$PhI(OCOCF_3)_2$-Mediated Metal-Free 2,3-Difunctionalization of Indoles: Direct Access to Carbochalcogenated Scaffolds

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Contents

1. Experimental Section

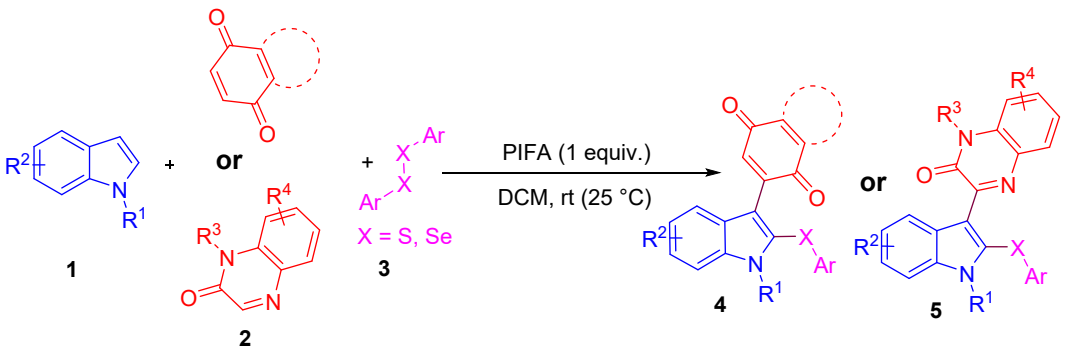
General Information

^{1}H NMR spectra were determined on a Bruker 400 (400 MHz) spectrometer as solutions in $CDCl_3$. Chemical shifts are expressed in parts per million (δ), and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet), and coupling constants *J* were given in Hz. $^{13}C\{^{1}H\}$ NMR spectra were recorded at 100 MHz in $CDCl_3$ solution. Chemical shifts are expressed in parts per million (δ) and are referenced to $CDCl_3$ (δ = 77.16) as an internal standard. TLC was done on a silica gel-coated glass slide (Merck, Silica gel G for TLC). Silica gel (60-120 mesh, SRL, India) was used for column chromatography. Petroleum ether refers to the fraction boiling in the range of 60-80 °C unless otherwise mentioned. All solvents were dried and distilled before use. Commercially available substrates were freshly distilled before the reaction. Solvents, reagents, and chemicals were purchased from Aldrich, Merck, and Spectrochem Chemicals. All reactions involving moisture-sensitive reactants were executed using oven-dried glassware. All the quinoxalin-2(1H)-ones were prepared[1] according to the reported method.

2. Experimental Procedures

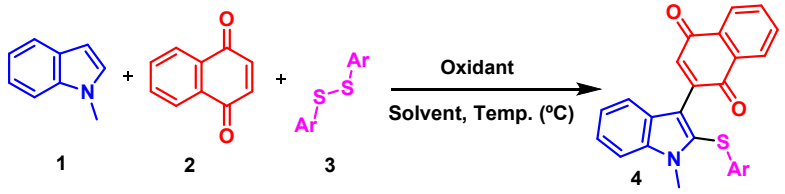
General procedure for the synthesis of 4(4aa-4aq) or 5 (5aa-5ag).

A reaction tube was equipped with a magnetic stir bar and was charged with the mixture of indole (**1**), 1,4-naphthoquinones or quinoxalin-2(1H)-one (**2**), and diaryl chalcogenides (**3**) in the presence of 1equiv. of PIFA and DCM as a solvent at room temperature for six hours. The reaction was monitored by thin-layer chromatography (TLC) analysis. Then 20 mL of water was added to the mixture, which was extracted with DCM three times (3×20mL). The extract was dried over anhydrous Na_2SO_4 and concentrated under a vacuum. Then this mixture of the crude product was purified by column chromatography on silica gel (eluent: petroleum ether/ EtOA).



3. Optimization of Reaction Conditions

Table 1. Optimization of Reaction Conditions.[a,b]



Entry	Oxidant	Solvent	Time(h)/Temp. (°C)	Yield (%)[b]
1	PIFA (1 equiv.)	DMSO	6/rt	22
2	PIFA (1 equiv.)	DMF	6/rt	19
3	PIFA (1 equiv.)	DMA	6/rt	23
4	PIFA (1 equiv.)	CH_3CN	6/rt	54
5	PIFA (1 equiv.)	DCM	6/rt	82
6	PIFA (1 equiv.)	DCE	6/rt	47
7	PIFA (1 equiv.)	toluene	6/rt	31
8	PIFA (1 equiv.)	1,4-dioxane	6/rt	36
9	PIFA (1 equiv.)	THF	6/rt	27
10	PIFA (1 equiv.)	EtOH	6/rt	23
11	PIDA (1 equiv.)	DCM	6/rt	trace
12	HTIB (1 equiv.)	DCM	6/rt	18
13	PIFA (0.5 equiv.)	DCM	6/rt	52
14	PIFA (0.8 equiv.)	DCM	6/rt	68
15	PIFA (1.5 equiv.)	DCM	6/rt	82
16	PIFA (2 equiv.)	DCM	6/rt	83
17	PIFA (1 equiv.)	DCM	6/50°C	79
18	PIFA (1 equiv.)	DCM	12/rt	81
19	-	DCM	6/rt	ND
20	PIFA (1 equiv.)	DCM	6/rt	79[c]

[a] Reaction conditions: **1** (1 mmol), **2** (1 mmol), and **3** (1.2 mmol), PIFA (1 equiv.) in 2 mL of solvent at room temperature (25 °C) for 6 h. [b] Isolated yield. [c] reaction under an argon atmosphere. ND = Not detected.

Based on our literature review, we optimized the reaction using N-methyl indole (**1**), naphthoquinone (**2**), and diphenyl disulfide (**3**) as model substrates. The reaction with one equiv. of PIFA in DMSO at room temperature for six hours gave the carbochalcogenated indole (**4aa**) in 22% yield (entry 1, Table 1). Although the yield was low, the product was promising. We then screened various solvents—DMF, DMA, MeCN, DCM, DCE toluene, 1,4-dioxane, THF, and ethanol (entries 2–10, Table 1) and found DCM to be the best solvent. Other hypervalent iodine reagents like phenyliodine(III) diacetate (PIDA), and hydroxy(tosyloxy)iodobenzene (HTIB), also known as Koser's Reagent, were less effective (entries 11–12, Table 1). Varying the PIFA amount (0.5–2 equiv.) showed no significant change (entries 13–16, Table 1). Regulating reaction time and temperature also gives minimal

effect, along with the best result at room temperature for six hours (entries 17–18, Table 1). Finally, we checked the necessity of the hypervalent iodine reagent by performing the reaction without PIFA, but the reaction did not proceed (entry 19, Table 1). Later, we observed that even under an argon atmosphere, the reaction proceeds well (entries 18, Table 1), to clarify the involvement of molecular oxygen in this reaction condition. Ultimately, the optimized conditions involved N-methyl indole (**1**), naphthoquinone (**2**), and diphenyl disulfide (**3**) in DCM at room temperature for six hours with 1 equiv. of PIFA, affording **4aa** in good yield (Table 1, entry 4).

4. Structure determination (X-ray crystallographic data for 3ar):

The red block crystal of **3an** was obtained by crystallization from a solution in dichloromethane/petroleum ether after purification by column chromatography. The chemical formula of compound **3an**: $C_{25}H_{16}BrNO_2S$.

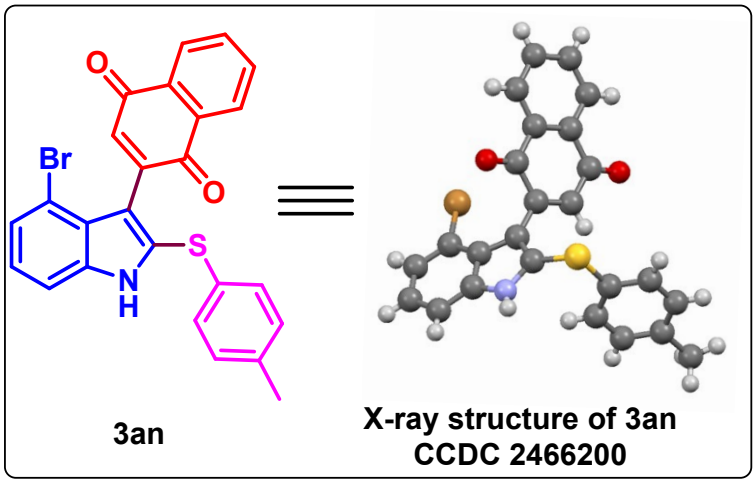
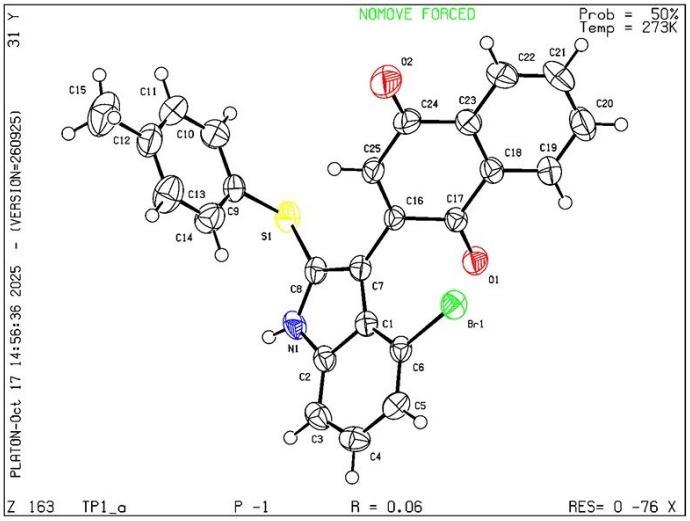
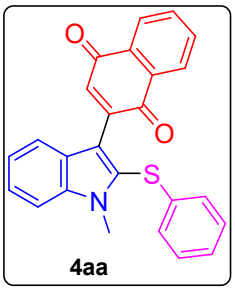


Table 2: Crystal  **data**

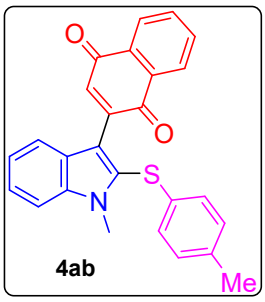
Wavelength	**0.71073Å**	
Formula	**$C_{25}H_{16}BrNO_2S$.**	
Crystal system	**Triclinic**	
Space group	**P -1**	
Unit cell dimensions	**a = 7.3740(3)Å**	**α = 92.277(2)**
	b = 8.7891(3)Å	**β = 94.132(2)**
	c = 16.2598(7)Å	**γ = 103.090(2)**
Volume	**1022.06(7)Å^3**	
Z	**2**	
R-factor (%)	**5.64**	

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication with a CCDC reference number CCDC **2466200**.

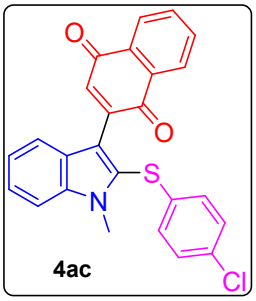
5. Spectroscopic Data of Synthesised Compounds:



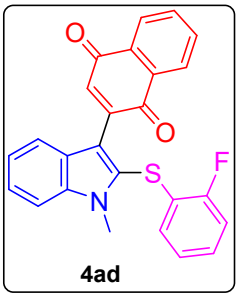
2-(1-methyl-2-(phenylthio)-1H-indol-3-yl)naphthalene-1,4-dione **(4aa):** Yield: 82%; 316 mg; red solid; Mp: 91-93 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.13-8.10 (m, 1H), 8.06-8.04 (m, 1H), 7.69-7.67 (m, 2H), 7.53 (d, J = 8 Hz, 1H), 7.30-7.26 (m, 2H), 7.18-7.16 (m, 1H), 7.14-7.10 (m, 2H), 7.05 (s, 1H), 7.04-7.01 (m, 1H), 6.93-6.91 (m, 2H), 3.66 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.3, 143.6, 138.4, 136.7, 136.3, 133.8, 133.7, 132.8, 132.4, 129.5, 129.0, 127.2, 126.8, 126.6, 126.2, 124.0, 121.3, 120.5, 116.9, 110.3, 30.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{18}NO_2S]^+$: 396.1053; Found : 396.1064.



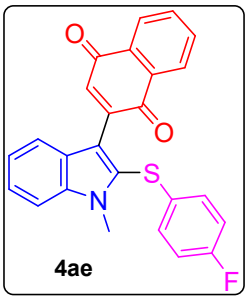
2-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione **(4ab):** Yield: 79 %; 332 mg; red solid; Mp: 106-109 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.07-8.05 (m, 1H), 8.00-7.99 (m, 1H), 7.64-7.61 (m, 2H), 7.47 (d, J = 8 Hz, 1H), 7.24-7.22 (m, 2H), 7.13-7.10 (m, 1H), 6.99 (s, 1H), 6.68 (d, J = 8 Hz, 1H), 6.78 (d, J = 8 Hz, 1H), 3.61 (s, 3H), 2.12 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.3, 143.6, 138.3, 136.6, 136.3, 133.7, 133.6, 132.8, 132.4, 130.2, 129.8, 129.2, 127.2, 127.1, 126.6, 126.0, 123.9, 121.3, 120.5, 116.9, 110.2, 30.7, 21. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{20}NO_2S]^+$: 410.1209; Found : 410.1216.



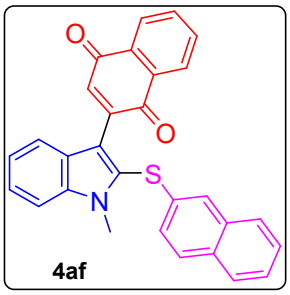
2-(2-((4-chlorophenyl)thio)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione **(4ac):** Yield: 80 %; 343 mg; red solid; Mp: 135-138 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19-8.17 (m, 1H), 8.14-8.12 (m, 1H), 7.78-7.76 (m, 2H), 7.67 (d, J = 8 Hz, 1H), 7.38-7.35 (m, 2H), 7.26-7.22 (m, 1H), 7.19-7.16 (m, 2H), 7.11 (s, 1H), 6.94-6.92 (m, 2H), 3.73 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.2, 184.2, 143.3, 138.4, 136.8, 134.8, 133.9, 133.8, 132.7, 132.3, 132.2, 129.6, 128.3, 128.0, 127.3, 126.6, 126.2, 124.3, 121.5, 120.5, 117.1, 110.3, 30.8. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{17}ClNO_2S]^+$: 430.0663; Found: 430.0671.



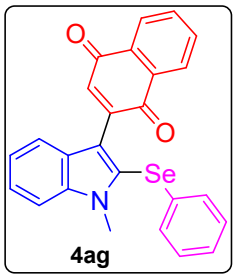
2-(2-((2-fluorophenyl)thio)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione **(4ad):** Yield: 81 %; 330 mg; red solid; Mp: 97-99 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.20-8.18 (m, 1H), 8.14-8.12 (m, 1H), 7.78-7.76 (m, 2H), 7.59 (d, J = 8 Hz, 1H), 7.41-7.35 (m, 2H), 7.26-7.22 (m, 1H), 7.19-7.16 (m, 2H), 7.11 (s, 1H), 7.11-7.09 (m, 1H), 7.05-6.99 (m, 1H), 6.67-6.63 (m, 1H), 3.77 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.2, 159.2 (d, J = 245 Hz), 143.4, 138.5, 137.6, 136.7, 133.8 (d, J = 7 Hz), 132.7, 132.3, 128.9, 128.0 (d, J = 8 Hz), 127.3, 126.6, 126.1, 125.2 (d, J = 4 Hz), 124.2, 123.5, 123.4, 121.4, 120.5, 117.5, 115.9 (d, J = 20 Hz), 110.4, 30.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{17}FNO_2S]^+$: 414.0959; Found: 414.0973.



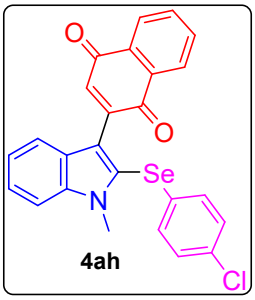
***2-(2-((4-fluorophenyl)thio)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione*(4ae):** Yield: 80 %; 334 mg; Mp: 109-111 °C; red solid; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.07-8.00 (m, 2H), 7.64-7.64 (m, 2H), 7.48 (d, J = 8 Hz, 1H), 7.26-7.20 (m, 2H), 7.13-7.10 (m, 1H), 7.02 (s, 1H), 6.92-6.88 (m, 2H), 6.81-6.77 (m, 2H), 3.60 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.1, 184.2, 161.5 (d, J = 245 Hz), 143.4, 138.3, 136.7, 133.7 (d, J = 9 Hz), 132.7, 132.3, 131.1, 131.0, 129.2, 128.9 (d, J = 7 Hz), 127.1, 126.5, 126.0, 124.1, 121.4, 120.4, 116.7 (d, J = 22 Hz), 110.2, 30.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{17}FNO_2S]^+$: 414.0959; Found: 414.0967.



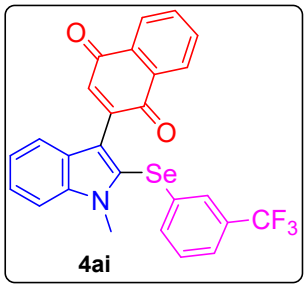
***2-(1-methyl-2-(naphthalen-2-ylthio)-1H-indol-3-yl)naphthalene-1,4-dione*(4af):** Yield: 80 %; 343 mg; Mp: 110-1113 °C; red solid; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19-8.16 (m, 1H), 8.10-8.08 (m, 1H), 7.74-7.71 (m, 3H), 7.67 (d, J = 8.8 Hz, 1H), 7.64-7.61 (m, 2H), 7.46 (s, 1H), 7.42-7.37 (m, 4H), 7.28-7.25 (m, 1H), 7.16 (s, 1H), 7.11-7.09 (m, 1H), 3.74 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.3, 143.5, 138.4, 136.6, 133.8, 133.8, 133.5, 132.8, 132.3, 131.8, 129.3, 129.1, 127.9, 127.2, 126.9, 126.7, 126.1, 126.0, 125.2, 124.9, 124.1, 122.2, 121.4, 120.5, 116.8, 110.3, 30.8. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{29}H_{20}NO_2S]^+$: 446.1209; Found : 446.1189.



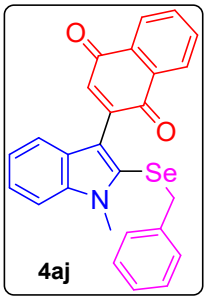
2-(1-methyl-2-(phenylselanyl)-1H-indol-3-yl)naphthalene-1,4-dione **(4ag):** Yield: 77 %; 340 mg; red solid; Mp: 90-93 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.20-8.28 (m, 1H), 8.24-8.22 (m, 1H), 7.86-7.84 (m, 2H), 7.71 (d, J = 8 Hz, 1H), 7.47 (d, J = 8.4 Hz, 1H), 7.44-7.40 (m, 1H), 7.35-7.30 (m, 2H), 7.24-7.23 (m, 5H), 3.86 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.7, 144.1, 138.7, 136.4, 134.1, 133.8, 132.8, 132.4, 131.8, 129.7, 127.7, 127.2, 127.0, 126.9, 123.7, 120.1, 117.0, 110.3, 30.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{18}NO_2Se]^+$: 444.497; Found : 444.509.



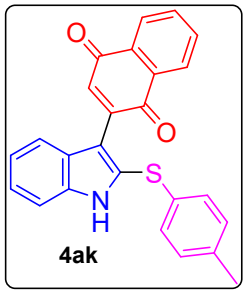
2-(2-((4-chlorophenyl)selanyl)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione **(4ah):** Yield: 79 %; 378 mg; Mp: 117-1119 °C; red solid; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.30-8.28 (m, 1H), 8.26-8.24 (m, 1H), 7.89-7.87 (m, 2H), 7.71 (d, J = 8 Hz, 1H), 7.61 (d, J = 8.4 Hz, 1H), 7.49 (d, J = 8 Hz, 1H), 7.46-7.42 (m, 1H), 7.36 (d, J = 4.8 Hz, 1H), 7.33 (s, 1H), 7.23 (d, J = 8 Hz, 1H), 7.19-7.16 (m, 2H), 3.87 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.6, 143.9, 138.8, 136.6, 133.9, 133.8, 132.8, 132.4, 131.0, 130.1, 129.9, 129.6, 127.3, 127.0, 126.2, 123.9, 121.4, 120.1, 117.2, 110.4, 30.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{17}ClNO_2Se]^+$: 478.0108; Found: 478.0114.



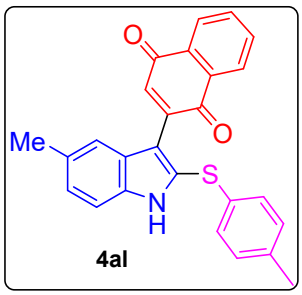
2-(1-methyl-2-((3-(trifluoromethyl)phenyl)selanyl)-1H-indol-3-yl)naphthalene-1,4-dione **(4ai):** Yield: 81%; 413 mg; red solid; Mp: 109-111 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19-8.17 (m, 1H), 8.15-8.13 (m, 1H), 7.78-7.76 (m, 2H), 7.62 (d, J = 8 Hz, 1H), 7.54 (s, 1H), 7.41 (d, J = 8.4 Hz, 2H), 7.37-7.33 (m, 1H), 7.29-7.26 (m, 1H), 7.24-7.22 (m, 1H), 7.16 (d, J = 8 Hz, 1H), 7.14 (s, 1H), 3.79 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.2, 184.5, 143.8, 138.8, 136.7, 133.9, 133.8, 133.2, 132.8, 132.4, 132.0, 131.7, 131.4, 129.9 (q, J= 32 Hz), 127.3, 126.9, 126.0 (q, J= 4 Hz), 125.0 (q, J= 272 Hz), 124.1, 123.8 (q, J= 4 Hz), 121.5, 120.1, 117.5, 110.5, 32.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{17}F_3NO_2Se]^+$: 512.0371; Found : 512.0379.



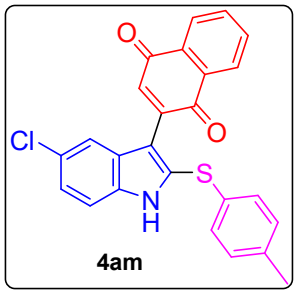
2-(2-(benzylselanyl)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione **(4aj):** Yield: 75%; 340 mg; red solid; Mp: 99-101 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.15-8.13 (m, 1H), 8.10-8.07 (m, 1H), 7.73-7.71 (m, 2H), 7.55 (d, J = 7.6 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 7.26-7.12 (m, 6H), 7.04 (s, 1H), 7.02-7.01 (m, 1H), 4.22 (s, 3H), 3.53 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.9, 144.6, 139.5, 138.0, 137.5, 135.3, 133.8, 133.6, 132.8, 132.4, 128.9, 128.2, 127.2, 127.1, 126.7, 126.0, 122.4, 121.0, 119.8, 109.5, 108.6, 32.1, 30.5. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{20}NO_2Se]^+$: 458.0654; Found : 458.0663.



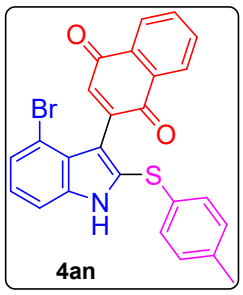
2-(2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione (**4ak**): Yield: 78%; 308 mg; red solid; Mp: 125-128 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/8); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.31 (s, 1H), 8.17-8.15 (m, 1H), 8.10-8.08 (m, 1H), 7.73-7.71 (m, 2H), 7.51 (d, J = 8 Hz, 1H), 7.24 (d, J = 8 Hz, 1H), 7.21-7.16 (m, 2H), 7.13-7.10 (m, 3H), 7.02 (d, J = 8 Hz, 1H), 2.23 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.2, 143.1, 137.9, 136.8, 136.1, 134.0, 133.9, 133.7, 132.8, 132.4, 130.7, 130.4, 130.2, 127.6, 127.2, 126.1, 123.8, 121.4, 120.1, 114.2, 111.0, 21.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{18}NO_2S]^+$: 396.1053; Found : 396.1062.



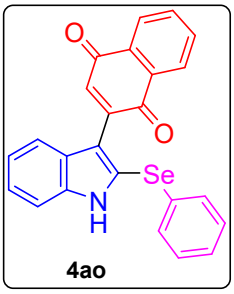
2-(5-methyl-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione (**4al**): Yield: 76%; 310 mg; red solid; Mp: 129-131 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/8); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.32 (s, 1H), 8.22-8.20 (m, 1H), 8.15-8.12 (m, 1H), 7.78-7.76 (m, 2H), 7.34 (s, 1H), 7.17 (d, J = 7.6 Hz, 1H), 7.16 -7.13 (m, 3H), 7.08-7.04 (m, 3H), 2.44 (s, 3H), 2.27 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.4, 184.2, 143.3, 137.6, 135.9, 135.1, 133.8, 133.7, 133.8, 131.1, 130.9, 130.5, 130.4, 129.9, 127.7, 127.3, 126.1, 125.4, 119.6, 114.0, 110.7, 21.7, 21.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{20}NO_2S]^+$: 410.1209; Found : 410.1213.



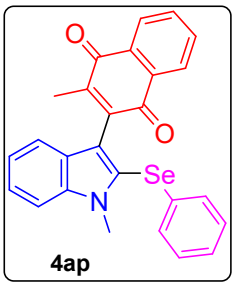
2-(5-chloro-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione **(4am):** Yield: 75%; 321 mg; red solid; Mp: 141-143 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/5); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.42 (s, 1H), 8.22-8.19 (m, 1H), 8.14-8.12 (m, 1H), 7.79-7.77 (m, 2H), 7.50 (s, 1H), 7.18-7.17 (m, 3H), 7.10 -7.06 (m, 3H), 6.99 (s, 1H), 2.28 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.2, 184.1, 142.6, 138.3, 136.2, 135.0, 134.0, 133.9, 133.0, 132.3, 130.7, 130.6, 129.9, 129.7, 128.6, 127.3, 126.4, 126.2, 124, 119.6, 112, 21.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{17}ClNO_2S]^+$: 430.0663; Found : 430.0674.



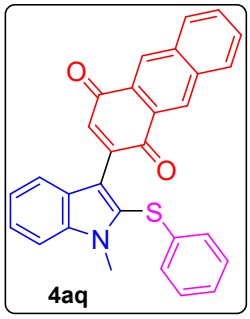
2-(4-bromo-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione **(4an):** Yield: 78%; 371 mg; red solid; Mp: 148-151 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/5); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.50 (s, 1H), 8.13-8.11 (m, 1H), 8.08-8.07 (m, 1H), 7.73-7.70 (m, 2H), 7.23 (d, J = 7.6 Hz, 1H), 7.20 (d, J = 7.6 Hz, 1H), 7.05-7.01 (m, 2H), 6.99 -6.97 (m, 2H), 6.91 (s, 1H), 2.20 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 185.2, 144.5, 137.8, 137.7, 137.7, 133.8, 133.7, 132.7, 132.5, 130.6, 130.4, 129.6, 129.3, 127.3, 127.0, 126.2, 125.3, 124.6, 115.8, 114.1, 110.5, 21.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{17}BrNO_2S]^+$: 474.0158; Found : 474.0164.



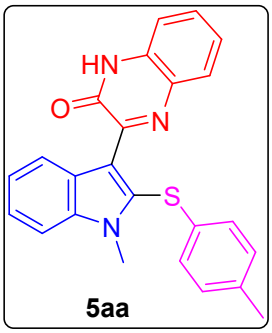
2-(2-(phenylselanyl)-1H-indol-3-yl)naphthalene-1,4-dione **(4ao)**: Yield: 81%; 347 mg; red solid; Mp: 121-123 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/5); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.41 (s, 1H), 8.23-8.21 (m, 1H), 8.16-8.14 (m, 1H), 7.79-7.77 (m, 2H), 7.61 (d, J = 8 Hz, 1H), 7.41-7.38 (m, 2H), 7.30 (d, J = 7.2 Hz, 1H), 7.29-7.20 (m, 5H), 7.19 (s, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.3, 184.7, 143.3, 137.6, 135.5, 134.0, 133.7, 132.7, 132.4, 132.4, 130.1, 129.9, 128.1, 127.6, 127.3, 126.1, 125.9, 123.6, 121.4, 119.8, 115.0, 111.0. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{24}H_{16}NO_2Se]^+$: 430.0341; Found : 430.0349.



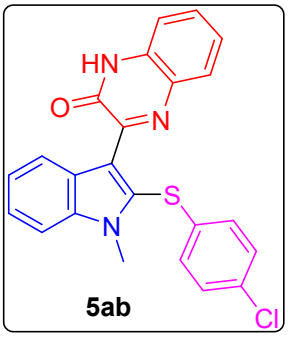
2-methyl-3-(1-methyl-2-(phenylselanyl)-1H-indol-3-yl)naphthalene-1,4-dione **(4ap):** Yield: 81%; 370 mg; red solid; Mp: 92-95 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.18-8.12 (m, 2H), 7.76-7.70 (m, 2H), 8.16-8.14 (m, 1H), 7.40 (d, J = 8 Hz, 1H), 7.32-7.28 (m, 2H), 7.19-7.13 (m, 6H), 3.80 (s, 3H), 2.07 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.8, 184.0, 146.3, 141.1, 138.6, 133.6, 133.5, 132.6, 132.5, 131.7, 130.0, 129.6, 129.3, 127.0, 126.9, 126.3, 126.1, 123.2, 120.6, 119.9, 116.5, 110.4, 31.9, 15.4. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{20}NO_2Se]^+$: 458.0654; Found : 458.0667.



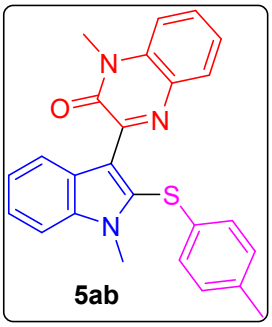
2-(1-methyl-2-(phenylthio)-1H-indol-3-yl)anthracene-1,4-dione **(4aq):** Yield: 79%; 351 mg; red solid; Mp: 131-133 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.74 (s, 1H), 8.67 (s. 1H), 8.10-8.07 (m, 2H), 7.70-7.65 (m, 3H), 7.41-7.31 (m, 3H), 7.24-7.22 (m, 2H), 7.17-7.15 (m, 5H), 3.79 (s, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.0, 184.4, 145.4, 138.7, 135.0, 131.9, 130.3, 130.3, 129.7, 139.7, 129.5, 129.5, 129.4, 129.2, 129.1, 128.9, 128.3, 127.8, 127.0, 126.9, 123.7, 121.3, 120.2, 117.2, 110.4, 32.2. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{29}H_{20}NO_2Se]^+$: 446.1209; Found : 446.1213.



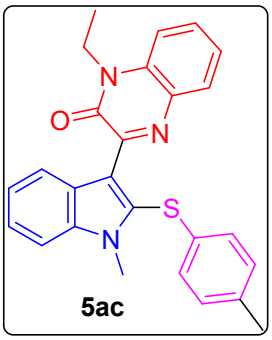
3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)quinoxalin-2(1H)-one **(5aa):** Yield: 78 %; 309 mg; yellow solid; Mp: 182-185 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 12.62 (s, 1H), 7.95-7.91 (m, 2H), 7.45-7.41 (m, 1H), 7.38-7.29 (m, 4H), 7.26-7.23 (m, 1H), 7.04 (d, J = 8 Hz, 2H), 6.98 (d, J = 8.4 Hz, 2H), 3.72 (s, 3H), 2.23 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 156.8, 153.0, 138.5, 136.1, 133.4, 132.9, 131.2, 130.0, 129.9, 129.0, 127.9, 126.9, 124.3, 123.6, 121.3, 121.3, 118.2, 116.0, 109.9, 30.80, 21.1. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{24}H_{20}N_3OS]^+$: 398.1322; Found : 398.1328.



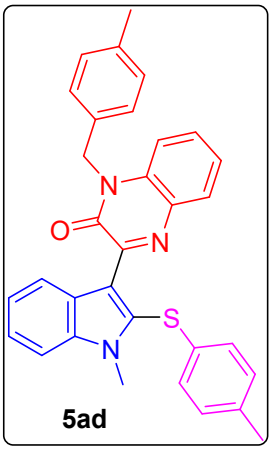
3-(2-((4-chlorophenyl)thio)-1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one **(5ab):** Yield: 75 %; 300 mg; yellow solid; Mp: 193-195 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 12.54 (s, 1H), 7.80 (d, J = 8 Hz, 2H), 7.80 (d, J = 8 Hz, 2H), 7.34-7.31 (m, 1H), 7.24-7.19 (m, 3H), 7.13-7.10 (m, 2H), 7.02 (d, J = 8 Hz, 2H), 6.92 (d, J = 8.8 Hz, 2H), 3.58 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 156.8, 152.7, 138.5, 135.4, 133.5, 131.9, 131.1, 130.2, 129.7, 129.4, 129.1, 128.7, 126.8, 124.0, 121.5, 121.3, 118.7, 115.9, 110.1, 30.7. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{23}H_{17}ClN_3OS]^+$: 418.0775; Found : 418.0781.



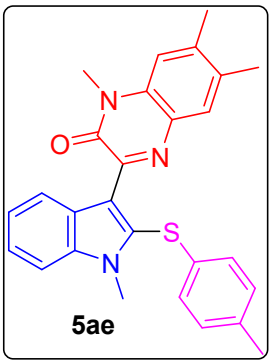
1-methyl-3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)quinoxalin-2(1H)-one **(5ac):** Yield: 75 %; 308 mg; yellow solid; Mp: 151-153 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.95-7.92 (m, 1H), 7.87-7.85 (m, 1H), 7.57-7.53 (m, 1H), 7.37-7.29 (m, 4H), 7.23-7.19 (m, 1H), 7.01-6.96 (m, 4H), 3.79 (s, 3H), 3.68 (s, 3H), 2.23 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 154.1, 137.4, 135.0, 132.4, 132.0, 130.4, 129.1, 128.9, 126.9, 125.9, 122.8, 122.5, 120.3, 120.2, 112.7, 108.9, 29.7, 28.7, 20.0. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{25}H_{22}N_3OS]^+$: 412.1478; Found : 412.1486.



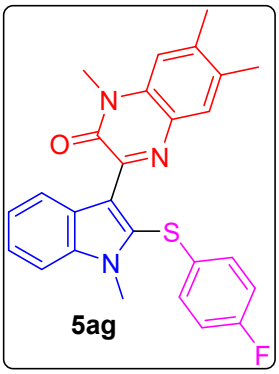
1-ethyl-3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)quinoxalin-2(1H)-one **(5ad):** Yield: 75 %; 318 mg; yellow solid; Mp: 118-121 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93-7.87 (m, 2H), 7.53-7.49 (m, 1H), 7.34-7.28 (m, 4H), 7.23-7.20 (m, 1H), 7.01-6.95 (m, 4H), 4.41-4.35 (m, 2), 3.66 (s, 3H), 2.21 (s, 3H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 154.5, 152.6, 138.3, 135.9, 133.7, 133.1, 132.2, 131.4, 130.4, 129.9, 129.8, 127.8, 126.9, 123.5, 123.4, 121.2, 121.2, 118.7, 113.5, 109.8, 37.8, 30.7, 21.0, 12.6. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{24}N_3OS]^+$: 426.1635; Found : 426.1644.



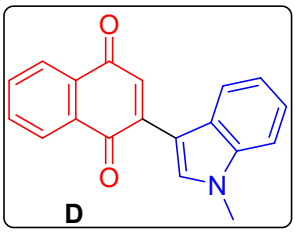
3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)-1-(4-methylbenzyl)quinoxalin-2(1H)-one **(5ae):** Yield: 75 %; 390 mg; yellow gummy mass; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94-7.90 (m, 2H), 7.43-7.39 (m, 1H), 7.35-7.29 (m, 4H), 7.26-7.24 (m, 3H), 7.11 (d, J = 8 Hz, 2H), 7.05-6.99 (m, 4H), 5.55 (s, 2H), 3.71 (s, 3H), 2.30 (s, 3H), 2.25 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 155.2. 152.7, 138.4, 137.4, 136.0, 133.7, 133.1, 132.7, 132.6, 131.4, 130.2, 130.0, 129.7, 127.8, 127.3, 126.9, 123.7, 123.5, 121.2, 121.2, 114.5, 109.8, 46.2, 30.7, 21.2, 21.0. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{32}H_{28}N_3OS]^+$: 502.1948; Found : 502.1953.



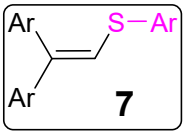
1,6,7-trimethyl-3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)quinoxalin-2(1H)-one **(5af):** Yield: 76 %; 333 mg; yellow solid; Mp: 163-165 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.79 (d, J = 8 Hz, 2H), 7.62 (s, 1H), 7.26-7.19 (m, 2H), 7.15-7.12 (m, 1H), 7.03 (s, 1H), 6.99-6.90 (m, 4H), 3.69 (s, 3H), 3.61 (s, 3H), , 2.36 (s, 3H), 2.30 (s, 3H), 2.17 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 155.1, 151.4, 139.8, 138.3, 135.9, 133.2, 132.5, 131.9, 131.4, 130.7, 130.2, 129.9, 127.8, 126.9, 123.3, 121.1, 121.0, 119.2, 114.3. 109.7, 30.6, 29.6, 21.0, 20.7, 19.3. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{27}H_{26}N_3OS]^+$: 440.1791; Found : 440.1798.



3-(2-((4-fluorophenyl)thio)-1-methyl-1H-indol-3-yl)-1,6,7-trimethylquinoxalin-2(1H)-one **(5ag):** Yield: 72 %; 319 mg; yellow solid; Mp: 127-129 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.84 (d, J = 8 Hz, 2H), 7.67 (s, 1H), 7.34-7.28 (m, 2H), 7.23-7.18 (m, 1H), 7.12-7.09(m, 3H), 6.90-6.86 (m, 2H), 3.77 (s, 3H), 3.68 (s, 3H), 2.44 (s, 3H), 2.36 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 161.4 (d, J = 244 Hz), 155.1, 151.2, 140.0, 138.3, 132.7, 131.9, 131.8 (d, J = 14 Hz), 131.4, 130.2, 130.1, 129.6 (d, J = 8 Hz), 126.9, 123.6, 121.2, 121.2, 119.3, 116.2 (d, J = 22 Hz), 114.3, 109.8, 30.6, 29.7, 21.8, 19.4. HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{23}FN_3OS]^+$: 444.1540; Found : 444.1553.



2-(1-methyl-1H-indol-3-yl)naphthalene-1,4-dione **(D)[2]:** Yield: 88 %; 252 mg; red solid; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/5); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (s, 1H), 8.05-8.01 (m, 1H), 7.90 (d, J = 7.6 Hz, 1H), 7.67-7.63 (m, 2H), 7.33 (s, 1H), 7.32-7.30 (m, 1H), 7.24-7.19 (m, 2H), 7.17-7.12 (m, 1H), 3.79 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 185.9, 185.3, 144.0, 138.1, 137.5, 135.8, 133.8, 133.3, 132.4, 129.6, 128.8, 126.9, 125.8, 123.1, 121.9, 120.8, 110.3, 33.6.



argio(2,2-diargiovinyl)sulfane **(7)[3]:** Yield: 34 %; 58 mg; yellowish white; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/50); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.45-7.44 (m, 2H), 7.40-7.37 (m, 5H), 7.33-7.26 (m, 5H), 7.17 (d, J = 8 Hz, 1H), 6.85 (s, 1H), 2.37 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.7, 140.3, 139.4, 137.1, 132.9, 130.2, 130.0, 129.9, 128.5, 128.4, 127.9, 127.3, 125.4, 21.2.

6. References:

1. Carrër, J.-D. Brion, S. Messaoudi and M. Alami, *Org. Lett.*, 2013, **15**, 5606–5609.

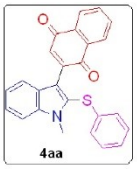
2. Y. Dong, H. Zhang, J. Yang, S. He, Z.-C. Shi, X.-M. Zhang and J.-Y. Wang, *ACS Omega*, 2019, **4**, 21567–21577.

3. N. Mukherjee and T. Chatterjee, *Green Chem.*, 2023, **25**, 8798–8807.

7. NMR spectra [^{1}H, and ^{13}C{^{1}H}] of synthesized products:

1H of VBSP-249/2

^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

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Current Data Parameters
NAME        Dr. A MAJEE 2021
EXPNO                  367
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211128
Time                  17.26
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       1
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9922944 sec
RG                    93.46
DW                   60.800 usec
DE                    6.50 usec
TE                   297.2 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1524711 MHz
NUC1                     1H
P1                    14.75 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                   16384
SF             400.1500414 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    2.00
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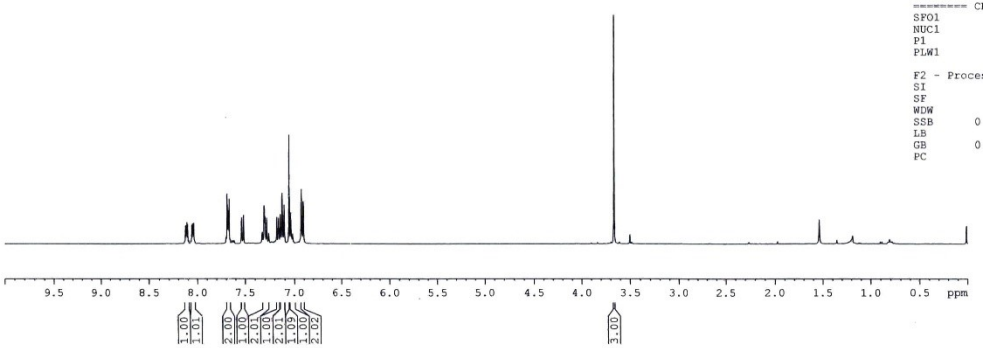
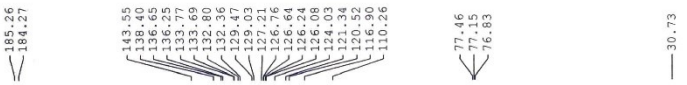
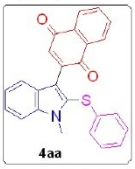


$^{13}C\{^1H\}$ NMR: 100 MHz; Solvent: $CDCl_3$



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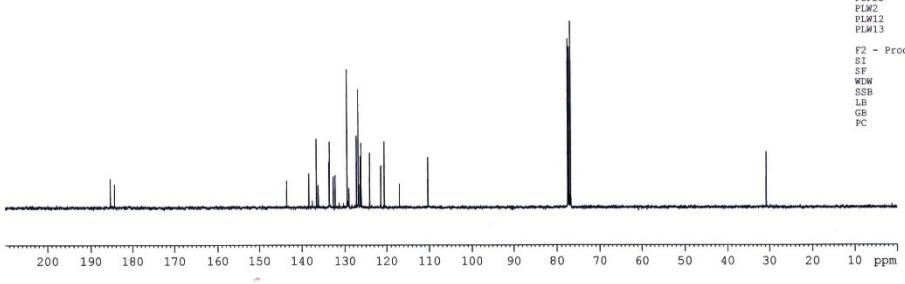
Current Data Parameters
NAME        Dr. A MAJEE 2021
EXPNO                  368
PROCNO                   1

F2 - Acquisition Parameters
Date_              20211128
Time                  17.50
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     400
DS                       2
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                    93.46
DW                   20.800 usec
DE                    6.50 usec
TE                   297.9 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

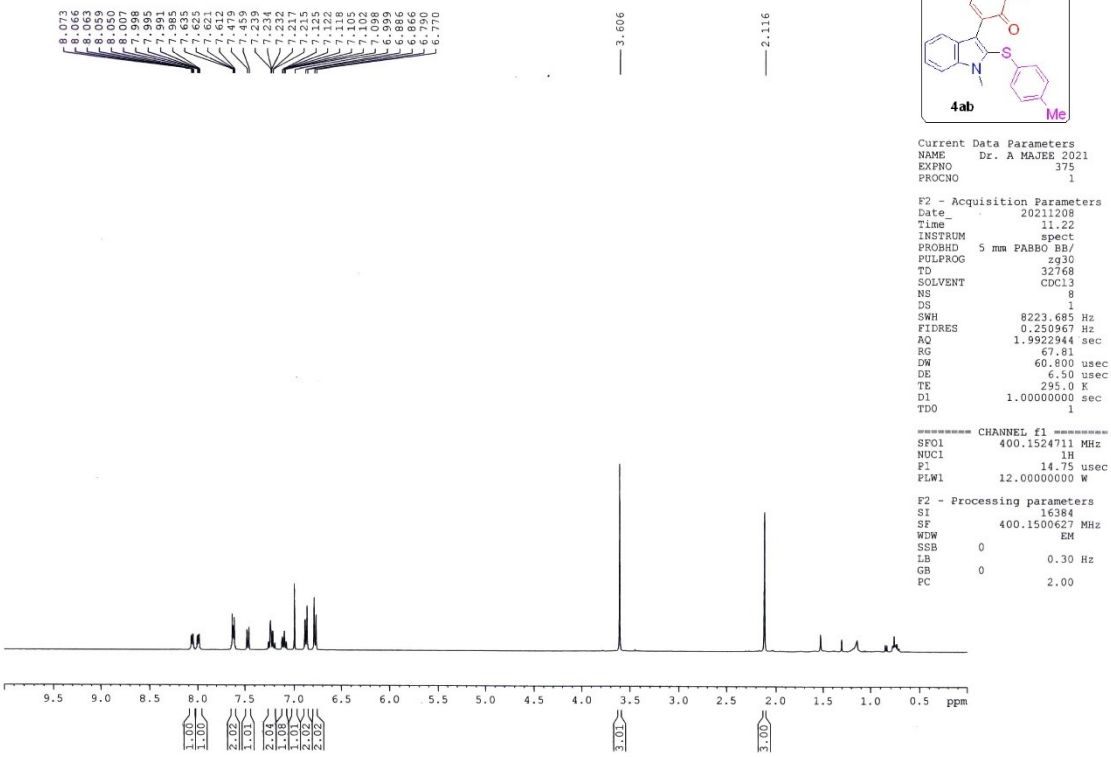
======== CHANNEL f1 ========
SFO1           100.6278588 MHz
NUC1                     13C
P1                    8.90 usec
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2           400.1516006 MHz
NUC2                     1H
CPDPRG[2          waltz16
PCPD2                90.00 usec
PLW2          12.00000000 W
PLW12          0.32231000 W
PLW13          0.16212000 W

F2 - Processing parameters
SI                   16384
SF             100.6177886 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.00
```



^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

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Current Data Parameters
NAME      Dr. A MAJEE 2021
EXPNO                375
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211208
Time              11.22
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ           1.9922944 sec
RG               67.81
DW              60.800 usec
DE               6.50 usec
TE              295.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1               1H
P1               14.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI               16384
SF          400.1500627 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               2.00
```
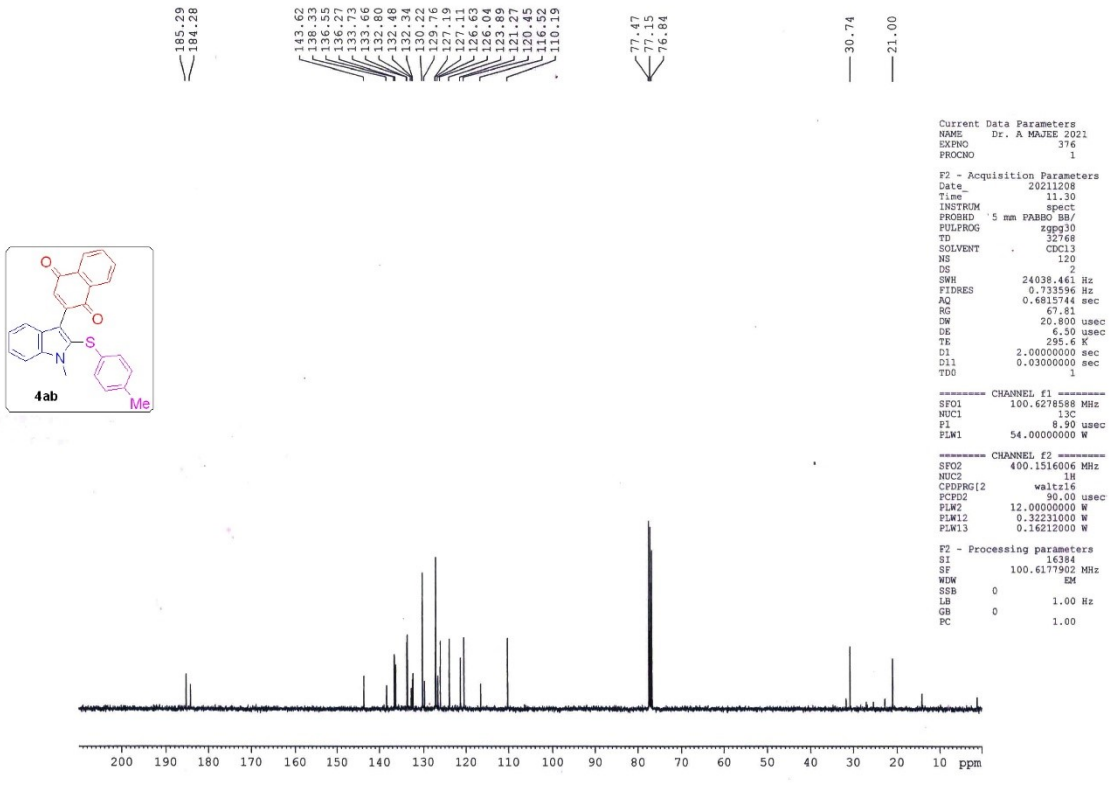

$^{13}C\{^1H\}$ NMR: 100 MHz; Solvent: $CDCl_3$

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Current Data Parameters
NAME      Dr. A MAJEE 2021
EXPNO                376
PROCNO                 1

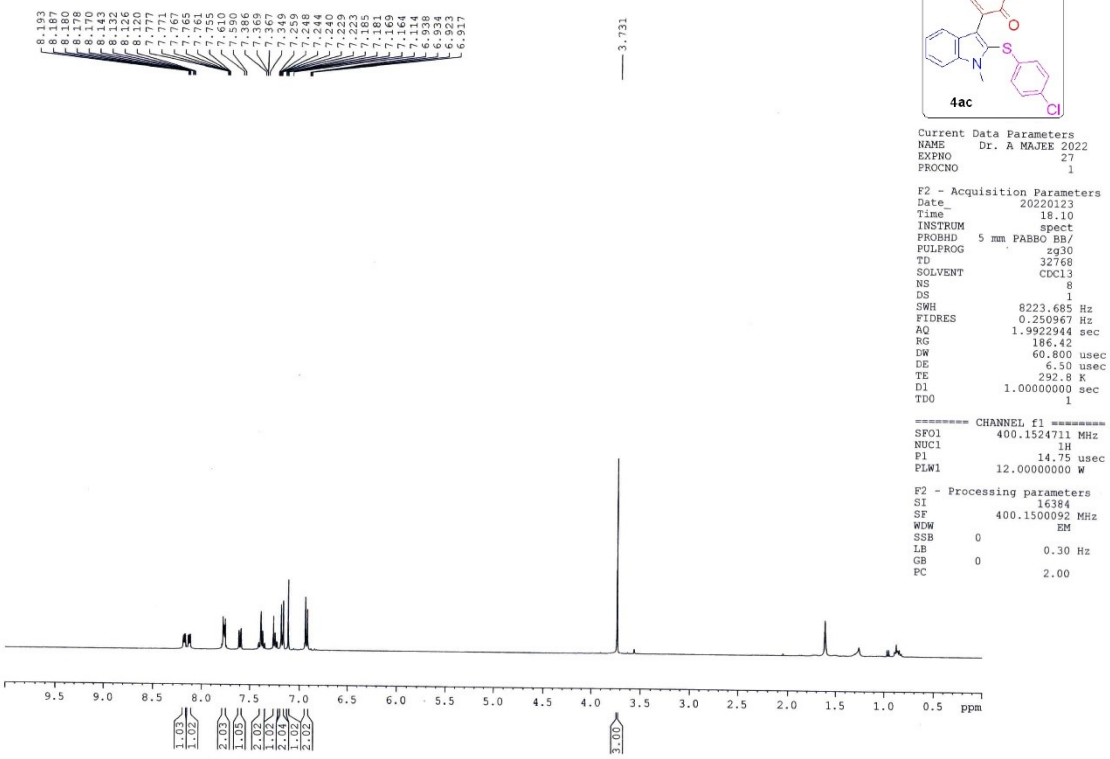
F2 - Acquisition Parameters
Date_           20211208
Time              11.30
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                 120
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ           0.6815744 sec
RG               67.81
DW              20.800 usec
DE               6.50 usec
TE              295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1               13C
P1               8.90 usec
PLW1        54.00000000 W

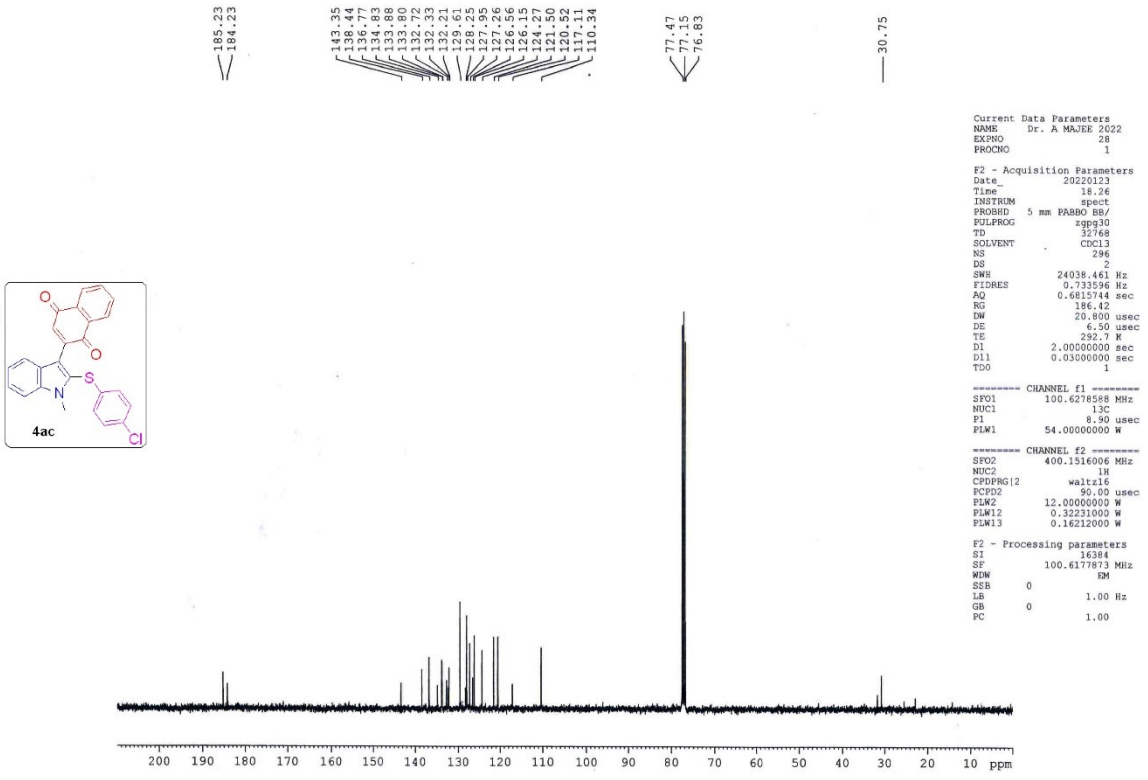
======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2           90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI               16384
SF          100.6177902 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.00
```

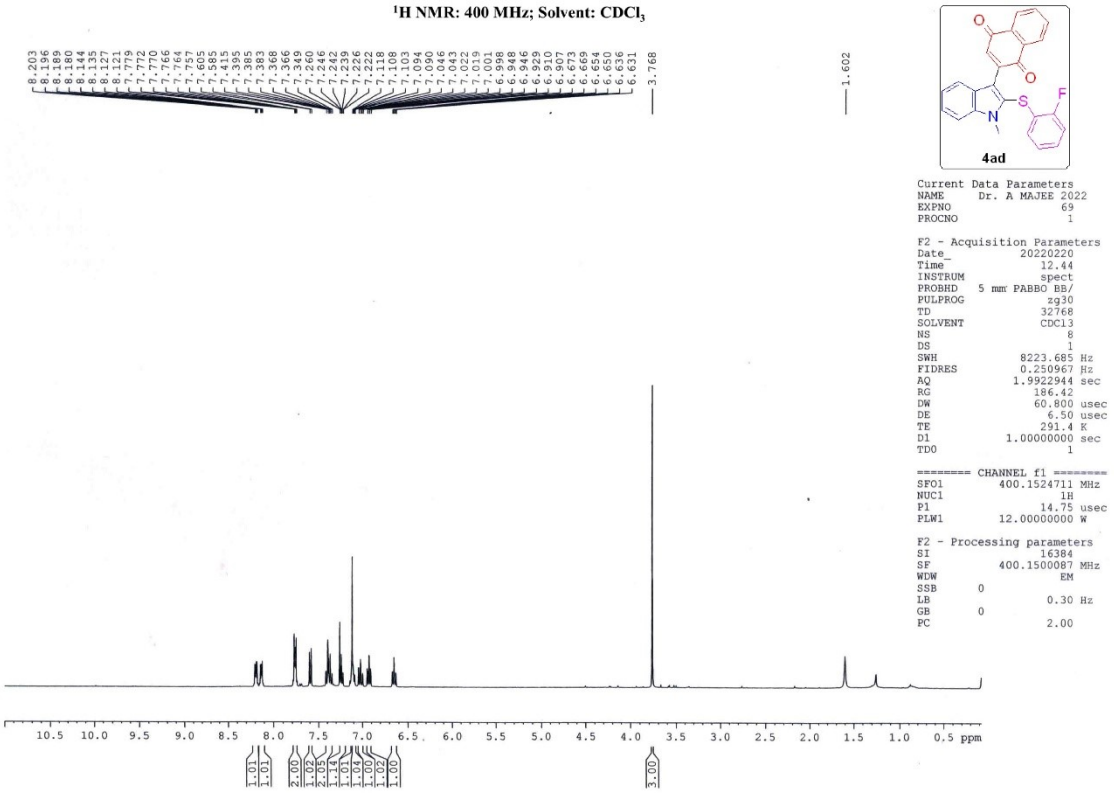
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



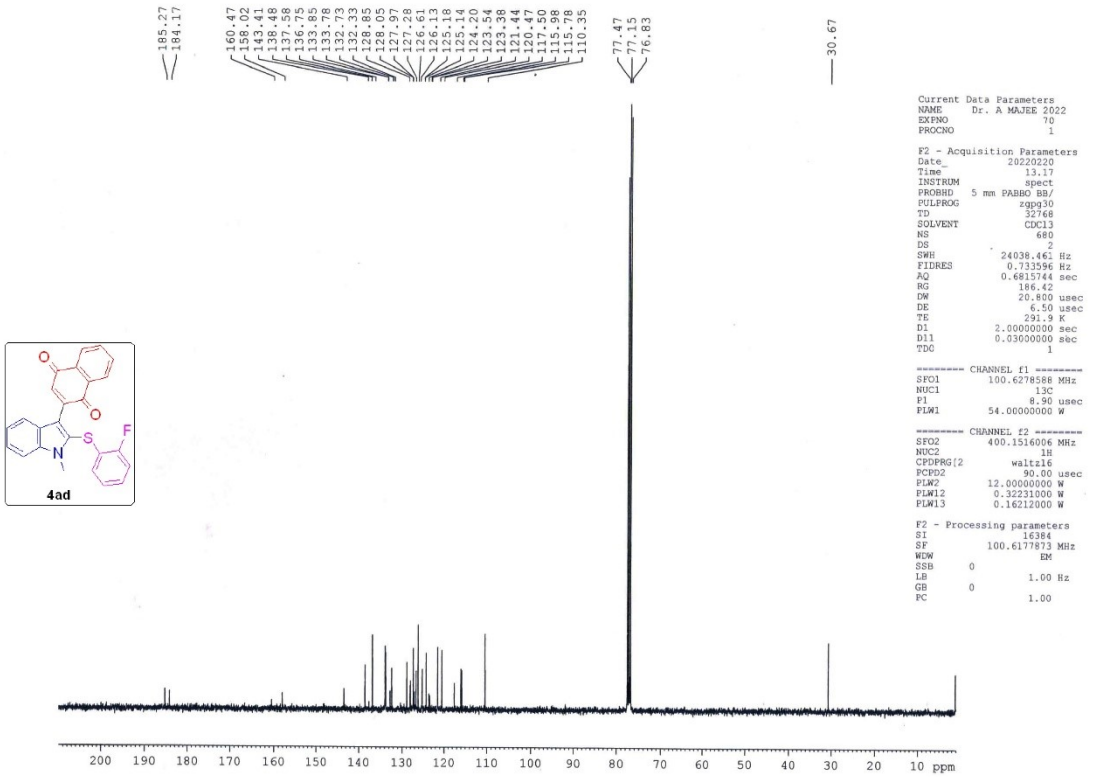

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                 69
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220220
Time              12.44
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               186.42
DW               60.800 usec
DE                6.50 usec
TE              291.4 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          400.1524711 MHz
NUC1                  1H
P1               14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF          400.1500087 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

$^{13}C\{^{1}H\}$ NMR: 100 MHz; Solvent: $CDCl_3$




```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                 70
PROCNO                 1

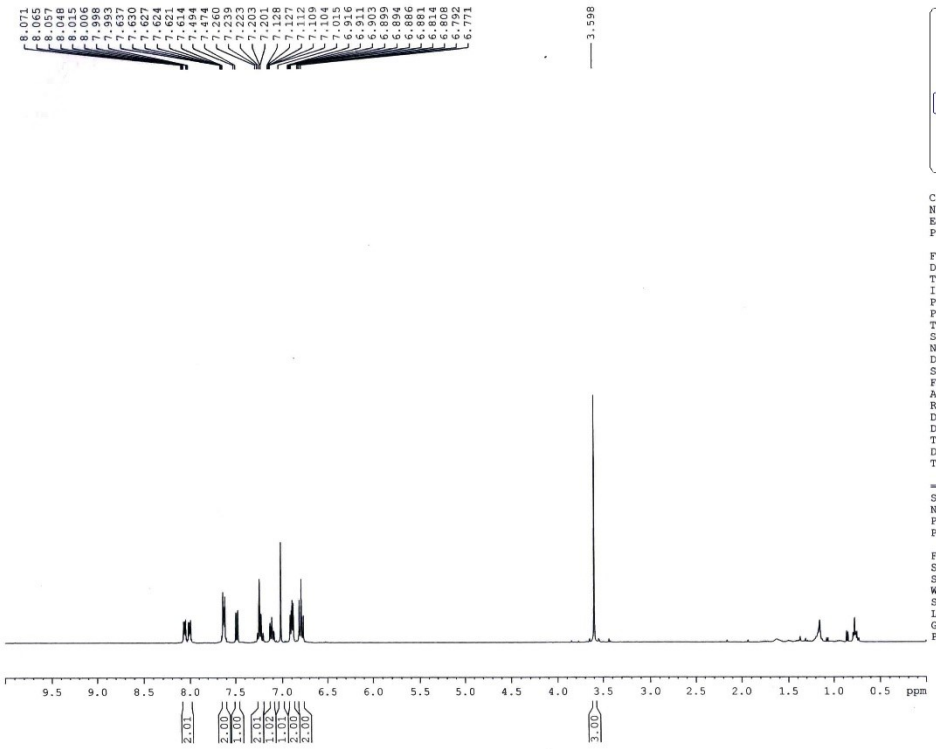
F2 - Acquisition Parameters
Date_           20220220
Time              13.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                  680
DS                    2
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               186.42
DW               20.800 usec
DE                6.50 usec
TE              291.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                  13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177873 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



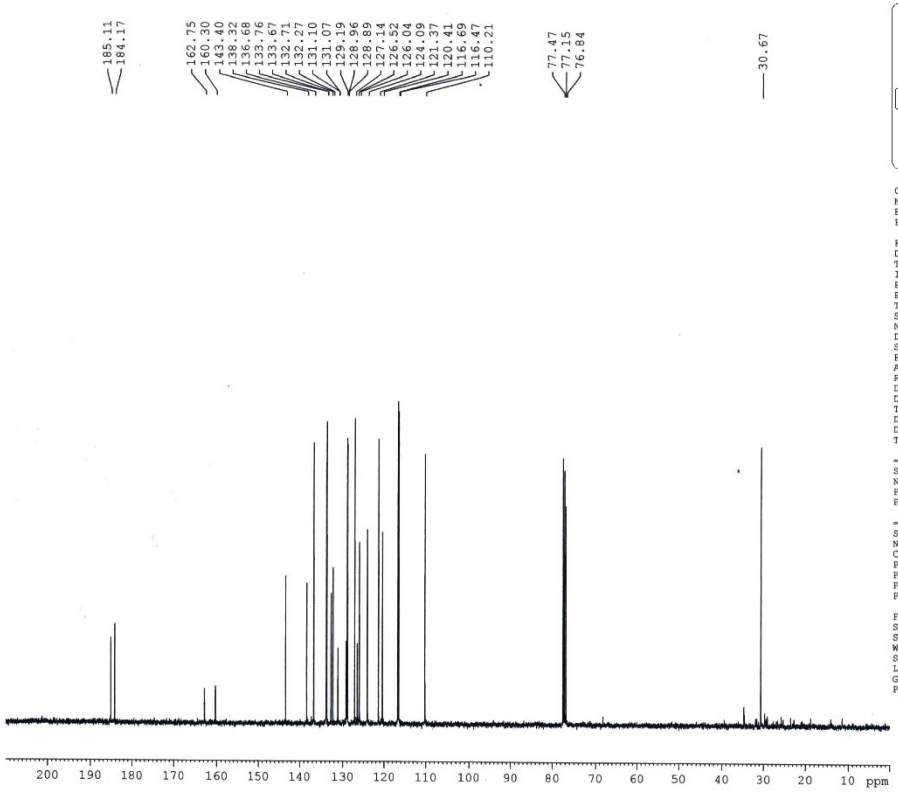

```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              638
PROCNO               1

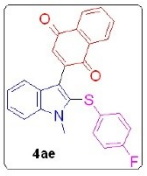
F2 - Acquisition Parameters
Date_           20230914
Time_              14.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9922944 sec
RG                37.83
DW                60.800 use
DE                 6.50 use
TE                298.5 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1               1H
P1                14.75 use
PLW1          12.00000000 W

F2 - Processing parameters
SI                16384
SF           400.1500624 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$






```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              639
PROCNO               1

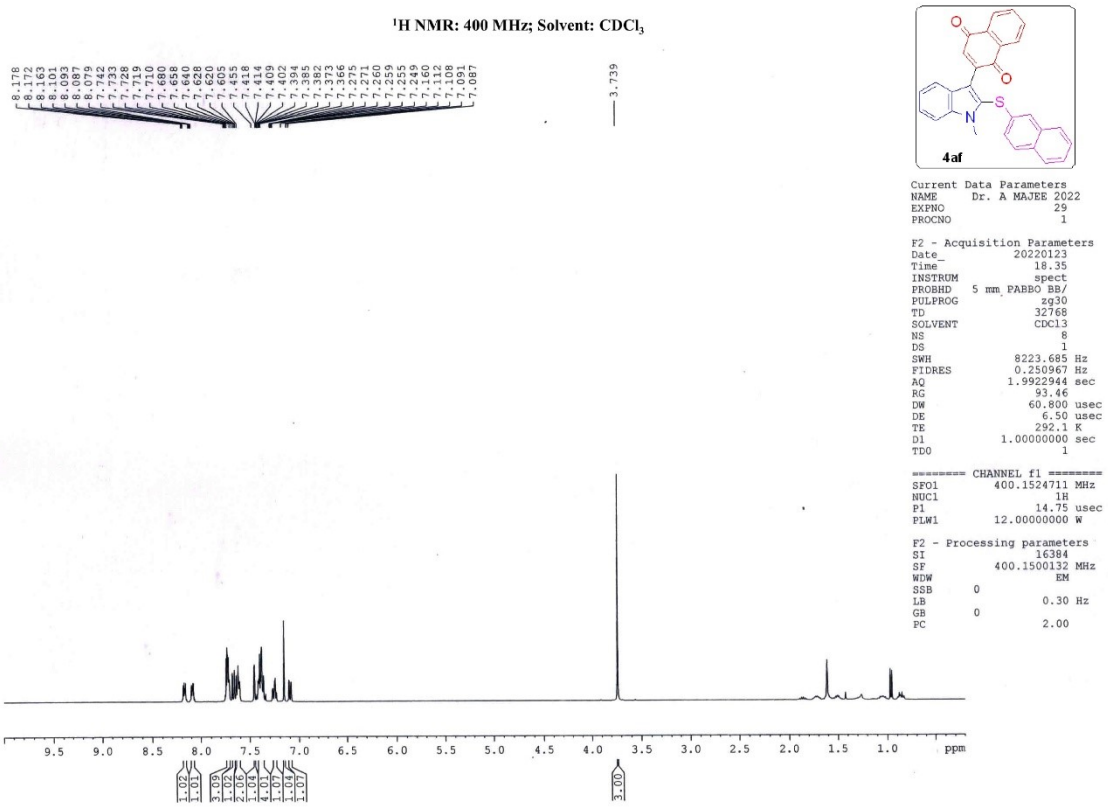
F2 - Acquisition Parameters
Date_           20230914
Time               14.56
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  240
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                37.83
DW                20.800 use
DE                 6.50 use
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1               13C
P1                 8.90 use
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 use
PLW2          12.00000000 W
PLW12          0.32231000 W
PLW13          0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177961 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



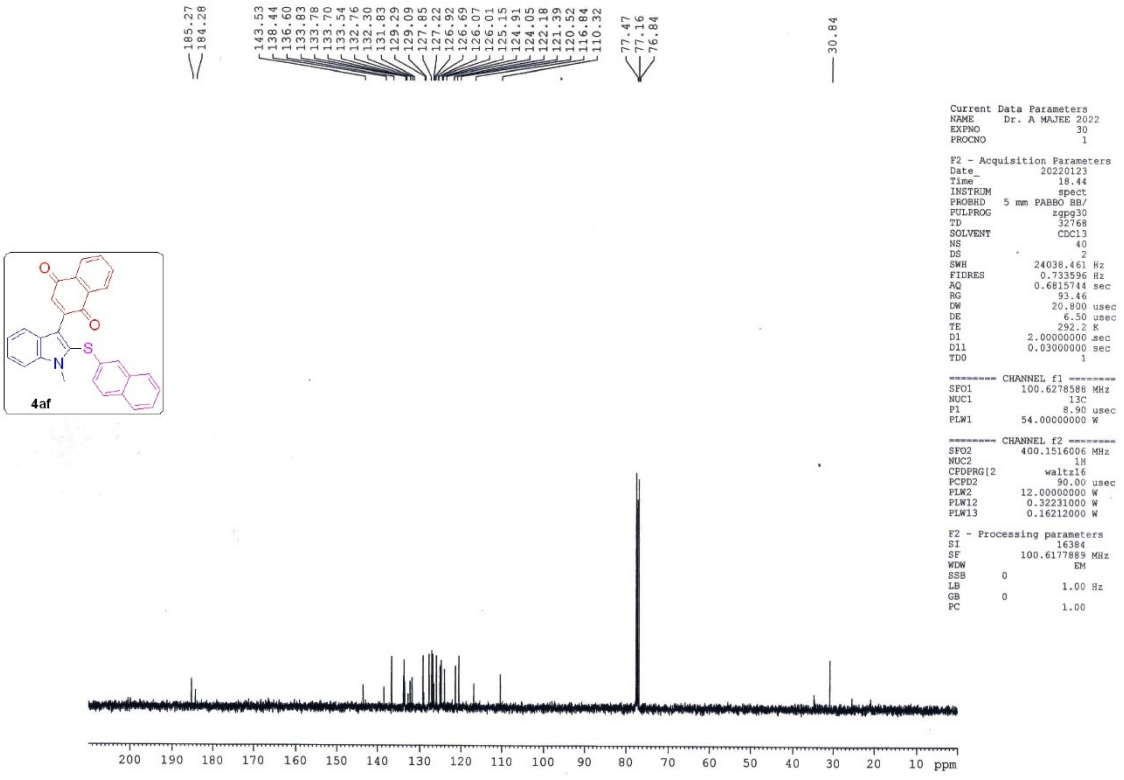

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                  29
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220123
Time              18.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                93.46
DW               60.800 usec
DE                6.50 usec
TE               292.1 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1                  1H
P1                14.75 usec
PLW1       12.00000000 W

F2 - Processing parameters
SI                16384
SF          400.1500132 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$

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Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                  30
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220123
Time              18.44
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                   40
DS                    2
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                93.46
DW               20.800 usec
DE                6.50 usec
TE               292.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1                 13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177889 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```
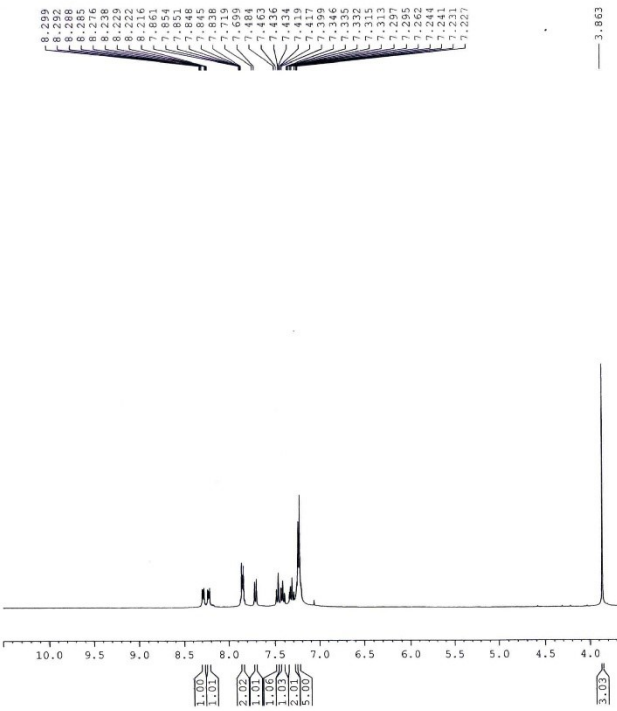
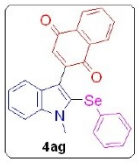
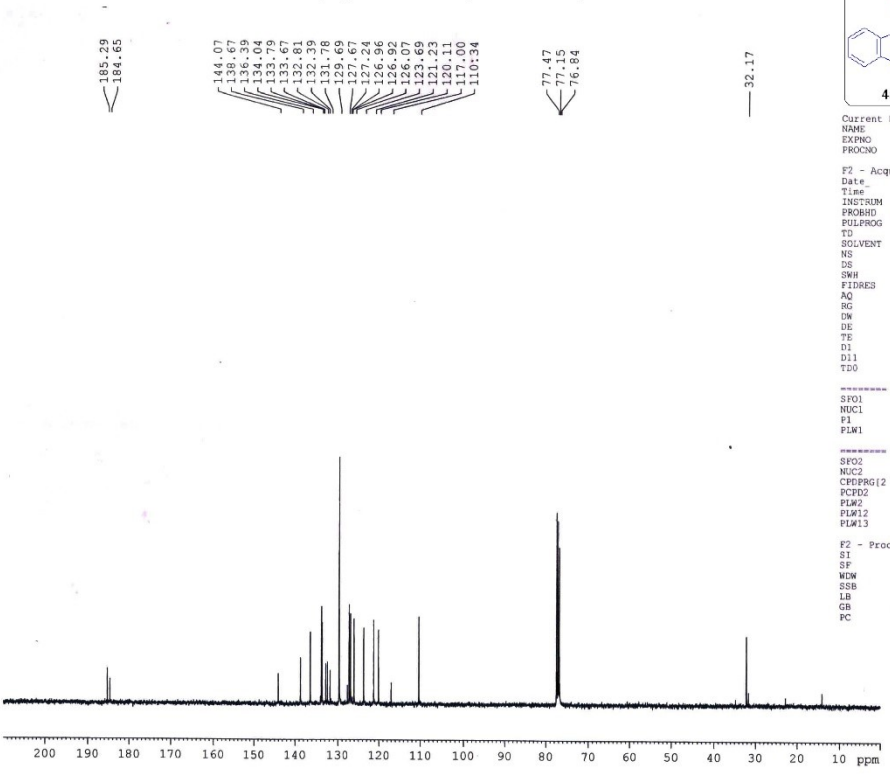

^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

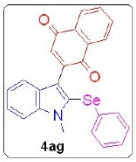





```
Current Data Parameters
NAME      Dr. A MAJEE 2021
EXPNO              294
PROCNO               1

F2 - Acquisition Parameters
Date_          20210926
Time             15.45
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG          zg30
TD              32768
SOLVENT          CDCl3
NS                   8
DS                   3
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               87.66
DW              60.800 usec
DE               6.50 usec
TE              297.1 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1              1H
P1               14.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI               16384
SF          400.1499745 MHz
WDW                 EM
SSB      0
LB               0.30 Hz
GB       0
PC               2.00
```

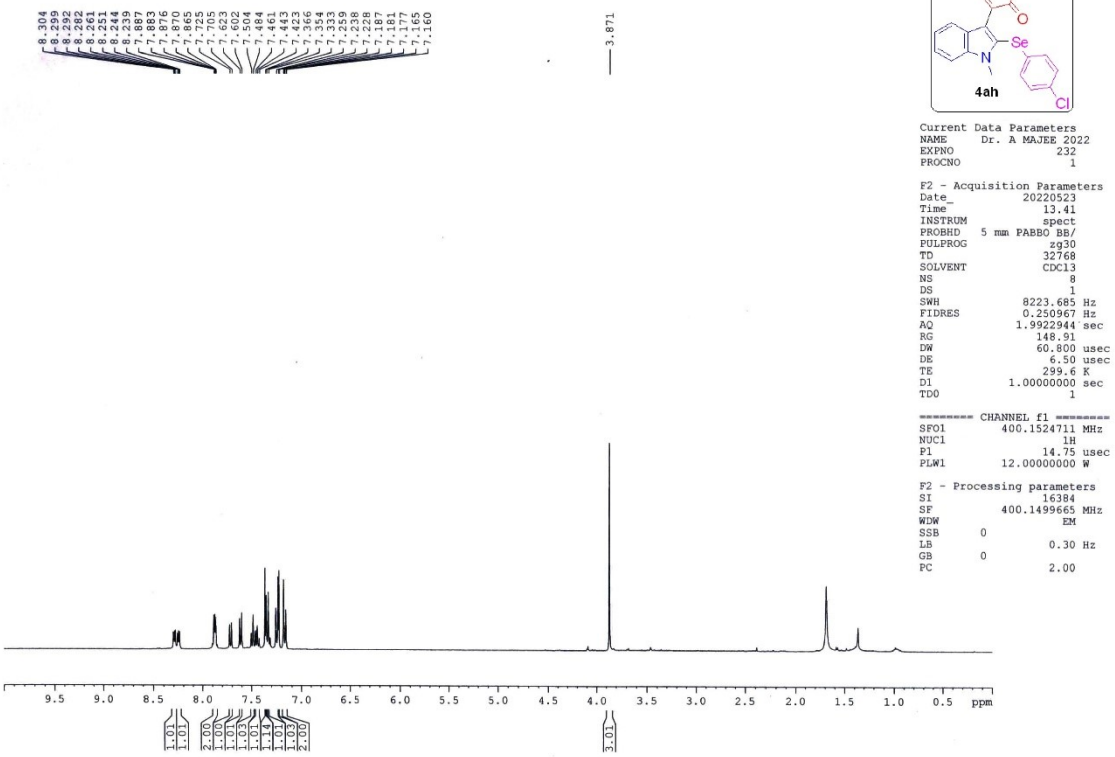
$^{13}C\{^1H\}$ NMR: 100 MHz; Solvent: $CDCl_3$



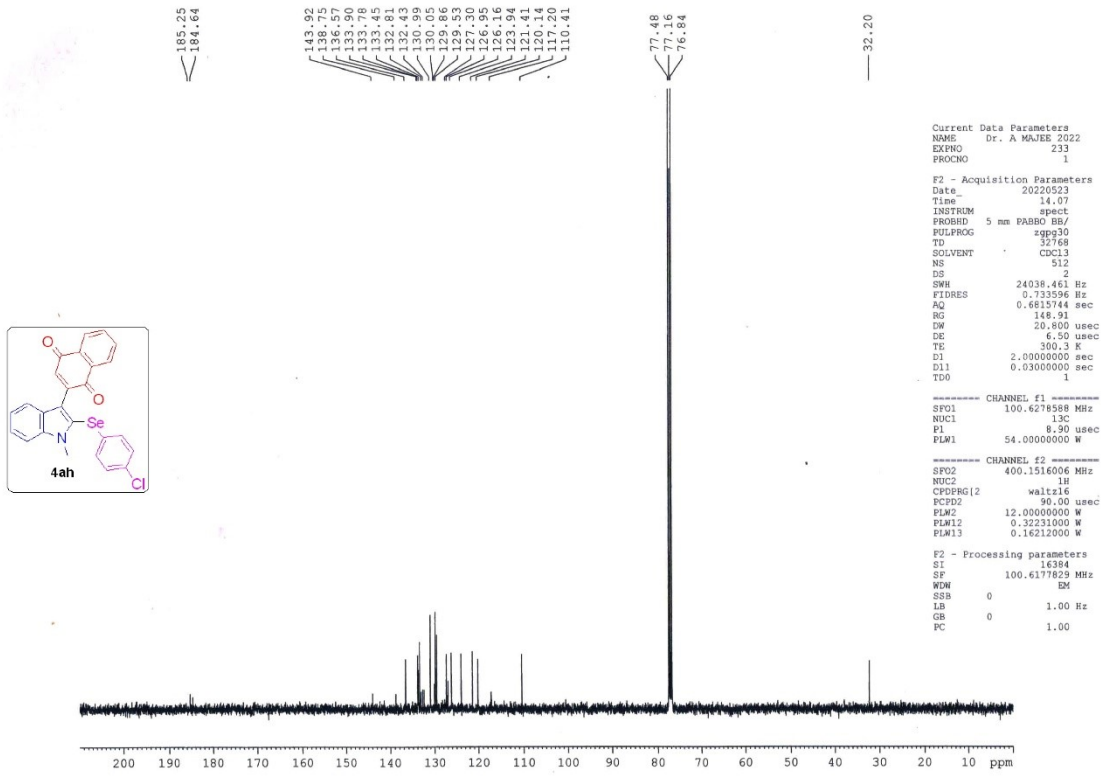



```
Current Data Parameters
NAME      Dr. A MAJEE 2021
EXPNO              295
PROCNO               1

F2 - Acquisition Parameters
Date_          20210926
Time             16.05
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD              32768
SOLVENT          CDCl3
NS                 400
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               87.66
DW              20.800 usec
DE               6.50 usec
TE              298.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI               16384
SF          100.6177889 MHz
WDW                 EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.00
```

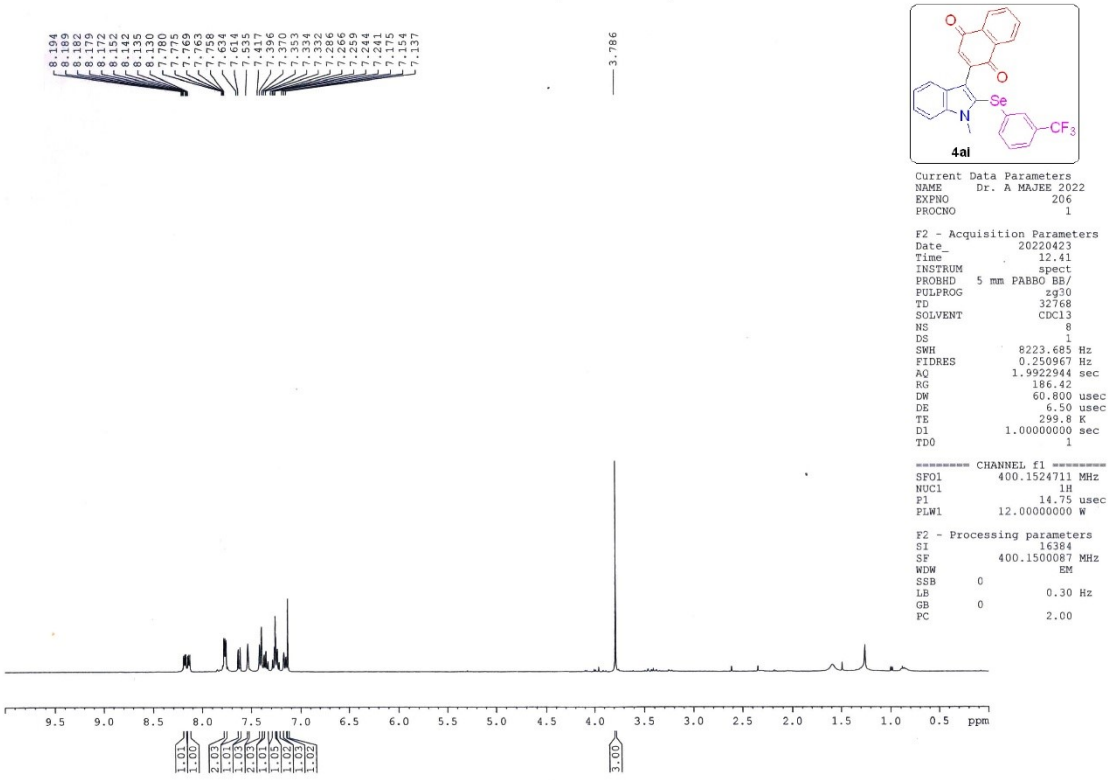
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



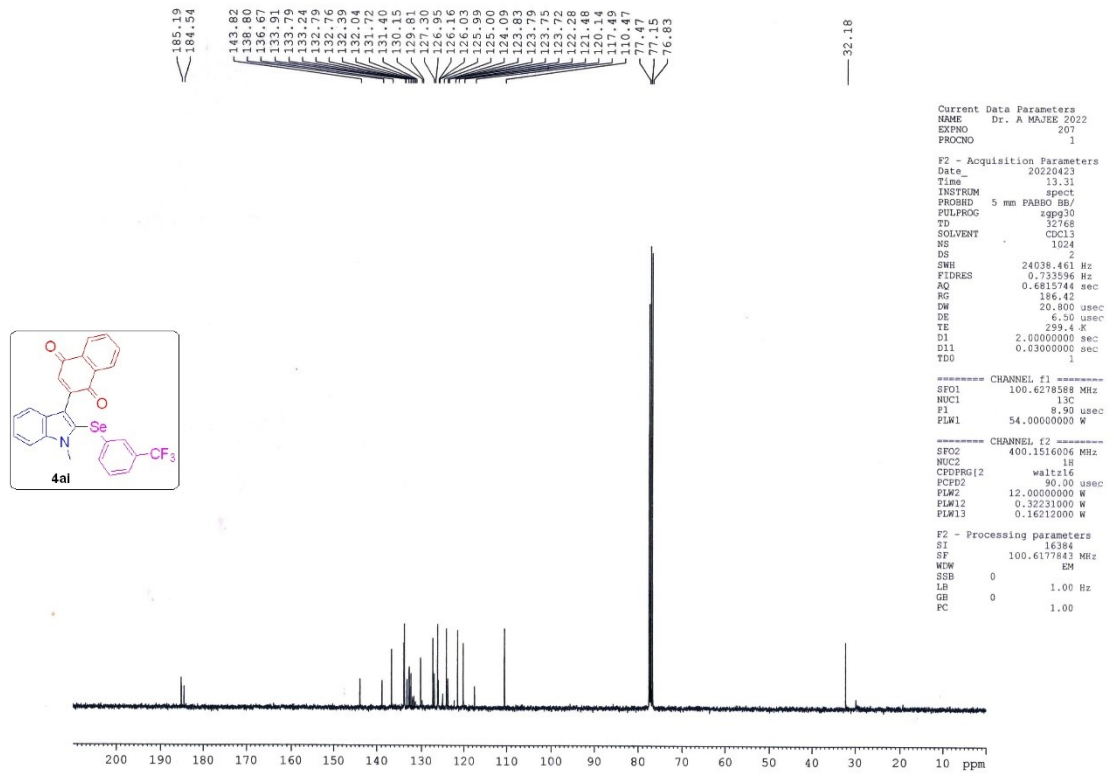
$^{13}C\{^{1}H\}$ NMR: 100 MHz; Solvent: $CDCl_3$



^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

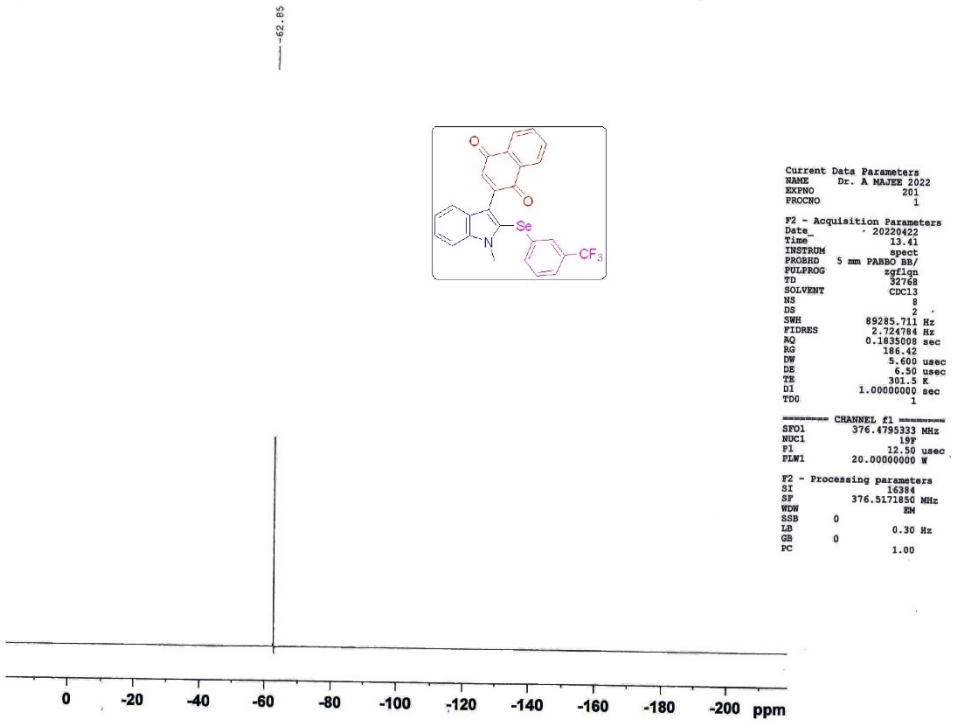


^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



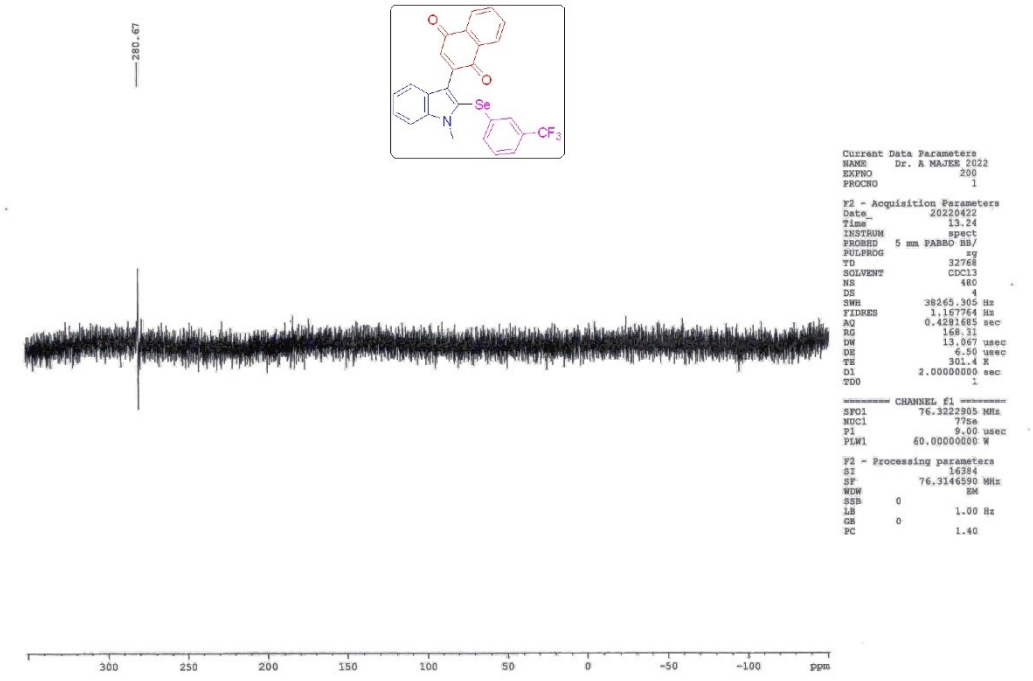
F19 1H coupled of VBSP-249/16

^{19}F NMR: 376 MHz; Solvent: $CDCl_3$

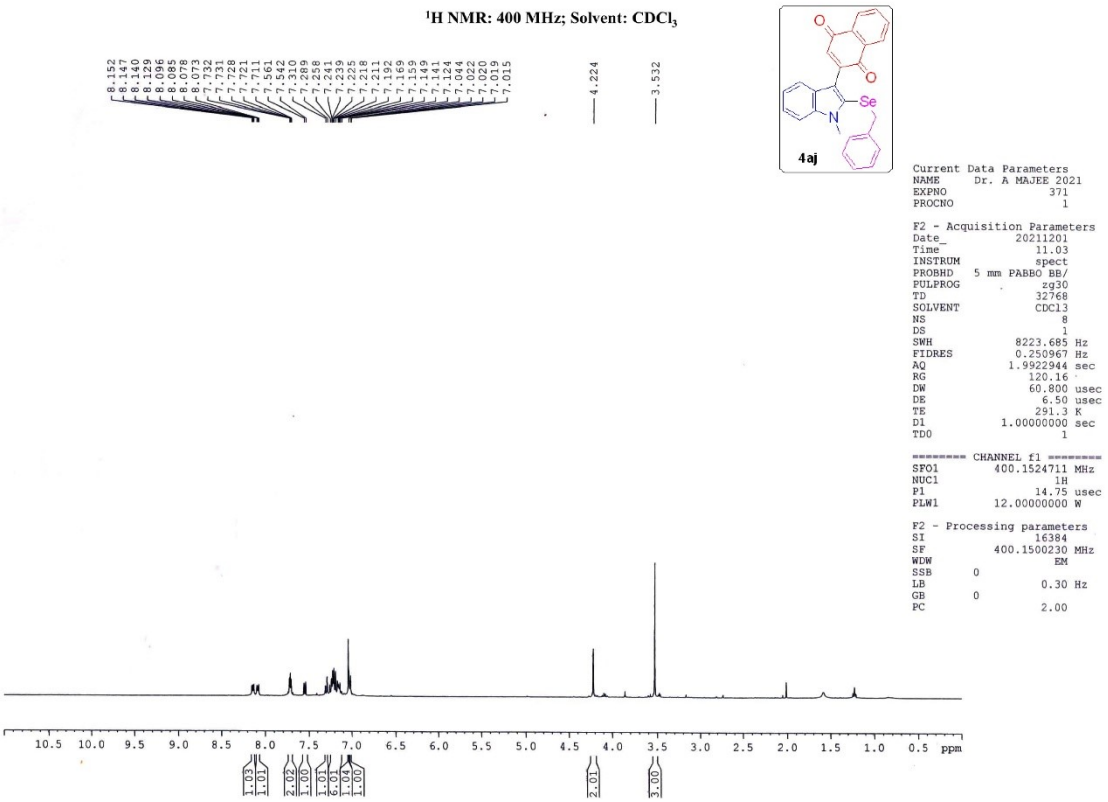


77Se of VBSP_249/16

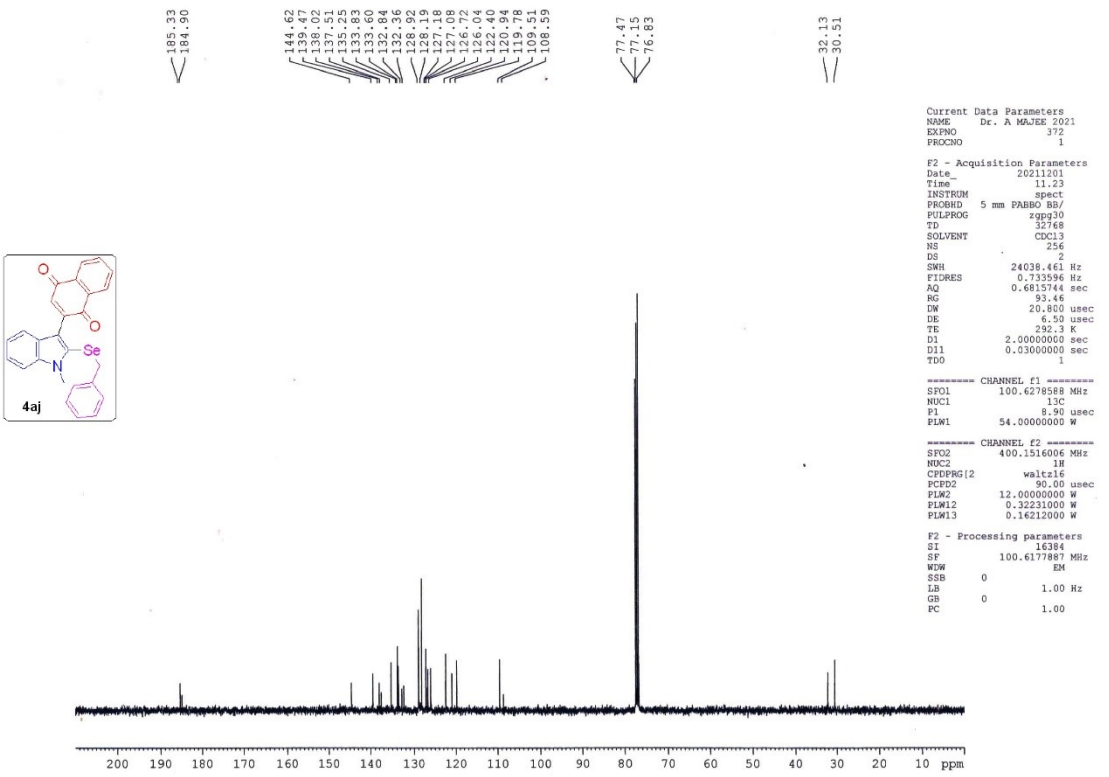
^{77}Se NMR: 76 MHz; Solvent: $CDCl_3$



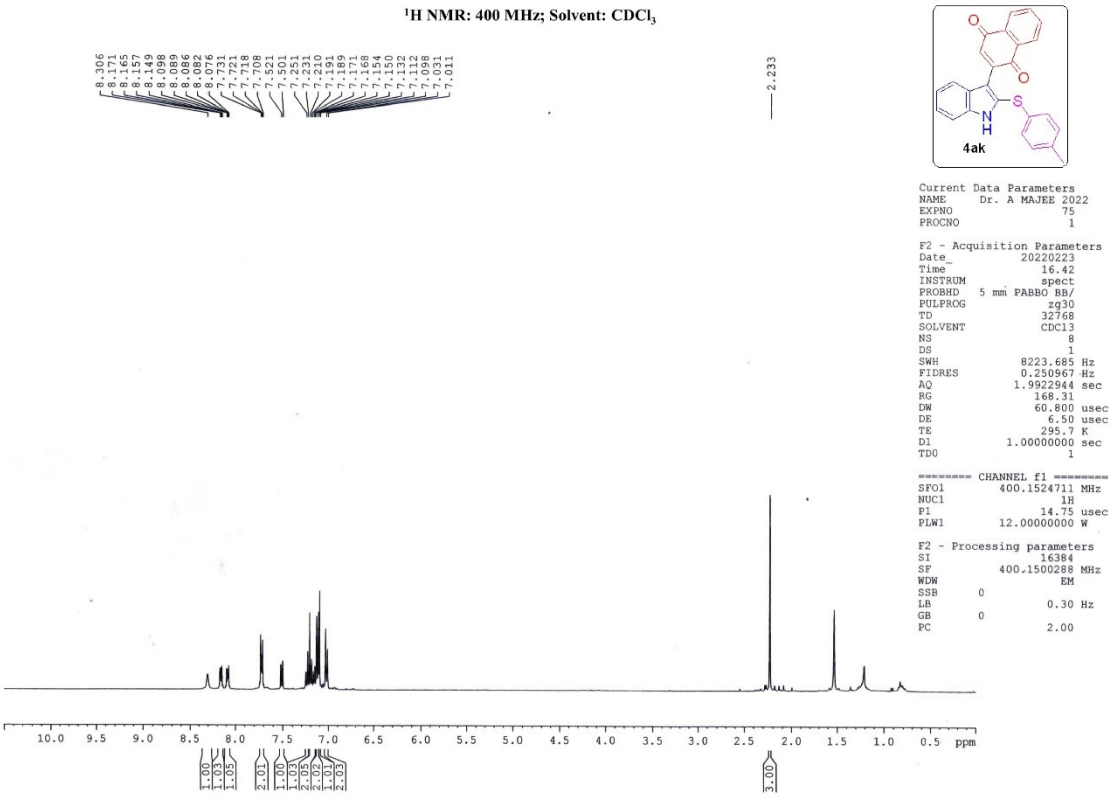
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



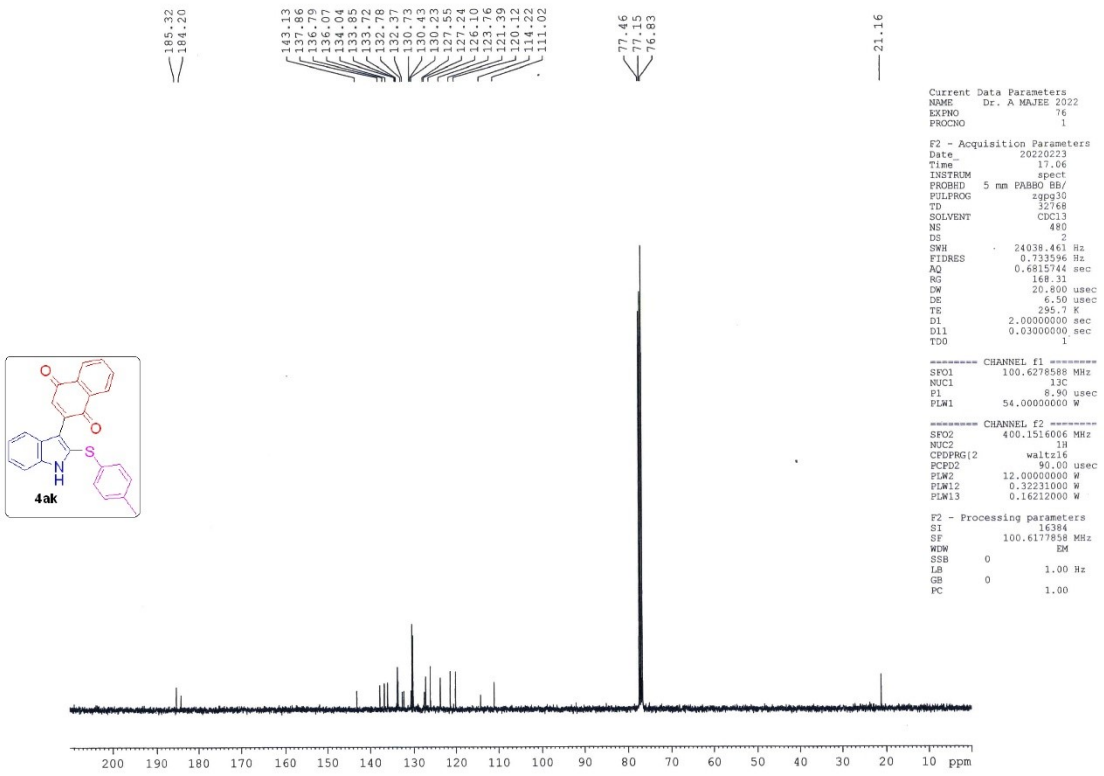
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



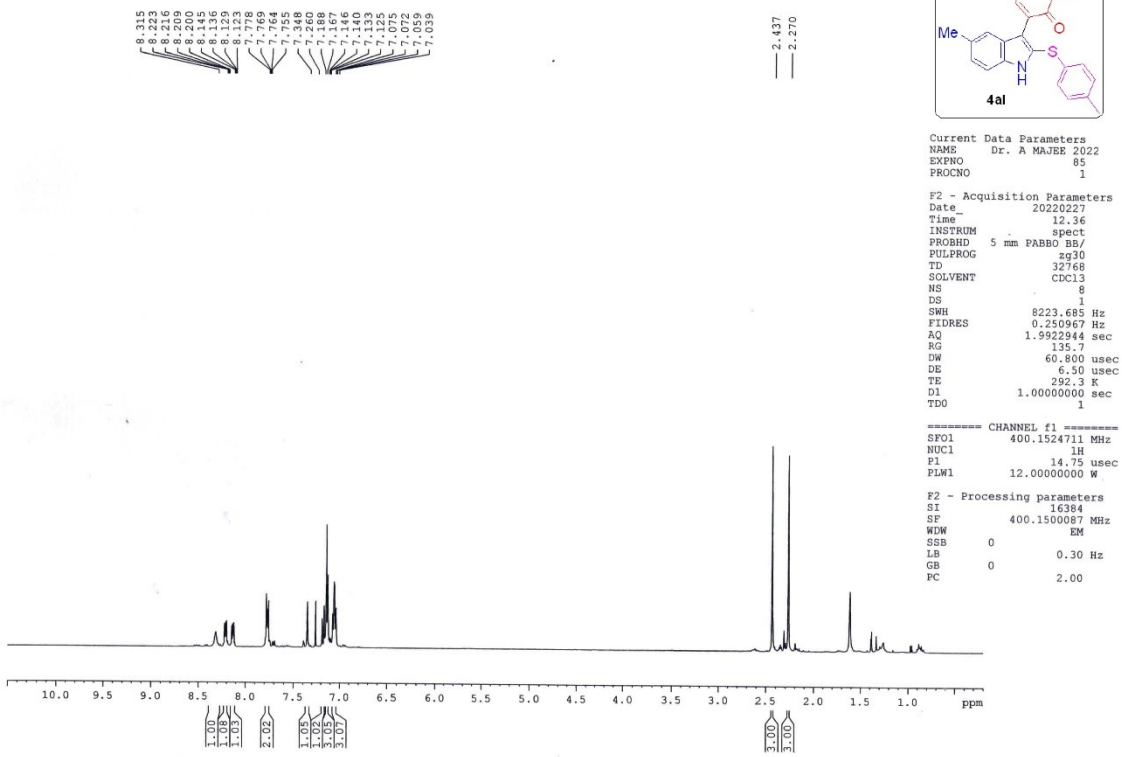
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



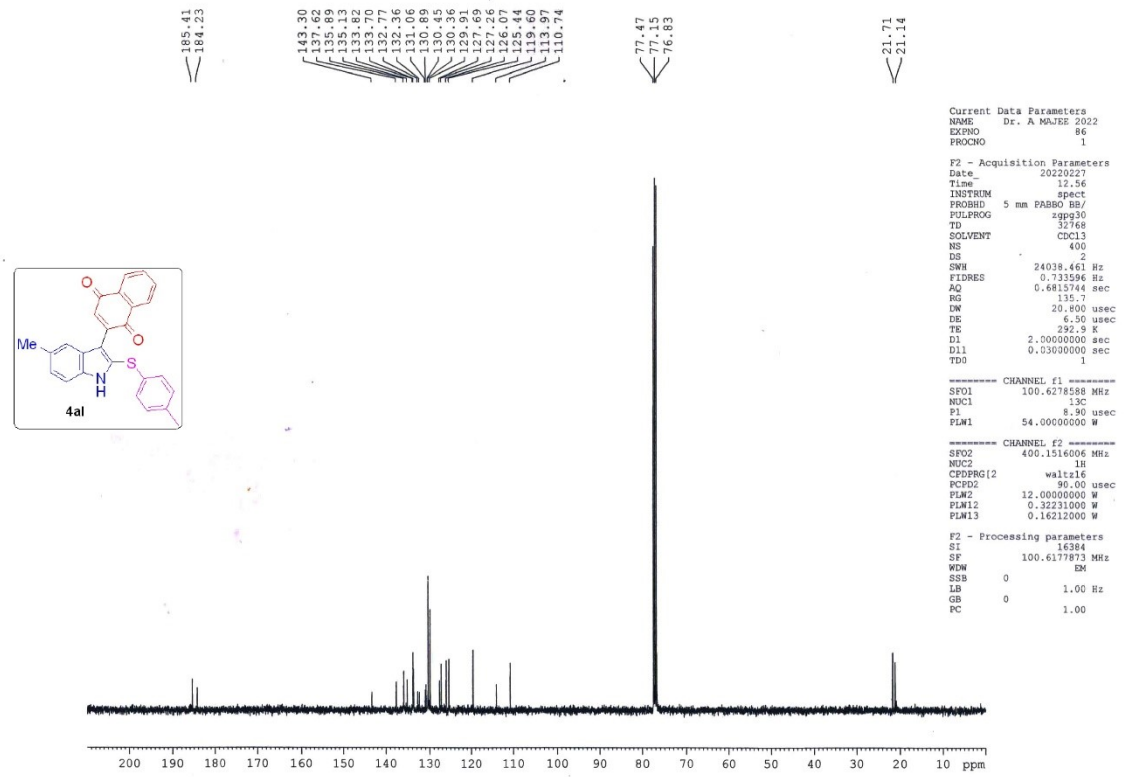
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



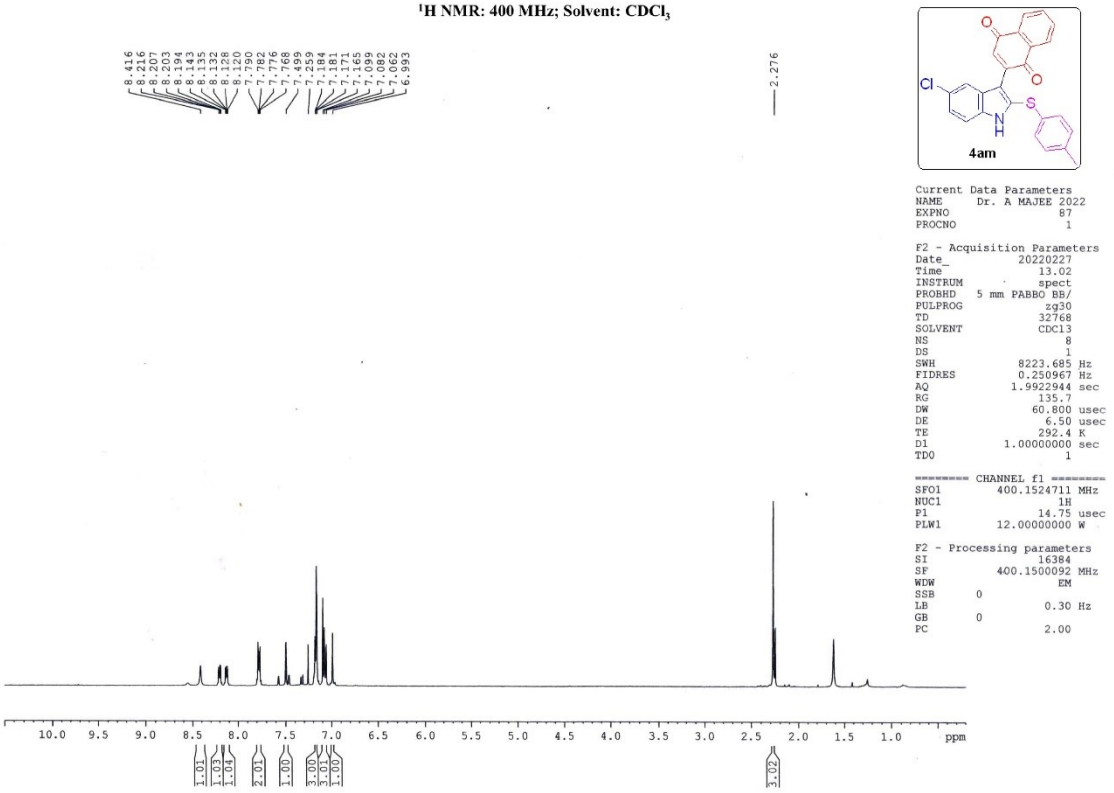
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



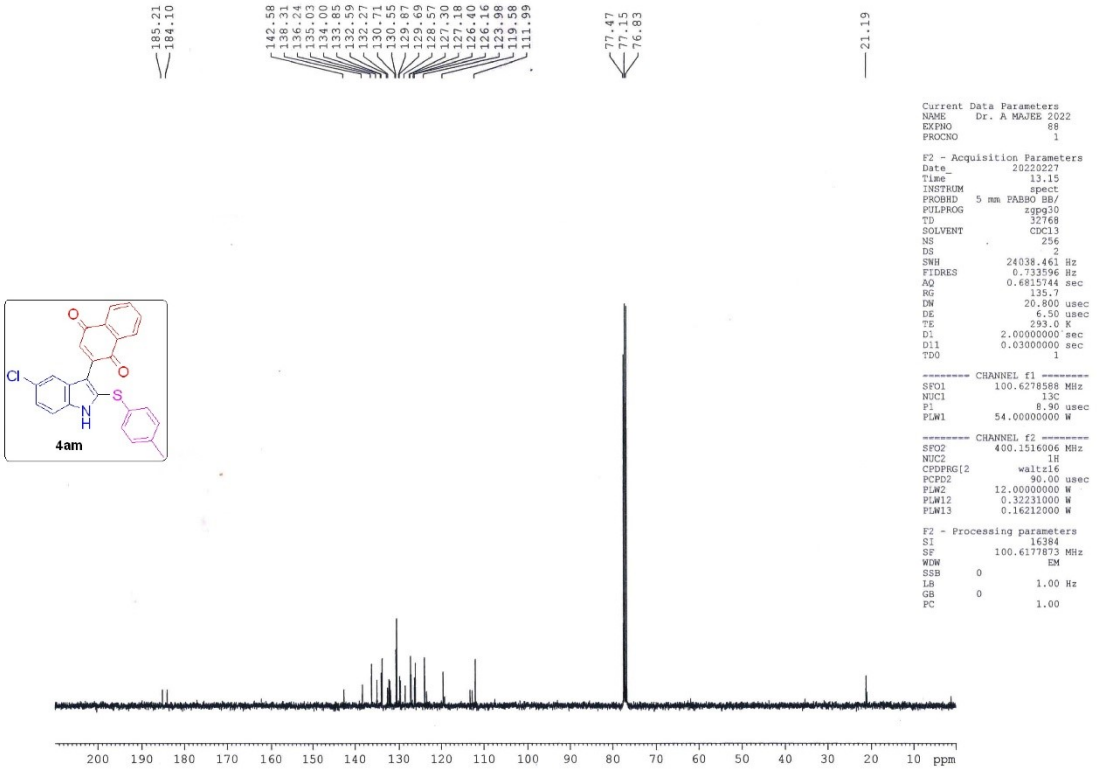
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



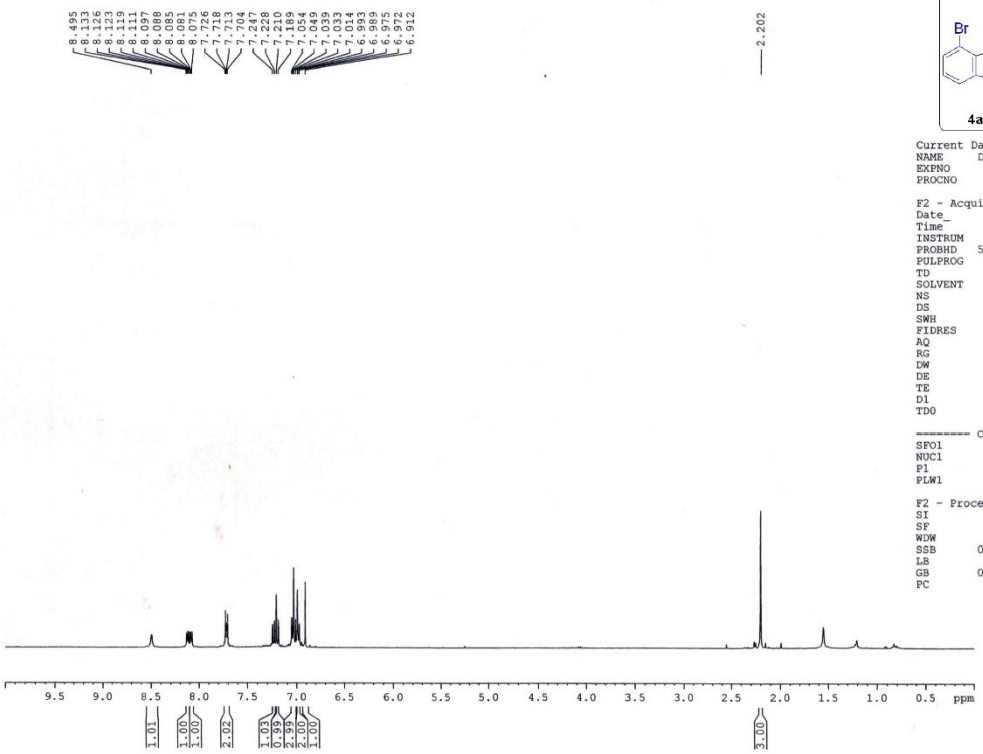
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$

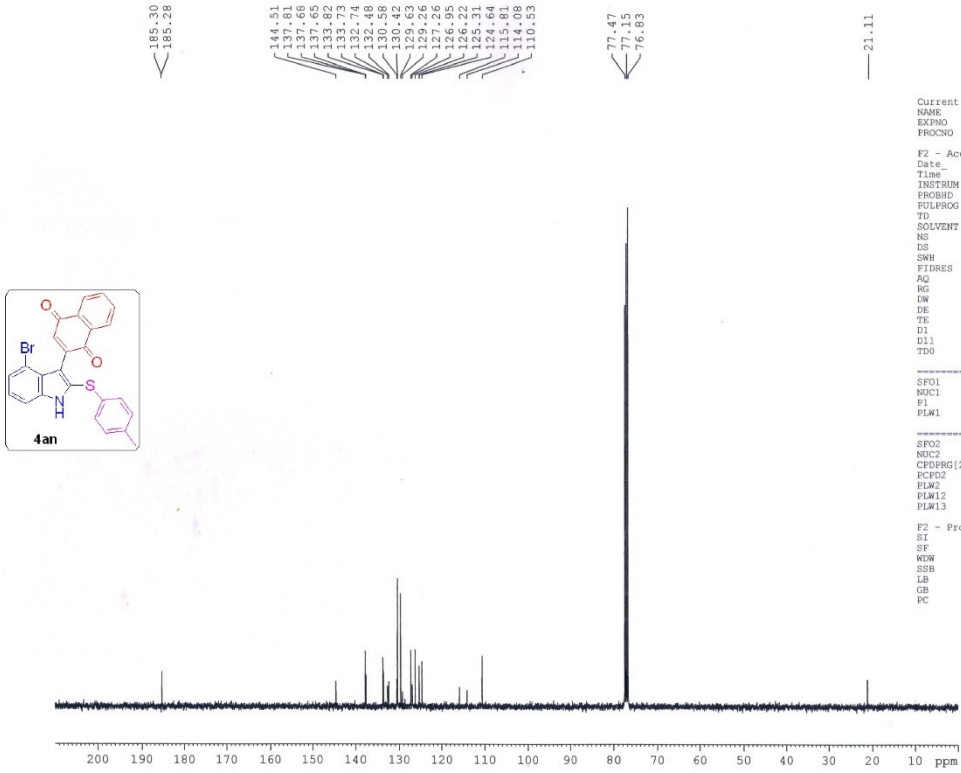


^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



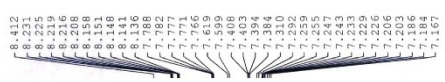

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                 73
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220223
Time              16.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9922944 sec
RG               168.31
DW               60.800 usec
DE                6.50 usec
TE               296.5 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1               1H
P1                14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF           400.1500288 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

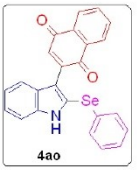
$^{13}C\{^{1}H\}$ NMR: 100 MHz; Solvent: $CDCl_3$



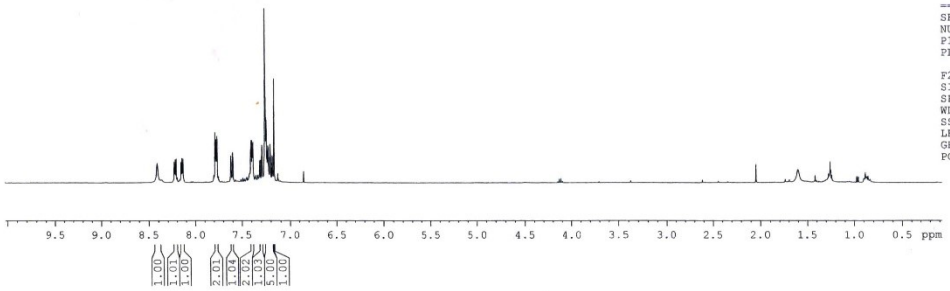

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                 74
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220223
Time              16.36
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                  480
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG               168.31
DW               20.800 usec
DE                6.50 usec
TE               296.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177858 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



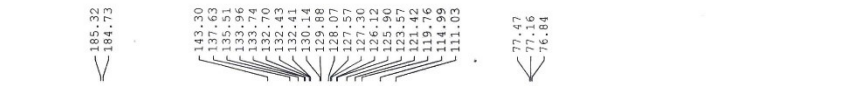


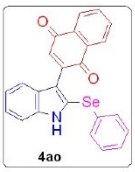
4ao



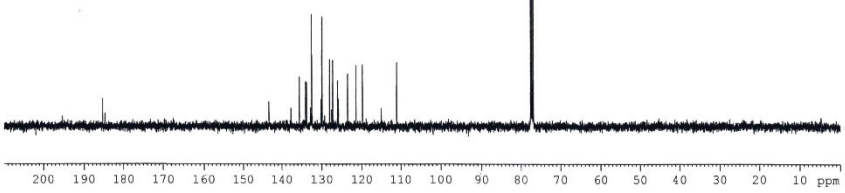

```
Current Data Parameters
NAME        Dr. A MAJEE 2023
EXPNO                  131
PROCNO                   1

F2 - Acquisition Parameter
Date_             20230226
Time                14.37
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             CDCl3
NS                      8
DS                      1
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9922944 se
RG                 186.42
DW                 60.800 us
DE                  6.50 us
TE                294.0 K
D1              1.00000000 se
TD0                     1

======== CHANNEL f1 ======
SFO1          400.1524711 MH
NUC1                   1H
P1                  14.75 us
PLW1          12.00000000 W

F2 - Processing parameters
SI                  16384
SF            400.1500097 MH
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  2.00
```

^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



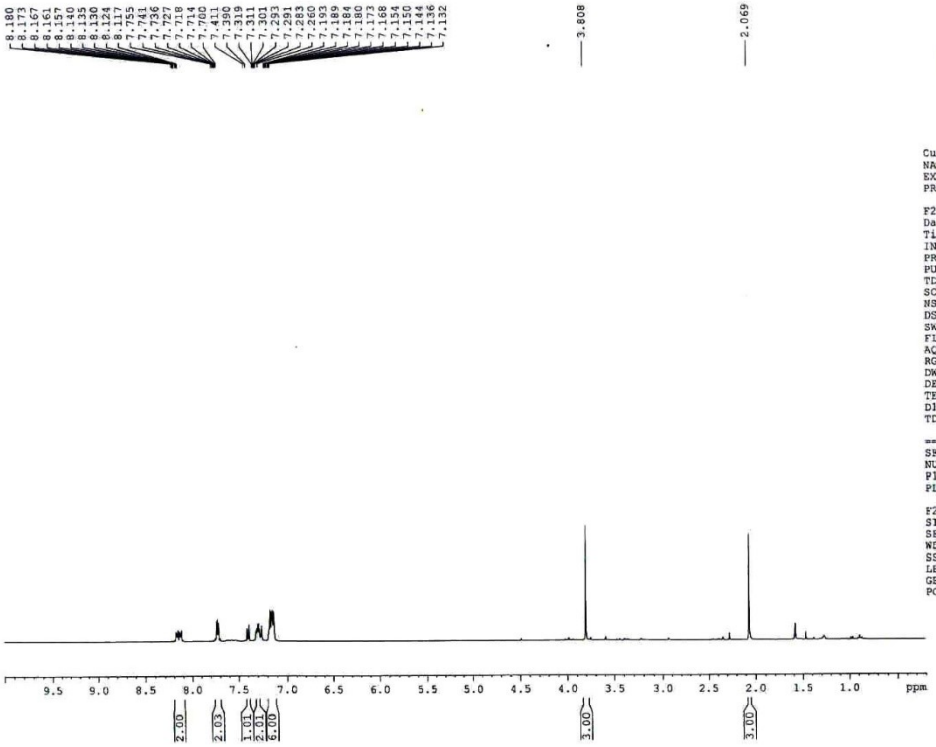


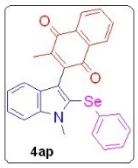
4ao




```
Current Data Parameters
NAME        Dr. A MAJEE 2023
EXPNO                  132
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230226
Time                15.03
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    400
DS                      2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 186.42
DW                 20.800 usec
DE                  6.50 usec
TE                294.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                   13C
P1                  8.90 usec
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.00000000 W
PLW12          0.32231000 W
PLW13          0.16212000 W

F2 - Processing parameters
SI                  16384
SF            100.6177858 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.00
```

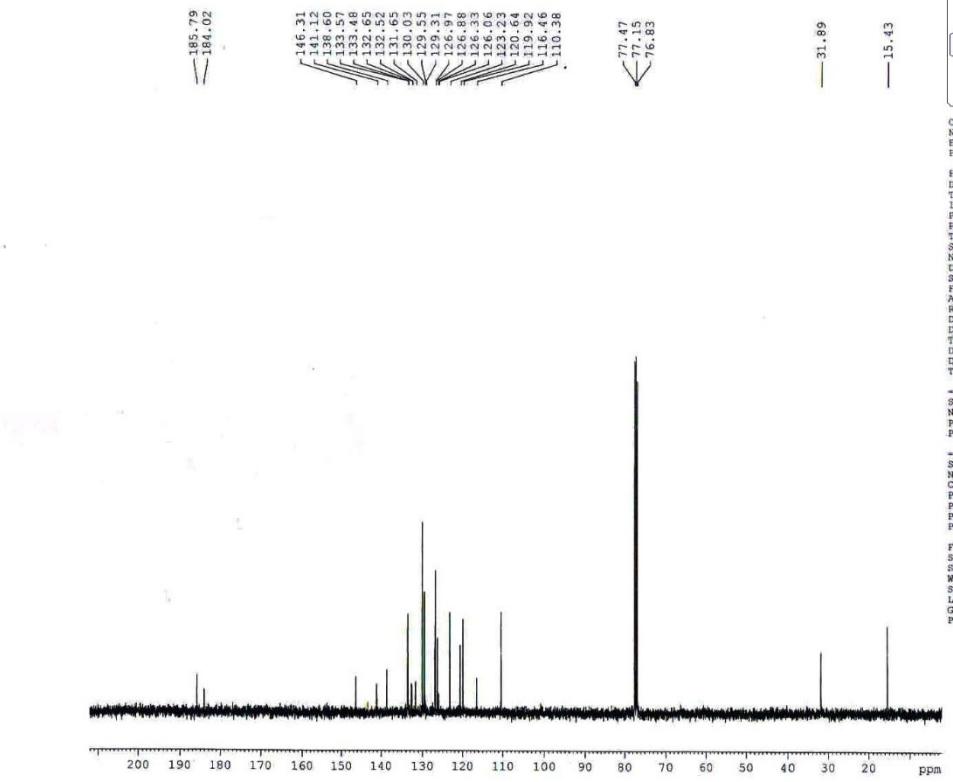
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

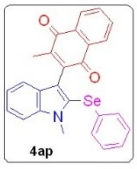





```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              112
PROCNO               1

F2 - Acquisition Parameters
Date_          20230221
Time              13.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   1
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               120.16
DW               60.800 usec
DE                6.50 usec
TE               301.4 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1               1H
P1               14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF           400.1500092 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

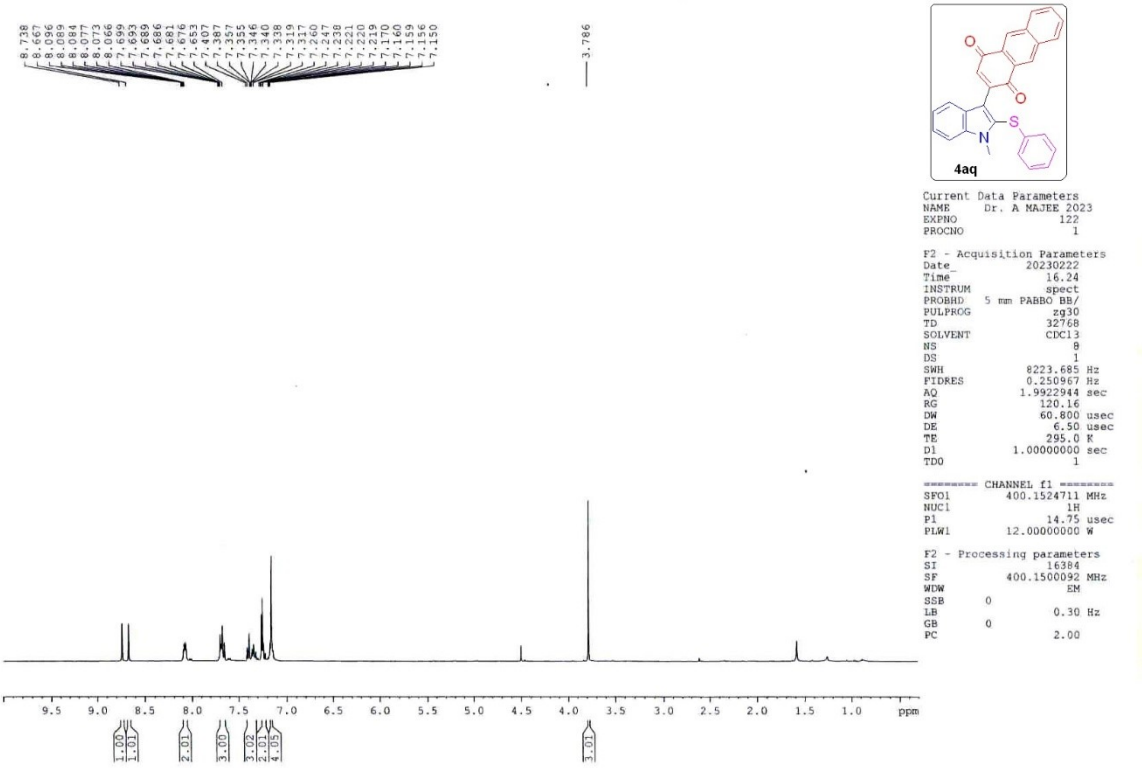
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



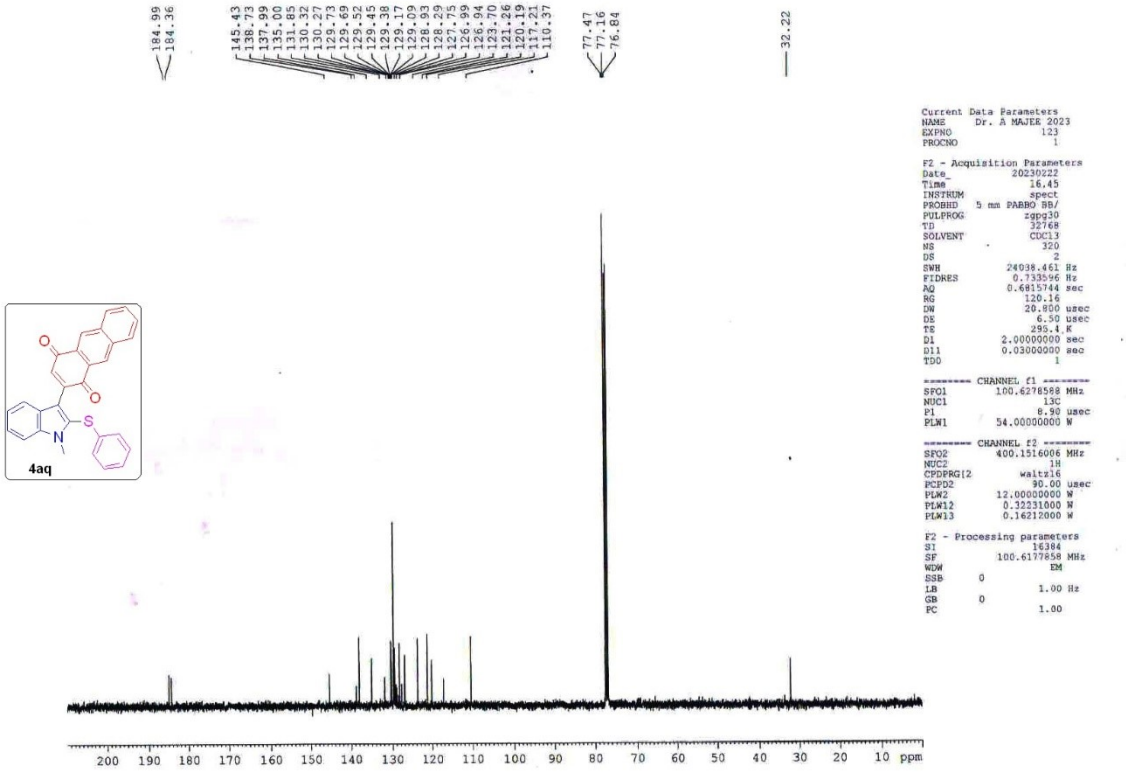



```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              113
PROCNO               1

F2 - Acquisition Parameters
Date_          20230221
Time              13.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                 120
DS                   2
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               120.16
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2               1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177858 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

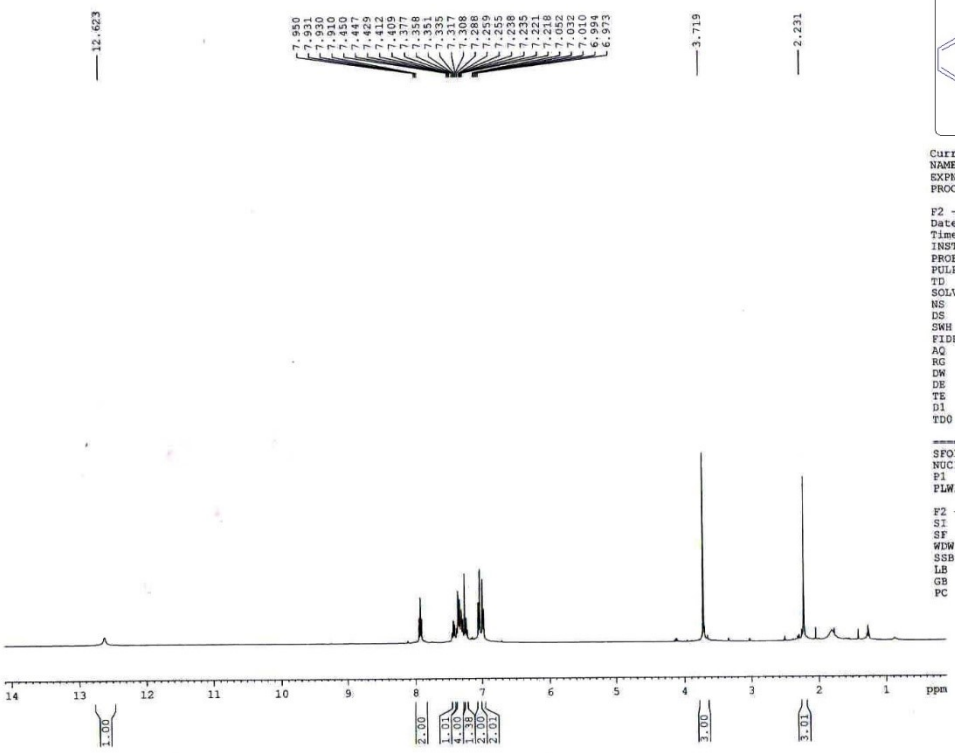
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

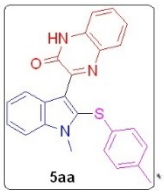


^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



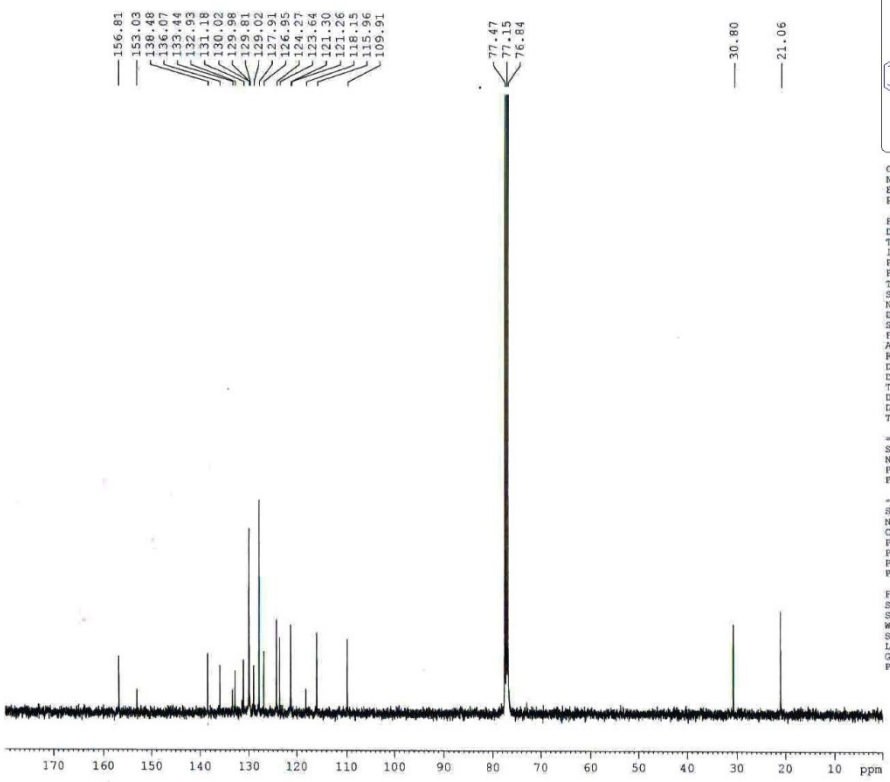
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

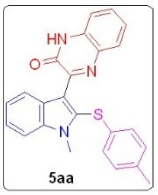




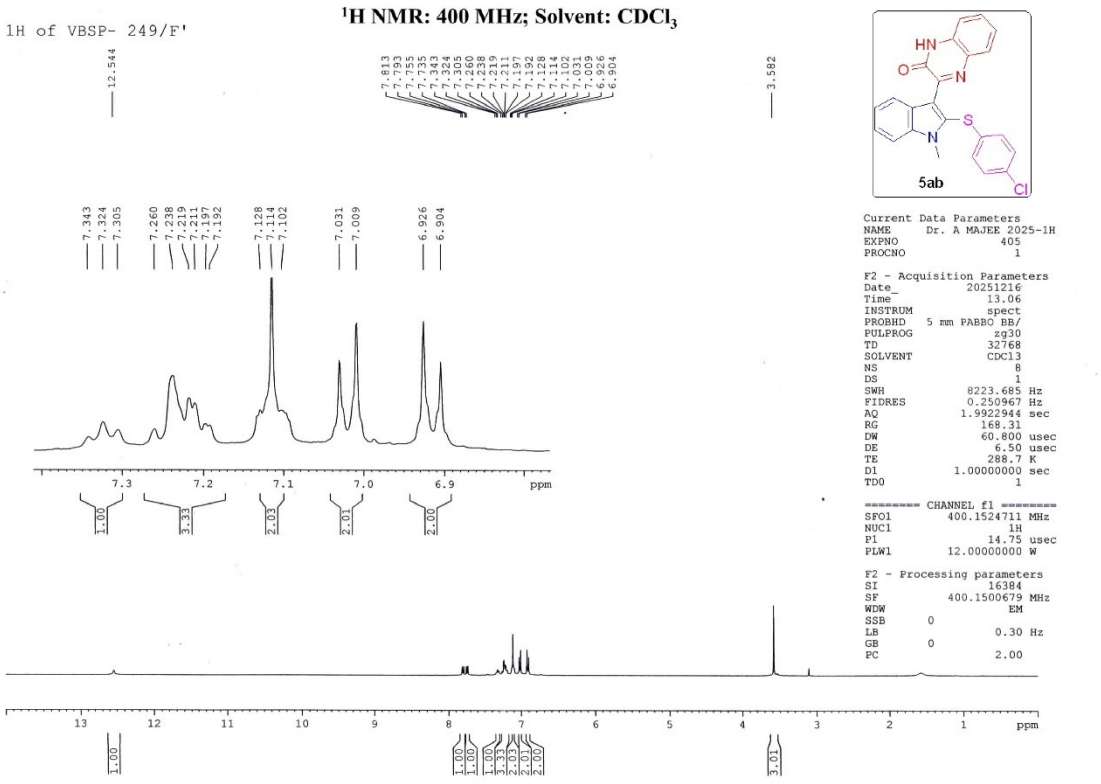

```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              472
PROCNO               1

F2 - Acquisition Parameters
Date_           20230708
Time              17.34
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                135.7
DW               60.800 use
DE                6.50 use
TE               296.5 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1                1H
P1                14.75 use
PLW1        12.00000000 W

F2 - Processing parameters
SI                16384
SF          400.1500097 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                2.00
```

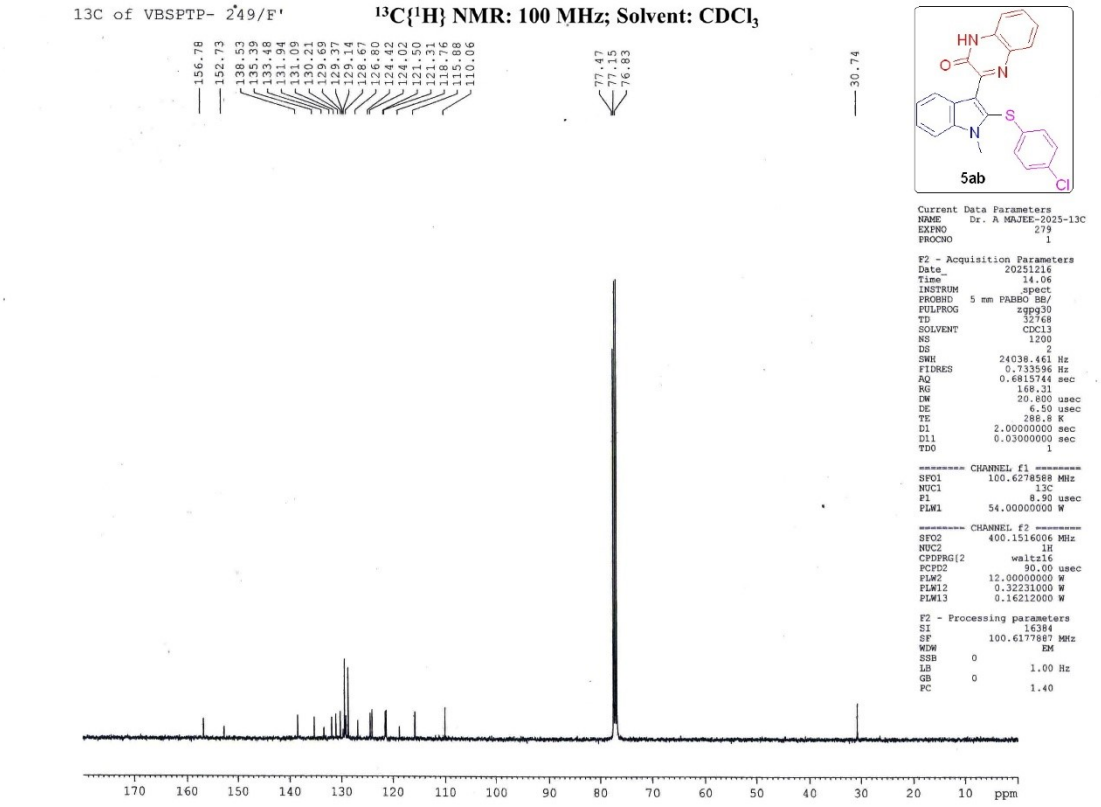
$^{13}C\{^1H\}$ NMR: 100 MHz; Solvent: $CDCl_3$



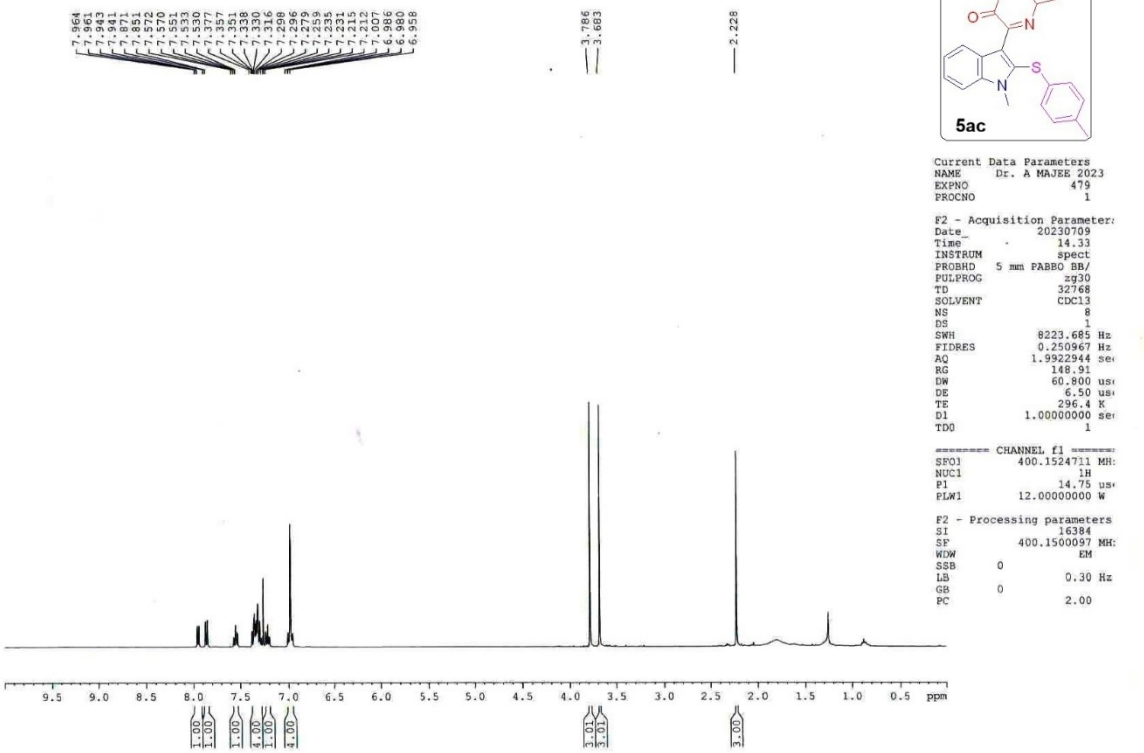



```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              473
PROCNO               1

F2 - Acquisition Parameters
Date_           20230708
Time              18.23
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                1024
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                135.7
DW               20.800 use
DE                6.50 use
TE               297.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1                13C
P1                8.90 use
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 use
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177858 MHz
WDW                  EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.00
```

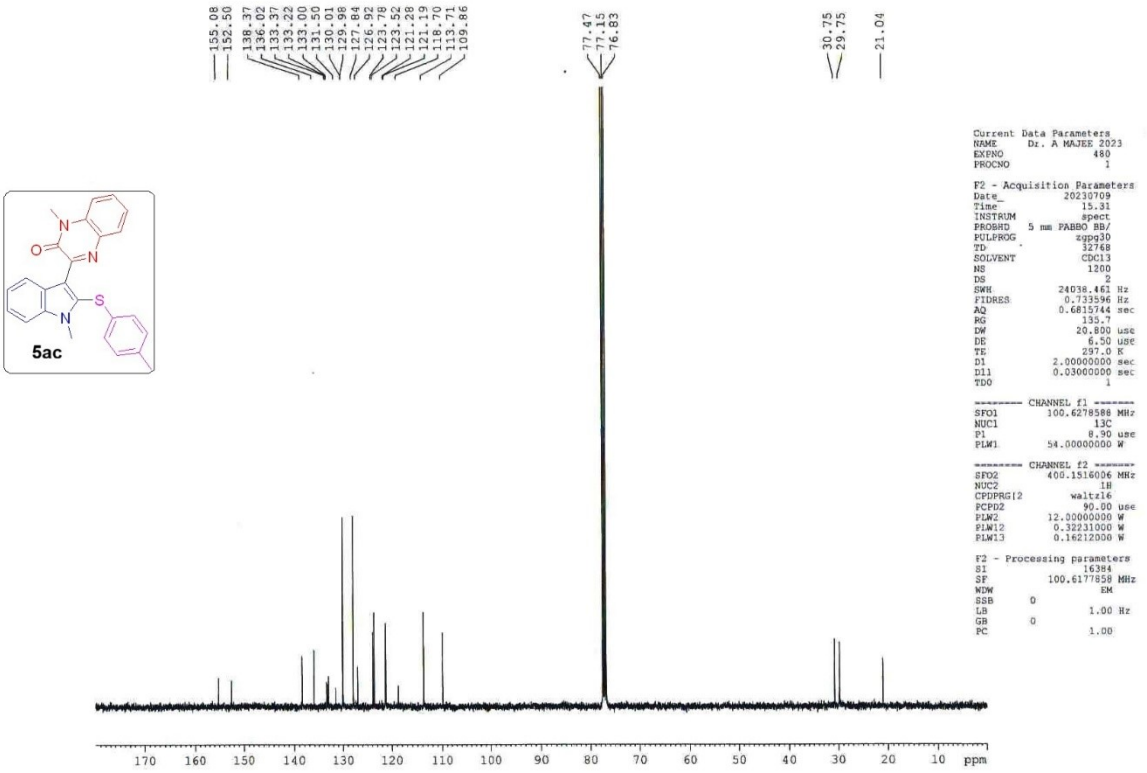

1H of VBSP- 249/F'
^{1}H NMR: 400 MHz; Solvent: CDCl$_3$
5ab
Current Data Parameters
NAME Dr. A MAJEE 2025-1H
EXPNO 405
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251216
Time 13.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 1
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 168.31
DW 60.800 usec
DE 6.50 usec
TE 288.7 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1524711 MHz
NUC1 1H
P1 14.75 usec
PLW1 12.00000000 W
F2 - Processing parameters
SI 16384
SF 400.1500679 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
ppm


13C of VBSPTP- 249/F'
^{13}C{^{1}H} NMR: 100 MHz; Solvent: CDCl$_3$
5ab
Current Data Parameters
NAME Dr. A MAJEE-2025-13C
EXPNO 279
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251216
Time 14.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 168.31
DW 20.800 usec
DE 6.50 usec
TE 286.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6278568 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
CHANNEL f2
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177887 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

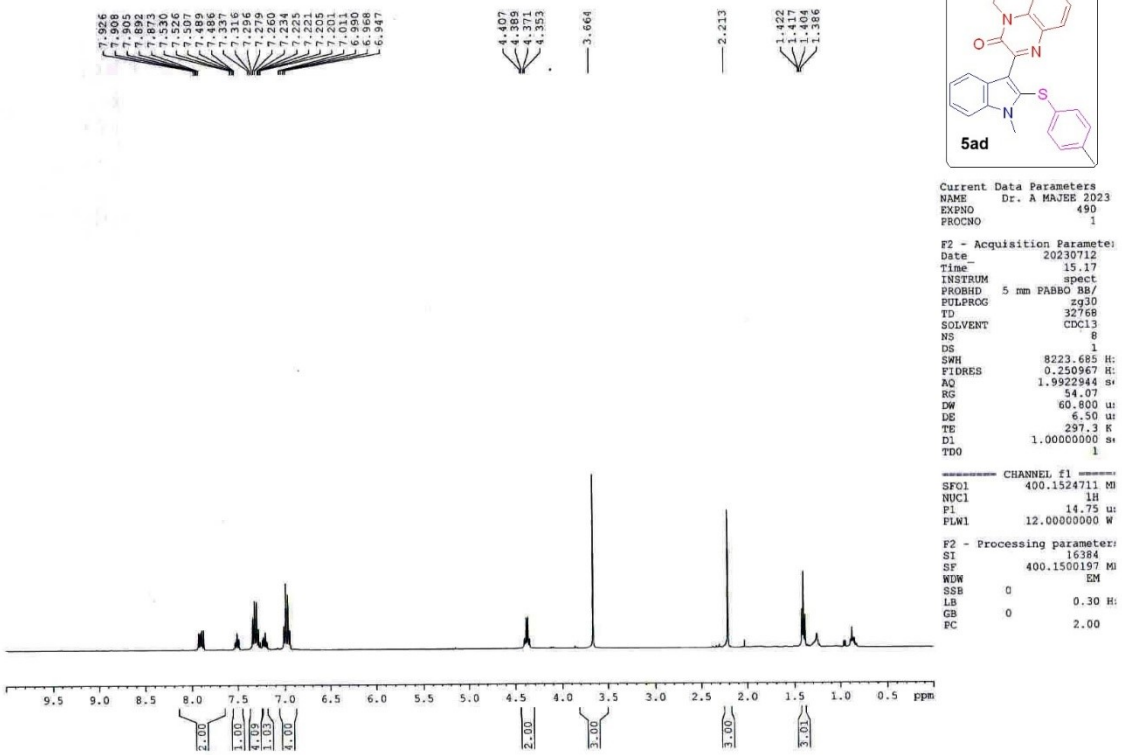
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



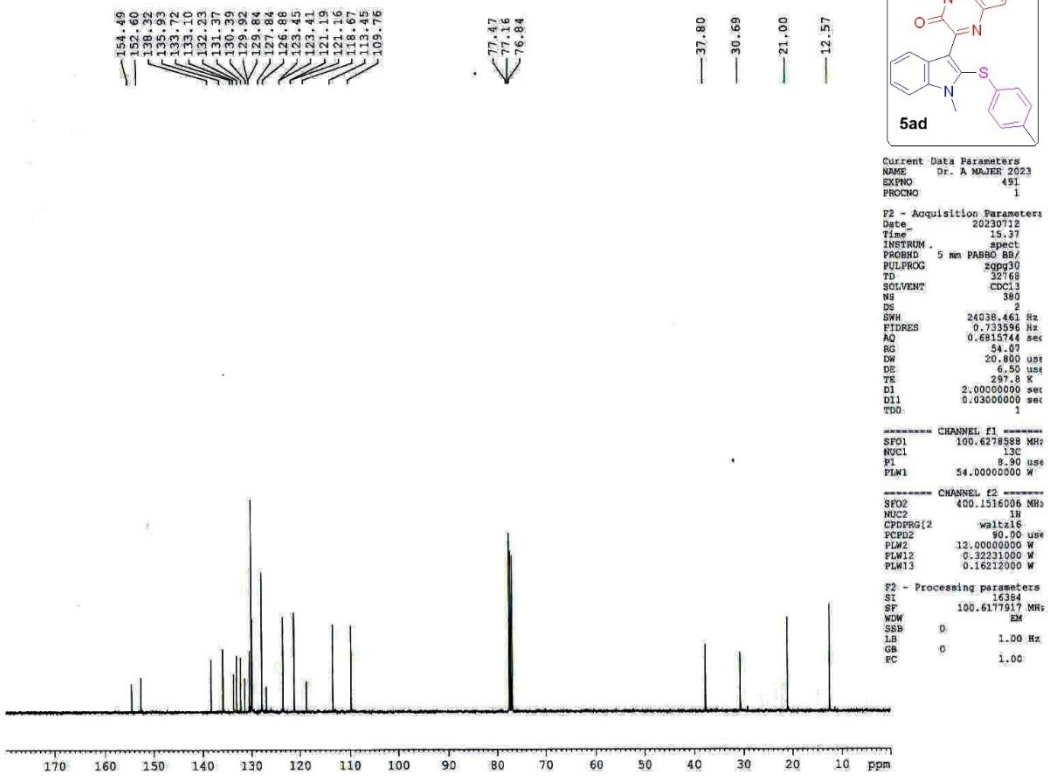
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



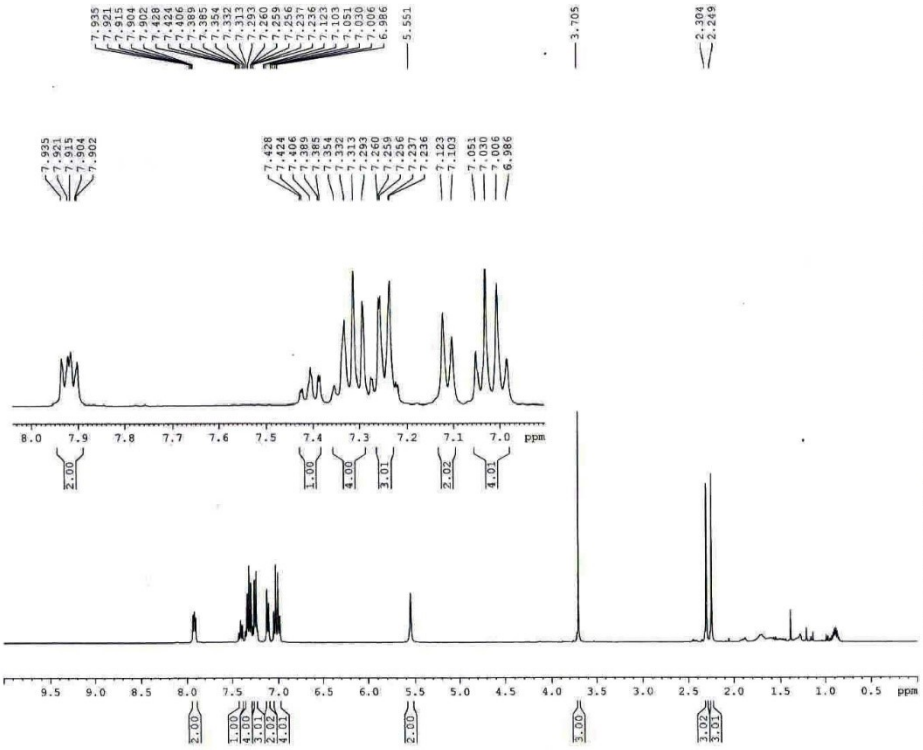
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

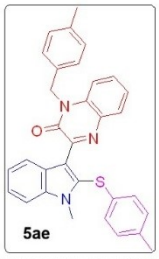


^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



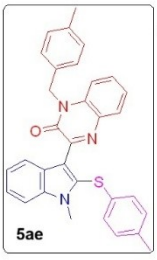
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

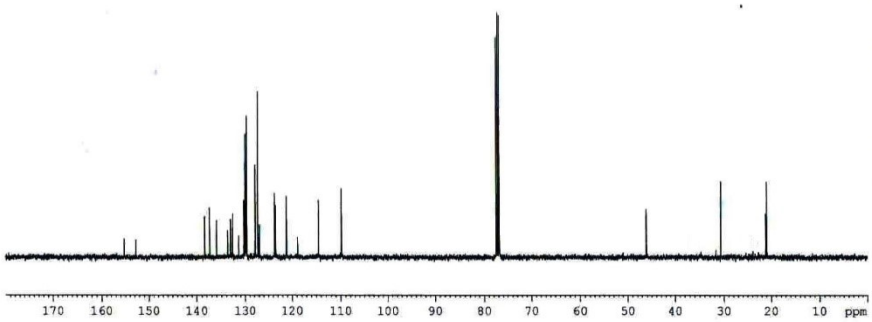





```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              546
PROCNO               1

F2 - Acquisition Parameters
Date_          20230730
Time              13.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                   8
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               67.81
DW               60.800 use
DE                6.50 use
TE              298.5 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1               1H
P1               14.75 use
PLW1        12.00000000 W

F2 - Processing parameters
SI                16384
SF          400.1500097 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

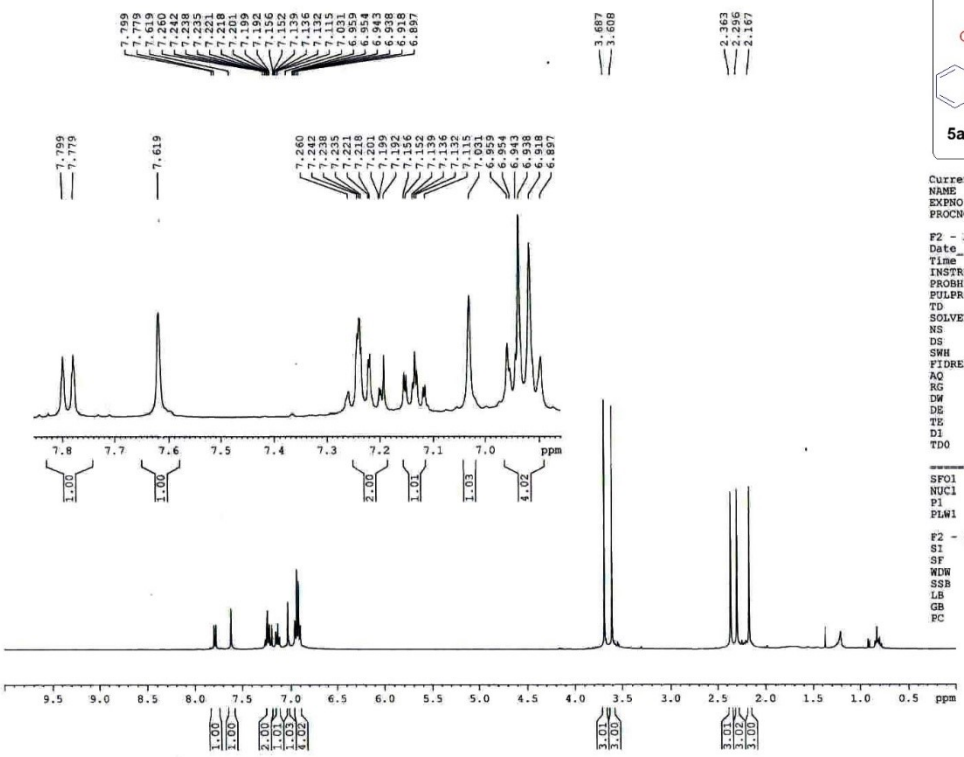
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$

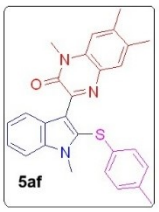





```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              547
PROCNO               1

F2 - Acquisition Parameters
Date_          20230730
Time              14.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                 256
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               67.81
DW               20.800 usec
DE                6.50 usec
TE              298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177887 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

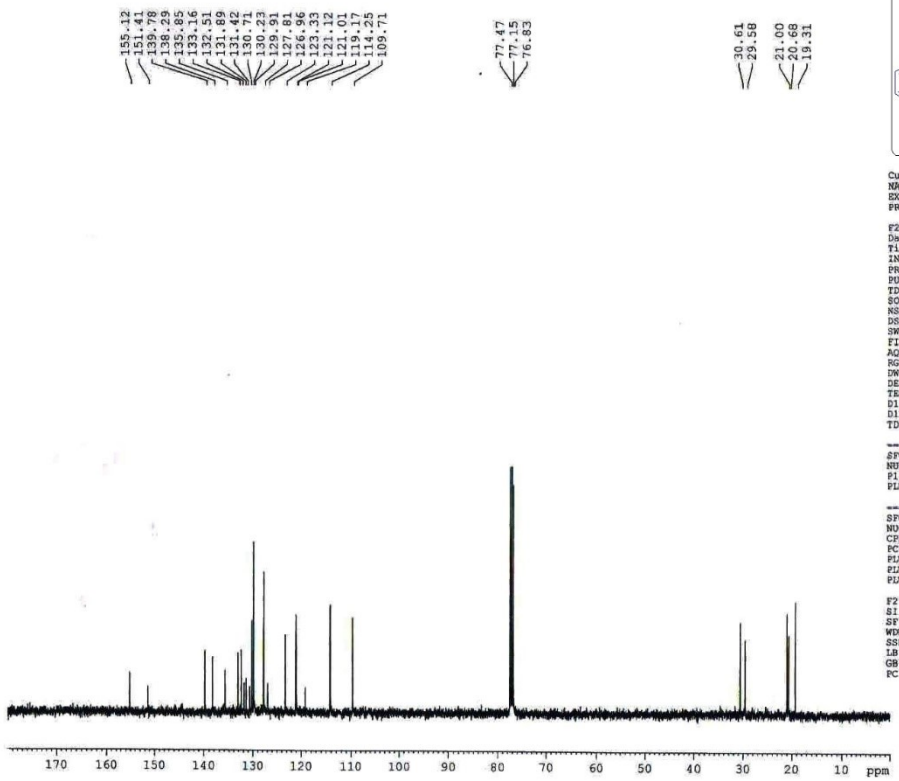
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

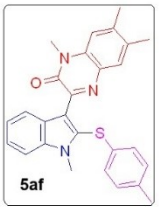




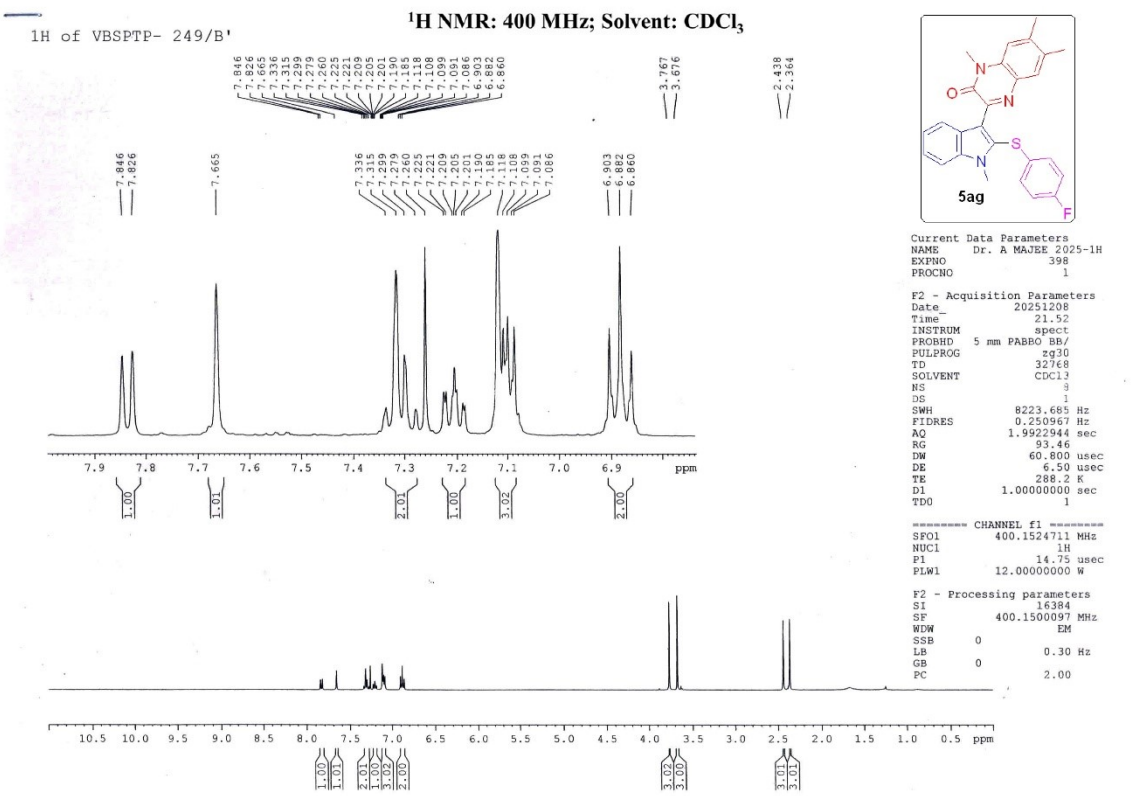

```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              569
PROCNO               1

F2 - Acquisition Parameters
Date_          20230814
Time              22.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               62.69
DW               60.800 use
DE                6.50 use
TE              298.9 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1               1H
P1                14.75 use
PLW1       12.00000000 W

F2 - Processing parameters
SI                16384
SF          400.1500367 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

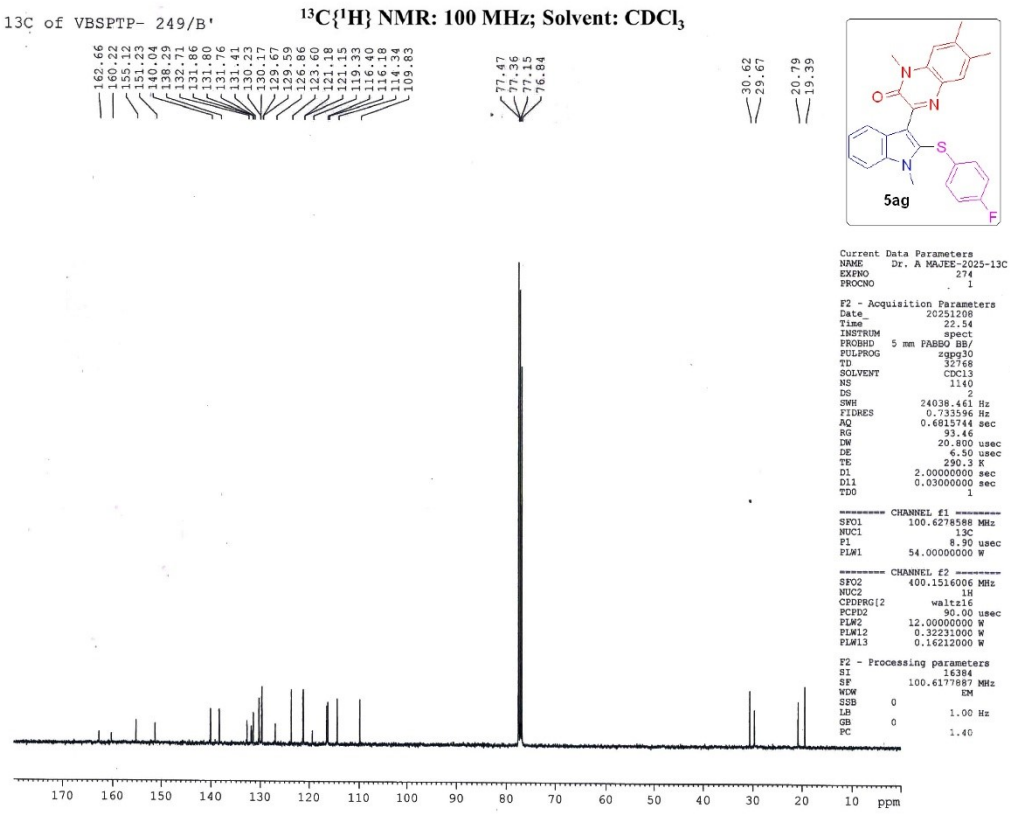
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$



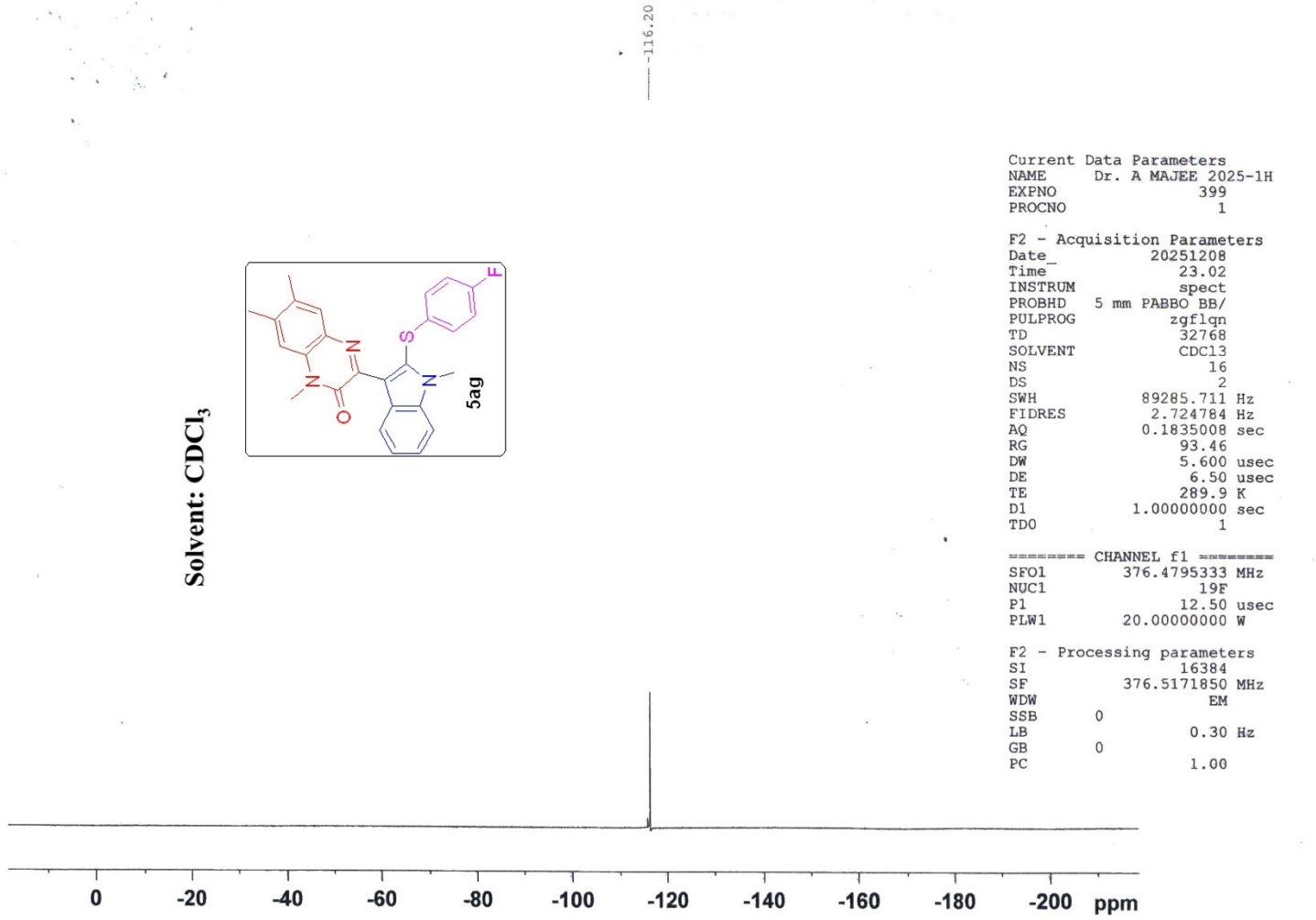



```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO              570
PROCNO               1

F2 - Acquisition Parameters
Date_          20230814
Time              23.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                 120
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               62.69
DW              20.800 usec
DE               6.50 usec
TE              299.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1       54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177902 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```


1H of VBSPTP- 249/B'
^{1}H NMR: 400 MHz; Solvent: CDCl$_3$
5ag
Current Data Parameters
NAME Dr. A MAJEE 2025-1H
EXPNO 398
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251208
Time 21.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 1
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 93.46
DW 60.800 usec
DE 6.50 usec
TE 288.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1524711 MHz
NUC1 1H
P1 14.75 usec
PLW1 12.00000000 W
F2 - Processing parameters
SI 16384
SF 400.1500097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

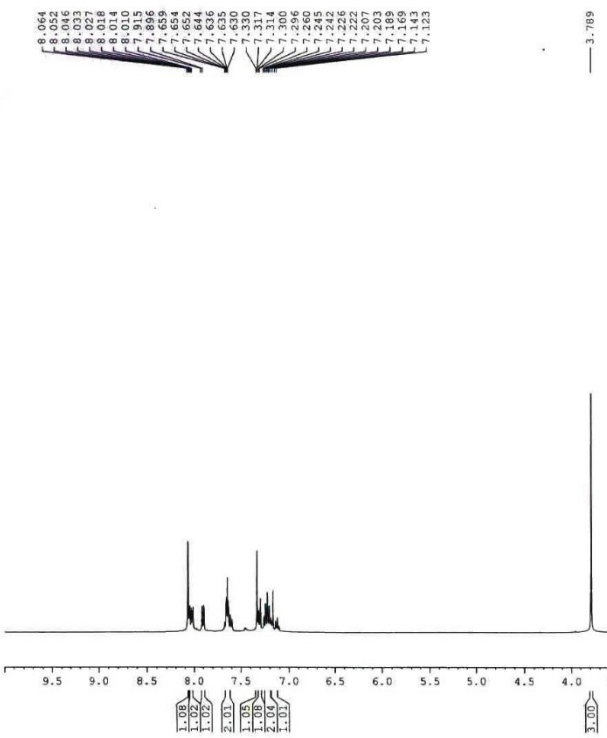

13C of VBSPTP- 249/B'
^{13}C{^{1}H} NMR: 100 MHz; Solvent: CDCl$_3$
5ag
Current Data Parameters
NAME Dr. A MAJEE-2025-13C
EXPNO 274
PROCNO 1
F2 - Acquisition Parameters
Date_ 20251208
Time 22.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1140
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 93.46
DW 20.800 usec
DE 6.50 usec
TE 290.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
CHANNEL f2
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177887 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

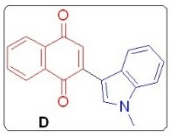
F19 1H coupled VBSPTP- 249/B'




```
Current Data Parameters
NAME      Dr. A MAJEE 2025-1H
EXPNO                399
PROCNO                 1

F2 - Acquisition Parameters
Date_           20251208
Time              23.02
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ            0.1835008 sec
RG                93.46
DW                5.600 usec
DE                6.50 usec
TE                289.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         376.4795333 MHz
NUC1                19F
P1                12.50 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                16384
SF           376.5171850 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

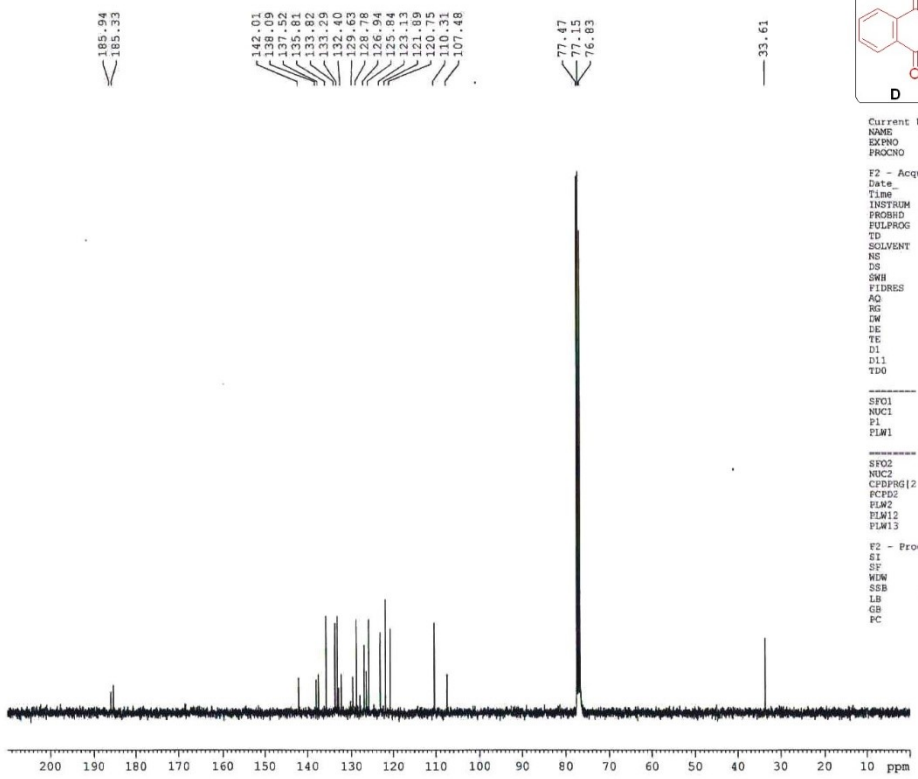
^{1}H NMR: 400 MHz; Solvent: $CDCl_3$

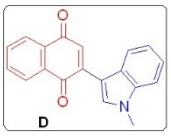





```
Current Data Parameters
NAME      Dr. A MAJEE 2021
EXPNO              387
PROCNO               1

F2 - Acquisition Parameters
Date_          20211212
Time              10.40
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               168.31
DW               60.800 usec
DE                6.50 usec
TE              291.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1               1H
P1                14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF           400.1500453 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

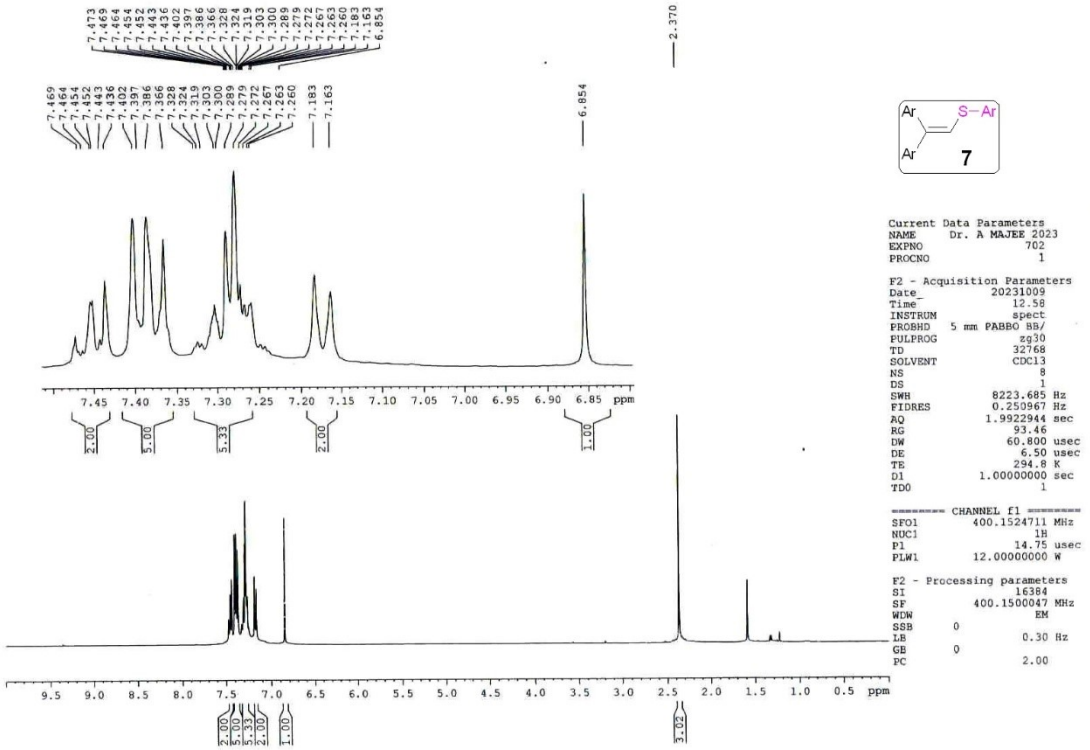
^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$






```
Current Data Parameters
NAME      Dr. A MAJEE 2021
EXPNO              388
PROCNO               1

F2 - Acquisition Parameters
Date_          20211212
Time              11.15
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                 512
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               168.31
DW               20.800 usec
DE                6.50 usec
TE              292.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1               13C
P1                 8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2               1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177874 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

^{1}H NMR: 400 MHz; Solvent: $CDCl_3$



^{13}C{^{1}H} NMR: 100 MHz; Solvent: $CDCl_3$