

## NHPI-catalyzed electrochemical C–H alkylation of indoles with alcohols to access di(indolyl)methanes via radical coupling

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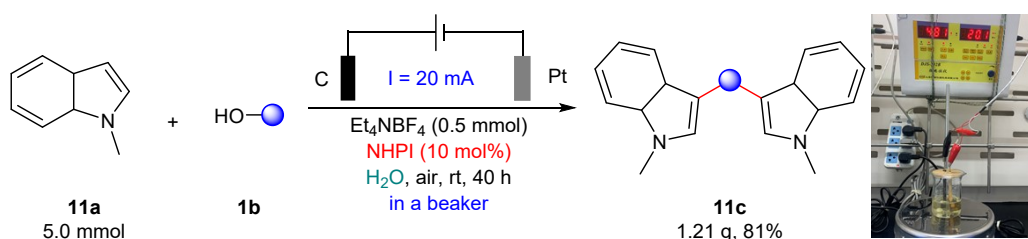
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## 1. General information

All glassware was oven dried at 100 °C for hours and cooled down under vacuum. Indoles was prepared according to reported procedures.<sup>1</sup> Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China), the carbon rods ( $\phi = 6$  mm), Ni plates (1.0 x 1.0 cm<sup>2</sup>), and Pt plates (1.0 x 1.0 cm<sup>2</sup>) was purchased from Xuzhou Xinke Instrument and Meter Co. LTD. The thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (b. p. 60-90 °C). <sup>1</sup>H, <sup>13</sup>C NMR, and <sup>19</sup>F NMR data were recorded with Bruker Advance III (500 MHz) spectrometers with tetramethylsilane as an internal standard. All chemical shifts ( $\delta$ ) are reported in ppm and coupling constants ( $J$ ) in Hz. All chemical shifts are reported relative to tetramethylsilane and *d*-solvent peaks (77.00 ppm, chloroform; 40.00 ppm, DMSO-*d*<sub>6</sub>), respectively.

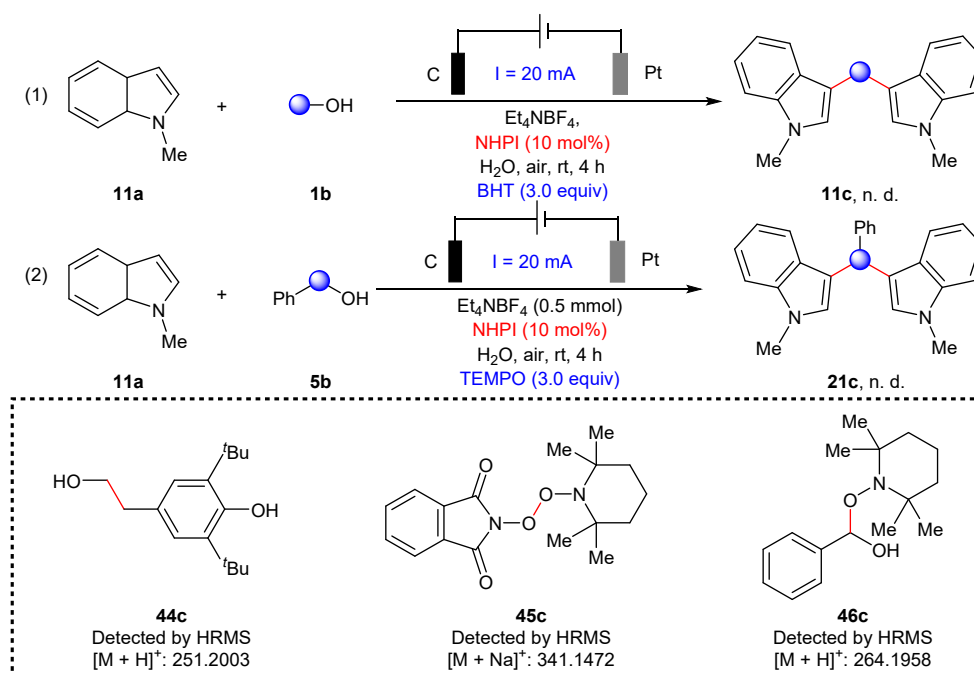
## 2. Large-scale synthesis of 11c.



In an oven-dried beaker (100 mL) equipped with a stir bar, **11a** (5.0 mmol, 0.665 g), **1b** (50.0 mmol, 1.6 g), and Et<sub>4</sub>NBF<sub>4</sub> (5.0 mmol, 1.085 g) were combined. The beaker was equipped with a carbon rods ( $\phi = 6.0$  mm) as the anode and Pt plates (1.0 × 1.0 cm<sup>2</sup>) as the cathode. Under the air, H<sub>2</sub>O (30.0 mL) was slowly injected into the reaction system. The reaction mixture was stirred and electrolyzed at a constant current of 20 mA under room temperature for 40 h. When the reaction was finished, the reaction mixture was concentrated, and then extracted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL × 3). The organic layers were combined, dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated again. The pure product **11c** was obtained in a yield of 81% by flash column chromatography on silica gel (EtOAc/petroleum ether = 1/100).

## 3. Preliminary mechanistic studies

### (1) Radical trapping experiments



In an oven-dried beaker (25 mL) equipped with a stir bar, **11a** (0.5 mmol, 66.5 mg), **1b** (5.0 mmol, 160.0 mg) or **5b** (5.0 mmol, 540.0 mg), NHPI (10.0 mol%, 4.1 mg), TEMPO or BHT (3.0 equiv), and Et<sub>4</sub>NBF<sub>4</sub> (0.5 mmol, 108.5 mg) were combined. The beaker was equipped with a carbon rods ( $\phi = 6$  mm) as the anode and Pt plates (1.0 × 1.0 cm<sup>2</sup>) as the cathode. Under the air, H<sub>2</sub>O (8.0 mL) was slowly injected into the reaction system. The reaction mixture was stirred and electrolyzed at a constant current of 20 mA under room temperature for 4 h. When the reaction was finished, the reaction mixture was washed with water and extracted with CH<sub>2</sub>Cl<sub>2</sub> (10 mL × 3). The organic layers were combined and concentrated in vacuum and not detected the desired product **11c** or **21c**. The compounds **44c-46c** can be detected by HRMS.

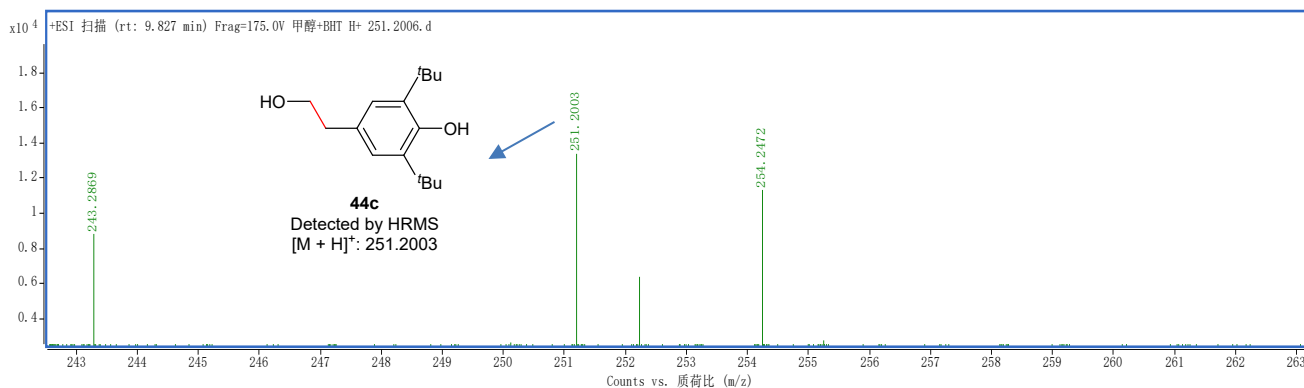


Fig. S1. The HRMS results of **44c**.

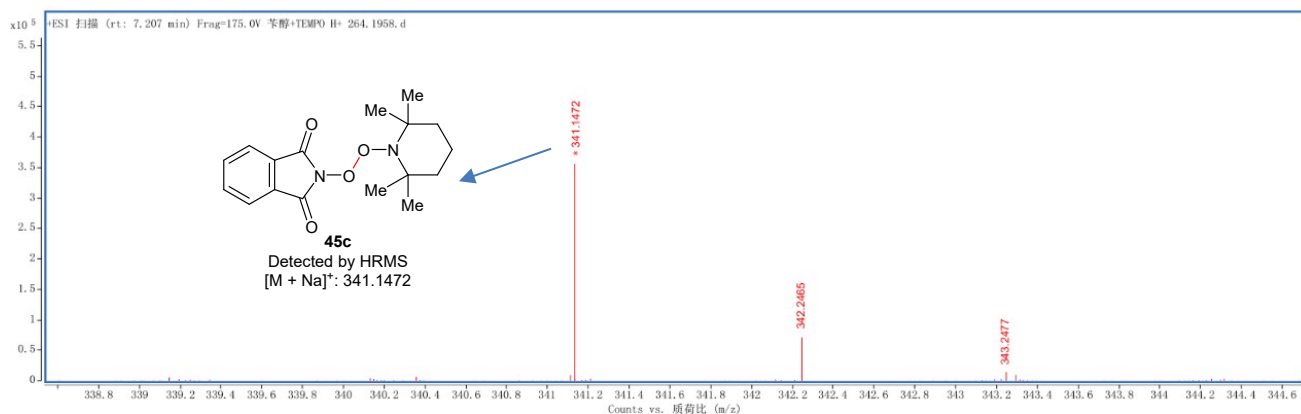


Fig. S2. The HRMS results of **45c**.

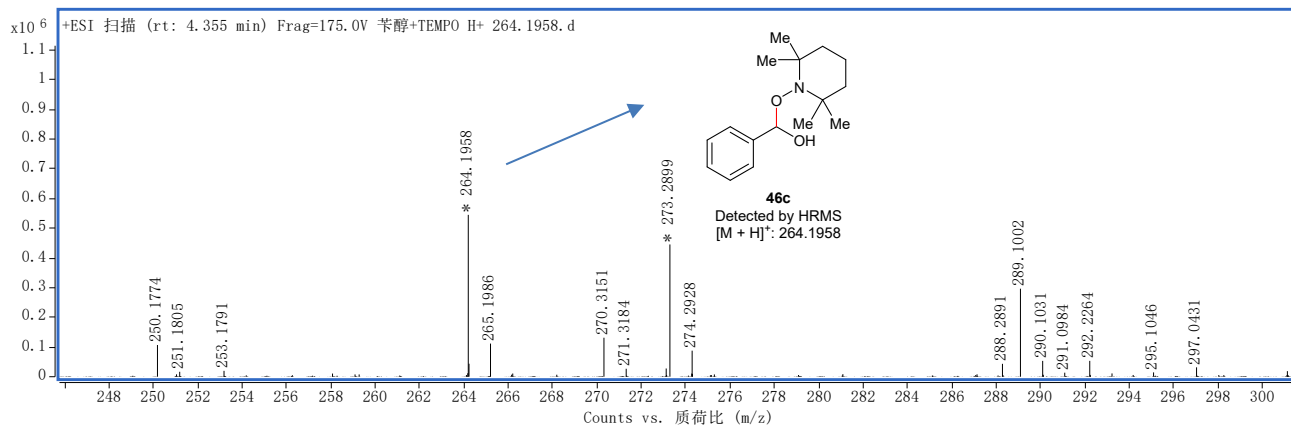
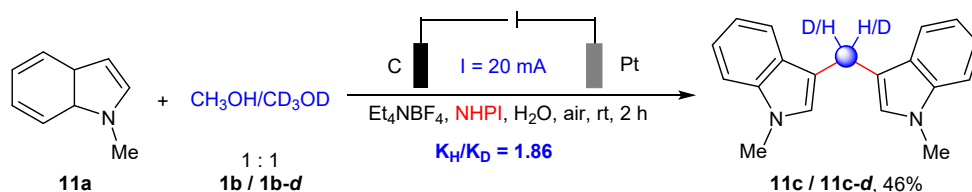
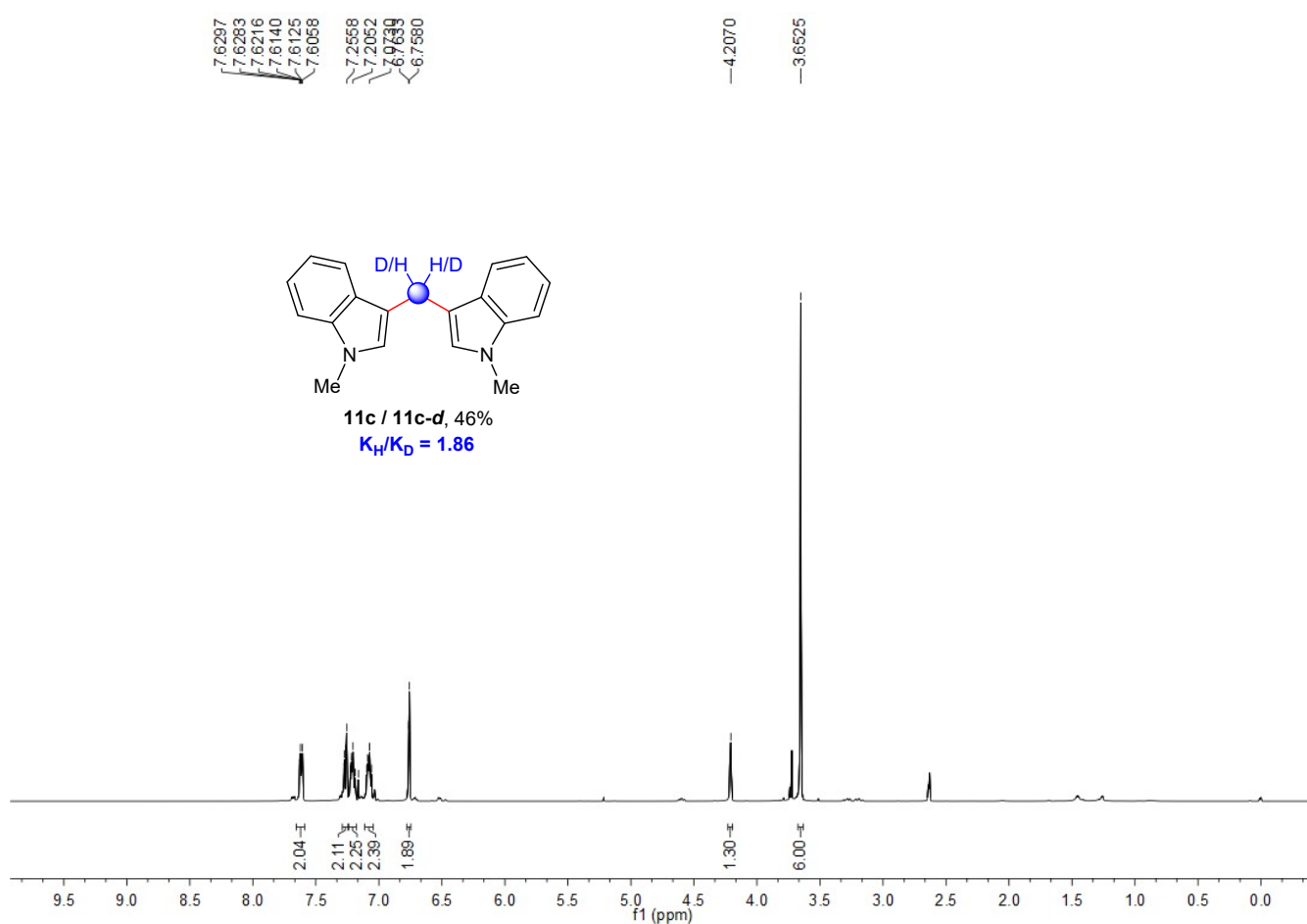


Fig. S3. The HRMS results of **46c**.

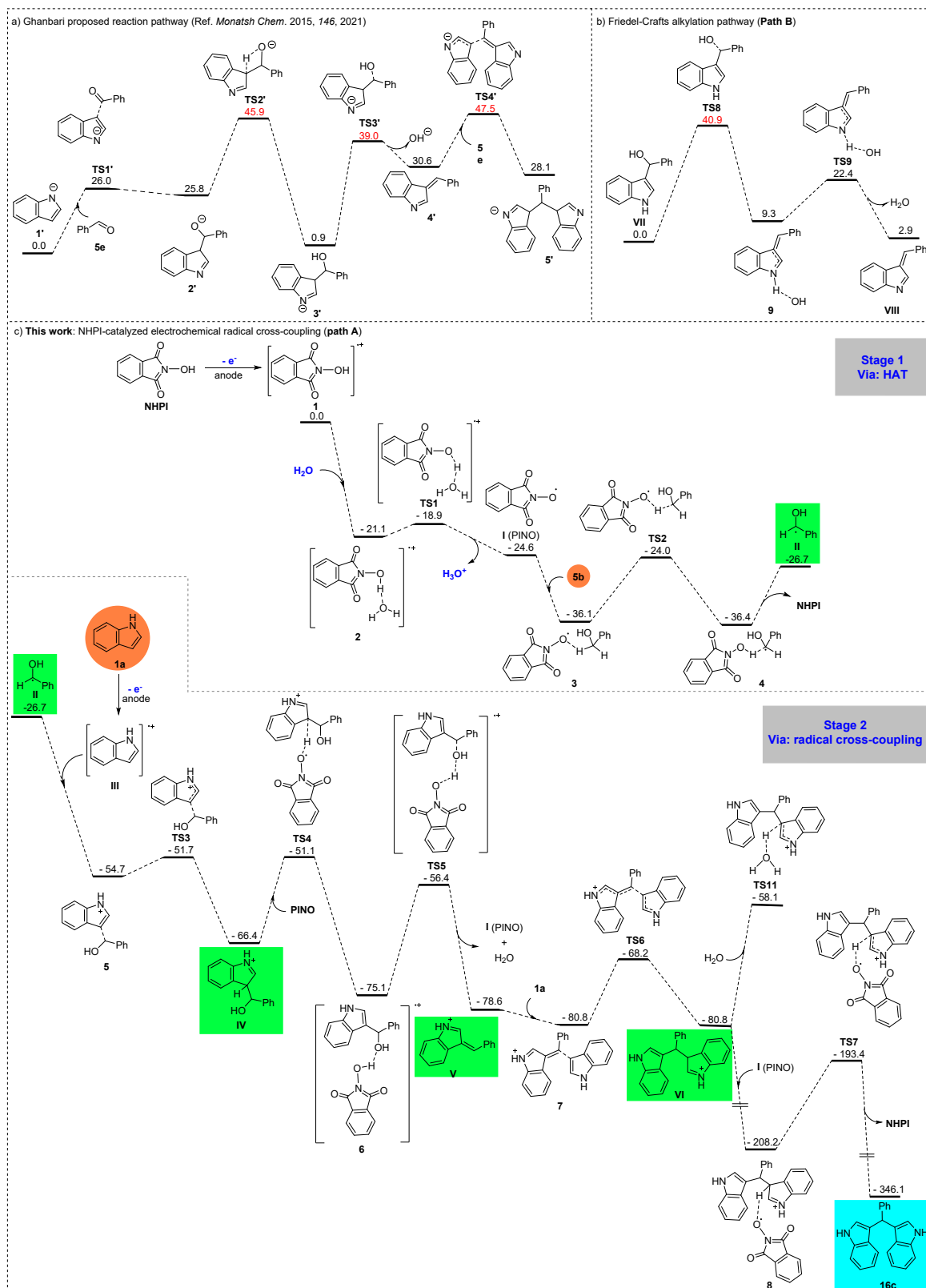
## (2) Intermolecular competitive kinetics experiments



In an oven-dried beaker (25 mL) equipped with a stir bar, **11a** (0.5 mmol, 66.5 mg), **CH<sub>3</sub>OH** (2.5 mmol), **CD<sub>3</sub>OD** (2.5 mmol), NHPI (10.0 mol%, 4.1 mg), and Et<sub>4</sub>NBF<sub>4</sub> (0.5 mmol, 108.5 mg) were combined. The beaker was equipped with a carbon rods ( $\phi = 6$  mm) as the anode and Pt plates ( $1.0 \times 1.0$  cm<sup>2</sup>) as the cathode. Under the air, H<sub>2</sub>O (8.0 mL) was slowly injected into the reaction system. The reaction mixture was stirred and electrolyzed at a constant current of 20 mA under room temperature for 2 h. The pure product **11c** was obtained in a yield of 46% by flash column chromatography on silica gel (EtOAc/petroleum ether = 1/100), A KIE value of 1.86 was determined by <sup>1</sup>H NMR.



**Fig. S4.** <sup>1</sup>H NMR results of **11c / 11c-d**.



**Fig. S5.** Summary of DFT calculation results, the relative free energies are given in kcal/mol. [a] For Ghanbari proposed reaction pathway (Ref. *Monatsh Chem.* 2015, 146, 2021). [b] For Friedel-Crafts alkylation pathway. [c] Path A is the proposed reaction pathway based on experimental and DFT data (this work).

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#### 4 Cartesian Coordinates of DFT Optimized Structures

Structure: NHPI

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -588.057577187 hartree

SCF Energy + ZPVE: -587.936943187 hartree

Free Energy: -587.971446 hartree

C	-2.473978811	0.402395901	-0.114242136
C	-3.760110355	0.588730183	0.397770762
C	-4.208729883	1.832636320	0.801885934
C	-3.314078966	2.903540871	0.676620838
C	-2.028587330	2.717776163	0.162284612
C	-1.584762055	1.452970462	-0.245959733
C	-2.304385587	-1.038630206	-0.443345510
H	-5.207814294	1.971584961	1.201849426
H	-3.624148485	3.896129563	0.986311724
H	-1.360509230	3.568889633	0.080355389
H	-0.587388039	1.303298819	-0.646393445
N	-3.554187992	-1.609446585	-0.191121635
O	-3.728077453	-2.958588026	-0.135589806
H	-4.122615428	-3.227775237	-0.983336396
O	-1.335443797	-1.646922908	-0.843973795
O	-5.551564797	-1.036242203	0.823618343
C	-4.455072968	-0.726615092	0.409914298

Structure: **1**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -587.785529270 hartree

SCF Energy + ZPVE: -587.667580270 hartree

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Free Energy: -587.703816 hartree

C	-2.438583291	0.392284953	-0.124152760
C	-3.753290860	0.595333884	0.404848575
C	-4.230579114	1.844342748	0.816126748
C	-3.356338266	2.899347443	0.685497168
C	-2.032102138	2.702335046	0.153357804
C	-1.561291166	1.418900170	-0.262049752
C	-2.287001210	-1.058354017	-0.436722819
H	-5.232468155	1.959872229	1.213620007
H	-3.643734149	3.902309402	0.980616793
H	-1.374459496	3.561177138	0.071651263
H	-0.560240443	1.291298703	-0.658273056
N	-3.533079141	-1.611760910	-0.115437825
O	-3.751966499	-2.944365547	-0.139082915
H	-4.080071250	-3.170515994	-1.030361084
O	-1.343545542	-1.666757799	-0.870030779
O	-5.565538252	-0.995137270	0.817578321
C	-4.457166498	-0.726577558	0.429463183

Structure: H<sub>2</sub>O

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -76.409061753 hartree

SCF Energy + ZPVE: -76.387722753 hartree

Free Energy: -76.406031 hartree

O	-4.799433343	-3.327955102	-2.286346416
H	-4.411956569	-4.066800872	-2.772170154
H	-5.577351378	-3.076248855	-2.800139911

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Structure: **2**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -664.250722045 hartree

SCF Energy + ZPVE: -664.105104045 hartree

Free Energy: -664.143548 hartree

C	-2.994165471	0.458465646	-0.166320823
C	-4.098041918	1.016183038	0.496947264
C	-4.013469913	2.239482349	1.141786068
C	-2.779882954	2.895662308	1.104022699
C	-1.678810262	2.339197918	0.442133454
C	-1.769150172	1.104944780	-0.207023345
C	-3.370618206	-0.832511385	-0.759992725
H	-4.870552072	2.665530052	1.651945636
H	-2.672131894	3.855818309	1.597045311
H	-0.737682282	2.878273119	0.433347415
H	-0.920737049	0.667746451	-0.722189738
N	-4.763475924	-1.003261228	-0.401259223
O	-5.471058888	-1.995680301	-0.715962184
H	-4.789302630	-3.133298499	-1.551709162
O	-2.768602706	-1.647222465	-1.408365003
O	-6.389709198	0.178423528	0.771902899
C	-5.258508032	0.119008165	0.375463890
O	-4.368645774	-3.858570355	-2.132272721
H	-3.409935477	-3.672906892	-2.186629825
H	-4.497685977	-4.736260208	-1.724580407

Structure: **TS1**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 1



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SCF Energy: -664.245666072 hartree

SCF Energy + ZPVE: -664.101660072 hartree

Free Energy: -664.139895 hartree

C	-2.847862437	0.481073390	-0.291919823
C	-3.974315550	0.853366520	0.458439365
C	-4.013717625	2.043243369	1.166894235
C	-2.880647681	2.858900032	1.104682363
C	-1.756238839	2.487214345	0.357888728
C	-1.722380100	1.287022819	-0.357317701
C	-3.078627994	-0.829133119	-0.919458135
H	-4.887378064	2.323238561	1.745622769
H	-2.869302098	3.797120481	1.649031250
H	-0.893006955	3.143798203	0.336885758
H	-0.853300085	0.992303226	-0.935613396
N	-4.410936212	-1.204315874	-0.485766223
O	-4.994422506	-2.275598659	-0.795788017
H	-4.257369267	-3.280581141	-1.639917699
O	-2.418568004	-1.533043164	-1.635051821
O	-6.107230921	-0.305126270	0.828994411
C	-5.005984352	-0.191404687	0.365534171
O	-3.848929932	-4.029764952	-2.206376464
H	-4.297964890	-4.880728706	-2.320108365
H	-2.997395418	-3.906196154	-2.651999277

Structure: H<sub>3</sub>O<sup>+</sup>

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -76.824015049 hartree

SCF Energy + ZPVE: -76.788822049 hartree

Free Energy: -76.807950 hartree

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H	-3.965850055	-3.520034539	-1.157743076
O	-4.246428843	-3.394623107	-2.087123661
H	-4.189903997	-4.251811063	-2.556509899
H	-5.174037225	-3.082712351	-2.098470283

Structure: **I** (PINO)

Charge = 0 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -587.414877411 hartree

SCF Energy + ZPVE: -587.306355411 hartree

Free Energy: -587.341065 hartree

C	-2.465275362	0.391921935	-0.109193617
C	-3.757524314	0.575109169	0.401615583
C	-4.209561136	1.822637832	0.800179229
C	-3.321172494	2.893984617	0.671202324
C	-2.030533411	2.711105805	0.161260803
C	-1.580214045	1.449806456	-0.239188639
C	-2.264974600	-1.029412034	-0.444635616
H	-5.210441251	1.957809056	1.196199394
H	-3.636121282	3.887277583	0.973127264
H	-1.366970393	3.565411217	0.077800870
H	-0.581318075	1.300867118	-0.635379741
N	-3.513088397	-1.668582431	-0.097160118
O	-3.744100062	-2.895438401	-0.240730428
O	-1.330453857	-1.631918263	-0.904187309
O	-5.571341008	-1.032382861	0.781056627
C	-4.464725983	-0.717902190	0.428782744

Structure: **5b**

Charge = 0 Multiplicity = 1

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Number of imaginary frequencies: 0

SCF Energy: -346.648858859 hartree

SCF Energy + ZPVE: -346.514329859 hartree

Free Energy: -346.545857 hartree

C	-6.234703006	-3.599367418	-5.649889147
C	-5.574175084	-3.170311434	-4.497563109
C	-5.872563938	-3.739240072	-3.257183235
C	-6.841527001	-4.745856231	-3.182962467
C	-7.501009216	-5.179093533	-4.331940750
C	-7.198168153	-4.604600020	-5.568424345
H	-5.998660838	-3.148211709	-6.609049932
H	-4.822317125	-2.387280963	-4.559878326
H	-7.078010754	-5.187972508	-2.217751475
H	-8.253453858	-5.959046343	-4.263007276
H	-7.714424541	-4.937063029	-6.464048828
C	-5.134031650	-3.313458777	-2.017427626
H	-4.680992482	-2.327357464	-2.168461116
O	-4.115350915	-4.284567868	-1.749335507
H	-3.669980796	-4.032966529	-0.928703244
H	-5.822338853	-3.257379431	-1.166257136

Structure: **3**

Charge = 0 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -934.081881295 hartree

SCF Energy + ZPVE: -933.837965295 hartree

Free Energy: -933.885151 hartree

C	-5.985914341	2.650551463	0.628911087
C	-6.417888220	2.260010653	1.902977199
C	-5.517826959	1.934934354	2.906247431

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C	-4.158676005	2.014332543	2.593032300
C	-3.727398746	2.406126235	1.319094499
C	-4.639291850	2.731905966	0.311819994
C	-7.155062927	2.881480424	-0.238876729
H	-5.859570576	1.622494564	3.887420510
H	-3.421610372	1.764053103	3.348546260
H	-2.663758751	2.452202547	1.110425728
H	-4.312736007	3.025301589	-0.680310812
N	-8.297112706	2.634799913	0.611470781
O	-9.491277928	2.661425865	0.221107414
O	-7.260461041	3.198329533	-1.394763034
O	-8.681335170	1.910855912	2.786474747
C	-7.889357569	2.217843427	1.930762367
C	-6.234668903	-0.328969628	-0.820572548
C	-7.625257191	-0.221730776	-0.796756795
C	-8.348922185	-0.583471108	0.345682610
C	-7.656270768	-1.038298652	1.471691648
C	-6.263709093	-1.139348864	1.451339834
C	-5.549023595	-0.788888298	0.305616472
H	-5.685922695	-0.034623225	-1.710822572
H	-8.156994342	0.156176257	-1.667902130
H	-8.207065138	-1.304763796	2.369338054
H	-5.736715898	-1.484649732	2.336190365
H	-4.465293950	-0.859484999	0.294404194
C	-9.860701373	-0.498414283	0.327253383
H	-10.170936503	0.288020451	-0.372554659
O	-10.438118507	-0.288758719	1.608056782
H	-10.129769593	0.563817192	1.952145857
H	-10.275744598	-1.444532090	-0.035228239

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Structure: **TS2**

Charge = 0 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -934.055298477 hartree

SCF Energy + ZPVE: -933.816873477 hartree

Free Energy: -933.860938 hartree

Structure: **4**

Charge = 0 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -934.080903980 hartree

SCF Energy + ZPVE: -933.838809980 hartree

Free Energy: -933.886360 hartree

C	-6.029078920	2.574378334	0.608854259
C	-6.544544868	2.296679113	1.875777335
C	-5.720744370	2.023746185	2.952527699
C	-4.340229095	2.036317329	2.716558582
C	-3.823848294	2.313260082	1.447350324
C	-4.667907445	2.590166602	0.364442595
C	-7.167517784	2.790898222	-0.324679812
H	-6.127679920	1.799480516	3.933338256
H	-3.657903978	1.823250178	3.532825441
H	-2.749143243	2.310168521	1.298231020
H	-4.273609490	2.797454477	-0.625200783
N	-8.304583653	2.685603555	0.476604906
O	-9.566001847	2.782729032	-0.020337625
O	-7.179412151	3.015642400	-1.516488191
O	-8.871267954	2.079907999	2.635462874
C	-8.030782850	2.319251178	1.794105967
C	-6.318561648	-0.502874660	-0.968795970

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C	-7.686374887	-0.386700973	-0.794297731
C	-8.282457906	-0.611782477	0.479364820
C	-7.429069728	-0.957785127	1.560649874
C	-6.057553212	-1.076495721	1.364705248
C	-5.488287663	-0.851548526	0.108593930
H	-5.886718267	-0.315190623	-1.947775138
H	-8.324601854	-0.108863562	-1.630127660
H	-7.833162111	-1.142598933	2.552652247
H	-5.423608765	-1.341578437	2.206160551
H	-4.415592968	-0.937868451	-0.031503873
C	-9.684153884	-0.464967043	0.599985428
H	-9.831958844	1.882761492	-0.291185115
O	-10.384244533	-0.588896931	1.755261276
H	-9.801358510	-0.591790457	2.529905262
H	-10.321157286	-0.329594684	-0.267607236

Structure: **II**

Charge = 0 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -346.007996069 hartree

SCF Energy + ZPVE: -345.887373069 hartree

Free Energy: -345.918805 hartree

C	-6.994652733	-4.616726906	-6.218356748
C	-6.288983294	-3.888813474	-5.274994880
C	-6.145148117	-4.371200767	-3.944819540
C	-6.744167552	-5.617462990	-3.615902480
C	-7.447755175	-6.332790367	-4.575618511
C	-7.581885308	-5.845105718	-5.880847594
H	-7.094089287	-4.229203752	-7.228200819
H	-5.836694195	-2.936959349	-5.541981987

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H	-6.647258111	-6.007901328	-2.607855167
H	-7.899171331	-7.283547290	-4.305848417
H	-8.134088008	-6.411021352	-6.624071837
C	-5.426330816	-3.610629555	-3.002697948
H	-4.967319642	-2.657489884	-3.240020545
O	-5.297362949	-4.075882065	-1.731495883
H	-4.788245631	-3.447258503	-1.200956714

Structure: **1a**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -363.688270823 hartree

SCF Energy + ZPVE: -363.557591823 hartree

Free Energy: -363.587839 hartree

C	-2.408575268	0.342355699	-0.061585380
C	-3.734200155	0.542303418	0.403093240
C	-4.221776948	1.805242421	0.763119876
C	-3.352636895	2.879616258	0.650613391
C	-2.027463567	2.705916981	0.191246240
C	-1.550181051	1.453726557	-0.163977894
C	-2.270670416	-1.063100165	-0.330084458
C	-3.476174417	-1.642062846	-0.028605062
H	-5.240511151	1.932631382	1.116587428
H	-3.695470303	3.873560988	0.921532309
H	-1.375207864	3.570968646	0.118529523
H	-0.530250549	1.329054687	-0.517040145
H	-1.391684562	-1.574686595	-0.696355975
N	-4.356849747	-0.683013184	0.413328064
H	-3.786553168	-2.675689977	-0.090710677
H	-5.314301399	-0.852545248	0.690294299

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Structure: **III**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -363.481281415 hartree

SCF Energy + ZPVE: -363.350800415 hartree

Free Energy: -363.381772 hartree

C	-2.406414640	0.351194254	-0.061741831
C	-3.734010744	0.551808758	0.403504159
C	-4.225958697	1.780709670	0.760780870
C	-3.334089549	2.870682350	0.643417471
C	-2.019905500	2.712300569	0.189254119
C	-1.536044941	1.457486227	-0.168981816
C	-2.261860838	-1.021310618	-0.325341092
C	-3.517395380	-1.632433899	-0.014385021
H	-5.241749425	1.917117184	1.115201421
H	-3.685829529	3.859948911	0.917069256
H	-1.373287968	3.579696123	0.119418904
H	-0.518868379	1.323644474	-0.522043861
H	-1.389719258	-1.546127413	-0.689940364
N	-4.361556190	-0.707960320	0.409662390
H	-3.801453386	-2.673694793	-0.086285294
H	-5.324362576	-0.878782476	0.690394691

Structure: **5**

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -709.558665211 hartree

SCF Energy + ZPVE: -709.301688211 hartree

Free Energy: -709.345202 hartree



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C	-2.241272524	0.360408735	0.140873110
C	-3.629940796	0.235939909	0.402434463
C	-4.464092073	1.348211802	0.573770133
C	-3.882959616	2.602577997	0.465446462
C	-2.504010322	2.752343543	0.195067265
C	-1.680351161	1.648184108	0.034860076
C	-1.723625197	-0.972438524	-0.004448582
C	-2.783068674	-1.827259378	0.177014724
H	-5.523990082	1.227591614	0.776099015
H	-4.499674999	3.487787551	0.587375940
H	-2.086100313	3.751085453	0.113222611
H	-0.620339448	1.770783113	-0.170969681
H	-0.702501386	-1.257437766	-0.217798983
N	-3.924969934	-1.108058326	0.425862910
H	-2.816922182	-2.907462303	0.144220521
H	-4.841857071	-1.506174293	0.580271256
C	-2.971294936	-4.095773730	-3.789086983
C	-3.177614113	-2.822335920	-3.280171912
C	-2.190361715	-1.835431256	-3.466554196
C	-0.995689117	-2.121647480	-4.158748872
C	-0.801657149	-3.397217862	-4.659454613
C	-1.786552704	-4.377525833	-4.473871342
H	-3.721520652	-4.866787651	-3.654572609
H	-4.086120729	-2.574949387	-2.737662344
H	-0.246180706	-1.348087245	-4.290870560
H	0.109548526	-3.640001257	-5.194836657
H	-1.624604208	-5.374958946	-4.871264861
C	-2.452622124	-0.548306509	-2.924987516
H	-3.388693146	-0.342316742	-2.401572855
O	-1.620271792	0.408822429	-3.080043421

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H	-1.916658657	1.240366051	-2.657135697
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Structure: **TS3**

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -709.554660388 hartree

SCF Energy + ZPVE: -709.298424388 hartree

Free Energy: -709.340392 hartree

C	-2.325934229	0.487620790	-0.092453685
C	-3.623376779	0.392541911	0.457323539
C	-4.332828513	1.503239289	0.914845376
C	-3.706299272	2.738667676	0.806057087
C	-2.414254661	2.860004884	0.256734413
C	-1.716314863	1.747249320	-0.197190777
C	-1.947418816	-0.844278464	-0.504996178
C	-2.993615867	-1.679038121	-0.114816070
H	-5.329073477	1.402494580	1.333282264
H	-4.222844165	3.628929619	1.150676039
H	-1.958831079	3.842913933	0.187531875
H	-0.718903576	1.846012641	-0.615687753
H	-0.965502373	-1.175378230	-0.814476853
N	-3.987997258	-0.947296729	0.427682591
H	-3.093866042	-2.750878858	-0.223117893
H	-4.878610590	-1.319354579	0.737939576
C	-2.798834125	-4.298598180	-3.708196344
C	-3.124515127	-3.048271194	-3.196997126
C	-2.175334689	-2.016707195	-3.233897587
C	-0.897803483	-2.237721392	-3.769511708
C	-0.577791576	-3.493942306	-4.269016881
C	-1.526576360	-4.520203510	-4.240883797

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H	-3.530345796	-5.099657659	-3.690703081
H	-4.106963453	-2.860250388	-2.770800028
H	-0.170365882	-1.432087318	-3.789249873
H	0.407962822	-3.675454794	-4.684249523
H	-1.271861722	-5.499235975	-4.635073060
C	-2.567091621	-0.709677387	-2.740757765
H	-3.599834773	-0.523317681	-2.449142964
O	-1.836663738	0.310725138	-3.087396478
H	-2.239319917	1.158164178	-2.822641335

Structure: **IV**

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -709.581777789 hartree

SCF Energy + ZPVE: -709.322687789 hartree

Free Energy: -709.363852 hartree

C	-2.499754703	0.724455480	-0.108625811
C	-3.545447296	0.521279727	0.792901735
C	-4.200641700	1.532000240	1.474076363
C	-3.756489945	2.829369353	1.215939733
C	-2.703437589	3.067691534	0.325999522
C	-2.060469934	2.021777841	-0.344149543
C	-2.073683615	-0.618331468	-0.642801042
C	-2.973650340	-1.541281301	0.102466198
H	-5.007725532	1.322633920	2.167724568
H	-4.232017943	3.663950585	1.719971823
H	-2.374017141	4.087498550	0.155351980
H	-1.233069623	2.224488678	-1.016406520
H	-1.028764568	-0.862250120	-0.402046910
N	-3.775173621	-0.879909868	0.868906103

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H	-3.013349421	-2.623368108	0.039797668
H	-4.484214159	-1.309309650	1.465628649
C	-2.595498613	-4.391435377	-3.369186118
C	-2.911440269	-3.084492370	-2.995230081
C	-1.901864365	-2.199357452	-2.613097763
C	-0.571061513	-2.629039724	-2.608183078
C	-0.254967348	-3.931602138	-2.988609896
C	-1.267305414	-4.815894296	-3.367351339
H	-3.386243329	-5.073473454	-3.666161300
H	-3.945751664	-2.749116497	-3.001095135
H	0.217869589	-1.943276941	-2.309668168
H	0.780372257	-4.258258633	-2.987013040
H	-1.020336783	-5.831640932	-3.660647805
C	-2.247946235	-0.791969066	-2.187692223
H	-3.294144501	-0.579869573	-2.435133291
O	-1.389296550	0.114331134	-2.853133173
H	-1.797569479	0.991420673	-2.860239458

Structure: **TS4**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 1

SCF Energy: -1296.987832350 hartree

SCF Energy + ZPVE: -1296.625553350 hartree

Free Energy: -1296.680639 hartree

C	-2.959181466	-1.991992852	-0.436118619
C	-3.558044805	-2.879520119	0.474444789
C	-3.654769643	-2.629009950	1.830500544
C	-3.141567523	-1.402356437	2.271720191
C	-2.571497375	-0.482585193	1.381527741
C	-2.464530615	-0.766015291	0.019656066

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C	-2.936633061	-2.656793041	-1.738215456
C	-3.683199153	-3.888742478	-1.525388788
H	-4.104663141	-3.341807080	2.513005280
H	-3.192087038	-1.159900710	3.328174694
H	-2.192797424	0.460432052	1.761652038
H	-1.999812688	-0.063798636	-0.666285568
N	-3.984378097	-4.008032980	-0.257901688
H	-3.922599515	-4.660960701	-2.246168753
H	-4.429587053	-4.826739251	0.155231391
C	-6.615652914	-1.192399871	-3.730061345
C	-5.411274864	-1.877331184	-3.580971036
C	-4.243478407	-1.178563194	-3.257883718
C	-4.290490055	0.205079021	-3.081921799
C	-5.498220244	0.889895465	-3.225947685
C	-6.661376959	0.192085369	-3.550133780
H	-7.518735665	-1.737966427	-3.985778368
H	-5.376450975	-2.954844537	-3.724450977
H	-3.379774994	0.746275353	-2.836798352
H	-5.527766298	1.966628262	-3.090844746
H	-7.600548279	0.724036928	-3.666082880
C	-2.932508356	-1.920404440	-3.063111998
H	-2.112677380	-1.191133109	-3.031888426
O	-2.697629893	-2.901246368	-4.058239729
H	-2.676162702	-2.462732133	-4.921048716
H	-1.735799656	-3.218597603	-1.725094612
C	0.561475748	-1.721215279	1.264881238
C	0.009411363	-2.853826896	1.877611936
C	-0.075685340	-2.966009027	3.255758675
C	0.416533180	-1.897684094	4.012632992
C	0.970156801	-0.768082560	3.399960955

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C	1.050514211	-0.660694075	2.006760498
C	0.434352130	-1.852228293	-0.202582980
H	-0.515574653	-3.841084481	3.722680529
H	0.364024579	-1.942229264	5.095230118
H	1.338335468	0.043617200	4.018513825
H	1.466902830	0.218469809	1.526565946
N	-0.157912219	-3.138313988	-0.396546978
O	-0.542431286	-3.583438544	-1.548686568
O	0.715403292	-1.110178566	-1.109862483
O	-1.039874632	-4.846964674	0.900967807
C	-0.476795651	-3.782065876	0.837914135

Structure: **6**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -1297.032464290 hartree

SCF Energy + ZPVE: -1296.664369290 hartree

Free Energy: -1296.718859 hartree

C	-2.919099699	1.511619951	-1.607145820
C	-1.858736670	1.339473669	-0.680974957
C	-0.974263763	2.338243684	-0.349336338
C	-1.165611346	3.579694385	-0.987216051
C	-2.202154614	3.788212917	-1.907179671
C	-3.088543573	2.766750908	-2.232616757
C	-3.608429876	0.276466070	-1.680202512
C	-2.929826876	-0.619218077	-0.786097096
H	-0.171226960	2.182303800	0.363029110
H	-0.484733979	4.393725853	-0.759899486
H	-2.308133428	4.759354378	-2.378357824
H	-3.884660255	2.922013885	-2.951943331

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N	-1.924501570	0.014727551	-0.212796827
H	-3.152845100	-1.656205163	-0.568716253
H	-1.278644564	-0.398960900	0.455752426
C	-6.081219104	-3.618275965	-1.980339252
C	-5.930195227	-2.237526107	-1.844484842
C	-5.026181700	-1.548394815	-2.653485328
C	-4.271752497	-2.243892108	-3.602680287
C	-4.428676919	-3.621578507	-3.742125435
C	-5.330650039	-4.311047570	-2.929387327
H	-6.788500544	-4.148842333	-1.350403428
H	-6.517547692	-1.692635252	-1.109368151
H	-3.567323245	-1.709308693	-4.234075327
H	-3.844894291	-4.157761955	-4.484027339
H	-5.450721106	-5.384468264	-3.039921817
C	-4.840622118	-0.056554268	-2.461413503
H	-5.694461060	0.328501177	-1.882605679
O	-4.756246855	0.664379989	-3.688339188
H	-5.576442491	0.533727639	-4.188900013
H	-3.393060909	0.531988048	-4.639116504
C	0.167661260	2.253548938	-3.844230557
C	0.337259413	1.007087476	-3.239388510
C	1.363408723	0.763888436	-2.344713782
C	2.231257810	1.828256482	-2.069091200
C	2.061281554	3.077168077	-2.673296950
C	1.017704434	3.311382885	-3.578389451
C	-1.044959956	2.195067785	-4.707334258
H	1.483485903	-0.205474012	-1.871112871
H	3.047394878	1.683314623	-1.368836800
H	2.748415988	3.882040075	-2.433427401
H	0.874040248	4.282709252	-4.041156329

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N	-1.519048052	0.892922718	-4.566313018
O	-2.600605489	0.418717910	-5.235796493
O	-1.561116338	3.050628341	-5.396305976
O	-1.021166299	-1.033439868	-3.390289913
C	-0.765409006	0.114899956	-3.692253685

Structure: **TS5**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 1

SCF Energy: -1296.999037140 hartree

SCF Energy + ZPVE: -1296.635944140 hartree

Free Energy: -1296.689028 hartree

Structure: **V**

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -633.169828830 hartree

SCF Energy + ZPVE: -632.938493830 hartree

Free Energy: -632.977230 hartree

C	-2.219106097	0.525050070	-1.138454932
C	-0.876406817	0.179616068	-1.333406771
C	0.187968383	0.977462269	-0.938012423
C	-0.141307100	2.180319842	-0.316778863
C	-1.479234965	2.552103800	-0.111929846
C	-2.531658152	1.735869166	-0.522003426
C	-3.023433116	-0.564048887	-1.702303408
C	-2.069795855	-1.523807758	-2.190670986
H	1.216800865	0.677481806	-1.105999572
H	0.652430451	2.842101132	0.013706145
H	-1.696941198	3.496951517	0.375426450



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H	-3.563794047	2.033895933	-0.365098368
N	-0.854962918	-1.078557577	-1.968426383
H	-2.230301827	-2.504067658	-2.620030899
H	-0.007206631	-1.596682986	-2.191140256
C	-7.364320575	-2.828851133	-2.238701305
C	-6.505581737	-1.869257954	-1.717803791
C	-5.241118898	-1.653706520	-2.299618304
C	-4.883521610	-2.371648094	-3.457240507
C	-5.754288828	-3.317321907	-3.983284127
C	-6.987138733	-3.556184301	-3.369365219
H	-8.330058664	-3.001423342	-1.775225916
H	-6.792583447	-1.290445948	-0.844554974
H	-3.955044115	-2.151607147	-3.973807476
H	-5.481239049	-3.858693193	-4.883092881
H	-7.663883864	-4.294794916	-3.787679952
C	-4.386572830	-0.665644467	-1.676240013
H	-4.905418623	0.092351185	-1.088512998

Structure: 7

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -996.886198542 hartree

SCF Energy + ZPVE: -996.520582542 hartree

Free Energy: -996.568637 hartree

C	-1.406843278	0.542716513	-1.004098045
C	-2.247610108	0.340600352	0.118678658
C	-2.465571044	1.333306872	1.082164601
C	-1.821275920	2.548061642	0.902174971
C	-0.985060601	2.776695640	-0.212910521
C	-0.774198588	1.790456273	-1.165011754

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C	-1.425994334	-0.679243340	-1.770209861
C	-2.260372582	-1.540193700	-1.100057128
H	-3.115607948	1.154208763	1.933001600
H	-1.965943071	3.340955457	1.629417961
H	-0.504167422	3.743334084	-0.325694110
H	-0.140127603	1.986937658	-2.025465494
N	-2.752798660	-0.933777025	0.029622352
H	-2.553468144	-2.552723518	-1.337621264
H	-3.401021570	-1.355208795	0.680988728
C	-1.728122974	-3.275759342	-5.809136771
C	-1.425756233	-2.125409081	-5.080032703
C	-0.983516228	-2.208744673	-3.754836281
C	-0.847004996	-3.476905866	-3.171421565
C	-1.145546556	-4.627880865	-3.900670834
C	-1.586628955	-4.531932023	-5.220980945
H	-2.071456351	-3.188188023	-6.835380233
H	-1.531402869	-1.148285312	-5.544910579
H	-0.512817140	-3.574357609	-2.142261159
H	-1.034648230	-5.601338267	-3.432729950
H	-1.819361410	-5.429646729	-5.785310126
C	-0.626138462	-0.930171288	-3.016381813
H	-0.789850792	-0.095647900	-3.708316026
C	1.436417931	-1.871036494	-1.692200460
C	2.384335091	-2.670424961	-2.331091719
C	3.053842259	-3.721860202	-1.728415001
C	2.733862323	-3.962701891	-0.391516686
C	1.798633707	-3.167898353	0.282589884
C	1.141392971	-2.111408551	-0.355121558
C	0.913697532	-0.873244707	-2.689059819
C	1.713053798	-1.206441600	-3.899137631

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H	3.783082223	-4.318452144	-2.265522186
H	3.224067577	-4.774993952	0.134358641
H	1.580277899	-3.376806628	1.324817510
H	0.420250751	-1.501046652	0.179363787
H	1.151403203	0.158064016	-2.394058142
N	2.503974776	-2.201943174	-3.669206959
H	1.666811043	-0.727611688	-4.871069600
H	3.135746144	-2.606925484	-4.361298128

Structure: **TS6**

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -996.864553783 hartree

SCF Energy + ZPVE: -996.501102783 hartree

Free Energy: -996.548473 hartree

C	-1.518657940	0.570536719	-1.009961722
C	-2.100395365	0.343376370	0.252504441
C	-2.299065109	1.358489800	1.188556655
C	-1.886888753	2.635275310	0.827351503
C	-1.300587924	2.887146959	-0.428792285
C	-1.110853806	1.867277787	-1.353482922
C	-1.473087831	-0.710102232	-1.691334621
C	-2.031429843	-1.635685621	-0.800620756
H	-2.753123685	1.154939142	2.152920015
H	-2.020305780	3.454871730	1.526057644
H	-0.993832864	3.898282487	-0.676620245
H	-0.663657782	2.072132137	-2.322575140
N	-2.407088313	-1.008636950	0.329064144
H	-2.230963820	-2.690540638	-0.922231925
H	-2.867428014	-1.458431653	1.112277744

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C	-1.287644546	-3.313777931	-5.854091619
C	-1.196403282	-2.145870691	-5.106059174
C	-1.000945905	-2.199133208	-3.714734710
C	-0.853295077	-3.450936369	-3.096451993
C	-0.933999175	-4.619865723	-3.851103785
C	-1.157630810	-4.555449424	-5.225904969
H	-1.452483836	-3.258182483	-6.925282365
H	-1.282167089	-1.177638903	-5.592494962
H	-0.638281096	-3.520396419	-2.034594070
H	-0.811440986	-5.581388039	-3.362505177
H	-1.219733146	-5.468523189	-5.809709472
C	-0.929839773	-0.925989489	-2.987116682
H	-0.916927785	-0.046687036	-3.628024398
C	1.487419591	-1.732210208	-1.684690396
C	2.065051176	-2.749655309	-2.469441559
C	2.378015425	-4.010558085	-1.968531680
C	2.073232598	-4.244300494	-0.631348068
C	1.481430262	-3.249365973	0.170352605
C	1.183564084	-1.989916134	-0.342198192
C	1.207454146	-0.623426822	-2.570526812
C	1.728116807	-0.997674343	-3.822692144
H	2.818216575	-4.776853081	-2.598365059
H	2.293536800	-5.214399061	-0.197562306
H	1.257317654	-3.471993705	1.208870505
H	0.730534170	-1.223211408	0.280801307
H	1.030210287	0.403342254	-2.279162867
N	2.194231796	-2.249525423	-3.765934719
H	1.739309714	-0.440336692	-4.749973912
H	2.550471251	-2.773405956	-4.558620856

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Structure: VI

Charge = 1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -996.886169228 hartree

SCF Energy + ZPVE: -996.520524228 hartree

Free Energy: -996.568590 hartree

C	-1.565501944	0.549535308	-1.033382231
C	-2.417335660	0.368476740	0.084588820
C	-2.612820544	1.365056073	1.048926981
C	-1.934646764	2.562046051	0.874360291
C	-1.086360516	2.769516262	-0.235768300
C	-0.897579883	1.779505543	-1.188630762
C	-1.615557683	-0.669427367	-1.802823796
C	-2.477242588	-1.508195105	-1.139158995
H	-3.272117919	1.202665870	1.895974436
H	-2.061407117	3.357377693	1.602301723
H	-0.578472332	3.722782034	-0.344046529
H	-0.253529359	1.959435605	-2.045412830
N	-2.957664947	-0.891010811	-0.010134881
H	-2.797700728	-2.511387667	-1.381029296
H	-3.621476241	-1.295228720	0.636412547
C	-1.992893755	-3.223801295	-5.858866339
C	-1.651945033	-2.090391693	-5.120348767
C	-1.214646875	-2.199391879	-3.795297311
C	-1.123156881	-3.476055857	-3.221631300
C	-1.460262970	-4.610184365	-3.960371236
C	-1.895969365	-4.488655454	-5.280367488
H	-2.331562862	-3.116403320	-6.884782112
H	-1.722795015	-1.106500555	-5.577478850
H	-0.793754984	-3.593456349	-2.192995160

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H	-1.383799857	-5.590606351	-3.500172955
H	-2.158656146	-5.373378301	-5.852016127
C	-0.817116719	-0.939370371	-3.045797336
H	-0.947973795	-0.094787513	-3.732521812
C	1.204983234	-1.959615774	-1.717879245
C	2.130409690	-2.783496532	-2.358644853
C	2.760811939	-3.862438975	-1.762478217
C	2.424030603	-4.105684243	-0.430132734
C	1.511117502	-3.286982946	0.246018414
C	0.893364957	-2.203045052	-0.385146625
C	0.721651333	-0.935802751	-2.708092214
C	1.517586775	-1.283201028	-3.916334403
H	3.473544642	-4.477514485	-2.300880852
H	2.883676160	-4.938882412	0.090630895
H	1.279196968	-3.498773871	1.284725473
H	0.189349334	-1.574312368	0.150850089
H	0.989567027	0.084567924	-2.400855695
N	2.274045753	-2.306175986	-3.691207182
H	1.492741710	-0.794118045	-4.883917542
H	2.896740970	-2.724934462	-4.383376934

Structure: **8**

Charge = 1 Multiplicity = 2

Number of imaginary frequencies: 0

SCF Energy: -1584.317478410 hartree

SCF Energy + ZPVE: -1583.842879410 hartree

Free Energy: -1583.907316 hartree

C	-0.348402174	-0.601164415	-4.519748338
C	0.101663325	0.737202780	-4.400374752
C	0.706568545	1.420603605	-5.462128191

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C	0.845755039	0.736859952	-6.662597806
C	0.394180315	-0.594036992	-6.807924949
C	-0.195526706	-1.269200883	-5.748993106
C	-0.911121292	-0.972694154	-3.246035552
C	-0.789491441	0.129167146	-2.435268921
H	1.059038523	2.441408453	-5.345429969
H	1.317577839	1.234150342	-7.505688510
H	0.522420679	-1.094577985	-7.763001929
H	-0.534212034	-2.295835511	-5.866590359
N	-0.182405437	1.152742424	-3.122762714
H	-1.090496666	0.278722692	-1.408009795
H	0.003418018	2.073512622	-2.748279384
C	-4.611341791	-2.937987607	-0.897574651
C	-3.703667322	-2.846677437	-1.952502033
C	-2.393188601	-2.402506426	-1.740066625
C	-2.005678782	-2.057135866	-0.437364456
C	-2.912605684	-2.149153878	0.618705036
C	-4.217349197	-2.588343866	0.393250600
H	-5.623625930	-3.282888684	-1.085787210
H	-4.014022964	-3.123745675	-2.957075446
H	-0.996581436	-1.708919027	-0.236968520
H	-2.596606388	-1.873827952	1.620412537
H	-4.920620213	-2.657404537	1.217524379
C	-1.447654955	-2.337899315	-2.926714331
H	-2.007275662	-2.686987328	-3.802361161
C	0.696458924	-3.149817118	-1.645990978
C	0.636012053	-4.268910185	-0.815669271
C	1.353617737	-4.412378807	0.359746838
C	2.184125133	-3.344675220	0.701823289
C	2.275139957	-2.210957484	-0.114831262

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C	1.538276908	-2.099356324	-1.297183796
C	-0.258419763	-3.361661962	-2.790724220
C	-0.785467354	-4.722598817	-2.496647807
H	1.273738263	-5.304153173	0.972055619
H	2.771015340	-3.397435621	1.612749921
H	2.934360711	-1.399537587	0.176910633
H	1.623155860	-1.217356930	-1.922010323
N	-0.280138328	-5.185699370	-1.401368568
H	-1.511364731	-5.286786734	-3.072449642
H	-0.509859322	-6.096130279	-0.999994830
C	4.129609672	-0.055764914	-6.685285609
C	4.107105651	0.797795387	-5.574442677
C	4.638189697	2.075320955	-5.630705973
C	5.203066690	2.478127401	-6.845421404
C	5.226501617	1.625432594	-7.954461365
C	4.686315599	0.336917349	-7.890996674
C	3.464930554	-1.326711894	-6.341192579
H	4.613241358	2.733217950	-4.768378904
H	5.628969802	3.472201299	-6.932124322
H	5.670632898	1.972876238	-8.881347055
H	4.696424040	-0.327101598	-8.748897689
N	3.055550379	-1.167888089	-4.967388242
O	2.441817887	-2.045181281	-4.308564097
O	3.263940636	-2.334487858	-6.968685064
O	3.200356923	0.467027539	-3.318172338
C	3.428355124	0.125057562	-4.450061108
H	0.259452480	-3.388313506	-3.761276347

Structure: **TS7**

Charge = 1 Multiplicity = 2



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Number of imaginary frequencies: 1

SCF Energy: -1584.291057090 hartree

SCF Energy + ZPVE: -1583.821889090 hartree

Free Energy: -1583.883080 hartree

C	-2.900263730	-1.893326774	-0.510462080
C	-3.379682774	-2.659630336	0.564490586
C	-3.351014591	-2.233511787	1.879896953
C	-2.829329011	-0.953234549	2.103487812
C	-2.374695872	-0.152471649	1.047018198
C	-2.396359044	-0.611771552	-0.270020386
C	-2.977341649	-2.720600047	-1.718180488
C	-3.660936350	-3.930761348	-1.262676979
H	-3.709081446	-2.857906390	2.691574603
H	-2.778164451	-0.574637542	3.119319148
H	-1.984378623	0.837366824	1.260130214
H	-2.022360300	0.000290359	-1.085640378
N	-3.840548499	-3.882603238	0.031126890
H	-3.957562553	-4.798891648	-1.840216211
H	-4.222909418	-4.646908539	0.587083382
C	-6.969860913	-2.060891516	-3.555105646
C	-5.653817368	-2.515087942	-3.489698810
C	-4.612282623	-1.625821924	-3.206406470
C	-4.904643995	-0.278231196	-2.985687781
C	-6.221711893	0.178708656	-3.053556760
C	-7.257099745	-0.711637697	-3.338057065
H	-7.770790663	-2.758785024	-3.779855753
H	-5.430818732	-3.564473893	-3.673098648
H	-4.096217777	0.417332504	-2.772293797
H	-6.436194841	1.230217065	-2.888022536
H	-8.281423346	-0.356401749	-3.394198075

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C	-3.170668219	-2.124818189	-3.105451372
H	-2.517232223	-1.243395446	-3.146613294
H	-1.737499337	-3.206845851	-1.719799342
C	0.631993972	-1.627259623	1.201186791
C	0.102654029	-2.749459199	1.850767453
C	0.069744699	-2.840634381	3.233268564
C	0.585881369	-1.759903225	3.954340606
C	1.112629806	-0.637882305	3.304274443
C	1.144655224	-0.553598515	1.908402684
C	0.473273658	-1.790560171	-0.259981817
H	-0.349089960	-3.709924730	3.729745712
H	0.574346091	-1.787771051	5.038830588
H	1.499510035	0.184975862	3.896348683
H	1.543201027	0.317757018	1.399128582
N	-0.135036932	-3.073286139	-0.411123967
O	-0.534410537	-3.549408519	-1.547653601
O	0.755328919	-1.076370902	-1.189427843
O	-0.961730169	-4.766926632	0.940576245
C	-0.409586191	-3.698566143	0.842006211
C	-2.964156087	-2.750401446	-5.626962088
C	-2.503394856	-3.874898018	-6.354090688
C	-2.512946226	-3.916701466	-7.753921024
C	-2.995474177	-2.800697558	-8.420621221
C	-3.458102212	-1.666891162	-7.716359971
C	-3.447993329	-1.630984711	-6.330084098
C	-2.804354836	-3.058170861	-4.227588191
C	-2.267341406	-4.320583392	-4.170595153
H	-2.155472363	-4.790134090	-8.290803585
H	-3.017503410	-2.797378980	-9.506101615
H	-3.826190131	-0.810818080	-8.273509739

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H	-3.804242679	-0.753242158	-5.796698126
N	-2.086287149	-4.812895658	-5.441411516
H	-1.983903750	-4.928039076	-3.321003081
H	-1.704906632	-5.722886050	-5.661564270

Structure: **16c**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -996.457518476 hartree

SCF Energy + ZPVE: -996.105254476 hartree

Free Energy: -996.155064 hartree

C	-0.281390000	0.187094000	-3.425693000
C	-0.373144000	1.521153000	-2.954703000
C	0.486827000	2.533566000	-3.399141000
C	1.455242000	2.184649000	-4.328597000
C	1.568632000	0.860889000	-4.809223000
C	0.713400000	-0.137930000	-4.367465000
C	-1.311757000	-0.568117000	-2.759721000
C	-1.964730000	0.314547000	-1.937508000
H	0.396516000	3.548962000	-3.025183000
H	2.141034000	2.942734000	-4.694600000
H	2.341197000	0.626405000	-5.535257000
H	0.808862000	-1.154475000	-4.741063000
N	-1.403977000	1.567825000	-2.048417000
H	-2.790235000	0.148002000	-1.258623000
H	-1.714074000	2.391547000	-1.551511000
C	-5.153753000	-2.708793000	-1.832329000
C	-4.031971000	-2.392194000	-2.598273000
C	-2.745018000	-2.479149000	-2.056904000
C	-2.602106000	-2.892858000	-0.728887000

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C	-3.722302000	-3.209440000	0.041391000
C	-5.001829000	-3.117493000	-0.506714000
H	-6.144760000	-2.636570000	-2.270815000
H	-4.153401000	-2.069644000	-3.630227000
H	-1.610674000	-2.971956000	-0.290841000
H	-3.593149000	-3.530916000	1.070766000
H	-5.872499000	-3.367149000	0.091991000
C	-1.552791000	-2.054486000	-2.904439000
H	-1.821237000	-2.253545000	-3.951411000
C	0.709170000	-2.603882000	-1.613312000
C	1.715570000	-3.588290000	-1.790474000
C	2.847406000	-3.664896000	-0.968243000
C	2.964687000	-2.727351000	0.046246000
C	1.979346000	-1.733498000	0.240829000
C	0.859423000	-1.663449000	-0.573605000
C	-0.288771000	-2.836345000	-2.629385000
C	0.151916000	-3.911161000	-3.358866000
H	3.600927000	-4.430874000	-1.124544000
H	3.830029000	-2.755452000	0.701366000
H	2.104871000	-1.013360000	1.043622000
H	0.106322000	-0.896719000	-0.412131000
N	1.348348000	-4.369349000	-2.858641000
H	-0.300840000	-4.388032000	-4.218153000
H	1.875640000	-5.150343000	-3.224453000

Structure: **VII**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -709.156189624 hartree

SCF Energy + ZPVE: -708.910493624 hartree

Free Energy: -708.952089 hartree

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C	-3.007566332	0.752144847	-0.849295118
C	-3.303545400	0.433744697	0.499024278
C	-3.752046905	1.393851604	1.414371648
C	-3.900716963	2.693061988	0.952343832
C	-3.612550598	3.033981388	-0.388243171
C	-3.168584111	2.078820977	-1.290218139
C	-2.583527797	-0.470618879	-1.485673342
C	-2.642171956	-1.448324571	-0.523023570
H	-3.974333503	1.127360496	2.443195614
H	-4.246903268	3.464092162	1.633821159
H	-3.741560476	4.061604626	-0.713767642
H	-2.945620138	2.347672184	-2.320106187
N	-3.071712480	-0.911407522	0.665191616
H	-2.419977035	-2.504592016	-0.592937241
H	-3.208428765	-1.429718975	1.522500654
C	-3.082321280	-4.011521634	-4.313919399
C	-3.132169746	-2.661321013	-3.968413092
C	-2.042068881	-2.048759681	-3.345198503
C	-0.895146554	-2.801468102	-3.077640044
C	-0.842200372	-4.151336767	-3.427254394
C	-1.935922758	-4.760129492	-4.043950372
H	-3.934813488	-4.476933695	-4.799388089
H	-4.023452746	-2.076252411	-4.182830034
H	-0.043837851	-2.331936979	-2.593532174
H	0.053141069	-4.727690316	-3.214208788
H	-1.894632114	-5.810561446	-4.315595339
C	-2.139380629	-0.602673700	-2.916238600
H	-2.874873592	-0.098802618	-3.558382688
O	-0.858286019	0.011972676	-3.125700114
H	-0.899801313	0.920328173	-2.795359761

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Structure: **TS8**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -709.086781663 hartree

SCF Energy + ZPVE: -708.845287663 hartree

Free Energy: -708.886848 hartree

C	-3.067101709	1.049110479	-0.245326399
C	-3.097852842	0.790133653	1.133033343
C	-2.431483801	1.570420014	2.071333282
C	-1.706098937	2.650080300	1.576057219
C	-1.652637268	2.924410203	0.198226799
C	-2.323430129	2.128731798	-0.726168087
C	-3.859766574	0.007070984	-0.887294597
C	-4.337089510	-0.816658930	0.168246235
H	-2.474139272	1.343912659	3.131465092
H	-1.167147353	3.290151796	2.267036929
H	-1.073038496	3.773899055	-0.148728189
H	-2.272968461	2.341745472	-1.789810664
N	-3.894977870	-0.347938338	1.325554832
H	-5.007702597	-1.664986239	0.135616072
H	-4.128805895	-0.743576499	2.232018720
C	-6.329558800	-1.893187044	-4.665024179
C	-5.607395971	-0.891951280	-4.025042808
C	-4.834994497	-1.191639244	-2.889600317
C	-4.744901732	-2.522896008	-2.444804847
C	-5.454012865	-3.522464526	-3.100374389
C	-6.255795519	-3.207883906	-4.200809232
H	-6.937984520	-1.652513036	-5.530619005
H	-5.647456033	0.132194894	-4.385357729

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H	-4.084341071	-2.777977166	-1.621480861
H	-5.372492167	-4.550667144	-2.763113848
H	-6.806180287	-3.993536643	-4.709125437
C	-4.131046108	-0.101966477	-2.236872733
H	-3.921192250	0.768533154	-2.851617114
O	-1.846586143	-0.639067739	-3.226700503
H	-2.257543324	-1.469472242	-3.496338584

Structure: **9**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -709.135593962 hartree

SCF Energy + ZPVE: -708.893744962 hartree

Free Energy: -708.937313 hartree

C	-3.301535897	0.690401023	-0.478322849
C	-3.389288544	0.194141118	0.833109250
C	-2.749732899	0.815576614	1.897965390
C	-2.006234380	1.966055507	1.620705157
C	-1.912700913	2.468368157	0.316292321
C	-2.556867960	1.833926495	-0.749905880
C	-4.085701266	-0.237820924	-1.302718227
C	-4.590430976	-1.215766145	-0.326242583
H	-2.827183845	0.418375191	2.906056787
H	-1.492514113	2.478597631	2.428015613
H	-1.329237065	3.364604498	0.129815674
H	-2.475441858	2.227150193	-1.759475007
N	-4.201834249	-0.967521563	0.886567334
H	-5.261719398	-2.040008204	-0.539819988
H	-4.552659821	-1.658166303	2.559279807
C	-6.439215661	-1.446066056	-5.438771797

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C	-5.722671581	-0.592205758	-4.606073277
C	-5.042614770	-1.093337641	-3.483485133
C	-5.048952460	-2.478150137	-3.246235585
C	-5.756967701	-3.330831313	-4.087929676
C	-6.461885057	-2.817354109	-5.178232055
H	-6.971989277	-1.044440646	-6.295047985
H	-5.695151799	0.474794600	-4.810280259
H	-4.466643554	-2.892548468	-2.429580077
H	-5.747745004	-4.399911941	-3.900327658
H	-7.013394263	-3.485829248	-5.832218546
C	-4.324968319	-0.144531416	-2.631368341
H	-3.961215247	0.751881479	-3.135553565
O	-4.720249675	-2.030148720	3.454870532
H	-4.452289159	-1.337540535	4.071642034

Structure: **TS9**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -709.111209386 hartree

SCF Energy + ZPVE: -708.873661386 hartree

Free Energy: -708.916374 hartree

Structure: **VIII**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -632.720370996 hartree

SCF Energy + ZPVE: -632.502722996 hartree

Free Energy: -632.541487 hartree

C	-3.229231233	0.820500332	-0.419666417
C	-3.341631022	0.419626183	0.922998400



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C	-2.678938790	1.093073459	1.940955239
C	-1.888953668	2.190908028	1.586724782
C	-1.772359382	2.595708326	0.251143397
C	-2.439746299	1.911308590	-0.769222253
C	-4.044317874	-0.134109385	-1.181680379
C	-4.587729374	-1.018818474	-0.136403405
H	-2.772059702	0.773656146	2.974657940
H	-1.357772585	2.738256290	2.359327382
H	-1.154266383	3.453212787	0.004113969
H	-2.343247096	2.227801937	-1.804333504
N	-4.198612366	-0.704582607	1.060070462
H	-5.288232755	-1.829860020	-0.300431453
C	-6.434903186	-1.568959918	-5.219673638
C	-5.694025040	-0.677140094	-4.450294659
C	-5.021335907	-1.115475745	-3.297476813
C	-5.061723033	-2.479777021	-2.964010916
C	-5.794096512	-3.371510958	-3.742620676
C	-6.490166745	-2.917871012	-4.864627587
H	-6.961946956	-1.215296764	-6.100387295
H	-5.641457651	0.372077449	-4.728455560
H	-4.487619445	-2.848611807	-2.119809305
H	-5.810261523	-4.424983734	-3.481306066
H	-7.060018046	-3.616046462	-5.470005253
C	-4.272912490	-0.129726559	-2.514466881
H	-3.874356936	0.712227034	-3.082278511

Structure: **1'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -363.204076725 hartree

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SCF Energy + ZPVE: -363.086868725 hartree

Free Energy: -363.116922 hartree

C	-2.284875488	0.234198105	-0.000000004
C	-3.724259161	0.206860952	0.000000004
C	-4.455784783	1.412794762	0.000000003
C	-3.769027829	2.618250095	0.000000003
C	-2.352218861	2.649868946	-0.000000001
C	-1.612362858	1.475766193	-0.000000009
C	-1.889401975	-1.135694717	0.000000009
C	-3.085641794	-1.855911490	-0.000000007
H	-5.544215228	1.391378469	0.000000004
H	-4.322065465	3.554039448	0.000000005
H	-1.841516535	3.609511332	-0.000000002
H	-0.524502179	1.515552855	-0.000000008
H	-0.882772444	-1.536090985	0.000000019
N	-4.200198084	-1.075491763	-0.000000009
H	-3.183190316	-2.938759202	-0.000000007

Structure: **5e**

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -345.449059260 hartree

SCF Energy + ZPVE: -345.338139260 hartree

Free Energy: -345.368809 hartree

C	-3.710845826	0.150117414	-0.317448624
C	-2.324096744	0.186030597	-0.179091689
C	-1.666587223	1.414036777	-0.061400100
C	-2.394416724	2.610880578	-0.076725652
C	-3.777647547	2.572596543	-0.212028544
C	-4.434264634	1.342944670	-0.333454094

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H	-4.224757520	-0.801242540	-0.413640319
H	-1.745606025	-0.734922371	-0.164525807
H	-1.868371427	3.556594027	0.018278837
H	-4.349167258	3.495575257	-0.223579397
H	-5.514729132	1.317735832	-0.441443537
C	-0.193353304	1.421030747	0.075035737
H	0.282592020	0.422764447	0.103689029
O	0.483008344	2.429548022	0.149827159

Structure: **TS1'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -708.632865135 hartree

SCF Energy + ZPVE: -708.403428135 hartree

Free Energy: -708.444278 hartree

C	-2.391459736	0.361710621	-0.114255778
C	-3.711185415	0.524250575	0.368747379
C	-4.197406909	1.773043869	0.759447805
C	-3.338744308	2.868704430	0.669600900
C	-2.027089576	2.716964799	0.190244542
C	-1.546129965	1.469057130	-0.212690202
C	-2.276883922	-1.042882946	-0.513402494
C	-3.536543464	-1.595022638	-0.030266739
H	-5.214220796	1.881897178	1.128252716
H	-3.685828050	3.851245068	0.976710927
H	-1.378448899	3.586860763	0.132619800
H	-0.534283754	1.361450082	-0.591379472
H	-1.350829971	-1.601232288	-0.397681640
N	-4.394923236	-0.704278298	0.403243244
H	-3.817687089	-2.643724293	-0.090272118

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C	-3.849007842	-4.398963569	-3.255907157
C	-3.724705121	-3.050160728	-2.919574968
C	-2.465090122	-2.475934050	-2.724333993
C	-1.327731453	-3.272214422	-2.884155613
C	-1.445911448	-4.622810333	-3.212776896
C	-2.708382230	-5.191292682	-3.399598624
H	-4.834168630	-4.831356860	-3.408491632
H	-4.615569912	-2.434271279	-2.803990684
H	-0.350367064	-2.814449096	-2.753829022
H	-0.553620181	-5.232489528	-3.328687985
H	-2.801613020	-6.241542449	-3.660928336
C	-2.319485980	-1.001815589	-2.369539508
H	-3.306184863	-0.493865063	-2.475768439
O	-1.277799781	-0.391177206	-2.804514952

Structure: **2'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -708.634619025 hartree

SCF Energy + ZPVE: -708.403902025 hartree

Free Energy: -708.444653 hartree

C	-2.477263451	0.483042331	-0.099067801
C	-3.726695153	0.634299412	0.528951204
C	-4.170590157	1.865299220	1.003013019
C	-3.326525420	2.966622773	0.840405898
C	-2.080957574	2.828716014	0.214688609
C	-1.646295253	1.586681207	-0.263825644
C	-2.374027539	-0.945342687	-0.521611766
C	-3.646274873	-1.480613209	0.054557724
H	-5.139539550	1.961122936	1.485389235

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H	-3.639808688	3.941496453	1.202894497
H	-1.443323878	3.700883832	0.099329057
H	-0.687275588	1.479976295	-0.760100061
H	-1.486642308	-1.476416850	-0.157765504
N	-4.419975714	-0.601590164	0.605106128
H	-3.948845646	-2.523981832	-0.001615742
C	-3.835195484	-4.456629678	-3.056681784
C	-3.691840230	-3.100146683	-2.757541851
C	-2.434943637	-2.552446490	-2.481516694
C	-1.317699861	-3.392247551	-2.524061458
C	-1.452916910	-4.750413880	-2.815129976
C	-2.714067120	-5.288541347	-3.082500165
H	-4.819484108	-4.863229101	-3.274185131
H	-4.569584253	-2.455094612	-2.739520718
H	-0.339490015	-2.955469721	-2.339334191
H	-0.574358203	-5.389920238	-2.840506665
H	-2.821164716	-6.343908000	-3.316909857
C	-2.256477335	-1.063729983	-2.140878443
H	-3.190092609	-0.555837079	-2.498465813
O	-1.121241859	-0.522942200	-2.571697686

Structure: **TS2'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -708.597224393 hartree

SCF Energy + ZPVE: -708.371096393 hartree

Free Energy: -708.412589 hartree

C	-2.622413448	0.592690858	-0.367364732
C	-3.473415007	0.505862109	0.758067123
C	-4.045418846	1.647506116	1.324730684

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C	-3.772494190	2.880438203	0.733847564
C	-2.939534105	2.971518271	-0.394388758
C	-2.353639084	1.833440123	-0.949877123
C	-2.163149037	-0.777240034	-0.627636453
C	-2.930524632	-1.550347863	0.342446092
H	-4.688841610	1.571344231	2.197616233
H	-4.209401095	3.784376085	1.148669144
H	-2.749580970	3.944597551	-0.838823894
H	-1.702723489	1.913522221	-1.817613877
H	-0.925856154	-0.906794544	-0.422046680
N	-3.637176039	-0.826631993	1.174183230
H	-2.894227498	-2.633464127	0.439885833
C	-4.012914312	-3.896873858	-3.281662499
C	-3.469917104	-2.682096594	-2.869815910
C	-2.149218900	-2.607149487	-2.406865128
C	-1.382868431	-3.772094717	-2.368280086
C	-1.923396815	-4.994379535	-2.780492066
C	-3.238367105	-5.061360639	-3.237823806
H	-5.038730581	-3.939698805	-3.637662888
H	-4.075756708	-1.777563822	-2.903217824
H	-0.359005832	-3.696350772	-2.014351113
H	-1.314780361	-5.894225935	-2.747266224
H	-3.658903396	-6.009189796	-3.561683755
C	-1.560084040	-1.277475259	-1.952392490
H	-1.793410123	-0.536878388	-2.743447075
O	-0.197500578	-1.321412500	-1.629586271

Structure: **3'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 0

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SCF Energy: -708.674654758 hartree

SCF Energy + ZPVE: -708.442858758 hartree

Free Energy: -708.484320 hartree

C	-2.237879505	0.410385114	0.091052015
C	-3.640068735	0.285655779	0.375954362
C	-4.510886859	1.365285160	0.124263077
C	-3.990634615	2.540074226	-0.400611096
C	-2.608309794	2.665303614	-0.682785285
C	-1.732914475	1.615496387	-0.440055882
C	-1.668269474	-0.849013722	0.454436365
C	-2.751473260	-1.607622230	0.915202176
H	-5.573637542	1.272672567	0.340220348
H	-4.651333743	3.379962237	-0.599739530
H	-2.231410454	3.598831872	-1.092487082
H	-0.671578238	1.725106211	-0.655574097
N	-3.939874994	-0.952920745	0.878529518
H	-2.705861920	-2.634679618	1.270085476
C	-0.044593104	-4.956550348	-0.359606961
C	-0.174371990	-3.577960559	-0.518575966
C	-0.010202121	-2.714324365	0.569656940
C	0.298158884	-3.253670929	1.819863053
C	0.428563104	-4.634961223	1.983637026
C	0.256004247	-5.490290940	0.895955416
H	-0.173885704	-5.614872883	-1.214090841
H	-0.410726841	-3.162630362	-1.496550094
H	0.442306990	-2.591768593	2.669323402
H	0.667136284	-5.041205522	2.962753401
H	0.359806024	-6.564032444	1.022830332
C	-0.217573668	-1.220648707	0.379524877
H	0.181191910	-0.951772969	-0.608644194

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O	0.574859464	-0.461571954	1.304277699
H	0.014673931	-0.256351136	2.064997038

Structure: **TS3'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -708.642851279 hartree

SCF Energy + ZPVE: -708.415154279 hartree

Free Energy: -708.423642 hartree

C	-2.447285839	0.421704577	0.047528756
C	-3.692543294	0.556901623	0.696832059
C	-4.462084043	1.710091406	0.557522979
C	-3.959748323	2.736442277	-0.244279464
C	-2.718046439	2.610273370	-0.887104590
C	-1.948087343	1.454454373	-0.745546555
C	-1.946668087	-0.895054608	0.434113091
C	-3.000929655	-1.414200586	1.301395858
H	-5.421146987	1.803285627	1.060005638
H	-4.535136967	3.648864228	-0.372112734
H	-2.351776955	3.426776036	-1.502714753
H	-0.985202899	1.365503262	-1.242405700
N	-4.006562614	-0.594930822	1.447048241
H	-3.014864282	-2.397422838	1.761331672
C	0.817041686	-4.855365792	-0.309191080
C	0.352447638	-3.575402954	-0.601348370
C	-0.301906672	-2.810576199	0.376172848
C	-0.445518558	-3.340876906	1.667796241
C	0.029745078	-4.616397962	1.961955026
C	0.654787799	-5.380543263	0.973951213
H	1.314125775	-5.438166572	-1.079034632



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H	0.490178274	-3.158922226	-1.596048071
H	-0.892670290	-2.736454994	2.451354718
H	-0.077308714	-5.011788308	2.967746198
H	1.025249146	-6.374342967	1.207648067
C	-0.788957168	-1.475840595	0.007075299
H	-0.231124703	-0.978153945	-0.778143316
O	1.293933493	-0.339186896	0.954853862
H	1.603928162	-1.134662166	1.405714562

Structure: OH-

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -75.877728569 hartree

SCF Energy + ZPVE: -75.868897569 hartree

Free Energy: -75.885150 hartree

O	-4.413899965	1.430917000	0.000000000
H	-5.378774035	1.430917000	0.000000000

Structure: 4'

Charge = 0 Multiplicity = 1

Number of imaginary frequencies: 0

SCF Energy: -632.730056975 hartree

SCF Energy + ZPVE: -632.512742975 hartree

Free Energy: -632.551789 hartree

C	-2.459593199	0.424563458	0.025920139
C	-3.694689144	0.582765582	0.680566672
C	-4.434105344	1.753817172	0.567518167
C	-3.906988603	2.779386102	-0.223157151
C	-2.676992808	2.628910153	-0.876601928
C	-1.937182671	1.448709636	-0.756820306

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C	-1.990536943	-0.918058598	0.393860284
C	-3.075477060	-1.426611019	1.256337210
H	-5.387411825	1.863749907	1.076504808
H	-4.458241402	3.708626161	-0.332821068
H	-2.292736153	3.442230540	-1.484919299
H	-0.981806574	1.339423531	-1.263391629
N	-4.044296064	-0.580566445	1.413042050
H	-3.120998112	-2.419341691	1.691886790
C	0.918677878	-4.818846099	-0.275407310
C	0.412064555	-3.560495223	-0.585275247
C	-0.340173917	-2.839066547	0.357100175
C	-0.527956593	-3.385244714	1.638147319
C	-0.009050929	-4.639034533	1.949171353
C	0.705590157	-5.362983289	0.992559561
H	1.485897353	-5.370934078	-1.018638613
H	0.583763992	-3.129525232	-1.568333269
H	-1.045551181	-2.813156283	2.401827857
H	-0.151538367	-5.047977531	2.944863383
H	1.108967653	-6.340303959	1.240566634
C	-0.862758585	-1.528011947	-0.035493808
H	-0.272542110	-0.998024055	-0.784470775

Structure: **TS4'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 1

SCF Energy: -995.932564555 hartree

SCF Energy + ZPVE: -995.596976555 hartree

Free Energy: -995.641767 hartree

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C	-3.918668418	0.608298344	0.865863177

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C	-4.981854031	1.502844926	0.692772977
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C	-1.922478270	-0.418838360	0.455653176
C	-2.593367522	-0.936374637	1.609905978
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H	-5.744559618	3.095555504	-0.531670192
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H	2.562993479	-4.859111873	1.022522112
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H	5.306508389	-1.405813736	-0.999974444
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Structure: **5'**

Charge = -1 Multiplicity = 1

Number of imaginary frequencies: 0

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SCF Energy + ZPVE: -995.623651885 hartree

Free Energy: -995.672753 hartree

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C	-3.628203892	2.509306616	-1.146700121
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C	-1.874727496	-0.501383262	0.398934320
C	-2.610877882	-1.131802084	1.407370053
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Structure: **TS11**

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Charge = 1 Multiplicity = 1

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C	-1.78521000	2.96356900	-0.11611400
C	-1.08409200	2.91569500	-1.34208600
C	-1.03132000	1.74724500	-2.09127600
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C	-2.51430500	-1.43525600	-1.13319300
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H	-2.82664900	-2.47047100	-1.11163300
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C	-3.86590700	-3.38481300	-4.83293700
C	-3.18632300	-2.37167800	-4.15926200
C	-1.79504600	-2.42178600	-3.99022200
C	-1.10344000	-3.51334100	-4.52500100
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H	-1.22286700	-5.37189400	-5.60168700
H	-3.69311900	-5.26795400	-5.87441400
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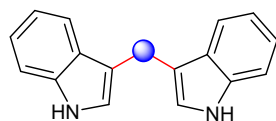
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C	1.21005100	-4.46156500	-0.63643700
C	0.34206500	-3.57621800	-1.32183600
C	0.39416000	-1.55214600	-3.00687900
C	1.47251000	-1.01655200	-3.76331800
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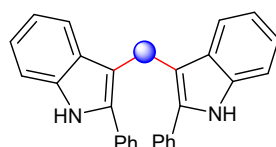
## 5 References

- (a) T. Benkovics; I. A. Guzei; T. P. Yoon, *Angew. Chem. Int. Ed.* **2010**, 49, 9153; (b) Bhattacharjee, P.; Boruah, P. K.; Das, M. R.; Bora, U., *New J. Chem.*, **2020**, 44, 7675.
- (a) Zheng, L.; Gao, F.; Yang, C.; Gao, G.; Zhao, Y.; Gao, Y.; Xia, W., *Org. Lett.* **2017**, 19, 5086; (b) Badigenchala, S.; Ganapathy, D.; Das, A.; Singh, R.; Sekar, G, *Synthesis*, **2014**, 46, 101; (c) Yadav, V.; Balaraman, E.; Mhaske, S. B., *Adv. Synth. Catal.* **2021**, 363, 4430; (d) Biswas, N.; Sharma, R.; Srimani, D., *Adv. Synth. Catal.* **2020**, 362, 2902; (e) Hikawa, H.; Yokoyama, Y., *RSC Adv.*, **2013**, 3, 1061; (f) Gopalaiah, K.; Chandrudu, S. N.; Devi, A., *Synthesis* **2015**; 47, 1766; (g) Kaswan, P.; Nandwana, N.K.; DeBoef, B.; Kumar, A., *Adv. Synth. Catal.*, **2016**, 358: 2108; (h) Dong, Y.; Lushnikova, T.; Golla, R.M.; Wang, X.; Wang, G., *Bioorgan. Med. Chem.*, **2017**, 25, 864; (i) Jin, J.; Li, Y.; Xiang, S.; Fan, W.; Guo, S.; Huang, D, *Org. Biomol. Chem.*, **2021**, 19, 4076; (j) Dipika; Sharma, Y. B.; Pant, S.; Dhaked, D. D.;

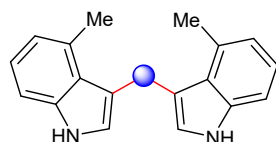
## 6 Detail descriptions for products



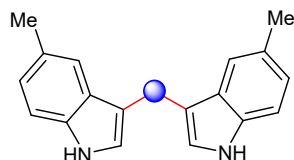
**di(1H-indol-3-yl)methane (1c).**<sup>2</sup> Yellow liquid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 79% isolated yield (48.6 mg). <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 10.75 (s, 2H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 1.8 Hz, 2H), 7.06 (t, *J* = 7.5 Hz, 2H), 6.95 (t, *J* = 7.4 Hz, 1H), 4.16 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO-*d*<sub>6</sub>) δ 136.8, 127.6, 123.2, 121.2, 119.1, 118.5, 114.7, 111.7, 21.4.



**bis(2-phenyl-1H-indol-3-yl)methane (2c).**<sup>2f</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 62% isolated yield (61.7 mg). <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 11.23 (s, 2H), 7.73 (d, *J* = 7.3 Hz, 4H), 7.49 (t, *J* = 7.7 Hz, 4H), 7.37 (t, *J* = 8.3 Hz, 4H), 7.07 (d, *J* = 8.0 Hz, 2H), 7.01 (t, *J* = 7.5 Hz, 2H), 6.74 (t, *J* = 7.5 Hz, 2H), 4.57 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO-*d*<sub>6</sub>) δ 136.5, 134.8, 133.6, 129.2, 129.0, 128.6, 127.6, 121.6, 119.6, 118.8, 111.5, 111.3, 21.7.



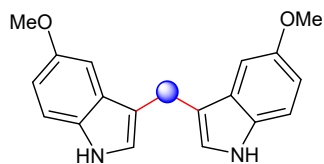
**bis(4-methyl-1H-indol-3-yl)methane (3c).**<sup>2</sup> White oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 70% isolated yield (47.9 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.84 (s, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.06 (t, *J* = 7.6 Hz, 2H), 6.83 (d, *J* = 7.1 Hz, 2H), 6.67 (s, 2H), 4.55 (s, 2H), 2.65 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 137.0, 131.3, 125.9, 122.9, 122.0, 120.7, 117.5, 109.0, 25.8, 20.1.



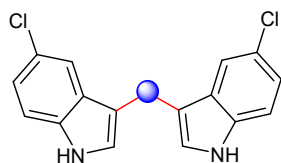
**bis(5-methyl-1H-indol-3-yl)methane (4c).**<sup>2</sup> White oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 74% isolated yield (50.7 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.75 (s, 2H), 7.40 (s, 2H), 7.22 (d, *J* = 8.3 Hz, 2H), 7.01 (d, *J* = 8.2 Hz, 2H), 6.83 (d, *J* = 0.9 Hz, 2H), 4.16 (s,



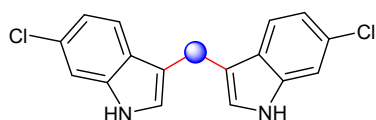
2H), 2.43 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 134.8, 128.3, 127.8, 123.4, 122.4, 118.8, 115.1, 110.7, 29.7, 21.5.



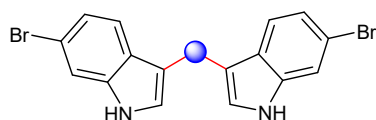
**bis(5-methoxy-1H-indol-3-yl)methane (5c).**<sup>2</sup> White oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/50) with 70% isolated yield (53.5 mg). <sup>1</sup>H NMR (500 MHz, DMSO *d*<sub>6</sub>) δ 10.57 (s, 2H), 7.23 (s, 1H), 7.21 (s, 1H), 7.09 (d, *J* = 2.1 Hz, 2H), 7.02 (d, *J* = 2.4 Hz, 2H), 6.71 (d, *J* = 2.4 Hz, 1H), 6.69 (d, *J* = 2.4 Hz, 1H), 4.07 (s, 2H), 3.71 (s, 6H). <sup>13</sup>C NMR (126 MHz, DMSO *d*<sub>6</sub>) δ 153.2, 132.0, 127.9, 123.9, 114.4, 112.3, 111.1, 101.1, 55.8, 21.3.



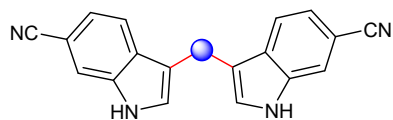
**bis(5-chloro-1H-indol-3-yl)methane (6c).**<sup>2</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 55% isolated yield (43.2 mg). <sup>1</sup>H NMR (500 MHz, DMSO *d*<sub>6</sub>) δ 10.99 (s, 2H), 7.51 (s, 2H), 7.34 (d, *J* = 8.6 Hz, 2H), 7.29 (d, *J* = 2.0 Hz, 2H), 7.03 (dd, *J* = 8.6, 1.9 Hz, 2H), 4.10 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO *d*<sub>6</sub>) δ 135.3, 128.6, 125.2, 123.2, 121.1, 118.3, 114.2, 113.3, 21.0



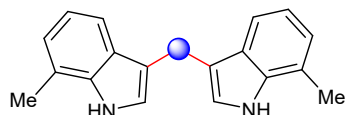
**bis(6-chloro-1H-indol-3-yl)methane (7c).**<sup>2</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 54% isolated yield (42.4 mg). <sup>1</sup>H NMR (500 MHz, DMSO *d*<sub>6</sub>) δ 10.92 (s, 2H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.37 (s, 2H), 7.20 (s, 2H), 6.93 (d, *J* = 8.4 Hz, 2H), 4.11 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO *d*<sub>6</sub>) δ 137.2, 126.3, 126.0, 124.4, 120.4, 118.8, 114.7, 111.4, 21.1.



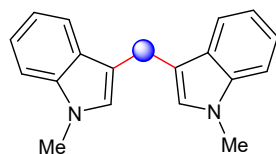
**bis(6-bromo-1H-indol-3-yl)methane (8c).**<sup>2</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 58% isolated yield (58.3 mg). <sup>1</sup>H NMR (500 MHz, DMSO *d*<sub>6</sub>) δ 10.92 (s, 2H), 7.50 (s, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.18 (s, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 4.10 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO *d*<sub>6</sub>) δ 137.7, 126.5, 124.3, 121.4, 120.8, 114.7, 114.3, 114.1, 21.0.



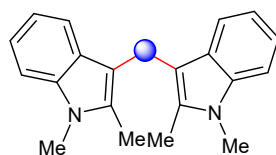
**3,3'-methylenebis(1H-indole-6-carbonitrile) (9c).**<sup>2h</sup> Brown oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/20) with 35% isolated yield (25.9 mg). <sup>1</sup>H NMR (500 MHz, DMSO *d*<sub>6</sub>) δ 11.39 (s, 2H), 7.82 (d, *J* = 0.6 Hz, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.50 (s, 2H), 7.26 (dd, *J* = 8.2, 1.3 Hz, 2H), 4.20 (s, 2H). <sup>13</sup>C NMR (126 MHz, DMSO *d*<sub>6</sub>) δ 135.5, 130.4, 128.1, 121.3, 121.2, 120.1, 116.7, 115.3, 102.6, 20.6.



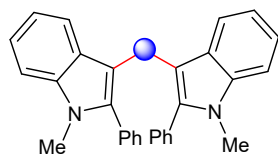
**bis(7-methyl-1H-indol-3-yl)methane (10c).**<sup>2</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 80% isolated yield (54.8 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.74 (s, 2H), 7.47 (d, *J* = 7.5 Hz, 2H), 7.00 - 6.99 (m, 4H), 6.87 (s, 2H), 4.21 (s, 2H), 2.45 (6, 1H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 136.0, 127.1, 122.4, 121.9, 120.2, 119.4, 117.0, 116.2, 29.7, 16.6.



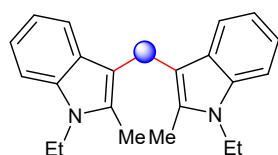
**bis(1-methyl-1H-indol-3-yl)methane (11c).**<sup>2d, 2i</sup> White oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 83% isolated yield (56.8 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.95 (d, *J* = 7.9 Hz, 2H), 7.55- 7.51 (m, 4H), 7.43 - 7.39 (m, 2H), 7.02 (s, 2H), 4.54 (s, 2H), 3.85 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 137.5, 128.3, 127.3, 121.7, 119.6, 118.9, 114.6, 109.4, 32.7, 21.3.



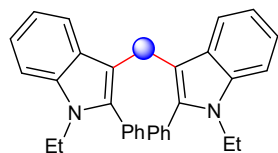
**bis(1,2-dimethyl-1H-indol-3-yl)methane (12c).**<sup>2i</sup> White oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 77% isolated yield (58.1 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.41 (d, *J* = 7.9 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.08 (t, *J* = 7.6 Hz, 2H), 6.95 (t, *J* = 7.4 Hz, 2H), 4.13 (s, 2H), 3.59 (s, 6H), 2.34 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 136.6, 132.7, 128.1, 120.3, 118.6, 118.5, 110.4, 108.4, 29.5, 20.0, 10.5.



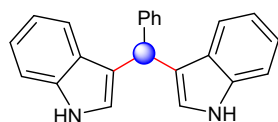
**bis(1-methyl-2-phenyl-1H-indol-3-yl)methane (13c).**<sup>2i</sup> Yellow solid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/75) with 75% isolated yield (79.8 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.42 – 7.33 (m, 6H), 7.30 – 7.26 (m, 4H), 7.24 (d, *J* = 7.9 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 7.12 (t, *J* = 7.6 Hz, 2H), 6.88 (t, *J* = 7.5 Hz, 2H), 4.20 (s, 2H), 3.52 (s, 6H). <sup>13</sup>C NMR (126 MHz, DMSO) δ 137.7, 137.3, 132.3, 130.9, 128.2, 128.1, 127.8, 121.3, 119.9, 118.9, 112.3, 109.0, 30.8, 21.1.



**bis(1-ethyl-2-methyl-1H-indol-3-yl)methane (14c).**<sup>2i</sup> White solid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 76% isolated yield (62.7 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.40 (d, *J* = 7.9 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.07 (t, *J* = 7.6 Hz, 2H), 6.94 (t, *J* = 7.4 Hz, 2H), 4.14 (s, 2H), 4.06 (q, *J* = 7.1 Hz, 4H), 2.33 (s, 6H), 1.26 (t, *J* = 7.2 Hz, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 135.5, 131.9, 128.4, 120.2, 118.6, 118.5, 110.5, 108.4, 37.7, 20.0, 15.4, 10.3.

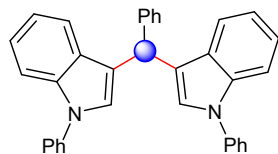


**bis(1-ethyl-2-phenyl-1H-indol-3-yl)methane (15c).**<sup>2i</sup> White solid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 79% isolated yield (89.6 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.40 – 7.33 (m, 6H), 7.27 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.17 (m, 6H), 7.11 (t, *J* = 7.6 Hz, 2H), 6.89 (t, *J* = 7.5 Hz, 2H), 4.10 (s, 2H), 3.97 (q, *J* = 7.1 Hz, 4H), 1.14 (t, *J* = 7.1 Hz, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 137.1, 135.9, 132.6, 130.7, 128.3, 128.1, 127.7, 121.1, 119.8, 118.7, 112.5, 109.2, 38.4, 20.7, 15.3.

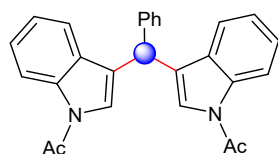


**3,3'-(phenylmethylene)bis(1H-indole) (16c).**<sup>2</sup> Yellow solid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/4) with 71% isolated yield (42.6 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.37 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 7.3 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.25 (t, *J* = 7.5 Hz, 2H), 7.19 (t, *J* = 7.2 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 2H), 6.98 (t, *J* = 7.5 Hz, 2H), 6.55 (d, *J* = 2.0 Hz, 2H), 5.85

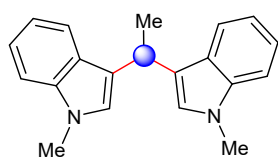
(s, 1H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  144.05, 136.7, 128.7, 128.2, 127.1, 126.1, 123.6, 121.9, 119.9, 119.7, 119.2, 111.0, 40.2.



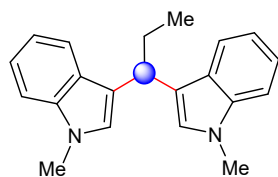
**3,3'-(phenylmethylene)bis(1-phenyl-1H-indole) (17c).**<sup>2f</sup> White solid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/50) with 78% isolated yield (92.4 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 (d,  $J$  = 8.3 Hz, 2H), 7.49 (d,  $J$  = 7.9 Hz, 2H), 7.46 – 7.39 (m, 10H), 7.30 (t,  $J$  = 7.5 Hz, 2H), 7.28 – 7.23 (m, 2H), 7.23 – 7.17 (m, 3H), 7.06 (t,  $J$  = 7.1 Hz, 2H), 6.89 (d,  $J$  = 0.8 Hz, 2H), 5.98 (s, 1H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  143.5, 139.8, 136.5, 129.5, 128.8, 128.5, 128.4, 127.3, 126.4, 126.1, 124.2, 122.4, 120.4, 120.3, 119.9, 110.5, 40.2.



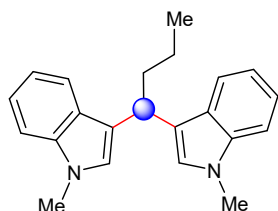
**1,1'-((phenylmethylene)bis(1H-indole-3,1-diyl))bis(ethan-1-one) (18c).** Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/20) with 76% isolated yield (77.1 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.44 (d,  $J$  = 5.6 Hz, 2H), 7.40 – 7.26 (m, 9H), 7.18 (t,  $J$  = 7.5 Hz, 2H), 6.86 (s, 2H), 5.73 (s, 1H), 2.45 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  168.6, 140.7, 136.3, 130.2, 129.7, 128.8, 128.5, 127.2, 125.5, 124.1, 123.6, 119.8, 116.7, 39.9, 24.0. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}_2$  407.1754; found: 407.1753.



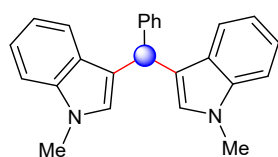
**3,3'-(ethane-1,1-diyl)bis(1-methyl-1H-indole) (21c).**<sup>2b</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/5) with 77% isolated yield (38.9 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.58 (d,  $J$  = 7.9 Hz, 2H), 7.27 (d,  $J$  = 8.2 Hz, 2H), 7.19 (t,  $J$  = 7.6 Hz, 2H), 7.03 (t,  $J$  = 7.4 Hz, 2H), 6.77 (s, 2H), 4.66 (q,  $J$  = 7.0 Hz, 1H), 3.69 (s, 6H), 1.78 (d,  $J$  = 7.1 Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.3, 127.3, 126.0, 121.3, 120.3, 119.8, 118.4, 109.1, 32.6, 28.0, 22.2.



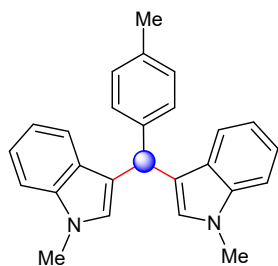
**3,3'-(propane-1,1-diyl)bis(1-methyl-1H-indole) (22c).**<sup>2b</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 62 % isolated yield (46.8 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.17 (t, *J* = 7.1 Hz, 2H), 7.02 (t, *J* = 7.0 Hz, 2H), 6.83 (s, 2H), 4.36 (t, *J* = 7.4 Hz, 1H), 3.69 (s, 6H), 2.22 (p, *J* = 7.3 Hz, 2H), 1.00 (t, *J* = 7.3 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 137.3, 127.6, 126.2, 121.2, 119.8, 119.0, 118.4, 109.1, 35.8, 32.6, 29.2, 13.2.



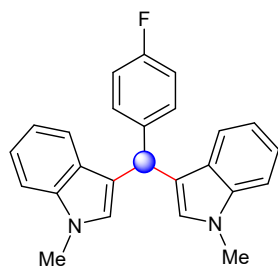
**3,3'-(butane-1,1-diyl)bis(1-methyl-1H-indole) (23c).**<sup>2b</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 32 % isolated yield (25.3 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.16 (t, *J* = 7.2 Hz, 2H), 7.02 (t, *J* = 7.5 Hz, 2H), 6.82 (s, 2H), 4.47 (t, *J* = 7.5 Hz, 1H), 3.65 (s, 6H), 2.17 (dd, *J* = 15.3, 7.6 Hz, 2H), 1.46 – 1.37 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 137.3, 127.6, 126.2, 121.3, 119.8, 119.3, 118.4, 109.1, 38.7, 33.6, 32.6, 21.6, 14.3.



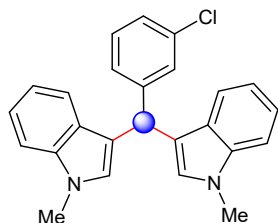
**3,3'-(phenylmethylene)bis(1-methyl-1H-indole) (24c).**<sup>2a</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 84% isolated yield (73.5 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.30 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 7.4 Hz, 2H), 7.19 (t, *J* = 8.0 Hz, 4H), 7.12 (dd, *J* = 14.9, 7.5 Hz, 3H), 6.91 (t, *J* = 7.3 Hz, 2H), 6.44 (s, 2H), 5.80 (s, 1H), 3.58 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 144.5, 137.4, 128.7, 128.3, 128.2, 127.5, 126.0, 121.4, 120.0, 118.6, 118.3, 109.1, 40.1, 32.7.



**3,3'-(p-tolylmethylene)bis(1-methyl-1H-indole) (25c).**<sup>2a</sup> White oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 74% isolated yield (67.3 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.38 (d, *J* = 7.9 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.18 (t, *J* = 7.6 Hz, 2H), 7.07 (d, *J* = 7.7 Hz, 2H), 6.98 (t, *J* = 7.5 Hz, 2H), 6.52 (s, 2H), 5.84 (s, 1H), 3.66 (s, 6H), 2.31 (s, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 141.4, 137.4, 135.3, 128.9, 128.5, 128.2, 127.5, 121.3, 120.1, 118.6, 118.4, 109.0, 39.6, 32.6, 21.1.

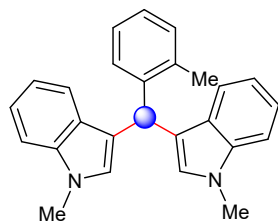


**3,3'-((4-fluorophenyl)methylene)bis(1-methyl-1H-indole) (26c).**<sup>2a</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 74% isolated yield (68.1 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.35 (d, *J* = 7.9 Hz, 2H), 7.28 (t, *J* = 7.8 Hz, 4H), 7.20 (t, *J* = 7.6 Hz, 2H), 7.00 (t, *J* = 7.5 Hz, 2H), 6.95 (t, *J* = 8.7 Hz, 2H), 6.50 (s, 2H), 5.86 (s, 1H), 3.68 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 161.3 (d, *J* = 243.8 Hz), 140.1, 137.4, 130.0 (d, *J* = 7.8 Hz), 128.2, 127.3, 121.5, 119.9, 118.7, 118.1, 114.9 (d, *J* = 21.1 Hz), 109.1, 39.3, 32.7. <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -117.5.

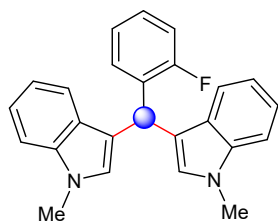


**3,3'-((3-chlorophenyl)methylene)bis(1-methyl-1H-indole) (27c).**<sup>2a</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 73% isolated yield (70.1 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.35 (d, *J* = 7.9 Hz, 2H), 7.32 (s, 1H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.18 (m, 2H), 7.17 (s, 1H), 7.17 (s, 1H), 7.16 – 7.14 (m, 2H), 6.98 (t, *J* = 7.5 Hz, 2H), 6.50 (s, 2H), 5.84 (s,

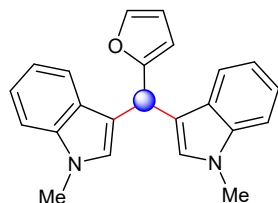
1H), 3.60 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 146.8, 137.5, 134.1, 129.6, 128.8, 128.4, 127.4, 127.0, 126.4, 121.7, 119.9, 118.9, 117.6, 109.3, 40.0, 32.7.



**3,3'-(*o*-tolylmethylene)bis(1-methyl-1H-indole) (28c).**<sup>2a</sup> White oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 73% isolated yield (66.4 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.34 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.16 (m, 3H), 7.15 – 7.09 (m, 2H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.99 (t, *J* = 7.1 Hz, 2H), 6.44 (s, 2H), 6.02 (s, 1H), 3.66 (s, 6H), 2.38 (s, 3H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 142.5, 137.4, 136.0, 130.1, 128.5, 128.4, 127.6, 125.9, 125.8, 121.4, 119.9, 118.6, 117.7, 109.0, 60.4, 32.6, 19.6.

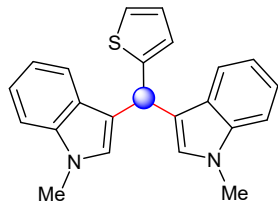


**3,3'-(2-fluorophenyl)methylenebis(1-methyl-1H-indole) (29c).**<sup>2a</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 74% isolated yield (68.1 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.36 (d, *J* = 7.8 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.15 (m, 4H), 7.05 (t, *J* = 9.2 Hz, 1H), 6.98 (q, *J* = 7.4 Hz, 3H), 6.58 (s, 2H), 6.19 (s, 1H), 3.66 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 160.4 (d, *J* = 245.7 Hz), 137.3, 131.2 (d, *J* = 14.2 Hz), 130.2 (d, *J* = 4.1 Hz), 128.1, 127.6 (d, *J* = 8.1 Hz), 127.1, 123.8 (d, *J* = 3.4 Hz), 121.4, 119.6, 118.6, 116.6, 115.1 (d, *J* = 22.3 Hz), 109.1, 32.6, 32.1 (d, *J* = 4.0 Hz). <sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) δ -118.7.

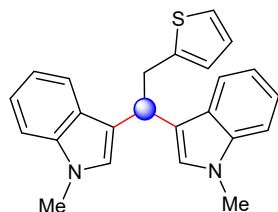


**3,3'-(furan-2-ylmethylene)bis(1-methyl-1H-indole) (30c).**<sup>2</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 64% isolated yield (54.4 mg). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.46 (d, *J* = 8.0 Hz, 2H), 7.33 (s, 1H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.18 (t, *J* = 7.6 Hz,

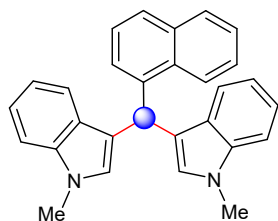
2H), 7.01 (t,  $J = 7.5$  Hz, 2H), 6.71 (s, 2H), 6.27 (dd,  $J = 3.0, 1.9$  Hz, 1H), 6.04 (d,  $J = 3.1$  Hz, 1H), 5.92 (s, 1H), 3.62 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  157.5, 141.2, 137.3, 127.7, 127.2, 121.5, 119.8, 118.9, 115.8, 110.2, 109.3, 106.5, 34.0, 32.7.



**3,3'-(thiophen-2-ylmethylene)bis(1-methyl-1H-indole) (31c).**<sup>2</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 63% isolated yield (56.1 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 (d,  $J = 7.9$  Hz, 2H), 7.29 (d,  $J = 8.2$  Hz, 2H), 7.20 (t,  $J = 7.6$  Hz, 2H), 7.14 (d,  $J = 4.9$  Hz, 1H), 7.02 (t,  $J = 7.4$  Hz, 2H), 6.93 – 6.87 (m, 2H), 6.71 (s, 2H), 6.15 (s, 1H), 3.69 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  149.2, 137.3, 127.8, 127.1, 126.4, 125.0, 123.4, 121.5, 119.8, 118.8, 118.2, 109.1, 35.2, 32.7.



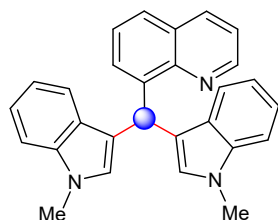
**3,3'-(2-(thiophen-2-yl)ethane-1,1-diyl)bis(1-methyl-1H-indole) (32c).**<sup>2</sup> Yellow oil was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 66% isolated yield (61.1 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 (d,  $J = 7.9$  Hz, 2H), 7.22 (d,  $J = 8.2$  Hz, 2H), 7.16 (dd,  $J = 11.1, 3.9$  Hz, 2H), 7.06 (dd,  $J = 4.9, 3.0$  Hz, 1H), 7.01 (t,  $J = 7.4$  Hz, 2H), 6.80 (d,  $J = 4.9$  Hz, 1H), 6.76 - 6.75 (m, 3H), 4.78 (t,  $J = 7.3$  Hz, 1H), 3.60 (s, 6H), 3.51 (d,  $J = 7.3$  Hz, 2H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  141.8, 137.4, 128.8, 127.5, 126.7, 124.6, 121.4, 121.2, 119.8, 118.6, 118.4, 109.2, 36.9, 35.4, 32.7.



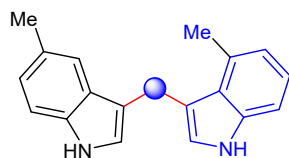
**3,3'-(naphthalen-1-ylmethylene)bis(1-methyl-1H-indole) (33c).**<sup>2b</sup> White solid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 46% isolated yield (46.1 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.17 (d,  $J = 8.5$  Hz, 1H), 7.87 (d,  $J = 8.0$  Hz, 1H), 7.73 (d,  $J = 7.9$  Hz, 1H),



7.44 (t,  $J = 7.0$  Hz, 1H), 7.37 (dd,  $J = 12.6, 4.5$  Hz, 3H), 7.33 – 7.25 (m, 4H), 7.20 (t,  $J = 7.6$  Hz, 2H), 6.98 (t,  $J = 7.4$  Hz, 2H), 6.66 (s, 1H), 6.44 (s, 2H), 3.63 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  140.0, 137.5, 133.9, 131.8, 128.9, 128.6, 127.4, 126.8, 126.1, 125.8, 125.5, 125.2, 124.3, 121.4, 119.9, 118.6, 117.9, 109.0, 35.6, 32.7.

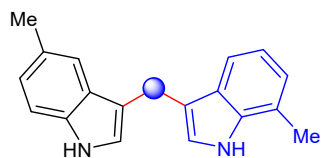


**8-(bis(1-methyl-1H-indol-3-yl)methyl)quinolone (34c).**<sup>2j</sup> White solid was obtained by column chromatography (eluent: EtOAc/petroleum ether = 1/100) with 36% isolated yield (36.1 mg).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.92 (dd,  $J = 4.1, 1.8$  Hz, 1H), 8.13 (dd,  $J = 8.3, 1.8$  Hz, 1H), 7.65 (dd,  $J = 15.5, 7.7$  Hz, 2H), 7.51 (s, 1H), 7.41 (d,  $J = 8.0$  Hz, 3H), 7.39 – 7.35 (m, 1H), 7.24 (d,  $J = 8.2$  Hz, 2H), 7.15 (t,  $J = 7.1$  Hz, 2H), 6.93 (t,  $J = 7.5$  Hz, 2H), 6.53 (s, 2H), 3.62 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  149.7, 146.2, 143.0, 137.5, 136.2, 129.4, 128.4, 128.3, 127.7, 126.3, 126.0, 121.2, 120.9, 120.5, 118.8, 118.4, 108.9, 32.8, 32.6.



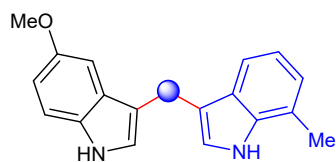
**37c**, 52%  
(**3c** : **4c** : **37c** = 23 : 25 : 52)

**5-methyl-3-((4-methyl-1H-indol-3-yl)methyl)-1H-indole (37c).** Brown oil was obtained 71.9 mg (**3c** : **4c** : **37c** = 23 : 25 : 52) by column chromatography (eluent: EtOAc/petroleum ether = 1/100).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47 (dd,  $J = 26.9, 14.0$  Hz, 3.85H), 7.38 (s, 2H), 7.11 (dd,  $J = 8.3, 2.2$  Hz, 2H), 7.07 – 7.01 (m, 4H), 6.98 (t,  $J = 7.7$  Hz, 2H), 6.81 (t,  $J = 5.8$  Hz, 2H), 6.67 (d,  $J = 1.3$  Hz, 0.85H), 6.59 (d,  $J = 1.6$  Hz, 1H), 6.51 (d,  $J = 1.2$  Hz, 1H), 6.46 (d,  $J = 1.6$  Hz, 0.85H), 4.48 (s, 0.9H), 4.28 (s, 2H), 4.11 (s, 0.95H), 2.61 (s, 2.75H), 2.58 (s, 3H), 2.42 (s, 3H), 2.40 (s, 2.75H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  137.0, 137.0, 131.4, 131.4, 128.4, 128.4, 127.8, 127.6, 126.2, 126.0, 123.6, 123.5, 123.1, 123.0, 122.9, 122.6, 122.0, 120.8, 120.8, 118.9, 117.4, 116.4, 116.1, 115.1, 110.9, 109.1, 29.8, 25.8, 23.5, 21.6, 21.2, 20.2, 20.1. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{19}\text{N}_2$  275.1543; found: 275.1541.



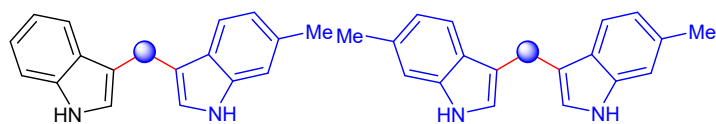
**38c**, 50%  
(**4c** : **10c** : **38c** = 25 : 25 : 50)

**7-methyl-3-((5-methyl-1H-indol-3-yl)methyl)-1H-indole (38c)**. Brown oil was obtained 83.0 mg (**4c** : **10c** : **38c** = 25 : 25 : 50) by column chromatography (eluent: EtOAc/petroleum ether = 1/100). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.53 (d, *J* = 15.2 Hz, 4H), 7.45 (d, *J* = 7.4 Hz, 2H), 7.38 (s, 2H), 7.13 (d, *J* = 8.2 Hz, 2H), 7.03 – 6.94 (m, 6H), 6.73 – 6.66 (m, 4H), 4.16 (s, 1H), 4.14 (s, 2H), 4.12 (s, 1H), 2.41 (s, 6H), 2.38 (s, 6H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 136.1, 136.0, 134.8, 134.7, 128.4, 127.9, 127.8, 127.2, 127.2, 123.5, 122.5, 122.4, 122.1, 120.3, 119.4, 119.0, 118.9, 117.1, 117.0, 116.3, 116.2, 115.2, 115.1, 110.8, 21.6, 21.4, 21.3, 21.2, 16.5. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> calcd for C<sub>19</sub>H<sub>19</sub>N<sub>2</sub> 275.1543; found: 275.1541.



**39c**, 52%  
(**5c** : **10c** : **39c** = 24 : 24 : 52)

**5-methoxy-3-((7-methyl-1H-indol-3-yl)methyl)-1H-indole (39c)**. Brown oil was obtained 77.3 mg (**5c** : **10c** : **38c** = 25 : 25 : 50) by column chromatography (eluent: EtOAc/petroleum ether = 1/100). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 19.6 Hz, 4H), 7.49 – 7.40 (m, 2H), 7.08 (dd, *J* = 8.8, 2.1 Hz, 2H), 7.03 (s, 2H), 7.00 (td, *J* = 7.4, 2.6 Hz, 2H), 6.95 (d, *J* = 6.9 Hz, 2H), 6.81 (dd, *J* = 8.7, 2.2 Hz, 2H), 6.69 (s, 3H), 4.15 (s, 0.95H), 4.12 (s, 2H), 4.09 (s, 0.95H), 3.76 (s, 5.5H), 2.35 (s, 5.5H). <sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) δ 153.8, 153.7, 136.1, 136.0, 131.7, 128.1, 128.0, 127.2, 127.1, 123.3, 123.2, 122.5, 122.4, 122.2, 122.1, 120.5, 120.4, 119.5, 119.4, 117.1, 117.0, 116.1, 116.0, 115.3, 115.2, 101.3, 101.2, 56.0, 21.5, 21.4, 21.3, 16.5. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> calcd for C<sub>19</sub>H<sub>19</sub>N<sub>2</sub>O 291.1492; found: 291.1490.

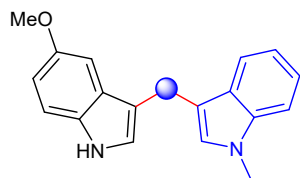


**40c**, 47%  
(**1c** : **40c** : **41c** = 32 : 47 : 21)

**41c** = **21a** + **1b** + **21a**

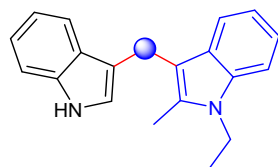
**3-((1H-indol-3-yl)methyl)-6-methyl-1H-indole (40c)**. Brown oil was obtained 51.7 mg (**1c** : **40c** : **41c** = 32 : 47 : 21) by column chromatography (eluent: EtOAc/petroleum ether = 1/100). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.58 (dd, *J* = 7.8, 3.7 Hz, 3H), 7.55 (s, 2H), 7.48 (s, 1.8H), 7.38 (s, 1.85H), 7.21 (d, *J* = 8.1 Hz,

2H), 7.16 (d,  $J = 7.1$  Hz, 2H), 7.13 (dd,  $J = 12.3, 6.5$  Hz, 2H), 7.07 (t,  $J = 7.4$  Hz, 2H), 6.98 (d,  $J = 8.2$  Hz, 1.85H), 6.70 (d,  $J = 12.9$  Hz, 4H), 4.17 (s, 1.35H), 4.14 (s, 2H), 4.12 (s, 0.9H), 2.41 (s, 5.6H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  136.5, 136.4, 134.8, 134.8, 128.5, 128.4, 127.8, 127.6, 123.5, 123.4, 122.6, 122.4, 121.9, 119.3, 119.2, 119.1, 118.9, 118.8, 115.7, 115.6, 115.1, 115.0, 111.2, 110.9, 21.6, 21.2, 21.1. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{18}\text{H}_{17}\text{N}_2$  261.1386; found: 261.1382.



**42c**, 37%  
(**5c** : **11c** : **42c** = 17 : 53 : 30)

**5-methoxy-3-((1-methyl-1H-indol-3-yl)methyl)-1H-indole (42c)**. Brown oil was obtained **42c**, 17.9 mg, 37% yield), **11c** (30.9 mg, 68%), **5c** (11.3 mg, 22%), (**5c** : **11c** : **42c** = 18 : 68 : 29) by column chromatography (eluent: EtOAc/petroleum ether = 1/100).  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.77 (s, 1H), 7.62 (d,  $J = 7.9$  Hz, 1H), 7.28 (d,  $J = 8.2$  Hz, 1H), 7.22 (dd,  $J = 4.7, 2.2$  Hz, 2H), 7.08 (t,  $J = 7.4$  Hz, 1H), 7.05 (d,  $J = 2.4$  Hz, 1H), 6.89 (d,  $J = 2.1$  Hz, 1H), 6.84 (dd,  $J = 8.8, 2.4$  Hz, 1H), 4.18 (s, 2H), 3.80 (s, 3H), 3.68 (s, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  153.8, 137.2, 131.6, 127.9, 127.8, 127.0, 123.0, 121.4, 119.3, 118.6, 115.5, 114.1, 112.0, 111.7, 109.1, 101.1, 55.9, 32.5, 21.1. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{19}\text{H}_{19}\text{N}_2\text{O}$  291.1492; found: 291.1490.



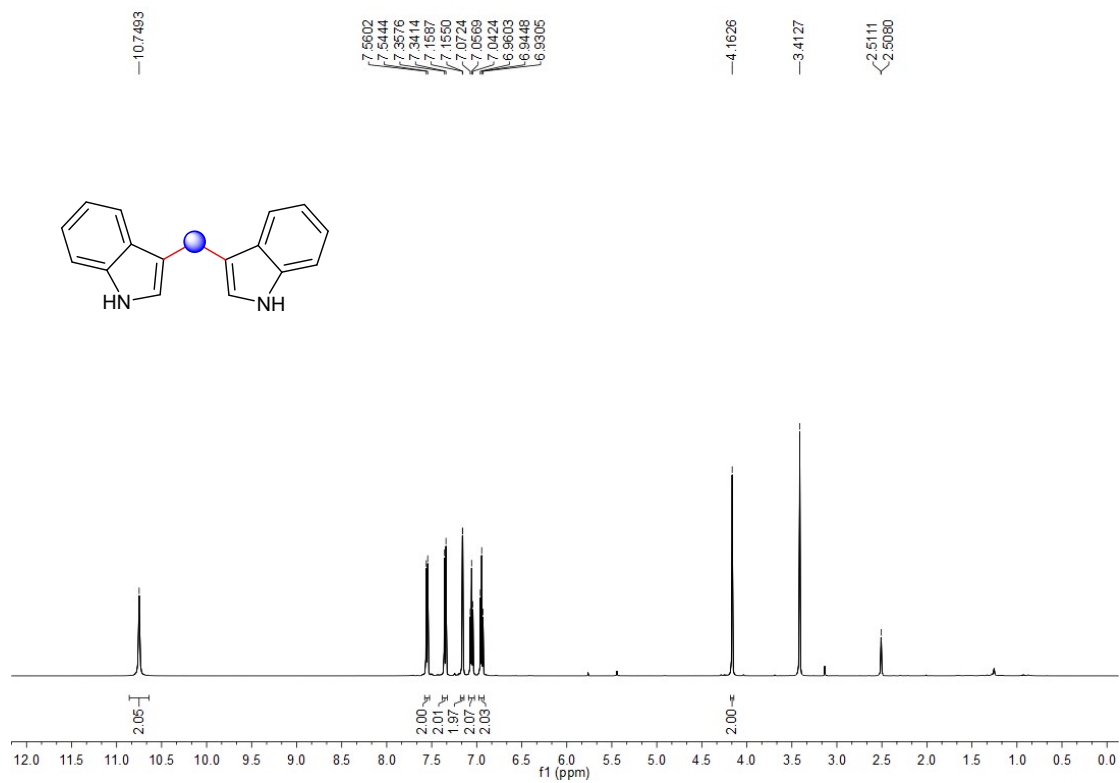
**43c**, 61%  
(**1c**, 15%)

**3-((1H-indol-3-yl)methyl)-1-ethyl-2-methyl-1H-indole (43c)**. Brown oil was obtained **43c** (43.9 mg, 61%), **1c** (9.2 mg, 15%) by column chromatography (eluent: EtOAc/petroleum ether = 1/100).  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ )  $\delta$  10.70 (s, 1H), 7.51 (d,  $J = 7.9$  Hz, 1H), 7.47 (d,  $J = 7.8$  Hz, 1H), 7.33 (dd,  $J = 8.1, 3.1$  Hz, 2H), 7.03 (dd,  $J = 15.1, 7.6$  Hz, 2H), 6.99 (s, 1H), 6.93 (dd,  $J = 15.5, 7.7$  Hz, 2H), 4.15 (q,  $J = 7.1$  Hz, 2H), 4.11 (s, 2H), 2.44 (s, 3H), 1.22 (t,  $J = 7.1$  Hz, 3H).  $^{13}\text{C}$  NMR (126 MHz,  $\text{DMSO } d_6$ )  $\delta$  136.8, 135.6, 132.5, 128.2, 127.5, 123.1, 121.2, 120.4, 118.9, 118.6, 118.5, 115.1, 111.7, 10.2, 109.2, 37.6, 20.3, 15.7, 10.3. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  calcd for  $\text{C}_{20}\text{H}_{21}\text{N}_2$  289.1699; found: 289.1694.

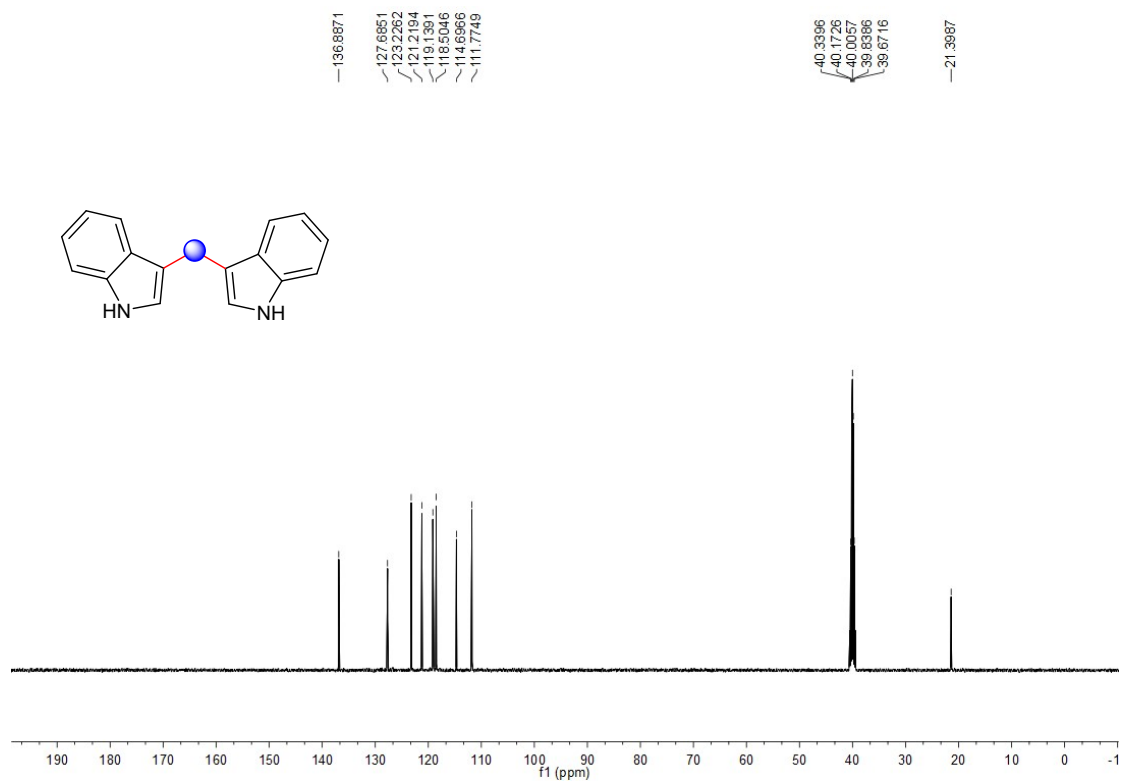
## 7 Copies of product NMR and HRMS Spectra

1c

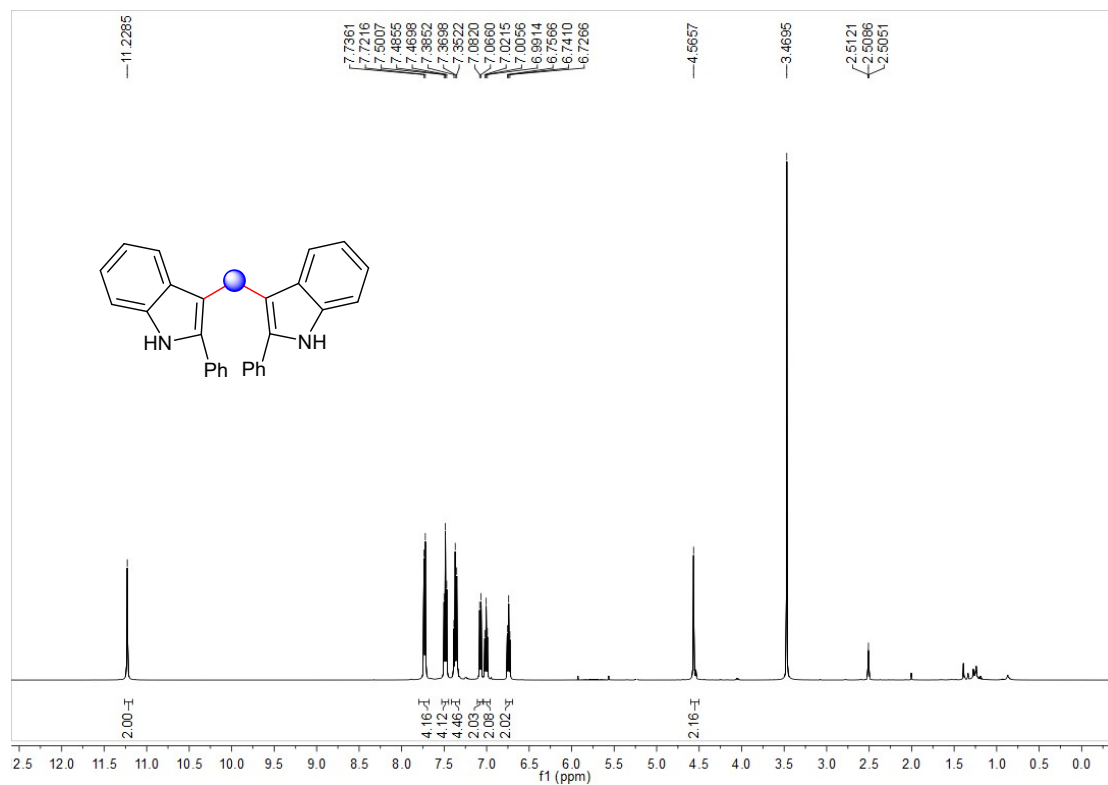
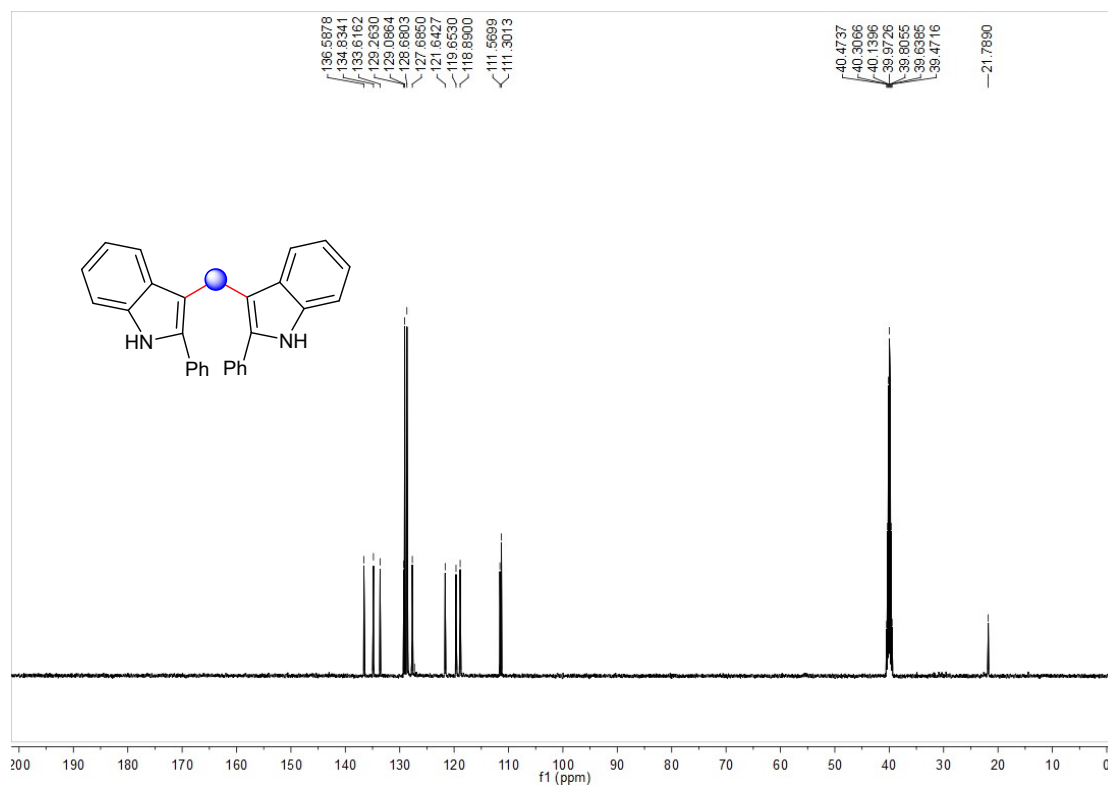
<sup>1</sup>H NMR



<sup>13</sup>C NMR

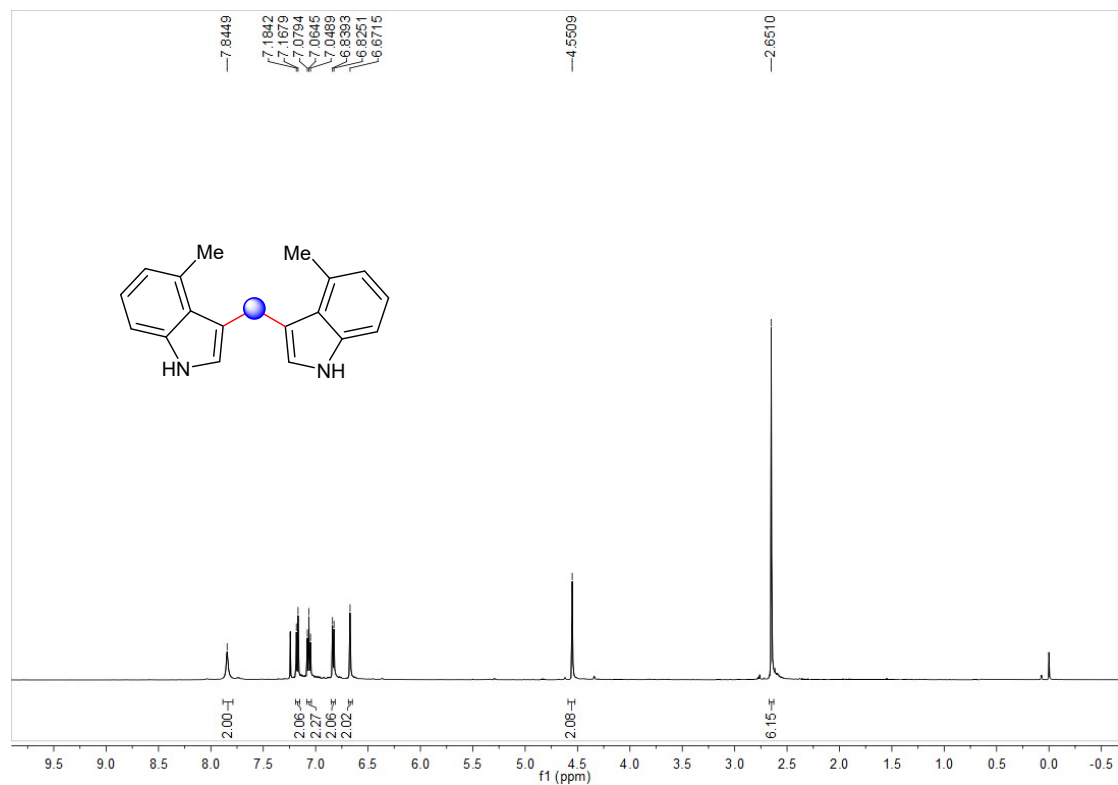


## 2c

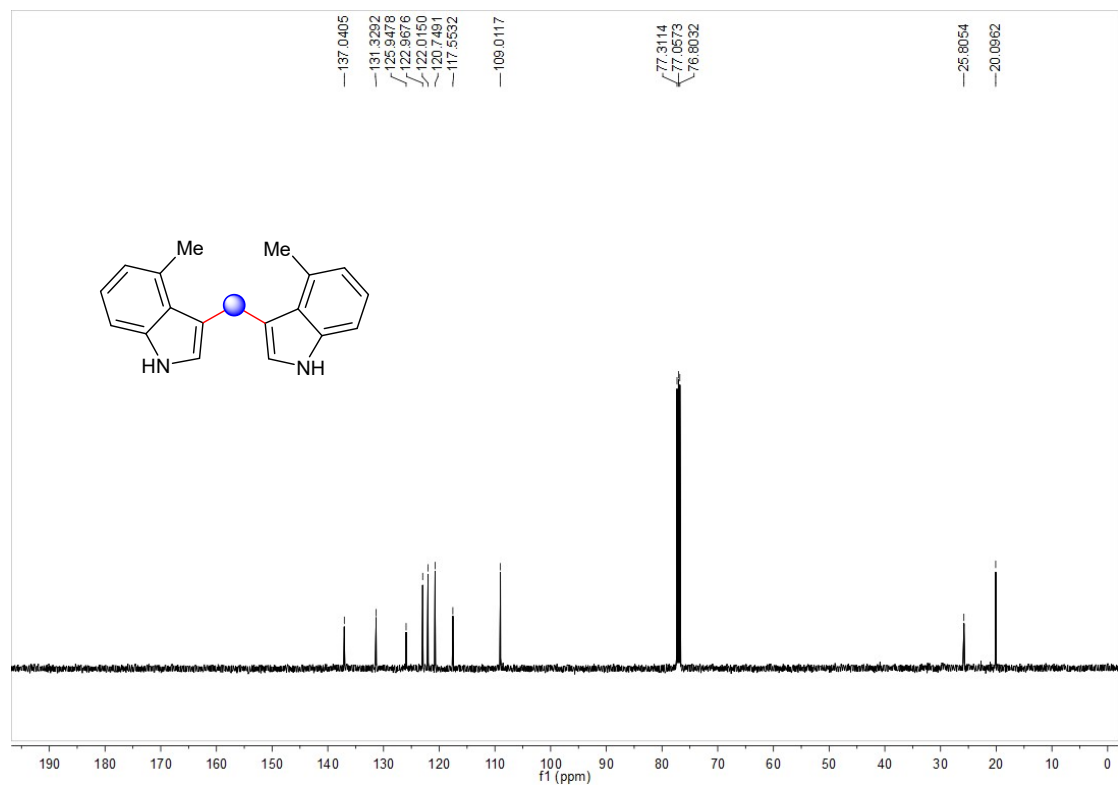
<sup>1</sup>H NMR<sup>13</sup>C NMR

3c

<sup>1</sup>H NMR



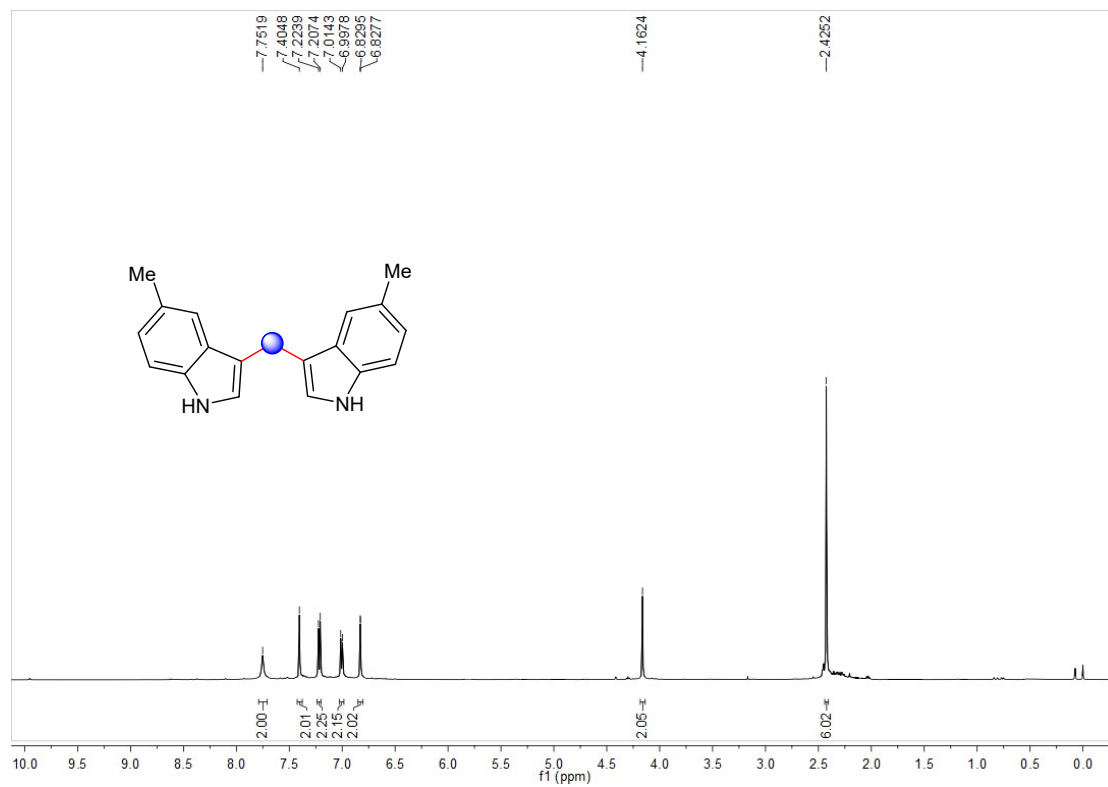
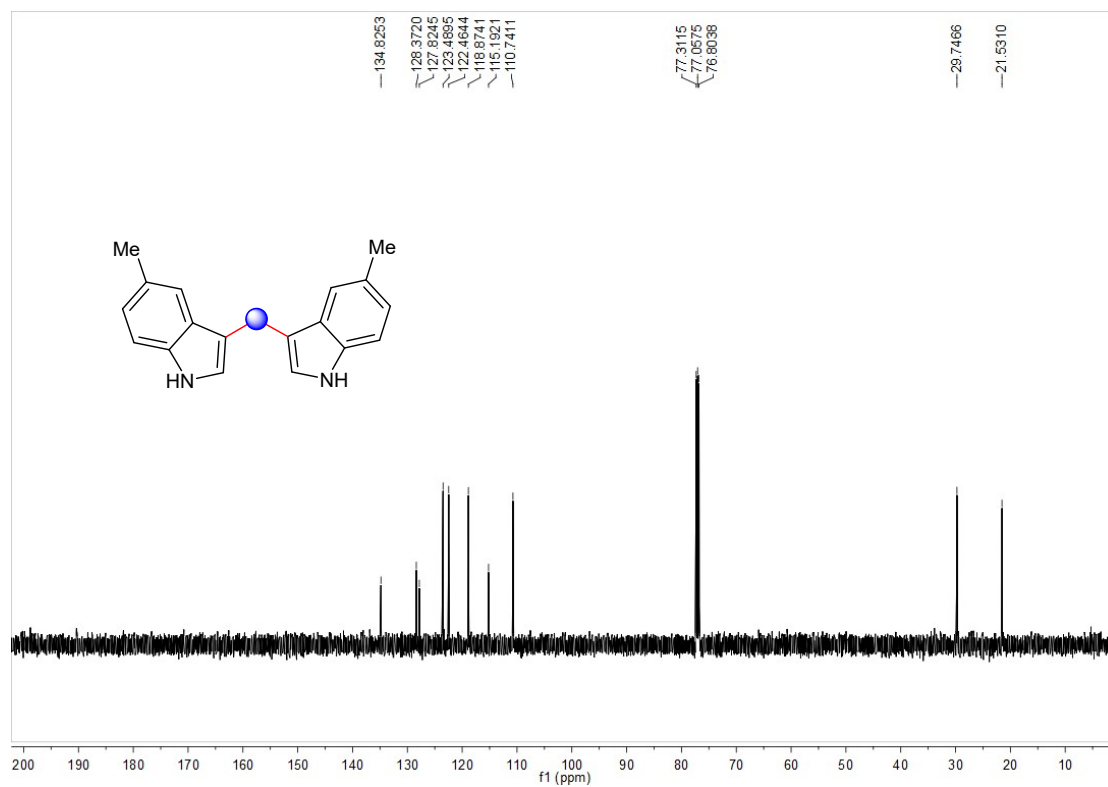
<sup>13</sup>C NMR



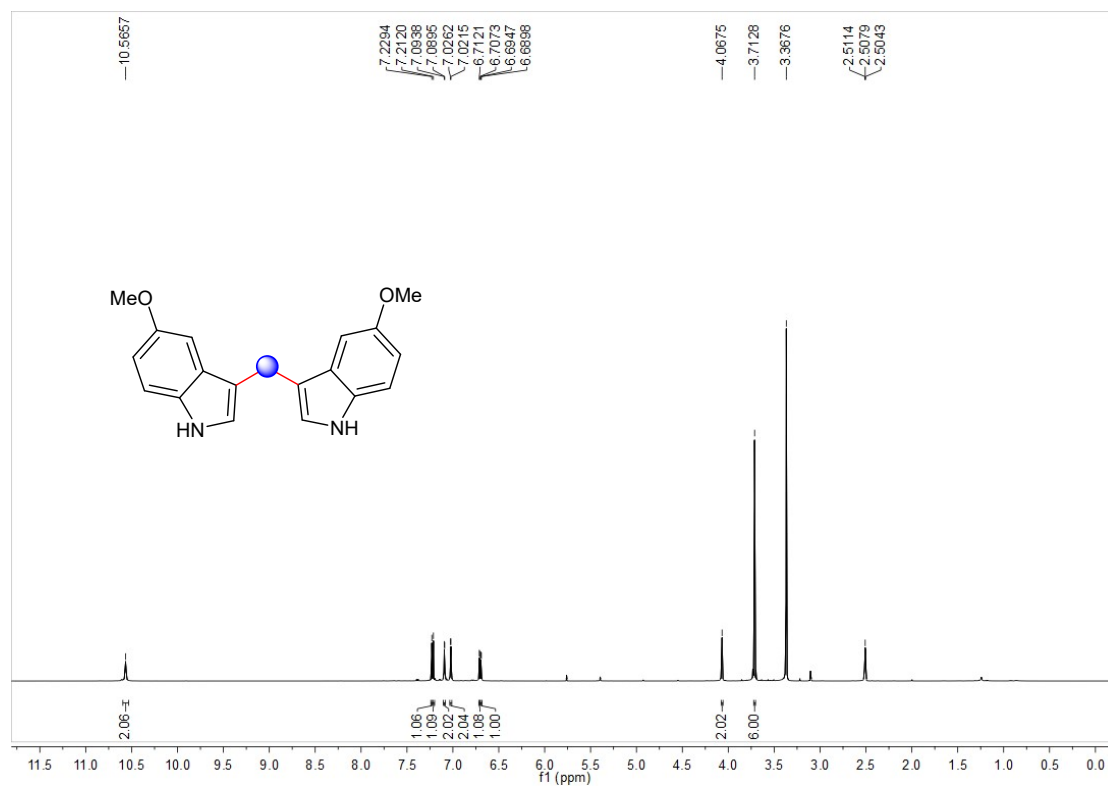
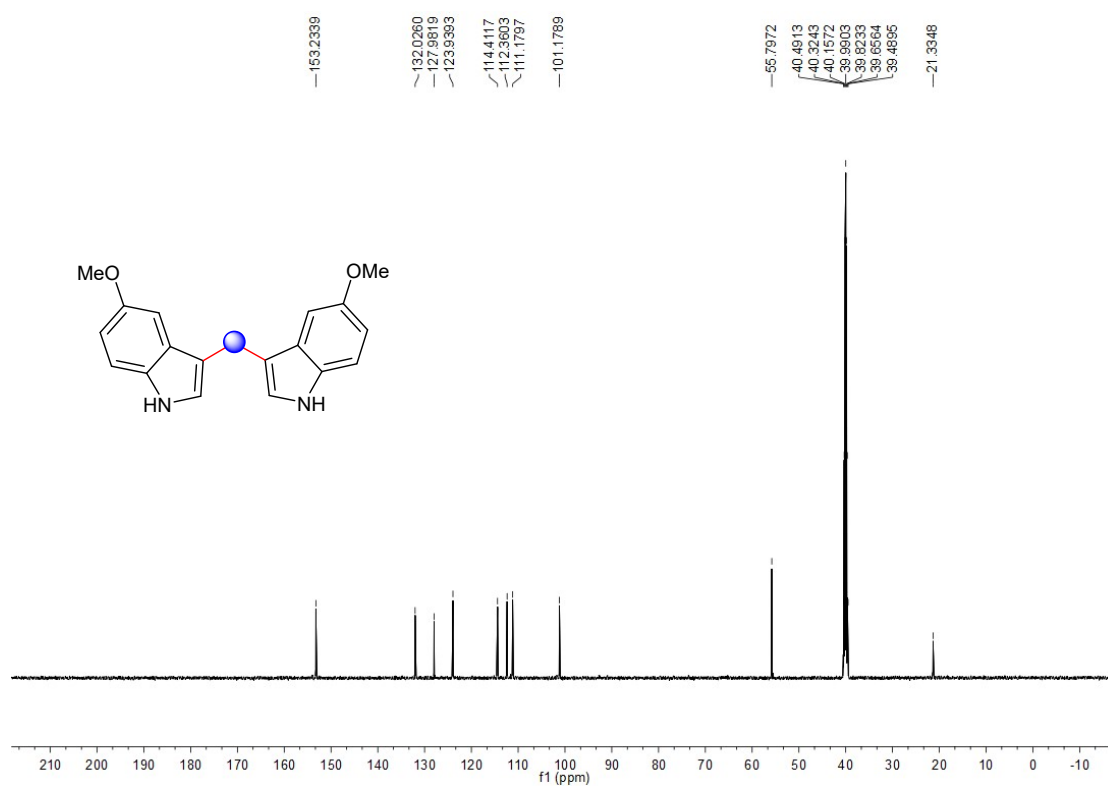




## 4c

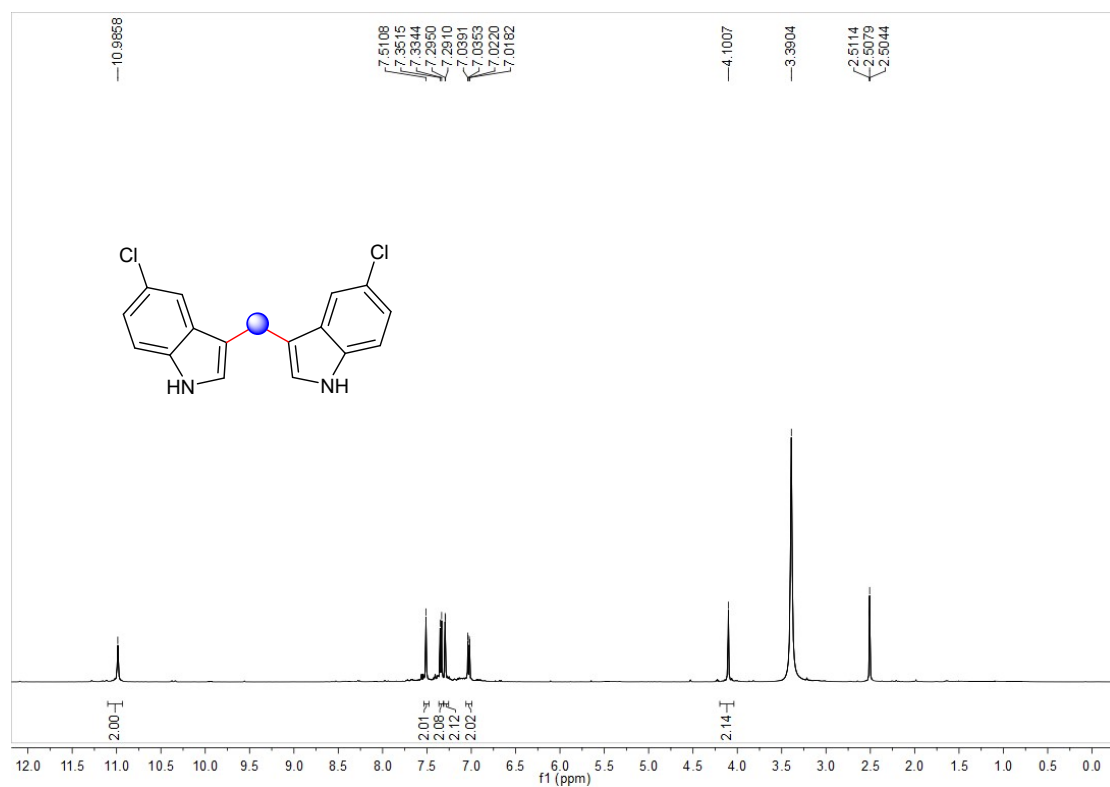
<sup>1</sup>H NMR<sup>13</sup>C NMR

## 5c

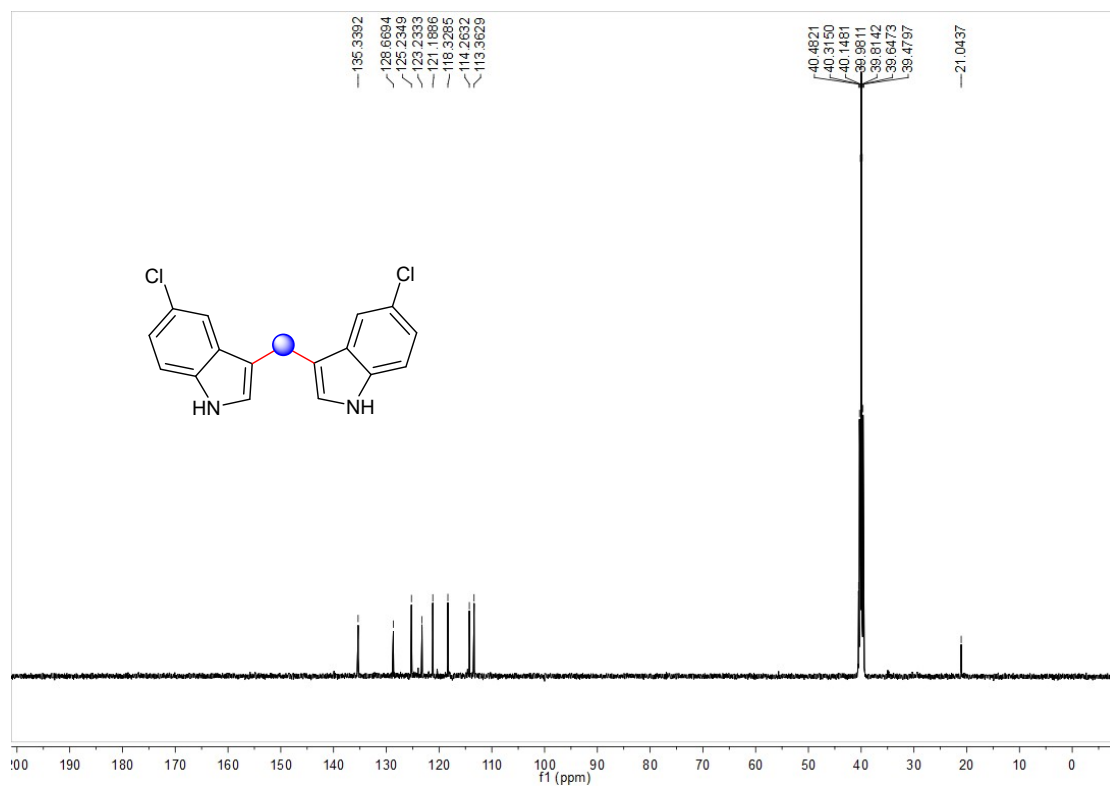
<sup>1</sup>H NMR<sup>13</sup>C NMR

6c

<sup>1</sup>H NMR

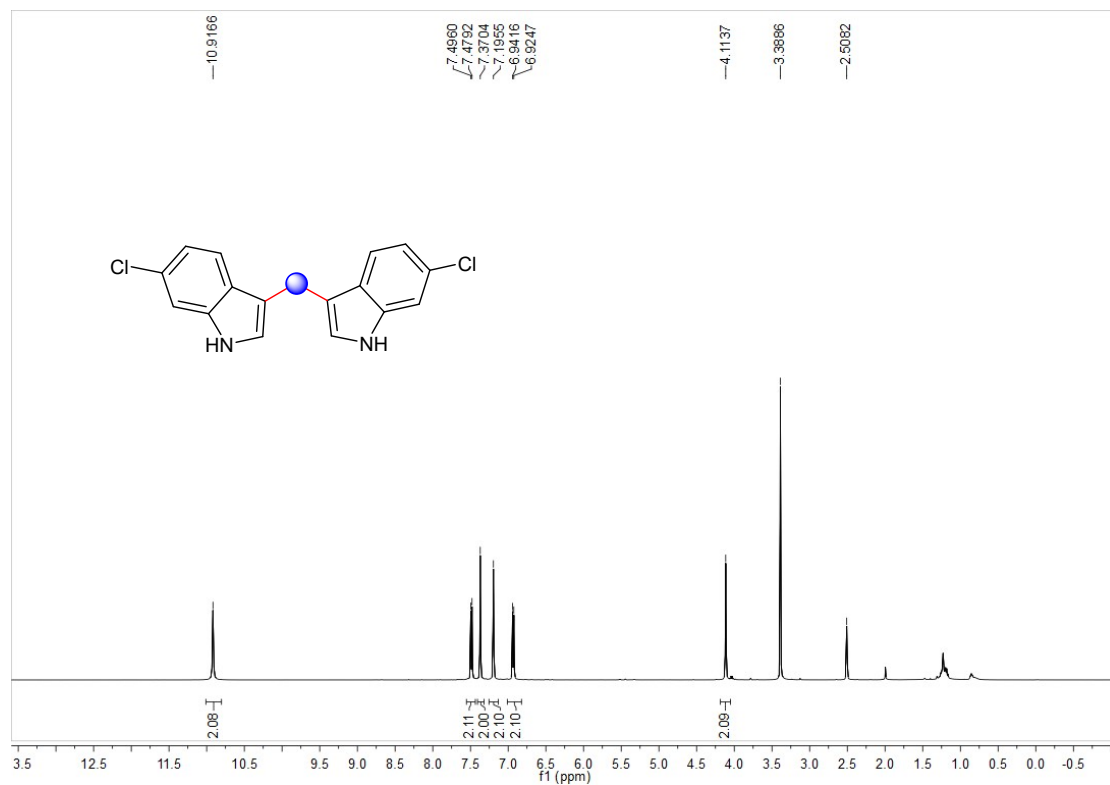


<sup>13</sup>C NMR

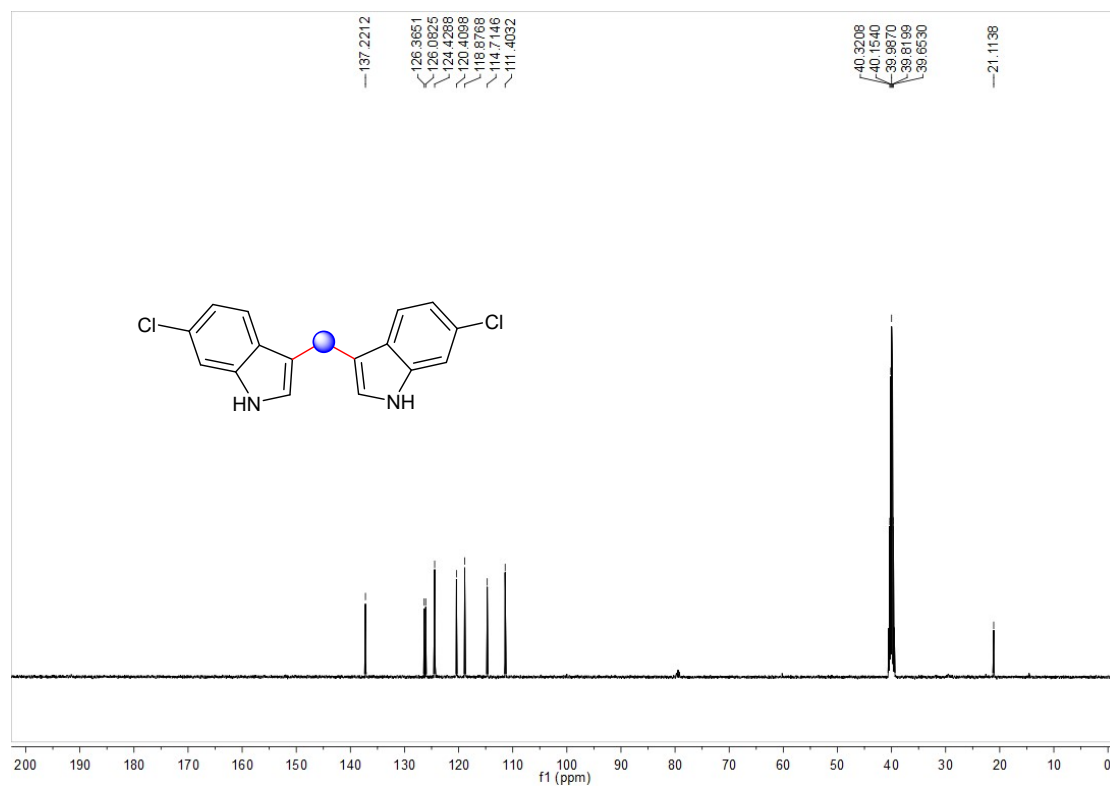


7c

<sup>1</sup>H NMR

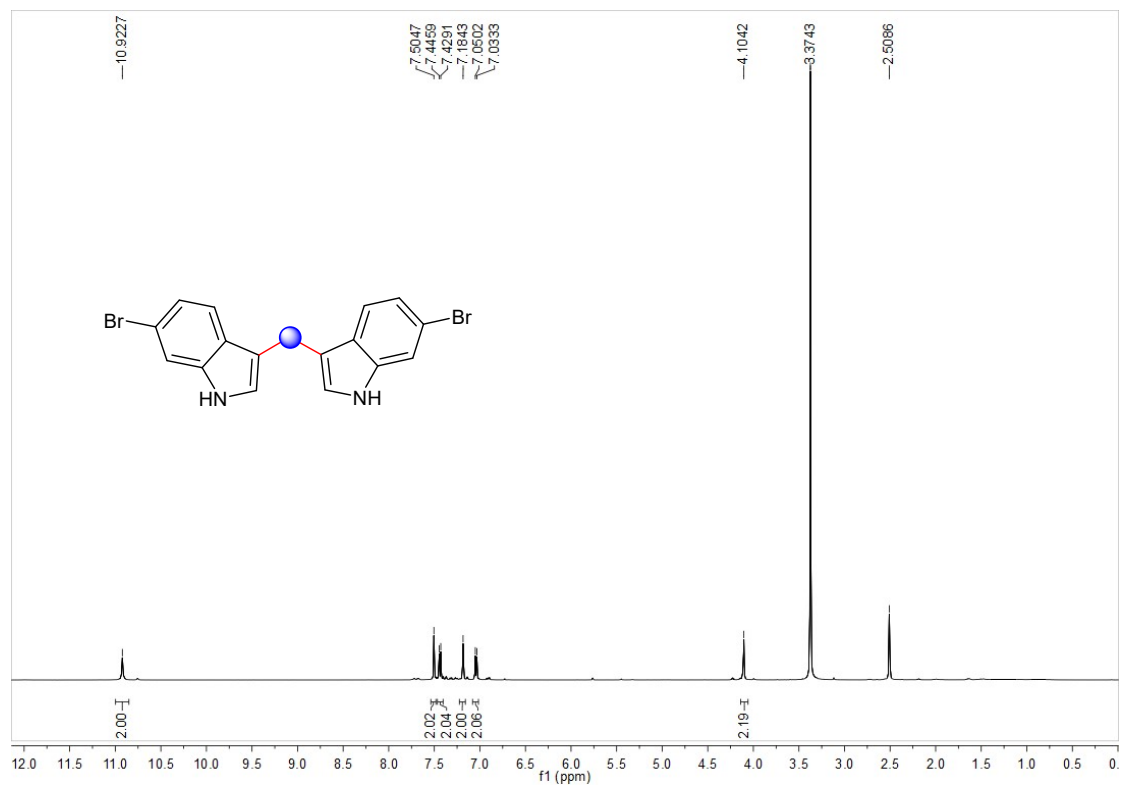


<sup>13</sup>C NMR

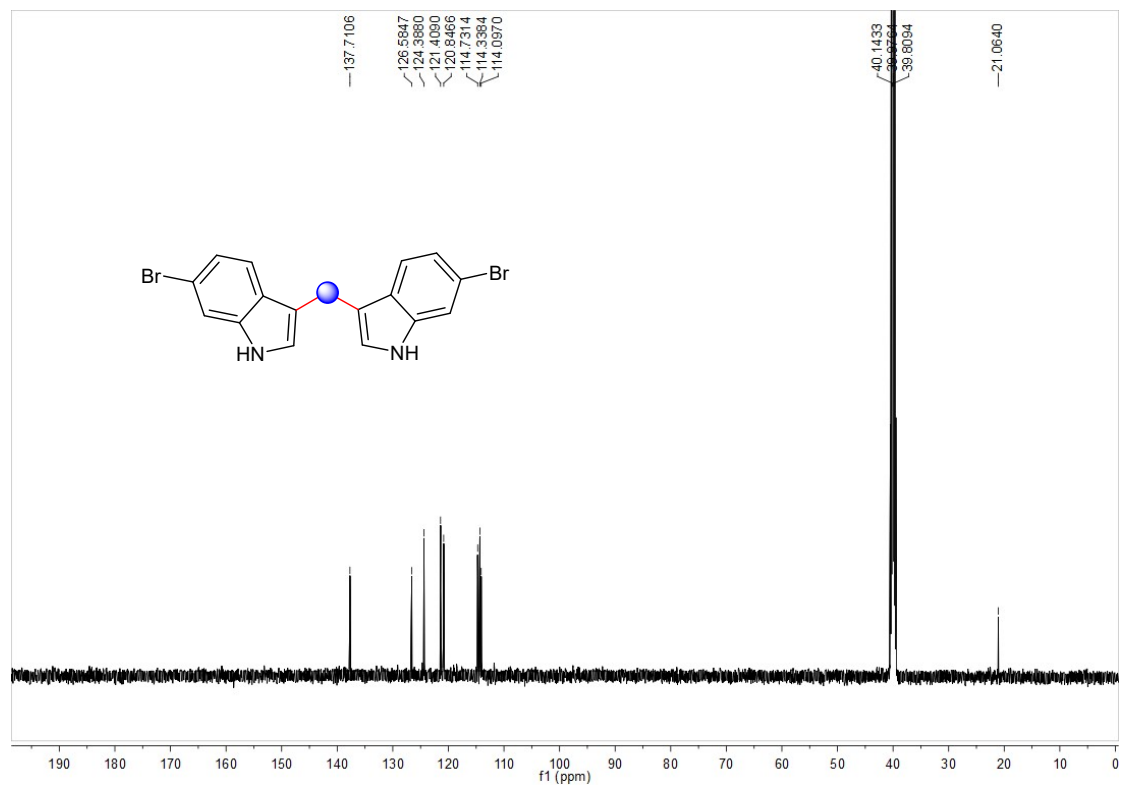


8c

<sup>1</sup>H NMR

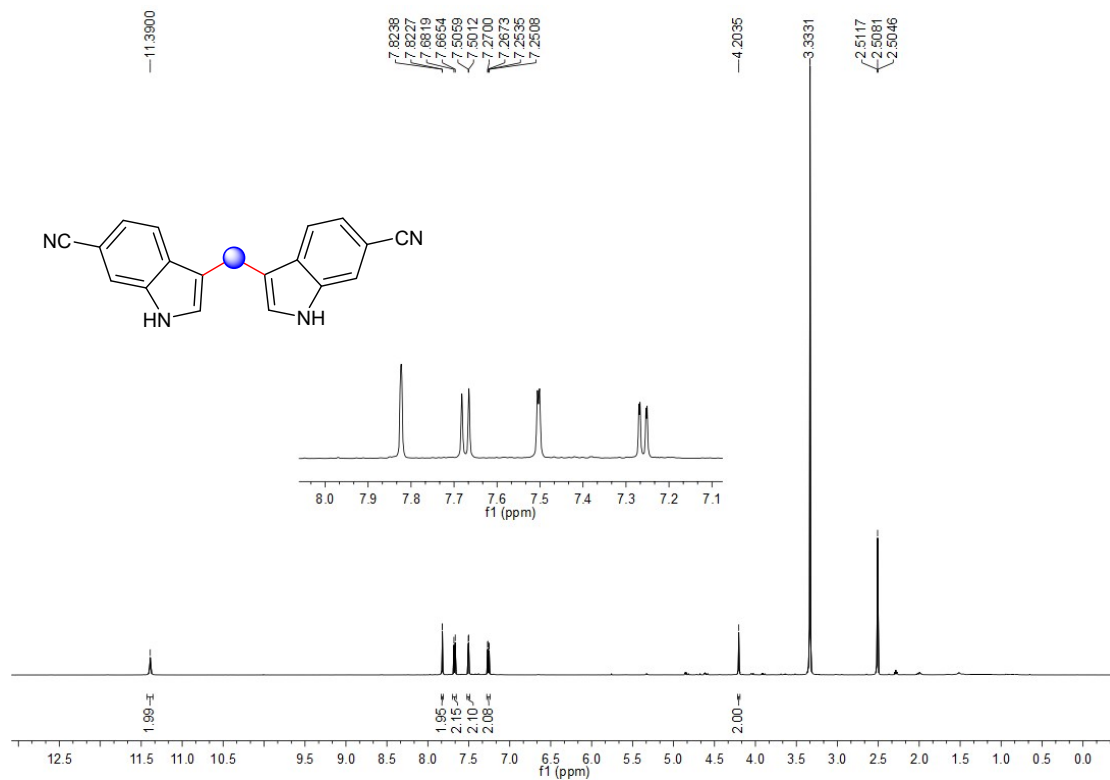


<sup>13</sup>C NMR

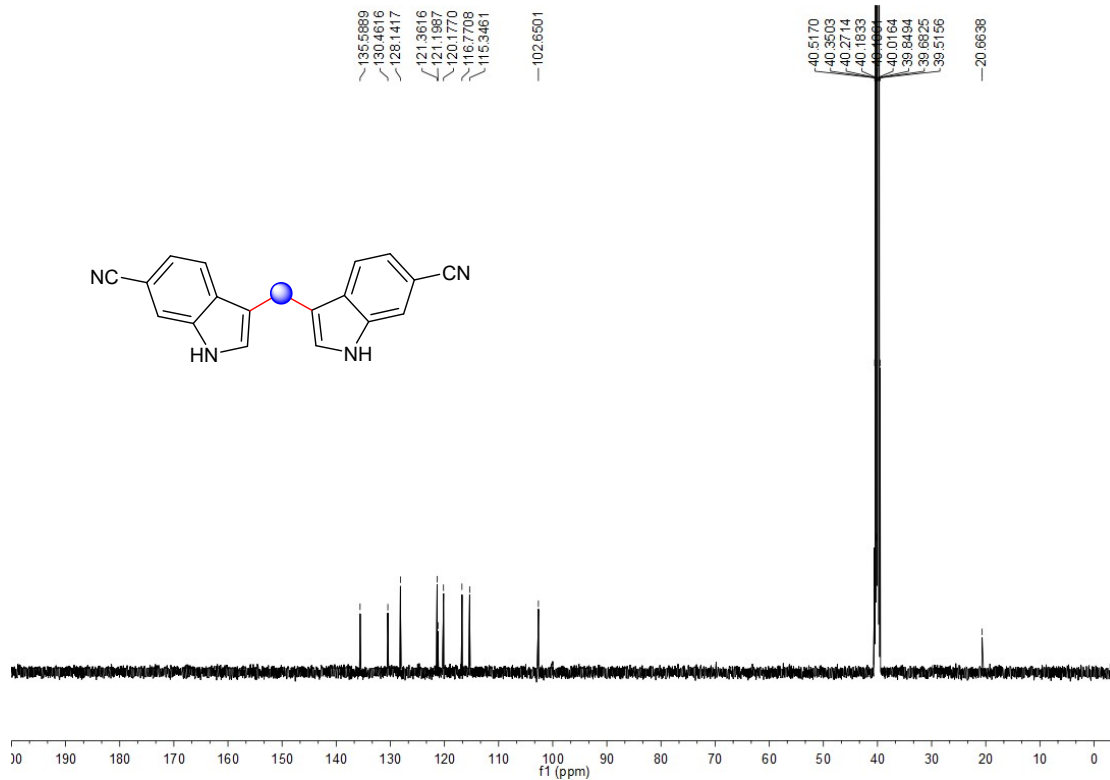


9c

<sup>1</sup>H NMR



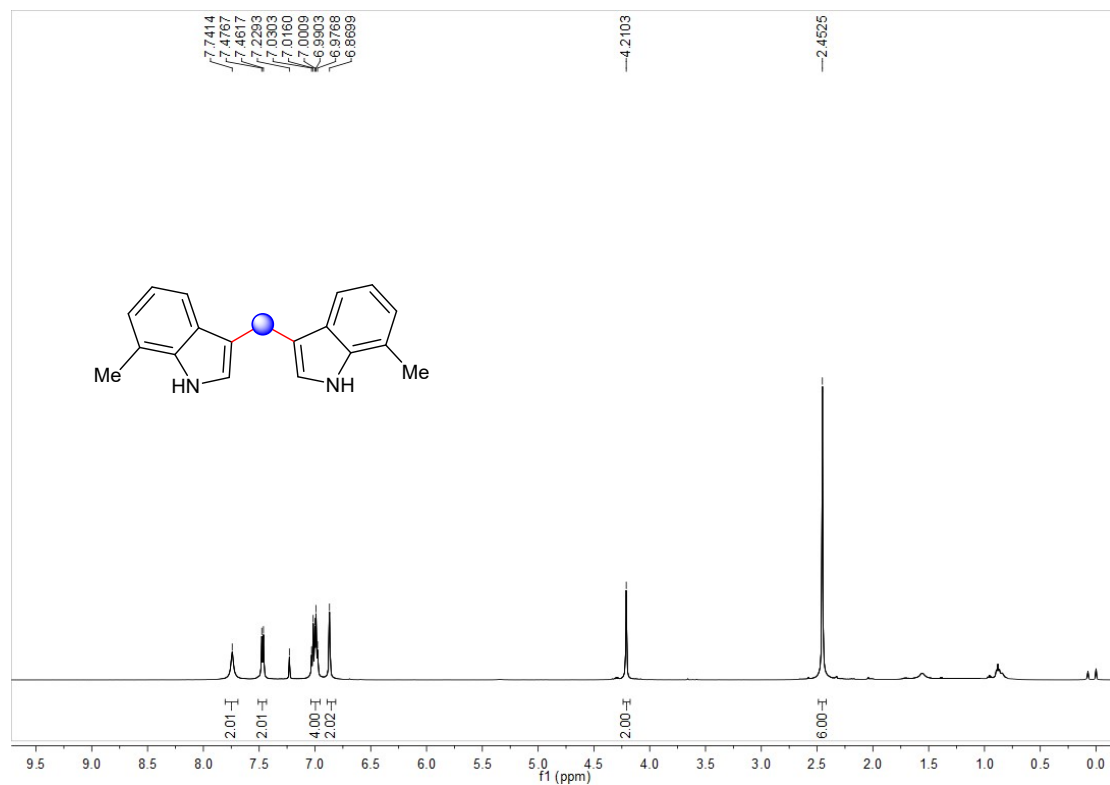
<sup>13</sup>C NMR



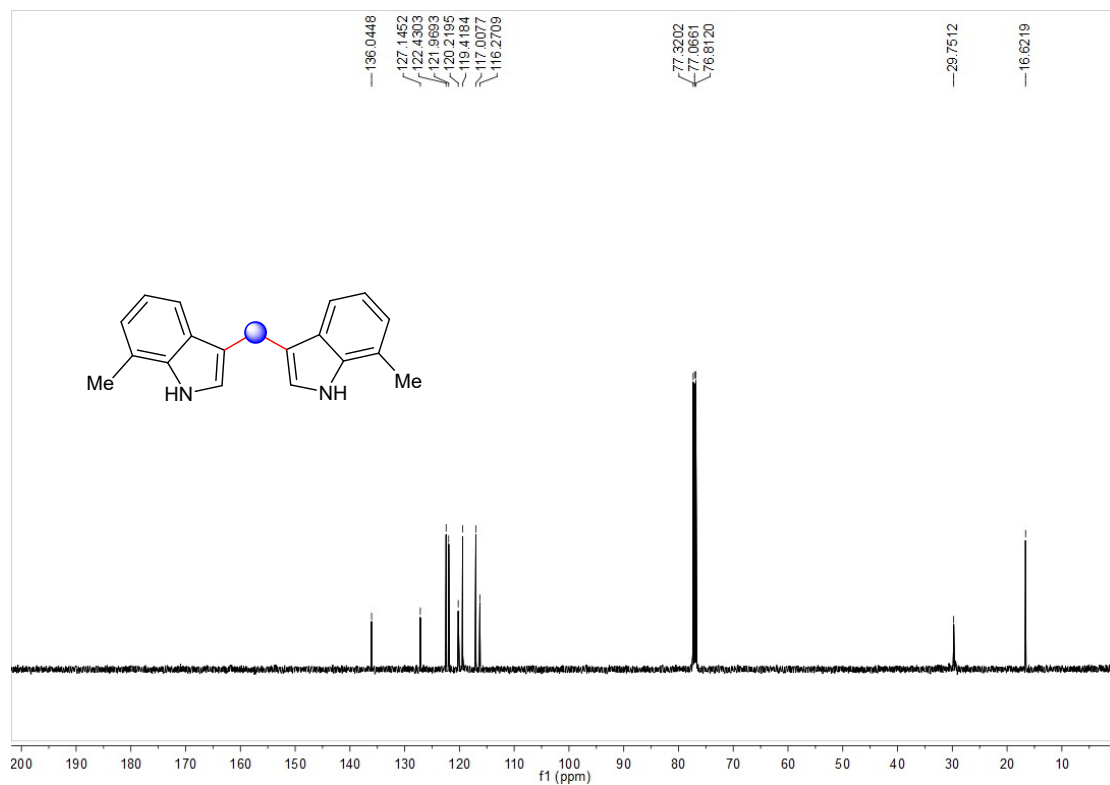


10c

<sup>1</sup>H NMR



<sup>13</sup>C NMR

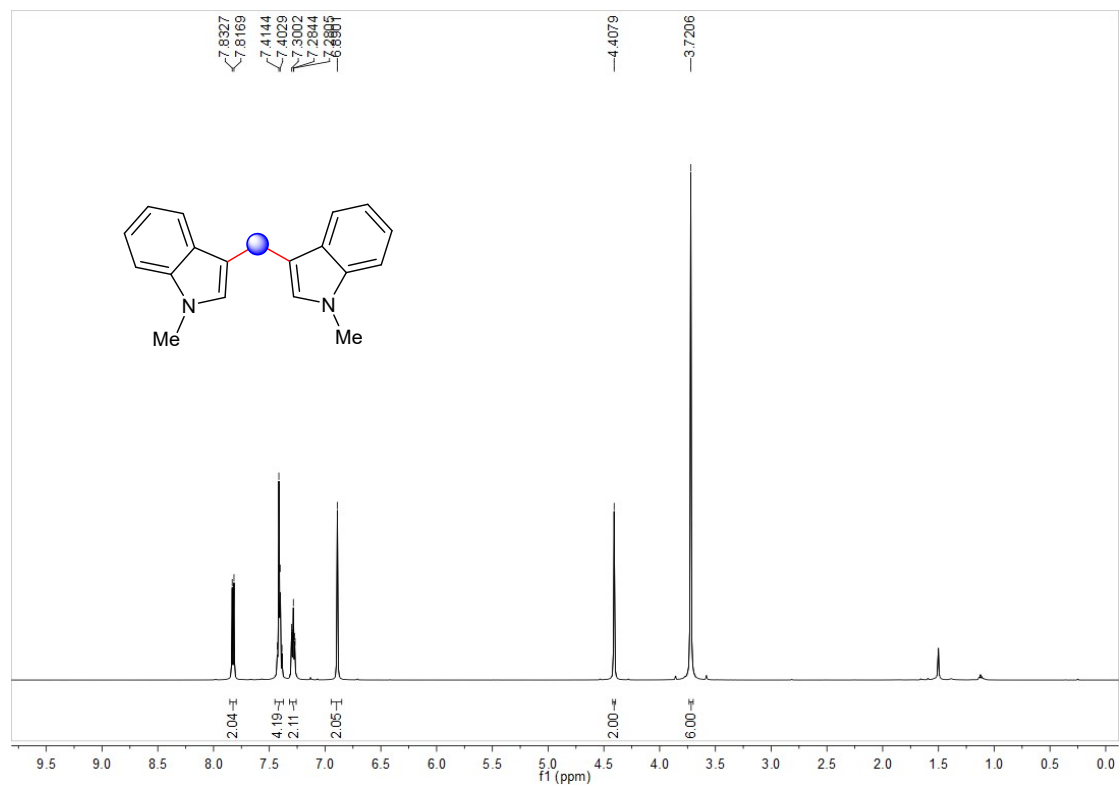




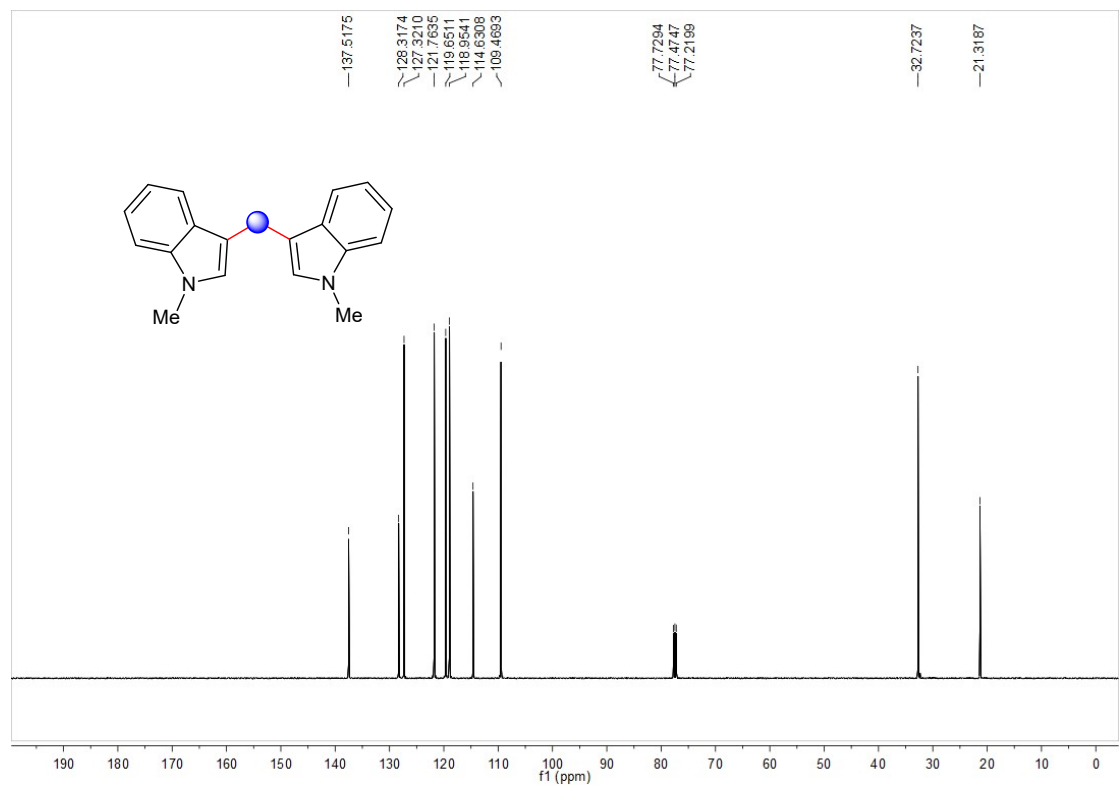


# 11c

## <sup>1</sup>H NMR

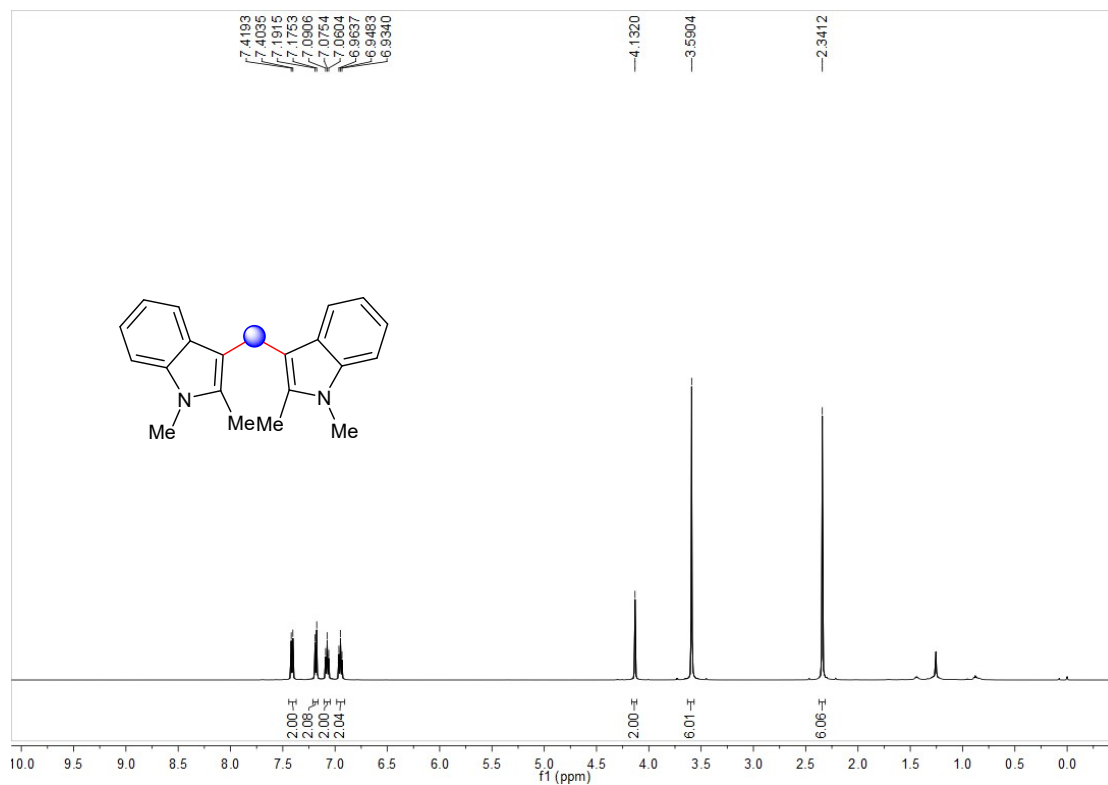


## <sup>13</sup>C NMR

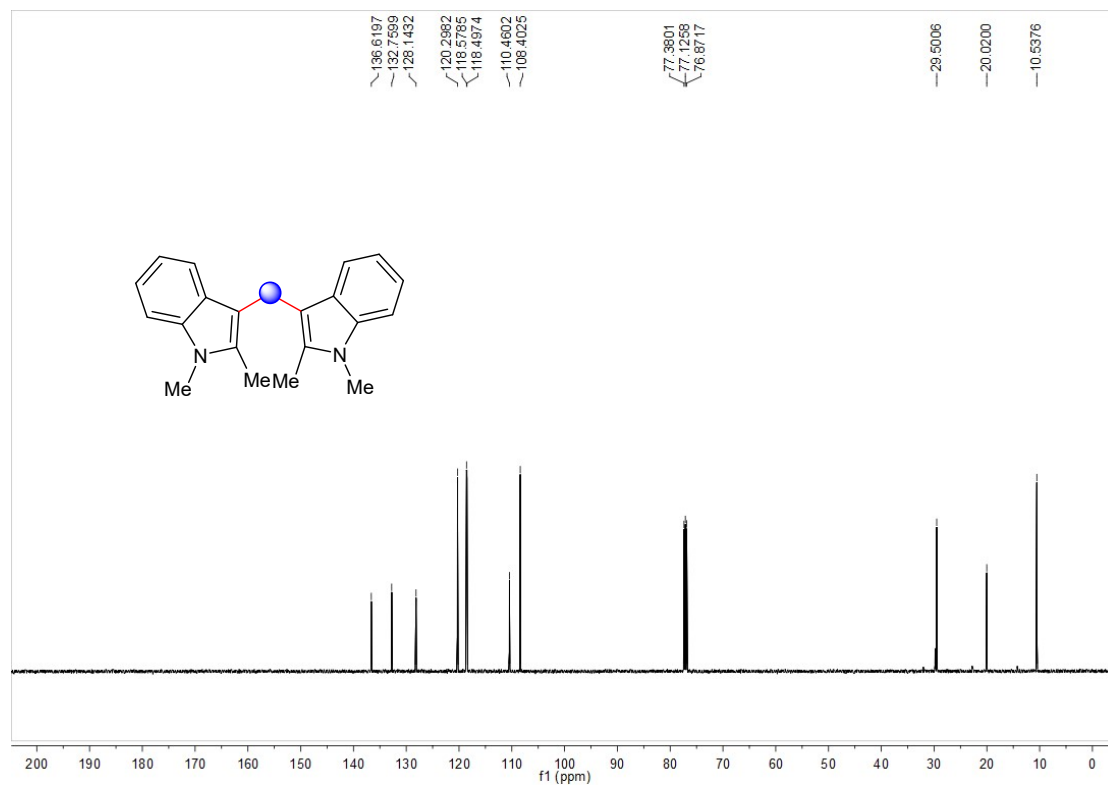


# 12c

## <sup>1</sup>H NMR



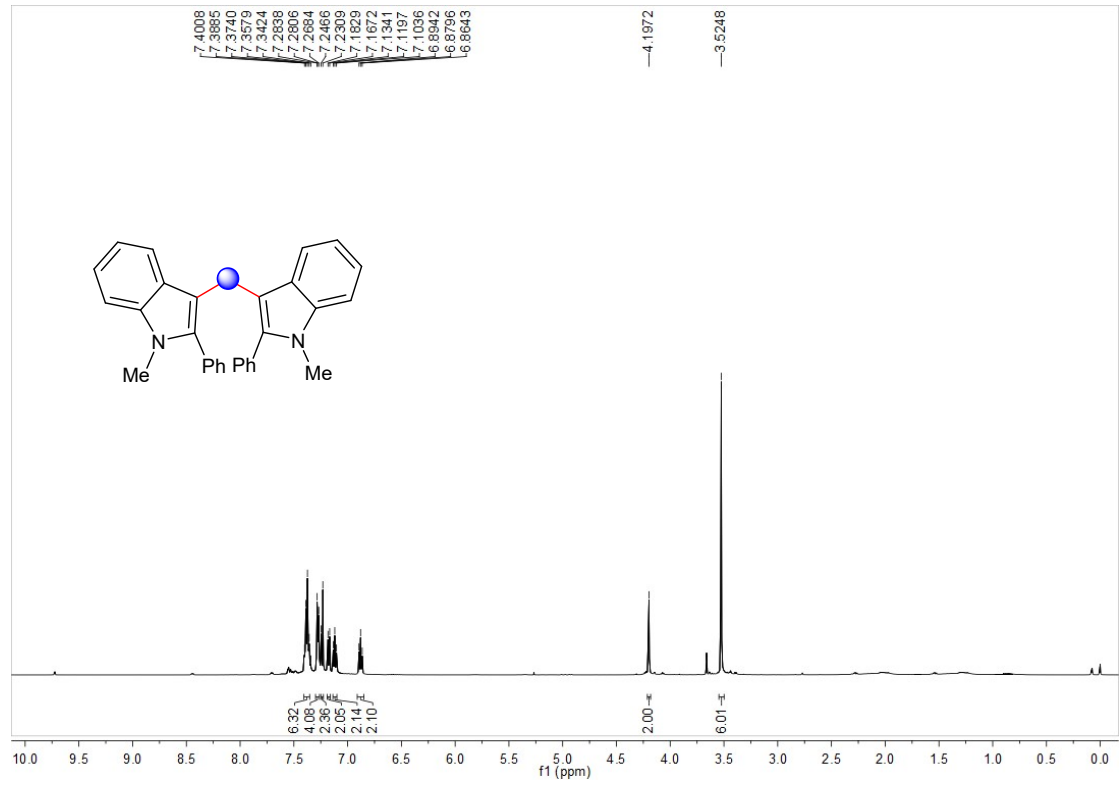
## <sup>13</sup>C NMR



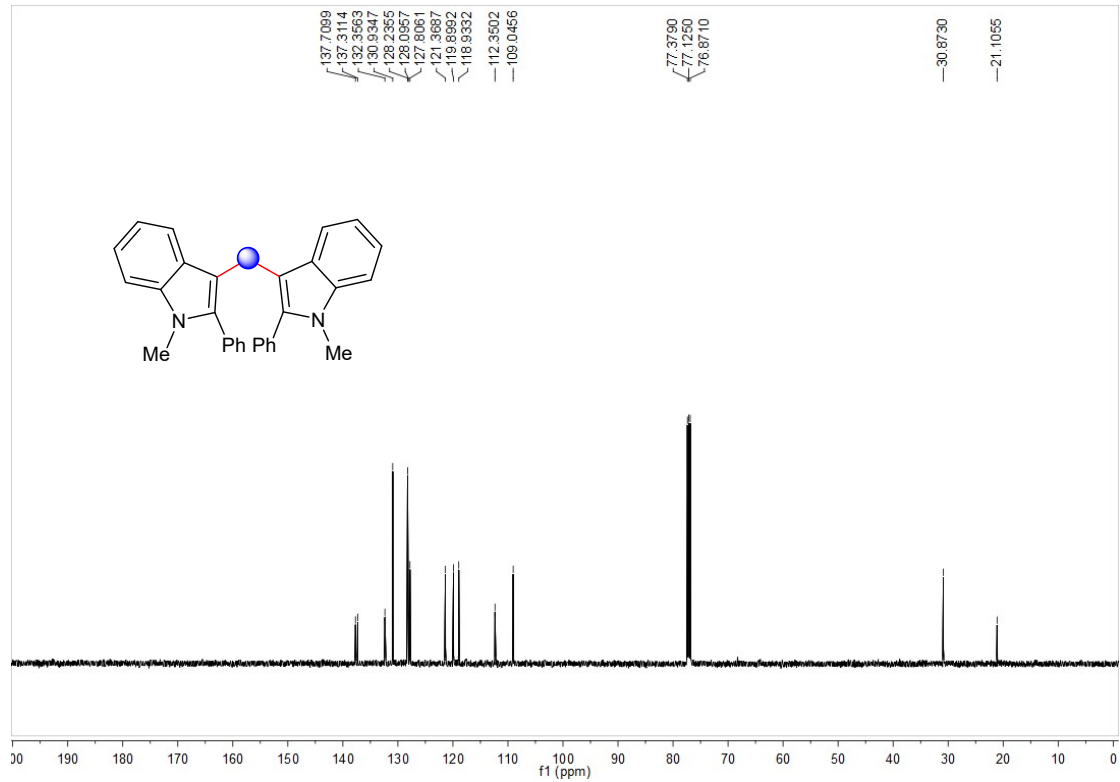


# 13c

## <sup>1</sup>H NMR



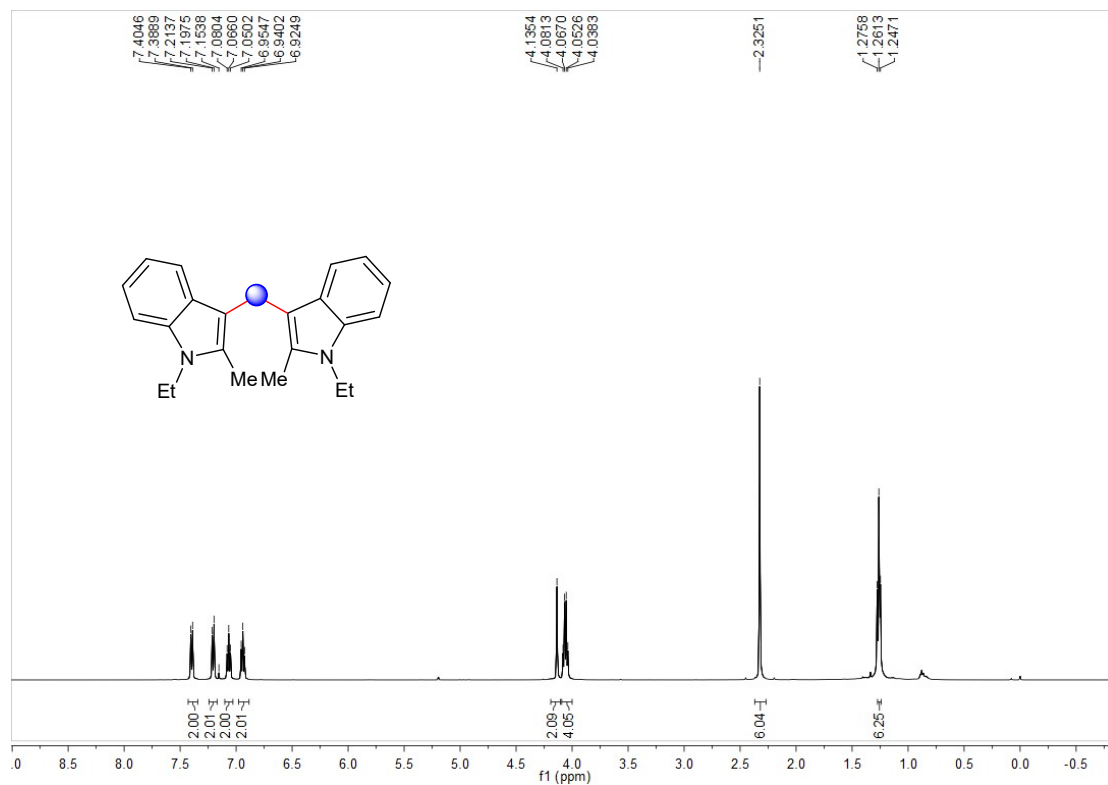
## <sup>13</sup>C NMR



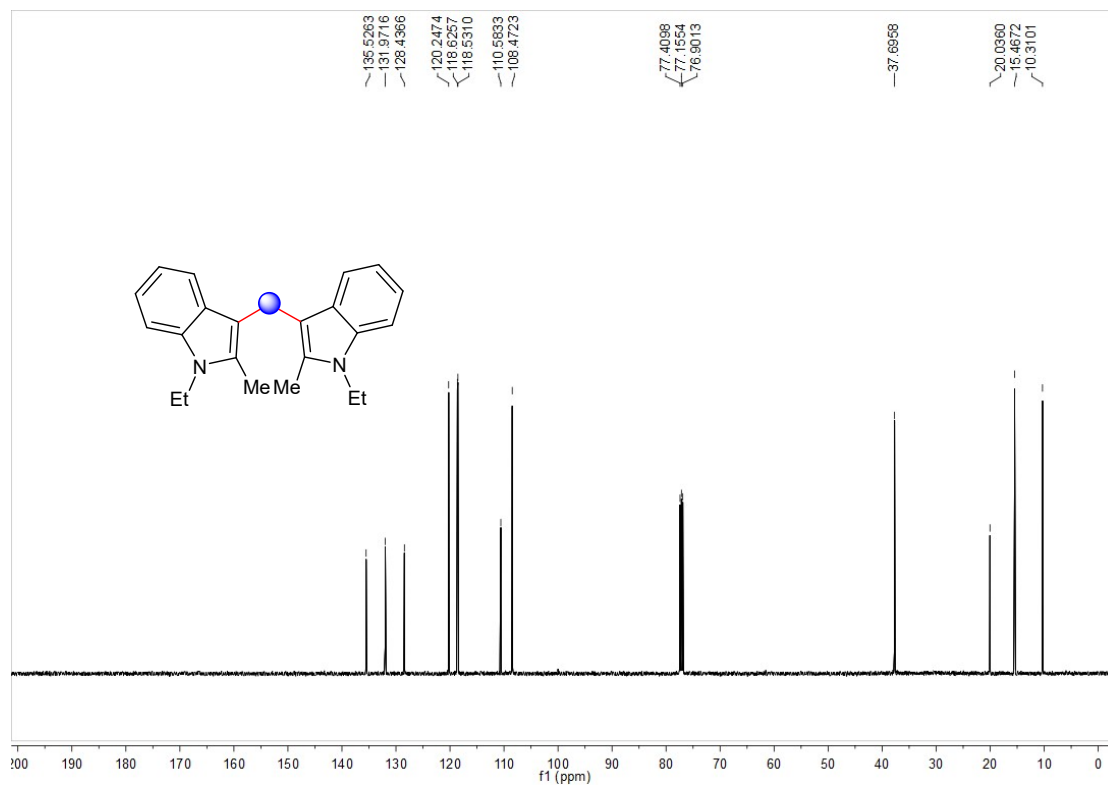


# 14c

## <sup>1</sup>H NMR



## <sup>13</sup>C NMR

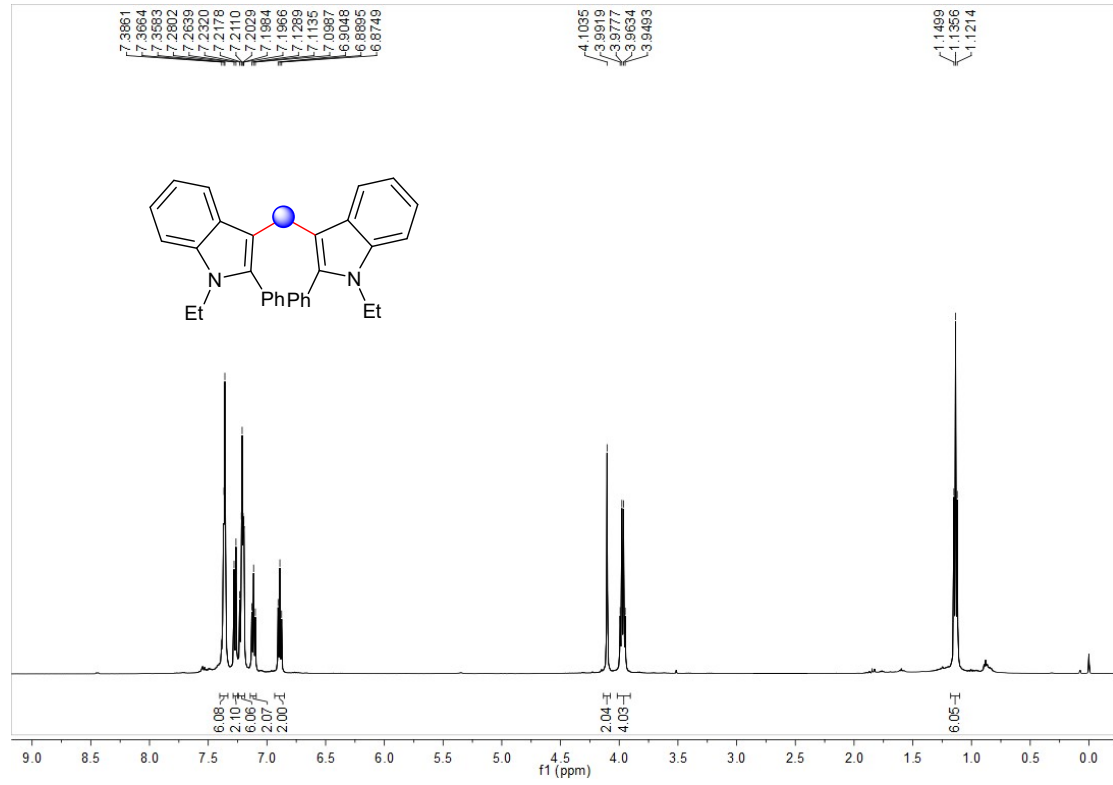




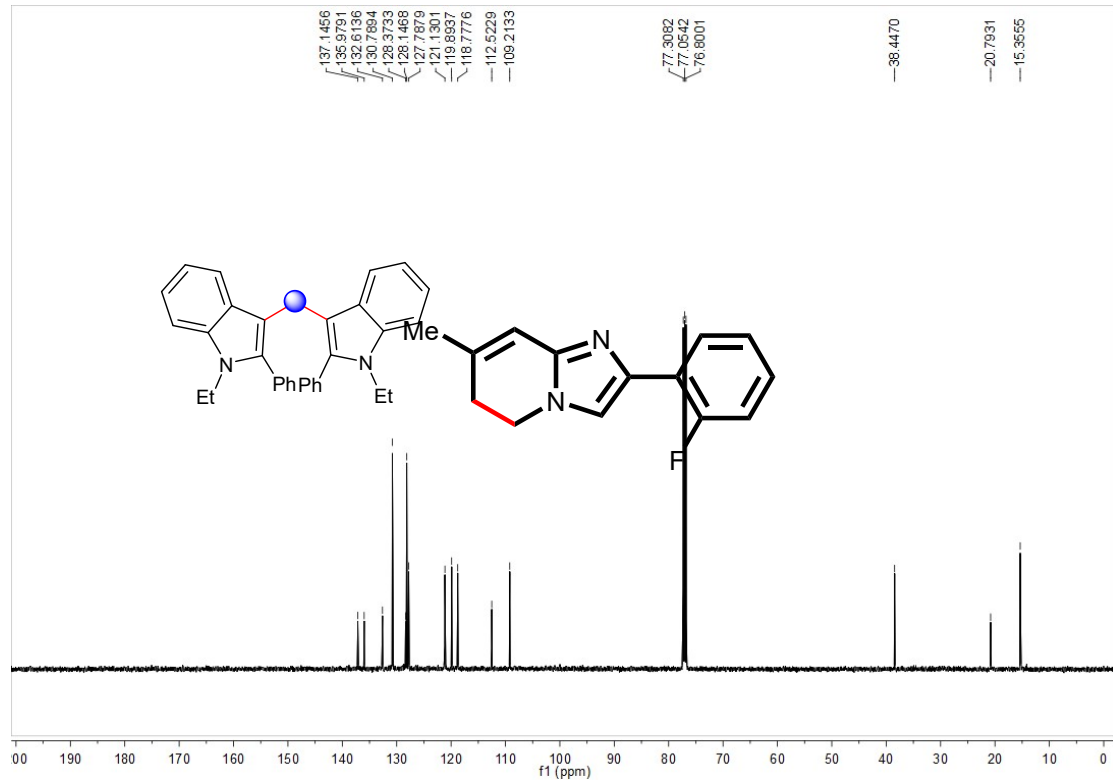


15c

<sup>1</sup>H NMR

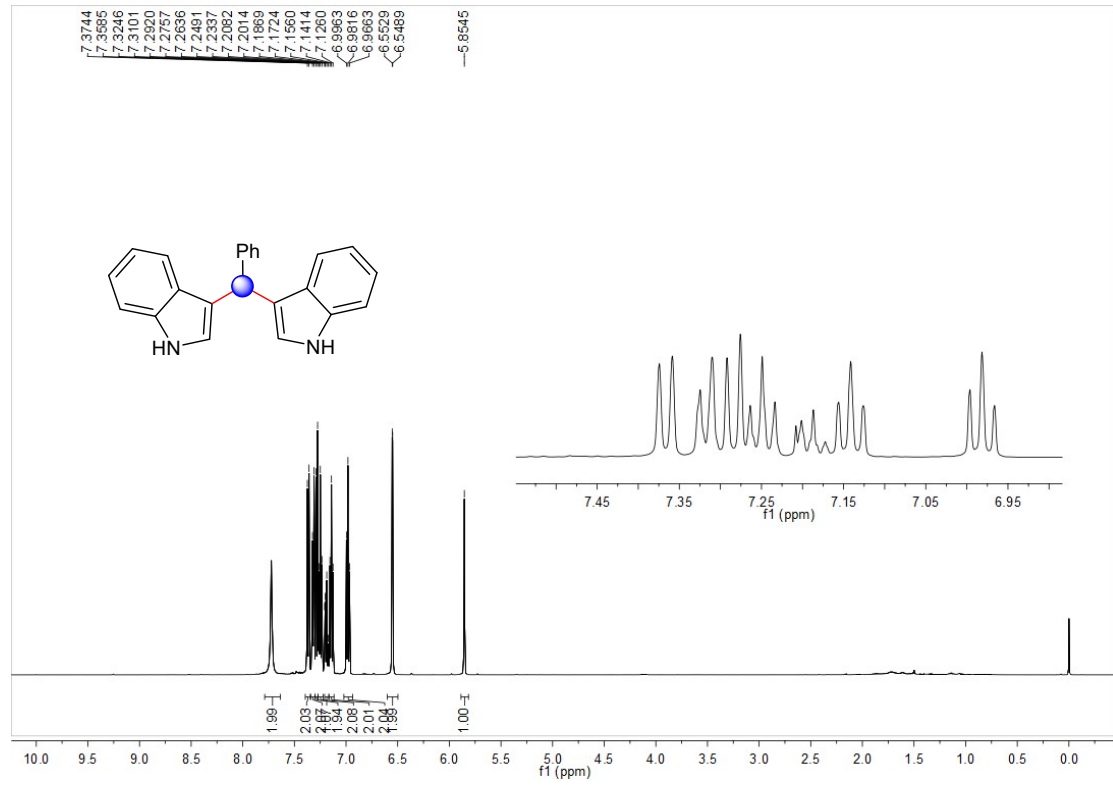


<sup>13</sup>C NMR

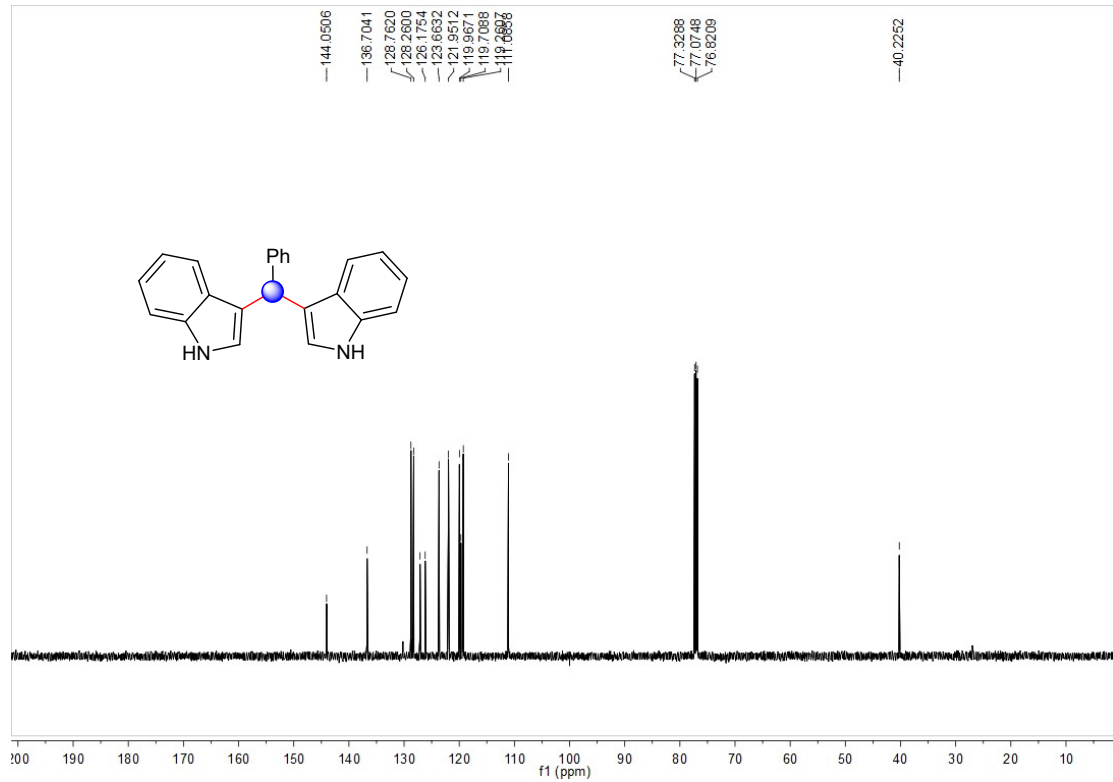


16c

<sup>1</sup>H NMR

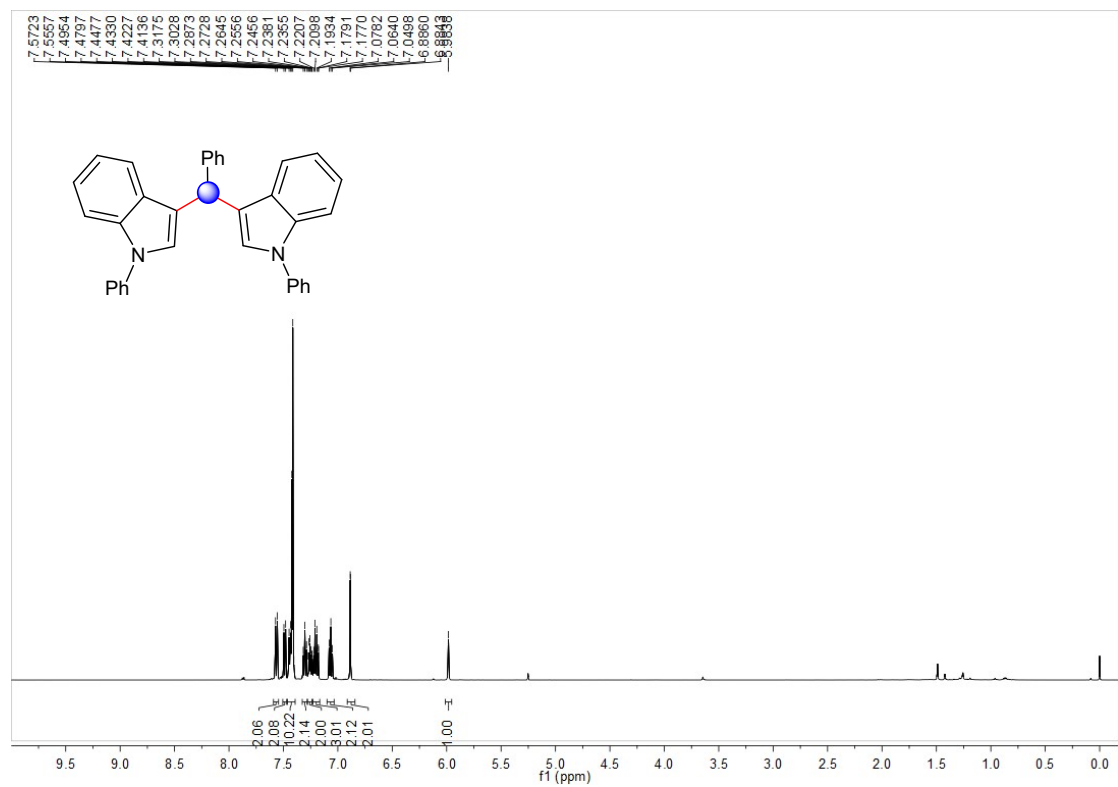
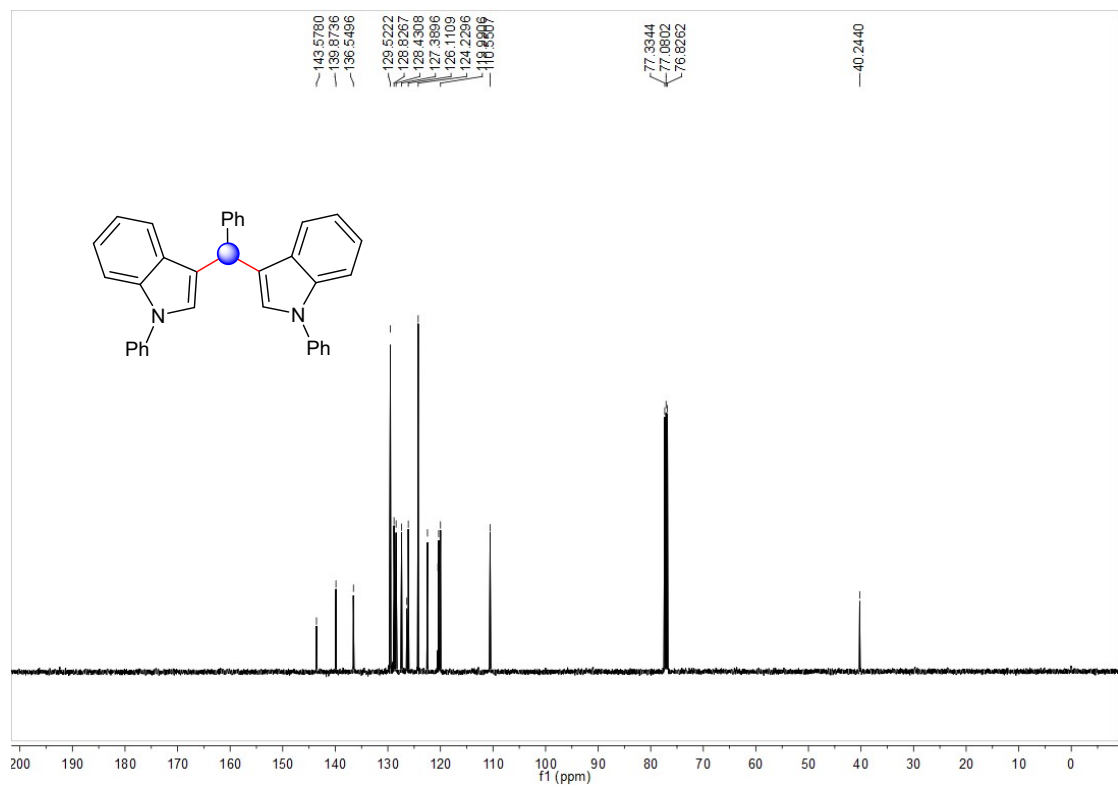


<sup>13</sup>C NMR





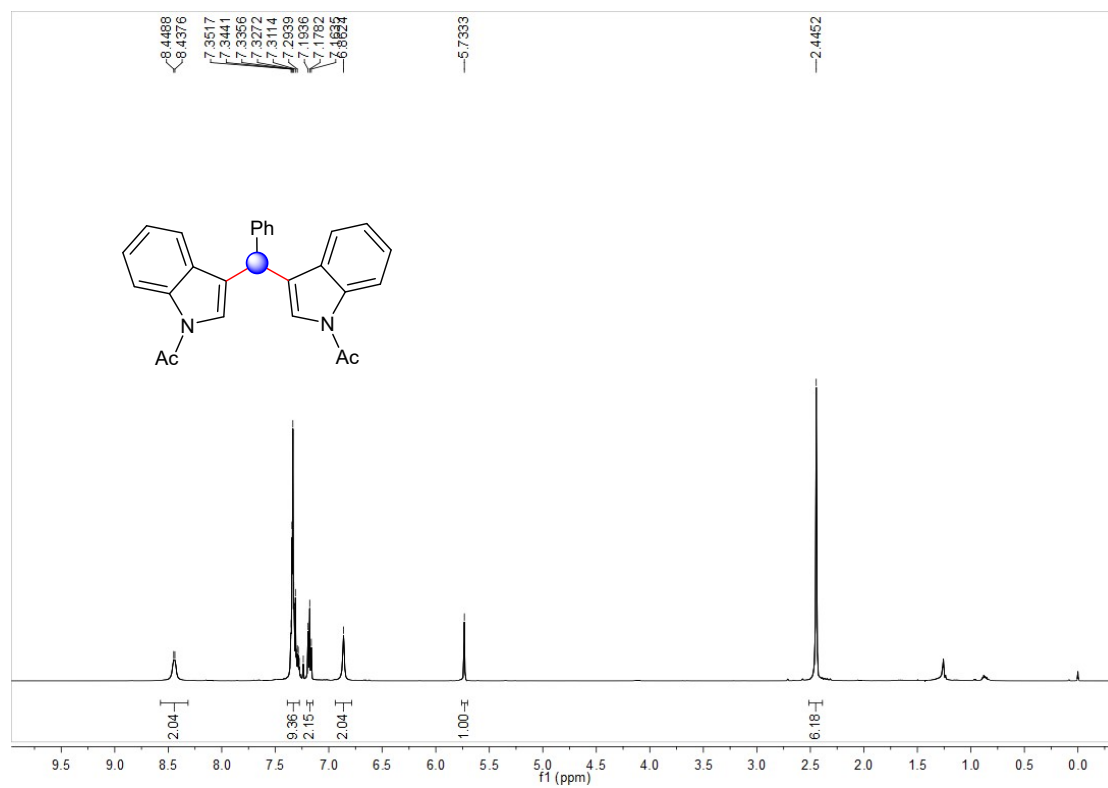
## 17c

<sup>1</sup>H NMR<sup>13</sup>C NMR

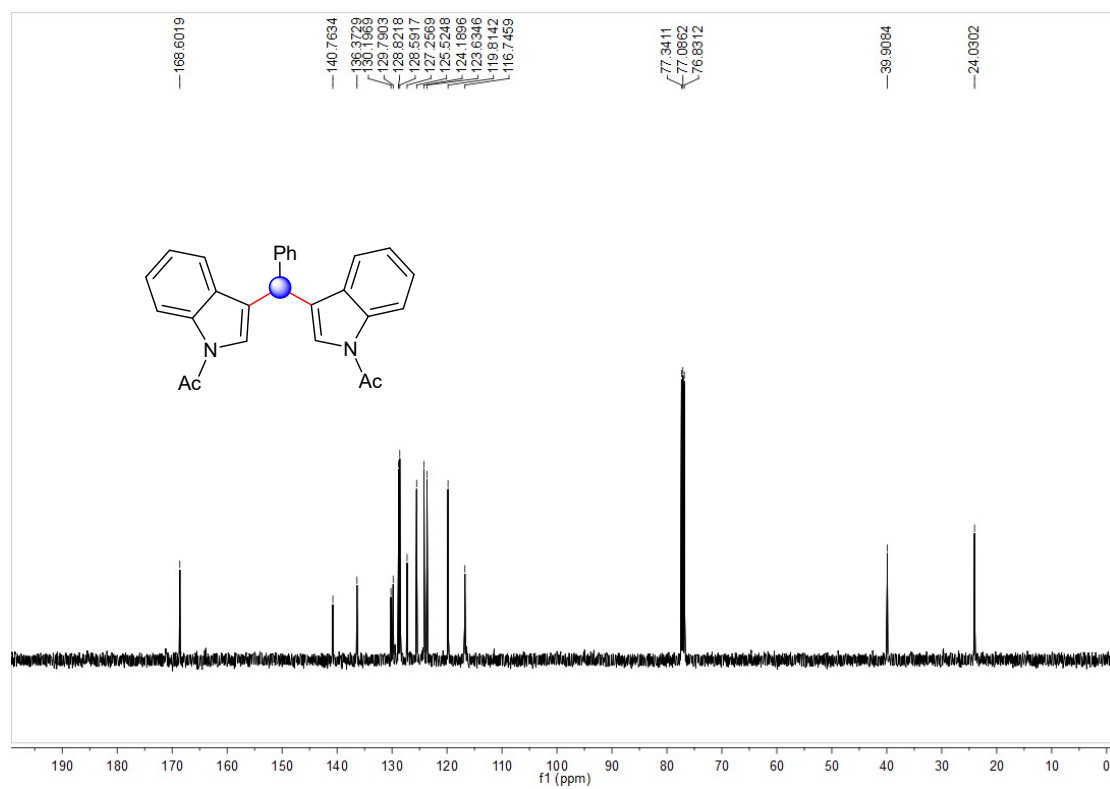


18c

<sup>1</sup>H NMR

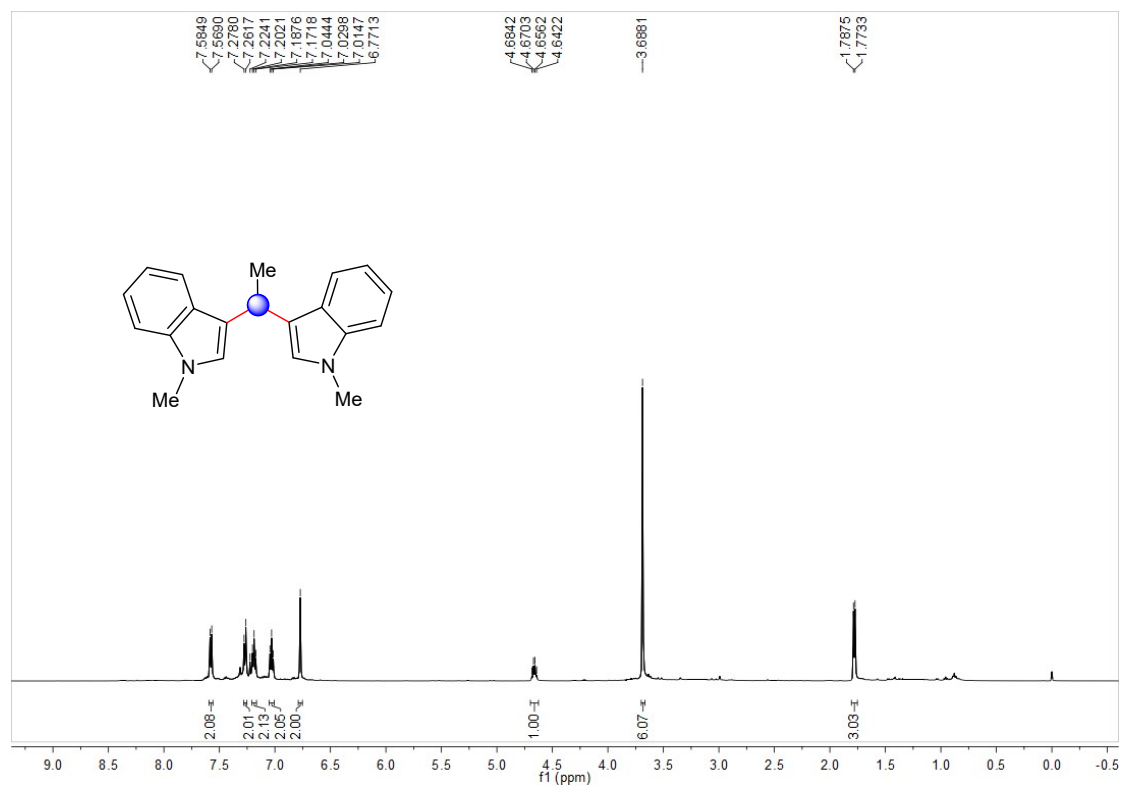


<sup>13</sup>C NMR

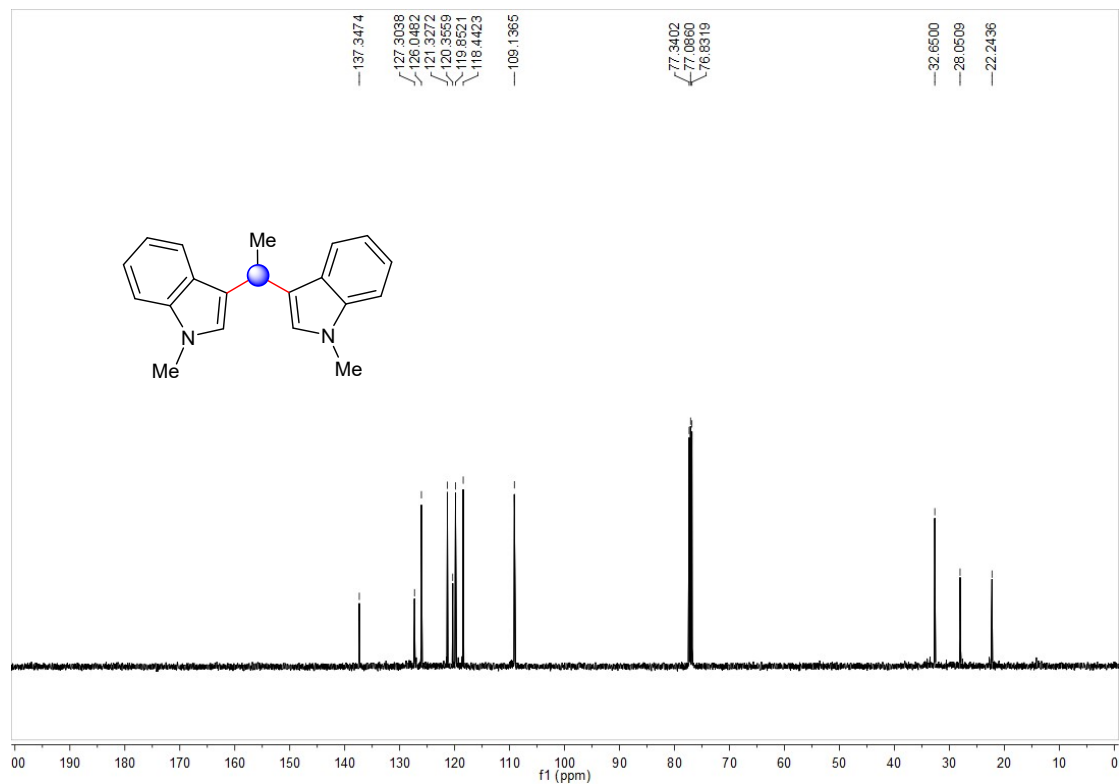


# 21c

## <sup>1</sup>H NMR



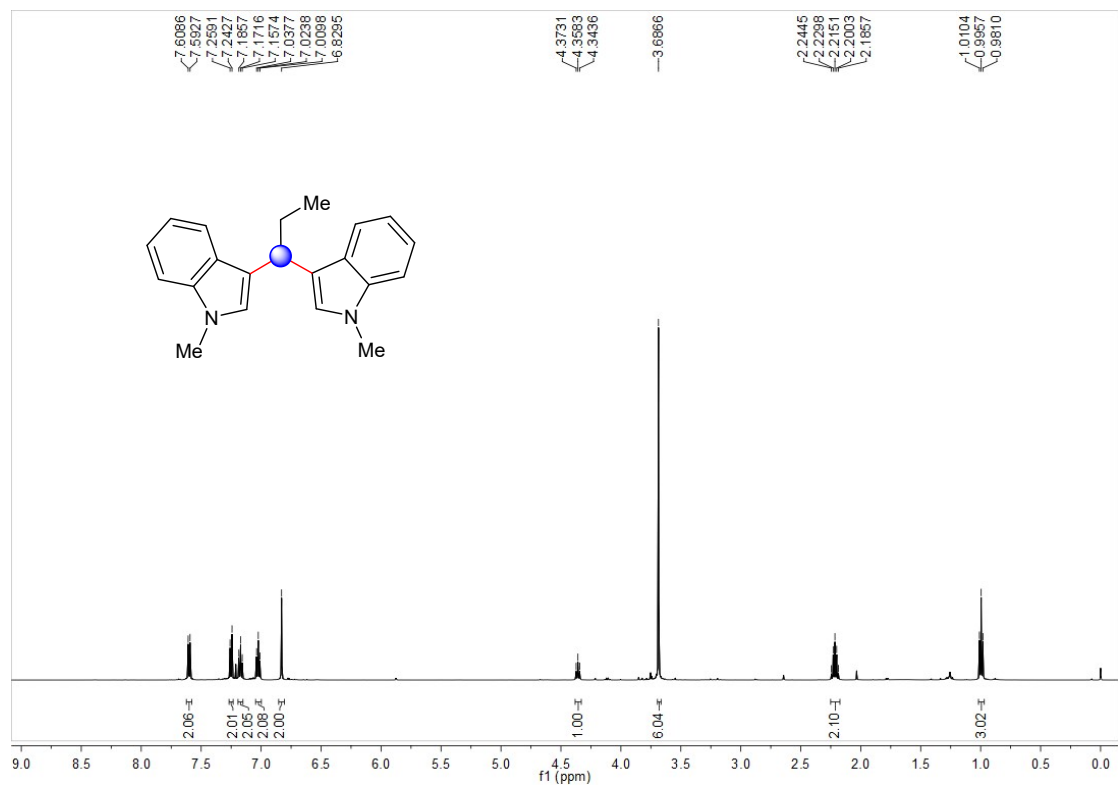
## <sup>13</sup>C NMR



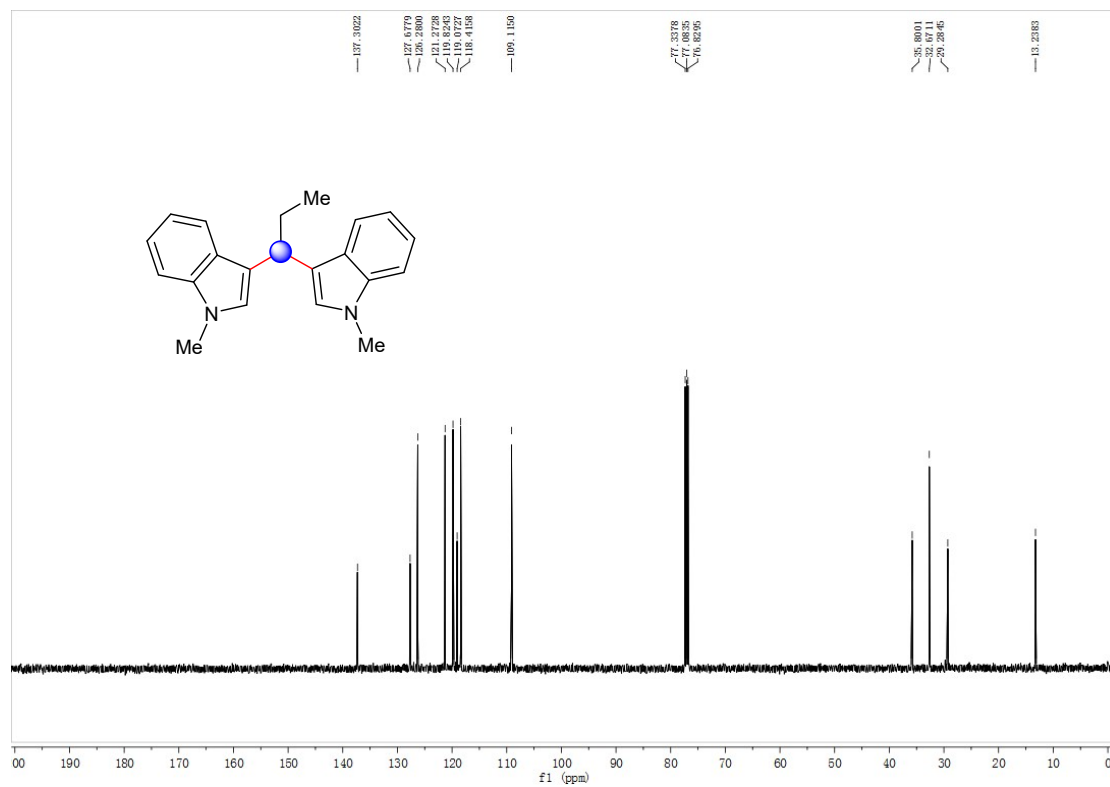


22c

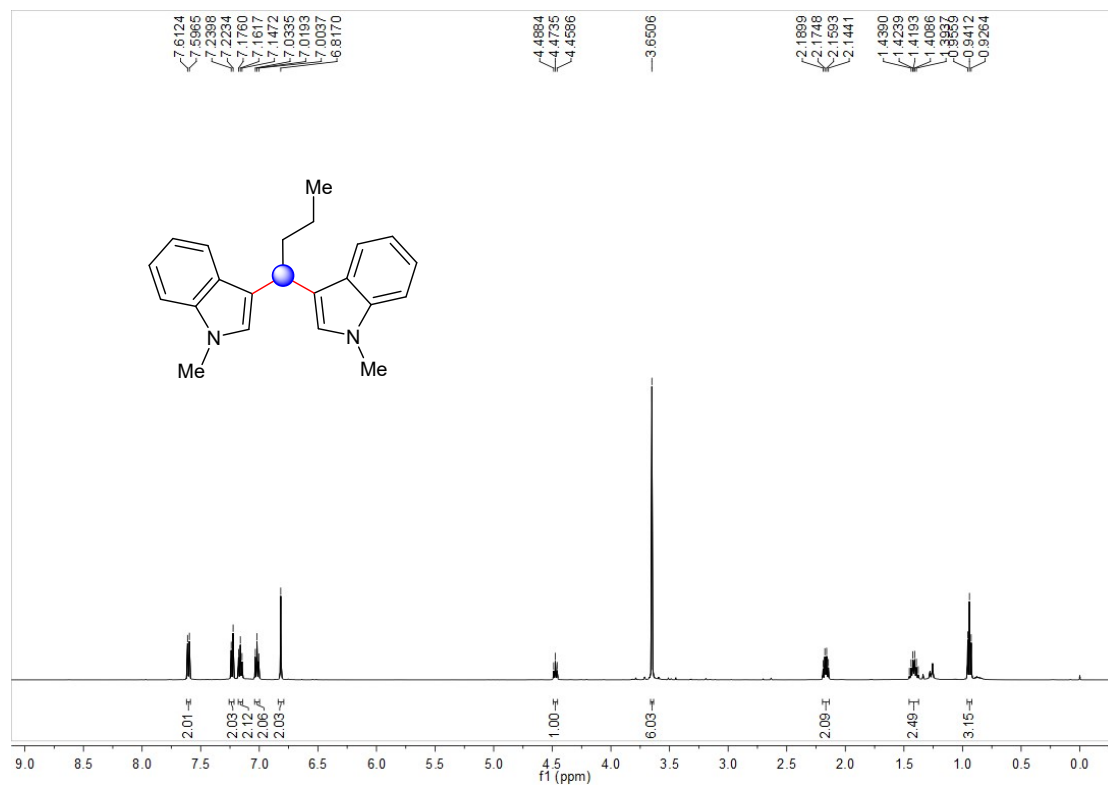
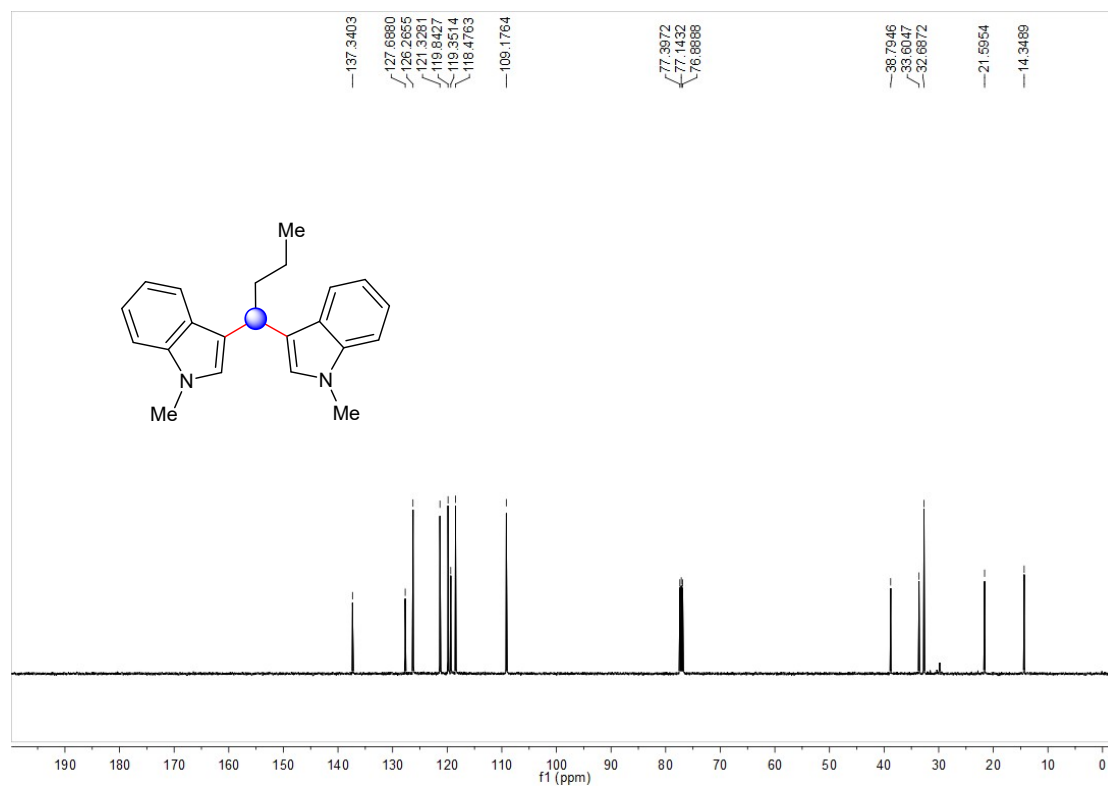
<sup>1</sup>H NMR



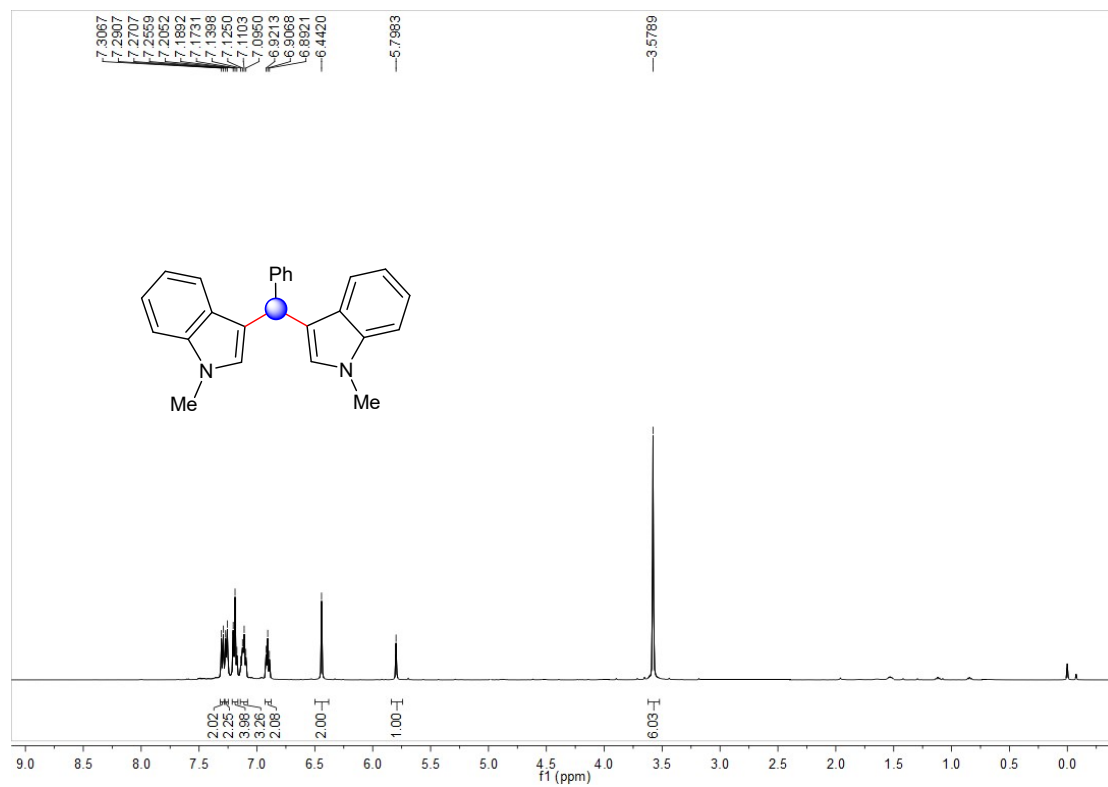
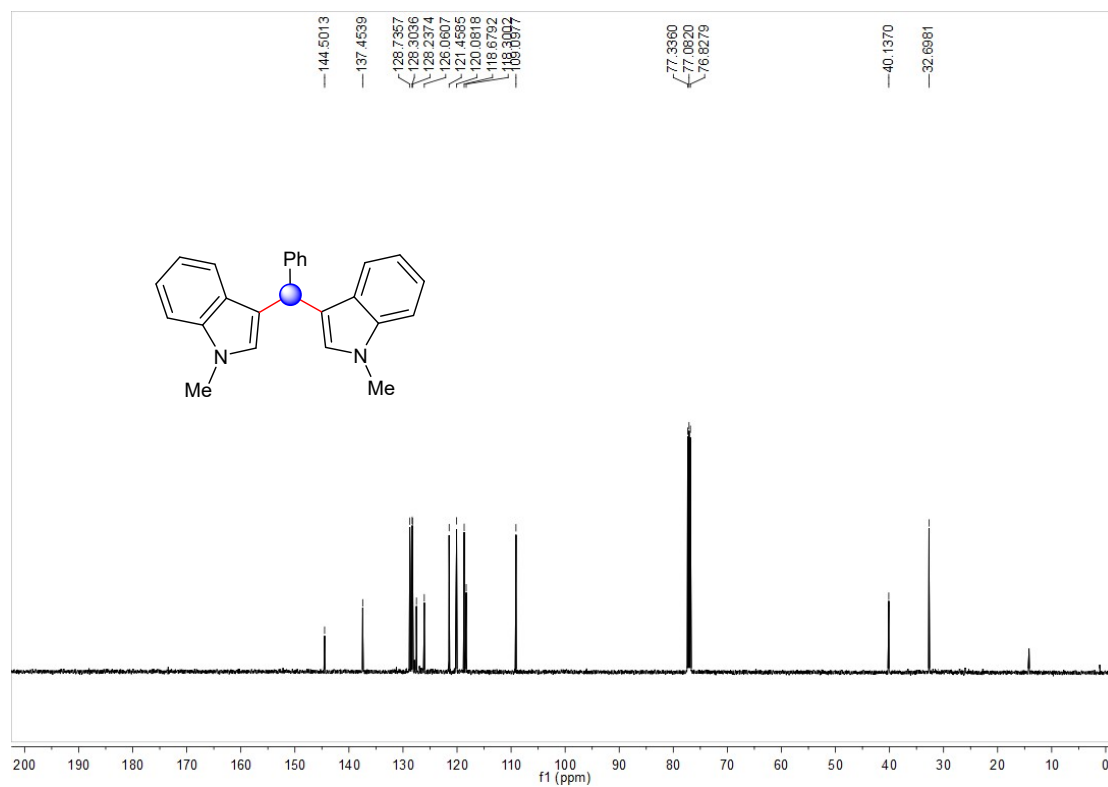
<sup>13</sup>C NMR



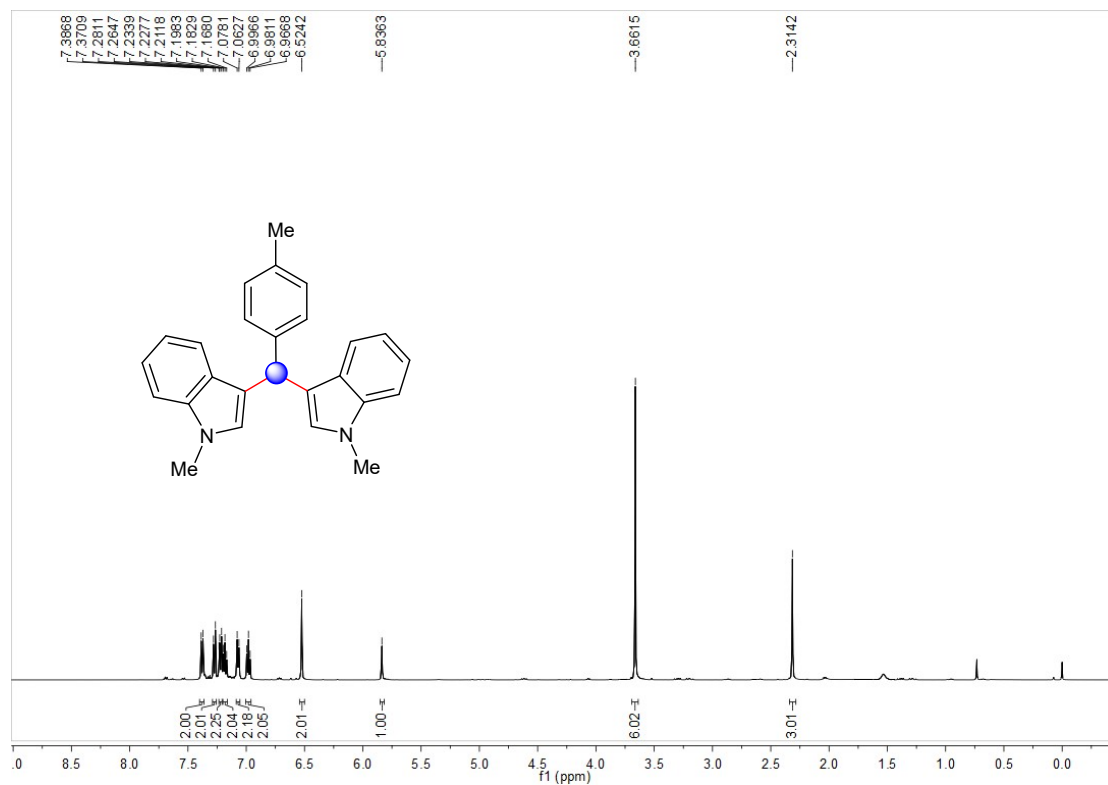
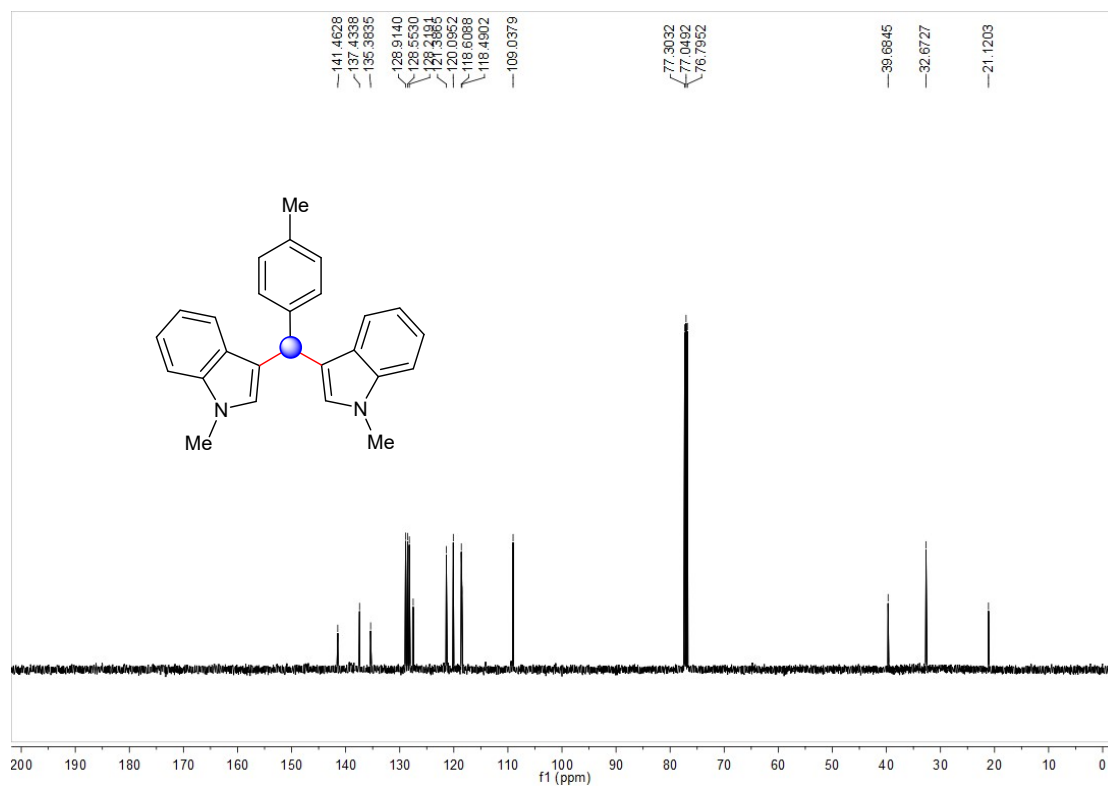
## 23c

<sup>1</sup>H NMR<sup>13</sup>C NMR

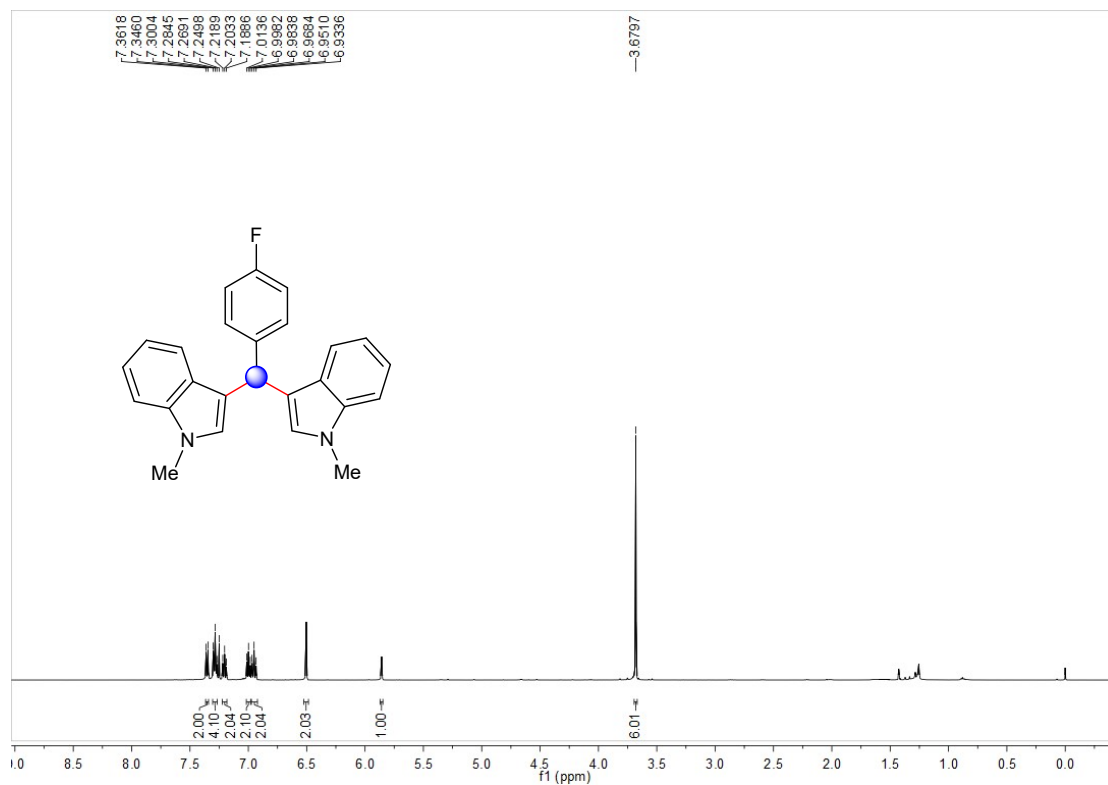
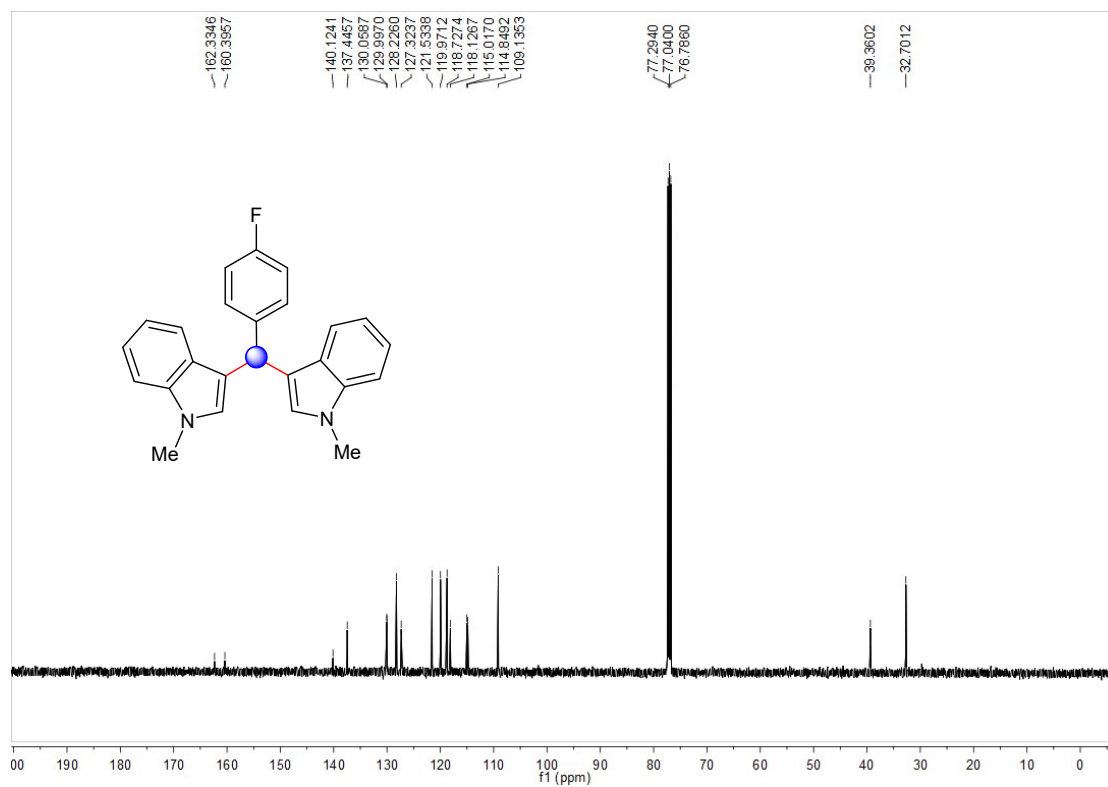
## 24c

<sup>1</sup>H NMR<sup>13</sup>C NMR

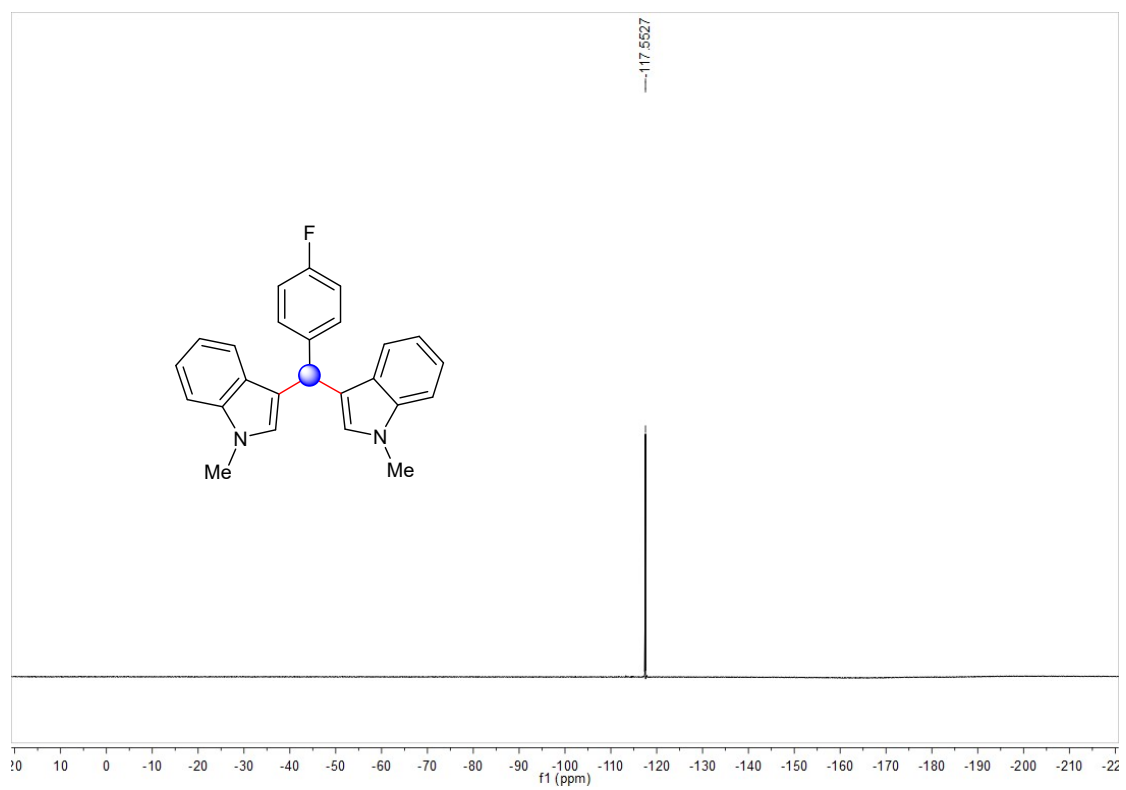
## 25c

<sup>1</sup>H NMR<sup>13</sup>C NMR

## 26c

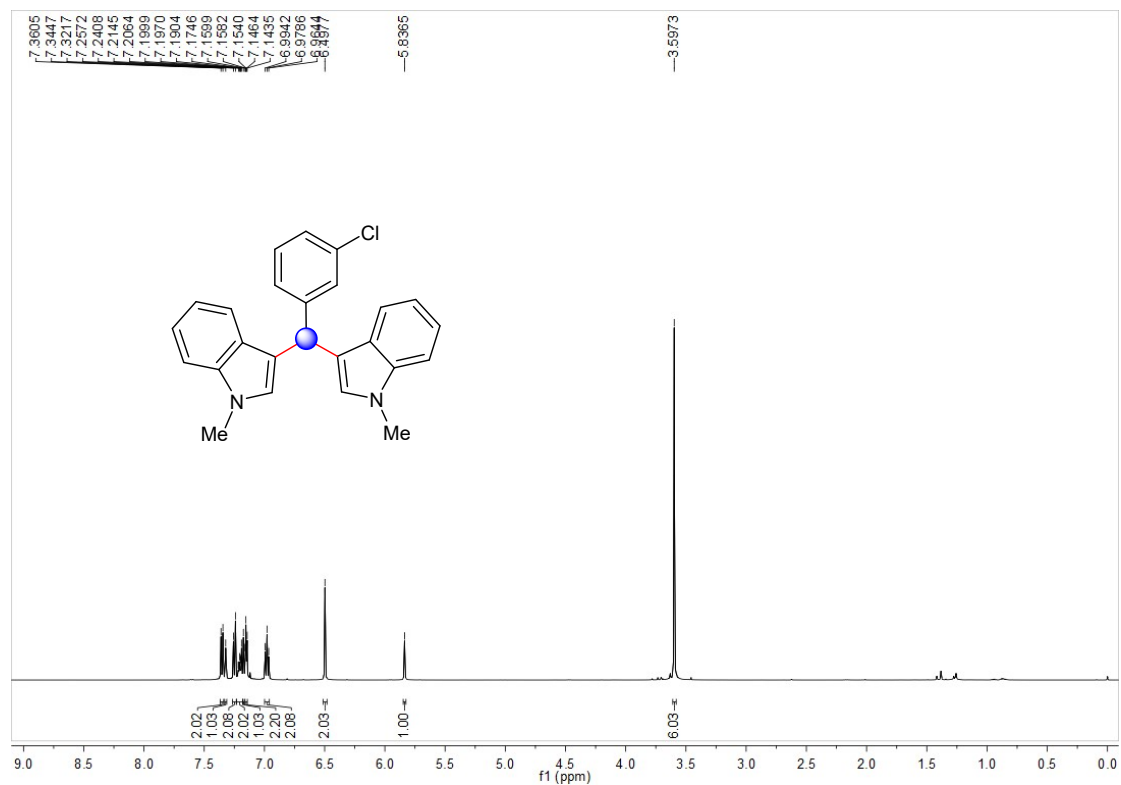
<sup>1</sup>H NMR<sup>13</sup>C NMR

**<sup>19</sup>F NMR**

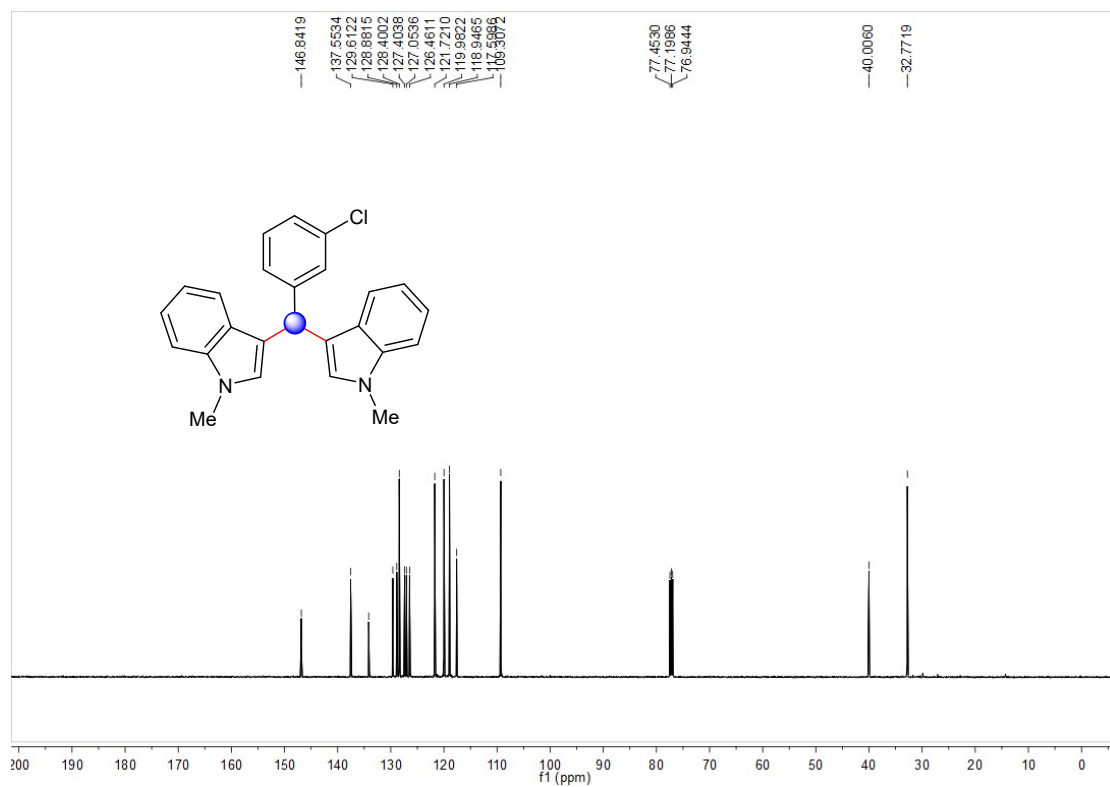


27c

<sup>1</sup>H NMR



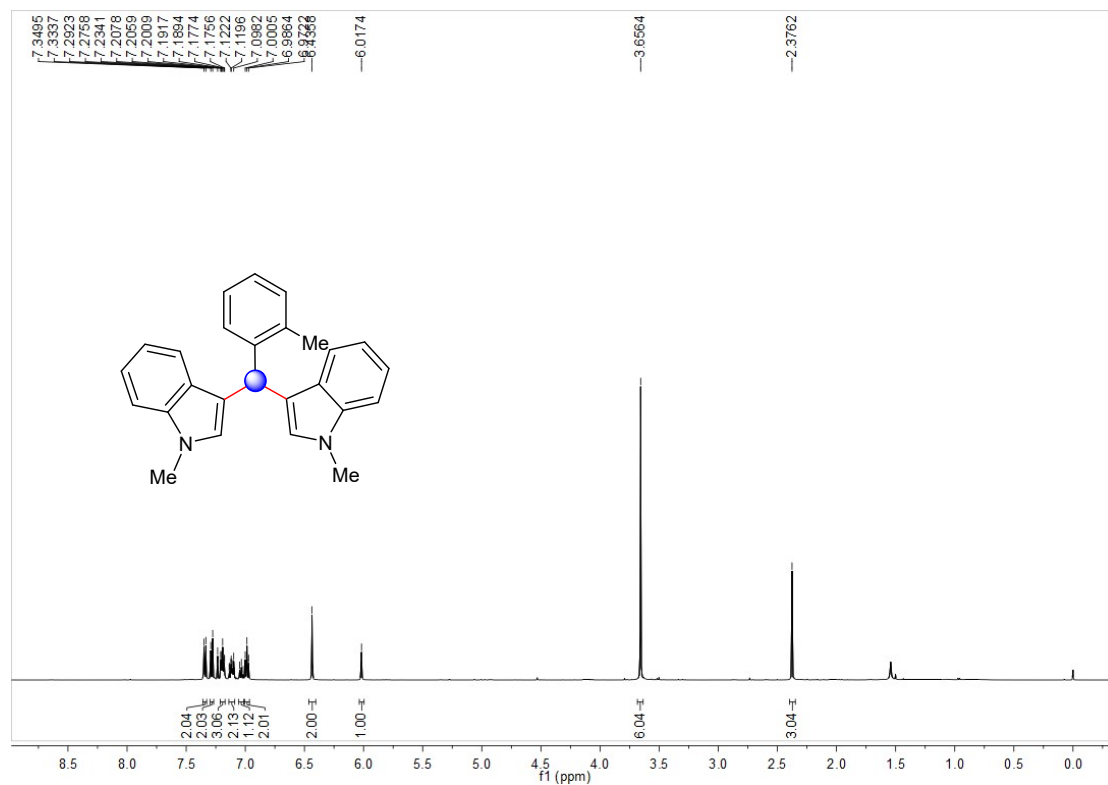
<sup>13</sup>C NMR



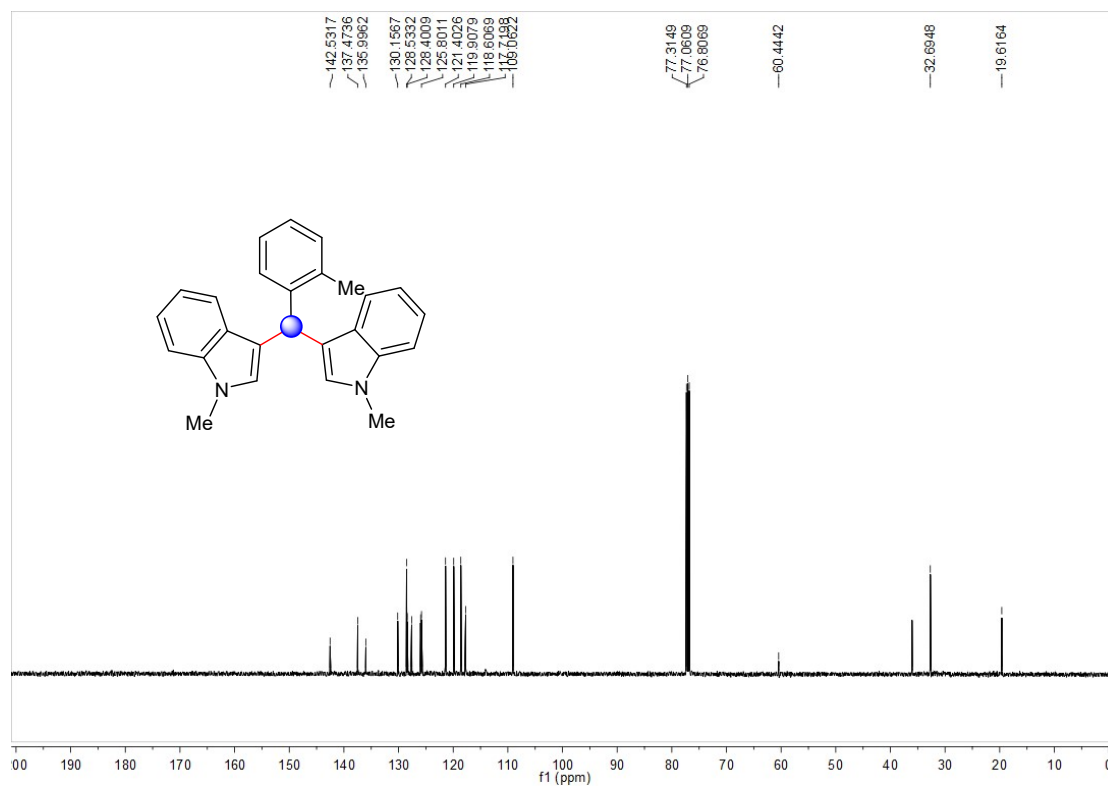


28c

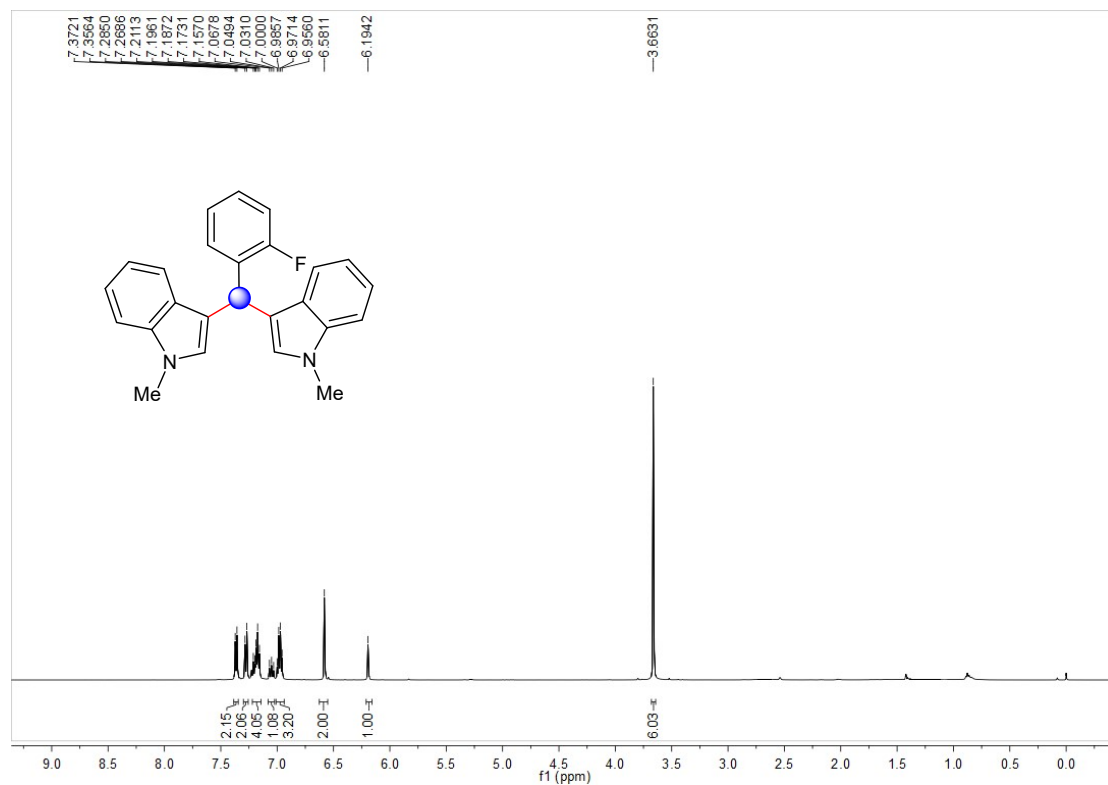
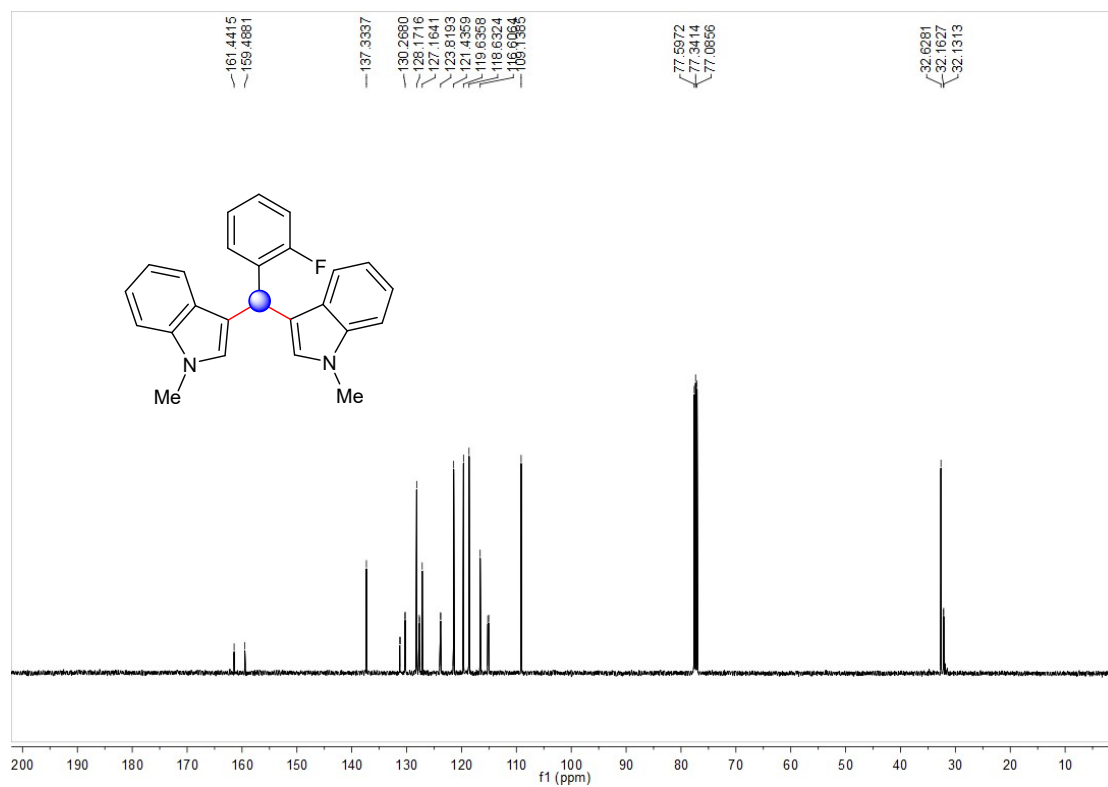
<sup>1</sup>H NMR



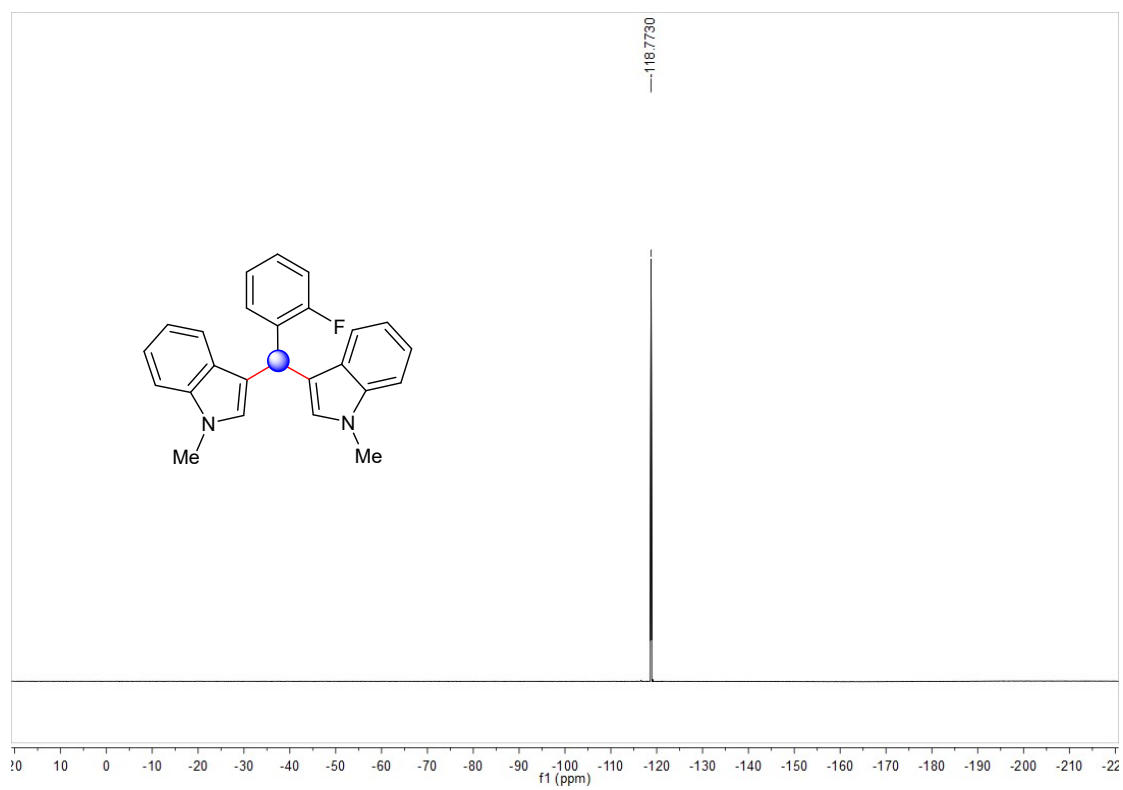
<sup>13</sup>C NMR



## 29c

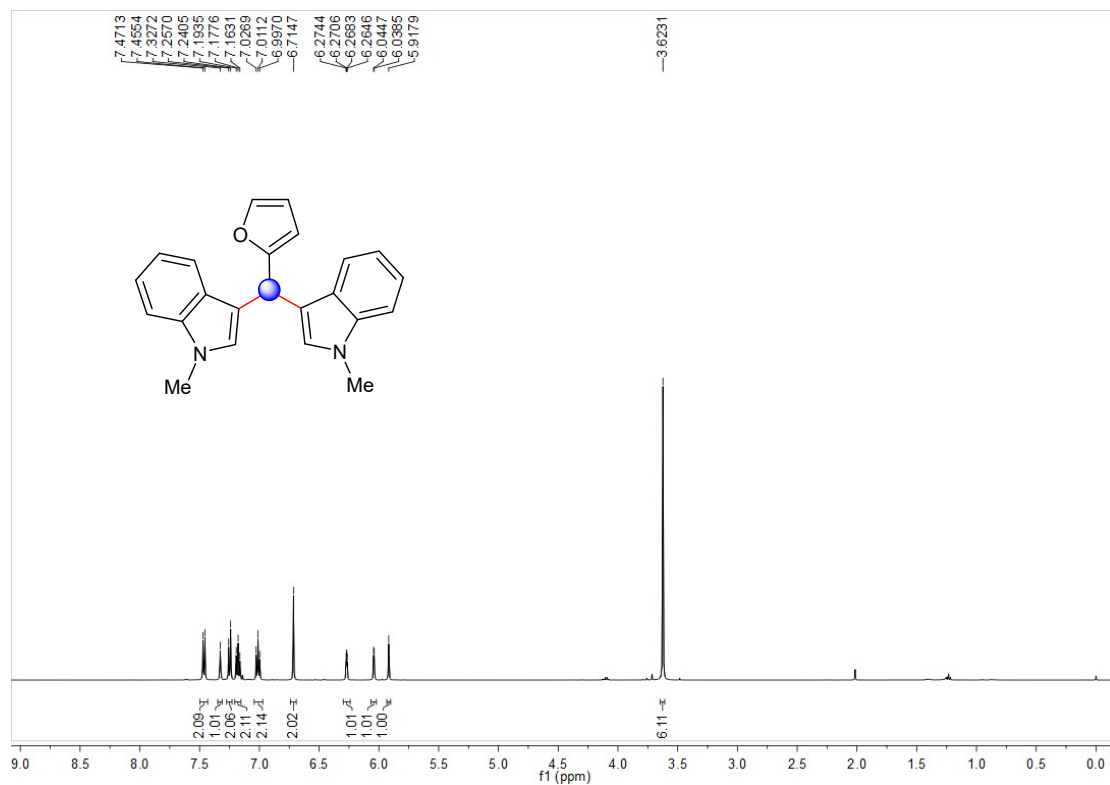
<sup>1</sup>H NMR<sup>13</sup>C NMR

**<sup>19</sup>F NMR**

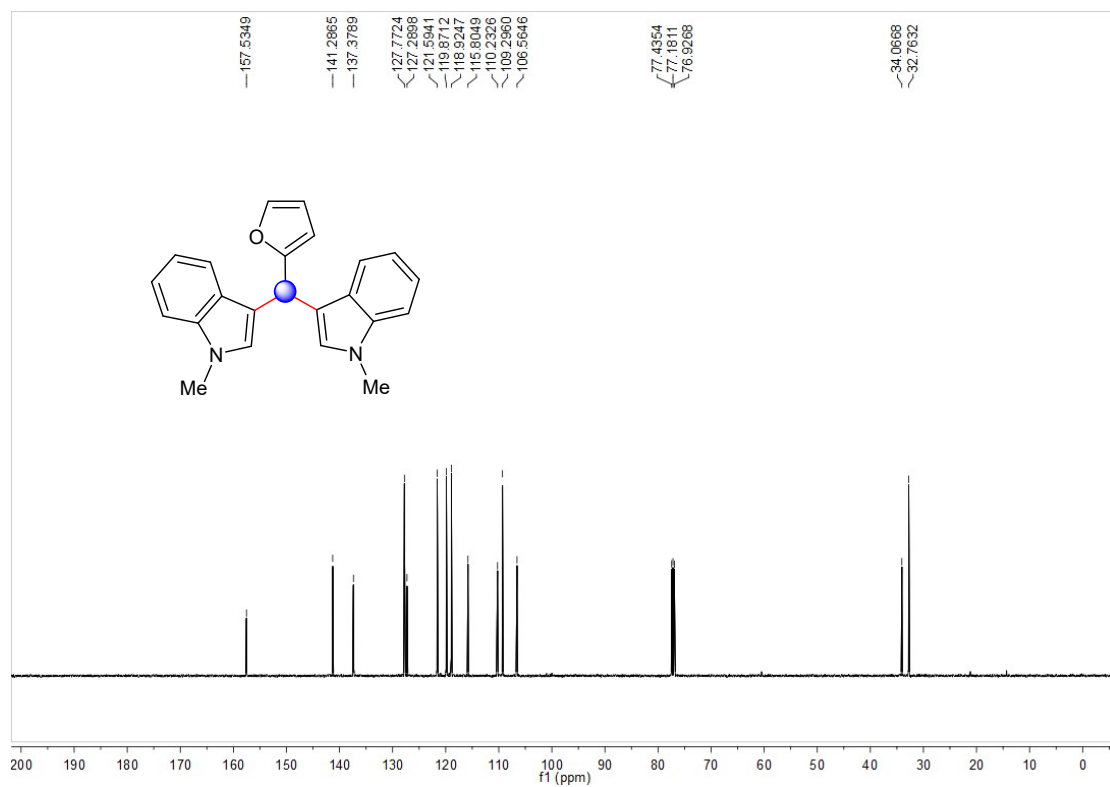


30c

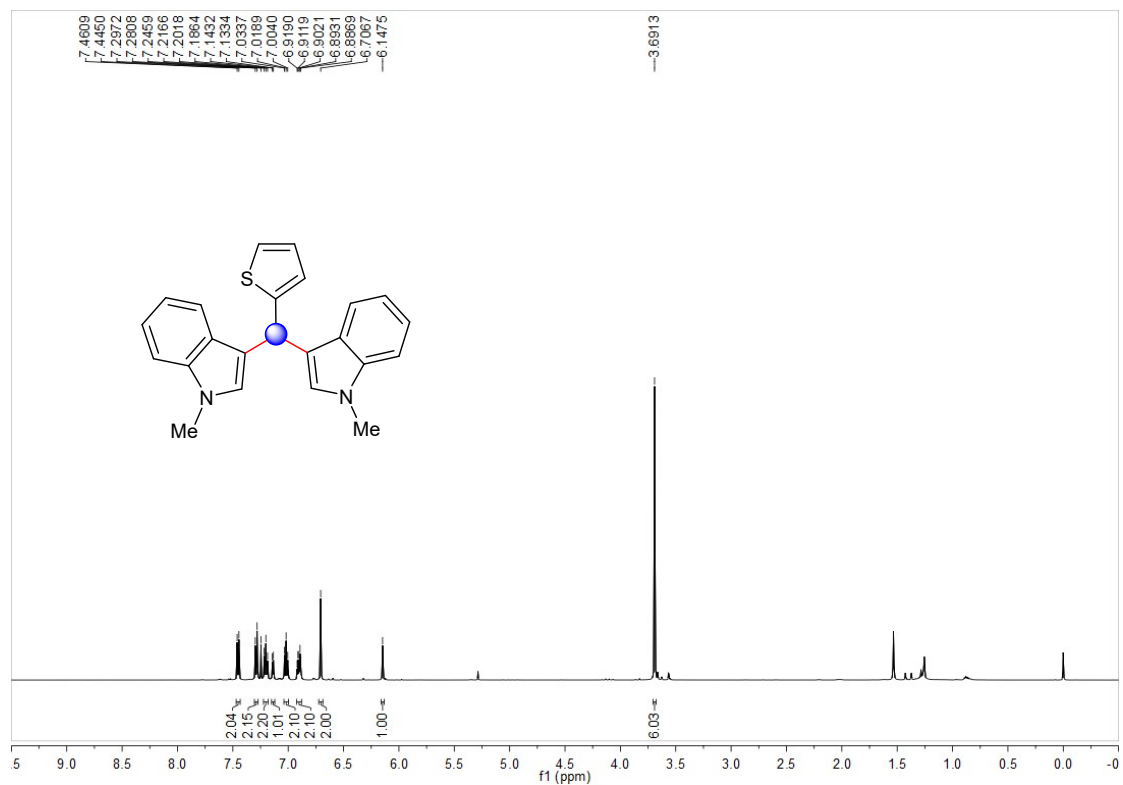
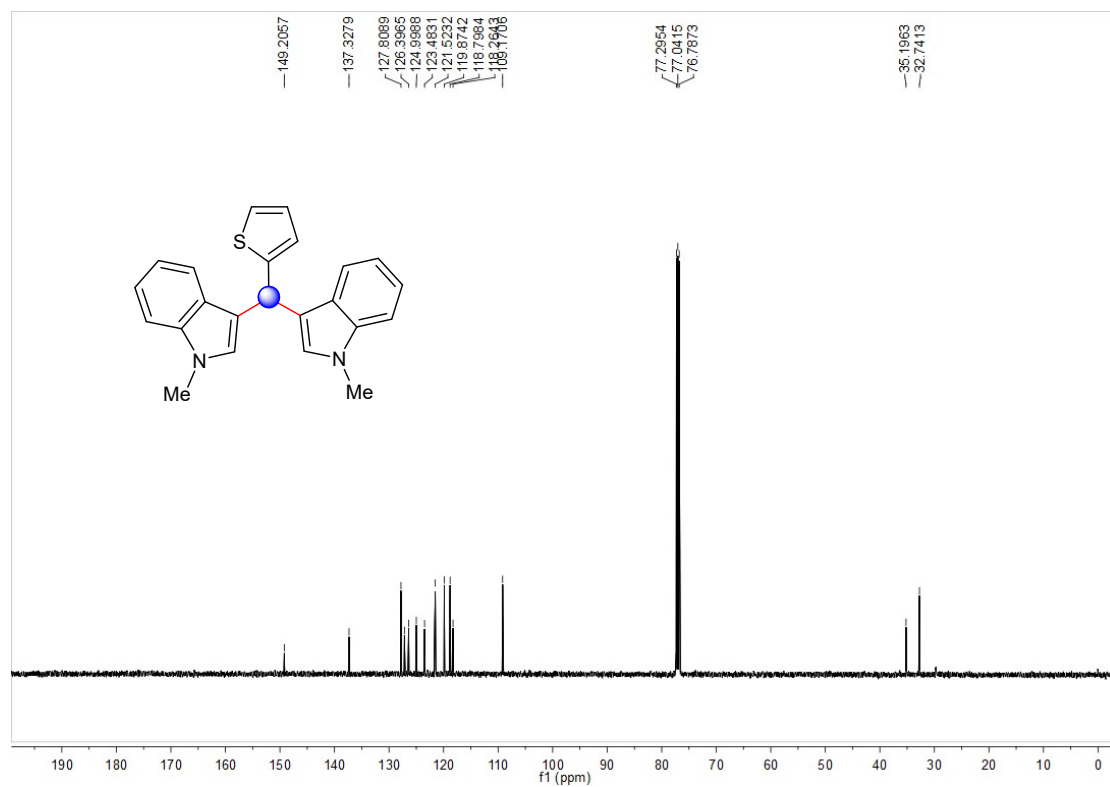
<sup>1</sup>H NMR



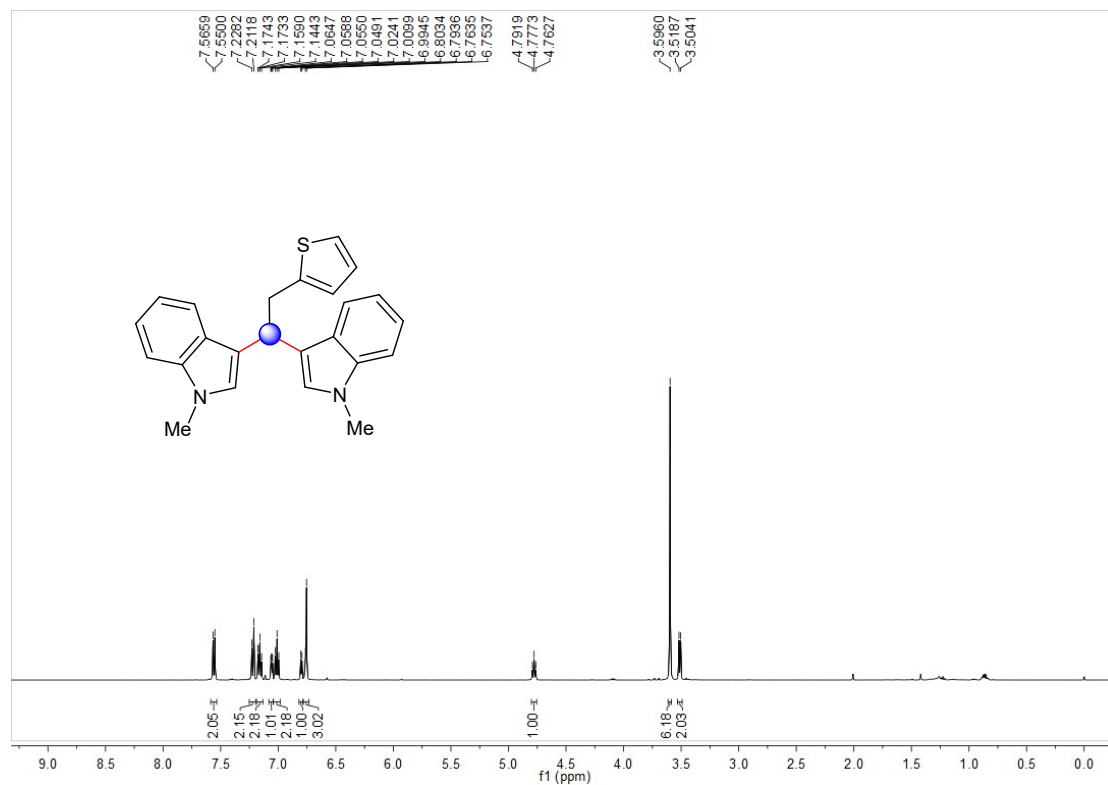
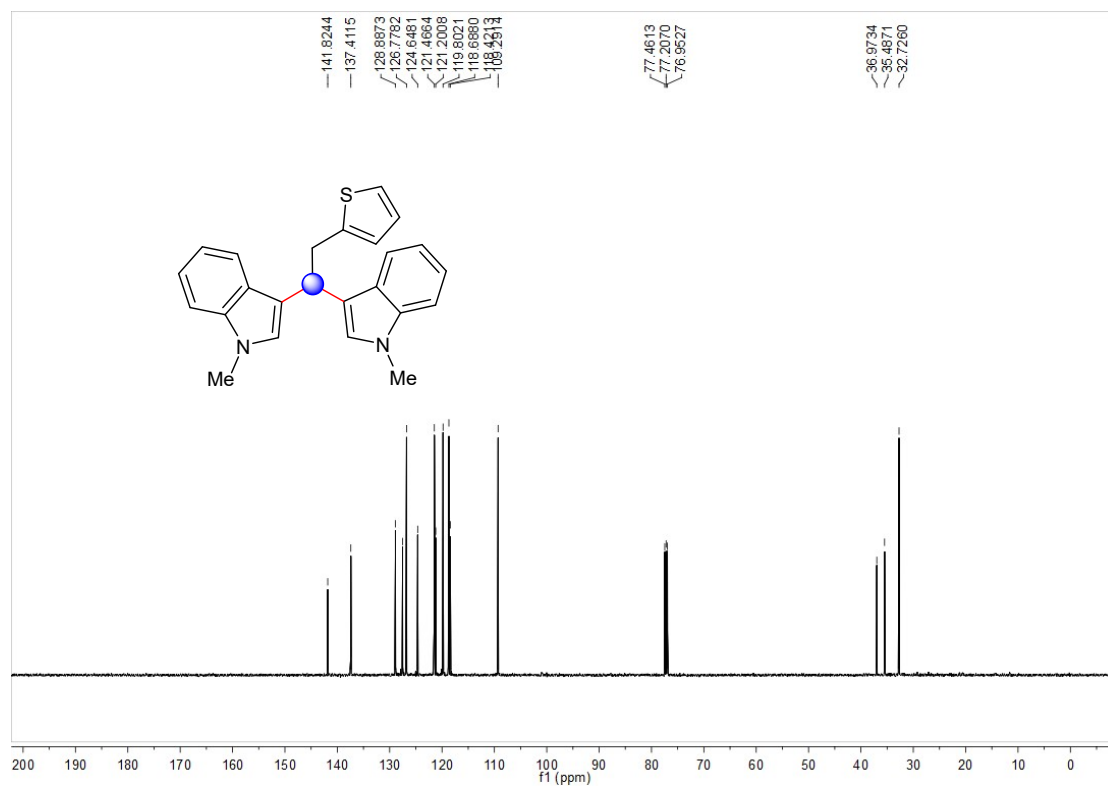
<sup>13</sup>C NMR



## 31c

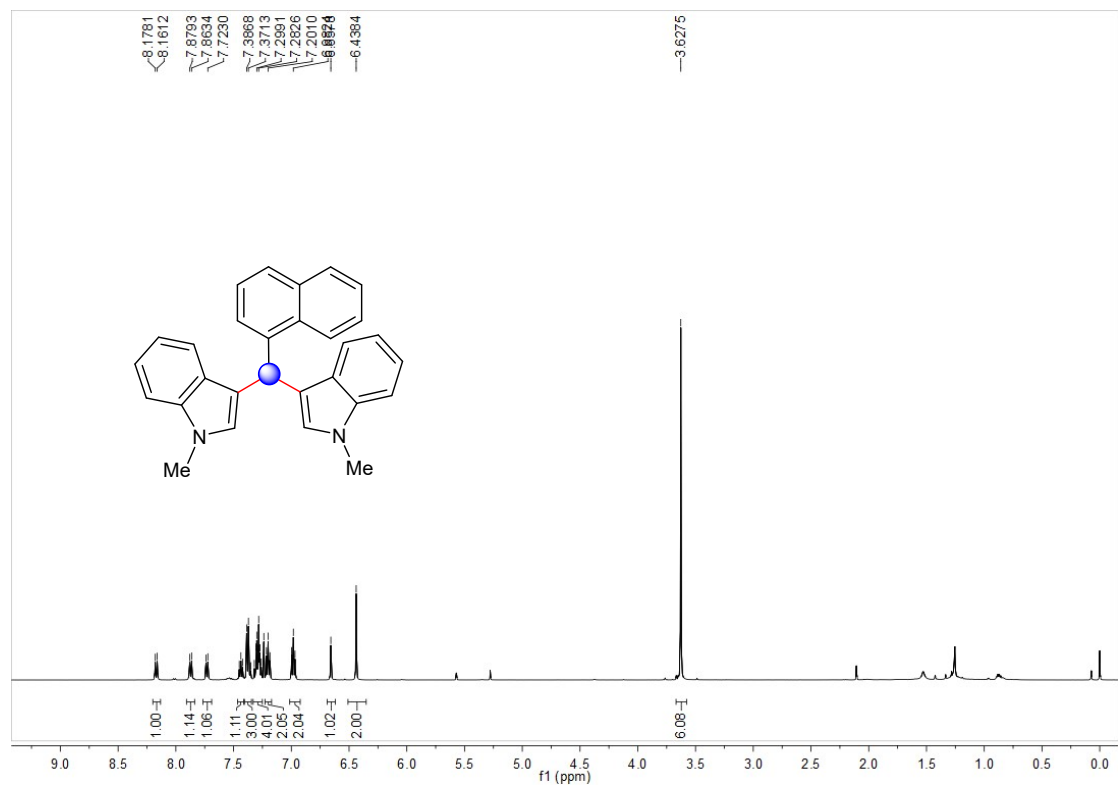
<sup>1</sup>H NMR<sup>13</sup>C NMR

## 32c

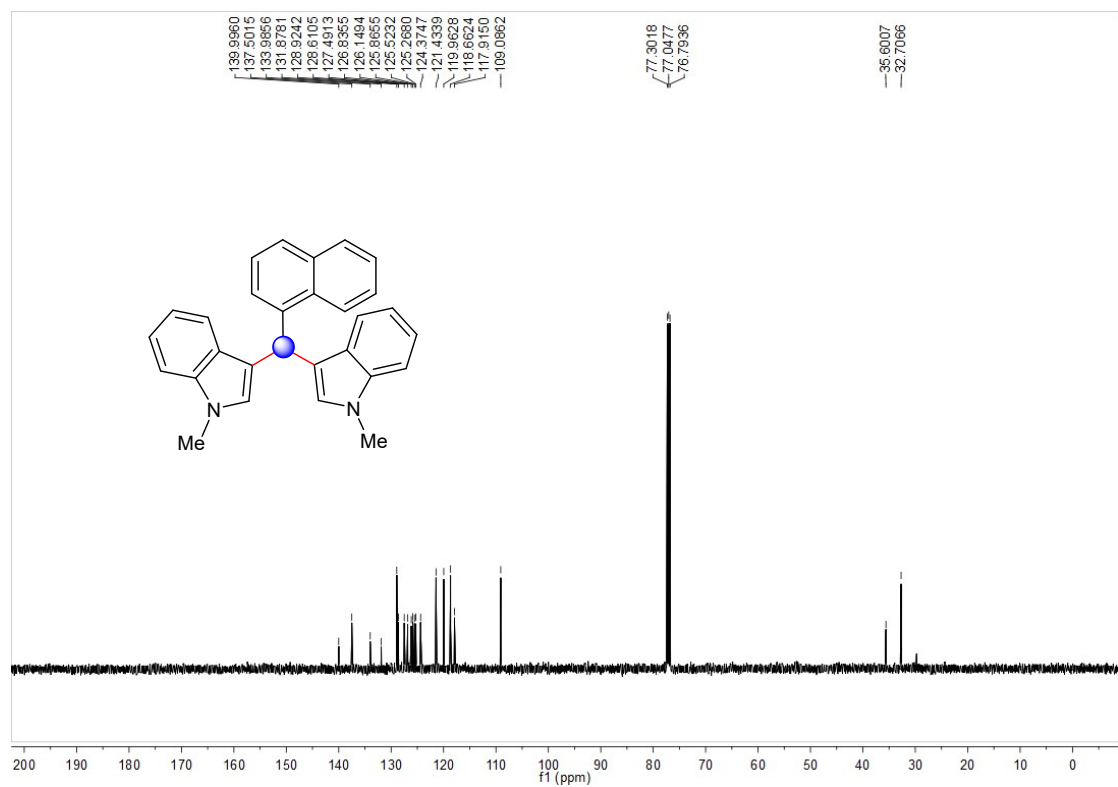
<sup>1</sup>H NMR<sup>13</sup>C NMR

33c

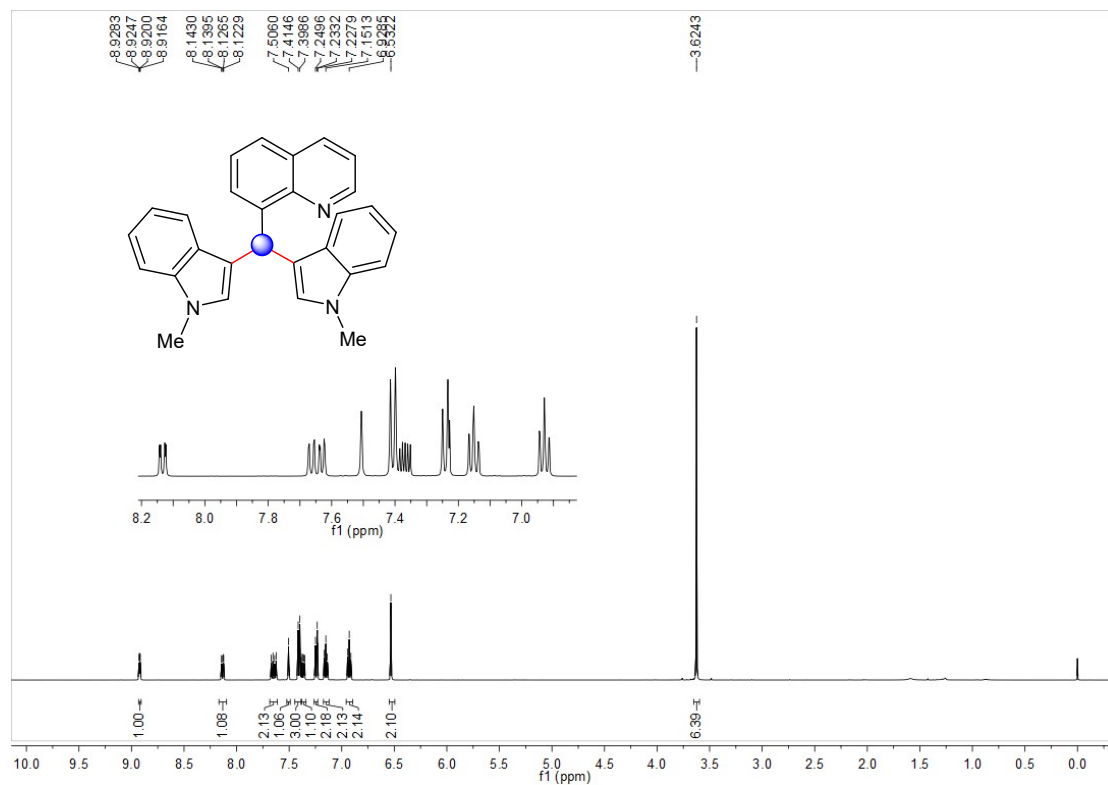
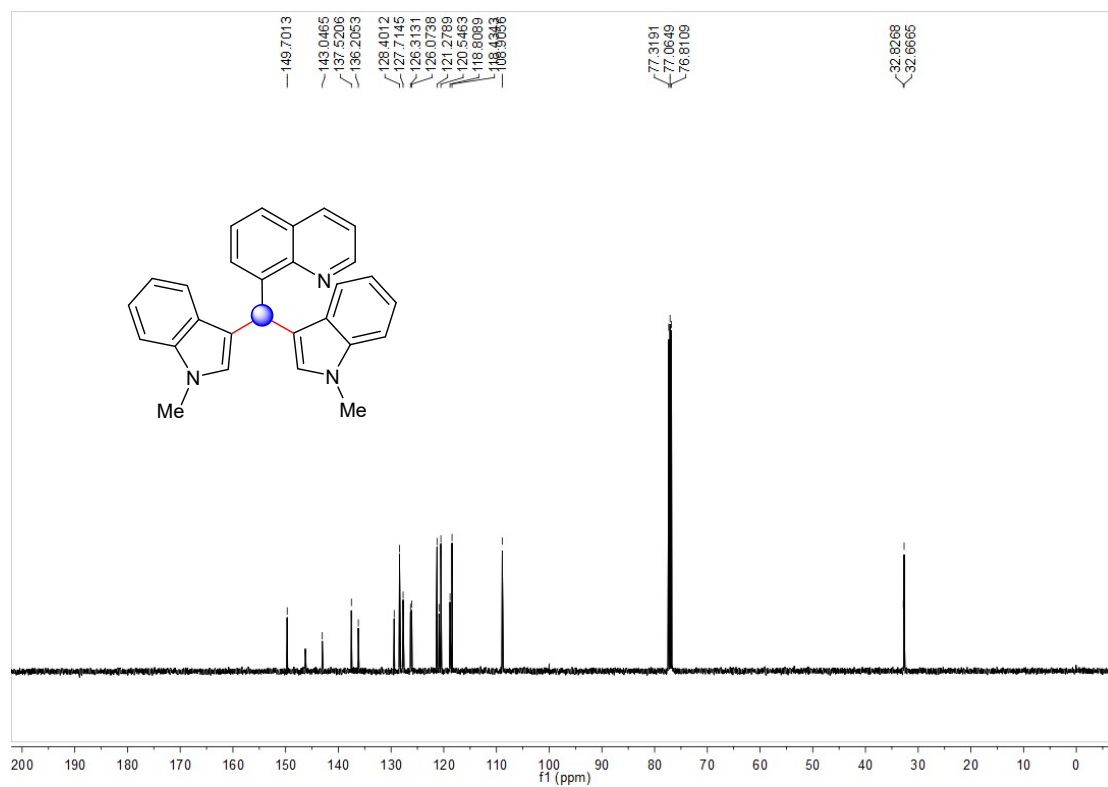
<sup>1</sup>H NMR



<sup>13</sup>C NMR



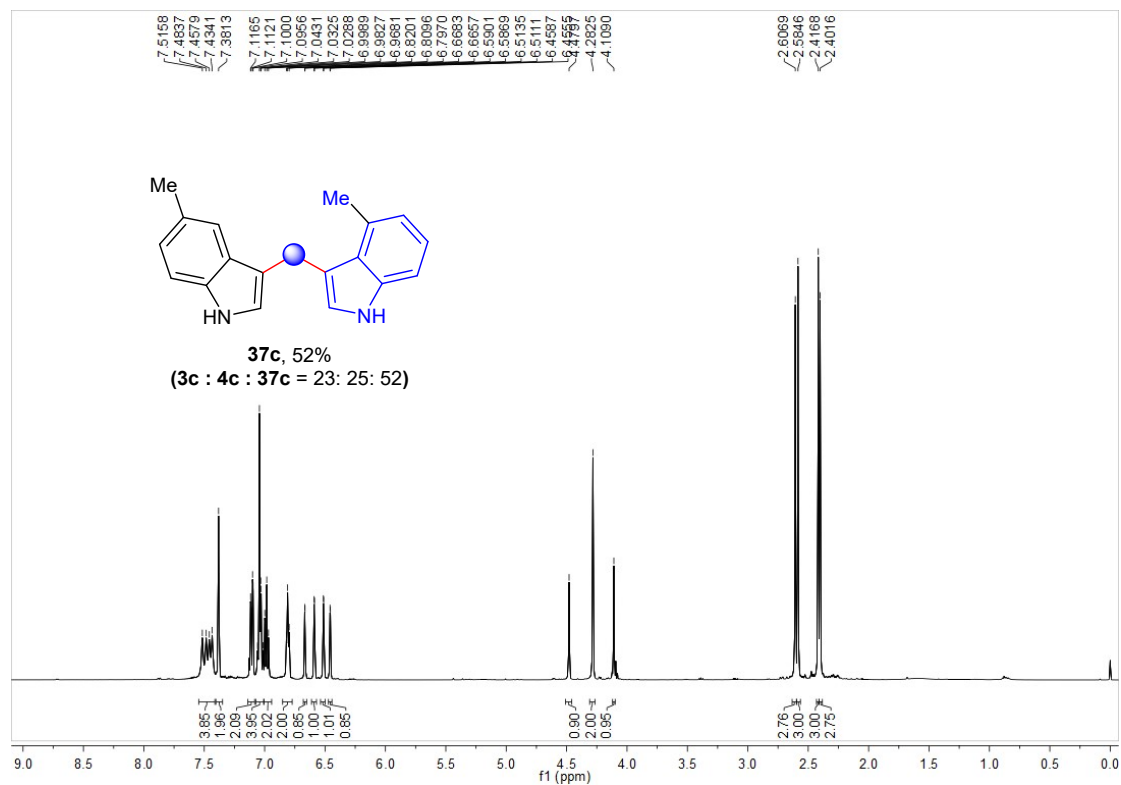
## 34c

<sup>1</sup>H NMR<sup>13</sup>C NMR

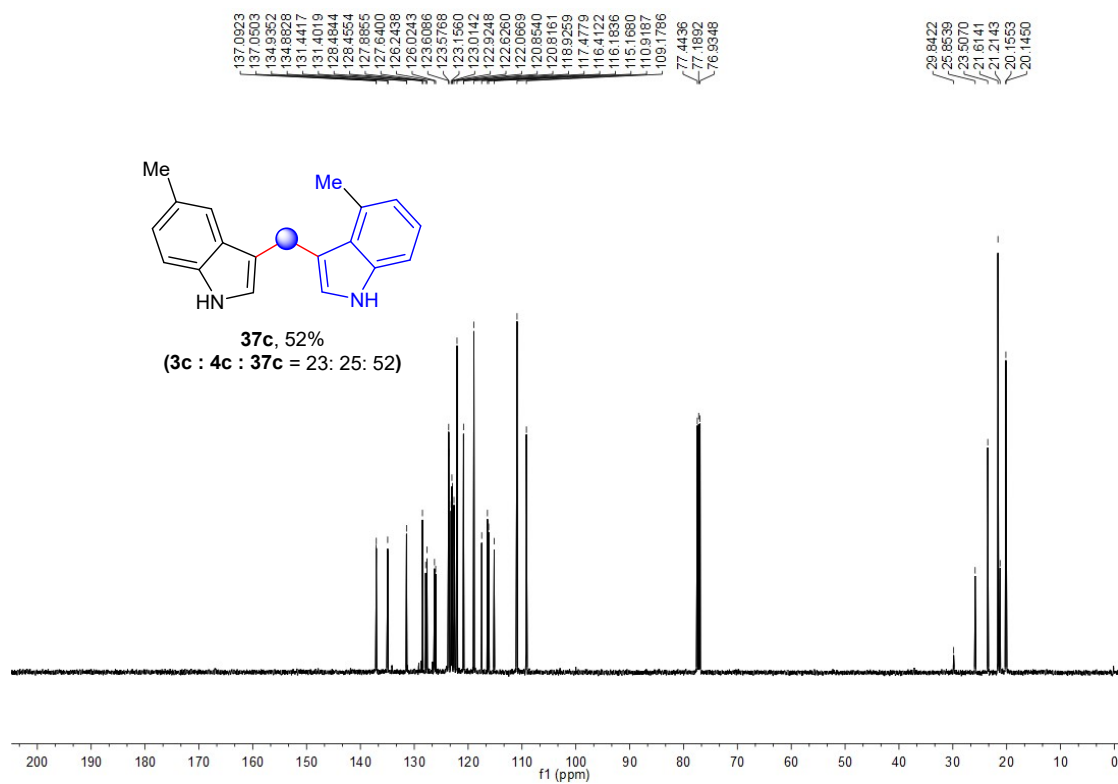


37c

<sup>1</sup>H NMR

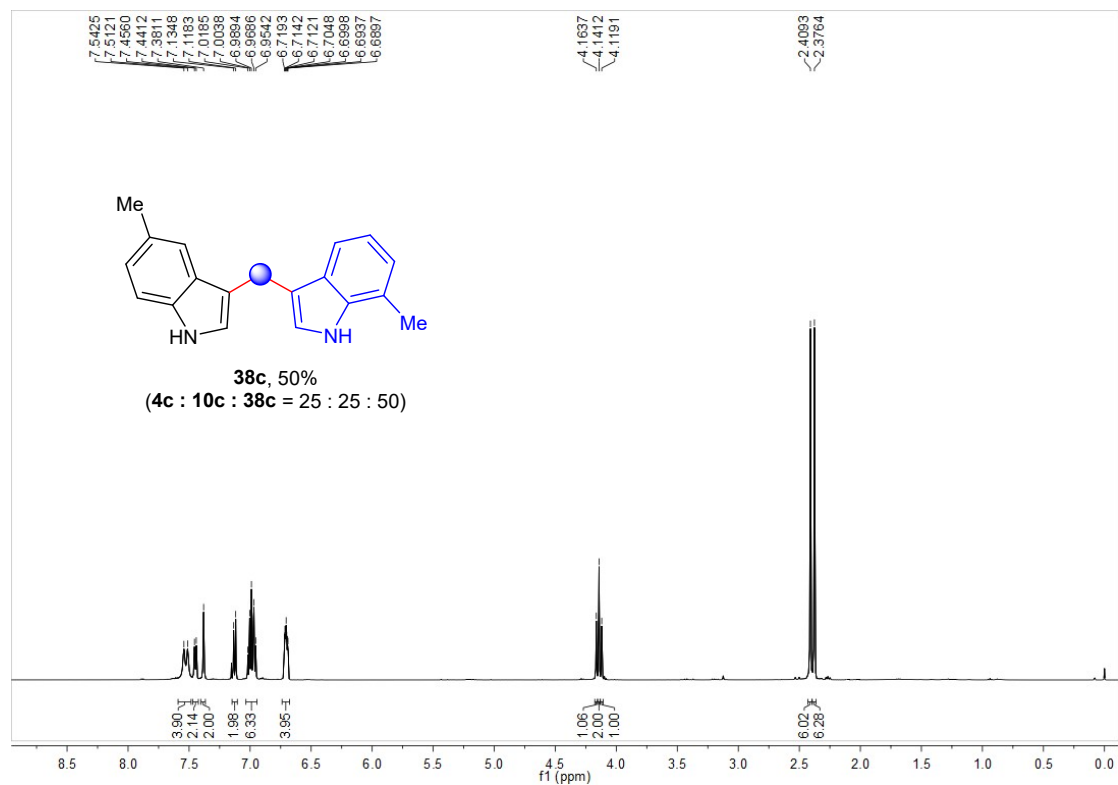


<sup>13</sup>C NMR

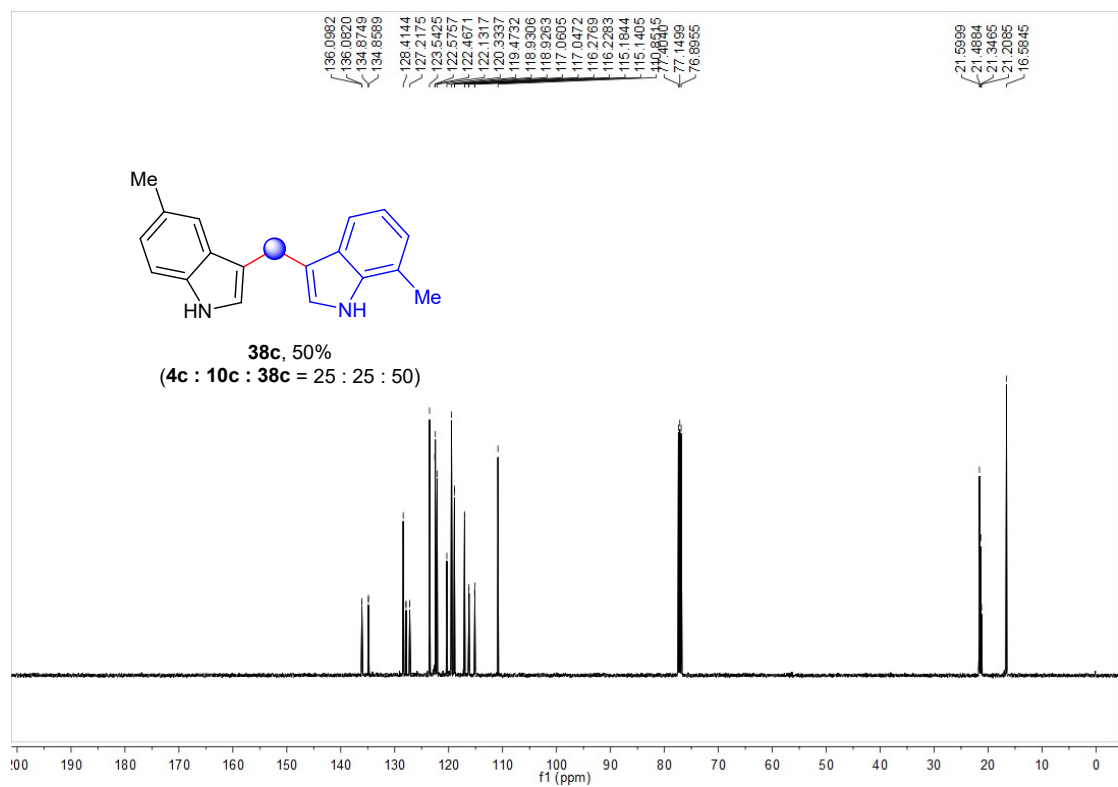


### 38c

#### <sup>1</sup>H NMR

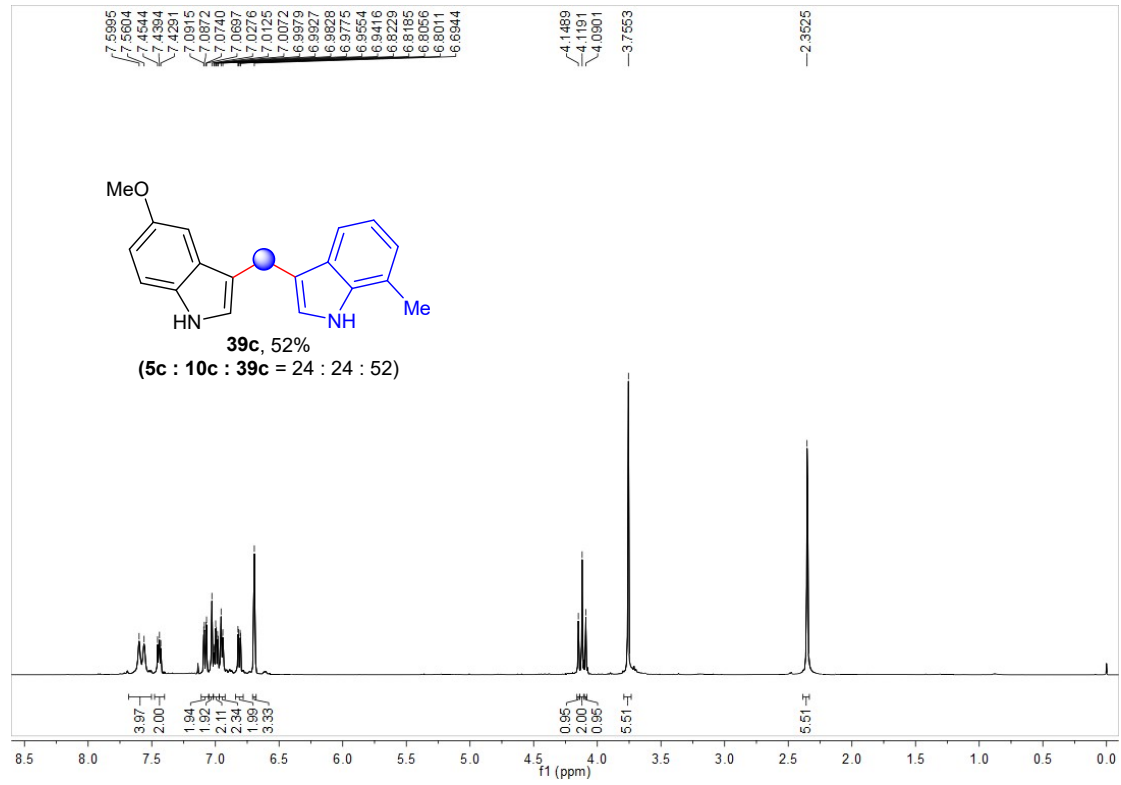


#### <sup>13</sup>C NMR

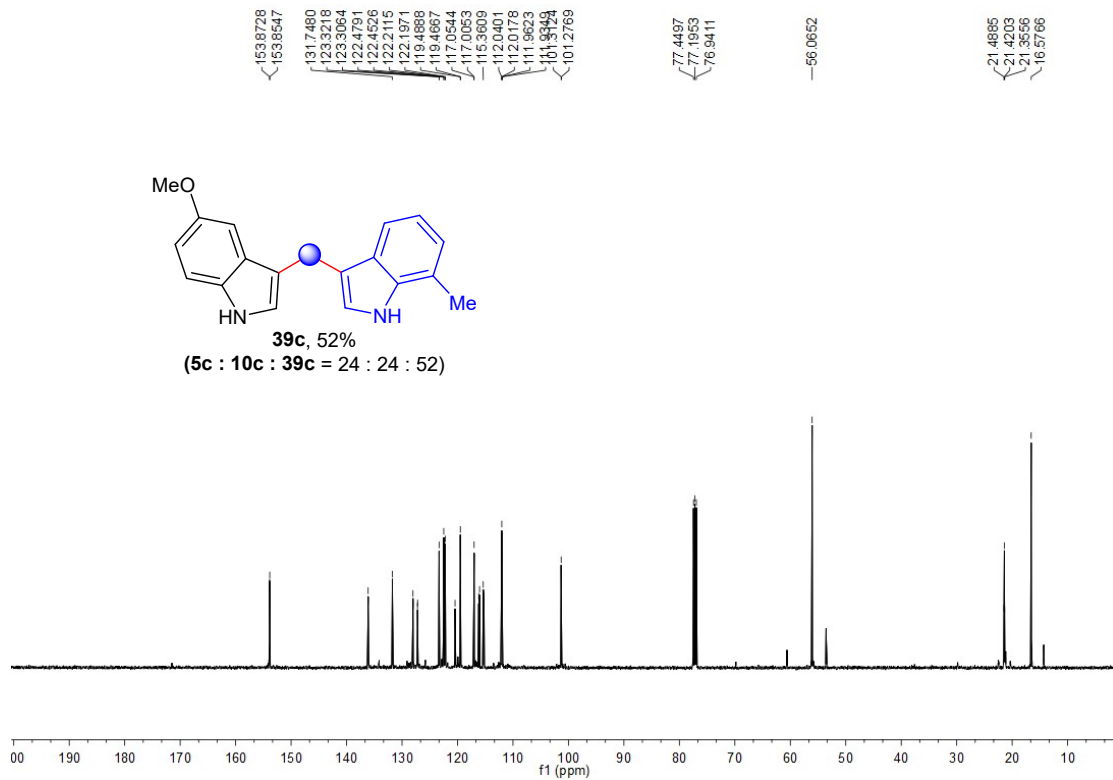


39c

<sup>1</sup>H NMR

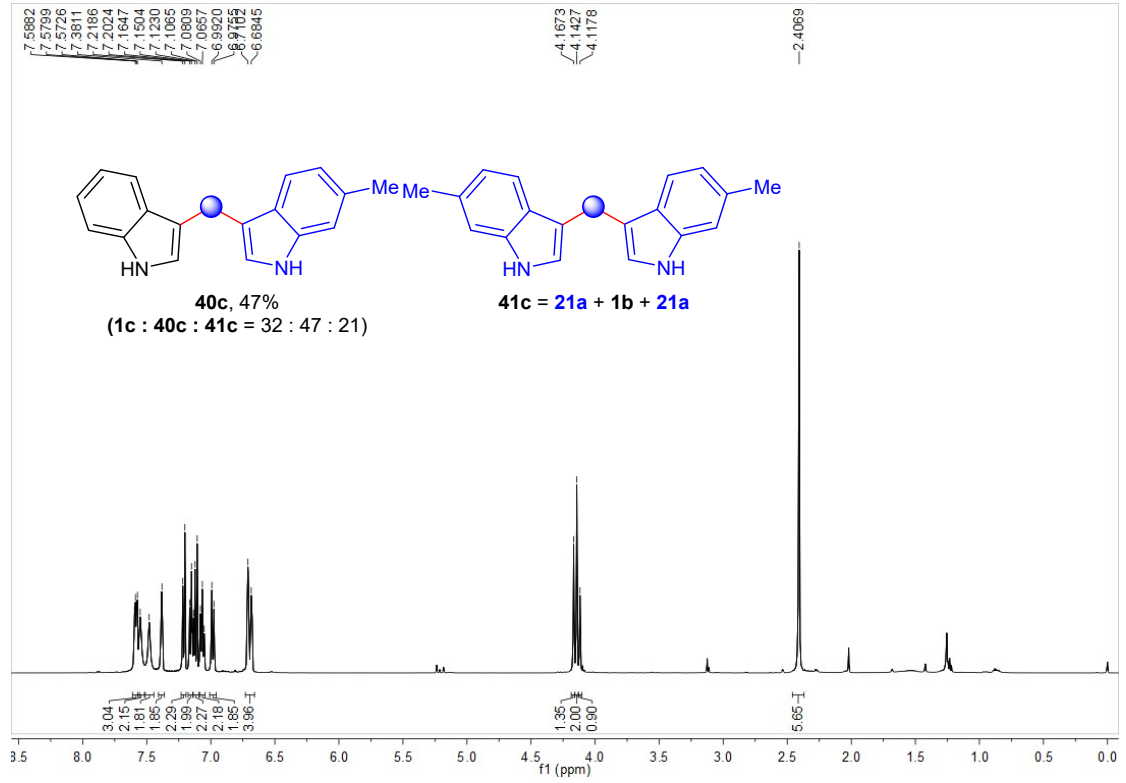


<sup>13</sup>C NMR

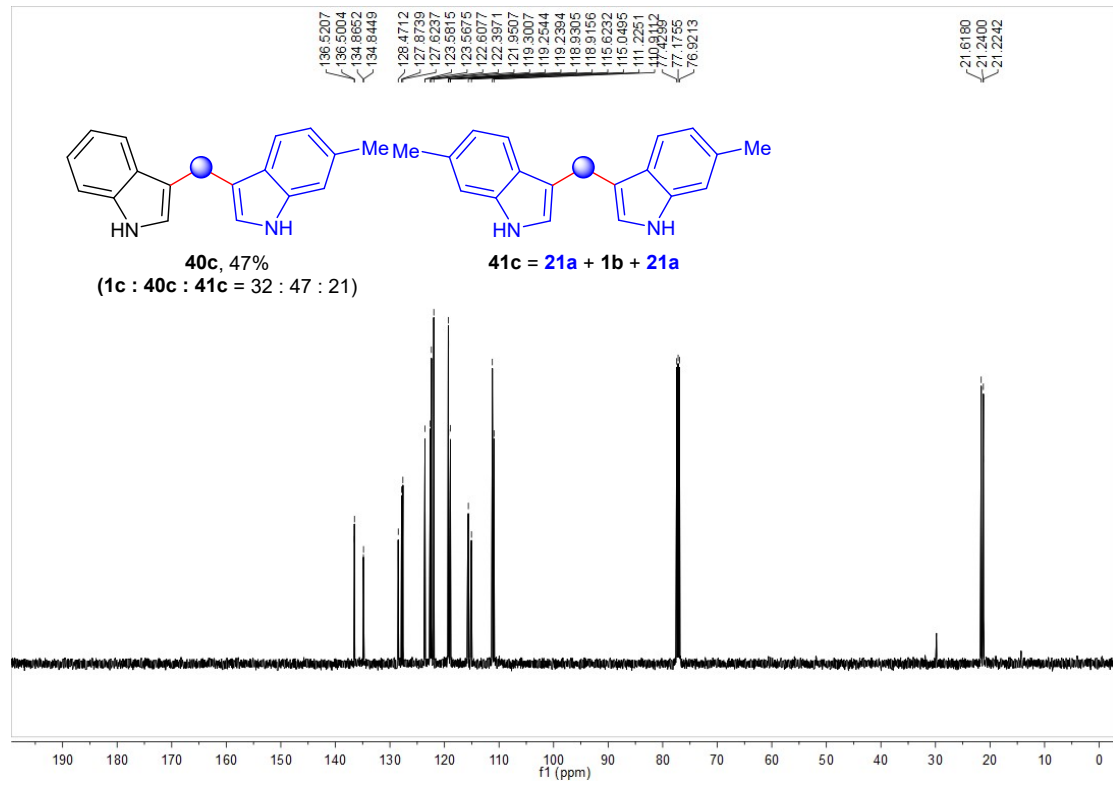


40c

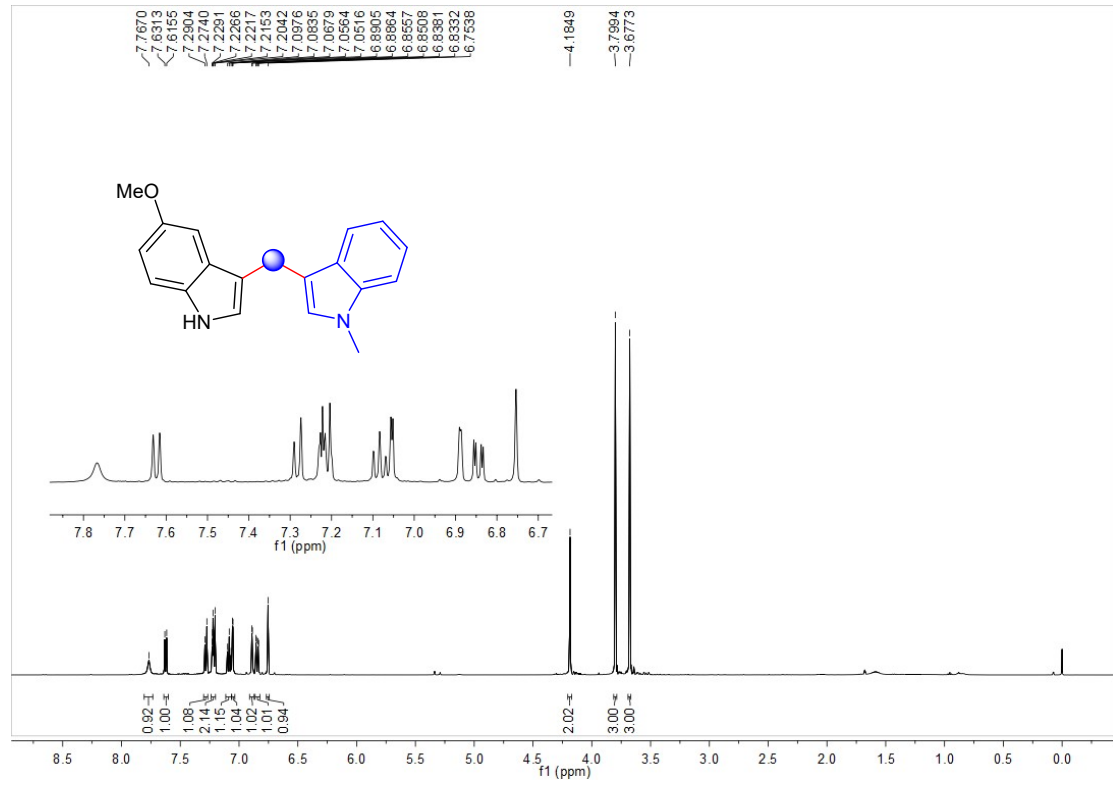
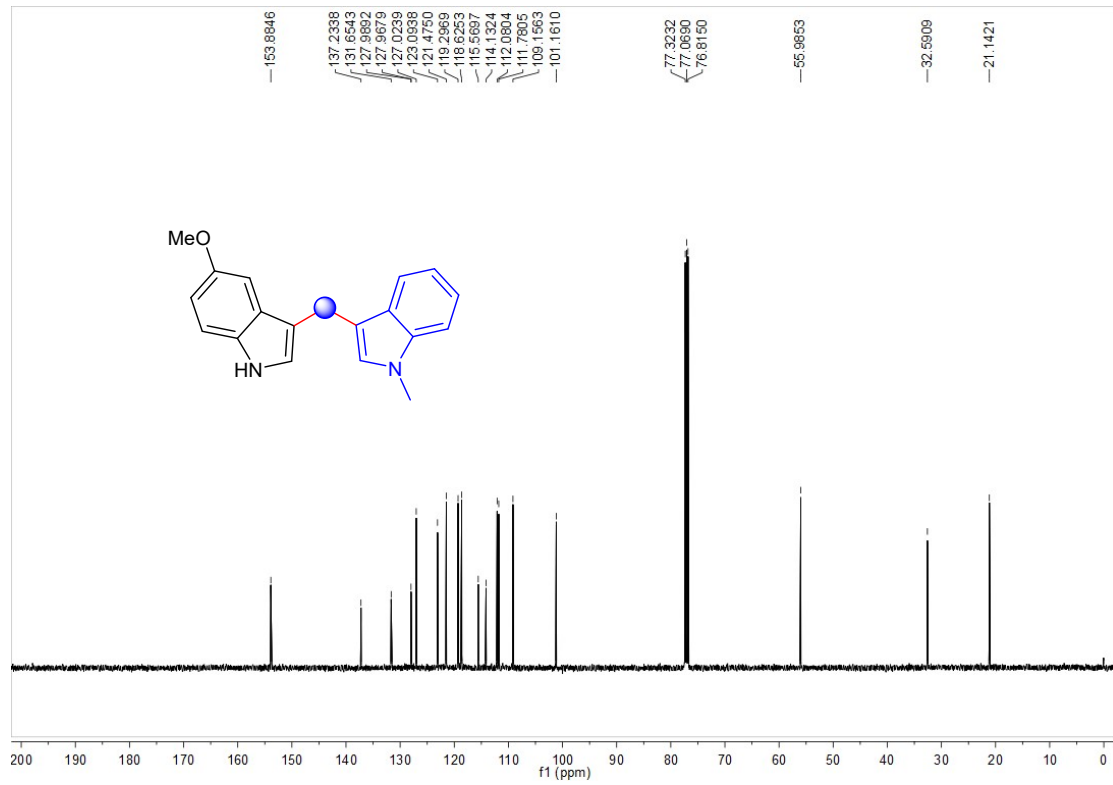
<sup>1</sup>H NMR



<sup>13</sup>C NMR

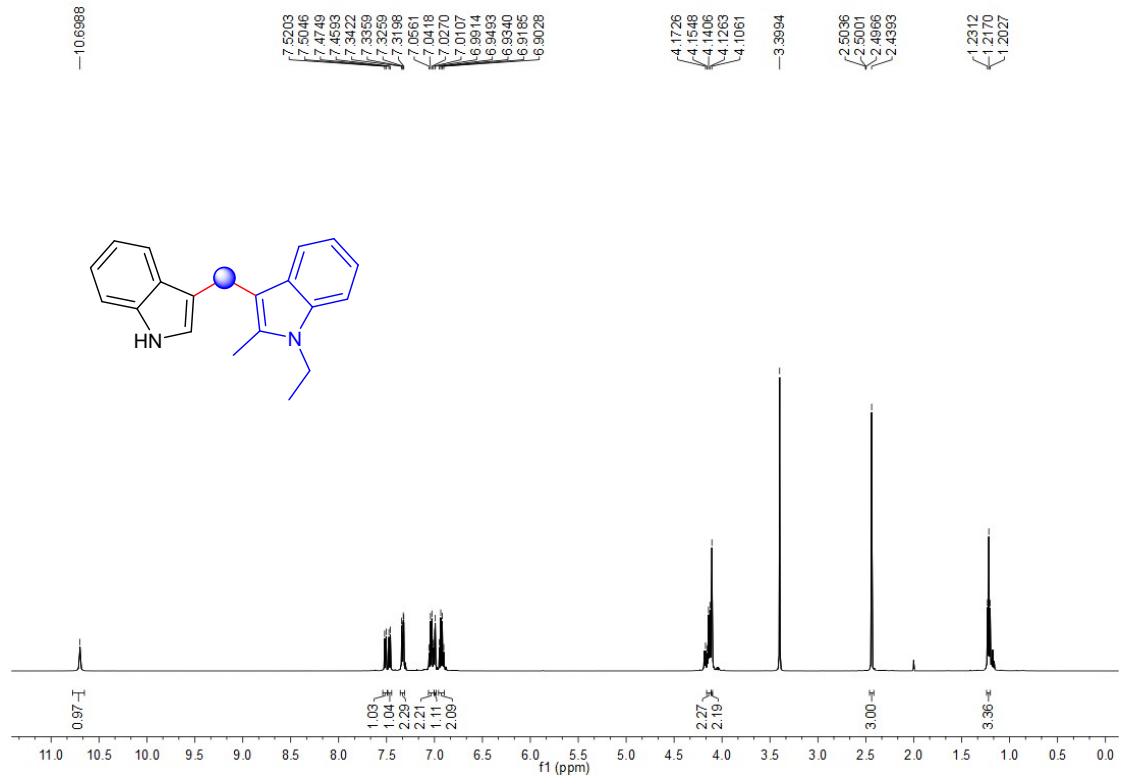


## 42c

<sup>1</sup>H NMR<sup>13</sup>C NMR

43c

<sup>1</sup>H NMR



<sup>13</sup>C NMR

