Electronic Supplementary Information

Pd(II)-Catalyzed intramolecular diarylation of alkynes via dual C-H activation: modular access to azafulvalene-based bis(polycyclic) aromatic enes

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1. General Information

1.1 General Information

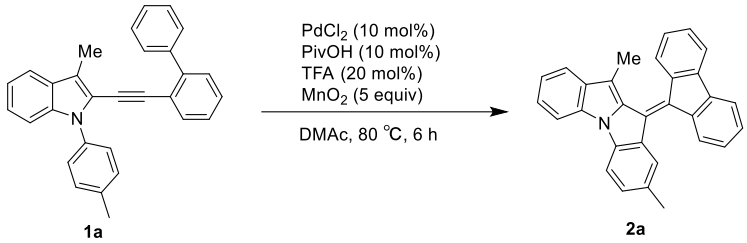
^{1}H NMR and ^{13}C NMR spectra were recorded on JEOL JNM AL 400 (400 MHz), JEOL JNM AL 600 (600 MHz), and Bruker AVANCE NEO 700 (700 MHz) spectrometers. ^{1}H NMR spectra are reported as follows: chemical shift in ppm (δ) relative to the chemical shift of $CDCl_3$ at 7.26 ppm, multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, m = multiplet, bs = broad singlet), and coupling constants (Hz). ^{13}C NMR spectra were recorded on JEOL JNM AL 400 (100 MHz) spectrometer with complete proton decoupling, and chemical shift reported in ppm (δ) relative to the central line for $CDCl_3$ at 77.16 ppm. ^{19}F NMR spectra were recorded on JEOL JNM AL 400 (376 MHz) spectrometer. High-resolution mass spectra were obtained on a Bruker Daltonics SolariX spectrometer using dithranol (DIT) as an exact matrix and FT-ICR-MS analyzer. UV/Vis absorption spectra were recorded on a JASCO V-650DS spectrometer. Redox potential values are measured by cyclic voltammograms (CV), which are versus $Ag/AgNO_3$ reference electrode; Pt wire as a counter electrode and glassy carbon as a working electrode; 0.1 M $TBAPF_6$ as a supporting electrolyte in dichloromethane; scan rate is 50 mV s^{-1}, and the energy level of Fc/Fc+ as -4.80 eV. Flash column chromatography was performed on silica gel 60N (spherical, neutral, 40-50 μm; Kanto Chemical Co., Inc.). Analytical thin-layer chromatography (TLC) was performed on 0.2 mm precoated plate Kieselgel 60 F254 (Merck).

1.2 Materials

Unless otherwise noted, materials were purchased from Wako Pure Chemical Industries, LTD., Tokyo Chemical Industry Co., LTD., Kanto Chemical Co., Inc., Aldrich Inc., and other commercial suppliers and were used without purification. Tetrahydrofuran and diethyl ether were supplied from Kanto Chemical Co., Inc. as “Dehydrated solvent system”. MnO_2 (activated, ~85%, <10 μm, Cat. No. 217646) and DMAc were purchased from Aldrich Inc. Other solvents were purchased from commercial suppliers as dehydrated solvents, and used under argon or nitrogen atmosphere. $CDCl_3$ was purchased from KANTO Chemical Co., Inc. All air- and moisture-sensitive manipulations were performed under argon atmosphere using oven-dried glassware, including standard Schlenk and glovebox techniques. The structure of **2f** was confirmed by means of X-ray crystallography. The structures of starting substrates and products were determined by ^{1}H, ^{13}C NMR, high resolution mass spectrometry (HRMS).

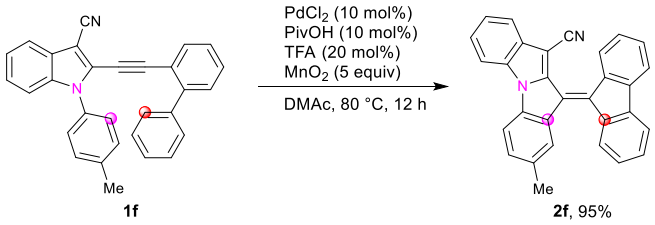
2. General procedures for the synthesis of 2a and 4a

2.1 General procedure for the Pd-catalyzed synthesis of 2a



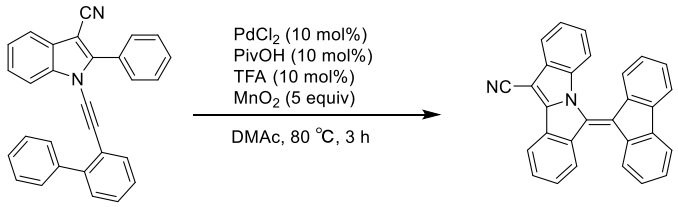
To an anhydrous DMAc (1.6 mL, 0.125 M) solution were added 2-(biphenyl-2-ylethynyl)-3-methyl-1-(*p*-tolyl)-1*H*-indole (**1a**) (79.5 mg, 0.2 mmol), $PdCl_2$ (3.5 mg, 0.02 mmol), PivOH (2.0 mg, 0.02 mmol), TFA (3.0 μL, 0.04 mmol) and MnO_2 (86.9 mg, 1.0 mmol). The reaction vial was purged with N_2 atmosphere and capped. The reaction mixture was stirred at room temperature for 5 min and then heated at 80 °C for 6 hours. After cooling to room temperature, the reaction mixture was passed through Celite using Et_2O as an eluent. The organic layer was washed with water and brine, dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography using hexane/DCM (2:1) as eluent to afford the desired product **2a** in 94% yield (74.4 mg, 0.19 mmol) as dark red solid.

2.2 Gram-scale synthesis of 2f



To an anhydrous DMAc (20 mL, 0.125 M) solution in Schlenk tube were added 2-(biphenyl-2-ylethynyl)-1-(*p*-tolyl)-1*H*-indole-3-carbonitrile (**1f**) (1.02 g, 2.5 mmol), $PdCl_2$ (44.3 mg, 0.25 mmol), PivOH (25.5 mg, 0.25 mmol), TFA (38.3 μL, 0.50 mmol) and MnO_2 (1.08 g, 12.5 mmol). This Schlenk tube was purged with N_2 atmosphere and capped. The reaction mixture was stirred at room temperature for 5 min and then heated at 80 °C for 12 hours. After cooling to room temperature, the reaction mixture was passed through Celite using Et_2O and DCM as an eluent. The organic layer was washed with water and brine, dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography using hexane/DCM (1:1) as eluent to afford the desired product **2f** in 95% yield (967 mg, 2.38 mmol) as dark red solid.

2.3 General procedure for the Pd-catalyzed synthesis of 4a

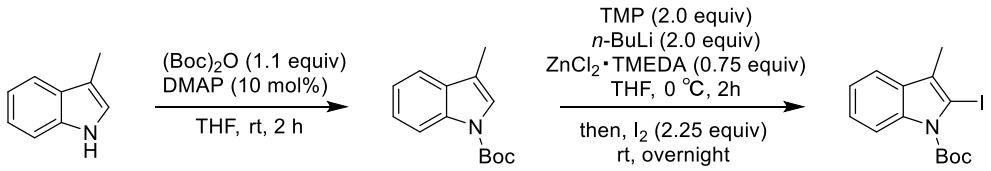


3a **4a**

To an anhydrous DMAc (1.6 mL, 0.125 M) solution were added 1-(biphenyl-2-ylethynyl)-2-phenyl-1*H*-indole-3-carbonitrile (**3a**) (78.9 mg, 0.2 mmol), $PdCl_2$ (3.5 mg, 0.02 mmol), PivOH (2.0 mg, 0.02 mmol), TFA (1.5 μL, 0.02 mmol) and MnO_2 (86.9 mg, 1.0 mmol). The reaction vial was purged with N_2 atmosphere and capped. The reaction mixture was stirred at room temperature for 5 min and then heated at 80 °C for 3 hours. After cooling to room temperature, the reaction mixture was passed through Celite using Et_2O as an eluent. The organic layer was washed with water and brine, dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography using hexane/AcOEt (10:1) as eluent to afford the desired product **4a** in 86% yield (66.7 mg, 0.17 mmol) as orange solid. Caution: The purification of compounds **4** by silica gel column chromatography should be carried out rapidly, as **4** is slightly unstable owing to the presence of an enamine moiety.

3. Synthetic methods of starting substrates

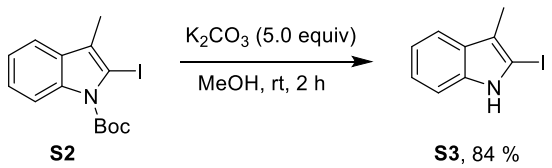
3.1 Synthetic methods of substrates 1



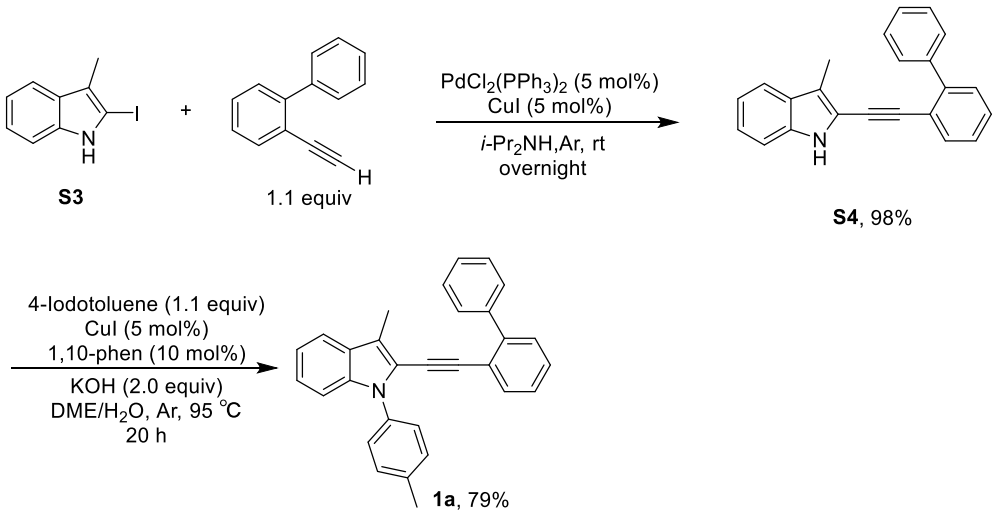
S1, 95 % **S2**, 97 %

Synthetic procedure of substrate S2:[1,2] To a mixture of 3-methyl-1*H*-indole (1.31 g, 10 mmol), $(Boc)_2O$ (2.4 g, 11 mmol), and DMAP (122 mg, 1 mmol) was added THF (80 mL). The mixture was stirred for 2 h at room temperature. Evaporation followed by column chromatography using a mixture of hexane/AcOEt (10/1) as eluent, to give *tert*-butyl 3-methyl-1*H*-indole-1-carboxylate (**S1**) as clear colorless oil (95% yield, 2.20 g). Next, *n*-BuLi (1.6 M hexanes solution, 4.2 mL, 6.8 mmol) was added successfully to a solution of 2,2,6,6-tetramethylpiperidine (TMP) (1.1 mL, 6.8 mmol) in THF (9 mL) at 0 °C, and the rection mixture was stirred for 5 min before adding $ZnCl_2$·TMEDA (568 mg, 2.3 mmol). The resulting mixture was stirred for 15 min at 0 °C and then **S1** (694 mg, 3.0 mmol) was

added at 0 °C. After stirring for 2 h at room temperature, a solution of I_2 (1.7 g, 6.8 mmol) in THF (8 mL) was added. The mixture was stirred overnight before addition of aqueous saturated solution of $Na_2S_2O_3$ and extracted with diethyl ether (3 x 40 mL). The combined organic layers were dried over $MgSO_4$ and filtered. After concentration under reduced pressure, the residue was purified by column chromatography using a mixture of hexane/AcOEt (20/1) as an eluent to give corresponding product *tert*-butyl 2-iodo-3-methyl-1*H*-indole-1-carboxylate (**S2**) in 97% yield (1.0 g, 2.9 mmol) as yellow oil.



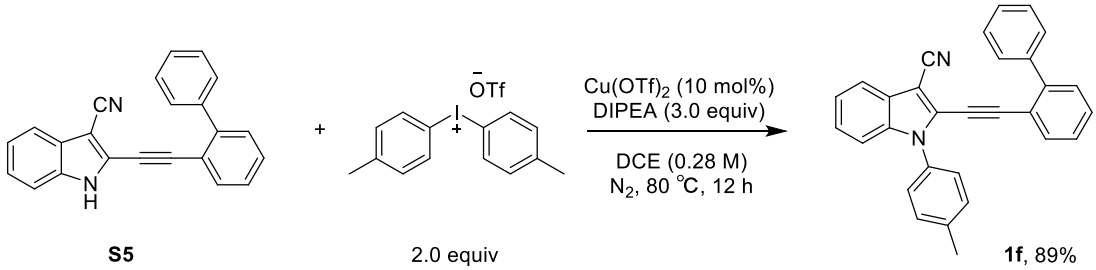
Synthetic procedure of substrate S3: A solution of **S2** (1.0 g, 2.9 mmol) and K_2CO_3 (2.0 g, 14.5 mmol) in methanol (9.6 mL) was stirred at room temperature for 2 hours. After completion of the reaction, the mixture was diluted with water and extracted with ethyl acetate. The combined organic layers were washed with water and brine, dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by column chromatography using a mixture of hexane/AcOEt (10/1) as an eluent to give corresponding product 2-iodo-3-methyl-1*H*-indole (**S3**) in 84% yield (625 mg, 2.4 mmol) as yellow oil.



Synthetic procedure of substrate 1a: A mixture of **S3** (563 mg, 2.2 mmol), 2-ethynyl-biphenyl (431 mg, 2.4 mmol), $PdCl_2(PPh_3)_2$ (77 mg, 0.1 mmol) and CuI (21 g, 0.1 mmol) were added *i*-Pr_2NH (8.8 ml) under Ar atmosphere. The reaction mixture was stirred at room temperature overnight. After filtration through Celite, the organic layer was washed successively with aq. NH_4Cl, water, and brine, dried over anhydrous $MgSO_4$, filtered, and

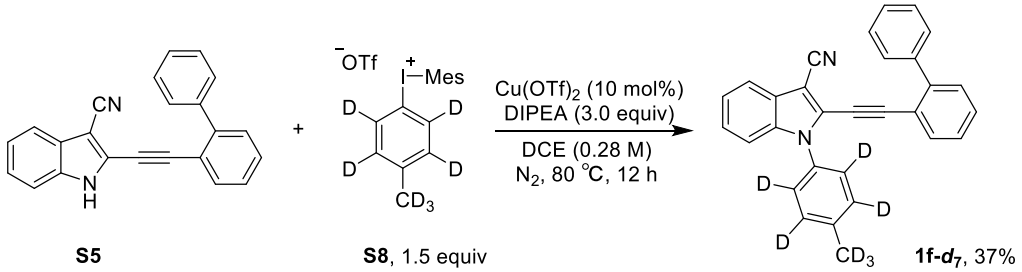
concentrated under reduced pressure. The crude product was purified by column chromatography using a mixture of hexane/AcOEt (10/1) as an eluent to give corresponding product 2-(biphenyl-2-ylethynyl)-3-methyl-1*H*-indole (**S4**) in 98% yield (661 mg, 2.2 mmol) as white solid. Next, a mixture of **S4** (513 mg, 1.7 mmol), 4-iodotoluene (401 mg, 1.8 mmol), CuI (16 mg, 0.08 mmol), 1,10-phenanthroline (30 mg, 0.17 mol), and KOH (187 mg, 3.3 mmol) was added to a solution of 1,2-DME/H_2O = 3:7 (v/v, 0.5 M) under Ar atmosphere. The mixture was heated at 90 °C for 20 h. After cooling to room temperature, the resulting mixture was quenched with aq. NH_4Cl and extracted with diethyl ether. The organic layer was separated and dried over $MgSO_4$. After filtration and evaporation of the solvent, the residue was purified by silica gel column chromatography using hexane/DCM (2/1) as eluent, giving 2-(biphenyl-2-ylethynyl)-3-methyl-1-(*p*-tolyl)-1*H*-indole (**1a**) in 79% yield (523 mg, 1.3 mmol) as white solid.

Synthetic procedure of substrate 1f [3]



S5 2.0 equiv **1f**, 89%

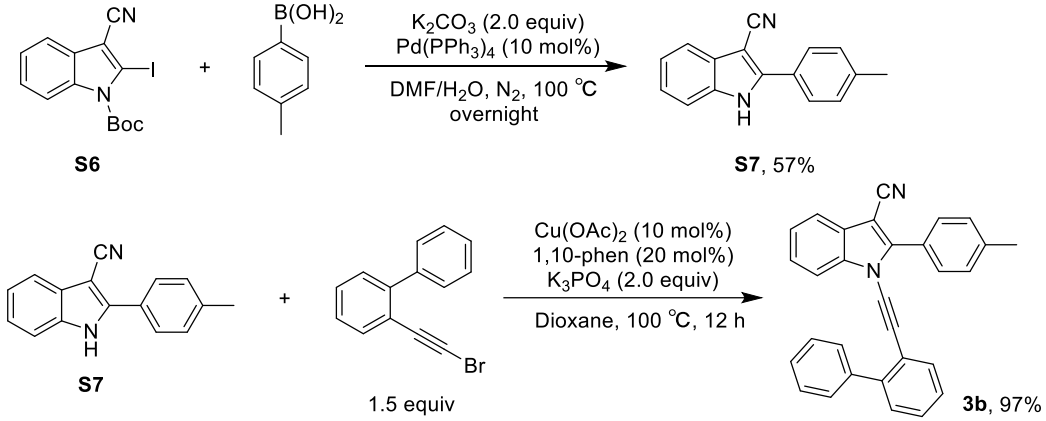
2-(Biphenyl-2-ylethynyl)-1*H*-indole-3-carbonitrile (**S5**) was synthesized from 3-cyanoindole according to the same procedure as described for **S4**. Next, a mixture of 2-**S5** (318 mg, 1.0 mmol), diphenyliodonium triflate (687 mg, 1.5 mmol), $Cu(OTf)_2$ (36 mg, 0.1 mmol), and DIPEA (0.5 ml, 3.0 mmol) was added to a solution of DCE (3.6 mL, 0.28 M) under an N_2 atmosphere. The reaction mixture was heated at 80 °C for 12 h. After cooling to room temperature, the reaction mixture was evaporated the solvent under reduce pressure. The crude product was purified by column chromatography using a mixture of hexane/DCM (1/3) as an eluent to give corresponding product 2-(biphenyl-2-ylethynyl)-1-(*p*-tolyl)-1*H*-indole-3-carbonitrile (**1f**) in 89% yield (363 mg, 0.9 mmol) as white solid.



S5 **S8**, 1.5 equiv **1f-*d*$_7$**, 37%

Synthetic procedure of substrate 1f-d_7: The known compound **S8** was synthesized according to the literature procedure.[4] The subsequent transformation to **1f-d_7** was carried out following the same procedure as that used for the synthesis of **1f**, affording **1f-d_7** in 37% yield (154 mg, 0.37 mmol) as white solid.

3.2 Synthetic methods of substrates 3

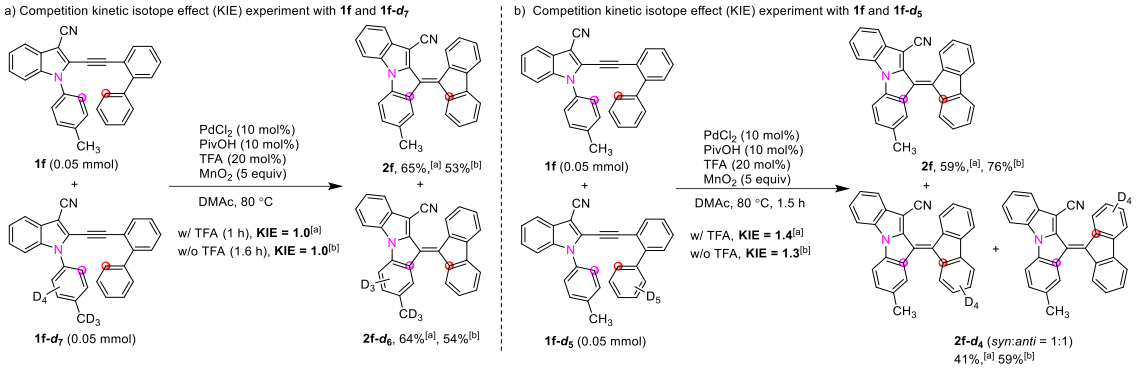


Synthetic procedure of substrate 3b:[5] *tert*-butyl 3-cyano-2-iodo-1*H*-indole-1-carboxylate (**S6**) was synthesized from 3-cyanoindole according to the same procedure as described for **S2**. Next, a mixture of **S6** (368 mg, 1.0 mmol), K_2CO_3 (276 mg, 2.0 mmol), $Pd(PPh_3)_4$ (116 mg, 0.1 mmol), and *p*-tolylboronic acid (204 mg, 1.5 mmol) was dissolved in a mixture of DMF/H_2O = 5:1 (v/v, 0.05 M) under Ar atmosphere. The reaction mixture was stirred at 100 °C overnight. The solution was warmed up to room temperature and extracted with Et_2O (3 x 20 mL). The combined organic layer was washed with water and brine, and dried over $MgSO_4$. After filtration and removal of solvent on a rotary evaporator, the crude product was purified by column chromatography using a hexane/AcOEt (10/1) as an eluent, giving 2-(*p*-tolyl)-1*H*-indole-3-carbonitrile (**S7**) in 57% yield (132 mg, 057 mmol).

To a mixture of **S7** (116 mg, 0.5 mmol), $Cu(OTf)_2$ (9 mg, 0.05 mmol), 1,10-phen (18 mg, 0.1 mmol), K_3PO_4 (212 mg, 1.0 mmol), and 2-(bromoethynyl)-biphenyl (190 mg, 0.75 mmol) was added dioxane (2.0 mL) under Ar atmosphere. The mixture was stirred for 24 h at 100 °C. The reaction mixture was allowed to cool to room temperature and was passed through a short pad of silica gel using DCM. The solvent was then removed under reduced pressure. The crude product was purified by column chromatography using a mixture of hexane/DCM (2/1) as an eluent to give corresponding product 2-(*p*-tolyl)-1*H*-indole-3-carbonitrile (**3b**) in 97% yield (179 mg, 0.46 mmol) as white solid.

4. Kinetic isotope effect (KIE) experiments

Kinetic isotope effect (KIE) values were determined based on the product yields measured by ^{1}H NMR spectroscopy, using CH_2Br_2 as an internal standard.



Scheme S1. KIE experiments. [a] With TFA. [b] Without TFA.

5. References

1. Y. Du, R. M. Pearson, C.-H. Lim, S. M. Sartor, M. D. Ryan, H. Yang, N. H. Damrauer, G. M. Miyake, *Chem. Eur. J.* **2017**, 23, 10962-10968.
2. J.-M. L'Helgoual'ch, A. Seggio, F. Chevallier, M. Yonehara, E. Jeanneau, M. Uchiyama, F. Mongin, *J. Org. Chem.* **2008**, *73*, 177-183.
3. M. K. Mehra, M. Malik, B. Kumar, D. Kumar, *Org. Biomol. Chem*. **2021**, *19*, 1109-1114.
4. R. A. Roberts, B. E. Metze, N. Javaly, T. M. McCormick, D. R. Stuart, *Chem. Sci*. **2025**, *16*, 5547.
5. Y. Zhang, R. P. Hsung, M. R. Tracey, K. C. M. Kurtz, E. L. Vera, *Org. Lett.* **2004**, *6*, 1151-1154.

6. DFT Calculations

6.1 DFT calculation data for the reaction mechanism: Path A

Density functional theory (DFT) calculations were performed using the Gaussian16[a] program package unless otherwise noted. Geometry optimizations for intermediates and transition states were carried out at the M06/def2-SVP level of theory. For all transition states, intrinsic reaction coordinate (IRC) calculations were performed to confirm the connection between the reactant and product.

[a] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci,

B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16*, Revision C.02; Gaussian, Inc.: Wallingford, CT, 2019.

Cartesian coordinates

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Structure: IM1A
Charge = 0, Multiplicity = 1
Final SCF Energy = -2104.65550074 Hartree
Gibbs Free Energy = -2104.182694 Hartree
Thermal Correction = 0.472807 Hartree
Imaginary Frequencies = none
Cartesian Coordinates (Angstrom):

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C	2.003353	-0.618220	0.570152
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C	3.399130	-2.245447	1.239796
C	0.935841	0.281240	0.388487
C	0.230689	1.285313	0.161606
C	-0.250551	2.633842	0.138086
C	0.318925	3.577895	-0.729126
C	-1.220116	3.029713	1.086667
C	-0.070416	4.908493	-0.648646
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C	-1.576113	4.375983	1.166983
C	-1.014114	5.308223	0.298388
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H	-2.318303	4.685775	1.909609

H	-1.317644	6.356942	0.358350
C	3.486744	0.599295	-1.042729
C	4.492077	1.533145	-0.781421
C	2.734022	0.680778	-2.217330
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C	2.991591	1.704602	-3.125242
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C	3.999196	2.635175	-2.872827
H	5.539155	3.275224	-1.497694
H	2.403010	1.767040	-4.045038
H	4.202772	3.432443	-3.593438
C	-1.760475	2.001709	1.997066
C	-1.475763	2.044072	3.360884
C	-2.491589	0.905448	1.478243
C	-1.872356	0.998238	4.196646
H	-0.904670	2.886849	3.763207
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H	-2.935740	0.983823	0.464973
C	-2.562764	-0.099018	3.686472
H	-1.621331	1.036490	5.260826
H	-3.451117	-0.976204	1.914164
H	-2.859057	-0.918627	4.346196
Pd	-1.156795	-0.358961	-0.041023
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H	5.912736	-4.450347	1.846799
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C	-5.877838	-1.340500	-2.212803
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H	-6.413718	-0.784429	-1.425691
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H	-4.228069	-3.619112	-0.182746
H	-5.570476	-2.537937	0.279043
C	-3.922753	-2.800128	-2.770696
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H	5.060143	1.460486	0.151181
Cl	-0.207058	-1.466203	-1.834297
C	0.986040	-2.269435	2.241390
H	0.218258	-1.506534	2.455625
H	0.473272	-3.107846	1.736641
H	1.367768	-2.648139	3.203042

****

Structure: $TS_{1\text{-}2}A$

Charge = 0, Multiplicity = 1

Final SCF Energy = -2104.64318198 Hartree

Gibbs Free Energy = -2104.173753 Hartree

Thermal Correction = 0.469429 Hartree

Imaginary Frequencies = -1566.83 cm^-1

Cartesian Coordinates (Angstrom):

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C	3.721534	-2.127378	1.069710
C	0.994136	0.181738	0.420927
C	0.201570	1.136331	0.279396
C	-0.418846	2.422565	0.355952
C	0.087849	3.490999	-0.399453
C	-1.487594	2.623871	1.258209

C	-0.466898	4.756242	-0.263447
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C	-2.019776	3.910934	1.383155
C	-1.522940	4.965709	0.625234
H	-0.072606	5.587616	-0.853869
H	-2.855346	4.074778	2.070841
H	-1.966044	5.960469	0.723712
C	3.505290	0.924338	-0.915002
C	4.381842	1.945550	-0.541348
C	2.771665	1.019601	-2.100669
C	4.532043	3.061302	-1.361312
C	2.919330	2.145599	-2.906617
H	2.083000	0.210231	-2.369810
C	3.799379	3.164597	-2.542651
H	5.220385	3.859567	-1.069482
H	2.346442	2.219954	-3.835430
H	3.917552	4.042594	-3.184240
C	-1.967983	1.495803	2.071850
C	-2.178347	1.673782	3.444910
C	-2.202775	0.221212	1.492799
C	-2.569337	0.607981	4.249209
H	-1.990191	2.654244	3.894040
C	-2.605942	-0.837466	2.329994
H	-2.903028	0.285066	0.407607
C	-2.777588	-0.656290	3.696236
H	-2.705542	0.764261	5.323366
H	-2.809449	-1.815735	1.878940
H	-3.087746	-1.491405	4.330408
Pd	-1.021894	-0.555996	-0.183843
N	3.346203	-0.210962	-0.078372
C	5.658352	-1.194627	-0.133716
C	6.406087	-2.263156	0.334607
C	5.840031	-3.256568	1.160365
H	7.460364	-2.340415	0.053093
C	4.507455	-3.199376	1.527655
H	6.465550	-4.083955	1.506794

H	4.066027	-3.976889	2.159242
H	6.096923	-0.430651	-0.781746
O	-3.906457	0.132958	-0.527722
C	-3.725237	-1.028505	-0.967795
O	-2.660552	-1.688464	-0.785756
C	-4.802895	-1.684714	-1.827346
C	-6.153914	-1.024588	-1.591276
H	-6.914724	-1.490514	-2.239912
H	-6.481318	-1.139805	-0.544831
H	-6.119018	0.052783	-1.812101
C	-4.877987	-3.178857	-1.532393
H	-5.640327	-3.646451	-2.178012
H	-3.912774	-3.672652	-1.717396
H	-5.163283	-3.368416	-0.483800
C	-4.351213	-1.462646	-3.275033
H	-5.077916	-1.921687	-3.966638
H	-4.288804	-0.386746	-3.509036
H	-3.362227	-1.914034	-3.455061
H	4.935269	1.857421	0.398690
Cl	0.169856	-1.535268	-1.937728
C	1.314469	-2.538695	1.994369
H	0.449310	-1.903947	2.246197
H	0.933400	-3.383686	1.393067
H	1.715988	-2.956129	2.931698

****

Structure: IM2A

Charge = 0, Multiplicity = 1

Final SCF Energy = -2104.68455492 Hartree

Gibbs Free Energy = -2104.211234 Hartree

Thermal Correction = 0.473321 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	4.236688	-1.312000	0.449959
C	2.138449	-0.569900	0.723696
C	2.235708	-1.703698	1.509750

C	3.569063	-2.187390	1.345446
C	1.047621	0.310267	0.555228
C	0.334494	1.315604	0.342669
C	-0.191697	2.638926	0.227654
C	0.514231	3.594903	-0.516945
C	-1.409389	2.966631	0.866472
C	0.009494	4.881839	-0.651339
H	1.458876	3.307408	-0.990286
C	-1.896954	4.267113	0.700251
C	-1.203151	5.213023	-0.048591
H	0.559231	5.624726	-1.235363
H	-2.854040	4.541436	1.152918
H	-1.617805	6.218119	-0.166453
C	3.601951	0.720177	-0.851470
C	4.582850	1.674195	-0.570738
C	2.855130	0.799033	-2.030266
C	4.822243	2.705871	-1.475187
C	3.091417	1.843635	-2.920015
H	2.092937	0.038322	-2.234988
C	4.074228	2.795094	-2.648134
H	5.592132	3.451087	-1.255839
H	2.506572	1.906385	-3.842107
H	4.260978	3.608385	-3.355315
C	-2.091735	1.964692	1.709735
C	-2.889914	2.395986	2.785761
C	-1.949655	0.576844	1.517535
C	-3.521080	1.498124	3.636367
H	-2.986410	3.468816	2.979729
C	-2.571791	-0.323827	2.381675
H	-1.757446	-1.824634	-2.407129
C	-3.361343	0.129177	3.437183
H	-4.127164	1.870040	4.467244
H	-2.463732	-1.402011	2.216040
H	-3.850408	-0.590122	4.101157
Pd	-0.976300	-0.330884	0.003479
N	3.353057	-0.328191	0.070907

C	5.564961	-1.523664	0.064052
C	6.219455	-2.621071	0.601468
C	5.577332	-3.496802	1.500655
H	7.258245	-2.814094	0.317921
C	4.260452	-3.291570	1.872979
H	6.129802	-4.351233	1.901513
H	3.759389	-3.978500	2.562516
H	6.061736	-0.849980	-0.639924
O	-2.749128	-1.960462	-2.536561
C	-3.397055	-1.702824	-1.442219
O	-2.884061	-1.247411	-0.419387
C	-4.884205	-2.000669	-1.505849
C	-5.489747	-1.129918	-2.610796
H	-6.573677	-1.321204	-2.674918
H	-5.348780	-0.056958	-2.398921
H	-5.040563	-1.351558	-3.590876
C	-5.538185	-1.682236	-0.168941
H	-6.618796	-1.892022	-0.227247
H	-5.112301	-2.291082	0.644542
H	-5.403867	-0.624214	0.106875
C	-5.071669	-3.479411	-1.851811
H	-6.148449	-3.711343	-1.900289
H	-4.620423	-3.727283	-2.824472
H	-4.621090	-4.132073	-1.085649
H	5.146337	1.601333	0.364568
Cl	0.100783	-1.639140	-1.776615
C	1.153508	-2.307352	2.326558
H	0.353997	-1.579552	2.539384
H	0.689439	-3.162476	1.802466
H	1.535630	-2.682165	3.289801

****

Structure: IM3A

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.44427923 Hartree

Gibbs Free Energy = -1930.857843 Hartree

Thermal Correction = 0.586436 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	3.793768	-0.761478	-1.091662
C	1.564747	-0.950188	-1.244548
C	1.946522	-0.178455	-2.326558
C	3.365012	-0.045094	-2.238928
C	0.267976	-1.307498	-0.824493
C	-0.752965	-1.778617	-0.281416
C	-1.726748	-2.647049	0.305033
C	-1.304150	-3.622416	1.219957
C	-3.093430	-2.504337	-0.026287
C	-2.234868	-4.447781	1.838197
H	-0.235356	-3.714010	1.441005
C	-4.006628	-3.342975	0.622411
C	-3.589433	-4.298016	1.544855
H	-1.902911	-5.203201	2.555430
H	-5.074313	-3.233248	0.411431
H	-4.331409	-4.930001	2.041101
C	2.669962	-2.070908	0.708817
C	3.374695	-3.274784	0.777502
C	1.943170	-1.613579	1.812344
C	3.360895	-4.018172	1.955079
C	1.925761	-2.370927	2.980775
H	1.402156	-0.664573	1.731389
C	2.634085	-3.569798	3.056767
H	3.914706	-4.959848	2.007855
H	1.357773	-2.013285	3.844435
H	2.622034	-4.156580	3.979758
C	-3.505452	-1.539241	-1.066500
C	-4.644425	-1.818918	-1.843773
C	-2.773885	-0.368968	-1.357313
C	-5.050602	-0.981569	-2.874293
H	-5.202731	-2.741842	-1.657610
C	-3.181434	0.462499	-2.402939
C	-4.313485	0.164728	-3.159620

H	-5.935172	-1.234461	-3.465672
H	-2.616636	1.375754	-2.619823
H	-4.617878	0.832210	-3.971709
Pd	-1.170808	0.308741	-0.356180
N	2.686273	-1.315376	-0.491121
C	5.136125	-0.786184	-0.697214
C	6.043965	-0.085035	-1.475604
C	5.639045	0.626403	-2.623599
H	7.099589	-0.079249	-1.188575
C	4.310345	0.652948	-3.009830
H	6.387679	1.167448	-3.209077
H	3.993140	1.215565	-3.893875
H	5.450784	-1.325204	0.200968
O	-0.169026	2.595922	2.022171
C	0.712662	2.155701	1.280706
O	0.606408	1.143441	0.504351
C	2.100062	2.831079	1.227332
C	2.399929	3.212643	-0.222406
H	3.369239	3.737845	-0.289379
H	2.448914	2.317122	-0.863461
H	1.622838	3.883704	-0.631097
C	3.153279	1.833730	1.707999
H	4.157576	2.292539	1.681275
H	2.957990	1.508916	2.745416
H	3.172689	0.938737	1.064687
C	2.120408	4.069629	2.111145
H	3.115359	4.547200	2.079832
H	1.373828	4.812433	1.782137
H	1.887670	3.817002	3.157670
H	3.923647	-3.623206	-0.102711
C	1.046188	0.453135	-3.322720
H	0.032723	0.022897	-3.283442
H	0.950646	1.538965	-3.135408
H	1.428099	0.333614	-4.349965
C	-2.523869	2.625692	0.915373
O	-2.105484	2.197619	-0.180427

N	-2.524871	3.951949	1.148195
C	-3.082847	1.703902	1.951583
H	-2.356224	1.628958	2.775476
H	-4.045958	2.057774	2.348677
H	-3.220320	0.706611	1.508587
C	-2.635627	4.476945	2.493573
H	-1.661923	4.394606	3.010897
H	-2.937542	5.533722	2.448500
H	-3.393438	3.940378	3.077942
C	-1.796800	4.793594	0.219642
H	-0.710194	4.724621	0.417102
H	-1.983983	4.475888	-0.812731
H	-2.122622	5.836421	0.342627

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Structure: $TS_{3\text{-}4}A$

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.42576173 Hartree

Gibbs Free Energy = -1930.834156 Hartree

Thermal Correction = 0.591606 Hartree

Imaginary Frequencies = -265.58 cm^-1

Cartesian Coordinates (Angstrom):

C	3.662832	-1.349358	-0.735963
C	1.500608	-0.980580	-1.229750
C	2.224073	-0.382569	-2.243226
C	3.601970	-0.619705	-1.949092
C	0.088237	-0.992420	-1.058296
C	-1.078397	-1.473604	-0.786835
C	-1.858507	-2.411637	-0.012359
C	-1.298165	-3.414879	0.784810
C	-3.252411	-2.216386	-0.033225
C	-2.129976	-4.209175	1.566786
H	-0.215512	-3.568306	0.788256
C	-4.074190	-3.009965	0.767207
C	-3.511581	-4.000689	1.567629
H	-1.692719	-4.997297	2.186847

H	-5.157379	-2.852757	0.767264
H	-4.156123	-4.620743	2.197182
C	2.010805	-2.116528	0.951797
C	2.406621	-3.415259	1.284846
C	1.274736	-1.349782	1.861070
C	2.070329	-3.946295	2.528080
C	0.927290	-1.899035	3.092682
H	0.977931	-0.321625	1.619237
C	1.324280	-3.191608	3.432141
H	2.386012	-4.961209	2.786624
H	0.349532	-1.295692	3.798806
H	1.055010	-3.611389	4.405586
C	-3.662254	-1.217851	-1.015555
C	-4.938293	-1.168219	-1.585903
C	-2.635187	-0.420680	-1.558777
C	-5.186042	-0.379575	-2.704140
H	-5.731439	-1.803747	-1.178670
C	-2.861593	0.281432	-2.748308
C	-4.141631	0.324059	-3.301338
H	-6.188194	-0.350956	-3.140821
H	-2.054283	0.841795	-3.233473
H	-4.318981	0.913300	-4.205574
Pd	-1.041024	0.668937	-0.766549
N	2.371095	-1.580761	-0.309021
C	4.881360	-1.656457	-0.122770
C	6.041700	-1.240686	-0.759923
C	6.001911	-0.533608	-1.977627
H	7.010126	-1.464810	-0.303084
C	4.792929	-0.219411	-2.575975
H	6.939586	-0.224323	-2.447981
H	4.758912	0.345674	-3.513189
H	4.917432	-2.192266	0.829951
O	0.354206	1.872856	1.722622
C	0.966776	2.214018	0.702724
O	0.615405	1.933019	-0.493334
C	2.308393	2.957741	0.828767

C	2.518141	3.928702	-0.326626
H	3.490222	4.441782	-0.221992
H	2.504348	3.403234	-1.293419
H	1.729698	4.700698	-0.355743
C	3.388511	1.872275	0.786501
H	4.390016	2.315221	0.929217
H	3.232345	1.122114	1.582910
H	3.384051	1.348462	-0.184404
C	2.377253	3.696370	2.158676
H	3.356072	4.194038	2.270795
H	1.595203	4.473322	2.229968
H	2.234503	3.005003	3.003044
H	2.972227	-4.003030	0.555314
C	1.686195	0.388240	-3.390702
H	0.585341	0.407450	-3.381660
H	2.032310	1.435652	-3.352796
H	2.012623	-0.031206	-4.357543
C	-2.346575	2.442463	1.163796
O	-2.305554	2.338101	-0.075234
N	-2.076036	3.620975	1.763512
C	-2.712744	1.272698	2.027633
H	-1.802785	0.920968	2.541553
H	-3.473721	1.524568	2.781276
H	-3.095669	0.465716	1.387835
C	-1.845867	3.727993	3.188184
H	-0.817835	3.402208	3.433359
H	-1.976117	4.776278	3.496603
H	-2.556205	3.122612	3.765452
C	-1.527129	4.705400	0.977887
H	-0.443375	4.806072	1.176654
H	-1.671755	4.500746	-0.088771
H	-2.018641	5.655460	1.243811

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Structure: IM4aA

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.47965393 Hartree

Gibbs Free Energy = -1930.886790 Hartree

Thermal Correction = 0.592864 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-1.237477	-3.194717	0.206394
C	-0.802028	-1.308795	-0.946883
C	-0.491290	-2.350669	-1.797466
C	-0.777942	-3.557183	-1.086115
C	-0.745523	0.111055	-1.194685
C	-1.801733	0.960297	-1.146427
C	-3.220917	0.758189	-0.817202
C	-4.031887	-0.370329	-0.883465
C	-3.733878	1.985869	-0.321471
C	-5.353018	-0.273187	-0.445513
H	-3.638824	-1.315686	-1.273949
C	-5.047073	2.065156	0.131730
C	-5.852686	0.927717	0.066276
H	-6.006654	-1.148776	-0.501845
H	-5.444455	3.006028	0.526164
H	-6.889809	0.978145	0.410429
C	-1.607823	-1.042259	1.415328
C	-2.851945	-1.234438	2.022665
C	-0.739942	-0.059159	1.900136
C	-3.235124	-0.432944	3.093995
C	-1.144640	0.757684	2.952654
H	0.258883	0.058627	1.463153
C	-2.390536	0.577213	3.550641
H	-4.213982	-0.584534	3.558094
H	-0.465094	1.533400	3.318594
H	-2.700931	1.218985	4.380080
C	-2.680608	3.004180	-0.416055
C	-2.592923	4.343706	-0.055104
C	-1.567121	2.387614	-1.021091
C	-1.398962	5.040352	-0.298465
H	-3.438340	4.855976	0.415542

C	-0.405728	3.089871	-1.327436
C	-0.313993	4.431238	-0.929943
H	-1.328754	6.094242	-0.014125
H	0.332373	2.683848	-2.066327
H	0.590803	5.005491	-1.149864
Pd	0.981116	1.103978	-1.084185
N	-1.245082	-1.817237	0.285391
C	-1.518338	-4.156883	1.181690
C	-1.351212	-5.490588	0.835760
C	-0.910828	-5.869799	-0.447277
H	-1.562003	-6.264704	1.579531
C	-0.621757	-4.914940	-1.408619
H	-0.790397	-6.931696	-0.680122
H	-0.262351	-5.206679	-2.401056
H	-1.841806	-3.867924	2.185574
O	2.611753	-0.064786	1.179851
C	2.601976	-0.865407	0.241380
O	2.003927	-0.681272	-0.879525
C	3.274407	-2.239724	0.399616
C	3.728567	-2.809435	-0.937953
H	4.210652	-3.790899	-0.786715
H	2.877773	-2.945358	-1.623451
H	4.456841	-2.146753	-1.436507
C	2.206085	-3.150982	1.010025
H	2.629915	-4.146280	1.231075
H	1.810289	-2.727791	1.949978
H	1.365504	-3.289103	0.311612
C	4.455808	-2.125966	1.355518
H	4.921818	-3.115578	1.501671
H	5.232217	-1.444456	0.964641
H	4.133774	-1.743845	2.336325
H	-3.529088	-1.997587	1.627272
C	0.057536	-2.236307	-3.171634
H	0.168026	-1.182941	-3.470524
H	1.057420	-2.700647	-3.234843
H	-0.581799	-2.740681	-3.916400

C	3.238569	2.433240	0.394644
O	2.803236	2.336317	-0.765922
N	4.527671	2.131866	0.655514
C	2.376364	2.923885	1.519212
H	2.237594	2.116962	2.255090
H	2.821176	3.794700	2.026510
H	1.394059	3.208143	1.116388
C	5.008153	1.943095	2.007833
H	4.709071	0.951407	2.393959
H	6.105138	2.019874	2.020539
H	4.616553	2.714492	2.684010
C	5.287241	1.500543	-0.405231
H	4.985324	0.444085	-0.538158
H	5.114018	2.017835	-1.357168
H	6.357657	1.539059	-0.159021

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Structure: IM4bA

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.46802914 Hartree

Gibbs Free Energy = -1930.880701 Hartree

Thermal Correction = 0.587328 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-1.713123	3.570586	-0.228213
C	-1.370494	1.356045	-0.522637
C	-1.999128	1.793181	-1.672625
C	-2.238936	3.194075	-1.492358
C	-0.942360	0.056912	-0.055139
C	-1.710867	-0.998106	0.303692
C	-3.186349	-1.119198	0.217255
C	-4.180113	-0.193104	-0.101495
C	-3.551539	-2.445545	0.546988
C	-5.513498	-0.602284	-0.111699
H	-3.925554	0.845581	-0.330813
C	-4.883918	-2.850306	0.525312

C	-5.865410	-1.920840	0.188755
H	-6.294732	0.123659	-0.355412
H	-5.157469	-3.879596	0.779285
H	-6.917168	-2.220677	0.169515
C	-0.432470	2.295762	1.534720
C	0.883869	1.792609	1.440335
C	-1.000129	2.553985	2.777462
C	1.592243	1.499151	2.615174
C	-0.271221	2.270844	3.933350
H	-2.023943	2.935215	2.832475
C	1.010741	1.724491	3.858836
H	2.616263	1.122688	2.528867
H	-0.725383	2.457394	4.910891
H	1.560720	1.493735	4.774823
C	-2.345521	-3.179822	0.917985
C	-2.176365	-4.492955	1.350521
C	-1.242142	-2.302001	0.813844
C	-0.900628	-4.927651	1.709991
H	-3.033478	-5.170003	1.424338
C	0.022664	-2.738116	1.208051
C	0.186910	-4.050577	1.653046
H	-0.754028	-5.952757	2.063325
H	0.882347	-2.053791	1.193052
H	1.175876	-4.391449	1.976215
Pd	1.026929	0.034176	-0.023121
N	-1.167628	2.442382	0.343663
C	-1.762655	4.887719	0.235228
C	-2.374377	5.828932	-0.580214
C	-2.919291	5.474771	-1.830087
H	-2.429954	6.869324	-0.247151
C	-2.853212	4.170998	-2.293563
H	-3.394515	6.245830	-2.443129
H	-3.269912	3.900580	-3.269234
H	-1.329272	5.165130	1.200515
O	3.166794	-0.041739	-0.007995
C	3.779333	1.052793	-0.279375

O	3.232364	2.147293	-0.425916
C	5.315745	0.963417	-0.332307
C	5.785505	-0.425390	-0.743729
H	6.888698	-0.460215	-0.781383
H	5.439478	-1.191978	-0.032672
H	5.404560	-0.696356	-1.743489
C	5.801602	1.274216	1.085428
H	6.905188	1.280798	1.125670
H	5.439843	2.263927	1.411886
H	5.441099	0.516453	1.802567
C	5.857204	2.009603	-1.298320
H	6.961239	1.995905	-1.300662
H	5.511732	1.817884	-2.328116
H	5.513934	3.016274	-1.018114
H	1.480649	1.980196	0.499987
C	-2.385309	0.965140	-2.842868
H	-1.933332	-0.036829	-2.779554
H	-3.480696	0.835572	-2.916823
H	-2.049524	1.424904	-3.787523
C	0.775679	-2.645961	-1.782351
O	0.949371	-1.426982	-1.646817
N	1.750483	-3.542053	-1.518943
C	-0.539099	-3.170053	-2.289726
H	-0.433623	-3.624149	-3.288641
H	-0.957835	-3.931832	-1.612068
H	-1.245163	-2.332438	-2.354904
C	3.019973	-3.120492	-0.957646
H	3.066474	-2.027157	-0.852350
H	3.161823	-3.577475	0.038383
H	3.847672	-3.456009	-1.605373
C	1.558172	-4.971364	-1.629562
H	0.871243	-5.232118	-2.445027
H	2.526477	-5.446743	-1.846554
H	1.164415	-5.401268	-0.688814

****

Structure: $TS_{4\text{-}5}A$

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.46168718 Hartree

Gibbs Free Energy = -1930.877316 Hartree

Thermal Correction = 0.584371 Hartree

Imaginary Frequencies = -1360.88 cm^-1

Cartesian Coordinates (Angstrom):

C	0.208131	3.861339	-0.294921
C	-0.662381	1.778775	-0.463210
C	-1.087186	2.455750	-1.588410
C	-0.552068	3.782951	-1.490219
C	-0.869445	0.426960	0.012020
C	-2.039288	-0.166560	0.355695
C	-3.410126	0.393883	0.286095
C	-3.880264	1.679655	0.013505
C	-4.336808	-0.631706	0.588754
C	-5.253980	1.919219	0.017424
H	-3.183135	2.497323	-0.188464
C	-5.708361	-0.389468	0.579027
C	-6.164517	0.893319	0.285467
H	-5.622236	2.928479	-0.189318
H	-6.416641	-1.191578	0.811288
H	-7.238163	1.102545	0.276455
C	0.768971	2.174750	1.489381
C	1.447707	0.931065	1.461477
C	0.676131	2.914614	2.668580
C	1.961210	0.438539	2.678384
C	1.216688	2.404340	3.845330
H	0.136469	3.866100	2.665732
C	1.847015	1.157918	3.860282
H	2.508398	-0.511605	2.665035
H	1.126066	2.980767	4.770736
H	2.261662	0.763084	4.791696
C	-3.594235	-1.840868	0.927836
C	-4.039144	-3.098995	1.327951
C	-2.212770	-1.553832	0.833084

C	-3.100088	-4.072853	1.666808
H	-5.110396	-3.315542	1.393212
C	-1.284291	-2.526365	1.204224
C	-1.733227	-3.780789	1.619892
H	-3.434341	-5.061495	1.995785
H	-0.209347	-2.300647	1.192290
H	-1.006498	-4.539827	1.928186
Pd	0.876295	-0.490490	-0.031299
N	0.149394	2.622031	0.313336
C	0.892885	5.022854	0.070006
C	0.783737	6.124028	-0.769353
C	0.017862	6.073214	-1.948264
H	1.309753	7.047373	-0.509996
C	-0.644665	4.912549	-2.317822
H	-0.046749	6.961477	-2.583310
H	-1.230938	4.871651	-3.241681
H	1.504359	5.061707	0.975763
O	2.833846	-1.424759	-0.172302
C	3.795078	-0.609079	-0.190257
O	3.669132	0.625065	0.009989
C	5.210171	-1.157475	-0.388745
C	5.176720	-2.554723	-0.992349
H	6.205038	-2.930203	-1.131568
H	4.635965	-3.260712	-0.342713
H	4.676707	-2.555523	-1.975296
C	5.837801	-1.206568	1.007166
H	6.872780	-1.585056	0.947494
H	5.860761	-0.203677	1.463482
H	5.269444	-1.878724	1.673354
C	6.009774	-0.213192	-1.280328
H	7.044802	-0.580376	-1.387899
H	5.568283	-0.144608	-2.288637
H	6.038465	0.801557	-0.856629
H	2.361778	0.816287	0.567471
C	-1.935138	1.923836	-2.685168
H	-2.031240	0.829145	-2.613231

H	-2.957150	2.345640	-2.666223
H	-1.505121	2.160787	-3.673064
C	-0.535112	-2.791520	-1.782507
O	0.158531	-1.777491	-1.638921
N	-0.053335	-4.028277	-1.525423
C	-1.946133	-2.677716	-2.287302
H	-2.068909	-3.166587	-3.267376
H	-2.658646	-3.139569	-1.584024
H	-2.191737	-1.612746	-2.387792
C	1.271015	-4.204957	-0.961765
H	1.813604	-3.250927	-0.924050
H	1.199201	-4.612314	0.063170
H	1.845561	-4.921553	-1.572436
C	-0.863157	-5.223358	-1.614797
H	-1.601136	-5.158981	-2.424779
H	-0.211066	-6.083618	-1.828249
H	-1.400807	-5.421522	-0.668010

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Structure: IM5A

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.49170801 Hartree

Gibbs Free Energy = -1930.902059 Hartree

Thermal Correction = 0.589649 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	0.175227	3.866935	-0.397698
C	-0.812483	1.832073	-0.354702
C	-1.334642	2.483258	-1.456562
C	-0.722503	3.778772	-1.493488
C	-0.952763	0.465803	0.111675
C	-2.105760	-0.164496	0.463362
C	-3.485212	0.377290	0.476844
C	-3.981673	1.672633	0.316179
C	-4.389150	-0.676635	0.749396
C	-5.355933	1.893605	0.392726

H	-3.301994	2.511459	0.145536
C	-5.762851	-0.452823	0.812328
C	-6.244942	0.839908	0.625057
H	-5.742297	2.910347	0.273679
H	-6.451367	-1.278409	1.021227
H	-7.320196	1.035195	0.674321
C	0.858045	2.240644	1.405139
C	1.250380	0.888899	1.477981
C	1.177747	3.132544	2.435300
C	1.965013	0.473294	2.608878
C	1.912869	2.697968	3.533838
H	0.815230	4.163033	2.386899
C	2.310585	1.366184	3.623721
H	2.271126	-0.576932	2.693553
H	2.157589	3.403265	4.333244
H	2.881085	1.017670	4.489977
C	-3.621102	-1.893257	0.983714
C	-4.040709	-3.181091	1.309904
C	-2.246033	-1.580352	0.865358
C	-3.082749	-4.164710	1.553078
H	-5.107634	-3.413469	1.391492
C	-1.298212	-2.566978	1.139411
C	-1.721437	-3.851761	1.483022
H	-3.396376	-5.177641	1.823802
H	-0.226759	-2.329521	1.103044
H	-0.976599	-4.620943	1.715093
Pd	0.818717	-0.418771	0.014277
N	0.105882	2.669214	0.291589
C	0.970336	5.000321	-0.202091
C	0.833871	6.053737	-1.099301
C	-0.071454	5.991862	-2.171837
H	1.449832	6.948088	-0.966240
C	-0.845768	4.859331	-2.378393
H	-0.157536	6.843368	-2.853119
H	-1.541818	4.802414	-3.221983
H	1.693104	5.058188	0.615115

O	2.864891	-1.350752	-0.113885
C	3.892176	-0.690771	-0.184044
O	3.905418	0.620463	-0.106314
C	5.267889	-1.312687	-0.311488
C	5.135107	-2.785775	-0.670978
H	6.136463	-3.238823	-0.753519
H	4.568451	-3.338074	0.094771
H	4.617112	-2.919422	-1.634712
C	5.937283	-1.163289	1.060147
H	6.937511	-1.626616	1.034766
H	6.053121	-0.104178	1.338558
H	5.350470	-1.666464	1.847263
C	6.082966	-0.575161	-1.372657
H	7.082473	-1.033571	-1.451261
H	5.604402	-0.637493	-2.363898
H	6.210534	0.488044	-1.120745
H	2.994528	0.931596	0.113021
C	-2.309174	1.959499	-2.446407
H	-2.466949	0.877320	-2.320928
H	-3.300565	2.440083	-2.351476
H	-1.962433	2.138246	-3.478794
C	-0.466689	-2.741333	-1.838181
O	0.355548	-1.844528	-1.630953
N	-0.135749	-4.044025	-1.660581
C	-1.853886	-2.428384	-2.321080
H	-2.010666	-2.791053	-3.350175
H	-2.620447	-2.886167	-1.674862
H	-1.982815	-1.338525	-2.305684
C	1.134188	-4.395106	-1.060517
H	1.723780	-3.488802	-0.869222
H	0.967841	-4.925500	-0.105321
H	1.706011	-5.063896	-1.726706
C	-1.064460	-5.135060	-1.850468
H	-1.786609	-4.921092	-2.648773
H	-0.505953	-6.037671	-2.143240
H	-1.625006	-5.357718	-0.922262

****

Structure: IM6A

Charge = 0, Multiplicity = 1

Final SCF Energy = -1872.36269334 Hartree

Gibbs Free Energy = -1871.787741 Hartree

Thermal Correction = 0.574952 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-1.377482	3.083748	-0.309434
C	0.234082	1.494342	-0.265160
C	0.687615	2.524215	0.544033
C	-0.323780	3.539634	0.526847
C	0.729947	0.138248	-0.424006
C	1.988190	-0.223947	-0.792937
C	3.105232	0.645205	-1.231972
C	3.153744	1.996363	-1.579837
C	4.280628	-0.136572	-1.333317
C	4.365737	2.557414	-1.981719
H	2.248553	2.610214	-1.550786
C	5.491488	0.431539	-1.722548
C	5.530970	1.787317	-2.040267
H	4.401527	3.614889	-2.260867
H	6.395457	-0.182446	-1.794397
H	6.472826	2.248146	-2.352636
C	-1.764364	0.964063	-1.609000
C	-2.566041	1.449342	-2.647259
C	-1.680118	-0.414285	-1.349294
C	-3.321557	0.566493	-3.416742
C	-2.410949	-1.283913	-2.163642
C	-3.243626	-0.803992	-3.178450
H	-3.949182	0.953797	-4.224676
H	-2.340365	-2.364731	-1.990780
H	-3.816560	-1.504442	-3.795639
C	3.939345	-1.522497	-1.031276
C	4.732239	-2.667881	-1.005635

C	2.551616	-1.590350	-0.768425
C	4.131261	-3.898339	-0.746129
H	5.808324	-2.604973	-1.198808
C	1.957879	-2.831419	-0.541109
C	2.751436	-3.978045	-0.531804
H	4.738220	-4.808665	-0.727853
H	0.877910	-2.904507	-0.372301
H	2.286085	-4.953004	-0.357378
Pd	-0.695585	-1.078790	0.249388
N	-1.011469	1.845215	-0.801474
C	-2.550347	3.828851	-0.468804
C	-2.644868	5.046861	0.195652
C	-1.598011	5.525199	1.000816
H	-3.556018	5.642841	0.087417
C	-0.441042	4.778543	1.174132
H	-1.701406	6.493658	1.499006
H	0.371143	5.148586	1.808932
H	-3.379052	3.464567	-1.081026
H	-2.575320	2.520334	-2.869070
C	1.945787	2.571937	1.330267
H	2.352146	1.559819	1.497160
H	2.742391	3.145153	0.819849
H	1.783186	3.053001	2.311628
C	1.297398	-1.231415	2.703044
O	0.463544	-1.811431	2.001140
N	0.984150	-0.116985	3.408071
C	2.703325	-1.755305	2.781369
H	3.382025	-1.085284	2.223282
H	3.077731	-1.843256	3.812236
H	2.731952	-2.735632	2.288103
C	1.914381	0.597442	4.252536
H	2.955176	0.421921	3.953172
H	1.729332	1.679745	4.164456
H	1.800098	0.318693	5.316653
C	-0.372654	0.394332	3.394379
H	-0.461817	1.277178	2.731044

H	-1.059314	-0.385039	3.037241
H	-0.663268	0.688542	4.416183
C	-3.631442	-1.672196	0.722087
O	-2.526293	-2.169404	0.971398
N	-4.637126	-2.428885	0.217152
C	-3.923759	-0.219342	0.972297
H	-4.210400	0.292721	0.038158
H	-4.745848	-0.094063	1.695680
H	-3.019030	0.266835	1.361926
C	-5.891940	-1.869228	-0.234100
H	-6.658408	-2.658670	-0.235192
H	-6.247223	-1.068447	0.427517
H	-5.810462	-1.464487	-1.261242
C	-4.389210	-3.802722	-0.164095
H	-4.469260	-3.918919	-1.260345
H	-3.381214	-4.092906	0.154097
H	-5.126586	-4.473393	0.307868

****

Structure: $TS_{6\text{-}7}A$

Charge = 0, Multiplicity = 1

Final SCF Energy = -1872.34608128 Hartree

Gibbs Free Energy = -1871.773072 Hartree

Thermal Correction = 0.573010 Hartree

Imaginary Frequencies = -255.08 cm^-1

Cartesian Coordinates (Angstrom):

C	-2.142840	2.648105	-0.594248
C	-0.233798	1.458823	-0.341114
C	-0.066482	2.592286	0.430662
C	-1.274368	3.360772	0.279901
C	0.481064	0.196125	-0.502848
C	1.812699	0.058001	-0.809434
C	2.759764	1.093350	-1.261255
C	2.583176	2.435743	-1.606970
C	4.043408	0.507909	-1.401122
C	3.678184	3.181460	-2.042043

H	1.593226	2.897914	-1.555760
C	5.134578	1.260966	-1.826145
C	4.948623	2.606025	-2.139145
H	3.537299	4.231214	-2.316850
H	6.122166	0.799006	-1.928224
H	5.795500	3.210560	-2.477040
C	-1.784578	0.372723	-1.732931
C	-2.635752	0.363774	-2.835190
C	-1.004732	-0.754528	-1.378084
C	-2.697364	-0.780878	-3.632504
C	-1.025300	-1.855603	-2.247401
C	-1.878397	-1.875558	-3.352809
H	-3.357449	-0.796507	-4.504699
H	-0.384880	-2.721033	-2.042861
H	-1.902257	-2.755665	-4.003167
C	3.938943	-0.909407	-1.075121
C	4.906420	-1.910542	-1.042010
C	2.589521	-1.189687	-0.751285
C	4.525219	-3.207674	-0.701459
H	5.950624	-1.684361	-1.282014
C	2.222365	-2.492144	-0.407498
C	3.191128	-3.494625	-0.394340
H	5.273181	-4.005789	-0.673974
H	1.187579	-2.717947	-0.119354
H	2.904280	-4.516571	-0.128812
Pd	-0.543414	-1.155863	0.581773
N	-1.480573	1.498709	-0.962407
C	-3.417222	3.121764	-0.911468
C	-3.814962	4.333175	-0.354609
C	-2.965734	5.059393	0.495936
H	-4.809515	4.725903	-0.585469
C	-1.701345	4.582425	0.817748
H	-3.308235	6.011970	0.910383
H	-1.045342	5.153371	1.483181
H	-4.089120	2.559265	-1.565476
H	-3.201163	1.261123	-3.102319

C	1.108974	2.949088	1.262234
H	1.676409	2.046321	1.547429
H	1.819277	3.608687	0.728819
H	0.804541	3.478514	2.182047
C	1.491378	-0.804945	2.941161
O	0.730758	-1.615262	2.410490
N	1.015995	0.283060	3.603554
C	2.980456	-0.985949	2.840067
H	3.405431	-0.217434	2.168987
H	3.495536	-0.916684	3.810050
H	3.174822	-1.966462	2.385580
C	1.841941	1.249722	4.287245
H	2.871252	1.248892	3.907069
H	1.435870	2.261600	4.125759
H	1.869093	1.068190	5.378101
C	-0.414628	0.489964	3.708779
H	-0.745444	1.309290	3.041081
H	-0.947814	-0.427816	3.425065
H	-0.676794	0.755657	4.746491
C	-3.211685	-1.924123	0.983331
O	-2.260932	-2.234122	1.713007
N	-3.715926	-2.790947	0.068413
C	-3.858890	-0.568593	1.088057
H	-3.866508	-0.051113	0.113861
H	-4.900652	-0.641188	1.441411
H	-3.282091	0.038205	1.799124
C	-4.756182	-2.446595	-0.874309
H	-5.325369	-3.354304	-1.129894
H	-5.466511	-1.724416	-0.451793
H	-4.338280	-2.026872	-1.809976
C	-3.046350	-4.050742	-0.172816
H	-2.652659	-4.079519	-1.204963
H	-2.212179	-4.158563	0.531219
H	-3.745265	-4.894423	-0.041234

****

Structure: IM7A

Charge = 0, Multiplicity = 1

Final SCF Energy = -1872.36892814 Hartree

Gibbs Free Energy = -1871.794510 Hartree

Thermal Correction = 0.574418 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-2.549179	1.918690	-1.112599
C	-0.410115	1.218095	-0.853122
C	-0.539418	2.309944	-0.015334
C	-1.895120	2.773803	-0.181089
C	0.477852	0.061755	-1.033390
C	1.885312	0.118994	-0.968887
C	2.710710	1.297425	-1.225910
C	2.389216	2.607910	-1.607004
C	4.081136	0.915805	-1.189889
C	3.408147	3.518895	-1.873684
H	1.345710	2.915076	-1.719599
C	5.093063	1.835103	-1.454165
C	4.753985	3.145657	-1.783153
H	3.149265	4.540634	-2.168307
H	6.143084	1.525209	-1.423112
H	5.538460	3.878596	-1.992967
C	-1.639114	-0.297400	-2.046035
C	-2.613237	-0.909554	-2.820054
C	-0.401134	-0.933098	-1.725540
C	-2.358296	-2.198516	-3.298440
C	-0.157477	-2.209428	-2.268633
C	-1.143770	-2.834089	-3.030404
H	-3.111789	-2.702298	-3.910944
H	0.805854	-2.698529	-2.109645
H	-0.954949	-3.832359	-3.434560
C	4.145445	-0.504071	-0.891536
C	5.239844	-1.342848	-0.690966
C	2.815700	-0.987768	-0.762887
C	5.020356	-2.675414	-0.349774

H	6.259676	-0.956355	-0.790990
C	2.616407	-2.316910	-0.365666
C	3.714064	-3.152415	-0.180224
H	5.869733	-3.346772	-0.192384
H	1.607430	-2.684941	-0.143634
H	3.551788	-4.190801	0.123916
Pd	-0.392188	-1.199954	0.506958
N	-1.614477	0.992661	-1.522562
C	-3.893792	2.080201	-1.444806
C	-4.593248	3.113112	-0.824710
C	-3.965533	3.969476	0.093808
H	-5.649415	3.263904	-1.066169
C	-2.622409	3.811862	0.415610
H	-4.543219	4.774250	0.557186
H	-2.139438	4.485901	1.130451
H	-4.387770	1.426289	-2.168268
H	-3.540278	-0.390035	-3.075483
C	0.467258	2.862419	0.921279
H	1.129783	2.064022	1.300635
H	1.127756	3.609061	0.441997
H	-0.019984	3.356256	1.778759
C	1.730060	-0.553690	2.830805
O	1.030877	-1.469241	2.407210
N	1.189297	0.517440	3.485503
C	3.220263	-0.561377	2.626549
H	3.514532	0.222615	1.905503
H	3.780030	-0.392904	3.559480
H	3.500867	-1.531879	2.196326
C	1.963065	1.599585	4.044247
H	2.913988	1.739904	3.513836
H	1.396865	2.541000	3.949211
H	2.179538	1.448989	5.119370
C	-0.232439	0.564270	3.744777
H	-0.688220	1.433049	3.231001
H	-0.715645	-0.353390	3.379899
H	-0.422371	0.670342	4.827829

C	-3.196852	-1.209389	1.514240
O	-2.179767	-1.682615	2.025299
N	-3.921819	-1.909472	0.598081
C	-3.679839	0.163887	1.898996
H	-3.630355	0.862750	1.046305
H	-4.718942	0.153713	2.263949
H	-3.025588	0.542888	2.693800
C	-5.078861	-1.409310	-0.100700
H	-5.989874	-1.973463	0.173023
H	-5.254617	-0.345793	0.103462
H	-4.932910	-1.519924	-1.190650
C	-3.482433	-3.227016	0.194796
H	-3.085219	-3.207907	-0.837460
H	-2.691634	-3.572582	0.871671
H	-4.329079	-3.933770	0.230244

****

Structure: IM3A'

Charge = 0, Multiplicity = 1

Final SCF Energy = -2111.10929112 Hartree

Gibbs Free Energy = -2110.620917 Hartree

Thermal Correction = 0.488374 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	3.811622	0.657645	1.232903
C	1.568601	0.586792	1.232236
C	1.966467	-0.227387	2.277891
C	3.394195	-0.190184	2.290368
C	0.270622	0.911901	0.776434
C	-0.687968	1.447672	0.176699
C	-1.607186	2.279828	-0.530394
C	-1.151640	3.006236	-1.640271
C	-2.957376	2.358036	-0.116878
C	-2.030889	3.808145	-2.356432
H	-0.101016	2.921946	-1.934075
C	-3.820214	3.162429	-0.868456

C	-3.368881	3.879200	-1.972875
H	-1.671982	4.369257	-3.223360
H	-4.877453	3.213677	-0.592680
H	-4.072248	4.492269	-2.543412
C	2.678648	1.979585	-0.545253
C	2.962602	3.337756	-0.386599
C	2.388487	1.463795	-1.809917
C	2.960855	4.179854	-1.495484
C	2.379275	2.313517	-2.913378
H	2.159332	0.402047	-1.930570
C	2.668095	3.668628	-2.759228
H	3.184853	5.242960	-1.370542
H	2.146537	1.905297	-3.900592
H	2.665919	4.331361	-3.629452
C	-3.409025	1.630512	1.085980
C	-4.480782	2.138857	1.842267
C	-2.794252	0.448188	1.539500
C	-4.931448	1.504126	2.992262
H	-4.949771	3.078563	1.534007
C	-3.244174	-0.188053	2.695507
C	-4.313163	0.333095	3.423091
H	-5.762303	1.932217	3.560014
H	-2.772840	-1.122114	3.023045
H	-4.661369	-0.180404	4.324310
Pd	-1.327299	-0.548765	0.625154
N	2.690932	1.123947	0.588588
C	5.162852	0.901254	0.966415
C	6.094902	0.282719	1.785266
C	5.702168	-0.561382	2.844131
H	7.160519	0.450715	1.603537
C	4.363888	-0.804216	3.101282
H	6.469782	-1.031563	3.465234
H	4.060549	-1.465725	3.919172
H	5.465886	1.551399	0.140571
O	0.035683	-0.987844	-2.257266
C	0.562241	-1.659921	-1.379281

O	0.218890	-1.831894	-0.174919
C	1.836910	-2.462328	-1.728047
H	3.183541	3.719207	0.615004
C	1.092268	-1.016345	3.181168
H	0.039329	-0.696180	3.111617
H	1.127110	-2.090066	2.925915
H	1.406152	-0.917903	4.233512
C	-2.600104	-2.557050	-0.834458
O	-2.625914	-2.250847	0.381199
N	-2.064986	-3.717783	-1.241273
C	-3.132950	-1.619087	-1.872579
H	-2.278230	-1.144292	-2.388290
H	-3.754714	-2.126558	-2.625049
H	-3.720976	-0.837664	-1.371339
C	-1.841158	-3.997041	-2.649717
H	-1.207574	-3.221798	-3.113900
H	-1.321019	-4.959810	-2.738506
H	-2.784416	-4.070153	-3.214148
C	-1.453055	-4.617154	-0.278267
H	-0.355007	-4.559251	-0.347562
H	-1.754827	-4.324046	0.732937
H	-1.779333	-5.650328	-0.475500
F	2.263309	-2.219724	-2.959865
F	1.593304	-3.777745	-1.640119
F	2.827590	-2.172093	-0.889529

****

Structure: $TS_{3\text{-}4}A'$

Charge = 0, Multiplicity = 1

Final SCF Energy = -2111.09028889 Hartree

Gibbs Free Energy = -2110.601843 Hartree

Thermal Correction = 0.488446 Hartree

Imaginary Frequencies = -277.69 cm^-1

Cartesian Coordinates (Angstrom):

C	3.658460	1.207502	0.967143
C	1.465021	0.742135	1.152049

C	2.116297	-0.155981	1.985003
C	3.510292	0.136248	1.880402
C	0.067590	0.873718	0.935032
C	-1.061679	1.458928	0.698019
C	-1.815917	2.437358	-0.050643
C	-1.234685	3.454909	-0.814987
C	-3.217002	2.287287	-0.023245
C	-2.046998	4.291984	-1.571424
H	-0.152366	3.593323	-0.803239
C	-4.018868	3.123088	-0.800919
C	-3.433339	4.117052	-1.579554
H	-1.589859	5.090725	-2.163079
H	-5.106123	2.997499	-0.796322
H	-4.062672	4.769868	-2.190978
C	2.173942	2.417002	-0.590463
C	2.484319	3.776830	-0.516319
C	1.686002	1.863901	-1.778321
C	2.313441	4.587415	-1.636564
C	1.506263	2.687153	-2.887427
H	1.453387	0.793274	-1.832797
C	1.822246	4.043697	-2.822766
H	2.560516	5.651345	-1.579275
H	1.123982	2.256107	-3.816866
H	1.687721	4.680686	-3.701819
C	-3.657097	1.300366	0.955437
C	-4.925031	1.297161	1.545434
C	-2.655726	0.468760	1.492521
C	-5.182400	0.524083	2.672484
H	-5.701980	1.957344	1.146462
C	-2.882741	-0.219367	2.689095
C	-4.154934	-0.211269	3.261318
H	-6.178434	0.533173	3.123637
H	-2.086058	-0.801508	3.164906
H	-4.339497	-0.785715	4.173477
Pd	-1.189747	-0.688036	0.609926
N	2.403743	1.587296	0.538448

C	4.917890	1.692257	0.599149
C	6.025833	1.104624	1.191099
C	5.897260	0.052584	2.120050
H	7.024541	1.464848	0.927292
C	4.650495	-0.438450	2.466500
H	6.797278	-0.383502	2.562426
H	4.548031	-1.267142	3.174305
H	5.023088	2.501735	-0.128592
O	0.723355	-1.280458	-1.892266
C	0.943549	-2.013271	-0.935677
O	0.319432	-2.119694	0.158262
C	2.104868	-3.025422	-1.053007
H	2.857812	4.186473	0.427216
C	1.523644	-1.204841	2.850707
H	0.423468	-1.172450	2.841785
H	1.818572	-2.207758	2.498287
H	1.864305	-1.100291	3.894800
C	-2.325329	-2.498972	-1.261445
O	-2.616988	-2.244586	-0.075822
N	-1.824418	-3.696628	-1.616461
C	-2.484970	-1.461437	-2.332127
H	-1.487314	-1.056112	-2.578593
H	-2.935546	-1.862043	-3.252369
H	-3.109865	-0.647345	-1.939274
C	-1.324828	-3.950082	-2.956106
H	-0.617211	-3.165451	-3.271676
H	-0.778501	-4.902690	-2.950482
H	-2.135080	-4.026708	-3.700944
C	-1.614444	-4.727680	-0.617105
H	-0.538215	-4.929686	-0.496650
H	-2.018997	-4.384107	0.341227
H	-2.123227	-5.658103	-0.918757
F	2.959037	-2.700317	-2.007807
F	1.597963	-4.233529	-1.361286
F	2.782601	-3.153764	0.081750

****

Structure: IM4aA'

Charge = 0, Multiplicity = 1

Final SCF Energy = -2111.14447411 Hartree

Gibbs Free Energy = -2110.653481 Hartree

Thermal Correction = 0.490993 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-0.191329	3.152412	0.329297
C	0.247265	1.367216	-0.973390
C	-0.620007	2.166153	-1.700684
C	-0.897293	3.308247	-0.891626
C	0.766842	0.063655	-1.280052
C	2.065066	-0.326686	-1.275294
C	3.319328	0.405829	-1.042672
C	3.661046	1.737527	-1.248961
C	4.248954	-0.497747	-0.464563
C	4.934542	2.167835	-0.874531
H	2.942095	2.430835	-1.698019
C	5.508072	-0.052625	-0.075141
C	5.844924	1.285180	-0.286659
H	5.224367	3.209385	-1.041741
H	6.225667	-0.740775	0.383276
H	6.835760	1.646166	0.004011
C	1.312462	1.421020	1.306522
C	2.418651	2.128516	1.783172
C	1.015465	0.157292	1.823618
C	3.238810	1.561797	2.754665
C	1.855927	-0.414177	2.774732
H	0.110347	-0.358329	1.484654
C	2.969665	0.283136	3.240284
H	4.108931	2.116457	3.117767
H	1.628385	-1.411777	3.163890
H	3.626049	-0.167066	3.990552
C	3.626283	-1.826111	-0.395736
C	4.002029	-3.046239	0.152100

C	2.363548	-1.720413	-1.012414
C	3.110580	-4.130622	0.087218
H	4.973300	-3.167301	0.642667
C	1.503081	-2.808409	-1.146067
C	1.876777	-4.025072	-0.552823
H	3.405187	-5.088752	0.524847
H	0.688800	-2.798176	-1.916564
H	1.215713	-4.893024	-0.629741
Pd	-0.466412	-1.495778	-1.000359
N	0.514642	1.971830	0.270077
C	-0.314597	4.075774	1.373218
C	-1.146718	5.165210	1.167685
C	-1.850178	5.342081	-0.041812
H	-1.267933	5.901449	1.967776
C	-1.733606	4.424080	-1.069894
H	-2.502230	6.212218	-0.158679
H	-2.293960	4.546734	-2.002386
H	0.214871	3.932478	2.319259
O	-2.212913	-0.285085	1.283128
C	-2.571896	0.100482	0.178417
O	-2.162342	-0.249125	-0.967130
C	-3.732398	1.122165	0.149295
H	2.644180	3.113835	1.363185
C	-1.167825	1.881585	-3.049766
H	-0.866597	0.883096	-3.400415
H	-2.269806	1.909940	-3.032881
H	-0.829314	2.624155	-3.793051
C	-2.256214	-3.179878	0.660797
O	-1.689960	-3.277904	-0.444409
N	-3.592741	-3.037266	0.744283
C	-1.459210	-3.230716	1.932074
H	-1.570584	-2.283262	2.481880
H	-1.778125	-4.059494	2.584064
H	-0.401075	-3.370146	1.669553
C	-4.283309	-2.728340	1.978782
H	-4.345788	-1.634499	2.122312

H	-5.303130	-3.140458	1.936370
H	-3.779479	-3.167385	2.848436
C	-4.382477	-2.870492	-0.460317
H	-4.790435	-1.846451	-0.507047
H	-3.752146	-3.042972	-1.339403
H	-5.224421	-3.582380	-0.461809
F	-3.600837	2.025205	1.106880
F	-4.884067	0.463030	0.369540
F	-3.852745	1.759348	-1.007119

6.2 Plausible reaction mechanism: Path B

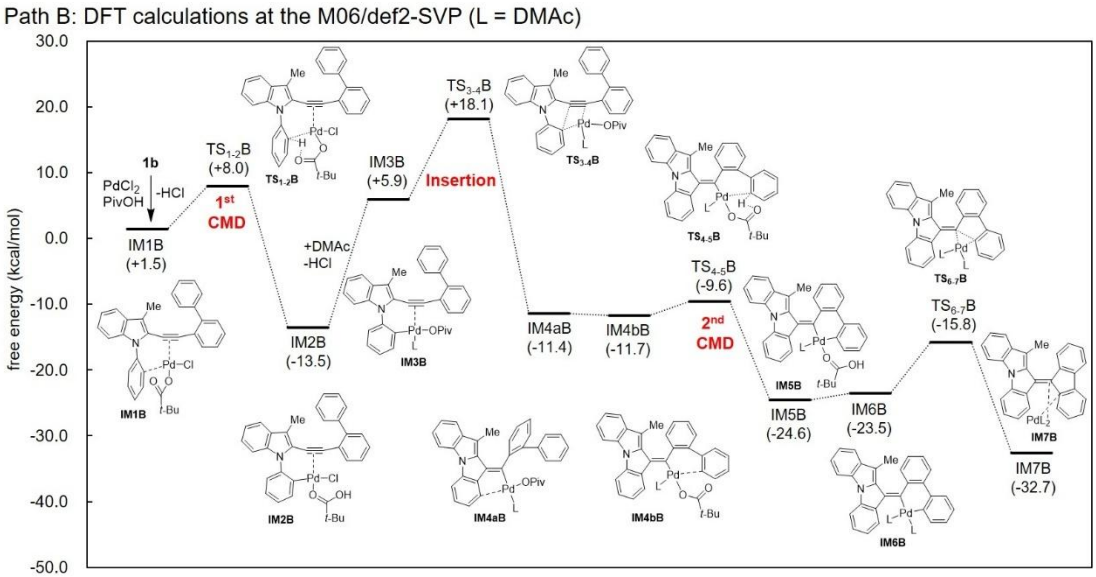

Figure S1. Plausible reaction mechanism Path B with energy diagram.

Cartesian coordinates

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Structure: IM1B

Charge = 0, Multiplicity = 1

Final SCF Energy = -2104.65311049 Hartree

Gibbs Free Energy = -2104.180380 Hartree

Thermal Correction = 0.472731 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-4.043670	-0.231789	0.621473
C	-2.252212	-0.929210	-0.540831
C	-3.336801	-1.151337	-1.370217
C	-4.485228	-0.718220	-0.637143
C	-0.895206	-1.282843	-0.694926
C	0.243829	-1.792521	-0.741533
C	1.261837	-2.788840	-0.912480
C	1.051265	-3.745613	-1.920653
C	2.393667	-2.884554	-0.075249
C	1.932737	-4.803385	-2.087647
H	0.175760	-3.640139	-2.567559

C	3.254134	-3.972794	-0.248857
C	3.033488	-4.923323	-1.240988
H	1.758654	-5.538438	-2.877855
H	4.128246	-4.053422	0.405303
H	3.731631	-5.756449	-1.360688
C	-1.775073	0.003257	1.693036
C	-0.818017	1.001767	1.428825
C	-1.778746	-0.670032	2.909062
C	0.163008	1.280164	2.388713
C	-0.812688	-0.357599	3.867283
H	-2.526243	-1.448216	3.089291
C	0.164211	0.599707	3.605041
H	0.913902	2.046514	2.171998
H	-0.812492	-0.889204	4.823232
H	0.928326	0.821696	4.354506
C	2.713603	-1.879604	0.969022
C	2.654320	-2.225876	2.324665
C	3.165939	-0.601363	0.611242
C	3.042147	-1.314233	3.303359
H	2.307340	-3.226122	2.605547
C	3.549438	0.310035	1.593906
H	3.250685	-0.333905	-0.447651
C	3.492665	-0.045942	2.938873
H	2.994579	-1.598120	4.359351
H	3.894543	1.303675	1.295103
H	3.804489	0.667270	3.708537
Pd	0.565566	0.348729	-0.536472
N	-2.676160	-0.356197	0.666037
C	-4.931477	0.289274	1.568515
C	-6.277574	0.299731	1.239433
C	-6.739432	-0.187255	-0.001056
H	-6.999270	0.699735	1.957432
C	-5.857588	-0.691152	-0.940519
H	-7.810288	-0.158677	-0.220202
H	-6.216071	-1.062091	-1.906026
H	-4.573065	0.676027	2.526793

O	-0.447077	3.094115	-0.905876
C	0.762973	3.153286	-0.726867
O	1.500348	2.146238	-0.375754
C	1.549925	4.450339	-0.954266
C	0.608230	5.641501	-0.847889
H	1.154790	6.576367	-1.060497
H	-0.226506	5.550201	-1.558445
H	0.174209	5.721160	0.162915
C	2.111605	4.349722	-2.374626
H	2.680910	5.262308	-2.623514
H	2.781213	3.480397	-2.476376
H	1.297737	4.239245	-3.110481
C	2.691853	4.587030	0.047014
H	3.221699	5.542095	-0.112573
H	2.319958	4.580029	1.086902
H	3.419328	3.768330	-0.059812
H	-0.966132	1.675641	0.560674
Cl	1.424368	0.177870	-2.674928
C	-3.307136	-1.728540	-2.736692
H	-2.274897	-1.914561	-3.070635
H	-3.863137	-2.680220	-2.789566
H	-3.773426	-1.044629	-3.465582

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Structure: $TS_{1\text{-}2}B$

Charge = 0, Multiplicity = 1

Final SCF Energy = -2104.64072377 Hartree

Gibbs Free Energy = -2104.169937 Hartree

Thermal Correction = 0.470787 Hartree

Imaginary Frequencies = -1581.13 cm^-1

Cartesian Coordinates (Angstrom):

C	-3.836696	-0.923397	0.634735
C	-1.923485	-1.502669	-0.393238
C	-2.926795	-2.092175	-1.133122
C	-4.152860	-1.732626	-0.486768
C	-0.519784	-1.588403	-0.525281

C	0.700208	-1.852491	-0.516827
C	1.911586	-2.619097	-0.562122
C	1.879191	-3.794323	-1.333545
C	3.073772	-2.287891	0.166428
C	2.971741	-4.647742	-1.373202
H	0.972432	-4.021898	-1.901376
C	4.155360	-3.172597	0.121691
C	4.113178	-4.338948	-0.636250
H	2.932082	-5.556148	-1.980133
H	5.055781	-2.919594	0.690709
H	4.980062	-5.005245	-0.658038
C	-1.668713	-0.133314	1.642692
C	-0.613780	0.710132	1.216545
C	-1.912309	-0.345548	3.000211
C	0.190731	1.298973	2.209076
C	-1.096127	0.259593	3.952257
H	-2.722735	-1.015008	3.302843
C	-0.035798	1.076941	3.561682
H	1.002268	1.965558	1.895558
H	-1.284476	0.075714	5.014067
H	0.608440	1.544872	4.311592
C	3.207169	-1.047435	0.974076
C	3.206282	-1.116098	2.371967
C	3.424358	0.189811	0.351437
C	3.419462	0.029603	3.135444
H	3.042228	-2.083085	2.859612
C	3.640538	1.333377	1.118254
H	3.436882	0.247068	-0.742333
C	3.641379	1.255408	2.509669
H	3.417667	-0.037655	4.227736
H	3.805717	2.291276	0.616178
H	3.817957	2.153476	3.110113
Pd	0.502028	0.320834	-0.653685
N	-2.463662	-0.783736	0.682008
C	-4.833446	-0.372384	1.446567
C	-6.151832	-0.669551	1.133987

C	-6.483702	-1.487467	0.036668
H	-6.952260	-0.252366	1.751717
C	-5.496783	-2.015426	-0.778498
H	-7.535621	-1.697642	-0.175538
H	-5.753368	-2.639304	-1.640678
H	-4.585835	0.279312	2.288609
O	-1.226433	2.753466	-0.334735
C	-0.103205	3.116978	-0.758843
O	0.897354	2.346747	-0.842945
C	0.089278	4.547210	-1.256594
C	-0.974741	5.464845	-0.670835
H	-0.839608	6.488206	-1.059448
H	-1.987523	5.123043	-0.931528
H	-0.909942	5.506183	0.429053
C	-0.056072	4.472252	-2.780055
H	0.089962	5.474107	-3.218349
H	0.688266	3.786624	-3.216314
H	-1.060784	4.117563	-3.063974
C	1.484050	5.045311	-0.892020
H	1.615903	6.079420	-1.252376
H	1.637620	5.047206	0.200880
H	2.265070	4.416832	-1.345092
H	-0.973674	1.568979	0.321435
Cl	1.579877	-0.019015	-2.701325
C	-2.764963	-2.930910	-2.346585
H	-1.708119	-3.001919	-2.646512
H	-3.145161	-3.954563	-2.187469
H	-3.325344	-2.511322	-3.199154

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Structure: IM2B

Charge = 0, Multiplicity = 1

Final SCF Energy = -2104.68161985 Hartree

Gibbs Free Energy = -2104.204220 Hartree

Thermal Correction = 0.477400 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-4.153622	0.682248	0.402624
C	-2.622364	-0.834817	-0.215364
C	-3.757513	-1.156103	-0.930782
C	-4.746170	-0.198315	-0.541178
C	-1.336124	-1.416713	-0.244036
C	-0.252162	-2.036350	-0.171307
C	0.641821	-3.155833	-0.073984
C	0.144992	-4.381765	-0.554919
C	1.922571	-3.108742	0.519105
C	0.884775	-5.548851	-0.440983
H	-0.845065	-4.397534	-1.019145
C	2.642042	-4.302999	0.634565
C	2.139375	-5.511445	0.163355
H	0.479734	-6.489654	-0.823135
H	3.632481	-4.266287	1.099721
H	2.733030	-6.424401	0.262392
C	-1.880929	0.772244	1.507554
C	-0.512633	0.731692	1.188801
C	-2.283587	1.272545	2.753461
C	0.413376	1.215070	2.109009
C	-1.348003	1.764276	3.656427
H	-3.342789	1.241923	3.022548
C	0.006077	1.740859	3.334957
H	1.479868	1.190640	1.863570
H	-1.682879	2.150647	4.623196
H	0.752760	2.120778	4.039150
C	2.564472	-1.869416	1.034334
C	2.719010	-1.681203	2.412752
C	3.128404	-0.934847	0.154616
C	3.420855	-0.582878	2.905296
H	2.284560	-2.412098	3.102924
C	3.833358	0.161119	0.650006
H	3.022547	-1.085359	-0.925307
C	3.983618	0.339486	2.024539
H	3.531819	-0.449366	3.985431

H	4.281606	0.872063	-0.053851
H	4.545365	1.195919	2.410596
Pd	0.232008	0.037976	-0.550626
N	-2.851610	0.268608	0.610589
C	-4.861633	1.780085	0.907032
C	-6.171067	1.957069	0.483005
C	-6.780242	1.073928	-0.427354
H	-6.739927	2.810745	0.862864
C	-6.074180	0.002513	-0.947992
H	-7.815925	1.246407	-0.732959
H	-6.534812	-0.676709	-1.672702
H	-4.399048	2.491519	1.594292
O	2.705916	1.689938	-2.347350
C	2.136580	2.355641	-1.390728
O	1.156416	1.965906	-0.754093
C	2.725416	3.727030	-1.110430
C	1.870583	4.714131	-1.915130
H	2.241538	5.740038	-1.754834
H	1.921250	4.497060	-2.994998
H	0.815797	4.674139	-1.599383
C	4.178671	3.812769	-1.562863
H	4.570459	4.819991	-1.345642
H	4.813807	3.083471	-1.032430
H	4.283748	3.627583	-2.642040
C	2.611858	4.031778	0.379698
H	3.016550	5.036502	0.584398
H	1.566035	3.999476	0.720756
H	3.184428	3.304197	0.980926
H	2.202026	0.834658	-2.549971
Cl	1.095735	-0.762836	-2.717318
C	-3.913634	-2.249604	-1.921488
H	-2.956730	-2.759130	-2.111758
H	-4.641289	-3.007255	-1.582717
H	-4.282137	-1.863271	-2.886856

****

Structure: IM3B

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.43763104 Hartree

Gibbs Free Energy = -1930.847195 Hartree

Thermal Correction = 0.590436 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	4.496212	-0.388782	-0.404200
C	2.477894	-0.028707	-1.311331
C	3.232421	-0.589788	-2.320737
C	4.525968	-0.823774	-1.756067
C	1.112869	0.346775	-1.308504
C	-0.024510	0.830540	-1.491216
C	-1.196193	1.410672	-2.076945
C	-1.611100	0.925587	-3.328902
C	-1.937335	2.423221	-1.430243
C	-2.736944	1.445918	-3.951443
H	-1.036455	0.120682	-3.795856
C	-3.085461	2.909315	-2.065093
C	-3.479516	2.439311	-3.313836
H	-3.043890	1.066805	-4.929992
H	-3.659942	3.697915	-1.568770
H	-4.372639	2.850797	-3.792510
C	2.735796	0.732202	1.023648
C	1.381022	0.617213	1.372901
C	3.593555	1.497157	1.825947
C	0.927793	1.220155	2.544017
C	3.129228	2.084001	2.998160
H	4.628967	1.647680	1.509222
C	1.795443	1.935618	3.368028
H	-0.129695	1.125523	2.818631
H	3.815742	2.669166	3.616781
H	1.419504	2.393536	4.288348
C	-1.516968	2.996531	-0.132778
C	-0.244546	3.563393	0.020923
C	-2.410303	3.030655	0.944874

C	0.119672	4.167307	1.219941
H	0.459898	3.543324	-0.817453
C	-2.043315	3.634846	2.144276
H	-3.387586	2.548064	0.842976
C	-0.782048	4.211033	2.281519
H	1.118449	4.601244	1.328155
H	-2.748130	3.649669	2.980758
H	-0.494020	4.685334	3.224863
Pd	-0.061138	-0.327892	0.354939
N	3.235910	0.119358	-0.149980
C	5.605138	-0.565472	0.432760
C	6.743493	-1.144152	-0.111250
C	6.796551	-1.548674	-1.457625
H	7.618611	-1.293754	0.527916
C	5.692947	-1.399161	-2.281153
H	7.714702	-1.995234	-1.849549
H	5.720217	-1.730016	-3.324611
H	5.576219	-0.280861	1.486582
O	-2.932407	-0.344195	0.941554
C	-2.813794	-1.040378	-0.071459
O	-1.699536	-1.301755	-0.646340
C	-4.077984	-1.629098	-0.724379
C	-4.794193	-0.468331	-1.414210
H	-5.730552	-0.816053	-1.885710
H	-5.042177	0.324660	-0.689360
H	-4.159750	-0.025045	-2.200182
C	-4.978311	-2.196309	0.368500
H	-5.919134	-2.580485	-0.062968
H	-4.489071	-3.033300	0.897811
H	-5.221915	-1.421958	1.112121
C	-3.743565	-2.707578	-1.744591
H	-4.668125	-3.118960	-2.187002
H	-3.115835	-2.309390	-2.556873
H	-3.186312	-3.542004	-1.283154
C	2.793260	-0.905855	-3.702757
H	1.721329	-0.698156	-3.841260

H	3.348000	-0.314340	-4.451575
H	2.964898	-1.968212	-3.947248
C	-1.207352	-2.348514	2.375444
O	-0.350334	-1.475520	2.156924
N	-1.257524	-3.488109	1.657912
C	-2.203723	-2.120051	3.470457
H	-3.143800	-1.774212	3.007229
H	-2.397800	-3.004133	4.093843
H	-1.826984	-1.301141	4.095193
C	-2.284534	-4.496023	1.787363
H	-2.727901	-4.702832	0.797524
H	-1.866721	-5.442672	2.174158
H	-3.093883	-4.171358	2.451377
C	-0.279107	-3.743360	0.616128
H	-0.672793	-3.436375	-0.368802
H	0.638433	-3.174444	0.815030
H	-0.038744	-4.818075	0.607507

****

Structure: $TS_{3\text{-}4}B$

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.41429546 Hartree

Gibbs Free Energy = -1930.827793 Hartree

Thermal Correction = 0.586503 Hartree

Imaginary Frequencies = -272.15 cm^-1

Cartesian Coordinates (Angstrom):

C	4.709661	-0.539952	-0.442325
C	2.769379	0.565498	-0.715026
C	3.590978	1.047668	-1.707678
C	4.837952	0.352628	-1.543942
C	1.394342	0.750588	-0.368498
C	0.258178	1.284296	-0.668282
C	-0.689263	2.312831	-1.005601
C	-1.050594	2.519065	-2.346332
C	-1.311439	3.064458	0.016675
C	-1.982973	3.492562	-2.683228

H	-0.591109	1.891849	-3.116228
C	-2.264316	4.020231	-0.345617
C	-2.589884	4.246636	-1.680147
H	-2.245970	3.655082	-3.732109
H	-2.746645	4.602149	0.446722
H	-3.329630	5.009874	-1.937962
C	2.732689	-0.817683	1.179031
C	1.358341	-0.506338	1.164526
C	3.329320	-1.324720	2.333060
C	0.634094	-0.568352	2.358930
C	2.563663	-1.485959	3.486011
H	4.401544	-1.532807	2.347836
C	1.230010	-1.086157	3.510394
H	-0.414927	-0.243784	2.388376
H	3.034862	-1.882676	4.389764
H	0.644472	-1.163529	4.431388
C	-0.987109	2.834367	1.445506
C	0.293839	3.099925	1.945404
C	-1.967068	2.341293	2.314757
C	0.587465	2.885104	3.288856
H	1.064596	3.484606	1.268817
C	-1.671209	2.125904	3.659003
H	-2.952245	2.077234	1.917350
C	-0.396387	2.400677	4.149548
H	1.591782	3.097924	3.666550
H	-2.443614	1.730890	4.325368
H	-0.164754	2.230159	5.205329
Pd	-0.190647	-0.647945	-0.222849
N	3.431946	-0.388587	0.051341
C	5.753335	-1.390071	-0.066695
C	6.937982	-1.316667	-0.788569
C	7.088811	-0.426399	-1.866040
H	7.769420	-1.972180	-0.513915
C	6.047449	0.404498	-2.251169
H	8.037488	-0.397786	-2.409374
H	6.160593	1.090075	-3.097323

H	5.644205	-2.105570	0.751397
O	-2.860638	-0.356587	0.794640
C	-3.007362	-0.444324	-0.429901
O	-2.056545	-0.645676	-1.262561
C	-4.412257	-0.258127	-1.031667
C	-4.666675	1.249447	-1.060243
H	-5.662682	1.465325	-1.485856
H	-4.627568	1.675626	-0.043568
H	-3.910187	1.765180	-1.676243
C	-5.441327	-0.929234	-0.129165
H	-6.462380	-0.765457	-0.515973
H	-5.275867	-2.019787	-0.071901
H	-5.381734	-0.529490	0.894172
C	-4.506578	-0.813414	-2.445715
H	-5.516953	-0.643646	-2.857732
H	-3.771160	-0.336674	-3.112017
H	-4.314546	-1.900729	-2.466911
C	3.255755	2.062705	-2.736432
H	2.180032	2.299973	-2.723822
H	3.802160	3.008509	-2.576719
H	3.516564	1.711582	-3.749362
C	-1.579950	-3.297225	0.339375
O	-0.451621	-2.820870	0.145228
N	-2.305999	-3.790169	-0.687908
C	-2.161044	-3.318643	1.722720
H	-2.944403	-2.543989	1.791208
H	-2.581643	-4.294609	2.006371
H	-1.359636	-3.049913	2.423040
C	-3.634177	-4.342517	-0.572807
H	-4.314647	-3.833896	-1.278770
H	-3.639605	-5.419390	-0.820813
H	-4.044543	-4.213888	0.435434
C	-1.782714	-3.725780	-2.038486
H	-2.274879	-2.915029	-2.602593
H	-0.707917	-3.513947	-2.005457
H	-1.955421	-4.688338	-2.547303

****

Structure: IM4aB

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.46141398 Hartree

Gibbs Free Energy = -1930.874792 Hartree

Thermal Correction = 0.586622 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	5.066101	-0.949801	-0.560926
C	3.030086	0.023141	-0.244437
C	3.864821	1.044203	-0.636167
C	5.159136	0.439537	-0.845609
C	1.643581	-0.316120	0.098668
C	0.439933	0.274363	-0.105464
C	0.217465	1.626325	-0.611791
C	0.202961	1.847652	-1.997300
C	0.108342	2.724199	0.268880
C	0.125004	3.134996	-2.513396
H	0.273182	0.981367	-2.663231
C	0.048726	4.015423	-0.269962
C	0.059077	4.225194	-1.645105
H	0.125628	3.291005	-3.596010
H	-0.022187	4.866467	0.415709
H	0.003901	5.242928	-2.042077
C	2.976201	-2.242961	0.245278
C	1.700681	-1.715841	0.513661
C	3.239246	-3.590323	0.451270
C	0.698302	-2.506318	1.056560
C	2.193657	-4.397422	0.927922
H	4.224265	-4.019557	0.253180
C	0.937383	-3.876309	1.232831
H	-0.198895	-2.044178	1.542251
H	2.384668	-5.461807	1.091446
H	0.155376	-4.518856	1.645003
C	0.109459	2.538588	1.738913

C	1.073173	3.183515	2.523903
C	-0.851964	1.736677	2.371351
C	1.090691	3.019728	3.906857
H	1.829087	3.808317	2.035094
C	-0.834818	1.578911	3.754655
H	-1.638403	1.249420	1.782260
C	0.137742	2.214067	4.525587
H	1.857703	3.521545	4.504085
H	-1.597679	0.958048	4.233438
H	0.149780	2.084522	5.611815
Pd	-1.025816	-1.052744	0.068478
N	3.761749	-1.184379	-0.196747
C	6.164430	-1.803283	-0.666164
C	7.374850	-1.246997	-1.065262
C	7.489016	0.123456	-1.352021
H	8.254397	-1.890773	-1.157031
C	6.392821	0.969662	-1.244819
H	8.456714	0.526194	-1.664625
H	6.488323	2.036570	-1.471880
H	6.082972	-2.870511	-0.444202
O	-3.688923	0.199164	0.747915
C	-3.334387	0.595570	-0.359149
O	-2.265403	0.218390	-0.975734
C	-4.136654	1.679635	-1.101016
C	-3.440511	3.003656	-0.779212
H	-4.009656	3.847746	-1.206534
H	-3.368736	3.157066	0.312107
H	-2.421797	3.028846	-1.197646
C	-5.565900	1.716318	-0.577417
H	-6.130009	2.526585	-1.070454
H	-6.094817	0.768442	-0.774741
H	-5.584455	1.884659	0.509585
C	-4.129795	1.451568	-2.608080
H	-4.695766	2.251846	-3.115916
H	-3.104066	1.444037	-3.007598
H	-4.604559	0.490208	-2.876291

C	3.582798	2.493502	-0.804414
H	2.611335	2.778575	-0.377504
H	4.360895	3.102725	-0.313332
H	3.571429	2.788895	-1.868950
C	-3.690640	-2.609528	0.301772
O	-2.460296	-2.721127	0.428431
N	-4.260637	-2.470117	-0.913378
C	-4.571908	-2.655848	1.511630
H	-4.851948	-1.620557	1.766281
H	-5.481652	-3.256882	1.369435
H	-3.984594	-3.064250	2.343074
C	-5.655038	-2.151006	-1.114270
H	-5.739169	-1.363375	-1.882740
H	-6.234313	-3.025558	-1.462819
H	-6.113828	-1.758018	-0.198618
C	-3.452582	-2.536437	-2.115216
H	-3.225726	-1.526677	-2.500069
H	-2.503340	-3.041656	-1.896222
H	-3.996261	-3.107240	-2.885501

****

Structure: IM4bB

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.46222741 Hartree

Gibbs Free Energy = -1930.875330 Hartree

Thermal Correction = 0.586898 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-4.941946	0.703975	0.263193
C	-2.908079	-0.289065	0.016234
C	-3.831872	-1.274266	-0.257803
C	-5.126847	-0.649186	-0.128013
C	-1.465770	-0.025547	0.163090
C	-0.415309	-0.746248	-0.297210
C	-0.436644	-2.009139	-1.024601
C	-0.960219	-2.133594	-2.320115

C	0.086152	-3.153254	-0.375958
C	-1.006393	-3.377298	-2.938317
H	-1.342769	-1.239684	-2.823800
C	-0.020520	-4.404106	-0.985174
C	-0.556106	-4.515463	-2.265937
H	-1.410680	-3.466540	-3.950797
H	0.361817	-5.287650	-0.463424
H	-0.603368	-5.493366	-2.752954
C	-2.706741	1.841597	0.867171
C	-1.402076	1.299917	0.818869
C	-2.964603	3.103771	1.388369
C	-0.350197	2.032402	1.359430
C	-1.886407	3.829655	1.903267
H	-3.977349	3.511605	1.415182
C	-0.596632	3.298062	1.900769
H	0.664509	1.611233	1.383703
H	-2.065709	4.819328	2.333931
H	0.227685	3.867659	2.341241
C	0.703524	-2.942117	0.943562
C	1.795669	-2.041784	1.050040
C	0.187822	-3.522684	2.101888
C	2.302671	-1.700256	2.316369
H	2.487443	-1.918209	0.168913
C	0.699810	-3.167869	3.349903
H	-0.656700	-4.215965	2.026351
C	1.740712	-2.243833	3.464919
H	3.158684	-1.020175	2.370708
H	0.264642	-3.607199	4.252590
H	2.123379	-1.969782	4.451584
Pd	1.450919	-0.140499	-0.113199
N	-3.581924	0.899643	0.343495
C	-6.018113	1.562260	0.490707
C	-7.299352	1.048927	0.319835
C	-7.504200	-0.284752	-0.069324
H	-8.162556	1.698670	0.490586
C	-6.430163	-1.136117	-0.294117

H	-8.525527	-0.654677	-0.197700
H	-6.597791	-2.174072	-0.599712
H	-5.870156	2.603173	0.788446
O	3.448232	0.584985	0.109641
C	4.397532	-0.197241	-0.258609
O	4.248665	-1.365335	-0.619270
C	5.819224	0.384207	-0.142503
C	6.733689	-0.286035	-1.159658
H	7.768444	0.082704	-1.048001
H	6.729057	-1.378367	-1.031219
H	6.405243	-0.074383	-2.191077
C	6.294040	0.049697	1.273446
H	7.333285	0.390768	1.425949
H	5.660404	0.543251	2.030414
H	6.261340	-1.039335	1.447282
C	5.827087	1.893804	-0.343682
H	6.857417	2.284376	-0.268629
H	5.434108	2.166698	-1.338327
H	5.209628	2.401430	0.413876
C	-3.636028	-2.720057	-0.544428
H	-2.693943	-3.101323	-0.122212
H	-4.458759	-3.309131	-0.106615
H	-3.618885	-2.943786	-1.625955
C	0.465734	2.526767	-1.610090
O	1.024984	1.423191	-1.566368
N	1.073238	3.651224	-1.175890
C	-0.915512	2.647067	-2.191900
H	-1.606528	3.137984	-1.486910
H	-0.912854	3.230294	-3.127099
H	-1.285955	1.636203	-2.407035
C	2.368756	3.592376	-0.525886
H	3.084901	4.244189	-1.054556
H	2.281577	3.955348	0.514210
H	2.760664	2.565011	-0.510609
C	0.441774	4.951761	-1.183304
H	-0.295679	5.046534	-1.990016

H	-0.062620	5.159403	-0.220551
H	1.210261	5.723922	-1.342458

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Structure: $TS_{4\text{-}5}B$

Charge = 0, Multiplicity = 1

Final SCF Energy = -1931.45436620 Hartree

Gibbs Free Energy = -1930.872001 Hartree

Thermal Correction = 0.582365 Hartree

Imaginary Frequencies = -1496.82 cm^-1

Cartesian Coordinates (Angstrom):

C	-5.035062	0.413939	0.256310
C	-2.926176	-0.411364	0.016766
C	-3.766486	-1.470694	-0.251174
C	-5.108037	-0.952737	-0.125928
C	-1.510647	-0.033696	0.171113
C	-0.402590	-0.671721	-0.278643
C	-0.333484	-1.922608	-1.024915
C	-0.887961	-2.062432	-2.306024
C	0.337067	-3.021686	-0.436742
C	-0.812203	-3.277482	-2.976243
H	-1.391418	-1.201931	-2.759710
C	0.359902	-4.249622	-1.103393
C	-0.203143	-4.377936	-2.369716
H	-1.242089	-3.373920	-3.977658
H	0.866237	-5.100663	-0.635866
H	-0.149478	-5.334895	-2.896231
C	-2.901107	1.730663	0.861294
C	-1.557017	1.294098	0.823216
C	-3.262111	2.969857	1.376605
C	-0.570652	2.110468	1.366515
C	-2.249158	3.780742	1.897459
H	-4.304419	3.295588	1.394966
C	-0.921287	3.353114	1.904832
H	0.472199	1.767028	1.392455
H	-2.510108	4.753571	2.324829

H	-0.148891	3.987077	2.351791
C	0.958513	-2.817303	0.879670
C	1.756058	-1.661912	1.108252
C	0.733986	-3.718317	1.925955
C	2.237313	-1.425597	2.412501
H	2.745602	-1.496383	0.291400
C	1.231667	-3.461515	3.200020
H	0.117047	-4.605422	1.747467
C	1.974657	-2.305995	3.452761
H	2.874655	-0.549465	2.583113
H	1.026888	-4.166196	4.011620
H	2.362599	-2.110129	4.456342
Pd	1.424265	0.047726	-0.125153
N	-3.695472	0.720345	0.336501
C	-6.178003	1.182824	0.476509
C	-7.413047	0.565525	0.307937
C	-7.507434	-0.783273	-0.071575
H	-8.326713	1.143863	0.473085
C	-6.366977	-1.545558	-0.289374
H	-8.494965	-1.236461	-0.197945
H	-6.448551	-2.596008	-0.587391
H	-6.115817	2.234509	0.766871
O	3.473418	0.768321	-0.025668
C	4.342520	-0.134805	-0.151271
O	4.075567	-1.363856	-0.175049
C	5.816558	0.273093	-0.201842
C	6.555219	-0.586389	-1.222581
H	7.627682	-0.326666	-1.230461
H	6.453864	-1.655956	-0.986192
H	6.160874	-0.427332	-2.240232
C	6.373398	0.005514	1.199183
H	7.444038	0.269993	1.241249
H	5.845376	0.609787	1.957220
H	6.267535	-1.057898	1.468079
C	5.963778	1.748751	-0.546195
H	7.031941	2.023954	-0.579517

H	5.521027	1.977391	-1.530018
H	5.464936	2.387001	0.199876
C	-3.453261	-2.896956	-0.532422
H	-2.471602	-3.192984	-0.133007
H	-4.212503	-3.550964	-0.072275
H	-3.441937	-3.125455	-1.613340
C	0.362031	2.744214	-1.530582
O	0.952316	1.658387	-1.517513
N	0.945279	3.874927	-1.072507
C	-1.026936	2.841290	-2.097033
H	-1.726746	3.286843	-1.371231
H	-1.049988	3.454131	-3.012903
H	-1.366950	1.826232	-2.341161
C	2.245863	3.827311	-0.433020
H	2.930622	4.542776	-0.918981
H	2.156787	4.111580	0.631289
H	2.678140	2.819550	-0.495573
C	0.272783	5.153731	-1.024989
H	-0.466296	5.257772	-1.829309
H	-0.241467	5.305037	-0.056872
H	1.015471	5.956723	-1.150275

****

Structure: IM5B
Charge = 0, Multiplicity = 1
Final SCF Energy = -1931.48390248 Hartree
Gibbs Free Energy = -1930.895861 Hartree
Thermal Correction = 0.588041 Hartree
Imaginary Frequencies = none
Cartesian Coordinates (Angstrom):

C	-5.097284	0.308483	0.438034
C	-2.977605	-0.472275	0.144062
C	-3.799739	-1.566468	-0.028946
C	-5.148502	-1.077846	0.129122
C	-1.567104	-0.058524	0.237083
C	-0.459100	-0.682905	-0.246518

C	-0.453566	-1.917463	-1.032224
C	-1.180834	-2.016354	-2.225951
C	0.356425	-3.005145	-0.622552
C	-1.128309	-3.169093	-3.004046
H	-1.802071	-1.169378	-2.536836
C	0.370080	-4.166018	-1.400917
C	-0.359947	-4.252808	-2.584598
H	-1.693953	-3.222474	-3.939130
H	0.997078	-5.009277	-1.093728
H	-0.312174	-5.163274	-3.188829
C	-2.977992	1.701993	0.897042
C	-1.625430	1.290127	0.845647
C	-3.354412	2.960486	1.350488
C	-0.645676	2.159124	1.315564
C	-2.348334	3.821256	1.799002
H	-4.403129	3.264714	1.374291
C	-1.011746	3.422032	1.793345
H	0.405982	1.844651	1.322952
H	-2.620339	4.810845	2.178679
H	-0.243090	4.096071	2.184826
C	1.150505	-2.870211	0.615525
C	1.615089	-1.599856	1.025820
C	1.447343	-3.990966	1.408142
C	2.327856	-1.491103	2.226994
H	3.358381	-1.462476	-0.427871
C	2.178927	-3.870405	2.584237
H	1.067075	-4.974324	1.111950
C	2.620120	-2.615167	2.998668
H	2.678665	-0.506467	2.559629
H	2.391157	-4.757843	3.187663
H	3.190154	-2.509068	3.927200
Pd	1.375000	0.045097	-0.098078
N	-3.764579	0.653324	0.440900
C	-6.250150	1.057467	0.673639
C	-7.474198	0.401153	0.593908
C	-7.547443	-0.967049	0.286263

H	-8.395277	0.963394	0.773198
C	-6.396810	-1.709904	0.054027
H	-8.526497	-1.451720	0.228676
H	-6.462297	-2.776147	-0.186367
H	-6.204195	2.123578	0.909407
O	3.501965	0.762878	0.107320
C	4.452253	0.030218	-0.125492
O	4.314081	-1.225277	-0.491186
C	5.892228	0.466509	0.050668
C	6.766843	-0.089591	-1.070285
H	7.808728	0.237512	-0.919051
H	6.751134	-1.189258	-1.091333
H	6.438524	0.275860	-2.057300
C	6.338312	-0.111806	1.399904
H	7.381828	0.182260	1.601193
H	5.711295	0.271101	2.222733
H	6.280603	-1.211980	1.404758
C	5.968425	1.986658	0.083143
H	7.013334	2.302548	0.235665
H	5.611195	2.426860	-0.862212
H	5.357649	2.403005	0.898619
C	-3.456294	-2.996633	-0.245625
H	-2.455434	-3.244187	0.138349
H	-4.183681	-3.645337	0.270110
H	-3.466141	-3.280285	-1.313534
C	0.386831	2.749190	-1.569720
O	1.226696	1.870327	-1.358889
N	0.655208	4.042177	-1.261597
C	-0.940583	2.433684	-2.195202
H	-1.776389	2.801727	-1.577671
H	-1.026703	2.890864	-3.194464
H	-1.023428	1.343535	-2.293869
C	1.861485	4.372501	-0.532742
H	2.481776	5.083313	-1.105467
H	1.603875	4.843579	0.432658
H	2.440913	3.458590	-0.346004

C	-0.294312	5.118053	-1.431297
H	-0.953989	4.947226	-2.291622
H	-0.922170	5.250902	-0.529260
H	0.251126	6.056925	-1.614766

****

Structure: IM6B

Charge = 0, Multiplicity = 1

Final SCF Energy = -1872.35389828 Hartree

Gibbs Free Energy = -1871.779588 Hartree

Thermal Correction = 0.574310 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	-4.919359	0.017186	-0.738092
C	-2.702022	0.431207	-0.449635
C	-3.306491	1.672170	-0.470785
C	-4.717990	1.420961	-0.627757
C	-1.390298	-0.235062	-0.424301
C	-0.192035	0.257693	-0.010126
C	0.017681	1.550326	0.643899
C	-0.727957	1.903088	1.777983
C	1.057679	2.412258	0.209104
C	-0.459301	3.072373	2.485194
H	-1.536921	1.236254	2.099395
C	1.298547	3.591117	0.920353
C	0.557497	3.922108	2.054433
H	-1.049502	3.322685	3.372990
H	2.109033	4.253278	0.597583
H	0.782237	4.840275	2.604753
C	-3.085434	-1.796043	-0.882549
C	-1.683796	-1.629618	-0.823842
C	-3.676064	-3.023543	-1.154761
C	-0.866291	-2.723689	-1.086785
C	-2.832795	-4.110142	-1.401222
H	-4.761950	-3.138260	-1.185030
C	-1.445721	-3.961508	-1.376513

H	0.223408	-2.609390	-1.061640
H	-3.271391	-5.086919	-1.625980
H	-0.803796	-4.821358	-1.587864
C	1.845624	2.029208	-0.980080
C	2.411197	3.002893	-1.818234
C	2.042693	0.663623	-1.281407
C	3.153611	2.645990	-2.940529
H	2.240532	4.063770	-1.604825
C	2.746935	0.320198	-2.440110
C	3.314384	1.298283	-3.259554
H	3.578453	3.422038	-3.584170
H	2.860551	-0.737473	-2.708590
H	3.871049	1.006652	-4.157063
Pd	1.513872	-0.749933	0.022803
N	-3.676805	-0.562275	-0.624006
C	-6.186258	-0.535211	-0.928630
C	-7.267050	0.337137	-1.004310
C	-7.091001	1.726131	-0.892075
H	-8.272139	-0.068361	-1.153117
C	-5.828135	2.273188	-0.705054
H	-7.963212	2.383683	-0.953446
H	-5.699069	3.357178	-0.618488
H	-6.333438	-1.614666	-1.014121
C	0.005363	-1.913174	2.444472
O	0.821228	-2.226491	1.570199
C	-2.694857	3.027084	-0.436906
H	-1.665214	3.023946	-0.826843
H	-3.284200	3.728390	-1.050535
H	-2.644438	3.449679	0.583354
C	-1.350306	-2.559448	2.472521
H	-2.108861	-1.844000	2.105889
H	-1.337521	-3.408917	1.777211
H	-1.651093	-2.900297	3.474240
N	0.300229	-0.985205	3.387965
C	1.617598	-0.384533	3.426342
H	2.323552	-1.002161	2.855074

H	1.602497	0.636137	2.997057
H	1.957645	-0.319563	4.473266
C	-0.627035	-0.489853	4.378598
H	-0.592975	0.613340	4.391788
H	-1.659164	-0.784101	4.154028
H	-0.369487	-0.850976	5.391155
C	4.596752	-1.345806	-0.459160
O	3.552222	-1.714120	0.086092
N	5.199092	-0.165719	-0.174845
C	5.255440	-2.238360	-1.476367
H	5.265972	-1.759683	-2.469362
H	6.296160	-2.479782	-1.209509
H	4.675342	-3.166902	-1.537807
C	4.629280	0.754528	0.786832
H	3.766087	0.295322	1.282898
H	5.388637	1.024911	1.540495
H	4.283713	1.675610	0.283469
C	6.279513	0.388245	-0.959813
H	6.884852	-0.390493	-1.438948
H	5.887681	1.066976	-1.742378
H	6.946058	0.971324	-0.304823

****

Structure: $TS_{6\text{-}7}B$

Charge = 0, Multiplicity = 1

Final SCF Energy = -1872.34143933 Hartree

Gibbs Free Energy = -1871.767262 Hartree

Thermal Correction = 0.574177 Hartree

Imaginary Frequencies = -256.57 cm^-1

Cartesian Coordinates (Angstrom):

C	-4.801454	-0.046875	-0.621539
C	-2.583047	0.397406	-0.385232
C	-3.204737	1.633503	-0.428004
C	-4.615034	1.361710	-0.551683
C	-1.270839	-0.248794	-0.379342
C	-0.043119	0.298853	-0.100375

C	0.175932	1.616457	0.513937
C	-0.447368	2.070387	1.677859
C	1.178750	2.407995	-0.093418
C	-0.077145	3.296037	2.234731
H	-1.233148	1.462277	2.141416
C	1.529121	3.636726	0.458812
C	0.907228	4.077877	1.629273
H	-0.569042	3.649375	3.147159
H	2.303581	4.249866	-0.015691
H	1.192824	5.037068	2.070557
C	-2.951245	-1.846508	-0.725634
C	-1.549628	-1.663279	-0.683226
C	-3.530727	-3.093061	-0.923869
C	-0.722193	-2.772768	-0.844796
C	-2.678316	-4.185954	-1.098429
H	-4.615471	-3.219658	-0.943655
C	-1.291970	-4.028756	-1.062049
H	0.367626	-2.657375	-0.776295
H	-3.108517	-5.178622	-1.260583
H	-0.643603	-4.899367	-1.194170
C	1.681711	1.793883	-1.324844
C	2.189304	2.496714	-2.419778
C	1.442587	0.397867	-1.418055
C	2.425201	1.841432	-3.628251
H	2.351750	3.577803	-2.342373
C	1.600757	-0.224963	-2.666824
C	2.105557	0.487561	-3.755188
H	2.813401	2.397853	-4.486511
H	1.352179	-1.286559	-2.784100
H	2.250077	-0.020051	-4.714621
Pd	1.603096	-0.794972	0.240947
N	-3.550542	-0.609156	-0.517283
C	-6.064147	-0.619393	-0.774261
C	-7.156732	0.237866	-0.851949
C	-6.996214	1.631425	-0.778513
H	-8.159219	-0.183292	-0.971396

C	-5.737377	2.198465	-0.629575
H	-7.877592	2.276445	-0.840122
H	-5.621494	3.285790	-0.572954
H	-6.199239	-1.702281	-0.829618
C	0.268756	-1.603350	2.826350
O	1.094843	-2.091775	2.051370
C	-2.610699	2.995616	-0.440613
H	-1.605920	3.002836	-0.891192
H	-3.244905	3.685189	-1.021277
H	-2.501548	3.426439	0.571951
C	-1.142240	-2.122431	2.851683
H	-1.820663	-1.373131	2.403593
H	-1.184663	-3.024875	2.227518
H	-1.506526	-2.355653	3.863306
N	0.596083	-0.571010	3.647800
C	1.936617	-0.023312	3.615191
H	2.598958	-0.692170	3.049521
H	1.936889	0.973461	3.132671
H	2.319251	0.086165	4.644091
C	-0.308020	0.083817	4.561656
H	-0.259960	1.177165	4.413357
H	-1.347438	-0.227405	4.402695
H	-0.037986	-0.125118	5.613247
C	4.361148	-1.203303	-0.465900
O	3.764812	-1.545920	0.561747
N	4.960409	0.009891	-0.575544
C	4.441128	-2.134076	-1.644428
H	3.971165	-1.679082	-2.532451
H	5.481686	-2.388099	-1.901916
H	3.901429	-3.053912	-1.385119
C	4.792250	0.992229	0.473247
H	4.321217	0.520218	1.343584
H	5.770343	1.409380	0.766624
H	4.145130	1.819903	0.127057
C	5.531631	0.514841	-1.803582
H	5.912494	-0.294592	-2.438633

H	4.792049	1.100122	-2.384068
H	6.381024	1.175000	-1.565193

****

Structure: IM7B

Charge = 0, Multiplicity = 1

Final SCF Energy = -1872.36490951 Hartree

Gibbs Free Energy = -1871.794137 Hartree

Thermal Correction = 0.570773 Hartree

Imaginary Frequencies = none

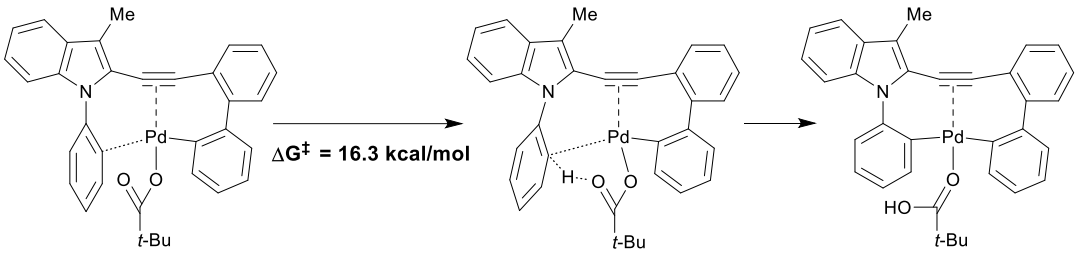
Cartesian Coordinates (Angstrom):

C	-4.849464	-0.224520	-0.502075
C	-2.627090	0.263712	-0.624385
C	-3.294066	1.425389	-1.013203
C	-4.697403	1.131742	-0.906670
C	-1.317631	-0.348583	-0.610432
C	-0.077238	0.313981	-0.759447
C	0.154296	1.722642	-0.368952
C	-0.515456	2.516755	0.558346
C	1.344979	2.200246	-0.971905
C	-0.025691	3.793829	0.845540
H	-1.423559	2.146026	1.046641
C	1.824835	3.474018	-0.686638
C	1.129346	4.273934	0.224011
H	-0.558862	4.429223	1.560644
H	2.741205	3.844537	-1.158714
H	1.493595	5.279142	0.454761
C	-2.962932	-1.966588	-0.228525
C	-1.568147	-1.774153	-0.404384
C	-3.516498	-3.208272	0.059353
C	-0.723510	-2.875139	-0.219729
C	-2.650807	-4.295272	0.183162
H	-4.593526	-3.330655	0.194789
C	-1.268584	-4.126569	0.054528
H	0.365878	-2.743417	-0.249123
H	-3.059912	-5.285020	0.405386

H	-0.603425	-4.983691	0.190866
C	1.888830	1.133134	-1.808539
C	2.962088	1.123575	-2.693894
C	1.059951	-0.024288	-1.649386
C	3.222326	-0.028782	-3.439285
H	3.580119	2.019303	-2.824761
C	1.328269	-1.169854	-2.428339
C	2.409858	-1.160938	-3.306808
H	4.057072	-0.040915	-4.147458
H	0.671674	-2.042243	-2.367735
H	2.616474	-2.049203	-3.911650
Pd	1.595605	-0.660075	0.375560
N	-3.576836	-0.727941	-0.339019
C	-6.102062	-0.814709	-0.349466
C	-7.223220	-0.027169	-0.597320
C	-7.096962	1.315431	-0.988893
H	-8.219425	-0.464074	-0.482784
C	-5.846981	1.899866	-1.145264
H	-7.998553	1.907005	-1.172861
H	-5.758307	2.947450	-1.451040
H	-6.209821	-1.858045	-0.043241
C	-0.142354	-0.503077	2.929989
O	0.704844	-1.261276	2.461162
C	-2.738736	2.688916	-1.555770
H	-1.793013	2.518158	-2.095626
H	-3.452855	3.153541	-2.255061
H	-2.509365	3.440055	-0.775952
C	-1.585851	-0.921813	2.988579
H	-2.181857	-0.333914	2.266338
H	-1.643199	-1.977824	2.692653
H	-2.035846	-0.794709	3.984929
N	0.186006	0.743121	3.377006
C	1.561548	1.189395	3.321945
H	2.209910	0.363603	2.998035
H	1.665291	2.030052	2.608771
H	1.887350	1.537265	4.318043

C	-0.739914	1.685734	3.953531
H	-0.575486	2.683922	3.511532
H	-1.782961	1.407214	3.759568
H	-0.600751	1.777169	5.047404
C	4.470257	-1.155691	0.355563
O	3.708202	-1.112284	1.322635
N	5.186750	-0.062354	-0.035463
C	4.637261	-2.428197	-0.432405
H	4.357764	-2.279205	-1.488677
H	5.672555	-2.803868	-0.400421
H	3.972753	-3.182236	0.008414
C	4.940483	1.215941	0.589715
H	4.213336	1.090751	1.401149
H	5.874721	1.640005	0.997385
H	4.526617	1.928908	-0.147852
C	6.097542	-0.026196	-1.151687
H	6.317256	-1.030189	-1.532916
H	5.682472	0.572489	-1.984052
H	7.053419	0.434939	-0.846356

6.3 Alternative reaction mechanism: Path C



IM3C (0 kcal/mol) **$TS_{3\text{-}4}C$** (+16.3 kcal/mol) **IM4C** (+13.7 kcal/mol)

****

Structure: **IM3c**

Charge = 0, Multiplicity = 1

Final SCF Energy = -1643.98437085 Hartree

Gibbs Free Energy = -1643.521644 Hartree

Thermal Correction = 0.462727 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	4.127938	0.029935	-0.362709
C	2.161187	-1.044760	-0.513337
C	2.926399	-1.525229	-1.560785
C	4.184659	-0.850219	-1.473585
C	0.873560	-1.439618	-0.074991
C	-0.167955	-1.968037	0.363273
C	-1.195570	-2.820157	0.887676
C	-0.898795	-3.717007	1.922009
C	-2.505495	-2.731147	0.361857
C	-1.894647	-4.522892	2.459916
H	0.125974	-3.765738	2.300501
C	-3.489307	-3.547617	0.928250
C	-3.193131	-4.429339	1.963697
H	-1.659403	-5.216753	3.271182
H	-4.518087	-3.473514	0.564774
H	-3.989062	-5.045031	2.391970
C	2.384440	0.580730	1.355307
C	2.877761	0.263440	2.620047
C	1.344422	1.508628	1.209740

C	2.316295	0.861591	3.746498
C	0.767240	2.075327	2.349046
H	1.033839	1.843642	0.206589
C	1.251740	1.751961	3.614678
H	2.700018	0.610701	4.739477
H	-0.066679	2.773658	2.231959
H	0.799570	2.199395	4.503773
C	-2.792902	-1.834288	-0.776209
C	-3.788016	-2.194242	-1.702781
C	-2.088855	-0.643415	-1.024046
C	-4.067931	-1.413386	-2.816731
H	-4.330986	-3.133645	-1.558304
C	-2.347998	0.139590	-2.144624
C	-3.344028	-0.246044	-3.042422
H	-4.844977	-1.727579	-3.519047
H	-1.777592	1.059704	-2.313139
H	-3.549958	0.375143	-3.919386
Pd	-0.696249	0.102597	0.198744
N	2.884817	-0.086830	0.209691
C	5.205351	0.848749	-0.008093
C	6.350847	0.763206	-0.783278
C	6.430874	-0.108025	-1.889275
H	7.212443	1.389262	-0.533822
C	5.360008	-0.911055	-2.241746
H	7.353310	-0.143123	-2.475505
H	5.422013	-1.583443	-3.103517
H	5.139650	1.529801	0.845303
O	-0.590327	2.738050	-1.074495
C	-1.545469	2.759271	-0.297540
O	-1.875124	1.778370	0.470065
C	-2.477303	3.976033	-0.213215
C	-1.833527	5.172907	-0.897963
H	-2.511632	6.043110	-0.861499
H	-0.886972	5.453275	-0.407070
H	-1.600356	4.951184	-1.950335
C	-2.788136	4.307224	1.243354

H	-3.467670	5.175458	1.300296
H	-3.264097	3.456978	1.754632
H	-1.869912	4.570148	1.798373
C	-3.766175	3.589868	-0.941719
H	-4.476236	4.435312	-0.936868
H	-3.560532	3.328559	-1.994546
H	-4.250908	2.724001	-0.462462
H	3.689199	-0.465351	2.708645
C	2.527857	-2.542179	-2.565547
H	1.493580	-2.882101	-2.406151
H	2.594419	-2.138081	-3.589930
H	3.186370	-3.426817	-2.529041

****

Structure: **$TS_{3\text{-}4}C$**

Charge = 0, Multiplicity = 1

Final SCF Energy = -1643.95776174 Hartree

Gibbs Free Energy = -1643.495677 Hartree

Thermal Correction = 0.462085 Hartree

Imaginary Frequencies = -1147.28 cm^-1

Cartesian Coordinates (Angstrom):

C	3.849029	-0.840718	-0.400874
C	1.718599	-1.519626	-0.572033
C	2.368719	-2.082137	-1.653871
C	3.731201	-1.658713	-1.554584
C	0.373533	-1.654168	-0.155155
C	-0.770378	-1.922341	0.261274
C	-1.952119	-2.533406	0.793971
C	-1.830107	-3.509611	1.792361
C	-3.223345	-2.131834	0.325122
C	-2.962686	-4.089350	2.349395
H	-0.830238	-3.799411	2.127300
C	-4.346359	-2.725260	0.912220
C	-4.222639	-3.687012	1.910073
H	-2.862780	-4.846392	3.131649
H	-5.343828	-2.408674	0.594645

H	-5.122416	-4.121696	2.354723
C	2.248405	-0.108407	1.398761
C	3.005256	-0.355035	2.547166
C	1.114448	0.726247	1.423917
C	2.637044	0.229660	3.755137
C	0.768359	1.284300	2.666348
H	0.949347	1.662013	0.426081
C	1.508937	1.045909	3.821159
H	3.228101	0.031807	4.654173
H	-0.101888	1.951795	2.718480
H	1.213929	1.500641	4.771319
C	-3.335122	-1.153538	-0.776023
C	-4.429088	-1.243259	-1.655703
C	-2.367356	-0.157526	-1.013354
C	-4.567313	-0.385035	-2.738543
H	-5.171358	-2.033732	-1.506049
C	-2.505464	0.691825	-2.112732
C	-3.598155	0.586313	-2.972227
H	-5.425164	-0.486616	-3.409234
H	-1.754305	1.465938	-2.302578
H	-3.688227	1.266446	-3.824882
Pd	-0.726536	0.229336	0.129179
N	2.609467	-0.758928	0.192694
C	5.062516	-0.235765	-0.052299
C	6.158732	-0.483463	-0.863977
C	6.064123	-1.307321	-2.003557
H	7.119712	-0.023602	-0.615581
C	4.860331	-1.891632	-2.357254
H	6.953851	-1.477880	-2.616119
H	4.781631	-2.522848	-3.248402
H	5.139505	0.415698	0.822346
O	0.821940	2.778651	-0.148717
C	-0.402929	3.086138	-0.074491
O	-1.313837	2.252377	0.164748
C	-0.782641	4.556069	-0.200145
C	0.167694	5.267049	-1.157023

H	-0.095041	6.336551	-1.216535
H	1.212489	5.181044	-0.823929
H	0.103048	4.845530	-2.173973
C	-0.629169	5.133482	1.211354
H	-0.868059	6.210453	1.205750
H	-1.313227	4.635545	1.919227
H	0.403637	5.011491	1.578179
C	-2.223153	4.700991	-0.672370
H	-2.484321	5.769557	-0.752573
H	-2.368994	4.240085	-1.663775
H	-2.927425	4.219985	0.022437
H	3.866436	-1.028258	2.491066
C	1.778523	-2.952399	-2.701330
H	0.693110	-3.069652	-2.563074
H	1.946479	-2.534596	-3.708588
H	2.231009	-3.958978	-2.695718

****

Structure: **IM4C**

Charge = 0, Multiplicity = 1

Final SCF Energy = -1643.96702507 Hartree

Gibbs Free Energy = -1643.499797 Hartree

Thermal Correction = 0.467229 Hartree

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	3.959601	-0.576075	-0.443419
C	1.925519	-1.497500	-0.234552
C	2.603707	-2.308891	-1.122529
C	3.903875	-1.731614	-1.266442
C	0.572184	-1.595228	0.172789
C	-0.590271	-1.985356	0.438740
C	-1.712067	-2.749826	0.893938
C	-1.495005	-3.746355	1.858339
C	-3.012800	-2.491468	0.404270
C	-2.557540	-4.485061	2.360357
H	-0.475167	-3.922243	2.212516

C	-4.066382	-3.240585	0.942175
C	-3.848536	-4.220116	1.905196
H	-2.381166	-5.256274	3.114894
H	-5.088473	-3.036893	0.610869
H	-4.697882	-4.777968	2.309926
C	2.370733	0.448023	1.233249
C	3.345498	0.848562	2.157538
C	1.032532	0.870475	1.348596
C	3.014403	1.712257	3.194748
C	0.735760	1.722821	2.425398
H	0.768256	2.237658	-0.193795
C	1.702091	2.156793	3.331689
H	3.783593	2.019871	3.909132
H	-0.297889	2.067487	2.562095
H	1.427972	2.829261	4.150373
C	-3.214330	-1.499980	-0.671246
C	-4.296111	-1.665890	-1.556144
C	-2.320868	-0.428668	-0.876393
C	-4.497705	-0.807876	-2.629238
H	-4.974118	-2.515254	-1.425236
C	-2.520990	0.402808	-1.983767
C	-3.598352	0.231160	-2.851570
H	-5.343171	-0.966731	-3.304791
H	-1.819612	1.222556	-2.187751
H	-3.729738	0.905961	-3.703649
Pd	-0.658855	0.144168	0.252380
N	2.742613	-0.450967	0.200470
C	5.093387	0.246876	-0.435292
C	6.169392	-0.121872	-1.230431
C	6.137149	-1.281528	-2.027128
H	7.061850	0.510731	-1.241190
C	5.009376	-2.084300	-2.055800
H	7.008081	-1.540056	-2.635935
H	4.969836	-2.977382	-2.688001
H	5.129092	1.163673	0.157553
O	0.378572	3.082021	-0.543639

C	-0.891134	3.107992	-0.226700
O	-1.486805	2.133380	0.224077
C	-1.568427	4.445212	-0.426959
C	-1.221522	4.989816	-1.812622
H	-1.717497	5.963577	-1.956403
H	-0.137641	5.132637	-1.936099
H	-1.573197	4.313058	-2.609549
C	-1.021220	5.378685	0.658914
H	-1.510234	6.363390	0.577382
H	-1.227396	4.980568	1.666970
H	0.066051	5.521987	0.558604
C	-3.075050	4.286130	-0.280547
H	-3.566088	5.259215	-0.443124
H	-3.476793	3.567008	-1.012784
H	-3.348220	3.922789	0.721717
H	4.361076	0.450874	2.080740
C	2.085425	-3.514230	-1.816288
H	1.016972	-3.674085	-1.606417
H	2.204982	-3.429832	-2.909995
H	2.627518	-4.424895	-1.507528

6.4 DFT and TD-DFT calculations for the ground-state geometry and excited state of products

Density functional theory (DFT) calculations were performed using the Gaussian16 program package. The ground-state geometry of products was optimized at the B3LYP/6-31G(d,p) level, and the time-dependent DFT (TD-DFT) calculations were conducted at the CAM-B3LYP/6-311+G(2d,p) level for the excited state calculation using the ground-state geometry.

****

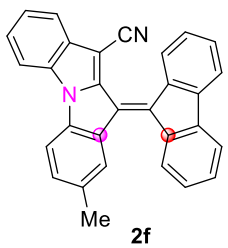
Structure: **2f**

Charge = 0, Multiplicity = 1

Final SCF Energy = -1263.57649167 Hartree

Gibbs Free Energy = -1263.240951 Hartree

Thermal Correction = 0.335541 Hartree



2f

Imaginary Frequencies = none

Cartesian Coordinates (Angstrom):

C	1.810202	1.738538	0.301212
C	0.397308	1.725005	0.223711
C	-0.051156	0.324904	0.048698
C	1.183836	-0.444919	-0.023881
C	1.691384	-1.691771	-0.410628
C	3.132580	-1.570142	-0.443839
C	3.459784	-0.228776	-0.107273
C	4.782678	0.219049	-0.073215
C	5.779473	-0.703304	-0.378552
H	5.034264	1.241886	0.180282
C	4.155249	-2.480205	-0.745543
C	5.471189	-2.036863	-0.709534
H	6.817276	-0.385327	-0.359696
H	3.913948	-3.506222	-1.005071
H	6.276513	-2.726978	-0.940695
C	0.996968	-2.855083	-0.805650
N	0.479614	-3.840933	-1.153251
N	2.260358	0.422270	0.138497
C	1.808669	4.074498	0.777735
C	0.405140	4.097819	0.758848
C	-0.291592	2.910833	0.499083
C	2.528435	2.896661	0.569007
H	2.351819	4.992754	0.983705
H	-1.374840	2.919879	0.521211
H	3.609526	2.892926	0.636581
C	-1.349269	-0.158499	0.012761
C	-1.838615	-1.435237	0.563789
C	-2.535782	0.520971	-0.544747
C	-1.197800	-2.411649	1.331687
C	-3.245561	-1.502916	0.383802
C	-2.655213	1.668337	-1.336720
C	-3.672386	-0.306171	-0.344277
C	-1.943787	-3.471857	1.851599
H	-0.135886	-2.353464	1.536804

C	-3.984510	-2.558076	0.906567
C	-3.906764	2.023577	-1.845551
H	-1.788758	2.274610	-1.573220
C	-4.916326	0.050438	-0.855807
C	-3.321559	-3.553628	1.631848
H	-1.443440	-4.240790	2.431624
H	-5.061204	-2.603625	0.770323
C	-5.031840	1.231020	-1.595621
H	-4.002426	2.919664	-2.451203
H	-5.782251	-0.586997	-0.702244
H	-3.884253	-4.387411	2.040886
H	-5.997014	1.521776	-1.999632
C	-0.343012	5.388394	1.001801
H	-0.420025	5.984313	0.083789
H	-1.361025	5.198823	1.353493
H	0.161630	6.009154	1.748479

****

Structure: **2n**

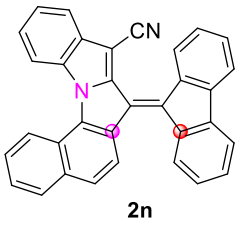
Charge = 0, Multiplicity = 1

Final SCF Energy = -1377.89434742 Hartree

Gibbs Free Energy = -1377.539236 Hartree

Thermal Correction = 0.355111 Hartree

Imaginary Frequencies = none



2n

Cartesian Coordinates (Angstrom):

C	-1.856203	-0.750271	0.088976
C	-0.567172	-1.293391	-0.026346
C	0.415364	-0.197062	-0.028634
C	-0.390205	1.010990	-0.024574
C	-0.292424	2.370467	-0.329187
C	-1.636817	2.854466	-0.529466
C	-2.524126	1.752592	-0.380633
C	-3.883021	1.890921	-0.685399
C	-4.345460	3.151811	-1.053929
H	-4.560468	1.049082	-0.677574
C	-2.125950	4.117277	-0.890296

C	-3.483995	4.259824	-1.138490
H	-5.397257	3.273322	-1.293813
H	-1.442129	4.953937	-0.993778
H	-3.882345	5.227999	-1.424888
C	0.860270	3.154448	-0.548017
N	1.774185	3.850603	-0.749019
N	-1.741794	0.654444	-0.005703
C	-2.788668	-2.970451	0.426799
C	-1.482934	-3.507440	0.250999
C	-0.388906	-2.694016	0.091288
C	-2.987631	-1.545402	0.420116
H	0.604426	-3.121402	0.055519
C	1.799452	-0.285001	0.007599
C	2.721710	0.593092	0.747379
C	2.643948	-1.304584	-0.641209
C	2.477307	1.641239	1.639373
C	4.044995	0.100940	0.593069
C	2.341930	-2.276926	-1.601284
C	4.001277	-1.055170	-0.305243
C	3.549506	2.225654	2.316996
H	1.470500	2.000459	1.816514
C	5.108117	0.683321	1.273649
C	3.373790	-3.044239	-2.147397
H	1.323235	-2.429817	-1.938787
C	5.025282	-1.819511	-0.855404
C	4.854278	1.760545	2.129318
H	3.364100	3.051969	2.995906
H	6.118455	0.301738	1.157364
C	4.702709	-2.828983	-1.767815
H	3.140335	-3.806885	-2.884087
H	6.062422	-1.624398	-0.598483
H	5.675516	2.229525	2.662923
H	5.492520	-3.433223	-2.204138
C	-5.299037	-1.894594	1.108227
C	-5.130976	-3.294708	1.013051
C	-3.896947	-3.815049	0.694498

C	-4.254550	-1.042814	0.823378
H	-6.254174	-1.486257	1.424261
H	-5.965765	-3.955908	1.224286
H	-3.743794	-4.890529	0.669444
H	-4.386307	0.021818	0.957399
H	-1.355492	-4.584607	0.306646

****

Structure: **2o**

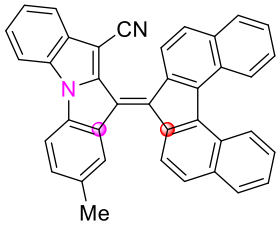
Charge = 0, Multiplicity = 1

Final SCF Energy = -1570.85546127 Hartree

Gibbs Free Energy = -1570.432670 Hartree

Thermal Correction = 0.422791 Hartree

Imaginary Frequencies = none



2o

Cartesian Coordinates (Angstrom):

C	3.311325	1.369302	0.642753
C	1.918656	1.621177	0.659647
C	1.216884	0.421535	0.157077
C	2.283571	-0.504947	-0.190164
C	2.539341	-1.676991	-0.912518
C	3.976511	-1.807465	-1.009958
C	4.556484	-0.679863	-0.366924
C	5.940202	-0.497308	-0.309521
C	6.739785	-1.469023	-0.904572
H	6.383962	0.362979	0.177126
C	4.804222	-2.772935	-1.600042
C	6.180352	-2.593845	-1.541022
H	7.819022	-1.355524	-0.875487
H	4.369618	-3.636331	-2.093916
H	6.837328	-3.330430	-1.992682
C	1.626279	-2.555081	-1.535877
N	0.921399	-3.307230	-2.081303
N	3.506075	0.085835	0.115870
C	3.743827	3.459526	1.704084
C	2.368167	3.728741	1.784844
C	1.461136	2.790219	1.276490

C	4.233507	2.273808	1.152037
H	4.449350	4.182377	2.104507
H	0.397382	2.975300	1.372465
H	5.296996	2.067845	1.145500
C	-0.151285	0.206179	0.071759
C	-0.867740	-1.040343	0.363096
C	-1.179351	1.192447	-0.282476
C	-0.366301	-2.256789	0.875916
C	-2.254756	-0.791146	0.300056
C	-1.022009	2.498739	-0.800225
C	-2.437437	0.554563	-0.285844
C	-1.244391	-3.226351	1.295519
H	0.700384	-2.428704	0.942339
C	-3.164965	-1.710607	0.903499
C	-2.119116	3.176368	-1.274724
H	-0.043750	2.962100	-0.834101
C	-3.542779	1.175488	-0.944386
C	-2.641760	-2.979331	1.345152
H	-0.871987	-4.182031	1.652635
C	-3.385368	2.540375	-1.380114
H	-2.016347	4.192779	-1.644485
C	1.874380	5.017463	2.400820
H	1.885959	5.837959	1.672541
H	0.847365	4.918105	2.763138
H	2.501355	5.324337	3.243525
C	-4.529670	-1.424737	1.198372
C	-5.350939	-2.365742	1.777733
C	-4.856474	-3.649923	2.105077
C	-3.526674	-3.938798	1.904294
H	-4.918565	-0.435529	0.996675
H	-6.384306	-2.114327	1.997907
H	-5.518329	-4.390247	2.544404
H	-3.121965	-4.903096	2.199845
C	-4.479950	3.204717	-1.993164
C	-5.660159	2.545447	-2.249239
C	-5.780427	1.174142	-1.925695

C	-4.751821	0.509204	-1.296302
H	-4.354774	4.243423	-2.287560
H	-6.484298	3.063598	-2.730368
H	-6.685897	0.635830	-2.189613
H	-4.848354	-0.549941	-1.099118

****

Structure: **4a**

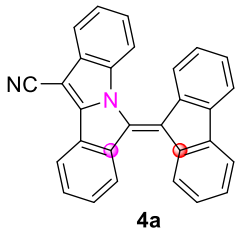
Charge = 0, Multiplicity = 1

Final SCF Energy = -1224.25886366 Hartree

Gibbs Free Energy = -1223.947237 Hartree

Thermal Correction = 0.311627 Hartree

Imaginary Frequencies = none



4a

Cartesian Coordinates (Angstrom):

C	-3.496315	-0.130205	0.013803
C	-3.044609	-1.438912	0.448275
C	-1.623223	-1.410981	0.495099
C	-2.360655	0.629321	-0.191113
C	-0.049444	0.633658	-0.005967
C	-0.523561	2.012845	-0.237872
C	-1.934899	1.988384	-0.403493
C	-3.735788	-2.584360	0.855000
C	-3.005746	-3.669975	1.329717
C	-1.605570	-3.613474	1.412722
C	-0.893352	-2.486911	0.999606
H	-4.820398	-2.609238	0.818397
H	-3.525474	-4.565554	1.655409
H	-1.058707	-4.462431	1.810861
H	0.184219	-2.454272	1.077958
N	-1.224384	-0.147561	0.023120
C	-4.832319	0.316669	-0.102077
N	-5.935069	0.682165	-0.202899
C	-2.657451	3.134481	-0.736662
C	0.165802	3.205618	-0.484214
C	-0.559446	4.352013	-0.809416
C	-1.956446	4.324109	-0.923491

H	-3.735059	3.091873	-0.856525
H	1.246009	3.248360	-0.429661
H	-0.027218	5.281831	-0.984988
H	-2.494411	5.232073	-1.177105
C	1.239913	0.140248	-0.014830
C	1.720626	-1.109624	-0.633360
C	2.437025	0.821350	0.510637
C	1.064939	-2.069604	-1.414153
C	3.136681	-1.155158	-0.518255
C	2.575457	1.948598	1.328947
C	3.576764	0.023146	0.227698
C	1.808372	-3.092225	-2.007357
H	-0.006445	-2.030007	-1.568544
C	3.870378	-2.177249	-1.115218
C	3.844835	2.315785	1.779914
H	1.710352	2.528263	1.631008
C	4.839636	0.391928	0.685982
C	3.197175	-3.156043	-1.850293
H	1.298299	-3.844007	-2.601939
H	4.952895	-2.204147	-1.028659
C	4.971449	1.552890	1.451120
H	3.954915	3.196921	2.404843
H	5.708708	-0.222233	0.467963
H	3.756960	-3.959895	-2.318888
H	5.950170	1.852301	1.813819

****

Structure: **4g**

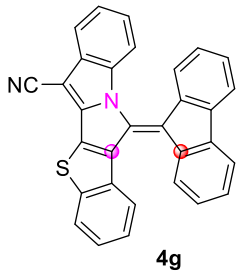
Charge = 0, Multiplicity = 1

Final SCF Energy = -1698.65308331 Hartree

Gibbs Free Energy = -1698.331337 Hartree

Thermal Correction = 0.321746 Hartree

Imaginary Frequencies = none



4g

Cartesian Coordinates (Angstrom):

C	0.060205	-0.060200	0.052320
C	2.370593	-0.281745	-0.034843

C	1.796564	-1.583354	-0.089407
C	0.411020	-1.479141	-0.013203
C	0.736657	-3.782491	-0.422336
C	-0.234690	-2.752536	-0.270168
S	2.400538	-3.182650	-0.347281
N	1.305047	0.620021	0.017448
C	3.231135	1.775296	0.381761
C	1.812233	1.887702	0.361531
C	1.180274	3.086292	0.688146
C	1.988837	4.183883	0.989490
C	3.389347	4.095924	0.970465
C	4.020741	2.892153	0.673712
C	3.569975	0.387549	0.137672
H	0.103583	3.171181	0.717534
H	1.515861	5.125942	1.248789
H	3.984945	4.972205	1.205918
H	5.102685	2.805527	0.688165
C	4.858801	-0.190436	0.158165
N	5.927882	-0.656042	0.171293
C	-1.178153	0.557844	0.026125
C	-2.387616	0.093203	0.718631
C	-1.569567	1.764406	-0.719398
C	-2.563000	-0.897784	1.691498
C	-3.457974	0.975768	0.412150
C	-0.873361	2.538895	-1.655507
C	-2.959417	1.989194	-0.517955
C	-3.817112	-1.053866	2.284926
H	-1.738596	-1.536832	1.989199
C	-4.703421	0.818543	1.015446
C	-1.545295	3.560318	-2.329590
H	0.174829	2.355866	-1.862748
C	-3.621476	3.008479	-1.197731
C	-4.881922	-0.211057	1.943520
H	-3.962724	-1.830258	3.029848
H	-5.520710	1.496078	0.785168
C	-2.904185	3.802237	-2.096675

H	-1.005019	4.170579	-3.046883
H	-4.684342	3.174892	-1.047090
H	-5.847795	-0.343661	2.421709
H	-3.408563	4.601315	-2.631639
C	-1.588918	-3.102254	-0.430652
C	0.382989	-5.112037	-0.657757
C	-0.965432	-5.427451	-0.781361
C	-1.939961	-4.422520	-0.681847
H	-2.356645	-2.343417	-0.367223
H	1.145623	-5.877622	-0.760078
H	-1.261716	-6.454241	-0.971686
H	-2.987749	-4.677891	-0.806412

Table S1. Excited state of **2f**.

state	*E* (eV)	λ (nm)	*f*	main configurations
S_1	2.4679	502.38	0.4570	HOMO → LUMO (0.70011)
S_2	2.7825	445.58	0.0024	HOMO-2 → LUMO (0.69403)
S_3	3.0232	410.11	0.0897	HOMO-1 → LUMO (0.68861)
S_4	3.7825	327.78	0.1485	HOMO-3 → LUMO (0.67205)

Table S2. Excited state of **2n**.

state	*E* (eV)	λ (nm)	*f*	main configurations
S_1	2.3707	522.99	0.4781	HOMO → LUMO (0.69924)
S_2	2.7436	451.90	0.0003	HOMO-2 → LUMO (0.68552) HOMO-1 → LUMO (-0.10158)
S_3	2.8820	430.21	0.1032	HOMO-2 → LUMO (0.10075) HOMO-1 → LUMO (0.68077)
S_4	3.6818	336.75	0.1680	HOMO-4 → LUMO (-0.19603) HOMO-3 → LUMO (0.63032) HOMO → LUMO+1 (0.12993)

Table S3. Excited state of **2o**.

state	*E* (eV)	λ (nm)	*f*	main configurations
S_1	2.0601	601.82	0.0036	HOMO-1 → LUMO (0.67046) HOMO → LUMO (0.17456)
S_2	2.3815	520.60	0.6641	HOMO-1 → LUMO (-0.17589) HOMO → LUMO (0.67589)
S_3	2.9372	422.12	0.1218	HOMO-2 → LUMO (0.68317)
S_4	3.4497	359.41	0.0319	HOMO-4 → LUMO (-0.24864) HOMO-3 → LUMO (0.61498) HOMO → LUMO+1 (0.10801)

Table S4. Excited state of **4a**.

state	*E* (eV)	λ (nm)	*f*	main configurations
S_1	2.6699	464.38	0.5805	HOMO → LUMO (0.69784)
S_2	3.0981	400.19	0.0005	HOMO-1 → LUMO (0.68656) HOMO-1 → LUMO+1 (-0.10323)
S_3	3.2065	386.66	0.0662	HOMO-3 → LUMO (-0.19674) HOMO-2 → LUMO (0.66530)
S_4	3.7923	326.94	0.0811	HOMO-3 → LUMO (0.62467) HOMO-2 → LUMO (0.19795) HOMO-2 → LUMO+1 (-0.12826) HOMO → LUMO+1 (-0.12645)

Table S5. Excited state of **4g**

state	*E* (eV)	λ (nm)	*f*	main configurations
S_1	2.3781	521.35	0.4900	HOMO-1 → LUMO (0.10939) HOMO → LUMO (0.68959)
S_2	2.7884	444.65	0.1124	HOMO-3 → LUMO (-0.10549) HOMO-2 → LUMO (-0.20062) HOMO-1 → LUMO (0.64598) HOMO → LUMO (-0.12323)
S_3	2.9497	420.33	0.0023	HOMO-2 → LUMO (0.64724) HOMO-1 → LUMO (0.21443)
S_4	3.4803	356.25	0.0023	HOMO-3 → LUMO (0.67505) HOMO-2 → LUMO (-0.11843)

7. Summary of single crystal 2f

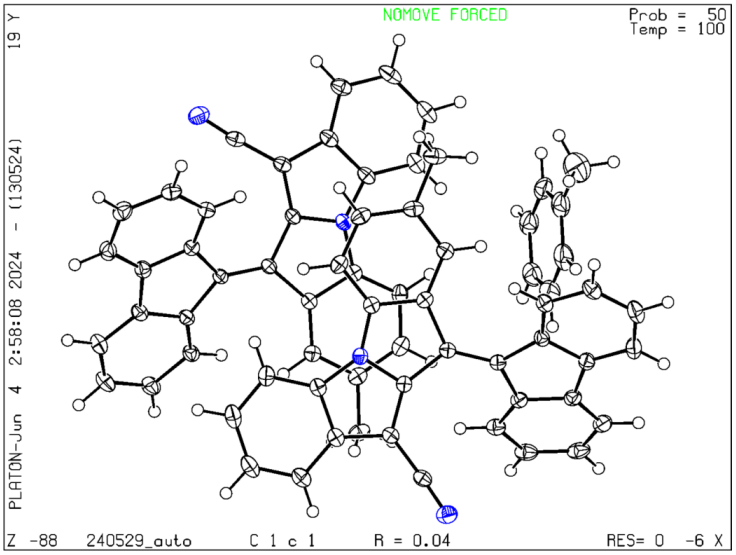
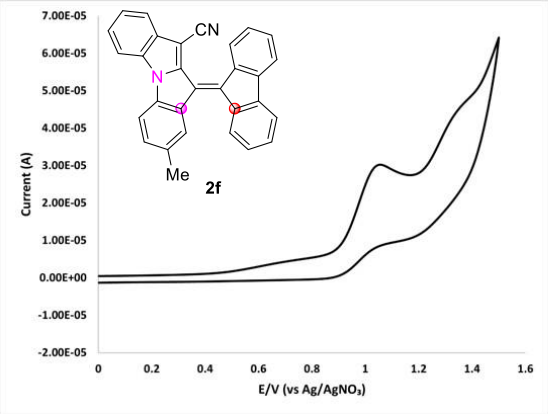


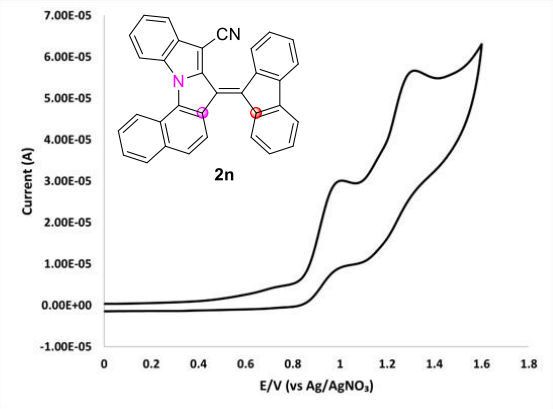
Table S6. Crystal data and structure refinement for **2f**

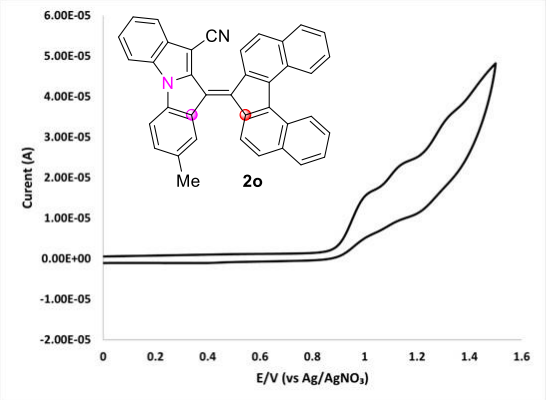
Identification code	**2f**
Empirical formula	$C_{67}H_{44}N_4$
Formula weight	905.06
Temperature/K	99.90(14)
Crystal system	monoclinic
Space group	Cc
a/Å	21.1210(3)
b/Å	15.8687(2)
c/Å	14.1284(2)
α/°	90
β/°	90.5909(14)
γ/°	90
Volume/Å^3	4735.08(12)
Z	4
ρ_{calc}g/cm^3	1.270
μ/mm^{-1}	0.074
F(000)	1896.0
Crystal size/mm^3	0.4 × 0.3 × 0.3
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	5.134 to 63.992

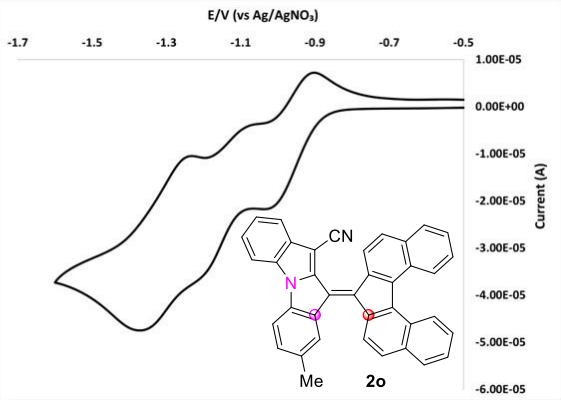
Index ranges	-30 ≤ h ≤ 30, -23 ≤ k ≤ 21, -20 ≤ l ≤ 19
Reflections collected	51619
Independent reflections	13566 [R_{int} = 0.0333, R_{sigma} = 0.0318]
Data/restraints/parameters	13566/2/644
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0369, wR_2 = 0.0936
Final R indexes [all data]	R_1 = 0.0403, wR_2 = 0.0958
Largest diff. peak/hole / e Å^{-3}	0.38/-0.25
Flack parameter	-0.6(6)

8. Cyclic voltammetry (CV) of products









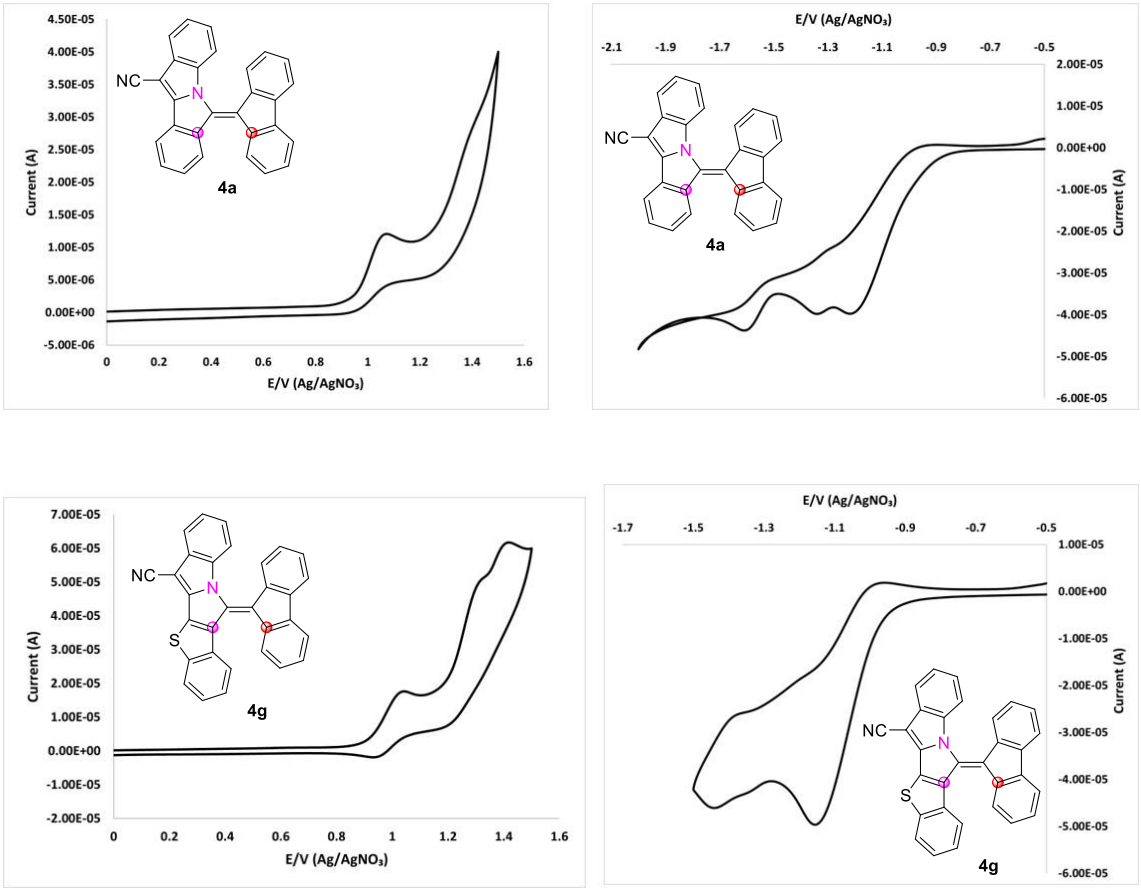
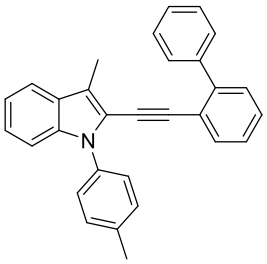


Figure S2. Cyclic voltammograms (CV) of BPAE products. First oxidation potentials measured by CV using $Ag/AgNO_3$ as a reference electrode, Pt wire as a counter electrode, glassy carbon as a working electrode, and Bu_4NPF_6 (0.1 M) as a supporting electrolyte in dichloromethane. The scan rate is 50 mV s-1 and the Fc/Fc^+ (-4.80 eV) was used as an external standard.

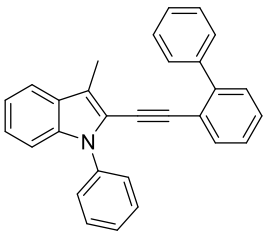
9. Analytical data of starting substrates and products

2-(biphenyl-2-ylethynyl)-3-methyl-1-(*p*-tolyl)-1*H*-indole (1a)



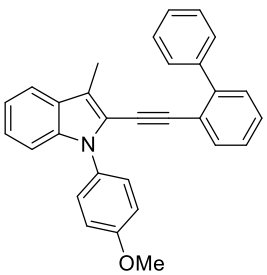
Purified by column chromatography (silica gel), [Hexane/DCM = 2:1 (v/v)] to give **1a** as white solid (1.32 mmol, 523.3 mg, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.53 (m, 3H), 7.42 (dd, *J* = 7.1, 1.1 Hz, 1H), 7.39-7.24 (m, 11H), 7.19 (td, *J* = 7.6, 1.4 Hz, 1H), 7.13 (td, *J* = 7.4, 1.1 Hz, 1H), 2.45 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 140.5, 137.3, 136.8, 135.4, 132.9, 129.7, 129.3, 128.5, 128.1, 128.0, 127.5, 127.1, 126.8, 123.8, 121.7, 120.3, 120.2, 119.3, 119.2, 110.5, 97.6, 84.2, 21.3, 9.8, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{23}N$, 397.1825; Found 397.1825; Mp. 76-78 °C.

2-(biphenyl-2-ylethynyl)-3-methyl-1-phenyl-1*H*-indole (1b)



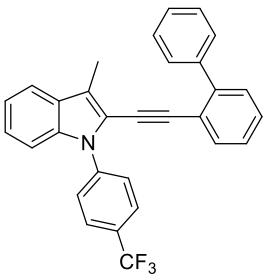
Purified by column chromatography (silica gel), [Hexane/DCM = 5:1 (v/v)] to give **1b** as white solid (0.71 mmol, 272.1 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.52 (m, 3H), 7.49-7.46 (m, 4H), 7.40-7.33 (m, 7H), 7.29 (dd, *J* = 7.3, 5.0 Hz, 2H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.3 Hz, 1H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 140.6, 138.0, 137.2, 132.9, 129.7, 129.3, 129.1, 128.6, 128.2, 128.1, 127.6, 127.2, 127.1, 127.0, 123.9, 121.6, 120.4, 120.2, 119.5, 119.4, 110.4, 97.7, 84.1, 9.8. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{21}N$, 383.1669; Found 383.1668; Mp. 126-128 °C.

2-(biphenyl-2-ylethynyl)-1-(4-methoxyphenyl)-3-methyl-1*H*-indole (1c)



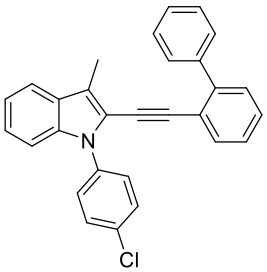
Purified by GPC to give **1c** as colorless oil (0.56 mmol, 231.8 mg, 56% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 6.9 Hz, 3H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.38-7.11 (m, 11H), 6.95 (d, *J* = 9.2 Hz, 2H), 3.89 (s, 3H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 143.3, 140.6, 137.5, 133.0, 130.9, 129.7, 129.3, 128.6, 128.3, 128.2, 127.9, 127.6, 127.1, 123.7, 121.6, 120.5, 120.1, 119.3, 118.9, 114.2, 110.4, 97.5, 84.1, 55.6, 9.8. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{23}NO$, 413.1774; Found 413.1774.

2-(biphenyl-2-ylethynyl)-3-methyl-1-(4-(trifluoromethyl)phenyl)-1*H*-indole (1d)



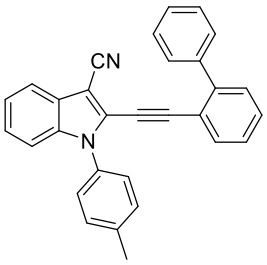
Purified by recrystallization ($CHCl_3$/hexane) to give **1d** as white solid (0.23 mmol, 104.0 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.2 Hz, 2H), 7.58-7.52 (m, 5H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.41-7.29 (m, 7H), 7.24-7.16 (m, 2H), 2.33 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.5, 141.0, 140.5, 136.8, 132.8, 129.8, 129.3, 128.9, 128.7 (q, J_F = 33.0 Hz), 128.5, 128.2, 127.7, 127.2, 126.8, 126.3 (q, J_F = 2.9 Hz), 124.4, 124.2 (q, J_F = 270 Hz), 121.3, 121.0, 120.7, 119.7, 119.6, 110.2, 98.4, 83.4, 9.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.1 (s, 3F). HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{20}F_3N$, 451.1542; Found 451.1543; Mp. 132-134 °C.

2-(biphenyl-2-ylethynyl)-1-(4-chlorophenyl)-3-methyl-1*H*-indole (1e)



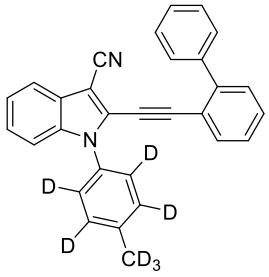
Purified by column chromatography (silica gel), [Hexane/AcOEt = 20:1 (v/v)] to give **1e** as white solid (0.99 mmol, 413.8 mg, 99% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57-7.52 (m, 3H), 7.46 (d, *J* = 7.3 Hz, 1H), 7.38-7.29 (m, 10H), 7.23-7.13 (m, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 140.5, 137.0, 136.5, 132.9, 132.6, 129.8, 129.2(8), 129.2(5), 128.7, 128.2, 128.1(6), 128.1(0), 127.7, 127.2, 124.1, 121.4, 120.6, 120.0, 119.5, 110.2, 98.1, 83.6, 9.8, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{20}ClN$, 417.1279; Found 417.1279; Mp. 113-115 °C.

2-(biphenyl-2-ylethynyl)-1-(*p*-tolyl)-1*H*-indole-3-carbonitrile (1f)



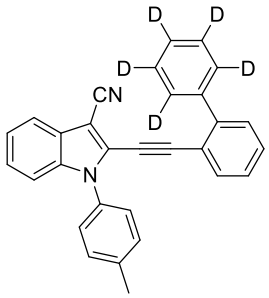
Purified by column chromatography (silica gel), [Hexane/DCM = 10:1 (v/v)] to give **1f** as white solid (0.89 mmol, 363.6 mg, 89% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.73 (m, 1H), 7.56-7.50 (m, 3H), 7.43-7.35 (m, 5H), 7.33-7.28 (m, 3H), 7.24-7.22 (m, 5H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 139.8, 138.8, 136.7, 134.0, 133.5, 130.1, 130.0, 129.8, 129.2, 129.1, 128.4, 127.8, 127.2, 127.0, 126.8, 125.4, 123.2, 119.8, 119.7, 115.2, 111.6, 100.6, 92.5, 80.5, 21.4. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{20}N_2$, 408.1620; Found 408.1621; Mp. 158-160 °C.

2-(biphenyl-2-ylethynyl)-1-(4-(methyl-d_3)phenyl-2,3,5,6-d_4)-1*H*-indole-3-carbonitrile (1f-d_7)



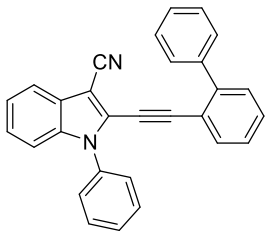
Purified by column chromatography (silica gel), [Hexane/AcOEt = 20:1 (v/v)] to give **1f-*d*$_7$** as white solid (0.37 mmol, 153.7 mg, 37% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.73 (m, 1H), 7.55 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.53-7.51 (m, 2H), 7.46-7.28 (m, 8H), 7.25-7.21 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 139.8, 138.5, 136.7, 134.1, 133.4, 130.0, 129.8, 129.2, 129.1, 128.4, 127.8, 127.2, 127.0, 125.4, 123.2, 119.8, 119.7, 115.2, 111.6, 100.6, 92.5, 80.5, sp^2 and sp^3 carbons adjacent to D cannot be identified due to their weak intensity and superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{13}D_7N_2$, 415.2060; Found 415.2060; Mp. 161-163 °C.

2-((biphenyl-2-yl-2',3',4',5',6'-*d*$_5$)ethynyl)-1-(*p*-tolyl)-1*H*-indole-3-carbonitrile (1f-*d*$_5$)



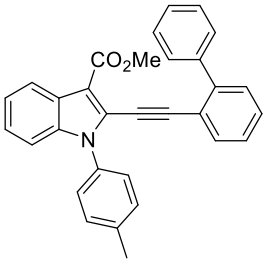
Purified by column chromatography (silica gel), [Hexane/AcOEt = 20:1 (v/v)] to give **1f-*d*$_5$** as white solid (0.48 mmol, 198.5 mg, 63% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.73 (m, 1H), 7.56-7.55 (m, 1H), 7.46-7.39 (m, 2H), 7.34-7.28 (m, 3H), 7.24-7.22 (m, 5H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 139.6, 138.8, 136.7, 134.1, 133.5, 130.2, 130.0, 129.8, 129.1, 127.2, 127.0, 126.8, 125.4, 123.2, 119.8, 119.8, 115.3, 111.6, 100.6, 92.5, 80.5, 21.4, sp^2 carbons adjacent to D cannot be identified due to their weak intensity and superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{15}D_5N_2$, 413.1935; Found 413.1935; Mp. 157-159 °C.

2-(biphenyl-2-ylethynyl)-1-phenyl-1*H*-indole-3-carbonitrile (1g)



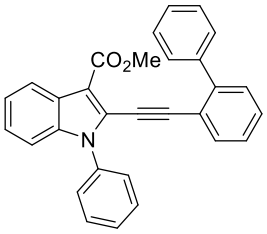
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **1g** as white solid (0.34 mmol, 132.1 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 9.2 Hz, 1H), 7.52 (d, *J* = 6.4 Hz, 3H), 7.46-7.21 (m, 14H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 139.7, 136.5, 136.0, 133.9, 130.0, 129.7, 129.5, 129.1, 128.9, 128.4, 127.9, 127.1, 127.0, 125.5, 123.3, 119.7, 119.6, 115.1, 111.5, 100.7, 92.7, 80.3, two sp^2 peaks not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{18}N_2$, 394.1465; Found 394.1465; Mp. 138-140 °C.

methyl 2-(biphenyl-2-ylethynyl)-1-(*p*-tolyl)-1*H*-indole-3-carboxylate (1h)



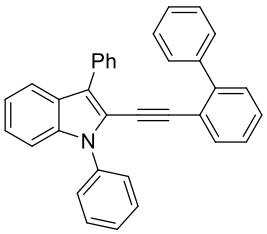
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **1h** as yellow solid (0.94 mmol, 415.0 mg, 94% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.3 Hz, 1H), 7.55 (d, *J* = 7.3 Hz, 1H), 7.51-7.49 (m, 2H), 7.42-7.36 (m, 2H), 7.32-7.15 (m, 11H), 3.84 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 143.6, 140.1, 138.4, 137.6, 134.1, 133.9, 129.9, 129.8, 129.4, 129.2, 128.1, 127.6, 127.3, 127.1, 126.9, 126.3, 124.4, 122.8, 122.1, 120.7, 111.5, 110.9, 99.9, 83.3, 51.2, 21.4. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{23}NO_2$, 441.1723; Found 441.1724; Mp. 117-119 °C.

methyl 2-(biphenyl-2-ylethynyl)-1-phenyl-1*H*-indole-3-carboxylate (1i)



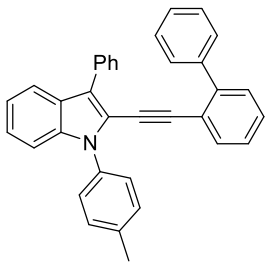
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **1i** as yellow solid (0.81 mmol, 346.0 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.3 Hz, 1H), 7.52-7.49 (m, 3H), 7.43-7.24 (m, 13H), 7.18 (d, *J* = 8.2 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 143.5, 139.9, 137.4, 136.4, 134.0, 129.7, 129.4, 129.2, 129.1, 128.5, 128.1, 127.6, 127.5, 127.0, 126.6, 126.2, 124.5, 122.8, 122.0, 120.5, 111.6, 110.8, 99.9, 83.1, 51.1. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{21}NO_2$, 427.1567; Found 427.1567; Mp. 46-48 °C.

2-(biphenyl-2-ylethynyl)-1,3-diphenyl-1*H*-indole (1j)



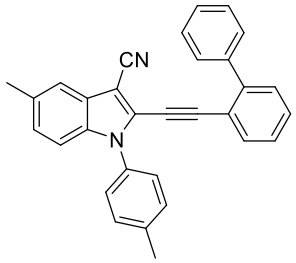
Purified by column chromatography (silica gel), [Hexane/DCM = 3:1 (v/v)] to give **1j** as white solid (0.49 mmol, 218.1 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.8 Hz, 1H), 7.74 (dt, *J* = 6.7, 1.5 Hz, 2H), 7.50-7.17 (m, 20H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 140.2, 137.8, 137.6, 134.2, 133.5, 129.8, 129.2(1), 129.1(6), 128.8, 128.6, 128.2, 127.7(3), 127.7(0), 127.6, 127.0, 126.8, 126.3, 124.2, 123.3, 121.3, 121.2, 120.3, 119.5, 110.8, 96.7, 84.4, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{34}H_{23}N$, 445.1825; Found 445.1825; Mp. 133-135 °C.

2-(biphenyl-2-ylethynyl)-3-phenyl-1-(*p*-tolyl)-1*H*-indole (1k)



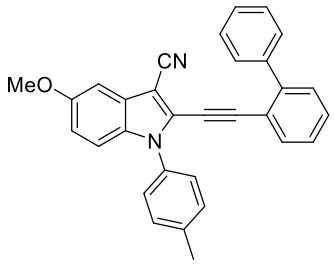
Purified by column chromatography (silica gel), [Hexane/DCM = 5:1 (v/v)] to give **1k** as white solid (0.67 mmol, 307.7 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.8 Hz, 1H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.45-7.16 (m, 19H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 140.2, 137.9, 137.4, 135.0, 134.3, 133.6, 133.2, 129.8(3), 129.7(6), 129.2, 128.8, 128.6, 128.1, 127.6, 127.3, 127.0, 126.7, 126.2, 124.1, 123.1, 121.3, 121.2, 120.2, 119.6, 110.8, 96.6, 84.6, 21.4. HRMS [APCI_positive] m/z: [M] calc For $C_{35}H_{25}N$, 459.1982; Found 459.1982; Mp. 123-125 °C.

2-(biphenyl-2-ylethynyl)-5-methyl-1-(*p*-tolyl)-1*H*-indole-3-carbonitrile (1l)



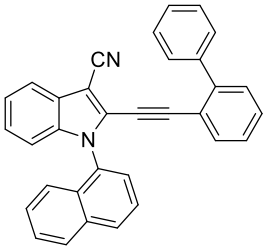
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **1l** as white solid (0.67 mmol, 307.7 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.51 (m, 4H), 7.45-7.29 (m, 6H), 7.21 (s, 4H), 7.11 (s, 2H), 2.47 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 139.8, 138.7, 135.1, 134.0, 133.7, 133.0, 130.1, 129.9, 129.8, 129.2, 128.8, 128.4, 127.8, 127.3, 127.2, 127.1, 126.7, 119.9, 119.2, 115.4, 111.3, 100.4, 92.0, 80.7, 21.5, 21.4. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{22}N_2$, 422.1778; Found 422.1778; Mp. 154-156 °C.

2-(biphenyl-2-ylethynyl)-5-methoxy-1-(*p*-tolyl)-1*H*-indole-3-carbonitrile (1m)



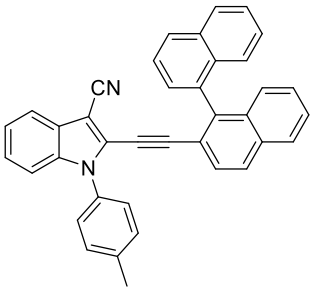
Purified by recrystallization ($CHCl_3$/hexane) to give **1m** as white solid (0.51 mmol, 223.7 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.35 (m, 9H), 7.33-7.29 (m, 1H), 7.21 (s, 4H), 7.13-7.10 (m, 1H), 6.92 (dd, J = 8.9, 2.5 Hz, 1H), 3.89 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 144.1, 139.8, 138.7, 134.0, 133.6, 131.7, 130.1, 129.9, 129.8, 129.1, 128.6, 128.4, 127.9, 127.8, 127.2, 126.6, 119.8, 116.4, 115.5, 112.6, 100.3, 100.1, 92.0, 80.6, 55.9, 21.4. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{22}N_2O$, 438.1727; Found 438.1727; Mp. 164-166 °C.

2-(biphenyl-2-ylethynyl)-1-(naphthalen-1-yl)-1*H*-indole-3-carbonitrile (1n)



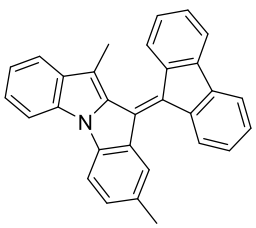
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **1n** as white solid (0.48 mmol, 213.2 mg, 56% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-7.99 (m, 2H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.44-7.29 (m, 7H), 7.24-7.13 (m, 7H), 6.82 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 139.5, 137.8, 134.5, 133.9, 132.6, 130.3, 130.2, 129.9, 129.6, 128.9, 128.6, 128.3, 127.8, 127.6, 127.0, 126.8(2), 126.7(6), 125.5, 125.4, 123.3, 122.9, 119.8, 119.5, 115.2, 112.0, 100.8, 92.4, 80.3, two sp^2 peaks are not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{33}H_{20}N_2$, 444.1621; Found 444.1621; Mp. 84-86 °C.

2-(binaphthalen-2-ylethynyl)-1-(*p*-tolyl)-1*H*-indole-3-carbonitrile (1o)



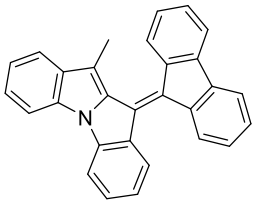
Purified by column chromatography (silica gel), [Hexane/DCM = 2:1 (v/v)] to give **1o** as white solid (0.54 mmol, 274.7 mg, 88% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 8.0, 4.8 Hz, 2H), 7.91 (d, *J* = 8.7 Hz, 2H), 7.69-7.64 (m, 2H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.51-7.45 (m, 3H), 7.29 -7.17 (m, 6H), 7.14-7.11 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 138.4, 136.6, 135.8, 133.6(3), 133.5(7), 133.2, 132.8, 132.5, 129.9, 128.9, 128.8, 128.5, 128.4, 128.2, 128.2, 127.3, 126.9, 126.3(4), 126.3(2), 126.2, 125.9, 125.6, 125.2, 123.1, 119.5(8), 119.5(6), 115.1, 111.6, 100.8, 92.6, 81.3, 21.4, three sp^2 peaks are not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{38}H_{24}N_2$, 508.1934; Found 508.1934; Mp. 238-240 °C.

10-(9*H*-fluoren-9-ylidene)-8,11-dimethyl-10*H*-indolo[1,2-*a*]indole (2a)



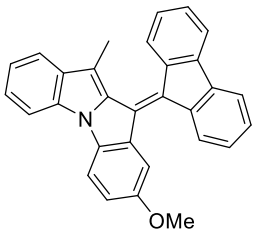
Purified by column chromatography (silica gel), [Hexane/DCM = 2:1 (v/v)] to give **2a** as dark red solid (0.19 mmol, 74.4 mg, 94% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.3 Hz, 1H), 8.24 (s, 1H), 7.82 (t, *J* = 6.9 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 8.2 Hz, 1H), 7.43-7.29 (m, 6H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.19 (d, *J* = 7.2 Hz, 1H), 2.37 (s, 3H), 2.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 139.4, 139.3, 139.2, 138.9, 138.2, 135.1, 134.3, 134.0, 132.7, 131.6, 131.0, 128.4, 128.0, 127.6, 127.0, 126.6, 126.5, 125.8, 125.5, 124.7, 121.1, 120.8, 120.2, 119.9, 117.5, 111.3, 111.0, 21.5, 14.6. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{21}N$, 395.1669; Found 395.1669; Mp. 140-142 °C.

10-(9*H*-fluoren-9-ylidene)-11-methyl-10*H*-indolo[1,2-*a*]indole (2b)



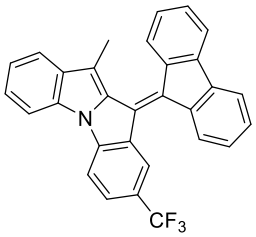
Purified by column chromatography (silica gel), [Hexane/DCM = 2:1 (v/v)] to give **2b** as dark red solid (0.09 mmol, 34.3 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 8.2 Hz, 1H), 8.34 (d, *J* = 7.3 Hz, 1H), 7.83-7.80 (m, 2H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 8.2 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 3H), 7.38-7.35 (m, 4H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.07 (t, *J* = 7.8 Hz, 1H), 2.11 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 140.6, 139.5, 139.1, 138.9, 138.2, 135.3, 134.1, 134.0, 132.9, 130.1, 128.1(4), 128.0(8), 127.7, 127.0, 126.6, 126.3, 125.9, 125.6, 124.7, 122.1, 121.4, 120.8, 120.2, 119.9, 117.6, 111.6, 111.1, 14.6. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{19}N$, 381.1512; Found 381.1512; Mp. 174-176 °C.

10-(9*H*-fluoren-9-ylidene)-8-methoxy-11-methyl-10*H*-indolo[1,2-*a*]indole (2c)



Purified by recrystallization ($CHCl_3$/hexane) to give **2c** as dark red solid (0.05 mmol, 22.3 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.8 Hz, 1H), 7.98 (d, *J* = 2.3 Hz, 1H), 7.81 (t, *J* = 6.6 Hz, 2H), 7.67 (t, *J* = 8.2 Hz, 2H), 7.53 (d, *J* = 8.2 Hz, 1H), 7.43-7.28 (m, 6H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.01 (dd, *J* = 8.7, 2.3 Hz, 1H), 3.79 (s, 3H), 2.09 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 140.6, 139.4, 138.8, 138.0, 135.8, 135.0, 134.9, 134.0, 132.7, 128.4, 128.2, 127.7, 127.1, 126.5, 125.7, 125.5, 124.7, 121.0, 120.8, 120.3, 119.9, 117.7, 117.1, 112.0, 111.0, 110.7, 56.0, 14.6, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{21}NO$, 411.1618; Found 411.1618; Mp. 203-205 °C.

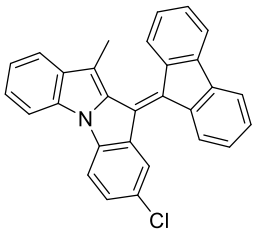
10-(9*H*-fluoren-9-ylidene)-11-methyl-8-(trifluoromethyl)-10*H*-indolo[1,2-*a*]indole (2d)



Purified by recrystallization ($CHCl_3$/hexane) to give **2d** as dark red solid (0.06 mmol, 28.8 mg, 64% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.24 (d, *J* = 7.3 Hz, 1H), 7.81 (t, *J* = 7.3 Hz, 2H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.71-7.66 (m, 3H), 7.46-7.25 (m, 7H), 2.13 (s, 3H). ^{13}C NMR (150MHz, $CDCl_3$) δ 142.7, 141.0, 139.8, 139.1, 138.5, 137.8, 135.5, 134.8, 134.3, 133.9, 133.7, 128.8, 128.4, 127.2, 126.9(5), 126.8(9) (q, J_F =4.4 Hz), 126.3, 125.9, 125.8, 124.8, 124.5 (q, J_F =270 Hz), 124.2 (q, J_F =31.7 Hz), 123.1 (q, J_F =4.4 Hz), 122.1, 121.0, 120.5, 120.1, 118.3, 111.3, 14.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.4 (s, 3F). HRMS [APCI_positive] m/z: [M] calc For

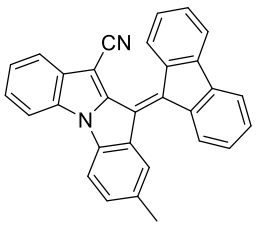
$C_{30}H_{18}F_3N$, 449.1386; Found 449.1386; Mp. 160-162°C.

8-chloro-10-(9*H*-fluoren-9-ylidene)-11-methyl-10*H*-indolo[1,2-*a*]indole (2e)



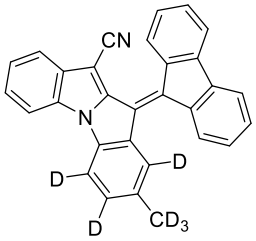
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **2e** as dark red solid (0.17 mmol, 70.7 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 1.8 Hz, 1H), 8.27 (d, *J* = 7.8 Hz, 1H), 7.80 (t, *J* = 6.6 Hz, 2H), 7.69 (t, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.7 Hz, 1H), 7.43-7.21 (m, 8H), 2.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 139.7, 139.4, 139.1, 138.6, 137.9, 135.4, 135.2, 133.9, 133.8, 129.7, 128.6, 128.2, 127.4, 127.2, 126.9, 126.7, 125.8, 125.7, 124.7, 121.6, 121.0, 120.4, 120.1, 118.0, 112.2, 111.0, 14.6, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{18}ClN$, 415.1122; Found 415.1122; Mp. 186-188 °C.

10-(9*H*-fluoren-9-ylidene)-8-methyl-10*H*-indolo[1,2-*a*]indole-11-carbonitrile (2f)



Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **2f** as dark red solid (0.20 mmol, 80.5 mg, 99% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.2 Hz, 1H), 8.22 (s, 1H), 8.00 (d, *J* = 7.3 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.73-7.69 (m, 2H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.52-7.32 (m, 5H), 7.28-7.24 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 142.9, 141.9, 140.7, 137.5, 137.2(9), 137.2(5), 133.6, 133.5, 131.9, 131.3, 130.8, 130.6, 130.4, 127.4, 127.0, 126.6, 126.5, 126.0, 125.9, 124.3, 123.1, 120.8, 120.4, 120.0, 115.4, 111.5, 111.4, 85.4, 21.4. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{18}N_2$, 406.1465; Found 406.1465; Mp. 255-257 °C.

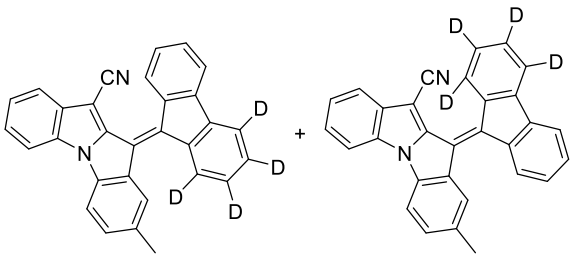
10-(9*H*-fluoren-9-ylidene)-8-(methyl-d_3)-10*H*-indolo[1,2-*a*]indole-11-carbonitrile-6,7,9-d_3 (2f-d_6)



Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **2f-d_6** as dark red solid (0.04 mmol, 17.6 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.8 Hz, 1H), 7.99 (dd, *J* = 7.1, 1.1 Hz, 1H), 7.82 (t, *J* = 7.1 Hz, 2H), 7.72-7.69 (m, 2H), 7.49-7.32 (m, 5H), 7.28-7.24 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 143.0, 142.2, 140.8, 137.7, 137.6, 133.7, 133.4, 132.3, 131.5, 130.9, 130.5, 127.6, 127.1, 126.7, 126.2, 126.1, 124.5, 123.3, 121.0, 120.6, 120.1, 115.5, 111.5, 85.7, sp^2 and sp^3 carbons adjacent to D cannot be identified due to their

weak intensity and superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{12}D_6N_2$, 412.1841; Found 412.1842; Mp. 250-252 °C.

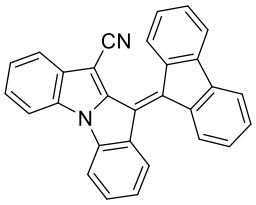
(*syn* and *anti*)-10-(9*H*-fluoren-9-ylidene-1,2,3,4-*d*$_4$)-8-methyl-10*H*-indolo[1,2-*a*]indole-11-carbonitrile (2f-*d*$_4$)



syn *anti*

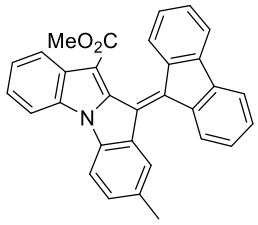
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **2f-*d*$_4$** as dark red solid (0.08 mmol, 33.5 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.8 Hz, 0.5H), 8.21 (s, 1H), 7.99 (d, *J* = 6.9 Hz, 0.5H), 7.84-7.81 (m, 2H), 7.72-7.69 (m, 1H), 7.60 (d, *J* = 8.2 Hz, 1H), 7.49-7.32 (m, 3.5H), 7.27-7.23 (m, 1.5H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 143.0, 142.3, 142.2, 140.8, 140.7, 137.8, 137.7, 137.6, 137.5, 133.7, 132.5, 131.6, 130.9, 130.8, 130.6, 127.6, 127.1, 126.8, 126.7(7), 126.7(5), 126.2, 126.1, 124.6, 123.3, 121.1, 120.6, 120.2, 115.5, 111.9, 111.5, 85.8, 21.6, sp^2 carbons adjacent to D cannot be identified due to their weak intensity and superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{14}D_4N_2$, 410.1712; Found 410.1712; Mp. 260-262 °C.

10-(9*H*-fluoren-9-ylidene)-10*H*-indolo[1,2-*a*]indole-11-carbonitrile (2g)



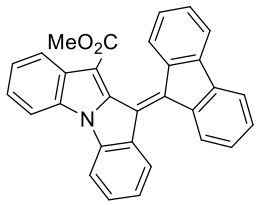
Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **2g** as dark red solid (0.09 mmol, 33.9 mg, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.2 Hz, 1H), 8.29 (d, *J* = 8.2 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 4.1 Hz, 1H), 7.84 (d, *J* = 3.2 Hz, 1H), 7.75-7.70 (m, 3H), 7.50-7.44 (m, 2H), 7.42-7.34 (m, 4H), 7.22-7.20 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 143.3, 142.4, 140.9, 139.7, 137.7, 137.6, 133.8, 132.4, 131.7, 131.0, 130.7, 130.1, 127.7, 127.2, 126.9, 126.5, 126.3, 124.3, 124.0, 123.5, 121.1, 120.6, 120.2, 115.4, 112.2, 111.6, 86.0, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{16}N_2$, 392.1308; Found 392.1308; Mp. 316-318 °C.

methyl 10-(9*H*-fluoren-9-ylidene)-8-methyl-10*H*-indolo[1,2-*a*]indole-11-carboxylate (2h)



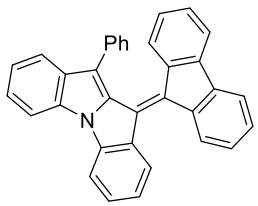
Purified by column chromatography (silica gel), [Hexane/DCM = 5:1 (v/v)] to give **2h** as dark red solid (0.17 mmol, 73.0 mg, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.8 Hz, 1H), 8.22 (d, *J* = 4.6 Hz, 2H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.43-7.35 (m, 2H), 7.32-7.29 (m, 3H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.10 (t, *J* = 7.8 Hz, 1H), 3.29 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 143.9, 141.9, 141.5, 140.0, 139.9, 137.9, 137.8, 133.0, 132.9, 132.4, 132.2, 130.5, 129.9, 127.5, 127.4, 126.9, 126.6, 126.0, 125.4, 123.2, 122.9(8), 122.9(5), 120.3, 119.9, 111.6, 111.0, 107.5, 50.7, 21.5, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{21}NO_2$, 439.1567; Found 439.1567; Mp. 226-228 °C.

methyl 10-(9*H*-fluoren-9-ylidene)-10*H*-indolo[1,2-*a*]indole-11-carboxylate (2i)



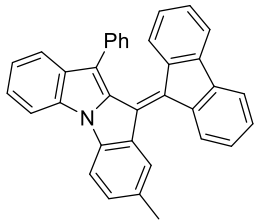
Purified by recrystallization ($CHCl_3$/hexane) to give **2i** as dark red solid (0.12 mmol, 49.8 mg, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 7.8 Hz, 1H), 8.30 (d, *J* = 7.3 Hz, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.72-7.62 (m 3H), 7.45-7.25 (m, 6H), 7.14-7.08 (m, 2H), 3.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 144.1, 141.9, 141.4, 140.1, 139.9, 139.8, 137.8, 132.8, 132.5, 132.3, 130.0, 129.7, 127.5, 127.0, 126.3, 125.7, 125.6, 123.5, 123.2, 123.1, 123.0, 120.4, 120.0, 112.0, 111.1, 107.7, 50.7, two sp^2 peaks are not shown due to superimposition.. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{19}NO_2$, 425.1410; Found 425.1410; Mp. 240-242 °C.

10-(9*H*-fluoren-9-ylidene)-11-phenyl-10*H*-indolo[1,2-*a*]indole (2j)



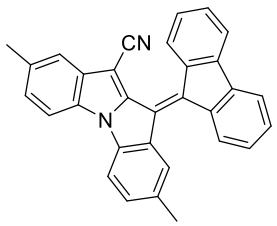
Purified by recrystallization ($CHCl_3$/hexane) to give **2j** as dark red solid (0.04 mmol, 19.1 mg, 43% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 7.8 Hz, 1H), 8.37 (d, *J* = 7.3 Hz, 1H), 7.84-7.80 (m, 2H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 6.4 Hz, 1H), 7.49 (d, *J* = 7.3 Hz, 1H), 7.45-7.40 (m, 2H), 7.32-718 (m,5H), 7.12-7.08 (m, 1H), 7.07-6.99 (m, 5H), 6.49 (t, *J* = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 140.4, 139.0, 138.0, 137.1, 136.7, 135.3, 134.9, 133.4, 133.3, 133.2, 129.9, 128.4, 128.3, 127.9, 127.5, 127.2, 126.9, 126.7, 126.6, 126.3, 126.1, 125.5, 124.9, 122.4, 121.8, 121.7, 120.1, 119.9, 118.7, 111.5, 111.0. HRMS [APCI_positive] m/z: [M] calc For $C_{34}H_{21}N$, 443.1669; Found 443.1669; Mp. 226-228 °C.

10-(9*H*-fluoren-9-ylidene)-8-methyl-11-phenyl-10*H*-indolo[1,2-*a*]indole (2k)



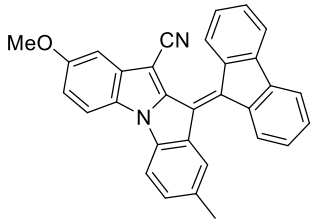
Purified by recrystallization ($CHCl_3$/hexane) to give **2k** as dark red solid (0.12 mmol, 54.5 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.3 Hz, 1H), 8.24 (s, 1H), 7.82 (d, *J* = 8.2 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.49 (d, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 7.1 Hz, 1H), 7.33-7.27 (m, 3H), 7.25-7.23 (m, 2H), 7.20-7.16 (m, 1H), 7.06-6.99 (m, 5H), 6.51-6.47 (m, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 139.0, 138.5, 138.0, 137.1, 136.9, 135.0(4), 135.0(0), 133.4, 133.3, 133.0, 131.9, 130.7, 128.4, 128.3, 127.8, 127.5, 127.2, 127.0(7), 127.0(5), 126.5, 126.3, 126.0, 125.4, 124.8, 121.7, 121.6, 120.1, 119.7, 118.7, 111.2, 110.9, 21.6. HRMS [APCI_positive] m/z: [M] calc For $C_{35}H_{23}N$, 457.1825; Found 457.1825; Mp. 231-233 °C.

10-(9*H*-fluoren-9-ylidene)-2,8-dimethyl-10*H*-indolo[1,2-*a*]indole-11-carbonitrile (2l)



Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **2l** as dark red solid (0.94 mmol, 39.5 mg, 94% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 7.8 Hz, 1H), 8.18 (s, 1H), 7.99 (d, *J* = 7.3 Hz, 1H), 7.71-7.66 (m, 3H), 7.61 (s, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.43-7.35 (m, 3H), 7.28-7.22 (m, 3H), 2.51 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 142.7, 142.3, 140.8, 137.9, 137.8, 137.7, 134.1, 133.6, 133.2, 132.5, 130.8, 130.5, 130.0, 127.8, 127.6, 127.1, 126.8, 126.2, 124.8, 120.8, 120.6, 120.2, 115.6, 111.7, 111.2, 85.4, 21.6, 21.6, two sp^2 peaks are not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{20}N_2$, 420.1621; Found 420.1621; Mp. 304-306 °C.

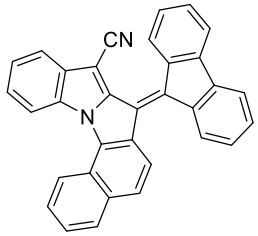
10-(9*H*-fluoren-9-ylidene)-2-methoxy-8-methyl-10*H*-indolo[1,2-*a*]indole-11-carbonitrile (2m)



Purified by column chromatography (silica gel), [Hexane/DCM = 1:1 (v/v)] to give **2m** as dark red solid (0.87 mmol, 38.2 mg, 87% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 7.8 Hz, 1H), 8.19 (s, 1H), 8.00 (d, *J* = 7.3 Hz, 1H), 7.72-7.68 (m, 3H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.41-7.36 (m, 3H), 7.28-7.22 (m, 3H), 7.08 (dd, *J* = 8.4, 2.0 Hz, 1H), 3.92 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 143.9, 142.7, 142.3, 140.8, 137.9, 137.8, 137.7, 134.9, 133.6, 132.5, 130.9, 130.8, 130.5, 127.6, 127.1, 126.9, 126.8, 126.7, 126.2, 124.9, 120.6,

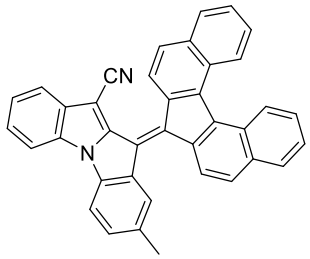
120.2, 116.9, 115.8, 112.4, 111.5, 101.9, 85.4, 56.0, 21.6. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{20}N_2O$, 436.1570; Found 436.1570; Mp. 323-325 °C.

7-(9*H*-fluoren-9-ylidene)-7*H*-benzo[*g*]indolo[1,2-*a*]indole-8-carbonitrile (2n)



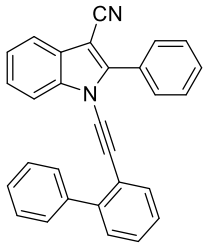
Purified by column chromatography (silica gel), [Hexane/DCM = 3:1 (v/v)] to give **2n** as dark red solid (0.32 mmol, 14.2 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 8.7 Hz, 1H), 8.38 (dd, *J* = 8.8, 3.2 Hz, 1H), 8.31 (d, *J* = 7.8 Hz, 1H), 8.25 (d, *J* = 7.8 Hz, 1H), 8.06 (d, *J* = 7.3 Hz, 1H), 7.93 (d, *J* = 8.7 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.73-7.58 (m, 5H), 7.51-7.47 (m, 1H), 7.44-7.29 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 142.3, 141.8, 140.8, 138.1, 137.9, 137.5, 135.6, 134.4, 133.7, 131.7, 130.8, 130.6, 129.3, 127.6, 127.3, 127.1, 127.0, 126.5, 126.4, 126.2, 125.4, 125.3, 124.4, 123.5, 122.8, 122.6, 121.3, 120.7, 120.3, 115.2, 113.8, 87.8. HRMS [APCI_positive] m/z: [M] calc For $C_{33}H_{18}N_2$, 442.1465; Found 442.1464; Mp. 288-290 °C.

10-(7*H*-dibenzo[*c*,*g*]fluoren-7-ylidene)-8-methyl-10*H*-indolo[1,2-*a*]indole-11-carbonitrile (2o)



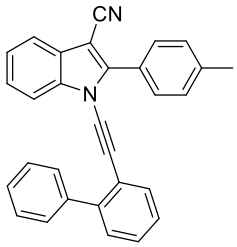
Purified by recrystallization ($CHCl_3$/hexane) to give **2o** as dark red solid (0.12 mmol, 58.5 mg, 57% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.3 Hz, 2H), 8.39 (d, *J* = 8.7 Hz, 1H), 8.27 (s, 1H), 8.13 (d, *J* = 8.2 Hz, 1H), 7.90-7.81 (m, 5H), 7.71 (d, *J* = 8.7 Hz, 1H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.57-7.47 (m, 5H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 143.8, 142.0, 140.7, 138.6, 138.0, 137.8, 136.6, 136.2, 133.8, 133.7, 132.4, 131.8, 131.1, 129.1(7), 129.1(0), 129.0, 128.9, 128.2, 127.9, 127.8, 127.7, 127.4, 126.8, 126.5, 126.4, 125.8, 125.7, 125.6, 123.4(4), 123.4(0), 122.9, 121.2, 115.7, 111.8, 111.6, 87.0, 21.5. HRMS [APCI_positive] m/z: [M] calc For $C_{38}H_{22}N_2$, 506.1778; Found 506.1778; Mp. 229-231 °C.

1-(biphenyl-2-ylethynyl)-2-phenyl-1*H*-indole-3-carbonitrile (3a)



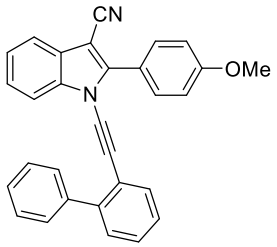
Purified by column chromatography (silica gel), [Hexane/DCM = 2:1 (v/v)] to give **3a** as white solid (0.71 mmol, 280.1 mg, 71 % yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 2H), 7.72 (d, *J* = 7.2 Hz, 1H), 7.54-7.49 (m, 6H), 7.45-7.31 (m, 8H), 7.18 (d, *J* = 7.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.5, 143.9, 140.7, 137.9, 132.6, 130.7, 129.8, 129.4, 129.3, 129.0, 128.4, 127.9, 127.6, 127.4, 126.9, 125.5, 124.4, 120.2, 119.8, 115.5, 112.4, 88.4, 80.6, 75.0, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{18}N_2$, 394.1465; Found 394.1465; Mp. 165-167 °C.

1-(biphenyl-2-ylethynyl)-2-(*p*-tolyl)-1*H*-indole-3-carbonitrile (3b)



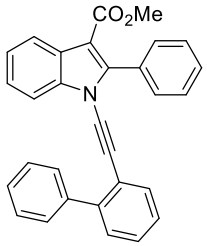
Purified by column chromatography (silica gel), [Hexane/DCM = 2:1 (v/v)] to give **3b** as white solid (0.46 mmol, 178.9 mg, 97% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.70 (m, 3H), 7.56-7.52 (m, 3H), 7.44-7.29 (m, 10H), 7.16 (d, *J* = 7.8 Hz, 1H), 2.47 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 143.9, 141.0, 140.6, 137.8, 132.6, 129.8, 129.6, 129.2, 128.9, 128.4, 127.8, 127.4, 126.9, 125.3, 124.7, 124.3, 120.3, 119.7, 115.6, 112.3, 87.9, 80.7, 74.9, 21.7, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{20}N_2$, 408.1621; Found 408.1622; Mp. 150-152 °C.

1-(biphenyl-2-ylethynyl)-2-(4-methoxyphenyl)-1*H*-indole-3-carbonitrile (3c)



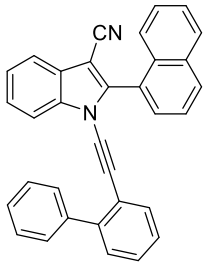
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **3c** as white solid (0.45 mmol, 191.0 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dt, *J* = 8.8, 2.5 Hz, 2H), 7.70 (dd, *J* = 7.0, 0.9 Hz, 1H), 7.56-7.52 (m, 3H), 7.45-7.29 (m, 8H), 7.18-7.17 (m, 1H), 7.00 (dt, *J* = 7.2, 2.4 Hz, 2H), 3.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 147.6, 143.8, 140.7, 137.7, 132.6, 130.9, 129.8, 129.3, 128.9, 128.4, 127.8, 127.4, 126.9, 125.2, 124.3, 120.3, 119.9, 119.6, 115.8, 114.4, 112.3, 87.4, 80.8, 74.9, 55.6. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{20}N_2O$, 424.1570; Found 424.1571; Mp. 144-146 °C.

methyl 1-(biphenyl-2-ylethynyl)-2-phenyl-1*H*-indole-3-carboxylate (3d)



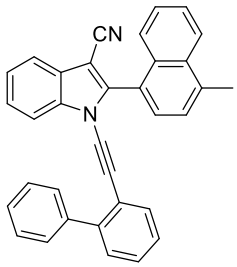
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **3d** as colorless oil (0.77 mmol, 329.2 mg, 99% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.8 Hz, 1H), 7.60-7.57 (m, 2H), 7.51-7.45 (m, 5H), 7.42-7.40 (m, 3H), 7.37-7.35 (m, 2H), 7.33-7.24 (m, 4H), 7.14 (d, *J* = 7.8 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 146.5, 143.5, 140.7, 137.8, 132.5, 130.9, 129.8, 129.7, 129.6, 129.2, 128.5, 128.4, 127.8, 127.7, 127.2, 126.2, 124.4, 124.0, 122.3, 120.7, 111.8, 107.6, 81.2, 75.0, 51.3. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{21}NO_2$, 427.1567; Found 427.1567.

1-(biphenyl-2-ylethynyl)-2-(naphthalen-1-yl)-1*H*-indole-3-carbonitrile (3e)



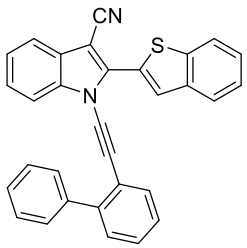
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **3e** as yellow solid (0.68 mmol, 302.3 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.2 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.78 (t, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 6.4 Hz, 1H), 7.63-7.52 (m, 3H), 7.43-7.27 (m, 9H), 7.20 (d, *J* = 7.3 Hz, 1H), 7.16-7.12 (m, 1H), 6.81 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.2, 143.3, 140.3, 137.5, 133.6, 132.3, 131.4, 130.0, 129.4, 129.0, 128.6(4), 128.6(2), 128.2, 127.6, 127.3, 127.0, 126.6, 126.5, 125.5, 125.4, 125.1, 124.4, 119.8, 119.7, 114.8, 112.3, 90.8, 80.4, 75.5, two sp^2 peaks are not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{33}H_{20}N_2$, 444.1621; Found 444.1621; Mp. 151-153 °C.

1-(biphenyl-2-ylethynyl)-2-(4-methylnaphthalen-1-yl)-1*H*-indole-3-carbonitrile (3f)



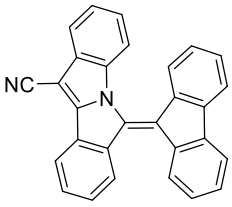
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **3f** as yellow solid (0.50 mmol, 229.3 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.7 Hz, 1H), 7.78 (d, *J* = 7.8 Hz, 2H), 7.64-7.60 (m, 2H), 7.55-7.51 (m, 1H), 7.46-7.13 (m, 12H), 6.84 (d, *J* = 7.3 Hz, 1H), 2.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 143.5, 140.5, 138.3, 137.5, 132.9, 132.4, 131.5, 129.8, 129.5, 129.1, 128.7, 128.2, 127.6, 127.1, 126.9, 126.6, 126.5, 126.2, 126.1, 125.4, 124.8, 124.3, 123.5, 120.0, 119.8, 115.0, 112.4, 90.8, 80.6, 75.4, 20.0. HRMS [APCI_positive] m/z: [M] calc For $C_{34}H_{22}N_2$, 458.1778; Found 458.1778; Mp. 181-183 °C.

1-(biphenyl-2-ylethynyl)-2-(benzo[*b*]thiophen-2-yl)-1*H*-indole-3-carbonitrile (3g)



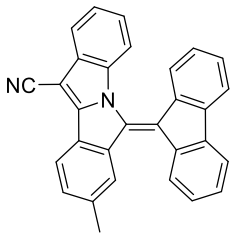
Purified by column chromatography (silica gel), [Hexane/AcOEt = 30:1 (v/v)] to give **3g** as yellow solid (0.18 mmol, 81.1 mg, 30% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.91-7.87 (m, 2H), 7.71 (t, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 6.4 Hz, 2H), 7.47-7.31 (m, 10H), 7.12 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 140.9, 140.6, 139.0, 138.0, 132.4, 129.9, 129.3, 129.1, 128.4, 127.8, 127.5, 127.1, 126.9, 126.2, 125.9, 125.1, 124.9, 124.7, 122.4, 120.2, 119.8, 115.4, 112.3, 88.5, 80.6, 76.7, two sp^2 peaks are not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{18}N_2S$, 450.1185; Found 450.1185; Mp. 177-179 °C.

6-(9*H*-fluoren-9-ylidene)-6*H*-isoindolo[2,1-*a*]indole-11-carbonitrile (4a)



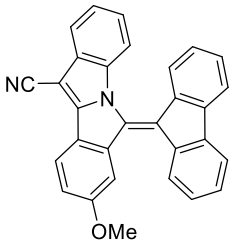
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **4a** as orange solid (0.17 mmol, 66.7 mg, 86% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.2 Hz, 1H), 8.23 (d, *J* = 7.8 Hz, 1H), 8.06 (d, *J* = 7.3 Hz, 1H), 7.85-7.77 (m, 3H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.44-7.30 (m, 6H), 7.24-7.13 (m, 2H), 7.04 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 140.9, 139.7, 139.6, 137.5, 136.8, 135.1, 133.0, 132.9, 130.6, 129.9, 128.9, 127.2, 127.0, 126.1, 125.8, 125.5, 125.4, 125.1, 124.1, 122.7, 121.2, 120.7, 120.3, 116.6, 115.2, 82.6, two sp^2 peaks are not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{29}H_{16}N_2$, 392.1308; Found 392.1308; Mp. 221-223 °C.

6-(9*H*-fluoren-9-ylidene)-8-methyl-6*H*-isoindolo[2,1-a]indole-11-carbonitrile (4b)



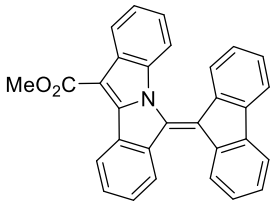
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **4b** as orange solid (0.08 mmol, 33.4 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.93 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 7.3 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.44-7.24 (m, 6H), 7.18-7.12 (m, 2H), 7.00 (d, *J* = 8.2 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 140.9, 140.5, 140.0, 139.6, 137.5, 136.9, 135.3, 133.0, 132.9, 131.8, 128.8, 127.2, 126.9, 126.5, 126.0, 125.8, 125.6, 125.3, 124.7, 124.0, 122.4, 121.0, 120.6, 120.2, 116.5, 115.3, 82.0, 22.3, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{18}N_2$, 406.1465; Found 406.1465; Mp. 293-295 °C.

6-(9*H*-fluoren-9-ylidene)-8-methoxy-6*H*-isoindolo[2,1-*a*]indole-11-carbonitrile (4c)



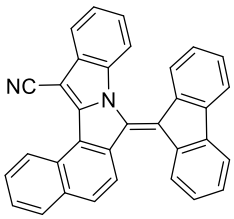
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **4c** as orange solid (0.08 mmol, 34.2 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 7.6 Hz, 1H), 8.02 (d, *J* = 2.0 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.42-7.23 (m, 6H), 7.15 (t, *J* = 7.8 Hz, 2H), 7.05 (dd, *J* = 8.7, 2.3 Hz, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 149.2, 141.4, 140.9, 139.6, 137.4, 136.8, 135.3, 133.1, 132.9, 128.9, 128.8, 127.2, 126.9, 125.8, 125.7, 125.1, 124.9, 123.9, 123.7, 122.2, 120.9, 120.7, 120.2, 117.6, 116.3, 115.4, 110.0, 81.4, 55.9. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{18}N_2O$, 422.1414; Found 422.1414; Mp. 281-283 °C.

methyl 6-(9*H*-fluoren-9-ylidene)-6H-isoindolo[2,1-*a*]indole-11-carboxylate (4d)



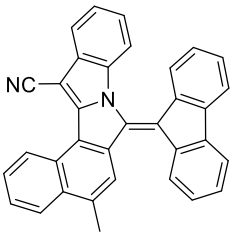
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **4d** as orange solid (0.09 mmol, 37.4 mg, 88% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 7.8 Hz, 1H), 8.49 (d, *J* = 8.2 Hz, 1H), 8.26 (t, *J* = 7.1 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.41-7.22 (m, 6H), 7.13 (t, *J* = 7.1 Hz, 2H), 7.01 (d, *J* = 8.2 Hz, 1H), 4.10 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 147.6, 140.7, 140.3, 139.3, 137.8, 137.1, 136.0, 133.2, 132.3, 130.4(4), 130.4(2), 129.4, 128.3(4), 128.3(0), 127.1, 126.8, 126.1, 126.0, 125.6, 125.0, 124.8, 123.8, 123.7, 123.5, 120.5, 120.1, 116.0, 105.5, 51.6. HRMS [APCI_positive] m/z: [M] calc For $C_{30}H_{19}NO_2$, 425.1410; Found 425.1410; Mp. 221-223 °C.

7-(9*H*-fluoren-9-ylidene)-7*H*-benzo[6,7]isoindolo[2,1-*a*]indole-13-carbonitrile (4e)



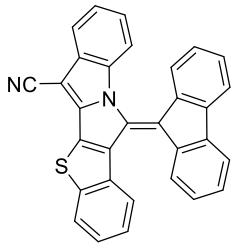
Purified by recrystallization ($CHCl_3$/hexane) to give **4e** as dark red solid (0.05 mmol, 20.1 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (d, *J* = 8.7 Hz, 1H), 8.43 (d, *J* = 8.7 Hz, 1H), 8.22 (d, *J* = 7.3 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 1H), 7.86-7.78 (m, 5H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.3 Hz, 1H), 7.39-7.31 (m, 4H), 7.23-7.14 (m, 2H), 7.07 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 147.6, 141.0, 139.8, 138.7, 137.5, 137.2, 135.8, 134.6, 134.2, 132.6, 130.7, 129.1, 129.0, 128.6, 128.0, 127.9, 127.4, 127.1, 126.9, 126.5, 126.4, 126.2, 125.7, 125.6, 124.1, 122.2, 121.4, 120.8, 120.4, 117.2, 116.2, 85.0, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{33}H_{18}N_2$, 442.1465; Found 442.1465; Mp. Over 350°C

7-(9*H*-fluoren-9-ylidene)-5-methyl-7*H*-benzo[6,7]isoindolo[2,1-*a*]indole-13-carbonitrile (4f)



Purified by recrystallization ($CHCl_3$/hexane) to give **4f** as dark red solid (0.04 mmol, 16.5 mg, 36% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.14 (d, *J* = 8.2 Hz, 1H), 8.31 (s, 1H), 8.25 (d, *J* = 7.3 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.86-7.78 (m, 4H), 7.67 (t, *J* = 7.1 Hz, 1H), 7.44 (t, *J* = 6.9 Hz, 1H), 7.39-7.29 (m, 4H), 7.21-7.13 (m, 2H), 7.04 (d, *J* = 8.2 Hz, 1H), 2.69 (s, 3H). ^{13}C NMR (176 MHz, $CDCl_3$) δ 148.0, 141.0, 139.7, 138.5, 137.7, 137.6, 137.2, 136.0, 134.3, 134.0, 132.6, 129.0(4), 129.0(1), 128.3, 128.0, 127.4, 127.0, 126.9, 126.4, 126.0, 125.7(2), 125.7(0), 125.4, 125.3, 124.0, 122.6, 121.3, 120.7, 120.3, 117.3, 116.1, 84.6, 20.7, one sp^2 peak is not shown due to superimposition. HRMS [APCI_positive] m/z: [M] calc For $C_{34}H_{20}N_2$, 456.1621; Found 456.1621; Mp. Over 350°C.

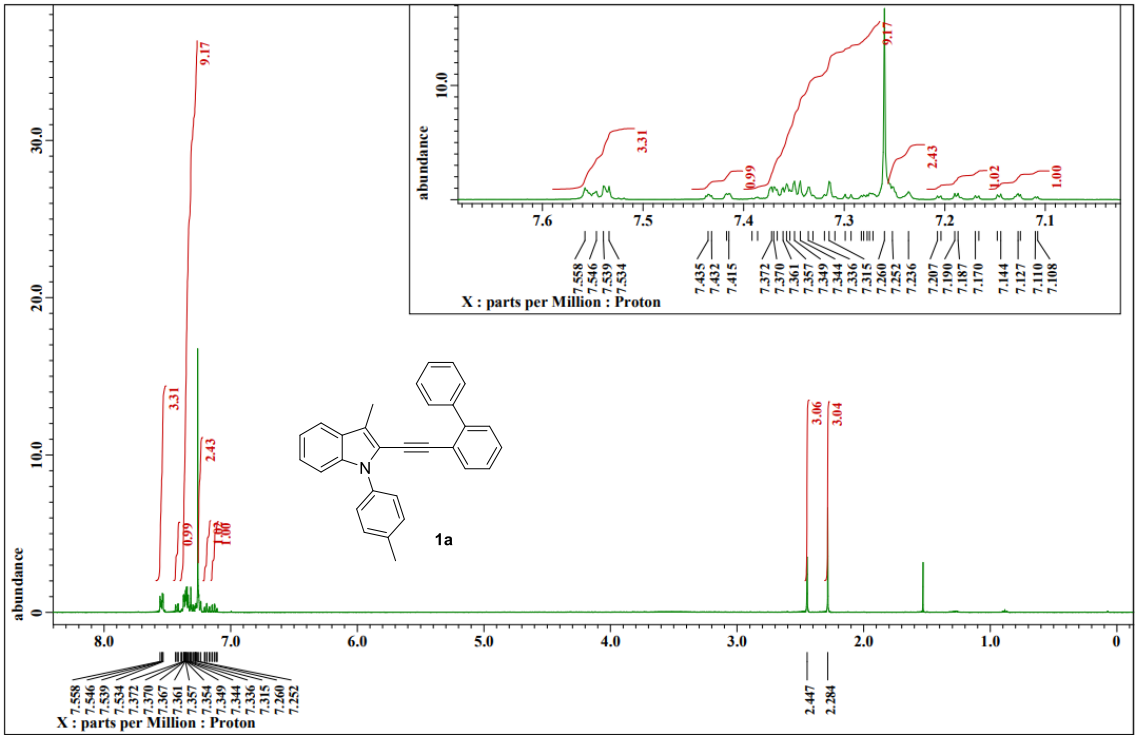
12-(9*H*-fluoren-9-ylidene)-12*H*-benzo[4',5']thieno[2',3':3,4]pyrrolo[1,2-*a*]indole-6-carbonitrile (4g)



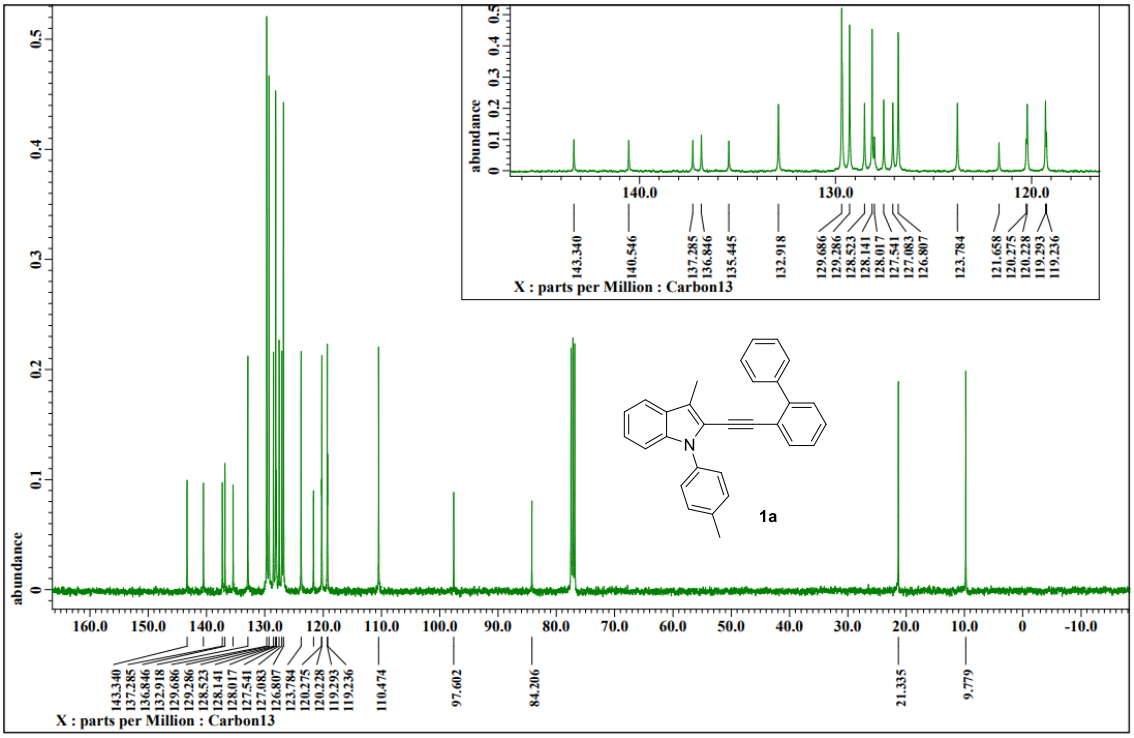
Purified by column chromatography (silica gel), [Hexane/AcOEt = 10:1 (v/v)] to give **4g** as dark red solid (0.08 mmol, 33.6 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 7.8 Hz, 2H), 7.70 (t, *J* = 8.5 Hz, 3H), 7.48-7.37 (m, 4H), 7.28-7.19 (m, 4H), 7.15 (t, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 144.6, 140.6, 140.4, 140.2, 138.2, 137.7, 135.1, 134.0, 132.9, 131.9, 131.6, 129.2, 129.0, 127.8, 127.3, 126.8, 126.5, 126.2, 126.0, 125.7, 125.6, 124.5, 124.1, 124.0, 121.6, 120.6, 120.5, 115.9, 114.8, 83.7. HRMS [APCI_positive] m/z: [M] calc For $C_{31}H_{16}N_2S$, 448.1029; Found 448.1028; Mp. 329-331 °C.

10. ^{1}H and ^{13}C NMR spectra of starting substrates and products

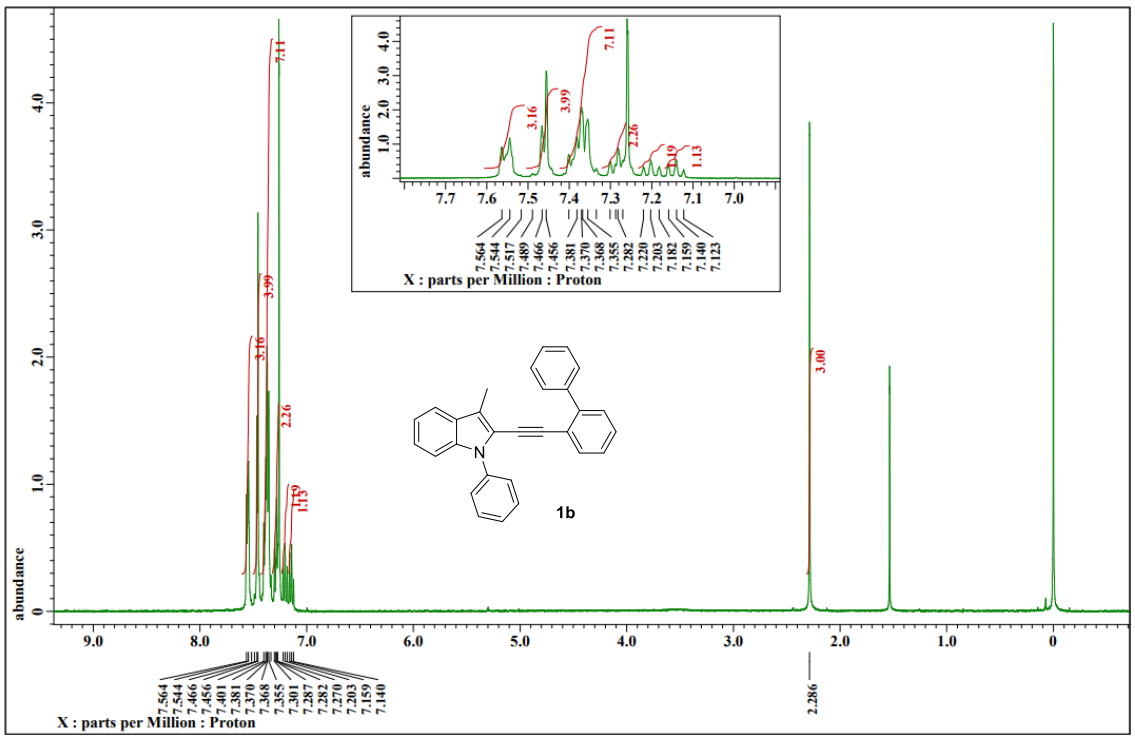
^{1}H NMR (400 MHz, $CDCl_3$)



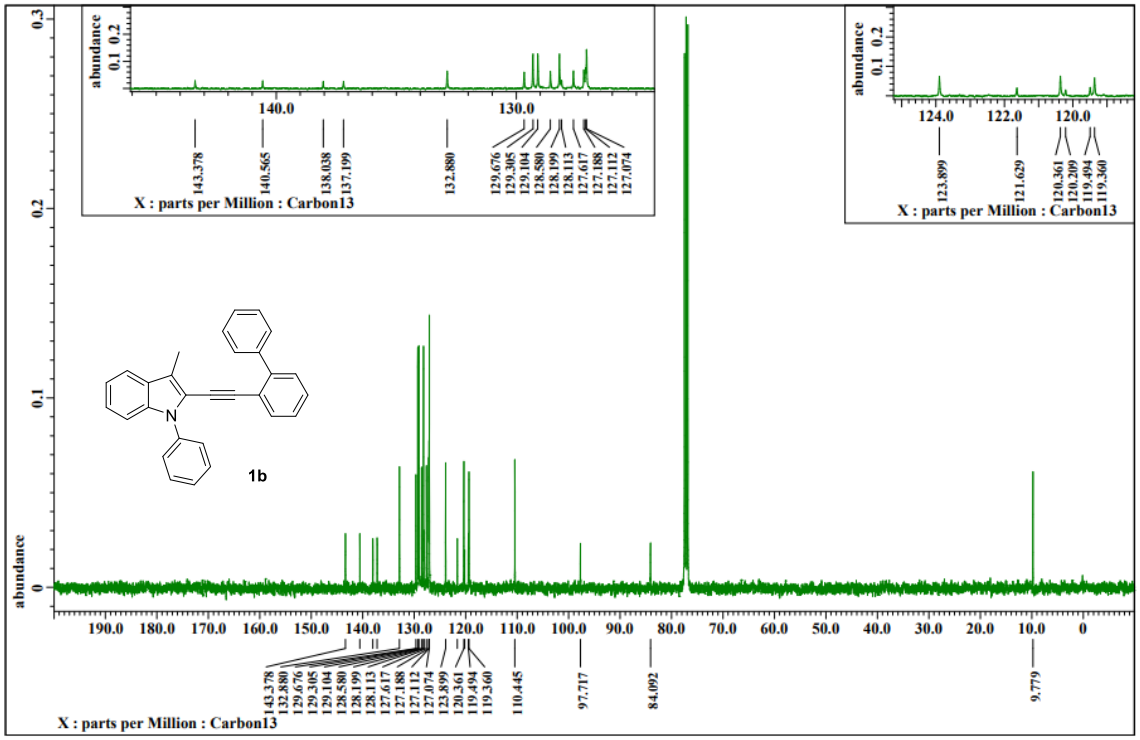
^{13}C NMR (100 MHz, $CDCl_3$)



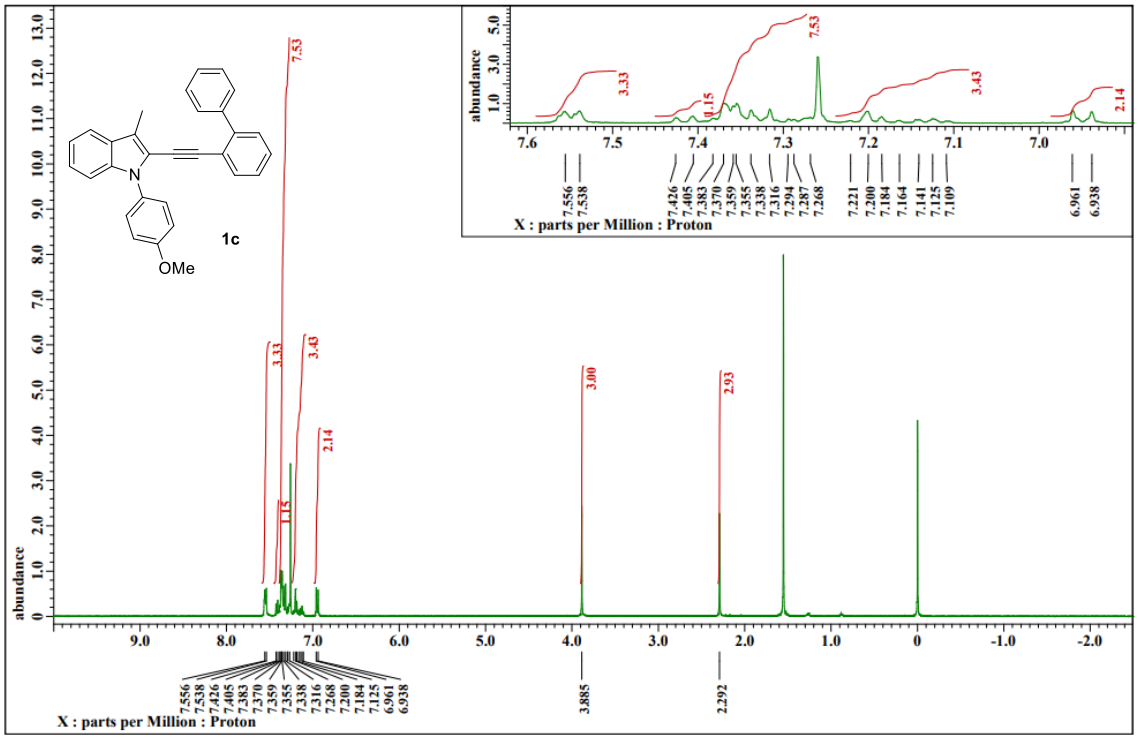
^{1}H NMR (400 MHz, $CDCl_3$)



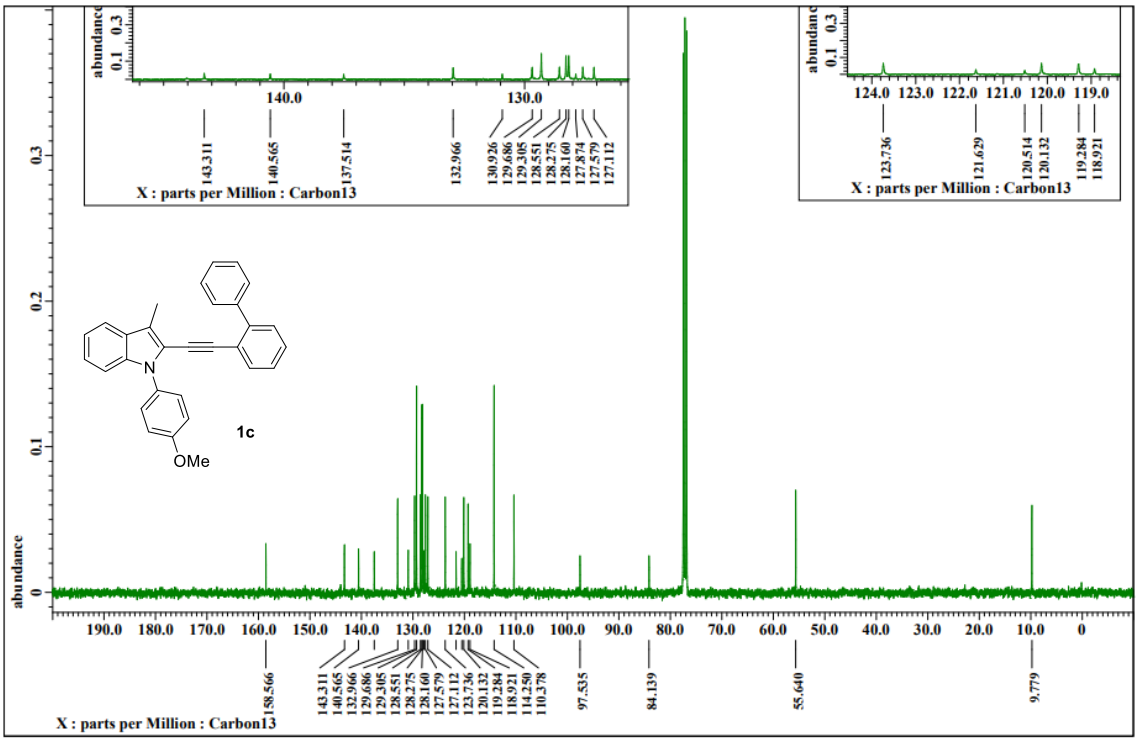
^{13}C NMR (100 MHz, $CDCl_3$)



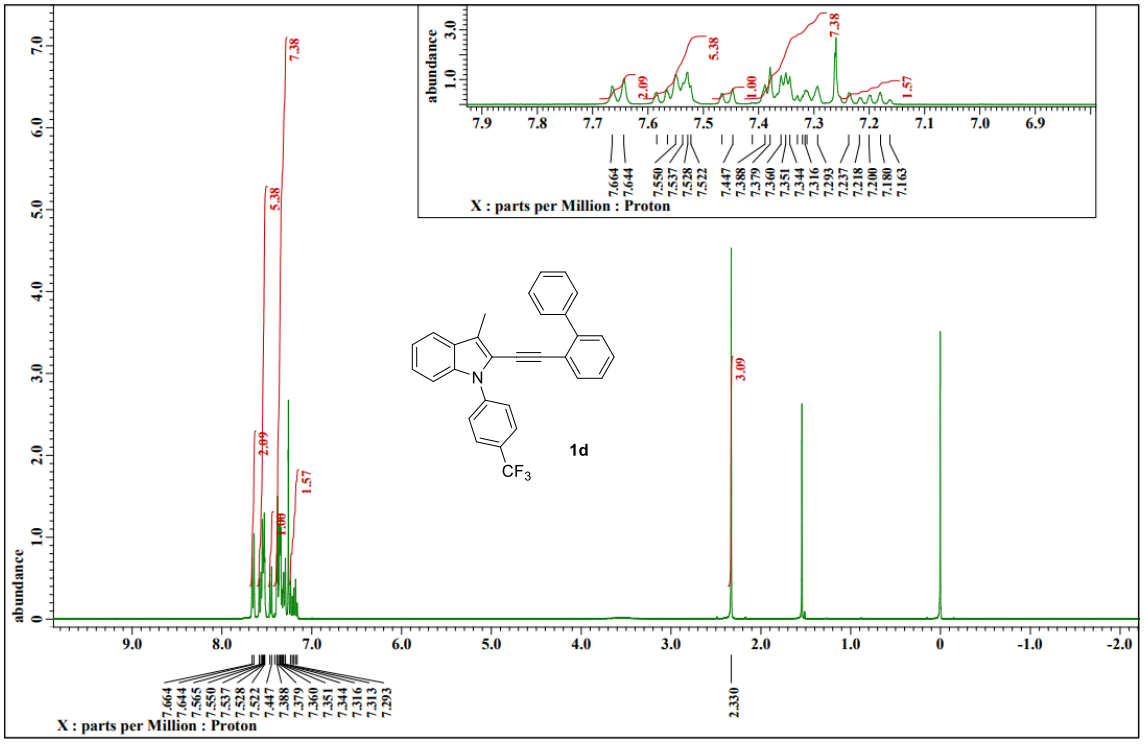
^{1}H NMR (400 MHz, $CDCl_3$)



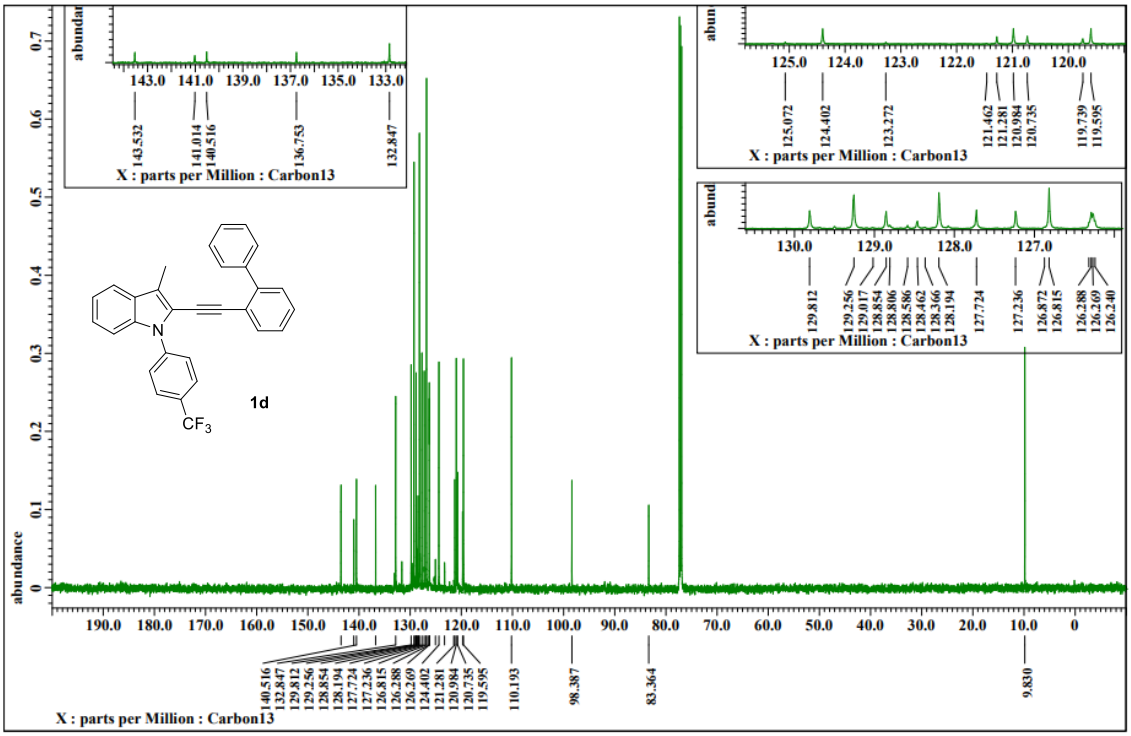
^{13}C NMR (100 MHz, $CDCl_3$)



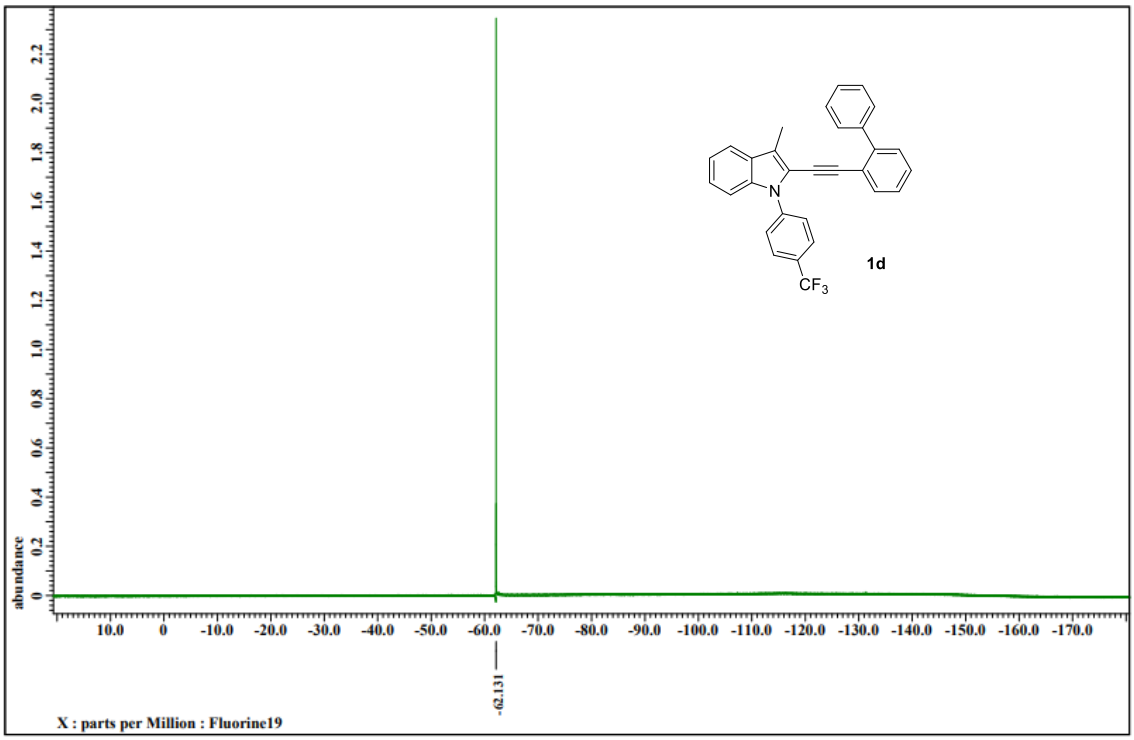
^{1}H NMR (400 MHz, $CDCl_3$)



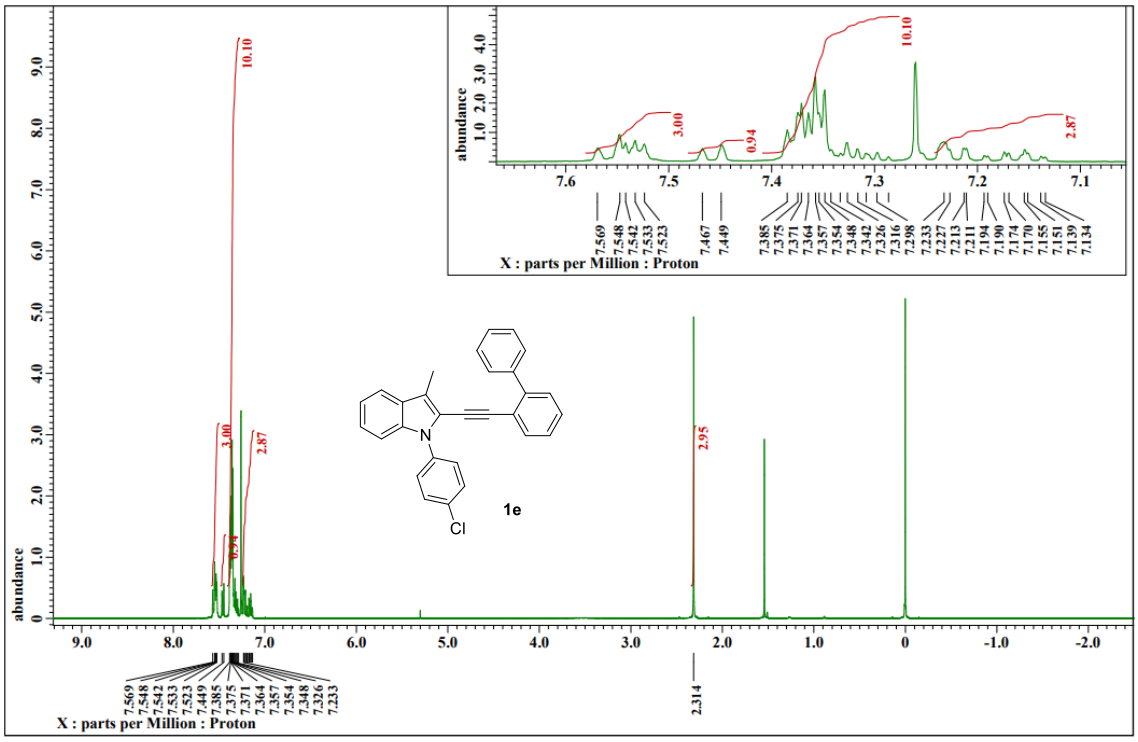
^{13}C NMR (150 MHz, $CDCl_3$)



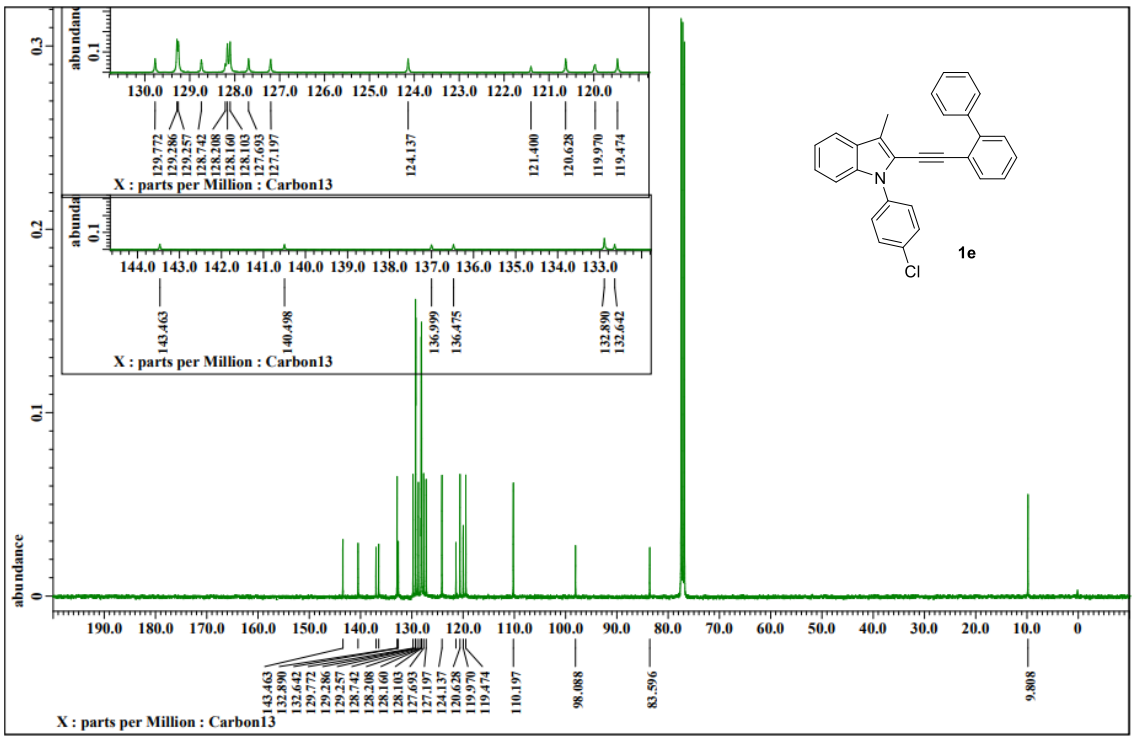
^{19}F NMR (376 MHz, $CDCl_3$)



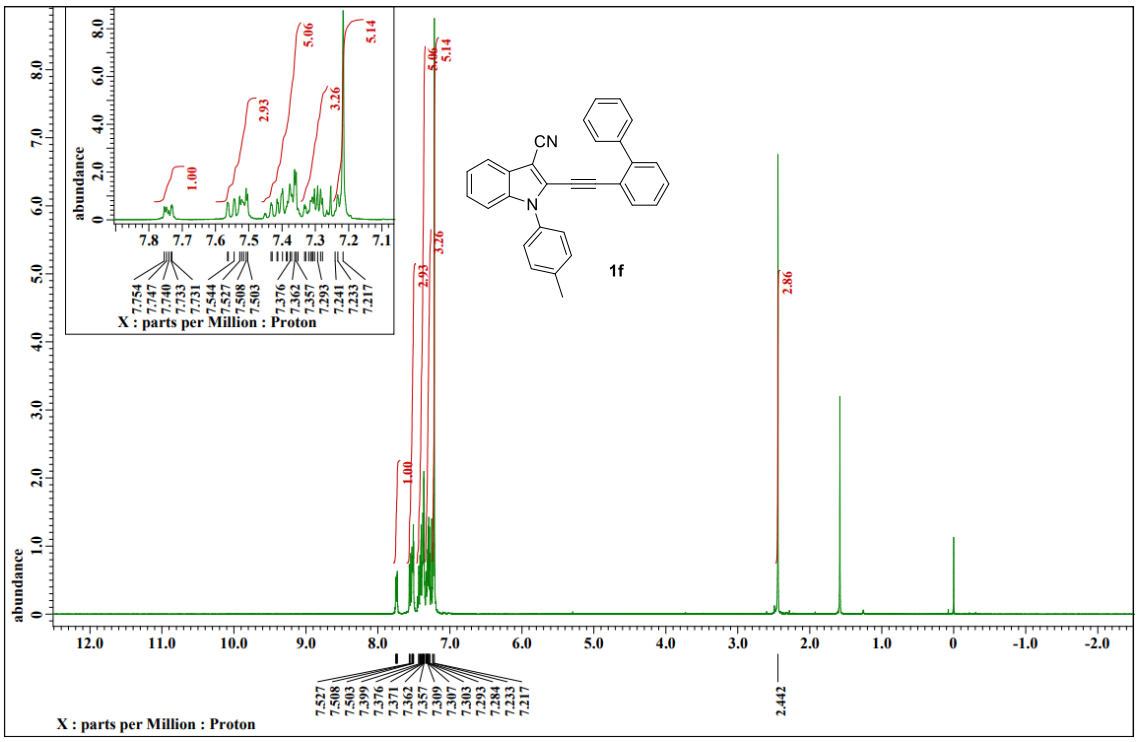
^{1}H NMR (400 MHz, $CDCl_3$)



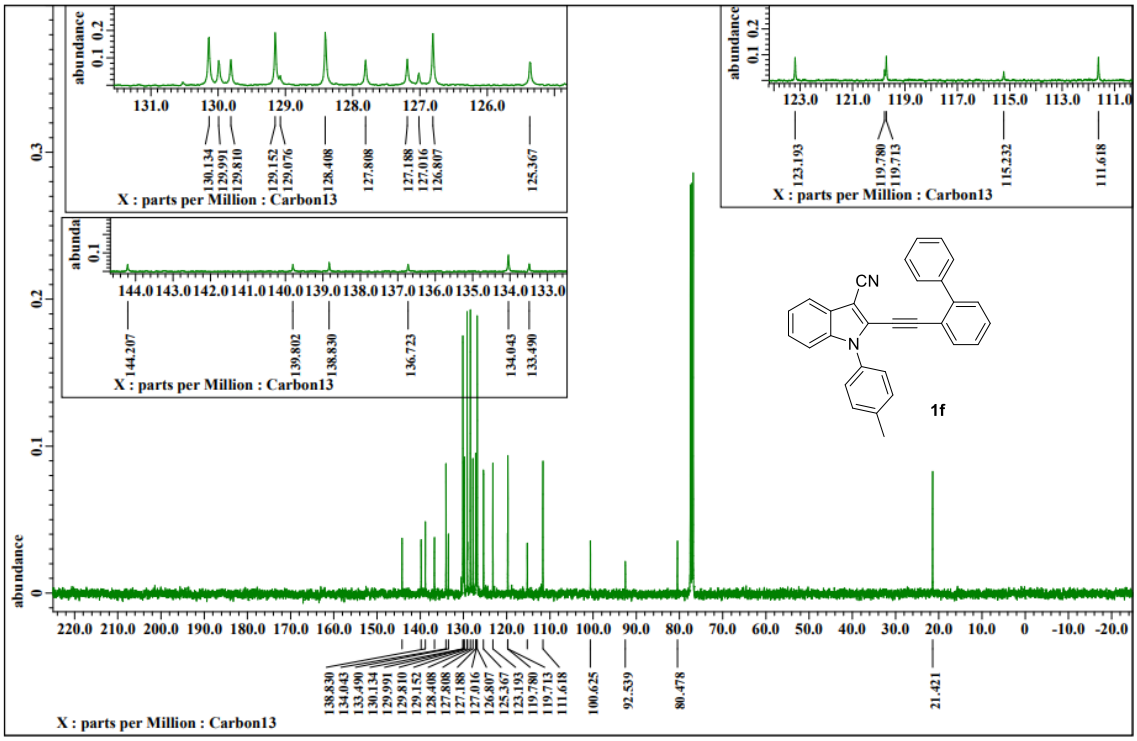
^{13}C NMR (100 MHz, $CDCl_3$)



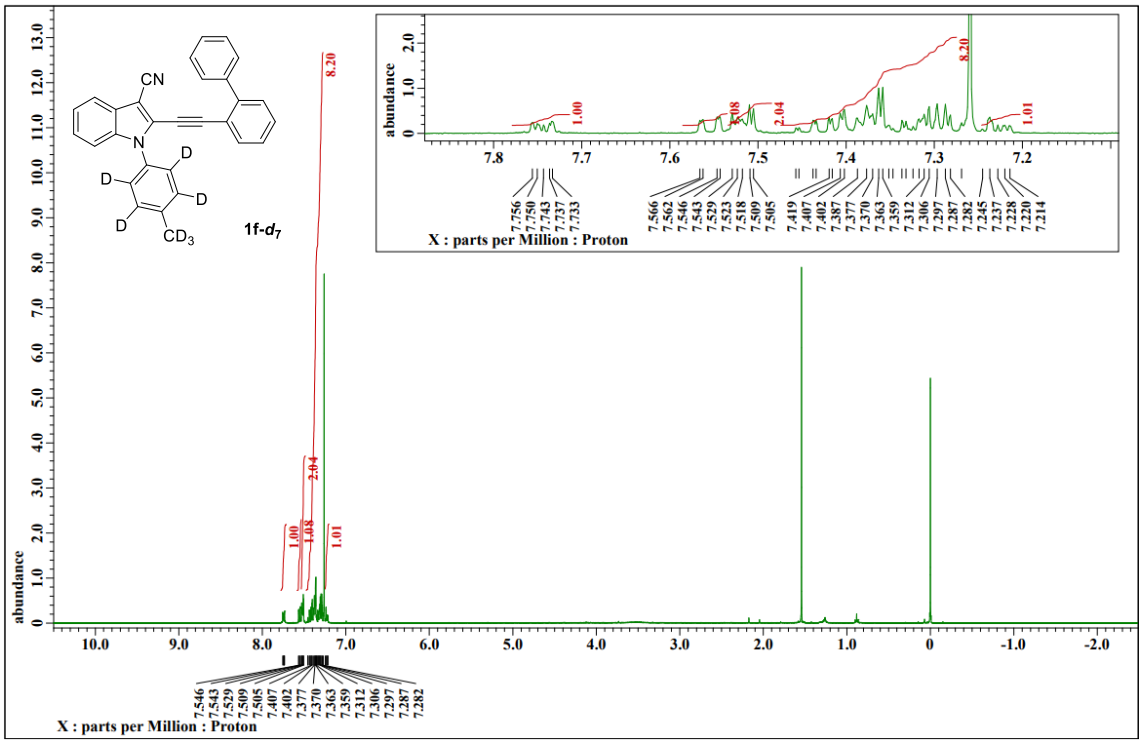
^{1}H NMR (400 MHz, $CDCl_3$)



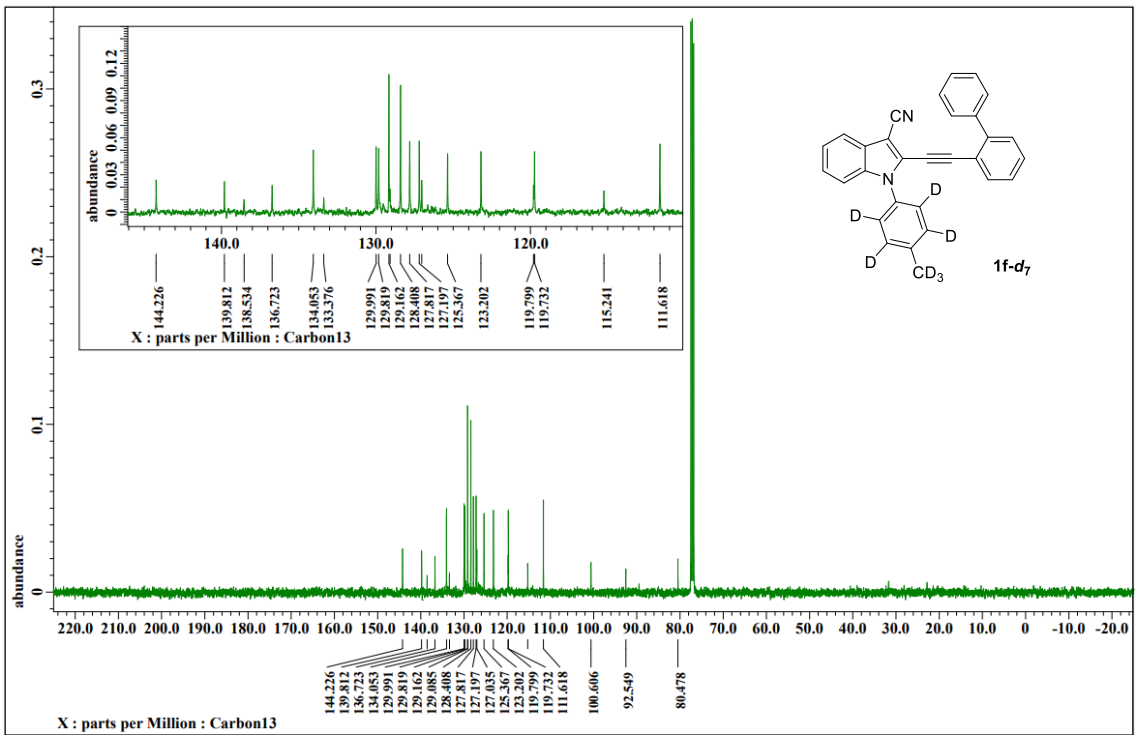
^{13}C NMR (100 MHz, $CDCl_3$)



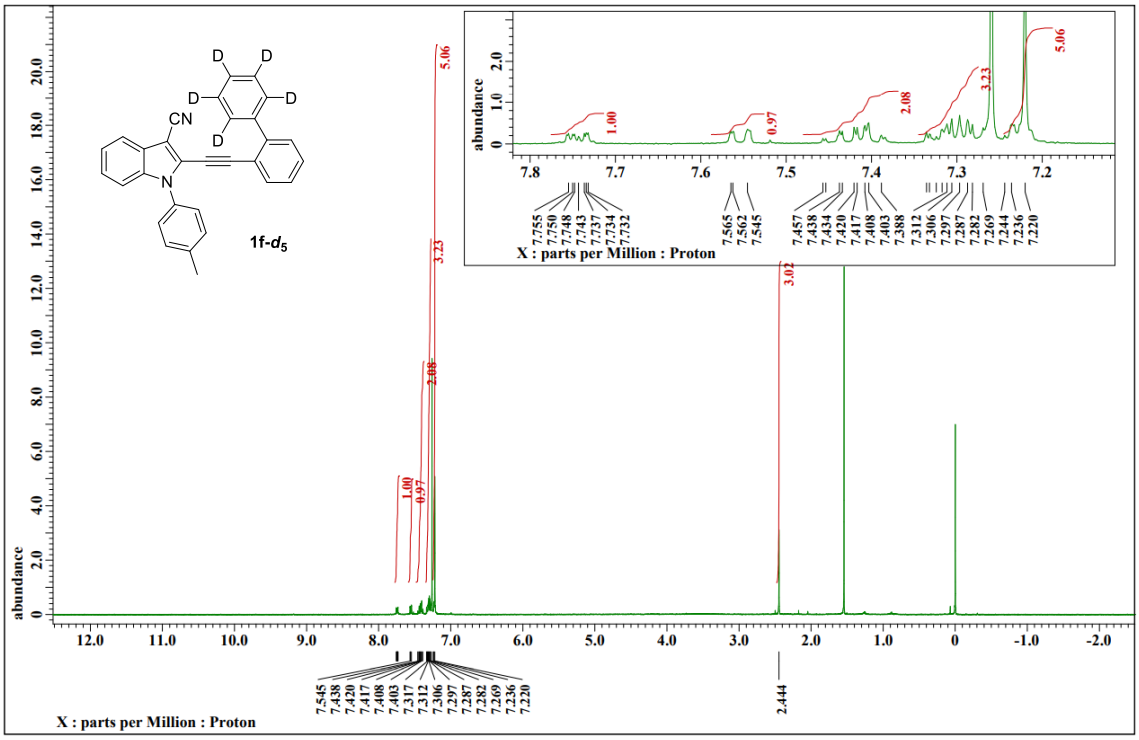
^{1}H NMR (400 MHz, $CDCl_3$)



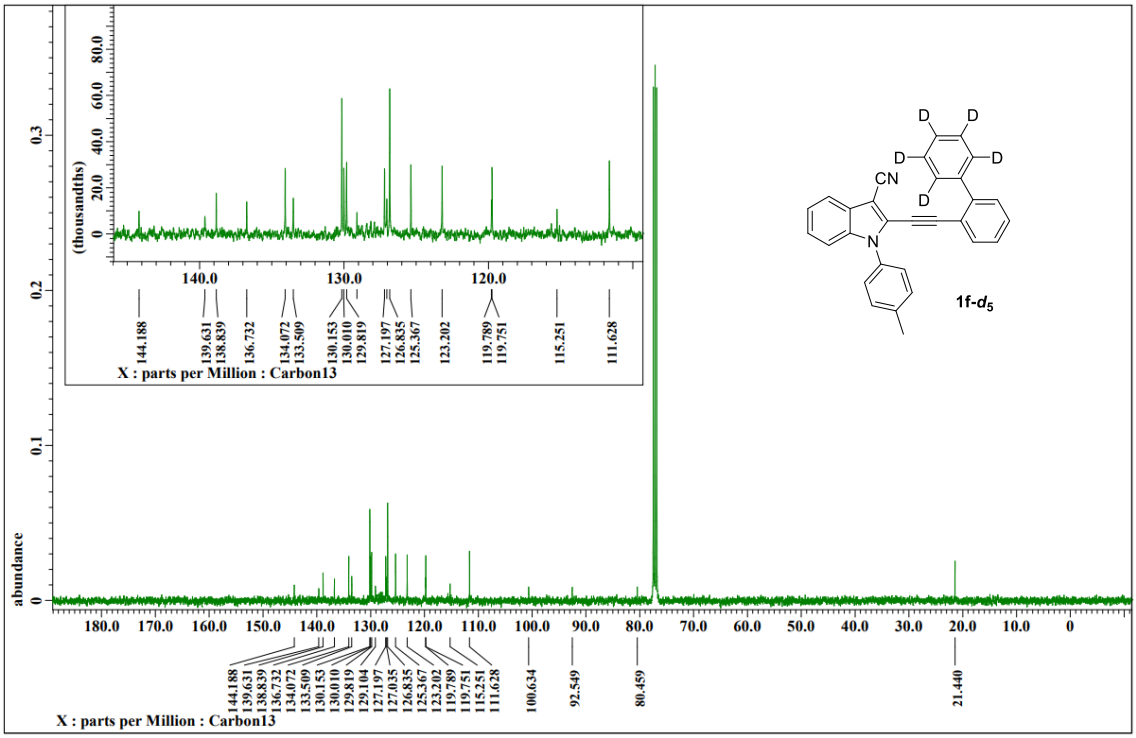
^{13}C NMR (100 MHz, $CDCl_3$)



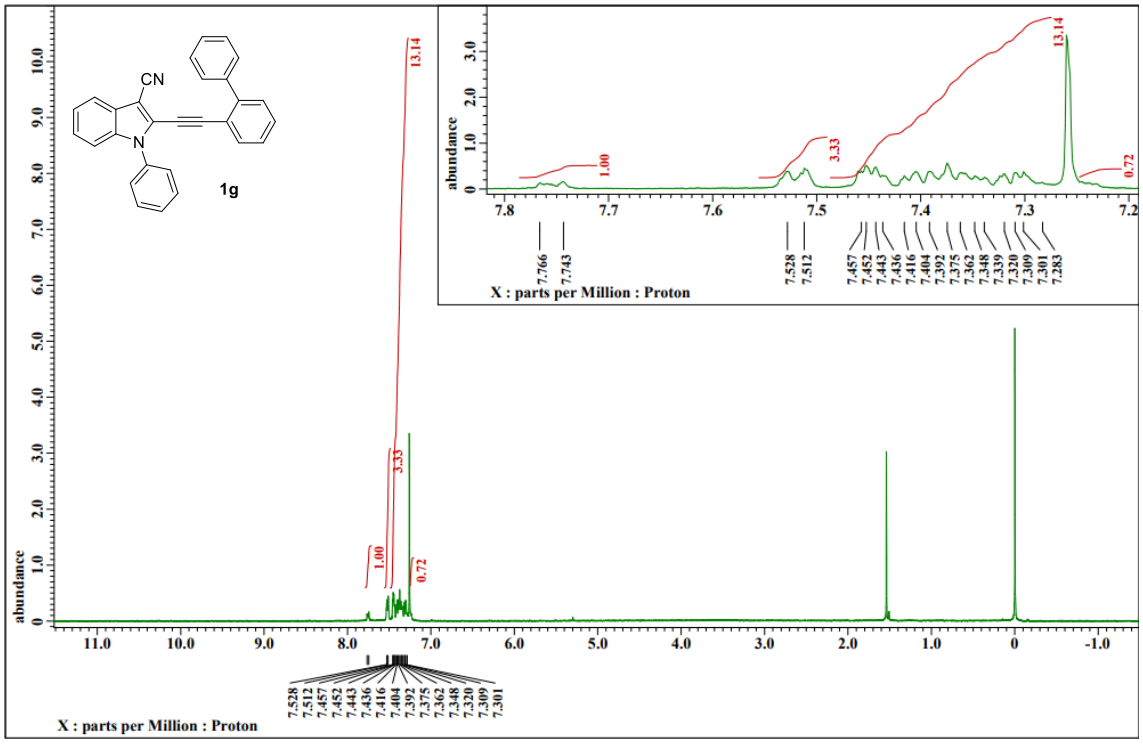
^{1}H NMR (400 MHz, $CDCl_3$)



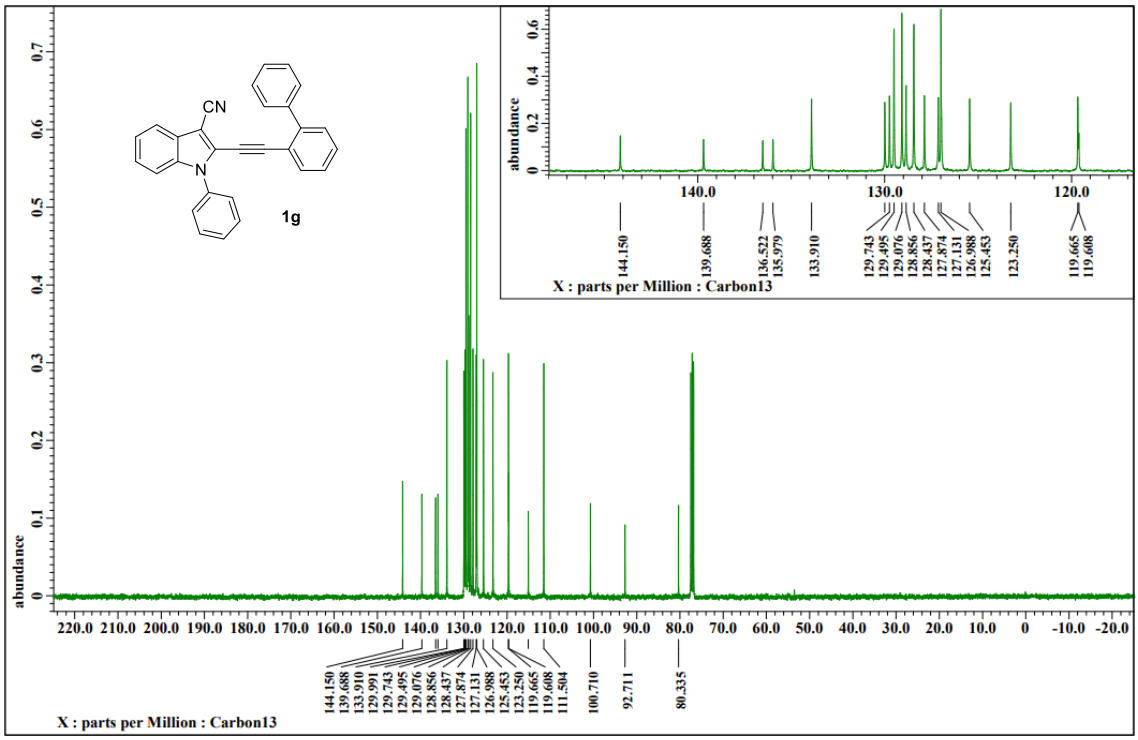
^{13}C NMR (100 MHz, $CDCl_3$)



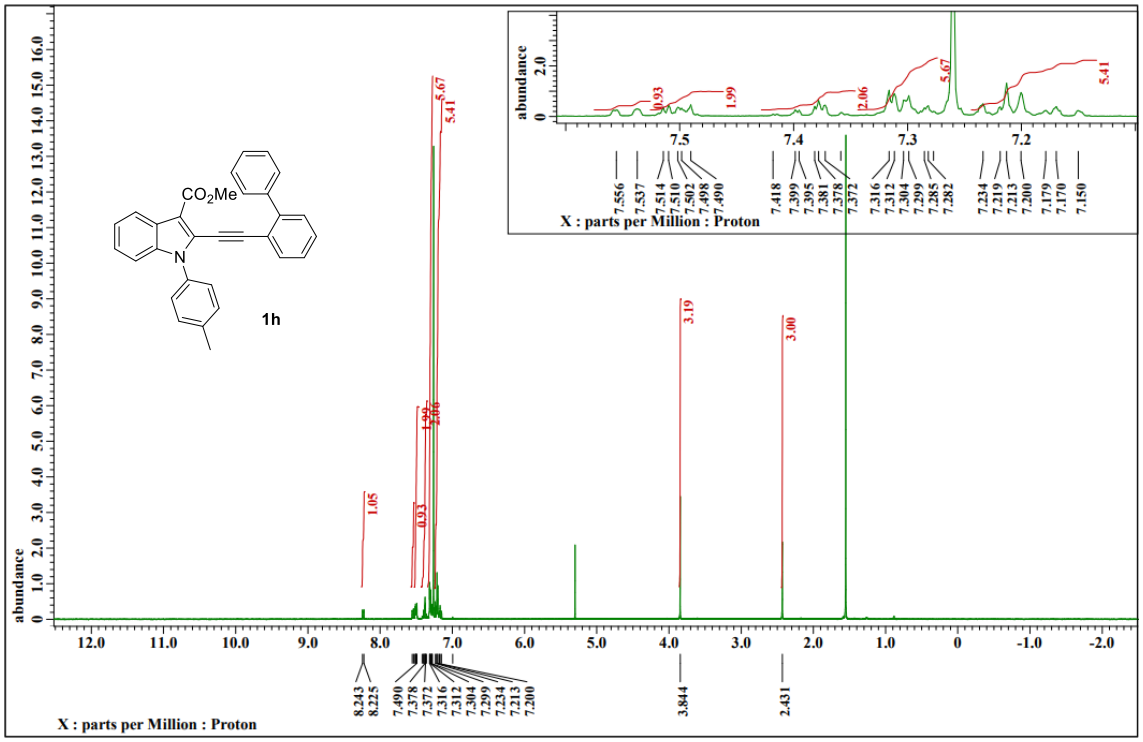
^{1}H NMR (400 MHz, $CDCl_3$)



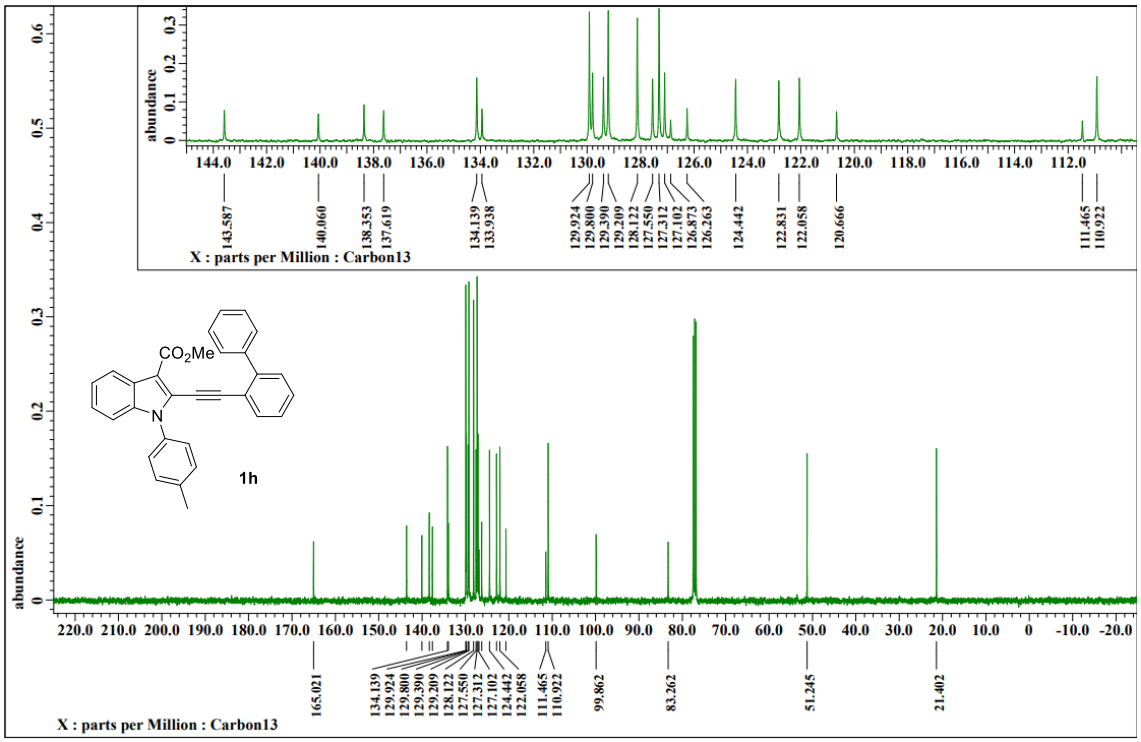
^{13}C NMR (100 MHz, $CDCl_3$)



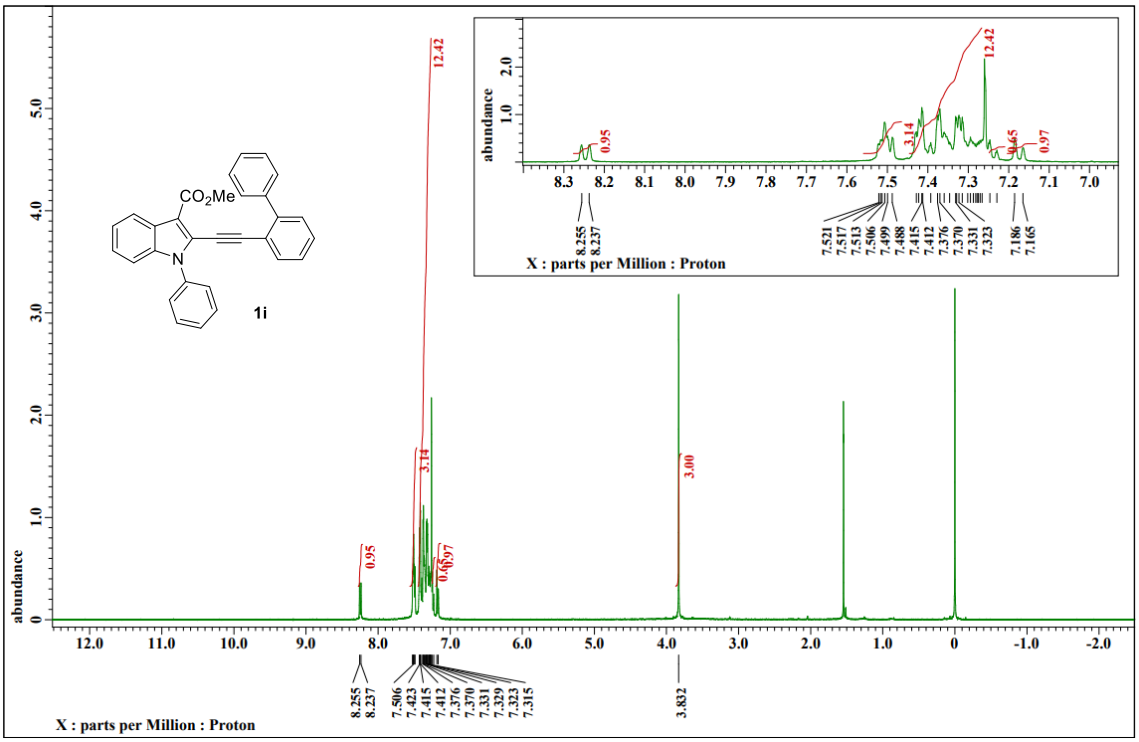
^{1}H NMR (400 MHz, $CDCl_3$)



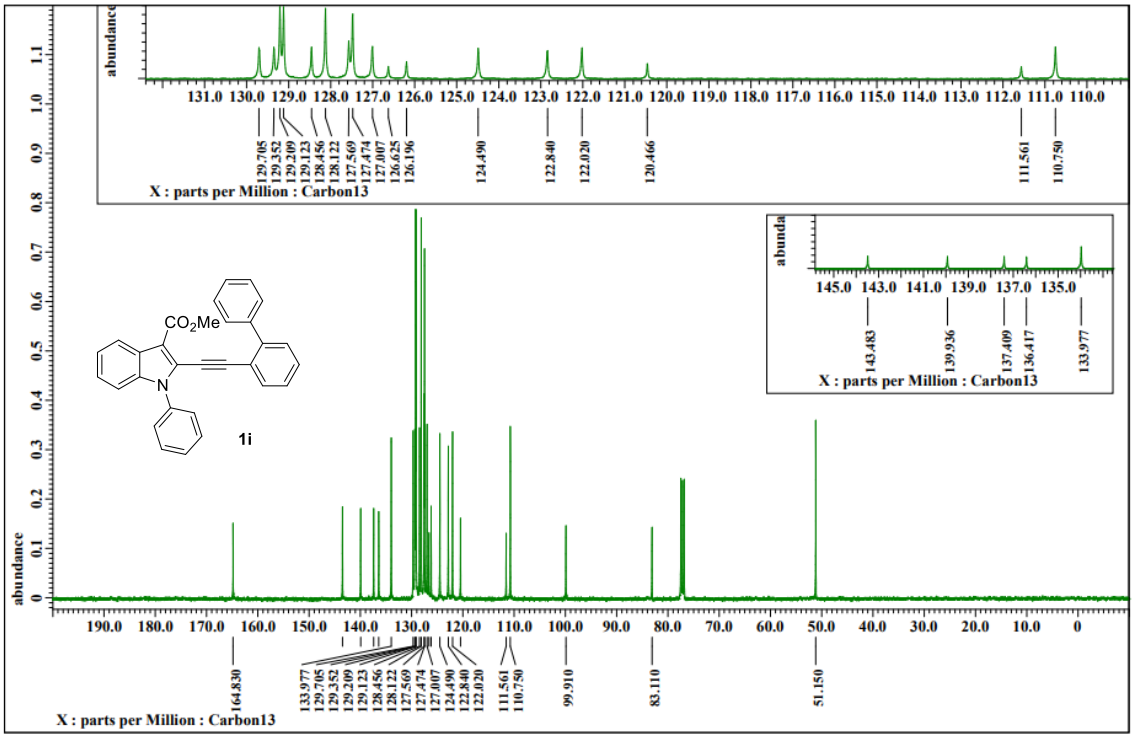
^{13}C NMR (100 MHz, $CDCl_3$)



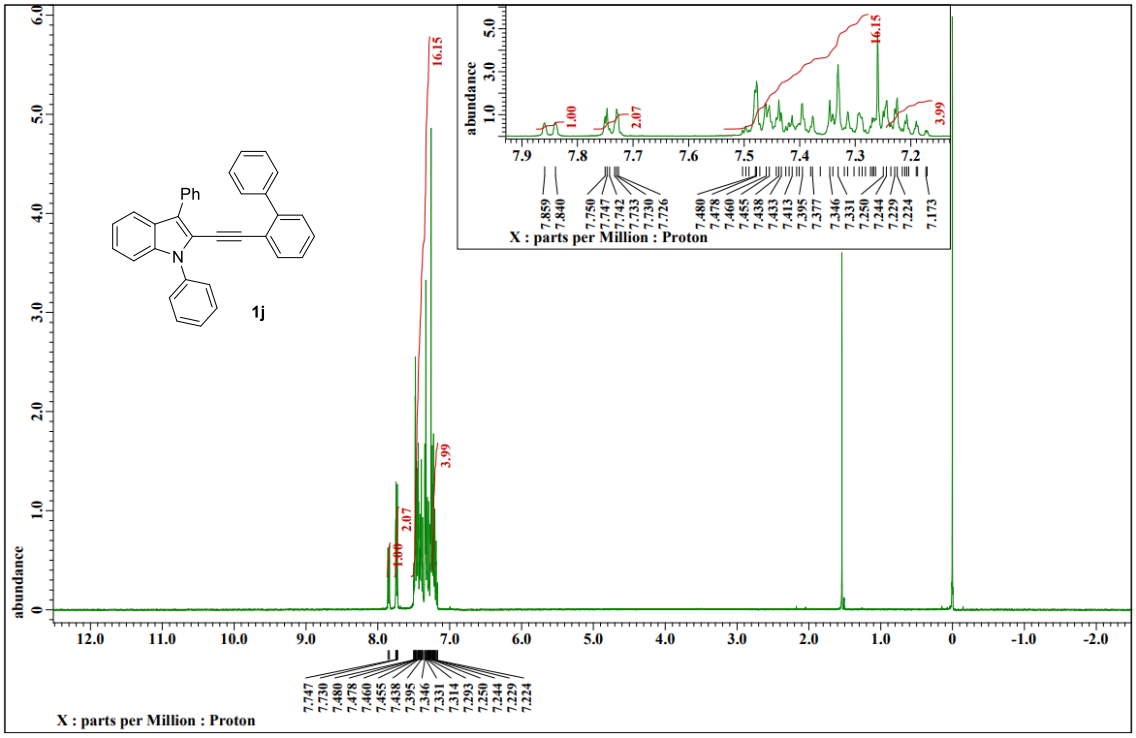
^{1}H NMR (400 MHz, $CDCl_3$)



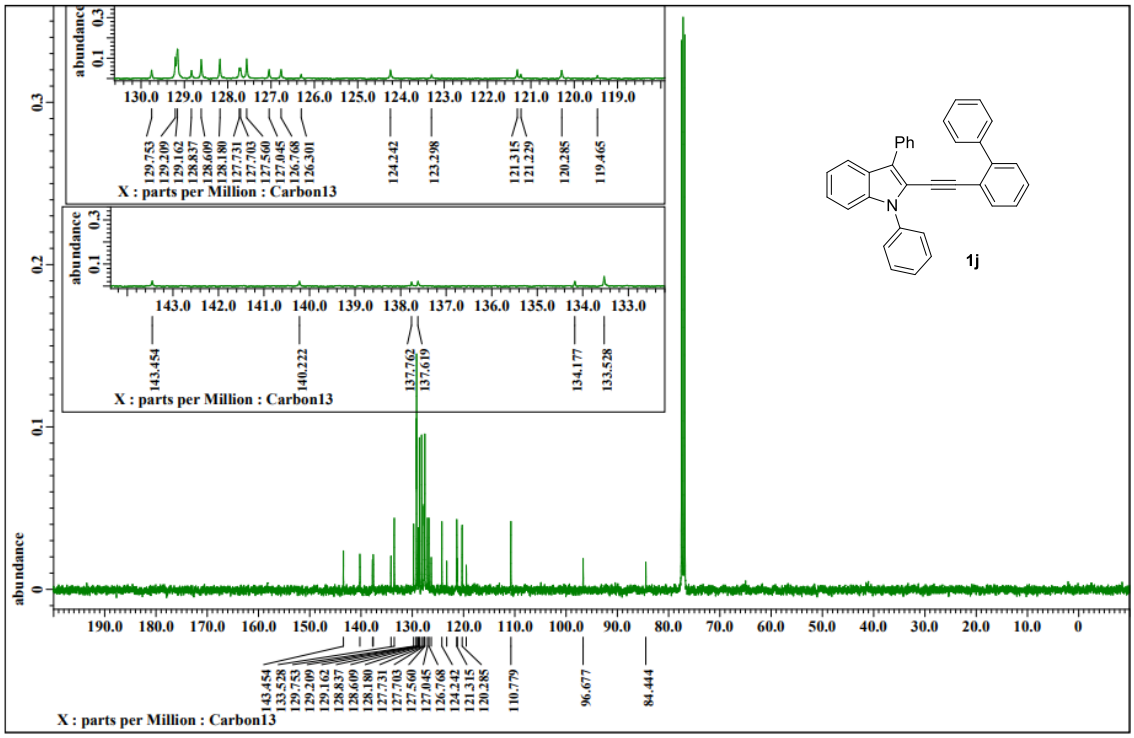
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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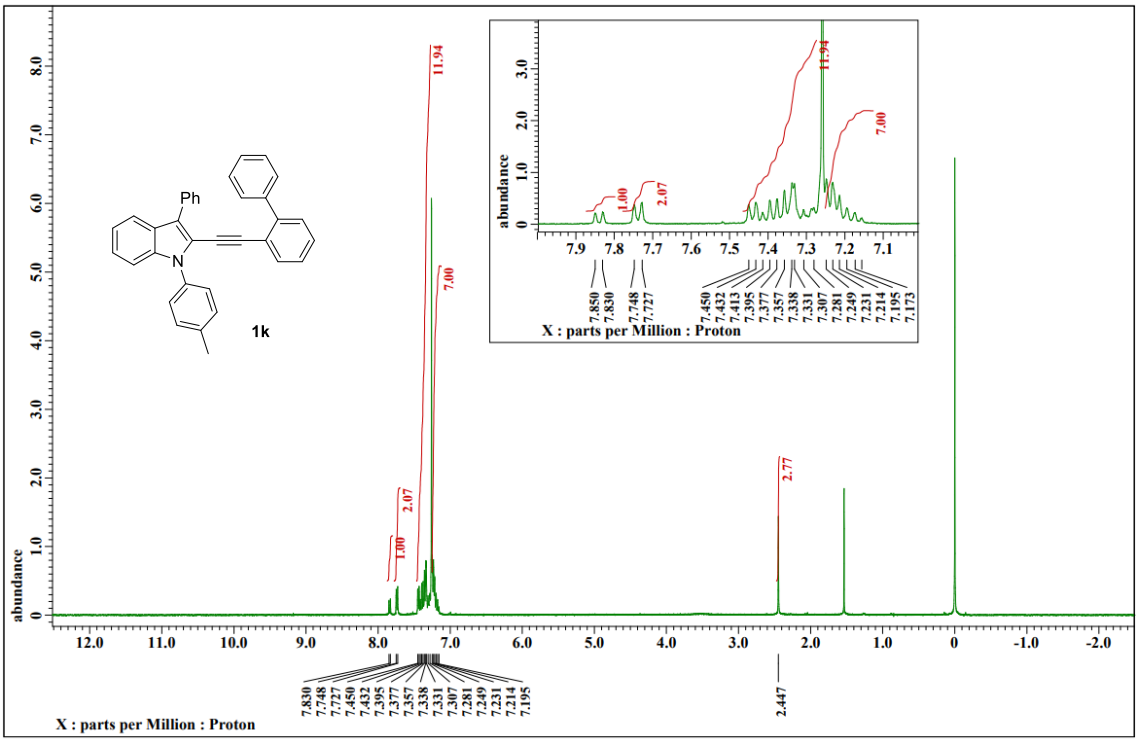

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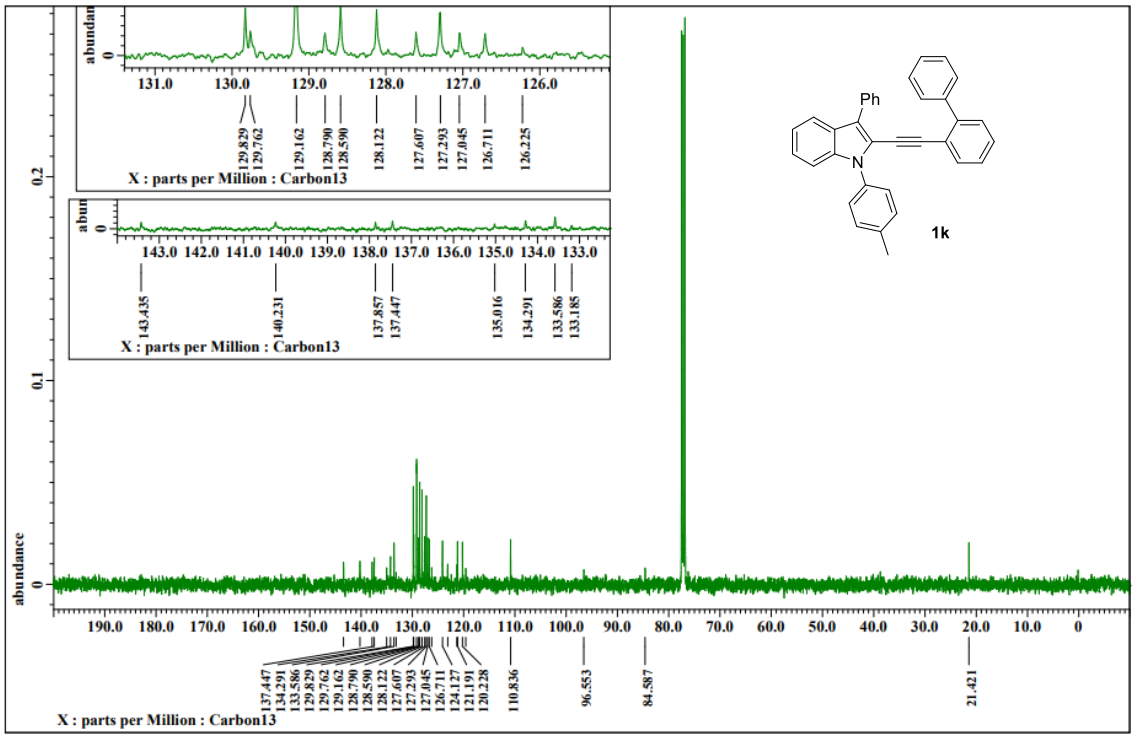
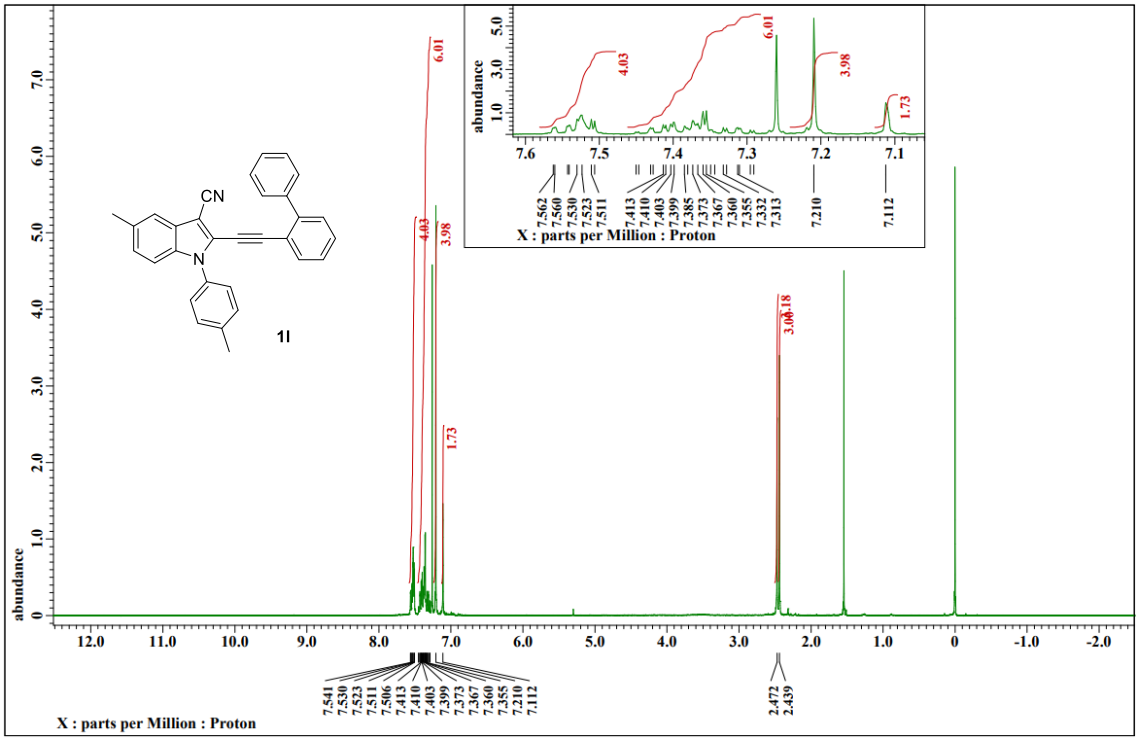


^{1}H NMR (400 MHz, $CDCl_3$)



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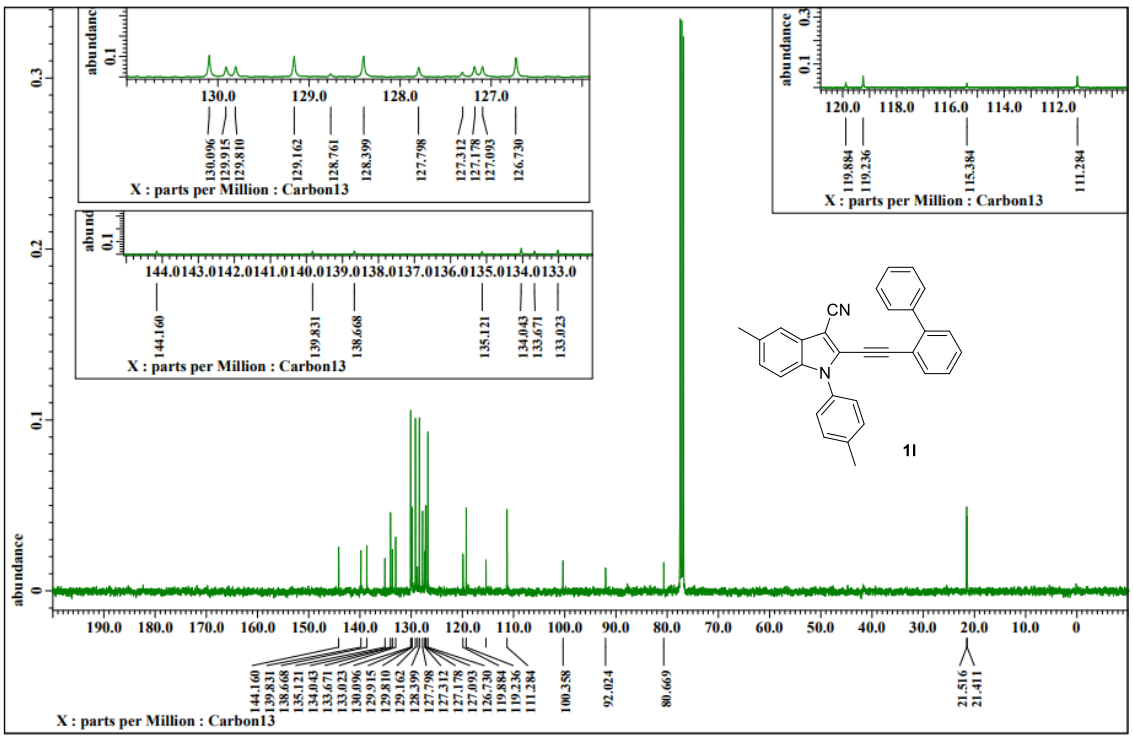

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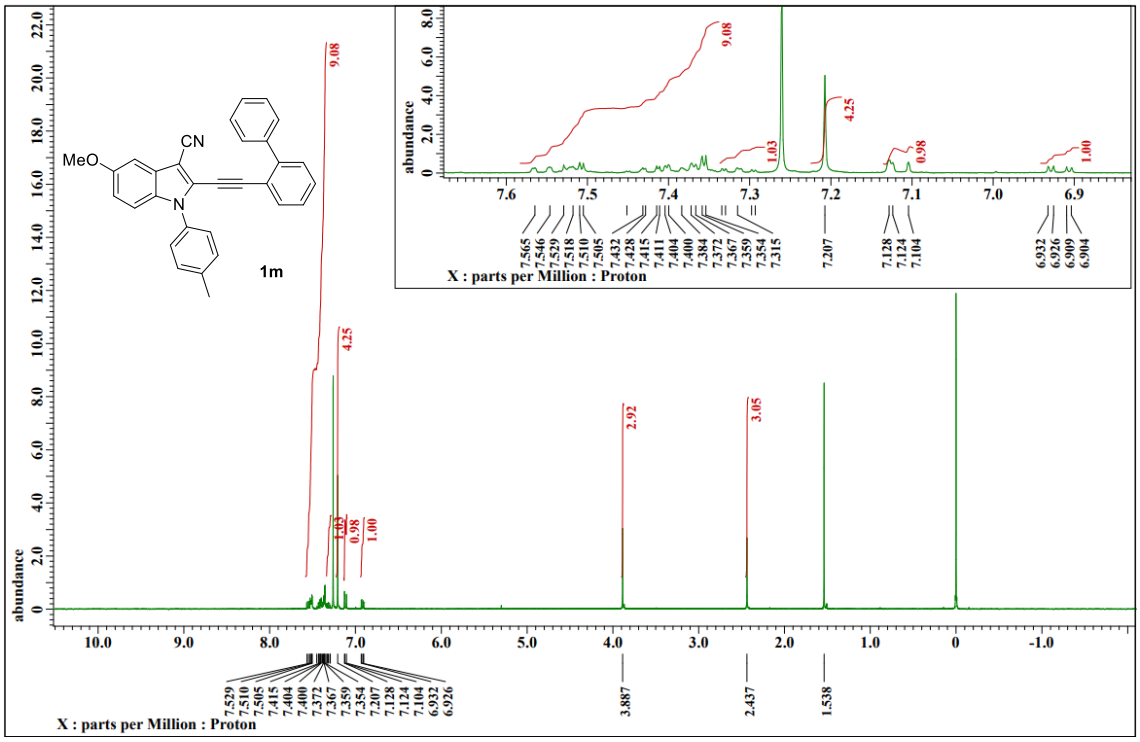

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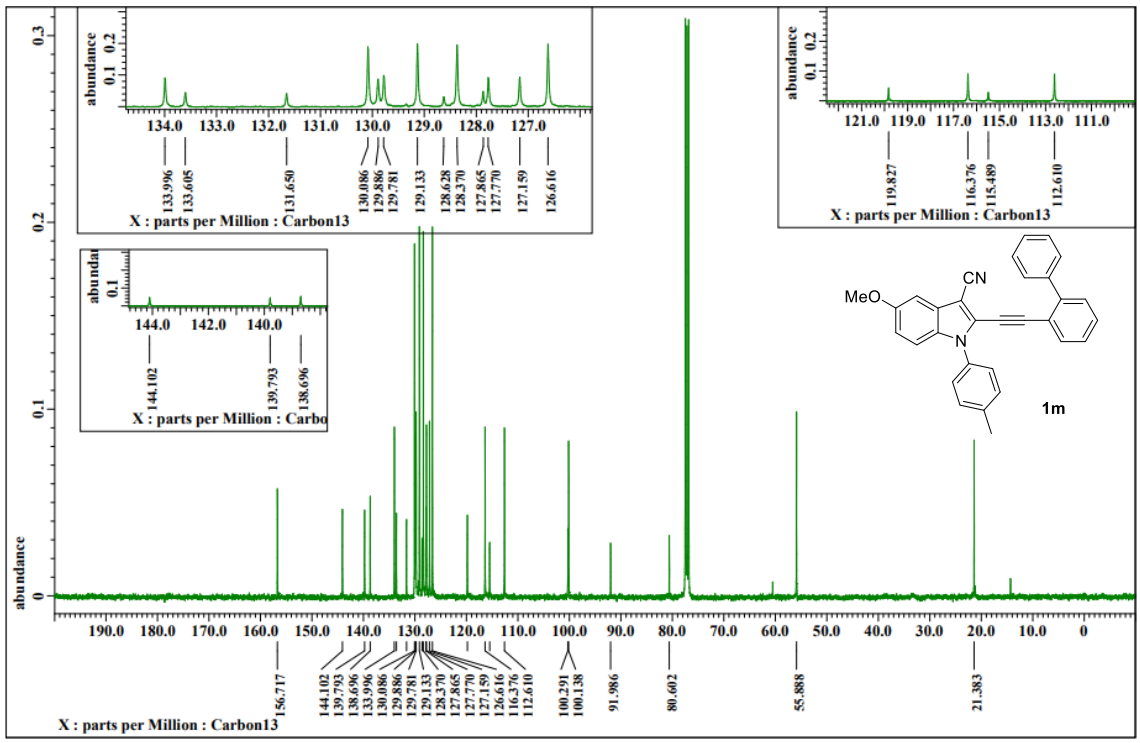

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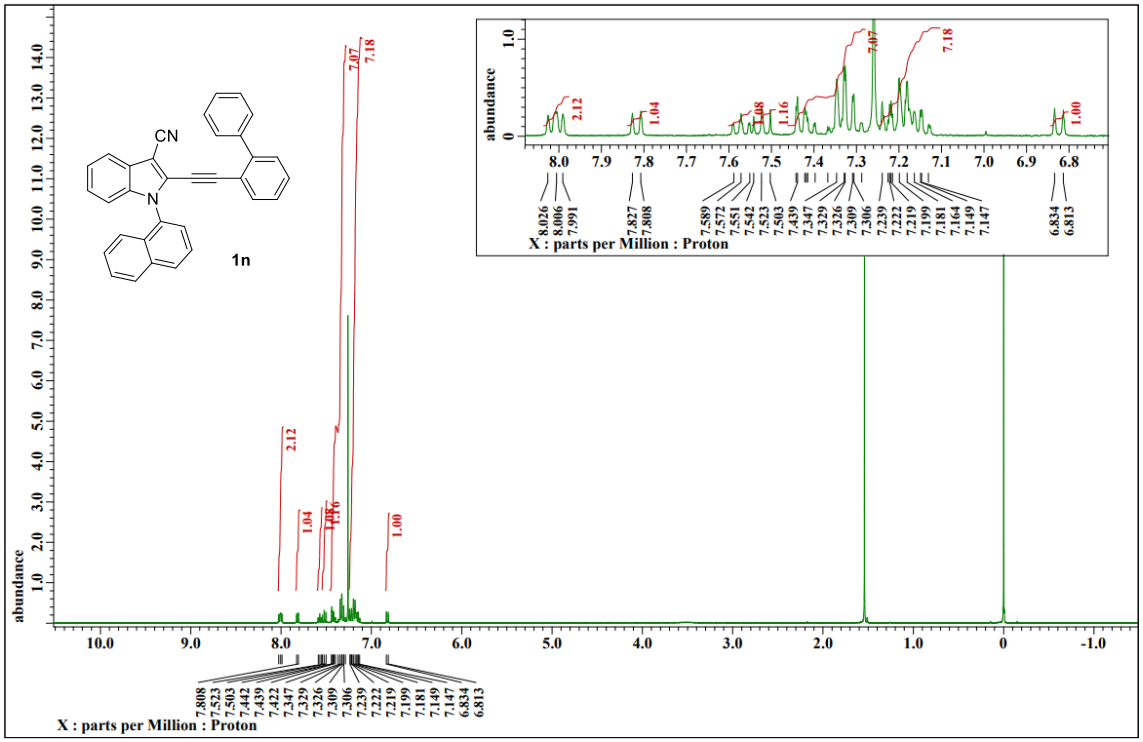

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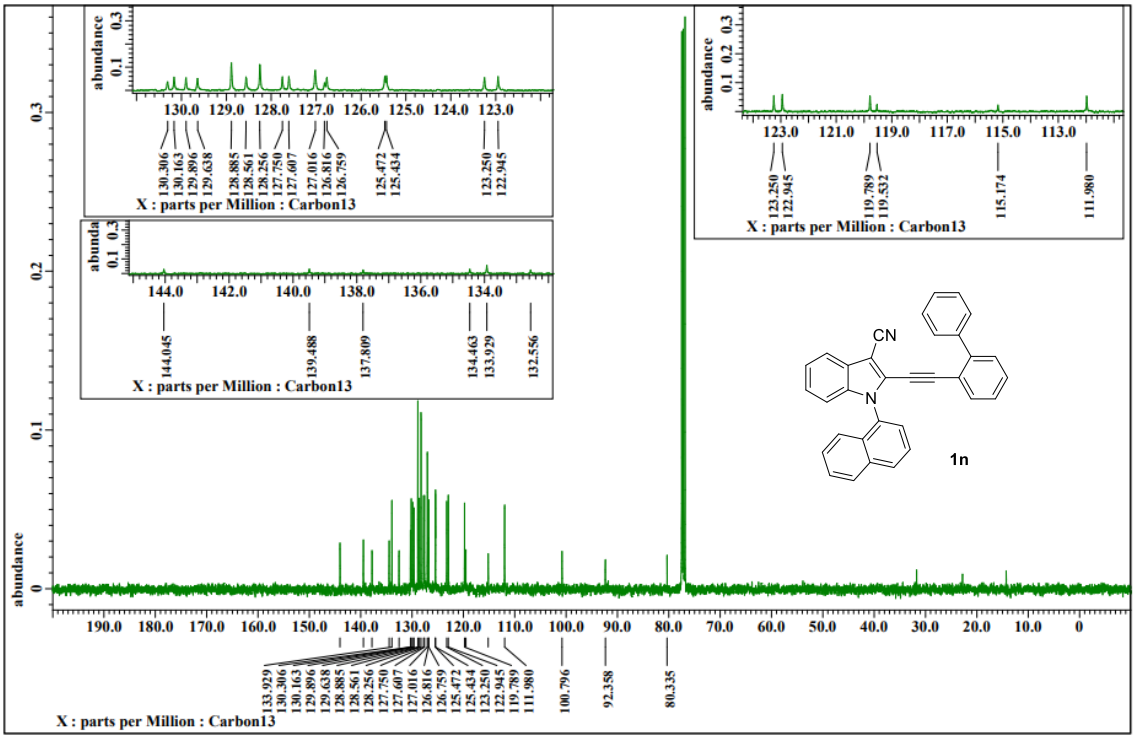

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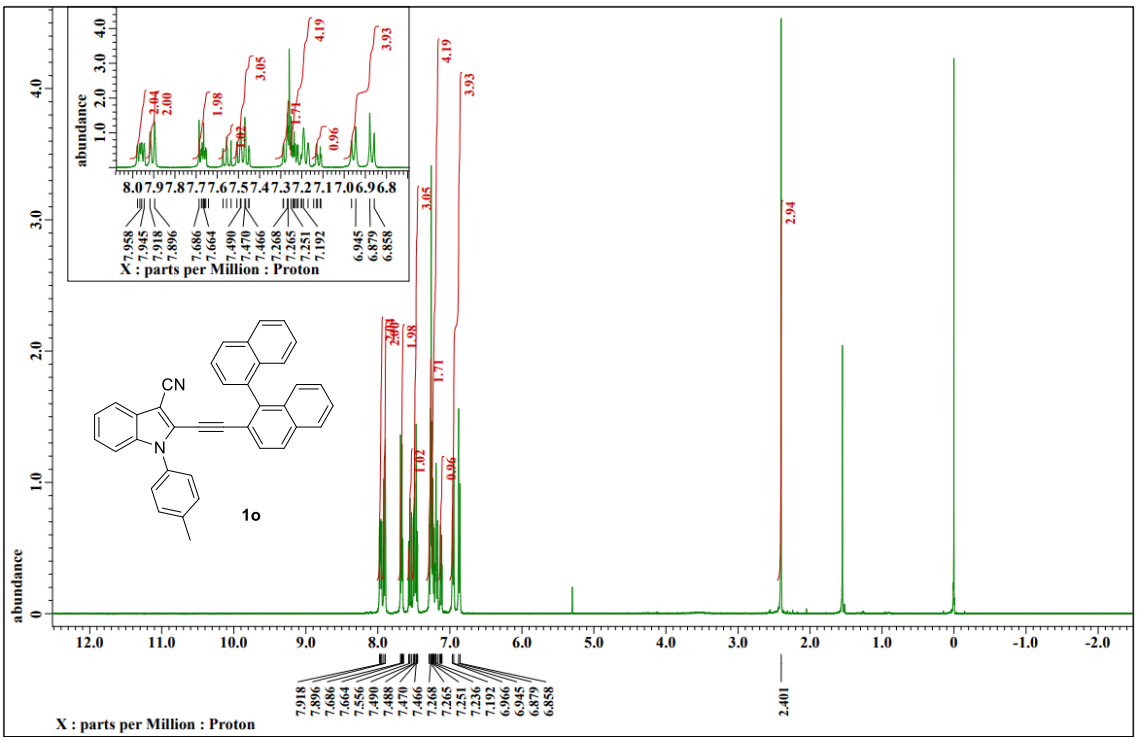

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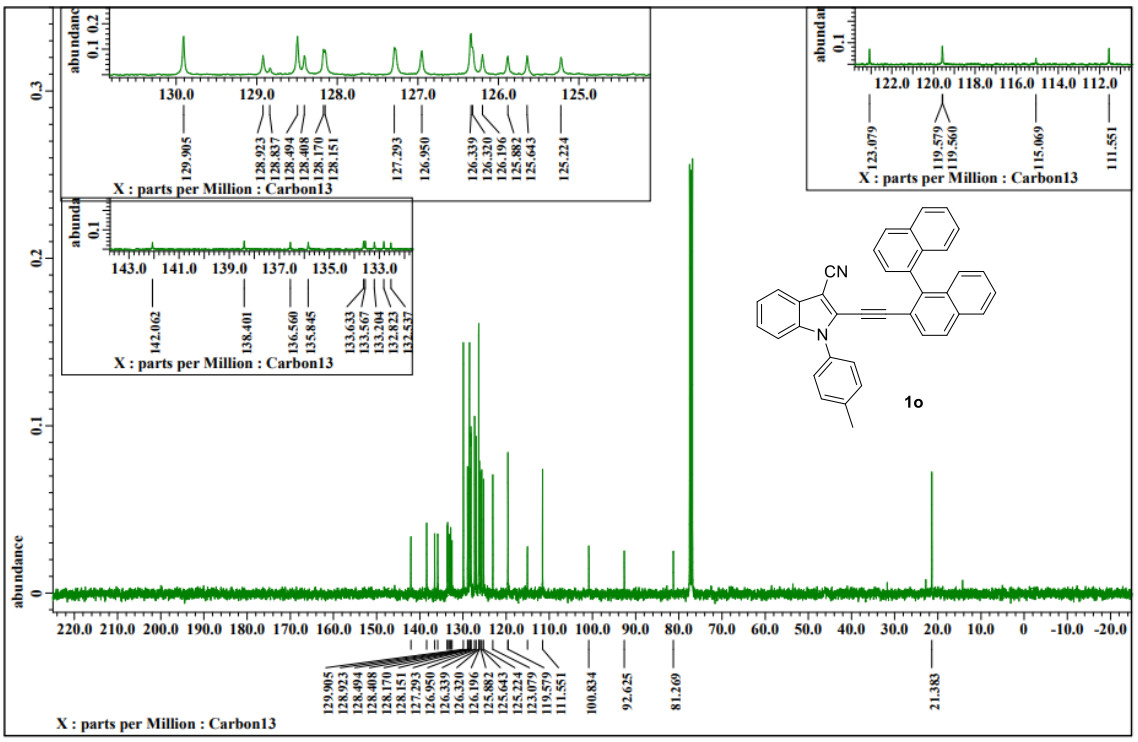
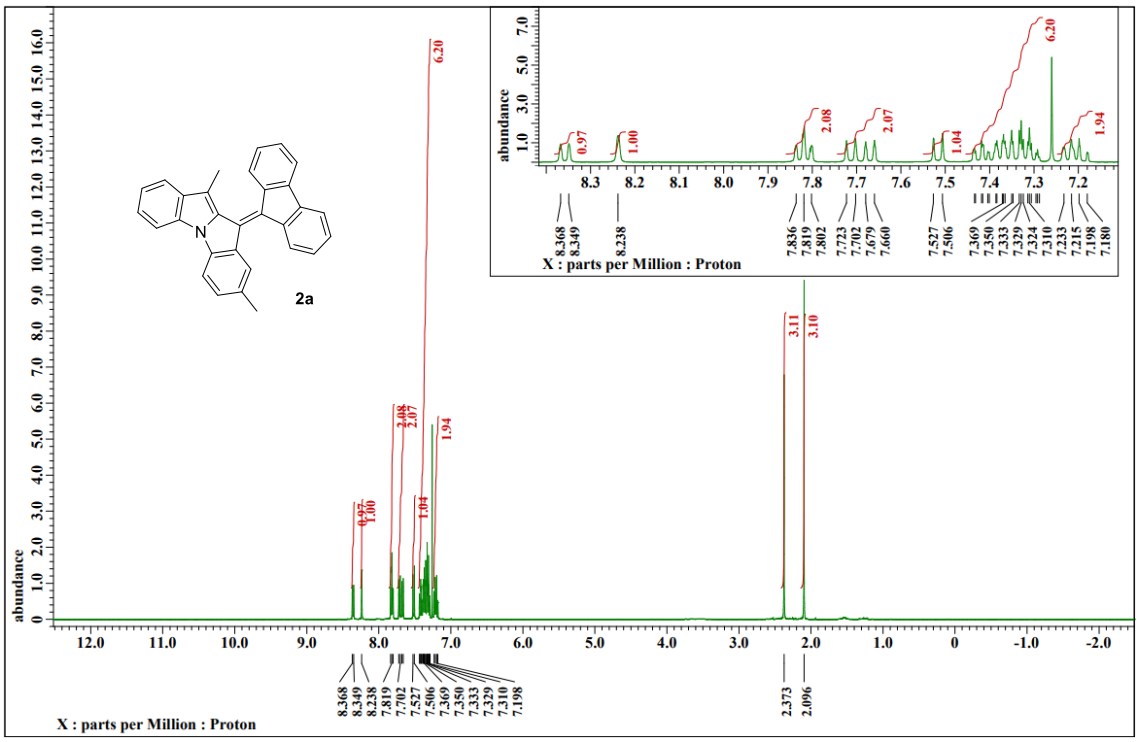
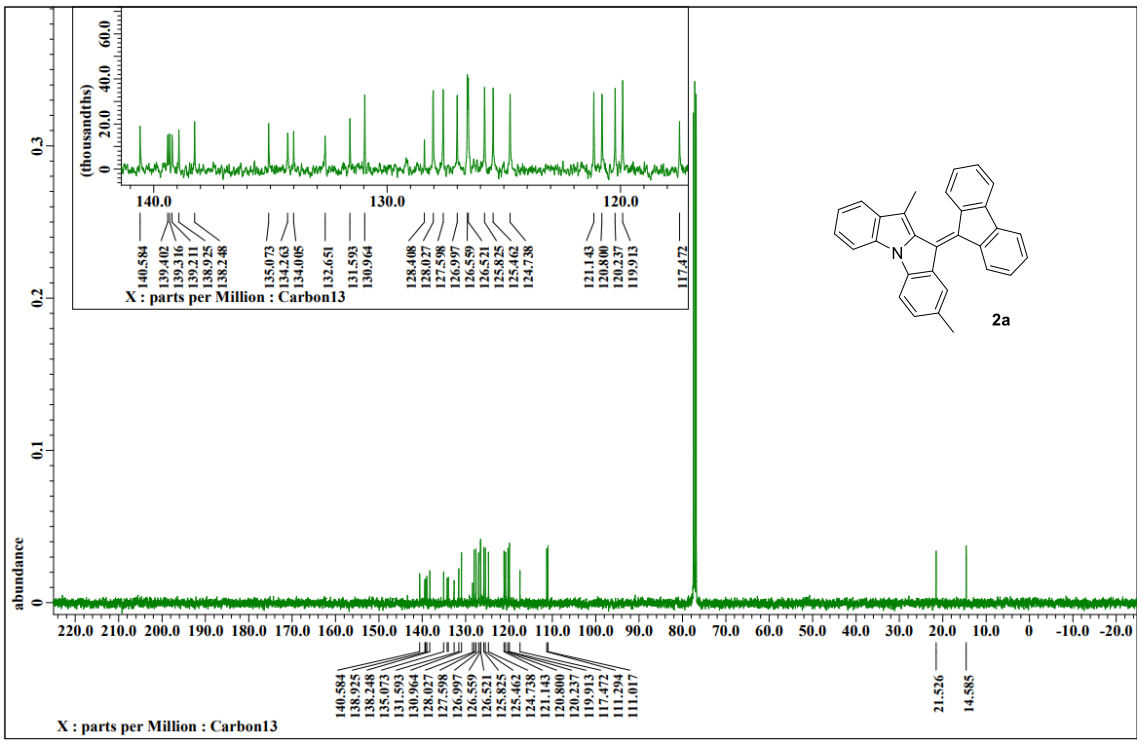


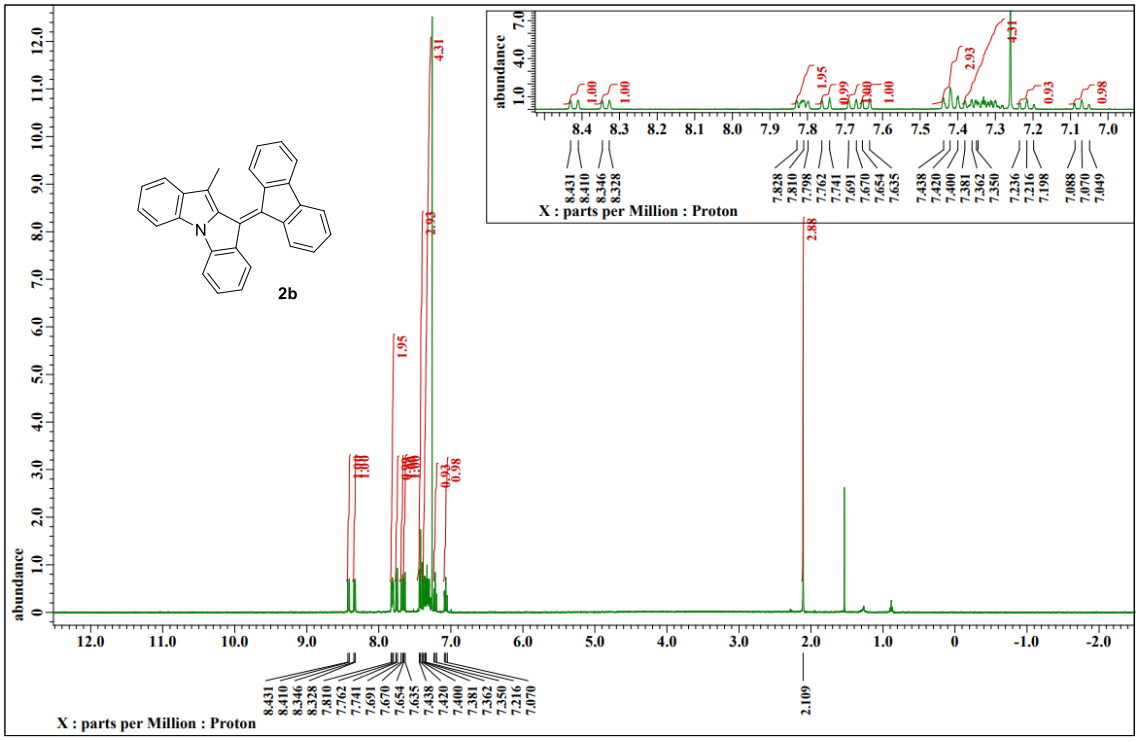
^{1}H NMR (400 MHz, $CDCl_3$)



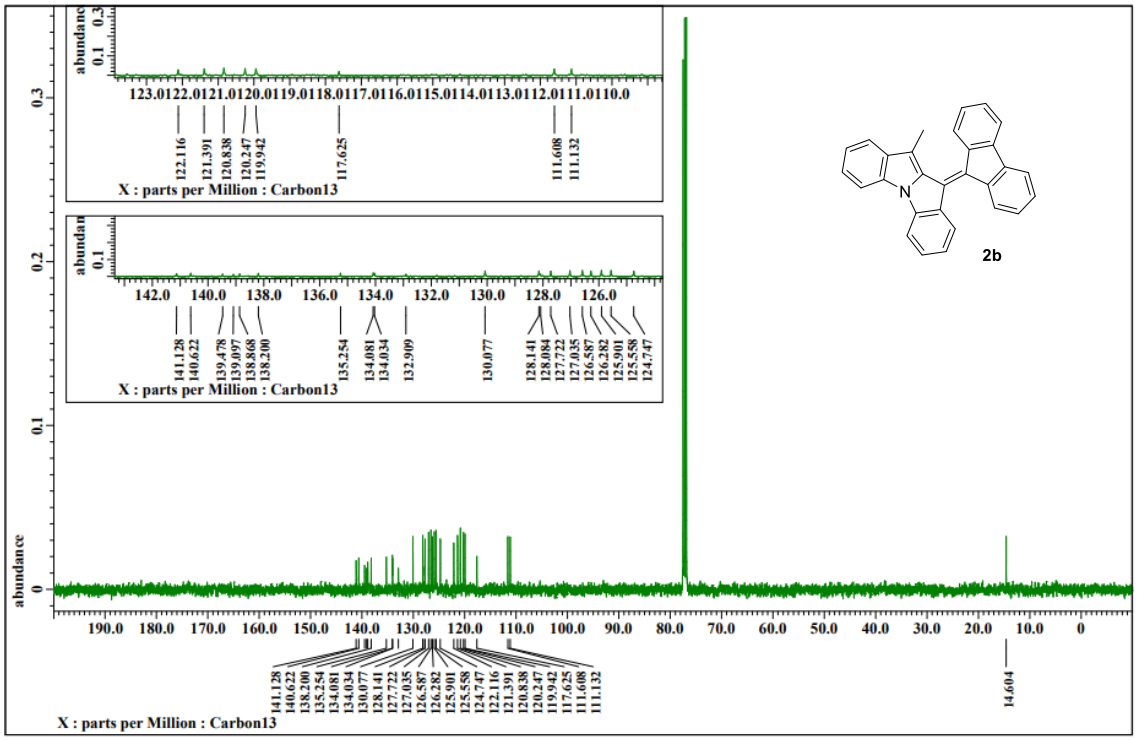
^{13}C NMR (100 MHz, $CDCl_3$)



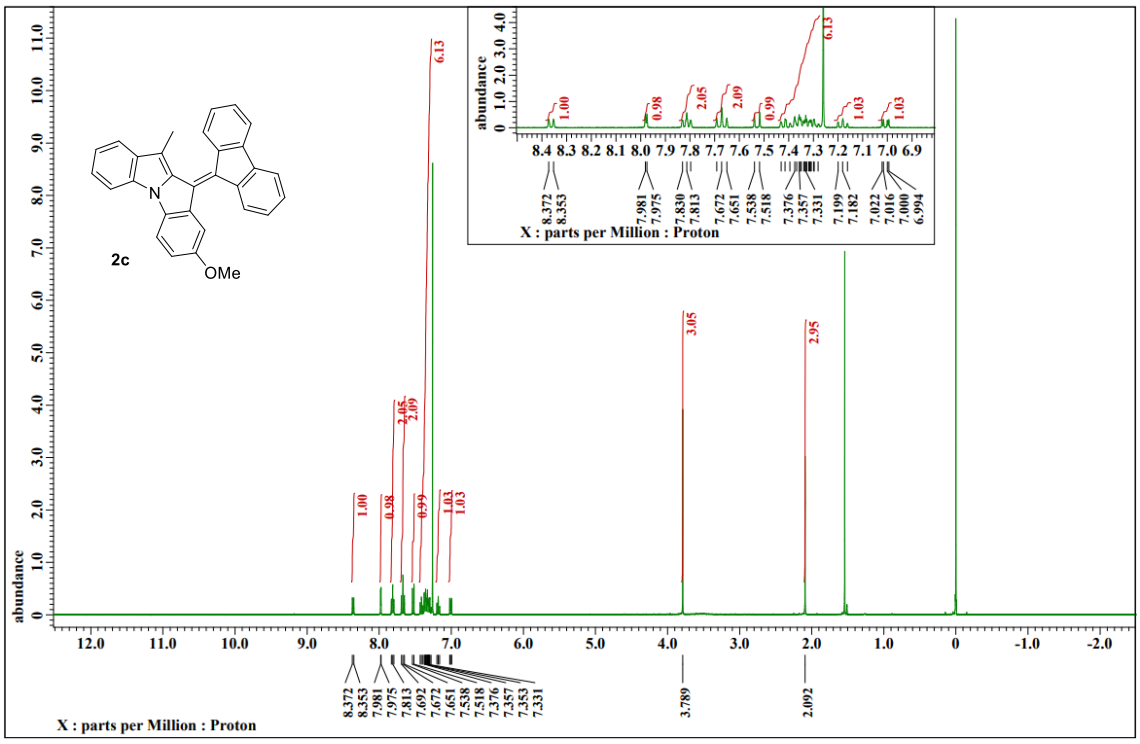
^{1}H NMR (400 MHz, $CDCl_3$)



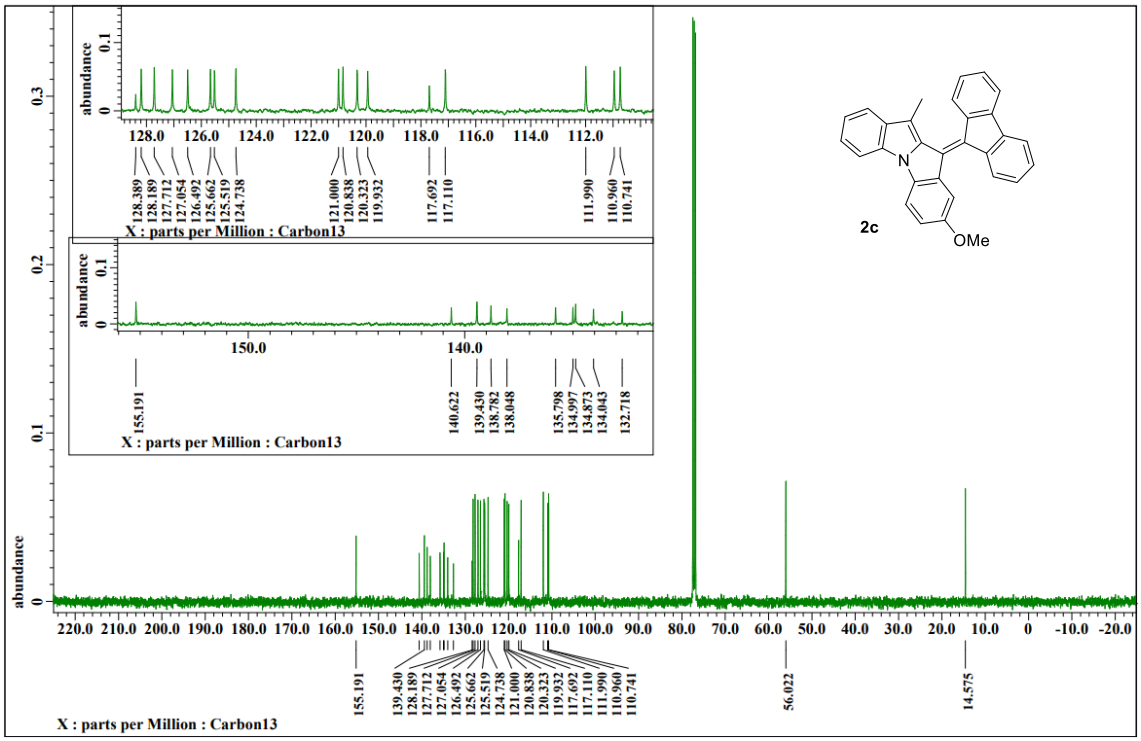
^{13}C NMR (100 MHz, $CDCl_3$)



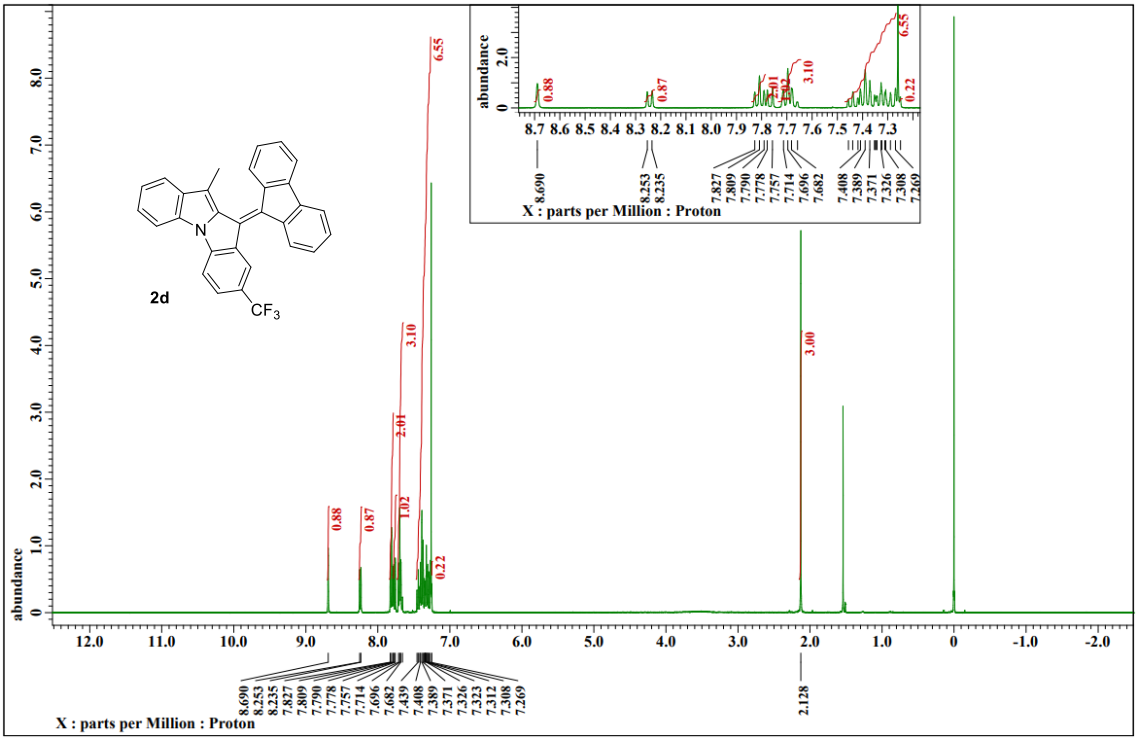
^{1}H NMR (400 MHz, $CDCl_3$)



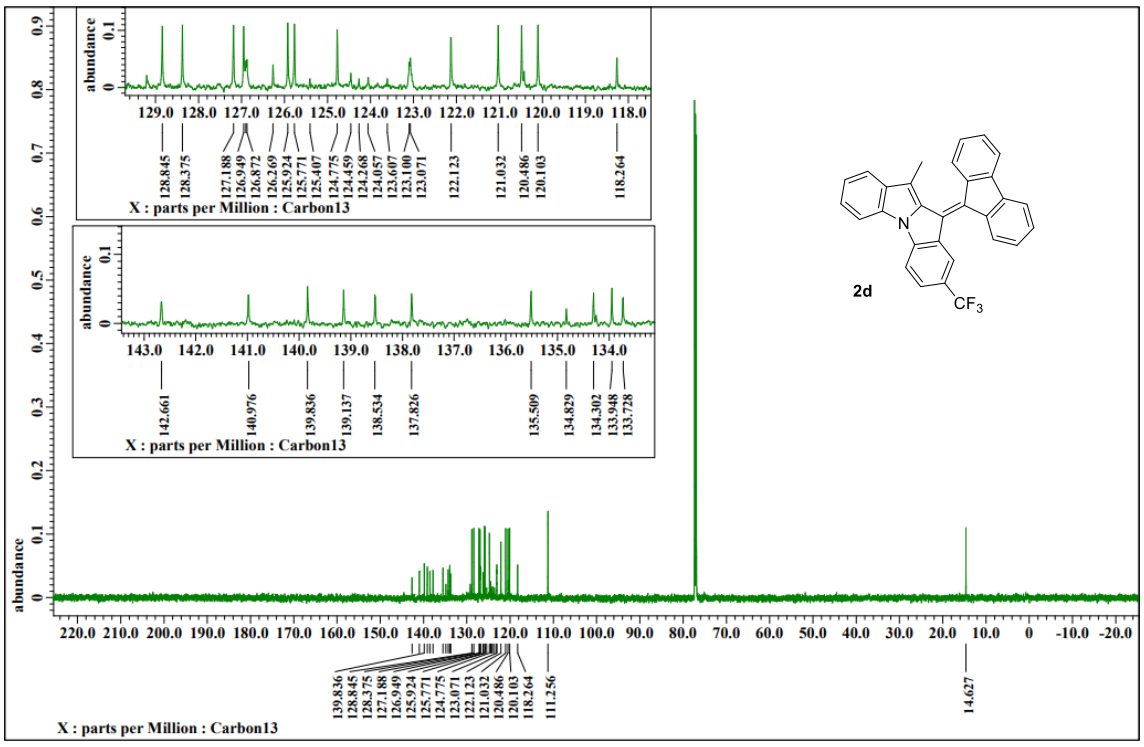
^{13}C NMR (100 MHz, $CDCl_3$)



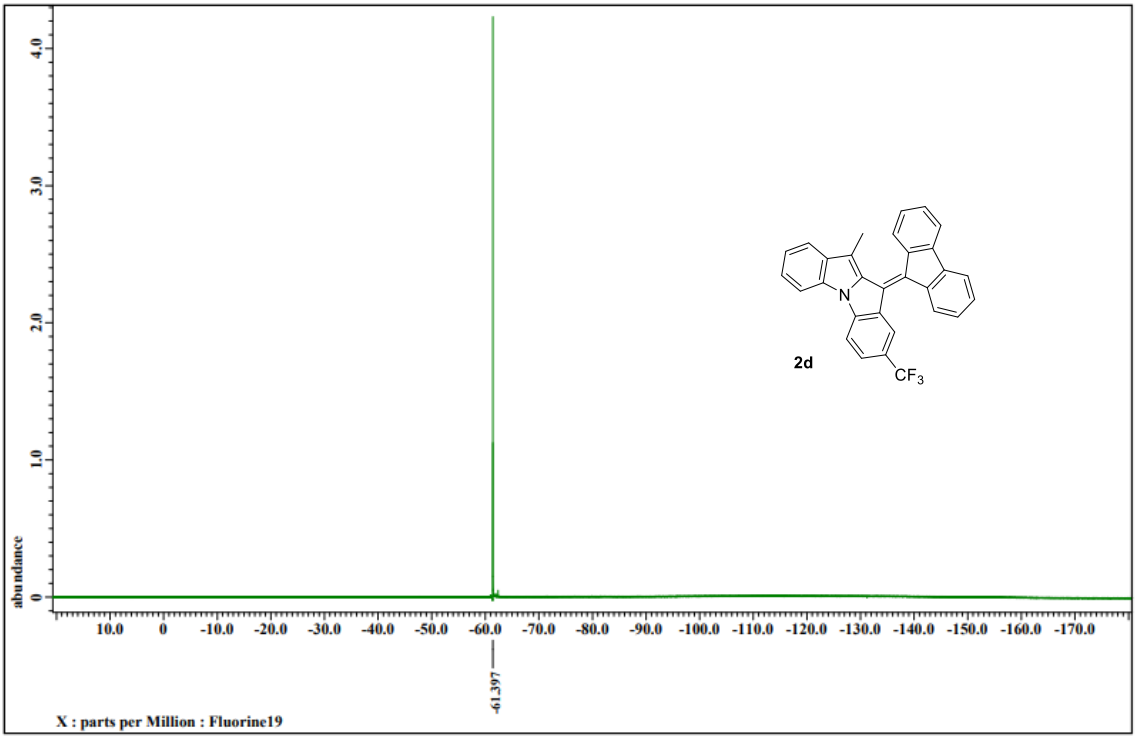
^{1}H NMR (400 MHz, $CDCl_3$)



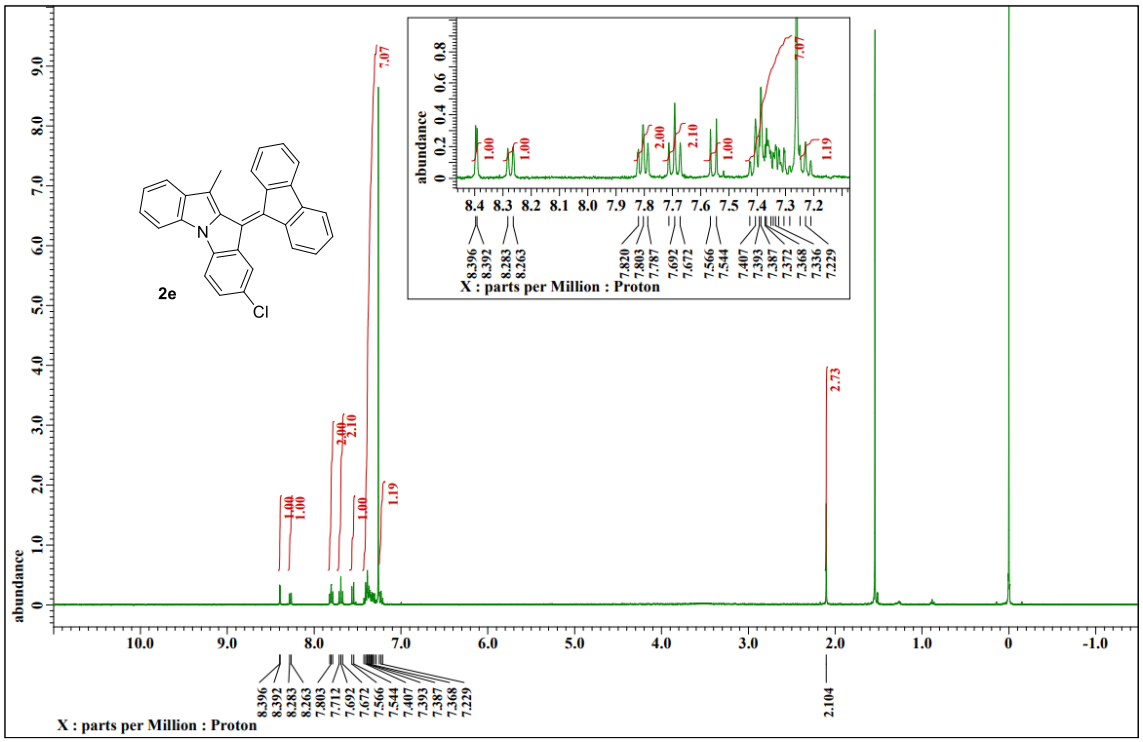
^{13}C NMR (150 MHz, $CDCl_3$)



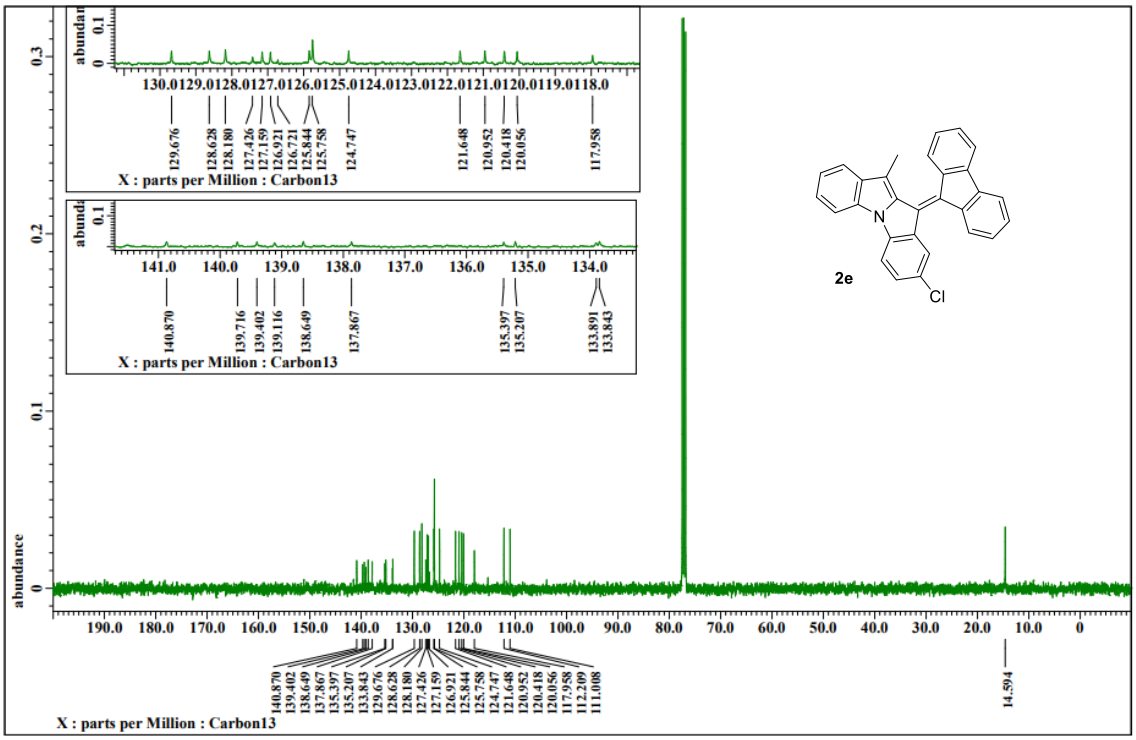
^{19}F NMR (376 MHz, $CDCl_3$)



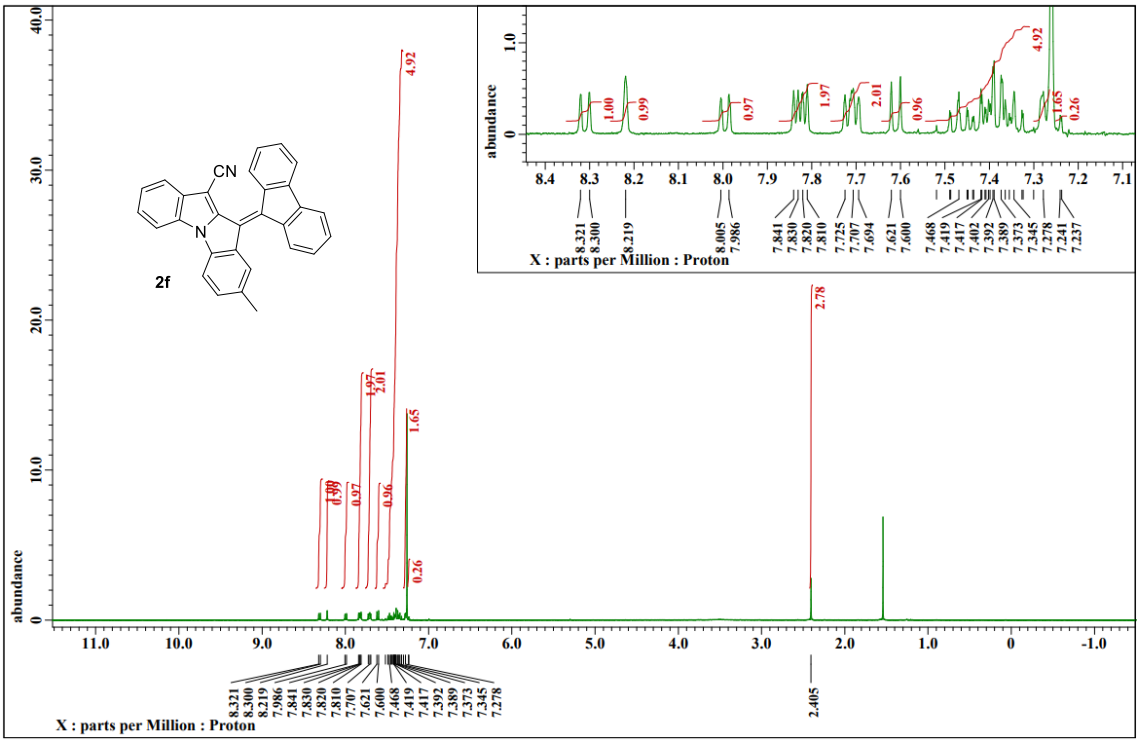
^{1}H NMR (400 MHz, $CDCl_3$)



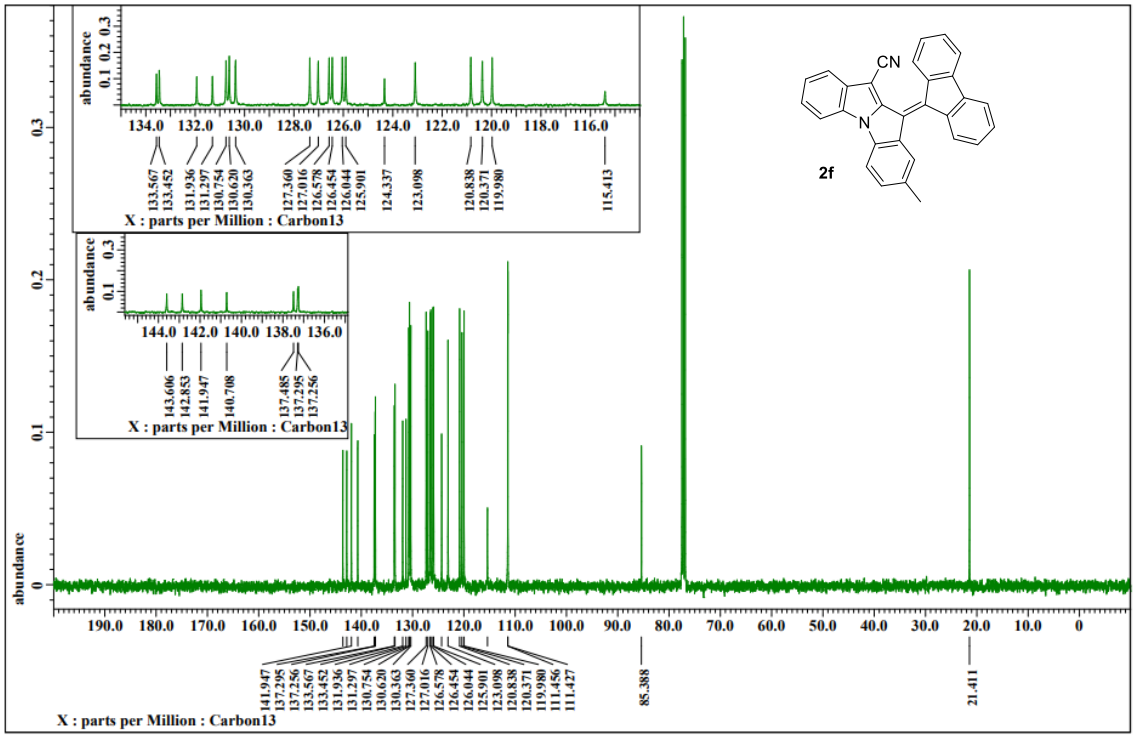
^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



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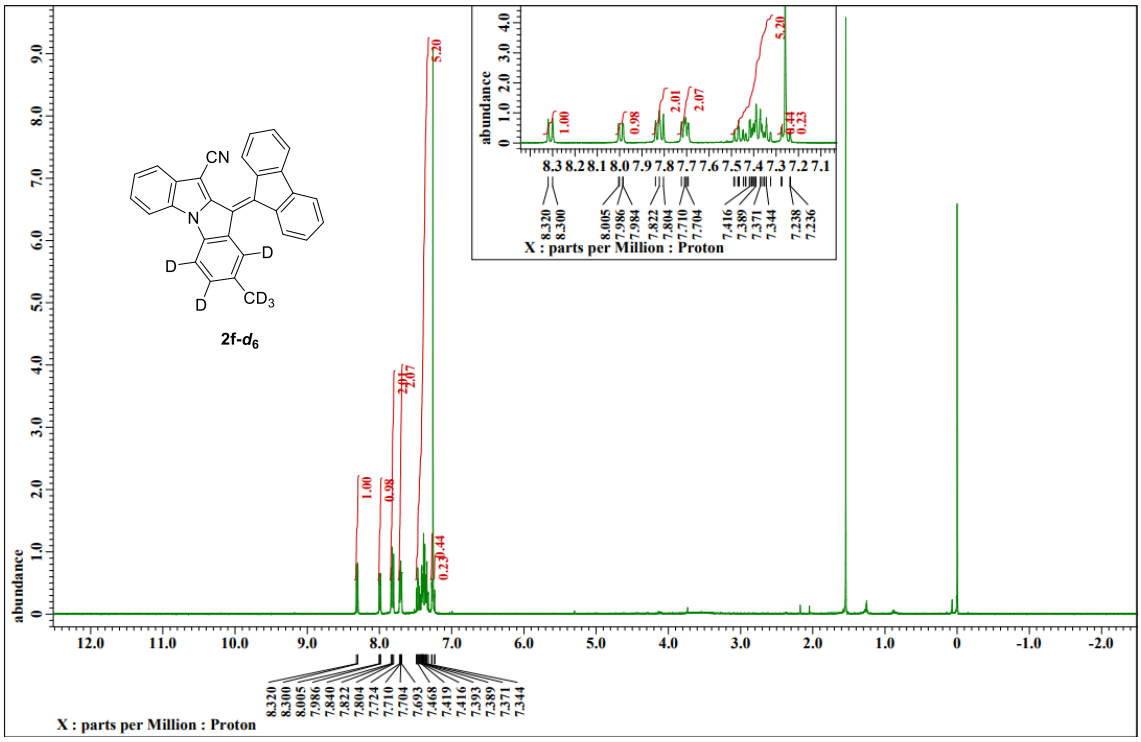

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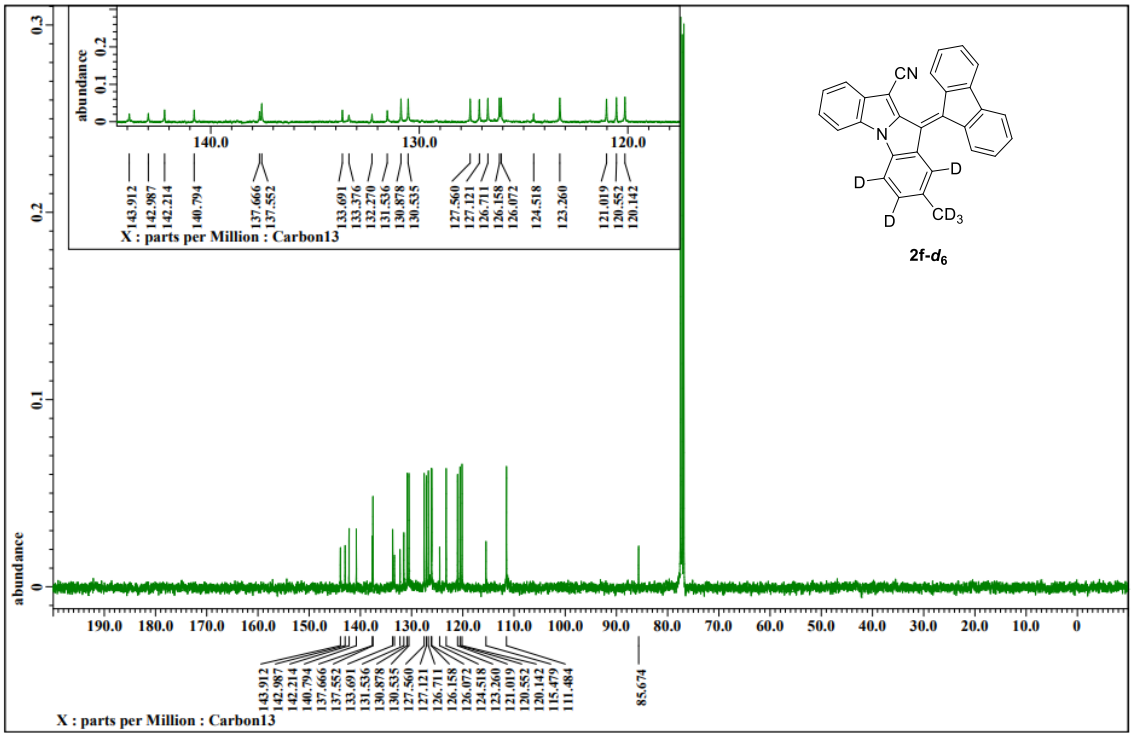
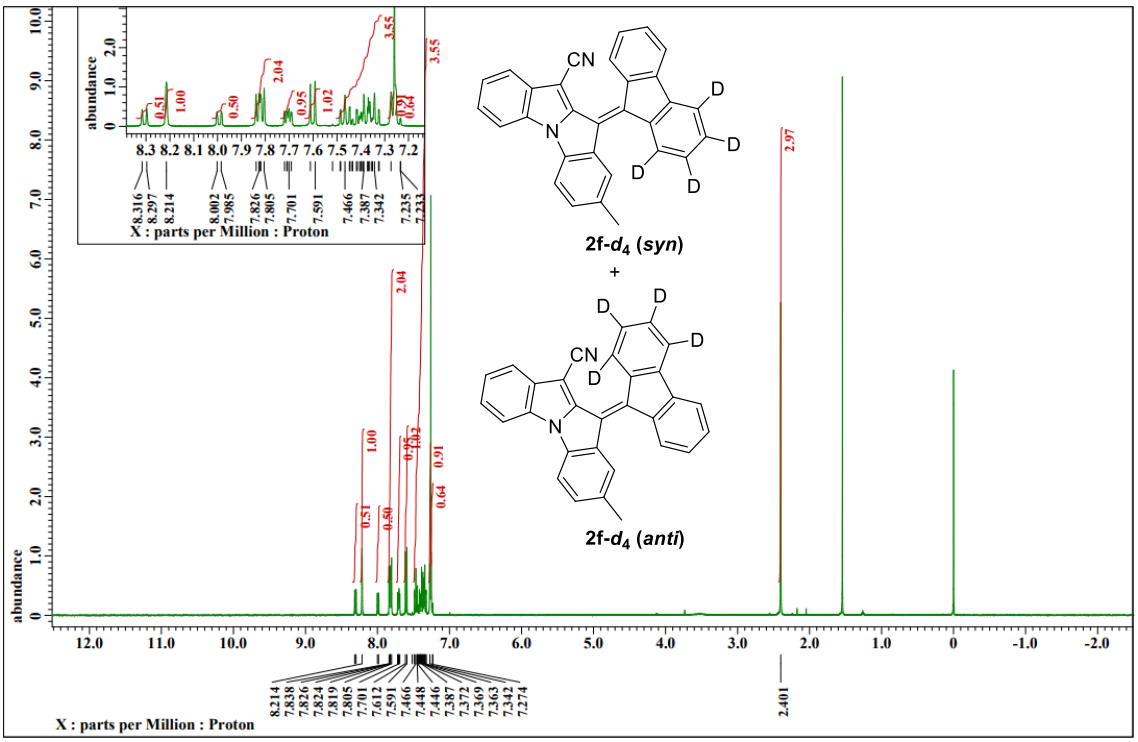


^{1}H NMR (400 MHz, $CDCl_3$)



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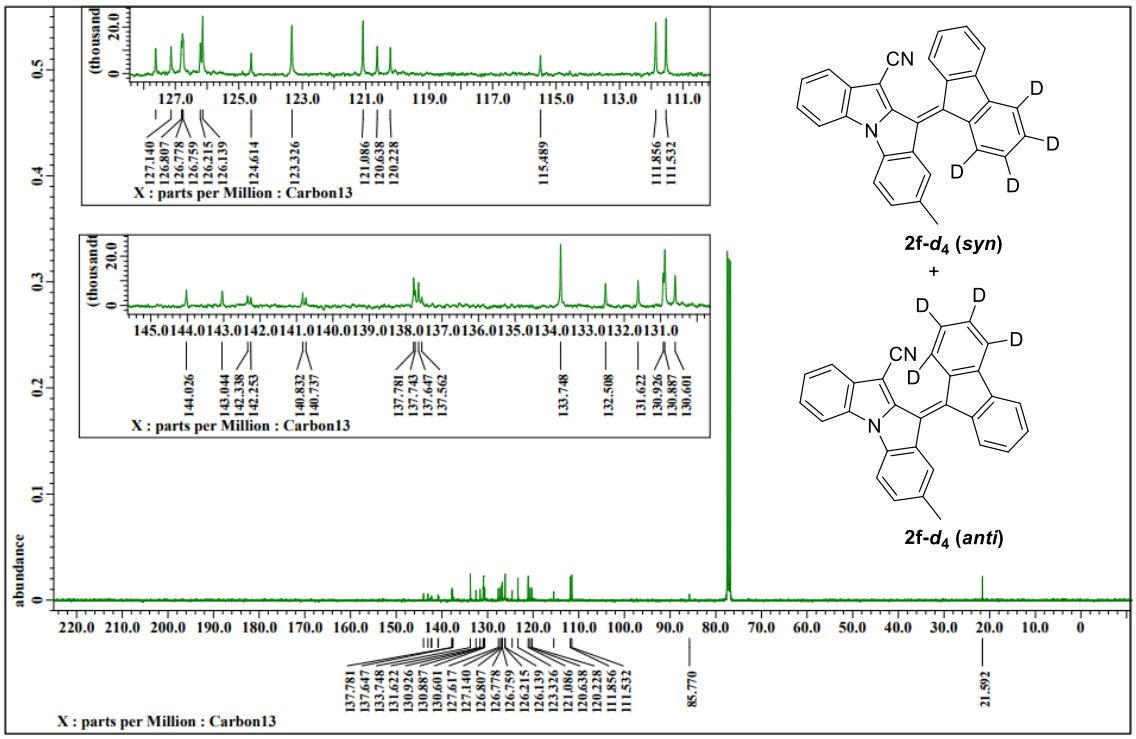
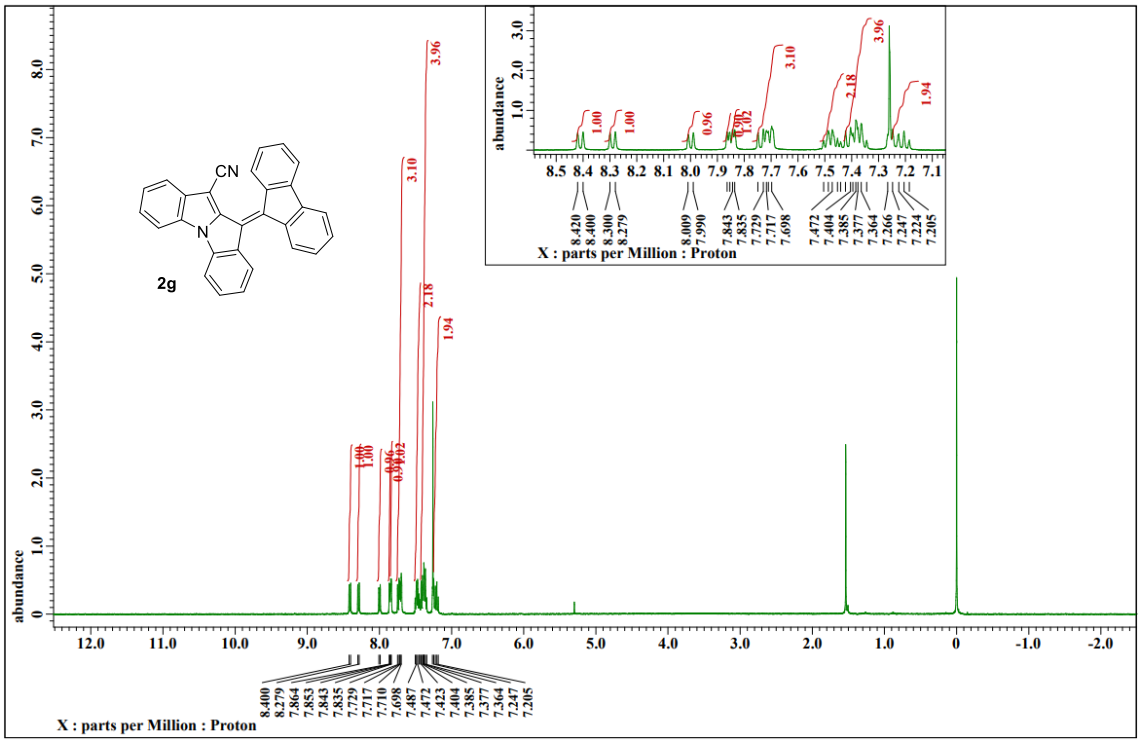


^{1}H NMR (400 MHz, $CDCl_3$)



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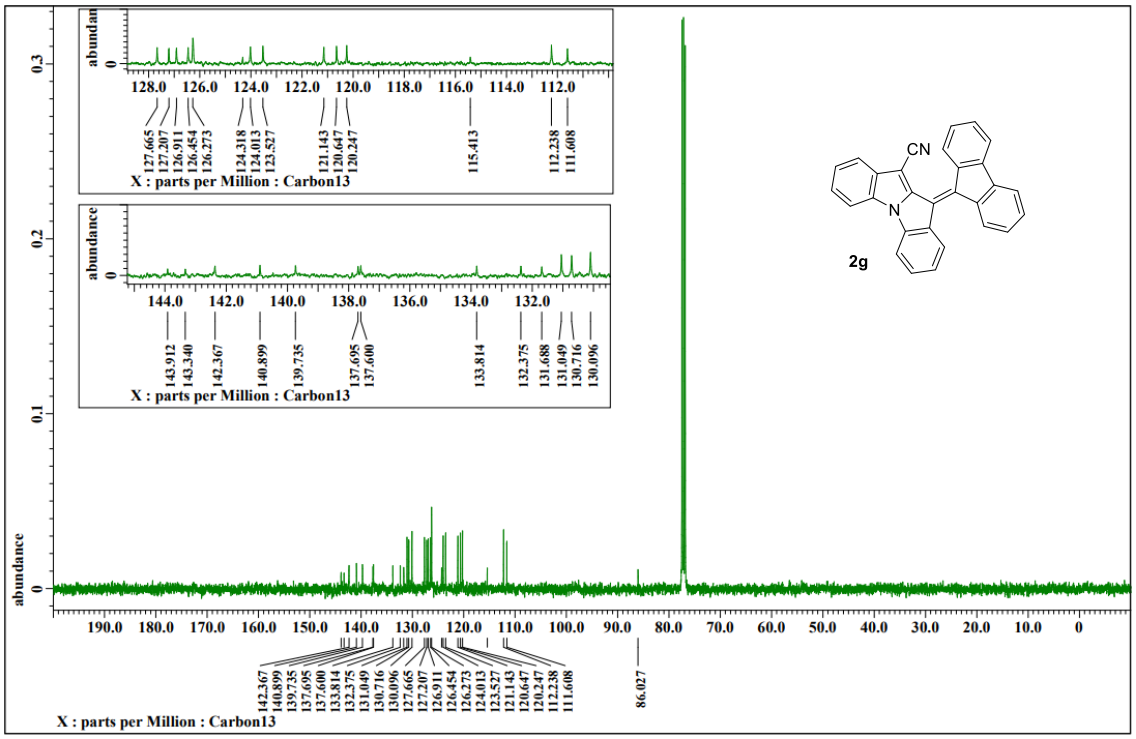
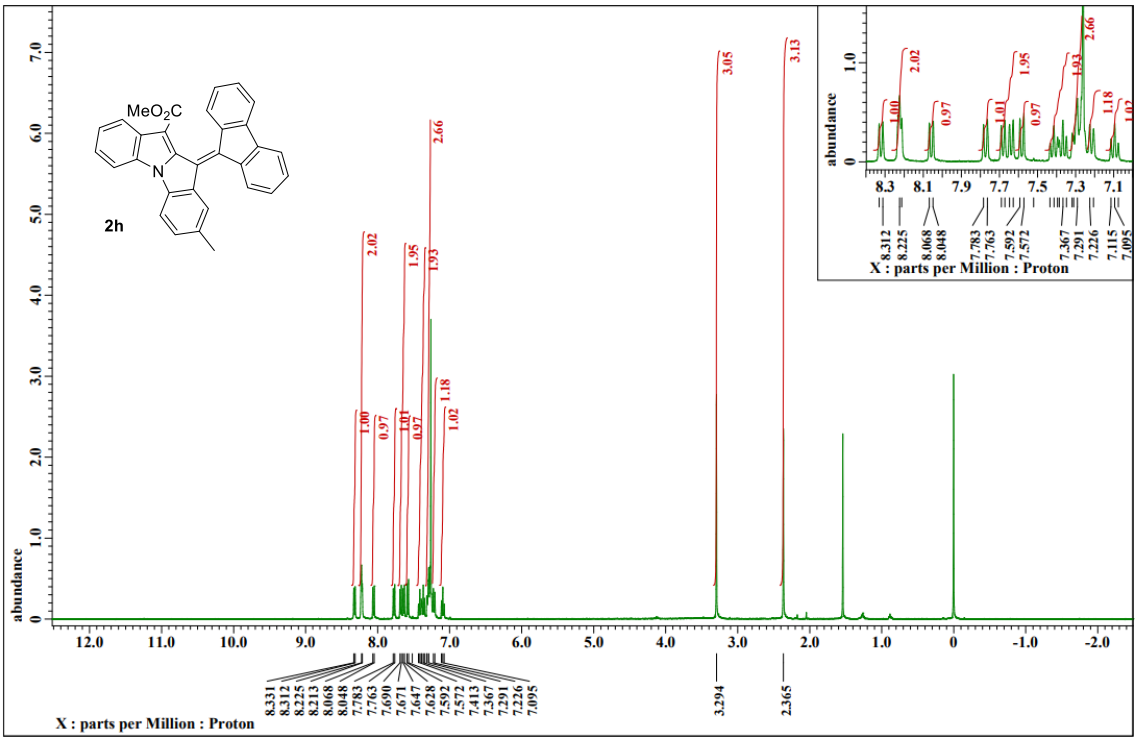


^{1}H NMR (400 MHz, $CDCl_3$)



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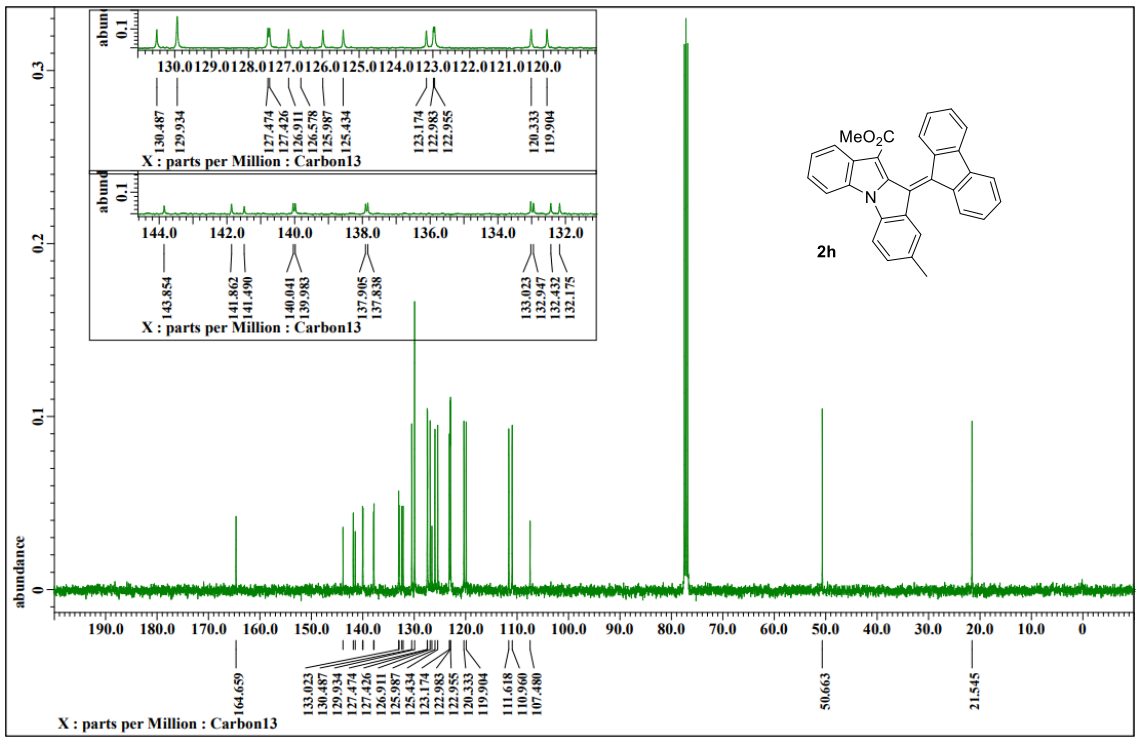

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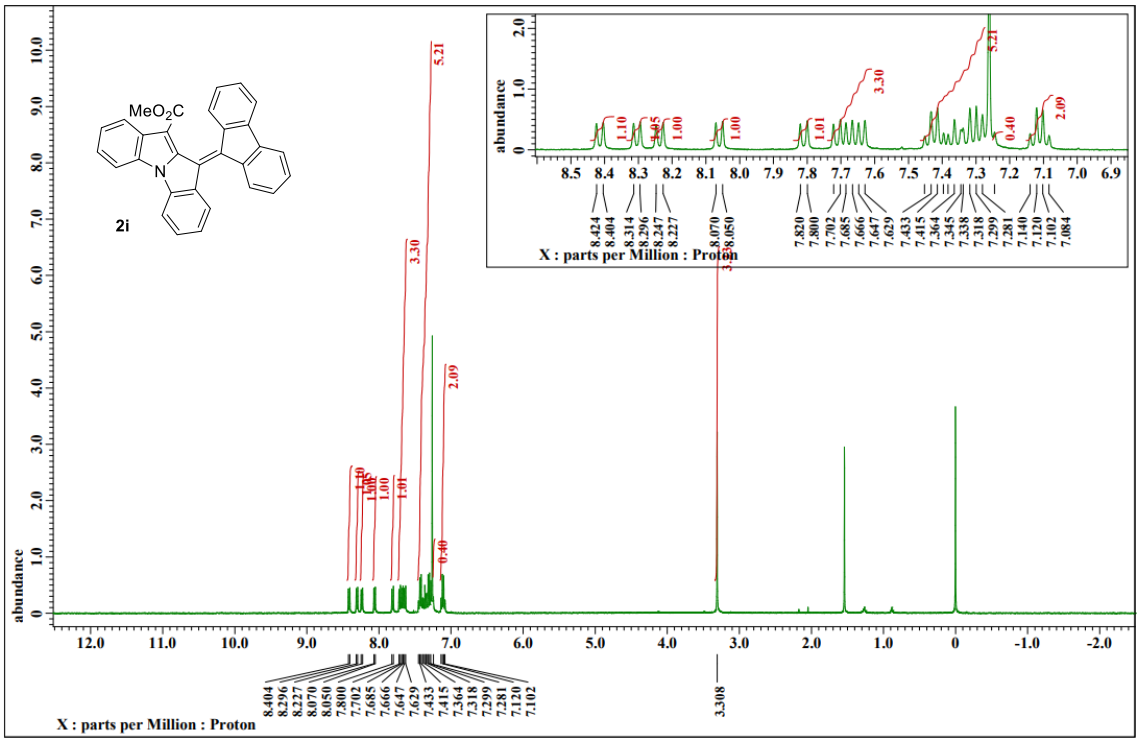
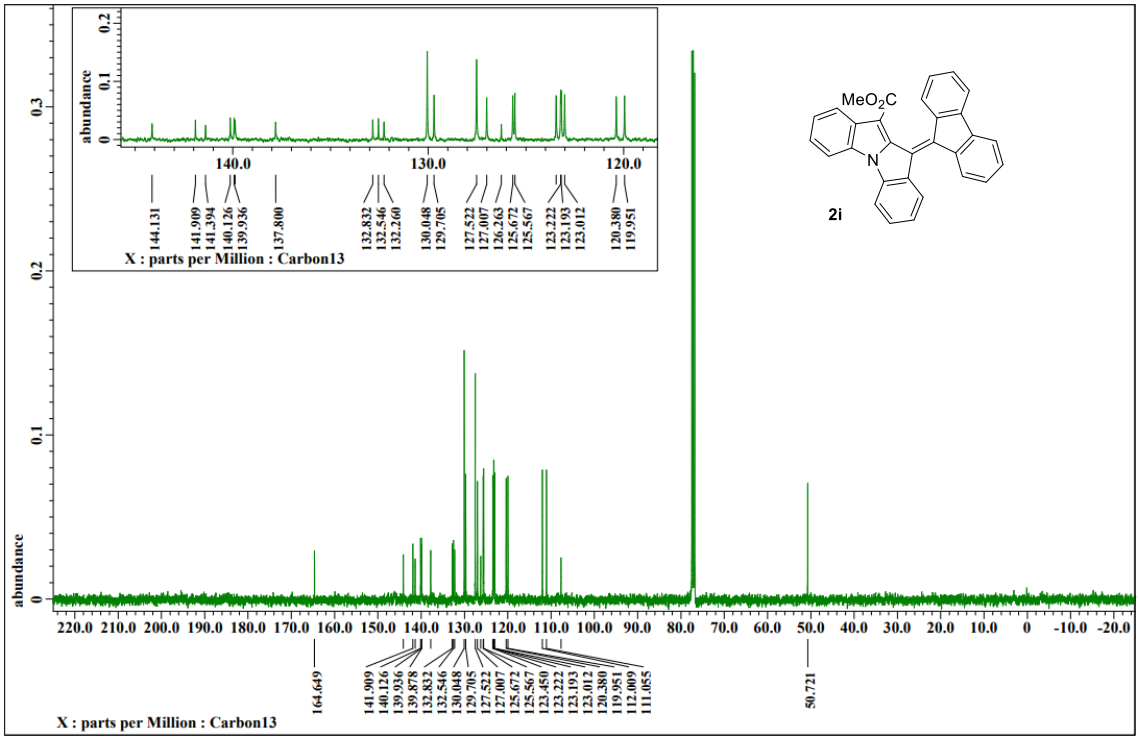


^{13}C NMR (100 MHz, $CDCl_3$)



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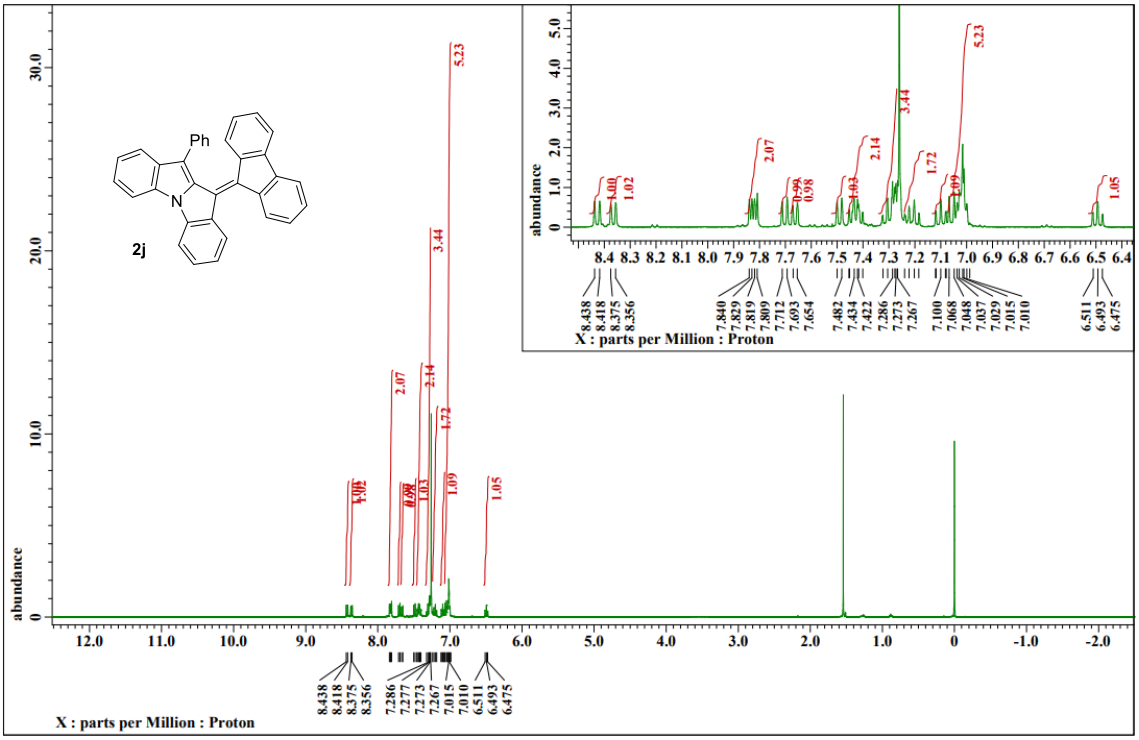
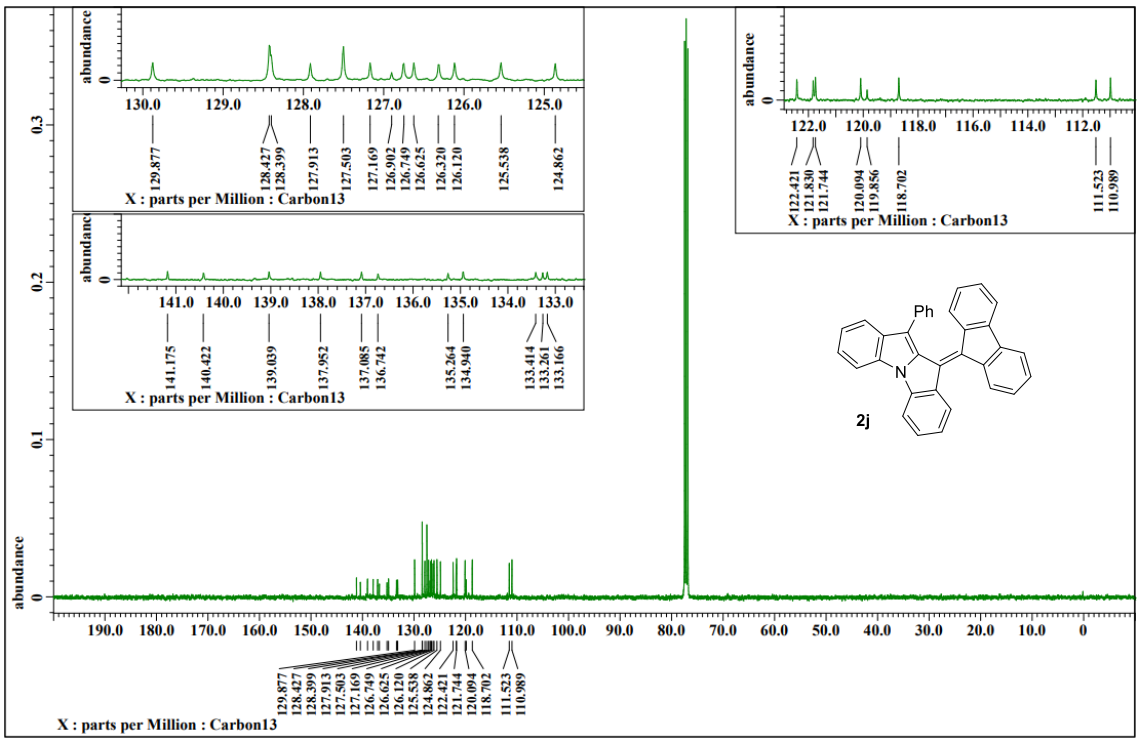
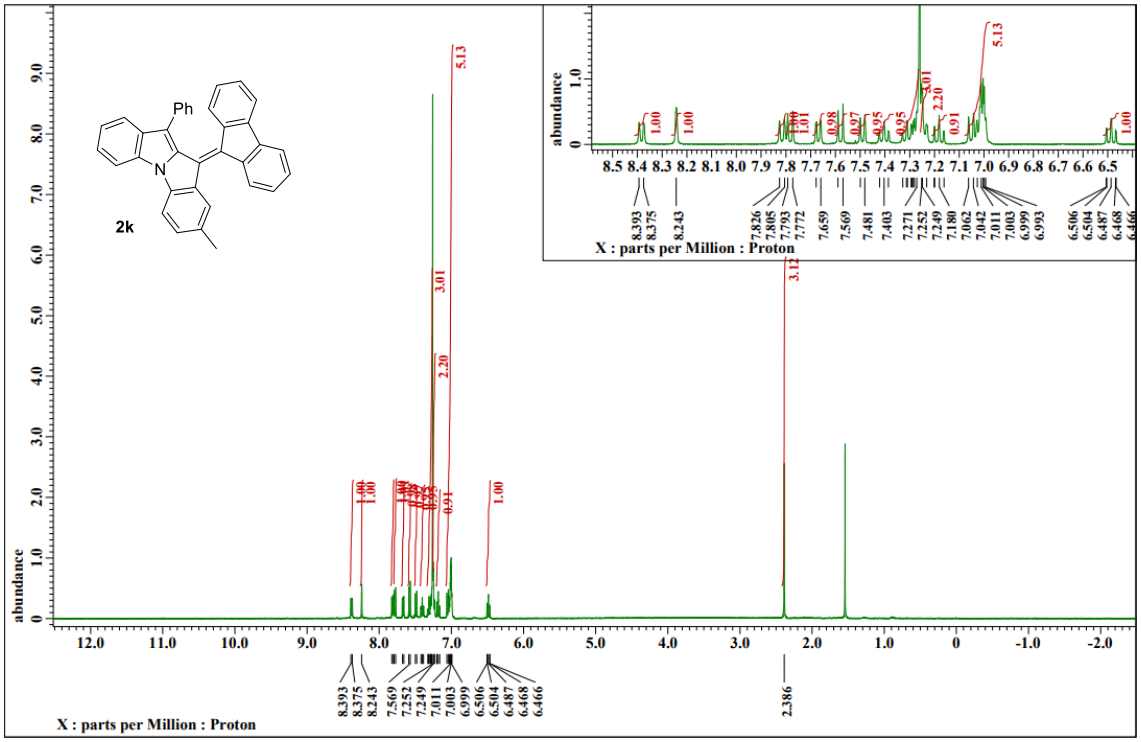


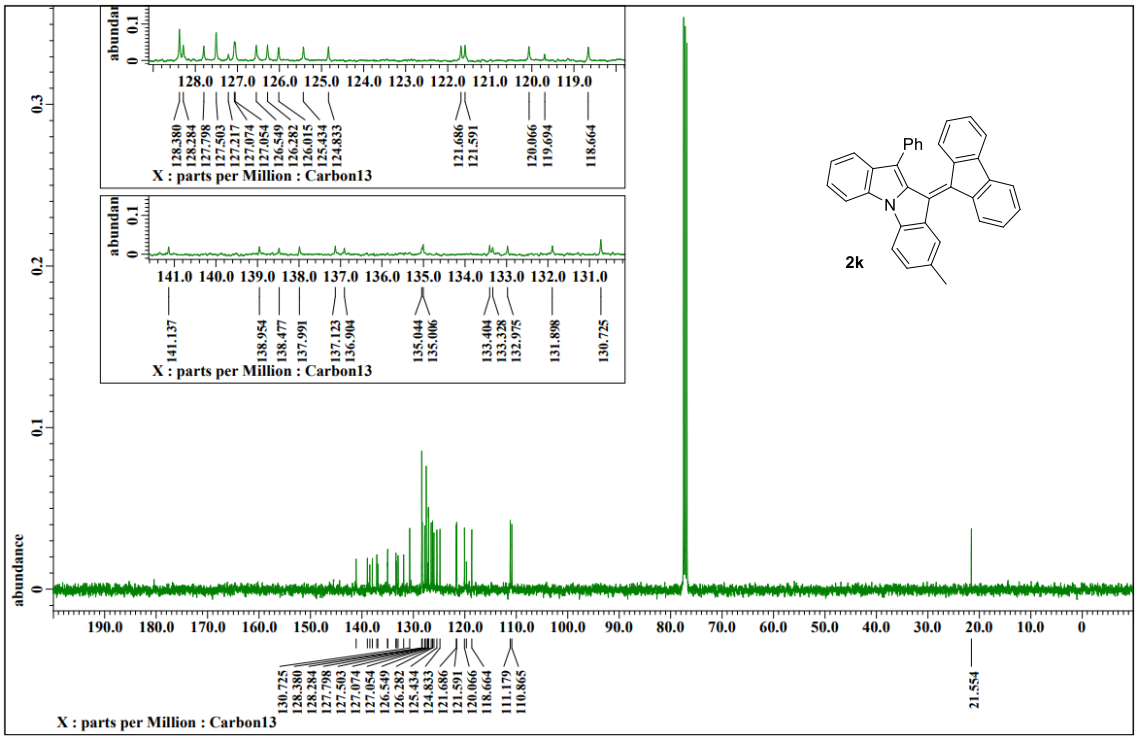
^{13}C NMR (100 MHz, $CDCl_3$)



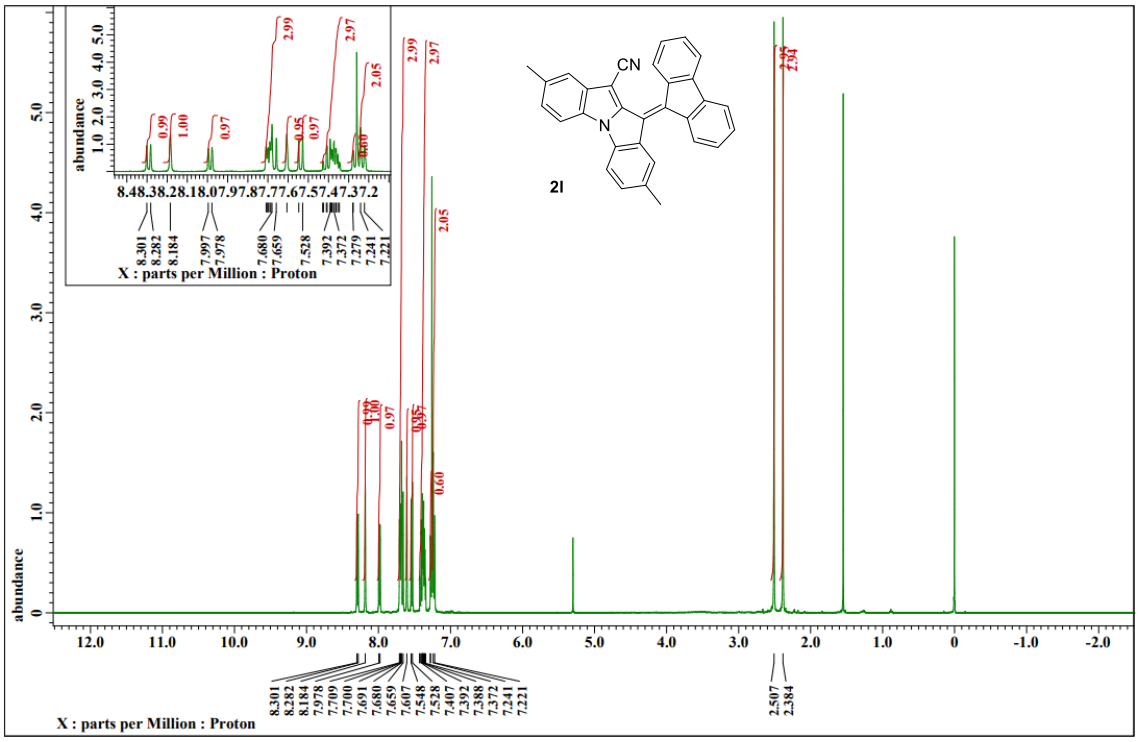
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



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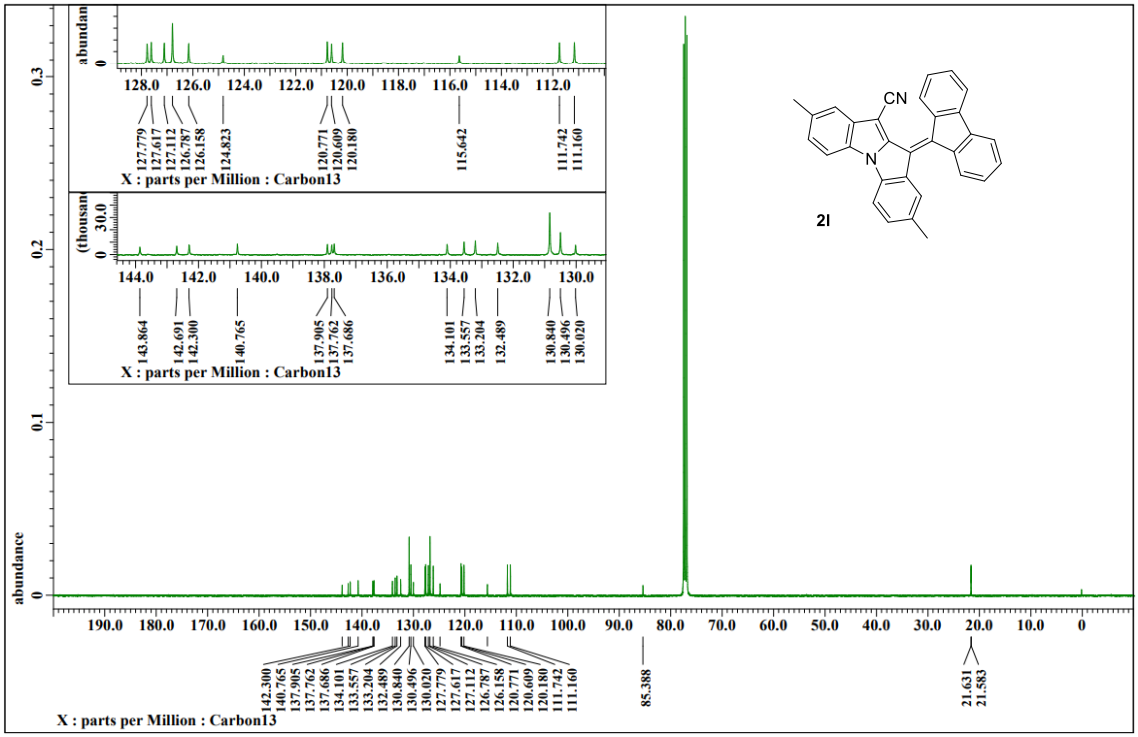

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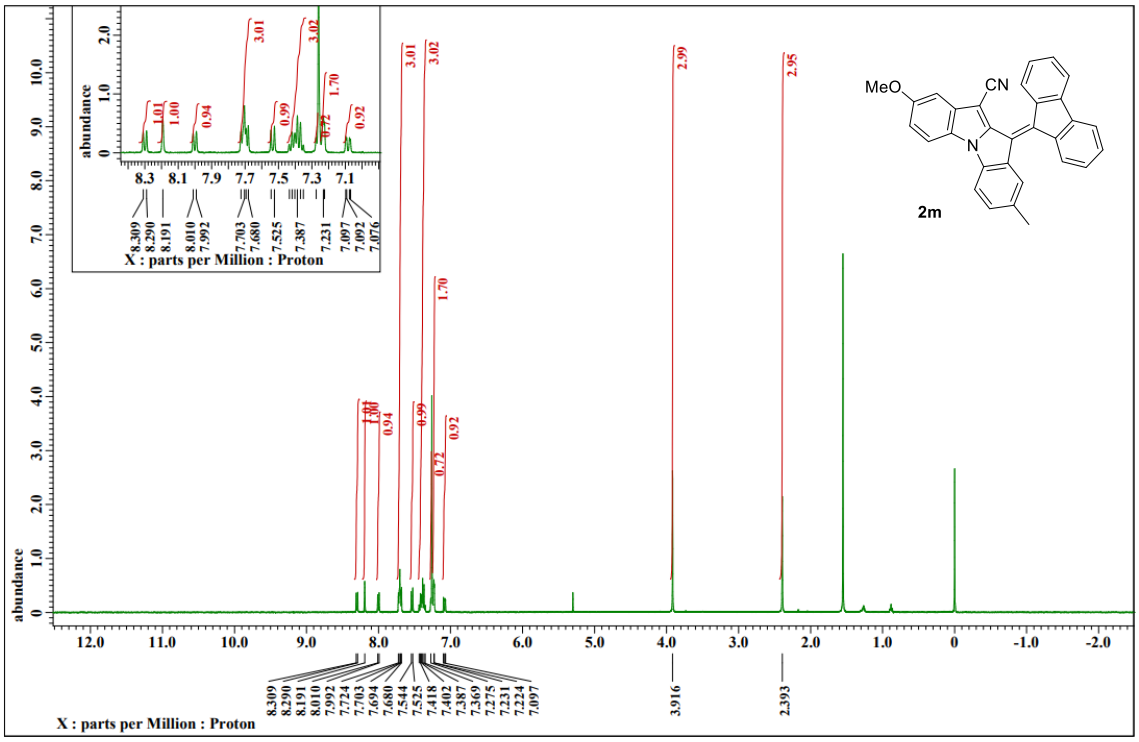

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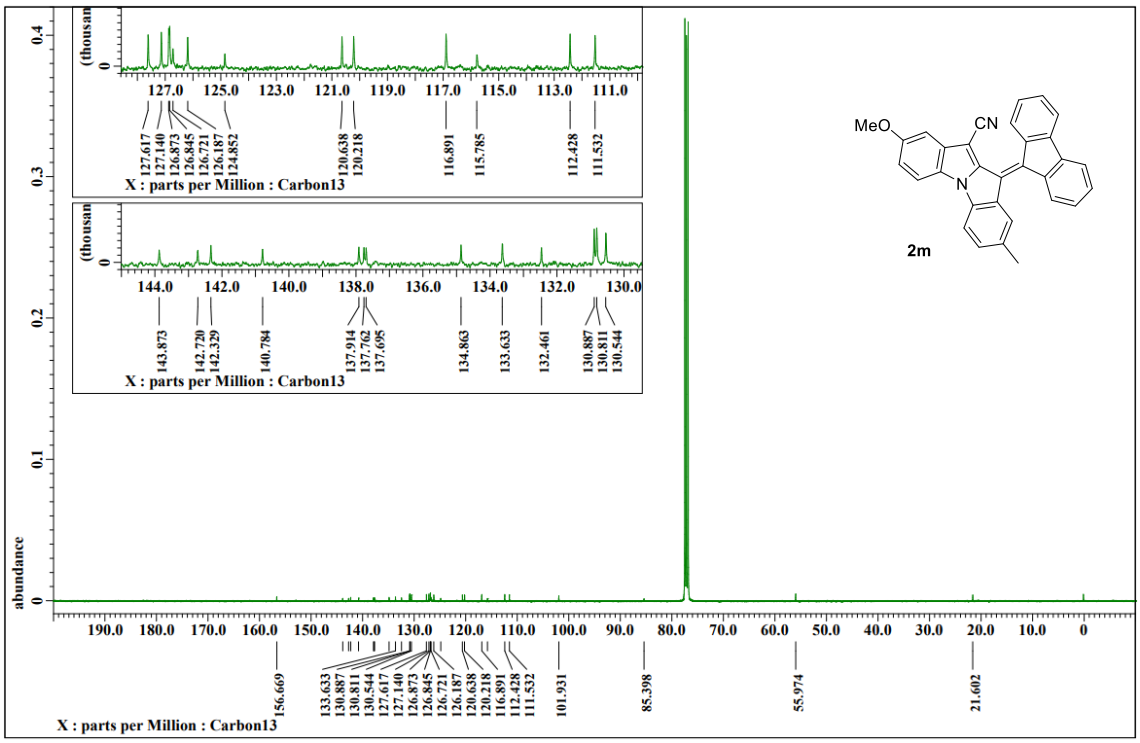

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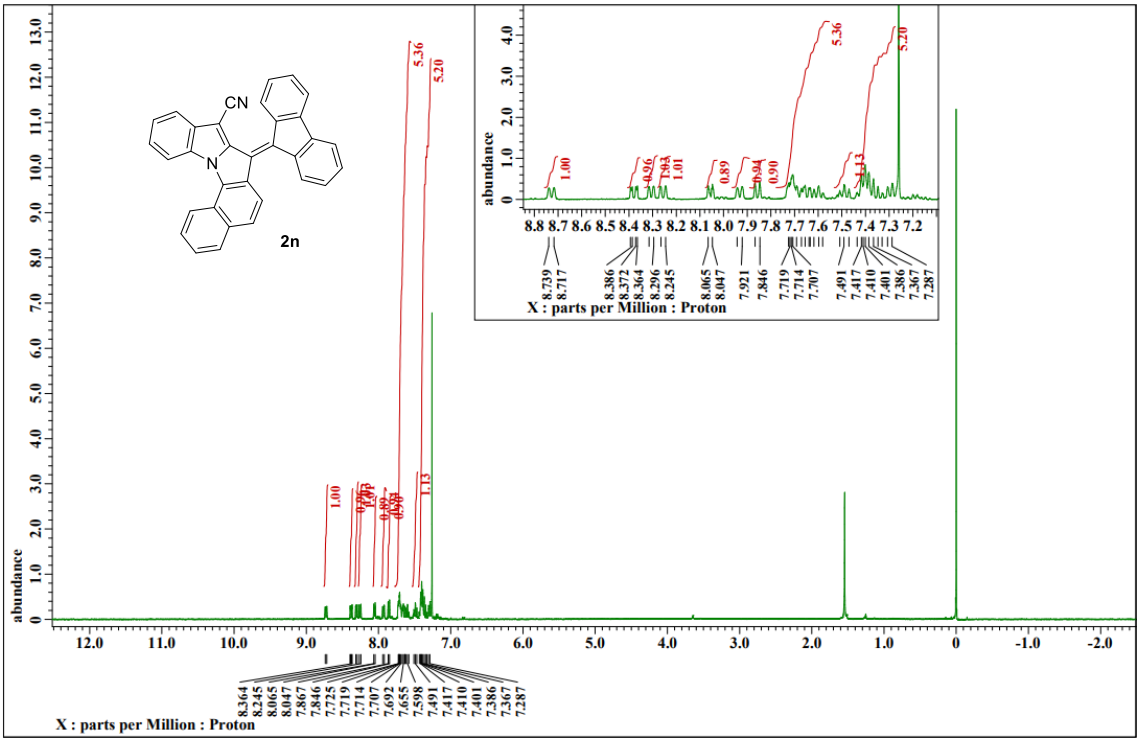

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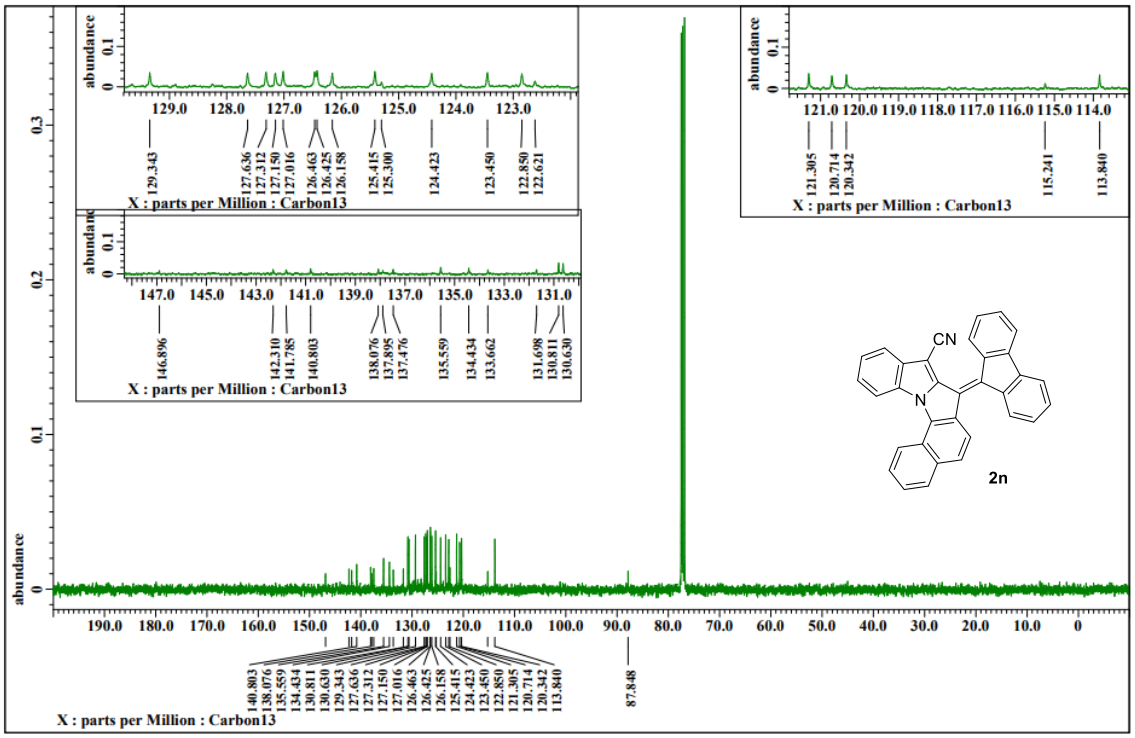

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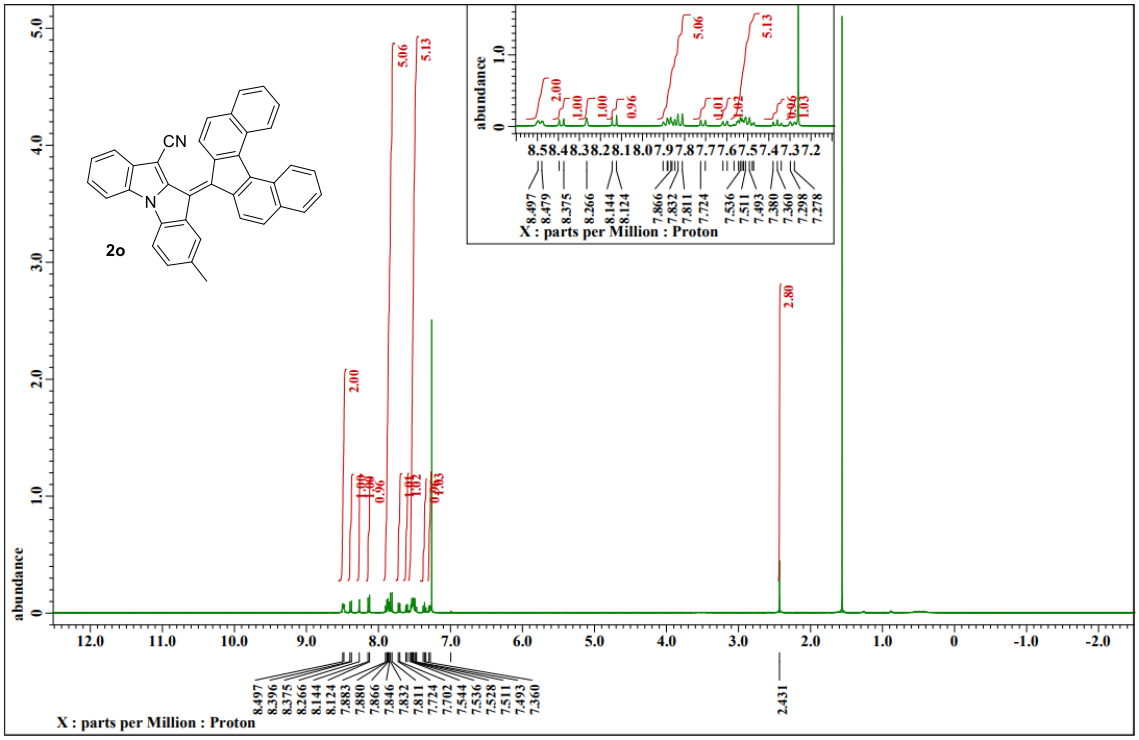

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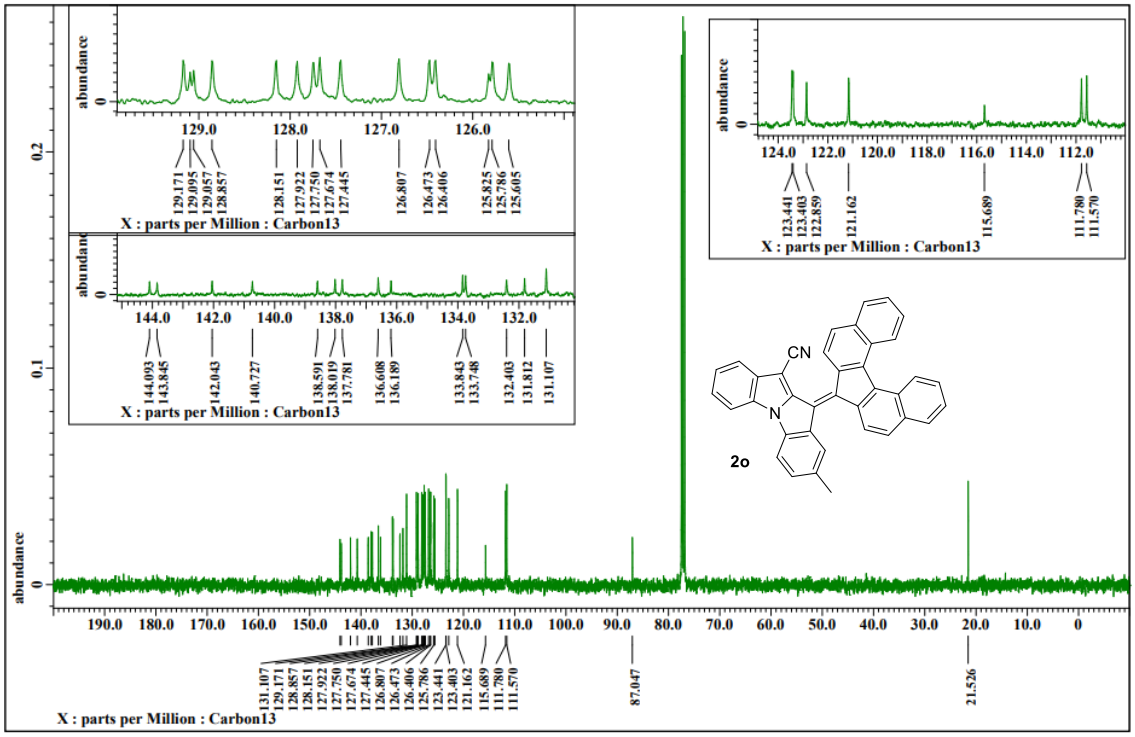

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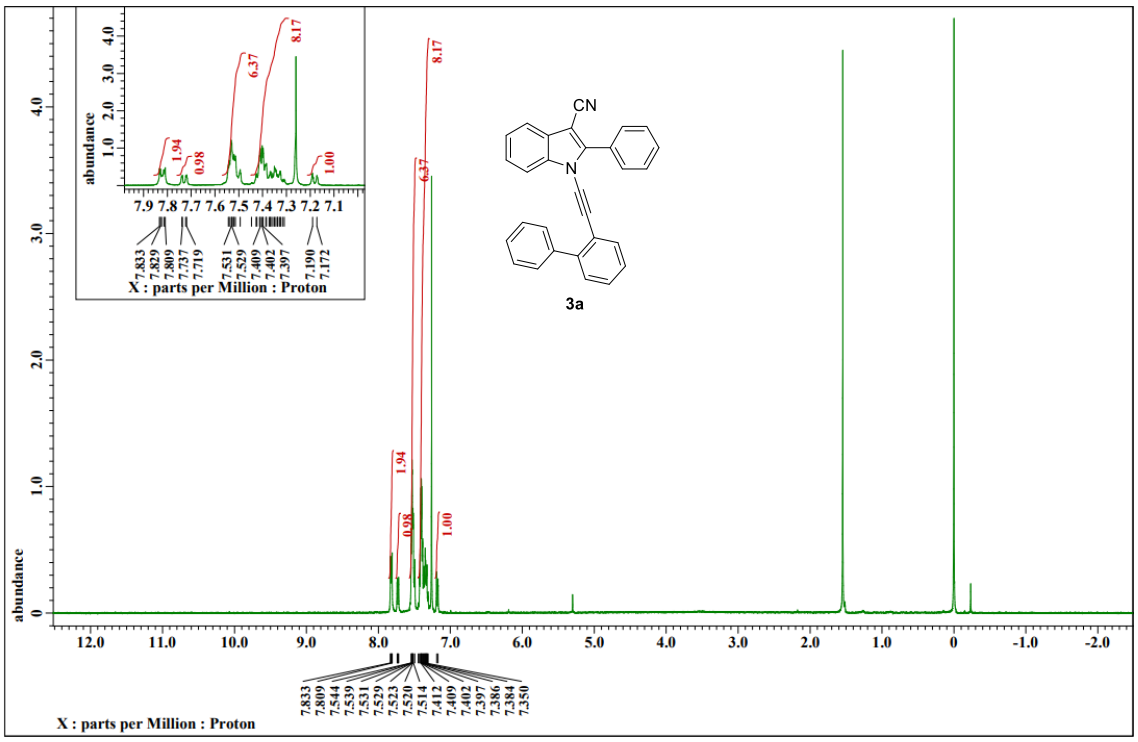
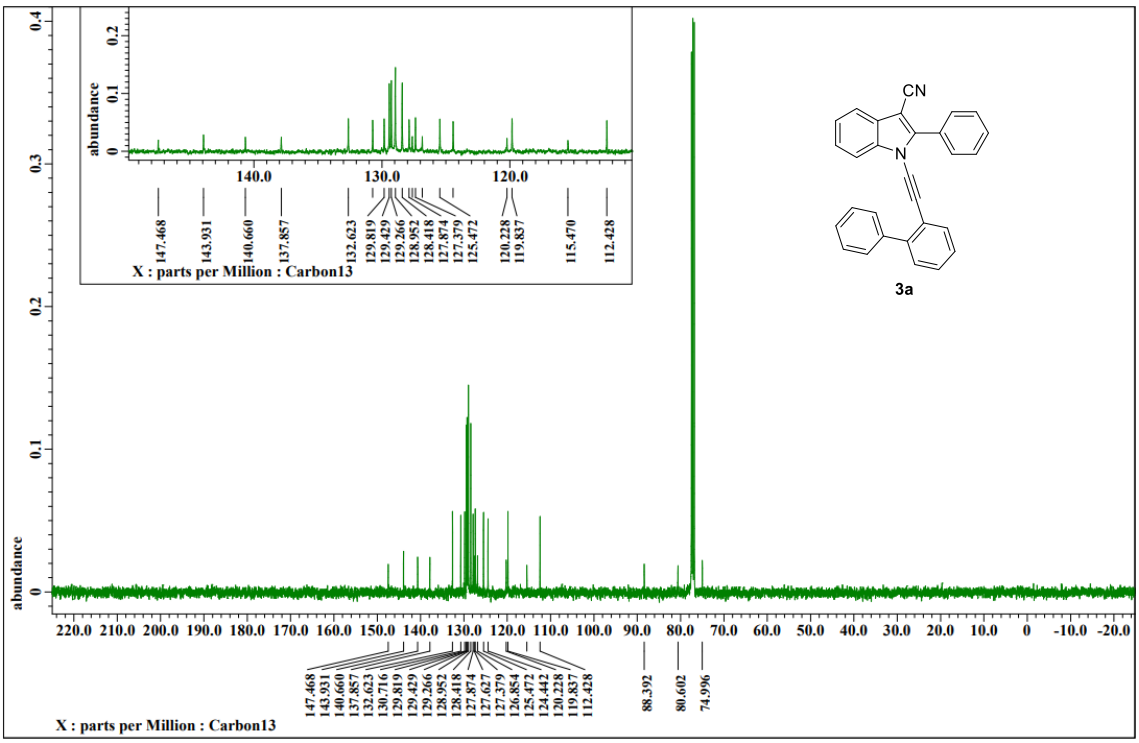


^{13}C NMR (100 MHz, $CDCl_3$)



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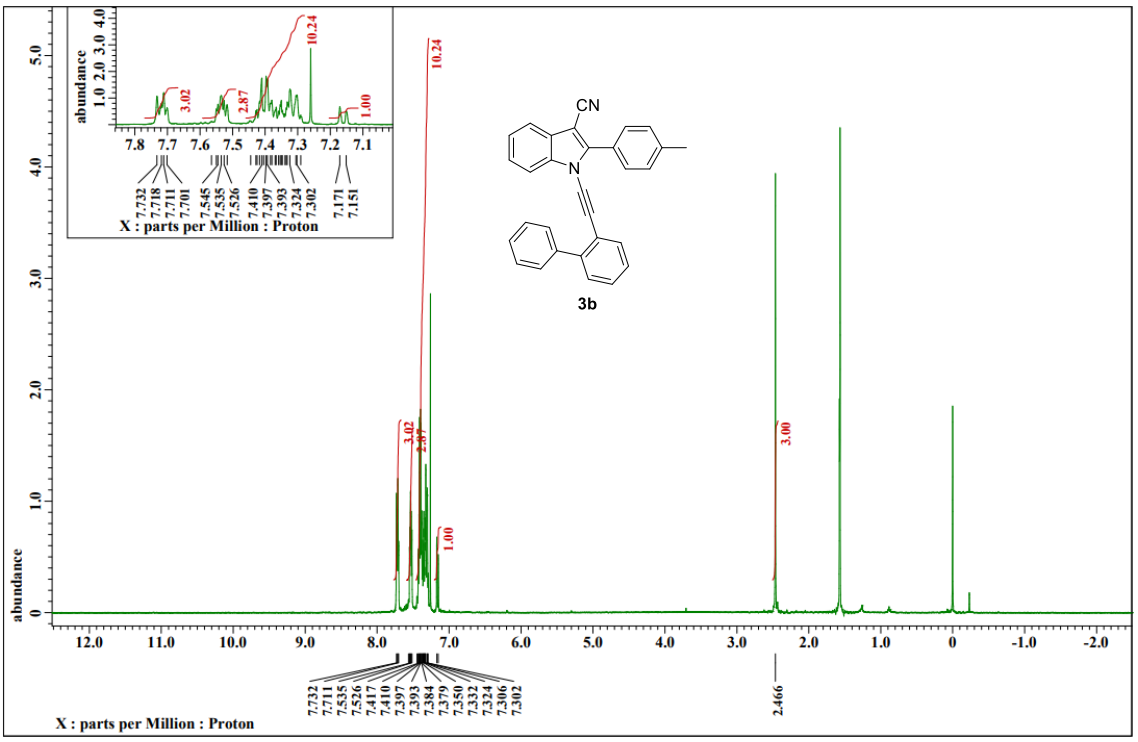

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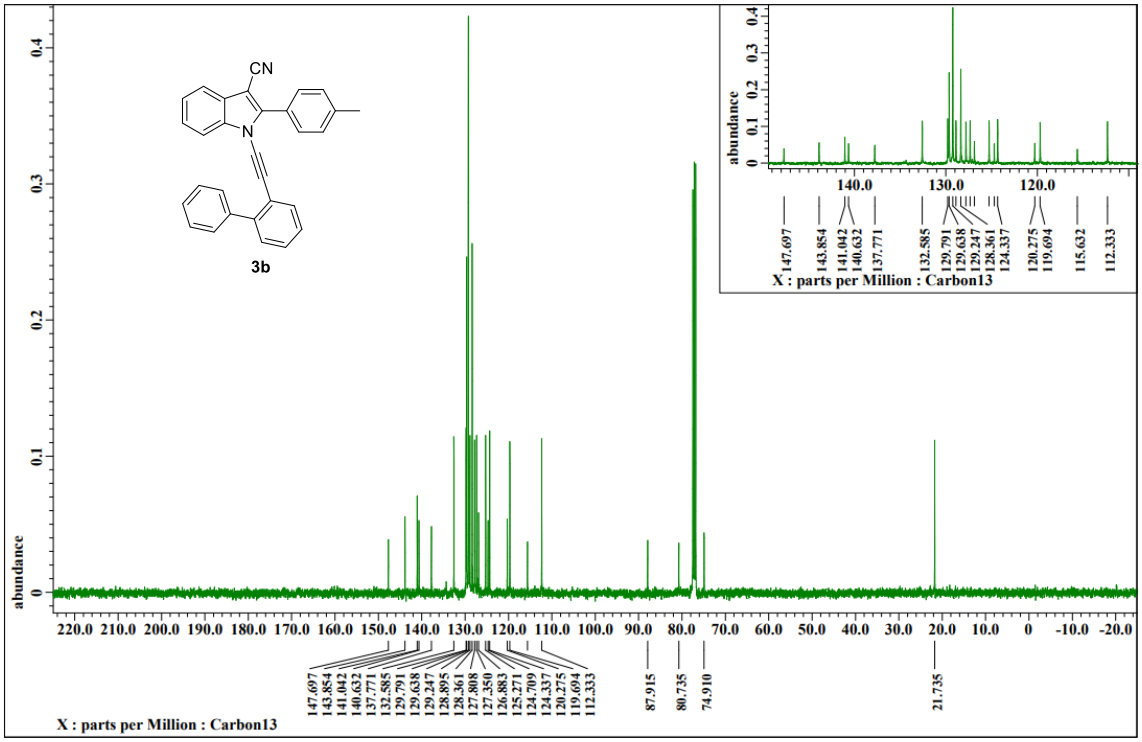

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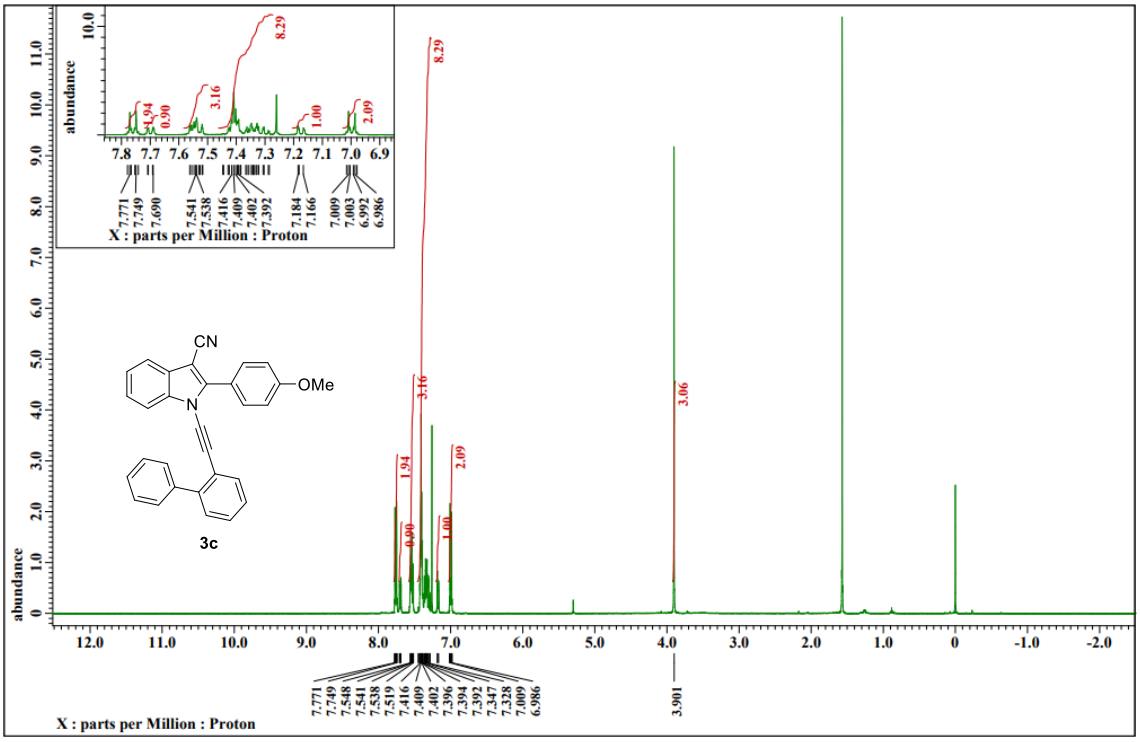
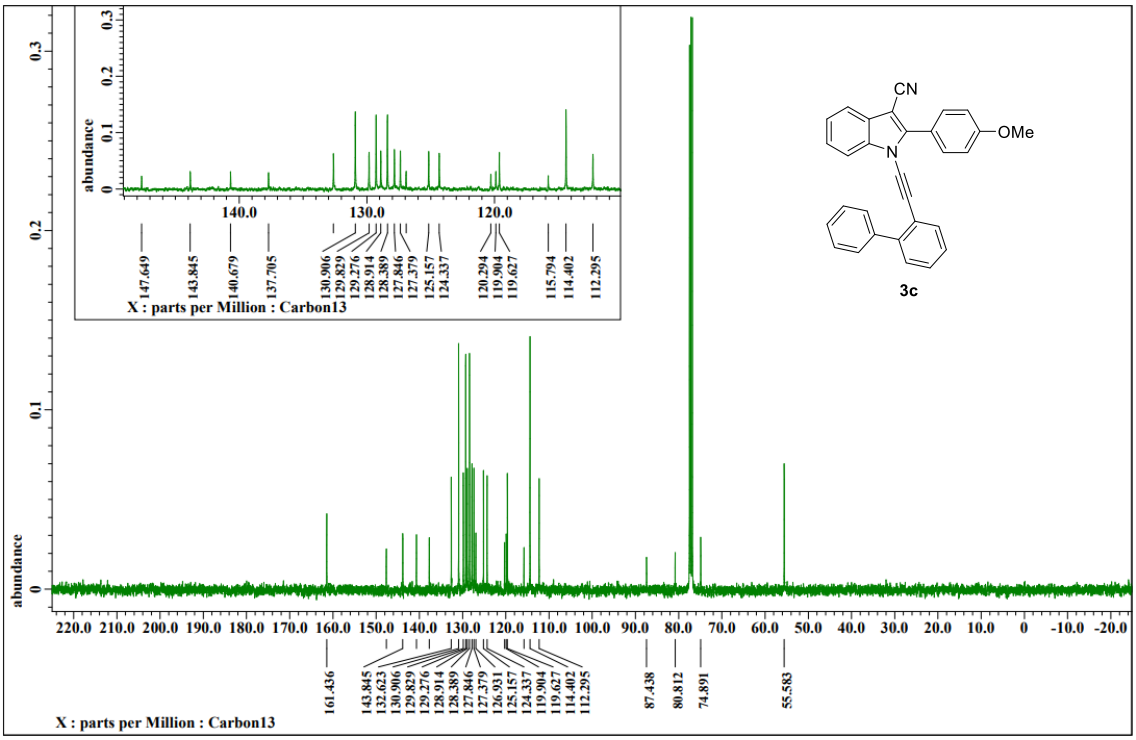
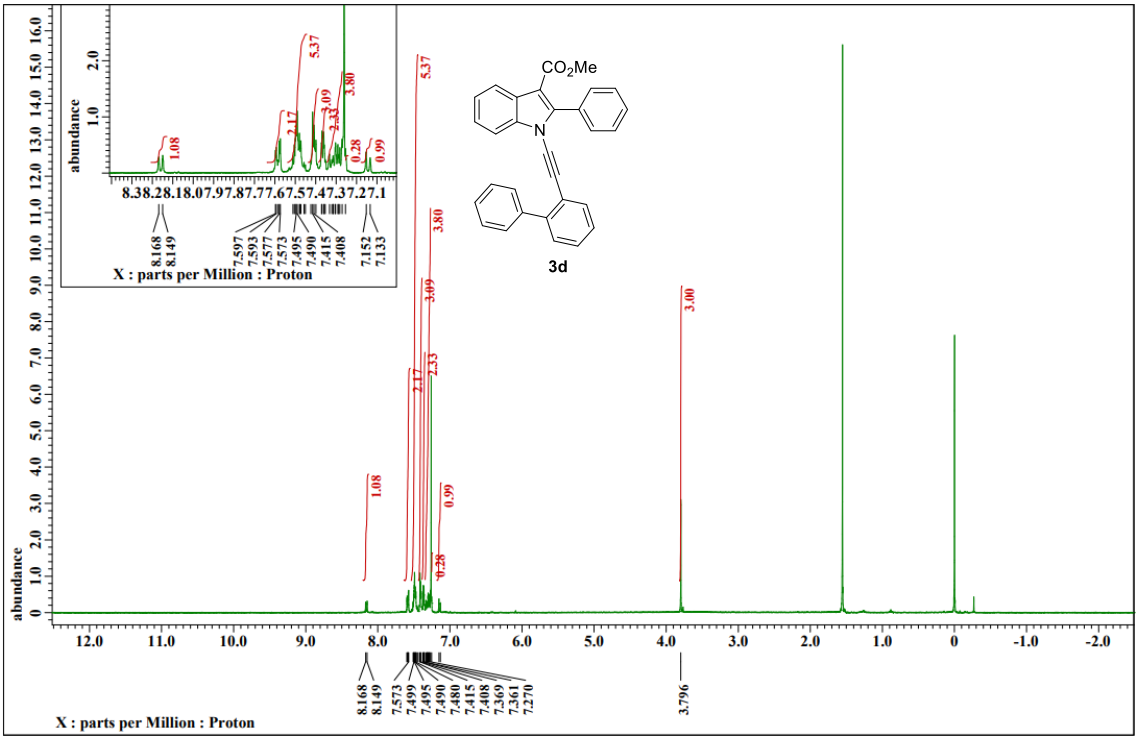


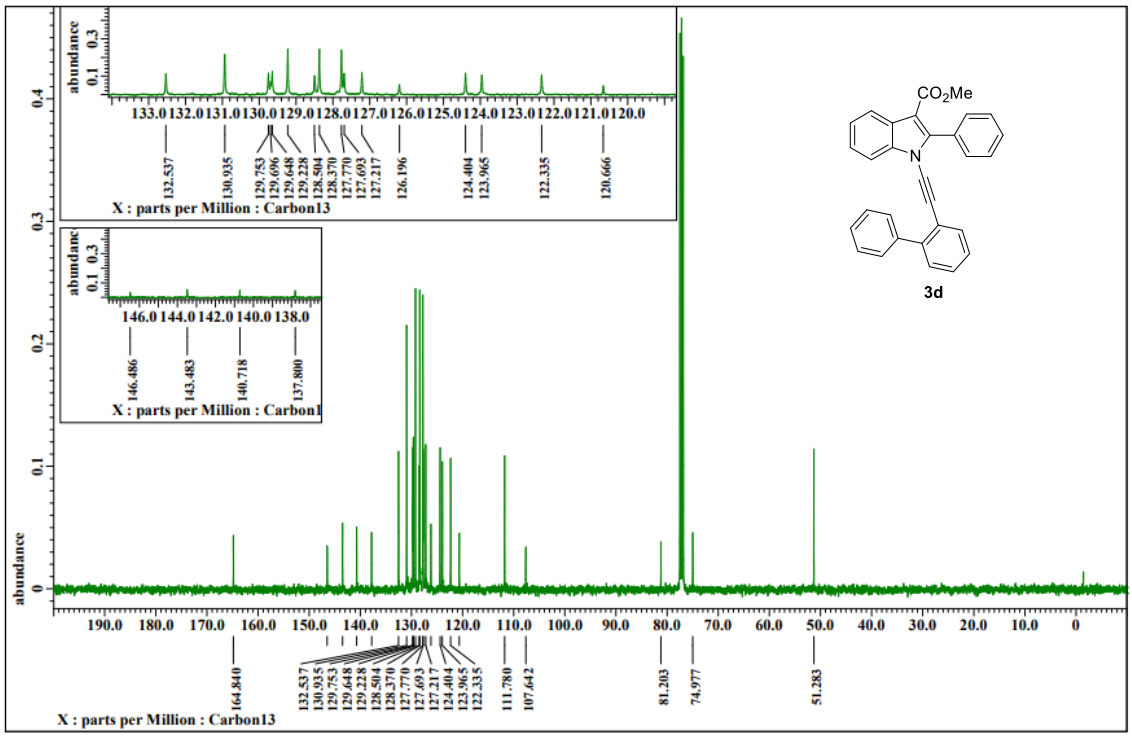
^{13}C NMR (100 MHz, $CDCl_3$)



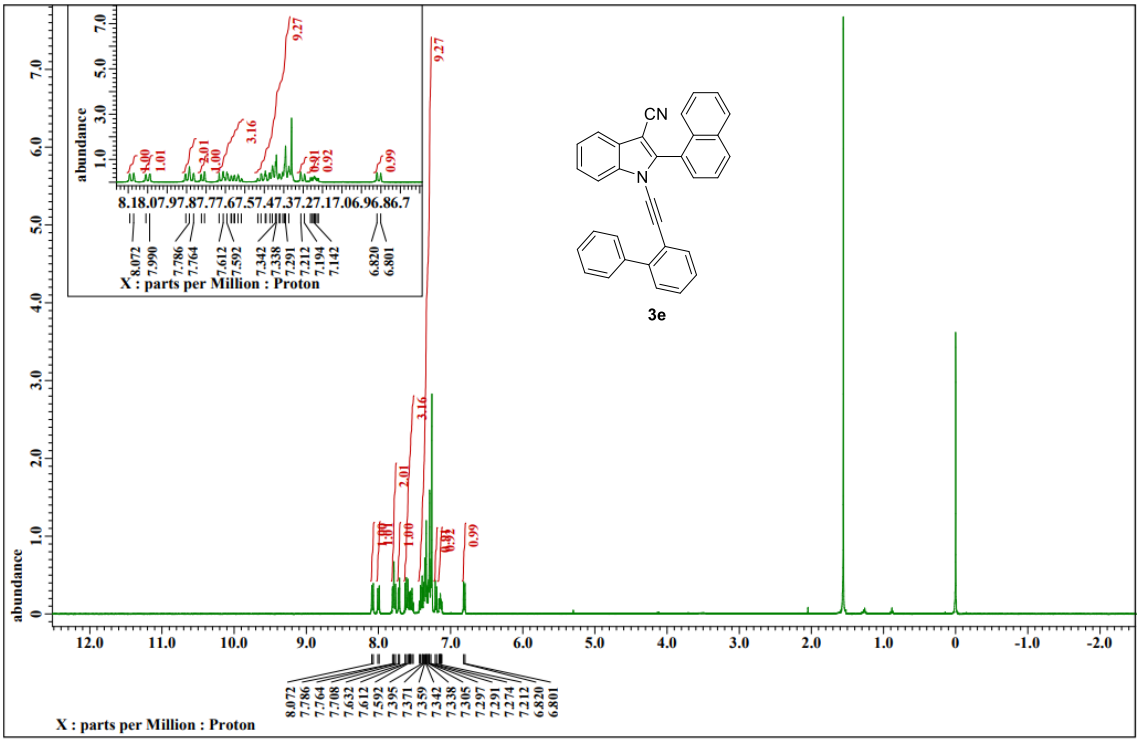
^{1}H NMR (400 MHz, $CDCl_3$)



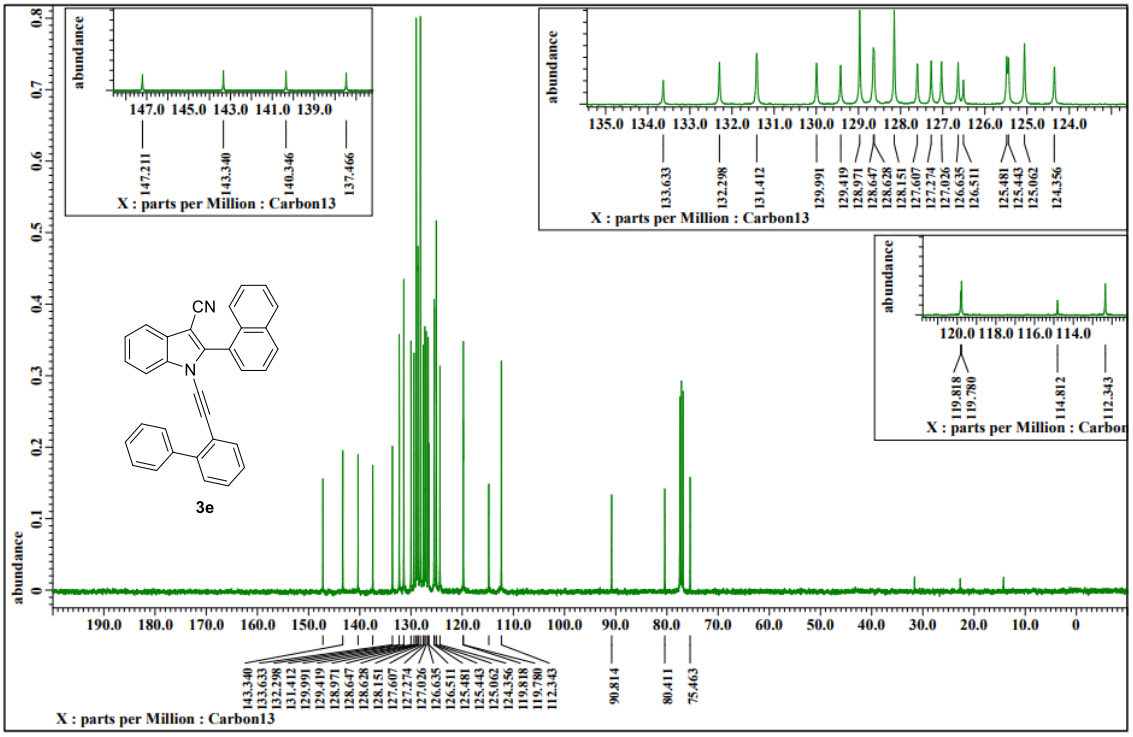
^{13}C NMR (100 MHz, $CDCl_3$)



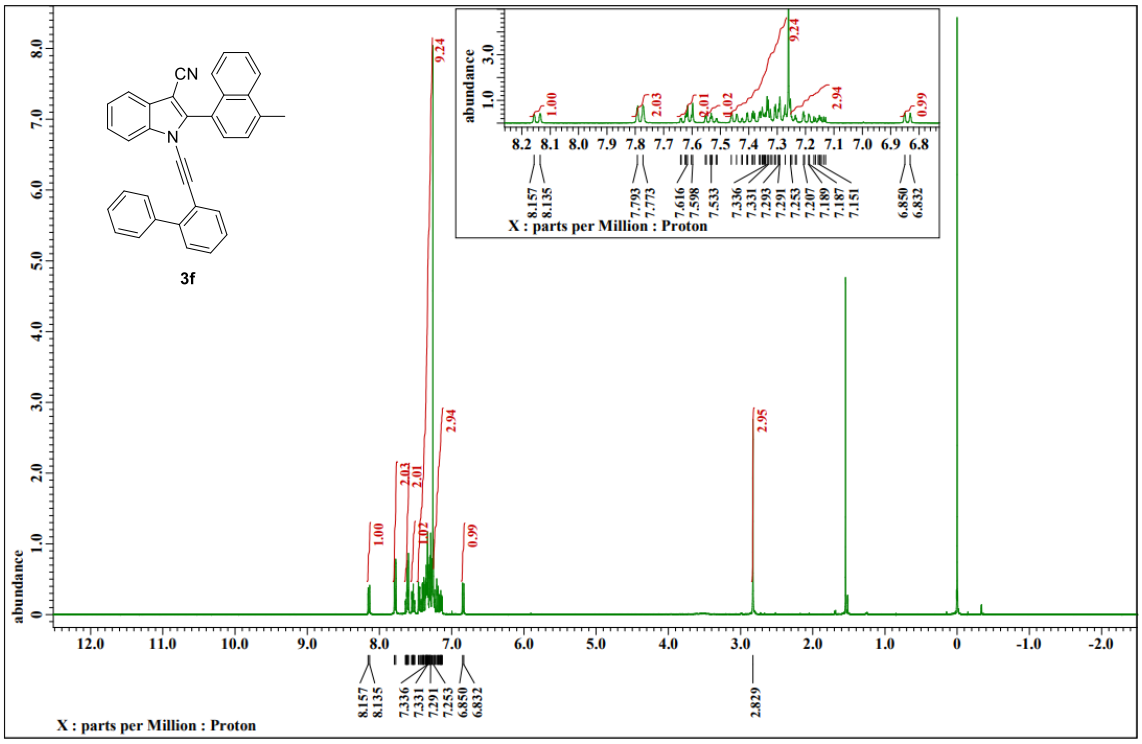
^{1}H NMR (400 MHz, $CDCl_3$)



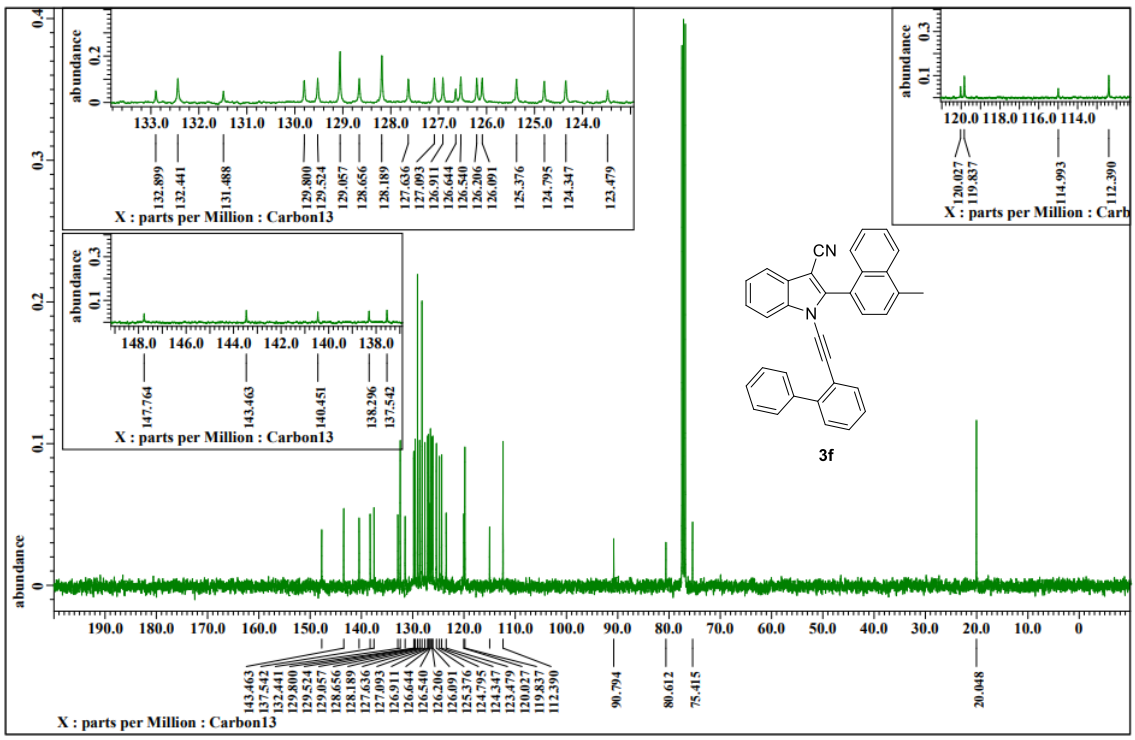
^{13}C NMR (100 MHz, $CDCl_3$)



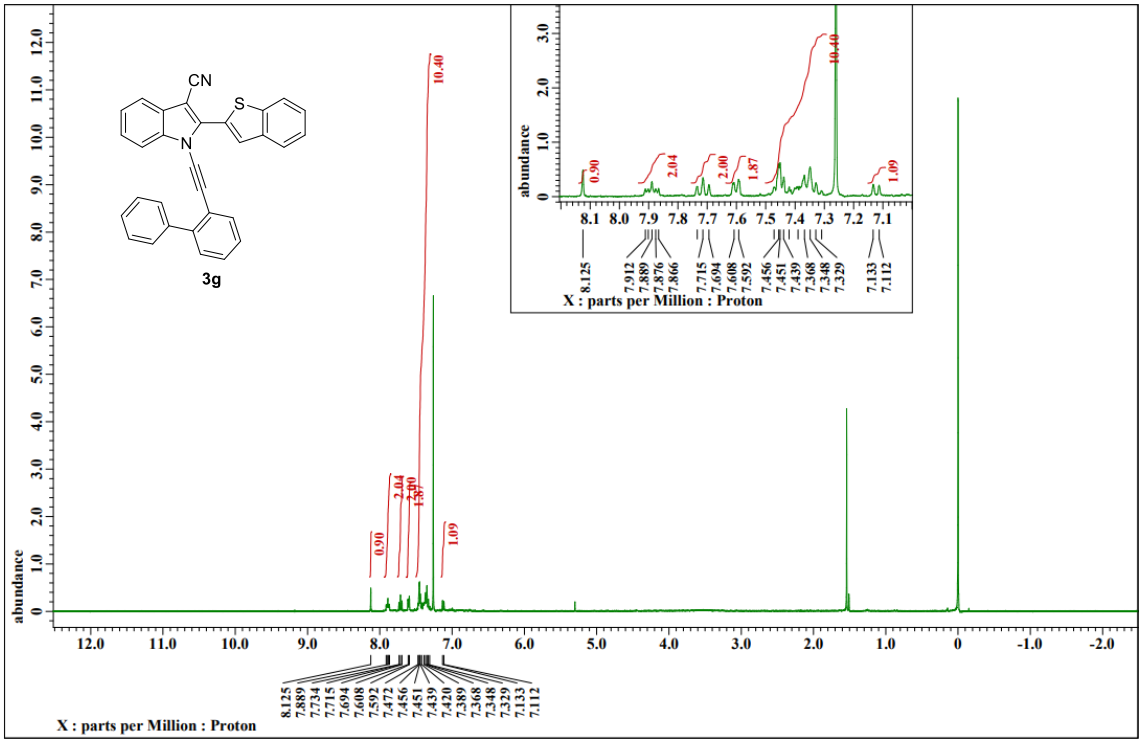
^{1}H NMR (400 MHz, $CDCl_3$)



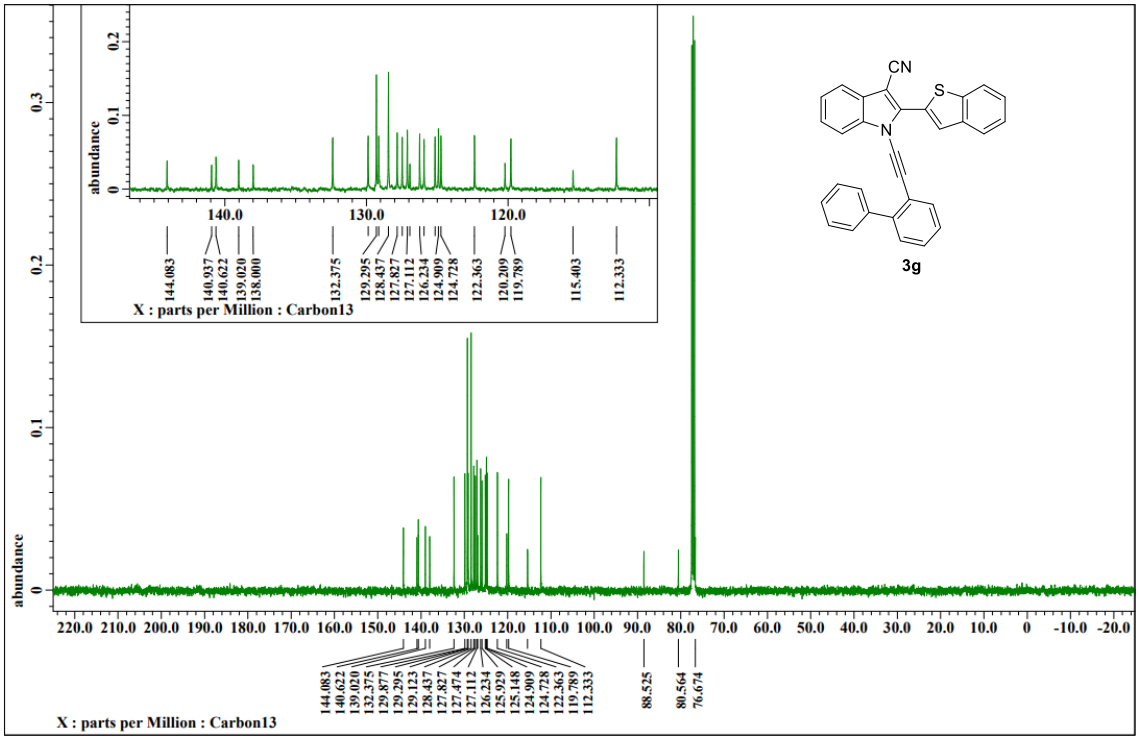
^{13}C NMR (100 MHz, $CDCl_3$)



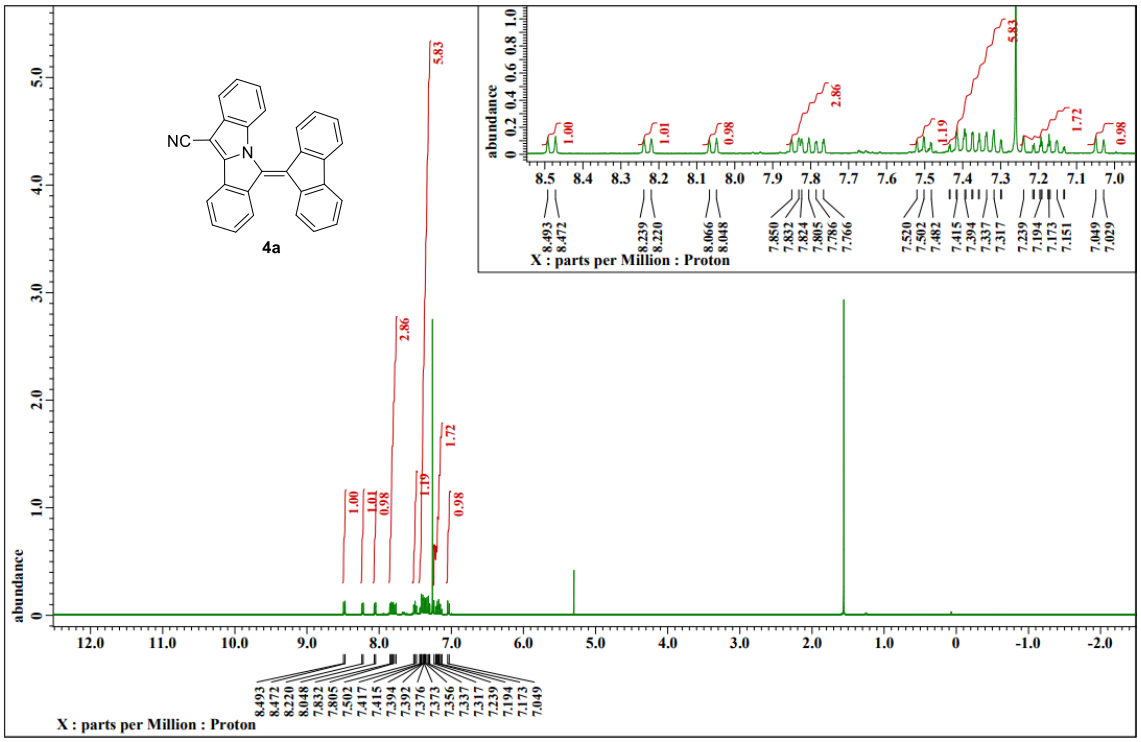
^{1}H NMR (400 MHz, $CDCl_3$)



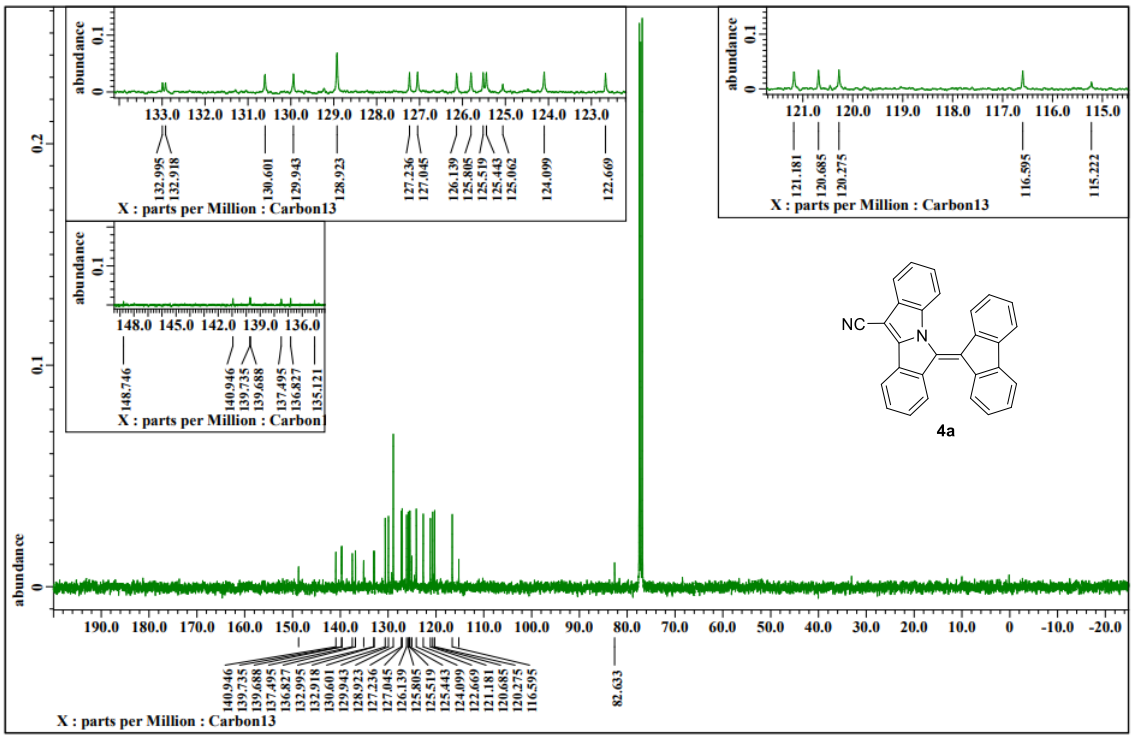
^{13}C NMR (100 MHz, $CDCl_3$)



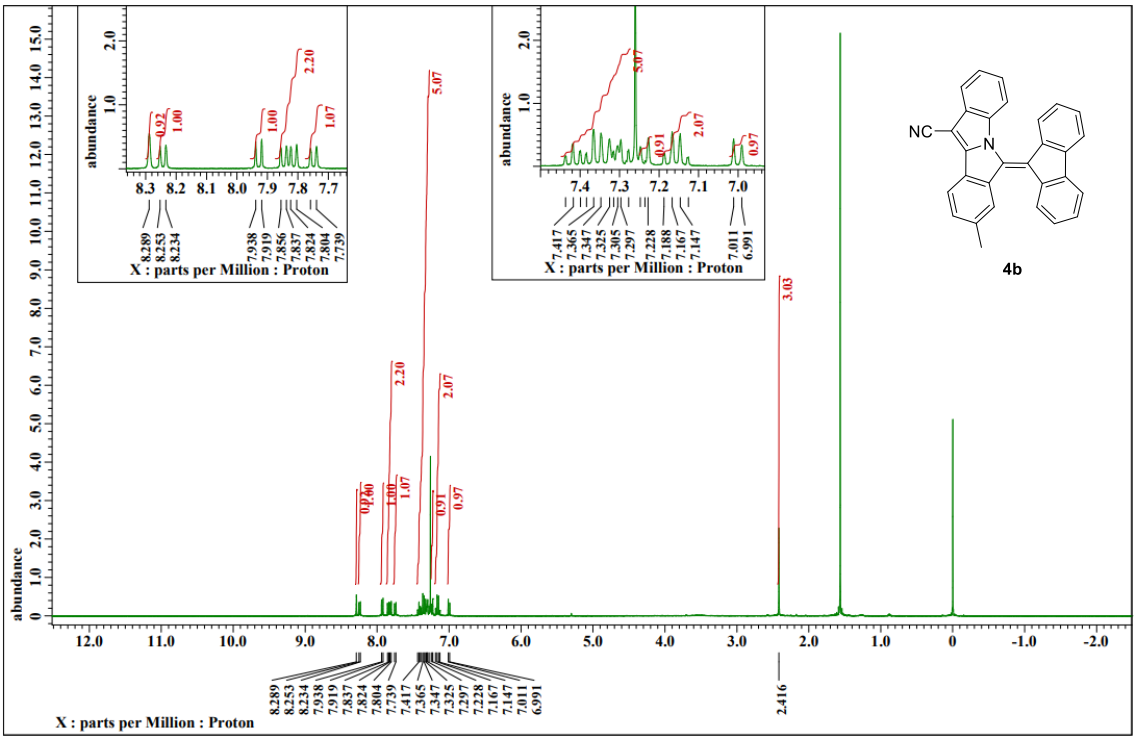
^{1}H NMR (400 MHz, $CDCl_3$)



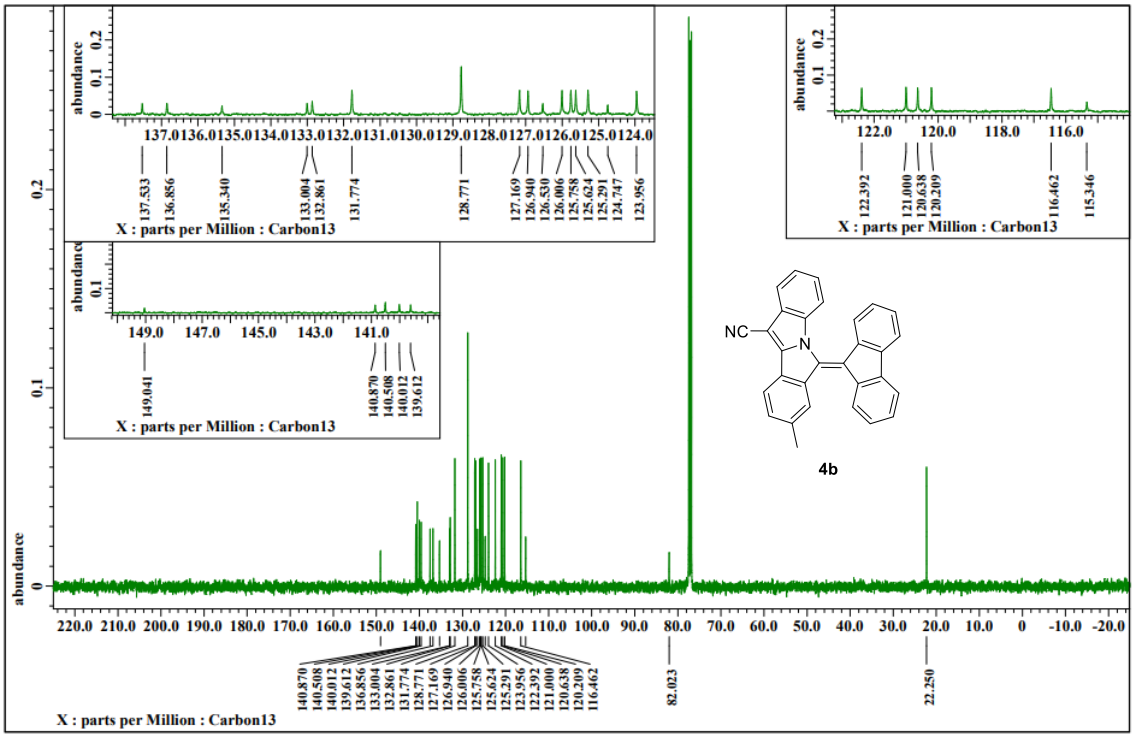
^{13}C NMR (100 MHz, $CDCl_3$)



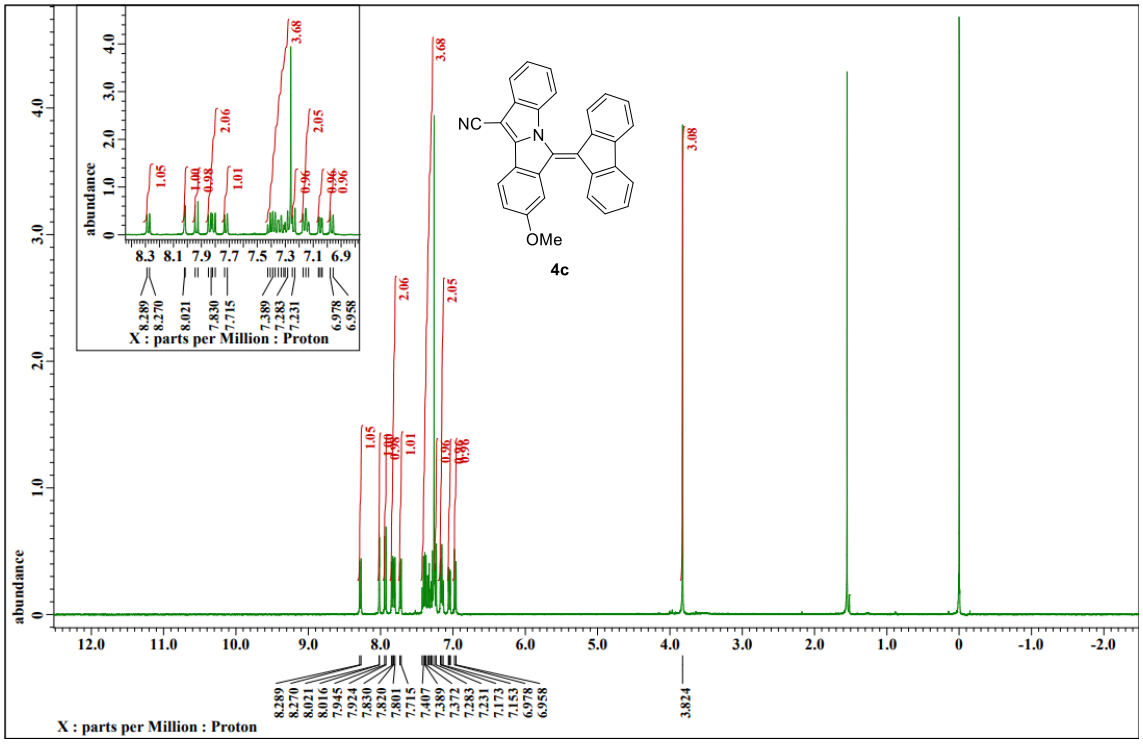
^{1}H NMR (400 MHz, $CDCl_3$)



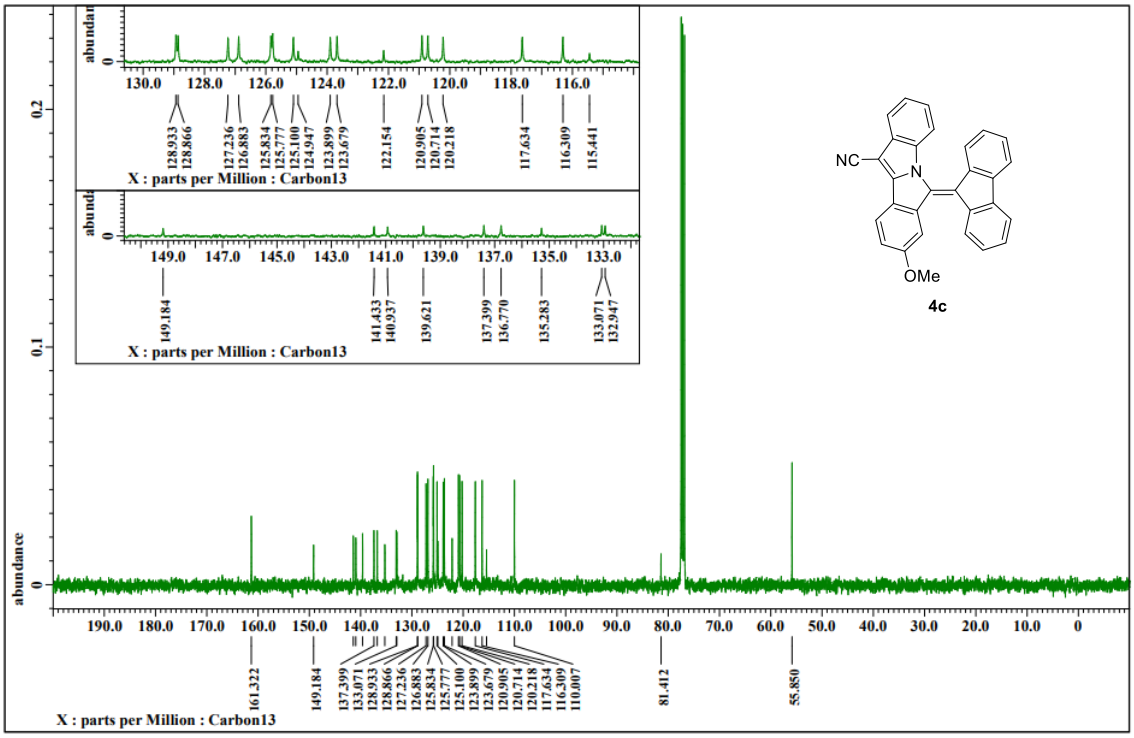
^{13}C NMR (100 MHz, $CDCl_3$)



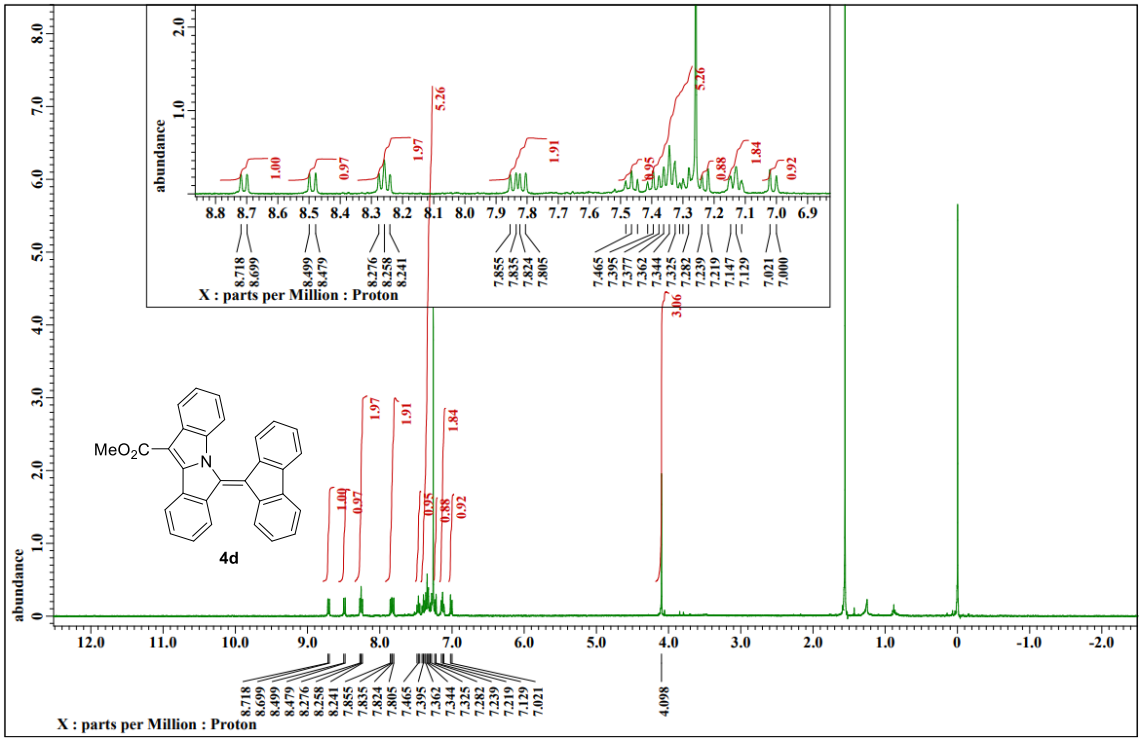
^{1}H NMR (400 MHz, $CDCl_3$)



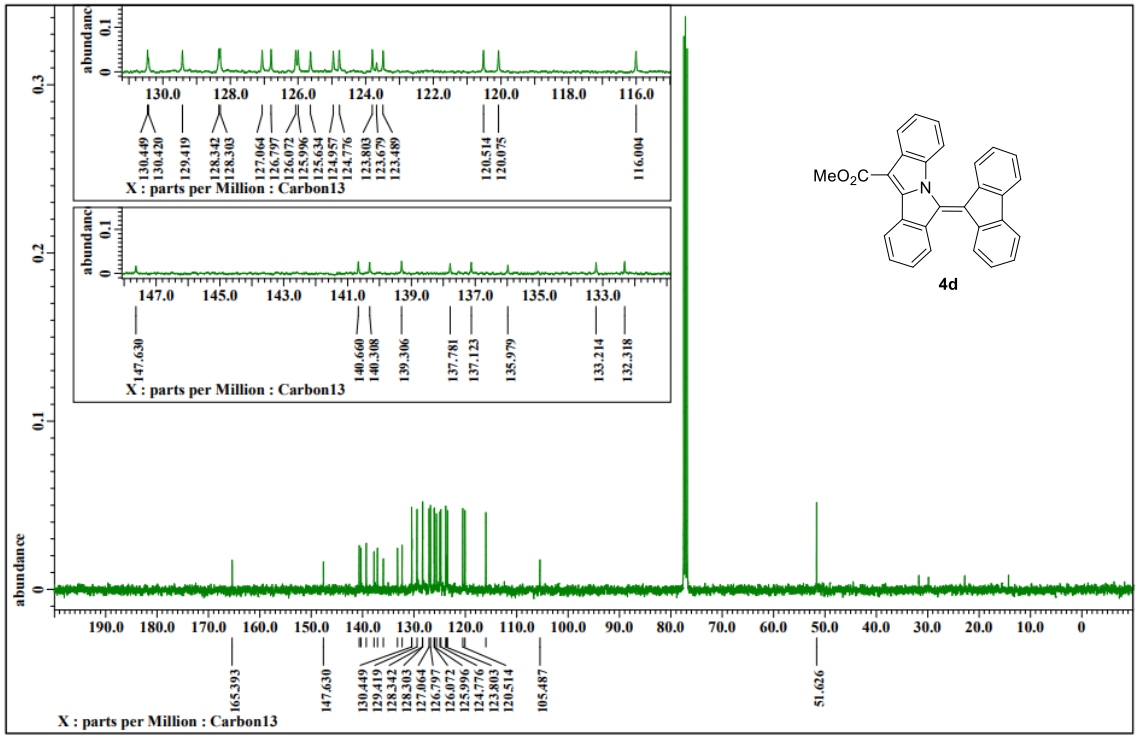
^{13}C NMR (100 MHz, $CDCl_3$)



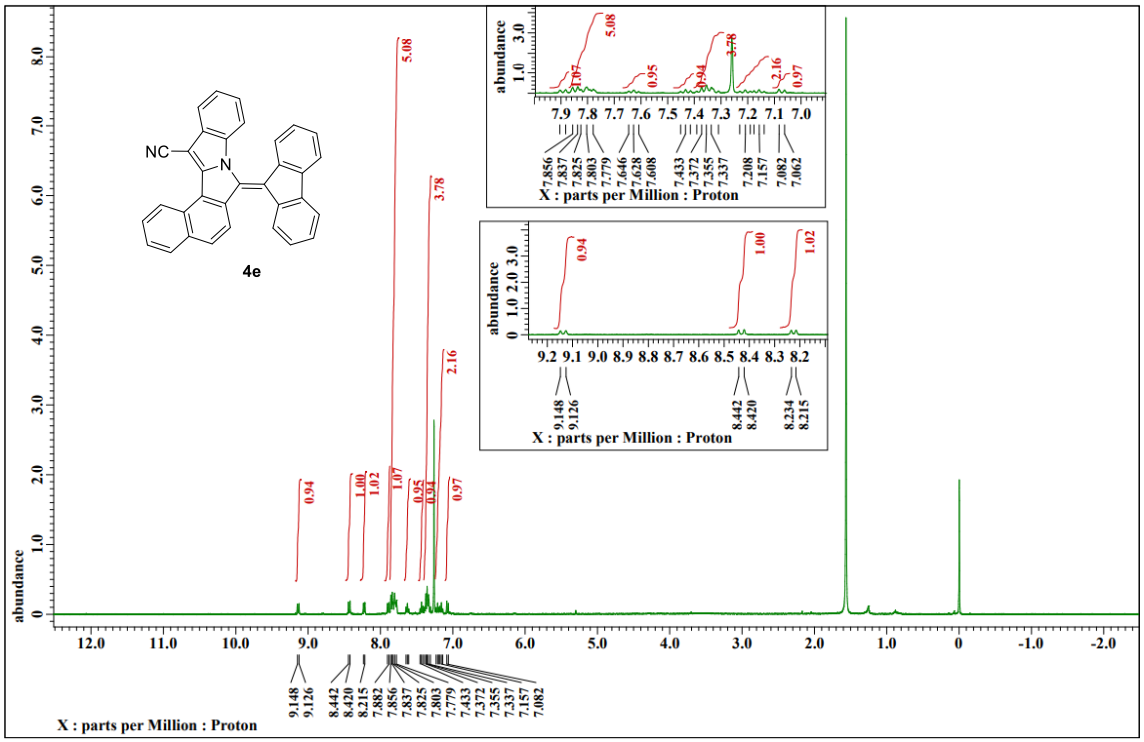
H NMR (400 MHz, $CDCl_3$)



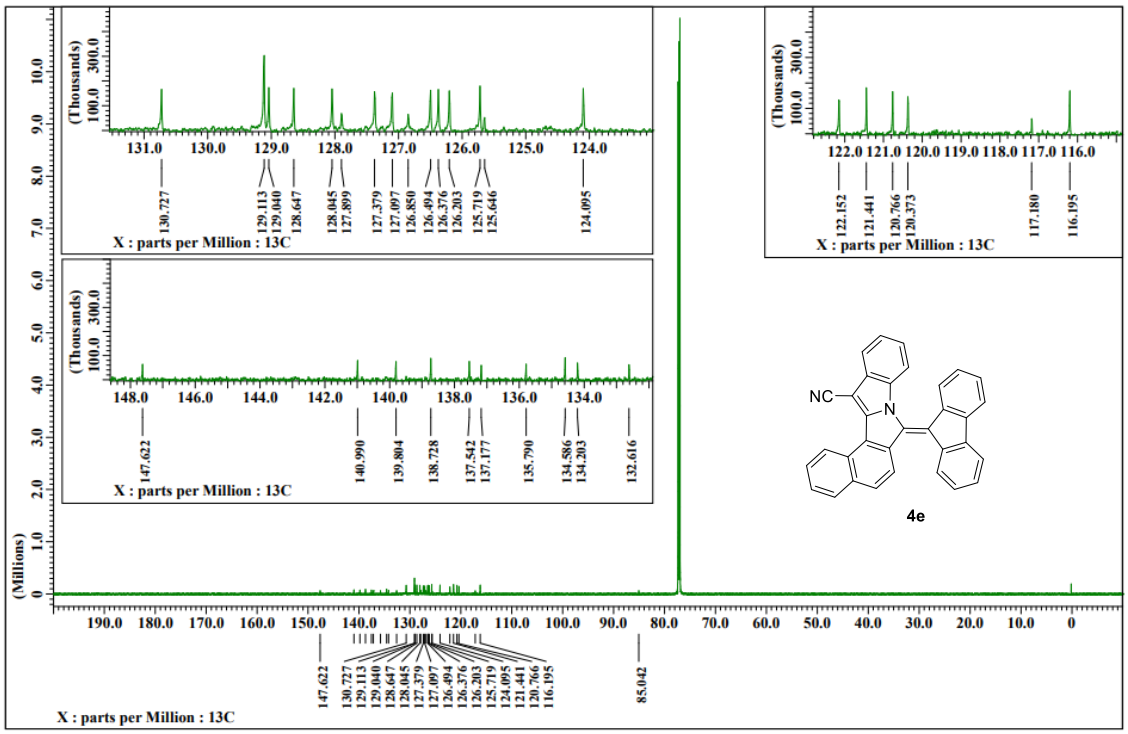
^{13}C NMR (100 MHz, $CDCl_3$)



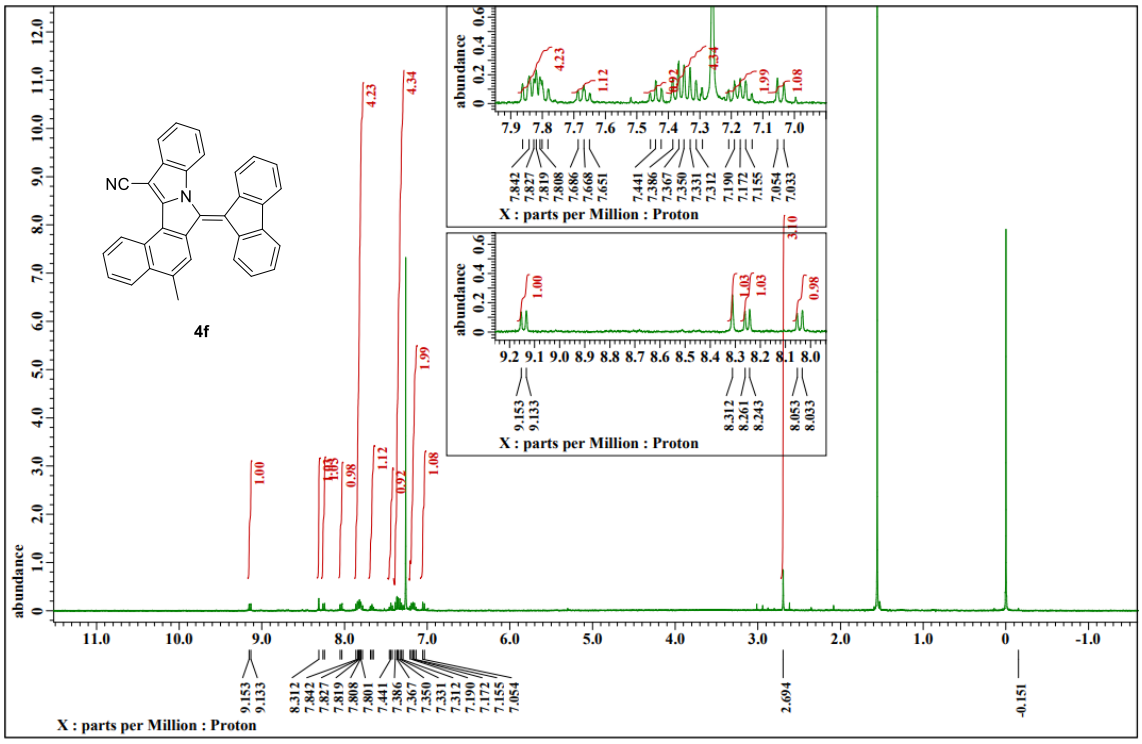
^{1}H NMR (400 MHz, $CDCl_3$)



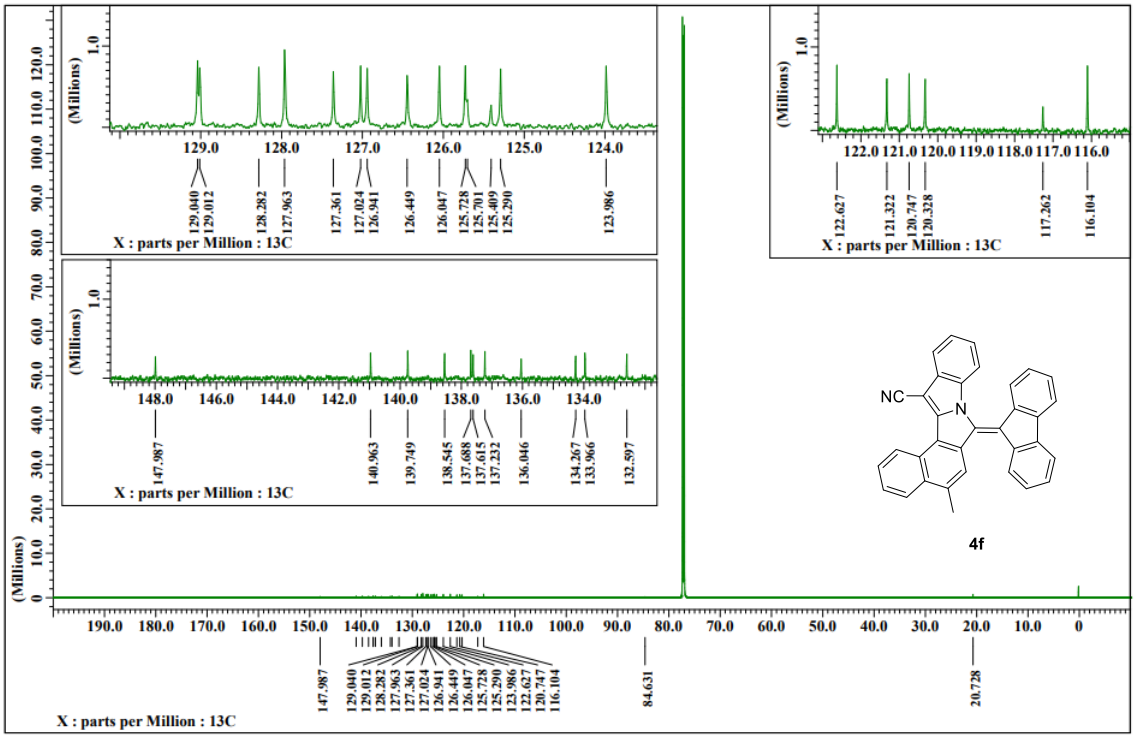
^{13}C NMR (176 MHz, $CDCl_3$)



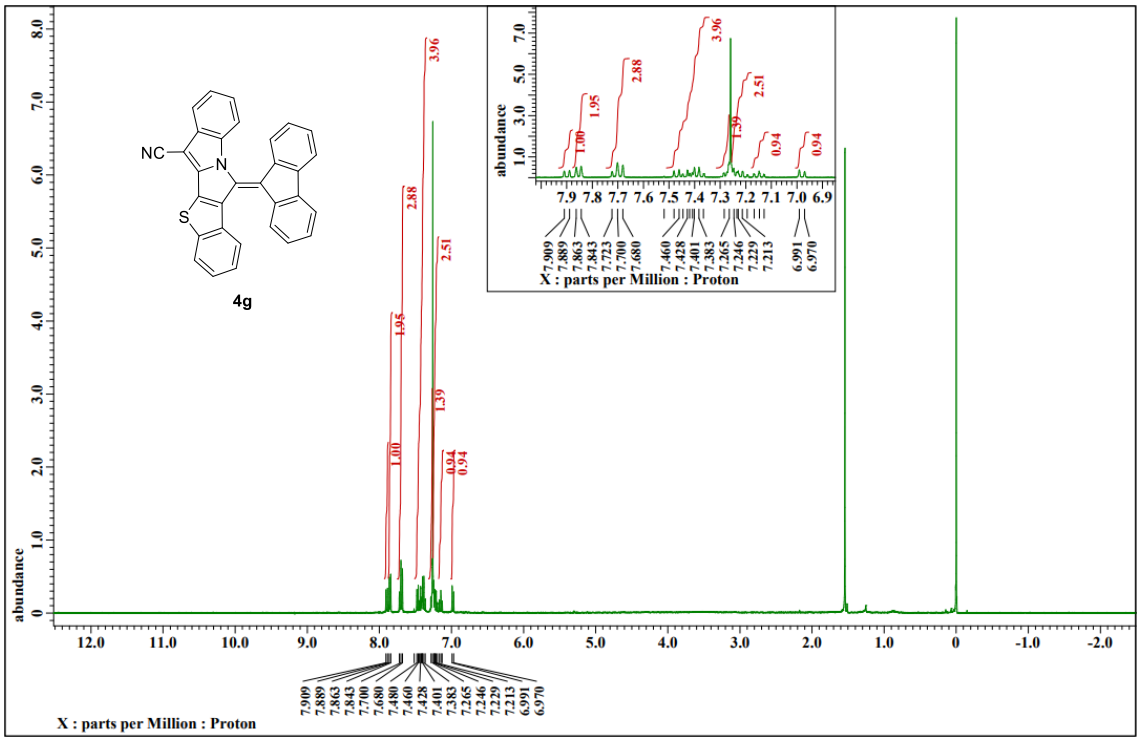
H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (176 MHz, $CDCl_3$)



^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (100 MHz, $CDCl_3$)