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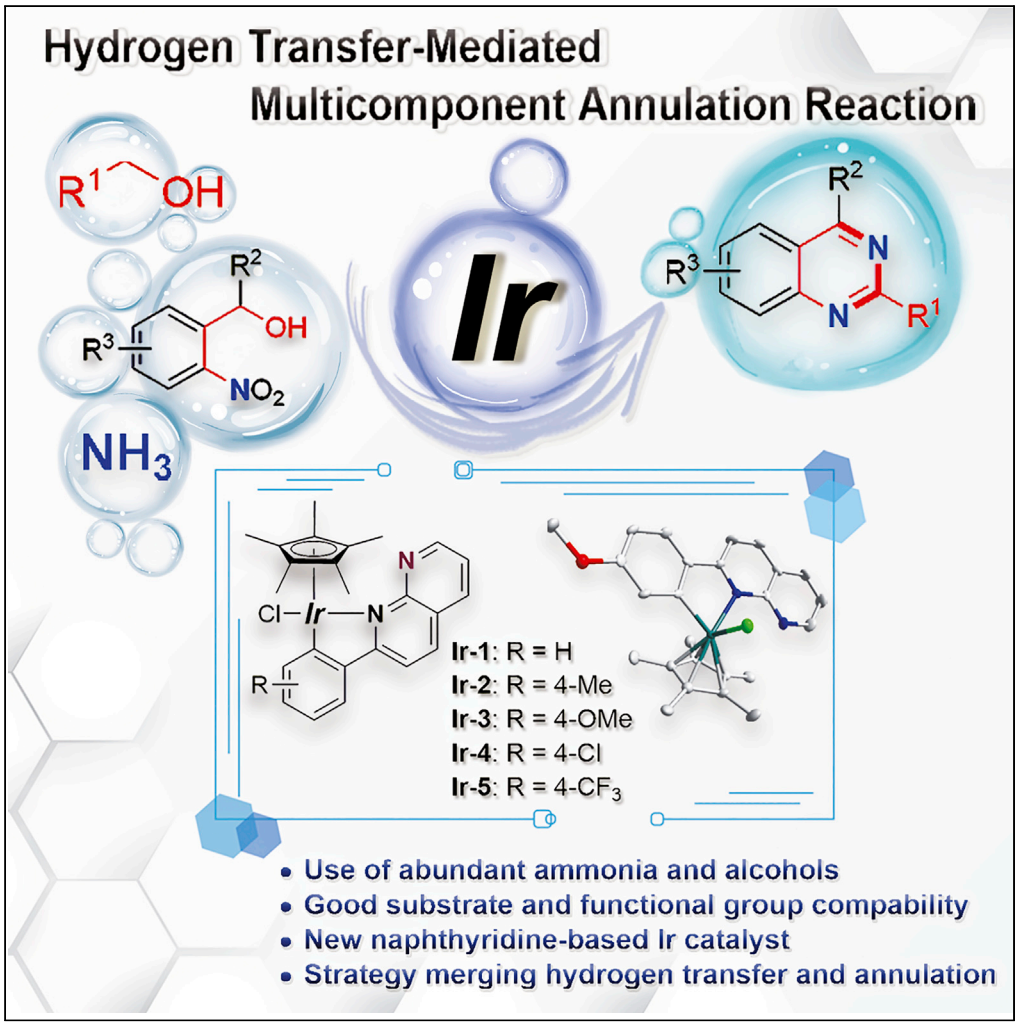

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HIGHLIGHTS

Use of abundant ammonia and alcohols

Good substrate and functional group compatibility

New naphthyridine-based Ir catalyst

Strategy merging hydrogen transfer and annulation

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Hydrogen Transfer-Mediated Multicomponent Reaction for Direct Synthesis of Quinazolines by a Naphthyridine-Based Iridium Catalyst

Zhenda Tan,[1] Zhongxin Fu,[2] Jian Yang,[1] Yang Wu,[1] Liang Cao,[1] Huanfeng Jiang,[1] Juan Li,[2,*] and Min Zhang[1,3,*]

SUMMARY

Selective linkage of renewable alcohols and ammonia into functional products would not only eliminate the prepreparation steps to generate active amino agents but also help in the conservation of our finite fossil carbon resources and contribute to the reduction of CO_2 emission. Herein the development of a novel 2-(4-methoxyphenyl)-1,8-naphthyridine-based iridium (III) complex is reported, which exhibits excellent catalytic performance toward a new hydrogen transfer-mediated annulation reaction of 2-nitrobenzylic alcohols with alcohols and ammonia. The catalytic transformation proceeds with the striking features of good substrate and functional group compatibility, high step and atom efficiency, no need for additional reductants, and liberation of H_2O as the sole by-product, which endows a new platform for direct access to valuable quinazolines. Mechanistic investigations suggest that the non-coordinated N-atom in the ligand serves as a side arm to significantly promote the condensation process by hydrogen bonding.

INTRODUCTION

Mass mining and consumption of fossil resources have resulted in a call for the development of new catalytic transformations, enabling production of functional chemicals from renewable resources with high step and atom efficiency (Goldemberg, 2007; Michlik and Kempe, 2013a, 2013b; Kozlowski and Davis, 2013). Among various alternative feedstocks, alcohols are a category of oxidized hydrocarbons that can be extensively derived from biomass including abundantly available lignocellulose via degradation (Zakzeski et al., 2010; Sun et al., 2018; Vispute et al., 2010). N-heteroarenes represent a class of highly important compounds, and they have been extensively employed for the development of valuable products, such as bioactive molecules, pharmaceuticals, agrochemicals, dyes, ligands, sensors, and materials (Boyarskiy et al., 2016; Preshlock et al., 2016; Bandini, 2011). Consequently, the linkage of alcohols into N-heteroaromatic frameworks is of high importance, as it not only helps in the conservation of our finite fossil carbon resources but also contributes to the reduction of CO_2 emission.

Over the past decade, the strategy of acceptorless dehydrogenative coupling (ADC) proceeded to renew the construction of N-heteroarenes. In this strategy, dehydrogenation is involved in the activation of alcohols via *in situ* formation of carbonyl intermediates, and H_2 and/or H_2O are generally generated as the by-products. Since 2013, significant progress has been made in this regard by the groups of Milstein (Srimani et al., 2013a, 2013b; Daw et al., 2016, 2017), Kempe (Michlik et al., 2013a, 2013b; Deibl et al., 2015; Hille et al., 2014, 2017; Deibl and Kempe, 2017; Kallmeier et al., 2017), Beller (Zhang et al., 2013a, 2013b), Kirchner (Mastalir et al., 2016), and others (Pan et al., 2016; Xu et al., 2017; Elangovan et al., 2015; Chen et al., 2014). However, it is important to note that these transformations mainly rely on the utilization of specific amines, whereas the synthesis of N-heteroarenes by combining alcohols with ammonia, an abundant and renewable nitrogen source, has been rarely explored, although the related transformations would eliminate prepreparation steps to generate active amino agents, and result in high step and atom efficiency. For instance, the Beller group has reported a Ru-catalyzed synthesis of pyrroles from ammonia, vicinal diols, and ketones (Scheme 1, Equation 1) (Zhang et al., 2013a, 2013b). Milstein and the co-workers have presented a synthesis of pyrroles and pyrazines from alcohols and ammonia (Scheme 1, Equation 2) (Daw et al., 2018).

In recent years, the so-called hydrogen-borrowing reaction has emerged as an appealing tool in achieving the alkylation of amines (Wang et al., 2014; Xiao et al., 2019; Kaloglu et al., 2016; Elangovan et al., 2016) and activated carbon nucleophiles (Blank and Kempe, 2010; Elangovan et al., 2015; Deibl and Kempe,

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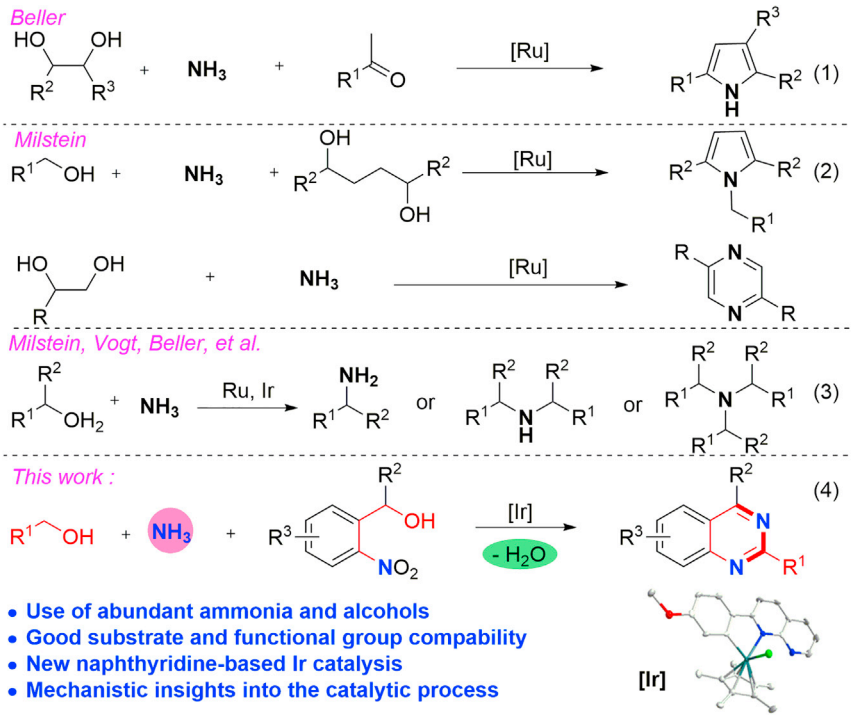


Scheme 1. Alcohols and Ammonia Utilized for the Synthesis of N-Heteroarene and Amine

2016; Peña-López et al., 2016). Interestingly, the synthesis of various alkylamines from alcohols and ammonia has also been nicely demonstrated (Scheme 1, Equation 3) (Ye et al., 2014; Pingen et al., 2010; Imm et al., 2010, 2011; Gunanathan and Milstein, 2008; Yamaguchi et al., 2008; Kawahara et al., 2010). In such transformations, the alcohols serve as both the hydrogen suppliers and coupling agents. So, there is no need for external reductants such as high-press H_2 gas. Despite these significant advances, the construction of functional N-heteroarenes involving alcohols and ammonia feedstocks through hydrogen autotransfer as a substrate-activating strategy remains a new subject to be explored. However, such a concept would encounter the challenges of difficult proton exchanges and selectivity control, as well as catalyst deactivation by the lone pair of electrons on the nitrogen of excess ammonia (Klinkenberg and Hartwig, 2011).

Among various N-heteroarenes, quinazolines constitute a class of structurally unique compounds, which have been found to exhibit diverse biological and therapeutic activities (Parhi et al., 2013; Ugale and Bari, 2014; Juvale et al., 2013; Ple et al., 2004), and have been extensively applied for the discovery of various functional products (Zhao et al., 2013; Zhang et al., 2011). However, the existing approaches for accessing such compounds generally require preinstalled reactants (Lin et al., 2014; Malakar et al., 2012; Portela-Cubillo et al., 2008; Yan et al., 2012; Zhang et al., 2010). In this context, the search for direct synthesis of quinazolines from easily available substrates, preferably abundant and sustainable ones, would be of great significance. Enlightened by our recent work on the synthesis and functionalization of N-heterocycles (C. Chen et al., 2017; Chen et al., 2018a, 2018b; X.-W. Chen et al., 2017; Liang et al., 2018, 2019; Xie et al., 2017, 2018, 2019), we wish herein to present, for the first time, a synthesis of quinazolines from 2-nitrobenzyl alcohols (Rajendran et al., 2015; Pasnoori et al., 2014), alcohols, and ammonia by a new iridium complex featuring a 2-(4-methoxyphenyl)-1,8-naphthyridyl ligand. In such a transformation, the hydrogen generated from dehydrogenation of alcohols and dehydroaromatization process is utilized for substrate activation through transfer hydrogenation (TH) of the nitro group, and there is no need for addition of external reductants.

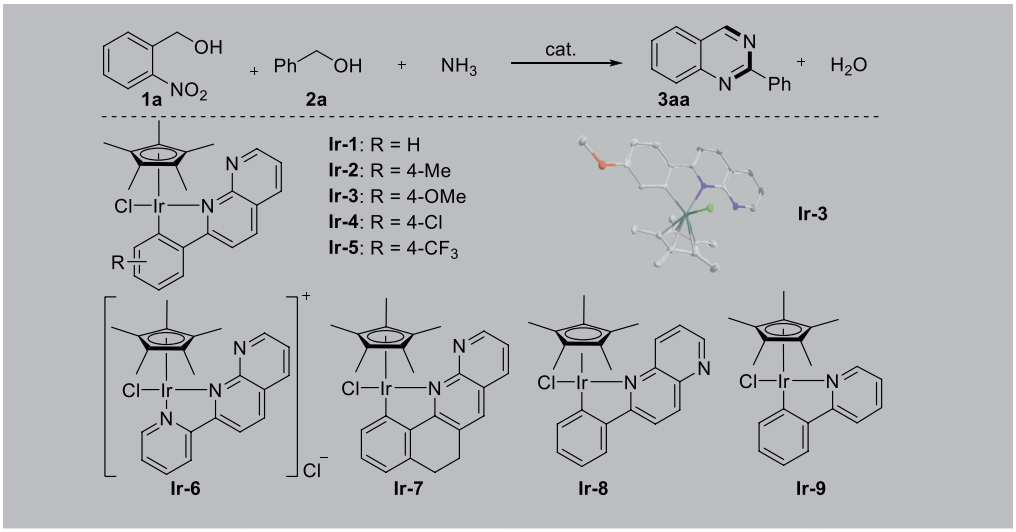
RESULTS AND DISCUSSION

We initiated our investigations by choosing the synthesis of quinazoline **3aa** from *o*-nitrobenzene methanol **1a**, alcohol **2a**, and ammonia as a model reaction. First, we tested the combinations of several metal

catalysts (i.e., Ru, Mn, Co, Fe, and Ni) with various phosphine ligands such as Xantphos, DPPE, DPPB, DPPP, Binap-dp, DPEphos, and Xphos (see Table S1), the privileged catalyst systems employed for the ADC and hydrogen-borrowing reactions. However, the low yields of product (<10%) disclosed that they were not suitable systems for the current synthetic purpose. When complex $[IrCp^*Cl_2]_2$ was employed, 15% yield of **3aa** was obtained. A further optimization of other reaction parameters involving solvents, bases, and temperatures (Table S2) slightly improved the yield to 18% by using *t*-BuONa as the base at 140°C. Enlightened by our recent synthesis of naphthyridines (Chen et al., 2017a, 2017b, 2018a, 2018b; Xiong et al., 2016), we believed that such compounds might serve as a class of useful N-ligands with tunable coordination modes, and the preparation of a suitable naphthyridyl Ir-complex might offer a solution to obtain the desirable catalytic efficiency. Thus, we prepared 9-cyclometalated iridium complexes, involving 8-naphthyridyl (**Ir-1**−**Ir-8**) and 1,2-phenylpyridyl (**Ir-9**) ones. Then, their catalytic performance toward the model reaction was evaluated (Table 1, entries 1–9). In comparison, complexes bearing a 1,8-naphthyridyl ligand (entries 1–7) exhibited appealing activity, and **Ir-3** (as confirmed by single-crystal X-ray diffraction, CCDC: 1848110, for detail, see Figure S101 and Tables S5–S10) was shown to be a preferred candidate, whereas complex with a 1,5-naphthyridyl or 2-pheynlpyridyl ligand only resulted in low product yield (entries 8–9). The results imply that the N-atom at position 8 in 1,8-naphthyridyl ligands plays a crucial role in affording a satisfactory product yield. Further optimization showed that the presence of iridium is essential in affording the product (entry 10), and the gaseous ammonia is relatively superior to other nitrogen sources (entries 11–15). A decrease of base amount to 30% resulted in a diminished yield (entry 16), and 40% *t*-BuONa was sufficient for the reaction (entry 17). The time-conversion profile at 2, 4, 8, and 16 h showed that the satisfactory product yield is due to the catalyst robustness (entry 18). Based on the results, the optimal (standard) conditions are as indicated in entry 17 of Table 1.

With the optimal reaction conditions established, we then examined the generality of the synthetic protocol. (2-nitrophenyl)methanol **1a** was further employed to couple with various primary alcohols (**2a**−**2t**, Scheme S1) and ammonia. As illustrated in Scheme 2, all the reactions proceeded smoothly and furnished the desired quinazolines in moderate to excellent yields upon isolation (Scheme 2, **3ab**−**3at**). Apart from the alkyl-substituted benzyl alcohols, other functional groups such as −OMe, −OH, $-NH_2$, −Cl, −Br, $-CF_3$, $-CO_2Me$, −COPh, −CN, and −C=C− are well tolerated in the transformation. The retention of these functionalities offers the potential for the elaboration of complex molecules via further chemical transformations. Moreover, except for the strong electron-withdrawing group $-CF_3$, the electronic property of these substituents has little influence on the reaction, whereas the relatively lower product yields using ortho-substituted benzyl alcohols might relate to the steric hindrance (**3ac** and **3ae**). Furthermore, heteroaryl methanols (**2o** and **2p**) were also amenable to the transformation and resulted in the 2-heteroaryl-substituted quinazolines (**3ao** and **3ap**) in good yields, and the obtained products have the potential to be applied as hemilabile bidentate ligands in organometallic chemistry and catalysis. Interestingly, cinnamyl alcohol **2q** underwent smooth hydrogen transfer-mediated annulation, affording the 2-alkenyl quinazoline **3aq** in 46% yield. The relatively low product yield is due to partial formation of 2-alkyl quinazoline via reduction of the alkenyl group. The relatively low product yield of **3aq** is due to the partial formation of 2-alkyl quinazoline via reduction of the alkenyl group. Aliphatic alcohols, such as methanol (**2r**), heptan-1-ol (**2s**), and cyclopropyl carbinol (**2t**), were efficiently transformed into the 2-non-substituted and 2-alkyl quinazolines (**3ar**, **3as,** and **3at**) in moderate yields.

Subsequently, we turned our attention to the transformation of different 2-nitrobenzyl alcohols **1**. First, various related substrates (**1b**−**1i**) in combination with different primary alcohols **2** and NH_3 were tested. As shown in Scheme 3, all the reactions smoothly delivered the multi-substituted quinazolines in moderate to excellent isolated yields. The electronic property of the substituents on the aryl ring of substrates **1** significantly influenced the product yields. In general, 2-nitrobenzyl alcohols **1** with electron-donating groups afforded the products in higher yields (**3ba**–**3ca** and **3ea**–**3fi**) than with electron-deficient ones (**3ga**–**3ia**). This phenomenon is rationalized as the catalyst has better stability toward the electron-rich aniline intermediates, arising from the TH of nitro group of substrates **1**. Gratifyingly, secondary alcohols, such as **1j** and **1k**, also underwent smooth annulation to give the 2,4-disubstituted quinazolines in good yields (**3ja**, **3jl**, and **3ka**). Similar to the results described in Scheme 2, a wide array of functionalities such as −Me, −OMe, −F, −Cl, −Br, −CN, −Ph, and ester are well tolerated in the transformation (Schemes 2 and 3). Noteworthy, the halogen groups did not undergo hydrodehalogenation, showing that the developed catalytic system exhibits unique chemoselectivity.



Entry	Catalyst	NH_3 Source	Yields of 3aa[a,b]
1	Ir-1	NH_4OAc	72
2	Ir-2	NH_4OAc	75
3	Ir-3	NH_4OAc	82
4	Ir-4	NH_4OAc	61
5	Ir-5	NH_4OAc	67
6	Ir-6	NH_4OAc	71
7	Ir-7	NH_4OAc	68
8	Ir-8	NH_4OAc	15
9	Ir-9	NH_4OAc	21
10	–	NH_4OAc	–
11	Ir-3	NH_4Cl	5
12	Ir-3	$HCOONH_4$	Trace
13	Ir-3	$NH_3 \cdot H_2O$	Trace
14	Ir-3	$(NH_4)_2SO_4$	22
15	Ir-3	NH_3 (g)	88[c]
16	Ir-3	NH_3 (g)	81[c,d]
17	Ir-3	NH_3 (g)	88[c,e]
18	Ir-3	NH_3 (g)	(12, 40, 65, 84)[f]

Table 1. Screening of Optimal Reaction Conditions

Also see Figure S101, Tables S5–S10 and Data S3.

[a]Unless otherwise stated, the reaction was performed with **1a** (0.5 mmol), **2a** (0.5 mmol), Ir (1 mol %), *t*-BuONa (50 mol %), NH_3 sources (1.0 mmol) in toluene (1.5 mL) for 24 h under Ar protection.

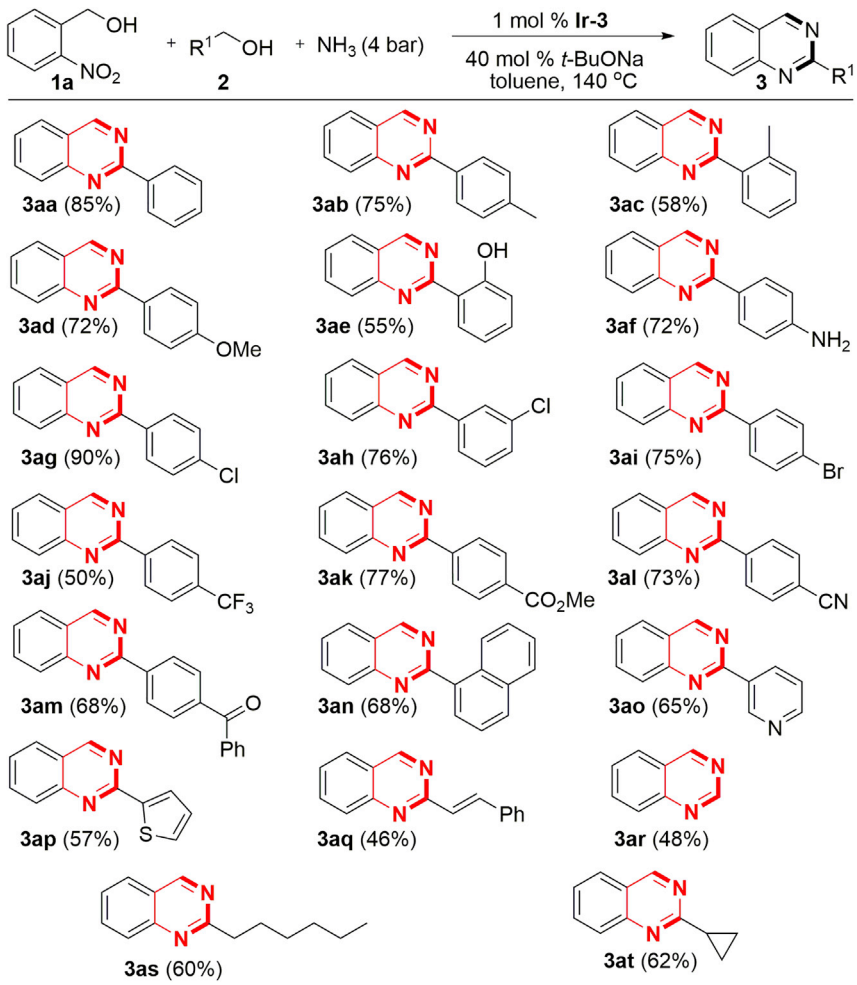
[b]Gas chromatography yields with the use of hexadecane as an internal standard.

[c]4 bar of NH_3.

[d]*t*-BuONa (30 mol %).

[e]*t*-BuONa (40 mol %).

[f]Conversions for 2, 4, 8, and 16 h.

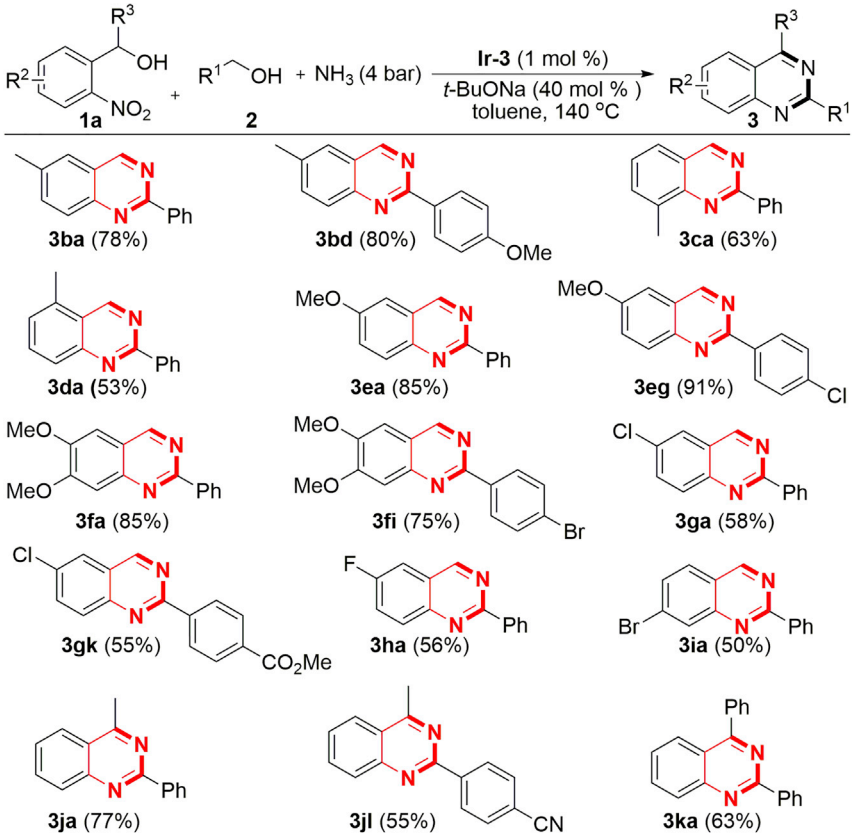


Scheme 2. Variation of Alcohols

Also see Scheme S1, Figures S1–S60 and Data S3.

To demonstrate the significance and practicality of the developed synthetic methodology, a gram-scale synthesis of compound **3aa** could be achieved by performing the reaction with 8 mmol of **1a** and 9 mmol of benzyl alcohol **2a**, which still afforded a good isolated product yield (78%) even with lower catalyst loading (Scheme 4, Equation a, 0.2 mol%). Furthermore, compound **3la**, a key ingredient used as a herbicide with the activity on Toll-like receptors, **20** could be prepared through the reduction of commercially available acifluorfen acid to 2-nitrobenzyl alcohol **1l** (Scheme S3) followed by the annulation reaction of **1l** with alcohol **2a** and ammonia (Equation b), and such a synthesis is far superior to the reported multi-step synthetic protocol (Mc Gowan et al., 2012; Munro and Bit, 1987; Sumida et al., 1995). Moreover, the extended π-conjugated system like compound **5ja** was successfully prepared by the halocyclization (Tan et al., 2016) of compound **3ja** and further Sonogashira coupling (Equation c), which offers a valuable basis for further development of optoelectronic materials.

To gain mechanistic insights into the catalytic transformation, a time-concentration profile of the model reaction is depicted in Figure 1 (also see Data S1). Substrates **1a** and **2a** with ammonia were converted into **3aa** in maximum yield within 24 h. 2-Aminobenzaldehyde **1a-4** and 1,2-dihydroquinazoline **3aa-1** were observed during the reaction, but they were consumed up after completion of the reaction (Figure 1). The subjection of compound **1a-4** with benzaldehyde **2a-1** and NH_3 or direct treatment of **3aa-1** under the standard conditions afforded product **3aa** in almost quantitative yields (see Equations 1 and 2 of Scheme S2, also see Data S1). These results support the fact that compounds **1a-4**, **2a-1,** and **3aa-1** are



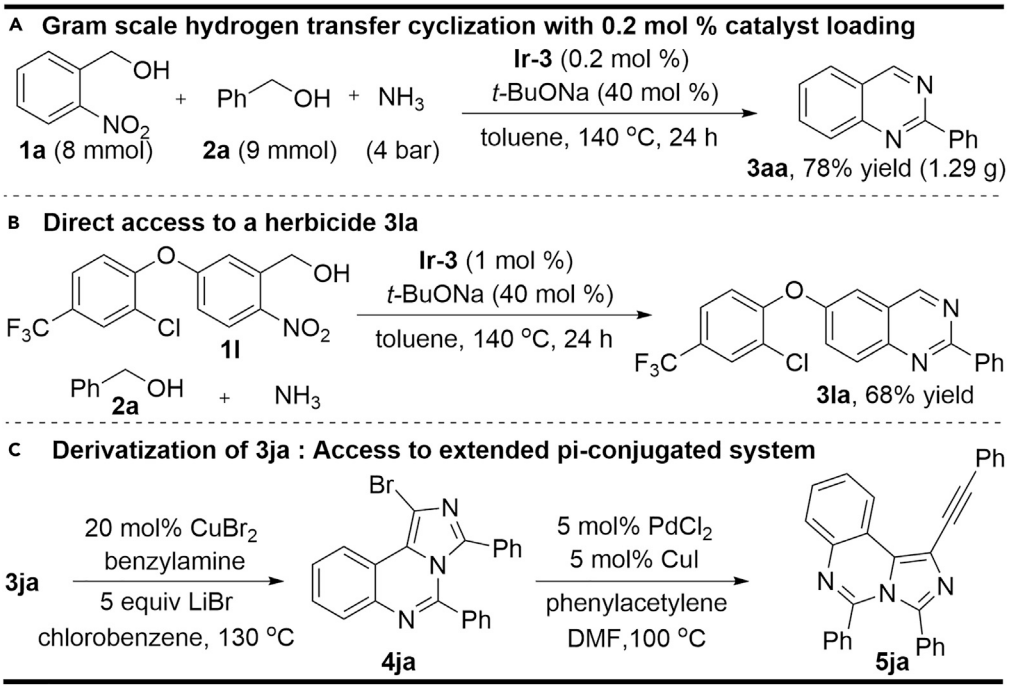
Scheme 3. Variation of *o*-Nitroaryl Alcohols

Also see Scheme S1, Figures S61–S91 and Data S3.

the reaction intermediates. Furthermore, both the iridium catalyst and base play crucial roles in the dehydrogenation of **3aa-1** to product **3aa** (Equation 2). An iridium hydride complex (**Ir-H**) was obtained from the reaction of equimolar **Ir-3** and benzyl alcohol, which can efficiently catalyze the reaction to afford **3aa**, showing that **Ir-H** as a catalytic species is involved in the reaction (Equations 3 and 4, Scheme S2, also see Data S2 and Figure S98).

With the above-mentioned preliminary experimental evidence in hand, the mechanism was further scrutinized by density functional theory calculations (geometry optimizations using B3LYP and single-point energy calculations using M06). For details, see Figures S99 and S100, Tables S3 and S4, Schemes S4–S8, and Data S4. The calculated free energy profile for the first TH (first TH) of **1a** to 2-nitrosobenzaldehyde **1a-2** is shown in Figure 2. Initially, the anion exchange between **Ir-3** and *t*-BuONa generates the alkoxy complex **Ir-O1**. One of the arms in 1,8-naphthyridyl ligand of **Ir-O1** dissociates, allowing the Ir center to coordinate with the hydroxyl group of **1a**. O–H bond cleavage occurs via transition state **TS1** with an energy barrier of 21.4 kcal/mol to give Ir-alkoxide complex **IN2**, which then undergoes β-hydride elimination by overcoming an energy barrier of 28.0 kcal/mol (**TS2**) relative to **IN2**, and generates complex **Ir-H** and *o*-nitrobenzaldehyde **1a-1**. The nitro group of **1a-1** further acts as a sacrificial hydrogen acceptor of **Ir-H** through two transition states **TS3** and **TS4**. Finally, 2-nitrosobenzaldehyde **1a-2** is generated with the regeneration of **Ir-O1**. In addition, the base-promoted intramolecular Meerwein-Ponndorf-Verley-Oppenauer-type transfer hydrogenation (MPV-O TH) is calculated to have an energy barrier of 33.1 kcal/mol (see Scheme S4), which is 3.5 kcal/mol higher than the overall barrier of the pathway shown in Figure 2. Thus, the MPV-O TH pathway is kinetically unfavorable.

The calculated free energy profiles for the second TH of 2-nitrosobenzaldehyde **1a-2** to 2-(hydroxyamino) benzaldehyde **1a-3** and the third TH of **1a-3** to 2-aminobenzaldehyde **1a-4** are shown in Figures S99 and



Scheme 4. The Synthetic Utility of the Developed Chemistry
Also see Scheme S1 and S3, Figures S92–S97 and Data S3.

S100 (also see Tables S3 and S4, Schemes S5–S8 and Data S4). In consideration that both 2-aminobenzaldehyde **1a-4** and benzaldehyde **2a-1** can condense with ammonia, two plausible pathways toward the formation of imines were investigated. For the reaction of **2a-1** and ammonia (black line in Figure 3), ammonia approaches benzaldehyde through the C–N bond linkage (**TS14**) giving **IN18**. The TH of the ammonia using other ammonia as the proton-transferring shuttle then takes place via **TS15** and leads to **IN20**. The calculated free energy barrier of transition state **TS15** is 22.8 kcal/mol relative to **IN16**. After rearranging to more stable **IN21** featuring two hydrogen bonds, the dehydration occurs via **TS16**, giving the imine complex **IN22**. Meanwhile, we performed calculations for the dehydration without the hydrogen-bonding between the OH group and the non-coordinated N-atom in the ligand (green line in Figure 3). The calculated free

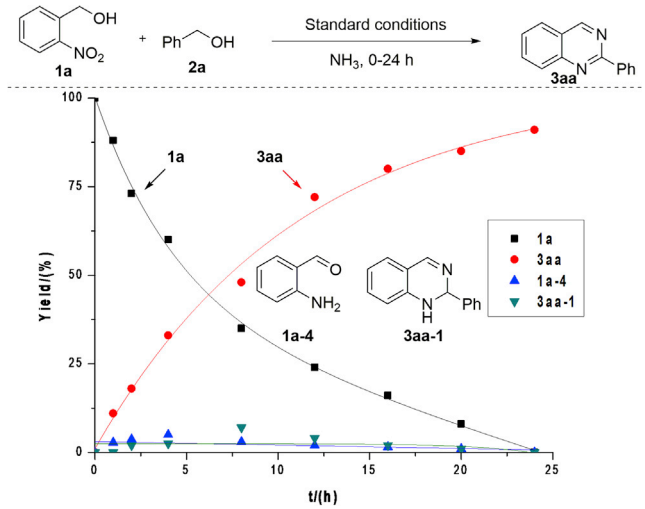


Figure 1. Time-Concentration Profile of the Model Reaction

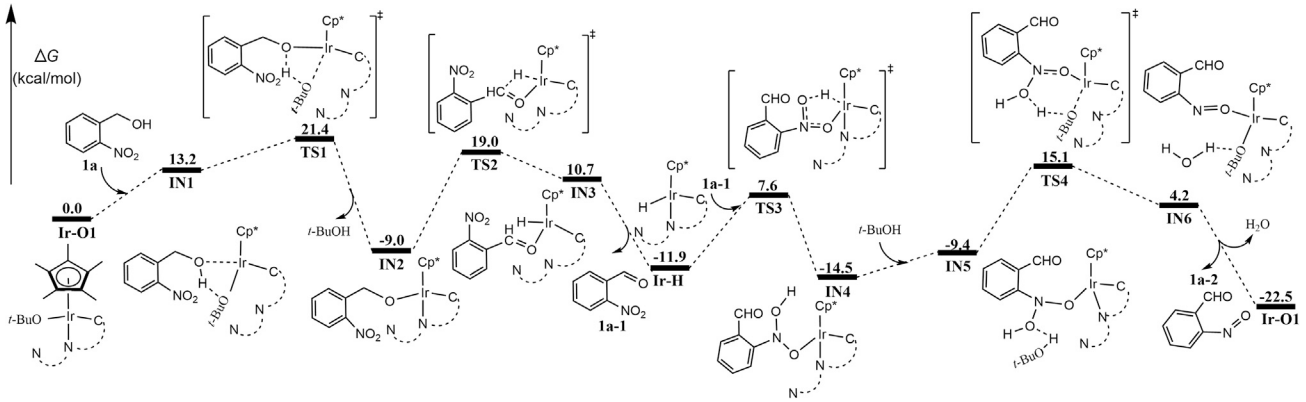


Figure 2. Calculated Energy Profiles for First TH

o-Nitrobenzene methanol **1a** → 2-nitrosobenzaldehyde **1a-2**. Values shown are relative free energies in kcal/mol. Also see Tables S3 and S4 and Data S4.

energy of transition state **TS16″** is −58.4 kcal/mol, which is higher than that of **TS16**. Therefore, the non-coordinated N-atom in the 1,8-naphthyridyl ligand plays a crucial role in the reaction, as it serves as a side-arm to significantly promote the dehydration by hydrogen bonding. An alkoxyl anion ligand rebounds to Ir center to give imine **2a-2** with regeneration of the **Ir-O2** catalyst. The reaction of **1a-4** and ammonia (purple line in Figure 3) follows similar mechanisms to those for **2a-1**. The relevant mechanistic details are therefore not discussed again, for simplicity. The highest energy point for the reaction of **1a-4** and ammonia is **TS16′**, which is energetically less favorable by 1.8 kcal/mol compared with that of **TS16** for the reaction of **2a-1** and ammonia. Therefore, from a kinetic point of view, the reaction of **1a-4** and ammonia is less kinetically favorable.

Based on all the above-mentioned findings, a plausible reaction pathway for the formation of product **3aa** is illustrated in Scheme 5. In the first TH process, the Ir-catalyzed dehydrogenation of **1a** via alkoxy anion exchange of **Ir-O1** with **1a** gives **IN2**, which is followed by β-H elimination to form the 2-nitrobenzaldehye **1a-1** and the **Ir–H** species. The successive TH to the nitro group of **1a-1** and *t*-BuOH-assisted dehydration forms 2-nitrosobenzaldehyde **1a-2** and regenerates the **Ir-O1** species. In the second TH process, the anion exchange of **Ir-O1** with **2a** gives a benzyloxy complex **Ir-O2**. The subsequent β-H elimination of **Ir-O2** followed by TH to the nitroso group and alcoholysis with **2a** delivers 2-(hydroxyamino)benzaldehyde **1a-3** and regenerates complex **Ir-O2**, respectively. In the

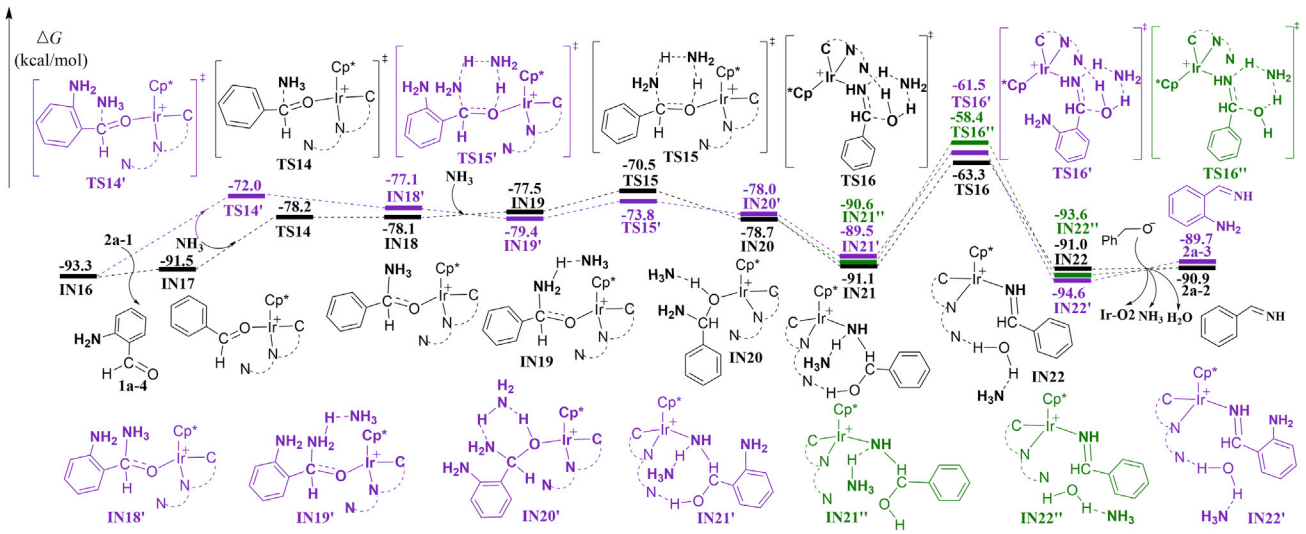
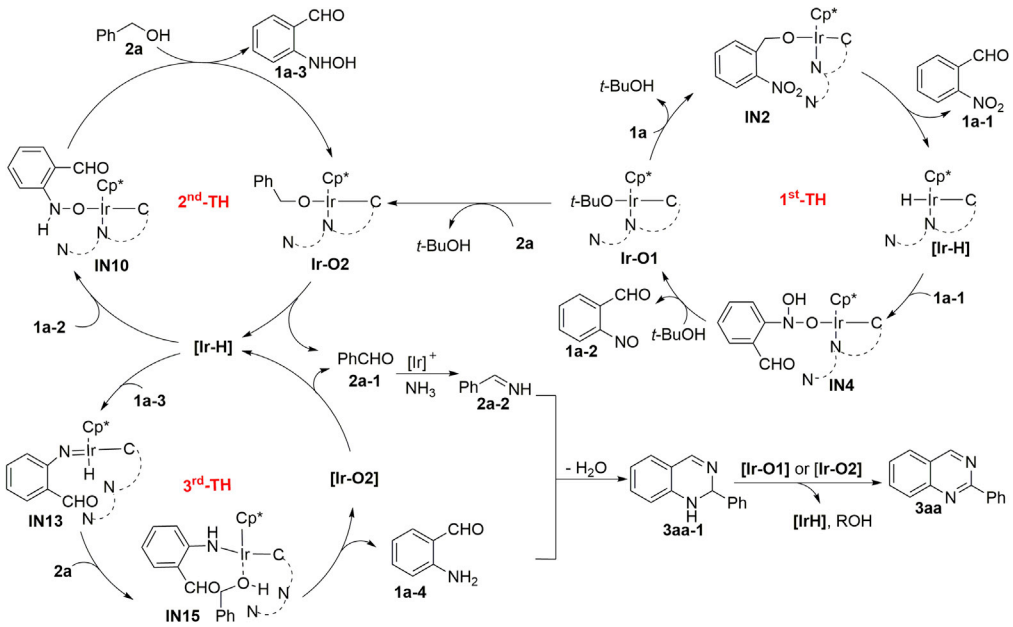


Figure 3. Calculated Energy Profiles for Coupling of Alcohol with Ammonia

Black line for benzaldehyde **2a-1** and purple line for 2-aminobenzaldehyde **1a-4**. The dehydration without the assistance of the non-coordinated N-atom in the ligand is shown in green line. Values shown are relative free energies in kcal/mol. Also see Tables S3 and S4 and Data S4.



Scheme 5. Plausible Reaction Pathway
Also see Data S1 and S2 and Figure S98.

third TH process, the **Ir-H** and benzaldehyde **2a-1** are generated via β-H elimination of **Ir-O2**. Subsequently, the Ir-promoted dehydration of **1a-3** forms a nitrene complex **IN13**, and the TH using **2a** as the proton-transferring shuttle generates 2-aminobenzaldehyde **1a-4** (Qu et al., 2014; Hou et al., 2017). Next, the successive formation of imine **2a-2** via the condensation of benzaldehyde **2a-1** with NH_3 and the cyclization between **2a-2** and **1a-4** affords the dihydroquinazoline **3aa-1**. Finally, the iridium alkoxy complex-catalyzed dehydroaromatization of **3aa-1** gives rise to product **3aa**, and the *in situ*-generated **Ir-H** and alcohol further take part in the TH of the nitro group.

Conclusion

In summary, we have prepared a series of cyclometalated iridium complexes. Among them, **Ir-3** featuring a 2-(4-methoxyphenyl)-1,8-naphthyridyl ligand exhibits the best catalytic performance toward the hydrogen transfer-mediated annulation of 2-nitrobenzyl alcohols with readily available alcohols and ammonia, which allows direct synthesis of a wide array of valuable quinazolines. Mechanistic investigation suggests that the non-coordinated N-atom in the ligand serves as a side arm to significantly promote the condensation step by hydrogen bonding. The catalytic transformation proceeds with the striking features of good substrate and functional group compatibility, liberation of H_2O as the sole by-product, high atom and step efficiency, and no need for additional reductants. The developed chemistry paves the avenues for further development of hydrogen transfer-mediated coupling reactions by design of catalysts bearing N-side arm ligands.

METHODS

All methods can be found in the accompanying Transparent Methods supplemental file.

DATA AND SOFTWARE AVAILABILITY

The crystallography data have been deposited at the Cambridge Crystallographic Data Center (CCDC) under accession number CCDC: 1848110 (**Ir-3**) and can be obtained free of charge from www.ccdc.cam.ac.uk/getstructures.

SUPPLEMENTAL INFORMATION

Supplemental Information can be found online at https://doi.org/10.1016/j.isci.2020.101003.

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AUTHOR CONTRIBUTIONS

Z.T. and M.Z. conceived and designed the study. Z.T., J.Y., Y.W., and L.C. performed the experiments and mechanism study and analyzed the data. Z.F. and J.L. performed DFT calculations and analyzed the data. Z.T., Z.F., H.J., J.L., and M.Z. co-wrote the paper. Z.T. and Z.F. contributed equally to this work.

DECLARATION OF INTERESTS

The authors declare no competing financial interests.

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Supplemental Information

Hydrogen Transfer-Mediated Multicomponent Reaction for Direct Synthesis of Quinazolines by a Naphthyridine-Based Iridium Catalyst

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Copies of product NMR spectra

Figure S1. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-1**, related to **Table 1**.

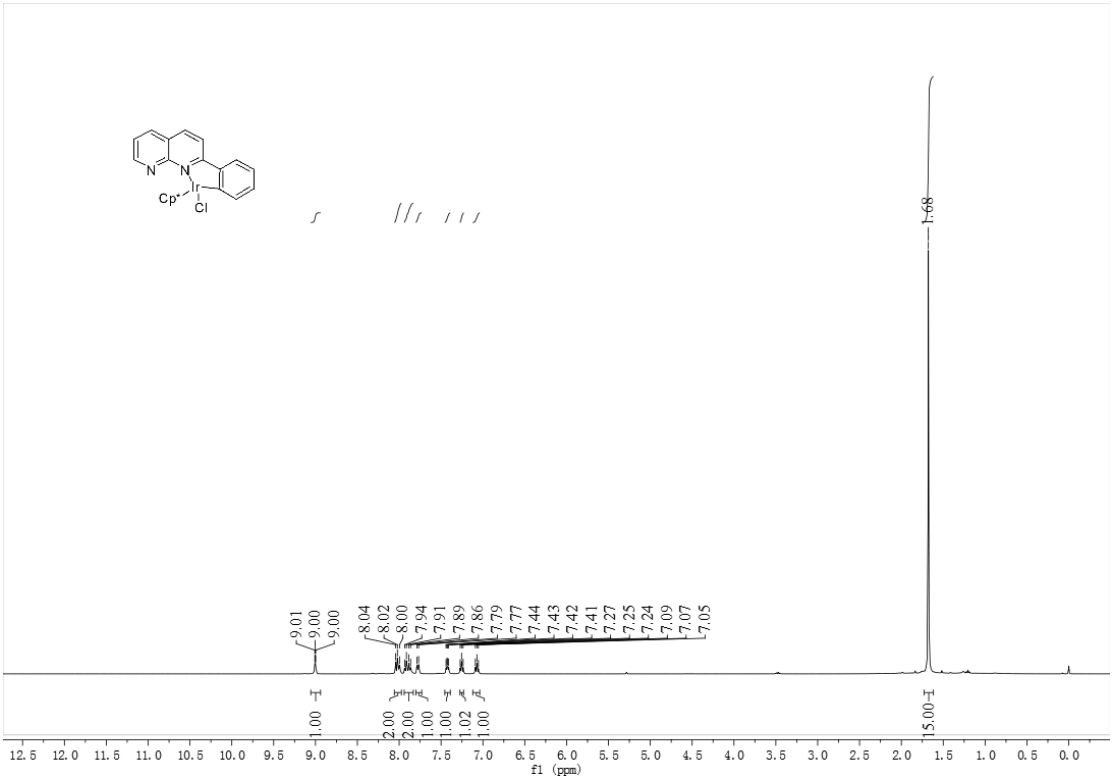


Figure S2. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-1**, related to **Table 1**.

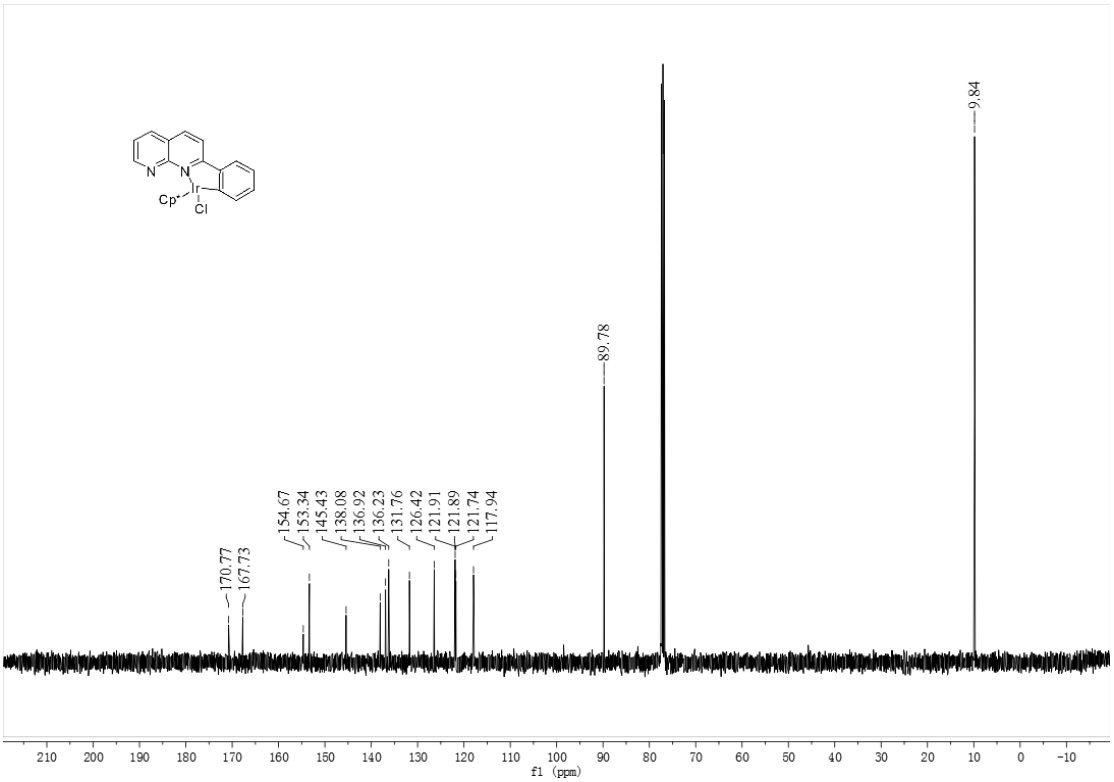


Figure S3. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-2**, related to **Table 1**.

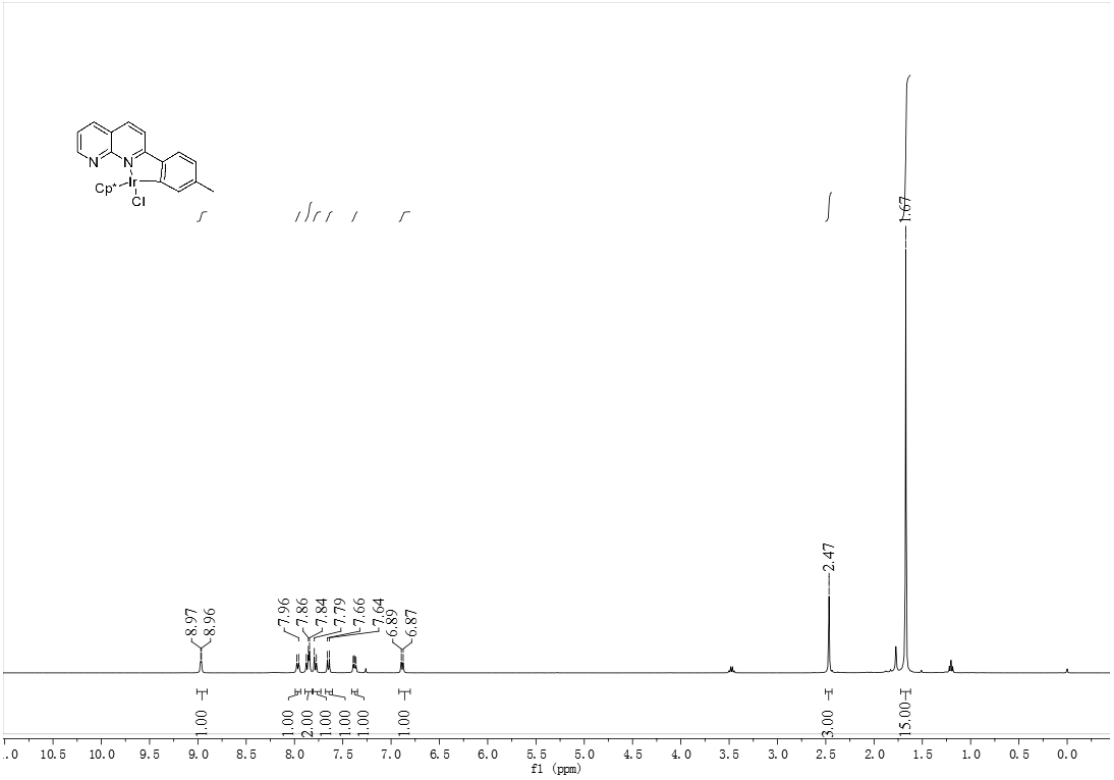


Figure S4. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-2**, related to **Table 1**.

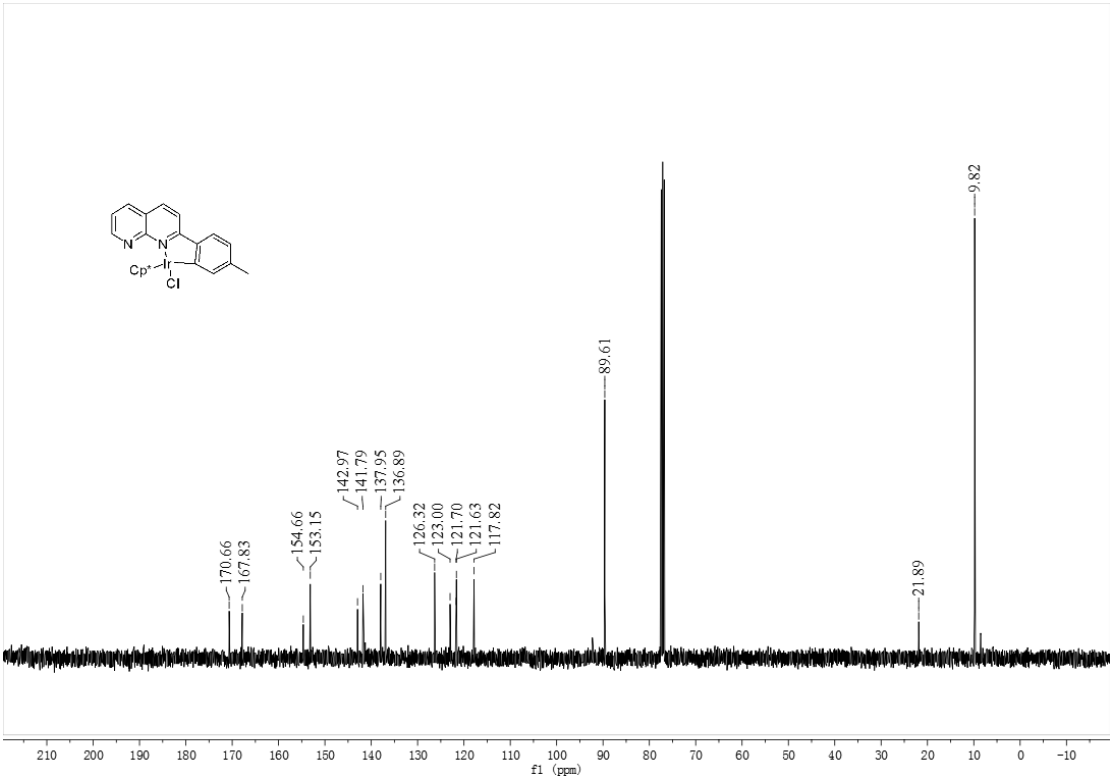


Figure S5. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-3**, related to **Table 1**.

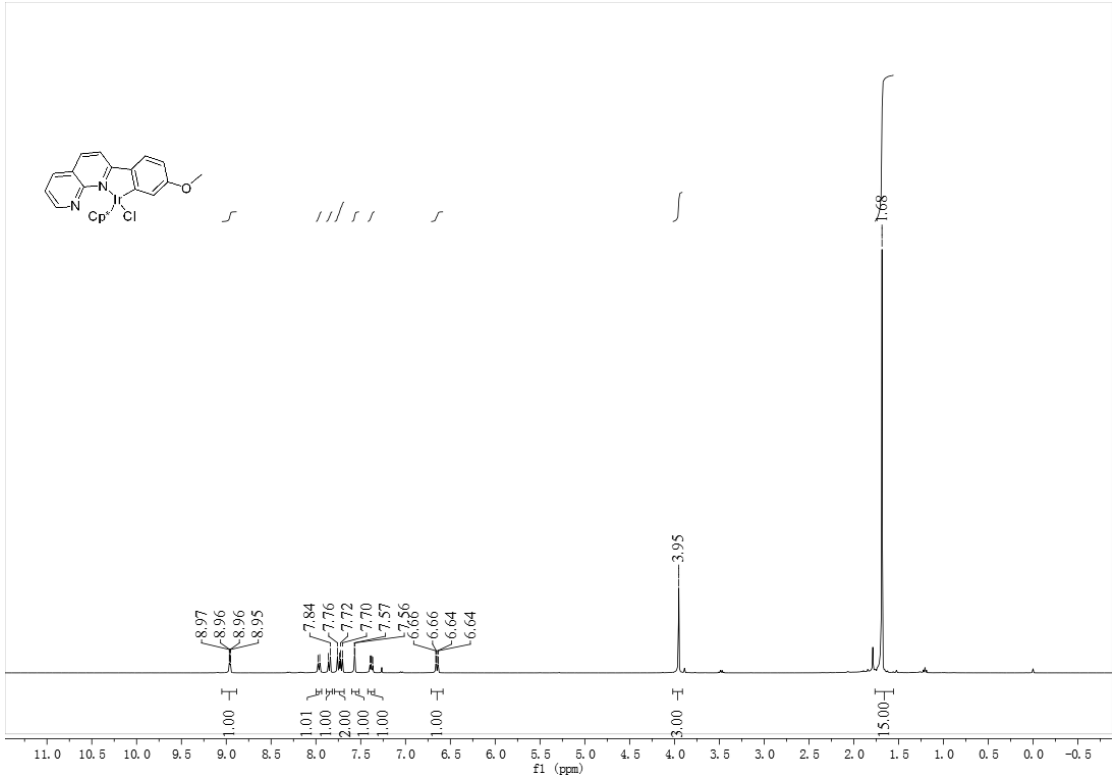


Figure S6. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-3**, related to **Table 1**.

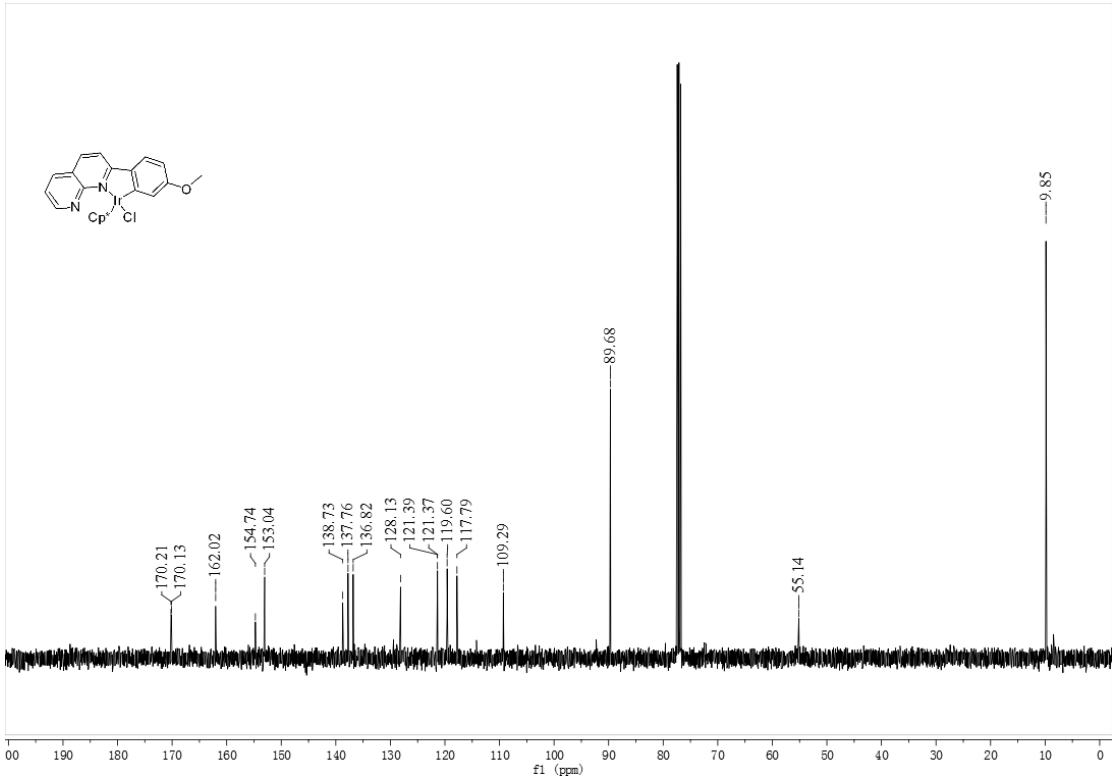


Figure S7. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-4**, related to **Table 1**.

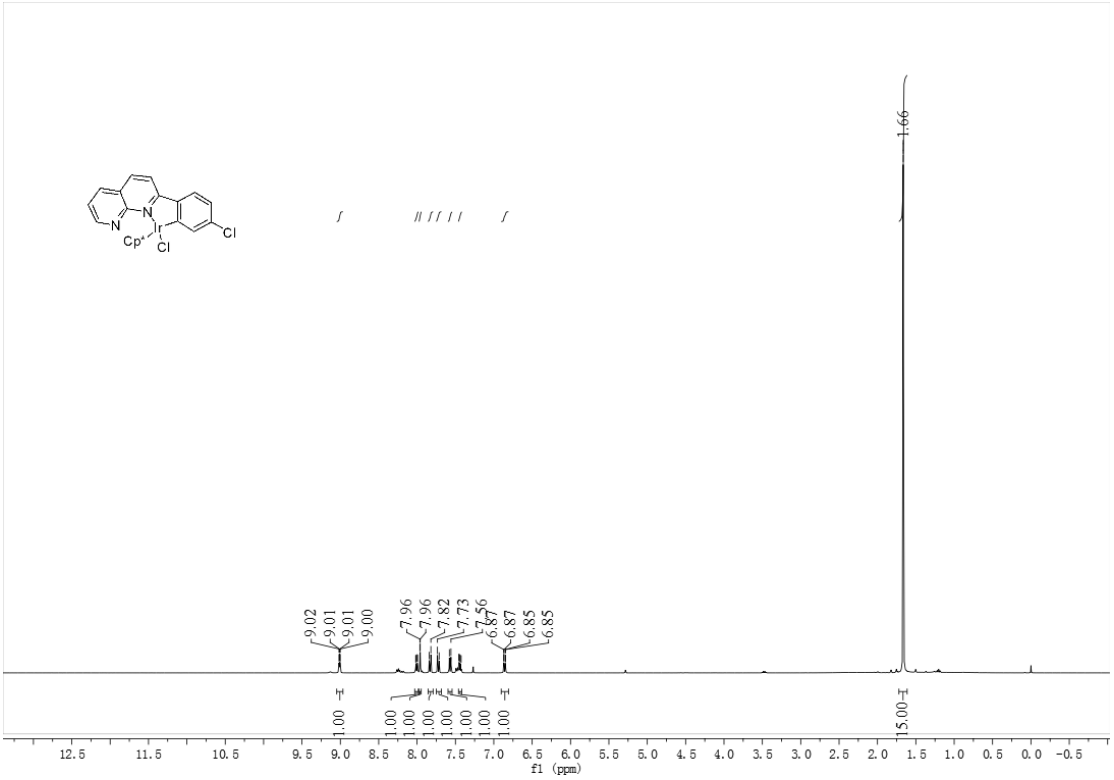


Figure S8. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-4**, related to **Table 1**.

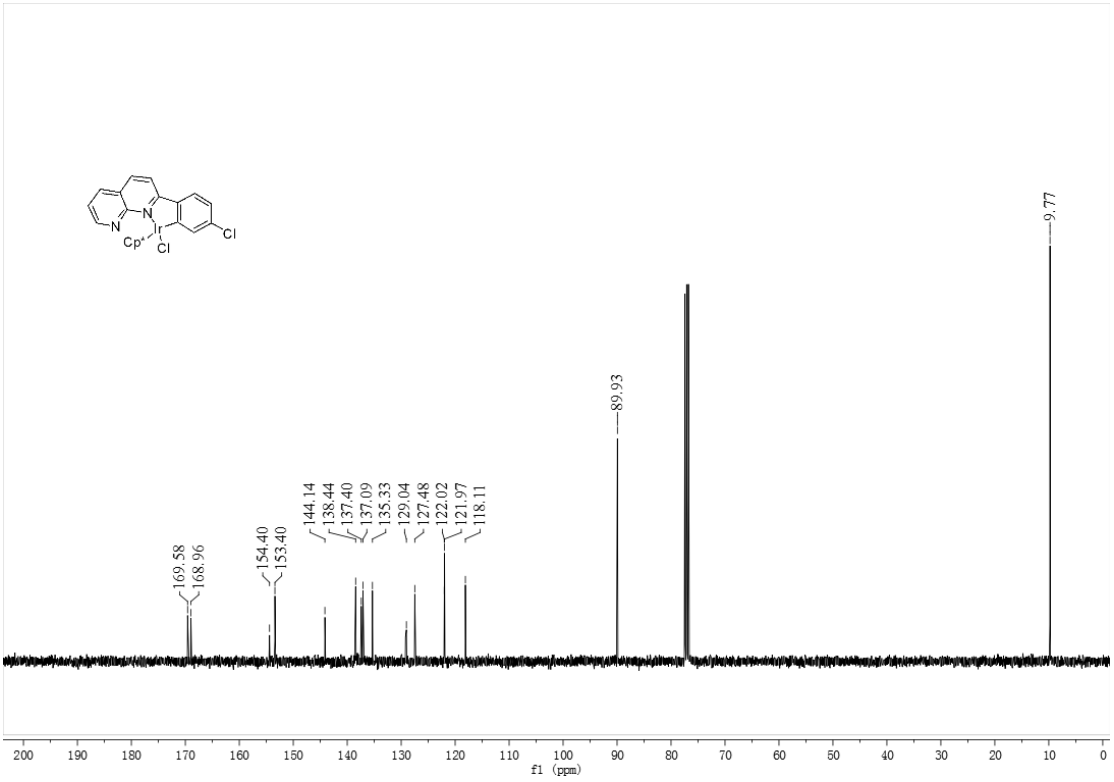


Figure S9. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-5**, related to **Table 1**.

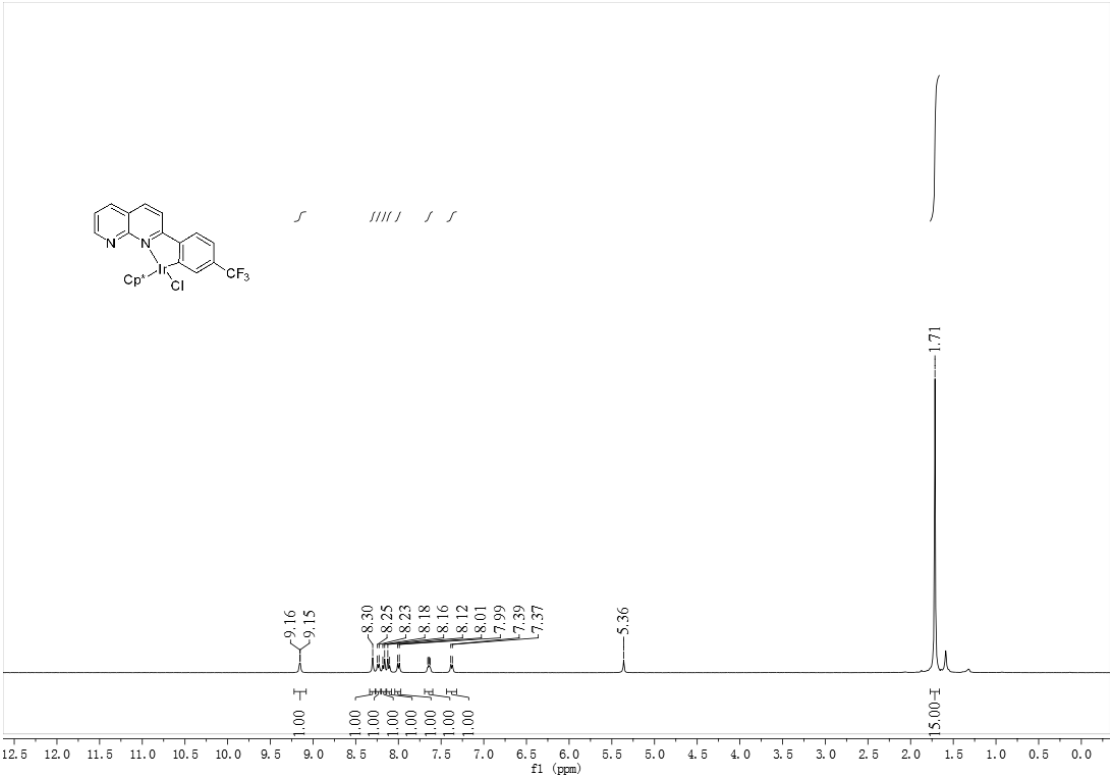


Figure S10. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-5**, related to **Table 1**.

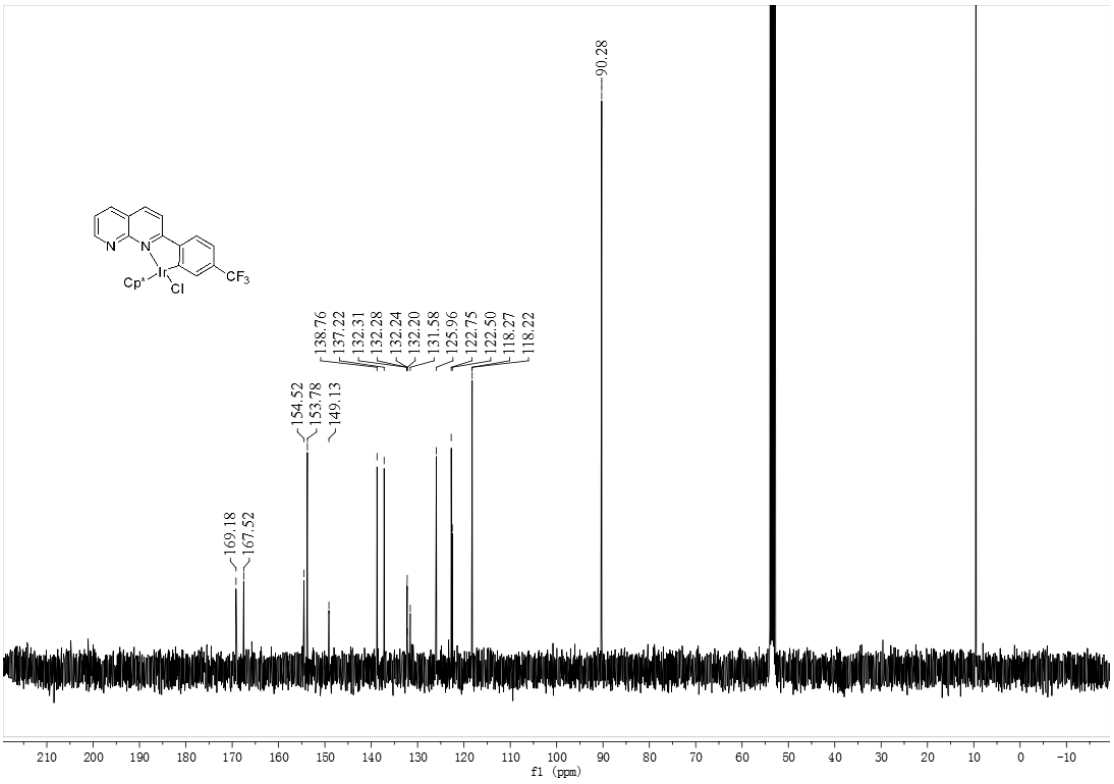


Figure S11. ^{19}F-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-5**, related to **Table 1**.

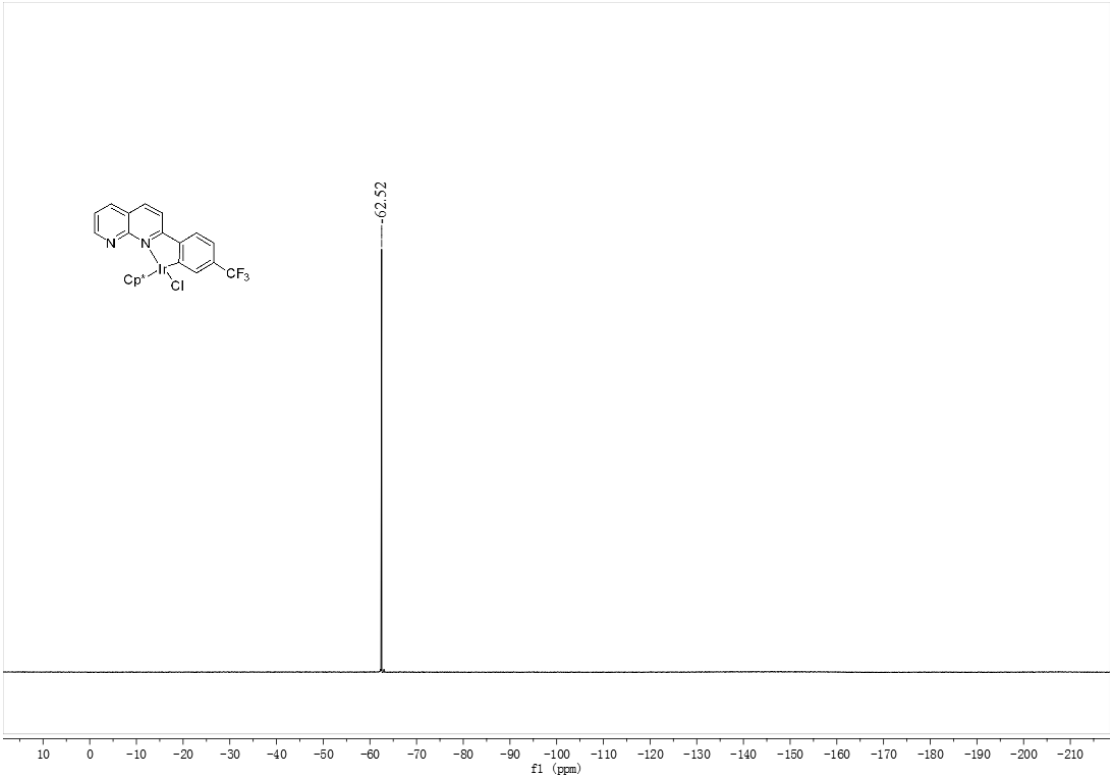


Figure S12. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-6**, related to **Table 1**.

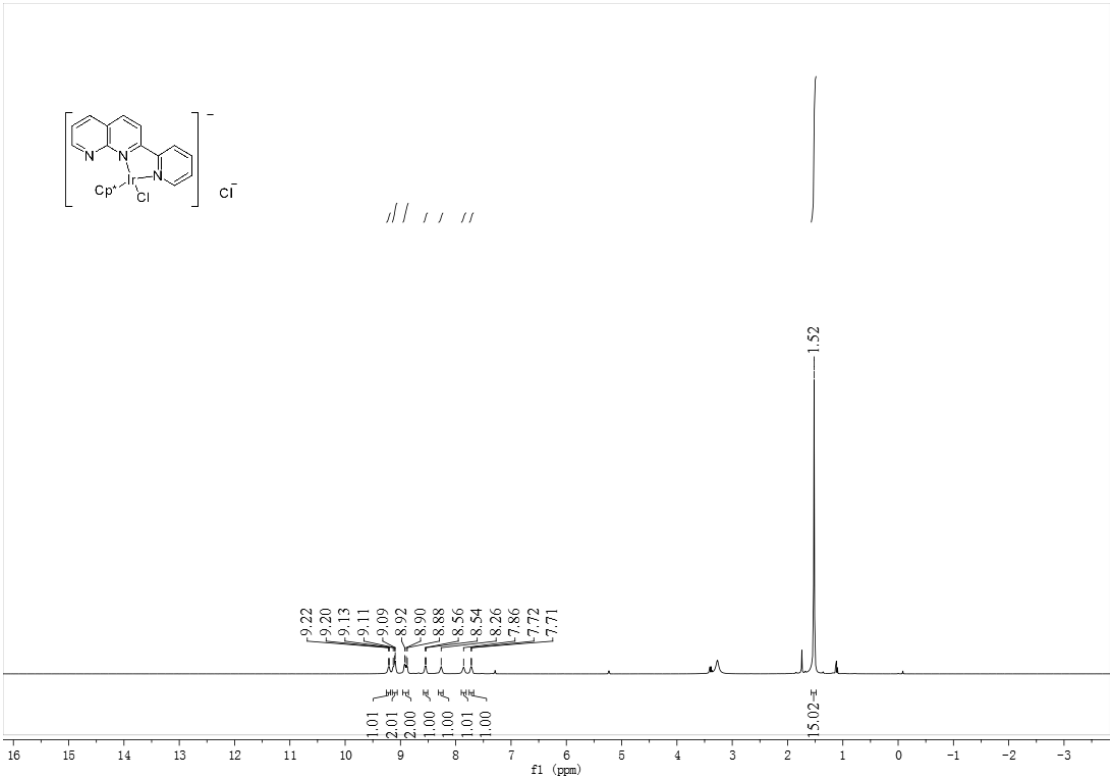


Figure S13. ^{13}C-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-6**, related to **Table 1**.

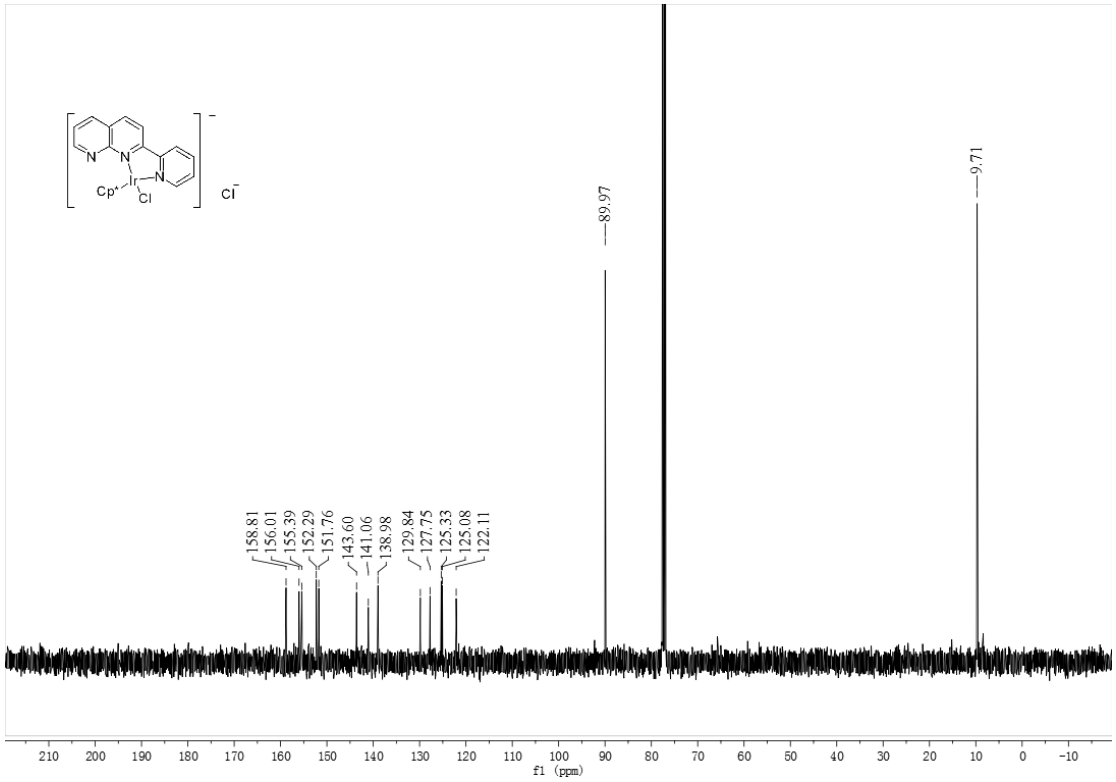


Figure S14. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-7**, related to **Table 1**.

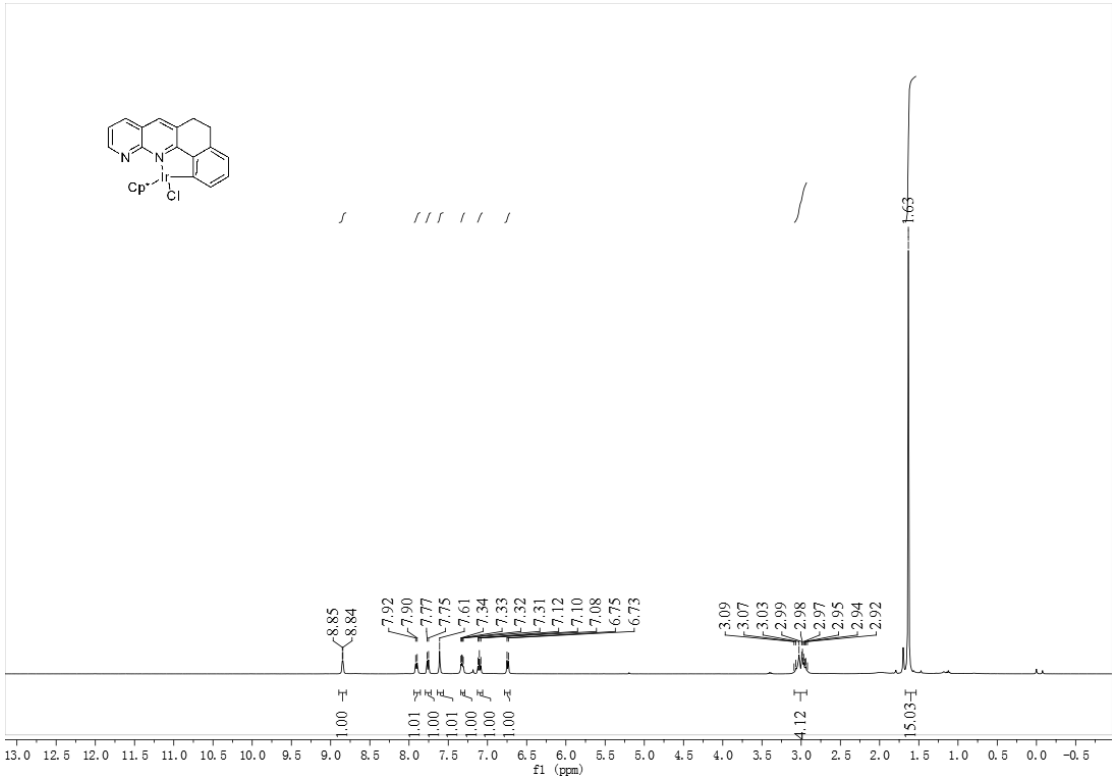


Figure S15. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-7**, related to **Table 1**.

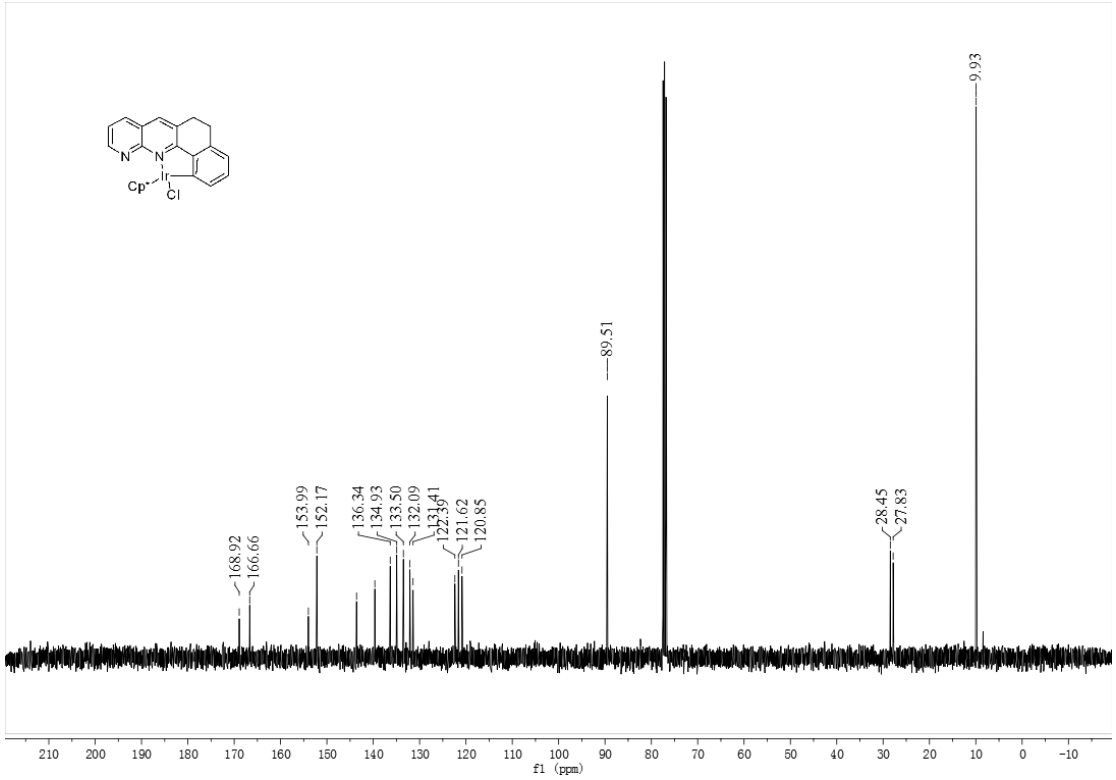


Figure S16. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-8**, related to **Table 1**.

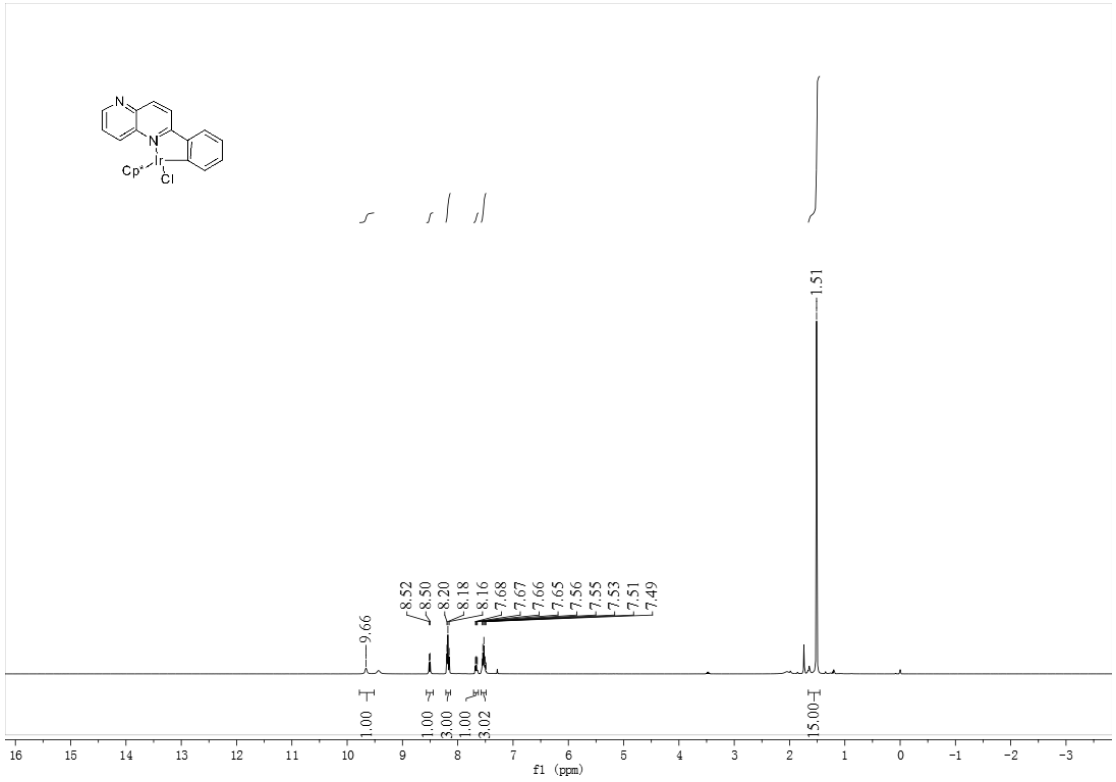


Figure S17. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-8**, related to **Table 1**.

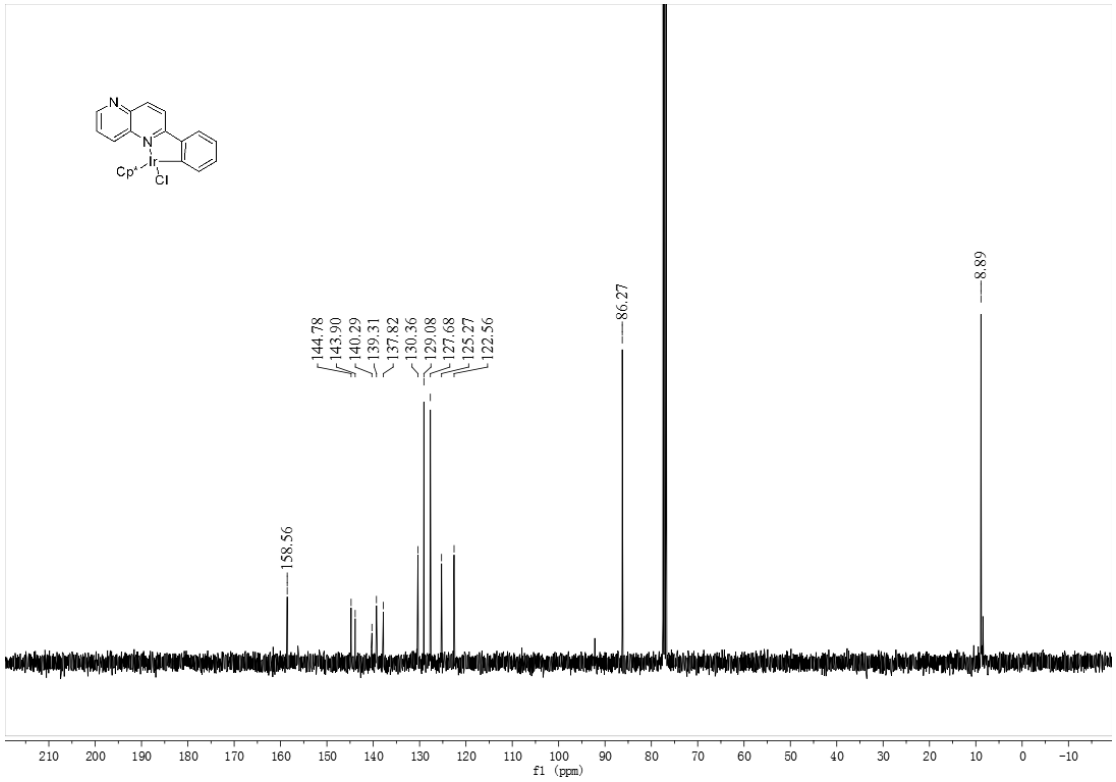


Figure S18. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **Ir-9**, related to **Table 1**.

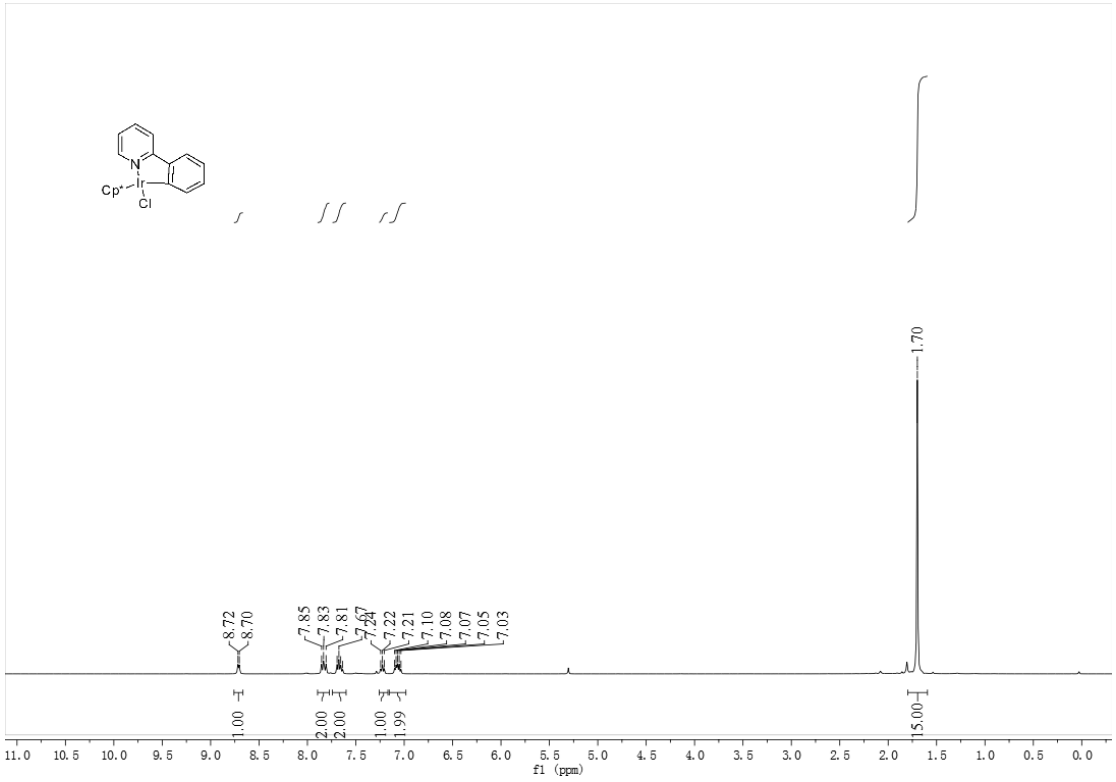


Figure S19. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **Ir-9**, related to **Table 1**.

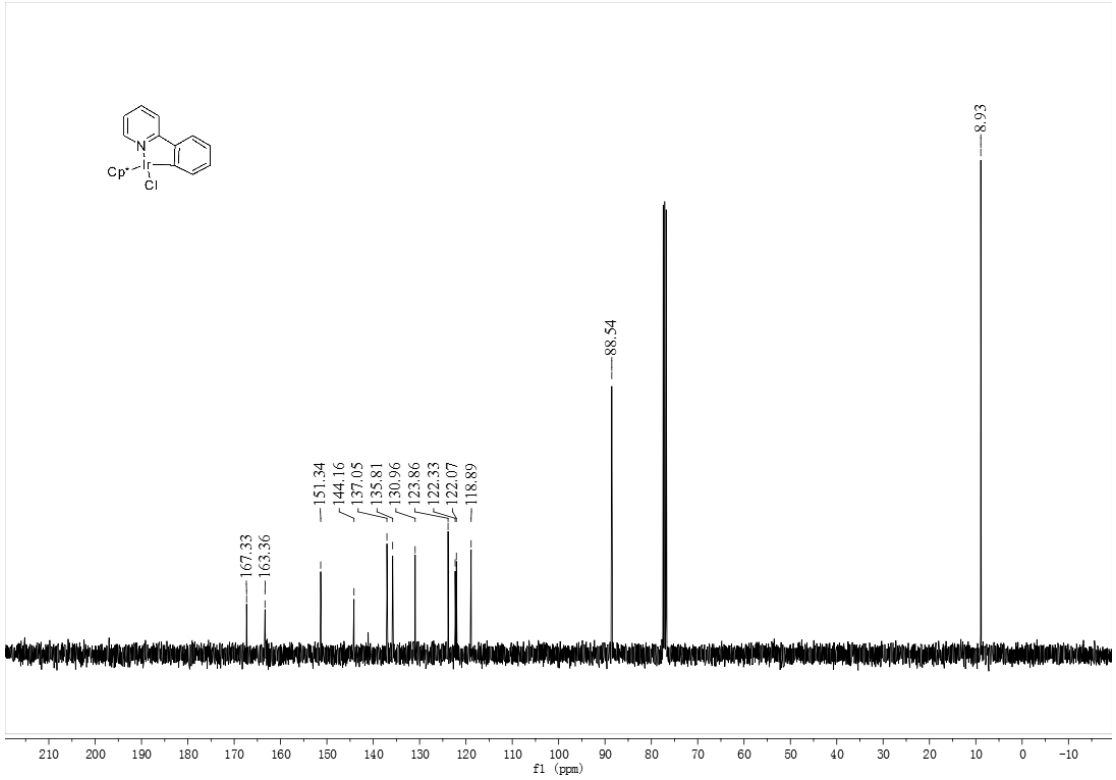


Figure S20. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3aa**, related to **Scheme 2**.

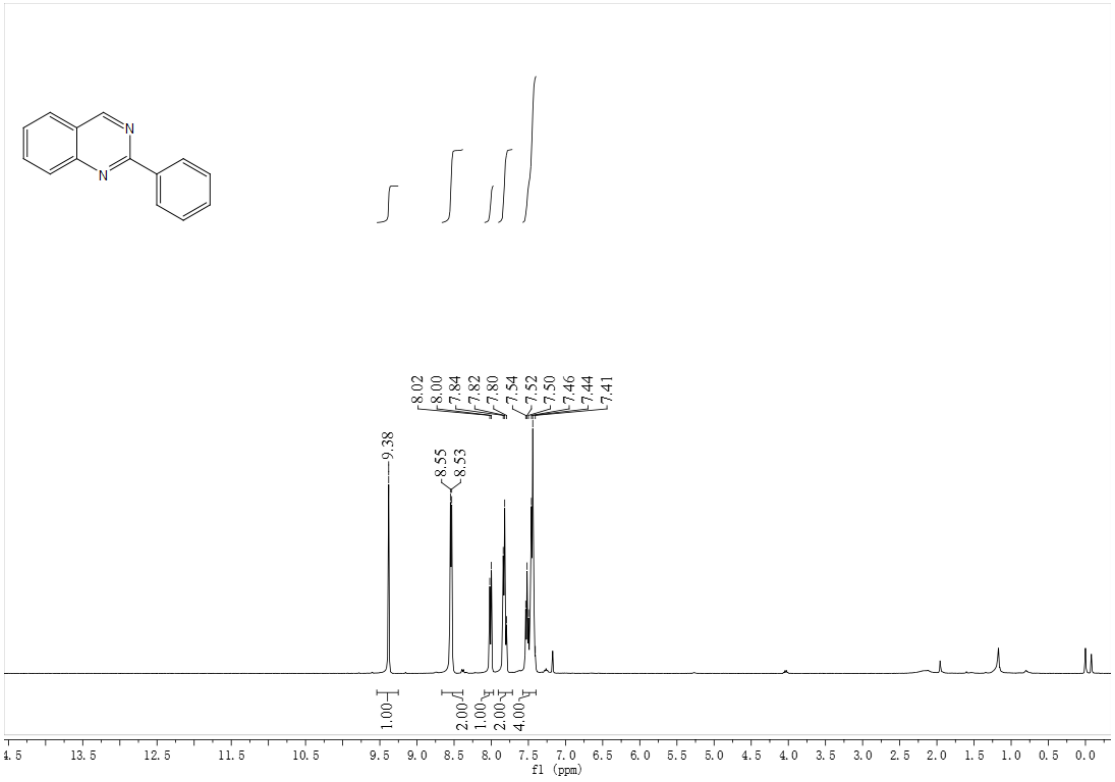


Figure S21. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3aa**, related to **Scheme 2**.

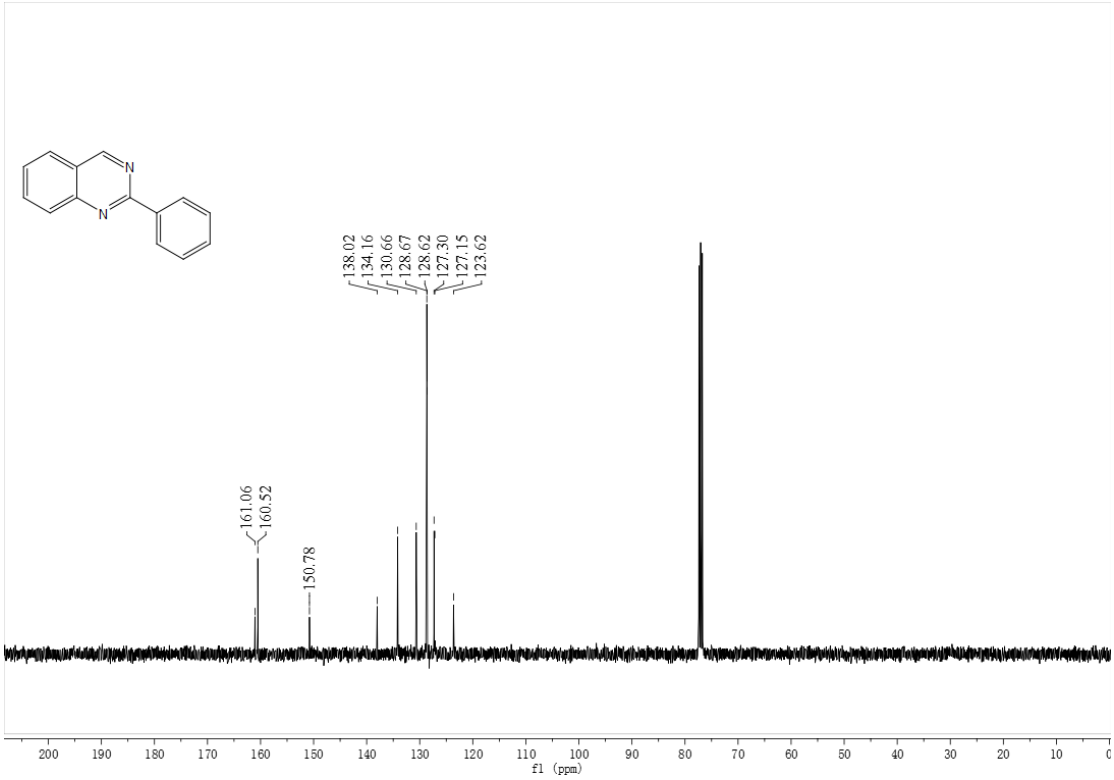


Figure S22. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ab**, related to **Scheme 2**.

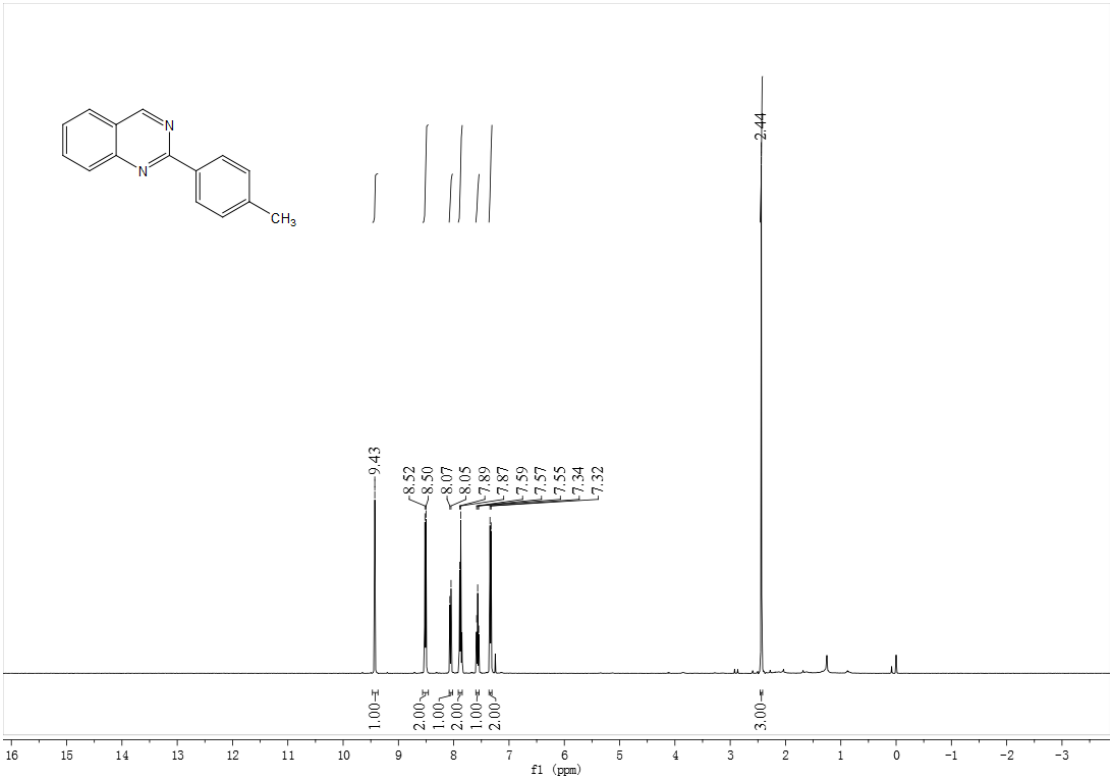


Figure S23. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ab**, related to **Scheme 2**.

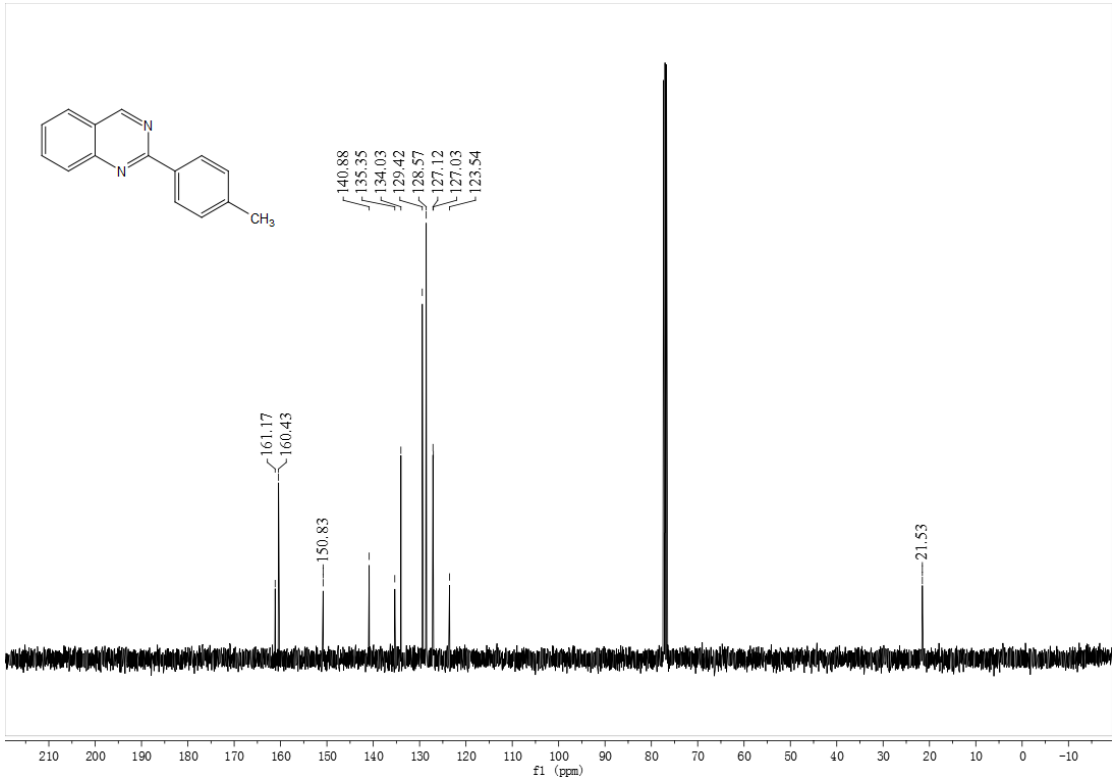


Figure S24. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ac**, related to **Scheme 2**.

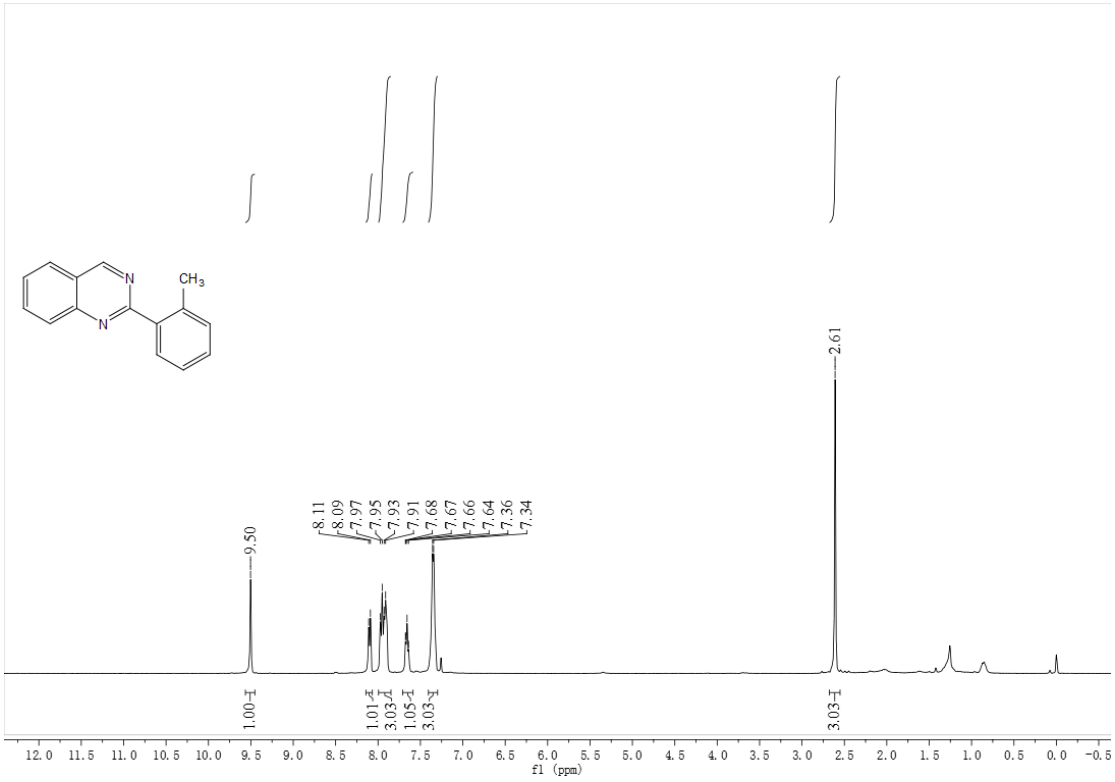


Figure S25. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ac**, related to **Scheme 2**.

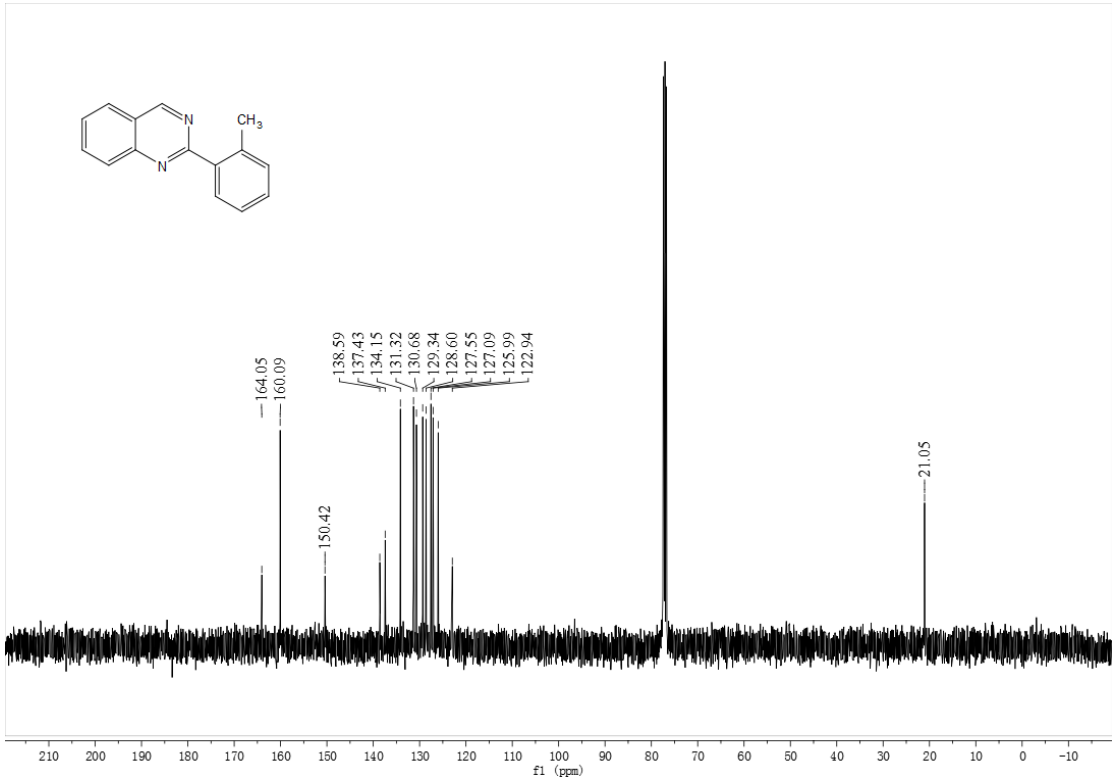


Figure S26. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ad**, related to **Scheme 2**.

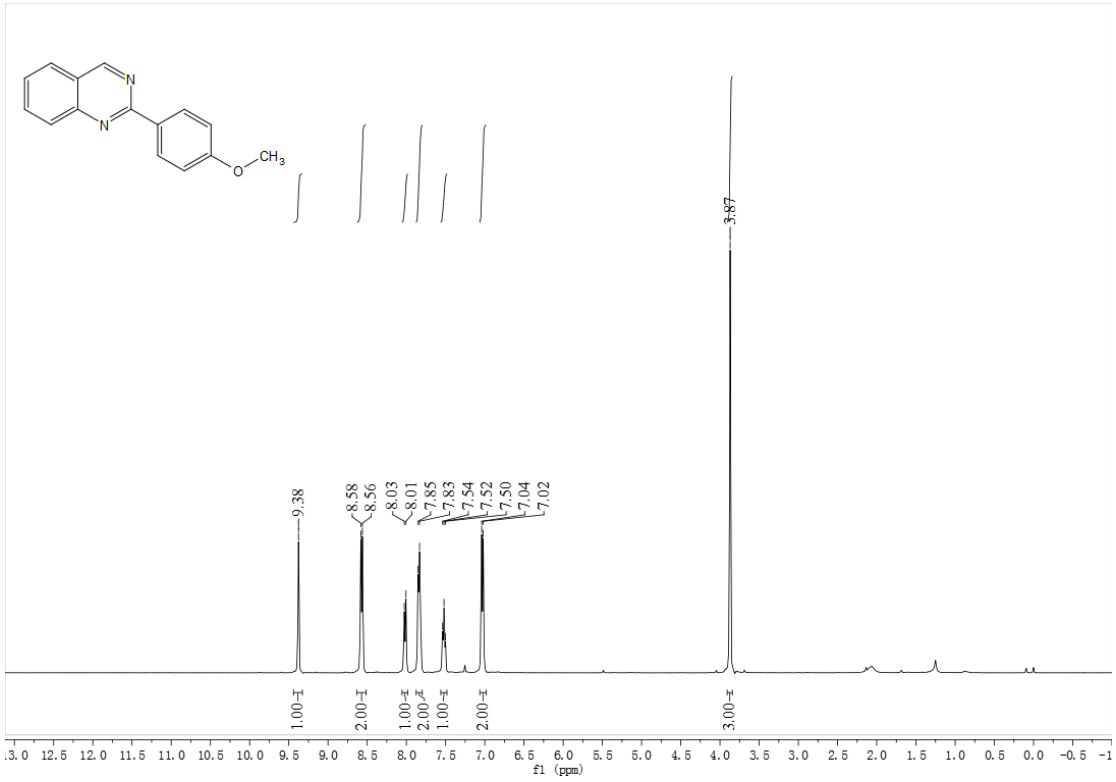


Figure S27. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ad**, related to **Scheme 2**.

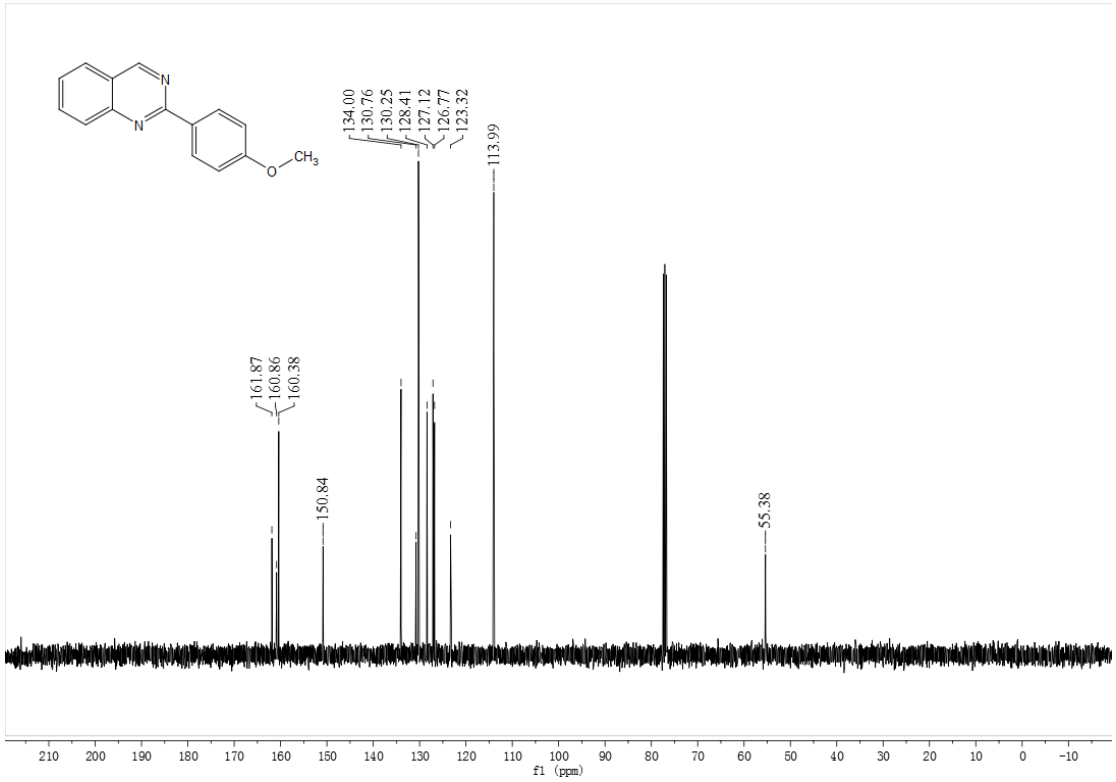


Figure S28. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ae**, related to **Scheme 2**.

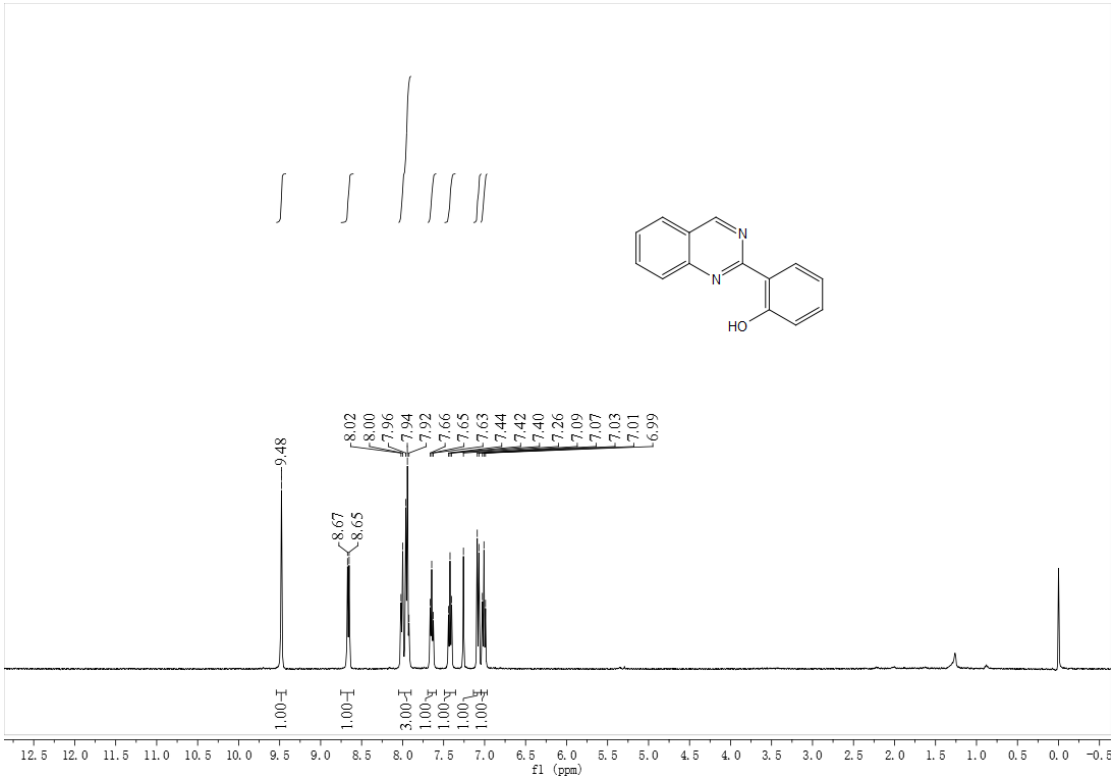


Figure S29. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ae**, related to **Scheme 2**.

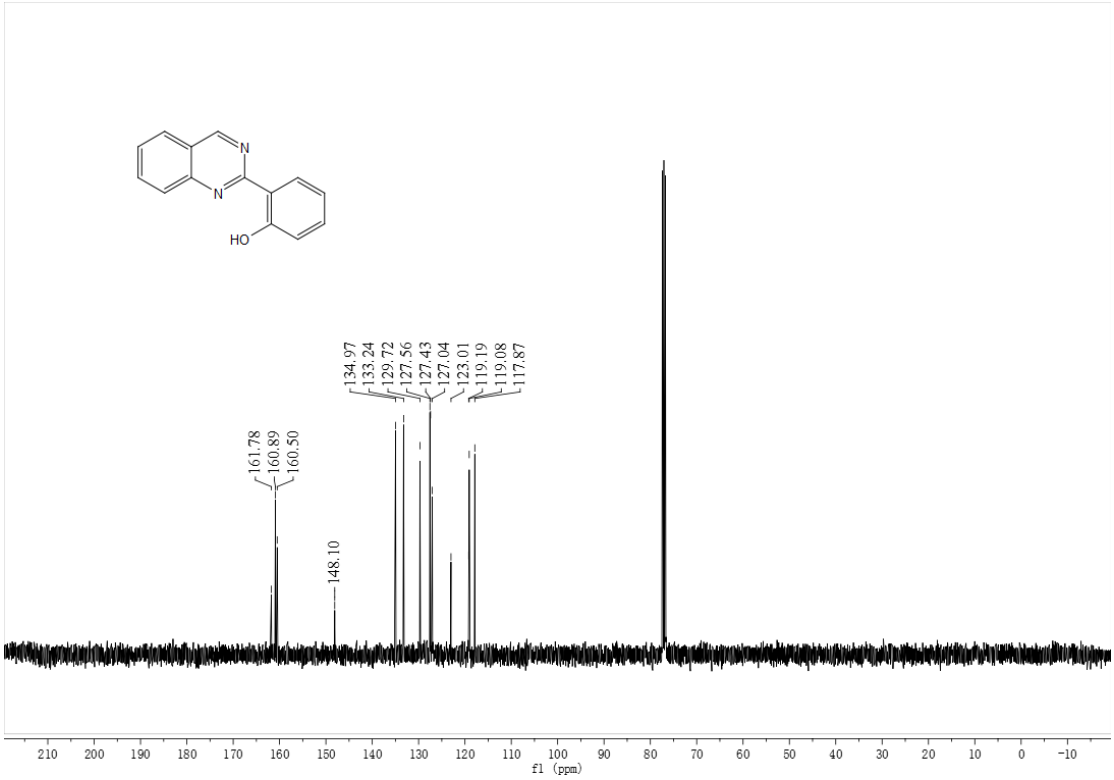


Figure S30. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3af**, related to **Scheme 2**.

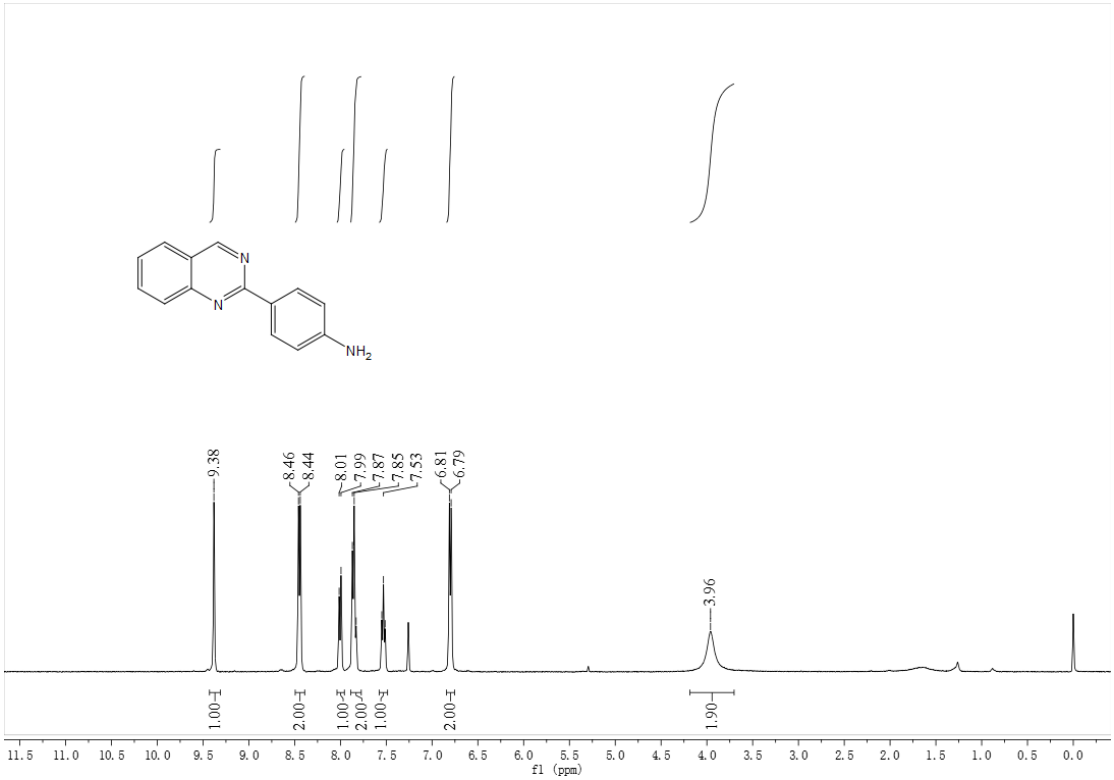


Figure S31. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3af**, related to **Scheme 2**.

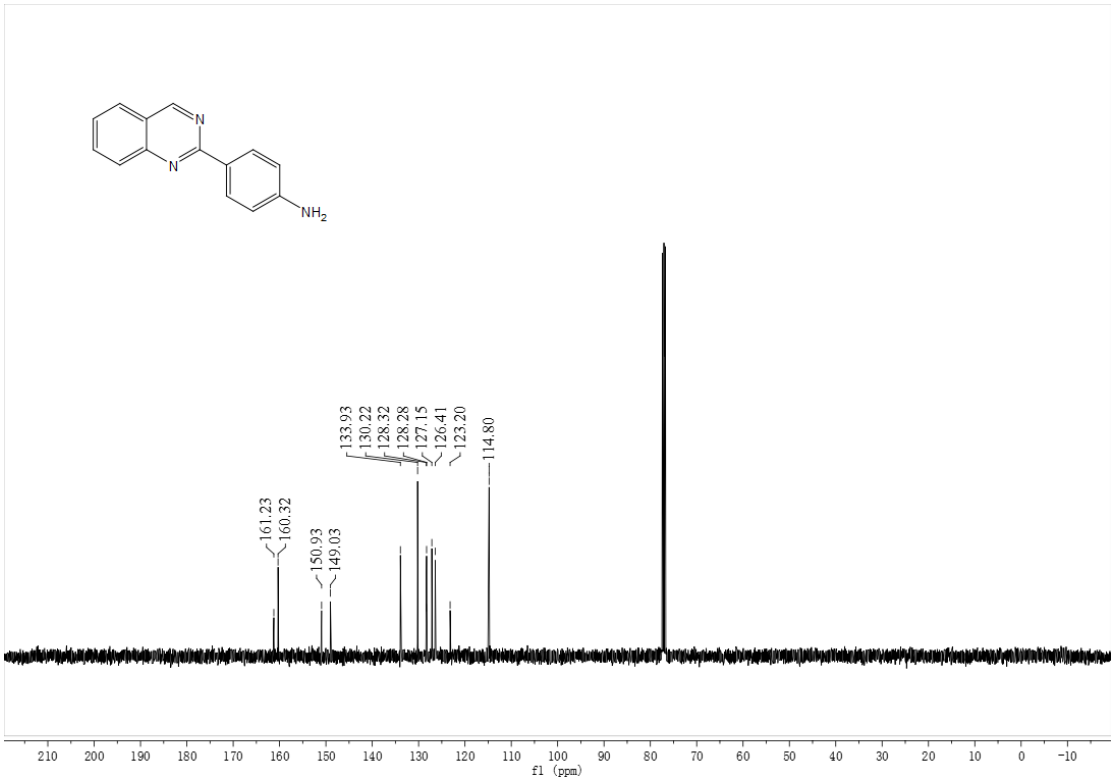


Figure S32. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ag**, related to **Scheme 2**.

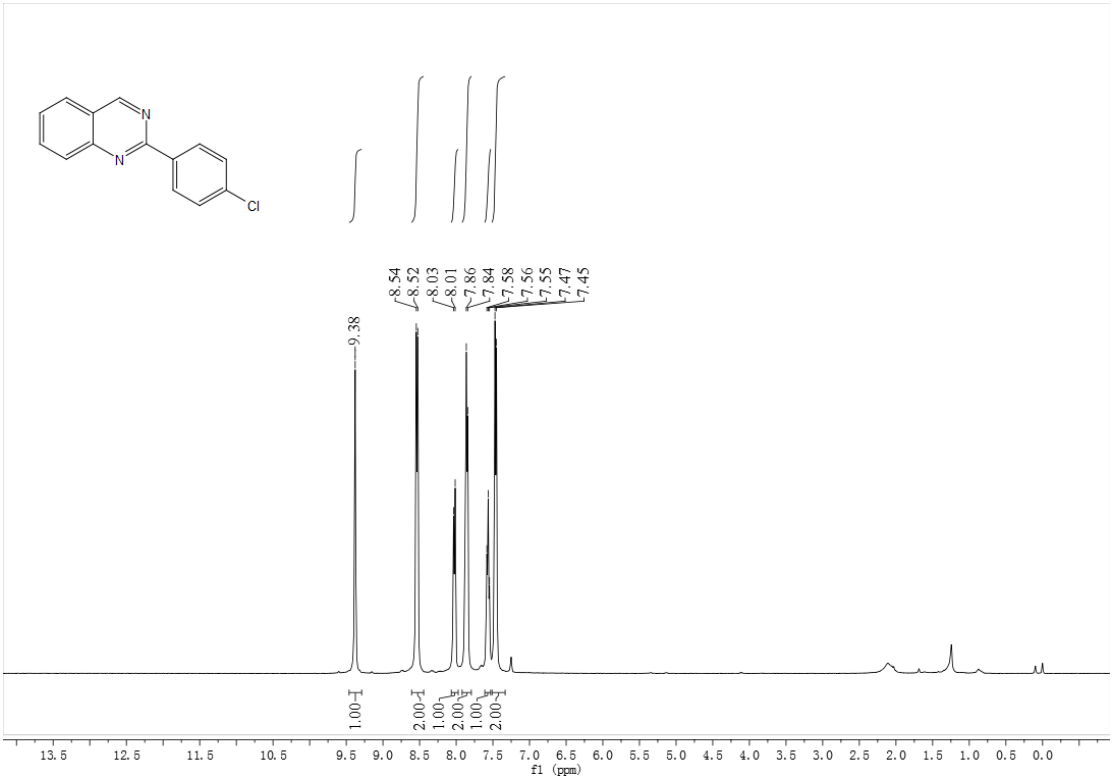


Figure S33. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ag**, related to **Scheme 2**.

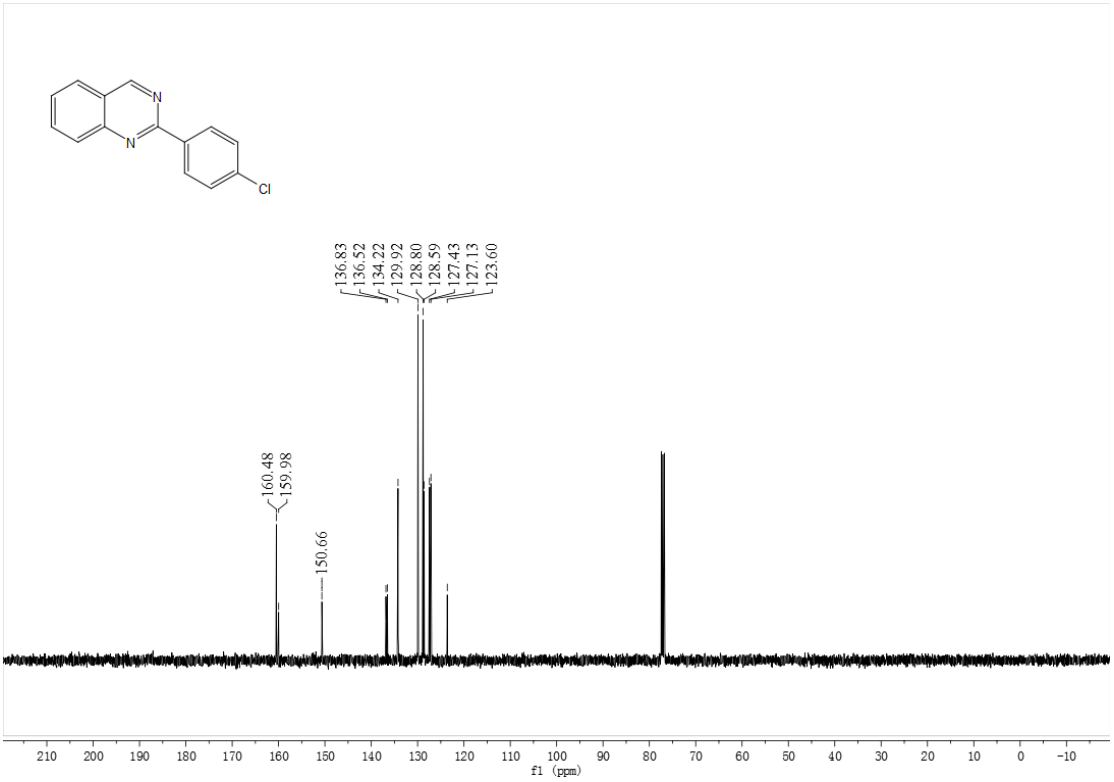


Figure S34. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ah**, related to **Scheme 2**.

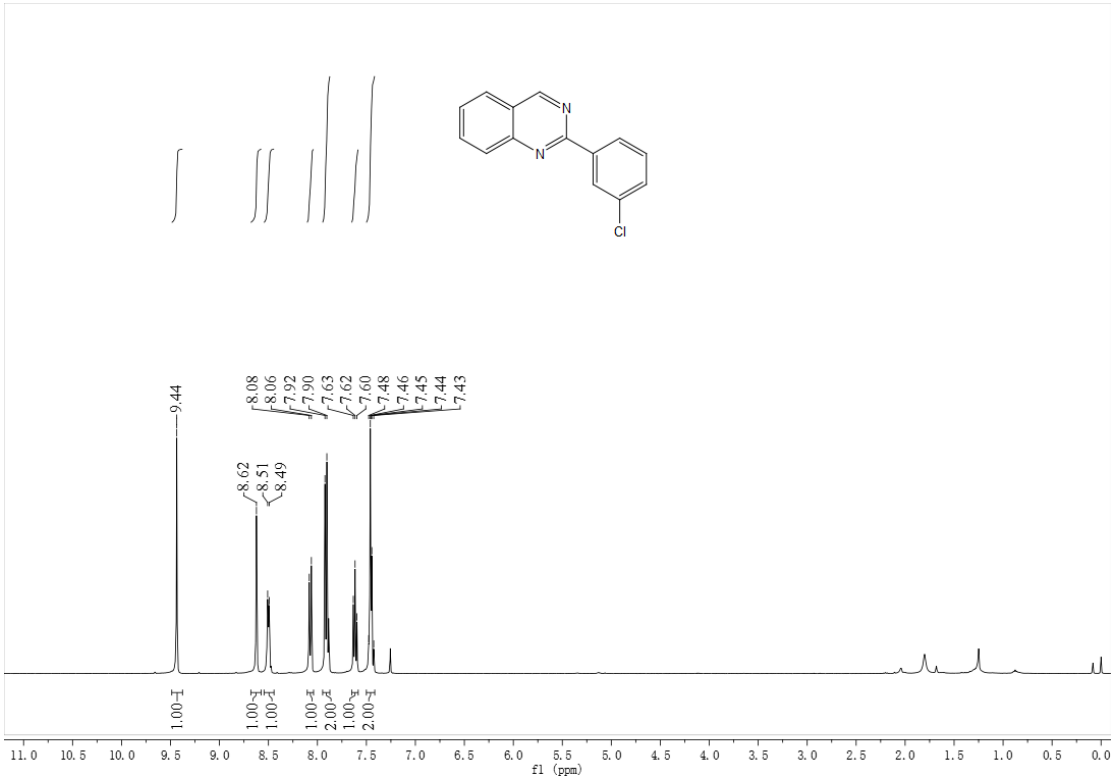


Figure S35. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ah**, related to **Scheme 2**.

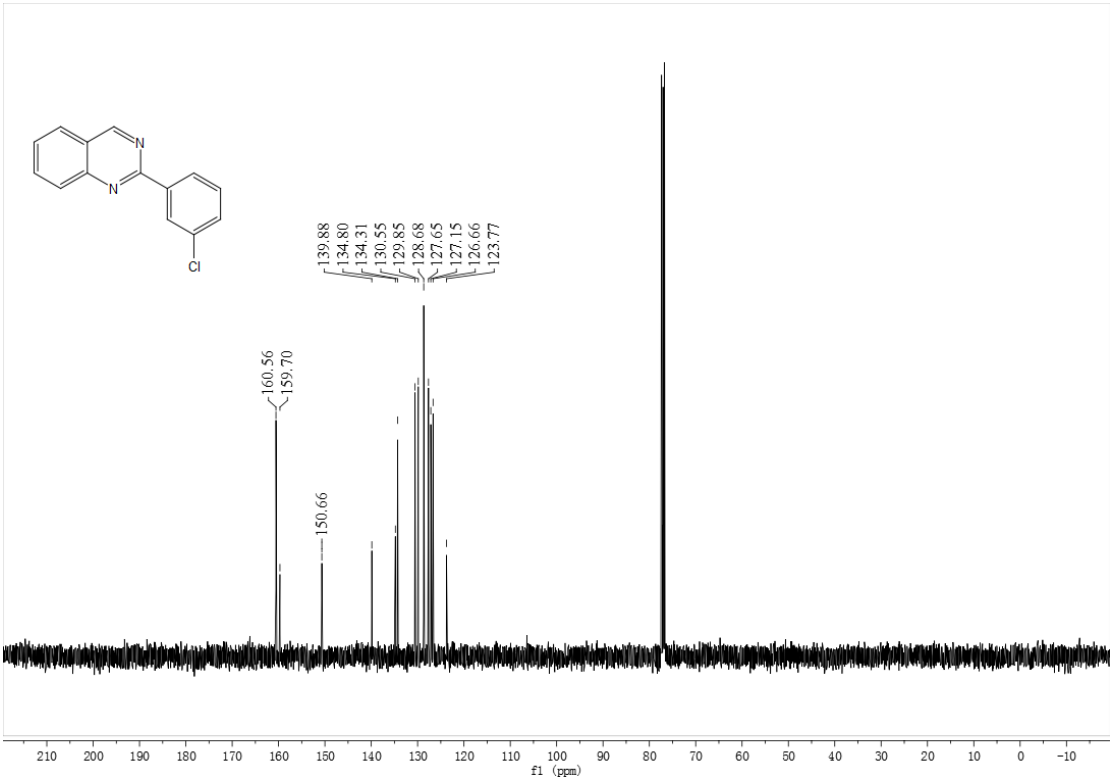


Figure S36. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ai**, related to **Scheme 2**.

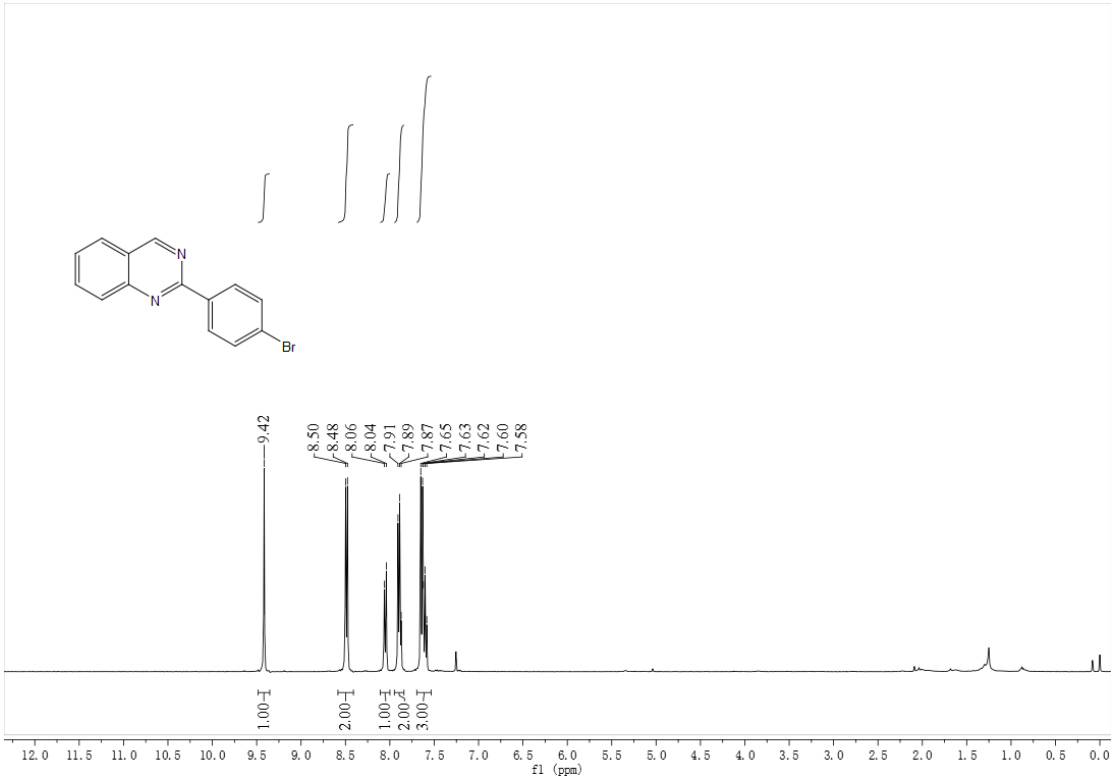


Figure S37. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ai**, related to **Scheme 2**.

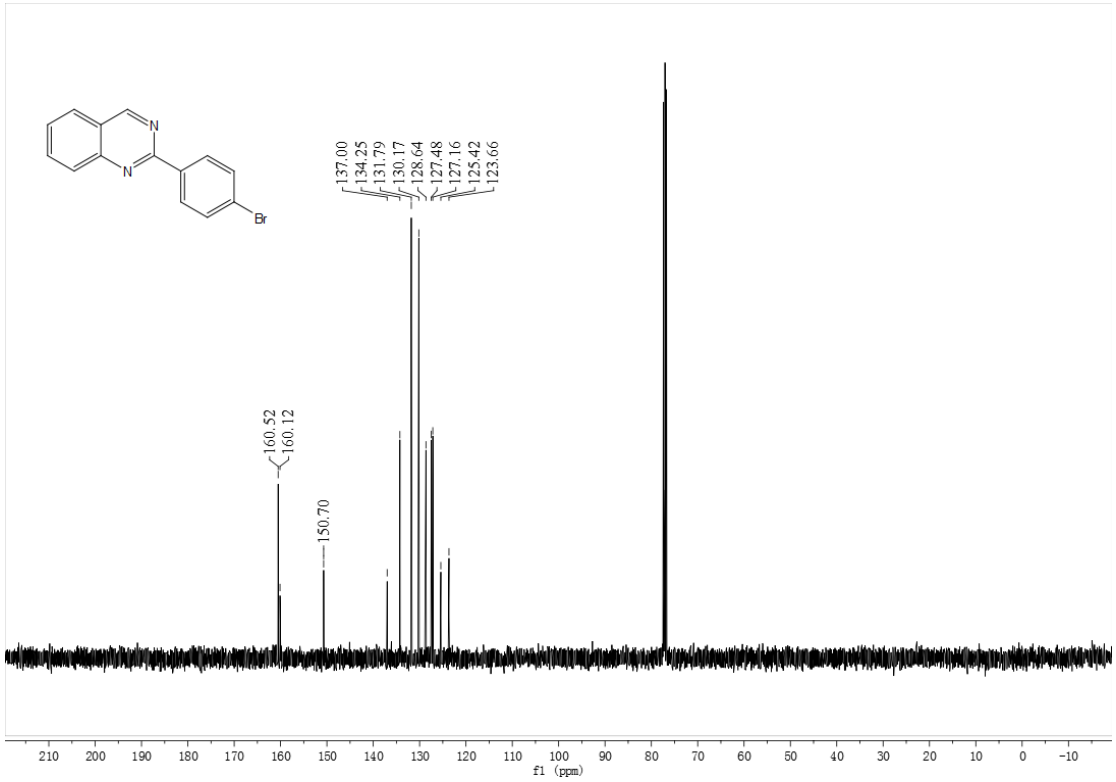


Figure S38. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3aj**, related to **Scheme 2**.

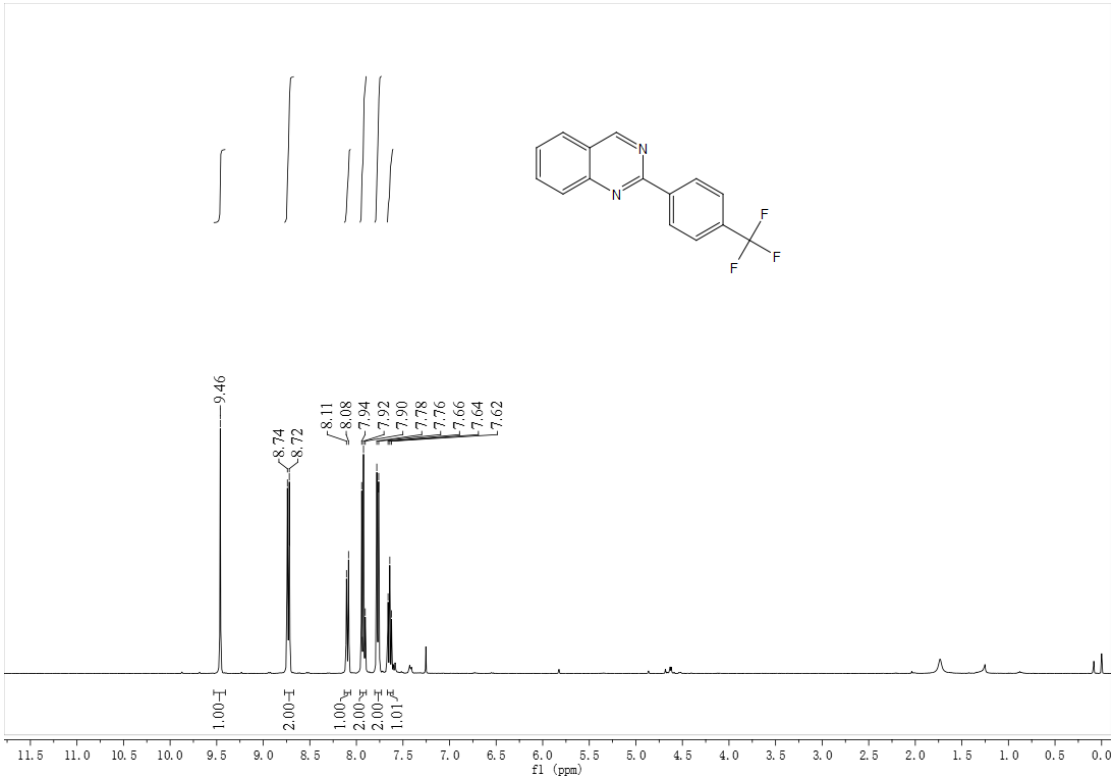


Figure S39. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3aj**, related to **Scheme 2**.

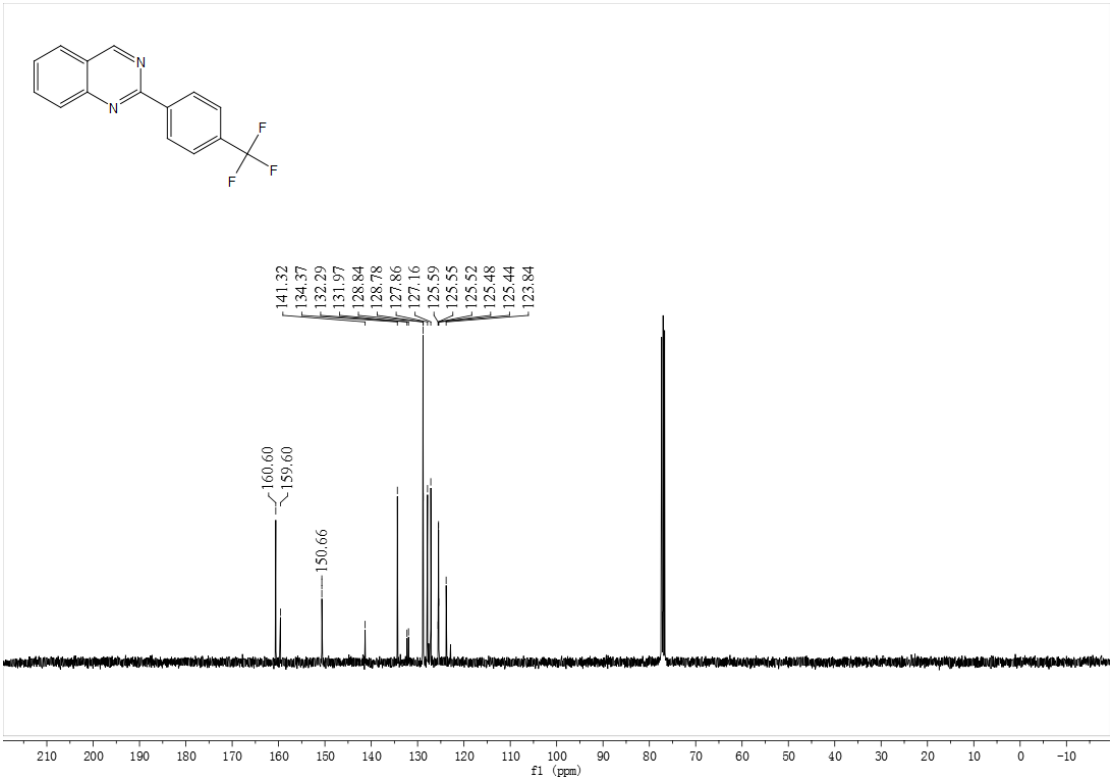


Figure S40. ^{19}F-NMR (100 MHz, $CDCl_3$) spectrum of **3aj**, related to **Scheme 2**.

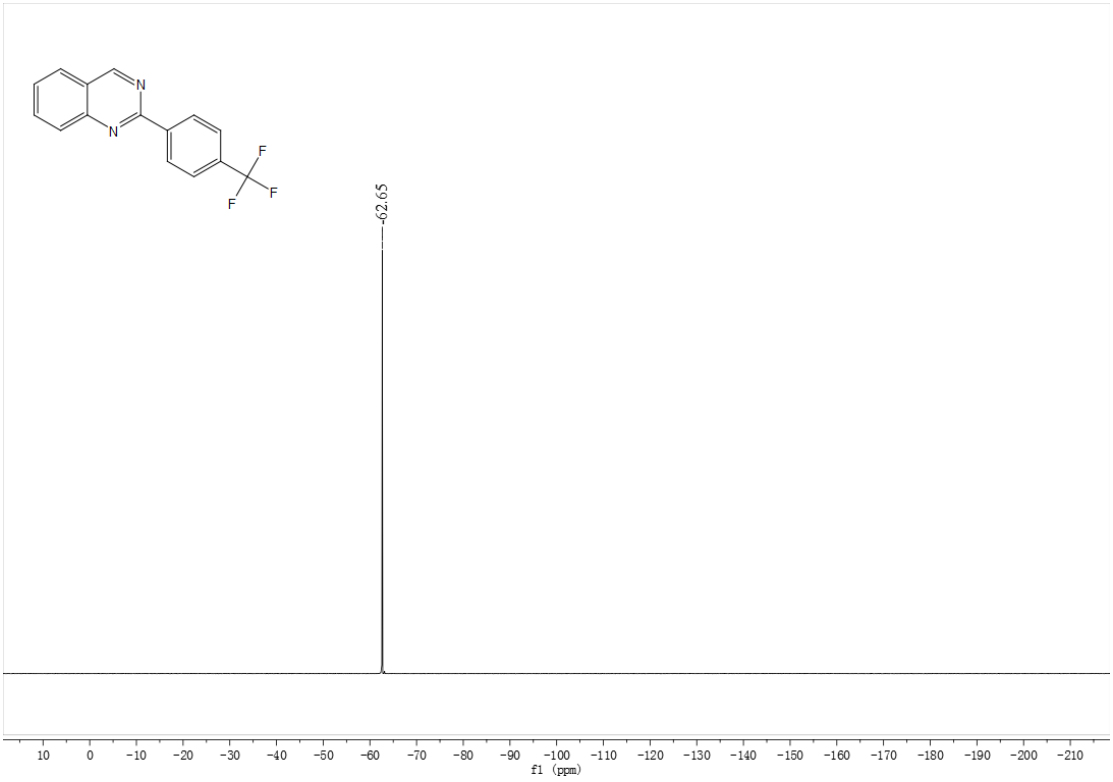


Figure S41. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ak**, related to **Scheme 2**.

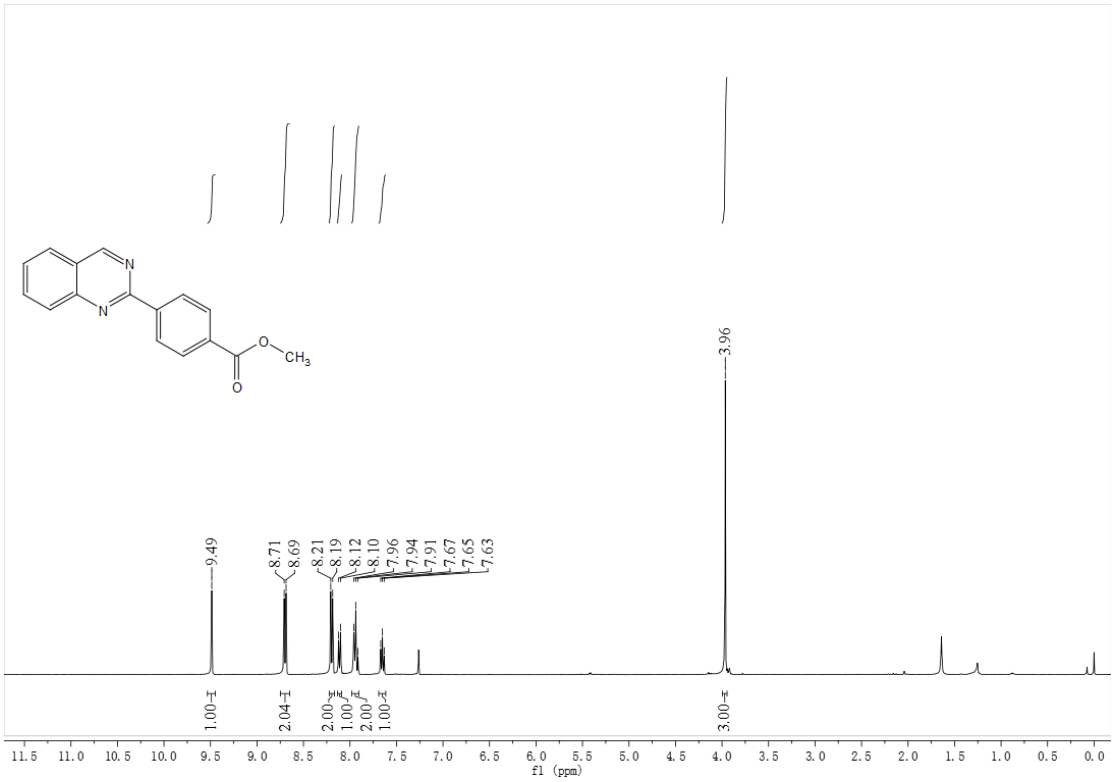


Figure S42. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ak**, related to **Scheme 2**.

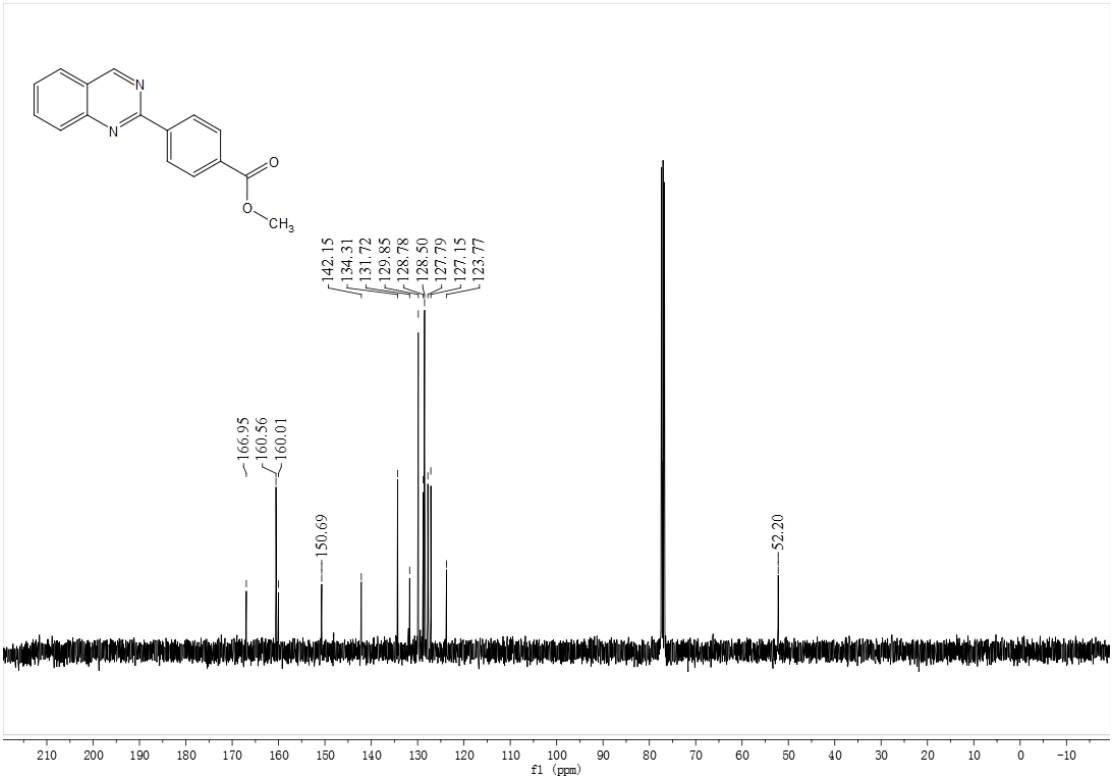


Figure S43. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3al**, related to **Scheme 2**.

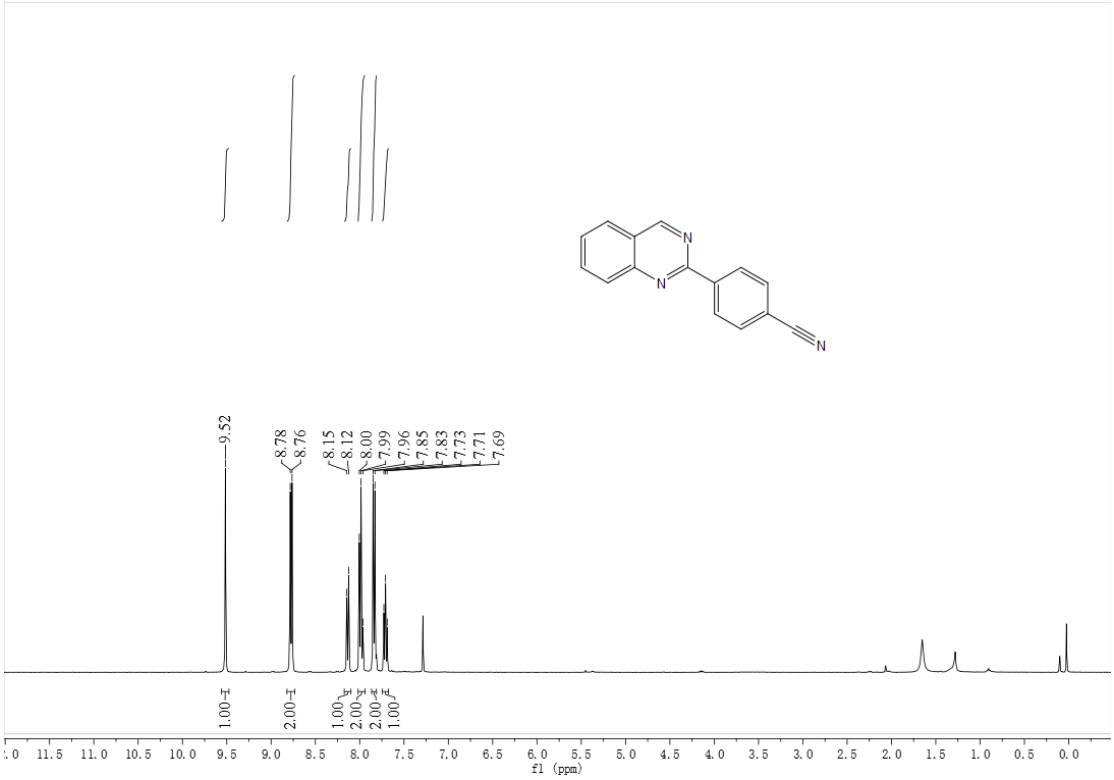


Figure S44. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3al**, related to **Scheme 2**.

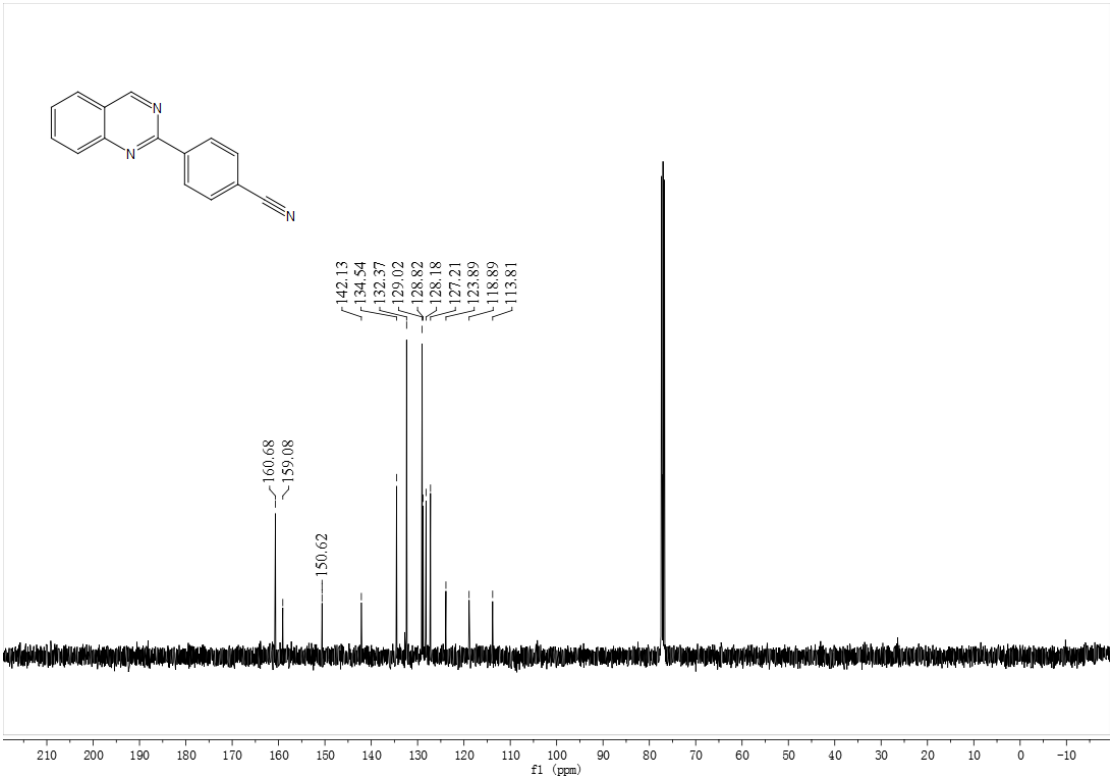


Figure S45. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3am**, related to **Scheme 2**.

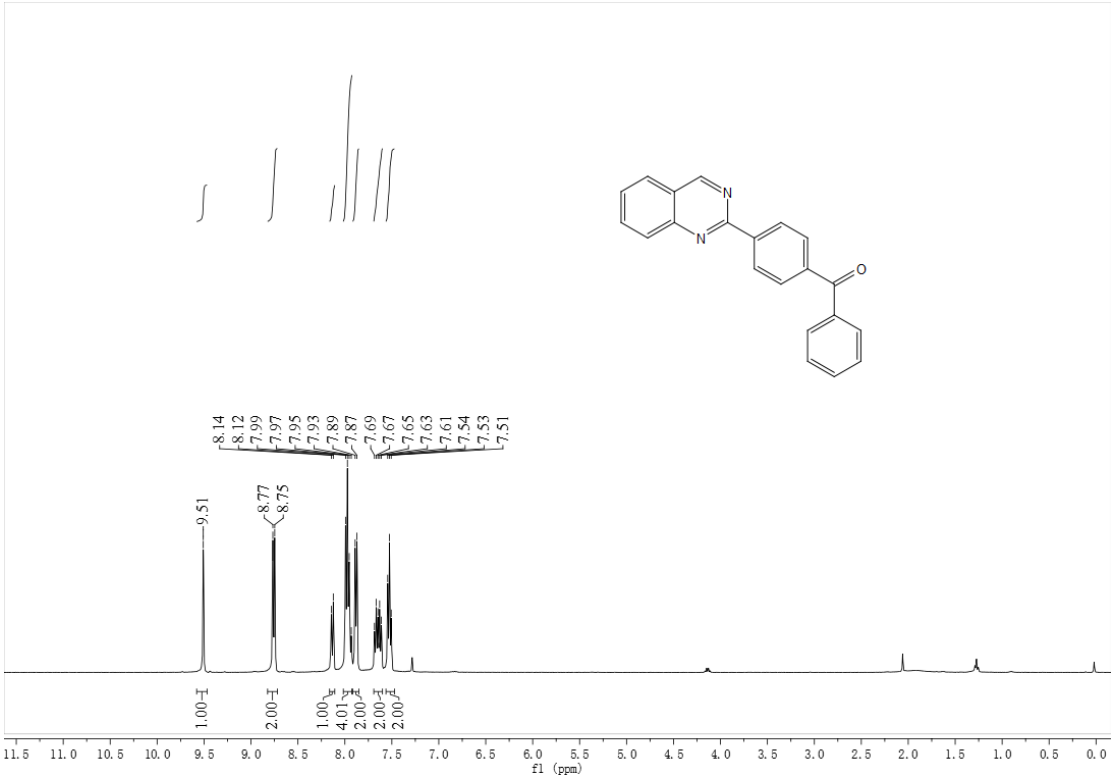


Figure S46. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3am**, related to **Scheme 2**.

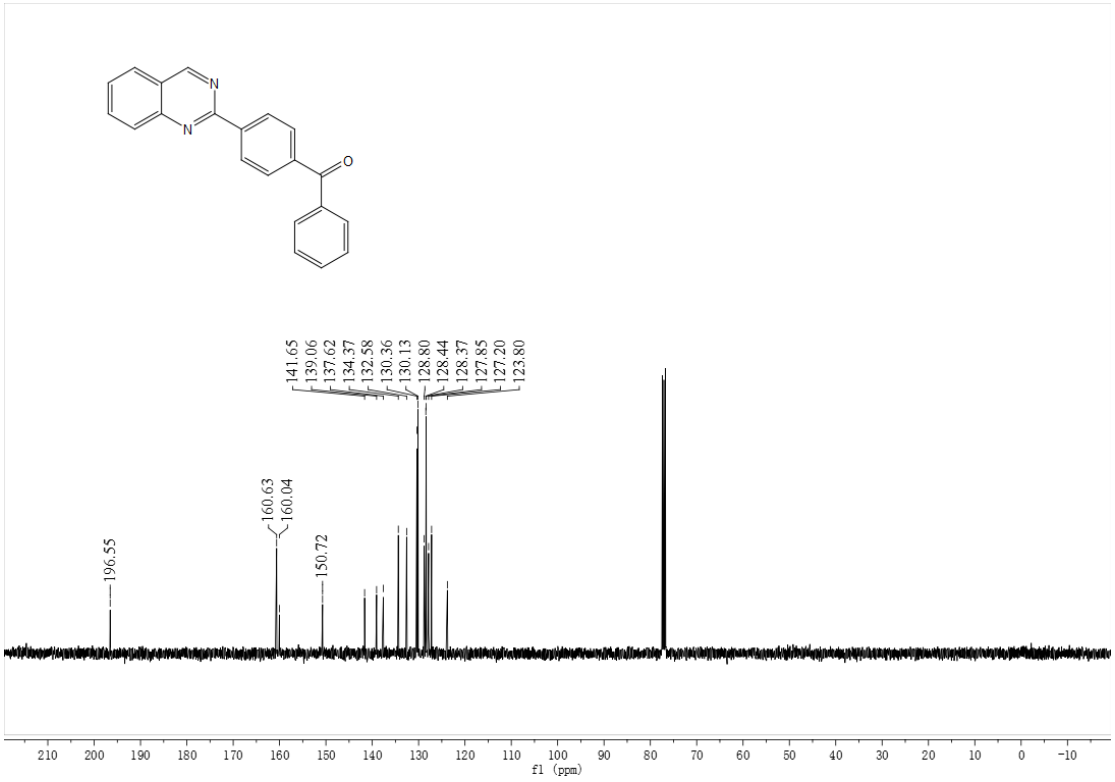


Figure S47. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3an**, related to **Scheme 2**.

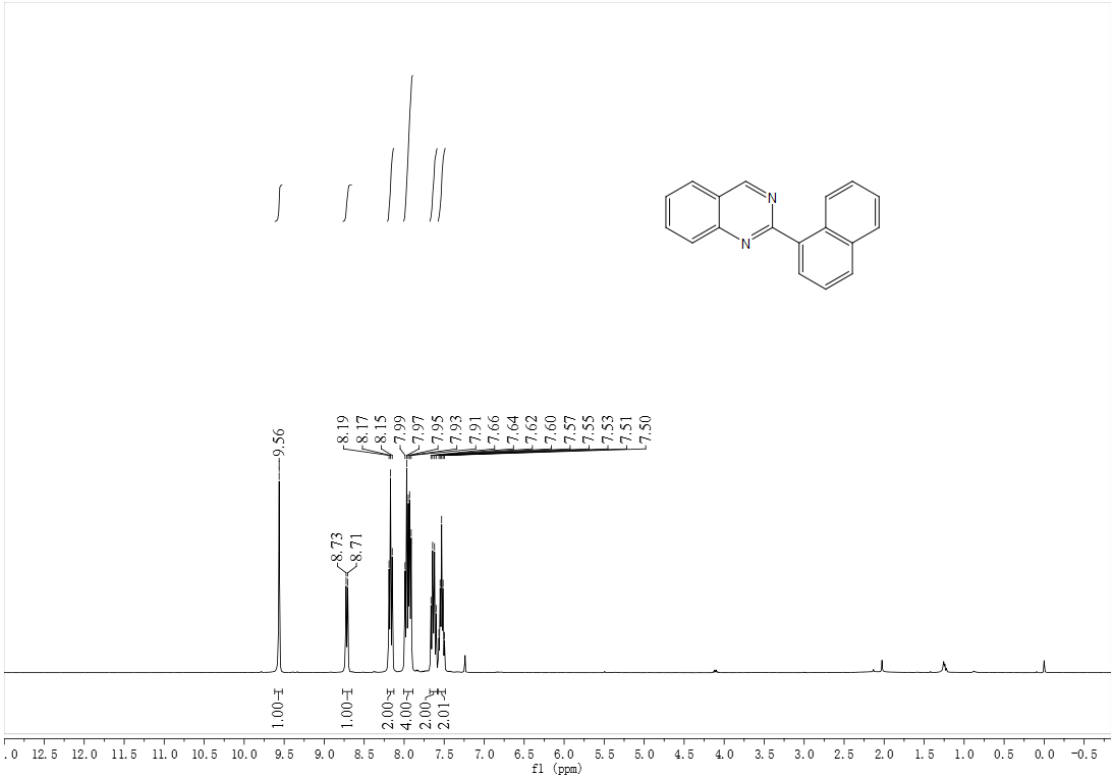


Figure S48. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3an**, related to **Scheme 2**.

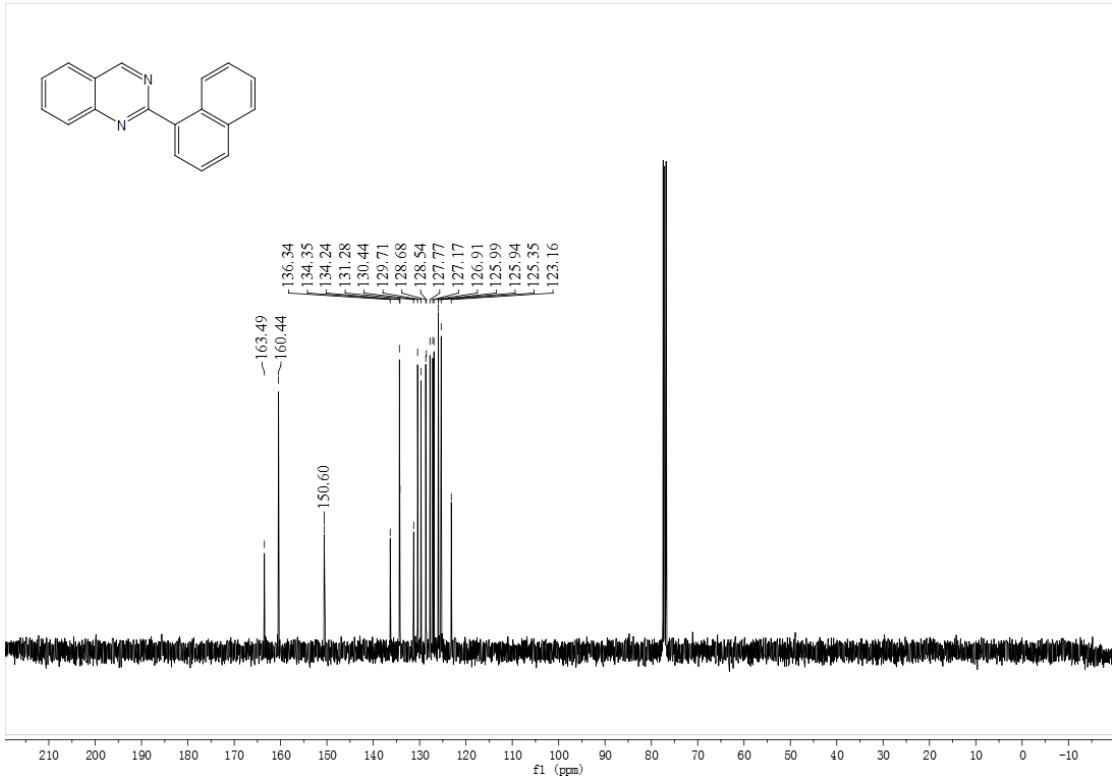


Figure S49. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ao**, related to **Scheme 2**.

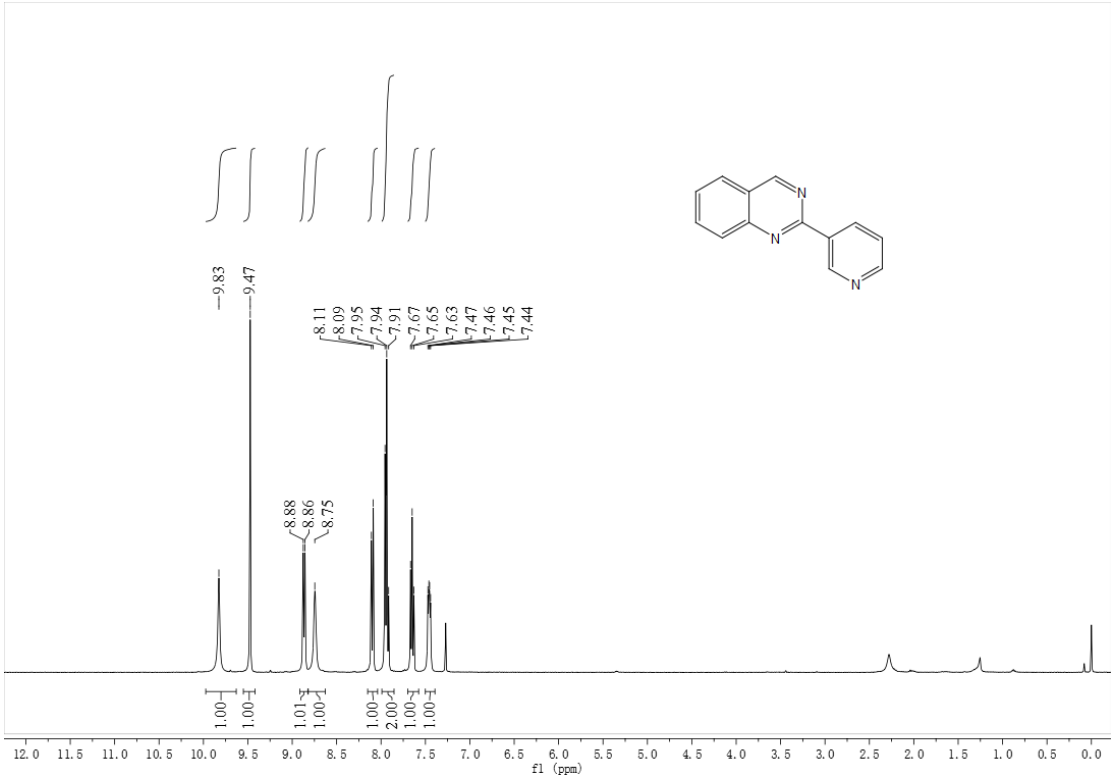


Figure S50. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ao**, related to **Scheme 2**.

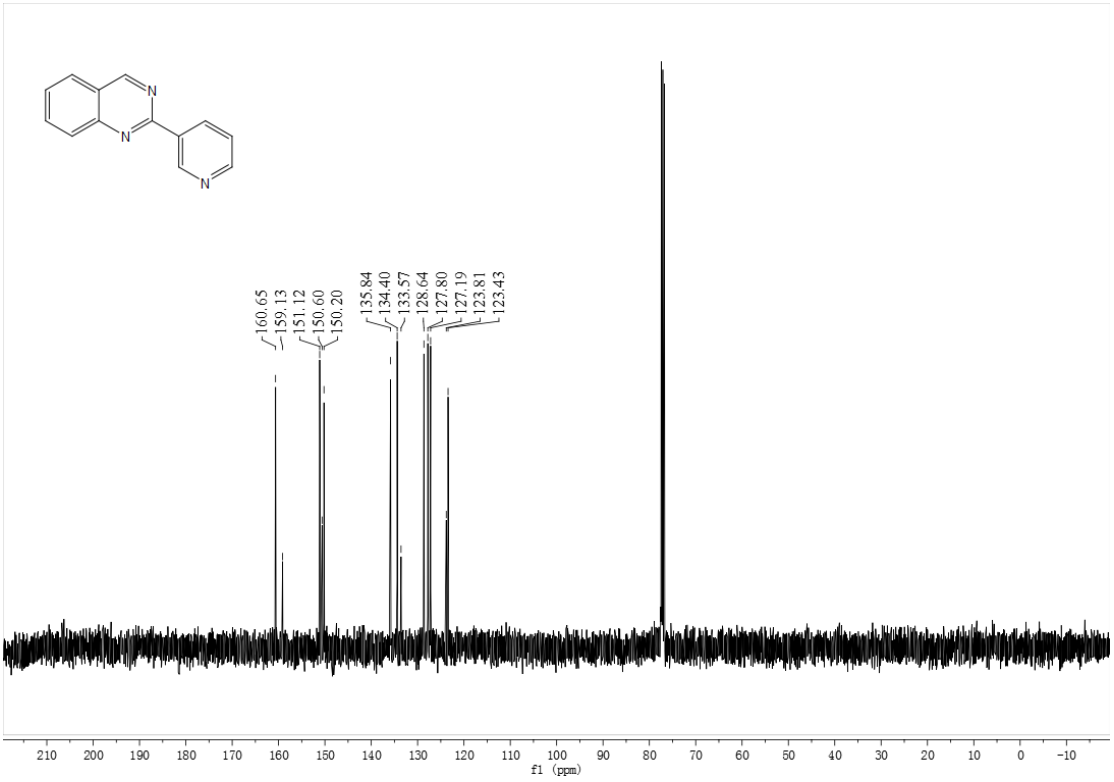


Figure S51. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ap**, related to **Scheme 2**.

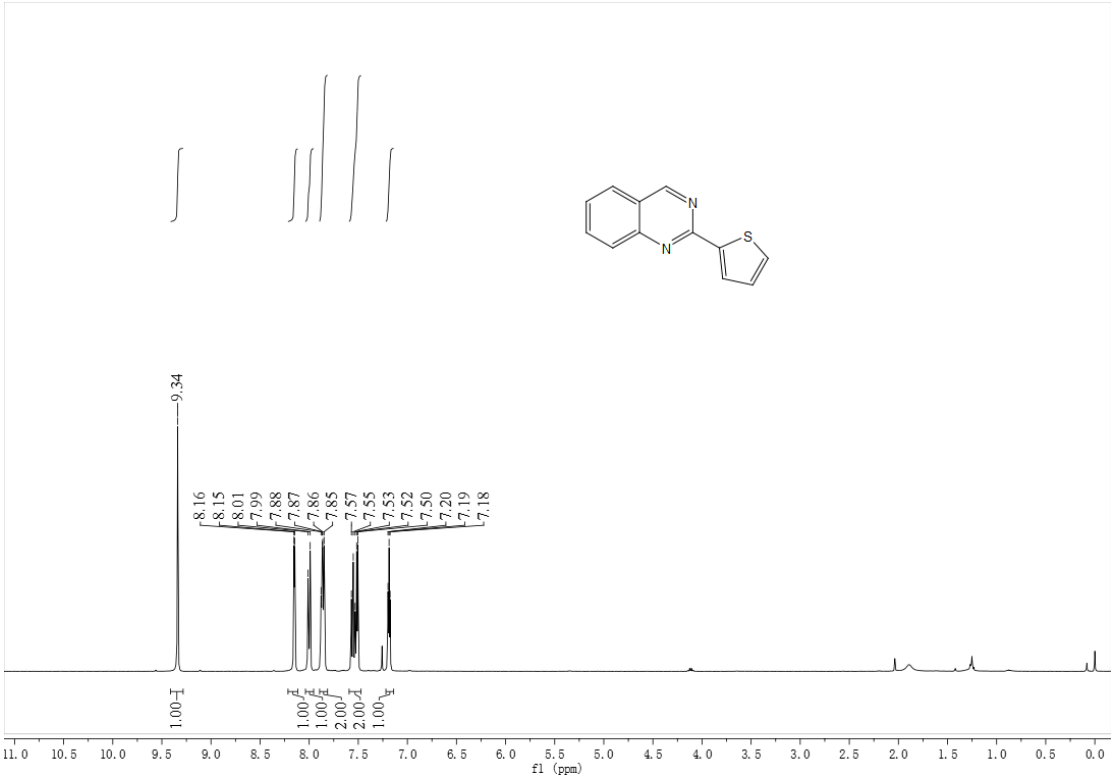


Figure S52. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ap**, related to **Scheme 2**.

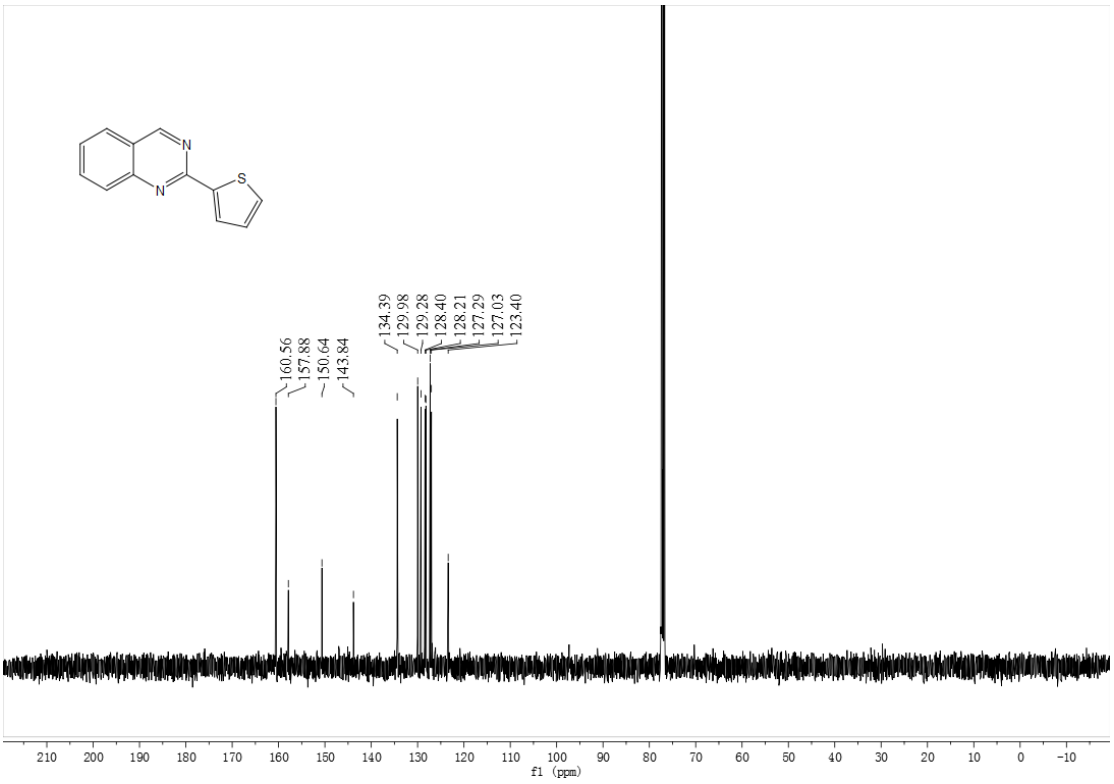


Figure S53. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3aq**, related to **Scheme 2**.

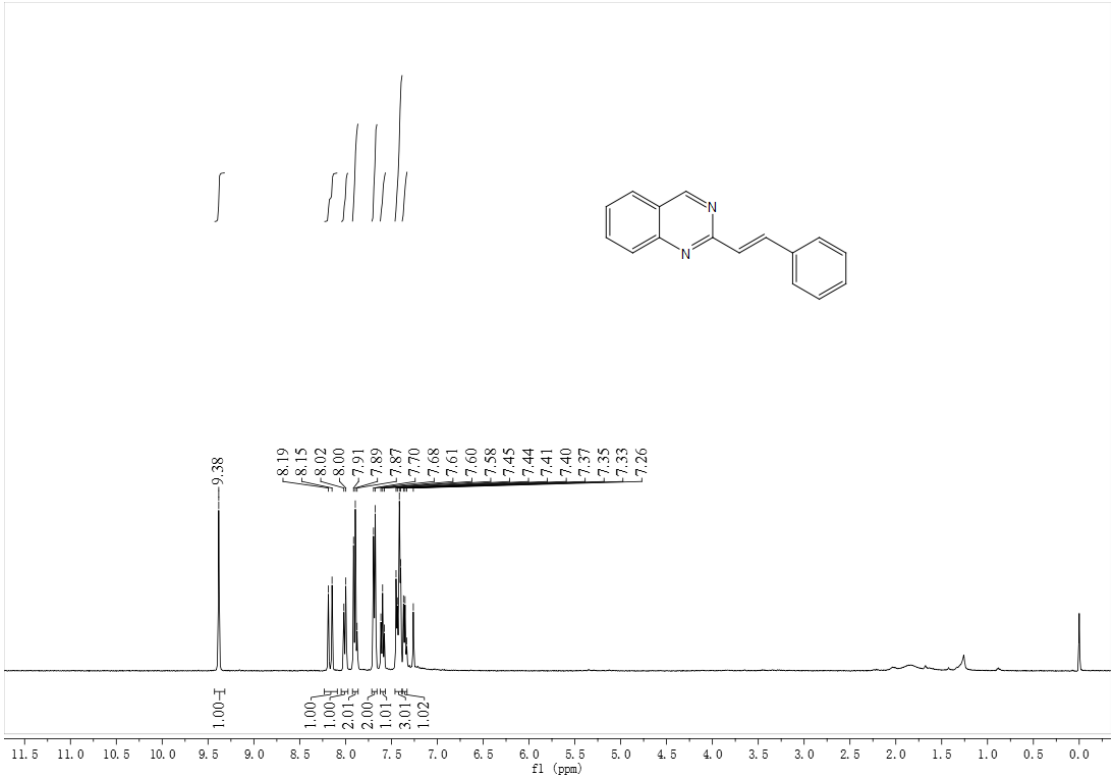


Figure S54. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3aq**, related to **Scheme 2**.

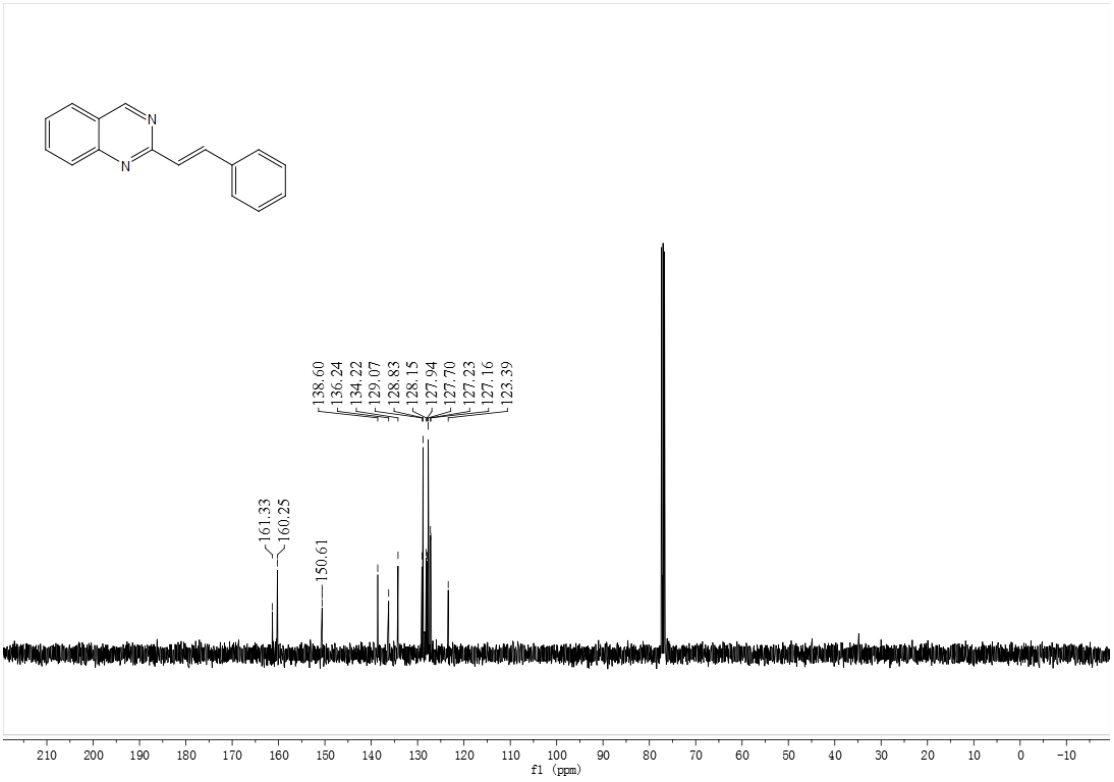


Figure S55. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ar**, related to **Scheme 2**.

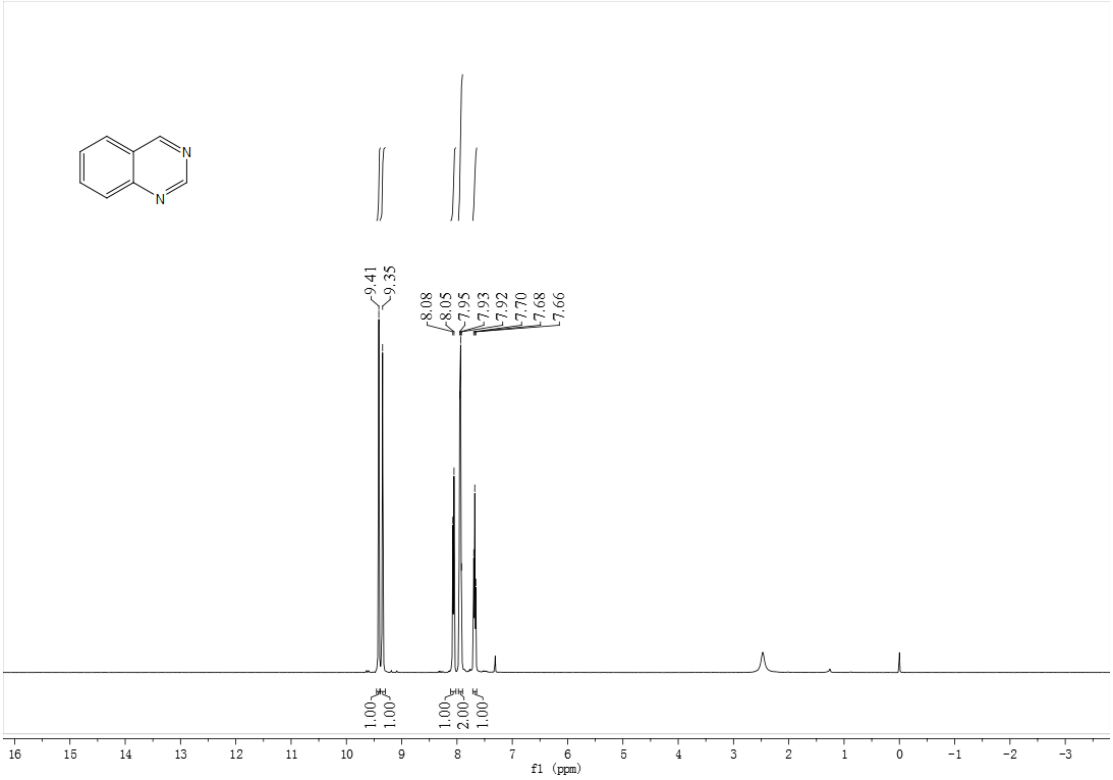


Figure S56. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ar**, related to **Scheme 2**.

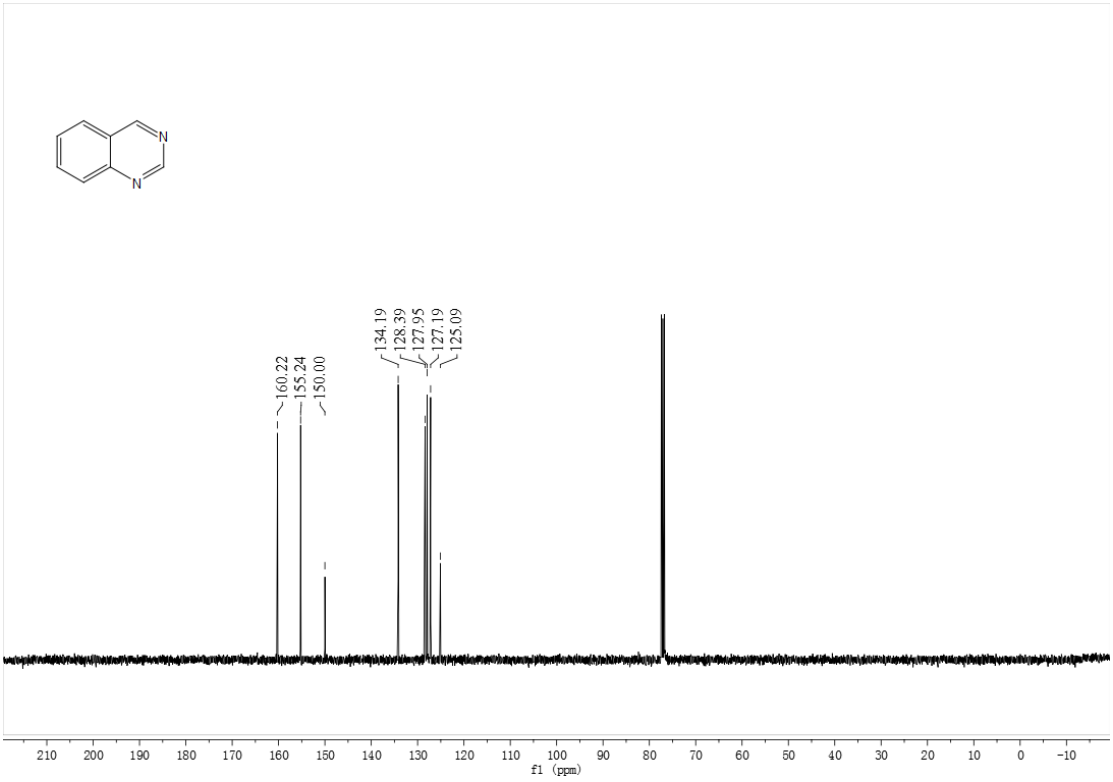


Figure S57. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3as**, related to **Scheme 2**.

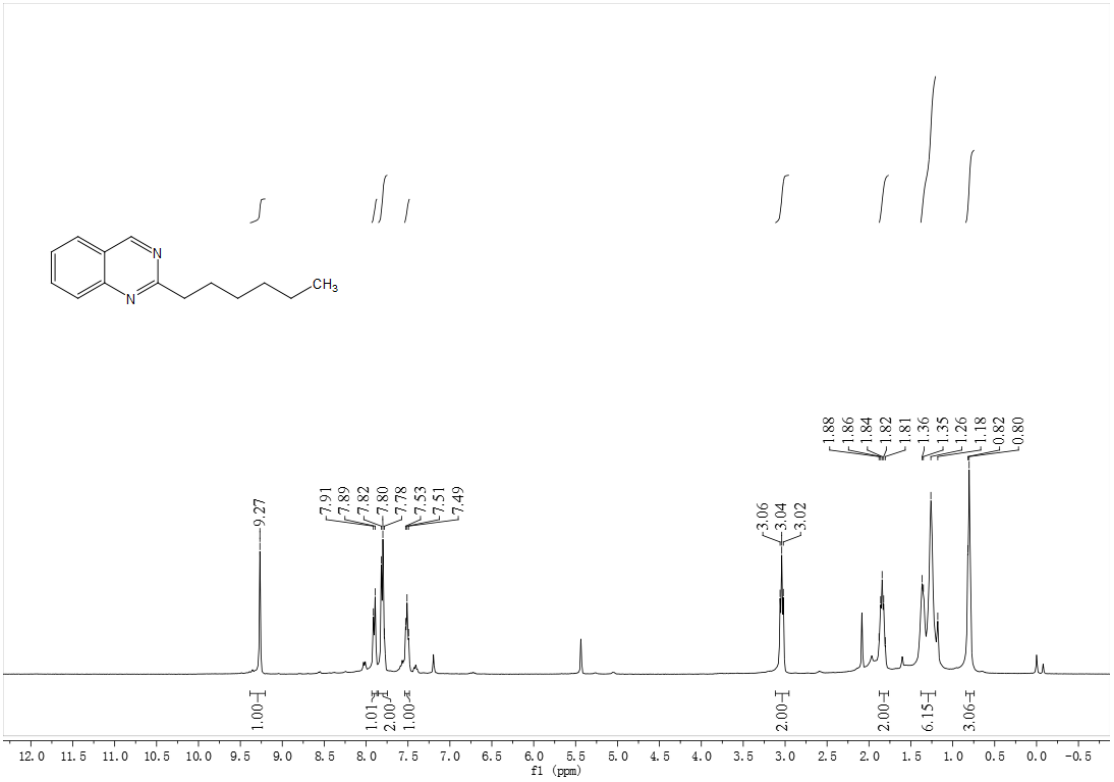


Figure S58. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3as**, related to **Scheme 2**.

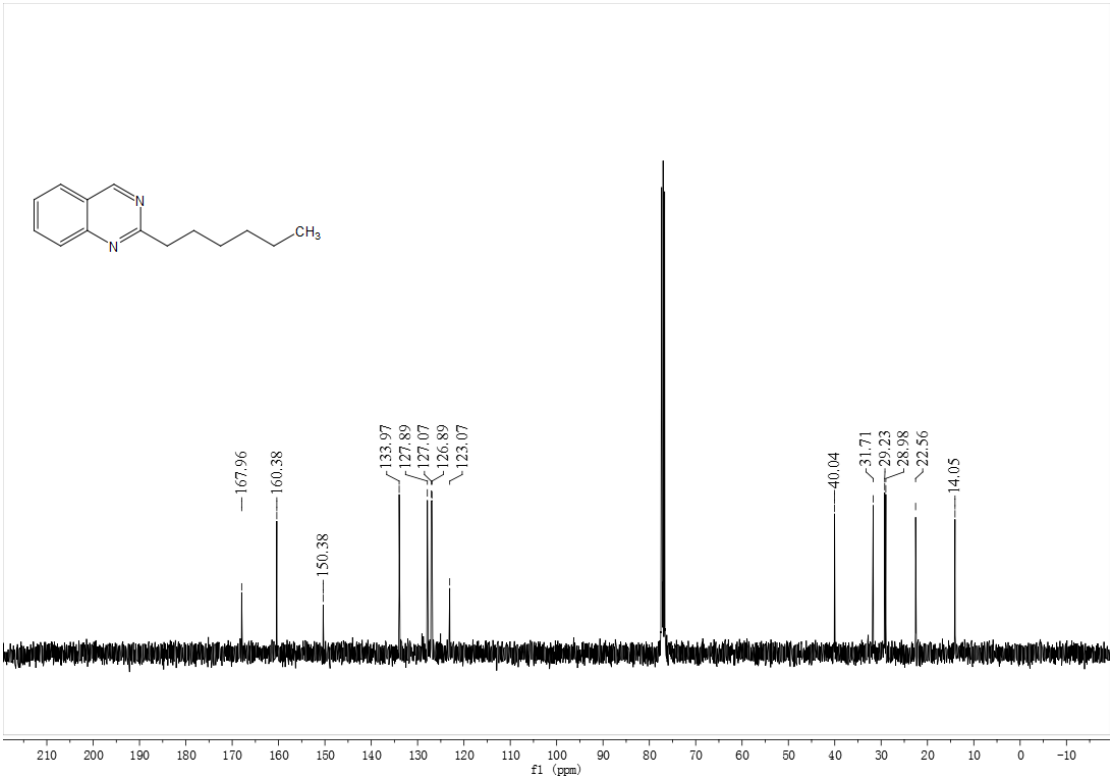


Figure S59. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3at**, related to **Scheme 2**.

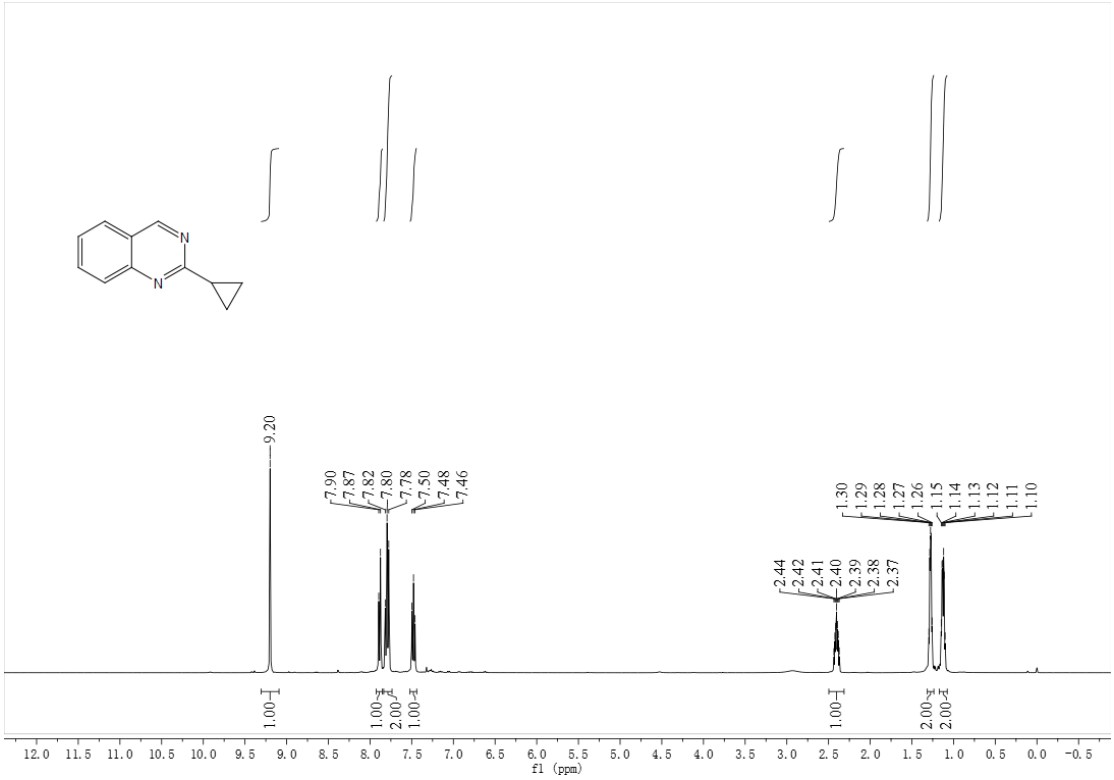


Figure S60. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3at**, related to **Scheme 2**.

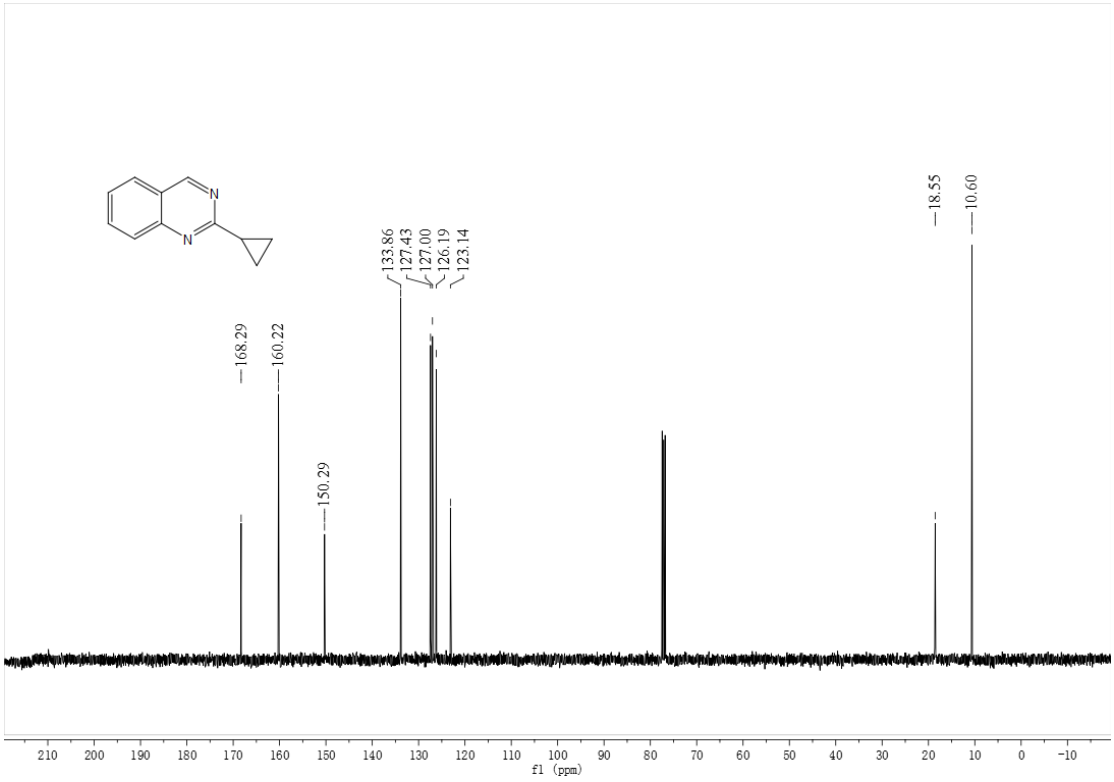


Figure S61. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ba**, related to **Scheme 3**.

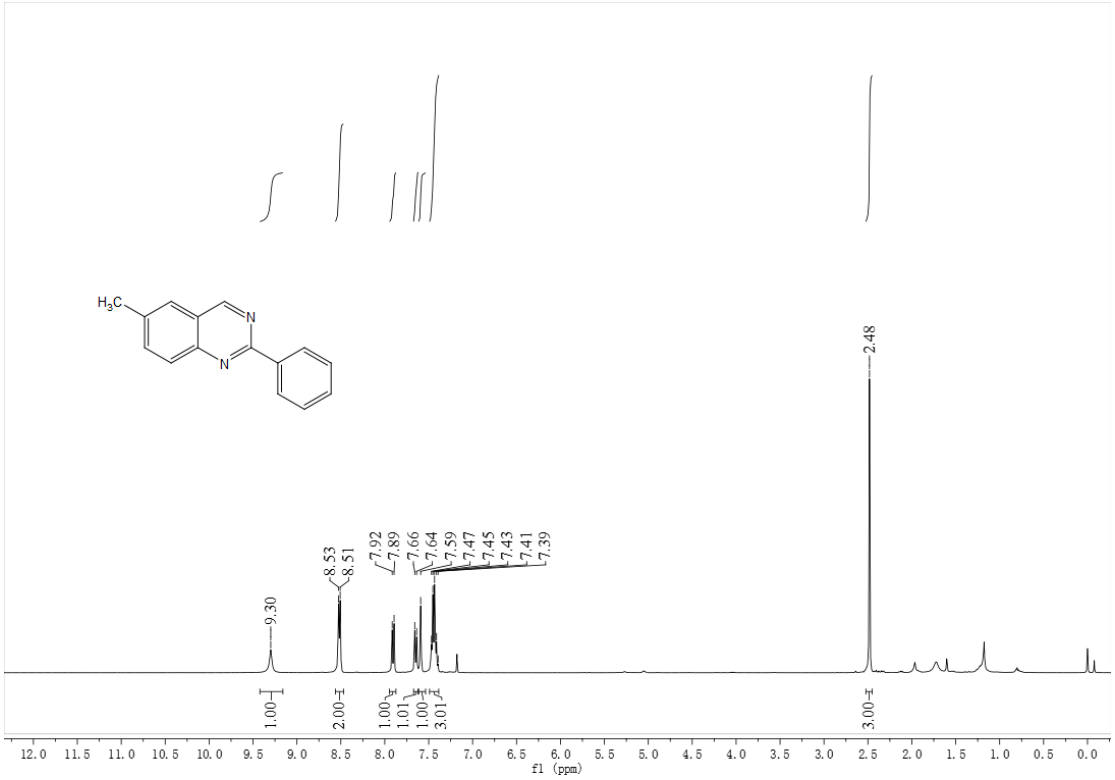


Figure S62. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ba**, related to **Scheme 3**.

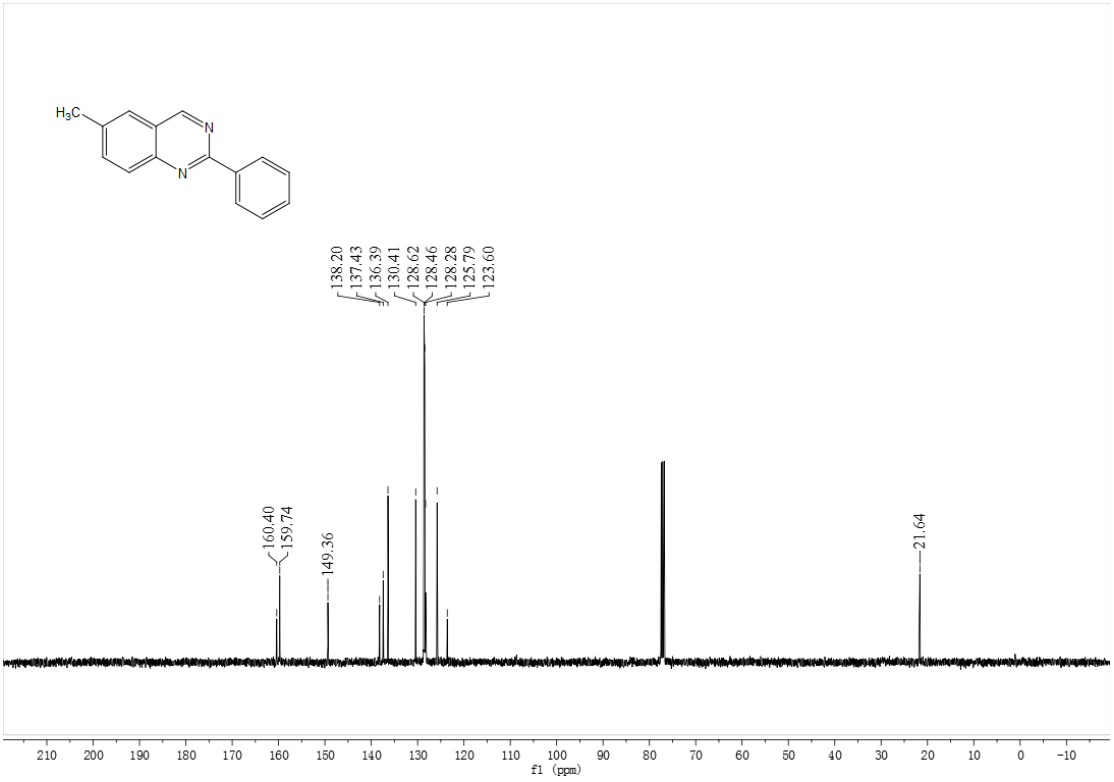


Figure S63. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3bd**, related to **Scheme 3**.

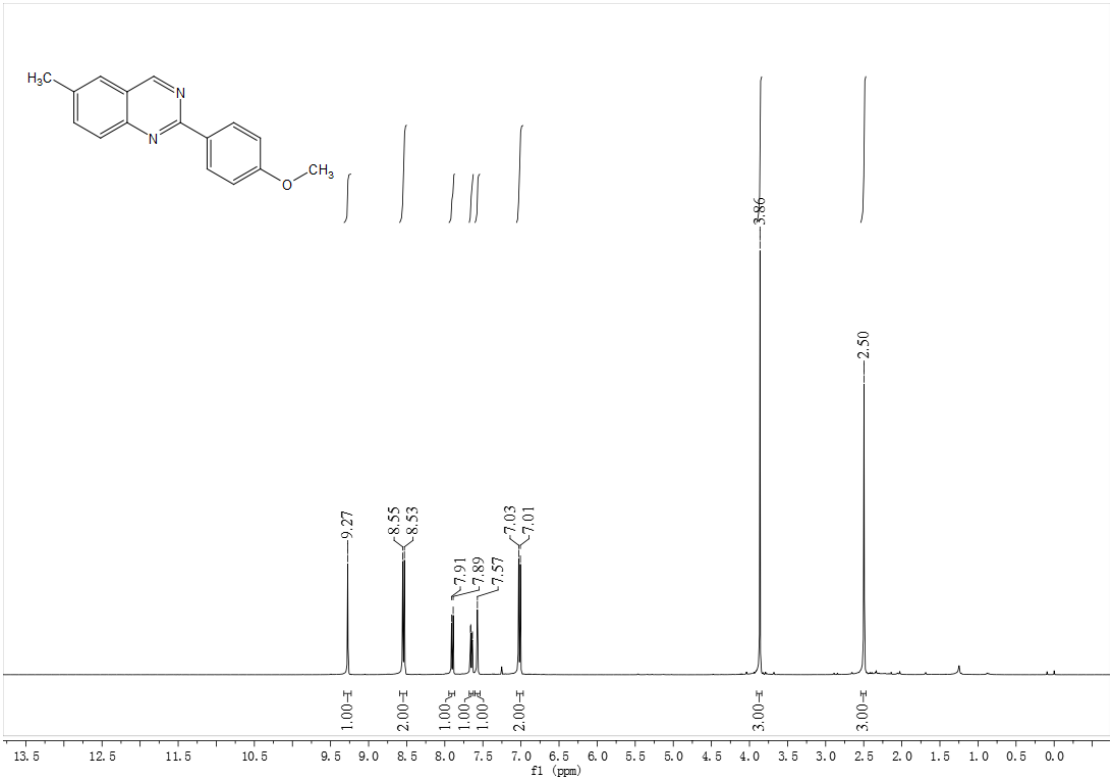


Figure S64. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3bd**, related to **Scheme 3**.

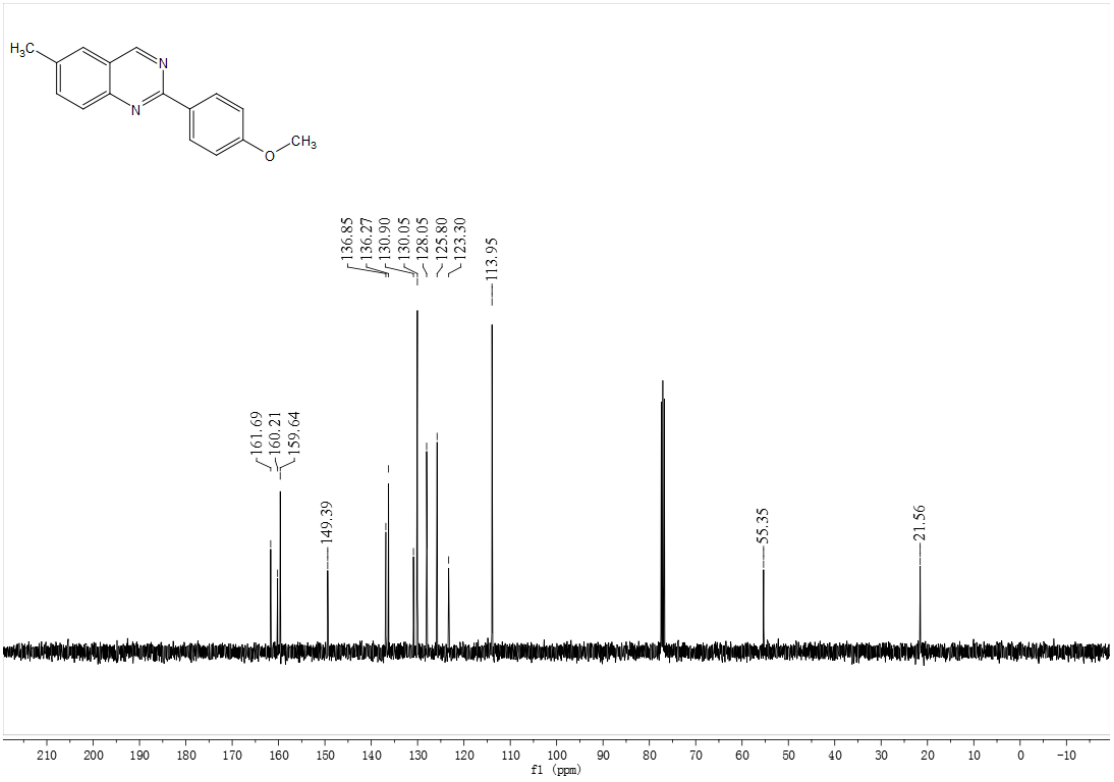


Figure S65. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ca**, related to **Scheme 3**.

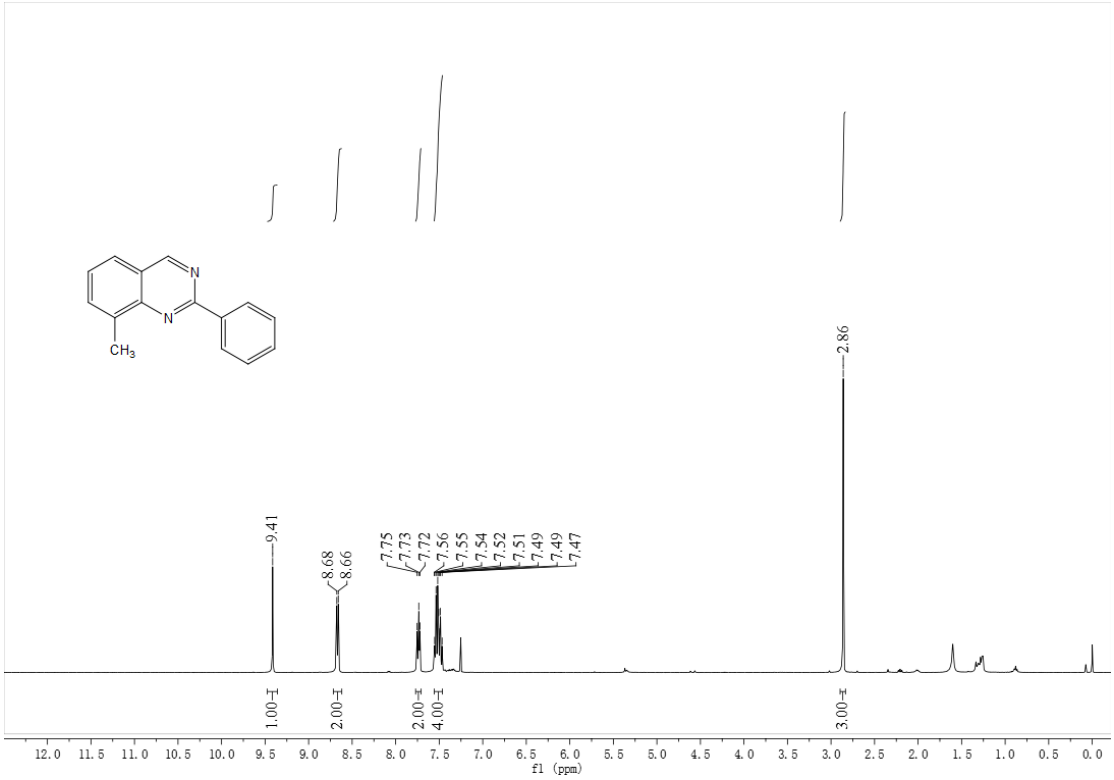


Figure S66. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ca**, related to **Scheme 3**.

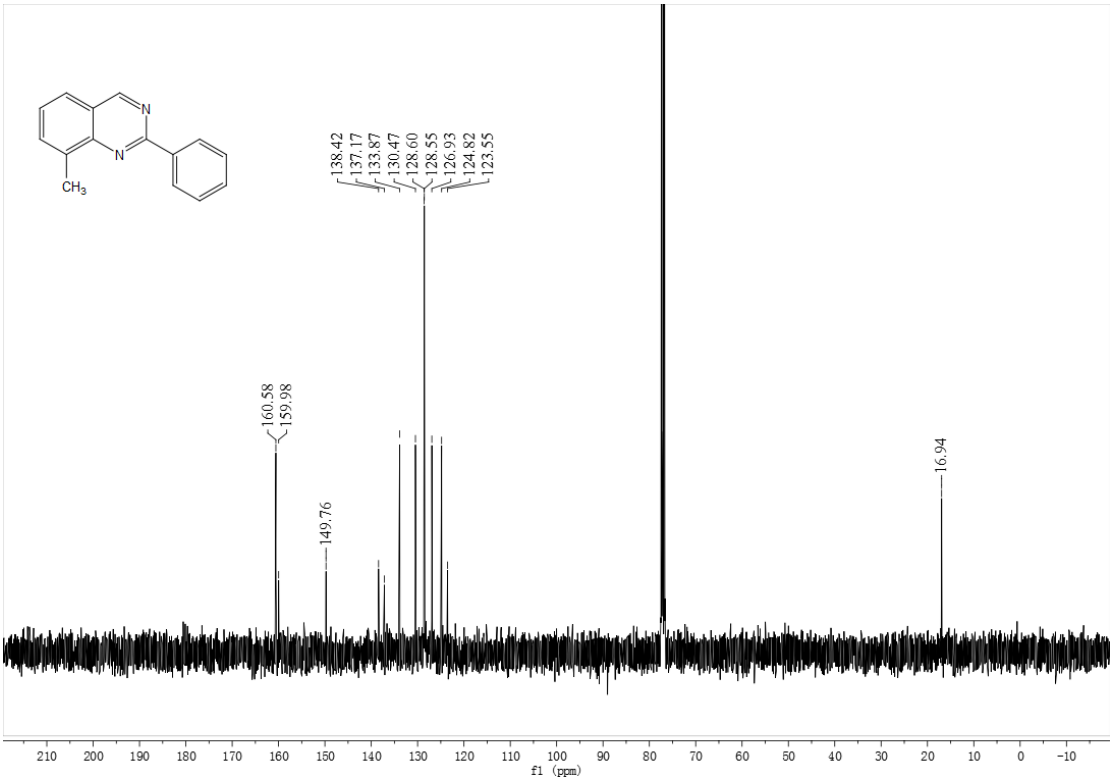


Figure S67. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3da**, related to **Scheme 3**.

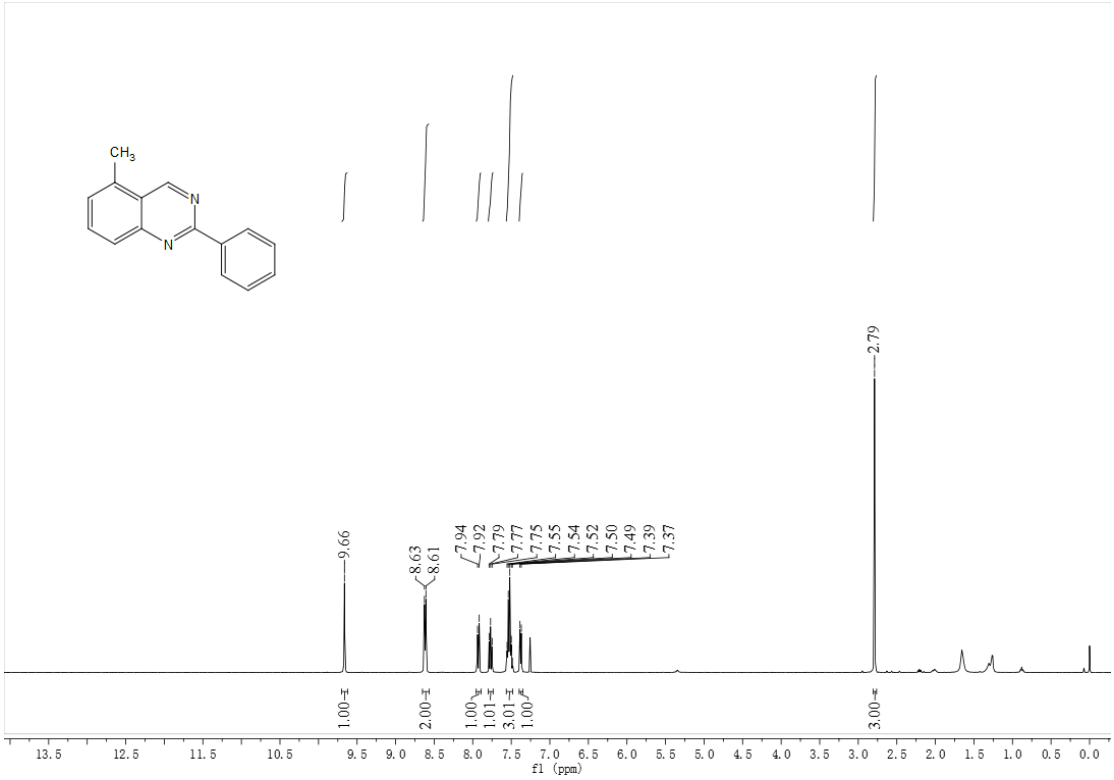


Figure S68. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3da**, related to **Scheme 3**.

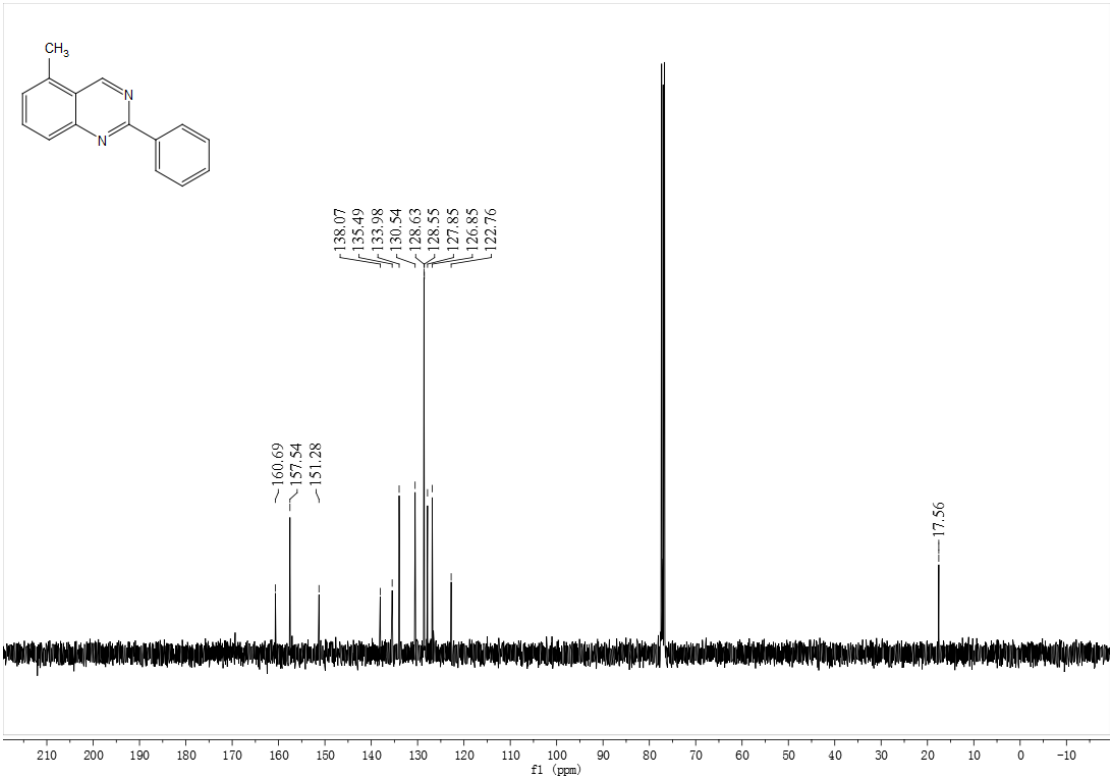


Figure S69. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ea**, related to **Scheme 3**.

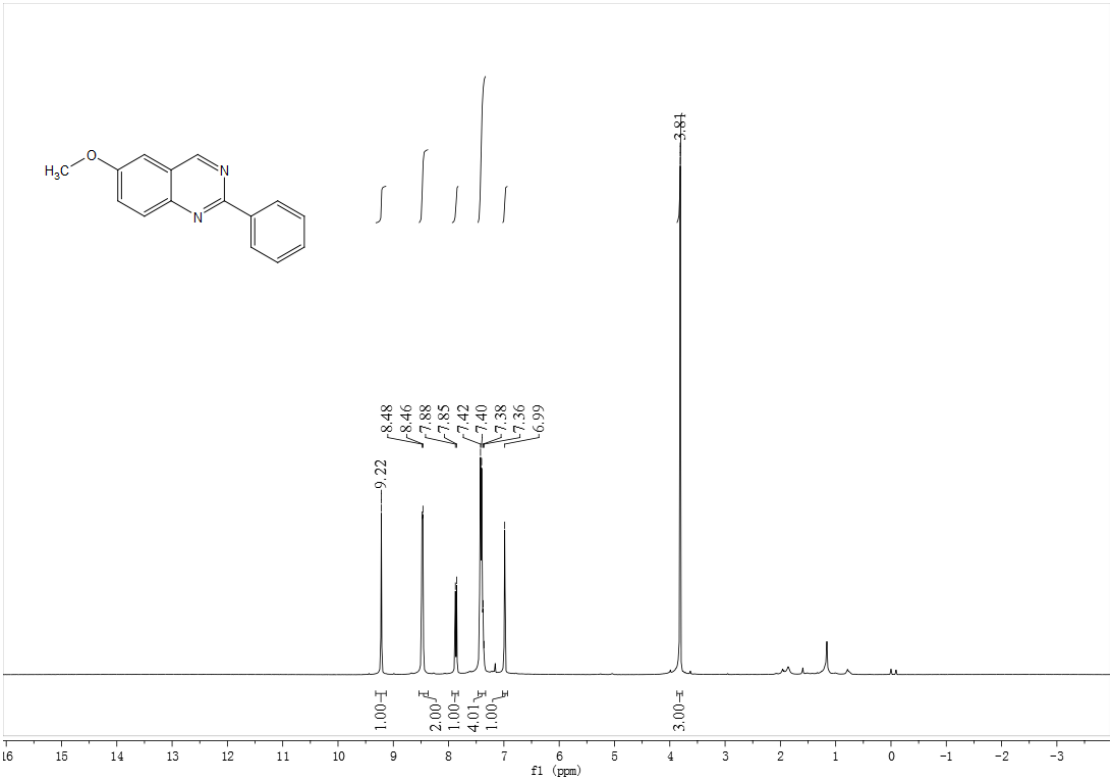


Figure S70. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ea**, related to **Scheme 3**.

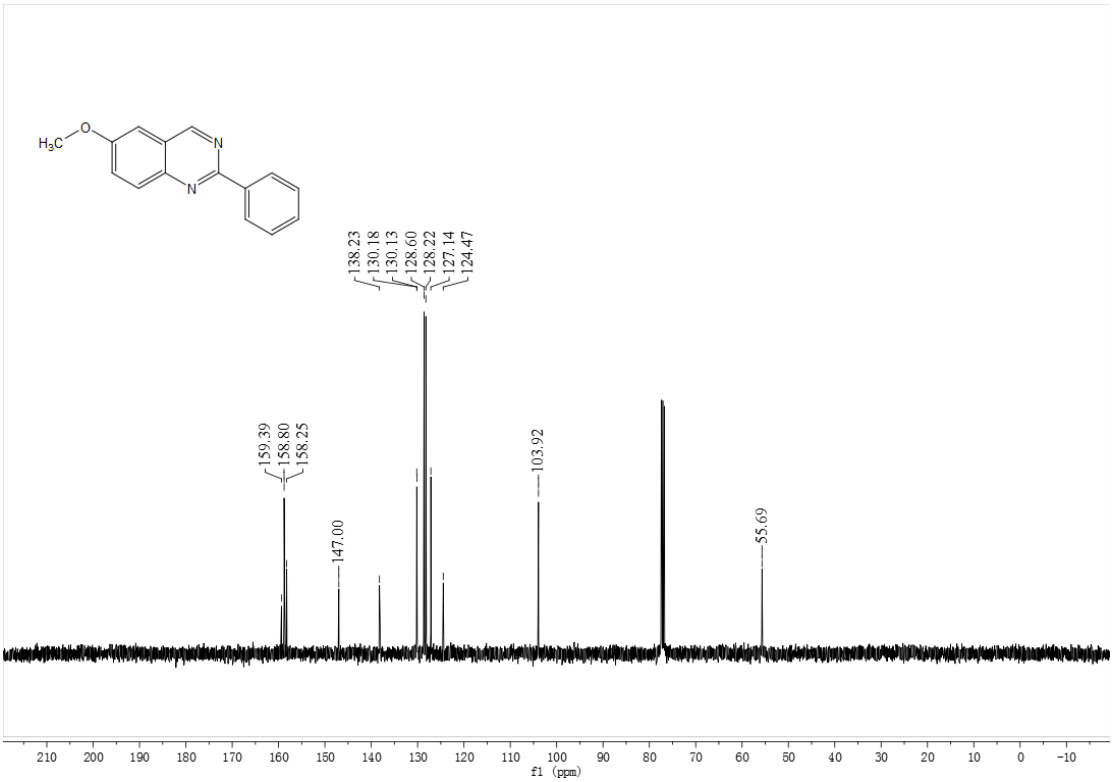


Figure S71. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3eg**, related to **Scheme 3**.

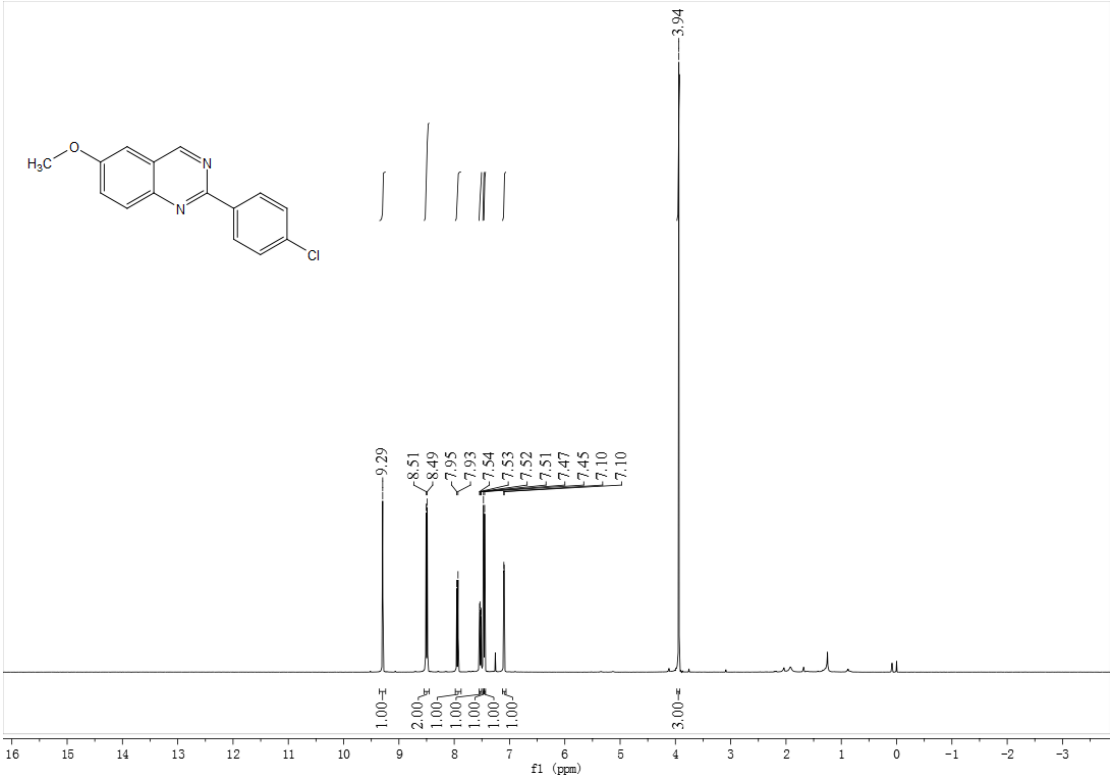


Figure S72. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3eg**, related to **Scheme 3**.

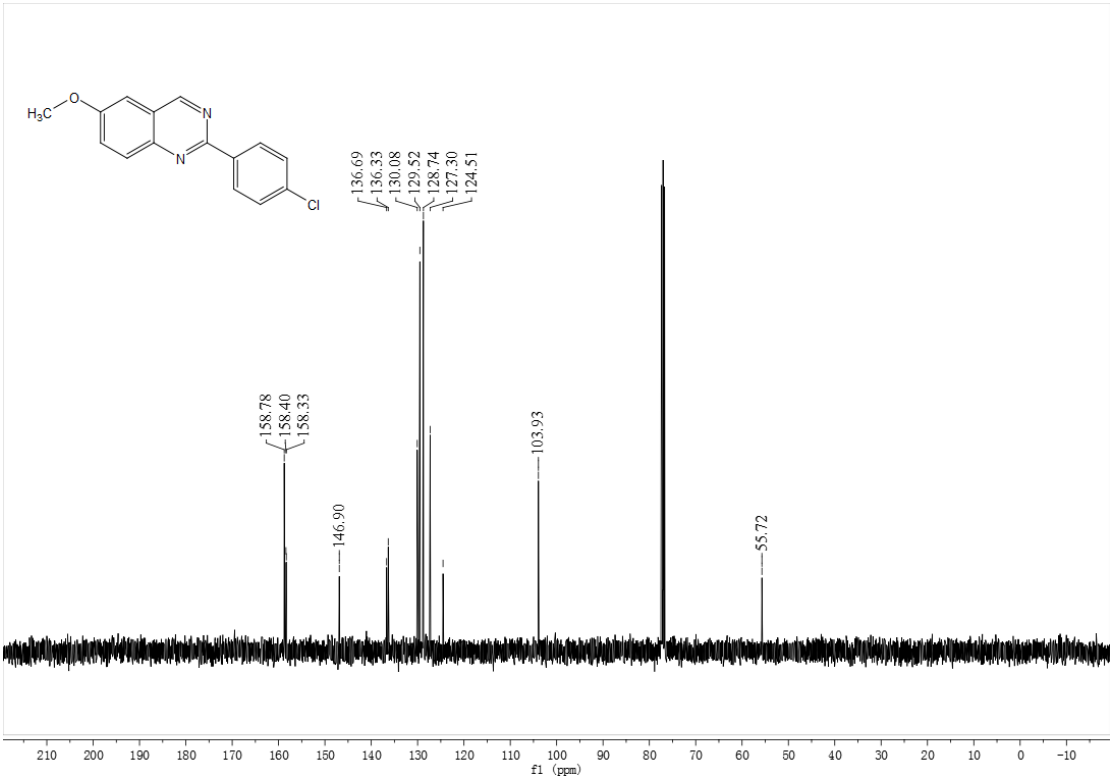


Figure S73. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3fa**, related to **Scheme 3**.

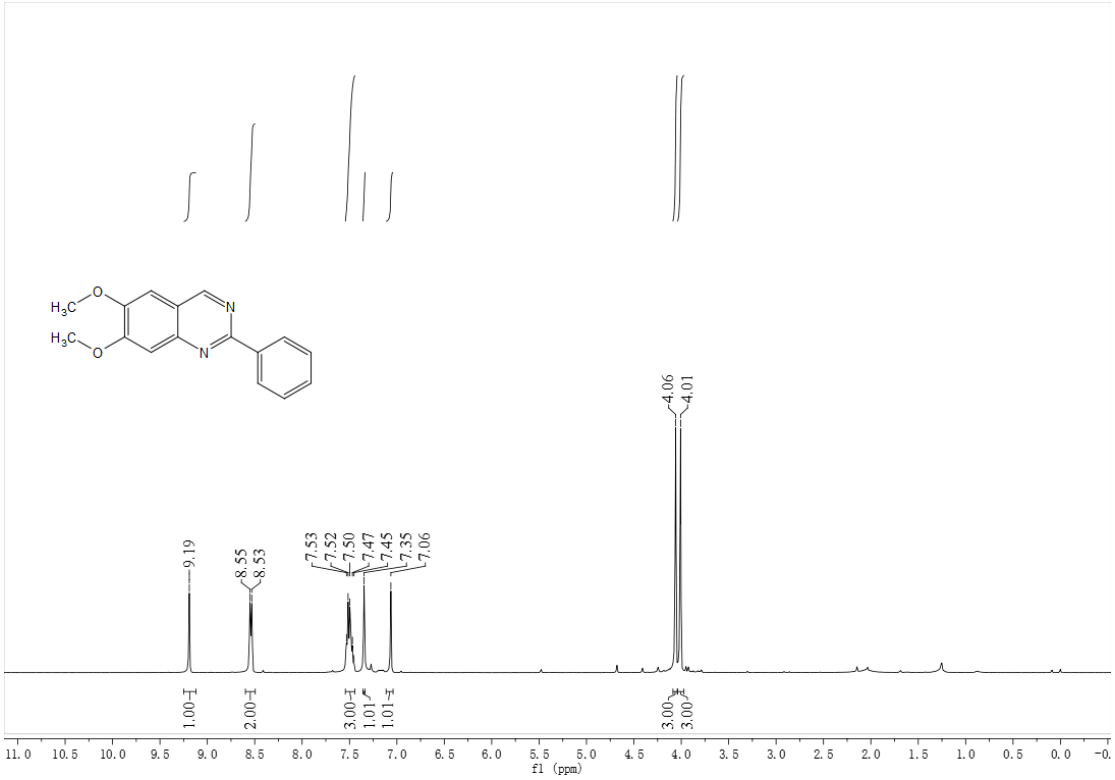


Figure S74. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3fa**, related to **Scheme 3**.

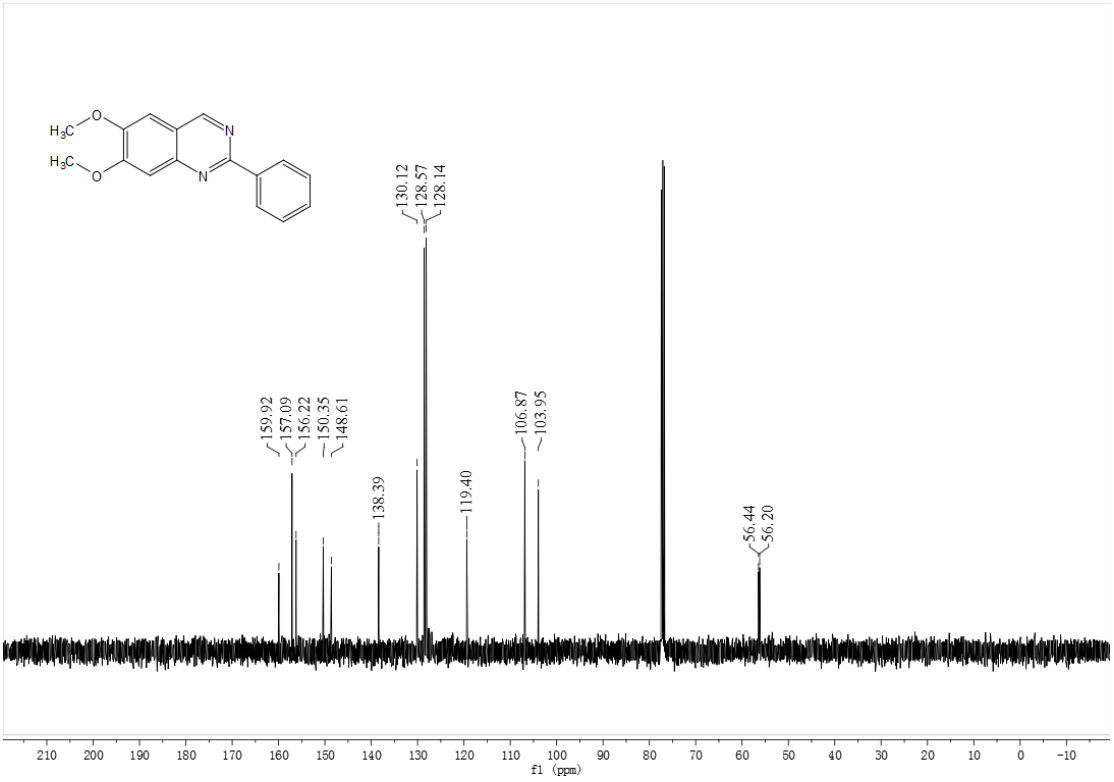


Figure S75. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3fi**, related to **Scheme 3**.

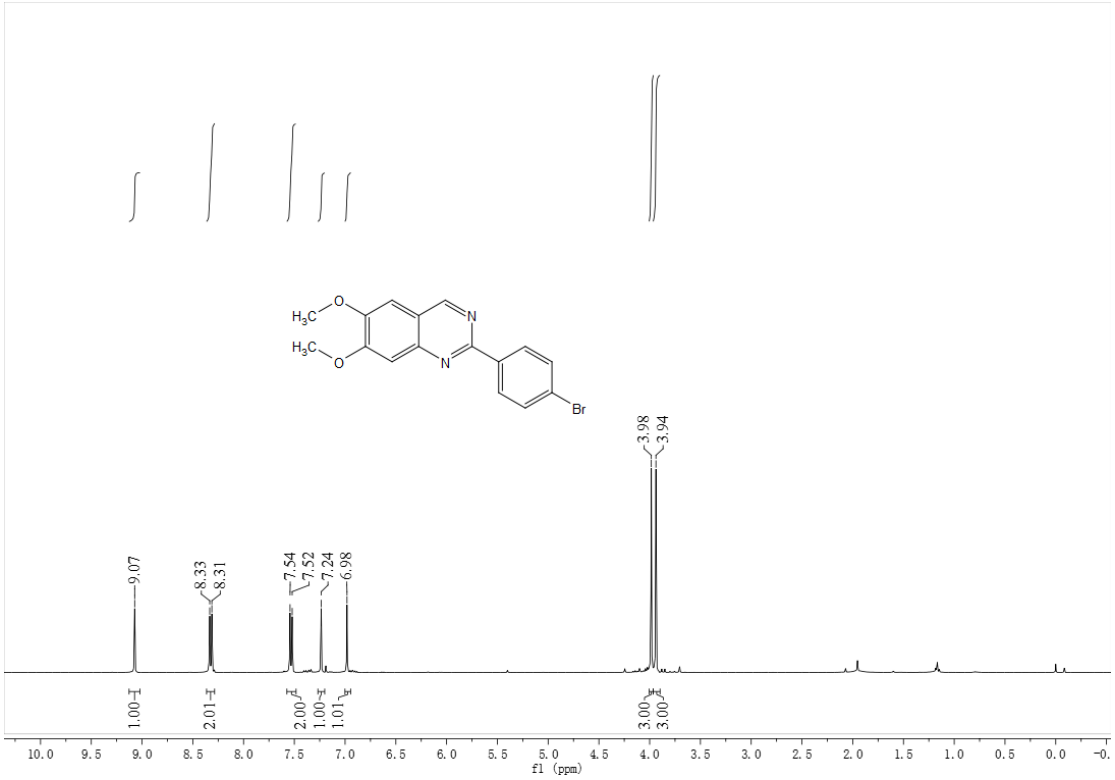


Figure S76. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3fi**, related to **Scheme 3**.

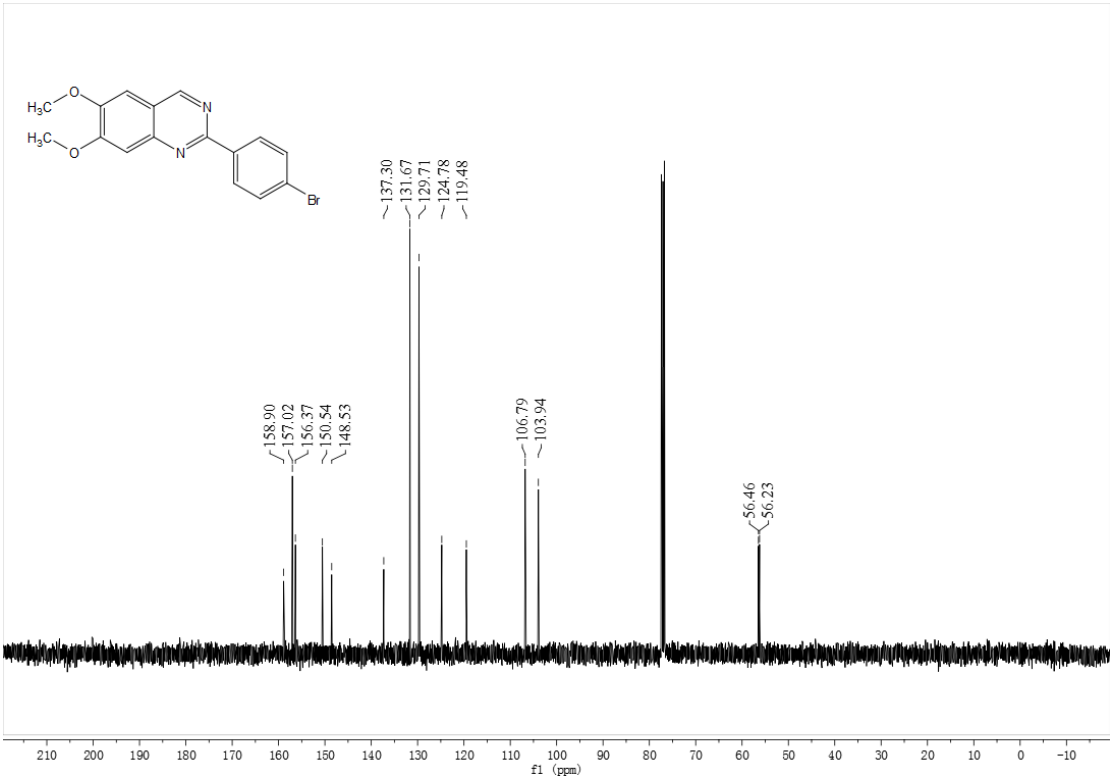


Figure S77. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ga**, related to **Scheme 3**.

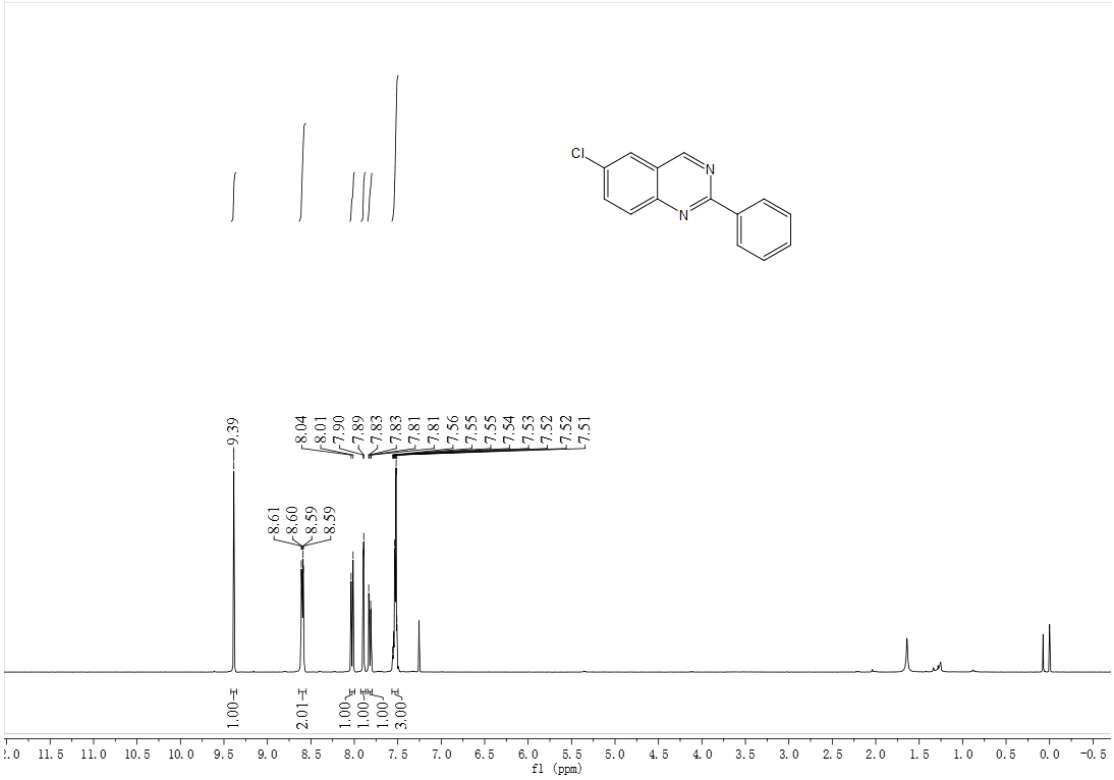


Figure S78. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ga**, related to **Scheme 3**.

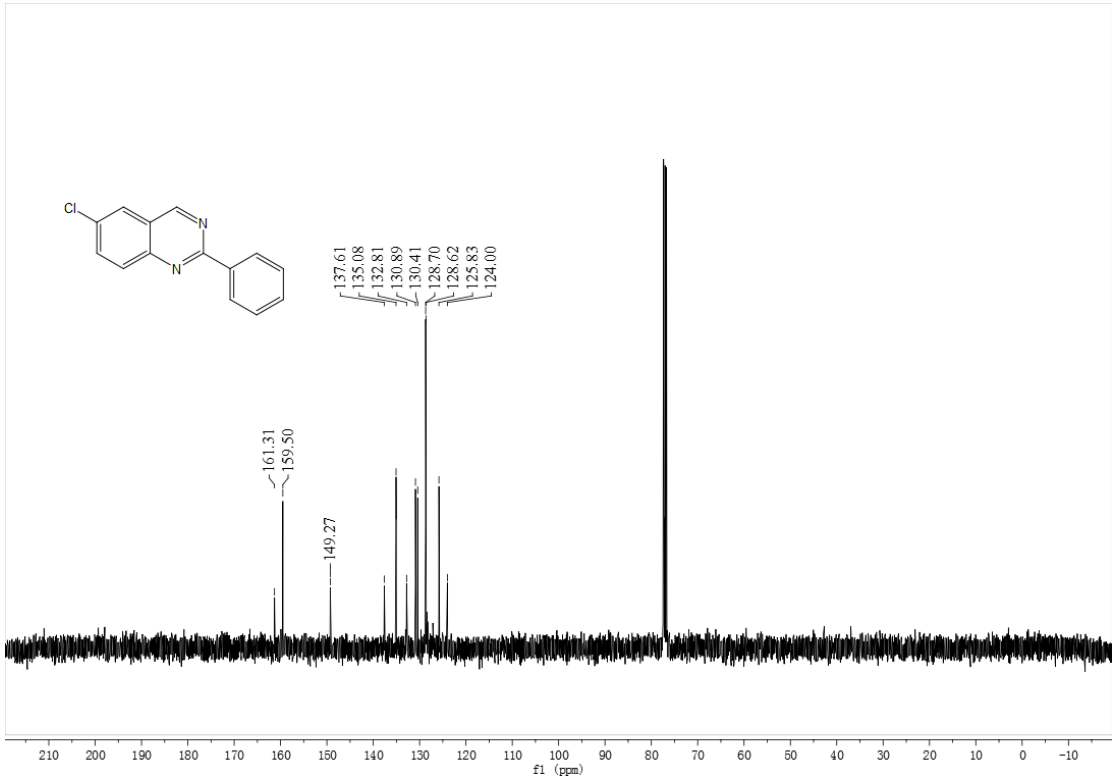


Figure S79. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3gk**, related to **Scheme 3**.

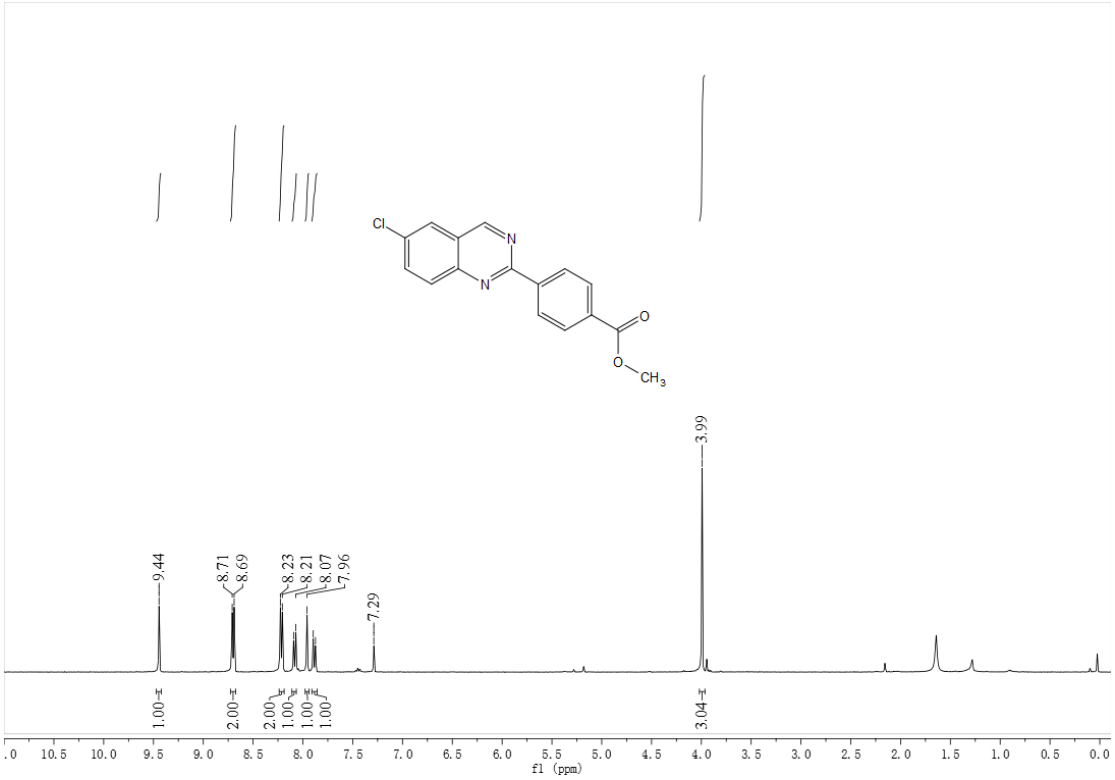


Figure S80. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3gk**, related to **Scheme 3**.

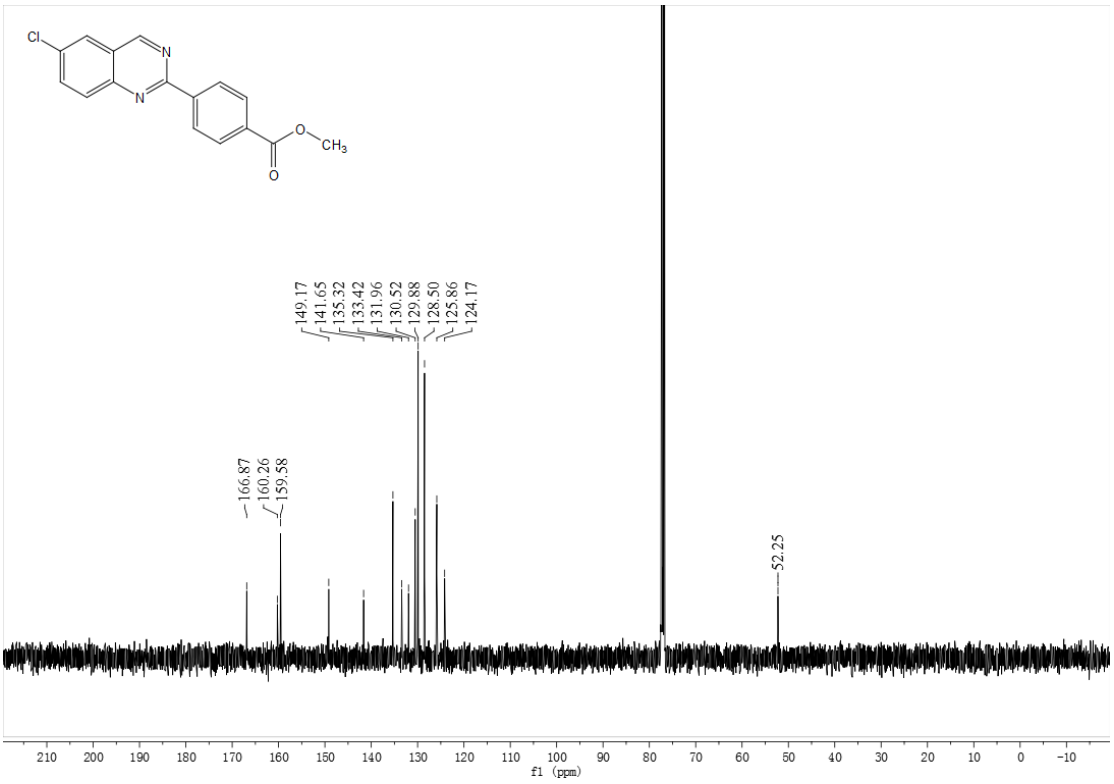


Figure S81. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ha**, related to **Scheme 3**.

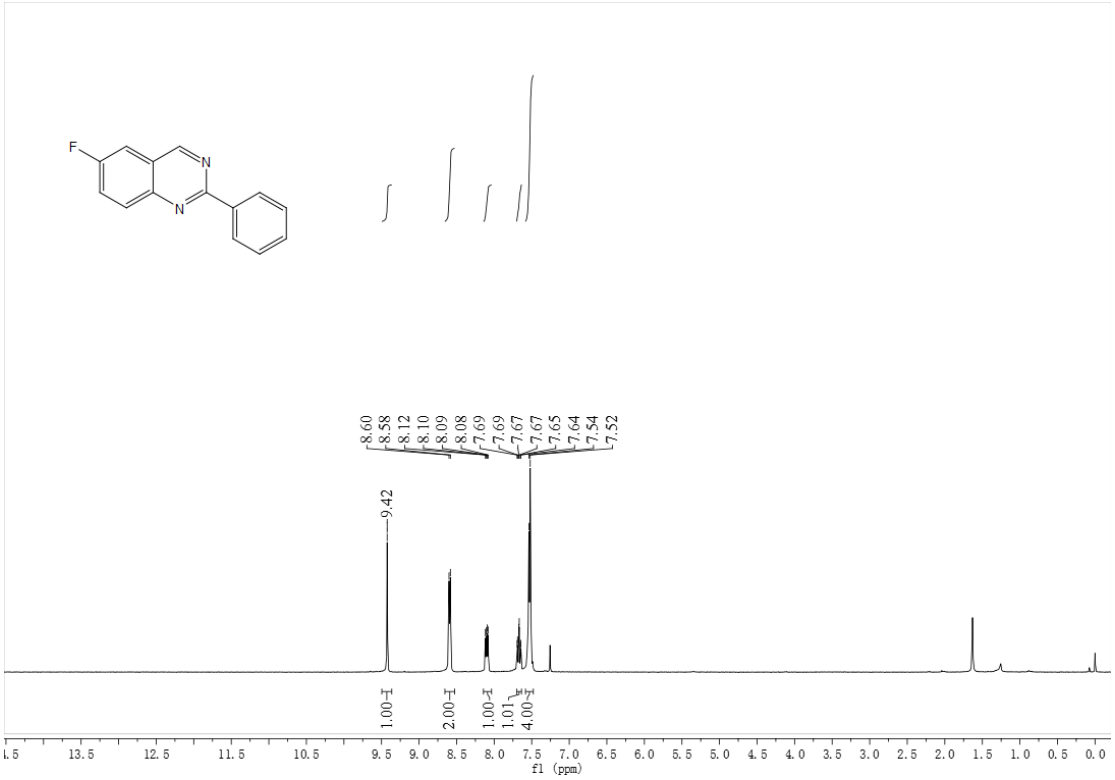


Figure S82. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ha**, related to **Scheme 3**.

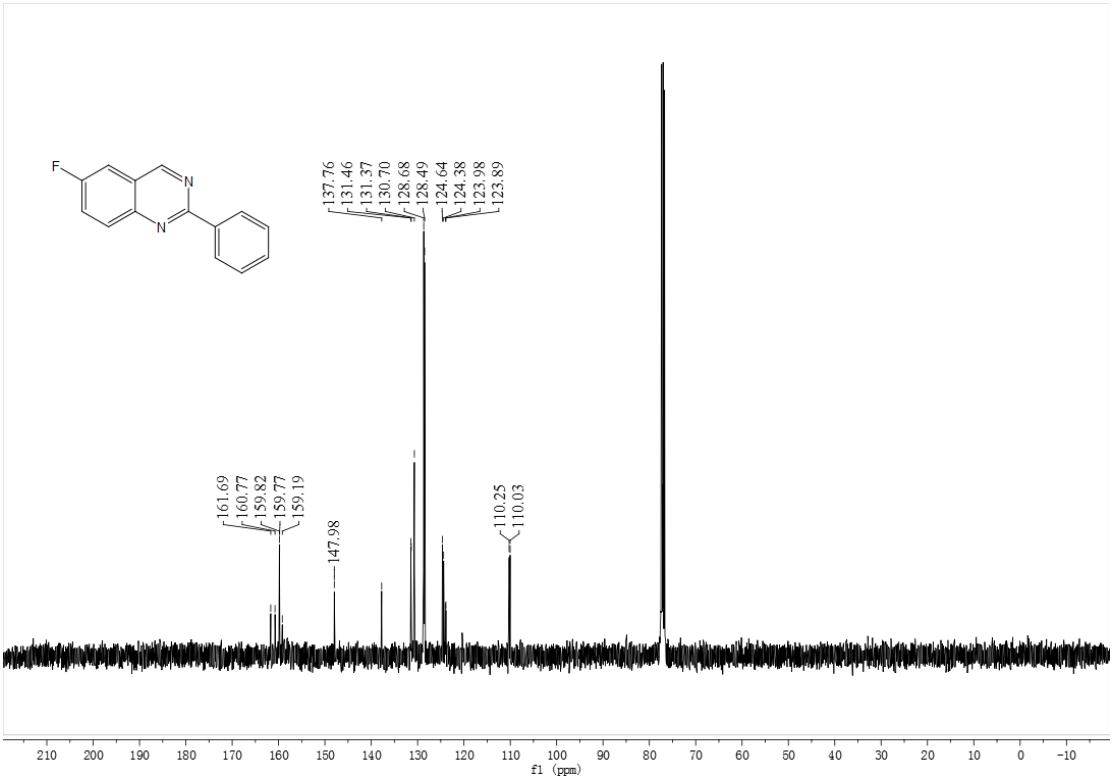


Figure S83. ^{19}F-NMR (400 MHz, $CDCl_3$) spectrum of **3ha**, related to **Scheme 3**.

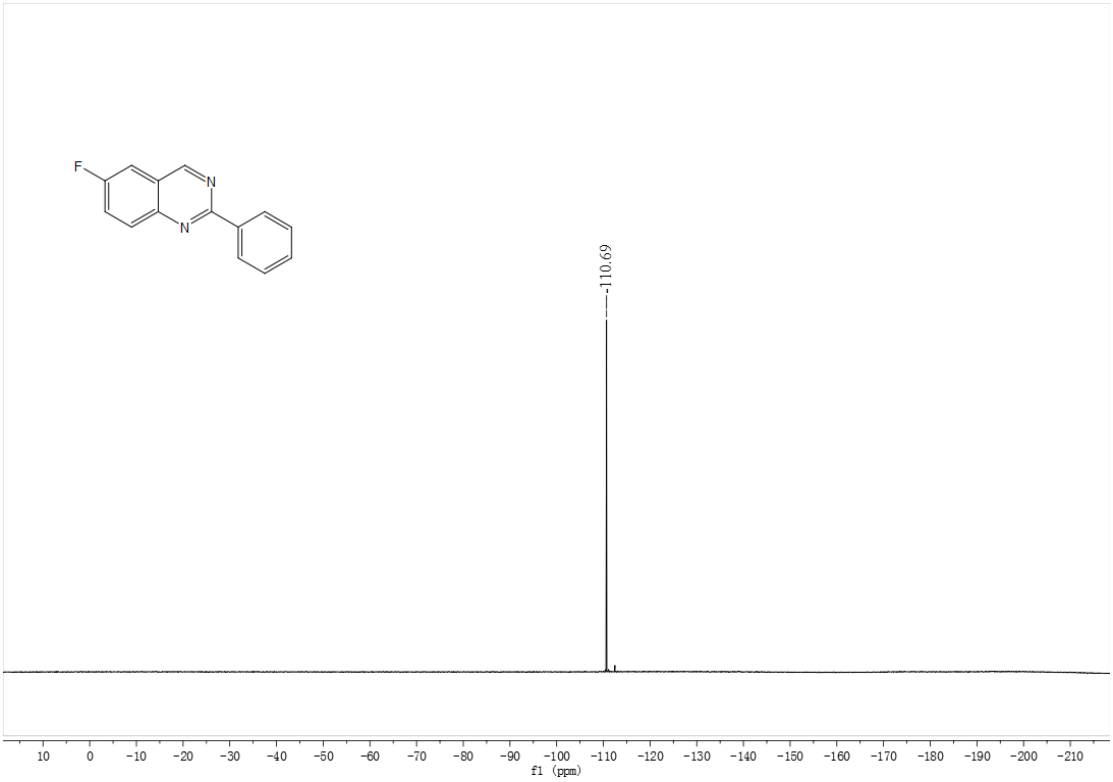


Figure S84. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ia**, related to **Scheme 3**.

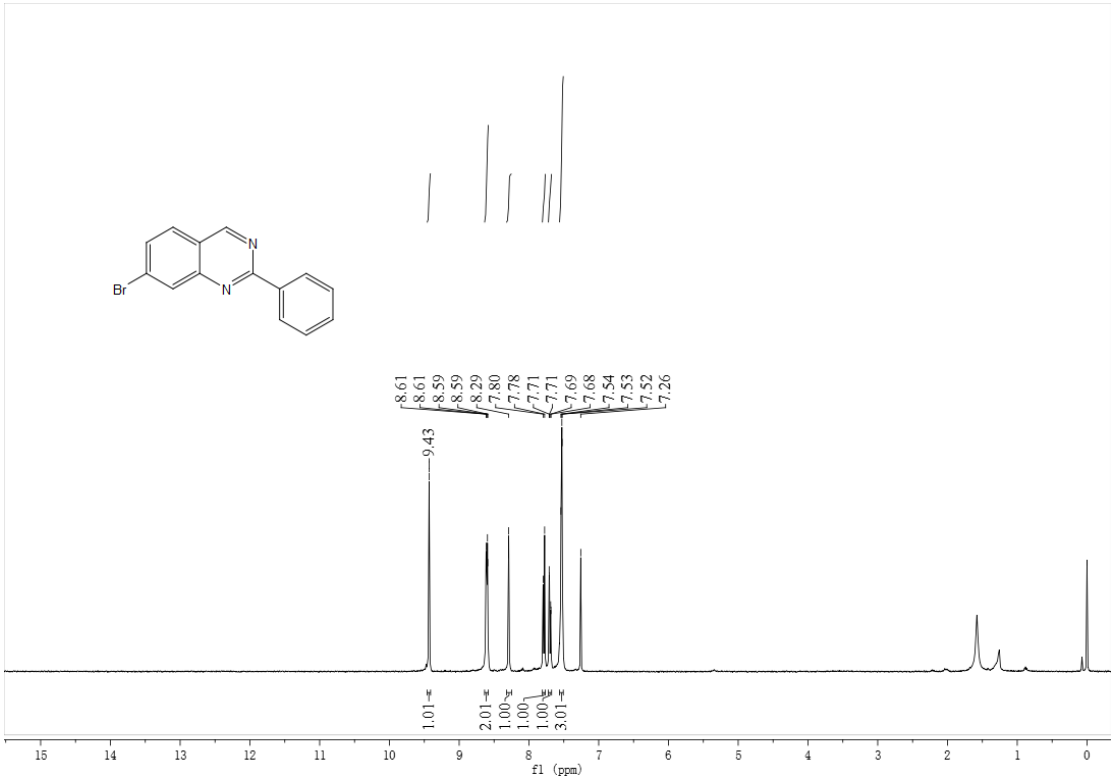


Figure S85. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ia**, related to **Scheme 3**.

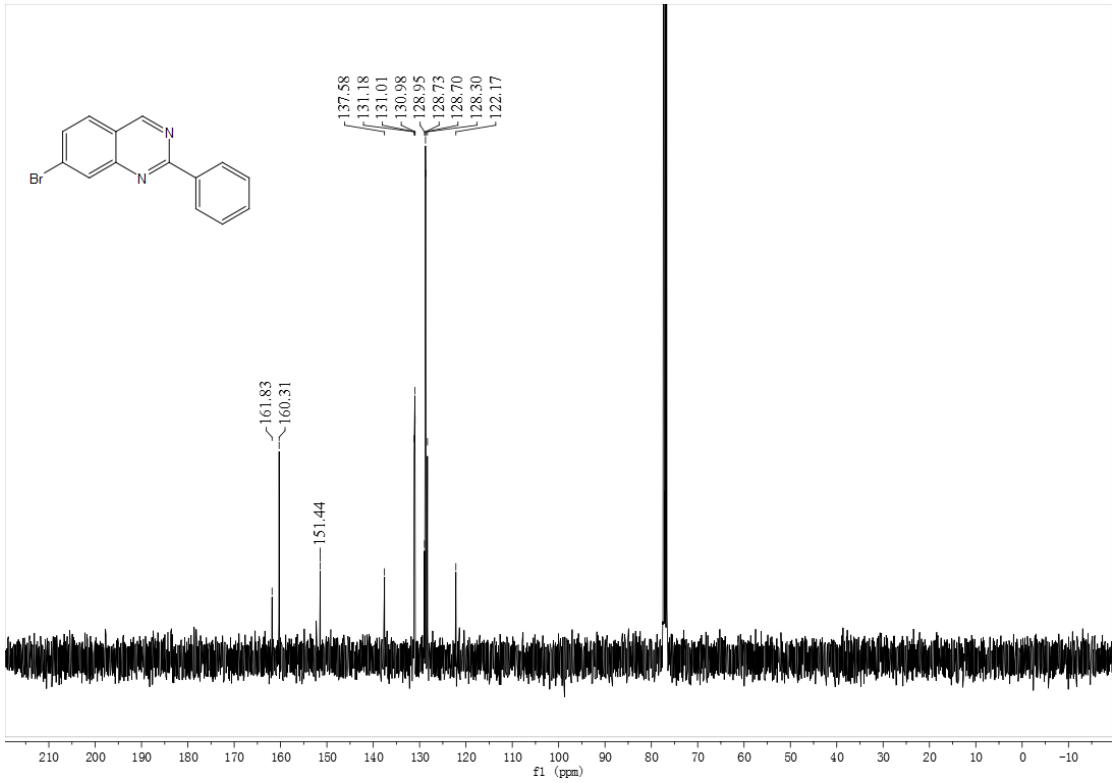


Figure S86. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ja**, related to **Scheme 3**.

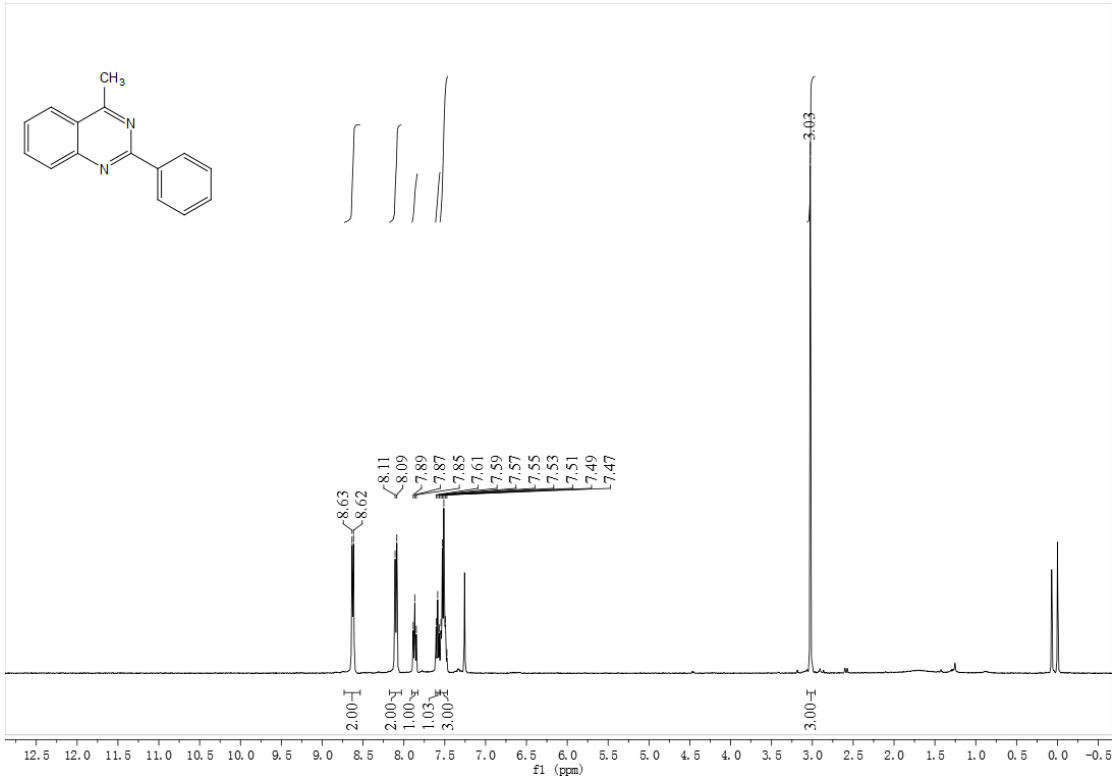


Figure S87. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ja**, related to **Scheme 3**.

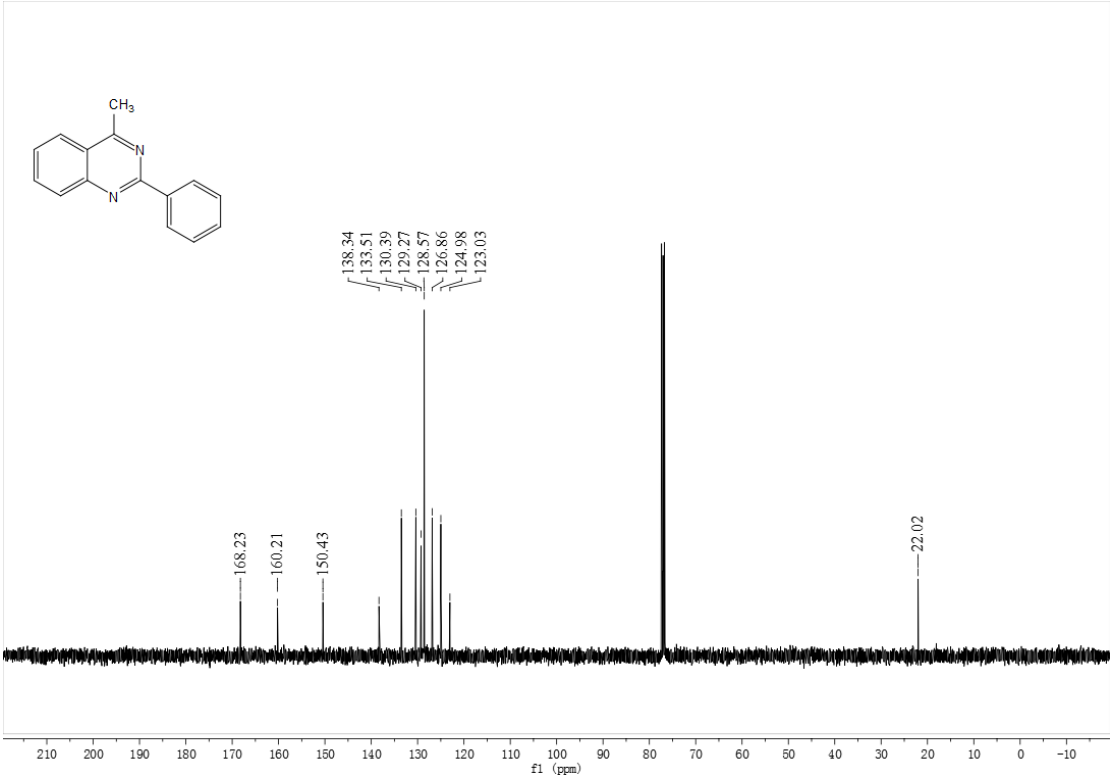


Figure S88. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3jl**, related to **Scheme 2**.

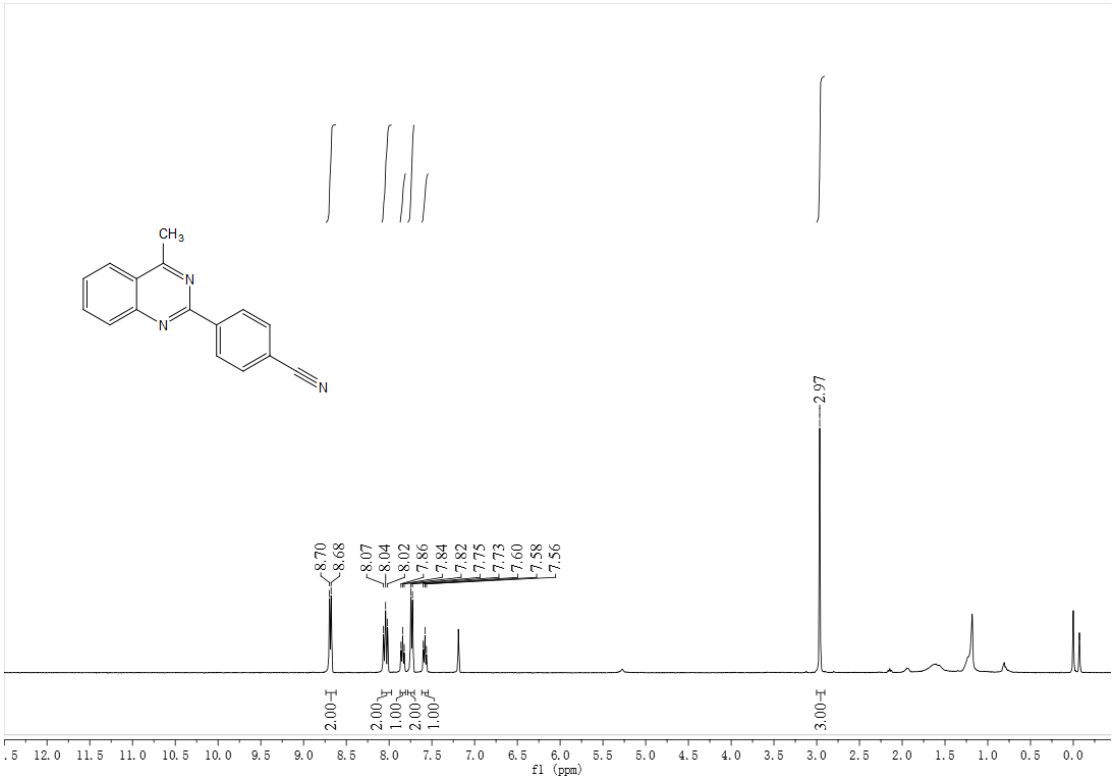


Figure S89. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3jl**, related to **Scheme 3**.

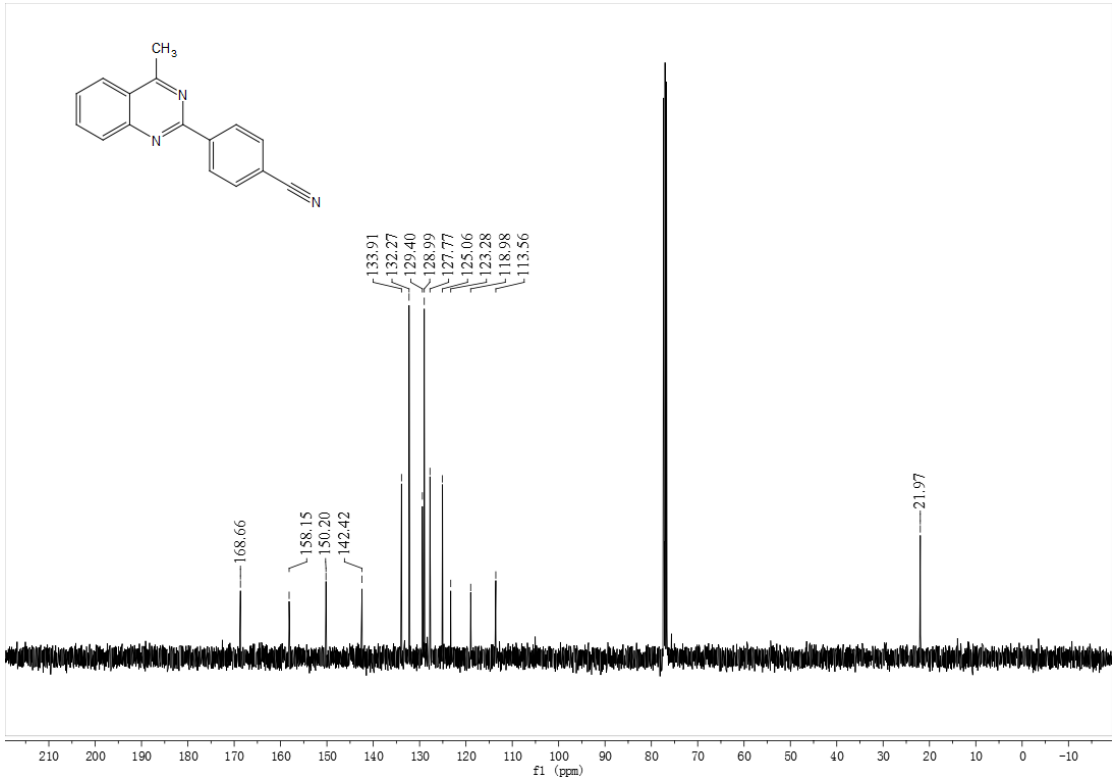


Figure S90. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3ka**, related to **Scheme 2**.

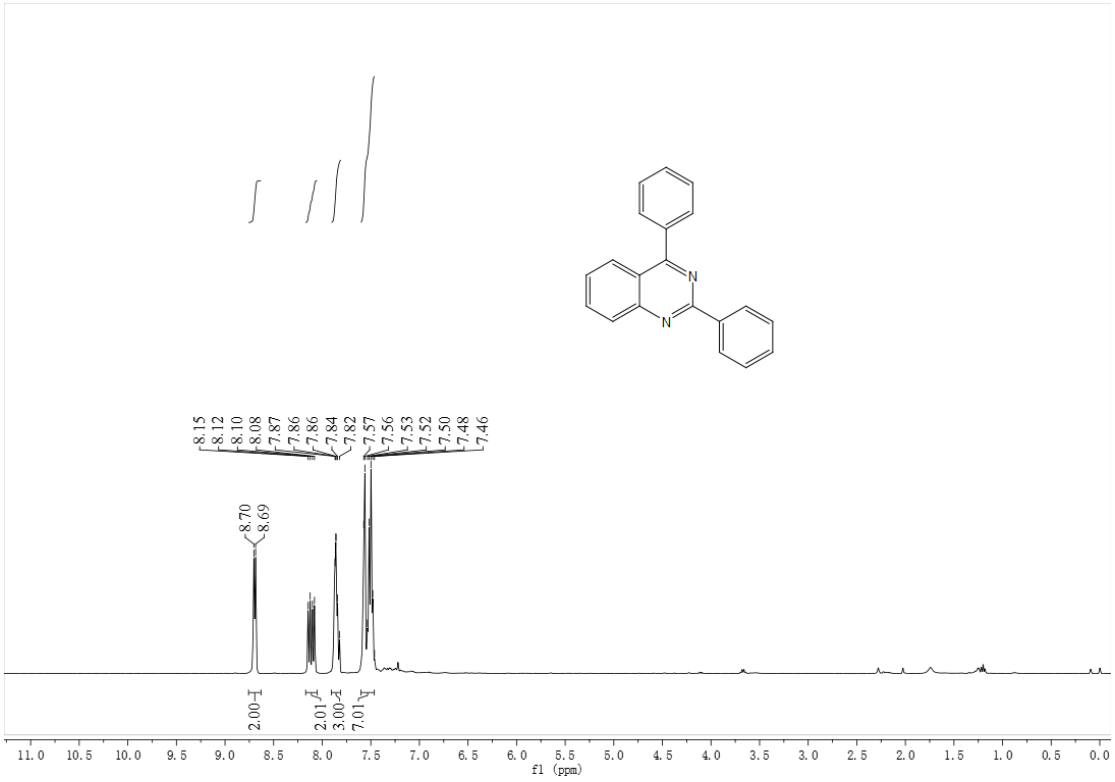


Figure S91. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3ka**, related to **Scheme 3**.

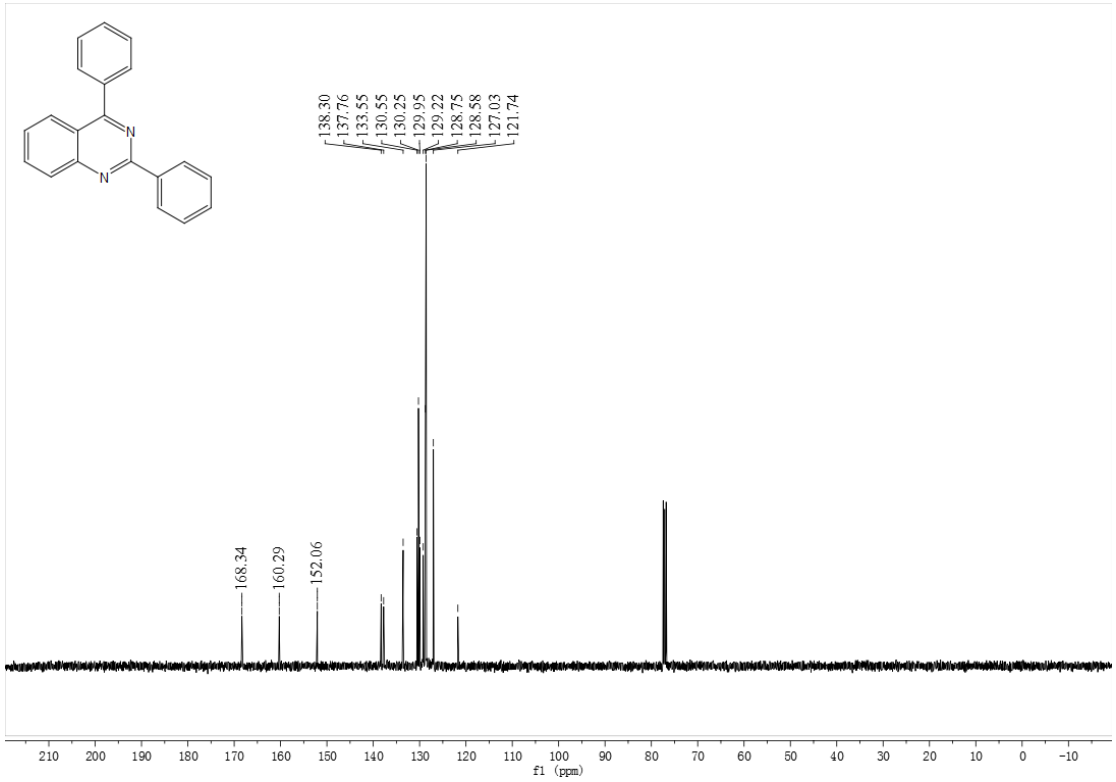


Figure S92. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **3la**, related to **Scheme 2**.

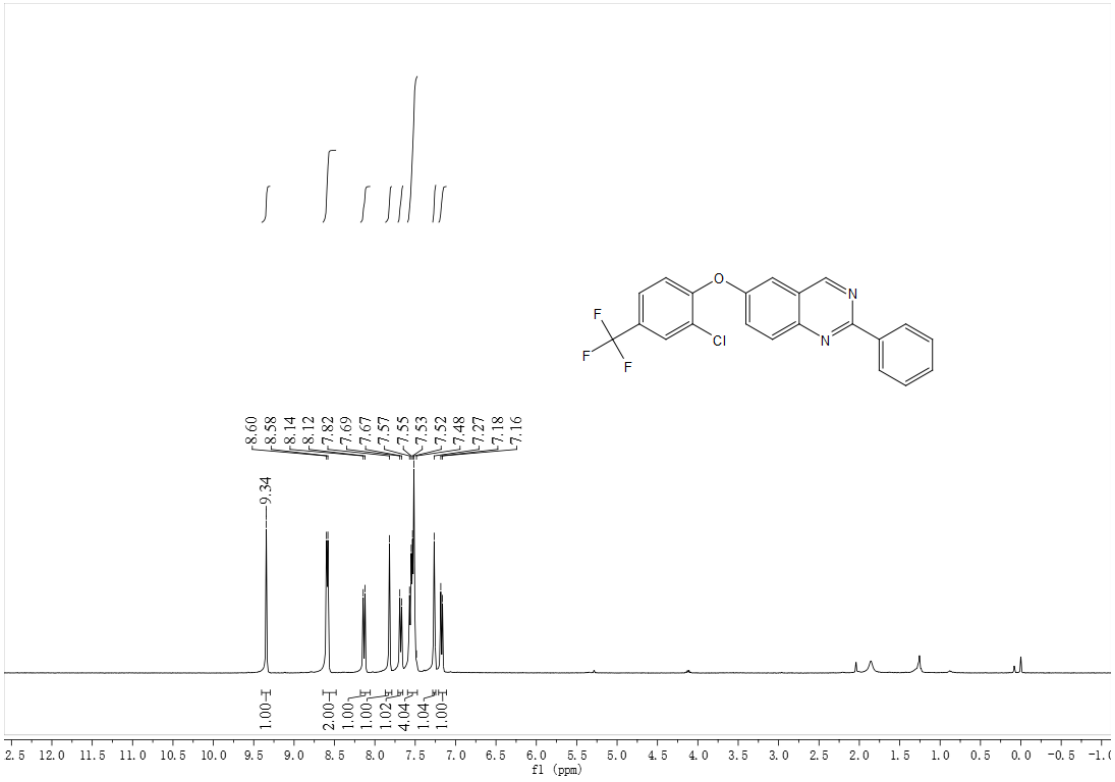


Figure S93. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **3la**, related to **Scheme 3**.

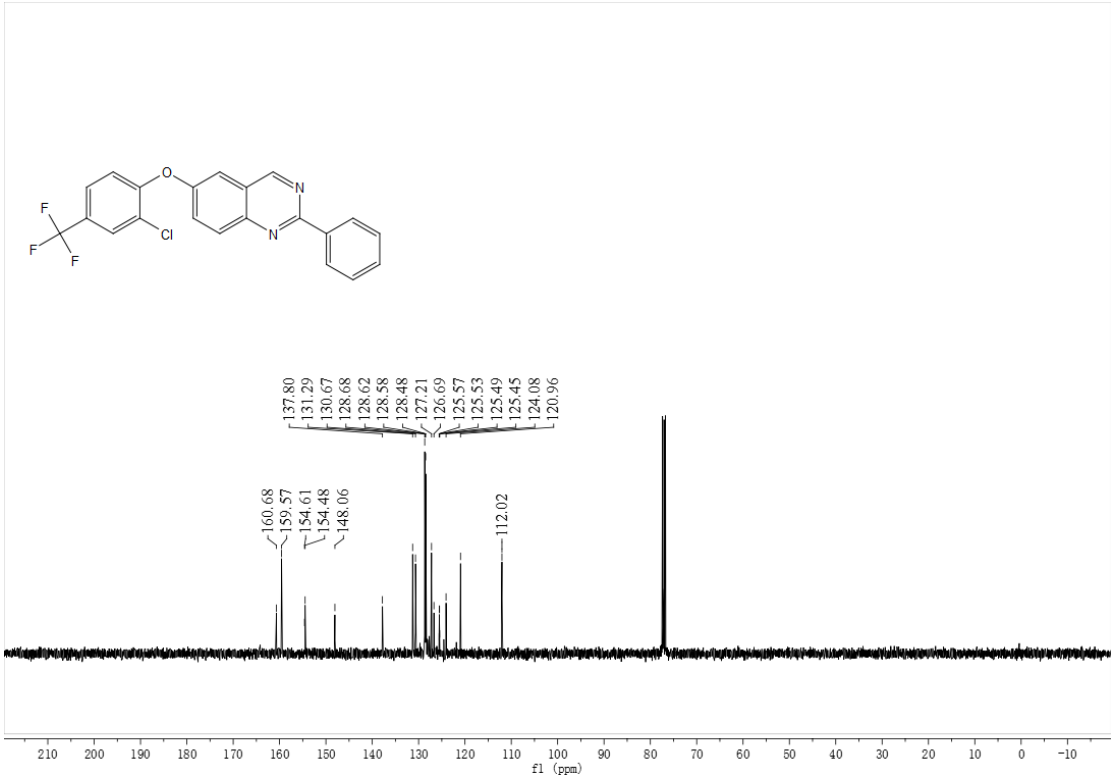


Figure S94. ^{19}F-NMR (100 MHz, $CDCl_3$) spectrum of **3la**, related to **Scheme 3**.

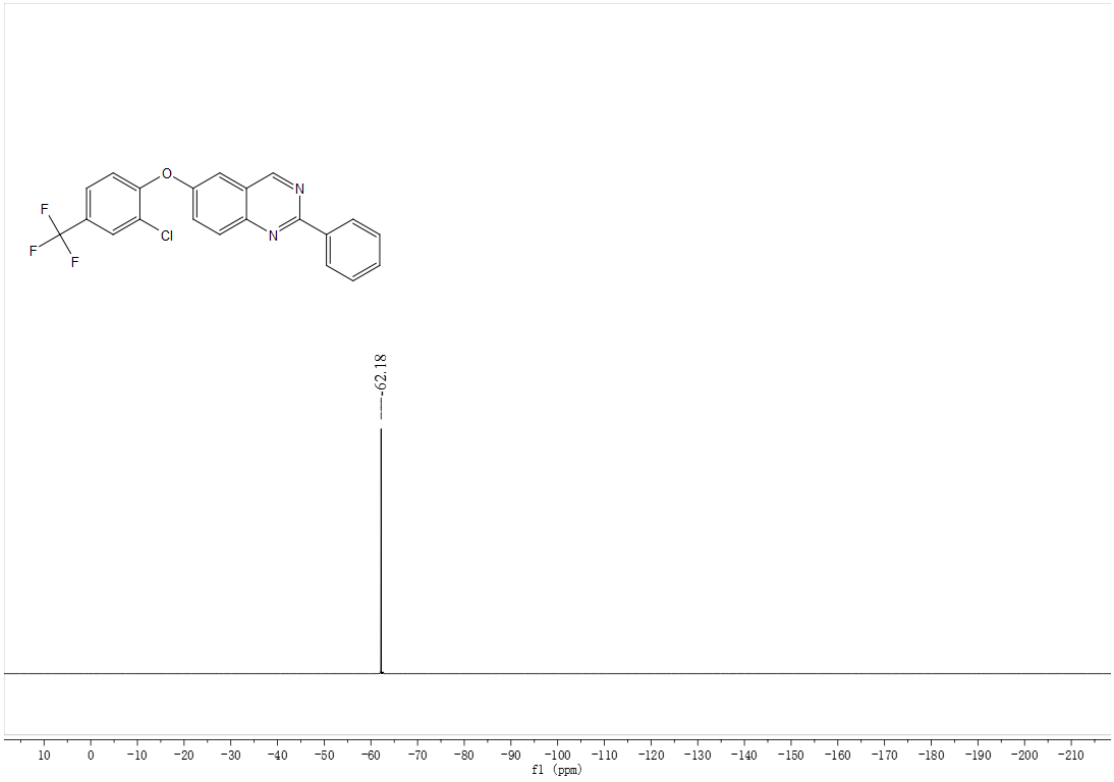


Figure S94. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **4ja**, related to **Scheme 4**.

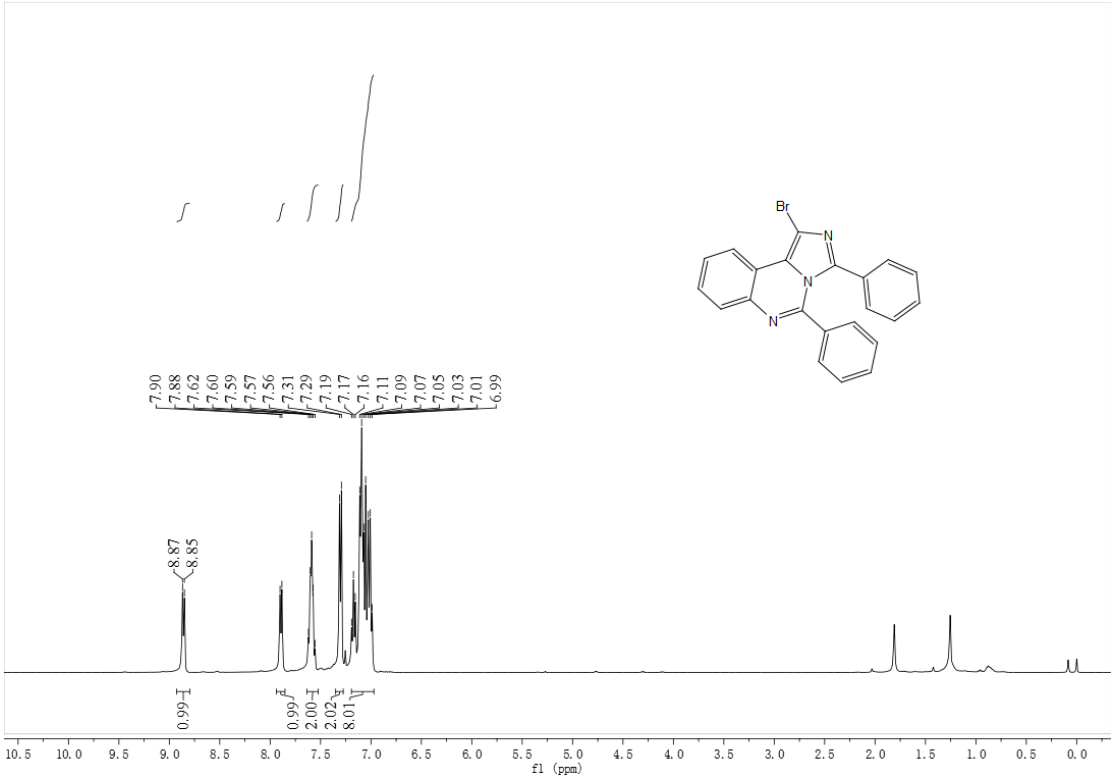


Figure S95. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **4ja**, related to **Scheme 4**.

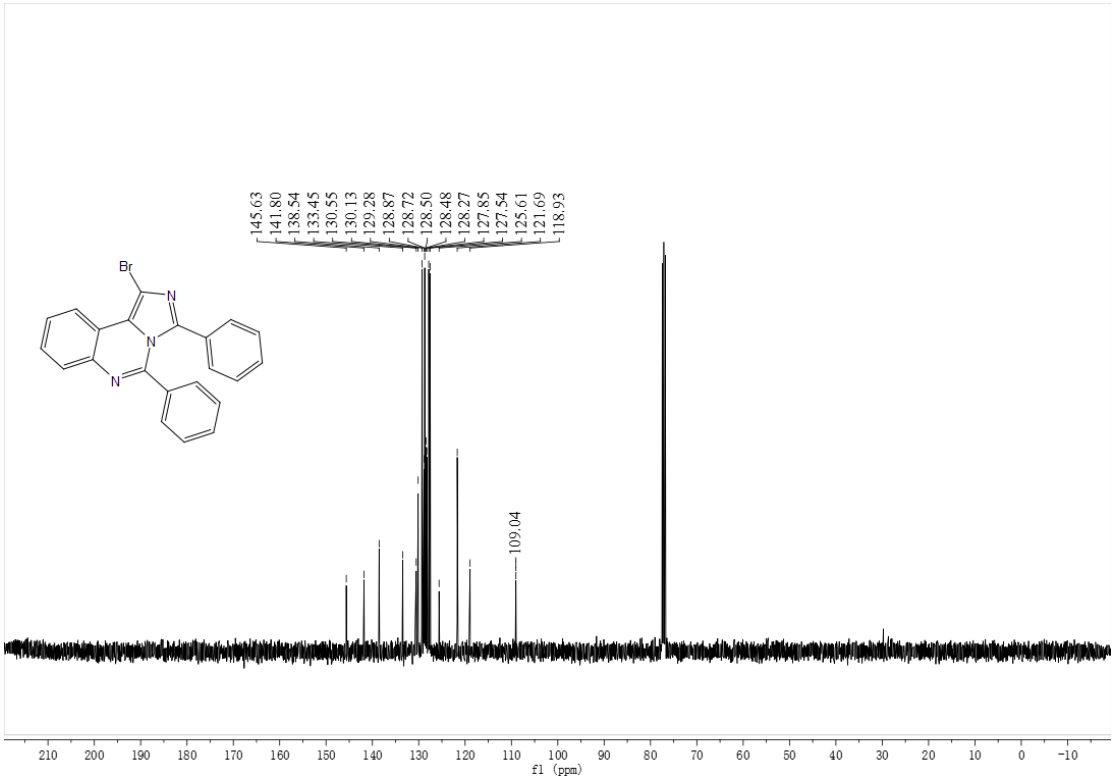


Figure S96. ^{1}H-NMR (400 MHz, $CDCl_3$) spectrum of **5ja**, related to **Scheme 4**.

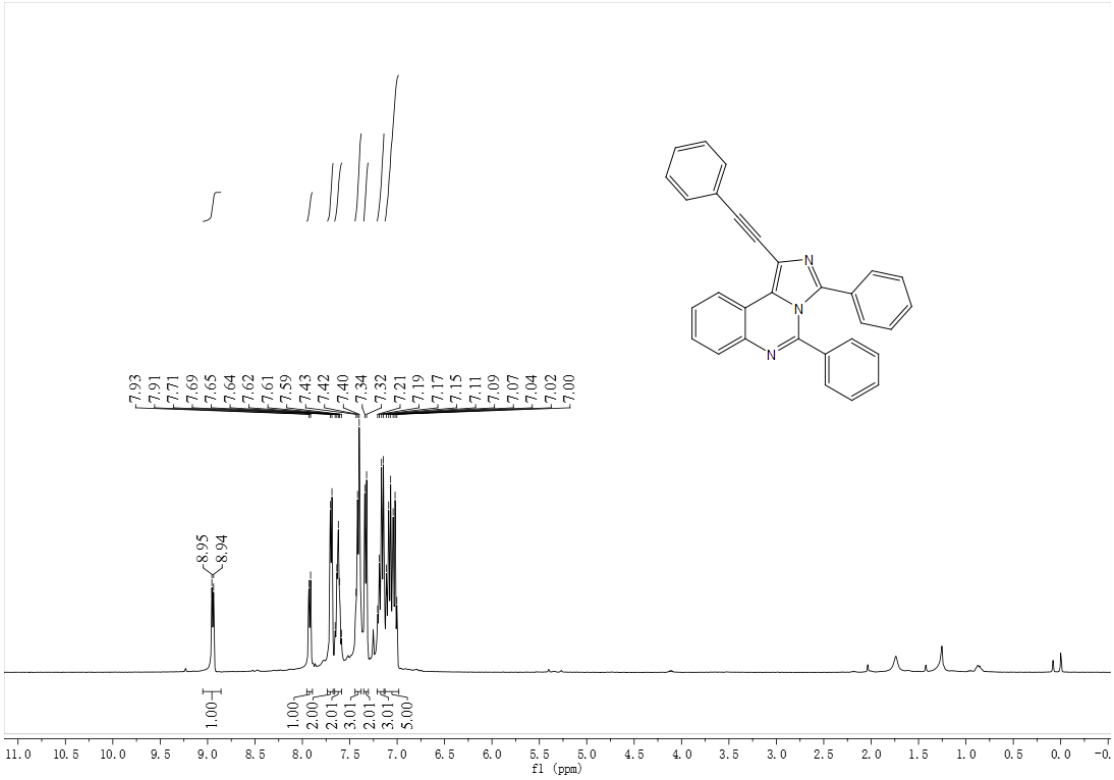
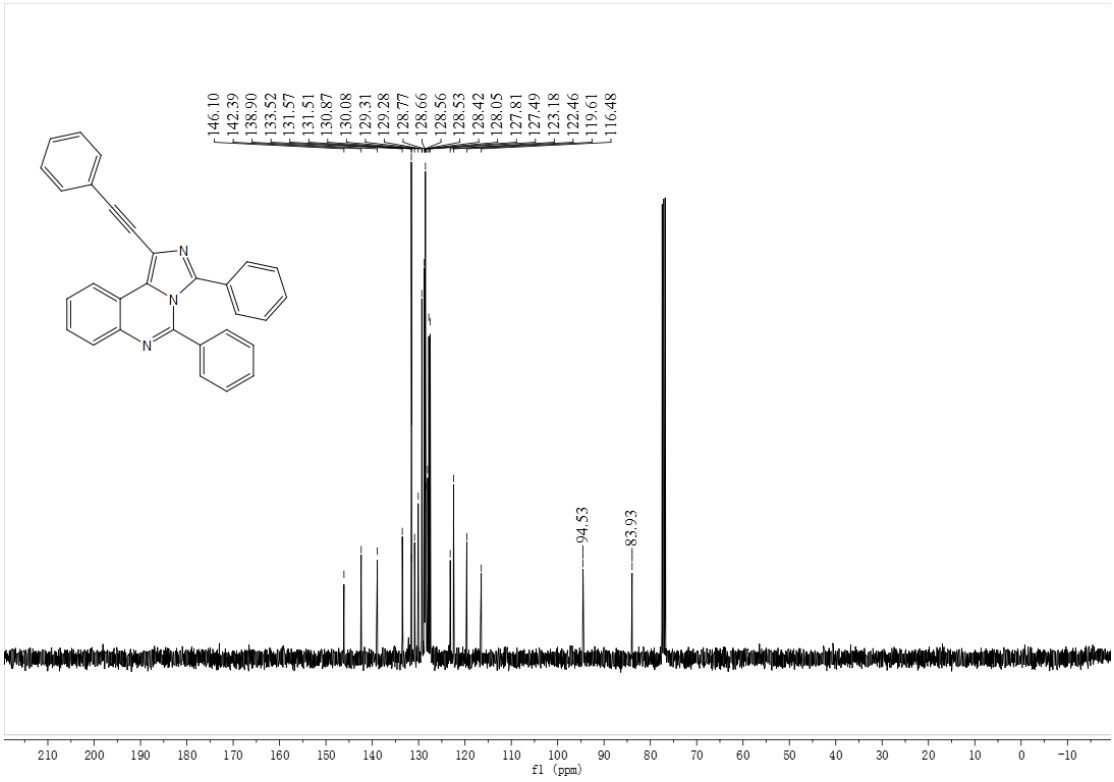


Figure S97. ^{13}C-NMR (100 MHz, $CDCl_3$) spectrum of **5ja**, related to **Scheme 4**.

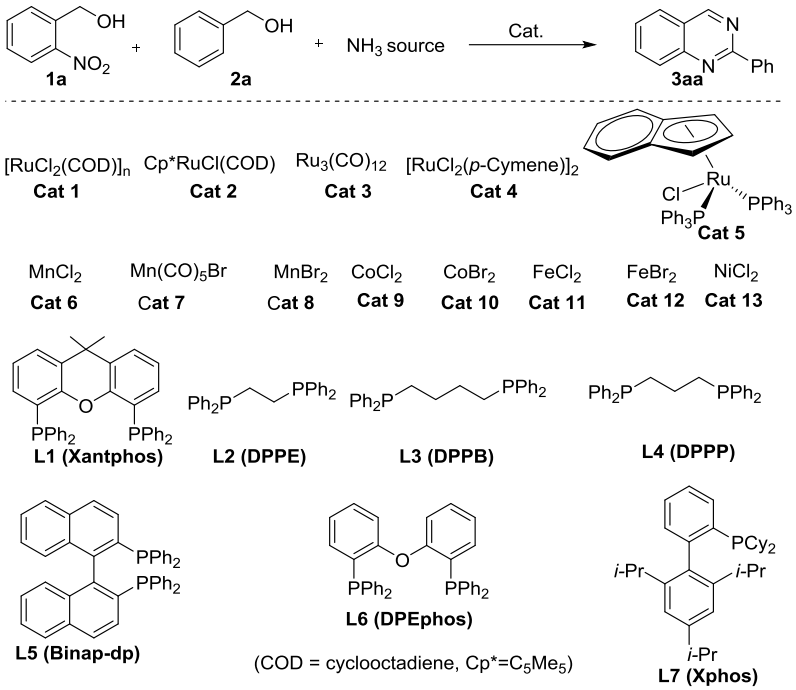


Transparent Methods.

All the obtained products were characterized by melting points (m.p), ^{1}H-NMR, ^{13}C-NMR and infrared spectra (IR). Melting points were measured on an Electrothemal SGW-X4 microscopy digital melting point apparatus and are uncorrected; IR spectra were recorded on a FTLA2000 spectrometer; ^{1}H-NMR and ^{13}C-NMR spectra were obtained on Bruker-400 and referenced to 7.26 ppm for chloroform solvent with TMS as internal standard (0 ppm). Chemical shifts were reported in parts per million (ppm, δ) downfield from tetramethylsilane. Proton coupling patterns are described as singlet (s), doublet (d), triplet (t), multiplet (m); TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF254), and visualization was effected at 254 nm; Unless otherwise stated, all the reagents were purchased from commercial sources (Energy Chemical, J&K Chemic, TCI, Fluka, Acros, SCRC), used without further purification. 1,8-naphthyridines were prepared by the condensation cyclization of 2-aminonicotinaldehyde with ketones in the presence of *t*-BuOK (Chen et al., 2017). 2-Nitrobenzyl alcohol **1l** was prepared by the reduction of Acifluorfen Acid (Rajendran et al., 2015). All calculations were performed for reactants in solution using the solvent model density (SMD) (Marenich et al., 2009) method (solvent = toluene) and employing the Gaussian 09 package (Frisch, M. J. Gaussian 09, Revision C.01; Gaussian, Inc: Wallingford, CT, 2010.). All stationary points were optimized without any constraints at the B3LYP level of theory. (Becke, 1993; Lee et al., 1988; Stephens et al., 1994) Frequency calculations at the same level of theory were also performed to identify all stationary points as minima (zero imaginary frequencies) or transition states (one imaginary frequency), and to calculate the free energies. Intrinsic reaction coordinate calculations were performed to verify the transition-state structures. (Fukui, 1970; Fukui, 1981) The LANL2DZ effective core potential method (Hay et al., 1985; Wadt et al., 1985) with an extra f-polarization function (α_f = 0.938) (Ehlers et al., 1993) was used as the basis set for Ir, while the 6-31G(d) (Krishnan et al., 1980; McLean et al., 1980) basis set was used for all other atoms (C, H, N, O, Na and Cl). To obtain better accuracy, energies of the optimized geometries were recalculated using M06 (Zhao et al., 2005; Zhao et al., 2008; Zhao et al., 2008; Zhao et al., 2009) single point calculations with a larger basis set, employing the LANL2TZ(f) (Roy et al., 2008) basis set for Ir and the 6-311++G** basis set for all other atoms. Empirical D3 dispersion corrections were included for the M06 functional. (Grimme et al., 2010) The final Gibbs free energies reported herein (ΔG_{sol}) represent the M06 single point energies with Gibbs free energy corrections.

Optimization of reaction conditions.

Table S1. Screening of different metal catalysts and ligands. Related to **Table 1**. Related to the first paragraph of “RESULTS AND DISCUSSION” in the main text.



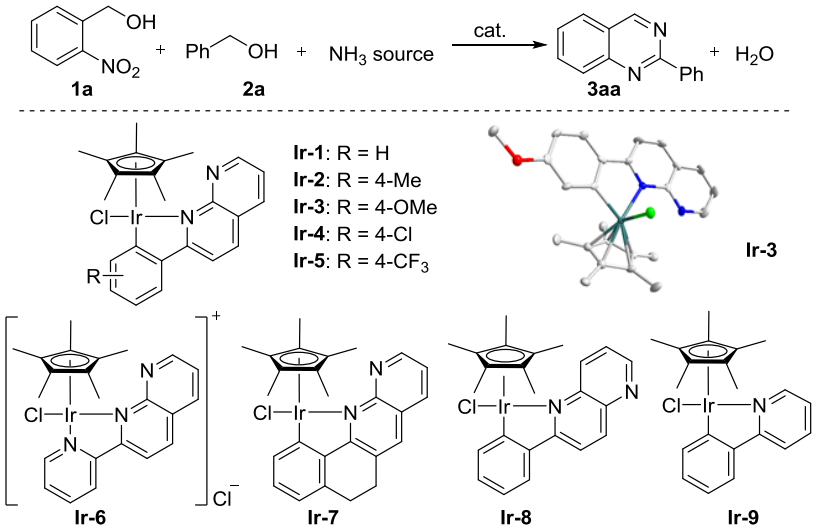
(COD = cyclooctadiene, Cp*=C_5Me_5)

Entry	Catalyst	Ligand	Additive	Solvent	Temperature	N source	Yields of **3aa** [a, b]
1	**Cat 3**	**L1**	*t*-BuOK	toluene	130	NH_4OAc	5%
2	**Cat 3**	**L2**	*t*-BuOK	toluene	130	NH_4OAc	-
3	**Cat 3**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	trace
4	**Cat 3**	**L4**	*t*-BuOK	toluene	130	NH_4OAc	<5%
5	**Cat 3**	**L5**	*t*-BuOK	toluene	130	NH_4OAc	-
6	**Cat 3**	**L6**	*t*-BuOK	toluene	130	NH_4OAc	<5%
7	**Cat 3**	**L7**	*t*-BuOK	toluene	130	NH_4OAc	-
8	**Cat 1**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	trace
9	**Cat 2**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	trace
10	**Cat 4**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	<5%
11	**Cat 5**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	trace
12	**Cat 6**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
13	**Cat 7**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
14	**Cat 8**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
15	**Cat 9**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
16	**Cat 10**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
17	**Cat 11**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
18	**Cat 12**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
19	**Cat 13**	**L3**	*t*-BuOK	toluene	130	NH_4OAc	-
20	**Cat 4**	**L6**	*t*-BuOK	toluene	130	NH_4OAc	<5%
21	**Cat 4**	**-**	*t*-BuOK	toluene	130	NH_4OAc	trace
22	**Cat 3**	**L1**	*t*-BuONa	toluene	130	NH_4OAc	5%
23	**Cat 3**	**L1**	NaOH	toluene	130	NH_4OAc	<5%
24	**Cat 3**	**L1**	KOH	toluene	130	NH_4OAc	<5%
25	**Cat 3**	**L1**	$NaOCH_3$	toluene	130	NH_4OAc	<5%
26	**Cat 3**	**L1**	*t*-BuOK	*p*-xylene	130	NH_4OAc	<5%
27	**Cat 3**	**L1**	*t*-BuOK	chlorobenzene	130	NH_4OAc	<5%
28	**Cat 3**	**L1**	*t*-BuOK	*t*-amyl alcohol	130	NH_4OAc	<5%
29	**Cat 3**	**L1**	*t*-BuOK	DMF	130	NH_4OAc	<5%
30	**Cat 3**	**L1**	*t*-BuOK	toluene	130	NH_4Cl	<5%
31	**Cat 3**	**L1**	*t*-BuOK	toluene	130	$HCOONH_4$	trace

32	**Cat 3**	**L1**	*t*-BuOK	toluene	130	$NH_3·H_2O$	trace

[a] The reaction was performed with **1a** (0.5 mmol), **2a** (0.5 mmol), catalyst (1 mol%), ligand (3 mol%), additive (50 mol%), NH_3 sources (1.0 mmol) in solvent (1.5 mL) for 24 h under Ar protection. [b] GC yield by using hexadecane as an internal standard.

Table S2. Optimization of reaction conditions with Ir catalysts. Related to **Table 1**. Related to the first paragraph of "RESULTS AND DISCUSSION" in the main text.



Entry	Catalyst	Additive	Solvent	Temperature	N source	Yields of **3aa**[a, b]
1	$[IrCp^*Cl_2]_2$	*t*-BuOK	toluene	130	NH_4OAc	15
2	$[IrCp^*Cl_2]_2$	*t*-BuOK	*p*-xylene	130	NH_4OAc	trace
3	$[IrCp^*Cl_2]_2$	*t*-BuOK	chlorobenzene	130	NH_4OAc	-
4	$[IrCp^*Cl_2]_2$	*t*-BuOK	*t*-amyl alcohol	130	NH_4OAc	14
5	$[IrCp^*Cl_2]_2$	*t*-BuOK	DMSO	130	NH_4OAc	10
6	$[IrCp^*Cl_2]_2$	*t*-BuOK	DMF	130	NH_4OAc	15
7	$[IrCp^*Cl_2]_2$	*t*-BuOK	1,4-dioxane	130	NH_4OAc	trace
8	$[IrCp^*Cl_2]_2$	*t*-BuONa	toluene	130	NH_4OAc	16
9	$[IrCp^*Cl_2]_2$	NaOH	toluene	130	NH_4OAc	15
10	$[IrCp^*Cl_2]_2$	NaOAc	toluene	130	NH_4OAc	11
11	$[IrCp^*Cl_2]_2$	Cs_2CO_3	toluene	130	NH_4OAc	12
12	$[IrCp^*Cl_2]_2$	NaOMe	toluene	130	NH_4OAc	9
13	$[IrCp^*Cl_2]_2$	-	toluene	130	NH_4OAc	10
14	$[IrCp^*Cl_2]_2$	*t*-BuONa	toluene	120	NH_4OAc	11
15	$[IrCp^*Cl_2]_2$	*t*-BuONa	toluene	140	NH_4OAc	18
16	$[IrCp^*Cl_2]_2$	*t*-BuONa	toluene	150	NH_4OAc	15
17	**Ir-1**	*t*-BuONa	toluene	140	NH_4OAc	72
18	**Ir-2**	*t*-BuONa	toluene	140	NH_4OAc	75
19	**Ir-3**	*t*-BuONa	toluene	140	NH_4OAc	82
20	**Ir-4**	*t*-BuONa	toluene	140	NH_4OAc	61
21	**Ir-5**	*t*-BuONa	toluene	140	NH_4OAc	67
22	**Ir-6**	*t*-BuONa	toluene	140	NH_4OAc	71
23	**Ir-7**	*t*-BuONa	toluene	140	NH_4OAc	68

24	**Ir-8**	*t*-BuONa	toluene	140	NH_4OAc	15
25	**Ir-9**	*t*-BuONa	toluene	140	NH_4OAc	21
26	-	*t*-BuONa	toluene	140	NH_4OAc	-
27	**Ir-3**	*t*-BuONa	toluene	140	NH_4Cl	5
28	**Ir-3**	*t*-BuONa	toluene	140	$HCOONH_4$	trace
29	**Ir-3**	*t*-BuONa	toluene	140	$NH_3{\cdot}H_2O$	trace
30	**Ir-3**	*t*-BuONa	toluene	140	$(NH_4)_2SO_4$	22
31	**Ir-3**	*t*-BuONa	toluene	140	NH_3	88 [c]
32	**Ir-3**	*t*-BuONa	toluene	140	NH_3	81[c, d]
33	**Ir-3**	*t*-BuONa	toluene	140	NH_3	88 [c, e]

[a] The reaction was performed with **1a** (0.5 mmol), **2a** (0.5 mmol), Ir (1 mol%), additive (50 mol%), N sources (1.0 mmol) in solvent (1.5 mL) for 24 h under Ar protection. [b] GC yield by using hexadecane as an internal standard. [c] 4 bar of NH_3. [d] With additive (30 mol%)). [e] With additive (40 mol%).

Typical procedure for the synthesis of complexes Ir-1 – Ir-5, Ir-7, Ir-8 and Ir-9.

Under N_2 atmosphere, $[Cp^*IrCl_2]_2$ (0.2 mmol), NaOAc (0.6 mmol) and 2-substituted 1,8-naphthyridine (0.4 mmol, Chen et al., 2017) and dichloromethane (5 mL) were introduced in a Schlenk tube, successively. Then the Schlenk tube was closed and the resulting mixture was stirred at 60 ^oC for 12 h. After cooling down to room temperature, the reaction mixture was filtered through celite, eluting with CH_2Cl_2, dried over $MgSO_4$ and filtered. The solvent was evaporated to give a crude solid followed by the addition of 1 mL of diethyl ether with washing for three times.

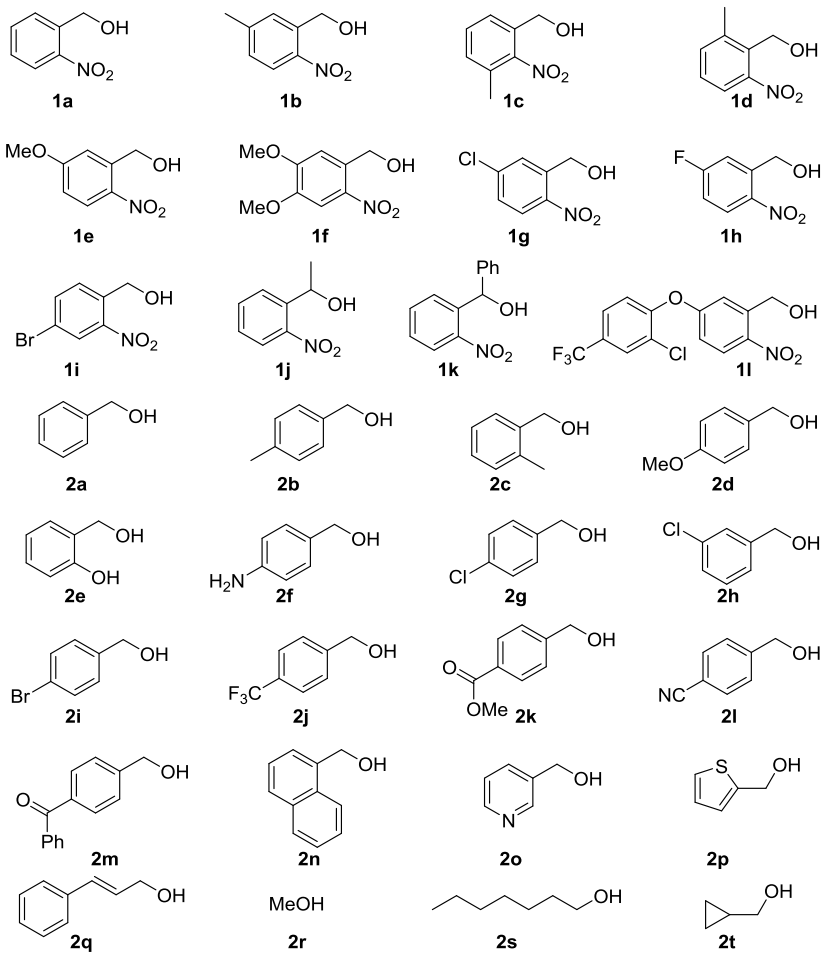
Typical procedure for the synthesis of complex Ir-6.

Under N_2 atmosphere, $[Cp^*IrCl_2]_2$ (0.2 mmol), and 2-(pyridin-2-yl)-1,8-naphthyridine (0.4 mmol) and dichloromethane (5 mL) were introduced in a Schlenk tube, successively. Then the Schlenk tube was closed and the resulting mixture was stirred at 60 ^oC for 12 h. After cooling down to room temperature, the reaction mixture was filtered through celite, eluting with CH_2Cl_2, dried over $MgSO_4$ and filtered. The solvent was evaporated to give a crude solid followed by the addition of 1 mL of diethyl ether with washing for three times.

Typical procedure for the synthesis of 3aa.

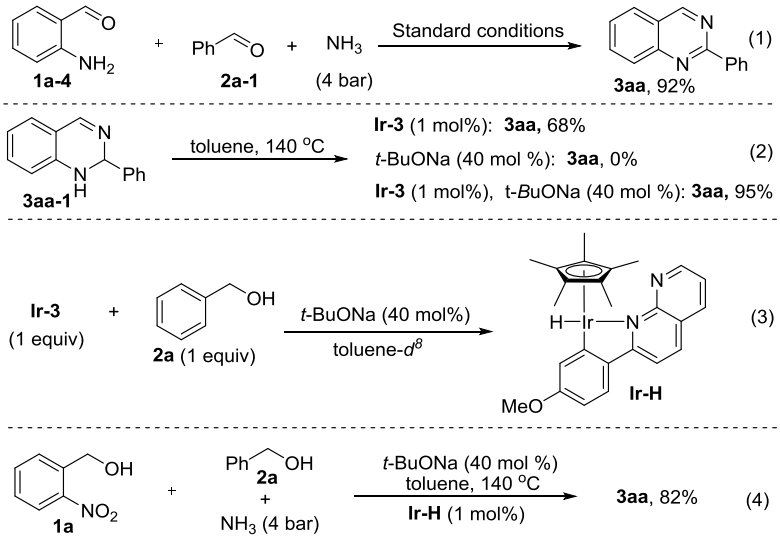
A vial was charged with (2-nitrophenyl)methanol **1a** (0.5 mmol), **Ir-3** (1 mol %), *t*-BuONa (40 mol %) in succession. The vial was transferred into the autoclave. Once sealed, the autoclave was purged with argon gas, and then was injected with phenylmethanol **2a** (0.5 mmol) in toluene (1.5 mL) under Ar atmosphere. Then the autoclave was aerated with NH_3, pressurized to 4 bar, heated up and kept at 140 °C for 24 h under thorough stirring. After the reaction, the autoclave was cooled to room temperature, depressurized, and the resulting mixture was purified by preparative TCL on silica to get 2-phenylquinazoline **3aa**.

Scheme S1. Substrates employed for the synthesis of quinazolines. Related to **Scheme 2, 3** & **4**. Related to the second and third paragraph of “RESULTS AND DISCUSSION” in the main text.



The Control Experiments. Related to the fifth paragraph of "RESULTS AND DISCUSSION" in the main text.

Scheme S2. Control experiments. Related to **Scheme 5**. Related to the fifth paragraph of "RESULTS AND DISCUSSION" in the main text.



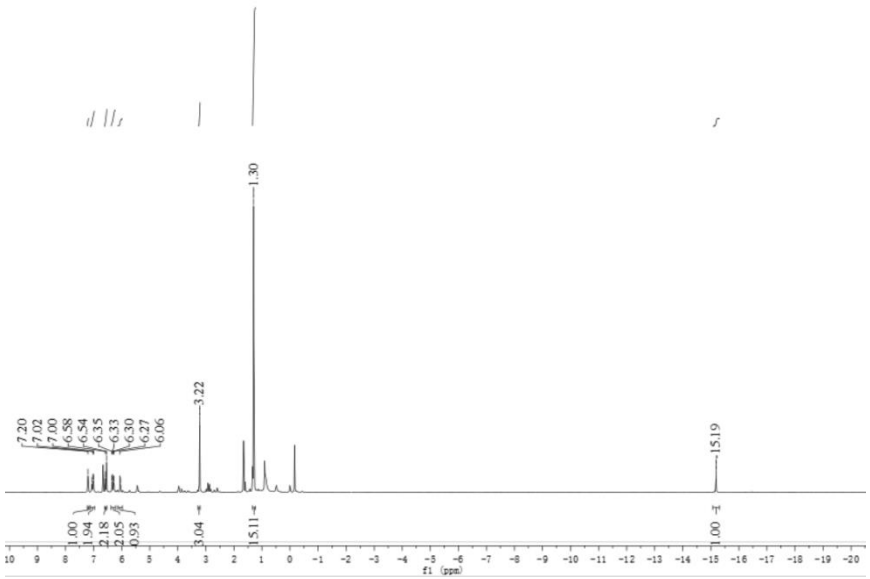
Data S1. The Experimental Procedure for the Time-Concentration Profile. Related to **Scheme 5**. Related to the fifth paragraph of "RESULTS AND DISCUSSION" in the main text.

A vial was charged with (2-nitrophenyl)methanol **1a** (0.5 mmol), **Ir-3** (1 mol %), *t*-BuONa (40 mol %) in succession, which was then transferred into the autoclave. Once sealed, the autoclave was purged with argon gas, and then was injected with phenylmethanol **2a** (0.5 mmol) in toluene (1.5 mL) under Ar atmosphere. Then the autoclave was aerated with NH_3, pressurized to 4 bar, heated up and kept at 140 °C for 0−24 h (1, 2, 4, 8, 12, 16, 20 h) under thorough stirring. After the reaction, the autoclave was cooled to room temperature, depressurized, and added hexadecane (25 mg) as an internal standard. The yield was determined by the GC-MS. For **1a-4**, MS (EI, m/z): 121.08 $[M]^+$; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 7.46 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.29 (t, *J* = 8.3 Hz, 1H), 6.73 (t, *J* = 7.8 Hz, 1H), 6.62 (d, *J* = 8.2 Hz, 1H), 6.05 (s, 2H). For **3aa-1**, MS (EI, m/z): 208.12 $[M]^+$; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1H), 7.50-7.53 (m, 2H), 7.31-7.45 (m, 3H), 7.14-7.21 (m, 2H), 6.70 (s, 1H), 6.56-6.63 (m, 2H), 5.97 (s, 1H).

Data S2. Preparation of Cyclometalated Iridium Hydride **Ir-H.** Related to **Scheme 5**. Related to the fifth paragraph of "RESULTS AND DISCUSSION" in the main text.

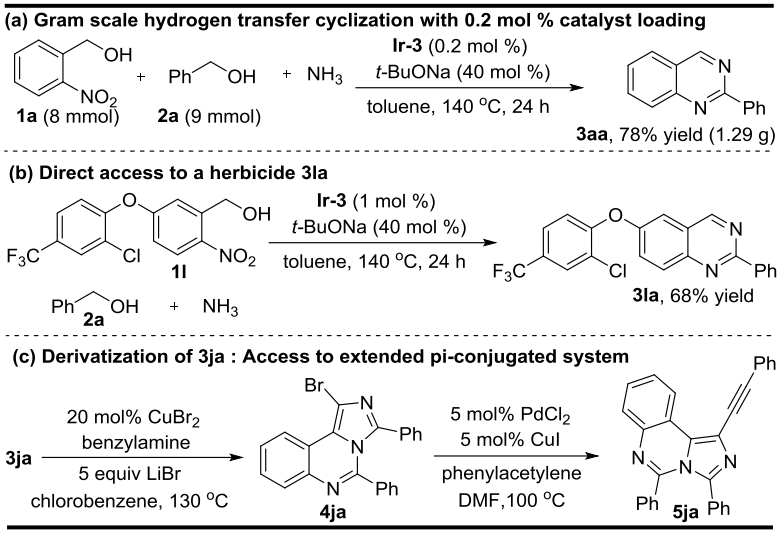
According to Xiao's reference method, (Wang et al., 2013) under N_2 atmosphere, **Ir-3** (1 equiv.) and HCOOH/Et_3N (F/T) azeotrope (4 equiv.) in methanol were introduced in a Schlenk tube, successively. The solution was left overnight; Crystals of **Ir-H** were collected after removing the liquid with syringe and washed with MeOH. 42% yield as red crystals; ^{1}H NMR (400 MHz, Tol) δ 7.20 (s, 1H), 7.05 (s, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.56 (d, *J* = 15.5 Hz, 2H), 6.34 (d, *J* = 7.8 Hz, 1H), 6.29 (d, *J* = 9.1 Hz, 1H), 6.05 (d, *J* = 7.8 Hz, 1H), 3.22 (s, 3H), 1.30 (s, 15H), -15.19 (s, 1H).

Figure S98. ^{1}H NMR spectrum of complex **Ir-H** in toluene-d^8. Related to **Scheme 5**. Related to the fifth paragraph of "RESULTS AND DISCUSSION" in the main text.



The details of the synthetic utility. Related to the fourth paragraph of "RESULTS AND DISCUSSION" in the main text.

Scheme S3. The synthetic utility of the developed chemistry. Related to **Scheme 4**.



(1) **Preparation of 1l：** To a solution of 5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic acid (Acifluorfen Acid, 2 mmol) in THF under N_2 atmosphere, BH_3-THF (1.0 M in THF. 2 mmol, 2 mL) was added at 0 °C over 1 hour. The resulting mixture was allowed to warm to room temperature over 32 hours. After reaction, THF was removed under vacuum; the reaction mixture was quenched with water, and extracted with EtOAc. The combined organic layer was dried with anhydrous sodium sulfate and solvent were removed under reduced pressure to give crude product. Crude product was purified by column chromatography to get **1l**.

(2) **Synthesis of a herbicide 3la**

A vial was charged with **1l** (0.5 mmol), **Ir-3** (1 mol %), *t*-BuONa (40 mol %) in succession. The vial was transferred into the autoclave. Once sealed, the autoclave was purged with argon gas, and then was injected with phenylmethanol **2a** (0.5 mmol) in toluene (1.5 mL) under Ar atmosphere. Then the autoclave was aerated with NH_3, pressurized to 4 bar, heated up and kept at 140 °C for 24 h under thorough stirring. After the reaction, the autoclave was cooled to room temperature, depressurized, and the resulting mixture was purified by preparative TCL on silica to get the product **3la**.

(3) **Synthesis of herbicide 4ja**

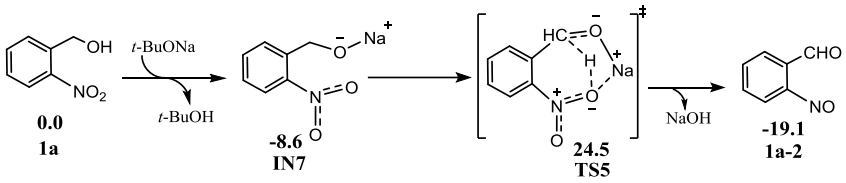
The mixture of **3ja** (0.5 mmol), benzylamine (1 mmol), lithium bromide (3 mmol), and $CuBr_2$ (0.1 mmol) in chlorobenzene (3 mL) was stirred at 120 °C for 32 h using an O_2 balloon. After being cooled to room temperature, the resulting mixture was extracted with chloroform, washed with 5% Na_2CO_3 solution, dried with anhydrous sodium sulfate, and then concentrated by removing the solvent under vacuum. Finally, the residue was purified by preparative TLC on silica to give the product **4ja**.

(4) **Synthesis of functionalized multi conjugate N-heteroaromatic 5ja**

Under N_2 atmosphere, **4ja** (0.5 mmol), ethynylbenzene (0.65 mmol), $PdCl_2$ (5 mol %), CuI (20 mol %), PPh_3 (10 mol %), $N(C_2H5)_3$ (1.5 mmol), and DMF (1.0 mL) were introduced in a Schlenk tube, successively. Then the Schlenk tube was closed, and the resulting mixture was stirred at 90 °C for 12 h. After being cooled to room temperature, the resulting mixture was extracted with chloroform, washed with 5% Na_2CO_3 solution, dried with anhydrous sodium

sulfate, and then concentrated by removing the solvent under vacuum. Finally, the residue was purified by preparative TLC on silica to give the product **5ja**.

Scheme S4. MPV-O TH pathway. Related to **Figure 2**. (Values shown are relative free energies in kcal/mol.) Related to the sixth paragraph of "RESULTS AND DISCUSSION" in the main text.



The calculated free-energy profile for the 2nd TH of **1a-2** to **1a-3** is shown in Figure S99. The reaction begins with coordination of **2a** to the Ir center of **Ir-O1** to form intermediate **IN8**, which is an endergonic process. Subsequent O–H deprotonation via four-centered transition-state **TS6** with an energy barrier of 23.3 kcal/mol relative to **Ir-O1** gives Ir–alkoxide intermediate **Ir-O2** and *t*-BuOH. From **Ir-O2**, C–H cleavage via transition state **TS7** gives Ir–benzaldehyde **IN9** with an energy barrier of 27.0 kcal/mol relative to **Ir-O2**. Intermediate **IN9** would then dissociate to give **Ir-H** together with the benzaldehyde. The next step is the TH from **Ir-H** to **1a-2**. We calculated two possible pathways: hydrogen migration to N atom via **TS8′** (blue line) and hydrogen migration to O atom via **TS8″** (red line). The results show that the barrier (24.7 kcal/mol) for hydrogen migration to O atom is higher than that (19.6 kcal/mol) for hydrogen migration to N atom, therefore the hydrogen migration to N atom is kinetically favorable. Previously, it has been shown that such a H-transfer could be facilitated by a transferring shuttle such as water or alcohol proton shuttle. We performed calculations for hydrogen migration to N atom when using benzyl alcohol **2a** as the proton transferring shuttle (black line). The calculated free energy of transition state **TS8** for the hydrogenation assisted by **2a** is -12.2 kcal/mol, which is lower than that of **TS8′**. Therefore, the hydrogen migration to the N atom using **2a** as the proton transferring shuttle constitutes a preferred mode. The relative instability of **TS8** compared with **TS8′** can be attributed to the ring strain associated with the four-membered ring in **TS8′**. **IN10** then isomerizes to the less stable intermediate **IN11** by coordination of **2a** to the Ir center and dissociation of one of the arms of the 1,8-naphthyridyl ligand. The TH is accomplished via transition state **TS9** with an energy barrier of 23.0 kcal/mol relative to **IN10**, which generates the 2-(hydroxyamino)benzaldehyde **1a-3** and complex **Ir-O2**.

Figure S99. Calculated energy profiles for transformation of 2-nitrosobenzaldehyde **1a-2** to 2-(hydroxyamino)benzaldehyde **1a-3**. Values shown are relative free energies in kcal/mol. Related to **Figure 2** & **Figure 3**. Related to the seventh paragraph of "RESULTS AND DISCUSSION" in the main text.

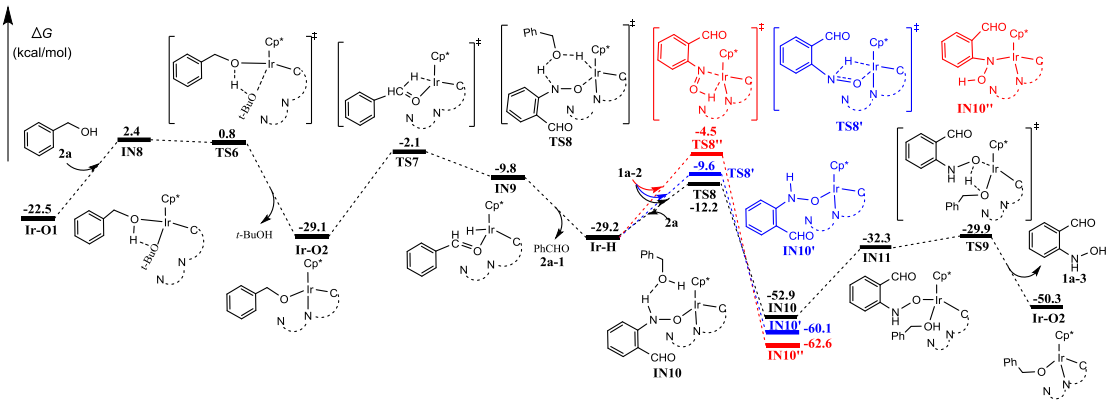
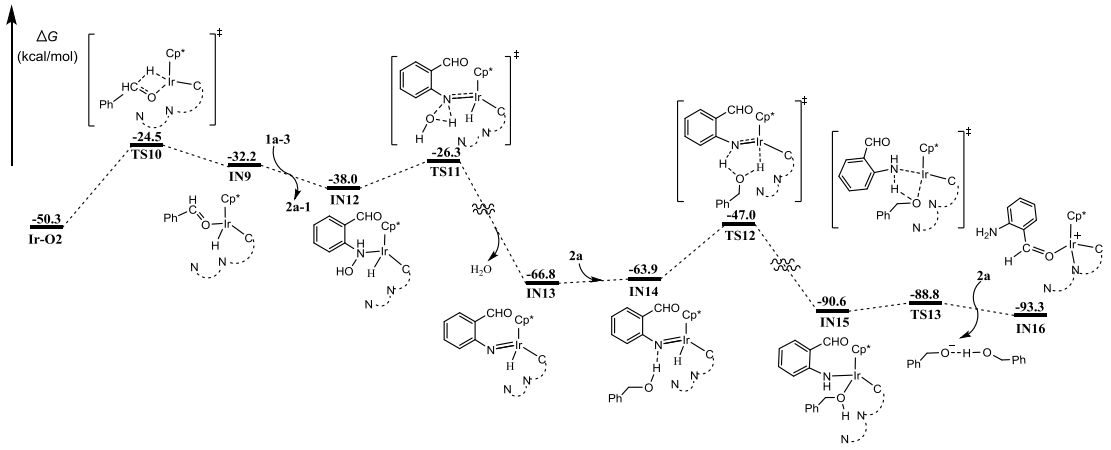
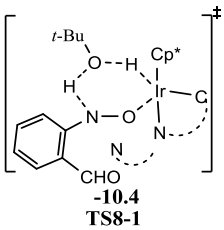


Figure S100. Calculated energy profiles for transformation of 2-(hydroxyamino)benzaldehyde **1a-3** to 2-aminobenzaldehyde. Values shown are relative free energies in kcal/mol. Related to **Figure 2** & **Figure 3**. Related to the seventh paragraph of "RESULTS AND DISCUSSION" in the main text.

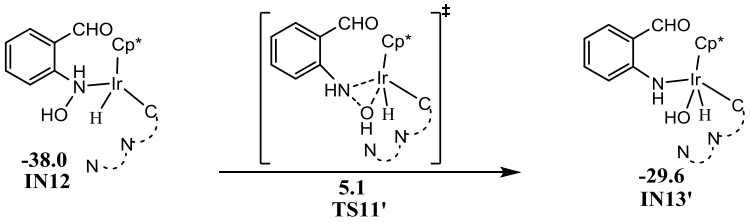


As shown in Figure S100 (3rd TH), **Ir-O2** is transformed to **IN9** through *β*-H elimination. The identified transition state is denoted as **TS10** and the calculated energy barrier is 25.8 kcal/mol. A molecule of **1a-3** enters and then the benzaldehyde dissociates to yield intermediate **IN12**. Subsequently, **IN12** undergoes dehydration by passing transition state **TS11**, affording an Ir-nitrene intermediate **IN13**. Binding of **IN13** with benzyl alcohol **2a** via a hydrogen bond affords intermediate **IN14**. From **IN14**, the TH using **2a** as the proton transferring shuttle takes place via **TS12** to give complex **IN15**, in which **2a** is bound to Ir. The hydrogen of **2a** is transferred to the nitrogen atom via **TS13** with a very small barrier of 1.8 kcal/mol. The iridium 2-aminobenzaldehyde **IN16** is generated with the formation of alcohol anion, which is stabilized by the hydrogen bonding by alcohol **2a**.

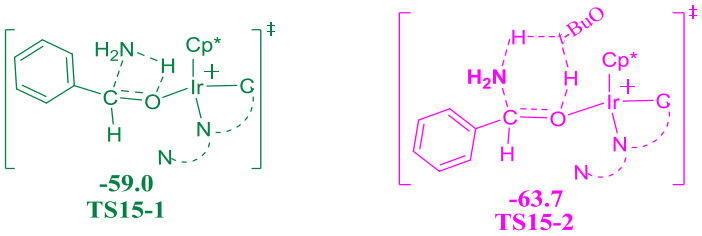
Scheme S5. Hydrogen migration to N atom using *t*-BuOH as the proton transferring shuttle. Values shown are relative free energies in kcal/mol. Related to **Figure 2** & **Figure 3**. Related to the seventh paragraph of "RESULTS AND DISCUSSION" in the main text.



Scheme S6. Other possible pathway started from **IN12**. Values shown are relative free energies in kcal/mol. Related to **Figure 2** & **Figure 3**. Related to the seventh paragraph of "RESULTS AND DISCUSSION" in the main text.



Scheme S7. Other possible pathway started from **IN19**. Values shown are relative free energies in kcal/mol. Related to **Figure 3**. Related to the seventh paragraph of "RESULTS AND DISCUSSION" in the main text.



Scheme S8. Other possible pathway started from **IN21**. Values shown are relative free energies in kcal/mol. Related to **Figure 3**. Related to the seventh paragraph of "RESULTS AND DISCUSSION" in the main text.

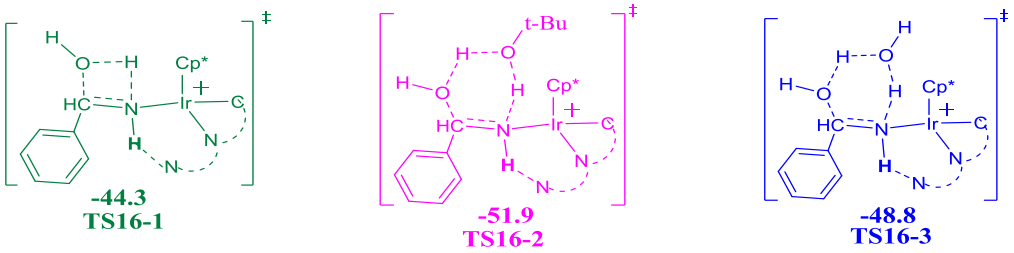


Table S3. Energies (in Hartree) for all TS and intermediates. Related to **Figure 2**, **Figure 3**, **Figure S99**, Figure **S100** and **Scheme S4**, **Scheme S5**, **Scheme S6**, **Scheme S7** & **Scheme S8**.

Geometry	E_0	E	$H_{413.15}$	$G_{413.15}$	$E_{(sol,M06)}$
Ir-O1	-1490.293732	-1490.229403	-1490.228095	-1490.402536	-1489.75506
1a	-551.134366	-551.117956	-551.116647	-551.187508	-551.0114631
IN1	-2041.416957	-2041.333032	-2041.331723	-2041.557112	-2040.745557

TS1	-2041.408804	-2041.326030	-2041.324722	-2041.544271	-2040.732445
IN2	-1807.908586	-1807.839290	-1807.837982	-1808.028124	-1807.287753
TS2	-1807.855907	-1807.786936	-1807.785627	-1807.974158	-1807.243077
IN3	-1807.870208	-1807.800571	-1807.799263	-1807.989963	-1807.25635
Ir-H	-1807.910263	-1807.839392	-1807.838084	-1808.037770	-1807.29225
TS3	-1807.877623	-1807.807900	-1807.806592	-1807.997863	-1807.261206
IN4	-1807.907399	-1807.836988	-1807.835680	-1808.027498	-1807.296366
***t*-BuOH**	-233.536268	-233.524255	-233.522947	-233.580384	-233.4931922
IN5	-2041.458380	-2041.374111	-2041.372803	-2041.595922	-2040.781565
TS4	-2041.404858	-2041.320656	-2041.319347	-2041.539368	-2040.742495
IN6	-2041.417579	-2041.331447	-2041.330139	-2041.555450	-2040.759786
1a-2	-474.748119	-474.733612	-474.732303	-474.799019	-474.619815
H_2O	-76.390125	-76.386179	-76.384871	-76.416321	-76.42743
***t*-BuONa**	-395.263703	-395.249546	-395.248238	-395.314796	-395.2140859
IN7	-712.877431	-712.858262	-712.856954	-712.936649	-712.7460679
TS5	-712.826173	-712.807984	-712.806675	-712.881912	-712.6933673
NaOH	-238.108646	-238.103584	-238.102276	-238.142390	-238.1421522
2a	-346.636496	-346.623523	-346.622215	-346.686686	-346.5400135
IN8	-1836.911027	-1836.831642	-1836.830334	-1837.042138	-1836.255335
TS6	-1836.913327	-1836.834518	-1836.833210	-1837.043820	-1836.257927
Ir-O2	-1603.408090	-1603.342829	-1603.341521	-1603.522468	-1602.81245
TS7	-1603.362712	-1603.297952	-1603.296643	-1603.474749	-1602.769385
IN9	-1603.377738	-1603.312241	-1603.310933	-1603.491010	-1602.78172
2a-1	-345.466000	-345.454515	-345.453207	-345.511975	-345.3587192
TS8	-2079.312101	-2079.229325	-2079.228017	-2079.448190	-2078.589596
IN10	-2079.384394	-2079.300413	-2079.299104	-2079.524868	-2078.654402
TS8'	-1732.657052	-1732.588403	-1732.587095	-1732.777218	-1732.045384
IN10'	-1732.735862	-1732.667536	-1732.666227	-1732.851169	-1732.126231
TS8''	-1732.641503	-1732.573418	-1732.572109	-1732.757193	-1732.037325
IN10''	-1732.728208	-1732.660113	-1732.658804	-1732.842567	-1732.129858
TS8-1	-1966.204210	-1966.122334	-1966.121026	-1966.336549	-1965.540029
IN11	-2079.347461	-2079.263782	-2079.262473	-2079.487346	-2078.621626
TS9	-2079.344560	-2079.261430	-2079.260122	-2079.482288	-2078.617761
1a-3	-475.953316	-475.937391	-475.936082	-476.005475	-475.8397945
TS10	-1603.362712	-1603.297952	-1603.296643	-1603.474749	-1602.769385
IN12	-1733.873484	-1733.803692	-1733.802383	-1733.991017	-1733.272035
TS11	-1733.844795	-1733.773839	-1733.772530	-1733.966068	-1733.253426
IN13	-1733.909215	-1733.837124	-1733.835815	-1734.033472	-1733.317896
TS11'	-1733.810514	-1733.740262	-1733.738954	-1733.929844	-1733.203408
IN13'	-1733.894687	-1733.824729	-1733.823420	-1734.012897	-1733.301025
IN14	-2004.142375	-2004.060198	-2004.058890	-2004.280108	-2003.425822
TS12	-2004.126634	-2004.045630	-2004.044321	-2004.261454	-2003.398905
IN15	-2004.184670	-2004.102997	-2004.101689	-2004.320682	-2003.468364
TS13	-2004.182515	-2004.101566	-2004.100258	-2004.317473	-2003.46559

IN16	-2350.855816	-2350.758697	-2350.757388	-2351.016560	-2350.016557
IN17	-2295.510124	-2295.415682	-2295.414374	-2295.666119	-2294.671788
1a-4	-400.801794	-400.787647	-400.786339	-400.850827	-400.6899132
NH_3	-56.514029	-56.509968	-56.508659	-56.540764	-56.5317547
TS14	-1659.203233	-1659.135024	-1659.133716	-1659.319764	-1658.58771
IN18	-1659.201798	-1659.133525	-1659.132216	-1659.318261	-1658.58754
TS14'	-1714.532549	-1714.463006	-1714.461698	-1714.648483	-1713.91008
IN18'	-1714.542462	-1714.473759	-1714.472451	-1714.656625	-1713.918227
IN19	-1715.733012	-1715.659948	-1715.658640	-1715.857467	-1715.118292
IN19'	-1771.060274	-1770.986486	-1770.985177	-1771.180845	-1770.452496
TS15	-1715.723377	-1715.652685	-1715.651377	-1715.840531	-1715.107175
IN20	-1715.728350	-1715.655572	-1715.654264	-1715.849553	-1715.120182
TS15'	-1771.062498	-1770.988987	-1770.987679	-1771.183810	-1770.443594
IN20'	-1771.064440	-1770.989750	-1770.988441	-1771.186668	-1770.450352
TS15-1	-1659.167866	-1659.100380	-1659.099072	-1659.284664	-1658.557134
TS15-2	-1892.729659	-1892.649609	-1892.648301	-1892.857627	-1892.057864
IN21	-1715.747857	-1715.675119	-1715.673811	-1715.868374	-1715.139997
IN21'	-1771.083117	-1771.008716	-1771.007408	-1771.204529	-1770.468709
TS16	-1715.703685	-1715.631683	-1715.630375	-1715.823540	-1715.095749
IN22	-1715.747576	-1715.673008	-1715.671699	-1715.873345	-1715.139803
TS16'	-1771.042429	-1770.968860	-1770.967551	-1771.161731	-1770.424036
IN22'	-1771.091888	-1771.015464	-1771.014156	-1771.217697	-1770.476703
IN21''	-1715.744916	-1715.672216	-1715.670908	-1715.866802	-1715.13918
TS16''	-1715.701957	-1715.630330	-1715.629021	-1715.820097	-1715.087871
IN22''	-1715.749138	-1715.673841	-1715.672532	-1715.877915	-1715.143996
TS16-1	-1659.137223	-1659.069786	-1659.068478	-1659.250792	-1658.533044
TS16-2	-1892.704617	-1892.624842	-1892.623534	-1892.832588	-1892.038956
TS16-3	-1735.561694	-1735.491091	-1735.489783	-1735.678620	-1734.968226
2a-2	-325.571476	-325.559576	-325.558268	-325.618207	-325.4553086
2a-3	-380.907260	-380.893214	-380.891906	-380.955684	-380.7845477

E_0 = Sum of electronic and zero-point Energies by B3LYP in solvent

E = Sum of electronic and thermal Energies by B3LYP in solvent

$H_{413.15}$ = Sum of electronic and thermal Enthalpies by B3LYP in solvent

$G_{413.15}$ = Sum of electronic and thermal Free Energies by B3LYP in solvent

$E_{(sol, M06)}$ = Single point energies calculated by M06 in solvent

Calculated imaginary frequencies of all transition states species

Table S4. Calculated imaginary frequencies of all transition states species for substrate. Related to **Figure 2**, **Figure 3**, **Figure S99**, Figure **S100** and **Scheme S4**, **Scheme S5**, **Scheme S6**, **Scheme S7** & **Scheme S8**.

Species	Frequency
TS1	-584.09
TS2	-743.09
TS3	-425.57

TS4	-715.20
TS5	-1746.69
TS6	-737.34
TS7	-686.33
TS8	-901.67
TS8'	-860.06
TS8''	-679.02
TS8-1	-860.46
TS9	-757.76
TS10	-686.33
TS11	-593.96
TS11'	-627.49
TS12	-563.41
TS13	-1148.07
TS14	-144.35
TS14'	-140.97
TS15	-57.07
TS15'	-316.98
TS15-1	-1654.38
TS15-2	-829.31
TS16	-697.59
TS16'	-281.04
TS16''	-716.03
TS16-1	-1584.06
TS16-2	-832.94
TS16-3	-1062.09

Crystallographic data of complex Ir-3.

Figure S101. Molecular structure of **Ir-3** is displayed with thermal ellipsoids set at 50% probability (Hydrogen atoms are omitted for clarity. CCDC: 1848110). Related to **Table 1**.

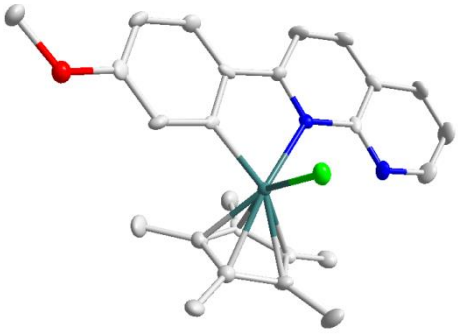


Table S5. Crystal data and structure refinement for **Ir-3**. Related to **Table 1**.

Identification code	**Ir-3**
Empirical formula	$C_{25}H_{26}ClIrN_2O$
Formula weight	598.13

Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.0070(4)
b/Å	14.7851(8)
c/Å	16.1262(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2147.52(17)
Z	4
ρ_{calc}g/cm^3	1.850
μ/mm^{-1}	6.361
F(000)	1168.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.052 to 49.994
Index ranges	-10 ≤ h ≤ 9, -12 ≤ k ≤ 17, -19 ≤ l ≤ 15
Reflections collected	14026
Independent reflections	3783 [R_{int} = 0.0488, R_{sigma} = 0.0487]
Data/restraints/parameters	3783/12/277
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0294, wR_2 = 0.0519
Final R indexes [all data]	R_1 = 0.0356, wR_2 = 0.0545
Largest diff. peak/hole / e Å^{-3}	1.03/-0.77
Flack parameter	-0.027(7)

Table S6. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **Ir-3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor. Related to **Table 1**.

Atom	*x*	*y*	*z*	U(eq)
C(1)	671(10)	6964(7)	59(6)	25(2)
C(2)	698(10)	7845(8)	-244(6)	29(3)
C(3)	1351(10)	8496(7)	223(6)	24(2)
C(4)	2021(9)	8266(6)	992(5)	18(2)
C(5)	1950(8)	7340(6)	1227(5)	14(2)
C(6)	2747(10)	8882(6)	1519(5)	23(2)
C(7)	3433(9)	8583(6)	2212(5)	20(2)
C(8)	3393(7)	7652(5)	2427(6)	15.3(18)
C(9)	4163(9)	7236(6)	3116(5)	16(2)
C(10)	5133(9)	7695(7)	3643(5)	18(2)

C(11)	5935(9)	7244(7)	4236(5)	20(2)
C(12)	5797(9)	6299(7)	4293(5)	18(2)
C(13)	4798(8)	5843(7)	3793(5)	16(2)
C(14)	3948(8)	6291(6)	3206(5)	11.5(19)
C(15)	7620(10)	6218(6)	5376(5)	24(2)
C(16)	192(9)	5757(7)	2999(5)	19(2)
C(17)	1123(9)	5157(7)	3447(6)	20(2)
C(18)	1600(10)	4445(6)	2885(5)	20(2)
C(19)	824(10)	4601(6)	2111(6)	20(2)
C(20)	-36(9)	5378(6)	2185(6)	20(2)
C(21)	-569(11)	6583(7)	3324(6)	30(3)
C(22)	1490(11)	5208(8)	4362(6)	31(3)
C(23)	2466(10)	3611(6)	3116(5)	24(2)
C(24)	994(11)	4030(7)	1348(6)	27(3)
C(25)	-1211(9)	5728(7)	1591(6)	25(2)
Cl(1)	4379(2)	5281.0(16)	1547.5(13)	18.9(5)
Ir(1)	2385.5(3)	5739.5(2)	2458.3(2)	12.78(10)
N(1)	1296(7)	6697(5)	765(4)	17.2(18)
N(2)	2595(7)	7057(4)	1966(4)	12.4(15)
O(1)	6620(6)	5772(5)	4823(3)	20.6(14)

Table S7. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **Ir-3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$. Related to **Table 1**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	15(5)	35(7)	25(6)	-4(5)	-8(4)	6(4)
C(2)	31(6)	36(8)	20(6)	5(5)	-10(4)	6(5)
C(3)	29(6)	21(7)	21(6)	10(5)	-2(4)	3(5)
C(4)	15(5)	18(6)	21(5)	7(4)	5(3)	4(4)
C(5)	6(4)	25(6)	12(5)	3(4)	3(3)	3(4)
C(6)	22(5)	14(5)	31(5)	4(4)	2(4)	-1(4)
C(7)	21(5)	9(5)	31(6)	1(4)	-4(4)	1(4)
C(8)	15(4)	16(5)	16(5)	-4(5)	1(4)	-1(3)
C(9)	19(5)	13(6)	16(5)	0(4)	9(4)	-3(4)
C(10)	16(5)	18(6)	19(5)	-5(4)	3(4)	2(4)
C(11)	15(5)	29(7)	16(5)	-7(5)	-1(4)	-6(4)
C(12)	14(5)	29(7)	11(5)	3(4)	5(3)	-1(4)
C(13)	11(4)	18(6)	19(5)	-5(4)	0(3)	-4(4)
C(14)	9(4)	14(5)	11(5)	-4(4)	5(3)	-1(4)
C(15)	23(5)	28(6)	21(5)	1(4)	-10(4)	-4(5)

C(16)	11(5)	25(6)	20(5)	7(5)	9(3)	3(5)
C(17)	19(2)	20(2)	20(2)	0.7(13)	1.0(13)	-1.3(13)
C(18)	20(3)	19(3)	19(3)	0.4(13)	0.2(13)	-1.3(13)
C(19)	22(5)	15(6)	24(5)	0(4)	-6(4)	-4(4)
C(20)	10(5)	23(6)	27(6)	4(4)	1(3)	1(4)
C(21)	36(6)	33(7)	23(6)	-3(5)	4(4)	0(5)
C(22)	37(6)	42(7)	14(5)	3(5)	4(4)	-9(5)
C(23)	33(6)	19(5)	20(5)	3(4)	0(5)	-11(5)
C(24)	32(6)	19(7)	30(6)	-6(5)	-16(4)	2(4)
C(25)	17(5)	26(6)	32(6)	4(5)	0(4)	0(5)
Cl(1)	21.8(12)	19.1(14)	15.7(12)	0.3(10)	1.6(9)	4.2(10)
Ir(1)	14.04(16)	12.03(17)	12.28(16)	-0.10(17)	-0.40(18)	-0.51(13)
N(1)	18(4)	20(5)	14(4)	1(4)	-2(3)	7(3)
N(2)	8(4)	15(4)	14(3)	2(3)	2(3)	2(3)
O(1)	19(3)	23(4)	20(3)	4(3)	-4(2)	1(3)

Table S8. Bond Lengths for **Ir-3**. Related to **Table 1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C(1)	C(2)	1.391(14)	C(14)	Ir(1)	2.024(8)
C(1)	N(1)	1.331(11)	C(15)	O(1)	1.429(9)
C(2)	C(3)	1.356(14)	C(16)	C(17)	1.418(12)
C(3)	C(4)	1.420(12)	C(16)	C(20)	1.443(12)
C(4)	C(5)	1.422(12)	C(16)	C(21)	1.494(13)
C(4)	C(6)	1.406(12)	C(16)	Ir(1)	2.160(8)
C(5)	N(1)	1.343(11)	C(17)	C(18)	1.454(13)
C(5)	N(2)	1.391(10)	C(17)	C(22)	1.514(13)
C(6)	C(7)	1.352(12)	C(17)	Ir(1)	2.139(9)
C(7)	C(8)	1.420(12)	C(18)	C(19)	1.450(12)
C(8)	C(9)	1.447(12)	C(18)	C(23)	1.505(12)
C(8)	N(2)	1.357(10)	C(18)	Ir(1)	2.154(9)
C(9)	C(10)	1.396(12)	C(19)	C(20)	1.391(13)
C(9)	C(14)	1.418(13)	C(19)	C(24)	1.499(12)
C(10)	C(11)	1.372(12)	C(19)	Ir(1)	2.263(9)
C(11)	C(12)	1.406(13)	C(20)	C(25)	1.517(12)
C(12)	C(13)	1.383(12)	C(20)	Ir(1)	2.288(9)
C(12)	O(1)	1.373(10)	Cl(1)	Ir(1)	2.417(2)
C(13)	C(14)	1.386(12)	Ir(1)	N(2)	2.112(6)

Table S9. Bond Angles for **Ir-3**. Related to **Table 1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N(1)	C(1)	C(2)	124.8(9)	C(18)	C(19)	Ir(1)	66.8(5)
C(3)	C(2)	C(1)	118.5(9)	C(20)	C(19)	C(18)	109.1(8)
C(2)	C(3)	C(4)	120.0(10)	C(20)	C(19)	C(24)	126.3(8)
C(3)	C(4)	C(5)	116.3(9)	C(20)	C(19)	Ir(1)	73.2(5)
C(6)	C(4)	C(3)	124.8(9)	C(24)	C(19)	Ir(1)	123.9(6)
C(6)	C(4)	C(5)	118.9(8)	C(16)	C(20)	C(25)	122.8(9)
N(1)	C(5)	C(4)	123.6(8)	C(16)	C(20)	Ir(1)	66.3(5)
N(1)	C(5)	N(2)	116.4(8)	C(19)	C(20)	C(16)	108.6(8)
N(2)	C(5)	C(4)	119.9(8)	C(19)	C(20)	C(25)	128.0(9)
C(7)	C(6)	C(4)	120.1(9)	C(19)	C(20)	Ir(1)	71.2(5)
C(6)	C(7)	C(8)	120.4(9)	C(25)	C(20)	Ir(1)	135.0(6)
C(7)	C(8)	C(9)	125.9(8)	C(14)	Ir(1)	C(16)	113.0(3)
N(2)	C(8)	C(7)	120.6(8)	C(14)	Ir(1)	C(17)	95.0(3)
N(2)	C(8)	C(9)	113.5(7)	C(14)	Ir(1)	C(18)	113.3(3)
C(10)	C(9)	C(8)	124.1(8)	C(14)	Ir(1)	C(19)	151.5(3)
C(10)	C(9)	C(14)	120.2(8)	C(14)	Ir(1)	C(20)	150.6(3)
C(14)	C(9)	C(8)	115.6(8)	C(14)	Ir(1)	Cl(1)	87.6(2)
C(11)	C(10)	C(9)	121.2(9)	C(14)	Ir(1)	N(2)	77.9(3)
C(10)	C(11)	C(12)	118.8(8)	C(16)	Ir(1)	C(19)	62.7(4)
C(13)	C(12)	C(11)	120.2(8)	C(16)	Ir(1)	C(20)	37.7(3)
O(1)	C(12)	C(11)	123.8(8)	C(16)	Ir(1)	Cl(1)	158.2(3)
O(1)	C(12)	C(13)	116.0(9)	C(17)	Ir(1)	C(16)	38.5(3)
C(12)	C(13)	C(14)	121.7(9)	C(17)	Ir(1)	C(18)	39.6(3)
C(9)	C(14)	Ir(1)	115.5(6)	C(17)	Ir(1)	C(19)	63.6(3)
C(13)	C(14)	C(9)	117.7(8)	C(17)	Ir(1)	C(20)	62.8(3)
C(13)	C(14)	Ir(1)	126.8(7)	C(17)	Ir(1)	Cl(1)	137.3(3)
C(17)	C(16)	C(20)	107.7(9)	C(18)	Ir(1)	C(16)	65.3(4)
C(17)	C(16)	C(21)	127.2(8)	C(18)	Ir(1)	C(19)	38.2(3)
C(17)	C(16)	Ir(1)	69.9(5)	C(18)	Ir(1)	C(20)	62.7(3)
C(20)	C(16)	C(21)	124.8(8)	C(18)	Ir(1)	Cl(1)	100.9(2)
C(20)	C(16)	Ir(1)	75.9(5)	C(19)	Ir(1)	C(20)	35.6(3)
C(21)	C(16)	Ir(1)	124.8(7)	C(19)	Ir(1)	Cl(1)	95.9(2)
C(16)	C(17)	C(18)	108.2(8)	C(20)	Ir(1)	Cl(1)	121.7(2)
C(16)	C(17)	C(22)	126.4(9)	N(2)	Ir(1)	C(16)	102.8(3)
C(16)	C(17)	Ir(1)	71.5(5)	N(2)	Ir(1)	C(17)	134.3(3)
C(18)	C(17)	C(22)	125.4(9)	N(2)	Ir(1)	C(18)	165.8(3)
C(18)	C(17)	Ir(1)	70.7(5)	N(2)	Ir(1)	C(19)	130.4(3)
C(22)	C(17)	Ir(1)	126.1(6)	N(2)	Ir(1)	C(20)	103.2(3)
C(17)	C(18)	C(23)	126.3(8)	N(2)	Ir(1)	Cl(1)	87.94(18)

C(17) C(18) Ir(1)	69.7(5)	C(1)	N(1)	C(5)	116.7(8)
C(19) C(18) C(17)	106.1(8)	C(5)	N(2)	Ir(1)	124.2(6)
C(19) C(18) C(23)	126.4(8)	C(8)	N(2)	C(5)	119.7(7)
C(19) C(18) Ir(1)	75.0(5)	C(8)	N(2)	Ir(1)	116.1(5)
C(23) C(18) Ir(1)	129.6(6)	C(12)	O(1)	C(15)	117.9(7)
C(18) C(19) C(24)	124.5(8)				

Table S10. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **Ir-3**. Related to **Table 1**.

Atom	*x*	*y*	*z*	U(eq)
H(1)	179.5	6529.69	-255.38	30
H(2)	278.59	7984.1	-755.41	35
H(3)	1360.63	9092.16	39.49	28
H(6)	2754.63	9494.83	1390.15	27
H(7)	3934.73	8990.1	2551.23	24
H(10)	5238.41	8317.93	3591.53	21
H(11)	6559.39	7557.2	4594.56	24
H(13)	4694.44	5220.43	3851.87	19
H(15A)	8361.16	6534.5	5061.52	35
H(15B)	8091.64	5778.45	5726.26	35
H(15C)	7080.1	6641.16	5712.29	35
H(21A)	-1582.4	6440.83	3453.81	46
H(21B)	-540.4	7050.56	2911.77	46
H(21C)	-70.98	6787.5	3816.27	46
H(22A)	1764.71	5816.42	4502.18	46
H(22B)	2300.14	4807.76	4482.86	46
H(22C)	636.42	5032.8	4680.29	46
H(23A)	3268.95	3775.21	3476.79	36
H(23B)	2856.32	3335.27	2622.84	36
H(23C)	1823.73	3191.27	3394.19	36
H(24A)	1987.92	3797.17	1322.17	41
H(24B)	800.31	4391.11	865.54	41
H(24C)	303	3536.37	1369.29	41
H(25A)	-2173.78	5537.53	1777.93	37
H(25B)	-1029.28	5489.81	1046.84	37
H(25C)	-1173.12	6376.16	1574.28	37

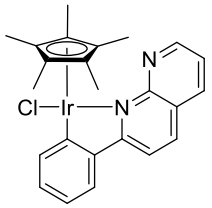
Crystal structure determination of Ir-3. Related to **Table 1**.

Crystal Data for $C_{25}H_{26}ClIrN_2O$ (*M* =598.13 g/mol): orthorhombic, space group $P2_12_12_1$ (no. 19), *a* = 9.0070(4) Å, *b* = 14.7851(8) Å, *c* = 16.1262(6) Å, *V* = 2147.52(17) Å^3, *Z* = 4, *T* = 100.00(10) K, μ(MoKα) = 6.361 mm^{-1}, *Dcalc* = 1.850 g/cm^3, 14026 reflections measured

(5.052° ≤ 2Θ ≤ 49.994°), 3783 unique (R_{int} = 0.0488, R_{sigma} = 0.0487) which were used in all calculations. The final R_1 was 0.0294 (I > 2σ(I)) and wR_2 was 0.0545 (all data).

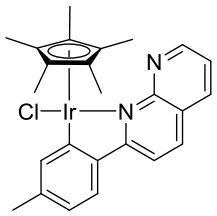
Data S3. Analytic data of the obtained compounds. Related to **Table 1, Scheme 2, Scheme 3** & **Scheme 4.**

Complex Ir-1



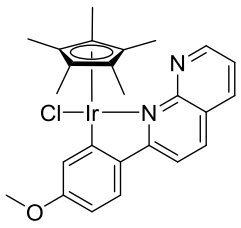
Orange red solid (107.9 mg, 95% Yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 – 8.94 (m, 1H), 8.02 (t, *J* = 9.2 Hz, 2H), 7.90 (dd, *J* = 20.0, 8.6 Hz, 2H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.43 (dd, *J* = 7.8, 4.2 Hz, 1H), 7.25 (t, *J* = 7.1 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 1.68 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.77, 167.73, 154.67, 153.34, 145.43, 138.08, 136.92, 136.23, 131.76, 126.42, 121.91, 121.89, 121.74, 117.94, 89.78, 9.84. IR (KBr): 3055, 2966, 2907, 1604, 1533, 1507, 1467, 1427, 1323, 1283, 847 cm^{-1}. HRMS (ESI): Calcd. for $C_{24}H_{24}IrN_2$ $[M\text{-}Cl]^+$: 533.1563; found: 533.1559.

Complex Ir-2



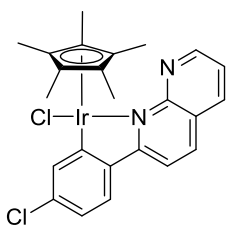
Orange red solid (105.9 mg, 91% Yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, *J* = 2.6 Hz, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.90 – 7.82 (m, 2H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.38 (dd, *J* = 7.8, 4.2 Hz, 1H), 6.88 (d, *J* = 7.8 Hz, 1H), 2.47 (s, 3H), 1.67 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.66, 167.83, 154.66, 153.15, 142.97, 141.79, 137.95, 136.89, 126.32, 123.00, 121.70, 121.63, 117.82, 89.61, 21.89, 9.82. IR (KBr): 3052, 2966, 2909, 2787, 1604, 1582, 1550, 1506, 1452, 1322, 1283, 846, 798 cm^{-1}. HRMS (ESI): Calcd. for $C_{25}H_{26}IrN_2$ $[M\text{-}Cl]^+$: 547.1720; found: 547.1723.

Complex Ir-3



Orange red solid (112.4 mg, 94% Yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (dd, *J* = 4.1, 1.6 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.85 (d, *J* = 8.6 Hz, 1H), 7.73 (dd, *J* = 13.8, 8.7 Hz, 2H), 7.57 (d, *J* = 2.4 Hz, 1H), 7.38 (dd, *J* = 7.9, 4.3 Hz, 1H), 6.65 (dd, *J* = 8.6, 2.4 Hz, 1H), 3.95 (s, 3H), 1.68 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.21, 170.13, 162.02, 154.74, 153.04, 138.73, 137.76, 136.82, 128.13, 121.39, 121.37, 119.60, 117.79, 109.29, 89.68, 55.14, 9.85. IR (KBr): 3056, 2966, 2907, 2789, 1605, 1536, 1508, 1465, 1425, 1292, 1264, 1220, 842 cm^{-1}. HRMS (ESI): Calcd. for $C_{25}H_{26}IrN_2O$ $[M\text{-}Cl]^+$: 563.1669; found: 563.1677. Crystals suitable for a single-crystal X-ray diffraction study were grown from a concentrated solution of $CHCl_3$ layered with *n*-hexane in degassed NMR tube.

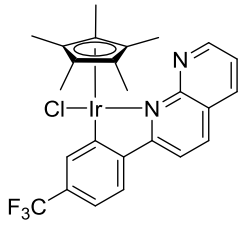
Complex Ir-4



Red solid (105.9 mg, 88% Yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (dd, *J* = 4.2, 1.9 Hz, 1H), 8.01 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.96 (d, *J* = 2.0 Hz, 1H), 7.83 (d, *J* = 8.6 Hz, 1H), 7.72 (d, *J* = 8.7 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.44 (dd, *J* = 7.9, 4.2 Hz, 1H), 6.86 (dd, *J* = 8.3, 2.0 Hz, 1H), 1.66 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.58, 168.96, 154.40, 153.40, 144.14, 138.44, 137.40, 137.09, 135.33, 129.04, 127.48, 122.02, 121.97,

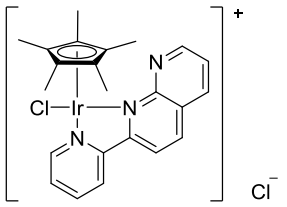
118.11, 89.93, 9.77. IR (KBr): 3056, 2966, 2910, 2788, 1603, 1531, 1508, 1451, 1318, 1275, 1087, 1028, 842, 734 cm^{-1}. HRMS (ESI): Calcd. for $C_{24}H_{23}ClIrN_2$ $[M\text{-}Cl]^+$: 567.1174; found: 567.1168.

Complex Ir-5



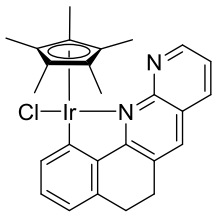
Brown solid (115.7 mg, 91% Yield); ^1H NMR (400 MHz, CD_2Cl_2) δ 9.15 (d, *J* = 2.2 Hz, 1H), 8.30 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 8.17 (d, *J* = 8.6 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 8.00 (d, *J* = 7.9 Hz, 1H), 7.64 (dd, *J* = 7.8, 4.2 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 1.71 (s, 15H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.18, 167.52, 154.52, 153.78, 149.13, 138.76, 137.22, 132.26 (q, $J_{C\text{-}F}$ = 3.8 Hz), 131.58, 125.96, 122.75, 122.50, 118.27, 118.22, 90.28, 9.53. ^{19}F NMR (376 MHz, CD_2Cl_2) δ -62.52. IR (KBr): 3076, 2964, 2915, 2790, 1603, 1510, 1453, 1428, 1318, 1109 cm^{-1}. HRMS (ESI): Calcd. for $C_{25}H_{23}F_3IrN_2$ $[M\text{-}Cl]^+$: 601.1437; found: 601.1437.

Complex Ir-6



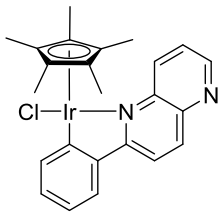
Brownish red solid (115.0 mg, 95% Yield); ^1H NMR (400 MHz, $CDCl_3$) δ 9.21 (d, *J* = 6.7 Hz, 1H), 9.15 – 9.07 (m, 2H), 8.96 – 8.84 (m, 2H), 8.55 (d, *J* = 7.2 Hz, 1H), 8.26 (s, 1H), 7.86 (s, 1H), 7.72 (d, *J* = 3.4 Hz, 1H), 1.52 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.81, 156.01, 155.39, 152.29, 151.76, 143.60, 141.06, 138.98, 129.84, 127.75, 125.33, 125.08, 122.11, 89.97, 9.71. IR (KBr): 3049, 2964, 2923, 2792, 1602, 1547, 1515, 1470, 1427, 1262, 1030, 859, 799 cm^{-1}. HRMS (ESI): Calcd. for $C_{23}H_{24}ClIrN_3$ $[M\text{-}Cl]^+$: 570.1283; found: 570.1272.

Complex Ir-7



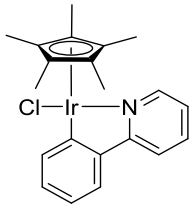
Brownish red solid (104.5 mg, 88% Yield); ^1H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 2.8 Hz, 1H), 7.91 (d, *J* = 7.7 Hz, 1H), 7.76 (d, *J* = 7.6 Hz, 1H), 7.61 (s, 1H), 7.32 (dd, *J* = 7.7, 4.2 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 6.74 (d, *J* = 7.2 Hz, 1H), 3.12 – 2.85 (m, 4H), 1.63 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.92, 166.66, 153.99, 152.17, 143.60, 139.66, 136.34, 134.93, 133.50, 132.09, 131.41, 122.39, 121.62, 120.85, 89.51, 28.45, 27.83, 9.93. IR (KBr): 3060, 2966, 2914, 2794, 1509, 1466, 1427, 1316, 1270, 1026, 845, 753, 732 cm^{-1}. HRMS (ESI): Calcd. for $C_{26}H_{26}IrN_2$ $[M\text{-}Cl]^+$: 559.1720; found: 559.1725.

Complex Ir-8



Yellow solid (96.6 mg, 85% Yield); ^1H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.51 (d, *J* = 8.4 Hz, 1H), 8.18 (t, *J* = 8.0 Hz, 3H), 7.66 (dd, *J* = 8.4, 5.2 Hz, 1H), 7.59 – 7.45 (m, 3H), 1.51 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.56, 144.78, 143.90, 140.29, 139.31, 137.82, 130.36, 129.08, 127.68, 125.27, 122.56, 86.27, 8.89. IR (KBr): 3045, 2965, 2906, 2794, 1607, 1568, 1489, 1439, 1273, 1028, 731 cm^{-1}. HRMS (ESI): Calcd. for $C_{24}H_{24}IrN_2$ $[M\text{-}Cl]^+$: 533.1563; found: 533.1560.

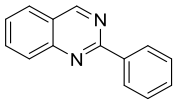
Complex Ir-9



Yellow solid (91.0 mg, 88% Yield); ^1H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 5.5 Hz, 1H), 7.89 – 7.78 (m, 2H), 7.67 (dd, *J* = 15.1, 7.7 Hz, 2H), 7.22 (t, *J* =

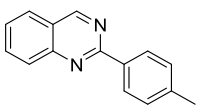
7.3 Hz, 1H), 7.14 – 6.99 (m, 2H), 1.70 (s, 15H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.33, 163.36, 151.34, 144.16, 137.05, 135.81, 130.96, 123.86, 122.33, 122.07, 118.89, 88.54, 8.93. IR (KBr): 3039, 2967, 2916, 1620, 1600, 1543, 1371, 1024, 753, 734 cm^{-1}. HRMS (ESI): Calcd. for $C_{21}H_{23}IrN$ [M-Cl]$^+$: 482.1454; found: 482.1456.

(1) 2-phenylquinazoline **(3aa)**



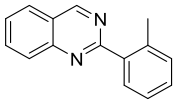
Pale yellow solid (87.6 mg, 85% Yield), m.p.: 99-100°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.54 (d, *J* = 7.2 Hz, 2H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.82 (t, *J* = 8.8 Hz, 2H), 7.58 – 7.38 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.06, 160.52, 150.78, 138.02, 134.16, 130.66, 128.67, 128.62, 127.30, 127.15, 123.62. IR (KBr): 3063, 2963, 2928, 1616, 1549, 772, 704 cm^{-1}. MS (EI, m/z): 206.15 [M]$^+$.

(2) 2-(p-tolyl)quinazoline **(3ab)**



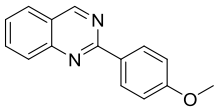
Pale yellow solid, (82.5 mg, 75% Yield), m.p.: 98-99°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.51 (d, *J* = 8.0 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 7.9 Hz, 2H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 7.9 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.17, 160.43, 150.83, 140.88, 135.35, 134.03, 129.42, 128.57, 127.12, 127.03, 123.54, 21.53. IR (KBr): 3028, 2919, 2795, 1619, 1550, 724 cm^{-1}. MS (EI, m/z): 220.14 [M]$^+$.

(3) 2-(o-tolyl)quinazoline **(3ac)**



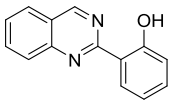
Pale yellow solid, (63.8 mg, 58% Yield), m.p.: 45-46°C (Ma et al., 2017); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.50 (s, 1H), 8.10 (d, *J* = 8.2 Hz, 1H), 8.01 – 7.87 (m, 3H), 7.66 (dd, *J* = 10.8, 3.8 Hz, 1H), 7.35 (d, *J* = 5.1 Hz, 3H), 2.61 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.05, 160.09, 150.42, 138.59, 137.43, 134.15, 131.32, 130.68, 129.34, 128.60, 127.55, 127.09, 125.99, 122.94, 21.05. IR (KBr): 3058, 2964, 2924, 1619, 1553, 769, 727 cm^{-1}. MS (EI, m/z): 220.16 [M]$^+$.

(4) 2-(4-methoxyphenyl)quinazoline **(3ad)**



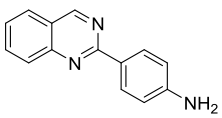
Pale yellow solid, (84.9 mg, 72% Yield), m.p.: 96-97°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.57 (d, *J* = 8.0 Hz, 2H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 7.3 Hz, 2H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.87, 160.86, 160.38, 150.84, 134.00, 130.76, 130.25, 128.41, 127.12, 126.77, 123.32, 113.99, 55.38. IR (KBr): 3055, 2969, 2833, 1605, 1585, 1407, 1247, 1162, 1028, 836, 796, 733 cm^{-1}. MS (EI, m/z): 236.15 [M]$^+$.

(5) 2-(quinazolin-2-yl)phenol **(3ae)**



White solid, (61.1 mg, 55% Yield), m.p.: 135-136°C (Gujjarappa et al., 2018); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.48 (s, 1H), 8.66 (d, *J* = 7.9 Hz, 1H), 8.07 – 7.87 (m, 3H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 8.1 Hz, 1H), 7.01 (t, *J* = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.78, 160.89, 160.50, 148.10, 134.97, 133.24, 129.72, 127.56, 127.43, 127.04, 123.01, 119.19, 119.08, 117.87. IR (KBr): 3351, 3041, 1584, 1476, 1382, 1280, 1239, 759 cm^{-1}. MS (EI, m/z): 222.12 [M]$^+$.

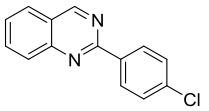
(6) 4-(quinazolin-2-yl)aniline **(3af)**



Pale yellow solid, (79.6 mg, 72% Yield), m.p.: 176-177°C (Saha et al., 2017); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.45 (d, *J* = 7.7 Hz, 2H),

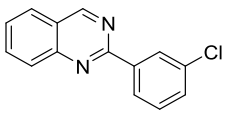
8.00 (d, *J* = 8.3 Hz, 1H), 7.85 (t, *J* = 8.3 Hz, 2H), 7.53 (t, *J* = 7.2 Hz, 1H), 6.80 (d, *J* = 7.7 Hz, 2H), 3.96 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.23, 160.32, 150.93, 149.03, 133.93, 130.22, 128.32, 128.28, 127.15, 126.41, 123.20, 114.80. IR (KBr): 3413, 3319, 1604, 1580, 1483, 1398, 1288, 1170, 836, 798, 734 cm^{-1}. MS (EI, m/z): 221.14 $[M]^+$.

(7) 2-(4-chlorophenyl)quinazoline **(3ag)**



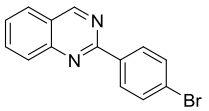
Pale yellow solid, (108 mg, 90% Yield), m.p.: 137-138°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.53 (d, *J* = 8.0 Hz, 2H), 8.02 (d, *J* = 8.3 Hz, 1H), 7.85 (d, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.0 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.48, 159.98, 150.66, 136.83, 136.52, 134.22, 129.92, 128.80, 128.59, 127.43, 127.13, 123.60. IR (KBr): 3052, 2968, 1619, 1551, 1487, 1409, 846, 796, 724 cm^{-1}. MS (EI, m/z): 240.10 $[M]^+$.

(8) 2-(3-chlorophenyl)quinazoline **(3ah)**



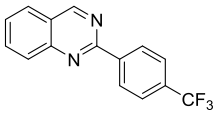
Pale yellow solid, (91.2 mg, 76% Yield), m.p.: 149-150°C (Han et al., 2012); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.62 (s, 1H), 8.50 (d, *J* = 6.6 Hz, 1H), 8.07 (d, *J* = 8.8 Hz, 1H), 7.91 (d, *J* = 7.7 Hz, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.50 – 7.40 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.56, 159.70, 150.66, 139.88, 134.80, 134.31, 130.55, 129.85, 128.68, 127.65, 127.15, 126.66, 123.77. IR (KBr): 3067, 2967, 1617, 1549, 780, 760, 716 cm^{-1}. MS (EI, m/z): 240.10 $[M]^+$.

(9) 2-(4-bromophenyl)quinazoline **(3ai)**



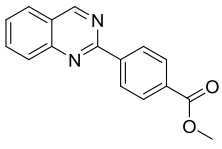
Pale yellow solid, (106 mg, 75% Yield), m.p.: 121-122°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 1H), 8.49 (d, *J* = 8.3 Hz, 2H), 8.05 (d, *J* = 8.8 Hz, 1H), 7.89 (t, *J* = 7.2 Hz, 2H), 7.69 – 7.55 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.52, 160.12, 150.70, 137.00, 134.25, 131.79, 130.17, 128.64, 127.48, 127.16, 125.42, 123.66. IR (KBr): 3066, 2926, 1618, 1549, 1407, 796, 724 cm^{-1}. MS (EI, m/z): 284.03 $[M]^+$.

(10) 2-(4-(trifluoromethyl)phenyl)quinazoline **(3aj)**



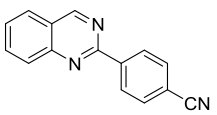
Pale yellow solid, (68.5 mg, 50% Yield), m.p.: 143-145°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.46 (s, 1H), 8.73 (d, *J* = 8.1 Hz, 2H), 8.10 (d, *J* = 8.8 Hz, 1H), 7.92 (t, *J* = 7.6 Hz, 2H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.64 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.60, 159.60, 150.66, 141.32, 134.37, 132.29, 131.97, 128.84, 128.78, 127.86, 127.16, 125.59, 125.50 (q, $J_{C\text{-}F}$ = 3.8 Hz), 123.84. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.65. IR (KBr): 3067, 2967, 1616, 1550, 1326, 1109, 855 cm^{-1}. MS (EI, m/z): 274.17 $[M]^+$.

(11) methyl 4-(quinazolin-2-yl)benzoate **(3ak)**



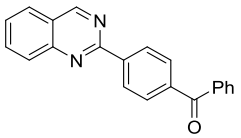
White solid, (101 mg, 77% Yield), m.p.: 162-163°C (Yamaguchi et al., 2016); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.49 (s, 1H), 8.70 (d, *J* = 8.3 Hz, 2H), 8.20 (d, *J* = 8.3 Hz, 2H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.94 (t, *J* = 9.0 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 3.96 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.95, 160.56, 160.01, 150.69, 142.15, 134.31, 131.72, 129.85, 128.78, 128.50, 127.79, 127.15, 123.77, 52.20. IR (KBr): 3062, 2968, 1720, 1619, 1549, 1286, 1113, 770, 711 cm^{-1}. MS (EI, m/z): 264.16 $[M]^+$.

(12) 4-(quinazolin-2-yl)benzonitrile **(3al)**



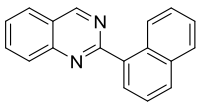
Pale yellow solid, (84.3 mg, 73% Yield), m.p.: 194-196°C (Yamaguchi et al., 2016); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.52 (s, 1H), 8.77 (d, *J* = 8.2 Hz, 2H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.98 (t, *J* = 8.2 Hz, 2H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.71 (t, *J* = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.68, 159.08, 150.62, 142.13, 134.54, 132.37, 129.02, 128.82, 128.18, 127.21, 123.89, 118.89, 113.81. IR (KBr): 3065, 2968, 2225, 1616, 1546, 1429, 852, 799 cm^{-1}. MS (EI, m/z): 231.15 $[M]^+$.

(13) phenyl(4-(quinazolin-2-yl)phenyl)methanone **(3am)**



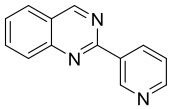
Pale yellow solid, (106.1 mg, 68% Yield), m.p.: 167-168°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.51 (s, 1H), 8.76 (d, *J* = 8.1 Hz, 2H), 8.13 (d, *J* = 8.3 Hz, 1H), 7.96 (dd, *J* = 16.0, 8.5 Hz, 4H), 7.88 (d, *J* = 7.5 Hz, 2H), 7.70 – 7.58 (m, 2H), 7.53 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.55, 160.63, 160.04, 150.72, 141.65, 139.06, 137.62, 134.37, 132.58, 130.36, 130.13, 128.80, 128.44, 128.37, 127.85, 127.20, 123.80. IR (KBr): 3061, 1656, 1577, 1274, 926, 861, 751, 706 cm^{-1}. MS (EI, m/z): 310.12 $[M]^+$.

(14) 2-(naphthalen-1-yl)quinazoline **(3an)**



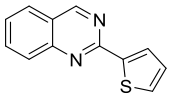
Pale yellow solid, (87.0 mg, 68% Yield), m.p.: 125-126°C (Ma et al., 2017); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.56 (s, 1H), 8.72 (d, *J* = 8.2 Hz, 1H), 8.17 (t, *J* = 8.0 Hz, 2H), 8.02 – 7.87 (m, 4H), 7.63 (dd, *J* = 17.6, 7.9 Hz, 2H), 7.58 – 7.47 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.49, 160.44, 150.60, 136.34, 134.35, 134.24, 131.28, 130.44, 129.71, 128.68, 128.54, 127.77, 127.17, 126.91, 125.99, 125.94, 125.35, 123.16. IR (KBr): 3053, 2967, 1618, 1551, 1467, 1429, 972, 760 cm^{-1}. MS (EI, m/z): 256.13 $[M]^+$.

(15) 2-(pyridin-3-yl)quinazoline **(3ao)**



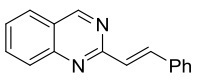
White solid, (67.2 mg, 65% Yield), m.p.: 94-95°C (Ma et al., 2017); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.83 (s, 1H), 9.47 (s, 1H), 8.87 (d, *J* = 7.9 Hz, 1H), 8.75 (s, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.93 (t, *J* = 8.1 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.46 (dd, *J* = 7.7, 4.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.65, 159.13, 151.12, 150.60, 150.20, 135.84, 134.40, 133.57, 128.64, 127.80, 127.19, 123.81, 123.43. IR (KBr): 3055, 2924, 2792, 1617, 1549, 1427, 1292, 759, 710 cm^{-1}. MS (EI, m/z): 207.13 $[M]^+$.

(16) 2-(thiophen-2-yl)quinazoline **(3ap)**



Pale yellow solid, (60.4 mg, 57% Yield), m.p.: 133-134°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 8.15 (d, *J* = 3.6 Hz, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.86 (dd, *J* = 7.2, 5.1 Hz, 2H), 7.60 – 7.46 (m, 2H), 7.19 (t, *J* = 4.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.56, 157.88, 150.64, 143.84, 134.39, 129.98, 129.28, 128.40, 128.21, 127.29, 127.03, 123.40. IR (KBr): 3065, 2966, 2789, 1616, 1551, 1425, 713 cm^{-1}. MS (EI, m/z): 212.08 $[M]^+$.

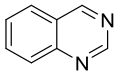
(17) (*E*)-2-styrylquinazoline **(3aq)**



White solid, (53.3 mg, 46% Yield), m.p.: 120-121°C (Han et al., 2012); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.38 (s, 1H), 8.17 (d, *J* = 16.0 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.89 (t, *J* = 7.7 Hz, 2H), 7.69 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.46 – 7.38 (m, 3H), 7.38 – 7.33 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.33, 160.25, 150.61,

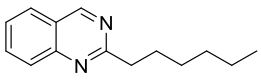
138.60, 136.24, 134.22, 129.07, 128.83, 128.15, 127.94, 127.70, 127.23, 127.16, 123.39. IR (KBr): 3057, 2966, 1613, 1550, 1376, 1234, 980, 750 cm^{-1}. MS (EI, m/z): 232.15 $[M]^+$.

(18) quinazoline **(3ar)**



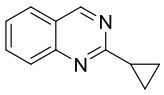
Brown solid, (31.2 mg, 48% Yield), m.p.: 45-46°C (Zhang et al., 2015); ^1H NMR (400 MHz, $CDCl_3$) δ 9.41 (s, 1H), 9.35 (s, 1H), 8.06 (d, *J* = 8.7 Hz, 1H), 7.93 (t, *J* = 7.0 Hz, 2H), 7.68 (t, *J* = 7.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.22, 155.24, 150.00, 134.19, 128.39, 127.95, 127.19, 125.09. IR (KBr): 3060, 2969, 1619, 1567, 1488, 1377, 754 cm^{-1}. MS (EI, m/z): 130.05 $[M]^+$.

(19) 2-hexylquinazoline **(3as)**



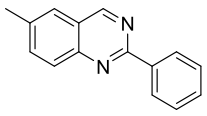
Pale yellow oil liquid (Zhang et al., 2015), (64.2 mg, 60% Yield); ^1H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 7.90 (d, *J* = 8.5 Hz, 1H), 7.80 (t, *J* = 7.5 Hz, 2H), 7.51 (t, *J* = 7.0 Hz, 1H), 3.04 (t, *J* = 7.7 Hz, 2H), 1.84 (dt, *J* = 15.0, 7.6 Hz, 2H), 1.40 – 1.22 (m, 6H), 0.81 (d, *J* = 6.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.96, 160.38, 150.38, 133.97, 127.89, 127.07, 126.89, 123.07, 40.04, 31.71, 29.23, 28.98, 22.56, 14.05. IR (KBr): 3063, 2959, 2927, 2858, 1619, 1529, 1466, 1428, 1232, 1141, 966, 753 cm^{-1}. MS (EI, m/z): 214.15 $[M]^+$.

(20) 2-cyclopropylquinazoline **(3at)**



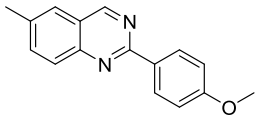
Pale yellow oil liquid (Zhang et al., 2015), (52.7 mg, 62% Yield); ^1H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.80 (t, *J* = 8.5 Hz, 2H), 7.48 (t, *J* = 7.5 Hz, 1H), 2.47 – 2.34 (m, 1H), 1.32 – 1.23 (m, 2H), 1.16 – 1.07 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.29, 160.22, 150.29, 133.86, 127.43, 127.00, 126.19, 123.14, 18.55, 10.60. IR (KBr): 3061, 3008, 1620, 1585, 1570, 1413, 1376, 758 cm^{-1}. MS (EI, m/z): 170.10 $[M]^+$.

(21) 6-methyl-2-phenylquinazoline **(3ba)**



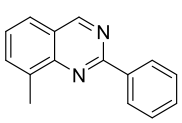
Pale yellow solid (85.8 mg, 78% Yield), m.p.: 129-130°C (Chen et al., 2014); ^1H NMR (400 MHz, $CDCl_3$) δ 9.30 (s, 1H), 8.52 (d, *J* = 7.3 Hz, 2H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.65 (d, *J* = 8.7 Hz, 1H), 7.59 (s, 1H), 7.50 – 7.35 (m, 3H), 2.48 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.40, 159.74, 149.36, 138.20, 137.43, 136.39, 130.41, 128.62, 128.46, 128.28, 125.79, 123.60, 21.64. IR (KBr): 3060, 2967, 2791, 1526, 1427, 831, 760 cm^{-1}. MS (EI, m/z): 220.18 $[M]^+$.

(22) 2-(4-methoxyphenyl)-6-methylquinazoline **(3bd)**



Pale yellow solid (100 mg, 80% Yield), m.p.: 119-120°C (Han et al., 2012); ^1H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.54 (d, *J* = 8.8 Hz, 2H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.65 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.57 (s, 1H), 7.02 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H), 2.50 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.69, 160.21, 159.64, 149.39, 136.85, 136.27, 130.90, 130.05, 128.05, 125.80, 123.30, 113.95, 55.35, 21.56. IR (KBr): 3047, 2962, 1602, 1552, 1514, 1425, 1244, 1026, 851, 827 cm^{-1}. MS (EI, m/z): 250.15 $[M]^+$.

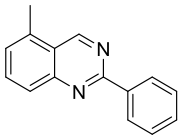
(23) 8-methyl-2-phenylquinazoline **(3ca)**



Pale yellow solid (69.3 mg, 63% Yield), m.p.: 59-60°C (Gopalaiah et al., 2017); ^1H NMR (400 MHz, $CDCl_3$) δ 9.41 (s, 1H), 8.67 (d, *J* = 6.7 Hz, 2H), 7.79 – 7.68 (m, 2H), 7.57 – 7.44 (m, 4H), 2.86 (s, 3H). ^{13}C NMR (101 MHz,

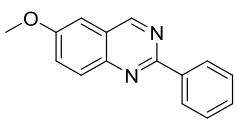
$CDCl_3$) δ 160.58, 159.98, 149.76, 138.42, 137.17, 133.87, 130.47, 128.60, 128.55, 126.93, 124.82, 123.55, 16.94. IR (KBr): 3064, 2967, 2791, 1528, 1468, 1427, 953, 760 cm^{-1}. MS (EI, m/z): 220.17 $[M]^+$.

(24) 5-methyl-2-phenylquinazoline **(3da)**



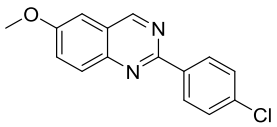
Pale yellow solid (58.3 mg, 53% Yield), m.p.: 115-117°C (Cheng et al., 2016); ^1H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.62 (d, *J* = 7.6 Hz, 2H), 7.93 (d, *J* = 8.5 Hz, 1H), 7.77 (t, *J* = 7.8 Hz, 1H), 7.58 – 7.47 (m, 3H), 7.38 (d, *J* = 7.0 Hz, 1H), 2.79 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.69, 157.54, 151.28, 138.07, 135.49, 133.98, 130.54, 128.63, 128.55, 127.85, 126.85, 122.76, 17.56. IR (KBr): 3059, 2966, 2796, 1525, 1467, 1427, 755, 703 cm^{-1}. MS (EI, m/z): 220.16 $[M]^+$.

(25) 6-methoxy-2-phenylquinazoline **(3ea)**



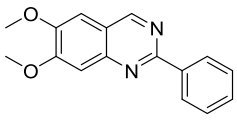
Pale yellow solid (100 mg, 85% Yield), m.p.: 120-121°C (Ma et al., 2017); ^1H NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.47 (d, *J* = 7.2 Hz, 2H), 7.87 (d, *J* = 9.1 Hz, 1H), 7.39 (dd, *J* = 17.8, 7.2 Hz, 4H), 6.99 (s, 1H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.39, 158.80, 158.25, 147.00, 138.23, 130.18, 130.13, 128.60, 128.22, 127.14, 124.47, 103.92, 55.69. IR (KBr): 3060, 2966, 2790, 1621, 1529, 1427, 1223, 1161, 1026, 834, 761 cm^{-1}. MS (EI, m/z): 236.16 $[M]^+$.

(26) 2-(4-chlorophenyl)-6-methoxyquinazoline **(3eg)**



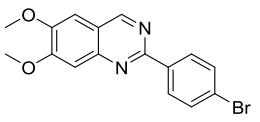
White solid (123 mg, 91% Yield), m.p.: 174-175°C (Cheng et al., 2016); ^1H NMR (400 MHz, $CDCl_3$) δ 9.29 (s, 1H), 8.50 (d, *J* = 8.6 Hz, 2H), 7.94 (d, *J* = 9.2 Hz, 1H), 7.53 (dd, *J* = 9.2, 2.7 Hz, 1H), 7.47 (s, 1H), 7.45 (s, 1H), 7.10 (d, *J* = 2.7 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.78, 158.40, 158.33, 146.90, 136.69, 136.33, 130.08, 129.52, 128.74, 127.30, 124.51, 103.93, 55.72. IR (KBr): 3065, 2966, 2790, 1531, 1469, 1428, 1318, 1223, 948, 837 cm^{-1}. MS (EI, m/z): 270.10 $[M]^+$.

(27) 6,7-dimethoxy-2-phenylquinazoline **(3fa)**



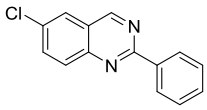
White solid (113 mg, 85% Yield), m.p.: 176-177°C (Gopalaiah et al., 2017); ^1H NMR (400 MHz, $CDCl_3$) δ 9.19 (s, 1H), 8.54 (d, *J* = 7.4 Hz, 2H), 7.57 – 7.42 (m, 3H), 7.35 (s, 1H), 7.06 (s, 1H), 4.06 (s, 3H), 4.01 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.92, 157.09, 156.22, 150.35, 148.61, 138.39, 130.12, 128.57, 128.14, 119.40, 106.87, 103.95, 56.44, 56.20. IR (KBr): 3061, 2966, 1619, 1500, 1412, 1229, 1155, 855, 759 cm^{-1}. MS (EI, m/z): 266.13 $[M]^+$.

(28) 2-(4-bromophenyl)-6,7-dimethoxyquinazoline **(3fi)**



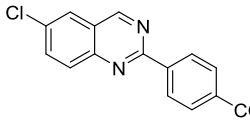
White solid, (129 mg, 75% Yield), m.p.: 157-159°C (unknown compound); ^1H NMR (400 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.32 (d, *J* = 8.5 Hz, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 7.24 (s, 1H), 6.98 (s, 1H), 3.98 (s, 3H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.90, 157.02, 156.37, 150.54, 148.53, 137.30, 131.67, 129.71, 124.78, 119.48, 106.79, 103.94, 56.46, 56.23. IR (KBr): 3071, 2965, 1615, 1498, 1421, 1230, 1154, 842 cm^{-1}. MS (EI, m/z): 344.08 $[M]^+$. HRMS (ESI): Calcd. for $C_{16}H_{14}BrN_2O_2$ $[M+H]^+$: 345.0233; found: 345.0235.

(29) 6-chloro-2-phenylquinazoline **(3ga)**



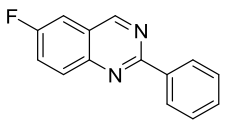
Pale yellow solid (69.6 mg, 58% Yield), m.p.: 157-158°C (Chen et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.39 (s, 1H), 8.60 (dd, *J* = 7.4, 2.1 Hz, 2H), 8.03 (d, *J* = 9.0 Hz, 1H), 7.89 (d, *J* = 2.2 Hz, 1H), 7.82 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.57 – 7.48 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.31, 159.50, 149.27, 137.61, 135.08, 132.81, 130.89, 130.41, 128.70, 128.62, 125.83, 124.00. IR (KBr): 3064, 2967, 1613, 1542, 1430, 837 cm^{-1}. MS (EI, m/z): 240.10 $[M]^+$.

(30) methyl 4-(6-chloroquinazolin-2-yl)benzoate **(3gk)**



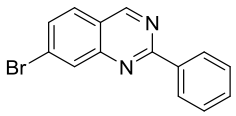
Pale yellow solid (81.9 mg, 55% Yield), m.p.: 198-199°C (unknown compound); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.70 (d, *J* = 7.8 Hz, 2H), 8.22 (d, *J* = 7.9 Hz, 2H), 8.08 (d, *J* = 9.1 Hz, 1H), 7.96 (s, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 3.99 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.87, 160.26, 159.58, 149.17, 141.65, 135.32, 133.42, 131.96, 130.52, 129.88, 128.50, 125.86, 124.17, 52.25. IR (KBr): 3066, 2966, 1539, 1473, 1429, 1374, 1277, 1107, 832, 765, 715 cm^{-1}. MS (EI, m/z): 298.12 $[M]^+$. HRMS (ESI): Calcd. for $C_{16}H_{12}ClN_2O_2$ $[M+H]^+$: 299.0582; found: 299.0579.

(31) 6-fluoro-2-phenylquinazoline **(3ha)**



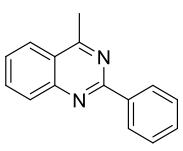
Pale yellow solid (62.7 mg, 56% Yield), m.p.: 140-141°C (Malakar et al., 2012); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 1H), 8.59 (d, *J* = 7.3 Hz, 2H), 8.10 (dd, *J* = 9.2, 5.0 Hz, 1H), 7.67 (td, *J* = 8.9, 2.3 Hz, 1H), 7.58 – 7.48 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ160.44 (d, $J_{C\text{-}F}$ = 251.0 Hz), 160.77, 159.79 (d, $J_{C\text{-}F}$ = 5.5 Hz), 147.98, 137.76, 131.41 (d, $J_{C\text{-}F}$ = 8.6 Hz), 130.70, 128.68, 128.49, 124.51 (d, $J_{C\text{-}F}$ = 25.8 Hz), 123.94 (d, $J_{C\text{-}F}$ = 9.3 Hz), 110.14 (d, $J_{C\text{-}F}$ = 21.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.69. IR (KBr): 3056, 2967, 1531, 1430, 1373, 1286, 837 cm^{-1}. MS (EI, m/z): 224.14 $[M]^+$.

(32) 7-bromo-2-phenylquinazoline **(3ia)**



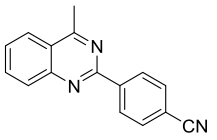
Pale yellow solid (71 mg, 50% Yield), m.p.: 125-127°C (Wang et al., 2014); ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.60 (dd, *J* = 7.3, 2.2 Hz, 2H), 8.29 (s, 1H), 7.79 (d, *J* = 8.6 Hz, 1H), 7.70 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.58 – 7.48 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.83, 160.31, 151.44, 137.58, 131.18, 131.01, 130.98, 128.95, 128.73, 128.70, 128.30, 122.17, 77.35, 77.03, 76.71. IR (KBr): 3066, 2966, 1540, 1428, 1379, 1319, 935, 759, 700 cm^{-1}. MS (EI, m/z): 284.06 $[M]^+$.

(33) 4-methyl-2-phenylquinazoline **(3ja)**



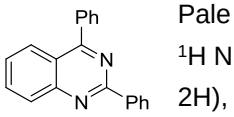
Pale yellow solid (84.7 mg, 77% Yield), m.p.: 89-90°C (Gopalaiah et al., 2017); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 7.4 Hz, 2H), 8.10 (d, *J* = 8.3 Hz, 2H), 7.87 (t, *J* = 7.7 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.56 – 7.46 (m, 3H), 3.03 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.23, 160.21, 150.43, 138.34, 133.51, 130.39, 129.27, 128.57, 126.86, 124.98, 123.03, 22.02. IR (KBr): 3063, 2966, 1616, 1547, 1430, 1338, 757, 708 cm^{-1}. MS (EI, m/z): 220.16 $[M]^+$.

(34) 4-(4-methylquinazolin-2-yl)benzonitrile **(3jl)**



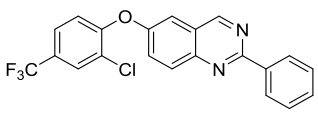
Brown solid (67.3 mg, 55% Yield), m.p.: 195-197°C (Yu et al., 2017); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 7.7 Hz, 2H), 8.11 – 7.99 (m, 2H), 7.84 (t, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 7.8 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 2.97 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.66, 158.15, 150.20, 142.42, 133.91, 132.27, 129.40, 128.99, 127.77, 125.06, 123.28, 118.98, 113.56, 21.97. IR (KBr): 3064, 2966, 2921, 2790, 2225, 1535, 1469, 1428, 854, 759 cm^{-1}. MS (EI, m/z): 245.15 $[M]^+$.

(35) 2,4-diphenylquinazoline **(3ka)**



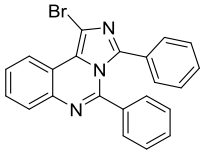
Pale yellow solid, (88.8 mg, 63% Yield), m.p.: 116-118°C (Cheng et al., 2016); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 7.3 Hz, 2H), 8.11 (dd, *J* = 17.7, 8.4 Hz, 2H), 7.91 – 7.80 (m, 3H), 7.61 – 7.45 (m, 7H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.34, 160.29, 152.06, 138.30, 137.76, 133.55, 130.55, 130.25, 129.95, 129.22, 128.75, 128.58, 127.03, 121.74. IR (KBr): 3060, 2966, 1559, 1536, 1440, 1338, 769, 702 cm^{-1}. MS (EI, m/z): 282.15 $[M]^+$.

(36) 6-(2-chloro-4-(trifluoromethyl)phenoxy)-2-phenylquinazoline **(3la)**



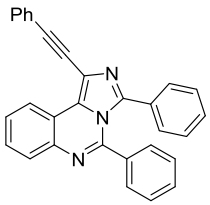
Pale yellow solid, (136 mg, 68% Yield), m.p.: 142-143°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.34 (s, 1H), 8.59 (d, *J* = 7.1 Hz, 2H), 8.13 (d, *J* = 9.1 Hz, 1H), 7.82 (s, 1H), 7.68 (d, *J* = 9.1 Hz, 1H), 7.59 – 7.46 (m, 4H), 7.27 (s, 1H), 7.17 (d, *J* = 8.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.68, 159.57, 154.61, 154.48, 148.06, 137.80, 131.29, 130.67, 128.68, 128.62, 128.58, 128.48, 127.21, 126.69, 125.51 (q, J_{C-F} = 4.0 Hz), 124.08, 120.96, 112.02. IR (KBr): 3060, 1562, 1537, 1486, 1340, 771, 702 cm^{-1}. HRMS (ESI): Calcd. for $C_{21}H_{13}ClF_3N_2O$ $[M+H]^+$: 401.0663; found: 401.0664.

(37) 1-bromo-3,5-diphenylimidazo[1,5-c]quinazoline **(4ja)**



Yellow solid, (95.7 mg, 48% Yield), m.p.: 229 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 7.4 Hz, 1H), 7.89 (d, *J* = 7.4 Hz, 1H), 7.65 – 7.53 (m, 2H), 7.30 (d, *J* = 7.7 Hz, 2H), 7.20 – 6.97 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.63, 141.80, 138.54, 133.45, 130.55, 130.13, 129.28, 128.87, 128.72, 128.50, 128.48, 128.27, 127.85, 127.54, 125.61, 121.69, 118.93, 109.04. MS (EI, m/z): 399.05 $[M]^+$.

(38) 3,5-diphenyl-1-(phenylethynyl)imidazo[1,5-c]quinazoline **(5ja)**



Yellow solid, (151 mg, 72% Yield), m.p.: 201-202°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, *J* = 7.2 Hz, 1H), 7.92 (d, *J* = 7.1 Hz, 1H), 7.70 (d, *J* = 6.9 Hz, 2H), 7.66 – 7.57 (m, 2H), 7.45 – 7.37 (m, 3H), 7.33 (d, *J* = 7.4 Hz, 2H), 7.22 – 7.12 (m, 3H), 7.12 – 6.99 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.10, 142.39, 138.90, 133.52, 131.57, 131.51, 130.87, 130.08, 129.31, 129.28, 128.77, 128.66, 128.56, 128.53, 128.42, 128.05, 127.81, 127.49, 123.18, 122.46, 119.61, 116.48, 94.53, 83.93. IR (KBr): 3061, 2219, 1548, 1477, 1330, 758, 697 cm^{-1}. HRMS (ESI): Calcd. for $C_{30}H_{20}N_3$ $[M+H]^+$: 422.1652; found: 422.1649.

Data S4. Cartesian coordinates. Related to **Figure 2**, **Figure 3**, **Figure S99**, **Figure S100** and **Scheme S4**, **Scheme S5**, **Scheme S6**, **Scheme S7** & **Scheme S8**.

69

Ir-O1 SCF Done: E(RM06) = -1490.22403005

C	0.65556600	-1.93376900	-1.77003100
C	-0.73969600	-1.66490900	-1.98479000
C	-1.50812100	-2.38720600	-0.96538800
C	0.76498600	-2.63814500	-0.50448600
C	-0.59464200	-2.95550500	-0.06758300
C	-1.34097600	-1.02188500	-3.20154700
H	-0.64607300	-0.32065600	-3.67298000
H	-1.61076000	-1.77852000	-3.95271200
H	-2.25318800	-0.47040300	-2.95331300
C	-2.99799000	-2.54865800	-0.95585700
H	-3.28965700	-3.44228100	-1.52770800
H	-3.38850100	-2.66338300	0.05928500
H	-3.49915500	-1.69072400	-1.40803600
C	-0.88421300	-3.69010000	1.20135100
H	-0.45951100	-4.70250900	1.17972100
H	-0.42448200	-3.14518600	2.03556000
H	-1.95757700	-3.77630200	1.39228600
C	1.99397000	-3.26943400	0.08485300
H	1.99346400	-4.35820700	-0.06901200
H	2.90807900	-2.88163700	-0.37359200
H	2.05243100	-3.08346300	1.16265500
C	1.77339200	-1.65298600	-2.72979500
H	1.54811000	-0.79843000	-3.37468000
H	2.71232100	-1.43705400	-2.21353900
H	1.94080600	-2.52602800	-3.37663500
C	-4.42583800	0.67558800	0.05254100
C	-2.30937800	1.52996500	-0.23579400
C	-2.83932200	2.83844800	-0.46984800
C	-4.24097500	3.00504400	-0.43793600
C	-5.04851600	1.91971700	-0.17424900
H	-5.03357500	-0.20135500	0.27072800
C	-1.93409000	3.90327400	-0.71657900
H	-4.66032600	3.99201600	-0.61723800
H	-6.12955600	2.00679400	-0.13631100
C	-0.59314200	3.64761300	-0.71326600
C	-0.10681600	2.32919100	-0.47845300
H	-2.31745800	4.90370600	-0.89930900
H	0.11568100	4.44655800	-0.89459200
N	-3.11684800	0.47825000	0.02099300
N	-0.95089900	1.29188200	-0.25047700
C	1.29848200	1.98906600	-0.44272700
C	2.34085200	2.92536300	-0.56779000
C	3.66886600	2.53928100	-0.45344900
C	3.95908700	1.18780200	-0.18614000
C	2.92527200	0.24967000	-0.06170500
C	1.58306700	0.61133500	-0.21370000
H	2.12593000	3.97506100	-0.74748500
H	4.45634100	3.27670700	-0.55400100
H	3.20903300	-0.77194100	0.16540300
Ir	0.01183500	-0.62795300	-0.12390700
O	5.22037400	0.69808000	-0.03426700
C	6.31848700	1.59606100	-0.12929400
H	6.26694300	2.38166500	0.63547200
H	7.21318100	0.99233800	0.03877100
H	6.37997500	2.05872500	-1.12305800
C	-1.67851400	-0.39160200	3.22323900
H	-1.83556400	-1.46554200	3.38284100
H	-2.24044000	-0.10300400	2.32981800
H	-2.10217300	0.14185100	4.08571700
C	-0.17546200	-0.09136700	3.04474400
C	0.05254800	1.43403400	3.00607200
H	-0.54687400	1.91010000	2.22561400
H	-0.22134000	1.89902400	3.96293500
H	1.10797600	1.65183300	2.81010100
C	0.59489300	-0.65879400	4.25916200
H	0.48000700	-1.74796900	4.30631700
H	1.66431600	-0.43628700	4.16660900
H	0.23323000	-0.23384300	5.20516400
O	0.36721400	-0.76092400	1.92891100

18

1a SCF Done: E(RM06) = -551.095580062

C	-1.23151900	-1.36260700	-0.19493900
C	-0.11523500	-0.55241700	0.03399600
C	-0.21816400	0.83818100	0.24400100
C	-1.51230800	1.37344000	0.20371000
C	-2.63652700	0.58434400	-0.03929000
C	-2.49724400	-0.78993800	-0.24163500
H	-1.09027200	-2.42641500	-0.34030000
H	-1.63302700	2.44051500	0.36866500
H	-3.62057100	1.04338400	-0.06885400
H	-3.36529000	-1.41297700	-0.43335100
O	1.18923900	-2.45142700	0.27175600
N	1.18112600	-1.24143000	0.05600700
O	2.21251400	-0.58673800	-0.15254500
C	0.95127800	1.77650300	0.51148100
H	1.60035100	1.36103800	1.29404200
H	0.54884600	2.72195700	0.88662200
O	1.68521300	2.09806900	-0.65823100
H	2.15466900	1.27824100	-0.89064900

87

IN1 SCF Done: E(RM06) = -2041.32132465

C	2.79540100	-0.66819000	-2.22001400
C	2.00676600	0.52486300	-2.40361500
C	0.65792400	0.08049200	-2.61546000
C	1.95608100	-1.83676900	-2.55362500
C	0.65480500	-1.37795200	-2.78811800
C	2.49546200	1.94238600	-2.40620400
H	3.42670100	2.04310300	-1.84134800
H	2.69160200	2.27193600	-3.43631900
H	1.75762500	2.61245500	-1.95804900
C	-0.52596400	0.93760900	-2.93464100
H	-0.72586400	0.88123000	-4.01517300
H	-1.42950300	0.59263600	-2.42195800
H	-0.36028800	1.98362500	-2.67713000
C	-0.54626200	-2.16556900	-3.21646400
H	-0.73334300	-2.01082400	-4.28854100

H	-0.41495100	-3.23922500	-3.05914600
H	-1.45094500	-1.84958400	-2.68735800
C	2.47283100	-3.23482700	-2.70011400
H	2.88697800	-3.36925600	-3.70976100
H	3.27873600	-3.44999400	-1.99312700
H	1.68935200	-3.98490900	-2.56428300
C	4.28248200	-0.72094000	-2.04235000
H	4.65396100	0.16295900	-1.51868100
H	4.59190500	-1.60464300	-1.47559700
H	4.77825100	-0.76487100	-3.02265200
C	-2.14200400	4.87588100	-2.16031000
C	-1.05970900	3.66778600	-0.52794400
C	-2.09070800	3.96122600	0.41843800
C	-3.17973100	4.76151200	-0.00170100
C	-3.20789300	5.22616600	-1.29688400
H	-2.14989800	5.23055300	-3.19073100
C	-1.95290700	3.41990700	1.72275000
H	-3.97549100	4.99622300	0.70174900
H	-4.02204200	5.84398000	-1.66294600
C	-0.84271900	2.67594000	2.02459700
C	0.16152700	2.45775200	1.02560900
H	-2.72887000	3.59877300	2.46375600
H	-0.71634600	2.23134200	3.00420900
N	-1.10978200	4.13180200	-1.80885700
N	0.03329500	2.92076500	-0.20940500
C	1.44189600	1.80390300	1.42916800
C	2.08742000	2.42561400	2.51318000
C	3.32385800	2.01176700	3.00326300
C	3.93416800	0.91336200	2.39396300
C	3.28807900	0.26549400	1.33231800
C	2.04683200	0.67170600	0.81499000
H	1.61602600	3.28923900	2.97687700
H	3.78321400	2.54119100	3.83020000
H	3.79036100	-0.60894000	0.93015700
Ir	1.33980500	-0.60987400	-0.64390900
O	5.14204400	0.39022100	2.76297500
C	5.82591400	0.99419700	3.85056700
H	5.24128400	0.94138100	4.77886500
H	6.75017300	0.42564600	3.97886500
H	6.07694100	2.04301200	3.64203900
C	0.09527600	-3.23633700	2.60274300
H	-0.90794600	-2.80928600	2.68868200
H	0.73957600	-2.73823400	3.33584800
H	0.04088200	-4.30159700	2.85817400
C	0.65838400	-3.04200100	1.18343700
C	2.06925400	-3.64995200	1.12377200
H	2.71915200	-3.16770100	1.86196800
H	2.04369000	-4.72563600	1.33884000
H	2.51669400	-3.51254300	0.13450600
C	-0.26428900	-3.71553000	0.15955500
H	-1.27349400	-3.29132000	0.20420900
H	0.11724300	-3.58192000	-0.85587000
H	-0.34436500	-4.79255800	0.35257100
O	0.75662400	-1.62141700	0.97360400
C	-5.24100600	-1.85077400	3.15232400
C	-4.03441300	-1.32885000	2.69044100
C	-3.80349000	-1.07950400	1.33003900
C	-4.86224300	-1.39539900	0.45099000
C	-6.07588700	-1.92946200	0.90084200
C	-6.27025500	-2.15332600	2.25703100
H	-5.37732800	-2.02362200	4.21658400
H	-3.23057400	-1.10195200	3.38001200
H	-6.84583100	-2.15924800	0.17530900
H	-7.21279100	-2.56093300	2.60962600
C	-2.46141500	-0.48944300	0.91716100
H	-2.04270200	-1.06557600	0.08676100
H	-2.63674600	0.52103100	0.52243000
O	-1.56497600	-0.44607000	2.00631800
H	-0.69474500	-0.79201600	1.69393900
N	-4.74514900	-1.19445900	-0.99668200
O	-3.76761800	-0.57120800	-1.42688500
O	-5.62739900	-1.65238000	-1.72605000

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TS1 SCF Done: E(RM06) = -2041.30885579

C	2.67403100	-0.66227900	-2.10613200
C	1.79289400	0.44018300	-2.45617000
C	0.49698700	-0.12884200	-2.71119900
C	1.93560000	-1.90526400	-2.35065300
C	0.61325000	-1.58849600	-2.70083300
C	2.17766500	1.87968400	-2.62402400
H	3.03411700	2.14000500	-1.99619700
H	2.45582600	2.07262900	-3.67000400
H	1.35100600	2.54218500	-2.35622500
C	-0.70786700	0.60320700	-3.21170600
H	-0.71729500	0.57596400	-4.31168000
H	-1.63636600	0.13343000	-2.87120600
H	-0.72276900	1.64628300	-2.89552900
C	-0.47980300	-2.53968800	-3.08906000
H	-0.54564800	-2.62400100	-4.18339100
H	-0.30842600	-3.54560700	-2.69457800
H	-1.45967300	-2.20601600	-2.73656400
C	2.55735000	-3.26760200	-2.32482100
H	3.10662300	-3.42726800	-3.26402900
H	3.27860000	-3.37909100	-1.51140800
H	1.81581200	-4.06571400	-2.24022500
C	4.16479500	-0.58164900	-1.95030000
H	4.47546500	0.38127700	-1.53791800
H	4.54858400	-1.36598700	-1.28995700
H	4.65840700	-0.70073400	-2.92577800
C	-3.27220400	4.00356300	-2.49850100
C	-1.84170000	3.29931900	-0.83637300
C	-2.80185400	3.63482800	0.17026100
C	-4.04583900	4.17191100	-0.23677800
C	-4.28741200	4.35959400	-1.57876700
H	-3.44273000	4.14789500	-3.56527300
C	-2.43574200	3.41049600	1.52185600
H	-4.78929100	4.43003100	0.51415700
H	-5.22609600	4.77029300	-1.93750900
C	-1.19371900	2.90563900	1.79946200
C	-0.28671800	2.60107900	0.73067500
H	-3.14220800	3.64104800	2.31621800
H	-0.88386700	2.71838500	2.82198800
N	-2.10114600	3.49700400	-2.16012500
N	-0.61666700	2.78386300	-0.53965300
C	1.09946800	2.17880500	1.08435500

C	1.75261100	3.03977800	1.98648000
C	3.06392300	2.84546500	2.41380400
C	3.74657200	1.72519800	1.93424300
C	3.10118900	0.84862300	1.05263800
C	1.78784900	1.03315100	0.59426700
H	1.22248100	3.91811700	2.34790500
H	3.52318900	3.55287100	3.09482000
H	3.66295200	-0.02584800	0.74465100
Ir	1.11007500	-0.48192400	-0.63305700
O	5.03085500	1.39354400	2.26836700
C	5.72405200	2.23878500	3.17320100
H	5.22180300	2.28996500	4.14876800
H	6.71329700	1.79360700	3.30495400
H	5.83986600	3.25580200	2.77439300
C	0.98580100	-2.97610700	3.20122800
H	-0.08819200	-2.78235600	3.30899800
H	1.52680100	-2.23871800	3.80413900
H	1.19168900	-3.97470000	3.60666700
C	1.41257600	-2.87307400	1.72473600
C	2.92281800	-3.12468700	1.61596600
H	3.47097800	-2.40270300	2.23059700
H	3.18389500	-4.13488500	1.95508700
H	3.26454800	-3.01473200	0.58229700
C	0.62229200	-3.89103200	0.88683700
H	-0.45678400	-3.76519600	1.03924800
H	0.83131600	-3.75804700	-0.17846700
H	0.87738600	-4.92239400	1.16082100
O	1.13904100	-1.53200300	1.31882800
C	-3.75571200	-0.67117900	3.45917500
C	-2.81461800	-0.58062000	2.43459000
C	-3.01167100	-1.18903600	1.18734400
C	-4.21997800	-1.90115500	1.02709000
C	-5.16945700	-2.00685900	2.04950700
C	-4.93998500	-1.38697600	3.27083900
H	-3.56070200	-0.18055900	4.40902000
H	-1.89616500	-0.02622500	2.58281600
H	-6.07331000	-2.57356800	1.86512500
H	-5.67709400	-1.46262300	4.06440600
C	-1.92351900	-1.06316900	0.12477100
H	-1.68532000	-2.05885700	-0.27055500
H	-2.30368600	-0.47587800	-0.71616700
O	-0.77012700	-0.42049300	0.62820600
H	-0.06474900	-1.10295100	1.21898000
N	-4.55348300	-2.57466400	-0.23293500
O	-3.86584400	-2.32981700	-1.22965400
O	-5.51073600	-3.35122200	-0.24538600

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IN2 SCF Done: E(RM06) = -1807.74615465

C	3.15928400	0.45314100	1.03261300
C	3.16524100	-0.96201500	0.78496000
C	2.40406800	-1.61480800	1.85404000
C	2.23773000	0.69658600	2.12901300
C	1.83518600	-0.61253600	2.65345000
C	4.03570500	-1.68147300	-0.20538300
H	4.24609300	-1.05999500	-1.08062600
H	4.99913600	-1.95908200	0.24645900
H	3.56492400	-2.60381300	-0.55970400
C	2.32547500	-3.09572800	2.06962700
H	2.33102100	-3.64351600	1.12480600
H	3.18972000	-3.44047200	2.65672900
H	1.41882000	-3.37944700	2.60969300
C	0.85970500	-0.78261400	3.77570000
H	1.16282200	-0.20644100	4.65876000
H	-0.12598000	-0.42152900	3.45118400
H	0.75835000	-1.83003200	4.07326000
C	2.02470700	1.99482700	2.85380300
H	2.64696600	2.04973700	3.75909500
H	2.28608200	2.85436300	2.22959800
H	0.98048200	2.11317200	3.16003600
C	4.03976000	1.46830200	0.36745900
H	4.29138700	1.17790000	-0.65676400
H	3.57009700	2.45382100	0.32381000
H	4.98025800	1.57132900	0.92714200
C	-0.46012000	-4.40863500	0.03416400
C	-0.07146300	-2.51601300	-1.20712500
C	-0.49823500	-3.17342200	-2.40310800
C	-0.89692400	-4.52483800	-2.31252200
C	-0.88212600	-5.15390000	-1.08645400
H	-0.44777100	-4.87522900	1.01808300
C	-0.52464700	-2.42892900	-3.61130300
H	-1.22226500	-5.04326500	-3.21104100
H	-1.19023100	-6.18804300	-0.97124000
C	-0.18015300	-1.10793900	-3.58913800
C	0.23107700	-0.49090600	-2.37217400
H	-0.83998800	-2.91261300	-4.53211700
H	-0.22327700	-0.51539600	-4.49474100
N	-0.06297700	-3.14667200	-0.01286200
N	0.32398500	-1.19824000	-1.22303100
C	0.53049500	0.92174600	-2.24358800
C	0.41214600	1.84998400	-3.29266300
C	0.60657200	3.20752300	-3.07433400
C	0.90273400	3.64746500	-1.77092400
C	1.02985800	2.72547700	-0.72165900
C	0.88184300	1.35098600	-0.92825800
H	0.15446800	1.52461400	-4.29688200
H	0.50902500	3.90567400	-3.89708500
H	1.24463300	3.12384600	0.26436800
Ir	1.12085200	-0.09358600	0.44732800
O	1.08814300	4.95261400	-1.43221700
C	0.95465800	5.94707900	-2.44011400
H	-0.05293900	5.94979100	-2.87533800
H	1.13115100	6.90273600	-1.94136400
H	1.69644400	5.81749900	-3.23894300
C	-5.54999300	1.18495800	1.35663600
C	-4.49148800	0.52757200	0.71580200
C	-3.14313900	0.72224400	1.08692000
C	-2.92070100	1.62353200	2.13860100
C	-3.96136500	2.29307700	2.77702600
C	-5.28664100	2.07438900	2.38896400
H	-6.56208800	0.98667000	1.02717300
H	-3.73874400	2.98853700	3.58249300
H	-6.10454600	2.59103800	2.88242900
C	-1.92987200	0.03131600	0.46101700
H	-1.86672700	0.37727700	-0.58276100
H	-2.14956600	-1.04833800	0.39825600

O	-0.77961600	0.29904600	1.18797200
N	-4.86702600	-0.37641600	-0.37492100
O	-3.97864300	-0.80970700	-1.11502400
O	-6.06082400	-0.66448200	-0.51365800
H	-1.88998400	1.77613900	2.43376900

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TS2 SCF Done: E(RM06) = -1807.69742740

C	-0.86124200	0.75545200	2.65374200
C	0.47530300	0.17093600	2.65327700
C	0.33120700	-1.23550600	2.39801900
C	-1.79795900	-0.31949200	2.40783400
C	-1.06600000	-1.54541600	2.25805900
C	1.74518900	0.87532000	3.02479200
H	1.66487700	1.95195200	2.85130100
H	1.96573700	0.72435300	4.09147800
H	2.58816600	0.50823500	2.43563000
C	1.44136300	-2.23925300	2.36297400
H	2.40177000	-1.78351600	2.11199400
H	1.53782700	-2.71613200	3.34964400
H	1.24390000	-3.03385800	1.63594200
C	-1.64180500	-2.92025400	2.08886500
H	-1.68904300	-3.44384600	3.05452300
H	-2.65789800	-2.88981000	1.68577400
H	-1.03514300	-3.53468500	1.41635800
C	-3.29199300	-0.17623900	2.40817000
H	-3.68073400	-0.26890600	3.43169300
H	-3.60145500	0.79909800	2.02265200
H	-3.77630600	-0.94710700	1.80195400
C	-1.21305700	2.13722200	3.12068100
H	-0.44860100	2.86638600	2.84172300
H	-2.16489700	2.47811400	2.70240600
H	-1.30780800	2.15411800	4.21586600
C	5.38770100	-2.34956900	0.66102800
C	3.97753400	-0.80885300	-0.31053700
C	4.50201200	-1.10533600	-1.60864300
C	5.51853400	-2.08297400	-1.71719200
C	5.96883900	-2.71087000	-0.57764800
H	5.72997600	-2.83616600	1.57430800
C	3.96383900	-0.38923400	-2.70894600
H	5.92943000	-2.32250600	-2.69557600
H	6.74899100	-3.46510400	-0.61245600
C	2.99124600	0.54699600	-2.48218800
C	2.53020200	0.79111900	-1.14673900
H	4.32545100	-0.59550200	-3.71395700
H	2.54863000	1.10090100	-3.30312000
N	4.43710300	-1.44455700	0.80540200
N	3.01066900	0.12556900	-0.10745700
C	1.55169900	1.89565500	-0.92626100
C	1.91733900	3.13376400	-1.48233500
C	1.14038500	4.28397800	-1.35434100
C	-0.06770400	4.18451500	-0.66094500
C	-0.45464700	2.94976000	-0.11956500
C	0.32358300	1.78663100	-0.21107800
H	2.86304300	3.21122000	-2.01422100
H	1.47979400	5.21805500	-1.78745500
H	-1.41854800	2.92460100	0.37833900
Ir	-0.45288600	0.05393900	0.63451400
O	-0.93985400	5.21767700	-0.46272900
C	-0.61525300	6.48325900	-1.01743500
H	-0.52591800	6.43761900	-2.11122600
H	-1.44175100	7.14812200	-0.75508700
H	0.31563700	6.88676500	-0.59618000
C	-4.28003500	-2.70528000	-1.92651000
C	-3.46188600	-1.58045200	-1.76897600
C	-2.06846000	-1.69023800	-1.56459200
C	-1.54174700	-2.99175200	-1.54214800
C	-2.34513200	-4.11659300	-1.70627800
C	-3.72261800	-3.97684900	-1.89983100
H	-5.34300300	-2.55866100	-2.07027900
H	-1.89432500	-5.10509100	-1.69053200
H	-4.35617300	-4.84829600	-2.03328900
C	-1.06685800	-0.55841700	-1.46344600
H	-1.65595500	0.40745800	-0.49208600
H	-1.20205300	0.21229800	-2.23303000
O	0.18416600	-0.88317800	-1.17912600
N	-4.13939300	-0.28129400	-1.80531800
O	-3.44555400	0.74143500	-1.78066400
O	-5.37078700	-0.26297700	-1.85850700
H	-0.47125700	-3.08728100	-1.40169300

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IN3 SCF Done: E(RM06) = -1807.71120778

C	-0.92972000	0.94462200	2.51188100
C	0.33573400	0.23271800	2.63881000
C	0.08309500	-1.14431200	2.39137400
C	-1.96676500	-0.05381600	2.25645400
C	-1.33301600	-1.32589200	2.15618300
C	1.64218000	0.84323700	3.05010500
H	1.67553200	1.90815800	2.80456500
H	1.77997700	0.74810800	4.13687300
H	2.48373200	0.36093700	2.54799300
C	1.07709400	-2.26250900	2.44640300
H	2.10519400	-1.90795500	2.35178900
H	0.98374100	-2.79674200	3.40361900
H	0.90057900	-2.99472100	1.65117400
C	-2.01153600	-2.65429200	2.00556200
H	-2.08666200	-3.15661800	2.98070700
H	-3.02635400	-2.55220400	1.61252900
H	-1.45863800	-3.32323200	1.33936300
C	-3.44572100	0.20794900	2.24646800
H	-3.86032300	0.07040300	3.25490400
H	-3.67225300	1.22969200	1.93128400
H	-3.97745900	-0.47204700	1.57521200
C	-1.17540800	2.35628100	2.96340000
H	-0.34290700	3.01538700	2.70485100
H	-2.08111800	2.77226200	2.51270100
H	-1.30213200	2.38895900	4.05458500
C	5.03593200	-2.87982700	1.00902100
C	3.83017500	-1.25745700	-0.09554000
C	4.33488600	-1.70248100	-1.35846900
C	5.22937800	-2.79808400	-1.37815100
C	5.58626400	-3.39339900	-0.18912400
H	5.30689000	-3.33688000	1.96070800
C	3.90614600	-1.00410200	-2.51713900
H	5.62260500	-3.15159800	-2.32881200

H	6.27159500	-4.23475600	-0.15571700
C	3.05413400	0.05765200	-2.37651500
C	2.60454100	0.44379900	-1.07165200
H	4.25718600	-1.32077800	-3.49684600
H	2.69978000	0.60908600	-3.24089400
N	4.19601300	-1.86261800	1.07056700
N	2.97716300	-0.20323300	0.02158300
C	1.79498300	1.69202200	-0.94034100
C	2.40767100	2.83495800	-1.48249100
C	1.85205600	4.11014800	-1.40178100
C	0.61818800	4.24420500	-0.76322600
C	-0.02034700	3.10832700	-0.24563800
C	0.52507200	1.81636800	-0.30610800
H	3.37829600	2.72814800	-1.96171800
H	2.37801500	4.95906200	-1.82336500
H	-0.99311200	3.27105300	0.20529600
Ir	-0.59223200	0.25270000	0.48473000
O	-0.05149000	5.42415700	-0.60232700
C	0.53854900	6.60244000	-1.13029700
H	0.66838600	6.53954400	-2.21909000
H	-0.15403000	7.41561500	-0.90039000
H	1.50948300	6.81592600	-0.66306500
C	-4.34243600	-2.54814300	-1.81527500
C	-3.46163700	-1.46687500	-1.70612300
C	-2.06862700	-1.64319000	-1.55135800
C	-1.61017200	-2.97330300	-1.52280300
C	-2.47491700	-4.05571000	-1.65383000
C	-3.84972100	-3.84706100	-1.80290400
H	-5.40239600	-2.34903300	-1.91402200
H	-2.07548600	-5.06627600	-1.64525800
H	-4.53089300	-4.68573300	-1.90929700
C	-1.03922000	-0.55914200	-1.46166600
H	-1.71769100	1.21407500	-0.06102500
H	-1.16034100	0.26194900	-2.16764100
O	0.18853800	-0.88579500	-1.11817300
N	-4.07517000	-0.13569400	-1.72367800
O	-3.37526800	0.83118600	-2.03151300
O	-5.27192600	-0.04817200	-1.43159700
H	-0.54324800	-3.12868700	-1.40701700

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Ir-H SCF Done: E(RM06) = -1807.73824524

C	1.11652700	1.74831000	2.15598100
C	1.91752400	2.46668300	1.17772000
C	3.03031200	1.64512800	0.83320000
C	1.84419500	0.52998500	2.49225900
C	2.99756000	0.46285100	1.68164900
C	1.67238700	3.87089400	0.70855900
H	2.06941100	4.59069300	1.43890600
H	2.16015900	4.07064200	-0.25046800
H	0.60760500	4.08511300	0.58358500
C	4.15126500	1.99551400	-0.10346800
H	4.51518300	1.11405900	-0.64212500
H	3.83838900	2.73137100	-0.85007900
H	5.00815600	2.42039500	0.44067100
C	4.09821500	-0.54989200	1.78149400
H	3.73074300	-1.51394200	2.14246300
H	4.58555900	-0.71800200	0.81827100
H	4.86951400	-0.20256500	2.48589900
C	1.45351800	-0.42873900	3.57941500
H	1.80486700	-0.06404700	4.55632600
H	0.37002300	-0.55542800	3.64384200
H	1.88877700	-1.41924200	3.41895400
C	0.00071200	2.32435900	2.98288200
H	-0.71753000	1.55337900	3.27768600
H	0.39004600	2.78661700	3.90241500
H	-0.54960800	3.09977100	2.44208500
C	3.39428800	-3.20794700	-0.59943300
C	1.92862400	-1.73661500	-1.58622800
C	1.96067300	-2.48075000	-2.80854200
C	2.77937700	-3.62886300	-2.86724800
C	3.50615200	-4.00371700	-1.75714300
H	3.94909100	-3.47868100	0.29800900
C	1.15953700	-2.03971600	-3.89507500
H	2.81711500	-4.20443900	-3.78906200
H	4.14330100	-4.88238800	-1.75991100
C	0.37141000	-0.93793000	-3.73164300
C	0.36747100	-0.22404100	-2.49762100
H	1.17486100	-2.59001400	-4.83230300
H	-0.26376000	-0.59456400	-4.53951100
N	2.64568700	-2.11999900	-0.51004300
N	1.15230600	-0.60409300	-1.45828600
C	-0.47534600	0.91787100	-2.23331400
C	-1.35972300	1.47853500	-3.17342300
C	-2.18426500	2.54194500	-2.83882700
C	-2.13435300	3.04545500	-1.52339200
C	-1.25988000	2.48987700	-0.58201000
C	-0.38805000	1.43773200	-0.90307500
H	-1.41316100	1.08713400	-4.18586900
H	-2.85458900	2.96164000	-3.57949600
H	-1.29135400	2.90359500	0.41982900
Ir	0.97590200	0.58613000	0.29602300
H	-0.20541400	-0.45126400	0.62652700
O	-2.90281700	4.07778700	-1.07840300
C	-3.86085900	4.64566200	-1.96128700
H	-4.59524600	3.90124300	-2.29457900
H	-4.37377900	5.42063200	-1.38717800
H	-3.38476200	5.10585800	-2.83726700
C	-3.01475500	-3.83329900	1.19102100
C	-2.99730500	-2.46349400	1.44547500
C	-3.83000500	-1.56395000	0.75637400
C	-4.71327200	-2.10158700	-0.18869500
C	-4.75526300	-3.47092800	-0.44451800
C	-3.90017500	-4.33732400	0.24041500
H	-2.35418400	-4.48531500	1.74919000
H	-5.35646800	-1.41313000	-0.72692200
H	-5.45071200	-3.86185500	-1.18149700
H	-3.92537100	-5.40485200	0.04405500
C	-3.79297100	-0.06824600	0.88448200
H	-2.84535700	0.38089600	1.21136800
O	-4.75055000	0.61705100	0.57848700
N	-2.11591500	-1.99813000	2.52573300
O	-2.40629200	-0.93703400	3.08492400
O	-1.16054400	-2.70684700	2.83557400

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TS3 SCF Done: E(RM06) = -1807.71121694

C	3.04265000	0.25970500	-1.29602900
C	3.38300400	0.88335200	-0.03676700
C	2.73068900	2.18362900	0.00203100
C	2.16757400	1.16729800	-1.99722100
C	2.00328800	2.36107100	-1.21219400
C	4.38486300	0.37373400	0.95566600
H	5.40104800	0.69489300	0.68225900
H	4.18015300	0.74839300	1.96300800
H	4.38320100	-0.71883300	1.00279100
C	2.89481300	3.19048200	1.09989100
H	2.02637100	3.84864600	1.16908600
H	3.02429900	2.70530300	2.07248400
H	3.78319700	3.81403900	0.92226400
C	1.28837000	3.59151900	-1.68489700
H	0.28412200	3.35800300	-2.04787300
H	1.19768500	4.33321000	-0.88913300
H	1.84446700	4.05888000	-2.51109700
C	1.62250400	0.96841700	-3.37777900
H	2.15239600	1.62218200	-4.08572600
H	1.75449300	-0.06282400	-3.71613100
H	0.55491000	1.20735400	-3.42727900
C	3.69551800	-0.95029800	-1.90095700
H	2.97958800	-1.58413300	-2.43310300
H	4.46503800	-0.64258600	-2.62311700
H	4.19234700	-1.56413900	-1.14513800
C	-1.12270200	4.20278900	1.02335400
C	-1.00275200	1.95661500	1.49682800
C	-2.12790500	2.05434600	2.37512100
C	-2.73715000	3.31630000	2.53815200
C	-2.23895800	4.40648600	1.85609500
H	-0.70080500	5.04170600	0.47142400
C	-2.58183300	0.88416300	3.03971100
H	-3.59523200	3.40610800	3.19980100
H	-2.68174800	5.39278300	1.95053700
C	-1.92654100	-0.29468800	2.82695700
C	-0.81362500	-0.35876900	1.94541500
H	-3.43683400	0.94252400	3.70786700
H	-2.25336300	-1.19928400	3.32513300
N	-0.52073600	3.03494200	0.85032800
N	-0.36921800	0.74478400	1.27716800
C	-0.07955400	-1.57011200	1.66880600
C	-0.35779500	-2.81190100	2.26617900
C	0.37973900	-3.94305900	1.94732700
C	1.41462000	-3.82803900	1.00081200
C	1.69462400	-2.59370300	0.39944400
C	0.97160300	-1.43352700	0.70899200
H	-1.16100500	-2.91223100	2.99073600
H	0.14581000	-4.89082300	2.41698000
H	2.49374900	-2.58269100	-0.33146700
Ir	1.21938600	0.41867800	-0.05283100
H	-0.09755200	-0.33546600	-1.29412900
O	2.20239600	-4.86595600	0.60593100
C	1.94606900	-6.15951500	1.13889700
H	0.93206600	-6.50288300	0.89742200
H	2.67143700	-6.82572200	0.66639000
H	2.09120100	-6.18638000	2.22682600
C	-4.08178800	0.68190500	-1.55917200
C	-3.12041900	-0.34102100	-1.70338000
C	-3.46922300	-1.68957100	-1.40490500
C	-4.75701300	-1.93444800	-0.89672500
C	-5.69175800	-0.92191400	-0.72576100
C	-5.34746900	0.39222200	-1.07425200
H	-3.79290100	1.69304300	-1.81524200
H	-5.00445900	-2.96587400	-0.66635100
H	-6.68239900	-1.14907700	-0.34277300
H	-6.06932600	1.19637500	-0.95835000
C	-2.63769500	-2.89236500	-1.68051300
H	-1.78538000	-2.76160200	-2.36198700
O	-2.90583700	-3.99682700	-1.22872400
N	-1.85727500	0.05393700	-2.17688700
O	-0.83807000	-0.78727500	-2.02852000
O	-1.59763500	1.25513800	-2.47833300

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IN4 SCF Done: E(RM06) = -1807.75190479

C	-1.64370400	0.50954800	-2.49714900
C	-1.70143500	-0.92606600	-2.46025500
C	-0.36033500	-1.44095300	-2.75751000
C	-0.24523000	0.88231800	-2.58066700
C	0.51764600	-0.35045300	-2.80784200
C	-2.95068200	-1.76025600	-2.44608800
H	-3.28779400	-1.98118200	-3.46910900
H	-2.78766000	-2.71811700	-1.94164200
H	-3.76814700	-1.24824000	-1.93012500
C	-0.03827800	-2.87840100	-3.02689800
H	1.01527500	-3.10216700	-2.84069300
H	-0.63716000	-3.55106300	-2.40877200
H	-0.24898800	-3.12073500	-4.07920200
C	1.99596100	-0.37814100	-3.04126100
H	2.51032100	0.26714500	-2.32215700
H	2.40664400	-1.38731200	-2.94881800
H	2.23414300	-0.00709200	-4.04812000
C	0.29916200	2.26253300	-2.81046300
H	0.42094900	2.46207800	-3.88533600
H	-0.36658700	3.03179000	-2.40880000
H	1.27454300	2.38913100	-2.33165300
C	-2.82177000	1.43445800	-2.57276900
H	-2.59808400	2.42412400	-2.16864800
H	-3.11790900	1.56476200	-3.62320800
H	-3.68611300	1.04176500	-2.02938100
C	0.76715000	-4.43355200	0.23900300
C	-0.57686600	-2.76602900	1.06875200
C	-0.94446500	-3.57624200	2.18861300
C	-0.40296700	-4.87717900	2.27513100
C	0.46314100	-5.31581500	1.29681600
H	1.45113000	-4.75042300	-0.54696500
C	-1.81499600	-3.02282300	3.16396600
H	-0.67161500	-5.50877200	3.11824700
H	0.90661200	-6.30573900	1.32803800
C	-2.24346300	-1.73428900	3.02344600
C	-1.84152400	-0.95994700	1.89493100
H	-2.11225400	-3.62330600	4.01988200
H	-2.88270900	-1.28513300	3.77354300
N	0.27093900	-3.21237100	0.11647800
N	-1.06332500	-1.48959100	0.92693000

C	-2.17939200	0.43801900	1.71512000
C	-2.94774700	1.18174000	2.62811500
C	-3.14210300	2.54562600	2.45706200
C	-2.53204200	3.18263400	1.36084500
C	-1.76914700	2.44388300	0.44340000
C	-1.60419100	1.06290700	0.56895000
H	-3.40018200	0.70403300	3.49276700
H	-3.73909900	3.09984700	3.17146300
H	-1.30076100	2.99327900	-0.36556800
Ir	-0.60189500	-0.14341000	-0.69124000
H	1.24692400	2.18586300	1.47158600
O	-2.62648400	4.51518500	1.10700200
C	-3.36570800	5.33316900	2.00592000
H	-2.94211200	5.30718500	3.01804700
H	-3.29171100	6.34966000	1.61342500
H	-4.42275600	5.03951000	2.04508900
C	3.51822500	-0.64997100	1.09710900
C	3.29217200	0.65948400	0.64580800
C	4.37168700	1.57867700	0.61968000
C	5.62172100	1.17587600	1.11733300
C	5.83405100	-0.11311900	1.59142600
C	4.77585900	-1.02745100	1.56286900
H	2.69320600	-1.34931100	1.08653500
H	6.42522100	1.90608500	1.09864800
H	6.81070800	-0.40875400	1.96439500
H	4.92566300	-2.04447400	1.91772400
C	4.28871100	2.92756300	0.00644300
H	3.45329500	3.09475000	-0.69274500
O	5.12076500	3.80381100	0.19141700
N	2.00576100	1.02677100	0.14352700
O	1.67189900	2.36810100	0.60538700
O	1.03664900	0.16955100	0.59862900

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t-BuOH SCF Done: E(RM06) = -233.585121245

C	0.68230500	1.26641400	-0.51554700
H	1.74205100	1.28398000	-0.22710200
H	0.20416300	2.16186300	-0.10328900
H	0.63689200	1.32275200	-1.60978600
C	-0.00598600	-0.00002600	0.01419500
C	-1.49358100	-0.00356100	-0.34475300
H	-1.98910900	0.88174100	0.06901200
H	-1.63488800	-0.00350800	-1.43104600
H	-1.98479100	-0.89157000	0.06836100
C	0.68858500	-1.26278700	-0.51610700
H	1.74847300	-1.27505500	-0.22787200
H	0.21508500	-2.16079600	-0.10406400
H	0.64327800	-1.31899400	-1.61035400
O	0.02842200	-0.00027500	1.45393000
H	0.96353300	0.00155300	1.71797100

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IN5 SCF Done: E(RM06) = -2041.35886610

C	-1.47080900	-1.58336000	-2.41450600
C	-2.14105700	-2.39965000	-1.41228200
C	-1.11555400	-3.03206000	-0.63067600
C	-0.04437000	-1.83771100	-2.29727900
C	0.18465500	-2.72641100	-1.21895400
C	-3.61958000	-2.63076800	-1.30745900
H	-4.18906700	-1.73168200	-1.55975600
H	-3.93211900	-3.42753600	-1.99724400
H	-3.91094400	-2.93417400	-0.29743000
C	-1.34587400	-4.00651700	0.48762600
H	-1.43015300	-5.02979300	0.09569700
H	-0.51938800	-3.99851900	1.20380200
H	-2.26708700	-3.78283500	1.03390300
C	1.49471700	-3.34936400	-0.83440900
H	1.66866800	-4.26199300	-1.42389300
H	2.34055100	-2.67860500	-1.01162400
H	1.50793400	-3.63708200	0.21939400
C	0.97661200	-1.17565600	-3.16825200
H	0.79083300	-1.41201100	-4.22427200
H	0.91383000	-0.08688200	-3.04756600
H	1.99693300	-1.47211000	-2.91828700
C	-2.11613300	-0.90969800	-3.59183600
H	-3.16360800	-0.66500600	-3.39604700
H	-1.59793100	0.01546200	-3.86352900
H	-2.09634500	-1.56919100	-4.47164300
C	2.30538000	-2.01258900	2.60886900
C	0.20388800	-1.06186700	2.49749700
C	0.09585400	-1.07759300	3.92296000
C	1.15132300	-1.64784600	4.66670400
C	2.26184400	-2.13567200	4.01050400
H	3.18942700	-2.33050200	2.05991200
C	-1.05263900	-0.49159700	4.51677100
H	1.07704000	-1.67993700	5.75068400
H	3.09629600	-2.57521100	4.54639600
C	-1.99551800	0.08297000	3.71445600
C	-1.86340300	0.03773500	2.29540600
H	-1.15615900	-0.48961200	5.59847600
H	-2.86482000	0.56170200	4.14837600
N	1.32309800	-1.50324900	1.87562000
N	-0.80898100	-0.57399500	1.70672200
C	-2.81624800	0.63271800	1.38188100
C	-3.90731100	1.41987000	1.79064600
C	-4.73178500	2.03838800	0.86083400
C	-4.44776300	1.87689700	-0.50756500
C	-3.36441900	1.08509100	-0.92048300
C	-2.54185800	0.43036600	-0.00190200
H	-4.11785400	1.57546500	2.84498300
H	-5.56444900	2.64479200	1.19648700
H	-3.18836500	1.00813400	-1.98784400
Ir	-0.99381700	-0.79230600	-0.43446700
O	-5.17225200	2.44801700	-1.50608000
C	-6.27208100	3.28331100	-1.16338100
H	-5.95199800	4.14990000	-0.57091400
H	-6.68814600	3.63166600	-2.11119400
H	-7.04473200	2.73041500	-0.61373600
H	1.94217100	-0.26804200	0.55627900
C	2.43604900	3.27117300	0.69182400
C	1.38641600	2.70048600	-0.07340600
C	0.69242300	3.50565200	-0.98885300
C	1.05880400	4.83696600	-1.17471100
C	2.12233700	5.39621300	-0.45884300
C	2.79691200	4.60942600	0.46728200
H	0.51226200	5.43977100	-1.89606700

H	2.40845300	6.43276400	-0.61355600
H	3.61124300	5.01446800	1.06053700
N	0.99162700	1.34540600	0.12992800
O	0.11175300	0.93351800	-0.83614600
O	2.21746400	0.52974900	0.04459700
C	5.36168600	0.95864100	-2.33868200
H	4.74838500	1.69485000	-1.80514300
H	4.98520400	0.88268900	-3.36522400
H	6.38873500	1.34241900	-2.37487500
C	5.29649300	-0.41039200	-1.64451500
C	6.12234300	-1.44659100	-2.41163900
H	5.76244800	-1.53502700	-3.44306300
H	7.18163400	-1.16665800	-2.43766200
H	6.03734700	-2.43144200	-1.93776300
C	5.77506300	-0.30493000	-0.18774700
H	5.16057700	0.40906400	0.37283500
H	5.70236900	-1.28115900	0.30671700
H	6.81746600	0.03150300	-0.12894700
O	3.94702600	-0.90192100	-1.67481300
H	3.36002800	-0.24373400	-1.24548900
H	-0.11880300	3.06541700	-1.55245300
C	3.11960200	2.55427200	1.79246900
H	2.62273600	1.63961900	2.15397700
O	4.14439600	2.94933900	2.33053500

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TS4 SCF Done: E(RM06) = -2041.31614895

C	2.42943500	-0.50009300	-2.32562500
C	1.23293200	0.25145200	-2.67793200
C	0.12934200	-0.68699700	-2.69769400
C	2.03111200	-1.88101100	-2.14871400
C	0.62828900	-2.00633700	-2.39910300
C	1.18768300	1.67681100	-3.13997400
H	2.01760500	2.25355100	-2.72230100
H	1.26479400	1.72137800	-4.23577000
H	0.25905600	2.16180000	-2.83116800
C	-1.28500100	-0.37770800	-3.07196500
H	-1.47358000	-0.72614400	-4.09767400
H	-1.98927100	-0.89601400	-2.41323900
H	-1.50377600	0.69042600	-3.02577600
C	-0.15806300	-3.28263700	-2.42289100
H	-0.14171900	-3.73758800	-3.42378800
H	0.25278600	-4.02440100	-1.72986200
H	-1.20798900	-3.11283900	-2.16637600
C	2.93180900	-3.01926800	-1.78108200
H	3.07559400	-3.67697600	-2.64887000
H	3.91591300	-2.67243500	-1.45736800
H	2.49881400	-3.61246900	-0.97095700
C	3.83988700	0.00265500	-2.41185800
H	3.90767300	1.06578100	-2.16960400
H	4.51032200	-0.53565400	-1.73526500
H	4.22447000	-0.13087800	-3.43304200
C	-4.06803800	2.86360600	-2.53224800
C	-2.41622700	2.67166400	-0.93858400
C	-3.32238300	3.08151300	0.09040300
C	-4.65858700	3.37918300	-0.26706900
C	-5.03834500	3.27151200	-1.58552300
H	-4.34948900	2.77469600	-3.58133300
C	-2.81357900	3.16234500	1.41142200
H	-5.36286100	3.68885200	0.50181600
H	-6.05189400	3.49043700	-1.90678500
C	-1.49642200	2.86271000	1.63867300
C	-0.65051400	2.47230600	0.54801600
H	-3.47353100	3.45436200	2.22524200
H	-1.08246700	2.90615500	2.64046400
N	-2.81377700	2.57407800	-2.23998500
N	-1.11325600	2.37338700	-0.69080400
C	0.80798700	2.28596600	0.80262700
C	1.40703800	3.34462300	1.50982400
C	2.77569300	3.42133600	1.76019000
C	3.58149300	2.38860000	1.27907400
C	2.99302700	1.31511500	0.59464800
C	1.61681900	1.19846200	0.34463600
H	0.78337800	4.17029100	1.84433500
H	3.18353500	4.27244100	2.29347600
H	3.67151300	0.54111600	0.25737800
Ir	1.01403400	-0.51901800	-0.66530400
O	4.93871500	2.32523600	1.42460200
C	5.58692900	3.38625500	2.11038300
H	5.23974700	3.47154300	3.14883600
H	6.65139800	3.13990000	2.10959900
H	5.44133400	4.34851000	1.60125900
H	-0.88709900	-3.51521900	0.18172700
C	-3.88896900	-1.89353000	1.03359400
C	-2.68614200	-1.21517000	1.32897900
C	-2.55149200	-0.51256400	2.53183100
C	-3.60740400	-0.48251200	3.43827400
C	-4.80718700	-1.14654200	3.15273600
C	-4.94234500	-1.84487100	1.95724100
H	-3.49523700	0.05686500	4.37500900
H	-5.62778200	-1.12008300	3.86413600
H	-5.86026500	-2.37016300	1.71332600
N	-1.64243200	-1.26011300	0.33794900
O	-0.72995100	-0.41306600	0.57442900
O	-0.80574900	-3.02990700	1.01943100
C	1.51664300	-1.10250900	3.23407000
H	0.44190000	-1.25269500	3.38343200
H	1.67828600	-0.08416000	2.87020500
H	2.00939900	-1.20007500	4.21007700
C	2.06987100	-2.13573000	2.24129900
C	3.57821200	-1.94919500	2.04581200
H	3.81482400	-0.93906000	1.70762700
H	4.11050700	-2.11816100	2.99019300
H	3.96151000	-2.66445800	1.30930700
C	1.80917400	-3.55983100	2.77272900
H	0.73786000	-3.74605100	2.89342400
H	2.20757300	-4.30837600	2.07735900
H	2.29957500	-3.70325200	3.74331800
O	1.40256600	-2.03464000	0.96263200
H	0.34960000	-2.54296200	1.01129900
H	-1.61852600	-0.00461600	2.74062200
C	-4.07495900	-2.66731900	-0.21800400
H	-3.21491300	-2.68326900	-0.90897100
O	-5.10423200	-3.26149100	-0.49437200

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IN6 SCF Done: E(RM06) = -2041.33327065

C	2.49424900	-0.99165500	-2.06057300
C	1.48899700	-0.08207100	-2.59070800
C	0.24242000	-0.79553100	-2.62884300
C	1.85386000	-2.29965700	-1.91337300
C	0.49060000	-2.18289200	-2.25211500
C	1.73047300	1.29830600	-3.12308100
H	2.57605600	1.77801600	-2.62402700
H	1.95645500	1.24959500	-4.19759800
H	0.85454500	1.93709800	-2.98567400
C	-1.05565400	-0.28029200	-3.16394200
H	-1.16988300	-0.58234500	-4.21549200
H	-1.90534400	-0.69028000	-2.61037500
H	-1.12603800	0.80571900	-3.10496700
C	-0.52154900	-3.29114100	-2.23055700
H	-1.50334900	-2.93614600	-2.55412700
H	-0.22393800	-4.09631900	-2.91582600
H	-0.62033500	-3.71340800	-1.22402300
C	2.53686200	-3.52212900	-1.39024500
H	1.93284500	-4.41877500	-1.55616100
H	3.51071200	-3.66909600	-1.87164500
H	2.69921400	-3.40512800	-0.31057800
C	3.98225900	-0.78842000	-2.07940900
H	4.25112900	0.27037100	-2.06219400
H	4.46788200	-1.27486400	-1.22744500
H	4.41112300	-1.21988100	-2.99522700
C	-4.26301000	2.62795900	-2.54754800
C	-2.53375600	2.53990300	-1.03075000
C	-3.39498300	2.99127000	0.02036400
C	-4.75249900	3.25183200	-0.28546000
C	-5.19362700	3.07031100	-1.57566600
H	-4.59368800	2.48297600	-3.57582000
C	-2.82613400	3.14891800	1.30908500
H	-5.42307100	3.59211700	0.50045000
H	-6.22500500	3.25798300	-1.85755800
C	-1.49245300	2.88595200	1.48632200
C	-0.69519600	2.45496400	0.37606900
H	-3.45152400	3.47464600	2.13732100
H	-1.02631100	2.99841100	2.45953200
N	-2.99222800	2.37022300	-2.30367200
N	-1.21410200	2.27273300	-0.83040900
C	0.78317600	2.34543600	0.55621100
C	1.37506400	3.51890800	1.05891700
C	2.75163700	3.68587100	1.19170500
C	3.57119400	2.62369800	0.80870500
C	2.99229600	1.43396300	0.34340600
C	1.61056300	1.23205000	0.21346700
H	0.73246300	4.35686300	1.31886200
H	3.15245400	4.62114000	1.56508000
H	3.68330500	0.63989000	0.09442500
Ir	1.01976500	-0.61855700	-0.51665500
O	4.93650100	2.63351400	0.86052400
C	5.57836600	3.80846100	1.33432600
H	5.29978700	4.03318700	2.37266800
H	6.65084700	3.60491100	1.28933800
H	5.35162600	4.67827000	0.70321600
H	0.32645200	-4.58403100	1.07587600
C	-4.00751500	-1.65456600	0.94772500
C	-2.77524100	-1.02967900	1.28031100
C	-2.61328300	-0.42381100	2.54371500
C	-3.65684200	-0.44163200	3.45774900
C	-4.87628800	-1.05553600	3.13232100
C	-5.04482900	-1.65352100	1.88670300
H	-3.52600000	0.02054900	4.43221800
H	-5.68743600	-1.06764300	3.85475900
H	-5.97824100	-2.13726800	1.61764800
N	-1.77133000	-1.07097700	0.30286700
O	-0.69308700	-0.51936000	0.65430700
O	-0.21011200	-3.77685200	1.04721900
C	1.30687900	-0.62804500	3.22632400
H	0.29165700	-1.02808900	3.32000800
H	1.25410300	0.34201700	2.72464200
H	1.70263700	-0.47031300	4.23844600
C	2.19469200	-1.60302400	2.43595300
C	3.65872400	-1.12302400	2.45372600
H	3.74977100	-0.08636500	2.12732700
H	4.07917300	-1.19145200	3.46574700
H	4.26946700	-1.75001600	1.79295700
C	2.14676100	-2.98724900	3.12505100
H	1.12920900	-3.38903800	3.12537600
H	2.79818800	-3.69856700	2.60184400
H	2.49173100	-2.91728500	4.16423000
O	1.72196200	-1.81093100	1.10421900
H	0.46663600	-3.04992400	1.07441100
H	-1.66855300	0.04682000	2.78305000
C	-4.23341300	-2.32628100	-0.36009800
H	-3.37215700	-2.35976400	-1.04562600
O	-5.30322200	-2.82329300	-0.67112800

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1a-2 SCF Done: E(RM06) = -474.675779651

C	1.03180400	-1.33220900	0.01250300
C	-0.12818600	-0.55552900	-0.06032800
C	-0.04526900	0.85525900	-0.07575200
C	1.21857900	1.45458500	-0.03320100
C	2.37567100	0.67787700	0.04634000
C	2.28083700	-0.71682200	0.06992000
H	0.93154300	-2.41249200	-0.00303400
H	1.29077700	2.53938500	-0.04280100
H	3.34908600	1.15787100	0.08417200
H	3.18088200	-1.32285600	0.12040100
O	-1.48744900	-2.33165900	0.11612600
N	-1.41884300	-1.17394500	-0.26705700
C	-1.23395400	1.74531800	-0.07260300
H	-1.00135000	2.79553700	-0.35269200
O	-2.36454200	1.41782000	0.22663300

3

H2O SCF Done: E(RM06) = -76.4222760449

O	0.00000000	0.00000000	0.12002100
H	0.00000000	-0.76170600	-0.48008200
H	0.00000000	0.76170600	-0.48008200

15

t-BuONa SCF Done: E(RM06) = -395.287318925

C	1.15477700	0.97578400	1.07835800

H	0.78239700	0.67710900	2.06706300
H	0.78653500	1.99032700	0.87676800
H	2.25264300	1.01348700	1.12360200
C	0.61924400	-0.00014500	-0.00004100
C	1.15334600	0.44648300	-1.38434200
H	0.77937300	1.45189100	-1.61799100
H	2.25111500	0.46753800	-1.44129400
H	0.78392000	-0.23537900	-2.16133900
C	1.15376100	-1.42245200	0.30535200
H	0.78116600	-1.75678700	1.28251700
H	0.78413800	-2.12781100	-0.45059700
H	2.25154100	-1.48066400	0.31993300
O	-0.75527600	0.00000000	0.00013600
Na	-2.71794400	0.00020700	0.00038900

18

IN7 SCF Done: E(RM06) = -712.810324879

C	1.51910700	1.43002600	-0.06034500
C	0.52865900	0.45365700	0.03590400
C	0.79195800	-0.91702600	0.06458400
C	2.14084800	-1.28923700	0.01870000
C	3.15949300	-0.33842700	-0.05472700
C	2.85163000	1.02459200	-0.09939400
H	1.24802500	2.48098200	-0.09268500
H	2.38808900	-2.34872100	0.01942000
H	4.19649000	-0.66095700	-0.09657200
H	3.64011000	1.76787000	-0.17098100
O	-1.37215800	1.51305600	-0.82577800
N	-0.85818600	0.93242900	0.14581000
O	-1.40265900	0.89362200	1.26127200
C	-0.36494600	-1.92900100	0.09151000
H	-0.41610000	-2.30695300	1.14322300
H	-0.00713100	-2.80503800	-0.49660600
O	-1.52853700	-1.40112100	-0.36027000
Na	-3.12507600	-0.11874100	-0.17324100

18

TS5 SCF Done: E(RM06) = -712.755776275

C	1.72815600	1.19925300	-0.47386300
C	0.52561100	0.52772100	-0.11530700
C	0.52081700	-0.88201600	0.17223200
C	1.79489900	-1.50112500	0.29559200
C	2.95657100	-0.84219200	-0.04162200
C	2.91792800	0.51530300	-0.45861600
H	1.67698300	2.25634900	-0.70427400
H	1.82293200	-2.55145200	0.57533700
H	3.90543800	-1.37137000	-0.01953600
H	3.83796600	1.02270100	-0.73459300
O	-0.51576900	2.56193900	0.33783500
N	-0.55336900	1.30705400	0.25289500
O	-1.58734500	0.65307900	0.79888400
C	-0.69263100	-1.66614700	0.41643300
H	-1.09508300	-0.52008100	1.16882100
H	-0.49570800	-2.56239000	1.03090900
O	-1.72631500	-1.72971600	-0.38514700
Na	-3.05923800	-0.12821100	-0.71532800

3

NaOH SCF Done: E(RM06) = -238.118923163

Na	0.04216600	-0.92733100	0.00000000
O	0.04216600	1.08048800	0.00000000
H	-0.80116000	1.55674300	0.00000000

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2a SCF Done: E(RM06) = -346.623269538

C	1.61938200	1.20796900	-0.07982200
C	0.24464900	1.20556300	0.16211200
C	-0.45759700	0.00048000	0.28975400
C	0.24387600	-1.20512600	0.16270100
C	1.61859800	-1.20852900	-0.07922300
C	2.30959800	-0.00052900	-0.20017600
H	2.15146500	2.15130700	-0.17253700
H	-0.29076300	2.14787800	0.25479100
H	-0.29213300	-2.14705600	0.25584600
H	2.15007900	-2.15225400	-0.17145400
H	3.38065100	-0.00092000	-0.38559200
C	-1.94906300	0.00098500	0.51700000
H	-2.23538200	-0.88554500	1.10408500
H	-2.23514000	0.88922700	1.10161400
O	-2.60550800	-0.00073000	-0.75485600
H	-3.56137400	-0.00166700	-0.58198600

85

IN8 SCF Done: E(RM06) = -1836.83696080

C	-2.60767100	-0.31319200	-1.98166300
C	-1.47837200	-1.20500100	-2.22516200
C	-0.40685500	-0.38497500	-2.70497600
C	-2.26276100	0.99767800	-2.55498900
C	-0.92625600	0.96395400	-2.96418000
C	-1.46510000	-2.69864400	-2.09079500
H	-2.18609500	-3.04004400	-1.34331400
H	-1.72921300	-3.16447000	-3.05091900
H	-0.47760600	-3.05795700	-1.79061100
C	0.92751700	-0.85902700	-3.19129100
H	0.88867100	-1.00399400	-4.28147100
H	1.71715000	-0.12683800	-2.99171700
H	1.22753400	-1.79959100	-2.73078900
C	-0.14356300	2.06390400	-3.61695200
H	-0.12023700	1.92813500	-4.70769100
H	-0.57463600	3.04936000	-3.41744400
H	0.89675700	2.07664500	-3.27732200
C	-3.23813600	2.11688700	-2.75324600
H	-3.84664600	1.90786400	-3.64524800
H	-3.92975200	2.22148700	-1.91416200
H	-2.74443900	3.07906700	-2.91267900
C	-4.00950500	-0.74620800	-1.66387200
H	-4.02162700	-1.65701400	-1.06069000
H	-4.55856800	0.02467500	-1.11396400
H	-4.56505300	-0.95249800	-2.59036000
C	4.49795200	-3.08518200	-2.17823800
C	2.97747100	-2.52554000	-0.54133000
C	4.02862000	-2.35162500	0.41399400
C	5.36314900	-2.56261800	-0.00569300
C	5.60467100	-2.93256000	-1.30935400
H	4.66793700	-3.38112700	-3.21344900
C	3.65866900	-1.98353800	1.73300700

H	6.17521400	-2.43277400	0.70629900
H	6.61158400	-3.10781500	-1.67542800
C	2.33168900	-1.82863700	2.03218600
C	1.33843200	-2.03141700	1.01713400
H	4.42924200	-1.83013200	2.48528000
H	2.01344900	-1.54352600	3.02920600
N	3.23973300	-2.89395700	-1.82757200
N	1.66333100	-2.35448600	-0.22570400
C	-0.09635900	-1.99049800	1.42506700
C	-0.40952200	-2.84205700	2.50155800
C	-1.69588800	-2.98084500	3.01667900
C	-2.71166800	-2.21014500	2.44659400
C	-2.40924300	-1.33899400	1.39278200
C	-1.12680600	-1.20216800	0.83946000
H	0.38391400	-3.44459400	2.93811000
H	-1.88271500	-3.66823100	3.83393300
H	-3.22667400	-0.73182800	1.02180600
Ir	-1.00862200	0.20413200	-0.66200900
O	-4.01941800	-2.22522000	2.84794100
C	-4.37462000	-3.06945300	3.93161100
H	-3.83530500	-2.80194300	4.85043300
H	-5.44546200	-2.92123100	4.09153100
H	-4.19093500	-4.12797400	3.70196900
C	-1.62452100	3.18936000	2.62168200
H	-0.54514600	3.36721500	2.69848300
H	-1.89670500	2.43099000	3.36392100
H	-2.14256300	4.12383700	2.87334600
C	-1.99182100	2.70137700	1.20551000
C	-3.50754500	2.44925100	1.14373300
H	-3.79883700	1.71944400	1.90691800
H	-4.07798900	3.37139200	1.31436400
H	-3.79788500	2.04788200	0.16815300
C	-1.57275800	3.77325300	0.18232500
H	-0.50692600	4.00898000	0.29095800
H	-1.73944700	3.42438400	-0.84101500
H	-2.13504800	4.70603500	0.31950900
O	-1.28604300	1.48456400	1.02114000
C	3.86617400	2.95042400	2.78460000
C	3.05292100	2.18657800	1.94445600
C	2.69821800	2.66153000	0.67586200
C	3.17270100	3.91525000	0.26651000
C	3.99315000	4.67542400	1.10144300
C	4.34161800	4.19499800	2.36595200
H	4.12785000	2.57170400	3.76962300
H	2.68314800	1.21976700	2.27001900
H	4.35090900	5.64660800	0.76874100
H	4.97346800	4.78870500	3.02147500
C	1.84368100	1.83837900	-0.27119800
H	1.26333700	2.50952500	-0.91869500
H	2.48403900	1.23052900	-0.92146500
O	0.98519600	0.91952300	0.40155700
H	0.26419500	1.41303400	0.93455400
H	2.89571500	4.30080600	-0.71294600

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TS6 SCF Done: E(RM06) = -1836.83635657

C	-2.60906900	-0.32241200	-2.02880800
C	-1.47196700	-1.19831700	-2.25529600
C	-0.39060000	-0.36789300	-2.71643600
C	-2.25170800	1.00100600	-2.55105600
C	-0.90827000	0.98186700	-2.95446500
C	-1.44722600	-2.69266200	-2.13230100
H	-2.17981400	-3.04684100	-1.40243000
H	-1.68712500	-3.15158500	-3.10195200
H	-0.46235900	-3.04531100	-1.81595900
C	0.94764000	-0.83911100	-3.19319200
H	0.91529700	-0.98762500	-4.28302300
H	1.73289400	-0.10349700	-2.98975400
H	1.24826800	-1.77662900	-2.72672400
C	-0.13058900	2.09674500	-3.58828800
H	-0.13297600	1.99727400	-4.68328400
H	-0.54917200	3.07856900	-3.34792400
H	0.91656700	2.09161700	-3.27122100
C	-3.21924700	2.13335600	-2.71012600
H	-3.79873000	1.98350700	-3.63268400
H	-3.93709200	2.18349100	-1.88799200
H	-2.72081200	3.10277200	-2.79141300
C	-4.01243700	-0.76227500	-1.72703300
H	-4.02689900	-1.68124500	-1.13611900
H	-4.56694100	-0.00046400	-1.16943800
H	-4.56402600	-0.95758100	-2.65820500
C	4.55088400	-2.98350900	-2.14634600
C	3.00632000	-2.45435700	-0.52193700
C	4.04640100	-2.25450000	0.44053900
C	5.38829400	-2.43601600	0.03085400
C	5.64755000	-2.80358800	-1.27006900
H	4.73511900	-3.27814700	-3.17951900
C	3.65929900	-1.89212500	1.75607200
H	6.19200300	-2.28548900	0.74822700
H	6.66084100	-2.95650300	-1.62852700
C	2.32730800	-1.76676200	2.04567900
C	1.34690400	-1.99141200	1.02373000
H	4.42103700	-1.71835200	2.51277700
H	1.99577900	-1.48659000	3.03971000
N	3.28607000	-2.81984100	-1.80538900
N	1.68656400	-2.31035200	-0.21635800
C	-0.09195400	-1.97877700	1.41741200
C	-0.40491700	-2.83290100	2.49100400
C	-1.69695600	-2.99323700	2.98656100
C	-2.71833300	-2.24468500	2.39753800
C	-2.41608500	-1.37213600	1.34433500
C	-1.12708400	-1.21225400	0.81321800
H	0.39255700	-3.41966200	2.94152500
H	-1.88389800	-3.68113800	3.80335400
H	-3.23989300	-0.78374400	0.95650100
Ir	-0.99769800	0.19476700	-0.68683100
O	-4.03208300	-2.28436100	2.77743900
C	-4.38953400	-3.13789400	3.85310200
H	-3.87333200	-2.86077300	4.78229500
H	-5.46608800	-3.01269600	3.99316100
H	-4.17910700	-4.19180800	3.62532900
C	-1.58437000	3.20281400	2.71611100
H	-0.50102100	3.34962100	2.79830000
H	-1.88041300	2.43812600	3.44234400
H	-2.07631700	4.14625000	2.98449300
C	-1.96668900	2.75959200	1.29142500

C	-3.48324600	2.54017300	1.21527200
H	-3.79536300	1.79404800	1.95388700
H	-4.03082000	3.47032900	1.41194000
H	-3.77479500	2.17702600	0.22508400
C	-1.51362300	3.82851300	0.28294100
H	-0.44054000	4.02866800	0.38674300
H	-1.70264200	3.50372400	-0.74481700
H	-2.04424900	4.77560700	0.44279100
O	-1.31148200	1.50906100	1.07146900
C	3.66059100	2.87133400	2.84738000
C	2.80027900	2.16465700	2.00221500
C	2.61479400	2.57080200	0.67609500
C	3.30936700	3.69758400	0.21240300
C	4.17418800	4.39956600	1.05234400
C	4.35167700	3.98878100	2.37662200
H	3.78902900	2.54642200	3.87716600
H	2.26319900	1.29517500	2.36571500
H	4.70308000	5.27201100	0.67641700
H	5.01940000	4.53848700	3.03509600
C	1.69740300	1.81487300	-0.27264000
H	1.13797500	2.54099800	-0.88194100
H	2.30507700	1.22042700	-0.96916800
O	0.82082700	0.92928600	0.39743800
H	-0.05688300	1.45534600	0.95269800
H	3.16941600	4.02952200	-0.81513900

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Ir-O2 SCF Done: E(RM06) = -1603.27002002

C	-1.91456300	-1.96744900	-1.29717600
C	-0.96814300	-2.80755200	-0.61803000
C	0.26983400	-2.81592700	-1.40417300
C	-1.20004900	-1.27722100	-2.35812700
C	0.12953000	-1.89219400	-2.44597400
C	-1.27669800	-3.76808400	0.49557200
H	-2.11222700	-3.41503500	1.10716800
H	-1.54744900	-4.75845400	0.10111100
H	-0.41656200	-3.90476400	1.15887400
C	1.43122200	-3.72981900	-1.16063800
H	1.25302400	-4.70335700	-1.64150600
H	2.36140100	-3.32467900	-1.56811100
H	1.58775800	-3.91326300	-0.09517100
C	1.12621800	-1.60575500	-3.52758300
H	0.89941300	-2.20874500	-4.41899500
H	1.10102000	-0.55666900	-3.83513500
H	2.14867500	-1.84278300	-3.21953900
C	-1.81940700	-0.43933800	-3.44127400
H	-2.13286200	-1.05959200	-4.29432400
H	-2.70548100	0.09316000	-3.08269600
H	-1.11886800	0.31227700	-3.81940700
C	-3.39409300	-1.93967000	-1.05045800
H	-3.63707800	-2.11716900	0.00129200
H	-3.84582300	-0.98791900	-1.33726800
H	-3.87967900	-2.72805900	-1.64318000
C	3.66250300	-1.98102100	1.22293400
C	1.71332200	-0.96728500	1.89092600
C	2.21625700	-0.80401300	3.21990100
C	3.51319200	-1.28366200	3.50436000
C	4.25016200	-1.87486900	2.50106200
H	4.22217100	-2.44221600	0.41037300
C	1.39350200	-0.15155900	4.17545500
H	3.91282700	-1.16988900	4.50905000
H	5.25380900	-2.24968800	2.67394000
C	0.17390800	0.32821500	3.79212200
C	-0.27793400	0.15467100	2.45018900
H	1.75289200	-0.02372800	5.19335800
H	-0.45361500	0.85659200	4.49941400
N	2.44601500	-1.55732700	0.92017500
N	0.46273600	-0.52059300	1.54912900
C	-1.50977800	0.71945600	1.93207100
C	-2.39835200	1.49297600	2.69845400
C	-3.49795800	2.11086300	2.11720100
C	-3.69680200	1.96945400	0.73218600
C	-2.81987000	1.18836000	-0.03514000
C	-1.73583600	0.52133200	0.53818700
H	-2.23680700	1.63257900	3.76390800
H	-4.17005300	2.70279400	2.72709700
H	-3.01256200	1.13563800	-1.10135900
Ir	-0.41796500	-0.65963300	-0.41506700
O	-4.71788400	2.55242700	0.04617500
C	-5.62020000	3.39530100	0.75118100
H	-5.10261500	4.24688600	1.21113100
H	-6.32677500	3.76659500	0.00549900
H	-6.17164100	2.84385900	1.52411100
C	1.57003100	1.25436400	-1.59521300
O	0.61732800	1.13259900	-0.59998500
H	1.12144300	1.27780100	-2.61274500
H	2.29099800	0.41203100	-1.60965800
C	2.37860700	2.54094800	-1.44160200
C	3.46206500	2.79517600	-2.29550700
C	2.05681700	3.49102400	-0.46729700
C	4.20635000	3.96940100	-2.18027000
H	3.72482500	2.06302700	-3.05837000
C	2.80075000	4.66904200	-0.34848700
H	1.21790700	3.28753500	0.18964500
C	3.87731400	4.91415700	-1.20272400
H	5.04413700	4.14800700	-2.85082700
H	2.53685600	5.39818300	0.41474700
H	4.45604300	5.83008600	-1.10968100

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TS7 SCF Done: E(RM06) = -1603.22749750

C	-1.45744300	0.70661000	2.39596000
C	-0.12445800	0.13192000	2.55090900
C	-0.22893200	-1.27623800	2.27496900
C	-2.34763600	-0.36993200	2.02546800
C	-1.59523100	-1.59339400	1.96326600
C	1.08085100	0.84345300	3.08899700
H	1.02385000	1.91820500	2.89399700
H	1.14968600	0.70493200	4.17799200
H	1.99965600	0.47585500	2.62768800
C	0.88694300	-2.27180900	2.35670000
H	1.86663300	-1.79922000	2.25813200
H	0.85243300	-2.78700700	3.32785800
H	0.79996600	-3.03660400	1.57801700
C	-2.14722600	-2.96552700	1.71228300
H	-2.40790400	-3.46081900	2.65902500

H	-3.05295400	-2.93439100	1.09997200
H	-1.42335700	-3.60579000	1.19962000
C	-3.83092400	-0.24915400	1.82742700
H	-4.35754700	-0.45134400	2.77046900
H	-4.11340400	0.75497700	1.49902600
H	-4.19855100	-0.96184300	1.08305000
C	-1.86539300	2.08655100	2.82032900
H	-1.09327400	2.82551900	2.59274400
H	-2.78806400	2.40809000	2.32828500
H	-2.04339000	2.11112500	3.90493100
C	5.06735000	-2.11422100	1.27171400
C	3.74079300	-0.63984200	0.10000300
C	4.44964100	-0.92066700	-1.11108700
C	5.51072700	-1.85490800	-1.06928000
C	5.82657500	-2.45721300	0.12784900
H	5.30125300	-2.58149000	2.22828500
C	4.03706800	-0.23420000	-2.28228800
H	6.06022300	-2.08291200	-1.98010400
H	6.63409400	-3.17848400	0.20780300
C	3.00262000	0.65865500	-2.20091300
C	2.35195500	0.88765700	-0.94403000
H	4.54078000	-0.42996500	-3.22639000
H	2.65267200	1.18695600	-3.08138800
N	4.06956200	-1.24945300	1.27551100
N	2.71660300	0.25182300	0.15882500
C	1.29969200	1.94370600	-0.87130600
C	1.66943800	3.19293800	-1.39890600
C	0.82529300	4.30257000	-1.38950500
C	-0.45221500	4.14857600	-0.84689500
C	-0.84025900	2.90176700	-0.33505800
C	-0.00195600	1.77639300	-0.31367500
H	2.66961400	3.31403100	-1.80928400
H	1.16852900	5.24801400	-1.79401200
H	-1.85314300	2.83316800	0.04962100
Ir	-0.79465500	0.01101200	0.44394400
O	-1.39373700	5.13806200	-0.77683400
C	-1.05860700	6.41659600	-1.29414600
H	-0.83187300	6.37512200	-2.36819300
H	-1.93953000	7.04465700	-1.14037000
H	-0.20582100	6.86071900	-0.76309200
C	-4.07902700	-2.60879300	-2.92371100
C	-3.23502800	-1.55039800	-2.58975900
C	-1.96214800	-1.79745200	-2.05658500
C	-1.53748700	-3.11983300	-1.88141200
C	-2.38005800	-4.17966500	-2.22288500
C	-3.65309500	-3.92830200	-2.74013600
H	-5.06570200	-2.40612800	-3.33233700
H	-2.03945400	-5.20359200	-2.09052600
H	-4.30742500	-4.75430100	-3.00643300
C	-1.02907400	-0.65479600	-1.75955700
H	-1.82846600	0.23830200	-0.87711200
H	-1.06616600	0.13489800	-2.53045200
O	0.16252100	-0.89653200	-1.24632200
H	-0.54071500	-3.29989200	-1.49170300
H	-3.56415800	-0.52387400	-2.74233000

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IN9 SCF Done: E(RM06) = -1603.24039221

C	-1.37496500	1.01855100	2.28527400
C	-0.18263400	0.21779500	2.54185400
C	-0.49964300	-1.13331800	2.24657900
C	-2.44921100	0.09257500	1.92621200
C	-1.89645600	-1.21533900	1.86651600
C	1.11532000	0.73139900	3.09044600
H	1.23764500	1.79881100	2.88615100
H	1.14684200	0.59746700	4.18149000
H	1.96778000	0.21024500	2.64862400
C	0.40405500	-2.31797300	2.38958400
H	1.45595000	-2.03005700	2.43473200
H	0.15700000	-2.86772800	3.31001700
H	0.28304800	-3.01752100	1.55554400
C	-2.64480500	-2.49152000	1.62327600
H	-2.88956700	-2.97919400	2.57813000
H	-3.58362000	-2.31945900	1.09082300
H	-2.05650600	-3.20319800	1.03731900
C	-3.89873100	0.45167700	1.76599900
H	-4.42788500	0.32743900	2.72130400
H	-4.02426200	1.49121200	1.45180100
H	-4.39446600	-0.18329400	1.02626900
C	-1.56820200	2.44315000	2.72290100
H	-0.66941800	3.04296700	2.55867500
H	-2.38921800	2.92360100	2.18252500
H	-1.80707300	2.48465300	3.79493400
C	4.47126700	-3.12492700	1.46837300
C	3.48668400	-1.46179300	0.21571700
C	4.10098800	-1.95729500	-0.97775600
C	4.92906000	-3.10027300	-0.88391700
C	5.11929800	-3.69102500	0.34509300
H	4.61063800	-3.57710400	2.45031200
C	3.84147400	-1.25795500	-2.18510000
H	5.40351900	-3.49348000	-1.78039300
H	5.74812700	-4.56782800	0.46521200
C	3.04039900	-0.14857900	-2.15257600
C	2.47325500	0.28614600	-0.91022500
H	4.27899700	-1.61160700	-3.11609200
H	2.81503500	0.40504700	-3.05786700
N	3.68844300	-2.06239700	1.42323300
N	2.68644500	-0.36110200	0.22430400
C	1.73025900	1.58144000	-0.87969900
C	2.46301900	2.67600800	-1.36998100
C	1.98003800	3.98316400	-1.36477400
C	0.69807200	4.20066900	-0.85754900
C	-0.05579000	3.11438200	-0.39150600
C	0.41136000	1.78943700	-0.37910100
H	3.46968600	2.50368500	-1.74440600
H	2.59661300	4.79110100	-1.74173900
H	-1.05648800	3.34476200	-0.04094400
Ir	-0.88222400	0.31291600	0.29784600
O	0.08499500	5.42075600	-0.78516100
C	0.79177700	6.55207200	-1.27013700
H	1.02599400	6.45834300	-2.33924300
H	0.12781500	7.40764000	-1.12476400
H	1.72198500	6.72230900	-0.71132700
C	-4.52931100	-1.94280900	-2.72179600
C	-3.51034300	-1.03559400	-2.43674100
C	-2.26943700	-1.48380200	-1.95623100

C	-2.06038000	-2.86125800	-1.79281600
C	-3.07755000	-3.76970200	-2.08918700
C	-4.31636400	-3.31462300	-2.54800900
H	-5.48761100	-1.58254800	-3.08746600
H	-2.90096400	-4.83569900	-1.96799900
H	-5.10781100	-4.02294400	-2.77873400
C	-1.16844000	-0.50981800	-1.71608600
H	-1.89960900	1.31152900	-0.38470600
H	-1.16401500	0.34443100	-2.40589700
O	-0.01552000	-0.89005800	-1.23406400
H	-1.08884900	-3.20504400	-1.45140100
H	-3.67248800	0.03065200	-2.58182600

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2a-1 SCF Done: E(RM06) = -345.423119235

C	1.73382700	1.06318400	-0.00000200
C	0.35821100	1.29187600	0.00000000
C	-0.53501500	0.21114300	0.00000200
C	-0.04223300	-1.10401800	0.00000300
C	1.33015300	-1.33072000	0.00000100
C	2.21814800	-0.24748400	-0.00000200
H	2.42612100	1.90049500	-0.00000400
H	-0.02996900	2.30830800	-0.00000100
H	-0.74978800	-1.92775700	0.00000600
H	1.71417200	-2.34712800	0.00000100
H	3.28995300	-0.42767400	-0.00000400
C	-1.99084900	0.46758200	0.00000500
H	-2.27077200	1.54384100	0.00001500
O	-2.85164600	-0.39493200	-0.00000700

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TS8 SCF Done: E(RM06) = -2079.15228870

C	0.18037600	-0.71195000	-2.86115800
C	0.53254900	-2.09412700	-2.57964400
C	1.88976600	-2.11073100	-2.13813100
C	1.35647000	0.10123800	-2.58083800
C	2.39293100	-0.75996500	-2.12351800
C	-0.32205600	-3.28934100	-2.88702200
H	-1.38061100	-3.08563000	-2.70223500
H	-0.21810300	-3.57671700	-3.94261900
H	-0.04053400	-4.15600100	-2.28111600
C	2.66946100	-3.33458300	-1.77017600
H	3.22796100	-3.70877700	-2.64011800
H	3.39232200	-3.12535900	-0.97830300
H	2.01479700	-4.14296600	-1.43067300
C	3.81203700	-0.35379400	-1.86265100
H	4.35662900	-0.25523900	-2.81298700
H	3.86836000	0.60725600	-1.34612600
H	4.33658200	-1.09430200	-1.25599900
C	1.47195400	1.56101600	-2.89000800
H	1.61578700	1.70053700	-3.97151900
H	0.56522000	2.09868800	-2.59992500
H	2.32070200	2.01753300	-2.37691600
C	-0.97252300	-0.25191200	-3.70763700
H	-1.79613500	-0.96986300	-3.70143900
H	-1.34885600	0.71851500	-3.37472900
H	-0.64035100	-0.14921000	-4.75018600
C	4.24804100	-1.42938800	1.70801000
C	1.98672400	-1.80936400	1.83594900
C	2.12200500	-2.34245000	3.15535700
C	3.41037200	-2.38117000	3.73114200
C	4.48781300	-1.91684800	3.00864500
H	5.08015300	-1.06437200	1.10790500
C	0.95763000	-2.81102400	3.81913500
H	3.52945300	-2.77709700	4.73644100
H	5.49448100	-1.92414600	3.41324000
C	-0.24763600	-2.74607200	3.18399000
C	-0.33864200	-2.19647700	1.87037500
H	1.04089600	-3.21338500	4.82531400
H	-1.14696400	-3.09127800	3.67842400
N	3.05518800	-1.37622100	1.13405700
N	0.75467000	-1.73792800	1.22807700
C	-1.58148600	-2.07558700	1.14119600
C	-2.80798600	-2.58868100	1.60067100
C	-3.97279000	-2.44758000	0.86192600
C	-3.91177300	-1.76781400	-0.36708000
C	-2.69239700	-1.25165700	-0.83191100
C	-1.50874700	-1.39308800	-0.10674700
H	-2.86404900	-3.11595300	2.54821700
H	-4.90435400	-2.85141700	1.23941800
H	-2.71730100	-0.71178400	-1.76974000
Ir	0.33213900	-0.76065000	-0.68341300
H	-0.75209800	0.47089000	-0.96170600
O	-4.98007300	-1.55769100	-1.17728800
C	-6.26488700	-1.99570700	-0.74560500
H	-6.55714600	-1.51506800	0.19604700
H	-6.96011300	-1.69645100	-1.53262600
H	-6.30182300	-3.08642400	-0.62906200
C	2.92640100	2.22695800	0.76089100
C	1.67709000	2.82729400	0.41997700
C	1.68237200	4.23458900	0.11050000
C	2.90050800	4.94016500	0.09781000
C	4.10660500	4.32965800	0.40193200
C	4.09866700	2.96170700	0.74238300
H	2.92703100	1.17766700	1.02383700
H	2.85325500	5.99821900	-0.14527900
H	5.03485200	4.89402500	0.39655100
H	5.03451800	2.46902000	1.00233900
C	0.45003100	4.98472400	-0.13791900
H	-0.49222800	4.43890600	0.05964400
O	0.40278800	6.15513500	-0.51091600
N	0.50746700	2.13504800	0.40830700
O	0.57333100	0.83587600	0.80630800
C	-3.17349500	1.88662600	2.82609800
C	-2.61796500	1.80082200	1.54527300
C	-3.24043300	2.43239700	0.46269600
C	-4.42378300	3.15150100	0.69155400
C	-4.98143900	3.23080600	1.96714600
C	-4.35492200	2.59618100	3.04375000
H	-2.67196200	1.39748700	3.65806600
H	-1.69382800	1.25329600	1.39441100
H	-4.91129800	3.65784300	-0.14024500
H	-5.89758000	3.79574500	2.12301300
H	-4.78085400	2.66249700	4.04197700
C	-2.71102000	2.34685000	-0.96242700
H	-3.35835000	1.66188700	-1.53143700

H	-2.83073300	3.33642400	-1.43431900
O	-1.37610000	1.91802100	-1.13457300
H	-0.59824000	2.24867000	-0.37769600

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IN10 SCF Done: E(RM06) = -2079.22221171

C	1.55973900	0.08200900	-2.73516300
C	2.04341100	-1.27863400	-2.58720800
C	3.23698600	-1.22118600	-1.79234200
C	2.59234800	0.96788100	-2.19199600
C	3.61172000	0.18564000	-1.63401000
C	1.48873000	-2.50431900	-3.25078200
H	0.41206700	-2.43179200	-3.41940100
H	1.96880100	-2.64581600	-4.22945200
H	1.67008300	-3.40484800	-2.65685300
C	4.12225500	-2.38239700	-1.43858400
H	4.91543700	-2.51454100	-2.18866200
H	4.61066900	-2.23474100	-0.47002000
H	3.55717300	-3.31761300	-1.38590800
C	4.90725500	0.66738800	-1.05688800
H	5.68448200	0.68845400	-1.83548800
H	4.82009700	1.67817200	-0.64937300
H	5.26116600	0.01427200	-0.25627100
C	2.53026100	2.46208400	-2.26070000
H	2.78787300	2.80966800	-3.27168200
H	1.52375000	2.82666800	-2.03840800
H	3.22233700	2.93475400	-1.55862600
C	0.44887500	0.54252400	-3.63461700
H	-0.28977300	-0.24632400	-3.80486000
H	-0.07659800	1.40152500	-3.20679200
H	0.83709700	0.84338600	-4.61874200
C	4.43954400	0.89942500	2.59468200
C	2.71348100	-0.58097400	2.26793500
C	2.80390300	-1.03251600	3.62218700
C	3.78930700	-0.45538000	4.45227800
C	4.61657700	0.52166500	3.94203800
H	5.07651700	1.67014500	2.16297600
C	1.88890200	-2.02286300	4.06636700
H	3.87363000	-0.78703000	5.48420100
H	5.38296600	0.99532200	4.54696500
C	0.93814300	-2.48834700	3.20447600
C	0.87925100	-2.00172700	1.86519600
H	1.94422000	-2.38334300	5.09032400
H	0.21201700	-3.22159900	3.53336200
N	3.53550800	0.37519300	1.78251100
N	1.77666700	-1.10190700	1.40893700
C	-0.14755800	-2.38397600	0.91616200
C	-1.17992400	-3.29314100	1.20502600
C	-2.19814300	-3.53590700	0.29249600
C	-2.19420300	-2.83311500	-0.92605800
C	-1.15865500	-1.93448900	-1.22521700
C	-0.10104300	-1.71041300	-0.34060000
H	-1.20576300	-3.82111600	2.15443300
H	-2.98468300	-4.24036000	0.53521400
H	-1.21919000	-1.40777800	-2.17125200
Ir	1.46651200	-0.48696300	-0.62547000
H	-4.02983200	1.85637200	-0.64643100
O	-3.15734300	-2.96168700	-1.87927000
C	-4.23072900	-3.86608800	-1.64542100
H	-4.81165600	-3.58595700	-0.75802100
H	-4.87095100	-3.80274200	-2.52816800
H	-3.87222800	-4.89791600	-1.53620500
C	0.66409100	3.55629300	0.90515100
C	-0.36848600	3.10111800	0.04962100
C	-1.30631600	4.05896100	-0.45087400
C	-1.22829200	5.39748800	-0.01899500
C	-0.22746300	5.82518500	0.83812000
C	0.72502800	4.88909700	1.28198800
H	1.38214200	2.83073000	1.26608000
H	-1.96884800	6.09033000	-0.40902500
H	-0.16965200	6.86369900	1.15099400
H	1.52464900	5.21148700	1.94593300
C	-2.30421200	3.70251900	-1.45998000
H	-2.10259000	2.76438900	-2.01582300
O	-3.29372000	4.37045500	-1.74994800
N	-0.45669700	1.77281900	-0.30227900
O	0.30691200	0.89061300	0.45628400
C	-7.12725500	-0.96574400	0.13772600
C	-5.82085400	-0.48436900	0.03799600
C	-5.26264200	0.27627400	1.07514800
C	-6.03737000	0.54623500	2.20955400
C	-7.34149200	0.05731200	2.31479500
C	-7.89071400	-0.69934600	1.27779400
H	-7.55161600	-1.54769100	-0.67681200
H	-5.22577300	-0.68693500	-0.84810100
H	-5.61822100	1.14680900	3.01425700
H	-7.93118600	0.27781400	3.20103300
H	-8.90856300	-1.07306900	1.35378600
C	-3.83503600	0.77555000	0.98190100
H	-3.68107600	1.61718000	1.67219900
H	-3.13187500	-0.01347700	1.27001400
O	-3.45067600	1.13363600	-0.34934400
H	-1.40476200	1.41449400	-0.42137400

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TS8' SCF Done: E(RM06) = -1732.49020995

C	-0.36403200	-2.83276800	0.36507000
C	-1.51296100	-2.75012300	-0.52149100
C	-2.61513800	-2.25711800	0.23191400
C	-0.79311900	-2.35392100	1.67051700
C	-2.16222300	-1.95356300	1.55561100
C	-1.55342700	-3.23757600	-1.94093900
H	-0.55722600	-3.23875200	-2.39212500
H	-1.94090700	-4.26485400	-1.99770100
H	-2.19782500	-2.61137700	-2.56765300
C	-4.00688100	-2.06479100	-0.28787100
H	-4.62717600	-2.94675900	-0.07209000
H	-4.49557800	-1.20136600	0.17131900
H	-4.01857400	-1.92316100	-1.37346900
C	-2.96293600	-1.39225000	2.69099400
H	-2.98358100	-2.08949700	3.53922600
H	-2.52051100	-0.45332000	3.04392400
H	-3.99790800	-1.19378500	2.40057700
C	-0.03524300	-2.46139800	2.95982200
H	-0.39695800	-3.32564100	3.53542200
H	1.03559600	-2.59526100	2.79190300

H	-0.16036200	-1.56518900	3.57213400
C	0.84184500	-3.69543400	0.12118500
H	1.15968400	-3.67481100	-0.92357800
H	1.69230700	-3.39780500	0.74058100
H	0.59881900	-4.73775400	0.37127700
C	-4.14262600	1.90555400	1.08664300
C	-2.48737900	1.65731400	-0.47812300
C	-2.99257200	2.75207100	-1.24353400
C	-4.13236100	3.42882500	-0.75711300
C	-4.71012900	3.01374700	0.42338300
H	-4.58793600	1.54540800	2.01249400
C	-2.32818900	3.09683500	-2.45102400
H	-4.53373200	4.26707900	-1.32063700
H	-5.58149300	3.51013100	0.83764500
C	-1.22225100	2.39568900	-2.83706000
C	-0.72631600	1.33380700	-2.02551200
H	-2.70497500	3.92076100	-3.05140500
H	-0.69869800	2.65266500	-3.74993100
N	-3.08092100	1.24022500	0.65803400
N	-1.36147400	0.97899000	-0.88678300
C	0.48013000	0.59264000	-2.30351500
C	1.30507000	0.82344400	-3.41871800
C	2.49703900	0.13528800	-3.58554800
C	2.88359600	-0.79461900	-2.60239700
C	2.06158100	-1.03827600	-1.49099700
C	0.84480600	-0.37719500	-1.32227200
H	1.02418600	1.55815900	-4.16749400
H	3.11928100	0.33184300	-4.45021000
H	2.42429000	-1.74976900	-0.75922800
Ir	-0.46735700	-0.62972300	0.19621100
H	0.97690700	-0.68176200	1.01162600
O	4.03433600	-1.50996900	-2.64276800
C	4.96151100	-1.26478200	-3.69596200
H	5.29901200	-0.22110500	-3.69842300
H	5.81404600	-1.91740400	-3.49764300
H	4.53580100	-1.51675000	-4.67552000
C	1.62735400	2.72559600	1.20315800
C	1.97495900	1.51821100	1.88296700
C	3.34192600	1.38725900	2.32543000
C	4.26977200	2.40904800	2.05147600
C	3.91003300	3.56353400	1.37506300
C	2.57016700	3.70759000	0.96037100
H	0.59798400	2.85712600	0.89625900
H	5.28682400	2.25845900	2.40397900
H	4.63785200	4.34578200	1.17800600
H	2.26524900	4.61382200	0.43891300
C	3.79122600	0.22321000	3.08601200
H	2.99676100	-0.50127300	3.35006300
O	4.94898900	0.01629800	3.44831500
N	1.09659300	0.51402300	2.15942300
O	-0.20000500	0.75956000	1.64615100

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IN10' SCF Done: E(RM06) = -1732.58402243

C	1.38757400	-2.88021300	0.15082000
C	2.55816000	-2.10278800	0.45296200
C	3.06751100	-1.54902900	-0.80247900
C	1.06058600	-2.65393000	-1.24330100
C	2.15187600	-1.86677000	-1.82030500
C	3.30719400	-2.10534300	1.75473700
H	2.64092200	-2.29748900	2.60082100
H	4.08341600	-2.88448900	1.75880500
H	3.80537300	-1.14738500	1.93485100
C	4.39149800	-0.86576700	-0.95840500
H	5.18813200	-1.61603000	-1.07249600
H	4.41511100	-0.21775300	-1.83777800
H	4.63729200	-0.25313600	-0.08870200
C	2.17396400	-1.41509800	-3.24710600
H	2.09379600	-2.26710600	-3.93398500
H	1.32240300	-0.74677800	-3.43113900
H	3.09064400	-0.87005400	-3.48785500
C	0.01536400	-3.36583000	-2.05535900
H	0.44377900	-4.23436800	-2.57621600
H	-0.80223800	-3.73757800	-1.43045100
H	-0.41654800	-2.70605200	-2.81507900
C	0.71855300	-3.84122400	1.08765100
H	0.69733900	-3.46143300	2.11303500
H	-0.31025100	-4.05821300	0.79274400
H	1.26802600	-4.79304400	1.09318700
C	3.87097600	2.68104400	-0.36024400
C	2.01688300	1.98515600	0.80333000
C	2.05515600	3.15541600	1.62513700
C	3.08503000	4.09437000	1.39819200
C	4.00208900	3.86454400	0.39563000
H	4.57975400	2.47111600	-1.16001100
C	1.04992600	3.32282800	2.61273500
H	3.13084200	4.98935000	2.01379200
H	4.80401500	4.56396500	0.18266700
C	0.06278000	2.38636700	2.72383400
C	0.05353600	1.24476700	1.87168600
H	1.06784800	4.20034200	3.25383700
H	-0.72763600	2.50590200	3.45468800
N	2.92844500	1.77180500	-0.16922500
N	1.03470800	1.03526500	0.96494200
C	-1.00062000	0.25065000	1.87067500
C	-2.15558700	0.32695300	2.66777200
C	-3.18184200	-0.59954000	2.53794900
C	-3.05158600	-1.62332500	1.58278100
C	-1.89155300	-1.71361000	0.79580000
C	-0.84164900	-0.79825900	0.91925200
H	-2.27874600	1.12915800	3.38989300
H	-4.06863300	-0.51330900	3.15422100
H	-1.85255300	-2.52170800	0.07219100
Ir	0.85859400	-0.77077700	-0.16460300
H	-1.83058000	-0.47040500	-1.49874900
O	-3.99418500	-2.57185400	1.34743900
C	-5.25442200	-2.46151200	2.00312500
H	-5.74991900	-1.51516900	1.75528100
H	-5.85719300	-3.29152900	1.62871500
H	-5.15357900	-2.55393100	3.09200400
C	-1.43892900	2.79249200	-1.76882900
C	-2.11964200	1.54836100	-1.70151200
C	-3.54916500	1.56717700	-1.57641800
C	-4.21753200	2.80833300	-1.51739400
C	-3.53904400	4.01176800	-1.58086100
C	-2.13648900	3.98541200	-1.70771100

H	-0.36273400	2.77626800	-1.88122500
H	-5.29904000	2.77783500	-1.42087400
H	-4.07390400	4.95615700	-1.53943000
H	-1.58319900	4.92074400	-1.76337500
C	-4.36062200	0.35242600	-1.50457900
H	-3.82403300	-0.61012800	-1.63620500
O	-5.57517000	0.32408800	-1.32726100
N	-1.41045100	0.38729700	-1.83286600
O	-0.03045200	0.40408400	-1.67518800

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TS8" SCF Done: E(RM06) = -1732.48776846

C	0.16026100	-2.89291400	0.30272900
C	-0.38328300	-3.01992400	-1.05874900
C	-1.74164100	-2.70931600	-1.00978200
C	-0.94043300	-2.65069400	1.19733900
C	-2.09249000	-2.40641200	0.38175400
C	0.43626500	-3.38420800	-2.25834000
H	0.78419500	-4.42480500	-2.19828900
H	-0.13280800	-3.27941200	-3.18669600
H	1.32820100	-2.75132300	-2.34051700
C	-2.71948600	-2.66467300	-2.14572900
H	-3.45389400	-3.47868400	-2.06570500
H	-3.28740900	-1.72687600	-2.15546900
H	-2.22346000	-2.76356900	-3.11565900
C	-3.50069800	-2.29444900	0.88819200
H	-3.53676300	-1.82149000	1.87270400
H	-4.12971500	-1.71164800	0.21169800
H	-3.94558000	-3.29691200	0.97843800
C	-0.92308200	-2.76477900	2.69307800
H	-1.35322200	-1.87263700	3.15482800
H	-1.48430100	-3.65413400	3.01231800
H	0.09936700	-2.86074700	3.06657800
C	1.49294600	-3.44487600	0.72959600
H	1.91924300	-2.89017200	1.56978300
H	1.38203500	-4.49101600	1.04956300
H	2.21968700	-3.43787600	-0.08696500
C	-4.57071000	1.30453000	0.46279100
C	-2.52931800	1.54749700	-0.56842400
C	-2.96982000	2.73804000	-1.22517300
C	-4.28990200	3.17977600	-0.98747300
C	-5.10264800	2.46521800	-0.13453300
H	-5.18259500	0.71472500	1.14318200
C	-2.06231400	3.42430900	-2.07320400
H	-4.64032400	4.08371600	-1.47909400
H	-6.12038500	2.77460000	0.07962400
C	-0.79652300	2.93830700	-2.22129700
C	-0.38927200	1.75645000	-1.53779300
H	-2.38298900	4.32765600	-2.58524200
H	-0.08398000	3.44939400	-2.85644100
N	-3.34291800	0.85695500	0.25385200
N	-1.24182700	1.07195000	-0.73928000
C	0.94112000	1.19981500	-1.63038200
C	1.97400900	1.75865400	-2.40240200
C	3.23266700	1.17466700	-2.44437500
C	3.46560400	0.01287700	-1.68952300
C	2.43756300	-0.53859400	-0.90382400
C	1.16395300	0.02495500	-0.86051700
H	1.80965400	2.66072300	-2.98445300
H	4.01437400	1.62113800	-3.04740100
H	2.69026300	-1.41454500	-0.32115300
Ir	-0.47796800	-0.71789500	0.13436700
H	-1.51860400	-0.14640100	1.26208200
O	4.64706200	-0.65134500	-1.65785500
C	5.75456500	-0.11610100	-2.37413800
H	6.01405900	0.88916300	-2.01967300
H	6.58952800	-0.79186700	-2.17841800
H	5.56019300	-0.08620100	-3.45408100
C	0.41737300	2.56977200	2.06181600
C	1.04305300	1.30945900	2.02449100
C	2.45978600	1.25659300	2.03032800
C	3.20321700	2.45000000	1.98545100
C	2.57177400	3.68489500	1.96415100
C	1.16846300	3.73661300	2.01442500
H	-0.66245200	2.59338700	2.13686800
H	4.28639600	2.37034500	1.99666900
H	3.15454400	4.60182900	1.93539700
H	0.66352100	4.70038700	2.02251200
C	3.18468400	-0.01594300	2.20524600
H	2.54340200	-0.88603800	2.42988500
O	4.40309600	-0.13041400	2.16296300
N	0.29487100	0.08629100	2.12052500
O	-0.88286300	0.33095300	2.72824100

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IN10" SCF Done: E(RM06) = -1732.58822788

C	0.24210200	-2.88626700	0.72325600
C	0.14286500	-2.88927800	-0.72440700
C	-1.20943500	-2.57293200	-1.06826700
C	-1.11516300	-2.74847300	1.24672900
C	-1.99739400	-2.55127200	0.16871300
C	1.22256500	-3.27915200	-1.68876900
H	1.15658100	-4.35750000	-1.89209700
H	1.13085400	-2.75436800	-2.64403600
H	2.22111200	-3.07987100	-1.29471700
C	-1.78325400	-2.55199600	-2.45588100
H	-2.12451200	-3.55485100	-2.75130500
H	-2.64577700	-1.88236800	-2.52906800
H	-1.04326200	-2.22457100	-3.19201500
C	-3.49293600	-2.46210500	0.22882200
H	-3.84031500	-2.09556400	1.19823700
H	-3.89314400	-1.79731000	-0.54077100
H	-3.93972200	-3.45442900	0.06930000
C	-1.45034100	-2.81450400	2.70453600
H	-2.48513200	-2.52571500	2.90055200
H	-1.30575500	-3.83888800	3.07590700
H	-0.80533800	-2.14789000	3.28244300
C	1.41902000	-3.34217100	1.53686500
H	1.43185900	-2.86419600	2.52084600
H	1.38538700	-4.42993800	1.69740800
H	2.36934400	-3.11573400	1.04503500
C	-4.46034300	1.18839300	0.34924400
C	-2.44256000	1.34556100	-0.76057400
C	-2.95805900	2.37654700	-1.60538100
C	-4.30756000	2.75581700	-1.44632800
C	-5.07466300	2.15375700	-0.46997500

H	-5.01958700	0.72427600	1.15912300
C	-2.07389200	2.98671400	-2.53464700
H	-4.71873700	3.53022900	-2.08890500
H	-6.11374700	2.42279500	-0.31234600
C	-0.76883000	2.59131700	-2.56810000
C	-0.30696100	1.53693200	-1.72353400
H	-2.44124700	3.77362200	-3.18786900
H	-0.07212900	3.06606300	-3.24771400
N	-3.20211000	0.79111000	0.21194000
N	-1.14957300	0.89602700	-0.87901200
C	1.06088300	1.07429100	-1.69560200
C	2.09965600	1.66307500	-2.44061300
C	3.40525400	1.20899000	-2.33385300
C	3.68000500	0.14534600	-1.45396800
C	2.64857100	-0.44300300	-0.70621900
C	1.32382600	-0.01325200	-0.80864600
H	1.90060700	2.49482700	-3.11019200
H	4.19100000	1.67839100	-2.91357800
H	2.93160000	-1.24149000	-0.03023500
Ir	-0.28855400	-0.85605500	0.07423800
H	-2.09606800	0.38411900	1.69126100
O	4.91420400	-0.38776100	-1.27147800
C	6.02374600	0.20582700	-1.93551200
H	6.15063600	1.25643900	-1.64605500
H	6.90007800	-0.36178300	-1.61547800
H	5.92803300	0.13468000	-3.02685300
C	-0.32932400	2.71683400	2.14692000
C	0.43276100	1.52528400	2.02139400
C	1.85381500	1.65250900	2.11879200
C	2.44789400	2.92630700	2.19056000
C	1.68410600	4.08186500	2.23053700
C	0.28393000	3.95782300	2.23419400
H	-1.40917700	2.64200700	2.16933500
H	3.53176700	2.96460100	2.25768200
H	2.15378200	5.05963700	2.29466600
H	-0.33649500	4.84961000	2.30374800
C	2.71174700	0.47938900	2.32806000
H	2.16557400	-0.47074200	2.47172400
O	3.93518400	0.51049100	2.41933700
N	-0.14413700	0.26704000	1.88217100
O	-1.47949300	0.29525200	2.45387600

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TS8-1 SCF Done: E(RM06) = -1966.10951799

C	0.80064400	-0.56136300	-2.57507800
C	1.15213700	0.83850800	-2.74972400
C	-0.06525000	1.59690300	-2.76198300
C	-0.63843100	-0.62467500	-2.43208600
C	-1.16264300	0.70839900	-2.52957600
C	2.51930700	1.36227000	-3.08053600
H	3.30267700	0.76457800	-2.60701400
H	2.69173400	1.33816100	-4.16563500
H	2.64764900	2.39782300	-2.74977000
C	-0.15329000	3.07457700	-2.98488400
H	-0.22468500	3.29354100	-4.05985900
H	-1.03057700	3.50430000	-2.49768000
H	0.73452100	3.59274800	-2.60874500
C	-2.62169900	1.05335600	-2.55741100
H	-3.08767700	0.65706000	-3.47068900
H	-3.15485600	0.62934200	-1.70265400
H	-2.77685800	2.13400500	-2.54919800
C	-1.44720500	-1.88310500	-2.42363000
H	-1.62486200	-2.20824000	-3.45944500
H	-0.92777300	-2.68880300	-1.90104200
H	-2.41869000	-1.73783700	-1.94838000
C	1.66494000	-1.74716300	-2.90028300
H	2.72718500	-1.49193000	-2.90430000
H	1.50502100	-2.57043900	-2.19872000
H	1.41634800	-2.11188400	-3.90658200
C	-2.80070000	3.58637500	0.17962900
C	-0.74140600	2.88103900	0.90447000
C	-0.74197900	3.85362100	1.95167800
C	-1.87042000	4.69269800	2.08115200
C	-2.91666900	4.55816300	1.19539600
H	-3.60483100	3.46613300	-0.54447500
C	0.39117500	3.93547000	2.80242500
H	-1.89289300	5.43157800	2.87815800
H	-3.80473100	5.17819100	1.25988000
C	1.44779800	3.09792300	2.59351000
C	1.39952300	2.13131700	1.54616900
H	0.40442200	4.66485400	3.60807900
H	2.32019000	3.14419900	3.23329300
N	-1.76205300	2.77922900	0.02882300
N	0.32236100	2.02218700	0.74442200
C	2.47189000	1.20583900	1.25693500
C	3.73103800	1.25745600	1.88051600
C	4.74468600	0.37470700	1.53726200
C	4.48509200	-0.59119400	0.55013800
C	3.22594900	-0.65740000	-0.06627700
C	2.19641200	0.22863400	0.25575600
H	3.93797500	2.00545300	2.64007200
H	5.70794300	0.43901200	2.02847900
H	3.08349400	-1.44631200	-0.79207300
Ir	0.36188900	0.33471500	-0.62239900
H	0.64029700	-1.28607000	-0.06588300
O	5.38815700	-1.51452000	0.12804800
C	6.68501400	-1.52415000	0.71683600
H	6.63635400	-1.71593500	1.79602900
H	7.22526300	-2.33967800	0.23173300
H	7.21670100	-0.58156100	0.53494200
C	-3.75532400	-0.07415200	1.03323300
C	-3.05855900	-1.30350400	0.78399800
C	-3.87662700	-2.48492900	0.60262100
C	-5.27727200	-2.39586900	0.74600200
C	-5.91880400	-1.20067900	1.01451200
C	-5.13015800	-0.03505400	1.14270300
H	-3.16183100	0.82048900	1.15782100
H	-5.83894400	-3.31712600	0.61493800
H	-6.99931800	-1.15437800	1.11766800
H	-5.61486400	0.91933000	1.34506000
C	-3.31232700	-3.77460500	0.22546400
H	-2.22378100	-3.77962800	0.03094800
O	-3.94890500	-4.82153700	0.09256300
N	-1.71094100	-1.38570600	0.77847500
O	-1.04699100	-0.18505700	0.91716300
C	1.19450400	-2.41479500	2.61687400

H	0.26780100	-1.90838400	2.90506100
H	1.92866600	-1.65332000	2.33960200
H	1.57745800	-2.95723600	3.49042800
C	0.93925800	-3.38328500	1.45369100
C	2.23951300	-4.03296700	0.97247000
H	2.97629900	-3.28095200	0.67564800
H	2.68335600	-4.64196100	1.76941700
H	2.04511600	-4.68589400	0.11377100
C	-0.05792600	-4.47092000	1.88436600
H	-0.99551800	-4.02814600	2.23711900
H	-0.28609000	-5.14383800	1.05045300
H	0.35863300	-5.07102700	2.70263000
O	0.35915800	-2.68019300	0.32007200
H	-0.64188000	-2.31750400	0.57277000

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IN11 SCF Done: E(RM06) = -2079.18976561

C	-0.59292800	-2.48153700	-2.06560900
C	0.85917500	-2.40624300	-1.98943200
C	1.25539800	-1.22100100	-2.70348700
C	-1.04914600	-1.34481600	-2.85413500
C	0.08804400	-0.58057400	-3.26726900
C	1.77160300	-3.45882000	-1.43437800
H	1.28236600	-4.02049200	-0.63342800
H	2.05091300	-4.17350900	-2.22227400
H	2.68191400	-3.02132600	-1.01975600
C	2.67014400	-0.78844800	-2.93063400
H	3.04478100	-1.25475800	-3.85354300
H	2.75145300	0.29487300	-3.06270400
H	3.32804900	-1.09133100	-2.11252400
C	0.07064100	0.62294900	-4.16446500
H	0.04279600	0.32678500	-5.22280900
H	-0.80545500	1.25261700	-3.97909000
H	0.96195100	1.24191200	-4.02695200
C	-2.47875200	-1.06290700	-3.19907000
H	-2.77104400	-1.63669200	-4.08945900
H	-3.14828100	-1.34598800	-2.38237300
H	-2.64253200	-0.00381400	-3.41190700
C	-1.43189200	-3.65574600	-1.65956400
H	-1.04799700	-4.13421100	-0.75528000
H	-2.47172900	-3.37109800	-1.47427700
H	-1.43309300	-4.40692000	-2.46217600
C	6.16243200	-0.87302900	-0.33521700
C	4.16690200	-0.75126900	0.81098400
C	4.74477600	0.12988800	1.77945400
C	6.10495900	0.49106000	1.63496900
C	6.82373700	-0.01435100	0.57484200
H	6.71249300	-1.27870400	-1.18409100
C	3.90218100	0.59092900	2.82398000
H	6.56228200	1.15880700	2.36178500
H	7.87061600	0.23169600	0.42650000
C	2.60322600	0.16135700	2.87178800
C	2.11109100	-0.74703500	1.87655100
H	4.29390500	1.28265800	3.56632100
H	1.93174800	0.51414300	3.64689600
N	4.89532100	-1.23212900	-0.23796700
N	2.87462500	-1.16717800	0.87770500
C	0.73428900	-1.29801900	2.02617500
C	0.42100200	-1.76710500	3.31490200
C	-0.79321700	-2.37194400	3.63399900
C	-1.74005300	-2.50882000	2.61707800
C	-1.44422900	-2.03581600	1.32918300
C	-0.23288900	-1.41638900	0.98115300
H	1.16997500	-1.68715100	4.09921100
H	-0.97434800	-2.72750800	4.64184800
H	-2.22526900	-2.15270400	0.58511300
Ir	-0.10162000	-0.71339900	-0.97098900
H	-2.64166900	0.10324700	1.04789300
O	-2.97518800	-3.07077700	2.77084200
C	-3.34420200	-3.53805200	4.06175300
H	-3.34462400	-2.72669600	4.80137400
H	-4.35916000	-3.92865700	3.96078700
H	-2.68087300	-4.34270300	4.40578600
C	-3.68817700	2.36202800	-1.07592100
C	-3.79479000	1.37014200	-0.07358300
C	-5.00064300	1.30952300	0.69299600
C	-6.02585200	2.24020800	0.43743500
C	-5.90648500	3.21073100	-0.54429300
C	-4.72421500	3.25742300	-1.30039600
H	-2.77515800	2.40867400	-1.65472600
H	-6.92328500	2.16260600	1.04410000
H	-6.70975900	3.91821100	-0.72731700
H	-4.60879000	4.01171000	-2.07583000
C	-5.23604500	0.29797200	1.73161500
H	-4.44784800	-0.47041700	1.86735000
O	-6.23980600	0.24123600	2.43207400
N	-2.77529300	0.45579300	0.10614500
O	-1.54522500	0.79961300	-0.45757600
C	1.37786000	2.20682500	-0.83149700
O	0.80459700	1.17766600	0.00875100
H	-0.15124800	1.42051200	0.18816400
H	2.33890000	1.81593300	-1.17029200
H	0.73320900	2.35629500	-1.70593300
C	1.55884000	3.50145900	-0.07459000
C	2.82393300	3.90594500	0.36887600
C	0.45097600	4.31608500	0.20318500
C	2.98190700	5.10071300	1.07453300
H	3.68984600	3.28286600	0.15810100
C	0.60457400	5.50585200	0.91489300
H	-0.53749700	4.01663500	-0.13940200
C	1.87216400	5.90173100	1.35069700
H	3.97058700	5.40537800	1.40816200
H	-0.26270800	6.12653300	1.12383400
H	1.99371400	6.83157800	1.90013000

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TS9 SCF Done: E(RM06) = -2079.18347504

C	0.08890000	-3.36008800	-1.13985500
C	1.45623800	-2.87952800	-1.03730900
C	1.71387800	-2.04079800	-2.20911300
C	-0.50143200	-2.70955400	-2.28045700
C	0.52527200	-1.93746200	-2.97357100
C	2.49938800	-3.41210800	-0.10332700
H	2.05263400	-3.73387500	0.84138500
H	2.99266700	-4.28437100	-0.55797600
H	3.25639100	-2.66195400	0.13225100

C	3.04889900	-1.44421000	-2.53028800
H	3.65747800	-2.18791500	-3.06434400
H	2.96568400	-0.56466800	-3.17446500
H	3.59451500	-1.16916600	-1.62319700
C	0.31973300	-1.19152600	-4.25882700
H	0.27948300	-1.88398400	-5.11122300
H	-0.61868300	-0.62753900	-4.25072400
H	1.13267300	-0.48493100	-4.44905800
C	-1.90249600	-2.89565700	-2.77779200
H	-1.92745500	-3.69111200	-3.53579200
H	-2.58364500	-3.18059300	-1.97180500
H	-2.28853100	-1.98186500	-3.23685300
C	-0.52710000	-4.43504100	-0.29660100
H	-0.21918900	-4.35593300	0.74903700
H	-1.61950100	-4.40464700	-0.32701100
H	-0.21353200	-5.42111700	-0.66659100
C	5.91408300	-0.13401800	0.86421000
C	3.72780800	0.02977000	1.57445300
C	4.02584800	1.22216400	2.30748100
C	5.35352800	1.70943200	2.29075500
C	6.30850400	1.02734200	1.57010200
H	6.65379600	-0.68079300	0.27965700
C	2.95248800	1.85080300	2.98957900
H	5.59966200	2.61354200	2.84325200
H	7.34031200	1.36241300	1.53065200
C	1.70595300	1.28748700	2.93693600
C	1.50156800	0.06775900	2.21023400
H	3.12836100	2.77764100	3.53064900
H	0.86347600	1.76653600	3.42322800
N	4.68705700	-0.62264800	0.85385100
N	2.48696600	-0.52154800	1.54889100
C	0.16375200	-0.58647600	2.26552300
C	-0.44947900	-0.60778400	3.53102400
C	-1.68976500	-1.19656400	3.77154200
C	-2.34893800	-1.79776200	2.69769000
C	-1.74421000	-1.79579100	1.42977300
C	-0.50161200	-1.19889500	1.15872800
H	0.07274200	-0.16608200	4.37590000
H	-2.11128000	-1.18427400	4.77003600
H	-2.30894600	-2.26474800	0.62967000
Ir	0.10325700	-1.22118800	-0.82228900
H	-2.54181400	0.20757700	0.46610500
O	-3.57329300	-2.39592600	2.76706800
C	-4.28502100	-2.33018100	3.99783100
H	-4.47683500	-1.29177400	4.29616600
H	-5.23836000	-2.83225100	3.81890100
H	-3.75087200	-2.85119600	4.80323700
C	-3.39083900	2.35309800	-1.86248100
C	-3.56096900	1.55459200	-0.71150700
C	-4.62164500	1.87445800	0.18911800
C	-5.43078800	2.99514800	-0.07147500
C	-5.24232900	3.78555100	-1.19518400
C	-4.21833000	3.44581000	-2.09164600
H	-2.60305200	2.09815700	-2.55992600
H	-6.22181600	3.21017100	0.64089700
H	-5.87983600	4.64424800	-1.38317800
H	-4.06012000	4.04584500	-2.98478900
C	-4.93271000	1.04601600	1.36348400
H	-4.37464400	0.09327600	1.45530100
O	-5.77329400	1.32553300	2.20932800
N	-2.75938500	0.44635900	-0.49608400
O	-1.59510100	0.35863200	-1.28352300
C	1.37845400	1.57455700	-1.41163000
O	0.52673900	0.88749600	-0.49686700
H	-0.65947400	0.93895600	-0.84572800
H	2.37063600	1.11375000	-1.38929200
H	0.99123000	1.46410000	-2.43854500
C	1.50534400	3.04757100	-1.07156000
C	2.76648300	3.62450600	-0.87954600
C	0.37146500	3.86803100	-0.97667200
C	2.89764500	4.98794800	-0.60247000
H	3.65498900	3.00033300	-0.94516300
C	0.49726300	5.22754300	-0.69141100
H	-0.61798500	3.44362900	-1.12745500
C	1.76220700	5.79326300	-0.50545200
H	3.88595700	5.41761900	-0.45803300
H	-0.39286800	5.84738200	-0.61874900
H	1.85986200	6.85358100	-0.28659300

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1a-3 SCF Done: E(RM06) = -475.918672462

C	-1.25635900	-1.13751100	-0.04698200
C	-0.65583400	0.12972000	-0.02729600
C	0.76166800	0.22292700	-0.00250400
C	1.52658500	-0.95610400	0.03599200
C	0.92677900	-2.20727400	0.02847500
C	-0.47040600	-2.28647000	-0.01978100
H	-2.33651600	-1.20595200	-0.06169600
H	2.60680700	-0.84983000	0.05981700
H	1.53020600	-3.10962000	0.05354100
H	-0.95854200	-3.25774700	-0.02749900
C	1.46815100	1.51562300	-0.06162700
H	0.83576900	2.41352400	-0.22015000
O	2.67975600	1.64534900	0.02643300
N	-1.43287300	1.30456200	-0.09655900
H	-1.13781200	2.01863700	0.56302300
O	-2.81425400	1.08637100	0.16716500
H	-3.23732600	1.31982300	-0.67757000

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TS10 SCF Done: E(RM06) = -1603.22749750

C	-1.45744300	0.70661000	2.39596000
C	-0.12445800	0.13192000	2.55090900
C	-0.22893200	-1.27623800	2.27496900
C	-2.34763600	-0.36993200	2.02546800
C	-1.59523100	-1.59339400	1.96326600
C	1.08085100	0.84345300	3.08899700
H	1.02385000	1.91820500	2.89399700
H	1.14968600	0.70493200	4.17799200
H	1.99965600	0.47585500	2.62768800
C	0.88694300	-2.27180900	2.35670000
H	1.86663300	-1.79922000	2.25813200
H	0.85243300	-2.78700700	3.32785800
H	0.79996600	-3.03660400	1.57801700
C	-2.14722600	-2.96552700	1.71228300
H	-2.40790400	-3.46081900	2.65902500

H	-3.05295400	-2.93439100	1.09997200
H	-1.42335700	-3.60579000	1.19962000
C	-3.83092400	-0.24915400	1.82742700
H	-4.35754700	-0.45134400	2.77046900
H	-4.11340400	0.75497700	1.49902600
H	-4.19855100	-0.96184300	1.08305000
C	-1.86539300	2.08655100	2.82032900
H	-1.09327400	2.82551900	2.59274400
H	-2.78806400	2.40809000	2.32828500
H	-2.04339000	2.11112500	3.90493100
C	5.06735000	-2.11422100	1.27171400
C	3.74079300	-0.63984200	0.10000300
C	4.44964100	-0.92066700	-1.11108700
C	5.51072700	-1.85490800	-1.06928000
C	5.82657500	-2.45721300	0.12784900
H	5.30125300	-2.58149000	2.22828500
C	4.03706800	-0.23420000	-2.28228800
H	6.06022300	-2.08291200	-1.98010400
H	6.63409400	-3.17848400	0.20780300
C	3.00262000	0.65865500	-2.20091300
C	2.35195500	0.88765700	-0.94403000
H	4.54078000	-0.42996500	-3.22639000
H	2.65267200	1.18695600	-3.08138800
N	4.06956200	-1.24945300	1.27551100
N	2.71660300	0.25182300	0.15882500
C	1.29969200	1.94370600	-0.87130600
C	1.66943800	3.19293800	-1.39890600
C	0.82529300	4.30257000	-1.38950500
C	-0.45221500	4.14857600	-0.84689500
C	-0.84025900	2.90176700	-0.33505800
C	-0.00195600	1.77639300	-0.31367500
H	2.66961400	3.31403100	-1.80928400
H	1.16852900	5.24801400	-1.79401200
H	-1.85314300	2.83316800	0.04962100
Ir	-0.79465500	0.01101200	0.44394400
O	-1.39373700	5.13806200	-0.77683400
C	-1.05860700	6.41659600	-1.29414600
H	-0.83187300	6.37512200	-2.36819300
H	-1.93953000	7.04465700	-1.14037000
H	-0.20582100	6.86071900	-0.76309200
C	-4.07902700	-2.60879300	-2.92371100
C	-3.23502800	-1.55039800	-2.58975900
C	-1.96214800	-1.79745200	-2.05658500
C	-1.53748700	-3.11983300	-1.88141200
C	-2.38005800	-4.17966500	-2.22288500
C	-3.65309500	-3.92830200	-2.74013600
H	-5.06570200	-2.40612800	-3.33233700
H	-2.03945400	-5.20359200	-2.09052600
H	-4.30742500	-4.75430100	-3.00643300
C	-1.02907400	-0.65479600	-1.75955700
H	-1.82846600	0.23830200	-0.87711200
H	-1.06616600	0.13489800	-2.53045200
O	0.16252100	-0.89653200	-1.24632200
H	-0.54071500	-3.29989200	-1.49170300
H	-3.56415800	-0.52387400	-2.74233000

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IN12 SCF Done: E(RM06) = -1733.74794620

C	0.77871700	2.97355300	1.19831900
C	-0.62981600	2.58037500	1.15139000
C	-1.12373900	2.89285100	-0.17772300
C	1.15260200	3.39735800	-0.09466200
C	-0.01780300	3.34363300	-0.96730900
C	-1.47361200	2.28285000	2.35707700
H	-0.90166400	1.73832400	3.11458500
H	-1.82790800	3.21825800	2.81631200
H	-2.33921500	1.66911900	2.10156300
C	-2.56370000	2.86448200	-0.59946900
H	-3.03157000	3.84011900	-0.40128100
H	-2.67025900	2.65766100	-1.66912900
H	-3.12723300	2.10706000	-0.04898900
C	-0.10014500	3.94346700	-2.34646900
H	-0.33482800	5.01747100	-2.29736900
H	0.84656300	3.86231800	-2.89434900
H	-0.88065400	3.47076300	-2.95135900
C	2.50482600	3.88353500	-0.53291100
H	2.49580300	4.97120800	-0.68947200
H	3.27702500	3.66489700	0.21036500
H	2.81309500	3.42329100	-1.47799100
C	1.62520200	2.96152600	2.43682500
H	1.46067900	2.05716900	3.03005000
H	2.69347300	3.01740700	2.20573200
H	1.38323700	3.82138400	3.07816500
C	-5.80963600	-0.09481200	0.78576700
C	-3.68584200	-0.98194100	0.84624800
C	-4.15431400	-2.21810100	0.29713300
C	-5.53271400	-2.34441500	0.00206800
C	-6.36953300	-1.28014200	0.24934800
H	-6.45674500	0.76016500	0.98124000
C	-3.19373300	-3.23822600	0.07895900
H	-5.90919000	-3.27618600	-0.41450600
H	-7.43380500	-1.33135900	0.04104800
C	-1.88328300	-3.00401000	0.40602600
C	-1.50165300	-1.74135900	0.96769100
H	-3.50563800	-4.18699200	-0.35244200
H	-1.12293300	-3.75686700	0.22772000
N	-4.53197800	0.06465100	1.07525600
N	-2.38493400	-0.77477900	1.17320400
C	-0.08206600	-1.54078800	1.38113900
C	0.46313900	-2.56128200	2.17834100
C	1.77288500	-2.53772200	2.65718200
C	2.57473400	-1.44728600	2.31475500
C	2.04175100	-0.42532000	1.51257700
C	0.72662900	-0.42174900	1.01064900
H	-0.16581500	-3.40406100	2.45678800
H	2.13914200	-3.34922200	3.27544100
H	2.71563200	0.39798600	1.28224100
Ir	0.26336000	1.16213400	-0.24476600
O	3.87607400	-1.28466100	2.69527400
C	4.50059500	-2.34340100	3.40869400
H	4.49532500	-3.27569000	2.82941000
H	5.53408400	-2.02821000	3.57112700
H	4.02284400	-2.51579800	4.38236600
H	-0.80199000	0.16820200	-0.87490200
C	0.25381000	-1.22719000	-3.06456300
C	1.35470000	-1.13166600	-2.20912800

C	2.11385900	-2.27872500	-1.90172600
C	1.71398100	-3.51613900	-2.44298500
C	0.61998000	-3.61075900	-3.28925400
C	-0.10607100	-2.45561400	-3.60738000
H	-0.32204500	-0.33673700	-3.28724600
H	2.30511100	-4.38934900	-2.18667400
H	0.33157900	-4.57136300	-3.70612600
H	-0.96312600	-2.51438500	-4.27232200
C	3.34205400	-2.27111000	-1.06892800
H	3.73465000	-1.28639100	-0.75192000
O	3.94681700	-3.28031700	-0.75080400
N	1.66354700	0.17488500	-1.65305900
O	1.97728500	1.07526000	-2.74939200
H	2.54073400	0.12986100	-1.13865000
H	1.22824500	1.69879400	-2.69701900

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TS11 SCF Done: E(RM06) = -1733.71965832

C	-1.16676400	0.32320400	2.58041800
C	0.14907100	-0.27639500	2.58307800
C	-0.00264800	-1.63788500	2.14025800
C	-2.11650400	-0.67405800	2.15516500
C	-1.39928200	-1.88690800	1.89278900
C	1.39803400	0.33239500	3.15216600
H	1.35378400	1.42506000	3.12888500
H	1.52714800	0.02776900	4.20066500
H	2.28275300	0.02826500	2.58893200
C	1.08611300	-2.66979200	2.10159700
H	1.12242300	-3.20794700	3.05990400
H	0.91346900	-3.41169800	1.31605400
H	2.06729700	-2.21831900	1.93366600
C	-2.00779400	-3.22281400	1.58522600
H	-2.25984100	-3.74471400	2.52004300
H	-2.92967000	-3.13292100	1.00463300
H	-1.32495600	-3.86637200	1.02624000
C	-3.60688300	-0.50788500	2.10971800
H	-3.89667600	0.51927900	1.86941800
H	-4.06762700	-1.16790600	1.36948100
H	-4.04966800	-0.75253200	3.08612000
C	-1.50572300	1.67226700	3.14058500
H	-0.70989600	2.39863300	2.96051300
H	-2.43038800	2.07591000	2.71747000
H	-1.64816400	1.59789400	4.22837700
C	5.39457000	-2.30816700	0.72190700
C	4.07344700	-0.61960900	-0.11075000
C	4.79562200	-0.61841300	-1.34557700
C	5.86669100	-1.53146400	-1.49818600
C	6.17236200	-2.38061100	-0.45970100
H	5.62047800	-2.97725000	1.55172700
C	4.37890100	0.29702500	-2.34475900
H	6.42810300	-1.54917100	-2.42946500
H	6.98496700	-3.09692400	-0.53024300
C	3.32754500	1.13887700	-2.08680400
C	2.66882400	1.08395600	-0.81634100
H	4.88766000	0.31267600	-3.30576400
H	2.97048400	1.83025600	-2.84204000
N	4.38870600	-1.47327700	0.90480400
N	3.03614200	0.22620900	0.12581200
C	1.56327000	2.04936400	-0.54443800
C	1.85948600	3.39295800	-0.83573500
C	0.94848300	4.43231800	-0.66221800
C	-0.33136900	4.11358600	-0.20406500
C	-0.64811700	2.77562000	0.07504000
C	0.26401500	1.71993200	-0.05744500
H	2.85507000	3.64134000	-1.19503700
H	1.24081100	5.45140500	-0.88763600
H	-1.66298600	2.58082000	0.40727300
Ir	-0.50999900	-0.14387800	0.42199600
O	-1.33580700	5.01423700	-0.00230200
C	-1.07557600	6.38229900	-0.28737200
H	-0.82060200	6.53441800	-1.34440400
H	-2.00094200	6.91747400	-0.06229100
H	-0.26848400	6.78094400	0.34131800
C	-2.79673700	-1.98568100	-1.81687400
C	-2.60418600	-0.59601900	-1.66976100
C	-3.68753400	0.27744100	-1.84309200
C	-4.96084700	-0.22711700	-2.10515500
C	-5.16709600	-1.60684300	-2.21095100
C	-4.08638700	-2.47330100	-2.07502100
H	-5.79309600	0.46090400	-2.22756800
H	-6.15957300	-1.99739500	-2.41716800
H	-4.20817600	-3.54603700	-2.19312700
N	-1.34967800	-0.03545000	-1.30179700
H	-0.97455900	0.58699300	-2.03259800
O	-0.18150300	-0.51367100	-3.09872200
H	0.61671700	-0.62918400	-2.55396100
H	0.88577600	-0.57286600	-0.16438800
H	-3.52429600	1.34729200	-1.74798300
C	-1.64980700	-2.93251700	-1.82885000
H	-0.67076300	-2.46489400	-2.01634300
O	-1.78418200	-4.14301200	-1.71962900

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IN13 SCF Done: E(RM06) = -1733.78227305

C	-0.90059000	-2.52363600	1.57523300
C	0.50600200	-2.53087000	1.28780100
C	0.65267900	-2.94256700	-0.08301100
C	-1.61708100	-3.03214200	0.41953100
C	-0.66538500	-3.28142700	-0.60378700
C	1.61004000	-2.32003500	2.28153300
H	1.31099100	-1.62137300	3.06855500
H	1.86854500	-3.27316600	2.76586300
H	2.50740700	-1.91672800	1.80988700
C	1.95512600	-3.21145200	-0.77892000
H	2.25259700	-4.25860900	-0.62322700
H	1.87749600	-3.04979800	-1.85844000
H	2.75568100	-2.57284000	-0.39596000
C	-0.95978600	-3.86613900	-1.95402500
H	-1.09440700	-4.95459100	-1.87651100
H	-1.87537800	-3.44283000	-2.38050000
H	-0.13911600	-3.68859100	-2.65541100
C	-3.08988600	-3.30293900	0.33654100
H	-3.29696700	-4.35788800	0.56891200
H	-3.65435500	-2.69809300	1.05258700
H	-3.48246600	-3.09829900	-0.66386100
C	-1.50831700	-2.25603200	2.91913700

H	-0.94391500	-1.50417900	3.47588200
H	-2.54339000	-1.91111300	2.84364300
H	-1.51373300	-3.17843900	3.51728800
C	5.81644100	-0.86937200	-0.26527200
C	3.97188300	0.41837800	0.22016400
C	4.63943200	1.60090100	-0.22883400
C	5.96678500	1.48379500	-0.70554600
C	6.56351100	0.24357800	-0.72171000
H	6.27126700	-1.85948500	-0.27676900
C	3.91330000	2.81808400	-0.17126200
H	6.49438800	2.37060900	-1.04938000
H	7.58059200	0.10540800	-1.07497300
C	2.63524800	2.81512100	0.32317800
C	2.05069100	1.58896400	0.78447000
H	4.37416400	3.73598500	-0.52905200
H	2.05112800	3.72812800	0.34857600
N	4.57784700	-0.80320700	0.18668500
N	2.70691900	0.43903900	0.71456400
C	0.69018200	1.62664000	1.39089200
C	0.45486300	2.69601900	2.27476100
C	-0.75777500	2.90087800	2.92777800
C	-1.80024500	2.00640100	2.67638000
C	-1.58518800	0.93200900	1.79994700
C	-0.36746600	0.69876600	1.14758400
H	1.26561400	3.38871300	2.48436900
H	-0.87032700	3.73668500	3.60873700
H	-2.43297100	0.27628200	1.62849500
Ir	-0.43310100	-0.93463000	-0.12001400
O	-3.04387100	2.08134300	3.22512800
C	-3.33519600	3.17735800	4.08289400
H	-3.22233700	4.13755500	3.56307300
H	-4.37788000	3.05349000	4.38346400
H	-2.69951100	3.17139900	4.97824700
H	0.89160400	-0.24908100	-0.60088300
C	-0.04420500	1.48839700	-2.63996100
C	-1.28084100	1.09768600	-2.06708200
C	-2.39251900	1.98437700	-2.22637700
C	-2.22508100	3.20804300	-2.89148300
C	-1.00358400	3.56815900	-3.44632000
C	0.08309700	2.69038300	-3.32459200
H	0.79656000	0.80795800	-2.55426800
H	-3.08905600	3.86227300	-2.96290300
H	-0.89177600	4.51349600	-3.96949500
H	1.04428000	2.95267700	-3.76045200
C	-3.72345700	1.64636700	-1.68418800
H	-3.81891300	0.63739200	-1.24452200
O	-4.68848700	2.39680800	-1.72511400
N	-1.45112700	-0.12431400	-1.44970900
O	-3.52663000	-1.73792400	-2.59120000
H	-2.79672200	-1.18990800	-2.20961300
H	-3.52992400	-1.51111600	-3.53430800

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TS11' SCF Done: E(RM06) = -1733.67223992

C	0.51144400	2.74310500	1.48971500
C	-0.87353600	2.36576600	1.21476800
C	-1.17752500	2.75764500	-0.15037900
C	1.05073100	3.26142000	0.28777600
C	0.00256100	3.34976200	-0.70931800
C	-1.87724300	1.98489600	2.26178700
H	-1.40827100	1.41630400	3.07070900
H	-2.32149600	2.88887800	2.70371800
H	-2.67495700	1.36924500	1.84229600
C	-2.54155700	2.75645700	-0.77776500
H	-3.03300400	3.72594200	-0.61005300
H	-2.48657900	2.59534500	-1.85896600
H	-3.18276300	1.98008200	-0.35537900
C	0.18401700	3.84523100	-2.10003400
H	0.79779400	4.75371400	-2.13520900
H	0.71358300	3.07192400	-2.69346900
H	-0.77276300	4.06123500	-2.58514800
C	2.45867900	3.72878200	0.06072900
H	2.51763100	4.82493200	0.11069900
H	3.14800800	3.33102700	0.81182200
H	2.82018500	3.43269300	-0.93014500
C	1.17395600	2.67879000	2.83220800
H	0.90717700	1.76787800	3.37653500
H	2.26542200	2.71114700	2.75235500
H	0.86834000	3.53218400	3.45562500
C	-6.07570900	0.07008100	-0.83127800
C	-4.08744200	-0.88581800	-0.17604000
C	-4.42874300	-2.11425300	-0.82605500
C	-5.67091300	-2.19715400	-1.50008700
C	-6.50293800	-1.10147700	-1.50358200
H	-6.72169800	0.94778800	-0.82528600
C	-3.49060100	-3.17383600	-0.74995200
H	-5.94861900	-3.12123700	-2.00219200
H	-7.46549000	-1.11833500	-2.00521500
C	-2.32225800	-2.98280200	-0.05822000
C	-2.06099800	-1.72139700	0.57175000
H	-3.70611400	-4.11994900	-1.24167500
H	-1.58134400	-3.77245800	0.00940700
N	-4.92640800	0.18944500	-0.19425500
N	-2.92053500	-0.71546500	0.49896500
C	-0.80770700	-1.58142800	1.37075800
C	-0.58253500	-2.60264500	2.30867700
C	0.55242200	-2.66307200	3.11747500
C	1.52350800	-1.67287100	2.95883700
C	1.31956600	-0.65277200	2.01702800
C	0.17394100	-0.55512200	1.20843000
H	-1.33467500	-3.37928700	2.42787100
H	0.66022200	-3.46394400	3.84000400
H	2.11378600	0.08219900	1.92689100
Ir	0.22155000	1.00575600	-0.11338400
O	2.69121500	-1.60606000	3.66239100
C	2.95468500	-2.62290800	4.61888800
H	3.00305200	-3.61584700	4.15243100
H	3.92894000	-2.38381400	5.05164400
H	2.20082900	-2.63453500	5.41735000
H	-0.67456600	0.03044200	-0.99641800
C	1.37984800	-2.14435400	-1.65015800
C	2.39691800	-1.16368500	-1.50868000
C	3.70539700	-1.45887500	-2.02357700
C	3.95464100	-2.72759300	-2.56812600
C	2.95045700	-3.68164000	-2.67433100
C	1.65456700	-3.37349500	-2.22445600

H	0.39280200	-1.91004400	-1.27142900
H	4.95940600	-2.93112000	-2.92567000
H	3.16278600	-4.65394100	-3.10911400
H	0.86096300	-4.11073000	-2.31341900
C	4.80653200	-0.48145200	-2.03157100
H	4.57253600	0.53972800	-1.66803900
O	5.93895500	-0.72286900	-2.42600900
N	2.09280100	0.01557600	-0.89620700
O	1.54305300	1.21454400	-2.31229700
H	2.89609000	0.61758400	-0.76008500
H	0.83162900	0.68025900	-2.71536600

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IN13' SCF Done: E(RM06) = -1733.77494719

C	0.68379400	2.78410500	1.18380100
C	-0.72829500	2.41575100	1.16500900
C	-1.25532900	2.84003800	-0.09442300
C	0.99762800	3.48088700	-0.02593400
C	-0.18181000	3.52947600	-0.80904700
C	-1.51370100	1.97467300	2.36276700
H	-0.91996200	1.33455100	3.02053800
H	-1.81978700	2.85795000	2.94167800
H	-2.40399200	1.41606400	2.07354300
C	-2.68816900	2.81839600	-0.53569000
H	-3.16271000	3.79168500	-0.34519500
H	-2.75766200	2.61389600	-1.60836700
H	-3.26002600	2.05043500	-0.00851200
C	-0.34329100	4.11507700	-2.16431400
H	0.54044900	4.67066600	-2.48902400
H	-0.53106900	3.28127500	-2.86214500
H	-1.21156000	4.78353000	-2.20519300
C	2.33485200	4.05963200	-0.38856900
H	2.42454200	5.09769500	-0.04008500
H	3.15547300	3.49626400	0.06671600
H	2.49429700	4.06224700	-1.47090700
C	1.55863600	2.72712100	2.39629600
H	1.34345400	1.85844600	3.02073400
H	2.62314100	2.71513900	2.14577200
H	1.37707300	3.62574600	3.00407200
C	-5.87472900	-0.42055400	0.30920800
C	-3.72331700	-1.16631200	0.62992300
C	-4.09501500	-2.49942300	0.27096400
C	-5.44318000	-2.74819900	-0.08146800
C	-6.34089000	-1.70548100	-0.06222300
H	-6.57279400	0.41589800	0.32905200
C	-3.07629600	-3.48596100	0.28559300
H	-5.74836500	-3.75406400	-0.36073600
H	-7.38481800	-1.84809100	-0.32345800
C	-1.80278900	-3.13283000	0.65035000
C	-1.51813600	-1.77615300	1.01339200
H	-3.31284800	-4.50713700	-0.00435800
H	-1.00010100	-3.86140700	0.63805800
N	-4.62753300	-0.14582200	0.64260200
N	-2.45471100	-0.83841100	0.98888000
C	-0.13534900	-1.42873800	1.45767200
C	0.43438700	-2.32730800	2.37949600
C	1.72557400	-2.19737900	2.88146600
C	2.50342100	-1.13320300	2.42110700
C	1.95510100	-0.23415500	1.49532000
C	0.64696200	-0.32291900	1.00791400
H	-0.16799900	-3.15907600	2.73479300
H	2.10238500	-2.91677200	3.59922900
H	2.61842300	0.55223200	1.15322400
Ir	0.10654800	1.09654500	-0.45534600
O	3.78716500	-0.87953000	2.79883200
C	4.42368800	-1.80196800	3.67505400
H	4.47044200	-2.80698000	3.23677600
H	5.43915300	-1.42654400	3.81875700
H	3.91738400	-1.85120900	4.64815000
H	-0.98502900	-0.00037600	-0.51954400
C	0.52700800	-1.83684900	-2.34427500
C	1.70866200	-1.19595300	-1.87563800
C	2.92048000	-1.96454800	-1.91342900
C	2.90695500	-3.27819300	-2.43416300
C	1.74639600	-3.87083400	-2.89179100
C	0.55001500	-3.12884700	-2.83568400
H	-0.39334900	-1.26416900	-2.34796400
H	3.85369500	-3.81061800	-2.44814600
H	1.75360400	-4.88294600	-3.28624200
H	-0.37725500	-3.57106700	-3.19425300
C	4.19992300	-1.46213900	-1.41073200
H	4.19051900	-0.45132700	-0.94985800
O	5.26451400	-2.07040400	-1.45024600
N	1.65660600	0.12196900	-1.48433000
O	-0.54685800	1.18853900	-2.37911100
H	2.55022600	0.45472400	-1.14108400
H	0.27265600	0.96311000	-2.85796400

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IN14 SCF Done: E(RM06) = -2003.98849307

C	-1.21366300	0.27128100	2.81043500
C	0.11273600	0.81232700	2.84211700
C	1.05969800	-0.28386200	2.91186900
C	-1.07831100	-1.16175000	2.71043500
C	0.33171200	-1.49629500	2.80868000
C	0.48799000	2.25656400	2.99126200
H	-0.33017900	2.91696800	2.69365000
H	0.73495900	2.47988900	4.03900400
H	1.35991200	2.49866100	2.37717000
C	2.52274600	-0.13043500	3.19359800
H	2.66644100	0.17971500	4.23955100
H	3.06012000	-1.07361100	3.06041700
H	2.99881900	0.62812000	2.56385900
C	0.89039200	-2.88617300	2.88629500
H	1.00296900	-3.20277700	3.93290600
H	0.23440000	-3.61106200	2.39566000
H	1.87377100	-2.95564800	2.41227900
C	-2.20809000	-2.15050700	2.75969900
H	-2.42063300	-2.43261400	3.80081300
H	-3.12483500	-1.73622600	2.33260200
H	-1.97078900	-3.06691100	2.21129300
C	-2.49520500	1.01809900	3.04545100
H	-2.42650600	2.05857400	2.71919700
H	-3.33985200	0.55927100	2.52252900
H	-2.73703700	1.02414000	4.11798600
C	5.87741200	1.42105700	0.73192200

C	3.82924300	1.67423400	-0.28789400
C	4.43906700	1.67460600	-1.58184400
C	5.84617000	1.54648100	-1.66198800
C	6.57415100	1.42383000	-0.50040700
H	6.43586800	1.31623600	1.66188800
C	3.58404700	1.78904400	-2.70726300
H	6.32921700	1.54421100	-2.63630400
H	7.65505700	1.32470300	-0.51289900
C	2.23472500	1.92400100	-2.51021600
C	1.70889800	1.94939900	-1.17830700
H	4.00632400	1.76368200	-3.70909700
H	1.55197800	2.00101900	-3.34926300
N	4.56747000	1.53699300	0.85007600
N	2.48538100	1.80361900	-0.11300900
C	0.26346900	2.26441000	-0.99036900
C	-0.16017800	3.44306200	-1.63012100
C	-1.45249800	3.94926800	-1.51963400
C	-2.37128100	3.23221500	-0.75190800
C	-1.97448700	2.03815100	-0.13328200
C	-0.67576800	1.52412000	-0.22042400
H	0.56269100	4.00669600	-2.21466800
H	-1.71789700	4.87220600	-2.02196800
H	-2.74195100	1.49727900	0.40450700
Ir	-0.30032300	-0.26982200	0.76998500
O	-3.67389000	3.59547800	-0.55497800
C	-4.13807700	4.78201100	-1.18509600
H	-4.06315300	4.71622500	-2.27849300
H	-5.18912800	4.88033800	-0.90410500
H	-3.58969100	5.66750000	-0.83711700
H	-1.71332600	-0.52056300	0.13714000
C	2.63503700	-1.65883800	-0.06663100
C	1.46931900	-1.89617000	-0.84172000
C	1.49463000	-3.02943200	-1.71788100
C	2.58622500	-3.90934700	-1.70523300
C	3.70237000	-3.66445500	-0.91368800
C	3.72835600	-2.51510400	-0.11173800
H	2.67065000	-0.76550400	0.54377500
H	2.54282700	-4.77378700	-2.36133200
H	4.55184300	-4.34139000	-0.93425000
H	4.60789100	-2.28698200	0.48565900
C	0.41526400	-3.28540600	-2.69533600
H	-0.24992000	-2.43352800	-2.90295500
O	0.27920500	-4.34401600	-3.29554300
N	0.36303100	-1.06471100	-0.80792100
C	-2.87347900	-1.79309900	-2.67463900
O	-1.88210300	-0.79284200	-2.84200700
H	-1.24435800	-0.82710900	-2.09470400
H	-3.30180900	-1.95412400	-3.67367600
H	-2.43316800	-2.75497700	-2.37091600
C	-3.99443700	-1.43087500	-1.71345300
C	-4.66683600	-2.43151800	-0.99903300
C	-4.41090700	-0.10208000	-1.56463000
C	-5.73537400	-2.11391200	-0.15675200
H	-4.35217000	-3.46833800	-1.10402600
C	-5.47226700	0.22053200	-0.71615200
H	-3.88449900	0.67657900	-2.10661000
C	-6.13987200	-0.78435400	-0.01037100
H	-6.24693800	-2.90341100	0.38869700
H	-5.76967800	1.25990500	-0.60363300
H	-6.96776500	-0.53384500	0.64830600

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TS12 SCF Done: E(RM06) = -2003.95986019

C	1.09030800	-1.30137500	2.58060000
C	-0.27281700	-1.73358700	2.58479500
C	-1.11185200	-0.63817000	3.04343500
C	1.07572100	0.11831000	2.84679900
C	-0.29475600	0.50270500	3.17662200
C	-0.76504300	-3.13284300	2.37170300
H	-0.05802400	-3.72300900	1.78353900
H	-0.90340500	-3.64015900	3.33718300
H	-1.72629200	-3.13418400	1.85011200
C	-2.56755400	-0.76526900	3.36090500
H	-2.72721700	-1.58189400	4.07819000
H	-2.95967000	0.15048500	3.81328700
H	-3.17172800	-0.98416200	2.47216500
C	-0.68779000	1.86672800	3.66264300
H	-0.30710200	2.03533400	4.67965000
H	-0.27357300	2.65862200	3.03001200
H	-1.77257500	1.99657900	3.68968600
C	2.28361900	0.97630200	3.08817200
H	2.58657500	0.91046000	4.14344800
H	3.13299800	0.66274700	2.47629300
H	2.08192800	2.02825400	2.86702100
C	2.31148700	-2.17368300	2.56196000
H	2.14649600	-3.10132200	2.00967300
H	3.17336400	-1.66561400	2.11995600
H	2.58398400	-2.44544800	3.59181100
C	-5.86290900	-0.24422700	0.58906200
C	-3.95110200	-0.87974400	-0.52774200
C	-4.58589400	-0.66554900	-1.79165800
C	-5.92815100	-0.21900700	-1.80562900
C	-6.57641400	-0.00879400	-0.60999300
H	-6.35726200	-0.08192600	1.54667500
C	-3.81620400	-0.90342900	-2.95742400
H	-6.42549500	-0.04862000	-2.75758300
H	-7.60643300	0.33138100	-0.57153200
C	-2.52725600	-1.34740300	-2.82680300
C	-1.97464600	-1.56775400	-1.52263300
H	-4.25143800	-0.72174200	-3.93725000
H	-1.90809300	-1.51246100	-3.70112200
N	-4.60980100	-0.65598200	0.64393800
N	-2.66596000	-1.31559500	-0.41792300
C	-0.60357200	-2.14028700	-1.42952600
C	-0.32664900	-3.20087000	-2.31265000
C	0.90546000	-3.84462200	-2.37271300
C	1.92816700	-3.38679700	-1.53888900
C	1.67879900	-2.32129600	-0.66164900
C	0.43275300	-1.69954500	-0.55772200
H	-1.11986500	-3.55619000	-2.96482600
H	1.05164200	-4.66984200	-3.05989800
H	2.51775100	-1.97566300	-0.07178000
Ir	0.21326700	-0.16813100	0.81995600
O	3.19045800	-3.89578800	-1.50211300
C	3.52283000	-4.93486200	-2.41390700
H	3.39623800	-4.61365500	-3.45583100

H	4.57559900	-5.16449400	-2.23533200
H	2.92359100	-5.83767300	-2.23582500
H	1.60450000	0.13546700	0.11069400
C	-2.23703400	2.20085400	0.46934400
C	-1.18216000	2.17773300	-0.47587800
C	-1.17768400	3.18698600	-1.49147700
C	-2.17483500	4.17388100	-1.48961900
C	-3.17978400	4.19348200	-0.53115600
C	-3.20885400	3.18987000	0.44801200
H	-2.28519100	1.41208300	1.21070300
H	-2.13580400	4.92066400	-2.27662100
H	-3.94321800	4.96609600	-0.54993500
H	-4.00307400	3.17520500	1.19000700
C	-0.17979100	3.23706000	-2.59744000
H	0.62249200	2.47948000	-2.59441000
O	-0.23364400	4.07734500	-3.48603700
N	-0.21338100	1.18870700	-0.45338500
C	2.78246000	2.32910100	-0.95141400
O	2.07408000	1.26460200	-1.46753200
H	0.73831700	1.30908900	-1.08812900
H	2.69263100	3.23700900	-1.59265900
H	2.40051900	2.66076800	0.04349900
C	4.27705200	2.05762400	-0.78688600
C	5.10823400	2.98111700	-0.13525200
C	4.84940500	0.88859700	-1.29893600
C	6.47612500	2.74326600	0.00222400
H	4.67761500	3.89784000	0.26670700
C	6.21962000	0.64534600	-1.16236900
H	4.19863800	0.18313100	-1.80533700
C	7.03877600	1.57015000	-0.51181200
H	7.10458600	3.47119500	0.51094600
H	6.64832100	-0.26887600	-1.56780300
H	8.10456500	1.38195200	-0.40556000

86

IN15 SCF Done: E(RM06) = -2004.03664376

C	-1.39447900	-2.04740300	-2.07294600
C	0.05676600	-2.13927300	-2.19354800
C	0.50583900	-0.91766200	-2.77829800
C	-1.80969300	-0.80321100	-2.72141100
C	-0.65242100	-0.10653300	-3.14084200
C	0.90071200	-3.33237900	-1.85883200
H	0.43474300	-3.94312800	-1.08044000
H	1.02771000	-3.96580100	-2.74849000
H	1.88654700	-3.03101000	-1.49855100
C	1.91188300	-0.58108900	-3.16550900
H	2.06561000	-0.83312400	-4.22550800
H	2.11521300	0.48972300	-3.06033100
H	2.65081000	-1.12734300	-2.57729200
C	-0.59338300	1.16684300	-3.93332600
H	-0.43530800	0.95068000	-4.99974400
H	-1.52068200	1.74042700	-3.85279100
H	0.23222000	1.81137800	-3.61402200
C	-3.23720800	-0.41281400	-2.95076600
H	-3.61677700	-0.92517400	-3.84615200
H	-3.87647500	-0.70370500	-2.11229800
H	-3.35599000	0.66179400	-3.10331200
C	-2.31781700	-3.17703800	-1.72402100
H	-1.87453500	-3.85059900	-0.98677100
H	-3.26823600	-2.81531100	-1.31971900
H	-2.54485200	-3.76862100	-2.62259100
C	5.87496400	-0.96814000	-1.49107500
C	4.11010100	-0.97153000	-0.01036900
C	4.88535200	-0.25927100	0.95906300
C	6.21654400	0.09138500	0.63150700
C	6.71967900	-0.26478500	-0.59944100
H	6.25448900	-1.25865900	-2.47053500
C	4.25852000	0.05183100	2.19369800
H	6.82203500	0.63203000	1.35571700
H	7.73599500	-0.02036000	-0.89246300
C	2.97046700	-0.35900200	2.40894700
C	2.27392700	-1.09659100	1.39464400
H	4.80476800	0.61200700	2.94936300
H	2.46021500	-0.12429900	3.33666700
N	4.62813100	-1.31164900	-1.22525000
N	2.82869000	-1.36612900	0.22214600
C	0.93815200	-1.67083600	1.72774400
C	0.90737200	-2.39016200	2.93673000
C	-0.22352200	-3.05586600	3.40481900
C	-1.38614100	-2.98358200	2.63629400
C	-1.37725100	-2.24666800	1.44192000
C	-0.24758700	-1.57767000	0.93840900
H	1.81823300	-2.46075200	3.52663600
H	-0.17984600	-3.61104500	4.33479900
H	-2.31704600	-2.21210100	0.89938900
Ir	-0.57473600	-0.52252300	-0.82509600
H	-2.04890000	0.08733600	1.27706400
O	-2.57119600	-3.58019000	2.95510400
C	-2.64375900	-4.32141300	4.16509600
H	-2.44832000	-3.68853100	5.04087400
H	-3.66536900	-4.70392400	4.22257200
H	-1.94292200	-5.16697000	4.16560800
C	-2.70108500	2.39091100	-0.97207800
C	-2.86150000	1.49051700	0.11743300
C	-4.07417000	1.61315000	0.87502700
C	-5.00834400	2.62218000	0.55608000
C	-4.81287500	3.49665800	-0.49706600
C	-3.64187600	3.36345900	-1.26631900
H	-1.79615400	2.31176300	-1.56579200
H	-5.90196100	2.67579900	1.17143200
H	-5.54449900	4.26497000	-0.72905700
H	-3.46406700	4.03768300	-2.10172100
C	-4.42283200	0.70431100	1.97365200
H	-3.73356600	-0.14553800	2.15469400
O	-5.42206700	0.80867500	2.67670400
N	-1.84632500	0.61514000	0.43483200
C	1.18152200	2.34042900	-0.46864000
O	0.69511200	1.17544400	0.23538800
H	-0.17870400	1.38726200	0.66249000
H	2.08222900	2.01085600	-0.99061400
H	0.44313500	2.65504900	-1.21588200
C	1.48674600	3.47941700	0.47594500
C	0.47284200	4.37181200	0.85340700
C	2.77205900	3.65203500	1.00640300
C	0.73590600	5.40955300	1.74883000
H	-0.52765100	4.25480800	0.44209300

C	3.03914500	4.69210200	1.89810500
H	3.56585400	2.96844300	0.71612700
C	2.02054600	5.57165100	2.27293500
H	-0.05977200	6.09328200	2.03256700
H	4.04182700	4.81790700	2.29866100
H	2.22781100	6.38211800	2.96685400

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TS13 SCF Done: E(RM06) = -2004.03045835

C	-1.65257800	-1.59177800	-2.24718800
C	-0.22235700	-1.82832100	-2.37252100
C	0.37688500	-0.59953600	-2.80941500
C	-1.90952300	-0.23589400	-2.71580600
C	-0.67607500	0.37648800	-3.05652600
C	0.48752700	-3.13396200	-2.17426500
H	-0.07838700	-3.79695500	-1.51375500
H	0.61260400	-3.64771000	-3.13808300
H	1.47238500	-2.97864700	-1.72736200
C	1.81444300	-0.40247600	-3.17654500
H	1.93200000	-0.54218900	-4.26151300
H	2.15993200	0.61044000	-2.94515000
H	2.47435600	-1.10920200	-2.67099600
C	-0.47798800	1.73003000	-3.67403000
H	-0.43810900	1.65613700	-4.77048600
H	-1.29336600	2.41540300	-3.42480600
H	0.45987800	2.19097100	-3.34948900
C	-3.27452700	0.36240500	-2.86452200
H	-3.70054000	0.06728900	-3.83382100
H	-3.95949700	0.01088700	-2.08781800
H	-3.25517000	1.45386000	-2.82671300
C	-2.70097600	-2.64092700	-2.01949400
H	-2.34564800	-3.42649100	-1.34821700
H	-3.61287500	-2.21777000	-1.58609600
H	-2.97942000	-3.11645000	-2.97088400
C	5.74242600	-1.33565400	-1.65518200
C	3.99091700	-1.29995000	-0.15998000
C	4.81428900	-0.68398900	0.83513700
C	6.16215100	-0.40053900	0.51149600
C	6.63433200	-0.72803800	-0.73967700
H	6.09702100	-1.60206700	-2.65079000
C	4.21725300	-0.39444900	2.08937200
H	6.80399700	0.06867000	1.25393300
H	7.66170600	-0.53189400	-1.03071100
C	2.90651100	-0.73039600	2.29604500
C	2.15694200	-1.36291100	1.25098500
H	4.80321600	0.09369300	2.86471500
H	2.41736400	-0.51084900	3.23875700
N	4.47826400	-1.61373800	-1.39430300
N	2.68612800	-1.61768500	0.06337400
C	0.78473500	-1.86094300	1.55921700
C	0.70791000	-2.68952700	2.69200900
C	-0.47015900	-3.30935200	3.10734900
C	-1.62715200	-3.07685400	2.36263000
C	-1.56869300	-2.22894700	1.24483900
C	-0.39304800	-1.60057800	0.79934900
H	1.61458300	-2.88482700	3.26025500
H	-0.46552100	-3.95343600	3.97917000
H	-2.50324700	-2.07301200	0.71451400
Ir	-0.62088200	-0.32540100	-0.82627800
H	-1.92979500	0.25952700	1.43987100
O	-2.85336000	-3.61127200	2.63647900
C	-2.97512900	-4.46566700	3.76467600
H	-2.72409700	-3.94452900	4.69812700
H	-4.02326200	-4.77174500	3.79837600
H	-2.34321100	-5.35870100	3.66779500
C	-2.50004500	2.89555200	-0.43135300
C	-2.75693100	1.78634300	0.40339800
C	-4.06071100	1.67241500	0.96359400
C	-5.03040200	2.65824900	0.68759300
C	-4.75407000	3.74167500	-0.12887900
C	-3.47235700	3.85226200	-0.68966900
H	-1.51035600	3.00075000	-0.86412800
H	-6.00864300	2.53220200	1.14174200
H	-5.51217300	4.49290800	-0.32968600
H	-3.22899900	4.69900600	-1.32701700
C	-4.47228000	0.55149100	1.83071000
H	-3.72171200	-0.24077700	2.01731400
O	-5.58150100	0.44590800	2.33511700
N	-1.71314900	0.88278200	0.66676000
C	1.31640800	2.14682900	-0.23991600
O	0.64640600	1.05901300	0.38076000
H	-0.48285700	1.27912300	0.74674400
H	2.09809000	1.74900700	-0.89626500
H	0.62168500	2.71483800	-0.88127600
C	1.93972600	3.08520000	0.77723200
C	1.15188000	3.70450500	1.75887700
C	3.30899700	3.37355400	0.73833800
C	1.72023300	4.58429000	2.67975600
H	0.08532300	3.49727300	1.80408500
C	3.88171600	4.26014400	1.65451700
H	3.93330100	2.89635200	-0.01397700
C	3.08863300	4.86673600	2.62941300
H	1.09475500	5.05388300	3.43485900
H	4.94704900	4.47245800	1.60792500
H	3.53102600	5.55487600	3.34520000

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IN16 SCF Done: E(RM06) = -2350.69258635

C	0.57823700	-2.93450100	-0.48780100
C	1.85507400	-3.17118300	0.16966900
C	2.91283700	-2.80427300	-0.78271900
C	0.85539900	-2.22430900	-1.69840300
C	2.31271500	-2.20265600	-1.89977200
C	2.06128100	-4.01248100	1.39629400
H	1.22152000	-3.91435200	2.08996500
H	2.15116400	-5.07539700	1.12996100
H	2.97214800	-3.72762900	1.93270300
C	4.36659400	-3.08737900	-0.56301200
H	4.56499100	-4.14904800	-0.76842700
H	5.00810200	-2.49301100	-1.21540200
H	4.66802000	-2.90112400	0.47210400
C	2.98684700	-1.61559900	-3.10358100
H	2.73391400	-2.18655600	-4.00706200
H	2.67194900	-0.58014700	-3.27539200
H	4.07473000	-1.61992500	-2.99921800
C	-0.15611700	-1.77545300	-2.70944700

H	-0.36552100	-2.59452500	-3.41338100
H	-1.10204900	-1.48136500	-2.22717700
H	0.22043000	-0.93285800	-3.29948400
C	-0.76080500	-3.43681700	-0.04613300
H	-0.83436000	-3.50047100	1.04287900
H	-1.57659300	-2.80575400	-0.41949500
H	-0.90078300	-4.45256200	-0.44494100
C	5.82361400	0.53871300	-0.64763600
C	4.18844400	0.42159600	0.96175300
C	5.03503000	1.06836100	1.91497500
C	6.34026500	1.42216200	1.51240500
C	6.74575600	1.15622800	0.22109900
H	6.11107800	0.33214100	-1.67774000
C	4.50933200	1.34071700	3.20704400
H	7.00274000	1.90715400	2.22486500
H	7.73914100	1.41515900	-0.13040400
C	3.21176100	1.02199500	3.48596400
C	2.39909000	0.38248900	2.50183500
H	5.14017500	1.82261800	3.94944000
H	2.78516200	1.25840800	4.45316100
N	4.59529200	0.17608600	-0.30494300
N	2.91296000	0.03993700	1.29856100
C	0.98843800	0.10870100	2.66296900
C	0.25086200	0.46881900	3.80473600
C	-1.12755700	0.31832000	3.83712700
C	-1.78153100	-0.18377600	2.69654400
C	-1.05287900	-0.56389400	1.55296800
C	0.33648600	-0.45614600	1.52283000
H	0.74445900	0.88380800	4.67892900
H	-1.68133900	0.60510100	4.72306900
H	-1.62771800	-0.91597300	0.70017400
Ir	1.57839200	-1.04038300	0.02059700
O	-3.12423700	-0.34854900	2.61320500
C	-3.94806400	0.10797700	3.68133900
H	-3.82213900	1.18421700	3.84999800
H	-4.97454700	-0.08899400	3.36673500
H	-3.74476200	-0.43954200	4.61080300
C	-0.96929100	4.13905200	-3.58809700
C	-0.89296600	3.10233700	-2.67905900
C	0.36295200	2.57934400	-2.27025900
C	1.57485800	3.12517700	-2.81461400
C	1.46325900	4.18612300	-3.74404400
C	0.22229000	4.67545600	-4.11430300
H	-1.93204100	4.53456900	-3.89556900
H	2.37133000	4.61125300	-4.16506200
H	0.17341900	5.49167500	-4.83134900
H	-1.78948400	2.65142200	-2.25259100
C	0.34767100	1.48653500	-1.34390200
H	-0.63242000	1.12210000	-1.01399000
O	1.39917200	0.94489500	-0.90538100
C	-6.12445100	-3.14408500	0.62244900
C	-5.06597000	-2.45417500	0.02218600
C	-4.97728500	-2.35194200	-1.36954200
C	-5.97521000	-2.95688800	-2.14862600
C	-7.03368700	-3.64533600	-1.55532300
C	-7.11255000	-3.74277800	-0.16162500
H	-6.17731200	-3.21519500	1.70746500
H	-4.29005500	-1.98028400	0.61553000
H	-5.91931000	-2.88741000	-3.23500500
H	-7.79733500	-4.10827000	-2.17730200
H	-7.93552900	-4.28015600	0.30427600
C	-3.81739600	-1.59263500	-2.02627800
H	-3.39452300	-2.28036000	-2.79745800
H	-4.27926200	-0.77230200	-2.62542400
O	-2.85691900	-1.12851900	-1.16034300
H	-2.92995600	0.29997200	-1.07000200
C	-5.19997000	4.84029500	1.56229900
C	-5.25555700	3.68190700	0.78540500
C	-4.09448000	2.95396100	0.48692600
C	-2.87110600	3.42184200	0.98216600
C	-2.80967600	4.58334300	1.75626100
C	-3.97323500	5.29757600	2.05163000
H	-6.11270900	5.39137900	1.77780600
H	-6.21347900	3.33819500	0.39825700
H	-1.96898800	2.86808700	0.74439700
H	-1.84861800	4.93312600	2.12735600
H	-3.92518400	6.20376400	2.65080500
C	-4.18120900	1.66938600	-0.32021700
H	-4.46435500	0.84988000	0.36307000
H	-5.02640400	1.77171100	-1.02855500
O	-2.98634100	1.35883700	-0.98217900
N	2.79672100	2.65047400	-2.46112700
H	3.62698500	3.01809700	-2.90190700
H	2.87231600	1.86742500	-1.82414600

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IN17 SCF Done: E(RM06) = -2295.33599550

C	-0.74249800	-2.89916900	0.39712600
C	-2.04360400	-3.04647800	-0.23843700
C	-3.06308600	-2.71613100	0.76780400
C	-0.96364300	-2.26139600	1.65841500
C	-2.41406200	-2.20598500	1.90195100
C	-2.31166600	-3.78463700	-1.51847700
H	-1.48998200	-3.65504600	-2.22842100
H	-2.42750900	-4.86207100	-1.33322300
H	-3.22809900	-3.42935700	-2.00047600
C	-4.52866700	-2.94839000	0.57249500
H	-4.73874600	-4.02408300	0.65955900
H	-5.13337600	-2.42616300	1.31536300
H	-4.86335300	-2.63573300	-0.42075000
C	-3.03775700	-1.69340200	3.16467900
H	-2.87413200	-2.39718900	3.99243300
H	-2.60248100	-0.73434000	3.46421800
H	-4.11524200	-1.54888100	3.05434900
C	0.09212400	-1.92884300	2.66904200
H	0.29273300	-2.80992700	3.29648800
H	1.03387400	-1.63117900	2.18085200
H	-0.23448200	-1.12685500	3.34030400
C	0.56441400	-3.42149500	-0.11232800
H	0.60776500	-3.41893700	-1.20484700
H	1.41397500	-2.84729800	0.27669500
H	0.67421000	-4.46516000	0.21818900
C	-5.91303700	0.63106600	0.83166400
C	-4.28249000	0.62144600	-0.78458000
C	-5.10825900	1.38417800	-1.66816700
C	-6.39751700	1.74892700	-1.22458000

C	-6.80889100	1.37569800	0.03716700
H	-6.21024900	0.32645700	1.83412900
C	-4.58283600	1.74904700	-2.93635000
H	-7.04207200	2.32601400	-1.88278400
H	-7.78887900	1.64056400	0.42042300
C	-3.30306200	1.40081500	-3.25854900
C	-2.50643200	0.65444500	-2.33988000
H	-5.19939300	2.31879200	-3.62675200
H	-2.87651700	1.69874800	-4.20846600
N	-4.70260600	0.25593900	0.44629900
N	-3.01625800	0.23848300	-1.15863800
C	-1.10896800	0.34298800	-2.54786100
C	-0.38058600	0.75349800	-3.67786900
C	0.99095800	0.55702200	-3.75006700
C	1.64761100	-0.04241000	-2.65993500
C	0.92649000	-0.47293000	-1.52883200
C	-0.45758500	-0.32080900	-1.46338700
H	-0.87566000	1.24313200	-4.51172600
H	1.53782700	0.88275700	-4.62687300
H	1.50346300	-0.90223200	-0.71365100
Ir	-1.68763600	-0.94493700	0.03218800
O	2.98497400	-0.25797700	-2.61583900
C	3.80260200	0.22834100	-3.67536500
H	3.71667700	1.31672400	-3.77853600
H	4.82703100	-0.02639500	-3.39773800
H	3.55690800	-0.25544000	-4.62958400
C	1.17856700	4.07902600	3.65398000
C	1.07485300	2.99427100	2.78336000
C	-0.19676800	2.58414500	2.33985400
C	-1.35531100	3.26279700	2.76936500
C	-1.23846100	4.34187500	3.63496000
C	0.02887600	4.74912000	4.07754000
H	2.15611200	4.40263700	3.99973800
H	-2.32735200	2.93057700	2.41797500
H	-2.12639800	4.87018400	3.97109900
H	0.11451300	5.59391400	4.75632600
H	1.95594200	2.45887200	2.42802700
C	-0.27882900	1.43074400	1.45132400
H	0.66342700	0.94605400	1.16657200
O	-1.36797000	1.00022200	1.02754100
C	5.93961200	-3.20655600	-0.95455500
C	4.91408800	-2.55226900	-0.26390900
C	4.85607500	-2.59003200	1.13274700
C	5.84896300	-3.30126100	1.82348200
C	6.87401100	-3.95560100	1.13955000
C	6.92390700	-3.91048800	-0.25811100
H	5.96936200	-3.16744100	-2.04207500
H	4.14162400	-1.99940000	-0.78939600
H	5.81658700	-3.34205400	2.91225900
H	7.63449500	-4.50193400	1.69401100
H	7.72124100	-4.41976700	-0.79474800
C	3.73647800	-1.86371300	1.88916200
H	3.29959800	-2.61167800	2.59279100
H	4.23834800	-1.12668000	2.55959100
O	2.77930200	-1.27723600	1.09547800
H	2.95248800	0.13779400	1.11021600
C	5.35075600	4.79697200	-1.17685400
C	5.38245900	3.58553800	-0.48329400
C	4.21052600	2.84858800	-0.26097100
C	3.00074300	3.36103000	-0.74618600
C	2.96298400	4.57450700	-1.43706700
C	4.13787800	5.29781500	-1.65727700
H	6.27139700	5.35453000	-1.33404800
H	6.32961900	3.20728000	-0.10215200
H	2.09040900	2.79923000	-0.56478200
H	2.01242400	4.95784900	-1.80192200
H	4.10863300	6.24461900	-2.19128000
C	4.26563800	1.50920600	0.45522400
H	4.50597100	0.72901700	-0.28782500
H	5.12614300	1.53221800	1.15182500
O	3.07138800	1.19746300	1.11763600

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1a-4 SCF Done: E(RM06) = -400.767869235

H	-0.70556100	2.98650300	0.18566300
C	-1.76681400	0.68457300	-0.01979800
C	-0.38824400	0.98502300	-0.00199700
C	0.53467800	-0.09692900	0.00350600
C	0.05185200	-1.42045800	0.02392700
C	-1.30459500	-1.69959600	0.01552000
C	-2.21280000	-0.62931400	-0.01405500
H	-2.48223900	1.50376100	-0.03185600
H	0.78949100	-2.21728200	0.03585600
H	-1.66061100	-2.72522800	0.02615500
H	-3.28218700	-0.82492500	-0.02454600
C	1.98837500	0.11250900	-0.04979100
H	2.32784700	1.16148200	-0.18150500
O	2.82422100	-0.77786900	0.01571800
N	0.01515600	2.31135300	-0.03899000
H	0.89868900	2.54432600	0.39354500

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NH3 SCF Done: E(RM06) = -56.5395147280

N	0.00000000	0.00000000	0.12054200
H	0.00000000	0.93751400	-0.28126500
H	-0.81191100	-0.46875700	-0.28126500
H	0.81191100	-0.46875700	-0.28126500

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TS14 SCF Done: E(RM06) = -1659.07548630

C	1.41923100	-0.92533400	2.45367400
C	0.57348700	-2.05527500	2.15298200
C	-0.80409400	-1.69633100	2.51748000
C	0.55288700	0.18810200	2.75635000
C	-0.81906600	-0.33531200	2.84769300
C	1.04339700	-3.45219100	1.86840300
H	1.99829000	-3.45270700	1.33528900
H	1.18209500	-4.01216000	2.80374300
H	0.31885600	-4.00218700	1.26012600
C	-1.94231400	-2.66456400	2.58760300
H	-1.88797200	-3.22264200	3.53347000
H	-2.91091400	-2.16086500	2.55416300
H	-1.91128600	-3.39349900	1.77495700
C	-2.00401800	0.49789700	3.22677300
H	-1.98781500	0.72467600	4.30148000
H	-2.00492500	1.45416700	2.69287600

H	-2.94586900	-0.00927700	3.00334700
C	0.98155500	1.53264600	3.26987700
H	1.12315700	1.50625100	4.35938300
H	1.92879700	1.85414300	2.82580800
H	0.22985200	2.30059200	3.06073000
C	2.91367700	-0.96282700	2.55844800
H	3.36355100	-1.60547000	1.79699800
H	3.36253300	0.02872100	2.47214300
H	3.19069800	-1.36555700	3.54238900
C	-3.70379300	-2.42047900	-0.62787700
C	-1.56836400	-2.02854100	-1.36702300
C	-1.82727300	-2.71595100	-2.59322000
C	-3.11145900	-3.27533200	-2.78185000
C	-4.06223100	-3.12645300	-1.79652500
H	-4.43716400	-2.28698700	0.16557000
C	-0.79071700	-2.78758000	-3.55946200
H	-3.32951700	-3.80759500	-3.70406200
H	-5.06193900	-3.53469200	-1.90157100
C	0.40382700	-2.17130600	-3.31024200
C	0.61142500	-1.48673400	-2.07929400
H	-0.96432000	-3.31656700	-4.49283600
H	1.19882800	-2.19493900	-4.04555300
N	-2.50879400	-1.89506400	-0.40756800
N	-0.33930300	-1.46318400	-1.12359800
C	1.80929100	-0.72607400	-1.76562700
C	2.89262300	-0.57168400	-2.64572200
C	3.96494700	0.25538600	-2.33144700
C	3.94423900	0.95909900	-1.11476800
C	2.86146400	0.80423500	-0.22660500
C	1.79480600	-0.05591100	-0.50684300
H	2.91034900	-1.09331400	-3.59855100
H	4.79120000	0.35303400	-3.02495600
H	2.90267800	1.36630800	0.70170800
Ir	0.21939700	-0.45697700	0.69459100
O	4.91607700	1.81098700	-0.70719300
C	6.06039100	2.00103200	-1.53915800
H	5.78409700	2.43051100	-2.51007200
H	6.70153700	2.70422600	-1.00446900
H	6.60345500	1.06123800	-1.69335600
N	0.54153200	2.90673200	-1.49780800
H	0.09707000	2.66156000	-2.38351900
H	0.79066400	3.89703400	-1.51784900
H	1.38521000	2.33880900	-1.38277600
C	-2.75106700	5.56321700	-0.09876100
C	-1.70645700	4.66546000	0.12195800
C	-1.79677300	3.34783800	-0.34711400
C	-2.94570500	2.93295300	-1.03290700
C	-3.98822500	3.83239700	-1.25411600
C	-3.89223900	5.14756600	-0.78997300
H	-2.67835500	6.58188000	0.27179500
H	-3.01552500	1.90501800	-1.37451300
H	-4.87930300	3.50722500	-1.78415600
H	-4.70754400	5.84520800	-0.96054200
C	-0.66843100	2.39136600	-0.09716500
H	0.02337000	2.71479300	0.69092600
O	-0.88620100	1.14113600	-0.25396300
H	-0.82052100	4.98599400	0.66720000

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IN18 SCF Done: E(RM06) = -1659.07752042

C	1.29494200	-0.80364200	2.53848300
C	0.45769600	-1.94666800	2.27374600
C	-0.93073000	-1.55721100	2.54974100
C	0.42481700	0.33106200	2.73146300
C	-0.95374600	-0.17894800	2.79567400
C	0.92829300	-3.36285100	2.10663000
H	1.92389400	-3.40464000	1.65558600
H	0.97992200	-3.87199300	3.07923300
H	0.24849900	-3.93870000	1.47076600
C	-2.07311200	-2.52003100	2.63010300
H	-2.05294300	-3.02594200	3.60622100
H	-3.03982600	-2.02171500	2.53311500
H	-2.01129500	-3.29283300	1.86068500
C	-2.15036100	0.67742900	3.07441700
H	-2.15854200	1.00024700	4.12433600
H	-2.14821800	1.58080900	2.45545300
H	-3.08447000	0.14511800	2.87891600
C	0.84570900	1.69849200	3.18893900
H	0.97749500	1.72000200	4.27980800
H	1.79580100	2.00432000	2.73972100
H	0.09384300	2.45411000	2.94034300
C	2.78085400	-0.83847200	2.73051300
H	3.27374700	-1.51522500	2.02769500
H	3.23707300	0.14853700	2.62936800
H	2.99796300	-1.19588700	3.74652700
C	-3.75894800	-2.36447000	-0.61264300
C	-1.60368300	-2.04849100	-1.33095600
C	-1.86343400	-2.76487200	-2.54048200
C	-3.15874700	-3.29744500	-2.73130500
C	-4.11891700	-3.09646200	-1.76468200
H	-4.49941300	-2.18900600	0.16588000
C	-0.81686200	-2.89099900	-3.48996500
H	-3.37746700	-3.85089400	-3.64080600
H	-5.12685300	-3.48331300	-1.87202200
C	0.39129600	-2.30299400	-3.23862700
C	0.60087000	-1.59275600	-2.02265200
H	-0.99286700	-3.43914200	-4.41175800
H	1.19581500	-2.36786200	-3.96096500
N	-2.55439400	-1.86274300	-0.39094200
N	-0.36347200	-1.50856000	-1.08477800
C	1.82058200	-0.86758200	-1.70882700
C	2.92756700	-0.79142100	-2.56888200
C	4.02925600	-0.00090500	-2.26184100
C	4.01482400	0.74571000	-1.07149300
C	2.90741600	0.67077200	-0.20242600
C	1.80764500	-0.15470800	-0.47205000
H	2.94217900	-1.34803800	-3.50180200
H	4.87302400	0.03482600	-2.94014600
H	2.96189600	1.25835900	0.70916700
Ir	0.18201100	-0.43108300	0.69432500
O	5.01534500	1.56770000	-0.67266600
C	6.19126300	1.66131500	-1.47706800
H	5.96543500	2.06186100	-2.47305500
H	6.85410100	2.35231100	-0.95308800
H	6.68649800	0.68805100	-1.57535800
N	0.61627300	2.72276600	-1.49732300

H	0.18866800	2.45044000	-2.38673200
H	0.90029000	3.70531100	-1.55360100
H	1.44151000	2.12961800	-1.33554700
C	-2.45264700	5.67839100	-0.35581400
C	-1.43625200	4.74864300	-0.13167800
C	-1.60533900	3.41061600	-0.51162200
C	-2.80487000	3.00789000	-1.10914200
C	-3.82090700	3.93836100	-1.33223900
C	-3.64619300	5.27353400	-0.95912100
H	-2.31794300	6.71288800	-0.05223500
H	-2.93498500	1.96415700	-1.37621800
H	-4.75277800	3.62031600	-1.79193900
H	-4.44074800	5.99486600	-1.12912000
C	-0.49210600	2.40661900	-0.27301100
H	0.12802100	2.69721500	0.58840100
O	-0.83208700	1.14277100	-0.36011000
H	-0.51417000	5.06383700	0.35459000

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TS14' SCF Done: E(RM06) = -1714.41743282

C	1.55945800	-0.18579000	2.54091400
C	1.15700800	-1.55815500	2.37444600
C	-0.28263600	-1.63966900	2.64812400
C	0.35581500	0.60345900	2.67832500
C	-0.76801100	-0.33449800	2.80310600
C	2.07843200	-2.73985300	2.27868700
H	3.02135100	-2.47296100	1.79281100
H	2.31519900	-3.12968500	3.27847600
H	1.62672800	-3.55631700	1.70661100
C	-1.04467200	-2.91682200	2.81682800
H	-0.91018600	-3.29125600	3.84204000
H	-2.11578200	-2.78054700	2.65171900
H	-0.69430700	-3.69584700	2.13635300
C	-2.18450000	0.08022500	3.05700600
H	-2.32063400	0.35216300	4.11288800
H	-2.46152700	0.95467100	2.45963800
H	-2.89054300	-0.72028400	2.82248000
C	0.29524900	2.06001600	3.04100200
H	0.37404600	2.19292400	4.12929000
H	1.11308300	2.62618600	2.58427800
H	-0.64718400	2.51975400	2.72647800
C	2.97075800	0.29793700	2.68302800
H	3.66073000	-0.25476500	2.03985200
H	3.07222800	1.36067100	2.45287100
H	3.29479300	0.15392100	3.72293400
C	-2.49030600	-3.70466000	-0.49026600
C	-0.56851800	-2.66794900	-1.19352300
C	-0.47901300	-3.52768200	-2.33207700
C	-1.47306100	-4.51902300	-2.49566100
C	-2.49116000	-4.61092200	-1.57275300
H	-3.28523300	-3.75296900	0.25226100
C	0.58887500	-3.33084200	-3.24507200
H	-1.42176500	-5.18732500	-3.35131900
H	-3.27779900	-5.35287300	-1.66235800
C	1.47186300	-2.30873800	-3.03469800
C	1.33323500	-1.46821600	-1.89345700
H	0.68119100	-3.98289600	-4.10970100
H	2.27745800	-2.12615700	-3.73557600
N	-1.56994200	-2.77368900	-0.29427700
N	0.36743700	-1.68444400	-0.97804900
C	2.15919500	-0.29842500	-1.64168800
C	3.19298900	0.12901200	-2.48948600
C	3.88369900	1.31189700	-2.24956800
C	3.51809500	2.09589800	-1.14284600
C	2.48434900	1.66921100	-0.28481600
C	1.80853800	0.45826100	-0.48334700
H	3.47263700	-0.45668900	-3.36049000
H	4.68208300	1.61428000	-2.91621200
H	2.26073500	2.30557800	0.56702600
Ir	0.38856500	-0.34512400	0.70528900
O	4.09803900	3.27692100	-0.81733600
C	5.17730300	3.75732800	-1.61876100
H	4.85962500	3.93889100	-2.65295600
H	5.48492200	4.70142200	-1.16557100
H	6.02299100	3.05956000	-1.61036200
N	-0.42541100	2.65034300	-1.54986400
H	-0.68202000	2.33728900	-2.49025600
H	-0.46876100	3.67126000	-1.50404600
H	0.54120600	2.35192900	-1.35733400
C	-4.71776900	3.76453200	-0.67546300
C	-3.34775100	3.53016400	-0.49591600
C	-2.82826900	2.24674100	-0.76533500
C	-3.68211400	1.24746200	-1.24893400
C	-5.03877000	1.49770500	-1.44752200
C	-5.56022100	2.75718500	-1.14349600
H	-5.11835900	4.75116600	-0.45255200
H	-5.68934000	0.70964700	-1.81609000
H	-6.61955800	2.95955800	-1.27645400
C	-1.39088200	1.88707300	-0.42426300
H	-1.05847800	2.43309300	0.46848900
O	-1.11335200	0.60072300	-0.48565000
H	-3.26720700	0.26064400	-1.42410000
N	-2.47337700	4.55655000	-0.00596600
H	-2.03804100	5.06747200	-0.77530800
H	-3.00549900	5.25343100	0.51283700

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IN18' SCF Done: E(RM06) = -1714.42821239

C	1.75865400	-0.56590700	2.41150300
C	1.34759800	-1.90649600	2.08791000
C	-0.06450900	-2.04550600	2.46157000
C	0.56870700	0.17909400	2.75844700
C	-0.53844500	-0.78385000	2.84411900
C	2.25879800	-3.05076500	1.75135400
H	3.16370100	-2.70573300	1.24320800
H	2.56876000	-3.58101900	2.66274000
H	1.76483500	-3.77894800	1.10047500
C	-0.80560200	-3.34540500	2.49918600
H	-0.56871500	-3.87618700	3.43269000
H	-1.88749300	-3.20113600	2.46312700
H	-0.52492700	-3.99947100	1.67082500
C	-1.93080200	-0.42192100	3.25996500
H	-1.96527600	-0.18868600	4.33277600
H	-2.29009300	0.46116200	2.72120600
H	-2.63517500	-1.23551200	3.06997700
C	0.52769600	1.56972800	3.32535800

H	0.65124200	1.55010600	4.41736600
H	1.32634900	2.19913900	2.91965900
H	-0.42897400	2.06022500	3.11732900
C	3.17719800	-0.09118700	2.50228800
H	3.80470300	-0.51588900	1.71416900
H	3.25735500	0.99642100	2.44885100
H	3.59665400	-0.40371100	3.46845600
C	-2.59961700	-3.62966900	-0.71057700
C	-0.74273000	-2.49516200	-1.43646400
C	-0.77316000	-3.17795900	-2.69224400
C	-1.79139700	-4.13504200	-2.90387300
C	-2.71789900	-4.36330100	-1.91100700
H	-3.31856400	-3.79161800	0.09086100
C	0.20644900	-2.84956300	-3.66414700
H	-1.83013000	-4.66938800	-3.84953200
H	-3.51974900	-5.08398300	-2.03311100
C	1.11859100	-1.86834400	-3.39244400
C	1.09877900	-1.20262100	-2.13395900
H	0.20920100	-3.36873700	-4.61884600
H	1.85767100	-1.58729800	-4.13263900
N	-1.65257700	-2.73714400	-0.46848800
N	0.21939400	-1.54978700	-1.17215000
C	1.96189700	-0.08211200	-1.79583400
C	2.91146100	0.47028600	-2.67078800
C	3.63762600	1.60573900	-2.32814000
C	3.39415800	2.21452900	-1.08515700
C	2.44052700	1.66652000	-0.20438000
C	1.73382100	0.49629900	-0.51070800
H	3.09550900	0.02173800	-3.64291200
H	4.36898500	2.00722200	-3.01907400
H	2.30410300	2.17302200	0.74660900
Ir	0.42444900	-0.47160400	0.67958700
O	4.02259300	3.33050600	-0.64276900
C	5.02952200	3.92493800	-1.46145000
H	4.61715600	4.26905500	-2.41802900
H	5.39910500	4.78421500	-0.89879200
H	5.85732200	3.22983000	-1.64589700
N	-0.55424600	2.64055700	-1.29527800
H	-0.86704500	2.22928100	-2.17891300
H	-0.75966900	3.65728000	-1.27719700
H	0.45178300	2.45835600	-1.18431600
C	-4.43027700	4.18339300	-0.45804000
C	-3.10493500	3.78029700	-0.25869600
C	-2.79317600	2.40348500	-0.24123100
C	-3.81873900	1.46653500	-0.39019000
C	-5.14003400	1.87394900	-0.57955900
C	-5.44107200	3.23606600	-0.62291400
H	-4.66570900	5.24534800	-0.47715700
H	-5.92653900	1.13414700	-0.69702700
H	-6.46494900	3.56711500	-0.77359500
C	-1.35281500	1.92511400	-0.08532100
H	-0.86304800	2.40820800	0.77896600
O	-1.20331500	0.61212200	-0.16830600
H	-3.55368200	0.41510100	-0.36106000
N	-2.05227100	4.73890300	-0.16330600
H	-2.40480500	5.69047600	-0.23757000
H	-1.53640300	4.66769000	0.71382400

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IN19 SCF Done: E(RM06) = -1715.63825136

C	-1.70138500	0.68806100	2.46481400
C	-1.14638500	1.97890700	2.15326400
C	0.27116800	1.96063900	2.53540800
C	-0.60030700	-0.18466700	2.80477400
C	0.60396600	0.65268600	2.90838100
C	-1.92597200	3.22110900	1.83038100
H	-2.86624500	2.98552700	1.32357600
H	-2.17045800	3.77660300	2.74669400
H	-1.35555400	3.89319000	1.18149300
C	1.15033300	3.17161500	2.58003900
H	0.97671400	3.71724900	3.51882600
H	2.20980400	2.91055500	2.53632300
H	0.93861900	3.86007600	1.75874800
C	1.94881800	0.13782400	3.31919000
H	1.93852900	-0.17762100	4.37102200
H	2.24164600	-0.72946600	2.71786100
H	2.72486300	0.89872100	3.20402200
C	-0.71053000	-1.57973900	3.35178500
H	-0.88133800	-1.56073900	4.43750700
H	-1.54203900	-2.13159700	2.90144500
H	0.20661300	-2.15177600	3.17889400
C	-3.16263400	0.36835300	2.55769700
H	-3.74496900	0.85925700	1.77353600
H	-3.35864200	-0.70448500	2.50330800
H	-3.54262000	0.72112700	3.52641800
C	3.02971400	3.21656700	-0.60683300
C	1.04723300	2.33967300	-1.35749700
C	1.17543700	3.02564300	-2.60546700
C	2.31005000	3.84596700	-2.79918900
C	3.25002000	3.94323100	-1.79721600
H	3.75775100	3.27425600	0.20077300
C	0.16997700	2.83246000	-3.58825700
H	2.42445000	4.38141300	-3.73818500
H	4.13792200	4.55734600	-1.90499300
C	-0.86466800	1.97655900	-3.33108100
C	-0.94624400	1.30831000	-2.07526100
H	0.24316000	3.35320200	-4.53939800
H	-1.62426200	1.79542900	-4.08200800
N	1.97427300	2.45048800	-0.38171700
N	-0.03140700	1.52598000	-1.10796200
C	-1.95356900	0.31357800	-1.74733200
C	-2.98175600	-0.08353900	-2.61817800
C	-3.84560000	-1.12239900	-2.29019900
C	-3.66321200	-1.79360600	-1.06821500
C	-2.64282900	-1.39169800	-0.18559600
C	-1.79528600	-0.31515300	-0.47386000
H	-3.12352600	0.41659100	-3.57202100
H	-4.63493600	-1.40499700	-2.97647600
H	-2.55782000	-1.93622200	0.74983900
Ir	-0.38179400	0.46577100	0.73396200
O	-4.41905800	-2.83829900	-0.64977700
C	-5.50331200	-3.27404300	-1.46823600
H	-5.15202500	-3.63293400	-2.44376000
H	-5.96939500	-4.09986700	-0.92770600
H	-6.24049000	-2.47537500	-1.61387200
N	0.30174500	-2.67367600	-1.30521500

H	0.84227900	-2.38037900	-2.17711200
H	0.19575700	-3.69283600	-1.31055400
H	-0.63313100	-2.24784400	-1.31627700
C	3.72458200	-4.85109700	0.37416600
C	2.48920600	-4.20057000	0.37123300
C	2.40032100	-2.84636600	0.02484800
C	3.56570500	-2.14395000	-0.30235000
C	4.80179600	-2.79400200	-0.29806600
C	4.88359100	-4.14845000	0.03579700
H	3.78340000	-5.90077400	0.64901500
H	3.48866300	-1.08710300	-0.53611400
H	5.70387400	-2.24080400	-0.54677200
H	5.84650500	-4.65175500	0.04300100
C	1.04484000	-2.14533400	0.00205700
H	0.40263200	-2.55186100	0.80045600
O	1.11761000	-0.81563600	-0.05806100
H	1.59197100	-4.75072600	0.65208000
H	2.82481300	-2.08313600	-3.28363800
N	1.85503300	-1.95979100	-3.57614000
H	1.73516600	-2.50313600	-4.43112300
H	1.75615700	-0.97846800	-3.83592600

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IN19' SCF Done: E(RM06) = -1770.98835794

C	1.09729400	1.42282200	2.52302500
C	2.25477500	0.62689300	2.21072700
C	1.94541300	-0.76972000	2.54283300
C	0.01224100	0.50883800	2.80930800
C	0.58824500	-0.84217400	2.87875400
C	3.63329900	1.15047400	1.92840200
H	3.59702300	2.12215500	1.42766900
H	4.20177700	1.27609900	2.86069800
H	4.19939800	0.46567800	1.28923800
C	2.95382100	-1.87463100	2.58208700
H	3.50332200	-1.83796000	3.53390000
H	2.48552100	-2.85867100	2.50638400
H	3.68721900	-1.78730400	1.77740700
C	-0.20058500	-2.06524800	3.23123600
H	-0.52244800	-2.03029200	4.28070200
H	-1.10132900	-2.14414400	2.61328200
H	0.38229500	-2.97899400	3.08888200
C	-1.34052200	0.87609800	3.34947300
H	-1.31312500	0.96822600	4.44451100
H	-1.69131800	1.83373800	2.95202500
H	-2.08864900	0.11394700	3.10758400
C	1.07693200	2.91585700	2.65802600
H	1.70985000	3.40494700	1.91232000
H	0.06948600	3.32666900	2.56520700
H	1.45541000	3.19195500	3.65185400
C	2.85834000	-3.48710700	-0.72206300
C	2.30195900	-1.36388400	-1.39272700
C	2.98255100	-1.54217100	-2.63768900
C	3.62570300	-2.77825100	-2.87292800
C	3.56343200	-3.76415800	-1.91308900
H	2.79338600	-4.24833600	0.05373200
C	2.96502800	-0.47788500	-3.57584100
H	4.15368700	-2.93281900	-3.81040000
H	4.03888700	-4.72926900	-2.05390700
C	2.27318900	0.66358600	-3.28145800
C	1.59872500	0.79138800	-2.03327700
H	3.48846200	-0.58769500	-4.52191400
H	2.23205800	1.47830800	-3.99439000
N	2.25552900	-2.33839400	-0.45907300
N	1.65757900	-0.18396400	-1.10312700
C	0.76803600	1.92715400	-1.67232600
C	0.52799900	3.02467000	-2.51610400
C	-0.36031600	4.03131500	-2.15559200
C	-1.03946800	3.92654900	-0.92881300
C	-0.79796300	2.83320800	-0.07646800
C	0.12528800	1.83177800	-0.39985500
H	1.03031400	3.10620300	-3.47590600
H	-0.52462900	4.87056000	-2.82055200
H	-1.34531400	2.81086700	0.86092300
Ir	0.64152700	0.25273900	0.73761300
O	-1.94980600	4.82622700	-0.48062000
C	-2.23541800	5.97277700	-1.28024300
H	-2.66165800	5.68930800	-2.25069300
H	-2.97254500	6.54972500	-0.71871400
H	-1.33971600	6.58559900	-1.43673400
N	-2.54585100	0.21478500	-1.44078900
H	-2.31316200	-0.39183700	-2.28418200
H	-3.55380400	0.44056300	-1.43483500
H	-1.99549600	1.07877900	-1.46972100
C	-5.41075800	-2.63329200	-0.04776200
C	-4.54722500	-1.53045000	-0.04315400
C	-3.15096600	-1.74355900	-0.06226700
C	-2.65872700	-3.05083900	-0.04978300
C	-3.52398100	-4.14695300	-0.04589400
C	-4.90309200	-3.93252300	-0.05544300
H	-6.48550800	-2.46499700	-0.03786700
H	-1.58205100	-3.18446800	-0.04879500
H	-3.12535200	-5.15740800	-0.03781200
H	-5.58988200	-4.77474600	-0.05459400
C	-2.17892700	-0.56446000	-0.11992900
H	-2.42633100	0.17416200	0.66189100
O	-0.89039000	-0.92107200	-0.15077300
H	-1.54439200	-2.34982200	-3.11821000
N	-1.95522000	-1.54643800	-3.59421900
H	-2.76965500	-1.89496900	-4.09993500
H	-1.27921000	-1.24813400	-4.29702800
N	-5.05798400	-0.20454300	-0.10598900
H	-6.07427300	-0.18634500	-0.07480200
H	-4.70854000	0.39184800	0.64306500

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TS15 SCF Done: E(RM06) = -1715.63381546

C	0.27872100	1.05393200	2.73551000
C	1.54471300	0.38834200	2.57165100
C	1.30337500	-1.05982400	2.63538600
C	-0.75166300	0.04331400	2.65829800
C	-0.08168200	-1.26553200	2.66442900
C	2.89397900	1.03923200	2.67216600
H	2.87344700	2.06039600	2.28105500
H	3.22459900	1.08837800	3.71919000
H	3.65375600	0.48168600	2.11608100
C	2.37895400	-2.09679000	2.73566300

H	2.72082400	-2.17285600	3.77796200
H	2.02627800	-3.08471900	2.43032000
H	3.25047800	-1.84549900	2.12674100
C	-0.80917500	-2.57397600	2.68342000
H	-1.29489700	-2.73070200	3.65605800
H	-1.59097200	-2.60245200	1.91799600
H	-0.13519000	-3.41590900	2.50559300
C	-2.21272600	0.25148200	2.93656600
H	-2.41425500	0.19287300	4.01566300
H	-2.55363800	1.23377500	2.59511700
H	-2.82978300	-0.50898200	2.44851500
C	0.08785600	2.50393000	3.06219500
H	0.83360700	3.13869500	2.57595200
H	-0.90203100	2.86703300	2.77763300
H	0.18936300	2.64112200	4.14775000
C	3.14233000	-3.18460600	-0.74291000
C	2.60141100	-0.98682400	-1.12752300
C	3.64493200	-0.86245400	-2.09678000
C	4.46529900	-1.98787100	-2.33679400
C	4.21775500	-3.16060400	-1.65659200
H	2.91381800	-4.10242600	-0.20388200
C	3.78494800	0.37435800	-2.78120700
H	5.27344300	-1.91282000	-3.05990900
H	4.82001800	-4.04922400	-1.81362100
C	2.90288500	1.38742800	-2.52608800
C	1.87645100	1.21936700	-1.54978900
H	4.58167100	0.49628200	-3.51023600
H	2.98666300	2.33049600	-3.05250100
N	2.36290000	-2.14679500	-0.47739600
N	1.77091200	0.07236500	-0.84065400
C	0.85649300	2.20885000	-1.26075000
C	0.71347600	3.41766400	-1.96475300
C	-0.34491000	4.27897700	-1.70725400
C	-1.29193800	3.91712700	-0.73136700
C	-1.15325400	2.70944000	-0.02243900
C	-0.07628100	1.84688200	-0.24150700
H	1.42467700	3.69854700	-2.73641000
H	-0.43343300	5.20543900	-2.26141200
H	-1.91327200	2.48269000	0.71932800
Ir	0.31681000	0.13522000	0.75574900
O	-2.37190300	4.66578000	-0.40359200
C	-2.57071000	5.91709000	-1.06047300
H	-2.71128200	5.78562800	-2.14046500
H	-3.48067000	6.33655700	-0.62777800
H	-1.73450100	6.60276400	-0.87838100
N	-2.42694800	0.19638000	-2.06076700
H	-1.18474700	-0.70408100	-3.23202400
H	-3.40570700	0.24877200	-2.34043500
H	-2.11965200	1.15105800	-1.86954800
C	-5.42125600	-2.78429500	-1.10387000
C	-4.58311400	-1.67390100	-1.00150100
C	-3.19217900	-1.83004000	-0.89830500
C	-2.66129200	-3.12441800	-0.88109700
C	-3.49936100	-4.23911600	-0.98395400
C	-4.87993300	-4.07299900	-1.09976900
H	-6.49628600	-2.64441200	-1.18057400
H	-1.58951800	-3.24868000	-0.76653000
H	-3.07197300	-5.23860400	-0.96704700
H	-5.53170600	-4.93905100	-1.17640200
C	-2.28966900	-0.59538300	-0.79877900
H	-2.62843800	0.01016700	0.05368100
O	-0.94772000	-0.94594700	-0.60451000
H	-5.01942300	-0.67616200	-0.99171900
H	-0.39519600	-1.29039900	-1.94475200
N	-0.34441800	-1.30687500	-3.05732300
H	-0.46252200	-2.24079600	-3.45460300
H	0.50530200	-0.87340600	-3.42199800

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IN20 SCF Done: E(RM06) = -1715.64321931

C	0.22472500	1.06196500	2.74923100
C	1.55292100	0.52447100	2.54841500
C	1.45723600	-0.94216100	2.61899200
C	-0.69485400	-0.04134900	2.67589500
C	0.10003500	-1.28100900	2.65878200
C	2.83356400	1.30123700	2.64726900
H	2.70859300	2.32730100	2.29041000
H	3.17503200	1.34842300	3.69070200
H	3.63146300	0.83567300	2.06113300
C	2.63026700	-1.86696800	2.70515800
H	2.98976200	-1.90554000	3.74351500
H	2.37284500	-2.88509800	2.40473500
H	3.46401100	-1.53024400	2.08507600
C	-0.49637000	-2.65364100	2.68104800
H	-0.90518800	-2.87664800	3.67596800
H	-1.31914800	-2.74196800	1.96433300
H	0.24465900	-3.42092800	2.44296100
C	-2.17254700	0.01818500	2.93515900
H	-2.38081200	-0.08904500	4.00898500
H	-2.60190200	0.97216600	2.61341800
H	-2.70506500	-0.78546400	2.41849200
C	-0.09492000	2.48451500	3.09050700
H	0.54781500	3.19160300	2.56009500
H	-1.13368900	2.74089900	2.87351700
H	0.06275200	2.63252100	4.16785400
C	3.33983600	-2.99015000	-0.75974200
C	2.66050100	-0.83459200	-1.15662500
C	3.65836100	-0.66650600	-2.16540400
C	4.53188000	-1.74793700	-2.42043400
C	4.37585000	-2.92169900	-1.71555900
H	3.18483700	-3.91010700	-0.19873700
C	3.70363800	0.56527300	-2.87068500
H	5.30648900	-1.63919700	-3.17526400
H	5.02052000	-3.77787300	-1.88366800
C	2.77563500	1.53073300	-2.59764600
C	1.79611600	1.31852600	-1.58467100
H	4.46361800	0.71822700	-3.63242400
H	2.78128700	2.46601400	-3.14404300
N	2.51411800	-1.99318400	-0.47922600
N	1.78078900	0.17953600	-0.85755500
C	0.72907800	2.25225600	-1.27715200
C	0.48700900	3.43523100	-1.99535400
C	-0.62720200	4.22220600	-1.72989400
C	-1.52677700	3.81081000	-0.73056500
C	-1.28158700	2.63232100	0.00056500
C	-0.15214100	1.84753200	-0.23286800

H	1.15986200	3.75303700	-2.78635600
H	-0.79398700	5.12887900	-2.29895300
H	-2.00545900	2.36739100	0.76523300
Ir	0.36627700	0.16503400	0.76759400
O	-2.65567800	4.48030300	-0.39671100
C	-2.96993300	5.68853300	-1.08827200
H	-3.11412000	5.50958600	-2.16083500
H	-3.90605300	6.04322100	-0.65340700
H	-2.19239000	6.44769100	-0.94185900
N	-2.40935700	0.05036300	-2.14246500
H	-0.84523800	-1.31121500	-3.48848900
H	-3.33286500	-0.05387800	-2.55431100
H	-2.22960000	1.04298300	-2.00261900
C	-5.43176600	-2.86172800	-1.02476800
C	-4.58880800	-1.75078700	-1.00763800
C	-3.19900300	-1.90662800	-0.89021900
C	-2.67194400	-3.19759700	-0.77593600
C	-3.51671200	-4.31175200	-0.79374700
C	-4.89639000	-4.14839000	-0.92027100
H	-6.50567500	-2.72279400	-1.11511000
H	-1.60101100	-3.32989700	-0.66696200
H	-3.09272500	-5.30868300	-0.70575800
H	-5.55165300	-5.01501700	-0.93184700
C	-2.31674900	-0.66045500	-0.87581300
H	-2.60146200	-0.03393400	-0.02293600
O	-0.93962600	-0.99331600	-0.61483900
H	-5.01635900	-0.75264200	-1.08095100
H	-0.51235900	-1.34145900	-1.48570600
N	-0.15489400	-1.89116200	-3.00782800
H	-0.39001000	-2.86574100	-3.19342900
H	0.75405200	-1.71328400	-3.43212100

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TS15' SCF Done: E(RM06) = -1770.98129215

C	0.51892100	1.02458300	2.74133000
C	1.73903700	0.28390000	2.54066400
C	1.41445100	-1.14827100	2.62128300
C	-0.56972200	0.07581800	2.68611100
C	0.02214400	-1.27136500	2.68533800
C	3.12767600	0.85083500	2.60930700
H	3.16108300	1.87300700	2.22175600
H	3.48539800	0.87482700	3.64824900
H	3.83817700	0.24972500	2.03373500
C	2.42872700	-2.24572200	2.70390600
H	2.77764900	-2.34642800	3.74183700
H	2.01592200	-3.21010000	2.39892100
H	3.30534900	-2.04123500	2.08514900
C	-0.77516000	-2.53693500	2.75912000
H	-1.15146200	-2.69004600	3.78018800
H	-1.64444000	-2.50707900	2.09528300
H	-0.17725700	-3.41180000	2.48981500
C	-2.00882200	0.36451700	3.00452800
H	-2.18610000	0.30746500	4.08788800
H	-2.30246800	1.36769100	2.67965900
H	-2.67847400	-0.35776500	2.52756900
C	0.42725700	2.48169400	3.07961700
H	1.18533200	3.07371200	2.55997200
H	-0.55138100	2.90375900	2.84187000
H	0.58763400	2.60694700	4.15945900
C	3.06959600	-3.34031600	-0.77572700
C	2.62275800	-1.12525200	-1.18119600
C	3.60402400	-1.08090800	-2.21979400
C	4.34254100	-2.25603700	-2.48611500
C	4.07851300	-3.39756500	-1.76078700
H	2.83032700	-4.23105300	-0.19744200
C	3.76638400	0.13088900	-2.94218600
H	5.10158300	-2.24289100	-3.26411800
H	4.61861400	-4.32221300	-1.93531900
C	2.97015100	1.20198000	-2.64635200
C	2.00724200	1.11600100	-1.59778100
H	4.51181100	0.18893000	-3.73099900
H	3.06816700	2.12495800	-3.20444600
N	2.36737000	-2.25502100	-0.48630100
N	1.86955800	-0.01562200	-0.87124000
C	1.07577500	2.17544300	-1.25945800
C	1.00046400	3.40309500	-1.94109100
C	0.00910900	4.32964800	-1.64625300
C	-0.93990200	4.01603600	-0.65614400
C	-0.85781000	2.79741400	0.04251500
C	0.15402100	1.86968000	-0.21281700
H	1.71567000	3.65160300	-2.72001700
H	-0.02746500	5.26977100	-2.18290900
H	-1.60773500	2.61527300	0.80611400
Ir	0.45923700	0.12723000	0.75821200
O	-1.96779200	4.82425000	-0.30215400
C	-2.11495900	6.08178500	-0.96143000
H	-2.27915700	5.95285300	-2.03838000
H	-2.99570200	6.54788400	-0.51605900
H	-1.24259100	6.72534200	-0.79587600
N	-2.44042100	0.35647700	-1.99133900
H	-1.23317000	-0.66108200	-3.29823700
H	-3.43933800	0.44927500	-2.18300300
H	-2.07901500	1.29743600	-1.83001600
C	-5.41704100	-2.60015100	-0.87171900
C	-4.58382200	-1.47316100	-0.80303100
C	-3.17944400	-1.64902200	-0.78027500
C	-2.66438100	-2.94856300	-0.79394200
C	-3.49789300	-4.06758300	-0.86252600
C	-4.88037600	-3.88550500	-0.91009700
H	-6.49541500	-2.45672600	-0.89106600
H	-1.58724600	-3.06927300	-0.73889300
H	-3.07241700	-5.06710800	-0.87380600
H	-5.54717200	-4.74227400	-0.96128700
C	-2.24838600	-0.43374000	-0.74707900
H	-2.49338600	0.17704100	0.13603600
O	-0.89630100	-0.81691500	-0.63937200
H	-0.47377100	-1.12817800	-1.88955300
N	-0.40641600	-1.24084400	-3.05935800
H	-0.52762400	-2.19934500	-3.39036400
H	0.44002600	-0.83944900	-3.46452300
N	-5.14631700	-0.18071800	-0.83084200
H	-6.14861000	-0.18274100	-0.66746200
H	-4.70269900	0.48463600	-0.20377800

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IN20' SCF Done: E(RM06) = -1770.99030775

C	0.52219600	1.09342600	2.74138600
C	1.81188500	0.48796800	2.48914700
C	1.64971600	-0.97110100	2.59030200
C	-0.45276300	0.03461400	2.72671600
C	0.28107500	-1.24218800	2.69759100
C	3.13120600	1.20335200	2.51322100
H	3.03926400	2.22757200	2.14151000
H	3.52190300	1.25280300	3.53913500
H	3.87897600	0.68973300	1.90170000
C	2.78009400	-1.95058600	2.63834000
H	3.17256700	-2.00692300	3.66389500
H	2.46559700	-2.95538900	2.34733400
H	3.60707300	-1.65388900	1.98947800
C	-0.38040400	-2.58274900	2.77573900
H	-0.74779900	-2.76699100	3.79454300
H	-1.24262800	-2.64203900	2.10397800
H	0.30704800	-3.39170100	2.51634100
C	-1.91084900	0.17045700	3.05993100
H	-2.06857700	0.09301000	4.14484700
H	-2.30912000	1.13914800	2.74189400
H	-2.50835600	-0.61529100	2.58765800
C	0.28696900	2.53383600	3.07731700
H	0.95411200	3.20084300	2.52540700
H	-0.74144600	2.84498500	2.88261000
H	0.47875300	2.68143500	4.14922100
C	3.30489100	-3.10371900	-0.84111000
C	2.68816200	-0.92981300	-1.23795100
C	3.62899500	-0.81849700	-2.30740500
C	4.43984800	-1.93962400	-2.59596400
C	4.27962700	-3.09451500	-1.86173900
H	3.14946100	-4.00676300	-0.25345300
C	3.68331500	0.40068500	-3.03331200
H	5.16914600	-1.87582700	-3.39945100
H	4.87542700	-3.98034900	-2.05497500
C	2.81224600	1.40763700	-2.72365500
C	1.87877200	1.24685300	-1.65904900
H	4.40450200	0.51253900	-3.83867900
H	2.82805400	2.33520300	-3.28286300
N	2.53930600	-2.06898000	-0.52893400
N	1.86368600	0.12143200	-0.91113400
C	0.85606600	2.21885500	-1.31673000
C	0.61402700	3.39733500	-2.04253600
C	-0.45797900	4.22605700	-1.73292900
C	-1.31682100	3.86118300	-0.68145500
C	-1.07445100	2.68478900	0.05334800
C	0.01420700	1.85826200	-0.22444000
H	1.25214100	3.67854600	-2.87504300
H	-0.62438400	5.12870500	-2.30838300
H	-1.76637900	2.45516200	0.85792100
Ir	0.52262200	0.17068100	0.76992700
O	-2.40304900	4.57441200	-0.29893300
C	-2.70357200	5.79093200	-0.98261200
H	-2.91148500	5.61227500	-2.04456000
H	-3.59966300	6.18695900	-0.50156200
H	-1.88833900	6.51756000	-0.88320000
N	-2.37529700	0.09683700	-2.04623000
H	-0.99658700	-1.32175800	-3.38058100
H	-3.35144100	0.10818500	-2.33966700
H	-2.07040200	1.06474700	-1.94911500
C	-5.41294900	-2.73921800	-0.72815300
C	-4.57274400	-1.61480200	-0.74953500
C	-3.16983300	-1.80014500	-0.70743600
C	-2.66228200	-3.10005400	-0.61845200
C	-3.50400400	-4.21397400	-0.59587000
C	-4.88522300	-4.02612700	-0.65858900
H	-6.49004600	-2.59056600	-0.76501600
H	-1.58715800	-3.23373000	-0.56402400
H	-3.08478100	-5.21367500	-0.52878400
H	-5.55775400	-4.87967100	-0.64168600
C	-2.25000600	-0.58377400	-0.76253100
H	-2.47066800	0.07660800	0.08778000
O	-0.87448500	-0.95186500	-0.55820000
H	-0.49584600	-1.32467600	-1.44333400
N	-0.24509600	-1.88473700	-2.97520300
H	-0.46809000	-2.86552400	-3.14180900
H	0.61270300	-1.67751400	-3.48424000
N	-5.12778100	-0.32907000	-0.89062700
H	-6.12779100	-0.30656100	-0.71568800
H	-4.66980600	0.39947900	-0.35102800

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TS15-1 SCF Done: E(RM06) = -1659.04212823

C	0.01394400	-0.80279100	2.73605200
C	-1.36540500	-0.40560900	2.57226900
C	-1.40446000	1.06333100	2.51597800
C	0.82389700	0.36972400	2.51894300
C	-0.08549700	1.52615800	2.44325200
C	-2.56336500	-1.28087300	2.80189200
H	-2.35486600	-2.32186100	2.53915900
H	-2.86345300	-1.25584800	3.85876900
H	-3.42182500	-0.94995000	2.20914800
C	-2.65654800	1.87828500	2.59373700
H	-2.96668300	1.96998100	3.64470500
H	-2.51679600	2.88657600	2.19850900
H	-3.48151200	1.41199700	2.05073600
C	0.37357100	2.94614000	2.31484200
H	0.81395300	3.29490200	3.25884000
H	1.13941500	3.04973300	1.53958100
H	-0.45170500	3.61616600	2.06083600
C	2.30854900	0.47184200	2.72080600
H	2.53958700	0.70818400	3.76899200
H	2.81795700	-0.46627100	2.48021100
H	2.74768800	1.26380700	2.10648600
C	0.48222700	-2.15828700	3.16881200
H	-0.11031200	-2.95925200	2.71934400
H	1.53135500	-2.33436000	2.92268900
H	0.38204200	-2.23852700	4.25998100
C	-3.57400800	2.68562400	-0.88150600
C	-2.72615500	0.57583100	-1.18162000
C	-3.72145400	0.27524900	-2.16218400
C	-4.67537700	1.27246300	-2.46640500
C	-4.60351300	2.49061300	-1.82731700
H	-3.49245400	3.64004400	-0.36428800
C	-3.68976500	-0.99757000	-2.78897100
H	-5.44464600	1.06381400	-3.20526200
H	-5.31077900	3.28651100	-2.03528600

C	-2.69341600	-1.87858900	-2.47280700
C	-1.71303600	-1.53090500	-1.50038000
H	-4.44772500	-1.25046000	-3.52548000
H	-2.64057500	-2.84520900	-2.95862400
N	-2.67241200	1.77159700	-0.55711300
N	-1.76784300	-0.35130000	-0.84448600
C	-0.56399000	-2.35717500	-1.17027800
C	-0.26266500	-3.57273800	-1.80658100
C	0.91772100	-4.25475700	-1.53414700
C	1.82601600	-3.69841700	-0.61622500
C	1.52346000	-2.48519600	0.03180200
C	0.32486700	-1.80639000	-0.19951600
H	-0.94427000	-4.00071500	-2.53617300
H	1.12530300	-5.19252300	-2.03525000
H	2.25525700	-2.11406100	0.74325600
Ir	-0.29061900	-0.10179500	0.69556100
O	3.01709700	-4.25385000	-0.28646300
C	3.38232100	-5.50398300	-0.87036100
H	3.47268900	-5.42652900	-1.96092600
H	4.35586300	-5.75584200	-0.44567600
H	2.66191900	-6.29035300	-0.61545400
N	1.98060800	0.16008300	-2.45128700
H	0.79855900	0.43223300	-2.06842200
H	2.41211700	0.63255700	-3.24771000
H	2.22756600	-0.83154200	-2.43782300
C	4.99017300	3.36880700	-1.11699300
C	4.27548200	2.17688900	-0.99244600
C	2.89048300	2.15777400	-1.20711500
C	2.22569300	3.34501900	-1.53965400
C	2.94314300	4.53617000	-1.66247500
C	4.32441200	4.55003200	-1.45381800
H	6.06285700	3.37642100	-0.94505100
H	1.15006200	3.33007600	-1.68290800
H	2.42196400	5.45515100	-1.91643100
H	4.87964800	5.47923300	-1.54680900
C	2.13926200	0.85153100	-1.10743800
H	2.61496200	0.16200300	-0.40732800
O	0.73754700	0.98397800	-0.89482000
H	4.79543700	1.25925000	-0.72492800

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TS15-2 SCF Done: E(RM06) = -1892.67026538

C	-0.82436800	-3.13213900	-0.01685000
C	-0.05361400	-2.97582000	1.19143000
C	1.36310300	-2.87352300	0.81755900
C	0.07113000	-2.88151700	-1.12628000
C	1.43248900	-2.80827700	-0.57734700
C	-0.55098000	-3.23870000	2.58378800
H	-1.59884800	-2.94820900	2.70112100
H	-0.47292000	-4.30888200	2.82069600
H	0.03489100	-2.69678800	3.33162800
C	2.51433600	-2.93136300	1.77332400
H	2.78557700	-3.97888900	1.96942900
H	3.40019100	-2.42992900	1.37499900
H	2.27131400	-2.47146600	2.73345200
C	2.67840200	-2.74624800	-1.40497500
H	2.99053700	-3.76545200	-1.67480200
H	2.52543400	-2.19965300	-2.33817000
H	3.50696800	-2.27455800	-0.87138000
C	-0.25142500	-3.12334100	-2.57393300
H	-0.08949000	-4.17863900	-2.83627700
H	-1.29551800	-2.88933200	-2.80094100
H	0.37905600	-2.52686900	-3.24105100
C	-2.24281000	-3.60938100	-0.09645800
H	-2.83241300	-3.27680800	0.76192300
H	-2.74660300	-3.26589400	-1.00241900
H	-2.25343700	-4.70818100	-0.10441200
C	2.95614500	0.53123100	3.11442900
C	0.71319200	0.62044800	2.63689400
C	0.45696600	1.39145400	3.81276200
C	1.55030800	1.70775000	4.65053900
C	2.81266400	1.28021300	4.30203100
H	3.94255000	0.18237300	2.81354300
C	-0.87598900	1.80556300	4.07068400
H	1.37733500	2.28798600	5.55316500
H	3.68059000	1.50532300	4.91286700
C	-1.86183000	1.49706200	3.17468300
C	-1.55709700	0.74153100	2.00559700
H	-1.09546300	2.37495900	4.97001300
H	-2.88091200	1.82119000	3.34732800
N	1.95561800	0.20224200	2.31118800
N	-0.30715800	0.28097800	1.77958900
C	-2.51467000	0.44567600	0.95370900
C	-3.82741300	0.94768600	0.92139600
C	-4.64950700	0.73545500	-0.17884900
C	-4.14157000	0.02080400	-1.27831500
C	-2.83361000	-0.49661500	-1.24472200
C	-2.00858400	-0.32404100	-0.13458900
H	-4.22283500	1.52486300	1.75245700
H	-5.65783800	1.13135700	-0.18292200
H	-2.50072400	-1.05310700	-2.11603500
Ir	-0.15468700	-1.08074100	0.11785100
O	-4.83785700	-0.22549900	-2.41497500
C	-6.18124900	0.24384100	-2.51573700
H	-6.23035000	1.33782100	-2.45234500
H	-6.53349000	-0.07532200	-3.49837700
H	-6.82040600	-0.19882900	-1.74207700
N	0.46392400	1.72633800	-3.05964600
H	0.53732900	2.80595300	-2.05480200
H	0.98301200	1.87060500	-3.92500700
H	-0.50886300	1.52529600	-3.29799800
C	4.59001000	0.50530300	-3.66832900
C	3.20109400	0.42358700	-3.56314100
C	2.56073400	0.66909900	-2.33904200
C	3.33335600	0.98434900	-1.21791300
C	4.72468100	1.06657200	-1.32318300
C	5.35598800	0.83067400	-2.54570500
H	5.07348900	0.31031500	-4.62185400
H	2.84005400	1.14405900	-0.26550900
H	5.31679300	1.31450700	-0.44587100
H	6.43793200	0.89353700	-2.62416400
C	1.03659300	0.58622200	-2.25106200
H	0.69691600	-0.35496400	-2.69853900
O	0.52701500	0.69868000	-0.95452200
H	2.61551500	0.15386200	-4.44125300
C	-1.75644800	3.83431700	-1.09415500

H	-2.09721400	2.90941300	-0.61877400
H	-1.80837800	3.70794900	-2.18160700
H	-2.45466900	4.63312000	-0.82082700
C	-0.34165400	4.20563600	-0.64617300
C	0.17986900	5.43844200	-1.38575900
H	0.16251500	5.28619800	-2.47123600
H	-0.44703700	6.30714600	-1.15835100
H	1.20803200	5.66520900	-1.08592200
C	-0.24820200	4.38541700	0.86584700
H	-0.63058100	3.50726100	1.39526800
H	0.78909600	4.55696000	1.17131800
H	-0.84498500	5.24993300	1.17602800
O	0.59642100	3.11846600	-1.00334800
H	0.44716800	2.06738000	-0.67490500

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IN21 SCF Done: E(RM06) = -1715.66456230

C	2.04550100	-0.59560500	2.24878600
C	1.64017300	-1.90413100	1.80756200
C	0.28300900	-2.13729200	2.30823000
C	0.88514100	0.05421900	2.81264500
C	-0.17549700	-0.95784900	2.91355100
C	2.54040800	-2.97089200	1.25336400
H	3.38089800	-2.54457200	0.69826000
H	2.95580000	-3.58471800	2.06452000
H	1.99990600	-3.64273600	0.57942500
C	-0.43409300	-3.45185600	2.28205800
H	-0.11467200	-4.05965500	3.14101600
H	-1.51732400	-3.32674300	2.35119400
H	-0.21220500	-4.02755100	1.38013100
C	-1.49436800	-0.78403400	3.61275600
H	-1.54784800	-1.44990200	4.48394200
H	-1.62113400	0.23698900	3.98177800
H	-2.34621200	-1.02057300	2.96638400
C	0.87457200	1.38705300	3.50508900
H	1.10883600	1.27548800	4.57275100
H	1.61626300	2.06791500	3.07661100
H	-0.10391300	1.87340900	3.43699300
C	3.44351300	-0.05832800	2.22001000
H	4.00153900	-0.40568500	1.34684500
H	3.46990000	1.03339900	2.22657000
H	3.97488700	-0.40638400	3.11659400
C	-2.67763300	-3.39918100	-0.74026100
C	-0.79739400	-2.28407700	-1.46688500
C	-0.79279100	-3.02170900	-2.68967000
C	-1.78386700	-4.01151900	-2.87190500
C	-2.73133700	-4.21112700	-1.89039700
H	-3.43421800	-3.50326700	0.03454400
C	0.19286800	-2.70460100	-3.66191000
H	-1.78988300	-4.59374600	-3.78956300
H	-3.51228900	-4.95674200	-1.99401200
C	1.07432500	-1.68911300	-3.41804300
C	1.03957600	-0.99045900	-2.17686300
H	0.22218700	-3.26098100	-4.59483100
H	1.81658500	-1.41511600	-4.15770200
N	-1.74759900	-2.47770900	-0.52421800
N	0.15662300	-1.33029600	-1.21005200
C	1.88502900	0.14287000	-1.85760000
C	2.75736800	0.75651500	-2.77315100
C	3.43417900	1.92437900	-2.44452600
C	3.22348900	2.49983000	-1.17840100
C	2.36078400	1.88069500	-0.25356200
C	1.70155800	0.69154400	-0.55525400
H	2.90552300	0.33757300	-3.76464100
H	4.09979600	2.38269900	-3.16593200
H	2.24937700	2.36243700	0.71372600
Ir	0.50283000	-0.37450300	0.68895900
O	3.80862800	3.64347700	-0.75313800
C	4.71608900	4.32166900	-1.62153600
H	4.21833600	4.65219000	-2.54127700
H	5.06040300	5.19510700	-1.06494800
H	5.57682700	3.69049200	-1.87359700
N	-0.99510900	1.09572500	0.07951500
H	-1.15672700	1.08521000	-0.95278900
H	-0.56439700	2.00483700	0.26161000
H	-2.34219900	-0.86331900	0.40426100
C	-4.94635800	3.23362900	-0.98867500
C	-4.19449400	2.12245400	-0.60042600
C	-3.18654800	2.25455600	0.36243000
C	-2.95165900	3.50999000	0.93729200
C	-3.69967700	4.62186200	0.54656800
C	-4.69867200	4.48573600	-0.42000800
H	-5.73421700	3.11965000	-1.72889200
H	-2.18834200	3.61951000	1.70607000
H	-3.51076400	5.58916900	1.00412000
H	-5.28796400	5.34793500	-0.72006200
C	-2.32517700	1.07025600	0.77700500
H	-2.09286100	1.16393500	1.84632600
O	-2.98387800	-0.12199600	0.49343200
H	-4.39452300	1.14409400	-1.02388800
N	-1.53375500	1.53892400	-2.82347300
H	-2.35263200	2.14500400	-2.76992400
H	-1.76533500	0.80656600	-3.49421200
H	-0.79252500	2.09355600	-3.25159800

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IN21' SCF Done: E(RM06) = -1771.01101043

C	1.76026100	0.06235900	2.55975700
C	1.73098600	-1.33242600	2.20928200
C	0.38181300	-1.83636300	2.49676400
C	0.40095700	0.46919500	2.83519300
C	-0.41720300	-0.75019300	2.87859600
C	2.93180800	-2.19684500	1.95013100
H	3.72791200	-1.64112900	1.44672400
H	3.34085200	-2.58043300	2.89517600
H	2.68323600	-3.06277700	1.32923400
C	-0.01175600	-3.28146700	2.50374200
H	0.26360000	-3.73270400	3.46780200
H	-1.08892700	-3.41404300	2.37514000
H	0.49691000	-3.85221600	1.72356600
C	-1.83757900	-0.81287100	3.35423900
H	-1.85474300	-1.00628900	4.43621700
H	-2.37128700	0.12787000	3.19465300
H	-2.40597200	-1.61323200	2.87152000
C	-0.02392900	1.80796800	3.36965100
H	0.04919000	1.83136800	4.46580000

H	0.60614500	2.61466500	2.98311500
H	-1.06158300	2.04225600	3.11039800
C	2.99252200	0.90029000	2.71496700
H	3.77826600	0.61325000	2.01162800
H	2.79036100	1.96454100	2.57922700
H	3.38792800	0.76518700	3.73121300
C	-1.29460600	-4.08457700	-0.93500100
C	0.31813500	-2.50486100	-1.40301500
C	0.81573500	-3.29146000	-2.48618100
C	0.21477300	-4.54619800	-2.72893900
C	-0.84108200	-4.95693200	-1.94266600
H	-2.15573700	-4.35707400	-0.32846200
C	1.87304400	-2.76046700	-3.27206100
H	0.58829000	-5.16650600	-3.53919400
H	-1.33195000	-5.91150500	-2.09835900
C	2.35919100	-1.51579400	-2.98795200
C	1.85047900	-0.78063600	-1.87790100
H	2.27121300	-3.34313500	-4.09806600
H	3.15041000	-1.08437200	-3.58869000
N	-0.74149200	-2.90835400	-0.66356400
N	0.88733100	-1.29718700	-1.08007200
C	2.28150000	0.55724800	-1.52640200
C	3.14378400	1.33853300	-2.31536700
C	3.41353500	2.66030600	-1.98695500
C	2.79743300	3.21989000	-0.85296100
C	1.94524200	2.43670600	-0.05097400
C	1.69136600	1.09998000	-0.34873800
H	3.60382600	0.92809500	-3.20979400
H	4.07712800	3.24547800	-2.61180400
H	1.50891800	2.91797300	0.81986900
Ir	0.55500700	-0.17924000	0.74031000
O	2.96751200	4.49941700	-0.44755300
C	3.81927100	5.35778000	-1.20671300
H	3.44978800	5.48219600	-2.23181300
H	3.79778700	6.32199100	-0.69588800
H	4.84930500	4.98196300	-1.22811700
N	-1.08511100	0.84743200	-0.29007800
H	-0.94997500	0.84696300	-1.32360400
H	-0.99099100	1.81800100	0.01137200
H	-2.01036400	-1.48363500	-0.42620800
C	-5.91785400	1.97687600	-0.34839700
C	-4.89637400	1.05043600	-0.08058600
C	-3.56083500	1.37677700	-0.42924600
C	-3.30329200	2.60136400	-1.05326500
C	-4.32583300	3.51353600	-1.32374100
C	-5.63492600	3.19595000	-0.95858700
H	-6.94050400	1.72685100	-0.07415400
H	-2.28762700	2.86022600	-1.33860000
H	-4.09902600	4.45908400	-1.80712600
H	-6.44324700	3.89514100	-1.15586400
C	-2.47749100	0.38753600	-0.02921000
H	-2.55647200	0.22359500	1.05103100
O	-2.69018200	-0.82986200	-0.71653400
N	-1.37657700	0.70073400	-3.24932400
H	-2.09822100	0.00032900	-3.07594500
H	-0.76962100	0.32502900	-3.97725000
H	-1.85407100	1.50331800	-3.65876200
N	-5.17095300	-0.15095700	0.57661400
H	-6.15729100	-0.38328400	0.61594600
H	-4.61447000	-0.92952200	0.23704600

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TS16 SCF Done: E(RM06) = -1715.61588804

C	1.90677700	-0.10707100	2.43548000
C	1.27148400	-1.39672700	2.37997200
C	-0.13364500	-1.25056400	2.64899700
C	0.87310900	0.86659500	2.73479900
C	-0.37569500	0.15792200	2.84612500
C	1.99081200	-2.69858100	2.18777500
H	2.87903200	-2.58386000	1.55983200
H	2.32730900	-3.08127900	3.16117000
H	1.34735600	-3.46013600	1.74088200
C	-1.12404500	-2.35889500	2.85212100
H	-1.15058400	-2.67696300	3.90426500
H	-2.13974800	-2.04913100	2.58453100
H	-0.87528400	-3.23665900	2.24962300
C	-1.67013500	0.78139100	3.27733400
H	-1.69431100	0.86642000	4.37246100
H	-1.79415300	1.78720900	2.86622600
H	-2.53583800	0.18365500	2.98107000
C	1.10085800	2.29834500	3.11797700
H	1.30286700	2.36607600	4.19630400
H	1.95806100	2.73019700	2.59585800
H	0.22564900	2.92164400	2.91138300
C	3.38180300	0.16691600	2.37689000
H	3.90317700	-0.56180600	1.74864600
H	3.58806500	1.16163500	1.97043600
H	3.83030900	0.11899300	3.37915500
C	-0.54160400	-4.32359700	-0.71948100
C	0.77413700	-2.48594900	-1.20587500
C	1.55971900	-3.25959200	-2.11584200
C	1.27729300	-4.63790400	-2.23555600
C	0.23356300	-5.18503700	-1.51805400
H	-1.41792400	-4.70401500	-0.19878300
C	2.56149400	-2.59297800	-2.87132800
H	1.88327800	-5.24674000	-2.90148100
H	-0.01433400	-6.23889500	-1.58351700
C	2.72034300	-1.24355300	-2.72658500
C	1.95246900	-0.52646000	-1.76238300
H	3.17368700	-3.16015000	-3.56715300
H	3.45984900	-0.71253200	-3.31410800
N	-0.28835300	-3.02853400	-0.55824200
N	1.05061000	-1.16152500	-0.97357500
C	2.06133000	0.89988900	-1.53690900
C	2.78223600	1.77127300	-2.37302600
C	2.75664500	3.14414000	-2.16735400
C	1.98333000	3.65684100	-1.10895200
C	1.27126800	2.78664400	-0.26280500
C	1.31028700	1.40354300	-0.43285300
H	3.35900200	1.38810900	-3.21027000
H	3.31514600	3.79872200	-2.82575200
H	0.70204800	3.24170100	0.54177300
Ir	0.43084300	-0.00055200	0.74521900
O	1.86598900	4.97542300	-0.82140100
C	2.57788000	5.92360100	-1.61385700
H	2.25306200	5.89646300	-2.66131100

H	2.34082900	6.90113300	-1.18970700
H	3.66092200	5.75896400	-1.55974400
N	-1.31425500	0.51423800	-0.30601000
H	-1.43099500	0.01573700	-3.16870100
H	-1.41943200	1.51542900	-0.42096100
H	-1.78756900	-1.95955500	-0.62861900
C	-6.17996400	0.93904900	0.00025500
C	-4.98316600	0.27857800	0.27944500
C	-3.79631200	0.63294000	-0.37625300
C	-3.83593300	1.66290100	-1.32741900
C	-5.03218300	2.32611600	-1.60842000
C	-6.20766600	1.96578000	-0.94607900
H	-7.08896100	0.65367500	0.52275400
H	-2.92872600	1.95912200	-1.84745500
H	-5.04449400	3.12774900	-2.34222200
H	-7.13775600	2.48358700	-1.16369700
C	-2.52402000	-0.12416500	-0.04653800
H	-2.62095400	-0.58509900	0.94239600
O	-2.59692600	-1.44341900	-0.90603900
H	-4.96791600	-0.52386300	1.01324100
N	-2.18218700	-0.67160100	-3.26067800
H	-2.40896900	-1.11450600	-2.05437100
H	-1.89015300	-1.39073800	-3.92465400
H	-3.00446500	-0.20022700	-3.64190200

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IN22 SCF Done: E(RM06) = -1715.65702672

C	1.71431500	-1.46886400	2.18272000
C	0.69446400	-2.38803600	1.76932100
C	-0.59366000	-1.89593900	2.27432800
C	1.05080500	-0.31179000	2.74849900
C	-0.37590000	-0.63677100	2.85782100
C	0.92970800	-3.76224900	1.21164300
H	1.84916300	-3.80573000	0.62105600
H	1.02318900	-4.49335500	2.02667700
H	0.10360600	-4.09100300	0.57486100
C	-1.87669300	-2.67001800	2.26931600
H	-1.93263700	-3.29490900	3.17261200
H	-2.74936800	-2.01255700	2.26064800
H	-1.94326700	-3.33819200	1.40731500
C	-1.39400500	0.22466400	3.54229700
H	-1.46502100	-0.06194100	4.60141400
H	-1.10753600	1.28031300	3.51745100
H	-2.38583900	0.12621500	3.09360100
C	1.71818300	0.83226000	3.45765600
H	1.77333900	0.63671100	4.53746700
H	2.74085300	0.98651300	3.10266200
H	1.17146200	1.77080000	3.32216700
C	3.19183200	-1.71120100	2.12281700
H	3.47005000	-2.32618300	1.26267400
H	3.76203200	-0.78139000	2.07039000
H	3.50754200	-2.24327000	3.03073300
C	-3.49116200	-2.23829700	-1.11529500
C	-1.32850300	-1.70636700	-1.70776100
C	-1.51194700	-2.31028800	-2.99221100
C	-2.75359100	-2.91715400	-3.27985500
C	-3.75314600	-2.89543400	-2.33229100
H	-4.26888200	-2.16842300	-0.35741400
C	-0.44069500	-2.26767000	-3.92129900
H	-2.89979200	-3.39017000	-4.24737300
H	-4.72009000	-3.35436500	-2.50906200
C	0.72209700	-1.64527800	-3.57116000
C	0.87339000	-1.08488400	-2.27047000
H	-0.56203000	-2.72134500	-4.90105400
H	1.54584500	-1.58692000	-4.27150100
N	-2.33514100	-1.66435900	-0.80362500
N	-0.11952500	-1.15318600	-1.35343400
C	2.07287500	-0.38742800	-1.84379900
C	3.15586500	-0.09770000	-2.69305500
C	4.22500200	0.67417800	-2.25629500
C	4.20379100	1.18739500	-0.94761100
C	3.12820700	0.88997100	-0.08944200
C	2.07169500	0.07906600	-0.49923500
H	3.17330100	-0.46078100	-3.71646200
H	5.04826800	0.88446800	-2.92838600
H	3.16483900	1.30589700	0.91240000
Ir	0.48843600	-0.47051500	0.63950900
O	5.17146800	1.97251500	-0.41937400
C	6.30643000	2.30133400	-1.21968700
H	6.01578000	2.86044100	-2.11746600
H	6.93836200	2.93173000	-0.59152500
H	6.86493200	1.40284000	-1.50862300
N	-0.21885000	1.42255700	0.11290800
H	-6.69960400	1.20087600	0.34798000
H	0.48769000	2.00640400	-0.33661600
H	-3.16379700	-0.45494500	0.61930000
C	-3.47348900	5.04483600	-0.20181000
C	-3.05027200	3.75942900	0.12946600
C	-1.71636300	3.36686600	-0.08729000
C	-0.81236900	4.29293800	-0.64326600
C	-1.23847700	5.57554400	-0.97095200
C	-2.56821300	5.95461900	-0.75129300
H	-4.50508500	5.33775700	-0.02915700
H	0.22626200	4.02302200	-0.81849900
H	-0.53461800	6.28518800	-1.39592800
H	-2.89376700	6.95895400	-1.00737100
C	-1.36174700	1.99544300	0.28748300
H	-2.15367800	1.40571600	0.75096900
O	-3.75080000	0.03570000	1.22516300
H	-3.74627100	3.04232900	0.55670800
N	-6.23310700	0.41965200	-0.11340700
H	-4.60396600	0.15847200	0.73101600
H	-6.20771600	0.65029200	-1.10649600
H	-6.86263900	-0.37718800	-0.01849000

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TS16' SCF Done: E(RM06) = -1770.96506678

C	1.63293400	0.38930800	2.59753400
C	1.62512900	-1.03363500	2.44461000
C	0.25032900	-1.50044000	2.65649900
C	0.25365100	0.82959700	2.72395300
C	-0.57023200	-0.37420500	2.84379400
C	2.83536700	-1.92080800	2.37530500
H	3.67763600	-1.41672200	1.89261700
H	3.15885800	-2.21250100	3.38451300
H	2.63481800	-2.84297900	1.82160700

C	-0.16708600	-2.93515100	2.78176400
H	-0.08054600	-3.26257900	3.82777500
H	-1.20534900	-3.08618700	2.47435600
H	0.46123600	-3.59999200	2.18399700
C	-2.02641800	-0.37045000	3.19643400
H	-2.13923900	-0.30315000	4.28793100
H	-2.55047300	0.48926500	2.76951700
H	-2.53939700	-1.28054200	2.87256900
C	-0.20774200	2.21520900	3.07612400
H	-0.28449500	2.33940000	4.16556800
H	0.48742800	2.97621900	2.71023800
H	-1.19208000	2.42960700	2.64835100
C	2.84889700	1.25966100	2.70560600
H	3.69891000	0.84467800	2.15674100
H	2.66771200	2.26818400	2.32681900
H	3.14323900	1.34861400	3.76041900
C	-0.90690000	-4.26096300	-0.73677000
C	0.64892200	-2.61318600	-1.17013900
C	1.36903400	-3.48582600	-2.04440100
C	0.91445700	-4.81623600	-2.18112500
C	-0.22096300	-5.21849100	-1.50958200
H	-1.84052900	-4.52779200	-0.24538200
C	2.48377800	-2.95798300	-2.74871800
H	1.46293400	-5.50167700	-2.82209800
H	-0.60182800	-6.23118300	-1.58693400
C	2.80928800	-1.63936300	-2.59396500
C	2.08927400	-0.82458300	-1.67143700
H	3.05073400	-3.60240300	-3.41505800
H	3.63883500	-1.21110800	-3.14378100
N	-0.49841800	-3.00908400	-0.56429500
N	1.07961400	-1.33295700	-0.92701200
C	2.35209500	0.58597400	-1.45708300
C	3.21307700	1.35309700	-2.26211000
C	3.33073800	2.72514100	-2.08073400
C	2.56122900	3.34611500	-1.07915600
C	1.70960000	2.58092900	-0.26148200
C	1.60534000	1.19668000	-0.40493600
H	3.79128100	0.88916800	-3.05669100
H	3.99754200	3.29781000	-2.71421800
H	1.14916500	3.11021600	0.50370100
Ir	0.51213500	-0.04997600	0.74756400
O	2.57674600	4.67696600	-0.82499500
C	3.43178300	5.51623100	-1.59858000
H	3.16295500	5.49231700	-2.66204300
H	3.28369100	6.52661700	-1.21308500
H	4.48515100	5.23472400	-1.47951600
N	-1.10522300	0.62122600	-0.39544500
H	-0.98713300	0.60840500	-2.96291800
H	-1.02467100	1.55825700	-0.76694400
H	-1.93786400	-1.72964500	-0.95447000
C	-5.97116200	1.45281400	-0.59269000
C	-4.88759100	0.57477200	-0.40612700
C	-3.56225700	1.07121200	-0.54736600
C	-3.38830900	2.42331300	-0.86805100
C	-4.46860900	3.28566800	-1.06047300
C	-5.76589700	2.79024700	-0.91503700
H	-6.98249000	1.06791600	-0.47986100
H	-2.38600500	2.83647600	-0.94286800
H	-4.29692900	4.33050100	-1.30162600
H	-6.62201800	3.44560400	-1.05273600
C	-2.39598100	0.13971800	-0.26867400
H	-2.56752600	-0.38856000	0.67212700
O	-2.62323700	-1.09182200	-1.26589400
N	-1.76024100	0.08254400	-3.38663800
H	-2.17857000	-0.52564300	-2.54074200
H	-1.41236300	-0.49204000	-4.15818400
H	-2.46177200	0.73898900	-3.74014500
N	-5.11107100	-0.74805800	-0.03125600
H	-6.06984000	-1.05682200	-0.14507300
H	-4.44078500	-1.39637500	-0.43518600

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IN22' SCF Done: E(RM06) = -1771.01136503

C	-1.67545300	-1.51502500	-2.21160700
C	-0.72762400	-2.45188100	-1.68503900
C	0.61223600	-2.02673100	-2.10011100
C	-0.92719000	-0.41033300	-2.77958100
C	0.48568800	-0.79309800	-2.76444900
C	-1.06074600	-3.78363700	-1.07672100
H	-1.99785000	-3.74760900	-0.51435800
H	-1.17295000	-4.54440700	-1.86165900
H	-0.27532500	-4.13067500	-0.39914900
C	1.87022300	-2.82594400	-1.94436500
H	2.00882500	-3.48286600	-2.81526000
H	2.74743400	-2.17878400	-1.86841400
H	1.83976100	-3.46308500	-1.05707600
C	1.58984700	-0.02074100	-3.42171800
H	1.77416000	-0.42810500	-4.42619500
H	1.32522500	1.03266300	-3.55062700
H	2.52308200	-0.07751700	-2.85439600
C	-1.49430700	0.72478200	-3.58402000
H	-1.49191100	0.48032600	-4.65531700
H	-2.52771600	0.94419900	-3.30235300
H	-0.91331400	1.64330700	-3.45456000
C	-3.16193000	-1.70266600	-2.25600400
H	-3.53084400	-2.26639700	-1.39459100
H	-3.69899100	-0.75245900	-2.28797200
H	-3.42759100	-2.26450100	-3.16205600
C	3.25370400	-2.18860400	1.61183600
C	1.03143000	-1.67250300	1.93176600
C	1.07086600	-2.24515900	3.24313900
C	2.27621900	-2.82656100	3.69068600
C	3.38020700	-2.81043900	2.86765200
H	4.11904100	-2.13070300	0.95447800
C	-0.09973500	-2.19399800	4.04314500
H	2.31322100	-3.27168500	4.68139500
H	4.32693500	-3.24512200	3.16990700
C	-1.21553300	-1.57861500	3.55601900
C	-1.21705400	-1.03503200	2.23868600
H	-0.08721900	-2.63111700	5.03778400
H	-2.11105100	-1.50896200	4.16060800
N	2.13618500	-1.64162500	1.14767800
N	-0.13268900	-1.13369900	1.43394800
C	-2.34609800	-0.31396500	1.67983500
C	-3.50793700	0.00765300	2.40574100
C	-4.50373700	0.80015700	1.85170800

C	-4.32934200	1.30160600	0.54924200
C	-3.17266700	0.97791100	-0.18354700
C	-2.18552400	0.14757500	0.34282100
H	-3.64564100	-0.34680400	3.42277500
H	-5.38839100	1.03639200	2.43044000
H	-3.08793700	1.39177100	-1.18301300
Ir	-0.52246600	-0.49435000	-0.62457800
O	-5.22053000	2.09778300	-0.08593800
C	-6.42718000	2.45749500	0.58599100
H	-6.22215900	3.03179200	1.49752700
H	-6.98083700	3.08330800	-0.11623200
H	-7.02692800	1.57340900	0.83337100
N	0.28015900	1.32181900	0.01937700
H	6.81323600	-1.15105100	-0.03956500
H	-0.23426600	1.74205400	0.79398700
H	3.07071200	-0.43066400	-0.24672600
C	3.44591100	4.99898600	0.46953900
C	3.08134500	3.71660100	-0.00531000
C	1.73005100	3.29097400	0.18339600
C	0.82424900	4.14286600	0.85604600
C	1.20641000	5.38787600	1.32255000
C	2.53114000	5.81183500	1.11645900
H	4.46976900	5.33642100	0.32669700
H	-0.21112100	3.82985400	0.97024100
H	0.49041600	6.03480600	1.81919100
H	2.84703100	6.79008700	1.46945800
C	1.31040400	2.01003800	-0.35686700
H	1.91338900	1.57859800	-1.15014400
O	3.71416900	0.04137100	-0.81191400
N	6.20837700	-1.26256700	-0.85322800
H	4.56904500	-0.46775300	-0.76641800
H	6.23132300	-2.25283500	-1.09631200
H	6.67292400	-0.77546200	-1.62043200
N	4.00691800	2.93154100	-0.64288000
H	4.96225700	3.26364900	-0.62157300
H	3.91512400	1.91084700	-0.64391100

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TS16-1 SCF Done: E(RM06) = -1659.02031275

C	0.45732600	-0.18220500	-2.62010800
C	-0.97556400	-0.28675700	-2.62695100
C	-1.33464400	-1.62954500	-2.16575000
C	0.97900800	-1.36512200	-1.97185800
C	-0.15300900	-2.27150900	-1.75644400
C	-1.92223100	0.67918000	-3.27796100
H	-1.54321300	1.70397000	-3.23715300
H	-2.06507200	0.41842100	-4.33578500
H	-2.90751600	0.66442100	-2.80290900
C	-2.70932800	-2.22314400	-2.21938500
H	-2.89934500	-2.63763800	-3.21979200
H	-2.83059600	-3.03519200	-1.49796200
H	-3.48559600	-1.48012000	-2.02192300
C	-0.03704900	-3.66612000	-1.21880700
H	0.15419100	-4.37172300	-2.03912800
H	0.79547200	-3.75943700	-0.51566400
H	-0.95341700	-3.98928000	-0.71585400
C	2.42555200	-1.76344000	-1.91409400
H	2.71337100	-2.29919100	-2.83007800
H	3.08010100	-0.89155700	-1.82599500
H	2.63514200	-2.42099800	-1.06676900
C	1.25484900	0.89152700	-3.29533000
H	0.76722200	1.86788900	-3.23241500
H	2.25832000	0.98796900	-2.87657100
H	1.36319300	0.63940900	-4.35934000
C	-4.35161700	-1.53626900	1.16431000
C	-3.04550800	0.33320700	0.87157400
C	-4.07024700	1.17494900	1.40263700
C	-5.29086700	0.57490900	1.78220100
C	-5.44020600	-0.79035900	1.65966200
H	-4.43111500	-2.61891400	1.08589400
C	-3.79355400	2.56055200	1.54866100
H	-6.08870200	1.19779900	2.17802500
H	-6.35837600	-1.29177900	1.94661100
C	-2.55310200	3.03493900	1.22908700
C	-1.56017600	2.15583200	0.70486700
H	-4.56258000	3.22200200	1.93841200
H	-2.31335800	4.08185000	1.36988800
N	-3.19820600	-1.00852900	0.77602600
N	-1.84098500	0.85596100	0.46677000
C	-0.19191600	2.54585900	0.42808200
C	0.31507500	3.83837000	0.65444700
C	1.65437500	4.13337900	0.43828800
C	2.51033100	3.10756900	-0.00208500
C	2.00814000	1.81500300	-0.23073100
C	0.65961800	1.50321600	-0.04807900
H	-0.33369400	4.63425000	1.00881600
H	2.02186700	5.13694300	0.61499500
H	2.71360400	1.06776100	-0.57813600
Ir	-0.25866600	-0.23479700	-0.53551200
O	3.83600000	3.26754900	-0.23851300
C	4.41125600	4.56533400	-0.09623300
H	4.33468600	4.92912200	0.93562400
H	5.46454300	4.45256300	-0.36001600
H	3.94372900	5.28698700	-0.77698300
N	-0.13844600	-1.04670600	1.49336600
H	1.42934300	-0.66581500	3.88774700
H	-1.08091700	-1.43810800	1.55638300
H	0.05024200	-0.43278000	2.78378200
C	4.15814600	-3.43305800	1.65904300
C	2.78938200	-3.29699200	1.89608900
C	2.19143100	-2.02798300	1.88696000
C	2.98606200	-0.89236200	1.66580300
C	4.35520500	-1.03036300	1.44528900
C	4.94254600	-2.29968500	1.43626200
H	4.61073400	-4.42025600	1.66127400
H	2.53405800	0.09343400	1.65682200
H	4.96319100	-0.14614900	1.27611400
H	6.00967900	-2.40338500	1.26129700
C	0.73636800	-1.92847500	2.17699000
H	0.30279500	-2.88312000	2.47403600
O	0.57047600	-1.05376600	3.61447800
H	2.18306000	-4.17794200	2.09169500

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TS16-2 SCF Done: E(RM06) = -1892.64971376

C	0.41828500	-2.86866900	1.29602600

C	1.79988600	-2.61224500	0.99975800
C	2.00478000	-2.80018700	-0.43914100
C	-0.27474400	-3.02306500	0.03362500
C	0.74707800	-3.04606300	-1.01504700
C	2.89947300	-2.48053500	2.01340100
H	2.53991400	-2.02942700	2.94245900
H	3.30727800	-3.47034800	2.26153100
H	3.72864100	-1.87216100	1.64111300
C	3.33693000	-2.84345000	-1.12357100
H	3.77314100	-3.84907200	-1.03616200
H	3.25648700	-2.61230000	-2.18914100
H	4.04705100	-2.14019600	-0.68229200
C	0.47603400	-3.35302800	-2.45700200
H	0.50467300	-4.44000200	-2.61777500
H	-0.51563500	-3.01081200	-2.76277500
H	1.21989800	-2.90480300	-3.12229900
C	-1.68768800	-3.50740200	-0.12858000
H	-1.72784000	-4.60477300	-0.06880200
H	-2.34145100	-3.11509400	0.65561000
H	-2.11436100	-3.21384900	-1.09112000
C	-0.16490700	-3.07702500	2.66083200
H	0.34835900	-2.48072700	3.42015200
H	-1.22645700	-2.82246400	2.69730600
H	-0.06606300	-4.13470600	2.94177500
C	4.21804100	0.75895100	-1.98412400
C	2.93340500	1.07782000	-0.10525100
C	3.80503500	2.10934300	0.36001900
C	4.94833700	2.40889300	-0.41347700
C	5.16375300	1.72928600	-1.59344700
H	4.34737700	0.22724100	-2.92499400
C	3.45916300	2.79239000	1.55632600
H	5.63458600	3.17916900	-0.07172200
H	6.02586300	1.93336100	-2.21954800
C	2.29130700	2.48094600	2.19416900
C	1.45320800	1.44170600	1.69205600
H	4.11437500	3.57150300	1.93639100
H	1.99422800	3.01780600	3.08720600
N	3.14739900	0.43120900	-1.27432300
N	1.81596600	0.71841900	0.61084600
C	0.15457500	1.10061800	2.23981800
C	-0.45433700	1.79513100	3.30051200
C	-1.74383400	1.48766300	3.71384000
C	-2.44216600	0.46471700	3.04617000
C	-1.83248200	-0.24204100	1.99483700
C	-0.53064700	0.03795500	1.57594300
H	0.07255400	2.59397400	3.81453300
H	-2.19393800	2.03664200	4.53225400
H	-2.41639100	-1.02612900	1.52465000
Ir	0.54359300	-0.97459600	0.19490700
O	-3.70952900	0.08600100	3.34756400
C	-4.38778300	0.74303700	4.41626400
H	-4.51292900	1.81431600	4.21480100
H	-5.37064200	0.27206600	4.47833500
H	-3.86173000	0.60732300	5.36904100
N	-0.12497600	0.43759200	-1.36966300
H	-1.88451100	1.32173300	-3.87021000
H	0.81711400	0.61659100	-1.72736300
H	-0.47801300	2.13414100	-1.14595100
C	-4.15011500	-1.71696900	-3.23666500
C	-2.82316700	-1.28979200	-3.31703000
C	-2.27286600	-0.47058800	-2.31796900
C	-3.07823200	-0.07650200	-1.24111600
C	-4.40340300	-0.50552900	-1.15965600
C	-4.94260200	-1.32492700	-2.15566500
H	-4.56146900	-2.35465300	-4.01405100
H	-2.66040200	0.54847700	-0.46212700
H	-5.01459200	-0.20191800	-0.31402900
H	-5.97480700	-1.65723700	-2.08859300
C	-0.86330200	0.01988200	-2.49372600
H	-0.31933200	-0.60344000	-3.20829000
O	-1.00685000	1.35109700	-3.44464800
H	-2.20740200	-1.59422700	-4.16089300
C	-1.60237100	5.00701700	-2.43900600
H	-2.17923300	4.50984100	-3.22772800
H	-0.63998300	5.31989800	-2.85715000
H	-2.15361100	5.90343100	-2.13704700
C	-1.39799900	4.08745000	-1.23586700
C	-0.58133800	4.77326700	-0.14155900
H	0.38813100	5.10055000	-0.53075600
H	-1.11755400	5.65177200	0.23336900
H	-0.41024200	4.09771000	0.70367400
C	-2.72462700	3.55058900	-0.69831800
H	-3.27816100	3.00787200	-1.47218000
H	-2.56525300	2.88002100	0.15330300
H	-3.35181400	4.38141100	-0.35658800
O	-0.57157800	2.97067000	-1.74123700
H	-0.90161200	2.31081000	-2.70147500

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TS16-3 SCF Done: E(RM06) = -1735.47695655

C	0.28257400	-0.29486100	-2.73910600
C	-1.14928100	-0.41392000	-2.65430100
C	-1.46604100	-1.73986000	-2.11410000
C	0.85461400	-1.44665300	-2.07692500
C	-0.25272300	-2.35264100	-1.75747300
C	-2.13970800	0.51618000	-3.29288400
H	-1.77250400	1.54609200	-3.30690400
H	-2.32761400	0.21594200	-4.33305300
H	-3.10182100	0.50719000	-2.77259400
C	-2.83139000	-2.35388200	-2.06356700
H	-3.05357300	-2.85201300	-3.01828500
H	-2.91080000	-3.10552500	-1.27379100
H	-3.61188400	-1.60754200	-1.89769500
C	-0.09081100	-3.73499600	-1.19995200
H	-0.00409900	-4.45910600	-2.02227700
H	0.81658000	-3.82692800	-0.59754800
H	-0.94795000	-4.03689400	-0.59033900
C	2.30698000	-1.82606800	-2.08943100
H	2.55158000	-2.38688900	-3.00293100
H	2.95357800	-0.94432300	-2.06396200
H	2.57308300	-2.45140700	-1.23422500
C	1.02984900	0.76250200	-3.49394300
H	0.53772600	1.73682300	-3.43313600
H	2.05282200	0.88073900	-3.13114000
H	1.08424300	0.47941300	-4.55418700
C	-4.31908600	-1.41366200	1.31625700

C	-3.01957000	0.42503100	0.84939300
C	-4.03180500	1.30798300	1.33536200
C	-5.24676800	0.74165600	1.78016400
C	-5.39996500	-0.62896300	1.76613700
H	-4.39824100	-2.49909500	1.32781900
C	-3.74583500	2.69960200	1.37487900
H	-6.03785000	1.39490200	2.13901400
H	-6.31464500	-1.10437700	2.10400400
C	-2.50858700	3.14207300	1.00082100
C	-1.53084600	2.22259100	0.51690900
H	-4.50461000	3.39188100	1.72959700
H	-2.26012700	4.19456800	1.06347200
N	-3.17278100	-0.91941100	0.86771200
N	-1.82406900	0.91086600	0.37446100
C	-0.16512400	2.57616500	0.19186700
C	0.37546600	3.86128200	0.37844900
C	1.72384700	4.10873400	0.16376100
C	2.55119900	3.04526400	-0.24215200
C	2.01088400	1.76461900	-0.45332000
C	0.65680800	1.49728900	-0.25442000
H	-0.25158700	4.68421000	0.70968400
H	2.12179000	5.10425900	0.31924900
H	2.69517500	0.98770800	-0.77700100
Ir	-0.30262700	-0.24810300	-0.62843800
O	3.88492700	3.15841000	-0.45684800
C	4.51102900	4.42366600	-0.25209800
H	4.40469600	4.76005900	0.78649500
H	5.56883100	4.27038400	-0.47413600
H	4.10696100	5.18570000	-0.92941100
N	-0.02911900	-0.90692200	1.47546100
H	1.47245900	-2.33497900	3.93642200
H	-0.99526300	-1.21296800	1.61583500
H	0.18390700	0.11561900	2.52528400
C	4.32532400	-3.17797800	1.30845400
C	2.93945500	-3.15580700	1.47440100
C	2.25911900	-1.93828100	1.63865300
C	2.99103400	-0.74130500	1.65977500
C	4.37508300	-0.76615400	1.49351200
C	5.04412800	-1.98097700	1.31516600
H	4.83954200	-4.12537400	1.17465600
H	2.48132900	0.20423500	1.80176300
H	4.93168100	0.16663400	1.50168100
H	6.12267300	-1.99372700	1.18538200
C	0.78354600	-1.97668100	1.87633700
H	0.36637100	-2.97130500	1.71616300
O	0.64247400	-1.97190900	3.57023500
H	2.37970700	-4.08869200	1.47593900
O	0.44331000	0.41892400	3.55520900
H	0.58559700	-0.83681800	3.79720400
H	-0.35980500	0.76871900	3.98068000

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2a-2 SCF Done: E(RM06) = -325.531677644

N	-2.97963400	0.29680500	-0.00022900
H	-2.67117200	1.27665600	-0.00086400
C	1.74666200	-1.06015300	-0.00009700
C	0.37005800	-1.28365600	-0.00008200
C	-0.53244400	-0.20833100	0.00010500
C	-0.02364600	1.10139700	0.00012000
C	1.35010900	1.32635100	0.00005000
C	2.23938600	0.24615100	-0.00005100
H	2.43287400	-1.90268100	-0.00015300
H	-0.70372800	1.94980800	0.00031300
H	1.73071700	2.34413000	0.00012300
H	3.31132000	0.42455200	-0.00011900
C	-1.98411900	-0.50429100	0.00020500
H	-2.22314600	-1.57415200	0.00091600
H	-0.01546500	-2.30075200	-0.00011900

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2a-3 SCF Done: E(RM06) = -380.876588693

N	2.83351200	-0.49766900	-0.26729100
H	2.66285000	0.43670500	-0.65318500
C	-2.02255900	-1.09673700	-0.02545200
C	-0.68724000	-1.46948000	0.08067700
C	0.35362300	-0.52404800	0.08581700
C	0.02111000	0.85710600	0.04464800
C	-1.33158500	1.22405500	-0.06275100
C	-2.33701300	0.26341200	-0.10939200
H	-2.80546300	-1.84891400	-0.04212100
H	-1.58579700	2.28137300	-0.10070500
H	-3.37321400	0.58091600	-0.19274400
C	1.73601100	-1.04337400	0.10923000
H	1.81303300	-2.07266500	0.48110900
H	-0.42240900	-2.52293100	0.14138300
N	1.00777000	1.84769500	0.07822900
H	0.63971600	2.77697700	0.25483400
H	1.78822000	1.65276000	0.69820200

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