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Arene Reduction by Energy Transfer Catalysis Enabled Hydrogen Atom Transfer: Advancing the Chemoselectivity

De-Hai Liu,[1,3] Kyogo Nagashima,[2,3] Hui Liang,[1] Xue-Lin Yue,[1] Yun-Peng Chu,[1] Shuming Chen,*[,2,4] and Jiajia Ma*[,1,4]

[1]Frontiers Science Center for Transformative Molecules, School of Chemistry and Chemical Engineering and Zhangjiang Institute for Advanced Study, Shanghai Jiao Tong University, Shanghai 200240, P. R. China

[2]Department of Chemistry and Biochemistry, Oberlin College, 119 Woodland St., Oberlin, Ohio 44074

[3]These authors contributed equally to the work.

[4]Lead contact

*Correspondence: shuming.chen@oberlin.edu

**Correspondence: majj@sjtu.edu.cn

SUMMARY

Arene reduction is one of the key avenues for synthesizing cyclic alkenes and alkanes which are fundamental matters in physical sciences. While catalytic hydrogenation and Birch reduction are two broadly utilized approaches for arene reduction across academia and industry over the last century, both methods have encountered significant chemoselectivity challenges. We hereby introduce a highly chemoselective arene reduction protocol operating through selective energy transfer (EnT) catalysis, which enables subsequent hydrogen atom transfer (HAT). The design of this protocol intelligently bypasses the conventional metric of reduction reaction, i.e., the reductive potential, but instead, relies on other physical parameters including chemical moieties' triplet energies, kinetic barriers of energy and hydrogen atom transfer events. Many reducing labile functional groups which were incompatible with previous arene reductions, are retained in this work. We anticipate this protocol to trigger further advancement of chemoselective arene reductions and enable the current arene-rich drug space escaping from flatland.

THE BIGGER PICTURE

Catalytic hydrogenation and Birch reduction are two key approaches for arene reduction. Typically, metric for determining the arene reduction reactivity in both methods is the reductive potential. In this work, the triplet energies of chemical moieties and the kinetic barriers of energy and hydrogen atom transfer events are taken as the metrics for reactivity evaluation. Arenes are reduced by energy transfer catalysis mediated hydrogen atom transfer. Consequently, the chemoselectivity issue which has been present for more than a century, is solved to a large extent. This work is anticipated to inspire further advancement in arene reduction and can be directly employed in late-stage drug modification.

INTRODUCTION

Organic molecules are fundamental matters in the physical science and can be generally divided into linear and cyclic varieties. Industrially, linear molecules are generated from the manufacturing of petroleum, whereas the cyclic ones are typically obtained from dearomative reduction of (hetero)arenes. In this context, catalytic arene hydrogenation (introduced in the 1900s)[1, 2] and Birch reduction (introduced in the 1930s)[3, 4] are two major protocols for producing partially or fully saturated cyclic hydrocarbons and heterocycles, which have been taught in undergraduate lectures (Figure 1a). Despite their wide application in industry and academia over the last century, both protocols have encountered significant chemoselectivity challenge. This challenge has drawn increasing attention in modern synthetic chemistry, especially when these arene reduction protocols

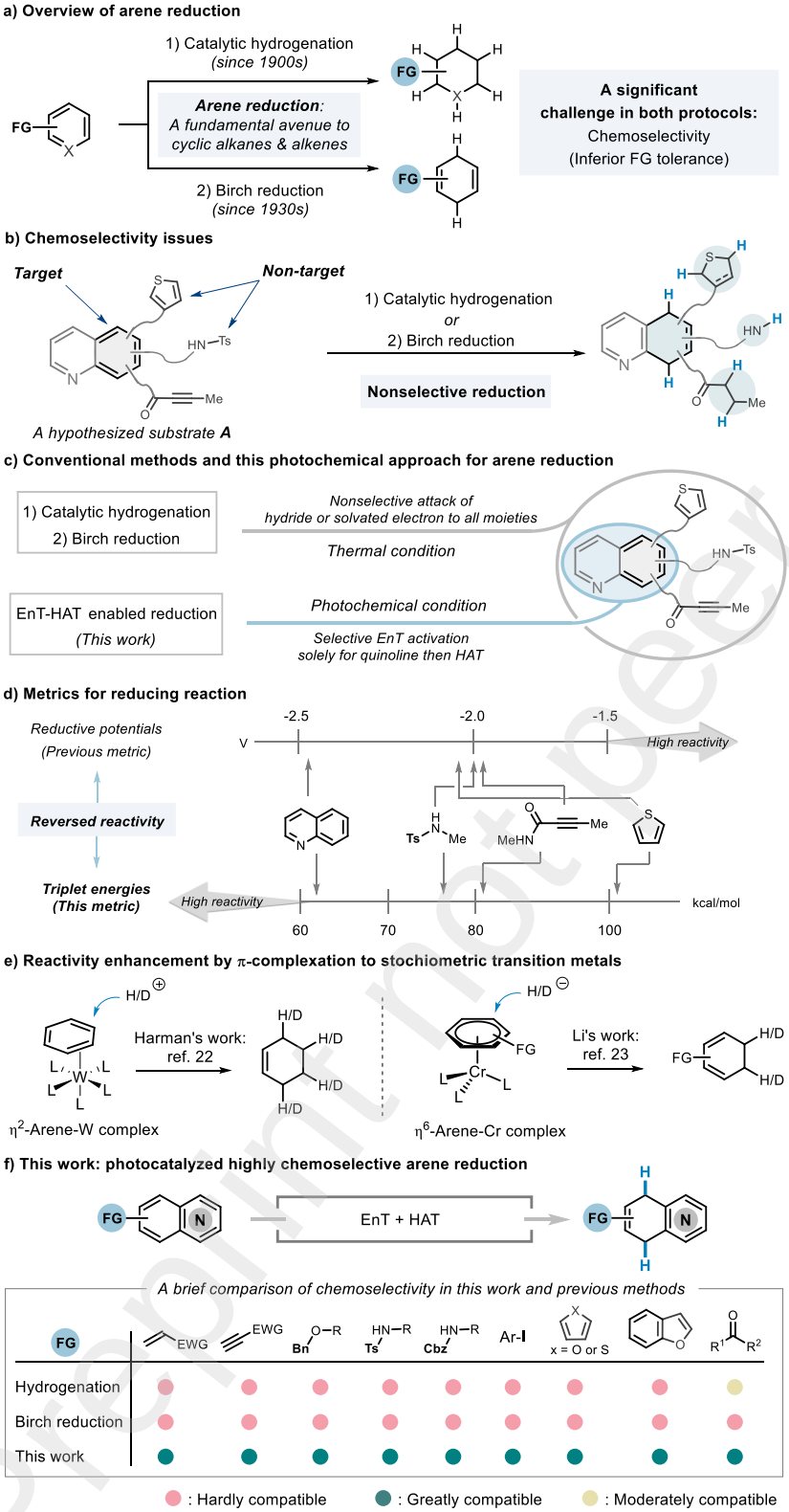


Figure 1. State of the art on arene reduction. FG = functional group; EnT = energy transfer; HAT = hydrogen atom transfer; EWG = electron withdrawing group.

are utilized in applied sciences, for instance, synthesis or modification of pharmaceuticals and materials.

To illustrate the chemoselectivity challenge, a hypothesized substate **A** containing quinoline, thiophene, benzsulfamide and electron deficient alkyne moieties is shown in Figure 1b, in which the quinoline is the target for reduction whereas the others are pendant functional groups. In case the catalytic hydrogenation (metal hydride)[5-7] or Birch reduction (solvated electrons)[8-11] protocol was utilized to reduce the benzenoid arene of quinoline, it's not surprising that none of the pendant functional groups can be compatible (Figure 1c). This can be attributed to that 1) the reductive potentials are taken as the metric in these reducing reactions and the target quinoline[12] encompasses lower reductive potentials than all other three functional groups[13-15], thus being less reactive (Figure 1d); 2) all moieties get attacked unselectively by highly aggressive hydride or solvated electron under the harsh conditions among the two protocols (Figure 1c) and 3) the thermal energy input for reducing benzenoid ring of quinoline is apparently sufficient for reducing thiophene, electron-deficient alkyne and the benzsulfamide. Overall, the intrinsic conflict of chemical moieties' reductive potentials and harsh thermal conditions lead to a totally unselective reaction. In addition, reactivity of arenes in reduction reactions can be enhanced by π-complexation to stochiometric transition metals.[16-21] Harman and coworkers demonstrated an elegant regiodivergent reductive deuteration protocol for accessing deuterated cyclohexenes through η^2-arene-tungsten complexes.[22] Li and coworkers further disclosed an intriguing regiodivergent 1,2-reduction of η^6-arene-chromium complexes to provide 1,3-cyclohexadienes with remarkable chemoselectivity. [23] In this context, we were intrigued to seek for an alternative metric besides the reductive potentials in reduction reactions. Interestingly, triplet energies of the four moieties in the hypothesized substrate **A** vary greatly and particularly the quinoline has the lowest value of 61.9 kcal/mmol whereas the others encompass much higher values (Figure 1d). This triggered us to pursue a chemoselective arene reduction strategy by using mild visible light-induced triplet energy transfer (EnT) catalysis.[24-31]

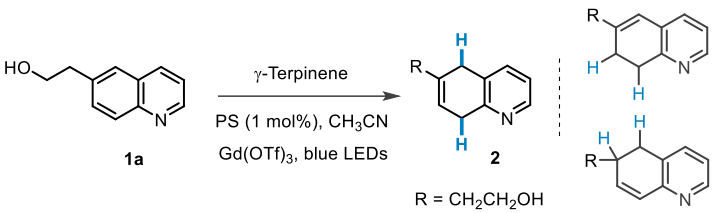
Although EnT catalysis have been recently disclosed for arene reduction, the existing examples are still far from sufficient for solving the chemoselectivity challenge. [32-35] In a seminal report, König and coworkers demonstrated proof-of-concept visible light mediated photochemical (hetero)arene reduction through consecutive energy transfer and single electron transfer.[32] Recently, Wang and Zhang expanded the scope of this protocol with a photoactive semiconductor-based system.[33] Miyake and coworkers demonstrated an excellent arene reduction protocol enabled by a tailored organic photoredox catalyst which operated through two consecutive photoinduced single electron transfers.[34] Key to the success of these methods is the harvest of two photon's energy and optionally in combination with sacrificial reductant to create a highly reducing condition (reductive potential of catalytic system low to -3.5 V vs SCE[36]).[37-44] Despite the notable reaction

efficiency, the highly reducing condition still resulted in inferior chemoselectivity among these works which is in accordance with previous thermal methods. In addition, Chirik disclosed an interesting visible light-induced arene reduction using a single iridium complex, in which an excited state arene is capable of abstracting two hydrogen atoms.[45, 46] However, only reactive polycyclic aromatics such as acridine and anthracene were shown to be reactive and the substrate scope was not evaluated. Lastly, (hetero)arene reduction under ultra violet (UV) light irradiation with stoichiometric reducing agents has been known for more than half a century. As early as in 1973, Barltrop pioneered this study which was further extended by many others and Qin recently introduced an elegant UV-enabled heteroarene reduction. [47-57] However, in all these reports, the requirement of a custom reaction apparatus significantly decreases the user friendliness and the indiscriminate activation of all UV-absorbing moieties leads to limited usefulness in applied science such as medicinal chemistry. The latter is understandable as drug molecules often encompass multiple "fancy" and sensitive functional groups which in case getting UV activation will lead to unpredictable side reactions.

Likewise, quinoline and isoquinoline are ubiquitous feedstocks in synthetic labs and are widespread frameworks among drugs and natural products.[58, 59] Dearomative reduction of quinoline and isoquinoline to access C(sp^3)-rich chemical space is a remarkable task in organic synthesis.[60-66] Typically observed regioselectivity in these dearomative reduction occurred on the less aromatic pyridinyl ring while few reports disclosed the reduction on the more inert benzenoid ring. To this end, advancing unforeseen and challenging regioselectivity of benzenoid ring within (iso)quinoline reduction is of great interest.

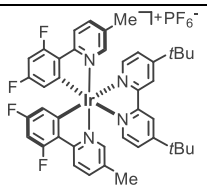
All in all, to search for a chemoselective and benzenoid-ring regioselective (iso)quinoline reduction, we questioned that if feasible to intertwine the energy transfer (EnT) catalysis with hydrogen atom transfer (HAT). Pleasingly, we herein report an efficient protocol for the benzenoid arene reduction of (iso)quinolines with broad scope and surprisingly excellent chemoselectivity that has been previously otherwise inaccessible (Figure 1e). Key to the excellent chemoselectivity is selective EnT to the (iso)quinoline moieties over other functional groups, followed by HAT to the excited state (iso)quinoline substrate. This reaction pathway intelligently bypasses the conventional highly reducing condition which is the bottleneck for obtaining high chemoselectivity. In particular, this method is very suited to the late-stage modification of drugs thus rapidly furnishing an intriguingly new C(sp^3)-rich drug space.

Table 1. Condition evaluation of quinoline reduction reaction. [a]

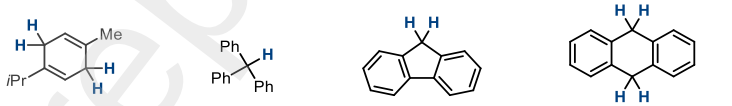


Entry	Deviation from standard conditions	Yield (%)[b]
1	None	62 (60[c])
2	Without $Gd(OTf)_3$	n.d.
3	LiCl instead of [Gd]	n.d.
4	$FeCl_3$ instead of [Gd]	n.d.
5	BF_3•Et_2O instead of [Gd]	27
6	CF_3CO_2H instead of [Gd]	52[d]
7	CH_2Cl_2 instead of CH_3CN	37
8	DMF instead of CH_3CN	n.d.
9	DMSO instead of CH_3CN	n.d.
10	Et_3SiH instead of γ-terpinene	<5
11	*n*-Bu_3SnH instead of γ-terpinene	n.d.
12	*p*-Toluenethiol instead of γ-terpinene	n.d.
13	$HC0_2Na$ instead of γ-terpinene	n.d.
14	Triphenylmethane instead of γ-terpinene	n.d.
15	9*H*-Fluorene instead of γ-terpinene	n.d.
16	9,10-Dihydroanthracene instead of γ-terpinene	n.d.
17	In the dark	n.d.
18	Under air	n.d.

[a]Standard conditions: **1** (0.10 mmol), $Gd(OTf)_3$ (0.2 mmol), γ-terpinene (0.3 mmol) in CH_3CN (2.0 mL, 0.05 M) were stirred for 6 hours under nitrogen and irradiated with 10 W blue LEDs (λ_{max} =455 nm). [b]Yields were determined by crude NMR analysis with 1,3,5-trimethoxybenzene as the internal standard. [c]Isolated yield. [d]0.3 mmol of CF_3CO_2H was employed. PS = Photosensitizer. n.d. = not detected.



PS: E_T = 62.9 kcal/mol



γ-Terpinene | Triphenylmethane | 9*H*-Fluorene | 9,10-Dihydroanthracene

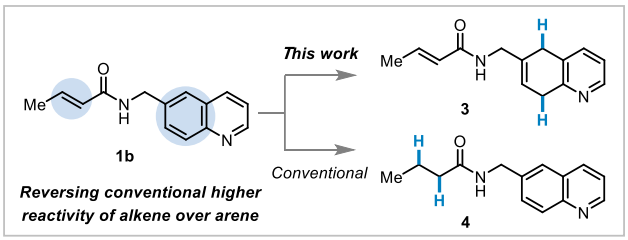
RESULTS

Reaction development

We commenced the experimental study by examining the reaction of quinoline substrate **1a**, γ-terpinene, $Gd(OTf)_3$ and an iridium-based photosensitizer (1 mol%) under the irradiation of blue LEDs (455 nm) (Table 1). Pleasingly, a 5,8-dihydrogenative product **2** (Birch-type product) was furnished smoothly as a single regioisomer with a remarkable 62% yield (entry 1). The Lewis acid $Gd(OTf)_3$ was found to be the most effective for this transformation. Removing $Gd(OTf)_3$ or using other metal-based Lewis acids such as LiCl and $FeCl_3$ instead didn't lead to product formation (entries 2-4). In contrast, the use of BF_3•Et2O or a Brønsted acid CF_3COOH proved capable of triggering this reducing reaction but with decreased yields (entry 5-6). Using CH_2Cl_2 instead of CH_3CN, decreased yield was also observed which could be traced back to the poor solubility of $Gd(OTf)_3$ in CH_2Cl_2 (entry 7). Notably, even though DMF and DMSO dissolve the $Gd(OTf)_3$ salt very well, the reaction is completed suppressed (entries 8-9), presumably due to competing coordination of the solvents over the substrate **1a**. Other hydrogen atom donor reagents such as silane, stannane, thiophenol, HCO2Na, triphenylmethane, 9*H*-fluorene and 9,10-dihydroanthracene didn't produce the desired product (entries 10-16). Control experiments revealed that both visible light and an inert atmosphere were essential to the reaction (entries 17-18). A comprehensive condition evaluation can be found in the Supplemental Information.

Having established the optimal reaction conditions, we proceeded to evaluate the chemoselectivity of this EnT-HAT mediated arene reduction. When the substrate **1b** with an acrylamide moiety was subjected to the standard condition, the Birch-type reduction product **3** was isolated in 64% yield (table 2, entry 1). Despite that the electron-deficient alkene of acrylamide is known to be more readily reduced than the aromatics in organic chemistry textbooks, but surprisingly retained under this highly chemoselective arene reduction protocol. In contrast, control experiments under conventional reducing conditions with $NaBH_4$ and hydrogen gas gave the complete alkene reduction product **4** (entries 2-3). In addition, the previously developed elegant and practical Birch reduction methods were tested for further featuring our protocol.[11, 67] Accordingly, Birch reduction conditions with lithium (or its related salt LiDBB) and amines lead to the full consumption of **1b** but afforded a complex mixture of products (entries 4-5). Collectively, our photochemical arene reduction of quinoline encompasses unforeseen chemoselectivity which was otherwise inaccessible under conventional conditions.

Table 2. Comparison of the current quinoline reduction protocol with previous protocols.



Entry	**Our approach**: Triplet energy transfer + HAT	**3** (%)	**4** (%)
1	PS (1 mol%), γ-Terpinene (3 eq.) $Gd(OTf)_3$ (3 eq.), CH_3CN, blue LEDs, r.t.	64	n.d.
	Conventional reduction conditions		
2	$NaBH_4$ (2 eq.), MeOH, r.t.	n.d.	80
3	H_2 (1 atm), Pd/C (10%), MeOH, r.t.	n.d.	76
	Previous chemical Birch reduction		
4 (ref. 11)	Li (3 eq.), *t*BuOH (2 eq.), $NH_2CH_2CH_2NH_2$ (6 eq.), THF, 0°C	Messy	
5 (ref. 67)	LiDBB (4 eq.) $(MeOCH_2CH_2)_2NH$ (1.2 eq.), THF, -78°C	Messy	

PS = Photosensitizer. n.d. = not detected.

Scope and generality evaluation

Having assessed the feasibility of the EnT-HAT mediated arene reduction, we next evaluated the scope and functional group compatibility (Figure 2). In general, the scope is broad and the regioselectivity (mostly >95:5 r.r.) is high. Quinolines bearing substituents at different positions were tested. Alkyl substituents on the pyridine ring did not impact the reaction outcome, and the corresponding products **5** and **6** were obtained in good yields. Quinolines bearing 5- and 8-alkyl substituents led to the Birch reduction products **7** and **10** with satisfactory yields and regioselectivities. Products **8** and **9** were afforded smoothly when installing a substituent at the 6 or 7 position on quinoline. It's worth noting that the 6-fluoro quinoline derivative is compatible thus providing **11** in 67% yield. The defluorination side reaction that occurs in many conventional Birch reductions was not observed in this case. Bis-substituted quinolines also underwent the reduction reaction thus providing the products **12** and **13**. In addition, aryl substituents (products **14** and **15**) also proved to be tolerated. Other azaarenes such as isoquinolines, phenanthridine, benzo[*f*]quinoline, 4,7-phenathroline were also reactive by furnishing products **16**-**20**. Next, functional group compatibility was evaluated. Many medicinally relevant carbocycles were found to be compatible, such as cyclopropanes (**21**-**23**), benzocyclobutene (**24**), fluorinated bicyclo[1.1.1]pentane (BCP) (**26**) and bicyclo[2.2.2]octane (**27**). Furthermore, this EnT-HAT mediated reduction protocol showed exclusive chemoselectivity for quinolines, whereas other (aza)arenes which would be reduced under previous arene reduction conditions were retained. For instance, naphthalene (**28**), Boc-protected indole (**29**), thiophene (**30**), furan (**31**) and benzofuran (**32**) all remained unreactive. Most intriguingly, a plethora of reducing

labile functional groups were compatible, such as cyano (**22**), ketones (**33, 34**), benzyl-protected amide (**35**), Cbz- and Ts-protected amines (**36, 37**), benzyl-protected alcohol (**38-39**) and halogens (**40, 41**). Most strikingly, electron-deficient alkenes (**3, 42-44**) and alkynes (**45**), which are typically more reactive than arenes under conventional reducing conditions, remained intact in this protocol. The electron-neutral alkene and alkyne also proved to be compatible (**46, 47**). The structures of compounds **32** and **36** were confirmed by X-ray crystallographic analysis.

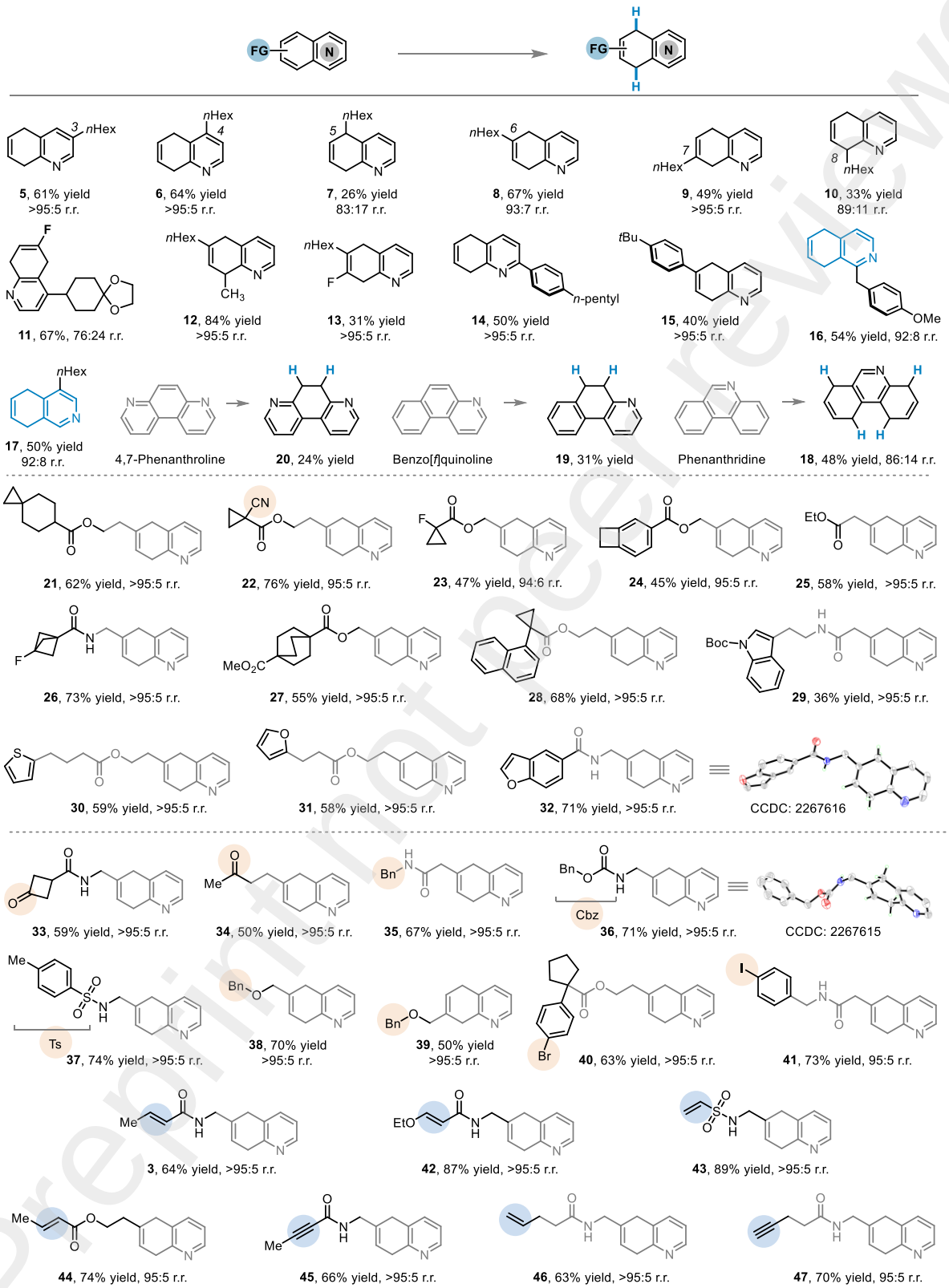


Figure 2. Scope and functional group compatibility evaluation of the EnT-HAT mediated benzenoid arene reduction. Reaction details are available in Supplemental Information.

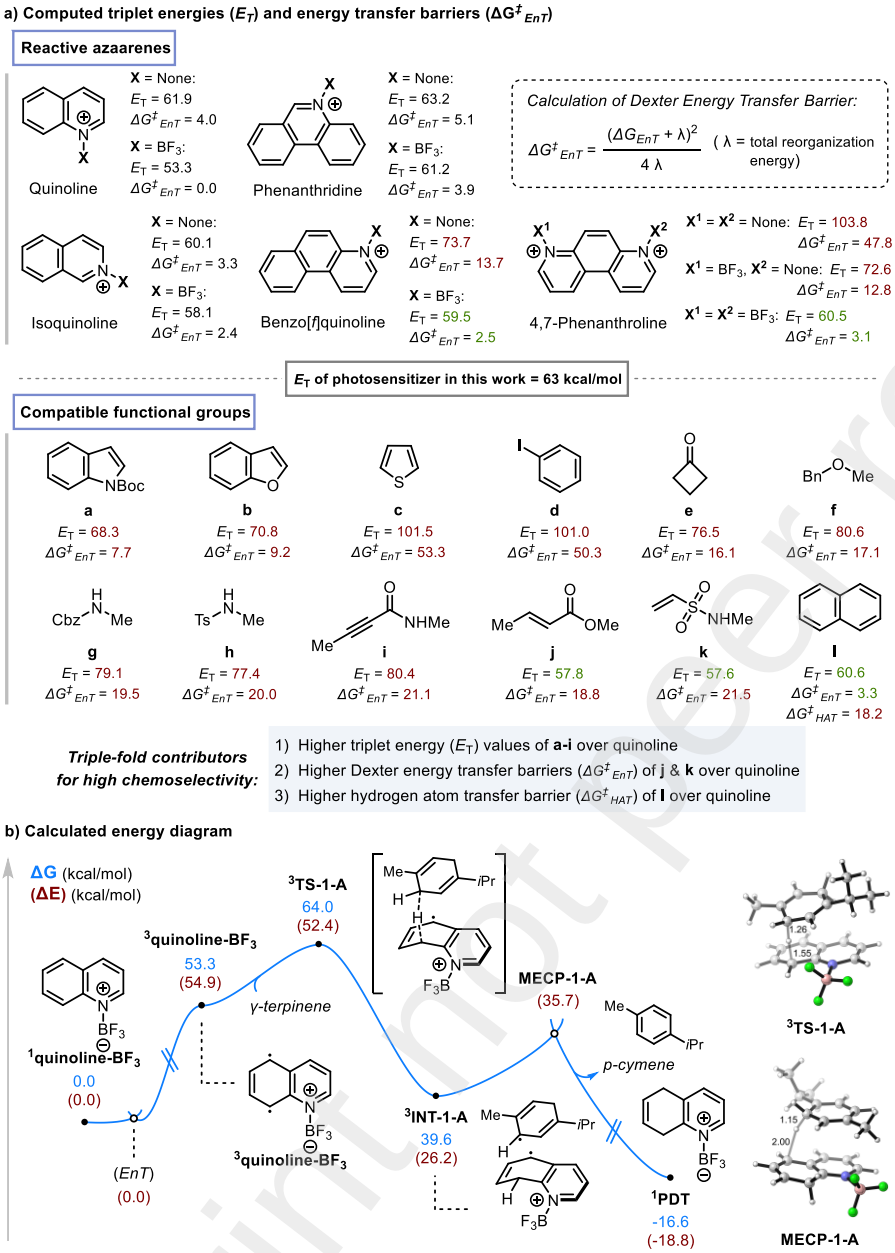


Figure 3. (a) Computed triplet energies (E_T) and energy transfer barriers ($\Delta G^{\ddagger}_{EnT}$) (both in kcal/mol) for azaarenes and pendant functional groups involved in the photochemical arene reduction protocol at the ωB97X-D/def2-TZVPP, SMD(MeCN)// ωB97X-D/def2-SVP level of theory. (b) Calculated energy diagram, transition state (TS) and minimum energy crossing point (MECP) structures. For MECPs, only potential energies can be calculated. Interatomic distances are in Å.

Mechanistic studies

To elucidate the origins of the excellent chemoselectivity of this EnT-HAT mediated arene reduction reaction, we performed density functional theory (DFT) calculations. We began by evaluating the triplet energies (E_T) of azaarene substrates (Figure 3a) and the pendant functional groups **a–l**, all of which have been shown to be compatible with the protocol.

Our results showed that Lewis acid coordination (modeled using BF_3) lowers the E_T of the nitrogen heterocycles (*N*-protonation was found to have a similar effect; see Supporting Information for details) which is consistent with our previous findings.[29, 30] This effect is especially pronounced in polycyclic azaarenes like benzo[*f*]quinoline and 4,7-phenanthroline. For example, the E_T of 4,7-phenanthroline was calculated to be 103.8 kcal/mol whereas the E_T of corresponding bis-BF_3 complexed congener was only 60.5 kcal/mol. In contrast, most compatible functional groups (**a**-**i**) were found to have significantly higher E_T values (~70-100 kcal/mol), indicating that they do not undergo energy transfer as readily under the reaction conditions (E_T of PS = 63 kcal/mol). However, compatible groups such as crotonate **j** (E_T = 57.8 kcal/mol), ethenyl sulfonamide **k** (E_T = 57.6 kcal/mol) and naphthalene **l** (E_T = 60.6 kcal/mol) were calculated to have E_T values lower than the E_T of the PS (63 kcal/mol). This observation suggests that E_T values are not the sole contributor to the experimentally observed chemoselectivity.

We then evaluated the Dexter energy transfer barriers ($\Delta G^{\ddagger}_{EnT}$) between these molecules and the excited triplet Ir photosensitizer. Following the method used by Baik and Yoon,[68, 69] these barriers were approximated using Marcus theory by treating the energy transfer process as a double electron exchange between the triplet donor and the singlet acceptor molecules. The calculated $\Delta G^{\ddagger}_{EnT}$ values revealed that Lewis acid coordination or *N*-protonation (see Supporting Information) also lowers energy transfer barriers between the excited Ir photosensitizer and the azaarene substrates. For quinoline, the energy transfer becomes essentially barrierless ($\Delta G^{\ddagger}_{EnT}$ = 0.0 kcal/mol). This result is consistent with Baik and Yoon's findings in photosensitized cycloadditions catalyzed by Brønsted acids. In contrast, the pendant functional groups with comparable E_T values to the azaarenes tend to have significantly higher energy transfer barriers, notably crotonate **j** ($\Delta G^{\ddagger}_{EnT}$ = 18.8 kcal/mol) and ethenyl sulfonamide **k** ($\Delta G^{\ddagger}_{EnT}$ = 21.5 kcal/mol). However, the energy transfer barrier ($\Delta G^{\ddagger}_{EnT}$) of naphthalene **l** was calculated to be 3.3 kcal/mol that indicates a third contributor for chemoselectivity. The initial hydrogen atm transfer barrier ($\Delta G^{\ddagger}_{HAT}$) was next evaluated and the value of naphthalene **l** was calculated to be 18.2 kcal/mol which explains why naphthalene was not reduced under the reaction conditions.

Collectively, these computational results point to triple-fold contributors for the excellent chemoselectivity in the EnT-HAT mediated arene reduction protocol: triplet energy (E_T), Dexter energy transfer barrier ($\Delta G^{\ddagger}_{EnT}$) and initial hydrogen atm transfer barrier ($\Delta G^{\ddagger}_{HAT}$), all of which rendering the arene reduction particularly facile and selective.

A computed full energy profile of a plausible mechanistic pathway for the EnT-HAT mediated quinoline reduction with Lewis-acid BF_3 is shown in Figure 3b. The reaction commences with the barrierless energy transfer from the excited Ir photosensitizer to ^{1}**quinoline-BF$_3$**, which undergoes an initial hydrogen atom transfer (HAT) with γ-terpinene on the triplet surface (^{3}**TS-1-A**) with a 10.7 kcal/mol activation free energy. This step results

in a triplet radical pair (³**INT-1-A**), which crosses over to the singlet surface through a minimum energy crossing point (**MECP-1-A**) with a 9.5 kcal/mol potential energy barrier. Once the crossover occurs, a second hydrogen atom is readily transferred to generate the reduced quinoline product (¹**PDT**) and *p*-cymene. Our further calculations found that this general mechanism may operate through a variety of isomeric transition states and MECPs that lie close in energy (see Supplementary Information for details).

Experimental investigations for probing the energy transfer pathway including the control experiments with triplet quenchers, various photosensitizers comparison, exclusion of redox process and so on, are available in the Supplementary Information.

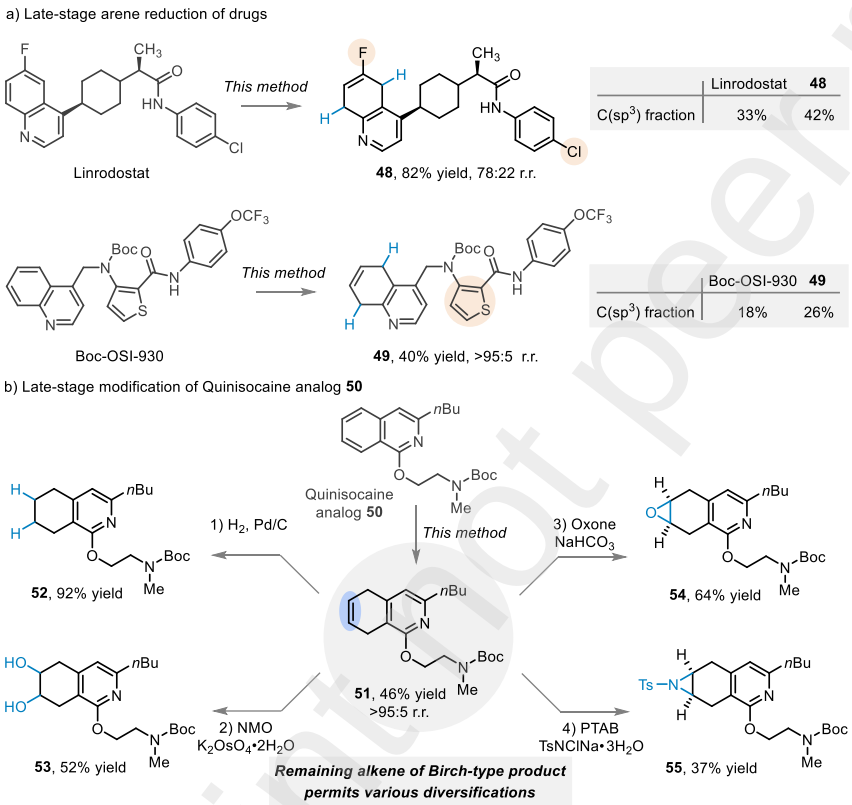


Figure 4. Synthetic applications. Reaction details are available in Supplemental Information.

Synthetic application

Due to its excellent chemoselectivity, this arene reduction protocol is an ideal tool for late-stage modification of drugs. Linrodostat, developed by Bristol Myers Squibb, has emerged as a significant antineoplastic drug and entered clinical trials for treating nearly twenty types of cancer such as advanced melanoma, glioblastoma, endometrial carcinosarcoma, advanced renal cell carcinoma, advanced gastric cancer and many others.[70] Although more than ten clinical trials have progressed to or completed the phase II stages, Linrodostat still faces high risk of attrition due to the severe evaluation before approval. In this context, the rapid derivatization of Linrodostat to provide back-up lead compounds is urgent. Our EnT-

HAT mediated arene reduction protocol can directly modify the Linrodostat, providing its analog **48** in excellent yield (Figure 4a). Both the reducing labile fluorine and chlorine substituents are hardly compatible in most previous arene reductions but remained intact under this protocol. The intriguing aspect of this late-stage modification is that 1) all pharmacophores (functional groups) remain unchanged and 2) the C(sp^3) fraction improves from original 33% to 42% (**48**), which has been shown to strongly correlate with higher clinical success.[71] Likewise, OSI-930 is a selective tyrosine kinase inhibitor with potential antineoplastic activity which encompasses multiple arene moieties including quinoline, benzene and thiophene. Typically, the reduction of quinoline results in the over-reduction of the thiophene. Under our protocol, the benzenoid ring of quinoline was selectively reduced to afford **49**, whereas the other (aza)arenes remained intact. Subsequent hydrogenation provided compound **50** with further increased C(sp^3) fraction. Next, the antipruritic drug quinisocaine's analog **51** also underwent efficient reduction with our protocol and the remaining alkene moiety in the Birch-type product **52** is a versatile synthon that permits various further diversifications. For example, oxidation of **52** by NMO and K_2OsO_4 led to diol **54**. Epoxidation and aziridination furnished **55** and **56**, respectively, which featured the additional small heterocycles. These frameworks are witnessing increasingly relevance in medicinal chemistry. Collectively, these examples show that our chemoselective arene reduction protocol is highly suitable for the late-stage modification of drugs and provides a practical avenue for extending the current drug space into C(sp^3)-rich territory.

SUMMARY

We report a highly chemoselective arene reduction protocol relying on energy transfer catalysis followed by hydrogen atom transfer. A plethora of reducing labile functional groups in previous arene reduction protocols hereby show great compatibility. The triplet energies of chemical moieties, the Dexter energy transfer barrier and initial hydrogen atm transfer barrier contribute to the unforeseen chemoselectivity. Due to the excellent chemoselectivity, this arene reduction protocol is particularly suitable for the late-stage modification of drugs thus intelligently meeting the medicinal chemists' request for exploring C(sp^3)-rich drug space.

EXPERIMENTAL PROCEDURES

Resource availability

Lead contact

Further information and requests for resources should be directed to and will be fulfilled by the lead contact, Jiajia Ma (majj@sjtu.edu.cn) and Shuming Chen (shuming.chen@oberlin.edu).

Materials availability

All materials generated in this study are available from the lead contact without restriction.

Data and code availability

Full experimental procedures and characterization data are provided in supplemental information. Crystallographic data of compounds **32** and **36** have been deposited in the Cambridge Crystallographic Data Center with CCDC numbers of 2267616 and 2267615, respectively.

SUPPLEMENTAL INFORMATION

Supplemental information can be found online at xxx

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AUTHOR CONTRIBUTIONS

J.M. conceived the concept. J.M. and S.C. supervised the research. J.M. and D.L. designed the synthesis. D.L., H.L., X.Y. and Y.C. performed the synthetic experiments. S.C. and K.N. conducted the computational study. J.M. and S.C. wrote the manuscript with contributions from all authors.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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Supplemental information for

Arene Reduction by Energy Transfer Catalysis Enabled Hydrogen Atom Transfer: Advancing the Chemoselectivity

De-Hai Liu,[1,3] Kyogo Nagashima,[2,3] Hui Liang,[1] Xue-Lin Yue,[1] Yun-Peng Chu,[1] Shuming Chen,*[,2,] and Jiajia Ma*[,1]

[1]Frontiers Science Center for Transformative Molecules, School of Chemistry and Chemical Engineering and Zhangjiang Institute for Advanced Study, Shanghai Jiao Tong University, Shanghai 200240, P. R. China
[2]Department of Chemistry and Biochemistry, Oberlin College, 119 Woodland St., Oberlin, Ohio 44074
[3]These authors contributed equally to the work
*Correspondence: shuming.chen@oberlin.edu; **Correspondence: majj@sjtu.edu.cn

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1. General Information

General remarks

Unless otherwise noted, all reactions were carried out under an atmosphere of argon or nitrogen in dried glassware. Reaction temperatures are referred to the ones of the heating/cooling media (heating block, cryogenic bath), unless otherwise stated. Dry solvents were either purchased from Adamas (H_2O < 50 ppm), stored under activated molecular sieves, withdrawn under positive argon pressure

Solvents for flash column chromatography (Acetone, petroleum ether, EtOAc, CH_2Cl_2) were purchased of technical grade and purified by atmospheric pressure distillation or purchased of reagent grade (MeOH) and used without additional purification. Reagents were purchased from TCI, Adamas, bidepharmand used without additional purification, unless otherwise stated.

Purification techniques

Flash chromatography was performed on silica gel (200-300 mesh) under a slight positive pressure. Thin layer chromatography (TLC) was carried out on YANTAI XINNUO silica gel $60F_{254}$ pre-coated glass sheets and were visualized using UV light (254 nm) and stained with basic aqueous potassium permanganate (2.0 g $KMnO_4$, 10.0 g K_2CO_3, 0.3 g of NaOH in 200 ml of deionized water) or alcoholic solution of phosphomolybdic acid (10.0 g of PMA in 100 ml of absolute EtOH) dips.

Analytical techniques

NMR-spectra were recorded on a Bruker Avance II 400 MHz or 500 MHz spectrometers. Chemicals shifts (δ) are quoted in ppm downfield of tetramethyl silane (0.00 ppm). The residual solvent signals were used as references for ^1H and ^{13}C NMR spectra ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; DMSO-d_6: δ_H = 2.50 ppm, δ_C = 39.52 ppm; CD_3OD: δ_H = 4.87 ppm, δ_C = 49.00 ppm; acetone-d_6: δ_H = 2.05 ppm, δ_C = 206.26 ppm). ^{19}F NMR spectra were calibrated using absolute referencing to the ^1H NMR spectrum, as suggested by IUPAC. (Harris et al., 2001) Coupling constants (*J*) are quoted in Hz and rounded to the nearest 0.1 Hz. The multiplicity abbreviations used (or combinations thereof) are: s = singlet, d = doublet, t = triplet, q = quartet,

hept = heptet, m = multiplet.

High Resolution Mass Spectrometry (HRMS) analysis was obtained using Electrospray Ionization (ESI) and reported as m/z (relative intensity). ESI was acquired using a Waters/Micromass LCT Classic (ESI-TOF).

2. State-of-the-Art of Birch Reduction

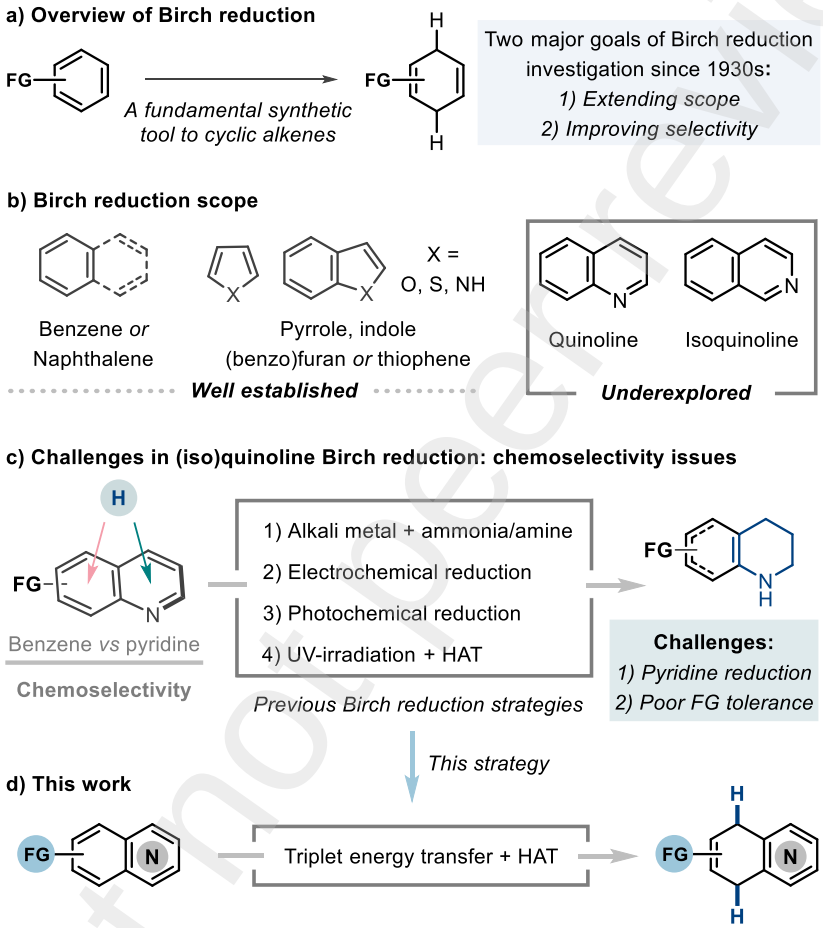


Figure S1. Birch reduction: scope and limitation.

Birch reduction was firstly introduced in 1930s and has been used to convert the arenes to 1,4-cyclohexadiene derivatives (Figure S1a). Comparing with the industrially and academically relevant arene hydrogenation which typically leads to fully saturated products, the intriguing feature of Birch reduction is that terminal cyclic products are often partially saturated. Therefore, the remaining alkene moieties can readily undergo various next round of synthetic transformations thus leading to a vastly extended chemical space which is otherwise inaccessible with the arene

hydrogenation protocol. As such, the advancement of Birch reduction is of utmost interest among synthetic chemistry.

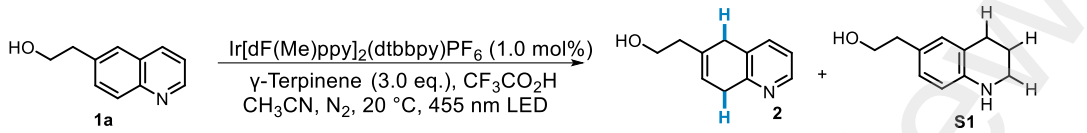
Since its invention in 1930s, **two of the most significant goals in Birch reduction** methodology advancements are 1) extending the scope of applicable aromatics and 2) improving the selectivity of the transformation. The state-of-art scope includes electron-neutral arenes such as benzene, naphthalene and electron-rich heteroarenes such as pyrrole, indole, (benzo)furan, (benzo)thiophene et. al (Figure S1b). Even though the electron-deficient heteroarenes quinoline and isoquinoline are ubiquitous feedstocks in synthetic labs and are widespread frameworks among drugs and natural products, the employment of them in Birch reduction is still a formidable challenge. Inferior yields and narrow scope are typically observed after subjecting (iso)quinolines to the conventional alkali metal/ammonia or the recently introduced electrochemical conditions. For example, Remers and coworkers reported a Birch reduction of quinolines under the condition of mixing lithium and liquid ammonia in methanol.[1] Only two examples were accomplished with up to 32% yield whereas sideproduct regioisomers of pyridine ring reduction were observed. In 2019, Baran and coworkers demonstrated an elegant electrochemical Birch reduction protocol which encompasses high efficiency and broad scope, and yet only one quinoline example was shown with 40% yield.[2,3] Except for these thermal reducing strategies, direct UV irradiation method is applicable.[4-8] However, the request for custom apparatus significantly decreases the user friendliness and the indiscriminate activation of most organic moieties leads to limited use in applied science such as medicinal chemistry. In this context, visible light photocatalysis has emerged as an intriguing tool for Birch reduction. In a seminal report, König and coworkers demonstrated the proof-of-concept of photochemical Birch reduction in which (iso)quinolines were reduced on the pyridine sphere whereas no “real” Birch products (1,4-cyclohexadiene derivatives) were afforded.[9] Very recently, Wang and Zhang leveraged this protocol to a new level with a photochemical semiconductor-based

system in which merely four isoquinolines were applicable and no quinolines were displayed.[10]

Overall, **quinolines and isoquinolines are still challenging substrates for Birch reduction which encounters remarkable limitations of narrow scope and inferior chemoselectivity**. **Our work is a new advance for Birch reduction which expanded its chemical space to quinolines, isoquinolines and related heteroarenes. In addition, the EnT-HAT strategy results in great chemoselectivity which was otherwise previously inaccessible.**

3. Reaction Optimization

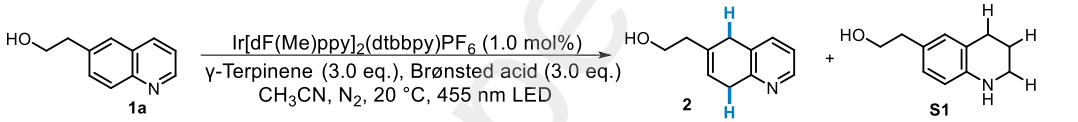
Table S1. Condition investigations on equivalent of CF_3CO_2H.



Entry[a]	CF_3CO_2H	product (%)[b]	S1 (%)[b]	S.M. (%)[b]	Entry[a]	CF_3CO_2H	product (%)[b]	S1 (%)[b]	S.M. (%)[b]
1	1.0 eq.	19	<5	30	**5**	**3.0 eq.**	**52**	<5	**0**
2	1.5 eq.	30	<5	19	6	4.0 eq.	50	<5	0
3	2.0 eq.	45	<5	0	7	5.0 eq.	50	<5	0
4	2.5 eq.	51	<5	0	8	6.0 eq.	49	<5	0

[a] Condition: **1a** (0.1 mmol, 17.3 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.001 mmol, 1.1 mg, 1 mol%), γ-terpinene (0.3 mmol, 48 μL, 3.0 equiv.), CF_3CO_2H, CH_3CN 2.0 mL, N_2, 20 °C, 6.0 hours. [b]Yields were determined by crude NMR analysis with 1,3,5-trimethoxybenzene as the internal standard.

Table S2. Condition investigations on Brønsted acids.

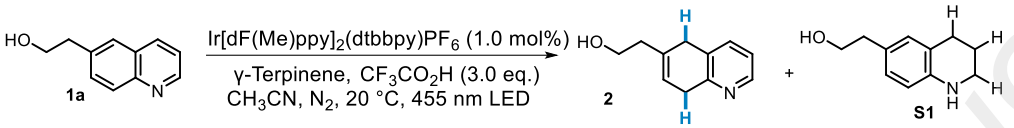


Entry[a]	Brønsted acid	product (%)[b]	S1 (%)[b]	S.M. (%)[b]	Entry[a]	Brønsted acid	product (%)[b]	S1 (%)[b]	S.M. (%)[b]
1	**CF_3COOH**	**52**	<5	**0**	7	HCl	0	40	0
2	AcOH	10	n.d.	35	8	HNO_3	42	<5	0
3	HCO_2H	22	n.d.	22	9	H_3PO_4	<10	<5	0
4	CF_3SO_2H	0	11	41	10[c]	H_3PO_4	21	<5	29
5	$PhCO_2H$	<10	n.d.	0	11	TsOH•H_2O	28	10	0
6	H_2SO_4	7	7	0					

Condition: **1a** (0.1 mmol, 17.3 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.001 mmol, 1.1 mg, 1 mol%), γ-terpinene (0.3 mmol, 48 μL, 3.0 equiv.), Brønsted acid (0.3 mmol, 3.0 equiv), CH_3CN 2.0 mL, N_2, 20 °C, 6.0 hours. [b]Yields were determined by crude NMR analysis with 1,3,5-trimethoxybenzene as the internal standard. [c]MeOH (2.0 mL) as solvent. n.d. = not detected

Notably, the pyridine ring reduction product **S1** were frequently detected when the Brønsted acids were employed. As shown in entry 7 of Table S2, the **S1** is the predominant product in the photochemical reaction.

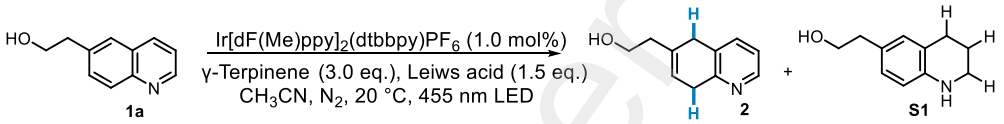
Table S3. Condition investigations on equivalent of γ-Terpinene.



Entry[a]	γ-Terpinene	Product (%)[b]	S1 (%)[b]	S.M. (%)[b]
1	1.0 eq.	43	<5	5
2	2.0 eq.	47	<5	0
3	**3.0 eq.**	**52**	**<5**	**0**
4	4.0 eq.	54	<5	0

[a] Condition: **1a** (0.1 mmol, 17.3 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.001 mmol, 1.1 mg, 1 mol%), γ-terpinene, CF_3CO_2H (0.3 mmol, 22.5 μL, 3.0 equiv.), CH_3CN 2.0 mL, N_2, 20 °C, 6.0 hours. [b]Yields were determined by crude NMR analysis with 1,3,5-trimethoxybenzene as the internal standard.

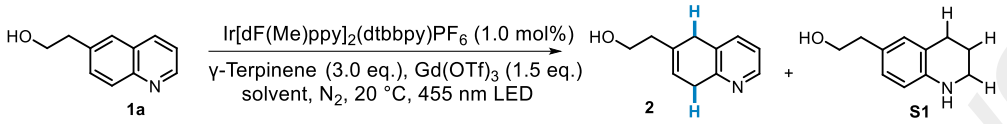
Table S4. Condition investigations on Lewis acids.



Entry[a]	Lewis acid	product (%)[b]	S1 (%)[b]	S.M (%)[b]	Entry[a]	Lewis acid	product (%)[b]	S1 (%)[b]	S.M (%)[b]
1[c]	$Et_2O•BF_3$	27	7	0	10	$Eu(OTf)_3$	27	<5	0
2[c]	$FeCl_3$	n.d.	<5	0	**11**	**$Gd(OTf)_3$**	**60**	**n.d.**	**0**
3[c]	LiCl	n.d.	n.d.	0	12	$Tb(OTf)_3$	49	n.d.	0
4	$SnCl_4$	20	n.d.	63	13	$Dy(OTf)_3$	58	n.d.	0
5	$Sc(OTf)_3$	45	5	0	14	$Ho(OTf)_3$	51	<5	0
6	$La(OTf)_3$	22	n.d.	48	15	$Sm(OTf)_3$	53	<5	0
7	$Ce(OTf)_3$	46	n.d.	3	16	$Tm(OTf)_3$	53	<5	0
8	$Pr(OTf)_3$	n.d.	n.d.	95	17	$Yb(OTf)_3$	41	n.d.	0
9	$Nd(OTf)_3$	53	n.d.	0	18	$Lu(OTf)_3$	56	<5	0

[a] Condition: **1a** (0.1 mmol, 17.3 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.001 mmol, 1.1 mg, 1.0 mol%), γ-terpinene (0.3 mmol, 48 μL, 3.0 equiv.), Lewis acid (0.15 mmol, 1.5 equiv.), CH_3CN 2.0 mL, N_2, 20 °C, 6.0 hours. [b]Yields were determined by crude NMR analysis with 1,3,5-trimethoxybenzene as the internal standard. [c]Lewis acid (0.2 mmo, 2.0 equiv.). n.d. = not detected

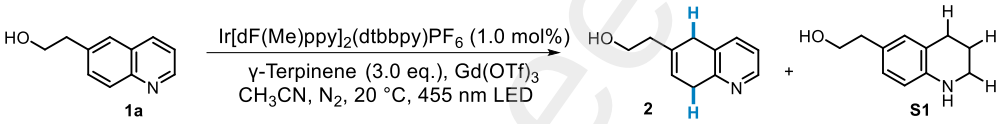
Table S5. Condition investigations on solvents.



Entry[a]	Solvent	product (%)[b]	S1 (%)[b]	S.M (%)[b]	Entry[a]	Solvent	product (%)[b]	S1 (%)[b]	S.M (%)[b]
1	EA	26	<5	18	**6**	**CH_3CN**	**60**	n.d.	**0**
2	$(CF_3)_2CHOH$	44	8	0	7[c]	DMF	n.d.	n.d.	0
3	NMP	6	n.d.	25	8[c]	DMSO	n.d.	n.d.	0
4	THF	22	<5	23	9[c]	DCM	37	<5	20
5	MeOH	30	n.d.	15					

[a] Condition: **1a** (0.1 mmol, 17.3 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.001 mmol, 1.1 mg, 1 mol%), γ-terpinene (0.3 mmol, 48 μL, 3.0 equiv.), Gd(OTf)$_3$ (0.15 mmol, 90.7 mg, 1.5 equiv.), solvent 2.0 mL, N_2, 20 °C, 6.0 hours. [b]Yields were determined by crude NMR analysis with 1,3,5-trimethoxybenzene as the internal standard. [c]Gd(OTf)$_3$ (0.2 mmol, 120.9 mg, 2.0 equiv.). n.d. = not detected

Table S6. Condition investigations on equivalent of Gd(OTf)$_3$

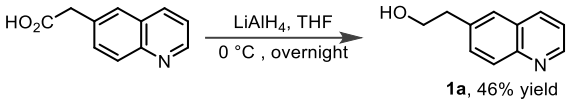


Entry[a]	Gd(OTf)$_3$	product (%)[b]	S1 (%)[b]	S.M (%)[b]	Entry[a]	Gd(OTf)$_3$	S1 (%)[b]	product (%)[b]	S.M (%)[b]
1	0.5 eq.	24	n.d.	21	**4**	**2.0 eq.**	n.d.	**62**	**0**
2	1.0 eq.	60	n.d.	0	5	2.5 eq.	n.d.	58	0
3	1.5 eq.	60	n.d.	0	6	3.0 eq.	n.d.	59	0

[a] Condition: **1a** (0.1 mmol, 17.3 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.001 mmol, 1.1 mg, 1.0 mol%), γ-terpinene (0.3 mmol, 48 μL, 3.0 equiv.), Gd(OTf)$_3$, CH_3CN 2.0 mL, N_2, 20 °C, 6.0 hours. [b]Yields were determined by crude NMR analysis with 1,3,5-trimethoxybenzene as the internal standard. n.d. = not detected

4. Synthesis of Starting Materials

Experimental Procedure A for synthesizing quinoline derivative 1a



1a, 46% yield

To a solution of 6-quinolineacetic acid (2.80 g, 15.0 mmol, 1.0 equiv.) in THF (80.0 mL) was added $LiAlH_4$ (0.68 g, 18.0 mmol, 1.2 equiv.) in batches and stirred for overnight at 0 °C. After completion of reaction, the resulting mixture was quenched by sat. NH_4Cl solution and extracted with CH_2Cl_2 (3 × 30 mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **1a** as a yellow solid (1.18 g, 46% yield).

Purification conditions: Acetone/CH_2Cl_2 = 1:6 to 1:3

R_f (**1a**) = 0.4 in Acetone/CH_2Cl_2 = 1:4.

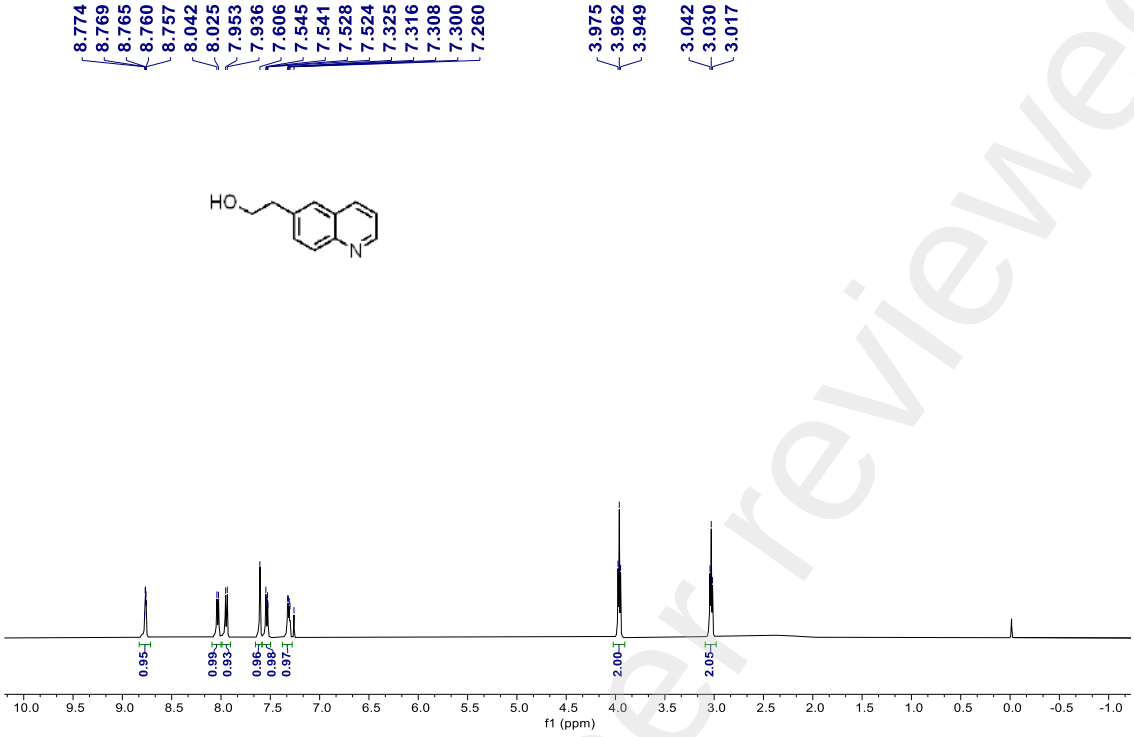
Analytical data of **1a**:

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 - 8.73 (m, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.61 (s, 1H), 7.53 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.31 (dd, *J* = 8.0, 4.5 Hz, 1H), 3.96 (t, *J* = 6.5 Hz, 2H), 3.03 (t, *J* = 6.5 Hz, 2H).

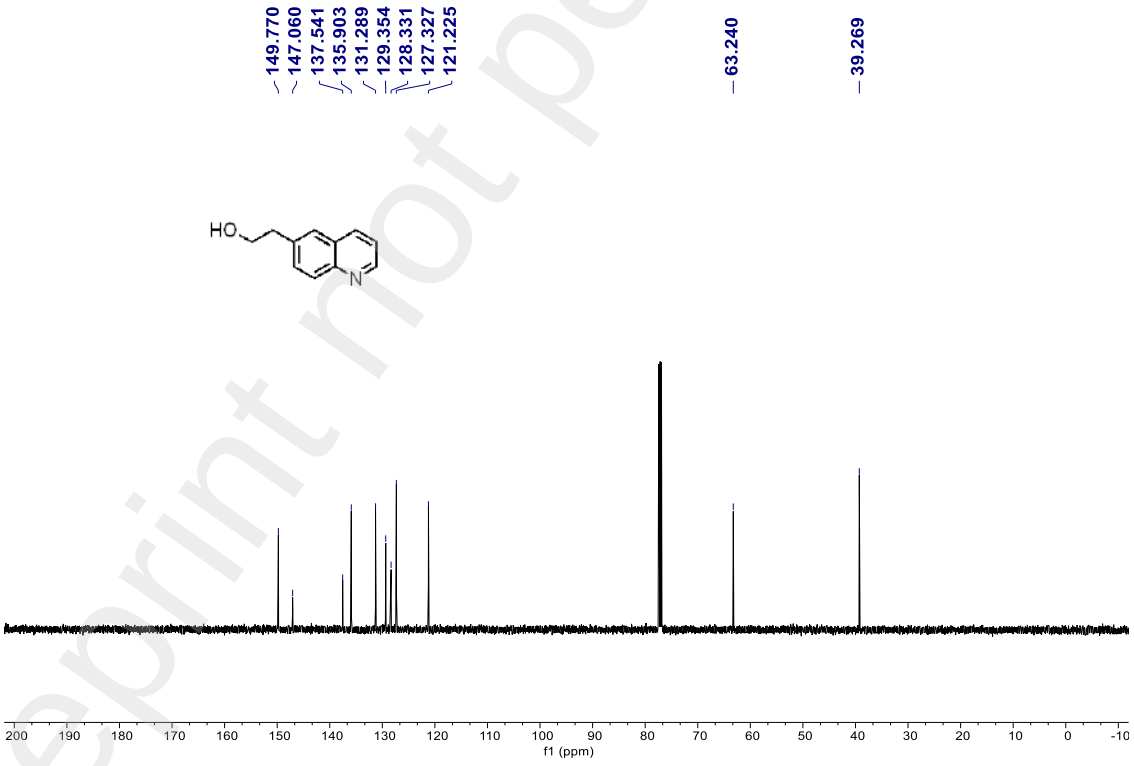
^{13}C NMR (126 MHz, $CDCl_3$) δ 149.8, 147.1, 137.5, 135.9, 131.3, 129.4, 128.3, 127.3, 121.2, 63.2, 39.3.

HRMS (ESI, *m*/*z*) calcd for $C_{11}H_{12}NO^+$ $[M+H]^+$: 174.0919, found: 174.0915.

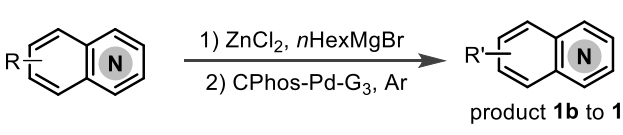
ldh-s.m.-oh.10.fid



ldh-s.m.-oh.11.fid



General procedure B for synthesizing quinoline derivatives 1b to **1j**[11]



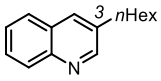
quinoline:
R= 3-Br, 4-Br, 5-Br, 6-I,7-Br
8-Br,6-Br-7-F, 6-Br-8-Me
Isoquinoline:
R= 3-Br

Step 1:

An oven-dried 10 mL flask equipped with a stir bar was cooled under vacuum. After evacuated/backfilled with N_2 (× 3), $ZnCl_2$•THF (2.0 M, 2.25 equiv.) was added at 0 ℃, subsequently, *n*HexMgBr (1.50 equiv.) was slowly dropwise and stirred for 2 hours.

Step2:

The tetrahydrofuran solution (2.0 M) of the quinoline (1.0 - 4.0 mmol, 1.0 equiv.) and CPhos-Pd-G3 (1.0 mol%) was added to the mixture prepared in step 1 under the argon atmosphere at 0 ℃. After stirred at the same temperature for 10 min, the reaction removes to the room temperature for 12 hours. The reaction was quenched with sat. NH_4Cl solution and extracted with CH_2Cl_2 (3 × 20 mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to afford the product **1b** to **1j.**



1b, 51% yield

According to the general procedure B, the 3-bromoquinoline (2.0 mmol, 416.0 mg, 1.0 equiv.) was converted to the product **1b** (218.6 mg, 51% yield) as a colorless oil.

Purification conditions: EtOAc/petroleum ether= 1:20 to 1:5

R_f(**1b**) = 0.35 in EtOAc/petroleum ether= 1:10

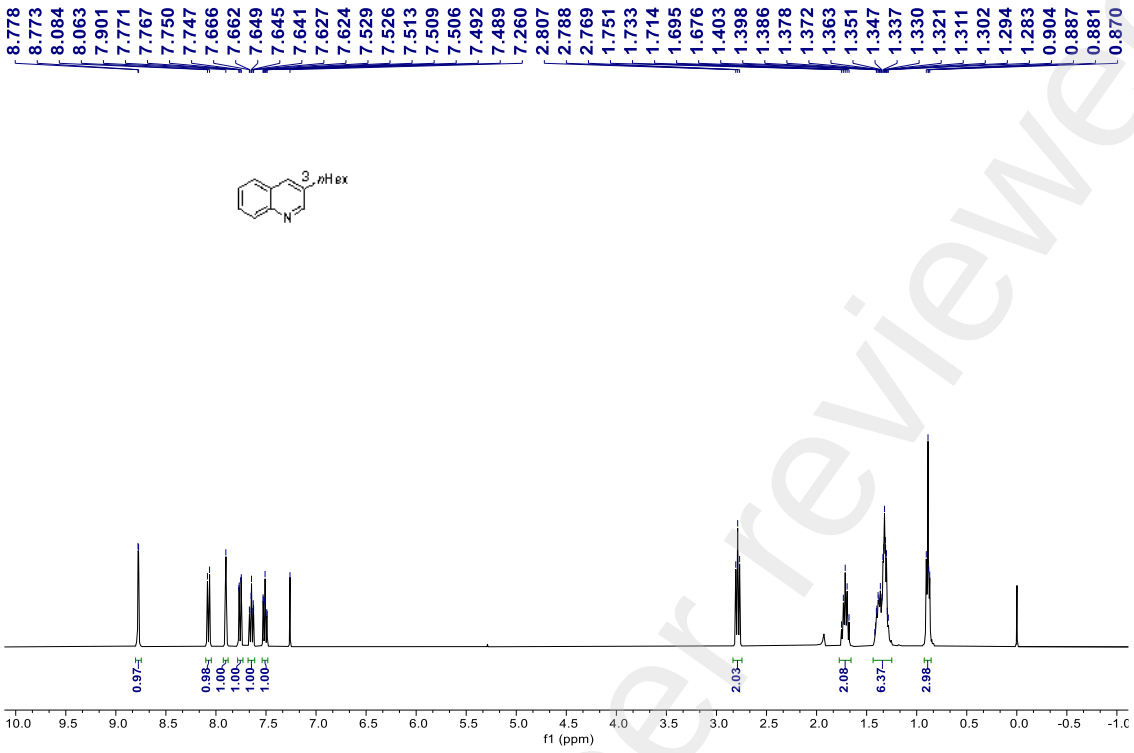
Analytical data of **1b**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 2.0 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.90 (br, 1H), 7.76 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.69 - 7.60 (m, 1H), 7.55 - 7.47 (m, 1H), 2.79 (t, *J* = 7.6 Hz, 2H), 1.71 (p, *J* = 7.4 Hz, 2H), 1.43 - 1.27 (m, 6H), 0.92 - 0.86 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.3, 146.9, 135.5, 134.2, 129.3, 128.6, 128.3, 127.4, 126.6, 33.3, 31.8, 31.2, 29.0, 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{20}N^+$ $[M+H]^+$: 214.1592, found: 214.1596.

Mar13-2023-majiajia-ldh02063-1p.10.fid



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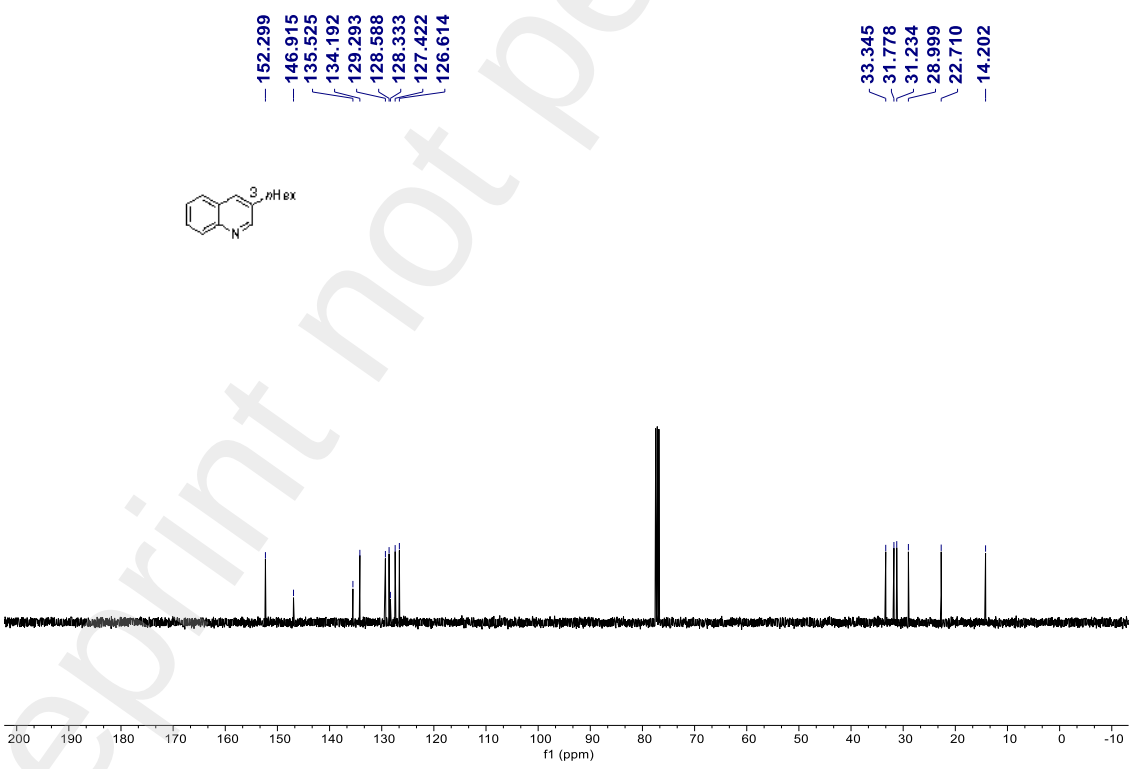
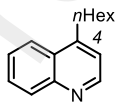




1c, 70% yield

According to the general procedure B, the 4-bromoquinoline (2.0 mmol, 416.0 mg, 1.0 equiv.) was converted to the product **1c** (298.6 mg, 70% yield) as a colorless oil.

Purification conditions: EtOAc/petroleum ether= 1:20 to 1:5

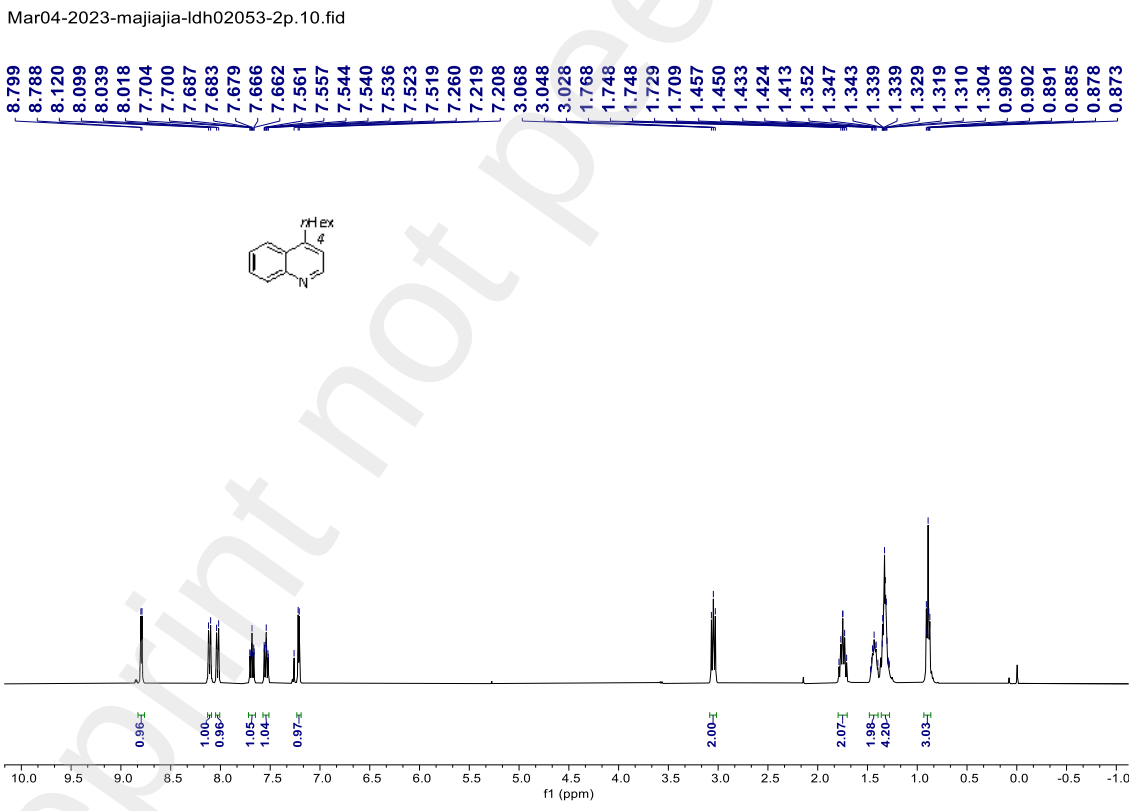
R_f(**1c**) = 0.4 in EtOAc/petroleum ether= 1:10

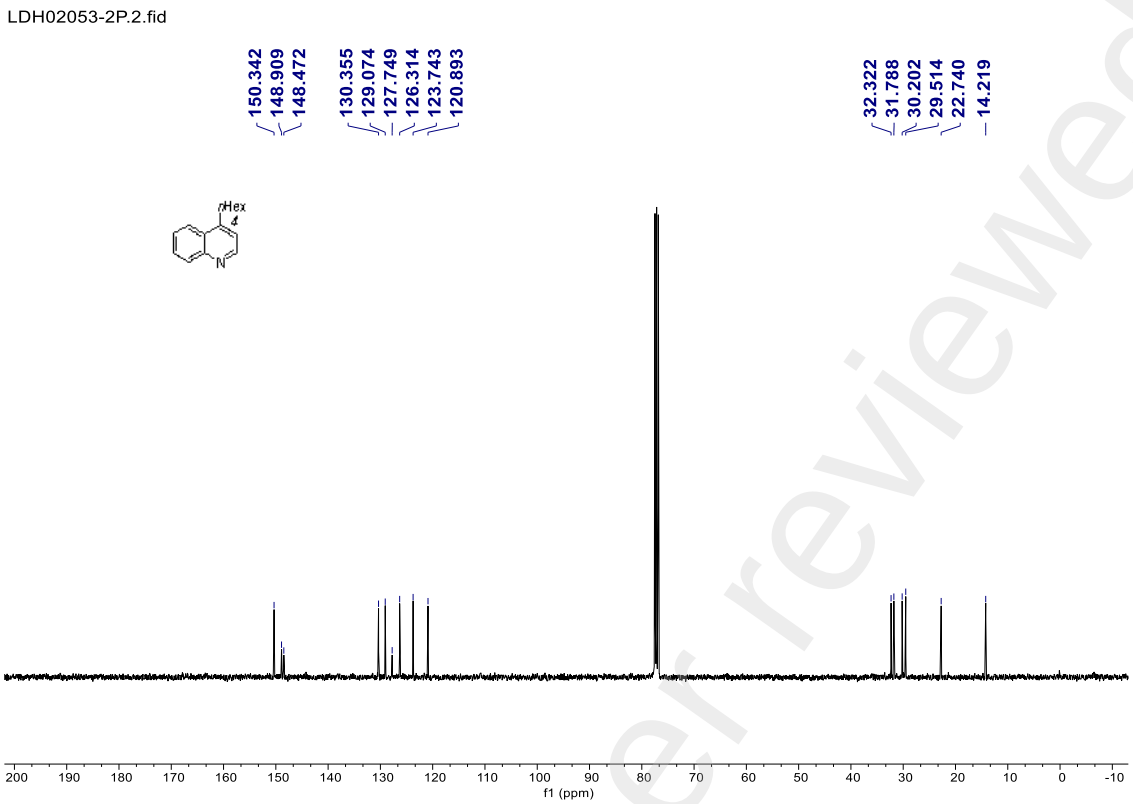
Analytical data of **1c**

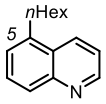
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.4 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.72 - 7.65 (m, 1H), 7.57 - 7.51 (m, 1H), 7.21 (d, *J* = 4.4 Hz, 1H), 3.05 (t, *J* = 8.0 Hz, 2H), 1.79 - 1.70 (m, 2H), 1.47 - 1.39 (m, 2H), 1.36 - 1.27 (m, 4H), 0.92 - 0.86 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 148.9, 148.5, 130.4, 129.1, 127.7, 126.3, 123.7, 120.9, 32.3, 31.8, 30.2, 29.5, 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{20}N^+$ [M+H]$^+$: 214.1596, found: 214.1592.







1d, 65% yield

According to the general procedure B, the 5-bromoquinoline (2.0 mmol, 416.0 mg, 1.0 equiv.) was converted to the product **1d** (277.3 mg, 65% yield) as a colorless oil.

Purification conditions: EtOAc/petroleum ether= 1:20 to 1:5

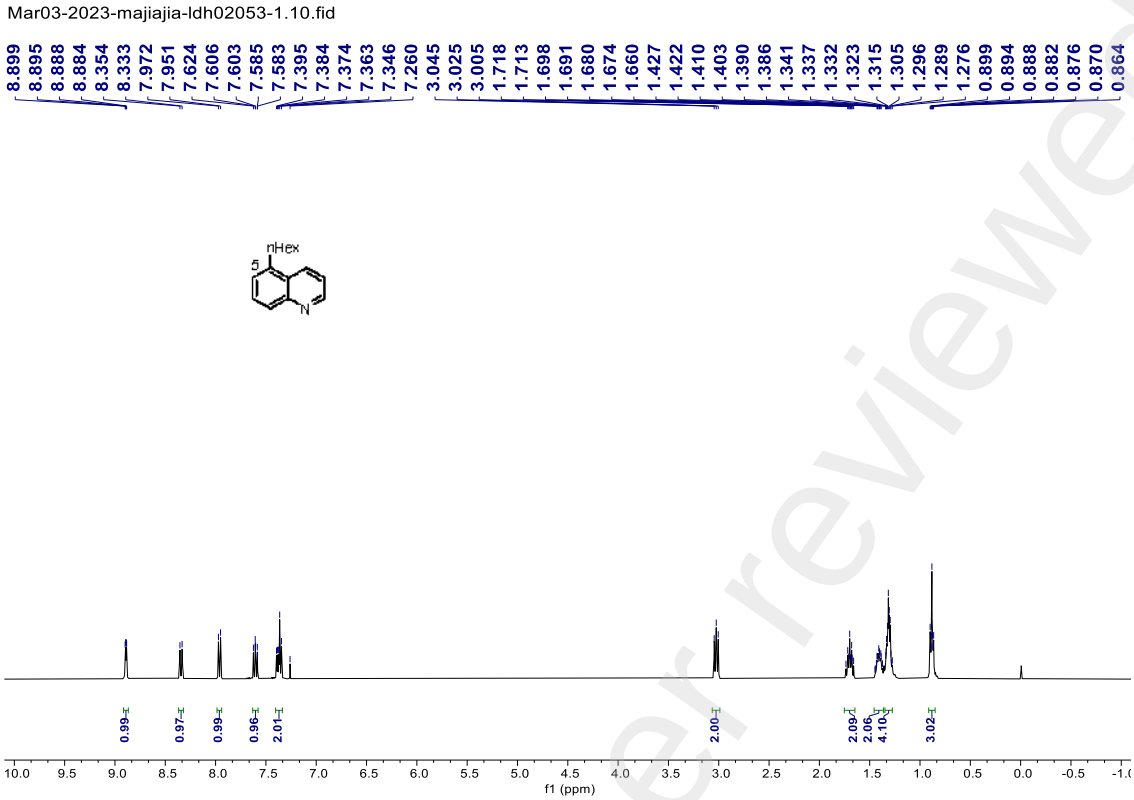
R_f(**1d**) = 0.4 in EtOAc/petroleum ether= 1:10

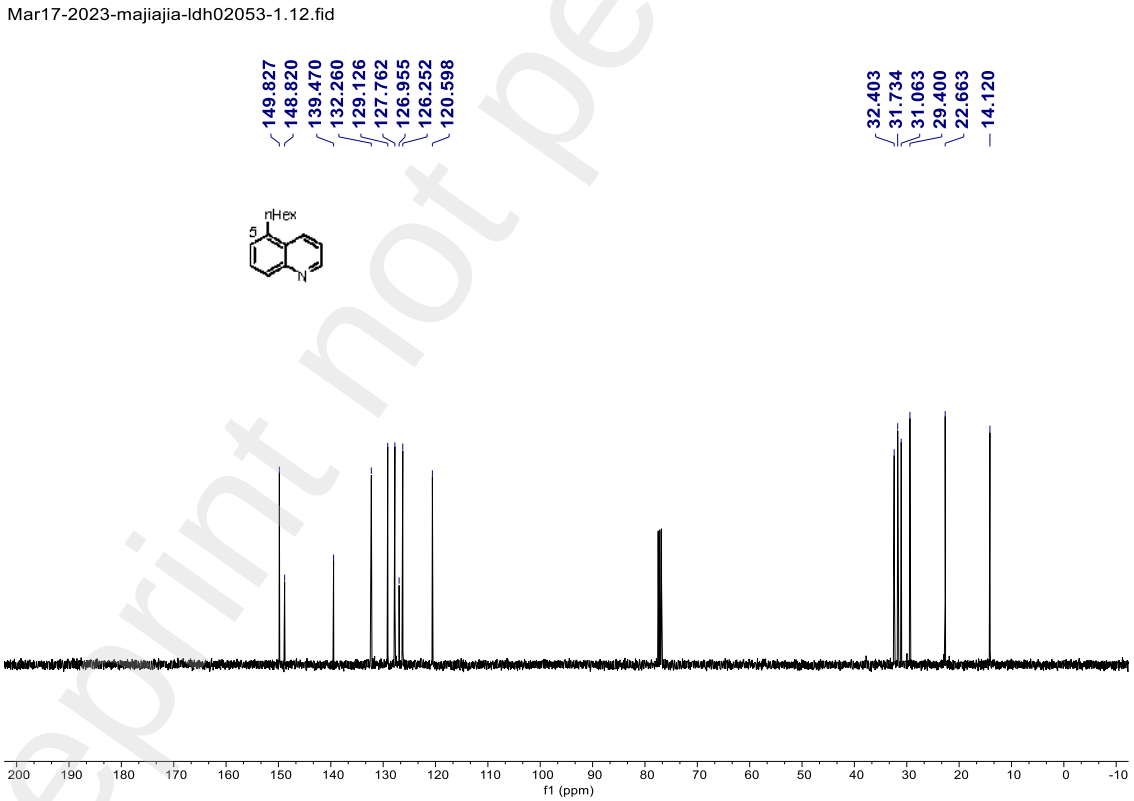
Analytical data of **1d**:

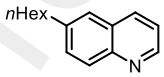
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.34 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 7.65 - 7.56 (m, 1H), 7.40 - 7.34 (m, 2H), 3.03 (t, *J* = 8.0 Hz, 2H), 1.74 - 1.65 (m, 2H), 1.45 - 1.37 (m, 2H), 1.35 - 1.28 (m, 4H), 0.92 - 0.84 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.8, 148.8, 139.5, 132.3, 129.1, 127.8, 127.0, 126.3, 120.6, 32.4, 31.7, 31.1, 29.4, 22.7, 14.1.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{20}N^+$ $[M+H]^+$: 214.1596, found: 214.1594.







1e, 89% yield

According to the general procedure B, the 6-Iodoquinoline (4.0 mmol, 1.02 g, 1.0

equiv.) was converted to the product **1e** (0.75 g, 89% yield) as a colorless oil.

Purification conditions: EtOAc/petroleum ether= 1:10 to 1:5

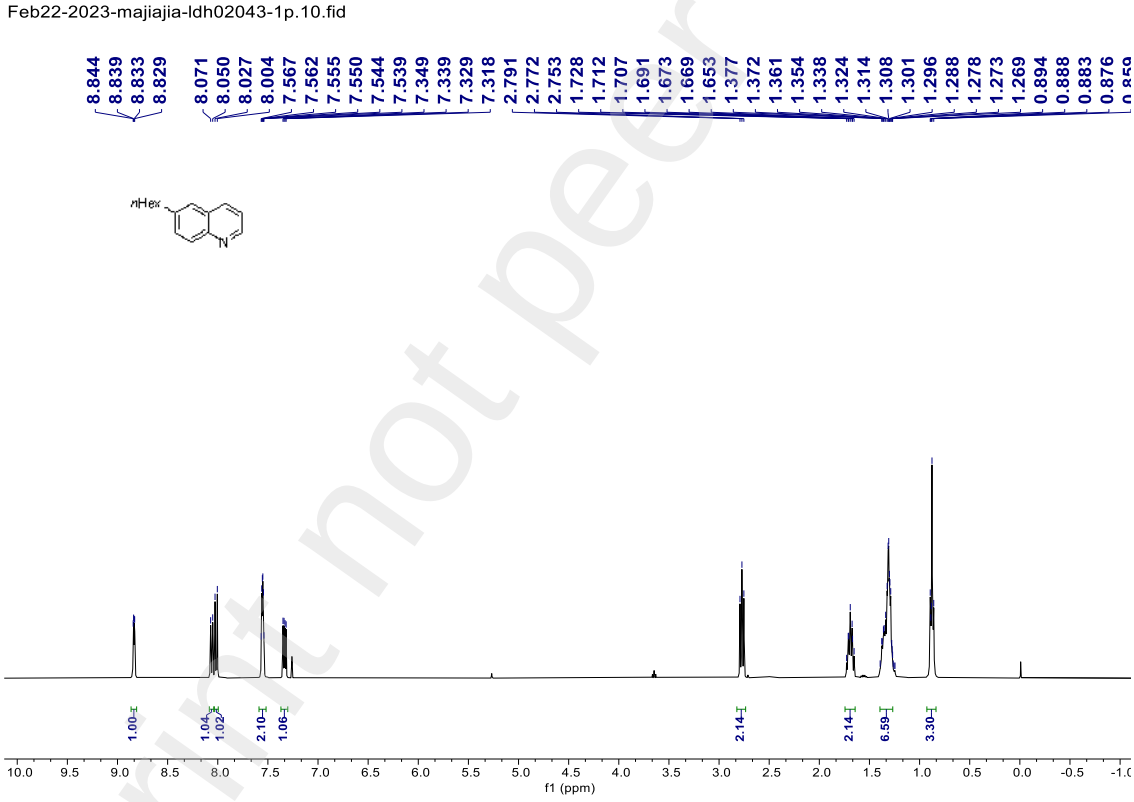
R_f (**1e**) = 0.4 in EtOAc/petroleum ether= 1:5

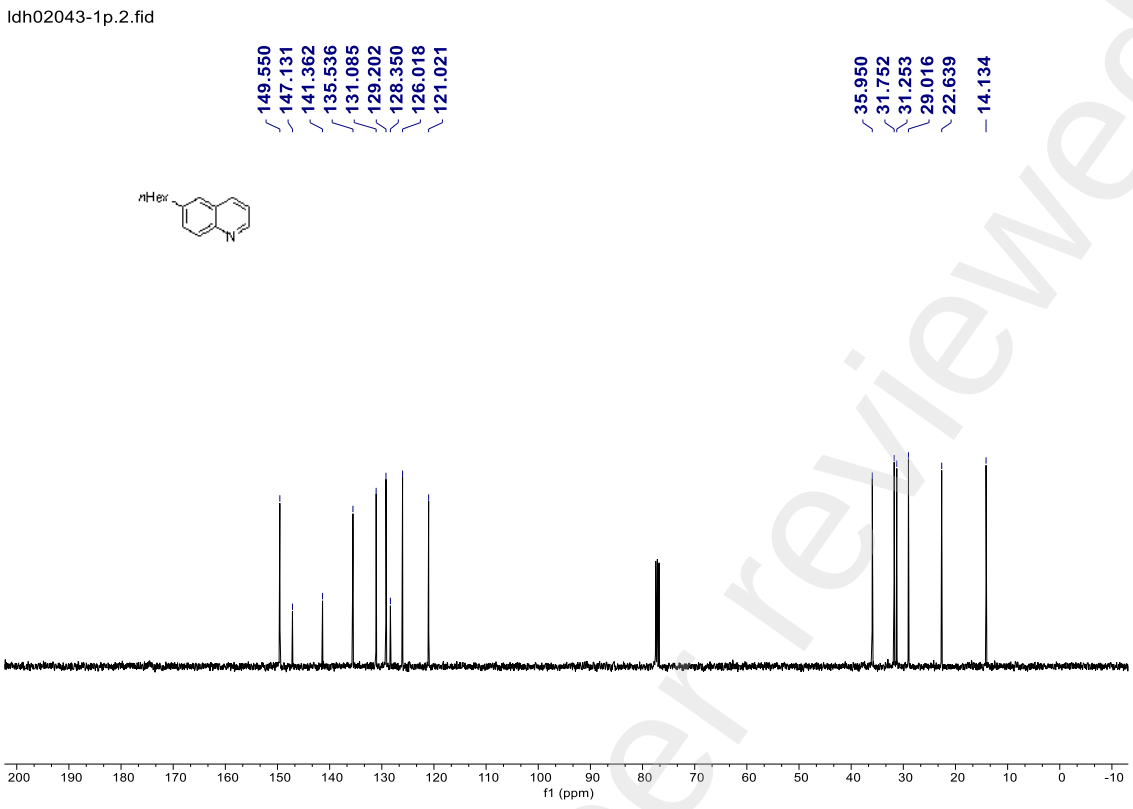
Analytical data of **1e**:

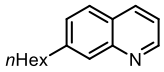
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (dd, *J* = 4.4, 2.0 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 9.2 Hz, 1H), 7.57 - 7.53 (m, 2H), 7.33 (dd, *J* = 8.0, 4.0 Hz, 1H), 2.77 (t, *J* = 7.6, 2H), 1.74 - 1.64 (m, 2H), 1.41 - 1.25 (m, 6H), 0.91 - 0.84 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.5, 147.1, 141.4, 135.5, 131.1, 129.2, 128.3, 126.0, 121.0, 35.9, 31.8, 31.3, 29.0, 22.6, 14.1.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{20}N^+$ [M+H]$^+$: 214.1596, found: 214.1592.







1f, 71% yield

According to the general procedure B, the 7-bromoquinoline (2.0 mmol, 416.0 mg, 1.0 equiv.) was converted to the product **1f** (311.0 mg, 71% yield) as a yellow oil.

Purification conditions: EtOAc/petroleum ether= 1:20 to 1:10

R_f (**1f**) = 0.45 in EtOAc/petroleum ether= 1:10

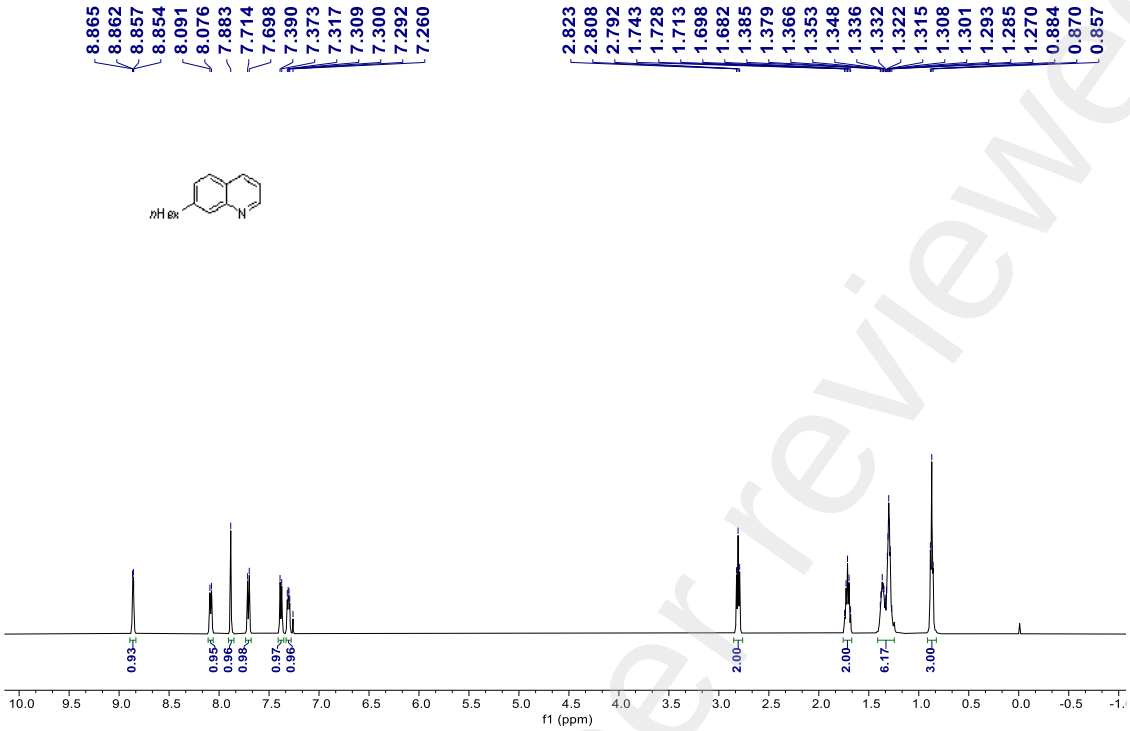
Analytical data of **1f**:

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.86 (dd, *J* = 4.0, 1.5 Hz, 1H), 8.08 (d, *J* = 7.5 Hz, 1H), 7.88 (s, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.5 Hz, 1H), 7.30 (dd, *J* = 8.5, 4.0 Hz, 1H), 2.81 (t, *J* = 7.5 Hz, 2H), 1.71 (p, *J* = 7.5 Hz, 2H), 1.40 - 1.25 (m, 6H), 0.90 - 0.84 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 150.4, 148.6, 144.8, 135.8, 128.3, 127.9, 127.5, 126.6, 120.4, 36.2, 31.8, 31.1, 29.0, 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{20}N^+$ $[M+H]^+$: 214.1596, found: 214.1592.

ldh02123p.10.fid



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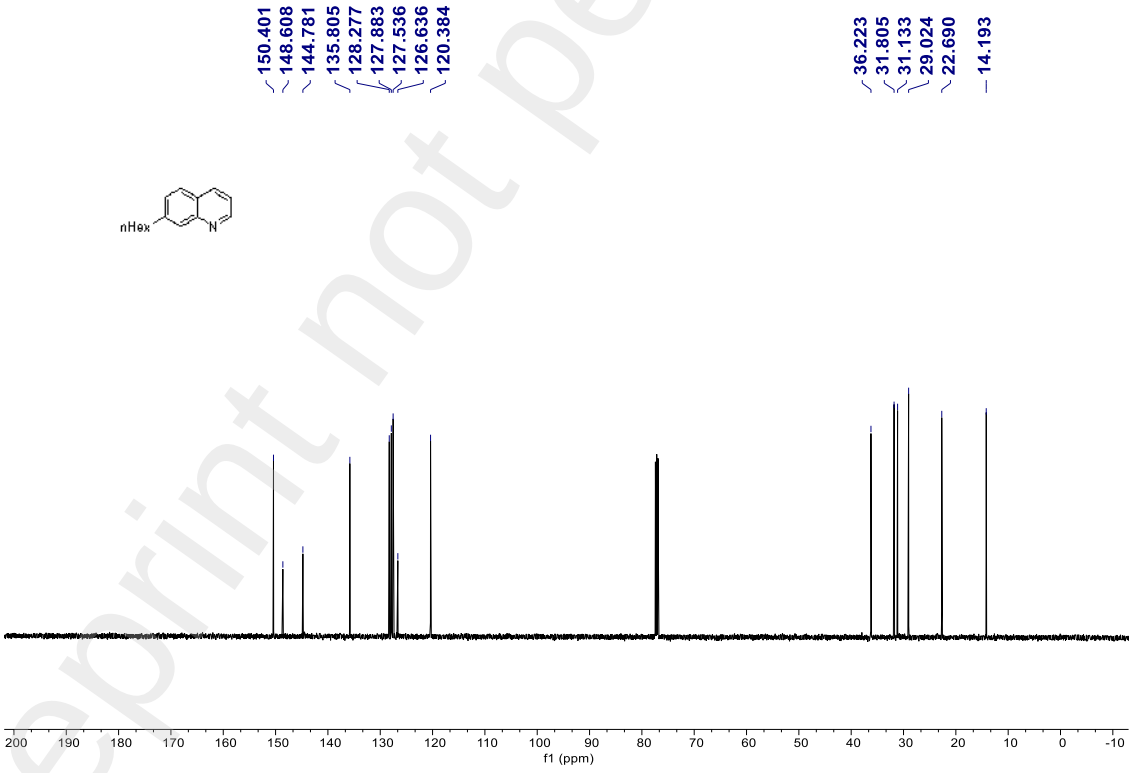
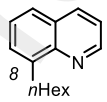




1g, 51% yield

According to the general procedure B, the 7-bromoquinoline (4.0 mmol, 832 mg, 1.0 equiv.) was converted to the product **1g** (434 mg, 51% yield) as a yellow oil.

Purification conditions: EtOAc/petroleum ether= 1:15 to 1:10

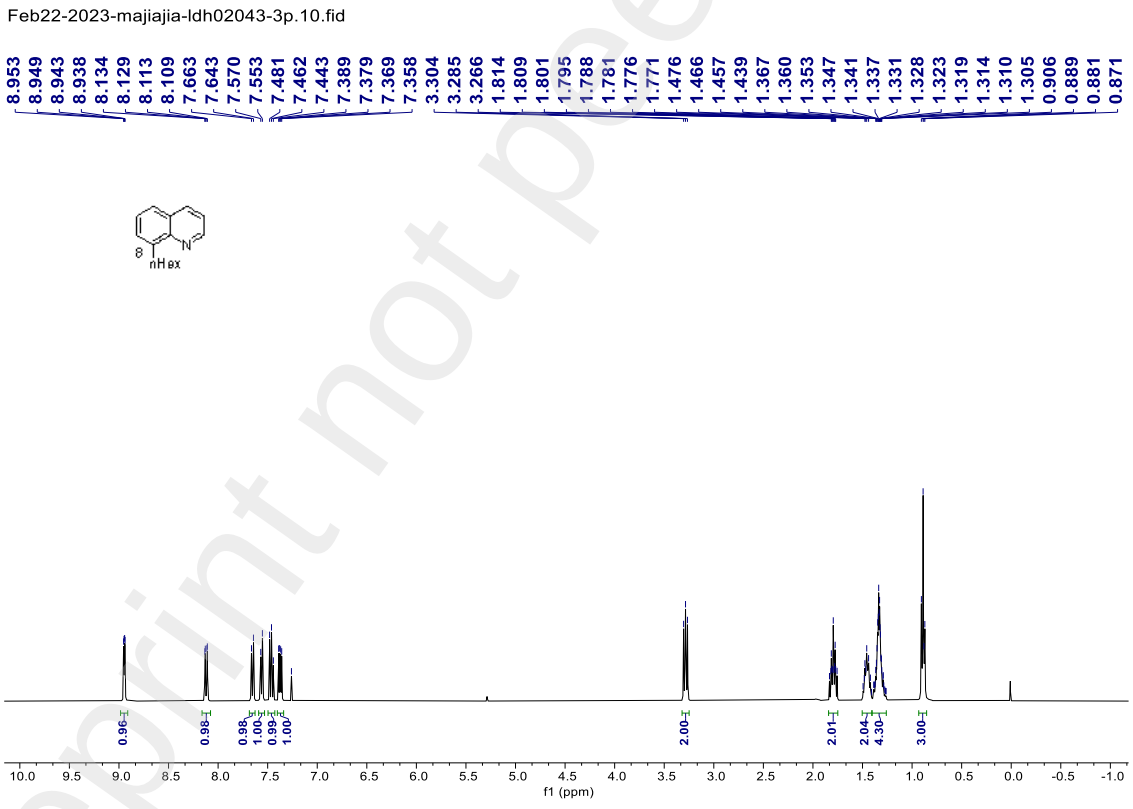
R_f (**1g**) = 0.3 in EtOAc/petroleum ether= 1:8

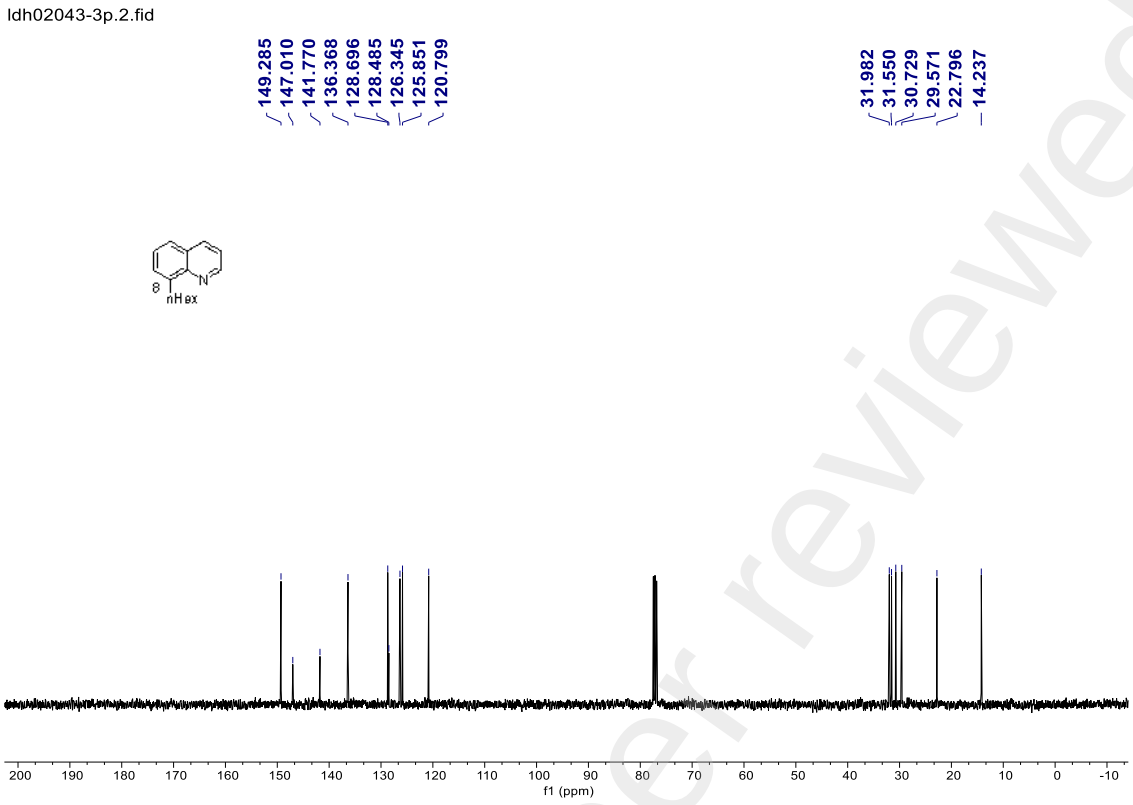
Analytical data of **1g**:

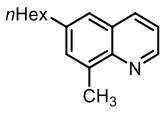
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (dd, *J* = 4.0, 1.6 Hz, 1H), 8.12 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 6.8 Hz, 1H), 7.49 - 7.43 (m, 1H), 7.37 (dd, *J* = 8.0, 4.0 Hz, 1H), 3.29 (t, *J* = 7.6, 2H), 1.84 - 1.74 (m, 2H), 1.50 - 1.41 (m, 2H), 1.40 - 1.26 (m, 4H), 0.92 - 0.86 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 147.0, 141.8, 136.4, 128.7, 128.5, 126.3, 125.9, 120.8, 32.0, 31.6, 30.7, 29.6, 22.8, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{20}N^+$ [M+H]$^+$: 214.1596, found: 214.1594.







1h, 86% yield

According to the general procedure B, the 8-methyl-6-bromoquinoline (2.0 mmol, 444.4 mg, 1.0 equiv.) was converted to the product **1h** (395.5 mg, 86% yield) as a yellow oil.

Purification conditions: EtOAc/petroleum ether= 1:10 to 1:5

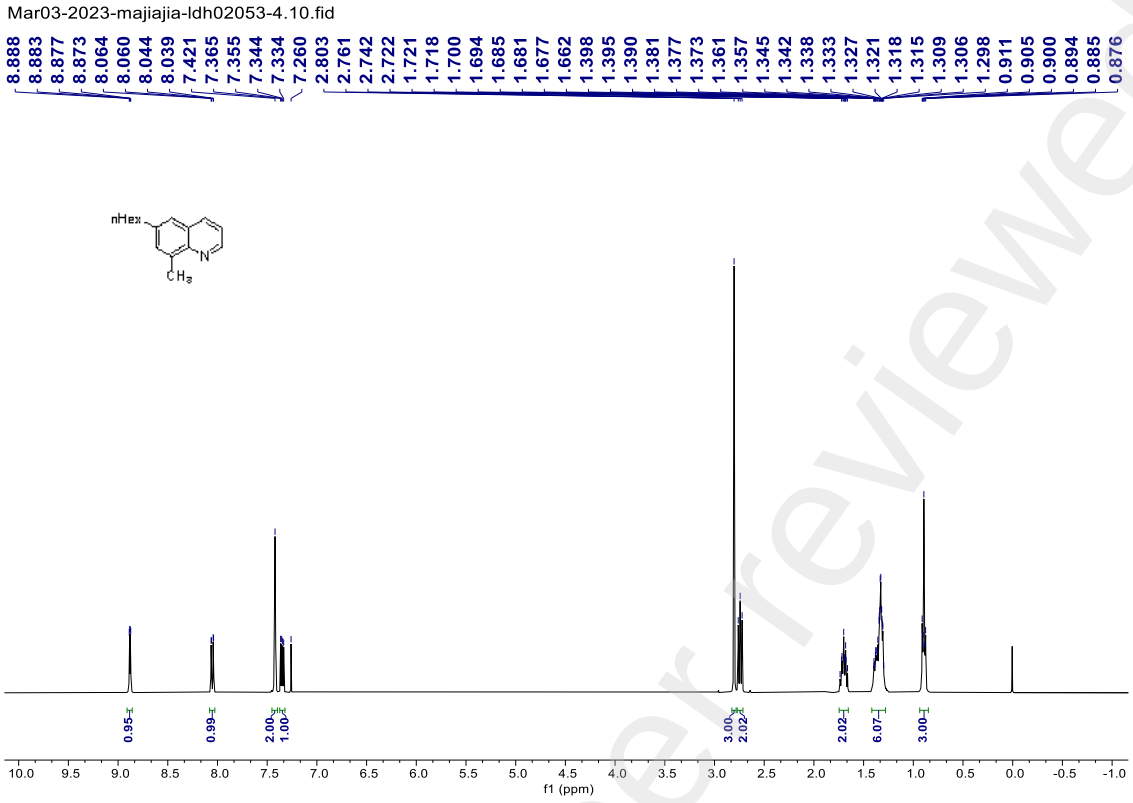
R_f (**1h**) = 0.5 in EtOAc/petroleum ether= 1:6

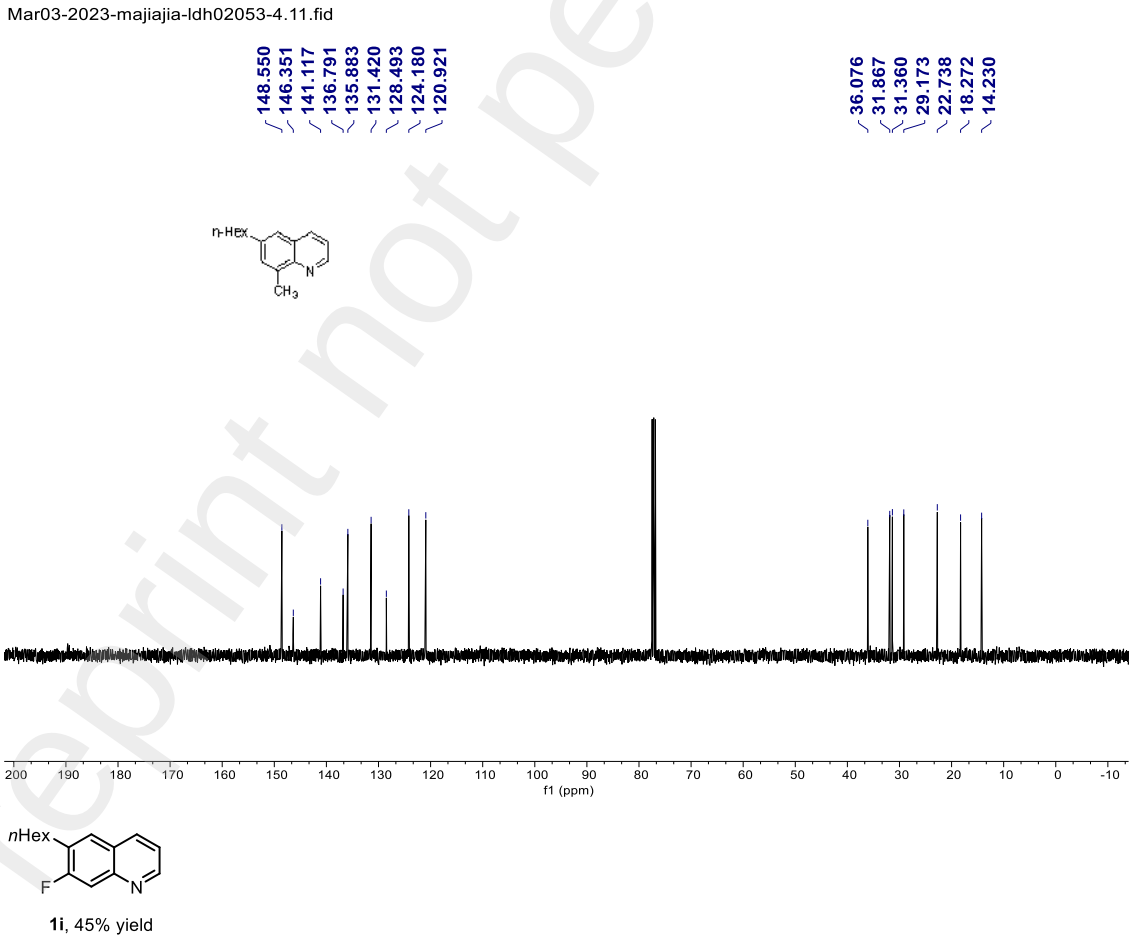
Analytical data of **1h**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (dd, *J* = 4.2, 2.0 Hz, 1H), 8.05 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.42 (s, 2H), 7.35 (dd, *J* = 8.4, 4.0 Hz, 1H), 2.80 (s, 3H), 2.74 (t, *J* = 8.0, 2H), 1.75 - 1.65 (m, 2H), 1.41 - 1.27 (m, 6H), 0.93 - 0.86 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.5, 146.4, 141.1, 136.8, 135.9, 131.4, 128.5, 124.2, 120.9, 36.1, 31.9, 31.4, 29.2, 22.7, 18.3, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{16}H_{22}N^+$ $[M+H]^+$: 228.1752, found: 228.1750.





1i, 45% yield

According to the general procedure B, the 6-bromo-7-fluoroquinoline (2.0 mmol,

452.1 mg, 1.0 equiv.) was converted to the product **1i** (208.1 mg, 45% yield) as a yellow oil.

Purification conditions: EtOAc/petroleum ether= 1:50 to 1:20

R_f (**1i**) = 0.5 in EtOAc/petroleum ether= 1:20

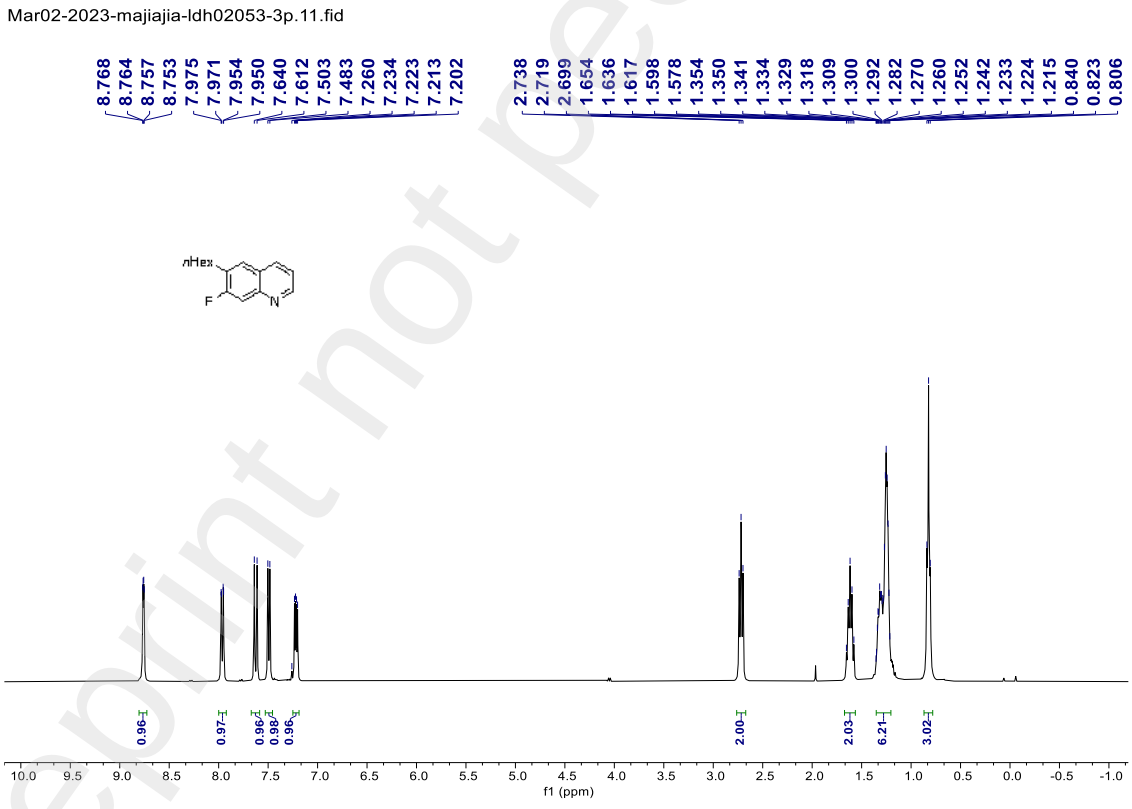
Analytical data of **1i**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (dd, *J* = 4.4, 1.6 Hz, 1H), 7.96 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.63 (d, *J* = 11.2 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.22 (dd, *J* = 8.4, 4.4 Hz, 1H), 2.72 (t, *J* = 7.6 Hz, 2H), 1.62 (m, 2H), 1.35 - 1.21 (m, 6H), 0.87 - 0.78 (m, 3H).

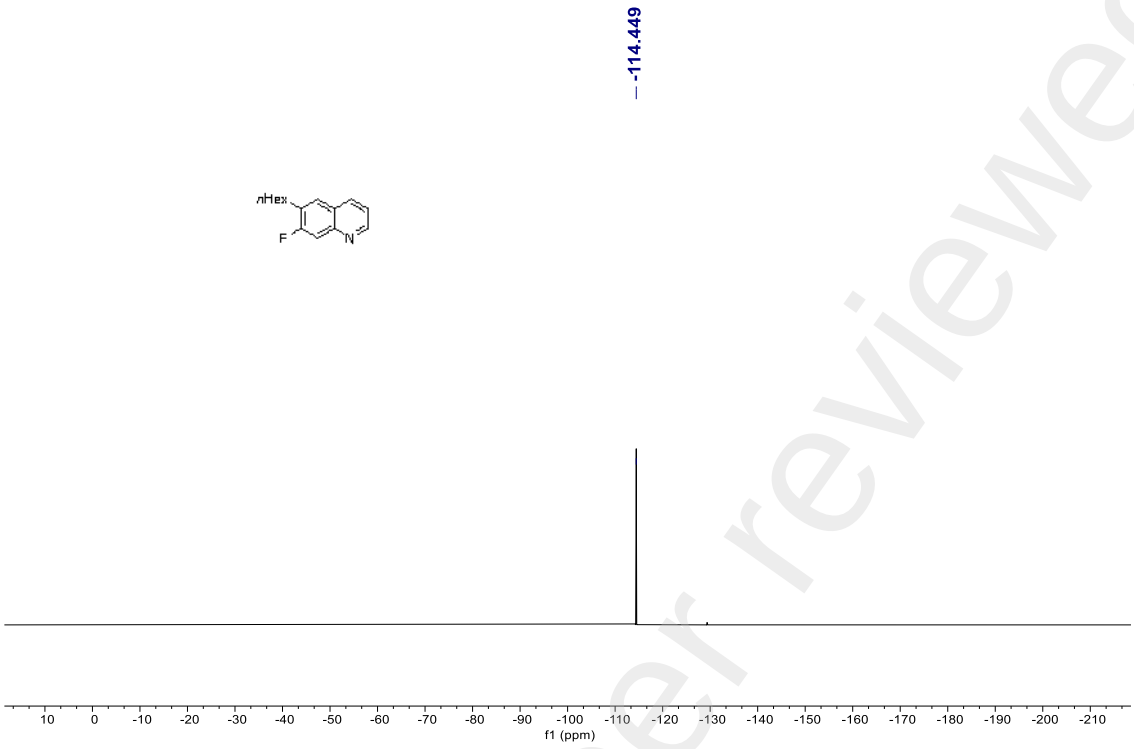
^{19}F NMR (376 MHz, $CDCl_3$) δ -114.45.

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2 (d, *J* = 250.8 Hz), 150.3, 148.0 (d, *J* = 12.9 Hz), 135.2 (d, *J* = 1.4 Hz), 131.7 (d, *J* = 20.0 Hz), 128.4 (d, *J* = 6.9 Hz), 125.4, 120.2 (d, *J* = 2.5 Hz), 112.6 (d, *J* = 21.6 Hz), 31.6, 29.9, 29.5 (d, *J* = 2.2 Hz), 29.0, 22.6, 14.0.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{19}NF^+$ $[M+H]^+$: 232.1502, found: 232.1497.



Mar02-2023-majiajia-ldh02053-3p.12.fid



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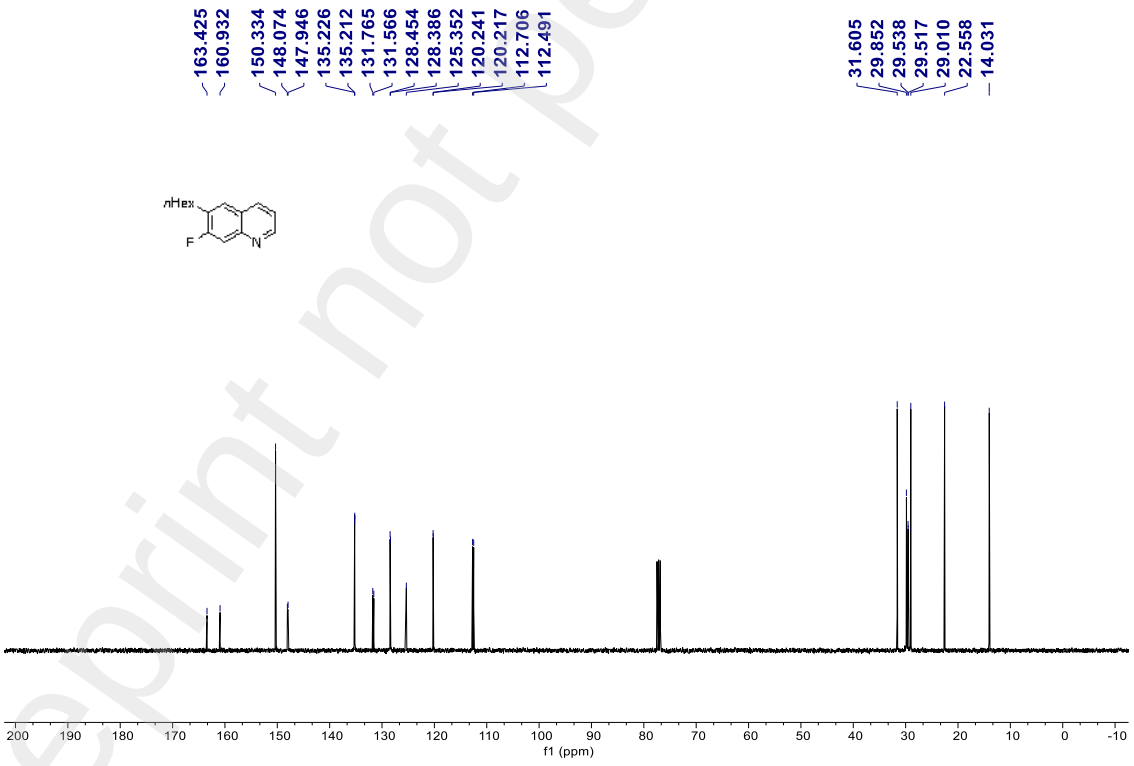
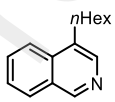




1j, 47% yield

According to the general procedure B, the 4-bromoisoquinoline (2.0 mmol, 416.1 mg, 1.0 equiv.) was converted to the product **1j** (202.3 mg, 47% yield) as a yellow oil.

Purification conditions: EtOAc/petroleum ether= 1:10 to 1:6

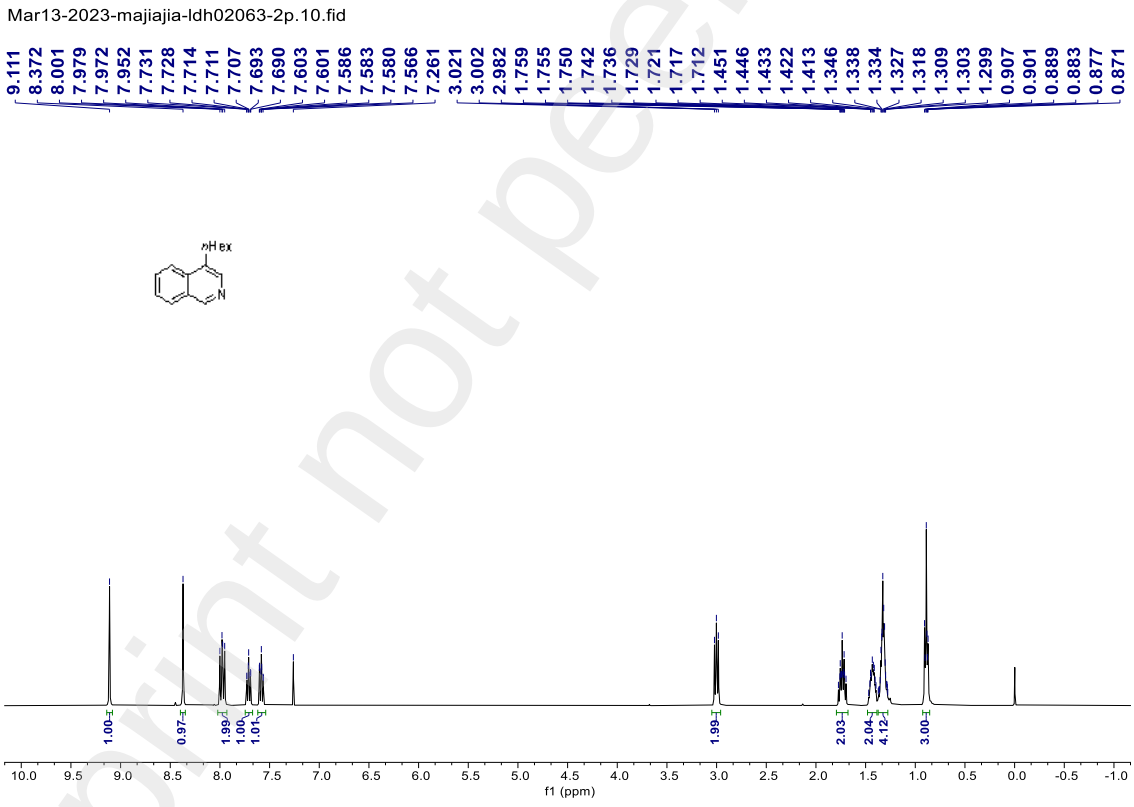
R_f (**1j**) = 0.35 in EtOAc/petroleum ether= 1:5

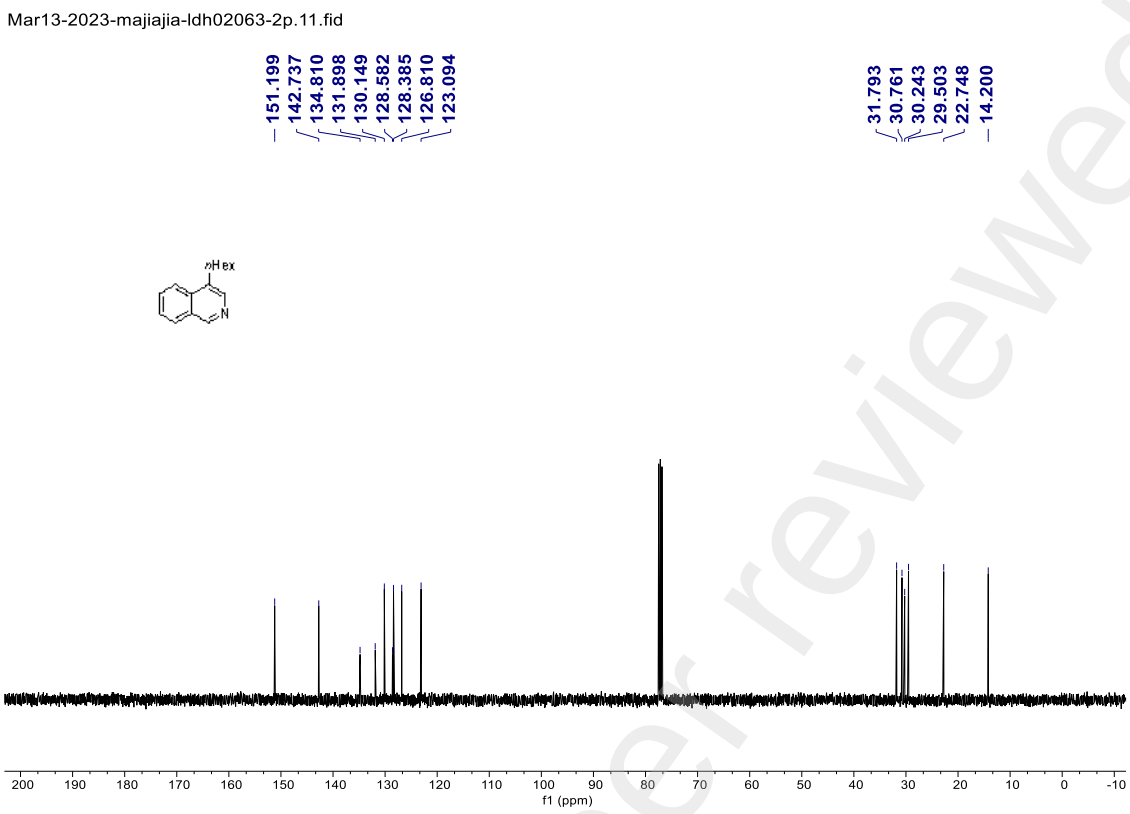
Analytical data of **1j**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.37 (s, 1H), 8.02 - 7.93 (m, 2H), 7.75 - 7.67 (m, 1H), 7.63 - 7.54 (m, 1H), 3.00 (t, *J* = 8.0 Hz, 2H), 1.80 - 1.67 (m, 2H), 1.47 - 1.39 (m, 2H), 1.37 - 1.28 (m, 4H), 0.92 - 0.87 (m, 3H).

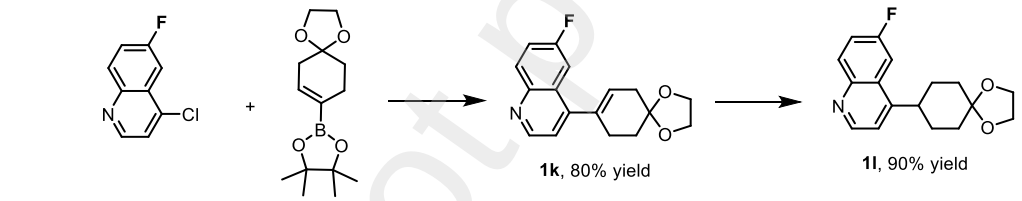
^{13}C NMR (101 MHz, $CDCl_3$) δ 151.2, 142.7, 134.8, 131.9, 130.1, 128.6, 128.4, 126.8, 123.1, 31.8, 30.8, 30.2, 29.5, 22.7, 14.2.

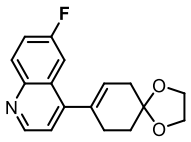
HRMS (ESI, *m/z*) calcd for $C_{15}H_{20}N^+$ $[M+H]^+$: 214.1596, found: 214.1593.





Experimental Procedure C for synthesizing quinoline derivatives 1l [12]





1k, 80% yield

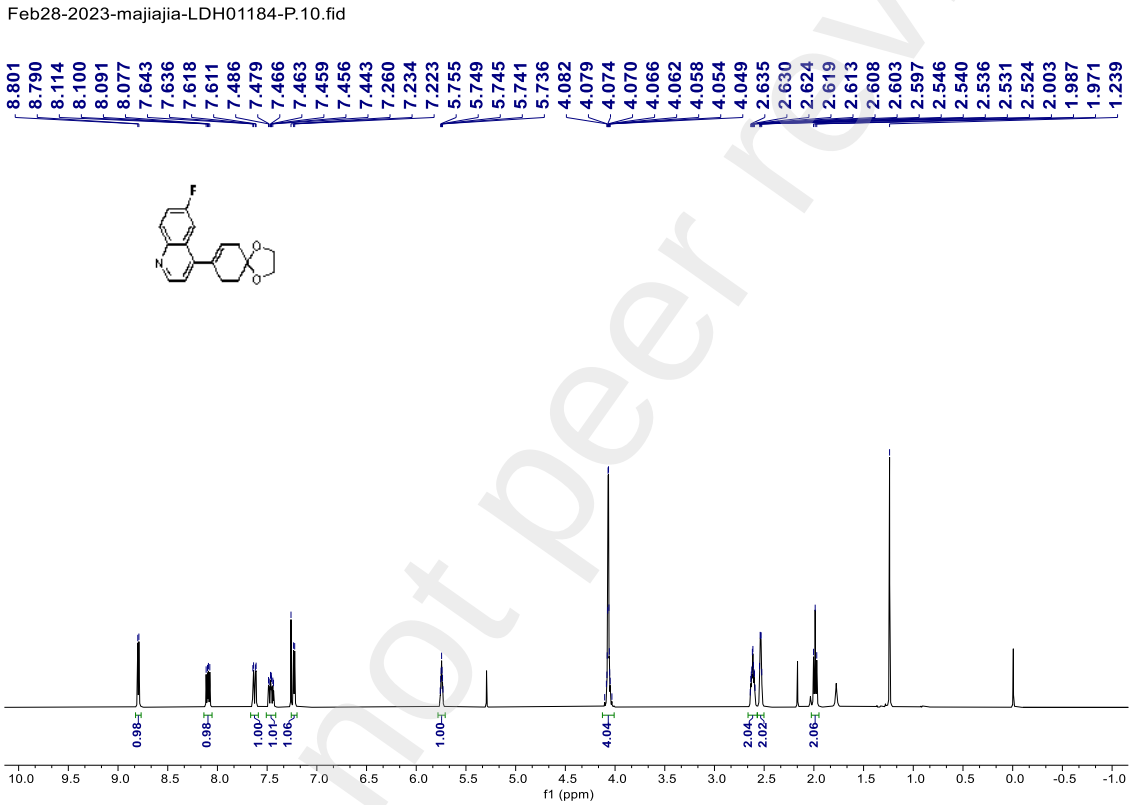
To a solution of 4-Chloro-6-fluoroquinoline (5.0 mmol, 908.0 mg, 1.0 equiv.), Pinacol ester (5.0 mmol, 1.33 g, 1.0 equiv.), K_2CO_3 (10.0 mmol, 1.38 g, 2.0 equiv.) and $Pd(PPh_3)_4$ (10.0 mol%, 578.0 mg) in 1,4-dioxane/H_2O (v/v = 10:1, 50 mL) were stirred for overnight under nitrogen atmosphere at 110 ℃. After completion of reaction, the resulting mixture was diluted by H_2O (100 mL) and washed with EtOAc (3 × 30mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **1k** as a white solid (1.14 g, 80% yield).

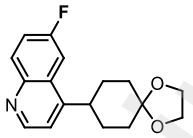
Purification conditions: EtOAc/petroleum ether = 1:3 to 1:1

R_f (**1k**) = 0.3 in EtOAc/petroleum ether = 1:1.

Analytical data of **1k**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 4.4 Hz, 1H), 8.10 (dd, *J* = 9.2, 5.6 Hz, 1H), 7.63 (dd, *J* = 10.2, 2.8 Hz, 1H), 7.51 - 7.42 (m, 1H), 7.23 (d, *J* = 4.4 Hz, 1H), 5.79 - 5.72 (m, 1H), 4.13 - 3.99 (m, 4H), 2.67 - 2.58 (m, 2H), 2.58 - 2.51 (m, 2H), 1.99 (t, *J* = 6.4 Hz, 2H).





1l, 90% yield

To a solution of **1k** (3.0 mmol, 855.0 mg, 1.0 equiv.) and Pd/C (Pd 5% on Carbon wetted with ca. 55% water, 86.0 mg) in MeOH (10 mL) was stirred for overnight under hydrogen atmosphere at room temperature. After completion of reaction, the resulting mixture was filtered by diatomaceous earth and washed with EtOAc (3 × 30mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the

product **1l** as a white solid (775.0 mg, 90% yield).

Purification conditions: Et_2O/petroleum ether = 1:3 to 1:1

R_f (**1l**) = 0.3 in Et_2O/petroleum ether = 1:1.

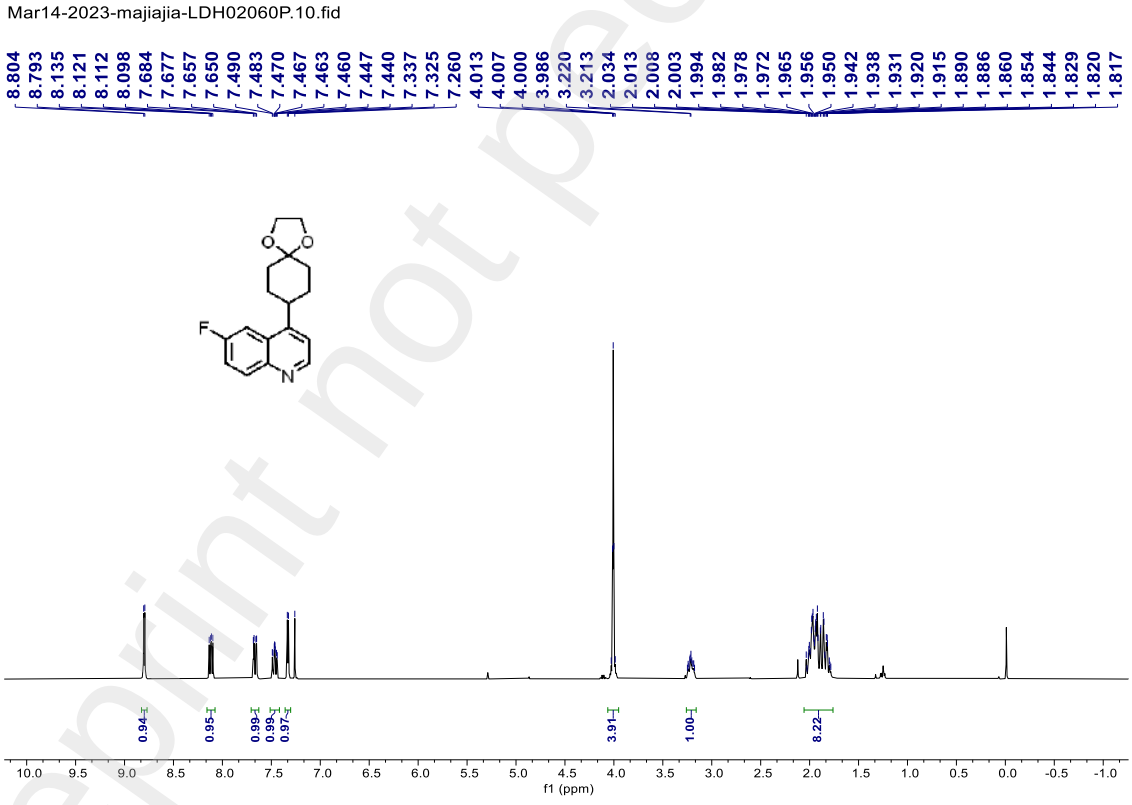
Analytical data of **1l**:

^1H NMR (400 MHz, $CDCl_3$) δ 8.80 (d, *J* = 4.4 Hz, 1H), 8.12 (dd, *J* = 9.2, 5.6 Hz, 1H), 7.67 (dd, *J* = 10.8, 2.8 Hz, 1H), 7.46 (ddd, *J* = 9.2, 8.0, 2.8 Hz, 1H), 7.33 (d, *J* = 4.8 Hz, 1H), 4.03 - 3.98 (m, 4H), 3.25 - 3.17 (m, 1H), 2.05 - 1.76 (m, 8H).

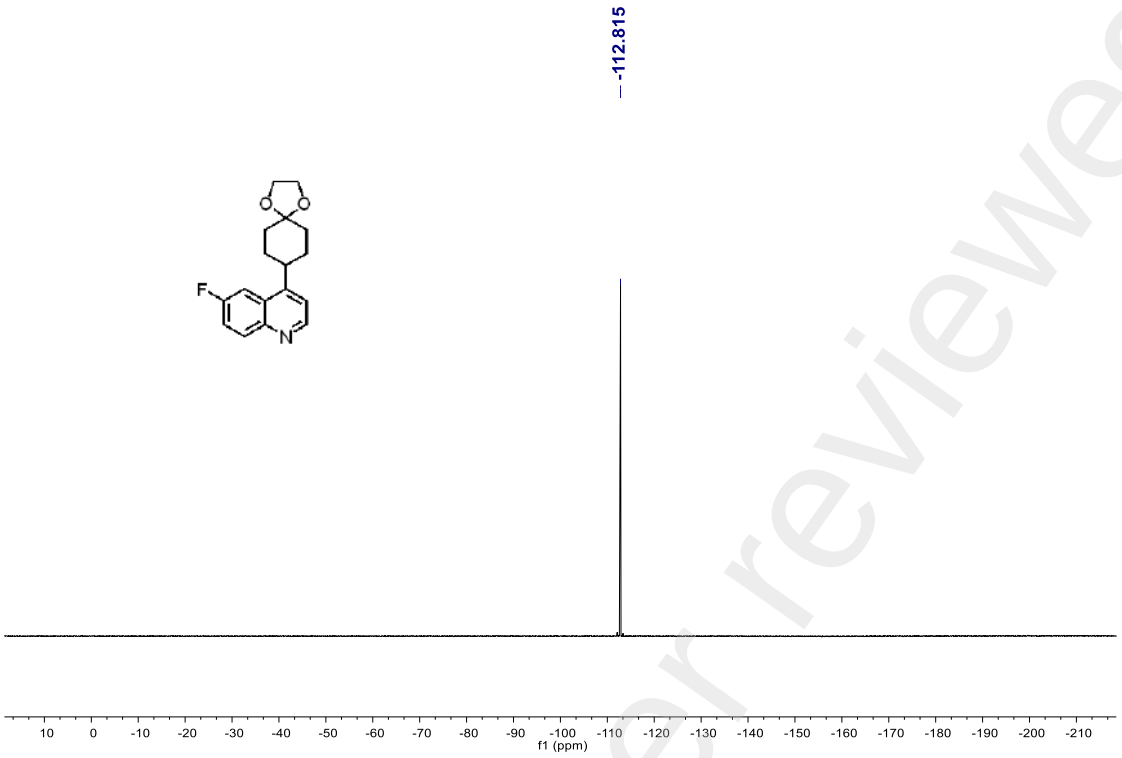
^{19}F NMR (376 MHz, $CDCl_3$) δ -112.81.

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7 (d, *J* = 247.0 Hz), 151.7 (d, *J* = 5.7 Hz), 149.76 (d, *J* = 2.6 Hz), 145.6, 133.0 (d, *J* = 9.2 Hz), 127.9 (d, *J* = 9.0 Hz), 119.2 (d, *J* = 25.7 Hz), 118.3, 108.3, 106.7 (d, *J* = 22.6 Hz), 64.6, 64.5, 38.0, 35.3, 30.5.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{19}NFO_2^+$ $[M+H]^+$: 288.1400, found: 288.1397.



Mar14-2023-majiajia-LDH02060P.11.fid



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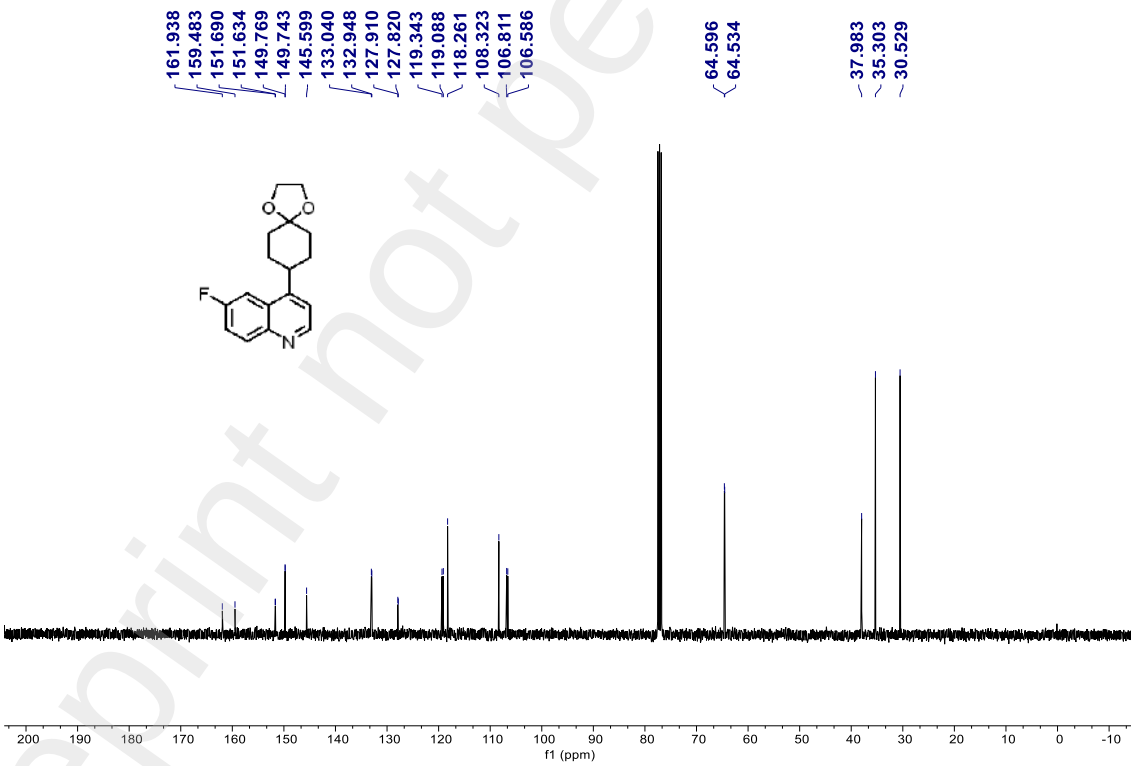
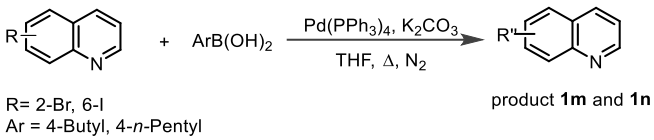


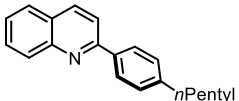
General procedure D for synthesizing quinoline derivatives 1m and 1n



R= 2-Br, 6-I
Ar = 4-Butyl, 4-*n*-Pentyl

product **1m** and **1n**

A dried 10 mL Schlenk tube was charged with started materials (1.0 mmol, 1.0 equiv.), $ArB(OH)_2$ (1.5 mmol, 1.5 equiv.), K_2CO_3 aq. (2.0 M, 5.0 equiv.) and $Pd(PPh_3)_4$ (5.0 mol%) in THF (0.5 M) under argon atmosphere. The reaction mixture was stirred vigorously at 80 ℃ until the full conversion of the starting material. Afterwards, the reaction was quenched by saturated aqueous $NaHCO_3$ and extracted with CH_2Cl_2 (10 mL × 3). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel (EtOAc/petroleum ether CH_2Cl_2/Acetone) to give the desired product **1m** and **1n.**



1m,79% yield

According to the general procedure D, the 2-bromoquinoline (4.0 mmol, 832.0 mg, 1.0 equiv.) was converted to the product **1m** (870.2 mg, 79% yield) as a white solid.

Purification conditions: EtOAc/petroleum ether= 1:10 to 1:5

R_f (**1m**) = 0.3 in EtOAc/petroleum ether= 1:5

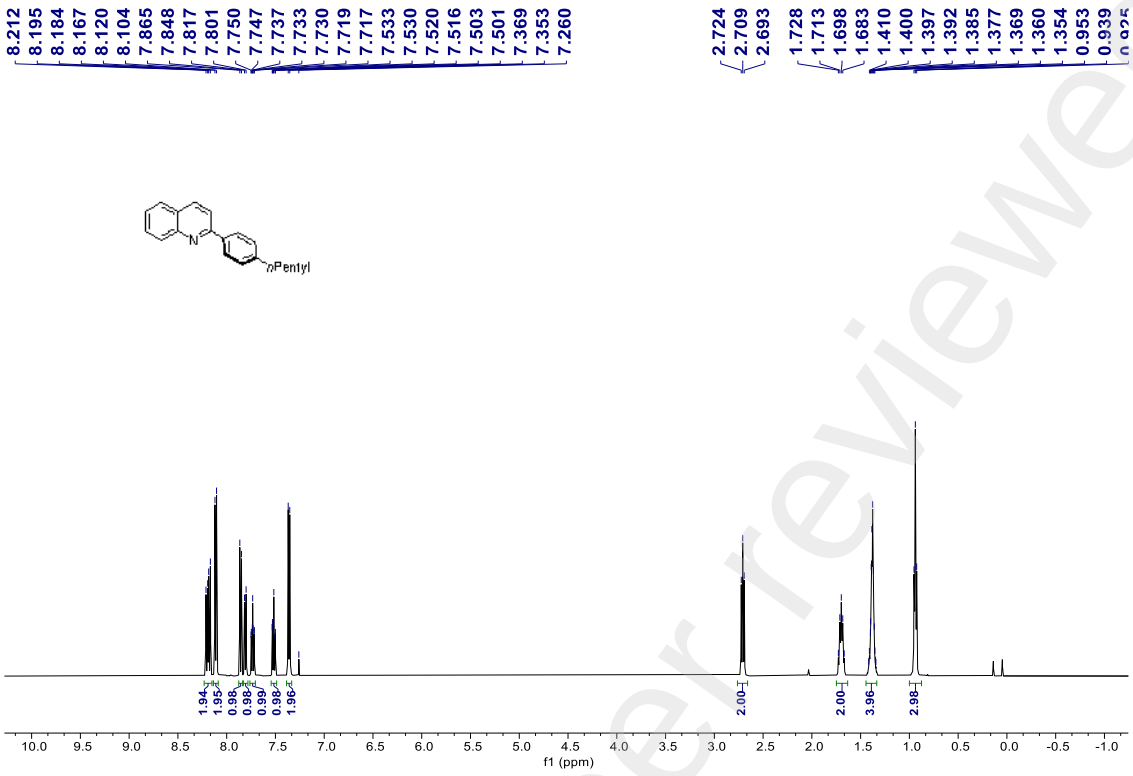
Analytical data of **1m**:

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 14.0, 8.5 Hz, 2H), 8.11 (d, *J* = 8.2 Hz, 2H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.77 - 7.70 (m, 1H), 7.55 - 7.48 (m, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.74 - 2.68 (m, 2H), 1.70 (p, *J* = 7.5 Hz, 2H), 1.43 - 1.33 (m, 4H), 0.94 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 148.4, 144.5, 137.2, 136.7, 129.8, 129.6, 129.1, 127.6, 127.5, 127.2, 126.1, 119.0, 35.8, 31.5, 31.2, 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{20}H_{22}N^+$ $[M+H]^+$: 276.1752, found: 276.1749.

LDH02028-11-S.M.10.fid



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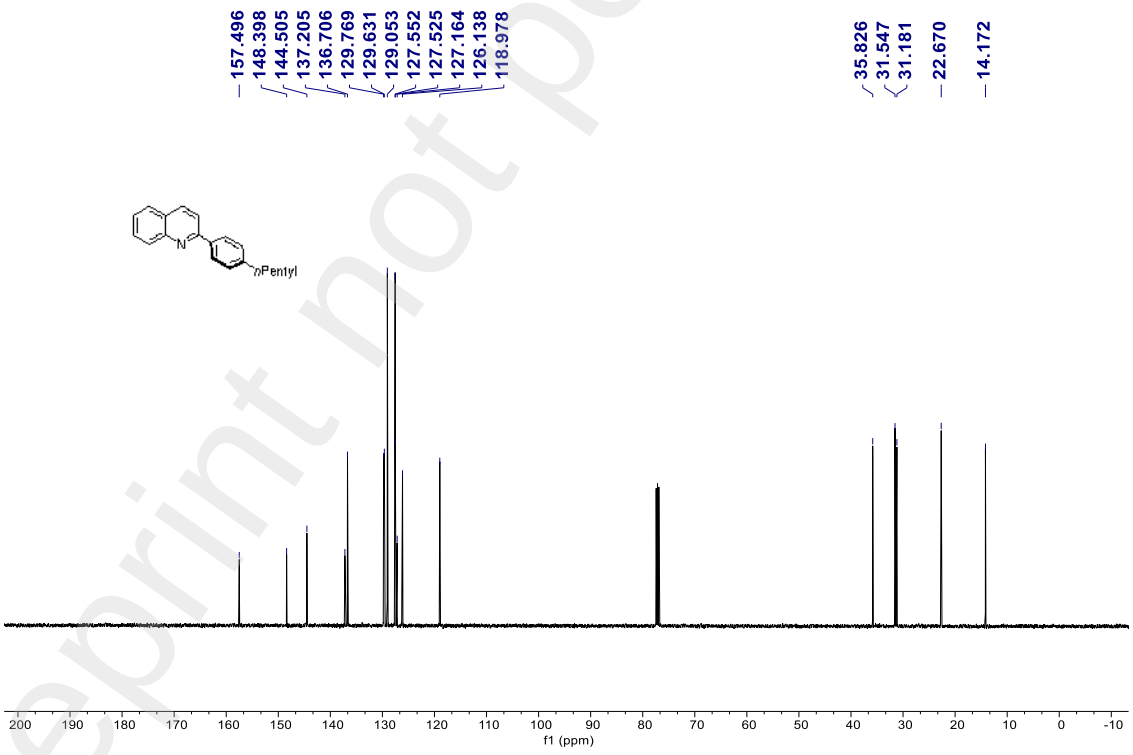
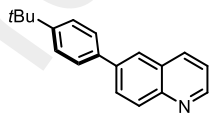




1n, 83% yield

According to the general procedure D, the 6-Iodoquinoline (1.0 mmol, 255.0 mg, 1.0 equiv.) was converted to the product **1n** (216.7 mg, 83% yield) as a white solid.

Purification conditions: Acetone/CH_2Cl_2 = 1:80 to 1:30

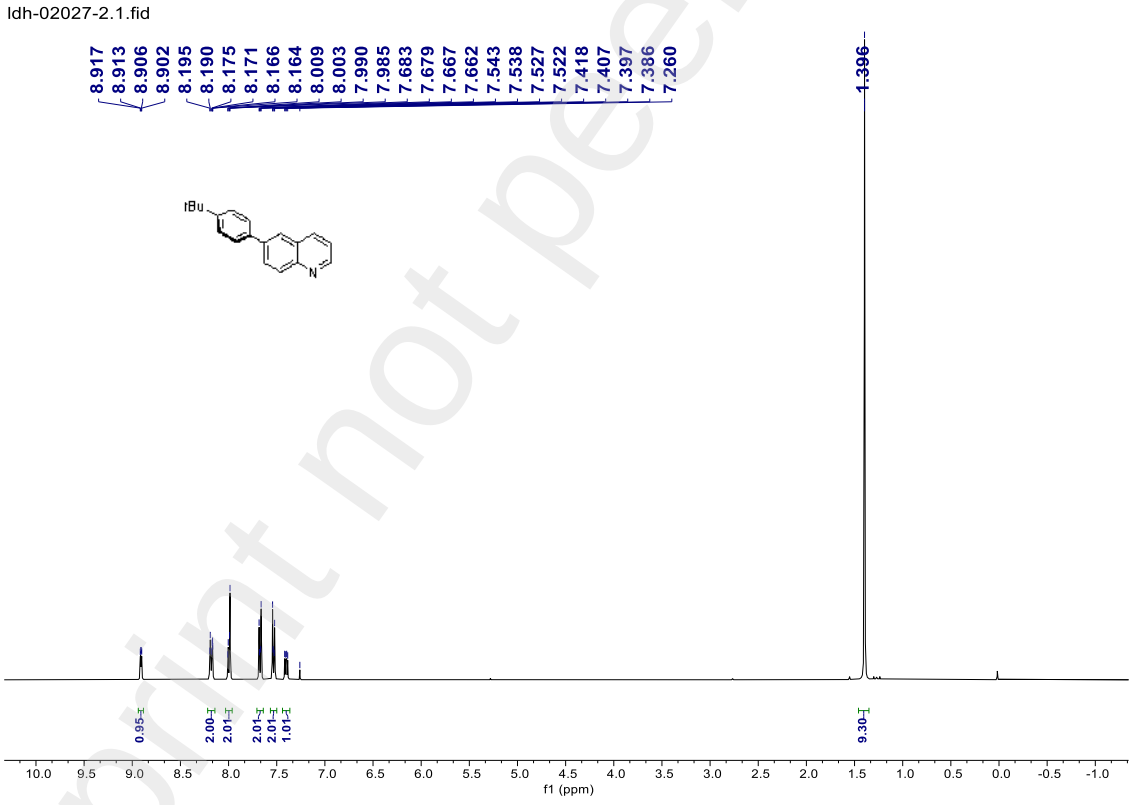
R_f (**1n**) = 0.4 in Acetone/CH_2Cl_2 = 1:40

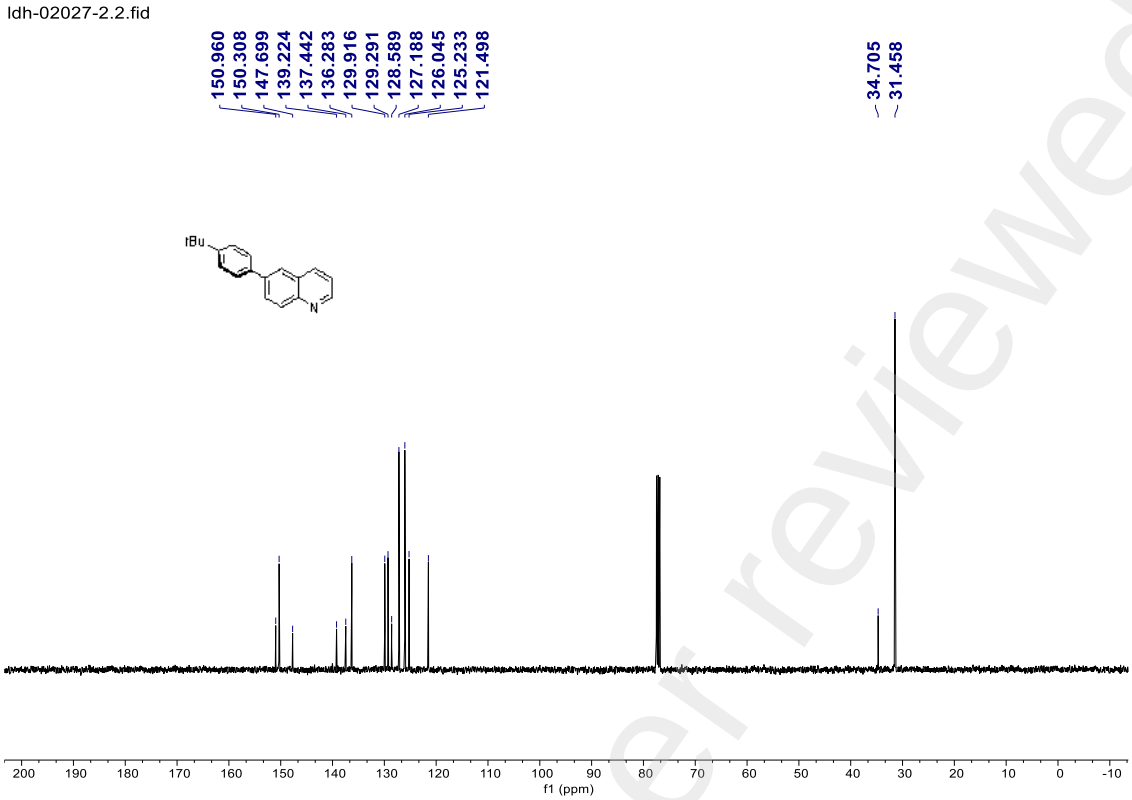
Analytical data of **1n**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.20 - 8.15 (m, 2H), 8.01 - 7.97 (m, 2H), 7.69 - 7.64 (m, 2H), 7.55 - 7.52 (m, 2H), 7.40 (dd, *J* = 8.4, 4.4 Hz, 1H), 1.40 (s, 9H).

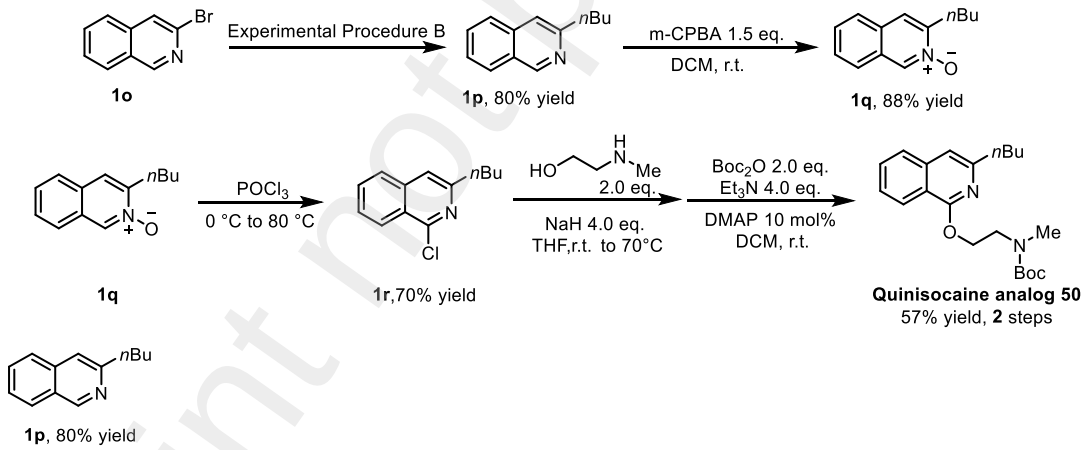
^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0, 150.3, 147.7, 139.2, 137.4, 136.3, 129.9, 129.3, 128.6, 127.2, 126.0, 125.2, 121.5, 34.7, 31.5.

HRMS (ESI, *m/z*) calcd for $C_{19}H_{20}N^+$ $[M+H]^+$: 262.1596, found: 262.1594.





Experimental Procedure E for synthesizing quinoline derivatives Quinisocaine analog 50 [13-14]



1p, 80% yield

According to the general procedure B, the 3-Bromoisoquinoline **1o** (20.0 mmol, 4.16 g, 1.0 equiv.) was converted to the product **1p** as a brown oil (0.77 g, 80% yield).

Purification conditions: EtOAc/petroleum ether= 1:10 to 1:5

R_f (**1p**) = 0.35 in EtOAc/petroleum ether = 1:5

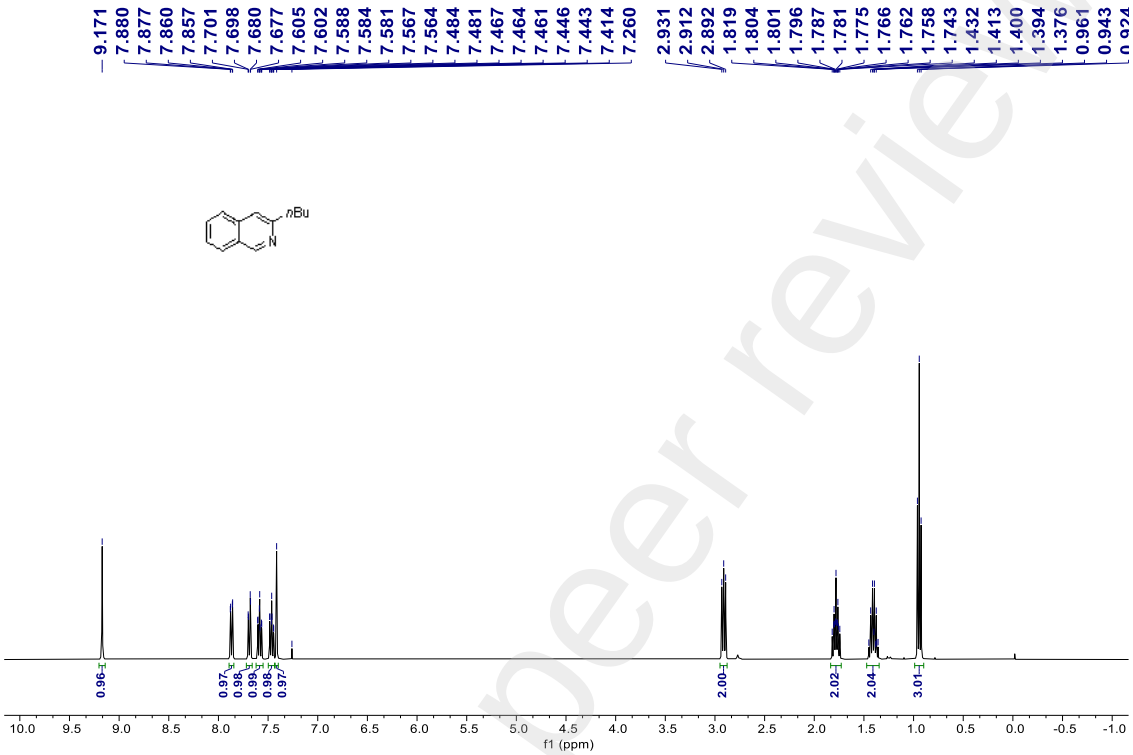
Analytical data of **1p**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 7.87 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.69 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.61 - 7.56 (m, 1H), 7.49 - 7.44 (m, 1H), 7.41 (s, 1H), 2.91 (t, *J* =

8.0, 2H), 1.83 - 1.74 (m, 2H), 1.47 - 1.35 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9, 152.1, 136.5, 130.2, 127.5, 127.1, 126.3, 126.1, 117.9, 37.9, 32.2, 22.6, 14.0.

Feb18-2023-majiajia-LDH02044-P.10.fid



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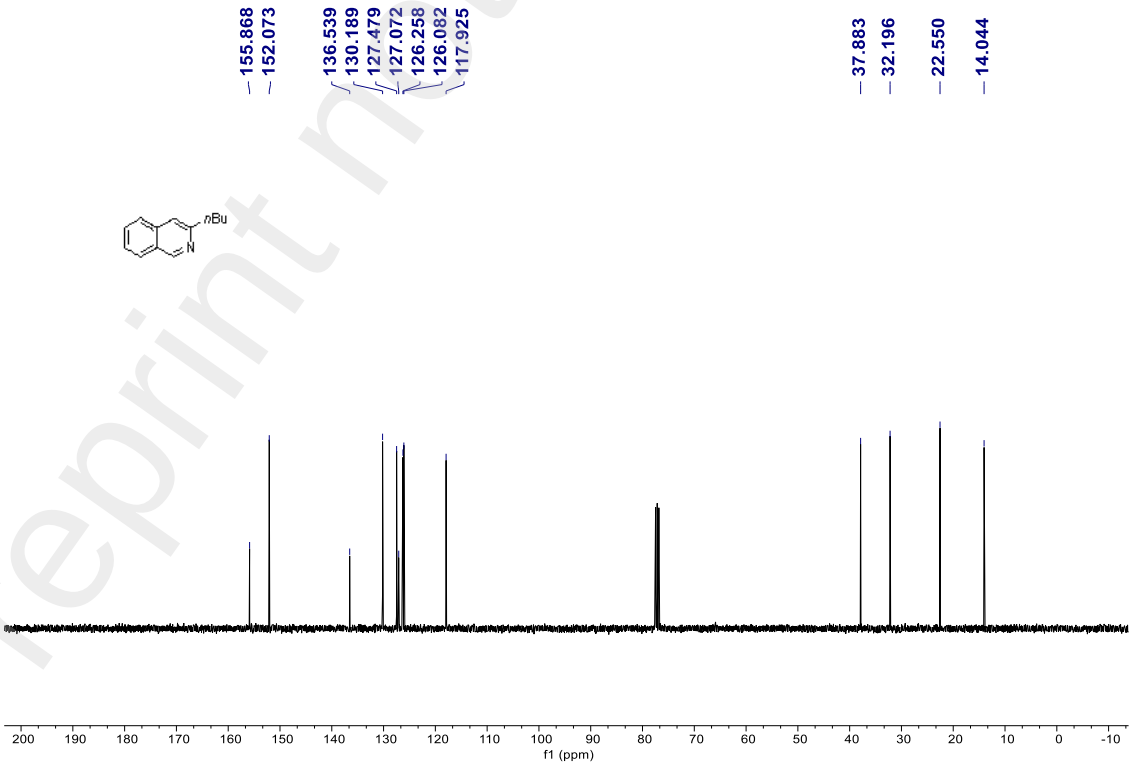
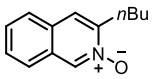




1q, 88% yield

To a solution of the substrate **1p** (20.0 mmol, 3.70 g, 1.0 equiv.) in CH_2Cl_2 (20 mL) was added the 3-Chloroperbenzoic acid (30.0 mmol, 6.10 g, 1.5 equiv.) at 0 °C. After stirring for 15 min at the same temperature, the mixture moves to the room temperature and stirred for 4 h. After completion of reaction, the resulting mixture was concentrated under reduced pressure and the crude residue was purified by flash chromatography on silica gel to give the product **1q** as a yellow solid (3.16 g, 88% yield).

Purification conditions: MeOH/ CH_2Cl_2 = 1:40 to 1:20

R_f (**1q**) = 0.3 in MeOH/ CH_2Cl_2 = 1:20.

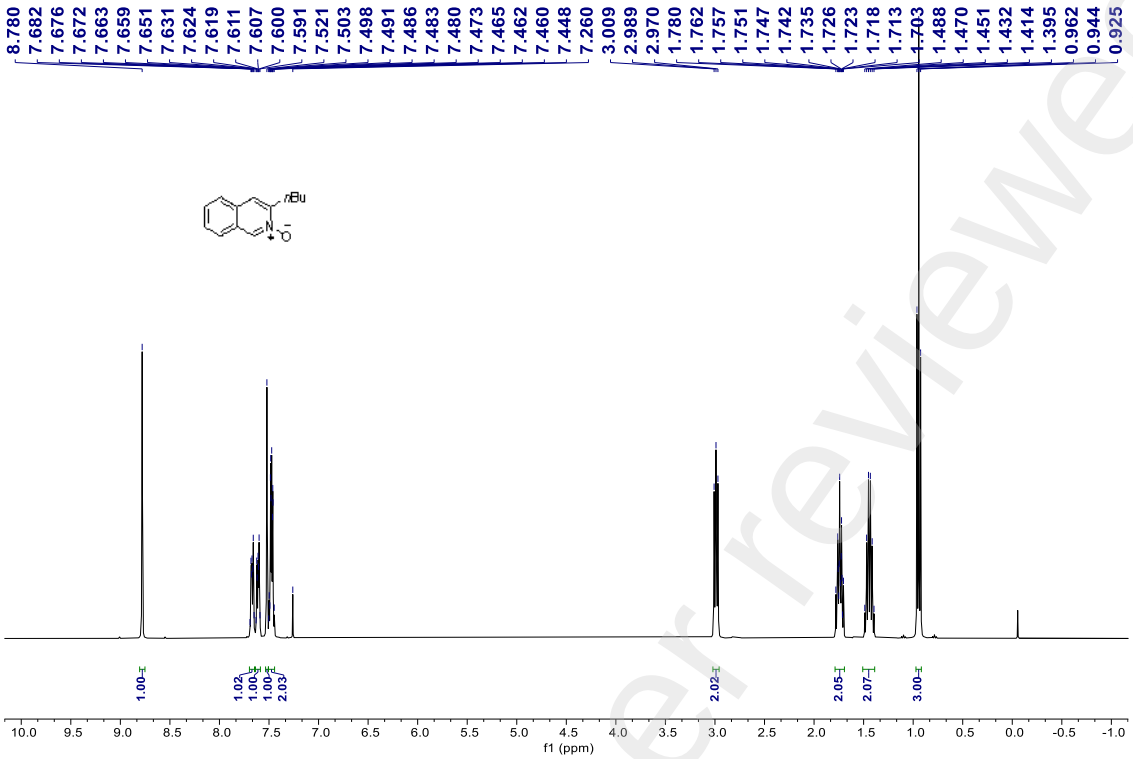
Analytical data of **1q**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (s, 1H), 7.70 - 7.65 (m, 1H), 7.63 - 7.58 (m, 1H), 7.52 (s, 1H), 7.51 - 7.44 (m, 2H), 2.99 (t, 2H), 1.79 - 1.69 (m, 2H), 1.44 (h, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).

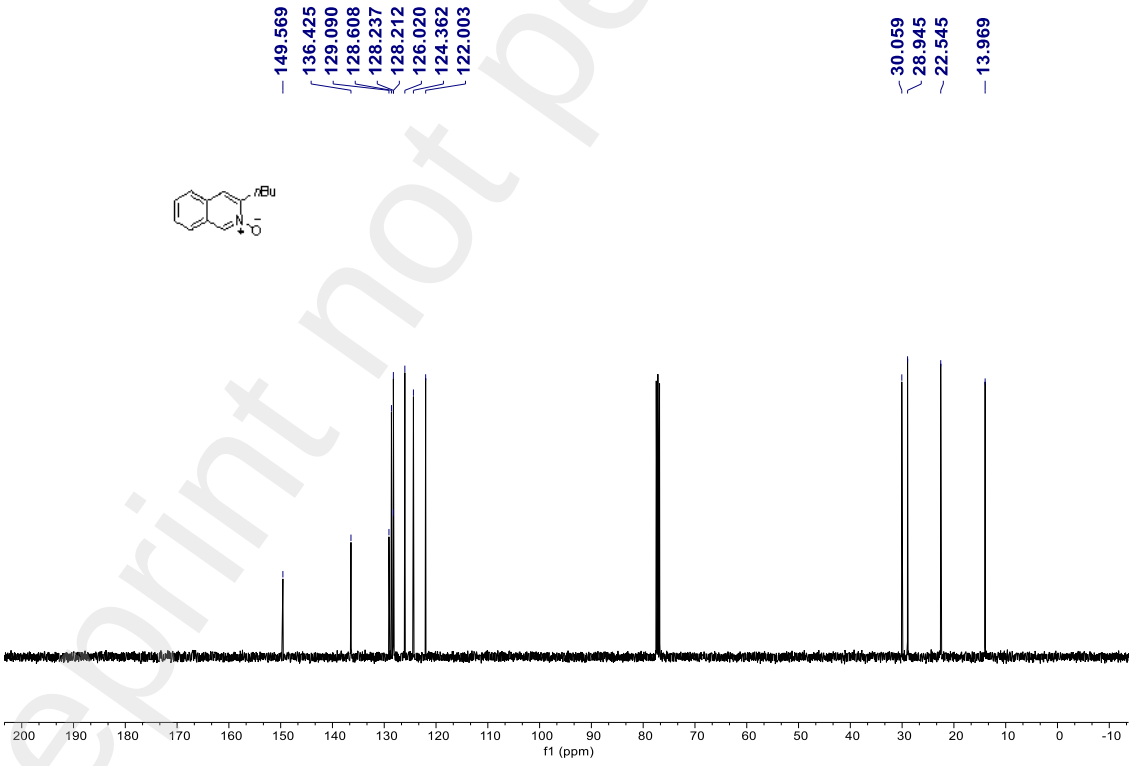
^{13}C NMR (101 MHz, $CDCl_3$) δ 149.6, 136.4, 129.1, 128.6, 128.2, 128.2, 126.0, 124.4, 122.0, 30.1, 28.9, 22.5, 14.0.

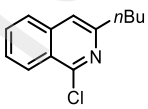
HRMS (ESI, *m*/*z*) calcd for $C_{13}H_{16}NO^+$ $[M+H]^+$: 202.1232, found: 202.1232.

Feb22-2023-majiajia-ldh02048-p.10.fid



Feb22-2023-majiajia-ldh02048-p.11.fid





1r, 70% yield

A $CHCl_3$ (10 mL) solution of **1q** (16.0 mmol, 3.21 g, 1.0 equiv.) was added dropwise to the $POCl_3$(20.0 mL) at 0 at 0 ℃. After stirring for 15 min at the same temperature, the mixture moves to 80 ℃ and stirred for 12 h. After completion of reaction, the resulting mixture was concentrated under reduced pressure. The crude residue was neutralized by saturated aqueous $NaHCO_3$ and extracted by CH_2Cl_2 (3 × 50 mL). The organic phases were concentrated and the crude residue was purified by flash chromatography on silica gel to give the product **1r** as a yellow oil (2.46 g, 70% yield).

Purification conditions: EtOAc/petroleum ether= 1:100

R_f (**1r**) = 0.5 in EtOAc/petroleum ether= 1:50

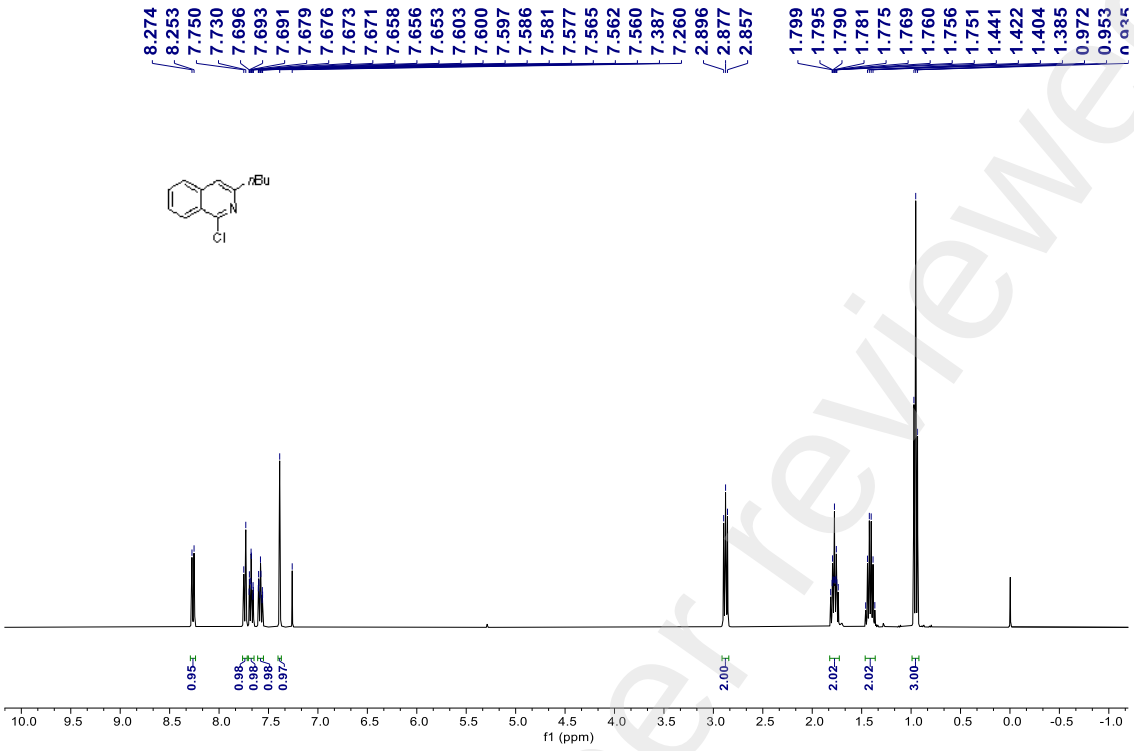
Analytical data of **1r**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.72 - 7.63 (m, 1H), 7.63 - 7.54 (m, 1H), 7.39 (s, 1H), 2.88 (t, *J* = 8.0 Hz, 2H), 1.84 - 1.71 (m, 2H), 1.46 - 1.36 (m, 2H), 0.95 (t, *J* = 7.6 Hz, 3H).

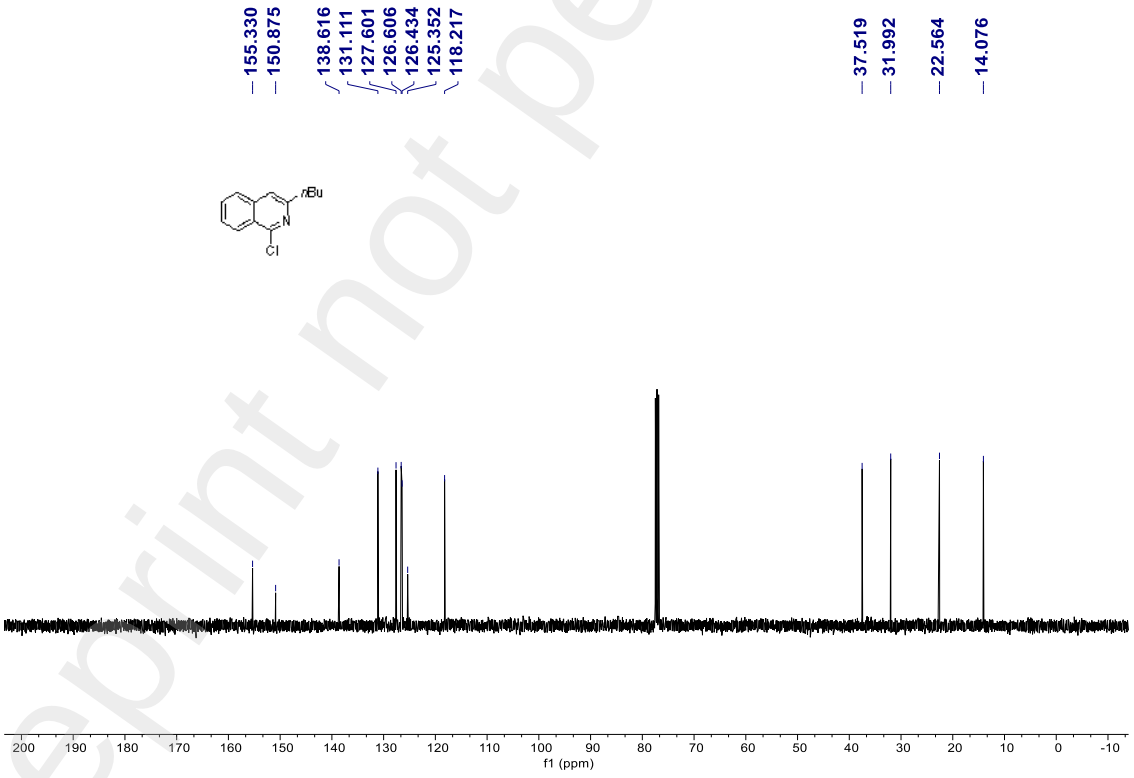
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 150.9, 138.6, 131.1, 127.6, 126.6, 126.4, 125.4, 118.2, 37.5, 32.0, 22.6, 14.1.

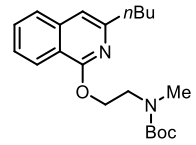
HRMS (ESI, *m*/*z*) calcd for $C_{13}H_{15}NCl^+$ $[M+H]^+$: 220.0893, found: 220.0898.

Mar09-2023-majiajia-LDH02048-2P.10.fid



Mar09-2023-majiajia-LDH02048-2P.11.fid





Quinisocaine analog 50
57% yield, **2** steps

Step 1:

To a solution of 2-Methylaminoethanol (15.3 mmol, 1.15g, 2.0 equiv.) in THF (50 mL) was in batches added NaH (30.6 mmol, 0.74 g, 4.0 equiv.) at 0 ℃. After stirring for 30 min at the same temperature, the substrate **1r** (7.65 mmol, 1.68 g, 1.0 equiv.) was added and the mixture moves to 70 ℃ for 12 h. After completion of reaction, the resulting mixture was diluted by H_2O (200 mL) and extracted by EtOAc (3× 50 mL). The organic phases were concentrated under reduced pressure and the crude residue was directly carried out for the next step.

Step 2:

To a CH_2Cl_2 (50 mL) solution of the crude in was added Boc_2O (15.3 mmol, 3.5 mL,), Et_3N (4.2 mL, 30.0 mmol) and DMAP (150.0 mg) and stirred for 6 h at the room temperature. After completion of reaction, the mixture was concentrated and the crude residue was purified by flash chromatography on silica gel to give the product **Quinisocaine analog 50** as a colorless oil (1.56 g, 57% yield, 2 steps).

Purification conditions: EtOAc/petroleum ether= 1:20 to 1:10

R_f (**Quinisocaine analog 50**) = 0.4 in EtOAc/petroleum ether= 1:10

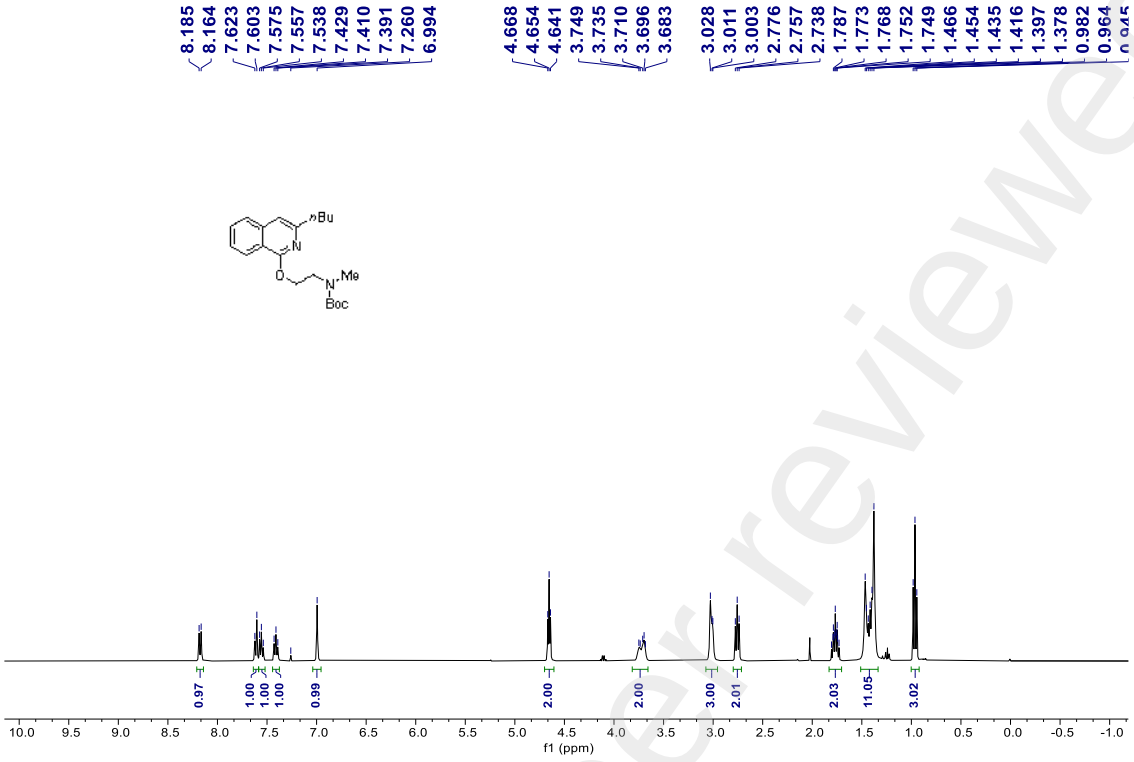
Analytical data of **Quinisocaine analog 50**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 6.99 (s, 1H), 4.65 (t, *J* = 5.2 Hz, 2H), 3.80 - 3.65 (m, 2H), 3.06 - 2.97 (m, 3H), 2.76 (t, *J* = 7.6 Hz, 2H), 1.81 - 1.72 (m, 2H), 1.49 - 1.35 (m, 11H), 0.96 (t, *J* = 7.4 Hz, 3H).

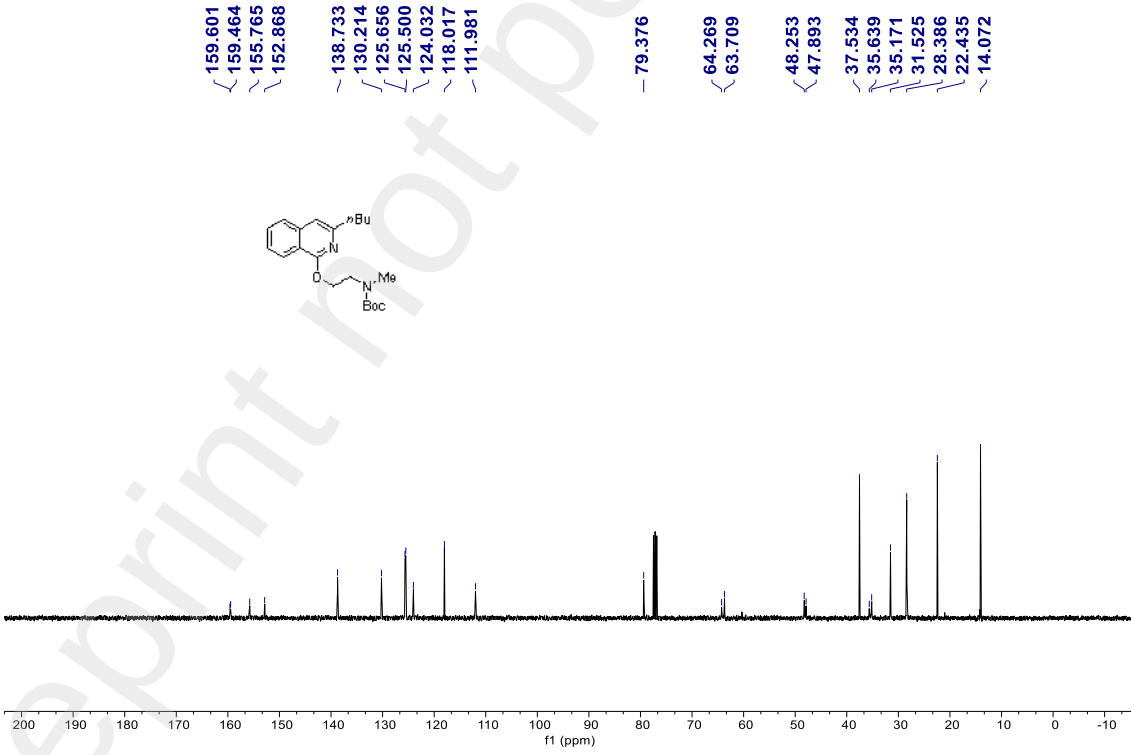
^{13}C NMR (101 MHz, $CDCl_3$, mixture of rotamers) δ 159.6 (rotamer), 159.5, 155.8, 152.9, 138.7, 130.2, 125.7, 125.5, 124.0, 118.0, 112.0, 79.4, 64.3 (rotamer), 63.7, 48.3, 47.9 (rotamer), 37.5, 35.6 (rotamer), 35.2, 31.5, 28.4, 22.4, 14.1.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{31}N2O_3^+$ $[M+H]^+$: 359.2335, found: 359.2329.

Mar03-2023-majiajia-ldh02054-2.11.fid

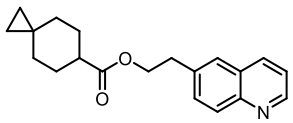


Mar03-2023-majiajia-ldh02054-2.10.fid



Experimental Procedure F for synthesizing quinoline derivatives 1s to 1aq

To a solution of N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride (2.6 mmol, 1.3 equiv.) in CH_2Cl_2 (10 mL) was added 4-Dimethylaminopyridine (0.2 mmol, 224.3 mg, 20 mol%), triethylamine (4.0 mmol, 202.3 mg, 2.0 equiv.), the material R_1OH or R_2NH_2 or EtOH (2.6 mmol, 1.3 equiv.) and the quinoline derivatives (2.0 mmol, 1.0 equiv.) and stirred at room temperature. After the reaction completed, the resulting mixture was diluted by H_2O (20 mL) and extracted with CH_2Cl_2 (3 × 20 mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **1s to 1aq**.



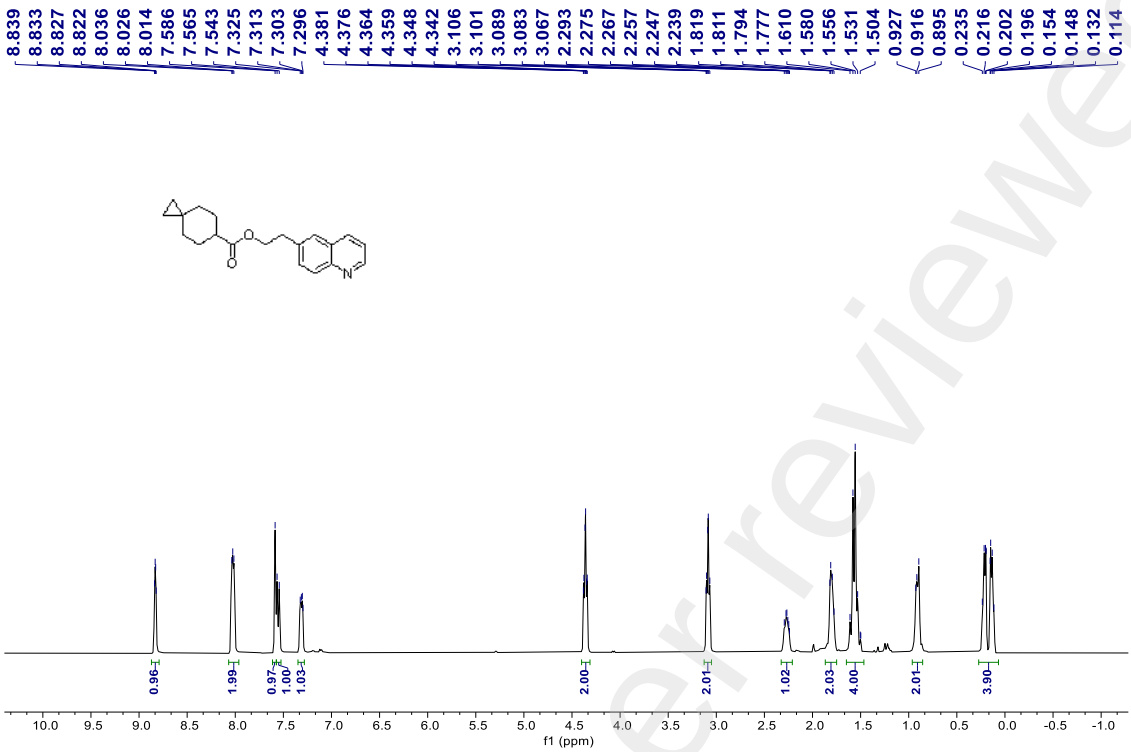
1s, 50% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 - 8.81 (m, 1H), 8.06 - 7.99 (m, 2H), 7.59 (s, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.34 - 7.29 (m, 1H), 4.40 - 4.33 (m, 2H), 3.12 - 3.04 (m, 2H), 2.32 - 2.21 (m, 1H), 1.87 - 1.76 (m, 2H), 1.65 - 1.48 (m, 4H), 0.96 - 0.87 (m, 2H), 0.25 - 0.11 (m, 4H).

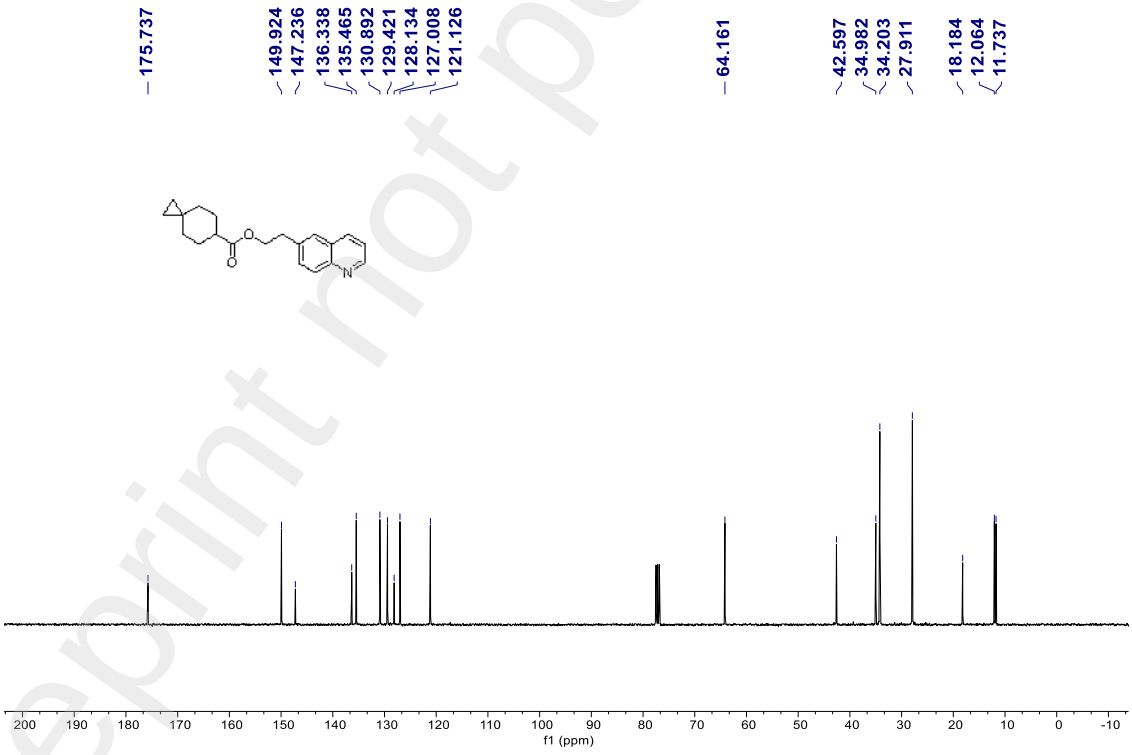
^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 149.9, 147.2, 136.3, 135.5, 130.9, 129.4, 128.1, 127.0, 121.1, 64.2, 42.6, 35.0, 34.2, 27.9, 18.2, 12.1, 11.7.

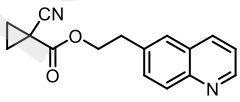
HRMS (ESI, *m*/*z*) calcd for $C_{20}H_{24}NO_2^+$ $[M+H]^+$: 310.1807, found: 310.1802.

yxl-145.1.fid



yxl-145.2.fid



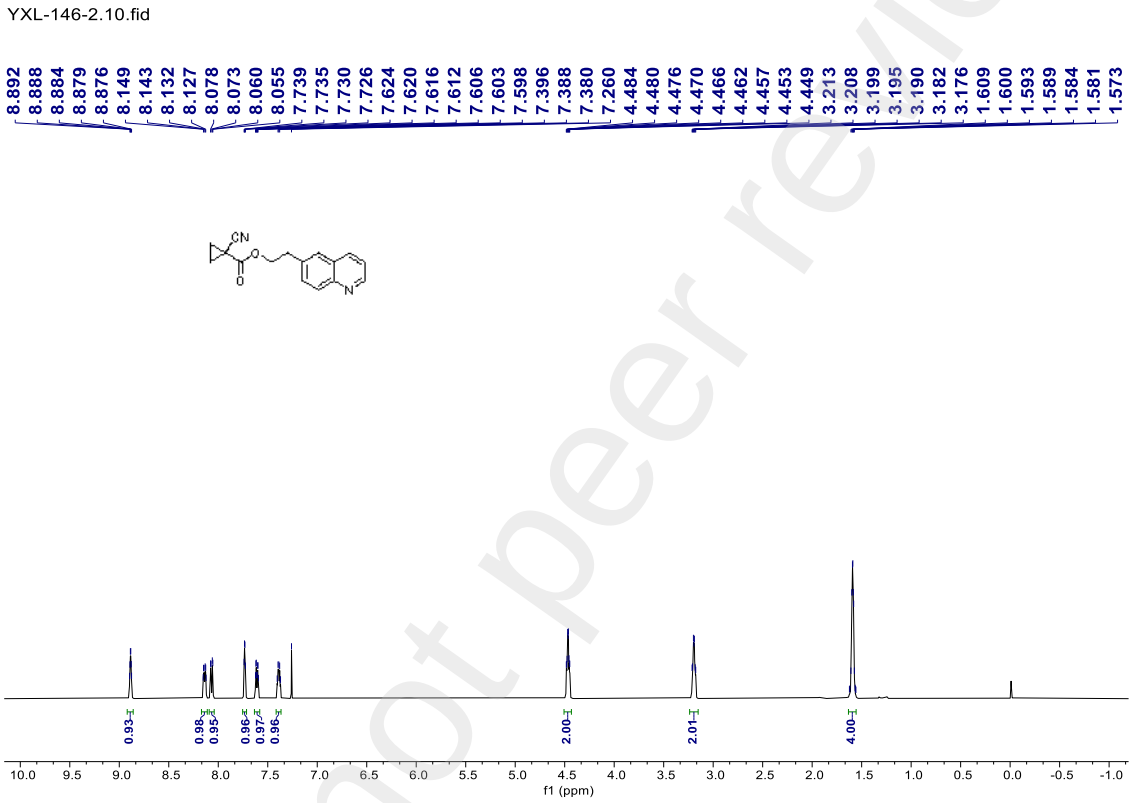


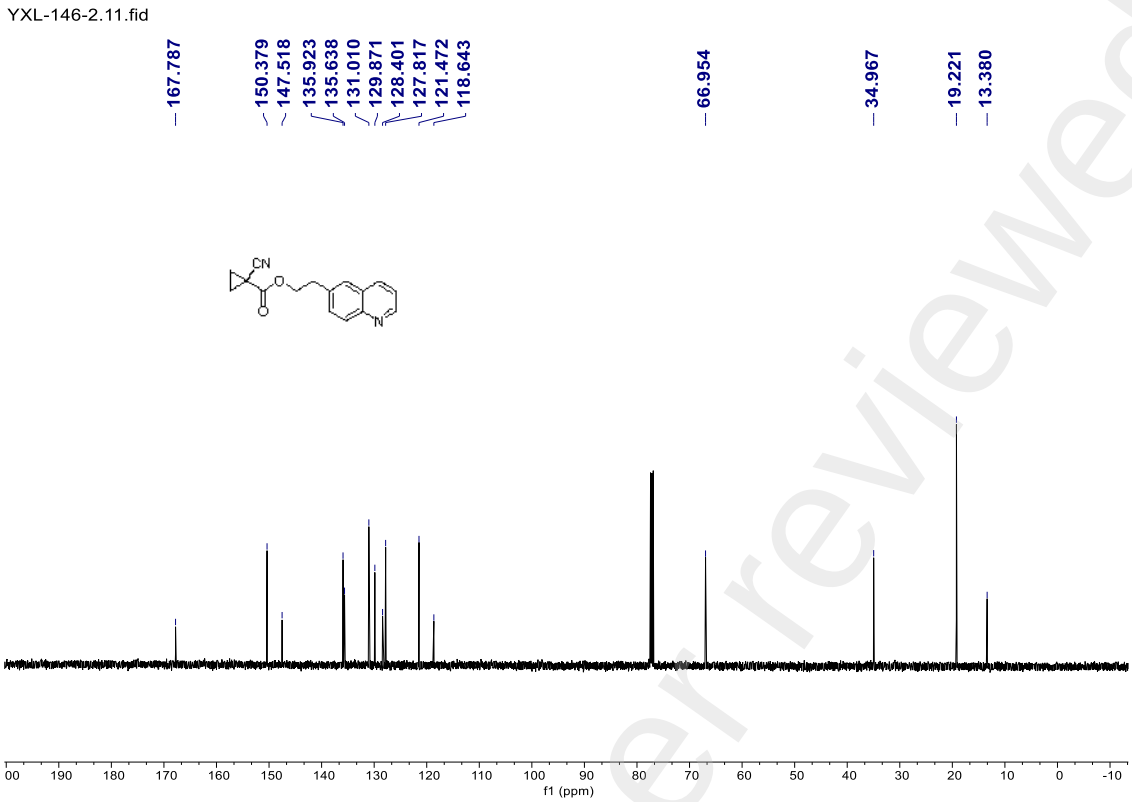
1t, 65% yield

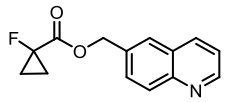
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.93 - 8.86 (m, 1H), 8.17 - 8.11 (m, 1H), 8.09 - 8.04 (m, 1H), 7.75 - 7.71 (m, 1H), 7.63 - 7.59 (m, 1H), 7.41 - 7.36 (m, 1H), 4.49 - 4.43 (m, 2H), 3.23 - 3.16 (m, 2H), 1.63 - 1.55 (m, 4H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 167.8, 150.4, 147.5, 135.9, 135.6, 131.0, 129.9, 128.4, 127.8, 121.5, 118.6, 67.0, 35.0, 19.2, 13.4.

HRMS (ESI, *m/z*) calcd for $C_{16}H_{15}N_2O_2^+$ $[M+H]^+$: 267.1134, found: 267.1132.







1u, 65% yield

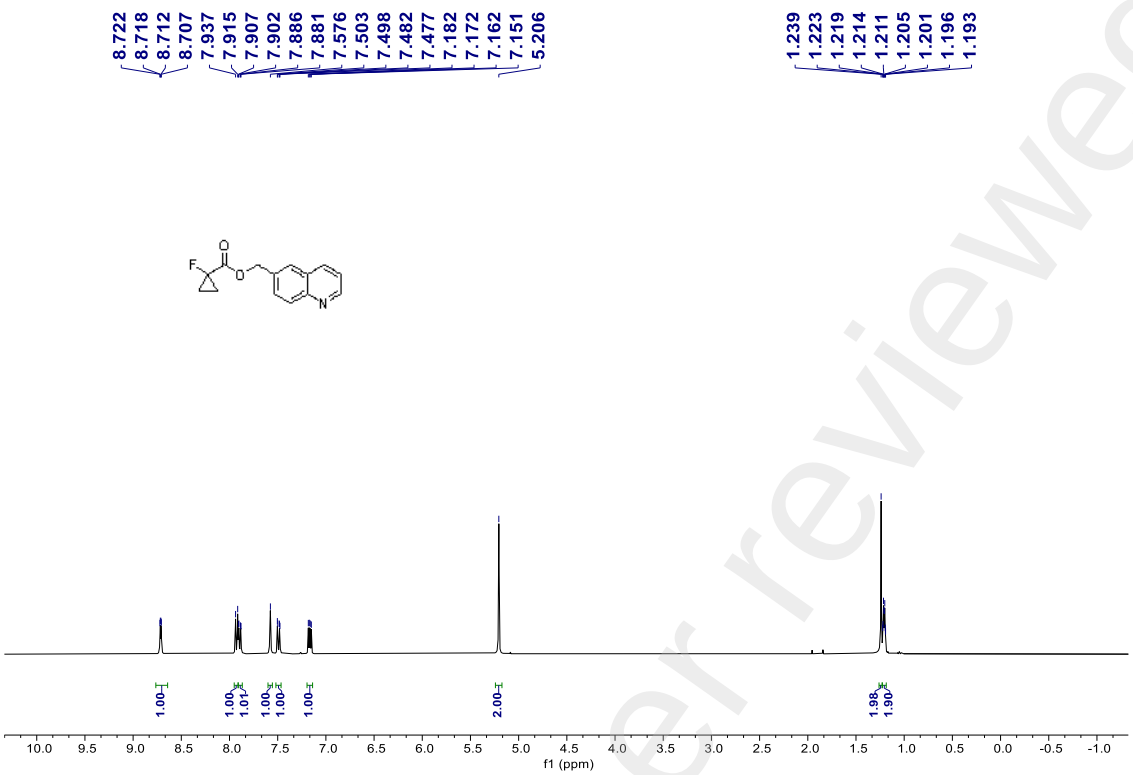
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (dd, *J* = 4.0, 1.6 Hz, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.89 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.58 (br, 1H), 7.49 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.17 (dd, *J* = 8.0, 4.0 Hz, 1H), 5.21 (s, 2H), 1.24 (s, 2H), 1.23 - 1.19 (m, 2H).

^{19}F NMR (376 MHz, $CDCl_3$) δ -198.07.

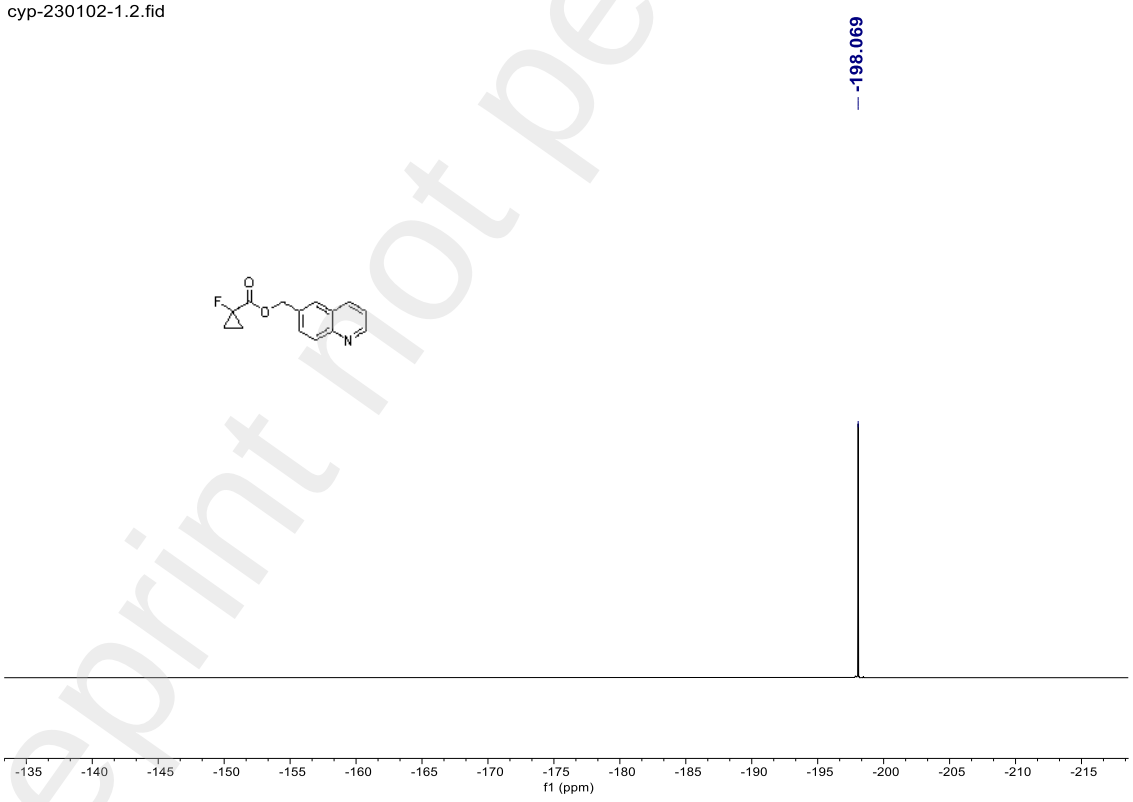
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.05 (d, *J* = 23.7 Hz), 150.51, 147.66, 135.74, 133.18, 129.64, 128.89, 127.59, 126.93, 121.20, 74.46 (d, *J* = 228.8 Hz), 66.42, 14.48 (d, *J* = 10.7 Hz).

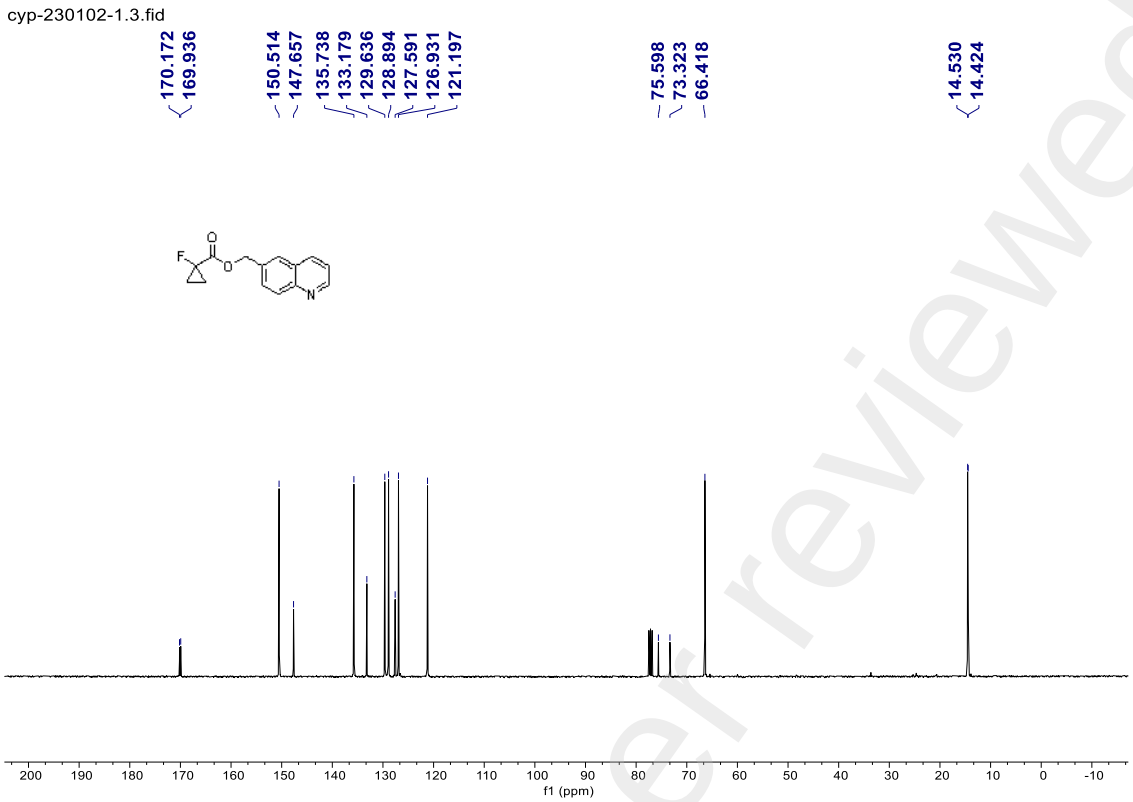
HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{13}NFO_2^+$ $[M+H]^+$: 246.0930, found: 246.0929.

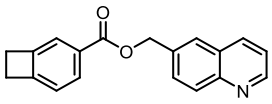
cyp-230102-1.1.fid



cyp-230102-1.2.fid







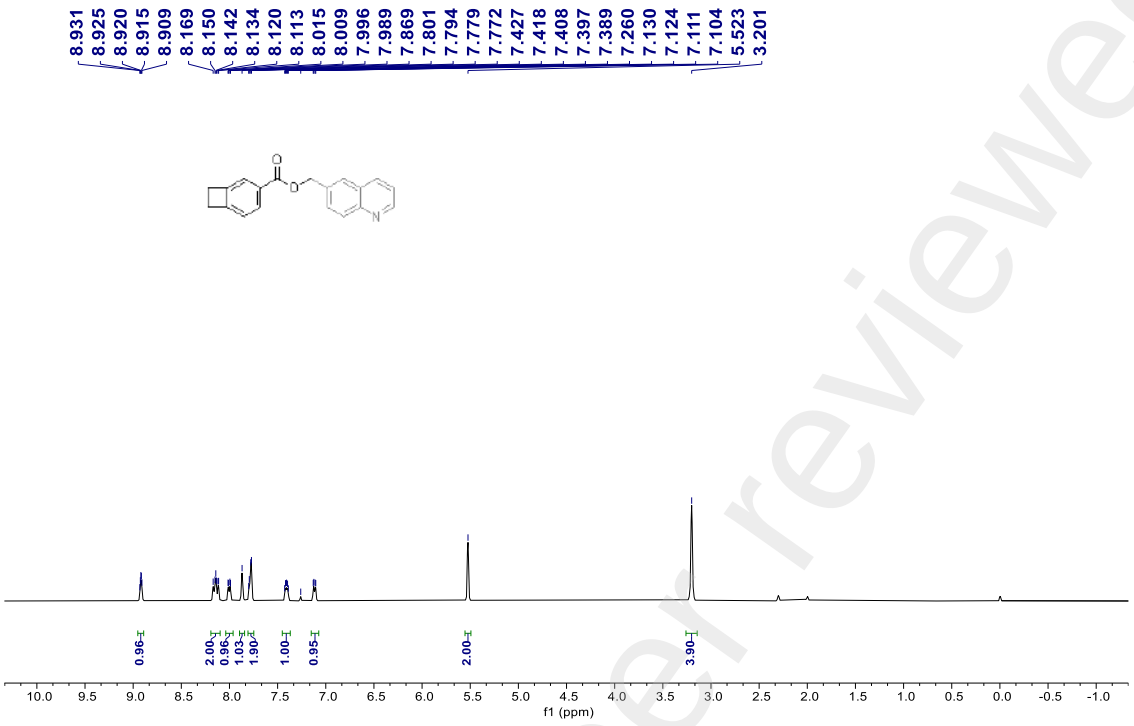
1v, 55% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 - 8.90 (m, 1H), 8.19 - 8.10 (m, 2H), 8.02 - 7.98 (m, 1H), 7.87 (s, 1H), 7.80 - 7.76 (m, 2H), 7.44 - 7.37 (m, 1H), 7.14 - 7.09 (m, 1H), 5.52 (s, 2H), 3.20 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 152.2, 150.8, 148.1, 146.0, 136.2, 134.7, 130.1, 129.4, 129.1, 128.6, 128.2, 126.9, 123.9, 122.6, 121.6, 66.2, 30.0, 29.5.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{16}NO_2^+$ $[M+H]^+$: 290.1181, found: 290.1178.

LH-20230104-1.1.fid



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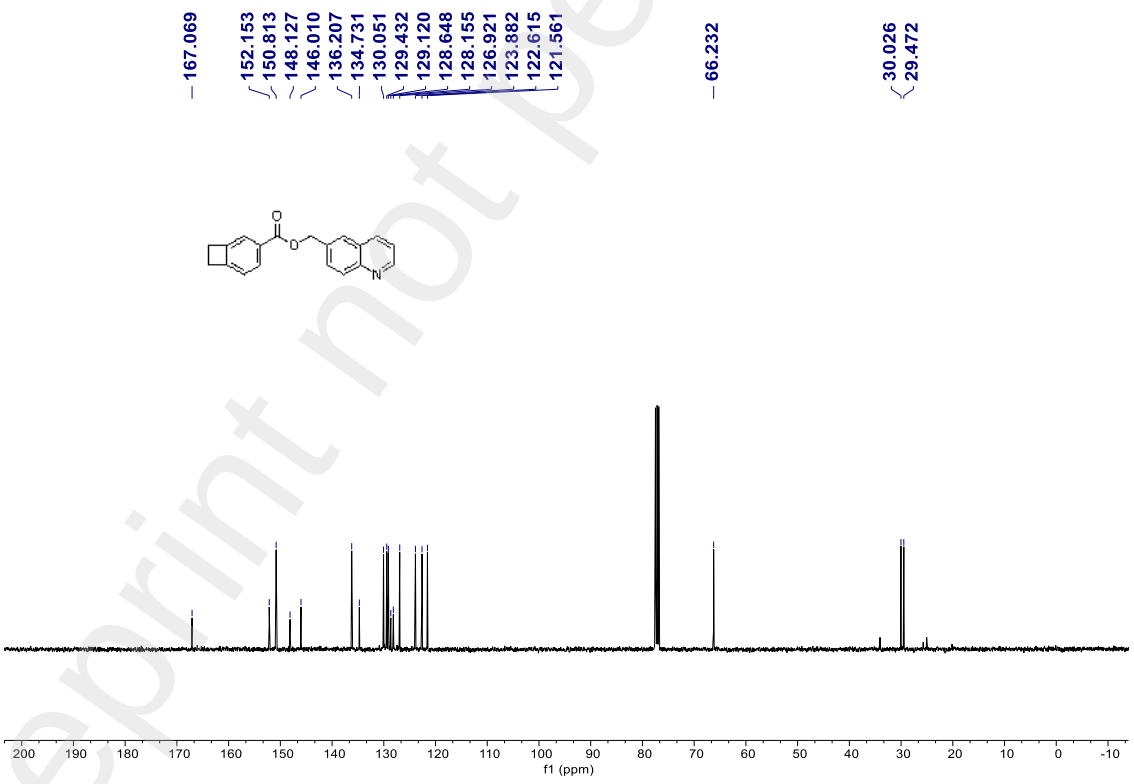
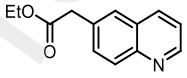


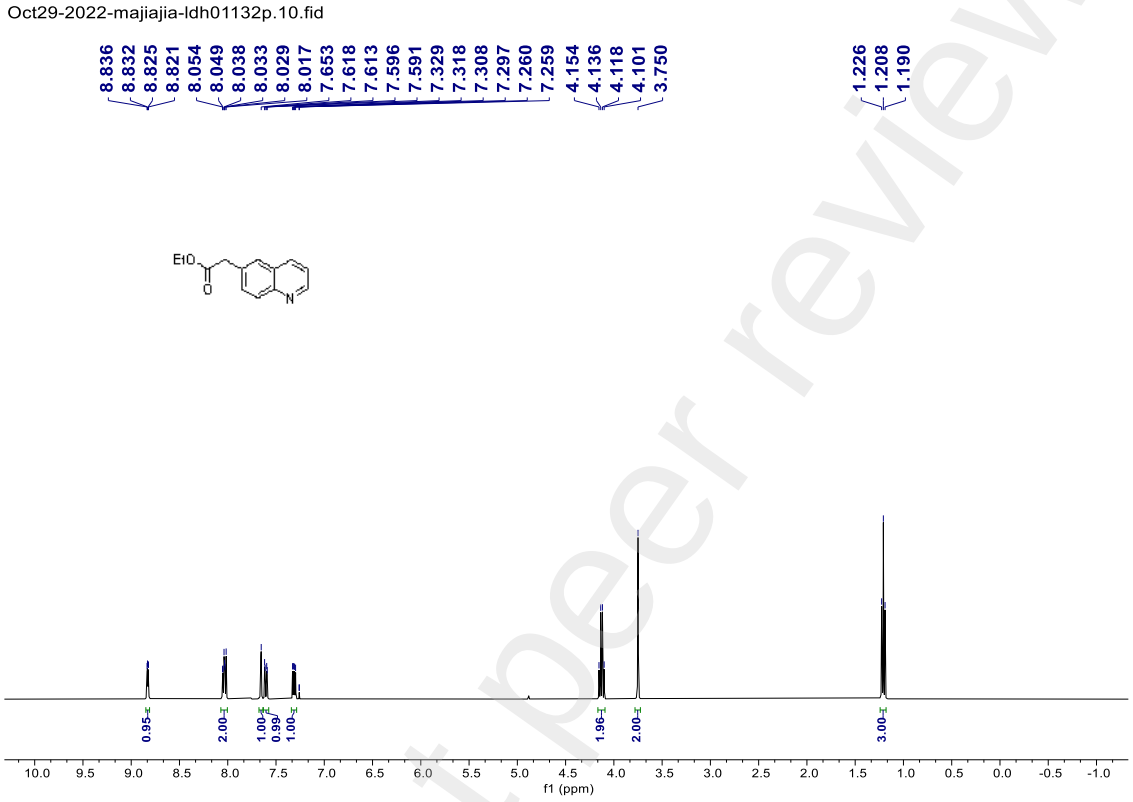


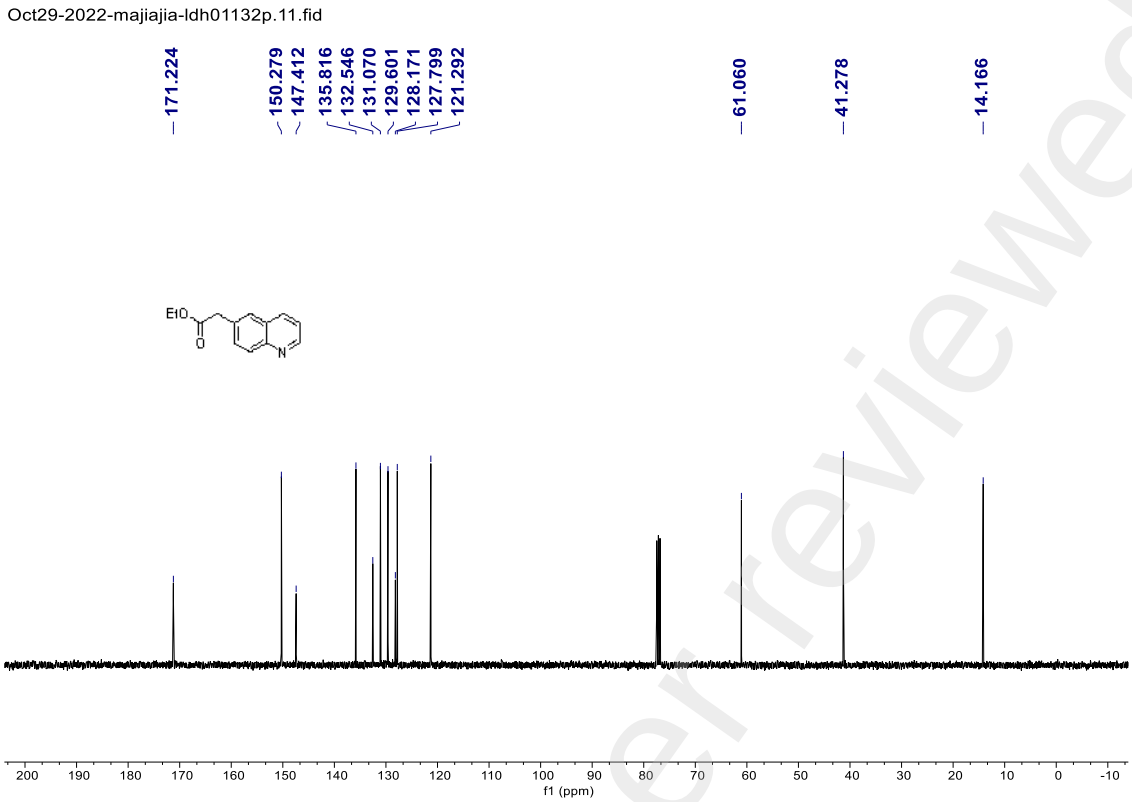
1w, 80% yield

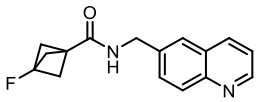
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.08 - 7.99 (m, 2H),

7.65 (s, 1H), 7.60 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.31 (dd, *J* = 8.4, 4.4 Hz, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.75 (s, 2H), 1.21 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 150.3, 147.4, 135.8, 132.5, 131.1, 129.6, 128.2, 127.8, 121.3, 61.1, 41.3, 14.2.







1x, 72% yield

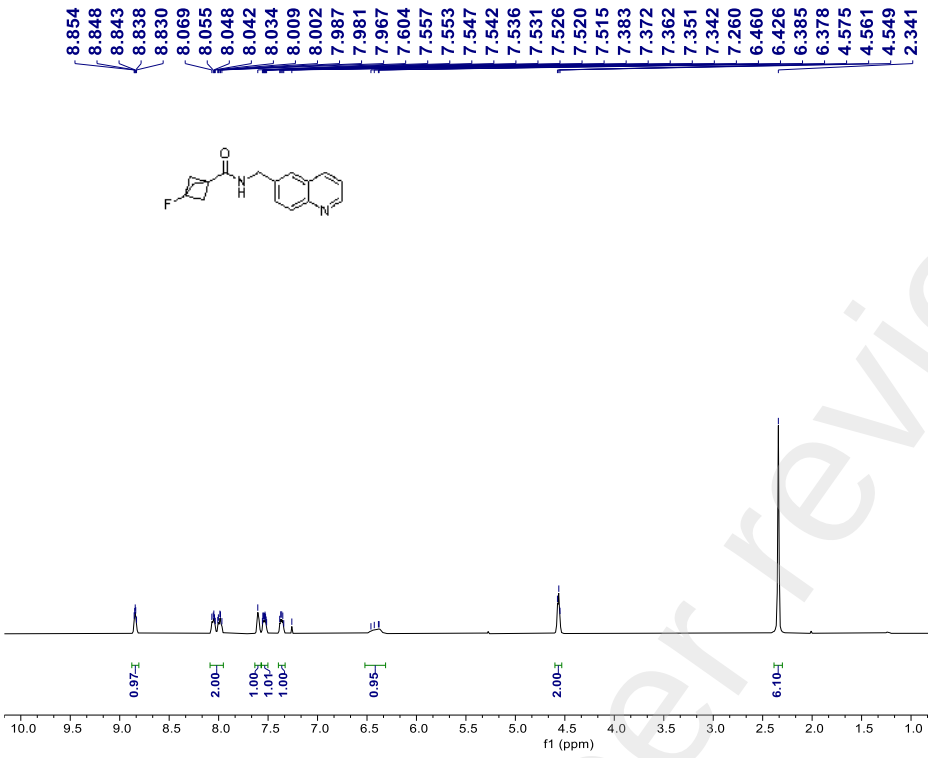
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 - 8.81 (m, 1H), 8.09 - 7.94 (m, 2H), 7.60 (s, 1H), 7.56 - 7.51 (m, 1H), 7.39 - 7.33 (m, 1H), 6.49 - 6.33 (m, 1H), 4.61 - 4.53 (m, 2H), 2.34 (s, 6H).

^{19}F NMR (376 MHz, $CDCl_3$) δ -149.78.

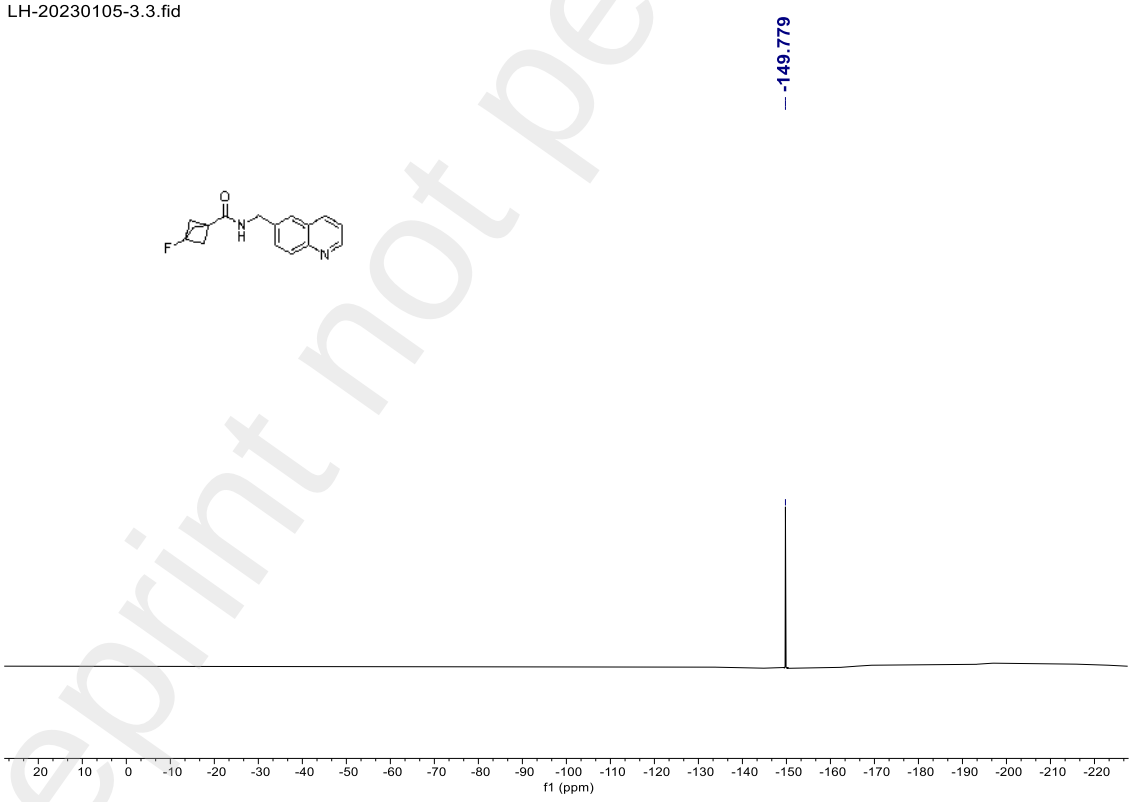
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.08 (d, J = 32.6 Hz), 150.53, 147.69, 136.27, 136.02, 130.06, 129.50, 128.17, 126.46, 121.57, 74.71 (d, J = 329.7 Hz), 55.03 (d, J = 21.6 Hz), 43.55, 29.54 (d, J = 42.6 Hz).

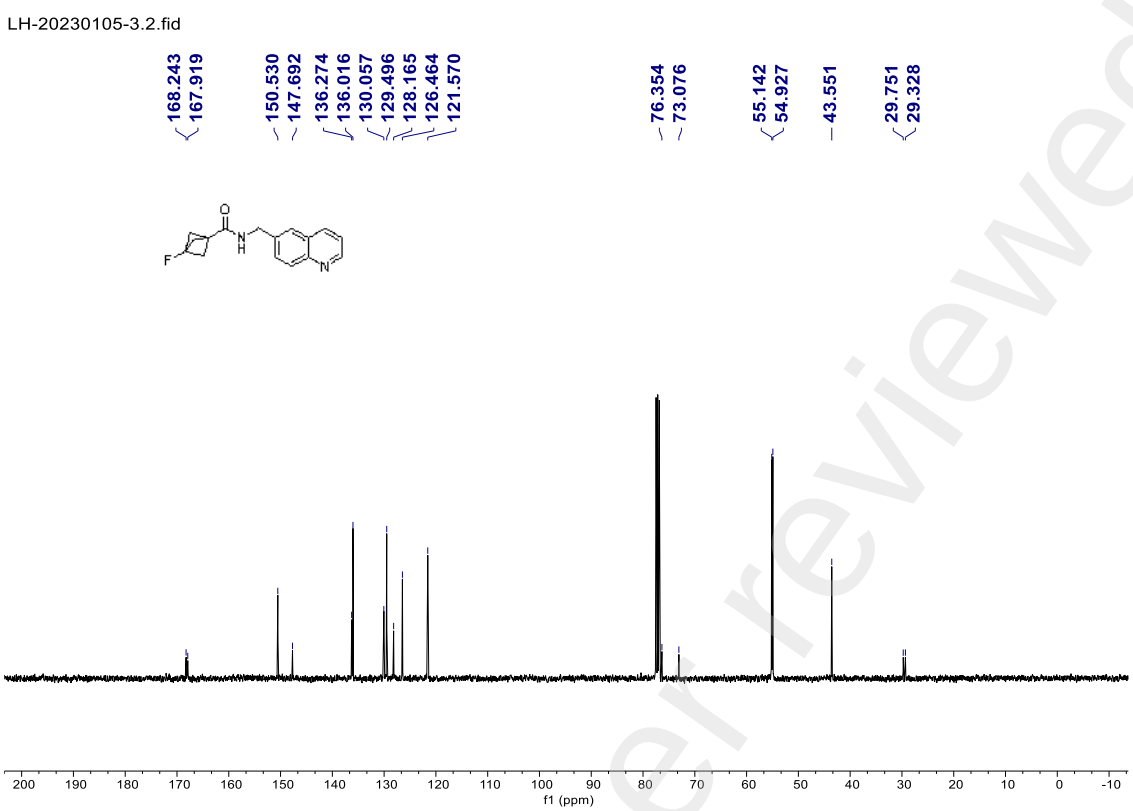
HRMS (ESI, *m/z*) calcd for $C_{16}H_{16}N_2OF^+$ $[M+H]^+$: 271.1247, found: 271.1245.

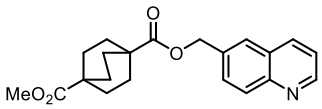
LH-20230105-3.1.fid



LH-20230105-3.3.fid







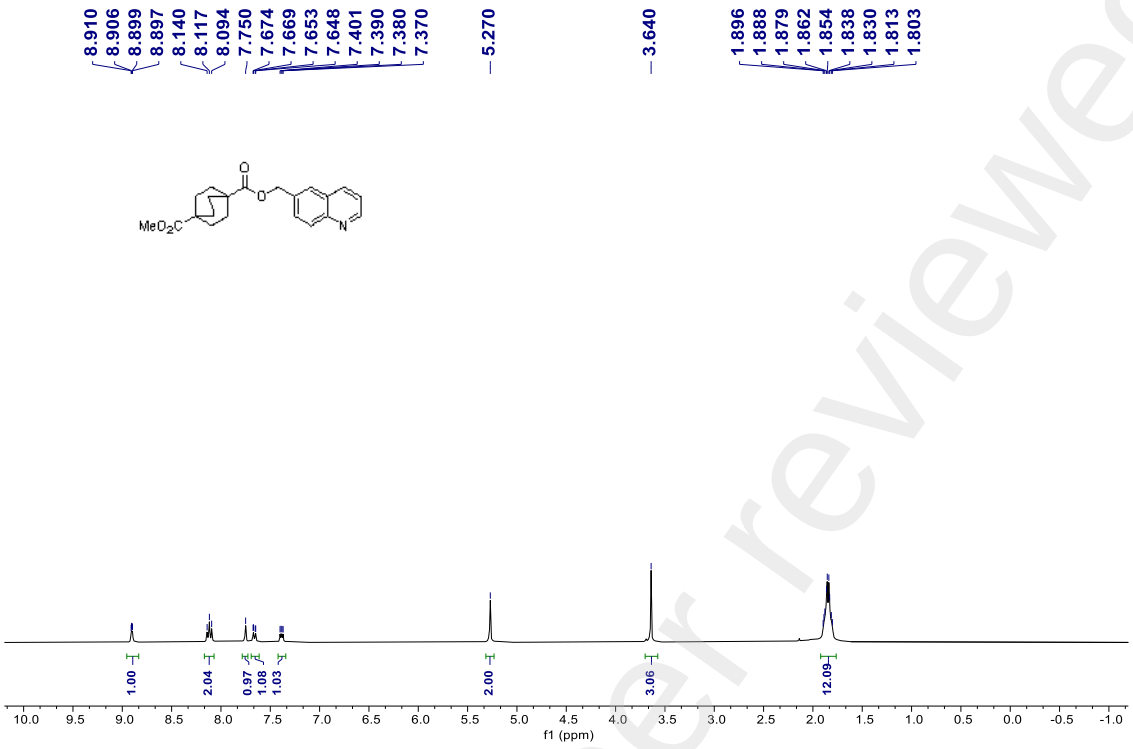
1y, 55% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 - 8.87 (m, 1H), 8.12 (t, *J* = 9.2 Hz, 2H), 7.75 (s, 1H), 7.66 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.39 (dd, *J* = 8.4, 4.4 Hz, 1H), 5.27 (s, 2H), 3.64 (s, 3H), 1.92 - 1.78 (m, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.5, 176.8, 150.5, 147.8, 135.9, 134.4, 129.7, 128.9, 127.8, 126.5, 121.3, 65.5, 51.6, 38.6, 38.5, 27.6, 27.5.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{24}NO_4^+$ $[M+H]^+$: 354.1698, found: 354.1705.

Jan05-2023-majiajia-CYP-230104-1.10.fid



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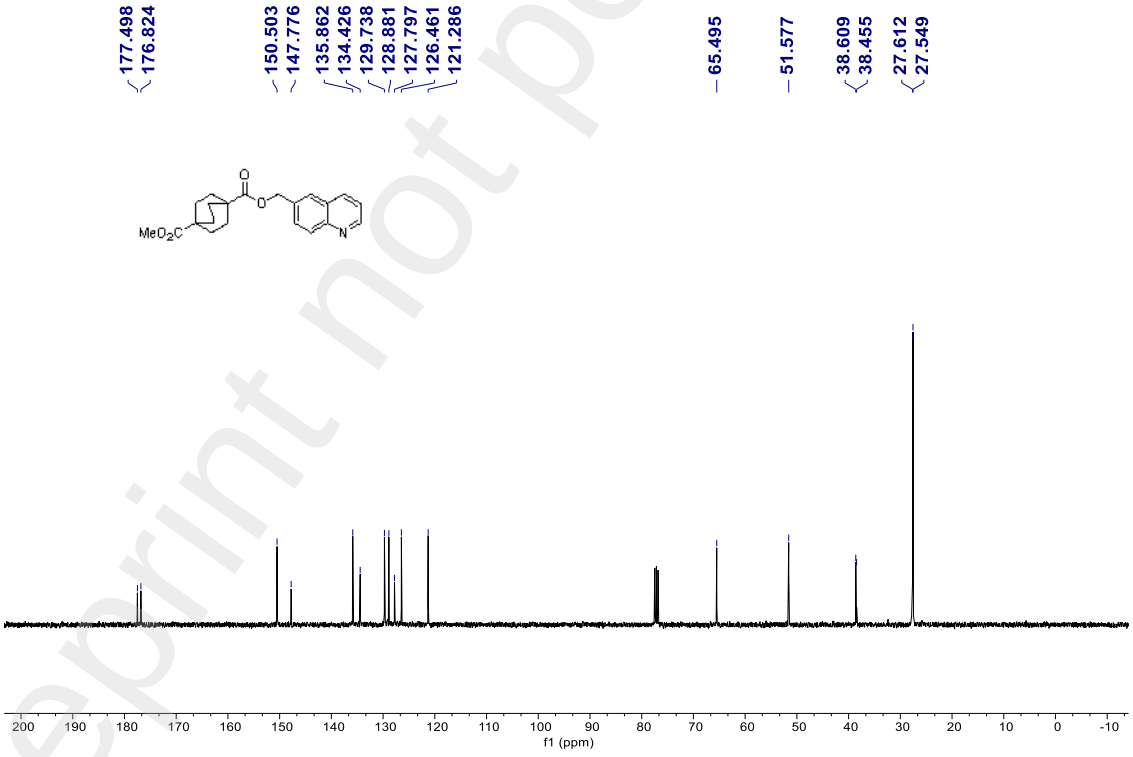
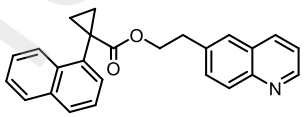


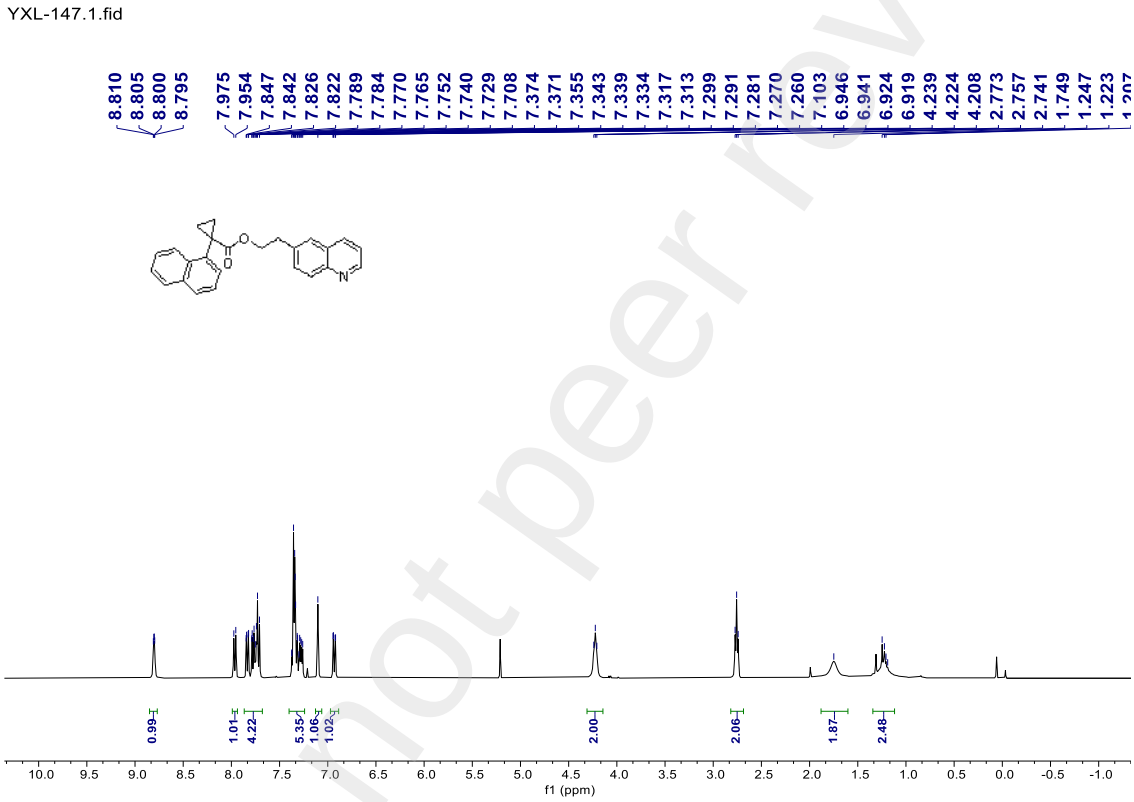


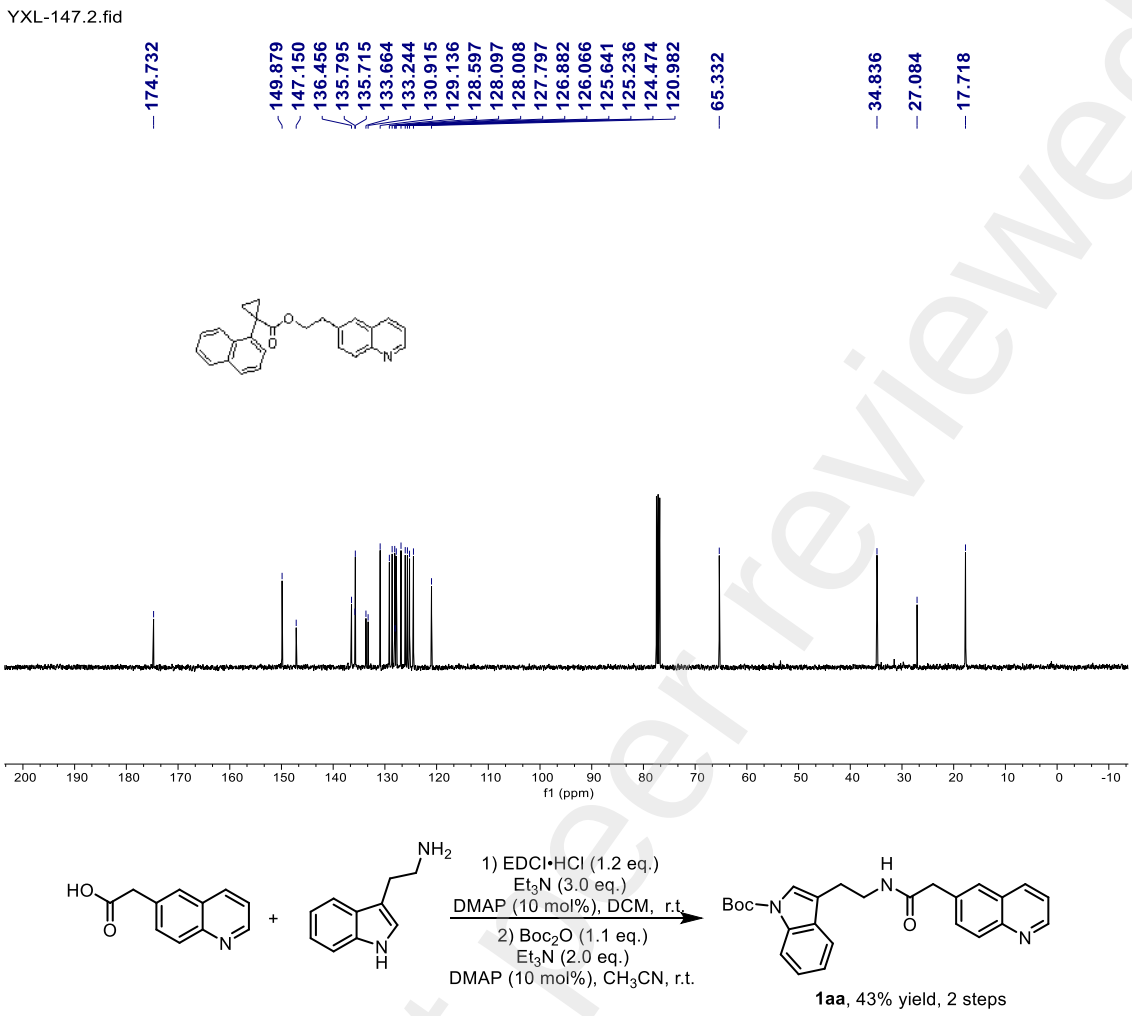
1z,45% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 - 8.77 (m, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.86 - 7.69 (m, 4H), 7.40 - 7.24 (m, 5H), 7.10 (s, 1H), 6.93 (dd, *J* = 8.6, 1.9 Hz, 1H), 4.22 (t, *J* = 6.3 Hz, 2H), 2.76 (t, *J* = 6.3 Hz, 2H), 1.75 (br, 1H) 1.27 - 1.15 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 149.9, 147.2, 136.5, 135.8, 135.7, 133.7, 133.2, 130.9, 129.1, 128.6, 128.1, 128.0, 127.8, 126.9, 126.1, 125.6, 125.2, 124.5, 121.0, 65.3, 34.8, 27.1, 17.7.

HRMS (ESI, *m*/*z*) calcd for $C_{25}H_{22}NO_2^+$ $[M+H]^+$: 368.1644, found: 368.1647.



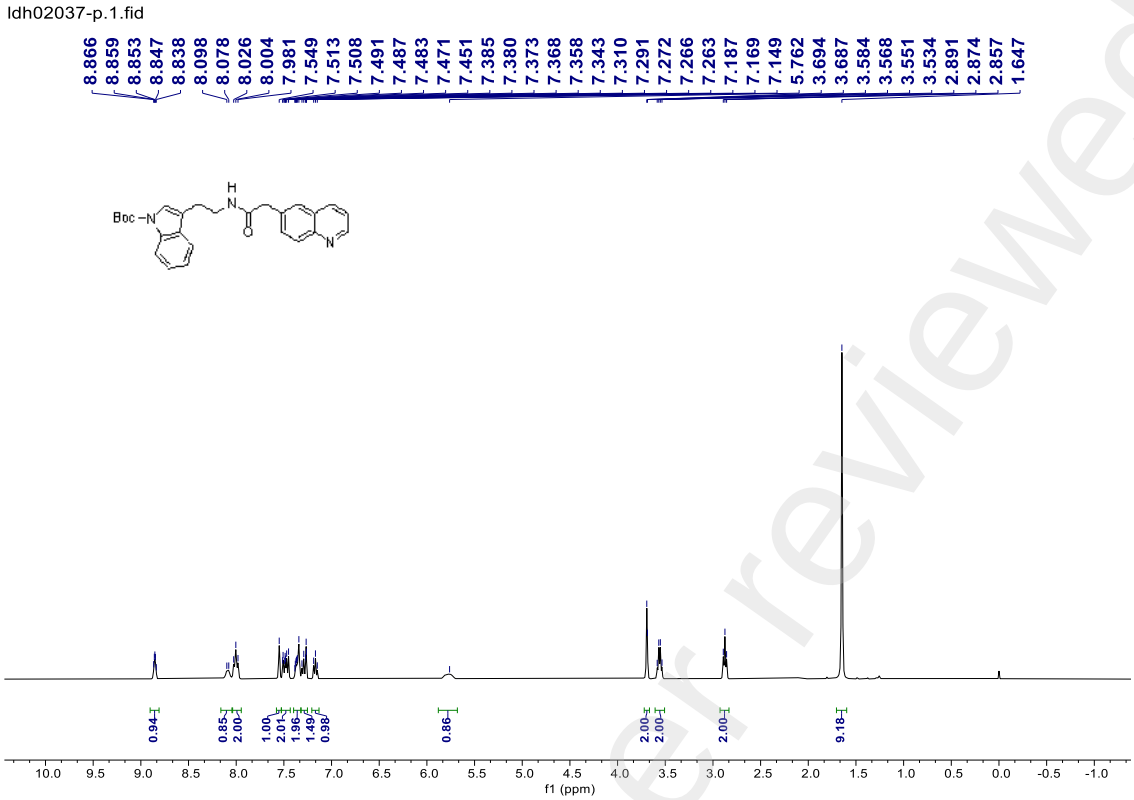


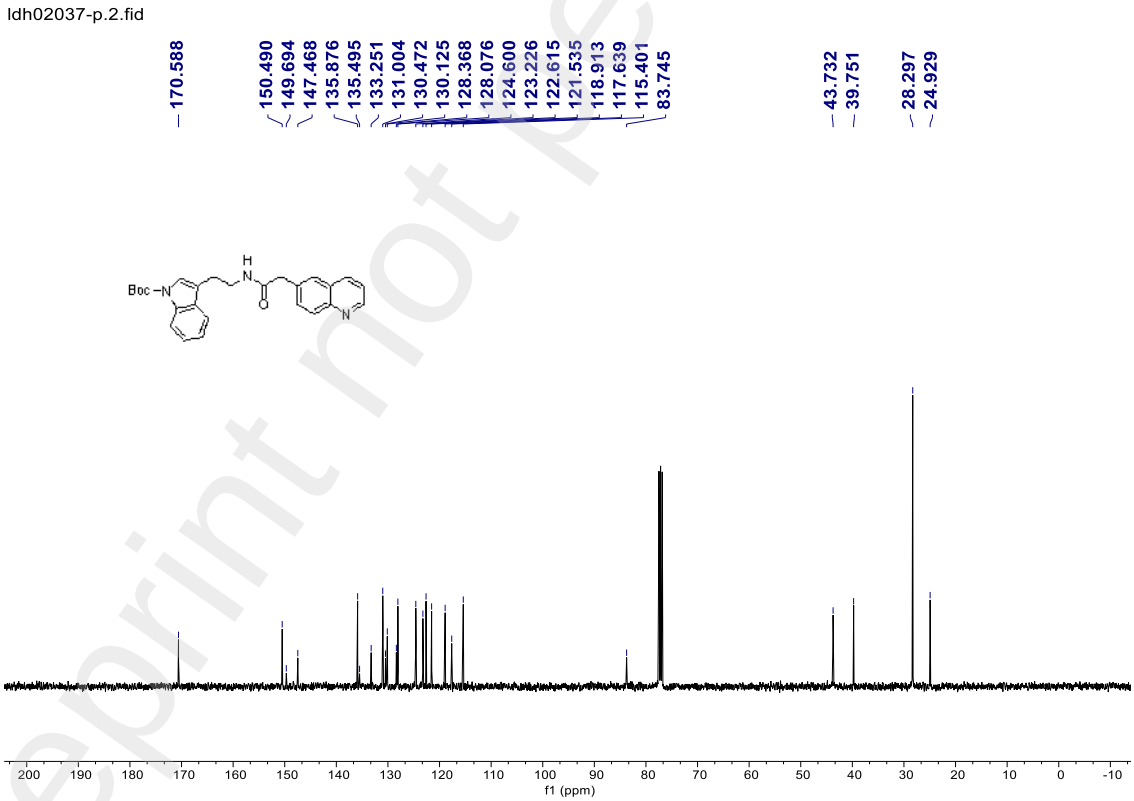
1aa, 43% yield, 2 steps

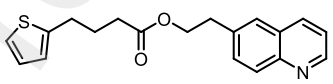
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 - 8.83 (m, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 8.00 (t, *J* = 8.8 Hz, 2H), 7.55 (s, 1H), 7.51 - 7.44 (m, 2H), 7.38 - 7.33 (m, 2H), 7.32 - 7.26 (m, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 5.76 (br, 1H), 3.69 (s, 2H), 3.56 (q, *J* = 6.8 Hz, 2H), 2.87 (t, *J* = 6.8 Hz, 2H), 1.65 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6, 150.5, 149.7, 147.5, 135.9, 135.5, 133.3, 131.0, 130.5, 130.1, 128.4, 128.1, 124.6, 123.2, 122.6, 121.5, 118.9, 117.6, 115.4, 83.7, 43.7, 39.8, 28.3, 24.9.

HRMS (ESI, *m/z*) calcd for $C_{26}H_{28}N_3O_3^+$ $[M+H]^+$: 430.2131, found: 430.2124.







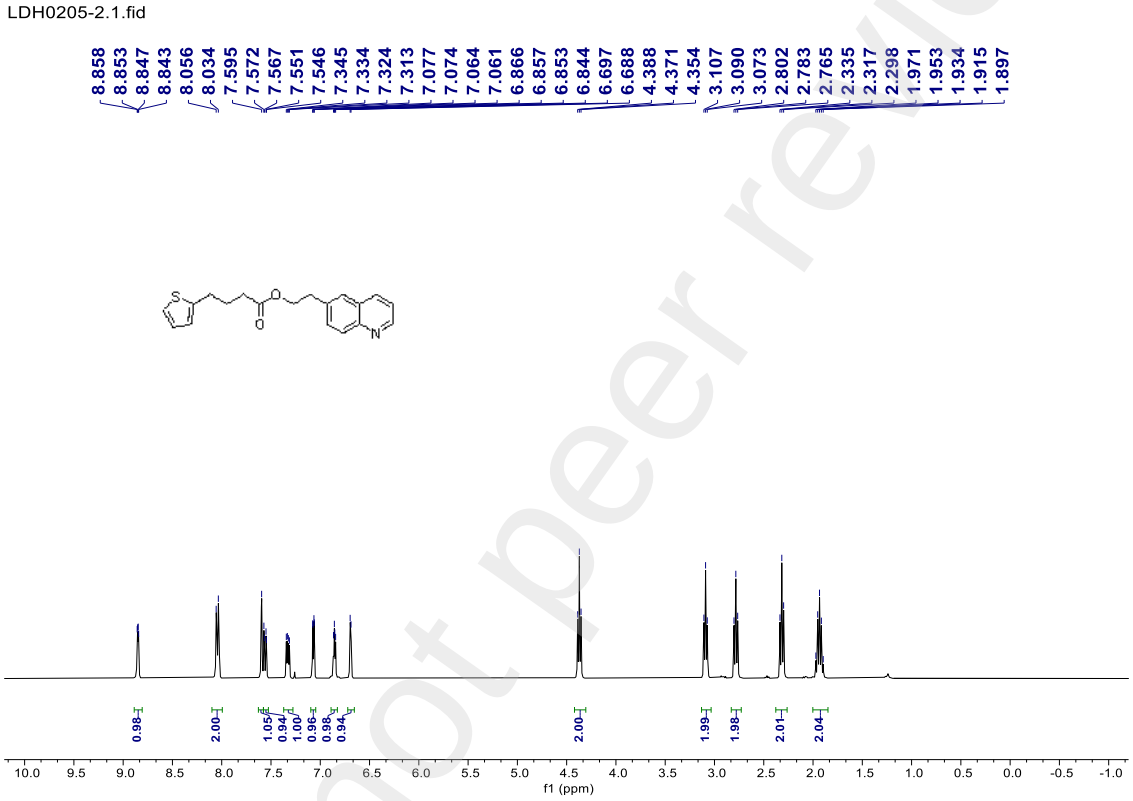
1ab, 75% yield

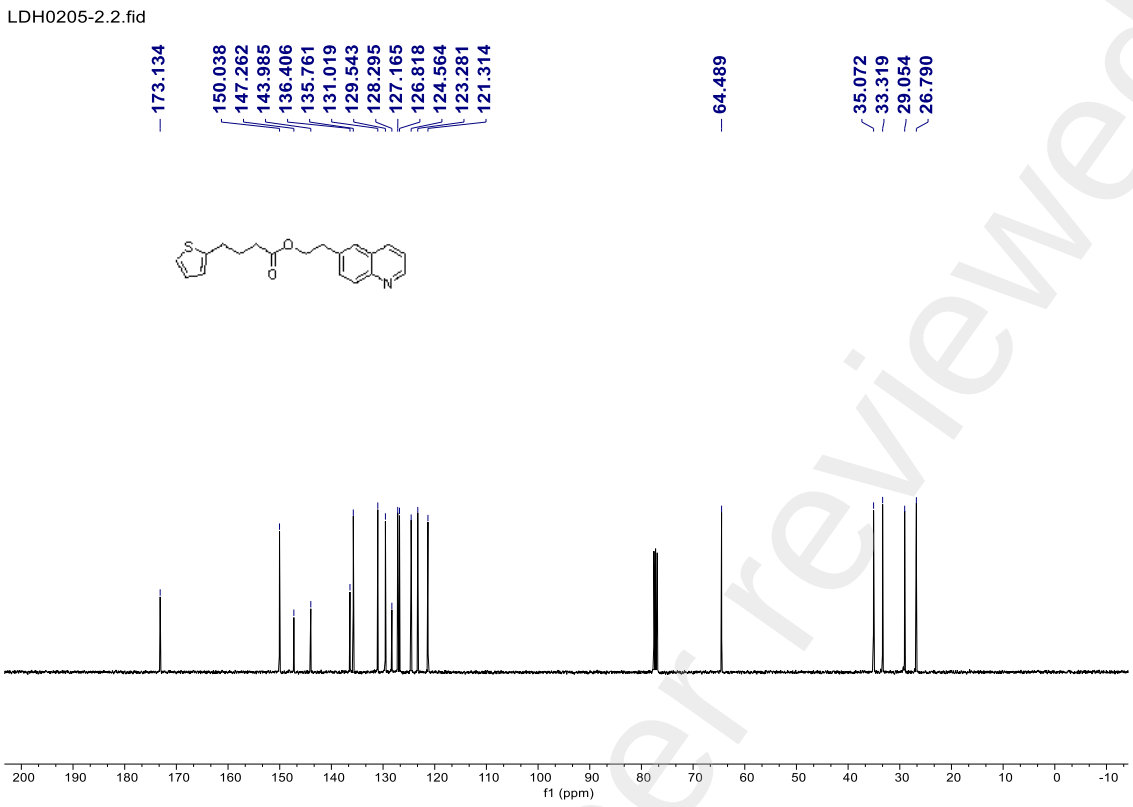
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (dd, *J* = 4.4, 2.0 Hz, 1H), 8.05 (d, *J* = 8.8 Hz, 2H), 7.60 (s,

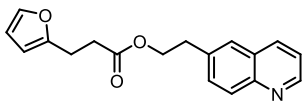
1H), 7.56 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.33 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.07 (dd, *J* = 5.2, 1.2 Hz, 1H), 6.85 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.69 (d, *J* = 3.6 Hz, 1H), 4.37 (t, *J* = 6.9 Hz, 2H), 3.09 (t, *J* = 6.8 Hz, 2H), 2.78 (t, *J* = 7.6 Hz, 2H), 2.32 (t, *J* = 7.4 Hz, 2H), 1.93 (p, *J* = 7.4 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.1, 150.0, 147.3, 144.0, 136.4, 135.8, 131.0, 129.5, 128.3, 127.2, 126.8, 124.6, 123.3, 121.3, 64.5, 35.1, 33.3, 29.1, 26.8.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{20}NO_2S^+$ $[M+H]^+$: 326.1215, found: 326.1209.







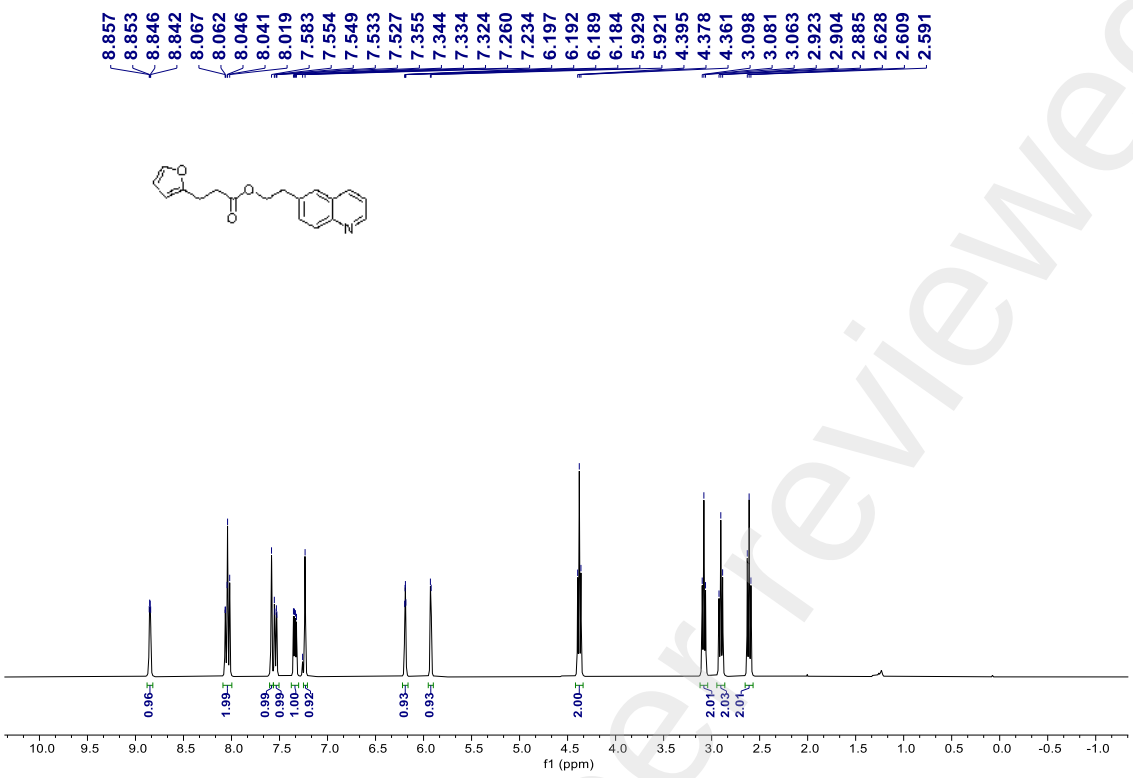
1ac, 78% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.16 - 7.94 (m, 2H), 7.58 (s, 1H), 7.54 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.34 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.23 (s, 1H), 6.25 - 6.11 (m, 1H), 5.92 (d, *J* = 3.2 Hz, 1H), 4.38 (t, *J* = 6.8 Hz, 2H), 3.08 (t, *J* = 7.0 Hz, 2H), 2.90 (t, *J* = 7.6 Hz, 2H), 2.61 (t, *J* = 7.4 Hz, 2H).

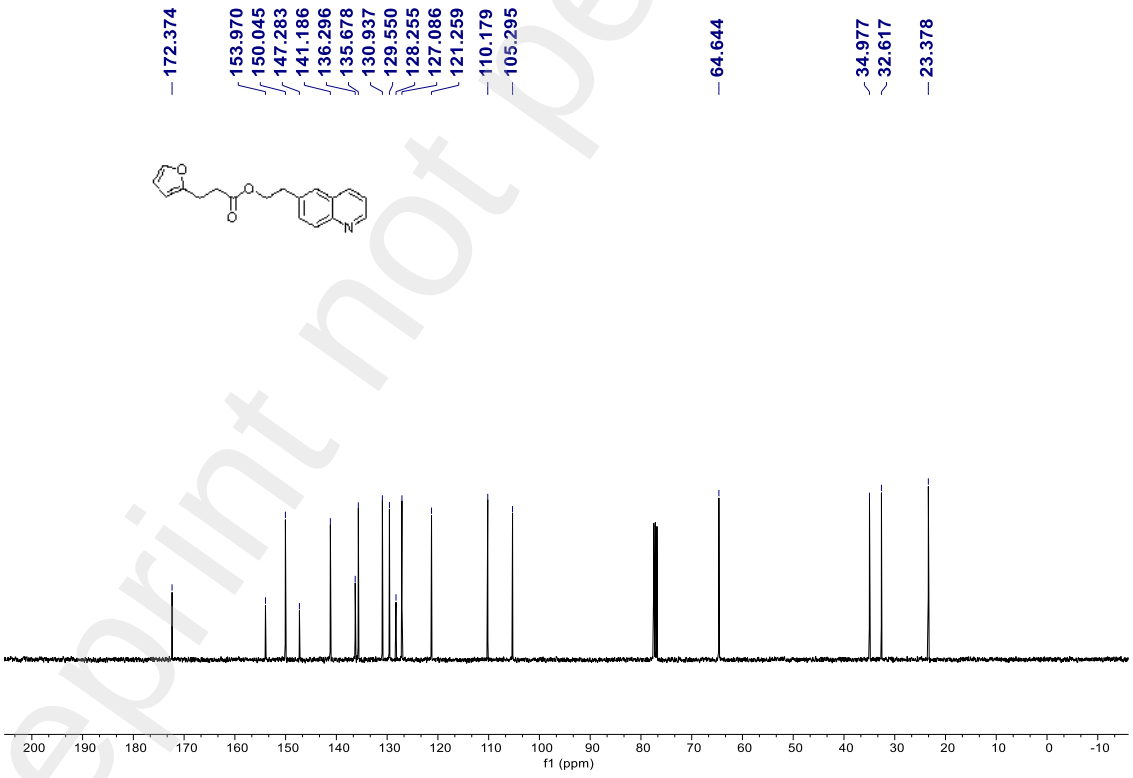
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4, 154.0, 150.0, 147.3, 141.2, 136.3, 135.7, 130.9, 129.6, 128.3, 127.1, 121.3, 110.2, 105.3, 64.6, 35.0, 32.6, 23.4.

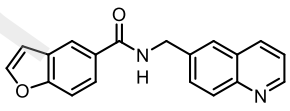
HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{18}NO_3^+$ $[M+H]^+$: 296.1287, found: 296.1282.

LDH0205-1.1.fid



LDH0205-1.2.fid



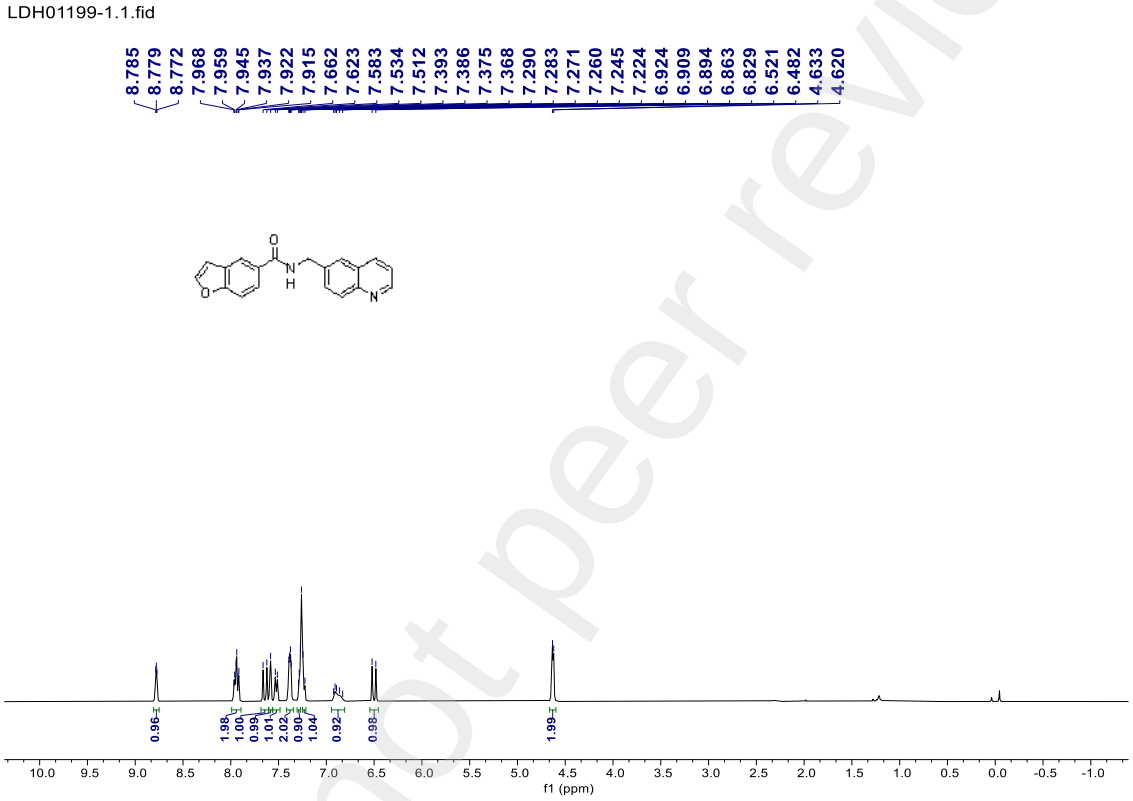


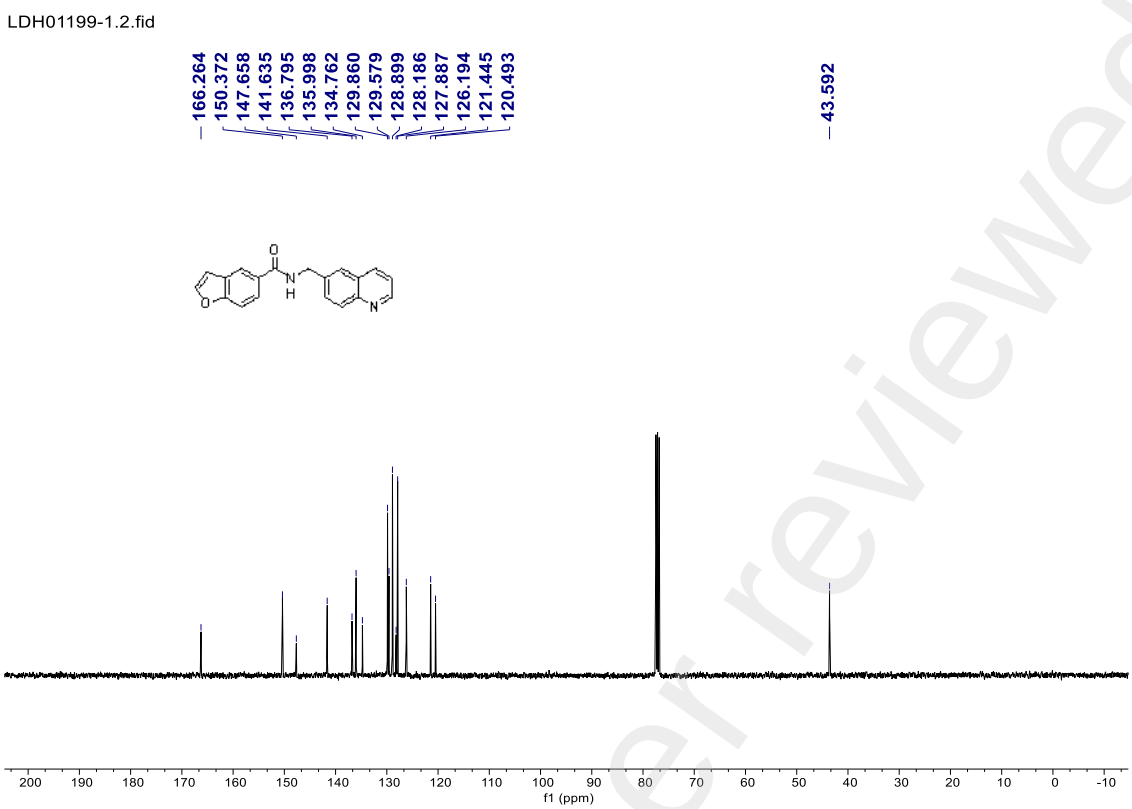
1ad, 90% yield

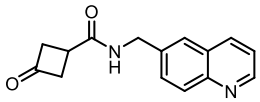
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 - 8.76 (m, 1H), 7.97 - 7.90 (m, 2H), 7.684 (d, *J* = 15.6 Hz, 1H), 7.58 (s, 1H), 7.52 (d, *J* = 8.8 Hz, 1H), 7.40 - 7.36 (m, 2H), 7.30 - 7.27 (m, 4H), 6.94 - 6.81 (m, 1H), 6.50 (d, *J* = 15.6 Hz, 1H), 4.63 (d, *J* = 4.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 150.4, 147.7, 141.6, 136.8, 136.0, 134.8, 129.9, 129.6, 128.9, 128.2, 127.9, 126.2, 121.4, 120.5, 43.6.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{15}N_2O_2^+$ $[M+H]^+$: 303.1134, found: 303.1131.







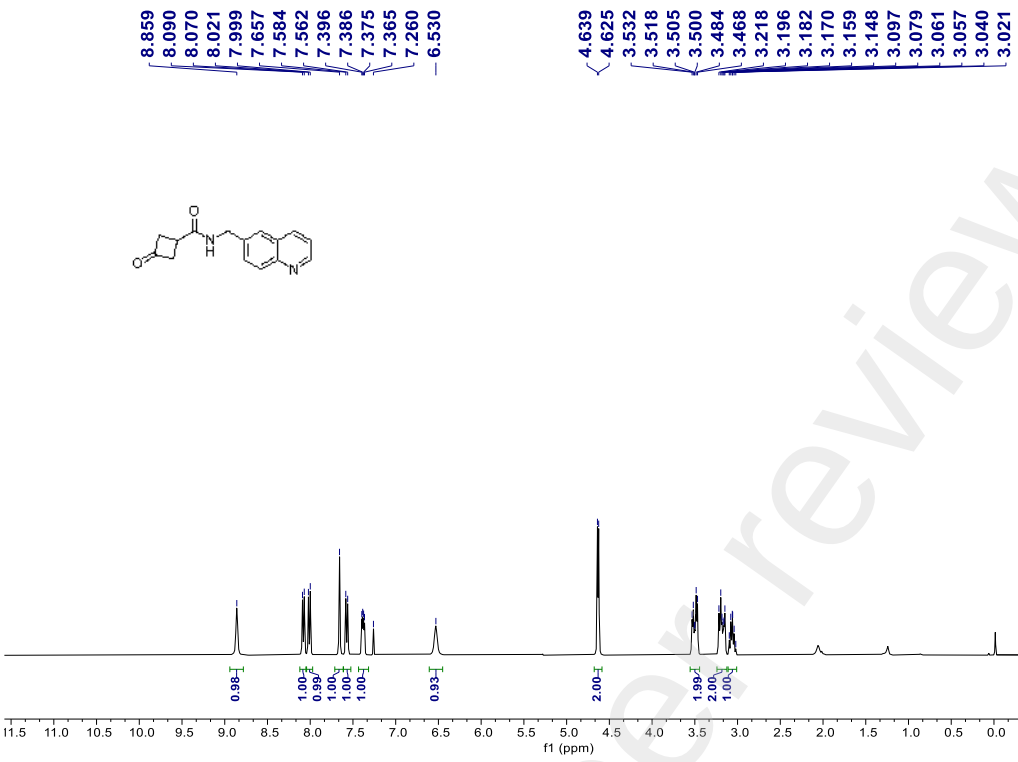
1ae, 63% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (br, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 7.66 (s, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.38 (dd, *J* = 8.4, 4.0 Hz, 1H), 6.53 (br, 1H), 4.63 (d, *J* = 5.6 Hz, 2H), 3.56 - 3.45 (m, 2H), 3.23 - 3.13 (m, 2H), 3.10 - 3.01 (m, 1H).

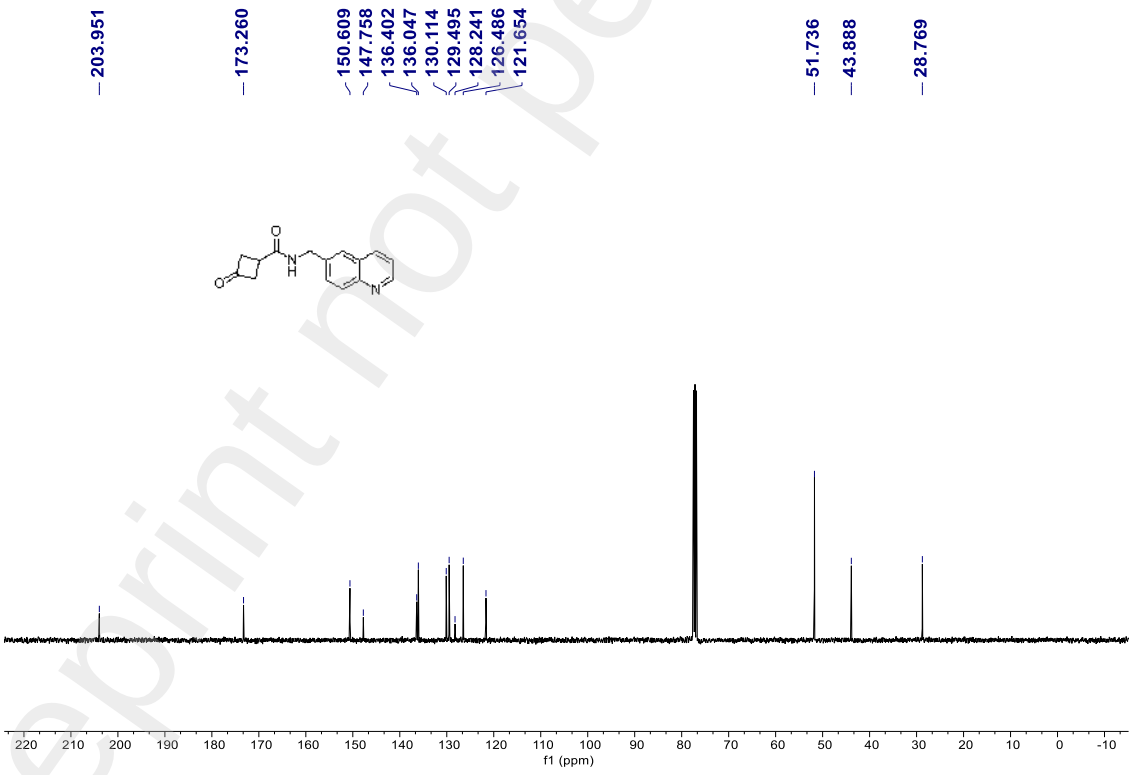
^{13}C NMR (101 MHz, $CDCl_3$) δ 204.0, 173.3, 150.6, 147.8, 136.4, 136.0, 130.1, 129.5, 128.2, 126.5, 121.7, 51.7, 43.9, 28.8.

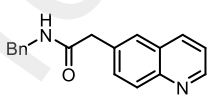
HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{15}N_2O_2^+$ $[M+H]^+$: 255.1134, found: 255.1131.

LH20230105-2.1.fid



LH20230105-2.2.fid





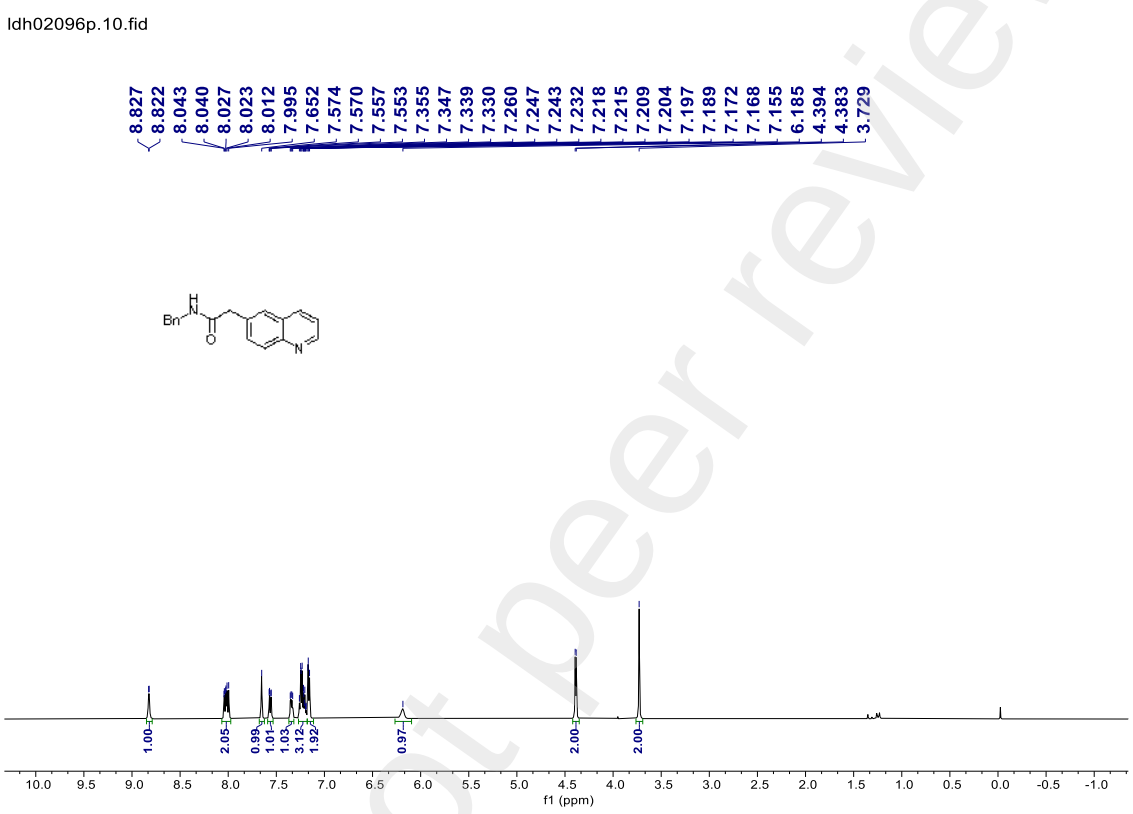
1af, 40% yield

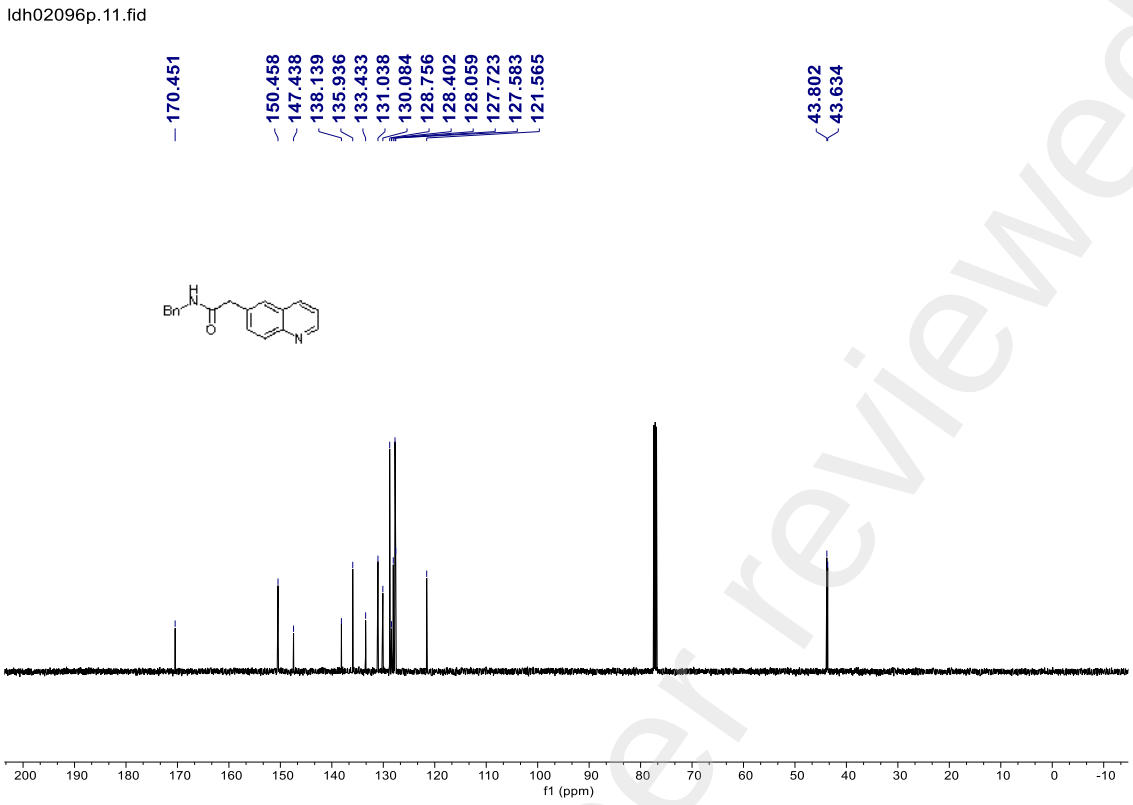
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.82 (d, *J* = 2.5 Hz, 1H), 8.05 - 7.98 (m, 2H), 7.65 (s,

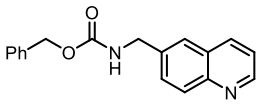
1H), 7.56 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.34 (dd, *J* = 8.5, 4.0 Hz, 1H), 7.27 - 7.18 (m, 3H), 7.18 - 7.13 (m, 2H), 6.18 (br, 1H), 4.39 (d, *J* = 5.5 Hz, 2H), 3.73 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.5, 150.5, 147.4, 138.1, 135.9, 133.4, 131.0, 130.1, 128.8, 128.4, 128.1, 127.7, 127.6, 121.6, 43.8, 43.6.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{17}N_2O^+$ $[M+H]^+$: 277.1341, found: 277.1336.







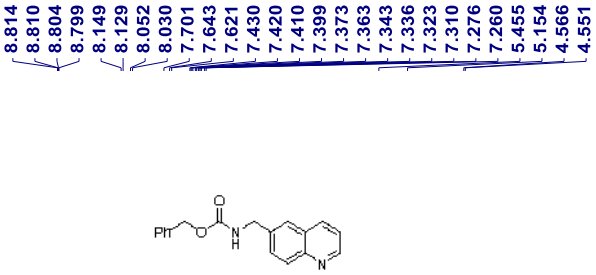
1ag, 55% yield

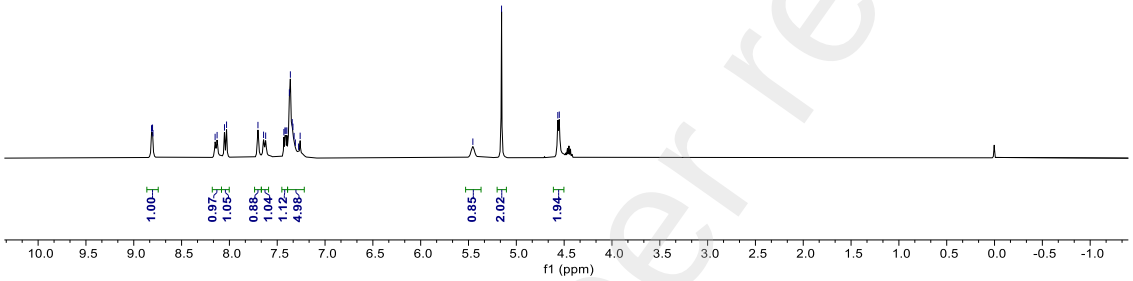
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 - 8.78 (m, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 8.04 (d, *J* = 8.7 Hz, 1H), 7.70 (s, 1H), 7.63 (d, *J* = 8.7 Hz, 1H), 7.41 (dd, *J* = 8.3, 4.3 Hz, 1H), 7.40 - 7.21 (m, 5H), 5.45 (br, 1H), 5.15 (s, 2H), 4.56 (d, *J* = 6.2 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 150.0, 147.1, 137.4, 136.9, 136.4, 129.7, 129.1, 128.7, 128.4, 128.3, 125.9, 121.6, 67.2, 44.9.

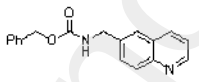
HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{17}N_2O_2^+$ $[M+H]^+$: 293.1290, found: 293.1286

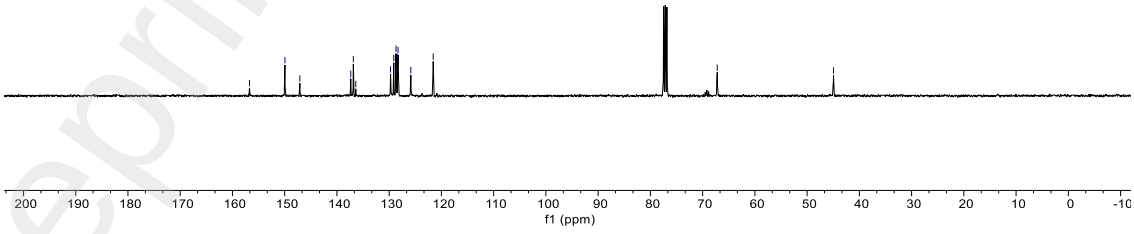
Jan02-2023-majiajia-LH20221230-NHCBZ.10.fid

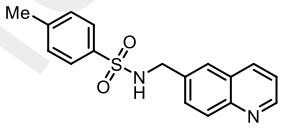




LH-20221230-S-NHCbz.2.fid





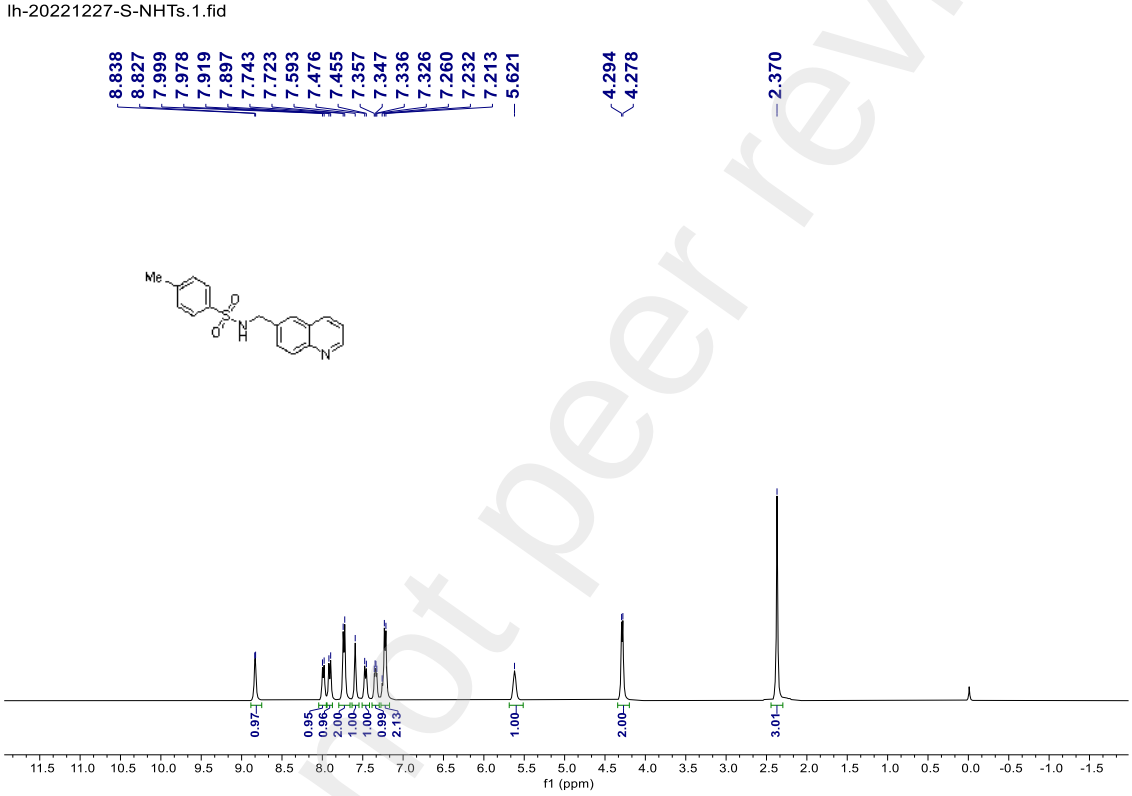


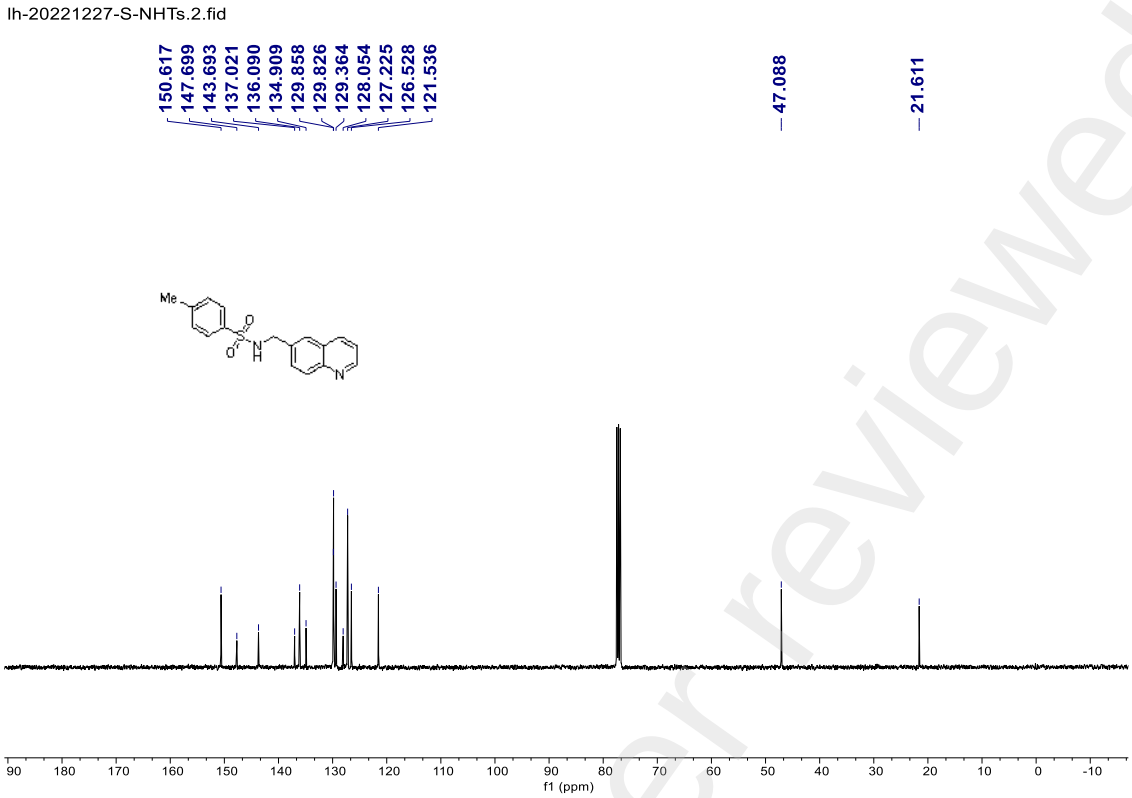
1ah, 75% yield

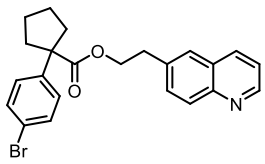
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 4.4 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 8.8 Hz, 1H)7.73 (d, *J* = 7.9 Hz, 2H), 7.59 (s, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.34 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 2H), 5.62 (br, 1H), 4.29 (d, *J* = 6.4 Hz, 2H), 2.37 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.6, 147.7, 143.7, 137.0, 136.1, 134.9, 129.9, 129.8, 129.4, 128.1, 127.2, 126.5, 121.5, 47.1, 21.6.

HRMS (ESI, *m/z*) calcd for $C_{17}H_{19}NO_2S^+$ $[M+H]^+$: 313.1011, found: 313.1006.





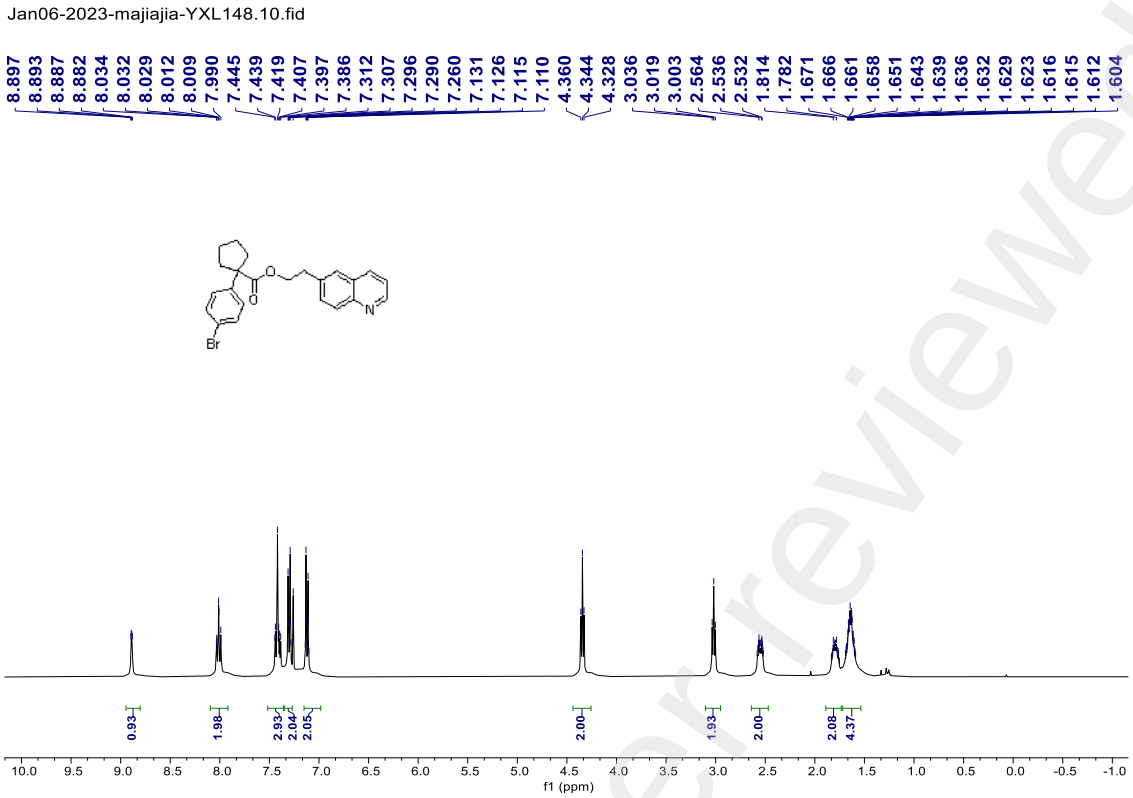


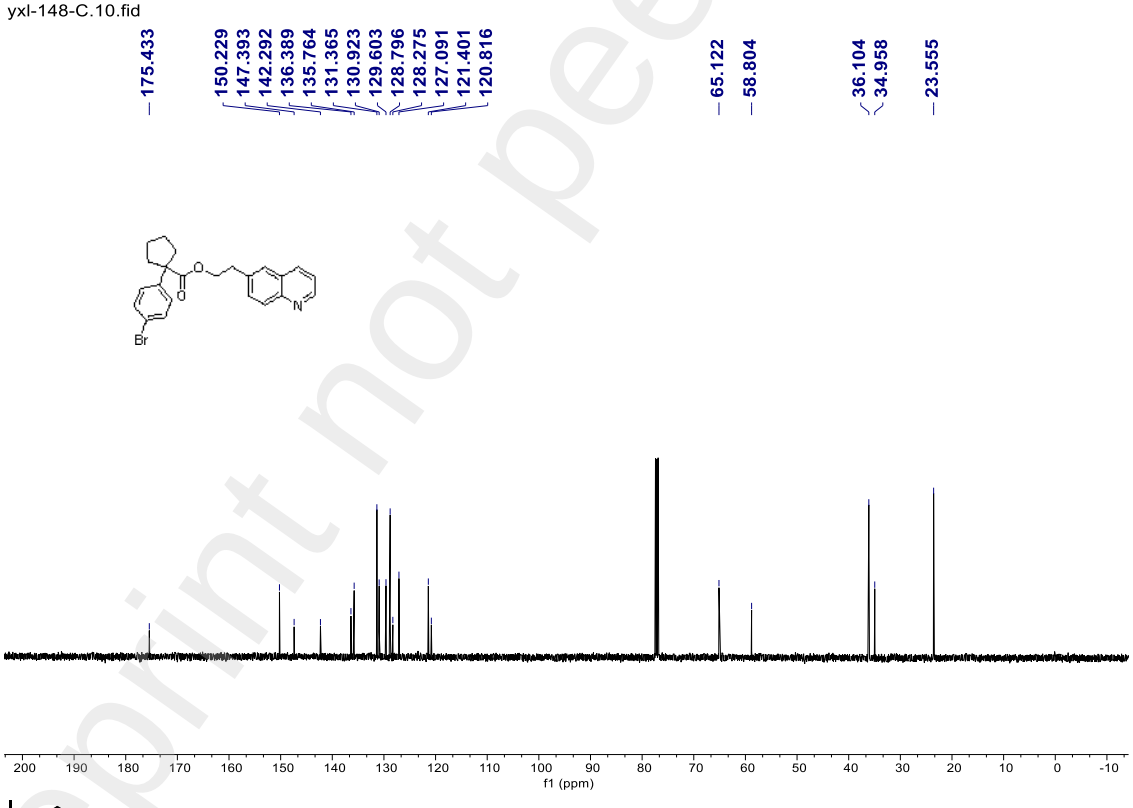
1ai, 66% yield

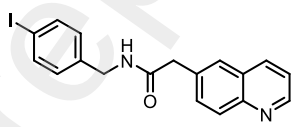
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (dd, *J* = 4.0, 1.6 Hz, 1H), 8.07 - 7.89 (m, 2H), 7.47 - 7.36 (m, 3H), 7.34 - 7.26 (m, 2H), 7.16 - 6.99 (m, 2H), 4.34 (t, *J* = 6.4 Hz, 2H), 3.02 (t, *J* = 6.4 Hz, 2H), 2.70 - 2.40 (m, 2H), 1.86 - 1.73 (m, 2H), 1.72 - 1.55 (m, 4H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 175.4, 150.2, 147.4, 142.3, 136.4, 135.8, 131.4, 130.9, 129.6, 128.8, 128.3, 127.1, 121.4, 120.8, 65.1, 58.8, 36.1, 35.0, 23.6.

HRMS (ESI, *m*/*z*) calcd for $C_{23}H_{23}BrNO_2$ $[M+H]^+$: 424.0907, found: 424.0904.







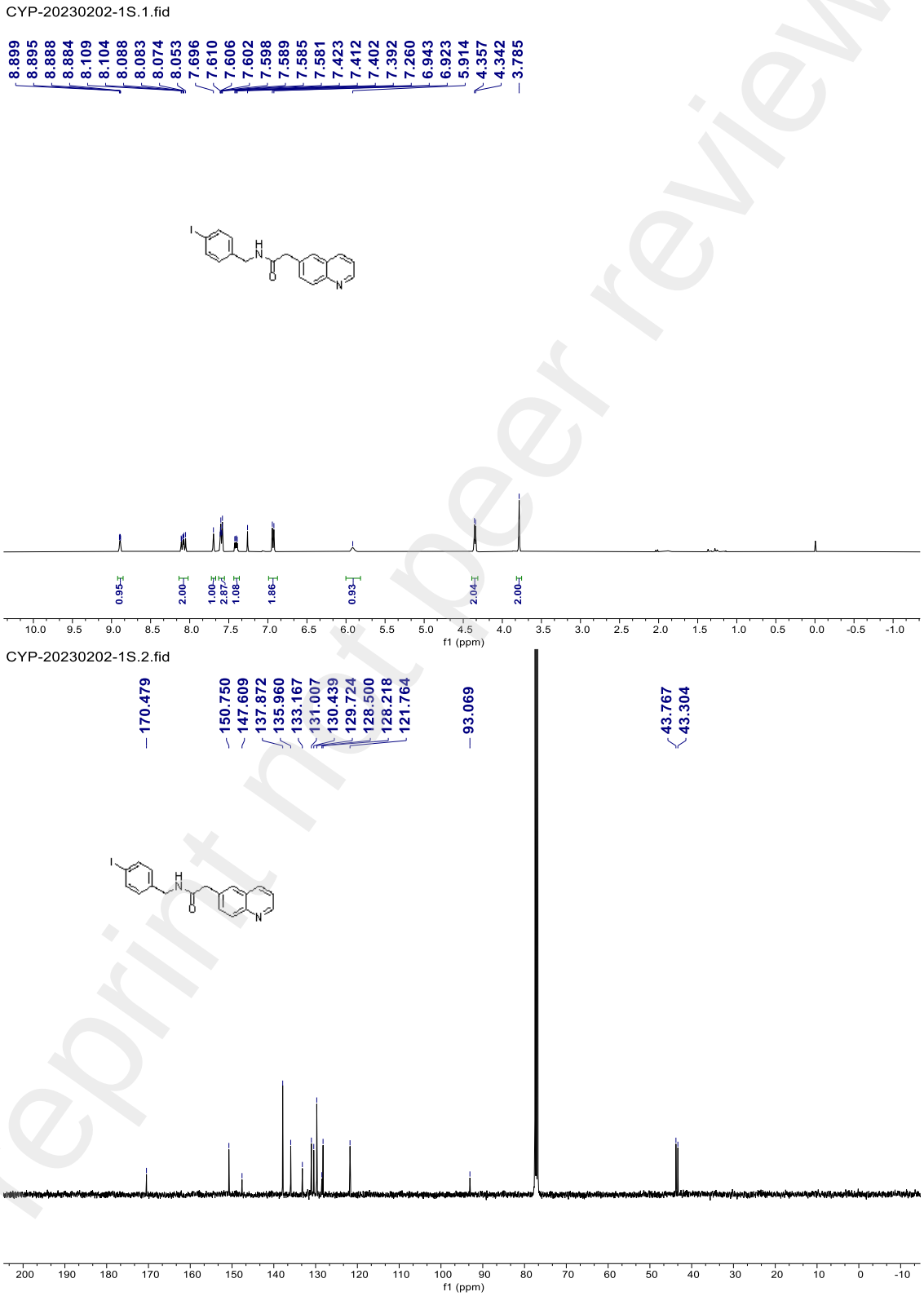
1aj, 47% yield

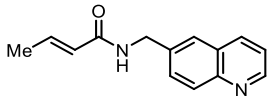
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (dd, *J* = 4.4, 1.6 Hz, 1H), 8.13 - 8.03 (m, 2H), 7.70 (s, 1H), 7.61 - 7.57 (m, 3H), 7.41 (dd, *J* = 8.0, 4.0 Hz, 1H), 6.93 (d, *J* = 8.0 Hz,

2H), 5.91 (br, 1H), 4.35 (d, J = 6.0 Hz, 2H), 3.78 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 150.7, 147.6, 137.9, 136.0, 133.2, 131.0, 130.4, 129.7, 128.5, 128.2, 121.8, 93.1, 43.8, 43.3.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{16}N_2OI^+$ [M+H]$^+$: 403.0307, found: 403.0302.





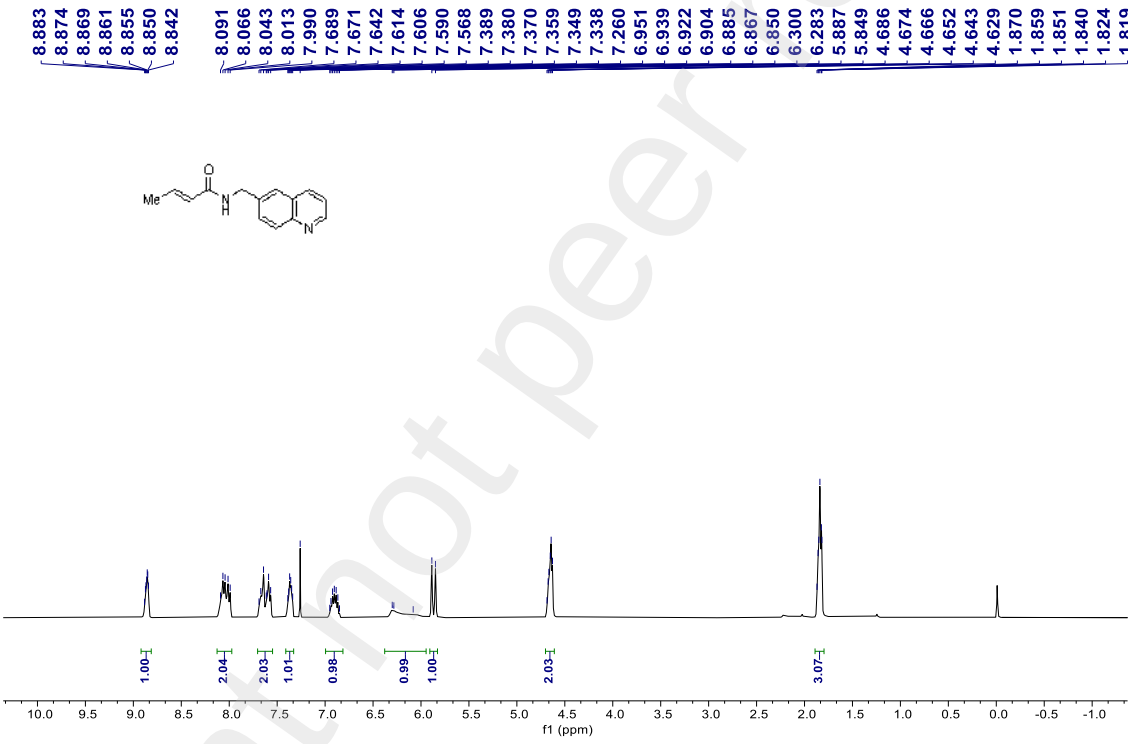
1ak, 67% yield

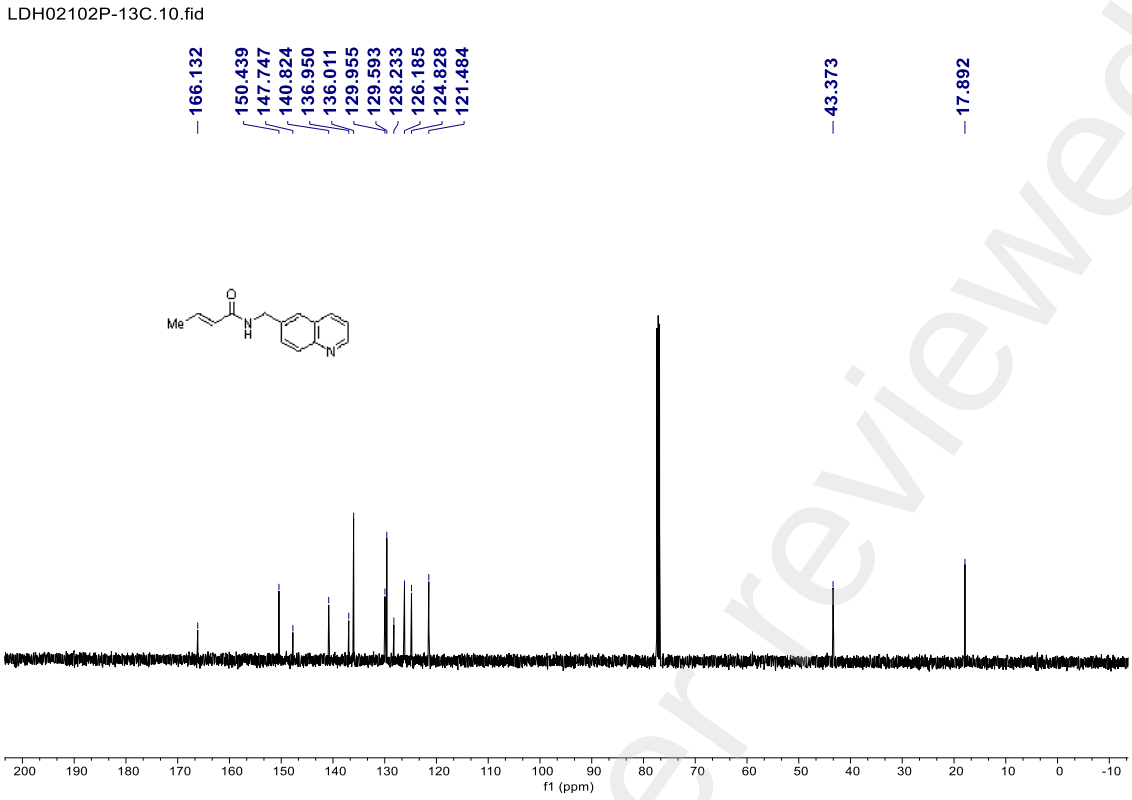
^{1}H NMR (400 MHz, $_{CD}Cl_3$) δ 8.91 - 8.82 (m, 1H), 8.11 - 7.97 (m, 2H), 7.71 - 7.54 (m, 2H), 7.41 - 7.31 (m, 1H), 6.97 - 6.83 (m, 1H), 6.37 - 5.97 (m, 1H), 5.87 (d, *J* = 15.2 Hz, 1H), 4.71 - 4.61 (m, 2H), 1.89 - 1.80 (m, 3H).

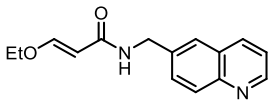
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.1, 150.4, 147.7, 140.8, 137.0, 136.0, 130.0, 129.6, 128.2, 126.2, 124.8, 121.5, 43.4, 17.9.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{15}N_2O^+$ $[M+H]^+$: 227.1184, found: 227.1183.

LDH02102.1.fid





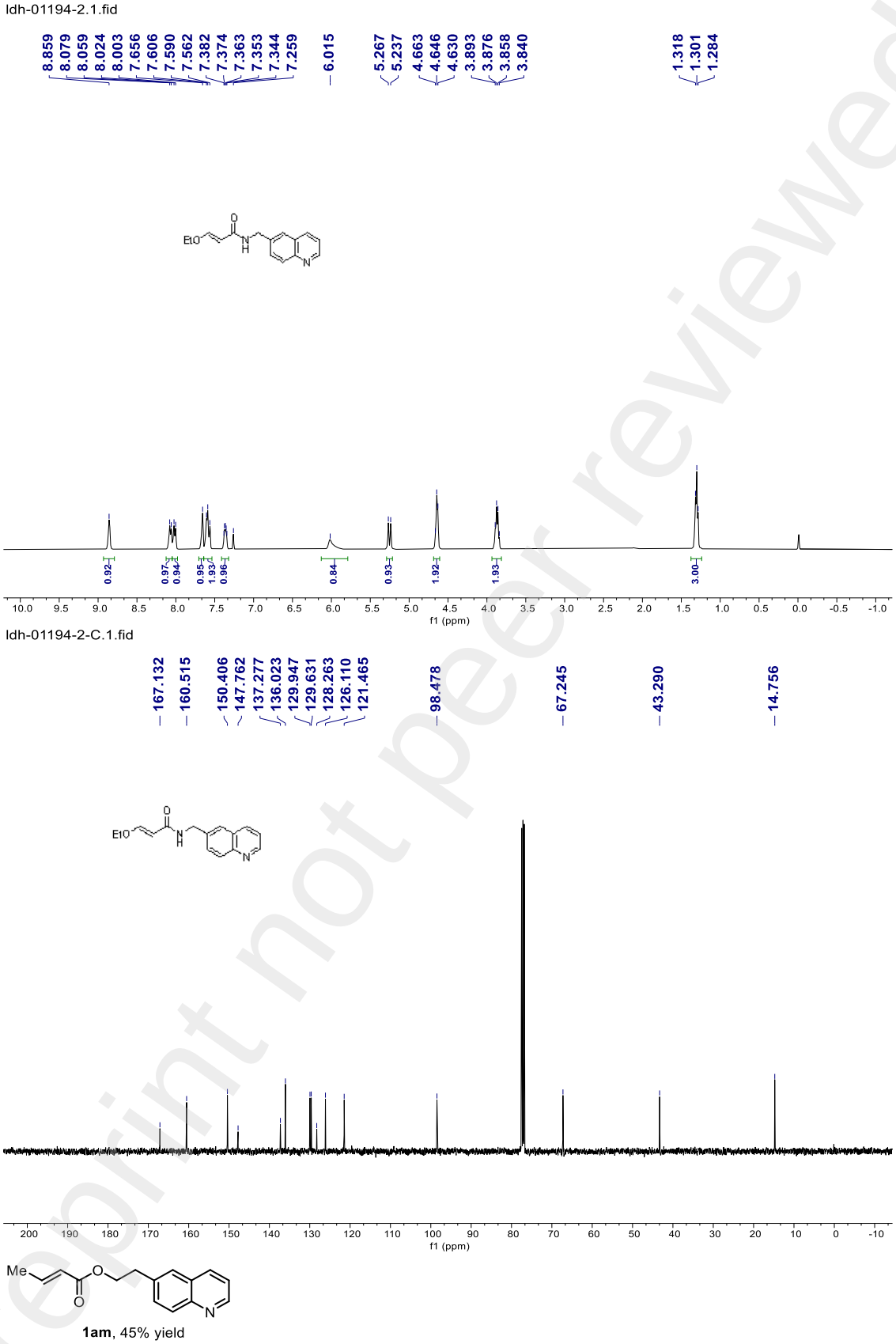


1al, 50% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (br, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.66 (br, 1H), 7.63 - 7.55 (m, 2H), 7.42 - 7.34 (m, 1H), 6.02 (s, 1H), 5.25 (d, *J* = 12.0 Hz, 1H), 4.68 - 4.60 (m, 2H), 3.92 - 3.82 (m, 2H), 1.36 - 1.26 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 160.5, 150.4, 147.8, 137.3, 136.0, 129.9, 129.6, 128.3, 126.1, 121.5, 98.5, 67.2, 43.3, 14.8.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{17}N_2O_2^+$ $[M+H]^+$: 257.1290, found: 257.1288.



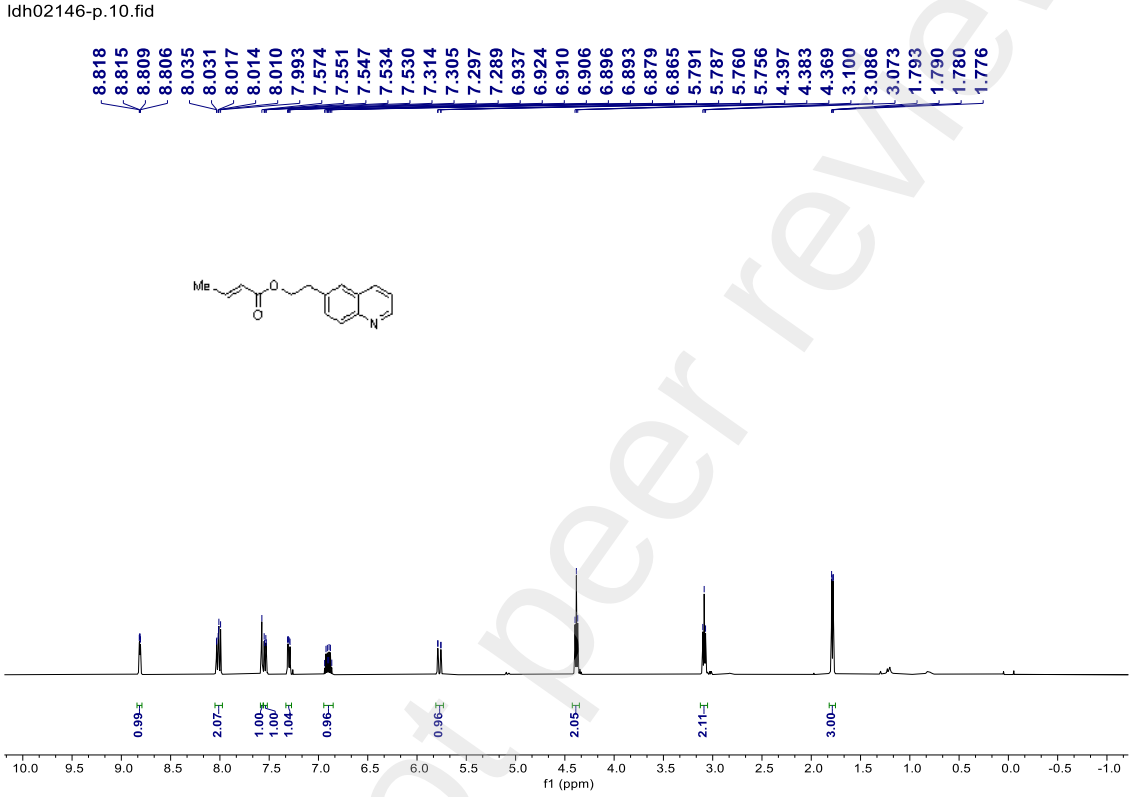
1am, 45% yield

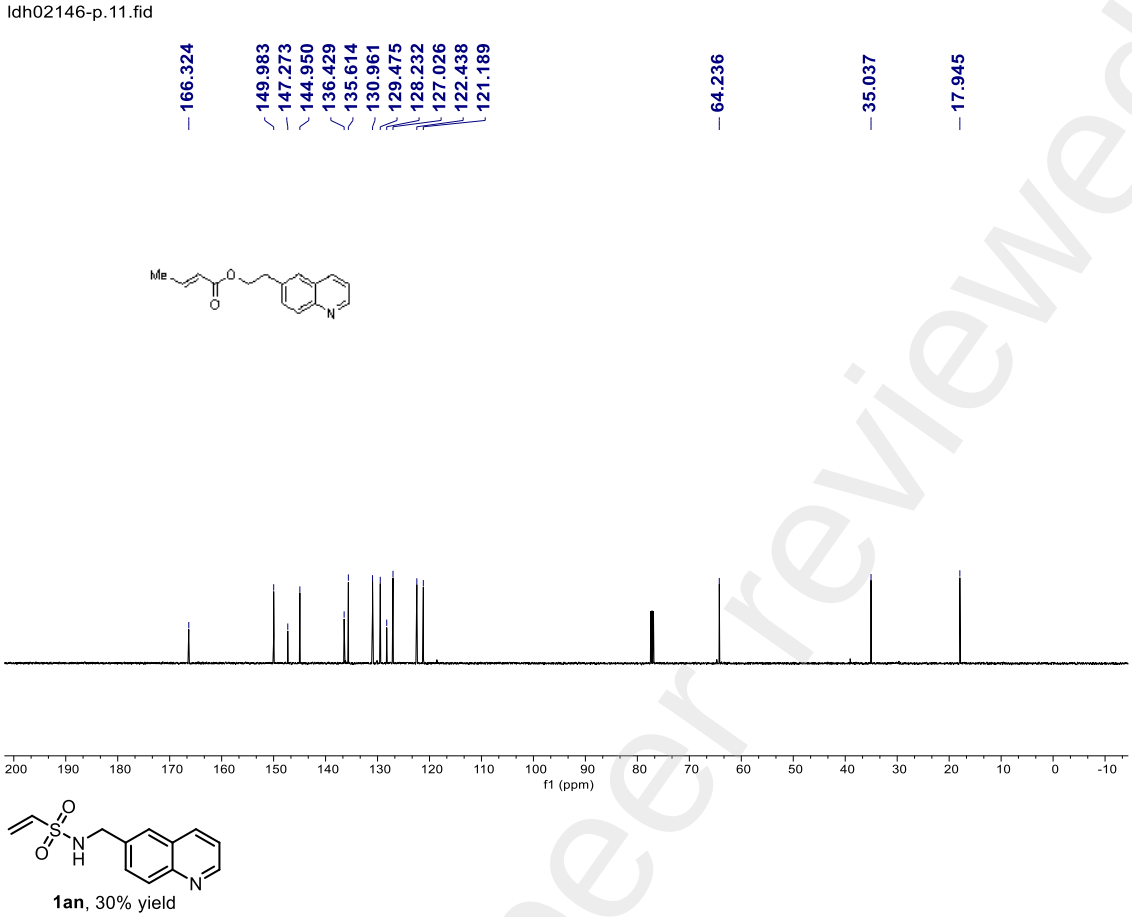
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (dd, *J* = 4.5, 1.5 Hz, 1H), 8.05 - 7.96 (m, 2H), 7.57 (s, 1H), 7.54 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.30 (dd, *J* = 8.0, 4.5 Hz, 1H), 6.95 - 6.85

(m, 1H), 5.77 (dd, *J* = 15.5, 2.0 Hz, 1H), 4.38 (t, *J* = 7.0 Hz, 2H), 3.09 (t, *J* = 6.9 Hz, 2H), 1.78 (dd, *J* = 6.5, 1.8 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.3, 150.0, 147.3, 144.9, 136.4, 135.6, 131.0, 129.5, 128.2, 127.0, 122.4, 121.2, 64.2, 35.0, 17.9.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{16}NO_2^+$ [M+H]$^+$: 242.1181, found: 242.1179.





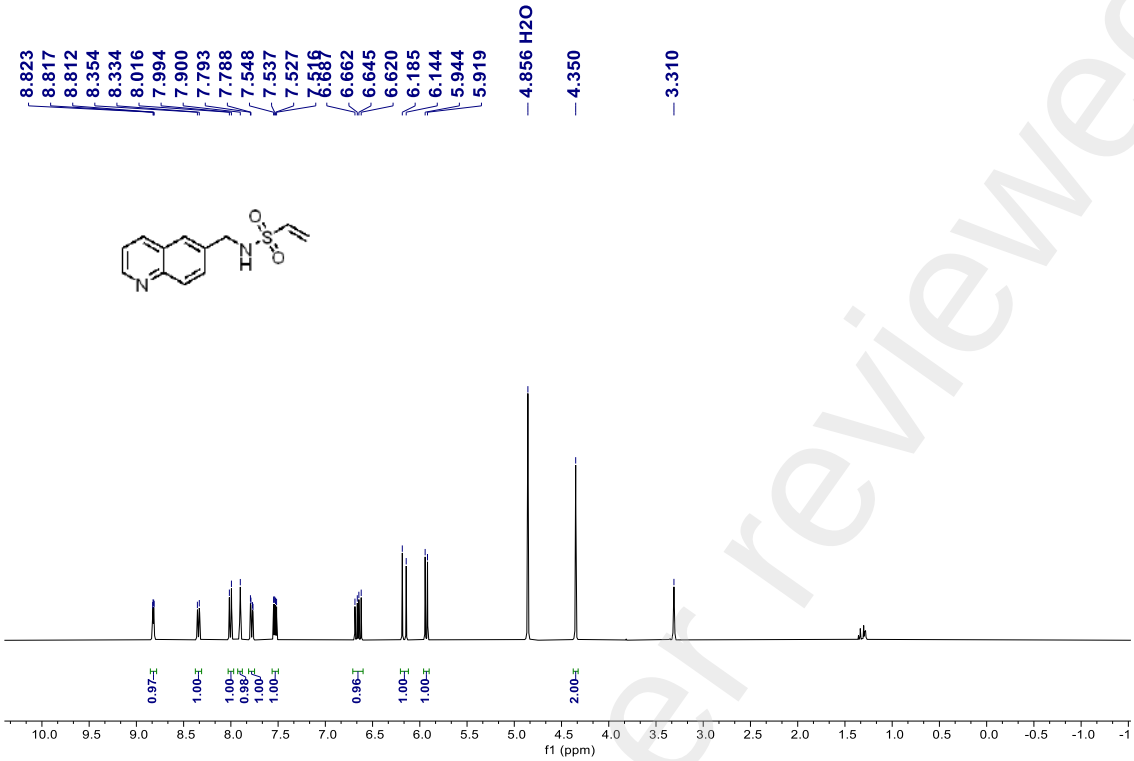
1an, 30% yield

^{1}H NMR (400 MHz, CD_3OD) δ 8.82 (dd, *J* = 4.4, 2.0 Hz, 1H), 8.34 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.90 (br, 1H), 7.78 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.53 (dd, *J* = 8.4, 4.4 Hz, 1H), 6.65 (dd, *J* = 16.8 10.0 Hz, 1H), 6.16 (d, *J* = 16.4 Hz, 1H), 5.93 (d, *J* = 10.0 Hz, 1H), 4.35 (s, 2H).

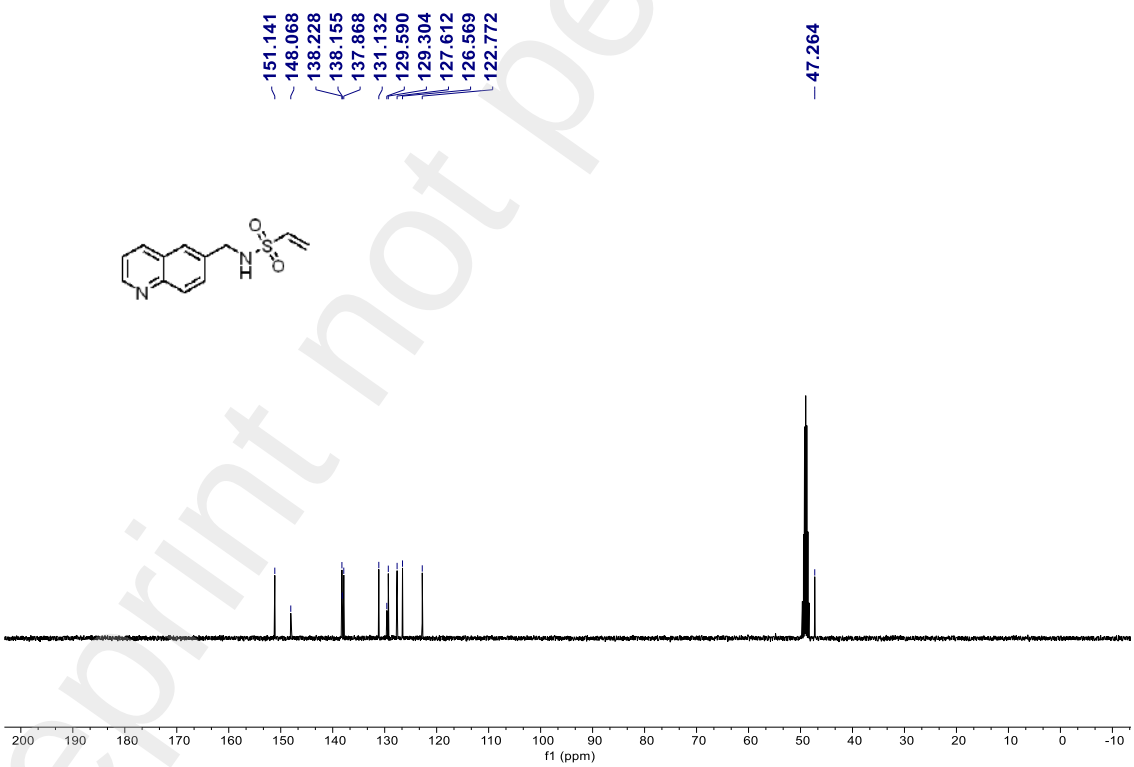
^{13}C NMR (101 MHz, CD_3OD) δ 151.1, 148.1, 138.2, 138.2, 137.9, 131.1, 129.6, 129.3, 127.6, 126.6, 122.8, 47.3.

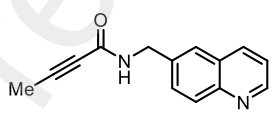
HRMS (ESI, *m*/*z*) calcd for $C_{12}H_{13}N_2O_2S^+$ $[M+H]^+$: 249.0698, found: 249.0697.

Mar09-2023-majiajia-ldh02059p.10.fid



Mar08-2023-majiajia-ldh02059p.13.fid





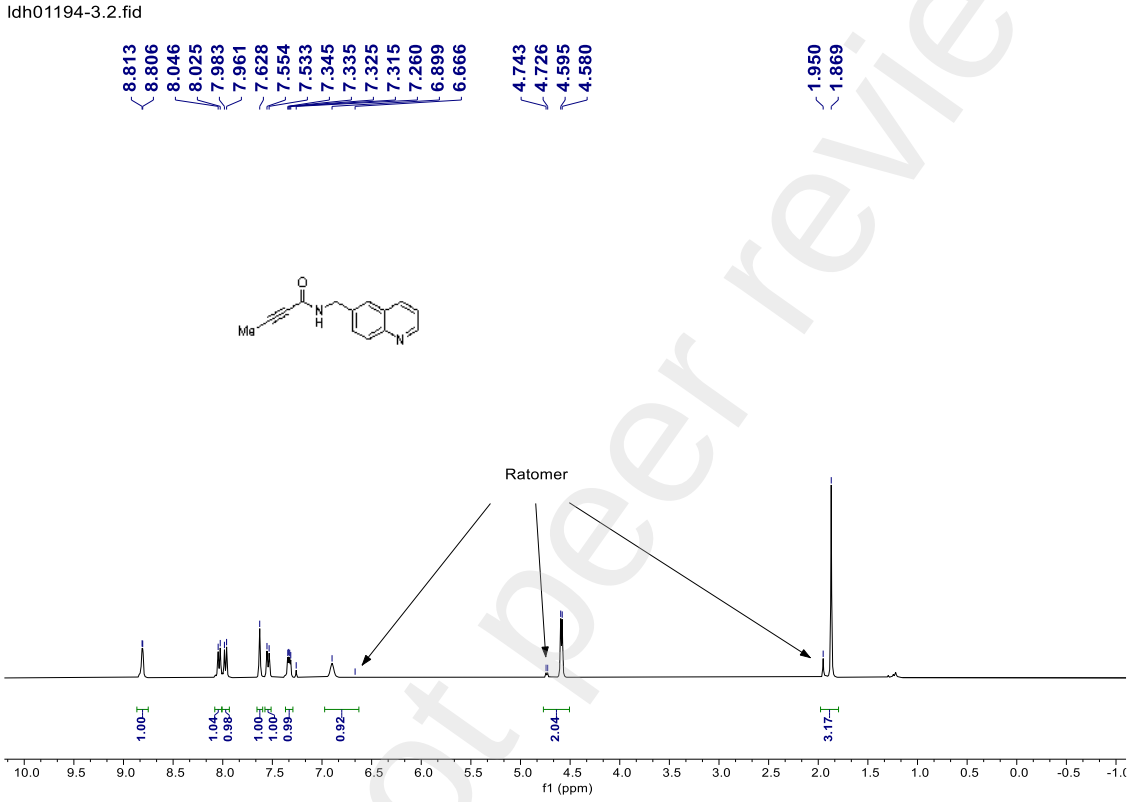
1ao, 60% yield

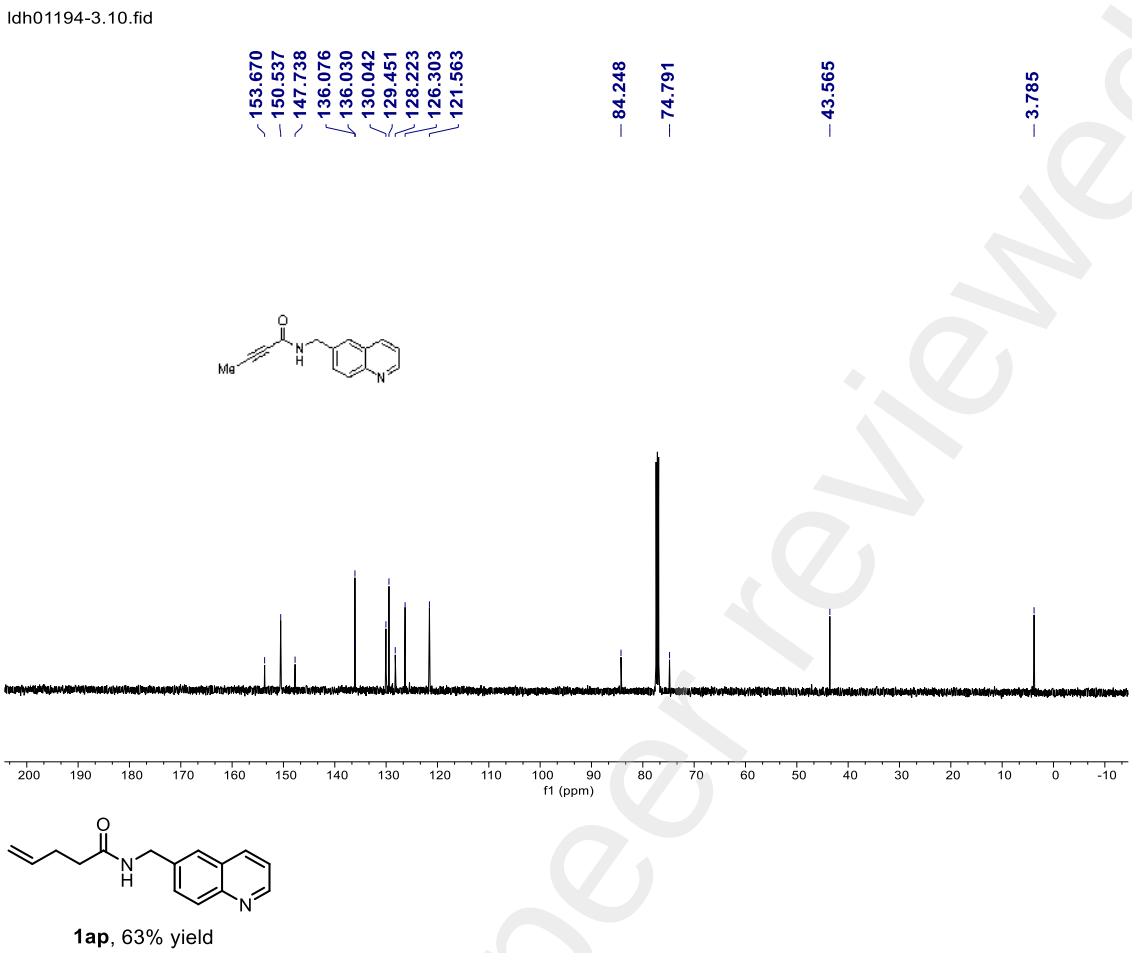
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (d, *J* = 2.6 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.97

(d, *J* = 8.8 Hz, 1H), 7.63 (s, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.33 (dd, *J* = 8.0, 4.0 Hz, 1H), 6.94 - 6.64 (m, 1H), 4.76 - 4.56 (m, 2H), 1.96 - 1.83 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.7, 150.5, 147.7, 136.1, 136.0, 130.0, 129.5, 128.2, 126.3, 121.6, 84.2, 74.8, 43.6, 3.8.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{13}N_2O^+$ $[M+H]^+$: 225.1028, found: 225.1025.





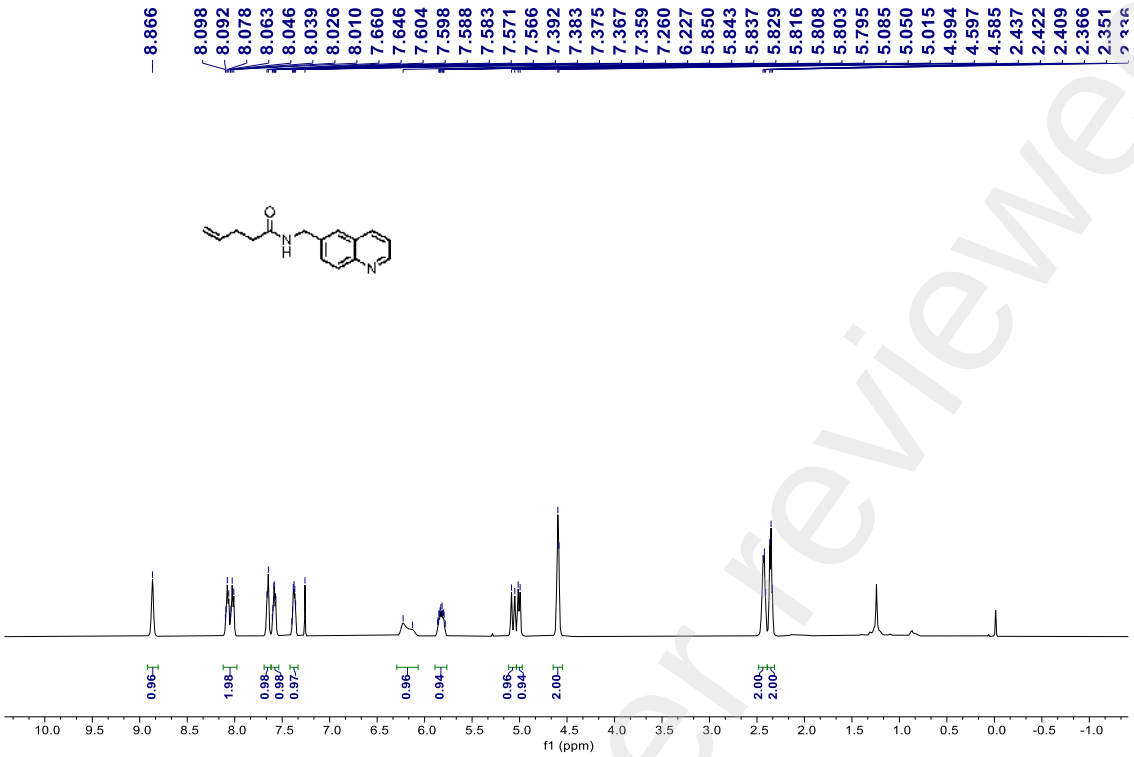
1ap, 63% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.87 (br, 1H), 8.12 - 7.98 (m, 2H), 7.69 - 7.62 (m, 1H), 7.61 - 7.54 (m, 1H), 7.41 - 7.34 (m, 1H), 6.28 - 6.07 (m, 1H), 5.88 - 5.77 (m, 1H), 5.07 (d, *J* = 17.5 Hz, 1H), 5.00 (d, *J* = 10.5 Hz, 1H), 4.59 (d, *J* = 6.0 Hz, 2H), 2.48 - 2.39 (m, 2H), 2.38 - 2.32 (m, 2H).

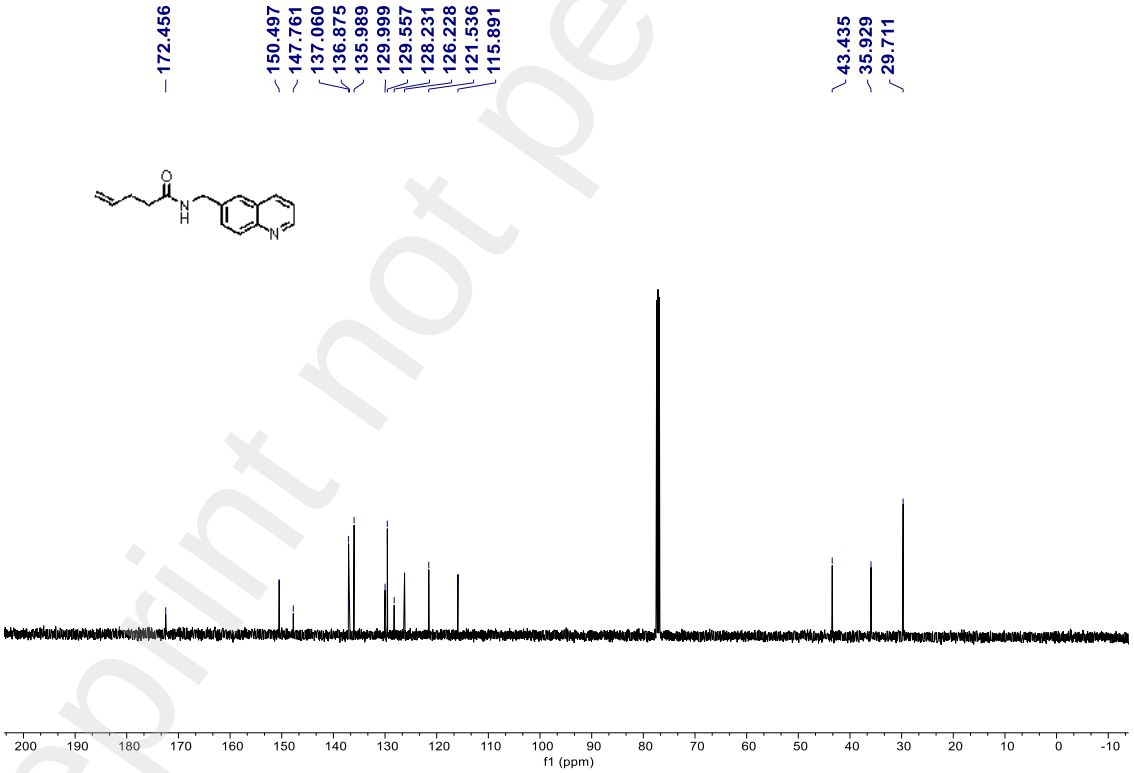
^{13}C NMR (126 MHz, $CDCl_3$) δ 172.5, 150.5, 147.8, 137.1, 136.9, 136.0, 130.0, 129.6, 128.2, 126.2, 121.5, 115.9, 43.4, 35.9, 29.7.

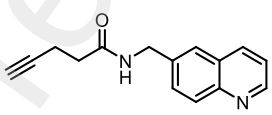
HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{17}N_2O^+$ $[M+H]^+$: 241.1341, found: 241.1337.

ldh02122p.10.fid



ldh02122p.11.fid



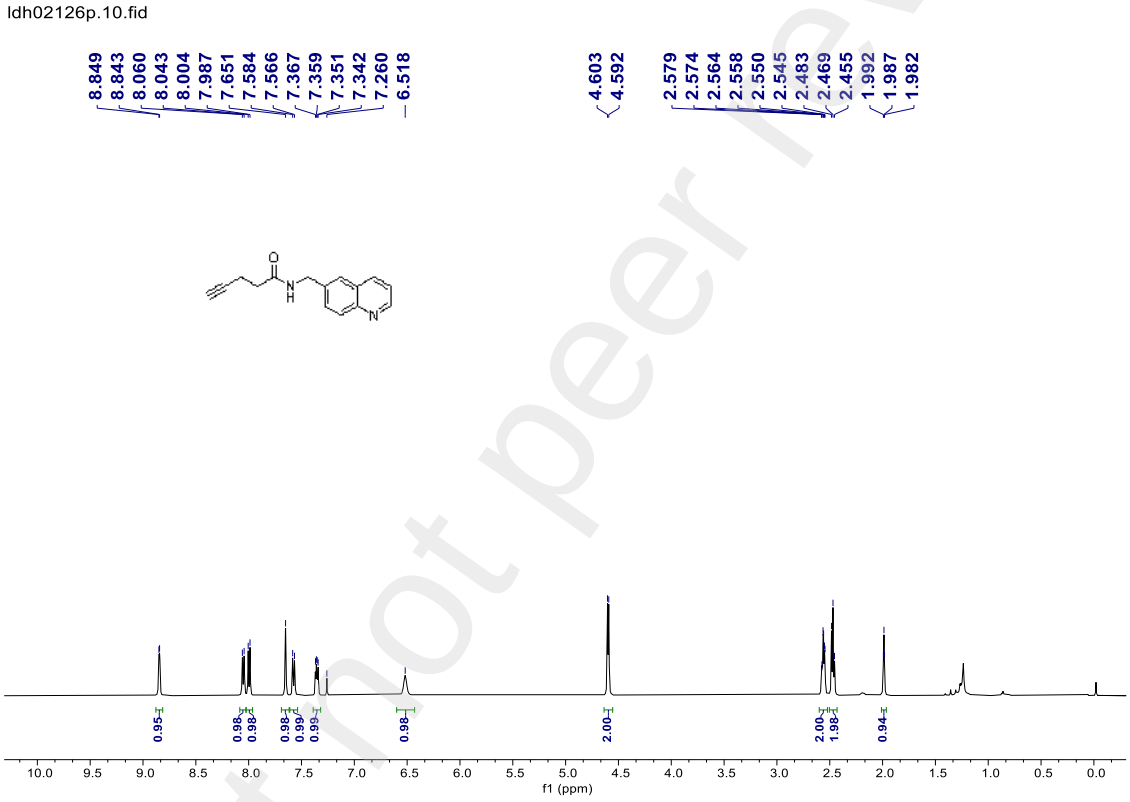


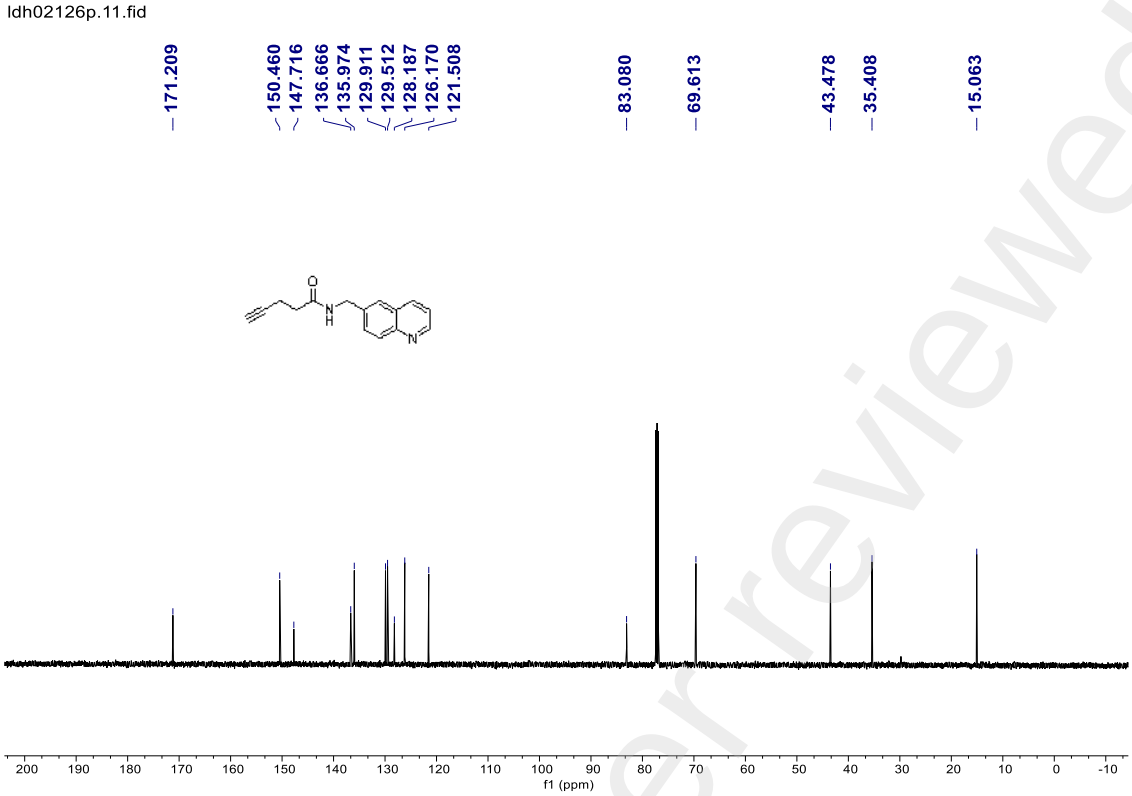
1aq, 62% yield

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (d, *J* = 3.0 Hz, 1H), 8.05 (d, *J* = 8.5 Hz, 1H), 8.00 (d, *J* = 8.5 Hz, 1H), 7.65 (s, 1H), 7.57 (d, *J* = 9.0 Hz, 1H), 7.36 (dd, *J* = 8.5, 4.0 Hz, 1H), 6.52 (br, 1H), 4.60 (d, *J* = 5.5 Hz, 2H), 2.59 - 2.53 (m, 2H), 2.47 (t, *J* = 7.0 Hz, 2H), 1.99 (t, *J* = 2.5 Hz, 1H)..

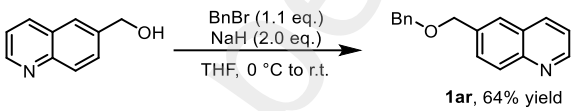
^{13}C NMR (126 MHz, $CDCl_3$) δ 171.2, 150.5, 147.7, 136.7, 136.0, 129.9, 129.5, 128.2, 126.2, 121.5, 83.1, 69.6, 43.5, 35.4, 15.1.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{15}N_2O^+$ $[M+H]^+$: 239.1184, found: 239.1180.





Experimental Procedure G for synthesizing quinoline derivatives 1ar and 1as



To a solution of 6-Quinolinylmethanol (6.0 mmol, 955 mg, 1.0 equiv.) in dry THF (30.0 mL) was added sodium hydride (60% in oil, 12.0 mmol, 480 mg, 2.0 equiv.) at 0 °C. After stirring for 30 minutes, BnBr (6.0 mmol, 1.03 g) was added to the reaction mixture, then stirred at 0 °C until the substrate was consumed completely. The resulting mixture was poured into saturated aqueous NaCl (50 mL), extracted with CH_2Cl_2 (3 × 20 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica to afford the product **1ar** as a yellow oil (946 mg, 60% yield).

Purification conditions: EtOAc/petroleum ether = 1:5 to 1:3

R_f(**1ar**) = 0.55 in EtOAc/petroleum ether = 1:1.

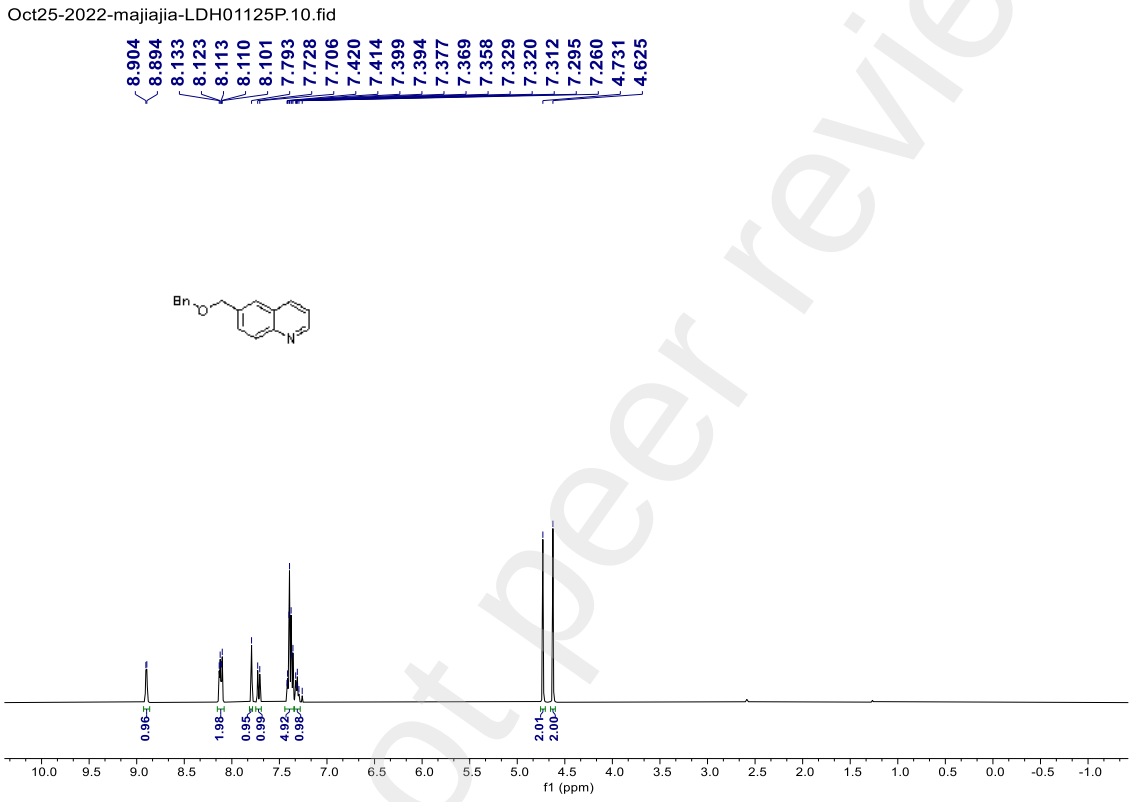
Analytical data of **1ar**:

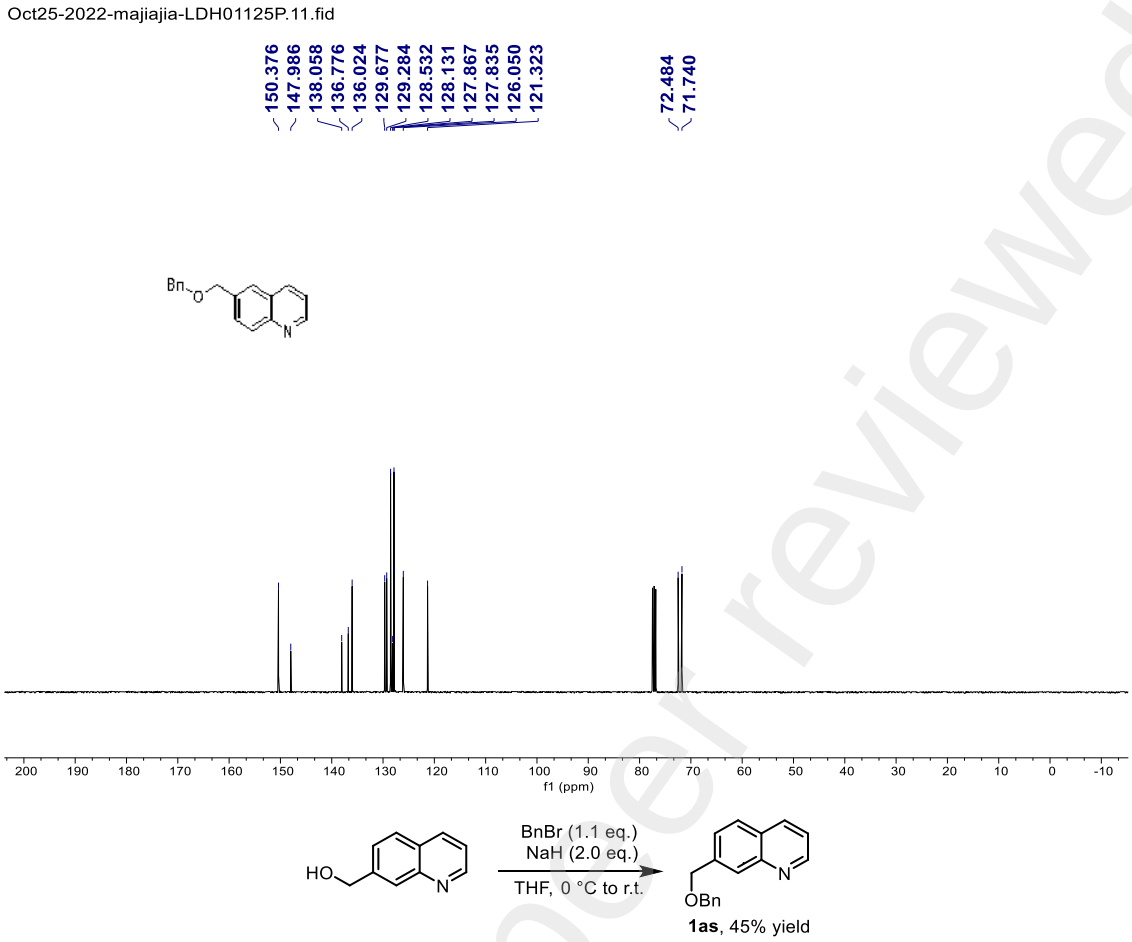
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 4.0 Hz, 1H), 8.14 - 8.08 (m, 2H), 7.79 (s,

1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.43 - 7.35 (m, 5H), 7.34 - 7.29 (m, 1H), 4.73 (s, 2H), 4.63 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 150.4, 148.0, 138.1, 136.8, 136.0, 129.7, 129.3, 128.5, 128.1, 127.9, 127.8, 126.0, 121.3, 72.5, 71.7.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{16}NO^+$ $[M+H]^+$: 250.1232, found: 250.1229.





To a solution of 6-Quinolinylmethanol (1.0 mmol, 344.0 mg, 1.0 equiv.) in dry THF (4.0 mL) was added sodium hydride (60% in oil, 1.5 mmol, 60.0 mg, 1.5 equiv.) at 0 °C. After stirring for 30 minutes, BnBr (1.1 mmol, 188.1 mg, 1.1 equiv.) was added to the reaction mixture, then stirred at 0 °C until the substrate was consumed completely. The resulting mixture was poured into saturated aqueous NaCl (10 mL), extracted with CH_2Cl_2 (3 × 5mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica to afford the product **1as** as a yellow oil (112.1 mg, 45% yield).

Purification conditions: EtOAc/petroleum ether = 1:5 to 1:3

R_f (**1as**) = 0.3 in EtOAc/petroleum ether = 1:2.

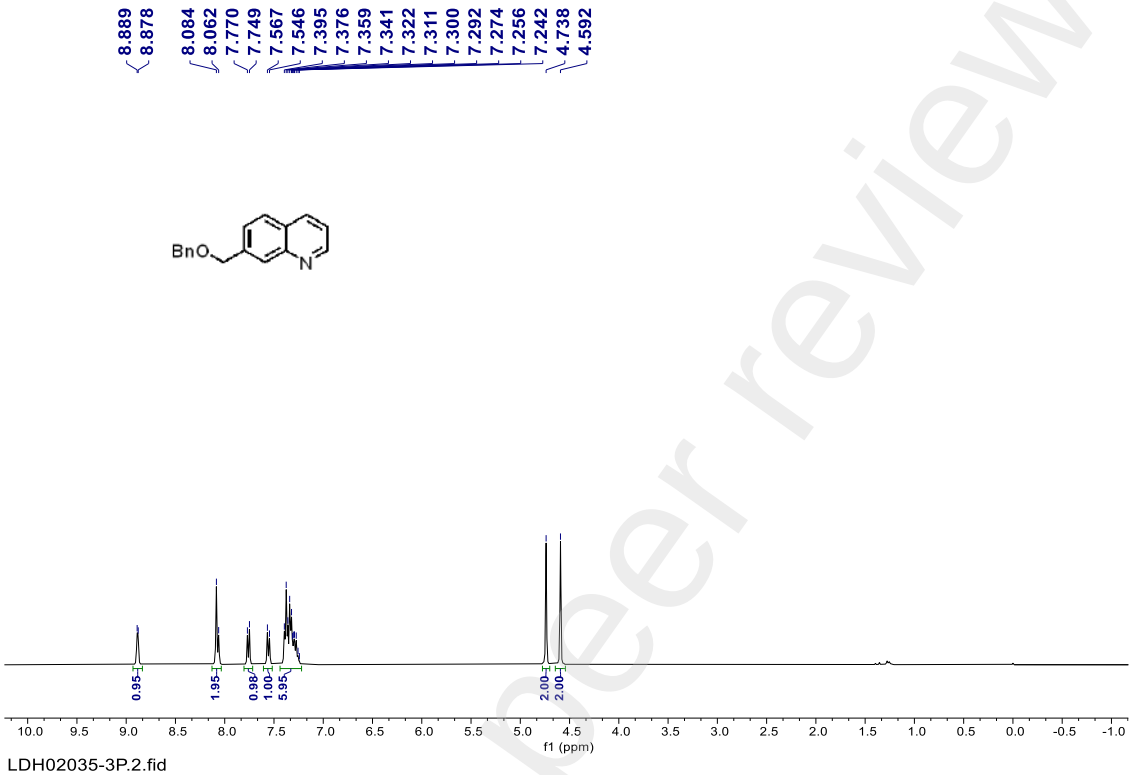
Analytical data of **1as**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (d, *J* = 4.4 Hz, 1H), 8.11 - 8.04 (m, 2H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.42 - 7.23 (m, 6H), 4.74 (s, 2H), 4.59 (s, 2H).

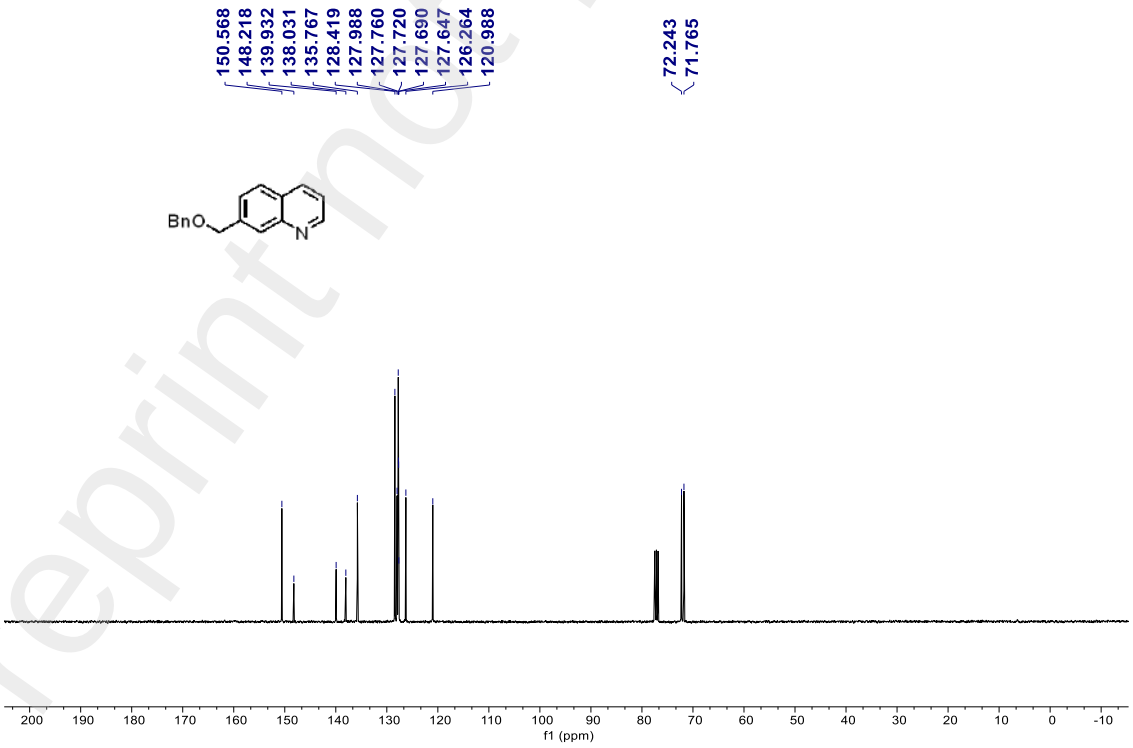
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.6, 148.2, 139.9, 138.0, 135.8, 128.4, 128.0, 127.8, 127.7, 127.7, 127.6, 126.3, 121.0, 72.2, 71.8.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{16}NO^+$ $[M+H]^+$: 250.1232, found: 250.1228.

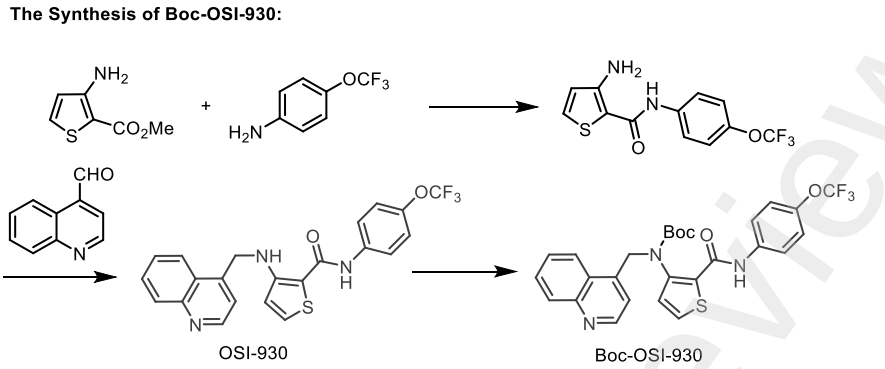
LDH02035-3P.1.fid



LDH02035-3P.2.fid



Experimental Procedure H for synthesizing Boc-OSI-930[15]



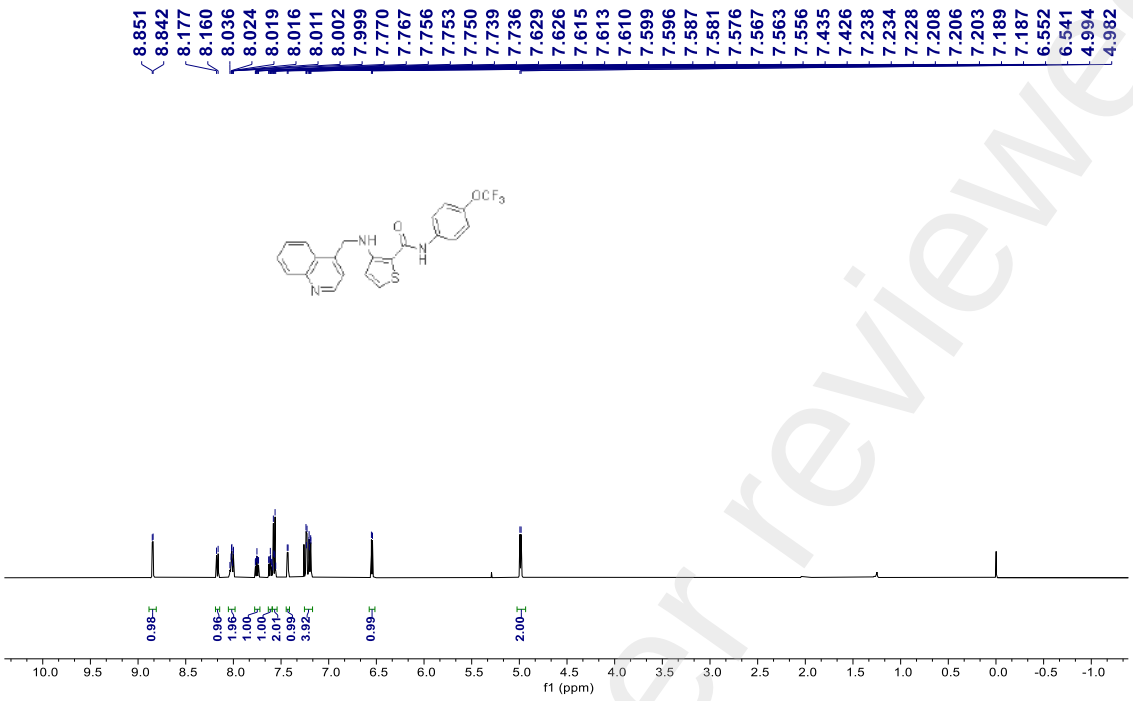
To a solution of **OSI-930** (6.0 mmol, 2.66 g, 1.0 equiv.) in CH_2Cl_2 (60 mL) was added 4-Dimethylaminopyridine (1.2 mmol, 147mg, 20 mol%), triethylamine (12.0 mmol, 1.21 g, 2.0 equiv.) and Di-tert-butyl decarbonate (9.0 mmol, 1.96 g, 1.5 equiv.) at 0 ℃ and stirred for 4 h. After completion of reaction, the resulting mixture was diluted by H_2O (100 mL) and extracted with CH_2Cl_2 (3 × 30 mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **Boc-OSI-930** as a white solid (1.96 g, 60% yield). *Note*: *According to the method from literature [15], the substrate **OSI-930** was prepared from the started material Ethyl 3-aminothiophene-2-carboxylate*.

Analytical data of **OSI-930**:

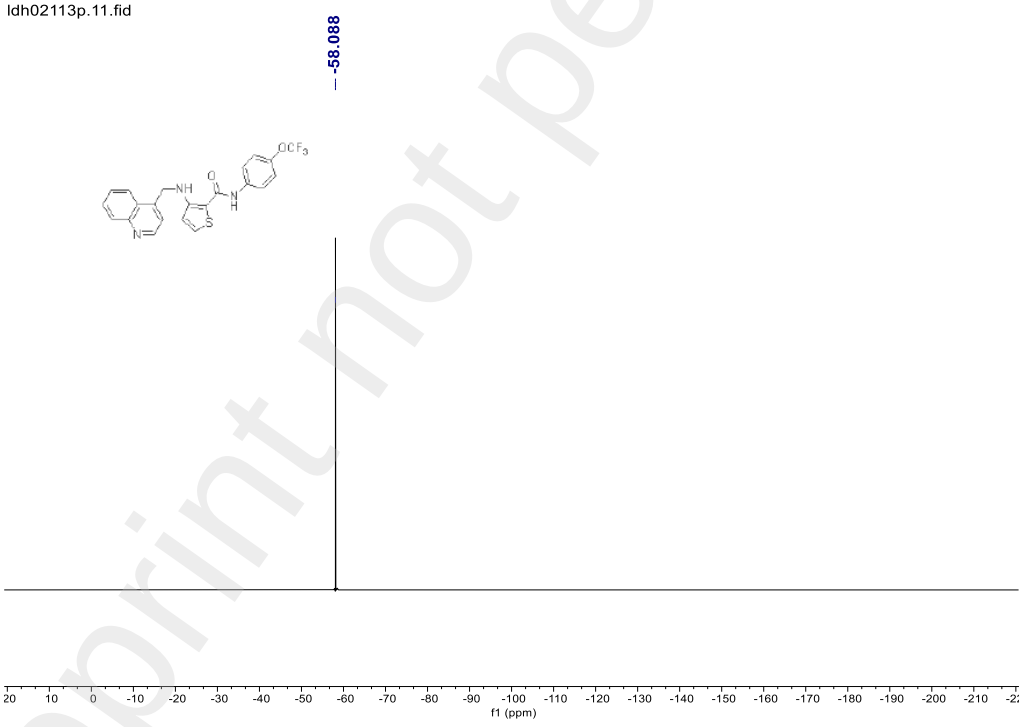
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (d, *J* = 4.5 Hz, 1H), 8.17 (d, *J* = 8.3 Hz, 1H), 8.05 - 8.00 (m, 2H), 7.79 - 7.72 (m, 1H), 7.65 - 7.58 (m, 1H), 7.59 - 7.55 (m, 2H), 7.43 (d, *J* = 4.4 Hz, 1H), 7.26 - 7.18 (m, 4H), 6.55 (d, *J* = 5.5 Hz, 1H), 4.99 (d, *J* = 6.2 Hz, 2H).

^{19}F NMR (471 MHz, $CDCl_3$) δ -58.09.

ldh02113p.10.fid



ldh02113p.11.fid



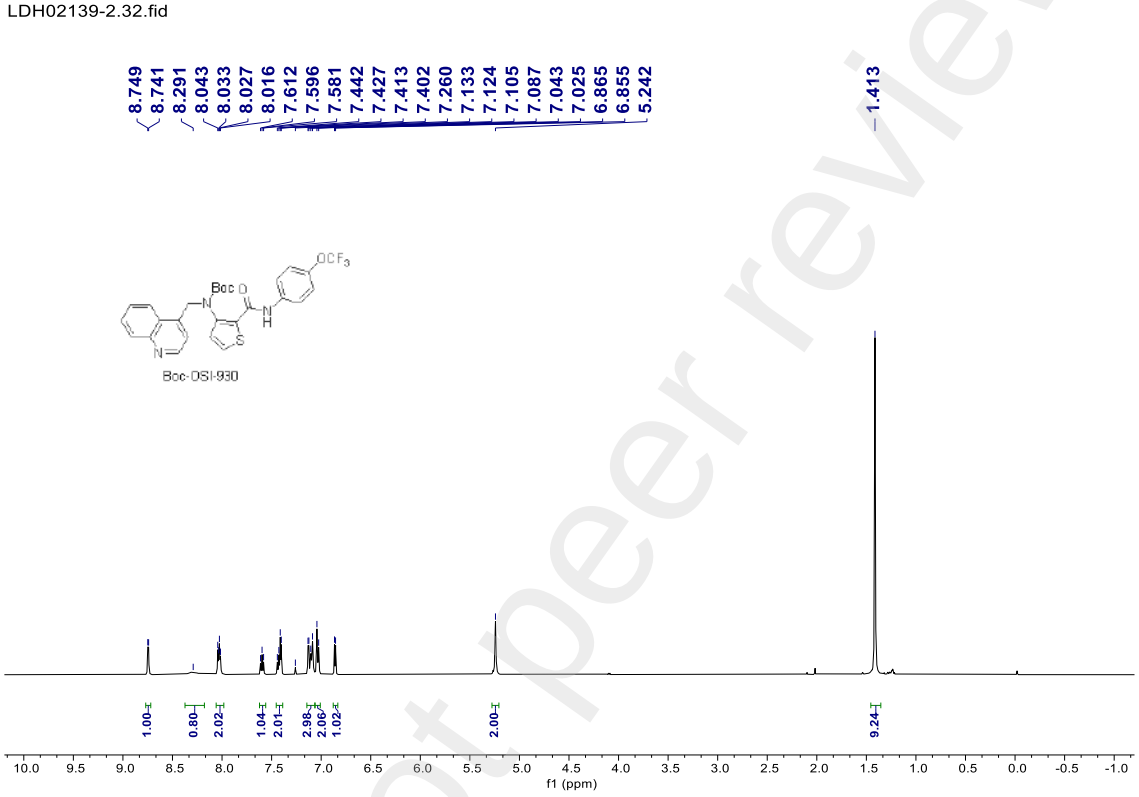
Analytical data of **Boc-OSI-930**:

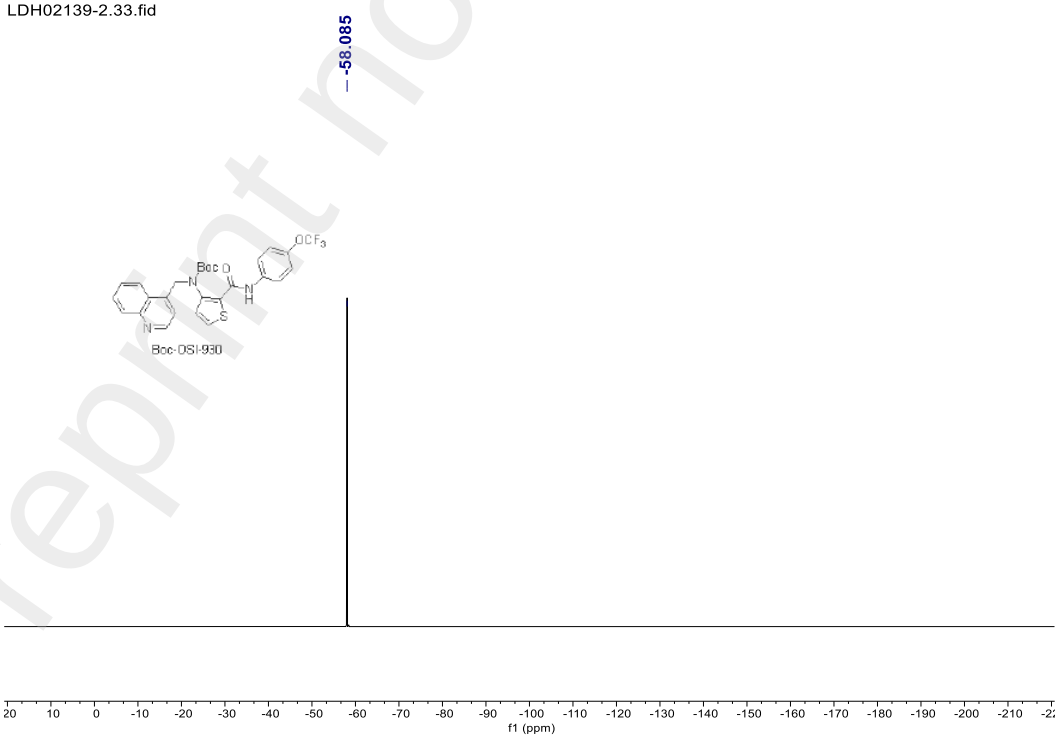
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.0 Hz, 1H), 8.29 (br, 1H), 8.06 - 8.00 (m, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.46 - 7.38 (m, 2H), 7.15 - 7.07 (m, 3H), 7.03 (d, *J* = 9.0 Hz, 2H), 6.86 (d, *J* = 5.0 Hz, 1H), 5.24 (s, 2H), 1.41 (s, 9H).

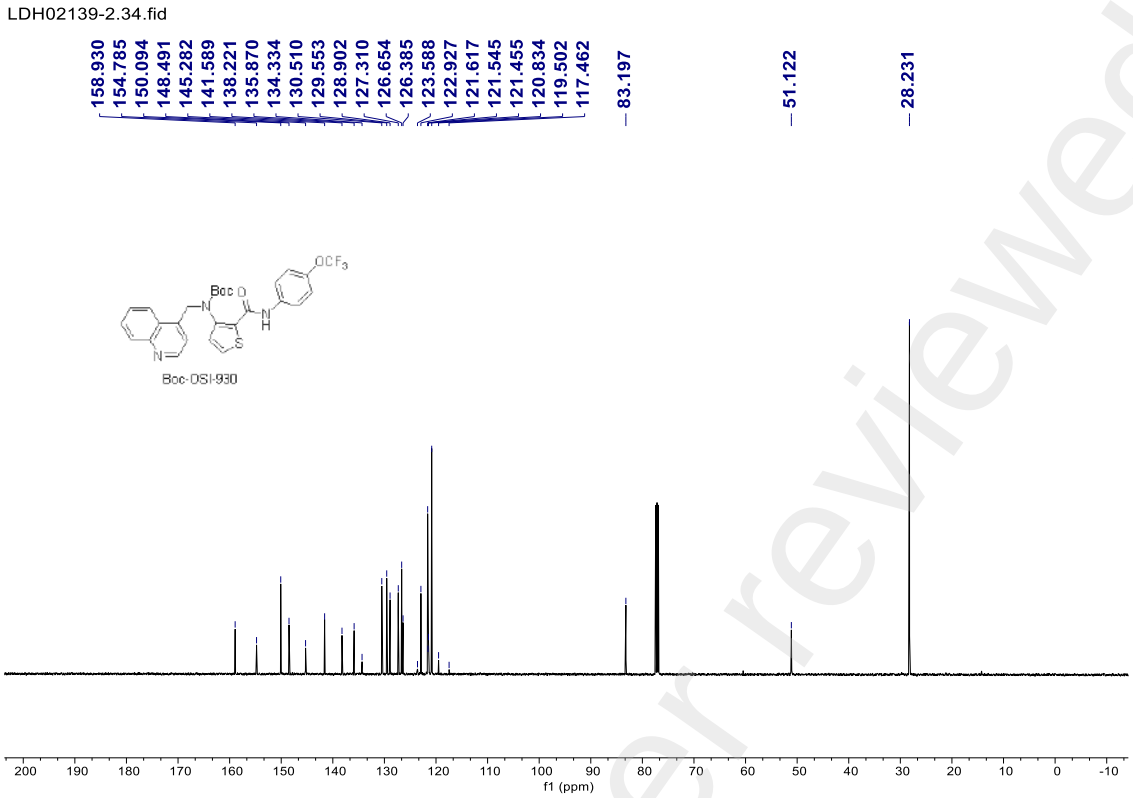
^{19}F NMR (471 MHz, $CDCl_3$) δ -58.09.

^{13}C NMR (126 MHz, $CDCl_3$) δ 158.93, 154.78, 150.09, 148.49, 145.28, 141.59, 138.22, 135.87, 134.33, 130.51, 129.55, 128.90, 127.31, 126.65, 126.39, 122.93, 121.62, 121.45, 120.83, 120.52 (q, J = 256.7 Hz), 83.20, 51.12, 28.23.

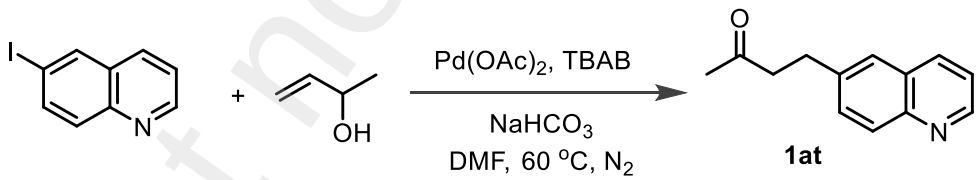
HRMS (ESI, *m*/*z*) calcd for $C_{27}H_{25}N_3O_4SF_3^+$ [M+H]$^+$: 544.1518, found: 544.1517.







Experimental Procedure I for synthesizing quinoline derivatives 1at



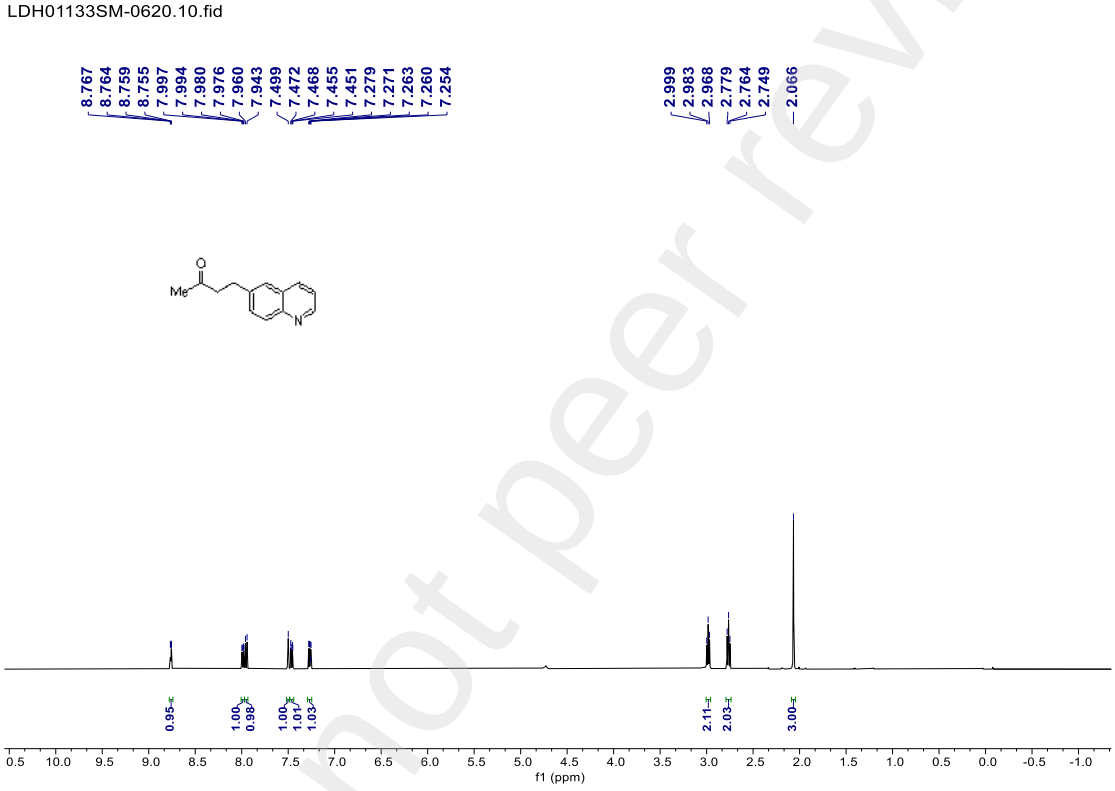
A dried 10 mL Schlenk tube was charged with the started material (5.0 mmol, 1.0 equiv.), the alcohol (7.5 mmol, 1.5 equiv.), $NaHCO_3$ (7.5 mmol, 1.5 equiv.), TBAB (5 mmol, 1.0 equiv.) and $Pd(OAc)_2$ (5.0 mol%) in DMF (0.6 M) under argon atmosphere. The reaction mixture was stirred vigorously at 60 ℃ until the full conversion of the starting material. Afterwards, the reaction was quenched by saturated aqueous $NaHCO_3$ and extracted with CH_2Cl_2 (30 mL × 3). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel (EtOAc/petroleum ether) to give the desired product **1at**

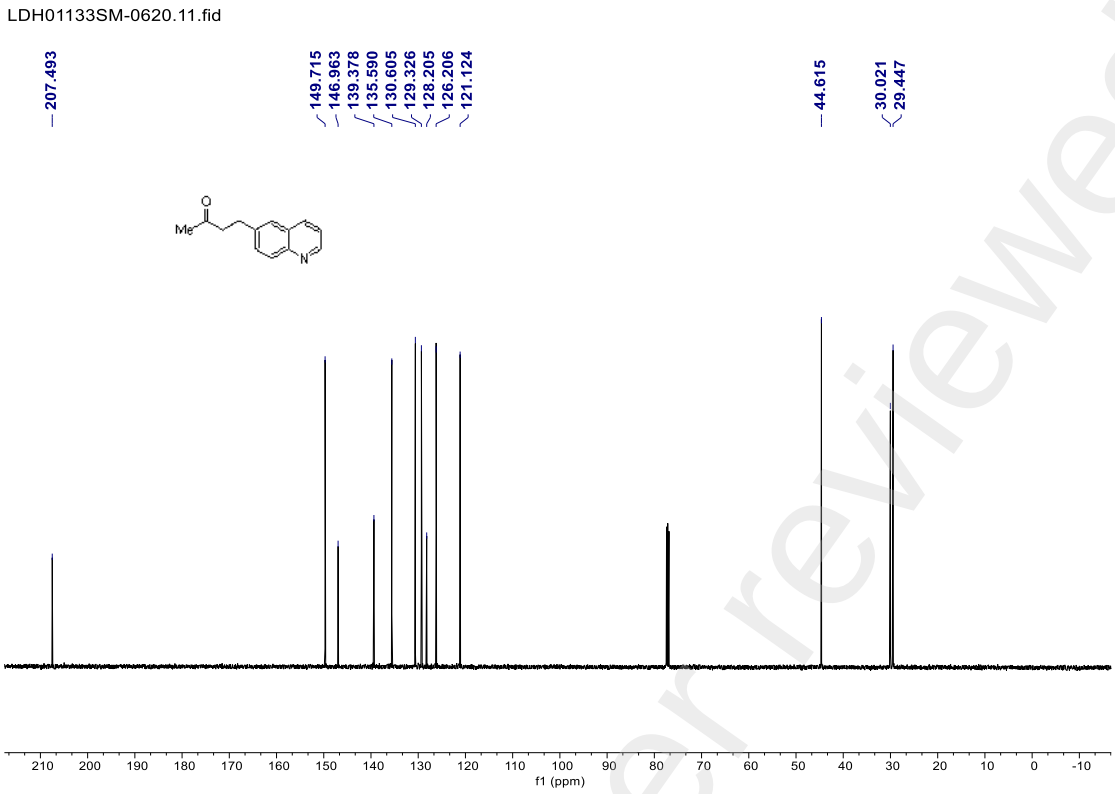
(530 mg, 53% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.76 (dd, *J* = 4.2, 1.8 Hz, 1H), 7.99 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.50 (s, 1H), 7.46 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.27 (dd, *J* = 8.3, 4.2 Hz, 1H), 2.98 (t, *J* = 7.5 Hz, 2H), 2.76 (t, *J* = 7.5 Hz, 2H), 2.07 (s, 3H).

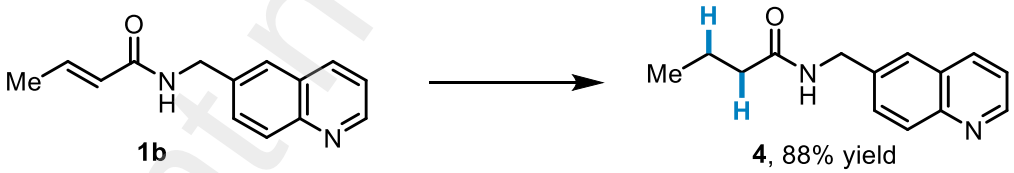
^{13}C NMR (126 MHz, $CDCl_3$) δ 207.5, 149.7, 147.0, 139.4, 135.6, 130.6, 129.3, 128.2, 126.2, 121.1, 44.6, 30.0, 29.4.

HRMS (ESI, *m*/*z*) calcd for $C_{13}H_{14}NO^+$ $[M+H]^+$: 200.1075, found: 200.1073.





5. Reduction of 1b with Conventional Hydrogenation



To a solution of the substrate **1b** (0.1 mmol, 22.6 mg, 1.0 equiv.) and Pd/C (Pd 5% on Carbon wetted with ca. 55% water, 10.0 mg) in MeOH (1.5 mL) were stirred for overnight under hydrogen atmosphere at room temperature. After completion of reaction, the resulting mixture was filtered by diatomaceous earth and washed with EtOAc (3 × 3mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **4** as a yellow solid (21.0 mg, 88% yield).

Purification conditions: Et_2O/petroleum ether = 1:3 to 1:1

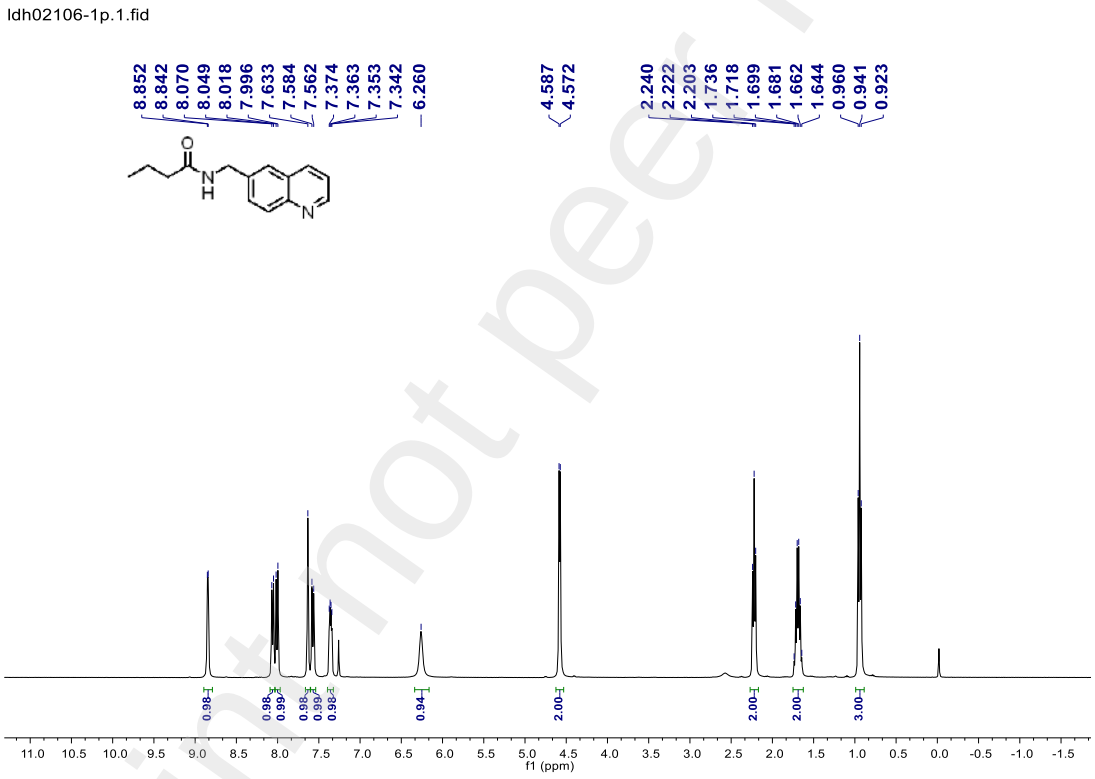
R_f (**4**) = 0.3 in Et_2O/petroleum ether = 1:1.

Analytical data of **4**:

^1H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 4.0 Hz, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 7.63 (s, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.36 (dd, *J* = 8.4, 4.4 Hz, 1H), 6.26 (br, 1H), 4.58 (d, *J* = 6.0 Hz, 2H), 2.22 (t, *J* = 7.6 Hz, 2H), 1.69 (h, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.1, 150.3, 147.5, 136.9, 135.9, 129.8, 129.4, 128.1, 126.0, 121.4, 43.2, 38.6, 19.2, 13.8.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{16}N_2ONa^+$ $[M+Na]^+$: 251.1152, found: 251.1155.



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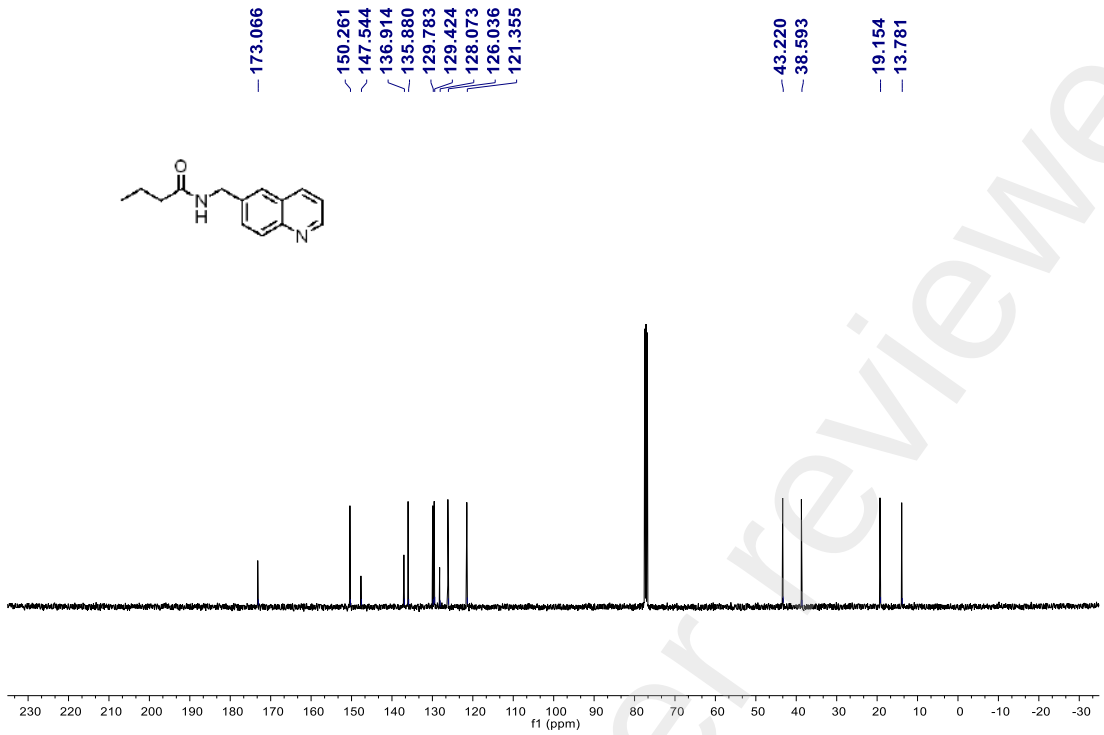
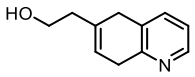


6. General Procedure for Quinolines Reduction and Characterization Data

A dried 10 mL Schlenk tube was charged with the starting material (0.2 mmol, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (1.0-3.0 mol%), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv.), γ-terpinene (0.6 mmol, 3.0-5.0 equiv.) and CH_3CN (4.0 mL, 0.05 M). The mixture was degassed by three cycles of freeze-pump-thaw, subsequently irradiated with 10 W blue LEDs (λ_{max} =455 nm) for 6 hours under nitrogen at 20 ℃. After the starting material was fully converted as checked by TLC, the reaction was quenched by saturated aqueous $NaHCO_3$ and extracted with CH_2Cl_2 or EtOAc (10 mL × 4). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel (petroleum ether/EtOAc, petroleum ether/acetone, EtOAc/CH_2Cl_2, petroleum ether/Et_2O or CH_2Cl_2/MeOH) to give the desired product.



2, 60% yield

According to the general procedure, a mixture of substrate **1a** (0.2 mmol, 34.6 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **2** as yellow oil (21.0 mg, 60% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:4 to 1:1

R_f(**2**) = 0.3 in EtOAc/petroleum ether = 1:1.

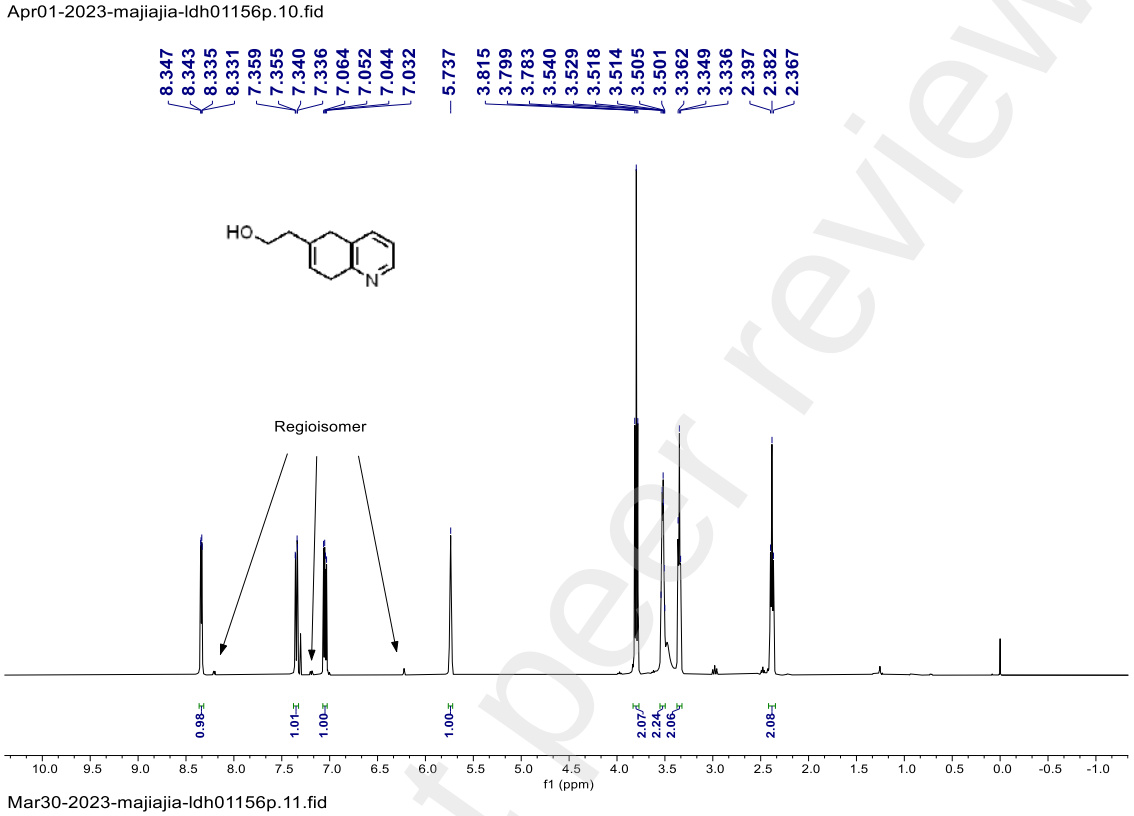
Analytical data of **2**:

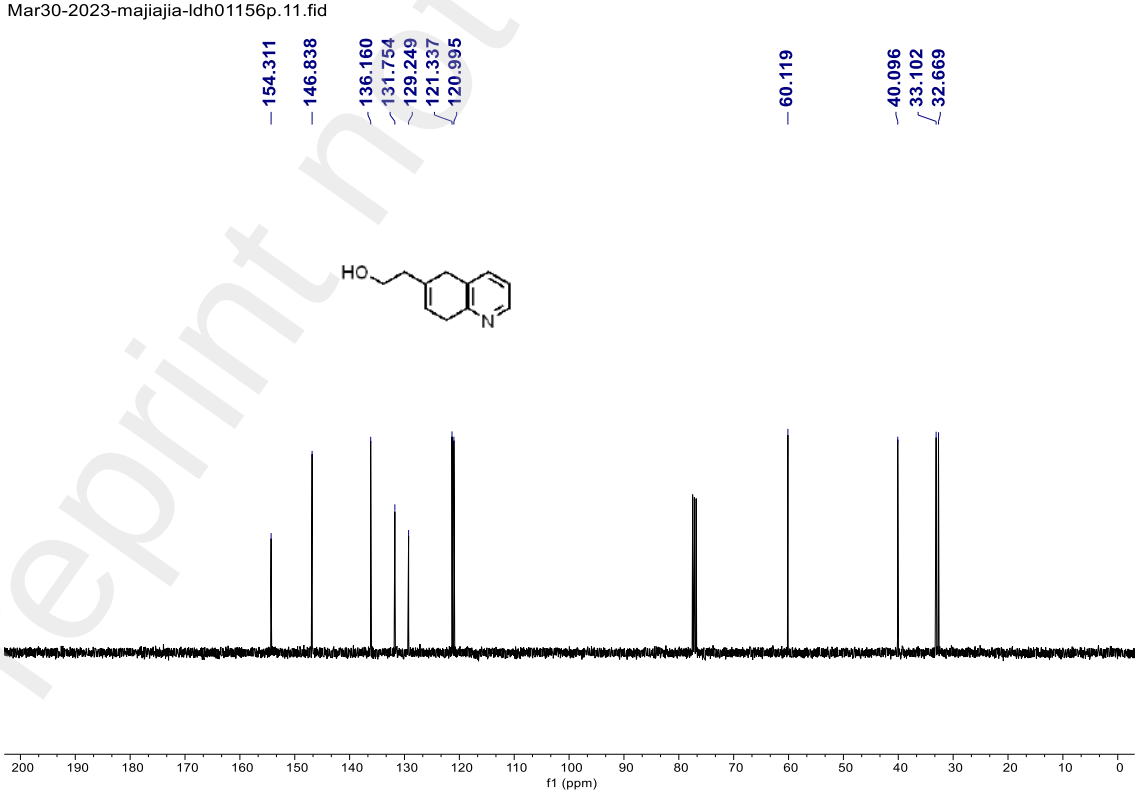
^1H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.35 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.05 (dd, *J* = 8.0, 4.8 Hz, 1H), 5.74 (br, 1H), 3.80 (t, *J* = 6.4 Hz, 2H), 3.55 - 3.50

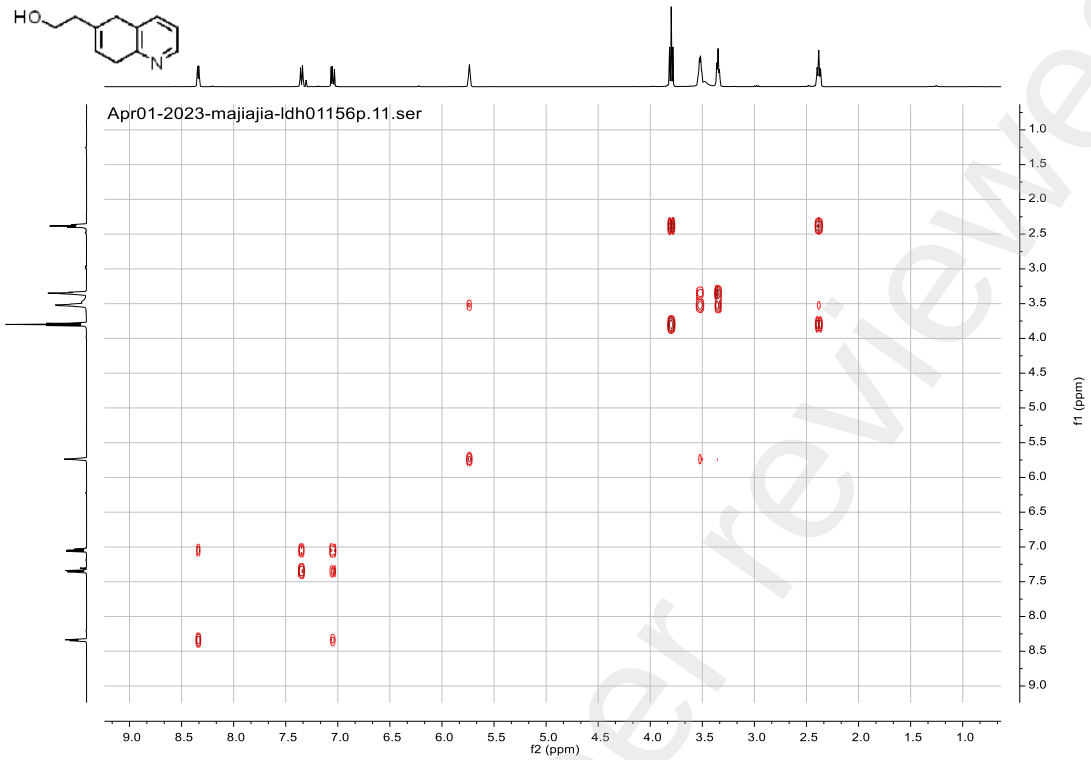
(m, 2H), 3.35 (t, *J* = 5.2 Hz, 2H), 2.38 (t, *J* = 6.0 Hz, 2H).

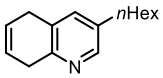
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.3, 146.8, 136.2, 131.8, 129.2, 121.3, 121.0, 60.1, 40.1, 33.1, 32.7.

HRMS (ESI, *m*/*z*) calcd for $C_{11}H_{14}NO^+$ $[M+H]^+$: 176.1070, found: 176.1079.









5, 61% yield

According to the general procedure, a mixture of **1b** (0.2 mmol, 42.6 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **5** as colorless oil (26.4 mg, 61% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:15 to 1:10

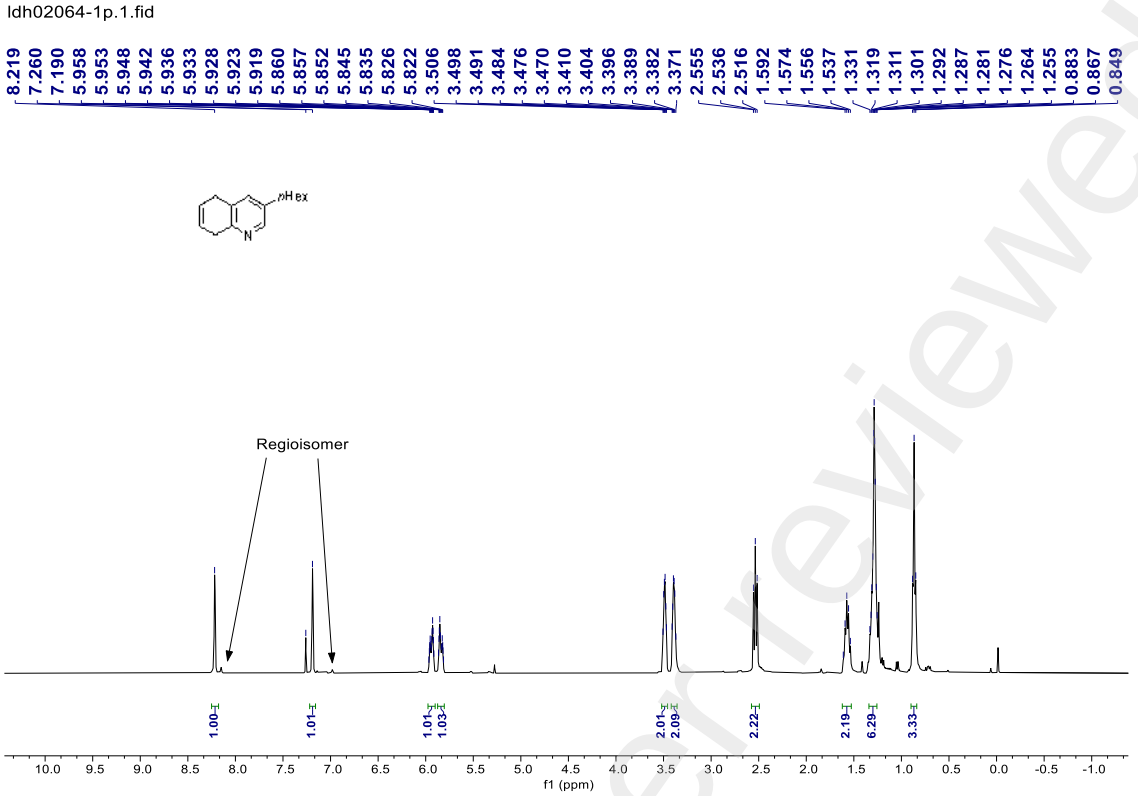
R*f* (**5**) = 0.35 in EtOAc/petroleum ether = 1:10.

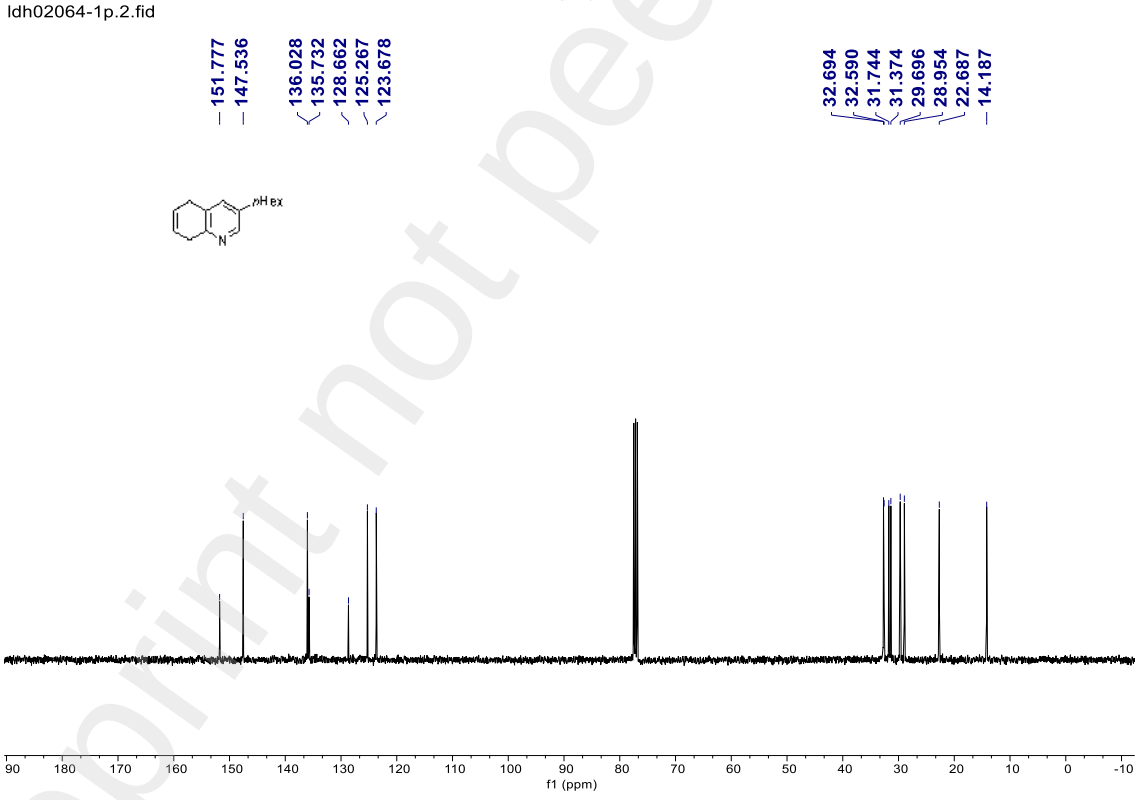
Analytical data of **5**:

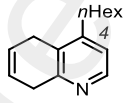
^1H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.19 (s, 1H), 5.98 - 5.90 (m, 1H), 5.87 - 5.80 (m, 1H), 3.52 - 3.46 (m, 2H), 3.42 - 3.36 (m, 2H), 2.54 (t, *J* = 8.0 Hz, 2H), 1.62 - 1.53 (m, 2H), 1.34 - 1.25 (m, 6H), 0.89 - 0.83 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 151.8, 147.5, 136.0, 135.7, 128.7, 125.3, 123.7, 32.7, 32.6, 31.7, 31.4, 29.7, 29.0, 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{22}N^+$ $[M+H]^+$: 216.1747, found: 216.1748.







6, 64% yield

According to the general procedure, a mixture of **1c** (0.2 mmol, 42.6 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol,

2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **6** as colorless oil (27.6 mg, 64% yield, >95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:10 to 1:5

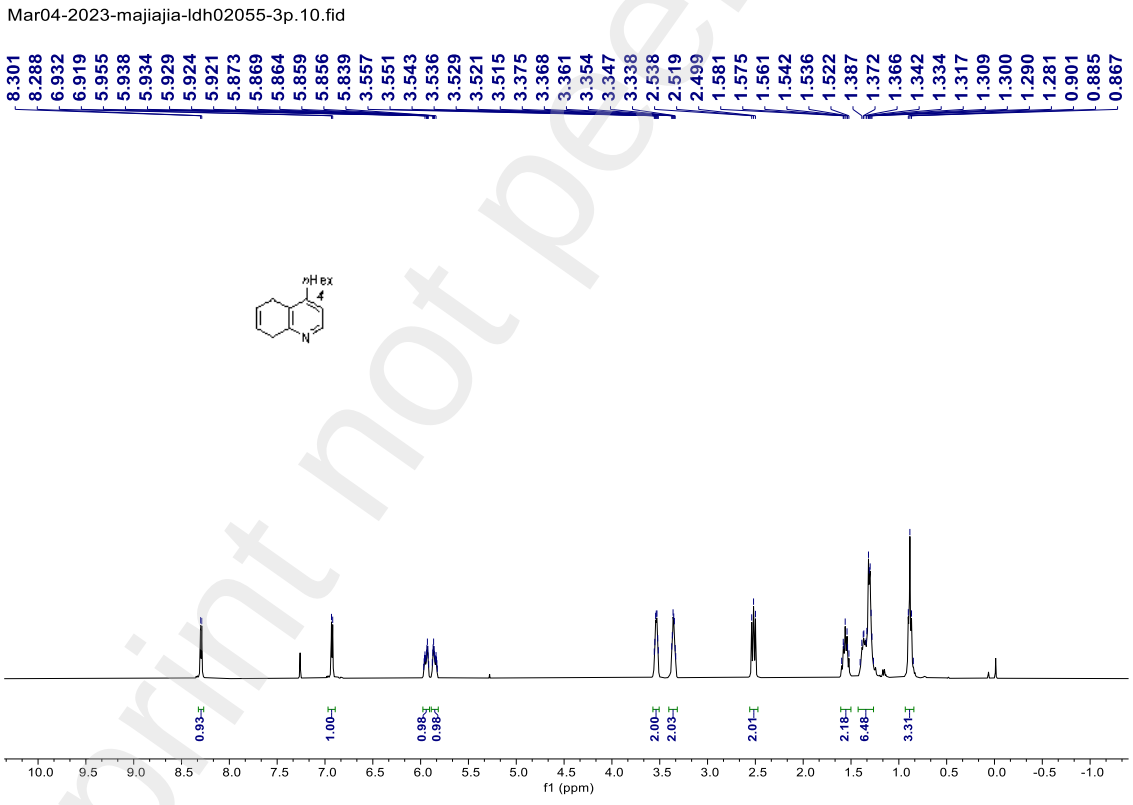
R_f (**6**) = 0.3 in EtOAc/petroleum ether = 1:5.

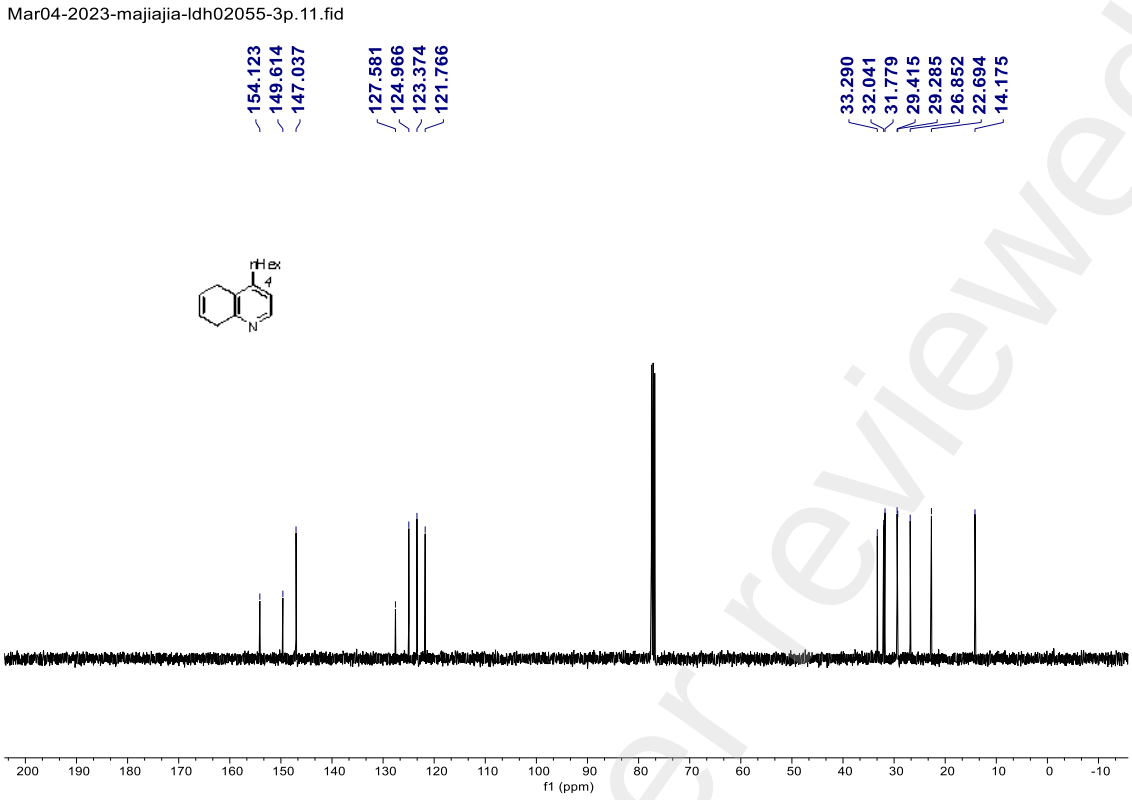
Analytical data of **6**:

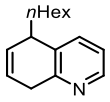
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 5.2 Hz, 1H), 6.93 (d, *J* = 5.2 Hz, 1H), 5.98 - 5.91 (m, 1H), 5.90 - 5.80 (m, 1H), 3.58 - 3.49 (m, 2H), 3.40 - 3.31 (m, 2H), 2.56 - 2.48 (m, 2H), 1.60 - 1.51 (m, 2H), 1.41 - 1.26 (m, 6H), 0.92 - 0.84 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.1, 149.6, 147.0, 127.6, 125.0, 123.4, 121.8, 33.3, 32.0, 31.8, 29.4, 29.3, 26.9, 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{22}N$ $[M+H]^+$: 216.1747, found: 216.1752.







7, 26% yield, 78:22 r.r.

According to the general procedure, a mixture of **1d** (0.2 mmol, 42.6 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **7** as colorless oil (11.1mg, 26% yield, 78:22 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:40 to 1:10

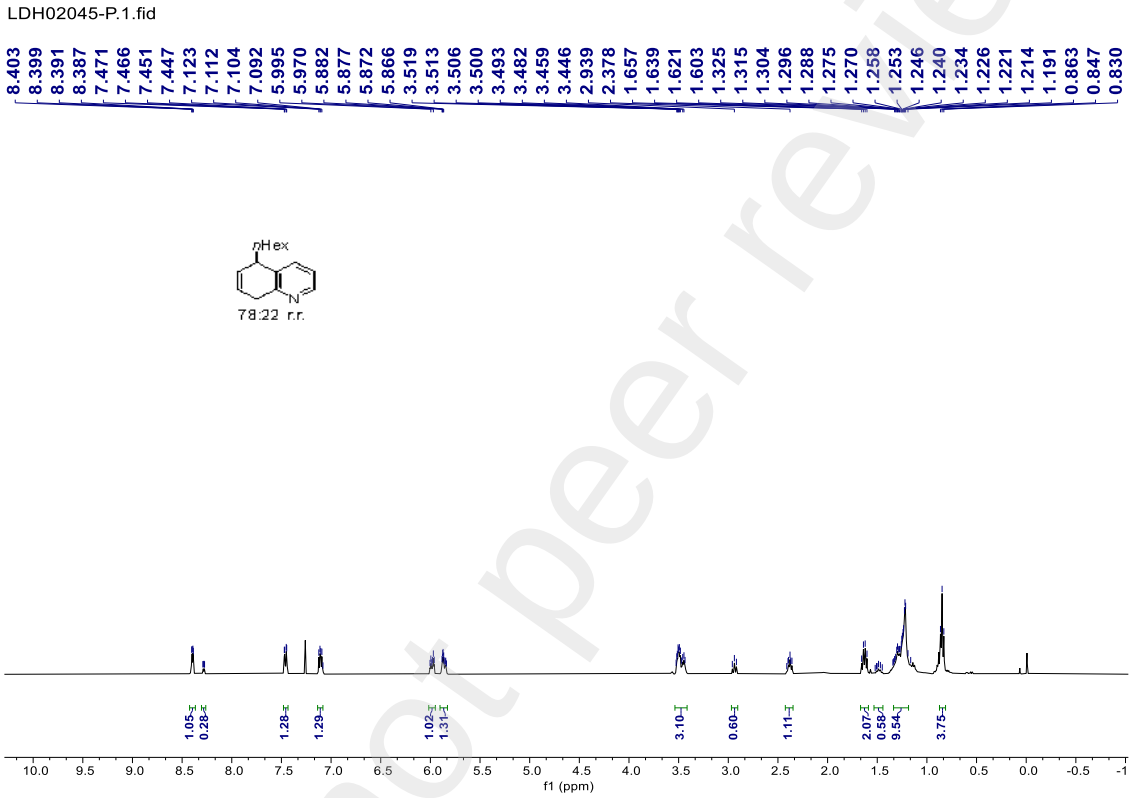
R_f (**7**) = 0.35 in EtOAc/petroleum ether = 1:8.

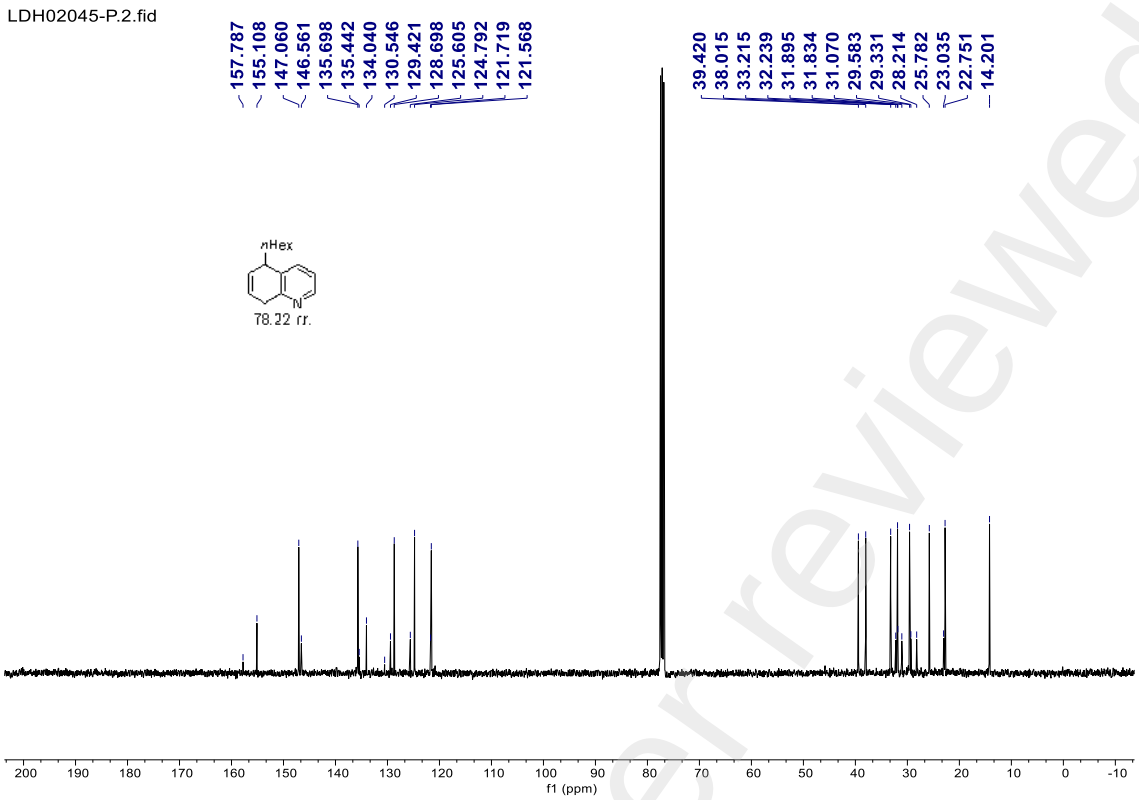
Analytical data of **7**:

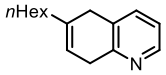
^{1}H NMR (400 MHz, $CDCl_3$, mixture of mixture of regioisomers) δ 8.40 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.28 (dd, *J* = 4.8, 1.6 Hz, 1H, minor), 7.48 - 7.44 (m, 1H, major; m, 1H, minor), 7.15 - 7.06 (m, 1H, major; m, 1H, minor), 6.03 - 5.94 (m, 1H), 5.90 - 5.82 (m, 1H, major; m, 1H, minor), 3.55 - 3.41 (m, 3H), 2.94 (t, *J* = 8.0 Hz, 2H, minor), 2.43 - 2.35 (m, 1H), 1.63 (q, *J* = 7.2 Hz, 2H), 1.54 - 1.43 (m, 2H, minor), 1.34 - 1.15 (m, 7H, major; m, 7H, minor), 0.90 - 0.81 (m, 3H, major; m, 3H, minor).

^{13}C NMR (101 MHz, $CDCl_3$, mixture of regioisomers) δ 157.8(minor), 155.1, 147.1, 146.6(minor), 135.7, 135.4(minor), 134.0, 130.5(minor), 129.4(minor), 128.7, 125.6(minor), 124.8, 121.7(minor), 121.6, 39.4, 38.0, 33.2, 32.2(minor), 31.9, 31.8(minor), 31.1(minor), 29.6, 29.3(minor), 28.2(minor), 25.8, 23.0(minor), 22.8, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{22}NO^+$ $[M+H]^+$: 216.1747, found: 216.1748.







8, 67% yield, 93:7 r.r.

According to the general procedure, a mixture of **1e** (0.2 mmol, 42.6 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **8** as colorless oil (28.9 mg, 67% yield, 93:7 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:10 to 1:5

R_f (**8**) = 0.4 in EtOAc/petroleum ether = 1:4.

Analytical data of **8**:

^{1}H NMR (500 MHz, $CDCl_3$, mixture of regioisomers) δ 8.38 (d, *J* = 4.5 Hz, 1H), 8.32 (d, *J* = 5.0 Hz, 1H, minor), 7.39 (d, *J* = 7.5 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H, minor), 7.06 (dd, *J* = 8.0, 5.0 Hz, 1H), 7.00 (dd, *J* = 7.5, 5.0 Hz, 1H, minor), 5.64 (br, 1H), 3.54 - 3.49 (m, 2H), 3.35 - 3.30 (m, 2H), 2.09 (t, *J* = 8.0 Hz, 2H), 1.52 - 1.42 (m, 2H), 1.34 - 1.24 (m, 6H), 0.90 - 0.85 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.1, 147.2, 146.7(minor), 137.0(minor), 136.1, 135.1, 129.6, 121.3, 120.9(minor), 118.7, 37.1, 36.2(minor), 35.5(minor), 33.8(minor),

33.5, 32.9, 32.2(minor), 32.0(minor), 31.9, 29.6(minor), 29.1, 27.6, 27.1(minor), 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{22}N^+$ $[M+H]^+$: 216.1747, found: 216.1748.

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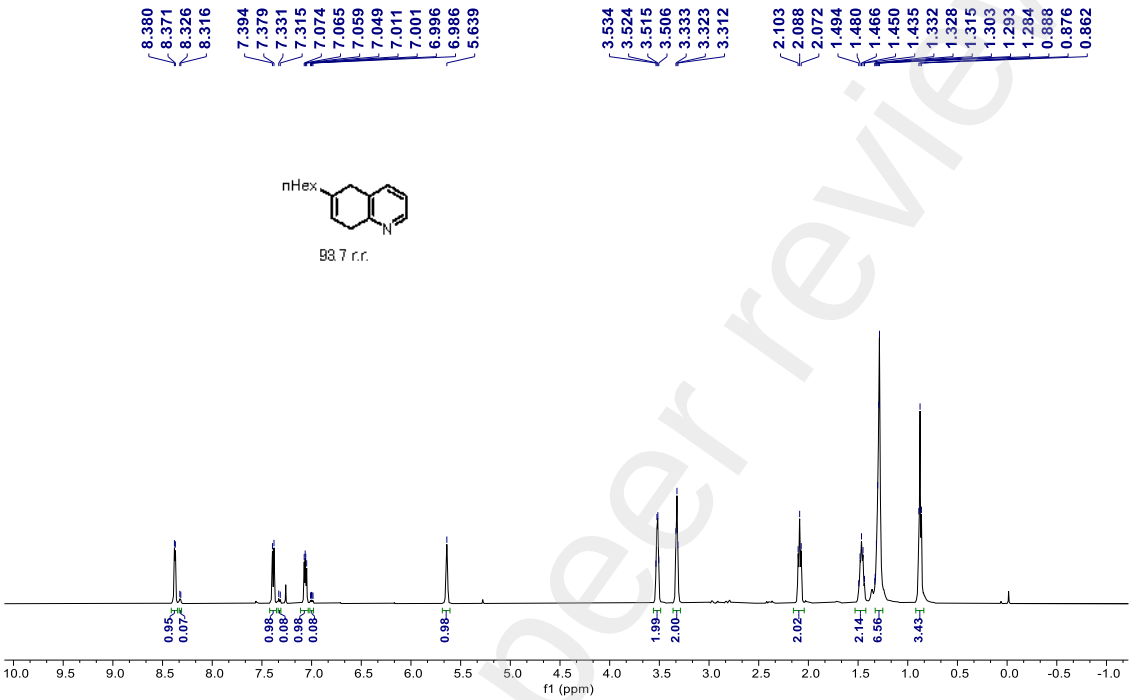

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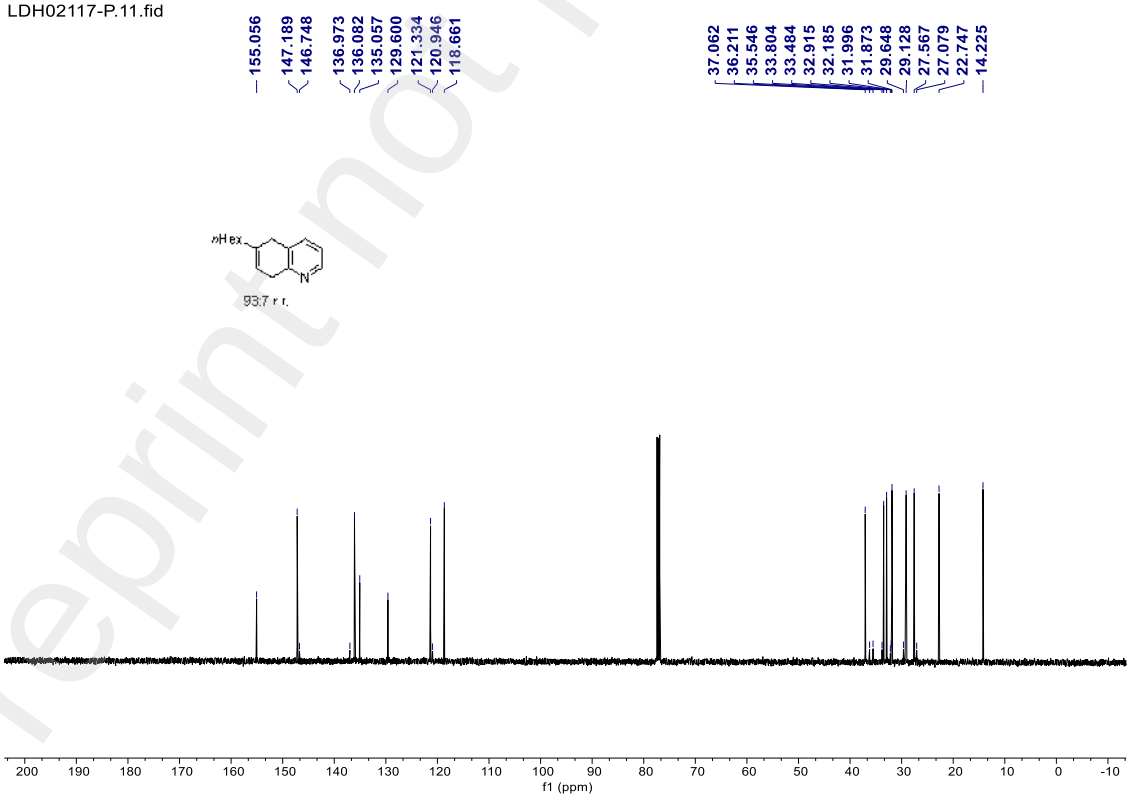
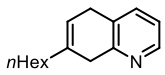




9, 49% yield

According to the general procedure, a mixture of **1f** (0.2 mmol, 42.6 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **9** as colorless oil (21.2 mg, 49% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:30 to 1:10

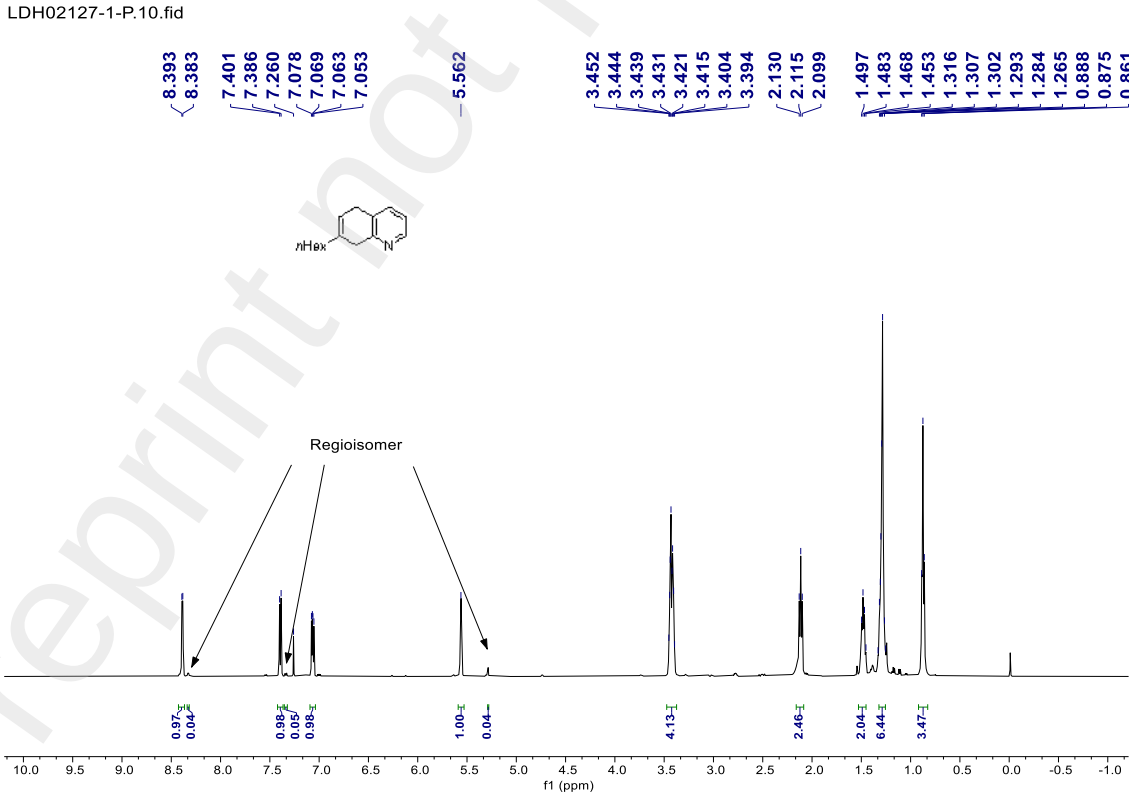
R_f (**9**) = 0.5 in EtOAc/petroleum ether = 1:10.

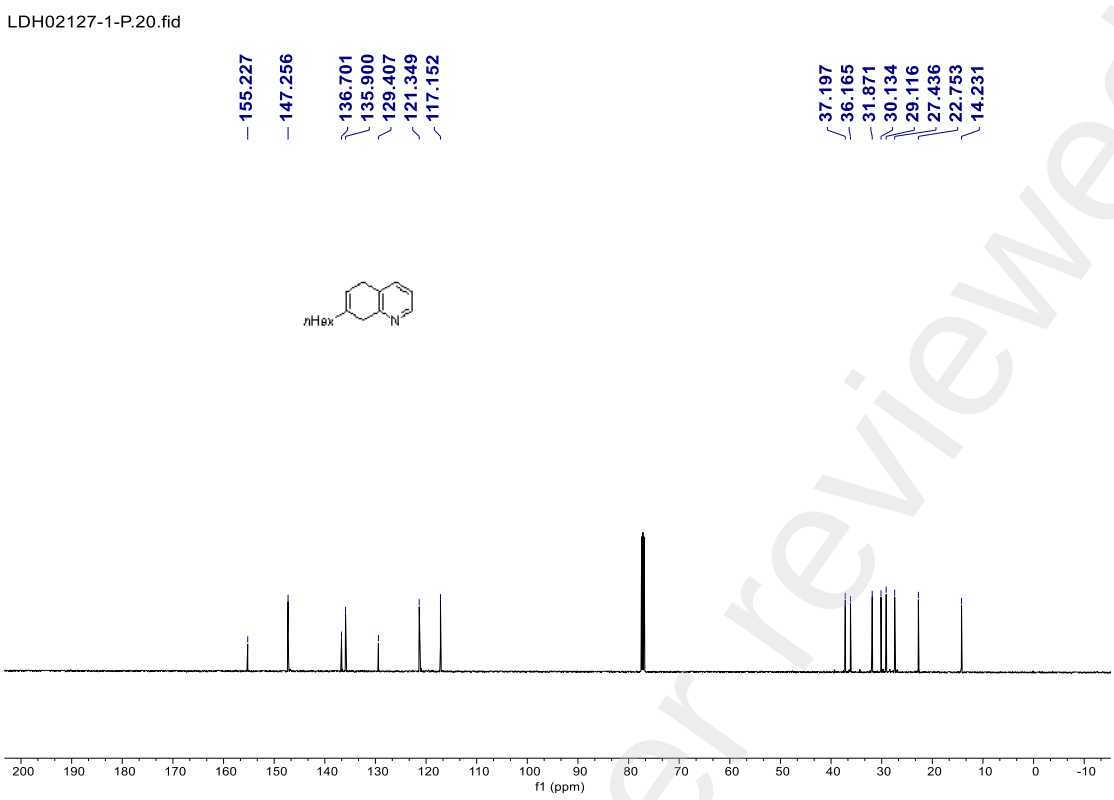
Analytical data of **9**:

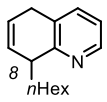
^1H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 5.0 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.07 (dd, *J* = 7.5, 4.5 Hz, 1H), 5.56 (br, 1H), 3.46 - 3.38 (m, 4H), 2.11 (t, *J* = 7.5 Hz, 2H), 1.51 - 1.44 (m, 2H), 1.32 - 1.26 (m, 6H), 0.91 - 0.84 (m, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 147.3, 136.7, 135.9, 129.4, 121.3, 117.2, 37.2, 36.2, 31.9, 30.1, 29.1, 27.4, 22.8, 14.2.

HRMS (ESI, *m/z*) calcd for $C_{15}H_{22}N^+$ $[M+H]^+$: 216.1747, found: 216.1748.







10, 33% yield, 89:11 r.r.

According to the general procedure, a mixture of **1g** (0.2 mmol, 42.6 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **10** as colorless oil (14.2 mg, 33% yield, 89:11 r.r.).

Purification conditions: Et_2O/petroleum ether = 1:30 to 1:10

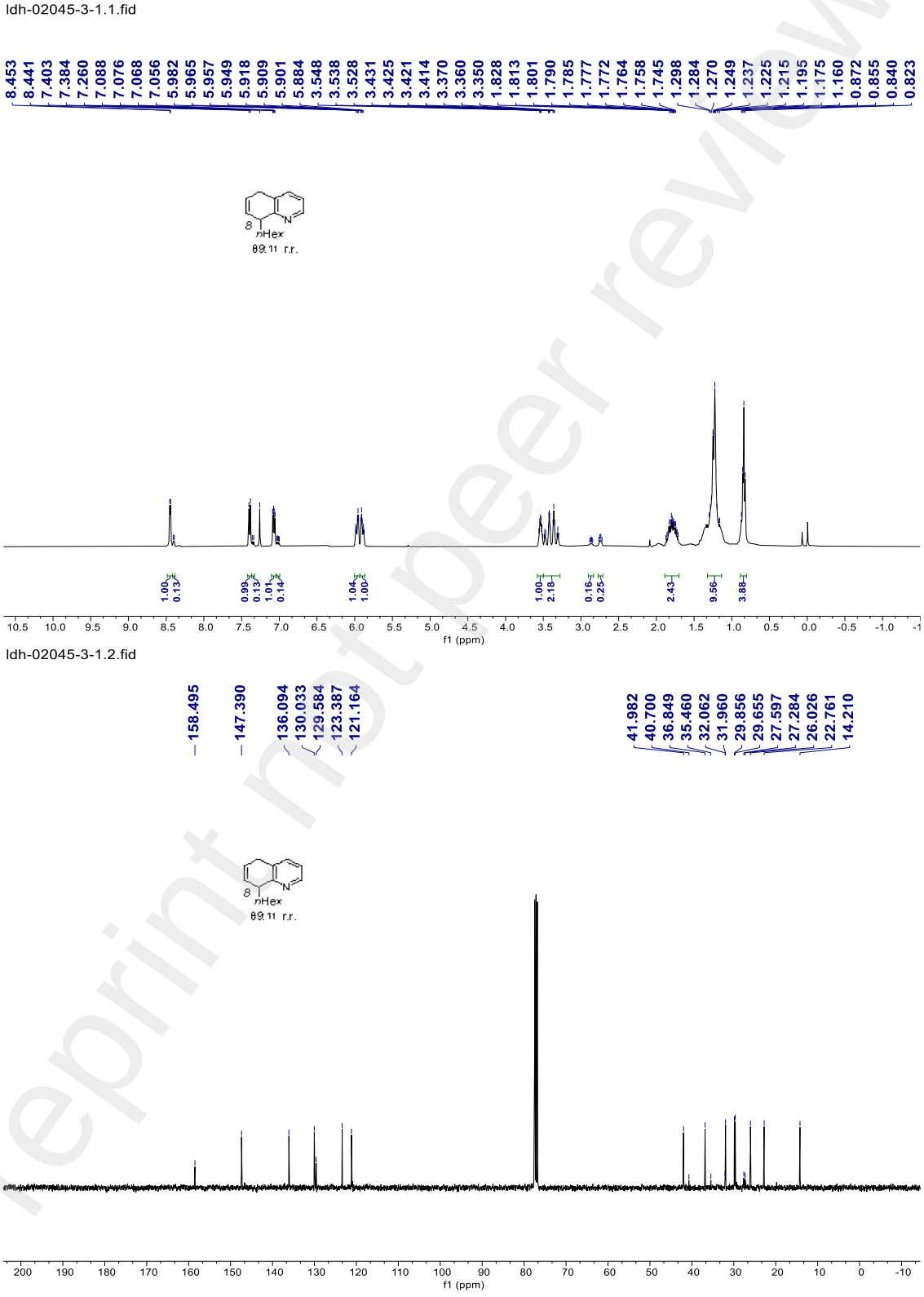
R_f (**10**) = 0.25 in Et_2O/petroleum ether = 1:10.

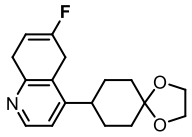
Analytical data of **10**:

^{1}H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.45 (d, *J* = 4.8 Hz, 1H), 8.40 (d, *J* = 4.8 Hz, 1H, minor), 7.39 (d, *J* = 7.8 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 1H, minor), 7.07 (dd, *J* = 8.0, 4.8 Hz, 1H), 7.02 (dd, *J* = 7.6, 4.8 Hz, 1H, minor), 6.00 - 5.94 (m, 1H), 5.93 - 5.86 (m, 1H), 3.57 - 3.50 (m, 1H), 3.49 - 3.29 (m, 2H), 2.90 - 2.83 (m, 1H, minor), 2.77 - 2.71 (m, 2H, minor), 1.88 - 1.69 (m, 2H), 1.23 (m, 8H, major; m,8H, minor), 0.85 (m, 3H, major; m, 3H, minor).

^{13}C NMR (101 MHz, $CDCl_3$, mixture of regioisomers) δ 158.5, 147.4, 136.1, 130.0, 129.6, 123.4, 121.2, 42.0, 40.7(minor), 36.8, 35.5 (minor), 32.1(minor), 32.0, 29.9, 29.7, 27.6(minor), 27.3(minor), 26.0, 22.8, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{22}N^+$ $[M+H]^+$: 216.1747, found: 216.1746.





11, 67%, 76:24 r.r.

According to the general procedure, a mixture of **1l** (0.2 mmol, 57.4 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **11** as yellow oil (38.8 mg, 67% yield, 76:24 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:3 to 1:1

R_f (**11**) = 0.3 in EtOAc/petroleum ether = 1:1.

Analytical data of **11**:

^{1}H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.36 (d, *J* = 5.2 Hz, 1H), 8.16 (d, *J* = 5.2 Hz, 1H, minor), 7.06 (d, *J* = 5.2 Hz, 1H), 6.98 (d, *J* = 5.6 Hz, 1H, minor), 6.23 (d, *J* = 13.6 Hz, 1H, minor), 5.49 - 5.38 (m, 1H), 3.97 (s, 4H, major; s, 4H, minor), 3.67 - 3.60 (m, 2H), 3.58 - 3.53 (m, 2H), 3.17 (td, *J* = 8.4, 2.8 Hz, 2H, minor), 2.70 - 2.56 (m, 2H), 1.91 - 1.80 (m, 1H, major; m, 3H, minor), 1.81 - 1.62 (m, 6H, major; m, 8H, minor).

^{19}F NMR (376 MHz, $CDCl_3$, mixture of regioisomers) δ -96.96(minor), -106.52.

^{13}C NMR (126 MHz, $CDCl_3$, mixture of regioisomers) δ 164.0 (d, *J* = 270.9 Hz, minor), 155.7 (d, *J* = 250.3 Hz), 153.6 (d, *J* = 3.1 Hz), 153.3(minor), 153.1 (d, *J* = 2.3 Hz), 148.8 (d, *J* = 6.5 Hz, minor), 148.0, 146.3 (d, *J* = 2.4 Hz), 125.8 (d, *J* = 9.9 Hz, minor), 124.8 (d, *J* = 12.9 Hz, minor), 119.0(minor), 118.6, 108.2(minor), 108.1, 100.1 (d, *J* = 20.3 Hz, minor), 99.9 (d, *J* = 16.7 Hz), 64.48 (d, *J* = 3.7 Hz), 64.46 (d, *J* = 3.6 Hz, minor), 38.1, 37.8(minor), 35.2, 35.1(minor), 32.4 (d, *J* = 8.3 Hz), 31.9 (d, *J* = 7.6 Hz, minor), 30.3, 30.0(minor), 27.2 (d, *J* = 29.6 Hz), 24.5 (d, *J* = 23.9 Hz, minor).

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{21}FNO_2$ $[M+H]^+$: 290.1551, found: 290.1552.

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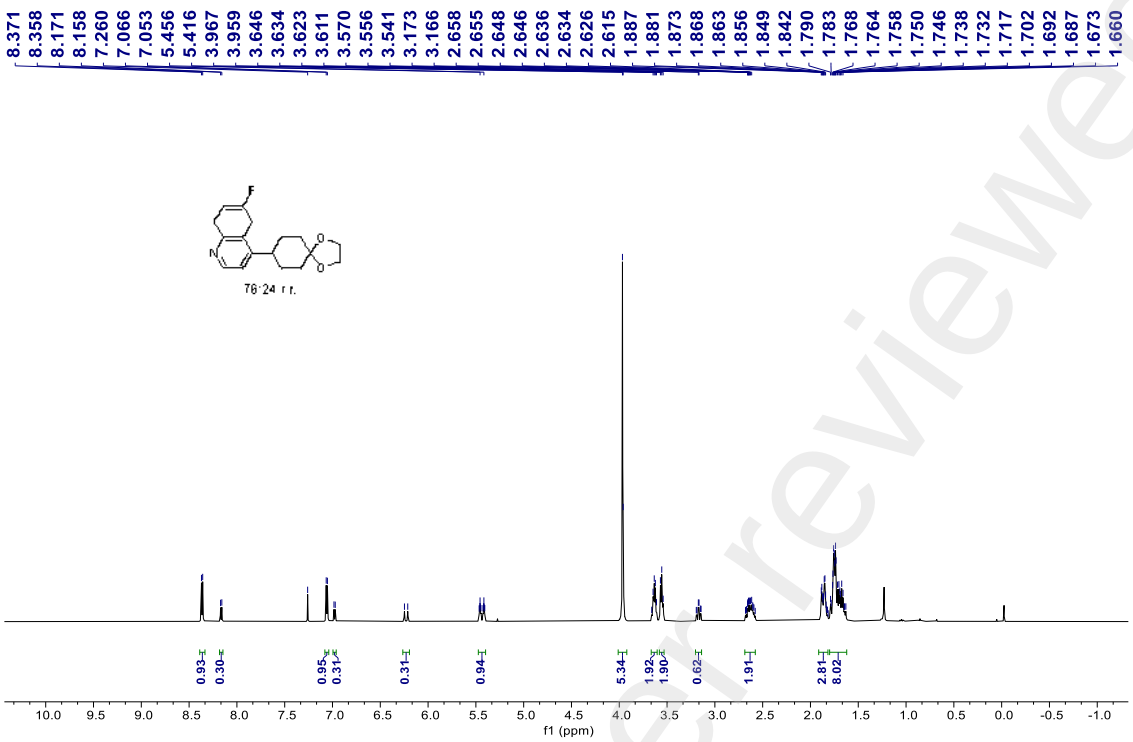

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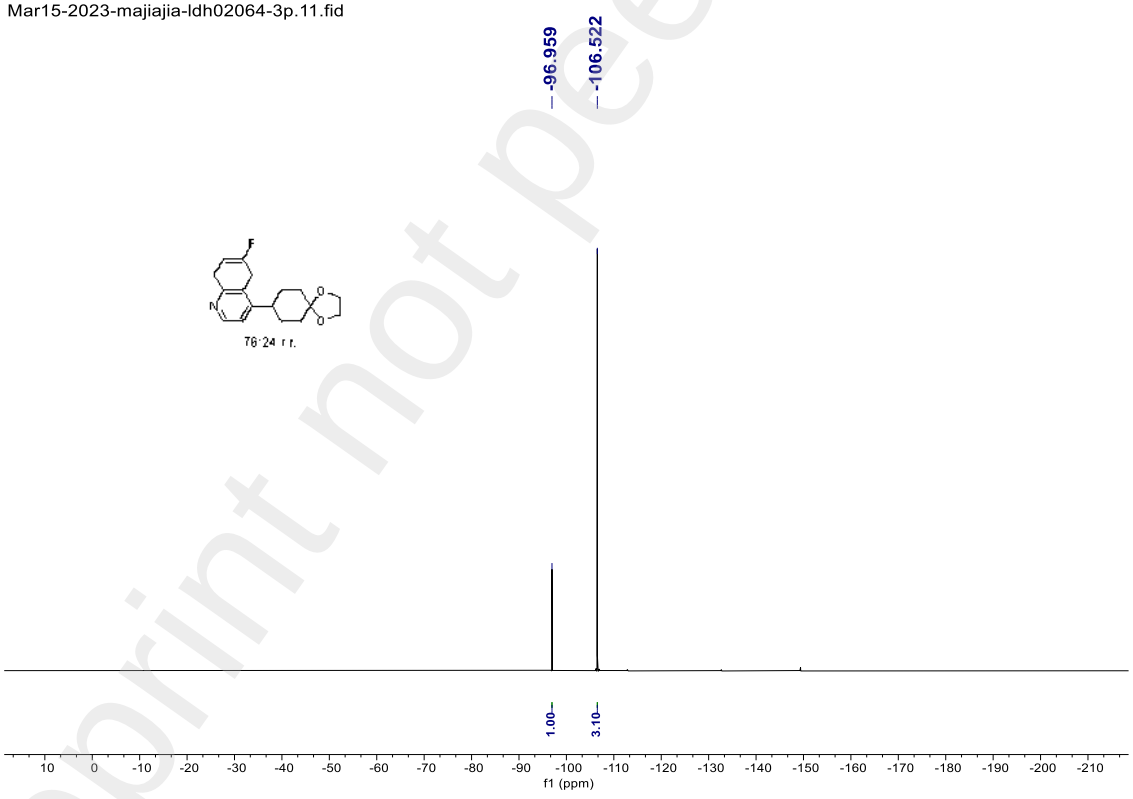
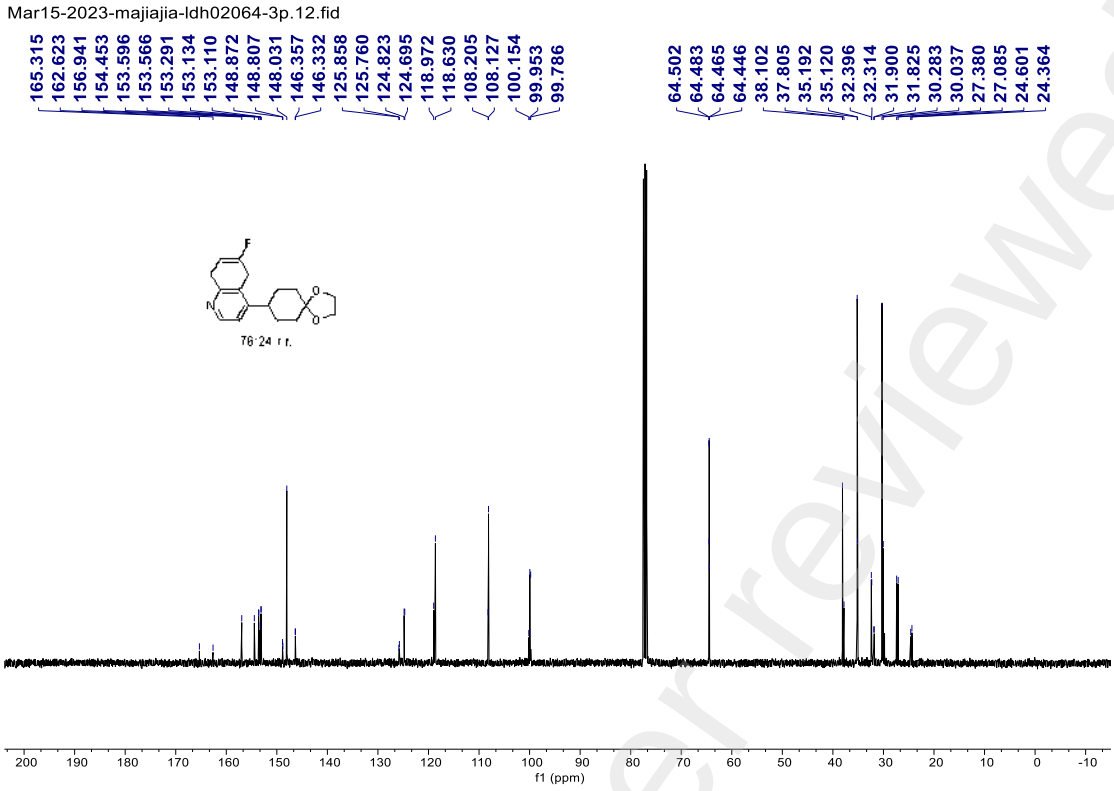
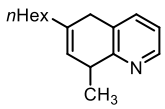






12, 84% yield

According to the general procedure, a mixture of **1h** (0.2 mmol, 45.5 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **12** as yellow oil (38.8 mg, 84% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:4

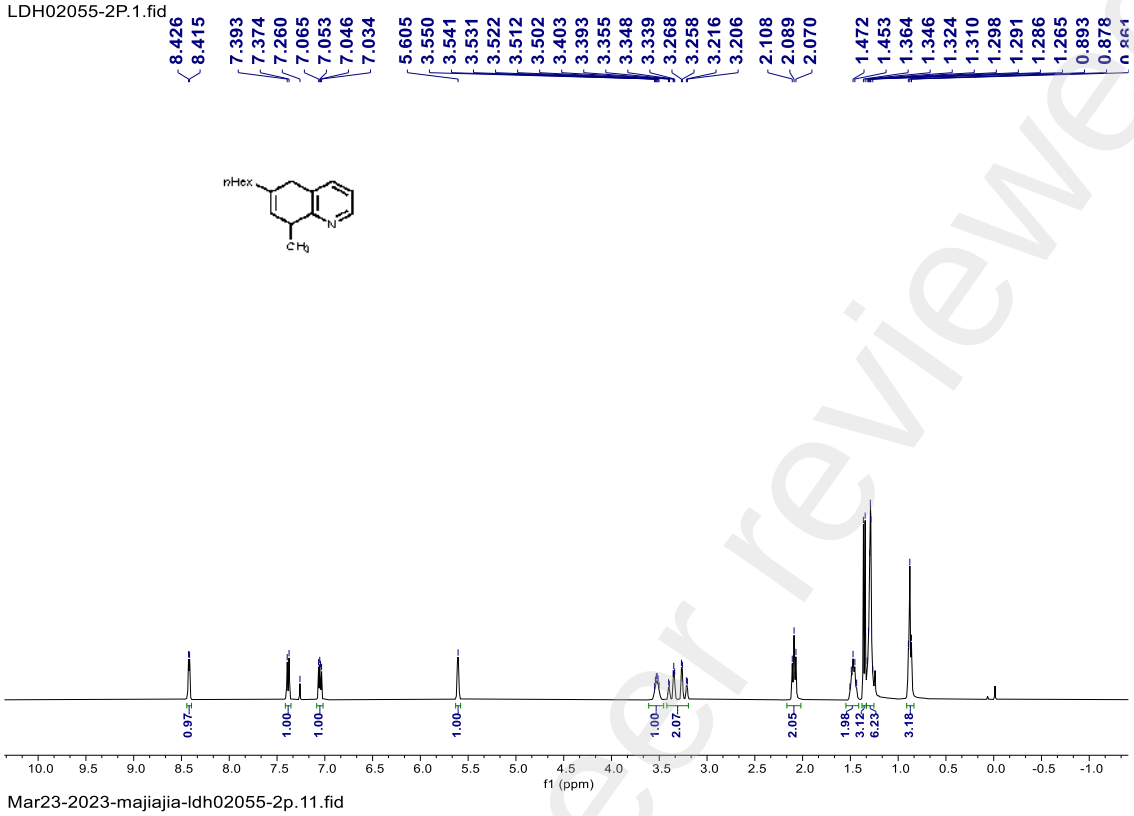
R_f (**12**) = 0.3 in EtOAc/petroleum ether = 1:5.

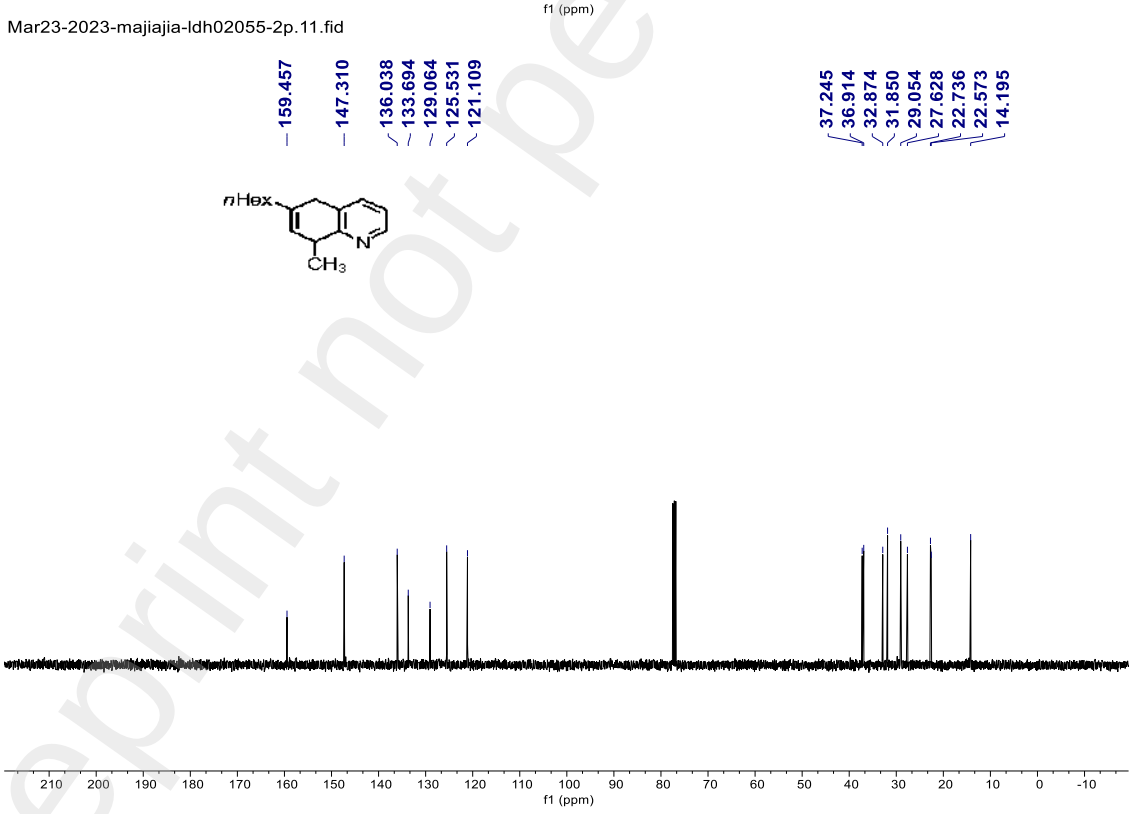
Analytical data of **12**:

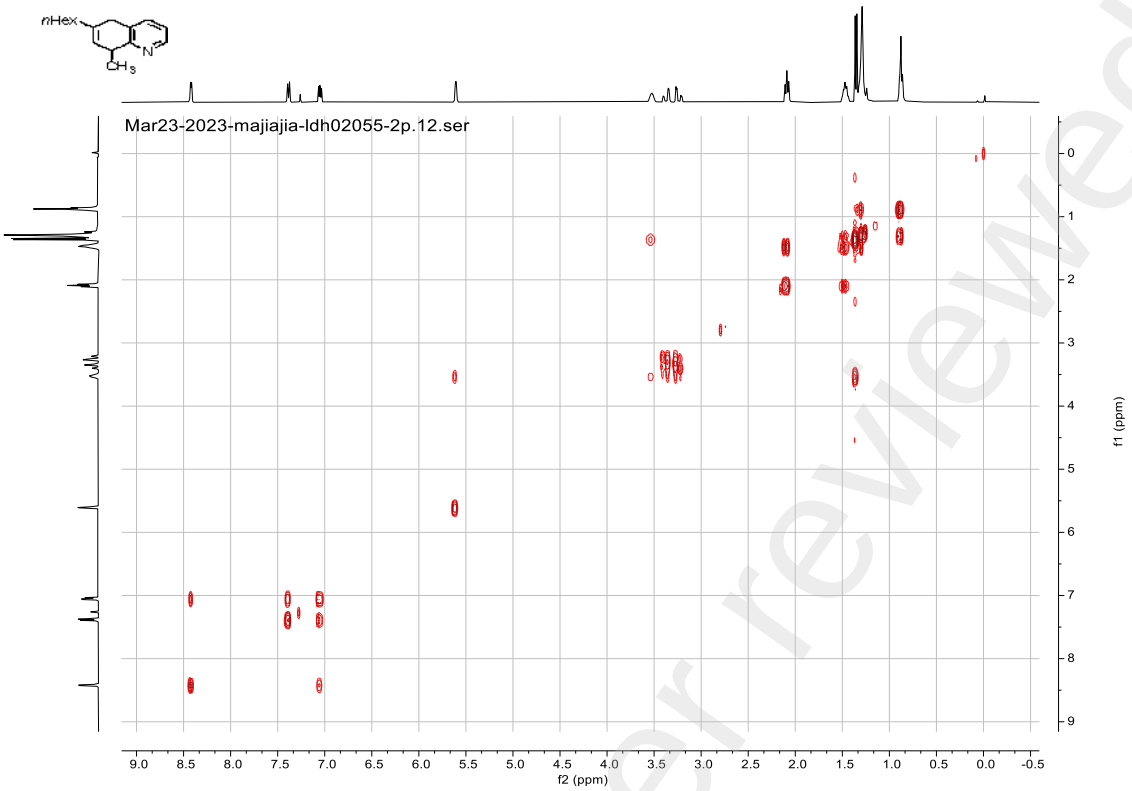
^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 4.4 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.26 (s, 1H), 7.05 (dd, *J* = 7.6, 4.8 Hz, 1H), 5.61 (br, 1H), 3.58 - 3.48 (m, 1H), 3.43 - 3.18 (m, 2H), 2.09 (t, *J* = 7.6 Hz, 2H), 1.53 -1.41 (m, 2H), 1.35 (d, *J* = 7.2 Hz, 3H), 1.35 - 1.24 (m, 6H), 0.91 - 0.84 (m, 3H).

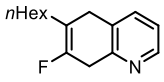
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 147.3, 136.0, 133.7, 129.1, 125.5, 121.1, 37.2, 36.9, 32.9, 31.8, 29.1, 27.6, 22.7, 22.6, 14.2.

HRMS (ESI, *m/z*) calcd for $C_{16}H_{24}NO^+$ $[M+H]^+$: 230.1907, found: 230.1903.









13, 31% yield

According to the general procedure, a mixture of **1i** (0.2 mmol, 46.3 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **13** as yellow oil (14.5 mg, 31% yield, > 95:5 r.r.).

Purification conditions: EtOAc/ CH_2Cl_2 = 1:80 to 1:40

R_f (**13**) = 0.45 in EtOAc/ CH_2Cl_2 = 1:40.

Analytical data of **13**:

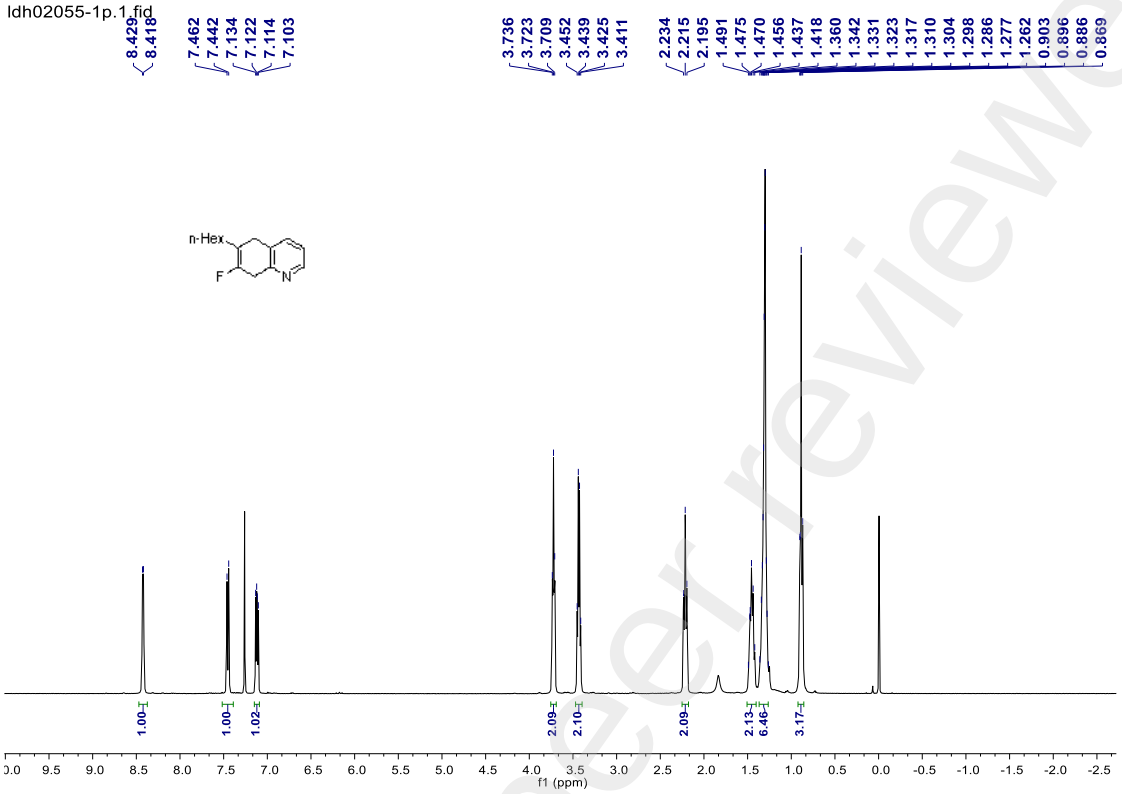
^1H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 4.4 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.12 (dd, *J* = 8.0, 4.8 Hz, 1H), 3.72 (t, *J* = 5.6 Hz, 2H), 3.43 (q, *J* = 5.6 Hz, 2H), 2.21 (t, *J* = 7.6 Hz, 2H), 1.51 - 1.40 (m, 2H), 1.38 - 1.24 (m, 6H), 0.93 - 0.85 (m, 3H).

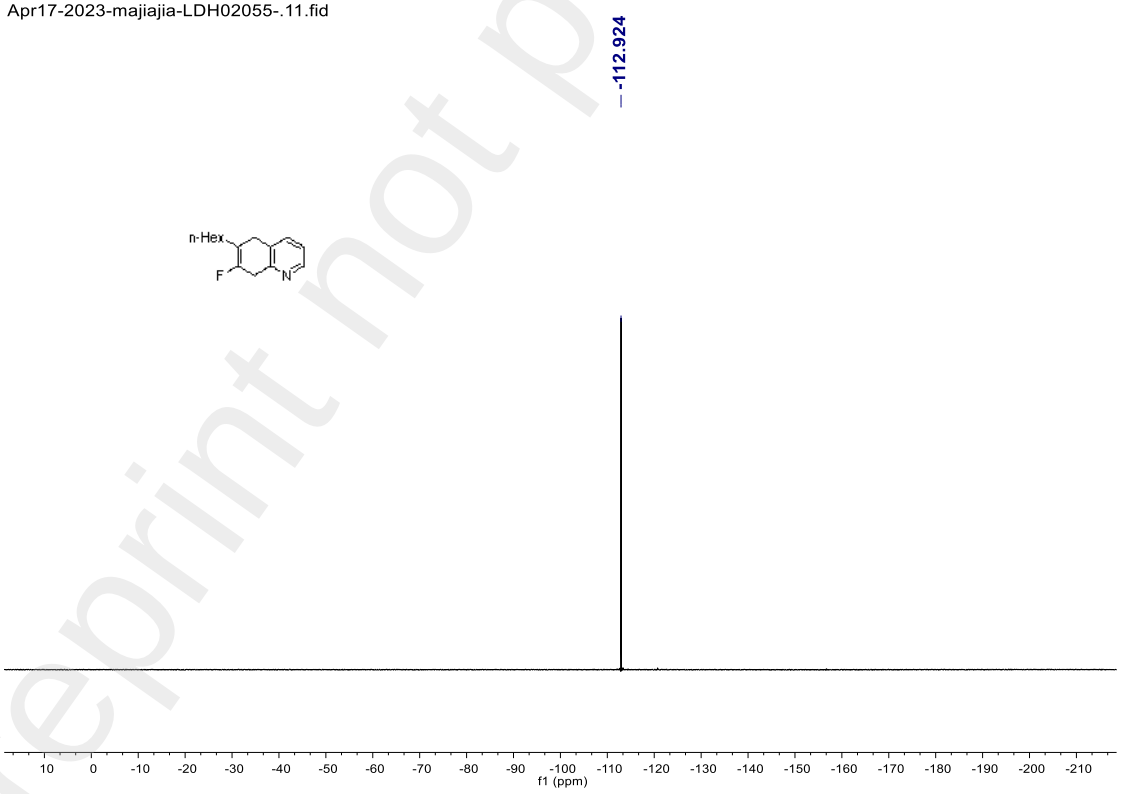
^{19}F NMR (376 MHz, $CDCl_3$) δ -112.92.

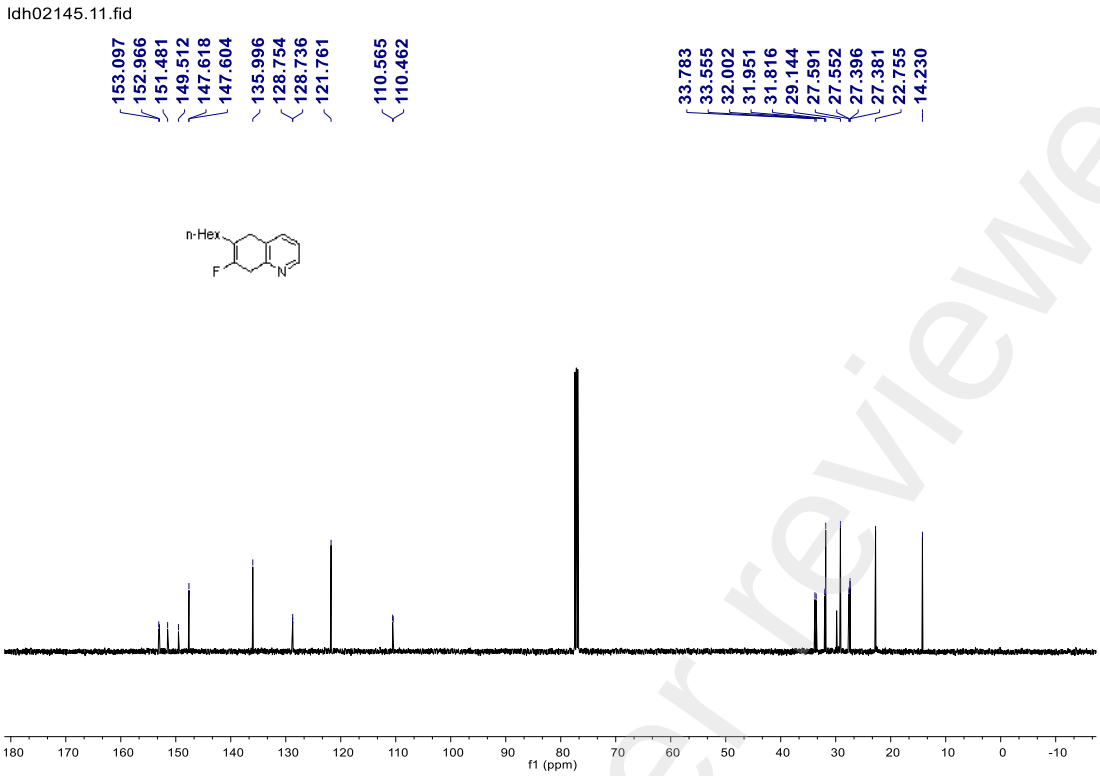
^{13}C NMR (126 MHz, $CDCl_3$) δ 153.0 (d, *J* = 16.5 Hz), 150.5 (d, *J* = 247.6 Hz), 147.6 (d, *J* = 1.8 Hz), 136.0, 128.7 (d, *J* = 2.2 Hz), 121.8, 110.5 (d, *J* = 13.0 Hz), 33.7 (d, *J* = 28.8 Hz), 32.0 (d, *J* = 6.3 Hz), 31.8, 29.1, 27.6 (d, *J* = 5.0 Hz), 27.4 (d, *J* = 1.9 Hz),

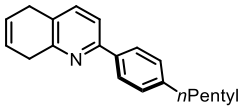
22.8, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{21}FN^+$ $[M+H]^+$: 234.1653, found: 234.1657.









14, 50% yield

According to the general procedure, a mixture of **1m** (0.2 mmol, 55.1 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.006 mmol, 3.0 mol%, 6.6 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (1.0 mmol, 5.0 equiv., 160 μL) and CH_3CN (1.0 mL, 2.0 M) were stirred for 6 h to give the desired product **14** as yellow oil (27.8 mg, 50% yield, >95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:5 to 1:2

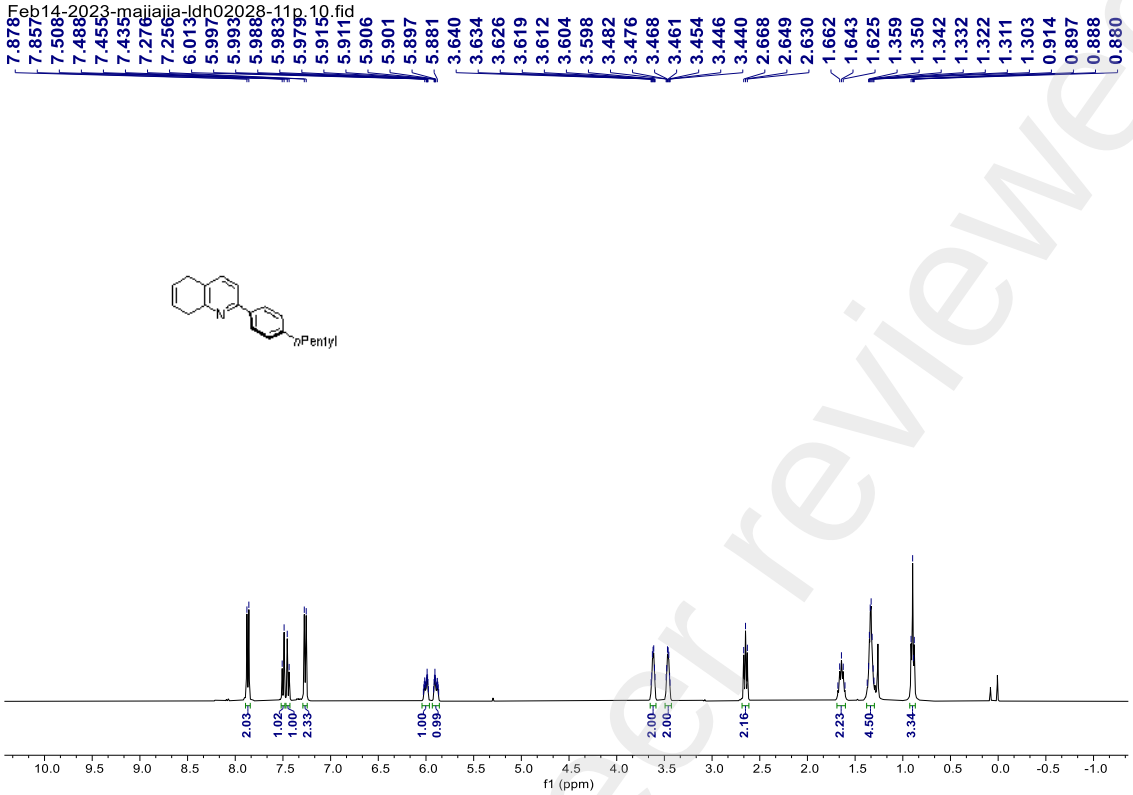
R_f (**14**) = 0.3 in EtOAc/petroleum ether = 1:2.

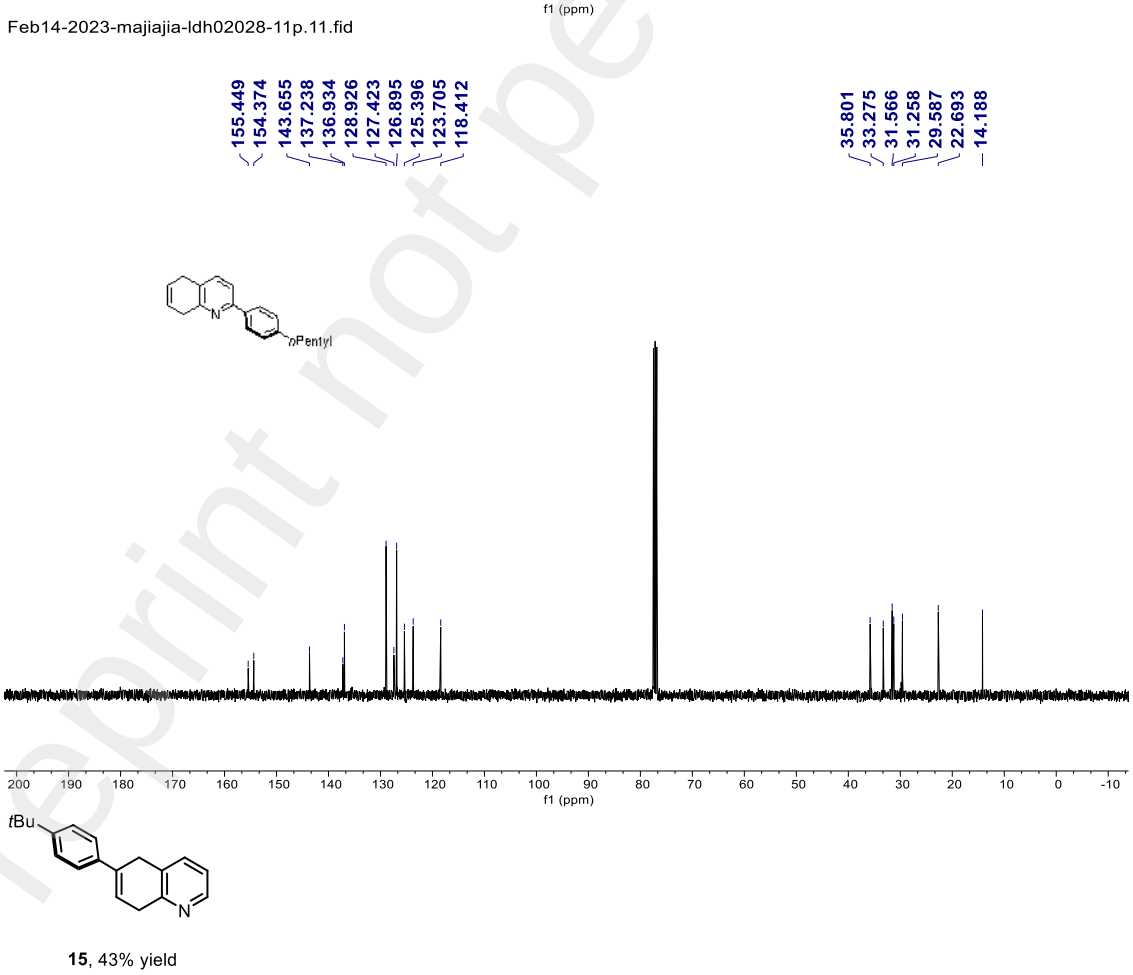
Analytical data of **14**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 6.05 - 5.95 (m, 1H), 5.94 - 5.84 (m, 1H), 3.66 - 3.58 (m, 2H), 3.50 - 3.42 (m, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 1.64 (p, *J* = 7.6 Hz, 2H), 1.38 - 1.30 (m, 4H) 0.92 - 0.87 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 155.4, 154.4, 143.7, 137.2, 136.9, 128.9, 127.4, 126.9, 125.4, 123.7, 118.4, 35.8, 33.3, 31.6, 31.3, 29.6, 22.7, 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{20}H_{24}N$ $[M+H]^+$: 278.1903, found: 278.1906.





15, 43% yield

According to the general procedure, a mixture of **1n** (0.2 mmol, 52.3 mg, 1.0 equiv.),

$Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.006 mmol, 3.0 mol%, 6.6 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 160 μL) and CH_3CN (1.0 mL, 1.0 M) were stirred for 6 h to give the desired product **15** as yellow oil (mg, 43% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:12 to 1:5

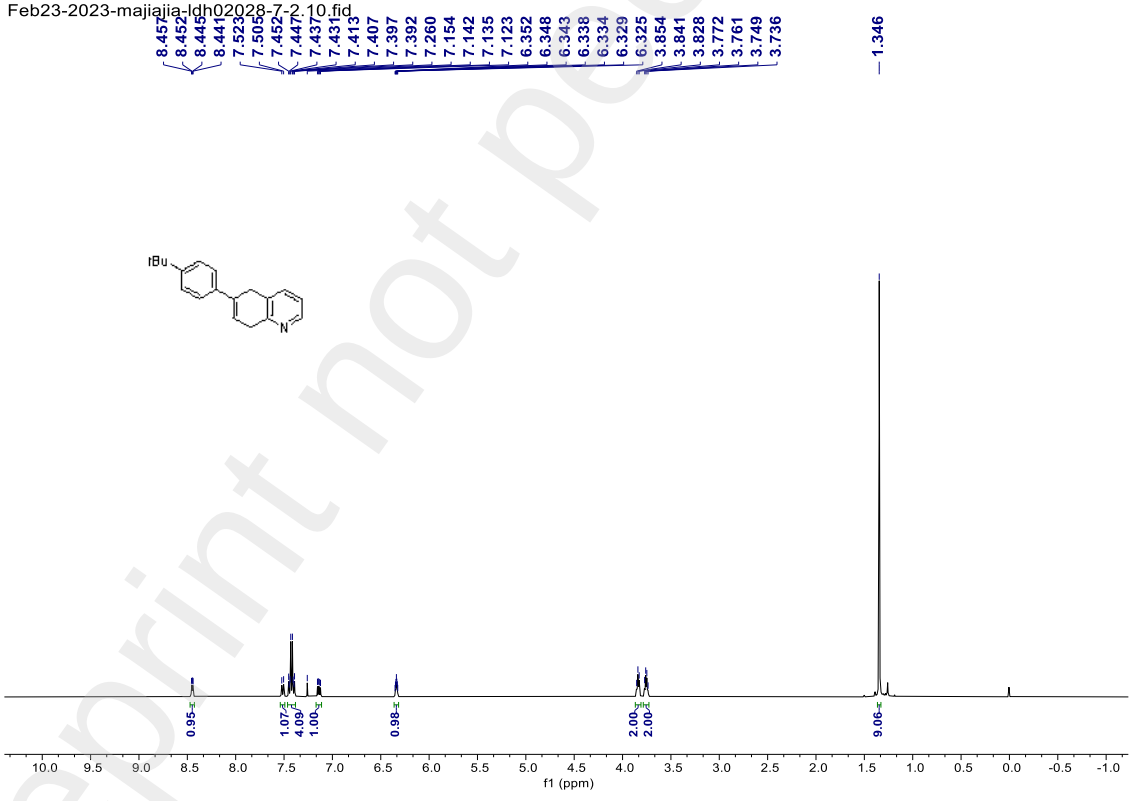
R_f (**15**) = 0.25 in EtOAc/petroleum ether = 1:6.

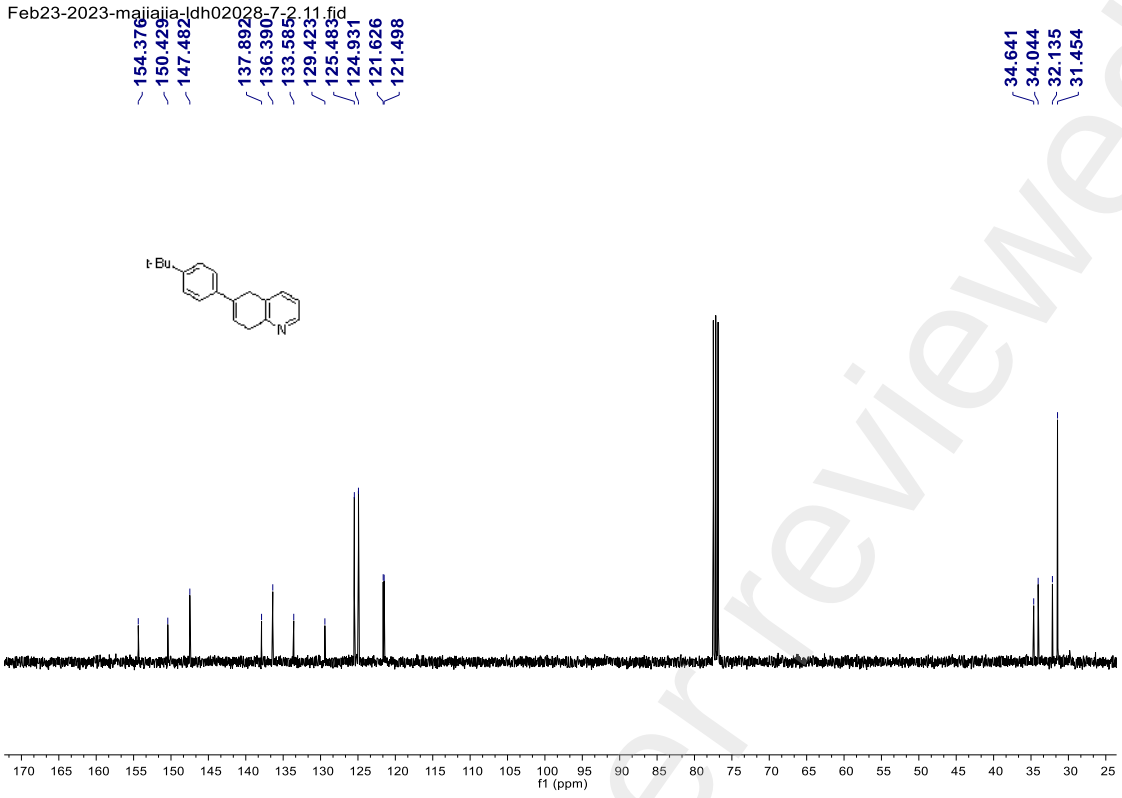
Analytical data of **15**:

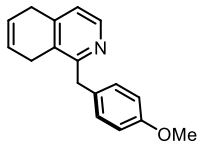
^1H NMR (400 MHz, $CDCl_3$) δ 8.45 (dd, *J* = 4.8, 2.0 Hz, 1H), 7.51 (d, *J* = 7.2Hz, 1H), 7.47 - 7.37 (m, 4H), 7.14 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.35 - 6.32 (m, 1H), 3.88 - 3.81 (m, 2H), 3.79 - 3.71 (m, 2H), 1.35 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.4, 150.4, 147.5, 137.9, 136.4, 133.6, 129.4, 125.5, 124.9, 121.6, 121.5, 34.6, 34.0, 32.1, 31.5.

HRMS (ESI, *m/z*) calcd for $C_{19}H_{22}NO^+$ $[M+H]^+$: 264.1747, found: 264.1751.







16, 54% yield, 92:8 r.r.

According to the general procedure, a mixture of **1-(4-methoxybenzyl)isoquinoline** (0.2 mmol, 49.8 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **16** as white solid (27.0 mg, 54% yield, 92:8 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:4

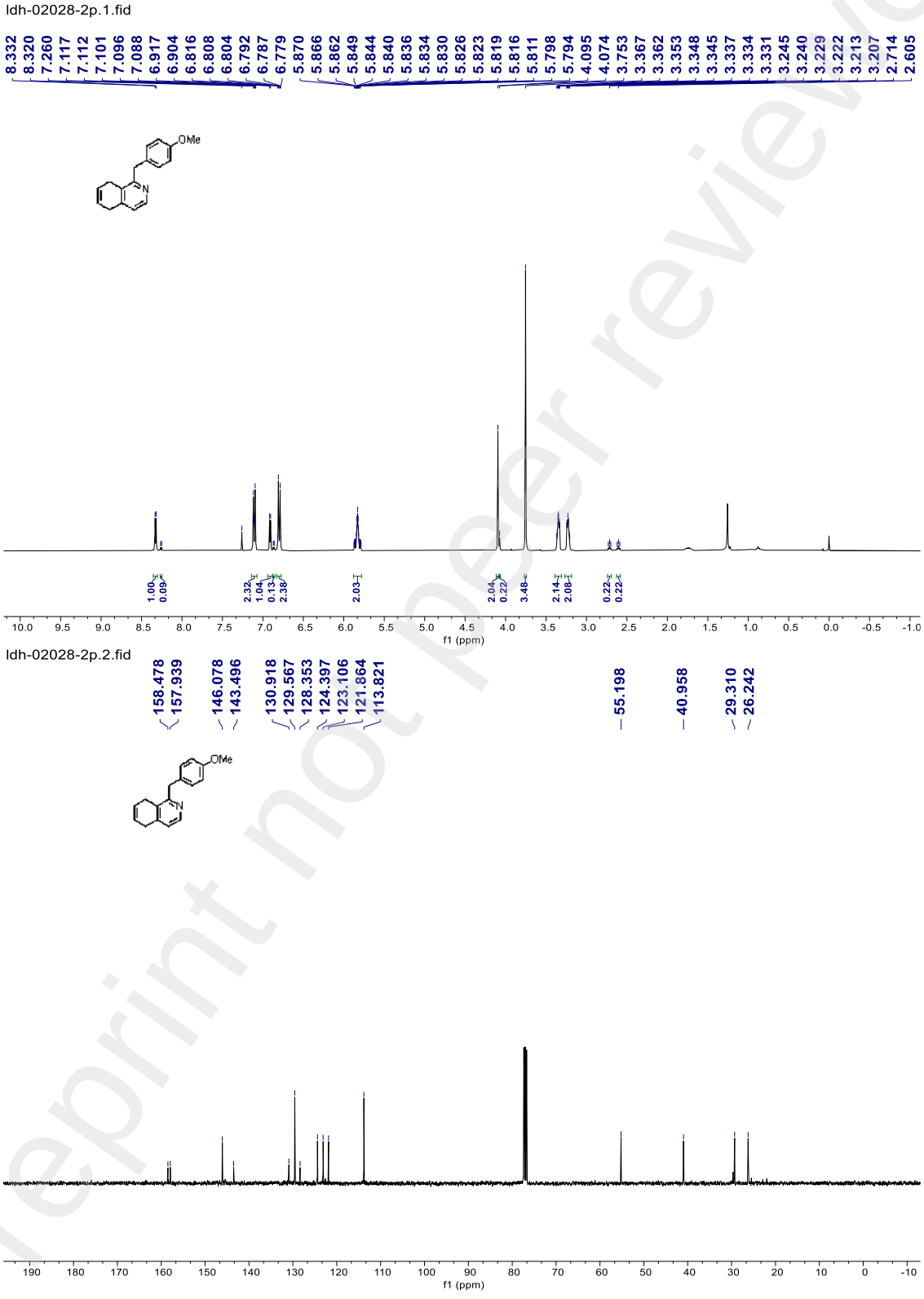
R_f (**16**) = 0.3 in EtOAc/petroleum ether = 1:3.

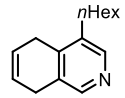
Analytical data of **16**:

^1H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.33 (d, *J* = 4.8 Hz, 1H), 8.26 (d, *J* = 4.8 Hz, 2H, minor), 7.14 - 7.07 (m, 2H, major; m, 2H, minor), 6.91 (d, *J* = 5.2 Hz, 1H), 6.87 (d, *J* = 5.2 Hz, 1H, minor), 6.84 - 6.76 (m, 2H, major; m, 2H, minor), 5.88 - 5.78 (m, 2H), 4.09 (s, 2H), 4.07 (s, 2H, minor), 3.75 (s, 3H, major; s, 3H, minor), 3.38 - 3.32 (m, 2H, major), 3.25 - 3.20 (m, 2H, major), 2.71 (t, *J* = 6.0 Hz, 2H, minor), 2.60 (t, *J* = 6.4 Hz, 2H, minor).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 157.9, 146.1, 143.5, 130.9, 129.6, 128.4, 124.4, 123.1, 121.9, 113.8, 55.2, 41.0, 29.3, 26.2.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{18}NO$ $[M+H]^+$: 252.1383, found: 252.1385.





17, 50% yield, 92:8 r.r.

According to the general procedure, a mixture of **1j** (0.2 mmol, 42.6 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **17** as colorless oil (21.5 mg, 50% yield, 92:8 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:3

R_f (**17**) = 0.3 in EtOAc/petroleum ether = 1:2.

Analytical data of **17**:

^{1}H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.20 (s, 1H), 8.18 (s, 1H), 8.13 (s, 1H, minor), 8.12 (s, 1H, minor), 5.98 - 5.92 (m, 1H), 5.91 - 5.86 (m, 1H), 3.41 - 3.33 (m, 2H), 3.33 - 3.25 (m, 2H), 2.73 (t, *J* = 6.0 Hz, 2H, minor), 2.67 (t, *J* = 6.0 Hz, 2H, minor), 2.59 - 2.50 (m, 2H, major; m, 2H, minor), 1.85 - 1.74 (m, 4H, minor), 1.60 - 1.50 (m, 2H, major), 1.41 - 1.26 (m, 6H, major; m, 6H, minor), 0.93 - 0.85 (m, 3H, major; m, 3H, minor).

^{13}C NMR (101 MHz, $CDCl_3$, mixture of regioisomers) δ 148.2 (minor), 147.7 (major), 147.4, 147.0 (minor), 141.1, 135.2, 129.6, 124.5, 123.6, 31.8, 30.2, 30.1, 30.0 (minor), 29.4, 27.0, 26.9 (minor), 26.2, 25.5 (minor), 22.7, 22.4 (minor), 14.2.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{22}N$ $[M+H]^+$: 216.1747, found: 216.1752.

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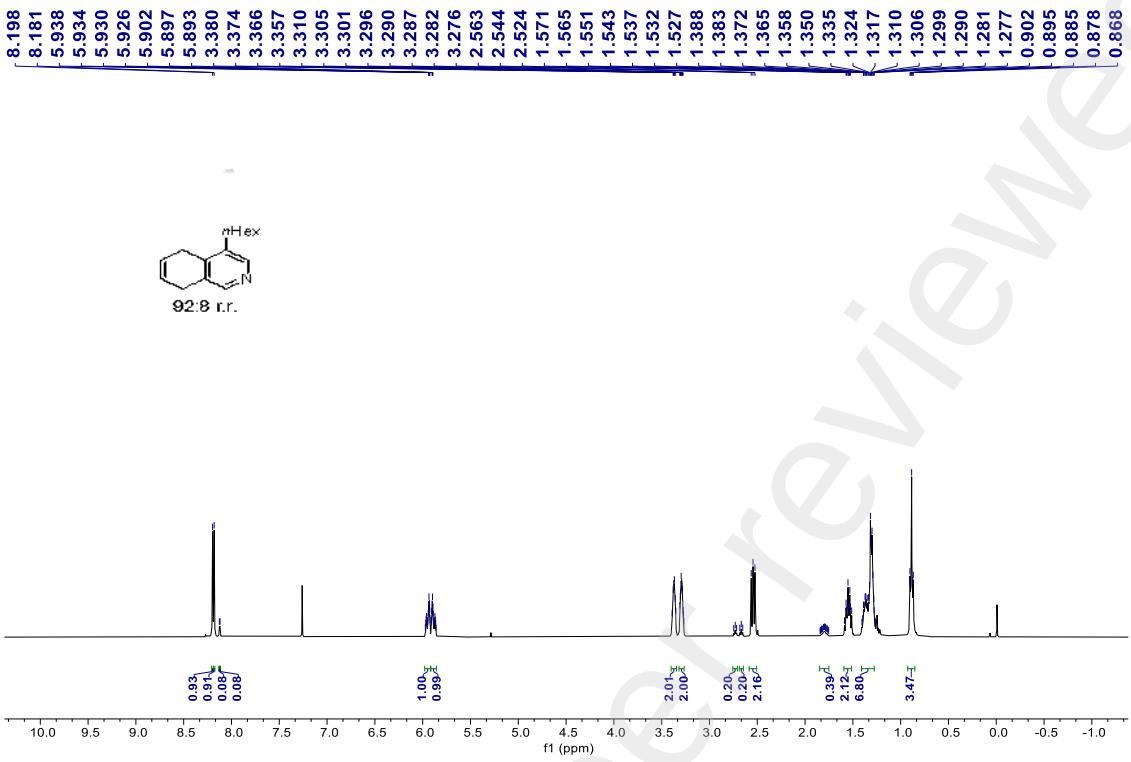

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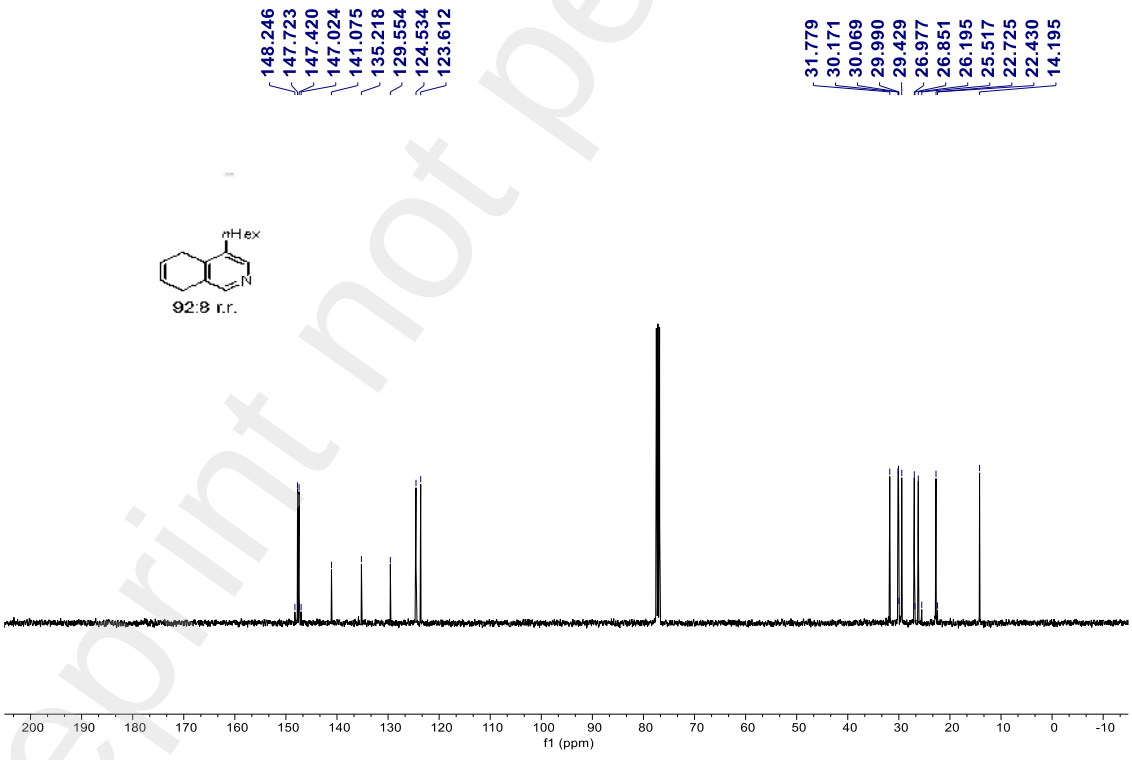
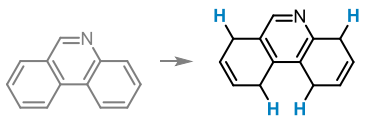




Phenanthridine **18**, 48% yield, 86:14 r.r.

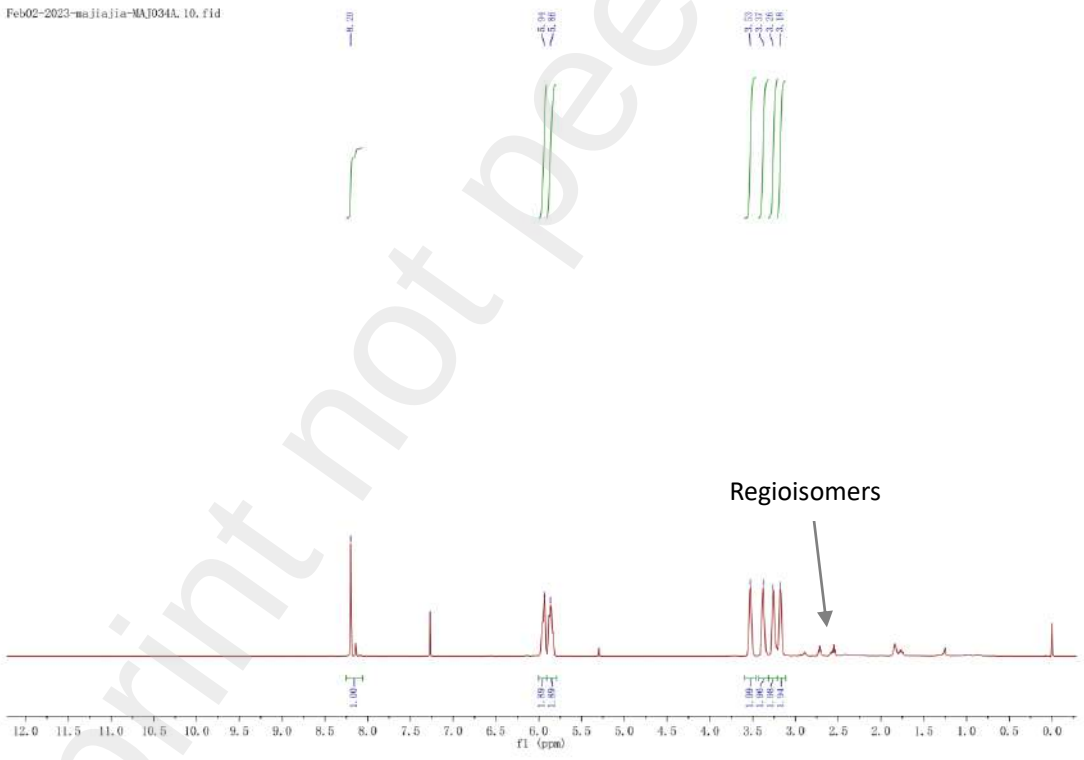
According to the general procedure, a mixture of phenanthridine (0.2 mmol, 35.8 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.004 mmol, 2.0 mol%, 4.4 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 5.0 equiv., 160 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 14 h to give the desired product **18** as pale yellow solid (17.1 mg, 48% yield, 86:14 r.r.).

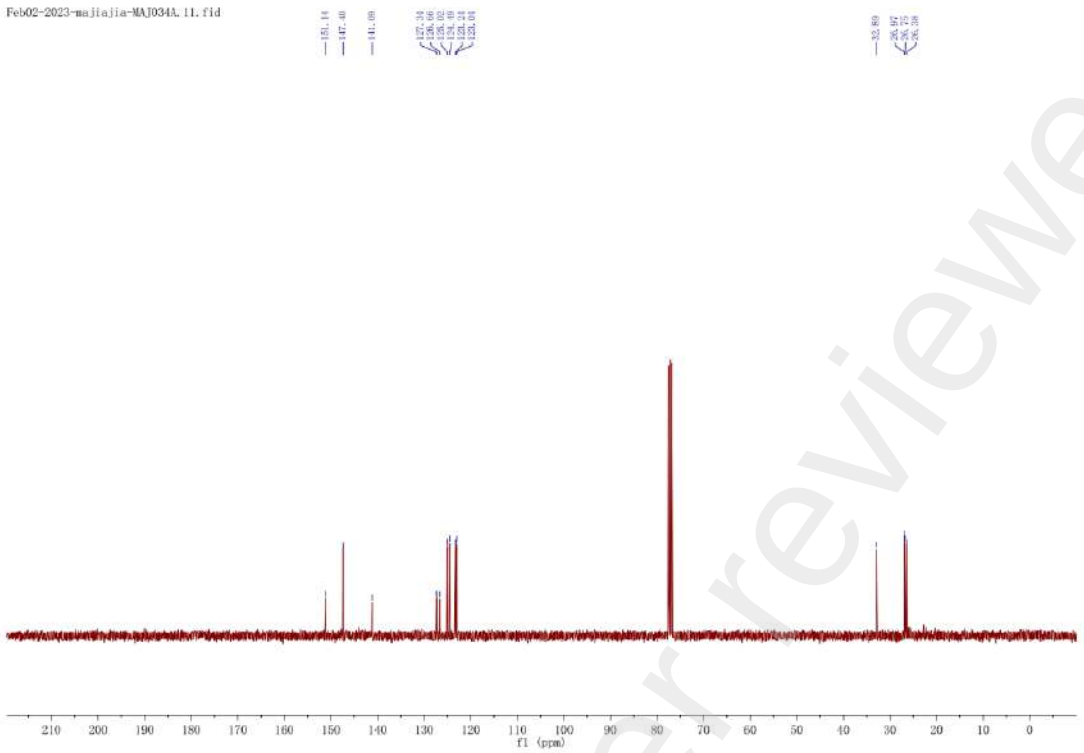
^1H NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 5.94 (m, 2H), 5.86 (m, 2H), 3.53 (m, 2H), 3.37 (m, 2H), 3.26 (m, 2H), 3.18 (m, 2H).

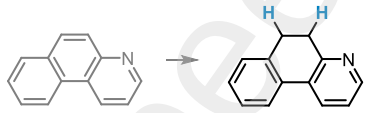
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.0, 138.0, 128.7, 128.5, 127.2, 62.9, 59.0, 51.1, 47.6, 41.1, 32.1, 30.5, 26.4, 26.12, 26.09, 12.0.

^{13}C NMR (100 MHz, $CDCl_3$) δ 151.14, 147.40, 141.09, 127.34, 126.66, 125.02, 124.49, 123.24, 123.04, 32.89, 26.97, 26.75, 26.38.

HRMS (ESI, *m*/*z*) calcd for $C_{13}H_{14}N^+$ $[M+H]^+$: 184.1126, found: 184.1120.







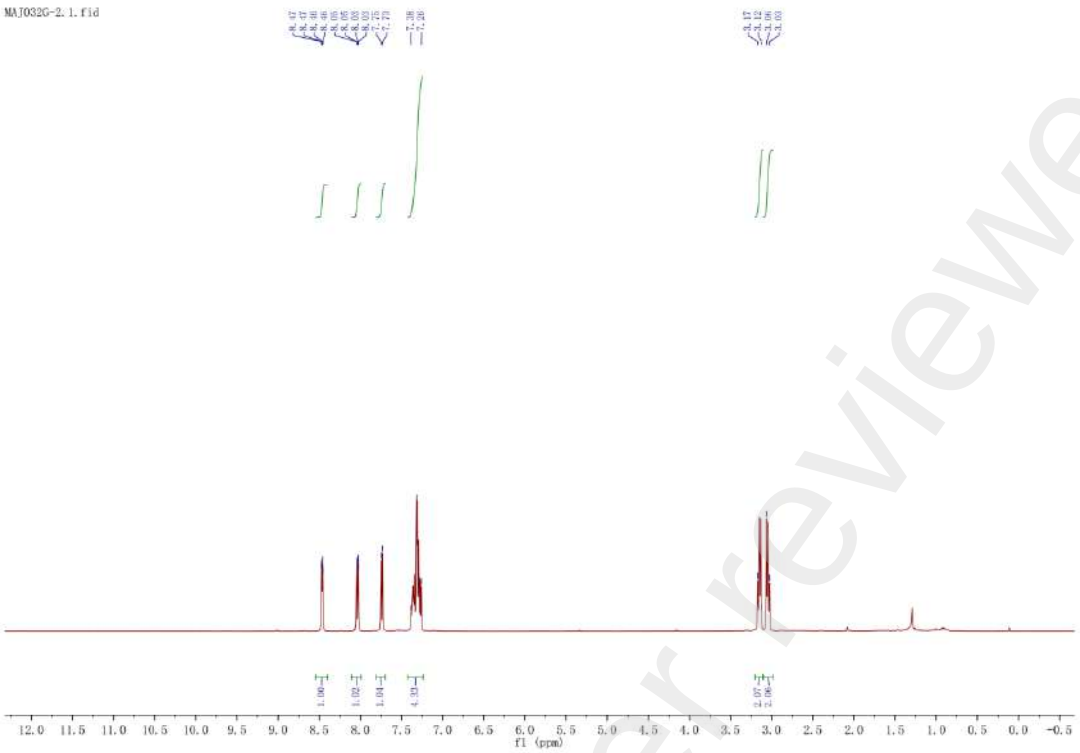
Benzo[*f*]quinoline **19**, 31% yield

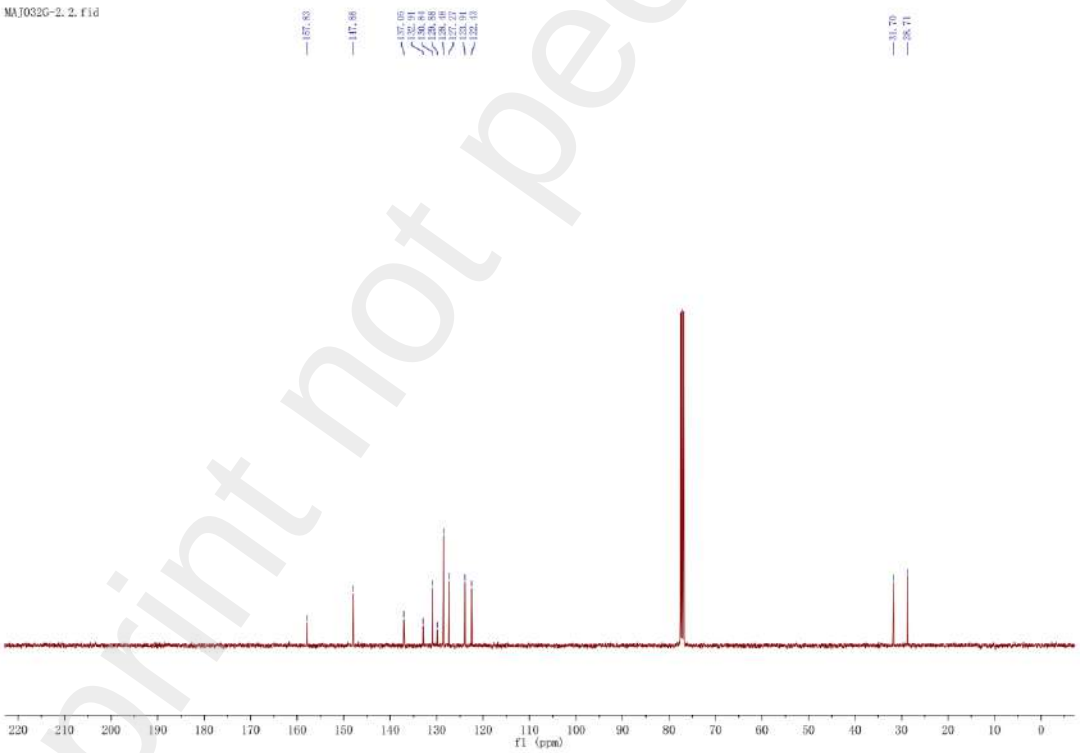
According to the general procedure, a mixture of benzo[*f*]quinoline (0.2 mmol, 36.0 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.004 mmol, 2.0 mol%, 4.4 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 14 h to give the desired product **19** as pale yellow solid (11.0 mg, 31% yield, 86:14 r.r.).

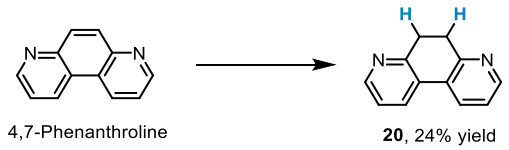
^1H NMR (400 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 4.9, 1.6 Hz, 1H), 8.04 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.38 - 7.26 (m, 4H), 3.17 - 3.12 (m, 2H), 3.06 - 3.03 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.83, 147.88, 137.05, 132.91, 130.84, 129.88, 128.48, 127.27, 123.91, 122.43, 31.70, 28.71.

HRMS (ESI, *m/z*) calcd for $C_{13}H_{12}N^+$ $[M+H]^+$: 182.0970, found: 182.0965.







4,7-Phenanthroline

20, 24% yield

According to the general procedure, a mixture of 4,7-Phenanthroline (0.2 mmol, 36.0 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.006 mmol, 3.0 mol%, 6.4 mg),

CF_3CO_2H (0.6 mmol, 3.0 equiv., 168 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 45 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 14 h to give the desired product **20** as brown solid (9.5 mg, 24% yield, >95:5 r.r.).

Purification conditions: Acetone/petroleum ether = 1:5 to 1:3

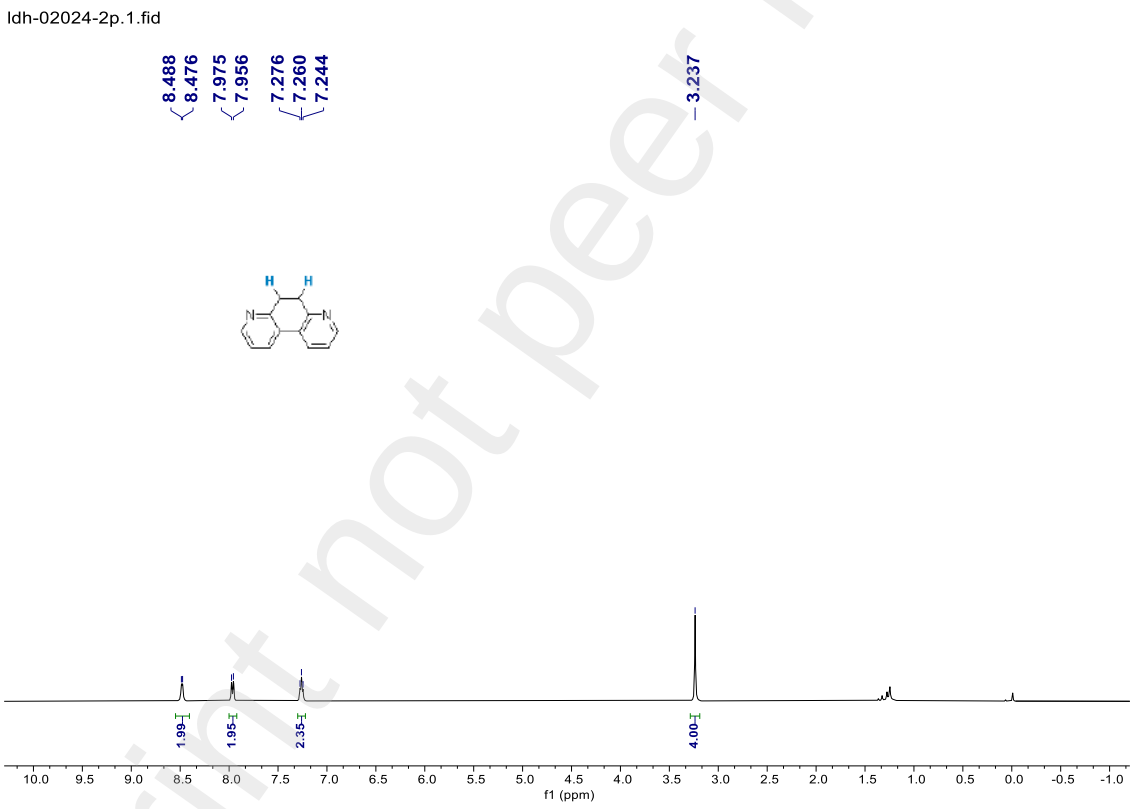
R_f (**20**) = 0.4 in Acetone/petroleum ether = 1:2.

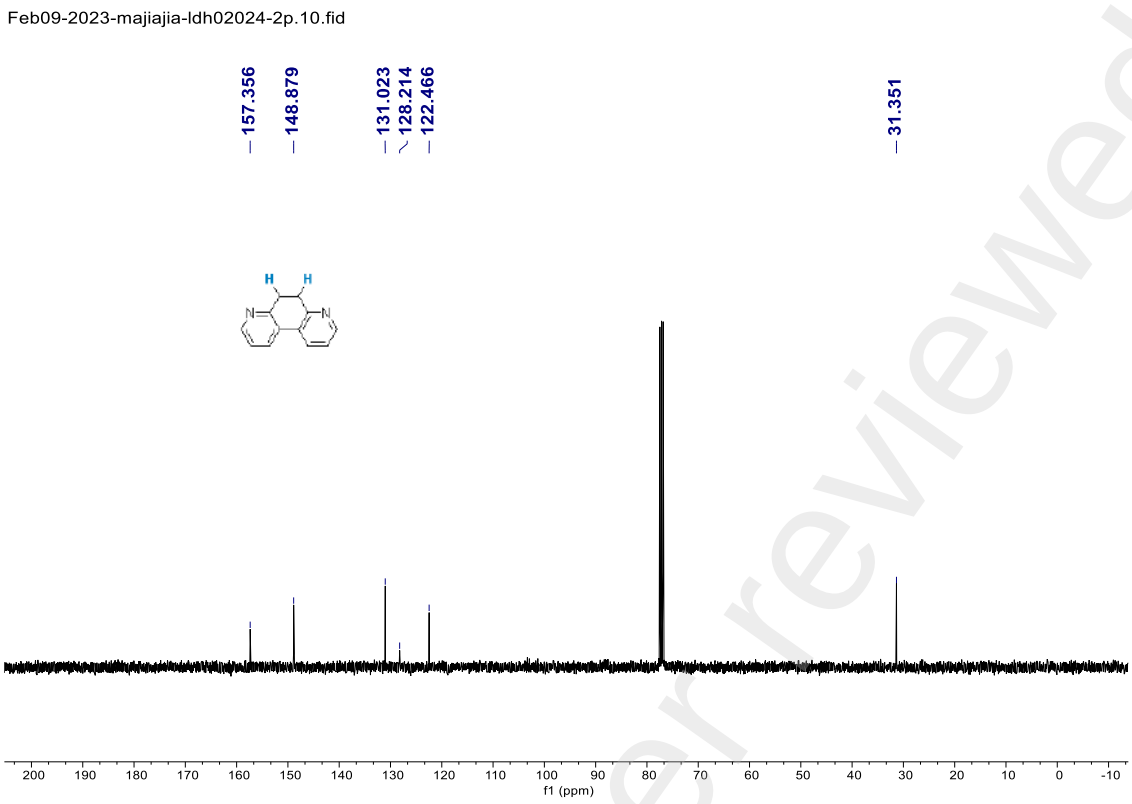
Analytical data of **20**:

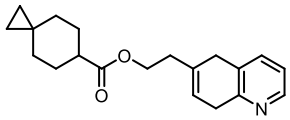
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 4.8 Hz, 2H), 7.97 (d, *J* = 7.6 Hz, 2H), 7.26 (t, *J* = 6.4 Hz, 2H), 3.24 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.4, 148.9, 131.0, 128.2, 122.5, 31.4.

HRMS (ESI, *m*/*z*) calcd for $C_{12}H_{11}N_2$ $[M+H]^+$: 183.0917, found: 183.0916.







21, 62% yield

According to the general procedure, a mixture of **1s** (0.2 mmol, 61.9 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **21** as yellow solid (38.6 mg, 62% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:3

R_f (**21**) = 0.3 in EtOAc/petroleum ether = 1:2.

Analytical data of **21**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 4.8 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.07 (dd, *J* = 8.0 4.8 Hz, 1H), 5.72 (br, 1H), 4.23 (t, *J* = 6.8 Hz, 2H), 3.56 - 3.48 (m, 2H), 3.44 - 3.35 (m, 2H), 2.43 (t, *J* = 6.8 Hz, 2H), 2.34 - 2.25 (m, 1H), 1.87 - 1.80 (m, 2H), 1.67 - 1.52 (m, 4H), 0.99 - 0.91 (m, 2H), 0.28 - 0.14 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 176.1, 154.5, 147.4, 136.0, 131.0, 129.0, 121.6, 121.4, 62.2, 42.9, 36.2, 34.4, 33.5, 32.9, 28.2, 18.4, 12.3, 11.9.

HRMS (ESI, *m*/*z*) calcd for $C_{20}H_{26}NO_2$ $[M+H]^+$: 312.1958, found: 312.1956.

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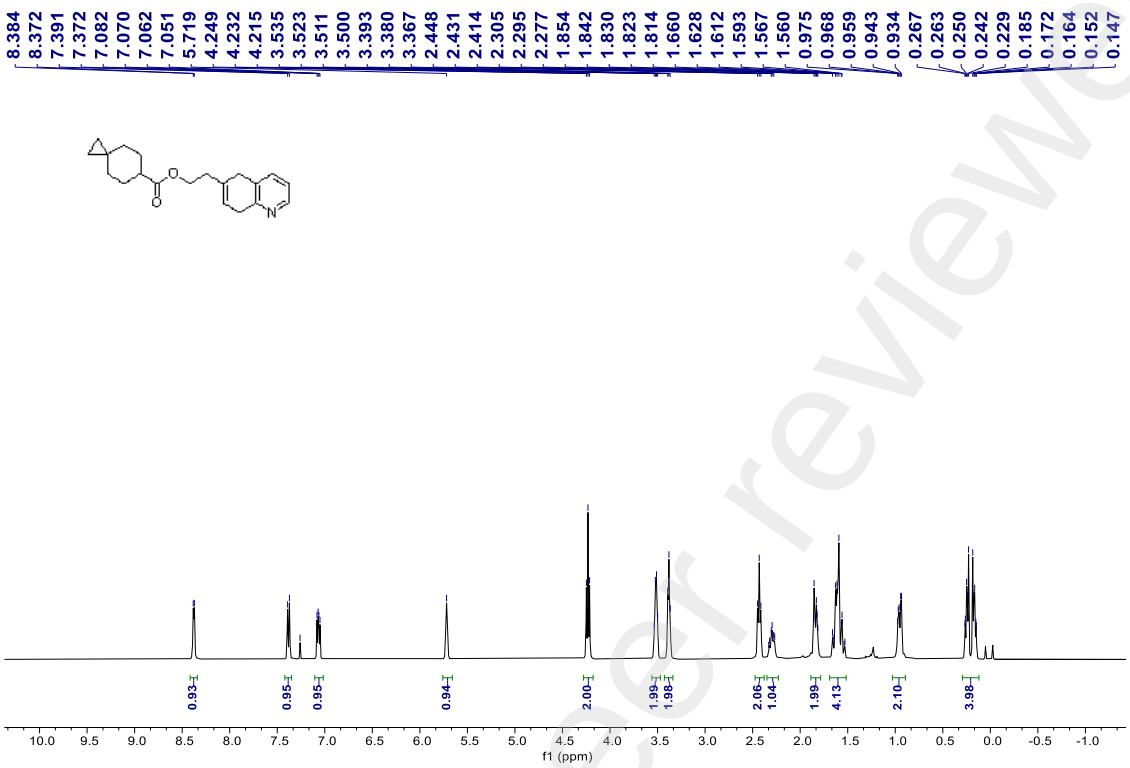

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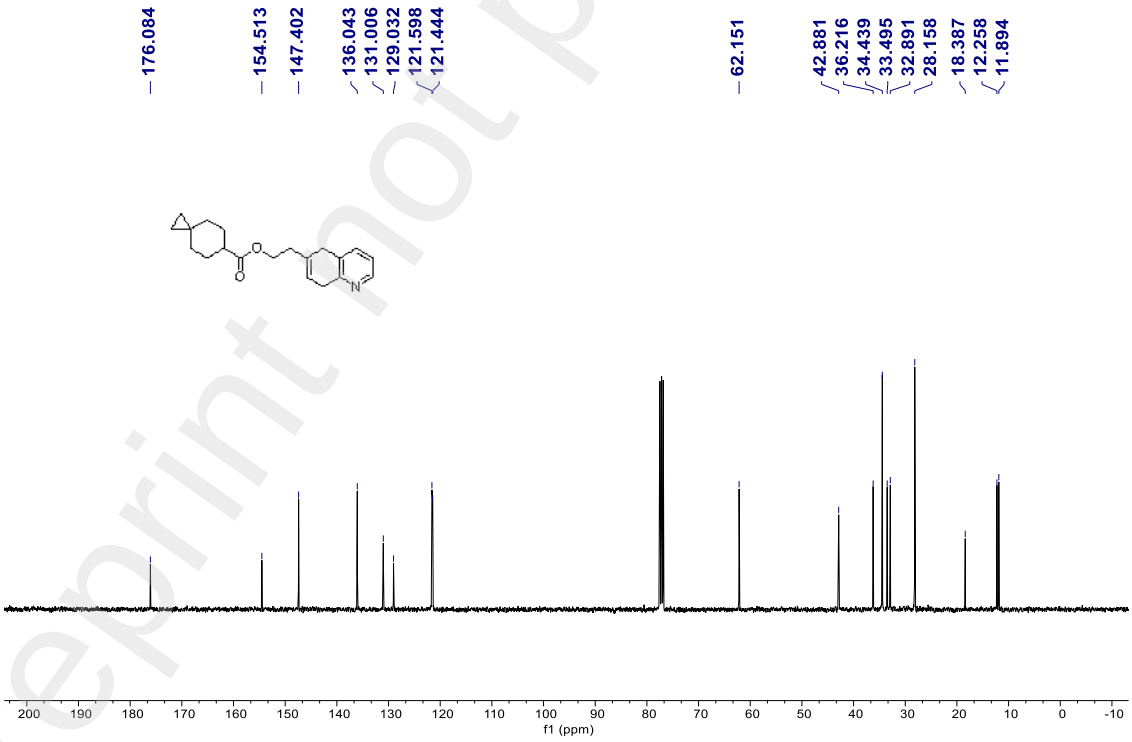
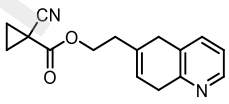




22, 76% yield

According to the general procedure, a mixture of **1t** (0.2 mmol, 53.2 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **22** as white solid (40.8 mg, 76% yield, 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:2

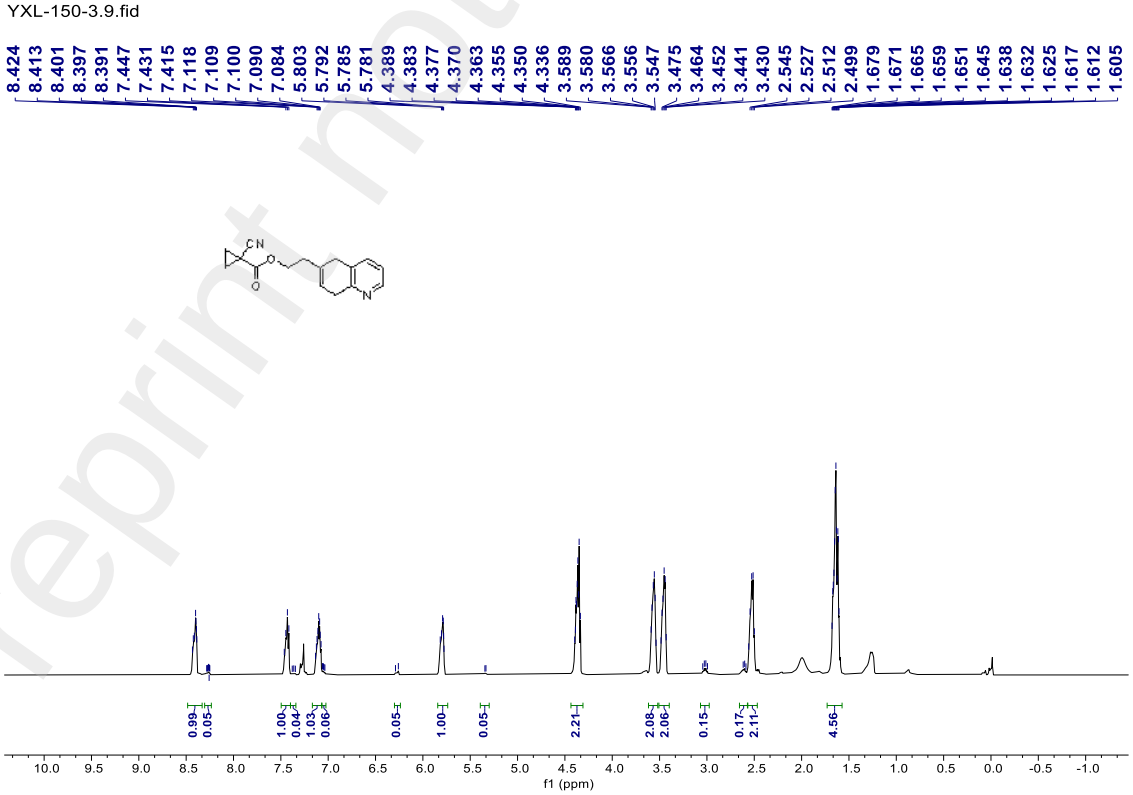
R_f (**22**) = 0.4 in EtOAc/petroleum ether = 1:2.

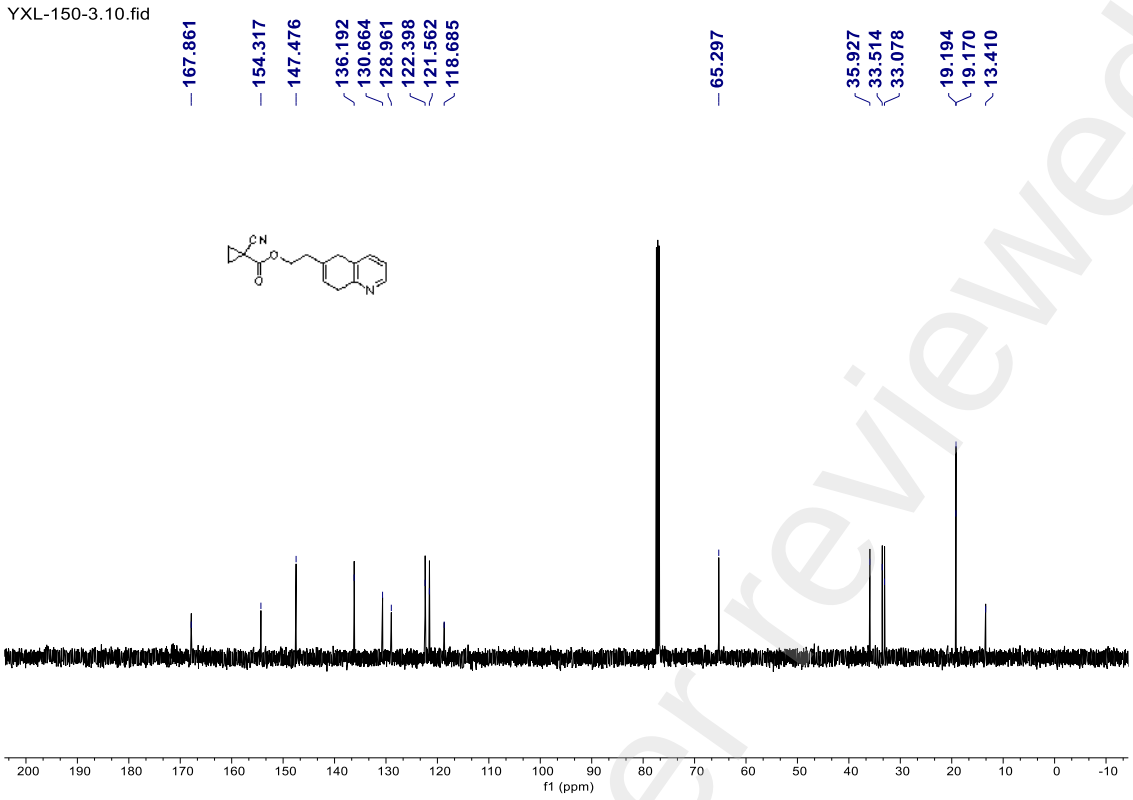
Analytical data of **22**:

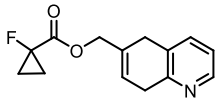
^{1}H NMR (500 MHz, $CDCl_3$, mixture of regioisomers) δ 8.47 - 8.36 (m, 1H), 8.30 - 8.23 (m, 1H, minor), 7.49 - 7.40 (m, 1H), 7.40 - 7.34 (m, 1H, minor), 7.15 - 7.06 (m, 1H), 7.06 - 7.03 (m, 1H, minor), 6.30 - 6.25 (m, 1H, minor), 5.84 - 5.75 (m, 1H), 5.39 - 5.32 (m, 1H, minor), 4.42 - 4.32 (m, 2H), 3.61 - 3.53 (m, 2H), 3.50 - 3.41 (m, 2H), 3.06 - 2.98 (m, 3H, minor), 2.65 - 2.58 (m, 2H), 2.57 - 2.49 (m, 2H), 1.72 - 1.58 (m, 4H, major; m, 4H, minor).

^{13}C NMR (126 MHz, CH_2Cl_2) δ 167.9, 154.3, 147.5, 136.2, 130.7, 129.0, 122.4, 121.6, 118.7, 65.3, 35.9, 33.5, 33.1, 19.2, 19.2, 13.4.

HRMS (ESI, *m/z*) calcd for $C_{16}H_{17}N_2O_2^+$ $[M+H]^+$: 269.1290, found: 269.1287.







23, 47% yield, 94:6 r.r.

According to the general procedure, a mixture of **1u** (0.2 mmol, 49.0 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **23** as colorless oil(23.2 mg, 47% yield, 94:6 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:6 to 1:2

R_f (**23**) = 0.3 in EtOAc/petroleum ether = 1:2.

Analytical data of **23**

^{1}H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.44 - 8.40 (m, 1H), 8.38 - 8.35 (m, 1H, minor), 7.43 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H, minor), 7.14 - 7.09 (m, 1H), 7.06 - 7.02 (m, 1H, minor), 6.04 (br, 1H), 4.75 (s, 2H), 4.24 - 4.20 (m, 2H, minor), 3.72 - 3.56 (m, 2H), 3.51 - 3.37 (m, 2H), 1.44 - 1.34 (m, 4H, major; m, 4H, minor).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.6 (d, *J* = 23.4 Hz), 153.6, 147.4, 136.5, 129.3, 128.4, 125.0, 121.7, 74.8 (d, *J* = 229.1 Hz), 68.8, 33.0, 30.4, 14.9, 14.8.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{15}FNO_2$ $[M+H]^+$: 248.1084, found: 248.1081

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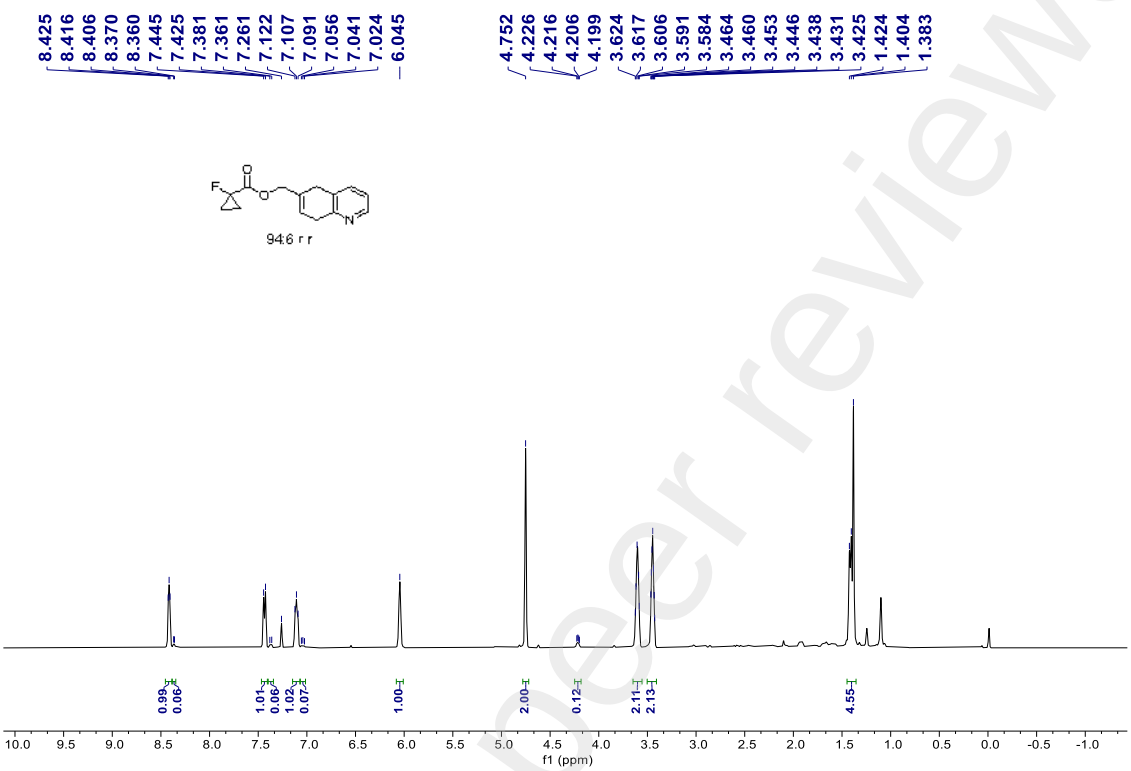

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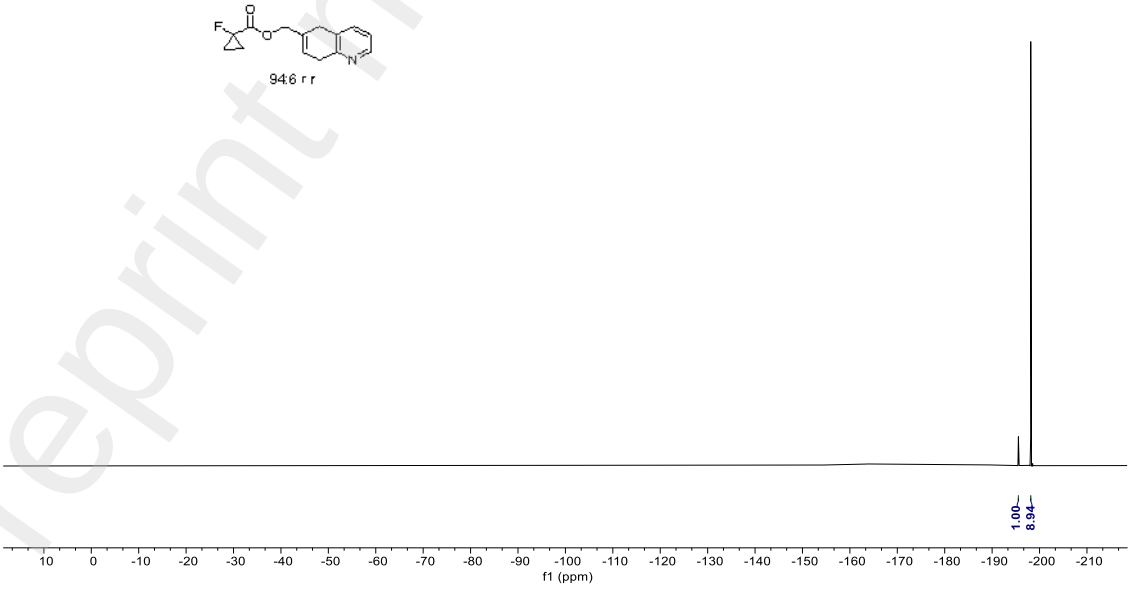
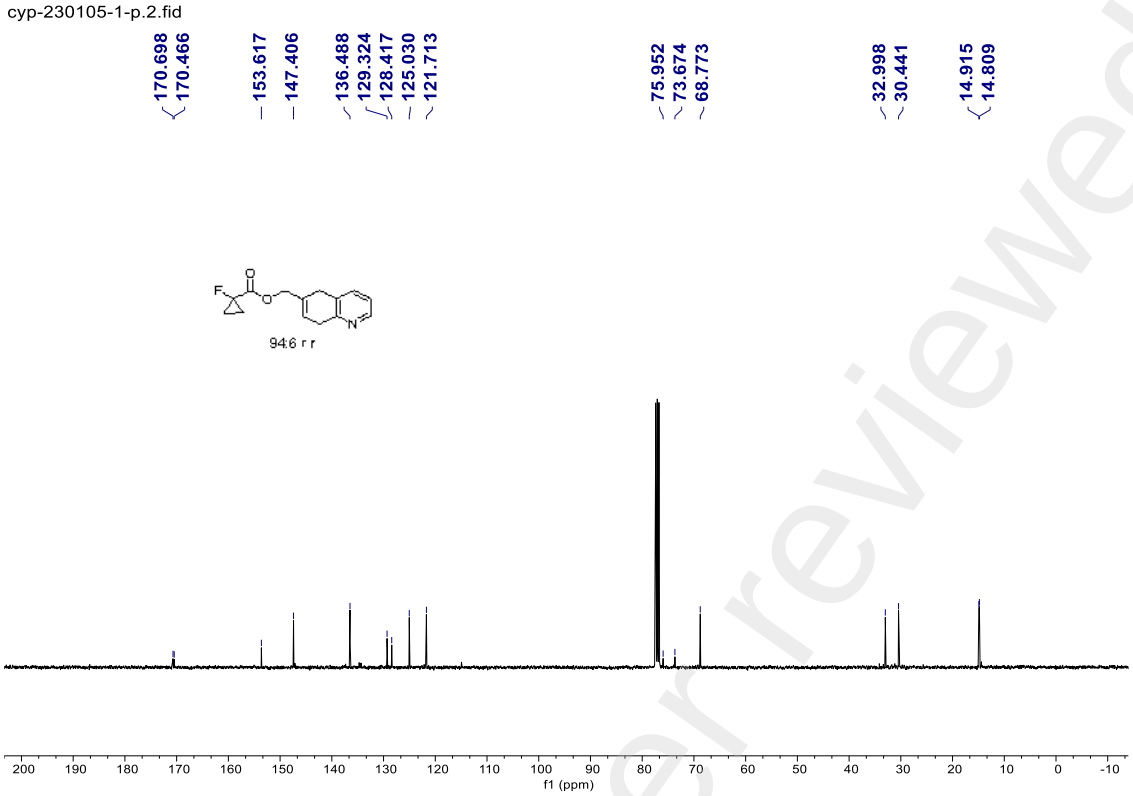
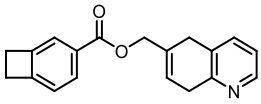






24, 45% yield, 95:5 r.r.

According to the general procedure, a mixture of **1v** (0.2 mmol, 57.8 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **24** a white solid (26.3 mg, 45% yield, 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:5 to 1:2

R_f (**24**) = 0.3 in EtOAc/petroleum ether = 1:2.

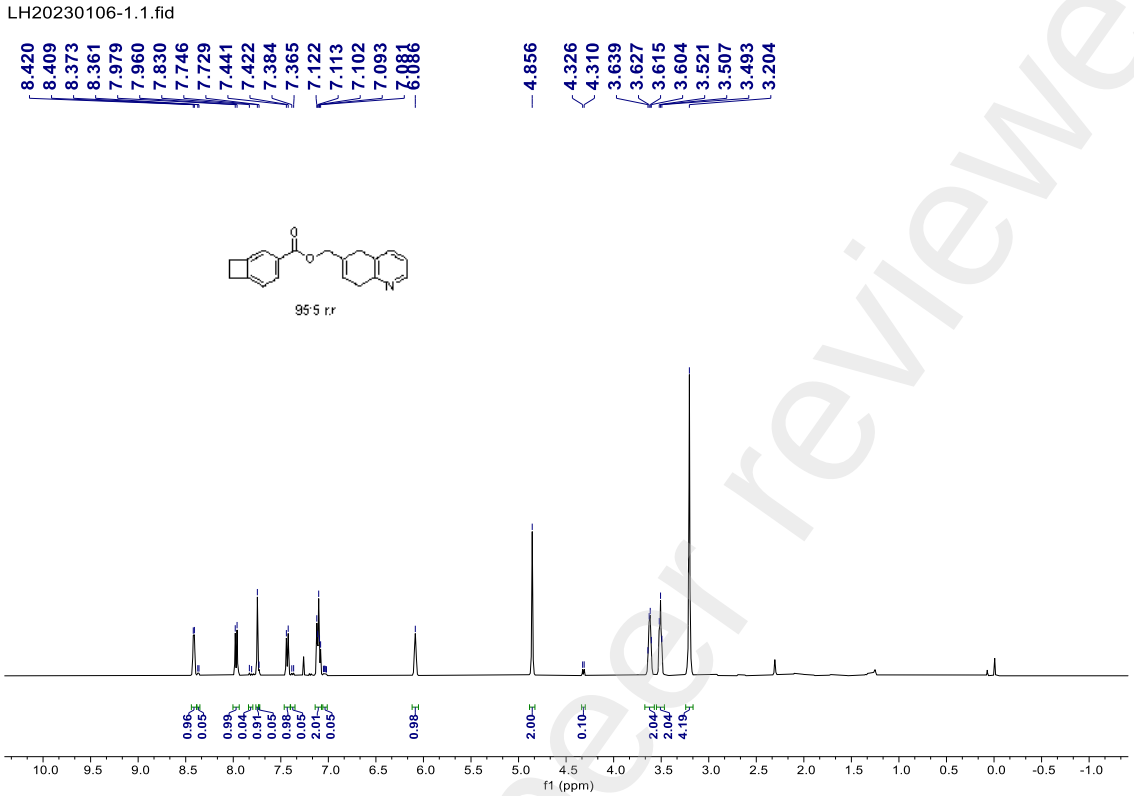
Analytical data of **24**:

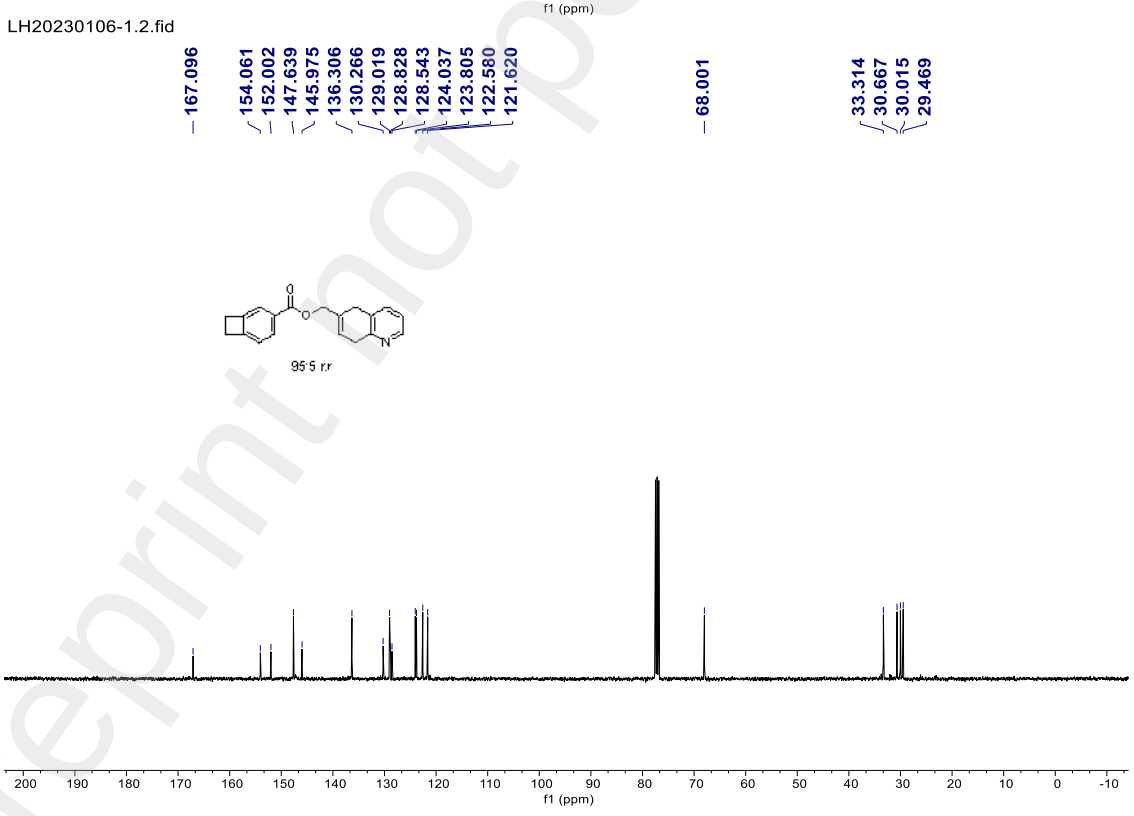
^{1}H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.41 (d, *J* = 4.4 Hz, 1H), 8.37 (d, *J* = 4.8 Hz, 1H, minor), 7.97 (d, *J* = 7.6 Hz, 1H), 7.82 (d, *J* = 9.2 Hz, 1H, minor), 7.75 (s, 1H), 7.73 (s, 1H, minor), 7.43 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 7.6 Hz, 1H, minor), 7.13 - 7.07 (m, 2H), 7.06 - 7.01 (m, 1H, minor), 6.09 (br, 1H), 4.86 (s, 2H), 4.32 (d, *J* = 6.4 Hz, 2H, minor), 3.66 - 3.57 (m, 2H), 3.55 - 3.47 (m, 2H), 3.20 (s, 4H).

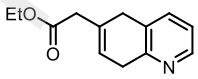
^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 154.1, 152.0, 147.6, 146.0, 136.3, 130.3, 129.0,

128.8, 128.5, 124.0, 123.8, 122.6, 121.6, 68.0, 33.3, 30.7, 30.0, 29.5.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{18}NO_2$ $[M+H]^+$: 292.2332, found: 292.2337.







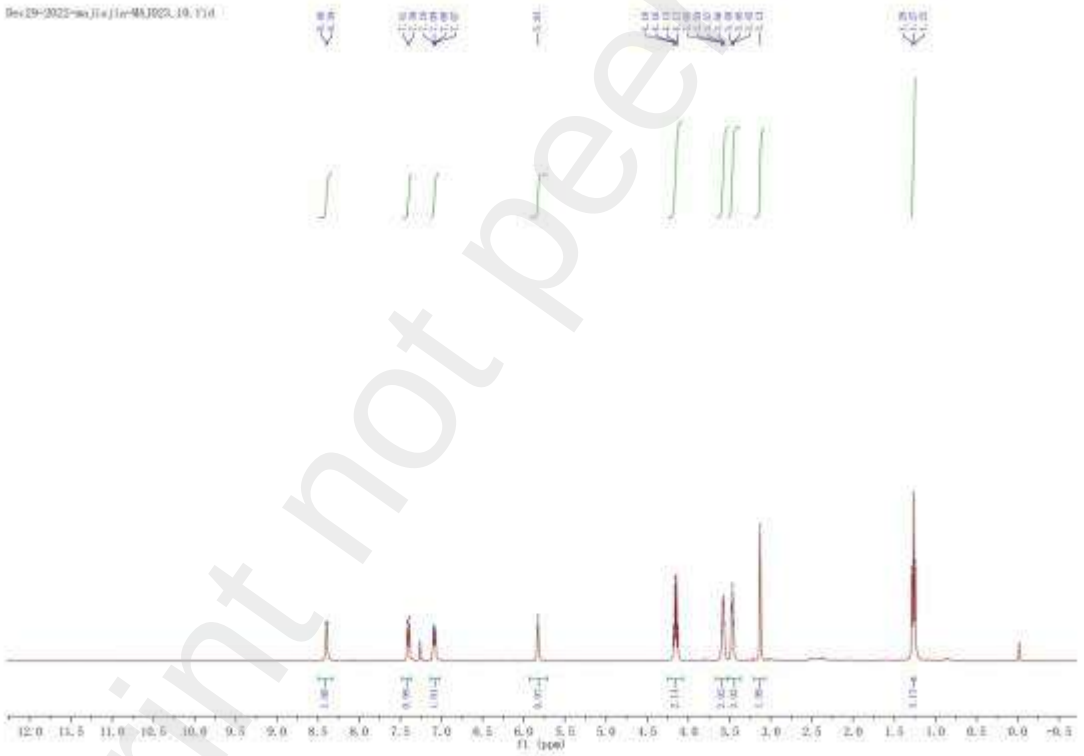
25, 58% yield

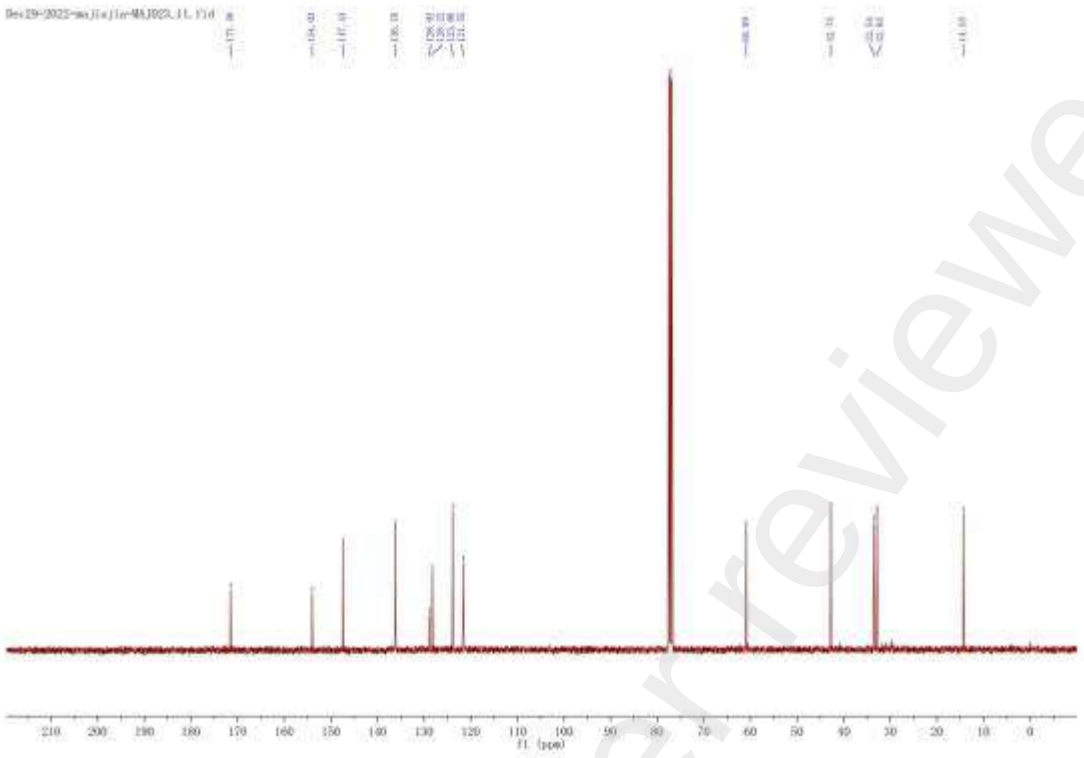
According to the general procedure, a mixture of **1w** (0.2 mmol, 43.8 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **25** as pale yellow oil (25.4 mg, 58% yield, >95:5 r.r.).

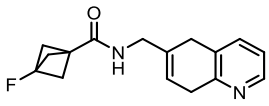
^1H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 4.8 Hz, 1H), 7.40 (d, *J* = 7.7 Hz, 1H), 7.09 (dd, *J* = 7.7, 4.7 Hz, 1H), 5.83 (s, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.58 (q, *J* = 4.7 Hz, 2H), 3.47 (d, *J* = 5.5 Hz, 2H), 3.13 (s, 2H), 1.26 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 154.0, 147.4, 136.2, 128.9, 128.2, 123.9, 121.6, 60.9, 42.8, 33.5, 32.9, 14.4.

HRMS (ESI, *m*/*z*) calcd for $C_{13}H_{16}NO_2^+$ $[M+H]^+$:218.1176, found: 218.1177







26, 73% yield

According to the general procedure, a mixture of **1x** (0.2 mmol, 54.1 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **26** as a white (39.8 mg, 73% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:1 to 2:1

R_f(**26**) = 0.3 in EtOAc.

Analytical data of **26**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.42 (d, *J* = 7.2 Hz, 1H), 7.10 (dd, *J* = 7.6, 4.8 Hz, 1H), 5.82 (br, 1H), 5.77 (br, 1H), 3.93 (d, *J* = 6.0 Hz, 2H), 3.56 - 3.51 (m, 2H), 3.38 - 3.33 (m, 2H), 2.35 (d, *J* = 2.4 Hz, 6H).

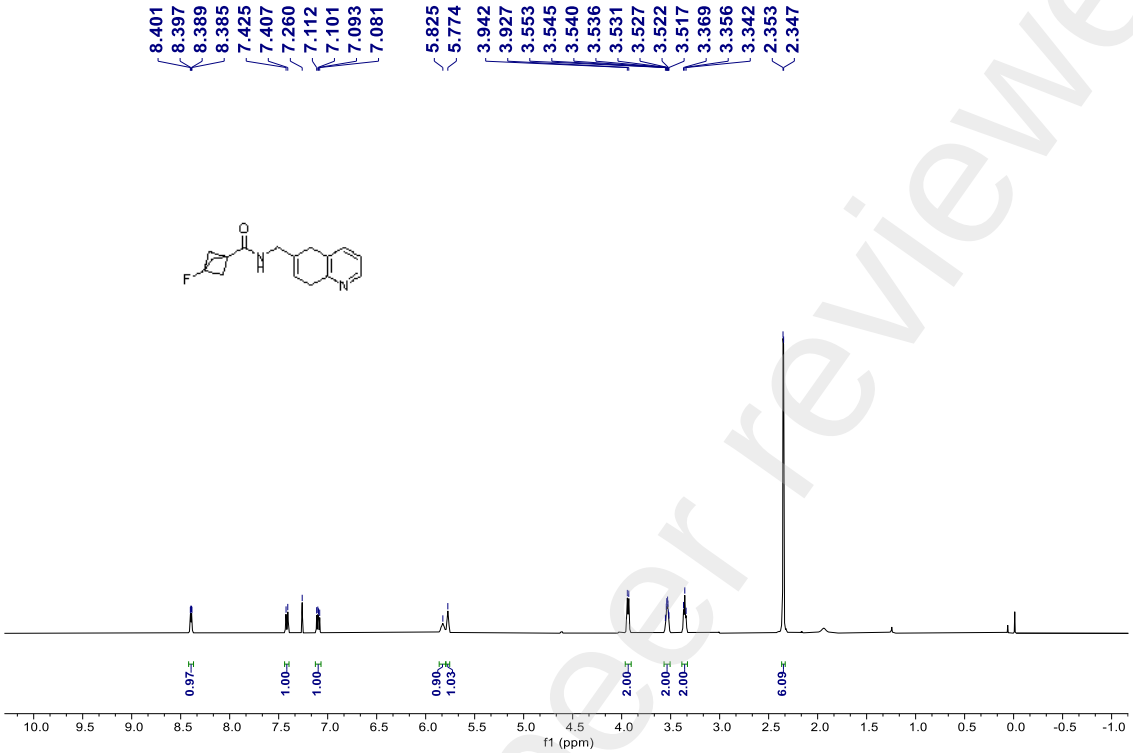
^{19}F NMR (376 MHz, $CDCl_3$) δ -149.8.

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2 (d, *J* = 32.4 Hz), 154.1, 147.6, 136.4, 131.6, 128.6, 121.9, 121.7, 74.7 (d, *J* = 329.8 Hz), 55.1 (d, *J* = 21.8 Hz), 44.7, 33.3, 31.0,

29.6 (d, J = 42.2 Hz).

HRMS (ESI, m/z) calcd for $C_{16}H_{18}FN_2O$ $[M+H]^+$: 273.1398, found: 273.1401.

Jan13-2023-majiajia-lh20230106-3.10.fid



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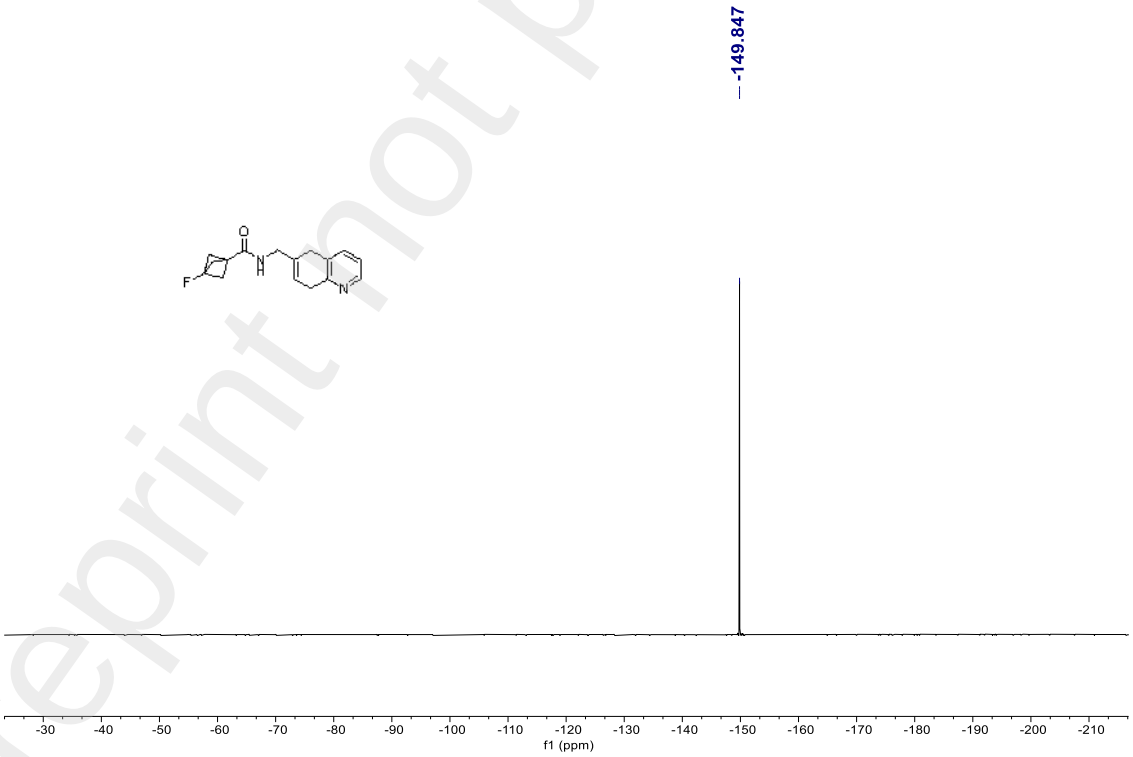
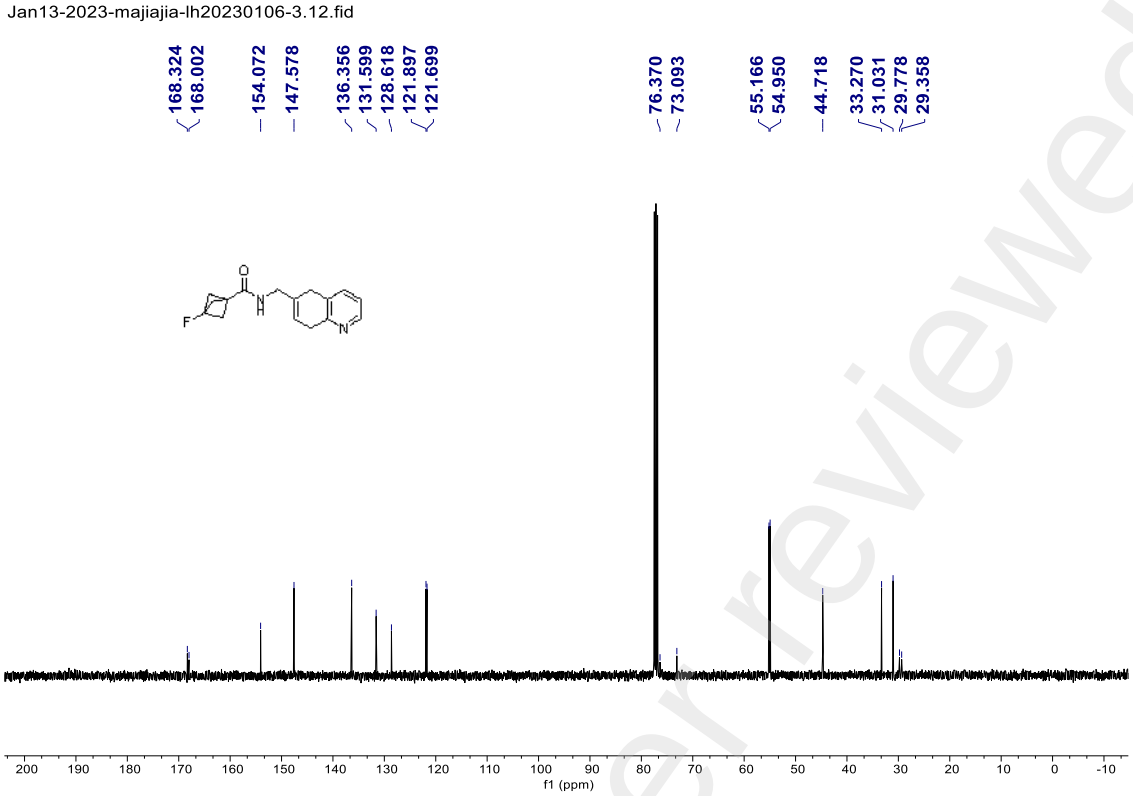
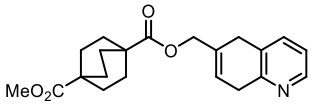






27, 55% yield

According to the general procedure, a mixture of **1y** (0.2 mmol, 70.6 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **27** as white solid (39.1 mg, 55% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:6 to 1:3

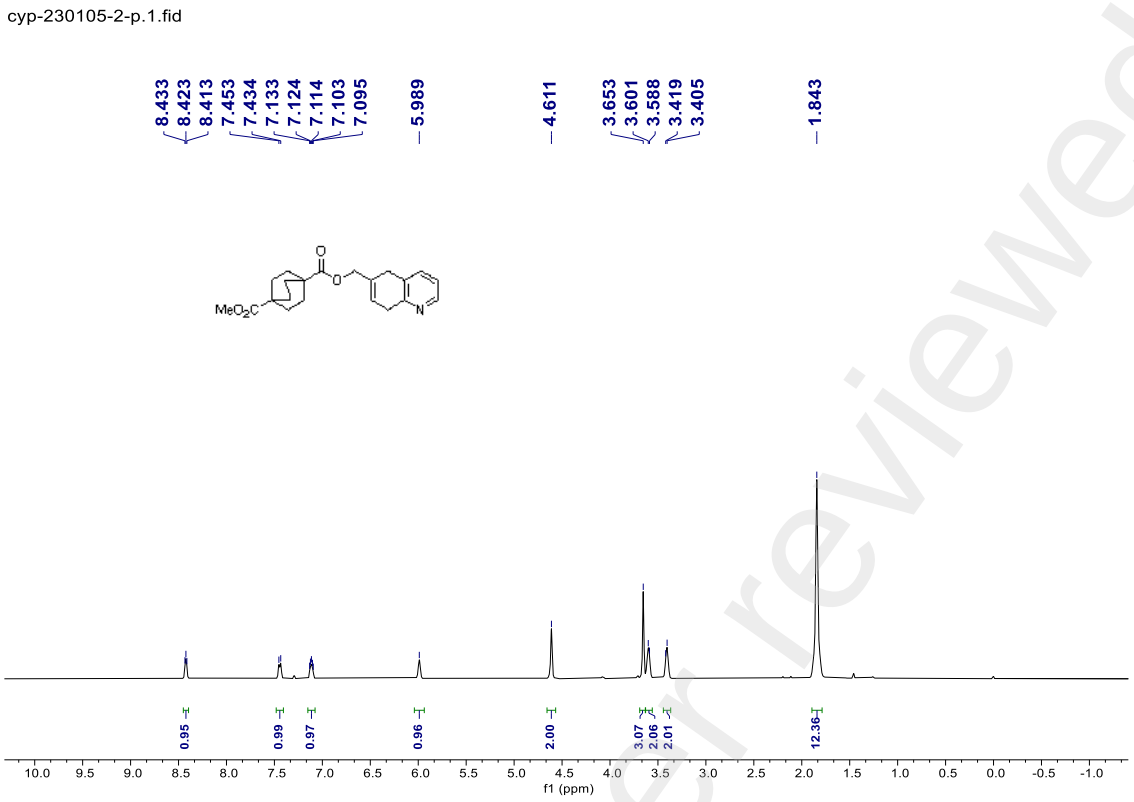
R_f (**27**) = 0.25 in EtOAc/petroleum ether = 1:3.

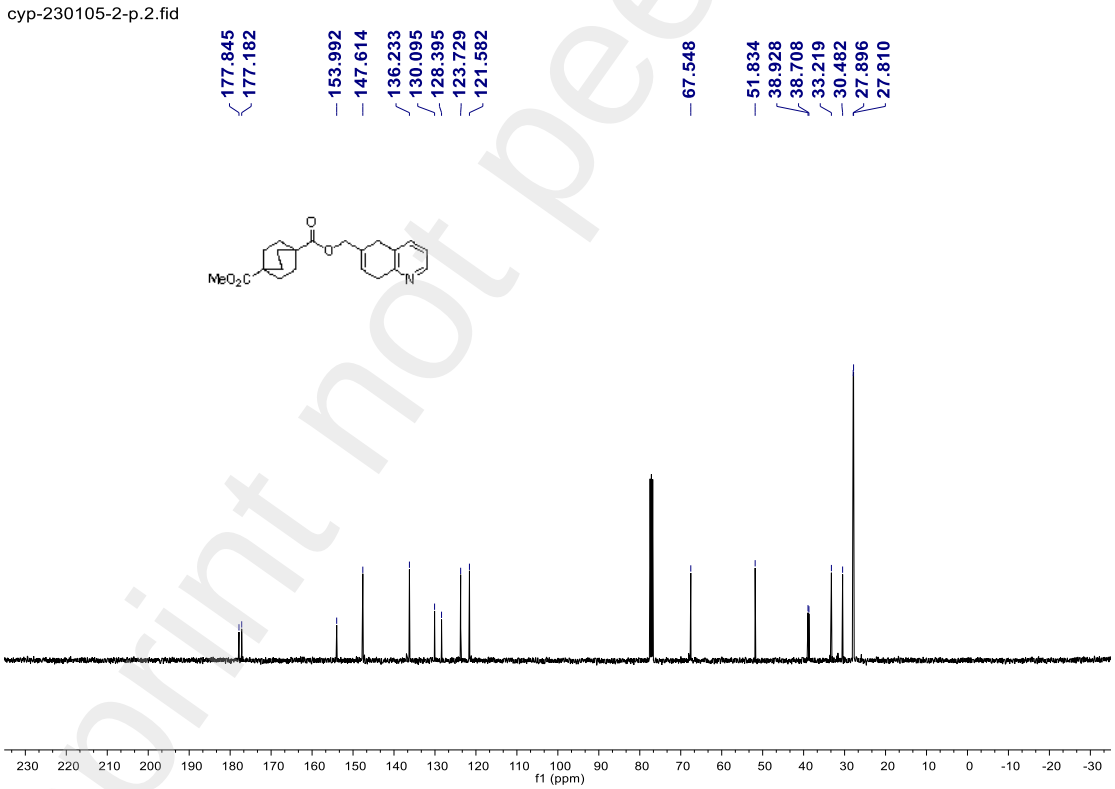
Analytical data of **27**:

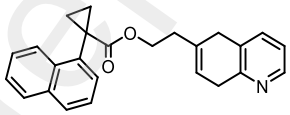
^1H NMR (400 MHz, $CDCl_3$) δ 8.46 - 8.39 (m, 1H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.16 - 7.07 (m, 1H), 5.99 (s, 1H), 4.61 (s, 2H), 3.65 (s, 3H), 3.63 - 3.56 (m, 2H), 3.44 - 3.36 (m, 2H), 1.84 (s, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.8, 177.2, 154.0, 147.6, 136.2, 130.1, 128.4, 123.7, 121.6, 67.5, 51.8, 38.9, 38.7, 33.2, 30.5, 27.9, 27.8.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{25}NO_4$ $[M+H]^+$: 356.1856, found: 356.1859.







28, 68% yield

According to the general procedure, a mixture of **1z** (0.2 mmol, 73.5 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol,

2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired **28** as a yellow oil (50.2 mg, 68% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether= 1:8 to 1:4

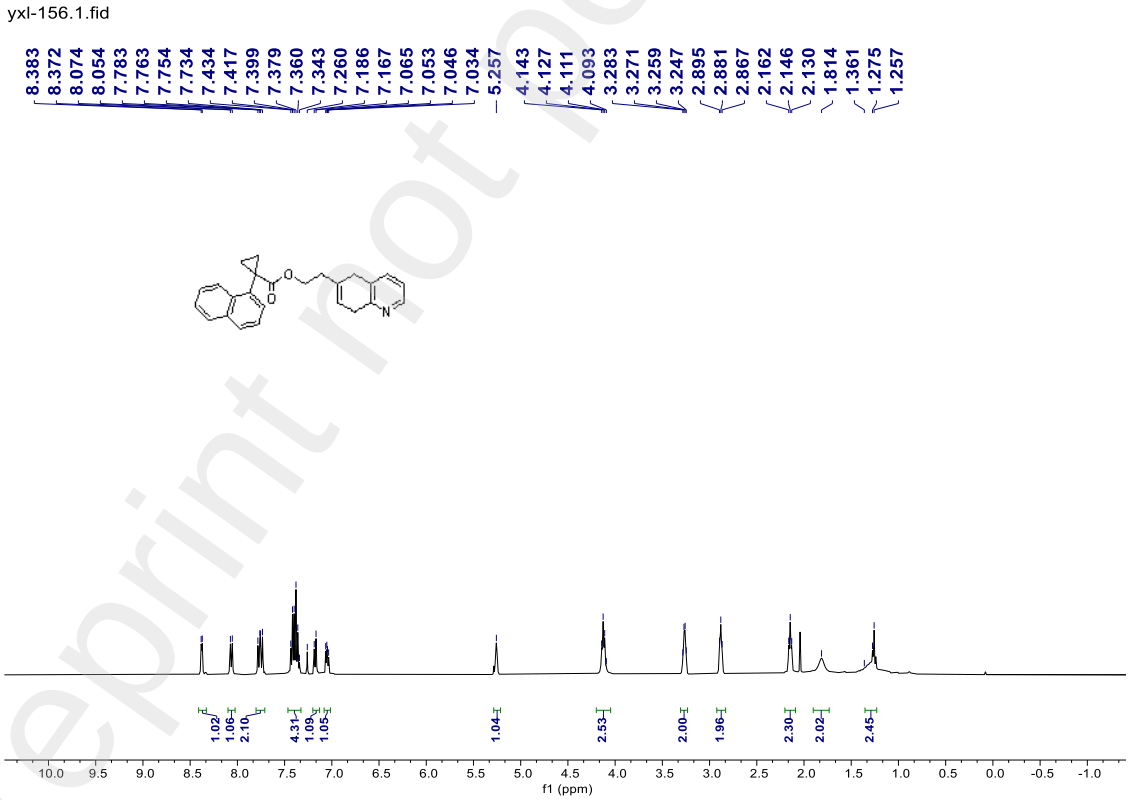
R_f (**28**) = 0.3 in EtOAc/petroleum ether= 1:3.

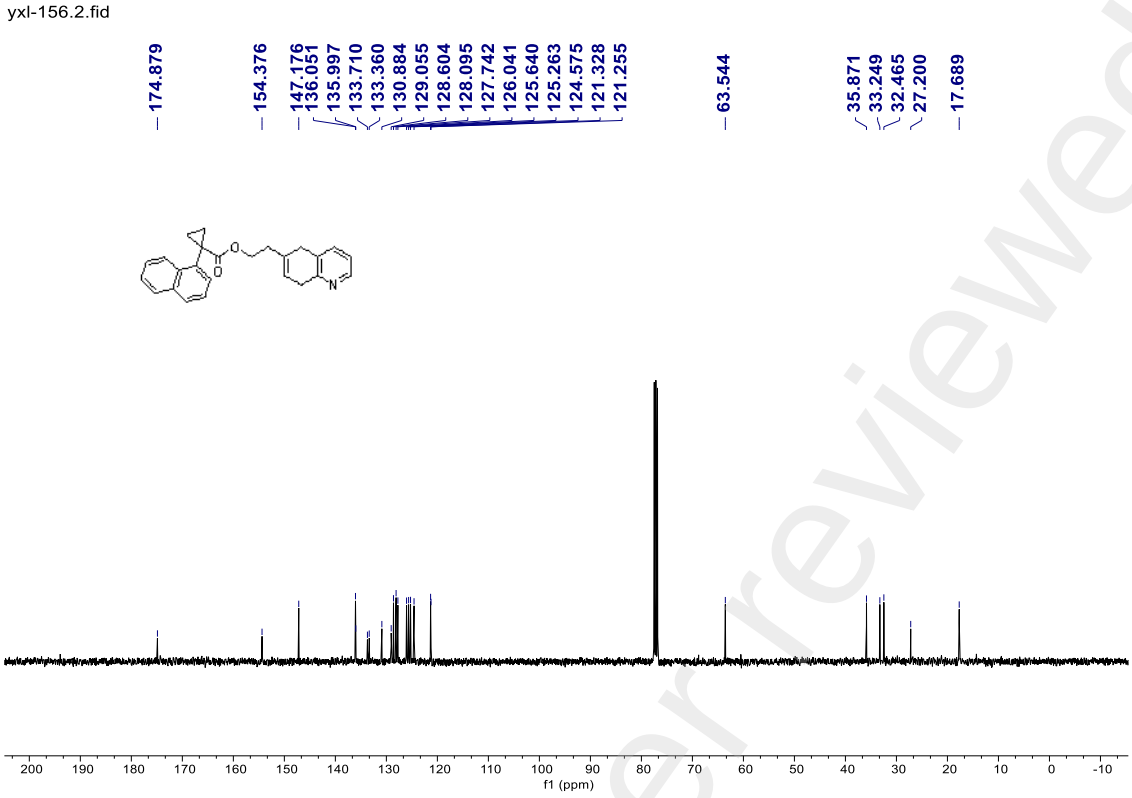
Analytical data of **28**:

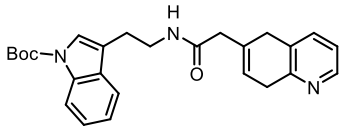
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 4.4 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.82 - 7.68 (m, 2H), 7.48 - 7.32 (m, 4H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.07 - 7.03 (m, 1H), 5.26 (br, 1H), 4.19 - 4.04 (m, 2H), 3.41 - 3.22 (m, 2H), 2.93 - 2.85 (m, 2H), 2.15 (t, *J* = 6.4 Hz, 2H), 1.81 (s, 2H), 1.34 - 1.24 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.9, 154.4, 147.2, 136.1, 136.0, 133.7, 133.4, 130.9, 129.1, 128.6, 128.1, 127.7, 126.0, 125.6, 125.3, 124.6, 121.3, 121.3, 63.5, 35.9, 33.2, 32.5, 27.2, 17.7.

HRMS (ESI, *m*/*z*) calcd for $C_{25}H_{24}NO_2$ $[M+H]^+$: 370.1802, found: 370.1800.







29, 36% yield

According to the general procedure, a mixture of **1aa** (0.1 mmol, 42.9 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.003 mmol, 3.0 mol%, 3.3 mg), Gd(OTf)$_3$ (0.2 mmol, 2.0 equiv., 121 mg), γ-terpinene (0.5 mmol, 5.0 equiv., 84 μL) and CH_3CN (0.5 mL, 0.5 M) were stirred for 15 h to give the desired product **29** as yellow oil (15.6 mg, 36% yield, >95:5 r.r.).

Purification conditions: Acetone/petroleum ether = 1:4 to 1:2

R_f (**29**) = 0.25 in EtOAc/petroleum ether = 1:1.

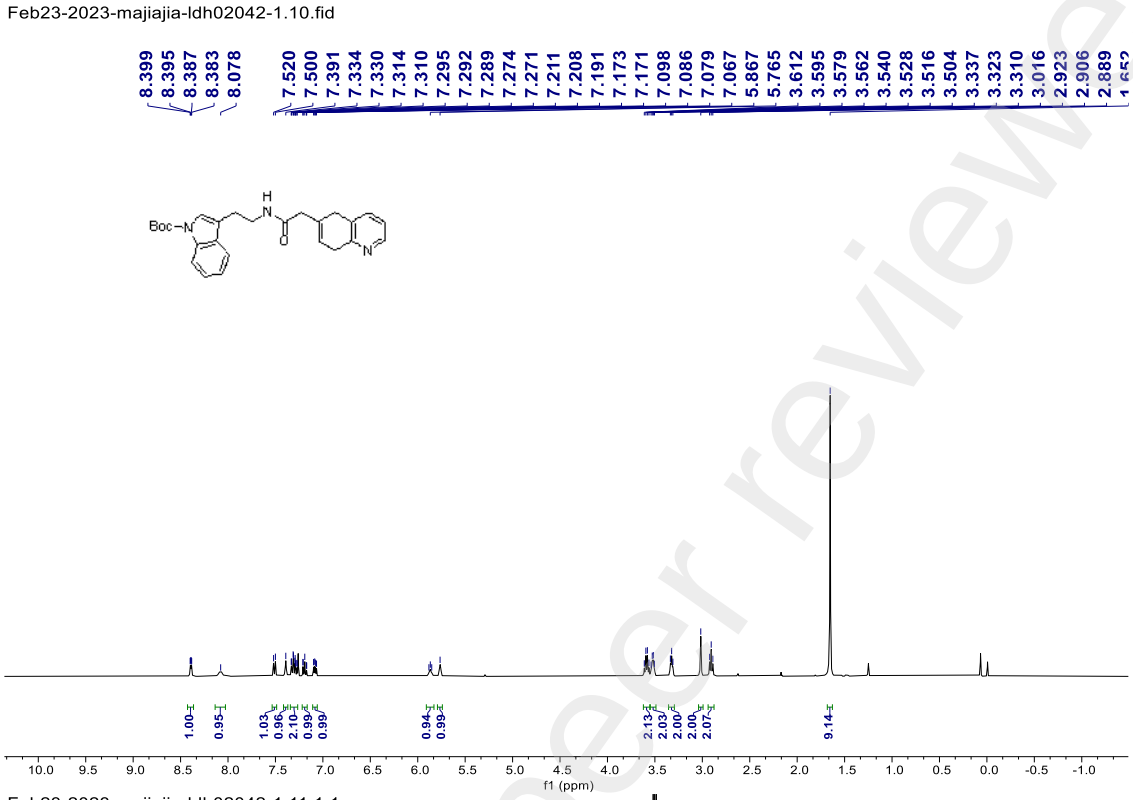
Analytical data of **29**:

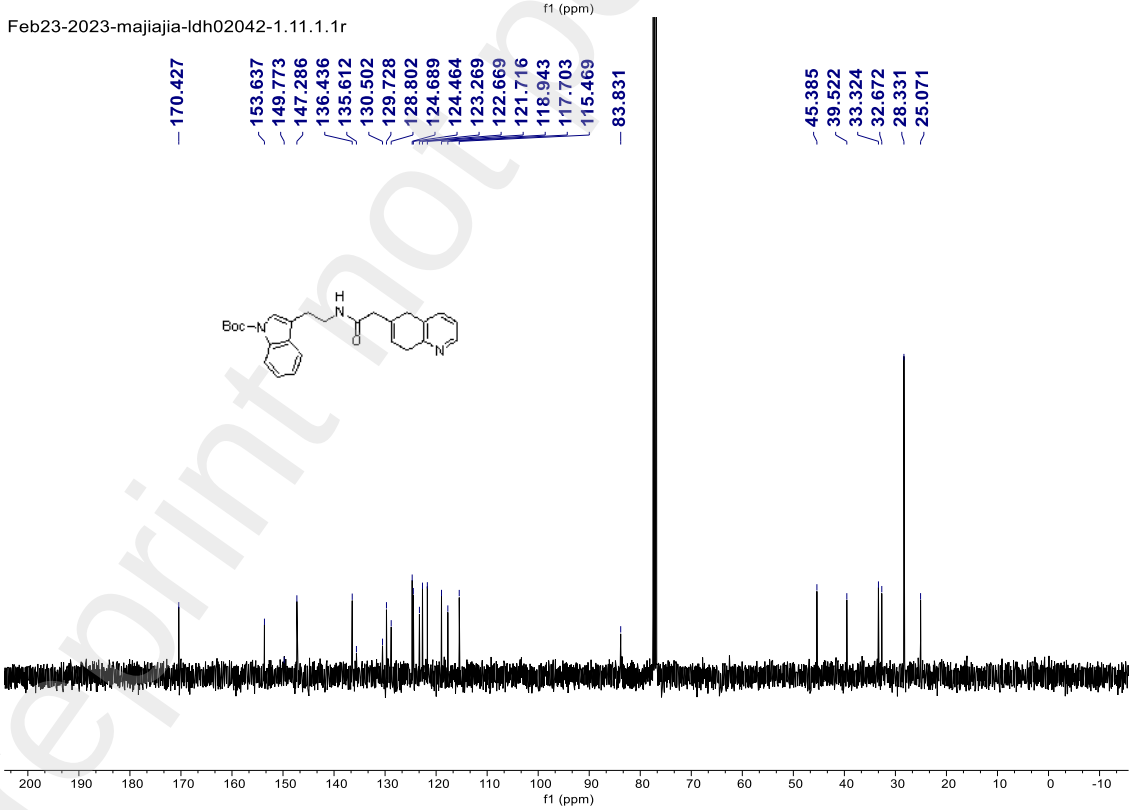
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.08 (br, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.39 (s, 1H), 7.34 - 7.27 (m, 2H), 7.23 - 7.15 (m, 1H), 7.08 (dd, *J* = 7.6, 4.8 Hz, 1H), 5.87 (t, *J* = 6.0 Hz, 1H), 5.76 (s, 1H), 3.59 (q, *J* = 6.8 Hz, 2H), 3.52 (q, *J* = 4.8 Hz, 2H), 3.36 - 3.29 (m, 2H), 3.02 (s, 2H), 2.91 (t, *J* = 6.8 Hz, 2H), 1.65 (s, 9H).

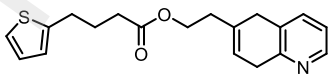
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 153.6, 149.8, 147.3, 136.4, 135.6, 130.5, 129.7, 128.8, 124.7, 124.5, 123.3, 122.7, 121.7, 118.9, 117.7, 115.5, 83.8, 45.4, 39.5, 33.3,

32.7, 28.3, 25.1.

HRMS (ESI, *m*/*z*) calcd for $C_{26}H_{30}N_3O_3$ $[M+H]^+$: 432.2282, found: 432.2282.







30, 59% yield

According to the general procedure, a mixture of **1ab** (0.2 mmol, 65.7 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **30** as yellow oil (38.3 mg, 59% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:5 to 1:2

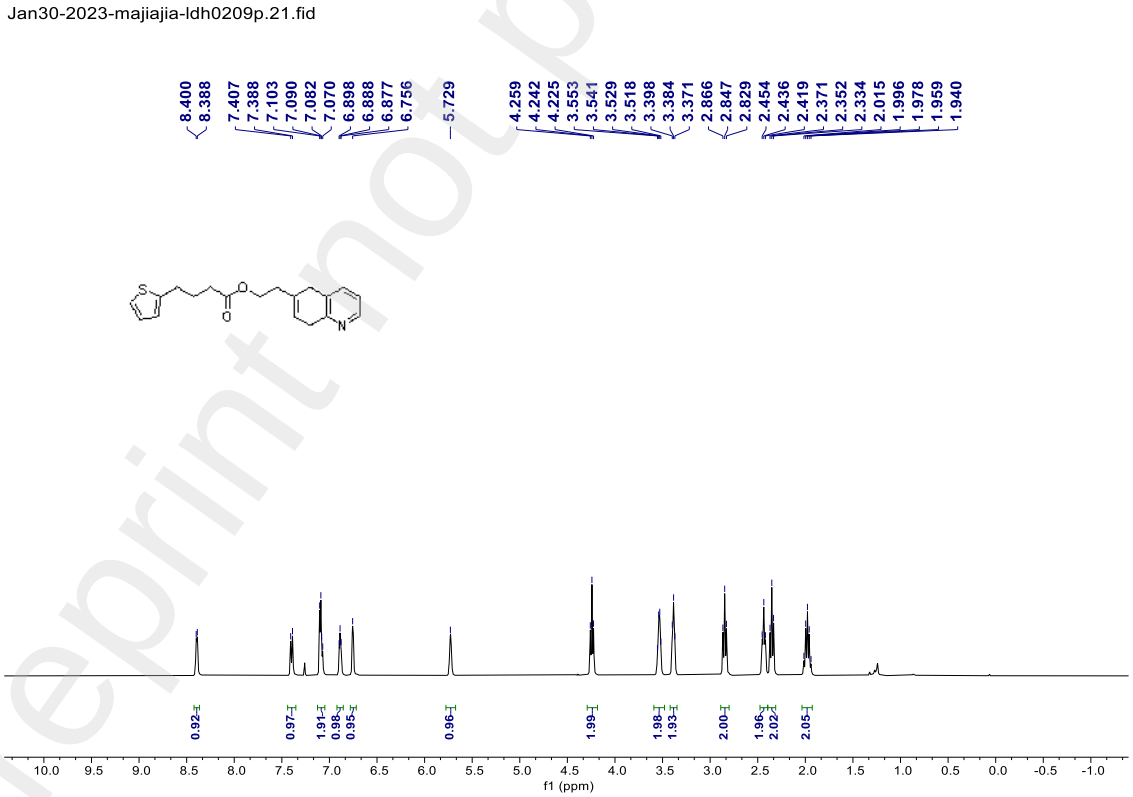
R_f (**30**) = 0.4 in EtOAc/petroleum ether = 1:1

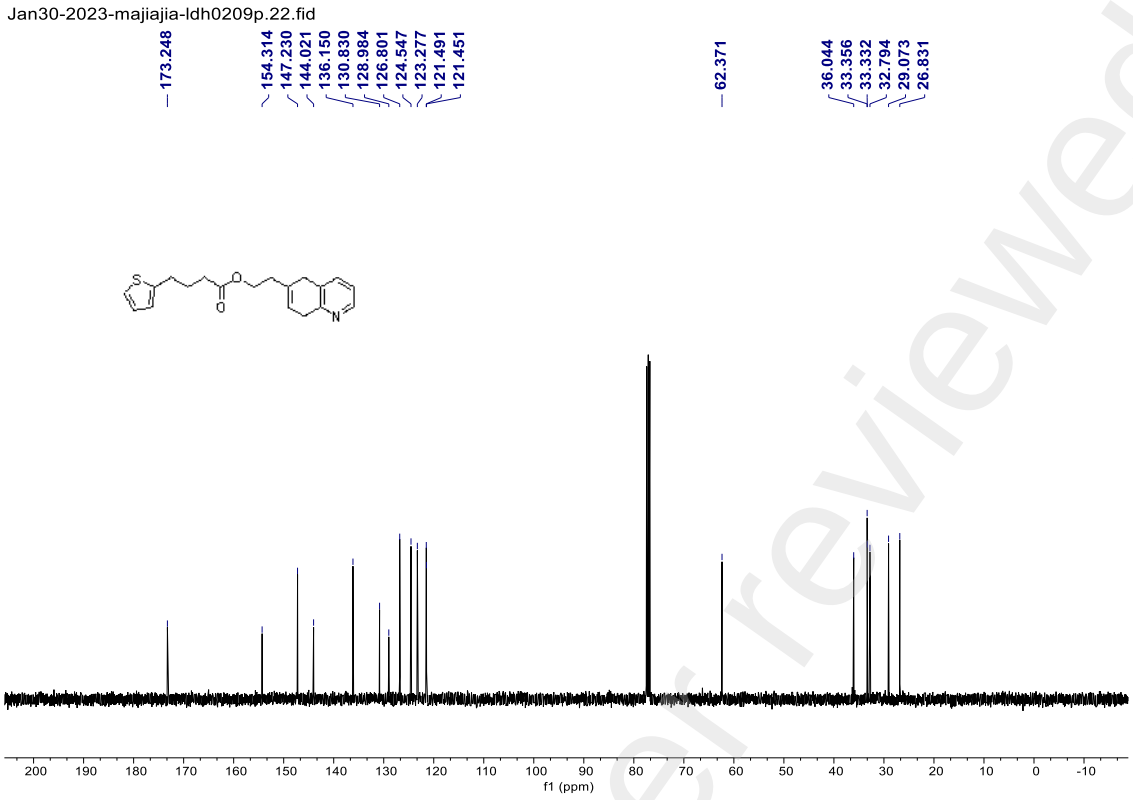
Analytical data of **30**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 4.8 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.12 - 7.06 (m, 2H), 6.89 (t, *J* = 4.4 Hz, 1H), 6.76 (br, 1H), 5.73 (br, 1H), 4.24 (t, *J* = 6.8 Hz, 2H), 3.58 - 3.49 (m, 2H), 3.43 - 3.35 (m, 2H), 2.85 (t, *J* = 7.6 Hz, 2H), 2.44 (t, *J* = 6.8 Hz, 2H), 2.35 (t, *J* = 7.4 Hz, 2H), 1.98 (p, *J* = 7.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 154.3, 147.2, 144.0, 136.2, 130.8, 129.0, 126.8, 124.5, 123.3, 121.5, 121.5, 62.4, 36.0, 33.4, 33.3, 32.8, 29.1, 26.8.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{22}NO_2S$ $[M+H]^+$: 328.1366, found: 328.1368.





31, 58% yield

According to the general procedure, a mixture of **1ac** (0.2 mmol, 59.3 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **31** as yellow oil (34.6 mg, 58% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:5 to 1:2

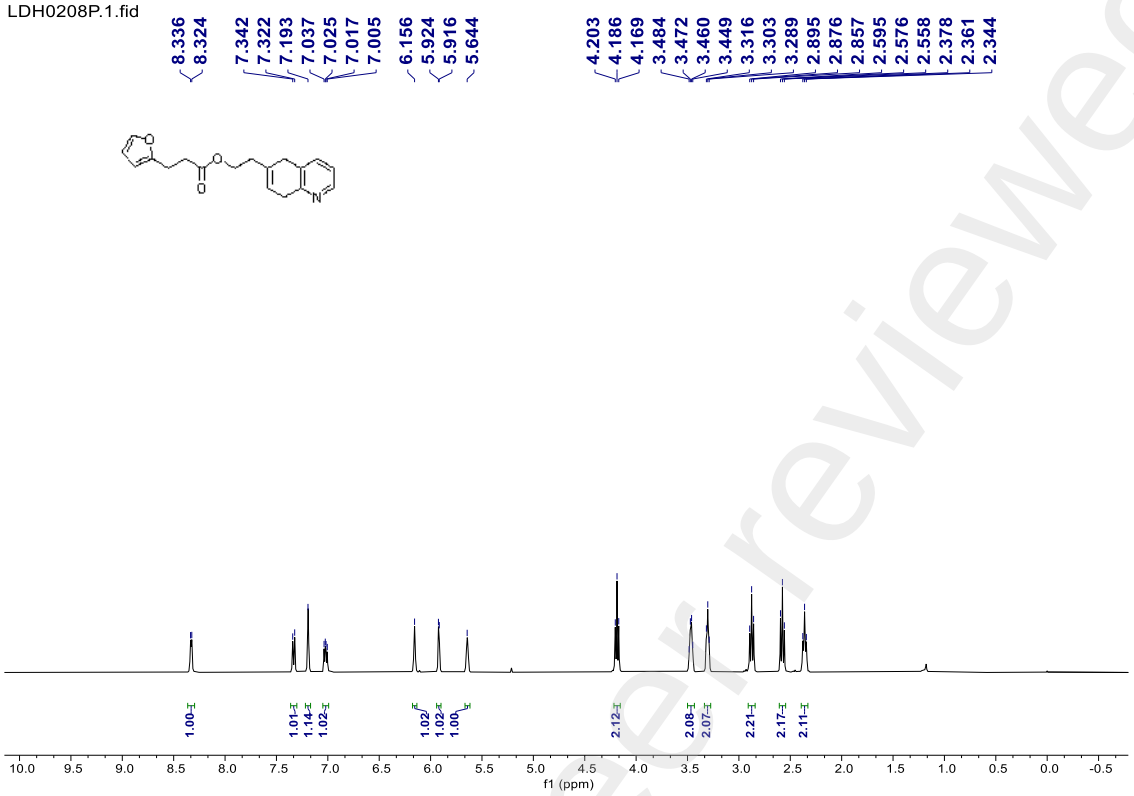
R_f (**31**) = 0.4 in EtOAc/petroleum ether = 1:1.

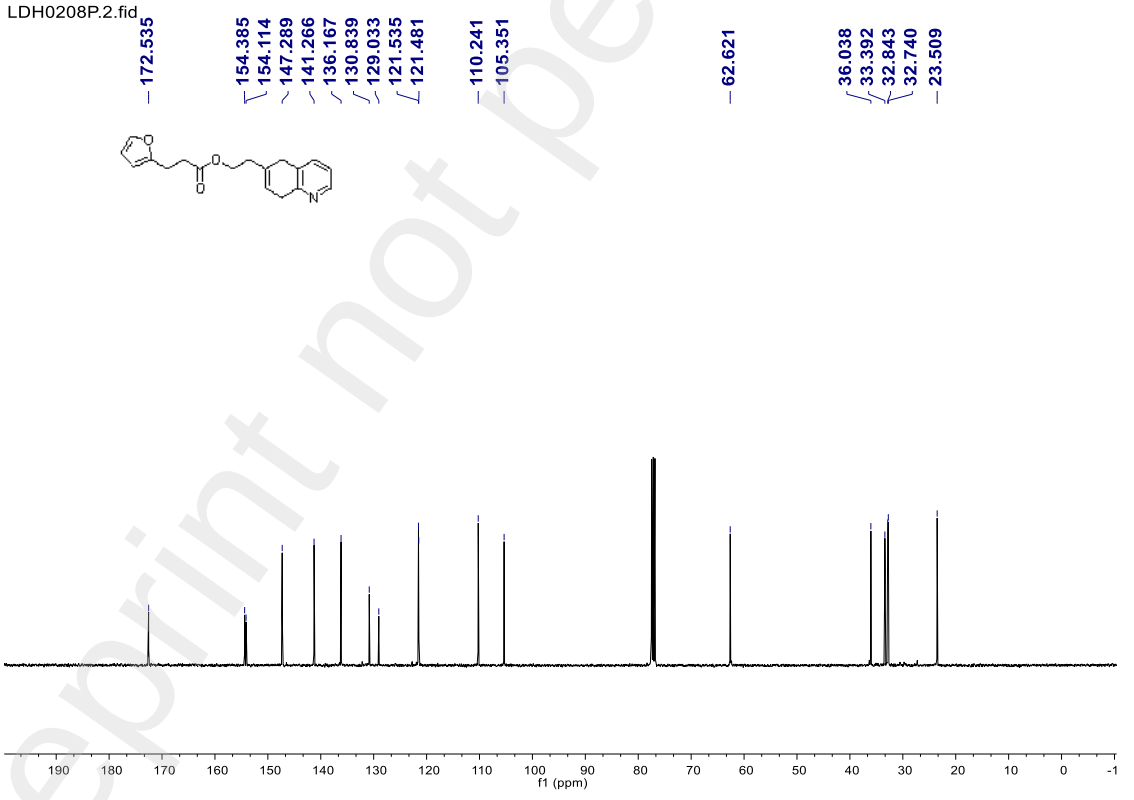
Analytical data of **31**:

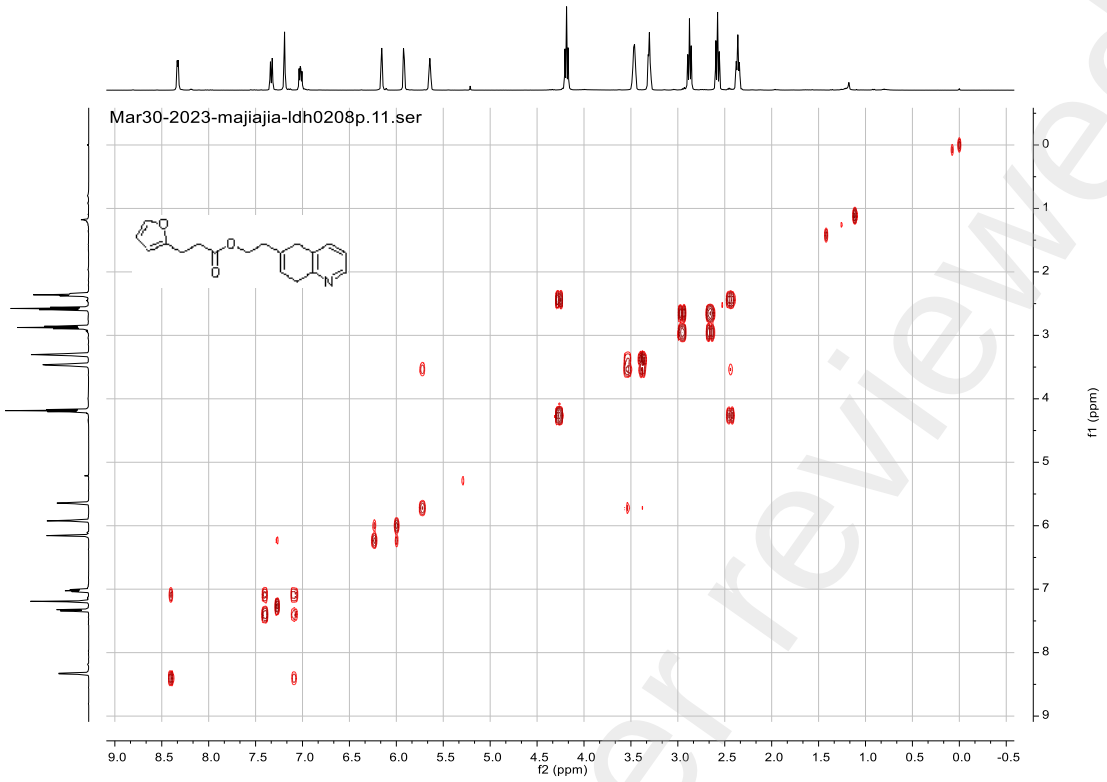
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 4.8 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.19 (br, 1H), 7.02 (dd, *J* = 8.0, 4.8 Hz, 1H), 6.16 (br, 1H), 5.92 (d, *J* = 3.2 Hz, 1H), 5.64 (br, 1H), 4.19 (t, *J* = 6.8 Hz, 2H), 3.50 - 3.44 (m, 2H), 3.33 - 3.28 (m, 2H), 2.88 (t, *J* = 7.6 Hz, 2H), 2.58 (t, *J* = 7.6 Hz, 2H), 2.36 (t, *J* = 6.8 Hz, 2H).

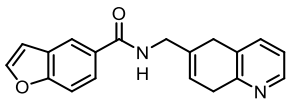
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 154.4, 154.1, 147.3, 141.3, 136.2, 130.8, 129.0, 121.5, 121.5, 110.2, 105.4, 62.6, 36.0, 33.4, 32.8, 32.7, 23.5.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{20}NO_3$ $[M+H]^+$: 298.1438, found: 298.1435.









32, 71% yield

According to the general procedure, a mixture of **1ad** (0.2 mmol, 60.5 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **32** as yellow solid (43.2 mg, 71% yield, > 95:5 r.r.).

Purification conditions: Acetone/petroleum ether = 1:5 to 1:2

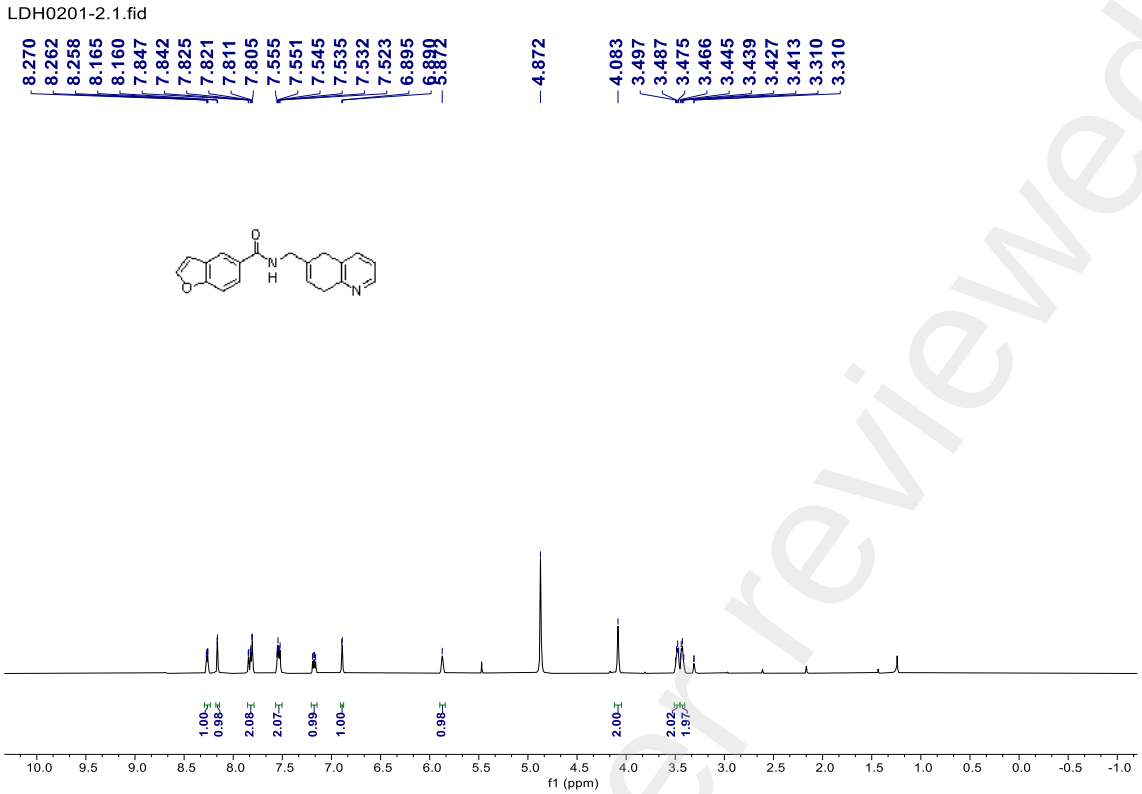
R_f (**32**) = 0.3 in Acetone/petroleum ether = 1:2.

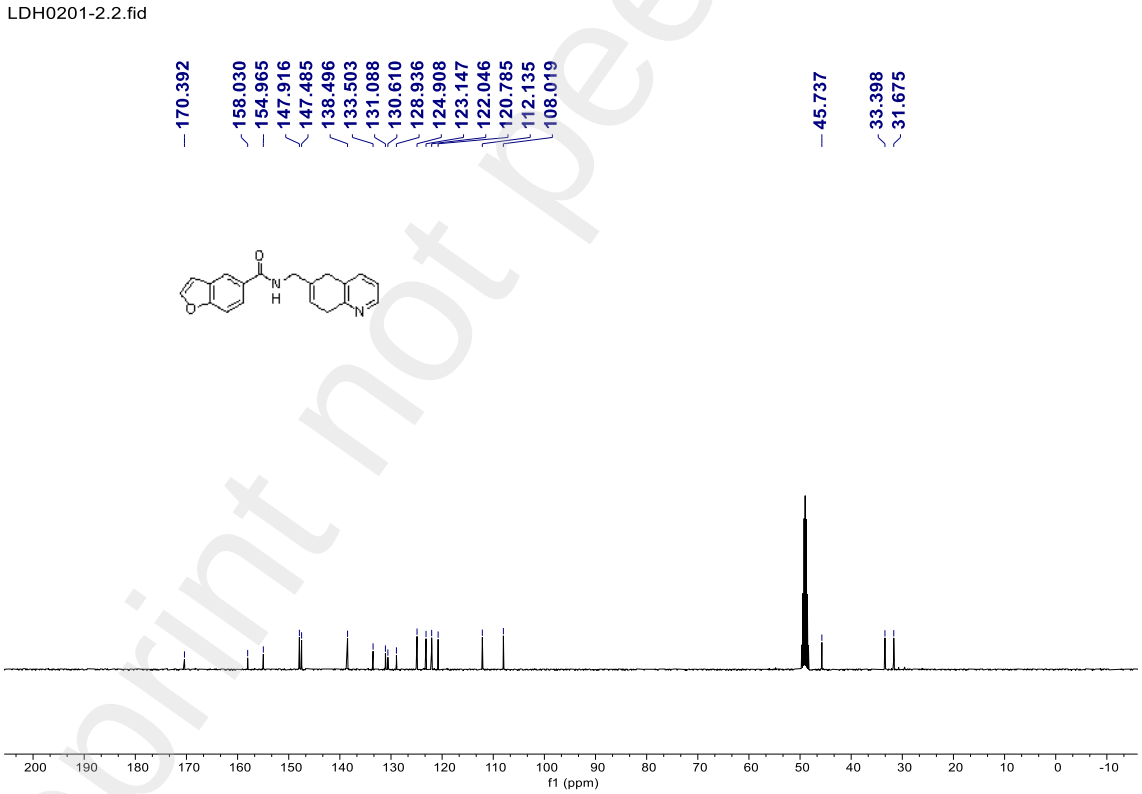
Analytical data of **32**:

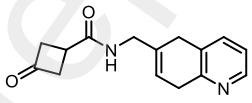
^{1}H NMR (400 MHz, CD_3OD) δ 8.27 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.16 (d, *J* = 2.0 Hz, 1H), 7.85 - 7.79 (m, 2H), 7.56 - 7.51 (m, 2H), 7.18 (dd, *J* = 8.0, 4.8 Hz, 1H), 6.89 (d, *J* = 2.0 Hz, 1H), 5.87 (br, 1H), 4.08 (s, 2H), 3.51 - 3.45 (m, 2H), 3.45 - 3.41 (m, 2H).

^{13}C NMR (101 MHz, CD_3OD) δ 170.4, 158.0, 155.0, 147.9, 147.5, 138.5, 133.5, 131.1, 130.6, 128.9, 124.9, 123.1, 122.0, 120.8, 112.1, 108.0, 45.7, 33.4, 31.7.

HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{17}N_2O_2$ $[M+H]^+$: 305.1285, found: 305.1288.







33, 59% yield

According to the general procedure, a mixture of **1ae** (0.2 mmol, 50.8 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol,

2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **33** as white solid (30.3 mg, 59% yield, > 95:5 r.r.).

Purification conditions: MeOH/CH_2Cl_2 = 1:40 to 1:20

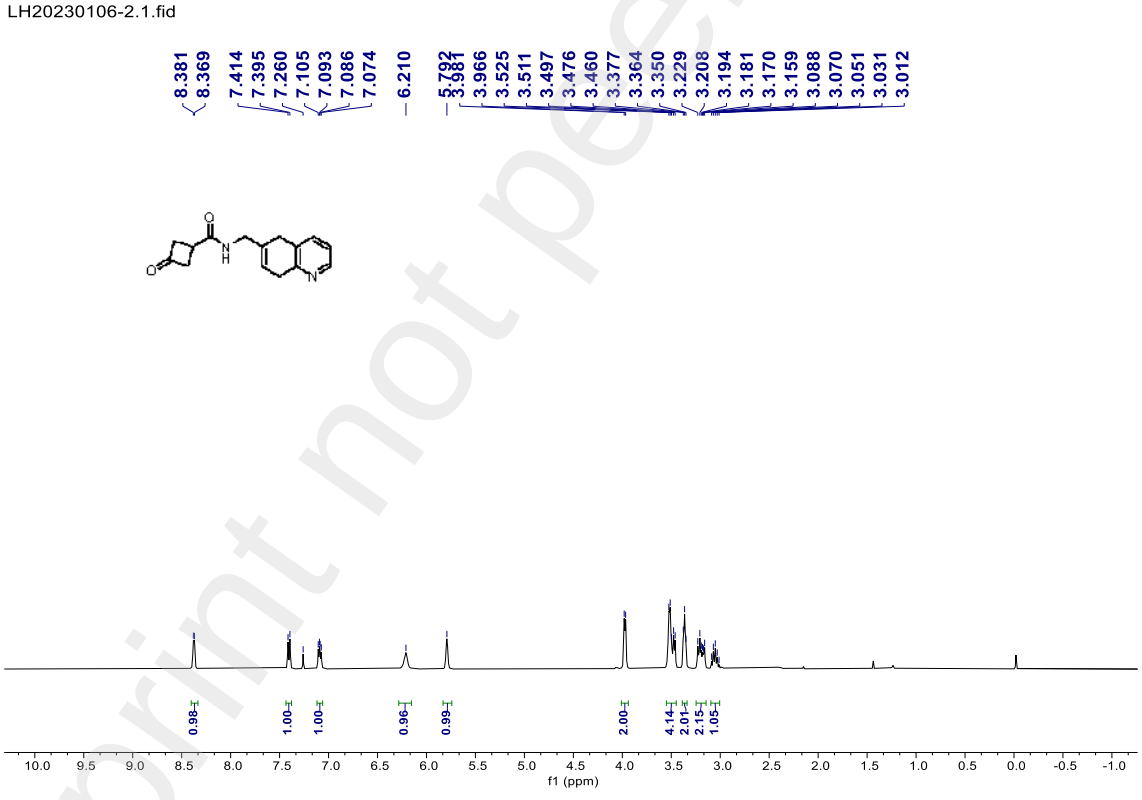
R_f (**33**) = 0.4 in MeOH/CH_2Cl_2 = 1:20

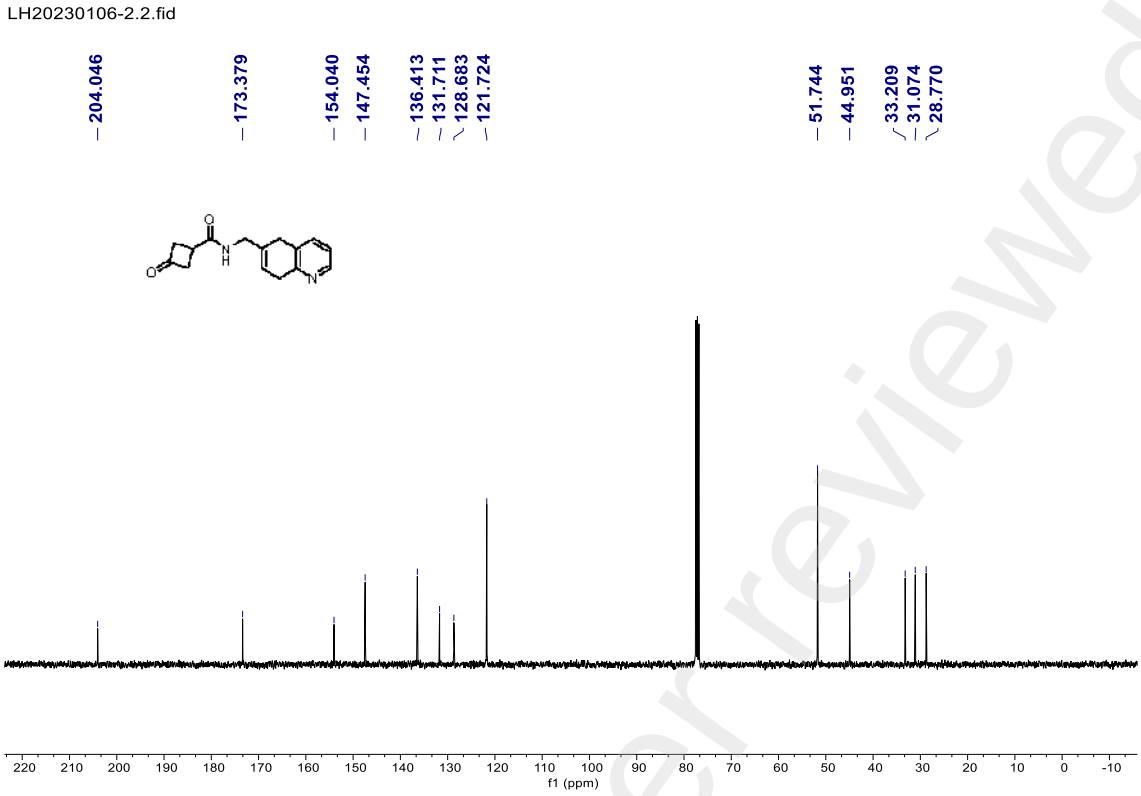
Analytical data of **33**:

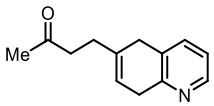
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 4.8 Hz, 1H), 7.40 (d, *J* = 7.6 Hz, 1H), 7.09 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.21 (br, 1H), 5.79 (br, 1H), 3.97 (d, *J* = 6.0 Hz, 2H), 3.55 - 3.44 (m, 4H), 3.40 - 3.33 (m, 2H), 3.25 - 3.14 (m, 2H), 3.10 - 3.01 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 204.0, 173.4, 154.0, 147.5, 136.4, 131.7, 128.7, 121.7, 51.7, 45.0, 33.2, 31.1, 28.8.

HRMS (ESI, *m*/*z*) calcd for $C_{15}H_{16}N_2O_2$ $[M+H]^+$: 257.1285, found: 257.1287.







34, 50% yield

According to the general procedure, a mixture of **4-(quinolin-6-yl)butan-2-one** (0.2 mmol, 39.8 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **34** as a yellow oil (20.0 mg, 50% yield, > 95:5 r.r.)

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:4

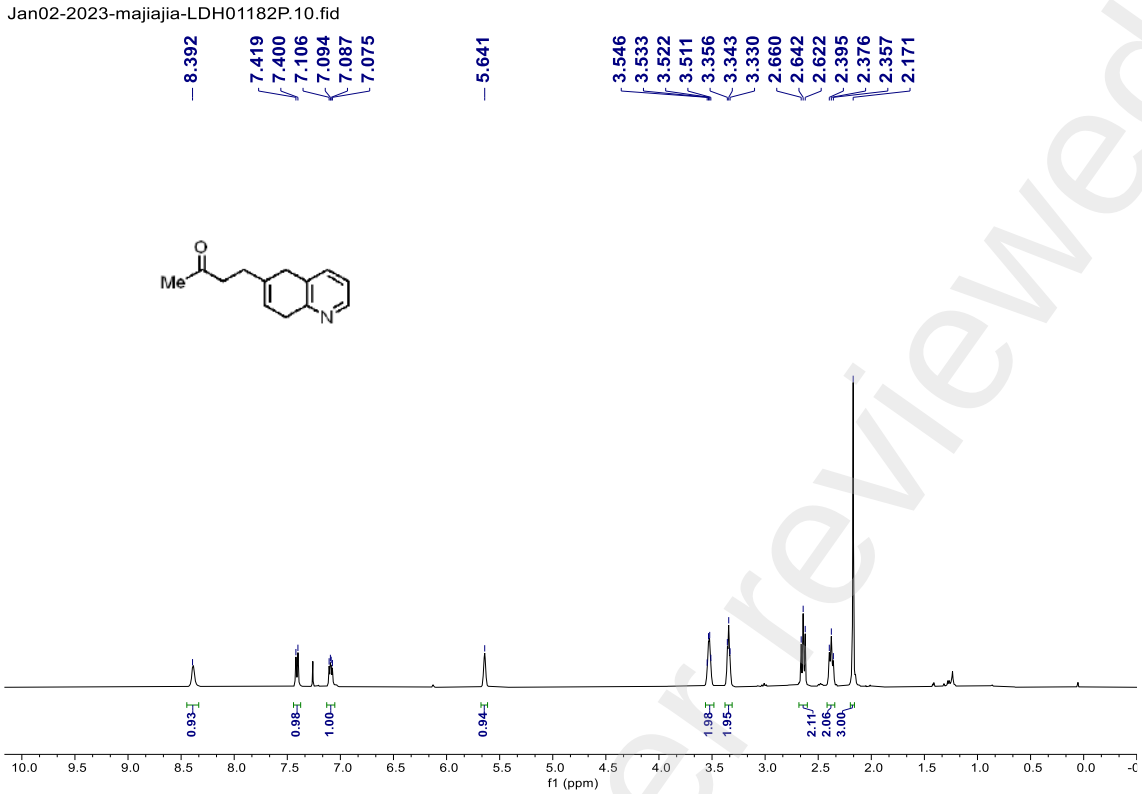
R_f (**34**) = 0.4 in EtOAc/petroleum ether = 1:3.

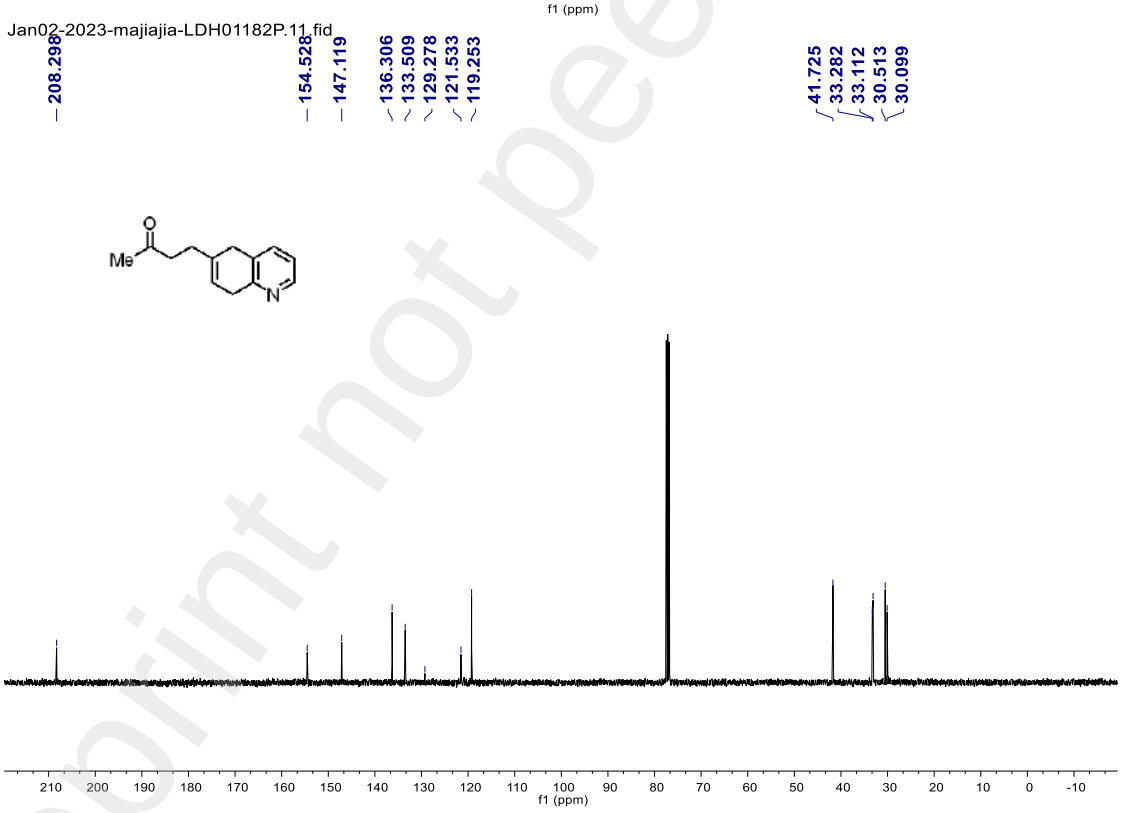
Analytical data of **34**:

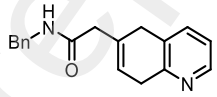
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (br, 1H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.09 (dd, *J* = 7.6, 4.8 Hz, 1H), 5.64 (br, 1H), 3.55 - 3.49 (m, 2H), 3.37 - 3.32 (m, 2H), 2.64 (t, *J* = 7.6 Hz, 2H), 2.38 (t, *J* = 7.6 Hz, 2H), 2.17 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 208.3, 154.5, 147.1, 136.3, 133.5, 129.3, 121.5, 119.3, 41.7, 33.3, 33.1, 30.5, 30.1.

HRMS (ESI, *m*/*z*) calcd for $C_{13}H_{16}NO$ $[M+H]^+$: 202.1226, found: 202.1234.







35, 67% yield

According to the general procedure, a mixture of **1af** (0.2 mmol, 55.3 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol,

2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **35** as yellow solid (37.4 mg, 67% yield, > 95:5 r.r.).

Purification conditions: MeOH/CH_2Cl_2 = 1:60 to 1:20

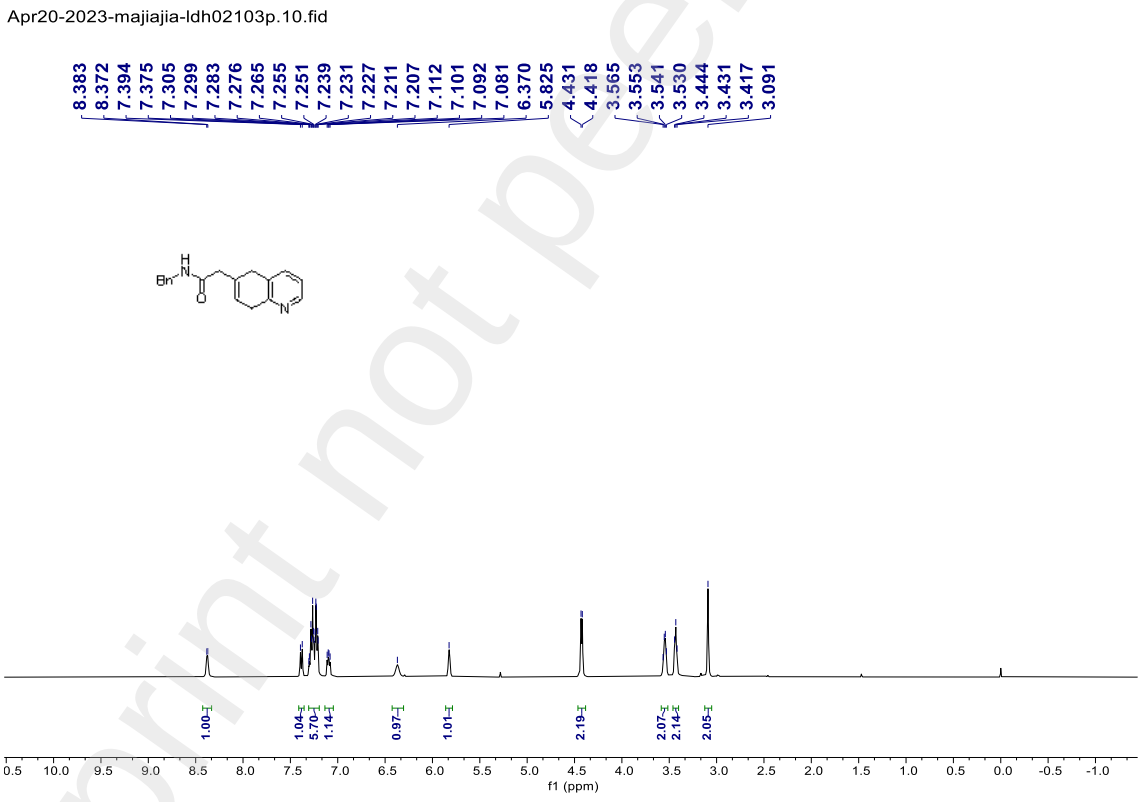
R_f (**35**) = 0.4 in EtOAc/petroleum ether = 1:30

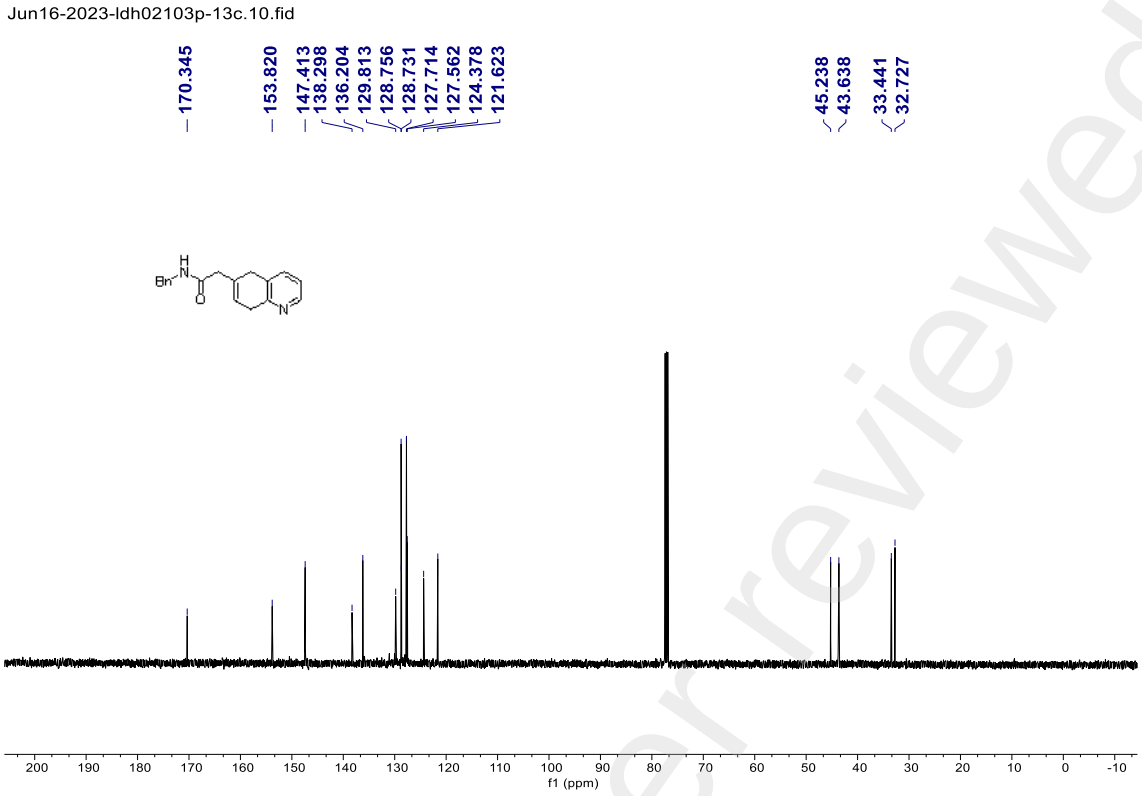
Analytical data of **35**:

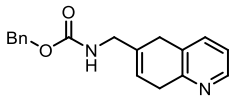
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 4.4 Hz, 1H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.31 - 7.19 (m, 5H), 7.10 (dd, *J* = 8.0, 4.4 Hz, 1H), 6.37 (br, 1H), 5.82 (br, 1H), 4.42 (d, *J* = 5.2 Hz, 2H), 3.59 - 3.52 (m, 2H), 3.47 - 3.40 (m, 2H), 3.09 (s, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.3, 153.8, 147.4, 138.3, 136.2, 129.8, 128.8, 128.7, 127.7, 127.6, 124.4, 121.6, 45.2, 43.6, 33.4, 32.7.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{19}N_2O^+$ $[M+H]^+$:279.1495, found: 279.1492.







36, 71% yield

According to the general procedure, a mixture of **1ag** (0.2 mmol, 58.5 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **36** as white solid (58.8 mg, 71% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:3 to 1:1

R_f (**36**) = 0.25 in EtOAc/petroleum ether = 1:1.

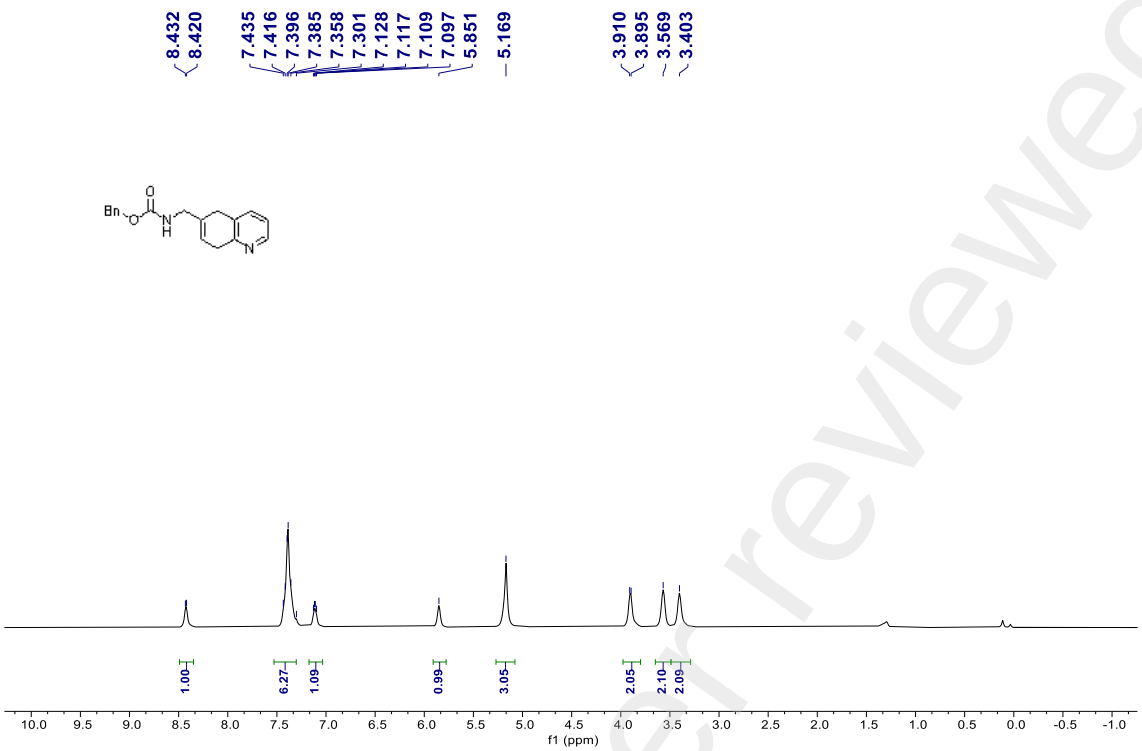
Analytical data of **36**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48- 8.33 (m, 1H), 7.48 - 7.27 (m, 6H), 7.18 - 7.02 (m, 1H), 5.85 (br, 1H), 5.17 (br, 3H), 3.93 - 3.87 (m, 2H), 3.57 (br, 2H), 3.40 (br, 2H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 154.3, 147.5, 136.5, 136.2, 132.0, 128.6, 128.2, 128.2, 121.5, 121.1, 66.9, 46.3, 33.2, 30.9.

HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{19}N_2O_2^+$ $[M+H]^+$: 295.1441, found: 295.1438.

LH-20221231-P-NHCbz.3.fid



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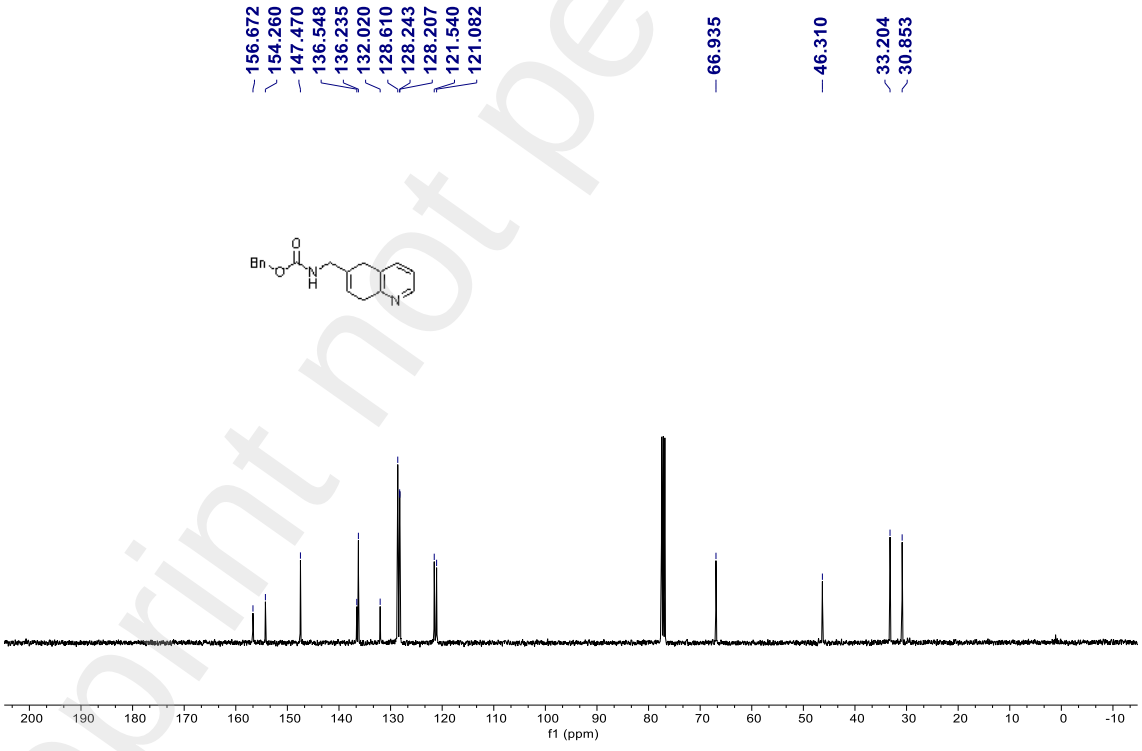
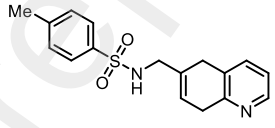




37, 74% yield

According to the general procedure, a mixture of **1ah** (0.2 mmol, 62.4 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol,

2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **37** as yellow solid (46.5 mg, 74% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:4 to 1:2

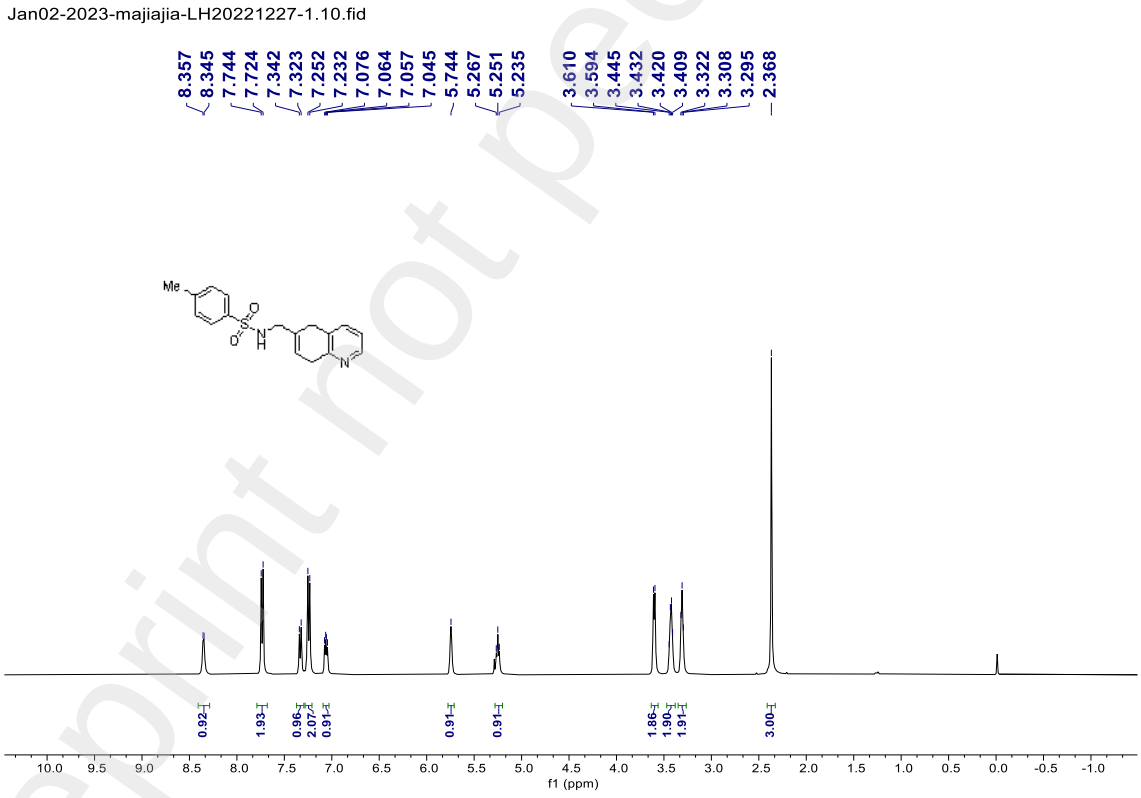
R_f (**37**) = 0.4 in EtOAc/petroleum ether = 1:1.

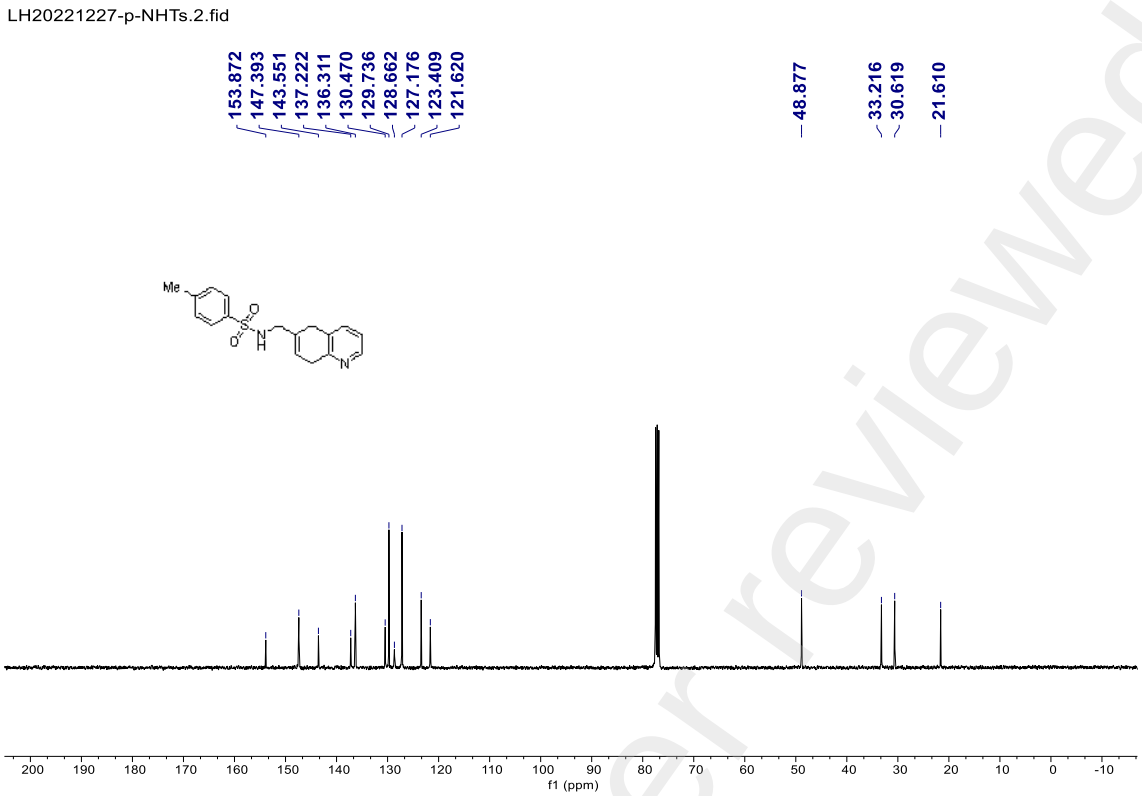
Analytical data of **37**:

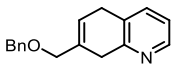
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 4.8 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.06 (dd, *J* = 7.6, 4.8 Hz, 1H), 5.74 (br, 1H), 5.25 (t, *J* = 6.4 Hz, 1H), 3.60 (d, *J* = 6.4 Hz, 2H), 3.47 - 3.38 (m, 2H), 3.34 - 3.27 (m, 2H), 2.37 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 153.9, 147.4, 143.6, 137.2, 136.3, 130.5, 129.7, 128.7, 127.2, 123.4, 121.6, 48.9, 33.2, 30.6, 21.6.

HRMS (ESI, *m/z*) calcd for $C_{17}H_{19}N_2O_2S$ $[M+H]^+$: 315.1162, found: 315.1156.







39, 50% yield

According to the general procedure, a mixture of **1ar** (0.2 mmol, 49.8 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **38** as yellow oil (34.9 mg, 70% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:3

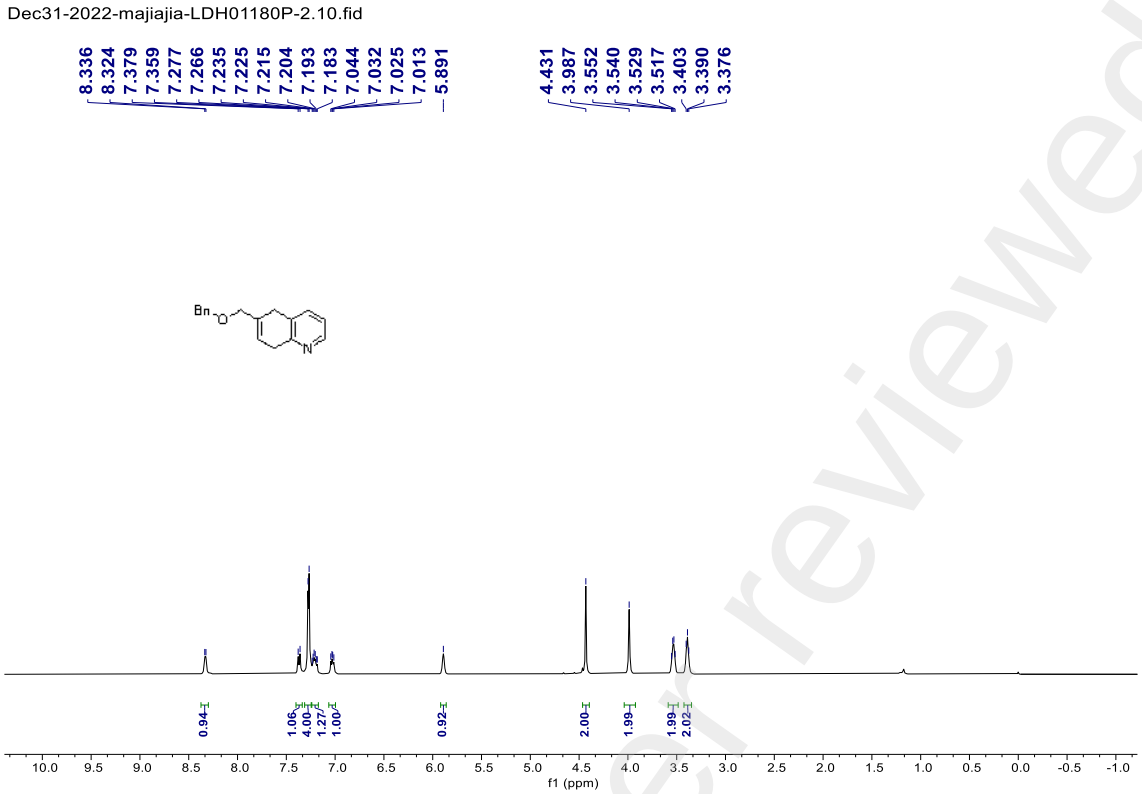
R*f* (**38**) = 0.35 in EtOAc/petroleum ether = 1:3.

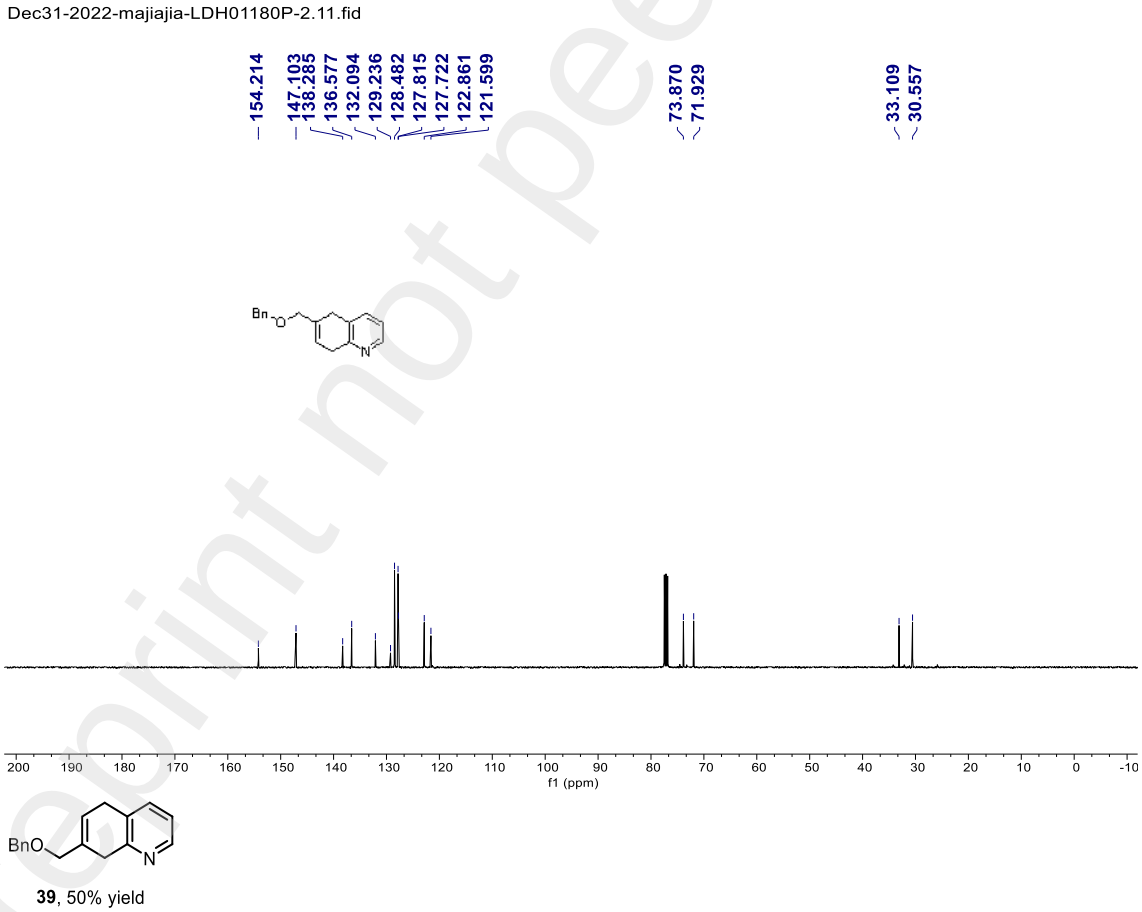
Analytical data of **38**:

^1H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 4.8 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 4.4 Hz, 4H), 7.24 - 7.17 (m, 1H), 7.03 (dd, *J* = 7.6, 4.8 Hz, 1H), 5.89 (br, 1H), 4.43 (s, 2H), 3.99 (s, 2H), 3.57 - 3.50 (m, 2H), 3.42 - 3.36 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.2, 147.1, 138.3, 136.6, 132.1, 129.2, 128.5, 127.8, 127.7, 122.9, 121.6, 73.9, 71.9, 33.1, 30.6.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{18}NO$ $[M+H]^+$: 252.1383, found: 252.1386.





39, 50% yield

According to the general procedure, a mixture of **1as** (0.2 mmol, 49.8 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol,

2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **39** as yellow oil (25.4 mg, 50% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:4

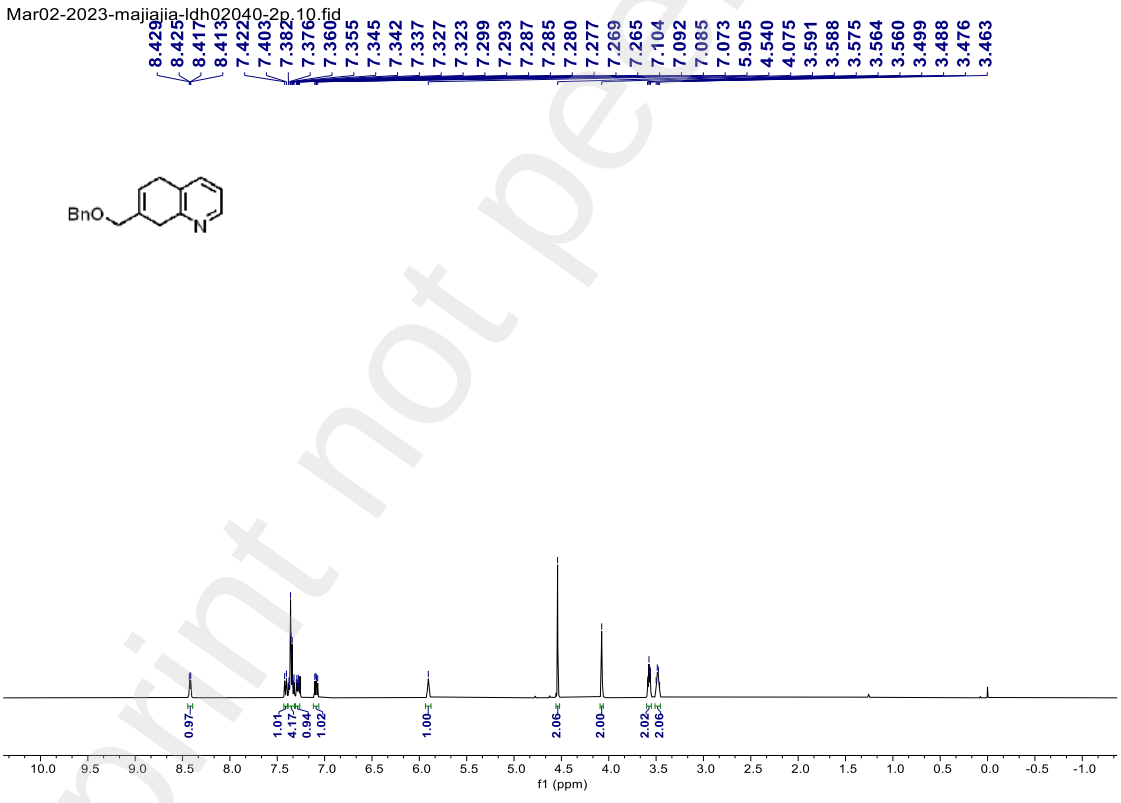
R_f(**39**) = 0.28 in EtOAc/petroleum ether = 1:3.

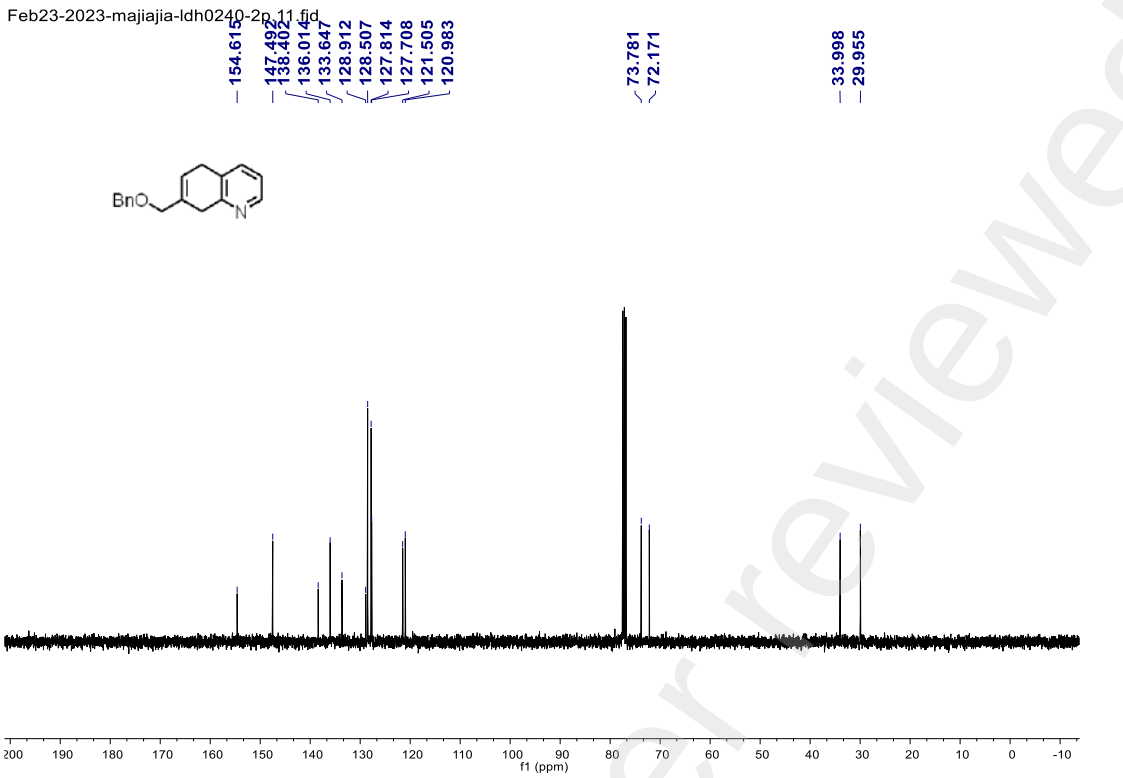
Analytical data of **39**:

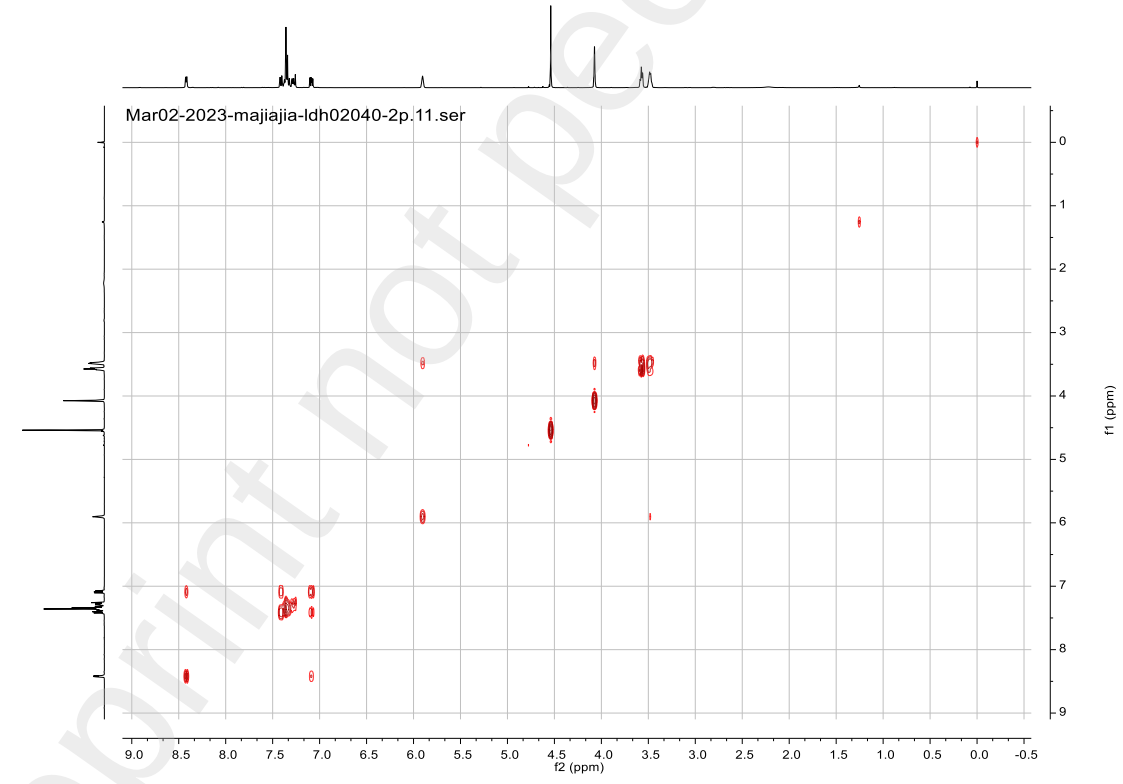
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.40 - 7.30 (m, 4H), 7.32 - 7.24 (m, 1H), 7.09 (dd, *J* = 7.6, 4.8 Hz, 1H), 5.91 (br, 1H), 4.54 (s, 2H), 4.07 (s, 2H), 3.59 - 3.55 (m, 2H), 3.51 - 3.46 (m, 2H).

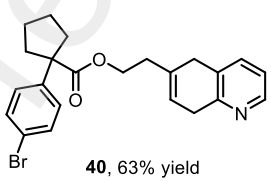
^{13}C NMR (101 MHz, $CDCl_3$) δ 154.6, 147.5, 138.4, 136.0, 133.6, 128.9, 128.5, 127.8, 127.7, 121.5, 121.0, 73.8, 72.2, 34.0, 30.0.

HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{18}NO^+$ $[M+H]^+$: 252.1383, found: 252.1383.









40, 63% yield

According to the general procedure xx, a mixture of 1ai (0.2 mmol, 84.6 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (2.1 mg, 1.0 mol%), $Gd(OTf)_3$ (0.4 mmol, 241.8 mg, 2.0 equiv.), γ-terpinene (0.6 mmol, 101 μL, 3.0 equiv.) and CH_3CN (4.0 mL, 0.05 M) were irradiated for 4 hours to afford product **40** as a yellow oil (53.7 mg, 63% yield).

Purification conditions: EtOAc/petroleum ether = 1:10 to 1:3

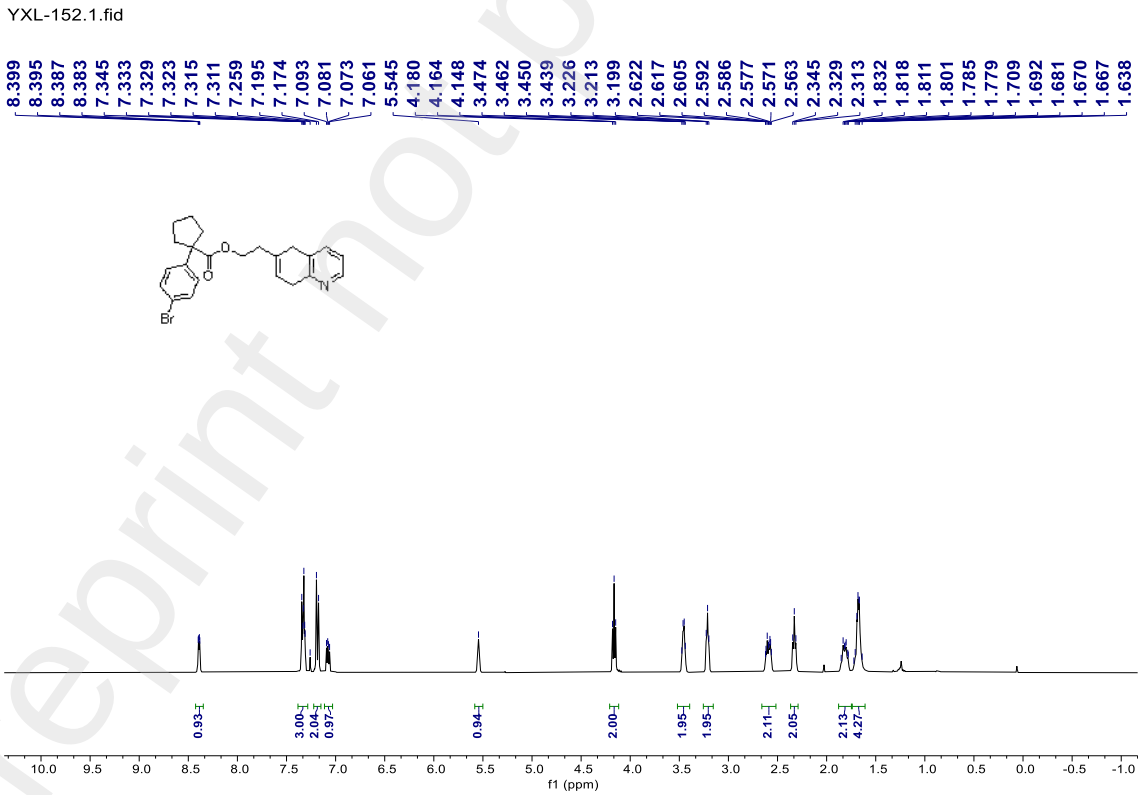
R_f (**40**) = 0.3 in EtOAc/petroleum ether = 1:4.

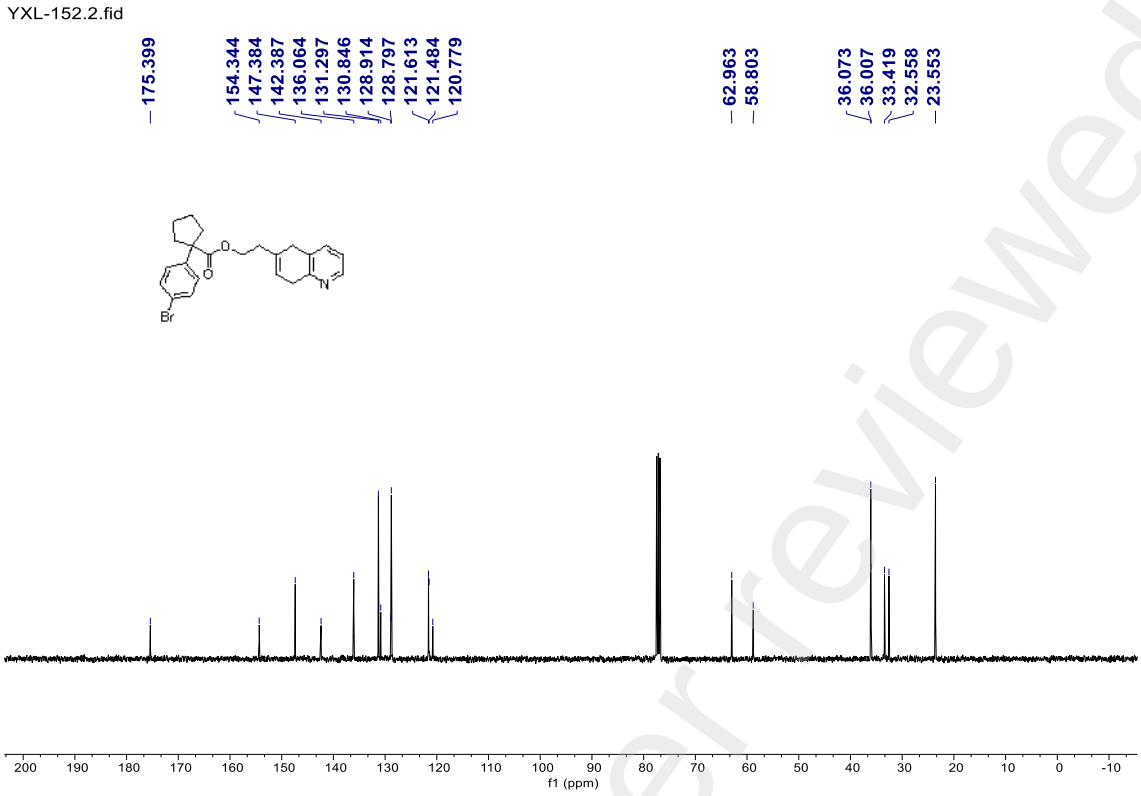
Analytical data of **40**:

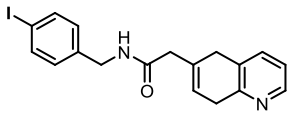
^1H NMR (400 MHz, $CDCl_3$) δ 8.39 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.36 - 7.29 (m, 3H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.08 (dd, *J* = 8.0, 4.8 Hz, 1H), 5.55 (br, 1H), 4.16 (t, *J* = 6.4 Hz, 2H), 3.49 - 3.42 (m, 2H), 3.25 - 3.17 (m, 2H), 2.69 - 2.50 (m, 2H), 2.33 (t, *J* = 6.4 Hz, 2H), 1.87 - 1.77 (m, 2H), 1.74 - 1.61 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.4, 154.3, 147.4, 142.4, 136.1, 131.3, 130.8, 128.9, 128.8, 121.6, 121.5, 120.8, 63.0, 58.8, 36.1, 36.0, 33.4, 32.6, 23.6.

HRMS (ESI, *m/z*) calcd for $C_{23}H_{25}BrNO_2$ $[M+H]^+$: 426.1063, found: 426.1060.







41, 73% yield

According to the general procedure, a mixture of **1aj** (0.2 mmol, 80.5 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **41** as yellow solid (59.0 mg, 73% yield, 95:5 r.r.).

Purification conditions: MeOH/CH_2Cl_2 = 1:50 to 1:20

R_f (**41**) = 0.3 in MeOH/CH_2Cl_2 = 1:20.

Analytical data of **41**:

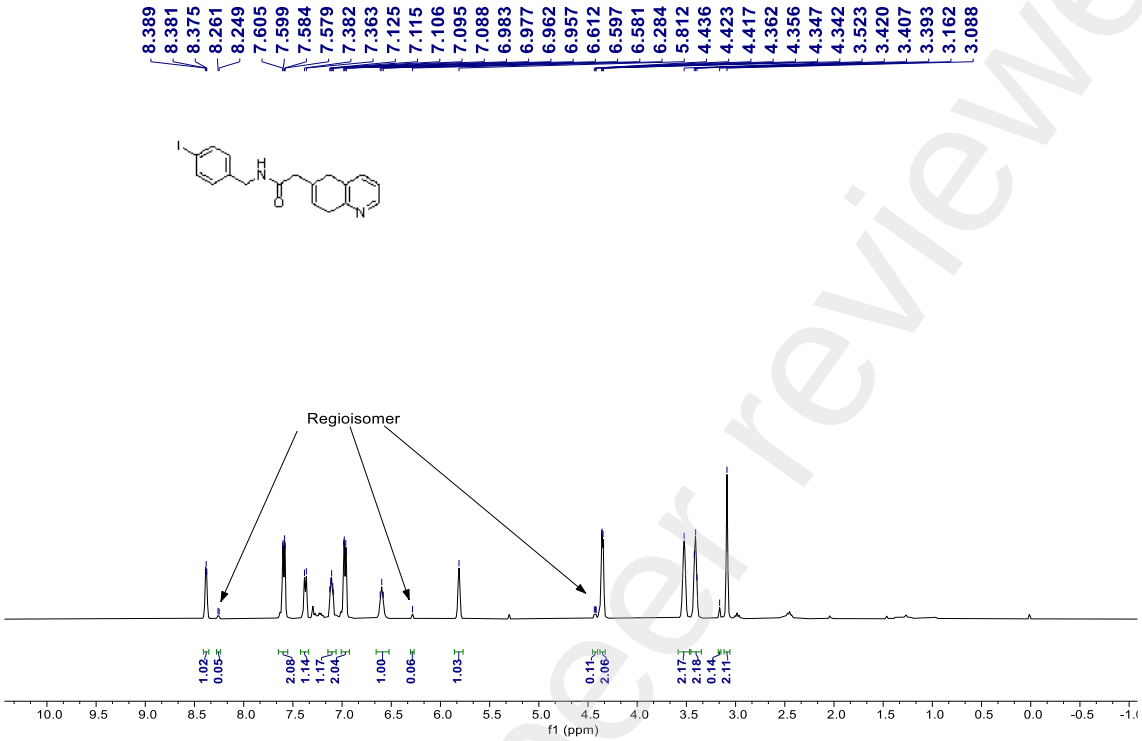
^{1}H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.41 - 8.35 (m, 1H), 8.27 - 8.24 (m, 1H, minor), 7.64 - 7.56 (m, 2H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.14 - 7.06 (m, 1H), 7.01 - 6.94 (m, 2H), 6.63 - 6.55 (m, 1H), 6.28 (br, 1H, minor), 5.81 (br, 1H), 4.44 - 4.40 (m, 2H, minor), 4.39 - 4.32 (m, 2H), 3.52 (br, 2H), 3.41 (br, 2H), 3.16 (br, 2H, minor), 3.09 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 153.8, 147.4, 138.1, 137.8, 137.7, 136.1, 129.6,

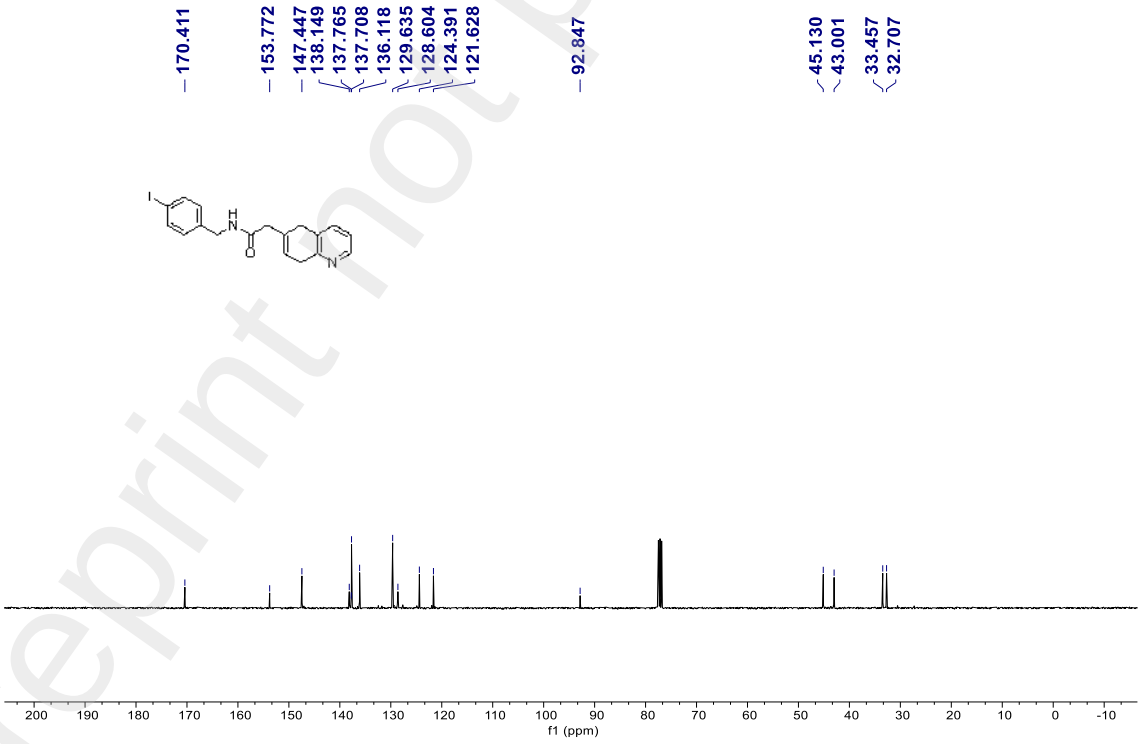
128.6, 124.4, 121.6, 92.8, 45.1, 43.0, 33.5, 32.7.

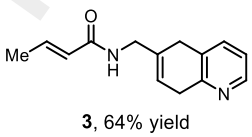
HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{18}IN_2O^+$ $[M+H]^+$: 405.0461, found: 405.0458.

cyp-230209-1p.1.fid



cyp-230209-1p.2.fid





3, 64% yield

According to the general procedure, a mixture of **1ak** (0.2 mmol, 45.2 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF_6 (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **3** as a white solid (29.0 mg, 64% yield, > 95:5 r.r.).

Purification conditions: MeOH/CH_2Cl_2 = 1:60 to 1:20

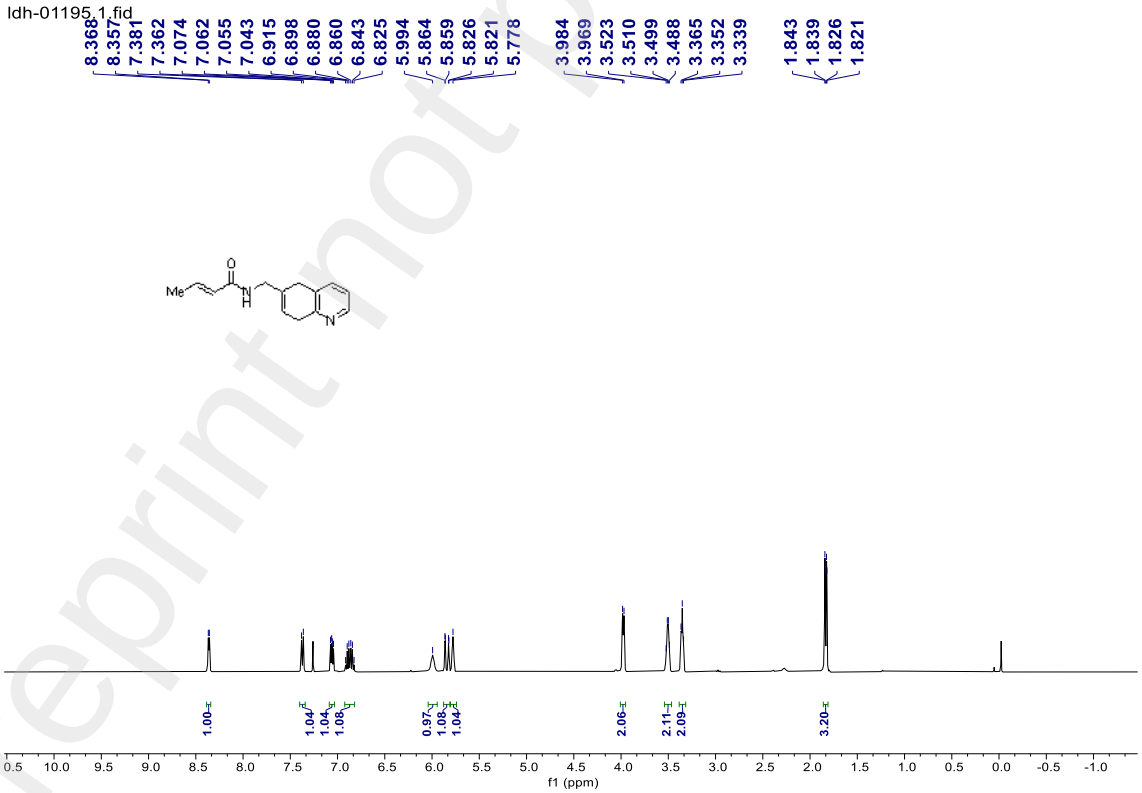
R_f (**3**) = 0.35 in MeOH/CH_2Cl_2 = 1:20.

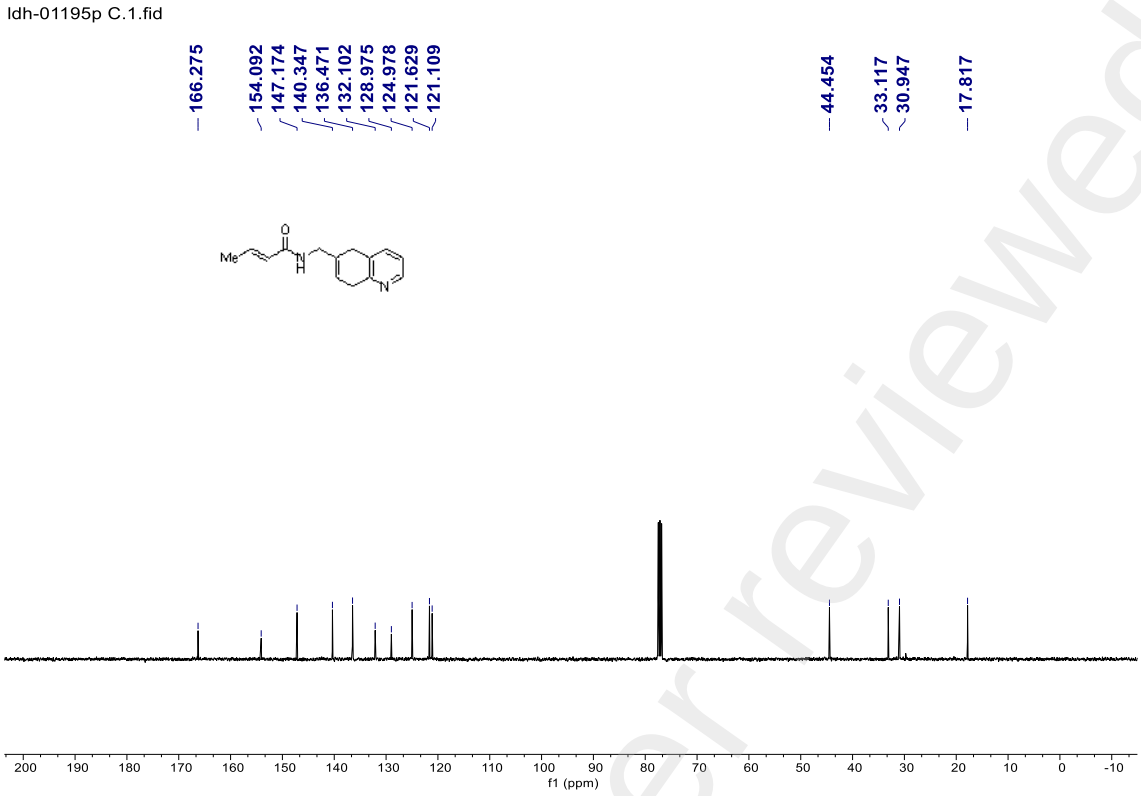
Analytical data of **3**:

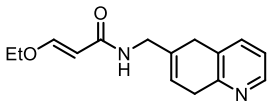
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 4.4 Hz, 1H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.06 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.94 - 6.80 (m, 1H), 5.99 (br, 1H), 5.84 (dd, *J* = 15.2, 2.0 Hz, 1H), 5.78 (br, 1H), 3.98 (d, *J* = 6.0 Hz, 2H), 3.55 - 3.47 (m, 2H), 3.39 - 3.32 (m, 2H), 1.83 (dd, *J* = 6.8, 1.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 154.1, 147.2, 140.3, 136.5, 132.1, 129.0, 125.0, 121.6, 121.1, 44.5, 33.1, 30.9, 17.8.

HRMS (ESI, *m*/*z*) calcd for $C_{14}H_{17}N_2O$ $[M+H]^+$:229.1335, found: 229.1340.







42, 87% yield

According to the general procedure, a mixture of **1al** (0.2 mmol, 51.3 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **42** as a yellow solid (44.9 mg, 87% yield, > 95:5 r.r.).

Purification conditions: Acetone/petroleum ether = 1:4 to 1:1

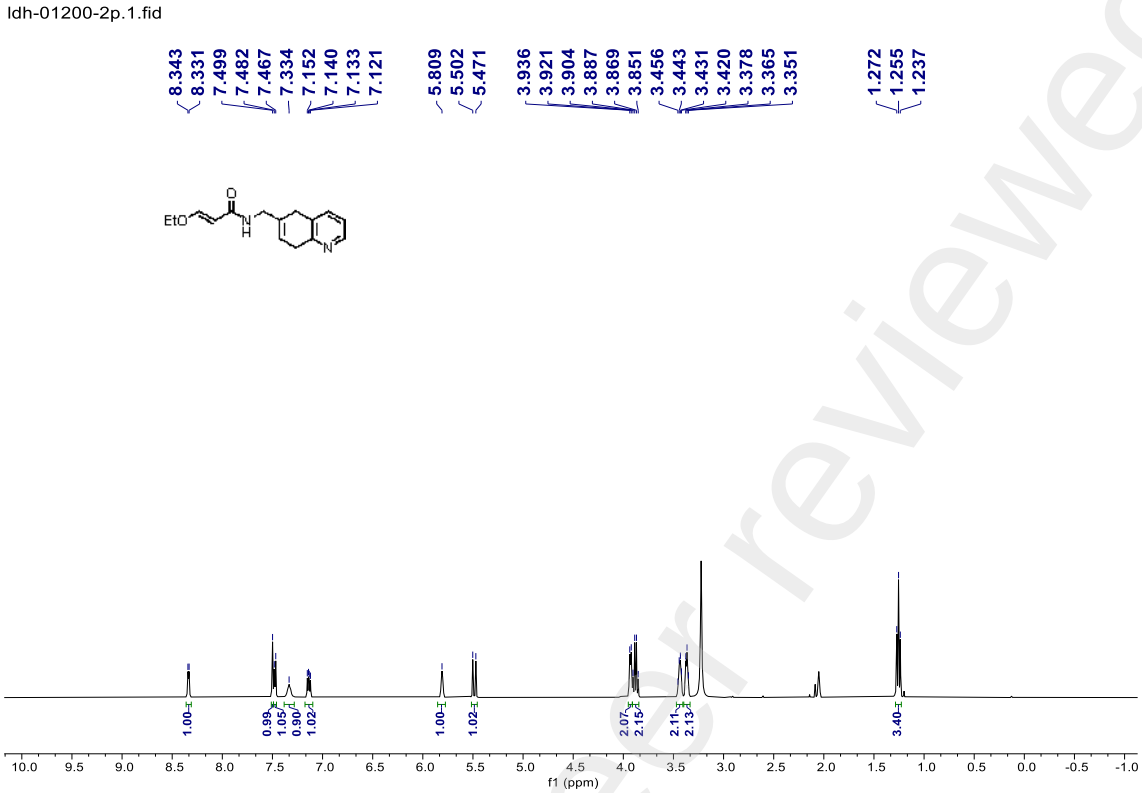
R_f (**42**) = 0.3 in Acetone /petroleum ether = 1:1.

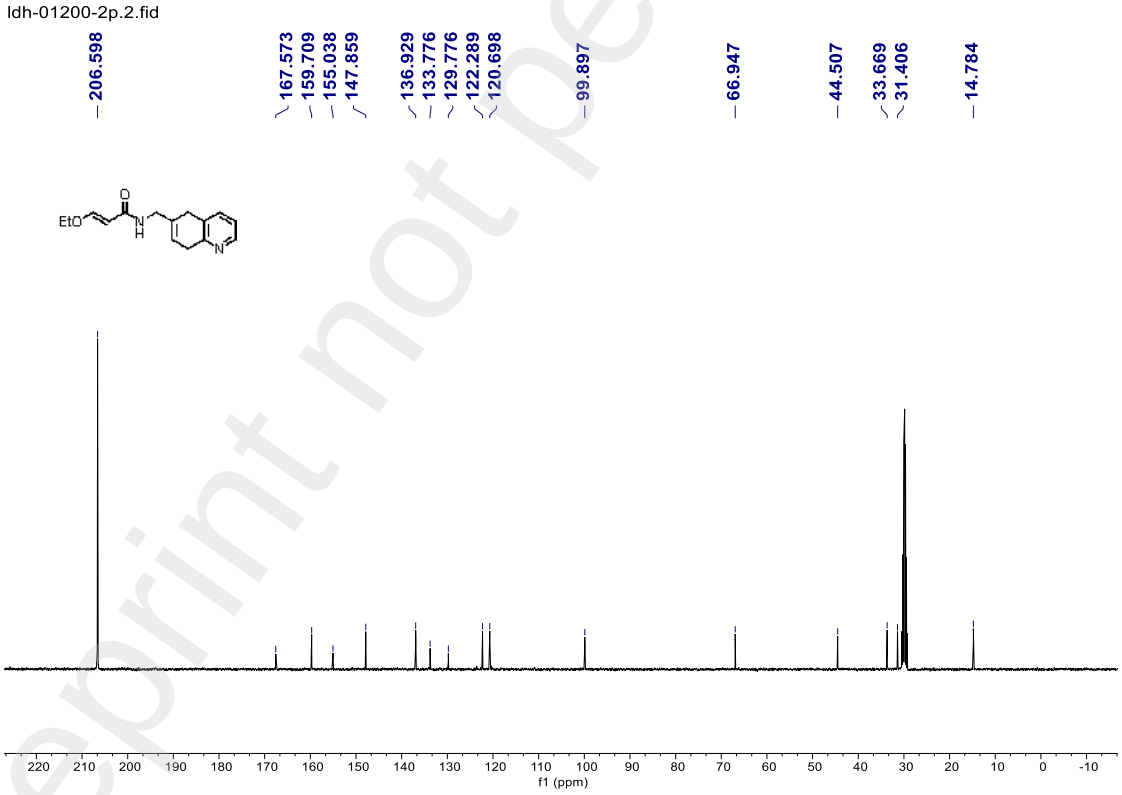
Analytical data of **42**:

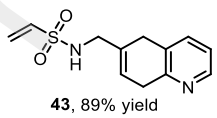
^{1}H NMR (400 MHz, Acetone-d_6) δ 8.34 (d, J = 4.8 Hz, 1H), 7.50 (br, 1H), 7.47 (d, J = 6.0 Hz, 1H), 7.33 (br, 1H), 7.14 (dd, J = 7.6, 4.8 Hz, 1H), 5.81 (br, 1H), 5.49 (d, J = 12.4 Hz, 1H), 3.93 (d, J = 6.0 Hz, 2H), 3.88 (q, J = 7.2 Hz, 2H), 3.48 - 3.40 (m, 2H), 3.40 - 3.33 (m, 2H), 1.25 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Acetone-d_6) δ 167.6, 159.7, 155.0, 147.9, 136.9, 133.8, 129.8, 122.3, 120.7, 99.9, 66.9, 44.5, 33.7, 31.4, 14.8.

HRMS (ESI, *m/z*) calcd for $C_{15}H_{19}N_2O_2$ $[M+H]^+$: 259.1441, found: 259.1445.







43, 89% yield

According to the general procedure, a mixture of **1an** (0.2 mmol, 49.6 mg, 1.0 equiv.),

$Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **43** as a yellow solid (44.5 mg, 89% yield, > 95:5 r.r.).

Purification conditions: Acetone/petroleum ether = 1:4 to 1:1

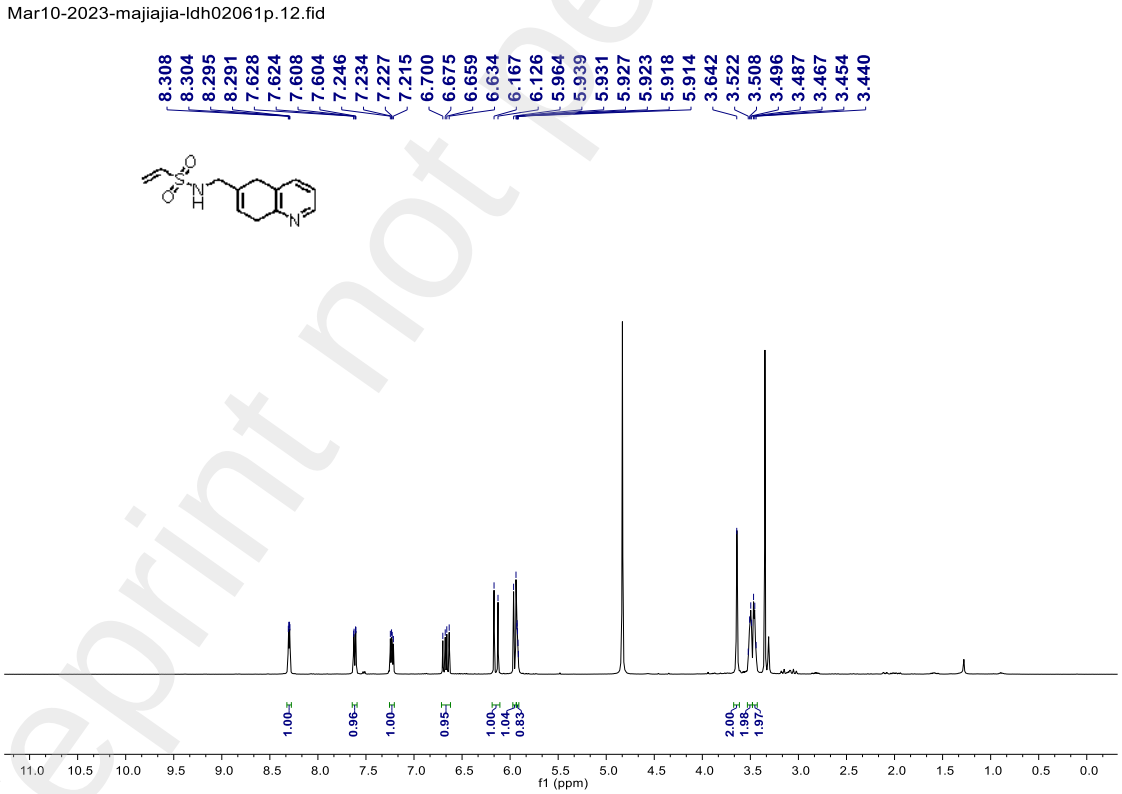
R_f (**43**) = 0.3 in Acetone /petroleum ether = 1:1.

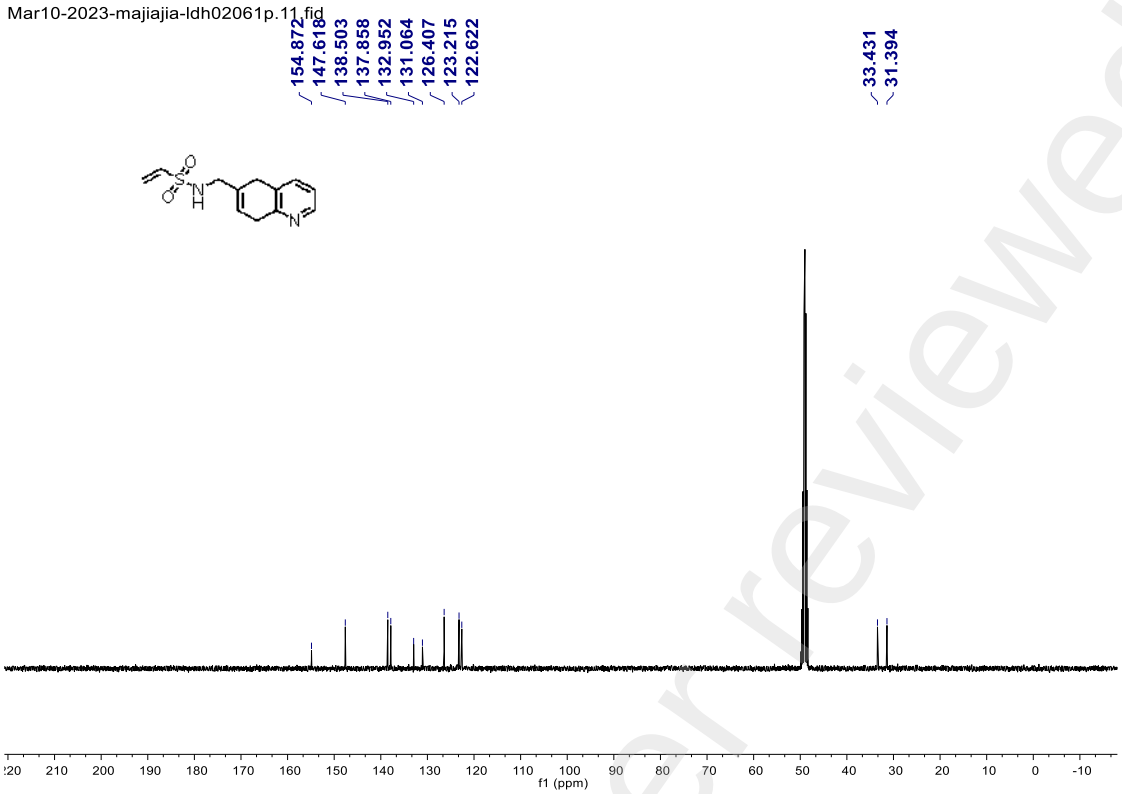
Analytical data of **43**:

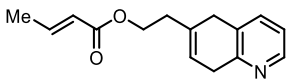
^1H NMR (400 MHz, CD_3OD) δ 8.30 (dd, *J* = 5.2, 2.0 Hz, 1H), 7.62 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.23 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.67 (dd, *J* = 16.4, 10.0 Hz, 1H), 6.15 (d, *J* = 16.4 Hz, 1H), 5.95 (d, *J* = 10.0 Hz, 1H), 5.93 - 5.91 (m, 1H), 3.64 (s, 2H), 3.53 - 3.48 (m, 2H), 3.48 - 3.43 (m, 2H).

^{13}C NMR (101 MHz, CD_3OD) δ 154.9, 147.6, 138.5, 137.9, 133.0, 131.1, 126.4, 123.2, 122.6, 33.4, 31.4.

HRMS (ESI, *m/z*) calcd for $C_{12}H_{15}N_2O_2S^+$ $[M+H]^+$: 251.0854, found: 251.0845.







44, 74% yield, 95:5 r.r.

According to the general procedure, a mixture of **1am** (0.2 mmol, 48.2 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **44** as a colorless oil (35.9 mg, 74% yield, 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:3

R_f (**44**) = 0.35 in EtOAc/petroleum ether = 1:2.

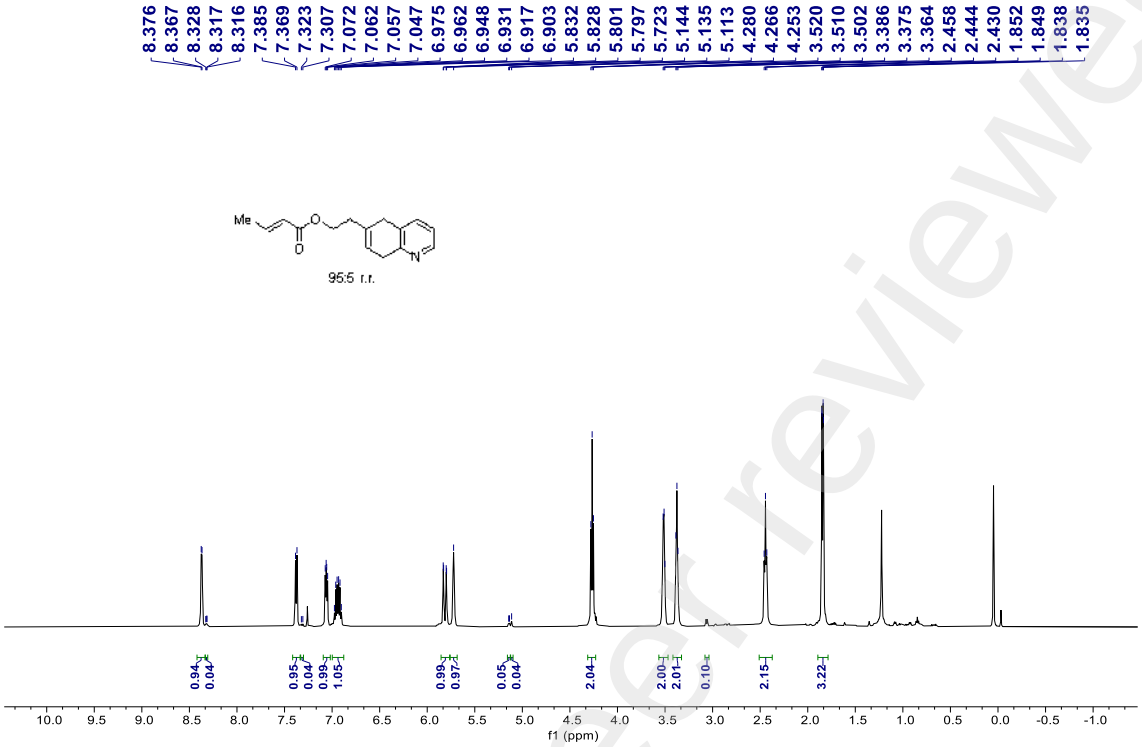
Analytical data of **44**:

^{1}H NMR (500 MHz, $CDCl_3$, mixture of regioisomers) δ 8.37 (d, *J* = 4.2 Hz, 1H), 8.33 - 8.31 (m, 1H, minor), 7.38 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H, minor), 7.09 - 7.03 (m, 1H), 6.98 - 6.90 (m, 1H), 5.81 (dd, *J* = 15.5, 2.0 Hz, 1H), 5.72 (br, 1H), 5.14 (d, *J* = 4.5 Hz, 1H, minor), 5.11 (s, 1H, minor), 4.27 (t, *J* = 6.8 Hz, 2H), 3.56 - 3.47 (m, 2H), 3.41 - 3.34 (m, 2H), 2.44 (t, *J* = 7.0 Hz, 2H), 1.84 (dd, *J* = 7.0, 1.5 Hz, 3H).

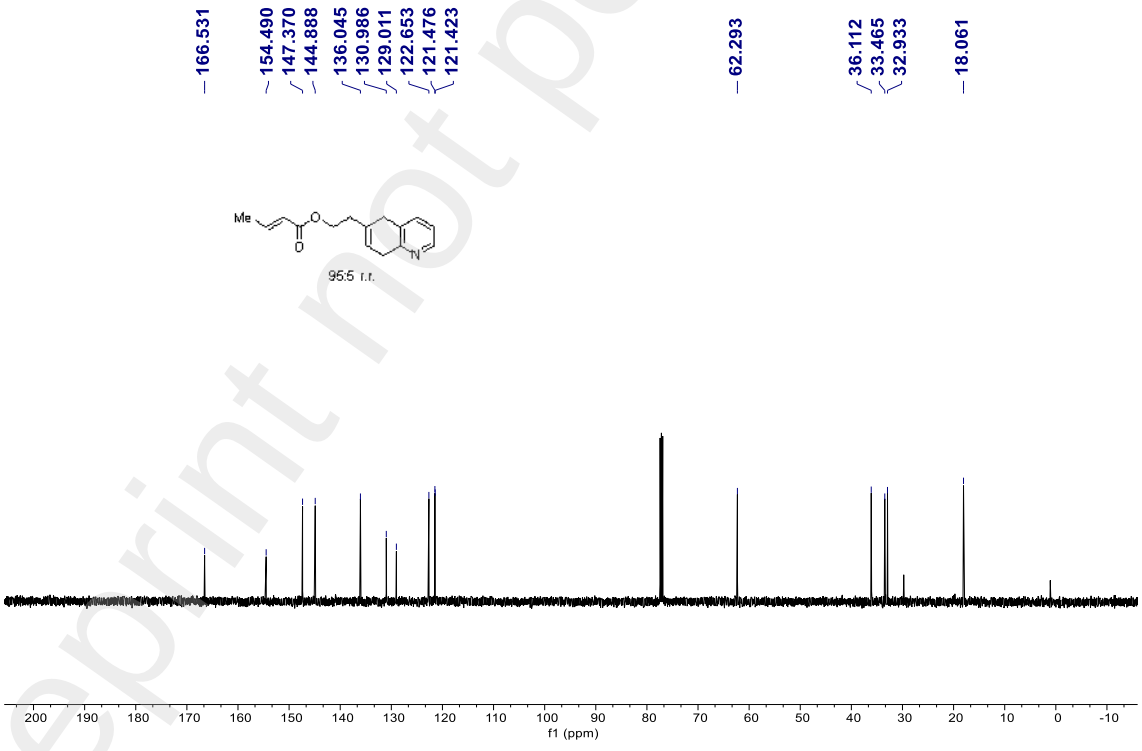
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.5, 154.5, 147.4, 144.9, 136.0, 131.0, 129.0, 122.7, 121.5, 121.4, 62.3, 36.1, 33.5, 32.9, 18.1.

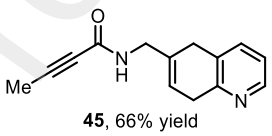
HRMS (ESI, *m/z*) calcd for $C_{15}H_{18}NO_2^+$ $[M+H]^+$: 244.1338, found: 244.1334.

LDH02147P.10.fid



LDH02147P.12.fid





45, 66% yield

According to the general procedure, a mixture of **1ao** (0.1 mmol, 22.4 mg, 1.0 equiv.),

$Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.001 mmol, 1.0 mol%, 1.1 mg), $Gd(OTf)_3$ (0.2 mmol, 2.0 equiv., 121 mg), γ-terpinene (0.3 mmol, 3.0 equiv., 48 μL) and CH_3CN (2.0 mL, 0.05 M) were stirred for 6 h to give the desired product **45** as yellow solid (15.0 mg, 66% yield, > 95:5 r.r.).

Purification conditions: $MeOH/CH_2Cl_2$ = 1:40 to 1:20

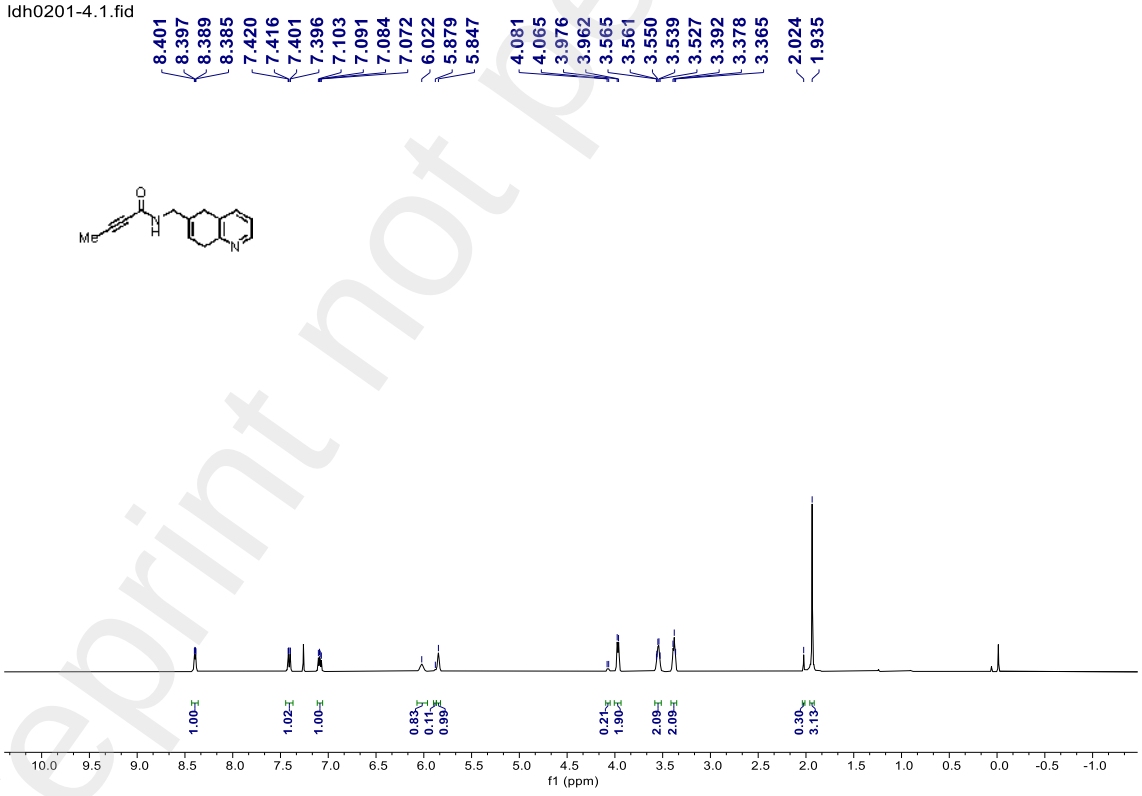
R_f (**45**) = 0.3 in $MeOH/CH_2Cl_2$ = 1:20.

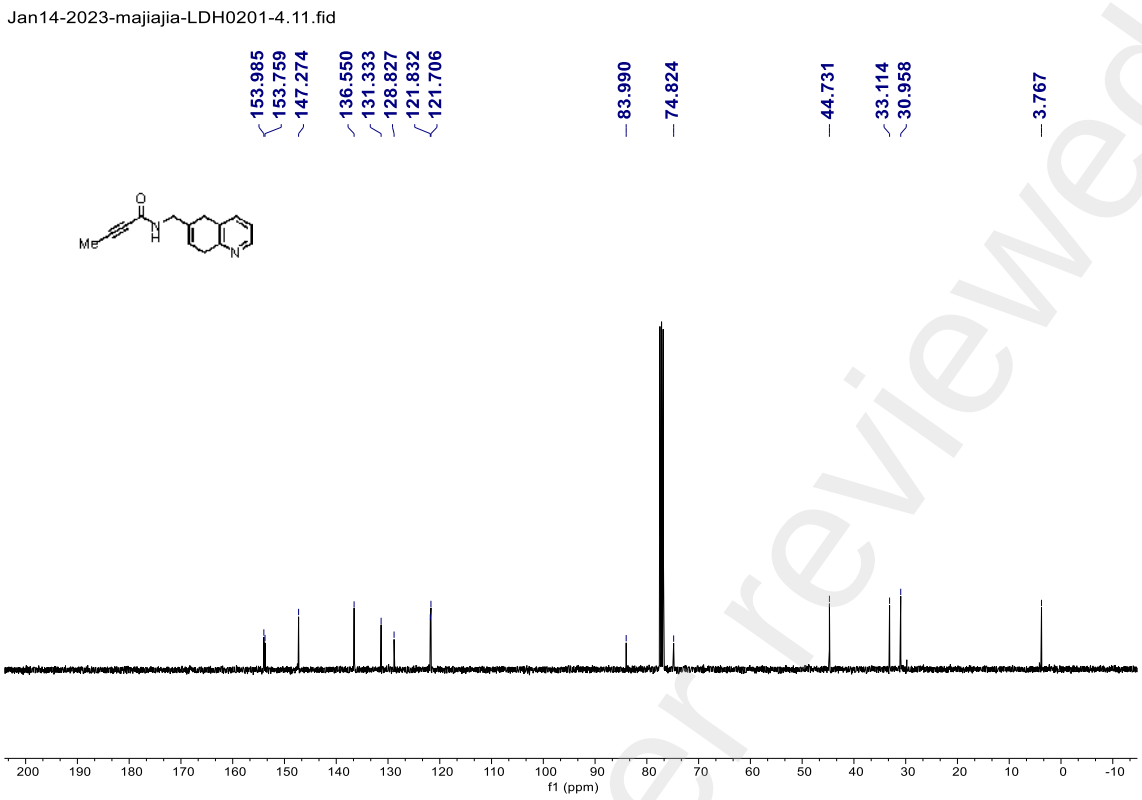
Analytical data of **45**:

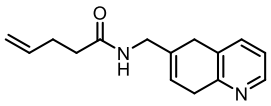
^1H NMR (400 MHz, $CDCl_3$, mixture of rotamer) δ 8.39 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.41 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.09 (dd, *J* = 7.6, 4.8 Hz, 1H), 6.02 (br, 1H), 5.88 (br, 1H, rotamer), 5.85 (br, 1H), 4.07 (d, *J* = 6.4 Hz, 2H, rotamer), 3.59 - 3.50 (m, 2H), 3.40 - 3.36 (m, 2H), 2.02 (s, 3H, rotamer), 1.94 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 154.0, 153.8, 147.3, 136.6, 131.3, 128.8, 121.8, 121.7, 84.0, 74.8, 44.7, 33.1, 31.0, 3.8.

HRMS (ESI, *m/z*) calcd for $C_{14}H_{14}N2O$ $[M+H]^+$: 227.1179, found: 227.1179.







46, 63% yield

According to the general procedure, a mixture of **1ap** (0.2 mmol, 48.0 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (2.0 mL, 0.05 M) were stirred for 6 h to give the desired product **46** as yellow solid (30.5 mg, 63% yield).

Purification conditions: MeOH/CH_2Cl_2 = 1:40 to 1:20

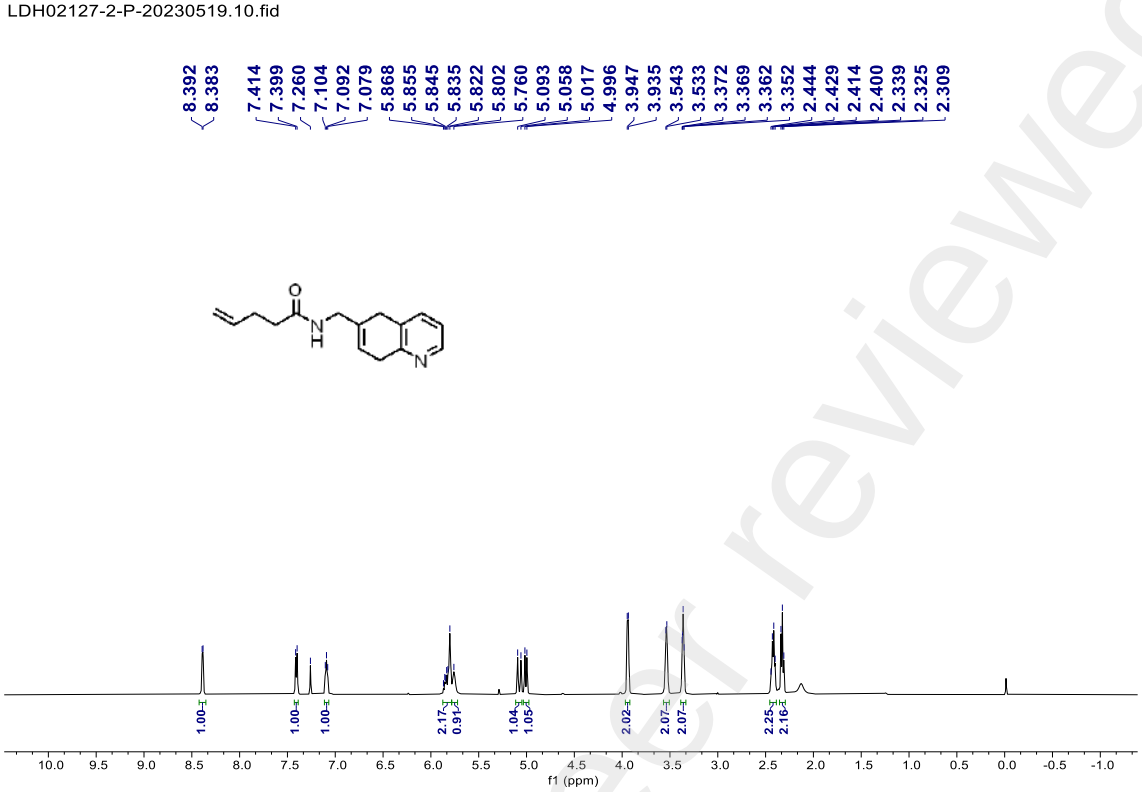
R_f (**46**) = 0.3 in MeOH/CH_2Cl_2 = 1:20.

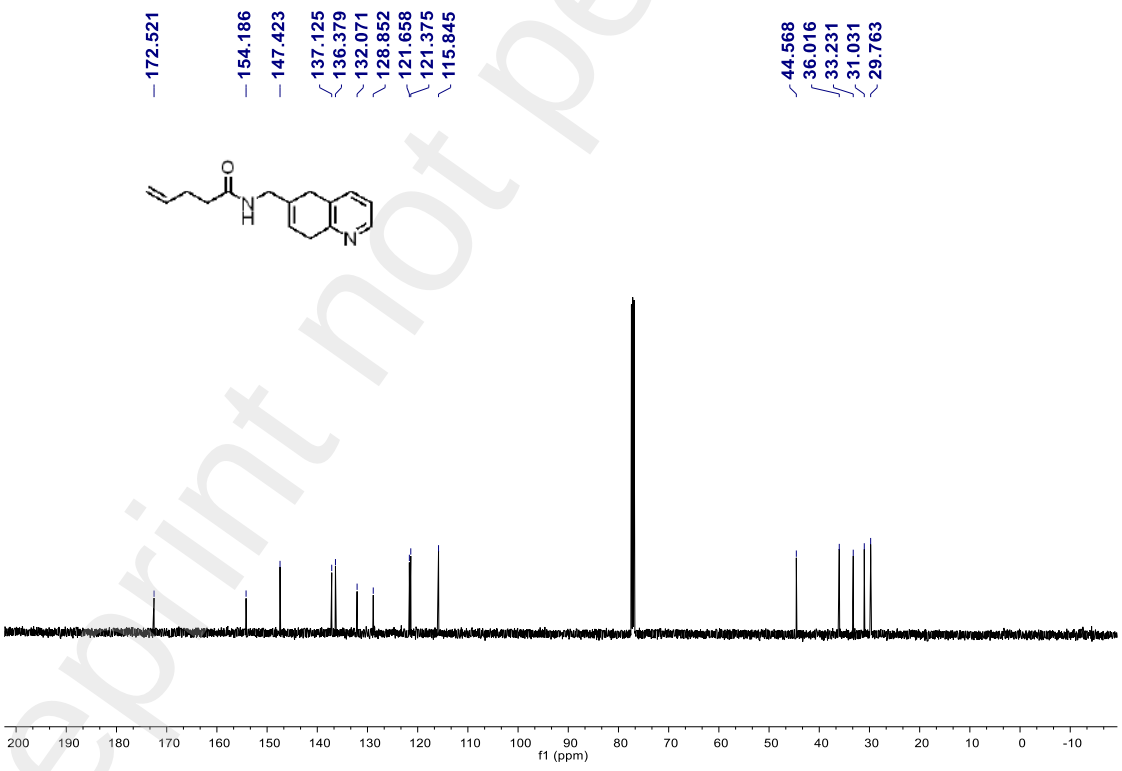
Analytical data of **46**:

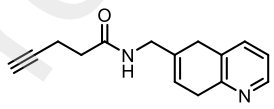
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 4.5 Hz, 1H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 6.0 Hz, 1H), 5.89 - 5.78 (m, 2H), 5.76 (br, 1H), 5.08 (d, *J* = 17.5 Hz, 1H), 5.01 (d, *J* = 10.5 Hz, 1H), 3.94 (d, *J* = 6.0 Hz, 2H), 3.57 - 3.51 (m, 2H), 3.39 - 3.33 (m, 2H), 2.45 - 2.39 (m, 2H), 2.35 - 2.30 (m, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.5, 154.2, 147.4, 137.1, 136.4, 132.1, 128.9, 121.7, 121.4, 115.8, 44.6, 36.0, 33.2, 31.0, 29.8.

HRMS (ESI, *m/z*) calcd for $C_{15}H_{19}N_2O^+$ $[M+H]^+$: 243.1497, found: 243.1500.







47, 70% yield

According to the general procedure, a mixture of **1aq** (0.2 mmol, 47.6 mg, 1.0 equiv.),

$Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 6 h to give the desired product **47** as yellow solid (33.6 mg, 70% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:2

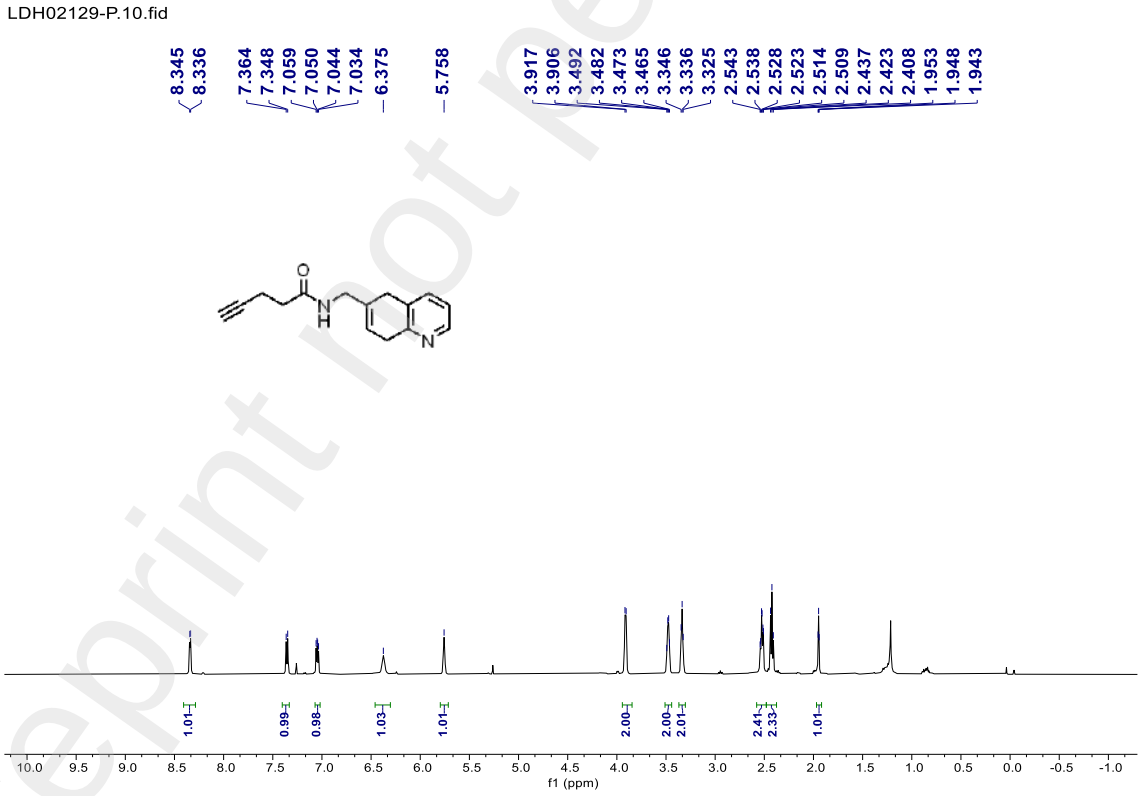
R_f (**47**) = 0.3 in EtOAc/petroleum ether = 1:22.

Analytical data of **47**:

^1H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 4.5 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.05 (dd, *J* = 7.5, 4.5 Hz, 1H), 6.38 (br, 1H), 5.76 (br, 1H), 3.91 (d, *J* = 5.5 Hz, 2H), 3.51 - 3.45 (m, 2H), 3.36 - 3.31 (m, 2H), 2.56 - 2.49 (m, 2H), 2.45 - 2.39 (m, 2H), 1.95 (t, *J* = 2.5 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 171.2, 154.2, 147.5, 136.3, 131.9, 128.8, 121.6, 121.5, 83.1, 69.5, 44.7, 35.5, 33.3, 31.0, 15.1.

HRMS (ESI, *m/z*) calcd for $C_{15}H_{17}N_2O^+$ $[M+H]^+$: 241.1341, found: 241.1338.



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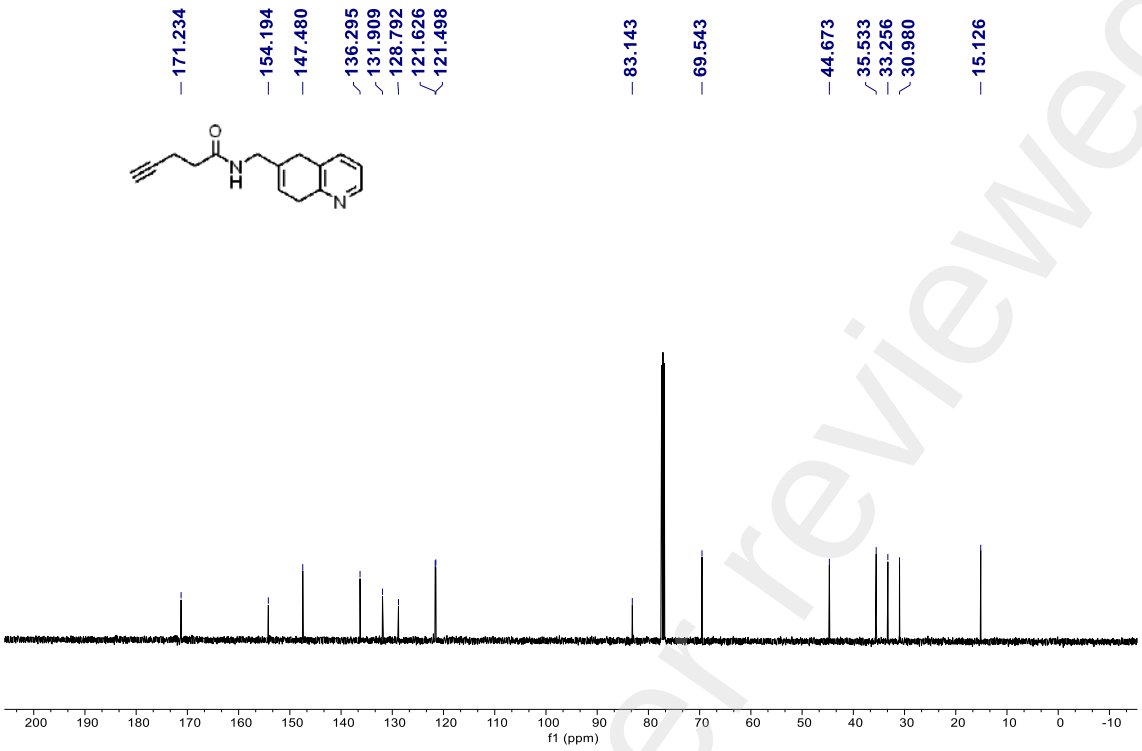
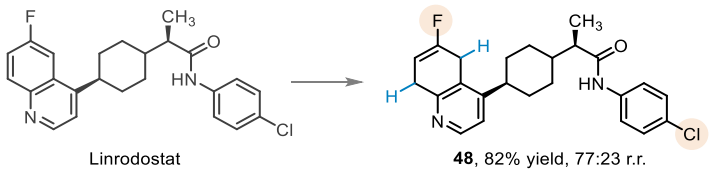


7. Late-Stage Reduction of Drugs and Synthetic Transformations



According to the general procedure, a mixture of **Linrodostat** (0.1 mmol, 41.1 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.001 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.2 mmol, 2.0 equiv., 121 mg), γ-terpinene (0.3 mmol, 3.0 equiv., 48 μL) and CH_3CN (2.0 mL, 0.05 M) were stirred for 4 h to give the desired product **48** as yellow oil (34.0 mg, 82% yield, 73:23 r.r.).

Purification conditions: Acetone/petroleum ether = 1:6 to 1:3

R_f (**48**) = 0.35 in Acetone/petroleum ether = 1:2.

Analytical data of **48**:

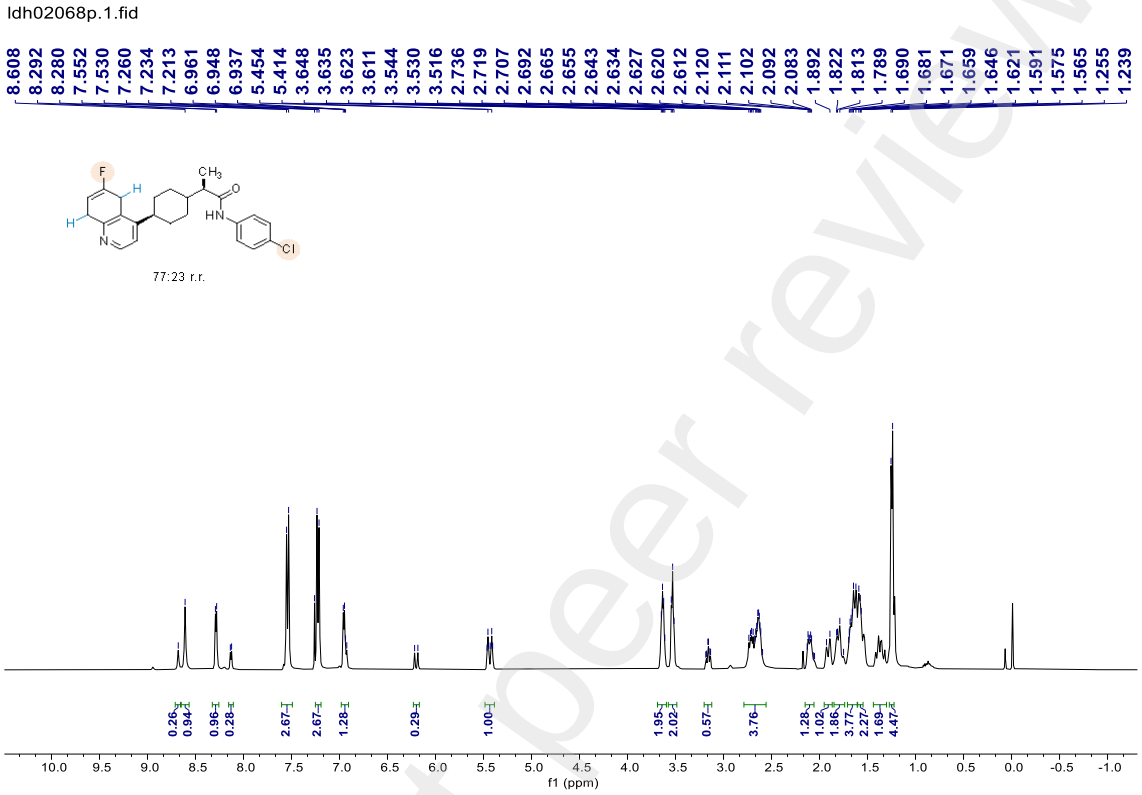
^{1}H NMR (400 MHz, $CDCl_3$, mixture of regioisomers) δ 8.68 (s, 1H, minor), 8.61 (s, 1H), 8.29 (d, *J* = 4.8 Hz, 1H), 8.13 (d, *J* = 5.2 Hz, 1H, minor), 7.54 (d, *J* = 8.8 Hz, 2H, major; d, *J* = 8.8 Hz, 2H, minor), 7.22 (d, *J* = 8.4 Hz, 2H, major; d, *J* = 8.4 Hz, 2H, minor), 6.98 - 6.90 (m, 1H, major; m, 1H, minor), 6.20 (d, *J* = 13.6 Hz, 1H, minor), 5.43 (dt, *J* = 15.2, 3.2 Hz, 1H), 3.67 - 3.59 (m, 2H), 3.57 - 3.49 (m, 2H), 3.16 (td, *J* = 8.8, 2.8 Hz, 2H, minor), 2.79 - 2.56 (m, 3H, major; m, 3H, minor), 2.16 - 2.03 (m, 1H, major; m, 1H, minor), 1.9 (d, *J* = 14.2 Hz, 1H), 1.85 - 1.73 (m, 1H, major; m, 2H, minor), 1.70 - 1.61 (m, 3H, major; m, 3H, minor), 1.61 - 1.55 (m, 1H, major; m, 1H, minor), 1.44 - 1.32 (m, 1H, major; m, 1H, minor), 1.27 - 1.19 (m, 3H, major; m, 3H, minor).

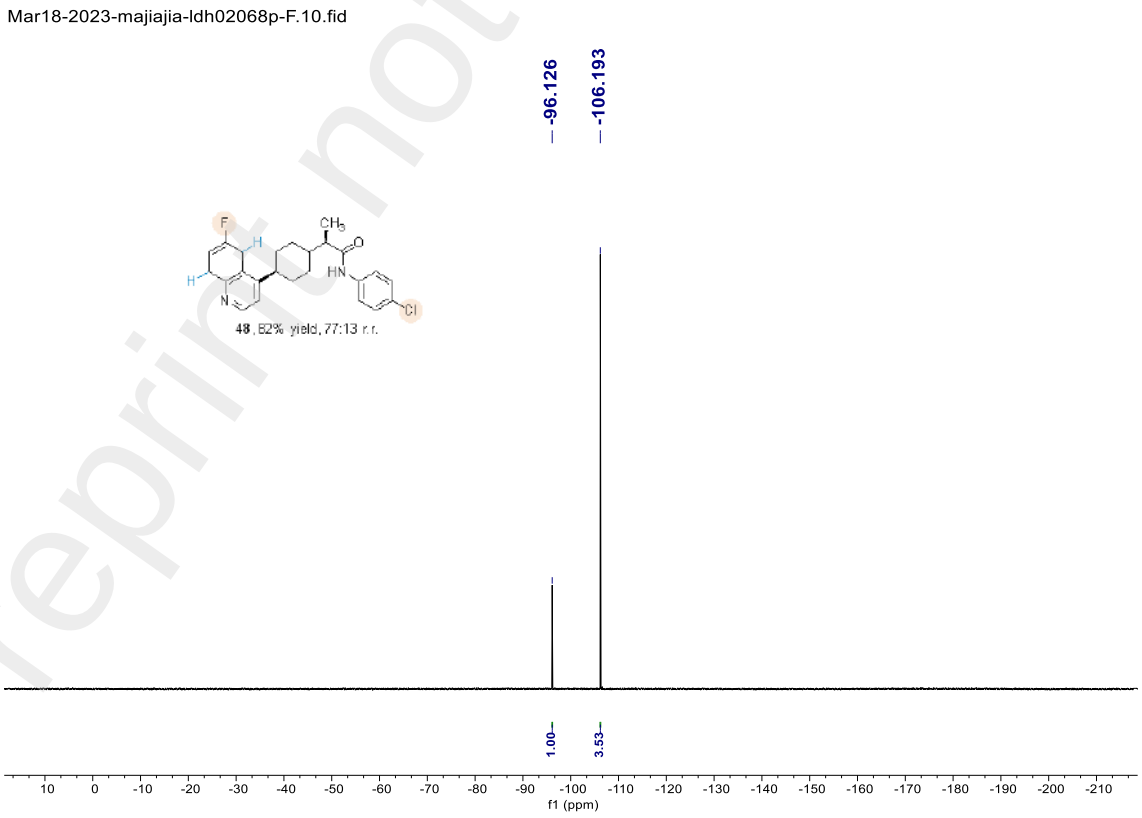
^{19}F NMR (376 MHz, $CDCl_3$) δ -96.13(minor), -106.19.

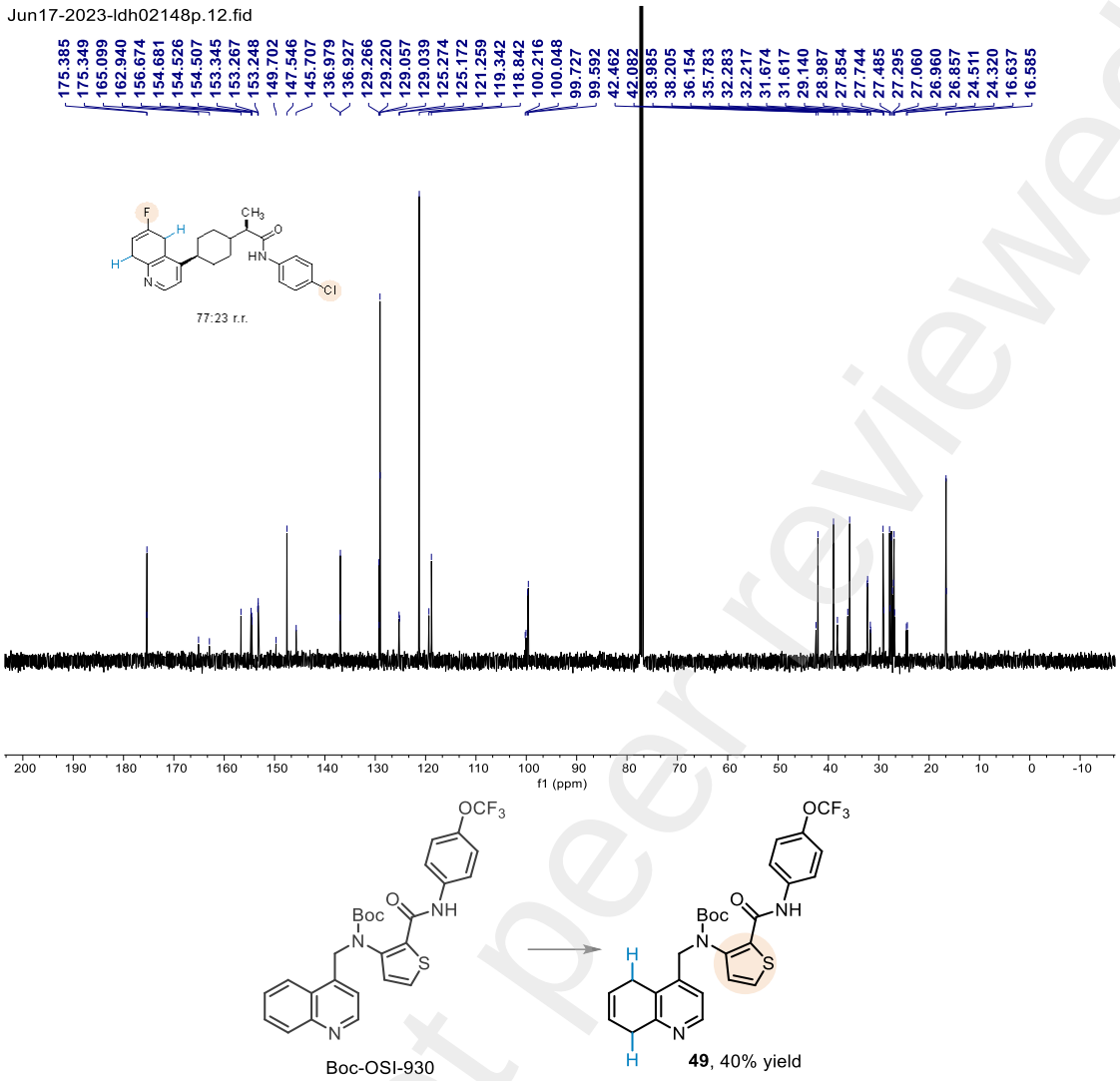
^{13}C NMR (126 MHz, $CDCl_3$) δ 175.39(minor), 175.35, 164.0 (d, *J* = 271.6 Hz, minor), 155.7 (d, *J* = 250.6 Hz), 154.5 (d, *J* = 2.3 Hz), 153.3, 153.26 (d, *J* = 2.3 Hz), 149.7(minor), 147.6, 145.7(minor), 137.0(minor), 136.9, 129.3, 129.2(minor), 129.1, 129.0 (minor), 125.2 (d, *J* = 12.8 Hz, minor), 121.3, 119.3(minor), 118.8, 100.1 (d, *J* = 21.0 Hz, minor), 99.7 (d, *J* = 17.0 Hz), 42.5(minor), 42.1, 39.0, 38.2(minor),

36.2(minor), 35.8, 32.3 (d, J = 8.2 Hz), 31.7 (d, J = 7.2 Hz, minor), 29.1, 29.0(minor), 27.9, 27.7(minor), 27.5, 27.2 (d, J = 29.6 Hz), 27.0, 26.9(minor), 24.4 (d, J = 24.0 Hz, minor), 16.6, 16.58(minor).

HRMS (ESI, m/z) calcd for $C_{24}H_{26}N_2OFCl^+$ $[M+H]^+$:413.1796, found: 413.1793.







According to the general procedure, a mixture of **Boc-OSI-930** (0.2 mmol, 108.7 mg, 1.0 equiv.), Ir[dF(Me)ppy]$_2$(dtbbpy)PF$_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), Gd(OTf)$_3$ (0.4 mmol, 2.0 equiv., 242 mg), γ-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **49** as white solid (43.8 mg, 40% yield, > 95:5 r.r.).

Purification conditions: EtOAc/petroleum ether = 1:4 to 1:1

R_f (**49**) = 0.4 in EtOAc/petroleum ether = 1:1.

Analytical data of **49**:

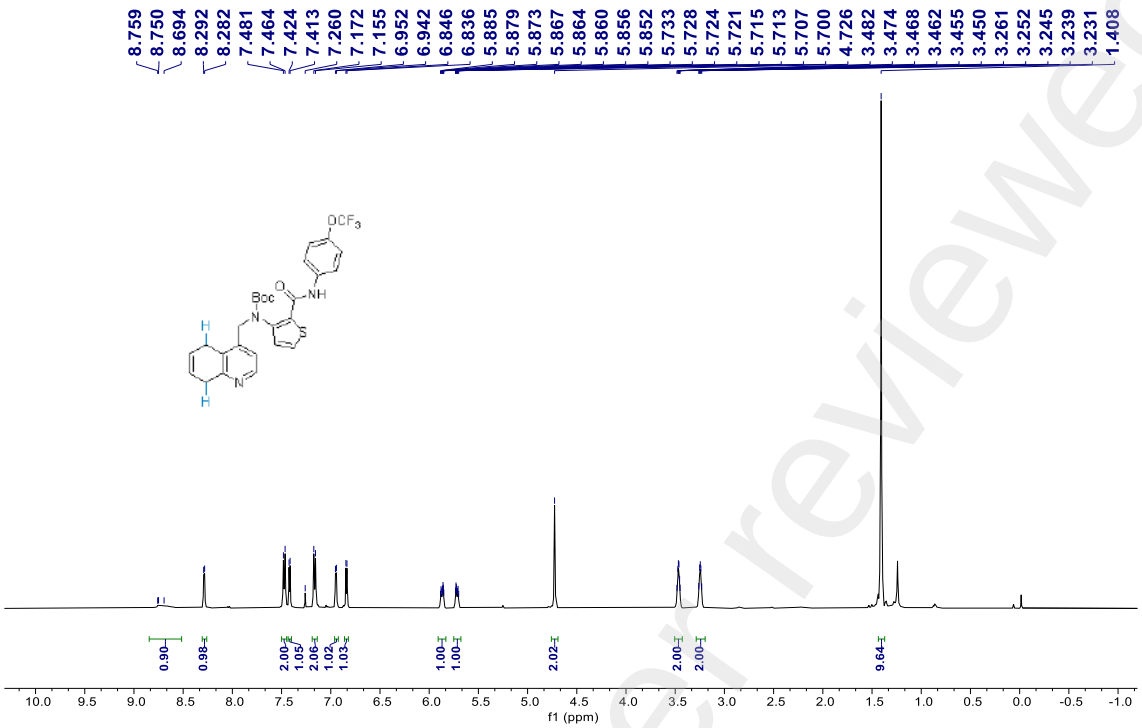
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.83 - 8.61 (m, 1H), 8.29 (d, *J* = 5.0 Hz, 1H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 5.5 Hz, 1H), 7.16 (d, *J* = 8.5 Hz, 2H), 6.95 (d, *J* = 5.0 Hz, 1H), 6.84 (d, *J* = 5.0 Hz, 1H), 5.90 - 5.84 (m, 1H), 5.75 - 5.68 (m, 1H), 4.73 (s, 2H), 3.50 - 3.43 (m, 2H), 3.28 - 3.21 (m, 2H), 1.41 (s, 9H).

^{19}F NMR (471 MHz, $CDCl_3$) δ -58.10.

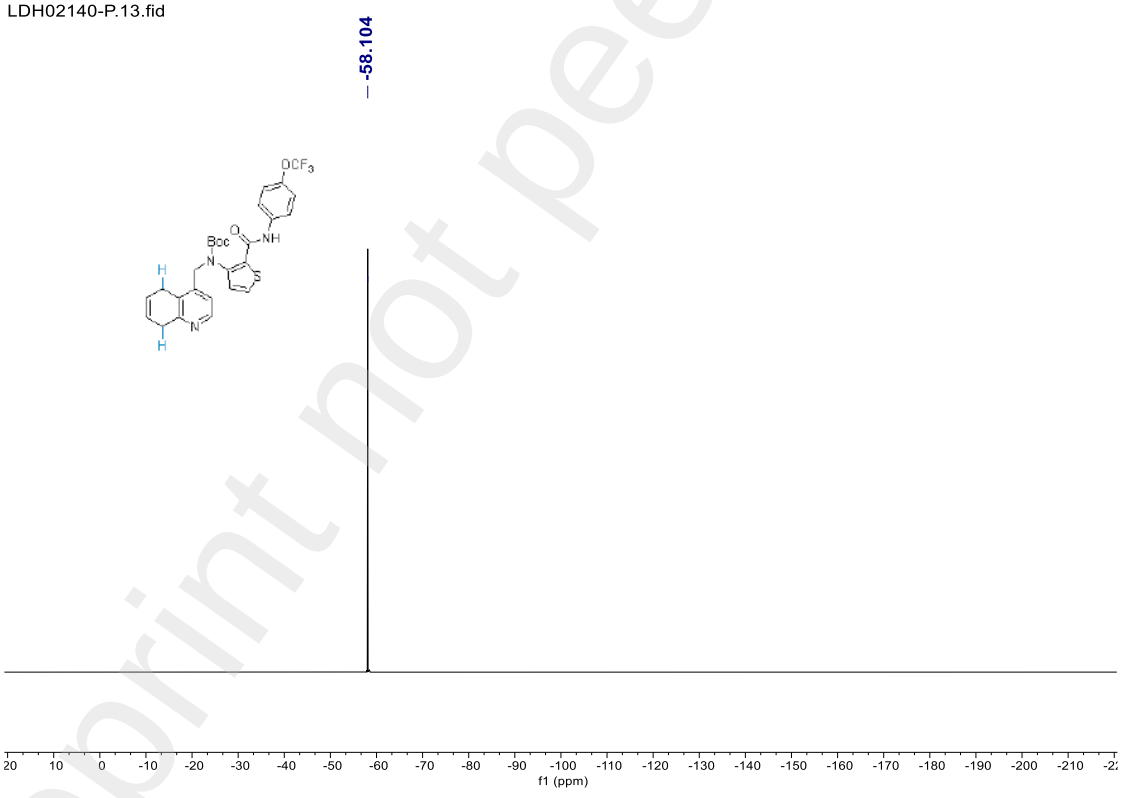
^{13}C NMR (126 MHz, $CDCl_3$) δ 159.28, 155.07, 147.42, 145.49, 143.34, 138.58, 136.30, 134.02, 128.78, 127.21, 126.70, 124.85, 122.46, 121.91, 121.59 (q, J = 257.4 Hz), 120.97, 120.64, 83.16, 50.89, 33.0, 28.3, 26.7.

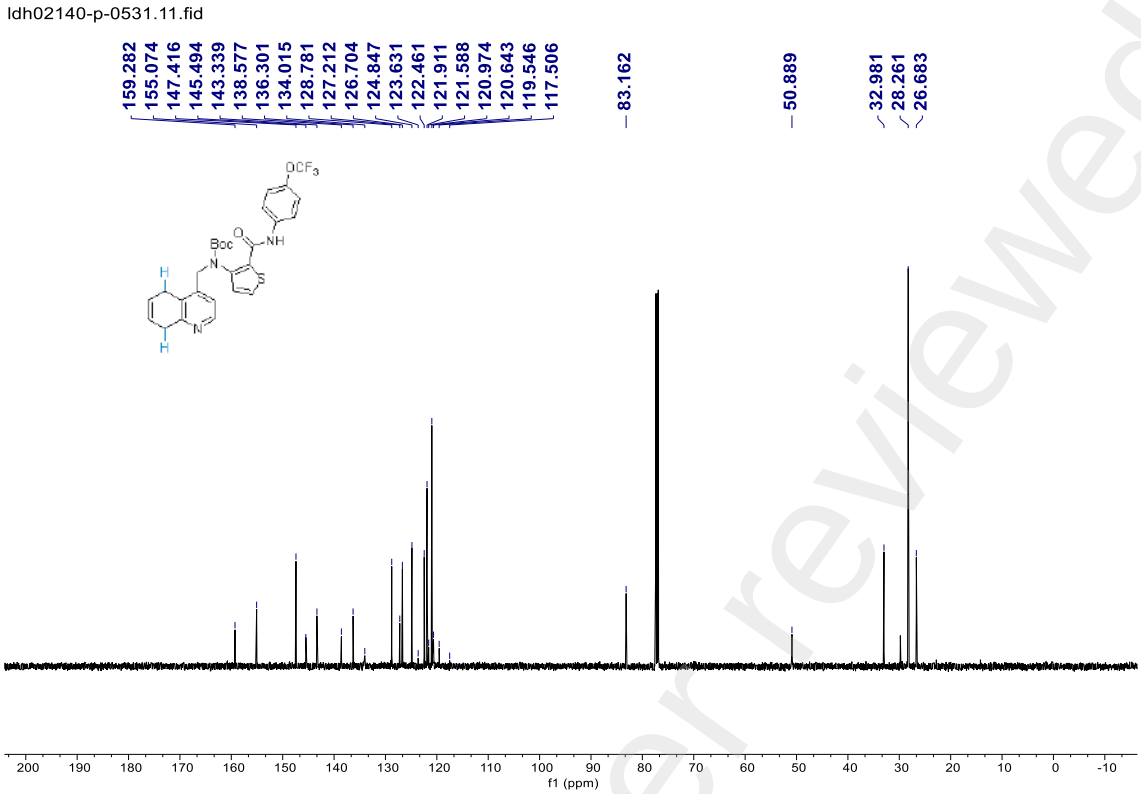
HRMS (ESI, *m*/*z*) calcd for $C_{27}H_{27}F_3N3O_4S^+$ $[M+H]^+$: 546.1669, found: 546.1659.

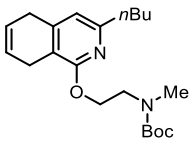
ldh02140-p-0531.10.fid



LDH02140-P.13.fid







51, 46% yield

According to the general procedure, a mixture of **Quinisocaine analog 50** (0.2 mmol, 71.6 mg, 1.0 equiv.), $Ir[dF(Me)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 1.0 mol%, 2.2 mg), $Gd(OTf)_3$ (0.4 mmol, 2.0 equiv., 242 mg), *γ*-terpinene (0.6 mmol, 3.0 equiv., 96 μL) and CH_3CN (4.0 mL, 0.05 M) were stirred for 4 h to give the desired product **51** as colorless oil (33.2 mg, 46% yield, > 95:5 r.r.).

Purification conditions: EtOAc/CH_2Cl_2 = 1:80 to 1:50

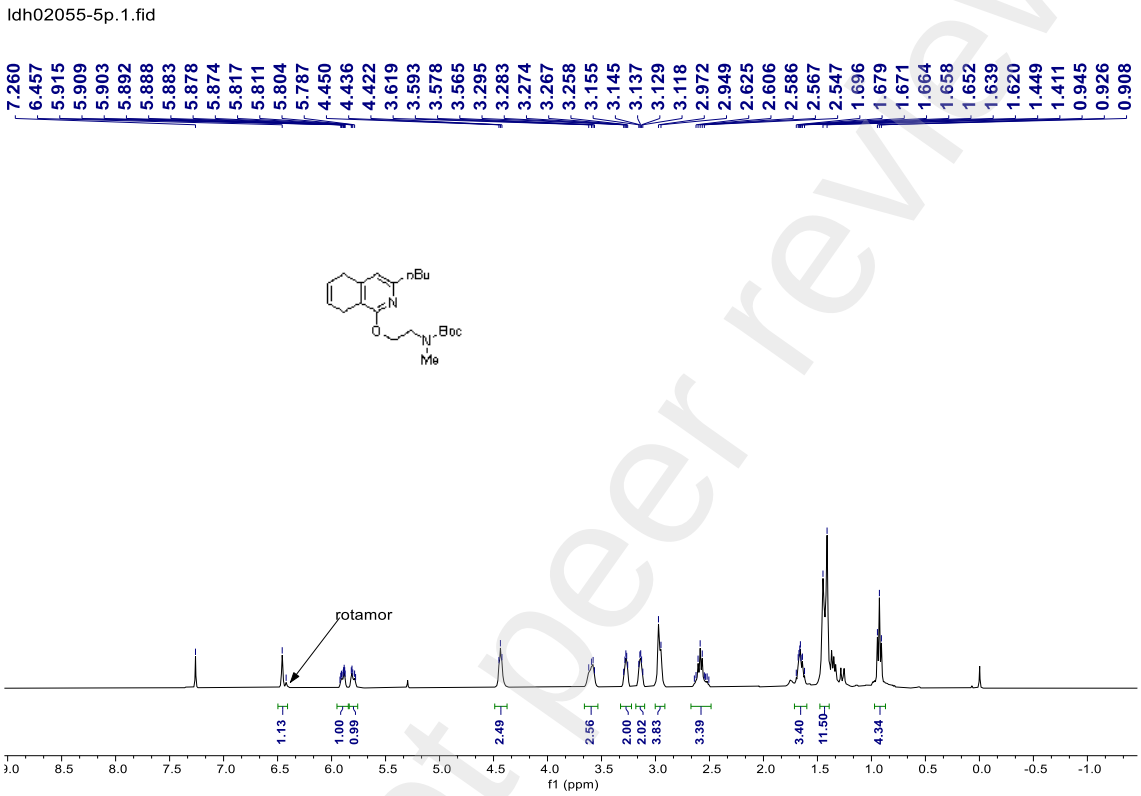
R_f (**51**) = 0.3 in EtOAc/CH_2Cl_2 = 1:40.

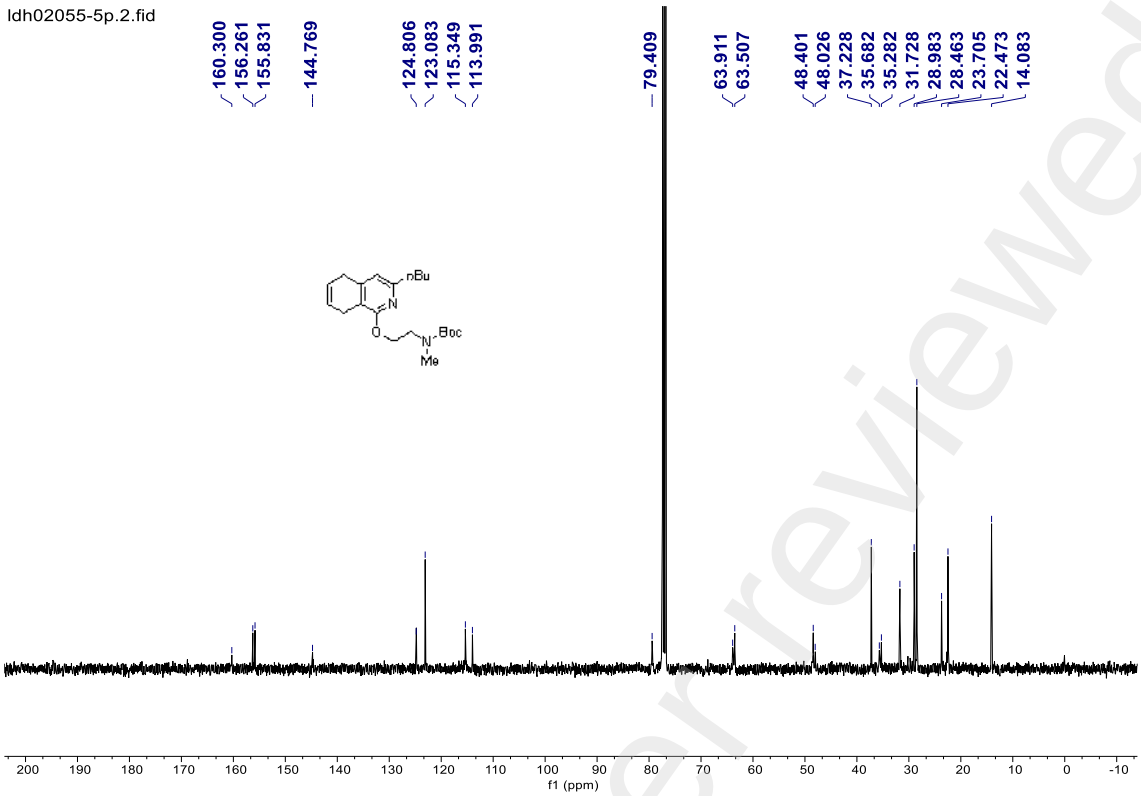
Analytical data of **51**:

^{1}H NMR (400 MHz, $CDCl_3$, mixture of rotamer) δ 6.46 (s, 1H), 5.95 - 5.85 (m, 1H), 5.84 - 5.76 (m, 1H), 4.47 - 4.40 (m, 2H), 3.66 - 3.54 (m, 2H), 3.32 - 3.23 (m, 2H), 3.14 (dt, *J* = 7.8, 4.3 Hz, 2H), 3.01 - 2.91 (m, 3H), 2.68 - 2.50 (m, 3H), 1.74 - 1.59 (m, 3H), 1.51 - 1.38 (m, 9H) 0.93 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.3, 156.3, 155.8, 144.8, 124.8, 123.1, 115.3, 114.0, 79.4, 63.9(rotamer), 63.5, 48.4, 48.0(rotamer), 37.2, 35.7(rotamer), 35.3, 31.7, 29.0, 28.5, 23.7, 22.5, 14.1.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{33}N_2O_3$ $[M+H]^+$: 361.2486, found: 361.2490.





Synthetic transformations of Birch-type product 50

To a solution of **51** (36.5 mg, 0.1 mmol, 1.0 equiv.) and Pd/C (Pd 5% on Carbon wetted with ca. 55% water, 10.0 mg) in MeOH (1.5 mL) was stirred for overnight under hydrogen atmosphere at room temperature. After completion of reaction, the resulting mixture was filtered by diatomaceous earth and washed with EtOAc (3 × 3mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **52** as a colorless oil (33.7 mg, 92% yield).

Purification conditions: Et_2O/petroleum ether = 1:50 to 1:10

R_f (**52**) = 0.4 in Et_2O/petroleum ether = 1:10.

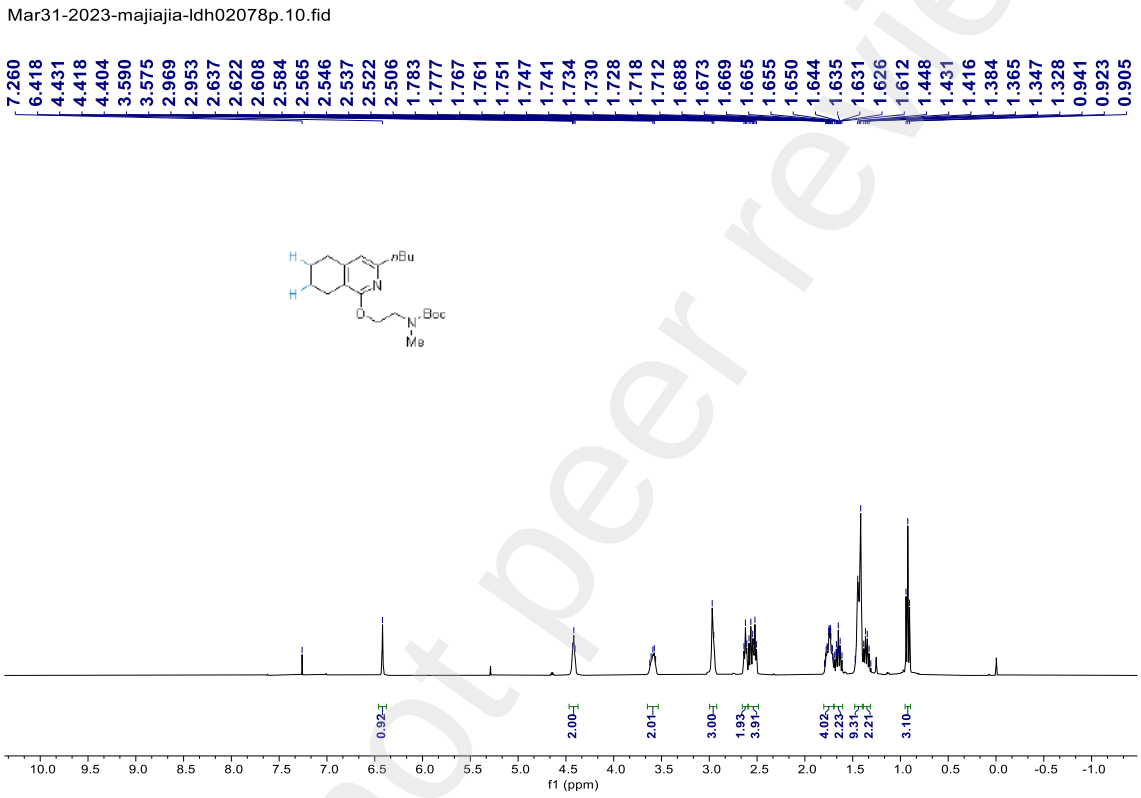
Analytical data of **52**:

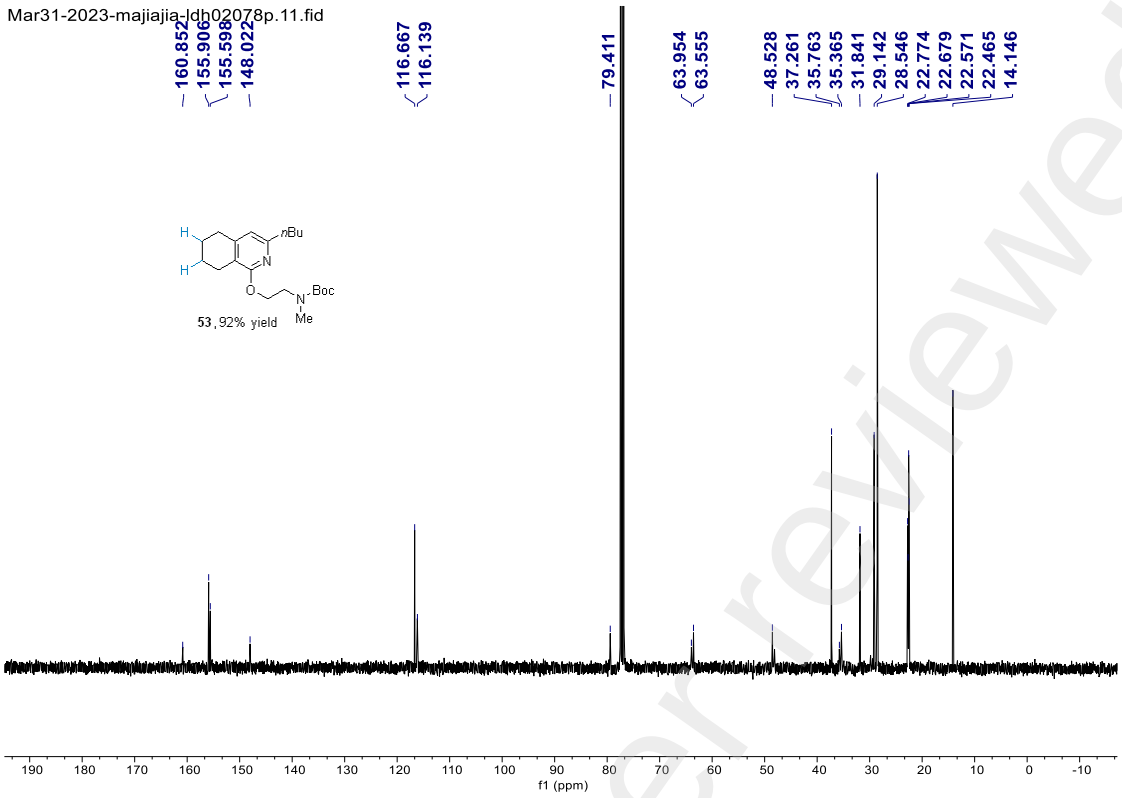
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.42 (s, 1H), 4.42 (t, *J* = 5.4 Hz, 2H), 3.64 - 3.54 (m, 2H), 2.99 - 2.93 (m, 3H), 2.62 (t, *J* = 5.6 Hz, 2H), 2.59 - 2.50 (m, 4H), 1.80 - 1.70 (m,

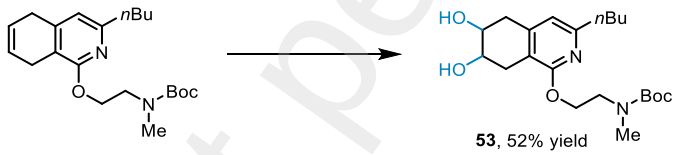
4H), 1.69 - 1.61 (m, 2H), 1.49- 1.40 (m, 9H), 1.39 - 1.30 (m, 2H), 0.92 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.9, 155.9, 155.6, 148.0, 116.7, 116.1, 79.4, 64.0 (rotamer), 63.6, 48.5 (rotamer), 37.3, 35.8 (rotamer), 35.4, 31.8, 29.1, 28.5, 22.8, 22.7, 22.6, 22.5, 14.1.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{35}N_2O_3$ $[M+H]^+$: 363.2639, found: 363.2642.







To a solution of **51** (46.2 mg, 0.128 mmol, 1.0 equiv.) and $K_2OsO_4 \cdot 2H_2O$ (2.4 mg, 5.0 mol%) in Acetone/H_2O (*v*/*v* = 1:1, 1.5 mL) was added 4-Methylmorpholine N-oxide (31.0 g, 0.256 mmol, 2.0 equiv.) in batches and stirred for overnight at room temperature. After completion of reaction, the resulting mixture was quenched by sat. $Na_2S_2O_3$ solution and extracted with CH_2Cl_2 (3 × 10mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **53** as a colorless oil (26.6 mg, 52% yield).

Purification conditions: EtOAc/petroleum ether = 1:2 to 1:1

R_f (**53**) = 0.25 in EtOAc/petroleum ether = 1:1.

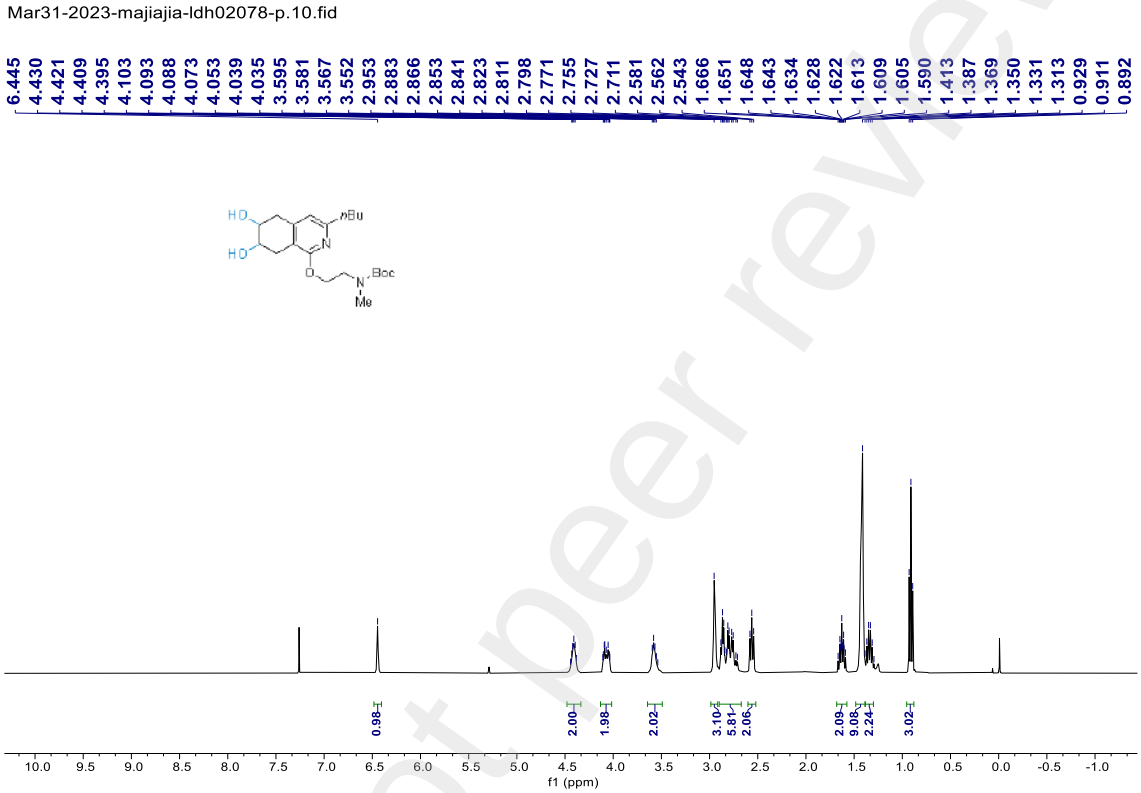
Analytical data of **53**:

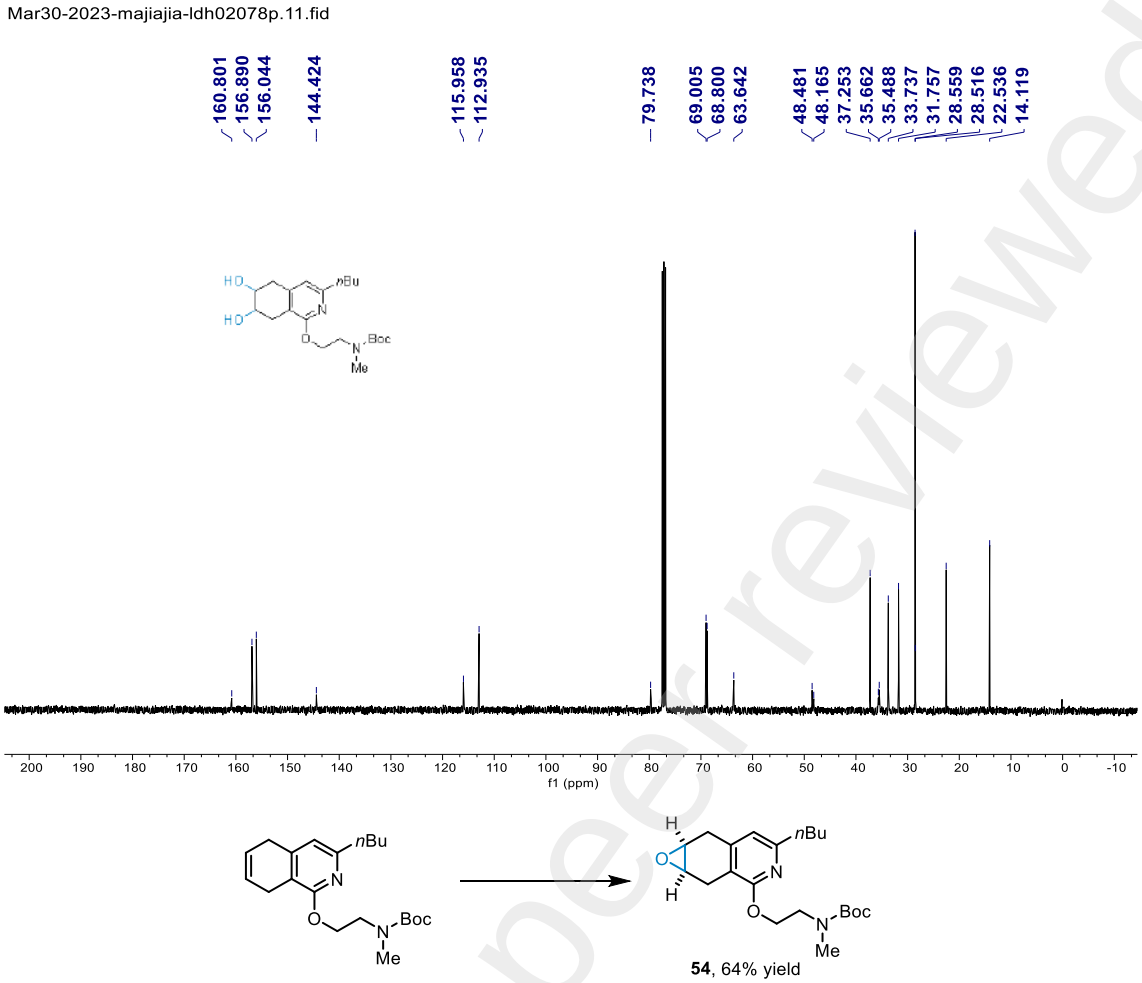
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.45 (s, 1H), 4.46 - 4.35 (m, 2H), 4.13 - 4.01 (m, 2H), 3.63 - 3.49 (m, 2H), 2.95 (br, 3H), 2.89 - 2.70 (m, 6H), 2.56 (t, *J* = 7.6 Hz, 2H), 1.67 -

1.58 (m, 2H), 1.42 (br, 9H), 1.38 - 1.29 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.8, 156.9, 156.0, 144.4, 116.0, 112.9, 79.7, 69.0, 68.8, 63.6, 48.5, 48.2(rotamer), 37.3, 35.7(rotamer), 35.5, 33.7, 31.8, 28.6, 28.5, 22.5, 14.1.

HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{34}N_2O_5Na$ $[M+Na]^+$:417.2360, found: 417.2356.





To a solution of **51** (36.5 mg, 0.1 mmol, 1.0 equiv.) in acetone (4.5 mL) was added saturated aqueous $NaHCO_3$ (3.0 mL). The resulting mixture was cooled to 0 ˚C and a solution of Oxone® (38.1 mg, 0.11 mmol, 1.1 equiv.) in H_2O (0.5 mL) was added dropwise over 5 minutes. The reaction mixture was stirred vigorously for 30 min at 0 ˚C. After completion of reaction, the mixture diluted with H_2O (10 mL) and extracted with EtOAc (3 x 5 mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **54** as a colorless oil (24.2 mg, 64% yield).

Purification conditions: EtOAc/petroleum ether = 1:20 to 1:8

R_f (**54**) = 0.25 in EtOAc/petroleum ether = 1:10.

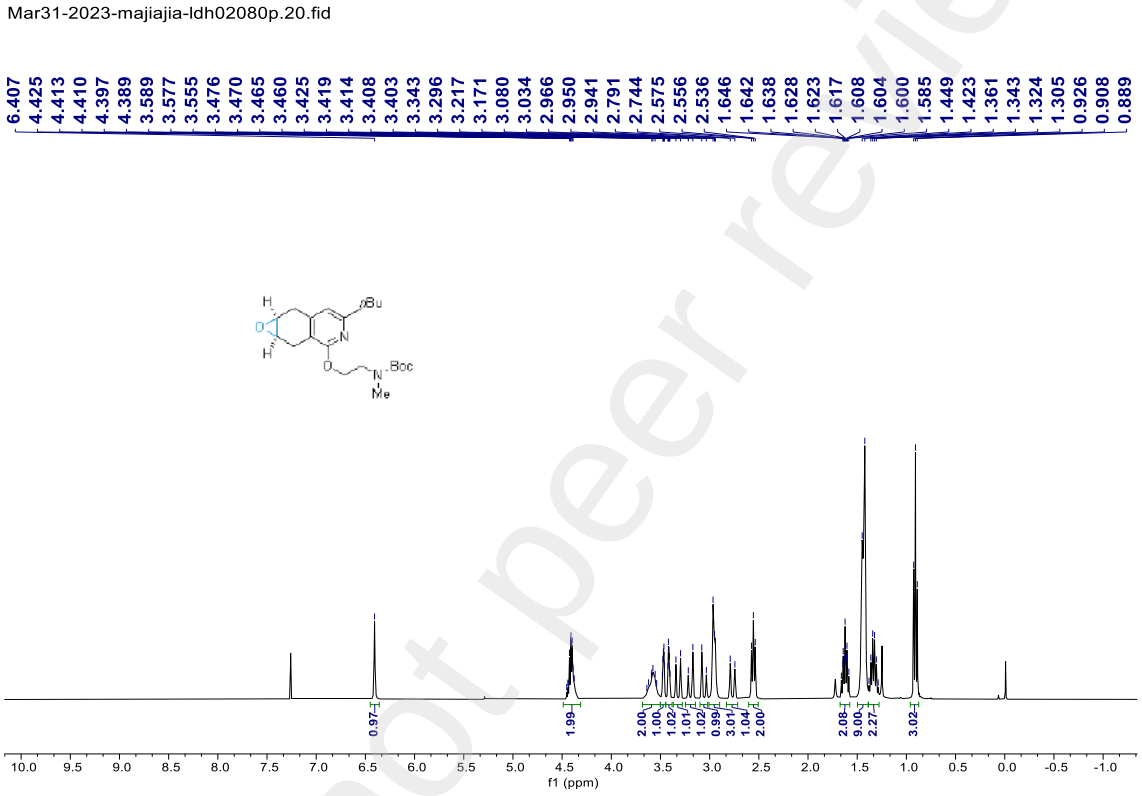
Analytical data of **54**:

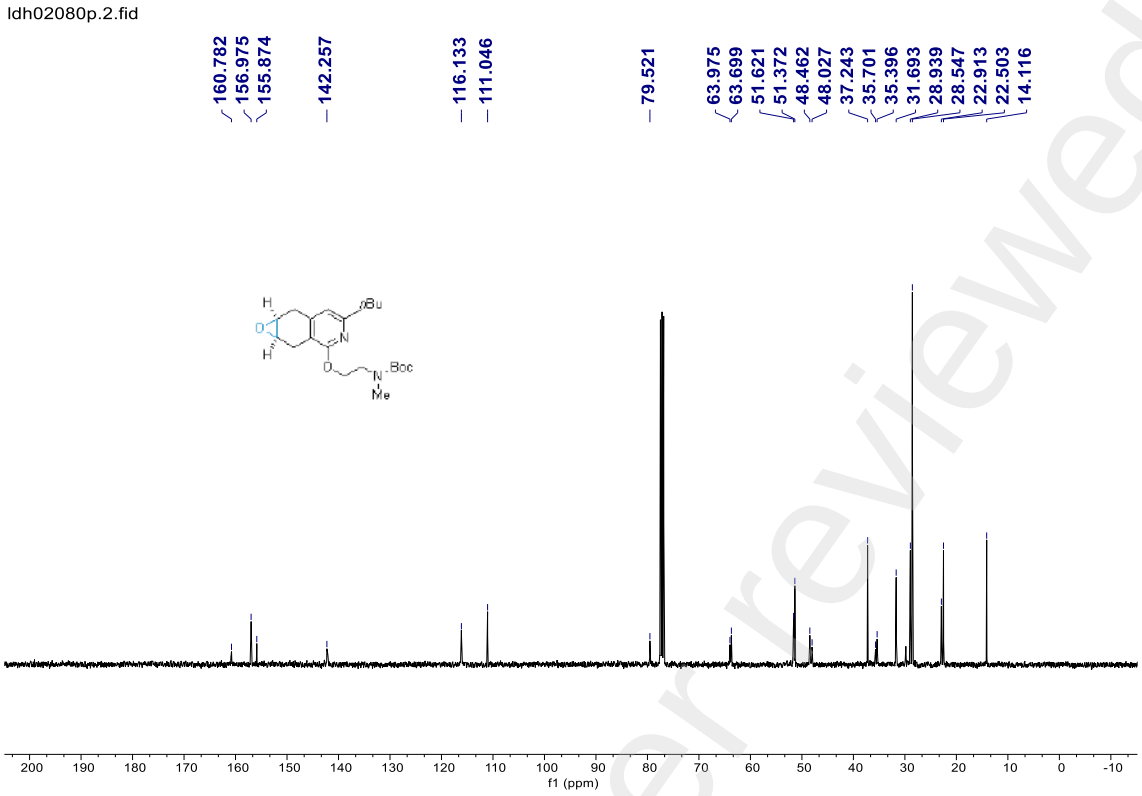
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.41 (s, 1H), 4.47 - 4.34 (m, 2H), 3.67 - 3.51 (m, 2H), 3.49 - 3.45 (m, 1H), 3.43 - 3.40 (m, 1H), 3.32 (d, *J* = 18.8 Hz, 1H), 3.19 (d, *J* = 18.4 Hz, 1H), 3.06 (d, *J* = 18.4 Hz, 1H), 2.99 - 2.92 (m, 3H), 2.77 (d, *J* = 18.8 Hz, 1H),

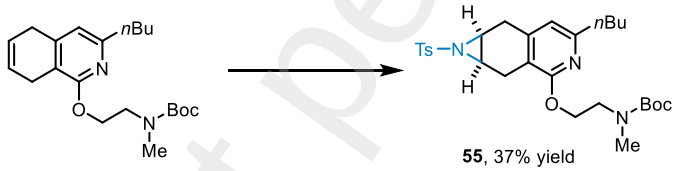
2.56 (t, *J* = 7.6 Hz, 2H), 1.67 - 1.58 (m, 2H), 1.48 - 1.40 (m, 9H), 1.39 - 1.28 (m, 2H), 0.91 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.8, 157.0, 155.9, 142.3, 116.1, 111.0, 79.5, 64.0 (rotamer), 63.7, 51.6, 51.4, 48.5, 48.0 (rotamer), 37.2, 35.7 (rotamer), 35.4, 31.7, 28.9, 28.5, 22.9, 22.5, 14.1.

HRMS (ESI, *m/z*) calcd for $C_{21}H_{32}N_2O_4Na^+$ $[M+Na]^+$: 399.2260, found: 399.2261.







To a solution of **51** (18.0 mg, 0.05 mmol, 1.0 equiv.) and chloramine T trihydrate (14.4 mg, 0.05 mmol, 1.0 equiv.) in MeCN (0.5 mL) was added phenyltrimethylammonium tribromide (2.0 mg, 10 mol%) at room temperature and the mixture was stirred for 20 hours at that temperature. After completion of reaction, the resulting mixture was diluted with H_2O (10 mL) and extracted with CH_2Cl_2 (3 × 5 mL). The organic phases were combined and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel to give the product **55** as a yellow oil (9.8 mg, 37% yield).

Purification conditions: EtOAc/petroleum ether = 1:8 to 1:3

R_f (**55**) = 0.3 in EtOAc/petroleum ether = 1:4.

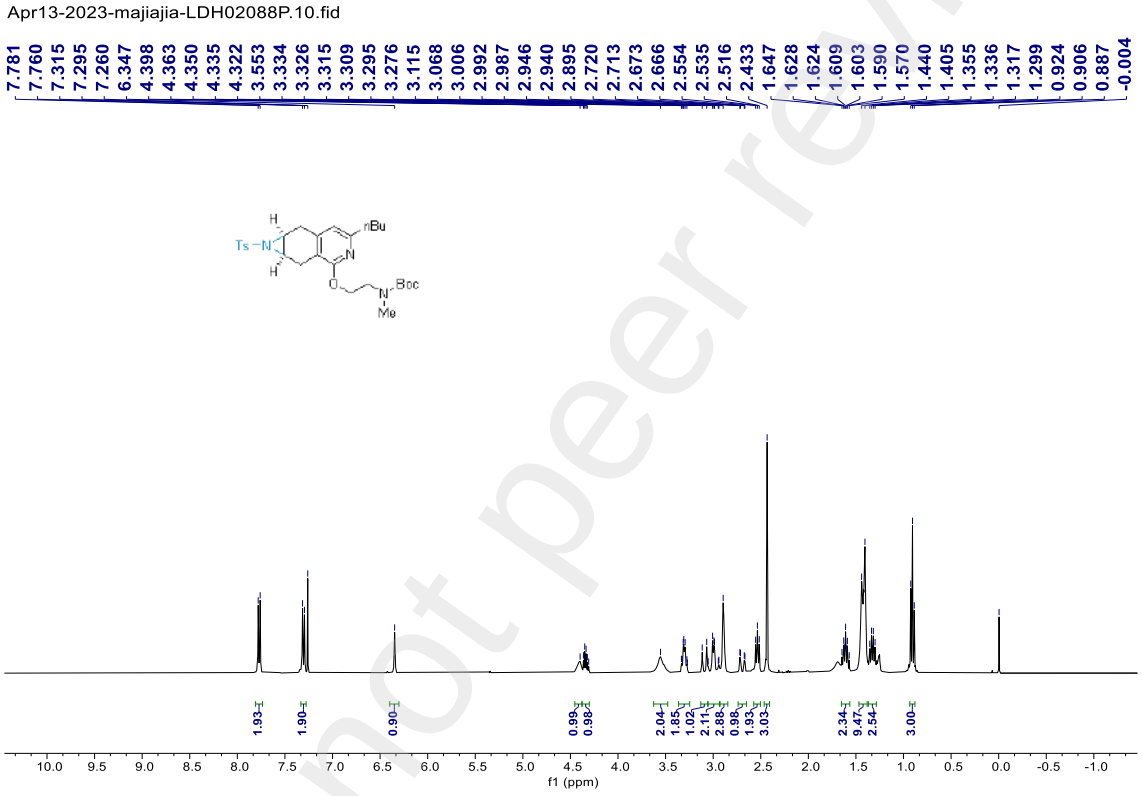
Analytical data of **55**:

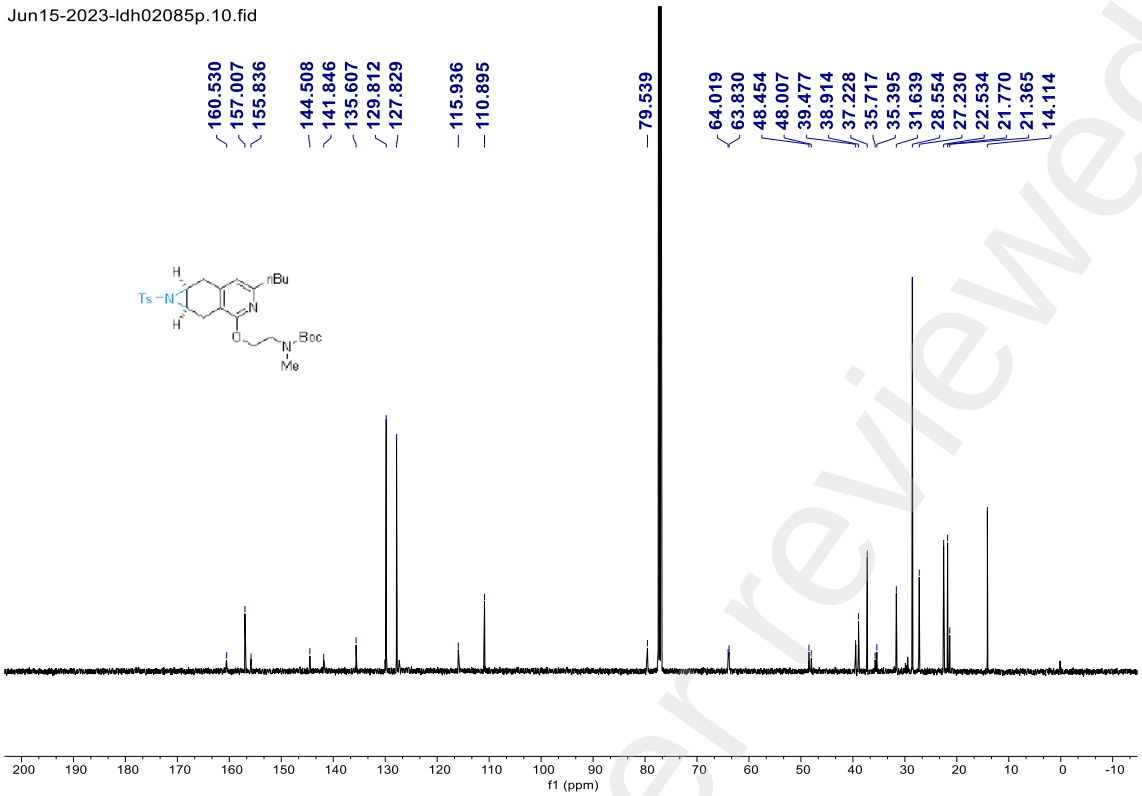
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.4 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 6.35 (s, 1H), 4.40 (br, 1H), 4.37 - 4.30 (m, 1H), 3.55 (br, 2H), 3.35 - 3.25 (m, 2H), 3.09 (d,

J = 18.8 Hz, 1H), 3.05 - 2.93 (m, 2H), 2.90 (s, 3H), 2.69 (dd, *J* = 18.8, 2.8 Hz, 1H), 2.56 - 2.51 (m, 2H), 2.43 (s, 3H), 1.65 - 1.56 (m, 2H), 1.47 - 1.38 (m, 9H), 1.37 - 1.29 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.5, 157.0, 155.8, 144.5, 141.8, 135.6, 129.8, 127.8, 115.9, 110.9, 79.5, 64.0 (rotamer), 63.8, 48.5, 48.0 (rotamer), 39.5, 38.9, 37.2, 35.7 (rotamer), 35.4, 31.6, 28.6, 27.2, 22.5, 21.8, 21.4, 14.1.

HRMS (ESI, *m*/*z*) calcd for $C_{28}H_{40}N_3O_5S^+$ $[M+H]^+$: 530.2689, found: 530.2693.





8. Single Crystal X-Ray Diffraction

Crystals of **32** and **36** were obtained by slow diffusion from a solution of the compounds in EtOAc layered with n-hexane at room temperature for several days (Figure S2-S3). Crystal data and details of the structure determination are presented in Table S7.

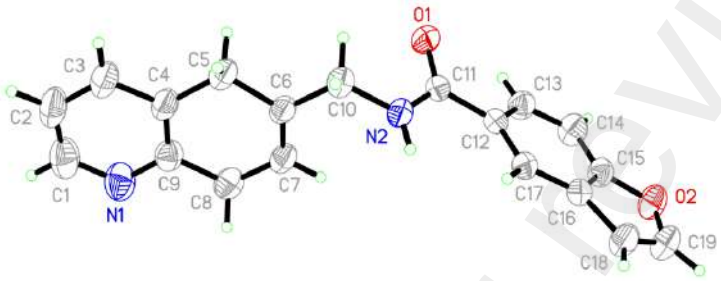


Figure S2. Crystal structure of **32**.

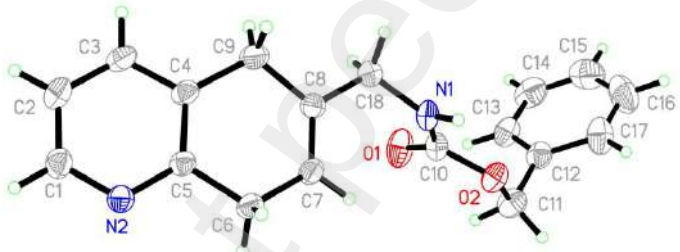


Figure S3. Crystal structure of **36**.

Table S7. Crystal data and details of the structure determination.

	32	**36**
Empiric formula	$C_{19}H_{16}N_2O_2$	$C_{18}H_{18}N_2O_2$
Formula weight	304.34	294.34
Crystal system, space group	Monoclinic, P 21/c	Monoclinic, Cc
a, *b*, *c* (Å)	15.7985(15), 11.3138(11), 8.6765(8)	16.6917(19), 13.5310(16), c=7.8355(9)
α, β, γ (°)	90, 103.085(5), 90	90, 116.430(5), 90
V (Å^3)	1510.6(2)	1584.7(3)
Z	4	4
μ (mm^{-1})	0.708	0.652
Crystal size (mm)	0.160 x 0.140 x 0.120 mm	0.160 x 0.150 x 0.140 mm
T_{min}, T_{max}	0.605, 0.753	0.612, 0.753
R(reflections)	0.0407 (2207)	0.0360 (2277)
wR2(reflections)	0.1177 (2778)	0.1084 (2494)
CCDC	2267616	2267615

9. Computational Study

I. Computational Methods

All density functional theory (DFT) computations were performed using Gaussian 16, Revision A.03.[16] Unless otherwise specified, molecular geometries were optimized using the long-range-corrected ωB97X-D[17] functional and the def2-SVP basis set. Frequency calculations were performed at the same level of theory as that used for geometry optimization to characterize the stationary points as either minima (no imaginary frequencies) or first-order saddle points (one imaginary frequency) on the potential energy surface. Intrinsic Reaction Coordinate (IRC) calculations were performed to confirm the first-order saddle points as real transition states connecting the expected reactants and products. Thermal contributions to Gibbs free energies were calculated from vibrational frequencies using the quasi-rigid rotor-harmonic oscillator (RRHO) approach of Grimme[18] implemented through Paton's GoodVibes[19] Python script. Single-point energies were calculated with the ωB97X-D functional and the def2-TZVPP basis set. Solvation effects were incorporated in single-point energy calculations using the SMD[20] model with acetonitrile as the solvent. Visualizations of optimized molecular structures were obtained using CYLview.[21] Monte Carlo conformational searches were performed with the Merck molecular force field (MMFF) implemented in Spartan '20.[22] All conformers within 10.0 kcal/mol of the lowest-energy conformer through Monte Carlo searches were reoptimized in Gaussian using the DFT methods described above. Minimum energy crossing points (MECPs) were located using easymecp,[23] a simplified Python wrapper developed by J. Rodríguez-Guerra and I. Funes-Ardóiz around the original MECP Fortran code from J. Harvey.[24] Triplet energies (E_T) were calculated by optimizing both the singlet ground state (S_0) and the first triplet state (T_1) geometries, evaluating their Gibbs free energies separately, and calculating the triplet energy using the equation E_T = G(T1) – G(S0).

II. Reorganization Energy and Dexter Energy Transfer Barrier Calculations

Vertical reorganization energies were evaluated using Nelsen's four-point model[25] as previously described in Baik and Yoon's study.[26] Vertical reorganization energies of the energy donor, λ_D(triplet), and the energy acceptor, λ_A(singlet), were calculated as follows:

$$\lambda_D(\text{triplet}) = E^3_{1_D} - E^3_{3_D}$$

$$\lambda_A(\text{singlet}) = E^1_{3_A} - E^1_{1_A}$$

Where E^x_y represents the single-point energy of state y (1 for singlet, 3 for triplet) computed in the gas-phase-optimized geometry of state x. The total reorganization energy, λ, was then calculated using the equation $\lambda = \lambda_A(\text{singlet}) + \lambda_D(\text{triplet})$. Table S8 shows the calculated vertical reorganization energies for azaarene substrates, functional groups and the Ir photosensitizer (**Ir-PS**). Energy transfer barriers calculated based on these values are also shown.

Table S8. Calculated vertical reorganization energies (kcal/mol) and energy transfer barriers (kcal/mol).

Molecule	$E^3_{3_D}$(Hartrees)	$E^3_{1_D}$(Hartrees)	**λ_D(triplet)**			
Ir-PS (Ir photosensitizer)*	-2347.446829	-2347.436434	6.5			
Molecule	$E^1_{1_A}$(Hartrees)	$E^1_{3_A}$(Hartrees)	**λ_A(singlet)**	**Total λ**	ΔG_{EnT}	$\Delta G^{\ddagger}_{EnT}$
quinoline	-401.941365	-401.920291	13.2	19.7	-2.0	4.0
quinoline-H^+	-402.404235	-402.386647	11.0	17.6	-5.8	2.0
quinoline-BF_3	-726.592864	-726.588407	2.8	9.3	-10.6	0.0
isoquinoline	-401.939866	-401.917988	13.7	20.3	-3.7	3.4
isoquinoline-H^+	-402.403479	-402.386041	10.9	17.5	-6.2	1.8
isoquinoline-BF_3	-726.609947	-726.589309	13.0	19.5	-5.8	2.4
phenanthridine	-555.590404	-555.565970	15.3	21.9	-0.7	5.1
phenanthridine-H^+	-556.052263	-556.036980	9.6	16.1	-3.8	2.4
phenanthridine-BF3	-880.255141	-880.232866	14.0	20.5	-2.7	3.9
benzo[f]quinoline	-555.589841	-555.549551	25.3	31.8	9.9	13.7
benzo[f]quinoline-H+	-556.052725	-556.038147	9.1	15.7	-4.9	1.9
benzofquinoline-BF_3	-880.254577	-880.236888	11.1	17.6	-4.3	2.5
4,7-phenanthroline	-571.629088	-571.612532	10.4	16.9	39.9	47.8
4,7-phenanthroline-H^+	-572.090060	-572.063401	16.7	23.3	8.8	11.0
4,7-phenanthroline-$2H^+$	-572.542994	-572.522622	12.8	19.3	-3.2	3.4
4,7-phenanthroline-BF_3	-896.292663	-896.252731	25.1	31.6	8.7	12.8
4,7-phenanthroline-$2BF_3$	-1220.953070	-1220.934367	11.7	18.3	-3.3	3.1
a	-385.901728	-385.881609	12.6	19.1	-3.2	3.3
b	-709.704188	-709.674421	18.7	21.0	4.4	7.7
c	-383.692391	-383.669754	14.2	20.7	7.0	9.2

d	-529.438978	-529.430176	5.5	12.0	37.2	50.3
e	-553.027827	-553.020475	4.6	11.1	37.6	53.3
f	-386.104122	-386.079291	15.6	22.1	16.7	17.1
g	-440.293905	-440.242692	32.1	42.0	15.2	19.5
h	-914.918515	-914.850464	42.7	49.2	13.5	20.0
i	-345.823970	-345.695897	80.4	86.9	-6.1	18.8
j	-324.702131	-324.641887	37.8	45.7	16.5	21.2
k	-721.931664	-721.785745	91.6	98.1	-6.3	21.5
l	-231.257372	-231.212884	27.9	34.4	12.6	16.1

* The Ir photosensitizer was optimized using the ωB97X-D functional with the SDD[27, 28] basis set (including effective core potential) for Ir, and the def2-SVP basis set for all other atoms. Single-point energy calculations were carried out using the ωB97X-D functional with the SDD basis set (including effective core potential) for Ir, and the def2-TZVPP basis set for all other atoms. Solvation effects were incorporated in single-point energy calculations using the SMD model with acetonitrile as the solvent.

III. Alternative Isomeric Transition States and MECPs

Alternative isomeric transition states (TSs) for the initial hydrogen atom transfer (HAT) are shown in Figures S4 and S5 for Lewis- and Brønsted-acid catalysis, respectively. The parameters varied in these TSs include the sites involved in the HAT process (5-position vs. 8-position on the quinoline substrate; hydrogen α to the isopropyl vs. methyl group on γ-terpinene), the π face of approach between the reactants, and the conformation about the transferring C...H...C bonds. Our calculations show that many of these isomeric TSs lie close in energy, often within 1.0 kcal/mol and well within the error margin for common DFT methods. This result suggests that the initial HAT step may operate through multiple possible isomeric TSs.

The subsequent crossover to the singlet surface can also be envisioned to occur through a variety of MECP structures (Figures S6 and S7). (While the site of the initial HAT step would dictate the range of MECP structures available to the system, molecular rotations and reorientations may occur in some cases, meaning that not every TS would necessarily have a unique ensuing MECP structure.) The potential energy barriers for these MECP structures vary (5.0–12.4 kcal/mol for the BF_3-catalyzed system, and 1.8–6.6 kcal/mol for the Brønsted-acid-catalyzed system).

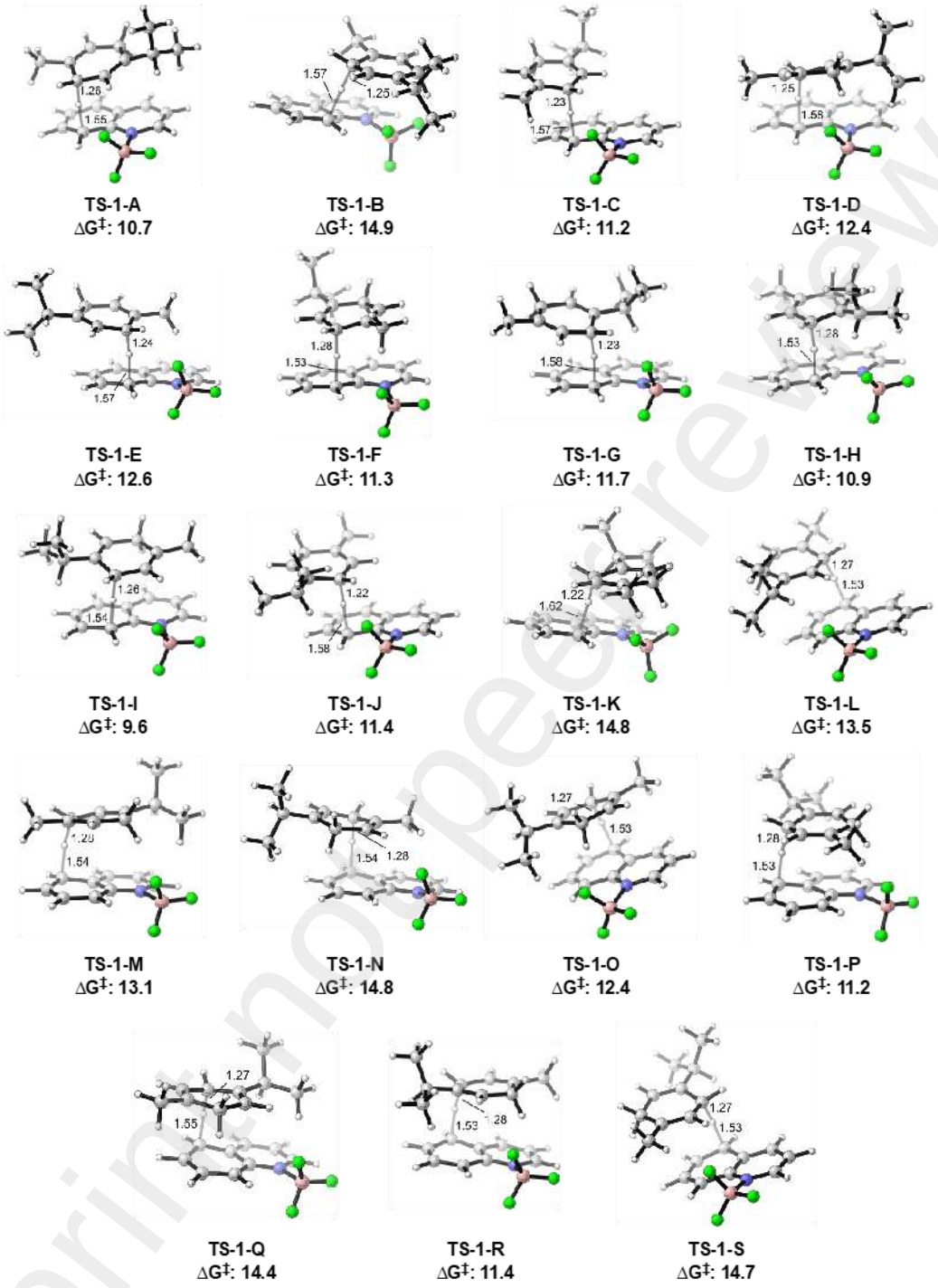


Figure S4. Calculated transition state (TS) structures of the initial hydrogen atom transfer (HAT) reaction between γ-terpinene and triplet quinoline coordinated to BF_3. Activation free energies (kcal/mol) are calculated with respect to isolated reactants. Interatomic distances are in Å.

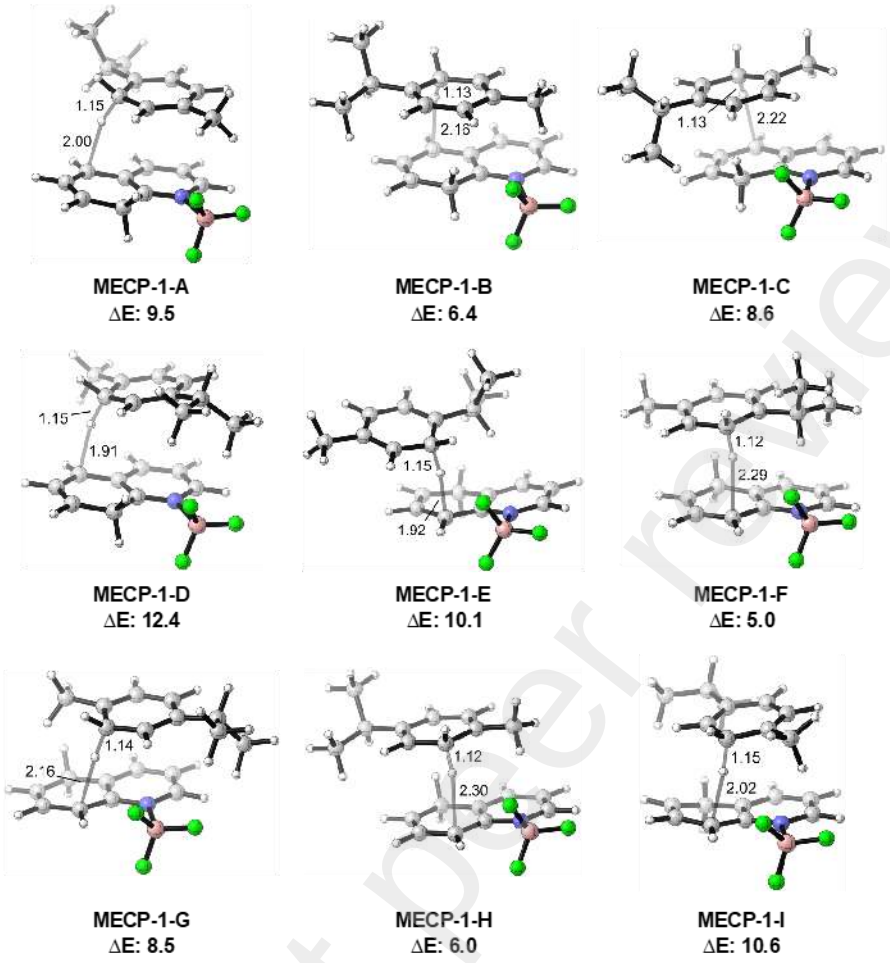


Figure S5. Calculated minimum energy crossing point (MECP) structures for the second hydrogen atom transfer (HAT) step with the quinoline substrate coordinated to BF_3. Potential energies (kcal/mol) are calculated with respect to the lowest-energy triplet diradical resting states prior to the MECPs. Interatomic distances are in Å.

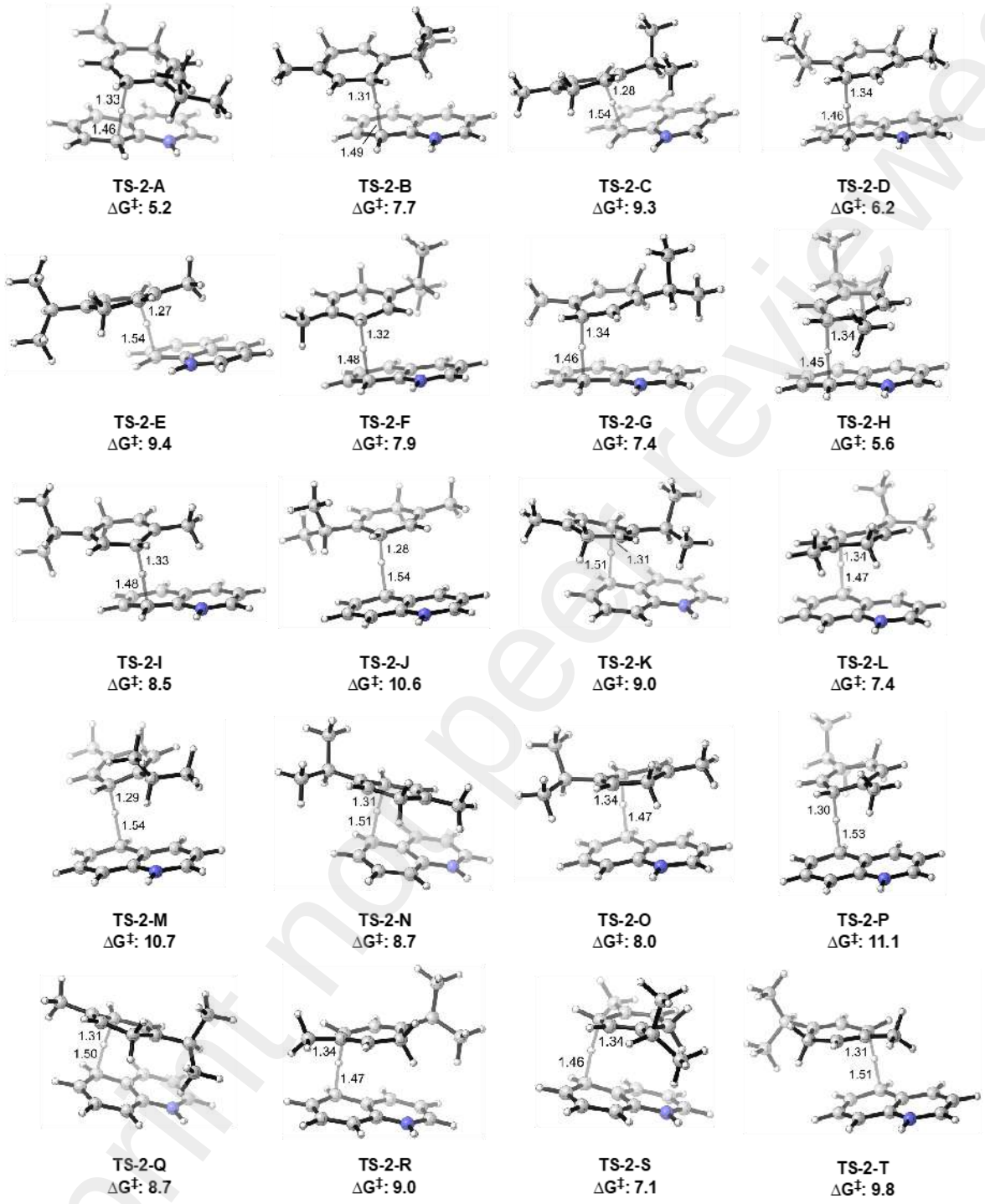


Figure S6. Calculated transition state (TS) structures of the hydrogen atom transfer (HAT) reaction between γ-terpinene and protonated triplet quinoline. Activation free energies (kcal/mol) are calculated with respect to isolated reactants. Interatomic distances are in Å.

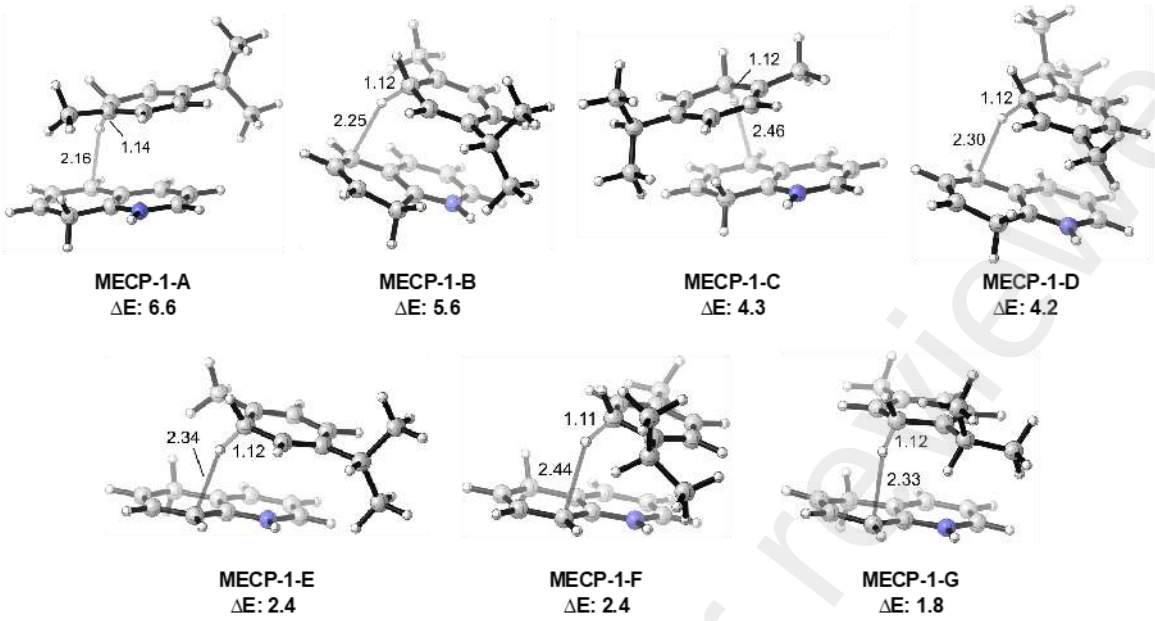
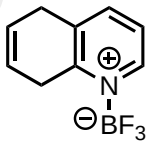
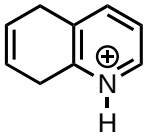


Figure S7. Calculated minimum energy crossing point (MECP) structures for the second hydrogen atom transfer (HAT) step with a protonated quinoline substrate. Potential energies (kcal/mol) are calculated with respect to the lowest-energy triplet diradical resting states prior to the MECPs. Interatomic distances are in Å.

IV. Computed Energies

Table S9. Calculated energies (in Hartrees) of azaarene substrates, products and the Ir photosensitizer.

Structure	**ΔG** [ωB97X-D/def2-SVP]	$\mathbf{E_{MeCN}}$ [ωB97X-D/def2-TZVPP, SMD (MeCN)]	$\mathbf{G_{MeCN}}$ (= ΔG + E_{MeCN})	**Imaginary Frequency** (cm^{-1})
γ-terpinene	0.198349	-390.714278	-390.515929	-
***p*-cymene** (oxidized product of γ-terpinene)	0.176933	-389.533939	-389.357006	-
	0.136624	-727.803201	-727.666577	-

	0.140515	-403.602611	-403.462096	-
^{1}quinoline	0.106117	-401.941365	-401.835248	-
^{3}quinoline	0.099002	-401.835634	-401.736632	-
^{1}quinoline-H^{+}	0.120007	-402.404235	-402.284228	-
^{3}quinoline-H^{+}	0.113436	-402.305094	-402.191658	-
^{1}quinoline-BF$_3$	0.111663	-726.592864	-726.481201	-
^{3}quinoline-BF$_3$	0.109029	-726.505297	-726.396268	-
^{1}isoquinoline	0.106127	-401.939866	-401.833739	-
^{3}isoquinoline	0.098619	-401.836546	-401.737927	-
^{1}isoquinoline-H^{+}	0.120077	-402.403479	-402.283402	-
^{3}isoquinoline-H^{+}	0.113779	-402.305225	-402.191446	-
^{1}isoquinoline-BF$_3$	0.115052	-726.609947	-726.494895	-
^{3}isoquinoline-BF$_3$	0.107833	-726.510162	-726.402329	-
^{1}phenanthridine	0.150106	-555.590404	-555.440298	-
^{3}phenanthridine	0.142340	-555.481966	-555.339626	-
^{1}phenanthridine-H^{+}	0.163968	-556.052263	-555.888295	-
^{3}phenanthridine-H^{+}	0.156916	-555.949408	-555.792492	-
^{1}phenanthridine-BF$_3$	0.159973	-880.255141	-880.095168	-
^{3}phenanthridine-BF$_3$	0.152372	-880.149988	-879.997616	-
^{1}benzo[f]quinoline	0.150083	-555.589841	-555.439758	-
^{3}benzo[f]quinoline	0.142646	-555.464877	-555.322231	-
^{1}benzo[f]quinoline-H^{+}	0.163892	-556.052725	-555.888833	-
^{3}benzo[f]quinoline-H^{+}	0.157482	-555.952336	-555.794854	-
^{1}benzo[f]quinoline-BF$_3$	0.159964	-880.254577	-880.094613	-
^{3}benzo[f]quinoline-BF$_3$	0.152697	-880.152415	-879.999718	-
^{1}4,7-phenanthroline	0.138209	-571.629088	-571.490879	-
^{3}4,7-phenanthroline	0.133599	-571.459057	-571.325458	-
^{1}4,7-phenanthroline-H^{+}	0.151878	-572.090060	-571.938182	-
^{3}4,7-phenanthroline-H^{+}	0.145036	-571.967405	-571.822369	-
^{1}4,7-phenanthroline-2H^{+}	0.165620	-572.542994	-572.377374	-
^{3}4,7-phenanthroline-2H^{+}	0.158836	-572.439495	-572.280659	-
^{1}4,7-phenanthroline-BF$_3$	0.148377	-896.292663	-896.144286	-
^{3}4,7-phenanthroline-BF$_3$	0.140840	-896.169468	-896.028628	-
^{1}4,7-phenanthroline-2BF$_3$	0.157080	-1220.953070	-1220.795990	-
^{3}4,7-phenanthroline-2BF$_3$	0.149784	-1220.849298	-1220.699514	-

^{1}a	0.117912	-385.901728	-385.783816	-
^{3}a	0.110387	-385.797543	-385.687156	-
^{1}b	0.217904	-709.704164	-709.486260	-
^{3}b	0.209956	-709.587356	-709.377400	-
^{1}c	0.088861	-383.692391	-383.603530	-
^{3}c	0.079702	-383.570362	-383.490660	-
^{1}d	0.059328	-529.438978	-529.379650	-
^{3}d	0.053075	-529.271707	-529.218632	-
^{1}e	0.040207	-553.027827	-552.987620	-
^{3}e	0.032298	-552.858232	-552.825934	-
^{1}f	0.130021	-386.104122	-385.974101	-
^{3}f	0.118939	-385.964607	-385.845668	-
^{1}g	0.122402	-440.299209	-440.176807	-
^{3}g	0.117286	-440.168034	-440.050748	-
^{1}h	0.145625	-914.918515	-914.772890	-
^{3}h	0.139450	-914.789002	-914.649552	-
^{1}i	0.091447	-345.823970	-345.732523	-
^{3}i	0.085134	-345.725610	-345.640476	-
^{1}j	0.078584	-324.704263	-324.625679	-
^{3}j	0.072766	-324.570379	-324.497613	-
^{1}k	0.075493	-721.931664	-721.856171	-
^{3}k	0.068399	-721.832847	-721.764448	-
^{1}l	0.062454	-231.257372	-231.194918	-
^{3}l	0.060228	-231.133254	-231.073026	-
^{1}lr-PS	0.656612	-2347.554351	-2346.897739	-
^{3}lr-PS	0.650873	-2347.446829	-2346.795956	-

Table S10. Calculated energies (in Hartrees) of transition states, intermediates and minimum energy crossing points (MECPs).

Structure	**ΔG** [ωB97X-D/def2-SVP]	**E_{MeCN}** [ωB97X-D/def2-TZVPP, SMD (MeCN)]	**G_{MeCN}** (= ΔG + E_{MeCN})	**Imaginary Frequency** (cm^{-1})
TS-1-A	0.328477	-1117.223584	-1116.895107	-828.11
TS-1-B	0.327433	-1117.215814	-1116.888381	-625.44
TS-1-C	0.327386	-1117.221688	-1116.894302	-662.42
TS-1-D	0.328052	-1117.220471	-1116.892419	-524.76

TS-1-E	0.32804	-1117.220079	-1116.892039	-792.05
TS-1-F	0.328984	-1117.223111	-1116.894127	-955.63
TS-1-G	0.328649	-1117.222265	-1116.893616	-640.59
TS-1-H	0.32922	-1117.224102	-1116.894882	-963.77
TS-1-I	0.329266	-1117.226096	-1116.89683	-817.91
TS-1-J	0.327435	-1117.221498	-1116.894063	-575.19
TS-1-K	0.329016	-1117.217655	-1116.888639	-323.53
TS-1-L	0.327952	-1117.2187	-1116.890748	-1133.14
TS-1-M	0.329912	-1117.221287	-1116.891375	-1121.27
TS-1-N	0.328865	-1117.217488	-1116.888623	-1216.24
TS-1-O	0.329087	-1117.221579	-1116.892492	-1080.97
TS-1-P	0.329776	-1117.224186	-1116.89441	-1092.53
TS-1-Q	0.32896	-1117.218247	-1116.889287	-1151.01
TS-1-R	0.329259	-1117.223308	-1116.894049	-1128.24
TS-1-S	0.328224	-1117.216939	-1116.888715	-1150.89
INT-1-A	0.331397	-1117.265366	-1116.933969	-
INT-1-B	0.331421	-1117.263343	-1116.931922	-
INT-1-C	0.331085	-1117.264602	-1116.933517	-
INT-1-D	0.331248	-1117.264764	-1116.933516	-
INT-1-E	0.331166	-1117.264749	-1116.933583	-
INT-1-F	0.330987	-1117.265727	-1116.93474	-
INT-1-G	0.331225	-1117.265116	-1116.933891	-
INT-1-H	0.331945	-1117.267853	-1116.935908	-
INT-1-I	0.331559	-1117.267147	-1116.935588	-
INT-1-J	0.33098	-1117.266233	-1116.935253	-
INT-1-K	0.331482	-1117.265949	-1116.934467	-
INT-1-L	0.331285	-1117.266197	-1116.934912	-
INT-1-M	0.331509	-1117.266089	-1116.93458	-
INT-1-N	0.330163	-1117.264804	-1116.934641	-
INT-1-O	0.331616	-1117.266467	-1116.934851	-
INT-1-P	0.330793	-1117.26774	-1116.936947	-
INT-1-Q	0.331407	-1117.267174	-1116.935767	-
INT-1-R	0.330617	-1117.267359	-1116.936742	-
INT-1-S	0.330652	-1117.266979	-1116.936327	-
MECP-1-A	-	-1117.250183	-	-
MECP-1-B	-	-1117.255605	-	-
MECP-1-C	-	-1117.254208	-	-
MECP-1-D	-	-1117.248167	-	-

MECP-1-E	-	-1117.250119	-	-
MECP-1-F	-	-1117.25853	-	-
MECP-1-G	-	-1117.254226	-	-
MECP-1-H	-	-1117.257823	-	-
MECP-1-I	-	-1117.250401	-	-
TS-2-A	0.330994	-793.0303404	-792.6993464	-851.4
TS-2-B	0.330574	-793.0259233	-792.6953493	-711.57
TS-2-C	0.329999	-793.0227987	-792.6927997	-390.7
TS-2-D	0.331257	-793.0289792	-792.6977222	-912.03
TS-2-E	0.329118	-793.0216774	-792.6925594	-424.96
TS-2-F	0.330142	-793.0251636	-792.6950216	-744.46
TS-2-G	0.330706	-793.0265255	-792.6958195	-927.43
TS-2-H	0.331047	-793.0297888	-792.6987418	-895.04
TS-2-I	0.32956	-793.0236782	-792.6941182	-808.93
TS-2-J	0.32824	-793.0189786	-792.6907386	-602.24
TS-2-K	0.330872	-793.0241553	-792.6932833	-822.21
TS-2-L	0.331151	-793.0269529	-792.6958019	-1078.13
TS-2-M	0.329442	-793.0199317	-792.6904897	-652.76
TS-2-N	0.329796	-793.0235909	-792.6937949	-846.42
TS-2-O	0.331143	-793.025963	-792.69482	-1101.65
TS-2-P	0.328623	-793.018569	-792.689946	-725
TS-2-Q	0.330221	-793.0240109	-792.6937899	-904.35
TS-2-R	0.330997	-793.0241717	-792.6931747	-1100.21
TS-2-S	0.33051	-793.0267223	-792.6962123	-1105.56
TS-2-T	0.330103	-793.022088	-792.691985	-879.46
INT-2-A	0.334384	-793.0643659	-792.7299819	-
INT-2-B	0.334298	-793.0643463	-792.7300483	-
INT-2-C	0.334266	-793.0628749	-792.7286089	-
INT-2-D	0.334567	-793.064687	-792.73012	-
INT-2-E	0.333781	-793.0625657	-792.7287847	-
INT-2-F	0.333748	-793.0632428	-792.7294948	-
INT-2-G	0.333758	-793.0632436	-792.7294856	-
INT-2-H	0.333171	-793.0614507	-792.7282797	-
INT-2-I	0.334526	-793.065458	-792.730932	-
INT-2-J	0.334556	-793.0654603	-792.7309043	-
INT-2-K	0.333786	-793.0656369	-792.7318509	-
INT-2-L	0.334251	-793.0673321	-792.7330811	-
INT-2-M	0.33375	-793.0649832	-792.7312332	-

INT-2-N	0.333503	-793.0636494	-792.7301464	-
INT-2-O	0.33427	-793.0645051	-792.7302351	-
INT-2-P	0.332198	-793.0622964	-792.7300984	-
INT-2-Q	0.334389	-793.0660423	-792.7316533	-
INT-2-R	0.334546	-793.0649242	-792.7303782	-
INT-2-S	0.332193	-793.0622973	-792.7301043	-
INT-2-T	0.333132	-793.0574239	-792.7242919	-
MECP-2-A	-	-793.053871	-	-
MECP-2-B	-	-793.0557557	-	-
MECP-2-C	-	-793.0577928	-	-
MECP-2-D	-	-793.0564854	-	-
MECP-2-E	-	-793.0617458	-	-
MECP-2-F	-	-793.060641	-	-
MECP-2-G	-	-793.0616336	-	-
TS-HAT-naphthalene	0.329461	-776.503598	-776.174137	-1354.07

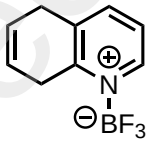
V. Cartesian Coordinates of Calculated Structures

γ-terpinene

C	0.14278500	-1.32002400	-0.00100600
C	1.64169800	-1.26353900	-0.00100400
C	2.20663300	0.13296900	0.00009300
C	1.40591700	1.20312500	0.00057400
C	-0.09366500	1.14658000	0.00004300
C	-0.66131500	-0.25120700	-0.00048800
H	2.03665000	-1.81697200	0.87282800
H	2.03662600	-1.81558300	-0.87573000
H	-0.30634300	-2.31963600	-0.00143300
H	1.85490200	2.20250200	0.00135800
H	-0.47960800	1.70358900	0.87392000
H	-0.47894900	1.70394200	-0.87390600
C	3.70486600	0.23874900	0.00059400
H	4.04177700	1.28496600	0.00134200
H	4.13395300	-0.26182500	0.88494400
H	4.13445800	-0.26071700	-0.88413800
C	-2.17157900	-0.40432900	-0.00031100
H	-2.37567300	-1.48838900	-0.00150400
C	-2.81291600	0.18296300	-1.26328900
H	-3.89018600	-0.04285200	-1.29192100
H	-2.70837500	1.27911200	-1.29997600
H	-2.35237000	-0.23258600	-2.17216700
C	-2.81220100	0.18002200	1.26440000
H	-3.88951900	-0.04557400	1.29297100
H	-2.35133700	-0.23788100	2.17203200
H	-2.70734100	1.27605000	1.30374500

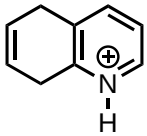
***p*-cymene**

C	0.62681300	0.22444600	-0.00249500
C	-0.21419300	1.33881600	-0.00644400
C	-1.60265900	1.19900900	-0.00172700
C	-2.20111200	-0.06252400	0.00637400
C	-1.35775500	-1.18161500	0.01203700
C	0.02571100	-1.04149600	0.00725200
H	0.22350100	2.34120000	-0.01180700
H	-1.79597200	-2.18381800	0.02149600
C	2.13763800	0.37985600	-0.00551000
H	2.34781000	1.46274100	-0.01667400
C	-3.69891100	-0.22697700	-0.00554200
H	-4.21075800	0.73126800	0.16090000
H	0.64991700	-1.93949100	0.01291600
H	-2.23183800	2.09343800	-0.00332500
C	2.76853300	-0.19814000	1.26585700
H	2.60897800	-1.28641500	1.32986000
H	3.85505800	-0.01961700	1.27995100
H	2.33334100	0.25733600	2.16768800
C	2.76667400	-0.22387300	-1.26573600
H	3.85310000	-0.04529500	-1.28511600
H	2.60763600	-1.31330400	-1.30726700
H	2.32999100	0.21290300	-2.17606200
H	-4.04501100	-0.62725600	-0.97196600
H	-4.03018300	-0.92869400	0.77500800



C	-2.04998500	-2.02032000	0.00007000
C	-0.63087000	-1.54749800	-0.00000600
C	-0.48119000	-0.05099100	-0.00002200
C	-1.59185800	0.80286900	-0.00003100
C	-3.00826400	0.27804700	-0.00006700
C	-3.11090600	-1.21605600	0.00002700
H	-2.19300800	-3.10411300	0.00014100
H	-0.08542600	-1.94969100	0.86829400
C	-1.37091000	2.18137700	0.00000300
H	-3.53997200	0.68837800	-0.87696000
C	-0.07896500	2.68673500	0.00004000
C	0.97339700	1.78786500	0.00004000
H	-2.22766100	2.86072100	0.00000400
H	0.11950700	3.75837400	0.00007800
H	2.01765700	2.09711700	0.00005600
N	0.76979700	0.46510800	0.00000500
H	-3.54006100	0.68849900	0.87671600
H	-4.11809300	-1.64095800	0.00006900
B	2.12991600	-0.51131400	-0.00000900

F	3.19921700	0.35163500	-0.00002900
F	2.05103200	-1.26248700	-1.15039400
F	2.05105700	-1.26247800	1.15038400
H	-0.08554300	-1.94971200	-0.86837000



C	2.44765900	-0.68617900	-0.00003900
C	1.18567200	-1.49985100	0.00001800
C	-0.05114300	-0.65228500	0.00000800
C	-0.04571600	0.74350100	0.00002500
C	1.24994900	1.51184200	0.00005500
C	2.47273500	0.64484000	-0.00002200
H	3.38192700	-1.25138400	-0.00009200
H	1.16360900	-2.16665100	-0.88134800
C	-1.27886900	1.40581700	0.00001200
H	1.26572800	2.18207900	0.87682000
C	-2.48415300	0.70384000	-0.00001400
C	-2.44120200	-0.67449100	-0.00003000
H	-1.29378400	2.49887900	0.00002200
H	-3.44515700	1.21805400	-0.00002300
H	-3.32562100	-1.31222100	-0.00005100
N	-1.24413800	-1.28875000	-0.00001900
H	1.26569900	2.18220200	-0.87661500
H	3.43426500	1.16312800	-0.00006200
H	1.16364300	-2.16657500	0.88144400
H	-1.23094000	-2.30846000	-0.00003200

^{1}quinoline

C	2.39573600	-0.71676900	-0.00000100
C	1.20650800	-1.40282000	-0.00000900
C	-0.03014200	-0.70147300	0.00001100
C	-0.01500100	0.72302400	0.00000600
C	1.23122100	1.40579100	-0.00000200
C	2.40964300	0.70111700	0.00000400
H	3.34138300	-1.26329600	-0.00000100
H	1.16819800	-2.49334300	-0.00001200
C	-1.26741900	1.39118800	-0.00000200
H	1.23529800	2.49881800	-0.00000700
H	3.36446500	1.23106900	0.00000400
C	-2.42130100	0.65068500	-0.00000600
C	-2.32032200	-0.76501900	0.00001200
H	-1.29545000	2.48406100	-0.00000300
H	-3.40364300	1.12601400	-0.00001600
H	-3.23632500	-1.36830900	-0.00001000
N	-1.18678000	-1.41848100	-0.00000300

^{3}quinoline

C	2.46518600	-0.68488400	0.00012900
C	1.20603800	-1.39994400	-0.00009200
C	-0.05378800	-0.70599200	-0.00012100
C	-0.03871100	0.74258900	-0.00011400
C	1.21453500	1.40984400	-0.00021400
C	2.47334400	0.66831300	0.00004400
H	3.39789800	-1.25178500	0.00044700
H	1.17363100	-2.49017800	-0.00009000
C	-1.27335300	1.39388800	0.00018400
H	1.23534300	2.50182500	-0.00051300
H	3.41199500	1.22533400	0.00035700
C	-2.46538400	0.61482000	0.00011300
C	-2.36425500	-0.74935200	-0.00009800
H	-1.31957400	2.48522300	0.00024500
H	-3.44391500	1.09773200	0.00015200
H	-3.25756400	-1.38031500	-0.00029500
N	-1.16849800	-1.41764700	0.00010100

^{1}quinoline–H^{+}

C	2.41129700	-0.71944000	0.00000100
C	1.21992500	-1.40892300	-0.00000200
C	0.01646500	-0.67692400	0.00000100
C	0.02036200	0.74487200	0.00000000
C	1.27220400	1.41756400	-0.00000200
C	2.44048300	0.69709700	0.00000100
H	3.35117100	-1.27456900	0.00000300
H	1.20329500	-2.50082700	-0.00000100
C	-1.22181800	1.42047700	0.00000000
H	1.28663300	2.50908100	-0.00000300

H	3.40171300	1.21316000	0.00000200
C	-2.41362300	0.71860500	0.00000100
C	-2.37069900	-0.67438300	0.00000200
H	-1.23084700	2.51324500	0.00000200
H	-3.37867800	1.22438900	-0.00000100
H	-3.26916200	-1.29380600	-0.00000100
N	-1.20137800	-1.31067600	0.00000000
H	-1.20206400	-2.32960300	-0.00000400

^{3}quinoline–H^{+}

C	2.48827700	-0.69109600	0.00000000
C	1.23098000	-1.37868100	0.00000100
C	0.00166700	-0.66500300	0.00000100
C	-0.01097400	0.76464300	0.00000000
C	1.24962300	1.41233700	0.00000000
C	2.49846000	0.66769200	-0.00000100
H	3.41145700	-1.27065600	-0.00000100
H	1.21253300	-2.47177100	0.00000000
C	-1.24875800	1.43410500	0.00000000
H	1.28132400	2.50374700	0.00000300
H	3.43768000	1.22313800	-0.00000200
C	-2.45416300	0.67733900	0.00000000
C	-2.41294200	-0.68266500	0.00000000
H	-1.28212400	2.52388200	0.00000100
H	-3.42163500	1.18026200	-0.00000100
H	-3.28821700	-1.32984000	-0.00000100
N	-1.17689300	-1.32177600	0.00000000
H	-1.16578700	-2.33835600	0.00000000

^{1}quinoline–BF$_3$

C	1.93927900	-2.08298900	0.00028000
C	0.65782200	-1.49236900	0.00007800
C	0.51647100	-0.05849800	0.00003500
C	1.67831800	0.75198900	-0.00013900
C	2.95184300	0.11712100	-0.00020600
C	3.07369000	-1.29328100	0.00002100
H	2.01975500	-3.17163900	0.00057500
H	-0.24150400	-2.11118500	-0.00015400
C	1.52575200	2.15466400	-0.00013000
H	3.85380300	0.73566200	-0.00033400
H	4.06702200	-1.74593400	0.00008900
C	0.24607600	2.68753000	0.00018800
C	-0.85136300	1.81862600	0.00036200
H	2.40370200	2.80519100	-0.00029700
H	0.07941500	3.76538700	0.00038100
H	-1.88291800	2.17918500	0.00059900
N	-0.71118300	0.49323700	0.00024100
B	-2.18573400	-0.52872400	-0.00003000
F	-3.16914100	0.39205800	0.00013000
F	-2.01668100	-1.24552300	1.14195100
F	-2.01636100	-1.24458600	-1.14267400

^{3}quinoline–BF$_3$

C	2.03148500	-2.04936600	-0.00053100
C	0.70205300	-1.47877200	-0.00178300
C	0.50189000	-0.06558200	-0.00079700
C	1.65321800	0.80153800	0.00000100
C	2.93922200	0.19959600	0.00095100
C	3.11544300	-1.23933200	0.00068500
H	2.13181300	-3.13517700	-0.00079400
H	-0.16995200	-2.12936500	-0.00384600
C	1.45080800	2.18425200	-0.00006400
H	3.81818400	0.84739000	0.00215900
H	4.12711900	-1.64799700	0.00150200
C	0.11835500	2.68544800	-0.00055900
C	-0.92882800	1.81762800	-0.00074800
H	2.30421600	2.86396600	0.00052100
H	-0.07298100	3.75871700	-0.00082500
H	-1.97163700	2.12721900	-0.00086700
N	-0.73921400	0.44825700	-0.00070700
B	-2.07461500	-0.52406700	0.00049600
F	-3.15786900	0.31971500	0.00155600
F	-1.98198000	-1.28948000	1.14544700
F	-1.98471500	-1.28964400	-1.14459200

^{1}isoquinoline

C	-2.41235500	0.70651900	0.00000000
C	-1.22594900	1.39753900	-0.00001100

C	0.00901900	0.69636200	0.00000400
C	0.01088000	-0.72422800	0.00000100
C	-1.23219900	-1.41401100	-0.00000100
C	-2.41250400	-0.71185400	0.00000500
H	-3.36233300	1.24489000	0.00000400
H	-1.21610500	2.49041100	-0.00000900
C	1.27411500	-1.37291400	-0.00000200
H	-1.23370200	-2.50654900	-0.00000200
H	-3.36467200	-1.24705300	0.00000900
C	2.41841400	-0.61454000	-0.00001800
H	1.33003000	-2.46364500	0.00001400
H	3.40225900	-1.09411900	0.00001800
C	1.26982100	1.35837100	0.00000700
H	1.28894900	2.45637500	-0.00000700
N	2.42287400	0.74174700	0.00000900

^{3}isoquinoline

C	2.45908700	-0.68470300	-0.00000900
C	1.20248600	-1.40253300	0.00000000
C	-0.02038900	-0.71477700	0.00000000
C	-0.00542000	0.73522900	0.00000200
C	1.23395300	1.40763100	0.00001800
C	2.47608500	0.67446900	0.00000000
H	3.39196700	-1.25203900	-0.00003200
H	1.20484600	-2.49464800	0.00001200
C	-1.24534600	1.38184900	-0.00001700
H	1.24716800	2.49975500	0.00004400
H	3.41969900	1.22274100	-0.00001300
C	-2.46207800	0.59269600	-0.00000400
H	-1.30728500	2.47201800	-0.00003000
H	-3.42664300	1.11576300	0.00000600
C	-1.27312400	-1.35760400	0.00000200
H	-1.32168900	-2.45045300	0.00001300
N	-2.48565500	-0.70095600	0.00000500

^{1}isoquinoline–H^{+}

C	2.44523400	-0.72037800	0.00000000
C	1.26232800	-1.41383300	-0.00000400
C	0.03312800	-0.69703800	0.00000000
C	0.03371100	0.73556900	-0.00000100
C	1.27324400	1.41638300	0.00000000
C	2.44737500	0.69847300	0.00000200
H	3.39471700	-1.25806900	0.00000200
H	1.25203400	-2.50560300	-0.00000400
C	-1.21863200	1.41153400	0.00000000
H	1.28692200	2.50763800	-0.00000100
H	3.40253400	1.22746200	0.00000500
C	-2.38289700	0.70268600	-0.00000300
H	-1.25580700	2.50175600	0.00000300
H	-3.37379000	1.15537300	-0.00000200
C	-1.20245600	-1.35813000	0.00000100
H	-1.28327800	-2.44696800	0.00000300
N	-2.33602300	-0.66533100	0.00000200
H	-3.21737700	-1.17586700	0.00000500

^{3}isoquinoline–H^{+}

C	2.50055200	-0.68791300	0.00000000
C	1.25081900	-1.40692000	-0.00000600
C	0.00579900	-0.72017300	-0.00000200
C	0.03106700	0.72130900	-0.00000300
C	1.27341500	1.38898400	0.00000200
C	2.52149100	0.67276900	0.00000600
H	3.43044100	-1.25937800	0.00000100
H	1.26227300	-2.49855300	-0.00001900
C	-1.20143300	1.41919400	-0.00000600
H	1.28135600	2.48174800	0.00000700
H	3.45943000	1.22801600	0.00001300
C	-2.39654900	0.70443000	-0.00000600
H	-1.23455600	2.50862800	-0.00000900
H	-3.36771500	1.20343800	0.00000800
C	-1.21954200	-1.37659200	0.00000300
H	-1.33223600	-2.45890000	0.00000000
N	-2.40063100	-0.62518900	0.00000600
H	-3.28829800	-1.11920200	0.00002800

^{1}isoquinoline–BF_3

C	-3.51284500	-1.23552500	0.00697700
C	-2.17977400	-1.56033000	-0.01341800

C	-1.20116800	-0.53063600	-0.01727400
C	-1.60384600	0.83349800	-0.00239000
C	-2.98978800	1.13767200	0.01838600
C	-3.91697400	0.12355500	0.02306600
H	-4.26921400	-2.02234300	0.01093400
H	-1.85604500	-2.60332500	-0.02582500
C	-0.58500300	1.82452100	-0.01142100
H	-3.30608400	2.18271700	0.03019200
H	-4.98220000	0.36338600	0.03917400
C	0.72743500	1.44915700	-0.03327700
H	-0.84770800	2.88332500	-0.00670800
H	1.55392400	2.15937500	-0.05352100
C	0.18306700	-0.81529700	-0.03690700
H	0.56590100	-1.83816300	-0.05155300
N	1.09020000	0.13583800	-0.03829200
B	2.70845800	-0.23145300	0.01251400
F	3.09647000	0.05131800	1.29739200
F	3.28273700	0.59742600	-0.92022100
F	2.78091700	-1.56855200	-0.30380100

^{3}isoquinoline–BF_3

C	-3.57451800	-1.21162100	0.00270500
C	-2.17086600	-1.54754600	-0.00356400
C	-1.18253400	-0.53862800	-0.00491300
C	-1.61116300	0.84548900	-0.00107200
C	-2.98573800	1.13788100	0.00497400
C	-3.97737300	0.08603800	0.00708400
H	-4.30752600	-2.02049800	0.00392600
H	-1.86585700	-2.59550900	-0.00707600
C	-0.61365700	1.83487200	-0.00461200
H	-3.30510100	2.18232900	0.00761300
H	-5.03572100	0.34905200	0.01192900
C	0.75834700	1.45431800	-0.00882200
H	-0.87197600	2.89424500	-0.00310500
H	1.56377900	2.19185800	-0.00968600
C	0.18285000	-0.81118300	-0.01210300
H	0.58398900	-1.82388400	-0.02060000
N	1.13318900	0.20540600	-0.01060000
B	2.72089600	-0.23147800	0.00377200
F	2.89029600	-0.91947800	1.18140700
F	3.42412700	0.95117100	-0.05353500
F	2.87996800	-1.02677800	-1.10628600

^{1}phenanthridine

C	3.54750900	-0.24482800	0.00000000
C	2.79828200	0.91265300	0.00007600
C	1.38828500	0.84952100	0.00000500
C	0.72992800	-0.40096400	-0.00001200
C	1.51907700	-1.57295900	-0.00004100
C	2.89759600	-1.49394000	-0.00006500
C	0.58533100	2.04709000	0.00003900
C	-0.72354100	-0.39308200	0.00001500
C	-1.38090400	0.86314100	-0.00004900
C	-2.79248300	0.91360500	-0.00004500
H	-3.25887000	1.90008000	-0.00008200
C	-3.53852300	-0.24569900	-0.00001700
C	-2.89043100	-1.49498700	0.00005300
C	-1.51172400	-1.56527500	0.00006700
H	1.10429600	3.01568800	0.00014100
H	4.63820100	-0.19726500	0.00000900
H	3.28501400	1.89134000	0.00009600
H	1.04306600	-2.55417800	-0.00011600
H	3.49041600	-2.41125600	-0.00010600
H	-4.62942400	-0.19704500	-0.00004200
H	-3.47986500	-2.41426800	0.00011000
H	-1.03088600	-2.54462500	0.00015300
N	-0.70462300	2.06655500	-0.00004600

^{3}phenanthridine

C	3.58010500	-0.24509700	0.00029300
C	2.82747000	0.92340000	0.00102800
C	1.40594300	0.87569000	0.00051100
C	0.76015800	-0.40772300	-0.00030300
C	1.53476300	-1.55122900	-0.00129700
C	2.94505700	-1.48493600	-0.00102700
C	0.62702800	2.03607800	0.00088600
C	-0.72404100	-0.40959600	-0.00000600
C	-1.40127100	0.89167300	-0.00102400

C	-2.85334200	0.90024000	-0.00112900
H	-3.33089700	1.88118900	-0.00208000
C	-3.57872700	-0.27036500	-0.00004700
C	-2.90990000	-1.50301300	0.00126800
C	-1.49142900	-1.54960000	0.00125400
H	1.09665600	3.02204300	0.00230000
H	4.67079600	-0.18865100	0.00064900
H	3.32073500	1.89830300	0.00190500
H	1.06243400	-2.53536200	-0.00236300
H	3.52933200	-2.40665900	-0.00181000
H	-4.67018600	-0.24073200	-0.00015600
H	-3.47566100	-2.43642400	0.00235600
H	-1.01182300	-2.53016600	0.00234500
N	-0.78889600	2.04333500	-0.00079700

^{1}phenanthridine–H^{+}

C	3.56492400	-0.26476600	0.00004100
C	2.83272500	0.89772300	0.00013900
C	1.41491600	0.83483800	0.00007600
C	0.73470200	-0.41843700	-0.00000900
C	1.51830100	-1.58870000	-0.00013500
C	2.89799800	-1.50803500	-0.00012100
C	0.65410700	2.02065900	0.00002000
C	-0.71798700	-0.42165200	0.00001700
C	-1.40559700	0.81176200	-0.00005400
C	-2.80873300	0.88368300	-0.00008000
H	-3.30880000	1.85495100	-0.00014700
C	-3.53927000	-0.28580500	-0.00001100
C	-2.88046600	-1.52950500	0.00010400
C	-1.50228800	-1.59653900	0.00011300
H	1.12609800	3.00581100	0.00002800
H	4.65520700	-0.23135000	0.00008000
H	3.32894500	1.87057500	0.00023100
H	1.04570600	-2.57016800	-0.00028700
H	3.48530000	-2.42853600	-0.00024100
H	-4.62955300	-0.24512100	-0.00003100
H	-3.46582500	-2.45025900	0.00019600
H	-1.01885100	-2.57296200	0.00023300
N	-0.66048400	1.98461000	-0.00007100
H	-1.17484000	2.86343300	-0.00015900

^{3}phenanthridine–H^{+}

C	3.58205900	-0.30515100	0.00002800
C	2.82668900	0.90419000	0.00013400
C	1.40332400	0.88926700	0.00005000
C	0.73572600	-0.38550600	-0.00002500
C	1.51863000	-1.55056400	-0.00014700
C	2.94930000	-1.51780500	-0.00012500
C	0.65877600	2.06022200	0.00004200
C	-0.70883100	-0.41732600	0.00002900
C	-1.42491800	0.83606400	-0.00005000
C	-2.83823400	0.85154200	-0.00010100
H	-3.36581500	1.80737500	-0.00018500
C	-3.53161500	-0.33398100	-0.00002500
C	-2.84775600	-1.57747100	0.00011500
C	-1.47442000	-1.61011200	0.00014300
H	1.09973400	3.05520900	0.00013600
H	4.67204500	-0.24531200	0.00006600
H	3.34971600	1.86258000	0.00029100
H	1.03390000	-2.52768400	-0.00027400
H	3.50760800	-2.45369900	-0.00022400
H	-4.62325300	-0.31965300	-0.00006400
H	-3.41782000	-2.50731700	0.00020600
H	-0.97259400	-2.57707100	0.00027300
N	-0.73182700	1.99693500	-0.00006600
H	-1.25311100	2.86681800	-0.00017200

^{1}phenanthridine–BF_3

C	-3.81767700	-1.58084600	-0.00029400
C	-2.50687000	-2.00237000	-0.00043900
C	-1.46000900	-1.05287400	-0.00018100
C	-1.73670700	0.33256300	0.00011800
C	-3.08942100	0.73717100	0.00048500
C	-4.10251400	-0.20127400	0.00026100
C	-0.10039900	-1.48016000	-0.00028500
C	-0.60832400	1.24769800	0.00004500
C	0.70574800	0.71933300	-0.00027600
C	1.81926000	1.58592300	-0.00050500

H	2.82193700	1.16599300	-0.00093500
C	1.62753300	2.95080100	-0.00034100
C	0.32965500	3.48876300	0.00001000
C	-0.76534200	2.65102100	0.00018700
H	0.15113600	-2.54272600	-0.00030300
H	-4.63221300	-2.30697700	-0.00064900
H	-2.26022400	-3.06645800	-0.00076000
H	-3.34800400	1.79581100	0.00101200
H	-5.14217900	0.13286600	0.00061900
H	2.49406000	3.61440300	-0.00052900
H	0.18628100	4.57088400	0.00008900
H	-1.76553300	3.08407500	0.00039100
N	0.91009800	-0.66088800	-0.00035000
B	2.44754400	-1.31856000	0.00028300
F	3.04699600	-0.85914400	-1.14674300
F	3.04569100	-0.85996300	1.14817200
F	2.25361800	-2.68126600	-0.00038800

^{3}phenanthridine–BF_3

C	-3.91980900	-1.46174200	0.00005900
C	-2.61820300	-1.94448800	0.00121800
C	-1.51116400	-1.04910600	0.00093100
C	-1.76418500	0.36186800	-0.00012400

^{1}benzo[f]quinoline

C	3.54381600	-0.27888400	0.00000100
C	2.81231900	0.88986500	0.00000700
C	1.39912300	0.86383000	0.00002700
C	0.72293400	-0.38327400	0.00000000
C	1.49731200	-1.56553300	-0.00003900
C	2.87698100	-1.51714400	-0.00002600
C	0.64001100	2.08740100	0.00001400
C	-0.73393800	-0.39367400	0.00001600
C	-1.44258800	0.83532100	0.00001600
C	-3.48076000	-0.21256400	-0.00004100
C	-2.88494700	-1.48780300	0.00002300
C	-1.50921100	-1.57256000	0.00005100
H	1.18560400	3.03431300	0.00001900
H	4.63520200	-0.24519000	0.00000800
C	-3.07100900	0.81181700	-0.00144500
C	-4.15693400	-0.08796900	-0.00139600
C	-0.20531600	-1.52229700	0.00153900
C	-0.58399800	1.25702000	0.00032000
C	0.74746600	0.66114500	0.00025000
C	1.90322300	1.53345700	-0.00008900
H	2.88936700	1.07537500	-0.00021700
C	1.75065000	2.90177700	0.00011300
C	0.46926300	3.46222600	0.00065500
C	-0.67624100	2.62935100	0.00075000
H	0.05166400	-2.57817600	0.00272000
H	-4.75766700	-2.16172500	0.00024900
H	-2.42476500	-3.01913100	0.00224500
H	-3.28803800	1.88120900	-0.00254800
H	-5.17734000	0.29811500	-0.00247100
H	2.63280500	3.54359700	-0.00003400
H	0.34110900	4.54611000	0.00094600
H	-1.65658400	3.10665100	0.00109400
N	0.92280500	-0.64941100	0.00054100
B	2.42106700	-1.35173500	-0.00052500
F	3.04615900	-0.90792300	-1.14703200
F	3.04814800	-0.90735900	1.14475500
F	2.19925100	-2.70758900	0.00007300
H	3.31953100	1.85789400	0.00001700
H	1.00702700	-2.53983400	-0.00007600
H	3.45190100	-2.44552900	-0.00004900
H	-4.57295700	-0.11954300	-0.00006300
H	-3.50551600	-2.38538200	0.00005000
H	-1.03033200	-2.55280200	0.00009700
C	-0.71485800	2.07688400	-0.00000900
H	-1.30370000	2.99522900	-0.00002600
N	-2.79198900	0.90709400	-0.00003300

^{3}benzo[f]quinoline

C	3.54119100	-0.30641600	0.05273700
C	2.83233900	0.86619600	0.11205900
C	1.40956300	0.86929600	0.06037600
C	0.71484500	-0.37589700	-0.04707100
C	1.48241200	-1.57019000	-0.11565900

C	2.85530900	-1.53924900	-0.06569200
C	0.67846500	2.08165700	0.09969500
C	-0.72431800	-0.38247300	-0.08739100
C	-1.39294000	0.86799700	-0.12034400
C	-3.51889900	-0.19626900	0.17355500
C	-2.94614200	-1.43042500	0.20424600
C	-1.53387800	-1.55584700	-0.01938300
H	1.22014500	3.02656000	0.17928800
H	4.63237200	-0.29280100	0.09212600
H	3.35257500	1.82358500	0.19639600
H	0.97711800	-2.53156600	-0.21499500
H	3.42174300	-2.47138800	-0.11878300
H	-4.56358000	0.01062100	0.41409400
H	-3.54709000	-2.30845100	0.44749300
H	-1.07476600	-2.53949800	0.06776400
C	-0.70061000	2.08037500	-0.00240700
H	-1.26715500	3.01267300	-0.01017500
N	-2.76219700	0.83110600	-0.36021900

^{1}benzo[f]quinoline–H^{+}

C	3.57679800	-0.26250800	0.00004300
C	2.84120800	0.90369500	0.00011600
C	1.42947800	0.86004100	0.00005800
C	0.76317700	-0.39477300	-0.00001900
C	1.53917700	-1.57238300	-0.00013400
C	2.91897400	-1.50528900	-0.00010500
C	0.66563600	2.07423800	0.00003800
C	-0.69154500	-0.40759900	-0.00000200
C	-1.38223900	0.83175300	-0.00006700
C	-3.48577100	-0.30405800	-0.00000900
C	-2.85675500	-1.53727000	0.00010800
C	-1.46719300	-1.58025700	0.00012400
H	1.20405200	3.02469900	0.00009200
H	4.66729600	-0.22398300	0.00008900
H	3.34263500	1.87370800	0.00019200
H	1.06531400	-2.55425700	-0.00029700
H	3.50323900	-2.42713100	-0.00020700
H	-4.56939700	-0.18051900	-0.00004200
H	-3.45403800	-2.44835800	0.00020500
H	-0.97657000	-2.55406900	0.00026600
C	-0.69578400	2.07667000	-0.00006000
H	-1.25905500	3.01195600	-0.00012300
N	-2.74689600	0.81071300	-0.00008300
H	-3.22616800	1.70940700	-0.00013200

^{3}benzo[f]quinoline–H^{+}

C	3.60798500	-0.29734600	-0.00001700
C	2.88742900	0.88511700	0.00010500
C	1.45132300	0.88408900	0.00010100
C	0.76025900	-0.38235200	0.00001800
C	1.51524000	-1.54510600	-0.00016600
C	2.92779300	-1.51571400	-0.00017400
C	0.74180400	2.07468200	0.00010100
C	-0.71051700	-0.41717600	0.00008000
C	-1.39594700	0.84366600	-0.00006300
C	-3.51907000	-0.30199200	-0.00008500
C	-2.88446300	-1.52018400	0.00014200
C	-1.47098500	-1.58400400	0.00024300
H	1.25181700	3.03781400	0.00016800
H	4.69872300	-0.27493100	-0.00000900
H	3.40577200	1.84637400	0.00020700
H	1.02982800	-2.52160300	-0.00031700
H	3.48017600	-2.45668000	-0.00030500
H	-4.60316900	-0.18887100	-0.00020900
H	-3.48133800	-2.43199600	0.00022700
H	-0.99516800	-2.56312000	0.00044800
C	-0.70509400	2.04086200	-0.00002300
H	-1.25545300	2.98511500	-0.00008100
N	-2.78553800	0.83591700	-0.00019300
H	-3.26696500	1.72922100	-0.00035300

^{1}benzo[f]quinoline–BF_3

C	-4.55470000	-0.69181500	-0.00002900
C	-3.46713800	-1.53834900	-0.00010700
C	-2.15078500	-1.02435900	-0.00005500
C	-1.94421100	0.37678500	0.00005100
C	-3.07637000	1.22254900	0.00016700
C	-4.35400900	0.70035300	0.00012700

C	-1.01606000	-1.90465200	-0.00008600
C	-0.57801700	0.88257300	0.00000800
C	0.50716600	-0.03055400	-0.00003900
C	2.05165900	1.72969800	-0.00014900
C	1.03573400	2.68538400	-0.00014800
C	-0.27453000	2.25798400	-0.00004700
H	-1.19786200	-2.98185500	-0.00013700
H	-5.56812300	-1.09763100	-0.00008800
H	-3.60883400	-2.62154900	-0.00020300
H	-2.95698300	2.30633500	0.00031500
H	-5.21315000	1.37397900	0.00022700
H	3.10874000	1.99505000	-0.00022100
H	1.29039400	3.74490500	-0.00018500
H	-1.07550000	2.99747300	-0.00000900
C	0.25908600	-1.44454000	-0.00004800
H	1.10303600	-2.12890100	-0.00005600
N	1.79390100	0.42954800	-0.00010200
B	3.09957800	-0.61817800	0.00005800
F	2.97439700	-1.36364400	1.14750300
F	4.21075200	0.19100700	-0.00006100
F	2.97442100	-1.36404100	-1.14711800

^{3}benzo[f]quinoline–BF_3

C	-4.60350500	-0.65926200	0.00012600
C	-3.52797700	-1.52946100	0.00023400
C	-2.18203300	-1.04529500	0.00008400
C	-1.95963300	0.38108100	-0.00001300
C	-3.05913700	1.21947100	-0.00020500
C	-4.37700700	0.71910100	-0.00014100
C	-1.10324200	-1.91624100	-0.00015300
C	-0.56404400	0.90638400	0.00000900
C	0.52880700	-0.03608000	-0.00011700
C	2.08835700	1.73488400	-0.00006800
C	1.08015400	2.68113700	0.00006400
C	-0.26386100	2.25270100	0.00017400
H	-1.25664600	-2.99562900	-0.00029100
H	-5.62330500	-1.04853800	0.00023300
H	-3.68984900	-2.60960900	0.00042800
H	-2.92671800	2.30200100	-0.00043100
H	-5.21603200	1.41681100	-0.00030900
H	3.14521700	2.00052500	-0.00010800
H	1.33283000	3.74098300	0.00003100
H	-1.05377700	3.00338500	0.00040000
C	0.27648600	-1.39983600	-0.00018700
H	1.10757100	-2.10117300	-0.00008700
N	1.83414400	0.42479600	-0.00008200
B	3.10964700	-0.62395100	0.00001900
F	2.97973100	-1.38105300	1.14559600
F	4.23946700	0.16060600	0.00014200
F	2.98005500	-1.38111600	-1.14554200

^{1}4,7-phenanthroline

C	-3.46828700	-0.19252300	0.00000200
C	-1.42051800	0.83555600	-0.00007300
C	-0.72705500	-0.40157700	-0.00000400
C	-1.51136400	-1.57394600	0.00004900
C	-2.88604000	-1.47447300	0.00002800
C	-0.67739000	2.06942400	-0.00001300
C	0.72706500	-0.40154600	-0.00001800
C	1.42051400	0.83558300	-0.00001400
C	3.46829900	-0.19251000	0.00003300
C	2.88605700	-1.47447500	-0.00002000
C	1.51138100	-1.57392200	-0.00004300
H	-1.25751700	2.99350200	0.00000000
H	-4.55941100	-0.08865100	-0.00008000
H	-1.04103600	-2.55872000	0.00007600
H	-3.51654900	-2.36498800	0.00002100
H	4.55942500	-0.08862500	0.00005900
H	3.51655400	-2.36499500	-0.00004300
H	1.04101500	-2.55868000	-0.00008600
C	0.67733700	2.06941800	0.00001500
H	1.25752800	2.99345500	0.00004300
N	2.76866000	0.92054800	0.00002900
N	-2.76866000	0.92054400	0.00002100

^{3}4,7-phenanthroline

C	-3.50720800	-0.22454200	0.00010300
C	-1.41939200	0.89115900	-0.00061800

C	-0.72505500	-0.39951400	-0.00084100
C	-1.51051400	-1.54535500	0.00026400
C	-2.91244500	-1.48379300	0.00098600
C	-0.69893200	2.08940900	0.00030200
C	0.72507300	-0.39950300	-0.00094500
C	1.41935100	0.89120500	-0.00037700
C	3.50723700	-0.22447500	0.00031000
C	2.91250000	-1.48375400	0.00047100
C	1.51057200	-1.54532700	-0.00040400
H	-1.25936800	3.02358300	0.00068300
H	-4.59521900	-0.09808400	-0.00099700
H	-1.02777300	-2.52516800	0.00035000
H	-3.52888300	-2.38236800	0.00126200
H	4.59525300	-0.09801900	-0.00046400
H	3.52899400	-2.38228500	0.00036000
H	1.02783100	-2.52514000	-0.00089500
C	0.69881200	2.08941900	0.00050000
H	1.25929300	3.02344400	0.00114100
N	2.76554700	0.85961200	0.00025500
N	-2.76556400	0.85959700	-0.00024700

^{1}4,7-phenanthroline–H^{+}

C	-3.50282200	-0.17020300	-0.00009300
C	-1.44757300	0.82890400	0.00001500
C	-0.76709300	-0.41331200	0.00003300
C	-1.55926400	-1.58252900	0.00013700
C	-2.93047200	-1.46086300	0.00010300
C	-0.70003700	2.05804000	0.00000300
C	0.68445800	-0.41611500	0.00001500
C	1.36020000	0.83062700	0.00007100
C	3.47359100	-0.28507100	-0.00001900
C	2.85720200	-1.52569200	-0.00011100
C	1.46891800	-1.58336100	-0.00010200
H	-1.27677800	2.98454100	-0.00005500
H	-4.59151900	-0.05439900	-0.00011200
H	-1.10812500	-2.57583000	0.00035200
H	-3.57202800	-2.34292200	0.00028600
H	4.55619500	-0.15212100	-0.00001000
H	3.46482200	-2.42997200	-0.00021000
H	0.98668200	-2.56171900	-0.00022100
C	0.65986800	2.07008500	0.00006700
H	1.21535300	3.01037500	0.00011400
N	2.72506500	0.82259200	0.00006200
N	-2.78973400	0.93355900	-0.00020000
H	3.19622800	1.72593700	0.00009800

^{3}4,7-phenanthroline–H^{+}

C	3.48119800	-0.35333900	0.00009400
C	1.38291500	0.84208700	0.00016500
C	0.68949200	-0.41736000	-0.00009300
C	1.43174900	-1.58934500	-0.00041500
C	2.84533500	-1.56333500	-0.00029000
C	0.71392500	2.06278200	0.00019200
C	-0.77679200	-0.39018600	-0.00006000
C	-1.40614800	0.92419900	-0.00026400
C	-3.58126800	-0.17847900	0.00004400
C	-2.99497300	-1.43809300	0.00043000
C	-1.58915800	-1.51687500	0.00037600
H	1.28260200	2.99419900	0.00033000
H	4.56626000	-0.24551000	0.00023400
H	0.93358400	-2.55907300	-0.00078200
H	3.42506200	-2.48491700	-0.00049000
H	-4.65860700	0.01291800	-0.00003600
H	-3.62875800	-2.32434700	0.00067900
H	-1.13817000	-2.50968400	0.00081100
C	-0.68454900	2.11317000	-0.00006800
H	-1.21179000	3.06590600	-0.00012500
N	-2.74786500	0.83363600	-0.00055700
N	2.76201900	0.79495800	0.00029900
H	3.26037800	1.67898300	0.00051900

^{1}4,7-phenanthroline–2H^{+}

C	3.50914400	-0.26841200	0.00004700
C	1.39193500	0.82532600	0.00002800
C	0.72739700	-0.41749000	-0.00001700
C	1.51653400	-1.59207900	-0.00011000
C	2.89790600	-1.52068000	-0.00008200
C	0.67927000	2.06536100	0.00001300

C	-0.72741800	-0.41744000	-0.00001000
C	-1.39196200	0.82540200	-0.00005600
C	-3.50918000	-0.26841200	0.00001000
C	-2.89792400	-1.52067700	0.00008700
C	-1.51653800	-1.59200200	0.00007900
H	1.22729300	3.01055100	0.00005800
H	4.59325000	-0.13321200	0.00012200
H	3.23161200	1.73848400	0.00018500
H	1.04867200	-2.57775400	-0.00023900
H	3.51514800	-2.41989500	-0.00017100
H	-4.59326700	-0.13308500	0.00000100
H	-3.51503100	-2.41998300	0.00017000
H	-1.04859600	-2.57763800	0.00016300
C	-0.67926900	2.06540700	-0.00005700
H	-1.22714800	3.01077100	-0.00011200
N	-2.75798200	0.83265900	-0.00005200
H	-3.23142800	1.73827500	-0.00008900
N	2.75800000	0.83272100	0.00009700

^{3}4,7-phenanthroline–2H^{+}

C	3.54490700	-0.28189600	0.00010500
C	1.42701100	0.84599600	0.00024400
C	0.74874400	-0.41954600	-0.00009100
C	1.50781400	-1.57639600	-0.00059100
C	2.91666100	-1.51888400	-0.00049400
C	0.74114700	2.04733000	0.00022000
C	-0.74869300	-0.41961900	0.00009200
C	-1.42702400	0.84606700	-0.00023600
C	-3.54490000	-0.28195400	-0.00009300
C	-2.91658800	-1.51897300	0.00048200
C	-1.50768000	-1.57645300	0.00058600
H	1.26360700	3.00607200	0.00052300
H	4.63063800	-0.16258700	0.00030500
H	3.29262800	1.73199100	0.00081700
H	1.03770000	-2.56049800	-0.00106700
H	3.51794400	-2.42896800	-0.00085500
H	-4.63064500	-0.16277200	-0.00028200
H	-3.51781200	-2.42909500	0.00081600
H	-1.03761600	-2.56057700	0.00105900
C	-0.74124500	2.04725300	-0.00025100
H	-1.26388800	3.00593600	-0.00056600
N	-2.80789700	0.83360800	-0.00041700
H	-3.29273800	1.73209500	-0.00076500
N	2.80779100	0.83365600	0.00044300

^{1}4,7-phenanthroline–BF$_3$

C	-4.44215800	-0.76713700	0.00023500
C	-2.16627600	-1.01048700	-0.00030000
C	-1.94948300	0.38801300	0.00003200
C	-3.09348400	1.21433100	0.00060300
C	-4.34469700	0.63853700	0.00068700
C	-1.03697300	-1.89956400	-0.00070900
C	-0.58591300	0.89225800	-0.00018400
C	0.49369600	-0.02625200	-0.00034300
C	2.04268300	1.72905400	-0.00052300
C	1.03020700	2.68949800	-0.00057700
C	-0.28137800	2.26726500	-0.00035300
H	-1.25254000	-2.96894100	-0.00103700
H	-5.42765200	-1.24601500	0.00016400
H	-3.00291100	2.30155900	0.00102300
H	-5.24692300	1.25184500	0.00113300
H	3.10072700	1.99095800	-0.00055200
H	1.28961100	3.74785100	-0.00073900
H	-1.08141700	3.00833900	-0.00044800
C	0.23838300	-1.44070600	-0.00068200
H	1.08126400	-2.12687900	-0.00101100
N	1.78127900	0.42986700	-0.00033300
N	-3.39761000	-1.56430700	-0.00024100
B	3.08660800	-0.62390500	0.00039200
F	2.95574900	-1.36643300	1.14800000
F	4.19780700	0.18414400	0.00050800
F	2.95683100	-1.36737300	-1.14670800

^{3}4,7-phenanthroline–BF$_3$

C	-4.49035000	-0.77285900	-0.19439300
C	-2.12740300	-1.01875500	0.14909900
C	-1.94443700	0.38942800	0.07790500
C	-3.10246800	1.19783000	-0.06326400

C	-4.37947400	0.58233000	-0.28047100
C	-1.04805200	-1.90382800	0.07911200
C	-0.58886900	0.87808800	0.07157300
C	0.50008500	-0.04643500	0.02207100
C	2.04083400	1.72176800	0.03915400
C	1.02093300	2.68262000	0.10410000
C	-0.28541100	2.25683100	0.12198100
H	-1.24417800	-2.97636500	0.10448800
H	-5.39600600	-1.34059300	-0.41596000
H	-3.01542100	2.27584900	-0.19253300
H	-5.24480100	1.18554600	-0.55858100
H	3.09646400	1.99400400	0.01887700
H	1.27948600	3.74043100	0.14050900
H	-1.09039600	2.99044100	0.18145600
C	0.25296100	-1.43608400	0.00561000
H	1.08837700	-2.13012100	-0.02971200
N	1.79311200	0.42718000	0.00295900
N	-3.42689700	-1.44044800	0.36858700
B	3.09685300	-0.61522600	-0.06902500
F	3.01233800	-1.39449300	1.05989800
F	4.20725300	0.19591000	-0.08366600
F	2.93469900	-1.32983800	-1.23168900

^{1}4,7-phenanthroline–2BF$_3$

C	-3.47989900	1.28842100	0.00014300
C	-1.41600100	0.19101100	-0.00007600
C	-0.72701600	1.42547600	0.00007800
C	-1.49208900	2.60962300	0.00043000
C	-2.86707700	2.54434500	0.00042500
C	-0.67797300	-1.04019000	-0.00017700
C	0.72680300	1.42555000	-0.00006100
C	1.41581200	0.19110200	0.00003600
C	3.47971300	1.28843000	-0.00025900
C	2.86686900	2.54436200	-0.00047200
C	1.49189500	2.60969900	-0.00036900
H	-1.22393000	-1.98030600	-0.00034800
H	-4.56307500	1.16354800	0.00010700
H	-1.00689600	3.58596700	0.00077300
H	-3.48069700	3.44476100	0.00069700
H	4.56288800	1.16356200	-0.00038500
H	3.48053400	3.44475400	-0.00054600
H	1.00670400	3.58604100	-0.00070000
C	0.67779800	-1.04013500	-0.00001200
H	1.22380500	-1.98021200	0.00011200
N	2.78049700	0.16477100	0.00001600
N	-2.78071200	0.16473300	-0.00005100
B	3.63782600	-1.29145700	0.00011500
F	3.24662800	-1.93198900	1.14687000
F	4.95696600	-0.91669300	0.00111800
F	3.24803900	-1.93141900	-1.14738600
B	-3.63754600	-1.29138500	-0.00009100
F	-3.24717300	-1.93154800	1.14716100
F	-3.24669600	-1.93183000	-1.14705300
F	-4.95690000	-0.91725400	-0.00045300

^{3}4,7-phenanthroline–2BF$_3$

C	-3.51455500	1.29565200	-0.09491300
C	-1.44900400	0.17161800	-0.01476400
C	-0.74621200	1.42615900	-0.03060100
C	-1.48595800	2.58933000	-0.11145700
C	-2.88916200	2.53425700	-0.14613200
C	-0.74046700	-1.02274700	-0.00932700
C	0.74633900	1.42612900	0.03045700
C	1.44907600	0.17157200	0.01445600
C	3.51467300	1.29553400	0.09499000
C	2.88934800	2.53412200	0.14622100
C	1.48610200	2.58926000	0.11147300
H	-1.26278500	-1.97588600	-0.03760200
H	-4.59891400	1.18177900	-0.10266000
H	-0.99844500	3.56351700	-0.15114700
H	-3.48801700	3.44236200	-0.20627400
H	4.59901500	1.18155800	0.10293000
H	3.48822300	3.44221200	0.20637800
H	0.99863500	3.56346500	0.15120800
C	0.74044000	-1.02278200	0.00846000
H	1.26270800	-1.97594300	0.03645700
N	2.82764100	0.15935600	0.03207900
N	-2.82761200	0.15947400	-0.03217200

B	3.68022300	-1.27958600	-0.05381700
F	3.30111000	-1.99470100	1.05715100
F	5.00096400	-0.91032200	-0.04332500
F	3.27837000	-1.86102400	-1.23070700
B	-3.68041100	-1.27968300	0.05405500
F	-3.30165300	-1.99472000	-1.05707300
F	-3.27813600	-1.86099300	1.23078200
F	-5.00103400	-0.91014700	0.04394900

^{1}a

C	2.43107800	-0.70847800	0.00000000
C	1.24503800	-1.40051100	0.00000000
C	1.24503800	1.40051100	0.00000000
C	2.43107800	0.70847800	0.00000000
H	3.38010300	-1.24917100	0.00000000
H	1.24272600	-2.49363000	0.00000000
H	1.24272600	2.49363000	0.00000000
H	3.38010300	1.24917100	0.00000000
C	0.00000000	-0.71311600	0.00000000
C	-1.24503800	-1.40051100	0.00000000
C	-2.43107800	-0.70847800	0.00000000
C	-2.43107800	0.70847800	0.00000000
C	-1.24503800	1.40051100	0.00000000
C	0.00000000	0.71311600	0.00000000
H	-1.24272600	-2.49363000	0.00000000
H	-3.38010300	-1.24917100	0.00000000
H	-3.38010300	1.24917100	0.00000000
H	-1.24272600	2.49363000	0.00000000

^{3}a

C	2.48505100	-0.67940000	0.00000000
C	1.23443700	-1.40109300	0.00000000
C	1.23443700	1.40109300	0.00000000
C	2.48505100	0.67940000	0.00000000
H	3.42254900	-1.23883700	0.00000000
H	1.24332800	-2.49342200	0.00000000
H	1.24332800	2.49342200	0.00000000
H	3.42254900	1.23883700	0.00000000
C	0.00000000	-0.72690600	0.00000000
C	-1.23443700	-1.40109300	0.00000000
C	-2.48505100	-0.67940000	0.00000000
C	-2.48505100	0.67940000	0.00000000
C	-1.23443700	1.40109300	0.00000000
C	0.00000000	0.72690600	0.00000000
H	-1.24332800	-2.49342200	0.00000000
H	-3.42254900	-1.23883700	0.00000000
H	-3.42254900	1.23883700	0.00000000
H	-1.24332800	2.49342200	0.00000000

^{1}b

C	-2.14771500	-1.45151800	-0.00007500
C	-3.97695600	0.72763400	-0.00077000
C	-4.42916200	-0.58442600	-0.00069300
C	-3.52216200	-1.65820600	-0.00034900
H	-1.44004900	-2.27780200	0.00019100
H	-4.68070100	1.56279100	-0.00103700
H	-5.50204600	-0.78831400	-0.00090100
H	-3.90377600	-2.68155600	-0.00029500
C	-1.79908000	2.17092900	-0.00049000
C	-2.59573100	0.96527800	-0.00050100
C	-1.70057600	-0.12700200	-0.00015700
C	-0.49613600	1.79544800	-0.00015000
N	-0.40369100	0.40081100	0.00007000
C	0.77487000	-0.34305400	0.00038000
O	0.79631800	-1.54672600	0.00039600
O	1.82484800	0.46892100	0.00035700
C	3.19312000	-0.03619500	0.00037800
C	3.44631900	-0.84856400	-1.26745800
H	4.51050100	-1.12123700	-1.31941800
H	2.84702900	-1.76710900	-1.27719100
H	3.20114900	-0.25205900	-2.15871300
C	3.44610600	-0.84883800	1.26807600
H	4.51026700	-1.12157300	1.32012400
H	3.20083800	-0.25251300	2.15942500
H	2.84677100	-1.76735900	1.27752900
C	4.02558500	1.24108800	0.00058000
H	5.09649900	0.99309500	0.00064200
H	3.80702900	1.84515300	-0.89180400

H	3.80688200	1.84496500	0.89305500
H	-2.16628300	3.19446700	-0.00070900
H	0.41150700	2.39037500	-0.00002600

^{3}b

C	-2.10561000	-1.42645500	-0.00018400
C	-4.03221900	0.70180400	-0.00069900
C	-4.44652200	-0.62253900	-0.00069900
C	-3.52081000	-1.67238200	-0.00044900
H	-1.38770400	-2.24326900	0.00000300
H	-4.75193000	1.52202800	-0.00089500
H	-5.51436500	-0.85195700	-0.00090100
H	-3.87285200	-2.70545000	-0.00045600
C	-1.90779800	2.15327800	-0.00033800
C	-2.62090200	0.98758500	-0.00042900
C	-1.69083400	-0.13041400	-0.00017800
C	-0.46234400	1.81079400	-0.00000800
N	-0.37505100	0.41609700	0.00005500
C	0.78392600	-0.32998000	0.00027400
O	0.80280700	-1.54117000	0.00023000
O	1.84425200	0.48253500	0.00031800
C	3.20274600	-0.03288600	0.00040300
C	3.45233200	-0.84879700	-1.26681900
H	4.51288700	-1.13633100	-1.31608000
H	2.83834200	-1.75760600	-1.27735900
H	3.21704800	-0.24874000	-2.15851500
C	3.45213500	-0.84887900	1.26760900
H	4.51268000	-1.13641900	1.31699700
H	3.21673100	-0.24887800	2.15931100
H	2.83813000	-1.75767900	1.27800000
C	4.04997500	1.23537300	0.00051200
H	5.11863100	0.97724700	0.00060400
H	3.83673600	1.84167800	-0.89177000
H	3.83657100	1.84163000	0.89278700
H	-2.30017200	3.16819600	-0.00047800
H	0.42370200	2.43293700	0.00000800

^{1}c

C	-0.90755600	-1.41407500	0.00000000
C	-0.96685100	1.43738700	0.00000000
C	-2.13830700	0.69167300	0.00000000
C	-2.10953300	-0.71606900	0.00000000
H	-0.86639300	-2.50384200	0.00000000
H	-0.99881000	2.52875400	0.00000000
H	-3.10276100	1.20370000	0.00000000
H	-3.05033800	-1.27036800	0.00000000
C	1.65478700	1.12736600	0.00000000
C	0.25895200	0.75474200	0.00000000
C	0.25535900	-0.64907400	0.00000000
C	2.34254600	-0.04023500	0.00000000
H	2.07951800	2.12775800	0.00000000
H	3.40742200	-0.25808300	0.00000000
O	1.52437200	-1.12227700	0.00000000

^{3}c

C	-0.81463100	-1.45240700	0.00000000
C	-1.04697200	1.43728000	0.00000000
C	-2.18568600	0.63472600	0.00000000
C	-2.10765300	-0.75722300	0.00000000
H	-0.75358900	-2.54001500	0.00000000
H	-1.11179600	2.52568600	0.00000000
H	-3.17032100	1.10784700	0.00000000
H	-3.02210000	-1.35258200	0.00000000
C	1.55297300	1.19622300	0.00000000
C	0.25710300	0.77657900	0.00000000
C	0.28826500	-0.67312100	0.00000000
C	2.38504300	0.00355500	0.00000000
H	1.92506300	2.21903000	0.00000000
H	3.45801300	-0.15392400	-0.00000200
O	1.58800900	-1.09996400	0.00000000

^{1}d

C	1.24596700	-1.21285300	-0.00000200
C	2.64056600	-1.20564200	-0.00003600
C	3.34009400	0.00001000	0.00004100
C	2.64046000	1.20570000	-0.00000800
C	1.24594700	1.21284500	-0.00003000
C	0.55567100	-0.00005800	0.00002600

H	0.70276800	-2.15928700	-0.00000800
H	3.18128300	-2.15437600	-0.00003000
H	4.43184200	0.00010100	0.00006100
H	3.18124200	2.15439400	0.00000000
H	0.70260300	2.15919500	-0.00003600
I	-1.55116900	-0.00000100	0.00000100

^{3}d

C	1.19289700	-1.26097700	0.00026300
C	2.62518300	-1.24971500	-0.00040100
C	3.28412600	0.00001000	0.00006100
C	2.62522200	1.24970600	0.00037000
C	1.19294000	1.26095000	-0.00038600
C	0.53893000	-0.00002500	-0.00005100
H	0.62016600	-2.18616800	0.00090900
H	3.19536300	-2.17722300	-0.00069500
H	4.37954300	0.00000800	0.00018400
H	3.19542100	2.17720200	0.00088000
H	0.62019300	2.18613300	-0.00105400
I	-1.52389600	0.00000700	0.00001200

^{1}e

C	-0.00468900	-1.23584800	0.00011100
C	-1.26944100	-0.71375500	-0.00015300
C	-1.26944100	0.71375500	0.00013000
C	-0.00468900	1.23584800	-0.00005300
S	1.19104700	0.00000000	-0.00001600
H	0.28739100	-2.28476700	0.00017200
H	-2.17099100	-1.32683400	-0.00024200
H	-2.17099000	1.32683500	0.00019500
H	0.28739200	2.28476700	-0.00008000

^{3}e

C	-0.00473100	-1.29387000	-0.00002800
C	-1.28211000	-0.71976900	0.00000200
C	-1.28213000	0.71974500	-0.00000400
C	-0.00476400	1.29386800	0.00004700
S	1.20221900	0.00001200	-0.00000300
H	0.30162900	-2.33448700	0.00007100
H	-2.19812800	-1.31183100	0.00004300
H	-2.19816200	1.31178600	-0.00007200
H	0.30157000	2.33449300	-0.00010200

^{1}f

O	-2.12429700	-0.00026400	-0.53021700
C	-3.50483900	-0.00017600	-0.34105200
H	-3.84823100	0.89532400	0.21503700
H	-3.98219300	-0.00083700	-1.33019300
H	-3.84818200	-0.89496400	0.21621300
C	0.07390800	0.00026700	0.36392000
C	0.76391200	1.20358800	0.19202800
C	0.76347800	-1.20334900	0.19237300
C	2.11841500	1.20607200	-0.13575200
H	0.23138800	2.15025600	0.31624700
C	2.11797700	-1.20641600	-0.13541800
H	0.23061400	-2.14979000	0.31686500
C	2.79829000	-0.00031700	-0.29974100
H	2.64607200	2.15379600	-0.26420300
H	2.64528500	-2.15437100	-0.26359900
H	3.86037700	-0.00054300	-0.55489800
C	-1.40099700	0.00054700	0.66921000
H	-1.66077200	0.89157900	1.27781900
H	-1.66085100	-0.88963000	1.27903900

^{3}f

O	-2.19536700	-0.24041200	-0.41065300
C	-3.54194800	-0.18226500	-0.05503100
H	-3.95163800	0.84303100	-0.14740300
H	-4.09935500	-0.84204800	-0.73322500
H	-3.71047400	-0.52202900	0.98640200
C	0.06003100	0.30925000	0.06603200
C	1.00696700	1.33787200	-0.07715800
C	0.54635600	-1.13170900	0.04408900
C	2.35202900	1.06558300	-0.13248500
H	0.66107300	2.37525600	-0.12121100
C	1.90382600	-1.39455200	0.05503600
H	-0.19946500	-1.92498700	-0.00844800
C	2.83525000	-0.36075100	-0.00810700

H	3.08423100	1.86412400	-0.25920600
H	2.25214700	-2.43059300	0.08345400
H	3.90699900	-0.56176500	0.00600900
C	-1.36675100	0.55509600	0.39537200
H	-1.61127600	1.63142600	0.28311800
H	-1.54388300	0.29972600	1.46924400

^{1}g

N	-2.05471500	-0.65022500	0.19538700
H	-1.63978600	-1.48369200	0.58674800
C	-3.49217800	-0.53119500	0.19506800
H	-3.74906700	0.42215900	-0.28252600
H	-3.95622700	-1.35348000	-0.37039800
H	-3.90425500	-0.52870300	1.21740500
C	-1.23685400	0.39645600	-0.11289000
O	-1.65650700	1.49711300	-0.41635700
C	0.24137500	0.11047500	-0.04585600
C	0.78616900	-1.16746500	-0.21338900
C	1.09752300	1.19722300	0.15789200
C	2.16561400	-1.35854900	-0.15385400
H	0.13948400	-2.02281100	-0.42509000
C	2.47422300	1.00548600	0.22627600
H	0.65696100	2.19099100	0.25672000
C	3.01075200	-0.27354100	0.07313600
H	2.58213600	-2.35815300	-0.29498900
H	3.13454600	1.85880500	0.39506100
H	4.09151900	-0.42378200	0.12192000

^{3}g

N	-2.24419100	-0.40394800	0.42663900
H	-2.95299700	-0.14830300	1.11216700
C	-2.75286200	-1.05913200	-0.76407300
H	-1.90749800	-1.45452900	-1.34294100
H	-3.40120000	-1.89474700	-0.46367700
H	-3.33316000	-0.37554400	-1.40605800
C	-1.20324200	0.55294700	0.31893000
O	-1.80781900	1.69267400	0.17565200
C	0.16165800	0.23428700	0.16461600
C	0.63363600	-1.09379200	0.35676000
C	1.10697200	1.24054100	-0.17847400
C	1.97919600	-1.38917000	0.20554100
H	-0.07419300	-1.87670800	0.63972700
C	2.44773700	0.92261600	-0.32182600
H	0.76142900	2.26520300	-0.33126800
C	2.90004900	-0.39018500	-0.13503400
H	2.32318000	-2.41494000	0.35956200
H	3.15913400	1.70860100	-0.58702400
H	3.95834100	-0.63145900	-0.25082300

^{1}h

N	-2.30918600	-0.32661300	-1.02841900
H	-2.18427400	0.25308500	-1.85308800
C	-2.16528100	-1.75808900	-1.20132600
H	-2.50188900	-2.25901900	-0.28424200
H	-2.81737300	-2.08237100	-2.02343900
H	-1.12896400	-2.07445400	-1.42285000
S	-1.69763500	0.40874800	0.32481900
O	-2.01220700	1.81730000	0.17733900
O	-2.13560100	-0.38193600	1.46070300
C	0.07535700	0.23359600	0.21104200
C	0.81518200	1.19377200	-0.47880700
C	0.69855900	-0.87477600	0.78015900
C	2.18962400	1.02738900	-0.60862100
H	0.31242700	2.07038100	-0.89207200
C	2.07577900	-1.02696100	0.63936200
H	0.10589100	-1.59863100	1.34233400
C	2.84166900	-0.08333700	-0.05513300
H	2.77207900	1.78055800	-1.14549600
H	2.56651100	-1.89546100	1.08586600
C	4.33496200	-0.23341700	-0.17298200
H	4.84341100	0.33362600	0.62341600
H	4.64353500	-1.28393700	-0.07980100
H	4.70246700	0.15056200	-1.13528700

^{3}h

N	-1.32288000	-1.07964900	-0.98235600
H	-1.18424200	-0.74998000	-1.93258300
C	-0.54916600	-2.22064400	-0.54153900

H	-0.84935000	-2.46889000	0.48504700
H	-0.77940800	-3.08489800	-1.18050600
H	0.54063000	-2.03959700	-0.56100900
S	-1.71874100	0.15593500	0.04858800
O	-2.50772600	1.07501600	-0.75252700
O	-2.21616500	-0.44323200	1.27454800
C	-0.20873100	1.00965800	0.45576700
C	0.54621500	1.53599400	-0.70316700
C	0.57041100	0.46891200	1.58611300
C	1.75813500	0.96981300	-0.95828200
H	0.10650100	2.30292300	-1.34410300
C	1.78742300	-0.05170900	1.30053200
H	0.13201500	0.42579200	2.58455400
C	2.38066000	0.08185100	-0.01675400
H	2.31693900	1.25202600	-1.85609200
H	2.37183000	-0.54236000	2.08496100
C	3.68292800	-0.58650900	-0.31838800
H	4.38595400	-0.49426400	0.52544800
H	3.54355900	-1.66865600	-0.49250200
H	4.15945400	-0.16799400	-1.21599800

^{1}i

C	0.57103800	0.17021200	0.00001200
C	-0.76642000	-0.46865700	0.00000300
C	-1.87581900	0.27735700	-0.00000100
C	-3.27192500	-0.24811900	-0.00000100
H	-3.82116400	0.11702800	0.88268400
H	-3.82113100	0.11712500	-0.88267800
H	-3.30024000	-1.34672600	-0.00005600
H	-0.79804900	-1.56144400	-0.00001600
H	-1.74276200	1.36600700	-0.00000800
O	0.78563900	1.35688700	0.00000400
O	1.54602000	-0.75004200	0.00001600
C	2.87251500	-0.25404600	-0.00001600
H	3.52977100	-1.13085200	-0.00013300
H	3.06193900	0.36189400	-0.89140800
H	3.06203200	0.36172000	0.89147800

^{3}i

C	0.46983900	-0.00362300	0.13404700
C	-0.68404400	-0.89905900	0.13090600
C	-2.01351600	-0.40556100	0.46366800
C	-2.82640000	0.36537500	-0.52350700
H	-3.86783200	0.47773700	-0.19043300
H	-2.40216900	1.37961800	-0.65591800
H	-2.82406500	-0.11216300	-1.51692300
H	-0.50660500	-1.94493000	-0.14833500
H	-2.29778000	-0.36931800	1.52306600
O	0.42214300	1.18364400	0.37525600
O	1.61089000	-0.64609000	-0.17337000
C	2.78152800	0.14823800	-0.20296700
H	3.60494400	-0.52487700	-0.46730700
H	2.69462700	0.95144900	-0.94989200
H	2.97017700	0.60982600	0.77777300

^{1}j

C	0.61234000	0.41844300	-0.00042300
C	-0.82528900	0.12617300	-0.00020800
C	-2.01784400	-0.08104100	-0.00008700
C	-3.45744400	-0.30968300	0.00000500
H	-3.93250500	0.22301600	-0.83693700
H	-3.69101200	-1.38013800	-0.09484800
H	-3.90548300	0.05929000	0.93445100
O	1.04952600	1.55025000	0.00012900
N	1.38964900	-0.70142500	-0.00047700
H	0.92460400	-1.59897300	0.00012100
C	2.83045200	-0.64542700	0.00037700
H	3.25185500	-1.12472100	0.89807400
H	3.25274000	-1.13310200	-0.89230500
H	3.12276400	0.41181100	-0.00423200

^{3}j

C	0.61678600	0.60477900	-0.17155600
C	-0.72079300	0.25838700	-0.07416400
C	-1.91155700	-0.03232000	-0.01315900
C	-3.32719600	-0.37149300	0.04307000
H	-3.94277000	0.37078300	-0.49022400
H	-3.50347800	-1.35024700	-0.42878200

H	-3.69131300	-0.43048700	1.08135200
O	1.23305500	1.63892300	0.33795300
N	1.64178000	-0.28279900	-0.57478300
H	2.35255600	0.16152800	-1.15250400
C	2.12487700	-1.31119300	0.32430300
H	2.75794000	-2.01343900	-0.23694300
H	2.71227700	-0.89977700	1.16297400
H	1.26518700	-1.85910900	0.73301700

^{1}k

C	1.51292300	-0.39421900	0.37624600
H	2.21714600	0.13823600	1.02181100
C	1.70486200	-1.62502900	-0.08260000
H	2.61040500	-2.17894900	0.17577000
H	0.96440900	-2.10620500	-0.72638500
S	0.08925700	0.59729100	0.01139400
O	-0.43107300	1.03289200	1.29699700
O	0.44465100	1.55689100	-1.01850900
N	-0.96887600	-0.47379600	-0.69709900
H	-1.28648200	-0.08147100	-1.57974400
C	-1.97758100	-1.11635500	0.13049400
H	-2.70102700	-0.40779200	0.56360900
H	-2.51107700	-1.85357500	-0.48458700
H	-1.48920800	-1.65496600	0.95416100

^{3}k

C	-1.31798500	0.37201700	0.77734000
H	-1.53997400	0.02938600	1.79531100
C	-2.12360400	1.30008900	0.02157400
H	-1.86580100	2.36327700	-0.02750600
H	-2.94596200	0.94156000	-0.60797400
S	-0.03470900	-0.55113200	-0.00590400
O	0.69081200	-1.24182300	1.04752800
O	-0.60689200	-1.26902500	-1.13439800
N	0.91855800	0.63412500	-0.67970600
H	1.07981200	0.41464700	-1.65942700
C	2.05596000	1.13604300	0.07223100
H	2.84432300	0.38231000	0.22775800
H	2.47531100	1.99738100	-0.46502000
H	1.72014400	1.48856300	1.05736600

^{1}l

C	1.47109500	0.00000000	-0.00003300
C	0.38248300	-1.10550400	-0.00029200
C	-0.67546400	0.00000000	0.00005100
C	0.38248200	1.10550400	0.00002000
H	2.11350500	-0.00012200	0.89048400
H	2.11377000	0.00012100	-0.89035600
H	0.34203200	-1.75088300	0.89089800
H	0.34195100	-1.75023600	-0.89195200
H	0.34202300	1.75058100	0.89143000
H	0.34195800	1.75054000	-0.89141900
O	-1.86985200	0.00000000	0.00030500

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C	1.46914900	0.00000300	0.02920000
C	0.38040100	-1.08767200	0.03370300
C	-0.66863600	-0.00000800	-0.35513100
C	0.38039500	1.08767400	0.03370400
H	2.15202700	0.00000400	0.88866300
H	2.06327600	0.00000800	-0.89444100
H	0.16757900	-1.49515900	1.03594700
H	0.46506800	-1.91124600	-0.69058600
H	0.16756800	1.49517300	1.03594100
H	0.46505300	1.91123200	-0.69060300
O	-1.85605400	0.00000000	0.10827800

TS-1-A

C	2.94911600	-1.82465300	0.91525400
C	2.01134100	-1.41063200	1.89194100
C	1.24525400	-0.22044500	1.74534600
C	1.38999700	0.54216900	0.53629100
C	2.21634100	0.01961600	-0.50925500
C	3.08193700	-1.11385500	-0.24322100
H	0.26077400	-0.29804400	3.67228000
H	3.56578600	-2.70567400	1.10255500
H	1.89445900	-1.98710300	2.81220700
H	2.45537300	0.67773600	-1.34423900

C	-0.18011700	2.11726100	1.32716800
C	-0.34579700	1.44487200	2.50687000
H	-0.70071900	3.04257900	1.09029100
H	-1.02458300	1.84555300	3.26036500
C	-1.09506400	-0.46596700	-1.39914200
C	0.05044600	-1.33317600	-1.66015500
C	0.10629400	-2.61509300	-0.93969900
C	-0.68285800	-2.79157800	0.14314600
C	-1.70379800	-1.79873400	0.58943300
C	-1.93530300	-0.66142200	-0.35702500
H	0.36828400	-1.36847500	-2.71211000
H	1.04479100	-0.70408400	-1.21107700
H	-1.23916500	0.38599300	-2.06530000
H	-0.61220500	-3.72365800	0.71240100
H	-2.65560600	-2.31891200	0.80519700
H	-1.40339100	-1.37611100	1.57408800
C	1.05010900	-3.66740200	-1.44223100
H	1.14671300	-4.50110100	-0.73310100
H	0.69254900	-4.07132200	-2.40360000
H	2.05145400	-3.24744000	-1.61987700
C	-3.17201900	0.19964000	-0.18816900
H	-2.92648500	1.19112800	-0.60376500
C	-3.60456700	0.39097700	1.26640800
H	-4.44036700	1.10421200	1.32081400
H	-3.95200700	-0.55265200	1.71635700
H	-2.78391700	0.78248800	1.88179200
C	-4.32374600	-0.38400900	-1.02154200
H	-5.22487700	0.24184600	-0.93063100
H	-4.05281800	-0.44566800	-2.08521500
H	-4.58412300	-1.39883200	-0.67867900
H	3.80637600	-1.40418400	-1.00601400
N	0.67594900	1.67545800	0.35063700
C	0.36619000	0.24975600	2.73389200
B	0.86842000	2.59661900	-0.97654400
F	2.17720200	3.03283200	-0.97456800
F	-0.04593700	3.62402000	-0.87954400
F	0.61289300	1.79386800	-2.09014900

TS-1-B

C	2.95791600	-2.58338300	-1.38801200
C	3.69686600	-1.74454100	-0.52179400
C	3.21537600	-0.48172900	-0.09172700
C	1.93151100	-0.03205800	-0.57252800
C	1.16427300	-0.92357200	-1.38375300
C	1.72739500	-2.18247900	-1.82671900
H	4.91454500	0.02192000	1.15417000
H	3.38119900	-3.53840100	-1.70444100
H	4.67721700	-2.06632900	-0.16292200
H	0.30570900	-0.51791000	-1.91601700
C	2.13995300	1.92926900	0.73867300
C	3.35942400	1.55444300	1.22238500
H	1.64956800	2.85696700	1.02505800
H	3.87593000	2.20272100	1.93070900
C	-1.90001000	-1.72679100	0.02526000
C	-0.58268500	-1.76256000	0.66294300
C	-0.33522900	-0.82202700	1.76518800
C	-1.20787500	0.19073000	1.97213100
C	-2.44121300	0.39233400	1.16715100
C	-2.77541500	-0.71747000	0.22045500
H	-0.16303300	-2.76924300	0.81600900
H	0.21330200	-1.40155100	-0.23446400
H	-2.14256400	-2.52324000	-0.68463500
H	-1.00751900	0.91833200	2.76353900
H	-3.29568800	0.60276800	1.83631000
H	-2.30588800	1.32553300	0.58604000
C	0.88714800	-1.02136500	2.61093000
H	1.02065200	-0.19928600	3.32679800
H	0.81892200	-1.96649700	3.17409300
H	1.79520600	-1.08204300	1.99270200
C	-4.09322400	-0.65763900	-0.51860700
H	-4.08741300	-1.49048800	-1.24156900
C	-4.22850900	0.64864700	-1.31133900
H	-5.11301300	0.60919200	-1.96492100
H	-4.35226500	1.51297400	-0.63998000
H	-3.33844100	0.83180600	-1.92933200
C	-5.28783600	-0.87141500	0.41954900
H	-6.22582600	-0.89891400	-0.15563500
H	-5.19803600	-1.81805900	0.97311300

H	-5.37768000	-0.05431400	1.15284400
H	1.13654600	-2.80439000	-2.50143400
C	3.93394900	0.33916600	0.79539400
N	1.43352100	1.16370700	-0.17016600
B	0.15774800	1.92135100	-0.81594200
F	0.62271100	2.66094000	-1.87778400
F	-0.79920700	0.98986200	-1.22882200
F	-0.37635900	2.71924000	0.19120200

TS-1-C

C	0.84299700	-0.67376100	2.39605700
C	0.54560700	-1.82460600	1.61329100
C	-0.59157700	-1.88608800	0.75574300
C	-1.43523400	-0.72828800	0.66022200
C	-1.05937800	0.45844700	1.37193400
C	0.04833400	0.42921800	2.30949800
H	-0.29892600	-3.91404800	0.06284500
H	1.70110100	-0.69268600	3.07094000
H	1.18822400	-2.70562300	1.67613800
H	-1.79330700	1.26129500	1.43863800
C	-2.80149000	-1.84052300	-0.91270600
C	-2.04809600	-2.98045300	-0.84714700
H	-3.68073600	-1.73916100	-1.54540700
H	-2.33006900	-3.84511800	-1.44831400
C	1.31951200	0.20558200	-1.00633600
C	0.49211100	1.38102600	-0.75650100
C	1.16335900	2.58983400	-0.23568900
C	2.42326300	2.49689500	0.22533100
C	3.21307100	1.22501700	0.21525300
C	2.58398300	0.08936000	-0.53890700
H	-0.30484400	1.56358700	-1.49073900
H	-0.25081200	1.04064300	0.16382700
H	0.86897200	-0.62778000	-1.55406300
H	2.91325400	3.38107700	0.64471000
H	4.23091400	1.41382300	-0.17431100
H	3.38383500	0.89960700	1.26133300
C	0.34739300	3.84761300	-0.19634400
H	0.88054600	4.66827600	0.30275100
H	0.08188000	4.17010900	-1.21545800
H	-0.60559100	3.67008800	0.32759900
C	3.41185600	-1.14842500	-0.80775600
H	2.70557700	-1.94273700	-1.10245000
C	4.17210400	-1.63185000	0.43082400
H	4.66068100	-2.59650900	0.22788800
H	4.96070300	-0.92187500	0.72596300
H	3.49696300	-1.76612900	1.28916600
C	4.36875100	-0.91937000	-1.98686500
H	4.93415200	-1.83720300	-2.20928300
H	3.81833100	-0.62655600	-2.89251200
H	5.09916800	-0.12587600	-1.76206400
H	0.25472000	1.32501000	2.89670800
N	-2.49483500	-0.72332000	-0.17770500
C	-0.91855800	-3.01782000	-0.00510500
B	-3.41052700	0.60656100	-0.37858000
F	-3.90733500	0.96392000	0.86123000
F	-2.56490900	1.59729000	-0.88341000
F	-4.40179000	0.27738800	-1.27402500

TS-1-D

C	3.75605800	1.06643700	-1.00405800
C	3.33340900	-0.09759300	-1.68759700
C	2.33129600	-0.96221400	-1.16753400
C	1.73241200	-0.63042900	0.09719100
C	2.06679100	0.61826200	0.70207100
C	3.16188100	1.41094700	0.17876400
H	2.33970300	-2.39067600	-2.79541400
H	4.55984000	1.67447000	-1.42313000
H	3.79383800	-0.36294800	-2.64202000
H	1.70737100	0.81568900	1.71134400
C	0.34289600	-2.54028200	-0.05508400
C	0.87280100	-2.90278000	-1.26159600
H	-0.43113500	-3.11268300	0.45123300
H	0.50721800	-3.80181700	-1.75844800
C	-0.61387800	2.88935000	0.01062900
C	0.04122600	1.85767500	-0.80809900
C	-0.76237900	0.72303400	-1.24674300
C	-1.98733500	0.45721100	-0.73435900
C	-2.58765900	1.37703800	0.28062400

C	-1.83969400	2.64461700	0.51557000
H	0.75691900	2.23611400	-1.55619000
H	0.89250800	1.35243200	-0.04953800
H	-3.64369900	1.59038400	0.03214500
H	-2.62701800	0.82719600	1.24186700
H	3.47114200	2.30046300	0.73004700
C	0.16648100	4.13628400	0.30314400
H	0.43115100	4.66723000	-0.62530200
H	-0.39270600	4.82529700	0.95042400
H	1.11352100	3.88433100	0.80961800
C	-2.77678400	-0.75540000	-1.17159900
H	-2.06834000	-1.41743000	-1.69723600
C	-3.87843600	-0.36678600	-2.16757900
H	-3.46070000	0.14422800	-3.04761300
H	-4.41562900	-1.26314700	-2.51326500
H	-4.61955700	0.30403800	-1.70426500
C	-3.34799100	-1.53151700	0.01981300
H	-2.57583000	-1.74628100	0.77225100
H	-4.15568300	-0.96916800	0.51488600
H	-3.77749300	-2.48554000	-0.32147300
H	-2.31608300	3.39066200	1.15879200
H	-0.32223100	0.03414400	-1.97417100
N	0.76536900	-1.41985500	0.62252500
C	1.89241100	-2.11691000	-1.83818800
B	0.10381200	-1.08807700	2.05582000
F	1.11329000	-1.08110300	2.99463800
F	-0.84645600	-2.06613400	2.30190000
F	-0.49625500	0.17176200	1.95973600

TS-1-E

C	0.80657600	1.50553100	-1.82351300
C	-0.06392500	2.33638600	-1.06587200
C	-1.30789300	1.86074900	-0.55138000
C	-1.63614900	0.47521900	-0.73434300
C	-0.67674500	-0.38261000	-1.36992200
C	0.49747900	0.19253200	-2.00837000
H	-1.99443800	3.74282900	0.26036800
H	1.71232800	1.93213600	-2.25895100
H	0.19182500	3.38528500	-0.90126300
H	-1.01733300	-1.37020400	-1.68109700
C	-3.67731400	0.80121400	0.40986000
C	-3.42466800	2.13170800	0.60092000
H	-4.57942400	0.30803600	0.76498700
H	-4.15724100	2.74728200	1.12333200
C	0.67377700	0.11024000	1.68340000
C	0.81115700	-1.11827300	0.88653500
C	2.14394000	-1.41974800	0.34514300
C	3.14444000	-0.51967600	0.31556400
C	2.94230200	0.85102000	0.89947500
C	1.65211100	1.04138100	1.63075900
H	0.24105600	-1.97938300	1.26173000
H	0.08689400	-0.88205200	-0.08936100
H	3.77976200	1.09643900	1.57870500
H	3.02049500	1.60587900	0.09386100
H	1.15096100	-0.46800200	-2.57966700
C	-0.57502200	0.27800000	2.49928100
H	-0.48028700	-0.28005500	3.44523700
H	-0.77180000	1.33202100	2.73882800
H	-1.44470100	-0.14371500	1.97833000
C	4.48353800	-0.84287600	-0.31335000
H	4.41011300	-1.87578700	-0.69224500
C	5.63065700	-0.80736100	0.70339900
H	5.41738700	-1.45599100	1.56590900
H	6.56659500	-1.15350600	0.23924000
H	5.81085500	0.21239800	1.07918700
C	4.77645500	0.06770800	-1.51275600
H	3.95096800	0.04527000	-2.24034100
H	4.92757900	1.11331900	-1.19995000
H	5.69343300	-0.25492400	-2.02864700
H	1.53036200	1.97673800	2.18638200
H	2.29632000	-2.41135500	-0.09183800
C	-2.22100100	2.68431800	0.11967700
N	-2.79212700	-0.02089100	-0.23883600
B	-3.09617900	-1.61741400	-0.23585300
F	-4.33914500	-1.79166500	0.32800000
F	-3.03911100	-2.07425800	-1.53996300
F	-2.08776600	-2.18542200	0.54655700

TS-1-F

C	-0.78227100	-2.22285700	-2.01752600
C	-0.92301700	-2.36553400	-0.61373800
C	-0.02501200	-1.74733200	0.30266400
C	1.05927400	-0.96802300	-0.22678700
C	1.07574000	-0.68503400	-1.63291500
C	0.20300600	-1.42686500	-2.52494100
H	-0.93875200	-2.48249200	2.12312900
H	-1.46016600	-2.76302500	-2.68111200
H	-1.71364300	-3.00247300	-0.21159100
H	1.96401400	-0.20514800	-2.04271600
C	1.84180700	-0.54489600	1.95693400
C	0.80528200	-1.23585600	2.52460700
H	2.62668000	-0.06501600	2.53764200
H	0.73542000	-1.30081000	3.61070200
C	-0.13754300	2.25132400	-0.15214000
C	-0.60048400	1.53749200	-1.35530500
C	-1.89075300	0.85999900	-1.27770300
C	-2.51260300	0.60807600	-0.10104000
C	-1.89684100	1.06725800	1.18273900
C	-0.73564700	1.99027000	1.03007800
H	-0.39979200	2.05078700	-2.30665400
H	0.23131200	0.58006000	-1.49997000
H	-2.66435000	1.53016300	1.83050800
H	-1.57241700	0.17018100	1.75571800
H	0.32971400	-1.29913300	-3.60116600
C	0.98893900	3.22884500	-0.29961400
H	0.70048700	4.04375200	-0.98320200
H	1.26421200	3.67047600	0.66767600
H	1.87736000	2.73311300	-0.71399700
C	-3.86621500	-0.06880400	-0.05283100
H	-3.97817800	-0.62906200	-0.99627100
C	-4.98620700	0.98110700	-0.00065200
H	-4.93650800	1.65755000	-0.86601300
H	-5.97376600	0.49475400	0.00099900
H	-4.91482600	1.59387100	0.91220200
C	-3.99808000	-1.06330300	1.10361900
H	-3.17985600	-1.79735000	1.09985500
H	-3.99014300	-0.55393700	2.07988000
H	-4.94822200	-1.61269800	1.02891300
H	-0.37631600	2.49072900	1.93389100
H	-2.34450500	0.51260400	-2.21008100
N	1.98844800	-0.43681600	0.59859400
C	-0.13550600	-1.87868700	1.69598700
B	3.41795000	0.11270900	0.03408800
F	4.10490100	0.60947300	1.11939400
F	4.03216300	-0.97074400	-0.55250500
F	3.16850700	1.11395900	-0.90884000

TS-1-G

C	-1.21696700	-0.09196900	2.67144800
C	-0.35625000	1.03170900	2.53606400
C	0.86634900	0.96685900	1.80450900
C	1.18054400	-0.24894200	1.10764000
C	0.24151200	-1.33151300	1.15500400
C	-0.91280700	-1.25730600	2.03621800
H	1.55571900	2.96350700	2.26595300
H	-2.10795000	-0.01250600	3.29710600
H	-0.60576800	1.97037700	3.03546700
H	0.58348600	-2.30638300	0.80698900
C	3.17569100	0.72543100	0.29766400
C	2.94130500	1.89758400	0.96043700
H	4.05150200	0.55552600	-0.32460500
H	3.66246500	2.71137800	0.88257300
C	-1.35168000	0.77643700	-1.00685700
C	-1.33651200	-0.69704100	-1.07328500
C	-2.60419200	-1.39849500	-0.82299100
C	-3.67447100	-0.79268200	-0.27761800
C	-3.62193300	0.66940100	0.06035000
C	-2.40710700	1.39150900	-0.42940900
H	-0.72102800	-1.12031700	-1.87775200
H	-0.58489200	-1.00842000	-0.15620800
H	-4.52787300	1.17072900	-0.33017200
H	-3.70507500	0.78581900	1.15956600
H	-1.55702300	-2.13337200	2.11942300
C	-0.15273500	1.50736100	-1.57965700
H	0.74060500	0.98364400	-1.20467900
C	-4.95426000	-1.51121200	0.02622300

H	-4.89660900	-2.57678500	-0.23462700
H	-2.41994400	2.47993100	-0.33528100
H	-2.64470500	-2.46612600	-1.05832700
C	-0.12262900	1.37441400	-3.10937900
H	-1.01012600	1.84697200	-3.55972300
H	0.77296200	1.86726800	-3.51583000
H	-0.08911600	0.32342000	-3.42822200
C	-0.05893000	2.97171500	-1.16310100
H	0.89260200	3.40077400	-1.50964400
H	-0.87165700	3.57049200	-1.60572300
H	-0.09965600	3.08668200	-0.07005500
H	-5.20090800	-1.43126100	1.09840600
H	-5.79775000	-1.06492400	-0.52598600
N	2.30506400	-0.33433400	0.36065700
C	1.76915500	2.03580900	1.73191800
B	2.58113600	-1.59453300	-0.62583600
F	1.54352500	-1.57292600	-1.56180700
F	3.80478300	-1.38333400	-1.21868000
F	2.55337400	-2.75461100	0.12769400

TS-1-H

C	-2.65667900	-1.42347900	-1.88564000
C	-2.72765100	-1.62304800	-0.48458700
C	-1.56525600	-1.63794000	0.33550900
C	-0.28568600	-1.43492400	-0.28720500
C	-0.24785700	-1.07468300	-1.67352800
C	-1.45031500	-1.18250200	-2.47758900
H	-2.56855100	-2.03335300	2.21322800
H	-3.56986600	-1.47478300	-2.48158900
H	-3.69488100	-1.80186200	-0.00965500
H	0.72008600	-1.07797500	-2.17331200
C	0.78161200	-1.66988800	1.80596600
C	-0.40757300	-1.84659200	2.45888500
H	1.74537700	-1.68393600	2.31018400
H	-0.40869800	-1.99454700	3.53910300
C	0.44049200	1.93413900	-0.00727700
C	-0.47691200	1.66378700	-1.12612200
C	-1.91094000	1.68786400	-0.85246200
C	-2.40193900	1.61310300	0.40612000
C	-1.47025700	1.59322400	1.57602500
C	-0.03748900	1.85185900	1.25446700
H	-0.17533800	2.09129800	-2.09271700
H	-0.27495100	0.43447400	-1.40350500
H	-1.81852000	2.31173600	2.34220200
H	-1.56711300	0.60645600	2.08076800
H	-1.37020900	-1.02624500	-3.55458300
C	1.86177500	2.33374300	-0.34751400
H	2.15766300	1.72504000	-1.21434000
C	-3.86690200	1.53996200	0.70494800
H	-4.08815700	0.63849300	1.30108000
H	0.63356900	2.01094300	2.10143600
H	-2.59809600	1.69224300	-1.70237700
C	1.89197500	3.81190900	-0.76389500
H	1.62128100	4.46052900	0.08462900
H	2.89953400	4.09626800	-1.10333200
H	1.18996900	4.02525900	-1.58486200
C	2.87079900	2.05329200	0.76200900
H	3.88702900	2.27901000	0.40724600
H	2.68921100	2.68190300	1.64918400
H	2.85545900	0.99662300	1.06058000
H	-4.19128000	2.40474100	1.30688300
H	-4.47196600	1.50547100	-0.21123800
C	-1.60981400	-1.85410300	1.72248200
N	0.84897700	-1.49178500	0.44719600
B	2.31787300	-1.56627500	-0.24862900
F	2.36080000	-2.75813100	-0.93538900
F	3.24131100	-1.49438800	0.77674100
F	2.45099500	-0.48173200	-1.11643800

TS-1-I

C	-1.39919300	-2.33658200	1.42444100
C	-0.77270700	-1.38645500	2.26787000
C	0.41729400	-0.70748600	1.88572500
C	0.96932100	-0.97395900	0.58613600
C	0.22749400	-1.79989000	-0.31667600
C	-0.90515900	-2.56314100	0.17185400
H	0.69126600	0.40832800	3.72154500
H	-2.26825000	-2.88782400	1.78831000

H	-1.18214500	-1.18774100	3.26079500
H	0.72158400	-2.12546800	-1.23161200
C	2.73233600	0.53735800	1.01131800
C	2.25263400	0.83717400	2.25653100
H	3.63710500	0.97876400	0.59926700
H	2.79060500	1.55262300	2.87933600
C	-0.09163700	1.49100300	-1.27773000
C	-1.09656900	0.43603700	-1.36547400
C	-2.26264100	0.52090700	-0.47027000
C	-2.20624200	1.35382900	0.59296100
C	-1.06177600	2.27386700	0.85621900
C	-0.04166100	2.35245200	-0.23626300
H	-1.30213300	0.08201800	-2.38531700
H	-0.49831800	-0.59758600	-0.95676700
H	-1.44019700	3.28611600	1.09371800
H	-0.54051600	1.96103500	1.78859200
H	-1.36513900	-3.29510500	-0.49401200
C	1.00588500	3.41591600	-0.11837300
H	0.55662900	4.41937600	-0.20981900
H	1.49233400	3.36982900	0.86928600
H	1.78065300	3.30758400	-0.88928900
C	-3.45742200	-0.34969200	-0.80432900
H	-3.04826300	-1.33304100	-1.09804400
C	-4.41385700	-0.57631000	0.36266900
H	-3.88657000	-0.96365600	1.24639200
H	-4.92672900	0.35527100	0.65039600
H	-5.19209900	-1.30137600	0.08202000
C	-4.20802400	0.21989000	-2.01765300
H	-5.02597300	-0.45204200	-2.31863300
H	-4.64383200	1.20138900	-1.77350500
H	-3.54776600	0.35361600	-2.88705300
H	-3.04102800	1.39955300	1.29638400
H	0.67362800	1.52129400	-2.05401600
N	2.10607100	-0.36109800	0.18474600
C	1.07942300	0.20710000	2.72117700
B	2.80612700	-0.71588300	-1.24043500
F	3.90995600	0.10227000	-1.35313800
F	3.12571600	-2.05717300	-1.20561700
F	1.87399800	-0.45153800	-2.24678100

TS-1-J

C	-0.23710700	2.09955000	2.01684400
C	0.74879200	2.66572200	1.15935400
C	1.70519500	1.86583600	0.46958900
C	1.62944600	0.43875900	0.61413900
C	0.56327700	-0.11620700	1.39416300
C	-0.31087100	0.74757700	2.16382700
H	2.79145700	3.48552200	-0.46745700
H	-0.91691600	2.75954600	2.55914200
H	0.79722900	3.74926000	1.03063800
H	0.60781200	-1.17792100	1.63453300
C	3.44806100	0.18053400	-0.87074300
C	3.58793800	1.53208400	-1.02530800
H	4.08623400	-0.54772100	-1.36656200
H	4.37808500	1.91905000	-1.66912300
C	-1.11278700	1.19964000	-1.25006700
C	-1.14943000	-0.19211800	-0.81379400
C	-2.41255000	-0.70817000	-0.24277200
C	-3.38189500	0.16226000	0.09106300
C	-3.27421300	1.64002200	-0.12958200
C	-2.07463400	2.08857500	-0.91141900
H	-0.59185800	-0.89749800	-1.44475100
H	-0.38469500	-0.23524000	0.14132900
H	-4.19120700	2.01742900	-0.62091400
H	-3.26548500	2.15887600	0.85110700
H	-1.05768100	0.28580300	2.81100400
C	-2.01024100	3.53497000	-1.29273200
H	-1.07812300	3.77582500	-1.82175900
H	-2.85990900	3.81019900	-1.93922300
H	-2.07543200	4.17359000	-0.39605200
C	-2.47008800	-2.20590100	-0.01722000
H	-1.47751300	-2.48958300	0.37632000
C	-3.52659000	-2.64206700	0.99382000
H	-3.41295400	-2.11526900	1.95345000
H	-4.54641300	-2.45549200	0.62026300
H	-3.44335000	-3.72142800	1.18813100
C	-2.64468100	-2.94720100	-1.35010400
H	-2.60713800	-4.03540700	-1.19298400

H	-3.61511300	-2.69775600	-1.80805300
H	-1.85060300	-2.69209100	-2.06637100
H	-4.30541800	-0.19269400	0.55514900
H	-0.24319200	1.53398200	-1.82309600
C	2.70545200	2.40317500	-0.35441300
N	2.47321100	-0.36367600	-0.07133800
B	2.33351600	-1.98287700	-0.02064800
F	3.33845600	-2.49677700	-0.80675700
F	2.43547100	-2.37431500	1.30130300
F	1.06870400	-2.28814200	-0.53565500

TS-1-K

C	2.06019900	-2.85524200	-1.60337000
C	2.93121600	-2.12682200	-0.75801500
C	2.69068400	-0.77531400	-0.39731700
C	1.50547500	-0.12605700	-0.90423800
C	0.61050500	-0.89333500	-1.70713100
C	0.93492600	-2.25240400	-2.08827600
H	4.46449700	-0.52509700	0.81889000
H	2.30194900	-3.88644700	-1.86677000
H	3.83024100	-2.60713200	-0.36508700
H	-0.18146000	-0.36964600	-2.23812200
C	2.10200600	1.84460700	0.26467700
C	3.24330000	1.28687200	0.75845900
H	1.80354500	2.86745900	0.48495400
H	3.89720100	1.88189800	1.39627700
C	-2.51379200	-1.62171700	-0.37804100
C	-1.23925800	-1.52115400	0.34625300
C	-1.11271900	-0.46081500	1.36311600
C	-2.03864900	0.52338100	1.39236200
C	-3.20361400	0.58831100	0.46942900
C	-3.43097000	-0.63472000	-0.36289300
H	-0.80412800	-2.49030500	0.63649300
H	-0.42680800	-1.22622600	-0.51220400
H	-4.12165100	0.84141000	1.03159200
H	-3.03908700	1.44806600	-0.21022800
H	0.24599700	-2.78225400	-2.74821500
C	-4.69233400	-0.68435300	-1.16849100
H	-4.77185200	-1.61271900	-1.75045800
H	-5.57924000	-0.60175000	-0.51924800
H	-4.72863800	0.16687600	-1.86808800
C	0.07434600	-0.52035300	2.30493300
H	0.96096400	-0.72453600	1.67920100
C	0.33047000	0.78776500	3.04942500
H	0.36338400	1.64013200	2.35690900
H	-0.45377000	0.98159300	3.79918100
H	1.29151500	0.73875600	3.58223100
C	-0.06208600	-1.68893100	3.29148800
H	0.83332100	-1.76330500	3.92699900
H	-0.93442800	-1.53958800	3.94720100
H	-0.18705900	-2.65520200	2.78037600
H	-1.93933900	1.34646900	2.10155300
H	-2.67648600	-2.50749300	-0.99930200
N	1.22269000	1.15121700	-0.54593300
C	3.55811900	-0.05192500	0.43756100
B	-0.01321800	2.05837500	-1.07034000
F	0.45558400	2.81507900	-2.11930100
F	-1.07558100	1.24408800	-1.46596500
F	-0.39426400	2.84326600	0.01298800

TS-1-L

C	-0.39480500	-0.36778400	2.24043600
C	0.74516300	0.03709200	1.47826300
C	1.37789300	-0.85313500	0.56950900
C	0.82108900	-2.15774500	0.37226700
C	-0.46609200	-2.44020600	0.97891700
C	-0.97244300	-1.58170000	2.03156900
H	-0.78906700	0.31710900	2.99339200
H	1.18714600	1.01805200	1.63730700
C	1.47039000	-3.04508100	-0.48181800
H	-0.82991100	-3.47011300	0.92097600
C	2.64768000	-2.63796900	-1.13765100
C	3.11868500	-1.36416400	-0.94056800
H	1.06394900	-4.04688600	-0.63561500
H	3.18303100	-3.31181600	-1.80670200
H	4.00704600	-0.97672600	-1.43554800
N	2.49725900	-0.48487500	-0.11344000
C	-1.23472300	0.19532800	-1.00941000

C	-1.87985600	-1.10915400	-1.02529600
C	-3.29409000	-1.17759900	-0.59598900
C	-3.84098000	-0.13045800	0.04456500
C	-3.09944200	1.13910900	0.32048800
C	-1.77671500	1.26939500	-0.37328400
H	-1.62034700	-1.73916400	-1.88956700
H	-1.27612000	-1.77893000	-0.13296400
H	-0.26630100	0.31059200	-1.50463100
H	-4.87451700	-0.19153000	0.39910800
H	-3.73351200	2.01305700	0.08374600
H	-2.92339700	1.22612900	1.41255700
C	-4.02196000	-2.46636300	-0.84369700
H	-5.04697100	-2.43929400	-0.44940700
H	-4.07131200	-2.69069600	-1.92133400
H	-3.49228500	-3.30811400	-0.36632500
C	-1.09605700	2.61766700	-0.38750100
H	-0.04683800	2.44378700	-0.66357000
C	-1.10329900	3.29812500	0.98430100
H	-0.49322600	4.21240500	0.95200500
H	-2.11882500	3.58773900	1.29944500
H	-0.67621300	2.64360700	1.75857900
C	-1.72388800	3.52424300	-1.45684600
H	-1.18970100	4.48529400	-1.49917800
H	-1.66835100	3.06061300	-2.45250400
H	-2.78268400	3.74002400	-1.23874700
H	-1.85464100	-1.89235500	2.59404100
B	3.05867900	1.04277800	-0.06151300
F	3.33098400	1.35466900	1.25608300
F	4.18044300	1.08467500	-0.85742400
F	2.03074500	1.83508400	-0.57231800

TS-1-M

C	1.77755200	-2.60789500	-0.52019700
C	0.44881400	-2.10945400	-0.62737500
C	-0.17864100	-1.44429300	0.46043600
C	0.57776700	-1.19211700	1.65129700
C	1.99191900	-1.48547000	1.62474500
C	2.52704700	-2.34479300	0.58715400
H	2.18088300	-3.20309300	-1.34091700
H	-0.12531000	-2.28803300	-1.53340200
C	-0.04379500	-0.56117900	2.72732800
H	2.53341400	-1.41242000	2.57260200
C	-1.39280600	-0.17463000	2.61104600
C	-2.07047400	-0.43630300	1.44866100
H	0.51775800	-0.36661800	3.64309900
H	-1.91052400	0.32187800	3.43213100
H	-3.11590000	-0.17306100	1.30245900
N	-1.48325600	-1.05984500	0.39022700
C	1.33041800	1.78491200	0.81101300
C	2.51802100	1.00992400	0.44775900
C	2.68336900	0.65543800	-0.96777900
C	1.64760700	0.83557900	-1.82151100
C	0.36436800	1.48744900	-1.44276800
C	0.30829800	2.01569300	-0.04535700
H	3.44417800	1.30868200	0.96204800
H	2.37359800	-0.12878900	1.00841500
H	1.27310000	2.17908000	1.83028100
H	1.75422000	0.52505000	-2.86530700
H	0.14027800	2.30011200	-2.16096500
H	-0.46822000	0.77332600	-1.60179200
C	3.99986400	0.08007300	-1.39733700
H	4.28775600	-0.76548600	-0.75285600
H	3.96925800	-0.27569900	-2.43619200
H	4.79722600	0.83663100	-1.31393500
C	-0.86932400	2.88672000	0.35202900
H	-1.04995100	2.70590100	1.42531700
C	-2.16011700	2.56972000	-0.40727700
H	-2.99914100	3.13314200	0.02713400
H	-2.08646400	2.86248000	-1.46609100
H	-2.42124900	1.50445200	-0.38275400
C	-0.49837300	4.36859700	0.18343800
H	-1.33821100	5.01503300	0.48149800
H	0.37690700	4.63562400	0.79339700
H	-0.25895500	4.59481700	-0.86822100
H	3.54614000	-2.72496900	0.68269000
B	-2.40118400	-1.38025200	-0.91368000
F	-2.47462300	-2.74871400	-1.03596700
F	-3.62735500	-0.78756800	-0.68595600

F	-1.76481800	-0.80434900	-2.01737300

TS-1-N

C	0.50795200	0.16382500	2.03023800
C	-0.66227100	-0.39533800	1.43176300
C	-1.59458700	0.42485000	0.73984900
C	-1.31217900	1.82086500	0.58389600
C	0.01489100	2.28227800	0.94587600
C	0.83456700	1.46858900	1.82529200
H	1.13707000	-0.47728900	2.65022500
H	-0.90112000	-1.44632500	1.57680700
C	-2.27689800	2.64099700	0.00453300
H	0.18991600	3.36189900	0.92154900
C	-3.47880300	2.07334200	-0.45877600
C	-3.66592800	0.71808500	-0.34918400
H	-2.08904600	3.71177500	-0.09823600
H	-4.25250200	2.68735800	-0.91985300
H	-4.55347800	0.21005600	-0.72141600
N	-2.74644500	-0.09387300	0.23417200
C	0.57419300	0.13470200	-1.61340800
C	1.35174100	1.34465100	-1.34588000
C	2.73679700	1.16432500	-0.88015000
C	3.21263000	-0.01387700	-0.43751500
C	2.33479900	-1.23383600	-0.45511900
C	1.01232900	-1.05541200	-1.12300900
H	1.20217700	2.15951900	-2.06956700
H	0.74014800	1.85737200	-0.34920700
H	2.86453400	-2.07433200	-0.94121600
H	2.17257500	-1.58896300	0.58038900
H	1.74209000	1.89651600	2.25476900
C	-0.69848100	0.24105800	-2.40170900
H	-0.46676000	0.29189100	-3.47858800
H	-1.34633200	-0.62669600	-2.22242800
H	-1.25409300	1.15606700	-2.14949300
C	4.61953700	-0.14782900	0.10662600
H	5.08221000	0.85040100	0.02979500
C	5.47595600	-1.11624000	-0.71752100
H	5.47439700	-0.84104900	-1.78269500
H	6.51797100	-1.10507500	-0.36349700
H	5.11404500	-2.15312500	-0.63240500
C	4.61195800	-0.53913200	1.59010500
H	3.99581800	0.15500900	2.18146600
H	4.21583900	-1.55643200	1.73813600
H	5.63312200	-0.52296300	2.00018700
H	0.38328400	-1.94088600	-1.24740300
H	3.37976500	2.04969100	-0.85271300
B	-3.00086400	-1.70359600	0.18856700
F	-2.97401100	-2.17710800	1.48525700
F	-4.22033200	-1.89609800	-0.42035400
F	-1.95470300	-2.23065500	-0.56957900

TS-1-O

C	0.16683700	0.11573600	2.79218400
C	-0.48874100	-0.56504000	1.72430100
C	-1.27949500	0.13805500	0.77625700
C	-1.35169100	1.56666700	0.85565300
C	-0.49215600	2.23596700	1.80811000
C	0.13912500	1.47523400	2.86682100
H	0.68541000	-0.47646100	3.54781200
H	-0.45188600	-1.65060000	1.67066800
C	-2.16136300	2.25197400	-0.04802200
H	-0.65550800	3.30721700	1.95888700
C	-2.82719500	1.53342500	-1.05799000
C	-2.71058600	0.16707700	-1.10033500
H	-2.25435900	3.33757900	0.01886500
H	-3.44465400	2.04203300	-1.79874900
H	-3.21627200	-0.44794400	-1.84194700
N	-1.97599200	-0.52466700	-0.18892100
C	1.02126100	2.14351300	-1.25330200
C	1.69611200	2.14863100	0.05862100
C	2.38872700	0.93105800	0.45427800
C	2.26257200	-0.24457600	-0.21402400
C	1.38964500	-0.33017300	-1.42660300
C	0.85592600	0.97777300	-1.90985700
H	2.22536900	3.08134000	0.30676200
H	0.73857300	2.27012600	0.89139700
H	1.93334700	-0.83718300	-2.24621200
H	0.55088900	-1.02351300	-1.21200400

H	0.64471800	2.00616700	3.67568800
C	0.51824000	3.45830300	-1.77364600
H	1.35942400	4.12060300	-2.03649700
H	-0.11133500	3.32908800	-2.66456800
H	-0.07524700	3.98246700	-1.00747500
C	3.08631800	-1.44997400	0.18626200
H	3.39215100	-1.29100600	1.23439000
C	4.36789500	-1.50884300	-0.66064400
H	4.95732100	-0.58536300	-0.56221000
H	4.99695700	-2.35527500	-0.34553800
H	4.13255400	-1.65031200	-1.72753600
C	2.32103500	-2.77155700	0.11138700
H	1.38576000	-2.73882500	0.68348600
H	2.04936500	-3.02737000	-0.92378100
H	2.94424300	-3.58914900	0.50343700
H	0.31294600	0.96923900	-2.85985800
H	3.03059100	0.97364900	1.33919200
B	-2.02530500	-2.15049700	-0.24853000
F	-2.49393400	-2.58729900	0.97208400
F	-0.71758500	-2.58700000	-0.47402600
F	-2.85366600	-2.48801900	-1.29537000

TS-1-P

C	0.98361200	2.01633900	2.13829900
C	1.59583800	1.12531700	1.21052200
C	1.09329300	-0.18665200	1.00982500
C	-0.09965900	-0.58821500	1.69599200
C	-0.82261500	0.42075800	2.43723100
C	-0.17309400	1.67035700	2.77057400
H	1.46048900	2.97867900	2.33100700
H	2.50156900	1.42413500	0.68809900
C	-0.56488200	-1.89208800	1.53516900
H	-1.65316700	0.07934100	3.06230300
C	0.11673400	-2.76300400	0.66376700
C	1.23865200	-2.32134500	0.01015300
H	-1.46090600	-2.21974800	2.06597500
H	-0.22870100	-3.78474300	0.50343300
H	1.81327500	-2.94664700	-0.67029400
N	1.73235100	-1.06589800	0.18713600
C	-2.31262000	0.11275100	-0.62642000
C	-2.08920500	1.36377700	0.12480000
C	-1.09870700	2.29642700	-0.38797300
C	-0.22199700	1.96603300	-1.37258700
C	-0.30300600	0.62627000	-2.03070600
C	-1.45213000	-0.22591100	-1.60800400
H	-2.99000800	1.83290100	0.54588000
H	-1.58619700	0.95716900	1.23013600
H	-0.31026800	0.75617500	-3.12998600
H	0.65664500	0.10302900	-1.84691400
H	-0.65626900	2.35085700	3.47437700
C	-3.49041300	-0.74041000	-0.19412000
H	-3.44191500	-0.78855500	0.91089300
C	0.84261000	2.89783500	-1.85611600
H	0.85242600	3.83887800	-1.28930300
H	-1.57666600	-1.16948500	-2.14387600
H	-1.03279000	3.28305100	0.07818700
C	-4.82108700	-0.07073200	-0.56777100
H	-4.91853900	-0.00087300	-1.66243600
H	-5.67172500	-0.65556200	-0.18624400
H	-4.90731300	0.94667700	-0.15894900
C	-3.45069600	-2.17249400	-0.72075200
H	-4.27103300	-2.76193300	-0.28502800
H	-3.57469100	-2.19919600	-1.81496400
H	-2.50141800	-2.66887600	-0.47411200
H	1.82451600	2.40808100	-1.76644600
H	0.69800500	3.13250000	-2.92362100
B	3.12364800	-0.67578800	-0.56077600
F	4.03344400	-0.33395300	0.41532000
F	3.50638800	-1.77626600	-1.29411000
F	2.83863800	0.41403100	-1.39182000

TS-1-Q

C	0.84270900	-2.22783500	1.11337900
C	-0.32414300	-1.79220400	0.41822400
C	-1.07344900	-0.66788900	0.86966100
C	-0.58996700	0.08888300	1.98479700
C	0.73490800	-0.22116200	2.48549100
C	1.34765100	-1.49588500	2.14234200

H	1.32265900	-3.15692500	0.80126400
H	-0.70107900	-2.36396500	-0.42620500
C	-1.37140300	1.13163900	2.47666400
H	1.04433400	0.27194000	3.41165400
C	-2.58912600	1.44286800	1.84020500
C	-2.98119900	0.71272200	0.74764200
H	-1.02986600	1.70684100	3.33965500
H	-3.21834400	2.25899600	2.19549400
H	-3.89799600	0.91175700	0.19588500
N	-2.24385300	-0.32652100	0.27248200
C	1.32656300	1.18770000	-0.58595200
C	2.26652800	1.11841100	0.54382200
C	3.44983100	0.25771600	0.38421700
C	3.55480500	-0.65835500	-0.59536100
C	2.45943000	-0.80625000	-1.61047700
C	1.38427800	0.22941400	-1.54258500
H	2.47030400	2.07878000	1.03795800
H	1.58214800	0.58410200	1.46494600
H	2.89633300	-0.80044000	-2.62757300
H	2.01139900	-1.81507000	-1.52374000
H	2.25371300	-1.80783200	2.66448400
C	0.32584400	2.32996600	-0.60375900
H	-0.15952300	2.33867200	0.38739300
C	4.73026100	-1.57798200	-0.73024100
H	5.48140700	-1.40121900	0.05187900
H	0.64053000	0.20894300	-2.34138300
H	4.24792500	0.34955800	1.12733200
C	1.05002400	3.67509200	-0.77244500
H	1.57351800	3.71087700	-1.74091400
H	0.32517100	4.50258500	-0.74889100
H	1.79146600	3.86286600	0.01805400
C	-0.76554300	2.18783900	-1.66114400
H	-1.52697500	2.96942300	-1.52308300
H	-0.35157500	2.30735200	-2.67549500
H	-1.26387700	1.21212900	-1.61890100
H	4.40693700	-2.63079100	-0.66638600
H	5.21678600	-1.45665900	-1.71199000
B	-2.77896800	-1.12218400	-1.04871400
F	-3.93327800	-0.48875700	-1.44968800
F	-2.98582200	-2.43536000	-0.68017600
F	-1.76774500	-1.01293700	-2.00148400

TS-1-R

C	0.82996400	-2.03432200	1.74236900
C	-0.29127200	-1.77394300	0.90942500
C	-0.99993500	-0.54510800	0.99378700
C	-0.53969700	0.46548600	1.90158100
C	0.74200500	0.26556400	2.53359700
C	1.33087000	-1.06046700	2.55509300
H	1.28679800	-3.02478200	1.71317800
H	-0.66223100	-2.54539500	0.23881600
C	-1.28553600	1.63498600	2.04331700
H	1.02771300	0.97427400	3.31679400
C	-2.44866600	1.80855800	1.26712000
C	-2.81953200	0.83112500	0.38127700
H	-0.95821300	2.40789900	2.74111900
H	-3.05379000	2.71135700	1.35374900
H	-3.69468000	0.91021500	-0.26086300
N	-2.10999300	-0.32444700	0.23914900
C	1.25963600	2.45708000	-0.03681500
C	2.12282000	1.33444400	0.33638500
C	2.17342900	0.18168900	-0.57233000
C	1.22087300	0.06164200	-1.52948500
C	0.19015400	1.10103300	-1.79964100
C	0.33404700	2.36735900	-1.01661900
H	3.08346200	1.61784200	0.79013000
H	1.56600400	0.84727000	1.38162900
H	0.17096400	1.32644900	-2.88320300
H	-0.80831400	0.65374700	-1.62570700
H	2.20081700	-1.24658000	3.18810700
C	-0.57777300	3.49868600	-1.38088000
H	-0.44612800	4.36251800	-0.71477000
H	-0.39621700	3.82790900	-2.41746500
H	-1.62956900	3.17541400	-1.32837800
C	3.30187900	-0.81243600	-0.38053300
H	3.39727900	-0.96847200	0.70902000
C	3.05242000	-2.17264700	-1.02599200
H	2.09018300	-2.60132300	-0.71227600

H	3.04770800	-2.10124200	-2.12497700
H	3.85073300	-2.87710700	-0.74909500
C	4.62637800	-0.21395500	-0.87923600
H	5.46298400	-0.89882400	-0.67344200
H	4.58522600	-0.04241900	-1.96625900
H	4.85494800	0.74806100	-0.39693000
H	1.18847400	-0.82032700	-2.17131100
H	1.34931200	3.38315600	0.53871100
B	-2.60024000	-1.40351100	-0.88213700
F	-3.69236000	-0.84692800	-1.51191800
F	-2.89979000	-2.57926200	-0.22705300
F	-1.52726000	-1.56265400	-1.75707900

TS-1-S

C	0.13570200	0.60857500	2.28214600
C	1.28758100	0.53777000	1.43716800
C	1.59031200	-0.63877400	0.70204900
C	0.69337900	-1.75312700	0.77266200
C	-0.58471900	-1.54359200	1.42602000
C	-0.76619100	-0.40981600	2.30943700
H	-0.00366400	1.49749100	2.89990700
H	1.98730600	1.36954400	1.39854800
C	1.02660900	-2.93015800	0.10811700
H	-1.23121200	-2.41678200	1.55230900
C	2.22404400	-2.99224800	-0.62977000
C	3.02082800	-1.87765400	-0.70952400
H	0.35904700	-3.79259500	0.16262300
H	2.51817600	-3.90213500	-1.15309500
H	3.93789600	-1.84391200	-1.29462700
N	2.70935000	-0.72026700	-0.07183700
C	-0.68895900	0.86999800	-0.95670400
C	-1.65192000	-0.20551900	-0.78384400
C	-3.02407800	0.15052300	-0.35616600
C	-3.25924700	1.38091800	0.13091200
C	-2.20765600	2.44258100	0.21235600
C	-0.91503300	2.12363200	-0.47534800
H	-1.58041400	-1.00871900	-1.53195300
H	-1.21984300	-0.86462300	0.21428100
H	-2.60058600	3.40175700	-0.17371700
H	-1.98131000	2.65828200	1.27768800
H	-1.66271300	-0.35543800	2.92953100
C	0.08381700	3.22881600	-0.59960500
H	1.05471000	2.86312900	-0.95509700
H	-0.28852200	4.00667800	-1.28756100
H	0.23112700	3.71949200	0.37698500
C	-4.06543700	-0.94720100	-0.45766500
H	-3.56428700	-1.87544700	-0.12353000
C	-5.28506200	-0.73648300	0.43610200
H	-4.99583800	-0.57977300	1.48603400
H	-5.87586700	0.13470900	0.11162200
H	-5.94798000	-1.61326800	0.39134100
C	-4.48967600	-1.15576900	-1.91849800
H	-5.17321200	-2.01360800	-2.00901200
H	-5.01005300	-0.26152500	-2.29552800
H	-3.62817800	-1.34275900	-2.57648300
H	-4.25339300	1.64989800	0.49587000
H	0.26303400	0.66037400	-1.45161500
B	3.60727700	0.59531100	-0.40464600
F	4.05461900	1.13395100	0.78584700
F	4.63872500	0.18287600	-1.21637400
F	2.74200700	1.46758500	-1.06919400

INT-1-A

C	-3.21143300	-1.98024200	-0.18793300
C	-2.79768700	-1.22991400	0.92476400
C	-1.40395900	-1.03153100	1.20256100
C	-0.42530300	-1.59617900	0.34981700
C	-0.82812700	-2.40491800	-0.85037300
C	-2.29959600	-2.54325400	-1.04103700
H	-1.70748800	0.18720500	2.96033200
H	-4.27977800	-2.11258100	-0.37306000
H	-3.52980500	-0.77356700	1.59287400
H	-0.34457800	-3.39618200	-0.78336600
C	1.28883800	-0.70164200	1.66573900
C	0.38691200	-0.11521700	2.53850700
H	2.36748200	-0.61268700	1.78064900
H	0.75487600	0.46096800	3.38763900
C	-0.08347300	1.13200700	-1.26694900

C	-1.48848900	1.09191800	-1.39128500
C	-2.31664600	1.90731900	-0.56025600
C	-1.72980000	2.73453900	0.35296400
C	-0.24656500	2.86494300	0.50961300
C	0.55739800	1.95644000	-0.37528200
H	-1.95146800	0.41884600	-2.11724800
H	-0.35992500	-1.95824900	-1.74510600
H	0.52525800	0.47516200	-1.89471200
H	-2.35627800	3.36378300	0.99320700
H	0.05614600	3.92026700	0.33121200
H	0.03329900	2.70153700	1.57112200
C	-3.81191800	1.84089900	-0.72801500
H	-4.33429900	2.43557100	0.03476300
H	-4.10933400	2.22235900	-1.71786200
H	-4.16944700	0.80162800	-0.66251900
C	2.07223300	2.03350900	-0.35787600
H	2.44928800	1.01518800	-0.55247100
C	2.66204600	2.50727000	0.97217800
H	3.75966600	2.43886300	0.94578000
H	2.40293400	3.55759100	1.18096900
H	2.31121100	1.90237700	1.82099600
C	2.56780200	2.92904700	-1.50510800
H	3.66811700	2.96975800	-1.52298200
H	2.22295800	2.55016300	-2.47761600
H	2.19181300	3.95892400	-1.39003000
H	-2.63503300	-3.12404100	-1.90281300
N	0.88301100	-1.41416900	0.60230400
C	-0.96790900	-0.27237200	2.30109200
B	2.06097300	-2.02079300	-0.39619200
F	1.91435500	-3.38846000	-0.37735400
F	3.25747400	-1.59702600	0.13366100
F	1.82845000	-1.47401100	-1.64671300

INT-1-B

C	-3.28337500	-0.65394900	2.15599900
C	-3.50859100	-0.75389200	0.77335600
C	-2.66106000	-0.07193100	-0.16379700
C	-1.57916300	0.71311400	0.30403700
C	-1.30803000	0.84686700	1.77438600
C	-2.25421300	0.10245300	2.65110900
H	-3.69679100	-0.75942400	-1.93137600
H	-3.94578000	-1.18515400	2.84285000
H	-4.33790600	-1.34872800	0.38624000
H	-1.28784800	1.92051600	2.03674500
C	-0.97919400	1.25265700	-1.89228900
C	-2.01283400	0.49674400	-2.41982500
H	-0.27843700	1.80973500	-2.51143700
H	-2.14046400	0.43799900	-3.50062000
C	1.24751000	-1.59459800	1.12631100
C	0.07116500	-2.25142300	0.70009900
C	-0.23619800	-2.35388900	-0.69134000
C	0.58199500	-1.74604000	-1.59982400
C	1.80763100	-0.97853100	-1.21442500
C	2.12176500	-0.99968800	0.25252700
H	-0.59518500	-2.70913000	1.43542300
H	-0.27165700	0.51417000	1.95871600
H	1.48134500	-1.57618600	2.19606000
H	0.35218400	-1.82031800	-2.66748500
H	2.67969200	-1.35110000	-1.79111300
H	1.72101400	0.07895800	-1.54491200
C	-1.42640100	-3.17079500	-1.12056000
H	-1.67282400	-3.00467800	-2.17923000
H	-1.22753700	-4.24619900	-0.98517100
H	-2.31363200	-2.93049600	-0.51404000
C	3.44380600	-0.43418600	0.72733200
H	3.27970100	-0.05427000	1.74972600
C	3.96876200	0.72643800	-0.12080200
H	4.87455400	1.14878100	0.34002200
H	4.24647500	0.39260200	-1.13360200
H	3.22453600	1.52724600	-0.21017300
C	4.48815500	-1.56013600	0.80820600
H	5.45192900	-1.17379400	1.17576000
H	4.15888000	-2.36494600	1.48191100
H	4.66294900	-2.00441900	-0.18545800
H	-2.09227500	0.17538400	3.72858200
C	-2.86639700	-0.16043300	-1.55083100
N	-0.78420600	1.35923900	-0.56629400
B	0.38142800	2.42995000	-0.06835900

F	-0.31203400	3.50218000	0.44308500
F	1.16057700	1.80480100	0.88183900
F	1.10894300	2.73816600	-1.19932000

INT-1-C

C	0.23721800	0.39273000	3.17405000
C	0.65609000	-0.78221500	2.52719800
C	-0.02406400	-1.26468200	1.35899300
C	-1.15899800	-0.57382200	0.86843200
C	-1.66698500	0.65693000	1.56267000
C	-0.84981500	1.09518000	2.72773700
H	1.26625700	-2.97027900	1.03753500
H	0.79281300	0.74746400	4.04480300
H	1.51463900	-1.34403500	2.89902100
H	-2.71526400	0.47932800	1.86499100
C	-1.38391000	-2.11295700	-0.88049400
C	-0.27934400	-2.83652900	-0.45852600
H	-1.97556300	-2.38783800	-1.75175300
H	0.03119500	-3.72056600	-1.01544400
C	1.26587400	0.23338300	-1.58352800
C	0.28438700	1.24771500	-1.59069900
C	0.37850200	2.35378700	-0.69026900
C	1.41414000	2.40106600	0.19735800
C	2.48766500	1.36074500	0.26593900
C	2.33568700	0.24197000	-0.72481500
H	-0.56285500	1.18619300	-2.27542500
H	-1.74792200	1.46675300	0.81966600
H	1.16962400	-0.59293400	-2.29580400
H	1.48665100	3.23762100	0.89916300
H	3.48311800	1.83983600	0.14131000
H	2.53043800	0.94663400	1.29502300
C	-0.66068100	3.44222900	-0.76066600
H	-0.61506400	4.10396500	0.11622500
H	-0.50815700	4.06208600	-1.65882600
H	-1.67109800	3.01477900	-0.83682900
C	3.42188200	-0.80814300	-0.81867200
H	2.96639000	-1.69971000	-1.28492600
C	3.98669800	-1.22878600	0.54099200
H	4.68090100	-2.07509300	0.42680600
H	4.54650700	-0.40832000	1.01700900
H	3.18997800	-1.53281800	1.23555400
C	4.55178000	-0.33346400	-1.74626000
H	5.33272200	-1.10410000	-1.84386400
H	4.16643600	-0.10236000	-2.74973200
H	5.02849400	0.57787600	-1.35075600
H	-1.16166000	2.01057000	3.23478500
N	-1.80837600	-1.02248100	-0.22056100
C	0.39741400	-2.41753100	0.67315900
B	-3.19771800	-0.29681300	-0.77573000
F	-4.09485400	-0.36736000	0.26633300
F	-2.86489900	1.00416900	-1.10552100
F	-3.58942400	-1.02561500	-1.87209600

INT-1-D

C	-3.75237700	0.63369500	0.63108900
C	-3.02115600	0.16282500	1.73399300
C	-1.83600600	-0.62583600	1.55029300
C	-1.38240600	-0.92390600	0.24119200
C	-2.09392700	-0.37369300	-0.96044900
C	-3.33922300	0.38211400	-0.65050400
H	-1.42535900	-0.90177500	3.65422700
H	-4.66516800	1.20790300	0.80404100
H	-3.35156000	0.37501700	2.75230000
H	-2.29619200	-1.19589000	-1.66760300
C	0.40622600	-2.16282300	1.10558100
C	0.03754600	-1.88709600	2.41168100
H	1.26869800	-2.77580600	0.85070100
H	0.63316800	-2.28184600	3.23473600
C	-0.41376700	2.75768700	-0.71879900
C	-0.36949100	2.32235000	0.64047000
C	0.72376300	1.56124000	1.11543400
C	1.77825700	1.20282200	0.31701300
C	1.79992400	1.62327500	-1.12388800
C	0.61281300	2.42407700	-1.55521000
H	-1.18783900	2.57946000	1.31719900
H	-1.37968300	0.27503100	-1.50364500
H	2.73251800	2.18976000	-1.33439300
H	1.88096000	0.72627100	-1.76690800

H	-3.91859400	0.75085300	-1.49954900
C	-1.59057600	3.57221300	-1.18850800
H	-1.65533700	4.52273300	-0.63543500
H	-1.52037800	3.80599300	-2.26005300
H	-2.53512100	3.03292800	-1.01399100
C	2.97365000	0.46578400	0.88176100
H	2.62209400	-0.06979700	1.78175600
C	4.05165300	1.46245200	1.33659400
H	3.65543600	2.16198700	2.08725500
H	4.91337400	0.93473600	1.77491200
H	4.42239000	2.05576600	0.48527600
C	3.56311100	-0.56759400	-0.08205500
H	2.80278100	-1.25859000	-0.47085100
H	4.03849400	-0.08007500	-0.94777400
H	4.34058700	-1.16137900	0.42268100
H	0.58368700	2.74521900	-2.60082700
H	0.72921400	1.24938100	2.16514000
N	-0.29608000	-1.69411100	0.05908500
C	-1.09726200	-1.12485600	2.63628900
B	0.18711000	-2.16913200	-1.45486700
F	-0.86203000	-2.89407400	-1.97224500
F	1.31898800	-2.93259100	-1.26642600
F	0.44796700	-1.01909200	-2.17247500

INT-1-E

C	0.92171400	1.80124000	-1.53956200
C	0.12185900	2.51525200	-0.63226400
C	-1.10835000	1.96315400	-0.14075700
C	-1.53334700	0.68384400	-0.57887500
C	-0.69836000	-0.11435600	-1.53742900
C	0.55757100	0.55509800	-1.97303200
H	-1.61318400	3.63939000	1.12732700
H	1.85471500	2.24515400	-1.89323700
H	0.42422500	3.50352900	-0.28143600
H	-1.32148500	-0.38734900	-2.40702500
C	-3.46440700	0.83444000	0.73814300
C	-3.10656300	2.08469200	1.21580400
H	-4.37843600	0.32434900	1.03636800
H	-3.75686500	2.59782900	1.92427100
C	0.63360100	-0.69121500	1.70669300
C	1.07678200	-1.80715200	0.93660400
C	2.31005900	-1.75946300	0.24296400
C	3.14345900	-0.67328300	0.28879600
C	2.76227400	0.52155200	1.11713900
C	1.42098300	0.42345700	1.77227700
H	0.44158500	-2.69222000	0.86093900
H	-0.46825600	-1.08607200	-1.06551100
H	3.53622200	0.69470200	1.89534200
H	2.80984200	1.44119700	0.49874300
H	1.19491300	0.00328600	-2.66658000
C	-0.68174000	-0.78007500	2.43552500
H	-0.57399600	-1.37122200	3.35914500
H	-1.05625600	0.21568300	2.71646400
H	-1.43639900	-1.28246400	1.81489200
C	4.45293000	-0.64516300	-0.46858000
H	4.56785700	-1.63655500	-0.93839700
C	5.65616600	-0.43441000	0.45968700
H	5.66163100	-1.17108500	1.27697700
H	6.59933100	-0.53632800	-0.09875500
H	5.64833600	0.57170700	0.90872500
C	4.44734700	0.39527100	-1.59698600
H	3.61149800	0.22343700	-2.29099400
H	4.35636800	1.41949000	-1.20049000
H	5.38403000	0.34897100	-2.17360600
H	1.08265800	1.28966700	2.34981900
H	2.60603900	-2.62690900	-0.35553300
C	-1.92336800	2.65356600	0.77296500
N	-2.69148900	0.16489400	-0.13465400
B	-3.22166500	-1.33670000	-0.62200600
F	-4.42339600	-1.53452100	0.01259600
F	-3.34229000	-1.27479200	-1.99128300
F	-2.25179000	-2.23042500	-0.20570400

INT-1-F

C	1.19438900	2.88304700	-0.11602500
C	0.96702300	2.26073200	1.12203700
C	-0.13736900	1.36284300	1.30559700
C	-1.03867400	1.12556600	0.24001100

C	-0.84865400	1.79781100	-1.08918200
C	0.35538500	2.67078800	-1.17725100
H	0.32083500	0.87184100	3.36020700
H	2.05732400	3.54292900	-0.22928900
H	1.62899300	2.44641500	1.96971100
H	-1.76549100	2.36803600	-1.32681400
C	-2.29595800	-0.32216000	1.58141000
C	-1.44642000	-0.14866600	2.66160700
H	-3.17203500	-0.96668500	1.61558900
H	-1.64532700	-0.67661900	3.59404600
C	0.05547400	-2.25373400	-0.07019300
C	0.32382500	-1.54333900	-1.28045500
C	1.49684000	-0.76817900	-1.41123500
C	2.42715100	-0.65283600	-0.40982000
C	2.19320500	-1.34160300	0.90402500
C	0.93674100	-2.15311800	0.96728600
H	-0.39545400	-1.59329600	-2.09885500
H	-0.82213000	1.01845200	-1.86949500
H	3.06720300	-1.98033300	1.15469900
H	2.19077200	-0.58743000	1.72154200
H	0.54495500	3.15760300	-2.13619400
C	-1.18555800	-3.10228100	0.01624500
H	-1.11467900	-3.96093900	-0.67009900
H	-1.33815500	-3.49396300	1.03232100
H	-2.07997400	-2.53479700	-0.27946200
C	3.74414600	0.05629500	-0.64719100
H	3.56160600	0.82030100	-1.42281300
C	4.78144900	-0.93094000	-1.20715900
H	4.42548500	-1.39086100	-2.14026700
H	5.73731100	-0.42389100	-1.41340000
H	4.98067300	-1.74168000	-0.48766900
C	4.29937300	0.76923400	0.58789500
H	3.56823400	1.47157900	1.01203900
H	4.57980100	0.05312000	1.37671600
H	5.20483200	1.33814500	0.32779500
H	0.73665700	-2.69031600	1.89976300
H	1.68148300	-0.25318500	-2.36009700
N	-2.08954600	0.30385800	0.41055500
C	-0.36477100	0.70426500	2.52615900
B	-3.21989500	0.06721700	-0.78631100
F	-4.10798200	-0.85505300	-0.28102400
F	-3.78707400	1.30142600	-1.00640400
F	-2.54630200	-0.41746800	-1.88978000

INT-1-G

C	-1.28117900	-2.84529600	0.20029600
C	-0.39192700	-2.69457500	1.27823800
C	0.78338400	-1.88022300	1.15696200
C	1.04811100	-1.19953100	-0.05867500
C	0.12273200	-1.33899400	-1.23188700
C	-1.05993000	-2.21067800	-0.99212600
H	1.52576300	-2.26135100	3.15159200
H	-2.16371100	-3.47709100	0.32315400
H	-0.57514100	-3.20354800	2.22611900
H	0.70728400	-1.69944300	-2.09712100
C	3.01326500	-0.29204600	0.83784500
C	2.82575800	-0.94012300	2.04769900
H	3.86615500	0.35316400	0.63574600
H	3.55349900	-0.80858500	2.84832400
C	-1.29646500	1.48743000	0.47635800
C	-1.69681500	1.58530800	-0.89367500
C	-2.81545200	0.86972300	-1.37779100
C	-3.58078100	0.07369800	-0.56688700
C	-3.25708400	-0.03474400	0.89371200
C	-2.02694000	0.70228500	1.32152300
H	-1.09603900	2.18026200	-1.58430000
H	-0.20416600	-0.33075500	-1.53964000
H	-4.12986100	0.31610000	1.48748400
H	-3.17167400	-1.10591500	1.17254900
H	-1.76481900	-2.32441800	-1.81786700
C	-0.07116000	2.27677400	0.91128300
H	0.71366800	2.04421900	0.17289400
C	-4.74633900	-0.72058800	-1.06557000
H	-4.92285600	-0.56329200	-2.13899600
H	-1.73870200	0.60253300	2.37040000
H	-3.06733600	0.94529300	-2.44009300
C	-0.34357000	3.78445800	0.83004400
H	-1.13482100	4.07327400	1.54069500

H	0.56391100	4.35758300	1.07487700
H	-0.66873800	4.08630600	-0.17588000
C	0.45422900	1.90427300	2.29406700
H	1.40422100	2.42310700	2.49295700
H	-0.25249300	2.19650600	3.08786700
H	0.63455700	0.82366100	2.38512000
H	-4.58524100	-1.80081800	-0.89800800
H	-5.67099700	-0.45729200	-0.52311800
N	2.14453600	-0.43055800	-0.17997400
C	1.70548900	-1.73876400	2.20922700
B	2.51825200	0.34689700	-1.60592800
F	1.45927700	1.19197700	-1.87782900
F	3.68416500	1.03123700	-1.36382900
F	2.66351000	-0.64770400	-2.54602500

INT-1-H

C	-3.33901300	-1.57486600	-0.14764700
C	-2.83749900	-1.04910100	1.05394700
C	-1.42428500	-0.98160100	1.29640200
C	-0.51648500	-1.46362500	0.32260600
C	-1.01489700	-2.05993100	-0.96204700
C	-2.49662400	-2.04986300	-1.11713700
H	-1.58146100	-0.07726900	3.25380000
H	-4.41893600	-1.59795200	-0.30856700
H	-3.51490300	-0.67402500	1.82332800
H	-0.61884600	-3.08891900	-1.04448500
C	1.29983300	-0.89799200	1.68466200
C	0.47107200	-0.40839300	2.68088200
H	2.38526400	-0.89675700	1.76419600
H	0.90718700	-0.00064200	3.59274800
C	0.68366500	1.90625000	-0.29428900
C	0.06494100	1.31319600	-1.44033000
C	-1.33908000	1.31611300	-1.59156400
C	-2.17652400	1.87556100	-0.66246500
C	-1.60259100	2.51397000	0.56773000
C	-0.10899000	2.47152000	0.66221800
H	0.68839300	0.81986900	-2.18700800
H	-0.53010900	-1.53329300	-1.80138200
H	-1.95535300	3.56576900	0.63628700
H	-2.05348000	2.03987400	1.46838000
H	-2.89964200	-2.45363200	-2.04833500
C	2.20333000	1.87580400	-0.21568700
H	2.50233300	0.82529900	-0.37219600
C	-3.66449000	1.89604000	-0.81190400
H	-4.15497500	1.42653600	0.05883400
H	0.33571000	2.92732400	1.54968800
H	-1.77364700	0.84954100	-2.48122200
C	2.82065300	2.69505400	-1.35704600
H	2.54966300	3.75871200	-1.25942900
H	3.91844000	2.61703400	-1.34097300
H	2.47552200	2.34831500	-2.34129100
C	2.77467200	2.32801200	1.12559600
H	3.86586600	2.18890900	1.13807100
H	2.57563300	3.39630200	1.30931100
H	2.35378500	1.75881400	1.96777500
H	-4.04456300	2.93138800	-0.86629500
H	-3.99163900	1.36211100	-1.71521600
C	-0.89853700	-0.45197300	2.48769100
N	0.80907400	-1.40960800	0.54371200
B	1.90759700	-2.01471700	-0.54849000
F	1.64021300	-3.36175900	-0.63423100
F	3.14770100	-1.74083900	-0.01860800
F	1.69912500	-1.35045900	-1.74152400

INT-1-I

C	-1.07918400	-0.72478000	2.85372200
C	-0.40020700	0.49927700	2.74901700
C	0.68516500	0.66284300	1.82365900
C	1.07728300	-0.41773000	0.99616000
C	0.38171400	-1.74509500	1.08698700
C	-0.72871300	-1.79776000	2.07785000
H	1.10972500	2.71711700	2.34429100
H	-1.90192200	-0.81703600	3.56607600
H	-0.68614200	1.34961200	3.37056400
H	1.13749800	-2.52208000	1.30111900
C	2.74730300	0.89401800	0.01367000
C	2.42893100	1.98772500	0.80163200
H	3.54527600	0.90824600	-0.72642900

H	2.99039700	2.91506600	0.68957900
C	-0.24393200	1.24214400	-1.71018200
C	-1.01057500	0.06521500	-1.55613100
C	-2.16731400	0.04431100	-0.71646300
C	-2.50970800	1.17736900	-0.03630900
C	-1.73821200	2.45554700	-0.13947800
C	-0.55812800	2.40896900	-1.06560700
H	-0.69159500	-0.84143000	-2.07303800
H	0.02073100	-2.01425400	0.07882400
H	-2.41610100	3.28166700	-0.44413000
H	-1.39709300	2.77142600	0.87232800
H	-1.26932500	-2.74240800	2.16706300
C	0.21613700	3.67659700	-1.24574800
H	-0.40607900	4.45561000	-1.72067300
H	0.54051800	4.08855500	-0.27393200
H	1.10819200	3.52606000	-1.87036100
C	-2.97422300	-1.24452500	-0.65216900
H	-2.24905200	-2.05509100	-0.45408300
C	-4.01949600	-1.28210500	0.45932200
H	-3.57473900	-1.07312300	1.44294500
H	-4.81977600	-0.54576900	0.28203600
H	-4.49291300	-2.27453000	0.50302600
C	-3.62459900	-1.53762500	-2.01109700
H	-4.15307300	-2.50330900	-1.99270800
H	-4.35491400	-0.75204500	-2.26247000
H	-2.88061500	-1.57429500	-2.81971300
H	-3.38197400	1.18693900	0.62062100
H	0.62896400	1.21061100	-2.36914700
N	2.08780700	-0.27169800	0.12222100
C	1.39128700	1.87257100	1.71065500
B	2.58429900	-1.51735200	-0.86259400
F	3.60940900	-1.00698000	-1.62178300
F	2.99117700	-2.52529100	-0.01719400
F	1.49015800	-1.87091600	-1.62894600

INT-1-J

C	-0.05066400	1.52869200	2.87092600
C	0.74761300	2.21387700	1.93920600
C	1.42812000	1.50884200	0.89114700
C	1.30852700	0.10061300	0.79388000
C	0.48753600	-0.66967600	1.78745500
C	-0.19104700	0.16807700	2.81464100
H	2.34004700	3.25844600	0.00677500
H	-0.56573400	2.09559500	3.64939400
H	0.85893400	3.29844700	1.99293400
H	1.13511300	-1.42713300	2.26469200
C	2.67939900	0.08120900	-1.10274700
C	2.84442200	1.45716300	-1.06524400
H	3.14385100	-0.55076100	-1.85737900
H	3.45918600	1.94703500	-1.82039900
C	-0.67423800	1.13064100	-1.89341900
C	-1.17630800	-0.14149500	-1.54478800
C	-2.13280300	-0.28990200	-0.49090600
C	-2.56541200	0.82218400	0.17087200
C	-2.11450500	2.20635800	-0.17537900
C	-1.07733800	2.27630700	-1.25739400
H	-0.80156000	-1.03155200	-2.05334900
H	-0.24943000	-1.27416900	1.23249700
H	-2.99233800	2.82293500	-0.47067300
H	-1.73641400	2.71910200	0.73390800
H	-0.81398400	-0.35227500	3.54528200
C	-0.53289600	3.62853400	-1.59260900
H	0.23836000	3.57837400	-2.37459300
H	-1.33108000	4.30696800	-1.94161200
H	-0.09025800	4.10722400	-0.70032900
C	-2.63242600	-1.69303500	-0.18269800
H	-1.74712800	-2.34899500	-0.22281000
C	-3.26454900	-1.84400600	1.19891400
H	-2.59477000	-1.48442900	1.99505700
H	-4.21110100	-1.28547300	1.27814400
H	-3.49152700	-2.90154100	1.40009100
C	-3.59921400	-2.16335000	-1.27757700
H	-3.90588300	-3.20705000	-1.10778200
H	-4.50496000	-1.53578600	-1.28912000
H	-3.13735400	-2.10473700	-2.27406500
H	-3.28562200	0.73336300	0.98737700
H	0.07658200	1.20045000	-2.68674100
C	2.22568500	2.17400500	-0.05653800

N	1.94087100	-0.56769200	-0.18684500
B	1.89562000	-2.22733800	-0.29027900
F	2.65376800	-2.55575800	-1.38756600
F	2.43144400	-2.68765500	0.89156400
F	0.56850700	-2.58144700	-0.44782300

INT-1-K

C	-1.12784800	-2.87918600	1.67264000
C	-0.14256500	-2.20287200	2.40840000
C	0.85275100	-1.40494200	1.74903600
C	0.83355700	-1.27623100	0.33733900
C	-0.22980100	-1.95034100	-0.47887500
C	-1.18496300	-2.77854800	0.30739600
H	1.90958700	-0.83758100	3.54744200
H	-1.86165600	-3.49045100	2.20235500
H	-0.10535500	-2.28447800	3.49610500
H	0.25697200	-2.54634100	-1.27090300
C	2.75461100	0.06046400	0.39748400
C	2.83126400	-0.01540700	1.77816200
H	3.47066800	0.61437900	-0.20645000
H	3.63595600	0.49979400	2.30250800
C	-2.81624100	0.09570800	0.66255600
C	-1.74215300	0.85860500	1.17370600
C	-0.97591900	1.71426100	0.32217100
C	-1.30012900	1.79067000	-1.00009600
C	-2.42125100	1.01493100	-1.61351200
C	-3.16905000	0.12704700	-0.66144200
H	-1.48509000	0.78081400	2.23322600
H	-0.77745000	-1.16930800	-1.03513300
H	-3.13546800	1.70922900	-2.10710300
H	-2.02387700	0.41578200	-2.46000100
H	-1.96367700	-3.30052800	-0.25245300
C	-4.27581100	-0.70544600	-1.22856500
H	-4.76517500	-1.31792700	-0.45779000
H	-5.04589400	-0.07479800	-1.70597600
H	-3.89725400	-1.38046600	-2.01660000
C	0.16257600	2.50988900	0.94173300
H	0.71618200	1.80263900	1.58499300
C	1.15071500	3.08215800	-0.07244900
H	1.51937700	2.31774900	-0.77102000
H	0.68972000	3.88430800	-0.67046600
H	2.01708300	3.52149400	0.44574600
C	-0.38511200	3.61806100	1.85055200
H	0.43330300	4.15164100	2.35894900
H	-0.95469000	4.35135700	1.25777600
H	-1.05997400	3.21669500	2.62115900
H	-0.71383200	2.41108800	-1.67908100
H	-3.36922000	-0.55654300	1.34477700
N	1.77782100	-0.55602100	-0.29184800
C	1.87552400	-0.75242400	2.45879900
B	1.85386800	-0.46359400	-1.95343100
F	2.12910800	-1.74566900	-2.37303700
F	0.63166200	-0.00837200	-2.40033300
F	2.86753400	0.42661800	-2.22464900

INT-1-L

C	0.32278500	-0.45176500	2.76040600
C	0.52572500	0.54284300	1.78579200
C	1.38634300	0.29408300	0.67029900
C	2.06895000	-0.94235700	0.56304600
C	1.88826000	-2.01810500	1.60220800
C	0.93695900	-1.67250300	2.69663400
H	-0.35444700	-0.23088200	3.58845200
H	0.04006500	1.51075000	1.87167100
C	2.91213100	-1.14671500	-0.52075800
H	2.87383000	-2.27497100	2.03664700
C	3.05133700	-0.16355000	-1.49607600
C	2.35031700	1.02108000	-1.34000900
H	3.46095800	-2.08841300	-0.60588700
H	3.69667000	-0.30223300	-2.36306100
H	2.41594200	1.84074700	-2.05438100
N	1.55831500	1.24739600	-0.28912600
C	-1.25407700	-0.26949000	-1.53173200
C	-0.39770700	-1.34815000	-1.84404100
C	-0.42050200	-2.54491700	-1.06473100
C	-1.26304300	-2.62666100	0.00623400
C	-2.19341700	-1.52365800	0.39949200
C	-2.14163400	-0.31245600	-0.48691100

H	0.28181800	-1.27317300	-2.69654000
H	1.55133500	-2.94373200	1.09991900
H	-1.21408700	0.63373900	-2.14665700
H	-1.28451400	-3.53962700	0.61029500
H	-3.23369200	-1.90895400	0.45097000
H	-1.98183700	-1.22131700	1.44632600
C	0.47857900	-3.68892000	-1.45328100
H	0.39113900	-4.53296100	-0.75389200
H	0.23063700	-4.05874600	-2.46069800
H	1.53395900	-3.37229000	-1.48422400
C	-3.12434500	0.81006700	-0.24232700
H	-2.75317000	1.68143400	-0.80240000
C	-3.21357800	1.22303300	1.22907700
H	-3.86743200	2.10113100	1.33955000
H	-3.63230800	0.42009700	1.85755100
H	-2.22273900	1.49563700	1.61621500
C	-4.51046300	0.44533500	-0.79578400
H	-5.21231100	1.28416100	-0.66771800
H	-4.45822700	0.20279300	-1.86750800
H	-4.93720000	-0.42596900	-0.27232400
H	0.75119700	-2.42548500	3.46557100
B	0.84520700	2.73954200	-0.17266200
F	1.32275300	3.28971600	0.99467800
F	1.23786100	3.42938200	-1.29662200
F	-0.51900800	2.52930400	-0.13649100

INT-1-M

C	1.95777700	-2.46018400	-1.06921800
C	0.59341300	-2.16029000	-0.89890000
C	0.13407300	-1.56688300	0.32045500
C	1.05328100	-1.26331200	1.35264300
C	2.51714600	-1.57844300	1.19955500
C	2.88879700	-2.20159700	-0.10172400
H	2.27205600	-2.91353600	-2.01174700
H	-0.12071700	-2.36994800	-1.69032300
C	0.58268100	-0.66393500	2.51345400
H	2.83782200	-2.23490500	2.03120200
C	-0.77142800	-0.37929800	2.65649100
C	-1.62616800	-0.71815900	1.62160900
H	1.28599200	-0.41339900	3.31168200
H	-1.16772900	0.09300300	3.55478400
H	-2.70064900	-0.54508800	1.66764100
N	-1.19126700	-1.29089500	0.49533700
C	0.92059900	2.30078600	0.84746200
C	2.23673900	1.89339700	0.53437400
C	2.53186500	1.30957500	-0.73616700
C	1.51833500	1.12804300	-1.63203800
C	0.10646700	1.54890100	-1.37749700
C	-0.12426200	2.17535000	-0.03343100
H	3.04002000	2.04561800	1.26035900
H	3.09259900	-0.64416900	1.34206300
H	0.73216200	2.76024000	1.82383000
H	1.73091600	0.66597200	-2.60083100
H	-0.21877000	2.25101800	-2.17553300
H	-0.57628900	0.68693900	-1.51752600
C	3.95428600	0.93964700	-1.06871800
H	4.42686200	0.36448800	-0.25660400
H	4.01074800	0.33871300	-1.98699800
H	4.56669500	1.84390200	-1.21585400
C	-1.47821300	2.78208400	0.27822400
H	-1.63344100	2.68336100	1.36796400
C	-2.65112500	2.10380400	-0.43149800
H	-3.60273800	2.53951400	-0.09197000
H	-2.59812500	2.24600500	-1.52185000
H	-2.69606300	1.02328500	-0.25192900
C	-1.45896200	4.28566900	-0.04587500
H	-2.42751000	4.75137500	0.19510600
H	-0.67317200	4.80719500	0.51988300
H	-1.26593800	4.44899300	-1.11846300
H	3.94009500	-2.44711600	-0.26678000
B	-2.31767900	-1.72668000	-0.63449400
F	-2.22835900	-3.09126000	-0.75342600
F	-3.53066800	-1.30366300	-0.13511900
F	-1.97868100	-1.06760200	-1.80458800

INT-1-N

C	0.31790100	-0.91449100	2.19122100
C	-0.83642700	-1.04091800	1.39617700

C	-1.51372300	0.12774000	0.92151800
C	-1.00325600	1.41470500	1.22348400
C	0.32478800	1.56622800	1.91547000
C	0.88173400	0.30083300	2.46912800
H	0.77173100	-1.82349800	2.59238000
H	-1.25522400	-2.01982200	1.17900400
C	-1.73610200	2.53000800	0.84139900
H	0.25467500	2.33660700	2.70324100
C	-2.94105400	2.37794000	0.15849800
C	-3.36052800	1.09645500	-0.15613600
H	-1.35921800	3.52842700	1.07808700
H	-3.53927400	3.23564800	-0.14766700
H	-4.26864200	0.89734400	-0.72376800
N	-2.66884300	0.01189100	0.20559700
C	0.60408000	0.62975500	-1.77604500
C	1.54598500	1.66493800	-1.49742600
C	2.77716000	1.36810000	-0.86407600
C	3.13058200	0.09506600	-0.49722600
C	2.18923200	-1.04374100	-0.76642100
C	0.90031600	-0.65395700	-1.41477800
H	1.31779100	2.69508700	-1.78261400
H	1.04924500	1.96923900	1.17794000
H	2.69791900	-1.81359900	-1.38520600
H	1.97164200	-1.58260400	0.17819900
H	1.78077700	0.36645300	3.08545600
C	-0.68849500	0.96326900	-2.47361900
H	-0.50836600	1.19869500	-3.53489700
H	-1.39258900	0.12152500	-2.42503100
H	-1.16649700	1.84737400	-2.02433100
C	4.48600300	-0.20620700	0.10430300
H	4.92251000	0.76045100	0.40902600
C	5.42929300	-0.82331400	-0.93969100
H	5.53153400	-0.16739300	-1.81653500
H	6.43104300	-0.98676700	-0.51265300
H	5.05495800	-1.79881900	-1.28891800
C	4.40355500	-1.09188600	1.35227500
H	3.70991900	-0.67189300	2.09584400
H	4.05837800	-2.10822900	1.10462400
H	5.39292900	-1.18841400	1.82460700
H	0.16284400	-1.44241500	-1.58790000
H	3.47869500	2.18637700	-0.67001300
B	-3.20994700	-1.45925400	-0.32926100
F	-3.44882200	-2.22968900	0.78503500
F	-4.34813100	-1.19944800	-1.05560900
F	-2.18431400	-1.95862800	-1.11276800

INT-1-O

C	0.07723200	0.15013300	2.74060900
C	-0.57207900	-0.56850700	1.71862200
C	-1.36170800	0.11829800	0.74531000
C	-1.48834700	1.52898600	0.80069300
C	-0.75978900	2.32649200	1.84999300
C	0.00624300	1.51137200	2.83385700
H	0.65853200	-0.41036300	3.47579400
H	-0.48861000	-1.65034500	1.66751800
C	-2.28323000	2.16619400	-0.14129200
H	-1.47437100	2.98539100	2.37750000
C	-2.90757600	1.42995500	-1.14479700
C	-2.73668100	0.05599600	-1.15599300
H	-2.40264000	3.25170800	-0.10006600
H	-3.52531300	1.90584100	-1.90591000
H	-3.20348400	-0.58729000	-1.90084500
N	-2.00308500	-0.57972800	-0.23690700
C	1.11577600	2.20215900	-1.22099500
C	2.12651300	2.28272200	-0.21619200
C	2.81740000	1.12165300	0.20561000
C	2.56371200	-0.11895600	-0.31829300
C	1.50475900	-0.28067700	-1.37187000
C	0.80927400	0.98484400	-1.75821900
H	2.38566600	3.25385600	0.21399900
H	-0.05866900	3.01590500	1.34022300
H	1.95010200	-0.73841400	-2.27953100
H	0.76450800	-1.03994200	-1.05081000
H	0.52997800	2.03912400	3.63363600
C	0.42502800	3.46284900	-1.67080900
H	1.13649700	4.14802700	-2.15850300
H	-0.38362100	3.24893900	-2.38376900
H	-0.00782800	4.01117000	-0.81730800

C	3.32678700	-1.34392700	0.13782100
H	4.17972000	-0.98120900	0.73670800
C	3.89740300	-2.14631600	-1.03798400
H	4.47373500	-1.50433300	-1.72176000
H	4.56610700	-2.93980400	-0.67126100
H	3.09785100	-2.63513100	-1.61643300
C	2.47528500	-2.24407700	1.04415700
H	2.16863600	-1.70449700	1.95185100
H	1.56618600	-2.59063400	0.53011700
H	3.04854000	-3.13157500	1.35467000
H	0.03151100	0.91249200	-2.52532200
H	3.59281100	1.22269200	0.97149300
B	-1.97465600	-2.23349600	-0.29061500
F	-2.51678500	-2.65990700	0.89679500
F	-0.64365600	-2.60622700	-0.42403100
F	-2.72033500	-2.58844300	-1.38964500

INT-1-P

C	-1.85380200	2.66515500	-0.89097800
C	-2.19603100	1.36015000	-0.49042300
C	-1.40049000	0.24640000	-0.90870900
C	-0.28842400	0.44849100	-1.76248500
C	0.09180900	1.83214200	-2.21864500
C	-0.77734200	2.92268700	-1.69382400
H	-2.47458900	3.49185100	-0.53908900
H	-3.06695200	1.18521600	0.13512600
C	0.44667300	-0.65435700	-2.17539700
H	0.09817400	1.86366400	-3.32521700
C	0.09010800	-1.93199700	-1.75371500
C	-0.99425600	-2.06622900	-0.90400000
H	1.30935500	-0.51165300	-2.83125400
H	0.64410800	-2.81563300	-2.06891100
H	-1.32537500	-3.03066800	-0.52080600
N	-1.71355000	-1.01650000	-0.49577500
C	2.59064200	-0.06666600	0.48584000
C	2.41013600	1.34412600	0.34952000
C	1.34366800	2.01034800	0.99806200
C	0.45370500	1.34921800	1.80254700
C	0.61138400	-0.12388400	2.03818700
C	1.72537800	-0.76820600	1.27620000
H	3.10521800	1.91738000	-0.27071900
H	1.14105900	2.02007500	-1.92304900
H	0.75261200	-0.30185600	3.12701900
H	-0.35346400	-0.62691400	1.83385500
H	-0.53528200	3.94829900	-1.98104900
C	3.76183700	-0.70684900	-0.24596100
H	3.74613200	-0.30118100	-1.27495300
C	-0.68015600	2.02634700	2.50380800
H	-0.78262500	3.07752600	2.19867000
H	1.83355600	-1.84909300	1.39118100
H	1.22166000	3.08728400	0.84590200
C	5.09084600	-0.28123600	0.39286000
H	5.15536400	-0.66034200	1.42503400
H	5.94674000	-0.68067000	-0.17321700
H	5.19129300	0.81319200	0.43384900
C	3.68377200	-2.22783200	-0.35154200
H	4.50114100	-2.61057300	-0.98099700
H	3.78155100	-2.70420600	0.63670100
H	2.73068400	-2.55753200	-0.78987300
H	-1.62503700	1.49721000	2.30156000
H	-0.53443700	1.99725800	3.59804500
B	-2.98028100	-1.30321100	0.52801200
F	-4.11020500	-0.84744600	-0.10855100
F	-2.99231500	-2.66093300	0.74455800
F	-2.69985400	-0.58983500	1.68337900

INT-1-Q

C	-3.45807100	0.25307600	-0.43536300
C	-2.29599900	1.04597500	-0.47505100
C	-1.28964800	0.89929700	0.53359300
C	-1.45867000	-0.04739500	1.57123800
C	-2.65851400	-0.95740500	1.59840400
C	-3.66244300	-0.69577600	0.52872000
H	-4.21518400	0.40888100	-1.20703400
H	-2.16306800	1.79308800	-1.25282200
C	-0.48928900	-0.13177300	2.56258800
H	-3.14282000	-0.90147500	2.59106000
C	0.61609400	0.71211900	2.53497300

C	0.73756900	1.60214200	1.48103500
H	-0.60520900	-0.86196500	3.36749900
H	1.38524400	0.67617500	3.30585600
H	1.58552000	2.27816800	1.38032900
N	-0.17507700	1.68603300	0.51067900
C	1.75633200	-1.31253200	-0.20873600
C	1.08421400	-2.34426000	0.52163300
C	-0.13052200	-2.89314900	0.05262100
C	-0.73317100	-2.46191300	-1.10127800
C	-0.08855200	-1.38120200	-1.91765300
C	1.19299400	-0.85002900	-1.36148200
H	1.51829100	-2.71755300	1.45267500
H	-2.30373500	-2.00292100	1.51425200
H	0.08091900	-1.75407000	-2.95103100
H	-0.79409900	-0.53831800	-2.06914900
H	-4.57262000	-1.29942300	0.52564900
C	3.08627200	-0.79952800	0.32498000
H	2.91958300	-0.55132000	1.38974500
C	-2.00409700	-3.05227000	-1.62685100
H	-2.42811900	-3.79761400	-0.93798400
H	1.65951000	-0.04251200	-1.92627000
H	-0.60294400	-3.69535900	0.62995000
C	4.14906500	-1.90599000	0.27567400
H	4.34614000	-2.19818900	-0.76798000
H	5.09629000	-1.55916300	0.71718400
H	3.83211400	-2.80787300	0.81985900
C	3.59825900	0.45886800	-0.37286400
H	4.49594100	0.83848500	0.13815400
H	3.88306400	0.24404500	-1.41508600
H	2.85266700	1.26578700	-0.39772300
H	-2.76157000	-2.26936300	-1.79937500
H	-1.83572800	-3.54600700	-2.60015300
B	0.10574000	2.74606300	-0.72496000
F	1.35337900	3.28197800	-0.48074000
F	-0.90071300	3.68123500	-0.67242100
F	0.07574800	2.00083200	-1.88846700

INT-1-R

C	0.94843700	-1.92504300	2.01993700
C	-0.03050900	-1.78247600	1.01945700
C	-0.90910300	-0.65268700	1.02670800
C	-0.80630700	0.31985600	2.05072100
C	0.26636000	0.22023800	3.10367500
C	1.11692100	-1.00081400	3.01397600
H	1.59442600	-2.80503100	1.98640300
H	-0.14286500	-2.53351500	0.24254000
C	-1.70539000	1.37722300	2.06113200
H	-0.19545500	0.28242300	4.10700600
C	-2.68005700	1.47862200	1.07311200
C	-2.71558200	0.51074400	0.08421500
H	-1.63912000	2.13246200	2.84860700
H	-3.39729800	2.29860400	1.05660900
H	-3.43986800	0.52818100	-0.72930800
N	-1.86234600	-0.51781200	0.06120300
C	0.93945600	2.51479200	0.12480900
C	1.92326600	1.51313500	0.29070200
C	2.05589100	0.44908600	-0.65326400
C	1.22076800	0.41734100	-1.73213300
C	0.17277400	1.45143700	-1.98616200
C	0.07849400	2.52430500	-0.94176200
H	2.59436800	1.55174900	1.15328800
H	0.90941900	1.11885700	3.03460000
H	0.34312700	1.92107700	-2.97938100
H	-0.81003000	0.95197500	-2.11452500
H	1.89273100	-1.13769900	3.77043600
C	-0.95409200	3.58718300	-1.14755600
H	-0.99821200	4.28928700	-0.30233500
H	-0.74549300	4.16757500	-2.06357800
H	-1.95617500	3.14519900	-1.28412400
C	3.14502500	-0.58621500	-0.42030700
H	3.11129700	-0.82995400	0.65655000
C	2.93949200	-1.88685100	-1.19361000
H	1.92543400	-2.28748700	-1.05246300
H	3.08774600	-1.73845900	-2.27503900
H	3.66620900	-2.64618700	-0.86685800
C	4.52743000	0.01153100	-0.71334500
H	5.32638000	-0.70978000	-0.48020900
H	4.61014600	0.28075100	-1.77835100

H	4.70975800	0.92291100	-0.12430500
H	1.27440600	-0.39924700	-2.45222300
H	0.86272100	3.30941300	0.87449800
B	-2.05014300	-1.64225900	-1.14283800
F	-3.01875800	-1.12933100	-1.97717600
F	-2.42950200	-2.80383000	-0.51407800
F	-0.82909100	-1.75856800	-1.77806900

INT-1-S

C	-1.55411500	2.69086800	-1.03727500
C	-2.02381300	1.43576000	-0.60525300
C	-1.31009900	0.24360700	-0.94897400
C	-0.13038400	0.32220700	-1.72798900
C	0.41815800	1.65417800	-2.16758300
C	-0.41028600	2.82958700	-1.77434400
H	-2.13071700	3.57798400	-0.76598000
H	-2.93145400	1.35908200	-0.01317400
C	0.52690400	-0.85304100	-2.06630700
H	0.56556400	1.64941200	-3.26391100
C	0.03258000	-2.08024300	-1.63679200
C	-1.11729200	-2.09217600	-0.86388800
H	1.44107900	-0.80598200	-2.66372500
H	0.52996800	-3.01757900	-1.88454700
H	-1.55876700	-3.01167500	-0.48136900
N	-1.76644200	-0.97325200	-0.53480700
C	0.36865800	-0.18980100	1.90249300
C	1.41143700	-0.91042600	1.28264800
C	2.48578600	-0.23561500	0.62310900
C	2.52301700	1.12875500	0.64310100
C	1.49082200	1.95931000	1.34159900
C	0.35533800	1.18135900	1.94089300
H	1.38048500	-2.00290900	1.27432000
H	1.43743500	1.76219700	-1.74735200
H	1.97417500	2.57036500	2.13575100
H	1.08136200	2.72576800	0.64999800
H	-0.07268600	3.81924700	-2.08994300
C	-0.74731100	1.95961800	2.58524000
H	-1.59957800	1.31533000	2.83628300
H	-0.39337700	2.46034000	3.50410000
H	-1.10650000	2.75693000	1.91246200
C	3.55000700	-1.08712000	-0.05173300
H	3.01218000	-1.91854700	-0.54335200
C	4.34779600	-0.35728700	-1.13025700
H	3.68909600	0.11774600	-1.87409900
H	4.98684700	0.42922800	-0.69890400
H	5.00990500	-1.05883000	-1.65975000
C	4.48549500	-1.70506500	0.99557200
H	5.21036600	-2.38796500	0.52566700
H	5.04689800	-0.91535900	1.51945500
H	3.92314200	-2.27175400	1.75205200
H	3.33871100	1.66695100	0.15315200
H	-0.47175600	-0.73483200	2.33904800
B	-3.12136200	-1.11774000	0.40622200
F	-4.15705600	-0.58178000	-0.32255300
F	-3.26968100	-2.46439900	0.64517300
F	-2.86289100	-0.40387900	1.56302200

MECP-1-A

C	1.17238100	3.10448300	-0.99235700
C	1.99208700	1.92205200	-0.59065600
C	1.31275500	0.99313100	0.37964700
C	0.07749500	1.35819200	0.98747600
C	-0.60917000	2.52185900	0.54745900
C	-0.03052400	3.38104600	-0.43540300
H	1.60085900	3.77011800	-1.74503200
H	2.31237500	1.34634300	-1.47141100
C	-0.46915900	0.47700000	1.94634900
C	0.18133100	-0.70400100	2.24826500
C	1.36924300	-1.00422200	1.60046100
H	-1.40613600	0.74219000	2.44138000
H	-0.22506000	-1.40961400	2.97306200
H	1.93987900	-1.91025500	1.79356200
N	1.92287000	-0.15521300	0.71361900
C	-0.63720400	-0.37736500	-1.69134800
C	-1.86114900	0.29375500	-1.21814000
C	-2.71458100	-0.48536800	-0.29107500
C	-2.31223600	-1.74073900	0.09966200
C	-1.11948600	-2.32132600	-0.37464400

C	-0.27659800	-1.64186700	-1.28591100
H	-0.58359600	4.26985100	-0.74723600
C	0.95971700	-2.32600700	-1.79986300
H	0.68667300	-3.20489700	-2.40458200
H	1.57635400	-1.65618900	-2.40901100
H	1.59060400	-2.67531200	-0.96947600
C	-3.99606400	0.17188300	0.17095300
H	-3.73183400	1.22195900	0.40362200
C	-5.03896100	0.20496700	-0.95889300
H	-4.65853600	0.70994100	-1.85852700
H	-5.32846900	-0.81919700	-1.24239800
H	-5.94504400	0.73949000	-0.63533500
C	-4.59780300	-0.44143300	1.43375300
H	-5.45564700	0.15664600	1.77441700
H	-4.96684600	-1.46288800	1.25141300
H	-3.86645100	-0.48631100	2.25475600
H	-2.92670600	-2.31560200	0.79562900
H	-0.01055700	0.15794800	-2.41019200
B	3.42186900	-0.54931100	0.12667700
F	3.67676300	-1.82707400	0.57496100
F	4.27590000	0.39203400	0.65447900
F	3.36263500	-0.49429600	-1.25449900
H	-1.55513600	1.24956600	-0.66561000
H	2.94936800	2.24380500	-0.13769100
H	-1.52816600	2.81246400	1.06014300
H	-2.43787900	0.73161600	-2.05545100
H	-0.84960400	-3.33083800	-0.05362600

MECP-1-B

C	-0.81899200	1.20277600	-1.96014300
C	0.41584100	0.45548700	-1.60546300
C	1.11353200	0.96202800	-0.37872600
C	0.54932600	2.00363400	0.40331800
C	-0.67120700	2.62720300	-0.00890000
C	-1.30014700	2.23706600	-1.20906000
H	-1.31834100	0.92124900	-2.88939500
H	0.17764600	-0.61652200	-1.42064300
C	1.20698500	2.35460500	1.59742700
C	2.37346300	1.70724800	1.96852900
C	2.89498500	0.73724100	1.12592700
H	0.78075100	3.13911700	2.22746600
H	2.89485900	1.95509600	2.89370500
H	3.82417900	0.20853900	1.32956600
N	2.27771700	0.39214000	-0.01582700
C	-0.71586400	-0.61164900	1.92797800
C	-1.94590700	0.04910900	1.42906700
C	-2.58591100	-0.58062400	0.24033600
C	-1.96691200	-1.65017700	-0.36256800
C	-0.74788400	-2.17459600	0.11096400
C	-0.12973600	-1.67084100	1.29215000
H	-2.20396500	2.76021100	-1.53084300
C	1.12791100	-2.31659600	1.80830000
H	1.48658600	-1.82280400	2.72252600
H	0.95607200	-3.37995900	2.03667400
H	1.92209500	-2.27510400	1.05033500
C	-3.90721400	0.00234100	-0.20932700
H	-3.77683400	1.10080400	-0.18436400
C	-4.30970800	-0.38883400	-1.62897300
H	-3.51707100	-0.14914200	-2.35265000
H	-4.52307100	-1.46716100	-1.70126500
H	-5.22367500	0.14453100	-1.92973700
C	-5.03431400	-0.34001300	0.77924200
H	-5.97475400	0.14591800	0.47701000
H	-5.20640100	-1.42723200	0.80734100
H	-4.80430400	-0.00919300	1.80256700
H	-2.41192600	-2.10672600	-1.24900800
H	-0.27210500	-0.22010500	2.84824100
B	3.05219400	-0.70614100	-0.99467000
F	4.18707800	-1.08026300	-0.31295000
F	3.32297500	-0.03338200	-2.16363700
F	2.18658800	-1.76836400	-1.17651600
H	-2.67285400	0.19809500	2.24994000
H	1.12559700	0.41817900	-2.44862500
H	-1.04854000	3.47134500	0.57065900
H	-1.69440100	1.11455400	1.14474300
H	-0.28379300	-3.01232000	-0.41265300

MECP-1-C

C	-0.79764200	-0.20228300	2.23512500
C	0.09633300	0.59970100	1.36041600
C	1.28841700	-0.14772700	0.84413800
C	1.44728000	-1.53341700	1.10964800
C	0.46392000	-2.23477900	1.87819100
C	-0.60138100	-1.53415200	2.47329100
H	-1.61418500	0.32646900	2.72785400
H	-0.46947100	0.97358100	0.47294800
C	2.59168200	-2.17267100	0.59463000
C	3.51244900	-1.46047900	-0.15118000
C	3.29161500	-0.10800800	-0.37123600
H	2.74075900	-3.23700200	0.79249300
H	4.40430800	-1.93400800	-0.56199200
H	3.97417800	0.52006300	-0.94011600
N	2.21381000	0.51881600	0.12426200
C	-0.49293300	-0.14443300	-1.98496600
C	-1.52705000	0.67770100	-1.48171100
C	-2.59292000	0.14643300	-0.71127900
C	-2.53253400	-1.17374700	-0.34110800
C	-1.44127300	-2.08076400	-0.77953400
C	-0.43790800	-1.48157500	-1.70178800
H	-0.88105300	-2.45776900	0.12675600
H	-1.85403900	-3.01862400	-1.20179100
H	-1.29347400	-2.07471800	3.12283700
C	0.58015600	-2.39851300	-2.30253600
H	1.38553800	-1.84070900	-2.80056200
H	1.02742500	-3.05219600	-1.53657500
H	0.10986300	-3.06217000	-3.04936300
C	-3.72974400	1.07949300	-0.31589800
H	-3.84253800	1.78412100	-1.15777700
C	-5.07311400	0.37466400	-0.13646600
H	-5.33663900	-0.22050400	-1.02312300
H	-5.07093800	-0.29572800	0.73772500
H	-5.87115400	1.11426900	0.02820900
C	-3.38165200	1.91021300	0.92432500
H	-4.14248900	2.68675300	1.09560100
H	-3.34981400	1.26946300	1.81878400
H	-2.40604900	2.40833600	0.82120600
H	-3.33239300	-1.61710000	0.25594400
H	0.27481600	0.31217500	-2.61369000
B	2.09979800	2.15394600	-0.16162600
F	3.19553000	2.47887700	-0.92717900
F	2.11702200	2.75870400	1.07577600
F	0.91460500	2.35641200	-0.84034500
H	-1.52843900	1.73733800	-1.74617500
H	0.42711000	1.52919900	1.85124300
H	0.62638700	-3.29255400	2.09121900

MECP-1-D

C	0.32485900	-2.89598000	1.84286000
C	1.25901800	-1.98749200	1.11109300
C	0.69138800	-1.39353300	-0.15146300
C	-0.59280000	-1.77867600	-0.62327200
C	-1.40287700	-2.65720000	0.15668800
C	-0.90243900	-3.21788500	1.37082400
H	0.68798000	-3.33072700	2.77670700
H	1.60552300	-1.16819200	1.76143100
C	-1.05914200	-1.19235000	-1.81773800
C	-0.27578700	-0.26953300	-2.48852200
C	0.97103700	0.04662400	-1.97864700
H	-2.03998400	-1.47549700	-2.20570700
H	-0.61842600	0.21000200	-3.40569900
H	1.65109700	0.74593800	-2.46027100
N	1.43899500	-0.52485100	-0.85211700
C	-2.87450200	1.53539400	-0.90578500
C	-1.74399600	2.27449000	-0.52307600
C	-0.98324200	1.93707400	0.62680600
C	-1.37474300	0.83935800	1.35949600
C	-2.55567500	0.02700300	1.01553300
C	-3.31298400	0.45268200	-0.17664300
H	-2.22288400	-1.06208500	0.82533100
H	-3.21316800	-0.14055400	1.89222000
H	-1.53598200	-3.91130700	1.92875500
C	-4.52897300	-0.33679000	-0.54316200
H	-5.03376000	0.06713700	-1.43143200
H	-4.26367800	-1.39108900	-0.74195400
H	-5.25507500	-0.35648000	0.28642100
C	0.14738900	2.87121600	1.04670300

H	-0.34629500	3.84415800	1.22885700
C	0.84472800	2.46045900	2.34075500
H	0.14282700	2.39005100	3.18496500
H	1.36103600	1.49702500	2.21848700
H	1.60956400	3.20483800	2.60611700
C	1.17923800	3.09107100	-0.06522800
H	1.89292500	3.87332000	0.23235200
H	1.75978000	2.18053000	-0.25133600
H	0.71760900	3.40814200	-1.01143400
H	-0.83585600	0.56639400	2.26865100
H	-3.43143100	1.84157500	-1.79605500
B	3.00646900	-0.18644600	-0.42641100
F	3.46095600	0.72779400	-1.34920700
F	3.67778000	-1.38598400	-0.48766600
F	2.97411200	0.34291200	0.85166900
H	-1.47147600	3.15795600	-1.10425500
H	2.19277600	-2.51873700	0.85120800
H	-2.33702400	-3.02430100	-0.27297000

MECP-1-E

C	0.55395400	-0.34376800	2.28664600
C	-0.49412200	-0.85818300	1.47114900
C	-1.47626900	0.02834400	0.94151600
C	-1.45249700	1.40914300	1.29356200
C	-0.49848800	1.90826000	2.35304400
C	0.62168900	0.96142600	2.65043300
H	1.35327400	-1.03007100	2.57794300
C	-2.33739200	2.27156900	0.67230400
C	-3.25256500	1.79155600	-0.27058400
C	-3.25001700	0.43985500	-0.55202400
H	-2.31750400	3.33522200	0.92445800
H	-3.96357000	2.45078100	-0.76750900
H	-3.93843600	-0.01557500	-1.26299600
N	-2.39184600	-0.41282600	0.02638400
C	2.46924300	-1.67585200	-0.51511100
C	1.41788900	-0.72308000	-0.89742600
C	1.77369200	0.70639400	-0.85698600
C	2.97603600	1.07827800	-0.28817300
C	3.90104200	0.12390600	0.16351800
C	3.65805000	-1.27169300	0.03378200
H	1.46214400	1.32974700	3.24211400
C	4.71147200	-2.25679600	0.46718100
H	4.35822200	-3.29178500	0.36447800
H	5.62466800	-2.14907500	-0.13910300
H	4.99523400	-2.09626900	1.51877400
C	0.80341400	1.67632100	-1.48951500
H	-0.20962000	1.29469800	-1.27169300
C	0.89549700	3.10231700	-0.95190200
H	0.83503600	3.12573700	0.14536100
H	1.83880300	3.58787700	-1.24852000
H	0.07435800	3.71347500	-1.35509100
C	0.97353800	1.66176300	-3.01780000
H	0.21634500	2.29915500	-3.49962700
H	1.96977900	2.04159500	-3.29441800
H	0.87097500	0.64707400	-3.42893500
H	3.23626800	2.13595800	-0.20722400
H	2.25049900	-2.74068200	-0.63575100
B	-2.44324300	-1.98602400	-0.46220300
F	-3.54107900	-2.09363900	-1.28688300
F	-2.55451400	-2.76210300	0.66989000
F	-1.25582300	-2.21567500	-1.14129000
H	0.86871600	-1.02160800	-1.80643000
H	-0.11097800	2.90031800	2.06601900
H	-1.06933900	2.09346500	3.28651200
H	-0.60260800	-1.92790100	1.31273500
H	0.56917900	-0.86050100	-0.13006800
H	4.84543200	0.46247000	0.59815100

MECP-1-F

C	0.79132000	-2.50665700	-1.23900400
C	-0.45263000	-1.87234100	-1.05462700
C	-0.79025900	-1.33140500	0.21795300
C	0.12545600	-1.42397400	1.30123900
C	1.49695800	-2.01205200	1.10255400
C	1.73992900	-2.56397700	-0.25699100
H	1.00702700	-2.94230400	-2.21712400
H	-1.18938400	-1.85358100	-1.85321300
C	-0.26444400	-0.95662000	2.54788400

H	1.69200000	-2.78249400	1.87067800
C	-1.52549000	-0.38971200	2.72777400
C	-2.34951100	-0.26794400	1.62277200
H	0.43033200	-1.03189500	3.38868800
H	-1.85887800	-0.02159700	3.69761000
H	-3.32862700	0.20639800	1.67289700
N	-1.99377200	-0.70876200	0.41213300
C	2.60473300	0.19594500	-1.44037800
C	1.29821500	0.90039900	-1.41135800
C	1.00029800	1.66738100	-0.16368200
C	1.90250100	1.63710200	0.86925000
C	3.12202500	0.92471800	0.78233400
C	3.48699900	0.21923600	-0.39333600
H	2.69541400	-3.05825700	-0.44397300
C	4.78660500	-0.53938300	-0.42848500
H	4.99020500	-0.94995600	-1.42691700
H	5.63283000	0.10240400	-0.14115700
H	4.76286500	-1.38018100	0.28449900
C	-0.30437900	2.43081900	-0.12490500
H	-1.07977200	1.72548600	-0.46692000
C	-0.69220400	2.93595600	1.26242600
H	-0.68152000	2.13055800	2.01059400
H	-0.01392000	3.73306400	1.60744500
H	-1.70810500	3.35676200	1.23704900
C	-0.30394100	3.59492100	-1.12913900
H	-1.28242600	4.09761800	-1.12334200
H	0.46662100	4.33732000	-0.86630700
H	-0.11921200	3.25621800	-2.15817100
H	1.68692000	2.17657700	1.79344200
H	2.86489300	-0.34234700	-2.35588000
B	-3.01561700	-0.41528700	-0.84788200
F	-4.05677800	0.32251200	-0.33047600
F	-3.41444500	-1.63511800	-1.34174500
F	-2.27245800	0.30996500	-1.76888700
H	2.24699100	-1.21313300	1.31273900
H	1.19222900	1.54694300	-2.30400400
H	0.47073100	0.16000300	-1.57341100
H	3.81731100	0.95343000	1.62554500

MECP-1-G

C	-3.36305200	0.85711500	-1.31051900
C	-2.01023600	1.21419400	-0.99883600
C	-1.45733100	0.85442000	0.24357300
C	-2.19348000	0.02240000	1.14592800
C	-3.62583500	-0.35897700	0.84504500
C	-4.13887000	0.13589900	-0.47049800
H	-3.77131100	1.19918400	-2.26473100
C	-1.59007000	-0.39978700	2.31401000
C	-0.27637700	-0.02096900	2.61207500
C	0.37100200	0.82214000	1.73022300
H	-2.14826700	-1.03650300	3.00572100
H	0.22008500	-0.33050100	3.53088100
H	1.37169100	1.20026900	1.92498000
N	-0.18188700	1.24248500	0.58798200
C	0.01508300	-2.65094800	0.37601800
C	1.32166400	-2.20099400	0.63482800
C	2.02871900	-1.37439600	-0.28264300
C	1.36239600	-0.94012700	-1.39689900
C	-0.04062000	-1.30110300	-1.68174100
C	-0.66589600	-2.27069800	-0.75546100
H	-0.66824300	-0.35188300	-1.65484500
H	-0.17386500	-1.60213400	-2.73837100
H	-5.17175200	-0.10158400	-0.73449800
C	-2.01349400	-2.80963900	-1.11511000
H	-2.47578500	-3.35727300	-0.28184700
H	-2.69016200	-1.99999100	-1.42924700
H	-1.93058500	-3.50364500	-1.96946800
C	3.49322100	-1.06280400	-0.00303900
H	3.97692900	-2.04446400	0.15419000
C	4.20414000	-0.37463700	-1.16525600
H	4.13846500	-0.96366000	-2.09224300
H	3.77504100	0.62197300	-1.35230100
H	5.26951700	-0.23909900	-0.92766000
C	3.67693700	-0.24711200	1.28235400
H	4.74347800	-0.18149800	1.54528000
H	3.30087600	0.77497200	1.13299100
H	3.14934800	-0.69616200	2.13780500
H	1.84962900	-0.28224200	-2.11522600

H	-0.46019400	-3.33544000	1.08405600
B	0.63665200	2.34656700	-0.29986200
F	1.89066700	2.46207500	0.27962600
F	-0.08961000	3.51098300	-0.23425100
F	0.73413300	1.86945000	-1.60223500
H	1.83402400	-2.56233800	1.53046200
H	-3.72819600	-1.45990800	0.89437100
H	-4.27529700	0.01503500	1.65955900
H	-1.44959300	1.86023000	-1.66898300

MECP-1-H

C	-0.25122000	2.43725600	0.49376500
C	0.98325300	1.84824900	0.15003600
C	1.38491100	0.63252900	0.76855300
C	0.54233000	0.00561000	1.72677400
C	-0.79997200	0.58949500	2.07456500
C	-1.12037300	1.86126700	1.37605500
H	-0.52057100	3.38182700	0.01538300
H	1.66204500	2.34669300	-0.53676200
C	0.96511000	-1.17519400	2.31988000
H	-0.89128800	0.71456000	3.16962200
C	2.19012200	-1.74359800	1.97457600
C	2.95367400	-1.10686800	1.01212300
H	0.32064100	-1.66375300	3.05534400
H	2.54362500	-2.66972500	2.42718200
H	3.90689500	-1.50303800	0.66445000
N	2.56558000	0.02889400	0.42408300
C	-1.28756500	-2.14653600	-0.16800300
C	-2.50215300	-1.53309200	0.20476200
C	-2.93180600	-0.30957400	-0.38581500
C	-2.10169800	0.30241100	-1.28405400
C	-0.78786100	-0.26094300	-1.68719000
C	-0.44052200	-1.57965900	-1.08798600
H	-0.69230500	-0.29936500	-2.79068500
H	0.02337300	0.47052500	-1.42389400
H	-2.06886300	2.34721900	1.61484100
C	0.81757100	-2.24118600	-1.55272200
H	1.14482100	-3.03012600	-0.86046600
H	0.66020300	-2.70497900	-2.54250900
H	1.62575500	-1.50602100	-1.67807500
C	-4.27674900	0.26258700	0.03761500
H	-4.27335800	0.27011700	1.14387800
C	-4.52248800	1.69538800	-0.42889800
H	-3.71020700	2.37049600	-0.12262200
H	-4.61319200	1.74904100	-1.52542800
H	-5.46180000	2.07833300	-0.00325800
C	-5.42308200	-0.65287200	-0.41276000
H	-6.39172900	-0.27435600	-0.05184500
H	-5.46347700	-0.70229200	-1.51232600
H	-5.30148200	-1.67945900	-0.03726300
H	-2.39102700	1.24625500	-1.74970100
H	-1.01536900	-3.10177200	0.28987600
B	3.48996200	0.60721000	-0.80975100
F	4.57090500	-0.24022900	-0.90842100
F	3.85009000	1.89601600	-0.49171100
F	2.67622100	0.54608200	-1.93354000
H	-1.57572400	-0.17231400	1.82047800
H	-3.14967800	-2.03460900	0.92934700

MECP-1-I

C	0.09161400	-2.37598900	-1.69183000
C	-1.01118300	-1.65548400	-1.15154000
C	-0.95313500	-1.17789400	0.18368000
C	0.19559000	-1.44645800	0.98570100
C	1.23815200	-2.42898800	0.51055500
C	1.19242800	-2.68748700	-0.96123600
H	0.04957400	-2.65580600	-2.74730200
H	-1.90945000	-1.50226900	-1.74227800
C	0.30652700	-0.83844300	2.22068100
H	1.09662700	-3.38928200	1.04869600
C	-0.70461900	0.00733000	2.68955800
C	-1.81416500	0.19778300	1.89185700
H	1.19340700	-1.02570600	2.83199800
H	-0.64581200	0.49001100	3.66437500
H	-2.65579400	0.81930800	2.19427900
N	-1.93697300	-0.36464100	0.68064900
C	0.57848000	2.51652400	0.37393900
C	1.84901100	1.97568200	0.62275500

C	2.45784200	1.04857000	-0.26062200
C	1.72993600	0.63358200	-1.35218400
C	0.36076500	1.11229900	-1.62959000
C	-0.15713500	2.17322600	-0.73957600
H	0.22379300	1.36402900	-2.69759700
H	-0.34380600	0.20741800	-1.55827600
H	2.02602900	-3.23080800	-1.41387200
C	-1.45093200	2.85481300	-1.05839900
H	-1.45886000	3.88181600	-0.66547500
H	-1.62863400	2.88754900	-2.14274800
H	-2.30539800	2.31821000	-0.62042300
C	3.90607800	0.63837900	-0.00920100
H	4.49074300	1.57430700	-0.06833900
C	4.11925900	0.07493700	1.40108500
H	3.75369000	0.75654700	2.18210500
H	3.59689000	-0.88518500	1.52507600
H	5.18902200	-0.10171000	1.59028200
C	4.46935800	-0.31348500	-1.06191200
H	5.51698500	-0.55890900	-0.83431400
H	3.90286000	-1.25781500	-1.09021200
H	4.44257400	0.12815800	-2.06918600
H	2.16561200	-0.05238900	-2.07949600
H	0.18549900	3.27382300	1.05758700
B	-3.35144500	-0.13820100	-0.12410400
F	-4.02758300	0.84728300	0.57332900
F	-3.99764400	-1.34809600	-0.11885900
F	-3.04545900	0.28949100	-1.40990200
H	2.23836600	-2.08483200	0.81559600
H	2.40506400	2.33554600	1.49207400

TS-2-A

C	-2.75942800	-0.66523900	1.78254900
C	-2.90784500	-0.04520500	0.52437800
C	-1.98465700	0.92058700	0.04801500
C	-0.87167700	1.23527900	0.88346200
C	-0.62538800	0.47831700	2.06354700
C	-1.66676700	-0.39124800	2.56548300
H	-2.96941100	1.38605400	-1.83214300
H	-3.52875400	-1.35490800	2.13319400
H	-3.77458600	-0.28136600	-0.09643200
H	0.12599400	0.85194800	2.76781400
C	-0.10477000	2.84446800	-0.74077200
C	-1.14917800	2.55140600	-1.57329600
H	0.77112000	2.43389600	1.08522700
H	0.66399000	3.58394100	-0.95907900
H	-1.23228800	3.07559500	-2.52552800
C	1.72878900	-0.58338700	-0.10715000
C	0.89628600	-1.44459800	0.73505200
C	-0.16168400	-2.22193800	0.13031400
C	-0.56272100	-2.01304200	-1.15429000
C	0.15484900	-1.01766900	-2.00471900
C	1.34596800	-0.37065600	-1.38850700
H	1.37926700	-1.88718000	1.61676500
H	0.18955800	-0.54104000	1.40749500
H	0.43798900	-1.48848100	-2.96605000
H	-0.56862800	-0.23182300	-2.31474400
H	-1.53483000	-0.86262000	3.54027300
C	2.95223000	0.04178200	0.53579500
H	2.62748500	0.40142300	1.53234500
C	-1.70136300	-2.75477700	-1.77500600
H	-2.18605800	-3.43679800	-1.06457400
H	1.92956500	0.28914900	-2.03420900
H	-0.67942700	-2.96081500	0.74654700
C	4.04015400	-1.01730000	0.77011500
H	4.40382500	-1.41025000	-0.19138500
H	4.89520300	-0.58028500	1.30559400
H	3.67451900	-1.86746400	1.36401900
C	3.52051500	1.23356200	-0.23127200
H	4.33049700	1.70499600	0.34291800
H	3.94804500	0.92257300	-1.19677300
H	2.75771100	2.00003700	-0.43711900
H	-2.45732300	-2.04685200	-2.15368100
H	-1.35873000	-3.34100100	-2.64277100
C	-2.11324900	1.59691100	-1.18969800
N	-0.00358800	2.19682000	0.47547000

TS-2-B

C	-0.24483500	-2.21272800	1.34687500

C	0.92300200	-1.50967800	1.71544200
C	1.85379300	-1.03856800	0.75592200
C	1.54549800	-1.25641800	-0.62014800
C	0.29183600	-1.81433600	-0.99449700
C	-0.54640000	-2.40584400	0.02354600
H	3.31748400	-0.21223200	2.13137600
H	-0.89329100	-2.61669600	2.12606300
H	1.14932500	-1.35361600	2.77232100
H	0.16019700	-2.14016900	-2.03203200
C	3.60626800	-0.16402200	-1.24948200
C	3.91967800	0.07130800	0.05965300
H	2.23755500	-1.03532700	-2.53218800
H	4.22718000	0.13398300	-2.09259700
H	4.84540100	0.59507800	0.29812000
C	-0.84019200	1.22003000	0.01979000
C	-1.21843900	0.53243100	-1.21176900
C	-2.56265400	-0.00680800	-1.34474900
C	-3.38870700	-0.13853100	-0.27873200
C	-2.93591300	0.32846900	1.06923600
C	-1.64831600	1.07481800	1.10395000
H	-0.75884400	0.91097700	-2.13569600
H	-0.48063200	-0.55115100	-1.10952200
H	-3.72889800	0.94363100	1.53591900
H	-2.86810000	-0.54781600	1.74760500
H	-1.44382700	-2.94479100	-0.28224600
C	0.42541100	2.05446500	0.01214000
H	1.19587400	1.45665300	-0.50794600
C	-4.76125400	-0.72411900	-0.37855500
H	-4.98665100	-1.07316000	-1.39453500
H	-1.38131900	1.54586000	2.05245500
H	-2.88614900	-0.34922900	-2.33119900
C	0.21010900	3.33404800	-0.81206000
H	-0.55063400	3.97387000	-0.33964900
H	1.14522400	3.90891500	-0.87621800
H	-0.12173500	3.12008200	-1.83865900
C	0.95655400	2.39109400	1.40216500
H	1.93625800	2.88292200	1.32209300
H	0.28670800	3.08649200	1.93162900
H	1.07897500	1.49162900	2.02315200
H	-4.87416600	-1.57283300	0.31553200
H	-5.52137100	0.02021900	-0.09153100
N	2.43406800	-0.83332500	-1.55851600
C	3.06072300	-0.37561300	1.08416600

TS-2-C

C	-1.43484800	3.02637600	0.92681800
C	-2.43405300	2.04650800	1.08194200
C	-2.54489300	0.93544600	0.20954500
C	-1.58149900	0.82410600	-0.84023300
C	-0.49087500	1.72612800	-0.90272300
C	-0.49204600	2.90047600	-0.06518700
H	-4.29500200	0.01635000	1.10991500
H	-1.42180900	3.88957400	1.59388200
H	-3.17078800	2.14827700	1.88150300
H	0.15884700	1.70460100	-1.78385900
C	-2.67372600	-1.18620200	-1.61985800
C	-3.59156900	-1.11906500	-0.61146700
H	-1.03106200	-0.26720300	-2.48185100
H	-2.65390800	-1.96590900	-2.37922800
H	-4.36122600	-1.88784500	-0.54225200
C	2.54275700	1.03965600	0.57060300
C	1.29267900	0.32578600	0.77118500
C	1.19065900	-1.07354200	0.34901300
C	2.16720100	-1.57283800	-0.45020000
C	3.37560600	-0.79790000	-0.84887300
C	3.53729300	0.54519500	-0.21013400
H	0.73476300	0.59368700	1.68266600
H	0.47745200	0.92849900	-0.00621900
H	4.27991500	-1.40757600	-0.65697900
H	3.39549700	-0.67661000	-1.95264200
H	0.29281600	3.64580600	-0.20060700
C	4.81901500	1.27555900	-0.45289000
H	4.82397300	2.26620600	0.01954000
H	5.67131900	0.69907400	-0.05838400
H	4.99752900	1.40173600	-1.53300900
C	0.00925700	-1.87974100	0.85152500
H	-0.87604200	-1.22286800	0.78756400
C	-0.27969000	-3.13491000	0.03280100

H	-0.37402200	-2.91215100	-1.04064200
H	0.51129400	-3.89100700	0.15608000
H	-1.22117100	-3.59389400	0.36597400
C	0.20294600	-2.22817300	2.33569200
H	-0.68373100	-2.74923500	2.72468600
H	1.07272900	-2.88964700	2.46753200
H	0.36264900	-1.33374100	2.95566800
H	2.11131200	-2.60477800	-0.80454000
H	2.65356200	2.02196900	1.03750500
N	-1.69060900	-0.21415000	-1.71472300
C	-3.55098600	-0.05524100	0.31590100

TS-2-D

C	0.82784700	-2.74315500	-0.14662100
C	-0.17259200	-2.30498900	-1.03691500
C	-1.28286100	-1.53729700	-0.60105500
C	-1.34075100	-1.19033000	0.78119200
C	-0.23237600	-1.45702700	1.63388200
C	0.79720800	-2.36362700	1.17165700
H	-2.31940500	-1.38701900	-2.50478200
H	1.62306000	-3.39426200	-0.51262000
H	-0.12655800	-2.59458900	-2.08873900
H	-0.37778800	-1.34717300	2.71439900
C	-3.45426400	-0.08544800	0.41830300
C	-3.41492300	-0.37879300	-0.91637200
H	-2.48076500	-0.30463900	2.22780400
H	-4.26226200	0.46029000	0.90261500
H	-4.23357800	-0.04962000	-1.55682500
C	-0.16619200	1.89423600	1.14144600
C	0.98754100	1.01490900	1.18199600
C	1.70601100	0.72349700	-0.05510100
C	1.10666600	1.04148900	-1.23265900
C	-0.19421600	1.75829200	-1.32200800
C	-0.75817700	2.24957800	-0.02790700
H	1.59049500	1.04822900	2.09944300
H	0.43729800	-0.18314500	1.41173900
H	-0.10769300	2.59966300	-2.03572900
H	-0.94769500	1.09700300	-1.80596400
H	1.56255100	-2.69428800	1.87503400
C	-1.94531900	3.15710000	-0.09626900
H	-2.35456800	3.37827500	0.89849500
H	-1.66884100	4.11258800	-0.57159900
H	-2.74042300	2.71413500	-0.71663900
C	3.07861700	0.09220000	0.05758200
H	3.00047000	-0.68135800	0.84317400
C	3.55985600	-0.58627600	-1.22147800
H	2.82826500	-1.31592800	-1.59832000
H	3.75493500	0.14744400	-2.01903400
H	4.50449600	-1.11644500	-1.03532600
C	4.09834700	1.13672900	0.53951300
H	5.08074900	0.66853400	0.69623500
H	4.21673300	1.93425100	-0.20978200
H	3.79785600	1.60718800	1.48731900
H	1.60035300	0.80364300	-2.17743500
H	-0.57245800	2.25895000	2.08907400
C	-2.33724000	-1.11713600	-1.44796900
N	-2.42633300	-0.51220700	1.23716400

TS-2-E

C	2.41106500	2.84615400	-0.39410800
C	3.37293900	1.82874200	-0.54882300
C	3.21236200	0.54344600	0.02407600
C	2.02047000	0.30194800	0.77374100
C	1.00005000	1.28349700	0.82933900
C	1.25332800	2.60282400	0.30408100
H	5.07762800	-0.33370900	-0.66409800
H	2.59828200	3.83073800	-0.82503100
H	4.28533100	2.03010000	-1.11402100
H	0.17894600	1.14717400	1.54156200
C	2.76329200	-1.95568900	1.21833300
C	3.90565200	-1.75637800	0.49768500
H	1.01862800	-1.07662200	1.90568700
H	2.50896200	-2.88742900	1.72055000
H	4.62147900	-2.57280800	0.40088700
C	-1.94660300	0.83090900	-0.81957100
C	-0.65083400	0.30350500	-1.22076700
C	-0.42078200	-1.14245300	-1.13754400
C	-1.30679600	-1.89634100	-0.43979800

C	-2.54356300	-1.34341600	0.18055200
C	-2.85434500	0.08627400	-0.13827500
H	-0.16901500	0.81331600	-2.06909900
H	0.14422700	0.75992700	-0.33678700
H	-2.16823500	1.87612700	-1.05247000
H	-1.14296700	-2.97438400	-0.34837900
H	-3.40544700	-1.98292500	-0.08865700
H	-2.48925100	-1.46345300	1.28298200
C	0.78182200	-1.71590800	-1.82548800
H	0.93360000	-2.77252400	-1.56899100
H	0.66354800	-1.64202400	-2.91810700
H	1.69846600	-1.16252300	-1.56855900
C	-4.19640200	0.64671900	0.27163600
H	-4.15360000	1.73306800	0.09088700
C	-4.48584000	0.42831600	1.76131900
H	-5.41013500	0.95094700	2.04576400
H	-4.63113600	-0.63776700	1.99664400
H	-3.67371100	0.81640100	2.39501700
C	-5.32164300	0.07800500	-0.60609700
H	-6.27558700	0.56365400	-0.35494400
H	-5.12389300	0.24884100	-1.67405900
H	-5.45379200	-1.00398200	-0.44872900
H	0.49751000	3.37796200	0.43755700
C	4.15816300	-0.50365100	-0.10302400
N	1.85088100	-0.91958800	1.35011400

TS-2-F

C	0.05621400	-1.61774300	2.19754600
C	0.96578000	-0.55453000	2.03163500
C	1.77581700	-0.42462700	0.87109100
C	1.62583500	-1.41202700	-0.14601600
C	0.60211200	-2.39443800	-0.04916300
C	-0.10198600	-2.55272800	1.20508200
H	2.86117600	1.36232200	1.45906300
H	-0.50478200	-1.70389400	3.12930300
H	1.08958900	0.17962700	2.83072100
H	0.63131200	-3.24318900	-0.74102900
C	3.31281400	-0.29483100	-1.46773400
C	3.47395600	0.66617900	-0.51000400
H	2.32943800	-2.04623100	-1.95954700
H	3.87082400	-0.32997100	-2.40195100
H	4.19950700	1.46303100	-0.67410700
C	-0.68285800	0.45155200	-1.23508000
C	-1.32961000	-0.83812000	-1.34685300
C	-2.55616600	-1.08734800	-0.58802600
C	-2.93656500	-0.18239900	0.34339600
C	-2.19224400	1.07904700	0.61474900
C	-1.03582300	1.36321500	-0.28822400
H	-1.25952600	-1.33331000	-2.32641000
H	-0.44619900	-1.61134200	-0.73944400
H	0.15518900	0.67166700	-1.90337000
H	-3.83932900	-0.36220000	0.93396800
H	-2.89135600	1.93765400	0.59795400
H	-1.83542800	1.06806100	1.66418800
C	-3.30104800	-2.36206500	-0.85180600
H	-4.16751300	-2.47225400	-0.18710500
H	-3.65863900	-2.39927200	-1.89251300
H	-2.64497200	-3.23639000	-0.70644900
C	-0.32668300	2.69202800	-0.18127800
H	0.65062800	2.56855100	-0.67762400
C	-0.07072900	3.11534800	1.26758800
H	0.55774600	4.01688600	1.29186200
H	-1.00635600	3.35783900	1.79458900
H	0.44736400	2.32749500	1.83450200
C	-1.10441900	3.77500500	-0.94711000
H	-0.55869500	4.72901800	-0.91158300
H	-1.24382700	3.49910200	-2.00199300
H	-2.09797100	3.94402200	-0.50331200
H	-0.79699900	-3.38563500	1.31854300
N	2.39912000	-1.31453500	-1.26138200
C	2.71976800	0.61184200	0.68044300

TS-2-G

C	-3.43097800	-0.02909800	-0.54251400
C	-2.52791500	0.77269800	-1.26744900
C	-1.45474000	1.45370700	-0.63718900
C	-1.28627400	1.26177600	0.76620300
C	-2.07354500	0.29794600	1.45764100

C	-3.24616900	-0.23988800	0.80108300
H	-0.69250500	2.50135500	-2.38083400
H	-4.28468700	-0.47311700	-1.05671600
H	-2.67523400	0.92195100	-2.33898000
H	-2.05217500	0.30857800	2.55310200
C	0.56992100	2.80201900	0.75611100
C	0.44253200	2.99615700	-0.59134900
H	-0.20902100	1.83334300	2.40602600
H	1.31652300	3.29258900	1.37834400
H	1.12456300	3.68084900	-1.09599600
C	1.01222400	-1.16936100	1.22362100
C	-0.28020200	-1.81024100	1.06759600
C	-0.69556600	-2.24136200	-0.26434500
C	-0.01516300	-1.76030100	-1.33703400
C	1.20241800	-0.91209400	-1.22137500
C	1.74536200	-0.74315400	0.16092400
H	-0.61277100	-2.43801800	1.90581800
H	-1.15613500	-0.82204400	1.26732300
H	1.40885300	-1.04800400	2.23612700
H	-0.33690800	-2.03540700	-2.34559600
H	1.98912600	-1.30123900	-1.89449100
H	0.99019300	0.09654100	-1.64247100
C	-1.84757300	-3.19372900	-0.38605000
H	-2.21673400	-3.25733800	-1.41809700
H	-1.53581300	-4.20251800	-0.07117400
H	-2.68418500	-2.89768700	0.26377900
C	3.15279600	-0.21569300	0.33573300
H	3.21301300	0.21481900	1.34964800
C	3.53895100	0.87079900	-0.66988000
H	4.53450000	1.26894100	-0.42754600
H	3.59071300	0.47699400	-1.69661900
H	2.82772400	1.70807000	-0.66018100
C	4.14437900	-1.39084400	0.27569500
H	5.17111900	-1.03000800	0.43404300
H	3.92241500	-2.14428100	1.04454600
H	4.11341700	-1.88707000	-0.70711100
H	-3.93863900	-0.85271000	1.37988900
N	-0.30047000	1.94646200	1.40283900
C	-0.56780100	2.32735800	-1.31120700

TS-2-H

C	-0.36730500	-2.12343300	2.14207500
C	-0.22711800	-2.35571100	0.75809600
C	-0.98183200	-1.63866500	-0.20622500
C	-1.89202500	-0.65036800	0.27322500
C	-1.89966100	-0.29100900	1.65180800
C	-1.21090900	-1.14295700	2.59837900
H	-0.22543900	-2.62530700	-1.98836300
H	0.18977300	-2.74226500	2.84713500
H	0.45064900	-3.13673800	0.40768000
H	-2.72774000	0.32646100	2.01725300
C	-2.57660400	-0.17768200	-1.99025900
C	-1.69805600	-1.10249400	-2.48354300
H	-3.34128200	0.68143300	-0.27477300
H	-3.24049000	0.42674800	-2.60602600
H	-1.63687900	-1.25524700	-3.56121700
C	-0.42805100	2.32713500	0.14118500
C	0.05512100	1.67109800	1.35630100
C	1.24261700	0.85151100	1.28641900
C	1.80800400	0.49220500	0.09931800
C	1.22408300	0.99149000	-1.18099000
C	0.11463600	1.97506700	-1.04780500
H	-0.11767600	2.20104100	2.30314700
H	-0.89376800	0.74463400	1.54064400
H	2.02360000	1.40690600	-1.82363700
H	0.86131900	0.11829400	-1.76639100
H	-1.33190400	-0.94978100	3.66509100
C	-1.54157000	3.32476900	0.27404200
H	-1.20948900	4.20881600	0.84012900
H	-1.90433000	3.66591900	-0.70474100
H	-2.39206400	2.89994100	0.83408800
C	3.06534300	-0.34334300	0.04803900
H	3.14667700	-0.85735600	1.01996100
C	4.29881100	0.56254300	-0.10035700
H	4.35938200	1.29468300	0.71731500
H	5.21657300	-0.04307100	-0.08589500
H	4.27997000	1.11410900	-1.05336600
C	3.02763900	-1.40875000	-1.05122600

H	2.12568300	-2.03454100	-0.97926500
H	3.05427300	-0.96047800	-2.05647000
H	3.90242500	-2.06891600	-0.96725700
H	-0.25415600	2.43581100	-1.96879500
H	1.67800000	0.49042000	2.22179900
N	-2.67092100	0.00628300	-0.62478700
C	-0.89923400	-1.85898900	-1.60256900

TS-2-I

C	-0.21488000	-2.10044300	-0.65578200
C	-1.31036800	-1.54088900	-1.34864600
C	-2.34687600	-0.84039900	-0.67995100
C	-2.22252500	-0.67539700	0.73234200
C	-1.02659000	-1.06760700	1.39671700
C	-0.08215600	-1.91030200	0.69529500
H	-3.60813700	-0.44334100	-2.40238600
H	0.51668200	-2.69756400	-1.20289500
H	-1.39933400	-1.68425400	-2.42749300
H	-1.02935400	-1.09082900	2.49193900
C	-4.35057600	0.46685900	0.78157200
C	-4.48357200	0.34604300	-0.57329200
H	-3.16274300	0.01292500	2.41246500
H	-5.08036300	0.94879100	1.42992000
H	-5.36847800	0.75776100	-1.05869300
C	0.09470900	1.63578600	-0.29509600
C	0.50572000	1.25763000	1.05259700
C	1.84963500	0.74548100	1.26283000
C	2.64776100	0.36547200	0.23468700
C	2.16201300	0.52096200	-1.17294200
C	0.87056100	1.24053300	-1.33923500
H	0.07900600	1.85384900	1.87176000
H	-0.25327400	0.18386400	1.23005800
H	2.93681100	1.01740300	-1.78705100
H	2.07694700	-0.48151300	-1.63915600
H	0.76187500	-2.32586400	1.24667200
C	-1.16268000	2.43442500	-0.47241000
H	-1.00422300	3.46909900	-0.12864300
H	-1.47991900	2.46790200	-1.52277800
H	-1.99230700	2.02510700	0.12328800
C	4.03057500	-0.19867900	0.46582900
H	4.14214200	-0.32314400	1.55527700
C	5.12251700	0.77384200	-0.00130200
H	5.00659100	1.76221500	0.46641300
H	6.11467900	0.38455600	0.26910300
H	5.11105900	0.90617000	-1.09459800
C	4.19698800	-1.57893500	-0.18241100
H	3.40353000	-2.27369400	0.13345000
H	4.18450100	-1.51644400	-1.28198700
H	5.16207300	-2.01932400	0.10618300
H	0.56396500	1.48660800	-2.36012300
H	2.20041900	0.63136600	2.29218800
C	-3.49395900	-0.31961100	-1.32483700
N	-3.22856200	-0.05432500	1.40304200

TS-2-J

C	1.21423600	-2.88814500	-0.44143100
C	2.32167200	-2.38936900	0.26688800
C	2.72157100	-1.05001100	0.13505400
C	1.99706300	-0.15064700	-0.70116100
C	0.81333100	-0.65433700	-1.32884500
C	0.48829400	-2.04548700	-1.25748500
H	4.35285300	-1.21778200	1.37124500
H	0.94866100	-3.94201600	-0.35142900
H	2.89706900	-3.05660200	0.91331500
C	2.42755300	1.19064100	-0.79805200
H	0.34004300	-0.03825600	-2.09914500
C	3.56485900	1.61495800	-0.08132000
C	4.25211600	0.73054800	0.70707500
H	1.88844400	1.88519100	-1.44342200
H	3.91656900	2.64442300	-0.15217700
H	5.14155000	0.98940600	1.27945000
N	3.82336800	-0.57121800	0.79764900
C	-2.26586000	-0.13233800	0.16218000
C	-0.95357800	0.25051800	0.68321300
C	-0.59762300	1.65427100	0.75874900
C	-1.33135900	2.61492300	0.13339500
C	-2.57337600	2.23136900	-0.60583700
C	-3.00133700	0.81026500	-0.47979300

H	-0.54267000	-0.39357100	1.47638000
H	-0.17703000	-0.20041500	-0.23396500
H	-3.40497200	2.89674600	-0.30125700
H	-2.44487100	2.48377800	-1.68038800
H	-0.36413300	-2.42126800	-1.82654900
C	-2.70266700	-1.56780400	0.36162600
H	-1.78720900	-2.18210900	0.27840500
C	-0.96171200	4.06300800	0.16381800
H	-0.01254300	4.23341500	0.68833300
H	-3.96791700	0.54893000	-0.91673800
H	0.31003800	1.92986600	1.30138000
C	-3.24542700	-1.75539100	1.78713700
H	-4.16781000	-1.17173300	1.92859600
H	-3.47978600	-2.81354500	1.97313300
H	-2.52166400	-1.43160000	2.54992100
C	-3.69840600	-2.06760800	-0.68233900
H	-3.88330200	-3.14248200	-0.54487900
H	-4.67187700	-1.56143700	-0.59097800
H	-3.32880600	-1.91396600	-1.70757300
H	-0.87460100	4.46499500	-0.85880900
H	-1.74571900	4.65237000	0.66638500

TS-2-K

C	-0.21874800	-2.21608400	1.35183200
C	0.95177500	-1.49549200	1.67531200
C	1.82660200	-1.04956200	0.67299100
C	1.52946700	-1.26738300	-0.70349600
C	0.26153400	-1.86767000	-1.00869700
C	-0.54356900	-2.43158100	0.03392300
H	3.21266600	-0.25830900	1.96508900
H	-0.84521800	-2.60698900	2.15454700
H	1.20586600	-1.31624600	2.72298300
C	2.43723400	-0.81031300	-1.68082000
H	0.09020900	-2.19304600	-2.03910600
C	3.60946600	-0.13508000	-1.28719700
C	3.87250500	0.06791600	0.04188700
H	2.23025900	-0.98852700	-2.73685900
H	4.31967600	0.22811600	-2.03008600
H	4.76035300	0.57576600	0.41553800
N	2.99115000	-0.39655300	0.98577000
C	-0.82623800	1.20296100	0.02412800
C	-1.21569600	0.52345900	-1.20892000
C	-2.57488000	0.02095300	-1.34446700
C	-3.39355800	-0.11861600	-0.27382600
C	-2.91097000	0.29839400	1.08065700
C	-1.62937400	1.05414900	1.11338000
H	-0.74121300	0.88880000	-2.13034300
H	-0.53019400	-0.58211100	-1.10381000
H	-3.69711200	0.87750600	1.60071600
H	-2.80922700	-0.60980200	1.71424400
H	-1.44696500	-2.98195800	-0.23458400
C	0.43376600	2.04487300	0.01213700
H	1.19693400	1.46231500	-0.53291100
C	-4.77961900	-0.67194900	-0.37086800
H	-5.02184300	-0.99628000	-1.39114300
H	-1.35909800	1.52112900	2.06299700
H	-2.91125700	-0.29473100	-2.33539500
C	0.19484900	3.33608400	-0.78751600
H	-0.56521300	3.96144000	-0.29489600
H	1.12389900	3.92013000	-0.85699100
H	-0.14857000	3.13236700	-1.81203500
C	0.98184500	2.36619300	1.40001000
H	1.95872400	2.86347000	1.31406700
H	0.31852700	3.05324400	1.94797600
H	1.10816700	1.46030200	2.01193100
H	-4.90528300	-1.53153800	0.30759500
H	-5.52048600	0.08331300	-0.06261400

TS-2-L

C	-2.73409600	-0.65377200	1.72513300
C	-2.82837300	-0.02286300	0.46648500
C	-1.88940800	0.94666400	0.07209600
C	-0.80166000	1.29661900	0.92385000
C	-0.61782000	0.49721500	2.10422300
C	-1.67042500	-0.37659600	2.54893400
H	-2.80917500	1.38970700	-1.70865900
H	-3.51212500	-1.35317600	2.03296500
H	-3.66229000	-0.26039100	-0.19869700

C	0.07566100	2.32184600	0.52676600
H	0.11141200	0.84942500	2.84020300
C	-0.09992500	2.94994800	-0.72213400
C	-1.13663700	2.58148900	-1.53708900
H	0.89340600	2.61841400	1.18473800
H	0.57737500	3.73869100	-1.05031800
H	-1.33702900	3.03111500	-2.50852200
N	-2.00694800	1.60143100	-1.12560200
C	1.71331600	-0.59733000	-0.10910400
C	0.89535800	-1.44304400	0.76022300
C	-0.16826400	-2.23314400	0.18158100
C	-0.58290400	-2.05960800	-1.10353500
C	0.12663200	-1.08569900	-1.98773000
C	1.31863800	-0.41664700	-1.39308300
H	1.39270300	-1.87342700	1.63976000
H	0.19372100	-0.53444400	1.45108000
H	0.41387300	-1.59044100	-2.93125400
H	-0.59891600	-0.31653700	-2.32961100
H	-1.57837400	-0.86418600	3.52120800
C	2.94129600	0.04926500	0.50255900
H	2.61638200	0.46063400	1.47766000
C	-1.71160000	-2.83809900	-1.69981000
H	-2.21164700	-3.47407500	-0.95766900
H	1.89459500	0.23106800	-2.05715000
H	-0.67901900	-2.95877400	0.81956700
C	4.02306500	-1.00441000	0.78594600
H	4.38178500	-1.44835900	-0.15516600
H	4.88262200	-0.54479700	1.29460700
H	3.65740000	-1.82112300	1.42523800
C	3.51522800	1.19911500	-0.32107100
H	4.33113700	1.68833900	0.22940100
H	3.93713500	0.83984600	-1.27259100
H	2.75573500	1.96094800	-0.55057600
H	-2.46092400	-2.16227400	-2.14448500
H	-1.34965200	-3.48190600	-2.51796200

TS-2-M

C	1.49370300	-2.94013800	1.02305500
C	2.49163500	-1.94956300	1.07435200
C	2.52507300	-0.90715900	0.13550400
C	1.53056900	-0.80780500	-0.88232800
C	0.45931300	-1.75591300	-0.83793600
C	0.51023200	-2.86904900	0.06037300
H	4.23154300	-0.03956000	0.87813600
H	1.51526000	-3.76223000	1.73925400
H	3.26870400	-2.00199700	1.84088200
C	1.61513400	0.24222500	-1.82256000
H	-0.22536900	-1.79364600	-1.69034600
C	2.66438500	1.17726900	-1.73366700
C	3.60008500	1.07290600	-0.73852400
H	0.87192500	0.31692100	-2.61713000
H	2.74637600	1.99281200	-2.45244600
H	4.43593800	1.75950700	-0.61428100
N	3.51459100	0.04204200	0.16628700
C	-2.59000700	-1.03974200	0.57316000
C	-1.34521300	-0.33332200	0.81894200
C	-1.21082900	1.05551000	0.38257000
C	-2.14307900	1.54999200	-0.47331900
C	-3.32867000	0.77199100	-0.92790400
C	-3.53885500	-0.55419600	-0.26917600
H	-0.82101500	-0.59885000	1.74976100
H	-0.51505700	-0.96350800	0.05746600
H	-4.24062900	1.38996500	-0.81504200
H	-3.27372400	0.62101600	-2.02748700
H	-0.27076200	-3.62991600	0.00713400
C	-4.81167100	-1.28020600	-0.56497200
H	-4.85089300	-2.25991500	-0.07167300
H	-5.67937000	-0.68865900	-0.23088200
H	-4.93186900	-1.42977800	-1.65020100
C	-0.04873000	1.86183600	0.92856900
H	0.83318600	1.19740000	0.89921200
C	0.27941100	3.10933000	0.11328400
H	0.42904600	2.87329600	-0.95029600
H	-0.51763700	3.86506000	0.19180300
H	1.20187400	3.57421900	0.48959000
C	-0.30428000	2.22198000	2.40065400
H	0.56390900	2.74861900	2.82297900
H	-1.17878600	2.88434600	2.48985500

H	-0.49113200	1.33334300	3.02149300
H	-2.05991000	2.57427100	-0.84325600
H	-2.73299100	-2.01268200	1.05101400

TS-2-N

C	0.50474800	0.00081500	2.43006500
C	1.67968400	0.51419000	1.84256100
C	2.30240800	-0.14745000	0.76895400
C	1.73934000	-1.33494800	0.21967800
C	0.47176600	-1.75993900	0.74468200
C	-0.06926400	-1.14028900	1.92001300
H	3.88840700	1.14914800	0.64625900
H	0.07102100	0.50494600	3.29439000
H	2.13581900	1.42254600	2.24433500
C	2.38526500	-1.95553900	-0.86704300
H	0.11098200	-2.75255700	0.45999100
C	3.57361700	-1.40245200	-1.38779400
C	4.10421100	-0.26874600	-0.83369600
H	1.97020500	-2.87005800	-1.29296400
H	4.08603600	-1.87319500	-2.22693300
H	5.02366600	0.20383400	-1.17598800
N	3.46795500	0.32693900	0.22831900
C	-0.06356700	0.85314600	-1.27210500
C	-1.02617000	-0.20362700	-1.05139800
C	-2.26553400	0.09226000	-0.32519300
C	-2.37787100	1.28639400	0.29845800
C	-1.32500500	2.34142300	0.24583000
C	-0.15212600	2.05414800	-0.63494800
H	-1.09399700	-0.96268200	-1.84406700
H	-0.37722600	-0.95537500	-0.20385500
H	-1.77677400	3.30657800	-0.05581200
H	-0.95777200	2.54694300	1.27278400
H	-0.98007600	-1.54840500	2.36180100
C	0.86946900	3.13161300	-0.80669000
H	1.72360100	2.79537400	-1.40955400
H	0.42587800	4.01170800	-1.30014600
H	1.23738900	3.47842900	0.17295300
C	-3.32211500	-0.99421500	-0.29580300
H	-2.77679800	-1.94740900	-0.15729600
C	-4.31819200	-0.86021900	0.85342200
H	-3.81293400	-0.78703700	1.82837000
H	-4.95842100	0.02731000	0.73200200
H	-4.98322100	-1.73486800	0.88166700
C	-4.04746700	-1.07333600	-1.64751800
H	-4.75299300	-1.91661000	-1.65765700
H	-4.61700600	-0.14963300	-1.83162400
H	-3.35045700	-1.21133000	-2.48746900
H	-3.27652600	1.52491300	0.87143800
H	0.78632800	0.64950200	-1.92972200

TS-2-O

C	0.83564400	-2.72223100	0.02378000
C	-0.15089600	-2.31957800	-0.89714500
C	-1.24982900	-1.54371200	-0.48516400
C	-1.37082000	-1.10989600	0.86698700
C	-0.25474700	-1.36489100	1.73476300
C	0.77454400	-2.28311900	1.32531100
H	-2.18225700	-1.55689300	-2.31233300
H	1.63884300	-3.38266700	-0.30443300
H	-0.09128600	-2.65033600	-1.93698200
C	-2.52016200	-0.39465000	1.25475400
H	-0.40583100	-1.20146200	2.80636800
C	-3.51707100	-0.09872300	0.30362900
C	-3.37265100	-0.50813500	-0.99452700
H	-2.63571900	-0.07838700	2.29198200
H	-4.41520800	0.44872000	0.59021800
H	-4.10563900	-0.32351200	-1.77843000
N	-2.24758600	-1.21007400	-1.36160200
C	-0.09358500	1.96649900	1.14836300
C	1.03882200	1.05932800	1.17200200
C	1.69724300	0.71139900	-0.08298800
C	1.05601900	1.00182000	-1.24697000
C	-0.22544100	1.75950800	-1.30821800
C	-0.72392200	2.30243200	-0.00566700
H	1.67899200	1.10546900	2.06306700
H	0.46601000	-0.11498100	1.46091200
H	-0.13101400	2.58296400	-2.04258600
H	-1.01631200	1.11885800	-1.75532000

H	1.53274100	-2.58598500	2.04993700
C	-1.90687600	3.21655800	-0.04941100
H	-2.24013500	3.50531000	0.95601700
H	-1.66654200	4.13494100	-0.60942800
H	-2.74954300	2.73689800	-0.57287100
C	3.05864300	0.05285100	-0.00779000
H	2.99506800	-0.69800500	0.80128400
C	3.47820400	-0.66747800	-1.28573800
H	2.71876800	-1.39052300	-1.61793800
H	3.65894900	0.04208700	-2.10813600
H	4.41780200	-1.21340400	-1.12065900
C	4.11891300	1.08603900	0.40805500
H	5.09614900	0.59931400	0.53830400
H	4.22514300	1.86205400	-0.36520500
H	3.86575100	1.58569500	1.35440800
H	1.50707300	0.72247200	-2.20182700
H	-0.46090800	2.35776600	2.10071100

TS-2-P

C	-2.44847300	2.79141400	0.35685300
C	-3.38026200	1.74531800	0.48630500
C	-3.14882200	0.49306100	-0.10372300
C	-1.95454300	0.24141600	-0.84097100
C	-0.97586100	1.28586400	-0.87138700
C	-1.27758700	2.58060200	-0.33825500
H	-4.92024500	-0.33818100	0.51970300
H	-2.66745500	3.76398600	0.79877900
H	-4.30691700	1.91026900	1.04153700
C	-1.76524900	-1.02988000	-1.42442000
H	-0.14567500	1.18653000	-1.57757600
C	-2.74098300	-2.03110300	-1.25302000
C	-3.87837900	-1.77051100	-0.53476000
H	-0.86488400	-1.22798900	-2.00693100
H	-2.60890200	-3.01957700	-1.69344000
H	-4.67423200	-2.49507100	-0.36995400
N	-4.06155000	-0.52417400	0.01399800
C	1.98194200	0.90491200	0.77418300
C	0.69081200	0.43084700	1.24079000
C	0.43593000	-1.00884600	1.27523500
C	1.29779400	-1.83226900	0.62535400
C	2.51475200	-1.34591900	-0.08072800
C	2.86059800	0.09542100	0.12615000
H	0.22155000	1.02042600	2.04230600
H	-0.10990200	0.83364000	0.30512000
H	2.22579400	1.96084100	0.92086800
H	1.11308600	-2.91027100	0.61746700
H	3.37904200	-1.98454300	0.18179500
H	2.39788300	-1.53136500	-1.17026300
C	-0.76744800	-1.50699300	2.01910800
H	-0.92874600	-2.58076500	1.85766900
H	-0.64782100	-1.33386000	3.10030300
H	-1.67673800	-0.97120300	1.70641100
C	4.19857100	0.60007300	-0.36049900
H	4.17757100	1.69781000	-0.26381900
C	4.44350200	0.26147000	-1.83566400
H	5.36911900	0.74160900	-2.18372200
H	4.56209900	-0.82245600	-1.99049100
H	3.62100900	0.61496400	-2.47602400
C	5.33848500	0.08117700	0.52926000
H	6.29342800	0.52578900	0.21392300
H	5.17440000	0.34057800	1.58504400
H	5.44605400	-1.01242500	0.45611800
H	-0.54734000	3.38415300	-0.45166400

TS-2-Q

C	0.01596900	-1.58791100	2.18874400
C	0.97872500	-0.57996600	1.98368500
C	1.75465200	-0.54444600	0.81010900
C	1.57228600	-1.51807400	-0.21288500
C	0.49403000	-2.45159400	-0.04193300
C	-0.19665000	-2.53512500	1.21375700
H	2.86296400	1.08890900	1.37141000
H	-0.53850900	-1.61915000	3.12718800
H	1.15543600	0.16617900	2.76233000
C	2.36611700	-1.44288400	-1.37373700
H	0.45342200	-3.30878700	-0.72052000
C	3.31951100	-0.41187100	-1.50751700
C	3.48347900	0.50691600	-0.50622600

H	2.24625700	-2.18841100	-2.16104900
H	3.94025300	-0.33986400	-2.40076000
H	4.20772800	1.31952600	-0.53740600
N	2.71305900	0.41644400	0.62789500
C	-0.67661700	0.45062000	-1.22521900
C	-1.38574800	-0.80520000	-1.32781400
C	-2.62996200	-0.97963000	-0.57170900
C	-2.96019200	-0.05465400	0.35733300
C	-2.14123300	1.16007400	0.63429700
C	-0.97936800	1.38423800	-0.27959400
H	-1.33819300	-1.30597400	-2.30569600
H	-0.55457000	-1.61783200	-0.71960000
H	0.16231500	0.62667700	-1.90477000
H	-3.87340600	-0.18074100	0.94566700
H	-2.78910300	2.05782700	0.63432400
H	-1.77456700	1.11533700	1.68026100
C	-3.44367000	-2.21138300	-0.83500300
H	-4.32218400	-2.26740700	-0.17933400
H	-3.79062000	-2.23650600	-1.87961500
H	-2.83902100	-3.12003900	-0.67697400
C	-0.21498900	2.68470200	-0.19701400
H	0.74017400	2.52402500	-0.72526800
C	0.10128100	3.10091800	1.24220700
H	0.75859200	3.98227500	1.24785900
H	-0.80840600	3.37270100	1.79914700
H	0.60482600	2.29487600	1.79762700
C	-0.97063200	3.79879500	-0.94003500
H	-0.38475500	4.72935100	-0.92667000
H	-1.15561100	3.52564400	-1.98845400
H	-1.94113100	4.01025600	-0.46491700
H	-0.93523300	-3.32512900	1.36128500

TS-2-R

C	-3.39855500	-0.01797200	-0.52127500
C	-2.47978800	0.78488300	-1.22533900
C	-1.43278600	1.44084100	-0.55383000
C	-1.24117100	1.26662300	0.84736300
C	-2.06620100	0.28794000	1.50055200
C	-3.22380400	-0.23500500	0.82494300
H	-0.75405700	2.44863600	-2.20743400
H	-4.24430800	-0.45625900	-1.05212800
H	-2.60821300	0.94433000	-2.29873000
C	-0.22009100	1.98895900	1.49335600
H	-2.05523200	0.27448800	2.59487800
C	0.59769600	2.86293400	0.75069200
C	0.40493100	3.00624000	-0.59741100
H	-0.07730300	1.87955600	2.56899600
H	1.38544800	3.43819500	1.23742300
H	0.99313200	3.66930400	-1.23005700
N	-0.58822300	2.28936500	-1.21973400
C	1.00198500	-1.21490600	1.21786700
C	-0.29427900	-1.84412200	1.05673300
C	-0.71927600	-2.24125400	-0.28212100
C	-0.03849500	-1.74949900	-1.35076600
C	1.19853300	-0.92869400	-1.22598800
C	1.73804300	-0.77850900	0.16149700
H	-0.62633200	-2.48803600	1.88270700
H	-1.16818400	-0.85516100	1.28756300
H	1.39417400	-1.09735700	2.23207500
H	-0.36864900	-2.00548300	-2.36185500
H	1.98026200	-1.34010700	-1.89310600
H	1.01875300	0.08316800	-1.65050000
C	-1.88645700	-3.17155900	-0.41823000
H	-2.25904000	-3.21398900	-1.45020900
H	-1.59123100	-4.18987500	-0.11836200
H	-2.71652900	-2.87313200	0.23965900
C	3.14010100	-0.24167300	0.34706200
H	3.19155400	0.17685700	1.36610400
C	3.51498500	0.86447200	-0.64147500
H	4.50440300	1.27300100	-0.39127000
H	3.57414800	0.48707200	-1.67427800
H	2.79248400	1.69274300	-0.61754100
C	4.14723500	-1.40238700	0.27253300
H	5.16921600	-1.03177800	0.43932500
H	3.93226400	-2.16914600	1.03005700
H	4.12521800	-1.88551900	-0.71717100
H	-3.93004700	-0.85093900	1.38502100

TS-2-S

C	-0.46449800	-1.74775600	2.42207400
C	-0.27966300	-2.17120800	1.08942700
C	-1.01401000	-1.59266400	0.03814200
C	-1.94555900	-0.54322400	0.29012000
C	-1.97943800	-0.00887100	1.62492100
C	-1.32673200	-0.71392900	2.69641700
H	-0.24886400	-2.81402400	-1.42195600
H	0.07231800	-2.25528800	3.22423700
H	0.41183800	-2.98864500	0.87161700
C	-2.70649800	-0.03512700	-0.77810100
H	-2.80505500	0.66472900	1.87450200
C	-2.51567100	-0.53952400	-2.08019100
C	-1.60477000	-1.53664500	-2.30301500
H	-3.43980200	0.75090700	-0.59392500
H	-3.09490000	-0.15264200	-2.91862900
H	-1.41304500	-1.98097600	-3.27861300
N	-0.87990900	-2.03905700	-1.24940200
C	-0.37866400	2.39737800	-0.12594300
C	0.05983700	1.84983200	1.15754900
C	1.21602500	0.98289800	1.18994100
C	1.78387600	0.48127200	0.05773800
C	1.24355500	0.87602500	-1.27971500
C	0.17237100	1.91230500	-1.26385500
H	-0.10021900	2.48230300	2.04149100
H	-0.93019700	0.98522700	1.42828200
H	2.07369900	1.20323000	-1.93537700
H	0.86329900	-0.03114000	-1.79524600
H	-1.47758500	-0.37343000	3.72253300
C	-1.46244800	3.43429700	-0.11660600
H	-1.13089900	4.34292400	0.40927500
H	-1.76453400	3.71723300	-1.13338400
H	-2.35356300	3.06442500	0.41707900
C	3.01255800	-0.39708900	0.11646600
H	3.06060500	-0.81227900	1.13680300
C	4.28123100	0.44370700	-0.10002400
H	4.35398400	1.25346300	0.63955900
H	5.17683500	-0.18750400	-0.00545900
H	4.29749400	0.89559000	-1.10415700
C	2.95767500	-1.56799000	-0.86882200
H	2.03727100	-2.15864400	-0.74337700
H	3.00660700	-1.22665500	-1.91443400
H	3.81038400	-2.24239700	-0.70680800
H	-0.16578400	2.29198500	-2.23209800
H	1.62441500	0.70288800	2.16476300

TS-2-T

C	0.29601800	2.10846200	-0.68873100
C	1.41201700	1.52065700	-1.32433400
C	2.37895300	0.82156000	-0.58531800
C	2.23182200	0.64158200	0.82136700
C	1.00464500	1.10004300	1.41181100
C	0.11024000	1.93238600	0.66144500
H	3.61754700	0.45889600	-2.18260700
H	-0.40085500	2.70821800	-1.27564900
H	1.55384600	1.64932400	-2.40020400
C	3.24142400	-0.03551300	1.53337600
H	0.94569300	1.11862800	2.50413100
C	4.36733100	-0.53716300	0.84954700
C	4.48157900	-0.36387700	-0.50416900
H	3.15112600	-0.15938100	2.61338800
H	5.15687700	-1.06343200	1.38602000
H	5.32426200	-0.72181500	-1.09383200
N	3.49915000	0.30824300	-1.18720300
C	-0.11348200	-1.59149300	-0.34099600
C	-0.51566400	-1.24586300	1.01804500
C	-1.87061400	-0.76681600	1.24915800
C	-2.67185100	-0.35428900	0.23703700
C	-2.17316800	-0.43059300	-1.17312900
C	-0.89449200	-1.16367700	-1.37111300
H	-0.06883300	-1.85069800	1.81962100
H	0.19893900	-0.16281900	1.20822000
H	-2.95043800	-0.85875200	-1.83287500
H	-2.05356600	0.60212100	-1.56418400
H	-0.75256100	2.37082700	1.16571500
C	1.13089200	-2.40219500	-0.54996300
H	0.94701500	-3.45002600	-0.26283500
H	1.45345000	-2.39121400	-1.59959600

H	1.95805400	-2.04281400	0.07942800
C	-4.06697000	0.17155400	0.48365500
H	-4.18008400	0.26660300	1.57584800
C	-5.13385000	-0.81790000	-0.00578600
H	-4.99631800	-1.81122800	0.44512600
H	-6.13635900	-0.45710600	0.26614600
H	-5.11370500	-0.93123400	-1.10117500
C	-4.26990900	1.56165000	-0.13154900
H	-3.49672600	2.27028700	0.20336200
H	-4.25314200	1.52606400	-1.23235800
H	-5.24731000	1.96855900	0.16460600
H	-0.59873300	-1.38690300	-2.40047500
H	-2.22175600	-0.70088500	2.28247800

INT-2-A

C	-3.58845800	0.28482900	-1.44389200
C	-3.50498900	-0.03958100	-0.07753700
C	-2.35222300	-0.71364500	0.44245700
C	-1.32605300	-1.08924700	-0.44899900
C	-1.43725200	-0.91147700	-1.92923300
C	-2.61906800	-0.09184300	-2.33648300
H	-2.95089700	-0.72744400	2.52229700
H	-4.45199800	0.85012700	-1.79919000
H	-4.29852200	0.25094600	0.61218700
H	-1.50601700	-1.91378300	-2.39981600
C	-0.00293800	-1.90575500	1.35412100
C	-0.99528500	-1.59592700	2.26513200
H	0.55376400	-1.84165900	-0.59977100
H	0.95540000	-2.34967000	1.61932700
H	-0.84122600	-1.81119700	3.32229600
C	2.26171300	0.45114500	0.12591600
C	1.50681200	0.92752000	-0.98776900
C	0.31627700	1.67195700	-0.79981800
C	-0.16753000	1.97358400	0.44582600
C	0.61920500	1.58178700	1.66266000
C	1.82731800	0.74388200	1.39023700
H	1.86816500	0.75229200	-2.00452600
H	-0.49851500	-0.47477100	-2.31545200
H	0.92727000	2.50696800	2.19675200
H	-0.04671200	1.08625300	2.39920200
H	-2.70795200	0.16422500	-3.39364900
C	-1.42408900	2.75201300	0.66617000
H	-1.20933800	3.70945000	1.17014800
H	-1.94597400	2.96876200	-0.27579300
H	-2.11623000	2.20269300	1.32844300
C	3.52620500	-0.35947200	-0.10935000
H	3.95212600	-0.58849400	0.88130000
C	4.57370100	0.44264400	-0.88842200
H	4.79004500	1.39718900	-0.38805900
H	5.51414400	-0.12238100	-0.96755100
H	4.23500600	0.66751500	-1.91190500
C	3.22563000	-1.69509500	-0.80058400
H	2.58240700	-2.34139800	-0.17748200
H	2.74254000	-1.54600400	-1.78126000
H	4.14870600	-2.26474900	-0.98231600
H	-0.23665400	2.01684400	-1.67900200
H	2.41112700	0.40972400	2.25362700
N	-0.21660200	-1.65711100	0.04461100
C	-2.16471900	-0.99426500	1.81255300

INT-2-B

C	-3.58504400	0.23013400	-1.46304600
C	-3.50683700	-0.04193000	-0.08499800
C	-2.35561100	-0.69456100	0.46487800
C	-1.32624200	-1.10406200	-0.40779500
C	-1.43356400	-0.98597200	-1.89426800
C	-2.61252500	-0.18071400	-2.33697300
H	-2.96093400	-0.62687400	2.54170200
H	-4.44687900	0.78196700	-1.84283000
H	-4.30296900	0.27473000	0.59007600
H	-1.50481700	-2.00656700	-2.32350100
C	-0.00789900	-1.84675100	1.43027900
C	-1.00354200	-1.50247600	2.32521100
H	0.55524300	-1.85845600	-0.52280600
H	0.95028500	-2.27818700	1.71583200
H	-0.85262600	-1.67557300	3.39054300
C	2.26397700	0.45503600	0.10920900
C	1.50648200	0.88887500	-1.01997200

C	0.31553500	1.63869000	-0.85754400
C	-0.16554900	1.98699000	0.37691100
C	0.62550100	1.64399600	1.60569600
C	1.83258100	0.79566700	1.36255200
H	1.86553200	0.67539000	-2.03021200
H	-0.49279000	-0.56850500	-2.29627200
H	0.93586200	2.59002100	2.10066300
H	-0.03756600	1.17898100	2.36424400
H	-2.69710900	0.03510300	-3.40343600
C	-1.42359200	2.77002300	0.57072800
H	-1.94704800	2.95165100	-0.37776900
H	-2.11368800	2.24288600	1.25293900
H	-1.21067400	3.74534000	1.04000100
C	3.52746700	-0.36484300	-0.09789900
H	3.95693700	-0.55393700	0.89960500
C	4.57254500	0.40442800	-0.91249100
H	4.79069700	1.37853100	-0.45221200
H	5.51261400	-0.16367900	-0.97142400
H	4.23077000	0.58740300	-1.94326800
C	3.22356800	-1.72715000	-0.73341500
H	2.58254800	-2.34731000	-0.08211400
H	2.73667900	-1.61725500	-1.71741500
H	4.14558800	-2.30430700	-0.89578200
H	-0.24030500	1.94865300	-1.74783500
H	2.41838500	0.49443500	2.23663200
C	-2.17223200	-0.92066200	1.84553200
N	-0.21769100	-1.65039300	0.11129600

INT-2-C

C	3.23572100	-0.73866100	1.81717700
C	2.00974500	-0.06427500	1.95504100
C	1.51482200	0.77054200	0.89860500
C	2.29173300	0.92903800	-0.26565100
C	3.63999600	0.29805100	-0.43690200
C	4.01706100	-0.59952800	0.69901700
H	-0.34473300	1.32935300	1.85199100
H	3.57312700	-1.39039600	2.62515800
H	1.40583800	-0.18043300	2.85579000
H	4.40248400	1.09586200	-0.54498900
C	0.62255600	2.33206700	-1.22689400
C	-0.16882900	2.21929600	-0.09977900
H	2.37845100	1.79128300	-2.09989600
H	0.34929400	2.91200400	-2.10781000
H	-1.13217200	2.72553000	-0.06229400
C	-2.34775200	-0.57338000	0.16461300
C	-1.94395700	-0.22296600	-1.15847000
C	-0.74548400	-0.73884500	-1.71247700
C	0.05348500	-1.62223000	-1.03577400
C	-0.36510700	-2.12010600	0.31711600
C	-1.57408900	-1.44474600	0.88198000
H	-2.56492400	0.44483100	-1.75984400
H	3.67051700	-0.26027800	-1.39158200
H	-0.55688700	-3.21408100	0.24903000
H	0.48702000	-2.06306300	1.02376000
H	4.96638300	-1.13139700	0.61608000
C	1.30076700	-2.21184100	-1.61676600
H	1.16597500	-3.28758900	-1.82300900
H	1.58861100	-1.72893300	-2.56252800
H	2.14201800	-2.14612200	-0.90467200
C	-3.63714300	-0.01243200	0.74224700
H	-3.73023000	-0.41354100	1.76490700
C	-4.85280700	-0.49690000	-0.05568100
H	-4.87738200	-1.59469800	-0.11141300
H	-5.78691200	-0.15739800	0.41615400
H	-4.84023300	-0.10748100	-1.08598800
C	-3.61787800	1.51535100	0.84980000
H	-2.79038200	1.86519800	1.48770400
H	-3.52294900	1.98983000	-0.14091500
H	-4.55229600	1.88522600	1.29696200
H	-0.46168400	-0.43371000	-2.72531300
H	-1.88327300	-1.73444300	1.89107100
N	1.80938100	1.69378700	-1.26071300
C	0.27527000	1.43955600	0.96056900

INT-2-D

C	3.19384600	1.77160500	-0.92798700
C	3.40433200	0.55110900	-0.26177800
C	2.41890100	0.03273500	0.64136800

C	1.23774500	0.77253500	0.85865100
C	0.99281300	2.10946100	0.23360600
C	2.06579100	2.52296500	-0.72051500
H	3.46463600	-1.78508700	1.17169900
H	3.95305400	2.12869600	-1.62617200
H	4.31562400	-0.02439700	-0.42987100
H	0.88973700	2.86924400	1.03381400
C	0.40246200	-0.91453900	2.31187600
C	1.55175400	-1.66723300	2.15495000
H	-0.58307100	0.77452800	1.75379100
H	-0.44722600	-1.21667800	2.92280300
H	1.64814400	-2.61848300	2.67779500
C	-0.76746500	-1.99115700	-0.51217100
C	-1.89978900	-1.26493400	-0.06790700
C	-2.19100200	0.02884400	-0.59660900
C	-1.39213200	0.53568200	-1.58596500
C	-0.22105200	-0.20413200	-2.15194000
C	0.08289400	-1.50903800	-1.47254900
H	-2.55677500	-1.70873700	0.68358100
H	0.00808600	2.08767200	-0.27323400
H	-0.39051400	-0.39495700	-3.23385300
H	0.68432500	0.43968000	-2.15888000
H	1.92694400	3.47049400	-1.24389600
C	1.28803300	-2.25868500	-1.94446700
H	1.44277000	-3.18888800	-1.38021700
H	1.19499100	-2.52102800	-3.01193100
H	2.19790700	-1.63866300	-1.85893400
C	-3.35648200	0.83248900	-0.04281100
H	-3.46666200	1.72390600	-0.68163400
C	-4.67823500	0.06172600	-0.09251300
H	-5.51321400	0.70734200	0.21707400
H	-4.88556900	-0.29859200	-1.11010100
H	-4.67034600	-0.81056900	0.57943600
C	-3.05112300	1.32513400	1.37791000
H	-2.88540600	0.47981400	2.06888500
H	-2.16718900	1.98904200	1.38978100
H	-3.88486200	1.91330900	1.78872200
H	-0.56698900	-2.97287900	-0.07255600
H	-1.63528100	1.50637100	-2.03084700
C	2.55609100	-1.19691800	1.31789500
N	0.30037100	0.26614000	1.67292600

INT-2-E

C	-0.03118000	-2.09349000	0.77880800
C	1.09336000	-1.58620700	1.44943100
C	2.14087500	-0.93193500	0.72531700
C	2.03515300	-0.82670600	-0.67941800
C	0.91324600	-1.44217600	-1.45434000
C	-0.14844700	-2.03156900	-0.58544200
H	3.38762400	-0.44326200	2.42367400
H	-0.83419400	-2.54535200	1.36312500
H	1.17576000	-1.66152400	2.53444000
H	1.32712300	-2.22651100	-2.12011800
C	4.10092100	0.36656800	-0.78113600
C	4.25893600	0.27299600	0.58800500
H	2.90719000	-0.11063900	-2.36100200
H	4.80778500	0.85998300	-1.44731400
H	5.14026500	0.70782700	1.05916200
C	-0.71212600	1.48056100	-1.13718000
C	-1.94375100	0.79146300	-1.03021300
C	-2.49006200	0.46379200	0.24742000
C	-1.79338900	0.81146600	1.37059100
C	-0.49644400	1.55449600	1.33682100
C	0.02221500	1.85008000	-0.04007900
H	-2.49529700	0.54273300	-1.93958600
H	0.46572600	-0.68504300	-2.12293000
H	-0.60173700	2.50919200	1.89578900
H	0.27614100	1.00976900	1.92256600
H	-1.03670000	-2.42084600	-1.08409800
C	1.28916200	2.64217500	-0.13644500
H	1.63812900	2.74306500	-1.17494600
H	1.14584700	3.66097300	0.26312000
H	2.09425200	2.19151100	0.46940800
C	-3.84021700	-0.22711000	0.34205500
H	-4.05631000	-0.35975300	1.41500000
C	-4.95236900	0.64727000	-0.24744800
H	-5.93571300	0.17759400	-0.09601500
H	-4.97064300	1.63903000	0.22717600

H	-4.81908600	0.79430100	-1.33097300
C	-3.82693600	-1.61824500	-0.29904300
H	-3.59333200	-1.56605800	-1.37506800
H	-3.08749400	-2.27521800	0.18395300
H	-4.81116100	-2.09992600	-0.20174000
H	-0.34787800	1.75058200	-2.13479900
H	-2.20848900	0.57911500	2.35594500
N	3.00634700	-0.18577500	-1.34963700
C	3.27901200	-0.36861600	1.33941200

INT-2-F

C	0.73148800	-0.49782900	2.82352300
C	0.31886200	0.67175300	2.15964100
C	0.99694800	1.11711700	0.98016600
C	2.08908600	0.36864100	0.49684800
C	2.59646500	-0.86234200	1.18068200
C	1.78985200	-1.24555600	2.37966800
H	-0.21523000	2.86964900	0.62133400
H	0.18824900	-0.81763400	3.71468400
H	-0.52853500	1.25250500	2.52601700
H	3.65252900	-0.70483900	1.47755700
C	2.36987400	1.88592200	-1.32143900
C	1.30906000	2.65574700	-0.88471600
H	3.50120900	0.23465500	-0.94962200
H	2.96024000	2.10599000	-2.21030800
H	1.02214200	3.54491400	-1.44559100
C	-1.32188300	0.20384100	-1.42306000
C	-0.20327400	-0.41078300	-2.03709000
C	0.36998200	-1.59801500	-1.49299900
C	-0.20520400	-2.16610600	-0.38952300
C	-1.46439200	-1.64634800	0.22413600
C	-1.93760500	-0.32600800	-0.31834300
H	0.22168200	0.02816300	-2.94366300
H	2.61508300	-1.69625400	0.45456000
H	-1.69404900	1.13595600	-1.85406400
H	0.21431500	-3.08551000	0.03119200
H	-2.26333900	-2.40518600	0.07878000
H	-1.36861200	-1.59133200	1.32632800
C	1.57168900	-2.21268200	-2.16258900
H	1.97230500	-3.06276400	-1.59167300
H	1.31094900	-2.58483700	-3.16541500
H	2.38084600	-1.47713400	-2.31135400
C	-3.12355800	0.30738300	0.37611900
H	-2.88625500	0.29936700	1.45816100
C	-3.38910900	1.75590000	-0.02880200
H	-2.49709100	2.38963900	0.09340200
H	-3.71379100	1.82926600	-1.07834500
H	-4.19027500	2.18420100	0.59019600
C	-4.39493200	-0.53882200	0.19354200
H	-5.23967900	-0.08429900	0.73141000
H	-4.66395700	-0.60389900	-0.87207500
H	-4.27341700	-1.56172000	0.57723500
H	2.09078200	-2.15072300	2.90975300
N	2.71827900	0.79198100	-0.61193800
C	0.62597500	2.27284700	0.26341300

INT-2-G

C	0.73209500	-0.49692400	2.82370800
C	0.31908800	0.67240100	2.15960900
C	0.99679600	1.11752500	0.97981300
C	2.08897500	0.36917800	0.49645000
C	2.59681300	-0.86146500	1.18053000
C	1.79051200	-1.24454200	2.37977600
H	-0.21571200	2.86984800	0.62103600
H	0.18914200	-0.81659900	3.71508900
H	-0.52825000	1.25318500	2.52605900
H	3.65287800	-0.70363800	1.47721700
C	2.36899400	1.88603300	-1.32229000
C	1.30809400	2.65574500	-0.88552400
H	3.50118500	0.23546900	-0.94996400
H	2.95906300	2.10601200	-2.21138400
H	1.02084100	3.54469200	-1.44655600
C	-1.32213400	0.20278400	-1.42341900
C	-0.20357900	-0.41208900	-2.03728400
C	0.37003900	-1.59882100	-1.49242000
C	-0.20486600	-2.16625800	-0.38846900
C	-1.46408200	-1.64633700	0.22501100
C	-1.93751100	-0.32637200	-0.31819300

H	0.22099300	0.02613300	-2.94438300
H	2.61548200	-1.69556400	0.45462600
H	-1.69450900	1.13455900	-1.85499400
H	0.21487900	-3.08530900	0.03278900
H	-2.26297400	-2.40534400	0.08014400
H	-1.36816600	-1.59060200	1.32715400
C	1.57174300	-2.21371500	-2.16175900
H	1.97257000	-3.06337200	-1.59037000
H	1.31092800	-2.58653100	-3.16432500
H	2.38082400	-1.47819800	-2.31116500
C	-3.12329700	0.30744700	0.37616300
H	-2.88565900	0.30016700	1.45813700
C	-3.38892100	1.75566900	-0.02972200
H	-2.49667900	2.38931600	0.09136800
H	-3.71421900	1.82824700	-1.07912700
H	-4.18960600	2.18461200	0.58945600
C	-4.39469400	-0.53891900	0.19459000
H	-5.23932700	-0.08398800	0.73228700
H	-4.66398800	-0.60487900	-0.87090200
H	-4.27303200	-1.56150000	0.57908600
H	2.09174800	-2.14952900	2.91002000
N	2.71780900	0.79235600	-0.61259900
C	0.62542300	2.27304700	0.26291400

INT-2-H

C	-0.25772000	2.69356300	1.55385400
C	-1.26382900	1.72031400	1.68354500
C	-1.78469700	1.05287000	0.52676600
C	-1.22873700	1.34101200	-0.73518100
C	-0.09139100	2.29533400	-0.92087100
C	0.29585400	3.00246800	0.33834300
H	-3.29362100	-0.11256900	1.54664400
H	0.08381600	3.22154700	2.44603700
H	-1.68667000	1.48174800	2.66003500
H	-0.33853000	3.02704700	-1.71260500
C	-2.75395900	-0.15520900	-1.78995500
C	-3.33725400	-0.46694600	-0.57643300
H	-1.31301600	0.93897100	-2.71950000
H	-3.06522200	-0.57983800	-2.74378600
H	-4.16400000	-1.17606900	-0.54312800
C	-0.48666100	-2.23826300	0.65316300
C	-0.16670300	-2.08277300	-0.73013000
C	0.95780500	-1.32165500	-1.13055200
C	1.78373700	-0.69278500	-0.23234800
C	1.46674400	-0.75725500	1.23442300
C	0.27365500	-1.58928200	1.58458000
H	-0.75472600	-2.61621000	-1.48171500
H	0.77898400	1.72364500	-1.30319400
H	2.35265600	-1.13145200	1.78858700
H	1.34135200	0.27066400	1.63625900
H	1.06263900	3.77473400	0.25854600
C	-1.61580800	-3.15207900	1.05134100
H	-1.32056200	-4.20512700	0.92187600
H	-1.90239400	-3.01518700	2.10348300
H	-2.50692000	-2.99577900	0.42376100
C	3.08933000	-0.06284100	-0.67162300
H	2.96623500	0.24520900	-1.72570900
C	3.48632000	1.17182100	0.14180100
H	2.68651000	1.92684400	0.17128100
H	3.73016800	0.90830600	1.18249800
H	4.37965900	1.64467700	-0.29100200
C	4.21350000	-1.11220300	-0.63745300
H	3.97522400	-1.97125300	-1.28033100
H	5.16280900	-0.67552900	-0.98221300
H	4.37075700	-1.48833200	0.38570500
H	1.21382500	-1.28274800	-2.19555500
H	0.04229800	-1.70409800	2.64790000
C	-2.84947200	0.13040400	0.57917500
N	-1.74079400	0.73311900	-1.81836400

INT-2-I

C	3.58548600	0.07794500	0.15903000
C	2.83812300	-0.45051700	-0.91004600
C	1.63625200	-1.15759200	-0.64583700
C	1.16863200	-1.37194300	0.66983500
C	1.93833800	-0.80888100	1.82970000
C	3.17616500	-0.06889400	1.45827700
H	1.23815100	-1.50921700	-2.62002300

H	4.50639200	0.62043200	-0.06147700
H	3.17605500	-0.32139000	-1.94029200
C	-0.00000900	-2.09868900	0.85048200
H	2.19313600	-1.62108300	2.53647000
C	-0.71616500	-2.60558600	-0.24287000
C	-0.24246400	-2.36248100	-1.51024200
H	-0.36448400	-2.27849700	1.86449000
H	-1.63842000	-3.16897200	-0.10662300
H	-0.73900300	-2.70922800	-2.41657800
N	0.90283600	-1.67191300	-1.67391600
C	-1.82874600	0.65967600	-0.03839100
C	-1.18228600	1.17302200	1.11854700
C	0.02116400	1.91801800	1.00935000
C	0.61047900	2.19374700	-0.19418500
C	-0.03754100	1.72352400	-1.46302700
C	-1.25879000	0.88486000	-1.26652900
H	-1.62191500	1.02430100	2.10581800
H	1.26952100	-0.14032900	2.40406700
H	-0.29442600	2.61070700	-2.08248200
H	0.71291300	1.20075300	-2.09606500
H	3.77066400	0.35727600	2.26897800
C	1.83597900	3.04079600	-0.32859200
H	1.59121500	4.00076500	-0.81464500
H	2.29388300	3.26212800	0.64531600
H	2.59248400	2.55425200	-0.96696000
C	-3.16978600	-0.05864800	0.04670800
H	-3.16340800	-0.83388000	-0.74063000
C	-4.30771000	0.91864100	-0.28112800
H	-4.17411300	1.37035800	-1.27443700
H	-5.28132600	0.40619300	-0.26493200
H	-4.34042800	1.73484900	0.45736700
C	-3.43583100	-0.75275900	1.38287100
H	-2.61405100	-1.42038200	1.68229500
H	-3.58588600	-0.02505300	2.19507200
H	-4.35333200	-1.35584000	1.32153100
H	0.47961800	2.30875500	1.92319300
H	-1.76081800	0.51104700	-2.16575500

INT-2-J

C	3.58418100	0.07701100	0.15984000
C	2.83718100	-0.45112900	-0.90964300
C	1.63512500	-1.15812300	-0.64607500
C	1.16726600	-1.37323200	0.66939700
C	1.93707800	-0.81134500	1.82975700
C	3.17449900	-0.07035700	1.45890900
H	1.23715000	-1.50823600	-2.62054900
H	4.50500200	0.61983600	-0.06020600
H	3.17539900	-0.32158500	-1.93974300
C	-0.00155700	-2.09983100	0.84937300
H	2.19282700	-1.62462900	2.53500200
C	-0.71777900	-2.60569400	-0.24441400
C	-0.24384400	-2.36186700	-1.51155700
H	-0.36625400	-2.28040200	1.86315900
H	-1.64025100	-3.16884100	-0.10859600
H	-0.74035400	-2.70784000	-2.41820100
N	0.90170800	-1.67155200	-1.67459300
C	-1.82754200	0.66043800	-0.03779300
C	-1.18049300	1.17329600	1.11902800
C	0.02315300	1.91796000	1.00956600
C	0.61191800	2.19406000	-0.19413600
C	-0.03669800	1.72432800	-1.46285800
C	-1.25798300	0.88577000	-1.26609600
H	-1.61972700	1.02438100	2.10644100
H	1.26820300	-0.14423300	2.40563900
H	-0.29374900	2.61174700	-2.08190600
H	0.71343800	1.20163400	-2.09634400
H	3.76855400	0.35581100	2.26992800
C	1.83753100	3.04088100	-0.32883100
H	1.59299100	4.00056800	-0.81554900
H	2.29527900	3.26275100	0.64502500
H	2.59409800	2.55385100	-0.96676800
C	-3.16861600	-0.05780800	0.04761200
H	-3.16177800	-0.83414200	-0.73863400
C	-4.30651200	0.91885400	-0.28220400
H	-4.17264300	1.36902900	-1.27618000
H	-5.28008600	0.40633700	-0.26555100
H	-4.33958000	1.73621500	0.45499200
C	-3.43529200	-0.74998400	1.38464100

H	-2.61294900	-1.41596000	1.68613000
H	-3.58696000	-0.02099800	2.19540300
H	-4.35203800	-1.35421500	1.32343500
H	0.48215100	2.30822200	1.92333800
H	-1.76038000	0.51219800	-2.16521900

INT-2-K

C	-2.96979100	-1.14991600	-1.74472800
C	-1.72785500	-0.48604900	-1.72334900
C	-1.50446100	0.55864300	-0.78859300
C	-2.50939600	0.98671300	0.11109200
C	-3.84974100	0.30180400	0.10420000
C	-3.98206500	-0.80270700	-0.88910600
H	0.46343400	0.78381500	-1.29536500
H	-3.12168300	-1.95668600	-2.46402600
H	-0.92947100	-0.76852600	-2.41189100
C	-2.21719000	2.02941500	0.98080500
H	-4.64563300	1.04934100	-0.07624600
C	-0.95995200	2.64768100	0.97559800
C	-0.00230600	2.18652700	0.09752500
H	-2.98204900	2.37259900	1.68202600
H	-0.72531800	3.46683400	1.65407800
H	1.01244900	2.57932500	0.04213100
N	-0.29927600	1.18707100	-0.74605300
C	2.39868100	-0.54480500	-0.10075500
C	1.99685700	-0.04837600	1.17836900
C	0.81880400	-0.52285500	1.80451000
C	0.06097200	-1.53069500	1.26562200
C	0.54712400	-2.24255300	0.03566300
C	1.67352200	-1.55630000	-0.67347900
H	2.59030900	0.72303200	1.67439900
H	-4.06880800	-0.08641000	1.11694500
H	0.88068300	-3.26284000	0.33291700
H	-0.29583700	-2.44993600	-0.65031600
H	-4.93515500	-1.33425100	-0.92580800
C	-1.20484800	-2.02750200	1.88893800
H	-1.11165800	-3.08656000	2.18355100
H	-1.47961200	-1.45002500	2.78263500
H	-2.04049300	-1.98367900	1.16767800
C	3.62077200	0.03635700	-0.79308000
H	3.71814700	-0.48207800	-1.76114500
C	4.89553700	-0.24077700	0.01096200
H	5.01767700	-1.31703200	0.19852400
H	5.78238700	0.11388900	-0.53476100
H	4.87743500	0.27152500	0.98572600
C	3.46487700	1.53228200	-1.08654200
H	2.58177800	1.73750000	-1.71649300
H	3.38127000	2.12116500	-0.15804800
H	4.33853300	1.91733500	-1.63250100
H	0.50148600	-0.06282500	2.74518500
H	1.98782100	-1.96633000	-1.63872500

INT-2-L

C	-2.47895200	-1.79397500	-1.63263000
C	-2.91191300	-0.70589000	-0.85051500
C	-2.21932500	-0.37728900	0.34419200
C	-1.09878300	-1.11789100	0.78664500
C	-0.60939100	-2.27909900	-0.03227600
C	-1.39618600	-2.55058100	-1.26703700
H	-3.44050100	1.20129900	0.78598300
H	-3.02512100	-2.03317800	-2.54678600
H	-3.78171400	-0.11874300	-1.15190600
C	-0.47796500	-0.74162800	1.96974000
H	-0.57739300	-3.18992100	0.59483700
C	-0.95249700	0.34301400	2.72220200
C	-2.04409100	1.04072600	2.26211100
H	0.39344500	-1.29963700	2.31832400
H	-0.46900200	0.64449900	3.65061300
H	-2.47443900	1.89787500	2.78042600
N	-2.64227200	0.66425600	1.11536600
C	0.48075700	2.00873600	0.12800600
C	1.61791500	1.22010700	0.42939600
C	2.08152400	0.22509800	-0.48233700
C	1.41406200	0.05048600	-1.66410100
C	0.23401400	0.87519100	-2.06936800
C	-0.22850200	1.85800800	-1.03339000
H	2.16056700	1.40260300	1.35961200
H	0.44475400	-2.09121900	-0.31063400

H	0.47395700	1.42642100	-3.00458000
H	-0.60982500	0.22357000	-2.37818500
H	-1.08146500	-3.38982200	-1.89063400
C	-1.42324700	2.69329500	-1.37177500
H	-1.70567700	3.36629000	-0.54904600
H	-1.23002900	3.31762400	-2.26047900
H	-2.29194600	2.06187300	-1.63452100
C	3.32309200	-0.58780700	-0.15294300
H	3.46672300	-1.30320700	-0.97979500
C	4.56688200	0.30590400	-0.09499000
H	5.47228700	-0.29845200	0.06438700
H	4.69222300	0.86955100	-1.03057000
H	4.50211100	1.03257500	0.73023100
C	3.16373400	-1.40016100	1.13630200
H	3.00970800	-0.74692400	2.01058800
H	2.31470600	-2.09978300	1.07311300
H	4.06525100	-1.99894900	1.33265800
H	0.16530800	2.76986900	0.84869500
H	1.77521200	-0.69146200	-2.38330300

INT-2-M

C	-0.03632600	-1.81360000	0.99786200
C	1.09955000	-1.21688900	1.57202700
C	2.15478000	-0.76794100	0.74198200
C	2.12451500	-0.93328200	-0.66666400
C	0.96543900	-1.65465400	-1.29560300
C	-0.12877000	-2.01857900	-0.35466500
H	3.25998600	-0.02949500	2.29456500
H	-0.85997900	-2.10983700	1.64862600
H	1.16252600	-1.07380200	2.65266000
C	3.18071400	-0.43875600	-1.41459800
H	1.33661900	-2.57550100	-1.78726400
C	4.27122200	0.20415200	-0.80286600
C	4.27639800	0.33476800	0.56435800
H	3.16698500	-0.55348100	-2.50124300
H	5.10393300	0.59187900	-1.38849800
H	5.08103700	0.81317100	1.12318000
N	3.23943100	-0.14352900	1.28385800
C	-0.72178300	1.26653600	-1.27687500
C	-1.95987200	0.60181900	-1.10734300
C	-2.54883900	0.47150800	0.18659300
C	-1.89711800	1.00201700	1.26470100
C	-0.61206100	1.75905800	1.15534700
C	-0.03231300	1.81608900	-0.22795900
H	-2.47642300	0.20646800	-1.98471000
H	0.55196600	-1.04542400	-2.11755500
H	-0.76047100	2.79603500	1.52787900
H	0.14077500	1.34932400	1.86431300
H	-1.02716000	-2.47201200	-0.77645600
C	1.25233300	2.56485500	-0.40147200
H	1.63317100	2.50093900	-1.43082600
H	1.12203300	3.63317700	-0.15718700
H	2.03368200	2.19061100	0.28391100
C	-3.89122000	-0.22302000	0.34321500
H	-4.14049300	-0.19934100	1.41696900
C	-4.99612000	0.53179700	-0.40390400
H	-5.97653900	0.06896200	-0.21660200
H	-5.04648300	1.58177100	-0.08125700
H	-4.82701300	0.52128200	-1.49229000
C	-3.83556300	-1.69332100	-0.08356300
H	-3.57835600	-1.79565300	-1.15050600
H	-3.09549900	-2.25620700	0.50644300
H	-4.81196400	-2.17809200	0.06397300
H	-0.31120900	1.36180700	-2.28772600
H	-2.34693200	0.92276500	2.25915300

INT-2-N

C	-2.47398700	-1.28035400	-1.58431000
C	-2.34161300	-0.96248600	-0.21887800
C	-1.16313800	-1.33041800	0.47744500
C	-0.10837700	-2.03479800	-0.15216500
C	-0.18840000	-2.31217700	-1.62678200
C	-1.47074100	-1.90995800	-2.27115300
H	-1.75260200	-0.45799600	2.22237000
H	-3.39637000	-1.00764100	-2.10019600
H	-3.13763600	-0.43547200	0.31023400
C	0.97722300	-2.42872200	0.61471000
H	0.00723500	-3.38252500	-1.81986700

C	1.05146600	-2.11529700	1.98051100
C	0.03041600	-1.38781600	2.54655900
H	1.79372700	-2.98283400	0.14547300
H	1.90307700	-2.41890700	2.58810400
H	0.02063600	-1.07264200	3.58996900
N	-1.02995200	-1.03519600	1.79832400
C	-0.41822400	2.10824500	1.32863300
C	0.85727700	1.56920600	0.99966700
C	1.15069900	1.14422300	-0.32202900
C	0.18483900	1.30174900	-1.29051400
C	-1.11172700	2.00243500	-1.04743600
C	-1.39799200	2.30288700	0.39531100
H	1.60968900	1.49146600	1.78480400
H	0.64635700	-1.78513500	-2.12985400
H	-1.11965000	2.96177500	-1.61272600
H	-1.95433800	1.44464100	-1.50108700
H	-1.59224700	-2.13423100	-3.33281300
C	-2.73219800	2.90001700	0.71836300
H	-2.85330300	3.08914100	1.79410100
H	-2.86680500	3.85940700	0.19063900
H	-3.55846600	2.25007900	0.38103800
C	2.50897300	0.55714500	-0.70284900
H	2.30699000	-0.41105400	-1.20087900
C	3.22494400	1.45522300	-1.72149200
H	4.18579600	1.01265500	-2.02376400
H	2.62463200	1.61086600	-2.62870200
H	3.42905500	2.44374000	-1.28194800
C	3.43356800	0.28004500	0.48178700
H	3.74286100	1.21542600	0.97333000
H	2.96336500	-0.35859100	1.24348900
H	4.34882300	-0.22368000	0.13862800
H	-0.60954300	2.39828900	2.36722400
H	0.39034200	0.98471400	-2.31810700

INT-2-O

C	0.89930000	-2.41844800	-0.30778400
C	-0.14005200	-2.04162000	-1.17570800
C	-1.31706300	-1.45438800	-0.65290200
C	-1.50215600	-1.25441800	0.73865200
C	-0.41117500	-1.65579900	1.69126500
C	0.79557500	-2.24451500	1.04854600
H	-2.18418200	-1.20403500	-2.48703400
H	1.80603000	-2.85208200	-0.73109200
H	-0.03881100	-2.18440100	-2.25340500
C	-2.69013700	-0.68998700	1.17501100
H	-0.81389300	-2.36278500	2.44078200
C	-3.68963300	-0.29908800	0.26758000
C	-3.47413600	-0.49741900	-1.07457700
H	-2.85082800	-0.54048000	2.24536700
H	-4.62071100	0.15267100	0.60754100
H	-4.19191300	-0.22514500	-1.84868800
N	-2.32114200	-1.06246300	-1.48901200
C	1.40470400	1.24374700	1.11583100
C	2.64501400	0.56230100	1.07929500
C	3.17234900	0.06116200	-0.14721200
C	2.47759800	0.28533100	-1.30202800
C	1.21680700	1.08696100	-1.35098000
C	0.66182000	1.48626200	-0.01139000
H	3.20439500	0.41563300	2.00627300
H	-0.10335100	-0.76914100	2.27622000
H	1.04069100	1.58450400	2.08804400
H	2.87551300	-0.07944400	-2.25390900
H	1.40303700	1.99907500	-1.95721000
H	0.43806400	0.55510300	-1.93992800
C	4.46673400	-0.70715600	-0.13254400
H	4.75306300	-1.04319000	-1.13844200
H	5.28531400	-0.08610900	0.26207400
H	4.39531900	-1.59286700	0.51917500
C	-0.67924900	2.18997700	-0.00626900
H	-1.38476600	1.51539400	-0.53519600
C	-1.24511400	2.44677800	1.38850900
H	-1.28264300	1.53101900	1.99834200
H	-0.63783800	3.18417100	1.93564600
H	-2.26628700	2.85010600	1.32088400
C	-0.64086900	3.50008800	-0.80995500
H	-1.62693300	3.98778600	-0.80251900
H	0.08670700	4.19927900	-0.36994500
H	-0.36139200	3.33772400	-1.86052300

H	1.62150300	-2.53416000	1.70060700

INT-2-P

C	-2.43493800	-2.45804800	0.60465300
C	-1.44457300	-1.56529600	0.15281800
C	-1.79625200	-0.22761800	-0.17145100
C	-3.12666400	0.24420600	-0.05959800
C	-4.20637000	-0.68986900	0.41899400
C	-3.74220400	-2.07033300	0.73978300
H	0.13171600	0.30684000	-0.66989000
H	-2.14583800	-3.48165600	0.84909500
H	-0.40837000	-1.88620800	0.04340300
C	-3.39151700	1.56482100	-0.39899000
H	-5.01032200	-0.74225100	-0.33959900
C	-2.37103500	2.41739400	-0.84219800
C	-1.08919500	1.91858400	-0.93290500
H	-4.41316400	1.94468500	-0.31862600
H	-2.57192900	3.45401200	-1.11018500
H	-0.22621900	2.50087100	-1.25744300
N	-0.84326100	0.64096300	-0.60460800
C	2.35135400	0.24973100	-0.98335100
C	2.32346400	1.65331400	-0.77669700
C	2.05010700	2.20036000	0.51469800
C	1.82307100	1.34689400	1.55864400
C	1.90650400	-0.14146000	1.43218000
C	2.14944000	-0.65019000	0.03706600
H	2.53574800	2.32178700	-1.61480700
H	-4.70231700	-0.25473200	1.30730100
H	2.56469800	-0.11762600	-1.99018800
H	1.61266000	1.75139500	2.55270900
H	2.70941000	-0.51978000	2.10027400
H	0.99655300	-0.61701300	1.85702300
C	2.02866000	3.69581400	0.69063500
H	1.73718400	3.98111800	1.71016500
H	3.02389000	4.12170600	0.49109300
H	1.33064700	4.17774500	-0.01274400
C	2.29044900	-2.14804400	-0.13393800
H	1.58760800	-2.62029700	0.57928600
C	1.95151900	-2.65295300	-1.53723500
H	0.96105700	-2.30988300	-1.87729800
H	2.69343900	-2.31861300	-2.27812900
H	1.95235600	-3.75219200	-1.55731100
C	3.70205900	-2.60127100	0.27754400
H	3.78491000	-3.69688000	0.22803000
H	4.45507700	-2.16927600	-0.39893700
H	3.95153000	-2.29370400	1.30319100
H	-4.49077900	-2.78299400	1.09192600

INT-2-Q

C	-1.47125800	-0.76880800	2.66919700
C	-0.54004600	-1.52020400	1.92613500
C	-0.67374600	-1.61194600	0.51710300
C	-1.74602300	-0.99849000	-0.17280700
C	-2.81129600	-0.27994400	0.60706100
C	-2.53816900	-0.15663900	2.06614600
H	1.01529200	-2.74098600	0.28437600
H	-1.33036800	-0.67686600	3.74756800
H	0.29726000	-2.01350200	2.42386900
C	-1.78879200	-1.09916500	-1.55593400
H	-3.77487400	-0.81099800	0.47180100
C	-0.81403800	-1.82230100	-2.26101300
C	0.19776700	-2.42829100	-1.55549600
H	-2.60297500	-0.61829800	-2.10302300
H	-0.84594400	-1.91007800	-3.34629000
H	0.99116600	-3.01291100	-2.02149600
N	0.23708500	-2.31598500	-0.21382300
C	1.19607900	0.88704800	-1.30206700
C	0.04479800	1.61023600	-1.70075500
C	-0.79579700	2.24162500	-0.73785700
C	-0.43861800	2.19211200	0.58075500
C	0.84367400	1.58604800	1.04939600
C	1.59197100	0.80191600	0.00769500
H	-0.20747400	1.67553700	-2.76196500
H	-2.98056800	0.71843400	0.16970100
H	1.77286600	0.38006000	-2.07875800
H	-1.06385900	2.68331500	1.33276000
H	1.49839900	2.40383600	1.42131300
H	0.67886900	0.96649300	1.95339600

C	-2.04745600	2.94115100	-1.19854300
H	-2.63606400	3.32481300	-0.35338100
H	-1.80044800	3.79563100	-1.84716900
H	-2.68905900	2.27044300	-1.79388900
C	2.77935800	-0.00751900	0.48514500
H	2.37192800	-0.74434700	1.21143500
C	3.50104800	-0.78255400	-0.61599400
H	2.82694800	-1.44240600	-1.18357200
H	3.97138200	-0.09826200	-1.33866900
H	4.29895900	-1.40568300	-0.18711200
C	3.78485900	0.85426500	1.26580500
H	4.63189100	0.24210700	1.60767000
H	4.18219300	1.65649700	0.62492500
H	3.33568900	1.31820200	2.15477900
H	-3.24669300	0.41962400	2.66467000

INT-2-R

C	0.70423600	-2.83107200	0.14786100
C	0.01386100	-2.24607800	-0.93058700
C	-1.11770800	-1.42842200	-0.68152600
C	-1.60673500	-1.20610600	0.62607200
C	-0.88562600	-1.81090900	1.79655100
C	0.30443900	-2.63297800	1.44248200
H	-1.41850900	-0.99399300	-2.65568000
H	1.57868900	-3.44942000	-0.06196300
H	0.34366800	-2.41450800	-1.95768700
C	-2.74081700	-0.42276900	0.78706200
H	-1.58955200	-2.41919000	2.39510400
C	-3.38947800	0.15097300	-0.31572300
C	-2.87213700	-0.06616400	-1.57094300
H	-3.13202500	-0.24834900	1.79220100
H	-4.27678600	0.77091900	-0.19513100
H	-3.30281600	0.35093300	-2.48133900
N	-1.78208900	-0.84334100	-1.71793100
C	-0.70960900	2.24941000	0.32805600
C	-0.06708100	1.68488900	1.47212100
C	1.12455400	0.93706500	1.33245200
C	1.72494200	0.71764700	0.11813200
C	1.10020400	1.27459900	-1.12793100
C	-0.17291000	2.03023300	-0.90909900
H	-0.47851600	1.86959900	2.46779000
H	-0.57474800	-0.99456500	2.47584800
H	1.83420700	1.92968100	-1.64410100
H	0.94563900	0.45920700	-1.86836100
H	0.86056300	-3.09255900	2.26208500
C	-1.93284800	3.10577000	0.52100400
H	-1.65649800	4.07435300	0.96628600
H	-2.44384800	3.31118900	-0.43022700
H	-2.65224000	2.63577200	1.20982800
C	3.09195900	0.06978700	0.03170900
H	3.15638000	-0.65917300	0.85851400
C	3.35266700	-0.67723300	-1.27808800
H	2.57977600	-1.43085700	-1.48796100
H	3.39585700	0.01107900	-2.13656100
H	4.32050900	-1.19711200	-1.23316800
C	4.18313400	1.12867400	0.26655000
H	4.05935000	1.61850600	1.24262100
H	5.18311400	0.67051900	0.23511700
H	4.14746400	1.90928300	-0.50986200
H	1.61133300	0.55077100	2.23438000
H	-0.64665800	2.47740300	-1.78914900

INT-2-S

C	-2.43557400	-2.45772900	0.60480600
C	-1.44492400	-1.56506000	0.15342700
C	-1.79634500	-0.22738400	-0.17110600
C	-3.12672200	0.24462600	-0.05957500
C	-4.20655800	-0.68908100	0.41943000
C	-3.74280500	-2.06981200	0.73968400
H	0.13177700	0.30670500	-0.66944800
H	-2.14671800	-3.48145200	0.84906200
H	-0.40872600	-1.88610500	0.04434000
C	-3.39139400	1.56512600	-0.39953100
H	-5.01112900	-0.74081900	-0.33852200
C	-2.37075400	2.41743700	-0.84288800
C	-1.08894300	1.91848100	-0.93316900
H	-4.41301300	1.94513200	-0.31948300
H	-2.57152700	3.45396300	-1.11131800

H	-0.22586600	2.50058600	-1.25775900
N	-0.84319000	0.64094200	-0.60438900
C	2.05069400	2.20011700	0.51489400
C	1.82363900	1.34656500	1.55877700
C	1.90658100	-0.14179500	1.43209200
C	2.14942000	-0.65041000	0.03691300
C	2.35139800	0.24961000	-0.98340800
C	2.32378900	1.65317700	-0.77658400
H	1.61351400	1.75099500	2.55293100
H	-4.70158200	-0.25394100	1.30827600
H	2.56453500	-0.11764700	-1.99032600
H	0.99633500	-0.61701100	1.85668300
H	-4.49160900	-2.78242700	1.09143100
C	2.02967400	3.69555500	0.69105600
H	3.02532500	4.12105300	0.49276600
H	1.33269600	4.17784800	-0.01308700
H	1.73713800	3.98081500	1.71029700
C	2.29004300	-2.14827400	-0.13424200
H	1.58689500	-2.62042100	0.57875500
C	1.95122000	-2.65293200	-1.53760700
H	0.96065500	-2.31015700	-1.87763200
H	2.69304600	-2.31826900	-2.27845000
H	1.95235400	-3.75217000	-1.55789900
C	3.70146000	-2.60192700	0.27743000
H	3.95089200	-2.29442600	1.30310700
H	3.78399300	-3.69756000	0.22792500
H	4.45468600	-2.17014800	-0.39895700
H	2.70917100	-0.52058600	2.10027500
H	2.53609400	2.32170500	-1.61464200

INT-2-T

C	3.05201900	-2.06482100	1.35503100
C	1.96957800	-1.22786000	1.02211100
C	2.16561900	-0.15027400	0.11732500
C	3.42698400	0.11558100	-0.46936000
C	4.60132700	-0.76371300	-0.13052700
C	4.30048800	-1.86744400	0.82627900
H	0.21121700	0.46614000	0.22714100
H	2.88363900	-2.88790000	2.05173700
H	0.97756400	-1.39304500	1.44456500
C	3.53713500	1.18869200	-1.34408300
H	5.42157500	-0.14161200	0.27527700
C	2.43020600	1.99478600	-1.64523900
C	1.22027500	1.70259200	-1.05305600
H	4.50352600	1.40765000	-1.80526600
H	2.51022200	2.83732700	-2.33120000
H	0.30033400	2.26205600	-1.22542700
N	1.12397200	0.66321500	-0.20829400
C	-1.86813900	1.63449000	1.17674800
C	-2.18477400	1.87278900	-0.19553700
C	-2.30184300	0.85963100	-1.10293000
C	-2.18611600	-0.59086000	-0.73451300
C	-1.73891600	-0.76324000	0.68876600
C	-1.63462900	0.28215200	1.56702400
H	-2.34237800	2.90538800	-0.52278700
H	5.02195800	-1.19060200	-1.06074000
H	-1.55739800	-1.78127800	1.04457900
H	-1.43763200	-1.06608100	-1.40408700
H	5.12254100	-2.53125300	1.10172500
C	-1.83191000	2.75203600	2.17342100
H	-1.17076700	2.52245600	3.02158600
H	-1.49801700	3.69547000	1.71673600
H	-2.83766300	2.93681300	2.58930300
C	-3.51911100	-1.35845100	-1.04344900
H	-3.74994900	-1.12475400	-2.09769300
C	-3.33946300	-2.87162000	-0.93485700
H	-2.49487900	-3.22768500	-1.54524500
H	-3.17079300	-3.19003300	0.10596100
H	-4.24418800	-3.38888200	-1.28570100
C	-4.67595700	-0.86222300	-0.17995900
H	-4.82402500	0.22323400	-0.28088400
H	-5.61351900	-1.35765700	-0.47135200
H	-4.49962200	-1.08210000	0.88508100
H	-2.55352600	1.09016200	-2.14239600
H	-1.36266200	0.08022500	2.60797500

MECP-2-A

C	3.36785600	-0.48431400	1.66728900

C	2.13138100	0.19743100	1.89690700
C	1.52138700	0.93461700	0.85961100
C	2.11115100	0.92215200	-0.43268000
C	3.44149900	0.28358300	-0.71171400
C	3.99216500	-0.46600600	0.46516600
H	-0.16953300	1.70368800	1.98627200
H	3.81808600	-1.03507200	2.49549500
H	1.69836700	0.23247200	2.89768000
H	4.15807000	1.07023500	-1.02294500
C	0.30938700	2.21014000	-1.32509600
C	-0.28813100	2.28529900	-0.07717400
H	1.93070000	1.53083000	-2.35249500
H	-0.08507100	2.67629300	-2.22626100
H	-1.22812700	2.82560000	0.02872500
C	-2.26469700	-0.57602200	0.23395600
C	-1.84545000	-0.44707400	-1.11962500
C	-0.64340900	-1.01335600	-1.57680000
C	0.19775800	-1.71233600	-0.73740400
C	-0.13453100	-1.80975800	0.70290100
C	-1.42820200	-1.22086000	1.10702600
H	-2.49664900	0.05613500	-1.83847100
H	3.35452100	-0.38740900	-1.58738300
H	-0.03975700	-2.85226900	1.06540100
H	0.69676200	-1.30580600	1.28917300
H	4.94016600	-0.98665400	0.31999800
C	1.38861700	-2.46465000	-1.24218100
H	1.13693200	-3.53396400	-1.34890100
H	1.71165100	-2.10996200	-2.23147000
H	2.23379000	-2.40796900	-0.54028000
C	-3.62664300	-0.06597300	0.67267500
H	-3.74002200	-0.33843500	1.73474500
C	-4.74865900	-0.76223600	-0.10582800
H	-4.65943400	-1.85619500	-0.04069600
H	-5.73144500	-0.47523300	0.29528400
H	-4.73646000	-0.48455800	-1.17168700
C	-3.73862800	1.45759100	0.57587500
H	-2.99711700	1.95443500	1.21971600
H	-3.59719100	1.80862300	-0.45949800
H	-4.73455300	1.79280600	0.89980200
H	-0.39495200	-0.93571600	-2.63942200
H	-1.73234800	-1.34903000	2.15019400
N	1.48713700	1.55677400	-1.43603100
C	0.29942700	1.65006100	1.00197200

MECP-2-B

C	-2.04891500	-1.91535700	-1.80704200
C	-2.64148600	-0.91133800	-0.99017400
C	-2.08066400	-0.59382000	0.26939600
C	-0.93686300	-1.31381100	0.71019000
C	-0.43230500	-2.53209400	-0.00364500
C	-0.97826000	-2.64486300	-1.39540300
H	-3.43784600	1.00554500	0.81831300
H	-2.45926900	-2.08378300	-2.80490600
H	-3.53275600	-0.37905800	-1.32498900
H	-0.73358000	-3.42576100	0.58305900
C	-0.74081400	0.07980900	2.63821400
C	-1.88489300	0.77582000	2.28682700
H	0.50826300	-1.43851700	2.11271600
H	-0.14835600	0.27589800	3.53032800
H	-2.24187700	1.57934500	2.93089100
C	0.43590500	2.29949700	0.30414400
C	1.50346700	1.39624600	0.48613300
C	1.75927800	0.34624700	-0.43623100
C	0.92640300	0.21577600	-1.52122800
C	-0.20580800	1.13585800	-1.77887200
C	-0.40628200	2.21566800	-0.77702100
H	2.17937500	1.54864600	1.33158400
H	0.67001600	-2.54393800	-0.00870300
H	-0.13755500	1.55942900	-2.80193200
H	-1.15949700	0.54516800	-1.84271800
H	-0.53948200	-3.40494200	-2.04416000
C	-1.52509600	3.17567900	-1.01708800
H	-1.66482700	3.86997900	-0.17759000
H	-1.33900900	3.77178700	-1.92653500
H	-2.47076100	2.63474900	-1.19465900
C	2.99821200	-0.52364500	-0.28409700
H	2.93741500	-1.30839100	-1.05743400
C	4.25468700	0.31149600	-0.56736000

H	5.15143900	-0.32489900	-0.58788600
H	4.17372200	0.82196200	-1.53755800
H	4.40687000	1.08098500	0.20683800
C	3.10487500	-1.22107700	1.07660000
H	3.08889200	-0.50437700	1.91364600
H	2.30016700	-1.96020800	1.22837700
H	4.04918200	-1.77964100	1.14975600
H	0.28961000	3.09819000	1.03610100
H	1.12735300	-0.55556300	-2.27038600
C	-2.54179000	0.45301900	1.10919400
N	-0.33934200	-0.93961000	1.84608900

MECP-2-C

C	0.56948800	-2.33512900	1.44952200
C	1.80847800	-1.66599400	1.51436700
C	2.28405000	-0.92419900	0.39691800
C	1.48872600	-0.86559300	-0.77385700
C	0.19039600	-1.59215900	-0.91545000
C	-0.22610200	-2.28809900	0.33729500
H	4.15033600	-0.24632700	1.26427400
H	0.22671000	-2.89273500	2.32367900
H	2.42968500	-1.73281700	2.40818300
H	0.25642600	-2.31251900	-1.75563300
C	3.08352500	0.55317500	-1.84513100
C	3.90207500	0.52180700	-0.72957900
H	1.33149300	-0.11335700	-2.64300700
H	3.30780300	1.10533100	-2.75661600
H	4.84170300	1.07462400	-0.73767500
C	-0.44028400	1.91252700	-0.50820200
C	-1.64303000	1.21558900	-0.76877100
C	-2.25773300	0.39709200	0.21802000
C	-1.62914200	0.25525000	1.42821800
C	-0.37927800	0.97673400	1.78306900
C	0.19853100	1.82934300	0.70318100
H	-2.13490900	1.35773500	-1.73448200
H	-0.59076200	-0.85987900	-1.22278200
H	-0.54275200	1.59108600	2.69307400
H	0.39465200	0.24804100	2.12694800
H	-1.17771700	-2.82082300	0.31641800
C	1.41203100	2.63595400	1.03839200
H	1.86825000	3.09043700	0.14762800
H	1.14671300	3.45192400	1.73260400
H	2.16906200	2.02400600	1.55485900
C	-3.58637200	-0.28177400	-0.06559000
H	-3.81958700	-0.89984800	0.81704600
C	-4.70274300	0.75763500	-0.21739800
H	-5.68494000	0.26697000	-0.28534600
H	-4.72304800	1.44715500	0.63841700
H	-4.56669400	1.35674700	-1.13174500
C	-3.53042200	-1.21103700	-1.28222600
H	-3.30499100	-0.65737800	-2.20799400
H	-2.77337900	-2.00069300	-1.16442900
H	-4.50070400	-1.70692400	-1.42984100
H	-0.02615500	2.56069800	-1.28643700
H	-2.08914800	-0.36053600	2.20629600
N	1.92957800	-0.14825500	-1.81950900
C	3.50862300	-0.21331200	0.38107500

MECP-2-D

C	1.82920300	-2.68394000	-0.92558300
C	0.95961100	-2.42489400	0.16942200
C	1.07208300	-1.22024200	0.90415800
C	2.08171200	-0.28872400	0.54739000
C	3.11550200	-0.57778200	-0.50057100
C	2.81465000	-1.81908600	-1.28620500
H	-0.58509800	-1.55047300	2.26174200
H	1.68323700	-3.60073000	-1.50060300
H	0.19753600	-3.15068900	0.45677000
H	4.10333200	-0.68846700	-0.00664900
C	1.30398600	1.25575200	2.19308000
C	0.31761700	0.37215000	2.59792100
H	2.88094800	1.52481500	0.93219500
H	1.47267600	2.23480300	2.63892200
H	-0.35937000	0.65932200	3.40233800
C	-1.78231200	1.39261100	0.18409100
C	-0.74311300	2.28540500	-0.15207700
C	0.23129100	1.96097700	-1.13731400
C	0.14211700	0.74924000	-1.77013200

C	-0.92875500	-0.23226600	-1.46964900
C	-1.90646500	0.16340000	-0.41538100
H	-0.71278000	3.26862400	0.32426100
H	3.22526900	0.29513500	-1.16919300
H	-2.49937500	1.69955300	0.94784900
H	0.85759200	0.48731400	-2.55559400
H	-1.45722300	-0.51909500	-2.40055900
H	-0.46018200	-1.20086900	-1.16480900
C	1.30652200	2.95995800	-1.47476800
H	2.05395900	2.54099600	-2.16296500
H	0.87602800	3.85104500	-1.95756000
H	1.82313000	3.32330300	-0.57071200
C	-3.01086900	-0.82078200	-0.10812300
H	-2.53879300	-1.82210400	-0.10948400
C	-3.67768500	-0.61956700	1.25214300
H	-2.94545600	-0.58517800	2.07364500
H	-4.26453200	0.31134100	1.28209900
H	-4.37467000	-1.44503200	1.45572600
C	-4.06540000	-0.81400300	-1.22938300
H	-4.82388200	-1.58886400	-1.04627600
H	-4.57401300	0.16146600	-1.26786500
H	-3.62468200	-1.00688000	-2.21822300
H	3.46500700	-2.03848700	-2.13451600
N	2.15210600	0.87145200	1.21211600
C	0.19307300	-0.84837600	1.95508800

MECP-2-E

C	-3.28140300	-0.75074100	-1.82276700
C	-1.98858400	-0.13943000	-1.88267000
C	-1.56046700	0.68646000	-0.84031000
C	-2.36575700	0.92271400	0.31638000
C	-3.73384200	0.29440000	0.40113300
C	-4.10716600	-0.56317900	-0.76539800
H	0.27419700	1.08955500	-1.66872500
H	-3.59938800	-1.37603900	-2.65934700
H	-1.36217700	-0.27068000	-2.76748800
C	-1.87306200	1.73705800	1.31782400
H	-4.49108100	1.09150000	0.52462700
C	-0.60018600	2.33572900	1.21867000
C	0.15794900	2.08401600	0.10367900
H	-2.48784900	1.92878700	2.20094600
H	-0.21308400	2.98244200	2.00459800
H	1.15080400	2.50170200	-0.05896700
N	-0.32631100	1.28741400	-0.87327500
C	2.37036100	-0.55988900	-0.16604700
C	1.97705800	-0.16631300	1.14799500
C	0.80691700	-0.66282200	1.75304700
C	-0.02678000	-1.54251600	1.10306600
C	0.31092100	-1.98387500	-0.27630300
C	1.56291300	-1.43064900	-0.84588100
H	2.61765000	0.50943700	1.72043000
H	-3.80837100	-0.29609400	1.33441500
H	0.31590600	-3.09126200	-0.33283900
H	-0.55171500	-1.72919200	-0.94833700
H	-5.09122100	-1.03489800	-0.74391100
C	-1.25340400	-2.12041300	1.73036400
H	-1.11063500	-3.19533300	1.93456700
H	-1.50589200	-1.62624800	2.67844100
H	-2.11498500	-2.04884100	1.04618500
C	3.66677800	-0.04783600	-0.76875700
H	3.75327700	-0.50370500	-1.76884600
C	4.87870300	-0.49852900	0.05316700
H	4.88485000	-1.58985400	0.18629700
H	5.81310100	-0.21079700	-0.45018200
H	4.88677600	-0.03554200	1.05243000
C	3.64982200	1.47230100	-0.95561700
H	2.82325200	1.79186300	-1.61145200
H	3.55734300	1.99908400	0.00846700
H	4.58372800	1.81724200	-1.42210300
H	0.56067500	-0.34077600	2.76826200
H	1.85439900	-1.77316200	-1.84399600

MECP-2-F

C	1.63607900	-3.00960700	-0.42610700
C	0.86143100	-2.24615300	0.49624200
C	1.24369400	-0.93732900	0.81384700
C	2.39580800	-0.32509000	0.23774500
C	3.22544800	-1.10554800	-0.75015900

C	2.73760500	-2.49174200	-1.02719900
H	-0.35088000	-0.59211500	2.05383200
H	1.32290500	-4.03158100	-0.64667200
H	-0.01650600	-2.68642200	0.97397300
C	2.72364700	0.96479000	0.61354700
H	4.27051100	-1.15273600	-0.39075900
C	1.93725100	1.68065600	1.53762100
C	0.81163700	1.08143600	2.04456900
H	3.61142400	1.43764600	0.18643300
H	2.19881400	2.69257400	1.84424400
H	0.13744700	1.56528800	2.75048600
N	0.50079100	-0.18051500	1.68242900
C	-2.07874800	1.28611400	0.32432400
C	-1.20631100	2.34266300	-0.01460100
C	-0.20170800	2.19667800	-1.01350200
C	-0.10859000	0.99963100	-1.66871000
C	-1.02583200	-0.13698200	-1.40270500
C	-2.00774400	0.06177500	-0.29553500
H	-1.31591900	3.30597900	0.49076900
H	3.28940700	-0.54020200	-1.69858100
H	-2.81758800	1.45724300	1.11039800
H	0.63906300	0.86789800	-2.45660900
H	-1.56550600	-0.40458500	-2.33576500
H	-0.43720500	-1.06186000	-1.20325500
C	0.70788300	3.35279100	-1.32647700
H	1.52730000	3.05506500	-1.99497300
H	0.15039300	4.16465600	-1.81886200
H	1.14487500	3.77466400	-0.40825100
C	-2.89936500	-1.11035900	0.04243900
H	-2.26323500	-2.01287900	-0.03616600
C	-3.47995300	-1.06811400	1.45575000
H	-2.70225100	-0.94028500	2.22720000
H	-4.20337400	-0.24736800	1.57362200
H	-4.01279700	-2.00352300	1.67768300
C	-4.02066800	-1.26459600	-1.00024300
H	-4.60985300	-2.17084600	-0.79877900
H	-4.69959400	-0.39937500	-0.96557200
H	-3.62512200	-1.34665500	-2.02260100
H	3.31277000	-3.09305500	-1.73387500

MECP-2-G

C	1.81207700	-1.20494100	-2.38110600
C	0.85680200	-1.85273700	-1.53860300
C	0.88477000	-1.61745600	-0.16069500
C	1.88970300	-0.79886400	0.44598200
C	3.02266100	-0.27898600	-0.40265100
C	2.79660600	-0.41916300	-1.87541900
H	-0.79970900	-2.71463100	0.24708500
H	1.72240200	-1.33753100	-3.46127000
H	0.10282200	-2.51631800	-1.96711400
C	1.82469300	-0.55848300	1.80106300
H	3.94644400	-0.83306600	-0.13891800
C	0.79788100	-1.10933300	2.60053300
C	-0.13961200	-1.90635800	2.00015000
H	2.58990900	0.06521700	2.26983400
H	0.75596600	-0.93133000	3.67421600
H	-0.95580900	-2.38802200	2.53926500
N	-0.08227600	-2.13107400	0.66781300
C	-1.50314300	1.17103800	1.02175300
C	-0.40285900	2.01526100	1.27810100
C	0.54900700	2.34448900	0.27711500
C	0.35120000	1.85077100	-0.98625300
C	-0.80807500	1.00189300	-1.33765500
C	-1.72904800	0.64089800	-0.22555400
H	-0.28434300	2.43565600	2.28034900
H	3.23959900	0.76816600	-0.13531300
H	-2.18038000	0.94537500	1.84734100
H	1.04182400	2.11766700	-1.79116800
H	-1.37111200	1.47790400	-2.16612200
H	-0.44714900	0.05873300	-1.81463600
C	1.72546800	3.21713800	0.61917200
H	2.35946200	3.40370000	-0.25843700
H	1.39487700	4.19165800	1.00870200
H	2.34656300	2.75243300	1.40185500
C	-2.85785700	-0.30734700	-0.55527800
H	-2.37812300	-1.17568100	-1.05406500
C	-3.62177500	-0.82164600	0.66250800
H	-2.95650000	-1.28150500	1.40916700

H	-4.17297800	-0.01052100	1.16240000
H	-4.35979400	-1.57664600	0.35661600
C	-3.82769000	0.30465100	-1.58015800
H	-4.62556600	-0.41158400	-1.82314000
H	-4.29601700	1.21278300	-1.17185300
H	-3.32732700	0.56903300	-2.52218200
H	3.50601600	0.07106000	-2.54532100

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C	-2.80151200	1.60600200	-1.53600200
C	-2.14001200	1.36548800	-0.32883400
C	-2.45200800	2.16839800	0.80103300
C	-3.41064500	3.18183200	0.66592500
C	-4.06748000	3.42891200	-0.52815300
C	-3.74555400	2.62338300	-1.61461500
H	-2.60956800	1.01047300	-2.42998400
H	-4.80992400	4.22222900	-0.60499900
C	-1.72030200	1.84470100	2.02969300
C	-1.87700300	2.44731300	3.28639600
C	-1.11915400	2.01293900	4.36023600
H	-2.60078700	3.24825000	3.40835300
C	-0.08559600	0.42799800	2.93457700
C	-0.18996700	0.97525800	4.20531500
H	-1.25183100	2.48321900	5.33768400
H	0.60945100	-0.39003500	2.73621400
N	-0.81825700	0.84136500	1.88855300
C	0.64271100	0.47075100	5.34940100
H	1.23983000	1.28286500	5.79017200
H	0.00466200	0.06244200	6.14749300
H	1.33122000	-0.32280700	5.02858700
F	-3.71999300	3.95930900	1.70578800
F	-4.36306400	2.84114300	-2.76862500
Ir	-0.70049800	-0.00000100	-0.00000200
C	-2.80149200	-1.60598500	1.53604300
C	-2.14001800	-1.36547600	0.32886100
C	-2.45204900	-2.16838000	-0.80100100
C	-3.41069300	-3.18180400	-0.66587300
C	-4.06750300	-3.42887900	0.52822000
C	-3.74554300	-2.62335600	1.61467600
H	-2.60952100	-1.01046000	2.43002200
H	-4.80995400	-4.22218900	0.60508100
C	-1.72036700	-1.84468900	-2.02967700
C	-1.87710400	-2.44729600	-3.28637800
C	-1.11927200	-2.01293000	-4.36023300
H	-2.60090000	-3.24822400	-3.40832000
C	-0.08566300	-0.42800500	-2.93459400
C	-0.19006900	-0.97526100	-4.20533000
H	-1.25197800	-2.48320600	-5.33767900
H	0.60940000	0.39001800	-2.73624500
N	-0.81830700	-0.84136400	-1.88855400
C	0.64259000	-0.47076300	-5.34943400
H	1.23968500	-1.28288400	-5.79022300
H	0.00453000	-0.06243900	-6.14750900
H	1.33112100	0.32278200	-5.02863300
F	-3.72007400	-3.95927500	-1.70573000
F	-4.36302800	-2.84111200	2.76870000
C	0.94304200	2.57449700	-0.69769900
C	2.23047400	0.72175600	-0.18426400
C	3.39266100	1.46970300	-0.33297000
C	3.34212900	2.82645100	-0.68106800
C	2.06871100	3.37152900	-0.86362500
H	-0.06332200	2.97890600	-0.83158600
C	2.23047200	-0.72177100	0.18423200
C	3.39265800	-1.46972000	0.33294000
C	3.34212200	-2.82646800	0.68103800
H	4.35881200	-0.99472700	0.16941100
C	0.94303600	-2.57451100	0.69766000
C	2.06870200	-3.37154500	0.86358600
H	-0.06333000	-2.97891800	0.83154300
N	1.01698800	-1.28282700	0.37047200
H	4.35881400	0.99470700	-0.16944200
H	1.92740700	4.41698500	-1.13263100
N	1.01699100	1.28281400	-0.37050600
H	1.92739500	-4.41700200	1.13258900
C	4.63454300	-3.62913700	0.83833900
C	4.63455300	3.62911400	-0.83837200
C	5.39950100	3.60382800	0.49864300
H	5.68056100	2.58303200	0.79812400

H	6.32759700	4.18767800	0.40955400
H	4.79798900	4.04371500	1.30839100
C	4.35634600	5.08779800	-1.22023300
H	5.30782600	5.62850500	-1.32420100
H	3.82780900	5.16799400	-2.18224400
H	3.76620700	5.60909800	-0.45138800
C	5.48917300	2.98137000	-1.94445400
H	4.95355700	2.97193000	-2.90581200
H	6.41981800	3.55191000	-2.08064600
H	5.77080600	1.94609100	-1.70026500
C	5.48913200	-2.98145600	1.94448300
H	6.41975900	-3.55202200	2.08068700
H	5.77079700	-1.94617400	1.70035000
H	4.95347700	-2.97204700	2.90581900
C	4.35632500	-5.08784200	1.22011100
H	3.76626100	-5.60911900	0.45119300
H	5.30780500	-5.62854000	1.32413600
H	3.82770700	-5.16808900	2.18207300
C	5.39952900	-3.60377600	-0.49865300
H	4.79804800	-4.04363400	-1.30843900
H	5.68058100	-2.58296200	-0.79807700
H	6.32763200	-4.18761700	-0.40956400

^{3}Ir-PS

C	-2.80151200	1.60600200	-1.53600200
C	-2.14001200	1.36548800	-0.32883400
C	-2.45200800	2.16839800	0.80103300
C	-3.41064500	3.18183200	0.66592500
C	-4.06748000	3.42891200	-0.52815300
C	-3.74555400	2.62338300	-1.61461500
H	-2.60956800	1.01047300	-2.42998400
H	-4.80992400	4.22222900	-0.60499900
C	-1.72030200	1.84470100	2.02969300
C	-1.87700300	2.44731300	3.28639600
C	-1.11915400	2.01293900	4.36023600
H	-2.60078700	3.24825000	3.40835300
C	-0.08559600	0.42799800	2.93457700
C	-0.18996700	0.97525800	4.20531500
H	-1.25183100	2.48321900	5.33768400
H	0.60945100	-0.39003500	2.73621400
N	-0.81825700	0.84136500	1.88855300
C	0.64271100	0.47075100	5.34940100
H	1.23983000	1.28286500	5.79017200
H	0.00466200	0.06244200	6.14749300
H	1.33122000	-0.32280700	5.02858700
F	-3.71999300	3.95930900	1.70578800
F	-4.36306400	2.84114300	-2.76862500
Ir	-0.70049800	-0.00000100	-0.00000200
C	-2.80149200	-1.60598500	1.53604300
C	-2.14001800	-1.36547600	0.32886100
C	-2.45204900	-2.16838000	-0.80100100
C	-3.41069300	-3.18180400	-0.66587300
C	-4.06750300	-3.42887900	0.52822000
C	-3.74554300	-2.62335600	1.61467600
H	-2.60952100	-1.01046000	2.43002200
H	-4.80995400	-4.22218900	0.60508100
C	-1.72036700	-1.84468900	-2.02967700
C	-1.87710400	-2.44729600	-3.28637800
C	-1.11927200	-2.01293000	-4.36023300
H	-2.60090000	-3.24822400	-3.40832000
C	-0.08566300	-0.42800500	-2.93459400
C	-0.19006900	-0.97526100	-4.20533000
H	-1.25197800	-2.48320600	-5.33767900
H	0.60940000	0.39001800	-2.73624500
N	-0.81830700	-0.84136400	-1.88855400
C	0.64259000	-0.47076300	-5.34943400
H	1.23968500	-1.28288400	-5.79022300
H	0.00453000	-0.06243900	-6.14750900
H	1.33112100	0.32278200	-5.02863300
F	-3.72007400	-3.95927500	-1.70573000
F	-4.36302800	-2.84111200	2.76870000
C	0.94304200	2.57449700	-0.69769900
C	2.23047400	0.72175600	-0.18426400
C	3.39266100	1.46970300	-0.33297000
C	3.34212900	2.82645100	-0.68106800
C	2.06871100	3.37152900	-0.86362500
H	-0.06332200	2.97890600	-0.83158600
C	2.23047200	-0.72177100	0.18423200

C	3.39265800	-1.46972000	0.33294000
C	3.34212200	-2.82646800	0.68103800
H	4.35881200	-0.99472700	0.16941100
C	0.94303600	-2.57451100	0.69766000
C	2.06870200	-3.37154500	0.86358600
H	-0.06333000	-2.97891800	0.83154300
N	1.01698800	-1.28282700	0.37047200
H	4.35881400	0.99470700	-0.16944200
H	1.92740700	4.41698500	-1.13263100
N	1.01699100	1.28281400	-0.37050600
H	1.92739500	-4.41700200	1.13258900
C	4.63454300	-3.62913700	0.83833900
C	4.63455300	3.62911400	-0.83837200
C	5.39950100	3.60382800	0.49864300
H	5.68056100	2.58303200	0.79812400
H	6.32759700	4.18767800	0.40955400
H	4.79798900	4.04371500	1.30839100
C	4.35634600	5.08779800	-1.22023300
H	5.30782600	5.62850500	-1.32420100
H	3.82780900	5.16799400	-2.18224400
H	3.76620700	5.60909800	-0.45138800
C	5.48917300	2.98137000	-1.94445400
H	4.95355700	2.97193000	-2.90581200
H	6.41981800	3.55191000	-2.08064600
H	5.77080600	1.94609100	-1.70026500
C	5.48913200	-2.98145600	1.94448300
H	6.41975900	-3.55202200	2.08068700
H	5.77079700	-1.94617400	1.70035000
H	4.95347700	-2.97204700	2.90581900
C	4.35632500	-5.08784200	1.22011100
H	3.76626100	-5.60911900	0.45119300
H	5.30780500	-5.62854000	1.32413600
H	3.82770700	-5.16808900	2.18207300
C	5.39952900	-3.60377600	-0.49865300
H	4.79804800	-4.04363400	-1.30843900
H	5.68058100	-2.58296200	-0.79807700
H	6.32763200	-4.18761700	-0.40956400

TS-HAT-naphthalene

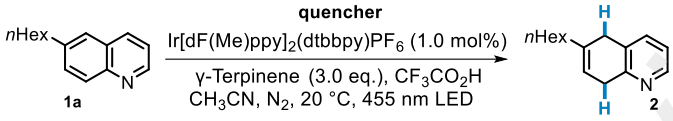
C	-3.42287100	-0.11507800	-0.47246300
C	-2.51516600	0.67077100	-1.24783000
C	-1.47504000	1.43541000	-0.61508100
C	-1.26703900	1.29196100	0.79485000
C	-2.04551400	0.29154600	1.51973600
C	-3.23770400	-0.27558500	0.86460600
H	-0.83055700	2.44782300	-2.40326600
H	-4.27474600	-0.58492000	-0.96957600
H	-2.65895300	0.76734400	-2.32582400
H	-2.05350300	0.36812500	2.61215800
C	0.50449300	2.96555300	0.68222300
C	0.31527900	3.09829800	-0.68208100
H	1.26454900	3.55869800	1.19529500
H	0.92620200	3.79518000	-1.25982000
C	1.05126800	-1.25620600	1.24532300
C	-0.29545400	-1.83074700	1.08664500
C	-0.66545700	-2.23148800	-0.28683900
C	0.00536400	-1.70535700	-1.33011400
C	1.18840900	-0.80061600	-1.17661200
C	1.77081300	-0.78304100	0.20995200
H	-0.55866200	-2.57222900	1.85590600
H	-1.10189500	-0.91028500	1.36826700
H	1.47127700	-1.21261200	2.25551800
H	-0.29770800	-1.96407100	-2.34951500
H	1.96230700	-1.07055100	-1.91741700
H	0.89756800	0.23856700	-1.44465000
C	-1.79064800	-3.21200500	-0.45182500
H	-2.10005900	-3.30316800	-1.50255600
H	-1.48528800	-4.20991500	-0.09470900
H	-2.66775000	-2.90784700	0.13892800
C	3.19147100	-0.28674900	0.38849500
H	3.32491200	-0.07404300	1.46277400
C	3.48217800	1.00268300	-0.38341200
H	4.49466500	1.36813700	-0.15278700
H	3.43209500	0.84093700	-1.47207300
H	2.76112300	1.79089800	-0.12795800
C	4.19287600	-1.38787800	0.00985300
H	5.22760600	-1.04698000	0.17127600
H	4.02995700	-2.29477400	0.61025300

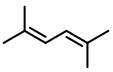
H	4.09737500	-1.66512800	-1.05246500	H	-0.12358400	1.94657900	2.49016300
H	-3.93540900	-0.86812900	1.46046400				
C	-0.67028100	2.33222900	-1.32807400				
C	-0.28389500	2.05669300	1.41458200				

10. Experimental Mechanistic Investigations

10.1 Control experiments with excited state quenchers

Table S11. Photochemical reduction reaction with triplet quenchers.



quencher		Yield (%)
none		62
$Cu(acac)_2$	(50 mol%)	30
$Ni(acac)_2$	(100 mol%)	45
	(50 mol%)	low conversion

10.2 Side products detection

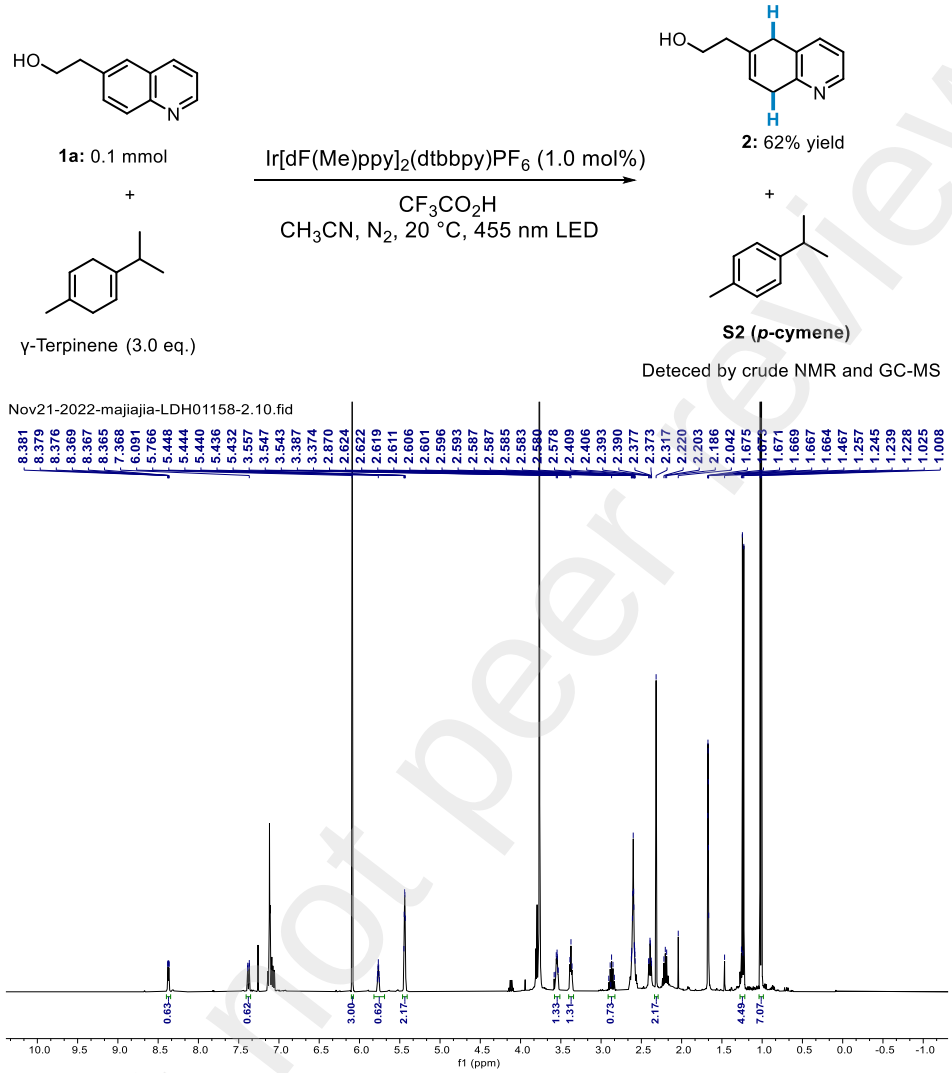


Figure S8. Crude ^{1}H NMR of the photochemical reduction of **1a**.

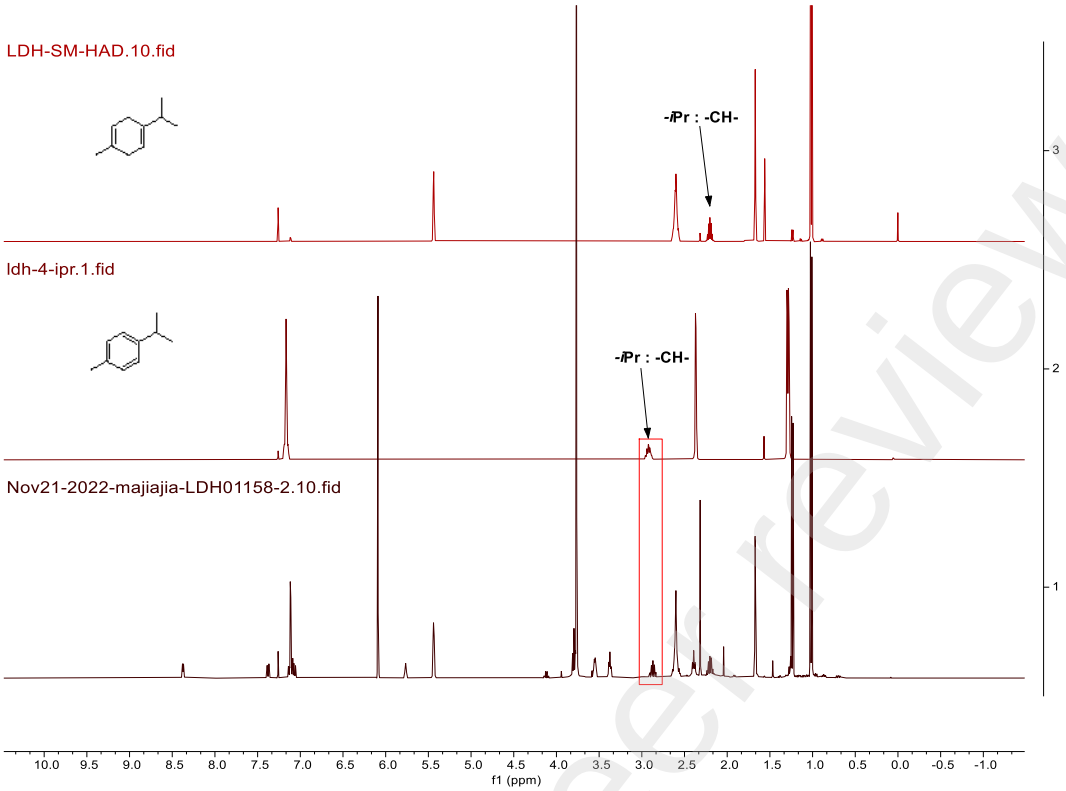
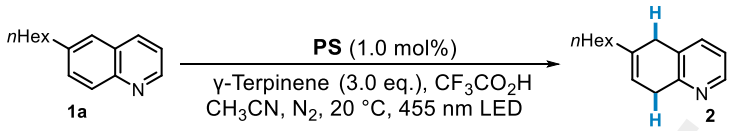


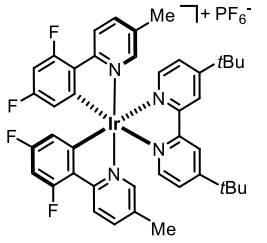
Figure S9. The γ-terpinene has been converted to **S2** (*p*-cymene) as detected by crude ^{1}H NMR analysis.

10.3 Comparison of various photosensitizers

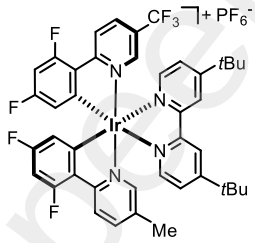
Table S12. Photochemical reduction reaction with various photosensitizers.



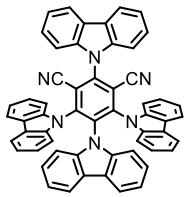
Entry	PS	E_T (kcal/mol)	$E_{1/2}^{II/III*}$ (V)	$E_{1/2}^{III*/IV}$ (V)	Yield (%)
1	**A**	62.9	+ 0.97	–0.92	62
2	**B**	61.8	+ 1.21	– 0.89	60
3	**C**	58.3	+ 1.49	– 1.24	53
4	**D**	46.5	+ 0.77	– 0.81	n.d.
5	**E**	44.7	+ 1.45	--	n.d.



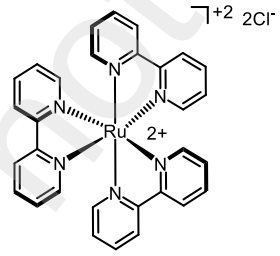
A: Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$



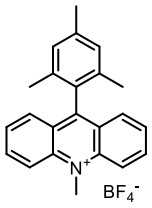
B: Ir[dF(CF$_3$)ppy$_2$(dtbbpy)]PF$_6$



C: 4CzIPN



D: Ru(bpy)$_3$Cl$_2$

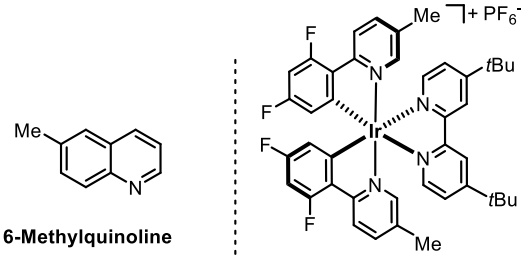


E: [Mes-Acr]BF$_4$

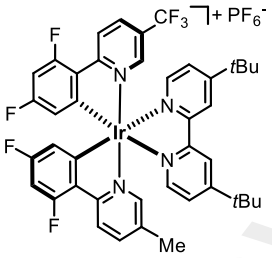
Control experiments were performed by conducting the photochemical reaction in the presence of various photosensitizers **A-E**. As shown in Table S12, yields of the reduction product **2** strongly correlate to the triplet energy of the photosensitizers rather than the redox potentials. These observations support the triplet energy transfer pathway over the single electron transfer (SET) event.

10.4 Exclusion of single electron transfer event

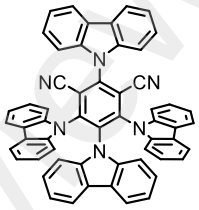
Table S13. Redox potential comparison of the quinoline with photosensitizers.



A: Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$



B: Ir[dF(CF$_3$)ppy$_2$(dtbbpy)]PF$_6$



C: 4CzIPN

$E_{1/2}^{red}$ = < –2.3 V (+ H^+)	$E_{1/2}^{PC+/PC*}$ = -0.92 V	$E_{1/2}^{PC+/PC*}$ = -0.89 V	$E_{1/2}^{PC+/PC*}$ = -1.24 V
$E_{1/2}^{ox}$ = > +1.8 V (+ H^+)	$E_{1/2}^{PC*/PC-}$ = +0.97 V	$E_{1/2}^{PC*/PC-}$ = +1.21 V	$E_{1/2}^{PC*/PC-}$ = +1.49 V
E_T (kcal/mol) = 61.2 (+ H^+)	E_T (kcal/mol) = 62.9	E_T (kcal/mol) = 61.8	E_T (kcal/mol) = 58.3
E_T (kcal/mol) = 58.9 (+ BF_3)			

As outlined in Table S13, reductive potential of an exemplified protonated quinoline has been determined to be < –2.3 V (*vs.* SCE) and the oxidative potential is > +1.8 V (*vs.* SCE) in a previous report.[29]

In this work, the photocatalysts **A-C** can smoothly enable the reduction of quinoline and related derivatives. Notably, neither the reductive potential (< -2.3 V) nor the oxidative one (> +1.8 V) of quinoline is amenable to the redox range of any these photosensitizers. In contrast, the triplet energy (58.9 kcal/mol) of the Lewis acid-bound 6-methylquinoline is amendable to all the photocatalyst.

This observation clearly excludes out the mechanism of single electron transfer between quinolines and the photocatalyst, but instead, supports the triplet-triplet energy transfer process.

11. References

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