

PhI(OCOCF₃)₂-Mediated Metal-Free 2,3-Difunctionalization of Indoles: Direct Access to Carbochalcogenated Scaffolds

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1. Experimental Section

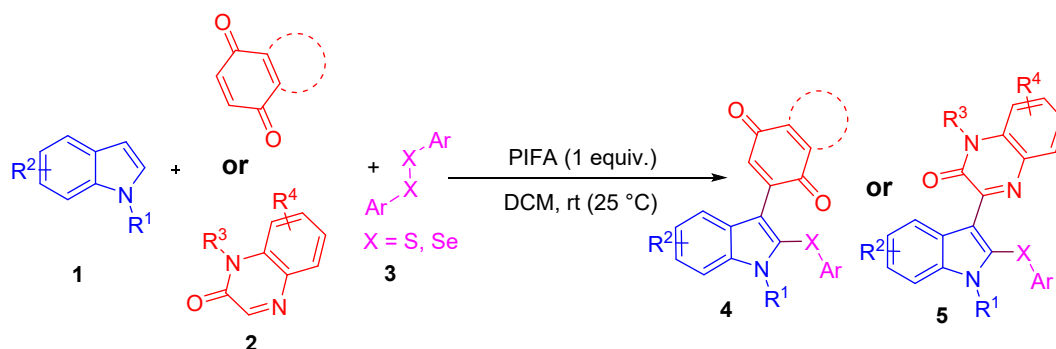
General Information

^1H 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. $^{13}\text{C}\{^1\text{H}\}$ 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 ($\delta = 77.16$) 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 $^\circ\text{C}$ 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 prepared¹ according to the reported method.

2. Experimental Procedures

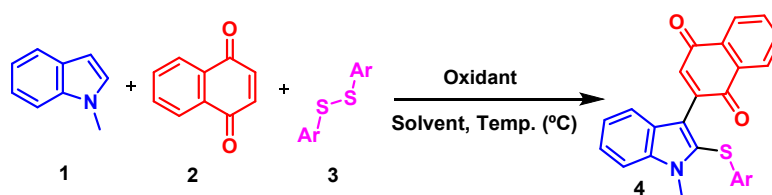
General procedure for the synthesis of 4(4aa-4aq) or 5 (5aa-5ag).

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 1 equiv. 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 ($3 \times 20\text{mL}$). 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 ₃ CN	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**: $C_{25}H_{16}BrNO_2S$.

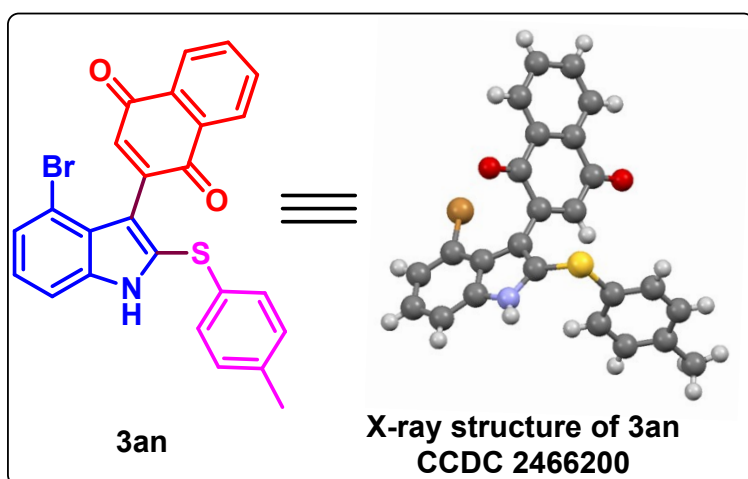
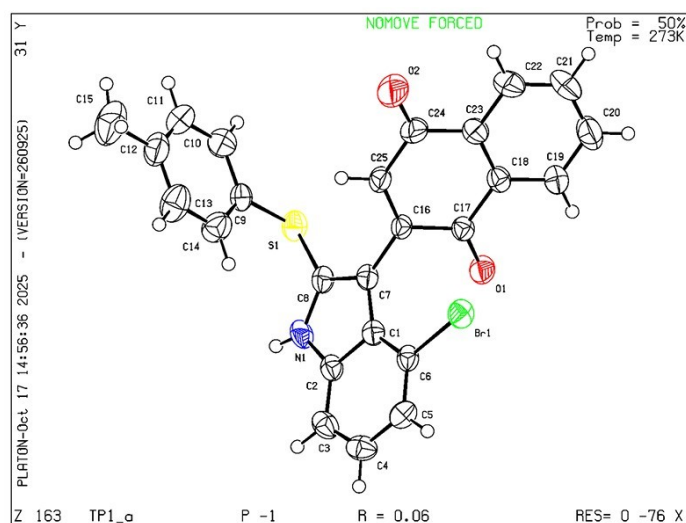


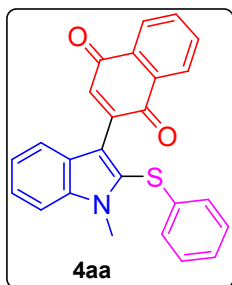
Table 2: Crystal



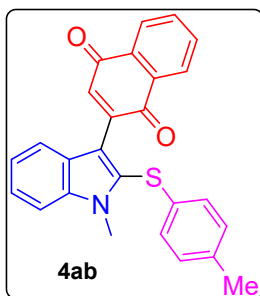
Wavelength	0.71073 Å	
Formula	C₂₅H₁₆BrNO₂S.	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.3740(3) Å	α = 92.277(2)
	b = 8.7891(3) Å	β = 94.132(2)
	c = 16.2598(7) Å	γ = 103.090(2)
Volume	1022.06(7) Å³	
Z	2	
R-factor (%)	5.64	

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

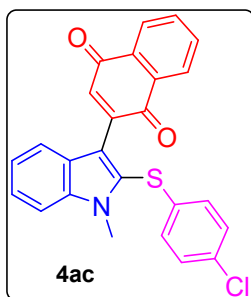
5. Spectroscopic Data of Synthesised Compounds:



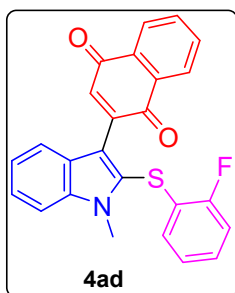
2-(1-methyl-2-(phenylthio)-1H-indol-3-yl)naphthalene-1,4-dione (4aa): Yield: 82%; 316 mg; red solid; Mp: 91-93 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.13-8.10 (m, 1H), 8.06-8.04 (m, 1H), 7.69-7.67 (m, 2H), 7.53 (d, J = 8 Hz, 1H), 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 $\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{18}\text{NO}_2\text{S}]^+$: 396.1053; Found : 396.1064.



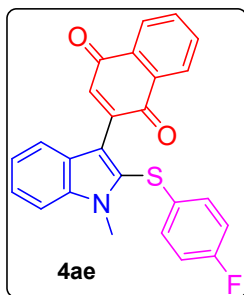
2-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione (4ab): Yield: 79 %; 332 mg; red solid; Mp: 106-109 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.07-8.05 (m, 1H), 8.00-7.99 (m, 1H), 7.64-7.61 (m, 2H), 7.47 (d, J = 8 Hz, 1H), 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 $\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{26}\text{H}_{20}\text{NO}_2\text{S}]^+$: 410.1209; Found : 410.1216.



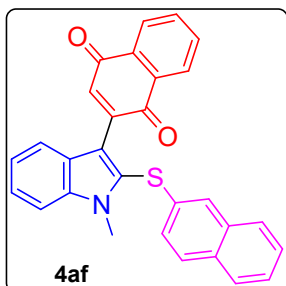
2-(2-((4-chlorophenyl)thio)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione (4ac): Yield: 80 %; 343 mg; red solid; Mp: 135-138 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.19-8.17 (m, 1H), 8.14-8.12 (m, 1H), 7.78-7.76 (m, 2H), 7.67 (d, J = 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{17}\text{ClNO}_2\text{S}]^+$: 430.0663; Found: 430.0671.



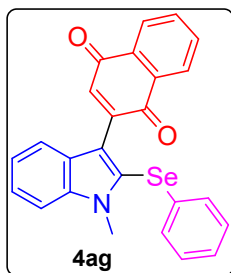
2-(2-((2-fluorophenyl)thio)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione (4ad): Yield: 81 %; 330 mg; red solid; Mp: 97-99 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.20-8.18 (m, 1H), 8.14-8.12 (m, 1H), 7.78-7.76 (m, 2H), 7.59 (d, J = 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{17}\text{FNO}_2\text{S}]^+$: 414.0959; Found: 414.0973.



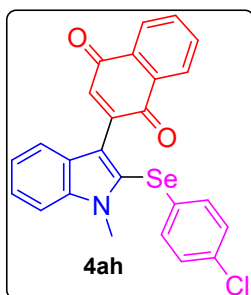
2-(2-((4-fluorophenyl)thio)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione(4ae): Yield: 80 %; 334 mg; Mp: 109-111 °C; red solid; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.07-8.00 (m, 2H), 7.64-7.64 (m, 2H), 7.48 (d, J = 8 Hz, 1H), 7.26-7.20 (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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{17}\text{FNO}_2\text{S}]^+$: 414.0959; Found: 414.0967.



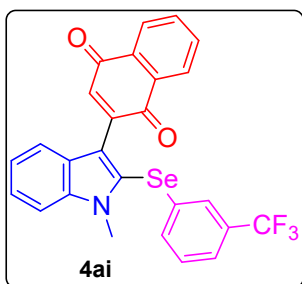
2-(1-methyl-2-(naphthalen-2-ylthio)-1H-indol-3-yl)naphthalene-1,4-dione(4af): Yield: 80 %; 343 mg; Mp: 110-1113 °C; red solid; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.19-8.16 (m, 1H), 8.10-8.08 (m, 1H), 7.74-7.71 (m, 3H), 7.67 (d, J = 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{29}\text{H}_{20}\text{NO}_2\text{S}]^+$: 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); ^1H 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{18}\text{NO}_2\text{Se}]^+$: 444.497; Found : 444.509.

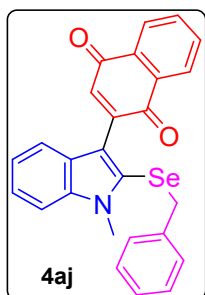


2-(2-((4-chlorophenyl)selanyl)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione (4ah): Yield: 79 %; 378 mg; Mp: 117-1119 °C; red solid; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.30-8.28 (m, 1H), 8.26-8.24 (m, 1H), 7.89-7.87 (m, 2H), 7.71 (d, 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{17}\text{ClNO}_2\text{Se}]^+$: 478.0108; Found: 478.0114.

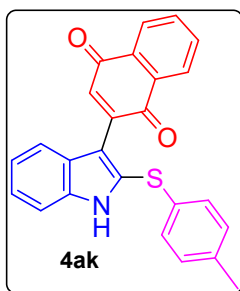


2-(1-methyl-2-((3-(trifluoromethyl)phenyl)selanyl)-1H-indol-3-yl)naphthalene-1,4-dione

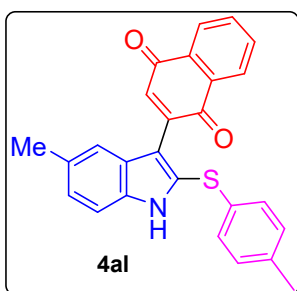
(4ai): Yield: 81%; 413 mg; red solid; Mp: 109-111 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ¹H NMR (CDCl₃, 400 MHz): δ 8.19-8.17 (m, 1H), 8.15-8.13 (m, 1H), 7.78-7.76 (m, 2H), 7.62 (d, *J* = 8 Hz, 1H), 7.54 (s, 1H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.37-7.33 (m, 1H), 7.29-7.26 (m, 1H), 7.24-7.22 (m, 1H), 7.16 (d, *J* = 8 Hz, 1H), 7.14 (s, 1H), 3.79 (s, 3H); ¹³C{¹H} NMR (CDCl₃, 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 [C₂₆H₁₇F₃NO₂Se]⁺ : 512.0371; Found : 512.0379.



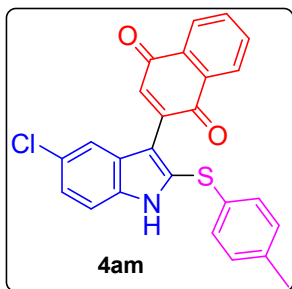
2-(2-(benzylselanyl)-1-methyl-1H-indol-3-yl)naphthalene-1,4-dione (4aj): Yield: 75%; 340 mg; red solid; Mp: 99-101 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ¹H NMR (CDCl₃, 400 MHz): δ 8.15-8.13 (m, 1H), 8.10-8.07 (m, 1H), 7.73-7.71 (m, 2H), 7.55 (d, *J* = 7.6 Hz, 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); ¹³C{¹H} NMR (CDCl₃, 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 [C₂₆H₂₀NO₂Se]⁺ : 458.0654; Found : 458.0663.



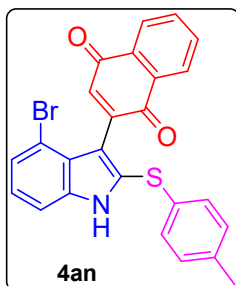
2-(2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione (4ak): Yield: 78%; 308 mg; red solid; Mp: 125-128 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/8); ^1H NMR (CDCl_3 , 400 MHz): δ 8.31 (s, 1H), 8.17-8.15 (m, 1H), 8.10-8.08 (m, 1H), 7.73-7.71 (m, 2H), 7.51 (d, J = 8 Hz, 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{18}\text{NO}_2\text{S}]^+$: 396.1053; Found : 396.1062.



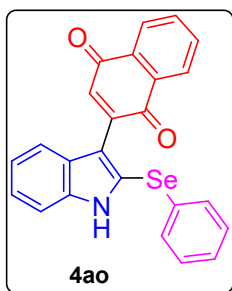
2-(5-methyl-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione (4al): Yield: 76%; 310 mg; red solid; Mp: 129-131 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/8); ^1H NMR (CDCl_3 , 400 MHz): δ 8.32 (s, 1H), 8.22-8.20 (m, 1H), 8.15-8.12 (m, 1H), 7.78-7.76 (m, 2H), 7.34 (s, 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{26}\text{H}_{20}\text{NO}_2\text{S}]^+$: 410.1209; Found : 410.1213.



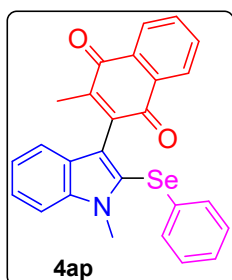
2-(5-chloro-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione (4am): Yield: 75%; 321 mg; red solid; Mp: 141-143 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/5); ^1H NMR (CDCl_3 , 400 MHz): δ 8.42 (s, 1H), 8.22-8.19 (m, 1H), 8.14-8.12 (m, 1H), 7.79-7.77 (m, 2H), 7.50 (s, 1H), 7.18-7.17 (m, 3H), 7.10-7.06 (m, 3H), 6.99 (s, 1H), 2.28 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ 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: $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{17}\text{ClNO}_2\text{S}]^+$: 430.0663; Found : 430.0674.



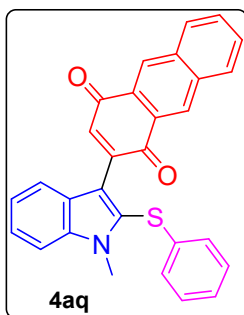
2-(4-bromo-2-(p-tolylthio)-1H-indol-3-yl)naphthalene-1,4-dione (4an): Yield: 78%; 371 mg; red solid; Mp: 148-151 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/5); ^1H NMR (CDCl_3 , 400 MHz): δ 8.50 (s, 1H), 8.13-8.11 (m, 1H), 8.08-8.07 (m, 1H), 7.73-7.70 (m, 2H), 7.23 (d, $J = 7.6$ 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); $^{13}\text{C}\{^1\text{H}\}$ 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: $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{17}\text{BrNO}_2\text{S}]^+$: 474.0158; Found : 474.0164.



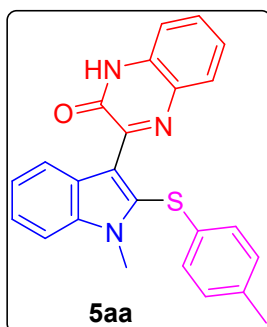
2-(2-(phenylselanyl)-1H-indol-3-yl)naphthalene-1,4-dione (4ao): Yield: 81%; 347 mg; red solid; Mp: 121-123 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/5); ^1H NMR (CDCl_3 , 400 MHz): δ 8.41 (s, 1H), 8.23-8.21 (m, 1H), 8.16-8.14 (m, 1H), 7.79-7.77 (m, 2H), 7.61 (d, J = 8 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{24}\text{H}_{16}\text{NO}_2\text{Se}]^+$: 430.0341; Found : 430.0349.



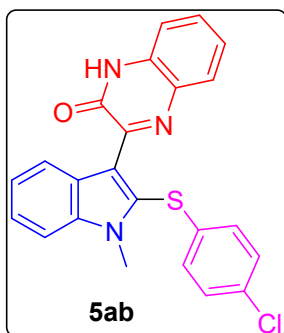
2-methyl-3-(1-methyl-2-(phenylselanyl)-1H-indol-3-yl)naphthalene-1,4-dione (4ap): Yield: 81%; 370 mg; red solid; Mp: 92-95 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.18-8.12 (m, 2H), 7.76-7.70 (m, 2H), 8.16-8.14 (m, 1H), 7.40 (d, J = 8 Hz, 1H), 7.32-7.28 (m, 2H), 7.19-7.13 (m, 6H), 3.80 (s, 3H), 2.07 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{26}\text{H}_{20}\text{NO}_2\text{Se}]^+$: 458.0654; Found : 458.0667.



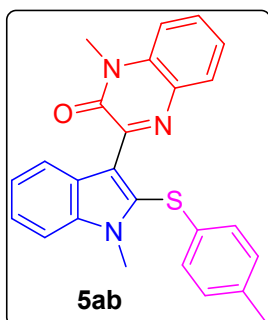
2-(1-methyl-2-(phenylthio)-1H-indol-3-yl)anthracene-1,4-dione (4aq): Yield: 79%; 351 mg; red solid; Mp: 131-133 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/10); ^1H NMR (CDCl_3 , 400 MHz): δ 8.74 (s, 1H), 8.67 (s, 1H), 8.10-8.07 (m, 2H), 7.70-7.65 (m, 3H), 7.41-7.31 (m, 3H), 7.24-7.22 (m, 2H), 7.17-7.15 (m, 5H), 3.79 (s, 1H); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{29}\text{H}_{20}\text{NO}_2\text{Se}]^+$: 446.1209; Found : 446.1213.



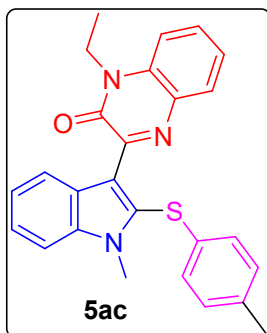
3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)quinoxalin-2(1H)-one (5aa): Yield: 78 %; 309 mg; yellow solid; Mp: 182-185 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^1H NMR (CDCl_3 , 400 MHz): δ 12.62 (s, 1H), 7.95-7.91 (m, 2H), 7.45-7.41 (m, 1H), 7.38-7.29 (m, 4H), 7.26-7.23 (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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{24}\text{H}_{20}\text{N}_3\text{OS}]^+$: 398.1322; Found : 398.1328.



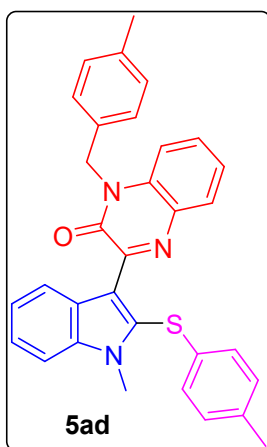
3-(2-((4-chlorophenyl)thio)-1-methyl-1H-indol-3-yl)quinoxalin-2(1H)-one (5ab): Yield: 75 %; 300 mg; yellow solid; Mp: 193-195 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^1H NMR (CDCl_3 , 400 MHz): δ 12.54 (s, 1H), 7.80 (d, J = 8 Hz, 2H), 7.80 (d, J = 8 Hz, 2H), 7.34-7.31 (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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{23}\text{H}_{17}\text{ClN}_3\text{OS}]^+$: 418.0775; Found : 418.0781.



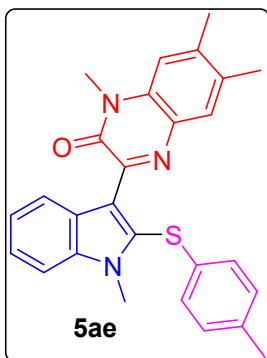
1-methyl-3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)quinoxalin-2(1H)-one (5ac): Yield: 75 %; 308 mg; yellow solid; Mp: 151-153 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^1H NMR (CDCl_3 , 400 MHz): δ 7.95-7.92 (m, 1H), 7.87-7.85 (m, 1H), 7.57-7.53 (m, 1H), 7.37-7.29 (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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{25}\text{H}_{22}\text{N}_3\text{OS}]^+$: 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); ^1H 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{26}\text{H}_{24}\text{N}_3\text{OS}]^+$: 426.1635; Found : 426.1644.

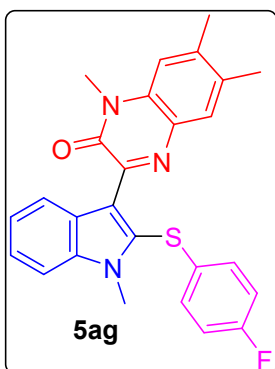


3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)-1-(4-methylbenzyl)quinoxalin-2(1H)-one (5ae): Yield: 75 %; 390 mg; yellow gummy mass; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^1H NMR (CDCl_3 , 400 MHz): δ 7.94-7.90 (m, 2H), 7.43-7.39 (m, 1H), 7.35-7.29 (m, 4H), 7.26-7.24 (m, 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{32}\text{H}_{28}\text{N}_3\text{OS}]^+$: 502.1948; Found : 502.1953.



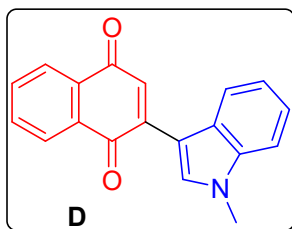
1,6,7-trimethyl-3-(1-methyl-2-(p-tolylthio)-1H-indol-3-yl)quinoxalin-2(1H)-one (5af):

Yield: 76 %; 333 mg; yellow solid; Mp: 163-165 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^1H 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{27}\text{H}_{26}\text{N}_3\text{OS}]^+$: 440.1791; Found : 440.1798.

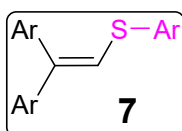


3-(2-((4-fluorophenyl)thio)-1-methyl-1H-indol-3-yl)-1,6,7-trimethylquinoxalin-2(1H)-one (5ag):

Yield: 72 %; 319 mg; yellow solid; Mp: 127-129 °C; column chromatography done (eluent: ethyl acetate/petroleum ether = 1/4); ^1H 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); $^{13}\text{C}\{^1\text{H}\}$ 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 : $[\text{M}+\text{H}]^+$ Calculated for $[\text{C}_{26}\text{H}_{23}\text{FN}_3\text{OS}]^+$: 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); ¹H NMR (CDCl₃, 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); ¹³C{¹H} NMR (CDCl₃, 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); ¹H NMR (CDCl₃, 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); ¹³C{¹H} NMR (CDCl₃, 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.

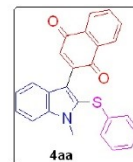
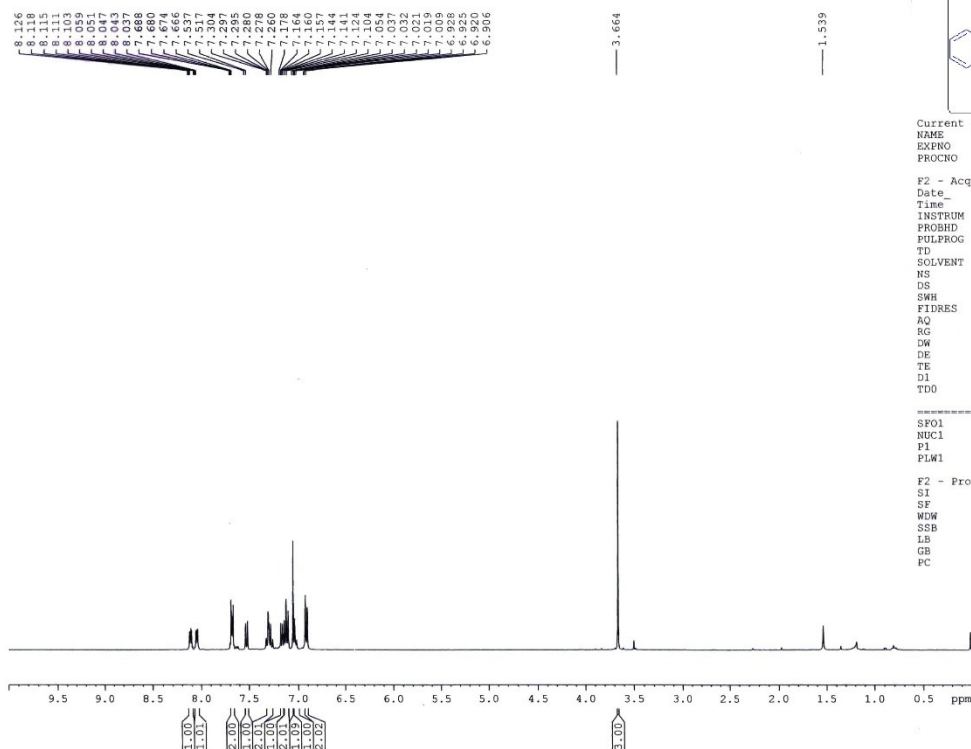
6. References:

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 [^1H , and $^{13}\text{C}\{^1\text{H}\}$] of
synthesized products:**

¹H of VBSP-249/2

¹H NMR: 400 MHz; Solvent: CDCl₃



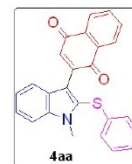
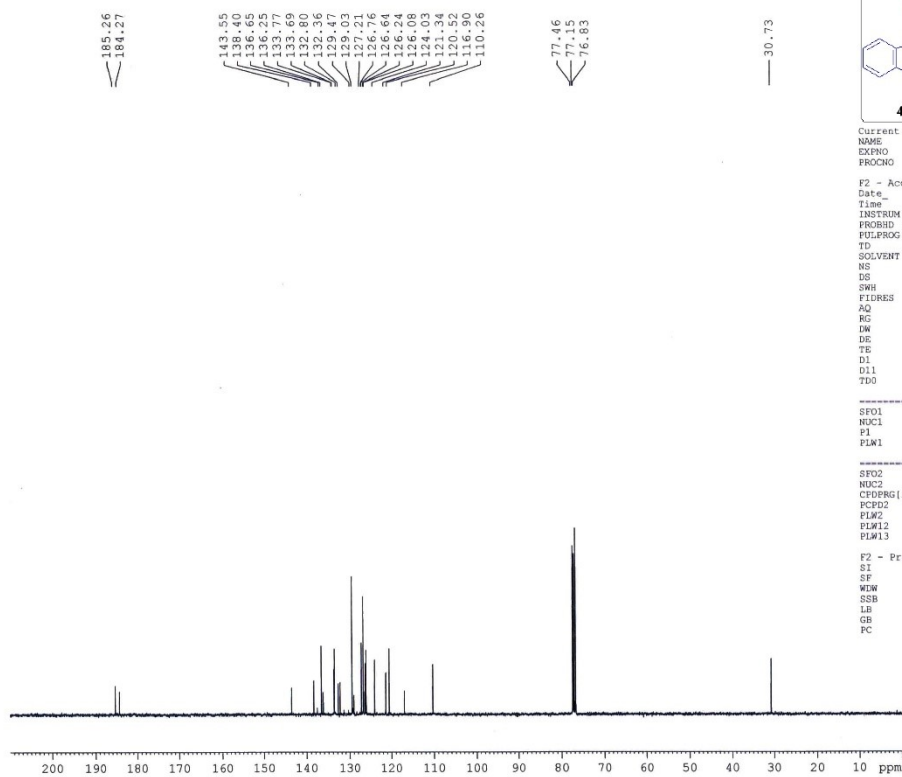
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EXPNO 367
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¹³C{¹H} NMR: 100 MHz; Solvent: CDCl₃



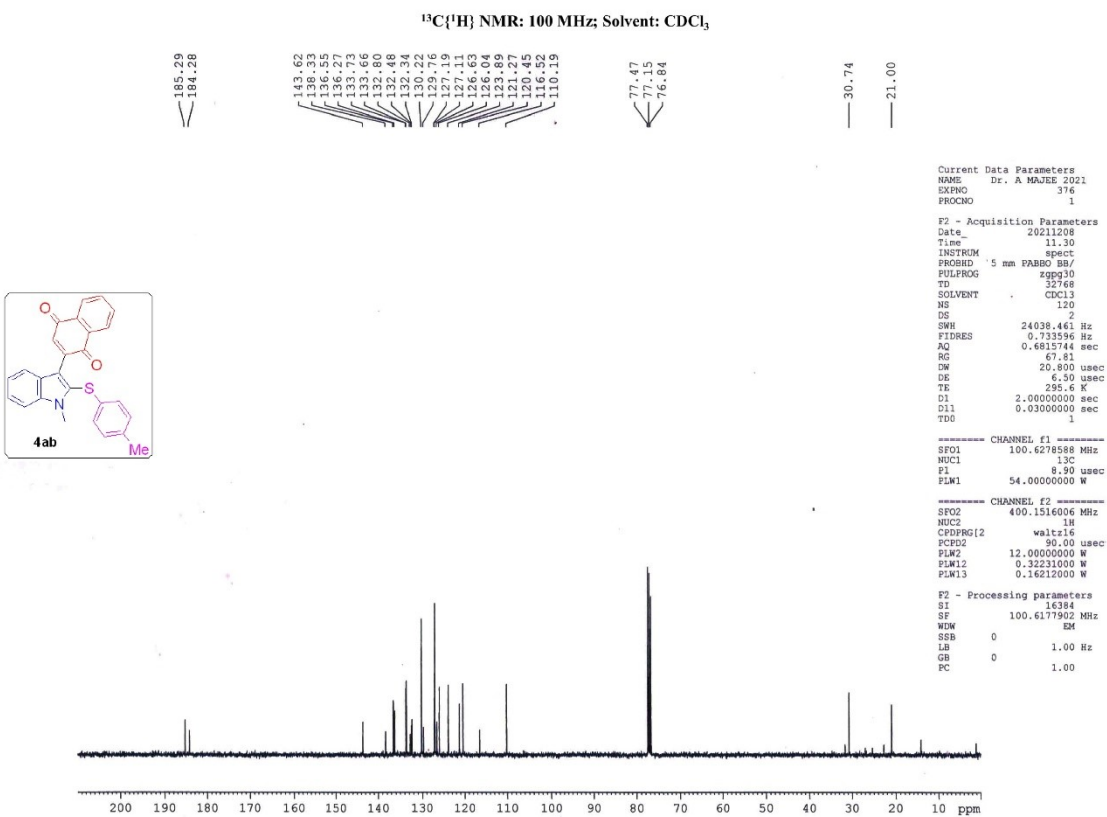
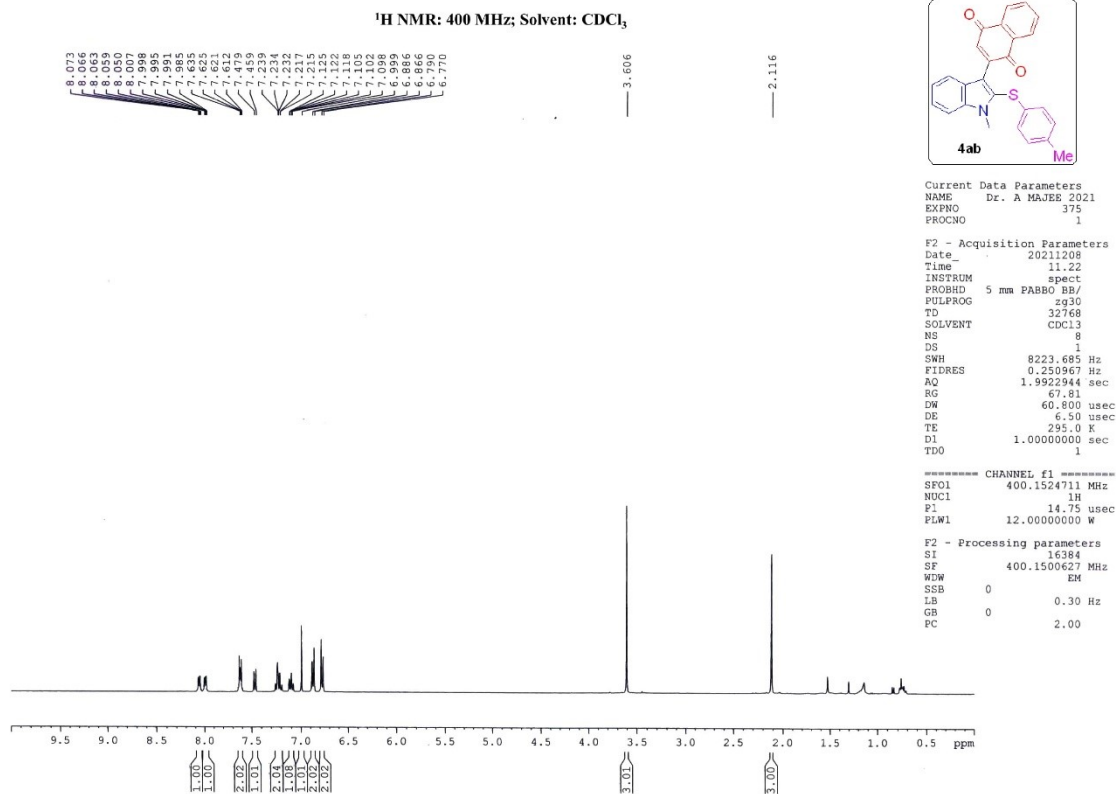
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PROCNO 1

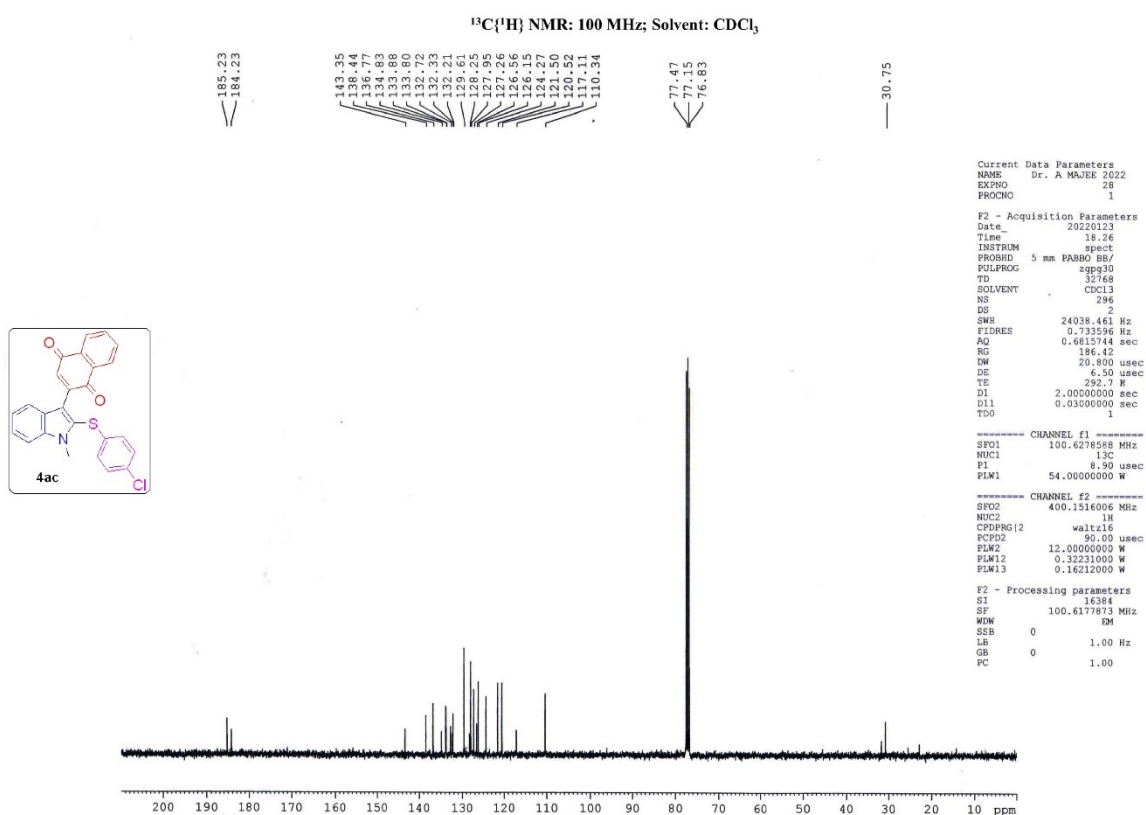
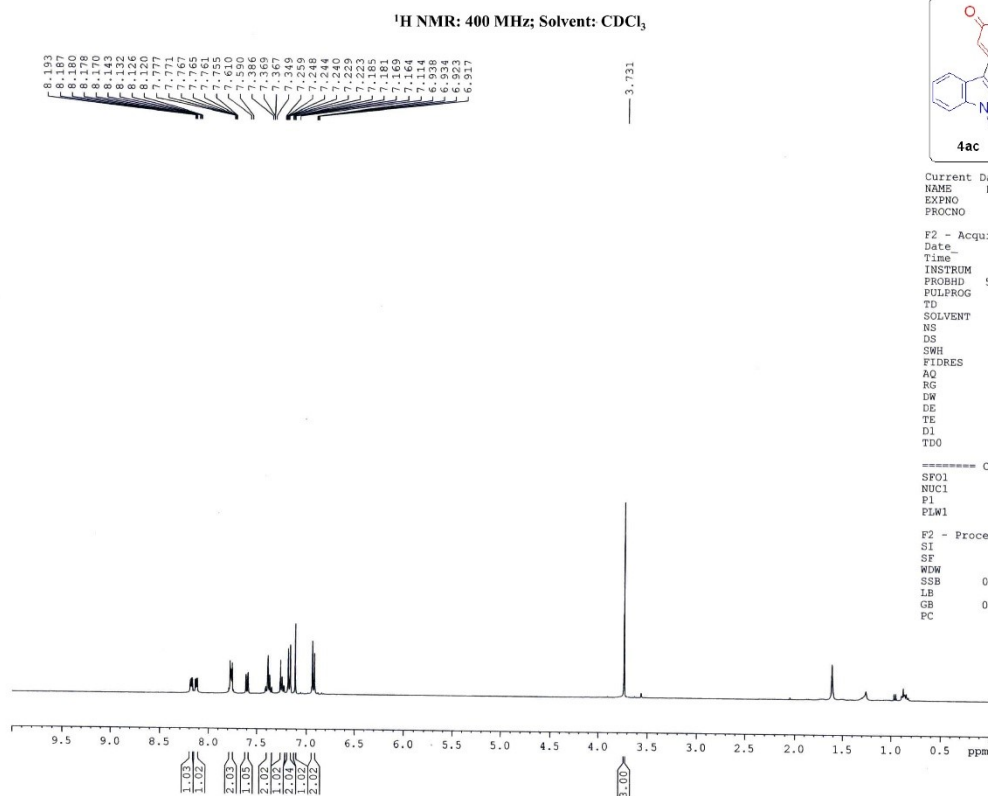
F2 - Acquisition Parameters
Date_ 20211128
Time_ 17.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 93.46
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

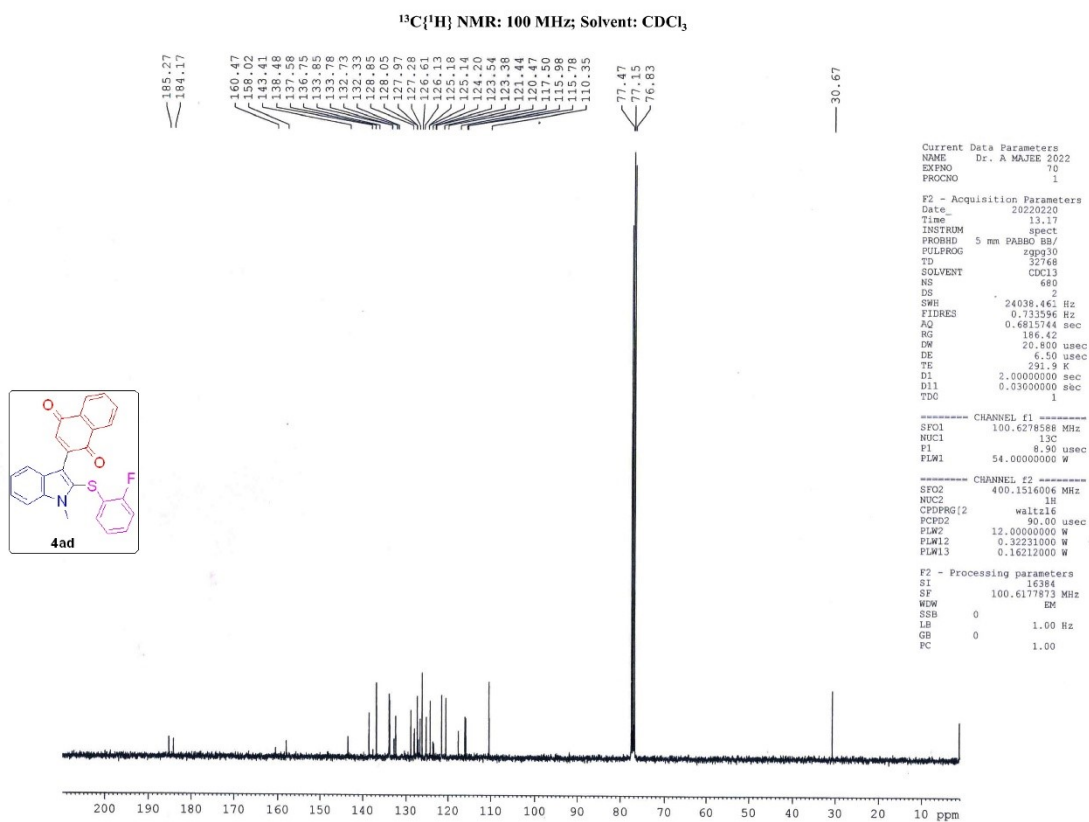
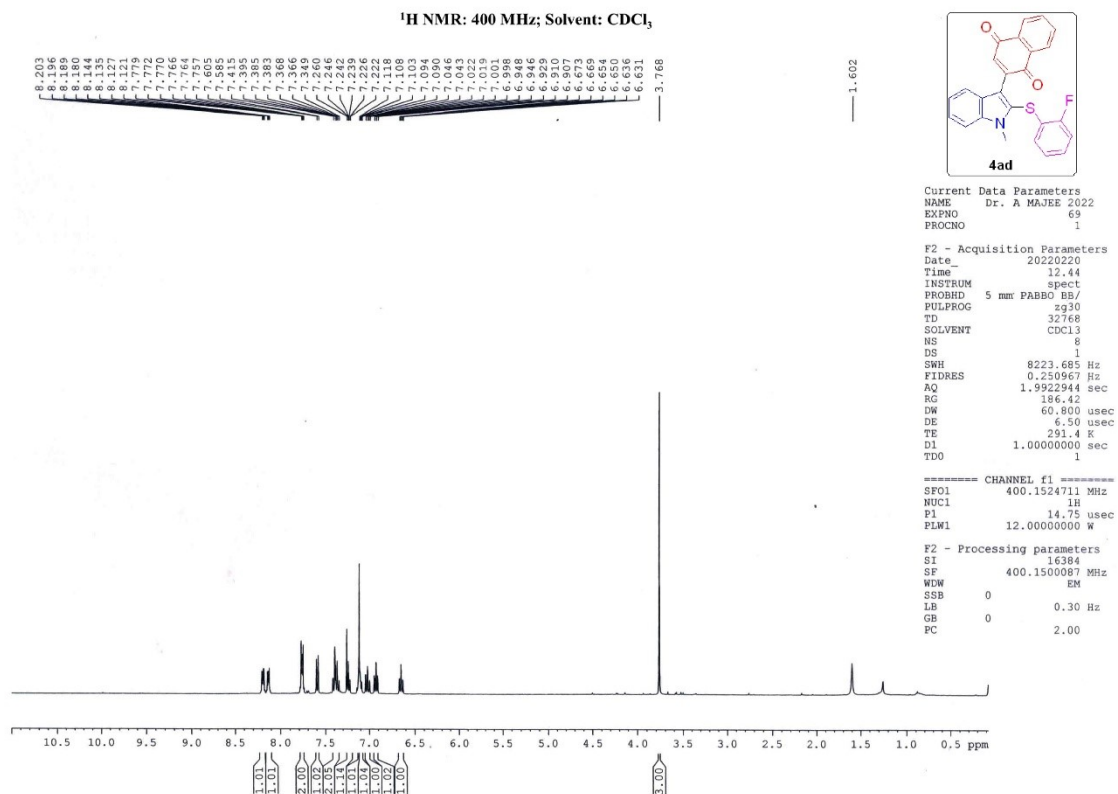
CHANNEL f1
SFO1 100.6278588 MHz
NUC1 13C
P1 8.50 usec
PLW1 54.00000000 W

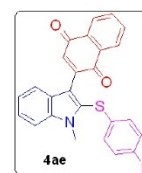
CHANNEL f2
SFO2 400.1516006 MHz
NUC2 1H
CFPRNG12 wall116
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

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







[illegible]

```

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    zgpg30
TD          32768
FIDRES     0.2300
SOLVENT    CDCl3
DS          8
US          1
SMH         8223.685 Hz
FIDRES      0.250967 Hz
AQ          1.9922254 sec
RG           37.83
DW           60.800 usec
DE          6.50 usec
TE          298.5 K
D1          1.00000000 sec
Time       1
===== CHANNEL f1 =====
SF01        400.1524711 MHz
NUC1         13C
P1           14.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI          1
SF          400.1500624 MHz
WDW         EM
SSB          0
GB           0.30 Hz
LB           0
PC           2.00

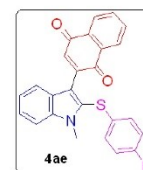
```

185.11
184.17

162.75
160.30
159.46
158.33
156.68
153.76
153.67
152.71
152.71
151.70
151.70
151.07
149.19
138.96
138.89
137.14
136.24
136.04
134.09
131.37
121.41
120.41
116.69
116.47
110.21

77.47
77.15
76.84

30.67



```

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

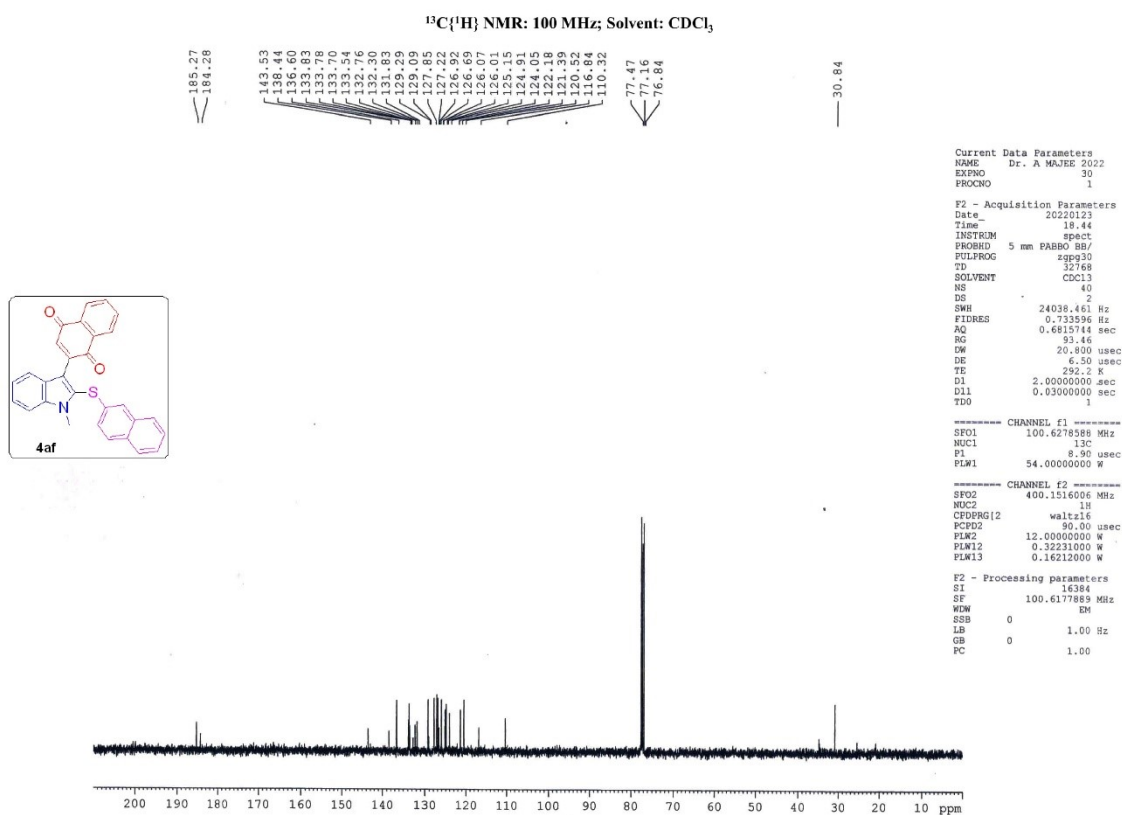
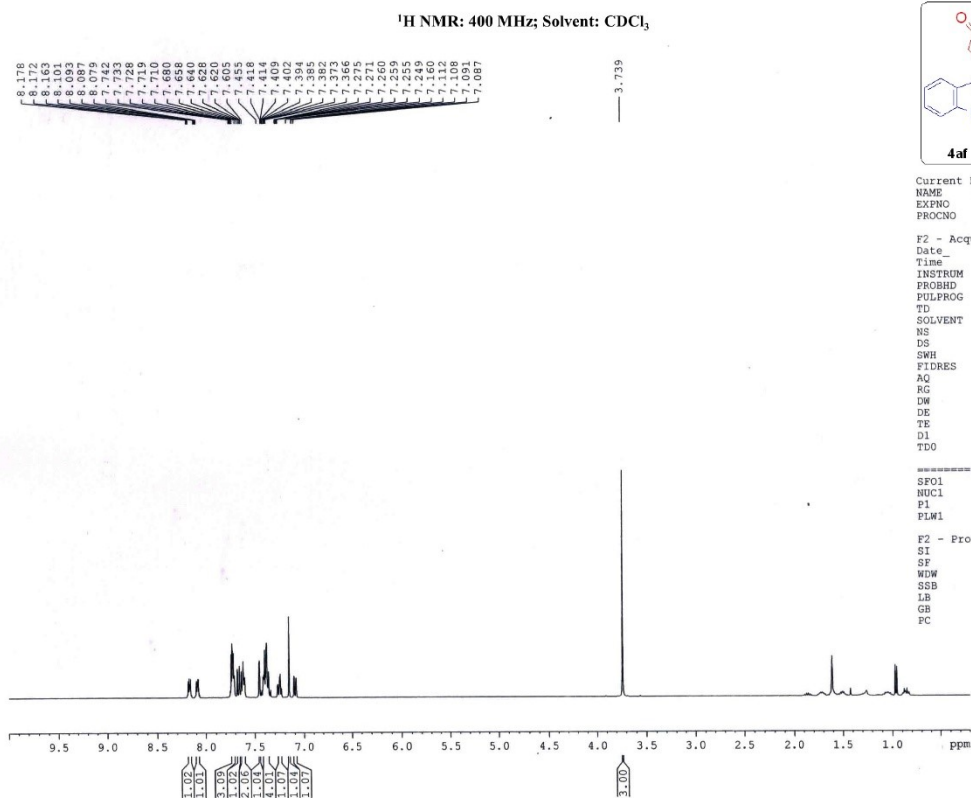
===== CHANNEL 1 =====
F2 - Acquisition Parameters
Date_     20230914
Time      14.56
INSTRUM    spect
PROBHD     5 mm BBO 1H/13
PULPROG    zgpg30
TD          32768
SOLVENT     CDCl3
NS          200
DS          2
SWH         24038.464 Hz
FIDRES     0.7373596 Hz
AQ          0.681734 sec
RG          28.860 usec
DE          6.50 usec
TE          298.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TDO         1

===== CHANNEL 12 =====
F301       100.6275858 MHz
NUC1        13C
P1          1.80 usec
PL1         54.00000000 W

===== CHANNEL 72 =====
F302       400.1516066 MHz
NUC2        1H
CPDPRG2    waltz16
PCPD2      90.00 usec
PL2         12.00000000 W
PLM12       0.32323100 W
PLM13       0.16212000 W

F2 - Processing parameters
SI          32768
SF          100.6177651 MHz
AQ          0.681734 sec
RG          28.860 usec
DE          6.50 usec
TE          298.2 K
D1          2.00000000 sec
D11         0.03000000 sec
TDO         1

```



4a

Current D
 NAME
 EXPNO
 PROCNO

F2 - Acq
 Date_
 Time_
 INSTRUM
 PROBHD
 PULPROG
 TD
 SOLVENT
 NS
 DS
 SWH
 FIDRES
 AQ
 RG
 DW
 DE
 TE
 D1
 TDO

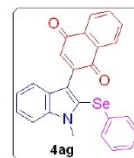
SF01
 NUC1
 P1
 FLW1

F2 - Proc
 SI
 SF
 WDW
 SSB
 LB
 GB
 PC

8.309
8.298
8.288
8.265
8.276
8.229
8.222
8.216
8.183
7.951
7.948
7.938
7.919
7.898
7.863
7.836
7.834
7.817
7.799
7.732
7.715
7.733
7.713
7.733
7.727
7.727
7.744
7.762
7.721
7.727
7.727

1.01
1.01
2.02
1.06
1.03
5.00
3.03

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm



```

Current Data Parameters
NAME      Dr. A NAEJE 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          1
SWH         8223.685 Hz
FIDRES     0.25066 Hz
AQ          1.999944 sec
RG          68
DE          60.800 usec
TE          30.0 usec
D0          297.1 K
D1          1.0000000 sec
D10         1

===== CHANNEL f1 =====
SF01        400.1524711 MHz
F1          1H
P1           14.75 usec
PLW1        12.0000000 W

F2 - Processing parameters
SI           1
SF           400.1499745 MHz
WDW          EM
GB           0
LB           0.30 Hz
RG           0
PC           2.00

```

Current
NAME
EXPNO
PROCNO

F2 - A
Date
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
D11
TD0

SF01
NUC1
P1
PLW1

SF02
NUC2
CPDPRG
PCFG
PLW2
PLW12
PLW13

F2 - Pr
SI
SF
WMW
SSB
LB
GB
PC

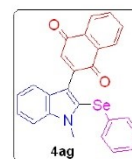
185.29
184.65

144.07
138.59
138.59
134.04
133.79
133.67
132.81
132.39
132.18
129.68
127.67
127.24
126.96
126.92
126.07
125.00
121.23
120.11
117.00
110.34

77.47
77.45
76.84

— 32.17 —

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



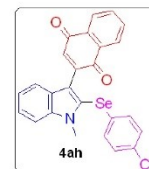
```

Current Data Parameters
Name      Dr. A MAJER 2021
EXPNO     1      295
PROCNO    1

F2 - Acquisition Parameters
-----
Time              20210926
Time              16.05
INSTRUM          spect
PROBHD          5 mm PABBO-BB
PULPROG          zgpg30
PC              12.648
TD              65536
SOLVENT          CDCl3
DS              4
SWH              24038.461 Hz
FIDRES          0.733556 Hz
AQ              0.681574 sec
RG              87.66
WDW              20.800 user
SSB              6.50 user
GB              0
TE              298.0 K
D1              2.0000000 sec
DELTA           0.0360000 sec
TDO              1
-----
CHANNEL f1
SFO1          100.6278589 MHz
NUC1           13C
P1              8.90 usec
PLM1          34.00000050 W
-----
CHANNEL f2
SFO2          400.1516006 MHz
NUC2           1H
PCPRG2         waltz16
P2              12.64800000 usec
PLW2           12.00000000 W
PLW12          0.32231000 W
PLW13          0.16212000 W

F2 - Processing parameters
-----
SF              100.6177889 MHz
WDW             HANN
SSB             0
GB              0
PC              1.00

```

[illegible]

```

Current Data Parameters
Name      Dr. A MAJEE 2022
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20220523
Time      12.41
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zgpg30
TD         32768
SOLVENT    CDCl3
NS          8
DS          1
SWH         8223.65 Hz
FIDRES      0.250967 Hz
AQ          1.9922944 sec
RG          148.91
DE          60.800 usec
TE          6.50 usec
DQ          295.6 K
TD0         1.0000000 sec
D1          1
D2          1

CHANNEL f1
SF01       400.1527411 MHz
P1          1.47 usec
PLW1       12.0000000 W

F2 - Processing parameters
SI          1
SF          16384
AQ          400.149665 MHz
RG          EM
SSB         0
LB          0.30 Hz
PC          0
GB          0
PC          0
DQ          2.00

```

Chemical Structure of 4ah:

O=C1C(=O)c2ccccc2C1c3c[nH]c4ccccc34Sc5ccc(Cl)cc5

13C NMR Peak List (ppm):

- 185.25
- 184.64
- 143.92
- 138.75
- 138.57
- 138.50
- 133.78
- 133.45
- 132.81
- 132.43
- 130.99
- 129.86
- 129.82
- 129.53
- 127.30
- 126.95
- 126.16
- 123.94
- 123.44
- 120.14
- 117.20
- 110.41
- 77.48
- 77.16
- 76.84

Current Data File Information:

NAME	EXPNO	PROCNO
F2 - Acquisition		
Date_		
Time		
INSTRUM		
PROBHD	5 mm	
PULPROG		
TD		
SOLVENT		
NS		
DS		
SWH		
FIDRES		
AQ		
RG		
DW		
DE		
TE		
D1	2	
D11	0	
TD0		

Channel List:

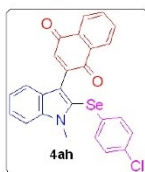
NAME	CHAN
SFO1	10
NUC1	
F1	
PLW1	54

Channel List (continued):

NAME	CHAN
SFO2	40
NUC2	
CPDPRG2	
PCPD2	
PLW2	12
PLW12	0
PLW13	0

F2 - Processing:

NAME	VALUE
SI	10
SF	
WDW	
SSB	0
LB	
GB	0
PC	



```

Name Data Parameters
Current Dr. A. MAJER 2022
EXPNO 1 233
PROCNO 1

F2 - Acquisition Parameters
Time 20250223
Date_ 14.07
INSTRUM spect
PROBHD 5 mm PABBO-BB1
PULPROG zgpg30
PCPDPRG2 waltz16
TD 658
TO SOLVENT CDCl3
NS 512
DS 2
SWH 24038.461 Hz
FIDRES 0.735556 Hz
AQ 0.6815744 sec
RG 148.91
DQ 26.600 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
D11 0.30000000 sec
D12 1
TD0 1

===== CHANNEL f1 =====
NUC1 100.627858 MHz
P1 13C
PL1 1
PLW1 54.00000000 W

===== CHANNEL f2 =====
SPR 400.151601 MHz
RUC2 1
PCPDPRG2 waltz16
PCPDPRG1 waltz16
PLW2 12.00000000 W
PLW1 0.32331000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.6177829 MHz
WDW 0
SSB 0
GB 0
LB 0
GB 0
TC 1.00

```

8.194
8.189
8.182
8.175
8.172
8.162
8.142
8.135
8.130
8.120
7.775
7.769
7.768
7.768
7.634
7.614
7.596
7.535
7.535
7.370
7.353
7.344
7.333
7.286
7.266
7.259
7.241
7.241
7.175
7.154
7.137

— 3.786

8.194
8.189
8.182
8.175
8.172
8.162
8.142
8.135
8.130
8.120
7.775
7.769
7.768
7.768
7.634
7.614
7.596
7.535
7.535
7.370
7.353
7.344
7.333
7.286
7.266
7.259
7.241
7.241
7.175
7.154
7.137

1.00
1.00
2.03
1.03
1.03
1.03
1.03
1.03
1.03
1.03
1.03
1.02

3.00

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

4a1

Current Data
NAME
EXPNO
PROCNO

F2 - Acquisition
Date
Time
INSTRUM
PROBHD 5
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
TD0

SF01
NUC1
P1
PLW1

F2 - Processing
SI
SF
WDW
SSB
LB
GB
PC



```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO      206
PROCNO     1
```

```

F2 - Acquisition Parameters
Date      20220423
Time      12.41
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         1.9222944 sec
RG         186.42
DW         60.800 usec
DE         6.50 usec
TE         299.8 K
D1         1.00000000 sec
TD0        1

```

```

000 000 000 000 000 000 CHANNEL f1 000 000 000 000 000 000
SF01      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
```

Chemical structure of **4al** is shown in the inset:

c1ccc(cc1)-c2nc3ccccc3n2-c4cc(=O)c5ccccc45

The ¹³C NMR spectrum displays the following chemical shifts (ppm):

- 185.19
- 184.54
- 143.82
- 138.80
- 136.67
- 133.91
- 133.79
- 132.79
- 132.76
- 132.39
- 132.04
- 131.72
- 131.10
- 129.81
- 129.30
- 126.95
- 126.16
- 126.03
- 125.00
- 124.09
- 123.83
- 123.79
- 123.75
- 123.22
- 121.48
- 120.14
- 117.49
- 110.47
- 77.47
- 77.15
- 76.03



```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO      207
PROCNO     1
```

```

F2 - Acquisition Parameters
Date_      20220423
Time       14:31
INSTRUM    spect
PROBHD      5 mm PARBO BB/
PULPROG     zgpg30
TD          32768
SOLVENT     CDCl3
NS          1024
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          299.4 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
```

```

SFO2      400.1516006 MHz
NUC2      1H
CPDPRG1[2  waltz16
PCPD2     90.00 usec
PLW2      12.00000000 W
PLW12     0.32231000 W
PLW13     0.16212000 W

```

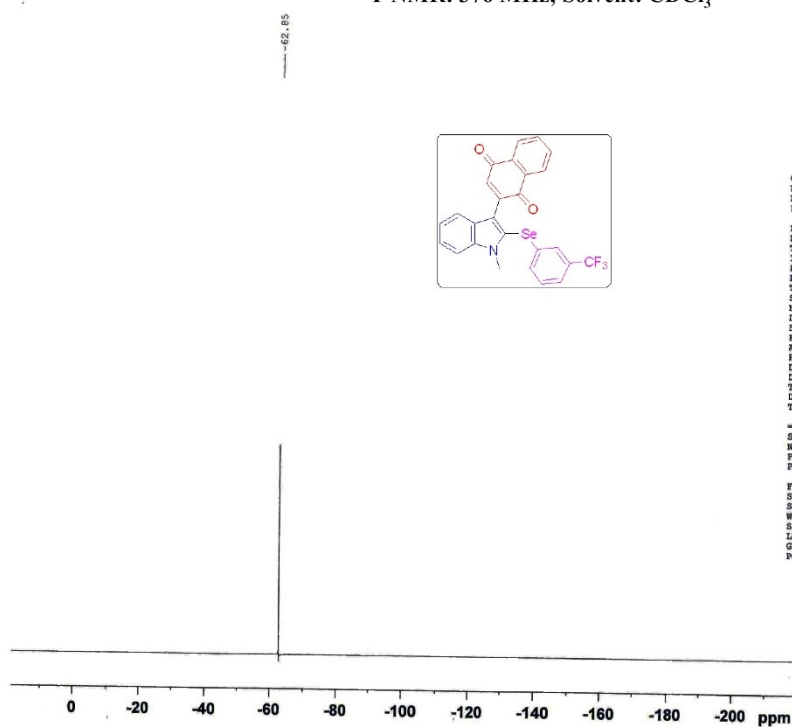
```

F2 - Processing parameters
SI                16384
SF                100.6177843 MHz
WDW               EM
SSB              0
LB                1.00 Hz
GB              0
PC                1.00

```

F19 1H coupled of VBSP-249/16

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



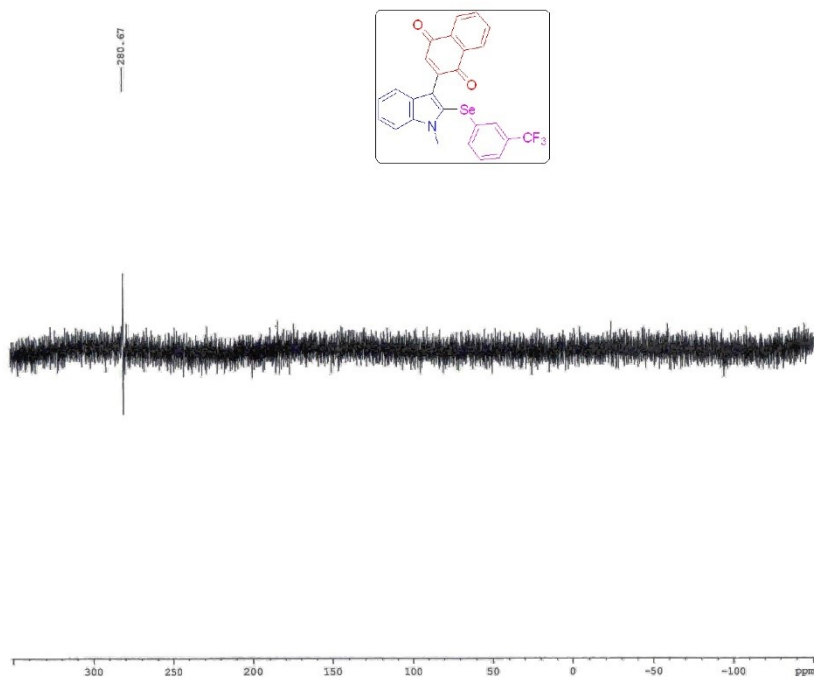
Current Data Parameters
NAME Dr. A MAJES 2022
EXPNO 201
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220422
Time 13.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl_3
NS 2
DS 4
SWH 89285.711 Hz
FIDRES 2.724784 Hz
AQ 0.1833008 sec
RG 186.42
DW 5.600 usec
DE 6.50 usec
TE 301.5 K
D1 1.00000000 sec
TDO 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

^{77}Se of VBSP_249/16 ^{77}Se NMR: 76 MHz; Solvent: CDCl_3



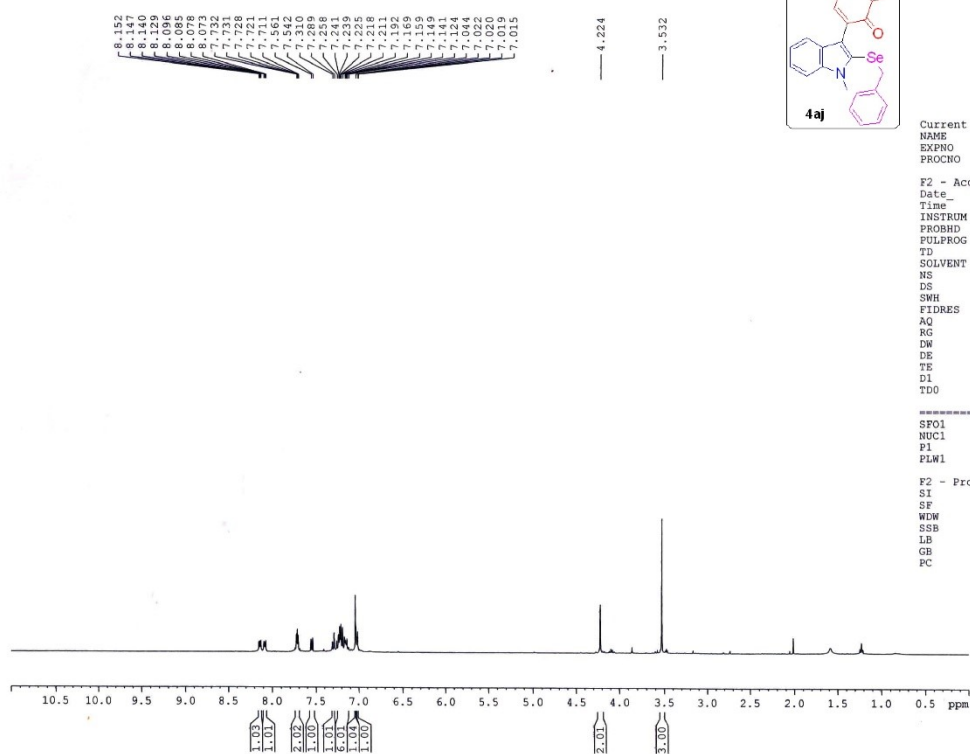
Current Data Parameters
NAME Dr. A MAJES 2022
EXPNO 200
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220422
Time 13.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl_3
NS 480
DS 4
SWH 38265.305 Hz
FIDRES 1.167764 Hz
AQ 0.4528185 sec
RG 168.31
DW 13.007 usec
DE 6.50 usec
TE 301.4 K
D1 2.00000000 sec
TDO 1

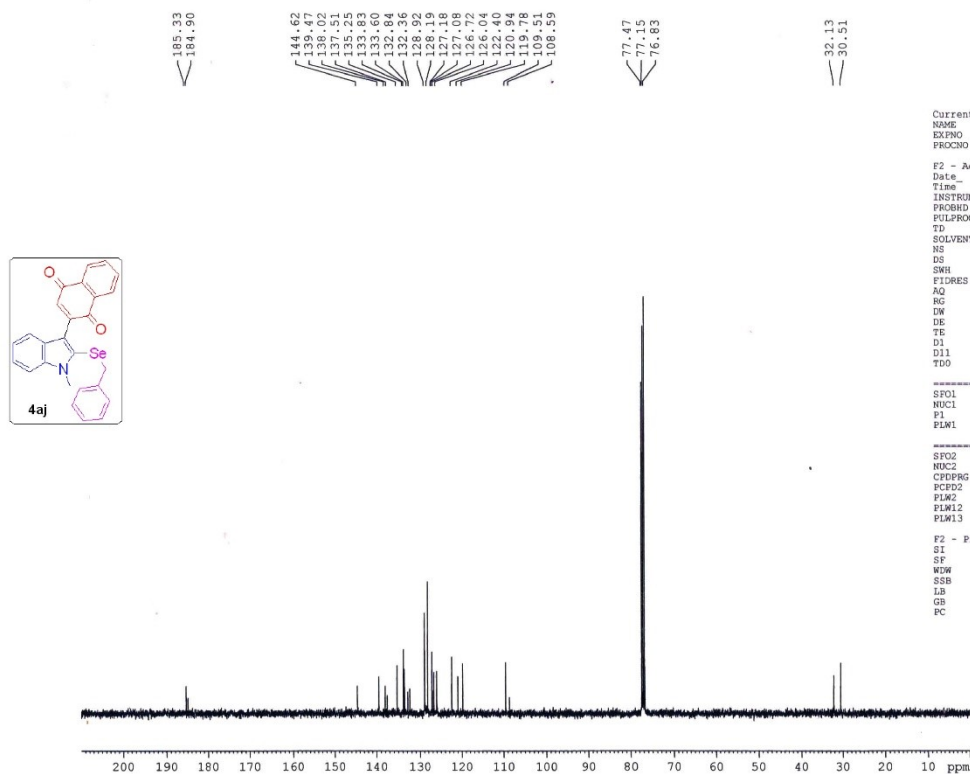
===== CHANNEL f1 =====
SFO1 76.3222905 MHz
NUC1 77Se
P1 9.00 usec
PLW1 60.00000000 W

F2 - Processing parameters
SI 16384
SF 76.3146590 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

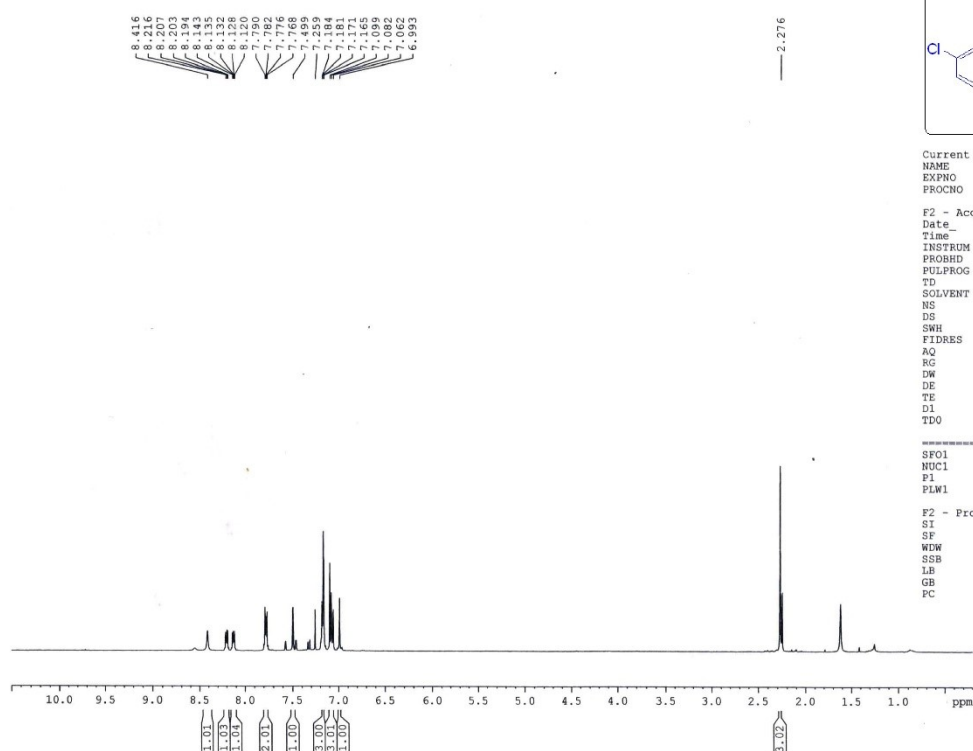
¹H NMR: 400 MHz; Solvent: CDCl₃



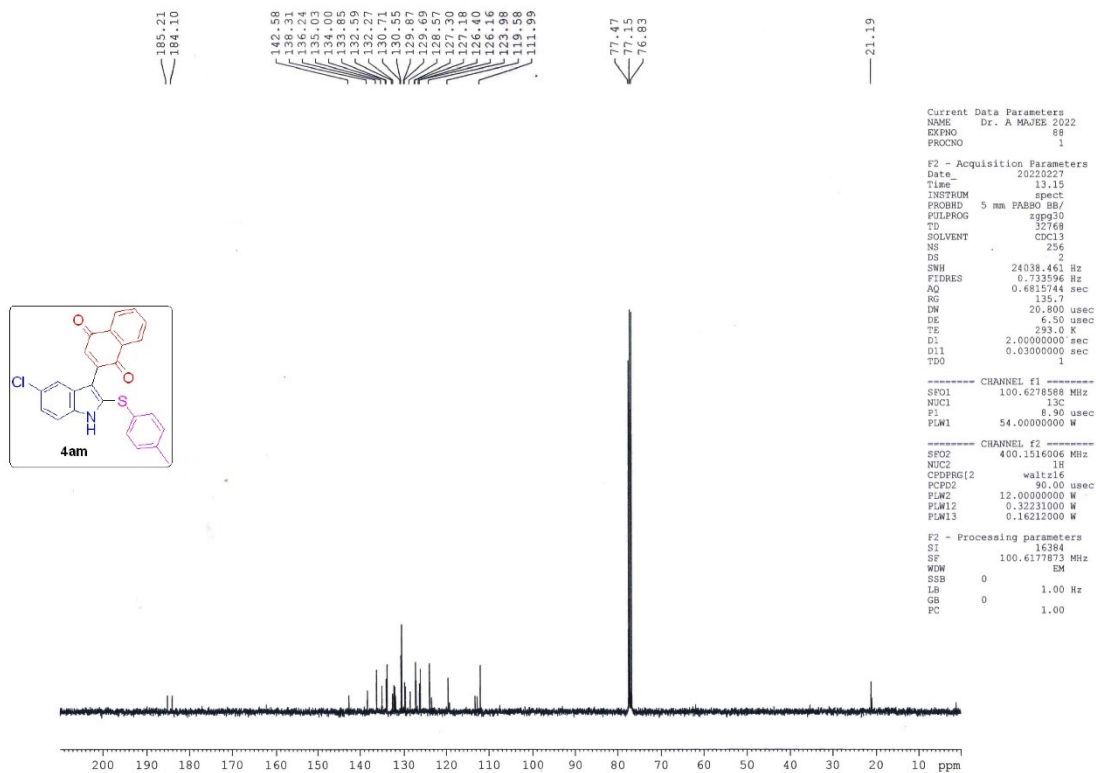
¹³C{¹H} NMR: 100 MHz; Solvent: CDCl₃

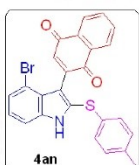
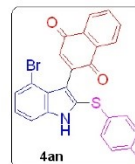


¹H NMR: 400 MHz; Solvent: CDCl₃



¹³C{¹H} NMR: 100 MHz; Solvent: CDCl₃





¹H NMR: 400 MHz; Solvent: CDCl₃



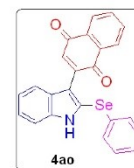
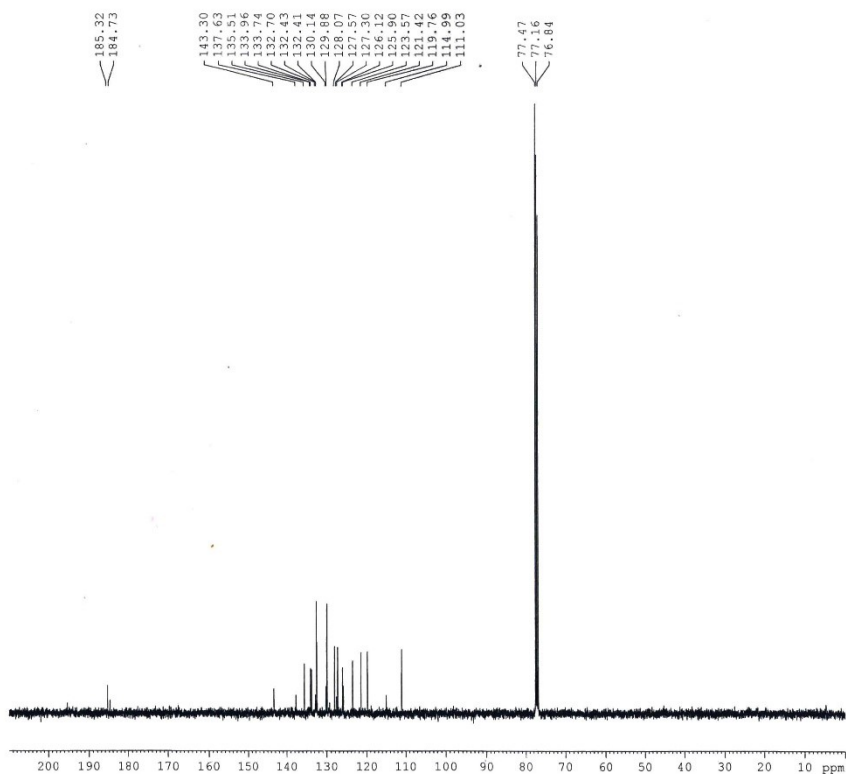
Current Data Parameters
NAME Dr. A MAJEE 2023
EXPNO 131
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230226
Time 14.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 8
DS 1
SWH 8223.693 Hz
FIDRES 0.230967 Hz
AQ 1.9922944 sec
RG 186.42
DW 60.800 us
DE 6.50 us
TE 294.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1524711 MHz
NUC1 1H
P1 14.75 us
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{¹H} NMR: 100 MHz; Solvent: CDCl₃



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

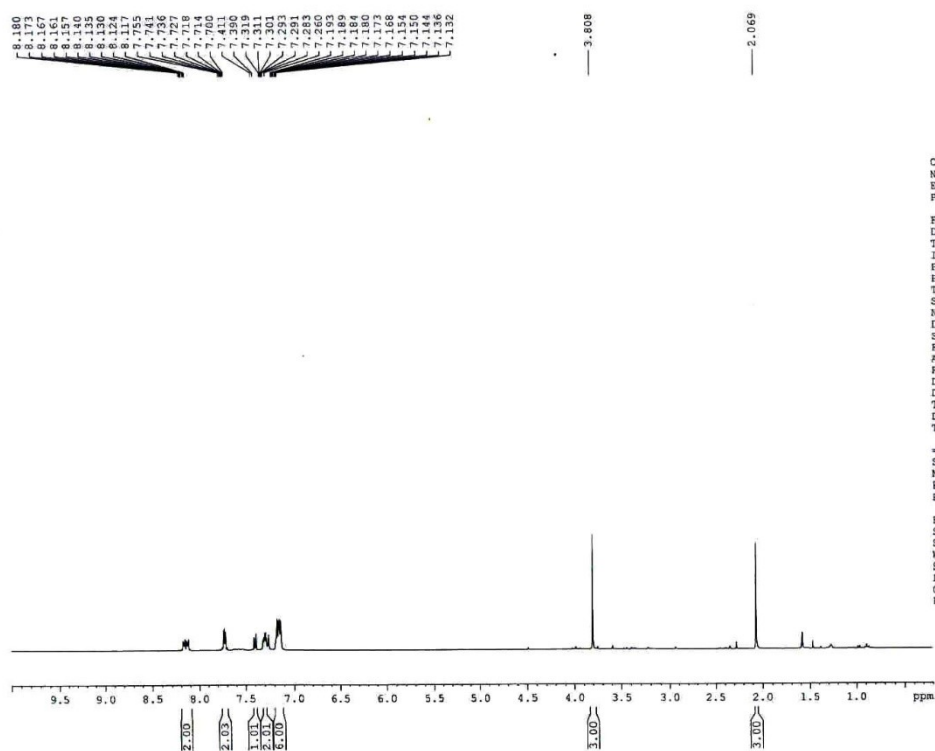
F2 - Acquisition Parameters
Date_ 20230226
Time 15.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl₃
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 186.42
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6278588 MHz
NUC1 13C
P1 9.90 usec
PLW1 54.00000000 W

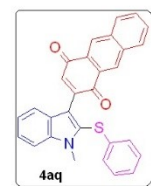
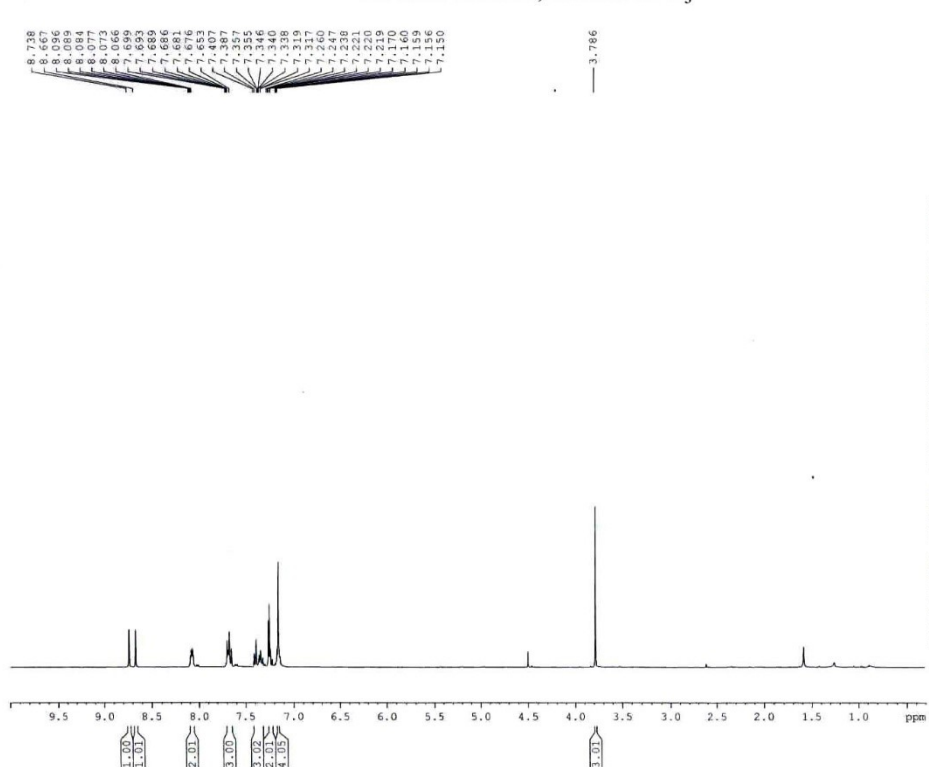
===== CHANNEL f2 =====
SF02 400.1516006 MHz
NUC2 1H
CPCPRG2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

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

¹H NMR: 400 MHz; Solvent: CDCl₃



¹H NMR: 400 MHz; Solvent: CDCl₃



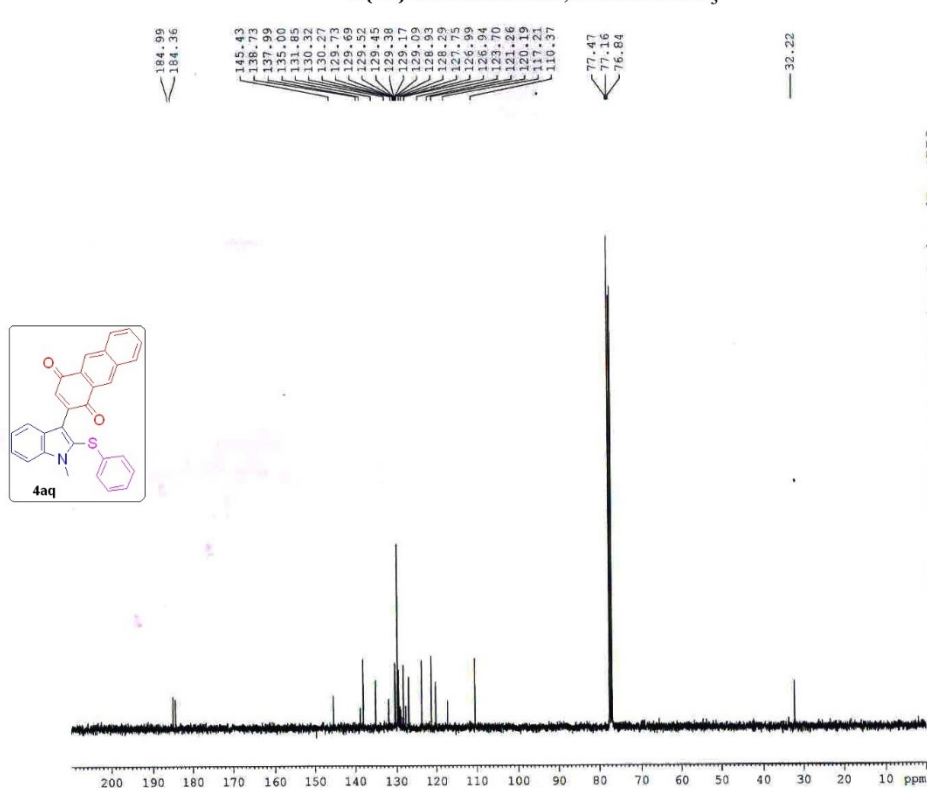
Current Data Parameters
NAME Dr. A MAJEE 2023
EXPNO 122
PROCNO 1

F2 - Acquisition Parameters
Date 20230222
Time 16.24
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 295.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 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

¹³C{¹H} NMR: 100 MHz; Solvent: CDCl₃



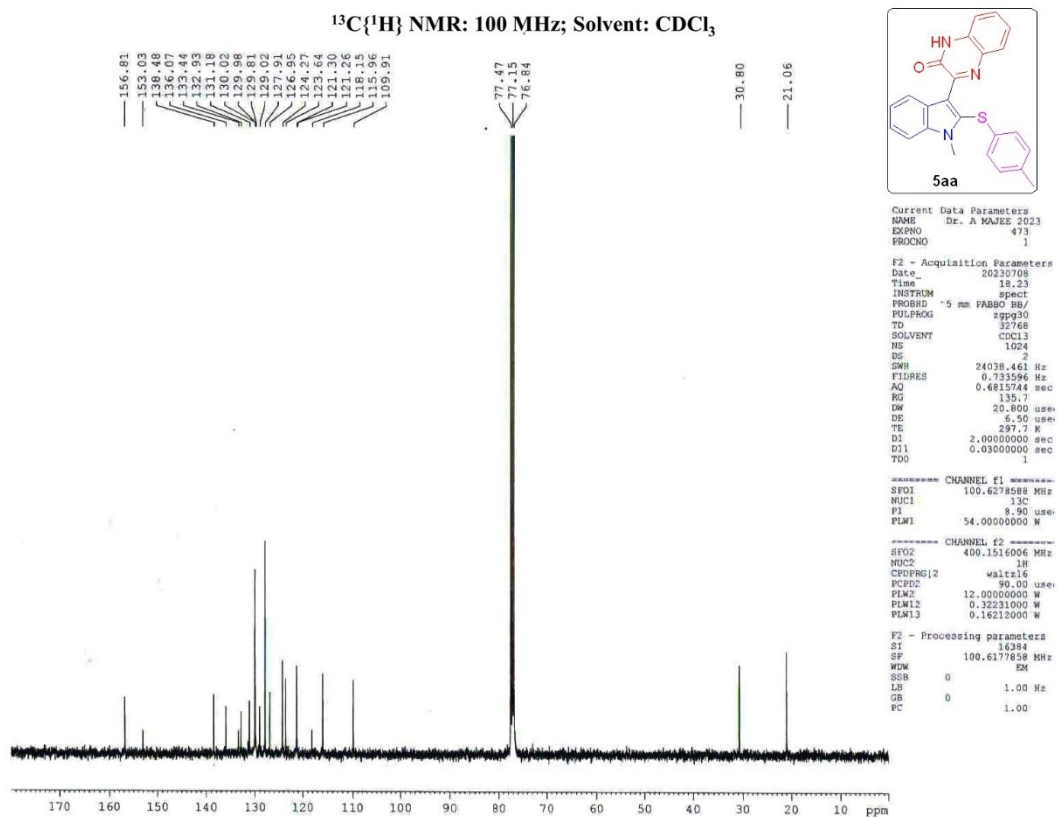
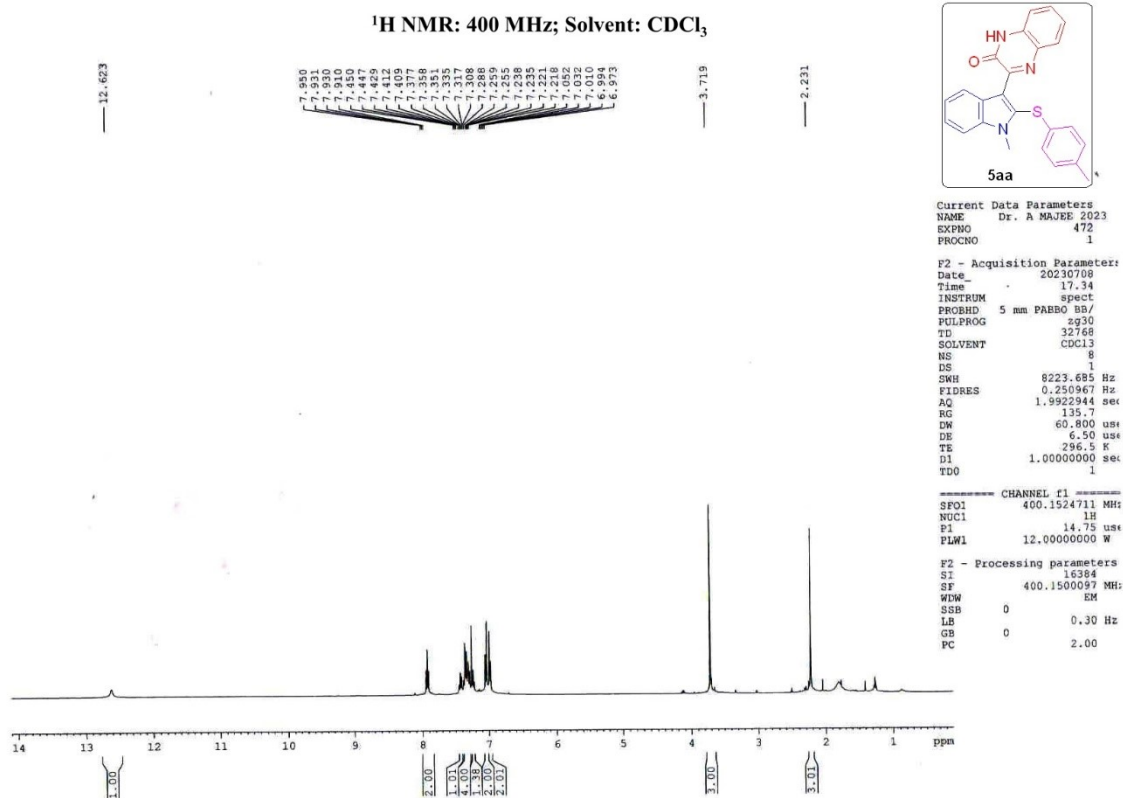
Current Data Parameters
NAME Dr. A MAJEE 2023
EXPNO 123
PROCNO 1

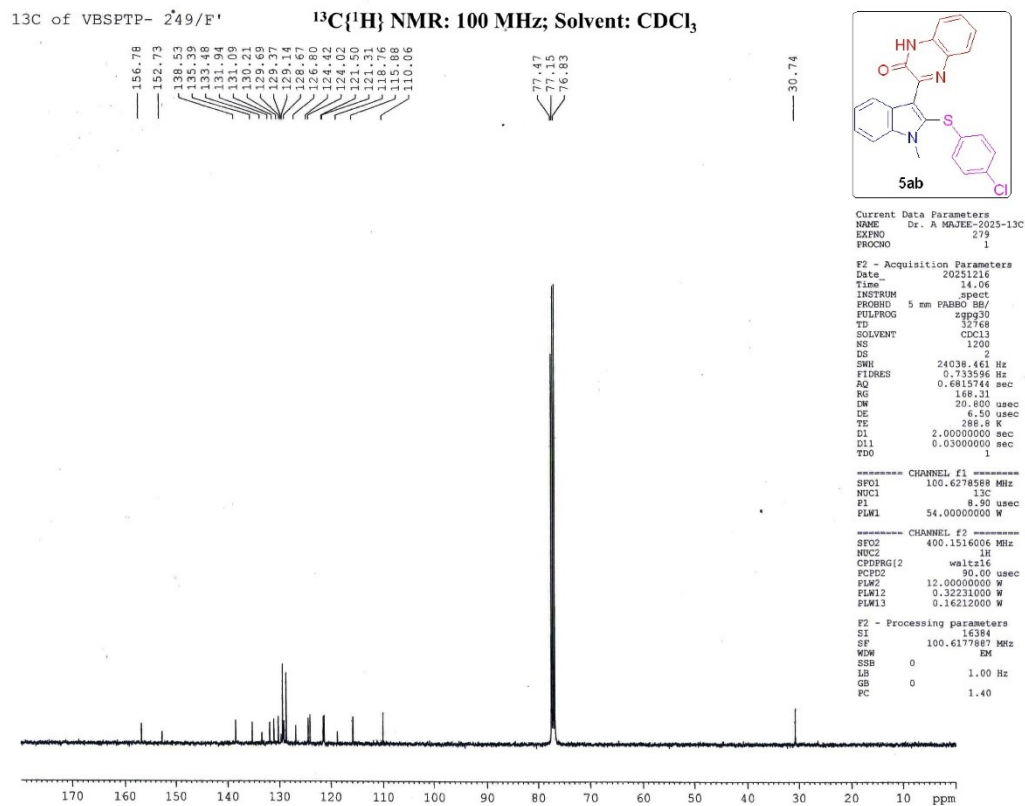
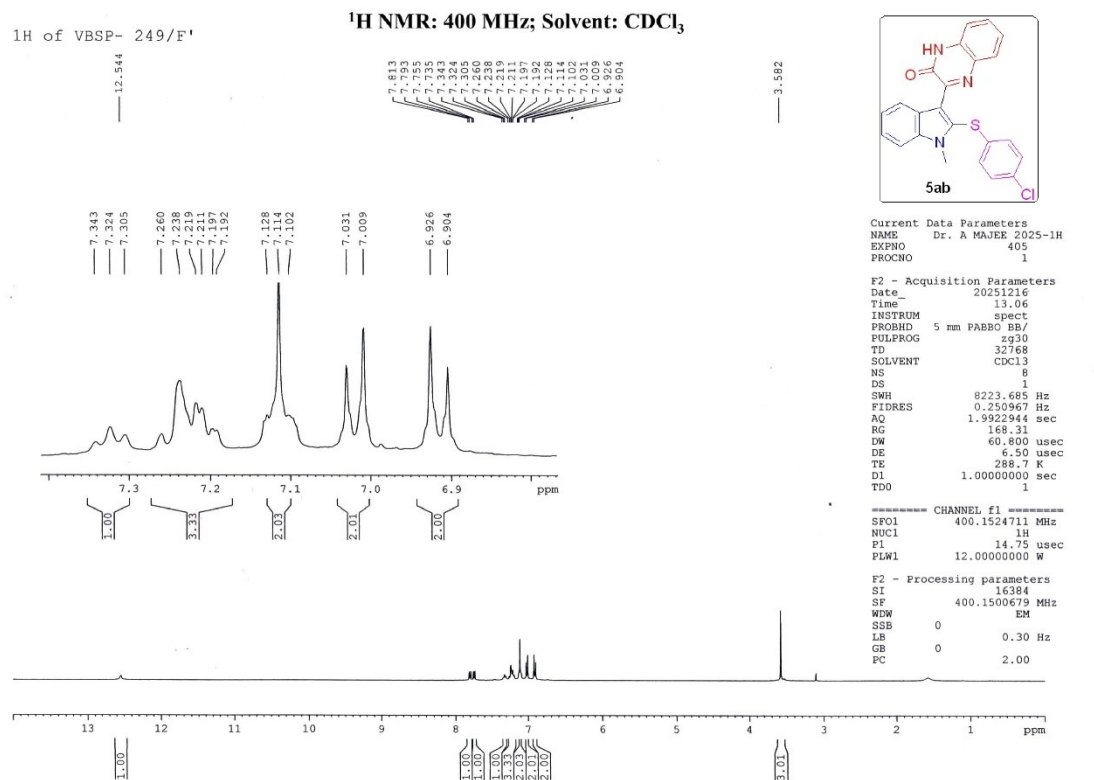
F2 - Acquisition Parameters
Date 20230222
Time 16.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 320
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 120.16
DW 20.850 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

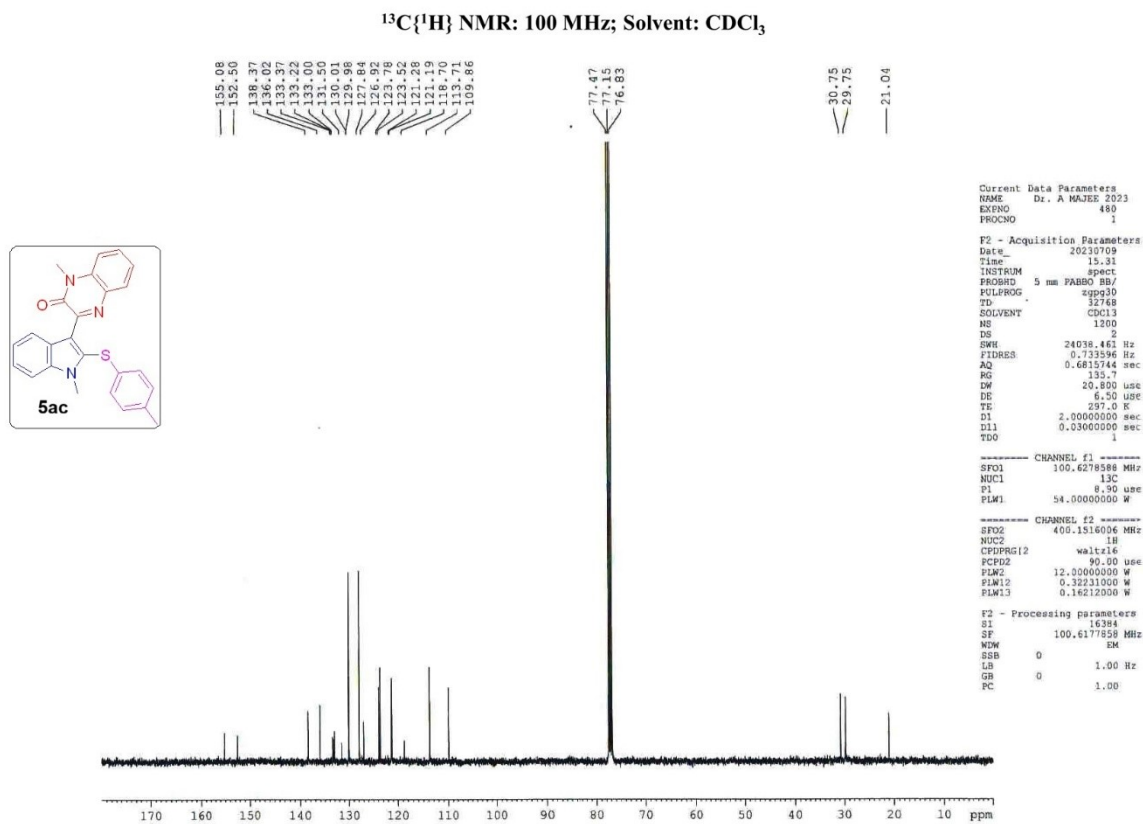
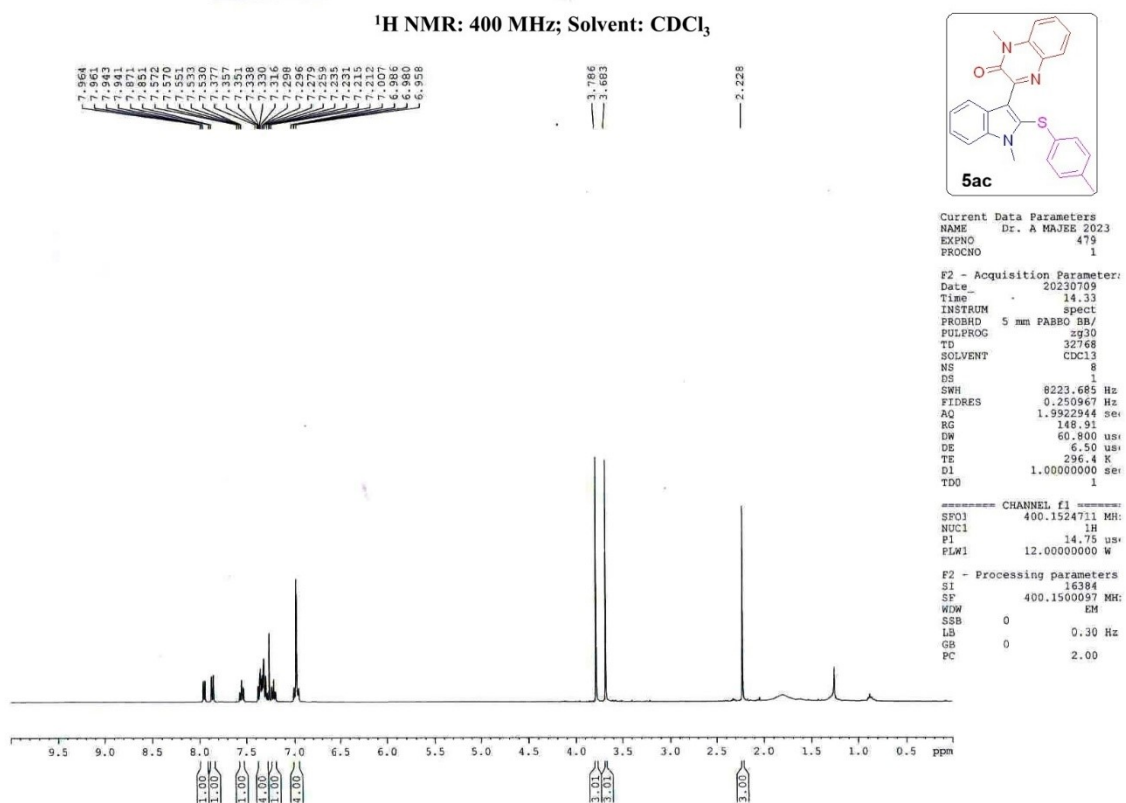
===== CHANNEL f1 =====
SF01 100.6278558 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

===== CHANNEL f2 =====
SF02 400.1516006 MHz
NUC2 1H
CPDPRG12 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

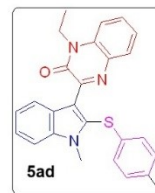
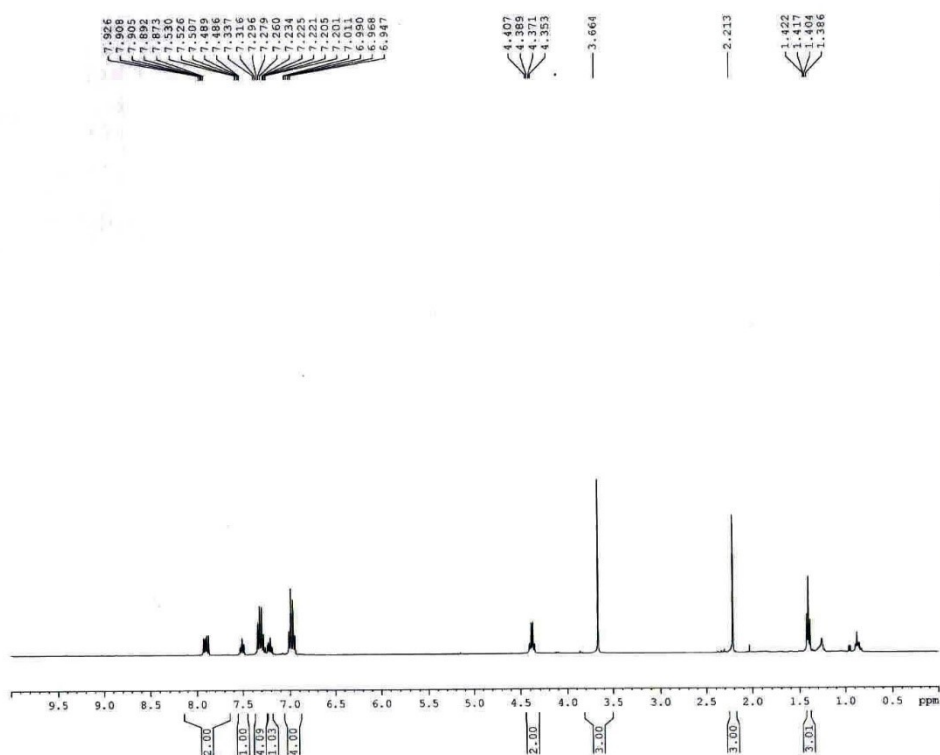
F2 - Processing parameters
SI 16384
SF 100.6177858 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00







¹H NMR: 400 MHz; Solvent: CDCl₃



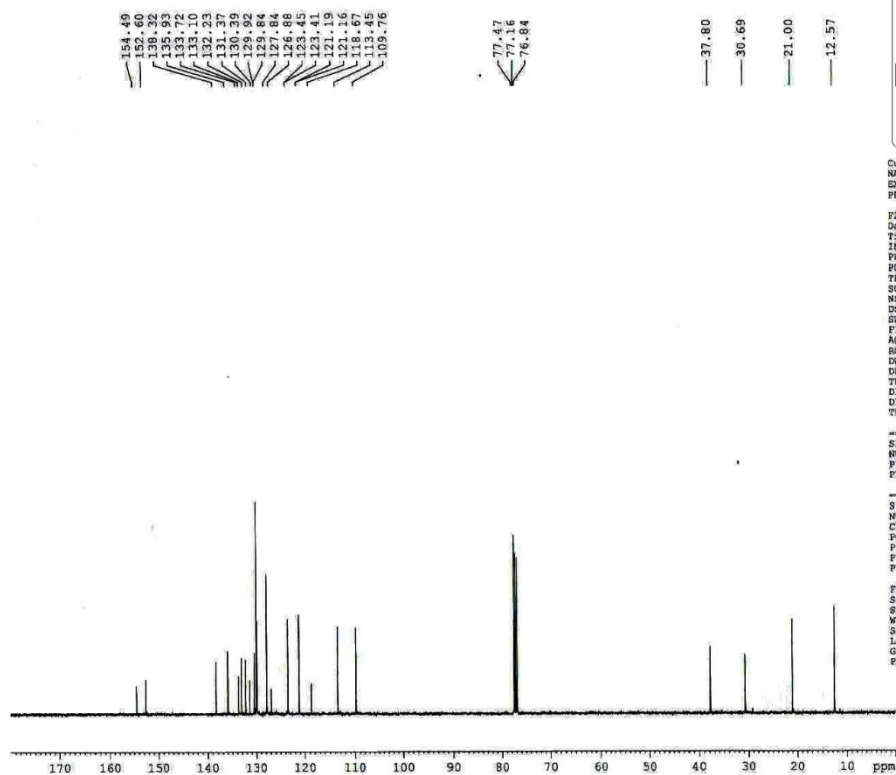
Current Data Parameters
NAME Dr. A MAJER 2023
EXPNO 490
PROCNO 1

F2 - Acquisition Parameters
Date 20230712
Time 15.17
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 s
RG 34.07
DW 60.800 us
DE 6.50 us
TE 297.3 K
D1 1.00000000 s
TDO 1

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

F2 - Processing parameters
SI 16384
SF 400.1500197 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

¹³C{¹H} NMR: 100 MHz; Solvent: CDCl₃



Current Data Parameters
NAME Dr. A MAJER 2023
EXPNO 491
PROCNO 1

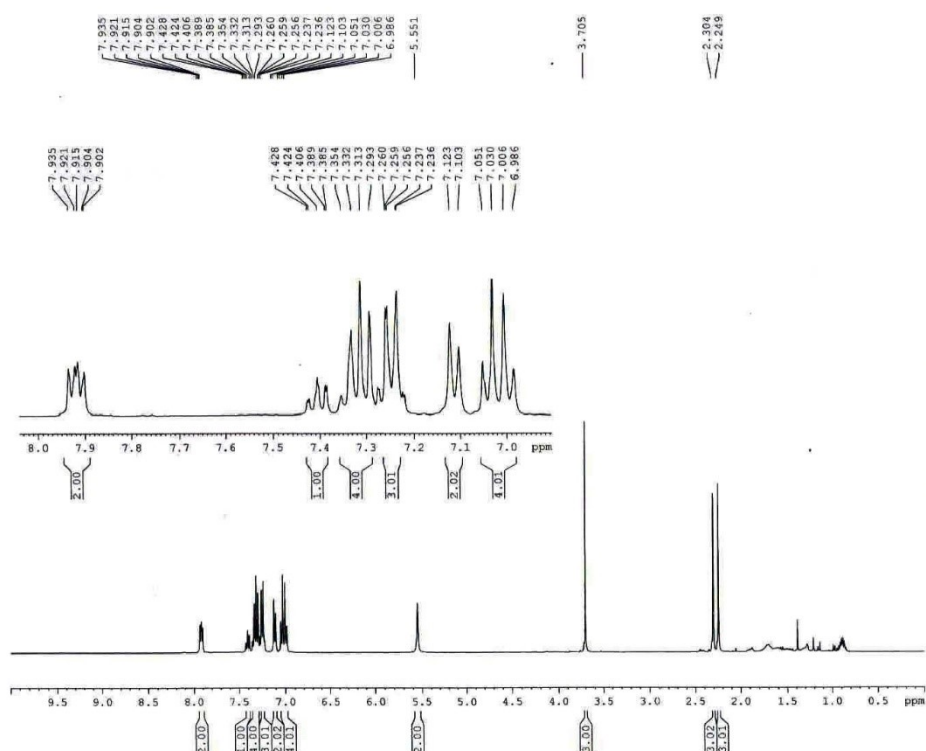
F2 - Acquisition Parameters
Date 20230712
Time 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 380
DS 2
SWH 24038.461 Hz
FIDRES 0.733996 Hz
AQ 0.6915744 sec
RG 34.07
DW 20.860 us
DE 6.50 us
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

CHANNEL f1
SFO1 100.6278988 MHz
NUC1 13C
P1 8.90 us
PLW1 54.00000000 W

CHANNEL f2
SFO2 400.1516096 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 us
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.6177817 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

5ae



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

```

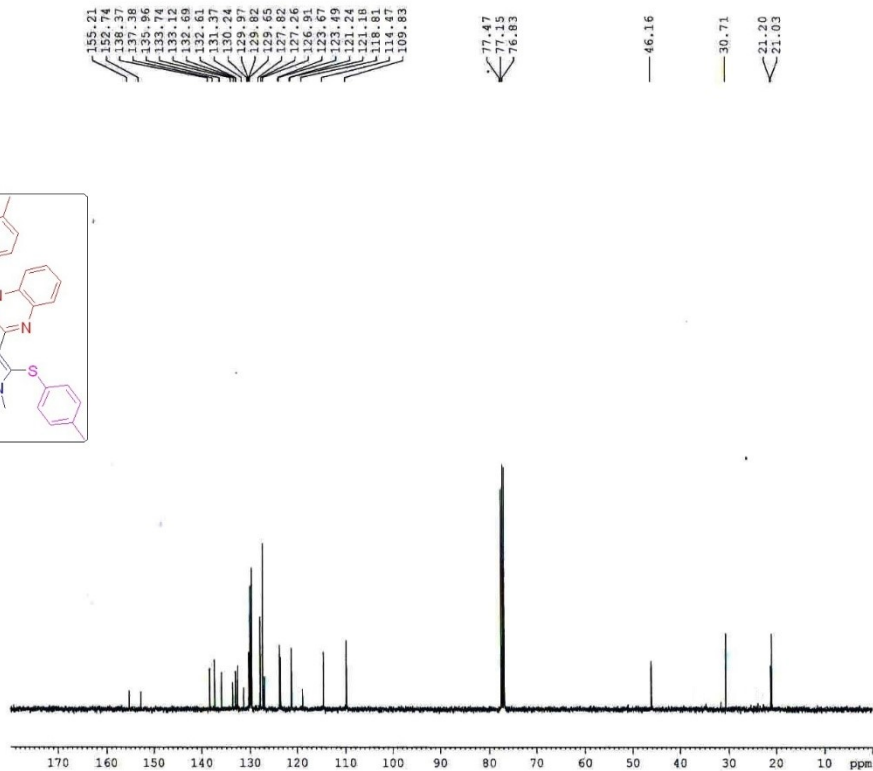
F2 - Acquisition Parameters
Date_      20230730
Time       13.43
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zg30
TD          32768
SOLVENT    CDCl3
NS          6
DS          1
SWH         8223.685 Hz
FIDRES     2.50947 Hz
AQ          1.992294 sec
RG          67.81
DW          60.800 usec
DE          6.50 usec
TE          298.5 K
D0          1.00000000 sec
TD0         1

```

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

```
F2 - Processing parameters
S1                      16384
SF                      400.1500097 MHz
WDW                      EM
SSB      0
LB                      0.30 Hz
GB      0
PC                      2.00
```

5ae



```
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
DE            20.800 usec
DW             6.50 usec
TE            298.2 K
D1            2.00000000
D11           0.03000000 sec
TD0            1

```

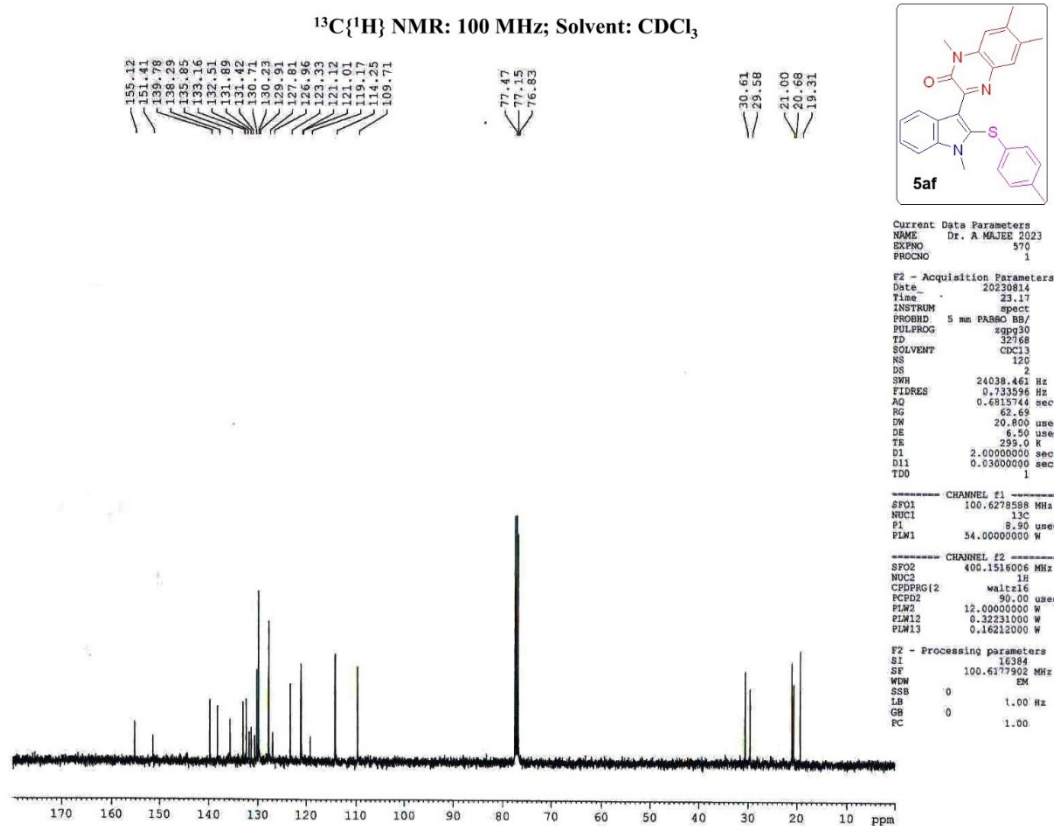
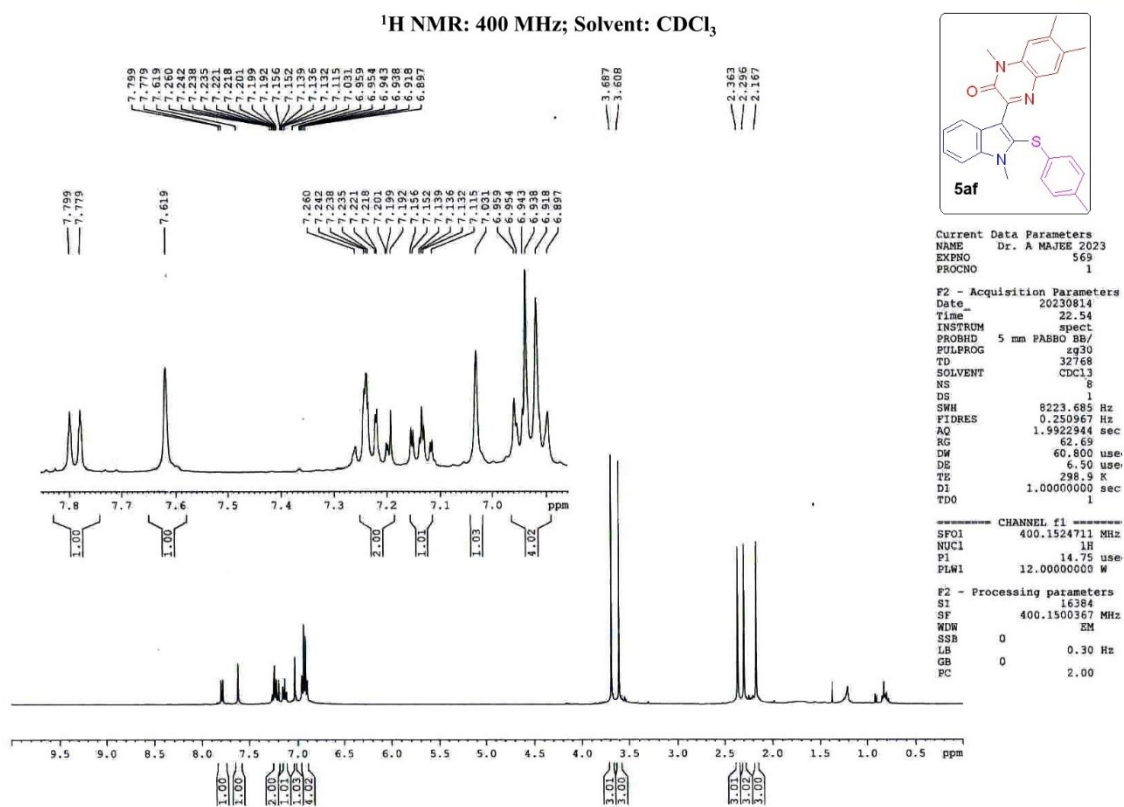
```
----- CHANNEL f1 -----
SF01      100.6278580 MHz
NUC1      13C
P1         8.90 usec
PLW1      54.00000000 W
```

```

----- CHANNEL f2 -----
SFO2      400.1516006 MHz
NUC2      1H
CPDPRG12  wait316
PCPD2     90.00 usec
PLW2      12.00000000 W
PLW12     0.32231000 W
PLW13     0.16212000 W

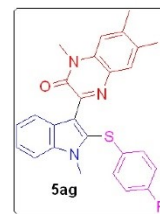
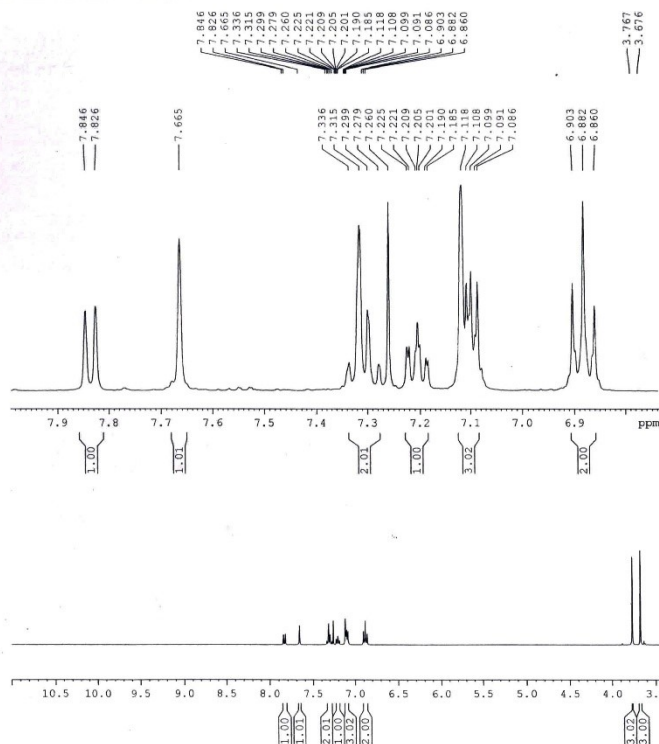
```

```
F2 - Processing parameters
S1                16384
SF                100.6177887 MHz
WDW               EM
SSB               0
LB                1.00 Hz
GB               0
PC                1.00
```



¹H of VBSPTP- 249/B'

¹H NMR: 400 MHz; Solvent: CDCl₃



Current Data Parameters
NAME Dr. A MAJEE 2025-1H
EXPNO 398
PROCNO 1

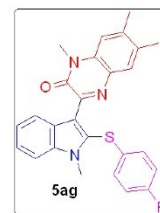
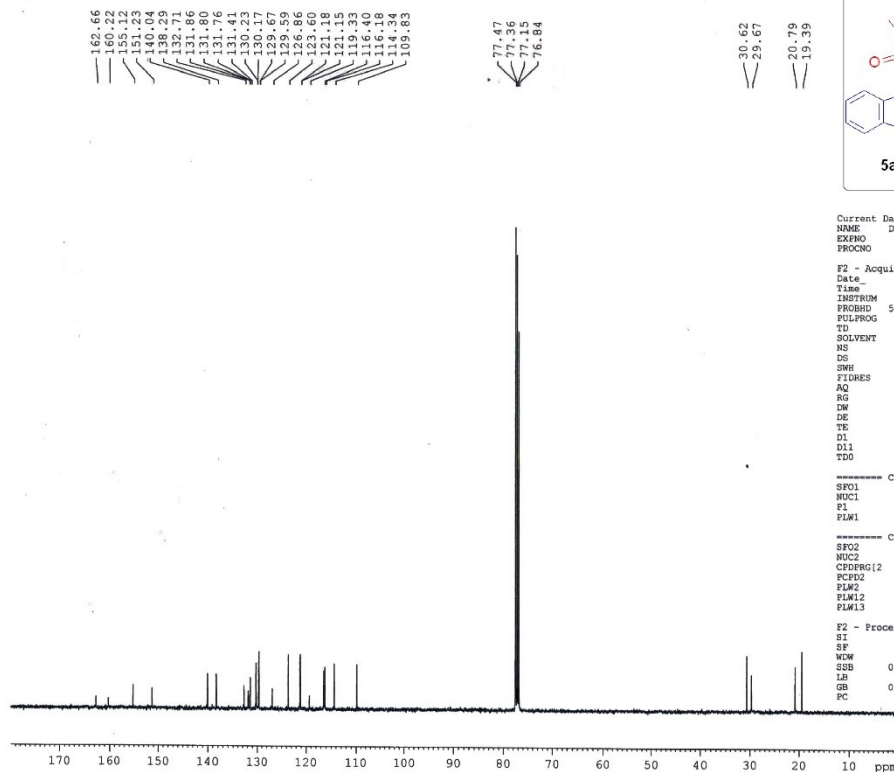
F2 - Acquisition Parameters
Date 20251208
Time 21.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 3
DS 1
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 93.46
DW 60.800 usec
DE 6.50 usec
TE 288.2 K
D1 1.00000000 sec
TDO 1

CHANNEL f1
SF01 400.1524711 MHz
NUC1 1H
P1 14.75 usec
PLW1 12.00000000 W

F2 - Processing parameters
S1 16384
SF 400.1500097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

¹³C of VBSPTP- 249/B'

¹³C{¹H} NMR: 100 MHz; Solvent: CDCl₃



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 0.6813744 sec
RG 93.46
DW 20.800 usec
DE 6.50 usec
TE 290.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

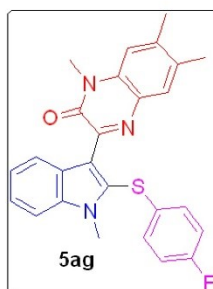
CHANNEL f1
SF01 100.6278588 MHz
NUC1 13C
P1 8.50 usec
PLW1 54.00000000 W

CHANNEL f2
SF02 400.1516006 MHz
NUC2 1H
CHPRG12 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

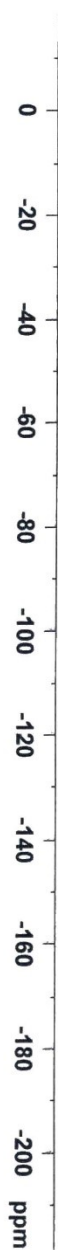
F2 - Processing parameters
S1 16384
SF 100.6177887 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

F19 1H coupled VBSPTP- 249/B'

-116.20



Solvent: CDCl₃



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

F2 - Acquisition Parameters
Date_ 20251208
Time_ 23.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
DS 16
SWH 89285.711 Hz
FIDRES 2.724784 Hz
AQ 0.1835008 sec
RG 93.46
DM 5.600 usec
DE 6.50 usec
TE 289.9 K
D1 1.00000000 sec
TD0 1

CHANNEL f1
SFO1 376.475333 MHz
NUC1 19F
P1 12.50 usec
PLM1 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

Cur: 3.789

NAME
EXP
PROC

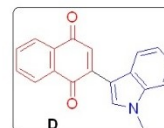
F2 -
Date:
Time:
INST:
PROB:
FULP:
TD:
SOLV:
MS
DS
SWH
FIDR:
AQ
RG
DW
DE
TE
D1
TDO

SPOL
NUC1
P1
PLW1

F2 -
S1
SF
WDW
SSB
LA
GB
PC

8.064
8.052
8.046
8.033
8.020
8.018
8.014
8.010
7.995
7.989
7.959
7.954
7.952
7.944
7.936
7.935
7.930
7.917
7.914
7.900
7.886
7.860
7.845
7.842
7.828
7.822
7.807
7.803
7.789
7.769
7.760
7.743
7.723

0.08
1.02
1.02
0.03
0.08
1.08
0.04
0.07
1.00



```

Current Data Parameters
Name      Dr. A MOJEE 2021
EXPNO     387
PROCNO    1
F2 - Acquisition Parameters
Date_     20211212
Time      10.40
INSTRUM    spect
PROBHD     5 mm PABBO BBO
PULPROG    zg30
TD         32768
SOLVENT     CDCl3
NS         8
DS         1
SWH         8223.65 Hz
FIDRES     0.250967 Hz
AQ         1.9999944 sec
RG         168.31
DE         60.800 usec
DU         6.50 usec
TE         295.0 K
D0         1.00000000 sec
T1         1
===== CHANNEL f1 =====
SF01       400.1527411 MHz
NUC1       1H
P1         14.75 usec
PLM1       12.00000000 W
F2 - Processing parameters
S1         S1      16384
SF         400.150453 MHz
WDW        EM
SSB         0
GB         0.30 Hz
LR         0
GB         0      2.00

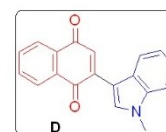
```

185.94
185.33
142.01
138.09
137.52
137.21
136.81
133.81
133.29
132.40
129.63
128.78
126.94
126.54
123.13
122.13
121.89
120.75
110.31
107.48
77.47
77.15
76.83
33.61

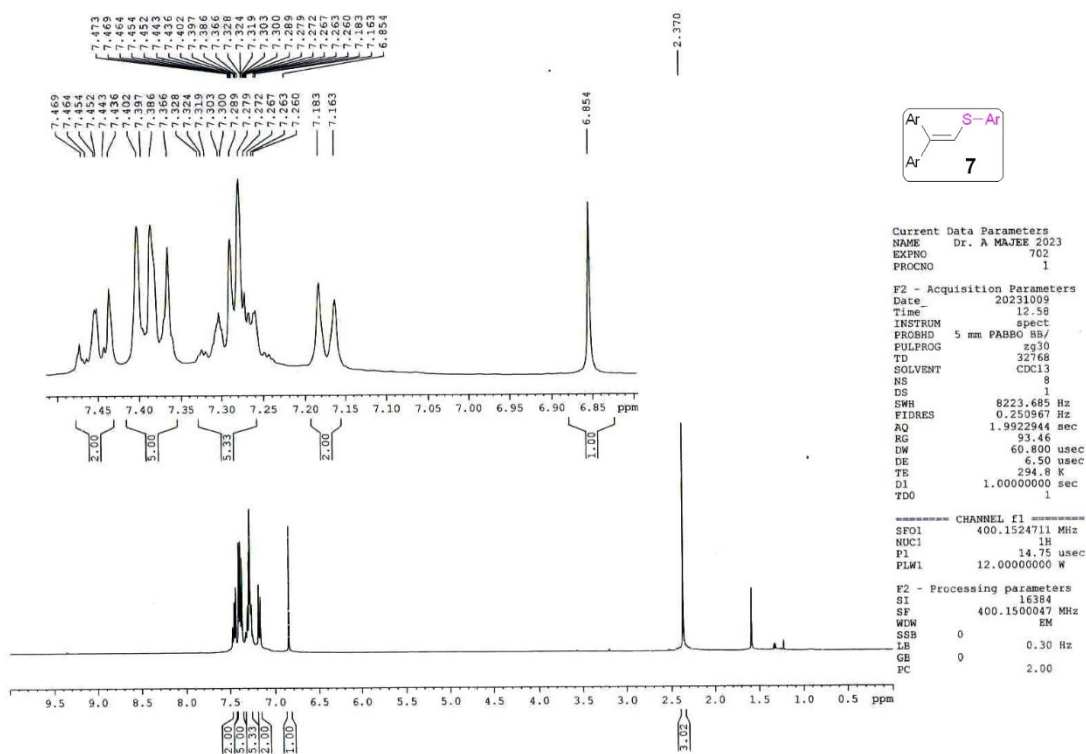
Current
NAME
EXPNO
PROCNO
F2 - Ac
Date_
Time_
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
RG
JW
DE
TE
D1
D11
TDO

SF01
NUC1
P1
PLM1

SF02
NUC2
CFPRG1
PCPS2
PLM2
PLM12
PLM13
F2 - P1
SI
SF
WDW
SSB
LB
GB
PC

[illegible]

¹H NMR: 400 MHz; Solvent: CDCl₃



¹³C{¹H} NMR: 100 MHz; Solvent: CDCl₃

