Supporting Information

One-pot C-C, C-N, and C-S Bond Construction for Synthesis of 3-Sulfenylindoles Directly from Unactivated Anilines Involving Dual Palladium Catalysis and Mechanistic Insights by DFT

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1. Synthesis of starting material.

General procedure for the synthesis of disulfides from respective thiols

In this work, disulfides were synthesized using the procedure reported in the literature.[S1, S2] The general experimental procedure followed as below;

A 25 mL round bottom flask filled with DMSO (1 equiv.) was added 20 mol% iodine. When iodine was homogenized in DMSO, thiophenol or alkyl-thiols (2 mmol) were added at rt and the progress of the reaction was monitored by thin-layer chromatography (TLC). After completion of the reaction (5-30 min.), it was quenched with EtOAc and hypo solution. The organic layer was separated and water layer was extracted again with EtOAc (3 x 25 mL). The combined organic layer was dried over sodium sulfate, filtered and organic layer was concentrated over rotary evaporator under reduced pressure. The resulting crude reaction mixture was purified by column chromatography using eluent EtOAc in *n*-Hexane. The pure disulfide was fully characterized by NMR and matched with the literature reports.

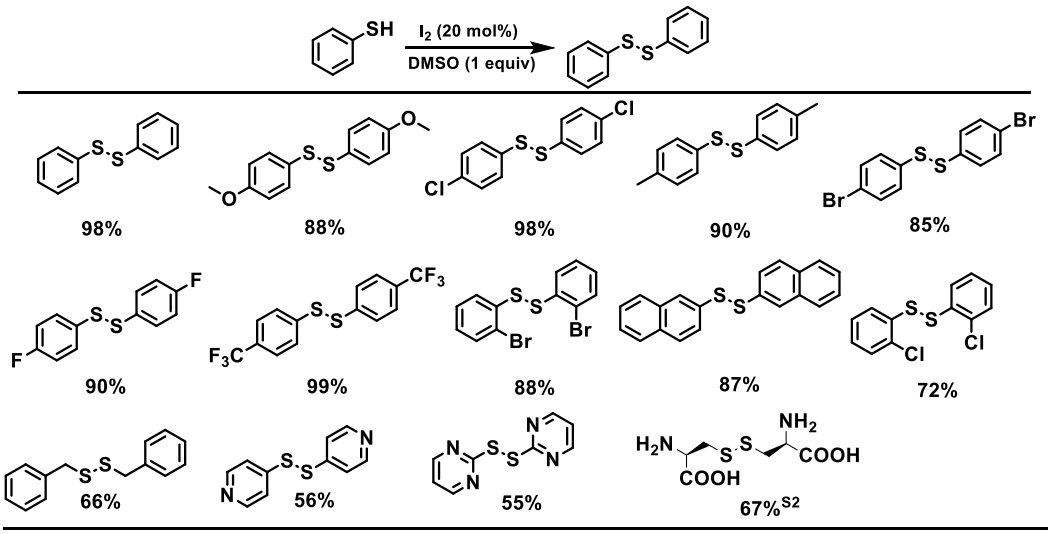
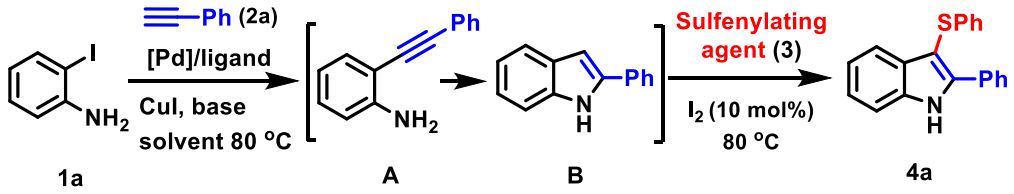


Figure S1. Synthesis of different disulfides



Entry	[Pd] (10 mol%)	Ligand (mol%)	Base (2.0 equiv)	Solvent	Sulfenylating agent	Time (h)	yield (%)[b] A	B	4a
1	$PdCl_2$	dppf (5)	iPr_2NH	CH_3CN	-	2	0	74	-
2	$Pd(PPh_3)_4$	dppf (5)	iPr_2NH	CH_3CN	-	3	91	0	-
3	$Pd(OAc)_2$	dppf (5)	iPr_2NH	CH_3CN	-	2	0	60	-
4	$PdCl_2$	(±)-BINAP (5)	iPr_2NH	CH_3CN	-	2	0	56	-
5	$PdCl_2$	dppe (5)	iPr_2NH	CH_3CN	-	2	0	33	-
6	$PdCl_2$	dppp (5)	iPr_2NH	CH_3CN	-	2	0	29	-
7	$PdCl_2$	PCy_3 (10)	iPr_2NH	CH_3CN	-	2	0	43	-
8	$PdCl_2$	P(*o*-tol)$_3$(10)	iPr_2NH	CH_3CN	-	2	0	46	-
9	$PdCl_2$	PPh_3 (10)	iPr_2NH	CH_3CN	-	2	0	87	-
10	$PdCl_2$	PPh_3 (10)	Et_2NH	CH_3CN	-	2	0	63	-
11	$PdCl_2$	PPh_3 (10)	K_2CO_3	CH_3CN	-	2	40	0	-
12	$PdCl_2$	PPh_3 (10)	Cs_2CO_3	CH_3CN	-	3	77	0	-
13	$PdCl_2$	PPh_3 (10)	Piperidine	CH_3CN	-	3	66	0	-
14	$PdCl_2$	PPh_3 (10)	NaOAc	CH_3CN	-	3	<10	0	-
15	$PdCl_2$	PPh_3 (10)	*t*-$BuNH_2$	CH_3CN	-	3	0	0	-
16	$PdCl_2$	PPh_3 (10)	Et_3N	CH_3CN	-	3	0	0	-
17	$PdCl_2$	PPh_3 (10)	Pyridine	CH_3CN	-	2.5	nd	nd	-
18	$PdCl_2$	PPh_3 (10)	iPr_2NH	MeOH	-	3	62	0	-
19	$PdCl_2$	PPh_3 (10)	iPr_2NH	DMF	-	3	52	0	-
20	$PdCl_2$	PPh_3 (10)	iPr_2NH	Toluene	-	3	46	0	-
21	$PdCl_2$	PPh_3 (10)	iPr_2NH	Dioxane	-	3	31	0	-
22	$PdCl_2$	PPh_3 (10)	iPr_2NH	DMSO	-	3	20	0	-
23	$PdCl_2$	PPh_3 (10)	iPr_2NH	DMA	-	3	41	0	-
24	$PdCl_2$	PPh_3 (10)	iPr_2NH	THF	-	2.5	0	0	-
25	$PdCl_2$	PPh_3 (10)	iPr_2NH	DCE	-	2.5	0	0	-
26	$PdCl_2$	PPh_3 (10)	iPr_2NH	HFIP	-	3	0	0	-
27	$PdCl_2$	-	iPr_2NH	CH_3CN	-	3	46	6	-
28	$PdCl_2$	PPh_3 (20)	iPr_2NH	CH_3CN	-	2	61	0	-
29[c]	$PdCl_2$	PPh_3 (10)	iPr_2NH	CH_3CN	-	2	0	0	
30[d]	$PdCl_2$	PPh_3 (10)	iPr_2NH	CH_3CN	PhSH	8[t]	0	0	9
31[d]	$PdCl_2$	PPh_3 (10)	iPr_2NH	CH_3CN	$PhSO_2NHNH_2$	8[t]	0	0	20
32[d]	$PdCl_2$	PPh_3 (10)	iPr_2NH	CH_3CN	$PhSO_2Cl$	4[t]	0	0	53
33[e]	$PdCl_2$	PPh_3 (10)	iPr_2NH	CH_3CN	$(PhS)_2$	2.5[t]	0	0	70
34[f]	$PdCl_2$	PPh_3 (10)	iPr_2NH	CH_3CN	PhSH	8[t]	0	0	0

[a]Reaction was conducted with 1a (0.5 mmol), 2a (0.75 mmol) and CuI (10 mol%) in 1.5 mL solvent for 2-3 h for first step. [b]Isolated yields are noted. [c]In the absence of CuI. [d]Sulfenylating agents (0.5 mmol) or [e]Sulfenlylated agents (0.25 mmol) and I_2 (10 mol%) were added. [f]Thiophenol was added in the beginning itself. [t]Stand for the second step time.

2. Table S1: Optimization for the reaction condition.

3. Spectral data for substituted sulfenylated indoles (4a-6h)

2-Phenyl-3-(phenylthio)-1H-indole (4a): General procedure was followed for the synthesis of 4a by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by phenyldisulfide (54.5 mg, 0.25 mmol). The reaction time was 4.5 h and pure compound 4a (105 mg, yield: 70%) was obtained as a white semisolid after column chromatography using 2% EtOAc in hexane as eluent. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (s, 1H), 7.73 (dd, *J* = 1.4, 8.4 Hz, 2H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.41 (dd, *J* = 8.0, 7.6 Hz, 3H), 7.38-7.34 (m, 1H), 7.28-7.24 (m, 1H), 7.17 (dd, *J* = 0.8, 7.1 Hz, 1H), 7.14 (d, *J* = 7.1 Hz, 2H), 7.09 (dd, *J* = 1.4, 8.5 Hz, 2H), 7.05-7.03 (m, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 142.1, 139.3, 135.9, 131.4, 131.2, 128.9, 128.8, 128.7, 128.1, 125.6, 124.7, 123.4, 121.2, 120.0, 111.2, 99.5. HRMS (ESI^+): m/z: $[M+H]^+$ calculated for $C_{20}H_{16}NS$: 302.1003, found: 302.0996.

2-Phenyl-3-(p-tolylthio)-1H-indole (4b): General procedure was followed for the synthesis of 4b by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1, 2-di-*p*-tolyldisulfide (61.5 mg, 0.25 mmol). The reaction time was 4.5 h and pure compound 4b (90 mg, yield: 59%) was obtained as a pale-yellow thick liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (s, 1H), 7.74 (dd, *J* = 1.5, 6.9 Hz, 2H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.43-7.39 (m, 3H), 7.35 (m, 1H), 7.25 (dd, *J* = 1.1, 7.0 Hz, 1H), 7.15 (dd, *J* = 1.2, 7.1 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 2.23 (s, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 141.9, 135.9, 135.6, 134.4, 131.5, 131.3, 129.6, 128.8, 128.7, 128.2, 125.8, 125.3, 121.2, 120.1, 111.2, 100.0, 20.9. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{21}H_{18}NS$: 316.1160, found: 316.1153.

3-((4-Chlorophenyl)thio)-2-phenyl-1H-indole (4c): General procedure was followed for the synthesis of 4c by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75mmol) followed by 1,2-bis(4-chlorophenyl)disulfide (72 mg, 0.25 mmol). The reaction time was 5 h and pure compound 4c (106 mg, yield: 63%) was obtained as a pale-yellow thick liquid after column chromatography using 3% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 7.74 (dd, *J* = 1.6, 8.0 Hz, 2H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.48-7.47 (m, 1H), 7.45-7.44 (m, 2H), 7.42-7.38 (m, 1H), 7.32-7.28 (m, 1H), 7.20 (dd, *J* = 1.0, 7.0 Hz, 1H), 7.13 (dd, *J* = 2.0, 6.6 Hz, 2H), 7.01 (dd, *J* = 2.1, 6.6 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 141.1, 136.8, 134.8, 130.2, 129.9, 129.4, 127.9, 127.8, 127.1, 125.8, 122.5, 120.3, 118.8, 110.2, 97.9. HRMS (ESI^-): *m/z:* $[M-H]^-$ calculated for $C_{20}H_{13}ClNS$: 334.0457, found: 334.0461.

3-((4-Bromophenyl)thio)-2-phenyl-1H-indole (4d): General procedure was followed for the synthesis of 4d by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(4-bromophenyl)disulfide (94 mg, 0.25 mmol). The reaction time was 5 h and pure compound 4d (114 mg, yield: 60%) was obtained as a pale-yellow thick liquid after column chromatography using 3% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.48 (s, 1H), 7.64 (dd, *J* = 1.6, 8.0 Hz, 2H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.37 (dd, *J* = 7.2, 7.3 Hz, 3H), 7.32 (d, *J* = 7.0 Hz, 1H), 7.22 (dd, *J* = 0.9, 7.0 Hz, 1H), 7.18 (dd, *J* = 1.7, 6.5 Hz, 2H), 7.10 (dd, *J* = 0.8, 7.9 Hz, 1H), 6.87 (dd, *J* = 2.0, 6.8 Hz, 2H). ^{13}C{1H} NMR (100 MHz, $CDCl_3$): δ 141.2, 137.6, 134.8, 130.7, 130.2, 129.9, 127.8, 127.1, 126.1, 122.5, 120.3, 118.8, 117.1, 110.2, 97.8. HRMS (ESI^+): *m/z:* $[M-H]^+$ calculated for $C_{20}H_{13}BrNS$: 377.9952, found: 377.9956.

3-((4-Fluorophenyl)thio)-2-phenyl-1H-indole (4e): General procedure was followed for the synthesis of 4e by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(4-fluorophenyl)disulfide (63.5 mg, 0.25 mmol).The reaction time was 4 h and pure compound 4e (91 mg, yield: 57%) was obtained as yellowish viscous liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (s, 1H),

7.71 (dd, *J* = 7.00 Hz, 2H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.43-7.34 (m, 4H), 7.24 (dd, *J* = 7.0, 8.1 Hz, 1H), 7.16 (dd, *J* = 7.2, 7.2 Hz, 1H), 7.05-7.02 (m, 2H), 6.83 (dd, *J* = 8.7, 8.8 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 160.8 (d, J^1 = 242.3 Hz), 141.9, 135.8, 134.1 (d, J^5= 3.0 Hz), 131.4, 131.0, 128.8 (d, J^4 = 3.1 Hz), 128.1, 127.4 (d, J^3= 7.7 Hz), 123.5, 121.3, 119.9, 116.0, 115.8 (d, J^2 = 21.9 Hz), 111.2, 100.0. ^{19}F NMR (375 MHz, $CDCl_3$): δ -118.5. HRMS (ESI^+): m/z: $[M+H]^+$ calculated for $C_{20}H_{15}FNS$: 320.0909, found: 320.0909.

2-Phenyl-3-((4-(trifluoromethyl)phenyl)thio)-1H-indole (4f): General procedure was followed for the synthesis of 4f by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(4-(trifluoromethyl)phenyl)disulfide (89 mg, 0.25 mmol). The reaction time was 3.5 h and pure compound 4f (101 mg, yield: 55%) was obtained as viscous liquid after column chromatography using 2% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.62 (s, 1H), 7.72 (dd, *J* = 1.6, 8.0 Hz, 2H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.47 (dd, *J* = 8.1, 8.5 Hz, 2H), 7.42-7.38 (m, 4H), 7.30 (m, 1H), 7.19 (dd, *J* = 0.9, 7.9 Hz, 1H), 7.06 (d, *J* = 8.2 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 144.6, 142.5, 135.9, 131.0, 130.8, 129.0, 128.9, 128.1, 126.7 (d, J^2= 25.8 Hz), 125.1, 125.6 (q, J^3 = 3.0 Hz), 124.3 (q, J^1= 215.0 Hz), 123.7, 121.5, 119.7, 111.3, 97.9. ^{19}F NMR (375 MHz, $CDCl_3$): δ -62.2. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{21}H_{15}F_3NS$: 370.0877, found: 370.0883.

3-((2-Bromophenyl)thio)-2-phenyl-1H-indole (4g): General procedure was followed for the synthesis of 4g by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(2-bromophenyl)disulfide (94 mg, 0.25 mmol). The reaction time was 4.5 h and pure compound 4g (108 mg, yield: 50%) was obtained as a white thick liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 7.67 (d, *J* = 6.9 Hz, 2H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.42-7.34 (m, 4H), 7.26 (dd, *J* = 7.2, 8.0 Hz, 1H), 7.15 (dd, *J* = 7.4, 7.6 Hz, 1H), 6.93 (dd, *J* = 7.4, 7.7 Hz, 1H), 6.87 (dd, *J* = 7.6, 7.3 Hz, 1H), 6.84 (d, *J* = 7.8, Hz, 1H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 142.6, 140.3, 136.0, 132.7, 131.1, 130.9, 128.9, 128.1, 127.7, 126.3, 125.7, 123.6, 121.4, 119.9, 111.3, 98.7. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{20}H_{15}BrNS$: 380.0108, found: 380.0107.

3-((2-Chlorophenyl)thio)-2-phenyl-1H-indole (4h): General procedure was followed for the synthesis of 4h by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(2-bromophenyl)disulfide (71 mg, 0.25 mmol). The reaction time was 4 h and pure compound 4h (113 mg, yield: 57%) was obtained as a white thick liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.57 (s, 1H), 7.69 (dd, *J* = 1.7, 8.3 Hz, 2H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.45-7.41 (m, 2H), 7.41-7.36 (m, 2H), 7.32 (dd, *J* = 1.6, 7.5 Hz, 1H), 7.30-7.25 (m, 1H), 7.19-7.14 (m, 1H), 7.00-6.88 (m, 2H), 6.68 (dd, *J* = 1.6, 7.7 Hz, 1H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 141.6, 137.2, 134.9, 130.1, 130.0, 129.3, 128.4, 127.8, 127.0, 126.0, 125.1, 124.3, 122.5, 120.3, 118.8, 110.2, 96.9. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{20}H_{15}ClNS$: 336.0613, found: 336.0857.

3-((2-Nitrophenyl)thio)-2-phenyl-1H-indole (4i): General procedure was followed for the synthesis of 4i by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(2-nitrophenyl)disulfide (77 mg, 0.25 mmol). The reaction time was 8 h and pure compound 4i (120 mg, yield: 70%) was obtained as a yellowish solid after column chromatography using 5% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (s, 1H), 8.29 (dd, J = 1.5, 8.2 Hz, 1H), 7.71 (dd, J = 1.6, 8.0 Hz, 2H), 7.51 (dd, J = 6.9, 7.4 Hz, 2H), 7.45-7.39 (m, 3H), 7.32-7.28 (m, 1H), 7.26-7.22 (m, 1H), 7.19-7.14 (m, 2H), 7.01 (dd, J = 1.4, 8.1 Hz, 1H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 145.1, 143.1, 140.0, 136.0, 133.6, 130.9, 130.6, 129.1, 129.0, 128.1, 127.7, 126.1, 124.5, 123.8, 121.6, 119.7, 111.4, 98.5. HRMS (ESI^+): m/z: $[M+Na]^+$ calculated for $C_{20}H_{14}N_2O_2SNa$: 369.0674, found: 369.0668.

2-Phenyl-3-((2,4,5-trichlorophenyl)thio)-1H-indole (4j): General procedure was followed for the synthesis of 4j by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(2,4,5-trichlorophenyl)disulfide (106 mg, 0.25 mmol). The reaction time was 5.3 h and pure compound 4j (101 mg, yield: 50%) was obtained as dirty white thick liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.62 (s, 1H), 7.67 (dd, J = 1.7, 8.2 Hz, 2H), 7.56 (d, J = 7.5 Hz, 1H), 7.45 (d, J = 3.9 Hz, 1H), 7.44-7.39 (m, 4H), 7.31 (m, 1H), 7.20 (m, 1H), 6.69 (s, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ δ143.0, 139.1, 136.0, 131.7, 130.8, 130.5, 130.5, 129.2, 129.0, 128.9, 128.7, 128.0, 126.8, 123.9, 121.7, 119.5, 111.5, 96.7. HRMS (ESI$^+$): *m/z*: $[M+H]^+$ calculated for $C_{20}H_{13}Cl_3NS$: 403.9834, found: 403.9826.

3-(naphthalen-1-ylthio)-2-phenyl-1H-indole (4k): General procedure was followed for the synthesis of 4k (95 mg) by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-di(naphthalen-2-yl)disulfide (80 mg, 0.25 mmol). The reaction time was 4.4 h and pure compound 4k (110 mg, yield: 63%) was obtained as white solid after column chromatography using 5% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (s, 1H), 7.84 (dd, J = 1.5, 8.0 Hz, 2H), 7.72 (dd, J = 7.1, 1.9 Hz, 1H), 7.65 (d, J = 8.6 Hz, 2H), 7.55 (dd, J = 1.8, 7.2 Hz, 1H), 7.47 (d, J = 8.1 Hz, 2H), 7.44-7.40 (m, 2H), 7.39-7.33 (m, 3H), 7.32-7.26 (m, 2H), 7.15 (dd, J = 0.9, 7.1 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 142.8, 137.0, 135.9, 133.9, 131.4, 131.3, 131.3, 128.8, 128.8, 128.4, 128.1, 127.7, 126.9, 126.3, 125.0, 124.6, 123.5, 123.0, 121.3, 120.0, 111.2, 99.3. HRMS (ESI$^+$): *m/z*: $[M+H]^+$ calculated for $C_{24}H_{18}NS$: 352.1160, found: 352.1164.

3-((2-Phenyl-1H-indol-3-yl)thio)phenol (4l): General procedure was followed for the synthesis of 4l by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82.2 µL, 0.75 mmol) followed by 3,3'-Dihydroxydiphenyl disulfide (62.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 4l (109 mg, yield: 69%) was obtained as a white thick solid after column chromatography using 12% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (s, 1H), 7.74 (dd, J = 1.6, 8.0 Hz, 2H), 7.62 (d, J = 7.9 Hz, 1H), 7.44 (dd, J = 8.3, 7.6 Hz, 3H), 7.40-7.36 (m, 1H), 7.3 (dd, J = 1.2, 7.0 Hz, 1H), 7.20-7.16 (m, 1H), 7.05 (dd, J = 7.8, 7.9 Hz, 1H), 6.74-6.72 (m, 1H), 6.54-6.50 (m, 2H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 156.1, 142.2, 141.1, 135.8, 131.4, 131.2, 129.9, 128.8, 128.8, 128.1, 123.4, 121.2, 120.0, 118.1, 112.2, 111.9, 118.1, 112.2, 111.9, 111.2, 99.1. HRMS (ESI$^+$): *m/z:* $[M+H]^+$ calculated for $C_{20}H_{16}NS$: 302.1003, found: 302.0996.

2-Phenyl-3-(pyrimidin-2-ylthio)-1H-indole (4m): General procedure was followed for the synthesis of 4m by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-di(pyrimidin-2-yl)disulfide (55.5 mg, 0.25 mmol). The reaction time was 6 h and pure compound 4m (100 mg, yield: 65%) was obtained as a white solid after column chromatography using 20% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (s, 1H), 8.43 (d, J = 4.8 Hz, 2H), 7.73 (dd, J = 1.6, 8.3 Hz, 2H), 7.61 (d, J = 7.9 Hz, 1H), 7.42-7.34 (m, 4H), 7.23 (m, 1H), 7.16 (dd, J = 1.0, 8.0 Hz, 1H), 6.91 (dd, J = 4.8, 4.8 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 173.5, 157.6, 135.8, 131.5, 131.1, 128.7, 128.7, 128.3, 123.3, 121.1, 119.7, 116.8, 111.4, 97.7. HRMS (ESI$^-$): *m/z*: $[M-H]^-$ calculated for $C_{18}H_{12}N_3S$: 302.0752, found: 302.0766.

2-Phenyl-3-(pyridin-4-ylthio)-1H-indole (4n): General procedure was followed for the synthesis of 4n (91 mg) by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1, 2-di(pyridin-4-yl)disulfide (55 mg, 0.25 mmol). The reaction time was 6.5 h and pure compound 4n (91 mg, yield: 60%) was obtained as a creamy solid after column chromatography using 15% EtoAc in hexane as eluent. ^{1}H NMR (400 MHz, DMSO-d_6): δ 12.25 (s, 1H), 8.29 (d, J = 4.9 Hz, 2H), 7.81 (dd, J = 1.4, 7.1 Hz, 2H), 7.57 (d, J = 8.1 Hz, 1H), 7.50 (dd, J = 7.2, 7.7 Hz, 2H), 7.42 (dd, J = 7.2, 7.5 Hz, 2H), 7.26 (dd, J = 1.0, 8.1 Hz, 1H), 7.13 (dd, J = 7.8, 7.8 Hz, 1H), 6.96 (d, J = 6.1 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ 150.9, 149.8, 143.3, 136.8,

131.3, 130.5, 129.2, 129.1, 128.6, 121.3, 120.0, 118.8, 112.7, 93.9. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{19}H_{15}N_2S$: 303.0956, found: 303.0996.

3-((Furan-2-ylthio)methyl)-2-phenyl-1H-indole (4o): General procedure was followed for the synthesis of 4o by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-bis(furan-2-ylmethyl)disulfide (46 µL, 0.25 mmol). The reaction time was 4.2 h and pure compound 4o (99 mg, yield: 65%) was obtained as a white viscous liquid after column chromatography using 2% EtOAc in hexane as eluent. ^1H NMR (400 MHz, $CDCl_3$): δ 8.35 (s, 1H), 7.72 (dd, *J* = 1.3, 7.7 Hz, 1H), 7.76 (dd, *J* = 1.5, 8.5 Hz, 2H), 7.45-7.41 (m, 2H), 7.40-7.34 (m, 2H) 7.26 (dd, *J* = 1.4, 6.8 Hz, 1H), 7.23-7.20 (m, 1H), 7.19-7.15 (m, 1H), 6.07 (dd, *J* = 1.8, 3.2 Hz, 1H), 5.73 (dd, *J* = 0.6, 3.2 Hz, 1H), 3.86 (s, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 151.3, 141.8, 141.5, 135.6, 131.7, 131.3, 128.5, 128.3, 128.2, 123.0, 120.8, 119.6, 111.0, 110.3, 107.8, 102.1, 32.8. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{19}H_{16}NOS$: 306.0952, found: 306.0941.

3-(Benzylthio)-2-phenyl-1H-indole (4p): General procedure was followed for the synthesis of 4p by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-dibenzyldisulfide (61.5 mg, 0.25 mmol). The reaction time was 4.5 h and pure compound 4p (83 mg, yield: 53%) was obtained as a white thick liquid after column chromatography using 2% EtOAc in hexane as eluent. ^1H NMR (500 MHz, $CDCl_3$): δ 8.27 (s, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 6.7 Hz, 2H), 7.37 (dd, *J* = 3.5, 7.9 Hz, 2H), 7.34 (m, 2H), 7.26-7.23 (m, 1H), 7.22-7.19 (m, 1H), 7.07 (dd, *J* = 1.5, 7.0 Hz, 3H), 6.95 (dd, *J* = 1.5, 6.7 Hz, 2H), 3.85 (s, 2H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 141.4, 138.3, 135.6, 131.7, 131.3, 128.9, 128.4, 128.3, 128.2, 128.1, 126.7, 123.0, 120.8, 119.7, 111.1, 102.4, 40.6. HRMS (ESI^-): *m/z:* $[M-H]^-$ calculated for $C_{21}H_{16}NS$: 314.1004, found: 314.1018.

2-Phenyl-3-(propylthio)-1H-indole (4q): General procedure was followed for the synthesis of 4q by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-dipropyldisulfide (39 µL, 0.25 mmol). The reaction time was 6.5 h and pure compound 4q (73 mg, yield: 55%) was obtained as a white thick liquid after column chromatography using 2% EtOAc in hexane as eluent. ^1H NMR (400 MHz, $CDCl_3$): δ 8.19 (s, 1H), 7.76 (dd, *J* = 1.4, 8.2 Hz, 2H), 7.74 (dd, *J* = 7.3, 1.8 Hz, 1H), 7.38 (dd, *J* = 7.2, 7.7 Hz, 2H), 7.31-7.25 (m, 2H), 7.17-7.10 (m, 2H), 2.55 (t, *J* = 7.2 Hz, 2H), 1.35 (m, 2H), 0.74 (t, *J* = 7.3 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 140.6, 135.7, 132.1, 131.7, 128.7, 128.3, 128.3, 123.0, 120.7, 119.9, 111.1, 103.6, 38.5, 23.1, 13.2. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{17}H_{18}NS$: 268.1160, found: 268.1145.

***S*-(2-Phenyl-1H-indol-3-yl)-D-cysteine (4r):** General procedure was followed for the synthesis of 4r by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-dipropyldisulfide (60 mg, 0.25 mmol). The reaction time was 7 h and pure compound 4r (56 mg, yield: 22%) was obtained as a white solid after crystallization in dichloromethane. ^1H NMR (400 MHz, DMSO-d_6): δ 11.95 (s, 1H), 8.03 (d, *J* = 7.6 Hz, 2H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.52 (dd, *J* = 7.4, 7.8 Hz, 2H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.41 (m, 2H), 7.18 (dd, *J* = 7.2, 7.6 Hz, 1H), 7.11 (dd, *J* = 7.7, 7.3 Hz, 1H), 3.13 (d, *J* = 10.4 Hz, 2H), 2.86 (t, *J* = 12.4 Hz, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6): δ 160.1, 143.1, 136.5, 131.2, 131.1, 129.3, 129.0, 128.6, 128.5, 128.2, 125.5, 123.0, 122.0, 120.7, 120.5, 119.4, 112.2, 101.9, 51.6. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{17}H_{17}N_2O_2S$: 313.1010, found: 313.1135.

3-(Phenylthio)-2-(*p*-tolyl)-1H-indole (5a): General procedure was followed for the synthesis of 5a by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with 1-ethynyl-4-methylbenzene (94 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 4 h and pure compound 5a (91 mg, yield: 58%) was obtained as a pale yellowish color thick liquid after column chromatography using 3% EtOAc in hexane as eluent. ^1H NMR (400 MHz, $CDCl_3$): δ 8.52 (s, 1H),

7.65 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.28-7.23 (m, 3H), 7.17-7.13 (m, 3H), 7.10 (dd, *J* = 1.6, 8.6 Hz, 2H), 7.06-7.01 (m, 1H), 2.38 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 142.3, 139.4, 138.8, 135.8, 131.3, 129.5, 128.8, 128.6, 128.0, 125.6, 124.6, 123.2, 121.1, 119.9, 111.1, 99.0, 21.3. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{21}H_{18}NS$: 316.1160, found: 316.1153.

2-(4-Methoxyphenyl)-3-(phenylthio)-1H-indole (5b): General procedure was followed for the synthesis of 5b by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with 1-ethynyl-4-methoxybenzene (97 µL) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 4 h and pure compound 5b (106 mg, yield: 64%) was obtained as pale yellowish thick liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.49 (s, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.24 (dd, *J* = 1.0, 8.2 Hz, 1H), 7.15 (dd, *J* = 7.9, 7.4 Hz, 3H), 7.10 (dd, *J* = 1.3, 8.5 Hz, 2H), 7.05-7.02 (m, 1H), 6.94 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 160.0, 142.2, 139.5, 135.7, 131.3, 129.4, 128.8, 125.5, 124.6, 124.0, 123.1, 121.1, 119.8, 114.3, 111.0, 98.4, 55.4. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{21}H_{18}NOS$: 332.1109, found: 332.1101.

4-(3-(Phenylthio)-1H-indol-2-yl)benzonitrile (5c): General procedure was followed for the synthesis of 5c by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with 4-ethynylbenzonitrile (100.5 mg, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 10 h and pure compound 5c (106 mg, yield: 70%) was obtained as yellowish solid after column chromatography using 8% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (s, 1H), 7.95 (d, *J* = 8.3 Hz, 2H), 7.75 (d, *J* = 8.3 Hz, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.37 (dd, *J* = 7.8, 7.6 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.13-7.12 (m, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 139.2, 138.3, 136.3, 135.8, 132.5, 131.1, 129.0, 128.5, 125.7, 125.1, 124.4, 121.7, 120.4, 118.6, 111.8, 111.5, 102.1. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{21}H_{15}N_2S$: 327.0956, found: 327.0948.

2-Butyl-3-(phenylthio)-1H-indole (5e): General procedure was followed for the synthesis of 5e by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with hex-1-yne (86 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 5e (64 mg, yield: 52%) was obtained as a pale yellowish color thick liquid after column chromatography using 3% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (s, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.13 (m, 1H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.11, (d, *J* = 7.9 Hz, 1H), 7.04-7.00 (m, 3H), 2.90 (t, *J* = 7.6 Hz, 2H), 1.67-1.59 (m, 2H), 1.37-1.31 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 145.5, 139.6, 135.5, 130.3, 128.6, 125.5, 124.5, 122.2, 120.7, 119.1, 110.8, 98.9, 31.6, 26.2, 22.4, 13.8. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{18}H_{20}NS$: 282.1316, found: 282.1305.

2-(3-Chloropropyl)-3-(phenylthio)-1H-indole (5f): General procedure was followed for the synthesis of 5f by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with 5-chloropent-1-yne (80 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 5f (64 mg, yield: 50%) was obtained as a pale yellow thick liquid after column chromatography using 3% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (s, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.21 (dd, *J* = 1.1, 7.0 Hz, 1H), 7.13 (dd, *J* = 6.6, 7.3 Hz, 3H), 7.03 (dd, *J* = 6.9, 8.3 Hz, 3H), 349 (t, *J* = 6.3 Hz, 2H), 3.09 (t, *J* = 7.2 Hz, 2H), 2.09 (m, 2H). $^{13}C\{1H\}$ NMR (125 MHz, $CDCl_3$): δ 143.3, 139.3, 135.5, 130.3, 128.7, 125.5, 124.6, 122.5, 120.9, 119.2, 111.0, 99.7, 44.3, 32.1, 23.7. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{17}H_{17}ClNS$: 302.0770, found: 302.0762.

2-Cyclohexyl-3-(phenylthio)-1H-indole (5g): General procedure was followed for the synthesis of 5g by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with ethynyl cyclohexane (98 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 5g (76 mg, yield: 50%) was obtained as a pale yellow thick liquid after column chromatography using 1% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (s, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.21 (m, 1H), 7.14-7.09 (m, 3H), 7.03-7.00 (m, 3H), 3.25-3.18 (m, 1H), 1.92 (d, J = 12.0, Hz, 2H), 1.85-1.75 (m, 4H), 1.50 (m, 2H), 1.43 (dd, J = 9.6, 7.6 Hz, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 149.8, 139.6, 135.3, 130.2, 128.6, 125.4, 124.4, 122.1, 120.7, 119.1, 110.8, 97.4, 35.9, 33.0, 26.4, 26.0. HRMS (ESI$^+$): *m/z*: $[M+H]^+$ calculated for $C_{20}H_{22}NS$: 308.1473, found: 308.1462.

2-Cyclopropyl-3-(phenylthio)-1H-indole (5h): General procedure was followed for the synthesis of 5h by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with ethynylcyclopropane (63 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 5h (70 mg, yield: 53%) was obtained as a pale yellow thick liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (s, 1H), 7.52 (d, J = 7.2 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.18 (dd, J = 7.1, 6.9 Hz, 1H), 7.15 (d, J = 1.3 Hz, 1H), 7.13 (dd, J = 4.6, 4.0 Hz, 1H), 7.11-7.07 (m, 2H), 7.06-7.01 (m, 2H), 2.40-2.33 (m, 1H), 1.10-1.05 (m, 2H), 0.91-0.87 (m, 2H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 145.8, 139.5, 134.9, 128.7, 125.5, 124.6, 122.2, 120.8, 118.7, 110.6, 99.4, 08.3, 07.9. HRMS (ESI$^+$): *m/z*: $[M+H]^+$ calculated for $C_{17}H_{16}NS$: 266.1003, found: 266.0992.

Ethyl 3-(phenylthio)-1H-indole-2-carboxylate (5i): General procedure was followed for the synthesis of 5i by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with ethyl propiolate (76 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 5i (90 mg, yield: 61%) was obtained as white solid after column chromatography using 5% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.26 (s, 1H), 7.61 (dd, J = 8.2, 8.2 Hz, 1H), 7.45 (d, J = 8.3 Hz, 1H), 7.36 (m, 1H), 7.18 (d, J = 4.3 Hz, 4H), 7.14 (dd, J = 0.9, 7.0 Hz, 1H), 7.10-7.06 (m, 1H), 4.39 (q, J = 7.1 Hz, 2H), 1.31 (t, J = 7.1 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 161.3, 137.9, 135.7, 130.1, 128.8, 128.7, 127.3, 126.1, 125.3, 121.8, 121.5, 112.1, 110.6, 61.5, 14.2. HRMS (ESI$^+$): *m/z*: $[M+H]^+$ calculated for $C_{17}H_{16}NO_2S$: 298.0901, found: 298.0897.

3-(Phenylthio)-1H-indole-2-carboxylic acid (5j): General procedure was followed for the synthesis of 5j by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with 4-ethynylbenzoic acid (46.3 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 4 h and pure compound 5j (91 mg, yield: 67%) was obtained as a white solid after column chromatography using 20% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.74 (s, 1H), 9.03 (s, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.1 Hz, 1H), 7.47 (d, J = 8.3 Hz, 1H), 7.38 (d, J = 7.4 Hz, 1H), 7.35-7.30 (m, 2H), 7.17-7.16 (m, 2H), 7.14 (d, J = 7.8 Hz, 1H). ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6): δ 163.6, 137.6, 129.4, 128.4, 127.2, 126.7, 125.2, 122.5, 120.8, 112.9, 108.4. HRMS (ESI$^+$): *m/z*: $[M+H]^+$ calculated for $C_{15}H_{12}NO_2S$: 270.0583, found: 270.0570.

6-Chloro-2-phenyl-3-(phenylthio)-1H-indole (6a): General procedure was followed for the synthesis of 6a by the reaction of 5-chloro-2-iodoaniline (126 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 6a (96 mg, yield: 57%) was obtained as a pale yellow thick liquid after column chromatography using 2% EtOAc in hexane as eluent. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.53 (s, 1H), 7.72 (d, J = 7.0 Hz, 2H), 7.52 (d, J = 8.4 Hz, 1H), 7.45-7.41 (m, 3H), 7.40-7.37 (m, 1H), 7.18-7.15 (m, 2H), 7.12 (dd, J = 1.6, 8.4 Hz, 1H), 7.08-7.04 (m, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 142.6, 138.8, 136.1, 131.0, 129.8, 129.2, 129.0, 128.9, 128.9, 128.1, 125.6, 124.9, 122.0, 121.0, 111.2, 99.9. HRMS (ESI$^+$): *m/z:* $[M+H]^+$ calculated for $C_{20}H_{15}ClNS$: 336.0613, found: 336.0614.

6-Fluoro-2-phenyl-3-(phenylthio)-1H-indole (6b): General procedure was followed for the 6b by the reaction of 5-fluoro-2-iodoaniline (118.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 6b (101 mg, yield: 63%) was obtained as a pale yellow thick liquid after column chromatography using 4% EtOAc in hexane as eluent. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.54 (s, 1H), 7.74 (d, J = 7.2 Hz, 2H), 7.52 (dd, J = 5.2, 8.6 Hz, 1H), 7.43 (dd, J = 7.0, 7.7 Hz, 2H), 7.37 (dd, J = 7.2, 7.3 Hz, 1H), 7.16 (dd, J = 7.9, 7.4 Hz, 2H), 7.14 (dd, J = 2.0, 9.2 Hz, 1H), 7.09-7.04 (m, 3H), 6.94-6.89 (m, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 160.6 (d, J^1= 238.2 Hz), 142.4, 138.9, 135.8, 135.7 (d, J^4= 12.5 Hz), 131.2, 128.9 (d, J^6= 3.6 Hz) 128.8, 128.0, 127.6, 125.6, 124.8, 121.0 (d, J^5= 10.0 Hz), 110.0 (d, J^3 = 24.3 Hz) 99.7, 97.7 (d, J^2 = 26.3 Hz). ^{19}F NMR (375 MHz, $CDCl_3$): δ -119.0. HRMS (ESI$^+$): *m/z:* [M+H]$^+$ calculated for $C_{20}H_{15}FNS$: 320.0909, found: 320.0909.

5-Chloro-2-phenyl-3-(phenylthio)-1H-indole (6c): General procedure was followed for the synthesis of 6c by the reaction of 4-chloro-2-iodoaniline (126 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 6c (109 mg, yield: 65%) was obtained as a pale-yellow color thick liquid after column chromatography using 2% EtOAc in hexane as eluent. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.57 (s, 1H), 7.72 (d, J = 7.0 Hz, 2H), 7.60 (d, J = 1.9 Hz, 1H), 7.42 (dd, J = 6.8, 7.6 Hz, 2H), 7.38 (dd, J = 7.0, 7.4 Hz, 1H), 7.34 (d, J = 8.5 Hz, 1H), 7.20 (dd, J = 1.9, 8.5 Hz, 1H), 7.17 (dd, J = 8.5, 6.9 Hz, 2H), 7.06 (dd, J = 7.4, 7.3 Hz, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.4, 143.4, 138.8, 134.2, 132.5, 131.0, 129.1, 129.0, 128.9, 128.1, 127.1, 125.6, 124.9, 123.8, 119.4, 112.3, 99.3. HRMS (ESI$^+$): *m/z:* [M+H]$^+$ calculated for $C_{20}H_{15}ClNS$: 336.0613, found: 336.0611.

5-Fluoro-2-phenyl-3-(phenylthio)-1H-indole (6d): General procedure was followed for the synthesis of 6d by the reaction of 4-fluoro-2-iodoaniline (118.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 6d (85 mg, yield: 53%) was obtained as a pale yellow thick liquid after column chromatography using 2% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 7.75 (d, J = 7.1 Hz, 2H), 7.44 (dd, J = 7.0, 7.6 Hz, 2H), 7.38 (d, J = 7.1 Hz, 1H), 7.37 (dd, J = 4.0, 8.6 Hz, 1H), 7.27 (dd, J = 2.4, 9.1 Hz, 1H), 7.17 (dd, J = 8.0, 7.3 Hz, 2H), 7.08 (d, J = 7.3 Hz, 2H), 7.06 (d, J = 7.2 Hz, 1H) 7.02-6.98 (m, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 158.8 (d, J^1 = 235.5 Hz), 143.8, 138.8, 132.2 (d, J^4 =12.0 Hz), 131.2, 129.0, 128.9 (d, J^5 = 5.3 Hz), 128.1, 125.6, 124.8, 112.0, 111.8 (d, J^2 = 27.2 Hz), 105.1 (d, J^3 = 24.15 Hz), 99.7. ^{19}F NMR (375 MHz, $CDCl_3$): δ -122.11. HRMS (ESI$^+$): *m/z*: [M+H]$^+$ calculated for $C_{20}H_{15}FNS$: 320.0909, found: 320.0909.

6-Chloro-3-(naphthalen-2-ylthio)-2-phenyl-1H-indole (6e): General procedure was fallowed for the synthesis of 6e by the reaction of 5-chloro-2-iodoaniline (126.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 1,2-di(naphthalen-2-yl)disulfane (79.5 mg, 0.25 mmol). The reaction time was 5 h and pure compound 6e (131 mg, yield: 63%) was obtained as white thick liquid after column chromatography using 3% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (s, 1H), 7.77 (dd, J = 8.3, 1.6 Hz, 2H), 7.72 (dd, J = 6.9, 2.1 Hz, 1H), 7.64 (d, J = 8.7 Hz, 1H), 7.53 (dd, J = 8.8, 1.9 Hz, 2H), 7.45 (d, J = 1.6 Hz, 1H), 7.43-7.41 (m, 2H), 7.39-7.32 (m, 4H), 7.25 (dd, J = 8.6, 1.9 Hz, 1H), 7.10 (dd, J = 8.5, 1.7 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 142.8, 136.5, 136.2, 133.9, 131.4, 131.0, 129.8, 129.1, 129.8, 129.2, 129.0, 128.9, 128.5, 128.1, 127.8, 126.9, 126.5, 125.1, 124.5, 123.1, 122.0, 120.9, 111.3, 99.6. HRMS (ESI$^+$): *m/z:* [M+H]$^+$ calculated for $C_{24}H_{17}ClNS$: 386.0770, found: 386.0769.

6-methyl-2-phenyl-3-(phenylthio)-1H-indole (6g): General procedure was fallowed for the synthesis of 6g by the reaction of 6-methyl-2-iodoaniline (116.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 6.5 h and pure compound 6g (104 mg, yield: 66%) was obtained as white thick liquid after column

chromatography using 1% EtOAc in hexane as eluent.^{1}H NMR (500 MHz, $CDCl_3$): δ 8.43 (s, 1H), 7.73 (d, *J* = 7.2 Hz, 2H), 7.49 (dd, *J* = 8.1 Hz, 1H), 7.41 (dd, *J* = 7.2, 7.7 Hz, 2H), 7.35 (d, *J* = 7.26 Hz, 1H), 7.23 (s, 1H) 7.14 (dd, *J* = 8.0, 7.2 Hz, 2H), 7.09 (d, *J* = 7.25 Hz, 2H), 7.03 (dd, *J* = 7.2 Hz, 1H), 6.99 (d, *J* = 8.05 Hz, 1H), 2.48 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 141.4, 139.4, 136.3, 133.4, 131.6, 129.1, 128.8, 128.5, 128.0, 125.6, 124.6, 122.9, 120.0, 111.1, 99.3, 21.8. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{21}H_{18}NS$: 316.1158, found: 316.1159.

2-(4-methoxyphenyl)-3-(phenylthio)benzofuran (6h): General procedure was followed for the synthesis of 6g by the reaction of 2-iodophenol (110 mg, 0.5 mmol) with 1-ethynyl-4-methoxybenzene (97 µL) followed by phenyl disulfide (54.5 mg, 0.25 mmol). The reaction time was 4 h and pure compound 6g (112 mg, yield: 68%) was obtained as a pale yellowish thick liquid after column chromatography using hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (d, *J* = 9.0 Hz, 2H), 7.53 (d, *J* = 8.2 Hz, 1H), 7.47 (d, *J* = 7.5 Hz, 1H), 7.32-7.28 (m, 1H), 7.22 (d, *J* = 7.0 Hz, 1H), 7.19-7.18 (m, 4H), 7.11-7.08 (m, 1H), 6.97 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ 160.6, 157.9, 153.8, 136.5, 131.1, 129.1, 129.0, 126.8, 125.4, 124.8, 123.4, 122.5, 120.1, 114.1, 111.2, 102.7, 55.4. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{21}H_{17}O_2S$: 333.0949, found: 333.0946.

4. Spectral data for other 3-functionalized indoles (Reaction with other electrophiles)

2-Phenyl-3-(phenylselanyl)-1H-indole (7): General procedure was followed for the synthesis of 7 by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82.2 µL, 0.75 mmol) followed by phenyldiselenide (78.3 mg, 0.25 mmol), instead of disulfide. The reaction time was 4.5 h and pure compound 7 (114 mg, yield: 65%) was obtained as a creamy white color thick liquid after column chromatography using 2% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.50 (s, 1H), 7.72 (dd, *J* = 1.5, 8.1 Hz, 2H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.43 (dd, *J* = 1.0, 7.2 Hz, 3H), 7.39-7.35 (m, 1H), 7.29-7.24 (m, 1H), 7.21-7.19 (dd, *J* = 1.6, 8.1 Hz, 2H), 7.17-7.15 (m, 1H), 7.14-7.06 (m, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 142.1, 136.2, 134.1, 132.1, 129.1, 128.7, 128.5, 128.3, 125.4, 123.3, 121.1, 121.0, 111.0, 95.9. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{20}H_{16}NSe$: 350.0448, found: 350.0433.

3-(2-Nitro-1-phenylethyl)-2-phenyl-1H-indole (8): General procedure was followed for the synthesis of 8 by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by β-nitrostyrene (74.5 mg, 0.5 mmol), instead of disulfide. The reaction time was 3.5 h and the pure compound 8 (85.5 mg, yield: 82%) was obtained as a brown thick liquid after column chromatography using 5% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.46-7.42 (m, 4H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.35-7.30 (m, 3H), 7.28-7.22 (m, 3H), 7.20 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.13-7.09 (m, 1H), 5.32 (t, *J* = 8.1 Hz, 1H), 5.21-5.10 (m, 2H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 139.4, 137.0, 136.1, 132.2, 129.0, 128.8, 128.7, 127.5, 127.2, 127.1, 122.5, 120.3, 120.0, 111.4, 110.0, 79.1, 40.8. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{22}H_{19}N_2O_2$: 365.1266, found: 365.1261.

3, 3'-((4-Methoxyphenyl)methylene)bis(2-phenyl-1H-indole) (9): General procedure was followed for the synthesis of 9 by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by 4-methoxybenzaldehyde (30.3 µL, 0.25 mmol), instead of disulfide. The reaction time was 2.5 h and pure compound 9 (101 mg, yield: 80%) was obtained as a white solid after column chromatography using 20% EtOAc in hexane as eluent. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00 (s, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.19 (dd, *J* = 1.6, 7.4 Hz, 4H), 7.16-7.14 (m, 6H), 7.09-7.06 (m, 3H), 7.03 (d, *J* = 7.7 Hz, 2H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.89-6.88 (m, 1H), 6.84-6.81 (m, 2H), 6.77 (dd, *J* = 2.5, 8.1 Hz, 1H), 6.08 (s, 1H), 3.65 (s, 3H). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 159.7,

146.6, 135.5, 133.1, 129.1, 129.0, 128.3, 127.4, 122.1, 121.8, 121.7, 119.6, 115.6, 115.4, 111.2, 110.5, 55.1, 40.1. HRMS (ESI^+): *m/z*: $[M+Na]^+$ calculated for $C_{36}H_{28}N_2ONa$: 527.2099, found: 527.2092.

3-Iodo-2-phenyl-1H-indole (10): General procedure was followed for the synthesis of 10 by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenyl acetylene (82 µL, 0.75 mmol) followed by iodine (126.5 mg, 0.5 mmol). The reaction time was 3.5 h and pure compound 10 (106 mg, yield: 66%) was obtained as yellow thick liquid after column chromatography using 3% EtOAc in hexane as eluent. ^1H NMR (500 MHz, $CDCl_3$): δ 8.45 (s, 1H), 7.79 (dd, J = 1.3, 8.4 Hz, 2H), 7.52-7.48 (m, 3H), 7.42 (dd, J = 7.3, 7.5 Hz, 1H), 7.36 (d, J = 7.9 Hz, 1H), 7.27 (dd, J = 1.2, 7.1 Hz, 1H), 7.24-7.21 (m, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 136.8, 132.2, 129.3, 128.8, 128.8, 128.6, 128.4, 128.4, 124.7, 123.6, 122.0. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{14}H_{11}IN$: 319.9936, found: 319.9929.

3-Bromo-2-phenyl-1H-indole (11): General procedure was followed for the synthesis of 11 by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82 µL, 0.75 mmol) followed by *N*-bromosuccinamide (88.5 mg, 0.5 mmol). The reaction time was 4 h and pure compound 11 (102 mg, yield: 75%) was obtained as white thick liquid which turn in to greenish solid after column chromatography using 3% EtOAc in hexane as eluent. Note- Decomposition of the (11) was observed in the air so covered it by aluminium foil and stored at 4 °C under N_2 atmosphere. ^1H NMR (500 MHz, $CDCl_3$): δ 8.28 (s, 1H), 7.82-7.77 (m, 2H), 7.49 (dd, J = 7.9, 8.0 Hz, 3H), 7.45-7.41 (m, 1H), 7.39-7.39 (m, 1H), 7.31-7.25 (m, 1H), 7.23-7.19 (m, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 135.3, 134.3, 131.4, 128.9, 128.9, 128.4, 127.7, 123.5, 121.0, 119.6, 111.1, 90.1. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{14}H_{11}BrN$: 272.0075, found: 272.0042.

3-Fluoro-2-phenyl-1H-indole (12): General procedure was followed for the synthesis of 12 by the reaction of 2-iodoaniline (109.5 mg, 0.5 mmol) with phenylacetylene (82.2 µL, 0.75 mmol) followed by selectfluor (177 mg, 0.5 mmol), instead of iodine and disulfide. The reaction time was 4.5 h and pure compound 12 (77 mg, yield: 72%) was obtained as white thick liquid after column chromatography using 2% EtOAc in hexane as eluent. ^1H NMR (500 MHz, $CDCl_3$): δ 7.79 (s, 1H), 7.72 (d, J = 7.4 Hz, 2H), 7.63 (d, J = 7.9 Hz, 1H), 7.47 (dd, J = 7.6, 7.9 Hz, 2H), 7.32 (dd, J = 7.4, 7.2 Hz, 2H), 7.22 (dd, J = 7.3, 7.0 Hz, 1H), 7.15 (dd, J = 7.3, 7.0 Hz, 1H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 140.4 (d, J^1 = 230.0 Hz), 134.8, 132.5 (d, J^2 = 14.8 Hz), 130.4, 130.3, 129.1, 127.5, 125.4, 125.4, 120.4, 117.0, 116.9, 111.3, 111.3. ^{19}F NMR (375 MHz, $CDCl_3$): δ -170.4. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{14}H_{11}FN$: 212.0875, found: 212.0866.

5. Synthetic Application of 3-Sulfenylindoles

Ethyl 1-oxo-9-(phenylthio)-2,3-dihydro-1H-pyrrolo[1,2-a]indole-2-carboxylate (13): To a solution of ethyl 3-(phenylthio)-1H-indole-2-carboxylate 5i (148.5 mg, 0.5 mmol) and potassium *tert*-butoxide (112 mg, 1.0 mmol) in THF (3 mL), ethyl acrylate (106.5 µL, 1 mmol) was added dropwise and refluxed for 3 h. The reaction mixture was diluted with water and extracted with ethyl acetate (3x10 mL), dried over sodium sulfate and purified using column chromatography to afford 13 (147 mg, yield: 84%) as greenish yellow thick liquid using 10 % EtOAc in hexane as eluent. ^1H NMR (500 MHz, $CDCl_3$): δ 7.68 (d, J = 8.2 Hz, 1H), 7.47 (d, J = 8.3 Hz, 1H), 7.42 (dd, J = 7.3, 7.6 Hz, 1H), 7.24-7.20 (m, 2H), 7.17 (dd, J = 7.5, 7.8 Hz, 3H), 7.11 (d, J = 7.2 Hz, 1H), 4.84 (m, 1H), 4.63-4.59 (m, 1H), 4.31-4.26 (m, 2H), 4.25-4.23 (m, 1H), 1.33 (t, J = 7.1 Hz, 3H). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 184.1, 167.0, 137.0, 135.5, 134.3, 134.2, 128.8, 128.2, 126.4, 125.9, 122.9, 122.6, 111.0, 104.8, 62.5, 56.7, 43.4, 14.2. HRMS (ESI^+): *m/z:* $[M+H]^+$ calculated for $C_{20}H_{18}NO_3S$: 352.1007, found: 352.1012.

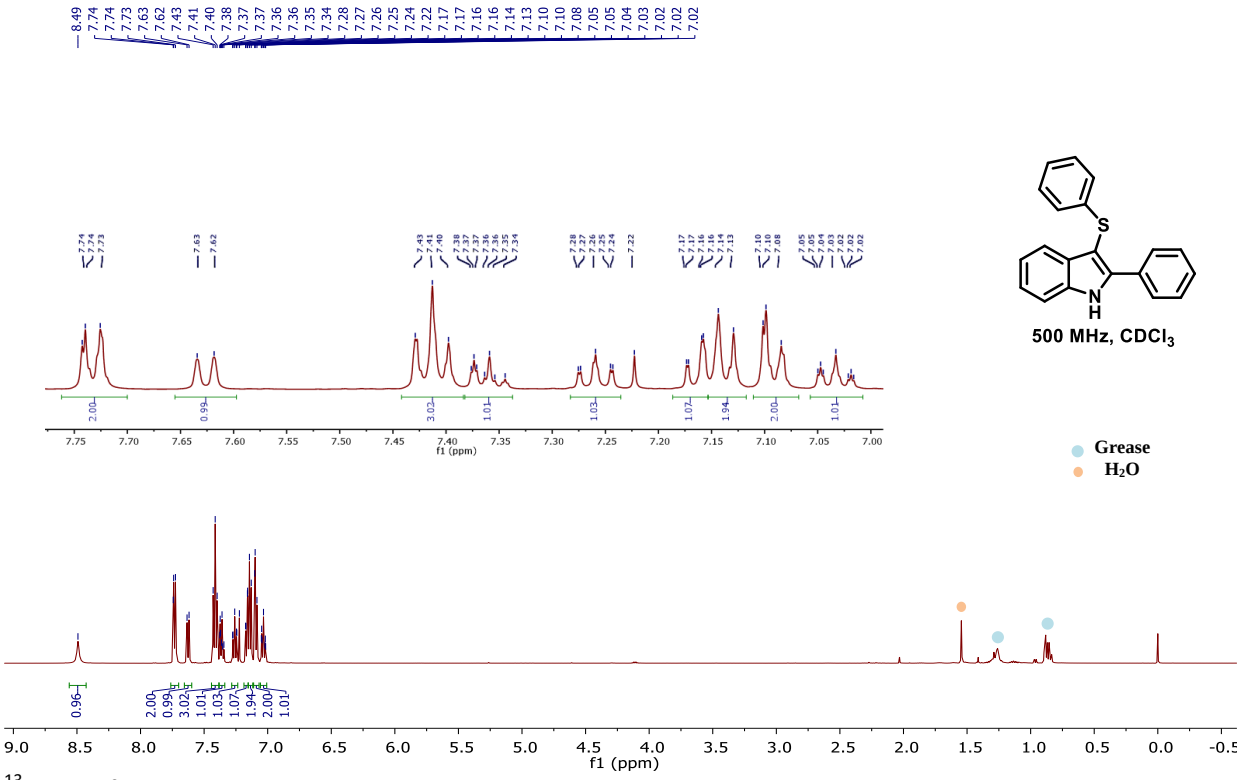
3-(Phenylthio)-1H-indole (14): A solution of ethyl 3-(phenylthio)-1H-indole-2-carboxylate 5i; (148.5 mg, 0.5 mmol) and sodium hydride (24 mg, 1.0 mmol) in toluene (3 mL) was stirred for 30 min. The reaction mixture was diluted with water and extracted with ethyl acetate (3x10 mL), dried over sodium sulfate and purified using column chromatography to afford 14 (108 mg, yield: 96%) as white solid using 5% EtOAc in hexane as eluent. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.39 (s, 1H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.48 (d, *J* = 2.6 Hz, 1H), 7.43 (d, *J* = 8.2 Hz, 1H), 7.27 (dd, *J*= 1.1, 7.1 Hz, 1H), 7.18-7.14 (m, 3H), 7.11-7.08 (m, 2H), 7.06-7.02 (m, 1H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): *δ* 139.2, 136.5, 130.7, 129.1, 128.7, 125.9, 124.8, 123.1, 120.9, 119.7, 102.9. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{14}H_{12}NS$: 226.0690, found: 226.0683.

2-Phenyl-3-(phenylsulfonyl)-1H-indole (15): 2-Phenyl-3-(phenylthio)-1H-indole (4a; 150.5 mg, 0.5 mmol) in 2 mL chloroform was taken in a 25 mL round bottom flask and *m*-perchlorobenzoic acid (262.8 mg, 1.5 mmol) was added portion wise at 0 °C for 3 h. After completion of reaction, $NaHCO_3$ (252 mg, 3 mmol) was added to the reaction mixture and stir at rt. for next 30 min. Now, solid was filtered off and filtrate was washed with water (3x10 mL). Organic layer was dried over Na_2SO_4 and concentrated to afford 15 (128 mg, yield: 77%) as a white solid after column chromatography. ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 9.02 (s, 1H), 8.22 (dd, *J* = 2.4, 5.5 Hz, 1H), 7.65 (dd, *J* = 8.2, 1.0 Hz, 2H), 7.51 (dd, *J* = 8.0, 1.1 Hz, 2H), 7.45-7.41 (m, 1H), 7.39-7.34 (m, 4H), 7.30-7.25 (m, 4H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): *δ* 143.9, 142.8, 134.6, 132.3, 130.2, 130.0, 129.8, 128.7, 128.1, 126.3, 125.9, 123.9, 122.6, 120.7, 112.6, 111.5. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{20}H_{16}NSO_2$: 334.0901, found: 334.0896.

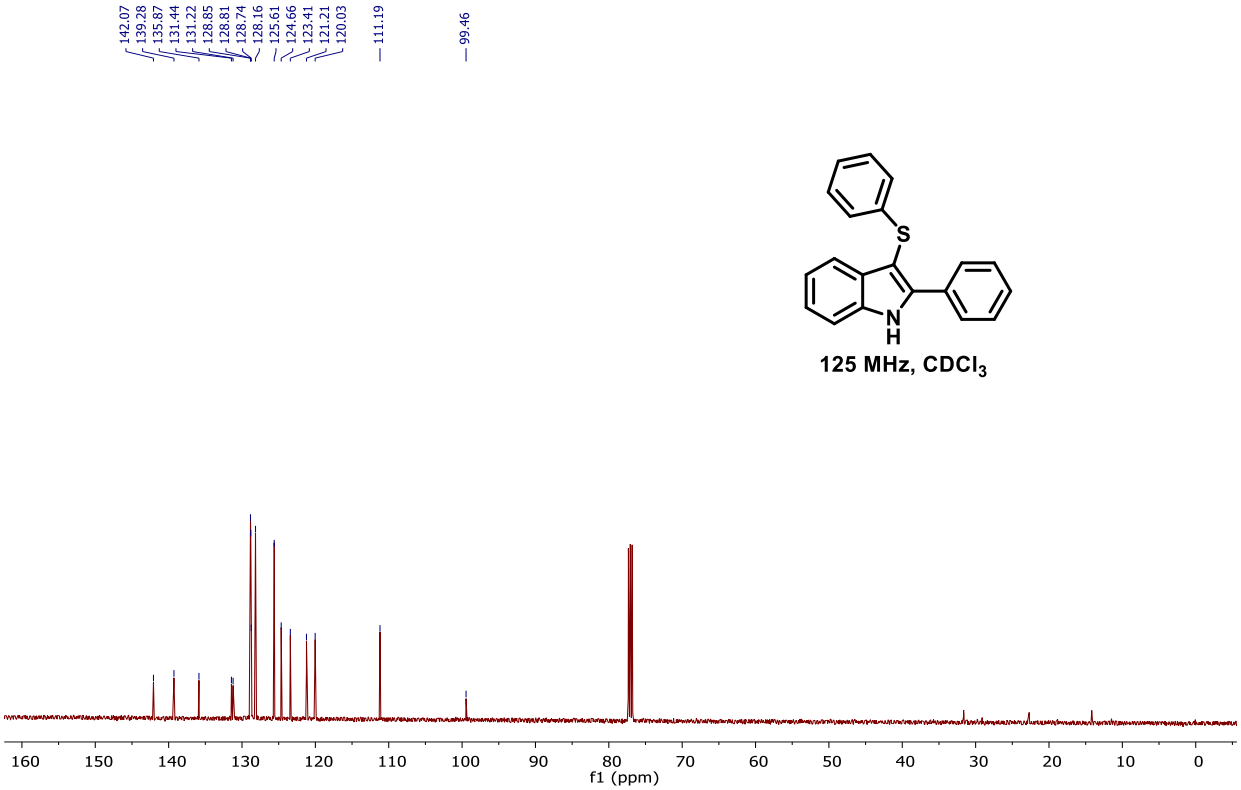
2-Phenyl-3-(phenylsulfinyl)-1H-indole (16): 2-phenyl-3-(phenylthio)-1H-indole (4a; 150.5 mg, 0.5 mmol) in 2 mL dichromethane was taken in a 25 mL round bottom flask and *m*-perchlorobenzoic acid (172.5 mg, 1 mmol) was added portion wise at -10°C for 5 h. After completion of reaction, $NaHCO_3$ (252 mg, 3 mmol) was added in reaction mixture and stirred at rt. for next 30 min. Solid was filtered and filtrate was washed with water (3x10 mL). Organic layer was dried over Na_2SO_4 and concentrated it to afford 16 (134 mg, yield: 86%) as a white solid. ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 9.87 (s, 1H), 8.22 (d, *J* = 7.5 Hz, 4H), 7.43-7.36 (m, 4H), 7.34 (d, *J* = 7.5 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 1H), 7.08 (dd, *J* = 8.1, 8.1 Hz, 1H), 6.90 (dd, *J* = 8.0, 7.3 Hz, 1H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): *δ* 144.4, 143.8, 136.3, 129.9, 129.8, 129.6, 128.9, 128.9, 125.2, 125.0, 123.5, 121.6, 120.1, 112.4, 111.9. HRMS (ESI^+): *m/z*: $[M+H]^+$ calculated for $C_{20}H_{16}NSO$: 318.0952, found: 318.0995.

6. Spectral data

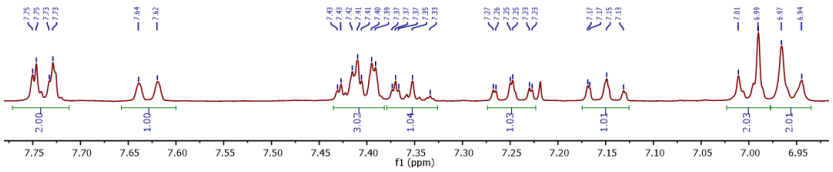
^{1}H NMR for 4a

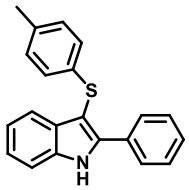


^{13}C NMR for 4a

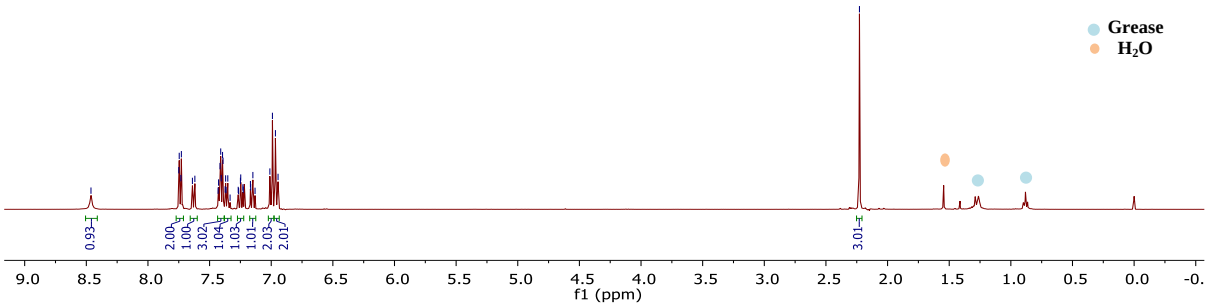


^{1}H NMR for 4b

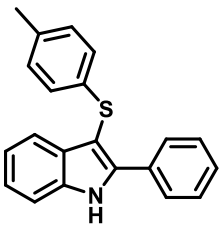




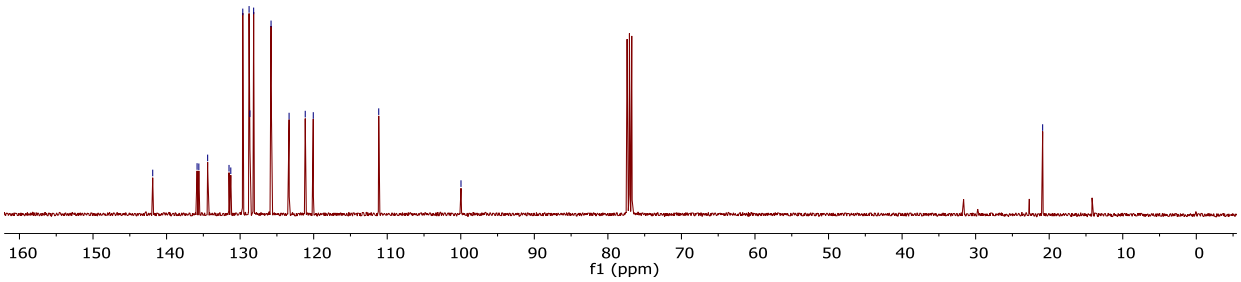
CDCl$_3$, 400 MHz



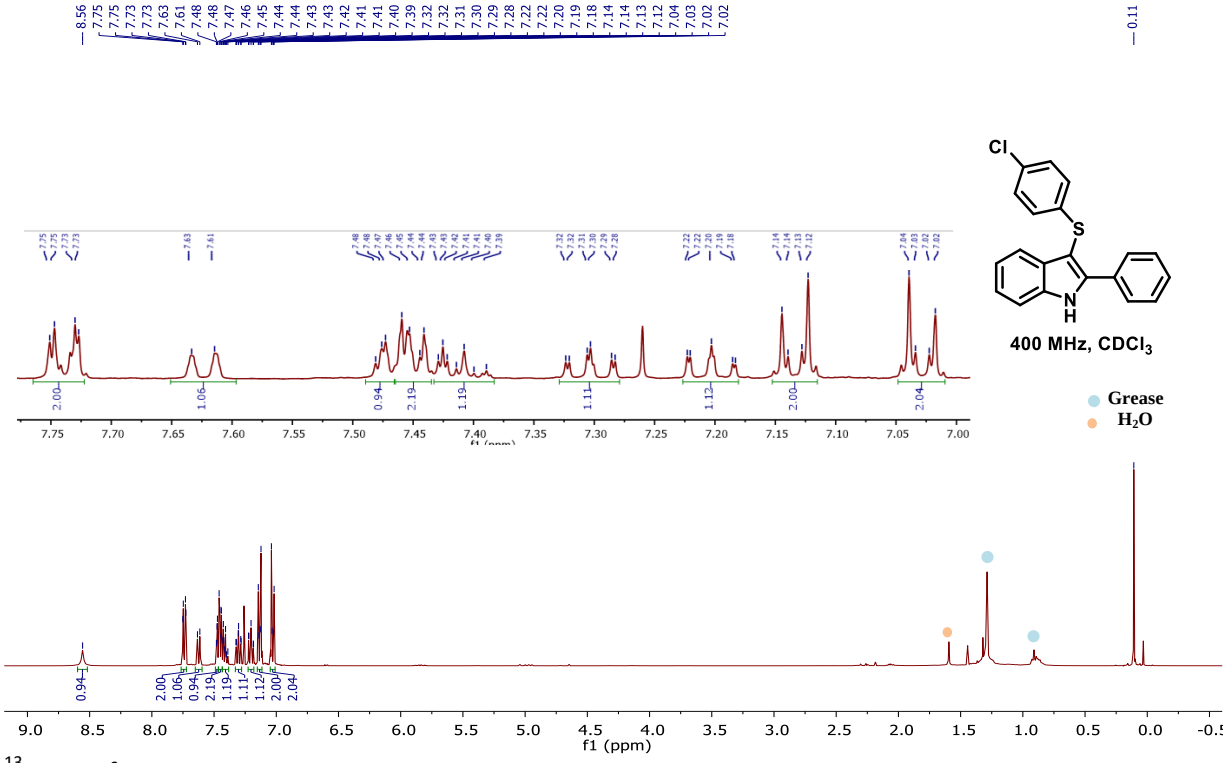
^{13}C NMR for 4b



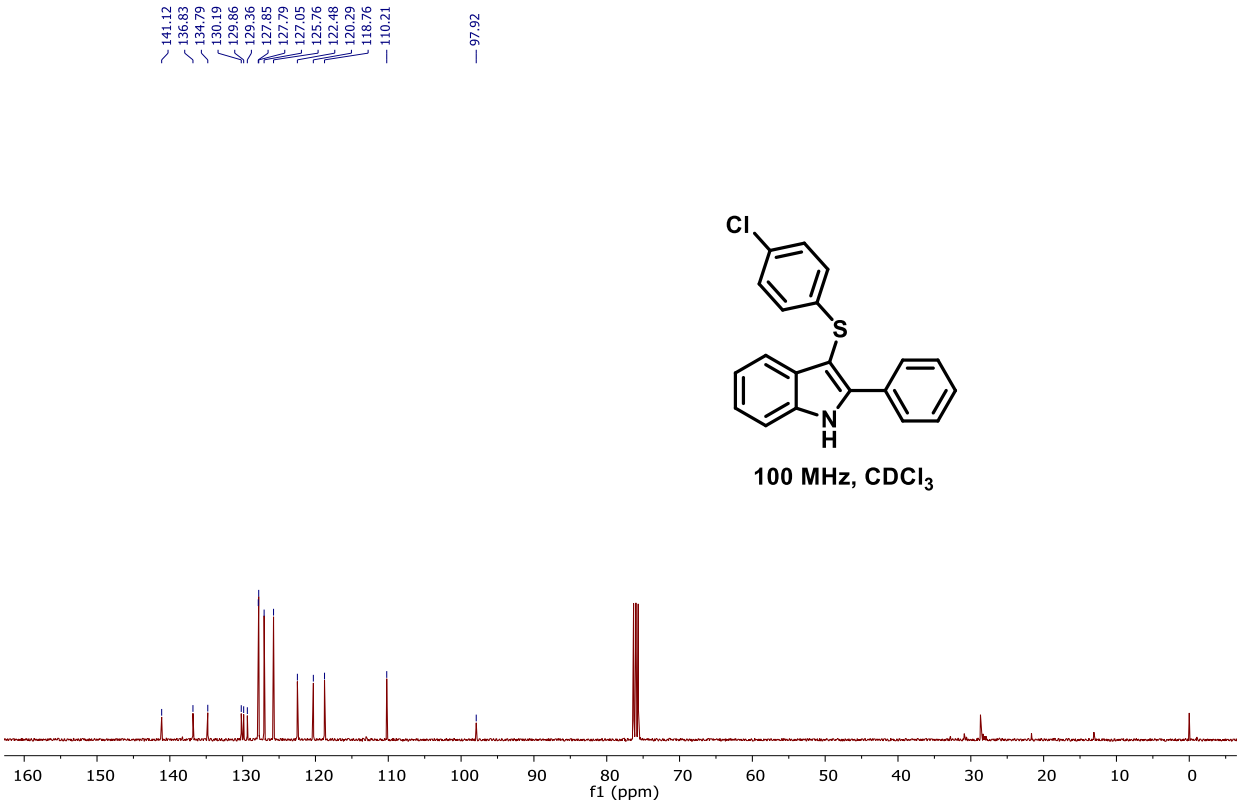
CDCl$_3$, 100 MHz



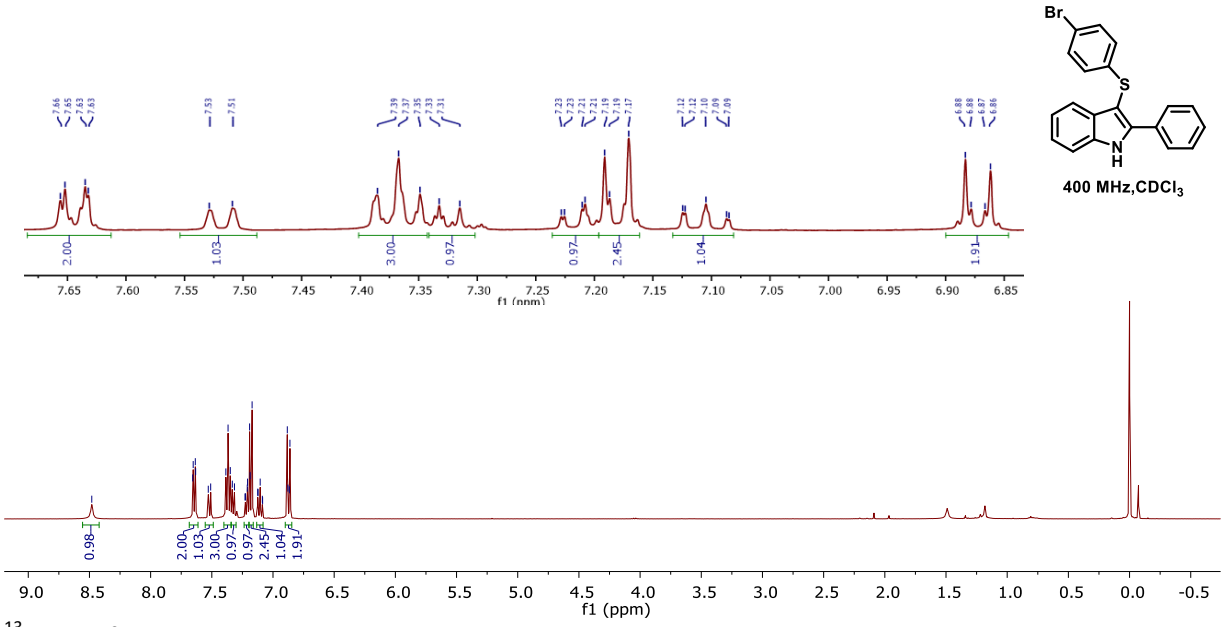
^{1}H NMR for 4c



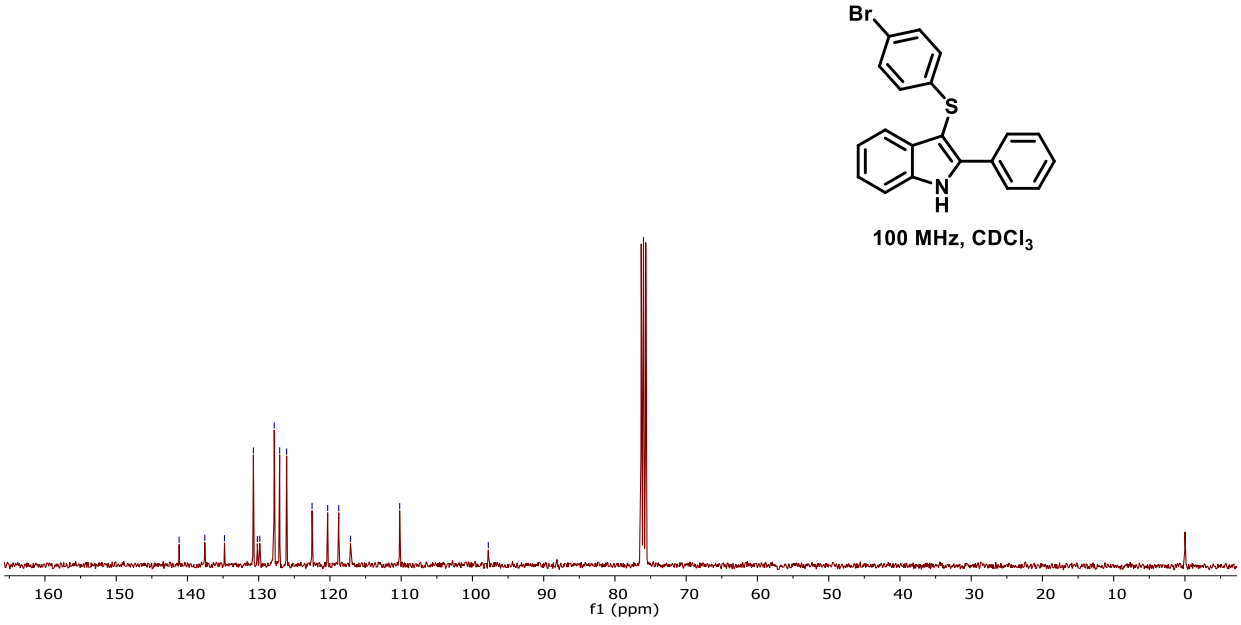
^{13}C NMR for 4c



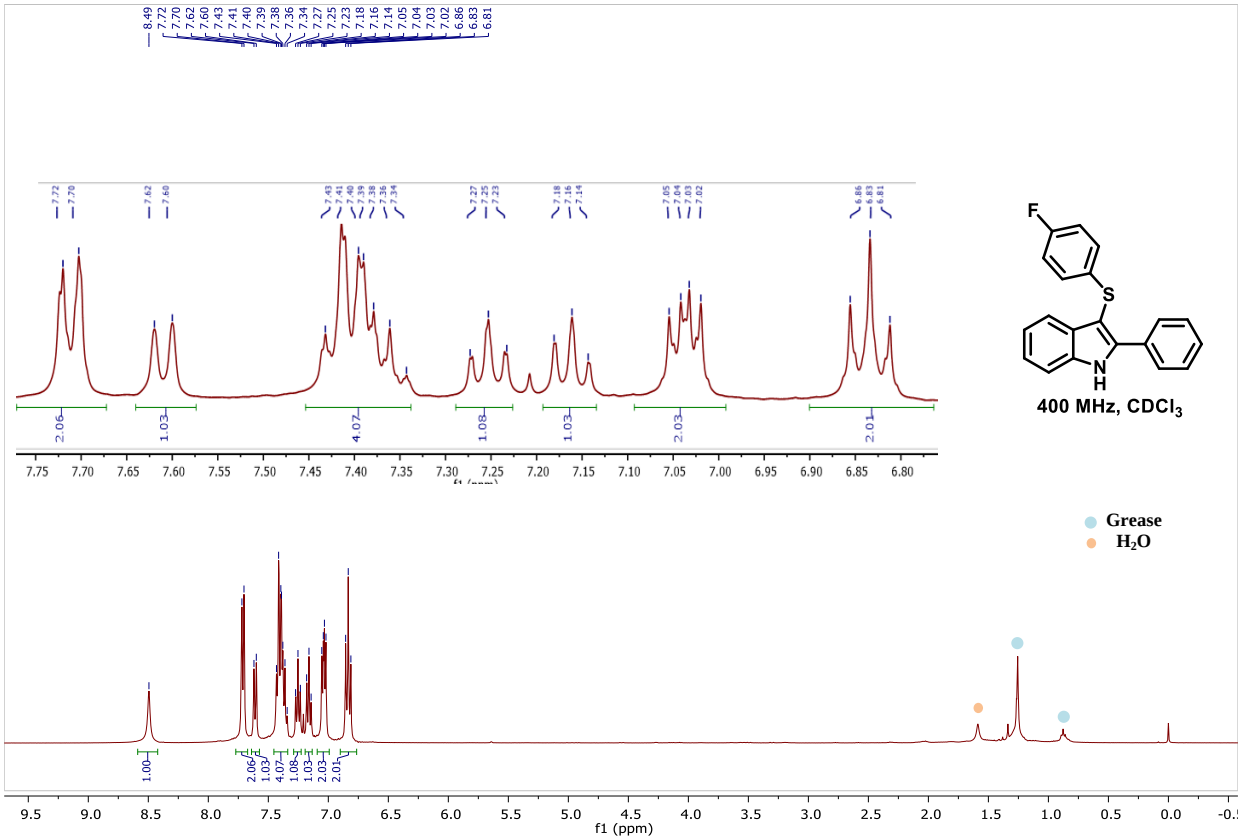
^{1}H NMR for 4d



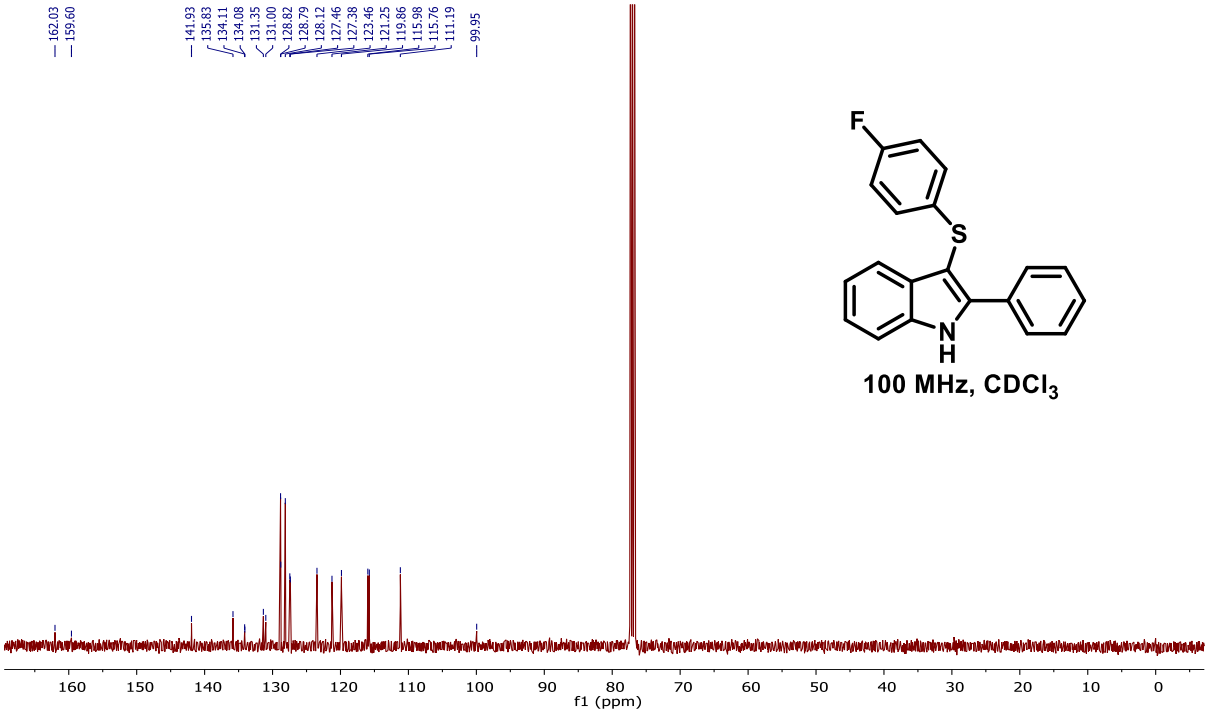
^{13}C NMR for 4d



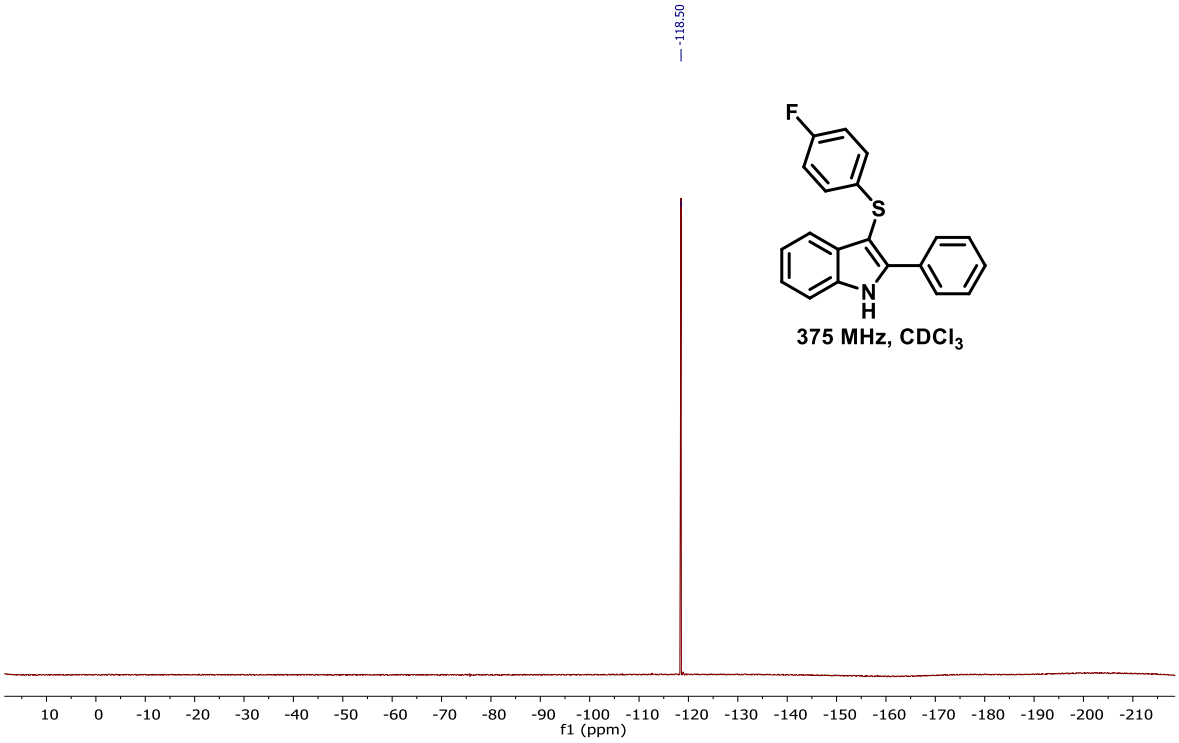
^{1}H NMR for 4e



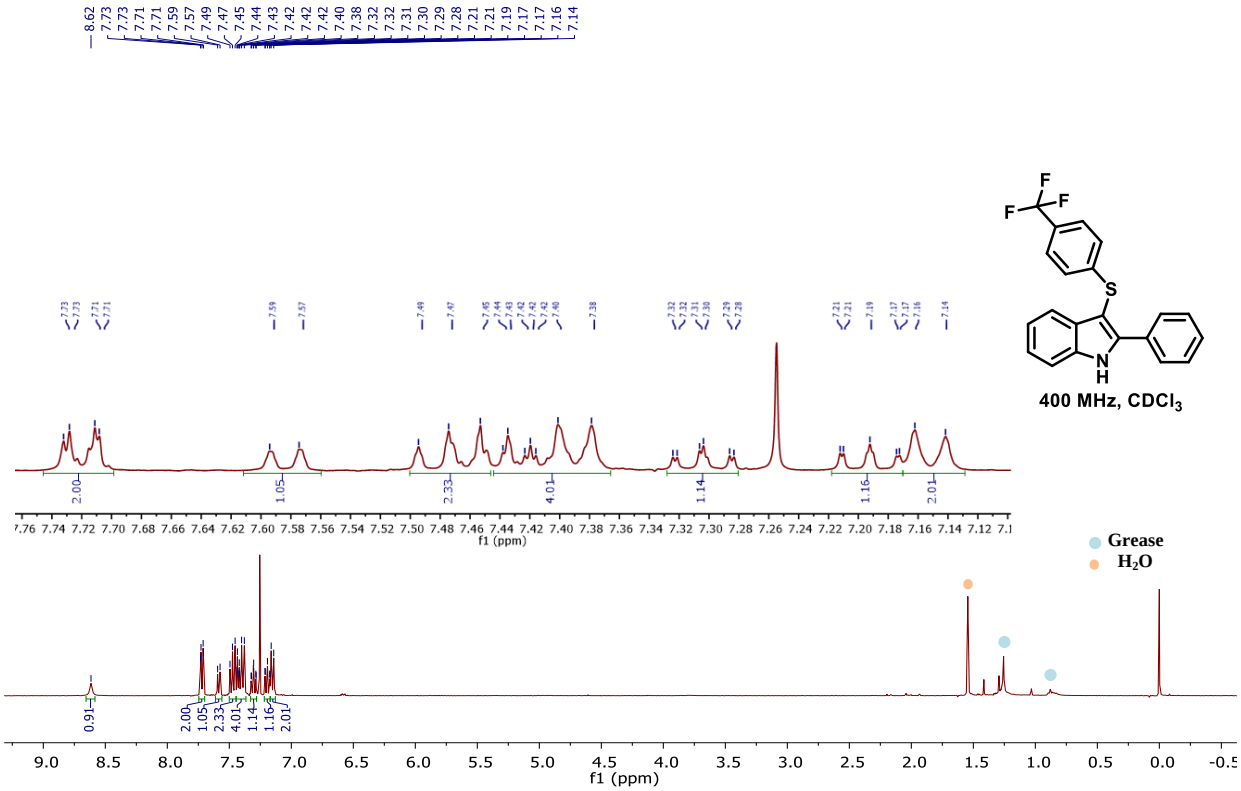
^{13}C NMR for 4e



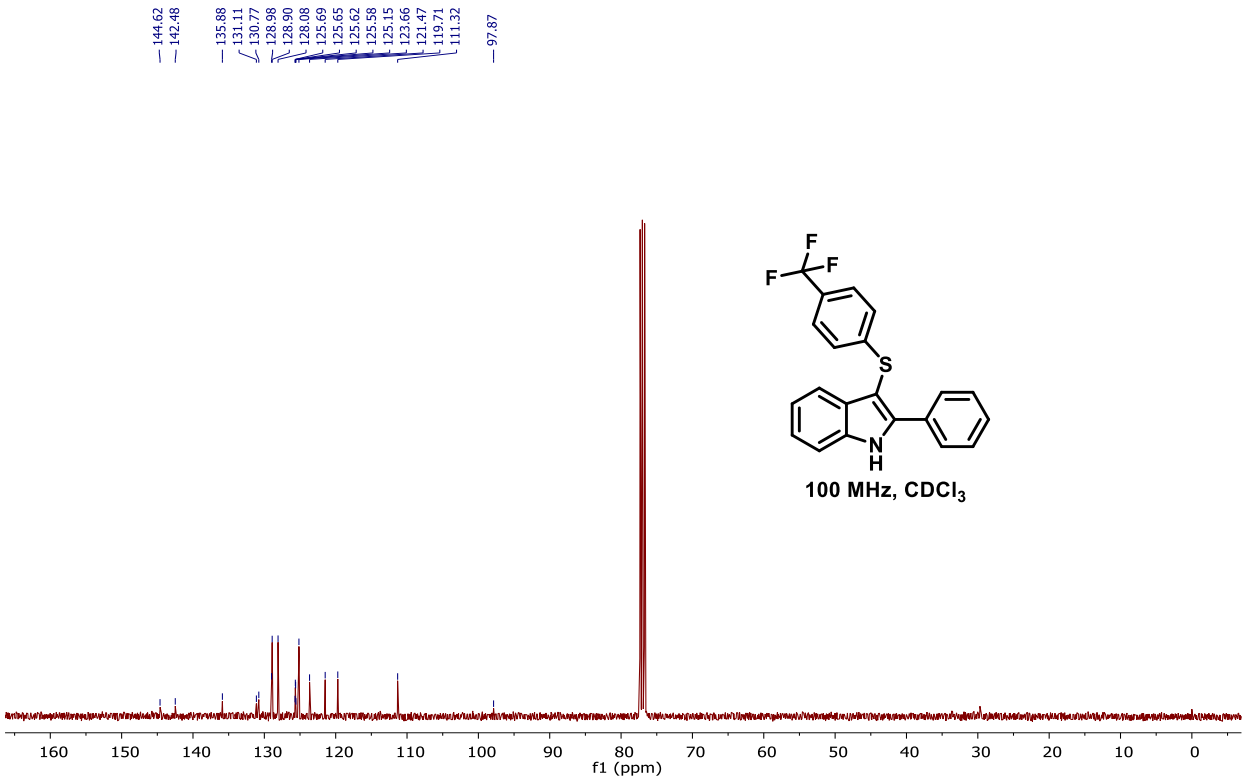
^{19}F NMR for 4e



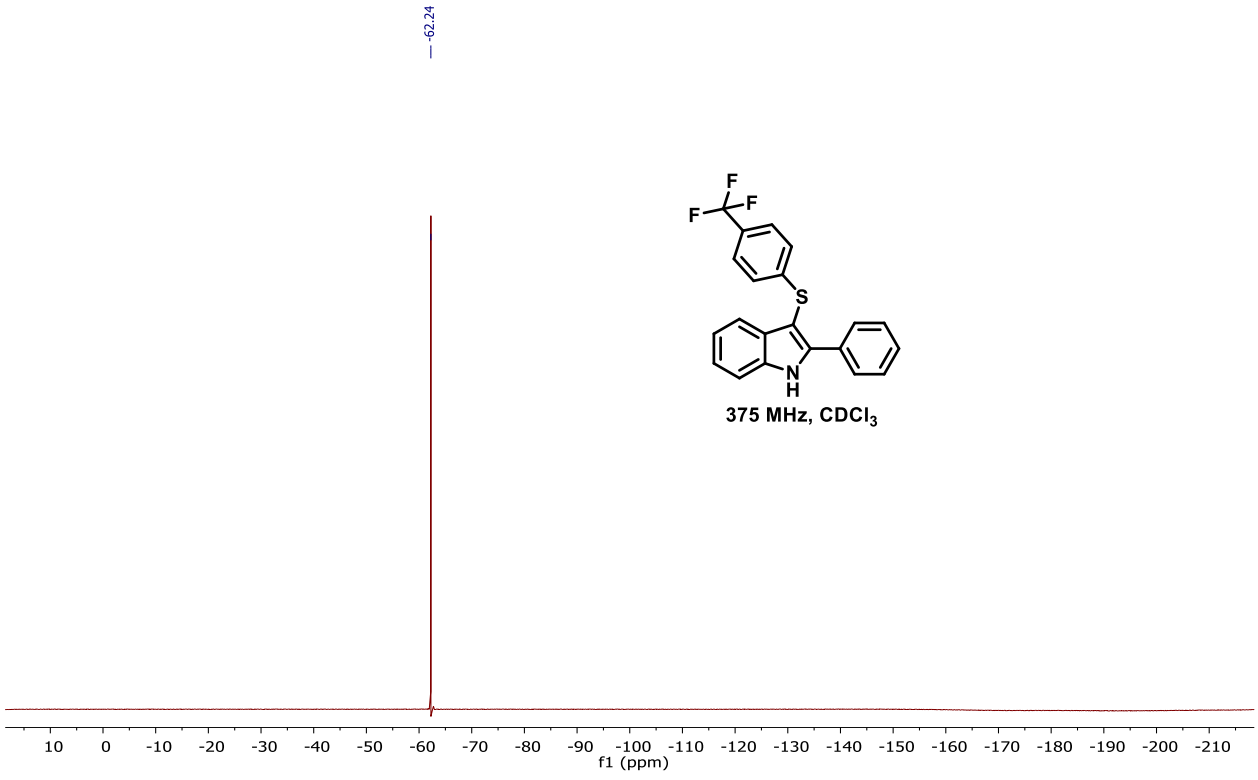
^{1}H NMR for 4f



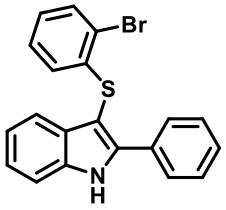
^{13}C NMR for 4f



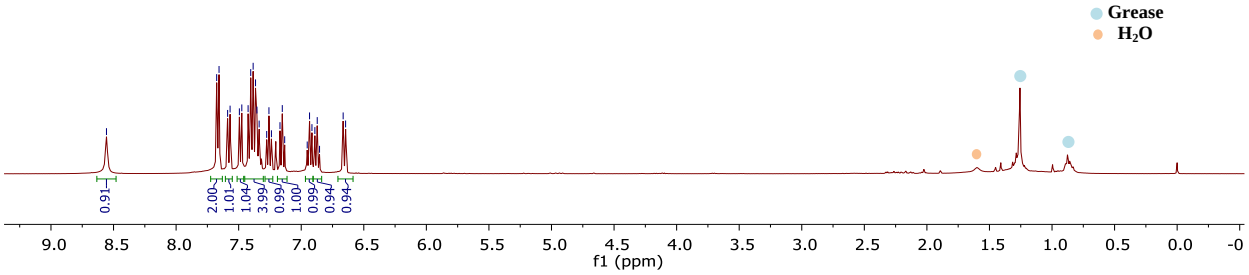
^{19}F NMR for 4f



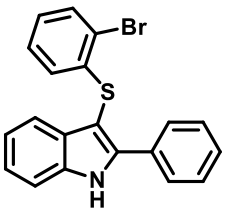
^{1}H NMR for 4g



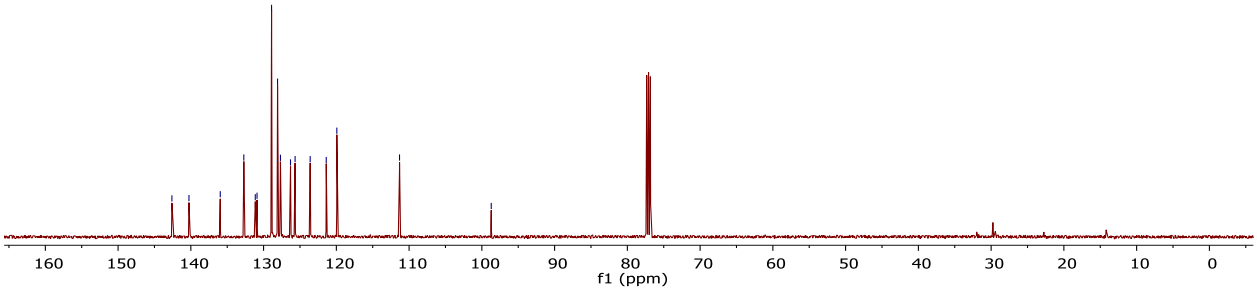
400 MHz, $CDCl_3$



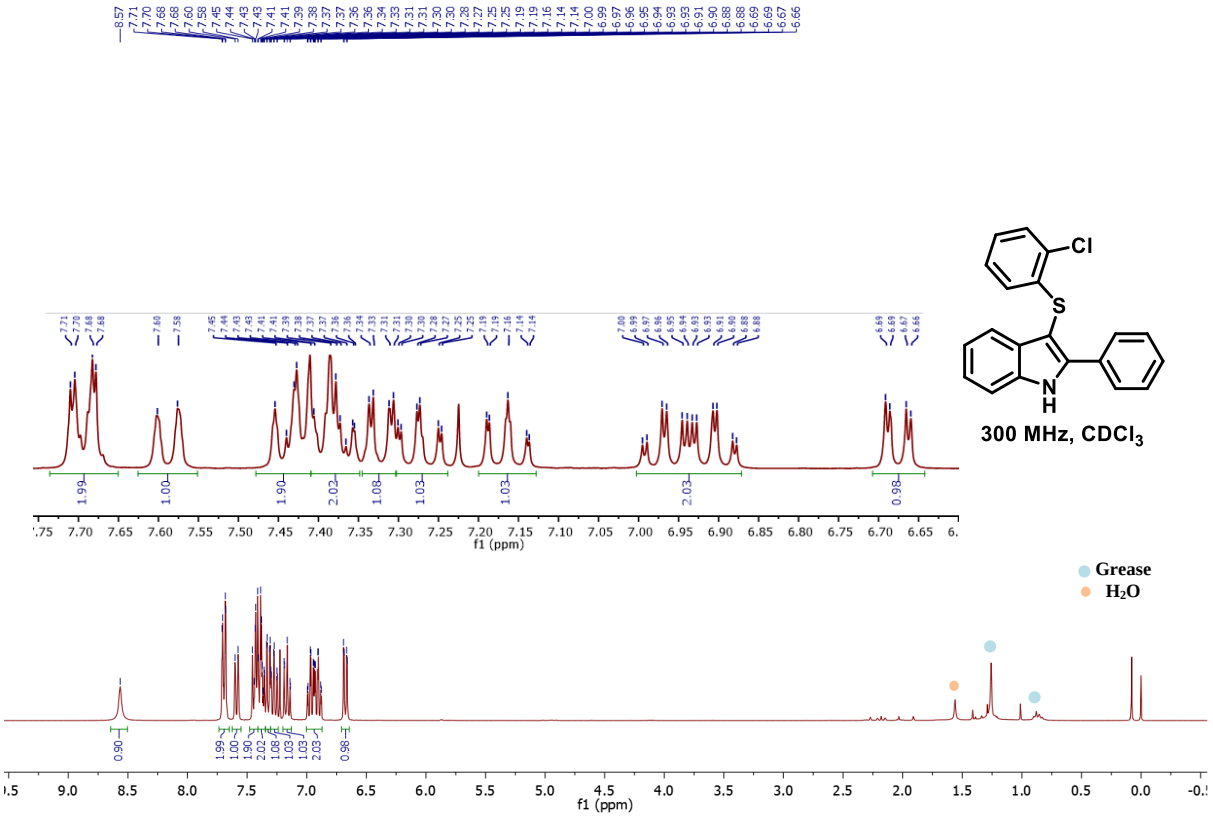
^{13}C NMR for 4g



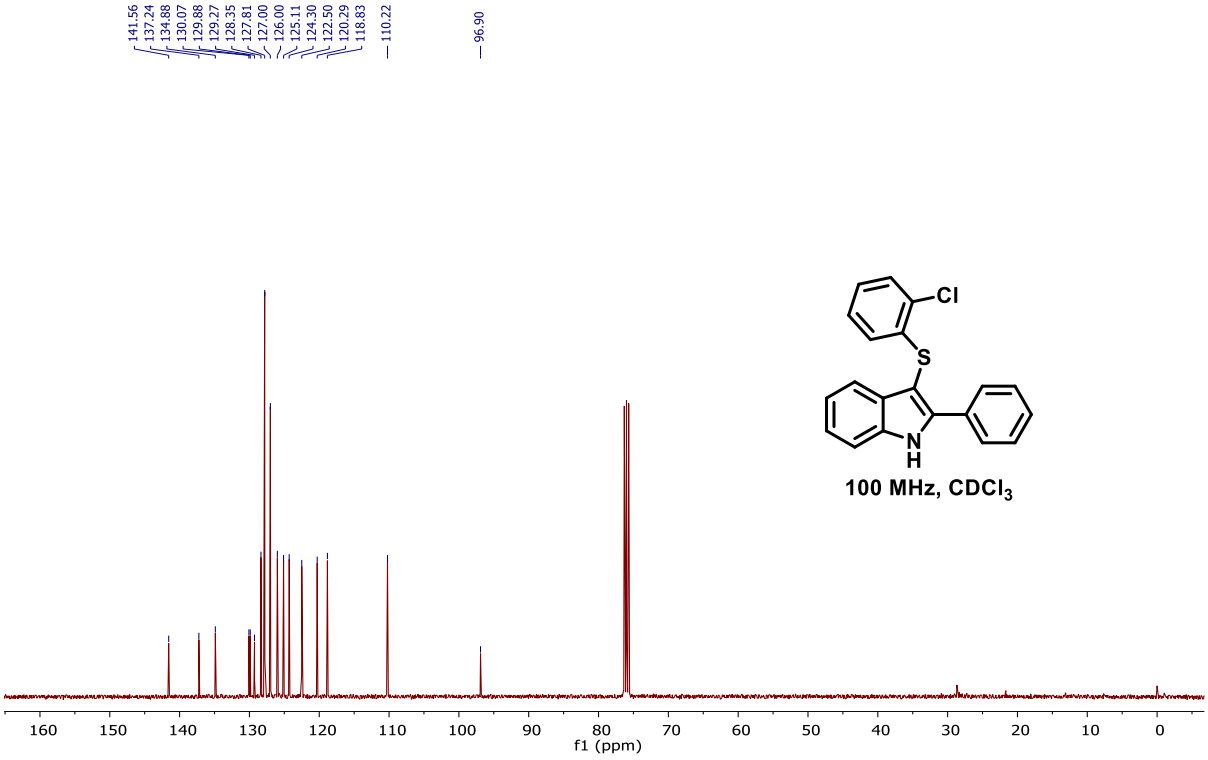
125 MHz, $CDCl_3$



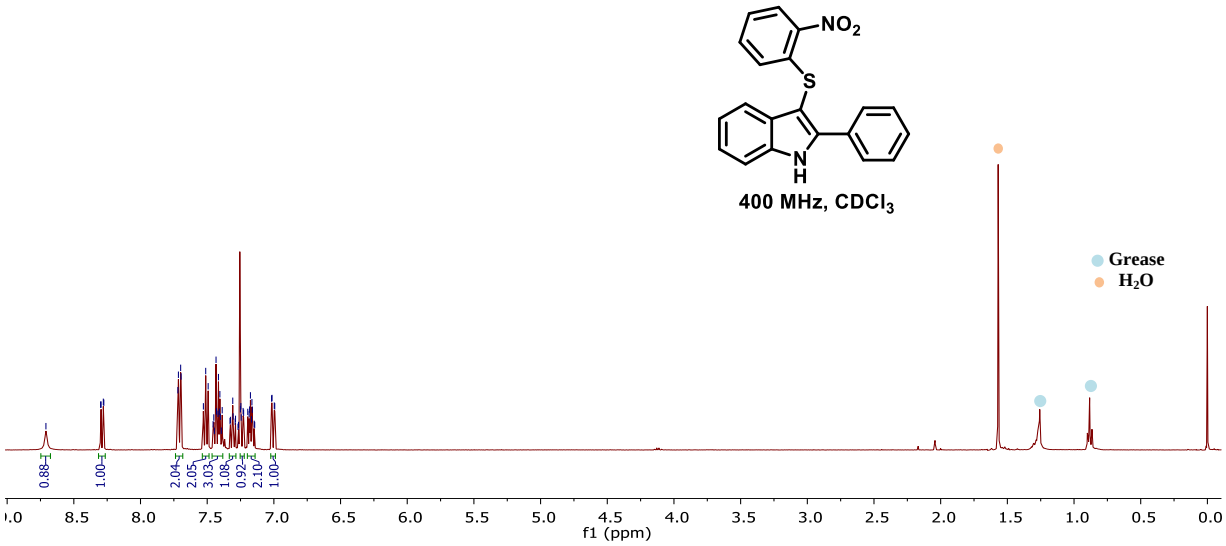
^{1}H NMR for 4h



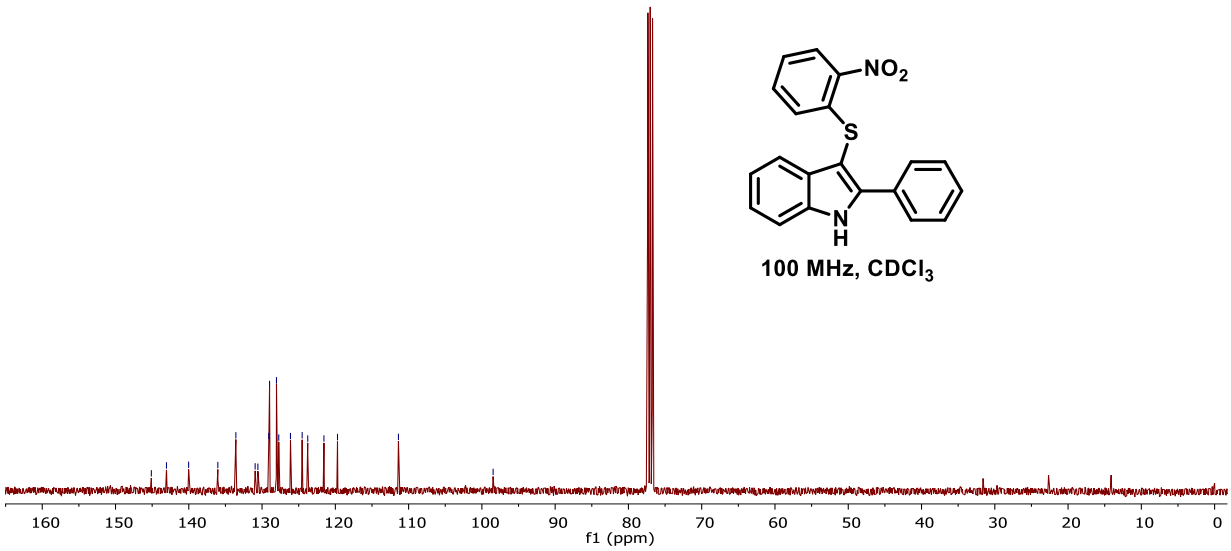
^{13}C NMR for 4h



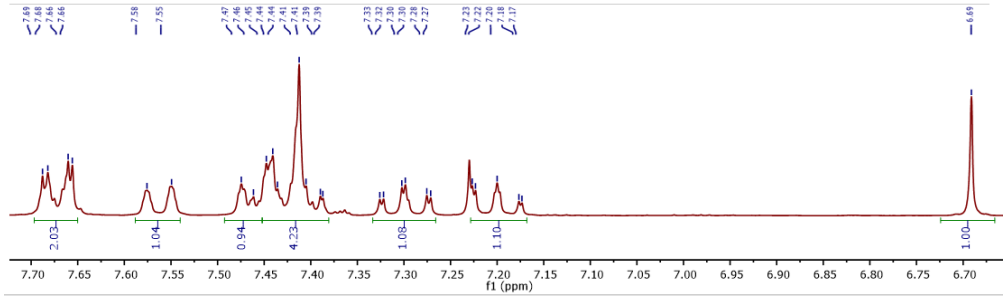
^{1}H NMR for 4i

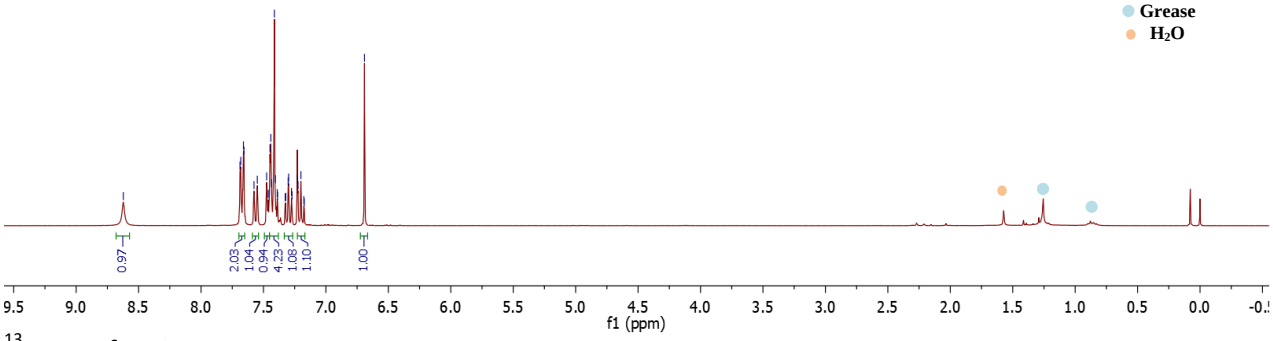


^{13}C NMR for 4i

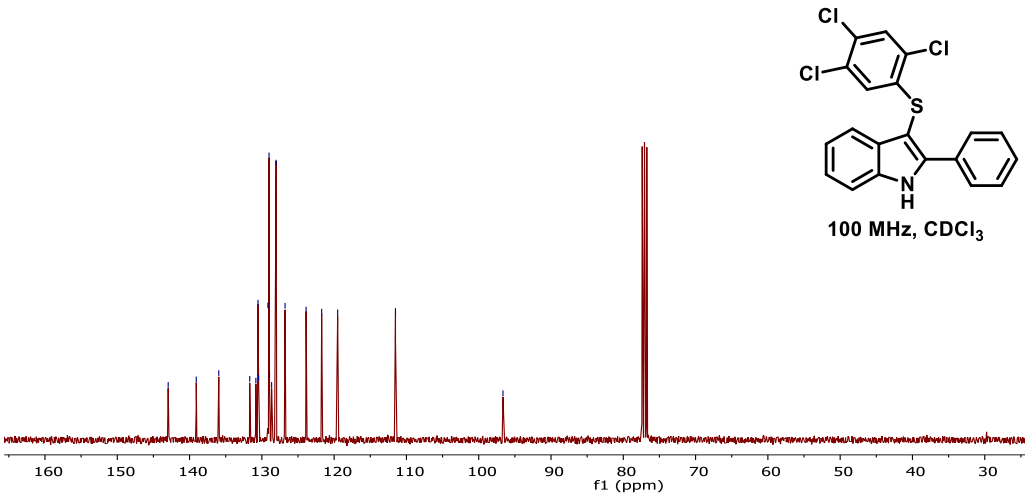


^{1}H NMR for 4j

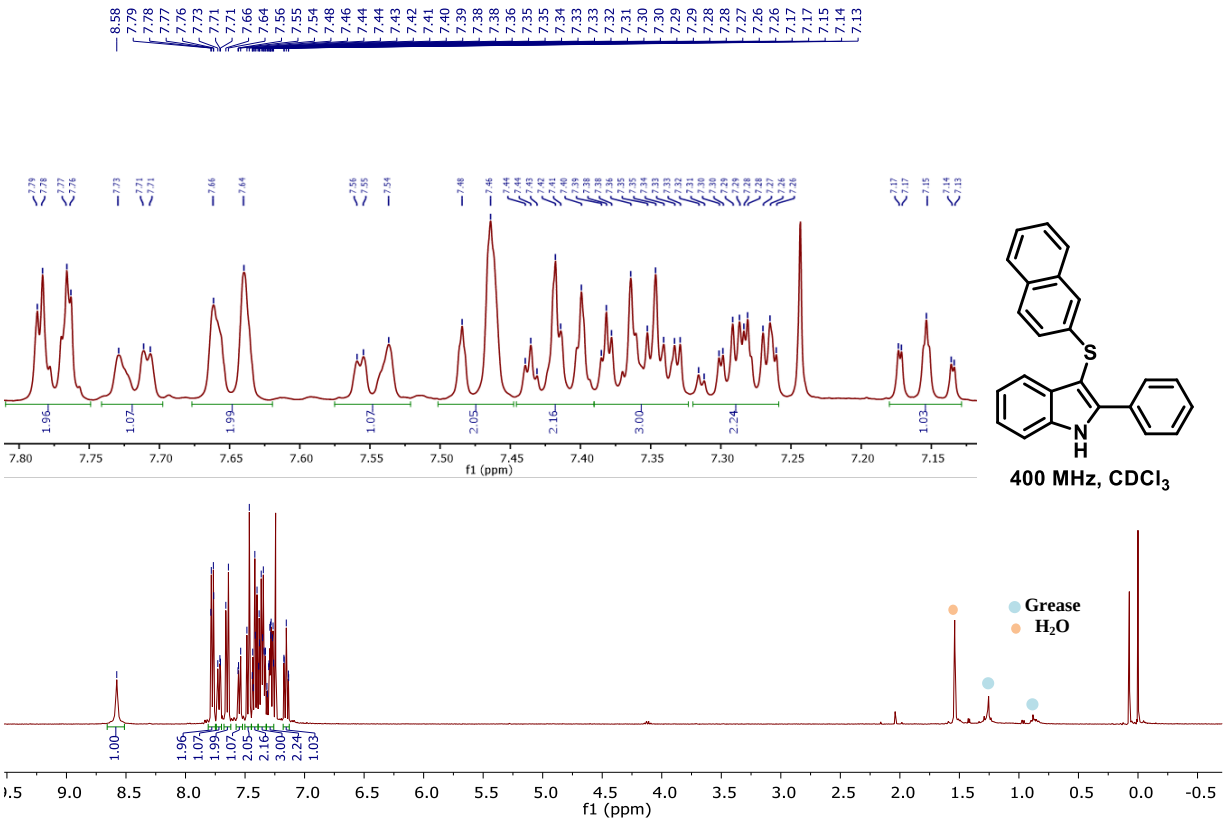




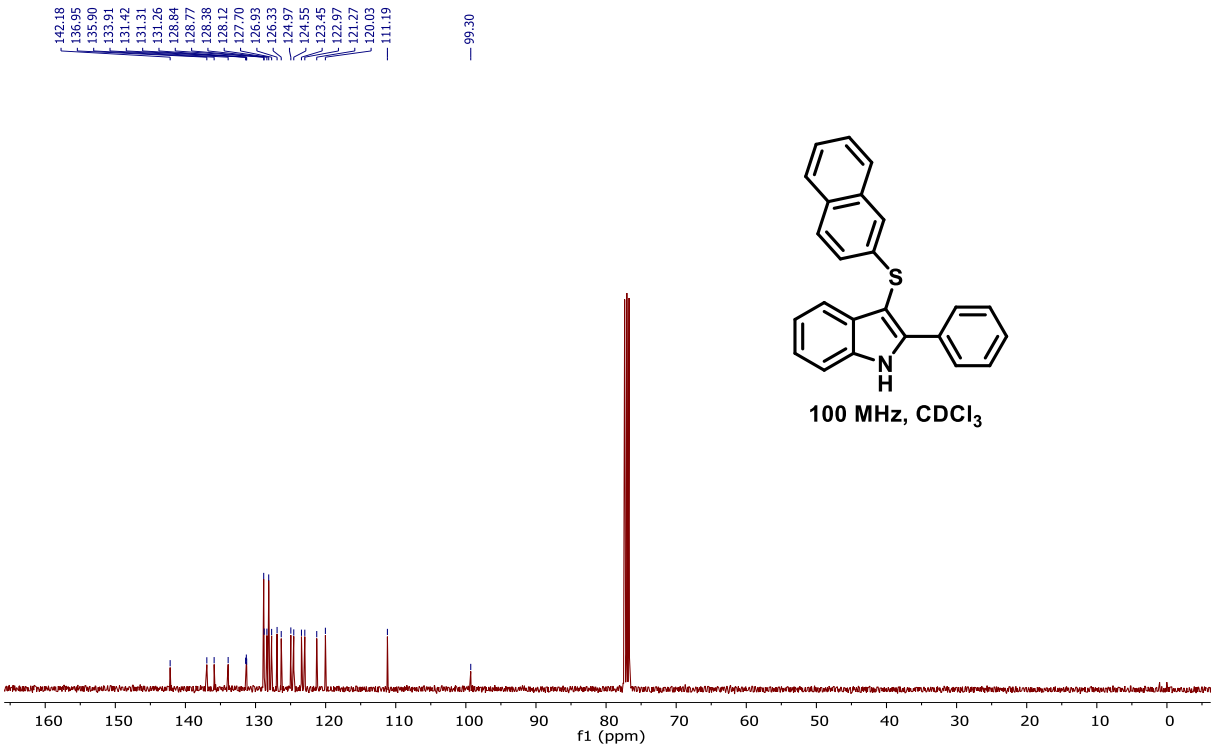
^{13}C NMR for 4j



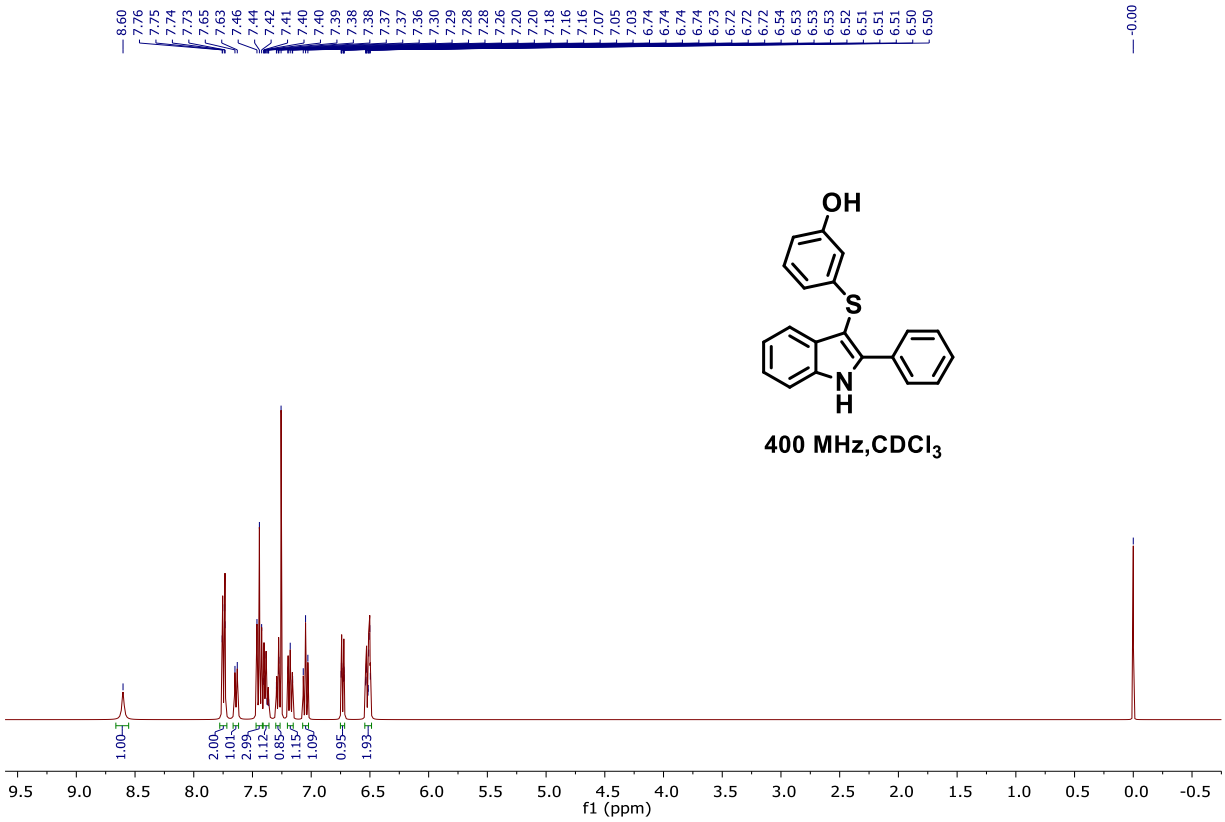
^{1}H NMR for 4k



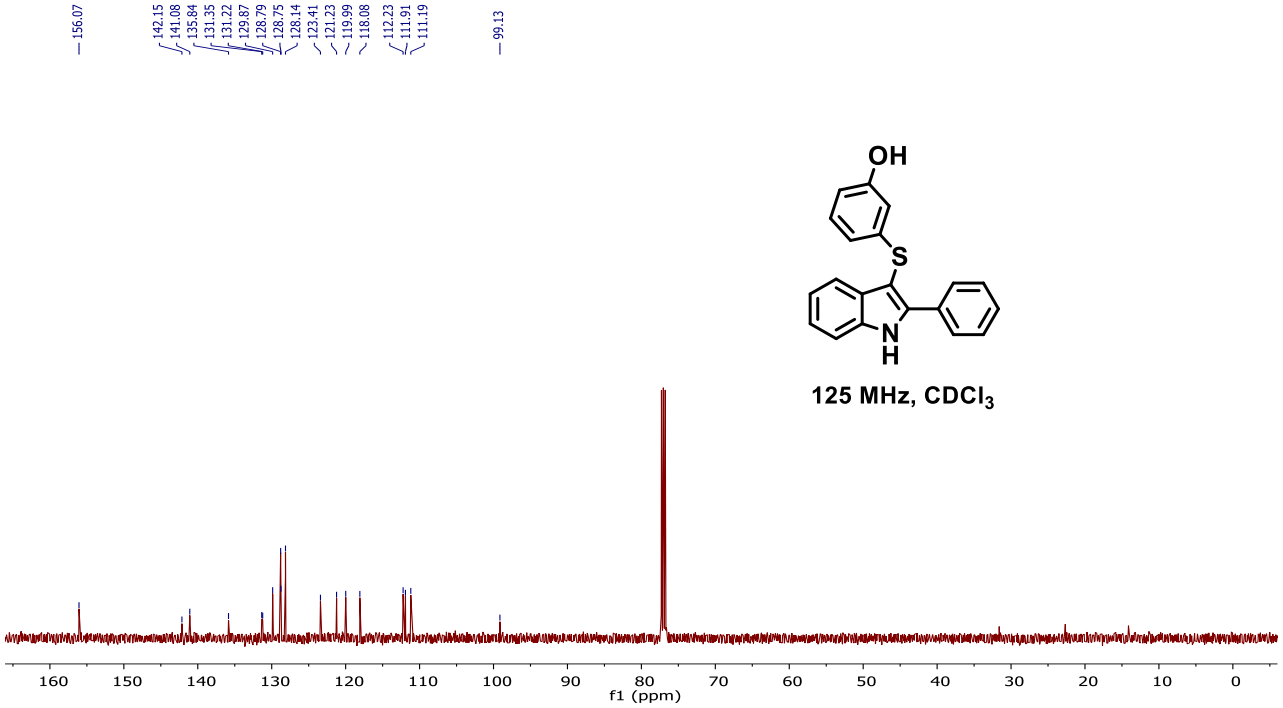
^{13}C NMR for 4k



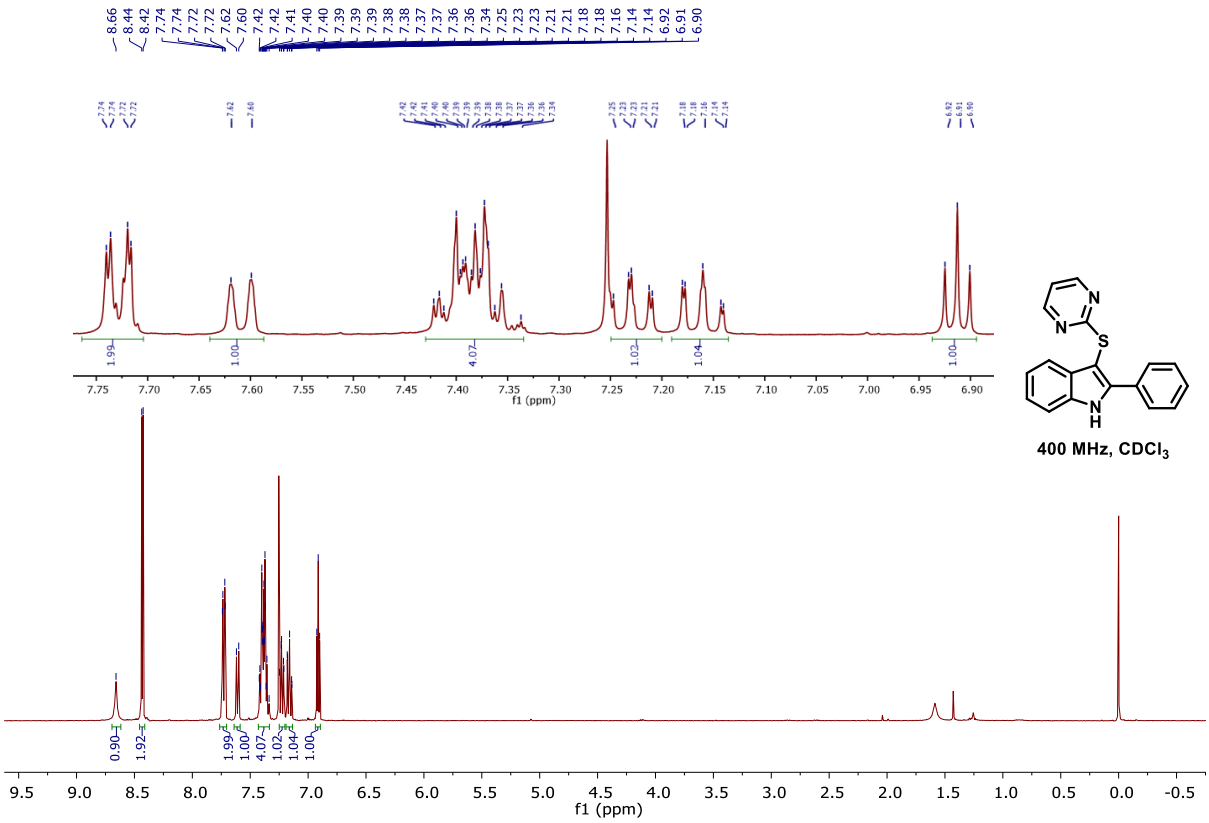
^{1}H NMR for 4l



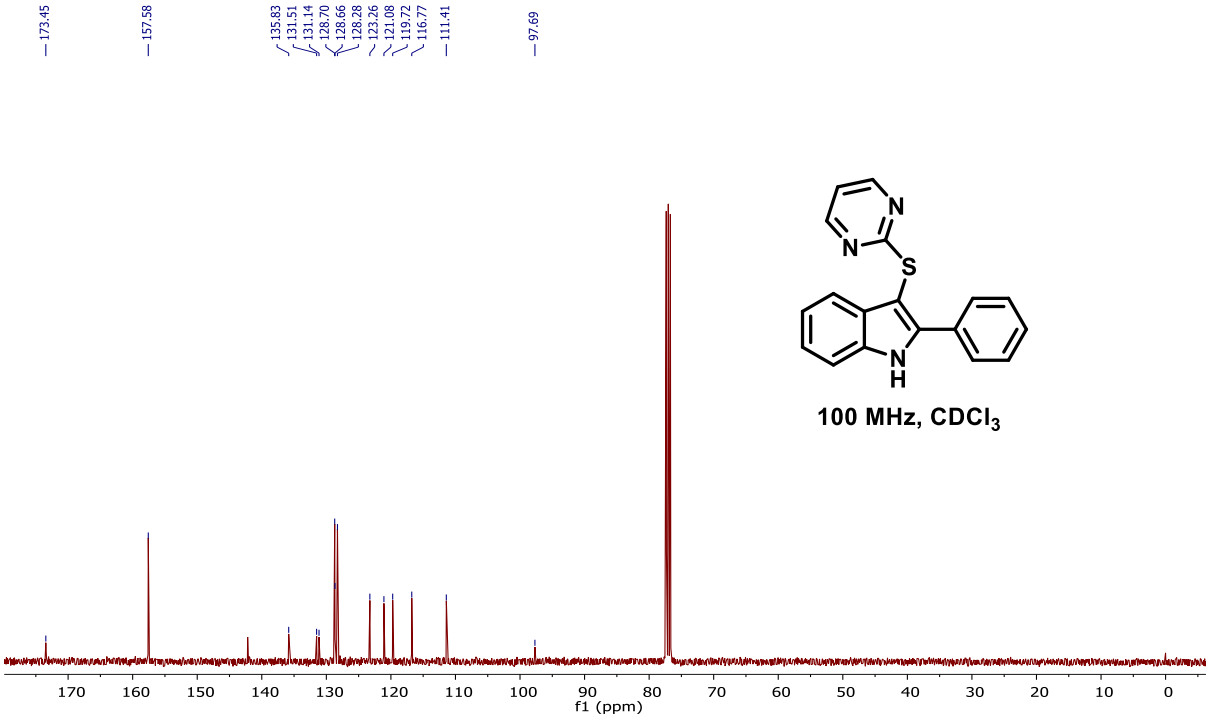
^{13}C NMR for 4l



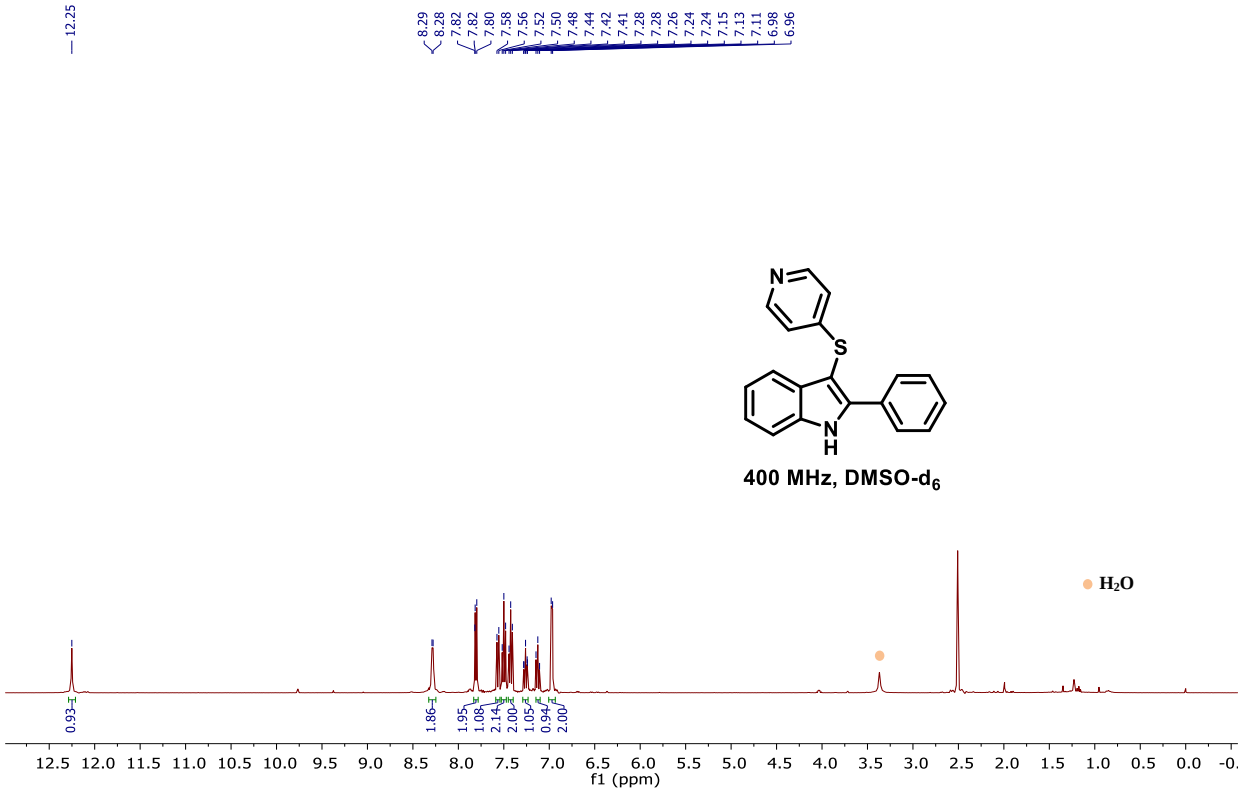
^{1}H NMR for 4m



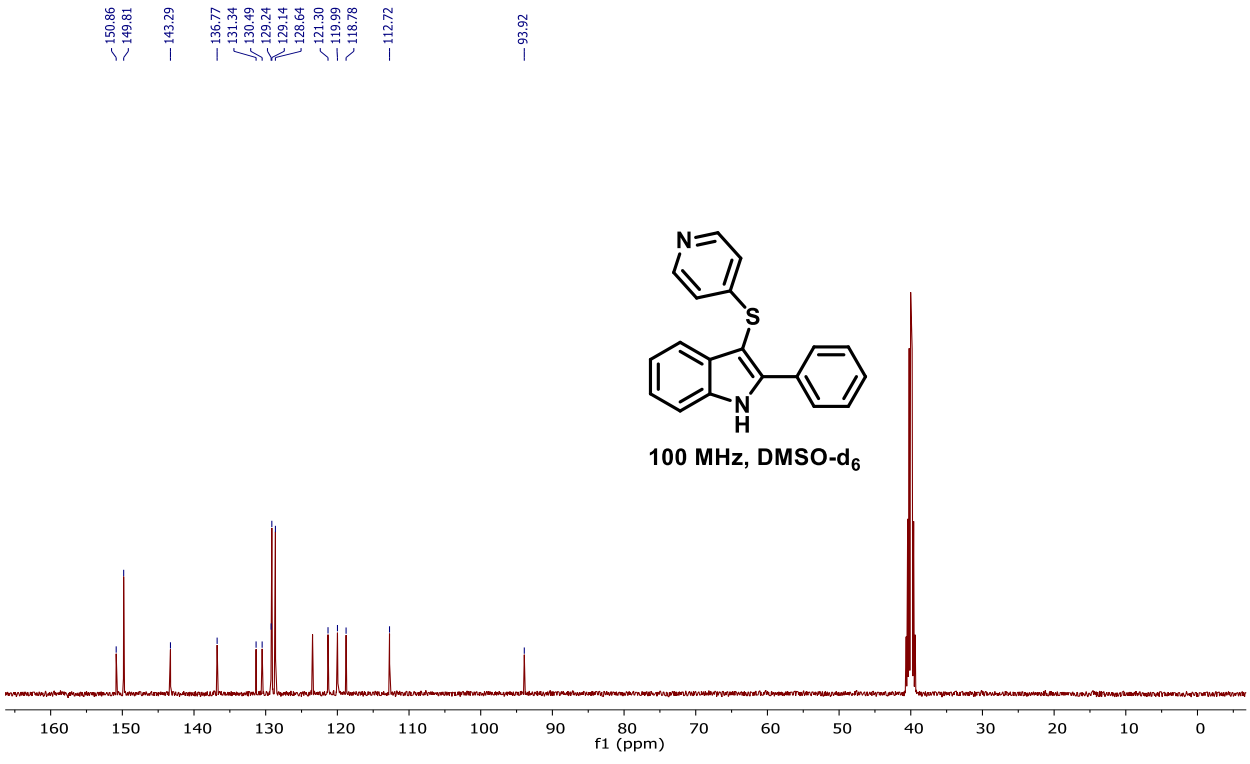
^{13}C NMR for 4m



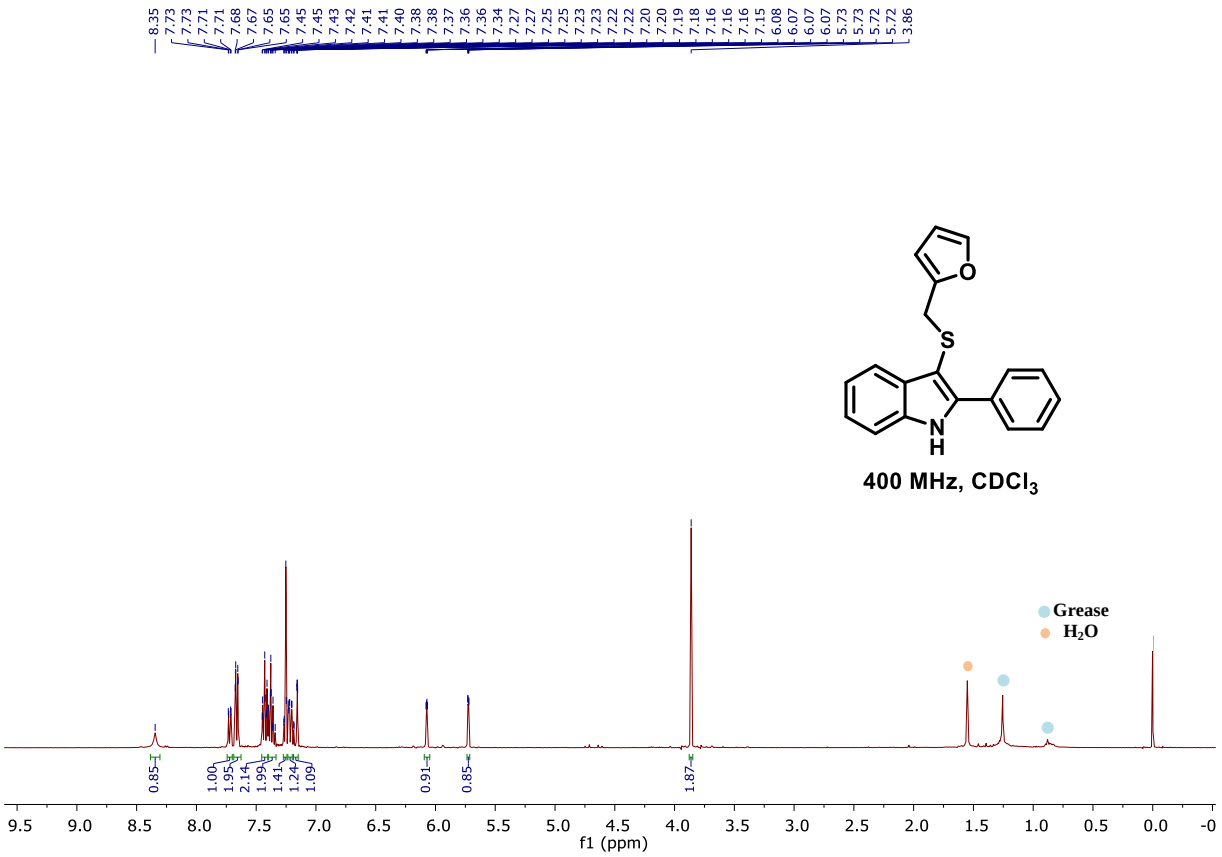
^{1}H NMR for 4n



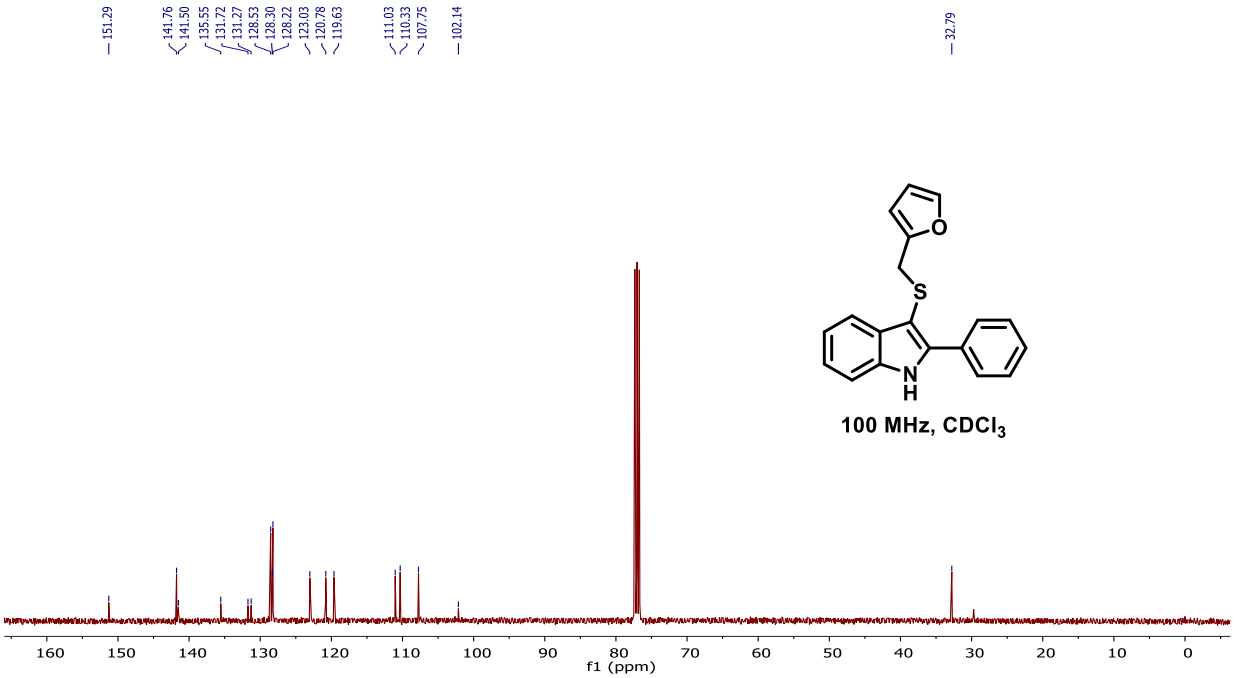
^{13}C NMR for 4n



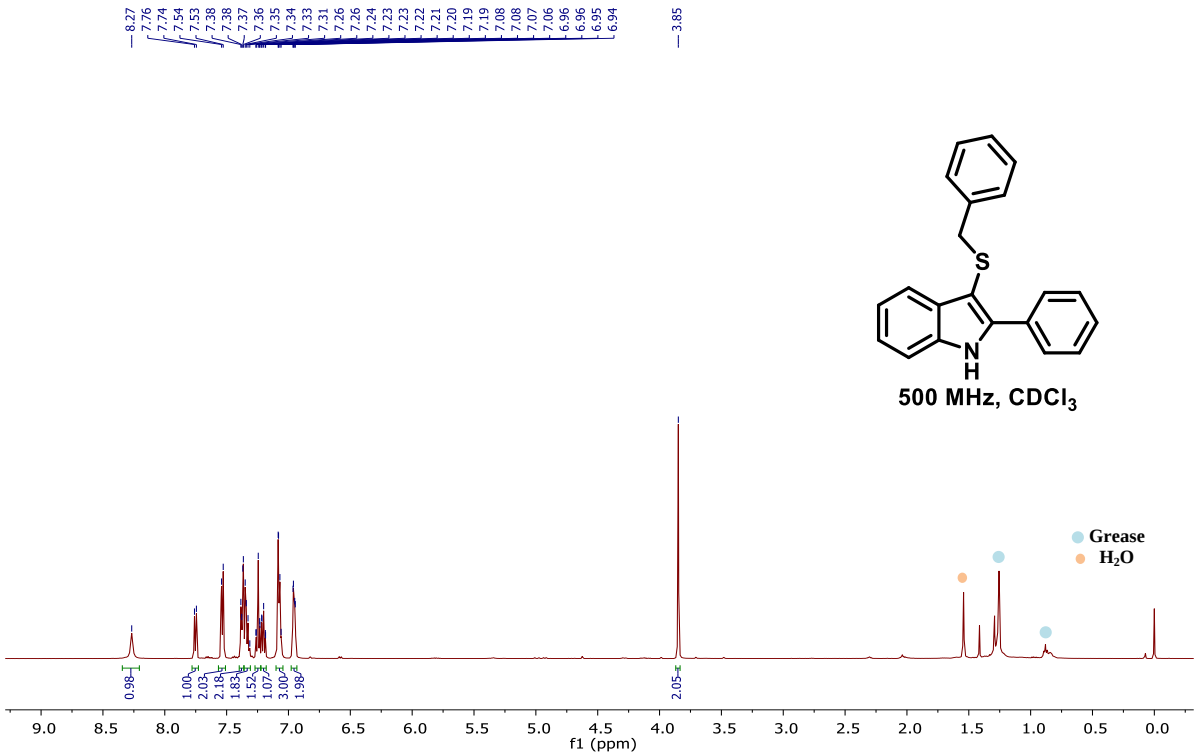
^{1}H NMR for 4o



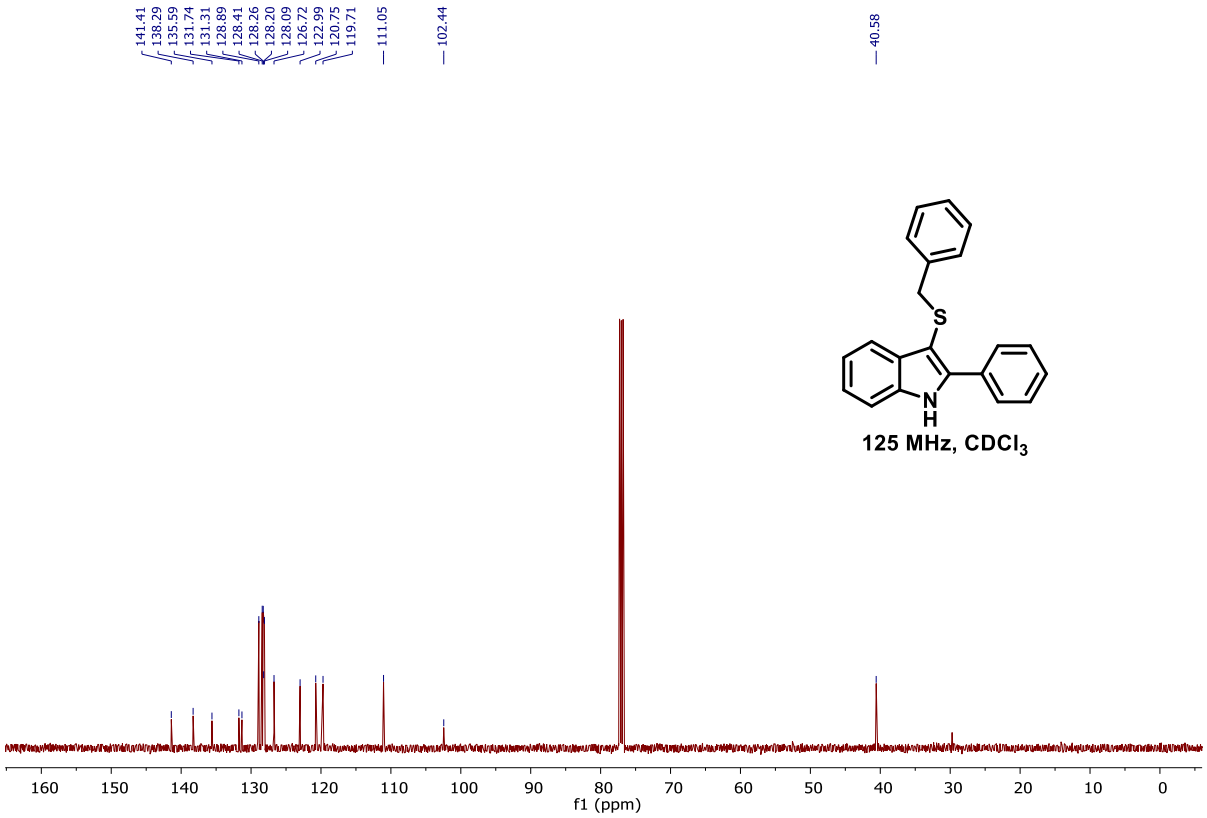
^{13}C NMR for 4o



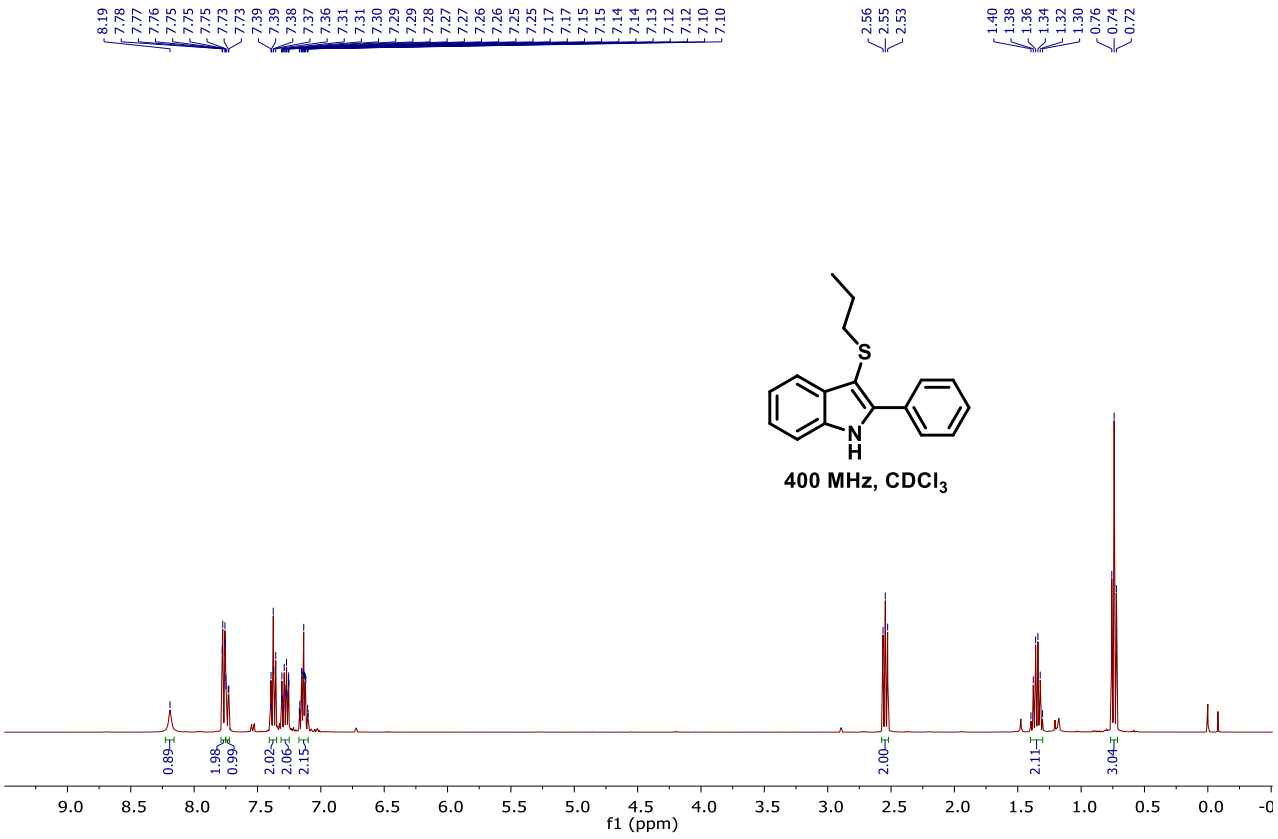
^{1}H NMR for 4p



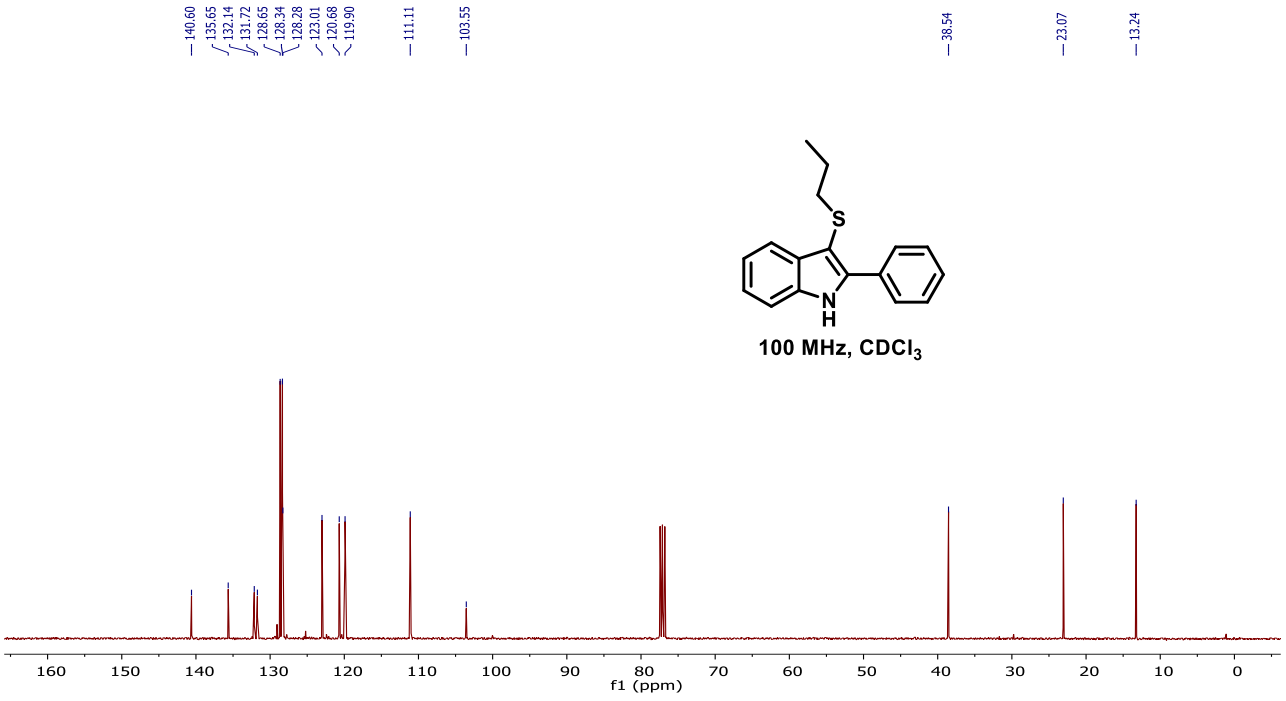
^{13}C NMR for 4p



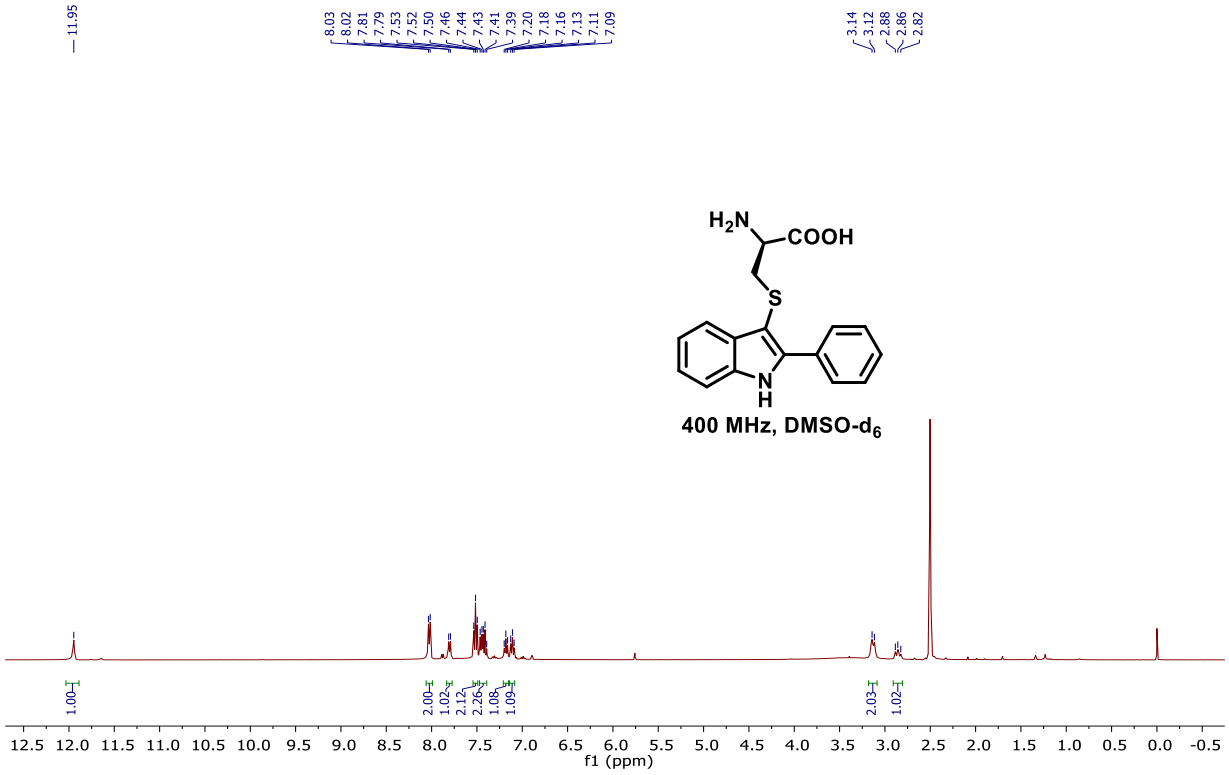
^{1}H NMR for 4q



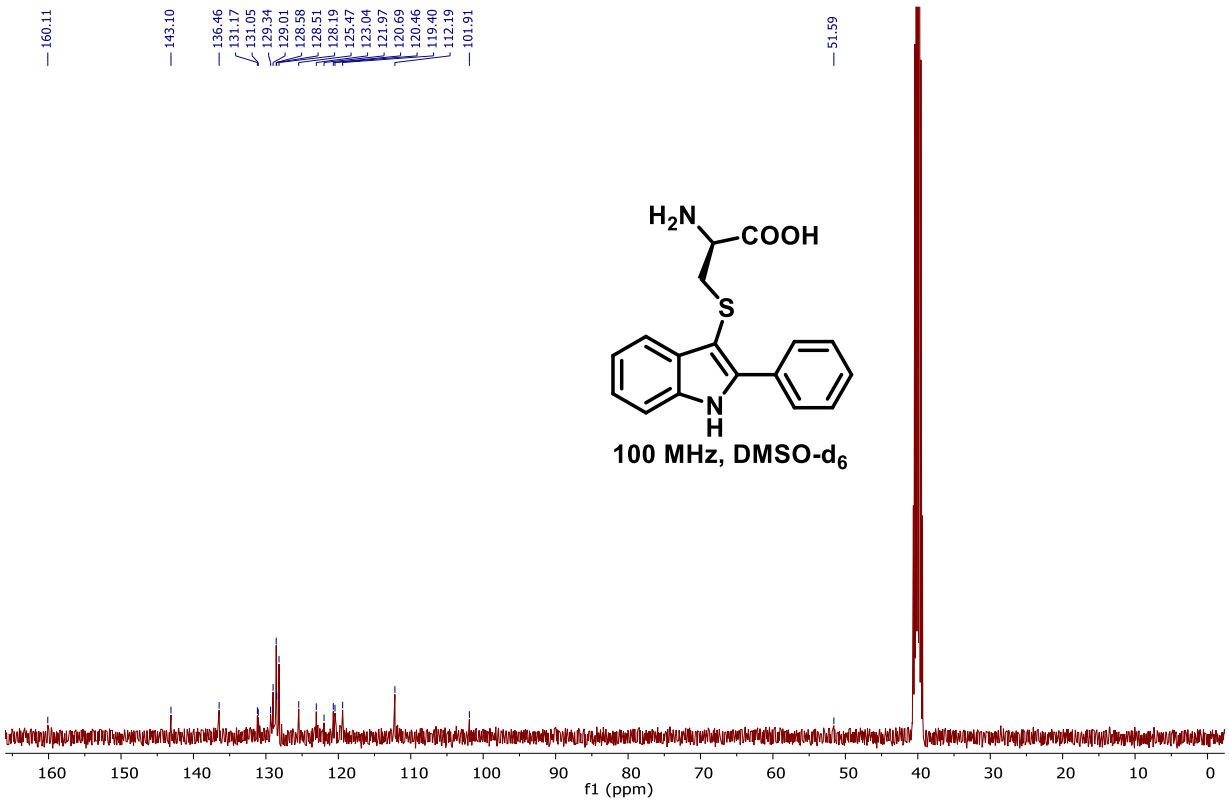
^{13}C NMR for 4q



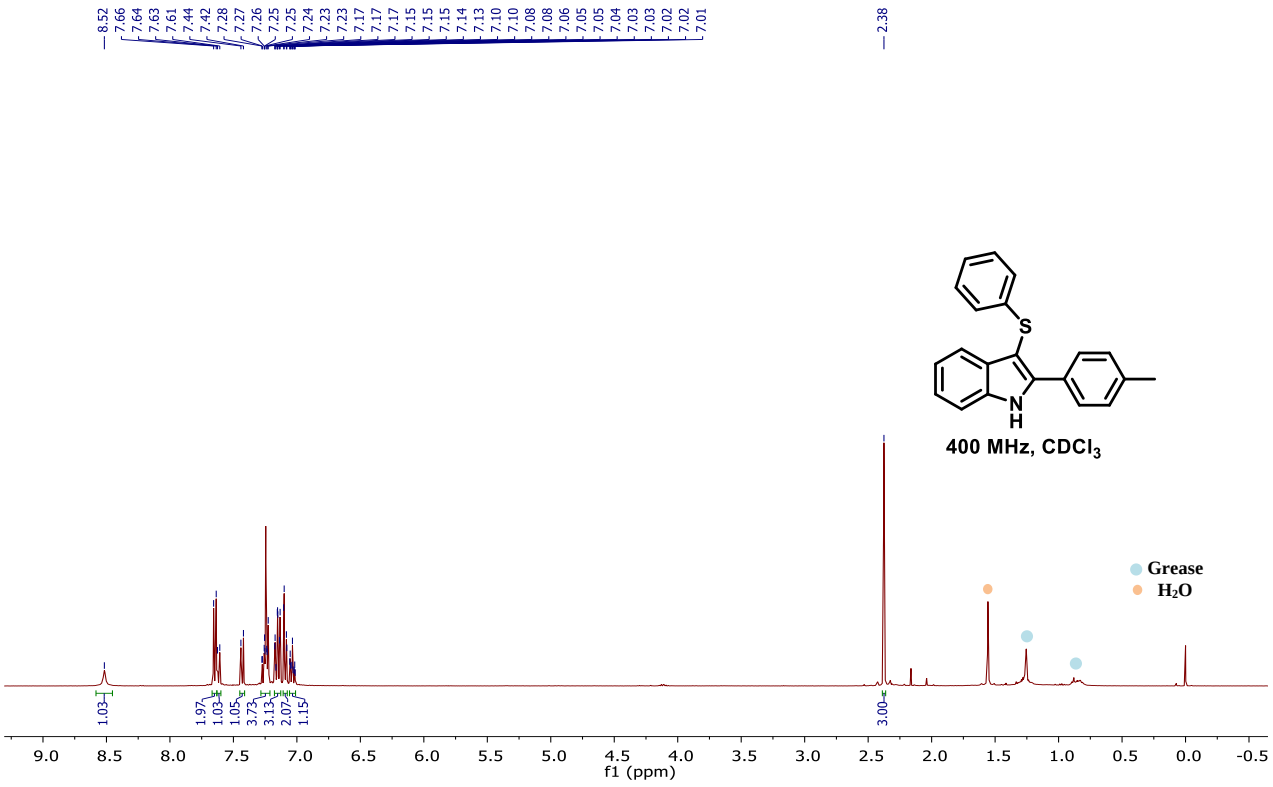
^{1}H NMR for 4r



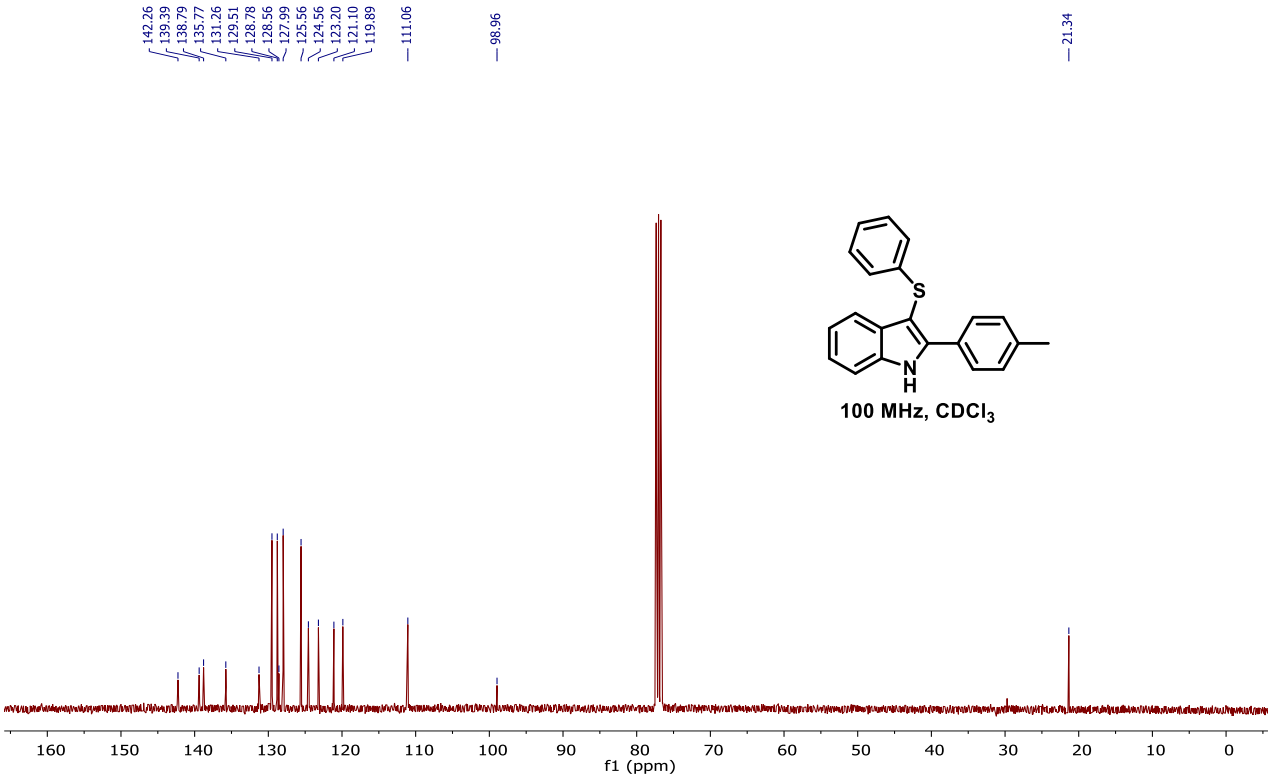
^{13}C NMR for 4r



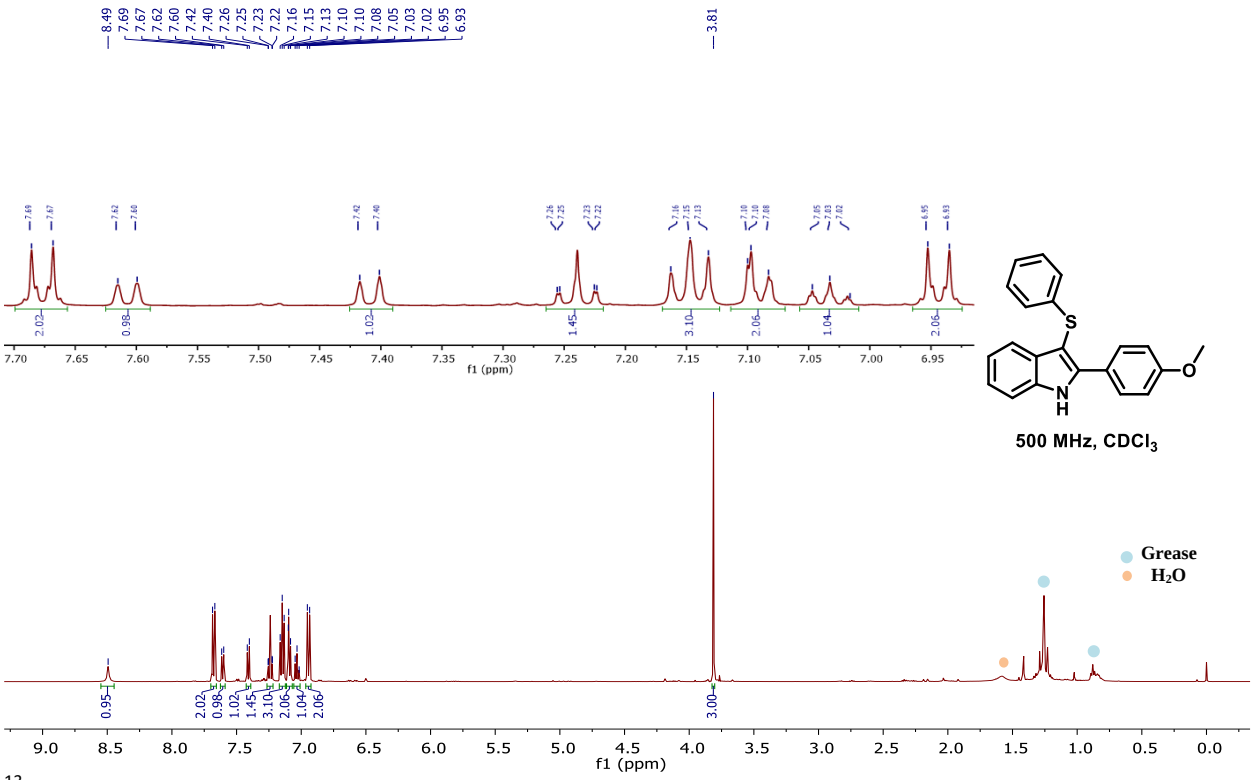
^{1}H NMR for 5a



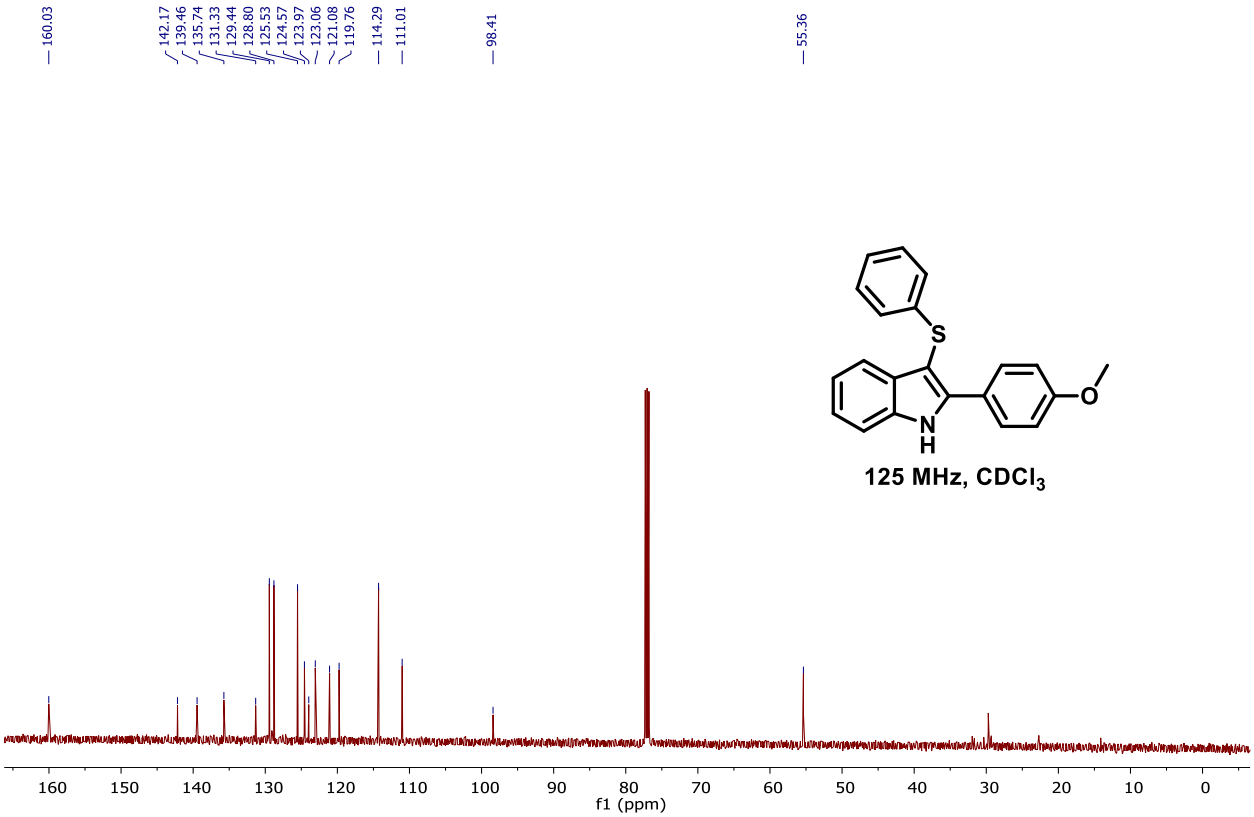
^{13}C NMR for 5a



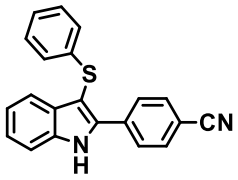
^{1}H NMR for 5b



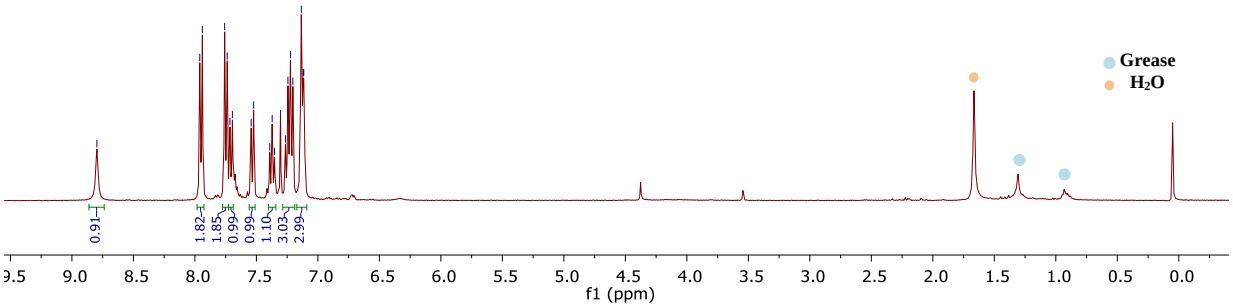
^{13}C NMR for 5b



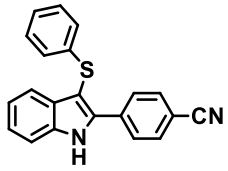
^{1}H NMR for 5c



400 MHz, $CDCl_3$

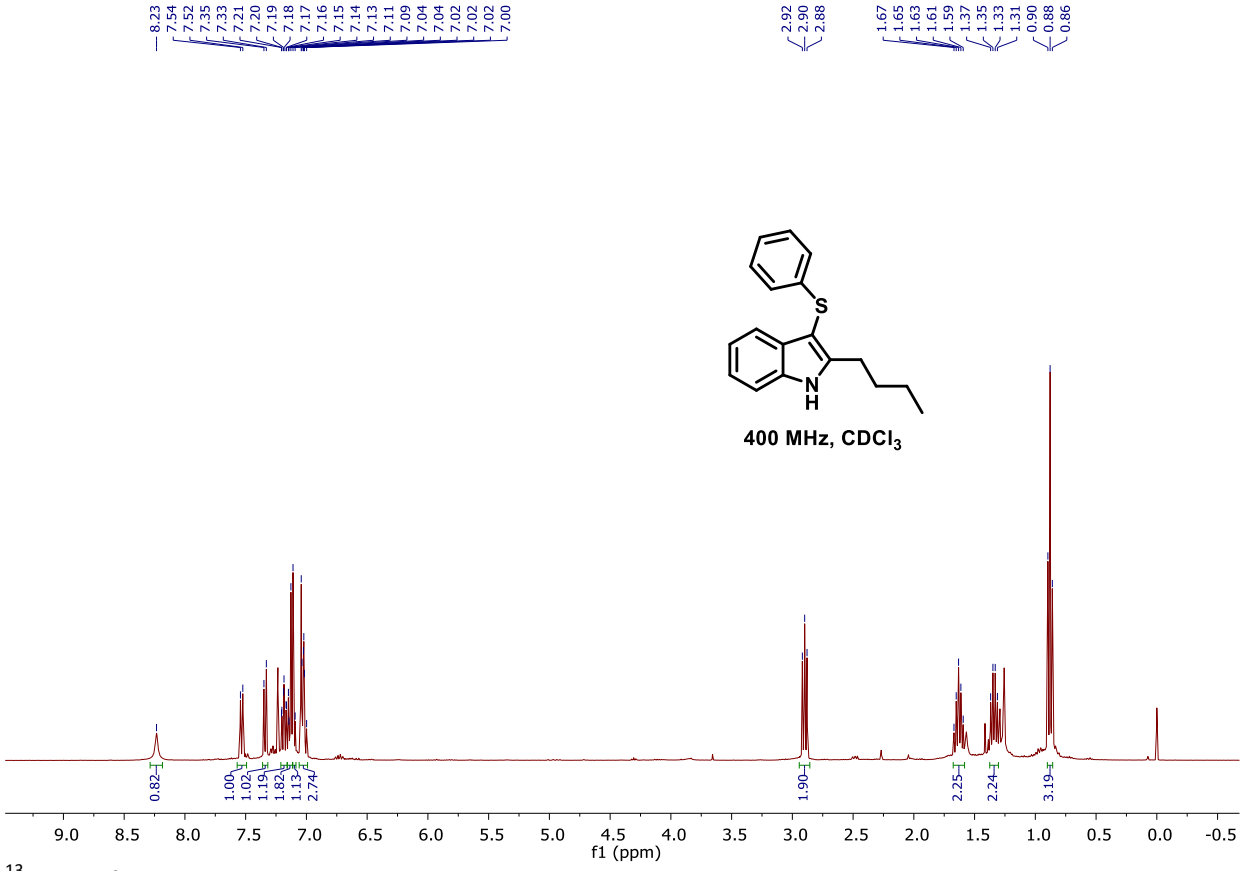


^{13}C NMR for 5c

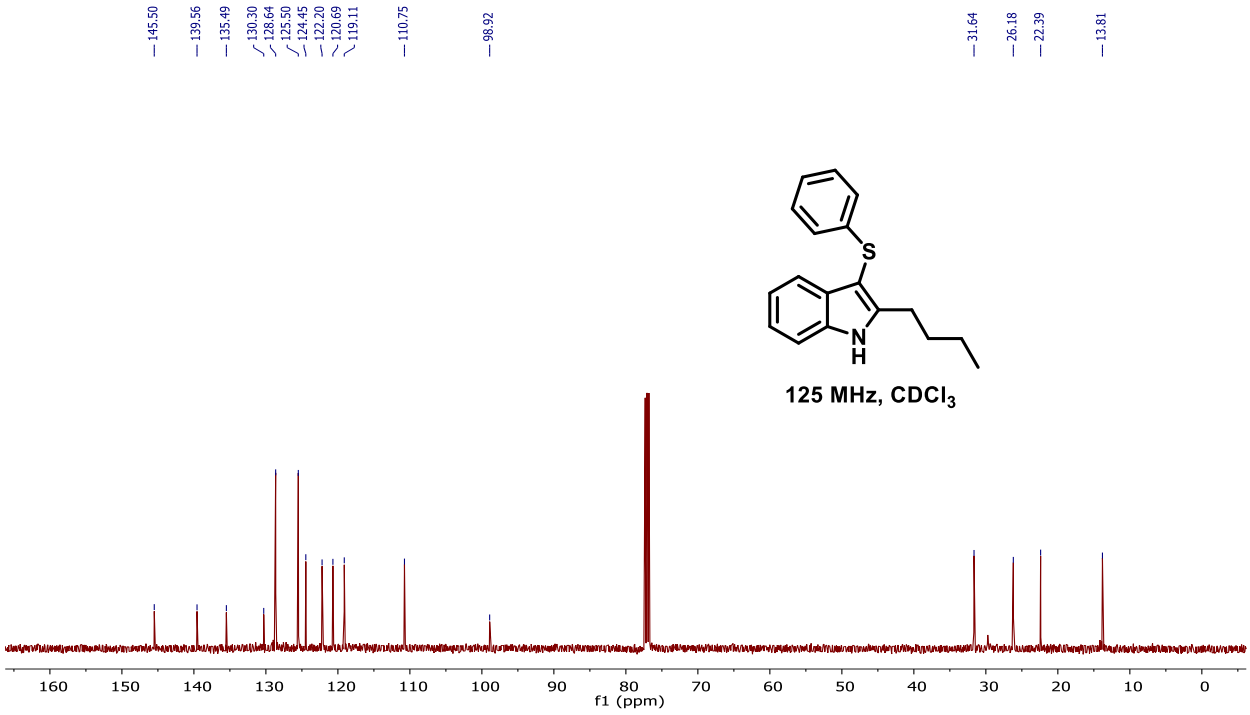


100 MHz, $CDCl_3$

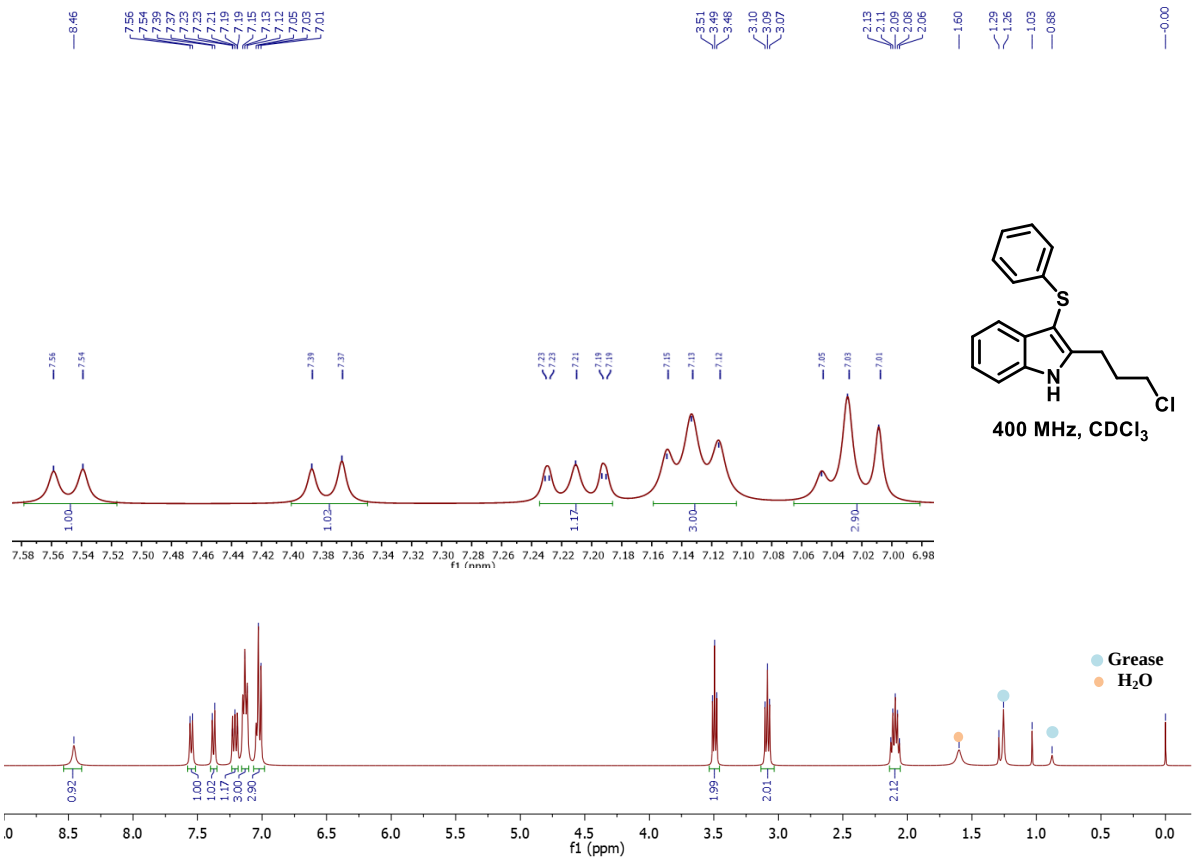
^{1}H NMR for 5e



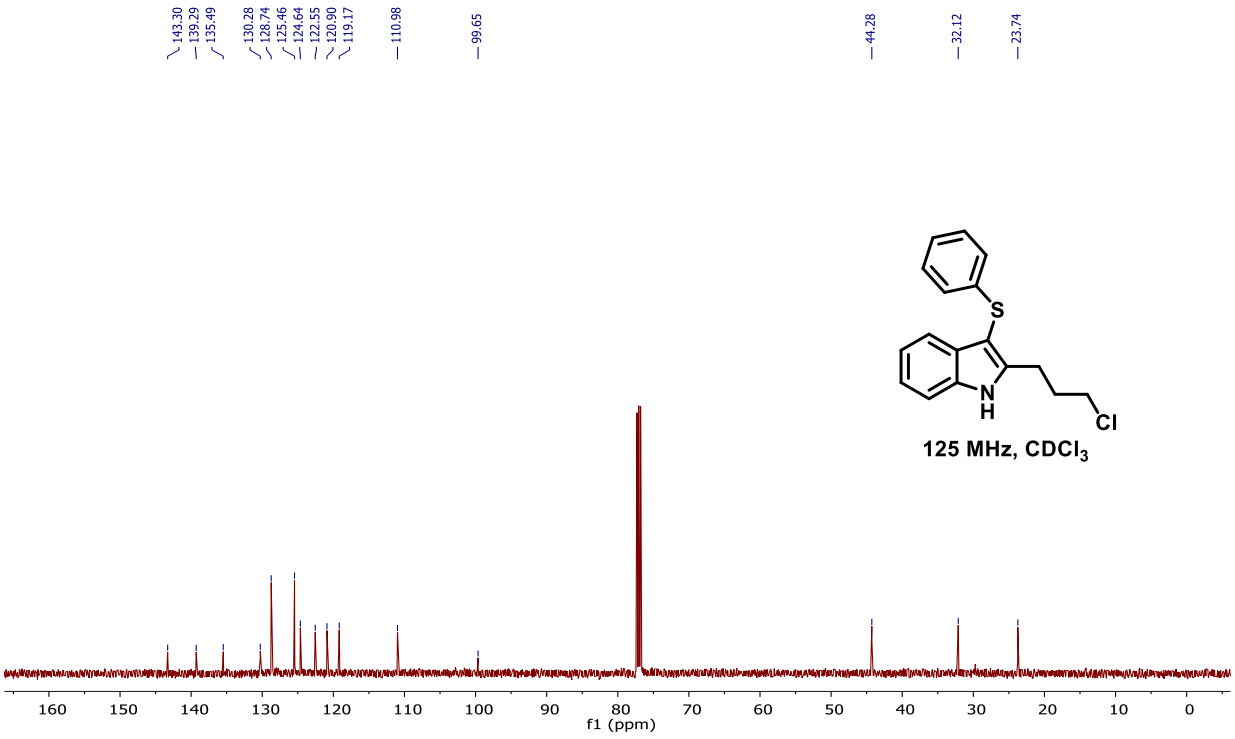
^{13}C NMR for 5e



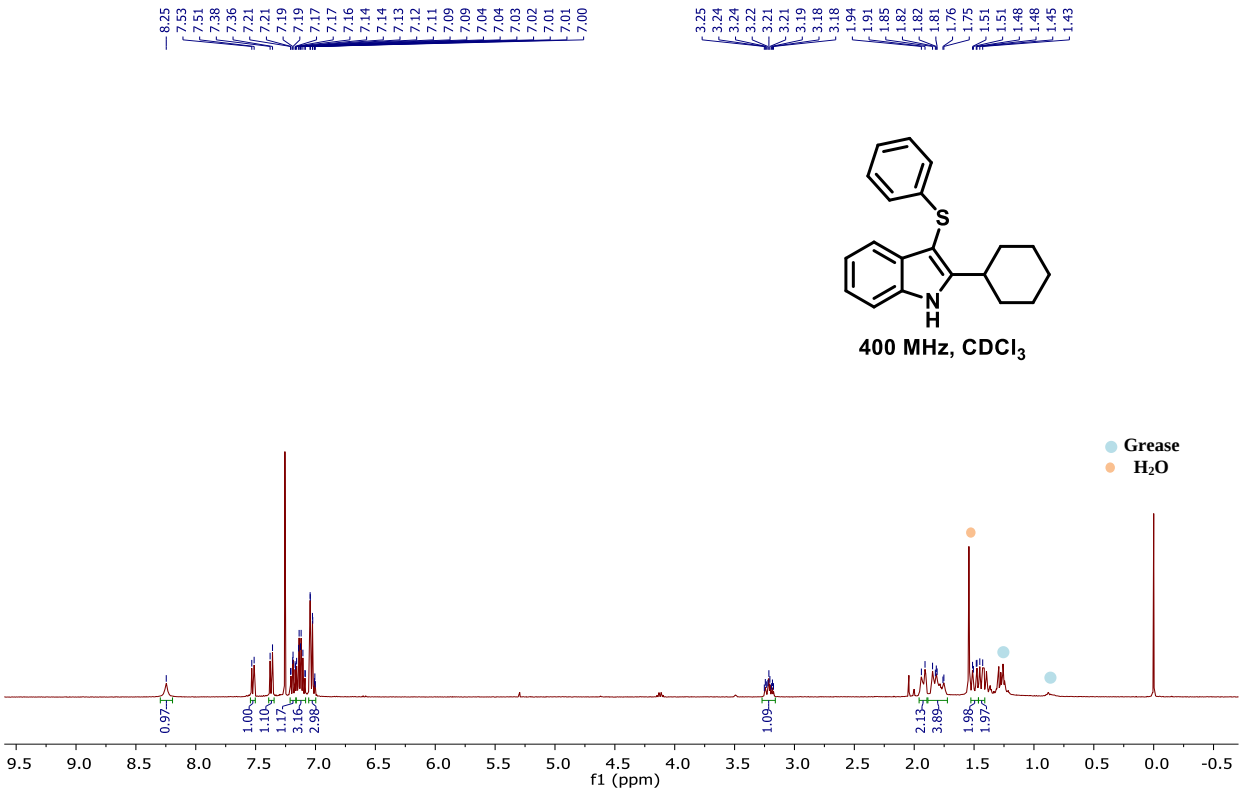
^{1}H NMR for 5f



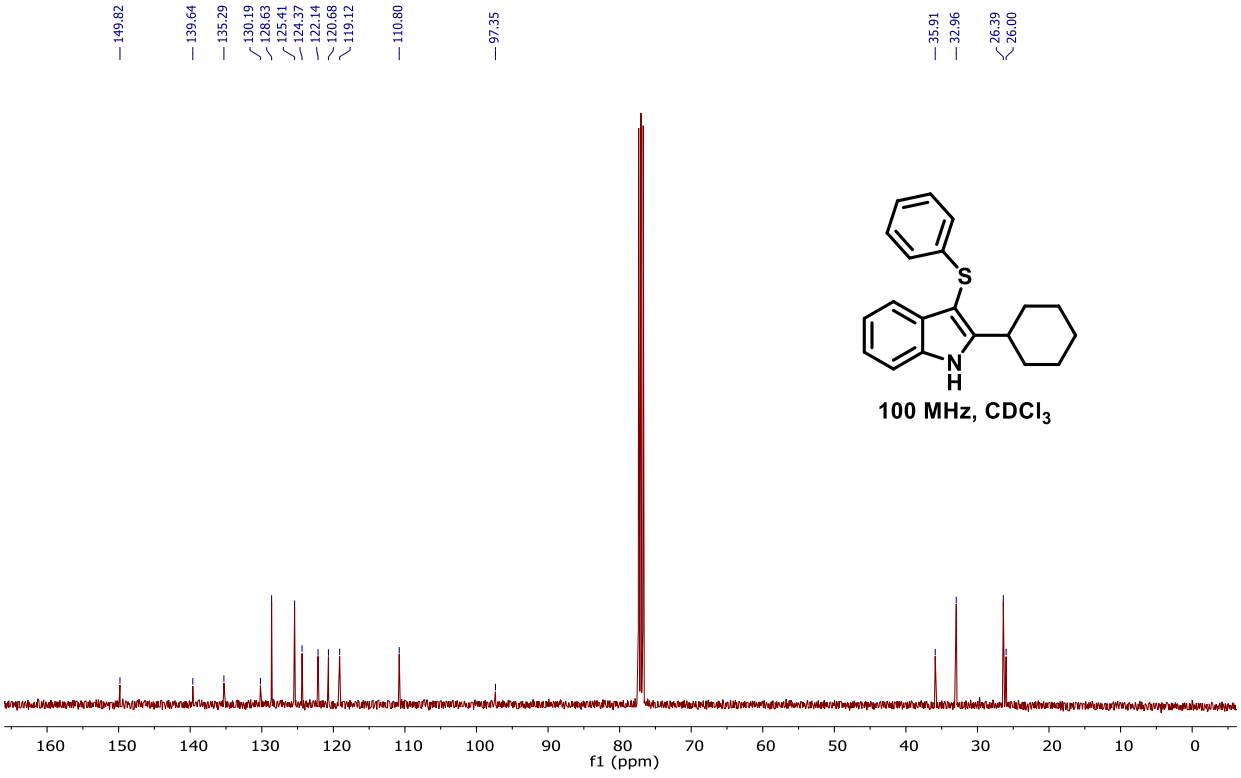
^{13}C NMR for 5f



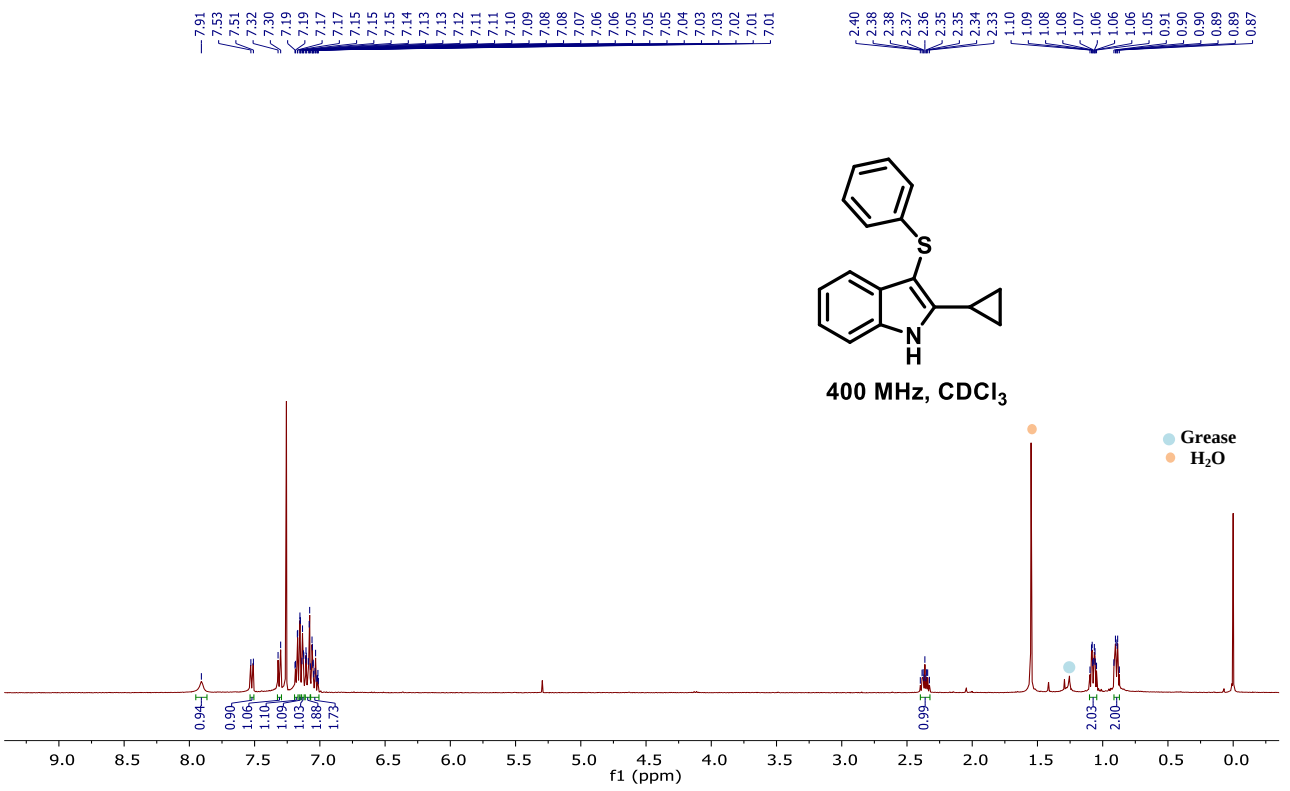
^{1}H NMR for 5g



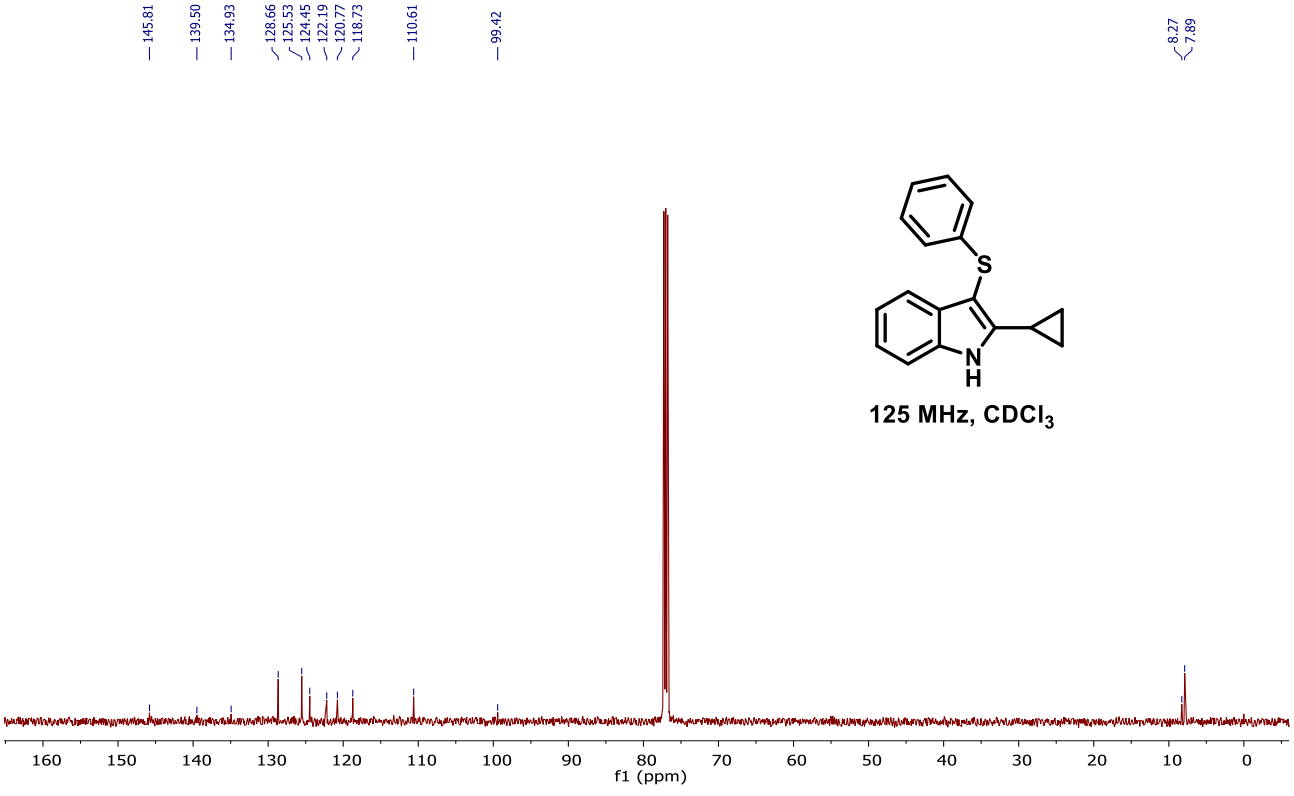
^{13}C NMR for 5g



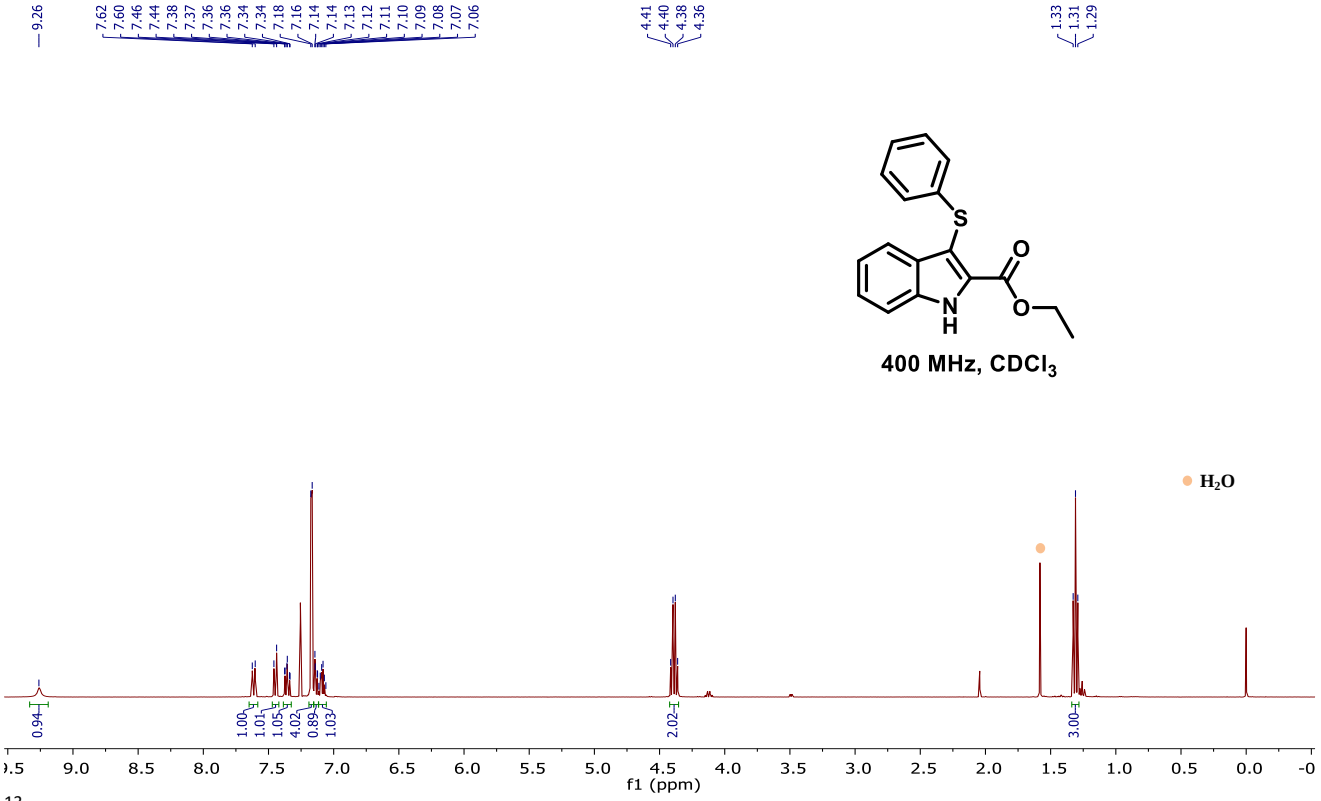
^{1}H NMR for 5h



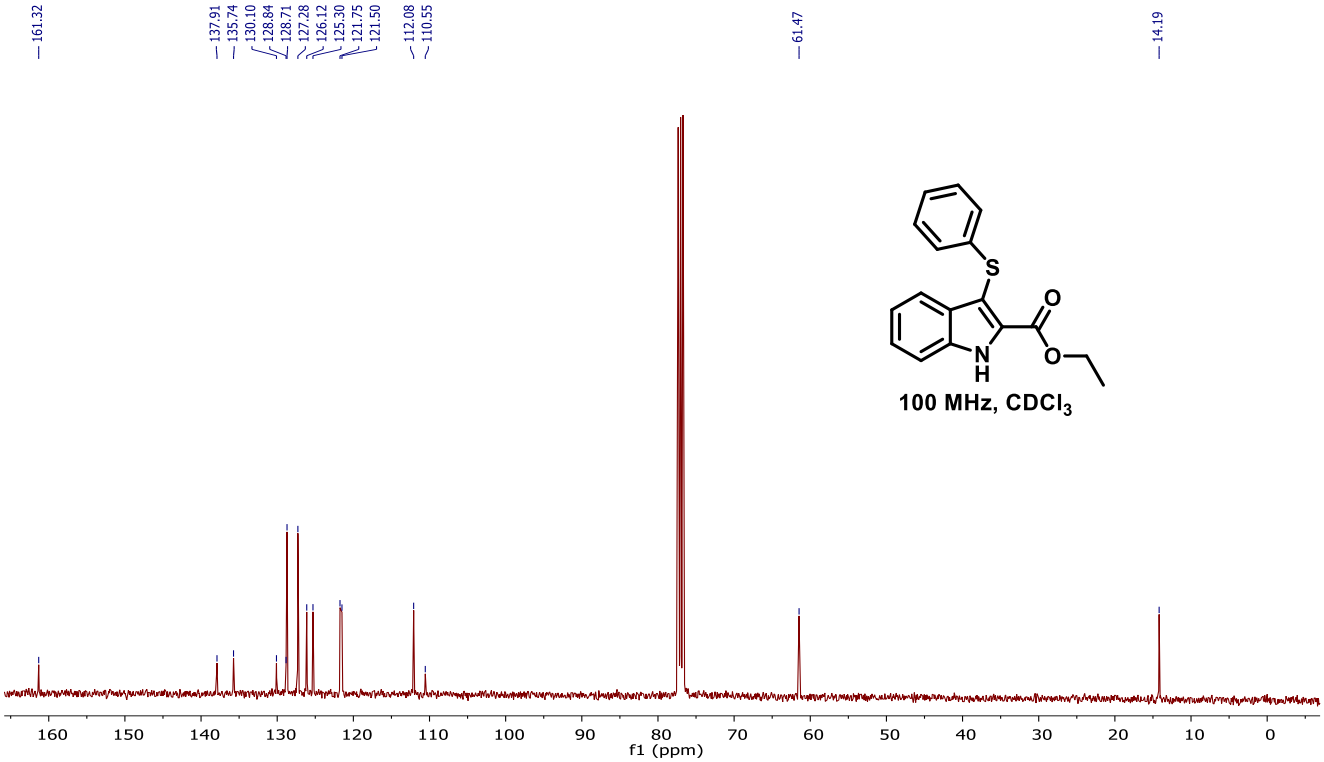
^{13}C NMR for 5h



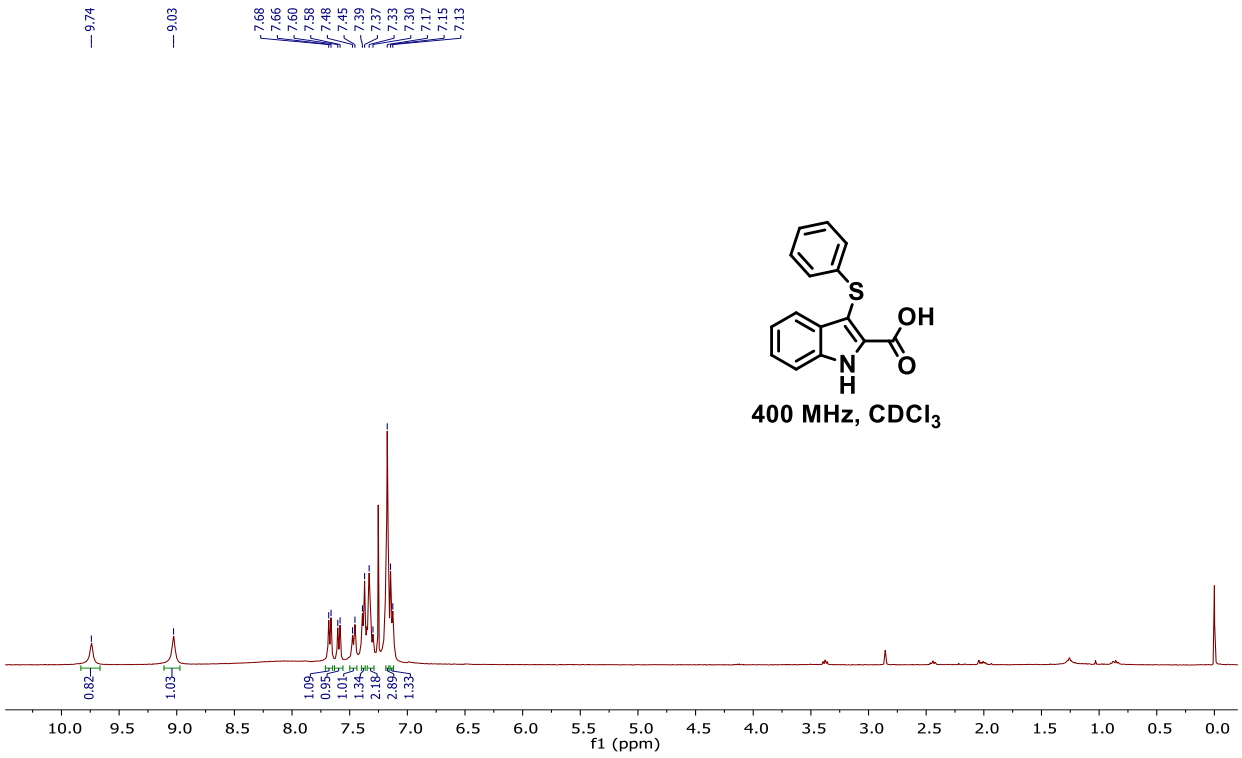
^{1}H NMR for 5i



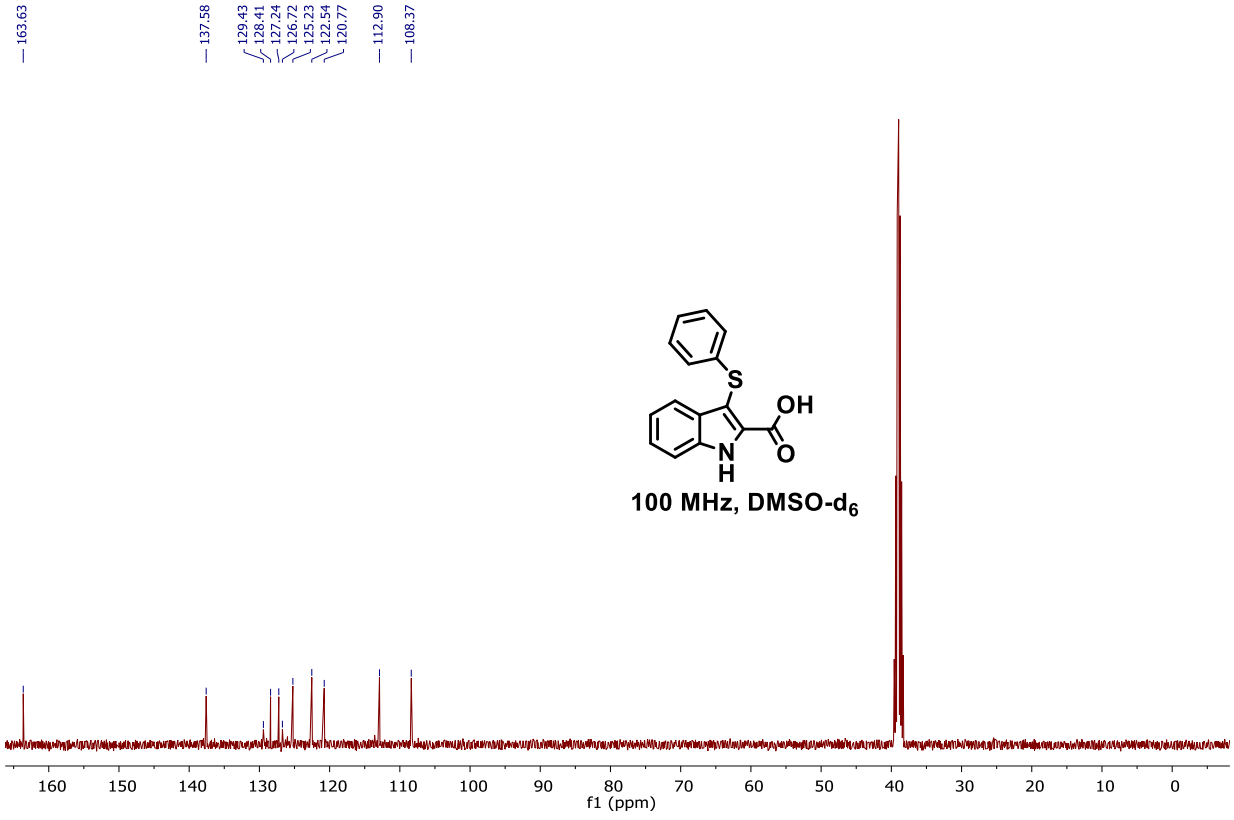
^{13}C NMR for 5i



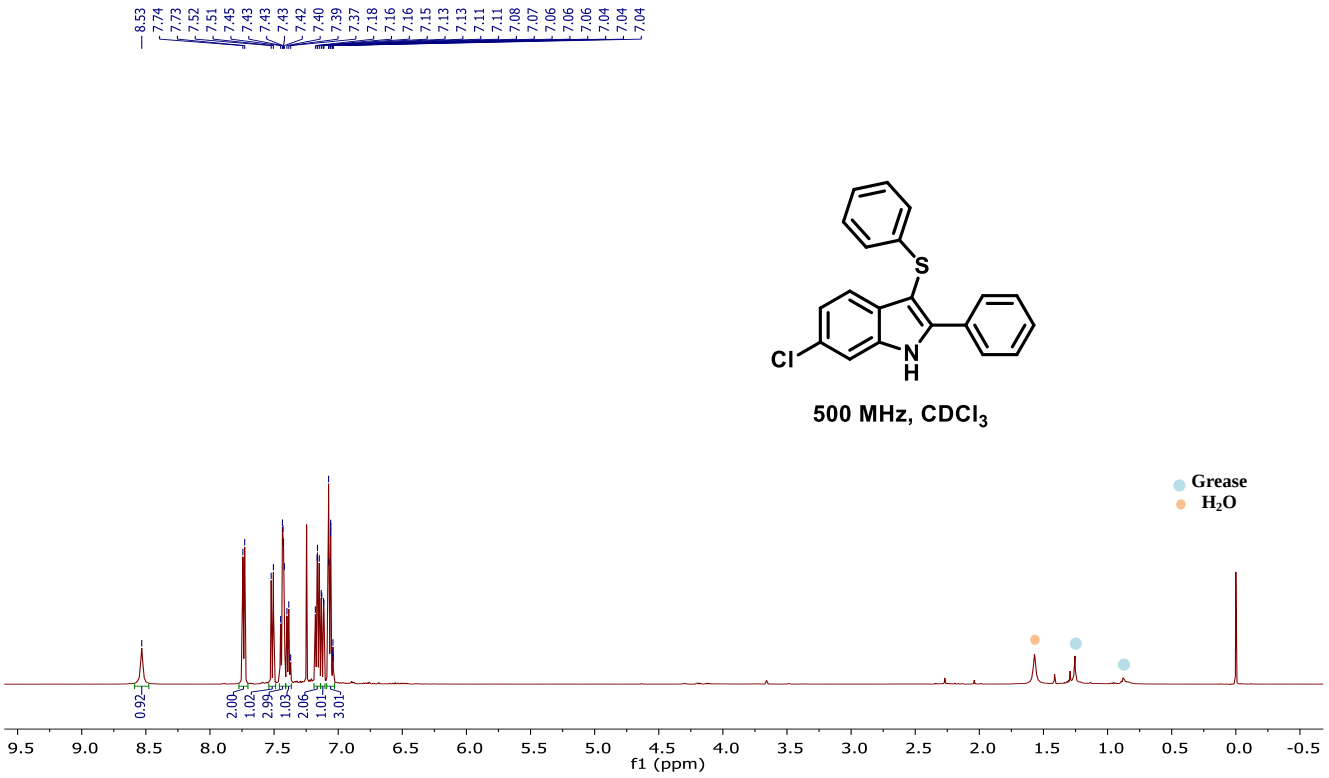
^{1}H NMR for 5j



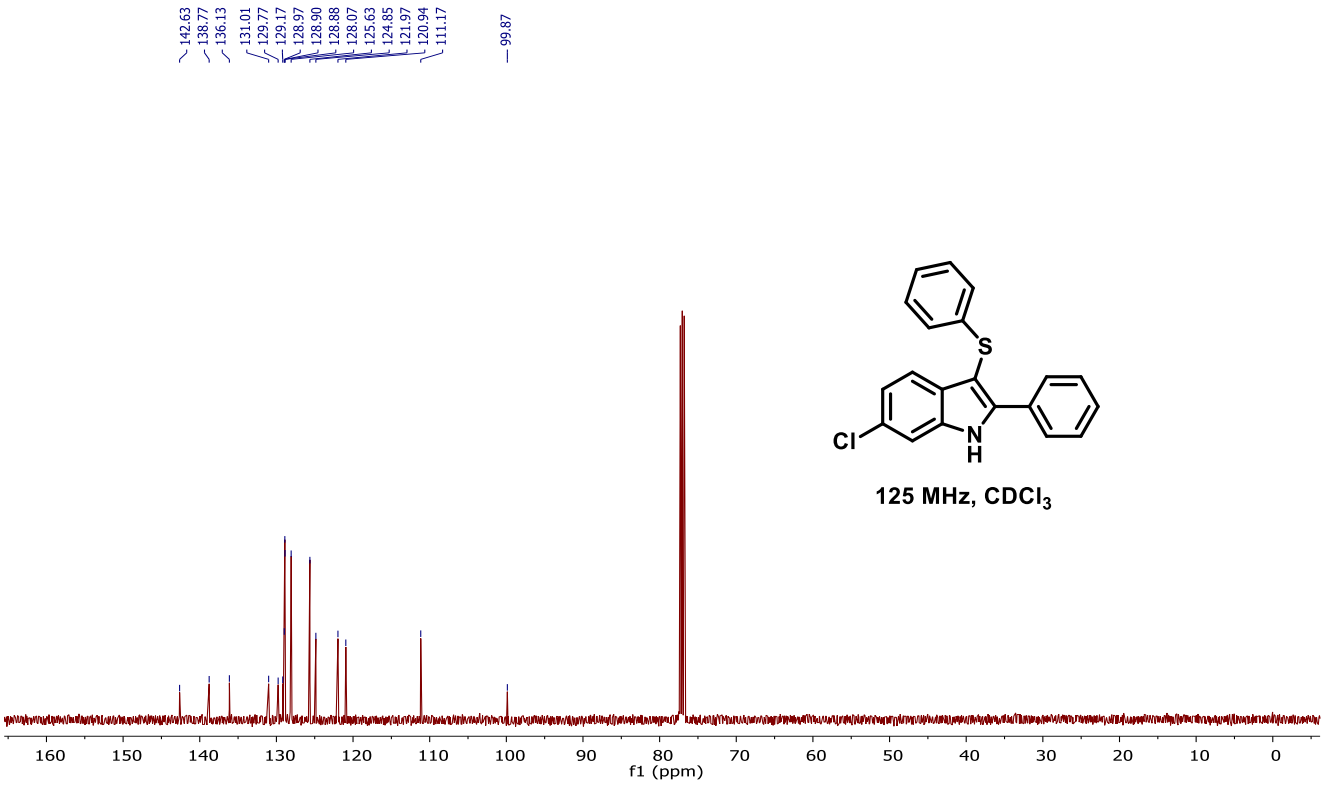
^{13}C NMR for 5j



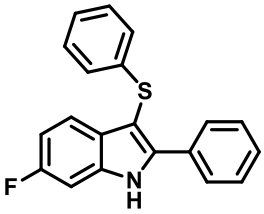
^{1}H NMR for 6a



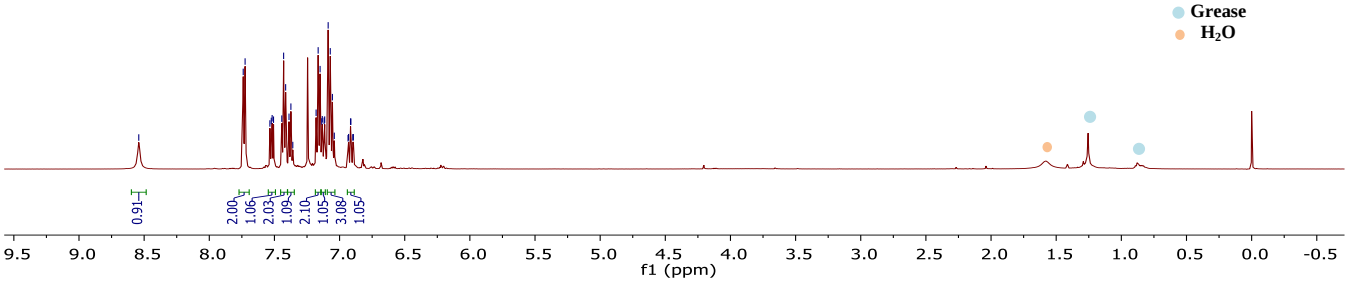
^{13}C NMR for 6a



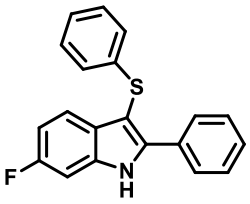
^{1}H NMR for 6b



500 MHz, $CDCl_3$

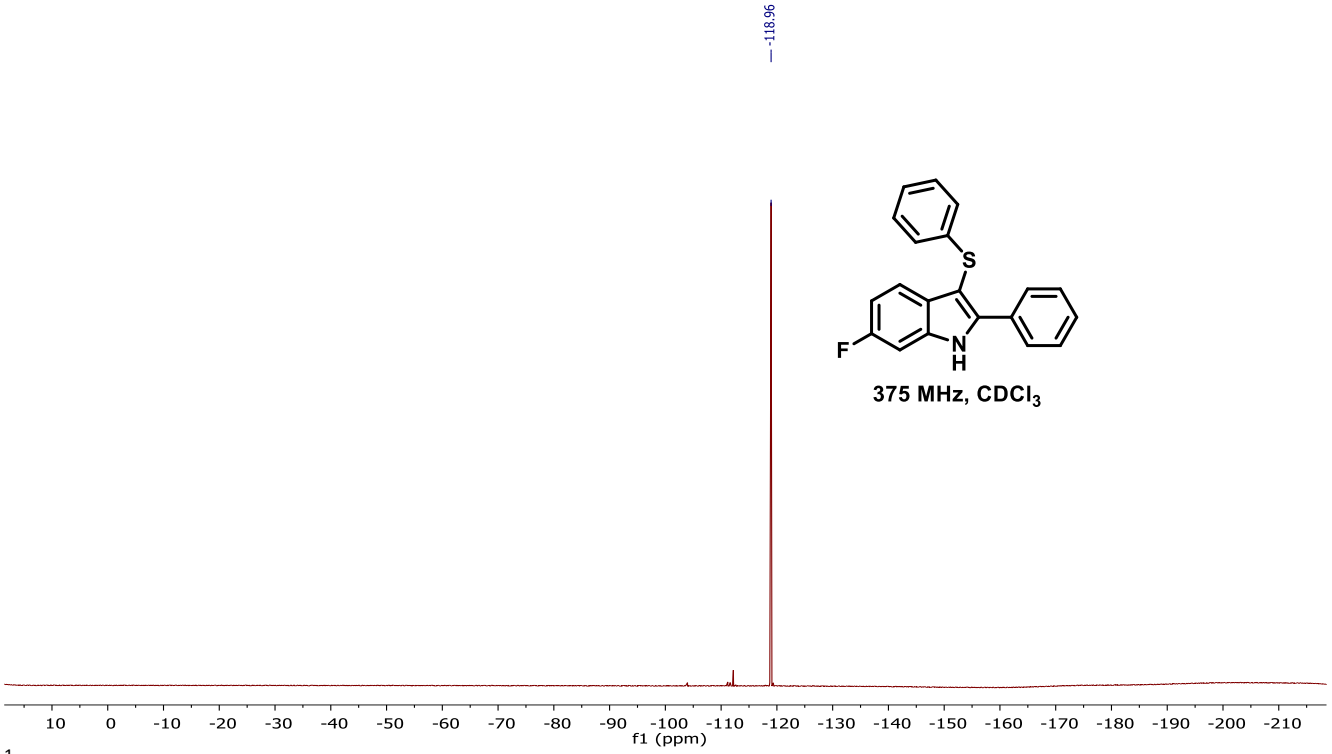


^{13}C NMR for 6b

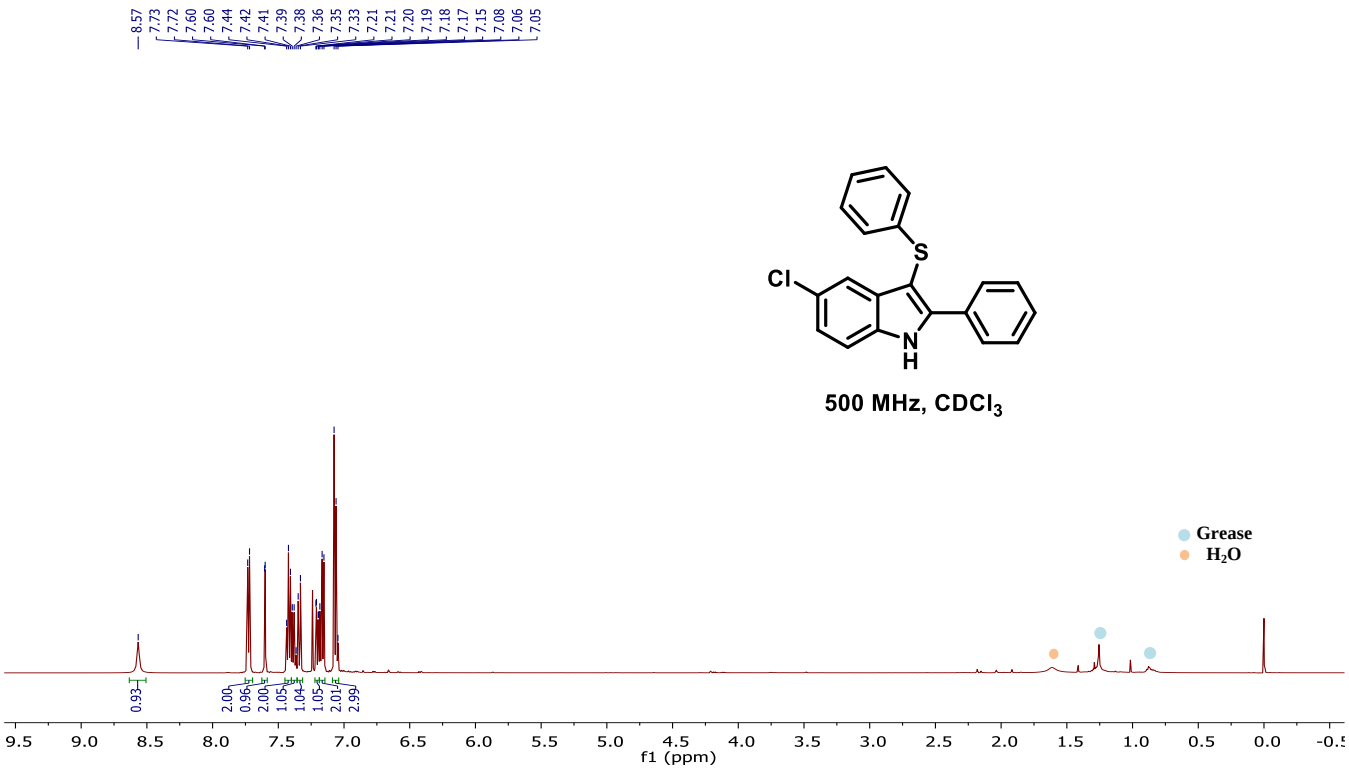


125 MHz, $CDCl_3$

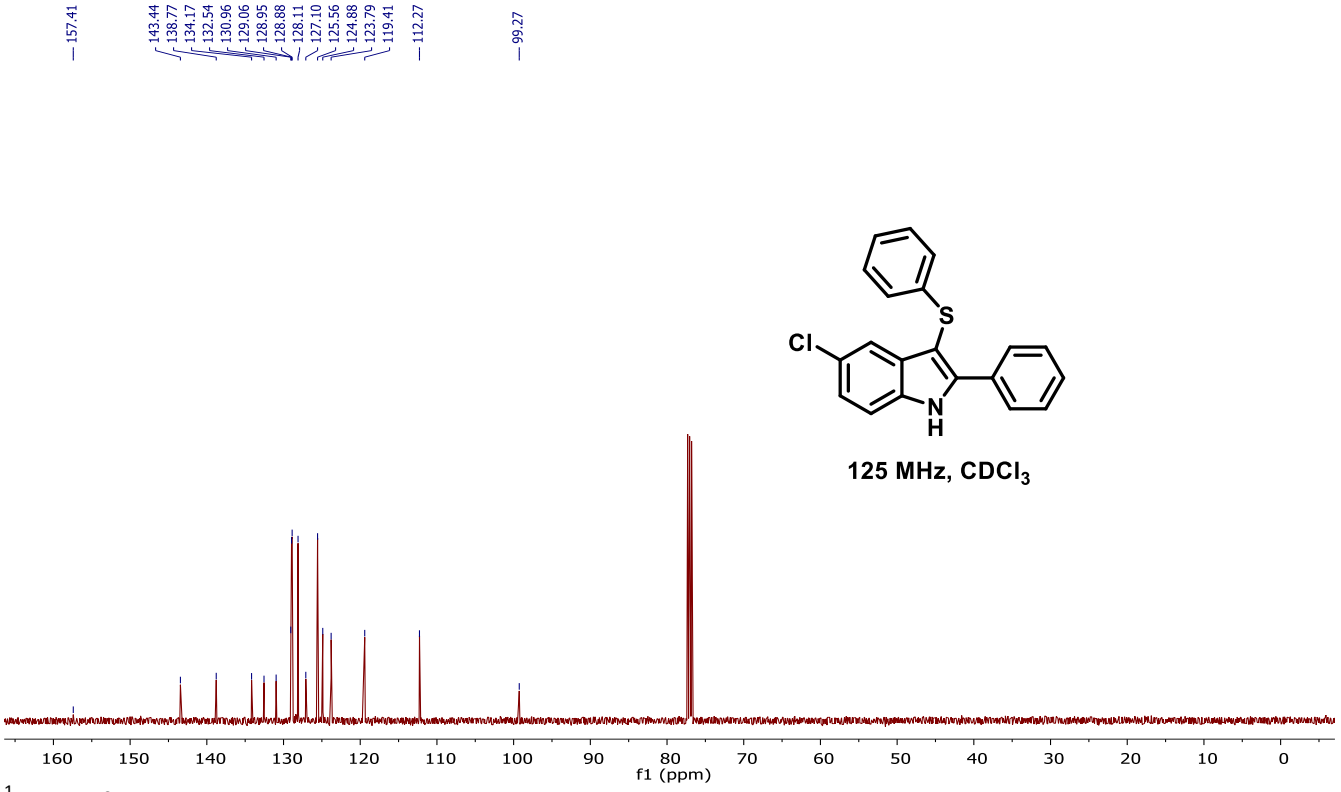
^{19}F NMR for 6b



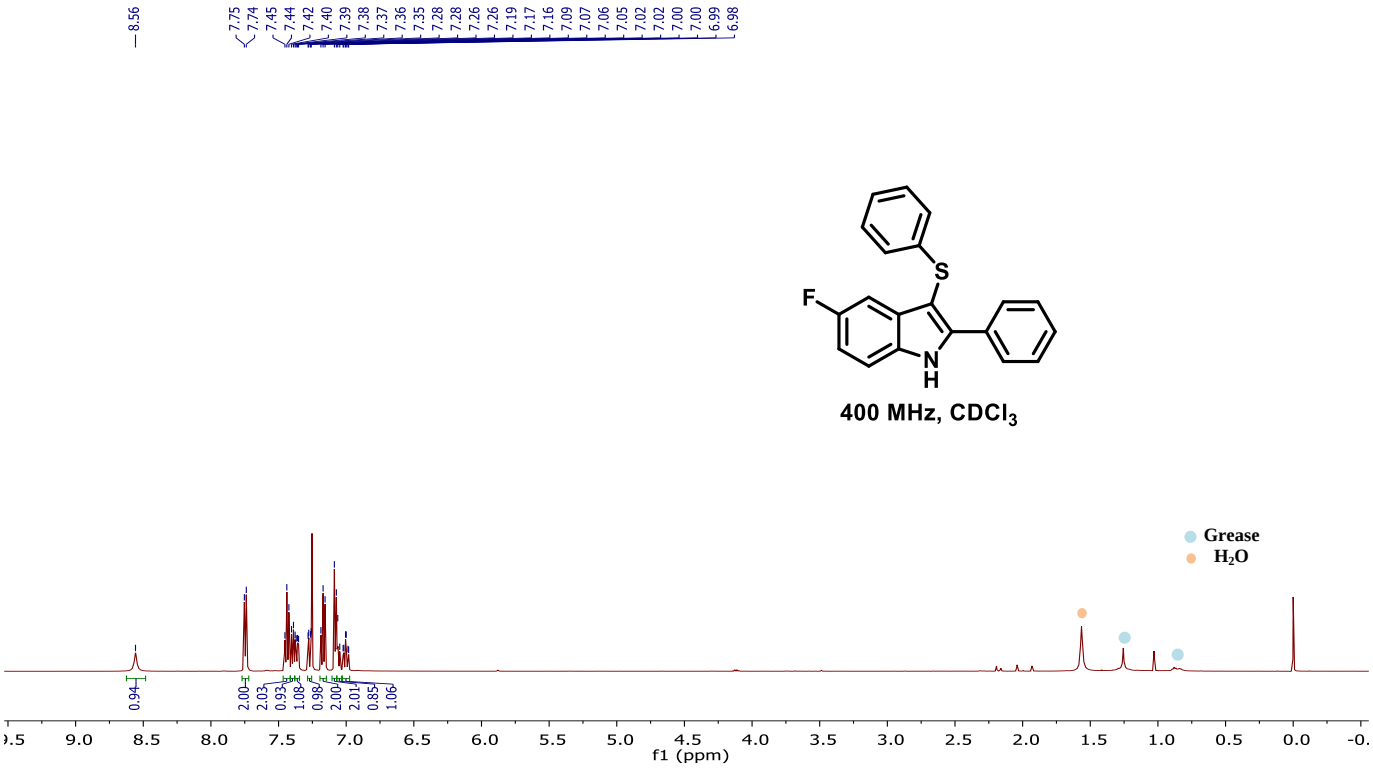
^{1}H NMR for 6c



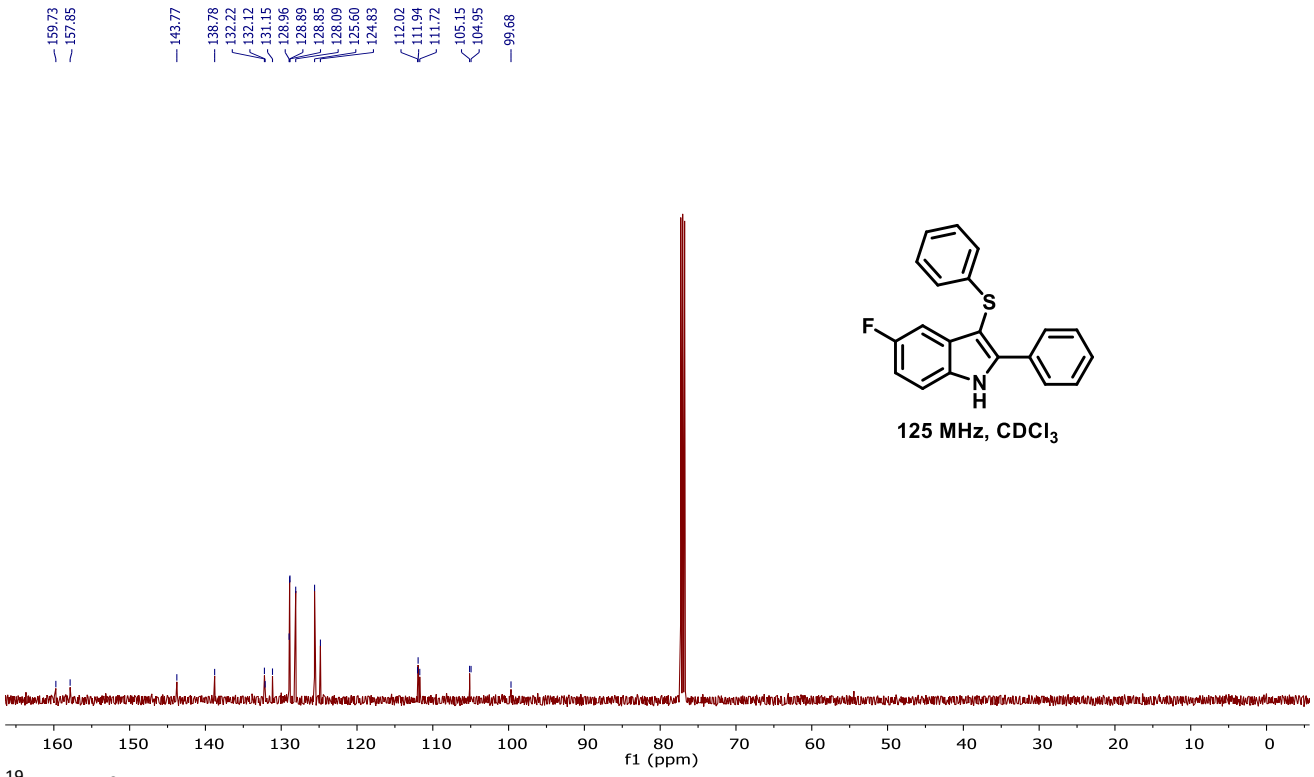
^{13}C NMR for 6c



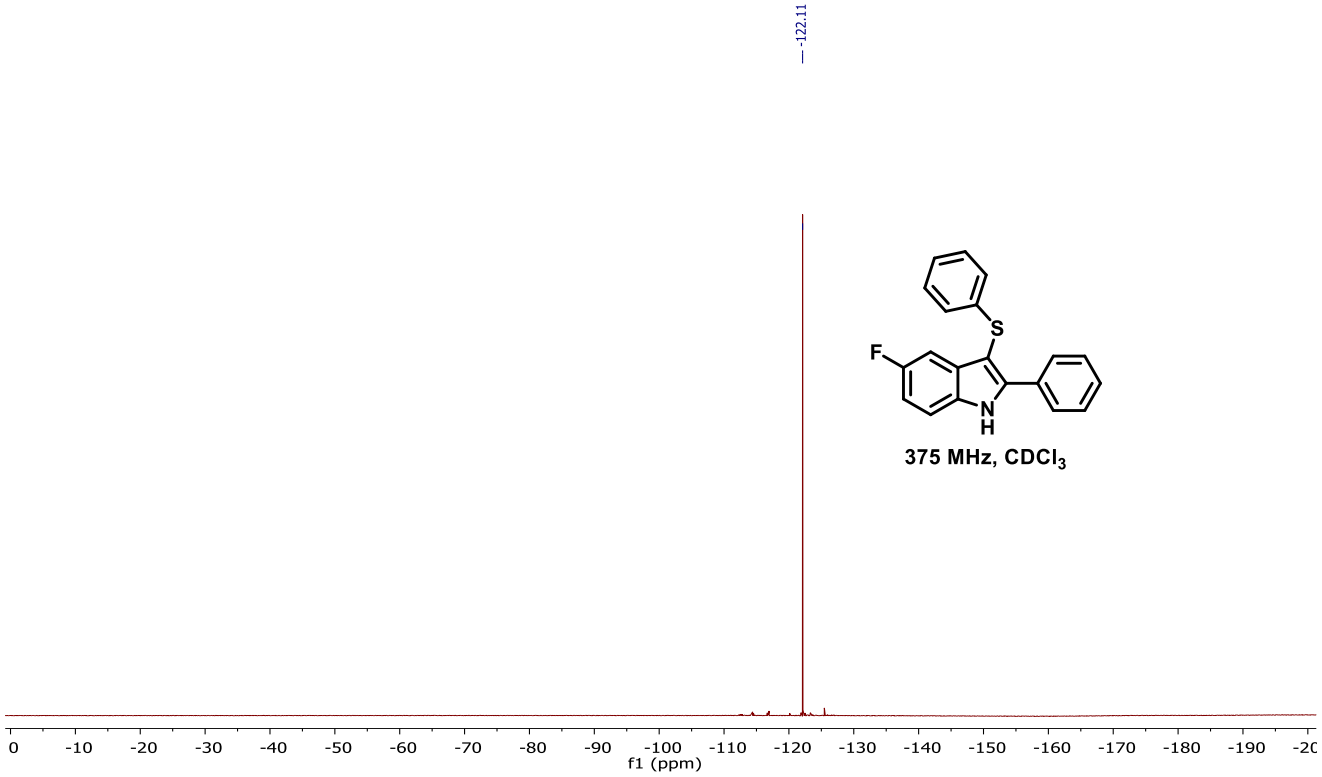
^{1}H NMR for 6d



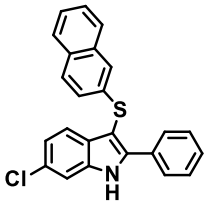
^{13}C NMR for 6d



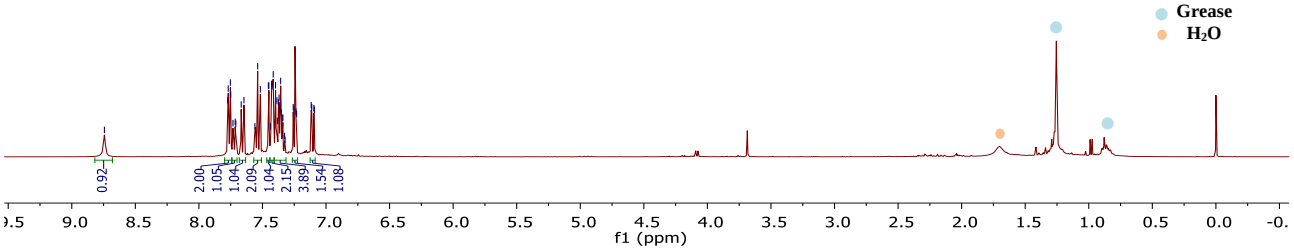
^{19}F NMR for 6d



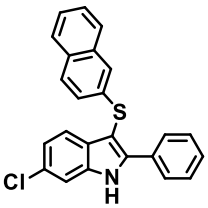
^{1}H NMR for 6e



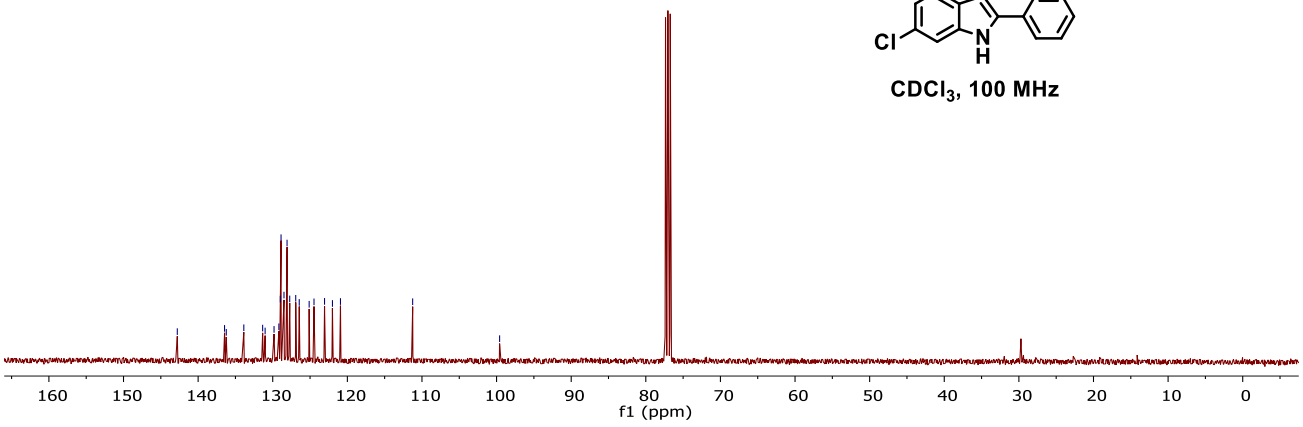
$CDCl_3$, 400 MHz



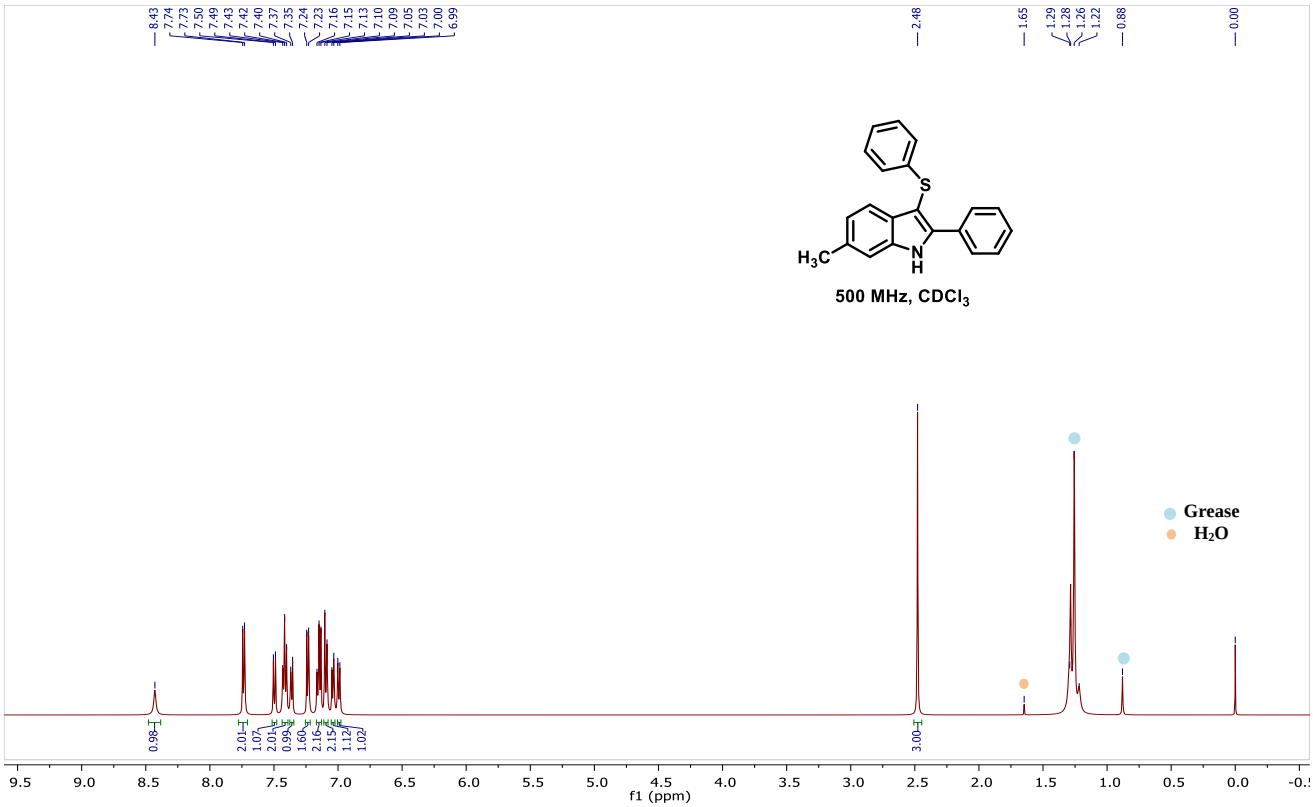
^{13}C NMR for 6e



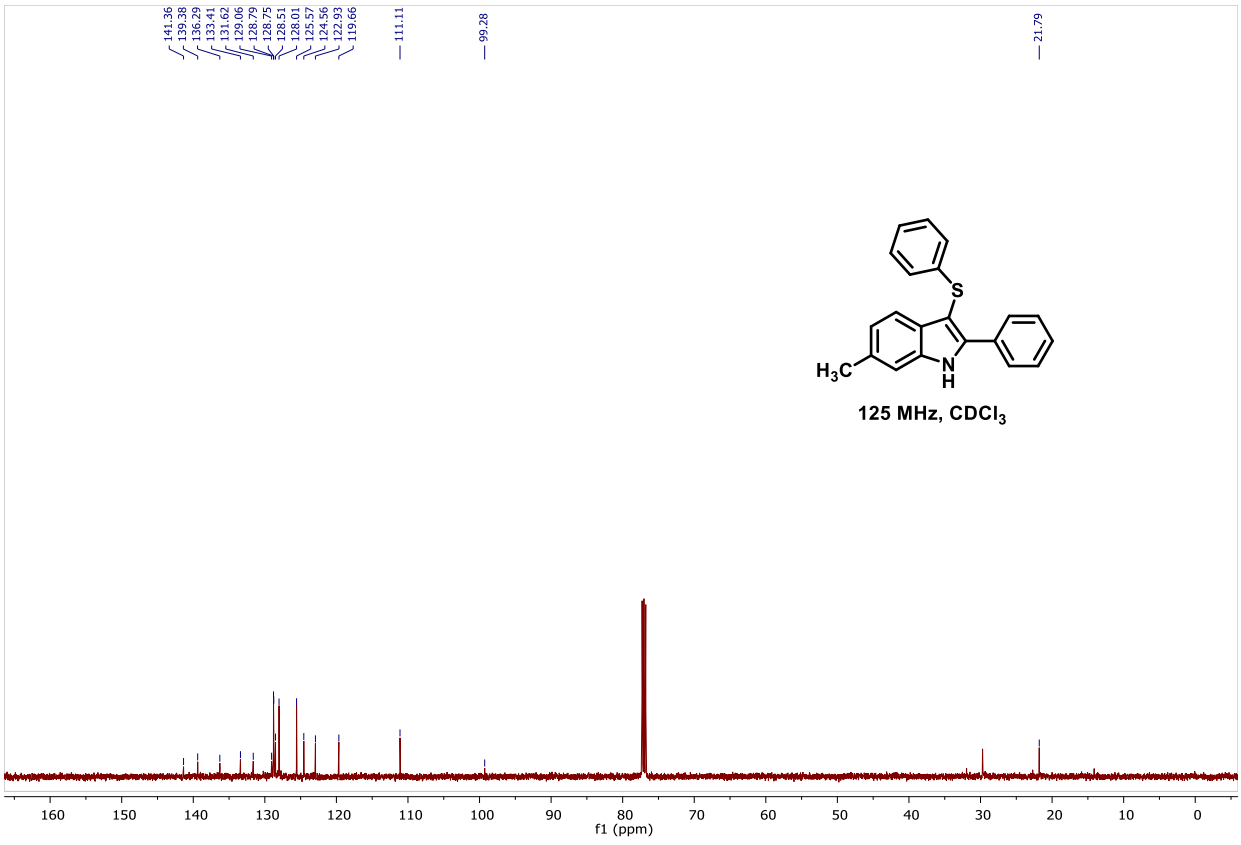
$CDCl_3$, 100 MHz



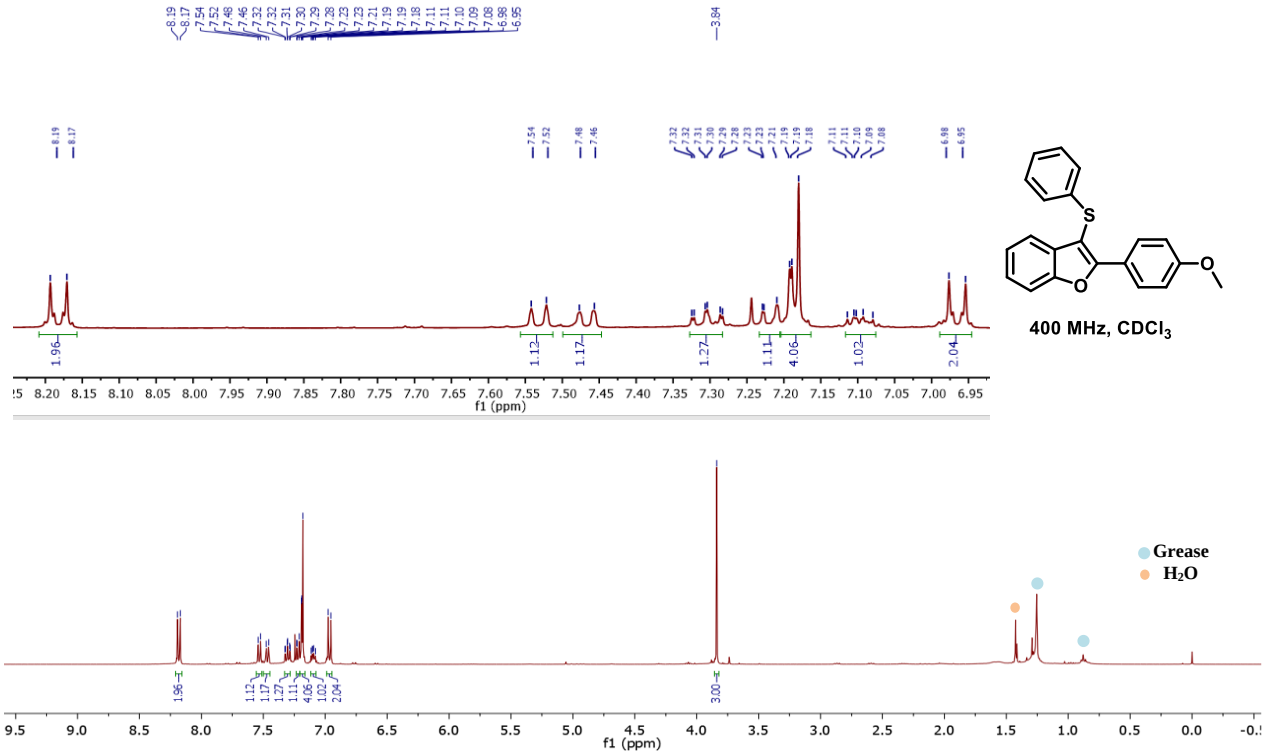
^{1}H NMR For 6g



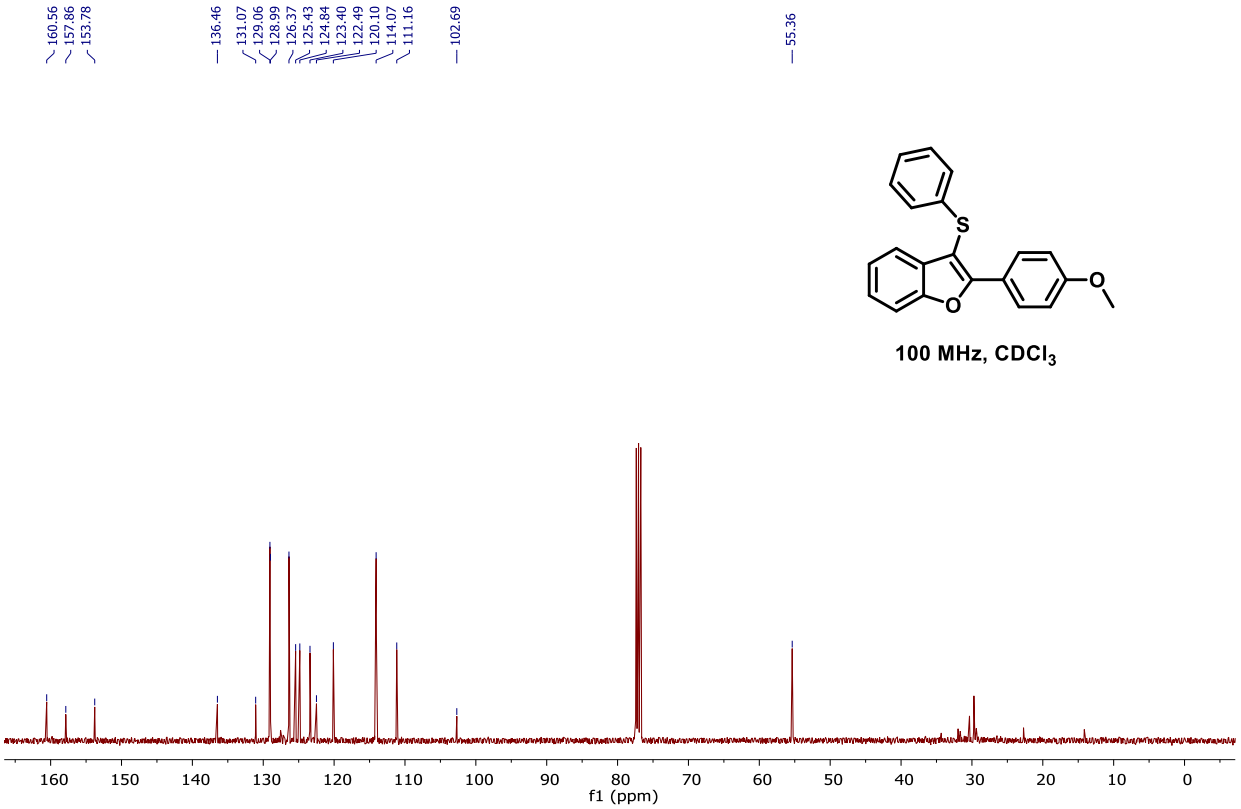
^{13}C NMR for 6g



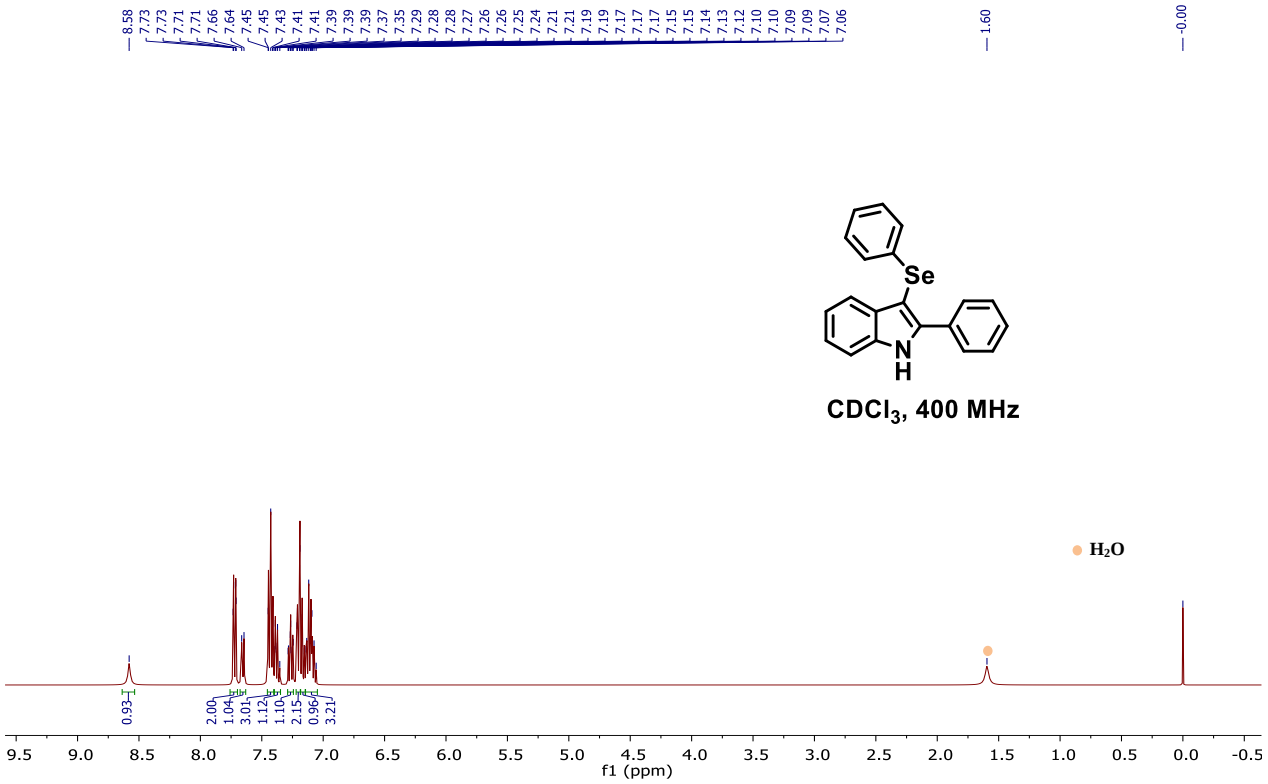
^{1}H NMR for 6h



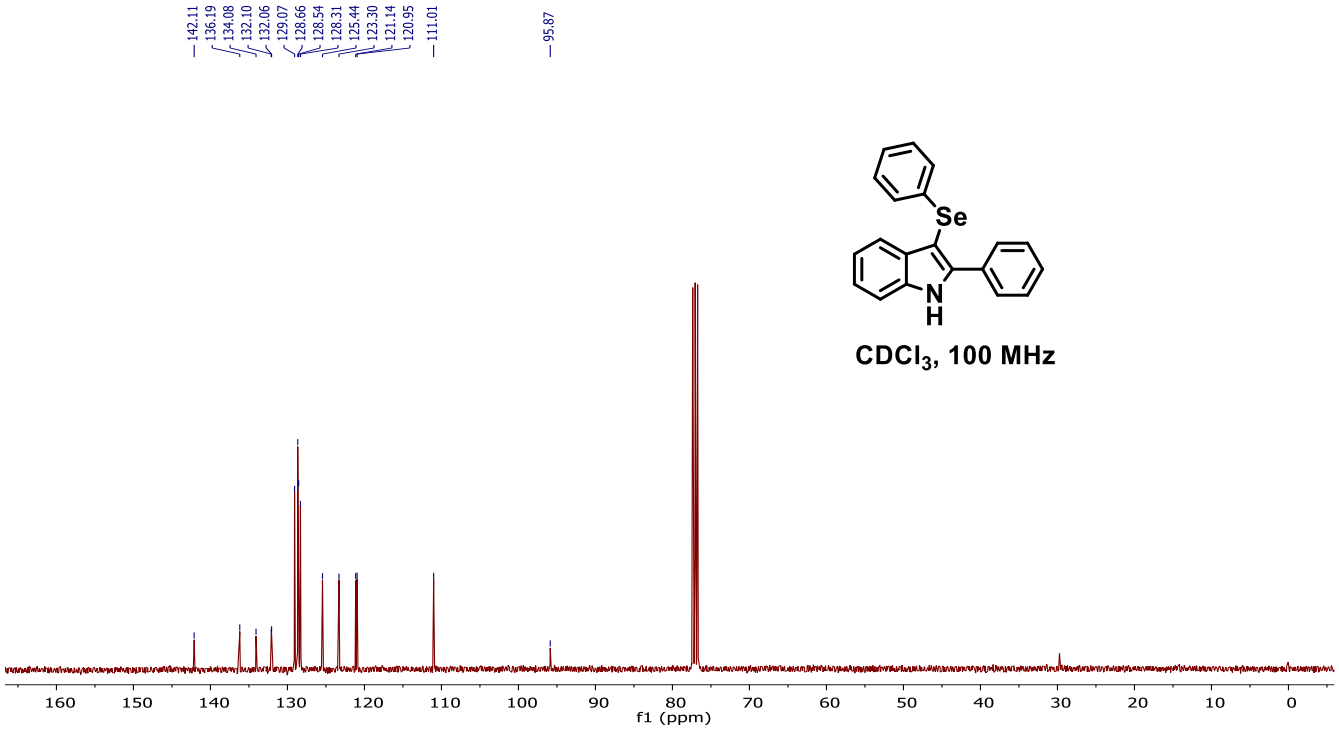
^{13}C NMR for 6h



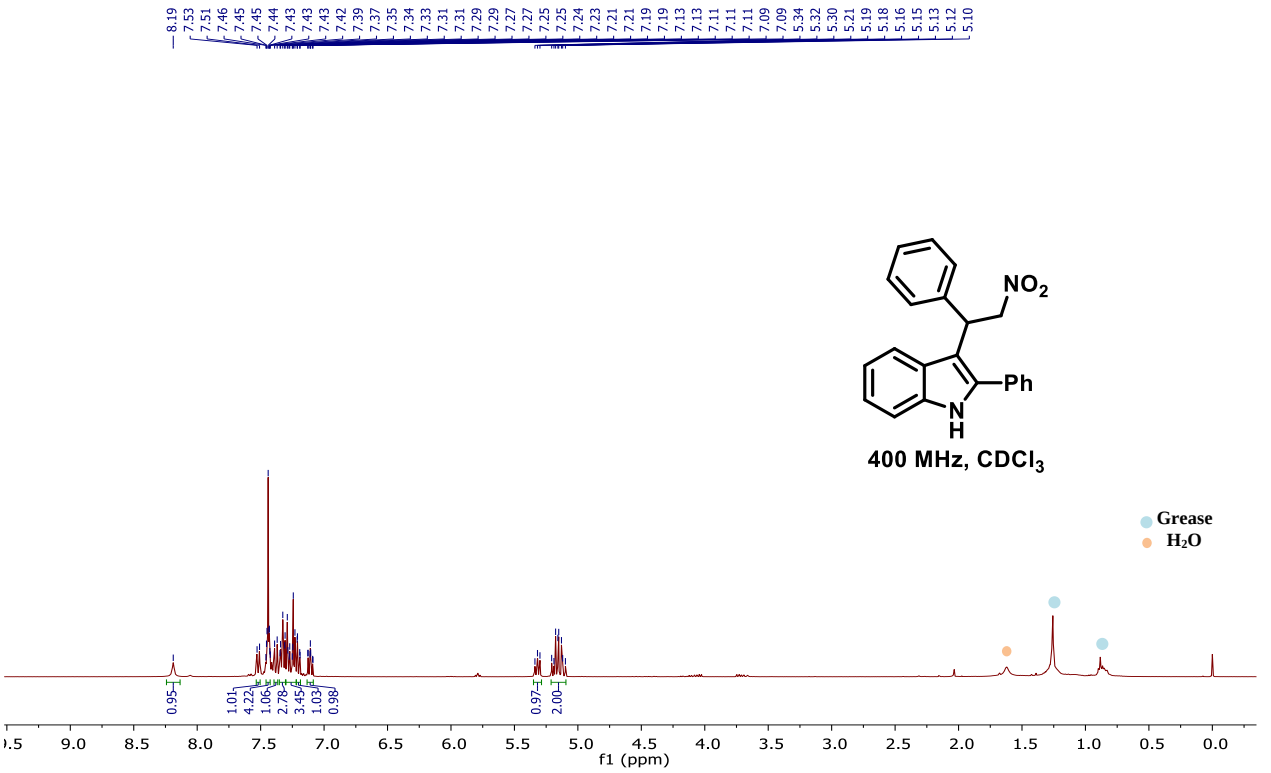
^{1}H NMR for 7



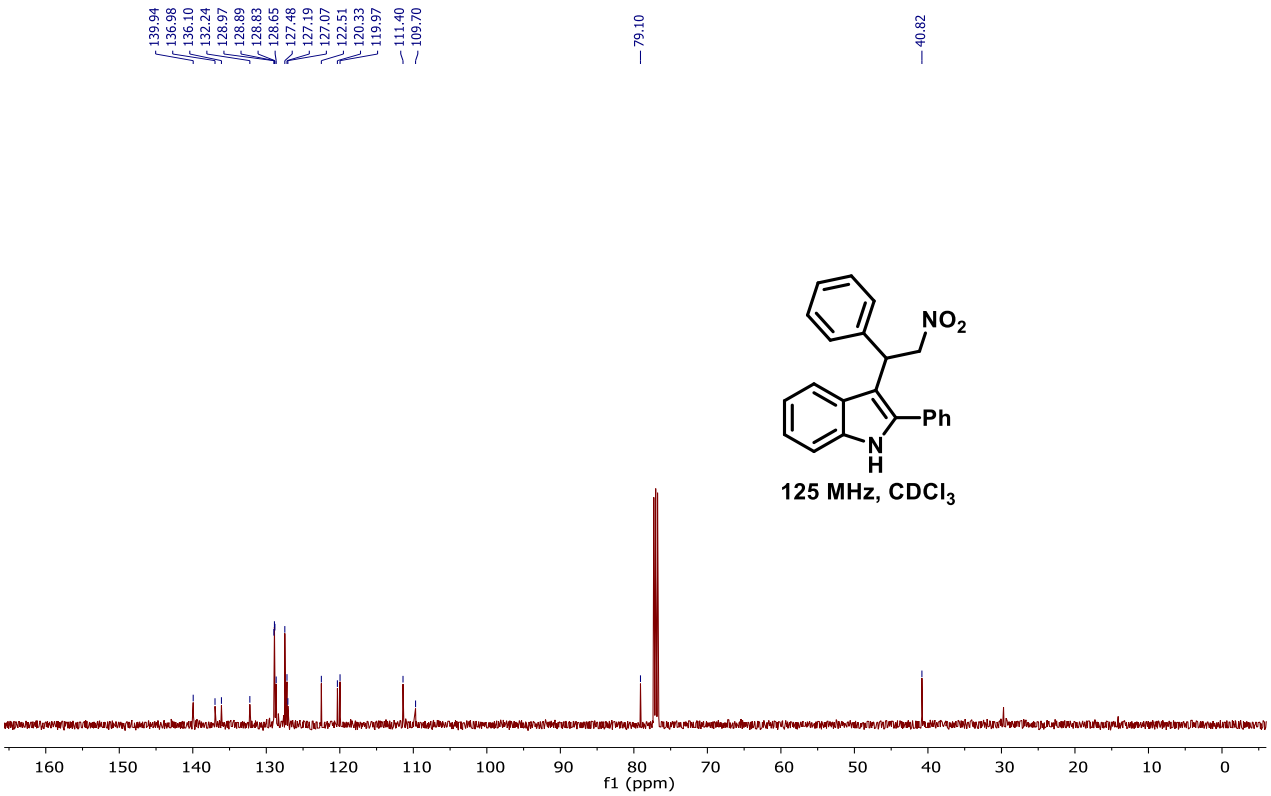
^{13}C NMR for 7



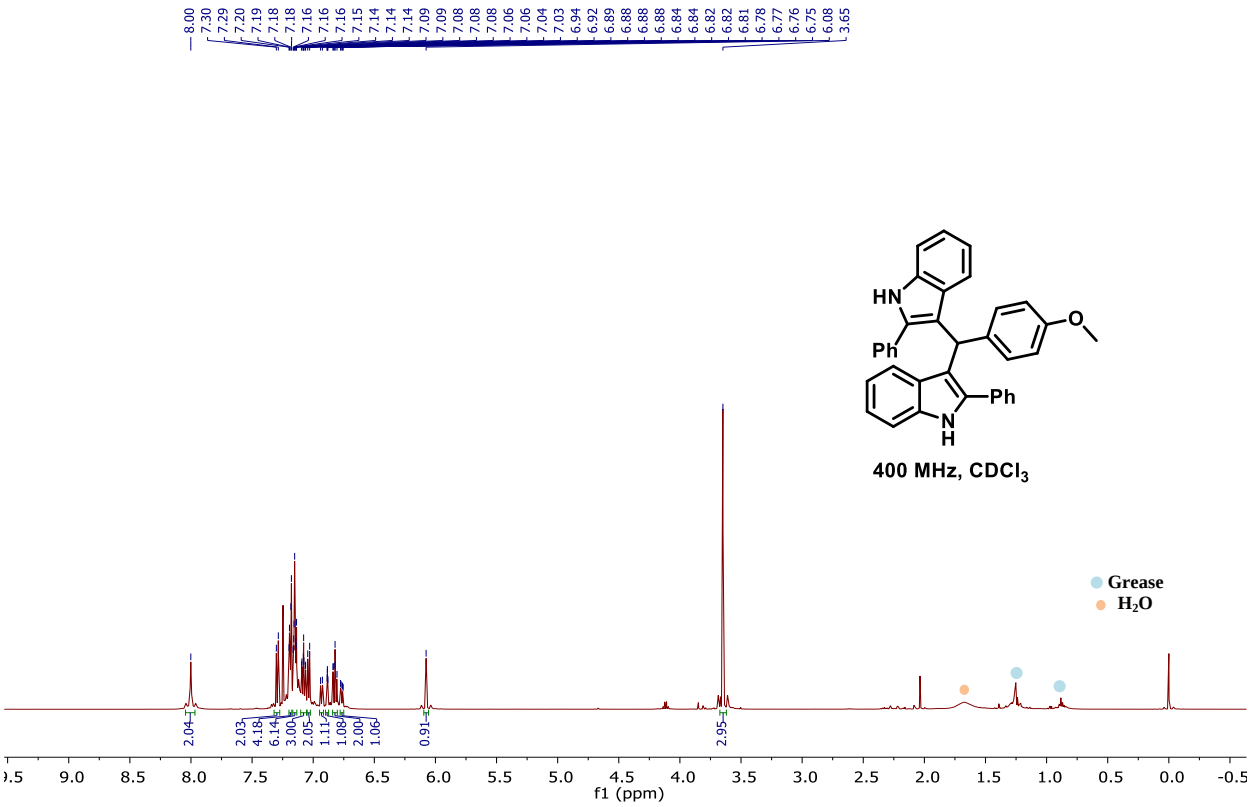
^{1}H NMR for 8



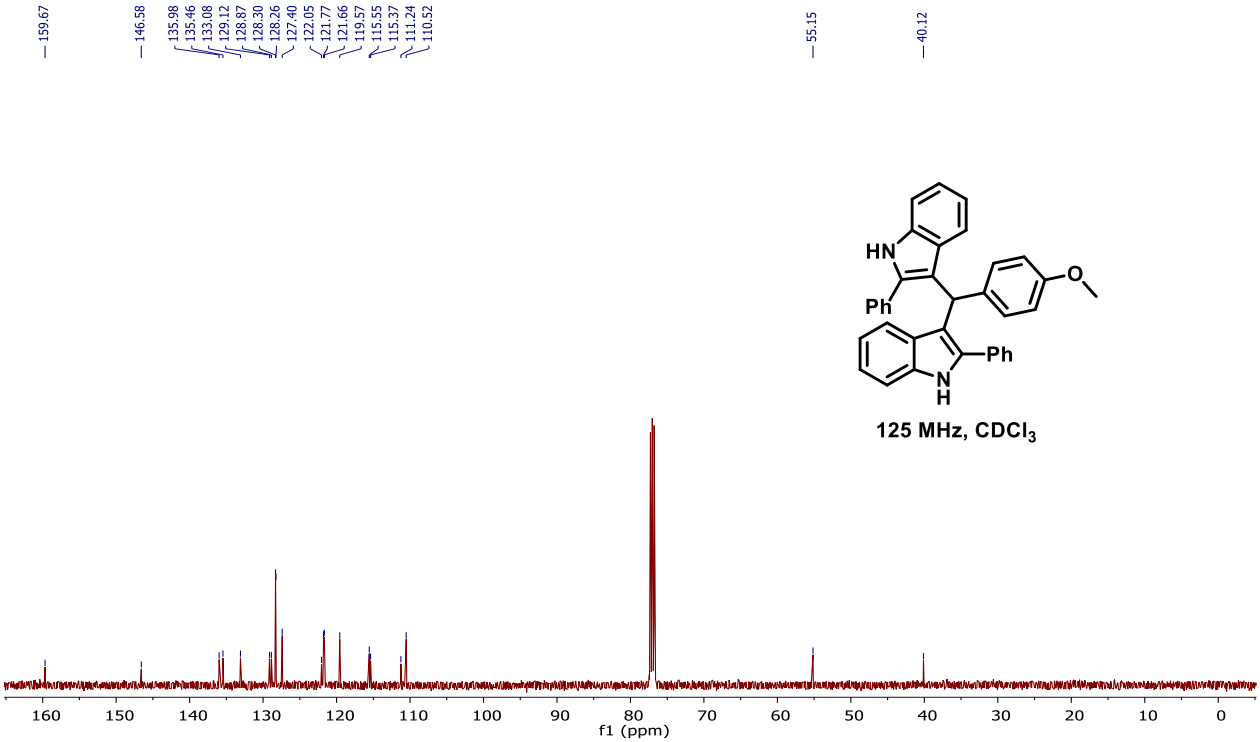
^{13}C NMR for 8



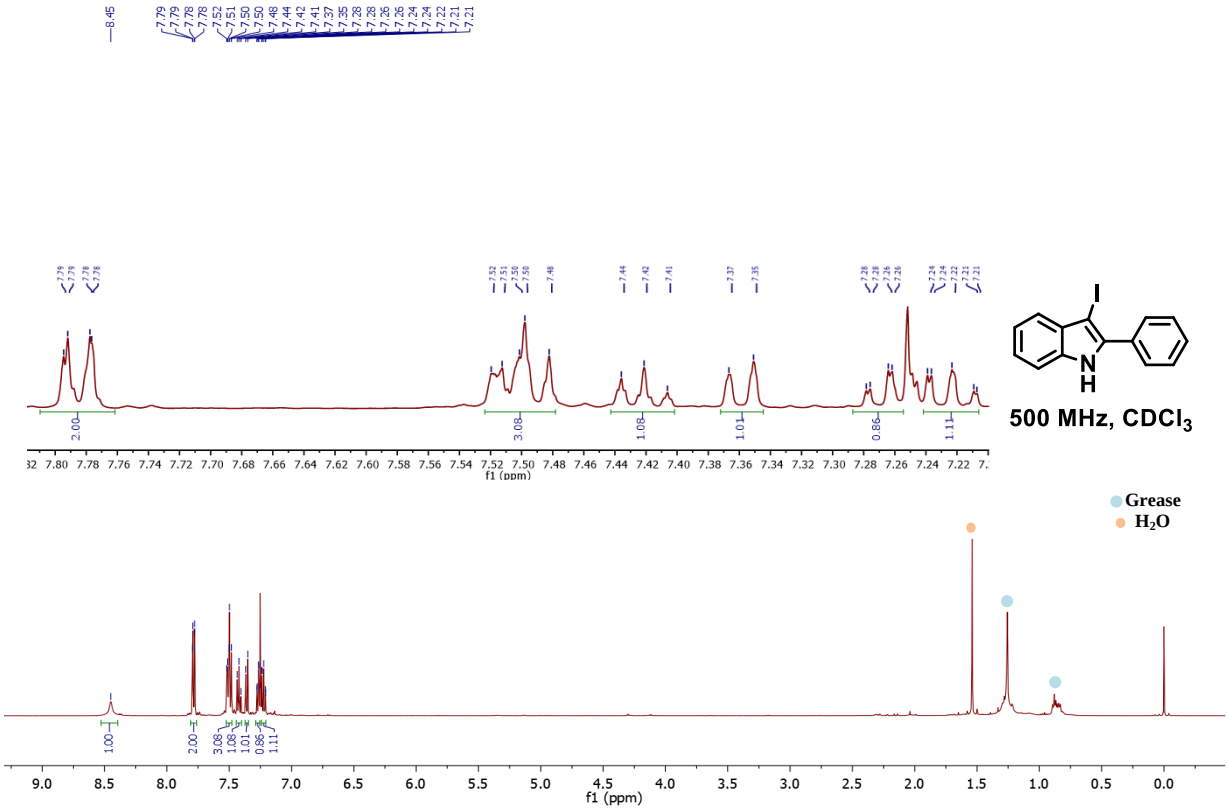
^{1}H NMR for 9



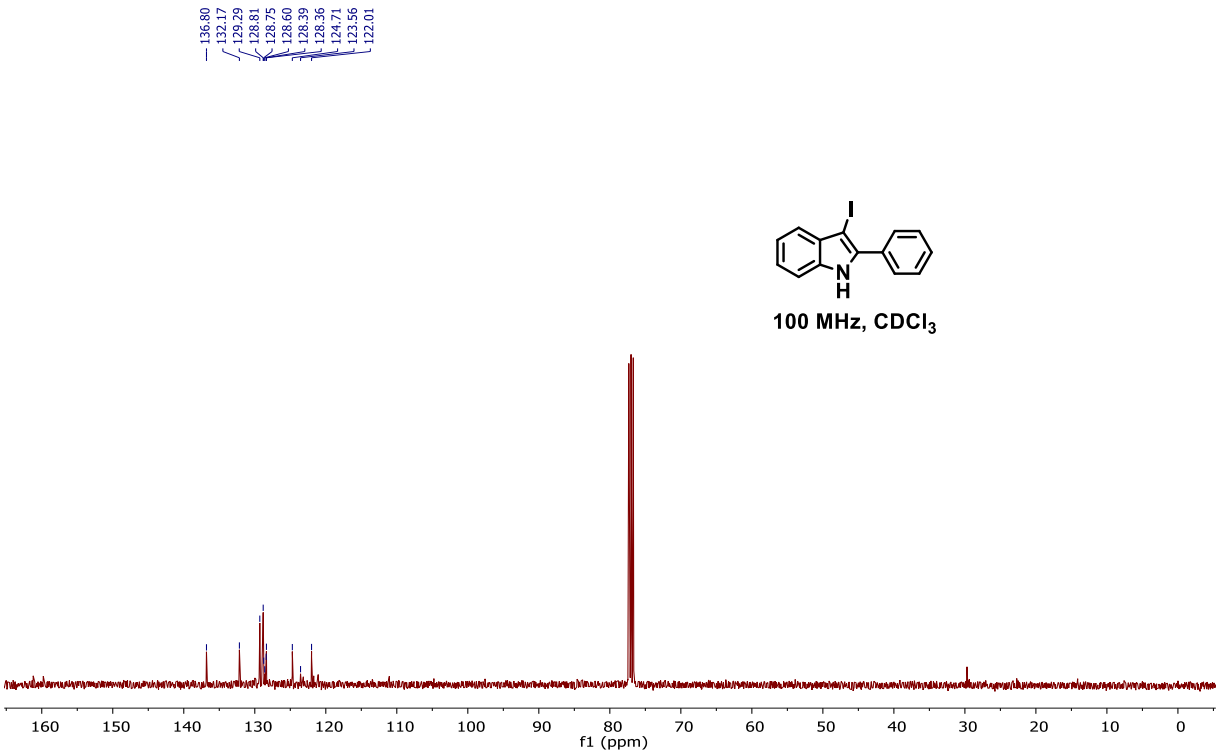
^{13}C NMR for 9



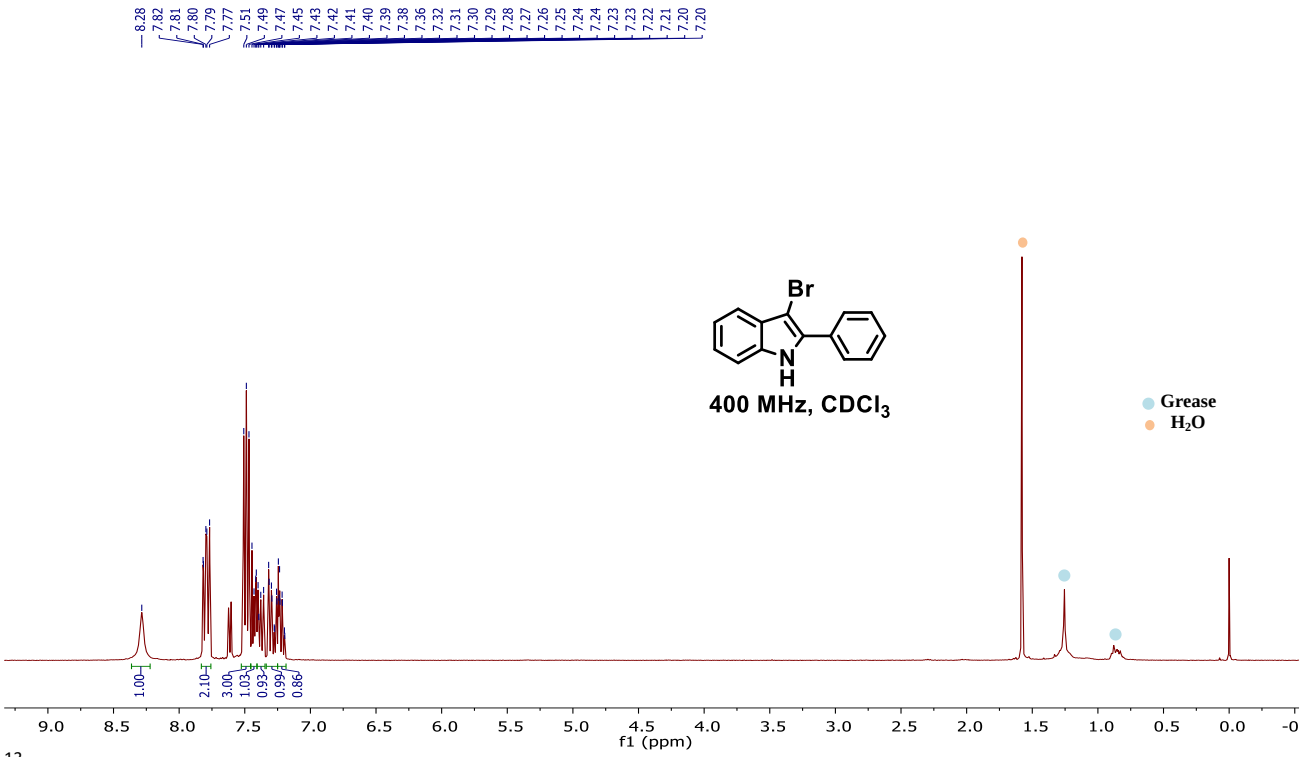
^{1}H NMR for 10



^{13}C NMR for 10



^{1}H NMR for 11



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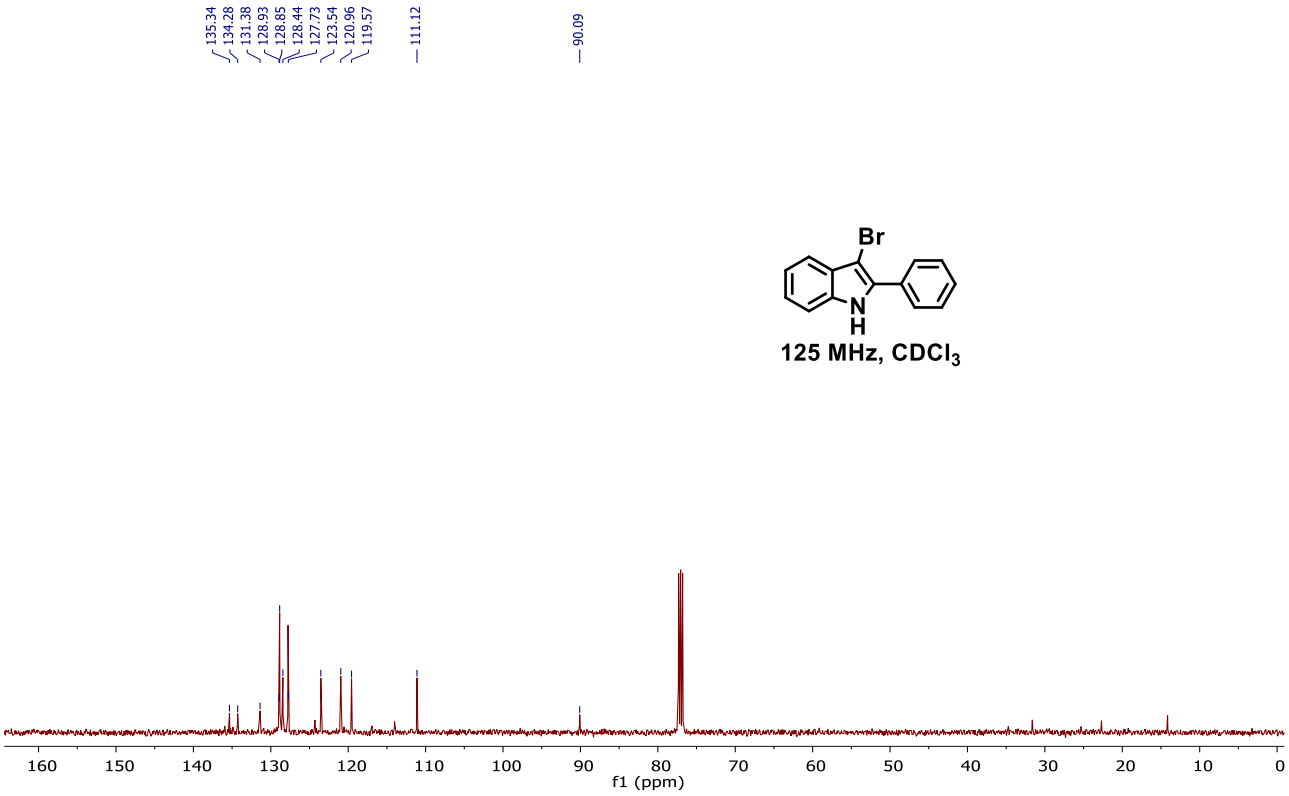
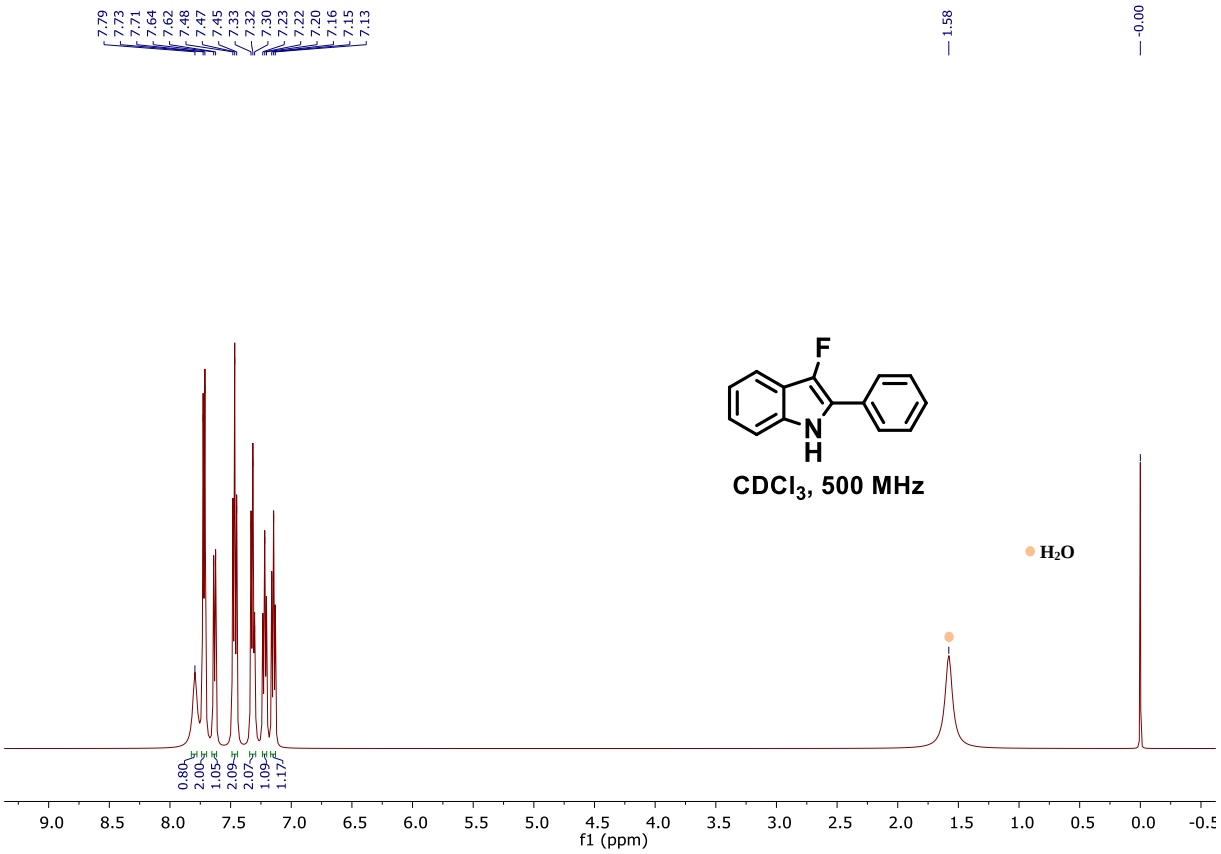
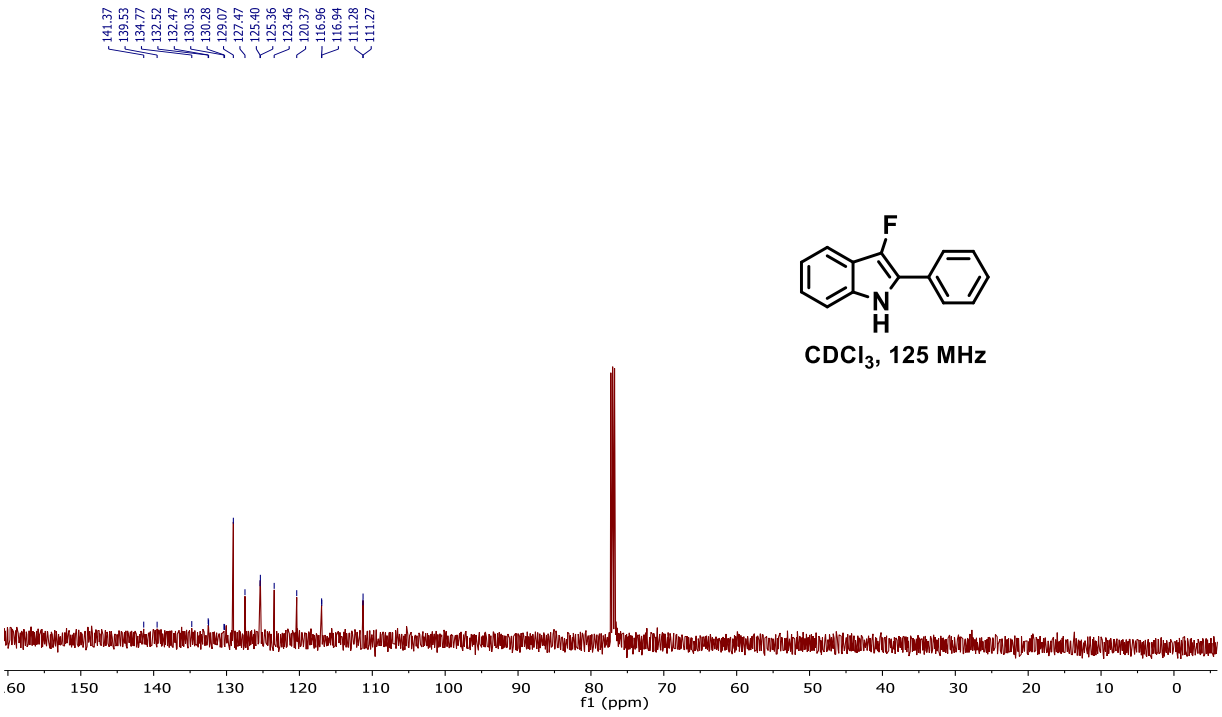


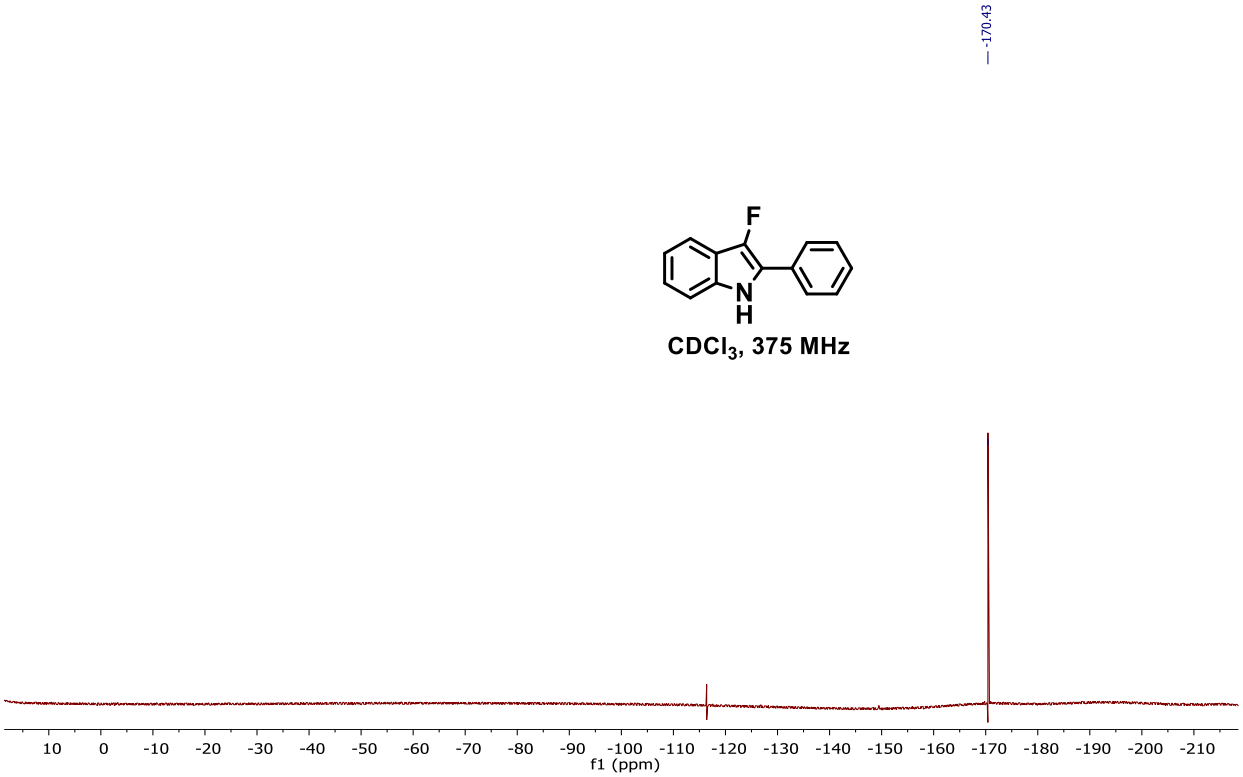
^{1}H NMR for 12



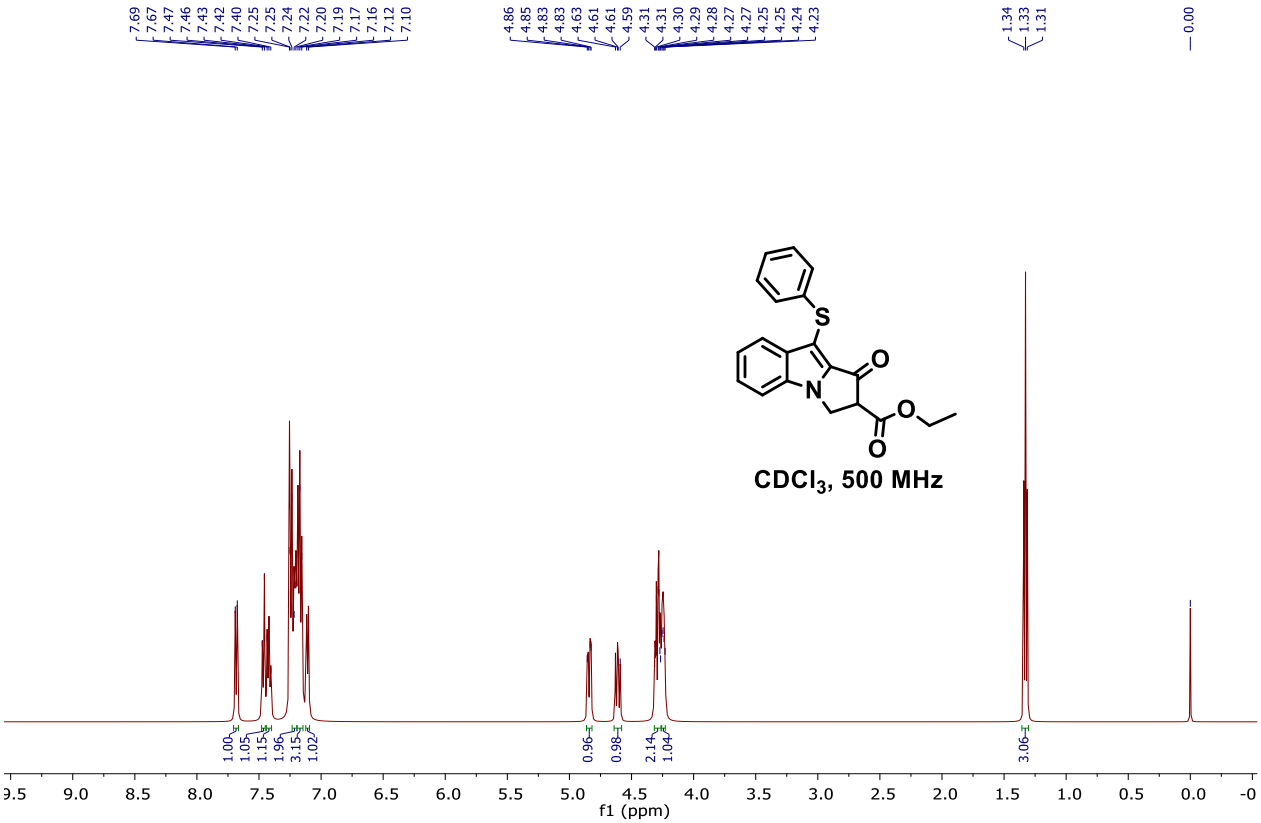
^{13}C NMR for 12



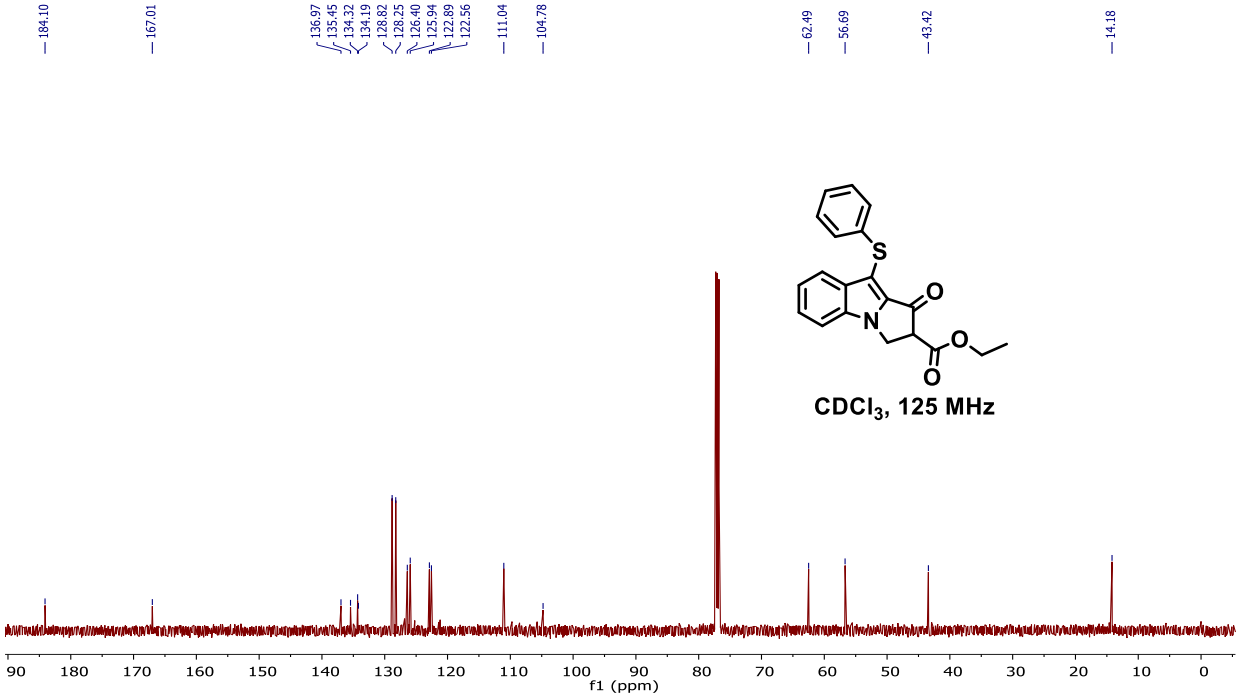
^{19}F NMR for 12



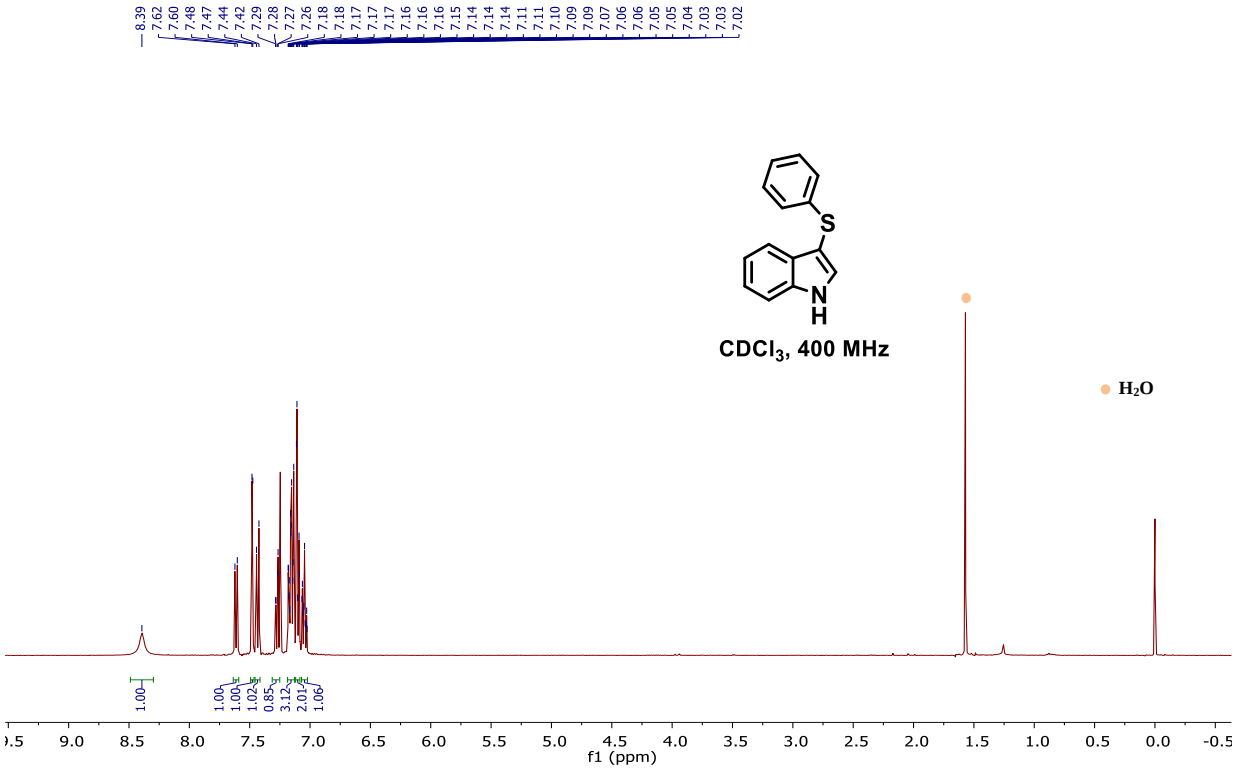
^{1}H NMR for 13



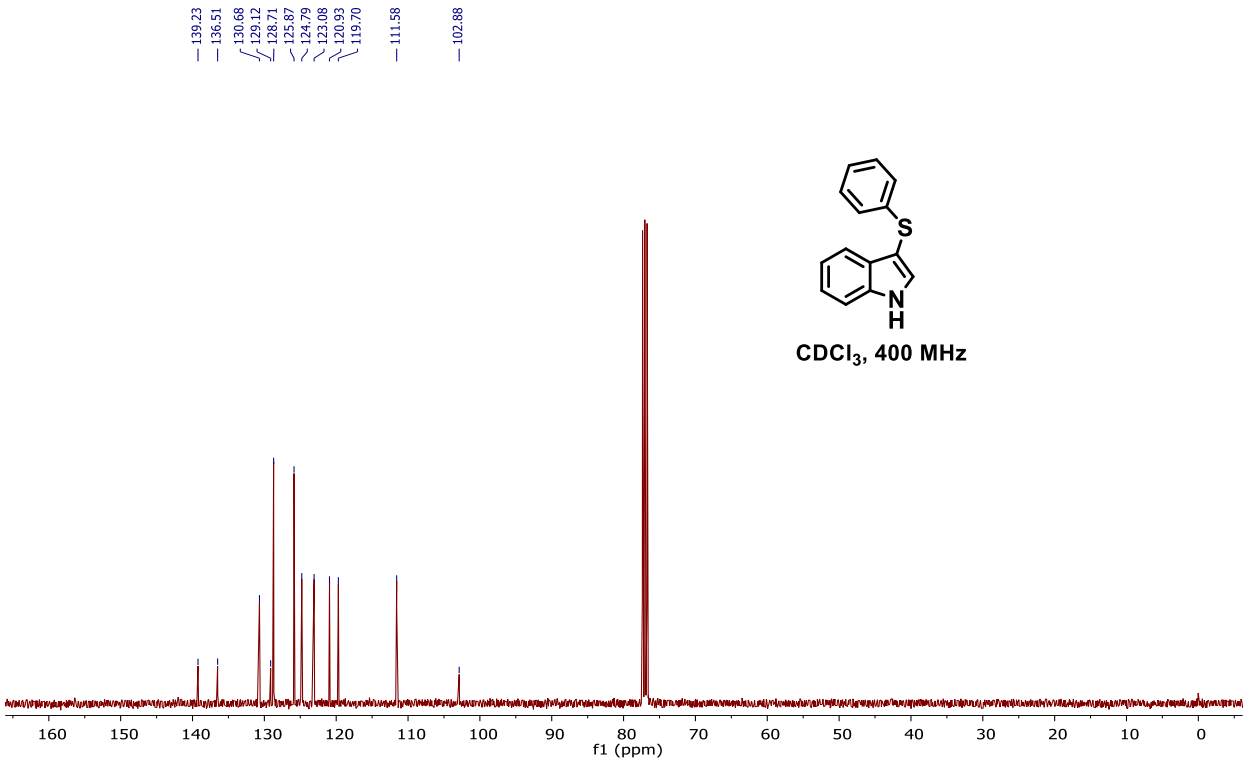
^{13}C NMR for 13



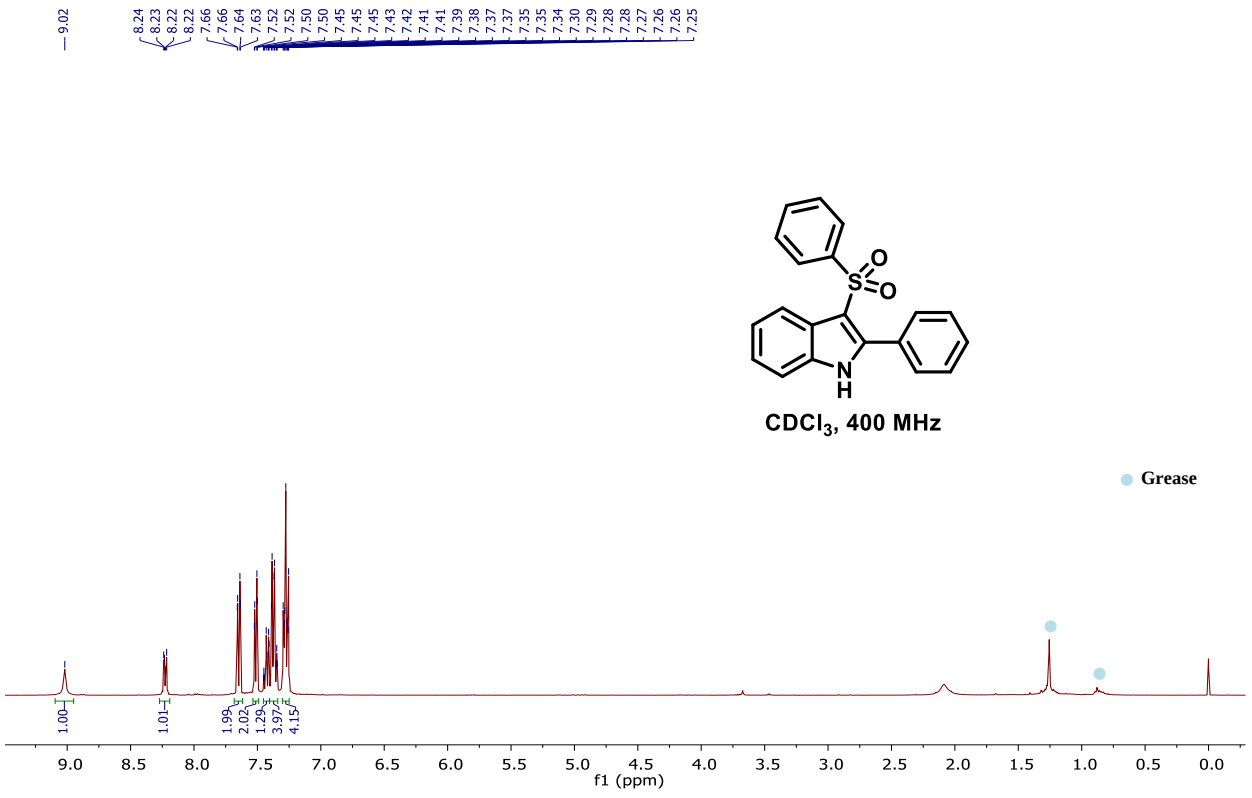
^{1}H NMR for 14



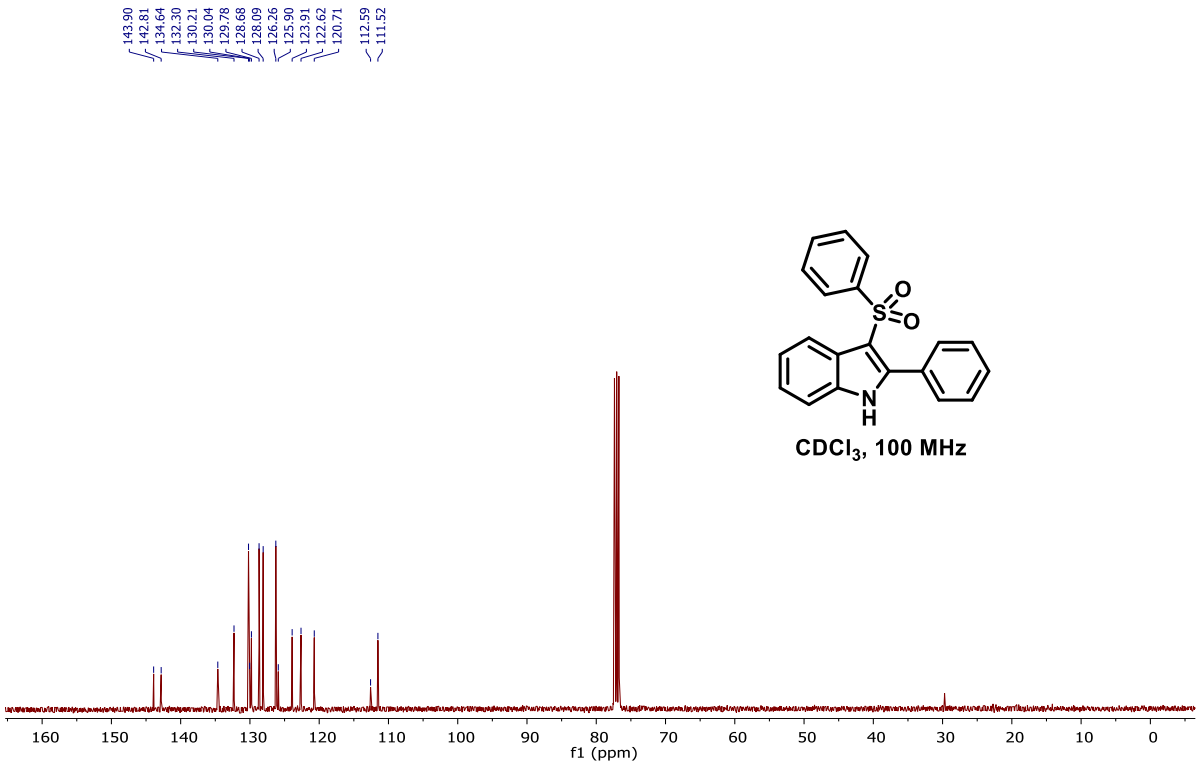
^{13}CNMR for 14



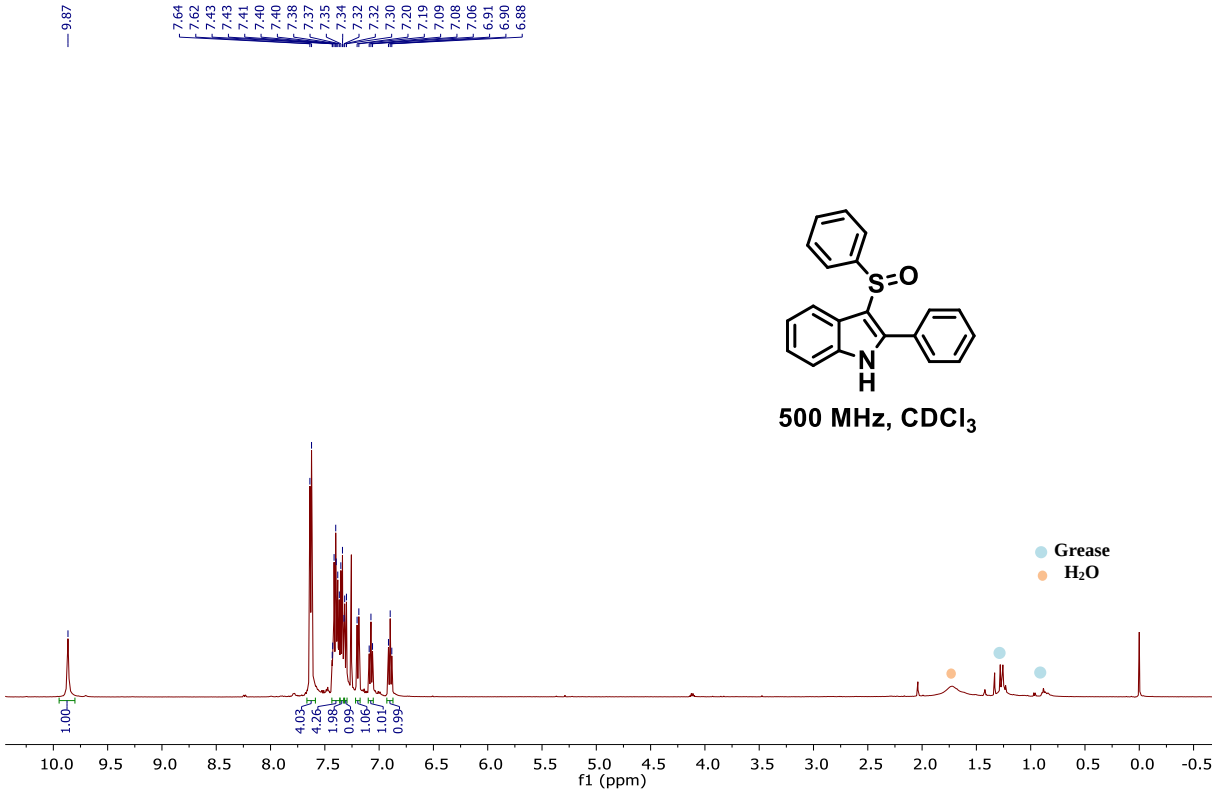
^{1}H NMR for 15



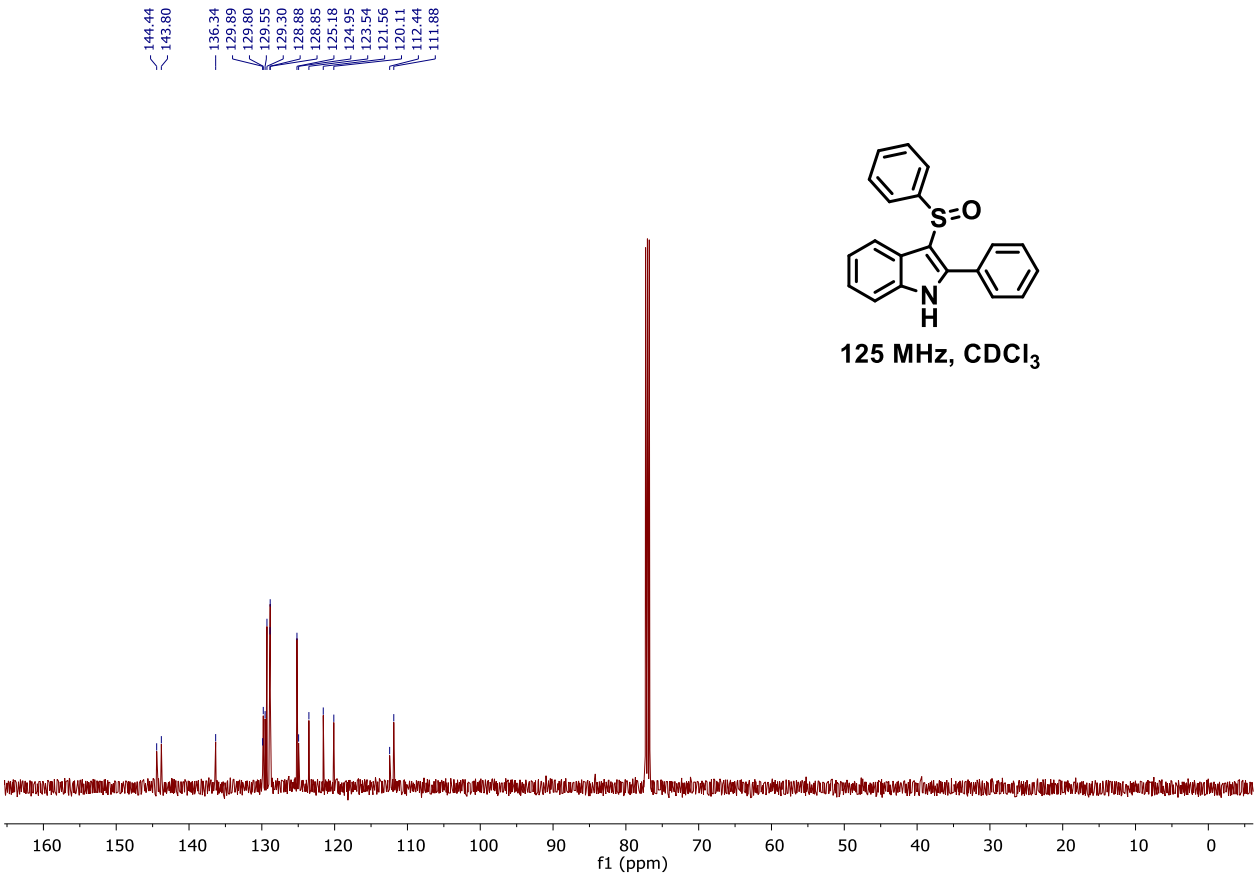
^{13}C NMR for 15



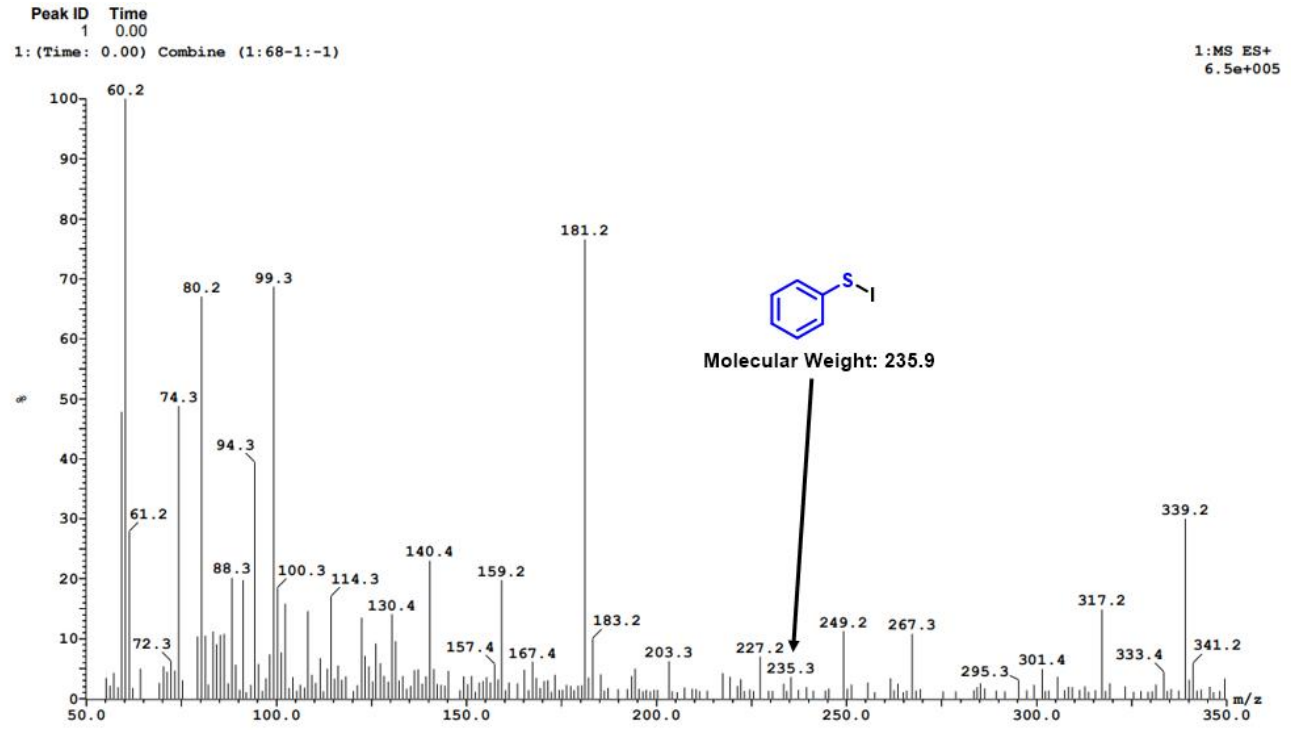
^{1}H NMR for 16

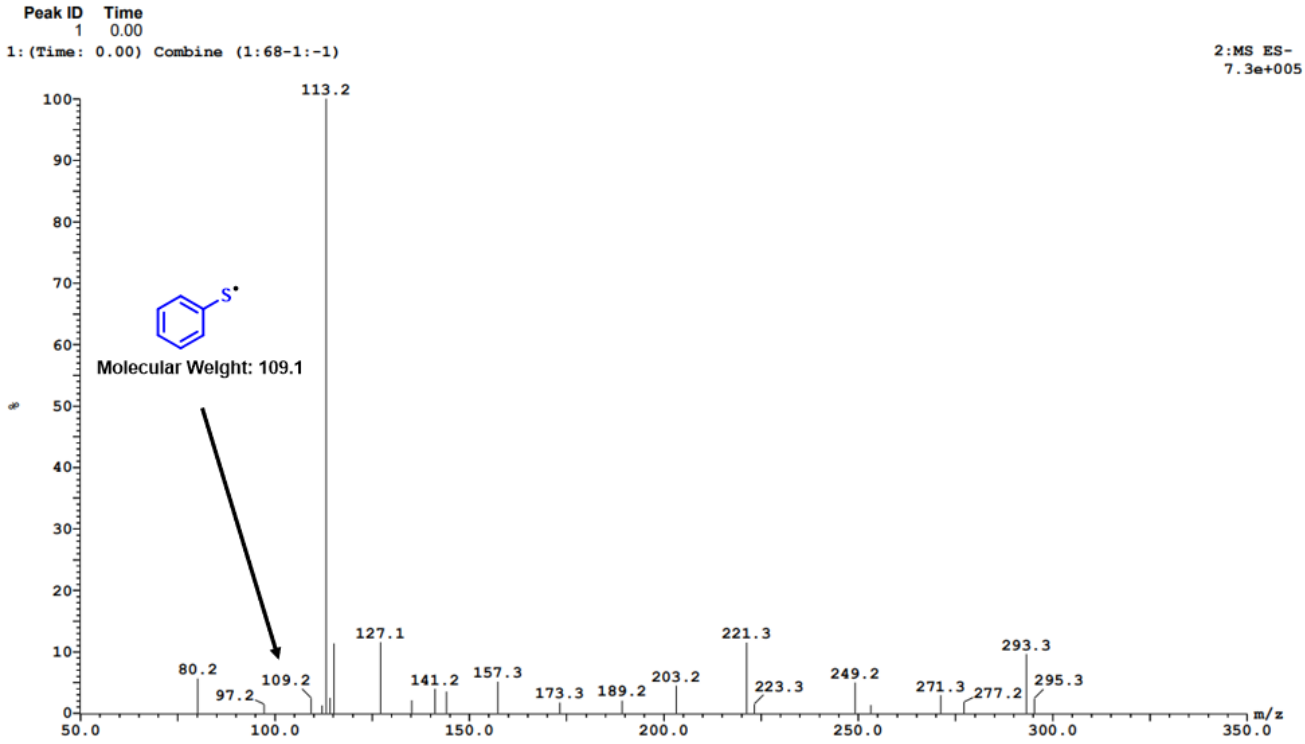


^{13}C NMR for 16



7. Identification of Intermediate for Sulfenylation step





8. Density Functional Theory Computational detail

Evaluation of Gibbs Free Energy:

The Gibbs free energy corresponding to different species in the catalytic cycle are evaluated using the following equations.

$G = H - TS$
$G = E+RT-TS$
$G = E+T(R-S)$
$G = E+(T\times (R-S) \times 1.5936\times 10^{-6})$
E = Sum of electronic and thermal energies

In the above equations, G is Gibbs free energy, H is the enthalpy, T is temperature in Kelvin, R is gas constant and S is entropy. E is the sum of electronic energy and thermal correction to energy.

The thermal correction to electronic energy can be obtained from the Gaussian output file. A part of sample Gaussian output (frequency run) of catalytic species $Pd(PPh_3)_2$ is shown below. The thermal correction to the electronic energy in this case is **0.598749**

Zero-point correction =	0.551782 (Hartree/Particle)
Thermal correction to Energy =	**0.598749**
Thermal correction to Enthalpy =	0.599867
Thermal correction to Gibbs Free Energy =	0.453362
Sum of electronic and zero-point Energies =	-2198.274307
Sum of electronic and thermal Energies =	-2198.227340
Sum of electronic and thermal Enthalpies =	-2198.226222
Sum of electronic and thermal Free Energies =	-2198.372727

In the evaluation of Gibbs free energy, we used the entropy value after correcting it for the translational motion. For details of this correction, see equation 2 of the following reference.

M. Mammen, E. I. Shaknovich, J. M. Deutch, G. M. Whitesides, *J. Org. Chem*. 1998, **63**, 3821-3830.

In Tables S2 and S3, the electronic energy calculated at B3PW91-D3/BSII level and the zero-point energy (ZPE), thermal energy correction along with the entropy correction ($\Delta S^{correction}$) all of these calculated at B3PW91/BSI level terms used for free energy evaluation are given. Using these values, the evaluation of Gibbs free energy of catalytic species $Pd(PPh_3)_2$ at 353.15 K is shown below.

$G = E+(T\times (R-S) \times 1.5936\times 10^{-6})$
$G = -2200.42195 + (353.15 \times (1.9827 - 236.146942) \times 0.00000159636) = -2199.955212$ a.u.

Table S2. The electronic energy (at B3PW91-D3/BSII level), zero-point energy (ZPE), thermal energy correction and the entropy correction ($\Delta S^{correction}$) both at B3PW91/BSI level) terms for free energy evaluation for the reaction with different catalyst (Entry 1 to 4 of Table S2).

Geometry	Electronic Energy	ZPE	Thermal Energy	$\Delta S^{correction}$	Free Energy
$Pd(PPh_3)_2$ in CH_3CN solvent entry No. 1 in Table 3					
$Pd(PPh_3)_2$	-2200.42195	0.551782	0.598749	236.146942	-2199.955212
1a	-582.8089429	0.10719	0.117136	68.555977	-582.7293379
RC	-2783.261453	0.658905	0.718196	276.944	-2782.698267
TS1	-2783.255055	0.659111	0.716432	267.173004	-2782.688125
Int1	-2783.319211	0.661448	0.719959	267.759003	-2782.749085
Cu(I) acetylide	-505.14294	0.100378	0.111137	73.820961	-505.0723022
CuI	-493.2901616	0.000565	0.004008	38.577538	-493.3067841
Int2	-2795.171208	0.76137	0.82758	312.862793	-2794.518888
TS2	-2795.150029	0.760134	0.82583	303.880798	-2794.494395
Int3	-2795.188531	0.760581	0.8254	300.001801	-2794.53114
TS3	-2795.137763	0.755825	0.819882	296.024811	-2794.483649
Int4	-2795.193256	0.763495	0.828039	301.833801	-2794.53426
TS4	-2795.160616	0.758606	0.819884	279.451782	-2794.497157
2-phenylindole	-594.7984601	0.211935	0.22731	89.020287	-594.6202179
$Pd(PPh_3)(CH_3CN)$ in CH_3CN solvent entry No. 2 in Table 3					
Int3	-1891.725961	0.533291	0.582286	238.750549	-1891.277154
TS3	-1891.654623	0.526628	0.574188	235.04454	-1891.211824
$Pd(CH_3CN)_2$ in CH_3CN solvent entry No. 3 in Table 3					
Int3	-988.2523765	0.304172	0.335386	164.071671	-988.0083689
TS3	-988.1842506	0.297709	0.328215	161.677673	-987.9460644
$Pd(PPh_3)_2CH_3CN$ in CH_3CN solvent entry No. 4 in Table 3					
Int3	-2927.950664	0.80814	0.876092	320.704712	-2927.253135
TS3	-2927.904994	0.803554	0.875852	327.217804	-2927.212495

Table S3. The electronic energy (at B3PW91-D3/BSII level), zero-point energy (ZPE), thermal energy correction and the entropy correction ($\Delta S^{correction}$) both at B3PW91/BSI level) terms for free energy evaluation for the reaction with different catalyst (Entry 5 to 10 of Table 3).

Geometry	Electronic Energy	ZPE	Thermal Energy	$\Delta S^{correction}$	Free Energy
$PdCl_2$ in CH_3CN solvent entry No. 5 in Table 3					
Int3	-1643.133915	0.212256	0.235597	129.754364	-1642.97035
TS3	-1643.088976	0.207205	0.229435	123.185349	-1642.92787
$PdCl_2$ in Toluene solvent entry No. 6 in Table 3					
Int3	-1643.137579	0.212514	0.235703	132.615814	-1642.975521
TS3	-1643.073709	0.207322	0.229466	127.49482	-1642.915001
$Pd(PPh_3)_2Cl_2$ in CH_3CN solvent entry No. 7 in Table 3					
Int3	-3715.623225	0.766845	0.836535	310.960876	-3714.960878
TS3	-3715.559451	0.761788	0.831806	313.408875	-3714.903213
$Pd(PPh_3)_2Cl_2$ in Toluene solvent entry No. 8 in Table 3					
Int3	-3715.609242	0.767085	0.837674	320.958344	-3714.951391
TS3	-3715.543648	0.761791	0.832803	325.680359	-3714.893331
$PdCl_2(CH_3CN)$ in CH_3CN solvent entry No. 9 in Table 3					
Int3	-1775.873898	0.257918	0.285774	165.545288	-1775.679216
TS3	-1775.855433	0.254999	0.284626	158.658691	-1775.659134
Int4	-1775.950219	0.26223	0.289191	142.236679	-1775.740097
TS4	-1775.927622	0.258815	0.28747	156.24469	-1775.727118
2-phenylindole	-594.7984601	0.211935	0.22731	89.020287	-594.6202179
$PdCl_2(CH_3CN)_2$ in CH_3CN solvent entry No. 10 in Table 3					
Int3	-1908.613881	0.30358	0.335951	201.336212	-1908.362273
TS3	-1908.600959	0.30162	0.335886	179.421997	-1908.362273

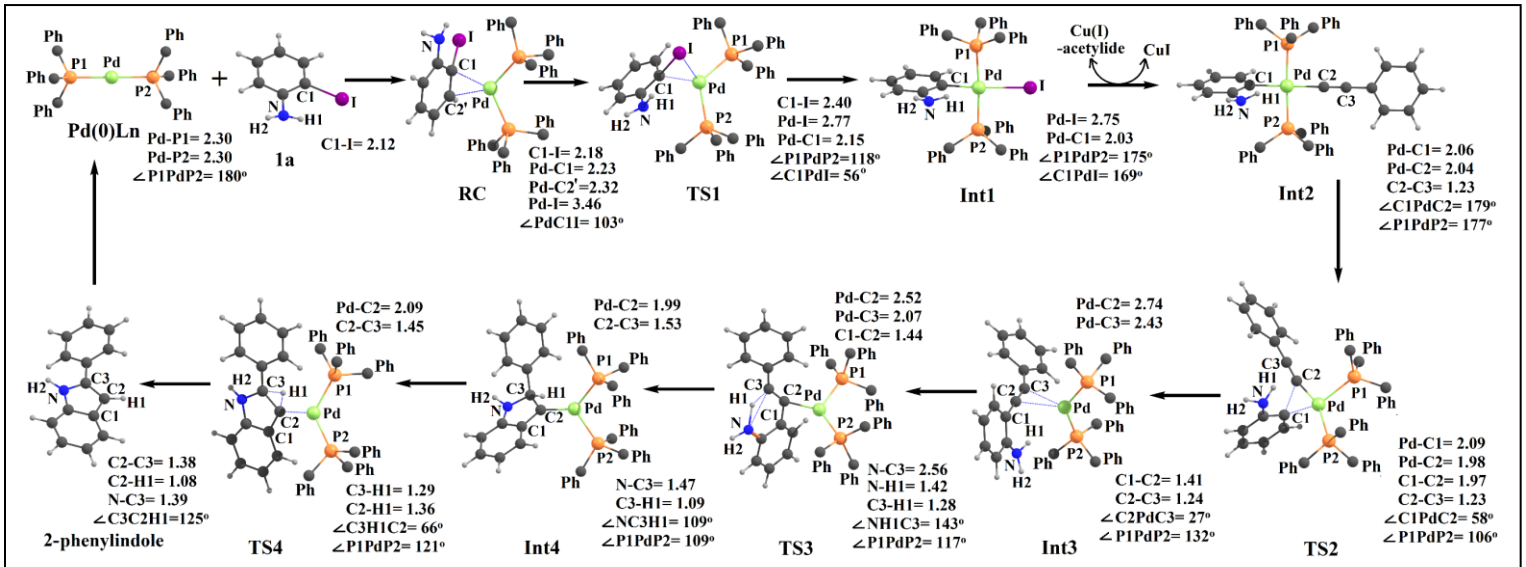


Figure S2. Geometrical changes during the catalytic cycle for the synthesis of 2-phenylindole by $Pd(PPh_3)_2$ catalyst. Bond distances are in Angstrom (Å) and angles are in Degree.

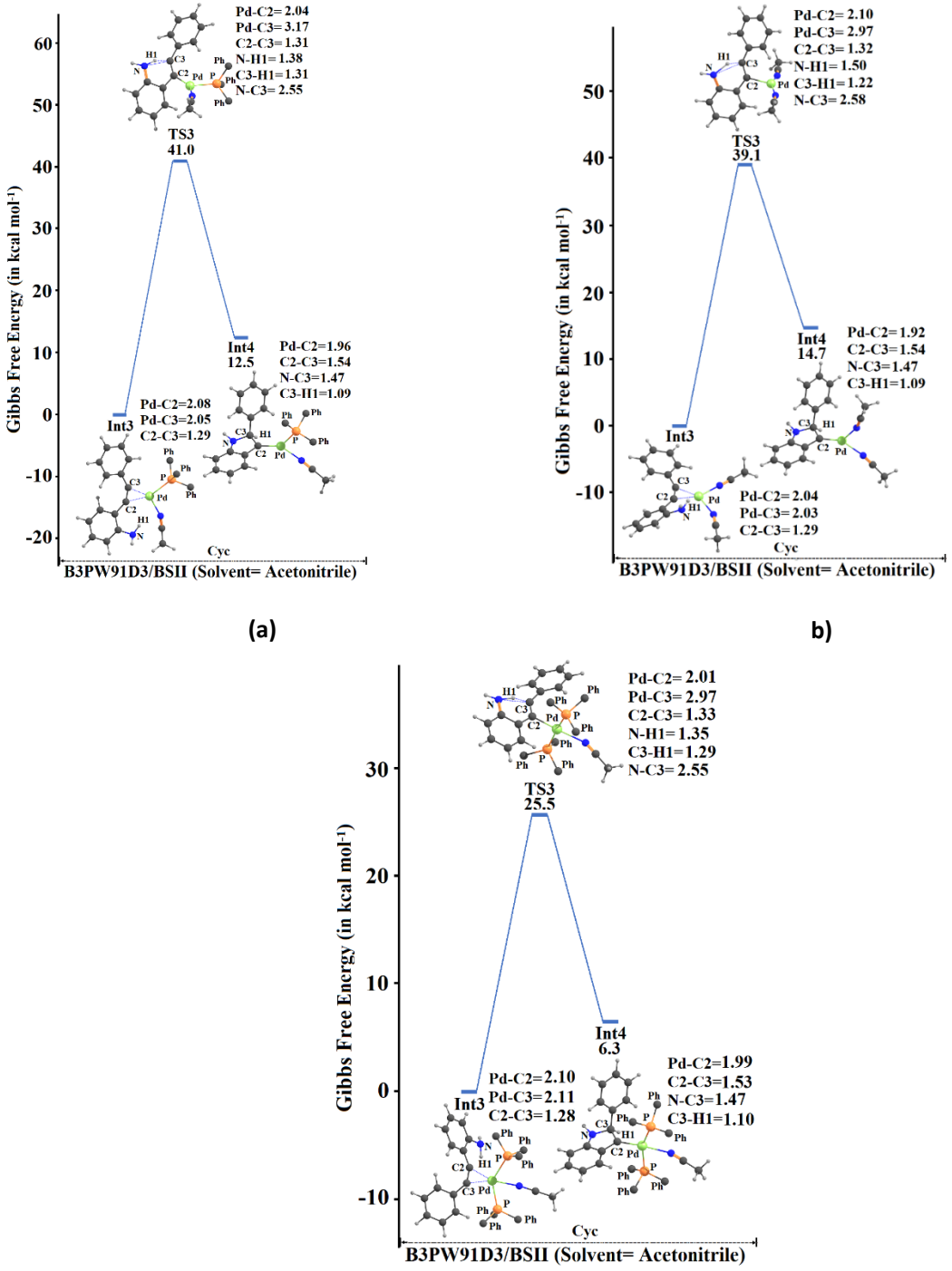


Figure S3. Gibbs energy changes during cyclization of Sonogashira intermediate **Int3** using (a) $Pd(PPh_3)(NCCH_3)$ in acetonitrile solvent (b) $Pd(NCCH_3)_2$ in acetonitrile solvent and (c) $Pd(PPh_3)_2(NCCH_3)$ in acetonitrile solvent. Bond distances are in Angstrom (Å).

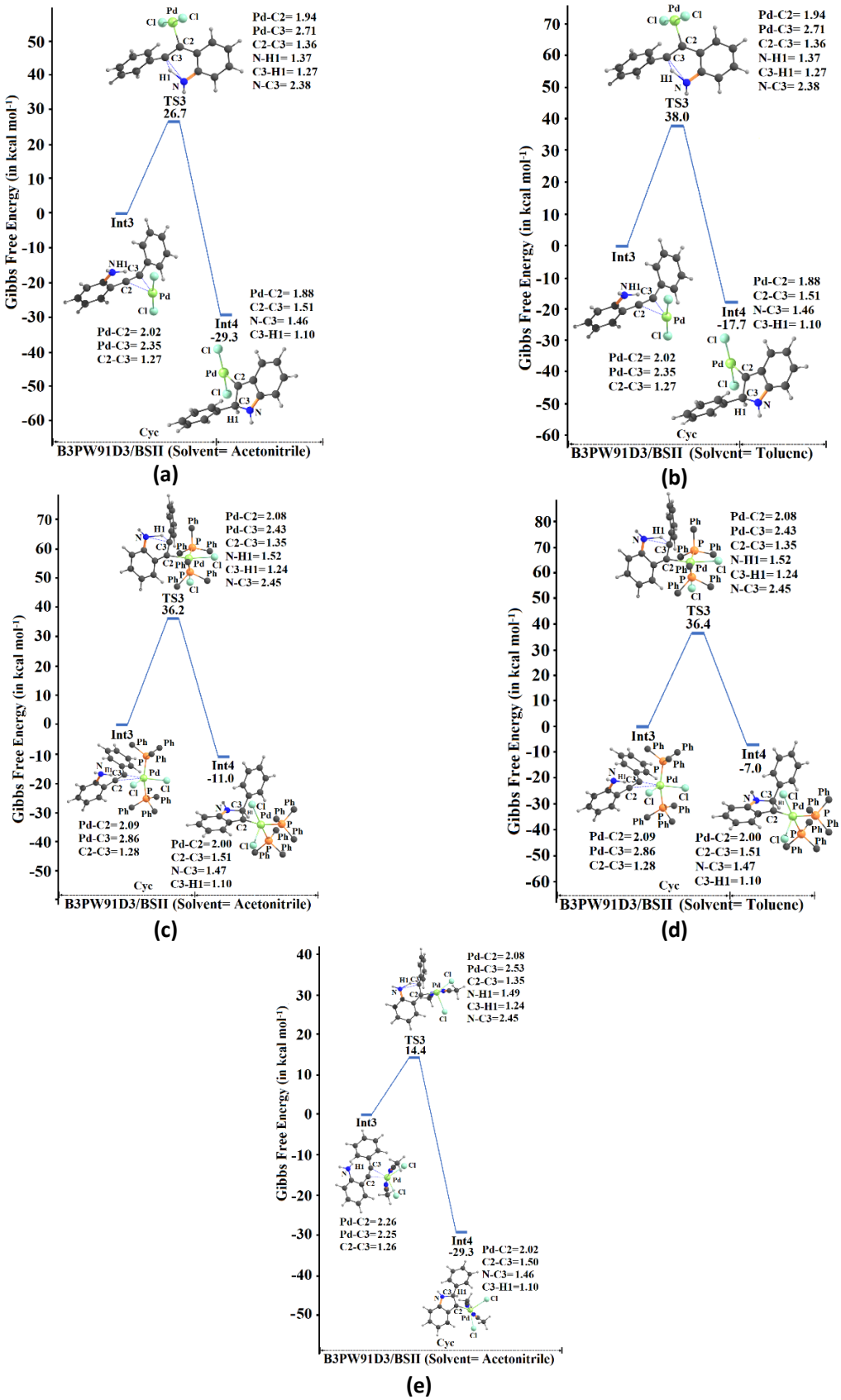


Figure S4. Gibbs energy changes during cyclization of Sonogashira intermediate **Int3** using (a) $PdCl_2$ in acetonitrile solvent (b) $PdCl_2$ in toluene solvent (c) $Pd(PPh_3)_2Cl_2$ in acetonitrile solvent (d) $Pd(PPh_3)_2Cl_2$ in toluene solvent, and (e) $PdCl_2(NCCH_3)_2$ in acetonitrile solvent. Bond distances are in Angstrom (Å).

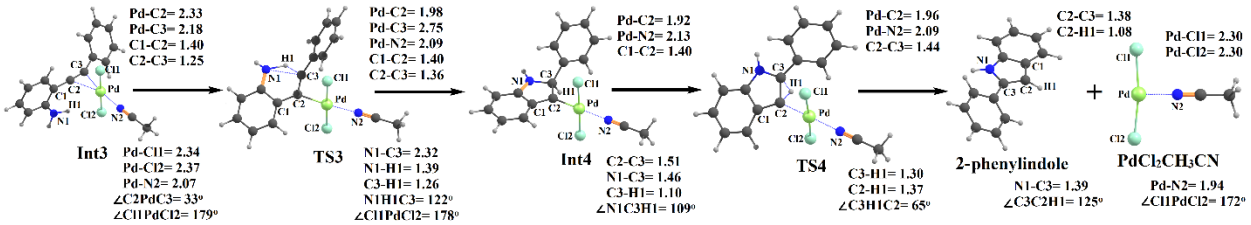


Figure S5. Geometrical changes during the cyclization step of catalytic cycle for synthesis of 2-phenylindole by $Pd(Cl)_2(CH_3CN)$ catalyst. Bond distances are in Angstrom (Å) and angles are in

9. Cartesian coordinates of optimized structures

B3PW91/BS-I Optimized Geometry of $Pd(PPh_3)_2$
Energy (B3PW91-GD3/BSII) = -2200.42195 a.u.

Pd	0.000004000	0.000250000	-0.001348000
P	-2.302277000	0.000182000	-0.000566000
P	2.302290000	-0.000254000	-0.000161000
C	3.085060000	-1.623799000	0.386669000
C	4.286114000	-2.064196000	-0.183988000
C	2.423540000	-2.455047000	1.302216000
C	4.819490000	-3.305424000	0.164161000
C	2.963034000	-3.689236000	1.656817000
C	4.162496000	-4.117596000	1.087222000
H	4.802312000	-1.441285000	-0.909656000
H	1.474050000	-2.128380000	1.722017000
H	5.749620000	-3.638282000	-0.290294000
H	2.439784000	-4.322494000	2.369060000
H	4.578899000	-5.085536000	1.355253000
C	3.084504000	1.146062000	1.213190000
C	4.284907000	0.871550000	1.880858000
C	2.423345000	2.354920000	1.474564000
C	4.817857000	1.793443000	2.782208000
C	2.962410000	3.278863000	2.366607000
C	4.161123000	2.999190000	3.023489000
H	4.801051000	-0.068420000	1.704388000
H	1.474394000	2.555553000	0.980882000
H	5.747511000	1.565959000	3.298406000
H	2.439430000	4.212566000	2.558390000
H	4.577256000	3.715116000	3.728062000
C	3.087098000	0.477061000	-1.598459000
C	4.287611000	1.192545000	-1.692495000
C	2.428068000	0.098961000	-2.777223000
C	4.822861000	1.512169000	-2.940584000
C	2.969444000	0.409387000	-4.022441000
C	4.168286000	1.118121000	-4.106602000
H	4.801816000	1.509882000	-0.789200000
H	1.479036000	-0.428928000	-2.705931000
H	5.752577000	2.073027000	-3.000008000
H	2.448114000	0.108502000	-4.927859000
H	4.586155000	1.370267000	-5.078171000
C	-3.085761000	-1.148447000	-1.210920000
C	-4.286733000	-0.875098000	-1.878048000
C	-2.425018000	-2.357923000	-1.470488000
C	-4.820635000	-1.798707000	-2.777076000
C	-2.965020000	-3.283557000	-2.360208000
C	-4.164290000	-3.005023000	-3.016556000
H	-4.802579000	0.065301000	-1.702998000
H	-1.475658000	-2.557740000	-0.977265000
H	-5.750725000	-1.572119000	-3.292884000
H	-2.442342000	-4.217710000	-2.550617000
H	-4.581160000	-3.722291000	-3.719326000
C	-3.085391000	1.623007000	-0.389751000
C	-4.285825000	2.064583000	0.181303000
C	-2.424792000	2.452430000	-1.307616000
C	-4.819504000	3.305157000	-0.168713000
C	-2.964599000	3.685946000	-1.664071000
C	-4.163439000	4.115484000	-1.094055000
H	-4.801293000	1.443130000	0.908739000
H	-1.475760000	2.124894000	-1.727773000
H	-5.749136000	3.638954000	0.286069000
H	-2.442064000	4.317778000	-2.378103000
H	-4.580075000	5.082917000	-1.363549000
C	-3.085478000	-0.474101000	1.599411000
C	-4.286388000	-1.188594000	1.695960000
C	-2.424806000	-0.094626000	2.776806000
C	-4.820433000	-1.505854000	2.945161000
C	-2.964963000	-0.402713000	4.023137000
C	-4.164222000	-1.110436000	4.109799000
H	-4.801837000	-1.507019000	0.793755000
H	-1.475470000	0.432449000	2.703557000
H	-5.750478000	-2.065954000	3.006545000
H	-2.442359000	-0.100796000	4.927475000
H	-4.581149000	-1.360752000	5.082245000

B3PW91/BS-I Optimized Geometry of 1a
Energy (B3PW91-GD3/BSII) = -582.8089429 a.u.

C	3.282473000	-0.375844000	0.003622000
C	2.524923000	-1.547264000	0.005141000
C	2.663231000	0.866032000	-0.001224000
H	3.003556000	-2.521943000	0.009765000
H	3.263377000	1.773821000	-0.009012000
C	1.135505000	-1.454402000	0.001969000
C	1.260298000	0.989827000	-0.007314000
H	0.527187000	-2.353574000	0.007044000
C	0.518437000	-0.206169000	-0.004270000
H	4.368176000	-0.427428000	0.007693000
I	-1.606182000	-0.133500000	0.000190000
N	0.671763000	2.238616000	-0.072681000
H	1.242534000	3.005709000	0.254254000
H	-0.288707000	2.295502000	0.241397000

B3PW91/BS-I Optimized Geometry of RC
Energy (B3PW91-GD3/BSII) = -2783.261453 a.u.

Pd	0.009353000	-0.647185000	0.213547000
P	-1.631480000	1.095351000	0.121848000
P	2.267571000	0.052479000	-0.092954000
C	-0.980717000	-2.623126000	0.495483000
C	0.405257000	-2.925150000	0.361037000
H	0.828358000	-3.060144000	-0.629519000
C	-1.634776000	-2.809604000	1.759714000
C	1.135363000	-3.403337000	1.480723000
C	0.500185000	-3.549973000	2.695287000
H	1.046383000	-3.927008000	3.556822000
C	-0.864298000	-3.240344000	2.836677000
H	-1.346178000	-3.346865000	3.806828000
H	2.178277000	-3.676994000	1.350838000
C	-1.522690000	2.341846000	1.480904000
C	-2.530850000	3.282251000	1.745878000
C	-0.381085000	2.335497000	2.292763000
C	-2.384995000	4.206031000	2.778862000
H	-3.441674000	3.280599000	1.152947000
C	-0.234344000	3.261054000	3.326052000
H	0.388218000	1.586869000	2.117819000
C	-1.234315000	4.200623000	3.568392000

H	-3.174891000	4.928274000	2.971080000
H	0.658821000	3.237242000	3.945191000
H	-1.124552000	4.919947000	4.376326000
C	-3.458595000	0.791206000	0.079540000
C	-4.202552000	0.852464000	-1.105591000
C	-4.115023000	0.425389000	1.265027000
C	-5.567300000	0.561138000	-1.105682000
H	-3.718855000	1.133840000	-2.036047000
C	-5.479420000	0.146677000	1.265206000
H	-3.554885000	0.351972000	2.192596000
C	-6.211862000	0.211422000	0.078656000
H	-6.126661000	0.616225000	-2.036554000
H	-5.971889000	-0.123482000	2.196566000
H	-7.276643000	-0.008407000	0.079327000
C	-1.407392000	2.081259000	-1.426190000
C	-1.653228000	3.455927000	-1.530103000
C	-0.986672000	1.383676000	-2.567509000
C	-1.485591000	4.115065000	-2.747465000
H	-1.967118000	4.020451000	-0.657025000
C	-0.834225000	2.039869000	-3.787700000
H	-0.773407000	0.319386000	-2.487355000
C	-1.080890000	3.408944000	-3.879631000
H	-1.674293000	5.184270000	-2.810561000
H	-0.511013000	1.482671000	-4.663501000
H	-0.952205000	3.924862000	-4.827945000
C	2.747654000	1.548477000	-1.066358000
C	3.785411000	1.556966000	-2.007799000
C	2.044439000	2.737866000	-0.829188000
C	4.111369000	2.728210000	-2.692714000
H	4.344364000	0.647726000	-2.208179000
C	2.378232000	3.908502000	-1.504538000
H	1.227184000	2.747191000	-0.113466000
C	3.412031000	3.906628000	-2.441206000
H	4.917833000	2.716499000	-3.422191000
H	1.819029000	4.819384000	-1.308206000
H	3.667210000	4.818486000	-2.975582000
C	3.303907000	-1.253134000	-0.885584000
C	4.496188000	-1.741305000	-0.338149000
C	2.840792000	-1.805037000	-2.091008000
C	5.208277000	-2.755568000	-0.981379000
H	4.872799000	-1.329467000	0.593740000
C	3.559610000	-2.805751000	-2.739454000
H	1.905751000	-1.448426000	-2.518953000
C	4.745825000	-3.287532000	-2.182988000
H	6.130062000	-3.126829000	-0.539793000
H	3.187609000	-3.217818000	-3.674271000
H	5.302337000	-4.076678000	-2.682235000
C	3.126382000	0.366423000	1.511193000
C	4.247602000	1.199688000	1.629928000
C	2.617176000	-0.253952000	2.661194000
C	4.848617000	1.402812000	2.871494000
H	4.647703000	1.696788000	0.750407000
C	3.223159000	-0.053149000	3.900873000
H	1.742724000	-0.895760000	2.577143000
C	4.338748000	0.776519000	4.008835000
H	5.715529000	2.054540000	2.949961000
H	2.816825000	-0.540901000	4.783573000
H	4.807200000	0.938820000	4.976594000
I	-2.183228000	-2.855301000	-1.308816000
N	-2.976403000	-2.518731000	1.928099000
H	-3.446548000	-3.050347000	2.647737000
H	-3.521489000	-2.434636000	1.078967000

B3PW91/BS-I Optimized Geometry of TS1
Energy (B3PW91-GD3/BSII) = -2783.255055 a.u.

Pd	-0.006550000	-0.624122000	0.022572000
P	2.169545000	0.462405000	0.136017000
P	-1.975397000	0.755275000	-0.092585000
C	-0.599284000	-2.601769000	0.637965000
C	0.254988000	-2.702752000	1.747662000
H	1.304889000	-2.445010000	1.643898000
C	-1.911318000	-3.130255000	0.688410000
C	-0.238943000	-3.158664000	2.974445000
C	-1.556501000	-3.600060000	3.056325000
H	-1.948590000	-3.985361000	3.994257000
C	-2.371881000	-3.599952000	1.924738000
H	-3.393577000	-3.969845000	1.991394000
H	0.421674000	-3.207463000	3.835767000
C	2.879687000	0.981228000	-1.481833000
C	4.249781000	1.209165000	-1.682843000
C	2.002884000	1.135839000	-2.564007000
C	4.724005000	1.611172000	-2.929784000
H	4.949609000	1.054410000	-0.865534000
C	2.478371000	1.540831000	-3.811249000
H	0.946916000	0.910953000	-2.427999000
C	3.838385000	1.783340000	-3.994524000
H	5.788058000	1.783837000	-3.072213000
H	1.785390000	1.652269000	-4.641278000
H	4.211268000	2.092535000	-4.967880000
C	3.518550000	-0.598841000	0.821436000
C	4.043294000	-0.414255000	2.107357000
C	3.975813000	-1.685586000	0.057491000
C	5.002141000	-1.291789000	2.614997000
H	3.708785000	0.420931000	2.715645000
C	4.937709000	-2.555075000	0.564891000
H	3.577307000	-1.851548000	-0.939538000
C	5.453838000	-2.362806000	1.847113000
H	5.400330000	-1.129644000	3.613854000
H	5.281701000	-3.387633000	-0.043781000
H	6.202559000	-3.044042000	2.243453000
C	2.286014000	1.956400000	1.211195000
C	3.167474000	3.022129000	0.991571000
C	1.442969000	1.995507000	2.330655000
C	3.210090000	4.097071000	1.878575000
H	3.817536000	3.021210000	0.121544000
C	1.498813000	3.061381000	3.226367000
H	0.730163000	1.187812000	2.485340000
C	2.382213000	4.116040000	3.000583000
H	3.895218000	4.920881000	1.692607000
H	0.838700000	3.075773000	4.089811000
H	2.419194000	4.954612000	3.691581000
C	-1.733122000	2.539154000	0.336005000
C	-2.595343000	3.251044000	1.179854000
C	-0.635088000	3.212160000	-0.219409000

C	-2.365987000	4.599457000	1.455461000
H	-3.452673000	2.754772000	1.623791000
C	-0.417131000	4.562740000	0.039958000
H	0.056051000	2.672513000	-0.861606000
C	-1.281596000	5.260704000	0.883056000
H	-3.044240000	5.133780000	2.116670000
H	0.440020000	5.063365000	-0.402318000
H	-1.106583000	6.312320000	1.096506000
C	-3.414230000	0.312906000	0.968270000
C	-4.743616000	0.568579000	0.603589000
C	-3.152728000	-0.264044000	2.217234000
C	-5.786678000	0.261202000	1.475286000
H	-4.962794000	1.011005000	-0.364297000
C	-4.196436000	-0.558237000	3.093954000
H	-2.127580000	-0.497164000	2.495546000
C	-5.514930000	-0.297338000	2.724815000
H	-6.813488000	0.463049000	1.179348000
H	-3.976684000	-1.006379000	4.059564000
H	-6.329666000	-0.533396000	3.405251000
C	-2.735643000	0.876256000	-1.775178000
C	-2.863762000	2.076727000	-2.485008000
C	-3.175281000	-0.313231000	-2.376475000
C	-3.408730000	2.085071000	-3.770245000
H	-2.542943000	3.012124000	-2.037193000
C	-3.731524000	-0.298885000	-3.652519000
H	-3.093352000	-1.246373000	-1.824217000
C	-3.843427000	0.899969000	-4.358536000
H	-3.498158000	3.026493000	-4.307339000
H	-4.073528000	-1.228920000	-4.100799000
H	-4.268277000	0.908810000	-5.359343000
I	0.502569000	-2.904293000	-1.475700000
N	-2.729514000	-3.138291000	-0.434980000
H	-3.516763000	-3.771149000	-0.362379000
H	-2.209974000	-3.284709000	-1.296858000

B3PW91/BS-I Optimized Geometry of Int1
Energy (B3PW91-GD3/BSII) = -2783.319211 a.u.

Pd	-0.004393000	-0.099362000	-0.019698000
P	2.380356000	-0.019243000	-0.057973000
P	-2.387366000	-0.006933000	-0.037543000
C	-3.058158000	0.006058000	1.673101000
C	-4.271538000	0.629207000	1.998165000
C	-2.343622000	-0.661919000	2.676970000
C	-4.757017000	0.586116000	3.304276000
C	-2.834970000	-0.705138000	3.980233000
C	-4.039745000	-0.079381000	4.297504000
H	-4.835835000	1.155497000	1.233899000
H	-1.412332000	-1.163810000	2.426030000
H	-5.697603000	1.075683000	3.544061000
H	-2.272341000	-1.229987000	4.747956000
H	-4.419220000	-0.109702000	5.315836000
C	-3.216688000	-1.420655000	-0.867859000
C	-4.429547000	-1.943738000	-0.407260000
C	-2.643057000	-1.946939000	-2.032524000
C	-5.060144000	-2.973290000	-1.104804000
C	-3.283415000	-2.963238000	-2.737020000
C	-4.492455000	-3.480452000	-2.272175000
H	-4.879996000	-1.557353000	0.502206000
H	-1.679732000	-1.575927000	-2.372014000
H	-5.996487000	-3.380096000	-0.731352000
H	-2.825536000	-3.366144000	-3.636555000
H	-4.985346000	-4.283908000	-2.813704000
C	-3.212030000	1.437799000	-0.838940000
C	-3.907505000	1.297910000	-2.048281000
C	-3.131920000	2.709322000	-0.249384000
C	-4.508575000	2.401349000	-2.653357000
C	-3.743842000	3.806016000	-0.851918000
C	-4.431558000	3.657638000	-2.055836000
H	-3.992077000	0.323262000	-2.518336000
H	-2.589337000	2.848336000	0.680460000
H	-5.046400000	2.271550000	-3.589292000
H	-3.670666000	4.781554000	-0.378775000
H	-4.906060000	4.516452000	-2.524274000
C	3.092189000	-0.135337000	1.633246000
C	4.370676000	0.360850000	1.929390000
C	2.349692000	-0.752673000	2.648148000
C	4.893984000	0.237066000	3.215092000
C	2.876978000	-0.874235000	3.932731000
C	4.148031000	-0.379251000	4.219327000
H	4.955216000	0.852653000	1.157351000
H	1.366342000	-1.155316000	2.420387000
H	5.885582000	0.626686000	3.431470000
H	2.290450000	-1.358377000	4.709290000
H	4.556726000	-0.471700000	5.222543000
C	3.242651000	1.453554000	-0.758649000
C	3.965806000	1.378168000	-1.955788000
C	3.184839000	2.679740000	-0.079036000
C	4.618380000	2.502115000	-2.460909000
C	3.843996000	3.797373000	-0.583647000
C	4.561758000	3.713568000	-1.776179000
H	4.029478000	0.439624000	-2.496517000
H	2.623017000	2.766968000	0.845513000
H	5.176639000	2.423712000	-3.390546000
H	3.786446000	4.738454000	-0.043135000
H	5.074298000	4.588462000	-2.168754000
C	3.130955000	-1.400466000	-1.007980000
C	4.280263000	-2.070796000	-0.578365000
C	2.546488000	-1.758267000	-2.230209000
C	4.837840000	-3.080509000	-1.362455000
C	3.114588000	-2.754701000	-3.018846000
C	4.260894000	-3.420595000	-2.584201000
H	4.736099000	-1.817082000	0.373900000
H	1.634161000	-1.263986000	-2.554053000
H	5.724516000	-3.603390000	-1.012982000
H	2.650962000	-3.024181000	-3.964266000
H	4.697179000	-4.208503000	-3.192959000
C	0.005695000	1.929125000	0.134833000
C	0.012491000	2.780561000	-0.986609000
C	0.002089000	2.485288000	1.415522000
C	0.023273000	4.171253000	-0.788366000
C	0.004706000	3.872337000	1.609472000
C	0.017602000	4.710397000	0.494562000
H	-0.009649000	1.830046000	2.284593000
H	0.038442000	4.830409000	-1.655134000
H	-0.002564000	4.284472000	2.615591000
H	0.022388000	5.790868000	0.620677000

I	0.007962000	-2.835881000	0.287610000
N	0.054865000	2.250951000	-2.274554000
H	-0.368288000	2.831679000	-2.987623000
H	-0.277776000	1.294035000	-2.315915000

B3PW91/BS-I Optimized Geometry of Cu(I)-acetylide
Energy (B3PW91-GD3/BSII) = -505.14294 a.u.

Cu	3.334173000	0.000106000	-0.000038000
C	-1.866485000	-1.210286000	0.000011000
C	-3.257339000	-1.205948000	-0.000049000
C	-3.958756000	0.000348000	-0.000057000
C	-3.256845000	1.206344000	-0.000050000
C	-1.865979000	1.210093000	0.000043000
C	-1.147295000	-0.000242000	0.000174000
H	-1.317811000	-2.147703000	-0.000005000
H	-3.797436000	-2.149662000	-0.000044000
H	-5.045810000	0.000564000	-0.000135000
H	-3.796536000	2.150290000	-0.000177000
H	-1.316935000	2.147294000	0.000022000
C	0.278314000	-0.000563000	0.000114000
C	1.504973000	-0.000390000	0.000053000

B3PW91/BS-I Optimized Geometry of CuI
Energy (B3PW91-GD3/BSII) = -493.2901616 a.u.

Cu	0.000000000	0.000000000	-1.557419000
I	0.000000000	0.000000000	0.852173000

B3PW91/BS-I Optimized Geometry of Int2
Energy (B3PW91-GD3/BSII) = -2795.171208 a.u.

Pd	-0.009203000	-0.399654000	0.032846000
P	-2.367653000	-0.195462000	0.077188000
P	2.342358000	-0.506307000	-0.010316000
C	3.125200000	0.701651000	1.128722000
C	4.362205000	1.292804000	0.847626000
C	2.482549000	0.997113000	2.337182000
C	4.948497000	2.164138000	1.765025000
C	3.076235000	1.857595000	3.257818000
C	4.309132000	2.444480000	2.972202000
H	4.866181000	1.080018000	-0.091085000
H	1.507955000	0.563329000	2.544552000
H	5.905958000	2.624400000	1.534108000
H	2.568215000	2.081242000	4.192315000
H	4.767558000	3.123862000	3.686496000
C	3.017542000	-0.088981000	-1.672843000
C	4.169429000	-0.702356000	-2.185630000
C	2.368861000	0.893054000	-2.436782000
C	4.658738000	-0.344357000	-3.441589000
C	2.866176000	1.249498000	-3.688677000
C	4.008090000	0.630138000	-4.196267000
H	4.683203000	-1.465036000	-1.608267000
H	1.487605000	1.386827000	-2.033834000
H	5.551140000	-0.830370000	-3.828211000
H	2.357309000	2.016040000	-4.267757000
H	4.390487000	0.906900000	-5.175696000
C	3.193280000	-2.079880000	0.416596000
C	2.972010000	-3.213367000	-0.380278000
C	4.033411000	-2.189619000	1.530965000
C	3.588513000	-4.422461000	-0.075559000
C	4.643584000	-3.406368000	1.838702000
C	4.425497000	-4.523096000	1.036463000
H	2.308001000	-3.154292000	-1.236562000
H	4.217386000	-1.326126000	2.162239000
H	3.400850000	-5.291332000	-0.700445000
H	5.292476000	-3.475140000	2.708266000
H	4.900491000	-5.470736000	1.277898000
C	-2.933839000	0.309322000	1.756668000
C	-4.125736000	-0.168895000	2.318048000
C	-2.157261000	1.225401000	2.482150000
C	-4.529023000	0.256028000	3.583853000
C	-2.569065000	1.650697000	3.743165000
C	-3.752122000	1.164723000	4.299601000
H	-4.739589000	-0.877364000	1.770673000
H	-1.240963000	1.613526000	2.043987000
H	-5.453953000	-0.126594000	4.008335000
H	-1.960353000	2.364973000	4.292038000
H	-4.067614000	1.493698000	5.286732000
C	-3.466976000	-1.611261000	-0.338951000
C	-4.395110000	-1.538987000	-1.385553000
C	-3.384645000	-2.792133000	0.414051000
C	-5.226790000	-2.621623000	-1.669098000
C	-4.222907000	-3.867615000	0.132346000
C	-5.145581000	-3.786778000	-0.910013000
H	-4.474066000	-0.637093000	-1.983513000
H	-2.657018000	-2.879989000	1.214081000
H	-5.941003000	-2.548494000	-2.485604000
H	-4.140724000	-4.775492000	0.723775000
H	-5.795541000	-4.629910000	-1.131391000
C	-2.984766000	1.134975000	-1.028788000
C	-4.059886000	1.956999000	-0.673680000
C	-2.386116000	1.295925000	-2.284374000
C	-4.529554000	2.923492000	-1.563035000
C	-2.864002000	2.253046000	-3.175896000
C	-3.935459000	3.071024000	-2.815677000
H	-4.528775000	1.847607000	0.300072000
H	-1.539356000	0.672129000	-2.556295000
H	-5.361393000	3.561176000	-1.274300000
H	-2.391325000	2.369062000	-4.147852000
H	-4.302916000	3.824286000	-3.508191000
C	-0.161755000	-2.456224000	0.096907000
C	-0.418581000	-3.205888000	-1.070584000
C	-0.033074000	-3.148727000	1.303932000
C	-0.553447000	-4.600919000	-0.997297000
C	-0.173789000	-4.539147000	1.385321000
C	-0.437628000	-5.261613000	0.223677000
H	0.182954000	-2.592692000	2.215623000
H	-0.758600000	-5.168729000	-1.904701000
H	-0.069490000	-5.046799000	2.341502000
H	-0.546278000	-6.343582000	0.260292000
N	-0.579138000	-2.548149000	-2.297629000
H	-0.416552000	-3.122687000	-3.115319000
H	-0.077331000	-1.668883000	-2.345868000
C	0.131557000	1.639905000	0.000443000
C	0.222733000	2.866884000	-0.019483000
C	0.328679000	4.289469000	-0.042956000
C	1.504129000	4.933695000	0.391279000
C	-0.738946000	5.086625000	-0.501126000

C	1.604268000	6.321086000	0.366736000
C	-0.631009000	6.473498000	-0.522985000
C	0.539169000	7.098589000	-0.089977000
H	2.332419000	4.327675000	0.746993000
H	-1.649269000	4.599153000	-0.837897000
H	2.520300000	6.799534000	0.706134000
H	-1.466520000	7.071512000	-0.880090000
H	0.620340000	8.182706000	-0.108127000

B3PW91/BS-I Optimized Geometry of TS2
Energy (B3PW91-GD3/BSII) = -2795.150029 a.u.

Pd	0.132427000	0.585664000	-0.194298000
P	0.847668000	-1.752287000	-0.083922000
P	-2.289538000	0.556873000	0.045283000
C	0.457794000	2.627450000	-0.520302000
C	0.415573000	3.091107000	-1.842326000
H	0.567755000	2.384661000	-2.654374000
C	0.313377000	3.555243000	0.536999000
C	0.204818000	4.439550000	-2.132513000
C	0.048241000	5.347253000	-1.084882000
H	-0.104253000	6.404043000	-1.290934000
C	0.106713000	4.907022000	0.235528000
H	-0.009204000	5.619417000	1.051253000
H	0.177007000	4.776201000	-3.165984000
C	2.226624000	-2.016545000	-1.276119000
C	2.251416000	-1.253021000	-2.449471000
C	3.221897000	-2.980341000	-1.070373000
C	3.240646000	-1.461862000	-3.409458000
H	1.501447000	-0.479893000	-2.597310000
C	4.218102000	-3.179437000	-2.024317000
H	3.223961000	-3.571865000	-0.158901000
C	4.226735000	-2.424524000	-3.197170000
H	3.247077000	-0.862696000	-4.316584000
H	4.990412000	-3.924287000	-1.849166000
H	5.004873000	-2.581283000	-3.940143000
C	-0.265671000	-3.172789000	-0.471902000
C	-0.125652000	-3.932308000	-1.641630000
C	-1.333455000	-3.461715000	0.392937000
C	-1.027265000	-4.955553000	-1.936235000
H	0.693876000	-3.731109000	-2.324693000
C	-2.224555000	-4.491169000	0.101346000
H	-1.466287000	-2.885813000	1.304175000
C	-2.076782000	-5.240658000	-1.065878000
H	-0.899909000	-5.535356000	-2.847295000
H	-3.040368000	-4.700866000	0.788076000
H	-2.776331000	-6.040681000	-1.294770000
C	1.591253000	-2.232525000	1.534617000
C	1.490809000	-3.521190000	2.076011000
C	2.316146000	-1.256705000	2.234998000
C	2.094869000	-3.824125000	3.296380000
H	0.936843000	-4.291985000	1.548628000
C	2.925053000	-1.566349000	3.449067000
H	2.415727000	-0.260247000	1.811860000
C	2.812215000	-2.848681000	3.986119000
H	2.005060000	-4.827834000	3.704887000
H	3.491008000	-0.801822000	3.975526000
H	3.283914000	-3.087182000	4.936242000
C	-2.816048000	-0.449117000	1.494204000
C	-3.958667000	-1.257741000	1.510430000
C	-2.009322000	-0.387207000	2.640290000
C	-4.287081000	-1.990652000	2.651302000
H	-4.588868000	-1.323746000	0.628191000
C	-2.342577000	-1.114902000	3.781157000
H	-1.117224000	0.235259000	2.630070000
C	-3.481107000	-1.921646000	3.787405000
H	-5.176137000	-2.616878000	2.650941000
H	-1.707331000	-1.058447000	4.661323000
H	-3.737921000	-2.495766000	4.674196000
C	-3.269532000	-0.106910000	-1.366367000
C	-4.611558000	0.240423000	-1.581902000
C	-2.644274000	-0.980532000	-2.264431000
C	-5.312584000	-0.288760000	-2.663775000
H	-5.104670000	0.936157000	-0.908414000
C	-3.347257000	-1.511422000	-3.344657000
H	-1.601048000	-1.242489000	-2.113984000
C	-4.682538000	-1.166715000	-3.546088000
H	-6.351426000	-0.008986000	-2.821115000
H	-2.847355000	-2.191178000	-4.029656000
H	-5.230004000	-1.574732000	-4.392219000
C	-3.139626000	2.161257000	0.356664000
C	-3.988502000	2.374224000	1.450294000
C	-2.941491000	3.201254000	-0.562129000
C	-4.634882000	3.599173000	1.614441000
H	-4.149965000	1.584220000	2.177262000
C	-3.594506000	4.420268000	-0.398606000
H	-2.264504000	3.066695000	-1.400657000
C	-4.443374000	4.623122000	0.688784000
H	-5.291260000	3.749224000	2.468370000
H	-3.423501000	5.216791000	-1.117586000
H	-4.948626000	5.577329000	0.817495000
C	5.450825000	1.564131000	-0.960456000
C	6.806690000	1.835614000	-0.820380000
C	7.298979000	2.410633000	0.352713000
C	6.414621000	2.714420000	1.388897000
C	5.056242000	2.450683000	1.256567000
C	4.544266000	1.868440000	0.077298000
H	5.070874000	1.108150000	-1.869836000
H	7.487262000	1.593903000	-1.633673000
H	8.360350000	2.620336000	0.457976000
H	6.786200000	3.164890000	2.306580000
H	4.369119000	2.697315000	2.061547000
C	3.159476000	1.596382000	-0.060011000
C	1.951165000	1.376822000	-0.188375000
N	0.355269000	3.108419000	1.859145000
H	0.590881000	3.833236000	2.526916000
H	0.964636000	2.302800000	1.960869000

B3PW91/BS-I Optimized Geometry of Int3
Energy (B3PW91-GD3/BSII) = -2795.188531 a.u.

Pd	-0.010584000	-0.271300000	0.049228000
P	-2.227054000	0.370730000	-0.220223000
P	2.032710000	0.854698000	-0.314715000
C	0.756463000	-3.775337000	-0.471688000
C	1.957216000	-4.496383000	-0.623251000
H	2.746790000	-4.331721000	0.104177000
C	-0.299321000	-3.975696000	-1.406478000

C	2.136983000	-5.387938000	-1.670786000
C	1.101846000	-5.568999000	-2.594520000
H	1.227744000	-6.260829000	-3.423910000
C	-0.093312000	-4.875402000	-2.467033000
H	-0.894723000	-5.032751000	-3.185990000
H	3.068486000	-5.937672000	-1.769453000
C	-3.620554000	-0.807127000	0.115209000
C	-3.511909000	-1.626453000	1.249569000
C	-4.752773000	-0.938298000	-0.700926000
C	-4.516302000	-2.535776000	1.571505000
H	-2.627776000	-1.555507000	1.879290000
C	-5.752088000	-1.859870000	-0.385134000
H	-4.857103000	-0.317834000	-1.586620000
C	-5.639097000	-2.657137000	0.752500000
H	-4.414096000	-3.159894000	2.455684000
H	-6.622370000	-1.951387000	-1.030979000
H	-6.418158000	-3.375222000	0.996162000
C	-2.636371000	0.937861000	-1.930820000
C	-2.082910000	0.220028000	-3.001913000
C	-3.458076000	2.037482000	-2.210742000
C	-2.363230000	0.576342000	-4.319062000
H	-1.411971000	-0.611058000	-2.793047000
C	-3.727088000	2.402791000	-3.530474000
H	-3.886936000	2.613919000	-1.395702000
C	-3.186533000	1.671035000	-4.586781000
H	-1.925519000	0.008815000	-5.136642000
H	-4.362483000	3.262108000	-3.731478000
H	-3.398924000	1.956489000	-5.614180000
C	-2.711274000	1.816189000	0.825171000
C	-4.007088000	2.007214000	1.325184000
C	-1.722623000	2.762625000	1.130678000
C	-4.306395000	3.124163000	2.105022000
H	-4.784170000	1.278848000	1.110476000
C	-2.025248000	3.882054000	1.903547000
H	-0.709534000	2.605983000	0.767591000
C	-3.318101000	4.064693000	2.393727000
H	-5.315022000	3.257018000	2.489288000
H	-1.244013000	4.602663000	2.131257000
H	-3.553552000	4.932959000	3.004523000
C	2.235063000	1.668458000	-1.961582000
C	1.081756000	2.103830000	-2.626700000
C	3.483177000	1.879035000	-2.564778000
C	1.171503000	2.747609000	-3.859814000
H	0.110501000	1.921815000	-2.173718000
C	3.571607000	2.514524000	-3.802555000
H	4.388803000	1.541690000	-2.068511000
C	2.417214000	2.952294000	-4.451713000
H	0.264202000	3.074762000	-4.361071000
H	4.546077000	2.666542000	-4.260780000
H	2.489029000	3.445363000	-5.418280000
C	3.631420000	-0.061162000	-0.167046000
C	4.751664000	0.419983000	0.522702000
C	3.713279000	-1.311014000	-0.797731000
C	5.927199000	-0.330367000	0.575735000
H	4.708625000	1.384378000	1.020851000
C	4.892600000	-2.050834000	-0.759063000
H	2.844687000	-1.707734000	-1.318013000
C	6.002972000	-1.563849000	-0.068310000
H	6.786853000	0.055357000	1.118846000
H	4.938646000	-3.013355000	-1.262456000
H	6.920934000	-2.145310000	-0.029171000
C	2.282011000	2.257991000	0.860398000
C	2.560775000	3.568722000	0.453073000
C	2.149009000	1.993081000	2.232855000
C	2.704955000	4.588451000	1.395595000
H	2.666438000	3.796897000	-0.603412000
C	2.308498000	3.008251000	3.172112000
H	1.914595000	0.984935000	2.565518000
C	2.583827000	4.312063000	2.755895000
H	2.918238000	5.601129000	1.061326000
H	2.207190000	2.780827000	4.230465000
H	2.700937000	5.107013000	3.488438000
C	-0.284685000	-0.581395000	3.405104000
C	-0.347853000	-0.278070000	4.763133000
C	0.239178000	-1.124634000	5.702622000
C	0.892485000	-2.282474000	5.275064000
C	0.952618000	-2.596252000	3.922331000
C	0.360196000	-1.749446000	2.964686000
H	-0.724245000	0.084003000	2.666046000
H	-0.856965000	0.627071000	5.084359000
H	0.190941000	-0.884466000	6.761739000
H	1.355224000	-2.947127000	6.000446000
H	1.454995000	-3.499170000	3.587769000
C	0.427844000	-2.119874000	1.575367000
C	0.586441000	-2.889874000	0.622014000
N	-1.500199000	-3.340843000	-1.231396000
H	-2.130350000	-3.294712000	-2.018156000
H	-1.510428000	-2.519224000	-0.634729000

B3PW91/BS-I Optimized Geometry of TS3
Energy (B3PW91-GD3/BSII) = -2795.137763 a.u.

Pd	0.010411000	0.476014000	0.396320000
P	-1.720383000	-1.093463000	0.491151000
P	2.125988000	-0.252573000	-0.570991000
C	0.177432000	2.456510000	1.943656000
C	0.309902000	1.627339000	3.086511000
H	-0.345242000	0.762943000	3.164092000
C	0.924920000	3.709806000	1.879339000
C	1.226195000	1.904591000	4.082120000
C	2.007601000	3.075342000	3.986421000
H	2.735473000	3.300504000	4.763387000
C	1.844237000	3.959807000	2.943713000
H	2.438396000	4.870542000	2.901614000
H	1.324340000	1.245061000	4.939738000
C	-3.048910000	-0.864525000	1.748707000
C	-3.558026000	0.426325000	1.948808000
C	-3.574746000	-1.926730000	2.497797000
C	-4.581980000	0.646347000	2.867985000
H	-3.137037000	1.262239000	1.396216000
C	-4.591438000	-1.700507000	3.424795000
H	-3.187981000	-2.932583000	2.361905000
C	-5.099268000	-0.415270000	3.609660000
H	-4.965992000	1.653024000	3.011606000
H	-4.985494000	-2.532160000	4.003928000
H	-5.890656000	-0.240656000	4.334416000
C	-1.027297000	-2.744138000	0.935079000

C	0.025442000	-2.789322000	1.860608000
C	-1.502598000	-3.944666000	0.391245000
C	0.584192000	-4.007280000	2.242131000
H	0.420103000	-1.860558000	2.266397000
C	-0.937280000	-5.163160000	0.768654000
H	-2.312241000	-3.928380000	-0.332870000
C	0.104799000	-5.197846000	1.694414000
H	1.403472000	-4.023125000	2.956052000
H	-1.313940000	-6.087130000	0.336382000
H	0.545659000	-6.148331000	1.984535000
C	-2.654157000	-1.448929000	-1.055292000
C	-4.042520000	-1.629502000	-1.087518000
C	-1.927748000	-1.535781000	-2.252725000
C	-4.689951000	-1.898503000	-2.293658000
H	-4.621247000	-1.556087000	-0.171545000
C	-2.575853000	-1.816224000	-3.453088000
H	-0.851751000	-1.380925000	-2.242659000
C	-3.959840000	-1.996086000	-3.476888000
H	-5.769002000	-2.031096000	-2.305509000
H	-1.996969000	-1.887005000	-4.370246000
H	-4.467045000	-2.206777000	-4.415207000
C	2.031168000	-1.449007000	-1.967447000
C	1.697091000	-2.787664000	-1.702346000
C	2.168032000	-1.041789000	-3.301333000
C	1.531520000	-3.696710000	-2.744211000
H	1.566904000	-3.122382000	-0.676504000
C	1.990205000	-1.953206000	-4.343032000
H	2.418782000	-0.010021000	-3.529557000
C	1.677399000	-3.283101000	-4.069072000
H	1.280128000	-4.729712000	-2.517756000
H	2.103941000	-1.619228000	-5.371554000
H	1.544996000	-3.993199000	-4.881542000
C	3.354101000	-1.014978000	0.573037000
C	4.281184000	-1.992525000	0.187842000
C	3.369441000	-0.547539000	1.894871000
C	5.204916000	-2.490313000	1.106210000
H	4.276973000	-2.376072000	-0.828795000
C	4.300517000	-1.039793000	2.807458000
H	2.650047000	0.205608000	2.210669000
C	5.218643000	-2.014075000	2.416574000
H	5.916633000	-3.251107000	0.794520000
H	4.302633000	-0.662633000	3.827063000
H	5.940689000	-2.402629000	3.130600000
C	3.064290000	1.164740000	-1.280695000
C	2.456108000	2.424815000	-1.303544000
C	4.372039000	1.027314000	-1.770900000
C	3.138883000	3.528580000	-1.816738000
H	1.453115000	2.558026000	-0.904102000
C	5.049717000	2.128740000	-2.285101000
H	4.863983000	0.058419000	-1.744226000
C	4.432412000	3.381709000	-2.310290000
H	2.651903000	4.499458000	-1.813381000
H	6.063153000	2.011789000	-2.661466000
H	4.966295000	4.241628000	-2.707780000
C	-2.851806000	4.539954000	-1.289196000
C	-3.676465000	4.675161000	-2.401500000
C	-3.913588000	3.582834000	-3.236595000
C	-3.311835000	2.355622000	-2.951689000
C	-2.482183000	2.219627000	-1.844164000
C	-2.242644000	3.308468000	-0.983740000
H	-2.674163000	5.389052000	-0.633742000
H	-4.137472000	5.636317000	-2.616908000
H	-4.558899000	3.687897000	-4.105367000
H	-3.484085000	1.497914000	-3.597176000
H	-1.999527000	1.270398000	-1.632004000
C	-1.397023000	3.206433000	0.187810000
C	-0.840914000	2.281359000	0.937480000
N	0.657912000	4.566100000	0.890285000
H	0.997651000	5.506323000	1.085868000
H	-0.660785000	4.202335000	0.512813000

B3PW91/BS-I Optimized Geometry of Int4
Energy (B3PW91-GD3/BSII) = -2795.193256 a.u.

Pd	0.344091000	-0.264046000	-0.258526000
P	-1.670488000	-1.376892000	0.252257000
P	-0.064377000	2.058716000	-0.479909000
C	2.637396000	-2.032008000	-1.433359000
C	2.428130000	-1.887728000	-2.816923000
H	1.678154000	-1.179986000	-3.160981000
C	3.621331000	-2.954263000	-0.972868000
C	3.186267000	-2.630409000	-3.709479000
C	4.162477000	-3.524563000	-3.229571000
H	4.754361000	-4.094534000	-3.942551000
C	4.395735000	-3.702564000	-1.870728000
H	5.149319000	-4.403622000	-1.520806000
H	3.038710000	-2.521304000	-4.780285000
C	-1.992779000	-2.910995000	-0.725039000
C	-0.917691000	-3.508883000	-1.395424000
C	-3.262003000	-3.501123000	-0.818450000
C	-1.103105000	-4.677555000	-2.132898000
H	0.062825000	-3.043517000	-1.337668000
C	-3.446289000	-4.666527000	-1.560531000
H	-4.109938000	-3.047262000	-0.313120000
C	-2.367645000	-5.258013000	-2.218464000
H	-0.257528000	-5.126475000	-2.648046000
H	-4.436226000	-5.111963000	-1.625806000
H	-2.514832000	-6.165102000	-2.799855000
C	-3.367297000	-0.639726000	0.304683000
C	-3.809461000	0.049748000	-0.835262000
C	-4.218492000	-0.716474000	1.415364000
C	-5.071891000	0.636688000	-0.867635000
H	-3.155297000	0.138154000	-1.698840000
C	-5.479407000	-0.118306000	1.385337000
H	-3.897827000	-1.245558000	2.308062000
C	-5.910534000	0.557229000	0.245114000
H	-5.393113000	1.168124000	-1.759633000
H	-6.126782000	-0.186560000	2.256656000
H	-6.892817000	1.022852000	0.223967000
C	-1.460120000	-1.992787000	1.977403000
C	-1.590754000	-3.338339000	2.341344000
C	-1.109936000	-1.055867000	2.964124000
C	-1.380881000	-3.738043000	3.662331000
H	-1.856425000	-4.078348000	1.592018000
C	-0.918362000	-1.455187000	4.284867000
H	-0.988883000	-0.009671000	2.691735000
C	-1.049462000	-2.799755000	4.637492000

H	-1.482255000	-4.787753000	3.927640000
H	-0.660332000	-0.715108000	5.038703000
H	-0.890793000	-3.112932000	5.666472000
C	-0.683002000	2.945126000	1.014736000
C	-1.960367000	2.630640000	1.507472000
C	0.109093000	3.850216000	1.733127000
C	-2.437541000	3.222799000	2.674364000
H	-2.588792000	1.924452000	0.971347000
C	-0.366704000	4.431545000	2.909017000
H	1.102040000	4.103640000	1.374351000
C	-1.640837000	4.124405000	3.381567000
H	-3.433184000	2.972639000	3.032364000
H	0.263094000	5.131663000	3.452947000
H	-2.011303000	4.582171000	4.295571000
C	-1.252723000	2.549260000	-1.804055000
C	-2.159893000	3.611048000	-1.702114000
C	-1.220534000	1.800642000	-2.990549000
C	-3.012391000	3.918429000	-2.763605000
H	-2.208124000	4.196467000	-0.788001000
C	-2.064725000	2.113946000	-4.053185000
H	-0.532633000	0.960917000	-3.068239000
C	-2.965668000	3.174303000	-3.941243000
H	-3.713300000	4.744459000	-2.668057000
H	-2.024956000	1.525261000	-4.966525000
H	-3.629211000	3.416819000	-4.767718000
C	1.422125000	3.060459000	-0.942870000
C	2.690330000	2.527735000	-0.686471000
C	1.323525000	4.333538000	-1.523334000
C	3.838977000	3.258389000	-0.991711000
H	2.765876000	1.530639000	-0.257828000
C	2.471636000	5.057185000	-1.837548000
H	0.346934000	4.758791000	-1.738732000
C	3.732456000	4.521704000	-1.569852000
H	4.816282000	2.831896000	-0.780924000
H	2.381681000	6.040094000	-2.294201000
H	4.627755000	5.087374000	-1.817205000
C	2.997351000	-0.246924000	2.789000000
C	3.695690000	0.750186000	3.468089000
C	4.938435000	1.177948000	3.002994000
C	5.475553000	0.603210000	1.851241000
C	4.774669000	-0.391222000	1.170510000
C	3.528109000	-0.827002000	1.633598000
H	2.029474000	-0.580432000	3.155432000
H	3.269638000	1.188463000	4.367334000
H	5.486253000	1.951422000	3.535343000
H	6.445398000	0.927802000	1.481240000
H	5.198205000	-0.830551000	0.270277000
C	2.749412000	-1.905766000	0.894380000
C	1.997947000	-1.365592000	-0.327700000
N	3.626707000	-2.974000000	0.391177000
H	4.445487000	-3.255865000	0.911730000
H	2.013986000	-2.335320000	1.586892000

B3PW91/BS-I Optimized Geometry of TS4
Energy (B3PW91-GD3/BSII) = -2795.160616 a.u.

Pd	0.099199000	-0.262050000	0.129225000
P	1.258266000	1.779642000	0.091729000
P	-2.227619000	-0.341289000	-0.105201000
C	1.497231000	-2.553734000	1.862532000
C	1.044174000	-2.158819000	3.126188000
H	0.415390000	-1.277410000	3.214841000
C	2.313830000	-3.700548000	1.751491000
C	1.414550000	-2.903190000	4.239617000
C	2.236728000	-4.035228000	4.103609000
H	2.515334000	-4.600328000	4.989768000
C	2.703739000	-4.452592000	2.862313000
H	3.339234000	-5.329167000	2.766465000
H	1.074283000	-2.607355000	5.228265000
C	3.027724000	1.625857000	0.608912000
C	3.881180000	0.840057000	-0.185878000
C	3.533127000	2.155611000	1.802342000
C	5.200414000	0.608324000	0.193383000
H	3.511270000	0.420504000	-1.119891000
C	4.851750000	1.909372000	2.189628000
H	2.895803000	2.765989000	2.435690000
C	5.691024000	1.139528000	1.388002000
H	5.847486000	0.010908000	-0.445047000
H	5.223127000	2.329214000	3.121679000
H	6.718851000	0.953310000	1.689334000
C	0.649582000	3.121842000	1.209375000
C	-0.153962000	2.738468000	2.292320000
C	0.939552000	4.481526000	1.032651000
C	-0.643282000	3.688503000	3.188330000
H	-0.405209000	1.686264000	2.413915000
C	0.440859000	5.432717000	1.921530000
H	1.548862000	4.800877000	0.191490000
C	-0.347624000	5.038461000	3.003010000
H	-1.265671000	3.373271000	4.022152000
H	0.667782000	6.485194000	1.767850000
H	-0.736016000	5.782584000	3.694264000
C	1.431317000	2.637424000	-1.537279000
C	2.546994000	3.404786000	-1.903913000
C	0.378653000	2.499942000	-2.453092000
C	2.601877000	4.025743000	-3.151194000
H	3.382258000	3.507633000	-1.216146000
C	0.430539000	3.128216000	-3.696625000
H	-0.481821000	1.893207000	-2.181525000
C	1.543085000	3.891328000	-4.049243000
H	3.475059000	4.615015000	-3.421734000
H	-0.398308000	3.015250000	-4.391223000
H	1.588157000	4.375518000	-5.021875000
C	-3.160243000	1.002305000	-0.977343000
C	-2.850852000	2.330276000	-0.640715000
C	-4.111732000	0.773496000	-1.979920000
C	-3.494906000	3.395485000	-1.265340000
H	-2.093774000	2.527447000	0.114887000
C	-4.740893000	1.841892000	-2.621111000
H	-4.364434000	-0.243019000	-2.265612000
C	-4.441033000	3.154336000	-2.262605000
H	-3.244958000	4.415009000	-0.982081000
H	-5.471903000	1.643082000	-3.401576000
H	-4.935188000	3.984967000	-2.760810000
C	-3.061604000	-0.393882000	1.545839000
C	-4.070336000	0.488301000	1.950990000
C	-2.624119000	-1.375806000	2.449988000
C	-4.624497000	0.393889000	3.229211000

H	-4.428708000	1.253280000	1.268515000
C	-3.186234000	-1.475932000	3.719573000
H	-1.837402000	-2.063361000	2.148651000
C	-4.186981000	-0.586952000	4.116276000
H	-5.406522000	1.088880000	3.526635000
H	-2.838351000	-2.247629000	4.402329000
H	-4.622241000	-0.660286000	5.110009000
C	-2.926900000	-1.861037000	-0.897092000
C	-4.211660000	-2.348109000	-0.615946000
C	-2.127900000	-2.555528000	-1.812981000
C	-4.685306000	-3.499844000	-1.242336000
H	-4.841579000	-1.827533000	0.101032000
C	-2.605478000	-3.701124000	-2.448660000
H	-1.118399000	-2.201100000	-2.007842000
C	-3.884509000	-4.176678000	-2.162917000
H	-5.681024000	-3.870245000	-1.009444000
H	-1.971349000	-4.227959000	-3.157616000
H	-4.254521000	-5.076206000	-2.649290000
C	2.616289000	-3.951459000	-2.481608000
C	2.691017000	-3.952503000	-3.872986000
C	2.293579000	-2.831562000	-4.599037000
C	1.805334000	-1.713358000	-3.921712000
C	1.721204000	-1.711245000	-2.533115000
C	2.137371000	-2.828503000	-1.792432000
H	2.900959000	-4.849710000	-1.940233000
H	3.056268000	-4.837148000	-4.388467000
H	2.354584000	-2.832414000	-5.684237000
H	1.481960000	-0.835505000	-4.475022000
H	1.313509000	-0.849592000	-2.002208000
C	2.073110000	-2.812181000	-0.312363000
C	1.243827000	-1.972146000	0.538097000
N	2.621318000	-3.874908000	0.417794000
H	3.425698000	-4.399751000	0.106345000
H	2.491763000	-1.662685000	0.094349000

B3PW91/BS-I Optimized Geometry of 2-Phenyl-Indole
Energy (B3PW91-GD3/BSII) = -594.7984601 a.u.

C	3.148640000	1.370585000	-0.273308000
C	1.890009000	0.758264000	-0.147825000
C	1.830895000	-0.636418000	0.121116000
C	2.978842000	-1.414955000	0.287002000
C	4.206689000	-0.777705000	0.167213000
C	4.290526000	0.600345000	-0.113641000
C	0.540036000	1.220199000	-0.229994000
C	-0.287811000	0.137432000	-0.022402000
N	0.501622000	-0.986783000	0.164988000
H	3.223687000	2.433895000	-0.487582000
H	2.916365000	-2.479706000	0.498304000
H	5.119995000	-1.354152000	0.289411000
H	5.269265000	1.064290000	-0.204800000
H	0.213223000	2.223923000	-0.466538000
H	0.150889000	-1.869633000	0.501480000
C	-1.747106000	0.054430000	-0.012441000
C	-2.414480000	-1.132541000	-0.357138000
C	-2.518252000	1.172924000	0.344221000
C	-3.804998000	-1.199448000	-0.339975000
C	-3.907167000	1.106704000	0.350135000
C	-4.558394000	-0.080704000	0.012554000
H	-1.842632000	-2.000678000	-0.677000000
H	-2.016569000	2.090807000	0.638210000
H	-4.301290000	-2.126728000	-0.615216000
H	-4.485004000	1.983406000	0.631827000
H	-5.643864000	-0.132621000	0.023875000

B3PW91/BS-I Optimized Geometry of $PdCl_2(NCCH_3)$
Energy (B3PW91-GD3/BSII) = -1181.129532 a.u.

Pd	0.672179000	0.003593000	-0.000011000
Cl	0.853934000	-2.290123000	0.000011000
Cl	0.821809000	2.299770000	0.000011000
N	-1.270703000	-0.009093000	0.000028000
C	-2.423506000	-0.014167000	0.000000000
C	-3.873862000	-0.019439000	-0.000013000
H	-4.246482000	1.009464000	-0.008570000
H	-4.241094000	-0.544170000	-0.887419000
H	-4.241169000	-0.529303000	0.895990000

B3PW91/BS-I Optimized Geometry of $PdCl_2(NCCH_3)$ -Int3
Energy (B3PW91-GD3/BSII) = -1643.133915 a.u.

Pd	-0.266967000	0.991421000	0.064960000
N	-0.308236000	3.063809000	0.127661000
C	2.073208000	-1.305843000	0.147779000
C	2.689205000	-1.531911000	1.402580000
H	2.060892000	-1.498195000	2.287196000
C	2.862066000	-1.284491000	-1.045595000
C	4.043630000	-1.775670000	1.492775000
C	4.813050000	-1.786177000	0.315726000
H	5.881909000	-1.977629000	0.374448000
C	4.244198000	-1.544777000	-0.920803000
H	4.861016000	-1.546254000	-1.816543000
H	4.509289000	-1.952912000	2.457033000
C	-2.803803000	-1.352828000	-1.020930000
C	-4.059637000	-1.951057000	-1.029927000
C	-4.418510000	-2.853338000	-0.027917000
C	-3.514657000	-3.159756000	0.990002000
C	-2.254554000	-2.571449000	1.008045000
C	-1.889545000	-1.668949000	-0.004223000
H	-2.512318000	-0.644442000	-1.790756000
H	-4.762684000	-1.708028000	-1.822291000
H	-5.403045000	-3.313995000	-0.037185000
H	-3.792604000	-3.857077000	1.775932000
H	-1.549135000	-2.794285000	1.802427000
C	-0.569374000	-1.084248000	0.016463000
C	0.681217000	-1.139079000	0.082604000
N	2.296395000	-1.055551000	-2.257867000
H	2.915799000	-0.867058000	-3.032266000
H	1.397410000	-0.576366000	-2.308401000
C	-0.383152000	4.212890000	0.201722000
C	-0.477371000	5.658384000	0.299875000
H	-0.955170000	6.063118000	-0.597441000
H	-1.070070000	5.931803000	1.178199000
H	0.523552000	6.089871000	0.397391000
Cl	-0.274472000	0.938810000	2.406971000
Cl	-0.311252000	1.050488000	-2.312471000

B3PW91/BS-I Optimized Geometry of $PdCl_2(NCCH_3)$ -TS3
Energy (B3PW91-GD3/BSII) = -1775.855433 a.u.

Pd	1.103341000	-0.473439000	-0.065019000
Cl	0.998838000	-0.635730000	-2.409522000
Cl	1.154330000	-0.372409000	2.297205000
C	-1.792613000	-1.341736000	0.266140000
C	-1.440499000	-2.648145000	0.685114000
H	-0.420728000	-2.819554000	1.014257000
C	-3.148871000	-1.058594000	-0.141695000
C	-2.375295000	-3.654789000	0.679138000
C	-3.686116000	-3.397394000	0.209104000
H	-4.414730000	-4.204442000	0.194432000
C	-4.058653000	-2.150153000	-0.233632000
H	-5.072495000	-1.963490000	-0.578735000
H	-2.107370000	-4.654053000	1.008792000
C	-1.456077000	3.274559000	-1.047200000
C	-1.268266000	4.619078000	-0.762318000
C	-0.649919000	4.992508000	0.434250000
C	-0.218797000	4.023351000	1.345104000
C	-0.405911000	2.676267000	1.071089000
C	-1.027699000	2.286693000	-0.136239000
H	-1.925317000	2.966856000	-1.977740000
H	-1.595710000	5.377438000	-1.467762000
H	-0.500219000	6.046201000	0.656561000
H	0.264403000	4.322406000	2.270969000
H	-0.060578000	1.908522000	1.759360000
C	-1.248591000	0.905825000	-0.450282000
C	-0.870614000	-0.298595000	0.044949000
N	-3.465424000	0.214654000	-0.435375000
H	-4.270736000	0.301951000	-1.059186000
H	-2.319969000	0.684334000	-1.069043000
N	3.183676000	-0.709199000	-0.142633000
C	4.325831000	-0.867391000	-0.194070000
C	5.762773000	-1.067228000	-0.263099000
H	6.110129000	-1.591149000	0.632575000
H	6.013154000	-1.661953000	-1.146874000
H	6.270761000	-0.100227000	-0.329392000

B3PW91/BS-I Optimized Geometry of $PdCl_2(NCCH_3)$ -Int4
Energy (B3PW91-GD3/BSII) = -1775.950219 a.u.

Pd	-1.127964000	-0.556536000	0.110124000
Cl	-1.416710000	0.035743000	2.389717000
Cl	-0.840561000	-1.174685000	-2.144487000
C	1.791761000	-1.308076000	0.093570000
C	1.764676000	-2.627996000	-0.427437000
H	0.816807000	-3.039725000	-0.757159000
C	3.040145000	-0.724835000	0.505248000
C	2.944828000	-3.325576000	-0.519687000
C	4.165955000	-2.731769000	-0.100886000
H	5.081563000	-3.312453000	-0.187787000
C	4.243360000	-1.451234000	0.409531000
H	5.191028000	-1.022857000	0.722135000
H	2.957409000	-4.335545000	-0.917322000
C	0.157542000	3.036178000	0.736671000
C	-0.121291000	4.241032000	0.093186000
C	0.551103000	4.583279000	-1.078684000
C	1.501145000	3.712137000	-1.611898000
C	1.780632000	2.506499000	-0.973410000
C	1.112551000	2.166019000	0.206454000
H	-0.378900000	2.756238000	1.639588000
H	-0.865663000	4.913020000	0.512440000
H	0.333888000	5.524033000	-1.578097000
H	2.021810000	3.967674000	-2.531171000
H	2.514156000	1.824967000	-1.396927000
C	1.407055000	0.849937000	0.906913000
C	0.770243000	-0.378982000	0.313557000
N	2.825041000	0.520716000	0.956440000
H	3.535573000	1.159977000	1.277600000
H	0.996529000	0.890104000	1.931829000
N	-3.236438000	-0.749941000	-0.108486000
C	-4.378716000	-0.852248000	-0.238840000
C	-5.816060000	-0.980349000	-0.404632000
H	-6.101826000	-2.036259000	-0.374690000
H	-6.333682000	-0.448030000	0.399102000
H	-6.118537000	-0.558002000	-1.367762000

B3PW91/BS-I Optimized Geometry of $PdCl_2(NCCH_3)$ -TS4
Energy (B3PW91-GD3/BSII) = -1775.927622 a.u.

Pd	1.180244000	-0.480764000	-0.021594000
Cl	1.196272000	-0.079651000	-2.366471000
Cl	0.990284000	-0.886653000	2.281270000
C	-1.688657000	-1.532282000	-0.084647000
C	-1.460878000	-2.912533000	-0.010869000
H	-0.444594000	-3.287156000	0.055480000
C	-3.010153000	-1.036766000	-0.136411000
C	-2.556460000	-3.760458000	-0.009882000
C	-3.866951000	-3.248728000	-0.088514000
H	-4.705372000	-3.940460000	-0.091068000
C	-4.120263000	-1.885929000	-0.156316000
H	-5.134581000	-1.501002000	-0.211419000
H	-2.409245000	-4.834728000	0.051083000
C	-2.094521000	2.954028000	0.824516000
C	-1.828639000	4.308884000	1.005724000
C	-0.775925000	4.912395000	0.320258000
C	0.012418000	4.153423000	-0.544404000
C	-0.245545000	2.798587000	-0.732410000
C	-1.303722000	2.191197000	-0.045656000
H	-2.893974000	2.479299000	1.387329000
H	-2.440140000	4.888679000	1.691905000
H	-0.568345000	5.969744000	0.462314000
H	0.833792000	4.617579000	-1.083513000
H	0.365754000	2.211018000	-1.412671000
C	-1.619813000	0.752684000	-0.207324000
C	-0.773873000	-0.409966000	-0.090258000
N	-2.945488000	0.338290000	-0.178513000
H	-3.710759000	0.946830000	-0.430574000
H	-1.025640000	0.264219000	-1.259813000
N	3.270489000	-0.603143000	0.078705000
C	4.418755000	-0.679021000	0.170120000
C	5.863219000	-0.774944000	0.289153000
H	6.152663000	-1.812757000	0.480829000
H	6.338567000	-0.437092000	-0.636708000
H	6.210198000	-0.151308000	1.118746000

10. References

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