Supporting Information for

Rhodium(III)-Catalyzed Mild and Regioselective Dearomative Spirocyclization of 2-Aryl-3-nitrosoindoles with Alkynes

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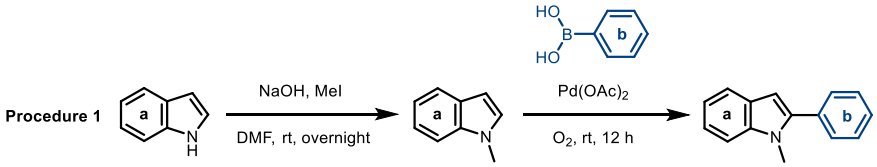
List of Contents

1. General Remarks

All reactions were carried out under air atmosphere. The column chromatography was performed using silica gel (200-300 mesh). ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on Bruker-AV (400, 100, and 376 MHz, respectively) instrument using $CDCl_3$/DMSO-d_6 as solvent and TMS as the internal standard. Mass spectra were measured on Agilent-8860-5977B GC-MS instrument (EI). High-resolution mass spectra (ESI) were obtained with the Thermo Scientific LTQ Orbitrap XL mass spectrometer. All reagents were obtained from commercial suppliers or prepared by our laboratory.

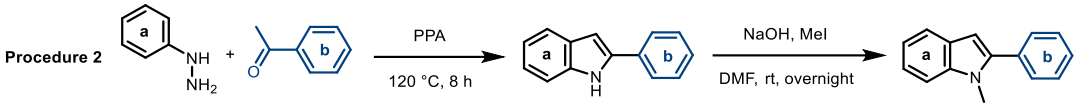
2. Raw Materials Preparation

2.1 Preparation of 2-Aryl-1-methyl-1-*H*-indoles



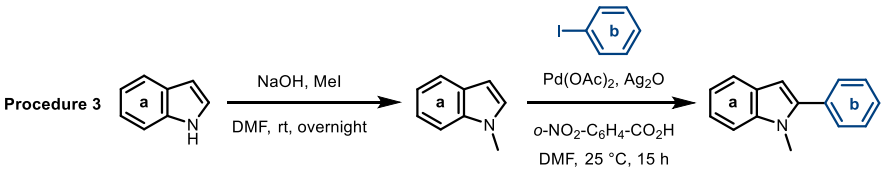
Synthesis of 2-aryl-1-methyl-1-*H*-indoles **01a**–**01c**, **01e**–**01g**, **01l**, **01n**, **01o**, and **01q**.[1]

Procedure 1: Indole (3.0 mmol, 1.0 equiv.), phenyl boronic acid (2 equiv.) and $Pd(OAc)_2$ (0.1 equiv.) were added to a Schlenk flask. AcOH (30 mL) was added by syringe and resulting solution was degassed twice and refilled with O_2 (1 atm). The reaction mixture was stirred for 12 h at room temperature. AcOH was recovered by distillation under reduced pressure, and the residue was dissolved in CH_2Cl_2 (80 mL), washed with aqueous $NaHCO_3$ (50mL×2). The organic layer was dried over Na_2SO_4. After removal of the solvent, the crude product was purified by flash chromatography on silica gel eluting with ethyl acetate and petroleum ether (1:20) to afford the corresponding 2-aryl indole.



Synthesis of 2-aryl-1-methyl-1-*H*-indoles **01d**, **01h**–**01j**.[2]

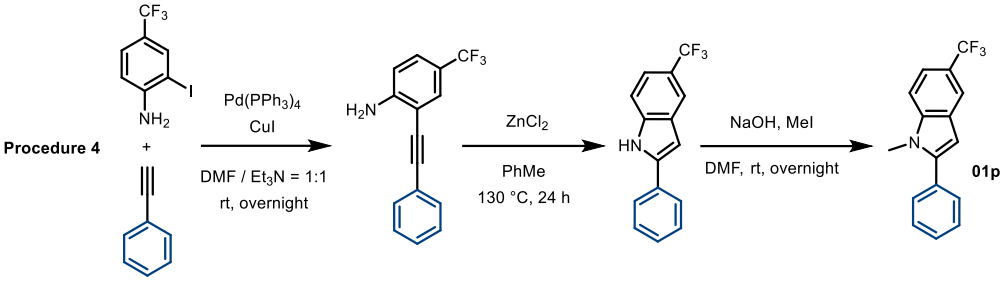
Procedure 2: Ketone (5 mmol) and substituted phenylhydrazine (9 mmol) were added to a flask with polyphosphoric acid (18 g), and the mixture was heated at 120 °C for 8 h. The resulting solution was poured into ice water (100 mL), neutralized by NaOH, and extracted with EtOAc (3 × 50 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated. The residue was purified by flash chromatography to get the desired product.



Synthesis of 2-aryl-1-methyl-1*H*-indoles **01k** and **01m**.[3]

Procedure 3: $Pd(OAc)_2$ (33.6 mg, 5 mol %), Ag_2O (522 mg, 2.25 mmol), 2-nitrobenzoic acid (753 mg, 4.5 mmol), indole (3.0 mmol) and aryl iodide (6.0 mmol) in dry DMF (6 mL) were stirred at room temperature for 15 h. The reaction mixture was filtered through a plug of silica gel and then evaporated to dryness under reduced pressure. The crude product was purified by column chromatography (ethyl acetate / petroleum ether = 1:30) to afford the corresponding 2-aryl indole.

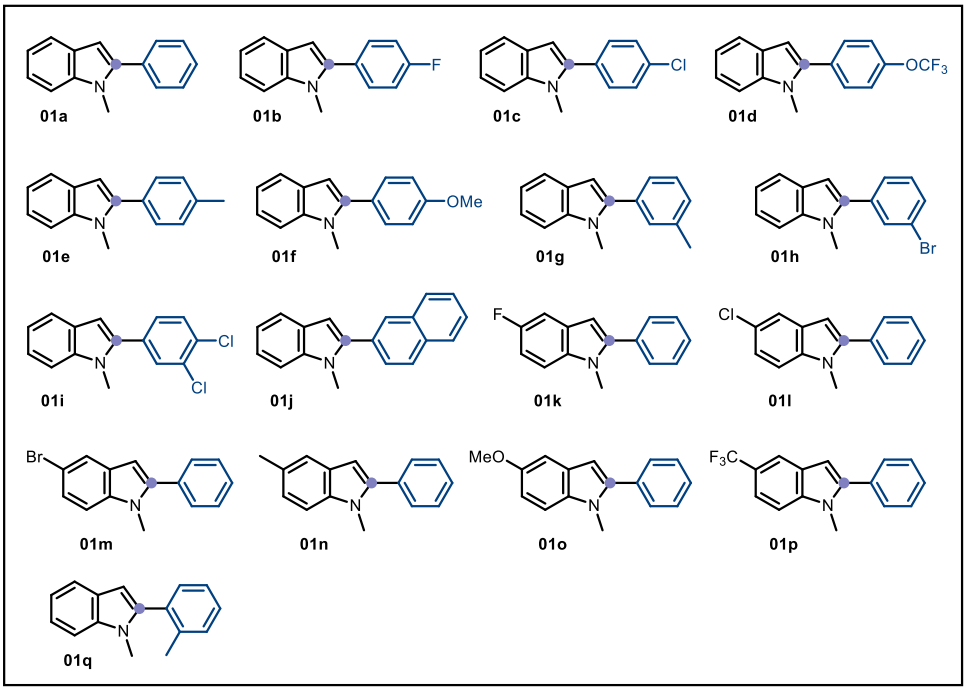
Synthesis of 1-methyl-2-phenyl-5-trifluoromethyl-1*H*-indole **01p**.



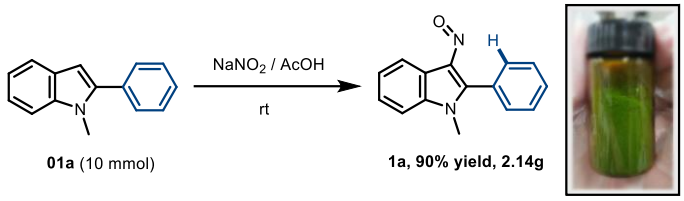
Procedure 4: $Pd(PPh_3)_4$ (115.6 mg, 2 mol%), CuI (19.0 mg, 2 mol%), 2-iodo-4-(trifluoromethyl)aniline (1434.5 mg, 5 mmol), ethynylbenzene (612.8 mg, 6 mmol) under argon, in DMF/Et_3N (10 mL, 1:1) were stirred at room temperature for overnight. The reaction mixture was filtered through a plug of silica gel and then evaporated to dryness under reduced pressure. The crude product was stirred with $ZnCl_2$ (681.5 mg, 5 mmol) in PhMe (10 mL) at 130 °C for 24 h. The reaction mixture was filtered through a plug of silica gel and then evaporated to dryness under reduced pressure. The crude product was purified by column chromatography to afford 2-(Phenylethynyl)-4-(trifluoromethyl)aniline. Then the methylation generated 1-methyl-2-phenyl-5-trifluoromethyl-1*H*-indole **01p**.with an overall yield of 30%.

01p. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (s, 1H), 7.52 – 7.38 (m, 8H), 6.63 (s, 1H), 3.75 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -60.13.

Table S1. Summary of 2-Arylindoles **01a**–**01q**

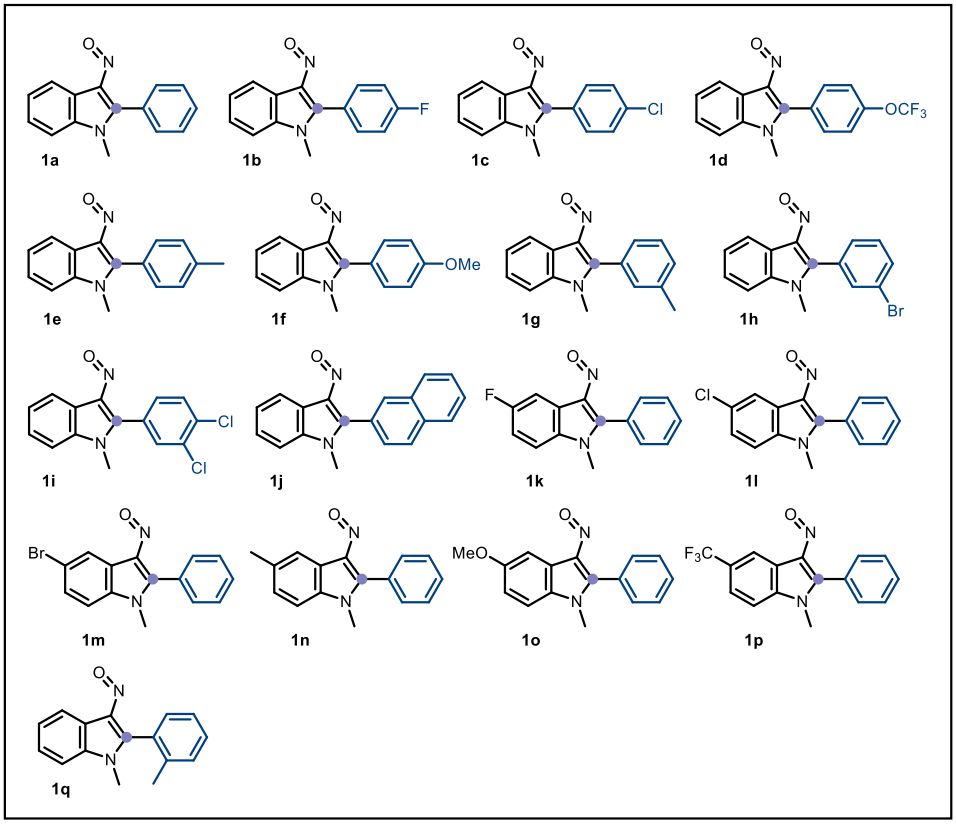


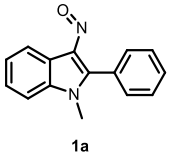
2.2 Preparation of 2-Aryl-1-methyl-3-nitroso-1-*H*-indoles



typical procedure: A solution of 1-methyl-2-phenylindole (**01a**, 2.07 g, 10 mmol) in 45 mL of mixed solvent (AcOH / MeCN = 15:30) and a solution of $NaNO_2$ (0.83 g, 12 mol) in water (5 mL) was added dropwise. The resulting reaction was stirred for 30 min at room temperature then diluted with water (50 mL). The mixture was filtered and the solid was washed with water. After dried under vacuum, 1-methyl-3-nitroso-2-phenyl-1*H*-indole (**1a**, 2.14 g, 90% yield) was provided.

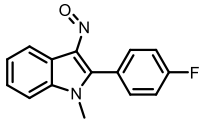
Table S2. Summary of 2-Aryl-3-nitrosoindoles **1a**–**1q**





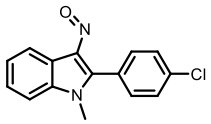
1a

1-Methyl-3-nitroso-2-phenyl-1*H*-indole (1a). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 – 8.28 (m, 1H), 7.88 – 7.83 (m, 2H), 7.64 – 7.58 (m, 3H), 7.46 – 7.38 (m, 3H), 3.89 (s, 3H). The NMR data agreed with those in a literature report.[4]



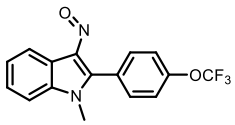
1b

2-(4-Fluorophenyl)-1-methyl-3-nitroso-1*H*-indole (1b). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 – 8.26 (m, 1H), 7.90 – 7.84 (m, 2H), 7.47 – 7.39 (m, 3H), 7.32 (t, *J* = 8.5 Hz, 2H), 3.90 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -108.87. The NMR data agreed with those in a literature report.[4]



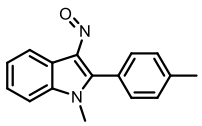
1c

2-(4-Chlorophenyl)-1-methyl-3-nitroso-1*H*-indole (1c). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.29 – 8.25 (m, 1H), 7.82 – 7.77 (m, 2H), 7.60 – 7.57 (m, 2H), 7.44 – 7.39 (m, 3H), 3.88 (s, 3H). The NMR data agreed with those in a literature report.[4]



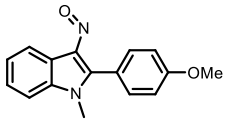
1d

1-Methyl-3-nitroso-2-(4-trifluoromethoxyphenyl)-1*H*-indole (1d). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 – 8.24 (m, 1H), 7.93 – 7.87 (m, 2H), 7.47 – 7.39 (m, 5H), 3.89 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.59.



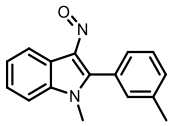
1e

1-Methyl-2-(4-methylphenyl)-3-nitroso-1*H*-indole (**1e**). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.34 – 8.28 (m, 1H), 7.75 (d, *J* = 7.8 Hz, 2H), 7.45-7.37 (m, 5H), 3.88 (s, 3H), 2.48 (s, 3H). The NMR data agreed with those in a literature report.[4]



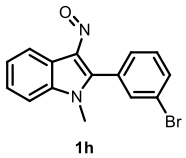
1f

1-Methyl-2-(4-methoxyphenyl)-3-nitroso-1*H*-indole (1f). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 – 8.27 (m, 1H), 7.82 – 7.77 (m, 2H), 7.41 – 7.34 (m, 3H), 7.13 – 7.07 (m, 2H), 3.90 (s, 3H), 3.87 (s, 3H). The NMR data agreed with those in a literature report.[4]



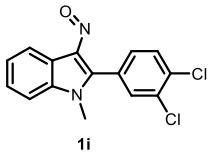
1g

1-Methyl-2-(3-methylphenyl)-3-nitroso-1*H*-indole (1g). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.33 – 8.29 (m, 1H), 7.68 (s, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.45 – 7.37 (m, 4H), 3.87 (s, 3H), 2.48 (s, 3H). The NMR data agreed with those in a literature report.[4]



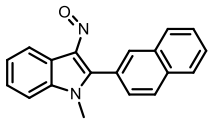
1h

2-(3-Bromophenyl)-1-methyl-3-nitroso-1*H*-indole (1h). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 – 8.24 (m, 1H), 8.03 – 7.97 (m, 1H), 7.82 – 7.73 (m, 2H), 7.51 – 7.40 (m, 4H), 3.88 (s, 3H). The NMR data agreed with those in a literature report.[4]



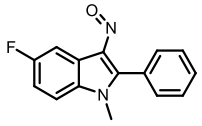
1i

2-(3,4-Dichlorophenyl)-1-methyl-3-nitroso-1*H*-indole (1i). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 – 8.21 (m, 1H), 7.95 (s, 1H), 7.71 – 7.67 (m, 2H), 7.46 – 7.39 (m, 3H), 3.89 (s, 3H).



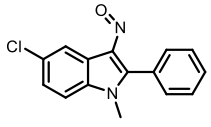
1j

1-Methyl-2-(naphthalen-2-yl)-3-nitroso-1*H*-indole (1j). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 1H), 8.35 – 8.31 (m, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.98 – 7.93 (m, 2H), 7.90 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.65 – 7.57 (m, 2H), 7.48-7.41 (m, 3H), 3.93 (s, 3H). The NMR data agreed with those in a literature report.[4]



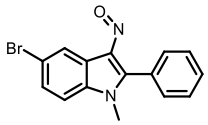
1k

5-Fluoro-1-methyl-3-nitroso-2-phenyl-1*H*-indole (1k). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 (dt, *J* = 8.9, 2.0 Hz, 1H), 7.85 – 7.79 (m, 2H), 7.64 – 7.55 (m, 3H), 7.30 (dd, *J* = 8.8, 4.1 Hz, 1H), 7.10 (td, *J* = 8.9, 2.5 Hz, 1H), 3.85 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -115.99. The NMR data agreed with those in a literature report.[4]



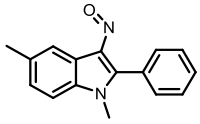
1l

5-Chloro-1-methyl-3-nitroso-2-phenyl-1*H*-indole (1l). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (d, *J* = 2.1 Hz, 1H), 7.85 – 7.79 (m, 2H), 7.63 – 7.56 (m, 3H), 7.34 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.28 (d, *J* = 8.6 Hz, 1H), 3.85 (s, 3H). The NMR data agreed with those in a literature report.[4]



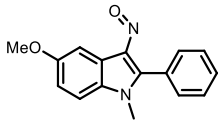
1m

5-Bromo-1-methyl-3-nitroso-2-phenyl-1*H*-indole (1m). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.48 – 8.45 (m, 1H), 7.88 – 7.84 (m, 2H), 7.65 – 7.60 (m, 3H), 7.52 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.29 (s, 1H), 3.89 (s, 3H). The NMR data agreed with those in a literature report.[5]



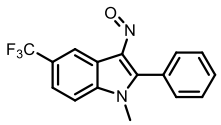
1n

1,5-Dimethyl-3-nitroso-2-phenyl-1*H*-indole (1n). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (s, 1H), 7.87 – 7.82 (m, 2H), 7.62 – 7.57 (m, 3H), 7.30 – 7.22 (m, 3H), 3.87 (s, 3H), 2.47 (s, 3H). The NMR data agreed with those in a literature report.[4]



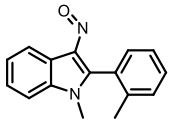
1o

1-Methyl-5-methoxy-3-nitroso-2-phenyl-1*H*-indole (1o). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 2.5 Hz, 1H), 7.85 – 7.80 (m, 2H), 7.59 (dd, *J* = 5.2, 1.9 Hz, 3H), 7.30 – 7.27 (m, 1H), 7.01 (dd, *J* = 8.9, 2.6 Hz, 1H), 3.88 (s, 3H), 3.86 (s, 3H).



1p

1-Methyl-3-nitroso-2-phenyl-5-(trifluoromethyl)-1*H*-indole (1p). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.55 (s, 1H), 7.88 – 7.83 (m, 2H), 7.67 – 7.60 (m, 4H), 7.51 – 7.46 (m, 1H), 3.92 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -61.16. The NMR data agreed with those in a literature report.[4]

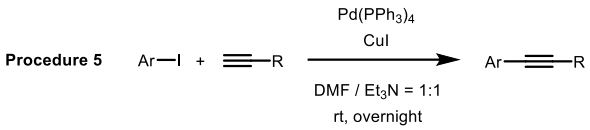


1q

1-Methyl-3-nitroso-2-(*o*-tolyl)-1*H*-indole (1q). Green solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 – 8.25 (m, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.54 – 7.49 (m, 1H), 7.48 – 7.38 (m, 5H), 3.69 (s, 3H), 2.30 (s, 3H). The NMR data agreed with those in a literature report.[4]

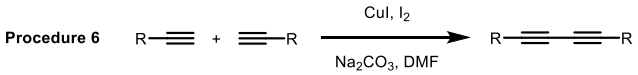
2.3 Preparation of Alkynes

Preparation of alkynes **2d**–**2h.**



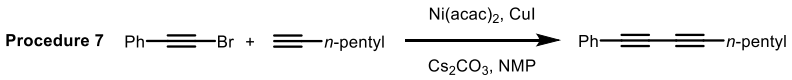
Procedure 5: $Pd(PPh_3)_4$ (2 mol%), CuI (2 mol%), aryl iodide (5 mmol), terminal alkyne (6 mmol) under argon, in DMF / Et_3N (10 mL, 1:1) were stirred at room temperature for overnight. The reaction mixture was filtered through a plug of silica gel and then evaporated to dryness under reduced pressure. The crude product was purified by column chromatography to afford the corresponding internal alkyne.

Preparation of 1,3-diynes **2i**–**2m**.[6a]



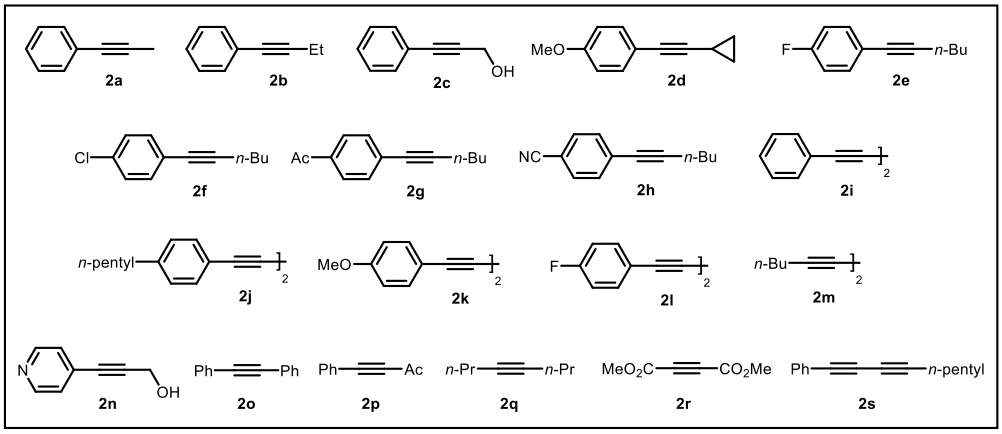
Procedure 6: To a stirred solution of alkyne (1 mmol) in DMF (1 mL), CuI (1 mmol), Na_2CO_3 (2 mmol), and iodine (1 mmol) were added successively. The resulting mixture was then allowed to react at 80 °C in air. Progress of this reaction was monitored by TLC. After completion of the reaction, 5 mL of ethyl acetate was added. The mixture was filtered through a pad of diatomite under reduced pressure, and the filtration residue was washed with ethyl acetate. The filtrate was then washed with saturated $Na_2S_2O_3$, saturated brine, and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure. The residue was then was purified by TLC using petroleum ether as eluent to afford the corresponding 1,3-diynes.

Preparation of 1,3-diynes **2s**.[6b]



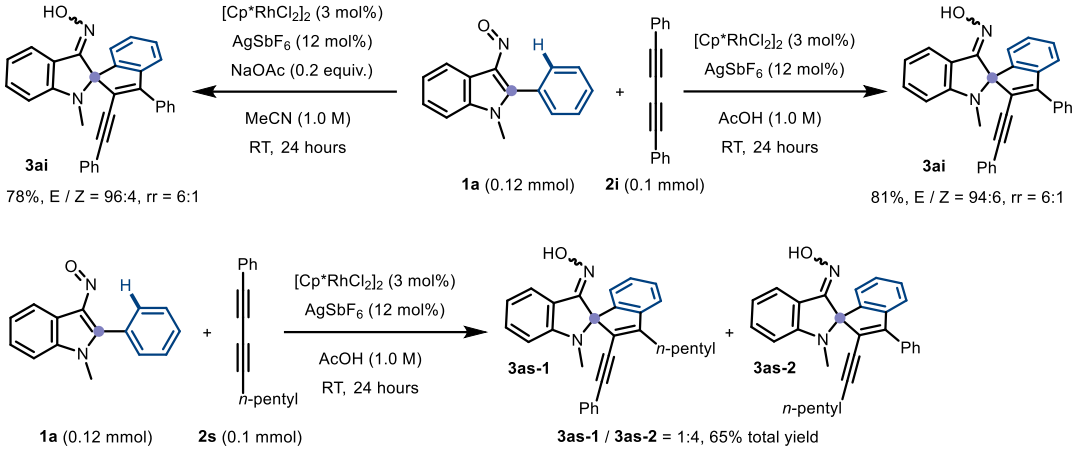
Procedure 7: In a 10 mL round bottom flask a mixture of 1-(2-bromoethynyl)benzene (181 mg, 1 mmol), hept-1-yne (115 mg, 1.2 mmol), Cs_2CO_3 (650 mg, 2 mmol), $Ni(acac)_2$ (13 mg, 0.05 mmol), CuI (10 mg, 0.05 mmol) and NMP (3 mL) was heated at 100 °C under argon for 9 h (TLC). The reaction mixture was then allowed to cool and was extracted with diethyl ether (3 × 20 mL). The extract was washed with water (10 mL) and brine (10 mL). Then the organic phase was dried over Na_2SO_4 and evaporated to leave the crude product, which was purified by column chromatography over silica gel to provide the 1,3-diyne.

Table S3. Summary of Alkynes **2a**–**2s**

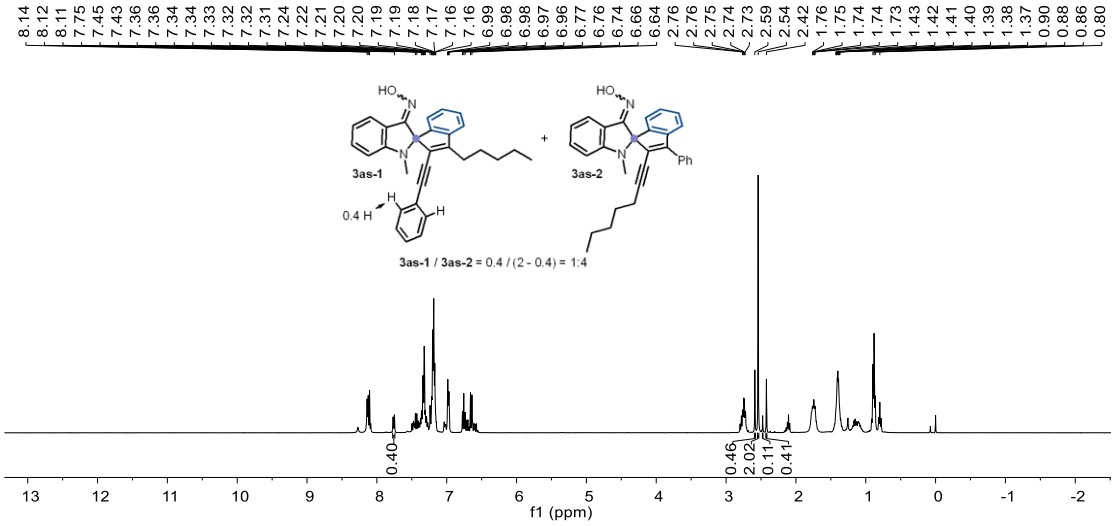


3. Supplementary Experiments

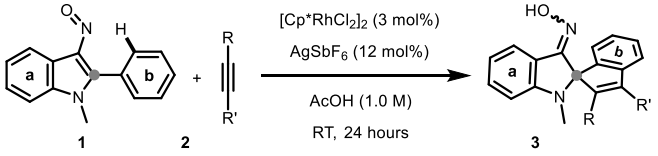
Scheme S1. Spirocyclization of 1,3-Diynes[a]

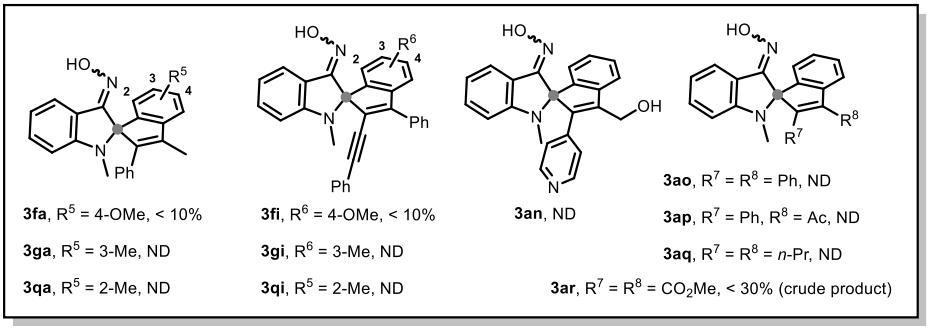


[a]Isolated yields were given. Ratios of E / Z isomers were determined by ^{1}H NMR. RT = room temperature. rr = regioisomer ratio.



Scheme S2. Supplementary Failed Substrates





3fa, R^5 = 4-OMe, < 10%

3ga, R^5 = 3-Me, ND

3qa, R^5 = 2-Me, ND

3fi, R^6 = 4-OMe, < 10%

3gi, R^6 = 3-Me, ND

3qi, R^5 = 2-Me, ND

3an, ND

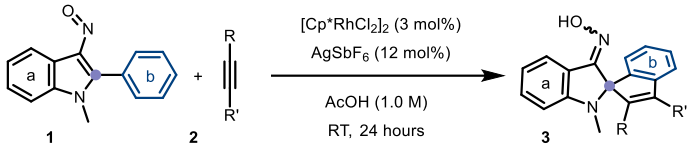
3ao, R^7 = R^8 = Ph, ND

3ap, R^7 = Ph, R^8 = Ac, ND

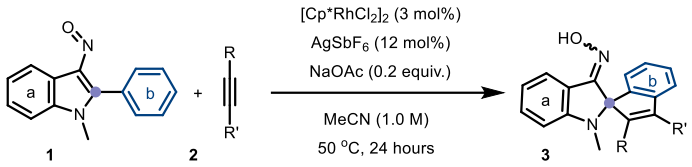
3aq, R^7 = R^8 = *n*-Pr, ND

3ar, R^7 = R^8 = CO_2Me, < 30% (crude product)

4. General Procedure



Conditions A: A 10 mL oven-dried reaction vessel was charged with 2-aryl-1-methyl-3-nitroso-1-*H*-indole **1** (0.12 mmol), alkyne **2** (0.1 mmol), $[Cp^*RhCl_2]_2$ (3 mol%, 1.9 mg), $AgSbF_6$ (12 mol%, 4.3 mg), AcOH (1.0 M). The sealed vessel was stirred at room temperature for 24 hours, under air. The reaction mixture was filtered through a plug of silica gel and then evaporated to dryness under reduced pressure. The crude product was purified by column chromatography to afford spirocyclicindolin-3-one oxime **3**.



Conditions B: A 10 mL oven-dried reaction vessel was charged with 2-aryl-1-methyl-3-nitroso-1-*H*-indole **1** (0.12 mmol), alkyne **2** (0.1 mmol), $[Cp^*RhCl_2]_2$ (3 mol%, 1.9 mg), $AgSbF_6$ (12 mol%, 4.3 mg), NaOAc (20 mol%, 1.6 mg), MeCN (1.0 M). The sealed vessel was stirred at 50 °C for 24 hours, under air. The reaction mixture was filtered through a plug of silica gel and then evaporated to dryness under reduced pressure. The crude product was purified by column chromatography to afford spirocyclicindolin-3-one oxime **3**.

5. DFT Calculations

All DFT calculations were carried out using Gaussian 09.[7] All structures were optimized using the B3LYP hybrid functional[8] combination with dispersion corrections with Becke-Johnson damping scheme D3(BJ)[9] at the basis set level of 6-31G(d)-Lanl2DZ (Rh).[10] Frequencies were analytically computed at the same level of theory to obtain the thermal correction to Gibbs free energies (at 298.15 K, 1.0 M) and in order to identify all structures as either intermediates (no imaginary frequency) or transition states (only one imaginary frequency). Solvation effects were incorporated using the SMD model[11] in geometry optimization, frequency analysis, as well as single-point calculations. The single-point calculations were performed at the M06/6-311+G(d,p)-SDD(Rh) level.[12,13] Graphical structures are visualized with CYLview.[14] Atomic charges (q) were obtained by natural population analysis.[15] Energy values are given in kcal/mol. Acetonitrile was used as the solvent in theoretical calculations. Bond lengths are in angstroms.

5.1 Supplementary Theoretical Study

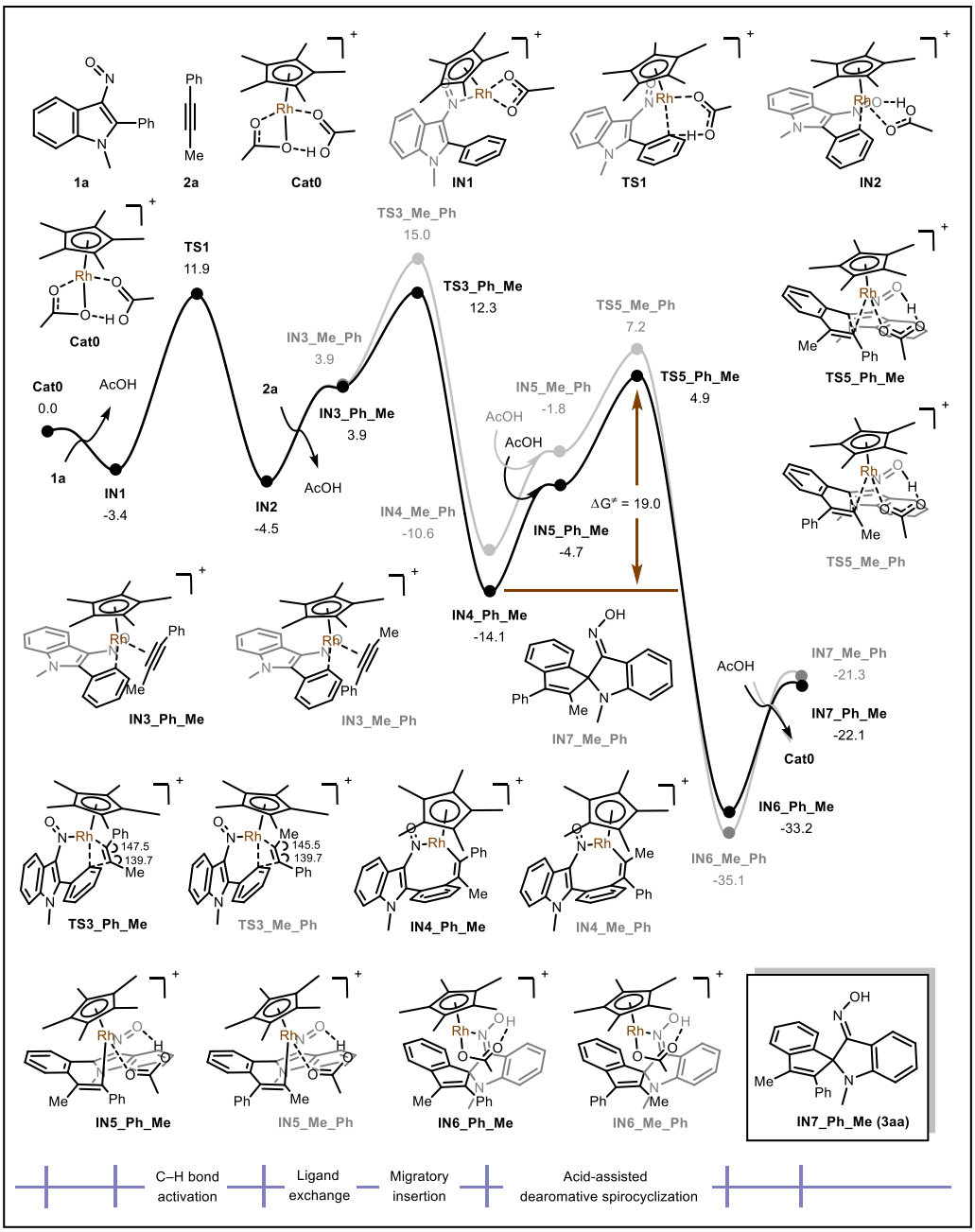


Figure S1. Free energy profiles for the reaction of indole **1a** with alkyne **2a** in acetonitrile at 298.15 K. Energy values are given in kcal/mol

The reaction employing phenyl methyl alkyne **2a** at 298.15 K was discussed (Figure S1). The complexation of **1a** with the in-situ generated rhodium acetate complex **Cat0** produces **IN1** with a free energy decrease of 3.4 kcal/mol. The subsequent C−H activation takes place *via* transition state **TS1** with an activation free energy of 15.3 kcal/mol, affording a six-membered rhodacycle **IN2**. Subsequent transformation can occur through two different channels. When the phenyl of alkyne is adjacent to Rh atom, the alkyne insertion has a lower overall activation free energy barrier ($\Delta G^{\ddagger}_{TS3\_Ph\_Me}$ = 16.7 kcal/mol *vs* $\Delta G^{\ddagger}_{TS3\_Me\_Ph}$ = 19.5 kcal/mol) and forms a more stable eight-membered rhodacycle ($\Delta\Delta G_{IN4\_Ph\_Me}$ = 0.0 kcal/mol *vs* $\Delta\Delta G_{IN4\_Me\_Ph}$ = 3.5 kcal/mol). Then the rate-determining acid-assisted

dearomative spirocyclization of **IN4_Ph_Me** has an overall activation free energy barrier as low as 19.0 kcal/mol, ensuring the reaction to be carried out smoothly at room temperature. Finally, desired product **IN7_Ph_Me** (**3aa**) is produced with the regeneration of catalyst **cat0**. Distortion–interaction analysis showed that the distortion energies of two transition states are really close ($\Delta E_{dist\_TS3\_Ph\_Me}$ = 36.2 kcal/mol *vs* $\Delta E_{dist\_TS3\_Me\_Ph}$ = 36.7 kcal/mol), and the energy difference is mainly contributed by interaction energy. Natural population analysis (NPA) shows that electron-donating methyl results in the stronger nucleophilicity of phenyl-linked carbon, which can better bond with the cationic Rh center *via* transition state **TS3_Ph_Me**.

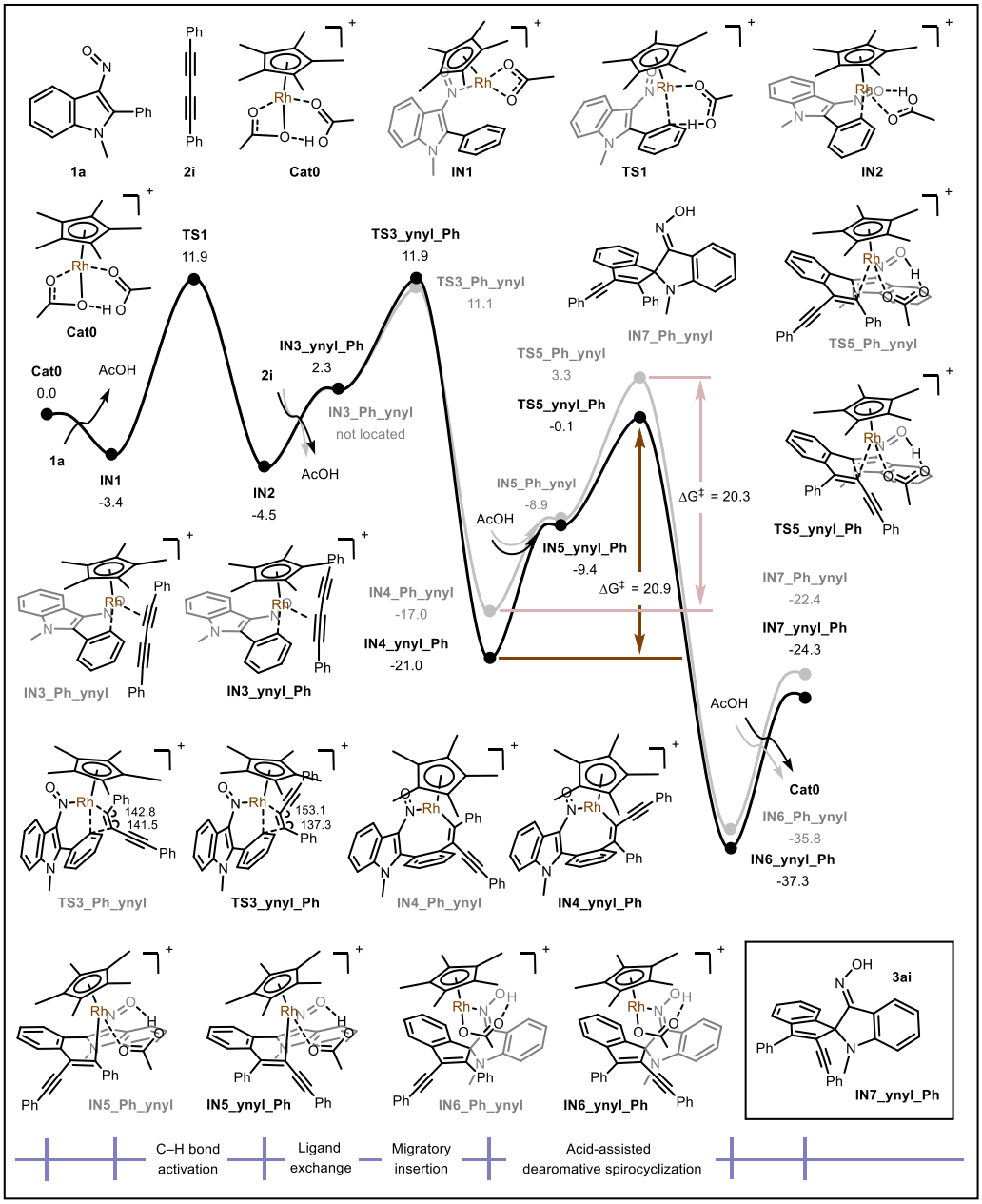


Figure S2. Free energy profiles for the reaction of indole **1a** with alkyne **2i** in acetonitrile at 298.15 K. Energy values are given in kcal/mol

The reaction using 1,3-diyne **2i** at 298.15 K was discussed (Figure S2). Rhodacycle **IN2** is generated *via* the same

C−H activation process as shown in figure S1. The following sequential ligand exchange and alkyne insertion convert intermediate **IN2** into corresponding eight-membered rhodacycle. Most notably, the reaction channel *via* transition state **TS3_Ph_ynyl** is slightly more favored in kinetics than that one *via* transition state **TS3_ynyl_Ph** ($\Delta G^{\ddagger}_{TS3\_Ph\_ynyl}$ = 15.5 kcal/mol *vs* $\Delta G^{\ddagger}_{TS3\_ynyl\_Ph}$ = 16.4 kcal/mol), but the relative free energies of two intermediates show a contrary trend in thermodynamics ($\Delta\Delta G_{IN4\_Ph\_ynyl}$ = 4.0 kcal/mol *vs* $\Delta\Delta G_{IN4\_ynyl\_Ph}$ = 0.0 kcal/mol). The sharp free energy drop make the reaction to be controlled majorly by thermodynamics ($\Delta G_{r\_IN4\_Ph\_ynyl}$ = -12.5 kcal/mol *vs* $\Delta G_{r\_IN4\_ynyl\_Ph}$ = -16.5 kcal/mol), that is mainly reflected in the intramolecular bond interaction (C(sp^2)−Rh = 2.78 Å vs C(sp)−Rh = 2.37 Å). Both two acid-assisted dearomative spirocyclization have relatively low activation free energy barriers ($\Delta G^{\ddagger}_{TS5\_Ph\_ynyl}$ = 20.3 kcal/mol *vs* $\Delta G^{\ddagger}_{TS5\_ynyl\_Ph}$ = 20.9 kcal/mol), that are rate-determining steps in corresponding pathways. Thus, the reaction can proceed smoothly at room temperature.

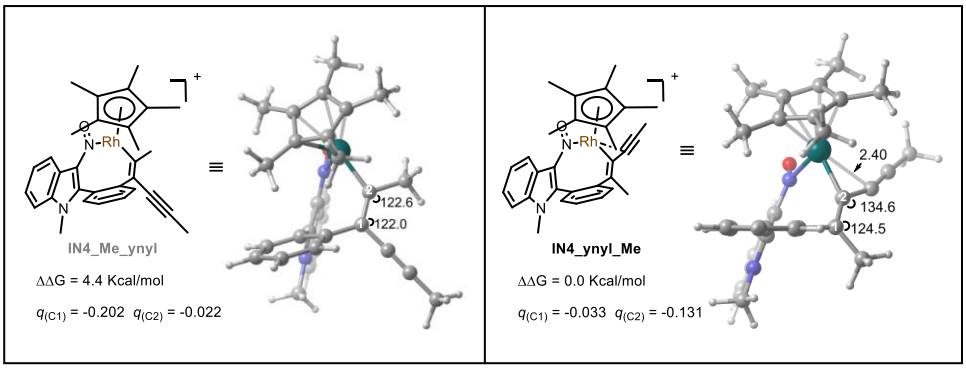


Figure S3. Eight-membered rhodacycle derived from aliphatic 1,3-diyne at 298.15 K (free energy in kcal/mol)

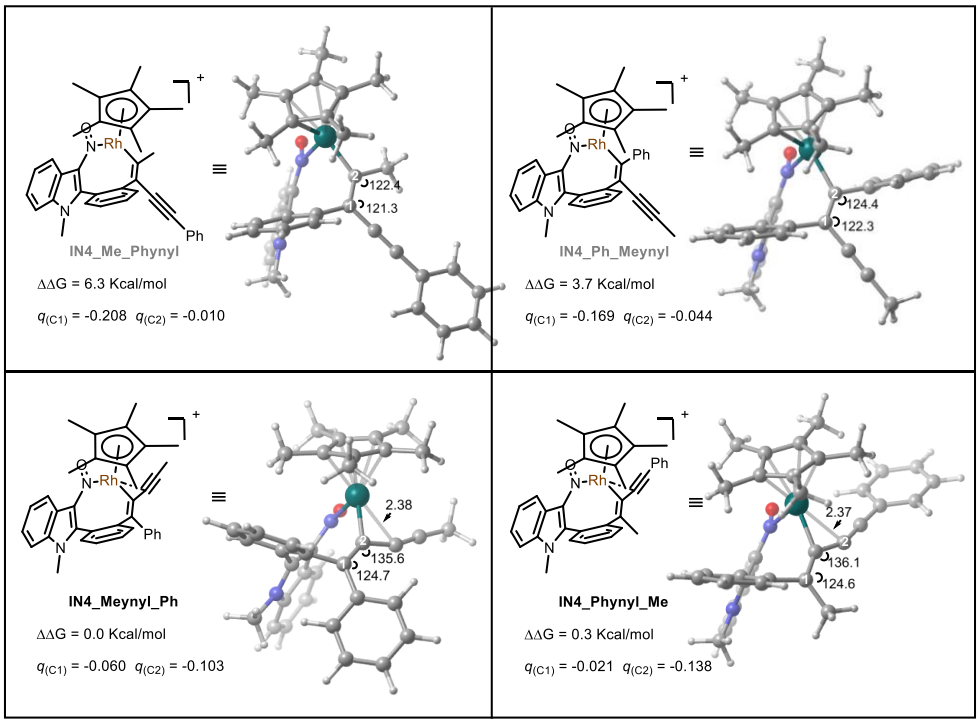
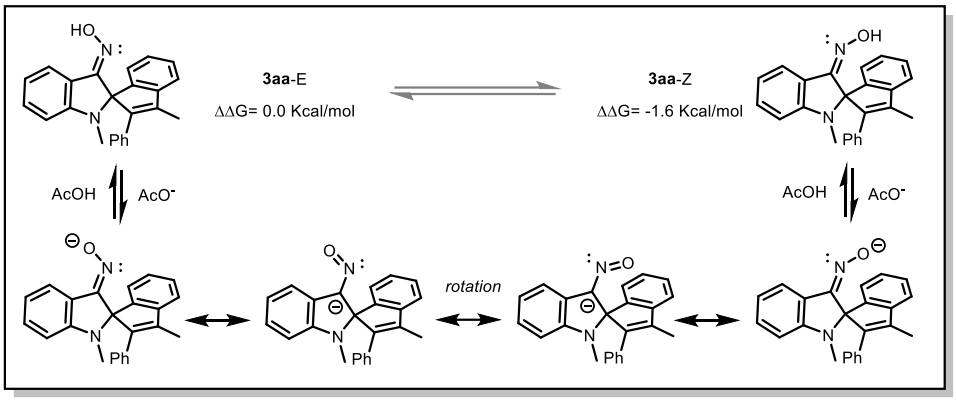


Figure S4. Eight-membered rhodacycle derived from unsymmetric 1,3-diyne at 298.15 K (free energy in kcal/mol)

Scheme S3. Possible conversion between E- and Z- product at 298.15 K (free energy in kcal/mol)



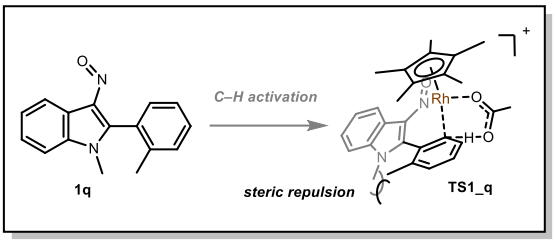


Figure S5. The origin of nonreactivity of indole **1q**.

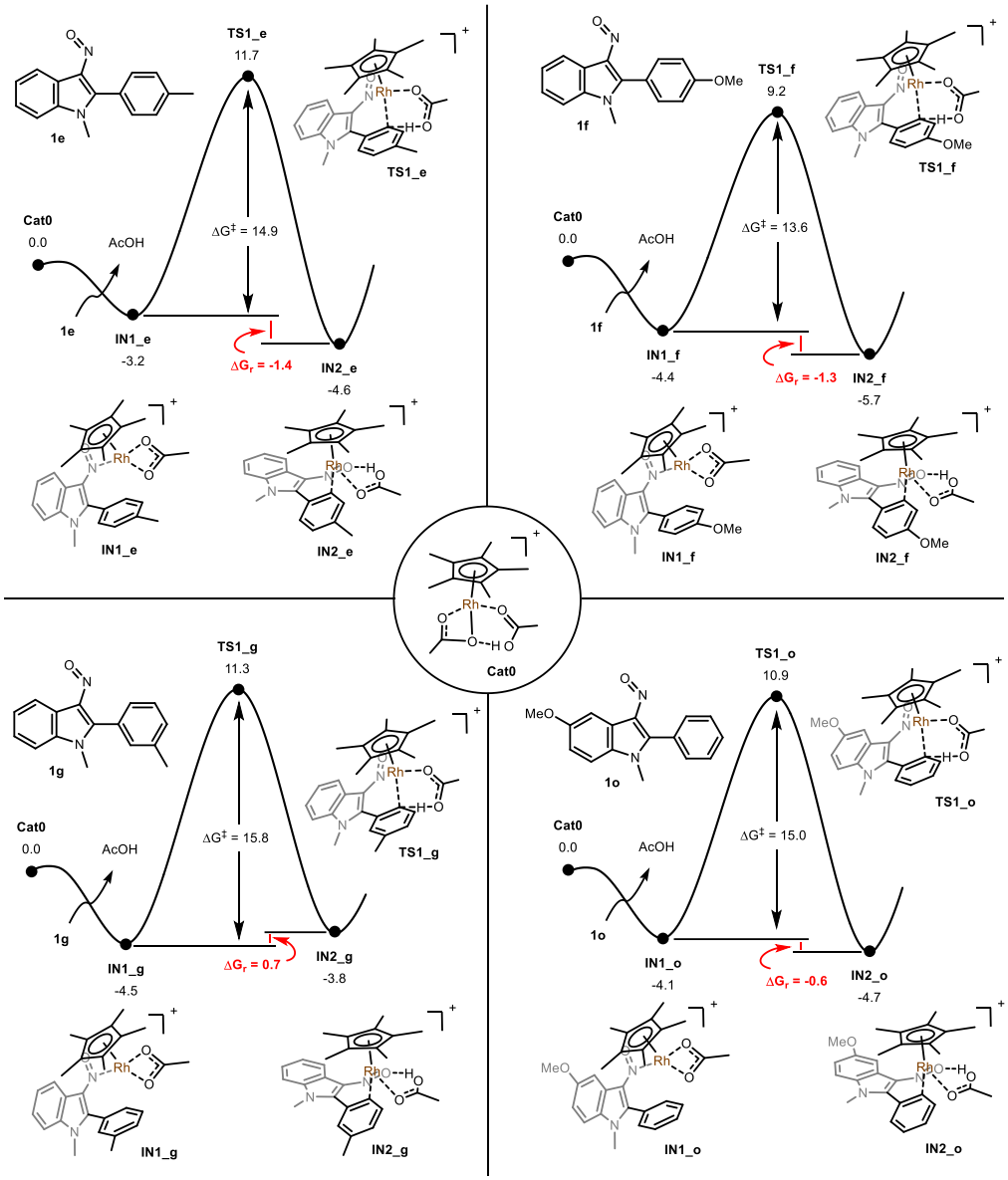


Figure S6. Substituted group effect in C–H activation at 298.15 K (free energy in kcal/mol)

Some indoles (*i.e.* **1f**, **1g** and **1o**) showed puzzling poor reactivities in the dearomative spirocyclization with aryl alky alkyne (**3fa**, **3ga** and **3oa**) or 1,3-diyne (**3fi**, **3gi** and **3oi**) under mild conditions. Thus, the C–H activation processes of four indoles, including a contrastive substrate **1e**, were discussed by DFT calculation (Figure S6). Indole **1g** showed the most special characteristic, that is the positive free energy change of reaction (ΔG_r = 0.7 kcal/mol). To a certain degree, the relative thermodynamic instability of C–H activation intermediate **IN2_g** can explain the nonreactivity of indole **1g**. However, the origins of low reactivities of indole **1f** and **1o** were difficult to disclosed based solely on calculated C–H activation processes.

5.2 Calculated Energy Data

Table S4. Single-point energies (***E***), thermal correction to Gibbs free energies (***TCG***), Gibbs free energies (***G***), and lowest frequencies of the structures calculated at the M06/6-311+G (d,p)-SDD, SMD (MeCN)//B3LYP-D3(BJ)/6-31G(d)-Lanl2DZ, SMD (MeCN) level of theory.

Structure	E (Hartree)	TCG (Hartree)	G (Hartree)	Lowest frequency (cm^{-1})
1a	-763.141523	0.195995	-762.945528	52.04
2a	-347.535360	0.103134	-347.432226	12.84
AcOH	-229.040442	0.034663	-229.005779	77.81
Cat0	-957.841295	0.284490	-957.556805	17.10
IN1	-1491.951948	0.450015	-1491.501933	23.17
TS1	-1491.926031	0.448391	-1491.477640	-1637.45
IN2	-1491.956659	0.453016	-1491.503643	27.11
IN3_Me_Ph	-1610.444518	0.527748	-1609.916770	21.87
IN3_Ph_Me	-1610.442700	0.525851	-1609.916849	18.08
TS3_Me_Ph	-1610.425003	0.525923	-1609.899080	-283.16
TS3_Ph_Me	-1610.430809	0.527349	-1609.903460	-391.08
IN4_Me_Ph	-1610.468324	0.528475	-1609.939849	25.90
IN4_Ph_Me	-1610.473852	0.528411	-1609.945441	28.21
IN5_Me_Ph	-1839.516844	0.585245	-1838.931599	24.22
IN5_Ph_Me	-1839.520221	0.584021	-1838.936200	16.41
TS5_Me_Ph	-1839.502095	0.584790	-1838.917305	-185.09
TS5_Ph_Me	-1839.505065	0.584080	-1838.920985	-216.76
IN6_Me_Ph	-1839.570914	0.586187	-1838.984727	19.34
IN6_Ph_Me	-1839.570408	0.588780	-1838.981628	15.53
IN7_Me_Ph	-1110.740635	0.329010	-1110.411625	27.17
IN7_Ph_Me (3aa_E)	-1110.741140	0.328236	-1110.412904	21.10
IN7_Ph_Me_Z (3aa_Z)	-1110.744626	0.329125	-1110.415501	26.82
2i	-615.294883	0.160710	-615.134173	20.71
IN3_Ph_ynyl	Not Located			
IN3_ynyl_Ph	-1878.202259	0.580937	-1877.621322	13.33
TS3_Ph_ynyl	-1878.185718	0.578447	-1877.607271	-351.19
TS3_ynyl_Ph	-1878.186865	0.580897	-1877.605968	-329.78
IN4_Ph_ynyl	-1878.234782	0.582729	-1877.652053	14.67
IN4_ynyl_Ph	-1878.24063	0.582264	-1877.658366	15.20
IN5_Ph_ynyl	-2107.282676	0.637737	-2106.644939	13.14

IN5_ynyl_Ph	-2107.286388	0.640624	-2106.645764	14.86
TS5_Ph_ynyl	-2107.263919	0.638375	-2106.625544	-220.16
TS5_ynyl_Ph	-2107.270839	0.639992	-2106.630847	-197.27
IN6_Ph_ynyl	-2107.329159	0.641343	-2106.687816	13.87
IN6_ynyl_Ph	-2107.331613	0.641410	-2106.690203	9.19
IN7_Ph_ynyl	-1378.498505	0.383096	-1378.115409	17.39
IN7_ynyl_Ph	-1378.502132	0.383672	-1378.118460	19.22
IN4_Me_ynyl	-1494.950086	0.482837	-1494.467249	10.35
IN4_ynyl_Me	-1494.960131	0.485925	-1494.474206	26.30
IN4_Me_Phynyl	-1686.589463	0.532331	-1686.057132	11.93
IN4_Ph_Meynyl	-1686.594963	0.533692	-1686.061271	26.13
IN4_Meynyl_Ph	-1686.600884	0.533755	-1686.067129	20.40
IN4_Phynyl_Me	-1686.600068	0.533420	-1686.066648	16.99
1e	-802.437447	0.219673	-802.217774	18.49
IN1_e	-1531.248109	0.474288	-1530.773821	18.28
TS1_e	-1531.223720	0.473605	-1530.750115	-1648.16
IN2_e	-1531.253230	0.477147	-1530.776083	20.27
1f	-877.637897	0.225701	-877.412196	39.83
IN1_f	-1606.449325	0.479123	-1605.970202	17.20
TS1_f	-1606.424526	0.475915	-1605.948611	-1626.38
IN2_f	-1606.456225	0.483979	-1605.972246	29.77
1g	-802.436897	0.220628	-802.216269	40.67
IN1_g	-1531.247971	0.473459	-1530.774512	10.69
TS1_g	-1531.222308	0.472963	-1530.749345	-1645.28
IN2_g	-1531.251585	0.478169	-1530.773416	25.96
1o	-877.635583	0.225641	-877.409942	40.44
IN1_o	-1606.446253	0.478804	-1605.967449	16.17
TS1_o	-1606.420623	0.477024	-1605.943599	-1630.65
IN2_o	-1606.451113	0.482702	-1605.968411	21.34

5.3 Coordinates of Optimized Structures

1a

Lowest frequency = 52.04 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.195995 Hartree

E = -763.141523 Hartree

G = -762.945528 Hartree

C	4.25768700	0.33170100	-0.06326300
C	4.14324700	-1.06463800	0.05657500
C	2.89541800	-1.68422200	0.12835200
C	1.77333300	-0.85907500	0.07856000
C	1.86641300	0.54770600	-0.03833500
C	3.12931100	1.14931700	-0.11251200
N	0.41782500	-1.21401300	0.13039400
C	-0.35321300	-0.09617800	0.03827400
C	0.50124500	1.02995300	-0.06586600
C	-1.81872600	-0.10930600	0.02448200
N	-0.00371100	2.28937900	-0.23362800
O	0.84460100	3.21000700	-0.30840400
C	-2.52568700	-1.01198000	-0.78971900
C	-3.91854700	-0.98998300	-0.81788800
C	-4.62234000	-0.07172400	-0.03524200
C	-3.92690600	0.83067800	0.77341800
C	-2.53437900	0.81684100	0.80353700
H	5.24517800	0.78083700	-0.11885300
H	5.04100700	-1.67480600	0.08986800
H	2.80617100	-2.76201300	0.21236800
H	3.21526400	2.22465700	-0.20455800
H	-1.98422100	-1.70941700	-1.42050300
H	-4.45319800	-1.68691100	-1.45654400
H	-5.70827300	-0.05823800	-0.05675100
H	-4.46960100	1.54533400	1.38522700
H	-1.99419600	1.51147300	1.43634300
C	-0.02576200	-2.58441300	0.36054700
H	-1.05384400	-2.57977600	0.71838100
H	0.03852700	-3.16978800	-0.56130500
H	0.61501000	-3.03703700	1.12067600

2a

Lowest frequency = 12.84 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.103134 Hartree

E = -347.535360 Hartree

G = -347.432226 Hartree

C	-2.60684400	0.00013000	-0.00047000
C	-1.39311300	0.00017000	-0.00021900
C	0.03687200	0.00009800	-0.00009100
C	0.75188600	-1.21363300	-0.00001000
C	0.75207200	1.21371600	-0.00001000
C	2.14496500	-1.20901300	0.00006200
H	0.20539300	-2.15174500	0.00002600
C	2.14515200	1.20887400	0.00006300
H	0.20573000	2.15191600	0.00003000
C	2.84615600	-0.00012400	0.00009000
H	2.68490200	-2.15170700	0.00012600
H	2.68523900	2.15148200	0.00012900
H	3.93243600	-0.00020900	0.00018100
C	-4.06567900	-0.00008000	0.00009000
H	-4.46087500	0.89133500	-0.50174200
H	-4.46055700	-0.88158300	-0.51924200
H	-4.46105600	-0.01031600	1.02346300

AcOH

Lowest frequency = 77.81 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.034663 Hartree

E = -229.040442 Hartree

G = -229.005779 Hartree

C	-0.09029300	0.12199800	-0.00000600
O	-0.64179500	1.20431300	-0.00005000
O	-0.77995800	-1.04209200	-0.00000400
H	-1.73137300	-0.80972100	-0.00004100
C	1.39447700	-0.11262400	0.00005100
H	1.68017600	-0.69365500	0.88357200
H	1.68023600	-0.69370700	-0.88341600
H	1.91988800	0.84306900	0.00004100

Cp*RhOAcAcOH (cat0)

Lowest frequency = 17.10 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.284490 Hartree

E = -957.841295 Hartree

G = -957.556805 Hartree

Rh	-0.11689000	0.15247300	-0.14502800
C	-2.24399800	0.23484100	-0.63657600
C	-2.03417100	0.57524800	0.74610800
C	-1.74654000	-1.10165400	-0.85196300
C	-1.45733200	-0.58700000	1.40465300
C	-1.27729600	-1.61174200	0.42041100
C	-1.11072300	-0.67295000	2.84915700
H	-2.00263000	-0.97875100	3.41248100
H	-0.32550800	-1.40999400	3.03102800
H	-0.78606800	0.29515800	3.23870700
C	-2.42441500	1.84832500	1.41550600
H	-2.40429300	2.68844500	0.71740900
H	-3.44578400	1.75560400	1.80737500
H	-1.76124500	2.07457300	2.25385900
C	-2.82126700	1.12351400	-1.68078400
H	-2.37049200	0.93359200	-2.65814700
H	-3.89793500	0.92268800	-1.76212500
H	-2.69150100	2.17811800	-1.42862700
C	-1.76843600	-1.85319700	-2.13821100
H	-0.93561700	-2.55790000	-2.20131600
H	-2.70175000	-2.42719400	-2.20969000
H	-1.72181200	-1.17693600	-2.99525500
C	-0.68690000	-2.96201600	0.63954400
H	-0.03047600	-2.97677200	1.51242800
H	-1.49423400	-3.68689100	0.80613900
H	-0.11774300	-3.28965100	-0.23381400
C	1.45521300	2.22514900	-0.22814900
O	1.34491400	1.52807500	0.85554600
O	0.72454000	1.91551200	-1.21047900
C	2.44954200	3.34225900	-0.29206900
H	2.33010100	3.99435900	0.57887700
H	3.46014600	2.91781700	-0.25247000
H	2.33296100	3.91734600	-1.21222800
C	2.68256100	-1.21692100	-0.12478700
O	1.65707100	-0.99598200	-0.79093600
O	3.05173200	-0.48892700	0.90796400
H	2.44041600	0.30109000	1.00726900
C	3.59699100	-2.35790800	-0.43776400
H	4.62343200	-1.99431800	-0.54684600
H	3.58128200	-3.06317300	0.40156000
H	3.27335300	-2.86361600	-1.34756800

IN1

Lowest frequency = 23.17 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.450015 Hartree

E = -1491.951948 Hartree

G = -1491.501933 Hartree

C	-4.77726200	-2.79815100	0.46726300
C	-5.71882300	-1.84419200	0.04920500
C	-5.35398900	-0.51238400	-0.15557800
C	-4.02282200	-0.17860800	0.07780400
C	-3.06078600	-1.11980900	0.50183100
C	-3.44504500	-2.45186500	0.69931300
N	-3.39451400	1.07093500	-0.05538400
C	-2.07045800	0.96663600	0.21642400
C	-1.80442300	-0.39365700	0.56872100
C	-1.17610900	2.12308700	0.21172500
N	-0.58814700	-0.94636800	0.82536600
O	-0.60090700	-2.11245400	1.27767800
C	-1.21880700	3.07058900	-0.83011600
C	-0.40179000	4.19571200	-0.78589100
C	0.46645600	4.39063900	0.29371400
C	0.51940900	3.45118200	1.32359500
C	-0.29692300	2.32175600	1.28687400
Rh	1.38233600	-0.48267300	0.08808000
H	-5.09228900	-3.82630100	0.61863200
H	-6.74811300	-2.14438000	-0.12159100
H	-6.07607100	0.22269200	-0.49299000
H	-2.72590100	-3.18852400	1.03082500
H	-1.87367100	2.91273500	-1.67986500
H	-0.43731000	4.91701100	-1.59663900
H	1.10098800	5.27147600	0.32719000
H	1.19731400	3.58946400	2.15890600
C	1.23851200	-1.67754100	-1.71245700
C	2.61089300	-1.69466500	-1.25800400
C	0.91114100	-0.31705900	-2.08283100

C	3.09864600	-0.34609900	-1.25834100
C	2.04675900	0.49991300	-1.79147900
C	4.46587600	0.10973800	-0.87056100
H	5.12448100	0.11040600	-1.74896400
H	4.44171600	1.12587100	-0.46881500
H	4.90688300	-0.54996800	-0.11888100
C	3.35781100	-2.90021700	-0.80822900
H	2.68655000	-3.64824500	-0.37934300
H	3.85725300	-3.35352500	-1.67507600
H	4.12279000	-2.64566300	-0.07167700
C	0.35532300	-2.86646800	-1.88873800
H	-0.69946400	-2.58635800	-1.83865300
H	0.53915100	-3.32055400	-2.87132700
H	0.54995800	-3.62362000	-1.12532500
C	-0.36487800	0.10926500	-2.72418800
H	-0.52311700	1.18404600	-2.63506900
H	-0.32903800	-0.14321100	-3.79215200
H	-1.22333800	-0.40958500	-2.29070100
C	2.17479300	1.96616300	-2.01134200
H	2.66170200	2.45374300	-1.16222200
H	2.80188900	2.14101100	-2.89588300
H	1.20641200	2.43787200	-2.17689800
C	2.84502500	-0.13740300	3.90484100
C	2.35557800	-0.22894700	2.48623700
O	2.10907800	0.81921700	1.81296200
O	2.14215000	-1.36698500	1.95230900
H	-0.26400700	1.60340200	2.09559800
C	-4.15573500	2.29048500	-0.31796000
H	-5.10966700	2.21887300	0.20711300
H	-3.60665800	3.15327800	0.05405400
H	-4.33775100	2.40343000	-1.39008600
H	1.97818200	-0.12682400	4.57742300
H	3.46271400	-1.00324100	4.15699500
H	3.40910900	0.78618400	4.05731900

TS1

Lowest frequency = -1637.45 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.448391 Hartree

E = -1491.926031 Hartree

G = -1491.477640 Hartree

C	-5.07397400	-2.32039100	-0.43351100
C	-5.88316700	-1.17479200	-0.50311600
C	-5.34104600	0.10515900	-0.37381200
C	-3.96571000	0.19327400	-0.17157300
C	-3.13742400	-0.94606800	-0.10304200
C	-3.69703800	-2.22246200	-0.23221100
N	-3.16633900	1.34143600	-0.00910600
C	-1.85587800	0.99731800	0.10380000
C	-1.79470300	-0.43788700	0.06579700
C	-0.75807400	1.93334100	0.33207100
N	-0.66670300	-1.17150200	0.18342400
O	-0.77202600	-2.41125200	0.28485600
C	-0.83899000	3.29104100	-0.03025000
C	0.17188300	4.17963900	0.33651500
C	1.27620700	3.73615900	1.06800900
C	1.40462800	2.37695200	1.35029000
C	0.42118200	1.44807100	0.97019800
Rh	1.21985700	-0.36770800	0.02136500
H	-5.52844600	-3.30102900	-0.53743400
H	-6.95143400	-1.28205000	-0.66421600
H	-5.97126000	0.98459600	-0.44026100
H	-3.07368400	-3.10499400	-0.17511400
H	-1.66511500	3.66315600	-0.62089400
H	0.08886900	5.22379100	0.05057500
H	2.04604600	4.43786200	1.37540700
H	2.28798600	2.01779900	1.87231700
C	1.64604300	-1.36320800	-1.92730100
C	2.82991600	-1.40233700	-1.13447700
C	1.30296900	0.03234500	-2.13685100
C	3.26726600	-0.03439800	-0.89418600
C	2.36624500	0.83179200	-1.57567700
C	4.51042700	0.35571600	-0.16267300
H	5.38363600	0.27717600	-0.82396400
H	4.45352400	1.38533600	0.19901300
H	4.68496000	-0.30098100	0.69455700
C	3.53755400	-2.61833900	-0.64053900
H	2.90035000	-3.50412400	-0.69336700
H	4.42995900	-2.80150200	-1.25344600
H	3.86725500	-2.48645900	0.39408400
C	0.88425800	-2.53803100	-2.44225200
H	-0.16548800	-2.28993700	-2.61370800
H	1.31449100	-2.86282100	-3.39879800
H	0.92960100	-3.38042300	-1.74806100
C	0.17588000	0.54689600	-2.97155700

H	-0.14585700	1.53482000	-2.63249000
H	0.49079600	0.63531700	-4.01978200
H	-0.68466900	-0.12589500	-2.93619300
C	2.49283300	2.30540500	-1.74354100
H	3.17539500	2.74529900	-1.01566600
H	2.89094400	2.50335000	-2.74835300
H	1.52596200	2.80705800	-1.66912400
C	1.25448100	-1.95057600	4.15104900
C	1.03256600	-1.10976200	2.92167500
O	1.73114800	-1.32919600	1.89366000
O	0.11812400	-0.21303700	2.97832900
H	0.24187000	0.49729600	1.96090500
C	-3.77339300	2.65960800	0.17153900
H	-4.77962000	2.51693200	0.56426900
H	-3.19546400	3.23601200	0.89241100
H	-3.82995000	3.19704100	-0.77868500
H	0.41538700	-2.64961400	4.25143400
H	2.18333500	-2.51763800	4.06967100
H	1.27074600	-1.31696200	5.04225300

IN2

Lowest frequency = 27.11 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.453016 Hartree

E = -1491.956659 Hartree

G = -1491.503643 Hartree

C	-4.71855800	-2.80683000	0.41298100
C	-5.63621800	-1.82658200	0.00779000
C	-5.25362800	-0.48996600	-0.14868800
C	-3.92628900	-0.17917000	0.12114400
C	-2.99252000	-1.15093500	0.53922700
C	-3.38615300	-2.48347900	0.68238800
N	-3.26954100	1.07070800	0.02638400
C	-1.97043600	0.95005100	0.37233700
C	-1.73127100	-0.44937300	0.64424600
C	-1.02688800	2.03124700	0.61046000
N	-0.51004300	-0.93698300	0.84026100
O	-0.38732000	-2.14559400	1.23278000
C	-1.47966700	3.30728900	1.02631000
C	-0.57267800	4.30449600	1.35602900
C	0.80101600	4.04491100	1.28956700
C	1.25798700	2.78343100	0.90474700
C	0.36464000	1.76269300	0.56396700
Rh	1.09721700	-0.01008200	-0.05899100
H	-5.05061700	-3.83431900	0.52590800
H	-6.66691800	-2.10611000	-0.18717500
H	-5.96794300	0.26335900	-0.46135200
H	-2.67682500	-3.23638600	1.00219000
H	-2.53827900	3.50495900	1.13977700
H	-0.93403300	5.27502400	1.68179000
H	1.51421000	4.82294200	1.54906900
H	2.32664400	2.59287700	0.86370400
C	1.17206600	-1.48794100	-1.87478400
C	2.49590600	-1.24669100	-1.49967700
C	0.53678700	-0.18845200	-2.14119800
C	2.73573600	0.20557500	-1.57304500
C	1.56493400	0.82765900	-2.08246100
C	4.04951400	0.85577000	-1.28554600
H	4.75544600	0.66856000	-2.10581600
H	3.94349400	1.93729200	-1.17080900
H	4.49524800	0.45366800	-0.37026300
C	3.53062700	-2.24195700	-1.08531400
H	3.08073900	-3.18616700	-0.76928200
H	4.20970300	-2.45255800	-1.92248400
H	4.14389700	-1.85783600	-0.26422900
C	0.46673800	-2.80262100	-1.94812000
H	-0.55148900	-2.73127200	-1.55629600
H	0.39342800	-3.13108500	-2.99337000
H	0.99731900	-3.57591800	-1.38734100
C	-0.84298300	-0.00865700	-2.68808000
H	-1.22924800	0.99226500	-2.47934200
H	-0.83443100	-0.14547000	-3.77784600
H	-1.53639400	-0.74109300	-2.26687100
C	1.40059900	2.26020000	-2.47242000
H	2.07734900	2.91146000	-1.91463600
H	1.62527200	2.37468300	-3.54114400
H	0.37772100	2.60645700	-2.30618900
C	3.94038200	-1.31598000	3.15086400
C	2.70960000	-1.22360300	2.30089700
O	2.36172900	-0.15390700	1.77539500
O	2.06190800	-2.36036200	2.17080000
H	1.16927400	-2.25727800	1.69964700
C	-3.94313900	2.25187500	-0.50844500
H	-4.59898400	1.92915900	-1.31892800
H	-4.53792800	2.74366700	0.26598500

H	-3.20193100	2.94216500	-0.90707100
H	3.67491500	-1.68016000	4.14879000
H	4.63030600	-2.04207100	2.70615100
H	4.42521400	-0.34206200	3.22267500

IN3_Me_Ph

Lowest frequency = 21.87 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.527748 Hartree

E = -1610.444518 Hartree

G = -1609.916770 Hartree

C	5.68872100	-0.40343300	-1.55776600
C	6.25369700	0.51643800	-0.66120500
C	5.45600100	1.26631100	0.20736700
C	4.08117900	1.06374900	0.13893000
C	3.49454700	0.14995400	-0.76270300
C	4.30736100	-0.59917800	-1.61971900
N	3.05947000	1.66582200	0.90044300
C	1.84341300	1.20041500	0.51016800
C	2.07329300	0.20554000	-0.49464000
C	0.55641600	1.70081300	0.95700800
N	1.11905700	-0.60251100	-0.99049400
O	1.43766700	-1.37911000	-1.92287700
C	0.43868300	3.02173600	1.46263800
C	-0.78051800	3.51323000	1.89997600
C	-1.91397000	2.69510400	1.83619300
C	-1.81884400	1.42161800	1.28280100
C	-0.60463300	0.90574800	0.80757300
Rh	-0.66500700	-0.94758000	-0.02626800
H	6.33685900	-0.96899800	-2.22049000
H	7.33043600	0.65425300	-0.64099600
H	5.89706900	1.97806600	0.89600700
H	3.87030700	-1.30333700	-2.31550800
H	1.29788800	3.67915300	1.46981900
H	-0.85151700	4.52954700	2.27507300
H	-2.87587000	3.06278100	2.18263200
H	-2.71853200	0.82348600	1.19398100
C	-0.19546900	-3.22183700	0.46522200
C	-1.57648000	-3.18596800	0.24536900
C	0.10772400	-2.25519200	1.52366100
C	-2.17256700	-2.22120200	1.17948200
C	-1.14988500	-1.76029900	2.04446100
C	-3.64048600	-1.96497400	1.29849800
H	-4.14302200	-2.81774400	1.77518800
H	-3.84408700	-1.07679500	1.90171900
H	-4.09806000	-1.82435200	0.31386200
C	-2.37909700	-4.03232300	-0.68514800
H	-1.76434300	-4.47579300	-1.47109500
H	-2.84460400	-4.85141500	-0.11947400
H	-3.18933100	-3.46240900	-1.14835400
C	0.82306600	-4.06576300	-0.22973900
H	1.69976900	-3.47709000	-0.51283200
H	1.16415500	-4.87227100	0.43297200
H	0.41414900	-4.52241400	-1.13454200
C	1.44907600	-2.06926400	2.15711300
H	1.54050000	-1.07884300	2.61105900
H	1.60181800	-2.81771100	2.94651200
H	2.25177100	-2.18786300	1.42443000
C	-1.31186900	-0.97851600	3.30585400
H	-2.21804500	-0.37021000	3.29879300
H	-1.38532300	-1.68139600	4.14711300
H	-0.45632000	-0.32537600	3.49171200
C	-1.95737600	0.31897500	-1.87399300
C	-1.60444200	-0.79137200	-2.26773400
C	-2.42245200	1.65161900	-1.65535900
C	-3.76409100	1.88852900	-1.30724600
C	-1.53440900	2.73606400	-1.78410600
C	-4.20665500	3.19141100	-1.08921100
H	-4.44355000	1.04852700	-1.20206400
C	-1.98500100	4.03344600	-1.56149800
H	-0.49775200	2.54594200	-2.04179100
C	-3.31939200	4.26436600	-1.21114500
H	-5.24340500	3.36916200	-0.81890500
H	-1.29400900	4.86605600	-1.65416800
H	-3.66599000	5.27827500	-1.03360200
C	-1.36113700	-1.94553200	-3.14123200
C	3.37221200	2.52476300	2.04108100
H	4.29999800	2.16552900	2.48881300
H	3.50203800	3.56440300	1.72811700
H	2.57549600	2.45504600	2.77966200
H	-0.40502100	-2.41627300	-2.90742300
H	-2.16089800	-2.68388000	-3.04418800
H	-1.33509700	-1.60474900	-4.18384600

IN3_Ph_Me

Lowest frequency = 18.08 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.525851 Hartree

E = -1610.442700 Hartree

G = -1609.916849 Hartree

C	4.25803300	-3.92576400	-0.21149800
C	5.45083700	-3.20816000	-0.03013300
C	5.46087500	-1.81110400	-0.00290500
C	4.23938800	-1.16580600	-0.16985600
C	3.03128300	-1.87141100	-0.36071500
C	3.03662800	-3.26987700	-0.37669100
N	3.96071000	0.21569000	-0.17438100
C	2.63534400	0.42877200	-0.38143800
C	2.00470000	-0.85718100	-0.44756200
C	2.00220500	1.71223900	-0.64128400
N	0.67003100	-1.03641300	-0.47179900
O	0.22050100	-2.19389200	-0.64365100
C	2.74501100	2.78743300	-1.19123600
C	2.12893600	3.98587700	-1.51861000
C	0.75236900	4.13607300	-1.31317300
C	0.00642100	3.07296500	-0.80890200
C	0.60339900	1.84874900	-0.47900000
Rh	-0.61488900	0.39272400	0.18760700
H	4.28671500	-5.01109200	-0.23059400
H	6.38692200	-3.74531100	0.08800400
H	6.38509700	-1.26130300	0.13505500
H	2.11661600	-3.82097400	-0.52372300
H	3.79824800	2.66950500	-1.40990300
H	2.71398700	4.79371300	-1.94727600
H	0.26024500	5.07177600	-1.56528100
H	-1.06579100	3.19068300	-0.68148100
C	-1.05807000	-0.72280400	2.27752000
C	-2.31107300	-0.22872700	1.92769400
C	-0.11545200	0.40608000	2.28156300
C	-2.19313200	1.22892600	1.73047000
C	-0.88981000	1.62186300	2.09766600
C	-3.34079600	2.12111700	1.38640200
H	-3.99847800	2.25382300	2.25663200
H	-2.99811500	3.10978000	1.06965400
H	-3.94799600	1.69004800	0.58399200
C	-3.59953400	-0.97428500	1.85698300
H	-3.44328900	-2.04857400	1.74197200
H	-4.16633000	-0.81383400	2.78528400
H	-4.22465200	-0.62203800	1.03445500
C	-0.67739200	-2.13798000	2.57036900
H	0.27766000	-2.39731000	2.10449600
H	-0.56414200	-2.28746500	3.65264100
H	-1.43410400	-2.83942300	2.20966700
C	1.28727600	0.33699900	2.79606600
H	1.89315500	1.16301500	2.41517500
H	1.28948700	0.39477500	3.89319700
H	1.76835100	-0.60246200	2.51126300
C	-0.39448300	3.01100100	2.33340400
H	-0.94200100	3.74731000	1.74095300
H	-0.53718600	3.26217000	3.39356900
H	0.66970600	3.10960600	2.10876300
C	-1.14714200	0.40054500	-2.39250300
C	-2.13836200	-0.11269900	-1.88957200
C	-0.09179000	0.87144000	-3.28848600
C	-3.34071000	-0.80966500	-1.54558000
C	-4.58210600	-0.14727100	-1.55796500
C	-3.29002800	-2.18663300	-1.25641100
C	-5.75261400	-0.85734200	-1.29280800
H	-4.61931700	0.91369400	-1.78348800
C	-4.46573100	-2.88645100	-0.99855700
H	-2.32524200	-2.68214300	-1.22782600
C	-5.69832400	-2.22614200	-1.01626600
H	-6.70774200	-0.34059100	-1.30455700
H	-4.42039500	-3.94906300	-0.77817600
H	-6.61256700	-2.77580800	-0.81211100
C	4.98701400	1.20070100	0.16069600
H	5.64881200	0.75827400	0.90710700
H	5.57182400	1.47480900	-0.72176100
H	4.51865700	2.08545200	0.58842600
H	0.87823800	0.44866400	-3.01067700
H	-0.32750000	0.55432000	-4.31173500
H	-0.00464800	1.96087600	-3.27389600

TS3_Me_Ph

Lowest frequency = -283.16 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.525923 Hartree

E = -1610.425003 Hartree

G = -1609.899080 Hartree

C	5.42514800	-2.05133800	-1.21173200
C	6.16282900	-0.91599800	-0.83727800
C	5.55859000	0.15551200	-0.17716200
C	4.19702900	0.04594600	0.09389000
C	3.43850800	-1.08895000	-0.27217300
C	4.06137000	-2.15313300	-0.93491100
N	3.34852900	0.96784400	0.72939200
C	2.08555900	0.46787500	0.79769600
C	2.08433400	-0.79986500	0.14920200
N	0.98678000	-1.57655200	-0.00054200
O	1.17425000	-2.73927100	-0.43436800
C	0.98000500	1.09637100	1.49036100
C	-0.34509100	0.92623300	1.01244500
Rh	-0.98838700	-0.87992400	0.03803100
H	5.92743300	-2.86864600	-1.72049000
H	7.22452900	-0.86951500	-1.05978000
H	6.13081100	1.02876600	0.11559100
H	3.49568300	-3.03157200	-1.21655800
C	-2.12823900	-2.76320400	-0.54502700
C	-2.97975700	-1.67152700	-0.85546500
C	-1.90297300	-2.74390900	0.89836600
C	-3.27260700	-0.96800300	0.36906000
C	-2.64308100	-1.66091200	1.46020400
C	-4.24736400	0.16201200	0.46684500
H	-5.26000400	-0.20953500	0.25926100
H	-4.25691400	0.60646100	1.46412800
H	-4.03532000	0.94677600	-0.26682700
C	-3.52561300	-1.28782200	-2.19236100
H	-3.02589300	-1.82339200	-3.00226700
H	-4.59728000	-1.52170300	-2.24269200
H	-3.41858500	-0.21265000	-2.37006300
C	-1.62867700	-3.82015700	-1.47483700
H	-0.56694600	-4.01119000	-1.30264400
H	-2.17464100	-4.75967900	-1.31524900
H	-1.76128100	-3.52674700	-2.51960300
C	-1.10792100	-3.77412300	1.62699300
H	-0.88330300	-3.46454500	2.65067100
H	-1.66650600	-4.71865000	1.66856000
H	-0.16708700	-3.96969600	1.10205700
C	-2.77376900	-1.31362100	2.90844400
H	-1.96424500	-1.75239300	3.49785400
H	-2.75595700	-0.23034000	3.06264800
H	-3.72390400	-1.68915100	3.31095800
C	1.21019900	1.85344000	2.66221500
C	0.16313500	2.48118900	3.32080600
C	-1.13462200	2.39347600	2.79807400
C	-1.37291300	1.64685600	1.65198400
H	2.21109400	1.91736700	3.07225200
H	0.35573100	3.04642300	4.22720800
H	-1.95773800	2.90656300	3.28721400
H	-2.37054000	1.62140700	1.23611800
C	-0.43676100	1.18376100	-0.99723700
C	-0.31918700	0.09253400	-1.66311300
C	0.01489800	-0.50436200	-2.96939700
C	-0.76694200	2.58767800	-1.21264300
C	-1.70439500	2.89271800	-2.21703200
C	-0.14954300	3.63445400	-0.50735500
C	-2.00838700	4.22033100	-2.51567900
H	-2.18772900	2.08152000	-2.75278500
C	-0.45531000	4.95789300	-0.81263200
H	0.56933200	3.40916900	0.27211000
C	-1.38539800	5.25521800	-1.81448200
H	-2.73473600	4.44440500	-3.29153700
H	0.03275800	5.76081700	-0.26788700
H	-1.62462000	6.28954400	-2.04416900
C	3.80057100	2.30629400	1.10010700
H	4.30333500	2.29407900	2.07112700
H	4.49804000	2.65445000	0.33614800
H	2.94773400	2.98206500	1.13461200
H	0.39563200	0.25923200	-3.65851700
H	0.77276500	-1.28909600	-2.85637700
H	-0.87147700	-0.96972300	-3.41373800

TS3_Ph_Me

Lowest frequency = -391.08 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.527349 Hartree

E = -1610.430809 Hartree

G = -1609.903460 Hartree

C	-4.93452900	-1.05997700	-1.55953100
C	-5.65168600	0.02542600	-1.02668800
C	-4.99927100	1.16561900	-0.55610500
C	-3.60829300	1.18011500	-0.63828900

C	-2.87168100	0.10164100	-1.18179200
C	-3.54336300	-1.03416200	-1.64831000
N	-2.70622700	2.15658100	-0.18605200
C	-1.42797500	1.73908700	-0.39583800
C	-1.48325200	0.45534000	-0.99913400
N	-0.38745300	-0.29239100	-1.27849100
O	-0.56210100	-1.29260900	-2.01285500
C	-0.23246500	2.50575000	-0.11029300
C	0.93263100	1.84071400	0.36664100
Rh	1.36848200	-0.21165800	-0.13126700
H	-5.47517500	-1.93254800	-1.91365000
H	-6.73541400	-0.02115800	-0.97895700
H	-5.55581800	1.99916700	-0.14251600
H	-2.99088800	-1.86921900	-2.05906100
C	2.38314900	-2.15500300	-0.85858300
C	2.86083200	-1.91031500	0.44997700
C	2.77552500	-1.01989700	-1.69005800
C	3.55362700	-0.63866900	0.44521800
C	3.54962600	-0.12215700	-0.89700500
C	4.29428600	-0.09028500	1.62211200
H	5.19914400	-0.68697800	1.80103400
H	4.60940900	0.94328400	1.46428000
H	3.68911900	-0.13676200	2.53291200
C	2.71627900	-2.78069100	1.65609900
H	1.98119300	-3.57245900	1.49810900
H	3.67798300	-3.25006000	1.90212700
H	2.40738400	-2.19583900	2.52873200
C	1.71003000	-3.38321100	-1.37689400
H	0.74869300	-3.13339100	-1.83381700
H	2.33398100	-3.85560000	-2.14675100
H	1.54420400	-4.11628400	-0.58392900
C	2.49684700	-0.92786100	-3.15272900
H	2.66659800	0.08229300	-3.53399300
H	3.14836200	-1.61691300	-3.70670100
H	1.46030100	-1.21470200	-3.35889100
C	4.25970500	1.09914200	-1.38604300
H	3.71502500	1.57804700	-2.20472300
H	4.39396100	1.83535100	-0.59040900
H	5.25692400	0.83159000	-1.76032500
C	-0.20889800	3.89886100	-0.33013500
C	0.93340500	4.64280600	-0.06920000
C	2.06701500	4.00524000	0.45271700
C	2.05428700	2.63634000	0.68266000
H	-1.08300400	4.38957200	-0.74346200
H	0.94060400	5.71095500	-0.26179300
H	2.96221300	4.57854800	0.67695000
H	2.92598100	2.16567500	1.11664500
C	0.44880100	0.63434600	1.80566200
C	-0.07467300	-0.47338600	1.40515600
C	-1.14416500	-1.41769000	1.52728400
C	-1.05263100	-2.72037100	1.00219000
C	-2.36522900	-0.99043400	2.09547500
C	-2.14807100	-3.57792300	1.05991900
C	-3.45612000	-1.85202400	2.14174100
H	-2.44644500	0.02453700	2.47154800
C	-3.35333300	-3.14754000	1.62313300
H	-2.06534400	-4.58138900	0.65220100
H	-4.39360600	-1.50843000	2.56932700
H	-4.21033300	-3.81412300	1.65081300
H	-0.12446400	-3.04161600	0.54775100
C	0.82278400	1.31944600	3.07130700
C	-3.13959600	3.35511300	0.52552500
H	-3.43477900	4.14010200	-0.17633100
H	-3.99208600	3.09273100	1.15489700
H	-2.32927500	3.71366000	1.15851800
H	1.91042100	1.32270000	3.20233100
H	0.47892600	2.35861400	3.08068000
H	0.37549300	0.77646500	3.91096500

IN4_Me_Ph

Lowest frequency = 25.90 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.528475 Hartree

E = -1610.468324 Hartree

G = -1609.939849 Hartree

C	3.47678700	-4.39205300	-1.62355300
C	4.63205900	-3.94013700	-0.96631600
C	4.58755300	-2.84589400	-0.10007700
C	3.35010600	-2.23534200	0.07886700
C	2.17654900	-2.67259900	-0.56868600
C	2.24099300	-3.76937300	-1.43622000
N	3.02455300	-1.12665900	0.87894900
C	1.70948300	-0.82742700	0.77540700
C	1.12929500	-1.76006600	-0.14029600
C	1.14746200	0.22035800	1.65093100

N	-0.15783100	-1.77777800	-0.54957900
O	-0.50695900	-2.73221400	-1.29114300
C	1.26754100	0.01711100	3.03850000
C	0.96143800	1.03508300	3.93534800
C	0.55971100	2.28218500	3.44827800
C	0.43310400	2.48423800	2.07570700
C	0.69054300	1.45671100	1.15440000
Rh	-1.70160200	-0.36614300	-0.50503100
H	3.54372100	-5.24693500	-2.28983000
H	5.57703900	-4.44862200	-1.13104300
H	5.47712600	-2.49351800	0.41013000
H	1.35386800	-4.12526900	-1.94225100
H	1.62388100	-0.94109100	3.40433300
H	1.05426800	0.86245500	5.00311200
H	0.34212500	3.09383800	4.13638400
H	0.12843500	3.45491100	1.69642300
C	-2.76142400	-0.20207000	1.36965700
C	-3.33434600	-1.43399100	0.80321400
C	-3.17482000	0.91531000	0.53873800
C	-3.94890700	-1.09801900	-0.39856300
C	-3.80046500	0.35875000	-0.60200700
C	-4.60474200	-2.00228200	-1.38755800
H	-5.68555300	-1.81149900	-1.41768500
H	-4.21848800	-1.82421000	-2.39757400
H	-4.44960900	-3.05450300	-1.13774600
C	-3.18192600	-2.78472700	1.42329900
H	-2.15938900	-2.93683600	1.78390000
H	-3.85145300	-2.88712500	2.28736600
H	-3.41865400	-3.58179300	0.71418300
C	-2.18424200	-0.11097100	2.73825100
H	-3.00401400	-0.12501700	3.47118800
H	-1.53277900	-0.96048700	2.95497200
H	-1.62085700	0.81055200	2.87830900
C	-2.98882500	2.36400700	0.85014000
H	-3.86199200	2.73896200	1.40049400
H	-2.10681600	2.52621200	1.47131200
H	-2.88449400	2.96036600	-0.05995400
C	-4.35686900	1.09623600	-1.77418800
H	-4.15655700	0.56073400	-2.70780300
H	-5.44722100	1.18959800	-1.67749500
H	-3.93677400	2.10188200	-1.85189300
C	0.54057300	1.72389600	-0.30428100
C	-0.36471900	1.04836900	-1.03643800
C	-0.55348400	1.15387300	-2.53122700
C	1.44334400	2.77311600	-0.85737500
C	0.97445400	3.77152100	-1.72756600
C	2.80337500	2.79068000	-0.49624600
C	1.83955500	4.74104600	-2.23802000
H	-0.07864400	3.79805200	-1.98879200
C	3.66847400	3.75672700	-1.00786400
H	3.18373800	2.03314500	0.18293700
C	3.19054000	4.73648000	-1.88351500
H	1.45399900	5.50638400	-2.90639900
H	4.71717200	3.74521800	-0.72282600
H	3.86343500	5.49180500	-2.27981200
C	4.03538800	-0.41214500	1.65466800
H	4.89880700	-0.23045300	1.01123000
H	3.63216900	0.53723900	1.99736900
H	4.34159300	-1.01556900	2.51344800
H	-0.84481700	0.17781000	-2.95371500
H	-1.35599200	1.85569800	-2.78848100
H	0.36210000	1.47166700	-3.04631300

IN4_Ph_Me

Lowest frequency = 28.21 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.528411 Hartree

E = -1610.473852 Hartree

G = -1609.945441 Hartree

C	-4.64685100	-3.15720900	-1.29563100
C	-5.65695300	-2.49157400	-0.58287600
C	-5.41214300	-1.26600700	0.03921500
C	-4.12974800	-0.74076300	-0.08686800
C	-3.10102200	-1.38840800	-0.80195000
C	-3.36383500	-2.61944700	-1.41510200
N	-3.61332200	0.45474000	0.43922400
C	-2.30841600	0.60091300	0.11363300
C	-1.92636900	-0.54546300	-0.65082400
C	-1.64593900	1.88734700	0.42103300
N	-0.68738400	-0.82611900	-1.12002300
O	-0.58939900	-1.79302000	-1.91711300
C	-2.17112200	3.03346400	-0.20189100
C	-1.74107800	4.30318200	0.17141400
C	-0.79876900	4.43709400	1.19454300
C	-0.27462400	3.30274400	1.81242200

C	-0.66592600	2.01252100	1.42373000
Rh	1.20153400	-0.17548900	-0.54508500
H	-4.86934400	-4.10802400	-1.77069800
H	-6.64612300	-2.93356900	-0.51360200
H	-6.18830900	-0.74912800	0.59253900
H	-2.59295500	-3.13357300	-1.97306500
H	-2.93252100	2.91859800	-0.96771900
H	-2.15049000	5.18026700	-0.32017700
H	-0.46955800	5.42347600	1.50835300
H	0.45754000	3.40984700	2.60716500
C	1.77089700	1.64919600	-1.54149500
C	1.93966400	0.63577400	-2.59627900
C	2.77422500	1.40852700	-0.52006400
C	2.91358300	-0.26263400	-2.16765900
C	3.40320400	0.18457700	-0.84861000
C	3.39167800	-1.50334600	-2.84576500
H	4.41953800	-1.36754200	-3.20782100
H	3.40439000	-2.35024700	-2.15072300
H	2.76232000	-1.76586300	-3.69945100
C	1.13223600	0.59781200	-3.85255000
H	0.08688100	0.85447900	-3.65500000
H	1.51816700	1.32973500	-4.57435400
H	1.16121700	-0.38869500	-4.32111300
C	0.96275400	2.88947800	-1.70021500
H	1.51142600	3.59537100	-2.34040000
H	0.00404100	2.68313400	-2.18075700
H	0.77798600	3.37472500	-0.74248300
C	3.08040600	2.29784300	0.64041000
H	3.86793500	3.01197000	0.36510300
H	2.20182200	2.86966300	0.94391700
H	3.43358000	1.72574400	1.50229200
C	4.48516300	-0.51123600	-0.09226200
H	4.31082700	-1.59136700	-0.05544900
H	5.44910200	-0.35209200	-0.59455800
H	4.56783900	-0.13959100	0.93055200
C	-0.09755500	0.81568100	2.09678100
C	0.59924900	-0.08478300	1.39173600
C	1.23572500	-1.30950400	1.90906900
C	0.75686100	-2.58081400	1.52351700
C	2.41091800	-1.24393000	2.68893200
C	1.43369300	-3.74253000	1.90229000
C	3.07597800	-2.40499900	3.07130300
H	2.79170700	-0.27041600	2.98328400
C	2.59476800	-3.65909700	2.67290400
H	1.04780500	-4.71208300	1.59965400
H	3.97513800	-2.33659200	3.67754900
H	3.12065700	-4.56272000	2.96758800
H	-0.15375200	-2.65161600	0.93591600
C	-0.37254600	0.70194600	3.58132000
C	-4.42388300	1.36407600	1.24591800
H	-4.98853400	0.77249300	1.96948300
H	-3.77629700	2.05949900	1.77464700
H	-5.11809500	1.91566600	0.60616800
H	-1.45364200	0.70370300	3.77578800
H	0.05280200	-0.21362900	4.00009400
H	0.04860900	1.55585200	4.12806100

IN5_Me_Ph

Lowest frequency = 24.22 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.585245 Hartree

E = -1839.516844 Hartree

G = -1838.931599 Hartree

C	-1.41824400	5.57201400	-0.91092500
C	-2.81246000	5.47813200	-0.78498900
C	-3.41690500	4.31446500	-0.30258700
C	-2.57179600	3.26872500	0.04951200
C	-1.16876500	3.34325800	-0.05929200
C	-0.58085000	4.51310500	-0.55084000
N	-2.90800800	1.99622600	0.55115800
C	-1.80512900	1.24612700	0.73816200
C	-0.67479300	2.03156300	0.33685800
C	-1.91580400	-0.01487800	1.49542900
N	0.60386700	1.62588800	0.32292600
O	1.45655500	2.57061300	0.24751300
C	-2.36224100	0.09296700	2.82600800
C	-2.70312000	-1.04313900	3.55148100
C	-2.63704800	-2.29573600	2.93305700
C	-2.18998700	-2.40134700	1.61903700
C	-1.78034600	-1.27314400	0.88609500
Rh	1.46054800	-0.28671700	0.04794300
H	-0.97851500	6.49093200	-1.28655200
H	-3.43499400	6.32230200	-1.06474300
H	-4.49412600	4.23542200	-0.20805700
H	0.49413900	4.59756600	-0.63797900

H	-2.46335200	1.07766400	3.27287800
H	-3.04381700	-0.95007700	4.57798300
H	-2.93370800	-3.18893600	3.47521600
H	-2.15759400	-3.37315900	1.13732900
C	1.75826300	-1.22737300	2.00339800
C	2.92844500	-0.34438900	1.88916100
C	1.88117600	-2.26292400	1.00283500
C	3.67247600	-0.76158600	0.78881500
C	2.97262100	-1.90177500	0.16795200
C	4.97097300	-0.20863700	0.30321300
H	5.79652200	-0.74586200	0.79001100
H	5.09271000	-0.34841800	-0.77391800
H	5.08045300	0.85255200	0.53629000
C	3.21060100	0.80195400	2.80438200
H	2.29273500	1.34551300	3.04866000
H	3.63869400	0.44174800	3.74934400
H	3.91943500	1.50509500	2.35924900
C	0.86073000	-1.22994700	3.19340800
H	1.40785600	-1.64268400	4.05284500
H	0.54888100	-0.21685000	3.45797300
H	-0.02743400	-1.83800500	3.03424700
C	1.06273700	-3.50467500	0.88326000
H	1.61489700	-4.34290400	1.32893200
H	0.11311100	-3.41193500	1.40767400
H	0.85922000	-3.75630200	-0.16069000
C	3.47635500	-2.65262200	-1.02070400
H	3.76743300	-1.96780900	-1.82301800
H	4.36194300	-3.24326700	-0.75012700
H	2.71784900	-3.33649600	-1.40884400
C	-1.34480900	-1.42531800	-0.52703800
C	-0.15808300	-0.99559600	-1.01180100
C	0.16615100	-1.10677600	-2.48337700
C	-2.35549300	-2.15871800	-1.35959200
C	-2.04923700	-3.38825800	-1.96331500
C	-3.65862500	-1.65314800	-1.49560100
C	-3.01219600	-4.08517600	-2.69595800
H	-1.04936100	-3.79813700	-1.84988300
C	-4.62149200	-2.34518600	-2.23081800
H	-3.91245100	-0.70766900	-1.02410100
C	-4.30154500	-3.56515400	-2.83388100
H	-2.75630400	-5.03689500	-3.15415500
H	-5.62219000	-1.93337700	-2.33194100
H	-5.05192500	-4.10727200	-3.40265700
C	-4.29206400	1.60603800	0.81171600
H	-4.88974600	1.85240200	-0.06877500
H	-4.34028900	0.53630600	0.99852000
H	-4.67400000	2.15387700	1.67725600
C	3.31681600	1.32569500	-2.09409000
O	2.41355700	0.49452500	-1.93973200
O	3.55814600	2.30075500	-1.24075500
H	2.83236600	2.29946000	-0.53914200
C	4.23375200	1.30257200	-3.27933600
H	4.12613900	2.23429800	-3.84518900
H	5.27194500	1.24261100	-2.93511800
H	4.00341800	0.44979100	-3.91843900
H	0.39116900	-0.12025600	-2.89995000
H	1.05797400	-1.72026700	-2.65566700
H	-0.66119400	-1.53726600	-3.05548100

IN5_Ph_Me

Lowest frequency = 16.41 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.584021 Hartree

E = -1839.520221 Hartree

G = -1838.936200 Hartree

C	2.59349700	-4.70948800	-2.08237100
C	3.94301500	-4.34625100	-1.96820000
C	4.33013200	-3.24381200	-1.20183300
C	3.31832000	-2.53896100	-0.56101900
C	1.95708100	-2.88855900	-0.65350900
C	1.58705600	-3.99148600	-1.43066900
N	3.42497200	-1.39573000	0.25526900
C	2.21411000	-0.98381700	0.67546800
C	1.23491400	-1.87276600	0.10365400
C	2.14794300	0.06857800	1.70931100
N	-0.09943400	-1.77294000	0.19358500
O	-0.74948100	-2.79306600	-0.21897700
C	2.78589400	-0.20426600	2.93336400
C	2.94461700	0.79817000	3.88453400
C	2.49109000	2.09030900	3.60411100
C	1.85624800	2.36008400	2.39289400
C	1.64670400	1.35380800	1.43758400
Rh	-1.38577900	-0.21111000	0.66821700
H	2.32318100	-5.57277000	-2.68285300
H	4.70227100	-4.92882300	-2.48053900

H	5.37199600	-2.95728300	-1.11381100
H	0.55062200	-4.28692200	-1.51452800
H	3.16991100	-1.20219100	3.12280200
H	3.43449100	0.57752500	4.82782400
H	2.63049800	2.88686100	4.32916900
H	1.51276700	3.36698100	2.17638700
C	-1.54096500	-0.01260900	2.83347000
C	-2.40924800	-1.16224900	2.54072100
C	-2.15493900	1.16910900	2.26016800
C	-3.44817900	-0.71783100	1.72732300
C	-3.25781500	0.72754400	1.49079900
C	-4.57433000	-1.51533200	1.16076700
H	-5.48227800	-1.35655300	1.75852600
H	-4.79666200	-1.20814900	0.13615900
H	-4.35157800	-2.58559000	1.16435700
C	-2.15076600	-2.55025200	3.02907800
H	-1.08444400	-2.79157300	2.97881800
H	-2.45967700	-2.64909300	4.07818300
H	-2.70059400	-3.29092000	2.44322100
C	-0.48040300	-0.03835800	3.87813300
H	-0.95970700	-0.04882000	4.86778000
H	0.13595200	-0.93630700	3.80156700
H	0.16383600	0.83702200	3.82521800
C	-1.72986000	2.58410900	2.47886900
H	-2.31418000	3.02071900	3.29996700
H	-0.67593500	2.64517900	2.75028700
H	-1.89379100	3.19726200	1.58895700
C	-4.19587300	1.57001800	0.69274800
H	-4.35866400	1.13343300	-0.29653700
H	-5.16827200	1.62985400	1.19978300
H	-3.81334000	2.58545000	0.56808400
C	1.02579400	1.66162900	0.12319900
C	-0.11355800	1.08100000	-0.28880200
C	-0.64841600	1.29054600	-1.65193200
C	-0.21330300	0.46978200	-2.70834400
C	-1.61894700	2.27157700	-1.91681400
C	-0.74178900	0.62059500	-3.98985600
C	-2.13940700	2.42907300	-3.20064600
H	-1.96335600	2.90613200	-1.10516500
C	-1.70830000	1.59982500	-4.24086600
H	-0.39876100	-0.02434000	-4.79461400
H	-2.88506000	3.19678700	-3.39030100
H	-2.11994700	1.71707500	-5.23941700
H	0.53469500	-0.29339500	-2.51160400
C	1.81812500	2.64687700	-0.71589400
C	4.71435400	-0.77052400	0.54508000
H	5.27897500	-0.70363500	-0.38698500
H	4.55439800	0.22720400	0.94597600
H	5.26922500	-1.37793600	1.26480300
C	-2.98119600	-1.31209000	-2.26659600
O	-2.87617400	-0.53657200	-1.31885500
O	-2.26783400	-2.42455500	-2.37364400
H	-1.71106000	-2.52076000	-1.55021100
C	-3.95823800	-1.11080000	-3.38768500
H	-3.49045200	-1.33826500	-4.34908000
H	-4.79791600	-1.80316700	-3.25051500
H	-4.33007000	-0.08609700	-3.38041100
H	2.82185700	2.25391600	-0.92954800
H	1.32340600	2.86280600	-1.66518000
H	1.95915500	3.59392900	-0.17910500

TS5_Me_Ph

Lowest frequency = -185.09 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.584790 Hartree

E = -1839.502095 Hartree

G = -1838.917305 Hartree

C	0.67479600	4.94431500	-0.67728000
C	1.96530200	5.44102500	-0.89673100
C	3.10430000	4.72637900	-0.50078900
C	2.98690900	3.48778100	0.13757700
C	1.70696200	2.98883400	0.38267400
C	0.56306800	3.71954000	-0.02779600
C	1.19602700	1.72002300	0.86142300
C	-0.25930700	1.77487600	0.85387100
N	-0.59118000	2.99675300	0.31952700
C	-1.95733100	3.43952500	0.11657700
C	-1.15300400	1.15046400	1.86692000
C	-2.18945400	0.34348600	1.36702300
C	-3.19774300	-0.09580300	2.23637600
C	-3.12186600	0.22213800	3.59264900
C	-2.04700100	0.96795000	4.09181200
C	-1.05130900	1.43399400	3.22891300
C	-2.05699600	0.08472400	-0.07016500
C	-0.76351400	0.10920200	-0.57252000

C	-3.26316000	-0.05713000	-0.90759700
N	1.80957100	0.55355100	0.92663800
O	3.10128100	0.54750300	1.02261900
C	-3.25532100	-0.91582700	-2.02394300
C	-4.39307900	-1.07290400	-2.81195000
C	-5.56239700	-0.37164300	-2.50399500
C	-5.58607500	0.48461400	-1.39923600
C	-4.45132000	0.63644400	-0.60521700
H	-0.19757000	5.49808400	-1.00615400
H	2.08103500	6.40159000	-1.38996500
H	4.08982500	5.14110500	-0.68927100
H	3.85923400	2.92482600	0.44625300
H	-2.40154900	2.90816600	-0.73232300
H	-2.54797500	3.23101000	1.01208400
H	-1.96778500	4.51156300	-0.07676700
H	-4.01838200	-0.69698200	1.85985100
H	-3.89730200	-0.12508500	4.26899700
H	-1.99959300	1.21106900	5.14898100
H	-0.24009000	2.05244200	3.60065000
H	3.67608300	-0.22436500	-0.19287600
H	-2.35471600	-1.47363100	-2.25805000
H	-4.36923500	-1.74666700	-3.66373900
H	-6.44951800	-0.49328700	-3.11893500
H	-6.48965300	1.03689800	-1.15702200
H	-4.47538100	1.31135500	0.24380900
Rh	0.81556500	-1.13393400	0.20540500
C	1.81831200	-3.20654900	0.30605600
C	0.47110400	-3.29436300	-0.26601200
C	1.71113000	-2.69294900	1.61104900
C	-0.45869300	-2.92785500	0.73949600
C	0.29725100	-2.44117200	1.87555300
C	-1.93841600	-3.08809200	0.66889200
H	-2.19477700	-4.10926300	0.98294500
H	-2.45413000	-2.39879500	1.33606400
H	-2.31851700	-2.94711500	-0.34443500
C	0.16187200	-3.81051100	-1.63270800
H	0.83799400	-3.37621500	-2.37565600
H	0.28527700	-4.90112000	-1.66800500
H	-0.86536200	-3.57518900	-1.92207000
C	3.06399100	-3.64649200	-0.38622600
H	3.94022200	-3.09451600	-0.03977500
H	3.23507800	-4.71152900	-0.17783200
H	2.98166300	-3.53929800	-1.47069200
C	2.82864500	-2.42536200	2.56343400
H	2.59580000	-1.58178600	3.21786800
H	2.99949100	-3.30472000	3.19875400
H	3.75845400	-2.20332800	2.03403800
C	-0.25308700	-2.05918000	3.20746800
H	-1.27190400	-1.68255100	3.12996300
H	-0.26627400	-2.94211400	3.86177600
H	0.36509600	-1.29804500	3.68932100
C	3.19744400	-0.80426800	-1.97915500
O	4.10522000	-0.53980300	-1.06758700
O	1.97562900	-0.79626500	-1.77155300
C	3.76199800	-1.11510500	-3.33436400
H	4.22972300	-0.21347400	-3.74628300
H	4.53975800	-1.88026000	-3.24488800
H	2.97235600	-1.45718600	-4.00422300
C	-0.49614900	0.52905400	-1.99632300
H	-0.24545200	-0.31247200	-2.64785800
H	-1.35114300	1.06360400	-2.42695200
H	0.37278100	1.19654100	-2.01559900

TS5_Ph_Me

Lowest frequency = -216.76 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.584080 Hartree

E = -1839.505065 Hartree

G = -1838.920985 Hartree

C	-4.92803200	0.68725600	-0.17700500
C	-5.60603000	-0.18055700	-1.04251700
C	-4.94847800	-0.82746200	-2.09745700
C	-3.58330300	-0.62395300	-2.32258800
C	-2.89809400	0.25319000	-1.48117100
C	-3.57595500	0.90369600	-0.41938600
C	-1.49866600	0.57989400	-1.29732800
C	-1.38280600	1.52837700	-0.19152000
N	-2.66386500	1.70766100	0.28504600
C	-2.98418600	2.51925900	1.44205300
C	-0.44953500	2.69135700	-0.17218400
C	0.32740900	2.84624400	0.98675300
C	1.04387400	4.03191300	1.18674300
C	1.03508200	5.01274800	0.19263200
C	0.31628600	4.81829100	-0.99173500
C	-0.43512200	3.65291900	-1.18030100

C	0.23930600	1.69757600	1.88947600
C	-0.08093200	0.49947000	1.29657500
C	0.38784300	1.94341600	3.36531000
N	-0.42827700	-0.05291500	-1.72675000
C	-0.55324500	-0.65535300	2.08956400
O	-0.53293100	-0.82361600	-2.76497700
C	-1.85096500	-1.17153500	1.93848500
C	-2.26435700	-2.28608900	2.66785000
C	-1.39123800	-2.91235400	3.56133000
C	-0.09800700	-2.40672200	3.72258000
C	0.31588200	-1.29297200	2.99377100
H	-5.44386700	1.16443100	0.64886900
H	-6.66577300	-0.35703000	-0.88391700
H	-5.50523500	-1.49590500	-2.74695800
H	-3.06183000	-1.12372800	-3.12960800
H	-2.72493100	1.97991800	2.36173000
H	-2.41779500	3.45223800	1.40510900
H	-4.04935400	2.74975200	1.44107500
H	1.62203700	4.17531700	2.09412100
H	1.59868600	5.92969100	0.33720300
H	0.31185700	5.58906000	-1.75660200
H	-1.03865800	3.52186100	-2.07327600
H	-0.49142900	-2.30813000	-2.24695300
H	-2.53892100	-0.71234800	1.23977800
H	-3.27378300	-2.66660800	2.53515600
H	-1.71434300	-3.78272600	4.12553400
H	0.59215300	-2.88179900	4.41499700
H	1.32665700	-0.91552200	3.10833500
Rh	1.12908600	-0.35242800	-0.38181600
C	2.92798900	-1.46763400	-1.16066400
C	3.13712900	-1.15240600	0.25476700
C	2.80231900	-0.25159600	-1.87011900
C	3.17088300	0.25620200	0.39342400
C	2.88166000	0.83638600	-0.90643400
C	3.47567100	1.02209400	1.63606500
H	4.55602600	1.21350800	1.68778700
H	2.96760700	1.98722400	1.64495300
H	3.18907100	0.46800800	2.53279300
C	3.35294000	-2.18140000	1.31393200
H	2.54766300	-2.92272100	1.30551500
H	4.29604600	-2.71223300	1.13008300
H	3.40114100	-1.73314600	2.30802800
C	2.90751900	-2.84228200	-1.73958200
H	2.27192500	-2.89310300	-2.62737100
H	3.92419300	-3.13139400	-2.03887400
H	2.55691700	-3.57765500	-1.01138500
C	2.59557900	-0.10607300	-3.34005000
H	2.17087300	0.87000900	-3.58576300
H	3.55609900	-0.20083600	-3.86304600
H	1.92040800	-0.87781200	-3.71773000
C	2.96763900	2.28107700	-1.26189800
H	2.75844700	2.91906900	-0.40449000
H	3.98454300	2.50697800	-1.61193900
H	2.27417800	2.53885200	-2.06512500
C	-0.31476400	-3.33394600	-0.62233700
O	-0.63272600	-3.25350800	-1.89677800
O	0.16772100	-2.40697300	0.03703700
C	-0.61084500	-4.66497700	0.00390600
H	-1.69777000	-4.78825600	0.07695000
H	-0.22463700	-5.47330500	-0.62455900
H	-0.17497600	-4.71554800	1.00203500
H	-0.13181500	2.86134000	3.66261800
H	0.01361400	1.10786200	3.95877500
H	1.44917600	2.08075000	3.61359400

IN6_Me_Ph

Lowest frequency = 19.34 cm^{-1}

Charge = 1, Multiplicity = 1

E = -1839.570914 Hartree

TCG = 0.586187 Hartree

G = -1838.984727 Hartree

C	5.46925500	0.69410800	-0.91013400
C	6.25168900	-0.45301900	-0.79493900
C	5.69743400	-1.70577000	-0.47554600
C	4.32845300	-1.83003300	-0.25572200
C	3.52101600	-0.68804500	-0.35875200
C	4.08772700	0.56979100	-0.70297000
C	2.10290700	-0.46884500	-0.18012200
C	1.83411400	1.03810700	-0.29765800
N	3.12528300	1.53934900	-0.80741100
C	3.40799500	2.96058400	-0.83480400
C	1.43293400	1.72494400	1.00335000
C	0.20575700	2.38359100	0.80680100
C	-0.32705200	3.17589000	1.82185300
C	0.39402400	3.31186700	3.01773700

C	1.60806700	2.64854500	3.20606500
C	2.13877700	1.83720800	2.18919700
C	-0.27378600	2.09717600	-0.57129900
C	0.66611400	1.36722900	-1.23300600
C	-1.55831800	2.57571200	-1.11830600
N	1.13511900	-1.31172400	-0.03234700
O	1.51379900	-2.65038200	0.00367700
C	-2.39935200	1.69829700	-1.82642400
C	-3.62380200	2.14160900	-2.32649600
C	-4.02918500	3.46442800	-2.13037800
C	-3.19692700	4.34534600	-1.43535800
C	-1.97245300	3.90563800	-0.93112500
H	5.91601300	1.65207700	-1.15184500
H	7.32381800	-0.37236200	-0.95292500
H	6.34121100	-2.57539100	-0.39128000
H	3.88712200	-2.78282300	0.00508500
H	2.49137300	3.49546100	-1.09409200
H	3.77831200	3.33508900	0.12904400
H	4.15332500	3.16631400	-1.60756500
H	-1.27565800	3.68642400	1.69620800
H	-0.00567700	3.93709100	3.81100700
H	2.14977800	2.76435000	4.14004400
H	3.09022800	1.33030100	2.32265000
H	0.84339900	-3.04768700	-0.64476300
H	-2.09749300	0.66607300	-1.96905800
H	-4.26454400	1.44918700	-2.86601900
H	-4.98475400	3.80683600	-2.51740100
H	-3.49900800	5.37823400	-1.28652700
H	-1.32546200	4.60192600	-0.40744800
Rh	-0.93555800	-1.01953700	0.28949900
C	-1.89478200	-2.69183300	1.18862000
C	-2.94367800	-1.74926100	0.82065400
C	-1.08204900	-2.07180100	2.22442800
C	-2.72079900	-0.55663000	1.55491200
C	-1.56752200	-0.75426200	2.43019200
C	-3.49761800	0.71017300	1.47169500
H	-4.16170300	0.78324300	2.34348900
H	-2.83428700	1.57944200	1.49018100
H	-4.10849000	0.75372000	0.56878900
C	-4.02188400	-2.01172100	-0.17436000
H	-3.65077400	-2.61537900	-1.00631800
H	-4.83783500	-2.56603400	0.30698300
H	-4.43095500	-1.08167600	-0.57512700
C	-1.80366000	-4.10964100	0.74698500
H	-0.78102800	-4.48522600	0.81576300
H	-2.43540400	-4.72113500	1.40645700
H	-2.15663300	-4.23519300	-0.27766300
C	0.05704400	-2.72339000	2.92797300
H	0.68294800	-1.98715300	3.43691000
H	-0.33603500	-3.42182600	3.67819000
H	0.67637300	-3.28808300	2.22707200
C	-1.09031300	0.21087700	3.45615200
H	-1.35397700	1.23362400	3.19217100
H	-1.56686800	-0.02431800	4.41762400
H	-0.00882500	0.15490900	3.59425200
C	-0.85300600	-2.44313800	-2.37788000
O	-0.13802100	-3.34103500	-1.88140800
O	-1.22957000	-1.36199300	-1.78715600
C	-1.38777000	-2.60570300	-3.78740000
H	-0.76534400	-3.29912300	-4.35744700
H	-2.40468600	-3.01416500	-3.73190000
H	-1.44270600	-1.63986200	-4.29655700
C	0.73870800	0.97964100	-2.66880000
H	1.68671100	1.33345200	-3.09467000
H	0.71340900	-0.10812400	-2.79047500
H	-0.08661600	1.40486800	-3.24371800

IN6_Ph_Me

Lowest frequency = 15.53 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.588780 Hartree

E = -1839.570408 Hartree

G = -1838.981628 Hartree

C	-4.95000000	-0.72755800	1.49582100
C	-5.15964200	-0.42515900	2.83971700
C	-4.10889200	-0.03587900	3.68996000
C	-2.80831000	0.05205600	3.20119300
C	-2.57113300	-0.25539500	1.85390600
C	-3.64365000	-0.62616000	0.99670000
C	-1.37166700	-0.26356800	1.04339700
C	-1.73756500	-0.83707800	-0.33044900
N	-3.21091400	-0.81489200	-0.29014100
C	-3.98222100	-1.49636600	-1.31012900
C	-1.19248000	-2.24873500	-0.52155200
C	-0.40338400	-2.26873100	-1.68179000

C	0.13054500	-3.46997800	-2.14529500
C	-0.11958400	-4.63894700	-1.41413200
C	-0.88005400	-4.60391200	-0.24149700
C	-1.43047600	-3.39505100	0.21725400
C	-0.34081000	-0.91003300	-2.25249700
C	-1.15845500	-0.07584600	-1.53722100
C	0.49169300	-0.61282600	-3.46027500
N	-0.18283400	0.16965900	1.29390700
C	-1.58259500	1.29384600	-1.84354400
O	-0.00943400	0.69944800	2.57183200
C	-1.58409300	1.77236300	-3.16946100
C	-1.99922900	3.06968800	-3.46775100
C	-2.44410400	3.92011300	-2.45369500
C	-2.47990400	3.45153900	-1.13763100
C	-2.05877500	2.15918100	-0.83741000
H	-5.77188100	-1.03036200	0.85665700
H	-6.16692600	-0.49837300	3.24083300
H	-4.31227300	0.18703500	4.73241700
H	-1.98553500	0.33599800	3.84376600
H	-3.48194600	-1.36592100	-2.27254700
H	-4.09217500	-2.57042900	-1.10795900
H	-4.97435100	-1.04228100	-1.37739600
H	0.72645000	-3.50389500	-3.05223700
H	0.28608500	-5.58441500	-1.76248500
H	-1.06089600	-5.52015800	0.31272500
H	-2.04211700	-3.36774000	1.11425700
H	0.41980600	1.58449800	2.33727300
H	-1.29002200	1.11840200	-3.98078300
H	-1.98805500	3.40931500	-4.49969600
H	-2.76960600	4.92999100	-2.68622700
H	-2.83241100	4.09610700	-0.33736000
H	-2.08363200	1.83835600	0.19526300
Rh	1.60573500	0.20950100	0.15296300
C	3.15332400	0.23111600	1.61122700
C	3.74725200	0.66857200	0.35592300
C	2.75648300	-1.16346000	1.45487300
C	3.62624000	-0.39525300	-0.57403600
C	3.05178100	-1.54615400	0.12371300
C	4.08254800	-0.39308900	-1.99320600
H	5.11937700	-0.75113600	-2.04727500
H	3.47069200	-1.05679500	-2.60842200
H	4.04951800	0.61175100	-2.42167000
C	4.33574800	2.01402100	0.10830200
H	3.86968700	2.77589400	0.73699200
H	5.40599000	1.98530900	0.35257100
H	4.23560700	2.30951400	-0.93837600
C	3.16587200	1.00369700	2.88360200
H	2.43980000	0.61096200	3.59671800
H	4.16572800	0.92603000	3.33212700
H	2.95024300	2.05941300	2.70663400
C	2.14726900	-2.01167000	2.52034800
H	1.58528700	-2.84322400	2.08881600
H	2.93488200	-2.42415200	3.16368700
H	1.47201400	-1.42307100	3.14638000
C	2.88631400	-2.89736100	-0.46982100
H	2.62780400	-2.84449600	-1.52810700
H	3.84301200	-3.43235200	-0.38861200
H	2.12560700	-3.48222900	0.04874800
C	0.93150900	3.10517000	0.37195000
O	0.83348300	2.98209300	1.61409200
O	1.16033000	2.15654900	-0.46621200
C	0.82974100	4.48571200	-0.24664800
H	0.09706600	5.08917800	0.29515700
H	1.80671300	4.97783200	-0.15828300
H	0.56254900	4.42987400	-1.30347800
H	0.78929000	0.43762600	-3.50396100
H	1.39588400	-1.22949400	-3.45473900
H	-0.05056300	-0.84978700	-4.38544100

IN7_Me_Ph

Lowest frequency = 27.17 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.329010 Hartree

E = -1110.740635 Hartree

G = -1110.411625 Hartree

C	3.98189500	-0.19243000	-1.78534100
C	5.20512900	-0.56372400	-1.22869800
C	5.31221800	-0.98159600	0.10606600
C	4.18212600	-1.00957100	0.92327300
C	2.94459200	-0.61290000	0.39886400
C	2.84243100	-0.24428600	-0.97084800
C	1.59904200	-0.52868100	0.95806200
C	0.66725000	0.00224600	-0.15089900
N	1.54135800	-0.00799900	-1.33215000
C	1.14689600	0.65719700	-2.55630300

C	0.11300800	1.38169400	0.18229600
C	-1.28963200	1.30687900	0.22112100
C	-2.03789500	2.43729800	0.54548000
C	-1.36319700	3.64019600	0.79776600
C	0.03070600	3.71044100	0.73463300
C	0.78505500	2.56658800	0.42879300
C	-1.70026500	-0.08301000	-0.09637300
C	-0.59774800	-0.83754900	-0.32796800
C	-3.10435900	-0.53277300	-0.14020400
N	1.07852900	-0.78185600	2.10690500
C	-0.48692700	-2.27130500	-0.71716900
O	1.98913000	-1.17638000	3.11433900
C	-3.50207000	-1.71225100	0.51128800
C	-4.82877200	-2.14027300	0.46207300
C	-5.78181500	-1.39558900	-0.23645600
C	-5.39921600	-0.21871300	-0.88516400
C	-4.07366900	0.21136800	-0.83532600
H	3.91311900	0.11837800	-2.82201300
H	6.09582100	-0.53269200	-1.85052200
H	6.27512000	-1.28118200	0.50697600
H	4.28125100	-1.35283200	1.94660600
H	0.06464800	0.56262100	-2.67212600
H	1.41130600	1.72378100	-2.56004600
H	1.62519500	0.17080400	-3.41129100
H	-3.12079100	2.39345600	0.60421500
H	-1.93511900	4.53003900	1.04622300
H	0.53503100	4.65276300	0.92854700
H	1.87009300	2.61105100	0.39095600
H	2.81240800	-0.66512800	2.98249700
H	-2.76842500	-2.28217200	1.07308100
H	-5.11873200	-3.05281900	0.97570800
H	-6.81543400	-1.72805400	-0.27311300
H	-6.13369600	0.36490300	-1.43339600
H	-3.78087700	1.11955500	-1.35328200
H	-1.44474500	-2.67716700	-1.05232100
H	0.24840900	-2.38730200	-1.52328200
H	-0.13553200	-2.88350600	0.12479400

IN7_Ph_Me

Lowest frequency = 21.10 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.328236 Hartree

E = -1110.741140 Hartree

G = -1110.412904 Hartree

C	-2.76614100	-1.50388500	-1.76757900
C	-3.89278400	-2.09432100	-1.19699500
C	-4.00482200	-2.28560300	0.18818400
C	-2.96261200	-1.90474500	1.03325700
C	-1.80455100	-1.33700300	0.48482600
C	-1.72888800	-1.09923700	-0.91582200
C	-0.56680200	-0.82510000	1.06696600
C	0.32020300	-0.33017000	-0.09993100
N	-0.58386900	-0.42660600	-1.24910500
C	-0.09124900	-0.26894700	-2.60036100
C	1.55779900	-1.21376200	-0.21093600
C	2.69333500	-0.42452000	0.02899400
C	3.96230700	-1.00274000	0.02668000
C	4.07102400	-2.37515900	-0.23575800
C	2.93519500	-3.15079800	-0.48640900
C	1.65672300	-2.56992300	-0.46911900
C	2.27643300	0.97625000	0.22300800
C	0.92446500	1.06840600	0.09583300
C	3.26945900	2.05197200	0.53054200
N	-0.09651200	-0.73646300	2.26035200
C	0.08974000	2.27543900	0.06971100
O	-0.89930300	-1.30103800	3.27684600
C	-1.22530500	2.27830900	0.57413600
C	-2.01229700	3.42696500	0.51883300
C	-1.51178000	4.60151100	-0.04761300
C	-0.21650000	4.61120300	-0.56977300
C	0.57090100	3.46242900	-0.51864800
H	-2.69961800	-1.35244200	-2.83935800
H	-4.70617100	-2.40822900	-1.84570600
H	-4.90117600	-2.73290600	0.60537600
H	-3.07597500	-2.04252300	2.10257100
H	0.71998300	0.46289200	-2.59344200
H	0.28575100	-1.21050500	-3.02330500
H	-0.88972900	0.11337800	-3.24268000
H	4.84978700	-0.40538900	0.21502600
H	5.05230200	-2.84144700	-0.24868800
H	3.04099600	-4.21166000	-0.69455100
H	0.77104400	-3.17132400	-0.65455400
H	-1.33459000	-2.09355500	2.90408900
H	-1.63489000	1.38360200	1.02725000
H	-3.02133700	3.40256700	0.92126600

H	-2.12764800	5.49538100	-0.09072400
H	0.17933200	5.51148700	-1.03189800
H	1.55789700	3.47372000	-0.96778000
H	3.84604600	2.32919300	-0.36209800
H	2.79111400	2.95411700	0.91846000
H	3.99086500	1.69401300	1.27509100

IN7_Ph_Me_Z

Lowest frequency = 26.82 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.329125 Hartree

E = -1110.744626 Hartree

G = -1110.415501 Hartree

C	-2.78241000	-1.82112400	-1.57993300
C	-3.82294300	-2.51226500	-0.95334100
C	-3.86934000	-2.67860800	0.43890200
C	-2.85137900	-2.15306800	1.23835300
C	-1.80370600	-1.46837200	0.62683500
C	-1.77330100	-1.28153800	-0.77315300
C	-0.61265300	-0.83315600	1.18106300
C	0.23847300	-0.34898400	-0.01467400
N	-0.68631600	-0.51902900	-1.14763400
C	-0.18652900	-0.46171800	-2.50561000
C	1.50996400	-1.18826900	-0.12442900
C	2.62331100	-0.33311200	-0.09881600
C	3.91446100	-0.85440900	-0.17672200
C	4.06634100	-2.24123000	-0.29707800
C	2.95203400	-3.08616100	-0.32992600
C	1.65404200	-2.56164700	-0.23557400
C	2.16015900	1.06245200	0.00851700
C	0.79634600	1.08696900	0.05489500
C	3.11798100	2.20767100	0.08294000
N	-0.37393000	-0.76212700	2.44240600
C	-0.09434700	2.25588300	0.01523400
C	-1.29689400	2.29112400	0.74525300
C	-2.14144000	3.39745200	0.67661100
C	-1.80890500	4.49155400	-0.12564400
C	-0.62531400	4.46572100	-0.86636200
C	0.21971600	3.35904200	-0.80121700
H	-2.76174500	-1.70583000	-2.65828800
H	-4.61456000	-2.93432700	-1.56677500
H	-4.69145400	-3.22286800	0.89317600
H	-2.86195800	-2.28191500	2.31662100
H	0.57265600	0.32164300	-2.56980500
H	0.25728600	-1.41250800	-2.83380900
H	-1.00313400	-0.19914000	-3.18380600
H	4.78316900	-0.20318300	-0.14948000
H	5.06360300	-2.66645300	-0.36634300
H	3.09184000	-4.15881300	-0.42765600
H	0.78772500	-3.21653000	-0.25151100
H	-1.56941600	1.45786300	1.38253100
H	-3.06157100	3.40422700	1.25426800
H	-2.46957800	5.35224100	-0.17860000
H	-0.36322100	5.30353500	-1.50657200
H	1.11763500	3.33439900	-1.40947100
H	3.58205100	2.39401900	-0.89444800
H	2.63089200	3.12877000	0.40985400
H	3.93047100	1.97364600	0.78117100
O	0.79402400	-0.10868800	2.83772400
H	1.14683200	0.40357800	2.07700900

2i

Lowest frequency = 20.71 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.160710 Hartree

E = -615.294883 Hartree

G = -615.134173 Hartree

C	-0.00000600	-1.90136700	0.00002800
C	0.00000000	-0.67949600	0.00004800
C	0.00000000	0.67949600	0.00004800
C	0.00000600	1.90136700	0.00002800
C	-0.00000100	-3.32202100	0.00000700
C	0.00023500	-4.03395400	1.21745600
C	-0.00023600	-4.03392400	-1.21746000
C	0.00023700	-5.42572200	1.21060400
H	0.00042400	-3.48584300	2.15418200
C	-0.00023600	-5.42569100	-1.21064200
H	-0.00042600	-3.48579000	-2.15417300
C	0.00000000	-6.12474700	-0.00002800
H	0.00042800	-5.96714500	2.15210100
H	-0.00042600	-5.96709200	-2.15215200
H	0.00000100	-7.21088300	-0.00004100

C	0.00000100	3.32202100	0.00000700
C	-0.00023500	4.03395400	1.21745600
C	0.00023600	4.03392400	-1.21746000
C	-0.00023700	5.42572200	1.21060400
H	-0.00042400	3.48584300	2.15418200
C	0.00023600	5.42569100	-1.21064200
H	0.00042600	3.48579000	-2.15417300
C	0.00000000	6.12474700	-0.00002800
H	-0.00042800	5.96714500	2.15210100
H	0.00042600	5.96709200	-2.15215200
H	-0.00000100	7.21088300	-0.00004100

IN3_ynyl_Ph

Lowest frequency = 13.33 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.580937 Hartree

E = -1878.202259 Hartree

G = -1877.621322 Hartree

C	-1.14832200	5.51814700	-1.39245000
C	-2.47773100	5.80411100	-1.04400000
C	-3.33713500	4.80551000	-0.57786400
C	-2.81775400	3.51833900	-0.48025500
C	-1.48577500	3.21084500	-0.83445000
C	-0.63595000	4.22310500	-1.29188600
N	-3.44725400	2.34174900	-0.02743500
C	-2.58711200	1.29214500	-0.09294700
C	-1.32763700	1.80329500	-0.54340000
C	-2.92114700	-0.10426900	0.12941900
N	-0.18612300	1.08803400	-0.54600400
O	0.83486400	1.59677700	-1.06114700
C	-4.24806800	-0.56685400	-0.06042500
C	-4.56605800	-1.90536200	0.10929400
C	-3.56366600	-2.81361100	0.46888900
C	-2.24996000	-2.37593600	0.61348800
C	-1.89693900	-1.03324400	0.42610400
Rh	0.05201600	-0.55059600	0.65412200
H	-0.50820600	6.31768700	-1.75318300
H	-2.85045400	6.81931300	-1.14004800
H	-4.36382300	5.03060900	-0.31194100
H	0.38694700	3.99946000	-1.56650100
H	-5.02172000	0.11513400	-0.38857800
H	-5.58539200	-2.24303800	-0.05071300
H	-3.80178500	-3.86452500	0.60848000
H	-1.47743300	-3.09781300	0.85743800
C	1.47757400	0.53448800	2.24388600
C	1.97026000	-0.77031800	2.20714600
C	0.04824400	0.45786500	2.56838500
C	0.86785100	-1.69484000	2.52081200
C	-0.25914300	-0.92617900	2.88394500
C	1.01958900	-3.17821200	2.62503700
H	1.55304700	-3.44832700	3.54681600
H	0.04806800	-3.67870300	2.64073600
H	1.59873000	-3.57519900	1.78501400
C	3.37135900	-1.21781900	1.96267600
H	3.99041600	-0.42034600	1.54902000
H	3.82109500	-1.53841700	2.91280200
H	3.40760400	-2.07419400	1.28366100
C	2.21724700	1.80592200	1.97661000
H	1.62667800	2.48145300	1.35111000
H	2.43277500	2.33117600	2.91665400
H	3.16638200	1.61823100	1.46818700
C	-0.81808200	1.63419100	2.88360600
H	-1.87816100	1.39134400	2.77550400
H	-0.64984600	1.95236500	3.92166500
H	-0.58854400	2.48276300	2.23395700
C	-1.51044400	-1.40223400	3.54427000
H	-1.72382300	-2.44783200	3.31414300
H	-1.38713400	-1.31538700	4.63263400
H	-2.37606200	-0.80098000	3.25773300
C	0.31037000	-1.94811400	-1.53764200
C	1.41292900	-1.43761300	-1.32264300
C	-0.83509500	-2.61008400	-2.06562400
C	-0.95528400	-4.00797100	-1.96299400
C	-1.86291900	-1.86123400	-2.67141900
C	-2.09098600	-4.64364500	-2.45900100
H	-0.16387900	-4.57816100	-1.48718200
C	-2.99296000	-2.50698100	-3.16104700
H	-1.76828300	-0.78259000	-2.73366400
C	-3.11204100	-3.89682500	-3.05307600
H	-2.18227200	-5.72255600	-2.37588800
H	-3.78710400	-1.92588100	-3.62000000
H	-4.00000300	-4.39561500	-3.43019000
C	-4.78154500	2.37338600	0.56759600
H	-4.89469000	3.32528200	1.08901400
H	-5.55701300	2.28765200	-0.19858800

H	-4.87949100	1.56347100	1.28873600
C	2.67707300	-0.94005600	-1.27682100
C	3.81545600	-0.50171000	-1.25049500
C	5.12753300	0.03352000	-1.18620000
C	6.21636600	-0.78806600	-0.82769600
C	5.34775300	1.39929600	-1.46232900
C	7.49749800	-0.24919600	-0.75197600
H	6.04318300	-1.83769000	-0.61298100
C	6.63396000	1.92539700	-1.38234200
H	4.50671300	2.02866800	-1.73541000
C	7.70983600	1.10504500	-1.02880100
H	8.33278400	-0.88615200	-0.47637500
H	6.79818100	2.97738600	-1.59618800
H	8.71161100	1.52012700	-0.96837400

TS3_Ph_ynyl

Lowest frequency = -351.19 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.578447 Hartree

E = -1878.185718 Hartree

G = -1877.607271 Hartree

C	5.01596400	-3.08140400	-0.09918900
C	4.45410800	-4.27438200	-0.58605100
C	3.19594900	-4.29104600	-1.18992000
C	2.52551400	-3.07404800	-1.28996800
C	3.08155300	-1.86240000	-0.81884900
C	4.34298200	-1.86537500	-0.21232400
N	1.24322500	-2.81076500	-1.80045100
C	0.95149900	-1.49030600	-1.66340500
C	2.06270500	-0.86203700	-1.03830600
N	2.09739900	0.45185600	-0.71030800
O	3.20928100	0.92481200	-0.38330100
C	-0.25615900	-0.84468100	-2.13896900
C	-0.83994100	0.20570000	-1.38224500
Rh	0.38113100	1.54574400	-0.16884900
H	5.99607800	-3.10649000	0.36745900
H	5.00775300	-5.20361100	-0.49216000
H	2.76424200	-5.21317100	-1.56266400
H	4.77683100	-0.94579600	0.15855700
C	1.37193500	3.41006800	0.73660400
C	0.09248900	3.28596600	1.33423800
C	1.17144500	3.59004200	-0.69950500
C	-0.90083700	3.39158800	0.28987000
C	-0.22793200	3.63126100	-0.96067600
C	-2.37574800	3.41398600	0.53383900
H	-2.64145200	4.30999400	1.11030700
H	-2.94003600	3.44160000	-0.40079000
H	-2.70231100	2.54483900	1.11417500
C	-0.22324700	3.09568700	2.78215500
H	0.64300500	2.73087200	3.33803000
H	-0.54166600	4.04696500	3.22884200
H	-1.04243600	2.38190800	2.91363400
C	2.69665600	3.50173500	1.41904200
H	3.39778100	2.77024300	1.00838800
H	3.12609700	4.50025900	1.26439700
H	2.60504500	3.33980400	2.49575200
C	2.28369000	3.80127200	-1.66980300
H	1.94529500	3.69136900	-2.70312000
H	2.70051200	4.81017700	-1.55028000
H	3.09112900	3.08573700	-1.48213200
C	-0.87825100	3.91194200	-2.27645400
H	-0.23493300	3.61585800	-3.10950000
H	-1.82914500	3.38343400	-2.37660200
H	-1.08358800	4.98607100	-2.37637400
C	-0.84423700	-1.23633000	-3.36028300
C	-2.00643000	-0.62946400	-3.81643500
C	-2.62324300	0.36044500	-3.03833900
C	-2.05798200	0.75095500	-1.83187900
H	-0.36471600	-1.99742700	-3.96550500
H	-2.43783700	-0.93155800	-4.76546000
H	-3.54433900	0.82694500	-3.37598600
H	-2.56648800	1.48239500	-1.21813400
C	-0.89908800	-0.26908200	0.52063200
C	0.23189100	-0.06987400	1.14011000
C	1.12618700	-0.65129100	2.09426200
C	2.18520700	0.08649200	2.65651500
C	1.00183100	-2.02443500	2.40549700
C	3.08682700	-0.52872000	3.52056000
C	1.91300600	-2.63176400	3.26188200
H	0.20024800	-2.59929800	1.95211700
C	2.95826500	-1.88769000	3.82201400
H	3.89863100	0.05043700	3.95101400
H	1.81515600	-3.68958700	3.48825600
H	3.67149300	-2.36771100	4.48564100
H	2.29057500	1.13263300	2.40418800

C	0.35452400	-3.87200400	-2.26516000
H	0.56333100	-4.12561700	-3.30816700
H	0.51613800	-4.75145200	-1.63928400
H	-0.68085400	-3.54999100	-2.16380300
C	-2.19748300	-0.68043200	0.74823900
C	-3.36143900	-1.02086400	0.88476400
C	-4.71924000	-1.41903000	0.99381800
C	-5.51998400	-1.48472400	-0.16655200
C	-5.28168400	-1.74775400	2.24428300
C	-6.85460400	-1.86721500	-0.07045200
H	-5.08209900	-1.23304800	-1.12751700
C	-6.61601600	-2.13630000	2.32589500
H	-4.66473500	-1.69643600	3.13576500
C	-7.40504000	-2.19517700	1.17279400
H	-7.46658200	-1.91301800	-0.96650800
H	-7.04336800	-2.39126100	3.29121300
H	-8.44613300	-2.49656100	1.24270400

TS3_ynyl_Ph

Lowest frequency = -329.78 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.580897 Hartree

E = -1878.186865 Hartree

G = -1877.605968 Hartree

C	-4.70422300	2.05475700	-1.44063900
C	-4.55310700	3.40079500	-1.06463400
C	-3.29167300	3.95456100	-0.83945000
C	-2.19230500	3.11472900	-1.00398500
C	-2.32470700	1.76117600	-1.39245100
C	-3.59789600	1.22286000	-1.61283900
N	-0.83051400	3.39040600	-0.79562100
C	-0.09264300	2.27019200	-1.01581400
C	-0.98362800	1.22324700	-1.37170700
N	-0.59327800	-0.05399500	-1.60824500
O	-1.44150400	-0.81233800	-2.13060800
C	1.35409900	2.18856200	-0.96494500
C	1.97006900	1.00641200	-0.47536700
Rh	1.05586800	-0.94583600	-0.65180700
H	-5.70082500	1.65540700	-1.60242200
H	-5.43334600	4.02539300	-0.94684800
H	-3.17822900	4.99256900	-0.54724200
H	-3.71440500	0.18713500	-1.90438200
C	0.58981000	-3.14334500	-1.01752000
C	1.40515400	-3.08364000	0.14301300
C	1.37283100	-2.62098200	-2.12969000
C	2.68671000	-2.53435100	-0.23317400
C	2.67641000	-2.28458500	-1.64812000
C	3.85201800	-2.39764700	0.69342300
H	4.20505400	-3.39290600	0.99418100
H	4.68716400	-1.87965200	0.21727400
H	3.58100000	-1.85862500	1.60721900
C	1.03119800	-3.51792300	1.52175500
H	-0.03671200	-3.37989500	1.71008200
H	1.26158600	-4.58315000	1.65734400
H	1.59169900	-2.95971200	2.27620700
C	-0.78196200	-3.72392500	-1.11880800
H	-1.42357900	-3.09461300	-1.73914000
H	-0.73931900	-4.72266600	-1.57384300
H	-1.24369800	-3.82305400	-0.13276700
C	0.88436400	-2.56162200	-3.53670200
H	1.54461800	-1.96461500	-4.17042700
H	0.82638100	-3.57457000	-3.95664000
H	-0.12287400	-2.13256300	-3.56844500
C	3.82749600	-1.79335900	-2.46489100
H	3.48486400	-1.30126300	-3.37901000
H	4.44048100	-1.08161100	-1.90542200
H	4.47490500	-2.63094100	-2.75680900
C	2.15305600	3.25498800	-1.42959400
C	3.53857500	3.16801600	-1.40082600
C	4.15223700	2.02524500	-0.86945200
C	3.37675000	0.97854300	-0.38923000
H	1.68095600	4.13607300	-1.84935100
H	4.13912500	3.98854600	-1.78057500
H	5.23539500	1.95617200	-0.82640900
H	3.86049100	0.12346400	0.06372900
C	1.08429100	0.44529800	1.21183100
C	-0.00201800	-0.23937000	1.03767000
C	1.92041300	0.86139300	2.33003100
C	2.04665500	-0.01272300	3.42678600
C	2.56210600	2.11141100	2.36623000
C	2.80754300	0.35721100	4.53418100
H	1.55014100	-0.97698000	3.39418100
C	3.31121200	2.47803400	3.48118200
H	2.46098600	2.79464600	1.53081700
C	3.44202900	1.60165100	4.56332100

H	2.90675100	-0.32776900	5.37114600
H	3.79536900	3.44981000	3.50610700
H	4.03617400	1.88877800	5.42604300
C	-0.36118000	4.67619900	-0.28836100
H	-0.24161300	5.39544300	-1.10347600
H	-1.09825100	5.05454200	0.42195600
H	0.58882600	4.53991800	0.22613700
C	-1.28159800	-0.58978500	1.35175300
C	-2.45830500	-0.91023200	1.45845100
C	-3.83679500	-1.22595300	1.55265200
C	-4.79562800	-0.18982900	1.57569800
C	-4.26719500	-2.56901700	1.58738300
C	-6.15169900	-0.49805400	1.63034400
H	-4.46384600	0.84234500	1.54108800
C	-5.62654300	-2.86274800	1.64518600
H	-3.52959000	-3.36519100	1.56670400
C	-6.57124600	-1.83163900	1.66605500
H	-6.88356900	0.30437500	1.64347800
H	-5.95093600	-3.89888800	1.67173300
H	-7.63070000	-2.06681900	1.70854200

IN4_Ph_ynyl

Lowest frequency = 14.67 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.582729 Hartree

E = -1878.234782 Hartree

G = -1877.652053 Hartree

C	1.23377600	4.89440000	-3.26055300
C	0.33629900	5.74480800	-2.59564200
C	-0.21169400	5.39192700	-1.36092500
C	0.17846800	4.16804400	-0.82607000
C	1.08150100	3.30000500	-1.47353700
C	1.61662200	3.66799700	-2.71368700
N	-0.21834500	3.56782100	0.38120700
C	0.37216100	2.36185500	0.53749200
C	1.18661600	2.13091800	-0.61627600
C	0.21221000	1.66848700	1.83496000
N	1.89509800	1.01237600	-0.89041600
O	2.65701900	1.05007600	-1.88996800
C	0.71441900	2.33140800	2.96881800
C	0.42680700	1.86679400	4.24874300
C	-0.39580100	0.74865500	4.40798200
C	-0.89079100	0.08390300	3.28737700
C	-0.57405000	0.51189400	1.99087100
Rh	1.74746700	-0.93632800	-0.18114600
H	1.64406000	5.19866800	-4.21878700
H	0.06273700	6.69417500	-3.04560700
H	-0.90652800	6.04577500	-0.84572000
H	2.31382400	3.02051200	-3.22788200
H	1.31407100	3.22685700	2.83592400
H	0.82518700	2.38600700	5.11483400
H	-0.64781300	0.39211800	5.40232300
H	-1.53210700	-0.78399400	3.40711600
C	2.82192300	-1.26346500	1.66264900
C	3.89541600	-1.23162200	0.65875700
C	2.01687100	-2.45058500	1.42738300
C	3.67274100	-2.28065400	-0.23167200
C	2.47066900	-3.01557800	0.21324500
C	4.44273800	-2.62804800	-1.46088800
H	5.00778800	-3.55623000	-1.30223200
H	3.77072600	-2.80081700	-2.30863500
H	5.14883300	-1.83960700	-1.73161000
C	4.97198700	-0.19710900	0.61971900
H	4.57238800	0.79457600	0.85327200
H	5.74282000	-0.42404300	1.36783400
H	5.45283200	-0.15349200	-0.36041700
C	2.80409900	-0.42084700	2.88859200
H	3.54202500	-0.81647300	3.60139900
H	3.07866500	0.61263200	2.66701300
H	1.82794900	-0.43091100	3.37182100
C	0.92992100	-2.96546400	2.31174300
H	1.35281700	-3.65608400	3.05327400
H	0.44014100	-2.15339200	2.85131000
H	0.17229000	-3.50811100	1.74082100
C	1.93142900	-4.22175800	-0.48009500
H	1.88914200	-4.06722400	-1.56303200
H	2.58831500	-5.08276300	-0.29648700
H	0.92959500	-4.47445200	-0.12774800
C	-1.09647900	-0.22941900	0.81037700
C	-0.26491100	-0.78359400	-0.10462600
C	-0.73119600	-1.52669200	-1.28963200
C	-0.47383900	-1.02648700	-2.58244600
C	-1.36304100	-2.77982100	-1.15940000
C	-0.84681600	-1.75873200	-3.71143700
C	-1.73358400	-3.50428900	-2.28955700

H	-1.55813700	-3.17218300	-0.16619200
C	-1.47484600	-2.99789800	-3.56940900
H	-0.65120800	-1.35648200	-4.70155000
H	-2.22464000	-4.46669800	-2.17480600
H	-1.76463400	-3.56643700	-4.44838800
H	0.00421600	-0.05812000	-2.69661400
C	-1.17243000	4.20111800	1.28930000
H	-1.99783300	4.59940700	0.69591100
H	-1.55427800	3.46255200	1.99017200
H	-0.68792800	5.01585200	1.83384500
C	-2.51060600	-0.34573800	0.68395900
C	-3.71600600	-0.45742500	0.54834200
C	-5.11027600	-0.63623500	0.32659200
C	-5.55143500	-1.41717800	-0.76295600
C	-6.06599000	-0.04477500	1.17741300
C	-6.91331300	-1.59623200	-0.99081800
H	-4.81639600	-1.87531600	-1.41786700
C	-7.42594200	-0.23189000	0.94074500
H	-5.73052800	0.55676600	2.01665500
C	-7.85481500	-1.00571200	-0.14191100
H	-7.24164900	-2.19867800	-1.83314600
H	-8.15396400	0.22831200	1.60281800
H	-8.91629200	-1.14780100	-0.32333300

IN4_ynyl_Ph

Lowest frequency = 15.20 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.582264 Hartree

E = -1878.24063 Hartree

G = -1877.658366 Hartree

C	1.41507200	-5.19880700	1.84660600
C	2.78736200	-5.23725400	1.55048600
C	3.48618800	-4.07512500	1.21936600
C	2.76017100	-2.88797600	1.20409300
C	1.38344200	-2.82403400	1.50260800
C	0.69834500	-4.00087500	1.82772800
N	3.20397100	-1.59091300	0.90099000
C	2.18574800	-0.70373000	0.96957200
C	1.00475300	-1.43215300	1.32122900
C	2.51318400	0.73987400	0.86848900
N	-0.25498700	-0.93854500	1.41688700
O	-1.12091100	-1.68747400	1.93244300
C	3.27215700	1.29762100	1.90921100
C	3.78745500	2.58690300	1.79383300
C	3.57390900	3.31665500	0.62182600
C	2.82715700	2.76383000	-0.41833300
C	2.27120100	1.48395200	-0.30258500
Rh	-1.07019000	0.77752400	0.56616200
H	0.90042100	-6.12019200	2.10239400
H	3.31662200	-6.18466900	1.57981400
H	4.54491200	-4.10005900	0.98631600
H	-0.35674900	-3.97738700	2.06523200
H	3.46943500	0.70729400	2.79897400
H	4.36604400	3.01184200	2.60818500
H	3.98670100	4.31567400	0.51770600
H	2.66141400	3.32661600	-1.33173600
C	-0.90540500	2.46445700	1.93324000
C	-2.00706200	1.64706900	2.45884600
C	-1.32479400	3.01051800	0.66335200
C	-3.02491000	1.61906700	1.49499800
C	-2.58037500	2.42288000	0.34995600
C	-4.32541900	0.88847100	1.55683000
H	-5.15435500	1.59787100	1.68170200
H	-4.51308500	0.32837900	0.63455800
H	-4.35020900	0.18728500	2.39467300
C	-1.99078700	0.96044400	3.78520300
H	-0.98186000	0.62747700	4.04394100
H	-2.32330500	1.65098400	4.57150000
H	-2.65172100	0.09073400	3.79408000
C	0.28956500	2.88762200	2.71785400
H	0.01309800	3.71241400	3.38988300
H	0.67454000	2.07226500	3.33503100
H	1.09169600	3.23690400	2.06698400
C	-0.57326700	4.00202100	-0.16354400
H	-0.92368800	5.01794500	0.06200500
H	0.49699400	3.96240000	0.04554700
H	-0.72190500	3.82781900	-1.23270900
C	-3.38749100	2.63851400	-0.88752800
H	-3.90183900	1.72053600	-1.18795200
H	-4.15553700	3.40300700	-0.70818200
H	-2.76371800	2.97543000	-1.71932100
C	1.43296500	0.89720300	-1.38052600
C	0.17956100	0.55316900	-1.02732400
C	2.02021700	0.66746300	-2.71502100
C	1.21351400	0.57995000	-3.86518900

C	3.41209800	0.51454000	-2.85990500
C	1.77870800	0.32800200	-5.11309200
H	0.14192300	0.72914800	-3.78064100
C	3.97480900	0.26227600	-4.11016400
H	4.05163800	0.57956200	-1.98554300
C	3.16163800	0.16637300	-5.24220800
H	1.13924700	0.26977500	-5.98957000
H	5.05057400	0.13868100	-4.19938700
H	3.60089500	-0.02575300	-6.21695300
C	4.59316900	-1.30805000	0.54980900
H	4.90911700	-2.02363000	-0.21227100
H	4.67309500	-0.29849400	0.15491300
H	5.22814300	-1.41191800	1.43383000
C	-0.85944800	-0.18241100	-1.59055000
C	-1.94533700	-0.77275900	-1.63247300
C	-3.18569500	-1.45265100	-1.73134900
C	-3.93841100	-1.42342100	-2.92352500
C	-3.68807700	-2.14228400	-0.60599600
C	-5.16497900	-2.07926400	-2.98462100
H	-3.55206500	-0.88883300	-3.78539200
C	-4.91724300	-2.79037800	-0.68153200
H	-3.10529100	-2.15149500	0.31000900
C	-5.65732400	-2.76225000	-1.86800800
H	-5.74038500	-2.05574200	-3.90533500
H	-5.29997000	-3.31758000	0.18748100
H	-6.61604100	-3.26957000	-1.92174600

IN5_Ph_ynyl

Lowest frequency = 13.14 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.637737 Hartree

E = -2107.282676 Hartree

G = -2106.644939 Hartree

C	2.70642800	-4.80732100	-1.87346900
C	4.05090000	-4.44207400	-1.71744700
C	4.41086200	-3.32528400	-0.95831900
C	3.37681200	-2.60840700	-0.36922900
C	2.01970400	-2.95820800	-0.50599300
C	1.67710500	-4.07627100	-1.27348900
N	3.45526900	-1.44971100	0.42933200
C	2.23195200	-1.02961200	0.79771400
C	1.27152800	-1.92761400	0.20512900
C	2.13363300	0.04470400	1.80581600
N	-0.06285900	-1.82232700	0.24330700
O	-0.70509700	-2.83828400	-0.19219100
C	2.73069600	-0.20327500	3.05532000
C	2.87743000	0.82155700	3.98443300
C	2.45690100	2.11393000	3.65802800
C	1.85836300	2.36071200	2.42399900
C	1.65908600	1.33004800	1.49491100
Rh	-1.36927400	-0.24754900	0.65151400
H	2.45731400	-5.68221300	-2.46618300
H	4.82781800	-5.03431700	-2.19061300
H	5.44899000	-3.03767100	-0.83653500
H	0.64460600	-4.37453200	-1.38901800
H	3.09551500	-1.20052400	3.28163900
H	3.33641700	0.61733500	4.94667400
H	2.59260700	2.92745400	4.36440000
H	1.53997800	3.36547700	2.16392900
C	-1.58220300	0.01374700	2.81362700
C	-2.42522500	-1.15057900	2.51535900
C	-2.18252600	1.17373200	2.18463700
C	-3.43758000	-0.73669400	1.64943000
C	-3.25906000	0.70557800	1.39185100
C	-4.52683100	-1.55982300	1.04902300
H	-5.47091000	-1.37125700	1.57782400
H	-4.68036900	-1.29953500	-0.00145000
H	-4.30845300	-2.62858400	1.11650000
C	-2.17204500	-2.52361900	3.04601000
H	-1.10194400	-2.75273600	3.04625400
H	-2.52425700	-2.59991900	4.08317200
H	-2.68861700	-3.28427300	2.45592500
C	-0.55784300	0.02561600	3.89334000
H	-1.07228200	0.04366500	4.86497900
H	0.06337800	-0.87159700	3.86636900
H	0.08429500	0.90226900	3.83649500
C	-1.76611600	2.59528000	2.37224800
H	-2.35159800	3.04344900	3.18611600
H	-0.71193700	2.66993900	2.63947800
H	-1.93736400	3.18768200	1.47008300
C	-4.17874900	1.51826700	0.54390400
H	-4.30394500	1.05785300	-0.44013300
H	-5.16785700	1.57657900	1.01734900
H	-3.80426200	2.53497600	0.40833300
C	1.04734500	1.61924900	0.17000200

C	-0.09389000	1.03873700	-0.28460300
C	-0.54767600	1.34556900	-1.65927300
C	-0.02840800	0.62115000	-2.74538000
C	-1.49435100	2.35227300	-1.90348400
C	-0.44952800	0.89750200	-4.04584100
C	-1.90761200	2.63411200	-3.20547400
H	-1.89992800	2.91310900	-1.06658000
C	-1.38993800	1.90586300	-4.28136800
H	-0.04109800	0.32894600	-4.87699900
H	-2.63487400	3.42228600	-3.38129500
H	-1.71649100	2.12165000	-5.29471600
H	0.70405800	-0.15983300	-2.56108800
C	4.73460600	-0.81842300	0.75119500
H	5.33304200	-0.77786600	-0.16090700
H	4.56170100	0.19035200	1.11770700
H	5.26001800	-1.40737300	1.50726400
C	-2.69094000	-1.28030800	-2.37530400
O	-2.67480200	-0.56431600	-1.37386100
O	-1.95857100	-2.37664500	-2.49376900
H	-1.48305400	-2.53208200	-1.62949100
C	-3.57471800	-1.00740200	-3.55551600
H	-3.04178000	-1.21014200	-4.48788400
H	-4.43987900	-1.68017400	-3.50794200
H	-3.92066400	0.02613400	-3.53213900
C	1.73717800	2.57356300	-0.63551400
C	2.31029200	3.38386500	-1.34162500
C	2.92211300	4.31422100	-2.22756500
C	4.10672300	4.99006200	-1.87111000
C	2.33972000	4.56864200	-3.48774200
C	4.68979200	5.89599000	-2.75420300
H	4.55789500	4.79690200	-0.90264000
C	2.93187500	5.47541800	-4.36290000
H	1.42752500	4.04838400	-3.76433800
C	4.10681100	6.14210100	-4.00093200
H	5.60235800	6.41183600	-2.46894800
H	2.47523300	5.66329900	-5.33061600
H	4.56508500	6.84910800	-4.68644000

IN5_ynyl_Ph

Lowest frequency = 14.86 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.640624 Hartree

E = -2107.286388 Hartree

G = -2106.645764 Hartree

C	-1.25423100	5.70622000	-0.62941800
C	-2.65412300	5.64341800	-0.55094100
C	-3.30390900	4.47492700	-0.14516300
C	-2.49707000	3.39194000	0.18313200
C	-1.08950100	3.43462000	0.11856400
C	-0.45558200	4.60900000	-0.29771900
N	-2.87953900	2.10717200	0.61655600
C	-1.80205600	1.32001100	0.79013100
C	-0.64278800	2.09179900	0.45788000
C	-1.94746900	0.03975200	1.51067700
N	0.61936400	1.63947900	0.45564500
O	1.51497800	2.54347000	0.49010200
C	-2.32601300	0.12890800	2.86251700
C	-2.67858700	-1.01222500	3.57551000
C	-2.69347600	-2.24995100	2.92554700
C	-2.31766500	-2.33847600	1.58845100
C	-1.90022800	-1.20633600	0.86559300
Rh	1.39718700	-0.27592400	-0.02451500
H	-0.78015400	6.63062100	-0.94498500
H	-3.24535400	6.51666500	-0.80841000
H	-4.38532400	4.41911900	-0.08956300
H	0.62392100	4.66725200	-0.34837600
H	-2.36426700	1.10446900	3.33807600
H	-2.96454800	-0.93240000	4.61964000
H	-2.99603700	-3.14514800	3.46083500
H	-2.33773300	-3.29871500	1.08350400
C	1.76891400	-1.34003100	1.83555800
C	2.94491300	-0.46903400	1.70939300
C	1.81864900	-2.31448400	0.76885200
C	3.62295800	-0.83316000	0.54383900
C	2.87338100	-1.92403300	-0.10233800
C	4.89838100	-0.27031100	0.01360100
H	5.73217500	-0.91107900	0.33240600
H	4.90963400	-0.25407800	-1.07944100
H	5.08934600	0.73874200	0.38321300
C	3.30142500	0.61156100	2.67627300
H	2.40819800	1.13851700	3.02388400

H	3.79469900	0.18291900	3.55877600
H	3.98067000	1.34219500	2.23023400
C	0.90640800	-1.39057100	3.05020400
H	1.45827100	-1.88358200	3.86281000
H	0.64177800	-0.38705700	3.39181700
H	-0.00933800	-1.95254300	2.87318300
C	0.95325700	-3.51984300	0.61757200
H	1.47274700	-4.38785900	1.04528100
H	0.00569800	-3.40345600	1.14294400
H	0.74607400	-3.73824600	-0.43277600
C	3.29374300	-2.60971100	-1.36060800
H	3.63638700	-1.88657400	-2.10612600
H	4.12504600	-3.29833400	-1.15781900
H	2.47219700	-3.18403000	-1.79432300
C	-1.49379000	-1.36607700	-0.55005000
C	-0.27885700	-0.96810800	-1.02223800
C	-2.49527600	-2.06837600	-1.40496900
C	-2.14905700	-3.17554600	-2.19675600
C	-3.83319700	-1.63675000	-1.40508900
C	-3.10656200	-3.81565300	-2.98435000
H	-1.12803200	-3.54064600	-2.18426500
C	-4.78872800	-2.27070800	-2.19874600
H	-4.11867700	-0.79069900	-0.78655400
C	-4.42839100	-3.36218500	-2.99398500
H	-2.82070700	-4.67502500	-3.58492800
H	-5.81494800	-1.91341100	-2.19513400
H	-5.17268300	-3.85964500	-3.60953800
C	-4.27461600	1.74803700	0.85712500
H	-4.85721600	2.01194000	-0.02832100
H	-4.34818400	0.67892900	1.03927900
H	-4.65232300	2.30080500	1.72145800
C	3.01867700	1.57690200	-2.16484800
O	2.08055200	0.78608800	-2.01051000
O	3.47404900	2.36222700	-1.20579200
H	2.85249300	2.29170800	-0.41824800
C	3.75590000	1.69961300	-3.46405000
H	4.02607100	2.74037100	-3.65939400
H	4.68251300	1.11609800	-3.39255300
H	3.15169900	1.29793300	-4.27788900
C	0.08111700	-1.18831500	-2.36468300
C	0.48603700	-1.36895100	-3.50270400
C	0.96168800	-1.58594100	-4.82264700
C	2.33042900	-1.41617600	-5.12329700
C	0.07798900	-1.97522600	-5.85132100
C	2.79541600	-1.62533900	-6.41910600
H	3.01120600	-1.12065000	-4.33219000
C	0.55368600	-2.18076500	-7.14403700
H	-0.97415800	-2.11223000	-5.62059500
C	1.91075100	-2.00588700	-7.43332700
H	3.85070500	-1.49051600	-6.63940900
H	-0.13566200	-2.47842200	-7.92913700
H	2.27682300	-2.16578800	-8.44340600

TS5_Ph_ynyl

Lowest frequency = -220.16 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.638375 Hartree

E = -2107.263919 Hartree

G = -2106.625544 Hartree

C	1.72700600	4.89101700	-0.11954600
C	2.96082500	5.25085000	-0.67464600
C	4.03175300	4.34822200	-0.73153800
C	3.90237200	3.05045200	-0.22771200
C	2.68580900	2.68349100	0.34925400
C	1.60993500	3.60589600	0.39952600
C	2.13511000	1.42691000	0.81385400
C	0.76079900	1.65714800	1.25685600
N	0.50169600	2.98725200	1.00033400
C	-0.78229200	3.61451300	1.24777500
C	0.15249700	1.05227800	2.47967000
C	-1.10172300	0.44624700	2.32168500
C	-1.84574500	0.06634500	3.44200200
C	-1.29280700	0.23590500	4.71268700
C	-0.01199300	0.77959600	4.86338900
C	0.71913600	1.19439300	3.74488700
C	-1.48393200	0.31853700	0.91198700
C	-0.44075600	0.29686200	-0.00725200
N	2.55262100	0.20086300	0.57925500
C	-0.71195500	0.58130400	-1.43325400
O	3.79388900	0.02024600	0.25592000
C	-0.11224700	1.66673700	-2.09142800
C	-0.35781500	1.90370200	-3.44393500
C	-1.19795000	1.05643300	-4.17042500
C	-1.79565900	-0.03189600	-3.52717400
C	-1.55656400	-0.26620800	-2.17404000

H	0.90011700	5.59208400	-0.09934200
H	3.08405100	6.25323500	-1.07373700
H	4.97334200	4.66069700	-1.17243200
H	4.72000600	2.34168500	-0.27160400
H	-1.51810400	3.25984800	0.51627400
H	-1.13029000	3.36318700	2.25264600
H	-0.67888900	4.69575100	1.16555700
H	-2.83194600	-0.36978100	3.31707300
H	-1.85838100	-0.06378500	5.58982000
H	0.40703100	0.91127800	5.85632900
H	1.69023100	1.66550900	3.86157400
H	3.81647500	-0.48563300	-1.22925200
H	0.55815000	2.32480300	-1.55308900
H	0.11415400	2.75289300	-3.93097100
H	-1.38357100	1.23978200	-5.22498100
H	-2.44706900	-0.70350000	-4.08038000
H	-2.01128200	-1.12171600	-1.68709000
Rh	1.13741700	-1.25270200	0.10378600
C	1.83144900	-3.37129500	-0.26495000
C	0.37501300	-3.30649800	-0.39291200
C	2.17811100	-3.00144300	1.05519400
C	-0.16167500	-2.95125500	0.87019500
C	0.94890700	-2.66556300	1.75952300
C	-1.60689200	-2.92081600	1.23535300
H	-1.91973200	-3.93372500	1.52315600
H	-1.79543900	-2.26308500	2.08391000
H	-2.23242100	-2.60322400	0.39844400
C	-0.37709700	-3.66323700	-1.63186800
H	0.02884900	-3.13614400	-2.50090900
H	-0.29186200	-4.74038800	-1.82617200
H	-1.43663400	-3.41574900	-1.54138100
C	2.76482000	-3.80507500	-1.34397500
H	3.74489000	-3.33233800	-1.24465000
H	2.91046700	-4.89230000	-1.28421800
H	2.36161900	-3.58237700	-2.33485400
C	3.55552900	-2.94620200	1.62489700
H	3.60338900	-2.26871200	2.48041600
H	3.85645300	-3.94536900	1.96650300
H	4.27842000	-2.60770200	0.87878600
C	0.85942000	-2.37811000	3.21982500
H	-0.07857400	-1.88797900	3.47767200
H	0.91361700	-3.32193600	3.77984100
H	1.68488200	-1.74495200	3.55245200
C	2.64803100	-0.73759800	-2.74870400
O	3.85407100	-0.61413600	-2.24008900
O	1.60983100	-0.80474800	-2.07910900
C	2.61048700	-0.78639800	-4.24718000
H	3.03208600	0.13954300	-4.65297200
H	3.22950700	-1.61720300	-4.60296100
H	1.58385700	-0.90890700	-4.59326200
C	-2.84544900	0.34378100	0.55512200
C	-4.02437600	0.32559600	0.24288000
C	-5.37044500	0.29526000	-0.20339700
C	-5.64496900	0.25382600	-1.58765100
C	-6.43990900	0.30327500	0.71599100
C	-6.96209500	0.22193200	-2.03490000
H	-4.81840100	0.25100200	-2.29150300
C	-7.75299900	0.26670900	0.25589300
H	-6.22649900	0.33593000	1.77974300
C	-8.01768500	0.22686800	-1.11692500
H	-7.16773400	0.19224400	-3.10091800
H	-8.57293200	0.27101000	0.96808600
H	-9.04420300	0.20043200	-1.47063300

TS5_ynyl_Ph

Lowest frequency = -197.27 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.639992 Hartree

E = -2107.270839 Hartree

G = -2106.630847 Hartree

C	3.34342800	1.70604500	2.73416600
C	4.40240500	0.84486500	3.04709900
C	4.22088200	-0.54209000	3.12829700
C	2.96583200	-1.11427700	2.89517400
C	1.89705800	-0.26772000	2.59730600
C	2.09378200	1.13378400	2.52300300
C	0.54775000	-0.48946800	2.11466700
C	-0.08484700	0.81241600	1.89631900
N	0.87725300	1.75180800	2.19016500
C	0.68482800	3.17868300	2.02104800
C	-1.52137700	1.14986700	2.10676300
C	-2.17639600	1.78292800	1.02948400
C	-3.46266100	2.30893800	1.21840900
C	-4.09300200	2.15355800	2.45284900
C	-3.45819000	1.46957400	3.49625400

C	-2.16786300	0.95775200	3.32551400
C	-1.37352300	1.79494900	-0.19197900
C	-0.41645500	0.77674400	-0.24600500
C	-1.48142900	2.85903100	-1.19191800
N	0.07850300	-1.56250300	1.51046900
O	0.64494400	-2.70463300	1.75586000
C	-1.18084200	2.58432500	-2.54230600
C	-1.27663000	3.58175100	-3.50753300
C	-1.66849500	4.87436500	-3.14428700
C	-1.96647900	5.16192200	-1.80900100
C	-1.87991700	4.16462600	-0.84082200
H	3.50232900	2.77538600	2.65037800
H	5.38713200	1.26722200	3.22360000
H	5.06485100	-1.18059600	3.37047500
H	2.81447400	-2.18526100	2.94396300
H	0.75024800	3.44420700	0.95922900
H	-0.29909800	3.46318000	2.39994900
H	1.45061100	3.71679300	2.57958100
H	-3.97367900	2.80642300	0.40153500
H	-5.09216600	2.55273800	2.59851800
H	-3.95854200	1.35548700	4.45300400
H	-1.65545100	0.46290700	4.14458400
H	1.42203400	-3.11587600	0.45892000
H	-0.89393300	1.57771800	-2.82757600
H	-1.05212000	3.35117200	-4.54485000
H	-1.74258300	5.65276400	-3.89822900
H	-2.26173800	6.16667400	-1.52099300
H	-2.09106000	4.40084100	0.19641500
Rh	-1.01093300	-1.32306200	-0.25031700
C	-1.87292900	-3.15770500	-1.25895700
C	-2.22871100	-1.95860400	-2.02145900
C	-2.43680700	-3.04535800	0.03123400
C	-3.06358000	-1.15241500	-1.20861000
C	-3.12688800	-1.76559600	0.10485700
C	-3.79347700	0.07264300	-1.64230100
H	-4.73410500	-0.22844900	-2.12328200
H	-4.04494400	0.71384800	-0.79780000
H	-3.22090700	0.65457700	-2.36745300
C	-1.83945500	-1.70873800	-3.44036900
H	-0.77751200	-1.92251600	-3.59524100
H	-2.41321600	-2.36058700	-4.11232900
H	-2.02949900	-0.67168200	-3.72750300
C	-1.08509000	-4.31106800	-1.78130900
H	-0.50511600	-4.79177600	-0.98912200
H	-1.77084000	-5.06306800	-2.19503000
H	-0.40806100	-4.00655000	-2.58241000
C	-2.31871400	-4.04428400	1.13336000
H	-2.55285100	-3.59484400	2.10117000
H	-3.01765100	-4.87375900	0.96507700
H	-1.30631300	-4.45378900	1.18285600
C	-3.98406900	-1.32402700	1.24118600
H	-4.16262000	-0.24996900	1.21449200
H	-4.95716700	-1.83107400	1.18215500
H	-3.53279000	-1.57789000	2.20289500
C	1.82938800	-2.60304200	-1.36781400
O	2.06824100	-3.33197700	-0.29976600
O	0.89817100	-1.79572200	-1.47232600
C	2.79301800	-2.83797600	-2.49487700
H	3.82100000	-2.73659000	-2.13459900
H	2.66717600	-3.86154200	-2.86674100
H	2.60732000	-2.12909500	-3.30230200
C	0.84316200	0.93985000	-0.83772100
C	2.03624900	1.01445100	-1.09221800
C	3.43873000	0.97365200	-1.30718300
C	4.08530300	1.86268300	-2.18866100
C	4.20832600	0.02440100	-0.59878800
C	5.46588800	1.79436400	-2.36169200
H	3.49667800	2.59715900	-2.72967800
C	5.58814100	-0.02930000	-0.77385100
H	3.71271300	-0.65234900	0.08901900
C	6.22103100	0.85193600	-1.65662100
H	5.95555700	2.48115800	-3.04618300
H	6.17075600	-0.75873300	-0.21839700
H	7.29768200	0.80641200	-1.79265900

IN6_Ph_ynyl

Lowest frequency = 13.87 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.641343 Hartree

E = -2107.329159 Hartree

G = -2106.687816 Hartree

C	-4.92434700	-0.75678300	1.63413600
C	-5.05770400	-0.47818600	2.99278400
C	-3.96054700	-0.10305200	3.78935700
C	-2.68953800	-0.00582600	3.23060100

C	-2.52873400	-0.29099200	1.86692100
C	-3.64806700	-0.64663100	1.06507800
C	-1.37493900	-0.29279900	0.99342100
C	-1.82182200	-0.83260700	-0.37153200
N	-3.28914800	-0.81139200	-0.24843500
C	-4.11926800	-1.47483600	-1.23480900
C	-1.28776100	-2.23598600	-0.64030400
C	-0.53588000	-2.21807200	-1.82122900
C	-0.00681100	-3.39262300	-2.34791200
C	-0.23923000	-4.58928200	-1.65815400
C	-0.97063400	-4.60090000	-0.46592400
C	-1.50633600	-3.41287200	0.05753100
C	-0.49631800	-0.83238700	-2.33668900
C	-1.29325400	-0.01437700	-1.56256300
N	-0.17154300	0.13169900	1.18027900
C	-1.67519500	1.37445900	-1.78858900
O	0.06654200	0.67158800	2.44480400
C	-1.51589800	1.97409200	-3.05605700
C	-1.88816100	3.29695400	-3.27689800
C	-2.43908700	4.05895100	-2.24270300
C	-2.61971300	3.47639100	-0.98610000
C	-2.24854000	2.15341500	-0.76186300
H	-5.78108500	-1.04727500	1.03635200
H	-6.04086700	-0.55821600	3.44855400
H	-4.10558600	0.10313100	4.84490200
H	-1.83213500	0.26928900	3.83034900
H	-3.66974000	-1.33735700	-2.22093000
H	-4.22750700	-2.54999000	-1.03876800
H	-5.10930600	-1.01158000	-1.24395800
H	0.56672700	-3.37978600	-3.26993000
H	0.15950700	-5.51951100	-2.05207200
H	-1.13707600	-5.53872100	0.05558000
H	-2.09113800	-3.42137400	0.97249900
H	0.48124800	1.55604900	2.17683500
H	-1.11637600	1.39412700	-3.87819000
H	-1.75672200	3.73042100	-4.26438700
H	-2.72895500	5.09129000	-2.41565200
H	-3.05114500	4.05316000	-0.17306800
H	-2.39449400	1.74058000	0.22707400
Rh	1.58759500	0.11721500	-0.00511600
C	3.22220900	0.21597300	1.34619900
C	3.75735500	0.48727400	0.01794300
C	2.76067800	-1.16715200	1.36657100
C	3.53330800	-0.66420700	-0.77692700
C	2.93526100	-1.69983700	0.06727900
C	3.86922000	-0.84165200	-2.21730300
H	4.79763800	-1.42115900	-2.30839900
H	3.08263600	-1.39116300	-2.73980700
H	4.01502800	0.11769000	-2.71734200
C	4.38328900	1.77010900	-0.40947200
H	3.96097900	2.61858900	0.13372700
H	5.45945200	1.73526500	-0.19486800
H	4.25577600	1.94111700	-1.48077900
C	3.34059400	1.11420200	2.52720400
H	2.63483600	0.83621000	3.31177100
H	4.35719300	1.02807700	2.93476700
H	3.16768100	2.15632200	2.25185700
C	2.19808400	-1.86932700	2.55475000
H	1.62010500	-2.74774000	2.25866400
H	3.01741000	-2.19920100	3.20639500
H	1.55343900	-1.20141200	3.13109400
C	2.65815000	-3.09726100	-0.35914800
H	2.48765000	-3.16295900	-1.43350700
H	3.53135300	-3.71955600	-0.11896900
H	1.79362600	-3.51688600	0.15879600
C	0.94852500	3.02921900	0.16820000
O	0.85124600	2.93522800	1.41279100
O	1.16706000	2.06090000	-0.65008400
C	0.86418100	4.39671500	-0.48125600
H	0.16403700	5.03351000	0.06481100
H	1.85659600	4.86314600	-0.43528200
H	0.56576600	4.32070500	-1.52833700
C	0.31916200	-0.48630900	-3.43230400
C	1.10987200	-0.24731200	-4.32727100
C	2.04892200	0.08807900	-5.33901000
C	2.87995900	-0.90413300	-5.89843700
C	2.17803000	1.42476800	-5.76991500
C	3.81808600	-0.56122800	-6.86820500
H	2.78069300	-1.93192600	-5.56385400
C	3.11922200	1.75498800	-6.74106700
H	1.54004100	2.18758600	-5.33449400
C	3.94050500	0.76589600	-7.29160900
H	4.45625700	-1.32985500	-7.29420100
H	3.21435600	2.78613500	-7.06846500
H	4.67458100	1.02878800	-8.04760500

IN6_ynyl_Ph

Lowest frequency = 9.19 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.641410 Hartree

E = -2107.331613 Hartree

G = -2106.690203 Hartree

C	-2.89728900	4.49449400	0.86171800
C	-3.43347200	5.10004500	-0.27309200
C	-3.08091500	4.69422700	-1.57281500
C	-2.16414500	3.66347700	-1.76001000
C	-1.60530300	3.04407000	-0.63295600
C	-1.98633300	3.44509600	0.67635100
C	-0.64857400	1.97218500	-0.47475700
C	-0.34898600	1.81729500	1.02176200
N	-1.37827200	2.67467900	1.63327700
C	-1.31656700	3.03006700	3.03728100
C	1.05796500	2.20054100	1.46157900
C	1.65093400	1.11112100	2.12886600
C	2.91844500	1.25319800	2.69605100
C	3.55961200	2.49632100	2.60681400
C	2.96160900	3.57002400	1.94309700
C	1.69488000	3.42480400	1.35482900
C	0.72103800	-0.03955800	2.09385900
C	-0.44810100	0.35629700	1.48619400
C	0.99910100	-1.37693000	2.63646500
N	-0.15334800	1.15150500	-1.33923700
O	-0.56330400	1.35813900	-2.65220600
C	0.60524600	-2.52455800	1.92216700
C	0.88700900	-3.79525500	2.42040600
C	1.55577100	-3.94437300	3.63898200
C	1.93604800	-2.81126300	4.36184100
C	1.66372800	-1.53662700	3.86522400
H	-3.17819400	4.82357200	1.85590500
H	-4.14269300	5.91345800	-0.14571300
H	-3.51895700	5.19255300	-2.43162000
H	-1.87046100	3.34735800	-2.75215100
H	-0.93162900	2.17782400	3.60183200
H	-0.67209400	3.89987600	3.22261300
H	-2.32489600	3.24925600	3.39841600
H	3.40687700	0.42609100	3.19801300
H	4.54144300	2.62041700	3.05405800
H	3.47668500	4.52387400	1.88216100
H	1.21938700	4.25717400	0.84450400
H	-0.87286700	0.41957300	-2.89446200
H	0.10588000	-2.41644800	0.96563100
H	0.58814100	-4.67165800	1.85180100
H	1.77613500	-4.93608500	4.02362500
H	2.44429700	-2.91776300	5.31590900
H	1.94092100	-0.66459100	4.44728300
Rh	1.21523200	-0.44900600	-1.12342100
C	2.18107200	-1.04694800	-2.91939500
C	2.60218800	-1.98214000	-1.88593400
C	2.71547900	0.26287700	-2.57939900
C	3.30443500	-1.23855900	-0.90132400
C	3.37430000	0.15646800	-1.32493900
C	3.86456700	-1.75494500	0.37693700
H	4.95380100	-1.85599800	0.27833400
H	3.67230200	-1.06021800	1.19871700
H	3.44952800	-2.72980700	0.63749600
C	2.30362300	-3.44282100	-1.88283300
H	1.27120500	-3.62952300	-2.19040800
H	2.96645200	-3.95687100	-2.59032100
H	2.45335500	-3.87960400	-0.89306800
C	1.50093300	-1.40267400	-4.19423800
H	0.91791800	-0.56508600	-4.58218900
H	2.26567600	-1.66001900	-4.94032200
H	0.84263400	-2.26448000	-4.07084800
C	2.57806800	1.48383500	-3.41856800
H	2.82139900	2.38556400	-2.85292800
H	3.26643600	1.41186200	-4.27072100
H	1.56110600	1.57523900	-3.80719100
C	4.12719000	1.23861200	-0.63262800
H	4.20059000	1.05296400	0.43796100
H	5.14713300	1.28625400	-1.03759400
H	3.65967200	2.21388300	-0.78422400
C	-1.32542900	-1.85576900	-1.98560500
O	-1.50243700	-1.03446400	-2.91292400
O	-0.39260400	-1.81061800	-1.10071700
C	-2.23619500	-3.06463700	-1.89023400
H	-3.26306400	-2.78596700	-2.13975200
H	-1.89854700	-3.80809500	-2.62359100
H	-2.20188100	-3.51458500	-0.89693100
C	-1.64619800	-0.34451000	1.31617500
C	-2.71730600	-0.88294500	1.10233700
C	-3.93282800	-1.55201600	0.80780700
C	-4.87531000	-0.95861900	-0.05742000
C	-4.19185000	-2.83142400	1.34144900

C	-6.04708400	-1.63691600	-0.38170000
H	-4.67131100	0.02469000	-0.46977700
C	-5.36773900	-3.49899600	1.01083300
H	-3.46301500	-3.28726600	2.00430700
C	-6.29668800	-2.90659700	0.14933900
H	-6.76721100	-1.17549100	-1.05114400
H	-5.56010400	-4.48488000	1.42403100
H	-7.21186700	-3.43229900	-0.10702400

IN7_Ph_ynyl

Lowest frequency = 17.39 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.383096 Hartree

E = -1378.498505 Hartree

G = -1378.115409 Hartree

C	4.79524700	-0.43503500	-1.43381300
C	5.96166700	-0.68271200	-0.71128900
C	5.97861600	-0.66905100	0.69135300
C	4.81539300	-0.37580000	1.40229700
C	3.63643300	-0.08829900	0.70104800
C	3.62101200	-0.16433500	-0.71899200
C	2.27635400	0.23535200	1.12291200
C	1.43984100	0.45004800	-0.16148800
N	2.35490000	0.00828000	-1.21713600
C	2.05586800	0.25820400	-2.61171700
C	1.04767900	1.91967300	-0.26973300
C	-0.34721300	2.02479400	-0.22139800
C	-0.97084000	3.26919300	-0.26334900
C	-0.16504400	4.40913700	-0.37146000
C	1.22834400	4.30010200	-0.43353500
C	1.85046400	3.04360000	-0.37785400
C	-0.92096900	0.66477700	-0.15271000
C	0.08362900	-0.27243300	-0.16984900
N	1.69197200	0.39856800	2.25585600
C	-0.02475600	-1.72735100	-0.21943600
O	2.52882100	0.31189500	3.39051600
C	1.05399300	-2.55246400	0.16159700
C	0.95086000	-3.94014200	0.10568300
C	-0.22553600	-4.54510600	-0.34134500
C	-1.29807500	-3.74314600	-0.74067300
C	-1.19979100	-2.35620200	-0.68514200
H	4.79574400	-0.46277700	-2.51786600
H	6.87851000	-0.89858900	-1.25317800
H	6.89767900	-0.88444300	1.22662800
H	4.84139000	-0.39152800	2.48565300
H	0.97677300	0.17202000	-2.75960700
H	2.37963700	1.25581100	-2.93888900
H	2.54640900	-0.49610800	-3.23321600
H	-2.05317200	3.35044200	-0.22038600
H	-0.62877100	5.39067100	-0.41150700
H	1.83553000	5.19608600	-0.52381100
H	2.93246600	2.95665100	-0.41776400
H	3.39441500	0.69799800	3.14901000
H	1.97681500	-2.11557700	0.52047600
H	1.79593000	-4.54979300	0.41308000
H	-0.30330000	-5.62766400	-0.38575500
H	-2.21359800	-4.19901400	-1.10750000
H	-2.03115000	-1.75262400	-1.02672500
C	-2.31310000	0.46034800	-0.06252700
C	-3.52352800	0.35702100	0.02561500
C	-4.92837100	0.16158400	0.12310300
C	-5.81197100	1.25861100	0.07564100
C	-5.45057500	-1.14076900	0.26556700
C	-7.18562100	1.05231200	0.16738900
H	-5.41006200	2.26107300	-0.03352100
C	-6.82576600	-1.33462600	0.35638800
H	-4.76910500	-1.98487500	0.30518300
C	-7.69619500	-0.24152000	0.30757200
H	-7.86013900	1.90281700	0.12993700
H	-7.22027200	-2.34065200	0.46606400
H	-8.76867300	-0.39761800	0.37938900

IN7_ynyl_Ph

Lowest frequency = 19.22 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.383672 Hartree

E = -1378.502132 Hartree

G = -1378.118460 Hartree

C	-2.36491000	-2.49149500	-1.67532300
C	-3.53792000	-2.88575100	-1.02753100
C	-3.60301000	-3.01412300	0.36643000
C	-2.47272800	-2.75846700	1.14629900

C	-1.28095400	-2.38300800	0.51751300
C	-1.23242400	-2.24183900	-0.89384300
C	0.03659000	-1.99826600	1.02113000
C	0.79013600	-1.35712800	-0.15783500
N	0.02073300	-1.84386600	-1.31617900
C	0.24007000	-1.25070000	-2.62273900
C	2.27346000	-1.64135900	-0.22073900
C	2.99162100	-0.43612200	-0.10440700
C	4.38723100	-0.45842400	-0.07163900
C	5.04150600	-1.69004500	-0.19406300
C	4.31948600	-2.87862500	-0.33619900
C	2.91699800	-2.86049700	-0.34215700
C	2.03707700	0.68590100	0.00063300
C	0.76459500	0.18455600	-0.03511200
C	2.39995800	2.10598000	0.10347200
N	0.62876300	-2.09983000	2.15631100
O	-0.10310400	-2.72435700	3.18086400
C	1.68711600	2.96616700	0.95782400
C	2.01198300	4.31888700	1.03442900
C	3.05186300	4.83800100	0.25866700
C	3.76575000	3.99357600	-0.59478700
C	3.44677300	2.63854100	-0.67043800
H	-2.34112800	-2.36698900	-2.75224000
H	-4.42615900	-3.07910400	-1.62271500
H	-4.53532800	-3.29661000	0.84448300
H	-2.55024300	-2.80668000	2.22717700
H	1.31130200	-1.08603900	-2.75787600
H	-0.09817600	-1.94403700	-3.39762000
H	-0.28862300	-0.29517300	-2.74522400
H	4.96003300	0.45419000	0.05260900
H	6.12725800	-1.72020000	-0.17561100
H	4.84678000	-3.82296900	-0.43464600
H	2.34809700	-3.78110300	-0.43493400
H	-0.74559500	-3.33723800	2.76746400
H	0.88924800	2.56529900	1.57390700
H	1.45570800	4.96765700	1.70524100
H	3.30415700	5.89287000	0.31951400
H	4.57084200	4.39038200	-1.20684000
H	3.99065100	1.99510700	-1.35397700
C	-0.46526700	0.85494300	-0.02666300
C	-1.59520900	1.31282800	-0.04111500
C	-2.92196600	1.81803700	-0.04887700
C	-4.01160900	0.92251100	-0.09040400
C	-3.16844700	3.20566200	-0.01411400
C	-5.31447200	1.41136900	-0.09647200
H	-3.82166100	-0.14549700	-0.11622700
C	-4.47661700	3.68162100	-0.02111900
H	-2.32930300	3.89367300	0.01784900
C	-5.55198800	2.78897200	-0.06224700
H	-6.14805100	0.71545500	-0.12784900
H	-4.65875800	4.75213800	0.00574400
H	-6.57083000	3.16537200	-0.06751400

IN4_Me_ynyl

Lowest frequency = 10.35 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.482837 Hartree

E = -1494.950086 Hartree

G = -1494.467249 Hartree

C	1.22294800	4.91499000	-3.25435100
C	0.35452000	5.77860400	-2.56846100
C	-0.18843200	5.42304000	-1.33220400
C	0.17612500	4.18254000	-0.81793900
C	1.04765600	3.29980500	-1.48783900
C	1.57888900	3.67130400	-2.72866000
N	-0.21905600	3.57919400	0.38853900
C	0.34933300	2.35990800	0.52703000
C	1.14061500	2.12182800	-0.64101300
C	0.18532700	1.64834100	1.81169300
N	1.83084000	0.99593700	-0.92512300
O	2.54751500	1.01205400	-1.95853900
C	0.66156400	2.30891600	2.95957500
C	0.37123500	1.82508600	4.23088200
C	-0.42845000	0.68708500	4.36749600
C	-0.89369400	0.02421700	3.23369200
C	-0.57324000	0.46964000	1.94272700
Rh	1.76253200	-0.95246700	-0.18949900
H	1.63073000	5.22161800	-4.21293100
H	0.10019900	6.74057000	-3.00272000
H	-0.85937400	6.08811900	-0.80000500
H	2.25232000	3.01269200	-3.25996800
H	1.24461700	3.21750700	2.84299000
H	0.74876100	2.34319500	5.10694200
H	-0.68478900	0.31374200	5.35463700
H	-1.51862300	-0.85751500	3.33772400

C	2.83562600	-1.25197800	1.65585300
C	3.92762600	-1.21173700	0.67179000
C	2.05018600	-2.45182000	1.41510400
C	3.72943100	-2.26204700	-0.21964500
C	2.52544900	-3.00889100	0.20577900
C	4.51843300	-2.60137400	-1.43909800
H	5.06644000	-3.54033900	-1.28555800
H	3.86011300	-2.75040000	-2.30226800
H	5.24057100	-1.81904400	-1.68401700
C	4.98875000	-0.16050100	0.64957500
H	4.56107900	0.83248700	0.82172600
H	5.72170900	-0.34231600	1.44645700
H	5.52133800	-0.14553500	-0.30433600
C	2.79570200	-0.40945300	2.88145100
H	3.53143900	-0.79690300	3.60109600
H	3.06113000	0.62704000	2.66254300
H	1.81546300	-0.43051600	3.35548800
C	0.97076200	-2.98706100	2.29696300
H	1.40646500	-3.66528700	3.04256700
H	0.46204400	-2.18381400	2.83198200
H	0.22647800	-3.54796800	1.72628900
C	2.01254300	-4.22437500	-0.49151000
H	1.98518900	-4.07457300	-1.57575500
H	2.67586100	-5.07785800	-0.29577700
H	1.00913400	-4.48965900	-0.15050900
C	-1.08248100	-0.27268800	0.75419000
C	-0.24993600	-0.85181700	-0.14162100
C	-0.75227000	-1.59486300	-1.35438500
C	-1.16085600	4.22011600	1.30414200
H	-1.97950900	4.63847500	0.71512900
H	-1.55506300	3.48193500	1.99847700
H	-0.66263600	5.02136000	1.85620000
C	-2.50697500	-0.37505700	0.64273600
C	-3.71837700	-0.44736200	0.56980500
C	-5.17205200	-0.53868100	0.47189300
H	-0.88895400	-2.66057500	-1.12610500
H	-1.71044300	-1.19643400	-1.71160700
H	-0.03348500	-1.53886800	-2.18465400
H	-5.55688500	-1.40944500	1.01796000
H	-5.65582700	0.35453600	0.88610700
H	-5.49103900	-0.63570200	-0.57327600

IN4_ynyl_Me

Lowest frequency = 26.30 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.485925 Hartree

E = -1494.960131 Hartree

G = -1494.474206 Hartree

C	-4.60815800	-3.31751000	-0.42681600
C	-5.63781800	-2.39003500	-0.20014900
C	-5.35997800	-1.03233600	-0.03562100
C	-4.02398200	-0.64867700	-0.11154000
C	-2.97359400	-1.56028100	-0.34290800
C	-3.27228700	-2.91959800	-0.50181400
N	-3.47005700	0.63364900	0.02030200
C	-2.12207900	0.59480400	-0.10705500
C	-1.75159300	-0.77198400	-0.31400900
C	-1.40088200	1.88779600	-0.17783700
N	-0.49547300	-1.27360900	-0.44173800
O	-0.40748200	-2.47750100	-0.78205100
C	-1.72107600	2.72936200	-1.25640300
C	-1.24618600	4.03734100	-1.30144000
C	-0.47463400	4.52822600	-0.24540800
C	-0.15867300	3.70007800	0.83107700
C	-0.58929800	2.36723100	0.87056500
Rh	1.35460300	-0.46162300	0.04179900
H	-4.85614700	-4.36716700	-0.55342000
H	-6.66749800	-2.73096400	-0.15373800
H	-6.15161500	-0.31243200	0.13944700
H	-2.48622700	-3.63881300	-0.68639900
H	-2.35505100	2.35293100	-2.05349300
H	-1.49187100	4.67282900	-2.14663700
H	-0.11508900	5.55287300	-0.26165500
H	0.44981000	4.07878600	1.64667800
C	2.08603100	0.68657600	-1.65417500
C	2.39032700	-0.70859500	-2.00666500
C	2.91462500	1.05355800	-0.52801000
C	3.28607200	-1.20477900	-1.05490100
C	3.56738500	-0.12878300	-0.09253800
C	3.85114600	-2.58252700	-0.94611500
H	4.92513400	-2.57305500	-1.17480900
H	3.74249500	-2.97436500	0.07205300
H	3.36277100	-3.27491400	-1.63596900
C	1.79259800	-1.42871300	-3.17144200
H	0.74275000	-1.15356700	-3.30802700

H	2.32456900	-1.16302200	-4.09465800
H	1.84893700	-2.51291900	-3.04765600
C	1.30288200	1.61928500	-2.51508300
H	1.91216000	1.92073000	-3.37888500
H	0.39778800	1.14138900	-2.89933800
H	1.01374600	2.52011100	-1.97270300
C	3.06115600	2.41886700	0.06035000
H	3.95004400	2.90954000	-0.35815900
H	2.19603700	3.04429200	-0.16337600
H	3.18443700	2.37834900	1.14613300
C	4.49898100	-0.26204200	1.06735100
H	4.39531000	-1.24026200	1.54653500
H	5.54032200	-0.16854500	0.73036600
H	4.31659000	0.51164100	1.81762100
C	-0.20126700	1.46999500	1.98711800
C	0.49796300	0.37276000	1.67250900
C	-0.62941400	1.83764800	3.38407200
C	-4.29389900	1.81092600	0.28611500
H	-5.03144700	1.54882400	1.04701600
H	-3.66818900	2.62056000	0.65415300
H	-4.80828200	2.12452700	-0.62633200
C	0.94103100	-0.75208300	2.38630900
C	1.43693900	-1.85770600	2.60257000
C	2.01887600	-3.14235300	2.95364600
H	-1.72427700	1.89263600	3.45152600
H	-0.26871500	1.10687900	4.11356500
H	-0.24359800	2.82684800	3.66326600
H	1.28297700	-3.95067500	2.86429100
H	2.86379500	-3.37649200	2.29262600
H	2.39255400	-3.13248400	3.98497700

IN4_Me_Phynyl

Lowest frequency = 11.93 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.532331 Hartree

E = -1686.589463 Hartree

G = -1686.057132 Hartree

C	1.20433600	4.87265300	-3.27757300
C	0.32301200	5.73288600	-2.60398900
C	-0.22203900	5.38288600	-1.36708400
C	0.15368000	4.15132300	-0.83958500
C	1.03843800	3.27226400	-1.49688800
C	1.57173200	3.63807400	-2.73847700
N	-0.24166800	3.55421700	0.37001300
C	0.33794900	2.34214700	0.52157100
C	1.13856600	2.10223900	-0.63990500
C	0.17300600	1.63929800	1.81114300
N	1.84037000	0.98041800	-0.91201500
O	2.56687400	0.99688100	-1.93829300
C	0.64167600	2.30817700	2.95680700
C	0.34766800	1.82954400	4.22953700
C	-0.44738700	0.68892000	4.36951100
C	-0.90508900	0.01715100	3.23752500
C	-0.58127300	0.45860300	1.94663200
Rh	1.77296600	-0.96714400	-0.16973000
H	1.61325900	5.17481600	-4.23707500
H	0.06008500	6.68779300	-3.04855800
H	-0.90311600	6.04525400	-0.84447300
H	2.25524700	2.98224100	-3.26028100
H	1.22087400	3.21891900	2.83786000
H	0.71915300	2.35411800	5.10432600
H	-0.70594700	0.32013400	5.35773000
H	-1.52518000	-0.86777500	3.34357800
C	2.84148400	-1.25397200	1.68043500
C	3.93436500	-1.21472200	0.69765000
C	2.05962400	-2.45709200	1.44368800
C	3.74060700	-2.27009600	-0.18940800
C	2.53875400	-3.01925500	0.23807400
C	4.53226600	-2.61219200	-1.40615600
H	5.08499500	-3.54730600	-1.24622200
H	3.87529600	-2.77006700	-2.26875300
H	5.25035800	-1.82746200	-1.65512300
C	4.99233500	-0.16051900	0.67104700
H	4.56223900	0.83154200	0.84213600
H	5.72741400	-0.33897400	1.46670200
H	5.52272500	-0.14620400	-0.28406600
C	2.79421200	-0.40387100	2.90042100
H	3.52746600	-0.78547800	3.62567600
H	3.05874300	0.63171300	2.67612100
H	1.81182700	-0.42410600	3.37017400
C	0.97936200	-2.99027500	2.32568500
H	1.41476400	-3.66718500	3.07262700
H	0.47080400	-2.18590800	2.85913000
H	0.23533000	-3.55206200	1.75559900
C	2.03052700	-4.23993000	-0.45330400

H	2.00586100	-4.09682200	-1.53845900
H	2.69540000	-5.09049100	-0.25034800
H	1.02685900	-4.50549100	-0.11331000
C	-1.07852800	-0.29013500	0.75758200
C	-0.23773400	-0.87320200	-0.13266100
C	-0.73485300	-1.61834700	-1.34569400
C	-1.19332900	4.19351700	1.27661100
H	-2.01427600	4.59794500	0.68113200
H	-1.58220600	3.45750200	1.97624200
H	-0.70503400	5.00471700	1.82294000
C	-2.49267100	-0.39448200	0.61861900
C	-3.70198500	-0.47931500	0.49006200
C	-5.10912100	-0.59341600	0.30655600
C	-5.62571600	-1.29282500	-0.80473400
C	-6.00749300	-0.01044900	1.22409600
C	-7.00166800	-1.40212500	-0.98867700
H	-4.93803300	-1.74263300	-1.51441100
C	-7.38213400	-0.12706300	1.03126300
H	-5.61564300	0.52921000	2.08080000
C	-7.88487100	-0.82126700	-0.07335500
H	-7.38634200	-1.94232800	-1.84922000
H	-8.06403500	0.32615400	1.74526400
H	-8.95747500	-0.90868800	-0.22055200
H	-0.00213800	-1.58502800	-2.16456900
H	-0.89444000	-2.67849300	-1.10654800
H	-1.68000000	-1.20746000	-1.72265800

IN4_Ph_Meynyl

Lowest frequency = 26.13 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.533692 Hartree

E = -1686.594963 Hartree

G = -1686.061271 Hartree

C	1.24230000	4.88709900	-3.27185100
C	0.34175200	5.73744000	-2.61098000
C	-0.21238000	5.38417200	-1.37910000
C	0.17476700	4.15996500	-0.84272400
C	1.08076500	3.29196300	-1.48623400
C	1.62206700	3.66037700	-2.72359600
N	-0.22763600	3.55946300	0.36252100
C	0.36240600	2.35336500	0.52126000
C	1.18189300	2.12283200	-0.62866500
C	0.19832700	1.65958300	1.81782000
N	1.89207900	1.00429600	-0.89872200
O	2.65925600	1.04221600	-1.89434500
C	0.69527500	2.32391300	2.95349400
C	0.40534400	1.85834300	4.23237900
C	-0.41425900	0.73735200	4.38840500
C	-0.90430000	0.07215100	3.26607800
C	-0.58541400	0.50077000	1.96998300
Rh	1.74399200	-0.94228700	-0.18735100
H	1.65748000	5.19172400	-4.22787300
H	0.07073100	6.68712400	-3.06183800
H	-0.90939500	6.03815300	-0.86699800
H	2.32170600	3.01287000	-3.23447400
H	1.29288400	3.22105500	2.82249700
H	0.79935100	2.37853600	5.09989900
H	-0.66808900	0.37943800	5.38184000
H	-1.54490600	-0.79651600	3.38390000
C	2.81077200	-1.26910600	1.66093400
C	3.88963500	-1.22943600	0.66258200
C	2.01354200	-2.45962500	1.41887900
C	3.67785000	-2.27747400	-0.23117300
C	2.47754600	-3.01951500	0.20612800
C	4.45775000	-2.61919300	-1.45593800
H	5.02952200	-3.54274600	-1.29419700
H	3.79233800	-2.79715800	-2.30777700
H	5.15921800	-1.82515600	-1.72254400
C	4.96117700	-0.18937000	0.63322000
H	4.55441800	0.80030600	0.86304700
H	5.72624000	-0.41219400	1.38849300
H	5.45083600	-0.14325500	-0.34244400
C	2.78436000	-0.43088400	2.88984400
H	3.51921100	-0.82700600	3.60557200
H	3.05744500	0.60406500	2.67345500
H	1.80553300	-0.44487200	3.36750100
C	0.92385500	-2.98204800	2.29569000
H	1.34538800	-3.66938700	3.04106300
H	0.42403800	-2.17306100	2.83087600
H	0.17440500	-3.53007600	1.71910600
C	1.95207300	-4.22920200	-0.49168100
H	1.90697800	-4.07122200	-1.57404900
H	2.62027400	-5.08235700	-0.31218200
H	0.95397400	-4.49627100	-0.13963700
C	-1.10840100	-0.23940300	0.78743500

C	-0.27262800	-0.79088900	-0.11986400
C	-0.71267800	-1.53892600	-1.31139600
C	-0.44810700	-1.03288100	-2.60140500
C	-1.30942500	-2.81029400	-1.19144500
C	-0.77469200	-1.77900900	-3.73559000
C	-1.63408700	-3.54826700	-2.32656600
H	-1.51026500	-3.20716700	-0.20103400
C	-1.36423500	-3.03799000	-3.60240700
H	-0.57228100	-1.37280200	-4.72276700
H	-2.09799300	-4.52496100	-2.21924700
H	-1.61704800	-3.61803000	-4.48532900
H	0.00149800	-0.05015000	-2.70858000
C	-1.18589900	4.19202300	1.26661200
H	-2.00726100	4.59314100	0.66954300
H	-1.57286000	3.45208200	1.96326600
H	-0.70357800	5.00466100	1.81622700
C	-2.53215300	-0.34100600	0.67655300
C	-3.74354100	-0.40692300	0.60883100
C	-5.19643300	-0.49861900	0.51043300
H	-5.50737800	-1.48530300	0.14516300
H	-5.66961600	-0.33886000	1.48704300
H	-5.59762300	0.25358800	-0.18063600

IN4_Meynyl_Ph

Lowest frequency = 20.40 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.533755 Hartree

E = -1686.600884 Hartree

G = -1686.067129 Hartree

C	-3.07313200	4.65371700	-1.45094500
C	-4.31406900	4.20441300	-0.97040400
C	-4.40931600	3.05437600	-0.18529900
C	-3.22200400	2.38562200	0.09821400
C	-1.96433400	2.81987300	-0.36992700
C	-1.88934600	3.97391900	-1.15938700
N	-3.03044800	1.21438900	0.84753000
C	-1.72361800	0.86375400	0.86702200
C	-1.00756100	1.82870600	0.09373200
C	-1.30812100	-0.23883700	1.76651400
N	0.31825100	1.81295300	-0.20183600
O	0.79436100	2.85714800	-0.70574800
C	-1.42832900	-0.02114700	3.14821800
C	-1.24158700	-1.06979200	4.04591300
C	-0.96522900	-2.35233500	3.56541900
C	-0.85123700	-2.57418600	2.19331500
C	-0.99685800	-1.52254800	1.27996100
Rh	1.66334500	0.21886800	-0.23675800
H	-3.03227700	5.55367500	-2.05729200
H	-5.21568000	4.75930900	-1.21105800
H	-5.36548800	2.70126500	0.18453100
H	-0.93580800	4.33133900	-1.52439700
H	-1.68473900	0.96964000	3.51092900
H	-1.32864500	-0.88903000	5.11285000
H	-0.83681600	-3.17871600	4.25819600
H	-0.63843800	-3.56990700	1.81676700
C	2.67824100	0.07110600	1.69116000
C	3.34008700	1.18616900	0.99887400
C	2.98960800	-1.14404900	0.97556700
C	3.94524700	0.67781800	-0.15699200
C	3.68230600	-0.76647700	-0.20579600
C	4.70465500	1.42475000	-1.20347900
H	5.77743500	1.20243300	-1.12697500
H	4.38533200	1.13215500	-2.21024600
H	4.57415200	2.50478300	-1.10070000
C	3.32274300	2.60141900	1.47635100
H	2.35756300	2.85519200	1.92363700
H	4.09144400	2.74773400	2.24681600
H	3.51930900	3.30337200	0.66279600
C	2.05822400	0.16294600	3.04432000
H	2.84711800	0.18228700	3.80954500
H	1.46948200	1.07736400	3.15261800
H	1.41053500	-0.69056600	3.24754700
C	2.64510400	-2.53466500	1.39882400
H	3.49325100	-2.98255600	1.93344900
H	1.78380500	-2.54381300	2.06837800
H	2.41867400	-3.17231800	0.53993300
C	4.17719500	-1.67670700	-1.28089700
H	4.11183800	-1.20008800	-2.26355100
H	5.23205200	-1.92863400	-1.10626600
H	3.60799500	-2.60935200	-1.30900900
C	-0.82723800	-1.73320600	-0.18236200
C	0.14339600	-1.01341500	-0.77535400
C	-1.74434000	-2.65105600	-0.88944200
C	-1.37406700	-3.27687500	-2.09433700
C	-3.02650300	-2.90853300	-0.36880800

C	-2.26332400	-4.11437200	-2.76422300
H	-0.37824400	-3.11931000	-2.49559300
C	-3.91473000	-3.74652600	-1.04152500
H	-3.33042300	-2.43850600	0.56088900
C	-3.53872100	-4.35234400	-2.24292600
H	-1.95560400	-4.59249700	-3.69014900
H	-4.90284200	-3.92498000	-0.62631500
H	-4.22918500	-5.00877600	-2.76482100
C	-4.13837300	0.50872000	1.48593300
H	-4.93634700	0.38017500	0.75129400
H	-3.80155400	-0.46596200	1.82984600
H	-4.51189800	1.09181300	2.33221900
C	0.52969000	-0.75356400	-2.09492900
C	1.14751200	-0.22922000	-3.02388300
C	1.82007300	0.30794800	-4.19403500
H	1.38456100	1.26884800	-4.49408900
H	2.88607700	0.46764200	-3.98620300
H	1.74104500	-0.38405700	-5.04166500

IN4_Phynyl_Me

Lowest frequency = 16.99 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.533420 Hartree

E = -1686.600068 Hartree

G = -1686.066648 Hartree

C	2.40819500	4.99699200	-1.12958500
C	3.68293400	4.95555200	-0.54186600
C	4.19113200	3.77080600	-0.00735600
C	3.37997900	2.64257300	-0.09112100
C	2.09990200	2.65862200	-0.68188200
C	1.60470900	3.85830500	-1.20819600
N	3.63539200	1.33999600	0.36534600
C	2.58603000	0.52294900	0.11132900
C	1.57588400	1.31096000	-0.52791400
C	2.77015900	-0.92902000	0.35404600
N	0.33678000	0.90629300	-0.90787800
O	-0.31423600	1.69634000	-1.63371100
C	3.74455500	-1.58011800	-0.41993400
C	4.12519200	-2.88744000	-0.12728300
C	3.55789700	-3.54416300	0.96718400
C	2.59550500	-2.90068400	1.74508400
C	2.17028000	-1.60149500	1.43862700
Rh	-0.78976500	-0.72689100	-0.29710800
H	2.04130400	5.93366000	-1.53852000
H	4.28611400	5.85738400	-0.50312500
H	5.17409900	3.73403700	0.44863000
H	0.62778200	3.89608100	-1.67056800
H	4.21145800	-1.04829900	-1.24347900
H	4.87182100	-3.38276000	-0.74025200
H	3.86150800	-4.55727800	1.21386900
H	2.15064000	-3.41273500	2.59289600
C	-0.35496200	-2.45398600	-1.54997800
C	-1.22311200	-1.59581000	-2.36917500
C	-1.13861200	-2.94667600	-0.44094100
C	-2.46318700	-1.49226600	-1.72503200
C	-2.39655100	-2.28774600	-0.49348500
C	-3.65557100	-0.69615900	-2.14344900
H	-4.46784600	-1.36313700	-2.46161800
H	-4.03958400	-0.08959900	-1.31574500
H	-3.42006200	-0.02833500	-2.97572800
C	-0.80170300	-0.94939500	-3.64835900
H	0.25409700	-0.66617300	-3.61678200
H	-0.93065000	-1.64932800	-4.48457300
H	-1.39050800	-0.05397800	-3.86018600
C	0.98403200	-2.95589100	-1.97250300
H	0.85880100	-3.77559600	-2.69414400
H	1.56975700	-2.17236200	-2.45938700
H	1.55452900	-3.33589900	-1.12457700
C	-0.70508900	-3.95663400	0.57135000
H	-1.00788200	-4.96201600	0.24960900
H	0.37920500	-3.95774600	0.69576900
H	-1.16257900	-3.76749200	1.54634900
C	-3.52571000	-2.42907600	0.47322700
H	-4.04416300	-1.47598200	0.61572500
H	-4.26090200	-3.15046600	0.09157100
H	-3.17807400	-2.78409800	1.44663600
C	1.11230100	-0.92671700	2.22994700
C	0.01775100	-0.53877300	1.56485200
C	1.34958300	-0.68955500	3.69768400
C	4.88514300	0.97933700	1.03158100
H	5.13798400	1.77034500	1.73987600
H	4.75655900	0.04247800	1.56858900
H	5.68808300	0.87877100	0.29623100
C	-1.11577000	0.22398800	1.85125700
C	-2.16040000	0.83762000	1.60710500

C	-3.36803800	1.54423100	1.37200600
C	-4.45455800	1.44640300	2.26552800
C	-3.49533500	2.32827700	0.20442700
C	-5.63761600	2.12981700	1.99653200
H	-4.35706700	0.83816800	3.15904800
C	-4.68565000	3.00186500	-0.05331000
H	-2.65873900	2.38793900	-0.48520400
C	-5.75746700	2.90697300	0.84030100
H	-6.47025300	2.05329600	2.68961600
H	-4.77829500	3.60127900	-0.95425000
H	-6.68409700	3.43475200	0.63460200
H	2.24806600	-0.07670400	3.84973500
H	0.49633500	-0.18578700	4.16052100
H	1.51964100	-1.63905400	4.22194000
H	3.60984800	2.21618300	-0.20055300
H	-1.61804300	-1.71936300	-1.39293500
H	-4.07772000	-1.68154200	-1.42437000
H	-4.07470000	1.58650300	1.36227100
H	-1.60852800	1.54536300	1.41225300
C	0.35309500	-2.58176400	0.36049000
H	-0.67005100	-2.57253700	0.73235500
H	0.40140000	-3.16559900	-0.56336100
H	1.00163900	-3.03980000	1.11067300
C	-5.76645800	-0.04330900	-0.02920000
H	-6.16652600	-0.50784800	-0.93592600
H	-6.16089900	-0.60295100	0.82965500
H	-6.15900100	0.97671200	0.04226600

1e

Lowest frequency = 18.49 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.219673 Hartree

E = -802.437447 Hartree

G = -802.217774 Hartree

C	4.64607400	0.31922000	-0.06544000
C	4.52676300	-1.07687400	0.05056300
C	3.27654100	-1.69211300	0.12166500
C	2.15734900	-0.86296200	0.07560100
C	2.25536000	0.54374400	-0.03754100
C	3.52031600	1.14090500	-0.11135100
N	0.80063100	-1.21314100	0.12860200
C	0.03231000	-0.09238800	0.03961100
C	0.89182500	1.03114500	-0.06346600
C	-1.43131400	-0.10152200	0.03001300
N	0.39327100	2.29237000	-0.23229500
O	1.24606400	3.20968000	-0.30598600
C	-2.14936800	-1.01003500	-0.76668900
C	-3.54080100	-0.97896400	-0.79253900
C	-4.26009100	-0.05198000	-0.02617200
C	-3.53785900	0.85643900	0.76196200
C	-2.14778600	0.83847300	0.79225800
H	5.63507100	0.76510600	-0.12075600
H	5.42229000	-1.69047700	0.08130900
H	3.18365900	-2.76987400	0.20227900

IN1_e

Lowest frequency = 18.28 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.474288 Hartree

E = -1531.248109 Hartree

G = -1530.773821 Hartree

C	-5.08486000	-2.45295200	0.50824400
C	-5.92686500	-1.41418100	0.08068900
C	-5.43117800	-0.12697300	-0.13476300
C	-4.07369000	0.07527200	0.09786800
C	-3.20988400	-0.95266100	0.53156200
C	-3.72495600	-2.23820000	0.73966200
N	-3.32500200	1.25521700	-0.04584600
C	-2.01598500	1.02319300	0.22523300
C	-1.88675300	-0.35516100	0.59061600
C	-1.01037800	2.07997100	0.20079900
N	-0.73321500	-1.02926300	0.84664000
O	-0.86439600	-2.18250700	1.31369100
C	-0.98443500	3.04515300	-0.82653900
C	-0.04776100	4.06996800	-0.80311000
C	0.89346200	4.16923000	0.23508000
C	0.86438000	3.20490700	1.24888000
C	-0.06962800	2.17241000	1.23741800
Rh	1.25735200	-0.77700100	0.08232000
H	-5.50016700	-3.44361400	0.66751500
H	-6.98069300	-1.61212100	-0.08969100
H	-6.07657800	0.67311300	-0.47949000

H	-3.08306900	-3.03998900	1.07846600
H	-1.68020600	2.97661500	-1.65543900
H	-0.03662300	4.80061200	-1.60740200
H	1.58437700	3.25539500	2.05939300
C	0.98124500	-1.96261500	-1.70558200
C	2.36127700	-2.08435300	-1.28491300
C	0.75275900	-0.58306400	-2.08127000
C	2.95008100	-0.77936100	-1.30490400
C	1.95402800	0.14432300	-1.81925000
C	4.35507200	-0.42588100	-0.94698000
H	4.99264100	-0.46960500	-1.83968600
H	4.41353000	0.58780600	-0.54257400
H	4.76268300	-1.11892600	-0.20665400
C	3.02477700	-3.34280000	-0.84867600
H	2.30569500	-4.04470300	-0.41955100
H	3.48468600	-3.82370800	-1.72247400
H	3.81152800	-3.14791900	-0.11664000
C	0.00733700	-3.08333600	-1.84920800
H	-1.02221100	-2.72348300	-1.78835900
H	0.14106500	-3.56723200	-2.82560400
H	0.15580000	-3.83977000	-1.07454900
C	-0.50022800	-0.05509100	-2.69199000
H	-0.58626000	1.02412200	-2.56259700
H	-0.49109300	-0.27024000	-3.76866700
H	-1.38589200	-0.53253300	-2.26640400
C	2.19309400	1.59379900	-2.05468800
H	2.74638800	2.04390900	-1.22592600
H	2.80245200	1.71215000	-2.96080300
H	1.26081300	2.14070800	-2.19220800
C	2.85019100	-0.65274300	3.86588300
C	2.31704200	-0.66255500	2.45968300
O	2.18218000	0.41732200	1.80635400
O	1.95431700	-1.75987800	1.92021300
H	-0.08050800	1.45022600	2.04328400
C	-3.96650200	2.54319500	-0.30067300
H	-4.91730200	2.56488400	0.23447700
H	-3.33252900	3.34803600	0.06600500
H	-4.14834600	2.67552200	-1.37067100
H	2.00856000	-0.54701400	4.56186600
H	3.36407200	-1.59088500	4.09086200
H	3.52650400	0.19289200	4.01411400
C	1.92814400	5.26288100	0.23129200
H	2.74996700	5.01411000	-0.45370300
H	1.50261400	6.21370800	-0.10771800
H	2.35926700	5.40752600	1.22665700

TS1_e

Lowest frequency = -1648.16 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.473605 Hartree

E = -1531.223720 Hartree

G = -1530.750115 Hartree

C	-5.42264300	-1.86886900	-0.16841000
C	-6.09792000	-0.64774400	-0.32337700
C	-5.40798900	0.56620400	-0.33251700
C	-4.02501200	0.51048000	-0.17963900
C	-3.32950400	-0.70709200	-0.02693400
C	-4.03611800	-1.91500300	-0.01796600
N	-3.09494200	1.56775500	-0.14675500
C	-1.82945500	1.08485600	-0.03118800
C	-1.93175600	-0.34605400	0.06271300
C	-0.62842800	1.90242200	0.07952800
N	-0.89022500	-1.19005700	0.22103800
O	-1.12999200	-2.40093600	0.41367600
C	-0.55252900	3.21371500	-0.42965900
C	0.56917000	4.00050400	-0.18541900
C	1.64641000	3.52494400	0.57904700
C	1.59315100	2.19798100	1.01654900
C	0.49826400	1.35899400	0.75819100
Rh	1.08225200	-0.63152400	0.02029400
H	-5.98984400	-2.79474200	-0.16471900
H	-7.17707000	-0.64277000	-0.44187200
H	-5.93500100	1.50443500	-0.46304300
H	-3.51553200	-2.85550400	0.10492700
H	-1.34313700	3.61933800	-1.04730800
H	0.60761000	5.00617400	-0.59553700
H	2.44023600	1.79273900	1.56558700
C	1.42911300	-1.89185200	-1.78298500
C	2.58818600	-1.95908100	-0.95644400
C	1.24477100	-0.50430300	-2.16955800
C	3.16245300	-0.62523200	-0.86070800
C	2.37435100	0.24199600	-1.67139900
C	4.42510200	-0.28044800	-0.13935400
H	5.29925200	-0.52987400	-0.75550400
H	4.47106400	0.78612200	0.09488800

H	4.50903300	-0.84149200	0.79605300
C	3.15099000	-3.17580000	-0.30425400
H	2.41830700	-3.98508000	-0.26288400
H	4.02043400	-3.53011600	-0.87372900
H	3.48771700	-2.95569100	0.71272100
C	0.55713300	-3.03460500	-2.18185900
H	-0.44932900	-2.69733000	-2.43908400
H	0.98300800	-3.53037800	-3.06411300
H	0.47790900	-3.77499500	-1.38236000
C	0.18929900	0.02255300	-3.08624300
H	-0.01188800	1.07846800	-2.88807600
H	0.51287500	-0.06963300	-4.13147500
H	-0.74585100	-0.53240100	-2.97467000
C	2.66195700	1.66367700	-2.00718800
H	3.38335900	2.11022500	-1.32203500
H	3.08594500	1.69821700	-3.02020300
H	1.75475900	2.27138100	-2.01035700
C	0.89701100	-1.77477100	4.29003700
C	0.78793000	-1.04230000	2.97892600
O	1.44131300	-1.46279000	1.98463700
O	0.01210800	-0.02260800	2.93653500
H	0.22050200	0.54919900	1.85171200
C	-3.53610500	2.96016900	-0.07759400
H	-4.53102200	2.97924300	0.36647000
H	-2.85880700	3.52916200	0.55767900
H	-3.57610500	3.40656000	-1.07456900
H	-0.05034700	-2.29216600	4.48276400
H	1.70585300	-2.50660500	4.25842600
H	1.05991800	-1.06248800	5.10410000
C	2.83997300	4.39773800	0.85593800
H	3.27101800	4.77856000	-0.07806500
H	2.55851500	5.27072100	1.45812700
H	3.61719600	3.84762700	1.39475600

IN2_e

Lowest frequency = 20.27 cm^{-1}

Charge =1, Multiplicity = 1

TCG = 0.477147 Hartree

E = -1531.253230 Hartree

G = -1530.776083 Hartree

C	5.09036000	-2.37002000	-0.67090000
C	5.90720400	-1.32456000	-0.21718100
C	5.38192400	-0.05789500	0.06123400
C	4.01811800	0.11621700	-0.13867100
C	3.18310000	-0.92155500	-0.60367600
C	3.71918800	-2.18392300	-0.86776900
N	3.23192500	1.27294500	0.07317900
C	1.94249100	1.03653800	-0.25365000
C	1.84803100	-0.36112000	-0.62358600
C	0.88673800	2.02106000	-0.38262500
N	0.68510600	-0.96865000	-0.83115800
O	0.68628200	-2.16653800	-1.28037800
C	1.18073300	3.38017800	-0.66357900
C	0.16528400	4.29378000	-0.88559500
C	-1.18296600	3.89328000	-0.85199900
C	-1.46899700	2.54545400	-0.60629200
C	-0.46680000	1.60130400	-0.36918200
Rh	-1.02027900	-0.27908700	0.08941300
H	5.53189200	-3.33957200	-0.88008300
H	6.97049100	-1.49580100	-0.08047500
H	6.01901300	0.74738500	0.40940900
H	3.08693700	-2.98700300	-1.22473100
H	2.20648300	3.71282000	-0.75814600
H	0.41371200	5.32804300	-1.10732200
H	-2.50904800	2.23048500	-0.58692500
C	-0.99847200	-1.90024200	1.78786900
C	-2.33436200	-1.74098900	1.41203400
C	-0.47754600	-0.57645800	2.16105500
C	-2.69397400	-0.32197200	1.58468300
C	-1.58751700	0.35148500	2.16541500
C	-4.05594200	0.23645500	1.32916600
H	-4.74793000	-0.06455200	2.12725100
H	-4.03963200	1.32845000	1.28986500
H	-4.46285000	-0.13659500	0.38405300
C	-3.27512600	-2.78148500	0.89692800
H	-2.74328300	-3.66517800	0.53647500
H	-3.96221300	-3.09888700	1.69280200
H	-3.88985900	-2.38963700	0.08034300
C	-0.18208100	-3.15145100	1.76928500
H	0.81738200	-2.96914700	1.36443300
H	-0.05810500	-3.53634800	2.79013200
H	-0.65649800	-3.93145700	1.16867300
C	0.87804900	-0.32686300	2.73943600
H	1.18473300	0.71386700	2.60647700
H	0.87254500	-0.54141200	3.81663100

H	1.63055900	-0.97009700	2.27600200
C	-1.55145500	1.75399600	2.67736100
H	-2.28558300	2.38748800	2.17471300
H	-1.78379600	1.75330000	3.75065200
H	-0.56413700	2.20412700	2.54908400
C	-3.63887500	-1.66934100	-3.27526200
C	-2.45675200	-1.50593800	-2.36879200
O	-2.23045800	-0.43541400	-1.78175200
O	-1.70669300	-2.58094300	-2.26863800
H	-0.83651700	-2.41321700	-1.77195000
C	3.78780800	2.47221200	0.69593000
H	4.51984800	2.15661500	1.44120200
H	4.27734300	3.10783100	-0.04686700
H	2.99153300	3.02262600	1.19423500
H	-3.28982100	-1.82881600	-4.30165300
H	-4.20814100	-2.55628200	-2.97802700
H	-4.27446000	-0.78439500	-3.23390400
C	-2.28536200	4.89455400	-1.06799300
H	-3.25299000	4.40121300	-1.20082700
H	-2.36681600	5.57181400	-0.20738000
H	-2.08731800	5.51812500	-1.94760300

C	-3.24592600	-0.83801700	-0.62281800
C	-3.88674100	0.15680500	0.12950200
C	-3.11735700	1.07504100	0.86486200
C	-1.73488800	0.99958800	0.84989600
H	6.01346000	0.58249500	-0.23914000
H	5.70957500	-1.85989800	0.00495700
H	3.43403100	-2.84786700	0.19612200
H	4.04472000	2.11088600	-0.29105400
H	-1.37439800	-1.66671900	-1.23649000
H	-3.81468800	-1.54834100	-1.21009700
H	-3.62736200	1.83658900	1.44627500
H	-1.15250300	1.70879300	1.42617000
C	0.61799500	-2.54299500	0.43494200
H	-0.38359300	-2.48348500	0.85794000
H	0.59319400	-3.14110500	-0.48073800
H	1.28294100	-3.02009500	1.15816900
C	-6.06003200	-0.59898900	-0.51338900
O	-5.22976200	0.31316300	0.20922900
H	-5.90712000	-1.62956800	-0.17280800
H	-7.08644200	-0.29409000	-0.30335000
H	-5.87306200	-0.53670100	-1.59160100

1f

Lowest frequency = 39.83 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.225701 Hartree

E = -877.637897 Hartree

G = -877.412196 Hartree

C	5.00952800	0.17666500	-0.15271900
C	4.83846000	-1.21157400	-0.01308500
C	3.56685600	-1.77566800	0.09789100
C	2.48014700	-0.90376800	0.06779600
C	2.63055400	0.49614200	-0.06886000
C	3.91561700	1.04138400	-0.18323600
N	1.11240400	-1.19874200	0.16175700
C	0.38503100	-0.04949900	0.07413100
C	1.28707700	1.03754300	-0.06922200
C	-1.07442300	-0.00085800	0.10679400
N	0.83694700	2.31407900	-0.25008400
O	1.72425900	3.19551200	-0.35996800
C	-1.85526100	-0.90974200	-0.62584600

IN1_f

Lowest frequency = 17.20 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.479123 Hartree

E = -1606.449325 Hartree

G = -1605.970202 Hartree

C	-5.56607300	-1.62043700	0.59448900
C	-6.21865200	-0.45092500	0.17518300
C	-5.50420700	0.72268500	-0.07485900
C	-4.12648000	0.67749700	0.11592400
C	-3.44946500	-0.48575200	0.53913000
C	-4.18258000	-1.65381600	0.78183700
N	-3.18312300	1.70292600	-0.06178700
C	-1.92863800	1.24396000	0.18085100
C	-2.03836900	-0.13581100	0.55867500
C	-0.75418200	2.09820500	0.10677000
N	-1.02089700	-1.00743700	0.78706000
O	-1.34963400	-2.13107400	1.23116400
C	-0.59302100	3.04911200	-0.92642800

C	0.51938300	3.86965200	-0.96435000
C	1.51188800	3.76448100	0.02898000
C	1.36373100	2.82863300	1.06105600
C	0.24068900	2.00825100	1.09142000
Rh	1.00982400	-1.09393500	0.06535400
H	-6.14842000	-2.51767100	0.78201600
H	-7.29569400	-0.45555200	0.03826400
H	-6.00411400	1.62367900	-0.41268800
H	-3.68596900	-2.55538900	1.11324000
H	-1.32704400	3.11928200	-1.72081600
H	0.65454300	4.58816600	-1.76605100
H	2.11397200	2.71818500	1.83231400
C	0.56722200	-2.18263100	-1.74597300
C	1.87582600	-2.58447500	-1.27709800
C	0.63881300	-0.78434600	-2.11462600
C	2.71849200	-1.42480400	-1.25830400
C	1.95305400	-0.31874200	-1.80410100
C	4.15015800	-1.36803500	-0.83931500
H	4.80394300	-1.52526900	-1.70708100
H	4.39456100	-0.39444600	-0.40655700
H	4.37688100	-2.14116600	-0.10090800
C	2.25135100	-3.95441300	-0.83452600
H	1.39462900	-4.48553200	-0.41273300
H	2.60527700	-4.52382800	-1.70452400
H	3.05449800	-3.93099800	-0.09491700
C	-0.60886000	-3.07909700	-1.94062100
H	-1.54458300	-2.51598100	-1.91002400
H	-0.54003700	-3.57109300	-2.91968200
H	-0.64613200	-3.85680800	-1.17374000
C	-0.45691500	-0.01518700	-2.76974600
H	-0.29134200	1.06003900	-2.70111300
H	-0.49923000	-0.28802600	-3.83242400
H	-1.42922700	-0.25057000	-2.32971200
C	2.48731900	1.05186200	-2.02380200
H	3.11979000	1.37184700	-1.19160400
H	3.10998000	1.04874000	-2.92881900
H	1.68907800	1.78137900	-2.15869900
C	2.43881200	-1.32194100	3.91701500
C	1.97599900	-1.20603900	2.49054200
O	2.04669600	-0.10087000	1.87130800
O	1.46648800	-2.21428000	1.89930800
H	0.13414500	1.30081900	1.90228600
C	-3.58898400	3.08363100	-0.31220700
H	-4.51731800	3.27152400	0.22996400
H	-2.82020100	3.76276300	0.05216900
H	-3.75239300	3.25017200	-1.38037500
H	1.60304000	-1.06735300	4.58075800
H	2.75511400	-2.34399800	4.14018100
H	3.25585300	-0.62264800	4.11238800
O	2.56906100	4.59495600	-0.10507400
C	3.62964400	4.49747600	0.84994900
H	4.37196300	5.23549600	0.54265200
H	3.27534600	4.73142200	1.86014900
H	4.07853500	3.49766800	0.83938800

TS1_f

Lowest frequency = -1626.38 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.475915 Hartree

E = -1606.424526 Hartree

G = -1605.948611 Hartree

C	-5.76752700	-1.05560100	-0.16575900
C	-6.22574400	0.26153100	-0.32421800
C	-5.33877500	1.34069600	-0.33854900
C	-3.98582800	1.05113400	-0.18631700
C	-3.50668700	-0.26608400	-0.03056700
C	-4.40807800	-1.33600600	-0.01700700
N	-2.89035900	1.93639000	-0.15735300
C	-1.72322600	1.24697100	-0.04319600
C	-2.06683400	-0.14720400	0.05504400
C	-0.40486600	1.84669600	0.05429800
N	-1.18423600	-1.15425800	0.20614500
O	-1.62335800	-2.31008800	0.39302600
C	-0.10994100	3.11923400	-0.46733800
C	1.12909700	3.71884600	-0.25614900
C	2.10509400	3.05695600	0.50439500
C	1.84257400	1.75992900	0.97472600
C	0.62492300	1.12515100	0.73278700
Rh	0.85922700	-0.94562300	0.02022100
H	-6.48323000	-1.87222000	-0.15854800
H	-7.28859800	0.44961200	-0.44153900
H	-5.69616100	2.35529600	-0.47322100
H	-4.05456300	-2.35106400	0.10705200
H	-0.82868300	3.64847500	-1.07935100
H	1.32128000	4.69446600	-0.68503100

H	2.62926600	1.24154500	1.51591700
C	0.99608700	-2.24129800	-1.78171800
C	2.10043300	-2.53203800	-0.92779800
C	1.09200700	-0.84347000	-2.16350700
C	2.91974900	-1.33372000	-0.81262100
C	2.33547200	-0.33234500	-1.63891800
C	4.20717700	-1.23829900	-0.06038100
H	5.03612900	-1.62317800	-0.66923100
H	4.43655500	-0.20320800	0.20506800
H	4.16927800	-1.82955900	0.85901400
C	2.40258800	-3.83310200	-0.26560400
H	1.53850000	-4.50127100	-0.28004200
H	3.22955600	-4.33059500	-0.78912900
H	2.71021200	-3.68092600	0.77305100
C	-0.07084600	-3.19434300	-2.20453400
H	-0.98227300	-2.66761300	-2.49606200
H	0.27676400	-3.77378800	-3.06985900
H	-0.32049900	-3.89486400	-1.40436800
C	0.18233800	-0.11943000	-3.10177400
H	0.18814100	0.95518200	-2.90184300
H	0.50581700	-0.27231200	-4.13988000
H	-0.84604600	-0.47938600	-3.01468700
C	2.90680600	1.00254800	-1.96798300
H	3.65879600	1.32080000	-1.24477600
H	3.39097400	0.93269900	-2.95194500
H	2.13220200	1.76891400	-2.03781900
C	0.46328000	-1.99344800	4.30113000
C	0.48050000	-1.27410700	2.97830400
O	1.04149000	-1.82109300	1.98869900
O	-0.09209900	-0.12915900	2.92322800
H	0.22036500	0.38276900	1.82670500
C	-3.09040400	3.38201500	-0.07671900
H	-4.06112200	3.56475600	0.38444000
H	-2.31716300	3.82490600	0.54991100
H	-3.07078300	3.83747600	-1.07040700
H	-0.57204800	-2.25310900	4.55010100
H	1.06510100	-2.90245600	4.25613400
H	0.83800100	-1.33051200	5.08718700
O	3.32743000	3.55624300	0.78445700
C	3.66182200	4.85524200	0.28407400
H	4.67676100	5.05228700	0.63161700
H	3.63788500	4.87226700	-0.81126900
H	2.98171400	5.61678400	0.68144700

IN2_f

Lowest frequency = 29.77 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.483979 Hartree

E = -1606.456225 Hartree

G = -1605.972246 Hartree

C	5.48995600	-1.51926100	-0.86659800
C	6.12745100	-0.37568000	-0.36563700
C	5.40290500	0.77079700	-0.01955600
C	4.02595700	0.72564200	-0.19928700
C	3.36965200	-0.41402200	-0.71004100
C	4.10383500	-1.55426600	-1.04352000
N	3.05977000	1.71883800	0.08638300
C	1.81858200	1.27931800	-0.22599300
C	1.95823200	-0.09322000	-0.67608100
C	0.60712500	2.06302200	-0.27407100
N	0.91364200	-0.87608900	-0.90941500
O	1.10218300	-2.01986900	-1.45382000
C	0.64268200	3.46767400	-0.49178900
C	-0.51797100	4.19419500	-0.64938800
C	-1.76654400	3.54075500	-0.60590400
C	-1.82133800	2.15225600	-0.41678200
C	-0.65331200	1.40891000	-0.25150700
Rh	-0.83485300	-0.56166100	0.12729300
H	6.08297700	-2.39049500	-1.12746600
H	7.20622500	-0.37328100	-0.24370100
H	5.90410800	1.65138800	0.36600700
H	3.60717700	-2.43299900	-1.43527100
H	1.58819200	3.98569800	-0.58936200
H	-0.48938700	5.26334400	-0.83132100
H	-2.77845000	1.64614900	-0.38627000
C	-0.39945000	-2.22439600	1.72018100
C	-1.75551900	-2.31909900	1.39661500
C	-0.13849900	-0.84638300	2.15991100
C	-2.38548700	-1.01659600	1.67641700
C	-1.41034600	-0.16425600	2.25792700
C	-3.84138000	-0.73174300	1.49866800
H	-4.42642200	-1.22335800	2.28750000
H	-4.04746600	0.34062600	1.54373200
H	-4.20116400	-1.11212000	0.53736500
C	-2.49110000	-3.50120900	0.85330400

H	-1.81034700	-4.23222400	0.41038400
H	-3.05131900	-4.00094900	1.65500600
H	-3.21876600	-3.19990400	0.09325100
C	0.64790000	-3.28215900	1.59416700
H	1.58090500	-2.87396200	1.19624700
H	0.87073200	-3.71002400	2.58062700
H	0.32207500	-4.09375400	0.93902300
C	1.16322200	-0.35332800	2.70484500
H	1.24178200	0.73376700	2.62311500
H	1.25155300	-0.61876300	3.76697700
H	2.00952000	-0.80164200	2.17817700
C	-1.62989400	1.19049600	2.84680900
H	-2.48336100	1.69688700	2.39080400
H	-1.83013200	1.09163000	3.92198200
H	-0.74927800	1.82642300	2.72749500
C	-3.34428600	-2.13728100	-3.24429600
C	-2.16094400	-1.83688000	-2.37471500
O	-2.11264100	-0.80932600	-1.67842900
O	-1.21429100	-2.74582200	-2.42661700
H	-0.36526000	-2.47202600	-1.93611400
C	3.41943700	2.96940200	0.74880900
H	4.22227700	2.75940600	1.45718600
H	3.76251500	3.71272400	0.02378700
H	2.55853700	3.35011200	1.29589600
H	-3.02488400	-2.19999100	-4.29005800
H	-3.75928900	-3.11234000	-2.96612700
H	-4.10480900	-1.36420200	-3.13151700
O	-2.84782500	4.33179200	-0.76380800
C	-4.14348700	3.72451300	-0.74482300
H	-4.85340400	4.54037100	-0.88763400
H	-4.24951300	2.99732400	-1.55758100
H	-4.33447800	3.23428300	0.21632300

1g

Lowest frequency = 40.67 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.220628 Hartree

E = -802.436897 Hartree

G = -802.216269 Hartree

C	-4.56392000	-0.00836200	0.24156900
C	-4.32026100	-1.37028700	-0.00878500
C	-3.02440800	-1.84959200	-0.20232300
C	-1.98753400	-0.92012000	-0.13856700
C	-2.21156500	0.45488800	0.10815000
C	-3.52034400	0.91428800	0.30374600
N	-0.60921200	-1.12619600	-0.29528800
C	0.05167400	0.05454100	-0.14694300
C	-0.90181800	1.07284300	0.10394300
C	1.50899900	0.19257600	-0.21897700
N	-0.51516800	2.35998400	0.35436300
O	-1.44473700	3.17761400	0.55615500
C	2.35001400	-0.69475600	0.47661500
C	3.73917200	-0.55728100	0.43843500
C	4.28556600	0.49113700	-0.31722400
C	3.46269900	1.38010800	-1.00773300
C	2.07679500	1.24006900	-0.96117800
H	-5.58541300	0.33026100	0.38944900
H	-5.15406400	-2.06498100	-0.04921900
H	-2.83656600	-2.90196800	-0.38729800
H	-3.70555000	1.96351700	0.49614300
H	1.91347400	-1.48636700	1.07800500
H	5.36549700	0.60971500	-0.36065400
H	3.90233700	2.18508800	-1.58961600
H	1.43511100	1.92429400	-1.50391000
C	-0.04596400	-2.41845000	-0.66979300
H	0.95729900	-2.27727800	-1.06765500
H	-0.00573400	-3.08552700	0.19628300
H	-0.67714900	-2.86636800	-1.44069500
C	4.63380600	-1.50475700	1.19751500
H	4.05393400	-2.28797600	1.69502900
H	5.35541900	-1.98782600	0.52764700
H	5.21248800	-0.97308200	1.96301700

IN1_g

Lowest frequency = 10.69 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.473459 Hartree

E = -1531.247971 Hartree

G = -1530.774512 Hartree

C	-4.73139800	-2.93057600	0.29108200
C	-5.64636100	-1.94347300	-0.10954000
C	-5.26645600	-0.60357300	-0.20795600

C	-3.94755800	-0.29489100	0.11312400
C	-3.01350500	-1.27076500	0.52401500
C	-3.41142600	-2.61011900	0.61286200
N	-3.30535400	0.95502400	0.09078700
C	-1.99707200	0.81853900	0.41970400
C	-1.75772400	-0.56273300	0.68924000
C	-1.08820300	1.95408500	0.55829800
N	-0.54660200	-1.13818300	0.91650500
O	-0.56500000	-2.32119200	1.32034200
C	-1.04860900	2.97433600	-0.41118600
C	-0.21566400	4.08174100	-0.25845400
C	0.57449100	4.16827200	0.89979400
C	0.54391800	3.16439300	1.86499400
C	-0.27761200	2.05061000	1.69861800
Rh	1.36251600	-0.64645000	0.06615100
H	-5.05870700	-3.96376300	0.35870700
H	-6.66711800	-2.22399400	-0.35053600
H	-5.96812700	0.15741500	-0.53066700
H	-2.71222000	-3.37132000	0.93274400
H	-1.65319600	2.88724800	-1.30783200
H	1.22120800	5.03113300	1.03807400
H	1.16627700	3.24118500	2.75037700
C	1.13652100	-1.80343900	-1.74259700
C	2.54865200	-1.72727500	-1.42397700
C	0.68314200	-0.46491500	-2.06129200
C	2.93167800	-0.34960300	-1.43646700
C	1.77793500	0.42662600	-1.86013500
C	4.28697300	0.20893800	-1.15708500
H	4.87114300	0.26029000	-2.08525700
H	4.21585000	1.22035600	-0.74878200
H	4.83592900	-0.41462700	-0.44686800
C	3.42392800	-2.88209400	-1.08471500
H	2.85959600	-3.68260200	-0.60046100
H	3.85377000	-3.28686000	-2.01081500
H	4.24715400	-2.58311200	-0.43205100
C	0.33262800	-3.05428500	-1.86477100
H	-0.72959600	-2.86219900	-1.69697600
H	0.44716100	-3.47113600	-2.87400900
H	0.66446200	-3.80971500	-1.14803300
C	-0.67526100	-0.11000500	-2.56257700
H	-0.92875800	0.92744800	-2.34040600
H	-0.69831800	-0.23963900	-3.65269500
H	-1.44305800	-0.75904800	-2.13610700
C	1.79739900	1.89830200	-2.08475200
H	2.20474200	2.42734300	-1.21807400
H	2.44942400	2.11815100	-2.94029200
H	0.80298900	2.28813600	-2.29800500
C	3.06787500	-0.53893500	3.78820500
C	2.50137400	-0.53891900	2.39582500
O	2.23553100	0.54876300	1.79959900
O	2.23763900	-1.64133600	1.80918100
H	-0.30570300	1.27256100	2.45130500
C	-4.04146200	2.19696300	-0.13177600
H	-5.01774600	2.10977600	0.34787200
H	-3.49697900	3.02934500	0.30982600
H	-4.17617800	2.37243700	-1.20264200
H	2.23734000	-0.53717400	4.50534300
H	3.66934100	-1.43470400	3.96241100
H	3.66840900	0.35842100	3.95749700
C	-0.13255300	5.13874200	-1.32924500
H	0.82051600	5.07044800	-1.86988800
H	-0.93981600	5.02936000	-2.05993500
H	-0.18858100	6.14566400	-0.90009600

TS1_g

Lowest frequency = -1645.28 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.472963 Hartree

E = -1531.222308 Hartree

G = -1530.749345 Hartree

C	-5.08628100	-2.45926400	-0.45692900
C	-5.88996100	-1.30909100	-0.51374200
C	-5.34175100	-0.03326400	-0.36965300
C	-3.96605800	0.04604500	-0.16604100
C	-3.14321000	-1.09807400	-0.11011200
C	-3.70894600	-2.37018200	-0.25400300
N	-3.16119900	1.18855500	0.00899800
C	-1.85226000	0.83665700	0.11753100
C	-1.79800400	-0.59833500	0.06434600
C	-0.74895500	1.76359200	0.35496200
N	-0.67294600	-1.33766500	0.17514900
O	-0.78331100	-2.57815700	0.26460600
C	-0.82333800	3.12374300	0.00323300
C	0.18374300	4.02470700	0.36590700
C	1.28231200	3.54983300	1.09963700

C	1.40810200	2.19231200	1.37302900
C	0.42451100	1.26340300	0.98879900
Rh	1.21480000	-0.53793000	0.01988200
H	-5.54542300	-3.43645700	-0.57228400
H	-6.95865600	-1.40940500	-0.67652200
H	-5.96756400	0.85004500	-0.42662200
H	-3.08969200	-3.25623200	-0.20687900
H	-1.65006000	3.49913700	-0.58558900
H	2.05755000	4.24506100	1.41183100
H	2.29284800	1.83182300	1.89210000
C	1.64475800	-1.52201500	-1.93723600
C	2.82920700	-1.56130700	-1.14696100
C	1.29449500	-0.12605100	-2.13511000
C	3.26022400	-0.19277400	-0.89605100
C	2.35453300	0.67452100	-1.56980100
C	4.50298300	0.19744300	-0.16369000
H	5.37572000	0.12779100	-0.82664200
H	4.44196000	1.22412200	0.20573600
H	4.68183200	-0.46466500	0.68850900
C	3.54353500	-2.77709700	-0.66178300
H	2.91242600	-3.66661300	-0.72452300
H	4.43932200	-2.94907900	-1.27298200
H	3.86890000	-2.65239900	0.37515800
C	0.88592000	-2.69560000	-2.45985000
H	-0.16701600	-2.45220800	-2.61819700
H	1.30855900	-3.00610800	-3.42451300
H	0.94269600	-3.54619300	-1.77657500
C	0.16427500	0.38965700	-2.96506000
H	-0.16282400	1.37277800	-2.61714600
H	0.47815300	0.48912700	-4.01263000
H	-0.69269400	-0.28798800	-2.93534600
C	2.47306700	2.15014200	-1.72762500
H	3.15893000	2.58789200	-1.00160800
H	2.86148900	2.35853800	-2.73405100
H	1.50408600	2.64588000	-1.64079600
C	1.25178300	-2.16284300	4.13562900
C	1.03038500	-1.30633100	2.91704600
O	1.72817100	-1.51268200	1.88640700
O	0.11599600	-0.40961300	2.98641200
H	0.23629500	0.31080100	1.98314400
C	-3.76171200	2.50705700	0.20858500
H	-4.76576500	2.36409500	0.60691500
H	-3.17591700	3.07297600	0.93130200
H	-3.82268300	3.05570100	-0.73492400
H	0.41154000	-2.86162800	4.22793900
H	2.17956700	-2.73045400	4.04618900
H	1.27002000	-1.54065100	5.03480500
C	0.09248700	5.47699200	-0.02041900
H	0.98219900	5.78851400	-0.58074800
H	-0.78975700	5.67238600	-0.63681700
H	0.03504200	6.11438000	0.87081700

IN2_g

Lowest frequency = 25.96 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.478169 Hartree

E = -1531.251585 Hartree

G = -1530.773416 Hartree

C	4.42185800	-3.32072900	-0.67577000
C	5.42098400	-2.48159000	-0.16155000
C	5.15813300	-1.14421200	0.15449100
C	3.86587100	-0.68620300	-0.07083100
C	2.85119900	-1.51372400	-0.59648400
C	3.12511400	-2.84977500	-0.89825500
N	3.32532300	0.59870900	0.17101100
C	2.02315200	0.63900800	-0.18386200
C	1.65956700	-0.69237200	-0.61687700
C	1.18466300	1.82080700	-0.29438300
N	0.40336100	-1.03745300	-0.88119500
O	0.17788000	-2.17815000	-1.41042100
C	1.75778400	3.09232800	-0.54850600
C	0.96883600	4.21565000	-0.76839500
C	-0.42799400	4.05837700	-0.73973600
C	-1.00708400	2.81186700	-0.51387700
C	-0.22315600	1.67360100	-0.29227600
Rh	-1.14244300	-0.07858400	0.08332400
H	4.66139500	-4.35305100	-0.91168400
H	6.42160500	-2.87296100	-0.00625100
H	5.93476000	-0.50043800	0.55164900
H	2.35315000	-3.49316300	-1.30136500
H	2.83269300	3.19947600	-0.62729200
H	-1.06488700	4.92371900	-0.91061300
H	-2.08989100	2.72409300	-0.50565100
C	-1.41220200	-1.75535100	1.69939400
C	-2.69593300	-1.37228000	1.30365200

C	-0.69854900	-0.54922400	2.14634800
C	-2.83367100	0.07629500	1.54523100
C	-1.64900200	0.54178500	2.17425800
C	-4.08118100	0.85538900	1.28465500
H	-4.84584200	0.61251000	2.03464500
H	-3.89669500	1.93165500	1.32528500
H	-4.49683200	0.61337600	0.30137800
C	-3.77810300	-2.23186100	0.73545300
H	-3.37894300	-3.15612600	0.31094100
H	-4.49770200	-2.50183400	1.52013600
H	-4.33673300	-1.70487100	-0.04427000
C	-0.80533800	-3.11874800	1.63623700
H	0.23055700	-3.07843800	1.28887100
H	-0.79807800	-3.57202500	2.63641100
H	-1.36694200	-3.77799600	0.96989000
C	0.66639000	-0.54093500	2.75657300
H	1.13449100	0.44323800	2.67383800
H	0.60438300	-0.79646100	3.82297500
H	1.31927100	-1.27411600	2.27565700
C	-1.40506600	1.90021700	2.74551300
H	-2.00140000	2.66438900	2.24182200
H	-1.68038400	1.90321300	3.80850800
H	-0.35248800	2.18391200	2.67173300
C	-3.99259800	-0.73720600	-3.31529700
C	-2.77946100	-0.85330600	-2.44305300
O	-2.34995000	0.11304800	-1.79304300
O	-2.24038200	-2.05208200	-2.43317000
H	-1.36004400	-2.08661300	-1.92929800
C	4.10449100	1.64265900	0.83280500
H	4.74578400	1.16382600	1.57446700
H	4.72548800	2.18092700	0.11156700
H	3.43165200	2.33339400	1.33812100
H	-3.74132800	-1.02283400	-4.34192600
H	-4.75889400	-1.43348000	-2.95603600
H	-4.38052400	0.28146600	-3.29217400
C	1.58650300	5.56206800	-1.05181500
H	1.28848100	6.30022500	-0.29681300
H	2.67933500	5.50486800	-1.05627000
H	1.26210300	5.94990400	-2.02534300

1o

Lowest frequency = 40.44 cm^{-1}

Charge = 0, Multiplicity = 1

TCG = 0.225641 Hartree

E = -877.635583 Hartree

G = -877.409942 Hartree

C	-3.60006900	0.30554400	0.00364800
C	-3.30629800	1.68449000	0.10604100
C	-1.99575900	2.14165900	0.15382100
C	-0.97860200	1.18781200	0.09861300
C	-1.25432300	-0.19231700	0.00029500
C	-2.57907900	-0.64782300	-0.05115100
N	0.41277700	1.36776300	0.12804900
C	1.03286100	0.16208400	0.04053800
C	0.03643300	-0.84751600	-0.03881100
C	2.48765300	-0.01362600	0.01274000
N	0.36868000	-2.16273700	-0.19431800
O	-0.59429000	-2.96656400	-0.24706900
C	3.29780200	0.78351800	-0.81551800
C	4.67678600	0.58622500	-0.85033600
C	5.26470200	-0.40535600	-0.06166900
C	4.46613100	-1.20502500	0.75981500
C	3.08675900	-1.01505600	0.79735200
H	-4.13527300	2.38398200	0.14278400
H	-1.78207900	3.20291900	0.22432000
H	-2.78052900	-1.70596700	-0.12827600
H	2.84474300	1.53671200	-1.45200300
H	5.29074400	1.20372900	-1.49936300
H	6.34009300	-0.55590600	-0.08859800
H	4.91845800	-1.97625000	1.37644800
H	2.46760800	-1.62966400	1.44056700
C	1.02920400	2.67327700	0.33196500
H	2.05346800	2.54353200	0.67722400
H	1.02659600	3.24953600	-0.59791100
H	0.46082300	3.21400100	1.09187300
O	-4.92811800	0.00299300	-0.03550600
C	-5.29315200	-1.37108300	-0.14477800
H	-6.38438800	-1.38909200	-0.16399400
H	-4.90392200	-1.81539500	-1.06897800
H	-4.93356500	-1.94959500	0.71500700

IN1_o

Lowest frequency = 16.17 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.478804 Hartree

E = -1606.446253 Hartree

G = -1605.967449 Hartree

C	-5.04659500	-0.96589600	0.17718200
C	-5.60649200	0.25337500	-0.26496700
C	-4.83004900	1.39759700	-0.39409100
C	-3.47811800	1.29769000	-0.06640900
C	-2.90440900	0.09280300	0.38140700
C	-3.68931800	-1.05973200	0.50971900
N	-2.47497500	2.27981700	-0.11865600
C	-1.27588200	1.75161800	0.22381600
C	-1.48781800	0.37016400	0.54162600
C	-0.05938200	2.55592600	0.32607200
N	-0.53475000	-0.55825600	0.81782100
O	-0.94388600	-1.66068300	1.24664000
C	0.26948800	3.50895900	-0.65826000
C	1.40215600	4.30373600	-0.51363300
C	2.22091300	4.16087400	0.61140800
C	1.90526700	3.21364900	1.58601700
C	0.77267600	2.41319800	1.44773900
Rh	1.45933900	-0.75585500	0.05843800
H	-6.66410400	0.27534500	-0.50622600
H	-5.26663700	2.32479400	-0.74810200
H	-3.24949800	-1.97822300	0.86601200
H	-0.34748500	3.60850600	-1.54417000
H	1.64990200	5.02932900	-1.28238000
H	3.10247500	4.78520000	0.72402000
H	2.53986000	3.09150500	2.45725300
C	0.90072600	-1.75703200	-1.78019900
C	2.19928700	-2.24357800	-1.37059700
C	1.03324600	-0.34953800	-2.09190200
C	3.10346500	-1.13137300	-1.33599700
C	2.37936100	0.03646400	-1.80356800
C	4.55024100	-1.17005200	-0.97045500
H	5.15788400	-1.37590800	-1.86134100
H	4.87709100	-0.21368300	-0.55475500
H	4.75239100	-1.95417600	-0.23622400
C	2.51687400	-3.64678500	-0.99008500
H	1.64677400	-4.15016100	-0.56155200
H	2.81643400	-4.20059500	-1.89004800
H	3.34149500	-3.69175700	-0.27530800
C	-0.32834300	-2.58106300	-1.97134700
H	-1.23215800	-1.98129000	-1.83954600
H	-0.34190100	-2.99513800	-2.98807000
H	-0.36067700	-3.41541100	-1.26638000
C	-0.03756900	0.49584600	-2.69131600
H	0.15058400	1.55829000	-2.53759900
H	-0.07086200	0.30926900	-3.77298600
H	-1.02024900	0.24748800	-2.28396900
C	2.97666700	1.38977200	-1.96839200
H	3.59914700	1.65586300	-1.10936600
H	3.62315000	1.38951700	-2.85622100
H	2.21338100	2.15654700	-2.09759300
C	2.96363800	-1.02111300	3.85904900
C	2.47373600	-0.91803900	2.44174800
O	2.57618900	0.17171400	1.79667800
O	1.90731900	-1.91219800	1.88000200
H	0.52494700	1.68877900	2.21287600
C	-2.78746700	3.68320300	-0.37972500
H	-3.75717100	3.90725900	0.06775200
H	-2.02824000	4.31843100	0.07280300
H	-2.83130200	3.87082000	-1.45597300
H	2.15119400	-0.72520600	4.53457100
H	3.25005900	-2.04879700	4.09626100
H	3.80760900	-0.34615200	4.02264200
O	-5.91819800	-2.00473100	0.25646600
C	-5.41674200	-3.26904000	0.68864500
H	-5.01639100	-3.21083400	1.70783400
H	-6.27045800	-3.94867700	0.67093600
H	-4.63815700	-3.64097600	0.01175800

TS1_o

Lowest frequency = -1630.65 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.477024 Hartree

E = -1606.420623 Hartree

G = -1605.943599 Hartree

C	-5.18905600	-0.71639100	-0.23569600
C	-5.65969700	0.61247000	-0.33323000
C	-4.78984300	1.69358700	-0.27928700
C	-3.43081600	1.41890900	-0.12376700

C	-2.94675300	0.10095400	-0.03236700
C	-3.82382100	-0.98825800	-0.08420800
N	-2.34434400	2.30911700	-0.03406100
C	-1.17534700	1.62524900	0.05732300
C	-1.50988800	0.22531500	0.07946800
C	0.14230400	2.23301500	0.21368700
N	-0.62239300	-0.78293600	0.20448200
O	-1.05643400	-1.94742400	0.33589700
C	0.42178700	3.54169500	-0.22227300
C	1.64482500	4.13923800	0.08286100
C	2.60641800	3.44910800	0.82498400
C	2.36863800	2.12252500	1.18201000
C	1.16069100	1.47770600	0.86475700
Rh	1.41835400	-0.54053900	0.03873600
H	-6.72617400	0.77128800	-0.45427300
H	-5.16567500	2.70678700	-0.36525900
H	-3.44406400	-1.99533500	-0.00442700
H	-0.29130800	4.09286400	-0.82082300
H	1.84053100	5.15114100	-0.25882900
H	3.54537200	3.92972900	1.08400200
H	3.13496500	1.56418300	1.71361100
C	1.61028300	-1.79625800	-1.79323600
C	2.75835500	-2.01591600	-0.97717500
C	1.58846000	-0.38789800	-2.14805600
C	3.48137300	-0.76101400	-0.85083300
C	2.79260000	0.21275800	-1.63469900
C	4.78390000	-0.58589000	-0.13927200
H	5.61332000	-0.93527000	-0.76861300
H	4.96654800	0.46319300	0.10555000
H	4.80682600	-1.16522000	0.78839300
C	3.17770100	-3.30208700	-0.35082600
H	2.35845400	-4.02443000	-0.32884900
H	4.00453700	-3.73930600	-0.92596400
H	3.53200000	-3.14307000	0.67162600
C	0.61137200	-2.81820300	-2.22109800
H	-0.37184800	-2.37144000	-2.38406500
H	0.93500800	-3.27377200	-3.16641500
H	0.50908900	-3.61405700	-1.47990100
C	0.59921700	0.27939100	-3.04643300
H	0.53239200	1.34883300	-2.83038100
H	0.90309200	0.16529300	-4.09544600
H	-0.39664100	-0.15768700	-2.93697500
C	3.23344600	1.60274100	-1.93461100
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H	3.63415500	1.62458400	-2.95722100
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C	1.00874100	-1.82002200	4.25224200
C	1.02691000	-1.02622300	2.97289200
O	1.62069500	-1.49914300	1.96450700
O	0.41750700	0.10127600	2.97033900
H	0.73572900	0.68098700	1.91313600
C	-2.56319800	3.74758700	0.11560000
H	-3.54617000	3.89491200	0.56285100
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H	1.67561500	-2.68096600	4.18384800
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IN2_o

Lowest frequency = 21.34 cm^{-1}

Charge = 1, Multiplicity = 1

TCG = 0.482702 Hartree

E = -1606.451113 Hartree

G = -1605.968411 Hartree

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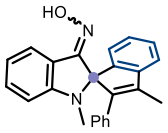
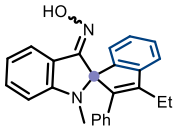
6. Characterization of Products



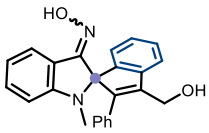
3aa, $CDCl_3$
E / Z = 96:4

3-Methyl-2-phenylspiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3aa), ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 1H), 8.08 (d, *J* = 7.6 Hz, 1H), 7.31 – 7.16 (m, 9H), 6.99 (d, *J* = 7.4 Hz, 1H), 6.65 (t, *J* = 7.6 Hz, 1H), 6.52 (d, *J* = 8.1 Hz, 1H), 2.47 (s, 3H), 2.22 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 156.7, 155.8, 144.9, 144.7, 141.5, 139.1, 134.8, 133.0, 130.0, 128.8, 128.6, 128.1, 127.1, 126.2, 121.2, 120.0, 119.3, 116.4, 106.5, 81.5, 28.2, 12.1. Conditions A. rr > 20:1. Light yellow solid, E / Z = 96:4, 94% yield, 33.2 mg. PE / EA = 10:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{24}H_{19}N_2O^-$ (M - H)$^-$ 351.1503, found 351.1497.



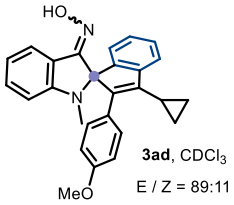
3ab, $CDCl_3$
E / Z = 91:9

3-Ethyl-2-phenylspiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ab). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.68 (s, 1H), 8.05 (d, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.29 (td, *J* = 7.4, 1.2 Hz, 1H), 7.25 – 7.18 (m, 6H), 7.08 (td, *J* = 7.4, 1.1 Hz, 1H), 7.00 (d, *J* = 7.3 Hz, 1H), 6.62 (t, *J* = 7.5 Hz, 1H), 6.50 (d, *J* = 8.1 Hz, 1H), 2.62 (q, J = 7.6 Hz, 1H), 2.49 (s, 3H), 1.29 (t, *J* = 7.6 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 156.3, 155.8, 145.3, 145.2, 143.6, 141.2, 135.0, 132.9, 129.9, 128.8, 128.5, 128.1, 127.2, 126.1, 121.6, 120.4, 119.4, 116.3, 106.5, 81.7, 28.2, 19.5, 13.6. Conditions A. rr > 20:1. Light yellow solid, E / Z = 91:9, 85% yield, 31.1 mg. PE / EA = 10:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{25}H_{21}N_2O^-$ (M - H)$^-$ 365.1659, found 365.1660.

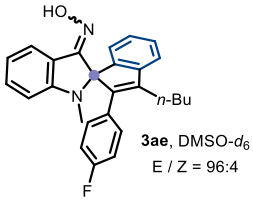


3ac, DMSO-d_6
E / Z = 95:5

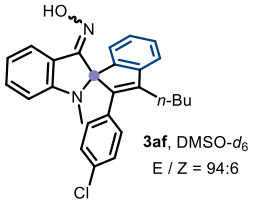
3-Hydroxymethyl-2-phenylspiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ac). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.10 (s, 1H), 8.04 (d, *J* = 7.5 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.35 – 7.24 (m, 7H), 7.12 (t, *J* = 7.5 Hz, 1H), 6.89 (d, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 8.1 Hz, 1H), 6.63 (t, *J* = 7.6 Hz, 1H), 5.23 (t, *J* = 5.2 Hz, 1H), 4.47 (d, *J* = 5.1 Hz, 2H), 2.42 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 155.6, 154.7, 146.1, 143.7, 143.7, 142.6, 134.9, 133.1, 129.3, 129.0, 128.8, 128.7, 128.2, 126.6, 122.1, 121.4, 120.1, 116.8, 107.4, 81.7, 56.0, 28.6. Conditions A. rr > 20:1. Light brown solid, E / Z = 99:1, 77% yield, 28.3 mg. PE / EA = 2:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{24}H_{19}N_2O_2^-$ (M - H)$^-$ 367.1452, found 367.1458.



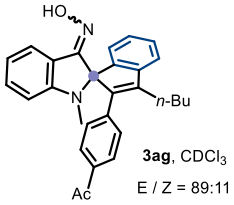
3-Cyclopropyl-2-(4-methoxyphenyl)spiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ad). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.92 (s, 1H), 8.08 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.45 (d, *J* = 7.4 Hz, 1H), 7.31 – 7.24 (m, 4H), 7.02 (td, J = 7.4, 1.1 Hz, 1H), 6.92 (d, *J* = 7.3 Hz, 1H), 6.73 – 6.69 (m, 2H), 6.65 (t, *J* = 7.4 Hz, 1H), 6.50 (d, *J* = 8.1 Hz, 1H), 3.71 (s, 3H), 2.40 (s, 3H), 1.87 – 1.82 (m, 1H), 0.94 – 0.88 (m, 1H), 0.86 – 0.82 (m, 1H), 0.66 – 0.59 (m, 1H), 0.56 – 0.50 (m, 1H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 158.5, 156.4, 155.8, 144.8, 144.5, 142.5, 142.2, 133.0, 130.2, 130.0, 128.5, 126.9, 125.7, 121.1, 120.7, 119.2, 116.3, 113.2, 106.5, 81.3, 55.0, 28.1, 8.8, 7.3, 6.9. Conditions A. rr > 20:1. Light brown solid, E / Z = 89:11, 81% yield, 33.1 mg. PE / EA = 5:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{27}H_{23}N_2O_2^-$ (M - H)$^-$ 407.1765, found 407.1772.



3-(*n*-Butyl)-2-(4-fluorophenyl)spiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ae). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.15 (s, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.34 – 7.12 (m, 7H), 6.89 (d, *J* = 7.3 Hz, 1H), 6.67 (d, *J* = 8.1 Hz, 1H), 6.61 (t, *J* = 7.6 Hz, 1H), 2.55 (t, *J* = 7.7 Hz, 2H), 2.43 (s, 3H), 1.62 – 1.54 (m, 2H), 1.36 – 1.30 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -114.37. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 161.9 (d, J_{CF} = 244.8 Hz), 155.6, 154.6, 145.9, 143.9, 143.6, 141.0, 133.0, 132.0 (d, J_{CF} = 3.2 Hz), 131.1 (d, J_{CF} = 8.0 Hz), 129.3, 129.0, 126.7, 121.6, 120.9, 120.1, 116.8, 115.8 (d, J_{CF} = 21.1 Hz), 107.5, 81.8, 30.9, 28.6, 25.7, 22.6, 14.2. Conditions A. rr > 20:1. Light yellow solid, E / Z = 96:4, 74% yield, 30.5 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{27}H_{24}FN_2O^-$ (M - H)$^-$ 411.1878, found 411.1887.



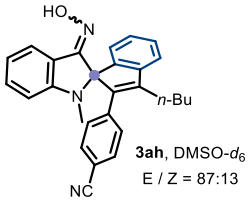
3-(*n*-Butyl)-2-(4-chlorophenyl)spiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3af). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.14 (s, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.31 (t, *J* = 7.3 Hz, 1H), 7.25-7.19 (m, 3H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 7.3 Hz, 1H), 6.65 (d, *J* = 8.1 Hz, 1H), 6.60 (t, *J* = 7.5 Hz, 1H), 2.54 (t, *J* = 7.7 Hz, 2H), 2.40 (s, 3H), 1.59-1.51 (m, 2H), 1.34-1.27 (m, 2H), 0.80 (t, *J* = 7.3 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 155.6, 154.5, 146.0, 144.1, 143.8, 140.7, 134.5, 133.1, 132.6, 130.8, 129.3, 129.0, 128.9, 126.8, 121.6, 121.1, 120.1, 116.9, 107.5, 81.8, 30.9, 28.6, 25.8, 22.6, 14.2. Conditions A. rr > 20:1. Light yellow solid, E / Z = 94:6, 85% yield, 36.4 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{27}H_{24}ClN_2O^-$ (M - H)$^-$ 427.1583, found 427.1600.



3ag, $CDCl_3$

E / Z = 89:11

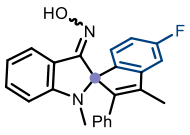
3-(*n*-Butyl)-2-(4-acetylphenyl)spiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ag). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.01 (s, 1H), 8.05 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.78 – 7.74 (m, 2H), 7.37 – 7.31 (m, 4H), 7.26 – 7.23 (m, 1H), 7.10 (td, *J* = 7.3, 1.2 Hz, 1H), 7.00 (d, *J* = 7.4 Hz, 1H), 6.64 (t, *J* = 7.5 Hz, 1H), 6.54 (d, *J* = 8.1 Hz, 1H), 2.63-2.57 (m, 2H), 2.49 (s, 3H), 2.49 (s, 3H), 1.70 – 1.63 (m, 2H), 1.42 – 1.36 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.9, 156.0, 155.7, 145.5, 145.1, 143.5, 140.2, 135.6, 133.1, 129.9, 129.0, 128.7, 128.3, 128.2, 126.5, 121.5, 120.7, 119.3, 116.6, 106.7, 81.7, 30.9, 28.3, 26.5, 26.2, 23.0, 13.8. Conditions A. rr > 20:1. Light yellow solid, E / Z = 89:11, 70% yield, 30.5 mg. PE / EA = 5:1, R_f = 0.15. HRMS (ESI) m/z calcd for $C_{29}H_{27}N_2O_2^-$ (M - H)$^-$ 435.2078, found 435.2097.



3ah, DMSO-d_6

E / Z = 87:13

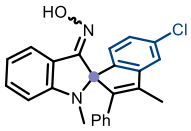
3-(*n*-Butyl)-2-(4-cyanophenyl)spiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ah). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.20 (s, 1H), 8.02 (d, *J* = 7.6 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 2H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.7 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 6.89 (d, *J* = 7.4 Hz, 1H), 6.70 (d, *J* = 8.1 Hz, 1H), 6.64 (t, *J* = 7.5 Hz, 1H), 2.62 – 2.57 (m, 2H), 2.42 (s, 3H), 1.61 – 1.55 (m, 2H), 1.36 – 1.30 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 155.6, 154.4, 146.0, 145.7, 143.5, 140.8, 140.1, 133.2, 132.8, 129.9, 129.4, 129.2, 127.2, 121.6, 121.4, 120.0, 119.3, 117.1, 110.5, 107.8, 81.9, 30.9, 28.6, 25.8, 22.6, 14.2. Conditions B. rr > 20:1. Light brown solid, E / Z = 87:13, 58% yield, 24.3 mg. PE / EA = 5:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{28}H_{24}N_3O^-$ (M - H)$^-$ 418.1925, found 418.1940.



3ba, $CDCl_3$

E / Z = 86:14

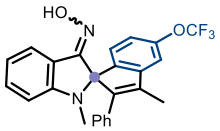
3-Methyl-2-phenylspiro[5-fluoroindene-1,2'-1'-methylindolin]-3'-one oxime (3ba). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (s, 1H), 8.09 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.27 – 7.20 (m, 6H), 7.01 – 6.98 (m, 1H), 6.96 – 6.93 (m, 1H), 6.79 – 6.74 (m, 1H), 6.66 (td, *J* = 7.5, 0.9 Hz, 1H), 6.52 (d, *J* = 8.1 Hz, 1H), 2.47 (s, 3H), 2.19 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -113.60 (major), -113.88. ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 163.7 (d, J_{CF} = 245.2 Hz), 156.6, 155.6, 147.2 (d, J_{CF} = 8.8 Hz), 143.8, 140.2 (d, J_{CF} = 2.6 Hz), 138.1 (d, J_{CF} = 2.8 Hz), 134.4, 133.2, 130.0, 128.7, 128.2, 127.4, 122.3 (d, J_{CF} = 9.1 Hz), 119.1, 116.6, 112.4 (d, J_{CF} = 23.0 Hz), 107.7 (d, J_{CF} = 23.8 Hz), 106.6, 80.9, 28.2, 12.0. Conditions A. rr > 20:1. Light yellow solid, E / Z = 86:14, 50% yield, 18.6 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{24}H_{18}FN_2O^-$ (M - H)$^-$ 369.1409, found 369.1419.



3ca, $CDCl_3$

E / Z = 96:4

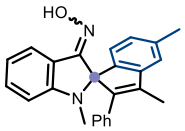
3-Methyl-2-phenylspiro[5-chloroindene-1,2'-1'-methylindolin]-3'-one oxime (3ca). ^1H NMR (400 MHz, Chloroform-*d*) δ 8.14 (s, 1H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.29 – 7.21 (m, 7H), 7.07 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 6.67 (t, *J* = 7.5 Hz, 1H), 6.52 (d, *J* = 8.1 Hz, 1H), 2.47 (s, 3H), 2.20 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, Chloroform-*d*) δ 156.6, 155.6, 146.7, 143.4, 143.1, 138.1, 134.6, 134.3, 133.3, 130.1, 128.7, 128.2, 127.5, 126.0, 122.28, 120.5, 119.1, 116.7, 106.7, 81.1, 28.2, 12.0. Conditions A. rr > 20:1. Light yellow solid, E / Z = 96:4, 74% yield, 28.6 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{24}H_{18}ClN_2O^-$ $(M - H)^-$ 385.1113, found 385.1131.



3da, $CDCl_3$

E / Z = 94:6

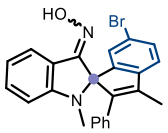
3-Methyl-2-phenylspiro[5-trifluoromethoxyindene-1,2'-1'-methylindolin]-3'-one oxime (3da). ^1H NMR (400 MHz, Chloroform-*d*) δ 8.29 (s, 1H), 8.06 (d, *J* = 7.7 Hz, 1H), 7.28 – 7.20 (m, 6H), 7.14 (s, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.95 – 6.91 (m, 1H), 6.67 (t, *J* = 7.5 Hz, 1H), 6.53 (d, *J* = 8.1 Hz, 1H), 2.47 (s, 3H), 2.20 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.62 (major), -57.66. $^{13}C\{^1H\}$ NMR (100 MHz, Chloroform-*d*) δ 156.4, 155.6, 150.0, 146.9, 143.9, 143.1, 138.0, 134.2, 133.3, 130.1, 128.7, 128.2, 127.6, 122.2, 120.5 (q, J_{CF} = 258.6 Hz), 119.1, 118.5, 116.8, 113.1, 106.7, 81.0, 28.2, 12.0. Conditions A. rr > 20:1. Light yellow solid, E / Z = 94:6, 73% yield, 31.8 mg. PE / EA = 10:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{25}H_{18}F_3N_2O_2^-$ $(M - H)^-$ 435.1326, found 435.1344.



3ea, $CDCl_3$

E / Z = 87:13

3-Methyl-2-phenylspiro[5-methylindene-1,2'-1'-methylindolin]-3'-one oxime (3ea). ^1H NMR (400 MHz, Chloroform-*d*) δ 8.33 (s, 1H), 8.08 (d, *J* = 7.6 Hz, 1H), 7.28 – 7.17 (m, 6H), 7.13 (s, 1H), 6.92 – 6.86 (m, 2H), 6.64 (t, *J* = 7.6 Hz, 1H), 6.51 (d, *J* = 8.1 Hz, 1H), 2.47 (s, 3H), 2.37 (s, 3H), 2.21 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, Chloroform-*d*) δ 157.0, 155.8, 144.9, 142.0, 141.8, 139.1, 138.4, 134.9, 133.0, 130.0, 128.8, 128.1, 127.1, 126.8, 121.0, 120.9, 119.3, 116.3, 106.5, 81.3, 28.2, 21.6, 12.1. Conditions A. rr > 20:1. Light yellow solid, E / Z = 87:13, 68% yield, 24.9 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{25}H_{21}N_2O^-$ $(M - H)^-$ 365.1659, found 365.1671.

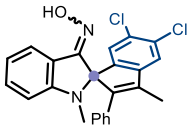


3ha, $CDCl_3$

E / Z = 90:10

3-Methyl-2-phenylspiro[6-bromoindene-1,2'-1'-methylindolin]-3'-one oxime (3ha). ^1H NMR (400 MHz,

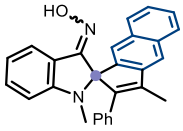
Chloroform-*d*) δ 8.43 (s, 1H), 8.07 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.44 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.29 – 7.15 (m, 7H), 7.12 (d, *J* = 1.8 Hz, 1H), 6.67 (t, *J* = 7.5 Hz, 1H), 6.53 (d, *J* = 8.1 Hz, 1H), 2.48 (s, 3H), 2.20 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, Chloroform-*d*) δ 156.2, 155.5, 146.9, 143.7, 142.1, 138.4, 134.3, 133.3, 131.7, 130.1, 128.7, 128.2, 127.4, 124.5, 121.3, 120.1, 119.0, 116.7, 106.7, 81.3, 28.2, 12.0. Conditions A. rr > 20:1. Light yellow solid, E / Z = 90:10, 89% yield, 38.3 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{24}H_{18}BrN_2O^-$ (M - H)$^-$ 429.0608, found 429.0626.



3ia, $CDCl_3$

E / Z = 92:8

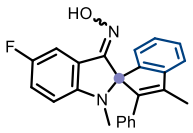
3-Methyl-2-phenylspiro[5,6-dichloroindene-1,2'-1'-methylindolin]-3'-one oxime (3ia). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 (s, 1H), 8.05 (d, *J* = 7.6 Hz, 1H), 7.36 (s, 1H), 7.28 (td, *J* = 7.8, 1.4 Hz, 1H), 7.22 – 7.20 (m, 5H), 7.07 (s, 1H), 6.69 (t, *J* = 7.5 Hz, 1H), 6.53 (d, *J* = 8.1 Hz, 1H), 2.49 (s, 3H), 2.17 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, Chloroform-*d*) δ 156.1, 155.4, 144.9, 144.5, 143.7, 137.6, 133.9, 133.4, 132.7, 130.1, 129.9, 128.7, 128.3, 127.7, 123.2, 121.8, 118.9, 117.0, 106.8, 81.0, 28.3, 12.0. Conditions A. rr > 20:1. Light yellow solid, E / Z = 92:8, 87% yield, 36.5mg. PE / EA = 10:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{24}H_{17}Cl_2N_2O^-$ (M - H)$^-$ 419.0723, found 419.0742.



3ja, $CDCl_3$

E / Z = 84:16

3-Methyl-2-phenylspiro[benzo[*d*]indene-1,2'-1'-methylindolin]-3'-one oxime (3ja). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.89 (s, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.68 – 7.64 (m, 2H), 7.45 – 7.43 (m, 1H), 7.41 (s, 1H), 7.40 – 7.37 (m, 1H), 7.33 – 7.29 (m, 3H), 7.24 – 7.20 (m, 3H), 6.69 (td, *J* = 7.5, 0.9 Hz, 1H), 6.56 (d, *J* = 8.1 Hz, 1H), 2.50 (s, 3H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ $^{13}C\{^{1}H\}$ NMR (100 MHz, Chloroform-*d*) δ 157.8, 155.7, 143.2, 142.9, 142.6, 139.4, 134.8, 134.3, 133.2, 132.6, 130.1, 128.9, 128.3, 128.2, 128.1, 127.4, 126.0, 125.5, 120.1, 119.2, 118.3, 116.6, 106.6, 81.1, 28.2, 12.1. Conditions A, solvent (0.5 M). rr > 20:1. Light yellow solid, E / Z = 84:16, 50% yield, 20.1 mg. PE / EA = 5:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{28}H_{21}N_2O^-$ (M - H)$^-$ 401.1659, found 401.1677.

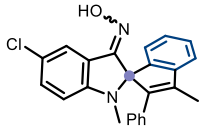


3ka, DMSO-d_6

E / Z = 99:1

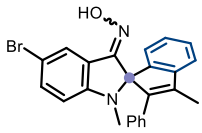
3-Methyl-2-phenylspiro[indene-1,2'-5'-fluoro-1'-methylindolin]-3'-one oxime (3ka). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.36 (s, 1H), 7.79 (dd, *J* = 8.8, 2.8 Hz, 1H), 7.41 (d, *J* = 7.4 Hz, 1H), 7.37 – 7.26 (m, 6H), 7.17 – 7.12 (m, 2H), 6.91 (d, *J* = 7.3 Hz, 1H), 6.67 (dd, *J* = 8.8, 4.1 Hz, 1H), 2.39 (s, 3H), 2.19 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -128.79. $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-d_6) δ 154.6 (d, J_{CF} = 231.3 Hz), 154.3 (d, J_{CF} = 2.7 Hz), 152.3, 145.6, 144.9, 141.5, 139.0, 135.3, 129.2, 129.0, 128.8, 127.9, 126.8, 121.3, 120.7, 120.1 (d, J_{CF} = 9.2 Hz),

119.6 (d, J_{CF} = 23.5 Hz), 115.4 (d, J_{CF} = 25.1 Hz), 107.8 (d, J_{CF} = 7.9 Hz), 82.1, 28.9, 12.5. Conditions A. rr > 20:1. Light yellow solid, E / Z = 99:1, 99% yield, 36.6 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{24}H_{18}FN_2O^-$ (M - H)$^-$ 369.1409, found 369.1425.



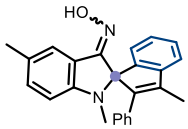
3la, DMSO-d_6
E / Z = 95:5

3-Methyl-2-phenylspiro[indene-1,2'-5'-chloro-1'-methylindolin]-3'-one oxime (3la). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.41 (s, 1H), 7.99 (d, J = 2.3 Hz, 1H), 7.41 (d, J = 7.4 Hz, 1H), 7.37 – 7.25 (m, 7H), 7.15 (t, J = 7.3 Hz, 1H), 6.93 (d, J = 7.2 Hz, 1H), 6.70 (d, J = 8.6 Hz, 1H), 2.41 (s, 3H), 2.19 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 154.2, 153.7, 145.5, 144.9, 141.5, 139.2, 135.2, 132.6, 129.2, 128.9, 128.9, 128.3, 127.9, 127.0, 121.4, 121.0, 120.7, 119.9, 108.6, 81.9, 28.5, 12.5. Conditions A, solvent (0.5 M). rr > 20:1. Light yellow solid, E / Z = 95:5, 82% yield, 31.7 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{24}H_{18}ClN_2O^-$ (M - H)$^-$ 385.1113, found 385.1132.



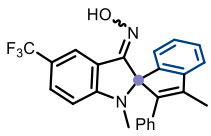
3ma, DMSO-d_6
E / Z = 99:1

3-Methyl-2-phenylspiro[indene-1,2'-5'-bromo-1'-methylindolin]-3'-one oxime (3ma). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.41 (s, 1H), 8.13 (d, J = 2.1 Hz, 1H), 7.41 – 7.24 (m, 8H), 7.15 (t, J = 7.3 Hz, 1H), 6.94 (d, J = 7.3 Hz, 1H), 6.66 (d, J = 8.6 Hz, 1H), 2.41 (s, 3H), 2.19 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 154.5, 153.6, 145.5, 144.9, 141.4, 139.2, 135.3, 135.1, 131.1, 129.2, 128.9, 128.9, 127.9, 127.0, 121.6, 121.4, 120.7, 109.2, 107.2, 81.8, 28.5, 12.5. Conditions A, solvent (0.5 M). rr > 20:1. Light yellow solid, E / Z = 99:1, 90% yield, 38.7 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{24}H_{18}BrN_2O^-$ (M - H)$^-$ 429.0608, found 429.0629.



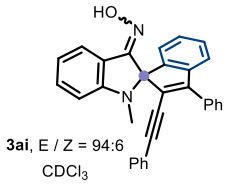
3na, $CDCl_3$
E / Z = 91:9

3-Methyl-2-phenylspiro[indene-1,2'-5'-methyl-1'-methylindolin]-3'-one oxime (3na). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (s, 1H), 7.92 (s, 1H), 7.33 – 7.26 (m, 4H), 7.23 – 7.18 (m, 3H), 7.10-7.05 (m, 2H), 6.97 (d, J = 7.3 Hz, 1H), 6.45 (d, J = 8.2 Hz, 1H), 2.44 (s, 3H), 2.27 (s, 3H), 2.23 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 156.8, 154.1, 144.9, 144.6, 141.4, 139.0, 134.9, 133.8, 130.2, 128.8, 128.5, 128.1, 127.0, 126.1, 125.5, 121.1, 120.0, 119.4, 106.5, 81.8, 28.4, 20.7, 12.1. Conditions A. rr > 20:1. Light yellow solid, E / Z = 91:9, 88% yield, 32.2 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{25}H_{21}N_2O^-$ (M - H)$^-$ 365.1659, found 365.1675.



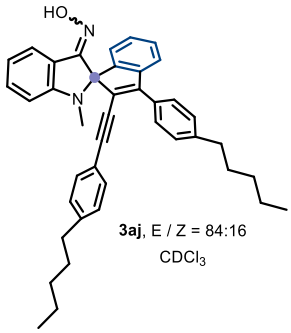
3pa, DMSO-d_6
E / Z = 99:1

3-Methyl-2-phenylspiro[indene-1,2'-1'-methyl-5'-trifluoromethylindolin]-3'-one oxime (3pa). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.50 (s, 1H), 8.24 (d, J = 2.0 Hz, 1H), 7.53 (dd, J = 8.6, 2.0 Hz, 1H), 7.40 (d, J = 7.4 Hz, 1H), 7.34 (td, J = 7.4, 1.1 Hz, 1H), 7.31 – 7.26 (m, 2H), 7.24 – 7.19 (m, 3H), 7.14 (td, J = 7.4, 1.2 Hz, 1H), 6.95 (d, J = 7.3 Hz, 1H), 6.78 (d, J = 8.6 Hz, 1H), 2.47 (s, 3H), 2.17 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -59.08. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 157.5, 153.4, 145.3, 144.9, 141.4, 139.5, 135.0, 130.4 (q, J_{CF} = 3.0 Hz), 129.4, 128.9, 128.8, 128.0, 127.1, 125.8 (q, J_{CF} = 3.4 Hz), 125.6 (q, J_{CF} = 270.4 Hz), 121.6, 120.7, 119.5, 116.4 (q, J_{CF} = 31.9 Hz), 107.1, 81.8, 28.3, 12.4. Conditions A. rr > 20:1. Light pink solid, E / Z = 99:1, 90% yield, 37.8 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{25}H_{18}F_3N_2O^-$ (M - H)$^-$ 419.1377, found 419.1395.



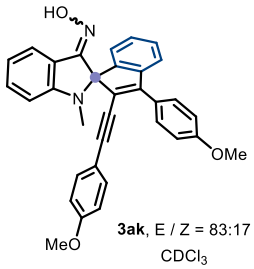
3ai, E / Z = 94:6
$CDCl_3$

3-Phenyl-2-phenylethynylspiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ai). ^{1}H NMR (400 MHz, Chloroform-d) δ 8.13 (d, J = 7.6 Hz, 1H), 8.10 (s, 1H), 7.84 (d, J = 7.3 Hz, 2H), 7.52 – 7.47 (m, 3H), 7.42 – 7.28 (m, 5H), 7.19 – 7.12 (m, 3H), 6.88 (dd, J = 7.3, 2.4 Hz, 2H), 6.77 (t, J = 7.6 Hz, 1H), 6.68 (d, J = 8.1 Hz, 1H), 2.63 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-d) δ 156.8, 156.4, 147.2, 144.4, 142.7, 133.4, 132.9, 131.4, 129.8, 129.1, 128.8, 128.6, 128.3, 128.1, 128.0, 127.6, 127.0, 124.0, 123.0, 121.7, 119.8, 117.0, 107.0, 100.0, 84.2, 81.8, 28.7. Conditions A. rr = 6:1. Light yellow solid, E / Z = 94:6, 81% yield, 35.5 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{31}H_{21}N_2O^-$ (M - H)$^-$ 437.1659, found 437.1681.



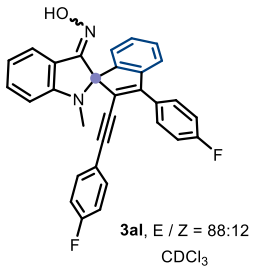
3aj, E / Z = 84:16
$CDCl_3$

3-(4-*n*-Pentylphenyl)-2-(4-*n*-pentylphenyl)ethynylspiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3aj). ^{1}H NMR (400 MHz, Chloroform-d) δ 8.26 (s, 1H), 8.12 (d, J = 7.5 Hz, 1H), 7.78 – 7.75 (m, 2H), 7.51 (d, J = 7.5 Hz, 1H), 7.35 – 7.25 (m, 6H), 6.96 (d, J = 7.9 Hz, 2H), 6.81-6.73 (m, 3H), 6.66 (d, J = 8.0 Hz, 1H), 2.69 – 2.65 (m, 2H), 2.61 (s, 3H), 2.52 – 2.48 (m, 2H), 1.71-1.66 (m, 2H), 1.55 – 1.50 (m, 2H), 1.39 – 1.35 (m, 4H), 1.30 – 1.24 (m, 4H), 0.92 (t, J = 6.5 Hz, 3H), 0.86 (t, J = 6.9 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-d) δ 156.9, 156.4, 146.6, 144.4, 143.5, 143.3, 143.0, 132.8, 131.3, 130.8, 129.8, 129.0, 128.6, 128.3, 128.1, 127.4, 126.6, 123.9, 121.7, 120.3, 119.9, 116.9, 106.9, 100.4, 83.9, 81.7, 35.9, 35.8, 31.6, 31.3, 31.1, 30.9, 28.6, 22.6, 22.5, 14.1, 14.0. Conditions A, solvent (0.5 M). rr =8:1. Light yellow solid, E / Z = 84:16, 85% yield, 49.1 mg. PE / EA = 10:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{41}H_{41}N_2O^-$ (M - H)$^-$ 577.3224, found 577.3248.



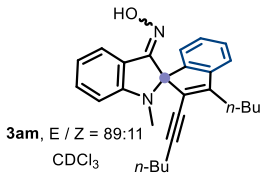
3ak, E / Z = 83:17
$CDCl_3$

3-(4-Methoxyphenyl)-2-(4-methoxyphenyl)ethynylspiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3ak). ^1H NMR (400 MHz, Chloroform-*d*) δ 8.26 (s, 1H), 8.12 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.81 – 7.78 (m, 2H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.35 – 7.30 (m, 2H), 7.25 – 7.20 (m, 2H), 7.02 – 6.98 (m, 2H), 6.83 – 6.79 (m, 2H), 6.76 (td, *J* = 7.6, 1.0 Hz, 1H), 6.68 – 6.65 (m, 3H), 3.86 (s, 3H), 3.73 (s, 3H), 2.61 (s, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, Chloroform-*d*) δ 159.7, 159.5, 157.0, 156.4, 145.7, 144.3, 143.1, 132.8, 132.8, 130.1, 130.0, 129.8, 129.0, 127.3, 126.1, 126.0, 123.9, 121.5, 119.8, 116.9, 115.3, 113.7, 106.9, 100.1, 83.3, 81.7, 55.3, 55.2, 28.6. Conditions A. rr = 11:1. Light yellow solid, E / Z = 83:17, 75% yield, 37.4 mg. PE / EA = 5:1, R_f = 0.15. HRMS (ESI) m/z calcd for $C_{33}H_{25}N_2O_3^-$ $(M - H)^-$ 497.1871, found 497.1900.



3al, E / Z = 88:12
$CDCl_3$

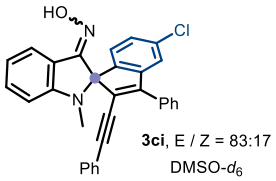
3-(4-Fluorophenyl)-2-(4-fluorophenyl)ethynylspiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3al). ^1H NMR (400 MHz, Chloroform-*d*) δ 8.42 (s, 1H), 8.09 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.81 – 7.77 (m, 2H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.39 – 7.33 (m, 2H), 7.27 – 7.24 (m, 2H), 7.19 – 7.14 (m, 2H), 6.86 – 6.82 (m, 4H), 6.76 (t, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 8.1 Hz, 1H), 2.62 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -110.32 (major), -110.46, -111.95 (major), -112.07. ^{13}C NMR (100 MHz, Chloroform-*d*) $^{13}C\{^1H\}$ NMR (100 MHz, Chloroform-*d*) δ 162.8 (d, J_{CF} = 248.6 Hz), 162.5 (d, J_{CF} = 250.2 Hz), 156.6, 156.3, 146.2, 144.2, 142.5, 133.3 (d, J_{CF} = 8.3 Hz), 133.0, 130.6 (d, J_{CF} = 8.1 Hz), 129.8, 129.4 (d, J_{CF} = 3.5 Hz), 129.2, 127.8, 126.9, 124.0, 121.5, 119.8, 119.0 (d, J_{CF} = 3.5 Hz), 117.1, 115.4 (d, J_{CF} = 21.9 Hz), 115.4 (d, J_{CF} = 21.9 Hz), 107.0, 99.1, 83.7 (d, J_{CF} = 1.6 Hz), 81.8, 28.7. Conditions A. rr = 9:1. Light yellow solid, E / Z = 88:12, 79% yield, 37.4 mg. PE / EA = 10:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{31}H_{19}F_2N_2O^-$ $(M - H)^-$ 473.1471, found 473.1494.



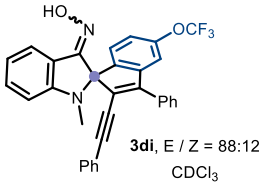
3am, E / Z = 89:11
$CDCl_3$

3-(*n*-Butyl)-2-(hexyne-1-yl)spiro[indene-1,2'-1'-methylindolin]-3'-one oxime (3am). ^1H NMR (400 MHz, Chloroform-*d*) δ 8.10 (d, *J* = 3.7 Hz, 1H), 8.07 (s, 1H), 7.31 – 7.25 (m, 3H), 7.17 – 7.14 (m, 1H), 7.12 – 7.08 (m, 1H), 6.68 (td, *J* = 7.5, 0.9 Hz, 1H), 6.60 (d, *J* = 8.1 Hz, 1H), 2.69 – 2.63 (m, 2H), 2.50 (s, 3H), 2.23 – 2.19 (m, 2H), 1.68 – 1.62 (m, 2H), 1.46 – 1.40 (m, 2H), 1.26 – 1.16 (m, 4H), 0.95 (t, *J* = 7.3 Hz, 3H), 0.76 (t, *J* = 7.2 Hz, 3H).

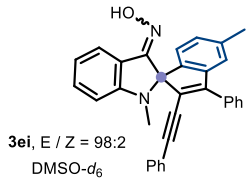
$^{13}C\{^{1}H\}$ NMR (100 MHz, Chloroform-*d*) δ 156.7, 156.1, 149.2, 144.3, 143.6, 132.7, 129.7, 128.8, 127.1, 126.8, 123.0, 120.0, 119.5, 116.5, 106.7, 101.2, 81.0, 74.3, 30.4, 30.4, 28.3, 26.7, 22.6, 21.5, 19.5, 14.0, 13.6. Conditions A. rr > 20:1. Light yellow oil, E / Z = 89:11, 61% yield, 24.3 mg. PE / EA = 10:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{27}H_{29}N_2O^-$ (M - H)$^-$ 397.2285, found 397.2306.



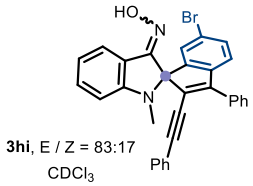
3-Phenyl-2-phenylethynylspiro[5-chloroindene-1,2'-1'-methylindolin]-3'-one oxime (3ci). ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.39 (s, 1H), 8.08 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.81-7.78 (m, 2H), 7.63-7.59 (m, 2H), 7.54-7.52 (m, 1H), 7.45-7.44 (m, 1H), 7.41 – 7.38 (m, 2H), 7.31 – 7.25 (m, 4H), 6.89 – 6.84 (m, 3H), 6.79 (t, *J* = 7.6 Hz, 1H), 2.61 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-*d*$_6$) δ 156.2, 154.3, 145.9, 144.7, 144.2, 134.4, 133.1, 132.6, 132.4, 131.5, 129.9, 129.7, 129.5, 129.5, 129.2, 128.8, 128.0, 125.8, 122.2, 121.7, 120.2, 117.7, 108.0, 100.6, 84.6, 81.6, 29.2. Conditions A. rr > 20:1. Light yellow solid, E / Z = 83:17, 64% yield, 30.2 mg. PE / EA = 10:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{31}H_{20}ClN_2O^-$ (M - H)$^-$ 471.1270, found 471.1293.



3-Phenyl-2-phenylethynylspiro[5-trifluoromethoxyindene-1,2'-1'-methylindolin]-3'-one oxime (3di). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 (s, 1H), 8.12 (d, *J* = 7.5 Hz, 1H), 7.84 – 7.80 (m, 2H), 7.56 – 7.51 (m, 2H), 7.49 – 7.46 (m, 1H), 7.40 – 7.35 (m, 2H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.22 – 7.14 (m, 4H), 6.90 – 6.87 (m, 2H), 6.81 (t, *J* = 7.5 Hz, 1H), 6.71 (d, *J* = 8.1 Hz, 1H), 2.66 (s, 3H). ^{19}F NMR (376 MHz, Chloroform-*d*) δ -57.56, -57.61 (major). $^{13}C\{^{1}H\}$ NMR (100 MHz, Chloroform-*d*) δ 156.2, 156.2, 150.1, 145.8, 144.9, 142.5, 133.1, 132.7, 131.5, 129.8, 129.1, 129.0, 128.6, 128.5, 128.5, 128.1, 125.0, 122.6, 120.4 (q, J_{CF} = 257.5 Hz), 119.8, 119.7, 117.4, 114.6, 107.2, 101.1, 83.7, 81.3, 28.8. Conditions A. rr > 20:1. Light yellow solid, E / Z = 88:12, 73% yield, 38.1 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{32}H_{20}F_3N_2O_2^-$ (M - H)$^-$ 521.1482, found 521.1504.

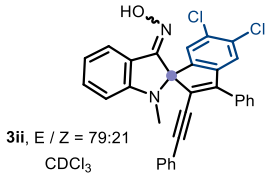


3-Phenyl-2-phenylethynylspiro[5-methylindene-1,2'-1'-methylindolin]-3'-one oxime (3ei). ^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 11.25 (d, *J* = 1.4 Hz, 1H), 8.08 (d, *J* = 7.4 Hz, 1H), 7.81 – 7.77 (m, 2H), 7.60 (t, *J* = 7.6 Hz, 2H), 7.53 – 7.48 (m, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.30 – 7.24 (m, 4H), 7.16 – 7.12 (m, 2H), 6.88 – 6.83 (m, 3H), 6.76 (t, *J* = 7.5 Hz, 1H), 2.59 (s, 3H), 2.36 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-*d*$_6$) δ 156.2, 154.8, 147.3, 142.7, 142.7, 139.1, 133.3, 133.0, 131.3, 129.6, 129.4, 129.3, 129.2, 129.0, 128.9, 128.9, 127.5, 124.0, 122.6, 122.6, 120.4, 117.4, 107.8, 99.5, 85.2, 81.7, 29.1, 21.7. Conditions A, solvent (0.5 M). rr = 4:1. Light brown solid, E / Z = 98:2, 54% yield, 24.4 mg. PE / EA = 10:1, Rf = 0.2. HRMS (ESI) m/z calcd for $C_{32}H_{23}N_2O^-$ (M - H)$^-$ 451.1816, found 451.1857.



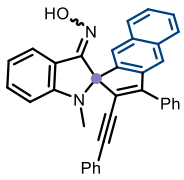
3hi, E / Z = 83:17
$CDCl_3$

3-Phenyl-2-phenylethynylspiro[6-bromoindene-1,2'-1'-methylindolin]-3'-one oxime (3hi). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (s, 1H), 8.12 (d, J = 7.6 Hz, 1H), 7.83-7.77 (m, 2H), 7.50 – 7.37 (m, 7H), 7.19 – 7.12 (m, 3H), 6.90-6.85 (m, 2H), 6.78 (t, J = 7.5 Hz, 1H), 6.68 (d, *J* = 8.1 Hz, 1H), 2.64 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 156.4, 156.1, 146.4, 146.3, 141.7, 133.1, 132.9, 132.2, 131.8, 131.4, 129.9, 128.9, 128.6, 128.4, 128.3, 128.0, 127.3, 122.8, 122.8, 121.9, 119.6, 117.3, 107.1, 100.5, 83.8, 81.4, 28.8. Conditions A, solvent (0.5 M). rr > 20:1. Light brown solid, E / Z = 83:17, 59% yield, 30.4 mg. PE / EA = 10:1, R_f = 0.2. HRMS (ESI) m/z calcd for $C_{31}H_{20}BrN_2O^-$ (M - H)$^-$ 515.0764, found 515.0789.



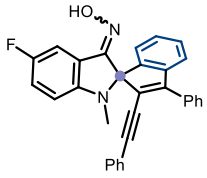
3ii, E / Z = 79:21
$CDCl_3$

3-Phenyl-2-phenylethynylspiro[5,6-dichloroindene-1,2'-1'-methylindolin]-3'-one oxime (3ii). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (s, 1H), 8.13 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.83 – 7.74 (m, 2H), 7.56 (s, 1H), 7.54 – 7.39 (m, 5H), 7.37 (s, 1H), 7.18-7.13 (m, 2H), 6.90 – 6.84 (m, 2H), 6.81 (t, *J* = 7.7 Hz, 1H), 6.70 (d, *J* = 8.1 Hz, 1H), 2.66 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 156.1, 154.8, 145.3, 144.0, 142.8, 133.4, 133.2, 132.5, 131.9, 131.5, 129.9, 129.1, 128.6, 128.5, 128.5, 128.1, 127.9, 125.9, 123.2, 122.5, 119.5, 117.6, 107.2, 101.3, 83.5, 81.2, 28.8. Conditions A. rr > 20:1. Light brown solid, E / Z = 79:21, 66% yield, 33.4 mg. PE / EA = 10:1, R_f = 0.25. HRMS (ESI) m/z calcd for $C_{31}H_{19}Cl_2N_2O^-$ (M - H)$^-$ 505.0880, found 505.0908.



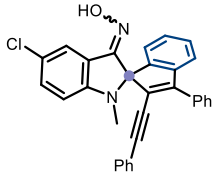
3ji, E / Z = 76:24
$CDCl_3$

3-Phenyl-2-phenylethynylspiro[benzo[*d*]indene-1,2'-1'-methylindolin]-3'-one oxime (3ji). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, *J* = 7.6 Hz, 1H), 8.03 (s, 1H), 7.93 – 7.90 (m, 2H), 7.87 (s, 1H), 7.82 – 7.80 (m, 1H), 7.76 – 7.73 (m, 1H), 7.70 (s, 1H), 7.55 (t, *J* = 7.5 Hz, 2H), 7.47 – 7.40 (m, 5H), 7.17-7.13 (m, 2H), 6.92 – 6.88 (m, 2H), 6.77 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 8.1 Hz, 1H), 2.66 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 157.8, 156.2, 147.3, 141.8, 140.7, 134.2, 133.4, 133.1, 133.0, 131.9, 131.5, 129.8, 128.9, 128.8, 128.5, 128.4, 128.4, 128.3, 128.0, 126.4, 126.2, 123.2, 122.9, 120.5, 119.5, 117.1, 106.9, 100.3, 84.3, 81.2, 28.6. Conditions A, solvent (0.5 M). rr > 20:1. Light yellow solid, E / Z = 76:24, 47% yield, 22.9 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{35}H_{23}N_2O^-$ (M - H)$^-$ 487.1816, found 487.1848.



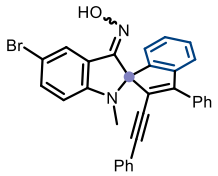
3ki, E / Z = 99:1
DMSO-d_6

3-Phenyl-2-phenylethynylspiro[indene-1,2'-5'-fluoro-1'-methylindolin]-3'-one oxime (3ki). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.58 (s, 1H), 7.84 (dd, J = 8.6, 2.8 Hz, 1H), 7.82 – 7.78 (m, 2H), 7.60 (t, J = 7.6 Hz, 2H), 7.53-7.48 (m, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.37 – 7.26 (m, 6H), 6.92 (dd, J = 7.7, 1.9 Hz, 2H), 6.86 (dd, J = 8.8, 4.1 Hz, 1H), 2.59 (s, 3H). ^{19}F NMR (376 MHz, DMSO-d_6) δ -128.13. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 155.1 (d, J_{CF} = 231.8 Hz), 154.1 (d, J_{CF} = 2.7 Hz), 152.9, 147.4, 145.3, 142.4, 133.2, 131.3, 129.7, 129.7, 129.5, 129.3, 129.3, 128.9, 128.5, 127.0, 124.4, 122.5, 122.0, 120.6 (d, J_{CF} = 9.4 Hz), 119.5 (d, J_{CF} = 23.6 Hz), 115.1 (d, J_{CF} = 25.0 Hz), 108.3 (d, J_{CF} = 8.1 Hz), 99.7, 85.0, 82.4, 29.5. Conditions A. rr = 5:1. Light yellow solid, E / Z = 99:1, 70% yield, 31.9 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{31}H_{20}FN_2O^-$ (M - H)$^-$ 455.1565, found 455.1595.



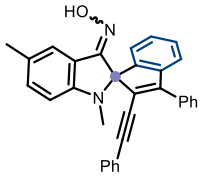
3li, E / Z = 99:1
DMSO-d_6

3-Phenyl-2-phenylethynylspiro[indene-1,2'-5'-chloro-1'-methylindolin]-3'-one oxime (3li). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.64 (s, 1H), 8.06 (d, J = 2.3 Hz, 1H), 7.82 – 7.79 (m, 2H), 7.60 (t, J = 7.5 Hz, 2H), 7.54 – 7.49 (m, 2H), 7.45 – 7.40 (m, 2H), 7.35-7.26 (m, 5H), 6.95 – 6.91 (m, 2H), 6.89 (d, J = 8.6 Hz, 1H), 2.59 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 154.8, 153.5, 147.5, 145.1, 142.4, 133.1, 132.5, 131.3, 129.8, 129.7, 129.6, 129.3, 129.3, 128.9, 128.5, 128.0, 126.8, 124.3, 122.4, 122.1, 121.4, 120.7, 109.1, 99.6, 84.9, 82.1, 29.1. Conditions A, solvent (0.5 M). rr = 5:1. Light yellow solid, E / Z = 99:1, 78% yield, 36.8 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{31}H_{20}ClN_2O^-$ (M - H)$^-$ 471.1270, found 471.1291.



3mi, E / Z = 99:1
DMSO-d_6

3-Phenyl-2-phenylethynylspiro[indene-1,2'-5'-bromo-1'-methylindolin]-3'-one oxime (3mi). ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (s, 1H), 8.19 (d, J = 2.2 Hz, 1H), 7.83 – 7.79 (m, 2H), 7.60 (t, J = 7.6 Hz, 2H), 7.54 – 7.49 (m, 3H), 7.43 (td, J = 7.4, 1.2 Hz, 1H), 7.37 – 7.27 (m, 5H), 6.95 – 6.90 (m, 2H), 6.85 (d, J = 8.6 Hz, 1H), 2.59 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) δ 155.2, 153.5, 147.5, 145.0, 142.4, 135.2, 133.1, 131.4, 130.8, 129.8, 129.8, 129.6, 129.4, 129.3, 128.9, 128.5, 126.8, 124.3, 122.4, 122.1, 122.0, 109.7, 108.0, 99.6, 84.9, 82.0, 29.0. Conditions A, solvent (0.5 M). rr = 5:1. Light yellow solid, E / Z = 99:1, 78% yield, 40.2 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{31}H_{20}BrN_2O^-$ (M - H)$^-$ 515.0764, found 515.0801.

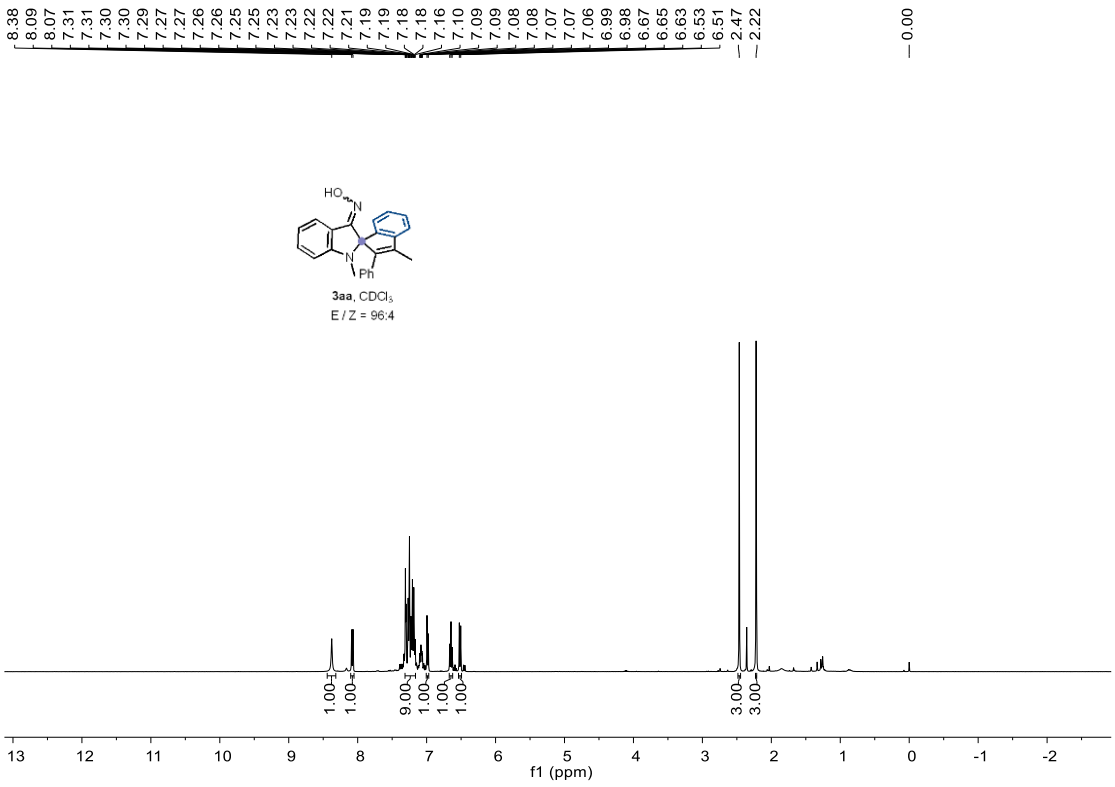


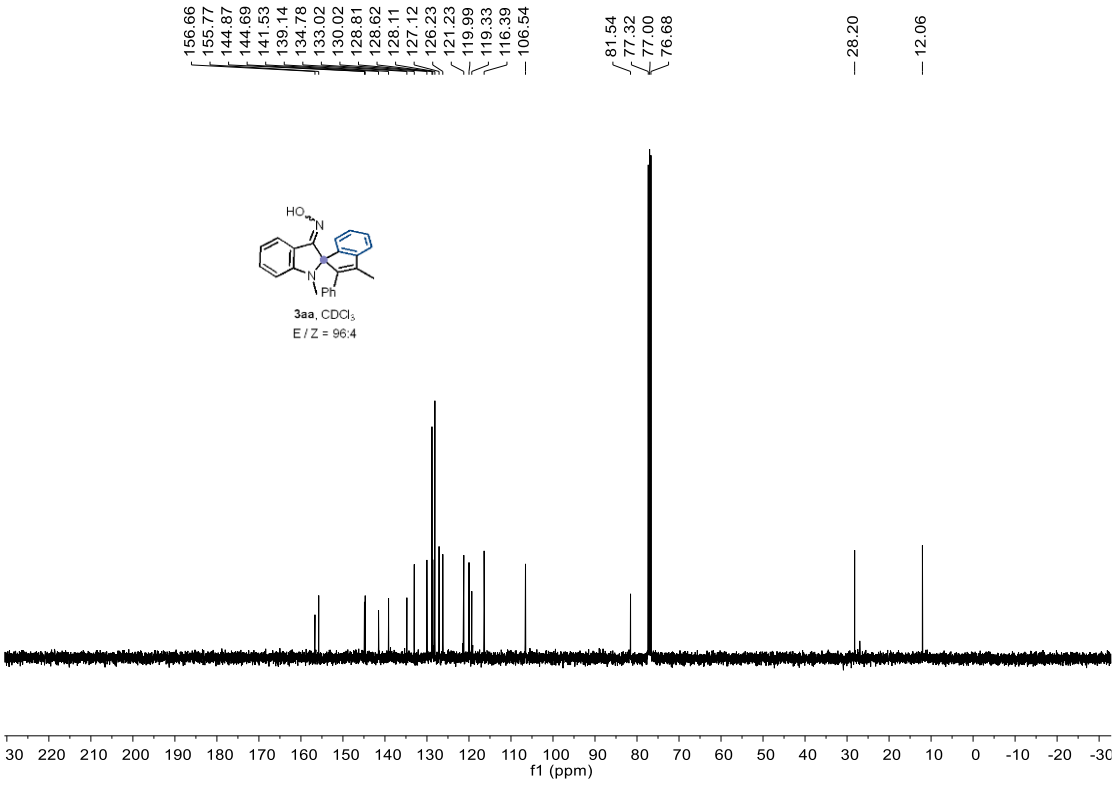
3ni, E / Z = 88:12

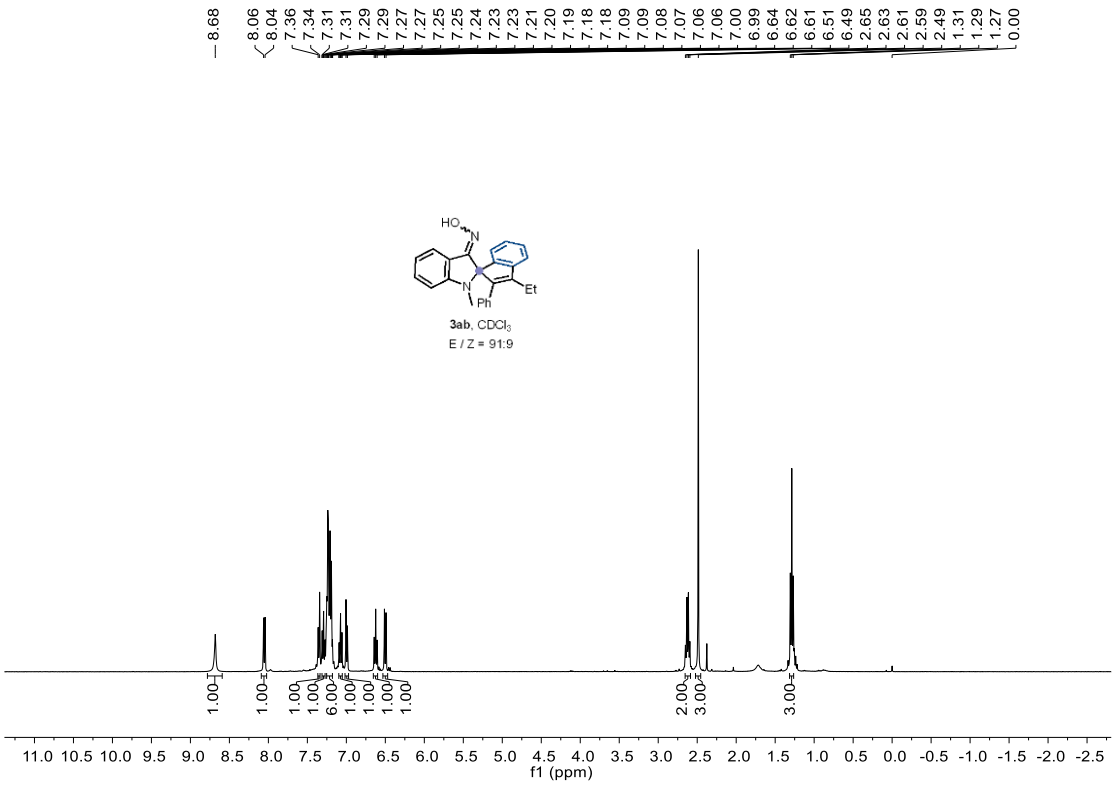
$CDCl_3$

3-Phenyl-2-phenylethynylspiro[indene-1,2'-5'-methyl-1'-methylindolin]-3'-one oxime (3ni). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (s, 1H), 7.98 (s, 1H), 7.85 – 7.82 (m, 2H), 7.51 – 7.47 (m, 3H), 7.44 – 7.40 (m, 1H), 7.35 – 7.26 (m, 3H), 7.21 – 7.12 (m, 4H), 6.91 – 6.87 (m, 2H), 6.61 (d, *J* = 8.1 Hz, 1H), 2.61 (s, 3H), 2.34 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, Chloroform-*d*) δ 156.9, 154.6, 147.3, 144.4, 142.6, 133.6, 133.4, 131.4, 130.0, 129.0, 128.8, 128.6, 128.3, 128.1, 128.0, 127.6, 127.1, 126.2, 123.9, 123.1, 121.7, 119.9, 107.0, 100.0, 84.4, 82.1, 28.9, 20.7. Conditions A. rr = 7:1. Light yellow solid, E / Z = 88:12, 65% yield, 29.4 mg. PE / EA = 5:1, R_f = 0.3. HRMS (ESI) m/z calcd for $C_{32}H_{24}N_2NaO^+$ $(M + Na)^+$ 475.1781, found 475.1765.

7. NMR Spectra of Products






8.68
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6.61
6.51
6.49
2.65
2.63
2.61
2.59
2.49
1.31
1.29
1.27
0.00
HO
N
N
Ph
Et
3ab, CDCl3
E / Z = 91:9
1.00
1.00
1.00
1.00
6.00
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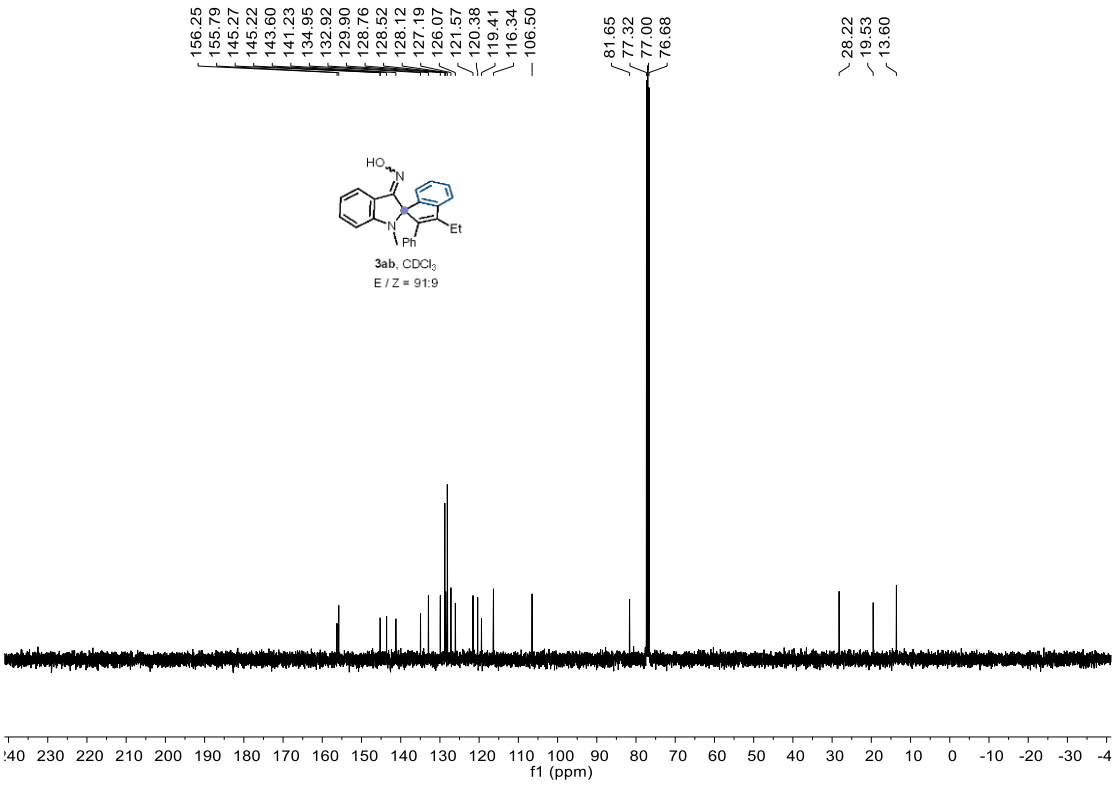
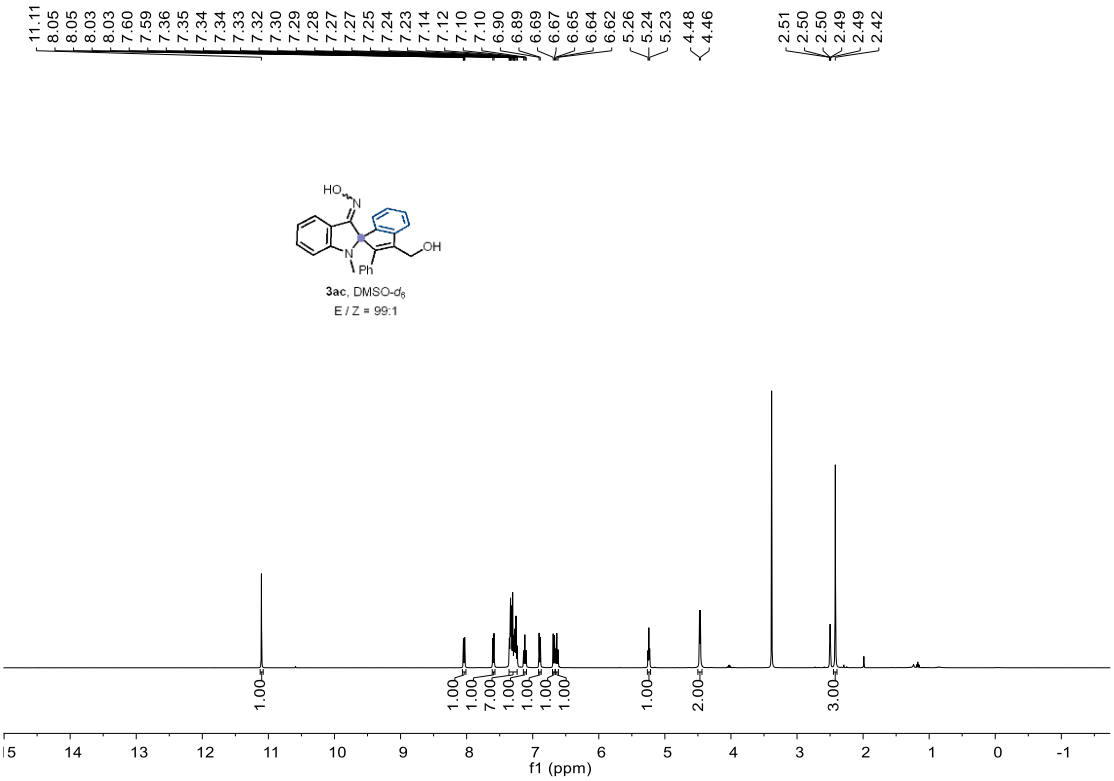
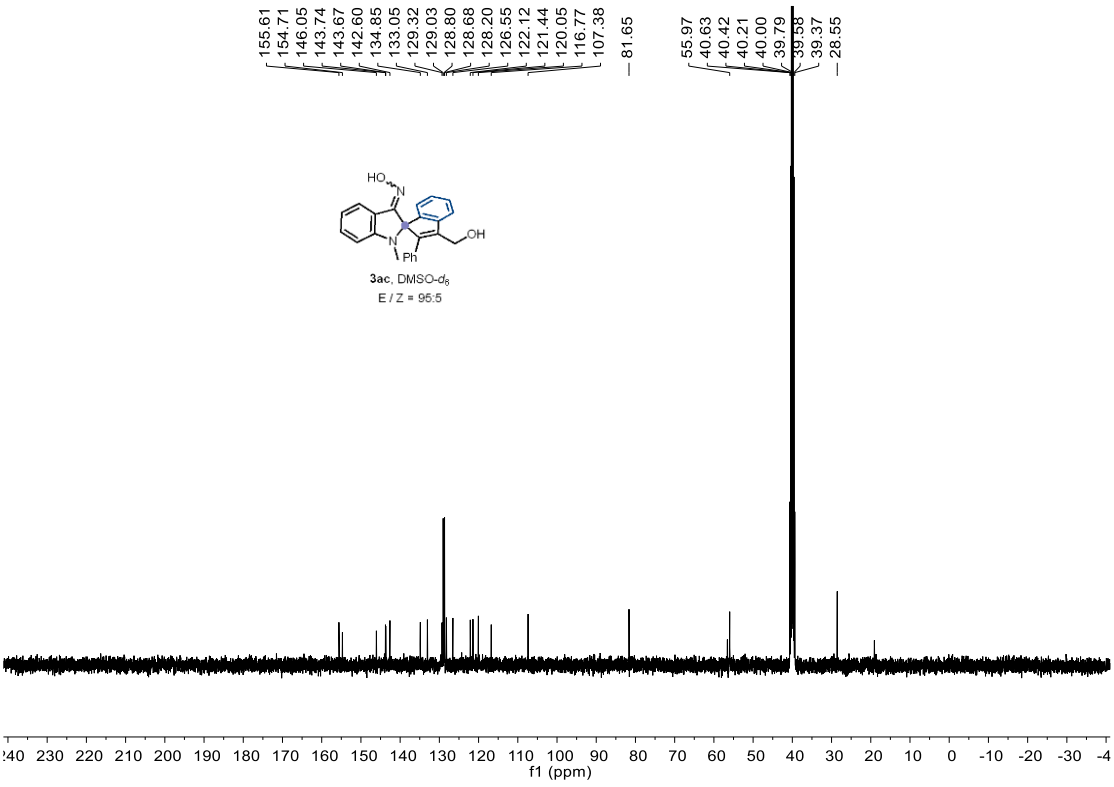
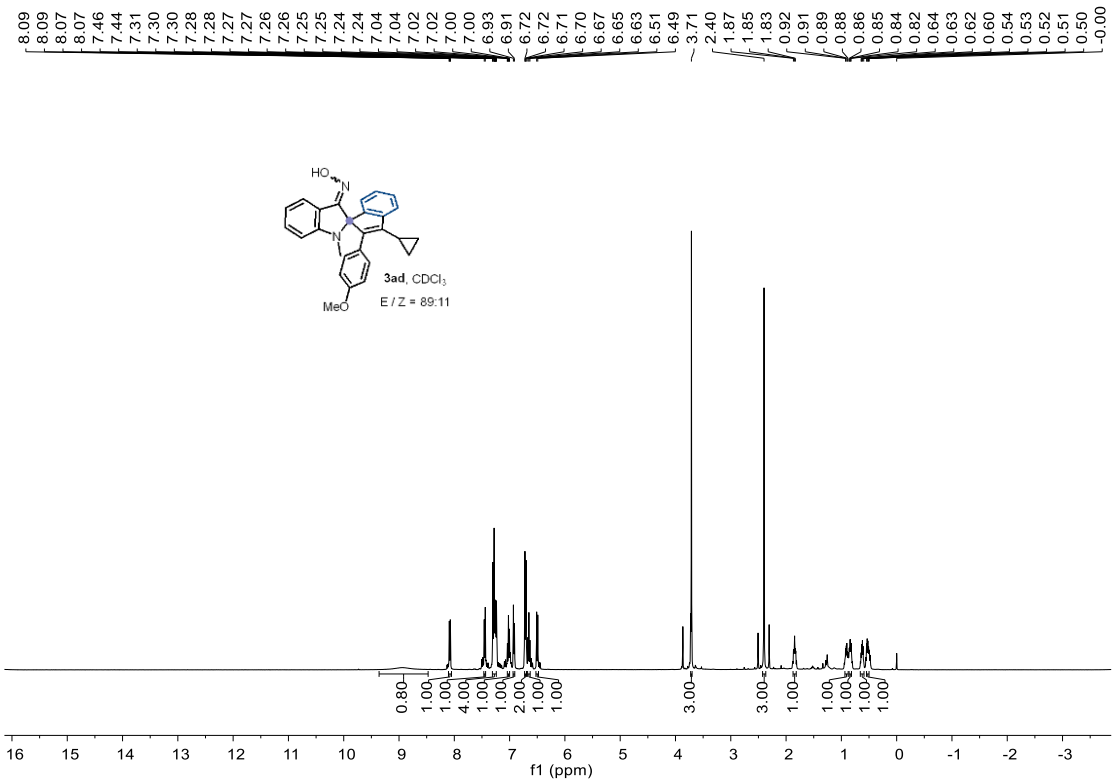
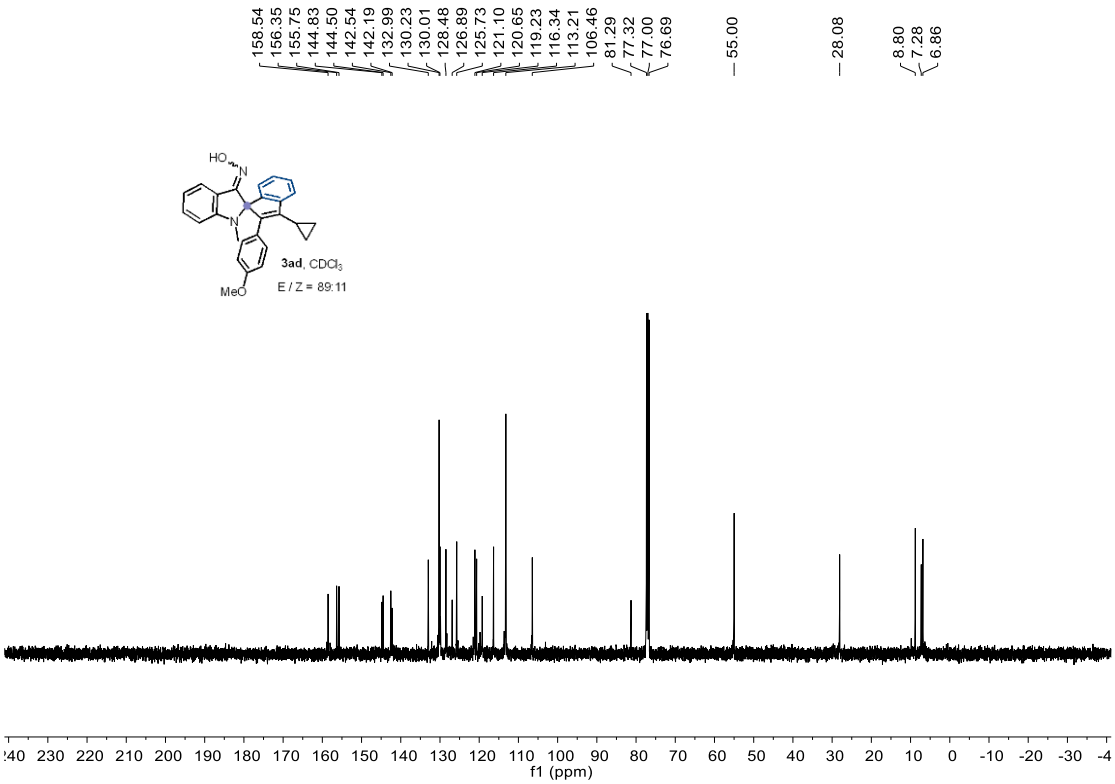
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

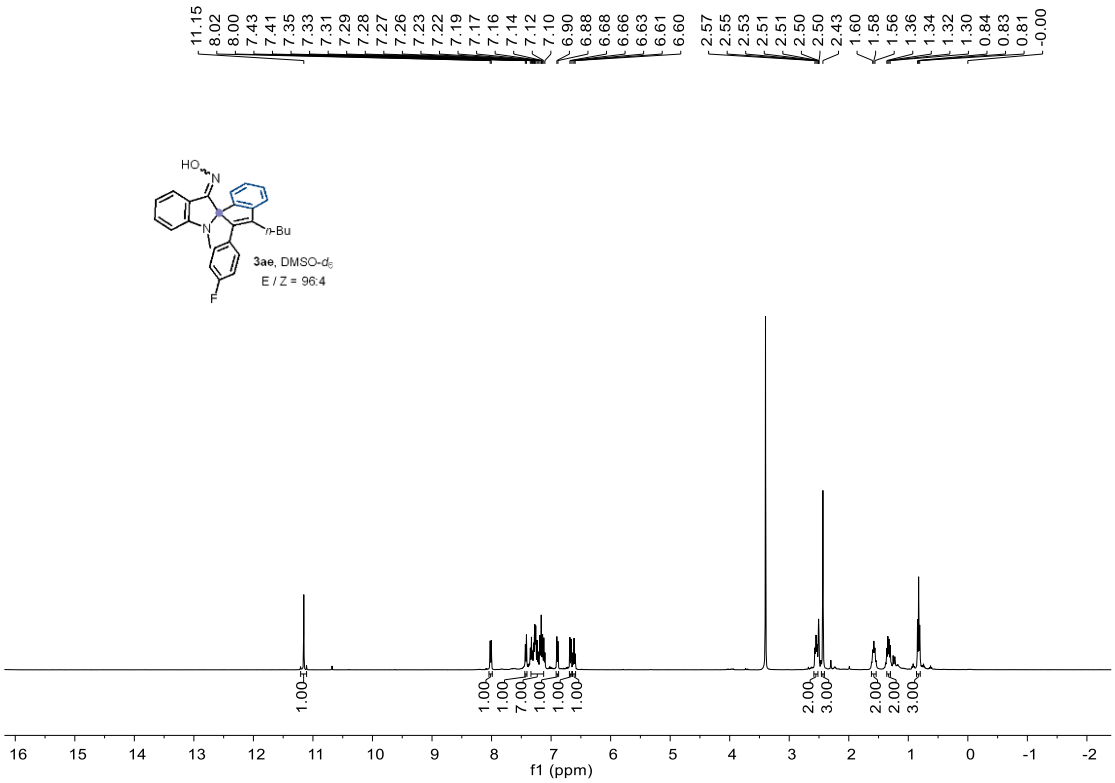

156.25
155.79
145.27
145.22
143.60
141.23
134.95
132.92
129.90
128.76
128.52
128.12
127.19
126.07
121.57
120.38
119.41
116.34
106.50
81.65
77.32
77.00
76.68
28.22
19.53
13.60
HO
N
N
Ph
Et
3ab, CDCl3
E / Z = 91:9
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

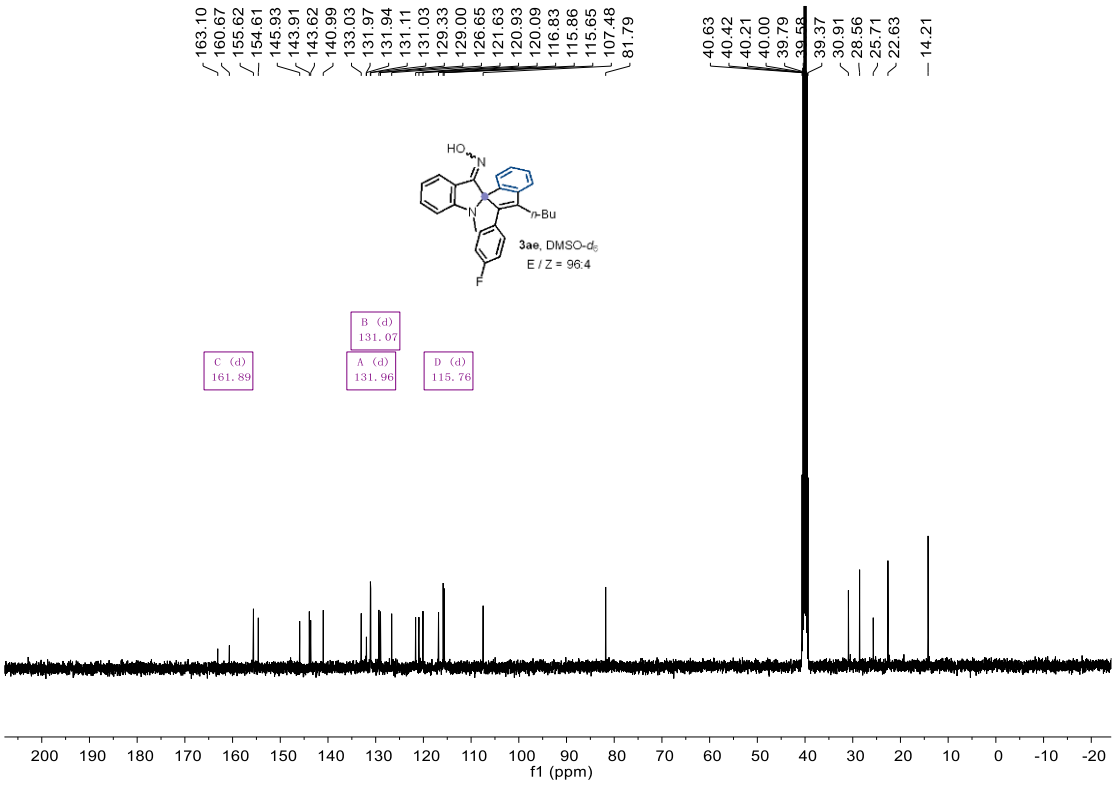

11.11
8.05
8.05
8.03
8.03
7.60
7.59
7.36
7.35
7.34
7.34
7.33
7.32
7.30
7.29
7.28
7.27
7.27
7.25
7.24
7.23
7.14
7.12
7.10
7.10
6.90
6.89
6.69
6.67
6.65
6.64
6.62
5.26
5.24
5.23
4.48
4.46
2.51
2.50
2.50
2.49
2.49
2.42
HO
N
OH
N
Ph
3ac, DMSO-d6
E / Z = 99:1
1.00
1.00
1.00
7.00
1.00
1.00
1.00
1.00
2.00
3.00
f1 (ppm)

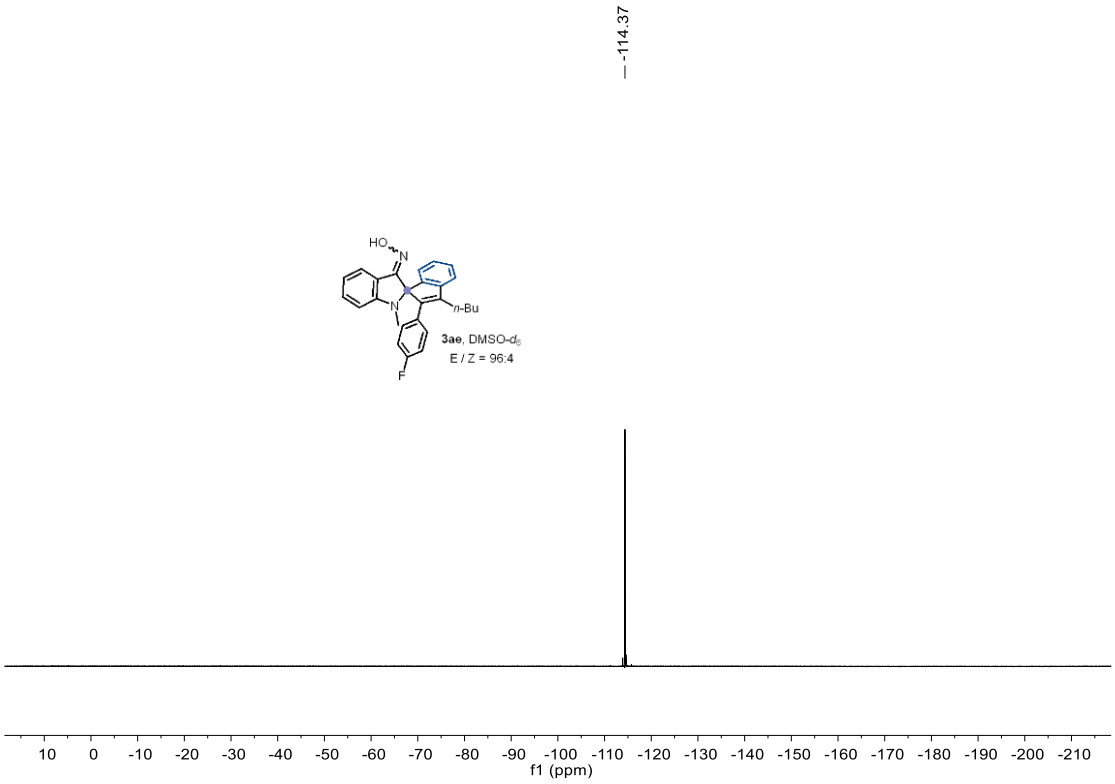

155.61
154.71
146.05
143.74
143.67
142.60
134.85
133.05
129.32
129.03
128.80
128.68
128.20
126.55
122.12
121.44
120.05
116.77
107.38
81.65
55.97
40.63
40.42
40.21
40.00
39.79
39.58
39.37
28.55
HO
N
OH
N
Ph
3ac, DMSO-d6
E / Z = 95:5
f1 (ppm)

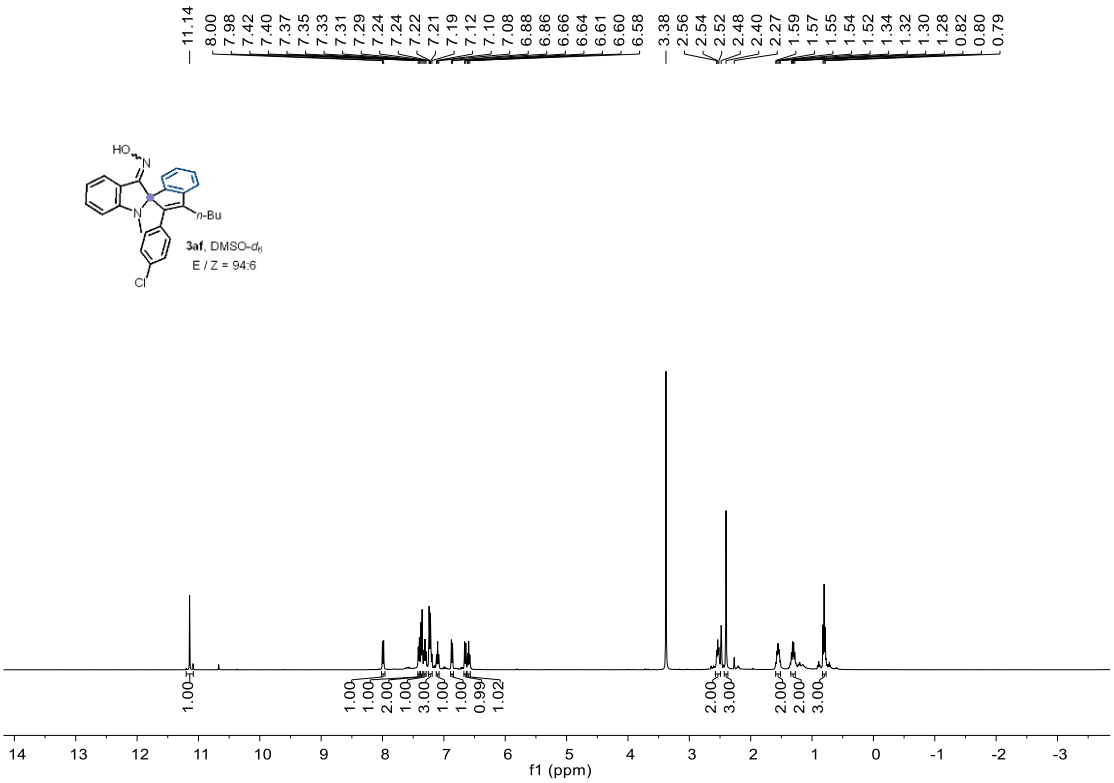

8.09 8.09 8.07 8.07 7.46 7.44 7.31 7.30 7.30 7.28 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.24 7.24 7.04 7.04 7.02 7.02 7.00 7.00 6.93 6.91 6.72 6.72 6.71 6.70 6.67 6.65 6.63 6.51 6.49 3.71 2.40 1.87 1.85 1.83 0.92 0.91 0.89 0.88 0.86 0.85 0.84 0.82 0.64 0.63 0.62 0.60 0.54 0.53 0.52 0.51 0.50 -0.00
HO
N
N
MeO
3ad, CDCl3
E / Z = 89:11
0.80 1.00 1.00 4.00 1.00 1.00 2.00 1.00 1.00 3.00 3.00 1.00 1.00 1.00 1.00 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

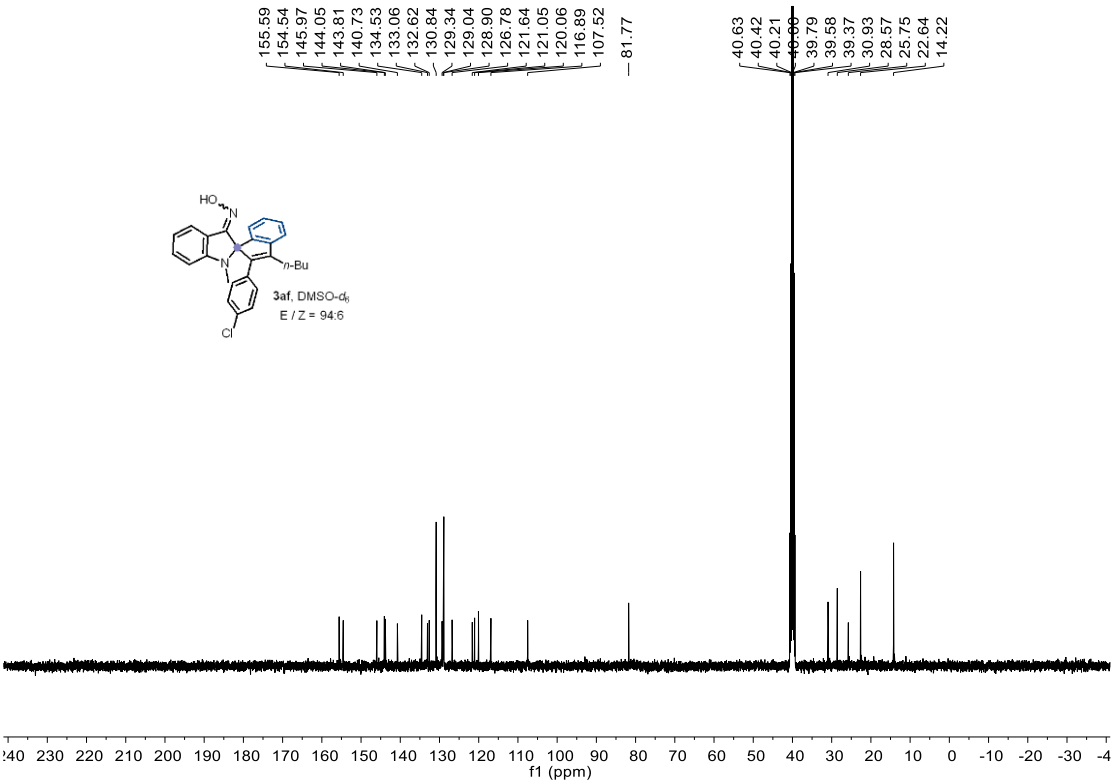

158.54 156.35 155.75 144.83 144.50 142.54 142.19 132.99 130.23 130.01 128.48 126.89 125.73 121.10 120.65 119.23 116.34 113.21 106.46 81.29 77.32 77.00 76.69 55.00 28.08 8.80 7.28 6.86
HO
N
N
MeO
3ad, CDCl3
E / Z = 89:11
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

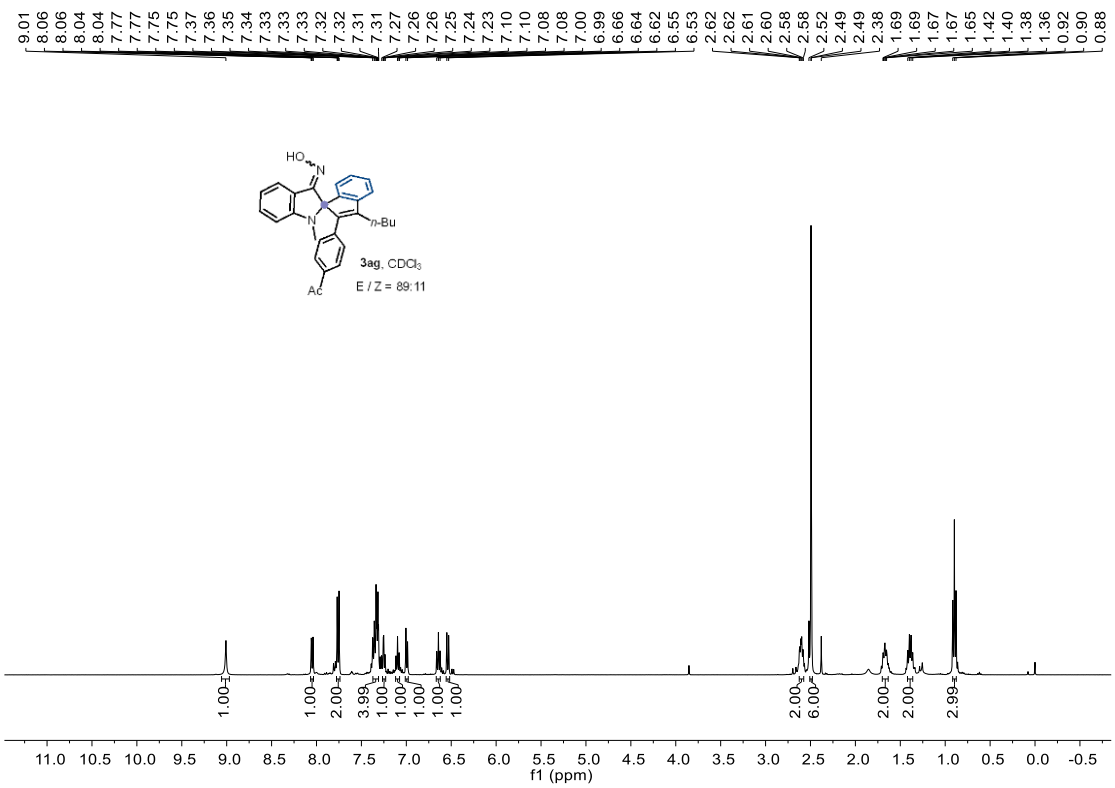

11.15
8.02
8.00
7.43
7.41
7.35
7.33
7.31
7.29
7.28
7.27
7.26
7.23
7.22
7.19
7.17
7.16
7.14
7.12
7.10
6.90
6.88
6.68
6.66
6.63
6.61
6.60
2.57
2.55
2.53
2.51
2.51
2.50
2.50
2.43
1.60
1.58
1.56
1.36
1.34
1.32
1.30
0.84
0.83
0.81
-0.00
HO
N
N
n-Bu
F
3ae, DMSO-d6
E / Z = 96:4
1.00
1.00
1.00
7.00
1.00
1.00
1.00
2.00
3.00
2.00
2.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

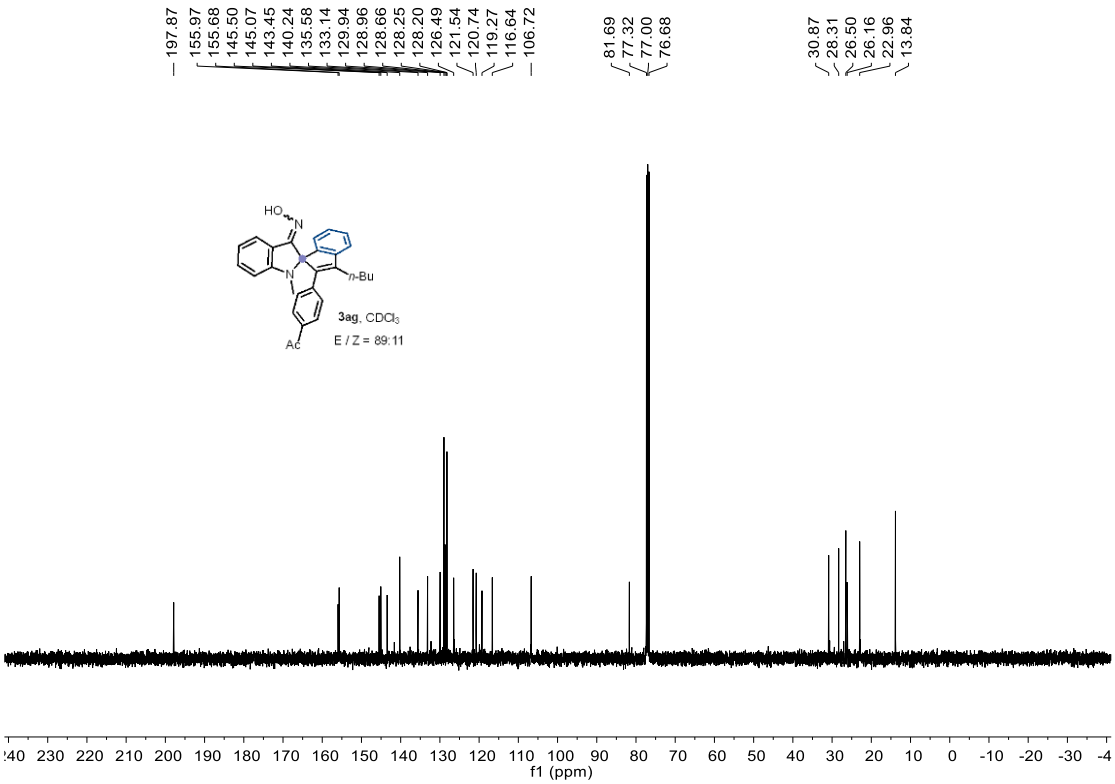

163.10
160.67
155.62
154.61
145.93
143.91
143.62
140.99
133.03
131.97
131.94
131.11
131.03
129.33
129.00
126.65
121.63
120.93
120.09
116.83
115.86
115.65
107.48
81.79
40.63
40.42
40.21
40.00
39.79
39.58
39.37
30.91
28.56
25.71
22.63
14.21
HO
N
N
n-Bu
F
3ae, DMSO-d6
E / Z = 96:4
B (d)
131.07
C (d)
161.89
A (d)
131.96
D (d)
115.76
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

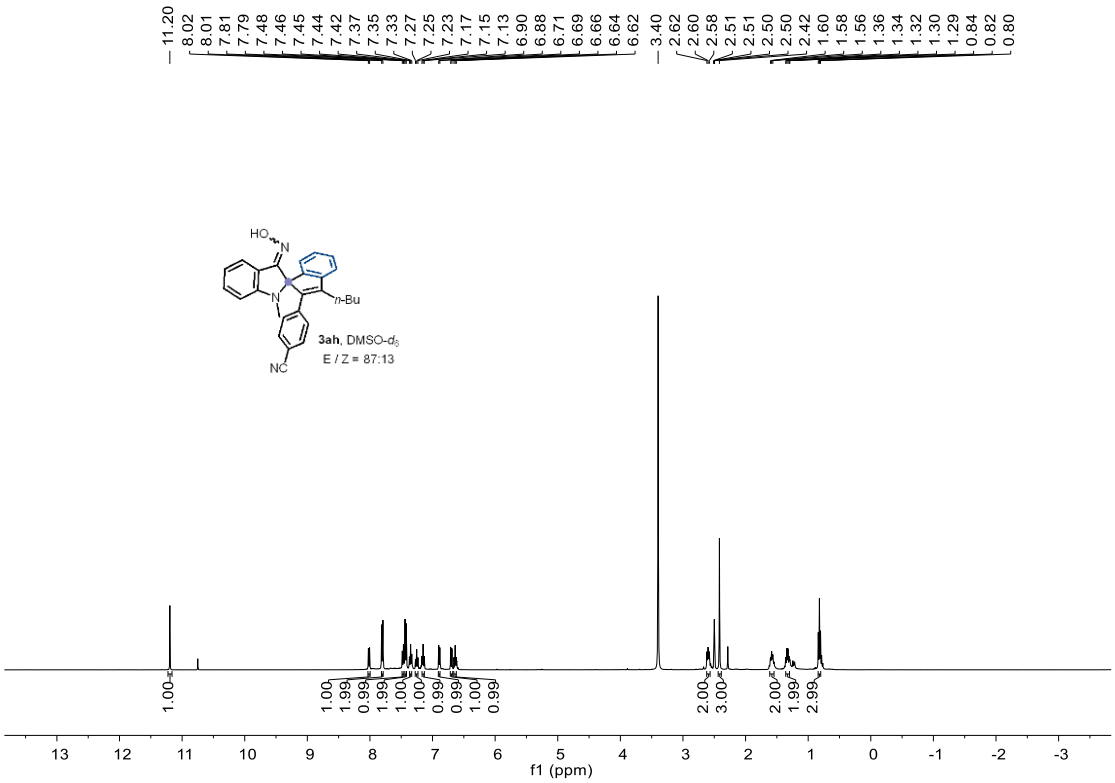

-114.37
HO
N
n-Bu
F
3ae, DMSO-d6
E / Z = 96:4
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

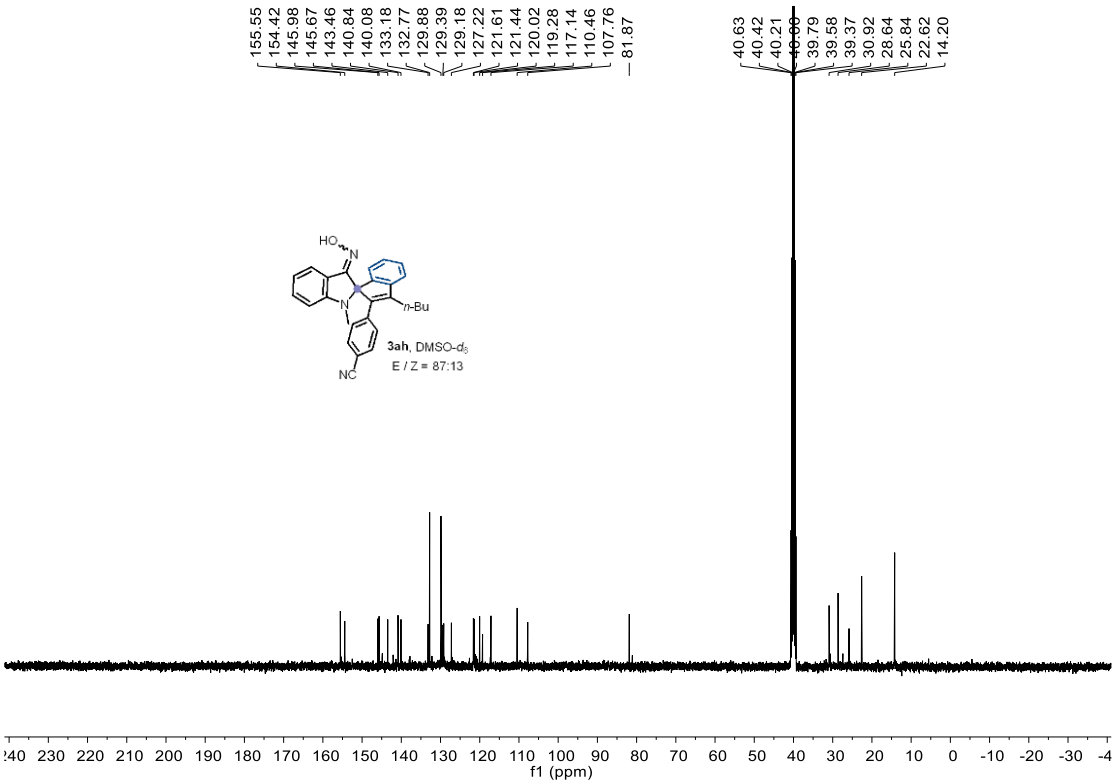

11.14
8.00
7.98
7.42
7.40
7.37
7.35
7.33
7.31
7.29
7.24
7.24
7.22
7.21
7.19
7.12
7.10
7.08
6.88
6.86
6.66
6.64
6.61
6.60
6.58
3.38
2.56
2.54
2.52
2.48
2.40
2.27
1.59
1.57
1.55
1.54
1.52
1.34
1.32
1.30
1.28
0.82
0.80
0.79
HO
N
n-Bu
Cl
3af, DMSO-d6
E / Z = 94:6
1.00
1.00
1.00
2.00
1.00
3.00
1.00
1.00
0.99
1.02
2.00
3.00
2.00
2.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

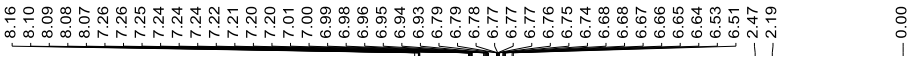

155.59
154.54
145.97
144.05
143.81
140.73
134.53
133.06
132.62
130.84
129.34
129.04
128.90
126.78
121.64
121.05
120.06
116.89
107.52
81.77
40.63
40.42
40.21
40.00
39.79
39.58
39.37
30.93
28.57
25.75
22.64
14.22
HO
N
n-Bu
Cl
3af, DMSO-d6
E / Z = 94:6
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

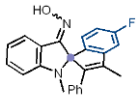

9.01 8.06 8.06 8.04 8.04 7.77 7.77 7.75 7.75 7.37 7.36 7.35 7.34 7.33 7.33 7.33 7.32 7.32 7.31 7.31 7.27 7.26 7.26 7.25 7.24 7.23 7.10 7.10 7.08 7.08 7.00 6.99 6.66 6.64 6.62 6.55 6.53
2.62 2.62 2.61 2.60 2.58 2.58 2.52 2.49 2.49 2.38 1.69 1.69 1.67 1.67 1.65 1.42 1.40 1.38 1.36 0.92 0.90 0.88
HO
N
n-Bu
Ac
3ag, CDCl3
E / Z = 89:11
1.00 1.00 2.00 3.99 1.00 1.00 1.00 1.00 1.00 2.00 6.00 2.00 2.00 2.99
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


197.87 155.97 155.68 145.50 145.07 143.45 140.24 135.58 133.14 129.94 128.96 128.66 128.25 128.20 126.49 121.54 120.74 119.27 116.64 106.72
81.69 77.32 77.00 76.68
30.87 28.31 26.50 26.16 22.96 13.84
HO
N
n-Bu
Ac
3ag, CDCl3
E / Z = 89:11
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)


11.20
8.02
8.01
7.81
7.79
7.48
7.46
7.45
7.44
7.42
7.37
7.35
7.33
7.27
7.25
7.23
7.17
7.15
7.13
6.90
6.88
6.71
6.69
6.66
6.64
6.62
3.40
2.62
2.60
2.58
2.51
2.51
2.50
2.50
2.42
1.60
1.58
1.56
1.36
1.34
1.32
1.30
1.29
0.84
0.82
0.80
HO
N
n-Bu
NC
3ah, DMSO-d6
E / Z = 87:13
1.00
1.00
1.99
0.99
0.99
1.99
1.00
1.00
0.99
0.99
1.00
0.99
2.00
3.00
2.00
1.99
2.99
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

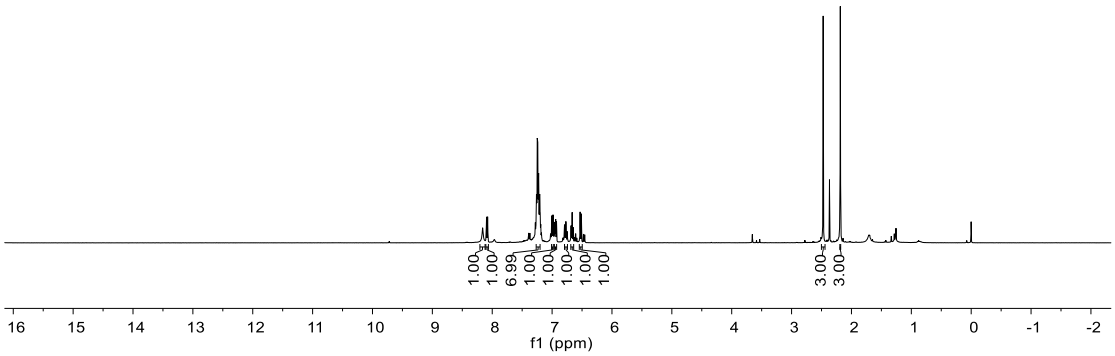

155.55
154.42
145.98
145.67
143.46
140.84
140.08
133.18
132.77
129.88
129.39
129.18
127.22
121.61
121.44
120.02
119.28
117.14
110.46
107.76
81.87
40.63
40.42
40.21
40.00
39.79
39.58
39.37
30.92
28.64
25.84
22.62
14.20
HO
N
n-Bu
NC
3ah, DMSO-d6
E / Z = 87:13
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

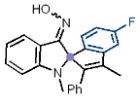




3ba, $CDCl_3$

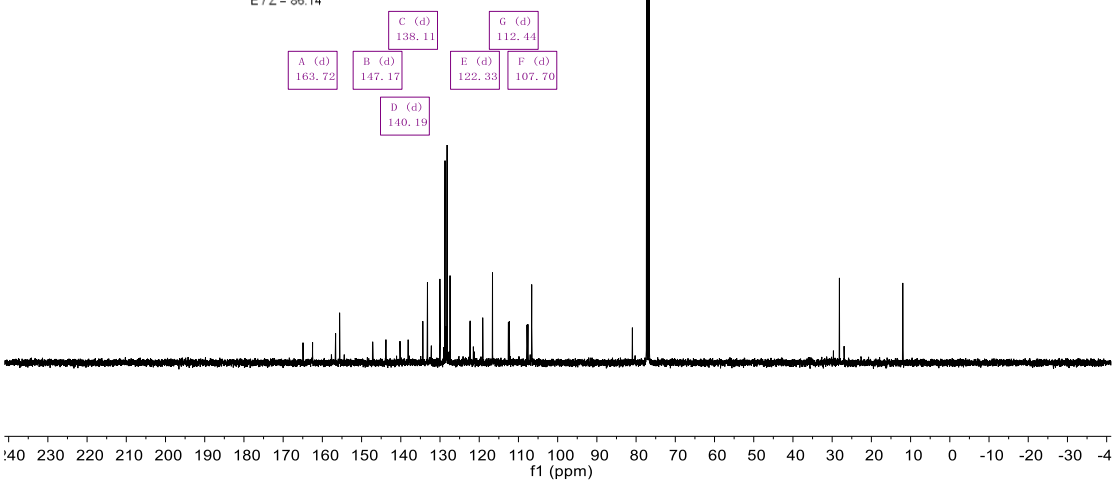
E / Z = 86:14

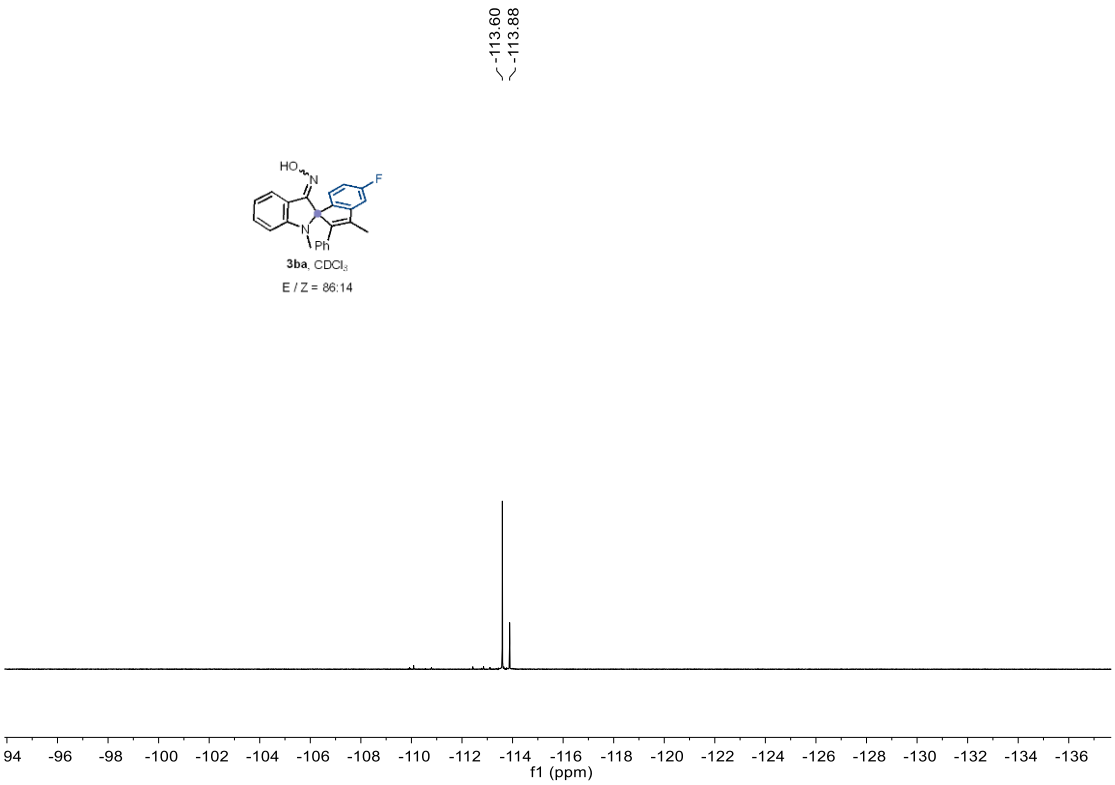


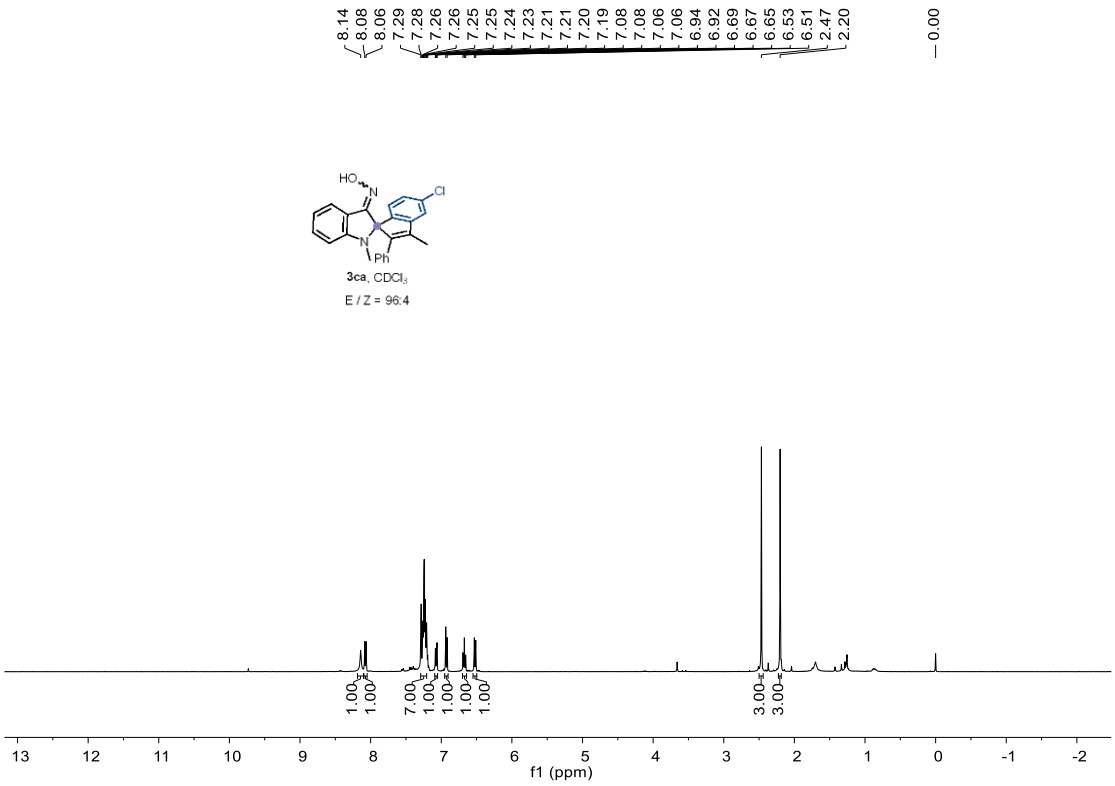


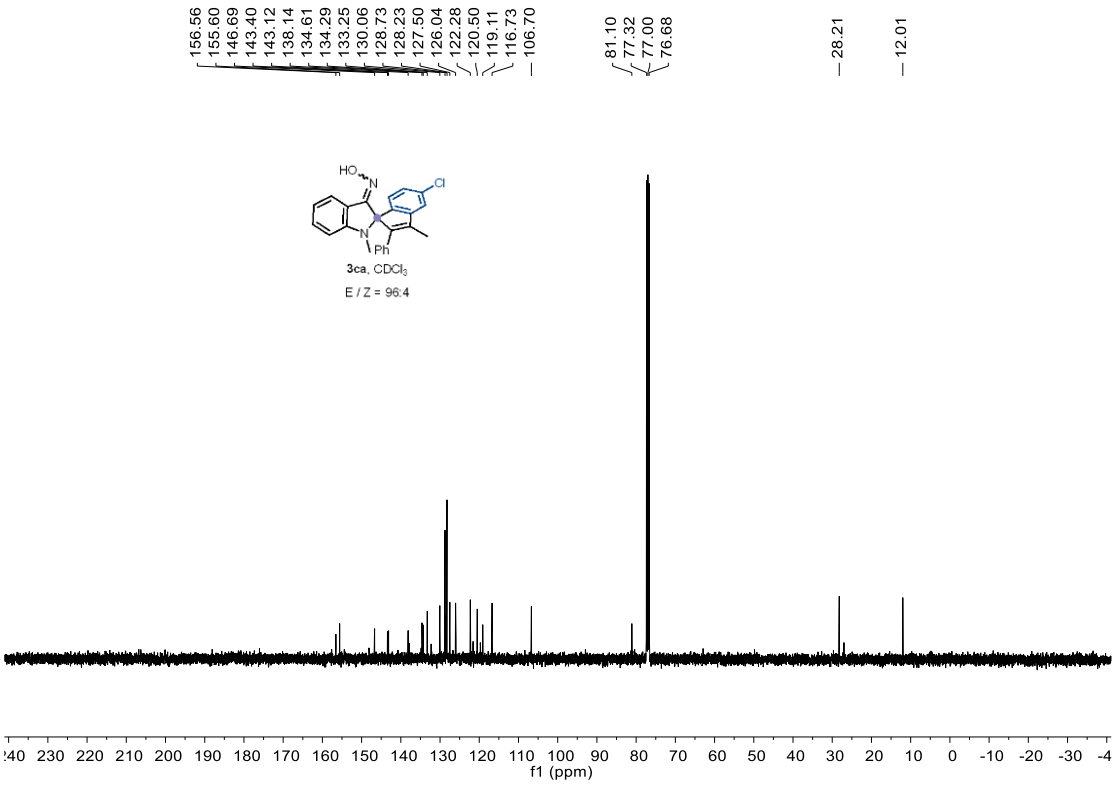
3ba, $CDCl_3$

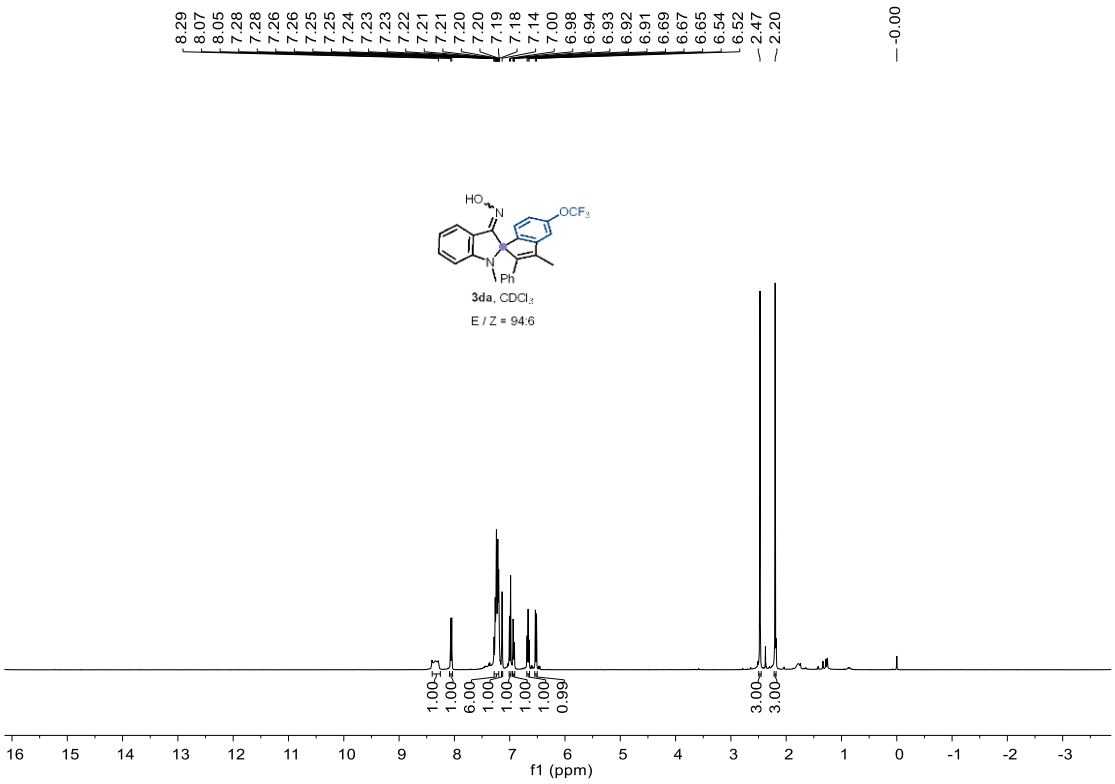
E / Z = 86:14

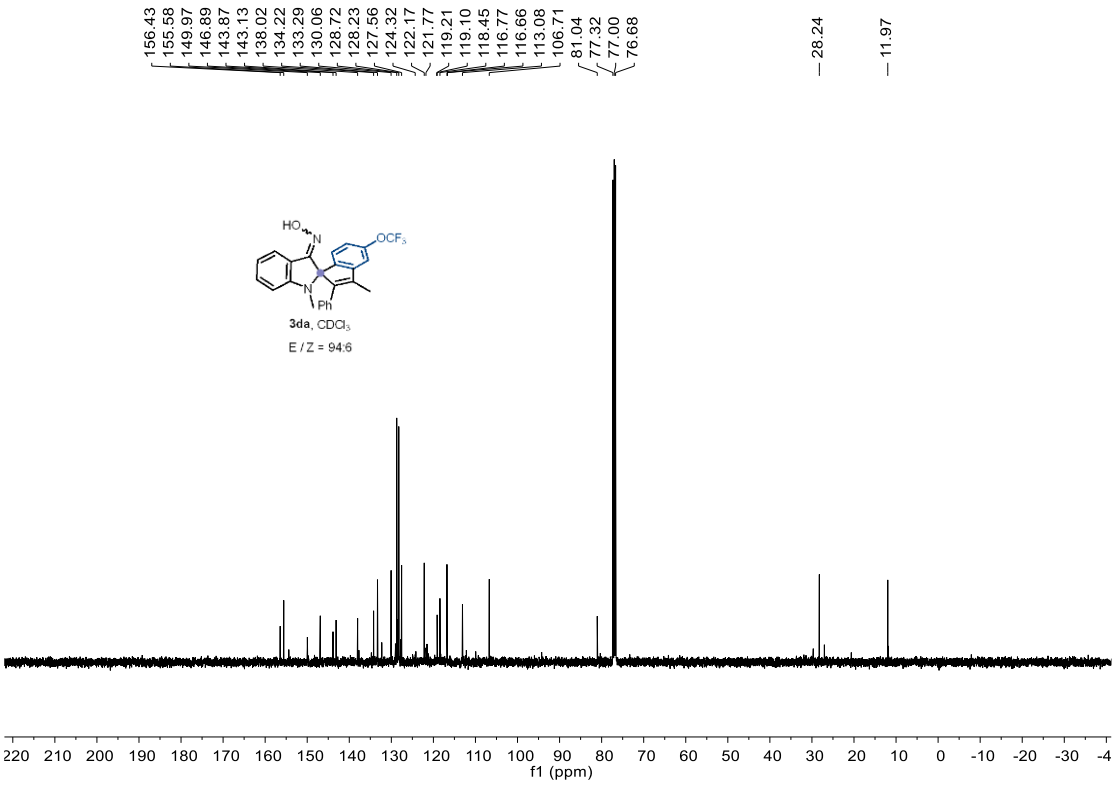


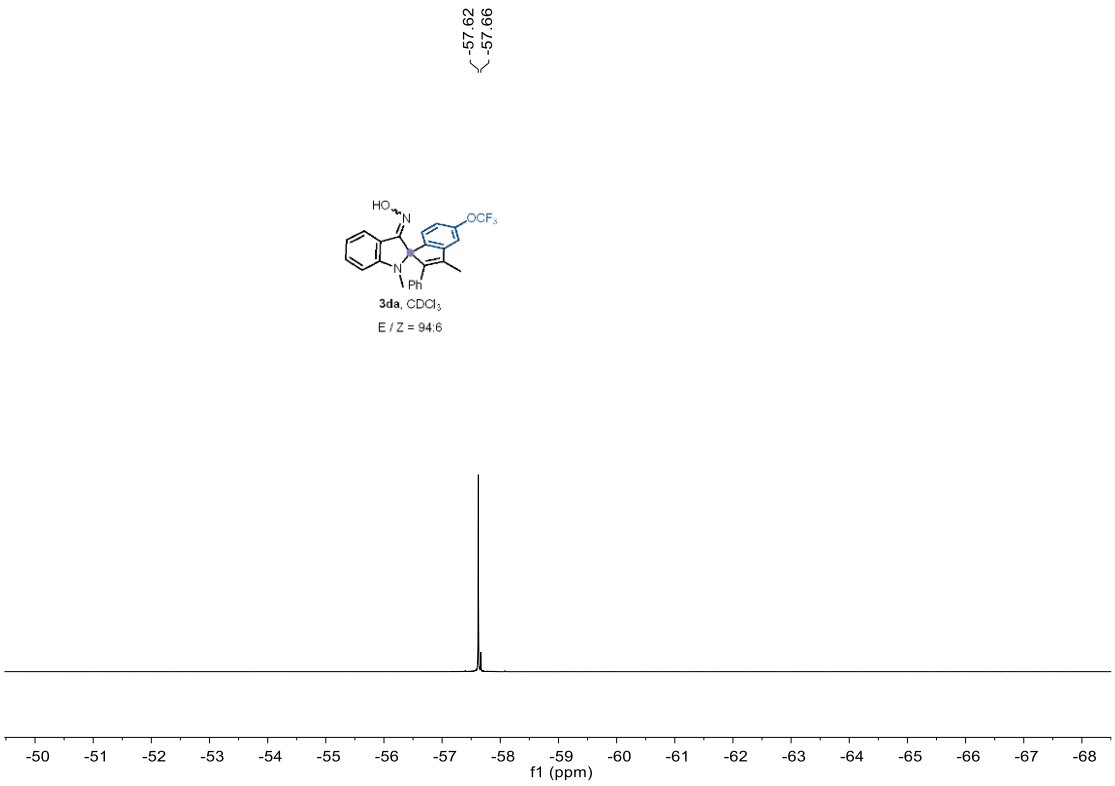

-113.60
-113.88
HO
N
F
N
Ph
3ba, CDCl3
E / Z = 86:14
94 -96 -98 -100 -102 -104 -106 -108 -110 -112 -114 -116 -118 -120 -122 -124 -126 -128 -130 -132 -134 -136
f1 (ppm)

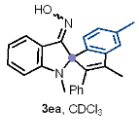

8.14
8.08
8.06
7.29
7.28
7.26
7.26
7.25
7.25
7.24
7.23
7.21
7.21
7.20
7.19
7.08
7.08
7.06
7.06
6.94
6.92
6.69
6.67
6.65
6.53
6.51
2.47
2.20
0.00
HO
N
Cl
N
Ph
3ca, CDCl3
E / Z = 96:4
1.00
1.00
7.00
1.00
1.00
1.00
1.00
3.00
3.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


156.56
155.60
146.69
143.40
143.12
138.14
134.61
134.29
133.25
130.06
128.73
128.23
127.50
126.04
122.28
120.50
119.11
116.73
106.70
81.10
77.32
77.00
76.68
28.21
12.01
HO
N
Cl
N
Ph
3ca, CDCl3
E / Z = 96:4
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)


8.29
8.07
8.05
7.28
7.28
7.26
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.21
7.20
7.20
7.19
7.18
7.14
7.00
6.98
6.94
6.93
6.92
6.91
6.69
6.67
6.65
6.54
6.52
2.47
2.20
0.00
HO
N
OCF3
N
Ph
3da, CDCl3
E / Z = 94:6
1.00
1.00
6.00
1.00
1.00
1.00
1.00
0.99
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

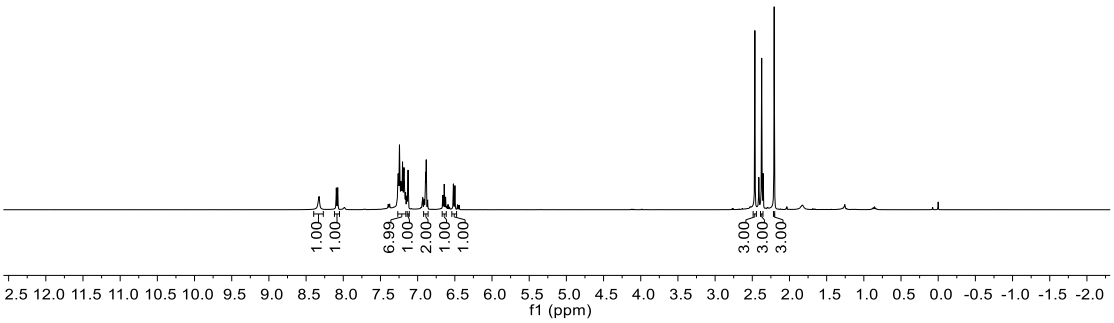

156.43
155.58
149.97
146.89
143.87
143.13
138.02
134.22
133.29
130.06
128.72
128.23
127.56
124.32
122.17
121.77
119.21
119.10
118.45
116.77
116.66
113.08
106.71
81.04
77.32
77.00
76.68
28.24
11.97
HO
N
OCF3
N
Ph
3da, CDCl3
E / Z = 94:6
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)


-57.62
-57.66
HO
N
OCF3
N
Ph
3da, CDCl3
E / Z = 94:6
-50
-51
-52
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
f1 (ppm)



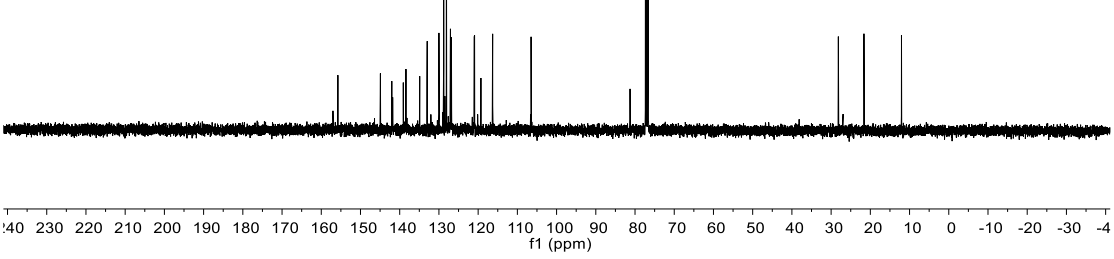
3ea, $CDCl_3$

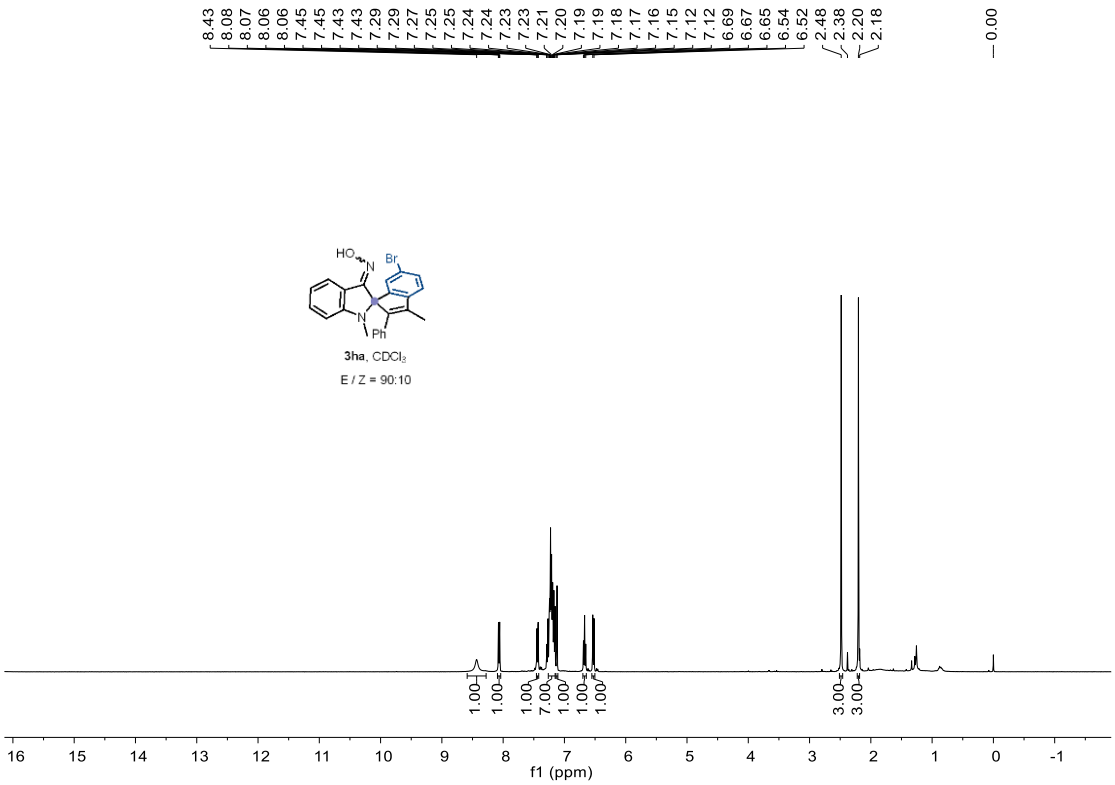
E / Z = 87:13

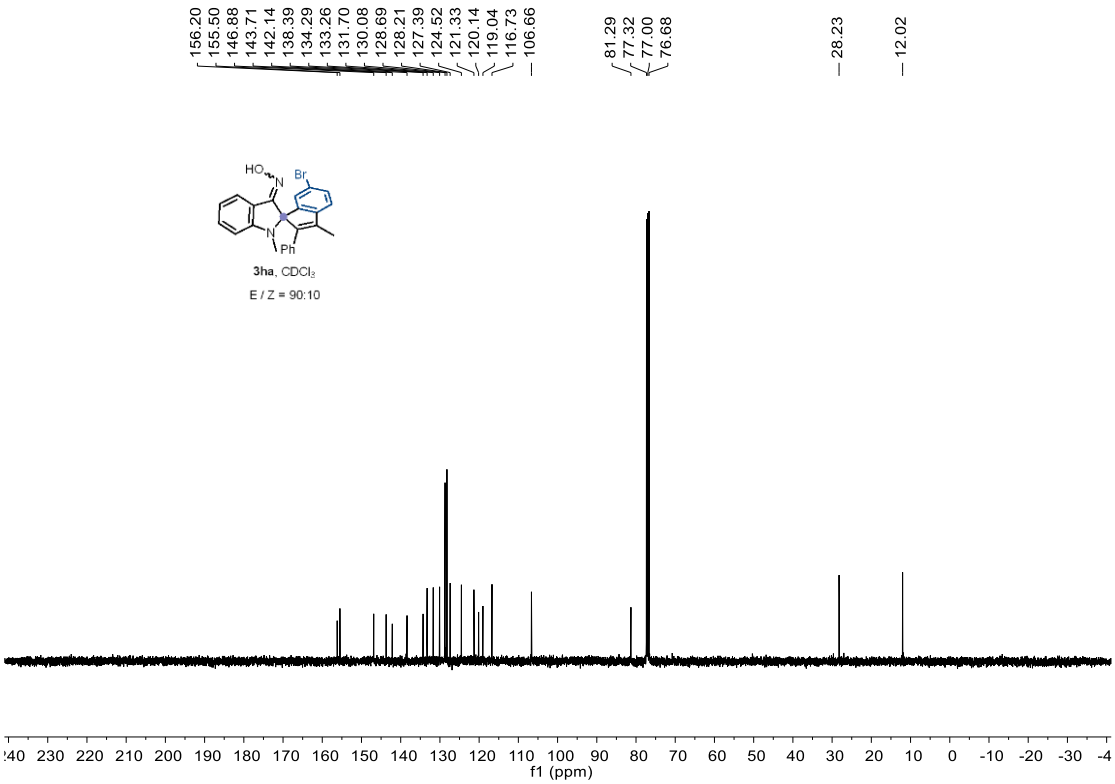


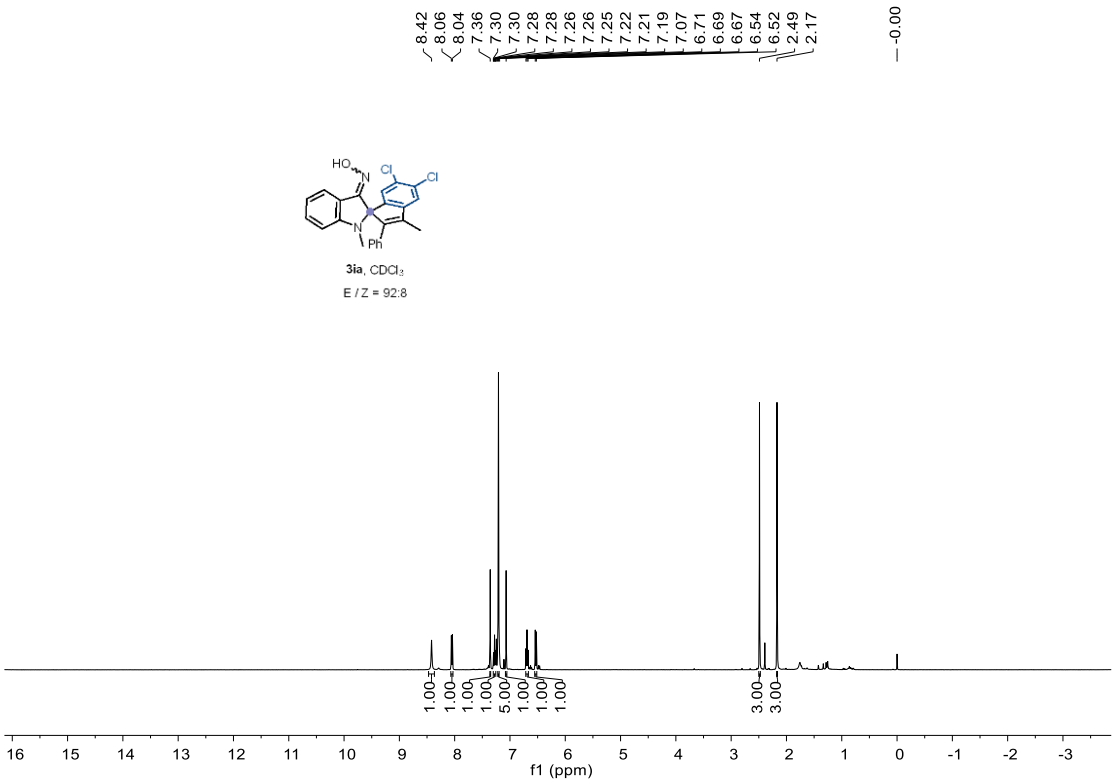
3ea, $CDCl_3$

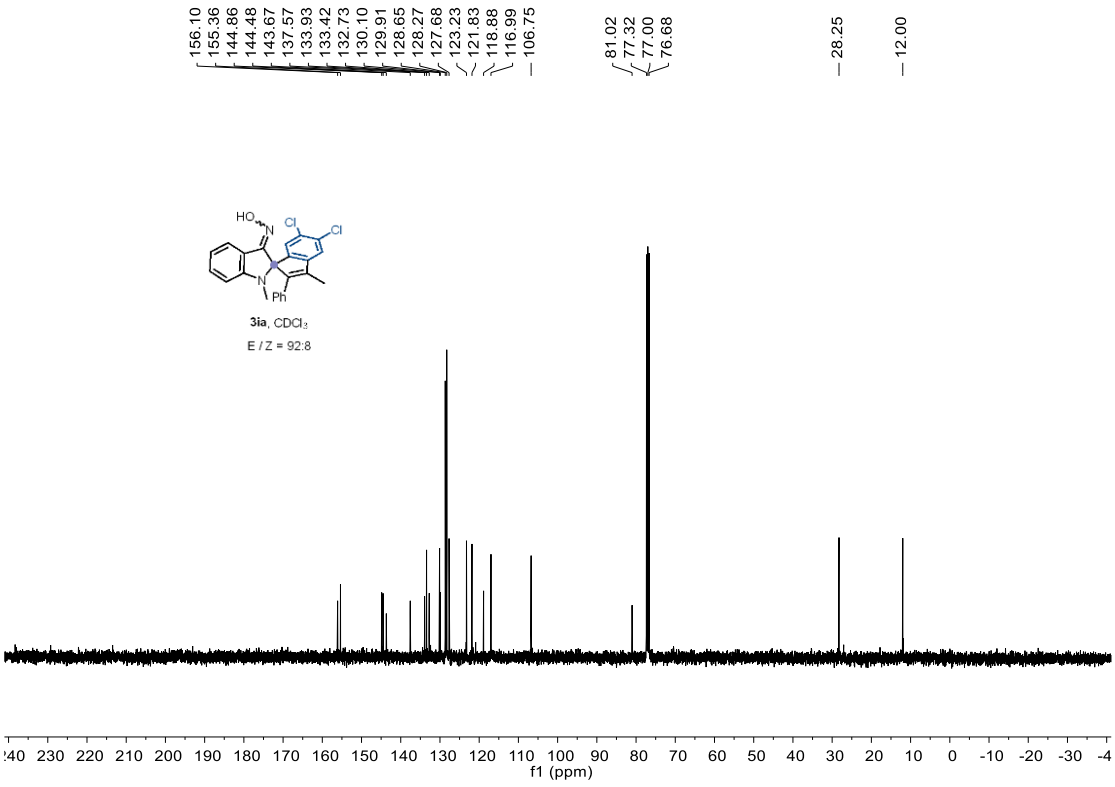
E / Z = 87:13

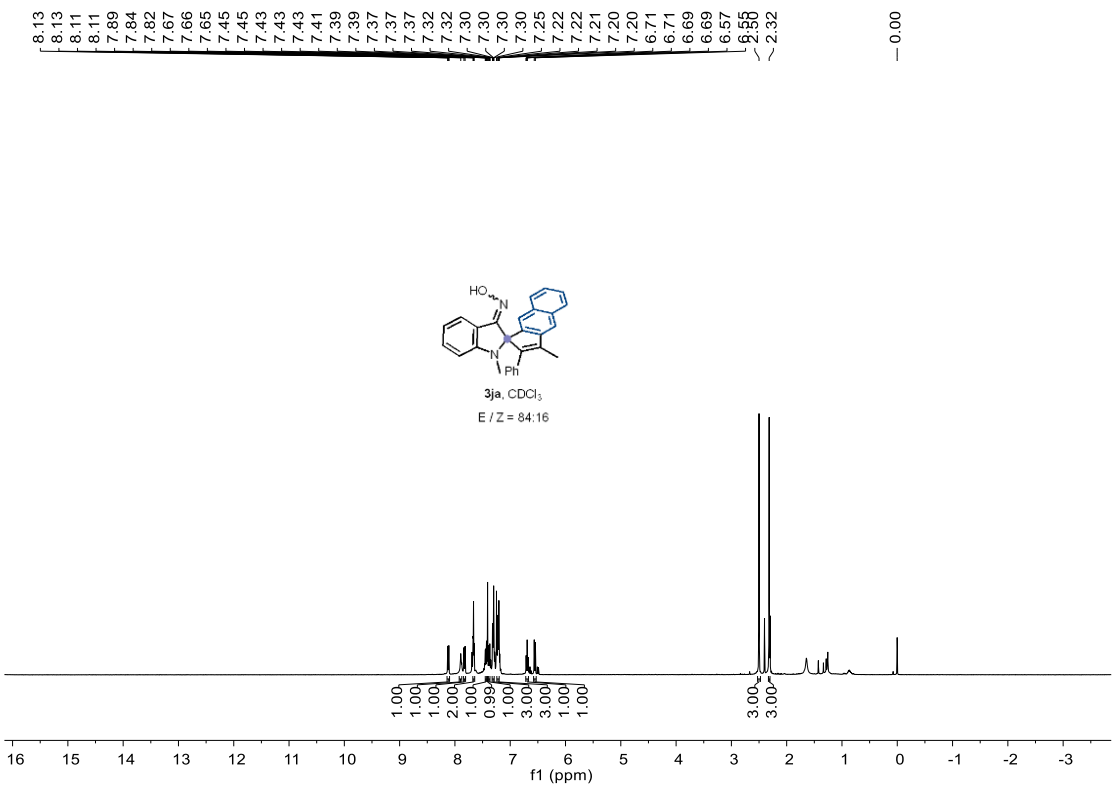


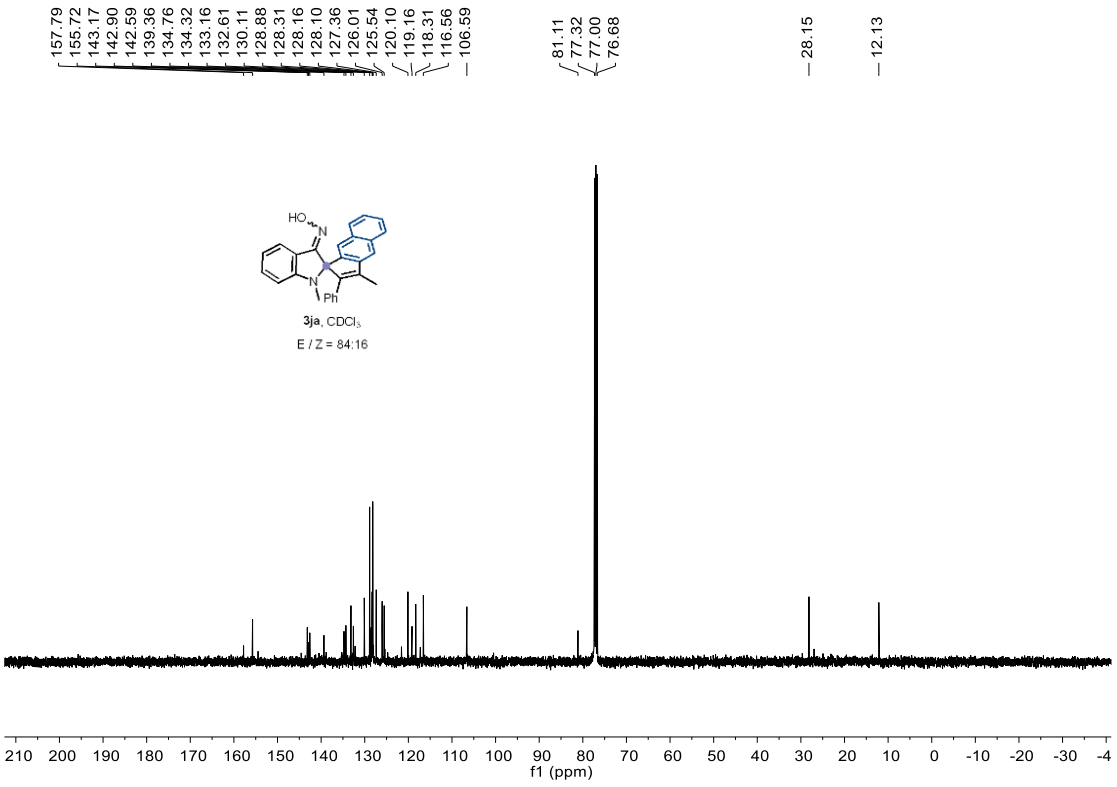

8.43
8.08
8.07
8.06
8.06
7.45
7.45
7.43
7.43
7.29
7.29
7.27
7.25
7.25
7.24
7.24
7.23
7.23
7.21
7.20
7.19
7.19
7.18
7.17
7.16
7.15
7.12
7.12
6.69
6.67
6.65
6.54
6.52
2.48
2.38
2.20
2.18
0.00
HO
N
Br
N
Ph
3ha, CDCl3
E / Z = 90:10
1.00
1.00
1.00
7.00
1.00
1.00
1.00
3.00
3.00
f1 (ppm)

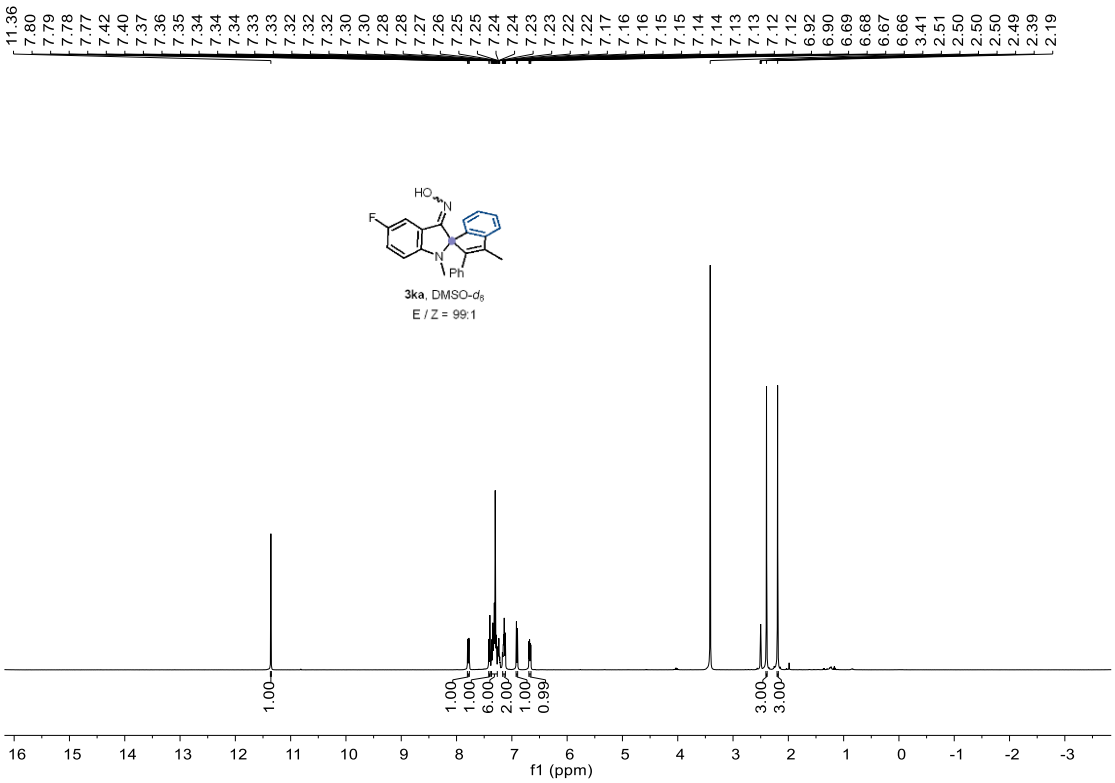

156.20
155.50
146.88
143.71
142.14
138.39
134.29
133.26
131.70
130.08
128.69
128.21
127.39
124.52
121.33
120.14
119.04
116.73
106.66
81.29
77.32
77.00
76.68
28.23
12.02
HO
N
Br
N
Ph
3ha, CDCl3
E / Z = 90:10
f1 (ppm)

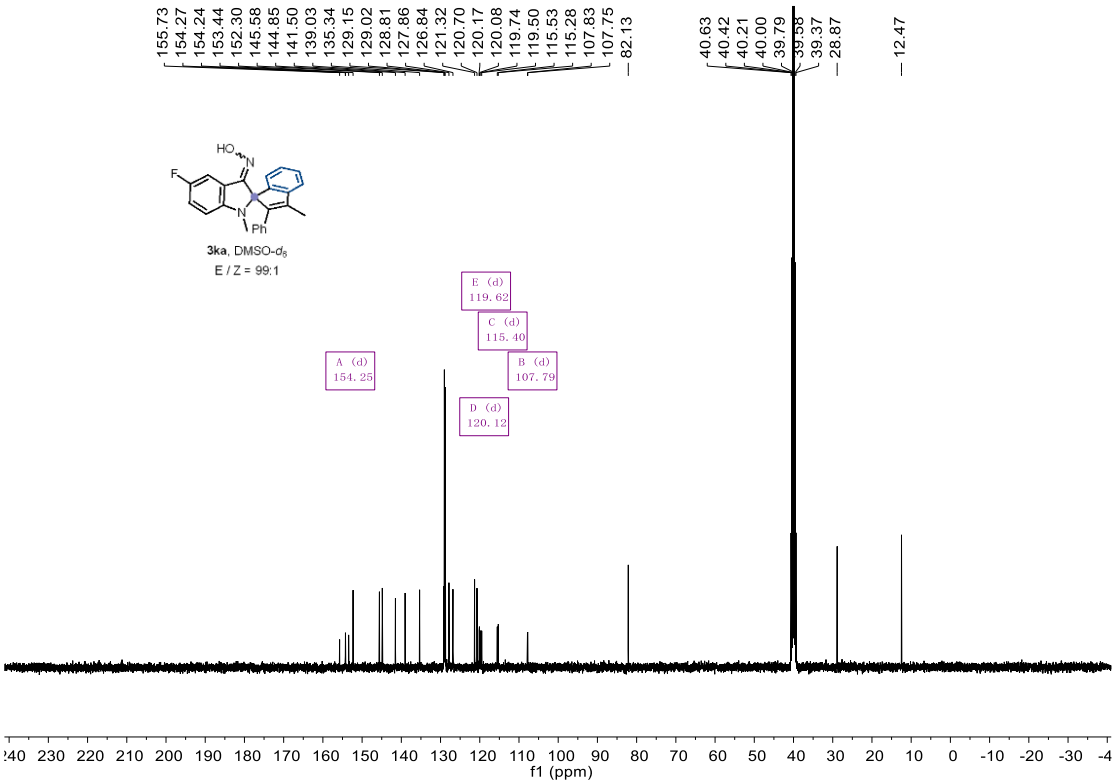

8.42
8.06
8.04
7.36
7.30
7.30
7.28
7.28
7.26
7.26
7.25
7.22
7.21
7.19
7.07
6.71
6.69
6.67
6.54
6.52
2.49
2.17
-0.00
HO
N
Cl
Cl
N
Ph
3ia, CDCl3
E / Z = 92:8
1.00
1.00
1.00
1.00
5.00
1.00
1.00
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

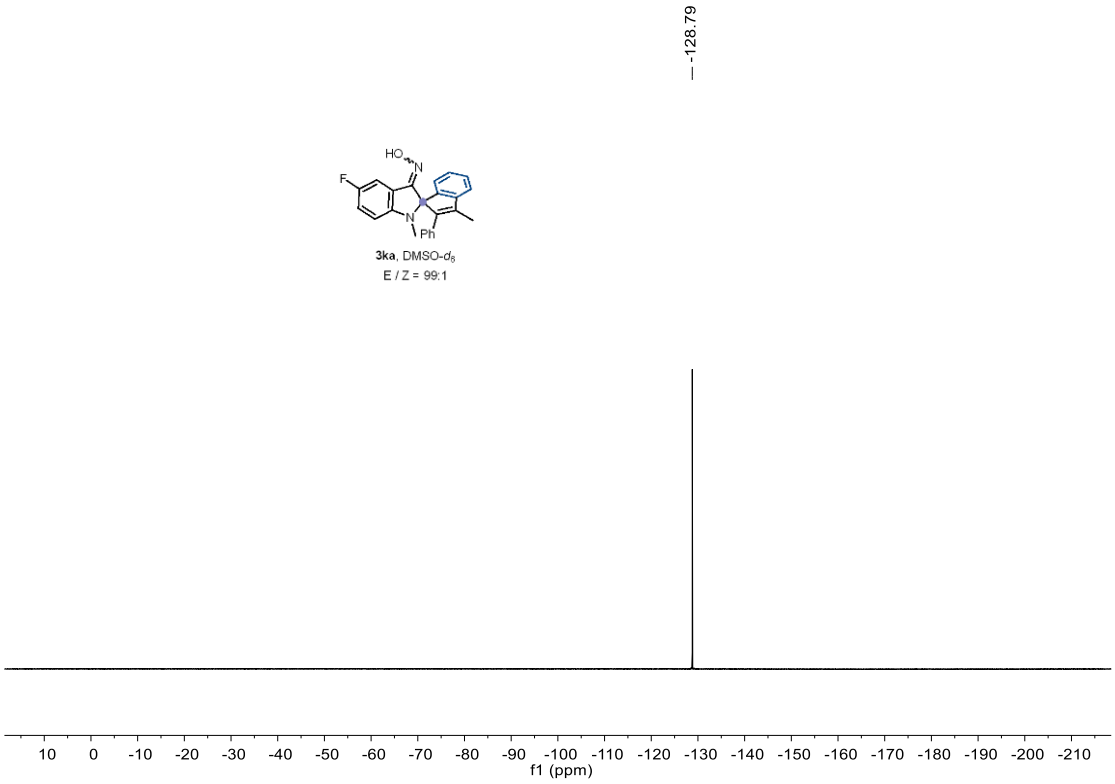

156.10
155.36
144.86
144.48
143.67
137.57
133.93
133.42
132.73
130.10
129.91
128.65
128.27
127.68
123.23
121.83
118.88
116.99
106.75
81.02
77.32
77.00
76.68
28.25
12.00
HO
N
Cl
Cl
N
Ph
3ia, CDCl3
E / Z = 92:8
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

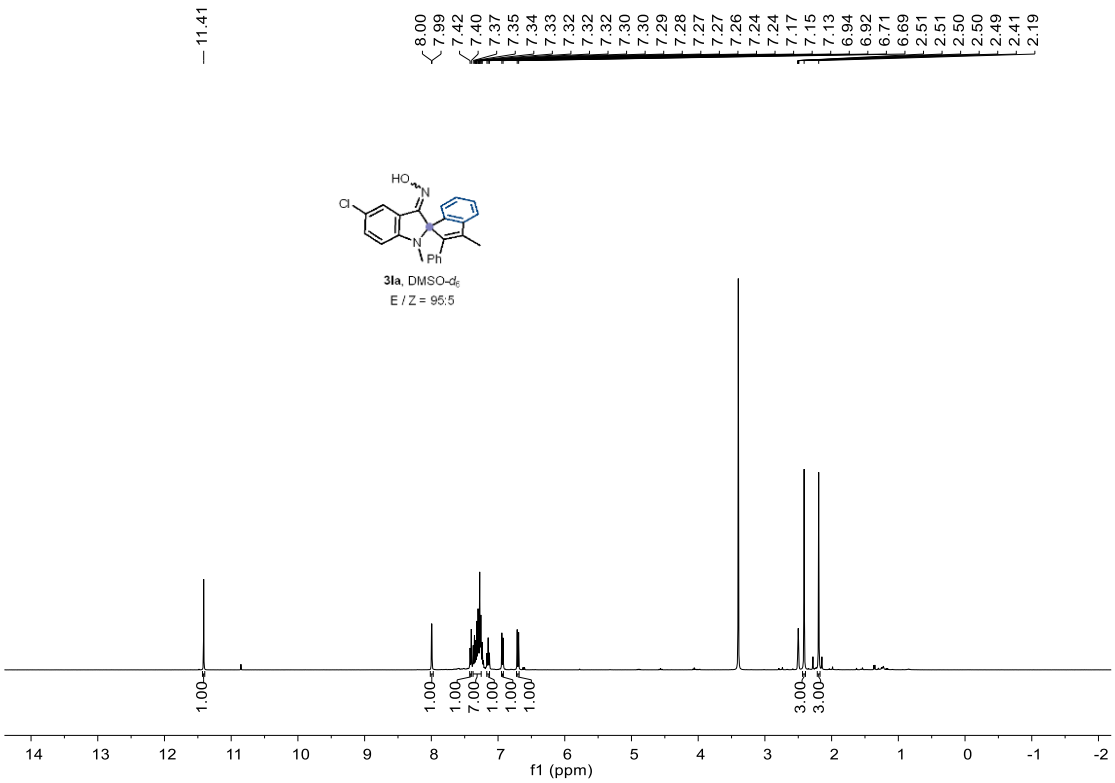

8.13
8.13
8.11
8.11
7.89
7.84
7.82
7.67
7.66
7.65
7.45
7.45
7.43
7.43
7.43
7.41
7.39
7.39
7.37
7.37
7.37
7.32
7.32
7.30
7.30
7.30
7.30
7.25
7.22
7.22
7.21
7.20
7.20
6.71
6.71
6.69
6.69
6.57
6.55
2.58
2.32
0.00
HO
N
N
Ph
3ja, CDCl3
E / Z = 84:16
1.00
1.00
1.00
2.00
1.00
0.99
1.00
3.00
3.00
1.00
1.00
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

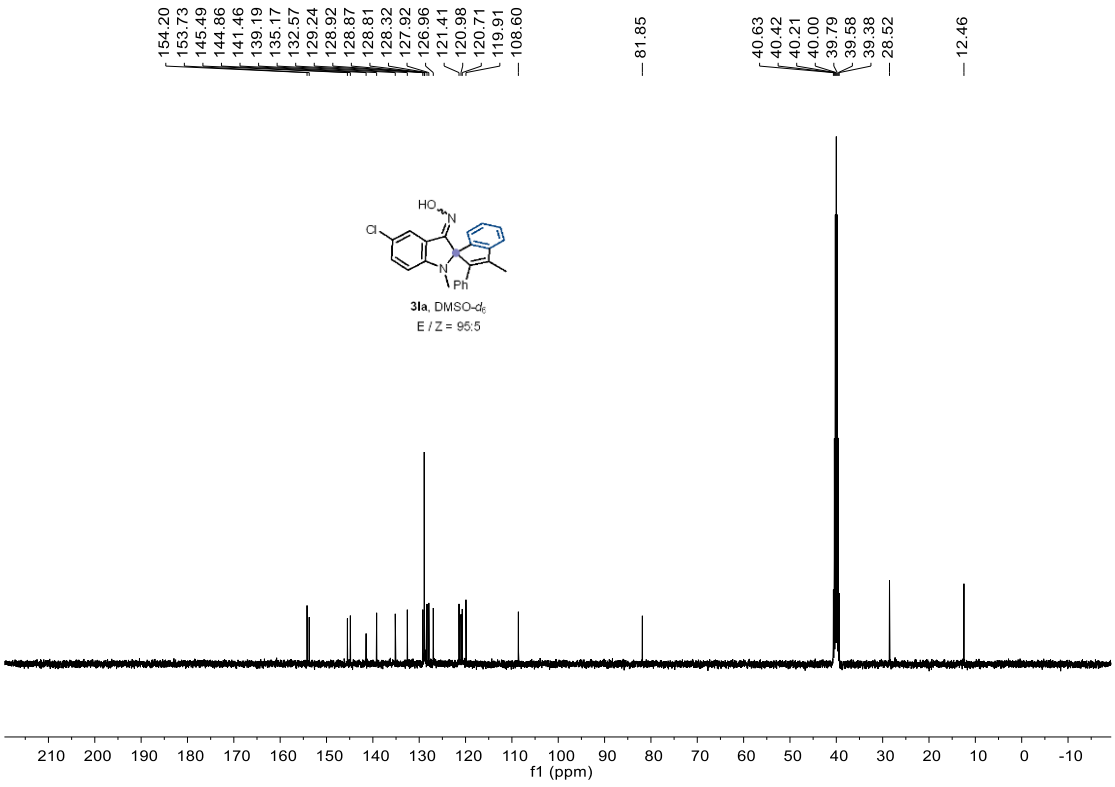

157.79
155.72
143.17
142.90
142.59
139.36
134.76
134.32
133.16
132.61
130.11
128.88
128.31
128.16
128.10
127.36
126.01
125.54
120.10
119.16
118.31
116.56
106.59
81.11
77.32
77.00
76.68
28.15
12.13
HO
N
N
Ph
3ja, CDCl3
E / Z = 84:16
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

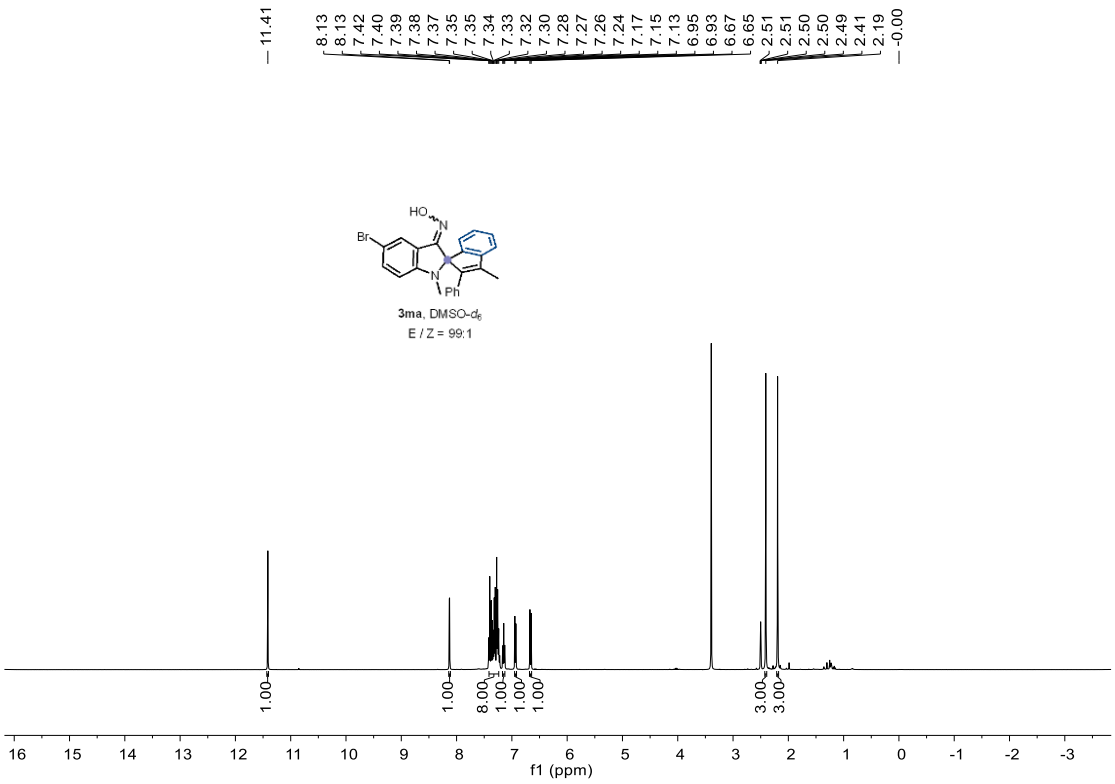

11.36
7.80
7.79
7.78
7.77
7.42
7.40
7.37
7.36
7.35
7.34
7.34
7.34
7.33
7.33
7.32
7.32
7.32
7.30
7.30
7.28
7.28
7.27
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.17
7.16
7.16
7.15
7.15
7.14
7.14
7.13
7.13
7.12
7.12
6.92
6.90
6.69
6.68
6.67
6.66
3.41
2.51
2.50
2.50
2.50
2.49
2.39
2.19
HO
N
F
N
Ph
3ka, DMSO-d6
E / Z = 99:1
1.00
1.00
1.00
6.00
2.00
1.00
0.99
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

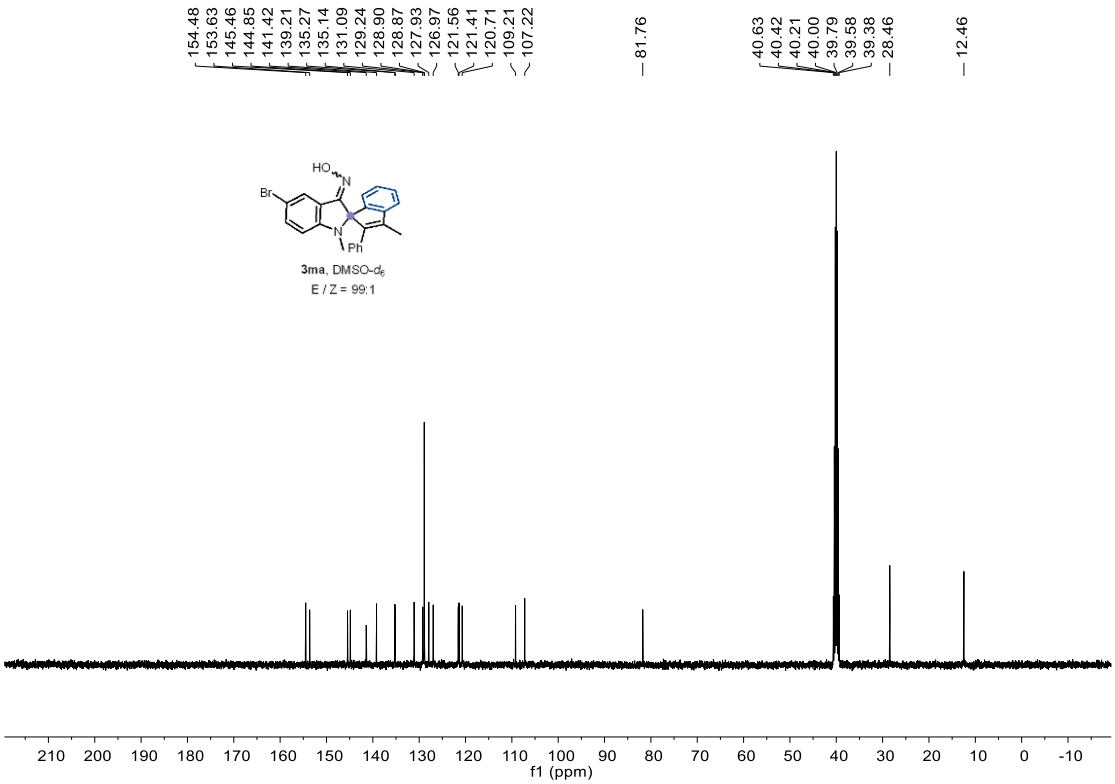

155.73
154.27
154.24
153.44
152.30
145.58
144.85
141.50
139.03
135.34
129.15
129.02
128.81
127.86
126.84
121.32
120.70
120.17
120.08
119.74
119.50
115.53
115.28
107.83
107.75
82.13
40.63
40.42
40.21
40.00
39.79
39.58
39.37
28.87
12.47
HO
N
F
N
Ph
3ka, DMSO-d6
E / Z = 99:1
E (d)
119.62
C (d)
115.40
A (d)
154.25
B (d)
107.79
D (d)
120.12
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)


-128.79
HO
N
F
N
Ph
3ka, DMSO-d6
E / Z = 99:1
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


11.41
8.00
7.99
7.42
7.40
7.37
7.35
7.34
7.33
7.32
7.32
7.32
7.30
7.30
7.29
7.28
7.27
7.27
7.26
7.24
7.24
7.17
7.15
7.13
6.94
6.92
6.71
6.69
2.51
2.51
2.50
2.50
2.49
2.41
2.19
HO
N
Cl
N
Ph
3la, DMSO-d6
E / Z = 95:5
1.00
1.00
1.00
7.00
1.00
1.00
1.00
3.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


154.20
153.73
145.49
144.86
141.46
139.19
135.17
132.57
129.24
128.92
128.87
128.81
128.32
127.92
126.96
121.41
120.98
120.71
119.91
108.60
81.85
40.63
40.42
40.21
40.00
39.79
39.58
39.38
28.52
12.46
HO
N
Cl
N
Ph
3la, DMSO-d6
E / Z = 95:5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


11.41
8.13
8.13
7.42
7.40
7.39
7.38
7.37
7.35
7.35
7.34
7.33
7.32
7.30
7.28
7.27
7.26
7.24
7.17
7.15
7.13
6.95
6.93
6.67
6.65
2.51
2.51
2.50
2.50
2.49
2.41
2.19
0.00
HO
N
Br
N
Ph
3ma, DMSO-d6
E / Z = 99:1
1.00
1.00
8.00
1.00
1.00
1.00
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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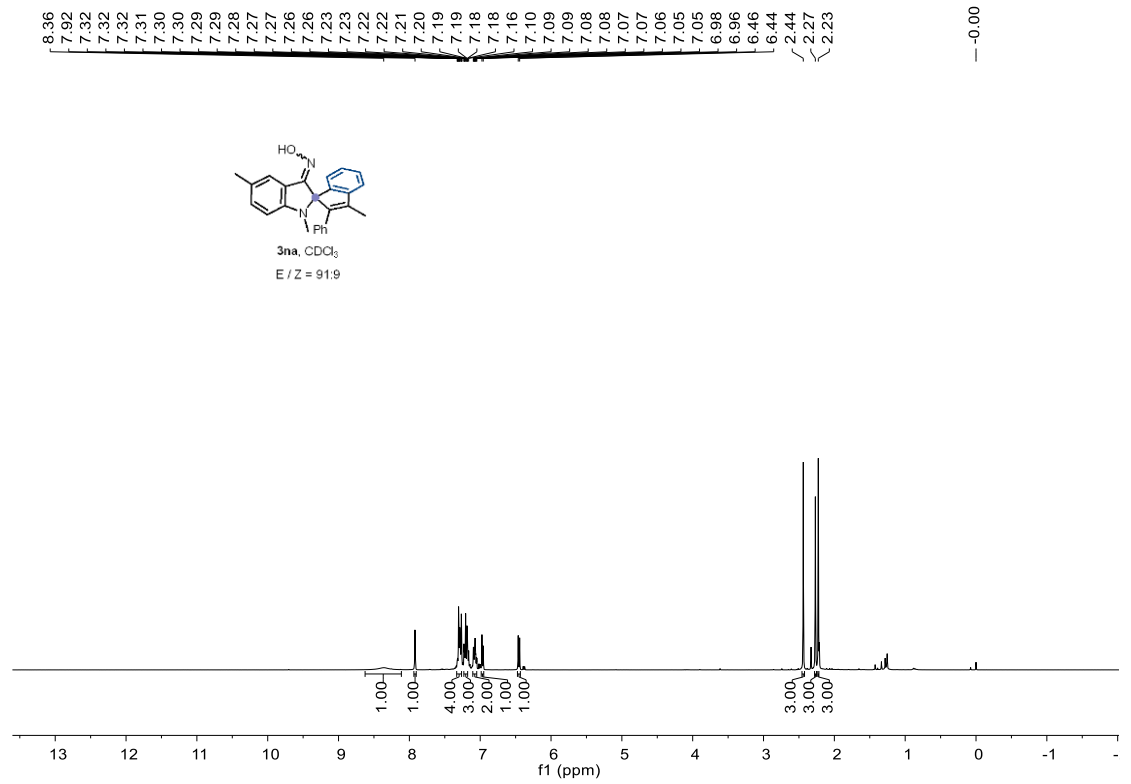
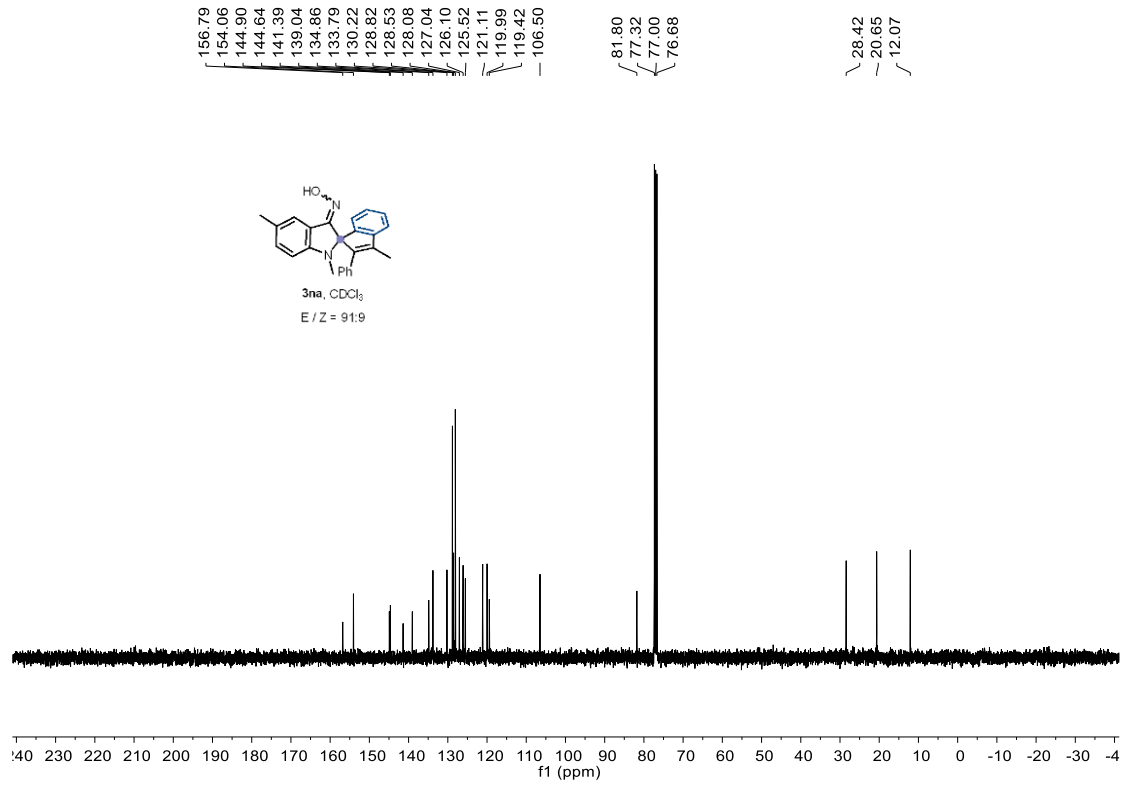
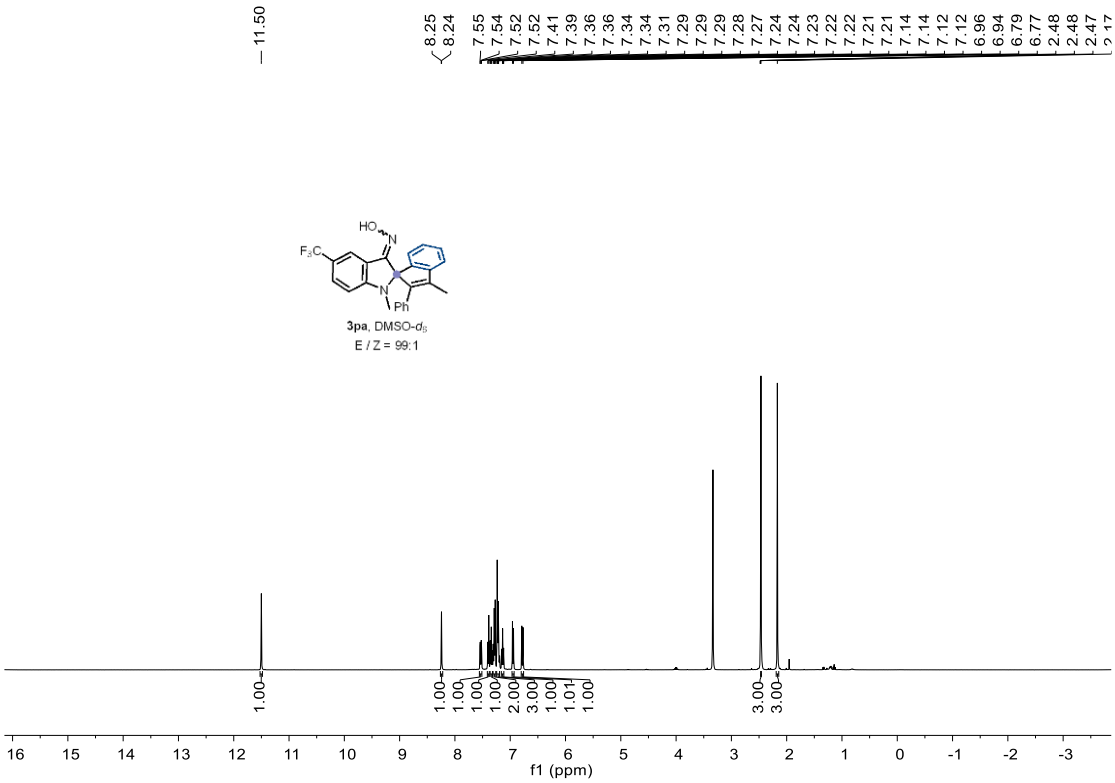
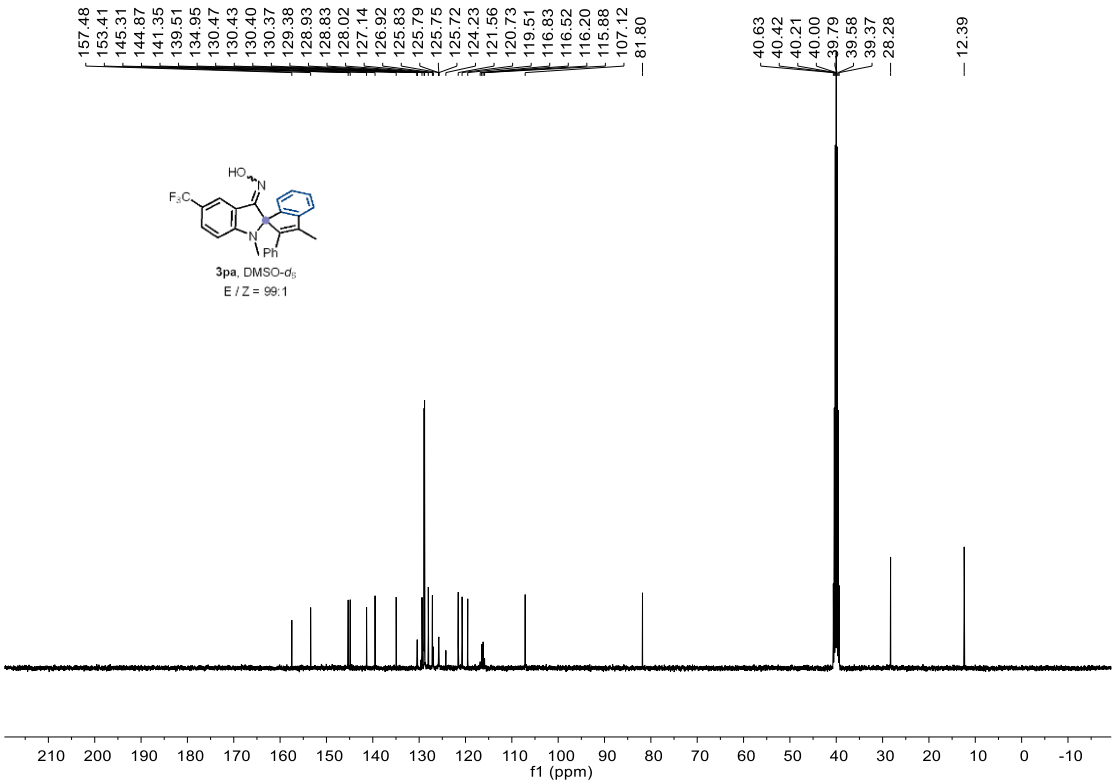
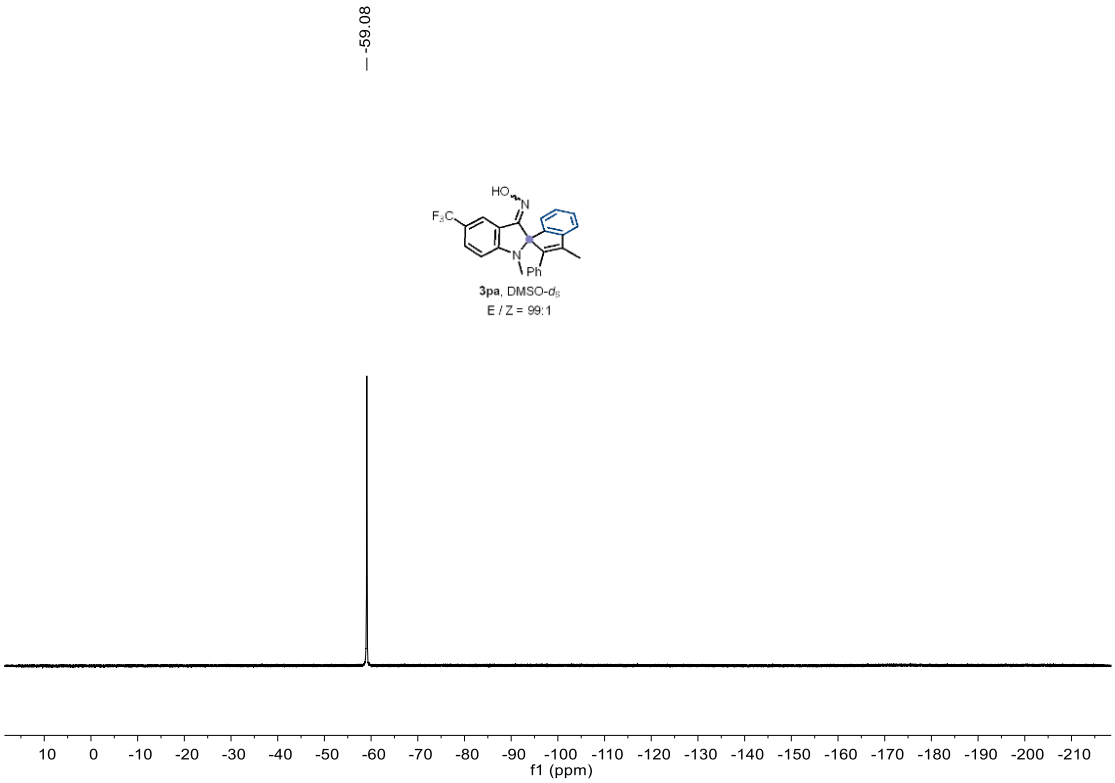
153.63
145.46
144.85
141.42
139.21
135.27
135.14
131.09
129.24
128.90
128.87
127.93
126.97
121.56
121.41
120.71
109.21
107.22
81.76
40.63
40.42
40.21
40.00
39.79
39.58
39.38
28.46
12.46
HO
N
Br
N
Ph
3ma, DMSO-d6
E / Z = 99:1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

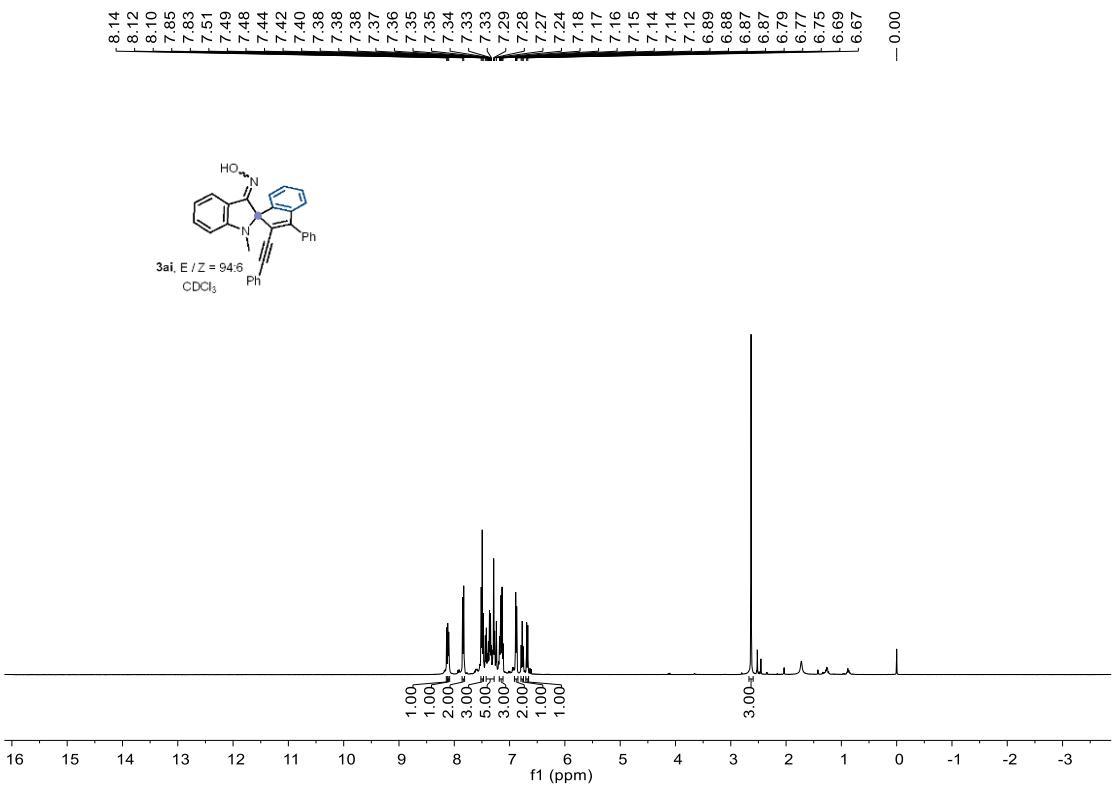

8.36
7.92
7.32
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.23
7.23
7.22
7.22
7.21
7.20
7.19
7.19
7.18
7.18
7.16
7.10
7.09
7.09
7.08
7.08
7.07
7.07
7.06
7.05
7.05
6.98
6.96
6.46
6.44
2.44
2.27
2.23
-0.00
HO
N
N
Ph
3na, CDCl3
E / Z = 91:9
1.00
1.00
4.00
3.00
2.00
1.00
1.00
3.00
3.00
3.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

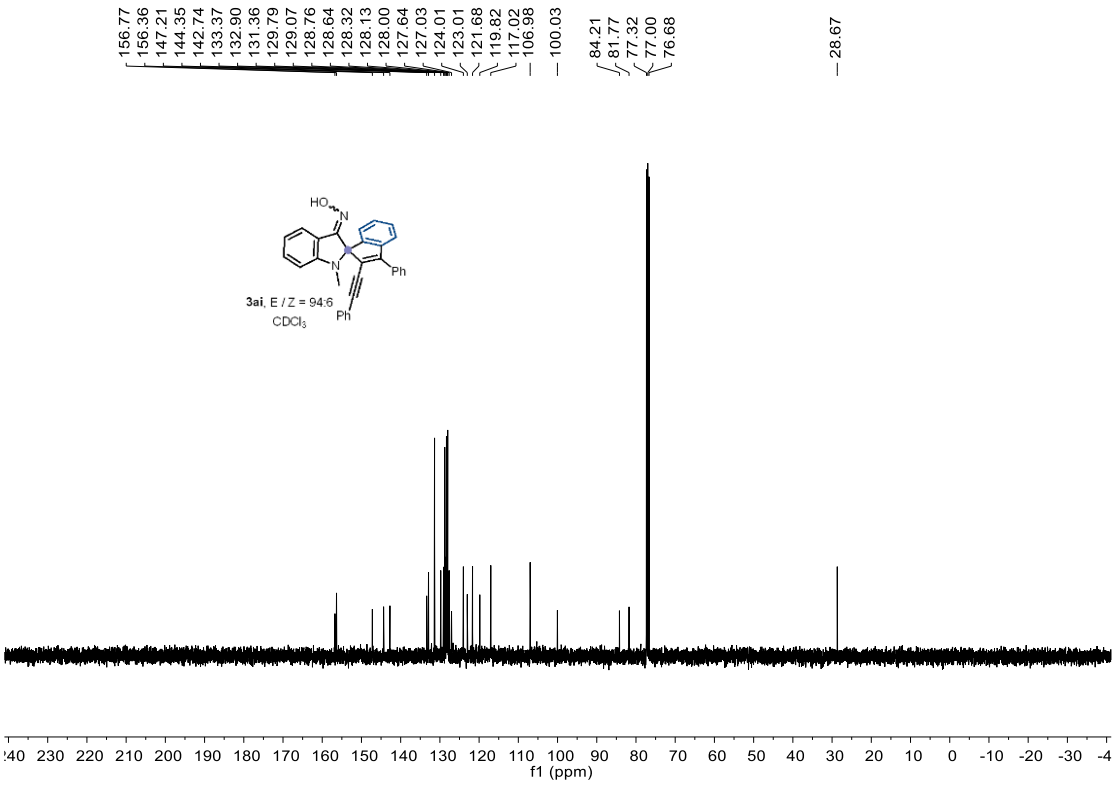

156.79
154.06
144.90
144.64
141.39
139.04
134.86
133.79
130.22
128.82
128.53
128.08
127.04
126.10
125.52
121.11
119.99
119.42
106.50
81.80
77.32
77.00
76.68
28.42
20.65
12.07
HO
N
N
Ph
3na, CDCl3
E / Z = 91:9
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

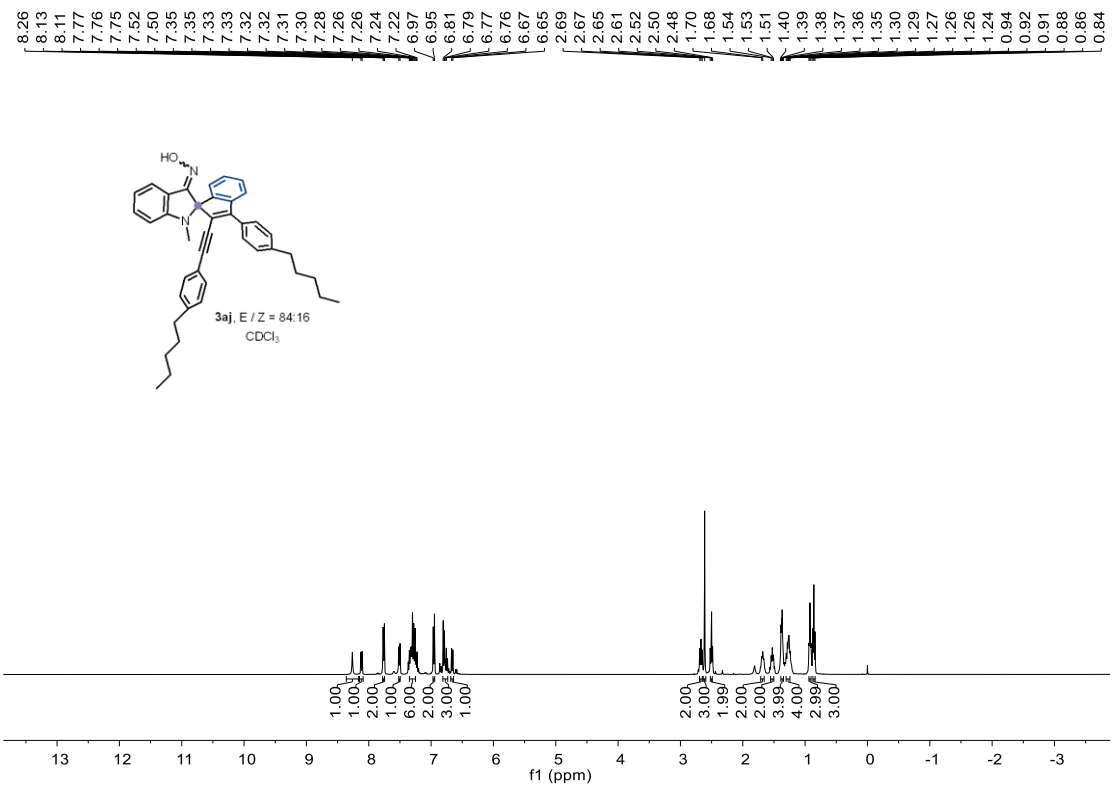

11.50
8.25
8.24
7.55
7.54
7.52
7.52
7.41
7.39
7.36
7.36
7.34
7.34
7.31
7.29
7.29
7.29
7.28
7.27
7.24
7.24
7.23
7.22
7.22
7.21
7.21
7.14
7.14
7.12
7.12
6.96
6.94
6.79
6.77
2.48
2.48
2.47
HO
N
F3C
N
Ph
3pa, DMSO-d6
E / Z = 99:1
1.00
1.00
1.00
1.00
1.00
2.00
3.00
1.00
1.01
1.00
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

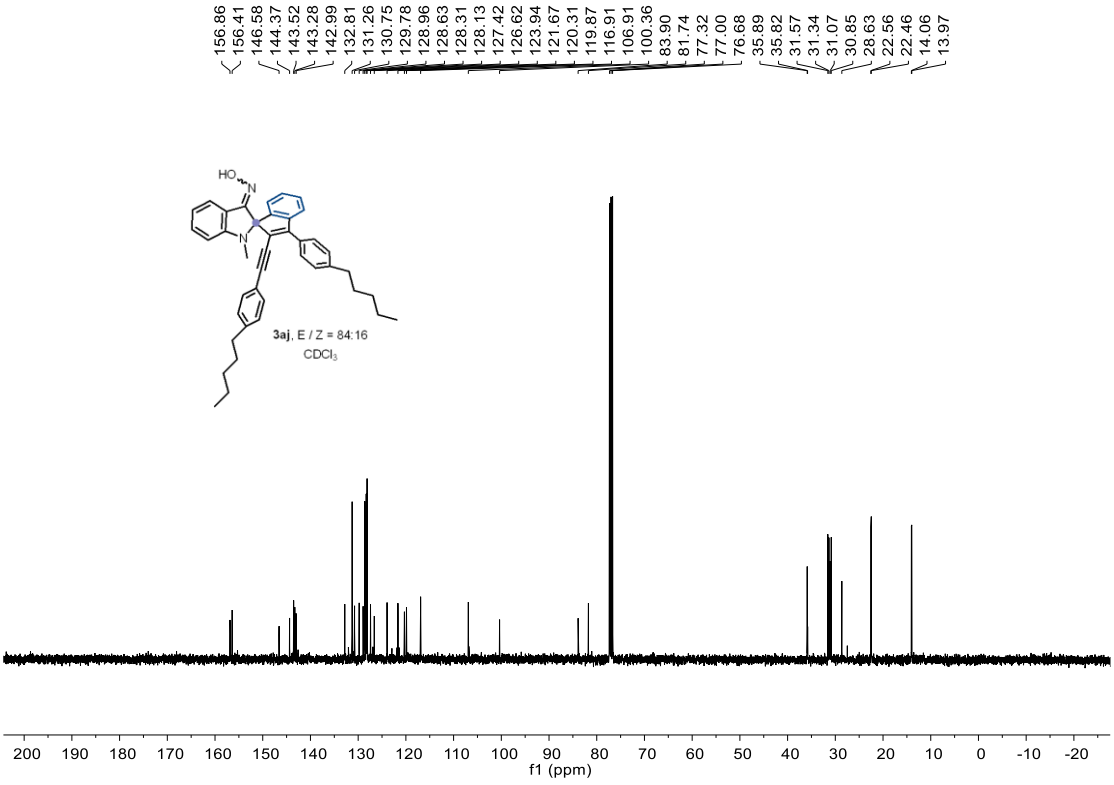

157.48
153.41
145.31
144.87
141.35
139.51
134.95
130.47
130.43
130.40
130.37
129.38
128.93
128.83
128.02
127.14
126.92
125.83
125.79
125.75
125.72
124.23
121.56
120.73
119.51
116.83
116.52
116.20
115.88
107.12
81.80
40.63
40.42
40.21
40.00
39.79
39.58
39.37
28.28
12.39
HO
N
F3C
N
Ph
3pa, DMSO-d6
E / Z = 99:1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

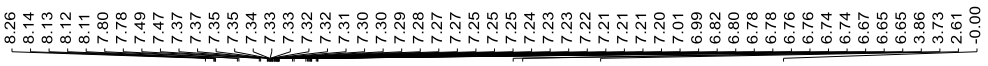

-59.08
HO
N
F3C
N
Ph
3pa, DMSO-d6
E / Z = 99:1
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

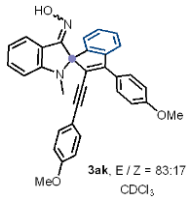

8.14
8.12
8.10
7.85
7.83
7.51
7.49
7.48
7.44
7.42
7.40
7.38
7.38
7.38
7.37
7.36
7.35
7.35
7.34
7.33
7.29
7.28
7.27
7.24
7.18
7.17
7.16
7.15
7.14
7.14
7.12
6.89
6.88
6.87
6.87
6.79
6.77
6.75
6.69
6.67
0.00
HO
N
Ph
N
Ph
3ai, E / Z = 94:6
CDCl3
1.00
1.00
2.00
3.00
5.00
3.00
2.00
1.00
1.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

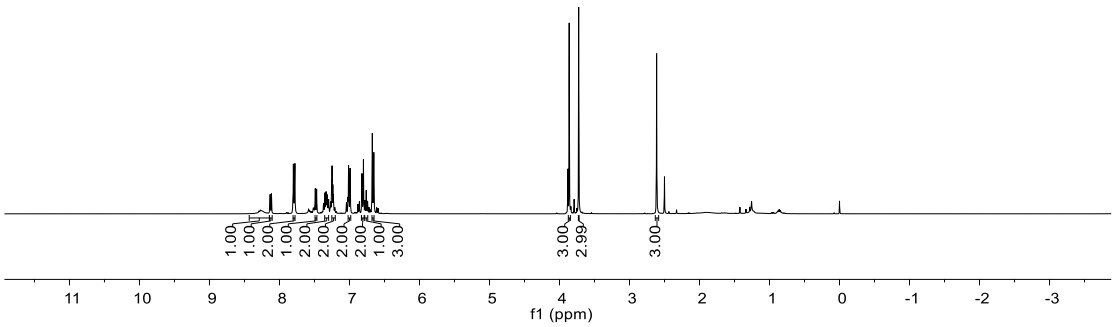

156.77
156.36
147.21
144.35
142.74
133.37
132.90
131.36
129.79
129.07
128.76
128.64
128.32
128.13
128.00
127.64
127.03
124.01
123.01
121.68
119.82
117.02
106.98
100.03
84.21
81.77
77.32
77.00
76.68
28.67
HO
N
Ph
N
Ph
3ai, E / Z = 94:6
CDCl3
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

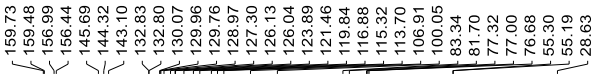

8.26
8.13
8.11
7.77
7.76
7.75
7.52
7.50
7.35
7.35
7.33
7.33
7.32
7.32
7.31
7.30
7.28
7.26
7.26
7.24
7.22
6.97
6.95
6.81
6.79
6.77
6.76
6.67
6.65
2.69
2.67
2.65
2.61
2.52
2.50
2.48
1.70
1.68
1.54
1.53
1.51
1.40
1.39
1.38
1.37
1.36
1.35
1.30
1.29
1.27
1.26
1.26
1.24
0.94
0.92
0.91
0.88
0.86
0.84
HO
N
N
3aj, E / Z = 84:16
CDCl3
1.00
1.00
2.00
1.00
6.00
2.00
3.00
1.00
2.00
3.00
1.99
2.00
2.00
3.99
4.00
2.99
3.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

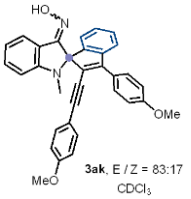

156.86
156.41
146.58
144.37
143.52
143.28
142.99
132.81
131.26
130.75
129.78
128.96
128.63
128.31
128.13
127.42
126.62
123.94
121.67
120.31
119.87
116.91
106.91
100.36
83.90
81.74
77.32
77.00
76.68
35.89
35.82
31.57
31.34
31.07
30.85
28.63
22.56
22.46
14.06
13.97
HO
N
N
3aj, E / Z = 84:16
CDCl3
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

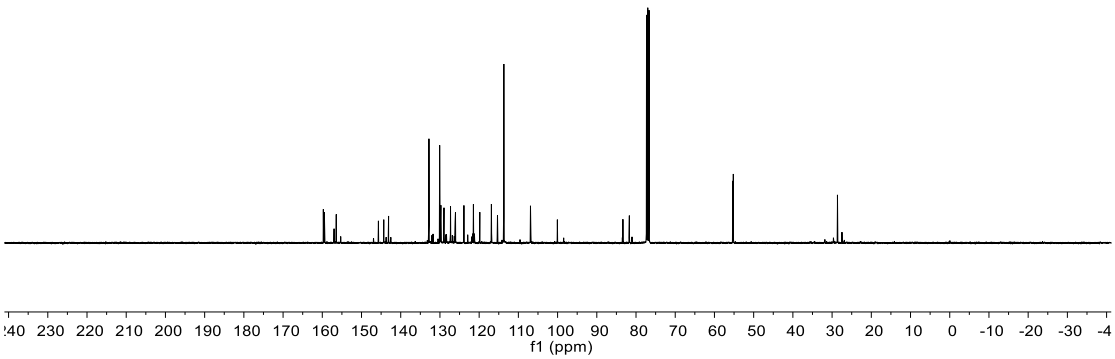

8.26
8.14
8.13
8.12
8.11
7.80
7.78
7.49
7.47
7.37
7.37
7.35
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.28
7.27
7.27
7.25
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.21
7.21
7.20
7.01
6.99
6.82
6.80
6.78
6.78
6.76
6.76
6.74
6.74
6.67
6.65
6.65
3.86
3.73
2.61
-0.00

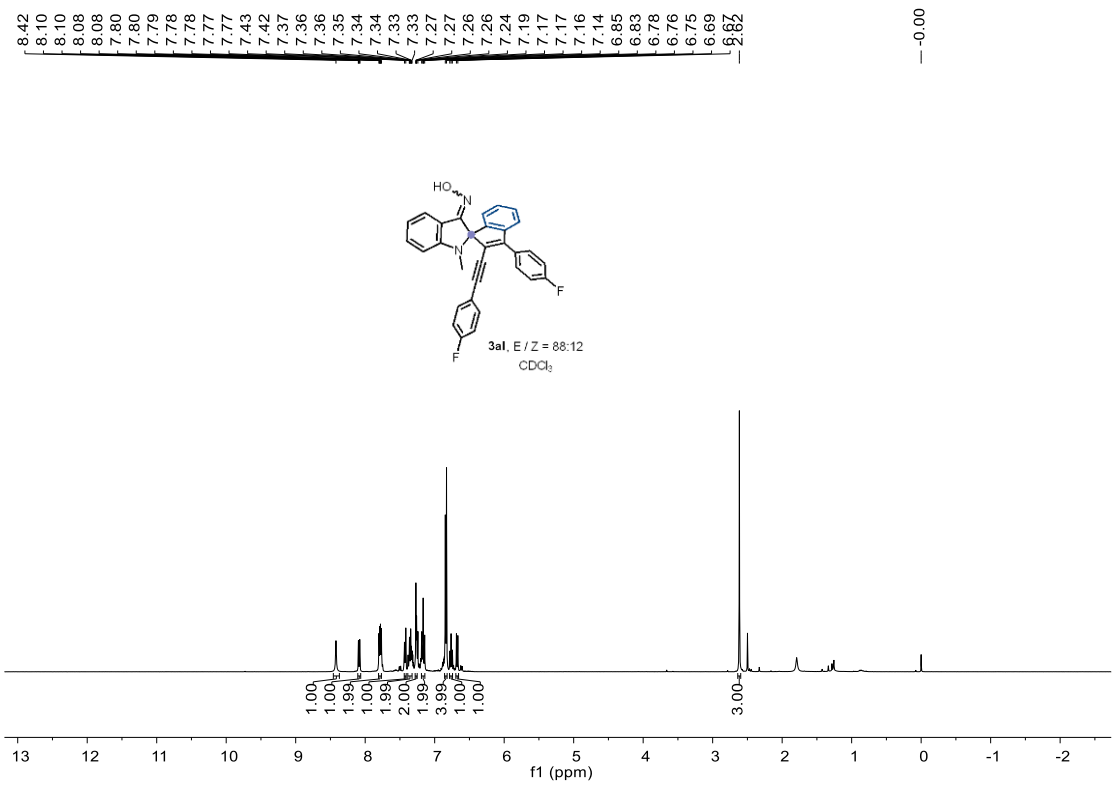

HO
N
N
OMe
MeO
3ak, E / Z = 83:17
CDCl3

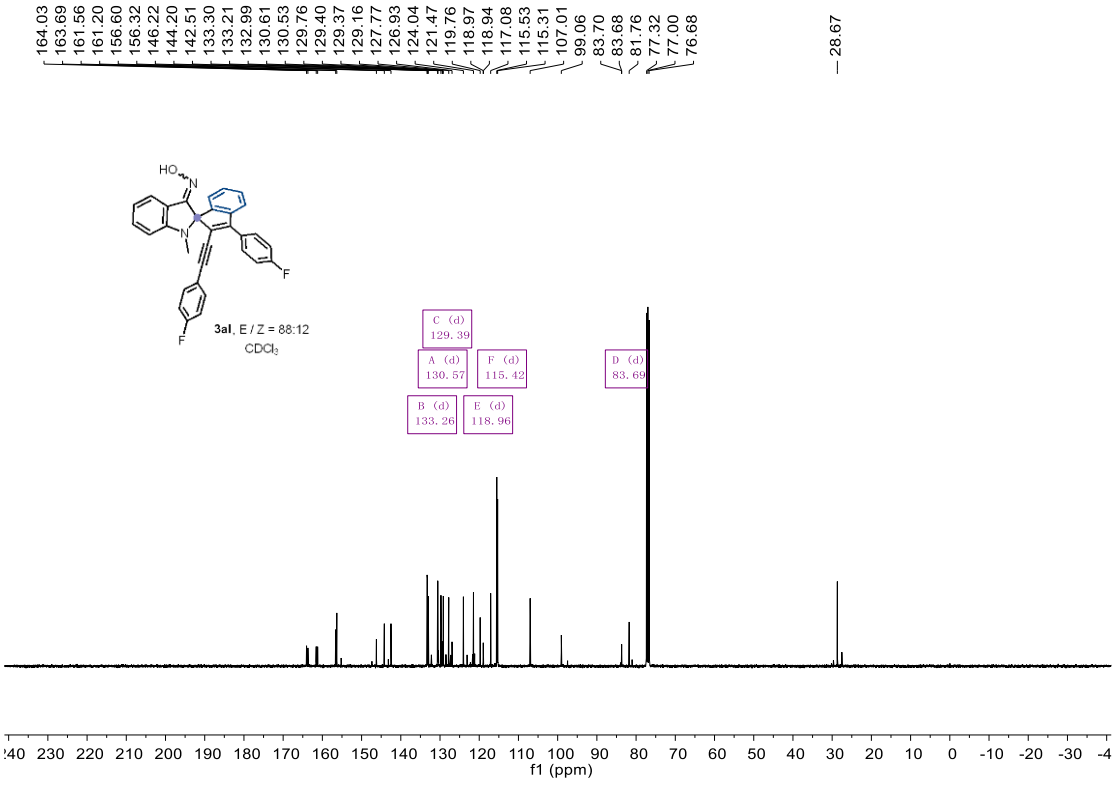

1.00
1.00
2.00
1.00
2.00
2.00
2.00
2.00
1.00
3.00
3.00
2.99
3.00
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)

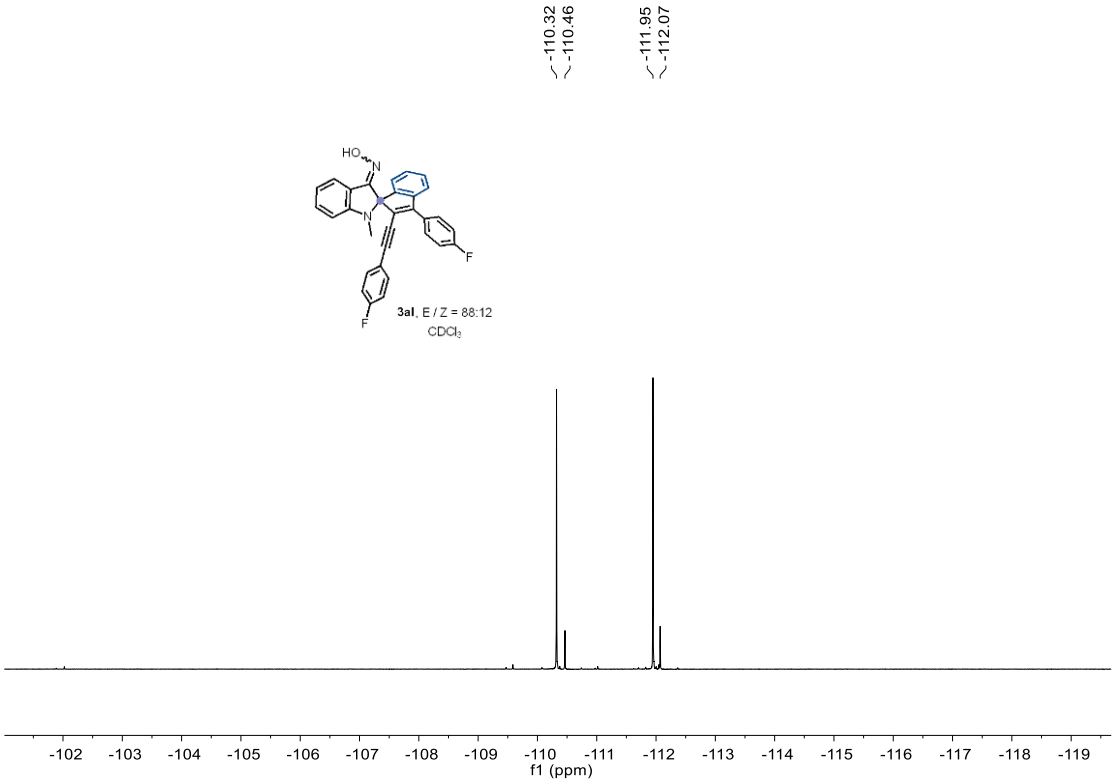

159.73
159.48
156.99
156.44
145.69
144.32
143.10
132.83
132.80
130.07
129.96
129.76
128.97
127.30
126.13
126.04
123.89
121.46
119.84
116.88
115.32
113.70
106.91
100.05
83.34
81.70
77.32
77.00
76.68
55.30
55.19
28.63

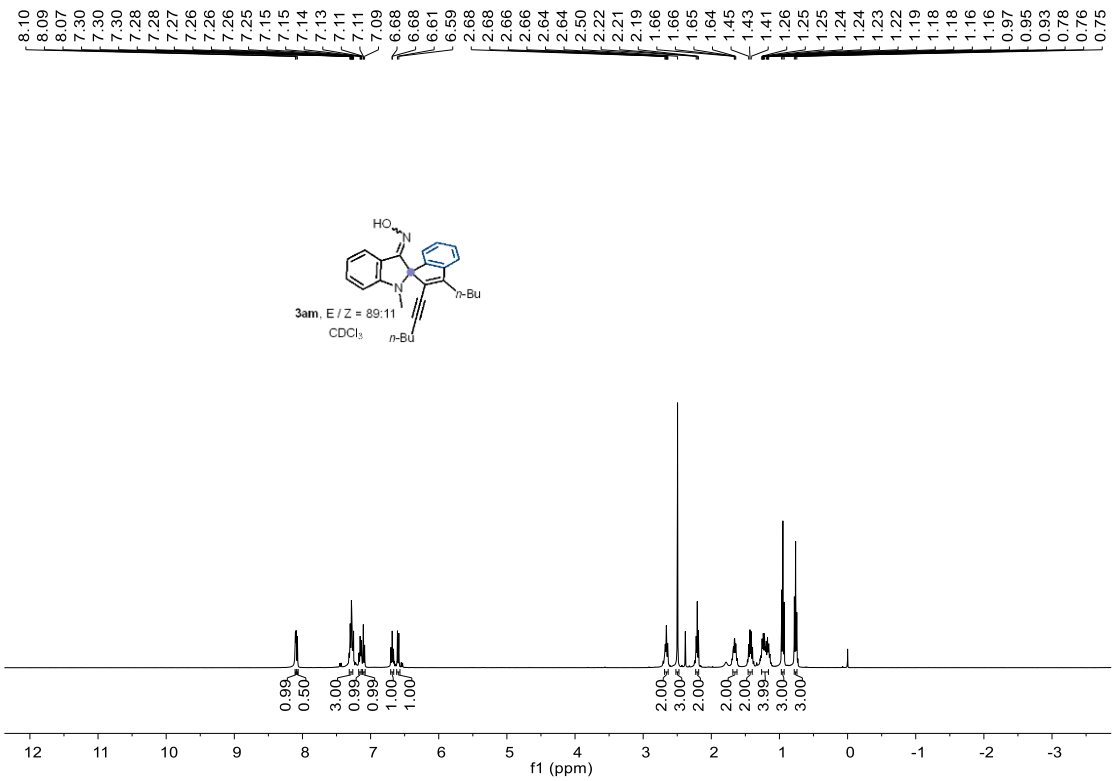

HO
N
N
OMe
MeO
3ak, E / Z = 83:17
CDCl3

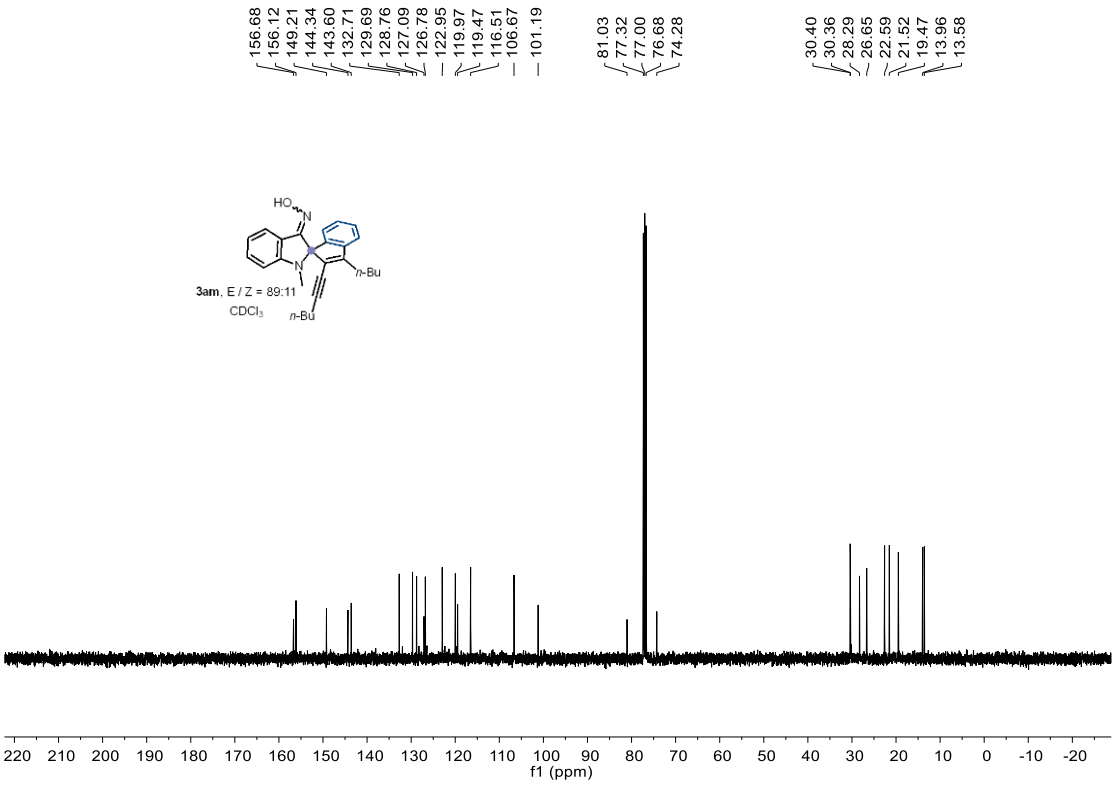

240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

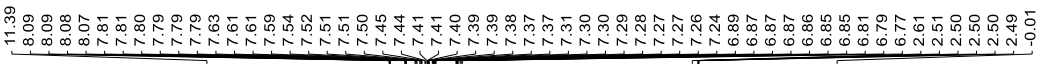

8.42
8.10
8.10
8.08
8.08
7.80
7.80
7.79
7.78
7.78
7.77
7.77
7.43
7.42
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.33
7.27
7.27
7.26
7.26
7.24
7.19
7.17
7.17
7.16
7.14
6.85
6.83
6.78
6.76
6.75
6.69
6.67
2.82
-0.00
HO
N
N
F
F
3al, E / Z = 88:12
CDCl3
1.00
1.00
1.99
1.00
1.99
2.00
1.99
3.99
1.00
1.00
3.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)

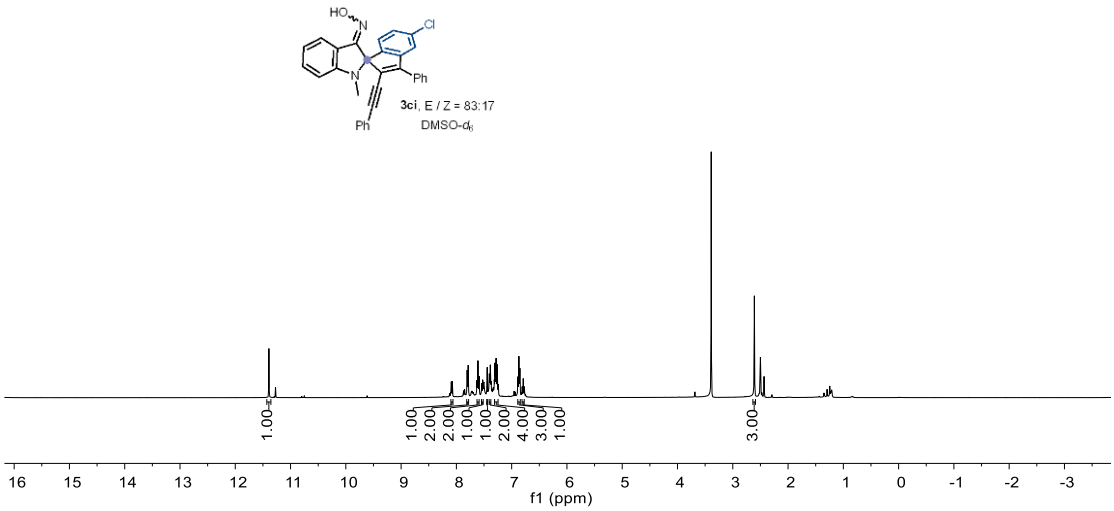

164.03
163.69
161.56
161.20
156.60
156.32
146.22
144.20
142.51
133.30
133.21
132.99
130.61
130.53
129.76
129.40
129.37
129.16
127.77
126.93
124.04
121.47
119.76
118.97
118.94
117.08
115.53
115.31
107.01
99.06
83.70
83.68
81.76
77.32
77.00
76.68
28.67
HO
N
N
F
F
3al, E / Z = 88:12
CDCl3
C (d)
129.39
A (d)
130.57
F (d)
115.42
D (d)
83.69
B (d)
133.26
E (d)
118.96
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-4
f1 (ppm)

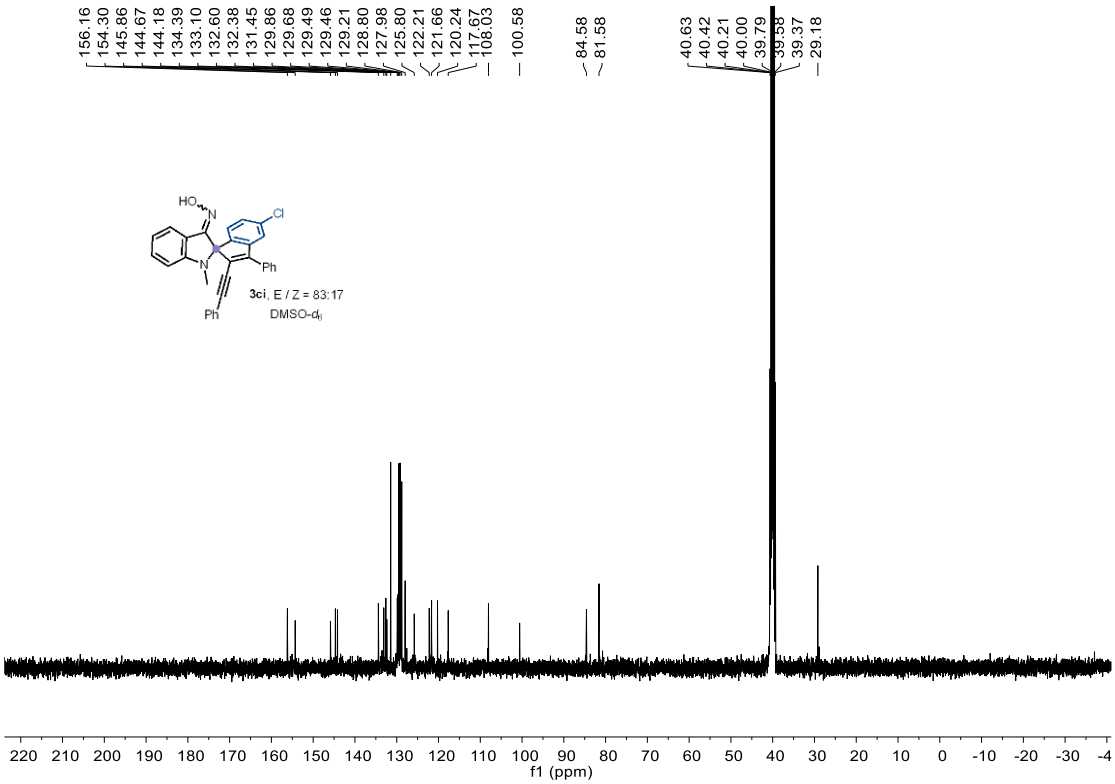

-110.32
-110.46
-111.95
-112.07
HO
N
N
F
F
3al, E / Z = 88:12
CDCl3
-102
-103
-104
-105
-106
-107
-108
-109
-110
-111
-112
-113
-114
-115
-116
-117
-118
-119
f1 (ppm)

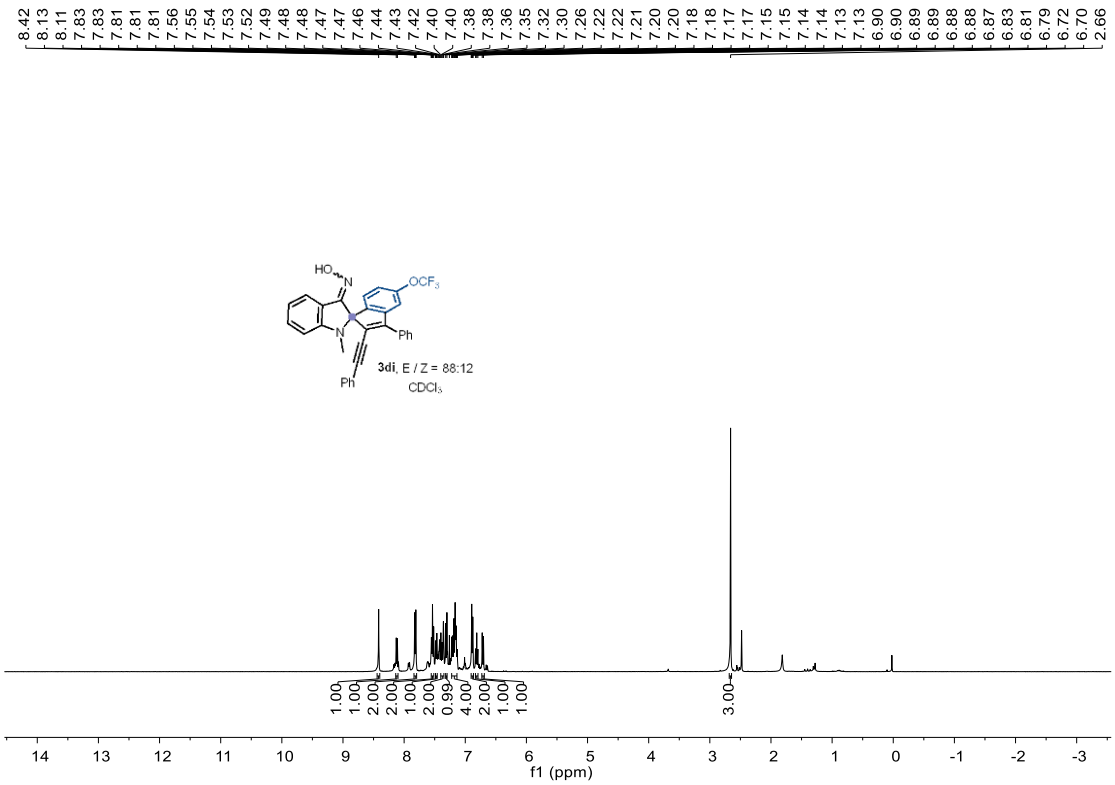

8.10 8.09 8.07 7.30 7.30 7.30 7.28 7.28 7.27 7.26 7.26 7.26 7.25 7.15 7.15 7.14 7.13 7.11 7.11 7.09 6.68 6.68 6.61 6.59 2.68 2.68 2.66 2.66 2.64 2.64 2.50 2.22 2.21 2.19 1.66 1.66 1.65 1.64 1.45 1.43 1.41 1.26 1.25 1.25 1.24 1.24 1.23 1.22 1.19 1.18 1.18 1.16 1.16 0.97 0.95 0.93 0.78 0.76 0.75
HO
N
n-Bu
3am, E / Z = 89:11
CDCl3
n-Bu
0.99 0.50 3.00 0.99 0.99 1.00 1.00 2.00 3.00 2.00 2.00 2.00 3.99 3.00 3.00
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

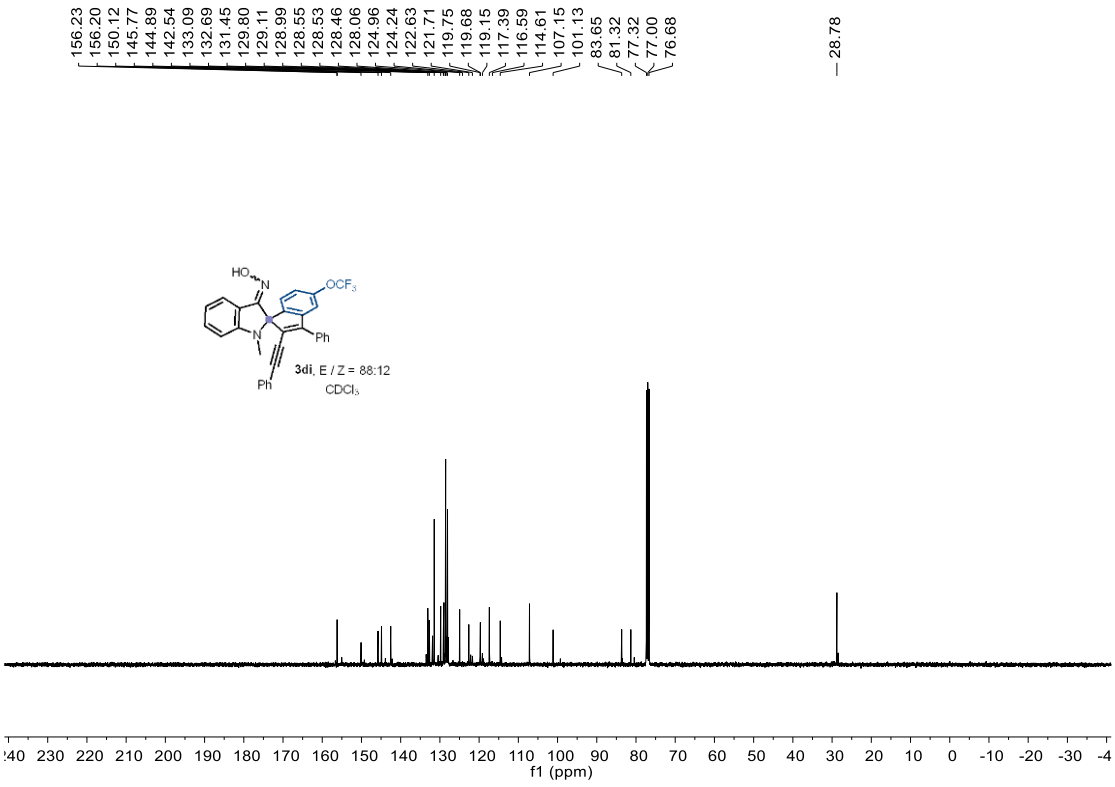

156.68 156.12 149.21 144.34 143.60 132.71 129.69 128.76 127.09 126.78 122.95 119.97 119.47 116.51 106.67 101.19
81.03 77.32 77.00 76.68 74.28
30.40 30.36 28.29 26.65 22.59 21.52 19.47 13.96 13.58
HO
N
n-Bu
3am, E / Z = 89:11
CDCl3
n-Bu
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

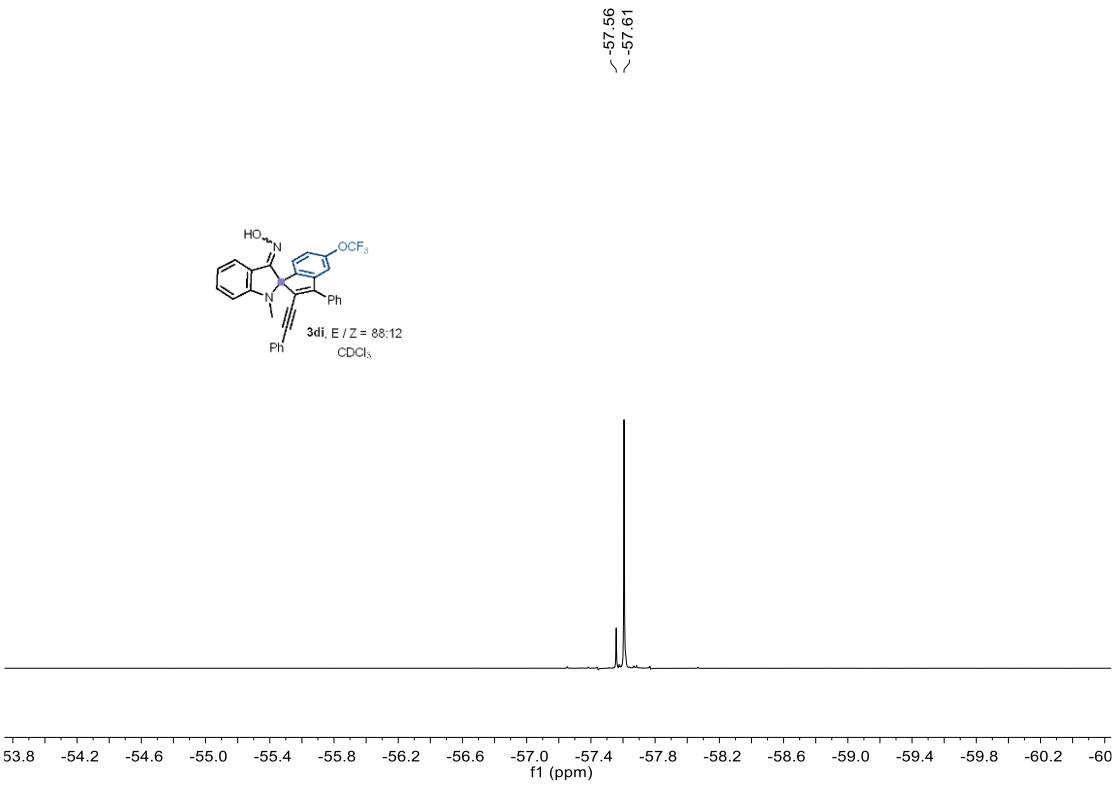

11.39
8.09
8.09
8.08
8.07
7.81
7.81
7.80
7.79
7.79
7.79
7.63
7.61
7.61
7.59
7.54
7.52
7.51
7.51
7.50
7.45
7.44
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
7.31
7.30
7.30
7.29
7.28
7.27
7.27
7.26
7.24
6.89
6.87
6.87
6.86
6.85
6.85
6.81
6.79
6.77
2.61
2.51
2.50
2.50
2.50
2.49
-0.01

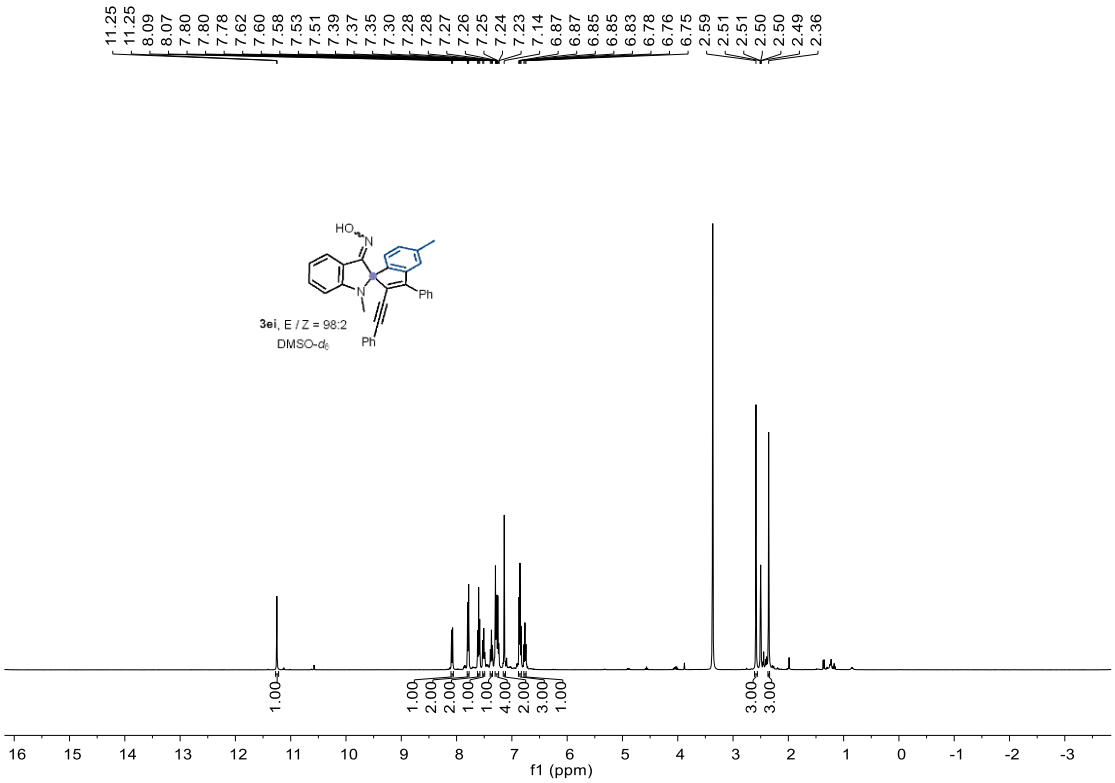

HO
N
Cl
N
Ph
Ph
3ci, E / Z = 83:17
DMSO-d6
1.00
1.00
2.00
2.00
1.00
1.00
2.00
4.00
3.00
1.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

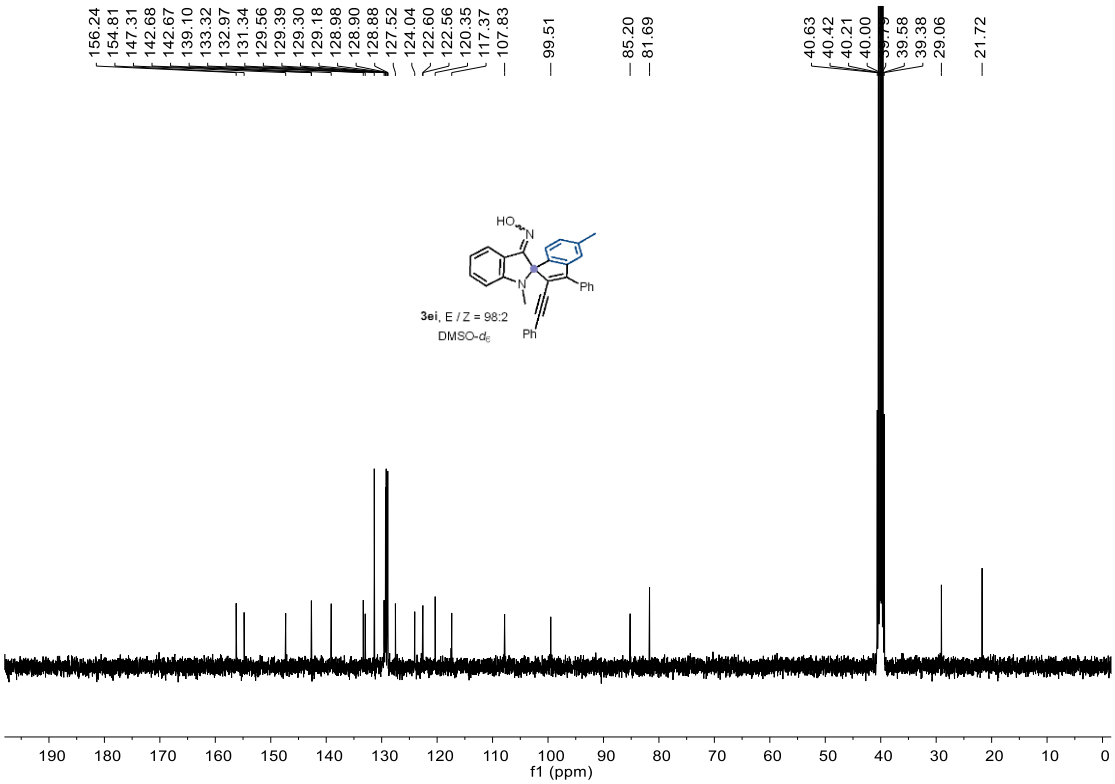

156.16
154.30
145.86
144.67
144.18
134.39
133.10
132.60
132.38
131.45
129.86
129.68
129.49
129.46
129.21
128.80
127.98
125.80
122.21
121.66
120.24
117.67
108.03
100.58
84.58
81.58
40.63
40.42
40.21
40.00
39.79
39.58
39.37
29.18
HO
N
Cl
N
Ph
Ph
3ci, E / Z = 83:17
DMSO-d6
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

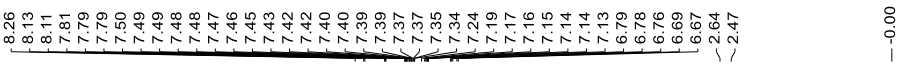

8.42
8.13
8.11
7.83
7.83
7.81
7.81
7.81
7.56
7.55
7.54
7.53
7.52
7.49
7.48
7.48
7.47
7.47
7.46
7.44
7.43
7.42
7.40
7.40
7.38
7.38
7.36
7.35
7.32
7.30
7.26
7.22
7.22
7.21
7.20
7.20
7.18
7.18
7.17
7.17
7.15
7.15
7.14
7.14
7.13
7.13
6.90
6.90
6.89
6.89
6.88
6.88
6.87
6.83
6.81
6.79
6.72
6.70
2.66
HO
N
OCF3
Ph
N
Ph
3di, E / Z = 88:12
CDCl3
1.00
1.00
2.00
2.00
1.00
2.00
0.99
4.00
2.00
1.00
1.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

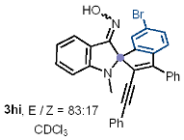

156.23
156.20
150.12
145.77
144.89
142.54
133.09
132.69
131.45
129.80
129.11
128.99
128.55
128.53
128.46
128.06
124.96
124.24
122.63
121.71
119.75
119.68
119.15
117.39
116.59
114.61
107.15
101.13
83.65
81.32
77.32
77.00
76.68
28.78
HO
N
OCF3
Ph
N
Ph
3di, E / Z = 88:12
CDCl3
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

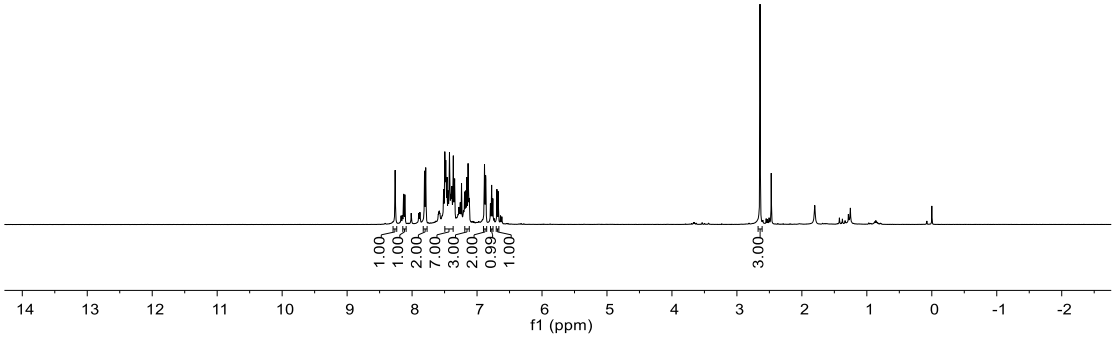

-57.56
-57.61
HO
N
OCF3
Ph
N
Ph
3di, E / Z = 88:12
CDCl3
53.8
-54.2
-54.6
-55.0
-55.4
-55.8
-56.2
-56.6
-57.0
-57.4
-57.8
-58.2
-58.6
-59.0
-59.4
-59.8
-60.2
-60
f1 (ppm)

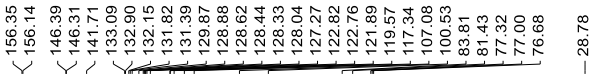

11.25
11.25
8.09
8.07
7.80
7.80
7.78
7.62
7.60
7.58
7.53
7.51
7.39
7.37
7.35
7.30
7.28
7.28
7.27
7.26
7.25
7.24
7.23
7.14
6.87
6.87
6.85
6.83
6.78
6.76
6.75
2.59
2.51
2.51
2.50
2.50
2.49
2.36
HO
N
N
Ph
Ph
3ei, E / Z = 98:2
DMSO-d6
1.00
1.00
2.00
2.00
1.00
1.00
4.00
2.00
3.00
1.00
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

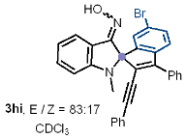

156.24
154.81
147.31
142.68
142.67
139.10
133.32
132.97
131.34
129.56
129.39
129.30
129.18
128.98
128.90
128.88
127.52
124.04
122.60
122.56
120.35
117.37
107.83
99.51
85.20
81.69
40.63
40.42
40.21
40.00
39.58
39.38
29.06
21.72
HO
N
N
Ph
Ph
3ei, E / Z = 98:2
DMSO-d6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.26
8.13
8.11
7.81
7.79
7.79
7.50
7.49
7.49
7.48
7.48
7.47
7.46
7.45
7.43
7.42
7.42
7.40
7.40
7.39
7.39
7.37
7.37
7.35
7.34
7.24
7.19
7.17
7.16
7.15
7.14
7.14
7.13
6.79
6.78
6.76
6.69
6.67
2.64
2.47
-0.00


HO
N
Br
Ph
Ph
3hi, E / Z = 83:17
CDCl3


1.00
1.00
2.00
7.00
3.00
2.00
0.99
1.00
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


156.35
156.14
146.39
146.31
141.71
133.09
132.90
132.15
131.82
131.39
129.87
128.88
128.62
128.44
128.33
128.04
127.27
122.82
122.76
121.89
119.57
117.34
107.08
100.53
83.81
81.43
77.32
77.00
76.68
28.78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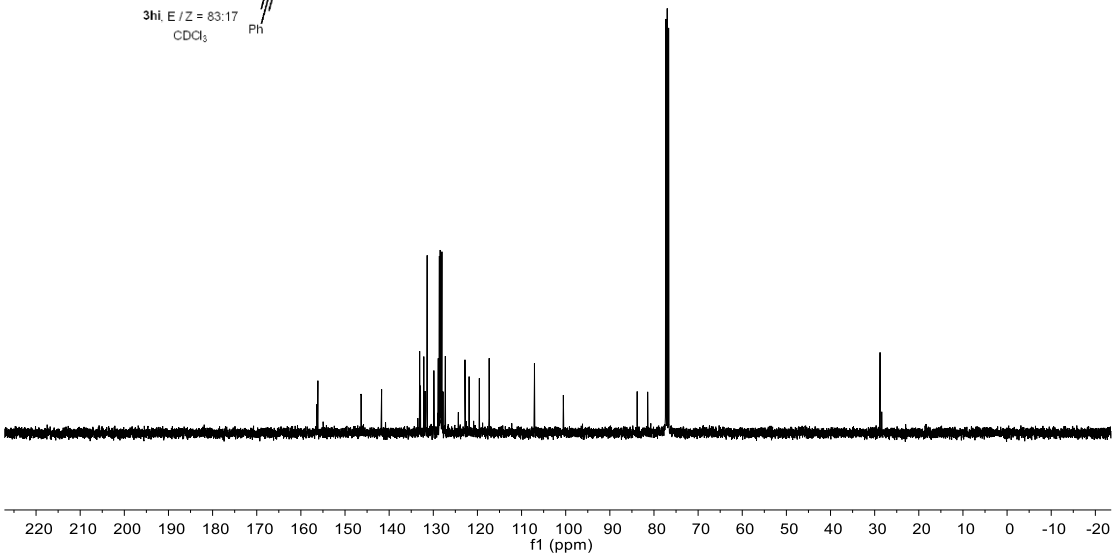
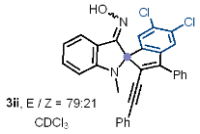
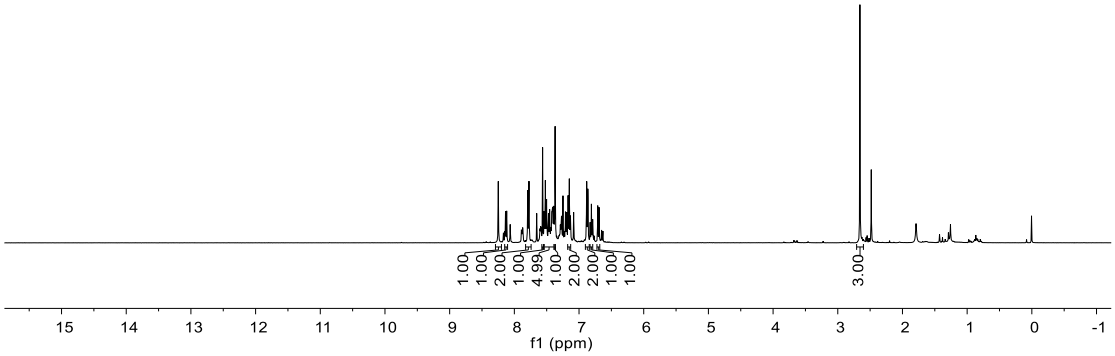
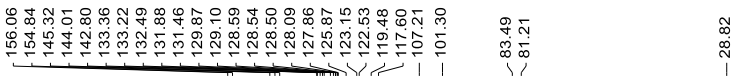
N
Br
Ph
Ph
3hi, E / Z = 83:17
CDCl3

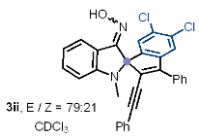

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


8.25
8.14
8.14
8.12
8.12
7.80
7.79
7.77
7.77
7.56
7.54
7.52
7.52
7.50
7.48
7.47
7.47
7.45
7.42
7.42
7.41
7.41
7.39
7.39
7.37
7.21
7.20
7.19
7.19
7.17
7.17
7.15
7.15
7.13
6.88
6.88
6.86
6.86
6.83
6.81
6.79
6.71
6.69
2.66
0.00

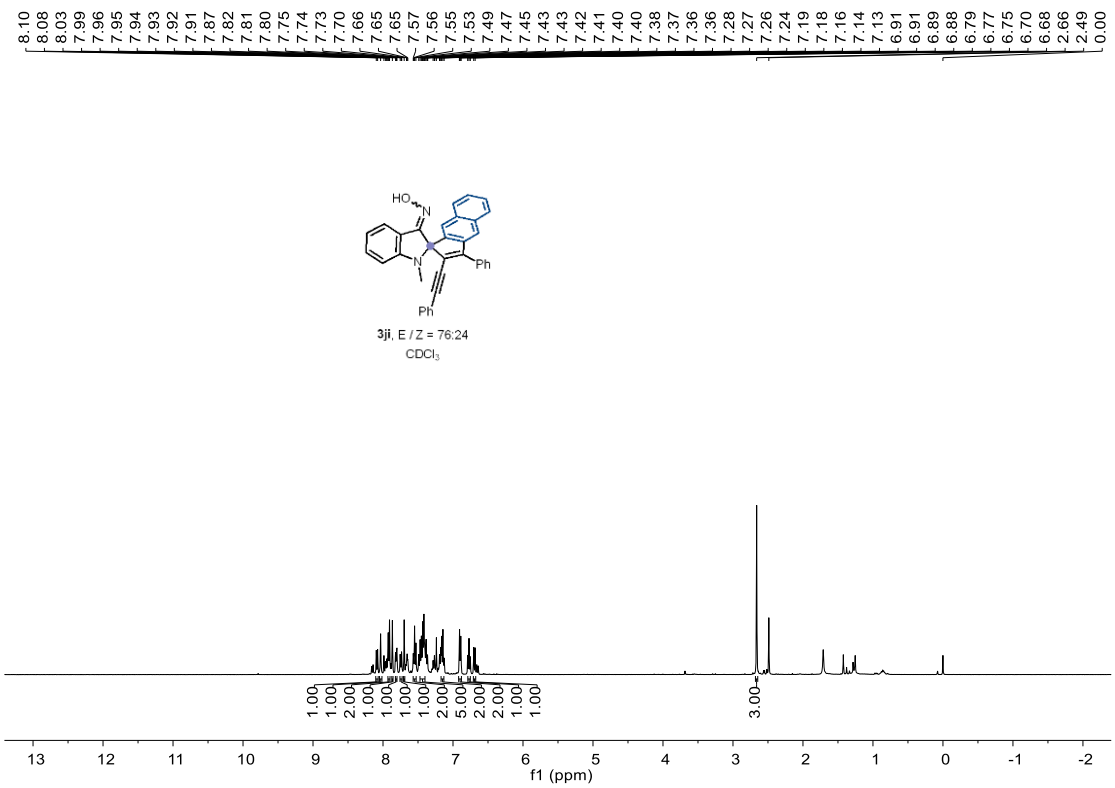

HO
N
Cl
Cl
Ph
Ph
3ii, E / Z = 79:21
CDCl3

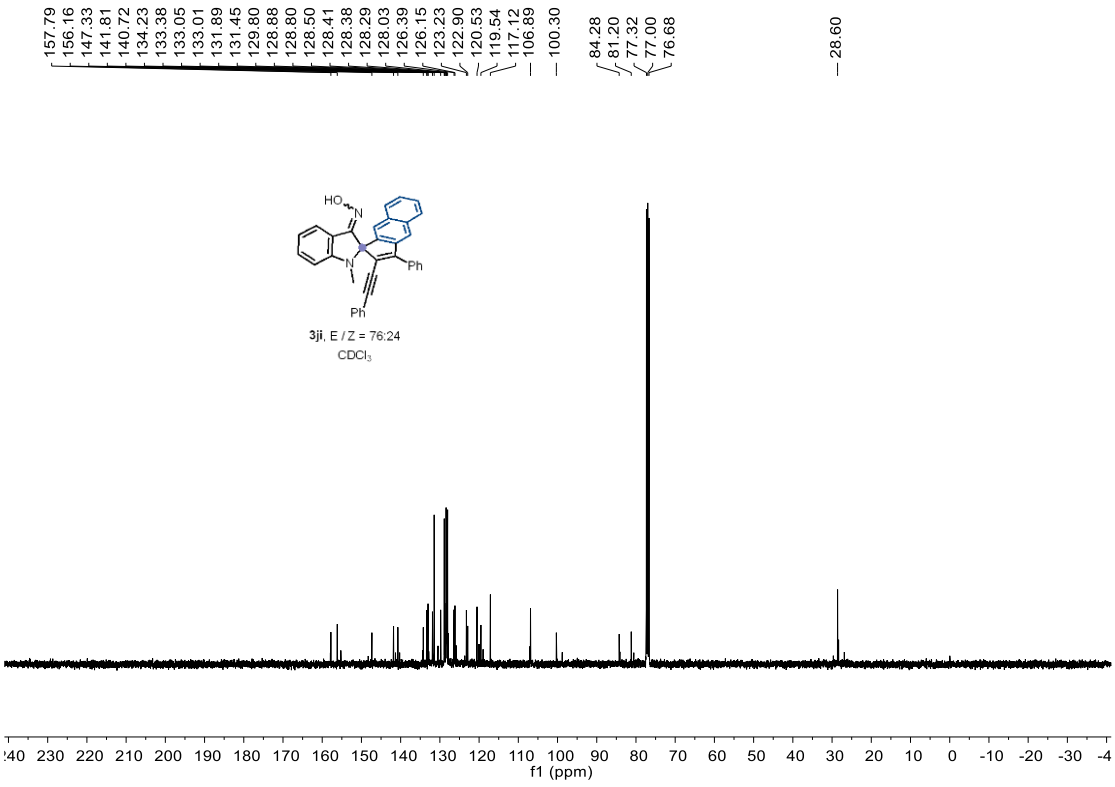

1.00
1.00
2.00
1.00
4.99
1.00
2.00
2.00
1.00
1.00
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

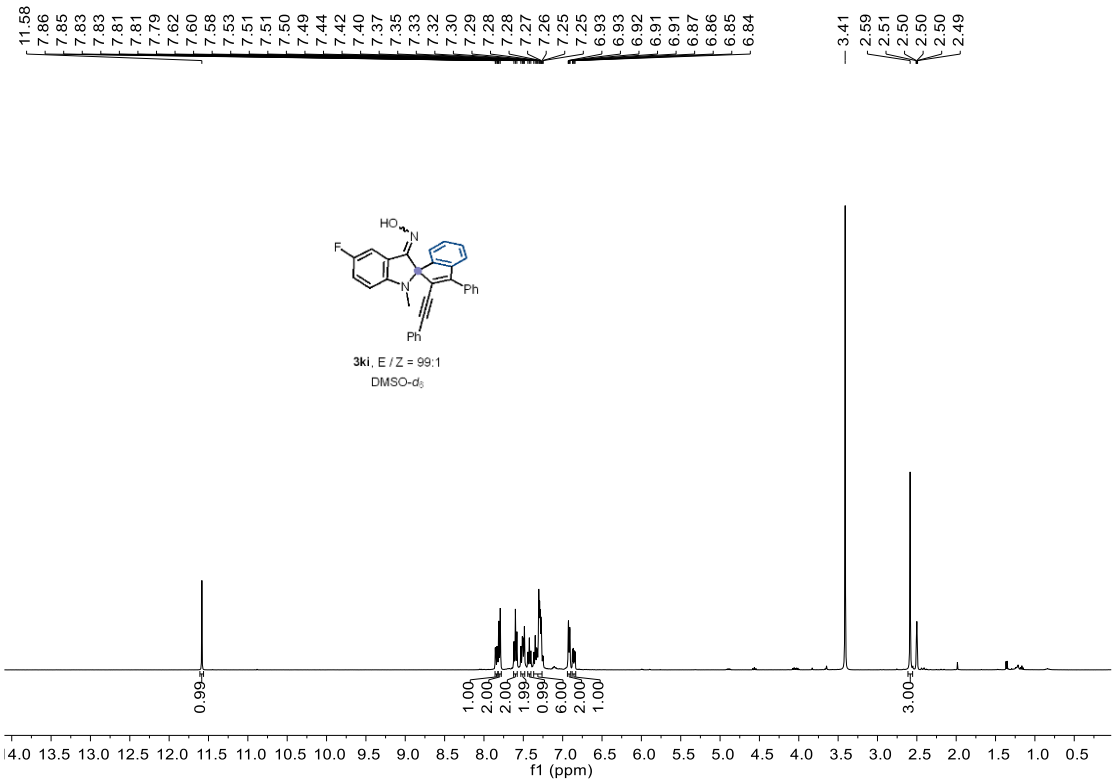

156.06
154.84
145.32
144.01
142.80
133.36
133.22
132.49
131.88
131.46
129.87
129.10
128.59
128.54
128.50
128.09
127.86
125.87
123.15
122.53
119.48
117.60
107.21
101.30
83.49
81.21
28.82

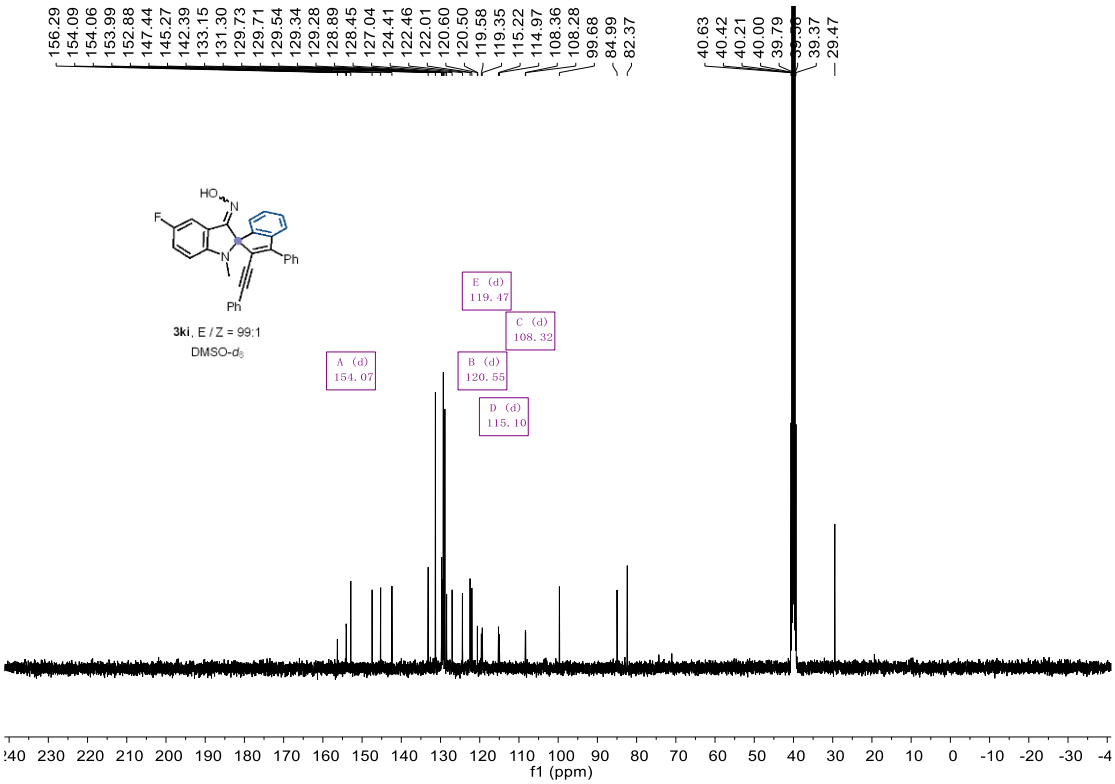

HO
N
Cl
Cl
Ph
Ph
3ii, E / Z = 79:21
CDCl3

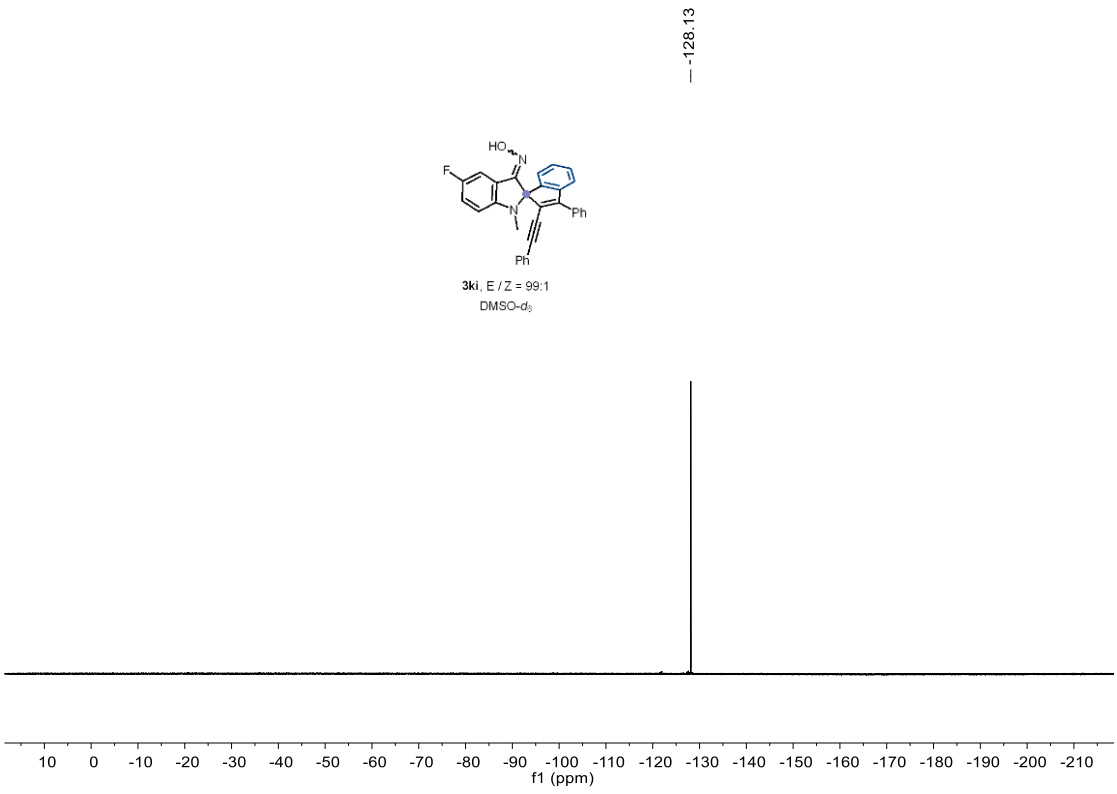
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

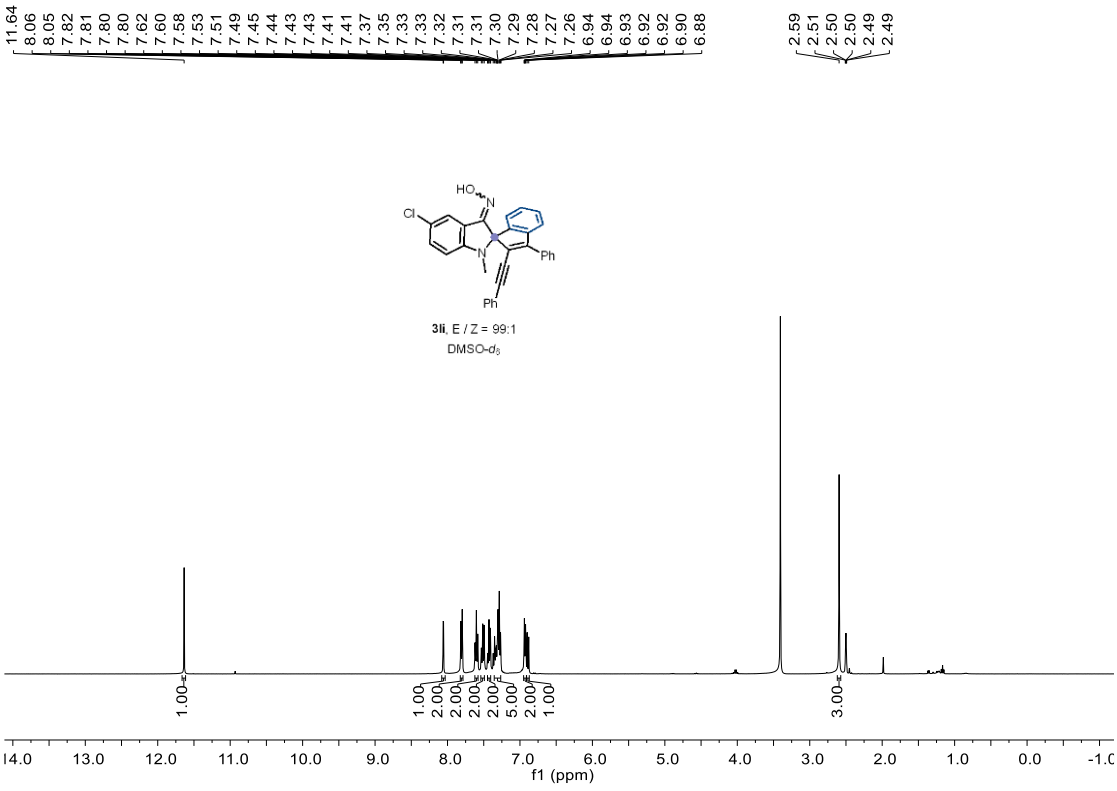

8.10 8.08 8.03 7.99 7.96 7.95 7.94 7.93 7.92 7.91 7.87 7.82 7.81 7.80 7.75 7.74 7.73 7.70 7.66 7.65 7.65 7.57 7.56 7.55 7.53 7.49 7.47 7.45 7.43 7.43 7.42 7.41 7.40 7.40 7.38 7.37 7.36 7.36 7.28 7.27 7.26 7.24 7.19 7.18 7.16 7.14 7.13 6.91 6.91 6.89 6.88 6.79 6.77 6.75 6.70 6.68 2.66 2.49 0.00
HO
N
N
Ph
Ph
3ji, E / Z = 76:24
CDCl3
1.00 1.00 2.00 1.00 1.00 1.00 1.00 2.00 5.00 2.00 2.00 1.00 1.00
3.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


157.79 156.16 147.33 141.81 140.72 134.23 133.38 133.05 133.01 131.89 131.45 129.80 128.88 128.80 128.50 128.41 128.38 128.29 128.03 126.39 126.15 123.23 122.90 120.53 119.54 117.12 106.89 100.30 84.28 81.20 77.32 77.00 76.68 28.60
HO
N
N
Ph
Ph
3ji, E / Z = 76:24
CDCl3
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)


11.58
7.86
7.85
7.83
7.83
7.81
7.81
7.79
7.62
7.60
7.58
7.53
7.51
7.51
7.50
7.49
7.44
7.42
7.40
7.37
7.35
7.33
7.32
7.30
7.29
7.28
7.28
7.27
7.26
7.25
7.25
6.93
6.93
6.92
6.91
6.91
6.87
6.86
6.85
6.84
3.41
2.59
2.51
2.50
2.50
2.50
2.49
HO
N
F
Ph
N
Ph
3ki, E / Z = 99:1
DMSO-d6
0.99
1.00
2.00
2.00
1.99
0.99
6.00
2.00
1.00
3.00
f1 (ppm)


156.29
154.09
154.06
153.99
152.88
147.44
145.27
142.39
133.15
131.30
129.73
129.71
129.54
129.34
129.28
128.89
128.45
127.04
124.41
122.46
122.01
120.60
120.50
119.58
119.35
115.22
114.97
108.36
108.28
99.68
84.99
82.37
40.63
40.42
40.21
40.00
39.79
39.58
39.37
29.47
HO
N
F
Ph
N
Ph
3ki, E / Z = 99:1
DMSO-d6
A (d)
154.07
B (d)
120.55
C (d)
108.32
D (d)
115.10
E (d)
119.47
f1 (ppm)


-128.13
HO
N
F
N
Ph
Ph
3ki, E / Z = 99:1
DMSO-d6
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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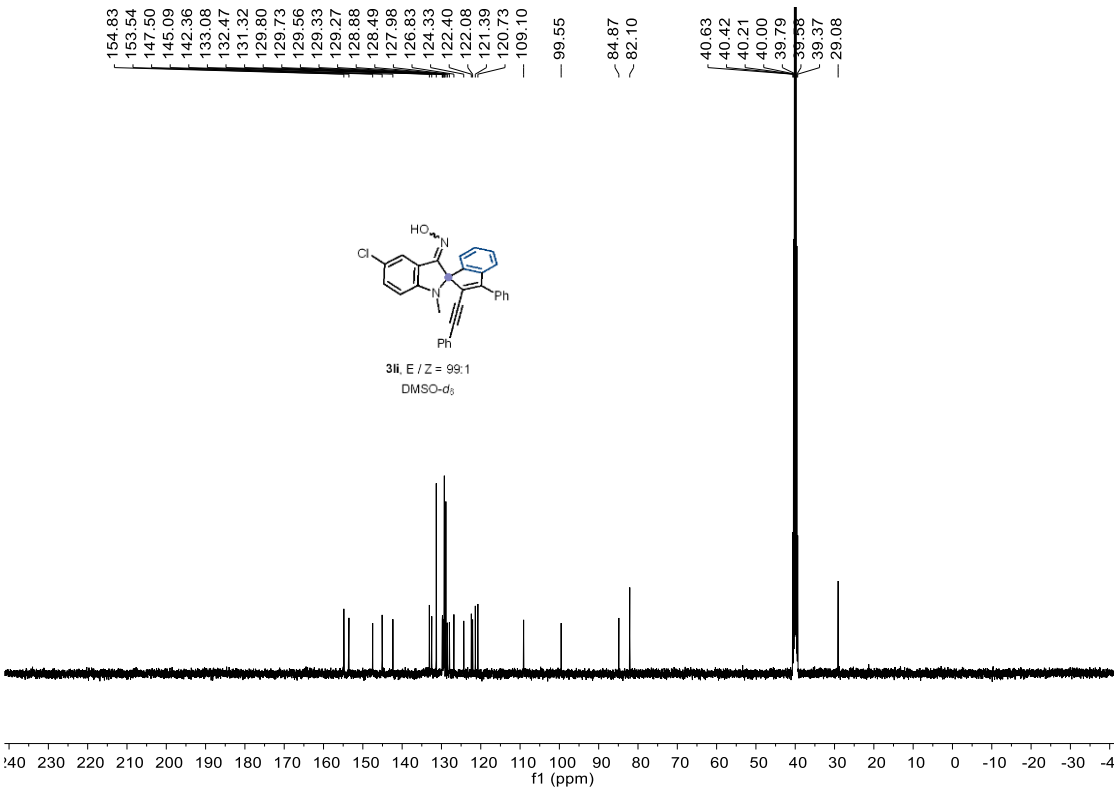
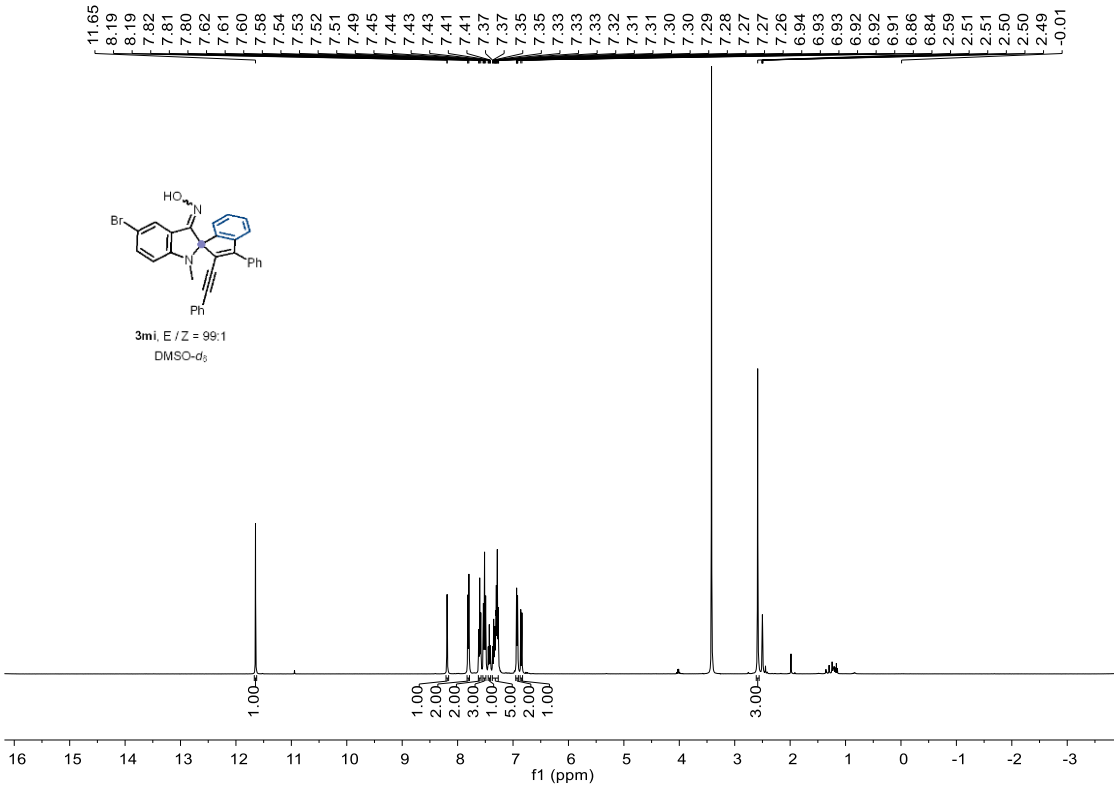
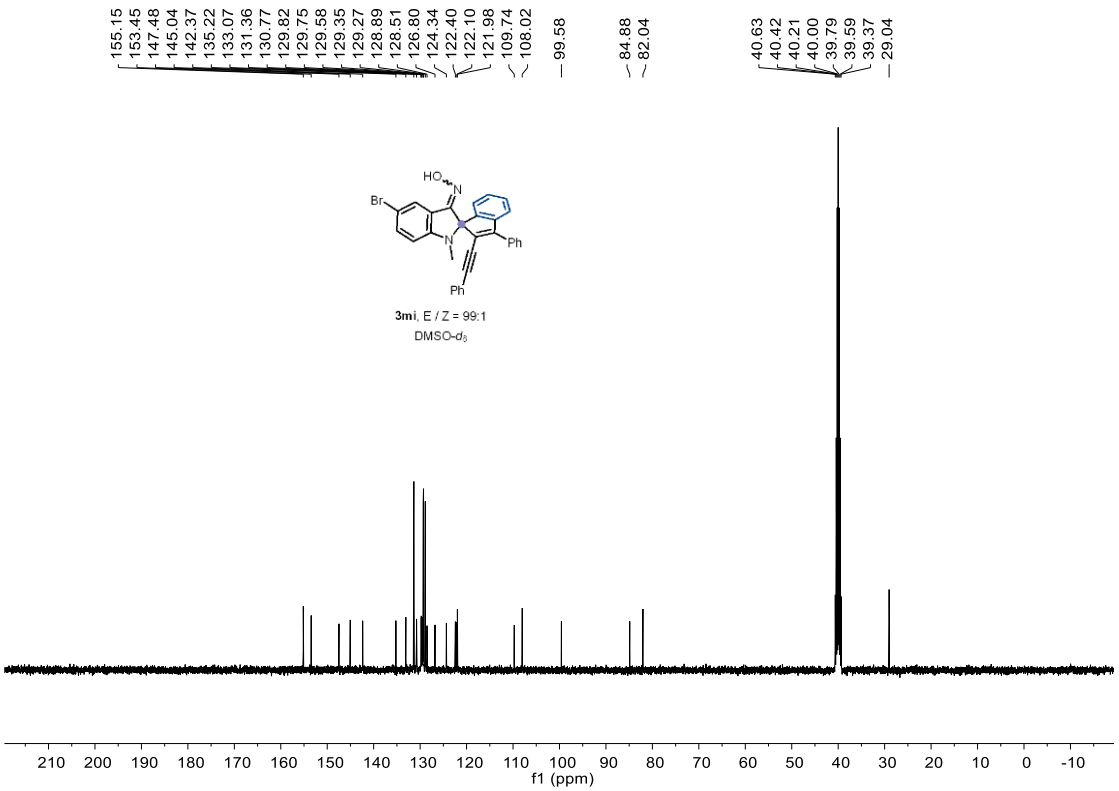
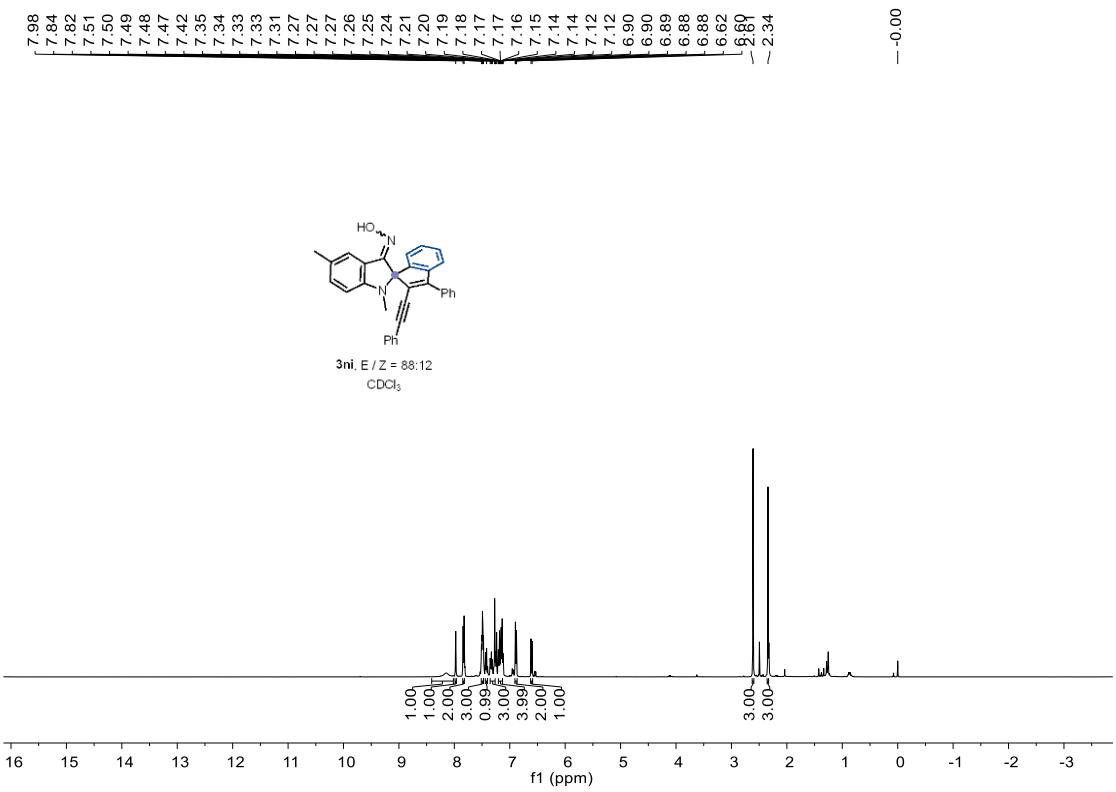
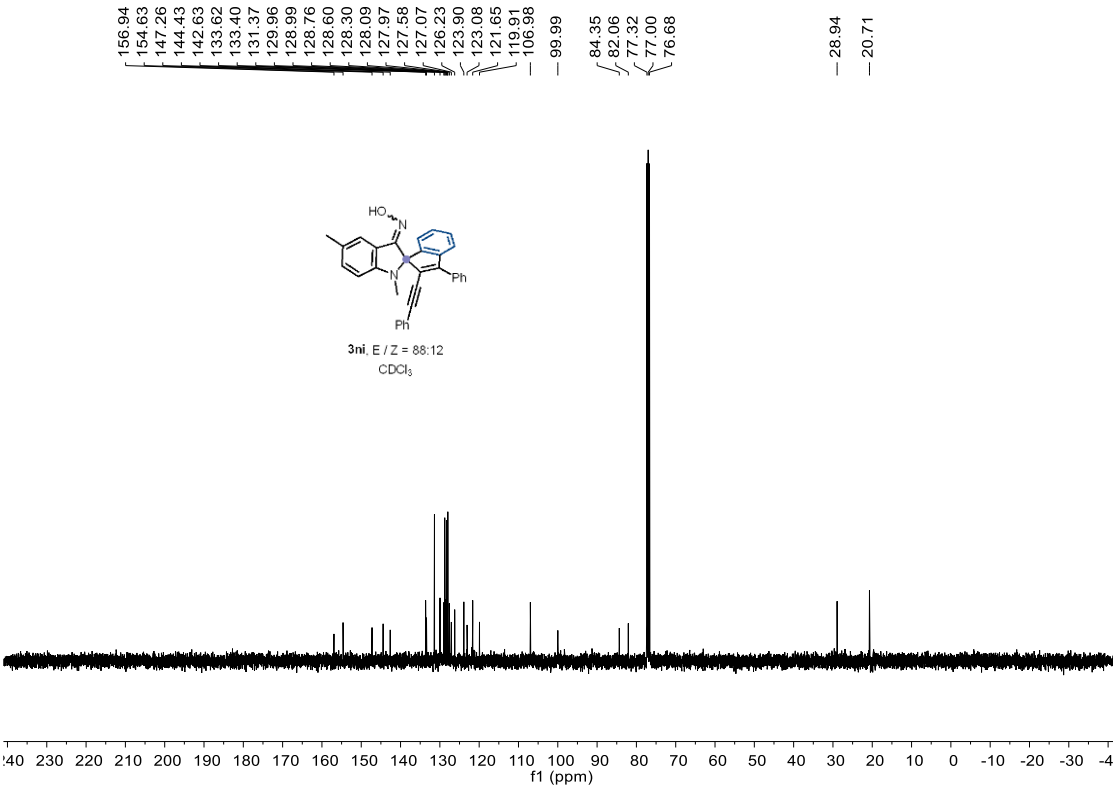
8.06
8.05
7.82
7.81
7.80
7.80
7.62
7.60
7.58
7.53
7.51
7.49
7.45
7.44
7.43
7.43
7.41
7.41
7.37
7.35
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.28
7.27
7.26
6.94
6.94
6.93
6.92
6.92
6.90
6.88
2.59
2.51
2.50
2.50
2.49
2.49
HO
N
Cl
N
Ph
Ph
3li, E / Z = 99:1
DMSO-d6
1.00
1.00
2.00
2.00
2.00
2.00
5.00
2.00
1.00
3.00
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


154.83
153.54
147.50
145.09
142.36
133.08
132.47
131.32
129.80
129.73
129.56
129.33
129.27
128.88
128.49
127.98
126.83
124.33
122.40
122.08
121.39
120.73
109.10
99.55
84.87
82.10
40.63
40.42
40.21
40.00
39.79
39.58
39.37
29.08
HO
N
Cl
N
Ph
Ph
3li, E / Z = 99:1
DMSO-d6
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-4
f1 (ppm)

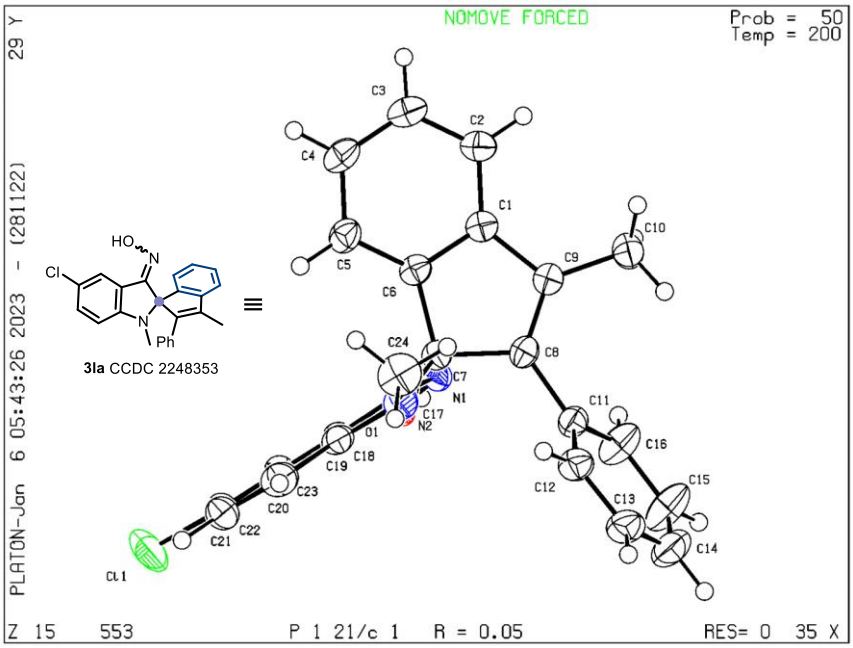

11.65
8.19
8.19
7.82
7.81
7.80
7.62
7.61
7.60
7.58
7.54
7.53
7.52
7.51
7.49
7.45
7.44
7.43
7.43
7.41
7.41
7.37
7.37
7.35
7.35
7.33
7.33
7.33
7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.27
7.27
7.26
6.94
6.93
6.93
6.92
6.92
6.91
6.86
6.84
2.59
2.51
2.51
2.50
2.50
2.49
-0.01
HO
N
Br
N
Ph
Ph
3mi, E / Z = 99:1
DMSO-d6
1.00
1.00
2.00
2.00
3.00
1.00
5.00
2.00
1.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


155.15
153.45
147.48
145.04
142.37
135.22
133.07
131.36
130.77
129.82
129.75
129.58
129.35
129.27
128.89
128.51
126.80
124.34
122.40
122.10
121.98
109.74
108.02
99.58
84.88
82.04
40.63
40.42
40.21
40.00
39.79
39.59
39.37
29.04
HO
N
Br
N
Ph
Ph
3mi, E / Z = 99:1
DMSO-d6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

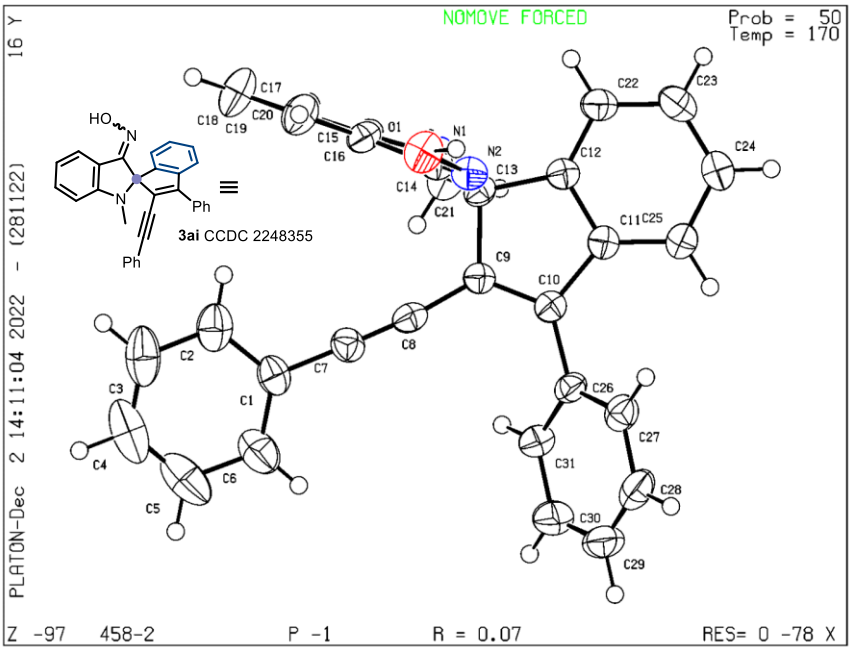

7.98
7.84
7.82
7.51
7.50
7.49
7.48
7.47
7.42
7.35
7.34
7.33
7.33
7.31
7.27
7.27
7.27
7.26
7.25
7.24
7.21
7.20
7.19
7.18
7.17
7.17
7.16
7.15
7.14
7.14
7.12
7.12
6.90
6.90
6.89
6.88
6.88
6.62
6.60
2.81
2.34
0.00
HO
N
Ph
Ph
3ni, E / Z = 88:12
CDCl3
1.00
1.00
2.00
3.00
0.99
3.00
3.99
2.00
1.00
3.00
3.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


156.94
154.63
147.26
144.43
142.63
133.62
133.40
131.37
129.96
128.99
128.76
128.60
128.30
128.09
127.97
127.58
127.07
126.23
123.90
123.08
121.65
119.91
106.98
99.99
84.35
82.06
77.32
77.00
76.68
28.94
20.71
HO
N
Ph
Ph
3ni, E / Z = 88:12
CDCl3
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -4
f1 (ppm)

8. X-ray Crystallographic Data for Compound 3la and 3ai.



Identification code	**3la**
Empirical formula	$C_{24}H_{19}ClN_2O$
Formula weight	386.86
Temperature/K	199.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.2188(4)
b/Å	20.7777(7)
c/Å	8.8300(3)
α/°	90
β/°	109.930(4)
γ/°	90
Volume/Å^3	1935.01(12)
Z	4
ρ_{calc}g/cm^3	1.328
μ/mm^{-1}	1.873
F(000)	808.0
Crystal size/mm^3	0.13 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.384 to 147.626
Index ranges	$-12 \le h \le 13$, $-25 \le k \le 23$, $-10 \le l \le 6$
Reflections collected	7351
Independent reflections	3811 [R_{int} = 0.0305, R_{sigma} = 0.0372]
Data/restraints/parameters	3811/0/257
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0476, wR_2 = 0.1347
Final R indexes [all data]	R_1 = 0.0524, wR_2 = 0.1402
Largest diff. peak/hole / e Å^{-3}	0.46/-0.51



Identification code	**3ai**
Empirical formula	$C_{31}H_{22}N_2O$
Formula weight	438.50
Temperature/K	169.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.2696(12)
b/Å	10.3708(13)
c/Å	12.6585(13)
α/°	90.132(9)
β/°	110.122(10)
γ/°	104.018(10)
Volume/Å^3	1222.8(3)
Z	2
ρ_{calc}g/cm^3	1.191
μ/mm^{-1}	0.072
F(000)	460.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.374 to 50
Index ranges	-12 ≤ h ≤ 12, -10 ≤ k ≤ 12, -15 ≤ l ≤ 12
Reflections collected	8691
Independent reflections	4303 [R_{int} = 0.0469, R_{sigma} = 0.0648]
Data/restraints/parameters	4303/2/312
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0653, wR_2 = 0.1626
Final R indexes [all data]	R_1 = 0.0921, wR_2 = 0.1861
Largest diff. peak/hole / e Å^{-3}	0.32/-0.26

9. References

1) Yang, S.-D.; Sun, C.-L.; Fang, Z.; Li, B.-J.; Li, Y.-Z.; Shi Z.-J. *Angew. Chem. Int. Ed.* **2008**, *47*, 1473.
2) Xie, R.; Ling, Y.; Fu, H. *Chem. Commun.* **2012**, *48*, 12210.
3) Lebrasseur, N.; Larrosa, I. *J. Am. Chem. Soc.* **2008**, *130*, 2926.
4) Wu, Y.; Pi, C.; Cui, X.; Wu, Y. *Org. Lett.* **2020**, *22*, 361.
5) Shoberu A.; Li C.-K.; Tao Z.-K.; Zhang G.-Y.; Zou J.-P. *Adv. Synth. Catal.* **2019**, *361*, 2255.
6) (a) Li, D.; Yin, K.; Li, J.; Jia, X. *Tetrahedron Lett.* **2008**, *49*, 5918. (b) Mukherjee, N.; Kundua D.; Ranu, B. *Chem. Commun.* **2014**, *50*, 15784-15787.
7) Frisch, M. J.; et al. Gaussian 09, revision A.1; Gaussian, Inc.: Wallingford, CT, **2009**.
8) (a) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
9) (a) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.* **2011**, *32*, 1456. (b) Grimme, S.; Antony, J; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.
10) (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270; (b) Wadt, W. R.; Hay, P. J. *J. Chem. Phys.* **1985**, *82*, 284; (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.
11) (a) Ho, J.; Klamt, A.; Coote, M. L. *J. Phys. Chem. A* **2010**, *114*, 13442; (b) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378-6396.
12) (a) Y. Zhao, D. G. Truhlar, Theor. Chem. Acc. 2008, 120, 215; (b) Y. Zhao, D. G. Truhlar, Acc. Chem. Res. 2008, 41, 157.
13) D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, H. Preuss, Theor. Chim. Acta 1990, 77, 123.
14) CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org).
15) Reed, A. E.; Weinstock, R. B.; Weinhold, F. *J. Chem. Phys.* **1985,** *83*, 735.