Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

Iodine(III)-Promoted Oxidative Carbotrifluoromethylation of Maleimides with Imidazopyridines and Langlois' Reagent

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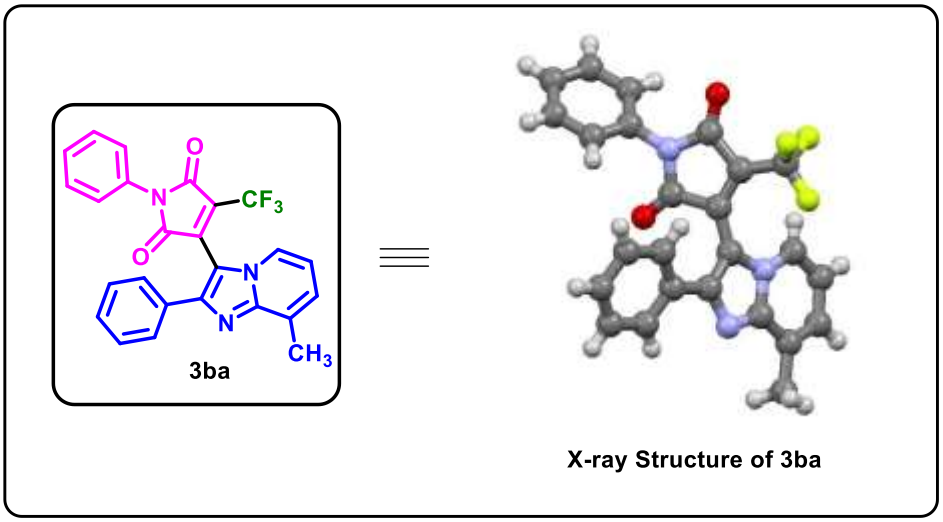
1. General information:

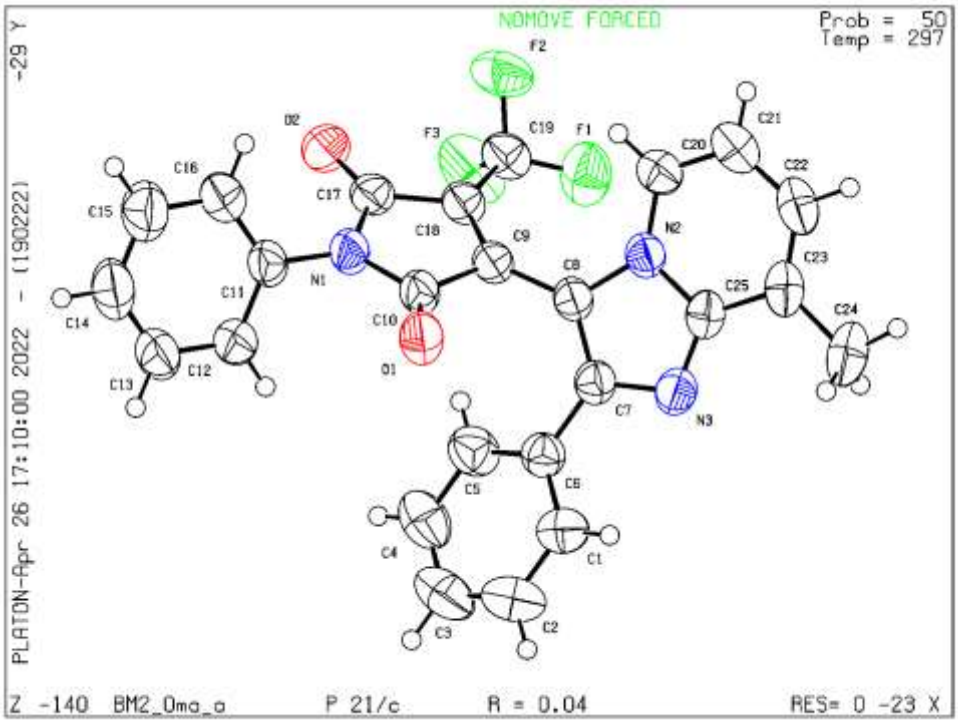
All reagents were purchased from commercial sources and used without further purification. ^{1}H NMR spectra were determined on a 400 MHz spectrometer as solutions in $CDCl_3$. Chemical shifts are expressed in parts per million (δ) and the signals were reported as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and coupling constants (J) were given in Hz. $^{13}C\{^{1}H\}$ NMR and ^{19}F NMR spectra were recorded at 100 MHz and at 376 MHz in $CDCl_3$ solution respectively. Chemical shifts are referenced to $CDCl_3$ (δ = 7.26 for ^{1}H and δ = 77.16 for $^{13}C\{^{1}H\}$ NMR) as internal standard. TLC was done on a silica gel-coated glass slide. All solvents were dried and distilled before use. Commercially available solvents were freshly distilled before the reaction. Melting points (M.p.) were determined after the re-crystallization of solid compounds from a solution of dichloromethane/petroleum ether (1:3). The crystallographic data for the compound **3ba** was collected by SCXRD-BRUKER D8QUEST and the crystal data was solved by APEX4 software.

Starting Materials: All the imidazopyridines (**1**)[1] and *N*-alkyl/aryl maleimides (**2**)[2] were prepared by previously reported methods.

2. Structure determination (X-ray crystallographic data for 3ba):

The brown block shaped crystal of **3ba** was obtained by crystallization from a solution in dichloromethane/petroleum ether after purification by column chromatography. The chemical formula of compound **3ba**: $C_{25}H_{16}F_3N_3O_2$.





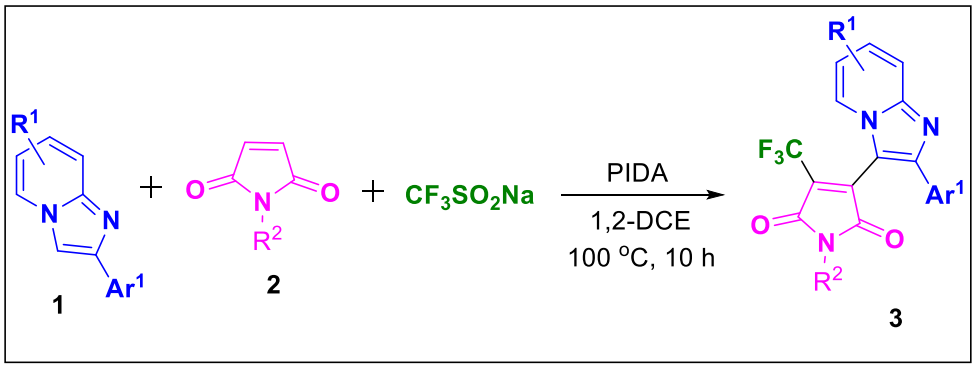
View of ORTEP diagram for the crystal structure of the compound **3-(8-Methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione** (**3ba**) (Thermal ellipsoid contour at 50% probability level).

Wavelength	0.71073Å	
Formula	$C_{25}H_{16}F_3N_3O_2$	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 11.571(4) Å	α = 90°
	b = 21.464(8) Å	β = 107.385(9)°
	c = 8.872(3) Å	γ =90°
Volume	2102.8 $Å^3$	
Z	4	

R-factor (%)	4.1

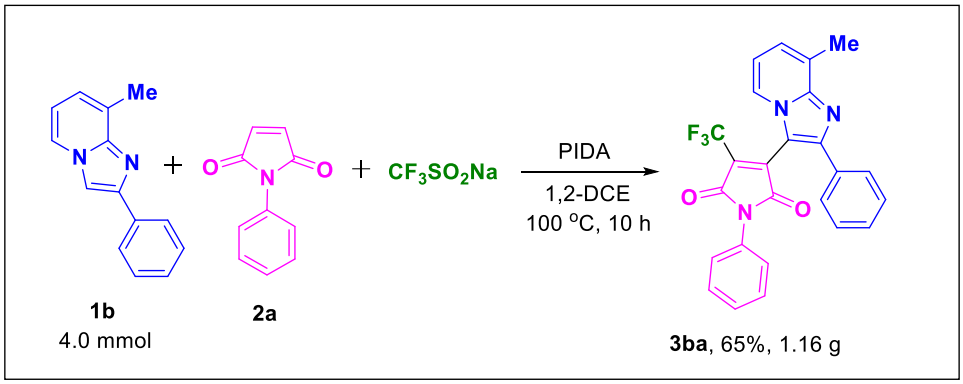
The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication with a CCDC reference number CCDC 2232229.

3. General experimental procedure for the synthesis of 3aa-3bh:



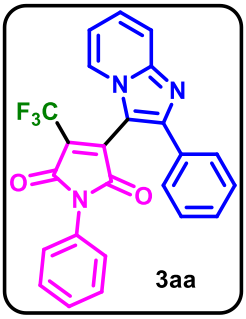
A mixture of 2-arylimidazo[1,2-*a*]pyridine (0.2 mmol) (**1**), *N*-aryl/alkyl maleimide (0.2 mmol) (**2**), CF_3SO_2Na (0.2 mmol, 31.2 mg) and PIDA (0.4 mmol, 128.8 mg) were taken in an oven-dried screw tube. Solvent 1,2-DCE (2 ml) was then added to the screw tube and the resultant mixture was stirred at 100 °C for 10 h. Progress of the reaction was monitored by TLC in regular intervals. After completion, the reaction mixture was allowed to cool to room temperature and then extracted with DCM (10 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude residue which was further purified by column chromatography using silica gel (100−200 mesh) and using mixture of petroleum ether and ethyl acetate as an eluent to afford the corresponding products **3**.

4. Gram scale synthesis of compound 3ba:

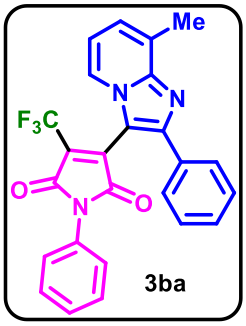


A mixture of 8-methyl-2-phenylimidazo[1,2-*a*]pyridine (4.0 mmol, 0.83 g) (**1b**), *N*-phenyl maleimide (4.0 mmol, 0.69 g) (**2a**), CF_3SO_2Na (4.0 mmol, 0.62 g) and PIDA (8.0 mmol, 2.57 g) were taken in an oven-dried round bottom flask. Then, 1,2-DCE (40 ml) was added to it and the resultant mixture was then stirred at 100 °C for 10 h. The progress of the reaction was monitored by TLC. After completion, the reaction mixture was allowed to cool to room temperature and then extracted with DCM (50 mL). The organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude residue which was further purified by column chromatography using silica gel (100−200 mesh) and using a mixture of petroleum ether and ethyl acetate (93:07) as an eluent to afford the corresponding product **3ba** (65%, 1.16 g) as a red solid.

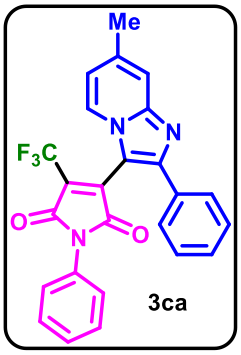
5. Characterization data of the synthesized compounds (3aa-3bh):



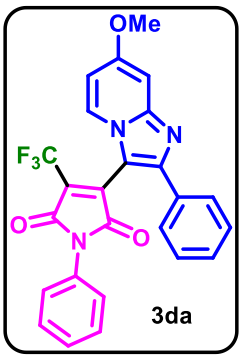
1-Phenyl-3-(2-phenylimidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3aa): Red solid (57.2 mg, 66%); M.p. 110–111 °C; R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.07 (d, J = 7.2 Hz, 1H), 7.78 (d, J = 8.8 Hz, 1H), 7.66-7.63 (m, 2H), 7.47-7.42 (m, 5H), 7.41-7.37 (m, 2H), 7.35-7.33 (m, 2H), 7.02-6.98 (m, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.5, 164.3, 152.6, 148.7, 134.8, 133.6, 130.7, 129.8, 129.4, 129.0, 128.7, 128.6, 128.1, 126.4, 125.9, 125.5, 120.1 (q, $J_{C\text{-}F}$ = 275.0 Hz), 118.4, 114.0, 108.1; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.52; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{24}H_{15}F_3N_3O_2]^+$: 434.1111; found: 434.1109.



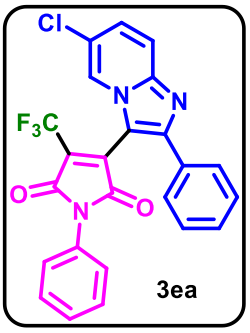
3-(8-Methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ba): Red solid (65.3 mg, 73%); M.p. 190–191 °C; R_f = 0.50 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94 (d, J = 6.8 Hz, 1H), 7.66-7.64 (m, 2H), 7.48-7.43 (m, 5H), 7.40-7.36 (m, 1H), 7.33-7.31 (m, 2H), 7.21 (d, J = 6.8 Hz, 1H), 6.91 (t, J = 7.2 Hz, 1H), 2.71 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.5, 164.3, 152.1, 149.1, 135.0, 134.9, 133.8, 130.7, 129.4, 129.2, 128.9, 128.8, 128.6, 126.9, 125.9, 123.7, 123.3, 120.1 (q, $J_{C\text{-}F}$ = 270.0 Hz), 114.0, 108.6, 17.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.43; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{25}H_{17}F_3N_3O_2]^+$: 448.1267; found: 448.1287.



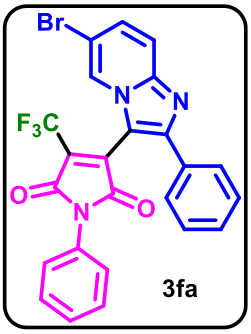
3-(7-Methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ca): Red solid (66.2 mg, 74%); M.p. 188-189 ^{o}C; R_f = 0.55 (PE : EA = 75 : 25); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.96 (d, J = 7.2 Hz, 1H), 7.64-7.62 (m, 2H), 7.52 (s, 1H), 7.48-7.41 (m, 5H), 7.40-7.36 (m, 1H), 7.34-7.32 (m, 2H), 6.84-6.82 (m, 1H), 2.48 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.6, 164.4, 153.0, 149.2, 139.9, 134.7, 133.8, 132.3, 130.7, 129.4, 129.3, 128.9, 128.7, 128.6, 125.9, 124.8, 120.2 (q, $J_{C\text{-}F}$ = 272.0 Hz), 116.8, 116.6, 107.9, 21.6; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.30; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{25}H_{17}F_3N_3O_2]^{+}$: 448.1267; found: 448.1275.



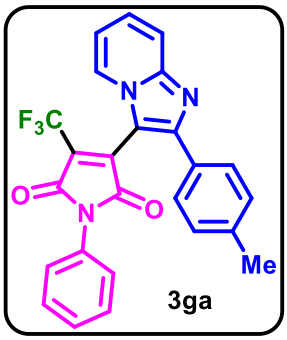
3-(7-Methoxy-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3da): Purple solid (70.4 mg, 76%); M.p. 190-191 ^{o}C; R_f = 0.45 (PE : EA = 70 : 30); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.90 (d, J = 7.6 Hz, 1H), 7.63-7.61 (m, 2H), 7.47-7.37 (m, 6H), 7.32 (d, J = 7.6 Hz, 2H), 7.03 (d, J = 2.4 Hz, 1H), 6.70-6.68 (m, 1H), 3.93 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.7, 164.5, 160.4, 153.6, 150.8, 134.4, 133.8, 130.7, 129.38, 129.36, 128.9, 128.7, 128.5, 126.2, 125.9, 121.9, 120.3 (q, $J_{C\text{-}F}$ = 272.0 Hz), 108.7, 107.6, 95.7, 56.0; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.09; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{25}H_{17}F_3N_3O_3]^{+}$: 464.1217; found: 464.1221.



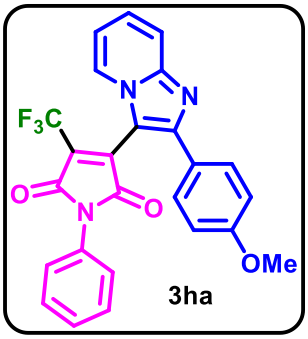
3-(6-Chloro-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ea): Red solid (59.8 mg, 64%); M.p. 184-185 ^{o}C; R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (s, 1H), 7.70 (d, J = 9.6 Hz, 1H), 7.63-7.61 (m, 2H), 7.49-7.41 (m, 6H), 7.39-7.34 (m, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.3, 164.0, 152.8, 146.8, 138.1, 134.3, 133.1, 130.5, 129.6, 129.4, 129.3, 129.0, 128.7, 128.6, 125.9, 123.4, 122.3, 119.8 (q, $J_{C\text{-}F}$ = 274.0 Hz), 114.6, 108.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.77; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{24}H_{14}{}^{35}ClF_3N_3O_2]^+$: 468.0721; found: 468.0705.



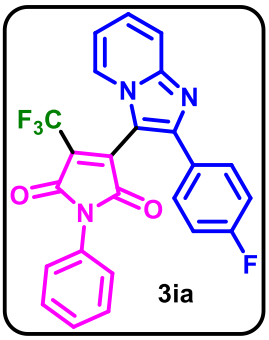
3-(6-Bromo-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3fa): Red solid (66.5 mg, 65%); M.p. 180-181 ^{o}C; R_f = 0.50 (PE : EA = 78 : 22); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.19 (s, 1H), 7.67-7.61 (m, 3H), 7.49-7.44 (m, 6H), 7.40-7.34 (m, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.3, 164.0, 152.6, 148.6, 146.9, 134.3, 133.0, 131.4, 130.5, 129.6, 129.4, 129.0, 128.7, 128.6, 125.9, 125.6, 119.8 (q, $J_{C\text{-}F}$ = 272.0 Hz), 118.8, 108.7, 108.0; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.77; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{24}H_{14}{}^{79}BrF_3N_3O_2]^+$: 512.0216; found: 512.0202.



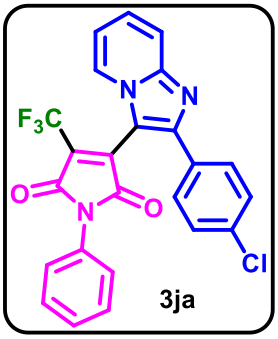
1-Phenyl-3-(2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ga): Red solid (62.6 mg, 70%); M.p. 190-191 ^{o}C; R_f = 0.50 (PE : EA = 75 : 25); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, J = 7.2 Hz, 1H), 7.76 (d, J = 8.8 Hz, 1H), 7.54 (d, J = 8.0 Hz, 2H), 7.49-7.44 (m, 2H), 7.42-7.39 (m, 1H), 7.37-7.33 (m, 2H), 7.27-7.25 (m, 3H), 6.99 (t, J = 7.2 Hz, 1H), 2.40 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.4, 164.2, 152.6, 148.6, 139.3, 134.87, 134.84, 130.6, 129.6, 129.2, 128.5, 127.9, 125.8, 125.7, 125.3, 123.8, 120.0 (q, $J_{C\text{-}F}$ = 277.0 Hz), 118.1, 113.8, 107.7, 21.4; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.45; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{25}H_{17}F_3N_3O_2]^{+}$: 448.1267; found: 448.1257.



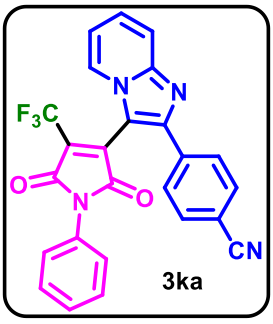
3-(2-(4-Methoxyphenyl)imidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ha): Red solid (66.7 mg, 72%); M.p. 128-129 ^{o}C; R_f = 0.45 (PE : EA = 70 : 30); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.05 (d, J = 6.8 Hz, 1H), 7.75 (d, J = 9.2 Hz, 1H), 7.59 (d, J = 8.8 Hz, 2H), 7.48-7.33 (m, 6H), 7.00-6.96 (m, 3H), 3.85 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.5, 164.3, 160.6, 152.5, 148.7, 134.9, 130.7, 130.1, 129.4, 128.6, 128.5, 128.1, 126.1, 125.9, 125.4, 120.2 (q, $J_{C\text{-}F}$ = 271.0 Hz), 118.1, 114.5, 113.8, 107.7, 55.4; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.38; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{25}H_{17}F_3N_3O_3]^{+}$: 464.1217; found: 464.1210.



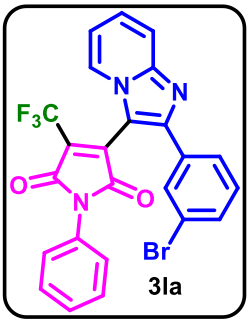
3-(2-(4-Fluorophenyl)imidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ia): Red solid (47.8 mg, 53%); M.p. 155-156 ^{o}C; R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.07 (d, J = 6.8 Hz, 1H), 7.77 (d, J = 9.2 Hz, 1H), 7.64-7.61 (m, 2H), 7.48-7.45 (m, 2H), 7.43-7.38 (m, 2H), 7.35-7.33 (m, 2H), 7.16 (t, J = 8.8 Hz, 2H), 7.02 (t, J = 7.2 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.4, 164.2, 163.5 (d, $J_{C\text{-}F}$ = 248 Hz), 151.5, 148.6, 134.4, 130.5 (d, $J_{C\text{-}F}$ = 9Hz), 129.7, 129.4, 128.7, 128.4, 126.4 (d, $J_{C\text{-}F}$ = 23 Hz), 125.9, 125.5, 120.0 (q, $J_{C\text{-}F}$ = 275 Hz), 118.2, 116.2, 116.0, 114.2, 107.9; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.51, -111.50; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{24}H_{14}F_4N_3O_2]^+$: 452.1017; found: 452.1012.



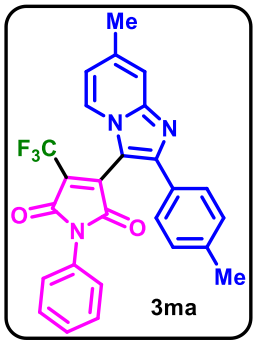
3-(2-(4-Chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ja): Red solid (62.6 mg, 67%); M.p. 135-136 ^{o}C; R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, J = 4.8 Hz, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.50-7.43 (m, 6H), 7.34 (d, J = 7.6 Hz, 2H), 7.03-7.00 (m, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.4, 164.1, 151.1, 148.6, 135.6, 134.5, 132.1, 130.6, 129.9, 129.4, 129.3, 128.7, 128.4, 125.9, 125.5, 124.9, 120.0 (q, $J_{C\text{-}F}$ = 275.0 Hz), 118.4, 114.3, 108.0; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.46; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{24}H_{14}{}^{35}ClF_3N_3O_2]^+$: 468.0721; found: 468.0717.



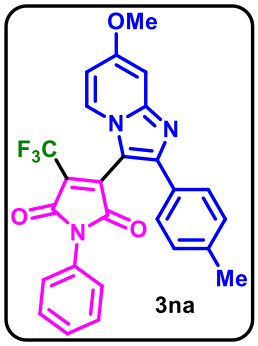
4-(3-(2,5-Dioxo-1-phenyl-4-(trifluoromethyl)-2,5-dihydro-1*H*-pyrrol-3-yl)imidazo[1,2-*a*]pyridin-2-yl)benzonitrile (3ka): Yellow solid (56.8 mg, 62%); M.p. 180-181 ^{o}C; R_f = 0.45 (PE : EA = 75 : 25); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.08 (d, J = 6.8 Hz, 1H), 7.80-7.72 (m, 5H), 7.50-7.46 (m, 3H), 7.42-7.38 (m, 1H), 7.33 (d, J = 7.6 Hz, 2H), 7.05 (t, J = 7.2 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.3, 163.9, 150.0, 148.6, 138.1, 133.9, 132.6, 130.4, 129.5, 129.2, 128.8, 128.6, 125.8, 125.5, 125.3, 124.9, 119.9 (q, $J_{C\text{-}F}$ = 272.0 Hz), 118.5, 114.6, 112.7, 108.5; ^{19}F NMR (376 MHz, $CDCl_3$): δ -61.52; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{25}H_{14}F_3N_4O_2]^{+}$: 459.1063; found: 459.1048.



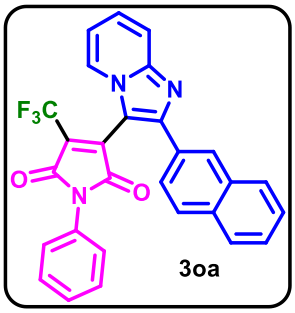
3-(2-(3-Bromophenyl)imidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3la): Red solid (59.4 mg, 58%); M.p. 140-141 ^{o}C; R_f = 0.55 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, J = 7.2 Hz, 1H), 7.87 (s, 1H), 7.78 (d, J = 8.8 Hz, 1H), 7.56-7.50 (m, 2H), 7.48-7.43 (m, 3H), 7.42-7.38 (m, 1H), 7.36-7.29 (m, 3H), 7.02 (t, J = 6.8 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.4, 164.1, 150.5, 148.6, 137.4, 135.5, 134.3, 132.3, 131.6, 130.5, 130.3, 129.4, 128.8, 128.4, 127.2, 126.0, 125.5, 123.1, 122.7 (q, $J_{C\text{-}F}$ = 272.0 Hz), 118.4, 114.3, 108.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.45; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{24}H_{14}{}^{79}BrF_3N_3O_2]^{+}$: 512.0216; found: 512.0201.



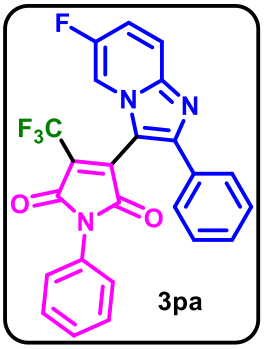
3-(7-Methyl-2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3ma): Red solid (71.9 mg, 78%); M.p. 198-199 ºC; R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94 (d, J = 7.2 Hz, 1H), 7.53-7.51 (m, 3H), 7.48-7.44 (m, 2H), 7.39 (d, J = 7.2 Hz, 1H), 7.33 (d, J = 7.6 Hz, 2H), 7.25-7.24 (m, 2H), 6.83-6.81 (m, 1H), 2.47 (s, 3H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.6, 164.5, 153.1, 149.2, 139.8, 139.4, 134.8, 130.9, 130.8, 129.7, 129.4, 128.6, 128.5, 126.0, 124.7, 122.7, 120.3 (q, $J_{C\text{-}F}$ = 273.0 Hz), 116.7, 116.5, 107.7, 21.6, 21.5; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.23; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{26}H_{19}F_3N_3O_2]^+$: 462.1424; found: 462.1428.



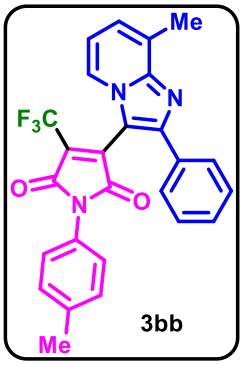
3-(7-Methoxy-2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3na): Purple solid (76.3 mg, 80%); M.p. 195-196 ºC; R_f = 0.45 (PE : EA = 75 : 25); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.85 (d, J = 7.6 Hz, 1H), 7.49 (d, J = 7.6 Hz, 2H), 7.44-7.40 (m, 2H), 7.36-7.29 (m, 3H), 7.22 (d, J = 8.0 Hz, 2H), 6.98-6.97 (m, 1H), 6.65-6.61 (m, 1H), 3.87 (d, J = 3.6 Hz, 3H), 2.36 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.7, 164.5, 160.3, 153.7, 150.8, 139.4, 134.5, 130.9, 130.7, 129.6, 129.3, 128.55, 128.50, 126.1, 125.9, 123.0 (q, $J_{C\text{-}F}$ = 271.0 Hz), 121.5, 108.5, 107.4, 95.6, 55.9, 21.5; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -60.96; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{26}H_{19}F_3N_3O_3]^+$: 478.1373; found: 478.1375.



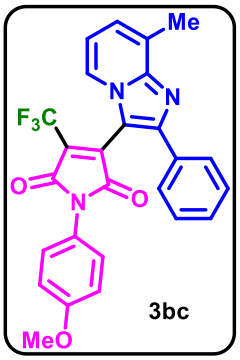
3-(2-(Naphthalen-2-yl)imidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3oa): Red solid (55.1 mg, 57%); M.p. 215-216 ^{o}C; R_f = 0.50 (PE : EA = 70 : 30); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.18 (s, 1H), 8.10 (d, J = 6.8 Hz, 1H), 7.94-7.86 (m, 3H), 7.82 (d, J = 9.2 Hz, 1H), 7.75-7.73 (m, 1H), 7.54-7.51 (m, 2H), 7.49-7.45 (m, 1H), 7.43-7.41 (m, 2H), 7.37 (d, J = 7.2 Hz, 1H), 7.28 (d, J = 7.6 Hz, 2H), 7.03 (t, J = 7.2 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.4, 164.3, 152.3, 148.7, 134.8, 133.6, 133.4, 131.0, 130.5, 129.4, 128.8, 128.6, 128.5, 128.4, 128.3, 127.9, 126.9, 126.7, 125.94, 125.91, 125.4, 124.1, 120.1 (q, $J_{C\text{-}F}$ = 271 Hz), 118.3, 114.1, 108.3; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.33; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{28}H_{17}F_3N_3O_2]^+$: 484.1267; found: 484.1262.



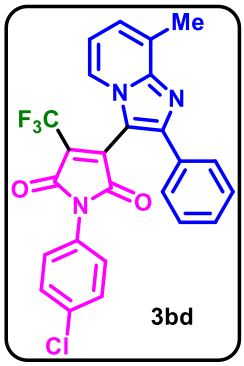
3-(6-Fluoro-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-phenyl-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3pa): Red solid (49.6 mg, 55%); M.p. 187-188 ^{o}C; R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (s, 1H), 7.63 (s, 2H), 7.47-7.36 (m, 10H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.1, 163.8, 152.8, 151.1, 144.9, 139.3, 136.8, 133.9, 131.7, 130.3, 129.9 (d, $J_{C\text{-}F}$ = 10.0 Hz), 129.4, 129.2, 128.7, 128.5, 128.4 (d, $J_{C\text{-}F}$ = 7.0 Hz), 126.0, 122.4 (q, $J_{C\text{-}F}$ = 277.0 Hz), 113.4 (d, $J_{C\text{-}F}$ = 34.0 Hz), 109.0; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.68, -136.31; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{24}H_{14}F_4N_3O_2]^+$: 452.1017; found: 452.1011.



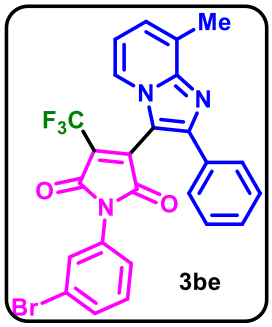
3-(8-Methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-1-(*p*-tolyl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3bb): Red solid (68.2 mg, 74%); M.p. 150-151 ^{o}C; R_f = 0.45 (PE : EA = 92 : 8); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, J = 7.2 Hz, 1H), 7.67-7.65 (m, 2H), 7.48-7.41 (m, 3H), 7.27-7.19 (m, 5H), 6.89 (t, J = 6.8 Hz, 1H), 2.71 (s, 3H), 2.37 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.6, 164.4, 152.0, 149.0, 138.7, 134.9, 133.8, 130.0, 129.1, 128.9, 128.8, 128.5, 126.9, 126.3, 125.8, 123.7, 123.3, 120.1 (q, $J_{C\text{-}F}$ = 271.0 Hz), 113.9, 108.5, 21.2, 17.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.46; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{26}H_{19}F_3N_3O_2]^+$: 462.1424; found: 462.1427.



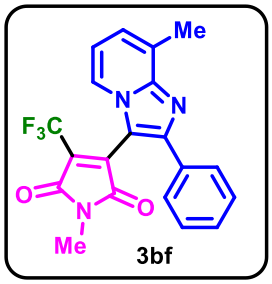
1-(4-Methoxyphenyl)-3-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3bc): Red solid (71.6 mg, 75%); M.p. 140-141 ^{o}C; R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, J = 6.8 Hz, 1H), 7.66-7.64 (m, 2H), 7.47-7.40 (m, 3H), 7.23-7.20 (m, 3H), 6.97-6.94 (m, 2H), 6.89 (t, J = 7.2 Hz, 1H), 3.81 (s, 3H), 2.71 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): 165.8, 164.6, 159.5, 152.0, 149.0, 134.9, 133.8, 129.2, 128.9, 128.8, 128.5, 127.6, 127.4, 126.9, 123.3, 123.1, 120.1 (q, $J_{C\text{-}F}$ = 271.0 Hz), 114.6, 113.9, 108.6, 55.6, 17.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.45; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{26}H_{19}F_3N_3O_3]^+$: 478.1373; found: 478.1378.



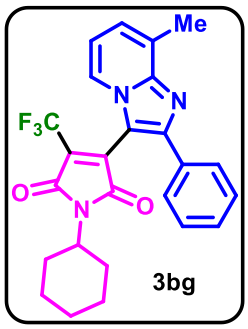
1-(4-Chlorophenyl)-3-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3bd): Red solid (65.5 mg, 68%); M.p. 123-124 ^{o}C; R_f = 0.50 (PE : EA = 85 : 15); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, J = 6.8 Hz, 1H), 7.65-7.63 (m, 2H), 7.48-7.41 (m, 5H), 7.30-7.24 (m, 3H), 6.93 (t, J = 6.8 Hz, 1H), 2.73 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.2, 164.0, 152.0, 148.9, 134.98, 134.96, 134.4, 133.5, 129.6, 129.4, 129.2, 129.0, 128.9, 128.6, 127.4, 127.0, 123.3, 120.1 (q, $J_{C\text{-}F}$ = 271.0 Hz), 114.3, 108.5, 17.3; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.42; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for [$C_{25}H_{16}{}^{35}ClF_3N_3O_2$]$^{+}$: 482.0878; found: 482.0896.



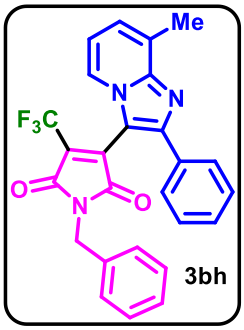
1-(3-Bromophenyl)-3-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3be): Red solid (63.1 mg, 60%); M.p. 160-161 ^{o}C; R_f = 0.45 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93 (d, J = 6.8 Hz, 1H), 7.65-7.63 (m, 2H), 7.54-7.50 (m, 2H), 7.48-7.42 (m, 3H), 7.35-7.28 (m, 2H), 7.24 (s, 1H), 6.93 (t, J = 7.2 Hz, 1H), 2.72 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.1, 163.9, 149.0, 134.9, 133.6, 131.8, 131.6, 130.6, 129.5, 129.4, 129.0, 128.9, 128.6, 127.8, 127.3, 125.0, 124.4, 123.3, 122.6, 119.8 (q, $J_{C\text{-}F}$ = 271.0 Hz), 114.2, 108.5, 17.3; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.43; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for [$C_{25}H_{16}{}^{79}BrF_3N_3O_2$]$^{+}$: 526.0373; found: 526.0377.



1-Methyl-3-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3bf): Red solid (56.2 mg, 73%); M.p. 152-153 ^{o}C; R_f = 0.40 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.85 (d, J = 6.8 Hz, 1H), 7.60-7.58 (m, 2H), 7.44-7.39 (m, 3H), 7.19 (d, J = 6.8 Hz, 1H), 6.87 (t, J = 7.2 Hz, 1H), 3.11 (s, 3H), 2.70 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.7, 165.6, 151.7, 148.9, 135.28, 135.23, 133.8, 129.1, 128.9, 128.8, 128.5, 126.7, 123.2, 120.0 (q, $J_{C\text{-}F}$ = 271.0 Hz), 113.9, 108.4, 24.9, 17.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.77; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{20}H_{15}F_3N_3O_2]^{+}$: 386.1111; found: 386.1109.



1-Cyclohexyl-3-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3bg): Red solid (67.1 mg, 74%); M.p. 110-111 ^{o}C; R_f = 0.50 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.83 (d, J = 6.8 Hz, 1H), 7.60-7.58 (m, 2H), 7.44-7.36 (m, 3H), 7.18 (d, J = 6.8 Hz, 1H), 6.86 (t, J = 7.2 Hz, 1H), 4.04-3.93 (m, 1H), 2.69 (s, 3H), 2.07-1.91 (m, 2H), 1.83-1.80 (m, 2H), 1.69-1.62 (m, 3H), 1.34-1.27 (m, 2H), 1.21-1.13 (m, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.3, 165.5, 151.3, 148.7, 134.8, 133.9, 129.0, 128.8, 128.7, 128.4, 126.6, 123.9, 123.1, 120.2 (q, $J_{C\text{-}F}$ = 271.0 Hz), 113.8, 108.5, 52.0, 29.8, 29.5, 25.88, 25.86, 24.8, 17.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.48; HRMS (ESI-TOF) m/z: [M + H]$^{+}$ Calcd for $[C_{25}H_{23}F_3N_3O_2]^{+}$: 454.1737; found: 454.1735.



1-Benzyl-3-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)-4-(trifluoromethyl)-1*H*-pyrrole-2,5-dione (3bh): Red solid (68.2 mg, 74%); M.p. 158-159 ^{o}C; R_f = 0.45 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81 (d, J = 6.8 Hz, 1H), 7.59-7.57 (m, 2H), 7.39-7.32 (m, 8H), 7.19 (d, J = 6.8 Hz, 1H), 6.87 (t, J = 7.2 Hz, 1H), 4.77-4.66 (m, 2H), 2.70 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.3, 165.1, 151.7, 149.0, 135.4, 135.2, 133.9, 129.0, 128.96, 128.90, 128.8, 128.5, 128.3, 126.8, 123.8, 123.1, 120.1 (q, $J_{C\text{-}F}$ = 271.0 Hz), 113.9, 113.8, 108.6, 42.5, 17.2; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -61.38; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{26}H_{19}F_3N_3O_2]^+$: 462.1424; found: 462.1429.

6. Control Experiments:

The productivity of this reaction was not found at all in the presence of radical scavengers like 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO), 2,6-di-*tert*-butyl-4-methyl phenol (BHT). Additionally, by employing *p*-benzoquinone (BQ) in the reaction, a trace amount of product was observed (Figure S1, eq A). Notably, the formation of radical-adduct (**4**) was detected by GC-MS in the presence of 1,1-DPE (Figure S1, eq B and ESI, Sl 7). These observations clearly highlight that the reaction likely proceeds through a radical pathway.

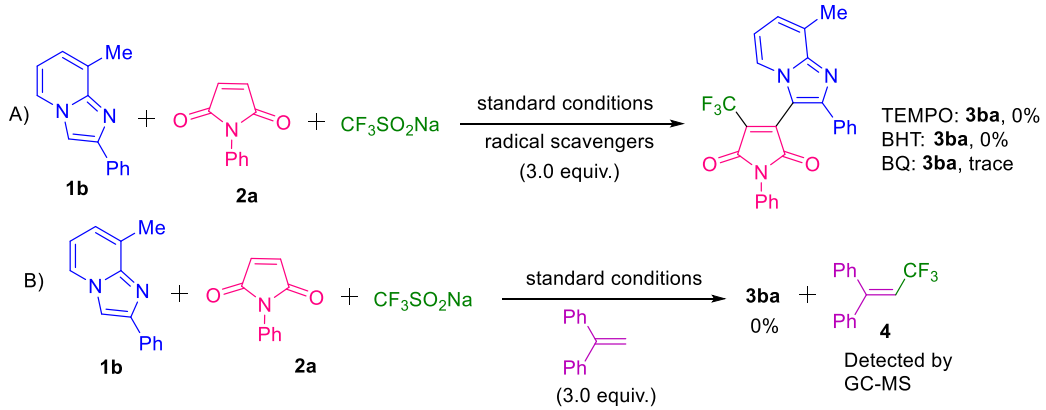
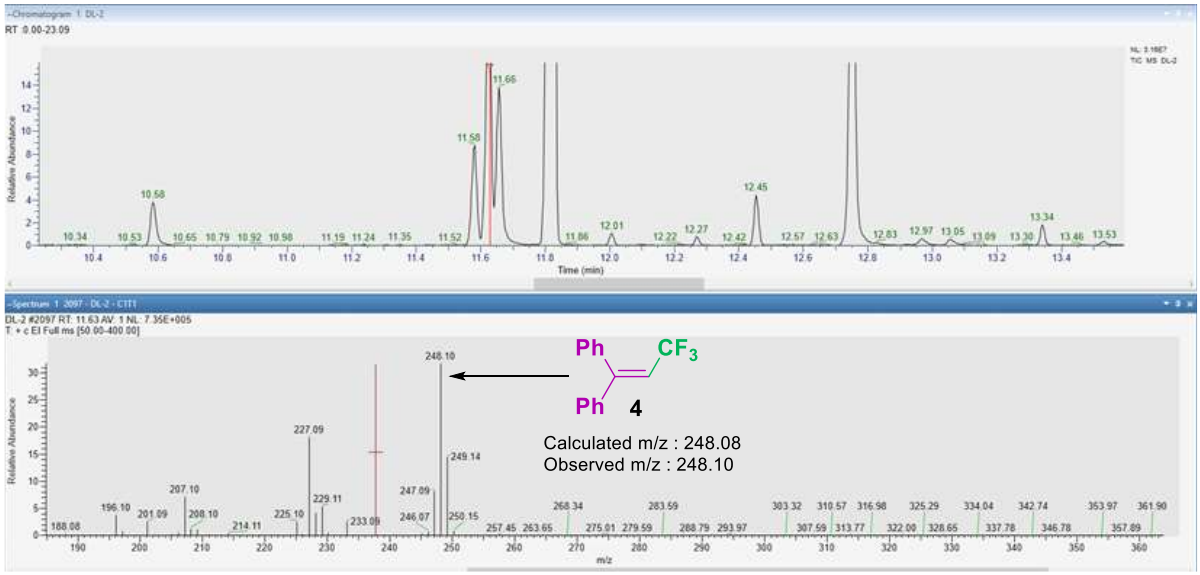


Figure: S1

7. GC-MS spectra of radical-adduct 4:



8. Computational Studies:

Geometry optimisation and energy calculations for all systems have been executed utilising Gaussian 16 software.[3] The resultant data were visualised, and the progression of calculations was meticulously tracked with various integrated scripts and graphic tools, including Gauss View. The electronic structure calculations were done using the UB3LYP hybrid density functional method.[4] The 6-31+G(d,p) basis set was utilized for all elements, with the LANL2DZ basis set specifically chosen for the iodine atom. Notably, unrestricted spin was taken into account for calculating the radical fragments. The influence of the bulk solvent was approximated by utilising the Polarization Continuum Model (PCM).[5] As dichloroethane (DCE) was employed as the solvent in the experimental process, established solvent-specific parameters were meticulously applied during the computational calculations.

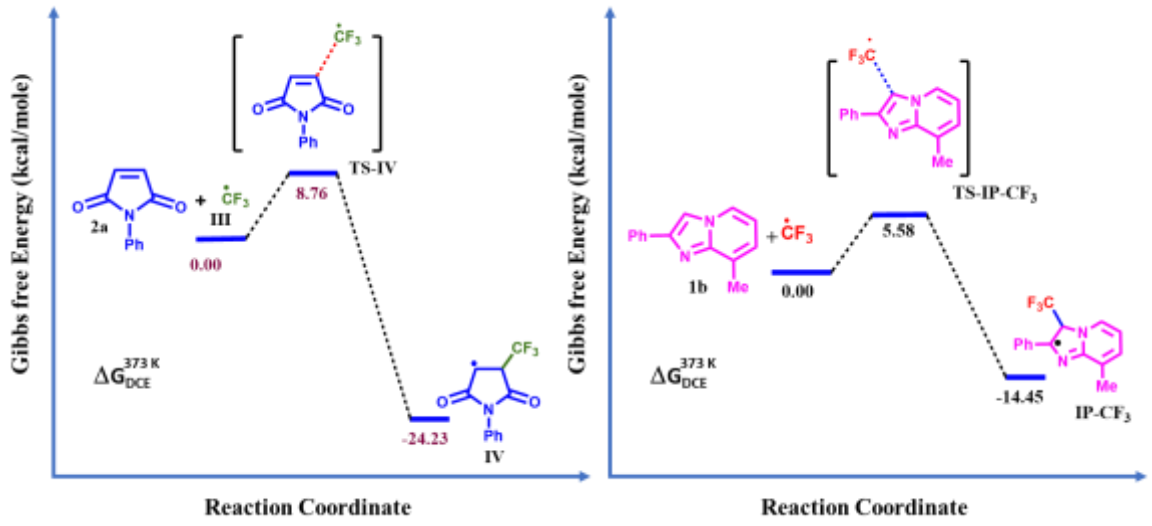
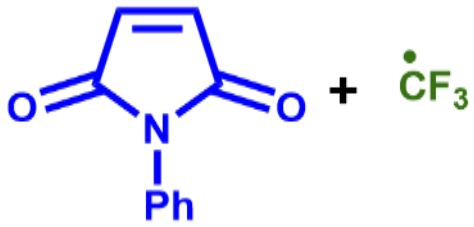
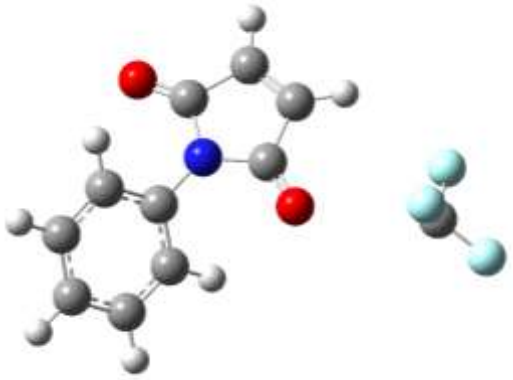


Figure 1: Potential energy surface for generated CF_3 maleimide radical intermediate **IV and** CF_3 imidazopyridine radical intermediate **IP-CF3**.

St.Pt.	General Structure	Ball & Stick model
2a + III		

Cartesian co-ordinate

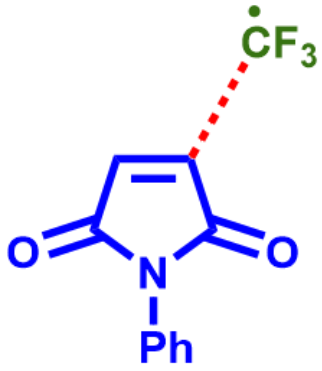
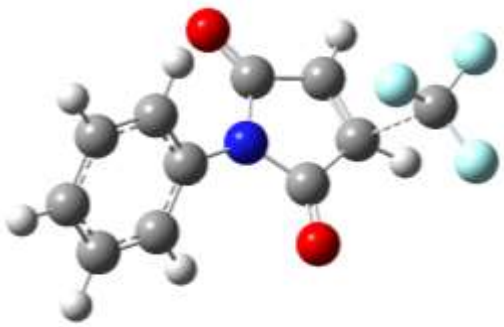
Atoms	X	Y	Z
F	5.06483	-1.51440	-0.47176
O	-2.55091	2.66738	-0.08826
F	4.18569	0.48143	-0.24291
O	0.92566	-0.35485	-0.12155
F	3.97795	-0.99891	1.36117
N	-1.09246	0.83274	-0.09230
C	-0.13395	2.95648	-0.15732
C	-1.43002	2.20392	-0.10874
C	0.87463	2.07982	-0.16787
C	0.30854	0.69175	-0.12644
C	-2.02984	-0.24607	-0.04704
C	4.05832	-0.81482	0.04901
C	-3.08878	-0.20761	0.86646
H	-3.19978	0.64027	1.53202
C	-1.88179	-1.33180	-0.91687
H	-1.05551	-1.35606	-1.61751
C	-3.86050	-2.35184	0.04129
H	-4.57254	-3.17091	0.07570
C	-4.00559	-1.25952	0.90042
H	-4.83101	-1.22478	1.60502
C	-2.79543	-2.38562	-0.86249
H	-2.67500	-3.23091	-1.53329
H	1.94209	2.25377	-0.19810
H	-0.10877	4.03802	-0.18004

Frequencies

8.7077	10.9563	16.5160
27.4395	32.1755	42.4595
46.1288	79.9807	109.1719
150.7642	265.6715	284.4427
289.6126	379.5341	415.4450
463.5633	492.9081	494.1369
507.4806	587.9322	621.3115
628.3370	633.6826	680.9610
694.4788	705.0926	720.0996
761.5616	767.2098	838.0491
843.5036	921.3780	963.1437
974.2283	978.3447	1001.0964
1017.2564	1041.2980	1051.7157
1061.3125	1084.1651	1107.0871
1153.8202	1186.0317	1202.8888
1215.3536	1225.4573	1234.9062
1330.8118	1345.6794	1361.8750
1406.6524	1490.5406	1535.6662
1637.7254	1649.4164	1654.9784
1777.3580	1834.7937	3185.6460
3196.1170	3207.3004	3226.4083
3227.4625	3250.1525	3270.7380

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.160857 Electronic Energy = -928.093644723
Internal Energy (E)= -927.909635723 Enthalpy (H)= -927.908454723
Gibbs Free Energy (G)=-928.003931723 Gibbs Free Energy of Solvation=-928.013016551

St.Pt.	General Structure	Ball & Stick model
TS-IV		

Cartesian co-ordinate

Atoms	X	Y	Z
F	3.37976	-1.75682	0.37328
O	-0.47708	2.71471	-0.07913
F	3.99592	0.30956	0.75079
O	0.34093	-1.65284	-1.31367
F	2.17061	-0.47216	1.67448
N	-0.44439	0.41550	-0.54358
C	1.47797	1.63275	-1.03076
C	0.09589	1.72352	-0.48394
C	1.75225	0.33640	-1.32085
C	0.50238	-0.47274	-1.08408
C	-1.76228	0.05418	-0.12119
C	2.96077	-0.51784	0.60435
C	-2.24349	0.50902	1.11137
H	-1.62117	1.13636	1.73834
C	-2.55970	-0.75007	-0.94274
H	-2.17633	-1.10364	-1.89238

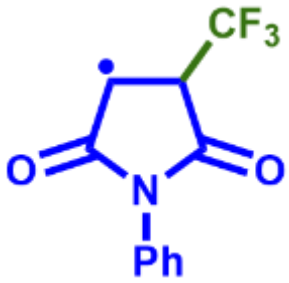
Frequencies

-223.6579	12.9585	29.4648
37.0144	57.8892	88.1554
102.4562	120.0199	129.1387
153.0693	268.0145	284.4574
301.8135	383.3039	415.1145
463.1334	496.8327	499.8923
508.2710	591.0941	619.1579
627.5235	640.0983	662.7620
697.1706	707.7923	721.4549
752.6871	768.5493	825.6253
843.2621	920.0514	922.4525
960.3614	978.6297	1001.3097
1010.3650	1017.5782	1038.7750
1051.3248	1071.6865	1106.7248
1151.7778	1186.1283	1202.5570
1217.4976	1222.1808	1235.6626
1327.9333	1346.0123	1362.3588
1399.0419	1490.6583	1533.7549
1535.7526	1637.5169	1648.9310
1775.0820	1830.4571	3185.7911
3196.4014	3207.5138	3228.2410

C	-4.33368	-0.64870	0.70562	3229.2821	3244.0723	3265.2093
H	-5.33405	-0.92220	1.02737			
C	-3.53281	0.16024	1.51599			
H	-3.90737	0.51902	2.46988			
C	-3.84204	-1.10420	-0.52036			
H	-4.45746	-1.73392	-1.15571			
H	2.58190	-0.06627	-1.88735			
H	2.10625	2.50654	-1.13999			

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.160718 Electronic Energy = -928.086799116
Internal Energy (E)= -927.904513116 Enthalpy (H)= -927.903332116
Gibbs Free Energy (G)=-927.988701116 Gibbs Free Energy of Solvation=-927.999062591

St.Pt.	General Structure	Ball & Stick model
IV		

Cartesian co-ordinate

Atoms	X	Y	Z
F	3.34522	-1.61105	0.27009
O	-0.56343	2.62389	-0.51267
F	4.08561	0.42622	0.06053
O	0.38847	-1.89995	-0.29758
F	2.57646	-0.03603	1.56857
N	-0.43677	0.28033	-0.33141
C	1.51236	1.44112	-0.76889
C	0.09184	1.59435	-0.53422
C	1.88924	0.00250	-0.72049
C	0.54863	-0.70611	-0.41670

Frequencies

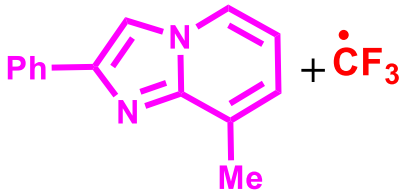
33.2174	41.4952	53.6343
76.7865	111.8773	139.3383
161.3490	247.7525	266.2823
273.4620	315.1406	334.7365
388.6575	412.9861	472.6318
500.7311	517.2110	530.8678
535.2749	582.4381	611.5025
628.4519	660.6114	688.1634
697.4095	710.5244	729.8511
767.3343	796.3255	842.2694
855.9367	924.6466	956.6881
979.3642	1002.8481	1017.1785
1040.6580	1050.6256	1059.5237
1111.1407	1120.3973	1166.3240

C	-1.82017	0.00957	-0.08119
C	2.97842	-0.31952	0.30856
C	-2.51963	0.79013	0.84624
H	-2.01847	1.59838	1.36441
C	-2.46086	-1.03012	-0.76505
H	-1.91011	-1.63589	-1.47426
C	-4.51616	-0.51243	0.40949
H	-5.56552	-0.71566	0.60060
C	-3.86879	0.52565	1.08449
H	-4.41179	1.13330	1.80183
C	-3.80848	-1.28830	-0.51234
H	-4.30391	-2.09749	-1.04004
H	2.27034	-0.36588	-1.68380
H	2.17264	2.27613	-0.95892

1175.8280	1187.1632	1202.8249
1215.0471	1244.9477	1269.0831
1305.4003	1347.5032	1349.8157
1363.4977	1380.3395	1491.1100
1532.7357	1636.5304	1646.9514
1725.5736	1825.0838	3036.4656
3187.5439	3198.5199	3209.0698
3231.7088	3233.9280	3266.8205

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.163293 Electronic Energy = -928.144653920
Internal Energy (E)= -927.96047192 Enthalpy (H)= -927.95929092
Gibbs Free Energy (G)=-928.03992992 Gibbs Free Energy of Solvation=-928.051626089

St.Pt.	General Structure	Ball & Stick model
1b + III		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-1.52497	-1.14078	-0.02286
C	-2.76687	-1.65085	0.44918
C	-3.92055	-1.13982	-0.10854
C	-3.87788	-0.13653	-1.11905
C	-2.68053	0.34906	-1.56513

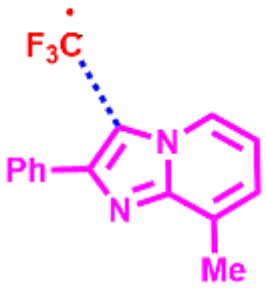
Frequencies

7.0034	13.5465	15.9725
19.7101	26.1772	33.9452
37.8828	68.6086	101.3131
121.4241	170.0364	188.0726
234.8406	261.4254	297.1023
328.6377	394.4036	412.0698
491.6932	492.5374	497.4423
518.2035	533.5024	558.6179

H	-4.88466	-1.50814	0.22913	573.3778	614.0455	633.4955
H	-4.79544	0.25373	-1.54420	661.0242	664.9156	680.8146
H	-2.57270	1.11195	-2.32621	698.4981	719.9539	750.9075
N	-1.52184	-0.15132	-1.01997	753.1758	767.2725	791.2114
N	-0.28282	-1.45699	0.33543	855.6937	881.1814	891.9966
C	-0.19900	0.14872	-1.26849	933.3937	944.9569	952.1203
C	0.54428	-0.67613	-0.42687	984.8204	986.5358	1004.2768
C	2.00852	-0.76353	-0.31055	1014.0908	1016.4742	1049.5948
C	2.58462	-1.63211	0.63215	1063.9327	1084.4383	1097.8573
C	2.85858	0.00308	-1.12711	1104.9123	1112.1248	1179.4239
C	3.97092	-1.72785	0.75427	1183.6221	1204.1224	1204.4854
H	1.92941	-2.22479	1.26093	1223.0760	1235.5637	1273.4122
C	4.24424	-0.09356	-1.00316	1288.5648	1316.2249	1360.3224
H	2.43951	0.67919	-1.86690	1370.2369	1381.7207	1399.9452
C	4.80760	-0.95998	-0.06108	1425.2418	1471.2156	1477.5893
H	4.39936	-2.40401	1.48880	1482.3669	1499.9771	1513.0100
H	4.88448	0.50717	-1.64290	1535.0405	1571.3032	1595.3755
H	5.88683	-1.03528	0.03534	1626.9665	1653.7647	1671.6055
C	-2.75594	-2.70806	1.51752	3044.2654	3101.9126	3129.2630
H	-2.20056	-3.59188	1.18545	3176.1308	3183.5817	3193.3040
H	-2.25288	-2.34423	2.41999	3193.3816	3203.9789	3218.3941
H	-3.77388	-3.00879	1.77867	3220.3176	3237.5308	3288.2300
C	-0.11311	2.63858	0.68041			
F	-1.13392	2.40322	1.50271			
F	-0.44975	3.55720	-0.23226			
F	0.96267	3.02776	1.35957			
H	0.08272	0.86825	-2.02058			

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.237945 Electronic Energy = -987.853776661
Internal Energy (E)= -987.588568661 Enthalpy (H)= -987.587386661
Gibbs Free Energy (G)=-987.691652661 Gibbs Free Energy of Solvation=-987.699686476

St.Pt.	General Structure	Ball & Stick model
TS-IP-CF$_3$		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

-151.9895	10.8048	29.4205
40.9625	49.6907	63.9248

C	-1.51371	-1.09089	-0.07455	90.0906	97.4975	113.2188
C	-2.74381	-1.71321	0.26442	119.0606	167.4150	194.0354
C	-3.90418	-1.11672	-0.19085	235.5470	253.0059	295.7120
C	-3.87561	0.07895	-0.96208	331.3041	394.7391	412.0256
C	-2.68400	0.67546	-1.27071	486.6681	487.9700	490.0815
H	-4.86270	-1.56800	0.04744	518.0475	523.1921	561.9413
H	-4.79737	0.53342	-1.30615	567.2181	614.8660	624.4226
H	-2.58448	1.59400	-1.83477	633.3108	661.4798	696.0217
N	-1.52351	0.08686	-0.83366	700.8381	749.3505	752.4767
N	-0.26338	-1.46340	0.21492	765.5543	789.0516	790.2576
C	-0.20202	0.49421	-0.95564	854.5600	887.0200	894.4824
C	0.55453	-0.53335	-0.34592	933.8993	942.5875	947.0770
C	2.01474	-0.63870	-0.27365	948.8826	985.5762	985.8064
C	2.60506	-1.77119	0.31725	1004.9038	1013.6670	1048.6913
C	2.85185	0.36663	-0.79135	1064.2323	1082.7639	1094.2292
C	3.99183	-1.89355	0.38249	1103.5679	1110.4570	1129.6040
H	1.95965	-2.54452	0.71880	1159.3890	1181.2227	1184.3545
C	4.23883	0.24045	-0.72536	1205.5651	1236.5460	1273.2610
H	2.42253	1.25884	-1.23642	1286.9960	1313.2587	1358.7519
C	4.81542	-0.89035	-0.13904	1366.1578	1376.1246	1399.9058
H	4.43222	-2.77406	0.84165	1425.2578	1460.7384	1476.6034
H	4.86956	1.02831	-1.12673	1478.1480	1492.8781	1499.2437
H	5.89595	-0.98713	-0.08667	1526.0460	1558.0638	1593.9500
C	-2.72197	-2.97167	1.08634	1624.6892	1649.8475	1665.6094
H	-2.13593	-3.75203	0.58928	3045.9196	3104.3569	3131.0865
H	-2.24726	-2.79385	2.05726	3179.3513	3187.8650	3194.8645
H	-3.73556	-3.34480	1.25362	3198.1714	3206.9453	3220.9139
C	-0.19414	2.31596	0.61930	3222.3945	3244.8688	3275.5252
F	-0.69118	1.92104	1.80332			
F	-1.01502	3.26371	0.10249			
F	1.01869	2.86624	0.81385			
H	0.08224	1.21443	-1.70686			

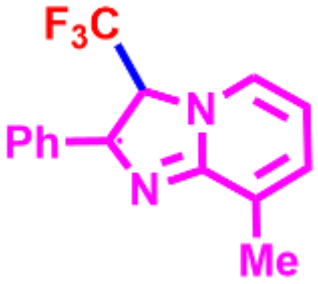
Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm

Zero-point correction= 0.237722 Electronic Energy = -987.852370110

Internal Energy (E)= -987.58885611 Enthalpy (H)= -987.58767411

Gibbs Free Energy (G)=-987.68211811 Gibbs Free Energy of Solvation=-987.690787183

St.Pt.	General Structure	Ball & Stick model
IP-CF_3		

Cartesian co-ordinate

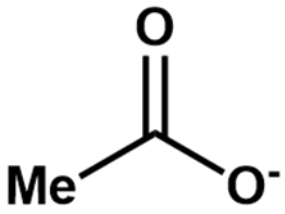
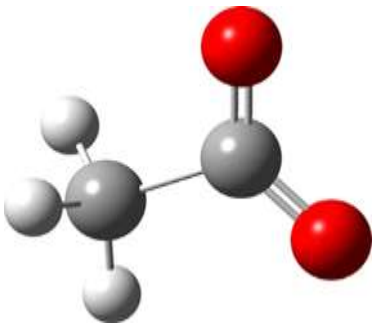
Atoms	X	Y	Z
C	-1.53362	-0.98932	-0.03061
C	-2.74268	-1.72551	0.09979
C	-3.91204	-1.11383	-0.30680
C	-3.92323	0.21214	-0.84398
C	-2.75712	0.91656	-0.93910
H	-4.84900	-1.65703	-0.22607
H	-4.84907	0.66824	-1.17308
H	-2.68996	1.92783	-1.31830
N	-1.59173	0.32795	-0.52086
N	-0.28666	-1.38512	0.20508
C	-0.23916	0.87888	-0.50904
C	0.55151	-0.37364	-0.11391
C	1.98362	-0.52748	-0.15932
C	2.57340	-1.71717	0.34121
C	2.84081	0.44649	-0.72662
C	3.94810	-1.90907	0.28428
H	1.92659	-2.47409	0.77033
C	4.21732	0.24085	-0.78532
H	2.43246	1.36830	-1.12605
C	4.78344	-0.93343	-0.27849
H	4.37633	-2.82592	0.68011
H	4.85173	1.00297	-1.22915
H	5.85745	-1.08764	-0.32112
C	-2.68611	-3.12404	0.64915
H	-2.02795	-3.75411	0.04140
H	-2.27394	-3.12847	1.66398
H	-3.68222	-3.57329	0.67262
C	-0.15422	2.04612	0.50711
F	-0.52325	1.67200	1.74646
F	-0.97598	3.06836	0.13414
F	1.09216	2.55563	0.57839
H	0.03986	1.30419	-1.48517

Frequencies

40.1176	49.9608	60.4769
62.7298	100.5241	113.2499
124.1980	176.7730	193.5846
231.2985	234.0801	266.2759
282.9604	292.2997	327.2430
399.0307	417.5894	421.7466
486.8662	510.1859	515.4336
526.8223	536.4464	569.9476
615.9451	622.5159	631.5075
653.8201	694.6264	695.1894
712.9430	745.9600	766.3718
772.3169	838.7338	843.5376
884.9075	891.0797	899.0308
912.5701	934.5582	968.3344
977.9781	995.4208	1001.0669
1016.7564	1049.3775	1063.0261
1067.6106	1091.1091	1106.7433
1113.0211	1166.2298	1175.1983
1181.2192	1200.2902	1211.4717
1240.8197	1247.0093	1251.4528
1274.4258	1336.3937	1336.6804
1361.1306	1364.3752	1370.3122
1401.5049	1426.0673	1467.5261
1476.7312	1479.2164	1490.5093
1510.7773	1543.6349	1582.1338
1602.6400	1628.2739	1644.3008
2997.4101	3045.1372	3103.2872
3130.4803	3177.7313	3185.3783
3193.1793	3201.4628	3211.3466
3221.1403	3226.0141	3250.3797

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.240163 Electronic Energy = -987.892383235
Internal Energy (E)= -987.627128235 Enthalpy (H)= -987.625946235
Gibbs Free Energy (G)=-987.714673235 Gibbs Free Energy of Solvation=-987.722713249

St.Pt.	General Structure	Ball & Stick model
Acetate ion		

Cartesian co-ordinate

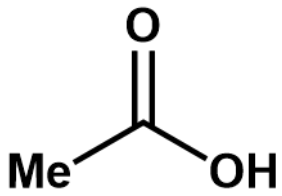
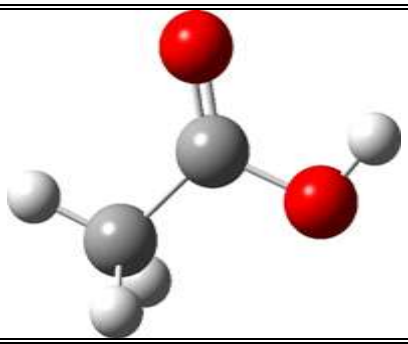
Atoms	X	Y	Z
C	-0.00028	-1.35371	0.00000
H	-0.48399	-1.75537	0.89495
H	1.04105	-1.69996	0.00000
H	-0.48399	-1.75537	-0.89495
C	-0.01115	0.18745	-0.00000
O	-0.00028	0.76301	-1.12926
O	-0.00028	0.76301	1.12926

Frequencies

43.9096	450.4062	603.4113
636.9904	895.4531	1016.5423
1046.2592	1353.8930	1396.0355
1459.5870	1479.3260	1583.4350
3034.0383	3100.6858	3126.7779

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.048358 Electronic Energy = -228.638898750
Internal Energy (E)= -228.58446375 Enthalpy (H)= -228.58328175
Gibbs Free Energy (G)=-228.62644775 Gibbs Free Energy of Solvation=-228.530426694

St.Pt.	General Structure	Ball & Stick model
Acetic Acid		

Cartesian co-ordinate

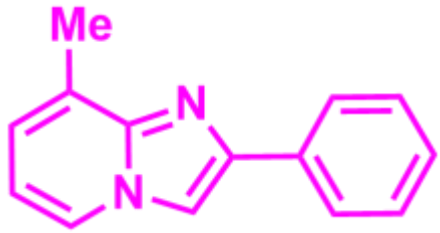
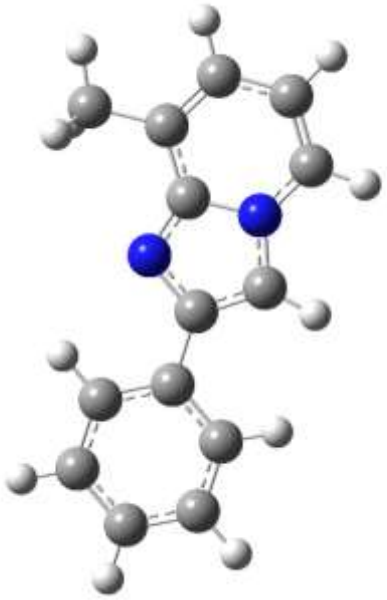
Atoms	X	Y	Z
C	1.39616	-0.12116	-0.00001
H	1.92586	0.83051	-0.00028
H	1.67670	-0.70460	-0.88204
H	1.67668	-0.70400	0.88243
C	-0.08735	0.12034	-0.00002
O	-0.79111	-1.03517	0.00002
O	-0.63301	1.20978	0.00001
H	-1.73908	-0.81383	-0.00009

Frequencies

61.5487	428.0033	545.2672
577.7843	648.9303	866.9908
1002.6795	1064.8413	1194.7045
1332.6039	1409.2903	1462.9659
1469.8960	1774.5123	3066.1544
3132.4456	3181.7000	3740.4508

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.061421 Electronic Energy = -229.113005988
Internal Energy (E)= -229.045102988 Enthalpy (H)= -229.043921988
Gibbs Free Energy (G)=-229.087420988 Gibbs Free Energy of Solvation=-229.080133806

St.Pt.	General Structure	Ball & Stick model
1b		

Cartesian co-ordinate

Atoms	X	Y	Z
N	-1.55859	-1.07318	-0.00223
N	-0.35612	0.83043	0.00207
C	-0.22935	-1.43829	-0.00296
C	0.49194	-0.25209	-0.00026
C	1.95601	-0.08772	-0.00006
C	-2.70056	-1.84082	-0.00432
H	-2.56627	-2.91511	-0.00697
C	-1.59209	0.32980	0.00092
C	-2.85047	0.99740	0.00248
C	2.81826	-1.20045	0.00754
H	2.40947	-2.20638	0.01405
C	-2.88361	2.50100	0.00613
H	-2.37069	2.90821	-0.87238
H	-2.37093	2.90384	0.88679
H	-3.91378	2.86534	0.00689
C	-3.98683	0.21465	0.00048
H	-4.96242	0.69130	0.00156
C	2.52446	1.19878	-0.00762
H	1.86847	2.06232	-0.01372
C	-3.91240	-1.20870	-0.00298
H	-4.81734	-1.80517	-0.00460
C	4.20337	-1.03103	0.00747
H	4.85024	-1.90365	0.01355

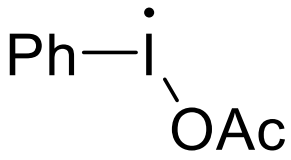
Frequencies

4.5664	66.8222	98.7844
126.1191	167.5276	185.7034
233.1027	263.1321	295.8058
329.2325	392.9829	414.0278
501.1839	517.4345	536.6705
558.1522	574.7442	612.9205
631.9747	659.8748	678.6087
701.9766	727.4434	749.0132
755.3150	773.5618	796.3666
855.4013	890.2523	890.6279
933.3259	951.6478	955.0253
984.5697	988.2613	1005.9437
1011.0777	1046.3964	1060.9804
1084.1540	1096.4795	1101.4852
1109.2776	1177.9482	1179.4450
1199.8662	1235.4400	1276.2173
1287.5531	1313.9404	1356.5599
1368.8820	1377.8249	1398.1511
1417.8880	1464.8161	1468.7152
1479.5425	1494.2093	1513.5945
1530.7618	1574.5195	1594.5275
1622.6037	1649.4062	1669.6825
3040.7400	3095.1763	3131.0563
3180.5580	3187.2012	3196.8176
3197.3058	3206.0134	3216.2595
3223.2914	3243.0896	3290.3759

C	3.91067	1.36677	-0.00759
H	4.32943	2.36920	-0.01354
C	4.75788	0.25394	-0.00005
H	5.83599	0.38492	0.00002
H	0.06703	-2.47502	-0.00562

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.225944 Electronic Energy = -650.282146028
Internal Energy (E)= -650.036939028 Enthalpy (H)= -650.035757028
Gibbs Free Energy (G)=-650.112155028 Gibbs Free Energy of Solvation=-650.10363081

St.Pt.	General Structure	Ball & Stick model
II		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-3.43343	0.79548	1.21188
C	-2.16460	0.20845	1.22137
C	-1.54847	-0.08319	0.00004
C	-2.16476	0.20774	-1.22138
C	-3.43359	0.79476	-1.21206
C	-4.06717	1.08914	-0.00014
H	-3.92164	1.02298	2.15464
H	-1.67386	-0.01732	2.16155
H	-1.67414	-0.01858	-2.16149
H	-3.92193	1.02170	-2.15489
H	-5.05204	1.54596	-0.00020
I	0.37632	-0.98503	0.00015
O	1.81284	1.27527	-0.00037
C	3.02986	0.83013	-0.00028
O	3.37179	-0.36083	-0.00013
C	4.07880	1.94822	-0.00010
H	4.70890	1.82384	-0.88531
H	3.62840	2.94089	-0.00302

Frequencies

16.8618	24.4084	32.9743
45.9228	85.9184	91.0605
146.6395	176.0562	226.3260
253.8506	410.5271	432.6667
453.7175	611.6293	617.7218
619.1477	657.3856	680.8767
746.5423	846.8819	901.2724
933.8484	991.6345	995.2729
1009.6645	1013.9339	1024.0068
1042.6070	1068.2818	1099.5903
1182.1742	1202.1460	1248.1913
1328.8207	1347.6985	1369.1912
1456.4479	1470.7867	1473.4494
1500.0783	1599.3258	1612.4737
1617.8166	3063.8230	3141.3196
3170.4517	3196.3065	3204.3921
3214.4623	3223.6012	3225.5666

H	4.70463	1.82736	0.88865	

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.139209 Electronic Energy = -471.479851960
Internal Energy (E)= -471.32304896 Enthalpy (H)= -471.32186696
Gibbs Free Energy (G)=-471.40054796 Gibbs Free Energy of Solvation=-471.390118143

St.Pt.	General Structure	Ball & Stick model
PhI	**PhI**	

Cartesian co-ordinate

Atoms	X	Y	Z
C	0.00000	1.20906	-2.66197
C	0.00000	1.21727	-1.26186
C	0.00000	0.00000	-0.57790
C	-0.00000	-1.21727	-1.26186
C	-0.00000	-1.20906	-2.66197
C	0.00000	0.00000	-3.36386
H	0.00000	2.15396	-3.19786
H	0.00000	2.15873	-0.72350
H	-0.00000	-2.15873	-0.72350
H	-0.00000	-2.15396	-3.19786
H	0.00000	0.00000	-4.44968
	0.00000	-0.00000	1.56658
O	1.81284	1.27527	-0.00037
C	3.02986	0.83013	-0.00028
O	3.37179	-0.36083	-0.00013
C	4.07880	1.94822	-0.00010
H	4.70890	1.82384	-0.88531
H	3.62840	2.94089	-0.00302
H	4.70463	1.82736	0.88865

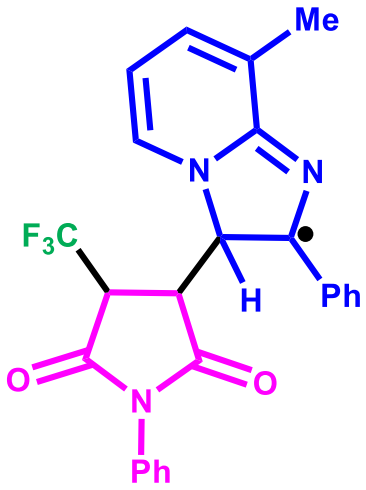
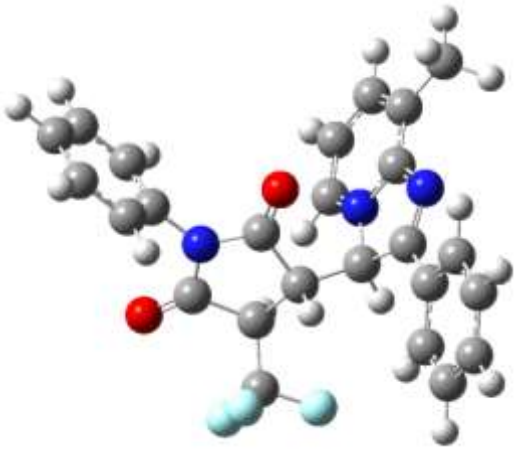
Frequencies

152.8235	222.4947	254.9545
412.0508	455.8428	621.2355
653.5494	683.2097	742.4813
846.8751	923.5638	987.0339
996.5714	1007.5715	1026.7224
1074.0994	1095.3416	1178.6720
1199.8623	1324.7740	1343.7525
1469.1700	1503.0526	1613.6696
1623.5826	3189.9324	3197.4115
3210.0188	3219.2892	3221.4817

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.089876 Electronic Energy = -243.042537542

Internal Energy (E)= -242.943828542	Enthalpy (H)= -242.942646542
Gibbs Free Energy (G)=-242.993698542	Gibbs Free Energy of Solvation=-242.990574237

St.Pt.	General Structure	Ball & Stick model
V		

Cartesian co-ordinate

Atoms	X	Y	Z
F	-1.01560	-3.32526	-2.78864
O	-0.51894	0.84328	1.37103
F	1.01780	-2.81035	-2.19834
O	-3.11758	-1.83077	-1.31017
F	-0.37800	-3.60429	-0.72249
N	0.94661	1.61398	-1.30241
N	-2.08362	-0.42084	0.21321
N	2.46624	1.86236	0.37794
C	0.18741	-0.66890	-0.42186
C	-0.80268	0.03926	0.50824
C	1.34510	0.23966	-0.91416
C	2.36568	0.57802	0.17902
C	-0.70662	-1.35973	-1.47517
C	3.14463	-0.40737	0.91485
C	0.11806	2.01298	-2.29678
H	-0.33516	1.25601	-2.92093
C	-2.12757	-1.27937	-0.88588
C	-3.25436	-0.04381	0.96638
C	1.61464	2.49875	-0.49757
C	1.43029	3.88203	-0.63439
C	-0.28253	-2.78859	-1.79803
C	3.33557	-1.71458	0.42178
H	2.91746	-2.01622	-0.53290
C	2.16441	4.84054	0.26037
H	3.24685	4.71414	0.16040
H	1.91237	4.66292	1.31041

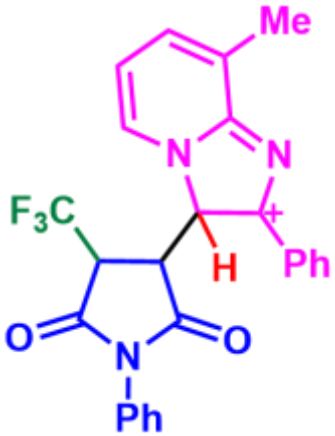
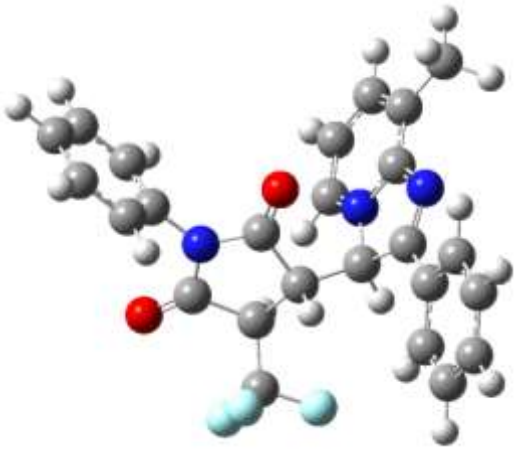
Frequencies

17.0464	17.9415	31.0234
38.5408	45.2839	53.7071
56.0052	57.1100	72.6274
80.9530	87.4428	93.3673
114.6232	128.5130	150.8126
169.3934	198.4161	203.1475
210.1300	239.1631	256.8821
267.9829	288.4277	310.5119
314.4177	336.0229	377.2680
407.5424	412.0594	418.3232
419.4886	466.5760	487.6172
497.7437	503.7304	511.4577
530.1258	530.6442	547.7264
567.2813	606.5916	615.3715
621.1899	628.4306	629.5060
631.1001	653.0341	665.3837
689.2002	695.7355	704.6364
723.8481	739.2704	761.5308
771.9751	785.2929	788.0734
804.9577	839.7218	852.7699
858.5073	879.6238	888.7426
911.3968	912.9265	939.1396
939.7189	957.5277	966.8463
990.5872	1000.9888	1001.5572
1010.5603	1011.3733	1015.8487
1016.3053	1022.7133	1034.7622
1047.0601	1055.6486	1058.3515
1067.8918	1084.5778	1096.6522
1102.1680	1113.8222	1117.3836

H	1.90811	5.87113	0.00902	1122.5593	1153.1003	1183.7687
C	0.55118	4.28884	-1.63928	1186.9642	1188.3773	1199.0472
H	0.37471	5.34932	-1.78797	1202.8326	1207.0771	1216.1055
C	3.73878	-0.03726	2.14039	1223.5644	1236.4575	1253.4874
H	3.58518	0.96608	2.52134	1260.3971	1277.0841	1291.8747
C	-0.09786	3.36416	-2.47336	1294.9493	1311.6935	1335.6130
H	-0.76219	3.69357	-3.26229	1338.4862	1351.1921	1356.3031
C	-3.55508	-0.72726	2.14591	1356.8727	1365.9654	1370.8731
H	-2.91260	-1.53279	2.48645	1398.8094	1403.1061	1420.9239
C	-4.06309	0.99337	0.49824	1457.8668	1472.1518	1479.4662
H	-3.80778	1.50888	-0.42197	1486.7877	1495.2276	1520.1288
C	4.10436	-2.62868	1.13965	1528.8071	1532.3245	1580.4694
H	4.25510	-3.62906	0.74764	1617.5776	1625.8338	1637.3905
C	-5.51029	0.67746	2.41507	1642.0163	1643.6651	1662.1116
H	-6.39258	0.95913	2.98136	1762.9075	1845.2291	3057.1968
C	-4.69027	-0.35914	2.87202	3073.5179	3092.6959	3113.6003
H	-4.93294	-0.88383	3.79052	3119.0694	3150.7694	3194.8194
C	4.49812	-0.95772	2.85460	3198.3375	3202.3510	3205.4144
H	4.94484	-0.66947	3.80063	3208.3708	3211.9445	3214.9940
C	4.68238	-2.25434	2.35684	3215.9161	3220.0327	3220.3456
H	5.27644	-2.97013	2.91645	3227.1721	3245.5732	3270.1260
C	-5.19759	1.35168	1.23033			
H	-5.83389	2.15583	0.87488			
H	-0.72803	-0.83001	-2.43098			
H	0.65642	-1.44110	0.19920			
H	1.84127	-0.23385	-1.76745			

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.395871 Electronic Energy = -1578.30912445
Internal Energy (E)= -1577.87201745 Enthalpy (H)= -1577.87083545
Gibbs Free Energy (G)=-1577.99844345 Gibbs Free Energy of Solvation=-1577.92691342

St.Pt.	General Structure	Ball & Stick model
VI		
Cartesian co-ordinate		**Frequencies**

Atoms	X	Y	Z
F	-1.01560	-3.32526	-2.78864
O	-0.51894	0.84328	1.37103
F	1.01780	-2.81035	-2.19834
O	-3.11758	-1.83077	-1.31017
F	-0.37800	-3.60429	-0.72249
N	0.94661	1.61398	-1.30241
N	-2.08362	-0.42084	0.21321
N	2.46624	1.86236	0.37794
C	0.18741	-0.66890	-0.42186
C	-0.80268	0.03926	0.50824
C	1.34510	0.23966	-0.91416
C	2.36568	0.57802	0.17902
C	-0.70662	-1.35973	-1.47517
C	3.14463	-0.40737	0.91485
C	0.11806	2.01298	-2.29678
H	-0.33516	1.25601	-2.92093
C	-2.12757	-1.27937	-0.88588
C	-3.25436	-0.04381	0.96638
C	1.61464	2.49875	-0.49757
C	1.43029	3.88203	-0.63439
C	-0.28253	-2.78859	-1.79803
C	3.33557	-1.71458	0.42178
H	2.91746	-2.01622	-0.53290
C	2.16441	4.84054	0.26037
H	3.24685	4.71414	0.16040
H	1.91237	4.66292	1.31041
H	1.90811	5.87113	0.00902
C	0.55118	4.28884	-1.63928
H	0.37471	5.34932	-1.78797
C	3.73878	-0.03726	2.14039
H	3.58518	0.96608	2.52134
C	-0.09786	3.36416	-2.47336
H	-0.76219	3.69357	-3.26229
C	-3.55508	-0.72726	2.14591
H	-2.91260	-1.53279	2.48645
C	-4.06309	0.99337	0.49824
H	-3.80778	1.50888	-0.42197
C	4.10436	-2.62868	1.13965
H	4.25510	-3.62906	0.74764
C	-5.51029	0.67746	2.41507
H	-6.39258	0.95913	2.98136
C	-4.69027	-0.35914	2.87202
H	-4.93294	-0.88383	3.79052
C	4.49812	-0.95772	2.85460
H	4.94484	-0.66947	3.80063
C	4.68238	-2.25434	2.35684
H	5.27644	-2.97013	2.91645
C	-5.19759	1.35168	1.23033
H	-5.83389	2.15583	0.87488
H	-0.72803	-0.83001	-2.43098
H	0.65642	-1.44110	0.19920
H	1.84127	-0.23385	-1.76745

17.0464	17.9415	31.0234
38.5408	45.2839	53.7071
56.0052	57.1100	72.6274
80.9530	87.4428	93.3673
114.6232	128.5130	150.8126
169.3934	198.4161	203.1475
210.1300	239.1631	256.8821
267.9829	288.4277	310.5119
314.4177	336.0229	377.2680
407.5424	412.0594	418.3232
419.4886	466.5760	487.6172
497.7437	503.7304	511.4577
530.1258	530.6442	547.7264
567.2813	606.5916	615.3715
621.1899	628.4306	629.5060
631.1001	653.0341	665.3837
689.2002	695.7355	704.6364
723.8481	739.2704	761.5308
771.9751	785.2929	788.0734
804.9577	839.7218	852.7699
858.5073	879.6238	888.7426
911.3968	912.9265	939.1396
939.7189	957.5277	966.8463
990.5872	1000.9888	1001.5572
1010.5603	1011.3733	1015.8487
1016.3053	1022.7133	1034.7622
1047.0601	1055.6486	1058.3515
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1122.5593	1153.1003	1183.7687
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1202.8326	1207.0771	1216.1055
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1338.4862	1351.1921	1356.3031
1356.8727	1365.9654	1370.8731
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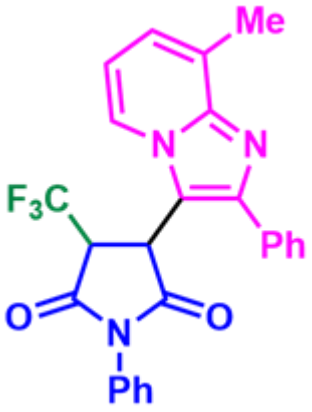
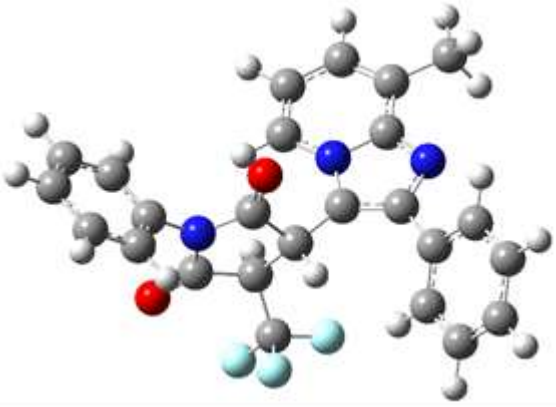
1457.8668	1472.1518	1479.4662
1486.7877	1495.2276	1520.1288
1528.8071	1532.3245	1580.4694
1617.5776	1625.8338	1637.3905
1642.0163	1643.6651	1662.1116
1762.9075	1845.2291	3057.1968
3073.5179	3092.6959	3113.6003
3119.0694	3150.7694	3194.8194
3198.3375	3202.3510	3205.4144
3208.3708	3211.9445	3214.9940
3215.9161	3220.0327	3220.3456
3227.1721	3245.5732	3270.1260

Statistical Thermodynamic Analysis

Temperature=373.15 K	Pressure=1 atm
Zero-point correction= 0.395871	Electronic Energy = -1578.30912445
Internal Energy (E)= -1577.87201745	Enthalpy (H)= -1577.87083545
Gibbs Free Energy (G)=-1577.99844345	Gibbs Free Energy of Solvation=-1577.92691342

St.Pt.	General Structure	Ball & Stick model
VII		

Cartesian co-ordinate

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O	3.19702	-0.66622	1.98694
F	0.69405	-2.84774	1.84336
N	-1.26857	1.76565	0.29895
N	2.39763	-0.11227	-0.11432
N	-3.29569	1.12804	-0.44984
C	0.05081	-0.40893	0.19482
C	1.17153	0.01413	-0.77510
C	-1.20192	0.39419	0.07185
C	-2.46744	0.03963	-0.39681
C	0.77382	-0.47436	1.57170
C	-2.94665	-1.27871	-0.86680
C	-0.31881	2.67252	0.71662
H	0.67995	2.30862	0.90946
C	2.27300	-0.45685	1.22979
C	3.66976	0.08393	-0.76198
C	-2.57290	2.16478	-0.02401
C	-2.95550	3.52732	0.12459
C	0.39031	-1.66613	2.43665
C	-2.69953	-2.46847	-0.16091
H	-2.17219	-2.43807	0.78548
C	-4.36405	3.93169	-0.21170
H	-5.08741	3.38316	0.40147
H	-4.59815	3.70454	-1.25757
H	-4.50809	5.00207	-0.04729

Frequencies

15.4306	18.1233	30.2838
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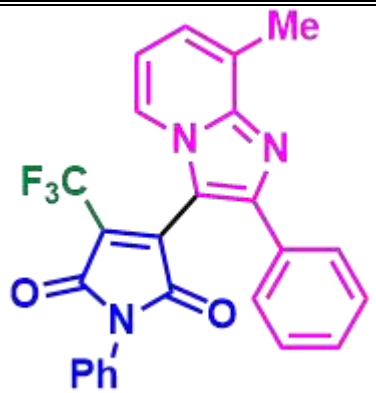
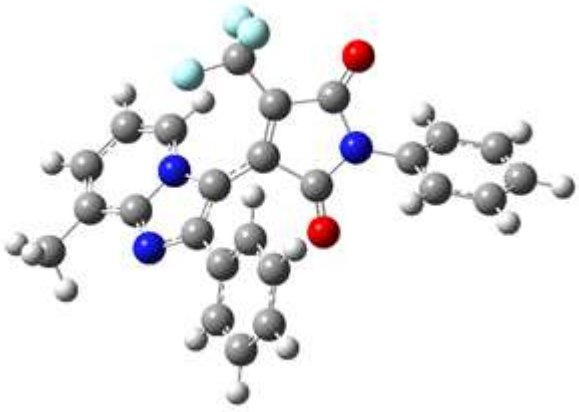
127.4160	130.5290	157.4843
175.6950	196.8082	200.2641
225.0018	238.5108	258.5326
267.1813	291.8583	309.3994
319.6657	342.2438	360.5210
397.0783	417.8761	420.1761
433.2583	475.3135	488.7914
504.6737	507.3408	521.5533
527.3246	534.6631	553.9193
584.7264	597.8388	622.0560
623.2764	628.5859	631.8764
633.9851	662.1599	676.7555
688.9116	705.1811	710.6506
726.0471	746.5771	750.1161
759.5621	769.9294	782.6131
788.2259	822.8863	853.4687
853.8543	863.5769	886.0773
890.1600	902.6080	931.1923
939.0650	941.9525	957.5383
975.8142	990.2020	993.2312
1009.4887	1012.8827	1013.9126
1016.3378	1028.9357	1046.3841
1048.9111	1054.3818	1062.0122
1067.1093	1097.3591	1100.9509
1101.3874	1102.3300	1140.3714
1150.8708	1179.9164	1181.3672

C	-1.99634	4.41500	0.56604	1184.9863	1190.0958	1197.9191
H	-2.25167	5.46301	0.68824	1200.2102	1204.1503	1215.8181
C	-3.69507	-1.34502	-2.05669	1236.8043	1253.6281	1264.8155
H	-3.89776	-0.43029	-2.60424	1276.7193	1284.0482	1317.2725
C	-0.67154	3.98580	0.85487	1334.6382	1337.7425	1356.3100
H	0.07798	4.69576	1.18432	1358.8392	1371.6043	1382.2795
C	4.24089	-0.96946	-1.47877	1391.8354	1398.4108	1413.9493
H	3.72853	-1.92416	-1.53996	1418.9106	1463.3804	1469.5923
C	4.30514	1.32336	-0.66405	1477.0853	1485.8614	1491.4815
H	3.84117	2.12807	-0.10298	1521.1217	1528.8239	1529.7419
C	-3.17002	-3.69361	-0.64292	1574.3261	1595.4444	1621.2377
H	-2.97405	-4.60138	-0.07976	1636.7613	1642.7141	1649.8851
C	6.12016	0.46136	-2.01736	1670.5539	1756.0064	1836.6557
H	7.07753	0.60878	-2.50767	3043.6611	3072.0709	3097.7963
C	5.47231	-0.77469	-2.10908	3099.4301	3133.9128	3184.1173
H	5.92335	-1.58798	-2.66872	3192.5876	3193.1161	3201.1645
C	-4.16614	-2.56825	-2.53514	3201.3724	3203.9611	3207.7201
H	-4.73735	-2.60039	-3.45845	3211.8525	3214.5722	3219.2179
C	-3.90128	-3.74916	-1.83228	3227.3768	3227.4385	3264.0720
H	-4.26739	-4.70124	-2.20499			
C	5.53758	1.50794	-1.29552			
H	6.03891	2.46797	-1.22388			
H	0.56706	0.41352	2.17774			
H	-0.19794	-1.42884	-0.12129			
H	1.84127	-0.23385	-1.76745			

Statistical Thermodynamic Analysis

Temperature=373.15 K Pressure=1 atm
Zero-point correction= 0.382956 Electronic Energy = -1577.88607903
Internal Energy (E)= -1577.46212303 Enthalpy (H)= -1577.46094203
Gibbs Free Energy (G)=-1577.58816603 Gibbs Free Energy of Solvation=-1577.56736877

St.Pt.	General Structure	Ball & Stick model
3ba		

Cartesian co-ordinate

Atoms	X	Y	Z

Frequencies

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55.3903	64.7396	71.6857

F	0.26656	-3.78911	1.17537	83.5022	107.5791	121.0982
O	-1.14825	1.12645	-1.35398	125.9346	143.3735	161.0673
F	1.50511	-2.15404	1.91841	177.2778	196.3227	214.2103
O	-2.71244	-2.47840	1.01310	226.0767	239.0952	260.7668
F	-0.40278	-2.59400	2.86860	270.0745	287.6936	305.8162
N	2.44051	-0.73185	-0.55189	323.1058	341.2687	347.6496
N	-2.30243	-0.54904	-0.23005	384.1388	415.5310	419.0912
N	3.14601	1.40539	-0.37647	425.3715	443.2829	493.2453
C	0.02312	-0.48627	0.08858	497.9293	508.7027	521.5025
C	-1.17453	0.18302	-0.59132	524.0559	538.1320	552.2547
C	1.34747	0.02926	-0.12150	578.4646	591.3437	626.1537
C	1.83845	1.34844	-0.02583	627.3327	628.8943	635.8297
C	-0.46602	-1.57158	0.74846	640.8805	666.0559	699.3292
C	1.13705	2.54270	0.47487	702.9145	705.9662	722.7041
C	2.54197	-2.05592	-0.90153	737.6734	759.5559	762.6714
H	1.65930	-2.66978	-0.79636	769.2632	775.0600	785.4821
C	-1.94202	-1.64823	0.56712	792.0683	807.0306	837.6265
C	-3.63587	-0.26806	-0.67655	851.8828	858.6350	861.0688
C	3.50484	0.15691	-0.71172	895.6238	906.0090	936.2579
C	4.75704	-0.31112	-1.18850	939.6846	967.1284	968.8684
C	0.22625	-2.52116	1.67104	985.8107	988.7481	991.2592
C	0.19701	2.46156	1.51719	1009.9994	1011.6682	1012.1386
H	-0.01152	1.50613	1.98851	1015.8029	1038.8966	1047.6959
C	5.89605	0.65890	-1.33931	1055.5836	1063.1947	1084.8260
H	6.13783	1.13248	-0.38172	1089.8710	1099.1955	1102.1008
H	5.63633	1.46324	-2.03597	1105.7350	1135.0307	1155.3195
H	6.78794	0.15023	-1.71202	1168.0890	1180.2402	1181.3632
C	4.85219	-1.65261	-1.50496	1189.2722	1195.1823	1198.7455
H	5.79307	-2.04900	-1.87356	1200.7973	1234.8076	1283.5646
C	1.43699	3.80286	-0.07285	1286.6807	1322.9082	1338.1879
H	2.16838	3.87201	-0.87128	1342.7872	1356.6034	1358.0448
C	3.73872	-2.52308	-1.37205	1362.3959	1382.7104	1407.9110
H	3.82121	-3.56912	-1.64206	1418.8771	1437.1101	1461.5794
C	-4.28266	0.88531	-0.22445	1470.2506	1477.0996	1486.1197
H	-3.77687	1.55420	0.46406	1492.1559	1501.6582	1523.6361
C	-4.26898	-1.14870	-1.55801	1531.4848	1548.9996	1598.8301
H	-3.74936	-2.03656	-1.90282	1620.7836	1635.2812	1643.2755
C	-0.44574	3.61065	1.98330	1647.0821	1654.6329	1668.2901
H	-1.16453	3.53235	2.79353	1746.6240	1815.3573	3045.6890
C	-6.22372	0.28327	-1.54378	3102.4127	3136.7682	3185.5046
H	-7.23295	0.49800	-1.88158	3191.3921	3192.4425	3199.8733
C	-5.57836	1.16157	-0.66744	3200.8759	3204.0912	3207.2503
H	-6.08338	2.05826	-0.32216	3208.7557	3214.3511	3214.6464
C	0.79230	4.94847	0.39313	3218.3668	3230.8312	3269.0713
H	1.02604	5.91364	-0.04651			
C	-0.15401	4.85652	1.42076			
H	-0.65362	5.74963	1.78408			
C	-5.56980	-0.87152	-1.98518			
H	-6.06743	-1.55465	-2.66640			
H	0.56706	0.41352	2.17774			
H	-0.19794	-1.42884	-0.12129			
H	1.84127	-0.23385	-1.76745			

Statistical Thermodynamic Analysis

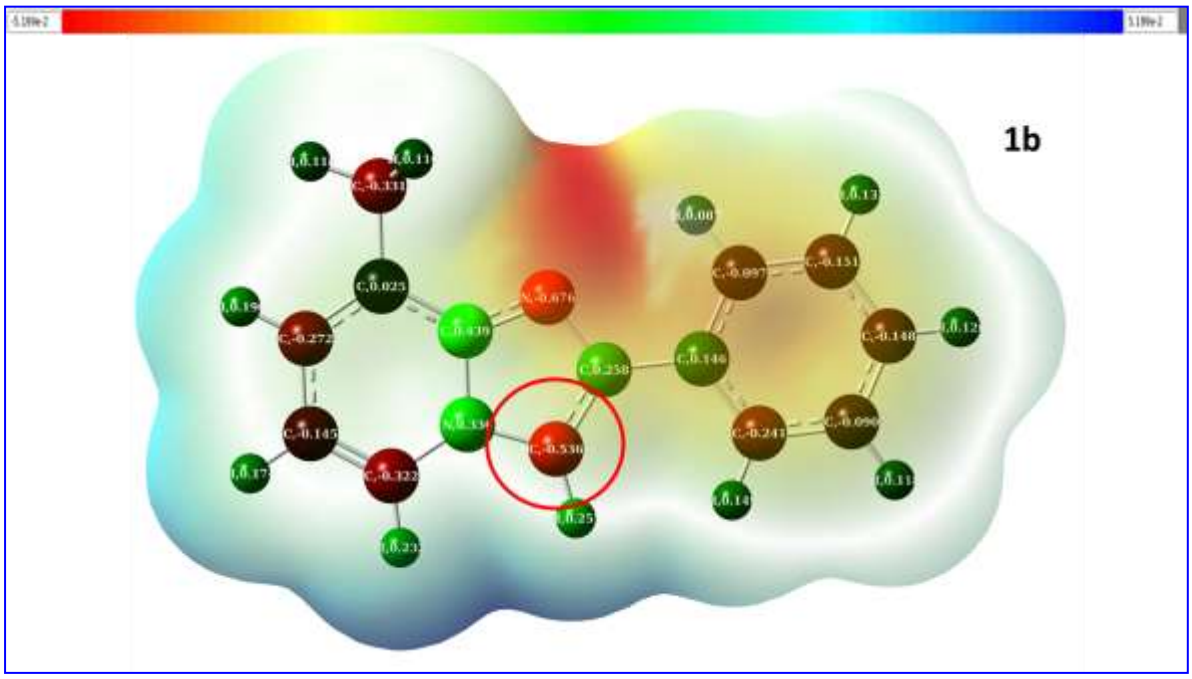
Temperature=373.15 K Pressure=1 atm

Zero-point correction= 0.358756 Electronic Energy = -1576.65655713

Internal Energy (E)= -1576.25716213 Enthalpy (H)= -1576.25598013

Gibbs Free Energy (G)=-1576.38175113 Gibbs Free Energy of Solvation=-1576.36371172

Merz Kollman Charges and Electron density mapped over electrostatic potential surface



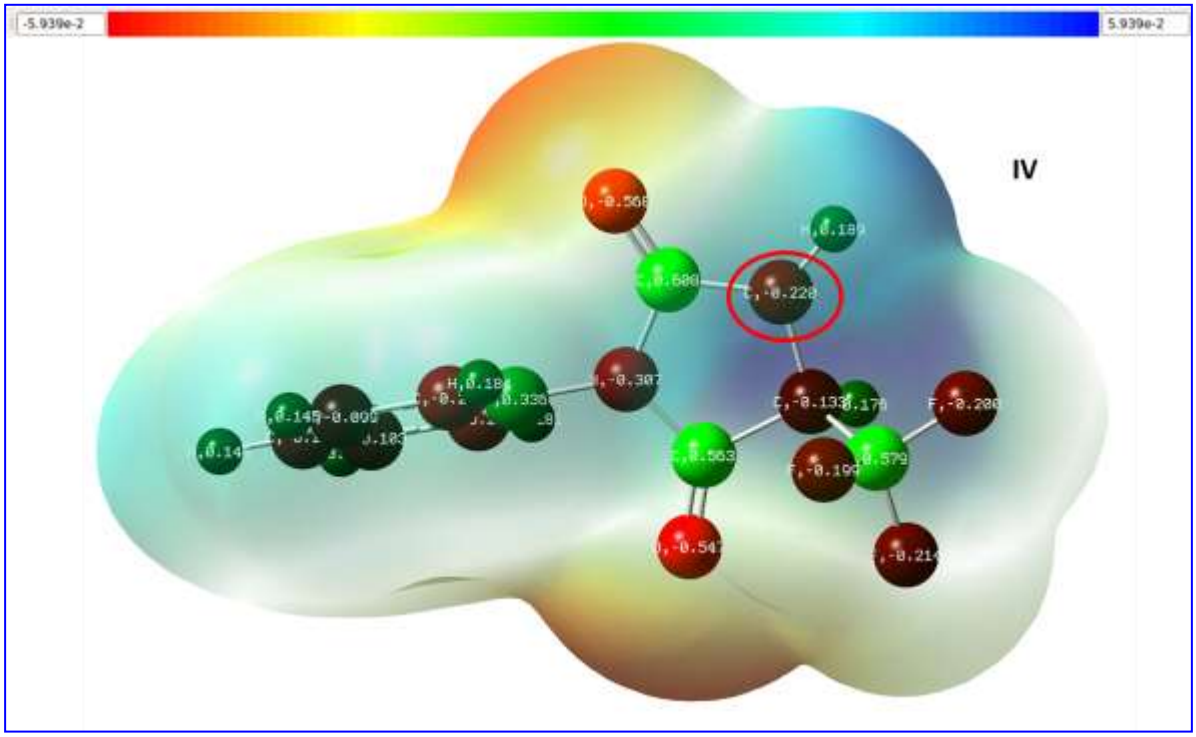


Figure 2: Merz Kollman Charges and Electron density mapped over electrostatic potential surface of intermediate **IV** and **1b** (DFT, Funtional UB3LYP, Basis 6-31+G(d,p))

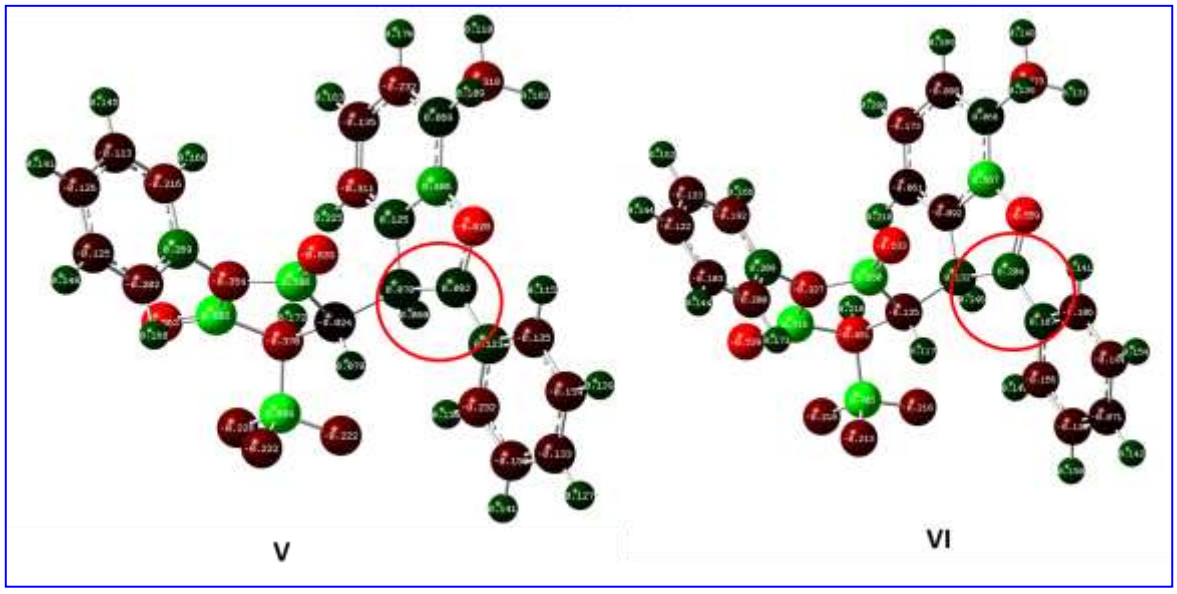


Figure 3: Increase in Merz Kollman charges from radical intermediate **V** to cationic intermediate **VI**, (DFT, Functional UB3LYP, Basis-6-31+G(d,p)). Increase in charge signifies single electron transfer.

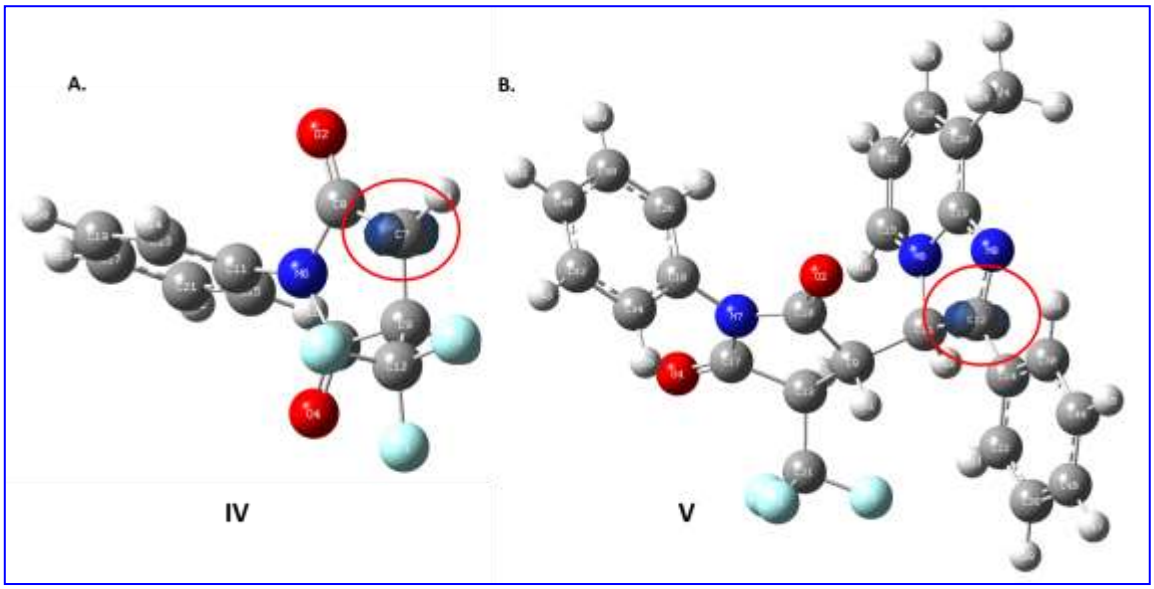


Figure 4: Spin density calculation for intermediate **IV** (iso value 0.05) and **V** (iso value 0.03), DFT-NBO calculation, Functional UB3LYP, Basis-6-31+G(d,p). Spin density signifies localization of the radical.

9. References:

(1) (a) A. K. Bagdi, M. Rahman, S. Santra, A. Majee and A. Hajra, *Adv. Synth. Catal*., 2013, **355**, 1741-1747; (b) B. S. Santaniello , M. J. Price and J. K. Murray Jr , *J. Chem. Educ.*, 2017, **94** , 388-391.

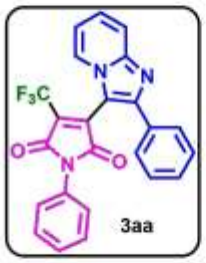
(2) (a) G. B. Deshmukh, N. S. Patil, V. B. Gaikwad, A. D. Bhole and S. V. Patil, *J. Chem. Pharm. Res.*, 2014, **6**, 393-399; (b) A. K. Ghosh, S. Samanta, P. Ghosh, S. Neogi and A. Hajra, *Org. Biomol. Chem.*, 2020, **18**, 3093-3097.

(3) Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

(4) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.

(5) J. Tomasi and M. Persico, *Chem. Rev.*, 1994, **94**, 2027–2094.

10. NMR spectra [^{1}H, ^{13}C{^{1}H} and ^{19}F] of synthesized products



^{1}H NMR: 400 MHz

Solvent: $CDCl_3$

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PROCNO                   1

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PULPROG           zg30
TD               32768
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DS                   2
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FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               168.31
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DE                6.50 usec
TE               300.0 K
D1            1.00000000 sec
TD0                  1

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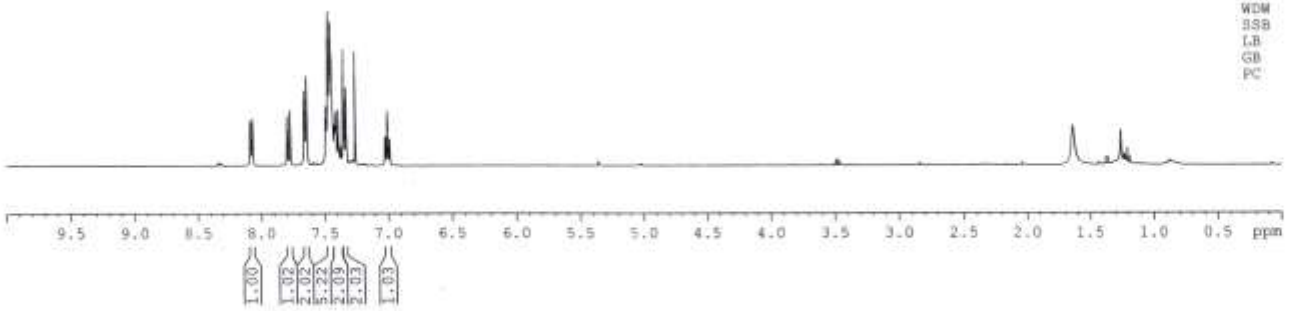

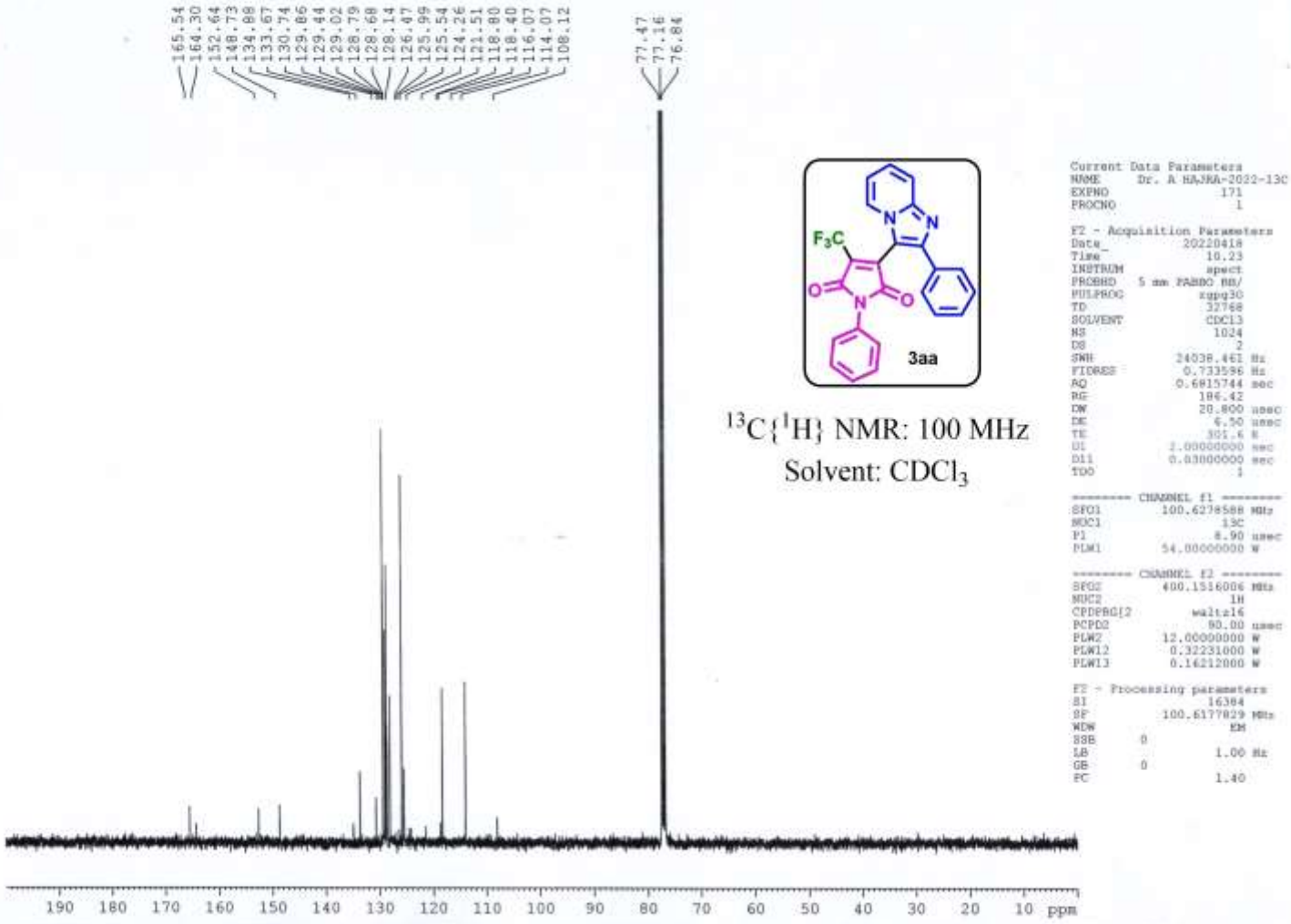


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SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
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D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

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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
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SF          100.6177829 MHz
WDW                   EM
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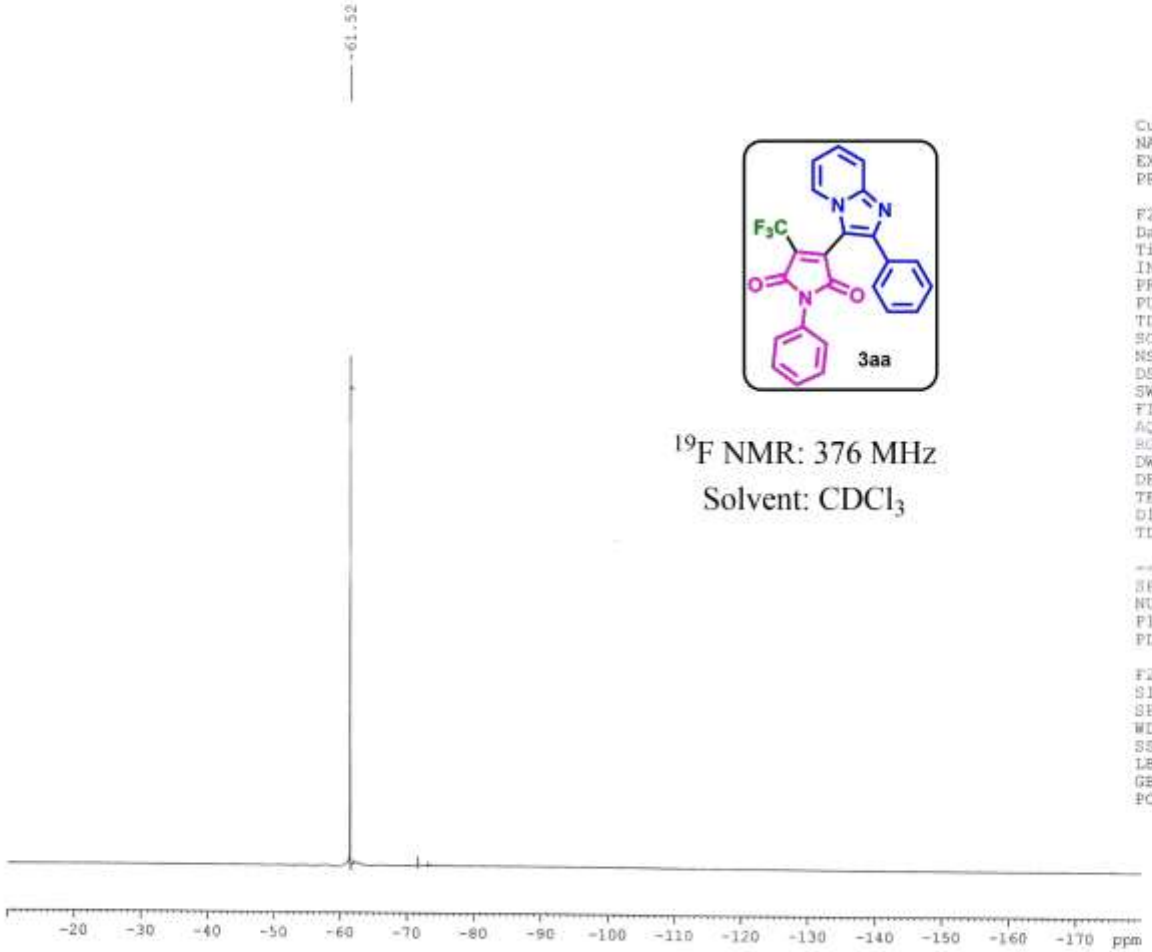

^{19}F NMR: 376 MHz

Solvent: $CDCl_3$

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EXPNO                  437
PROCNO                   1

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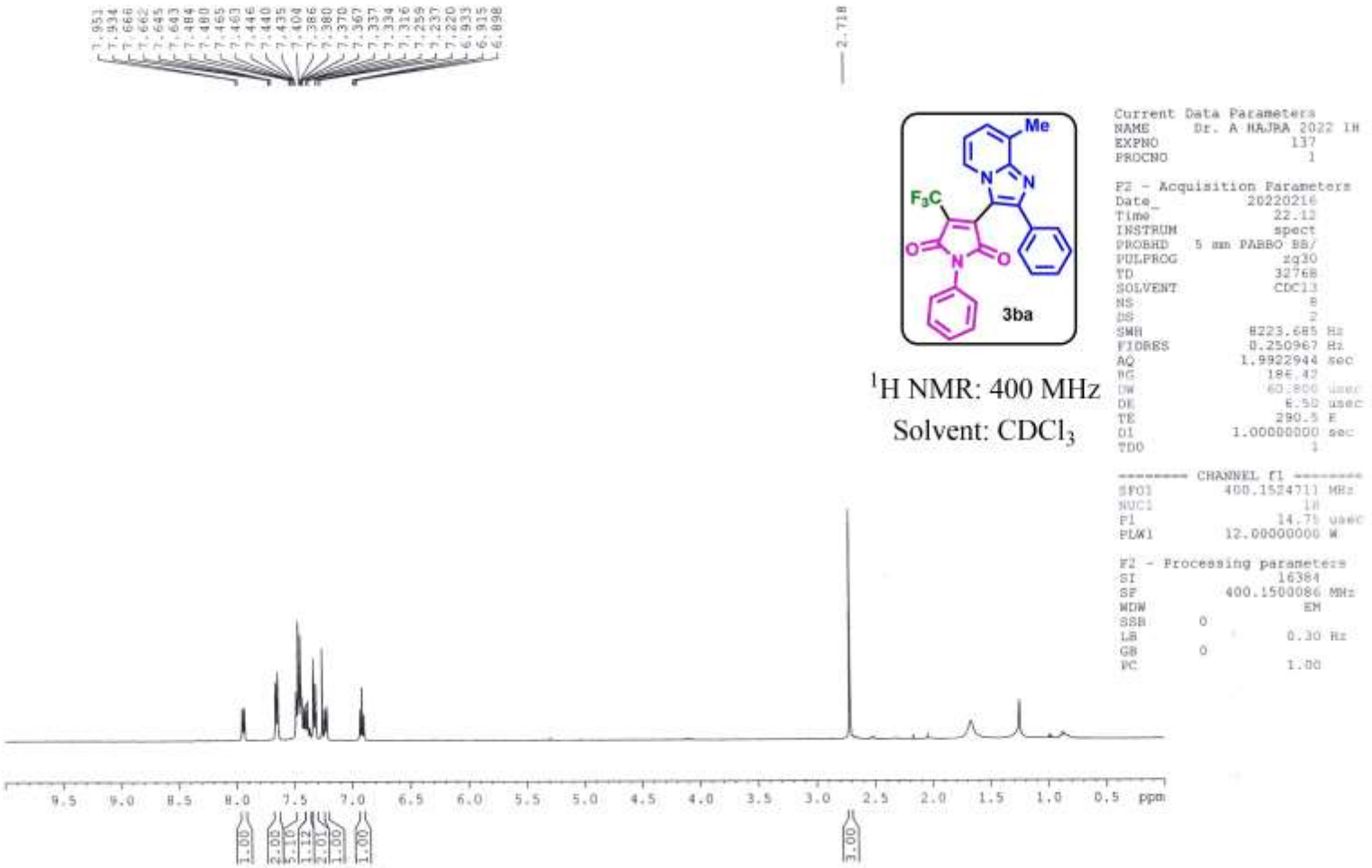
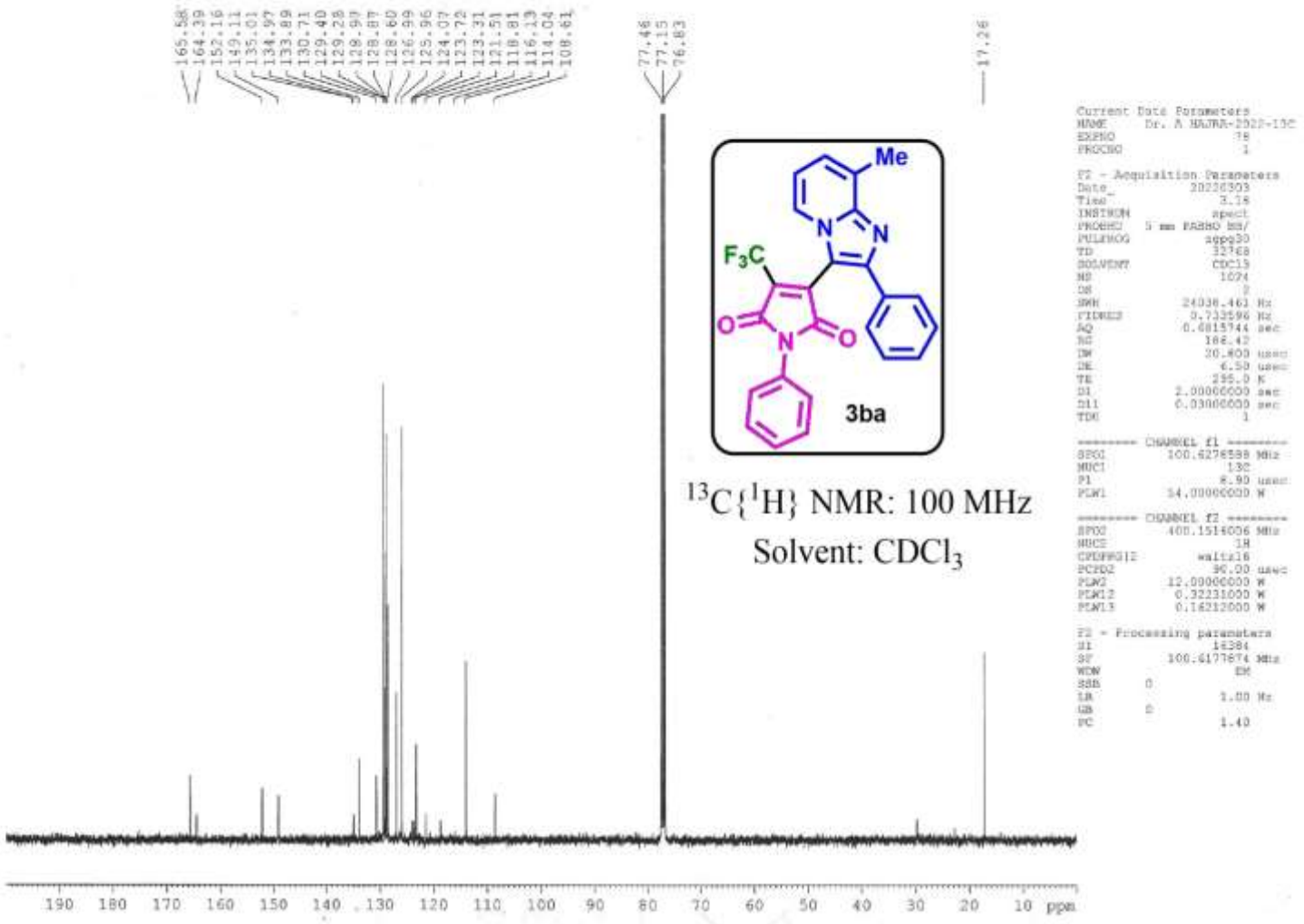
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG                168.31
DW                5.600 usec
DE                6.50 usec
TE                300.7 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
```


7.953
7.934
7.666
7.662
7.645
7.643
7.484
7.480
7.465
7.463
7.446
7.440
7.435
7.404
7.386
7.380
7.370
7.367
7.337
7.334
7.316
7.259
7.237
7.220
6.933
6.915
6.898
2.718
Me
N
N
F3C
O
O
N
3ba
1H NMR: 400 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A HAJRA 2022 1H
EXPNO 137
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220216
Time 22.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 186.42
DW 60.800 usec
DE 6.50 usec
TE 290.5 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 400.1500086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
1.00
2.00
2.10
1.12
2.01
1.00
1.00
3.00



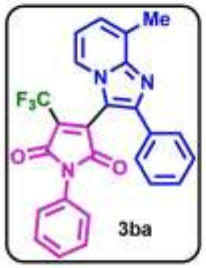

```
Current Data Parameters
NAME       Dr. A HAJRA-2022-15C
EXPNO                        78
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20220303
Time                       3.18
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                        168.42
DW                        20.800 usec
DE                         6.50 usec
TE                        295.0 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                100.6278588 MHz
NUC1                        13C
P1                         8.90 usec
PLW1                14.00000000 W

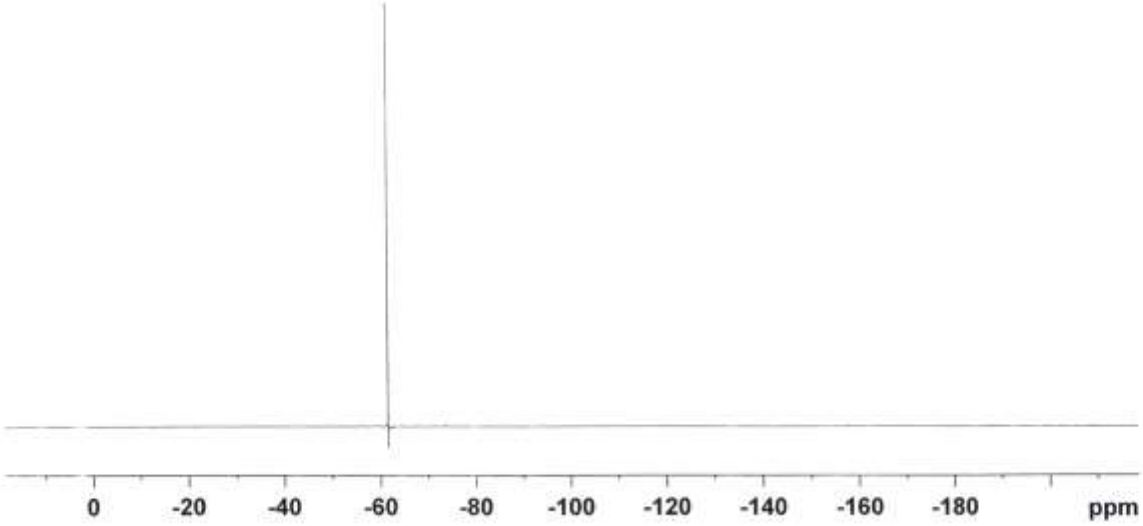
======== CHANNEL f2 ========
SFO2                400.1516006 MHz
NUC2                        1H
CPDPRG2                 waltz16
PCPD2                     90.00 usec
PLW2                12.00000000 W
PLW12                0.32231000 W
PLW13                0.16212000 W

F2 - Processing parameters
SI                         16384
SF                  100.6177674 MHz
WDW                           EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
```



^{19}F NMR: 376 MHz

Solvent: $CDCl_3$

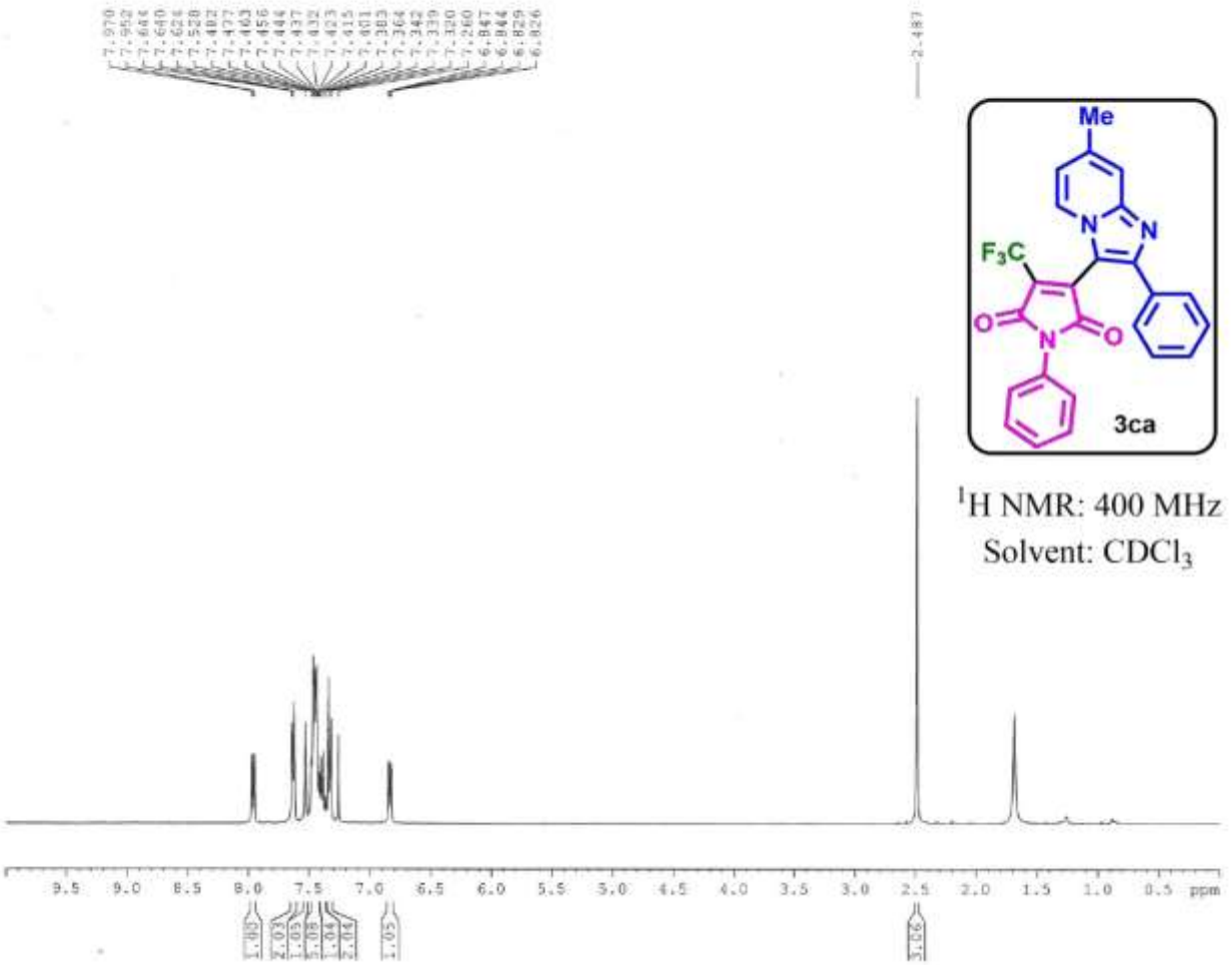



```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  138
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220216
Time                 22.14
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            zgflqn
TD                  32768
SOLVENT             CDCl3
NS                      4
DS                      2
SWH              89285.711 Hz
FIDRES           2.724784 Hz
AQ               0.1835008 sec
RG                  186.42
DW                  5.600 usec
DE                  6.50 usec
TE                  290.5 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
```

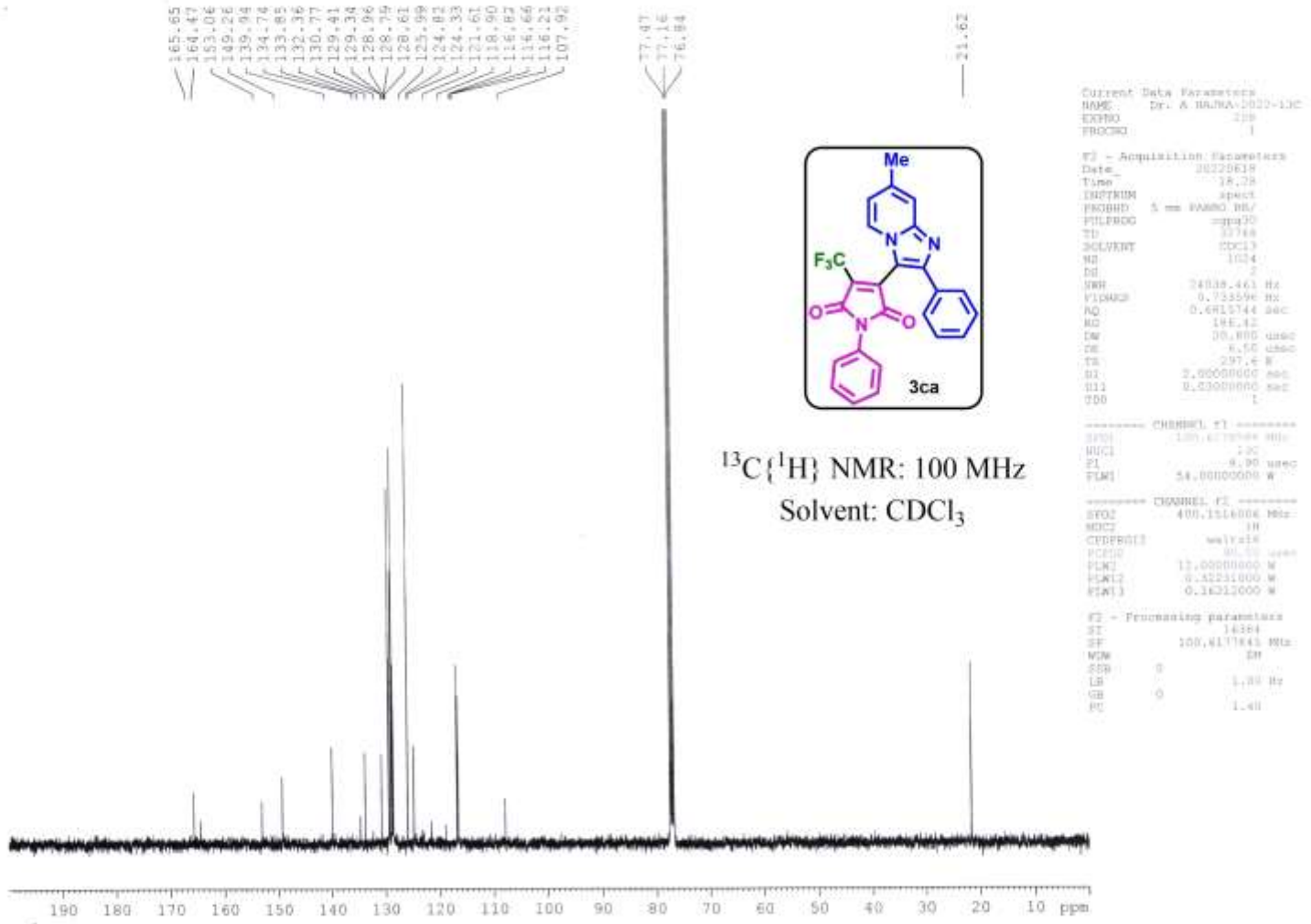



```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO              587
PROCNO               1

F2 - Acquisition Parameters
Date_          20220618
Time              17.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              120.16
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          400.1500087 MHz
WDW                 SM
SSB          0
LB               0.30 Hz
GB           0
PC               1.00
```



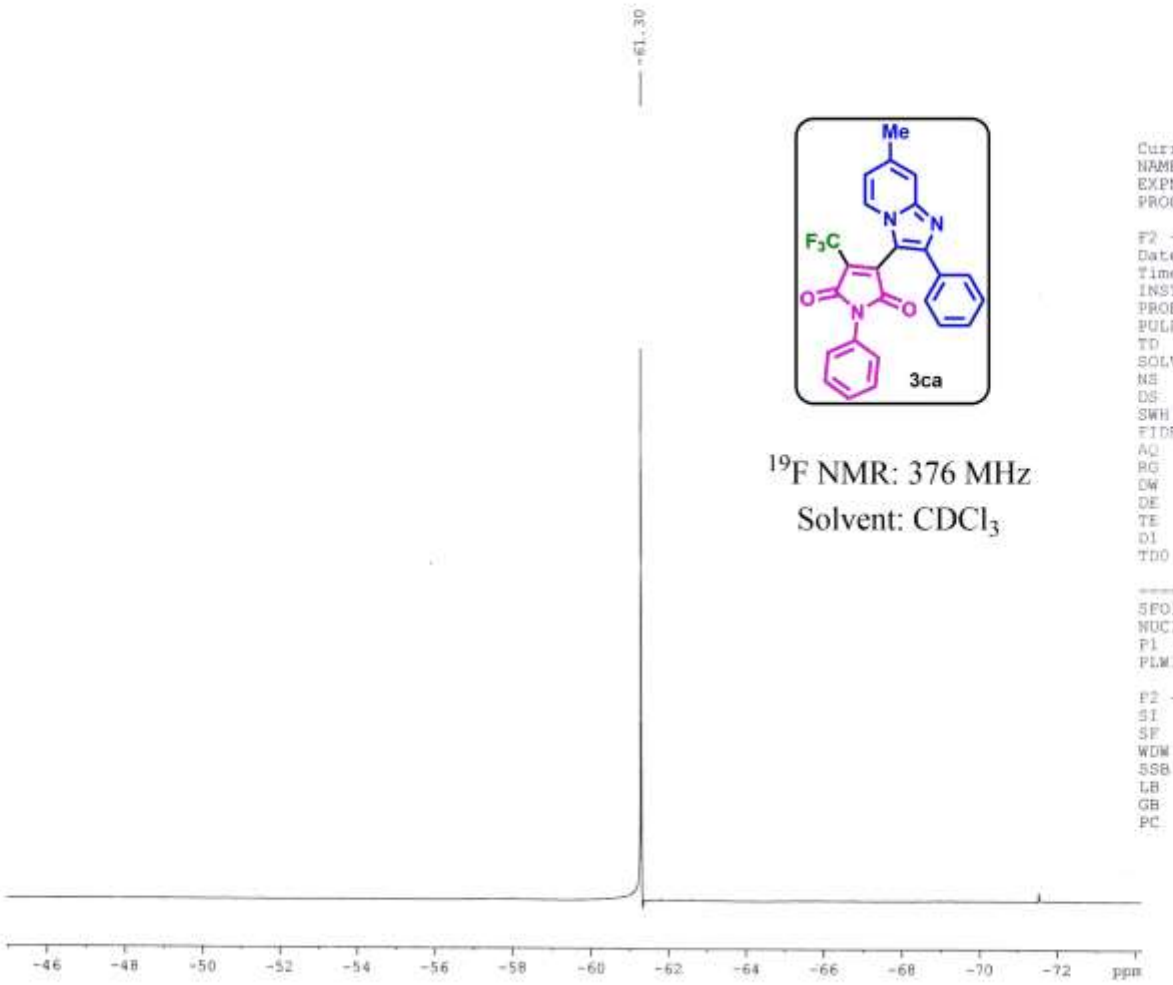
Current Data Parameters
NAME Dr. A RAJRA-2022-13C
EXPNO 220
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220619
Time 18.28
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 181.42
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6178566 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 11.00000000 W
PLW12 0.42231000 W
PLW13 0.16312000 W

F2 - Processing parameters
SI 16384
SF 100.6177841 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^{19}F NMR: 376 MHz

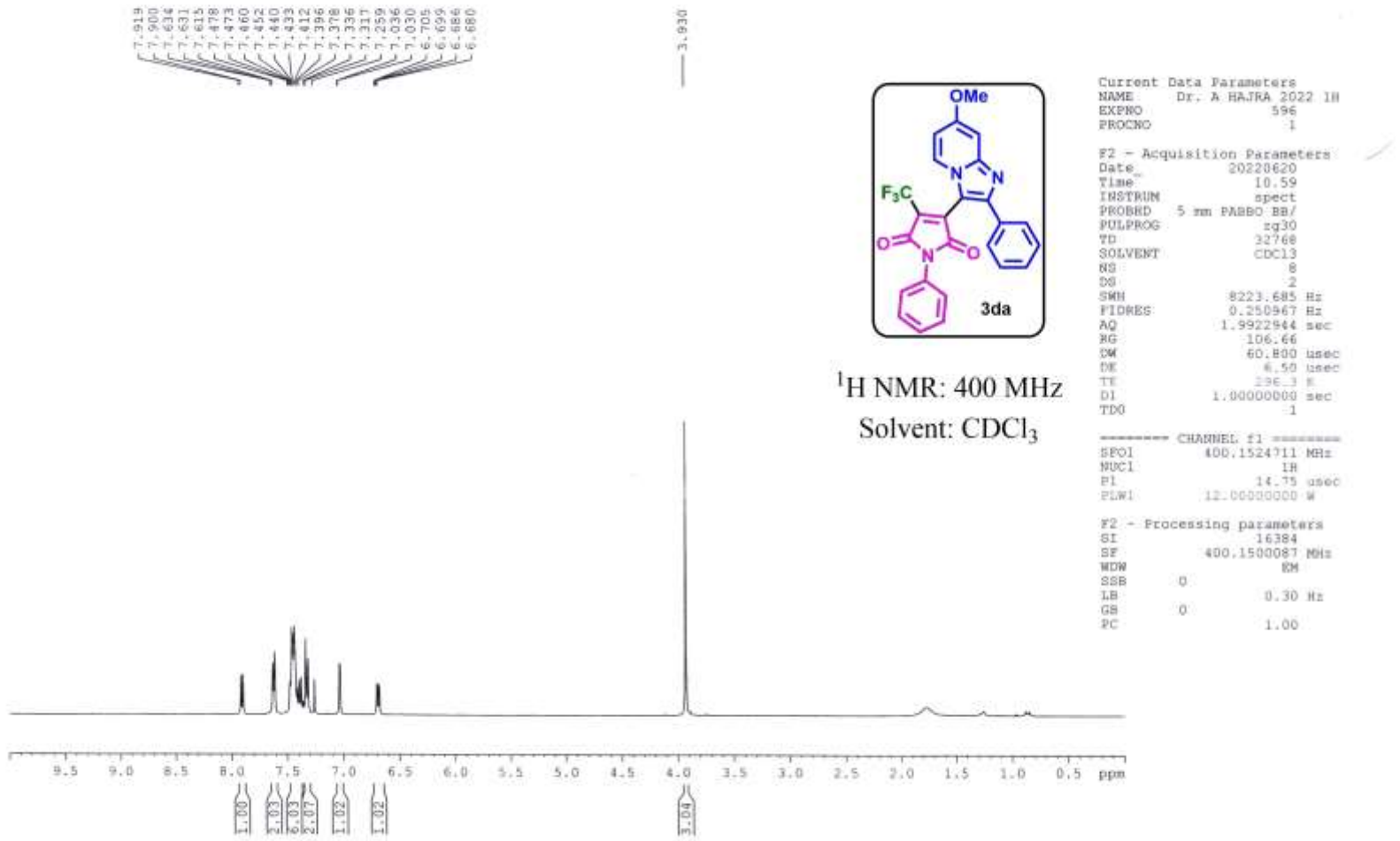
Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  572
PROCNO                   1

F2 - Acquisition Parameters
Date_             20220617
Time                 15.42
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgflqn
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       2
SWH              89285.711 Hz
FIDRES            2.724784 Hz
AQ                0.1835008 sec
RG                  186.42
DW                  5.600 usec
DE                  6.50 usec
TE                  297.2 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
```

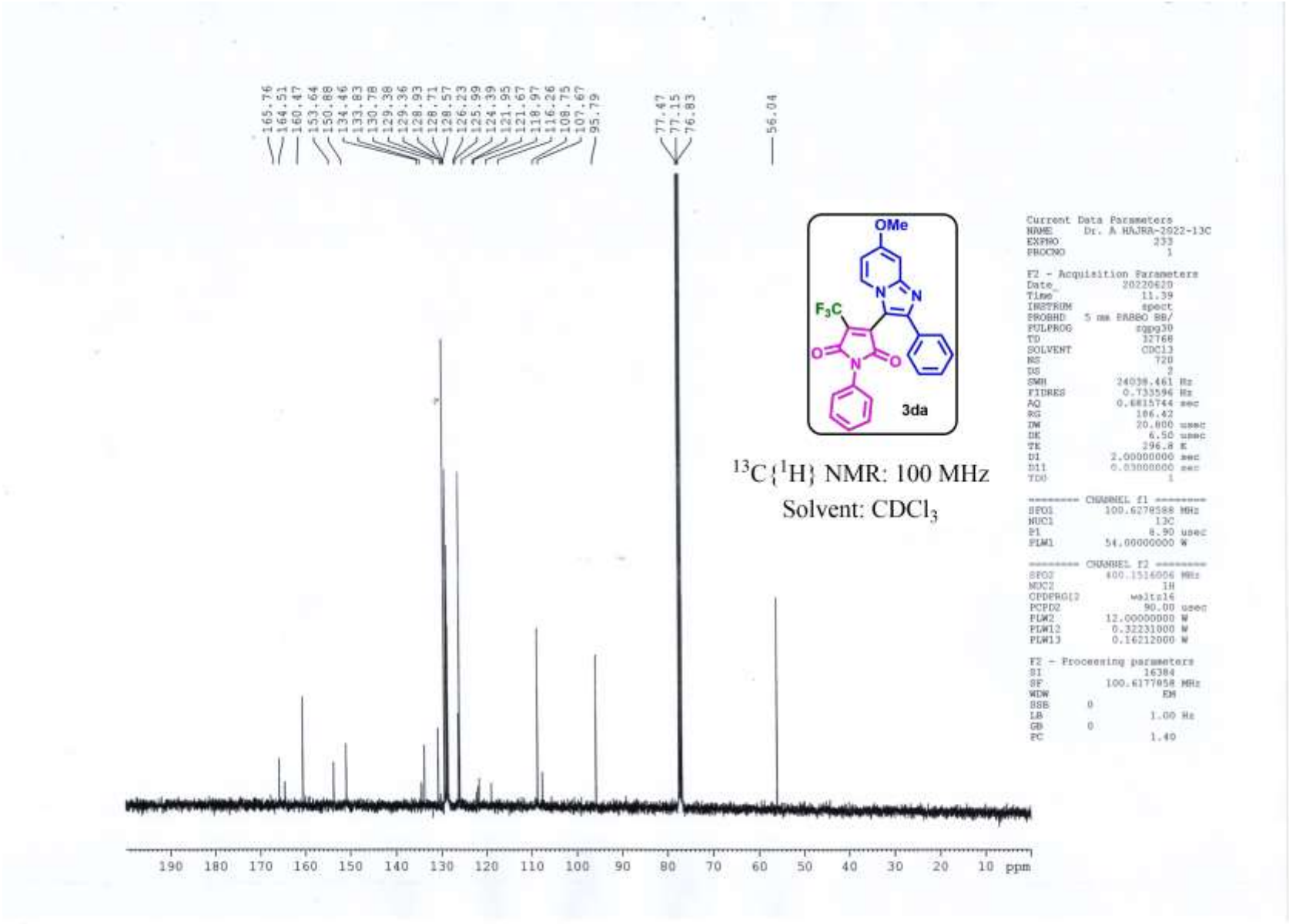



```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  596
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220620
Time_              10.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                106.66
DW                60.800 usec
DE                 6.50 usec
TE                296.3 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                1.00
```



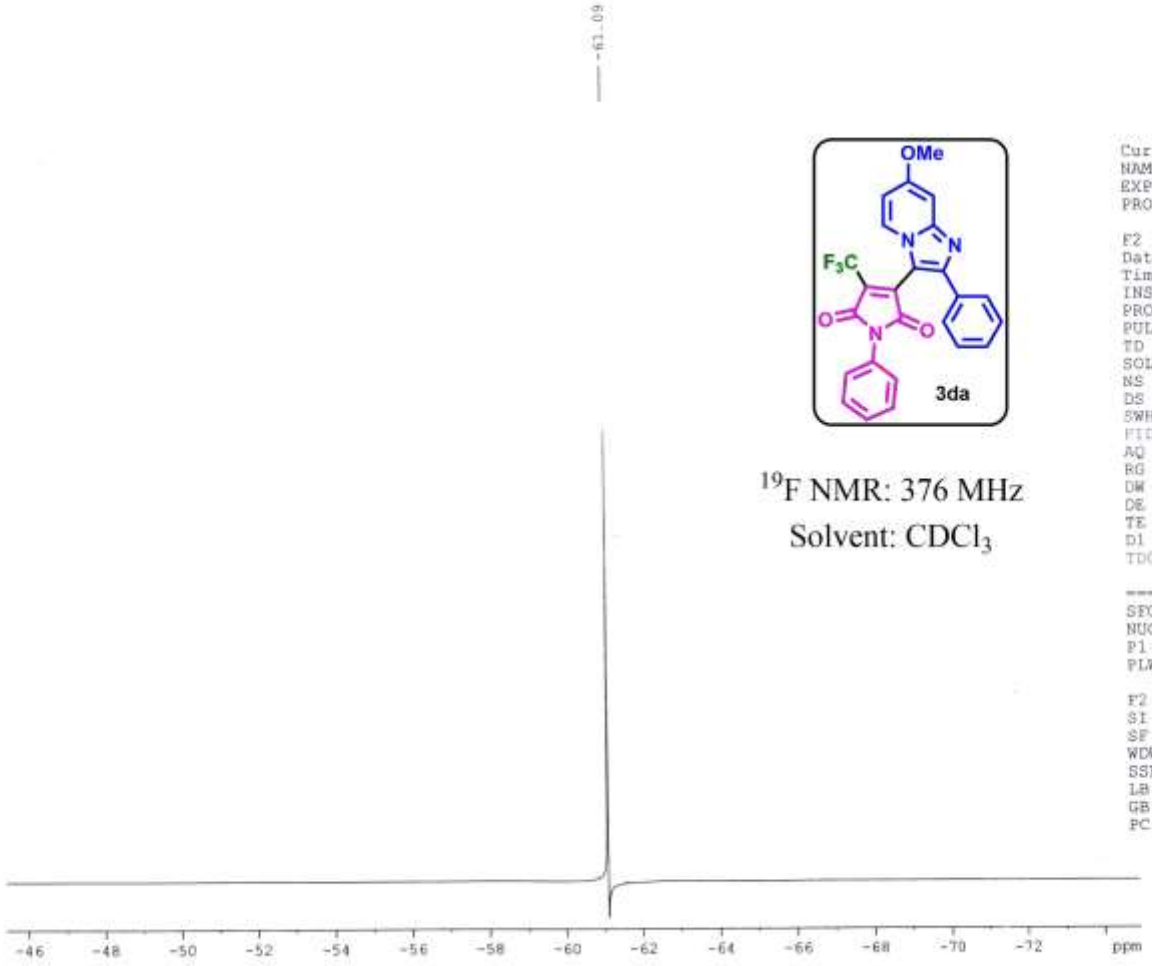

```
Current Data Parameters
NAME       Dr. A HAJRA-2022-13C
EXPNO                 233
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220620
Time_              11.39
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  720
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               296.8 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          100.6177058 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



^{19}F NMR: 376 MHz

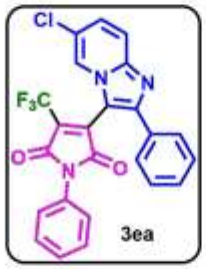
Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                597
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220620
Time              11.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ            0.1835008 sec
RG              186.42
DW                5.600 usec
DE                6.50 usec
TE              296.2 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

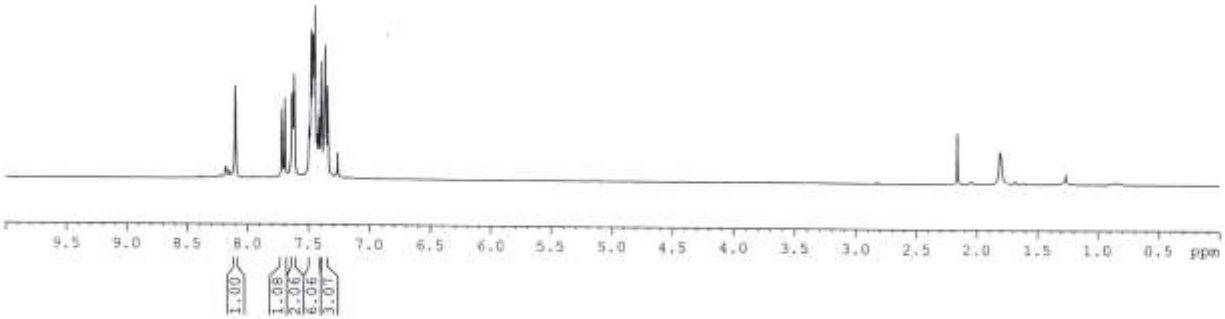
Solvent: $CDCl_3$

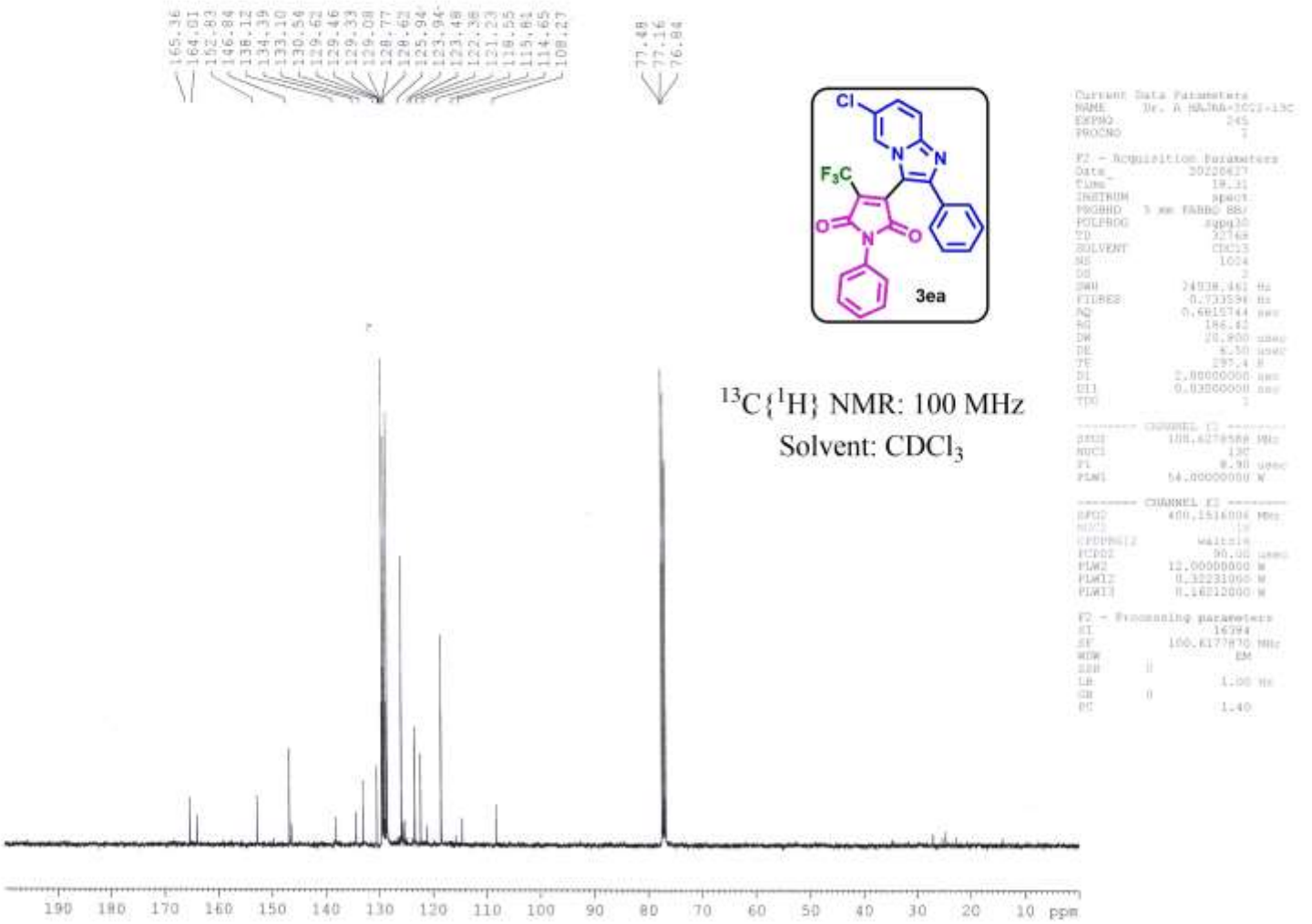
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  627
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220627
Time              20.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               87.66
DW              60.800 usec
DE               6.50 usec
TE              298.1 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          400.1500084 MHz
WDW                 EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```





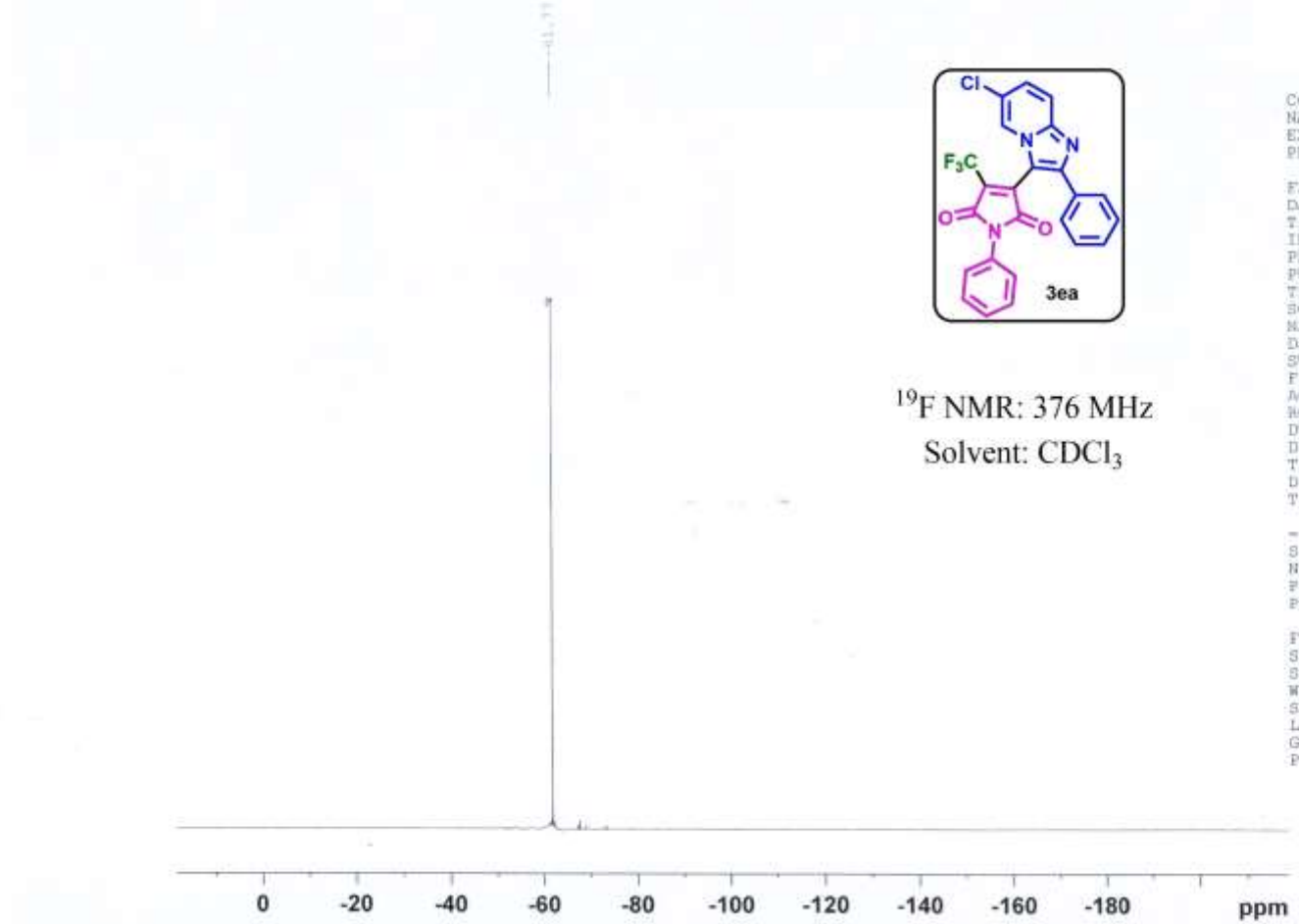
Current Data Parameters
NAME Dr. A MAJNA-3CC2-13C
EXPNO 245
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220627
Time 19.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 2
SWH 24038.461 Hz
FIDRES 0.733594 Hz
AQ 0.6815744 sec
RG 186.62
DW 20.800 usec
DE 6.50 usec
TE 297.4 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

======== 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 100.6177870 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^{19}F NMR: 376 MHz

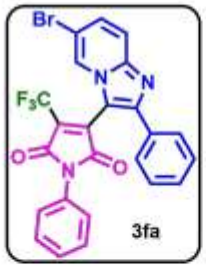
Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  625
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220627
Time              17.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG                87.66
DW                5.600 usec
DE                6.50 usec
TE                296.8 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

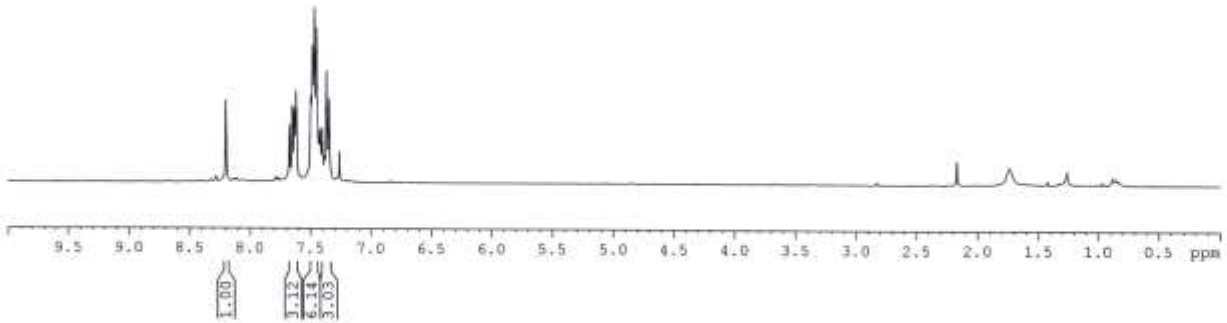
Solvent: $CDCl_3$

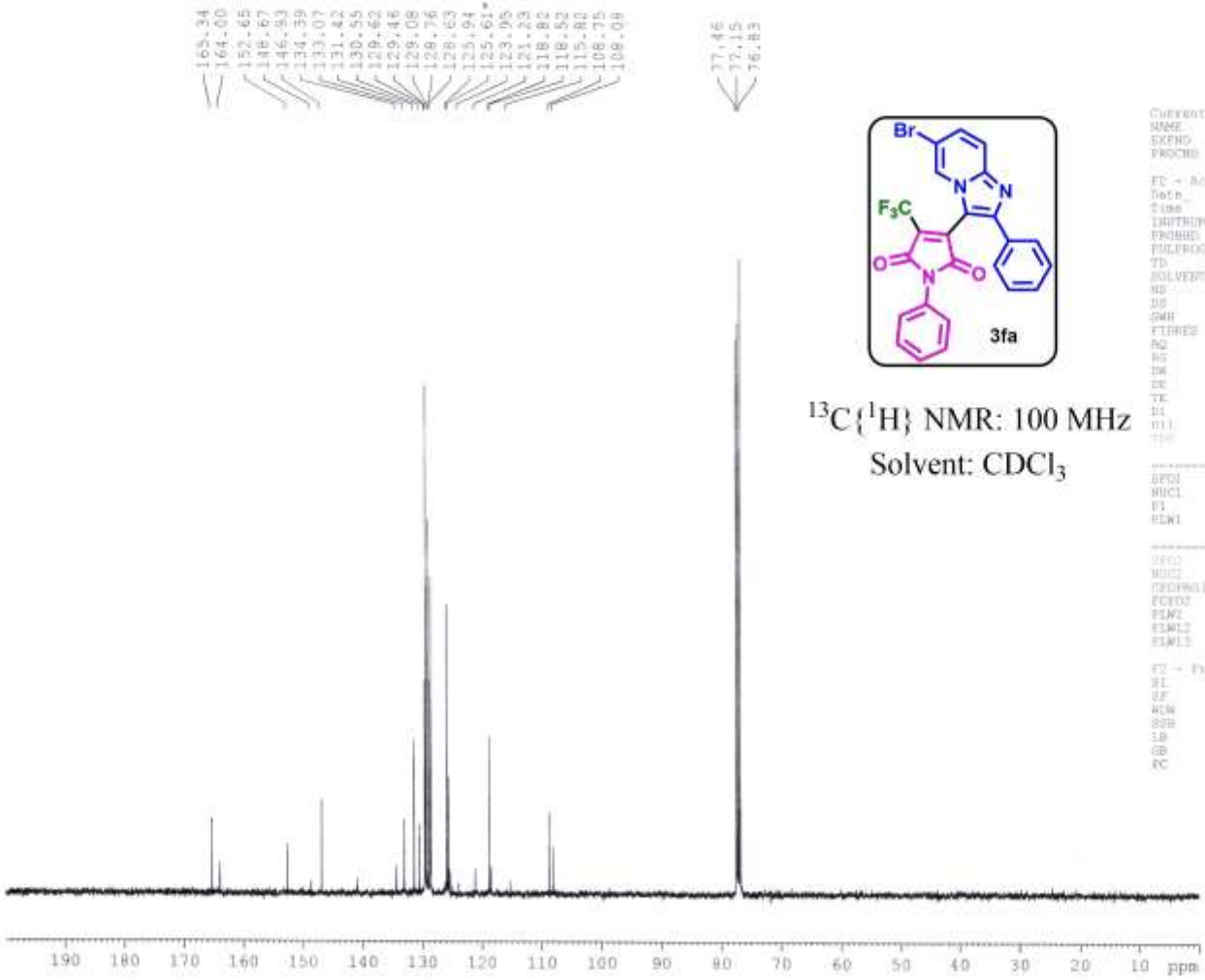
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                636
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220701
Time              20.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              106.66
DW               60.800 usec
DE                6.50 usec
TE              297.8 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          400.1500084 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





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

Solvent: $CDCl_3$

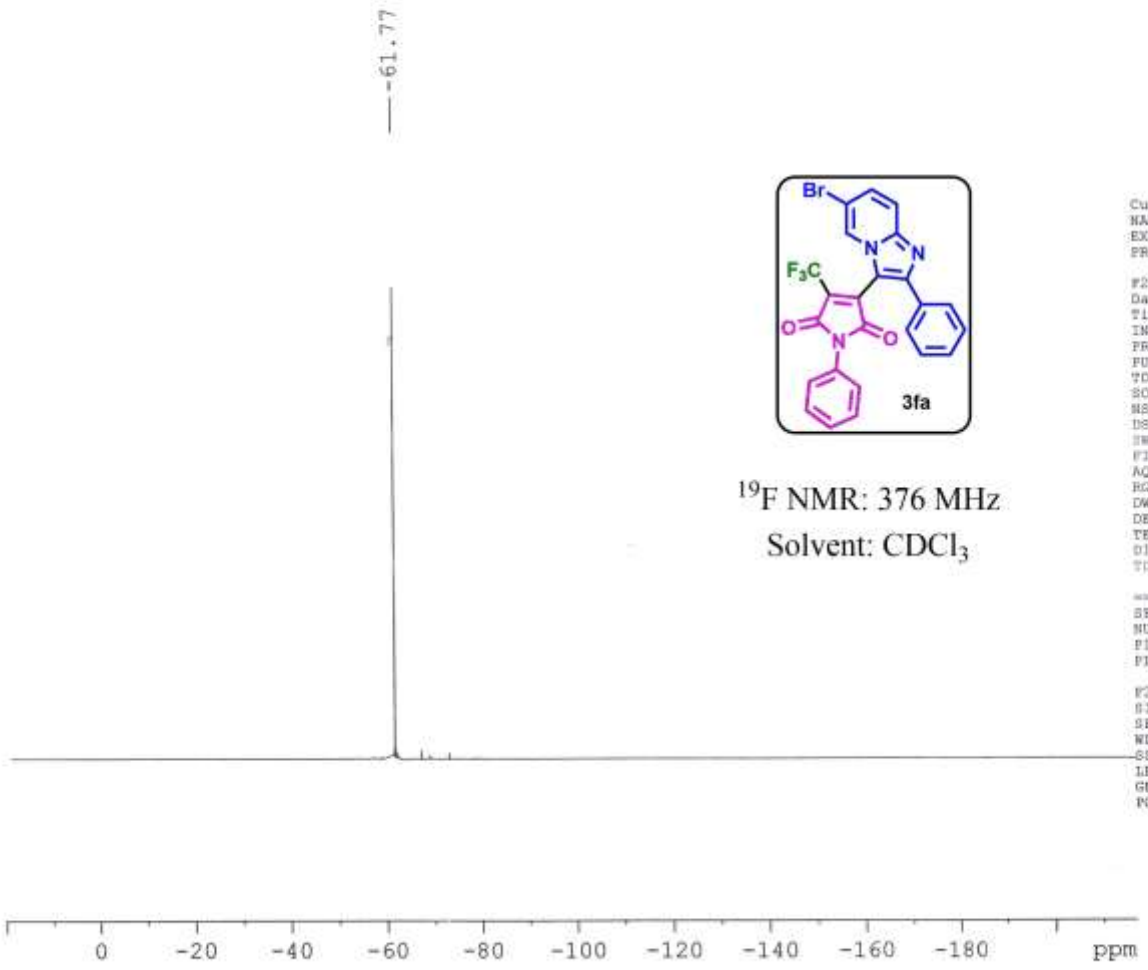
Current Data Parameters
NAME Dr. A MAJNA-2022-13C
EXPNO 259
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220701
Time 21.07
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 106.66
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 9.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.22231000 W
PLW13 0.16211000 W

F2 - Processing parameters
SI 16384
SF 100.6177873 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

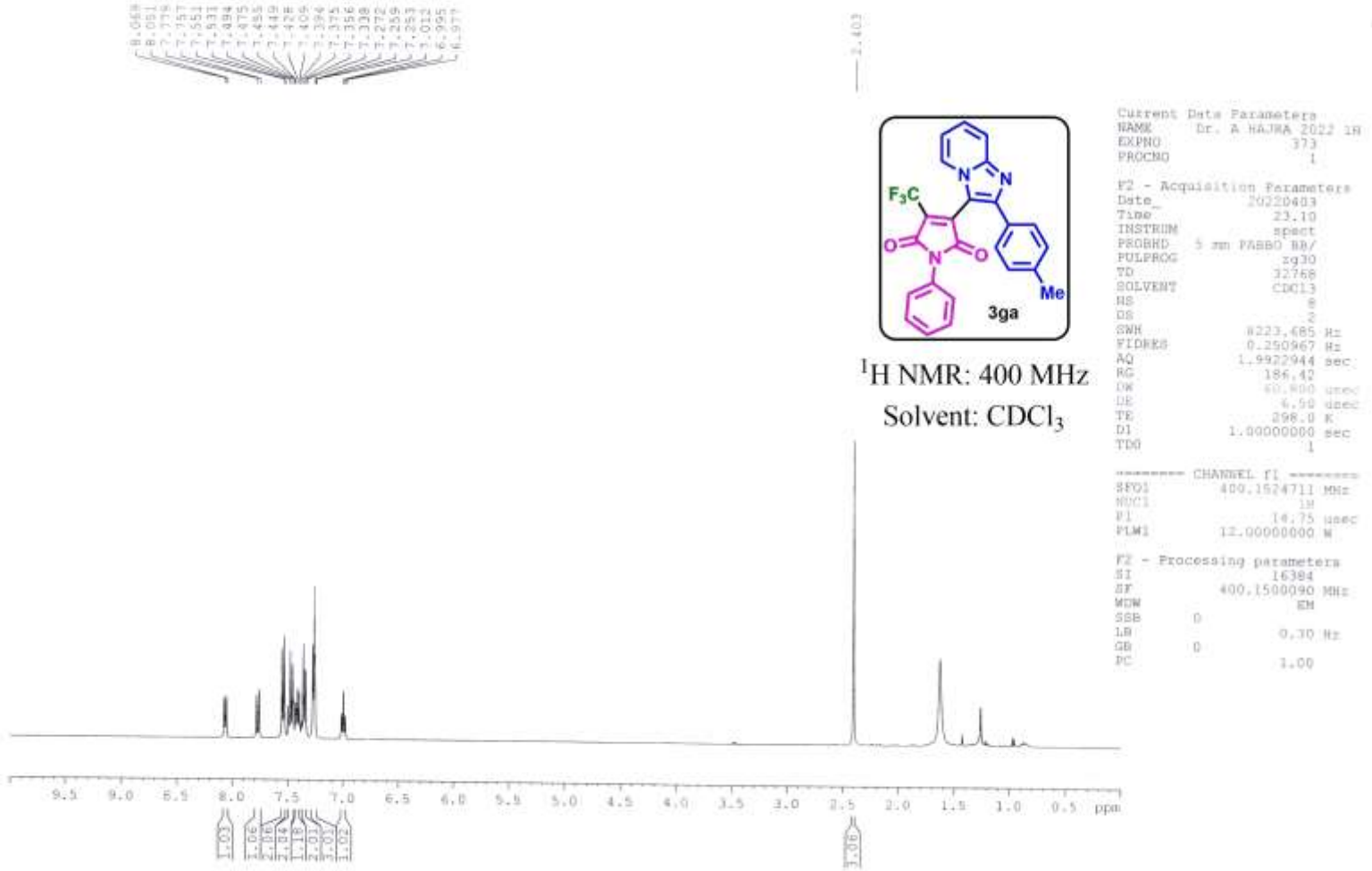


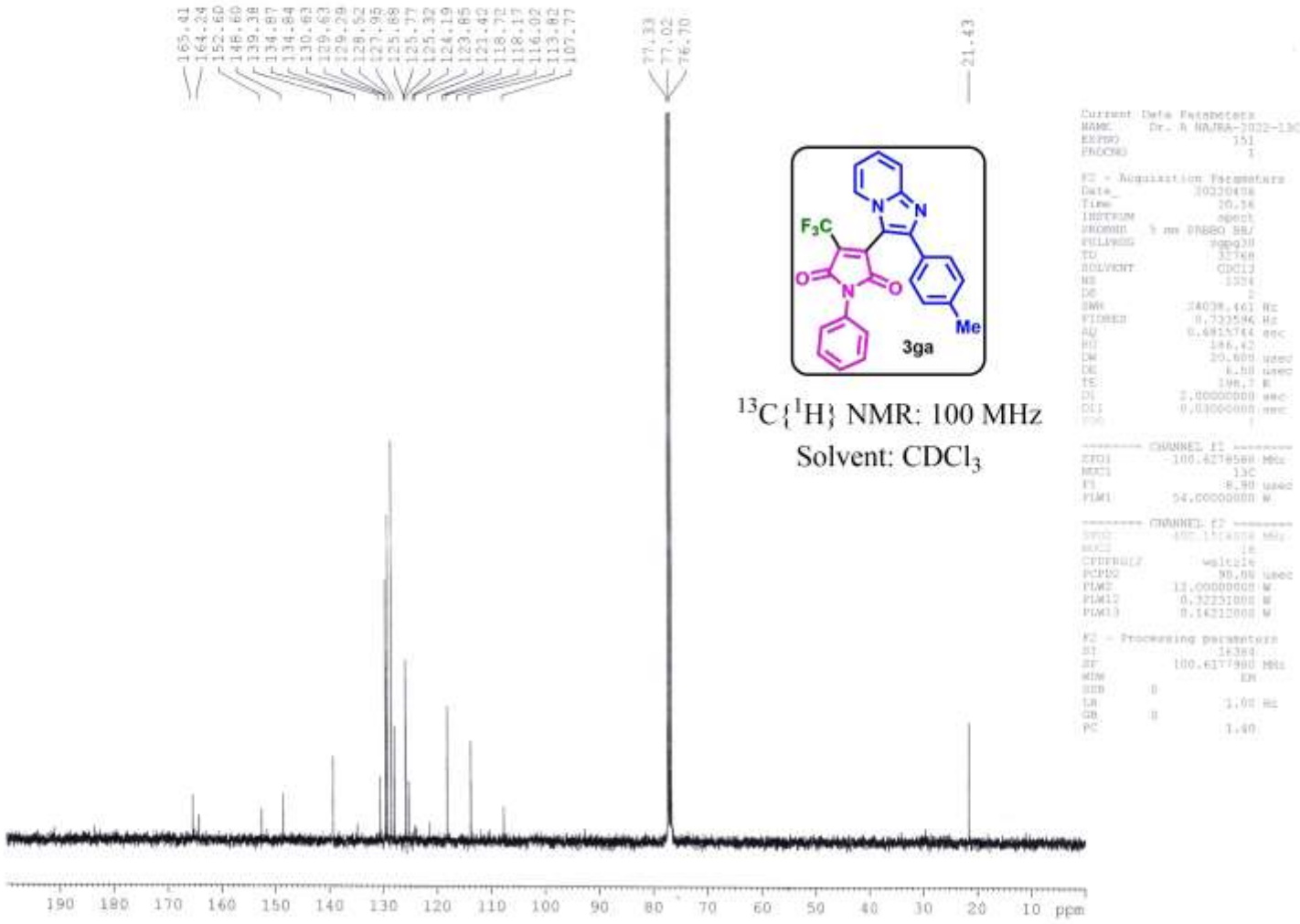

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  637
PROCNO                   1

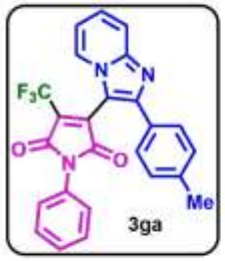
F2 - Acquisition Parameters
Date_           20220701
Time              20.15
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724384 Hz
AQ             0.1835008 sec
RG                106.66
DW                 5.600 usec
DE                 6.50 usec
TE                297.7 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
```


8.069
8.061
7.779
7.757
7.551
7.531
7.494
7.475
7.455
7.419
7.428
7.409
7.394
7.375
7.356
7.338
7.272
7.259
7.253
7.012
6.995
6.977
2.403
F3C
O
N
O
N
N
Me
3ga
1H NMR: 400 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A HAJRA 2022 1H
EXPNO 373
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220403
Time 23.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 186.42
DW 60.800 usec
DE 6.50 usec
TE 298.0 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 400.1500090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
1.03
2.90
1.04
2.18
1.01
1.01
1.02
3.06


165.41
164.24
152.60
146.60
139.38
134.87
134.84
130.63
129.63
129.29
128.52
127.95
125.68
125.77
125.32
124.19
123.85
121.42
118.72
118.17
116.02
113.82
107.77
77.33
77.02
76.70
21.43
F3C
N
N
O
O
N
Me
3ga
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



^{19}F NMR: 376 MHz

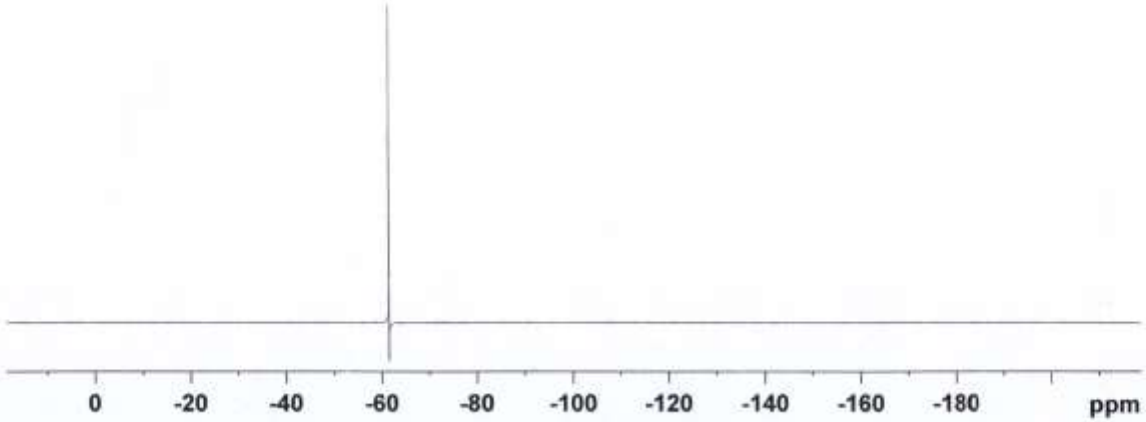
Solvent: $CDCl_3$

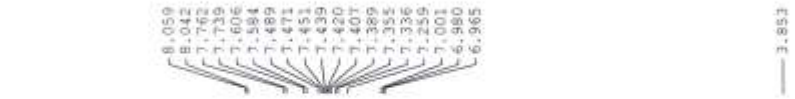
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  342
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220330
Time              21.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG               148.91
DW                5.600 usec
DE                6.50 usec
TE              298.6 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

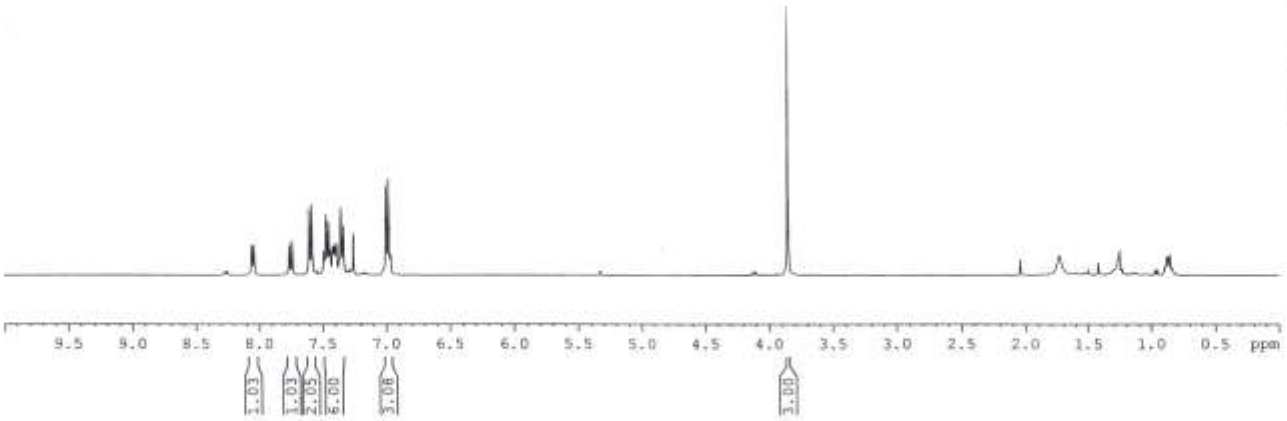
Solvent: $CDCl_3$

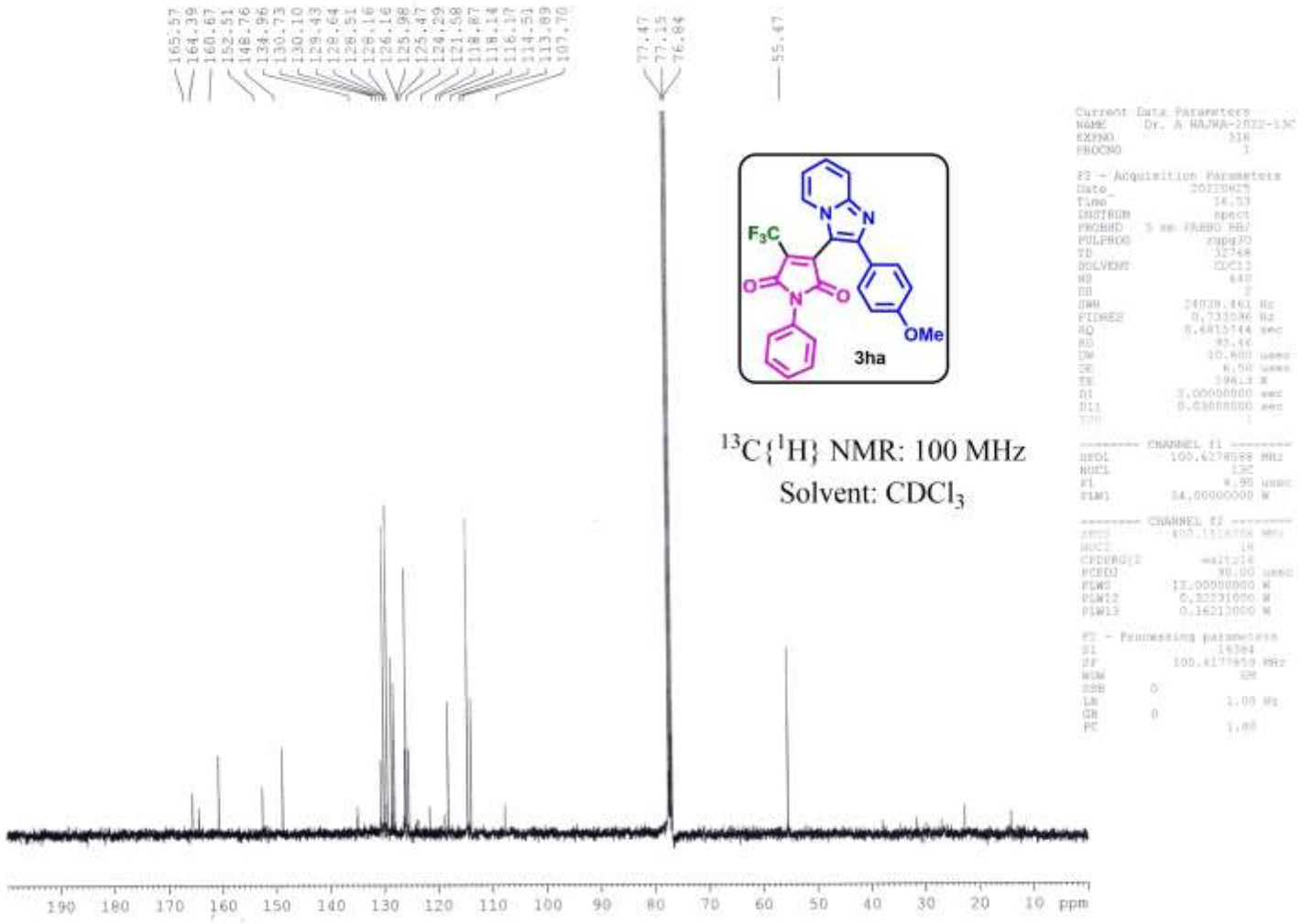
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  763
PROCNO                   1

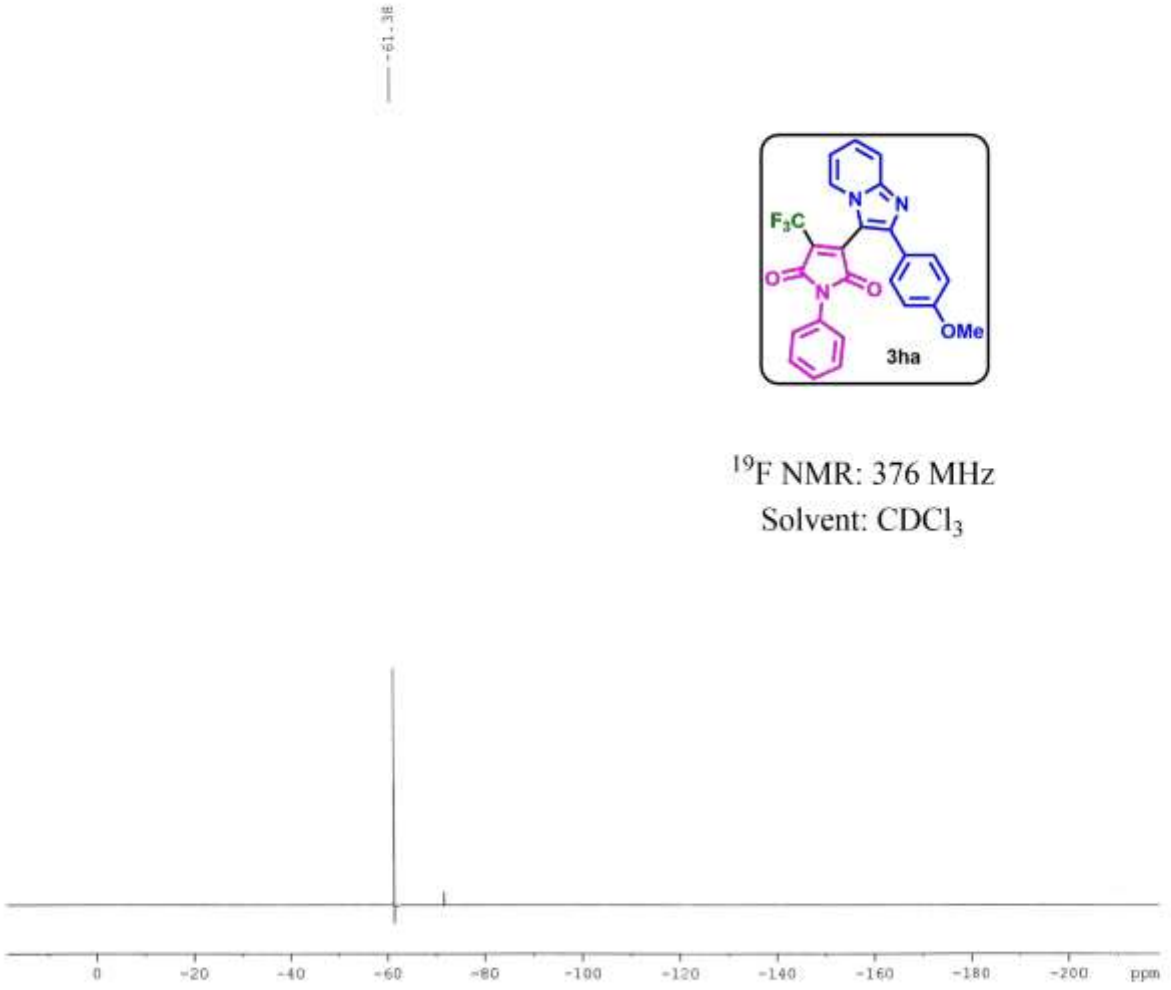
F2 - Acquisition Parameters
Date_           20220825
Time              16.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              93.46
DW              60.800 usec
DE               6.50 usec
TE              295.8 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              1.00
```




165.57
164.39
160.67
152.51
148.76
134.96
130.73
130.10
129.43
129.64
126.51
126.16
126.16
125.98
125.47
124.29
121.58
118.87
118.14
116.17
114.51
113.89
107.70
77.47
77.15
76.84
55.47
F3C
N
N
O
O
N
OMe
3ha
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



^{19}F NMR: 376 MHz

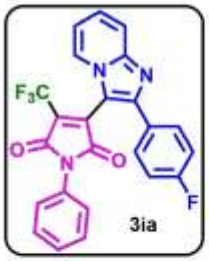
Solvent: $CDCl_3$

```
Current Data Parameters
NAME       Dr. A HAJRA 2022 1H
EXPNO                  764
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220825
Time                16.21
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgflqn
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH            69285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG                 93.46
DW                 5.600 usec
DE                 6.50 usec
TE                 295.8 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

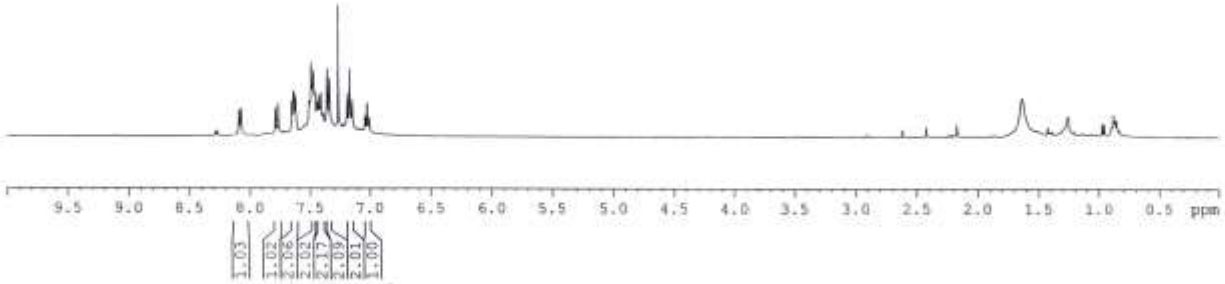
Solvent: $CDCl_3$

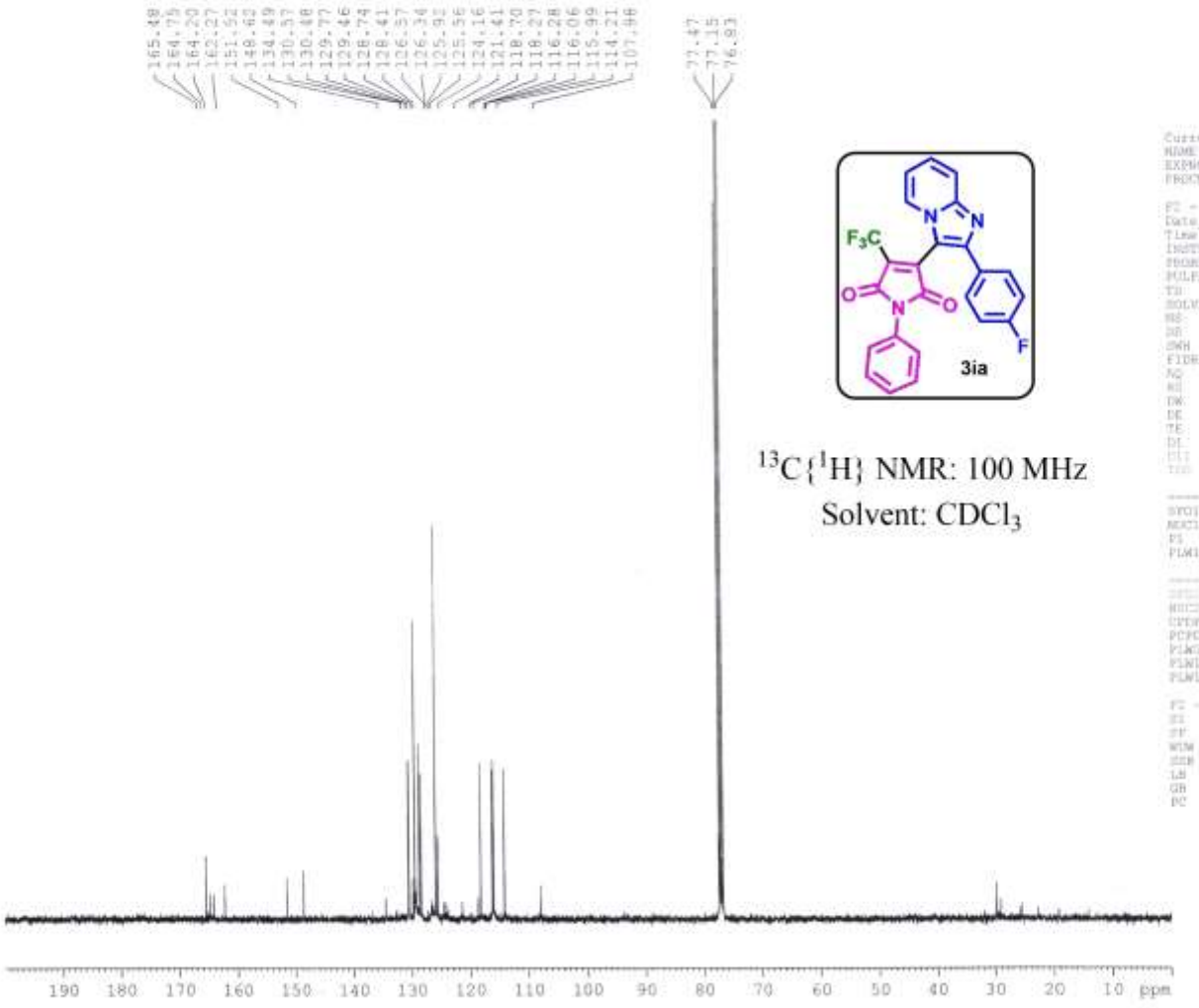
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  960
PROCNO                   1

F2 - Acquisition Parameters
Date_           20221031
Time              10.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                135.7
DW               60.800 usec
DE                6.50 usec
TE               294.1 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          400.1500084 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





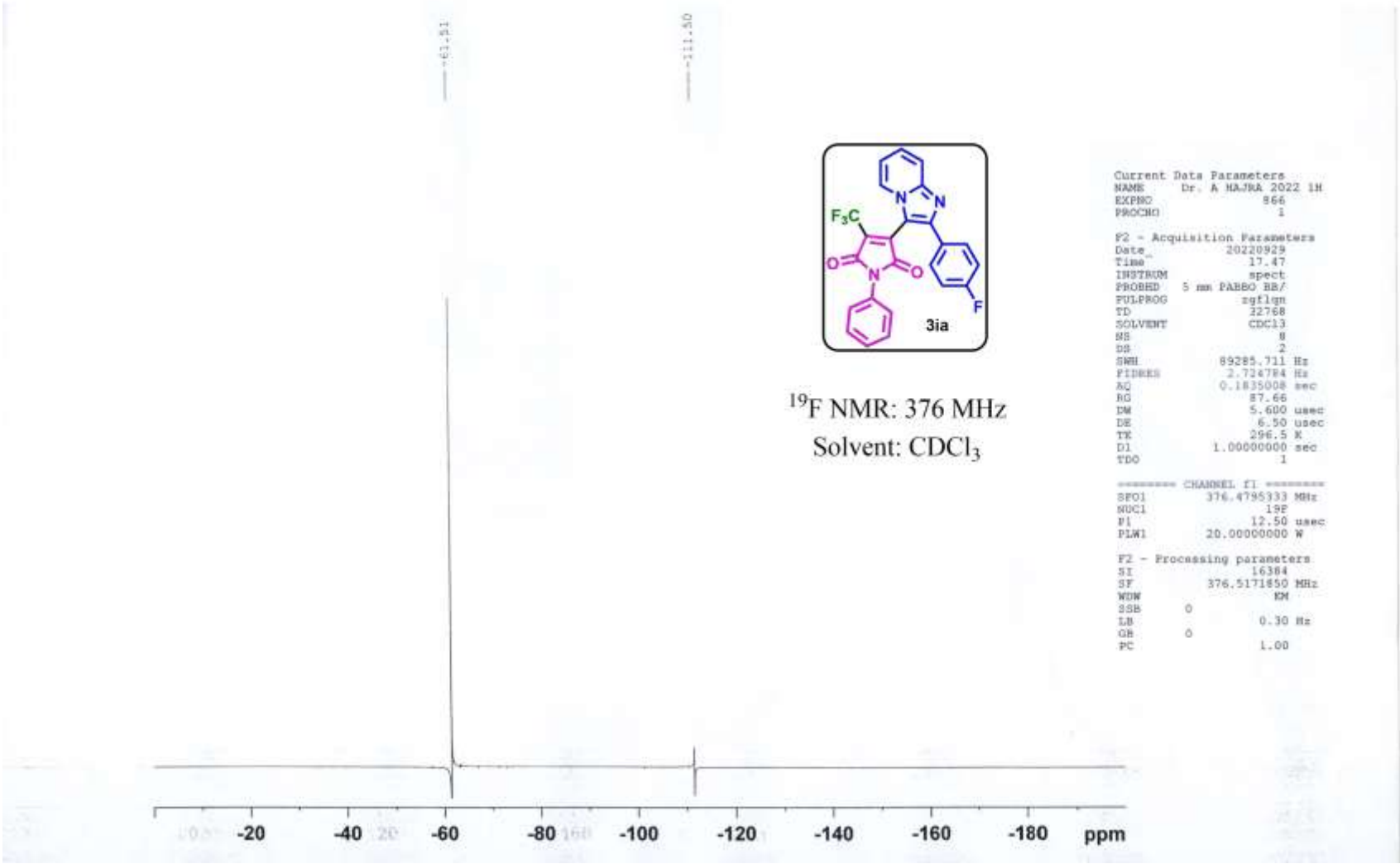
Current Data Parameters
NAME Dr. A MAJNA-2025-13C
EXPNO 455
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221219
Time 12.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 2
SWH 28030.661 Hz
FIDRES 0.855596 Hz
AQ 0.6815744 sec
RG 188.42
DW 20.800 usec
DE 6.50 usec
TE 292.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6278568 MHz
NUC1 13C
P1 8.90 usec
PLW1 59.00000000 W

======== CHANNEL f2 ========
SFO2 400.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 11.00000000 W
PLW12 0.35231000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.6177866 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

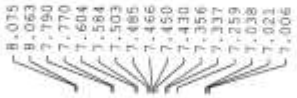


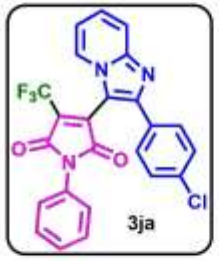

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO              866
PROCNO               1

F2 - Acquisition Parameters
Date_           20220929
Time              17.47
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD               22768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           89285.711 Hz
FIDRES        2.724784 Hz
AQ            0.1835008 sec
RG                87.66
DW                5.600 usec
DE                6.50 usec
TE               296.5 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

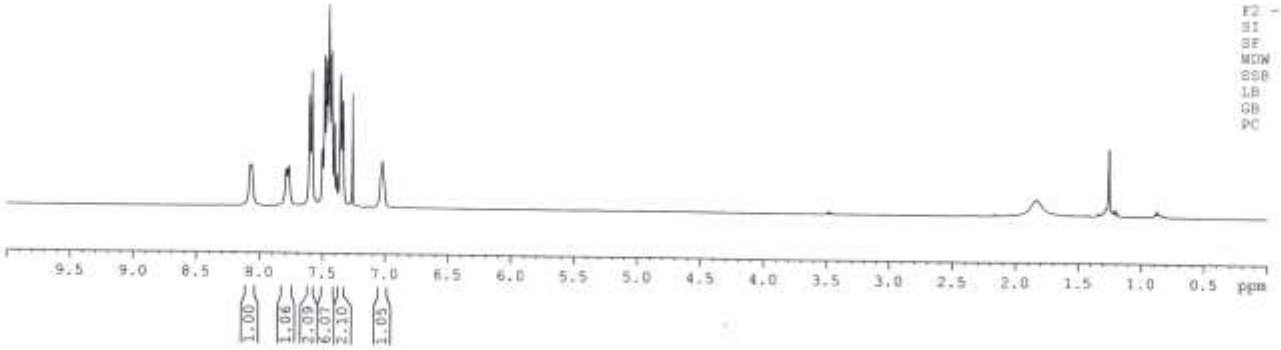
Solvent: $CDCl_3$

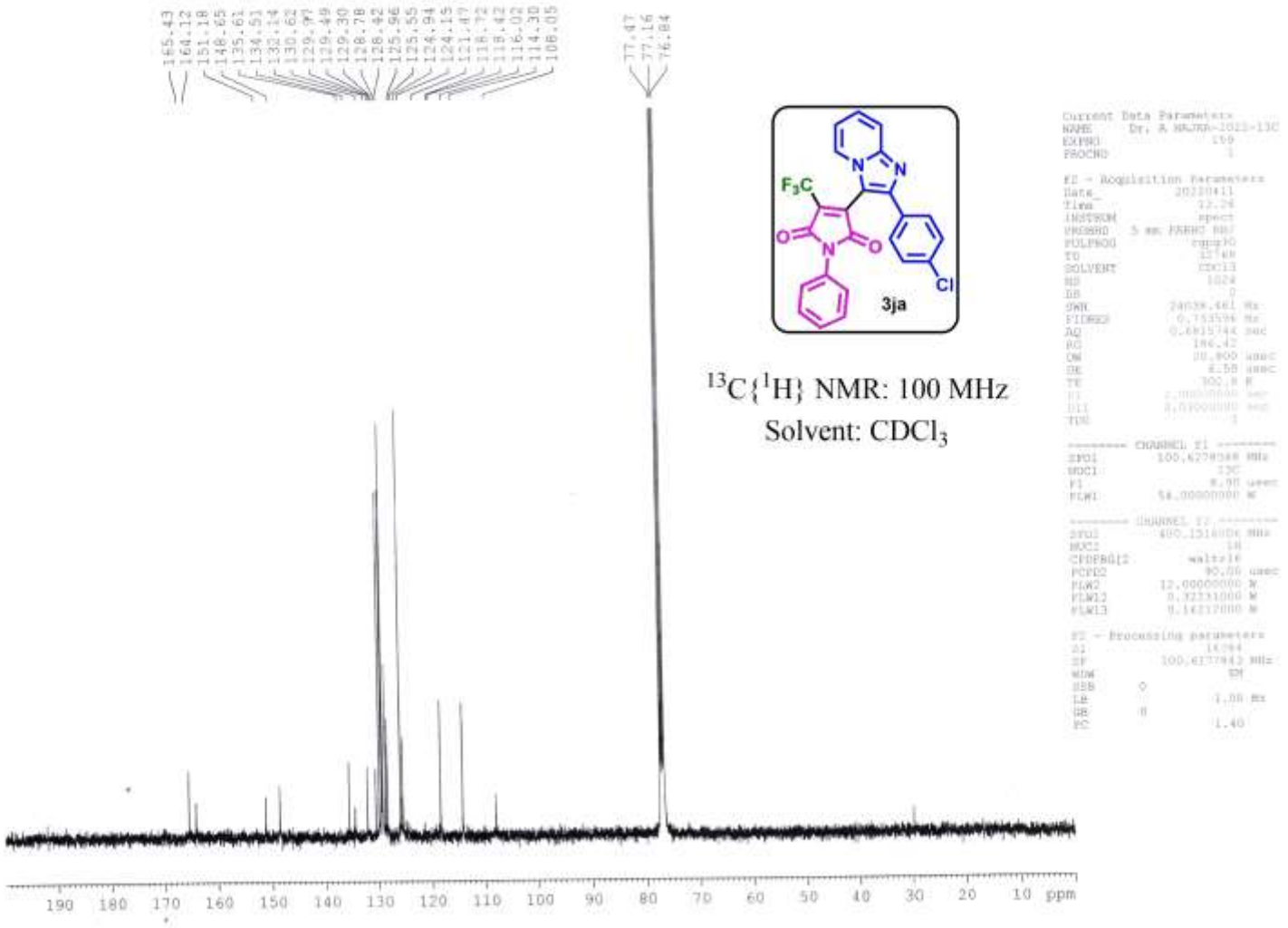
```
Current Data Parameters
NAME       Dr. A HAJRA 2022 1H
EXPNO              399
PROCNO               1

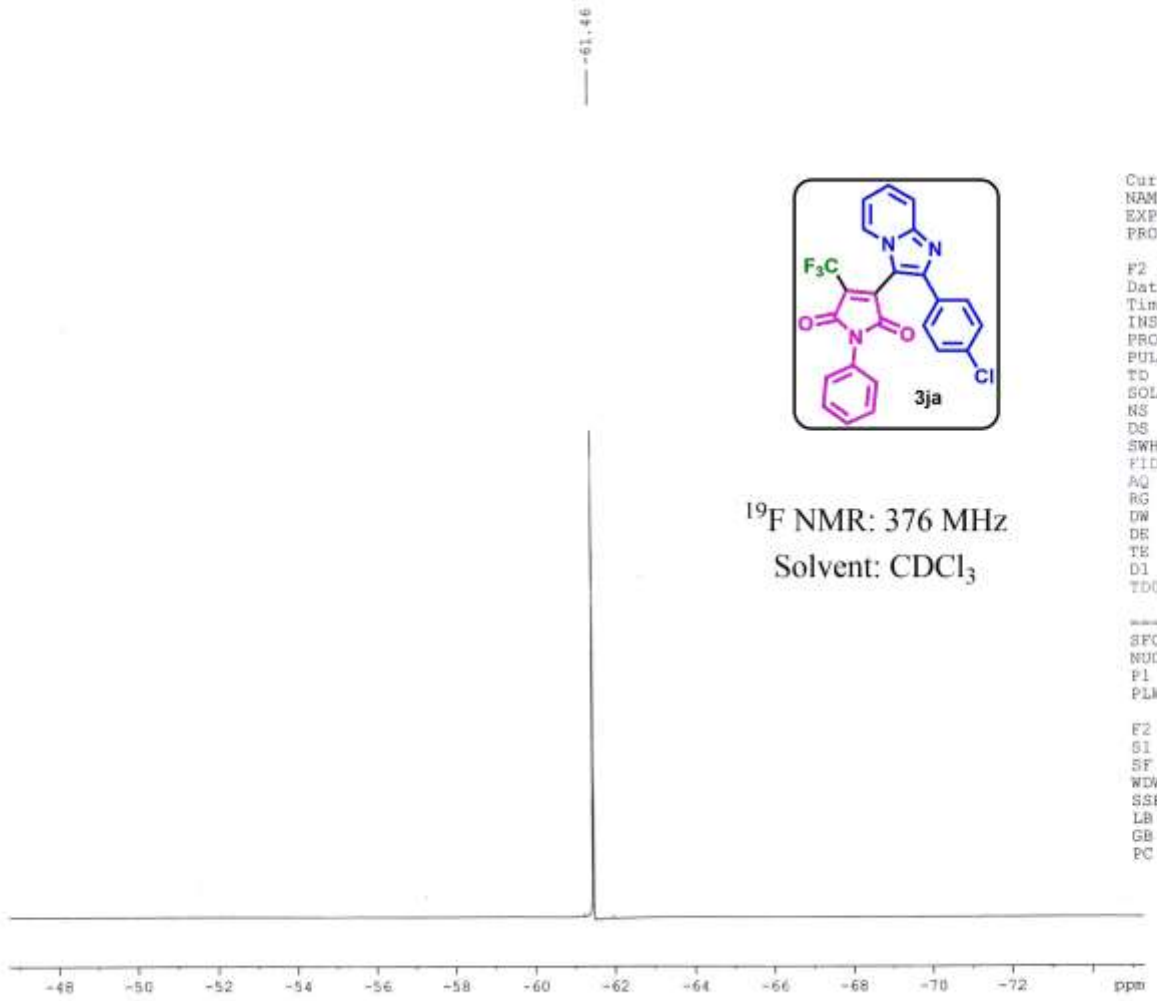
F2 - Acquisition Parameters
Date_          20220410
Time              12.52
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              106.66
DW               60.800 usec
DE                6.50 usec
TE               297.9 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                1.00
```




165.43
164.12
151.18
140.65
135.61
134.51
132.14
130.62
129.97
129.49
129.30
128.78
128.42
125.96
125.55
124.94
124.15
121.47
118.72
118.42
116.02
114.30
106.05
77.47
77.16
76.84
F3C
O
N
N
O
Cl
3ja
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



^{19}F NMR: 376 MHz

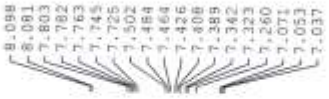
Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  400
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220410
Time                12.46
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zgflqn
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      2
SWH           89285.711 Hz
FIDRES         2.724704 Hz
AQ             0.1835008 sec
RG                  135.7
DW                  5.600 usec
DE                  6.50 usec
TE                  297.9 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

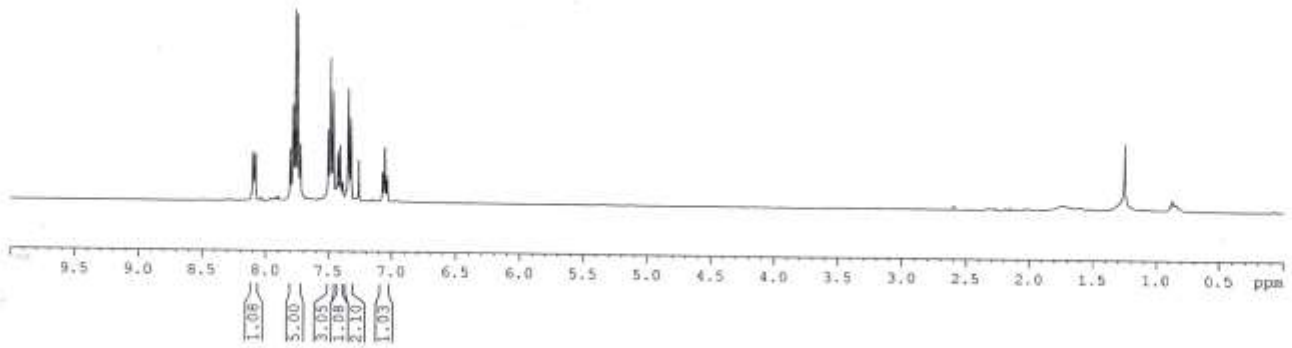
Solvent: $CDCl_3$

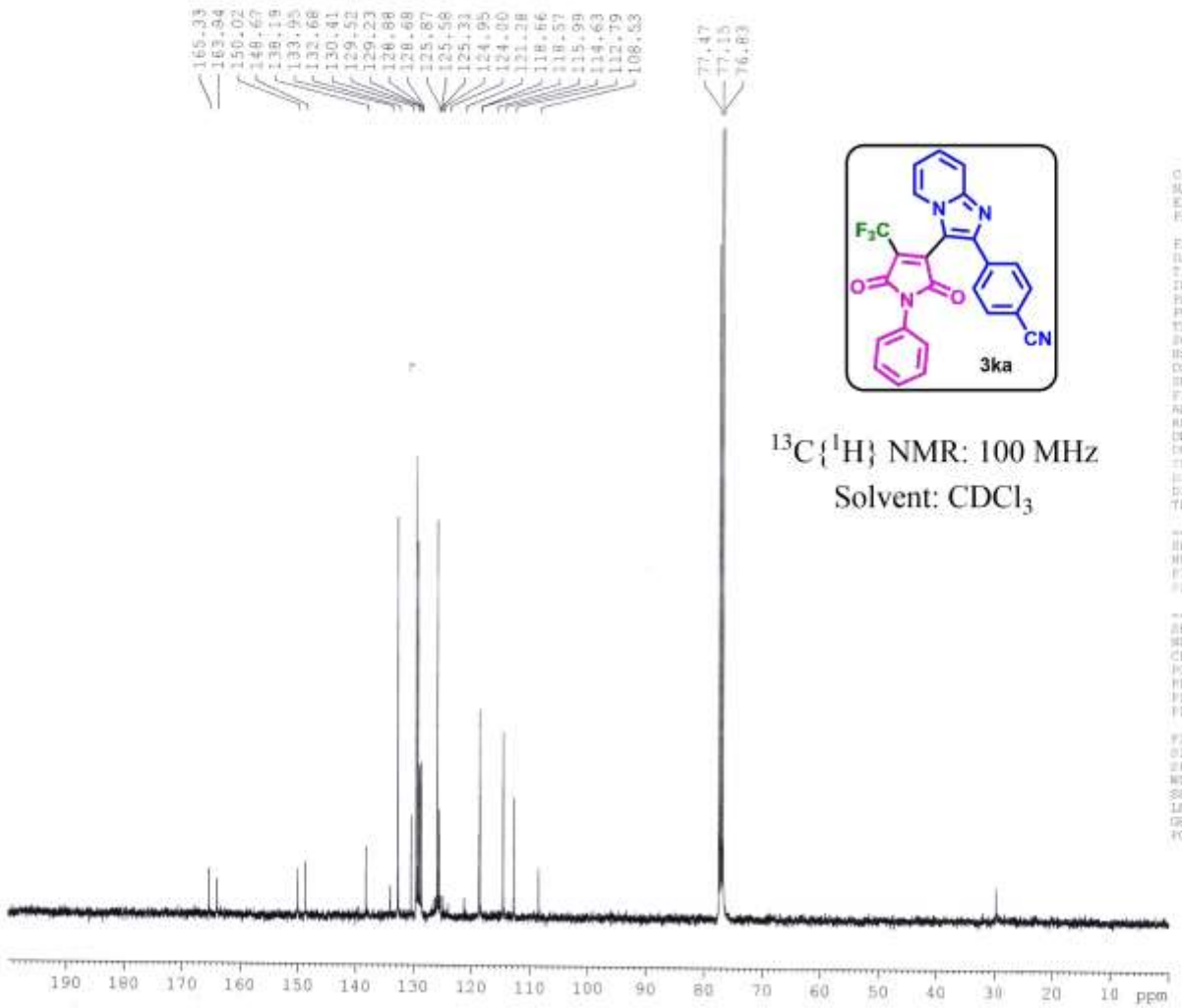
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO              212
PROCNO               1

F2 - Acquisition Parameters
Date_          20220303
Time              12.51
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              106.66
DW               60.800 usec
DE                6.50 usec
TE              294.6 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         400.1500086 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





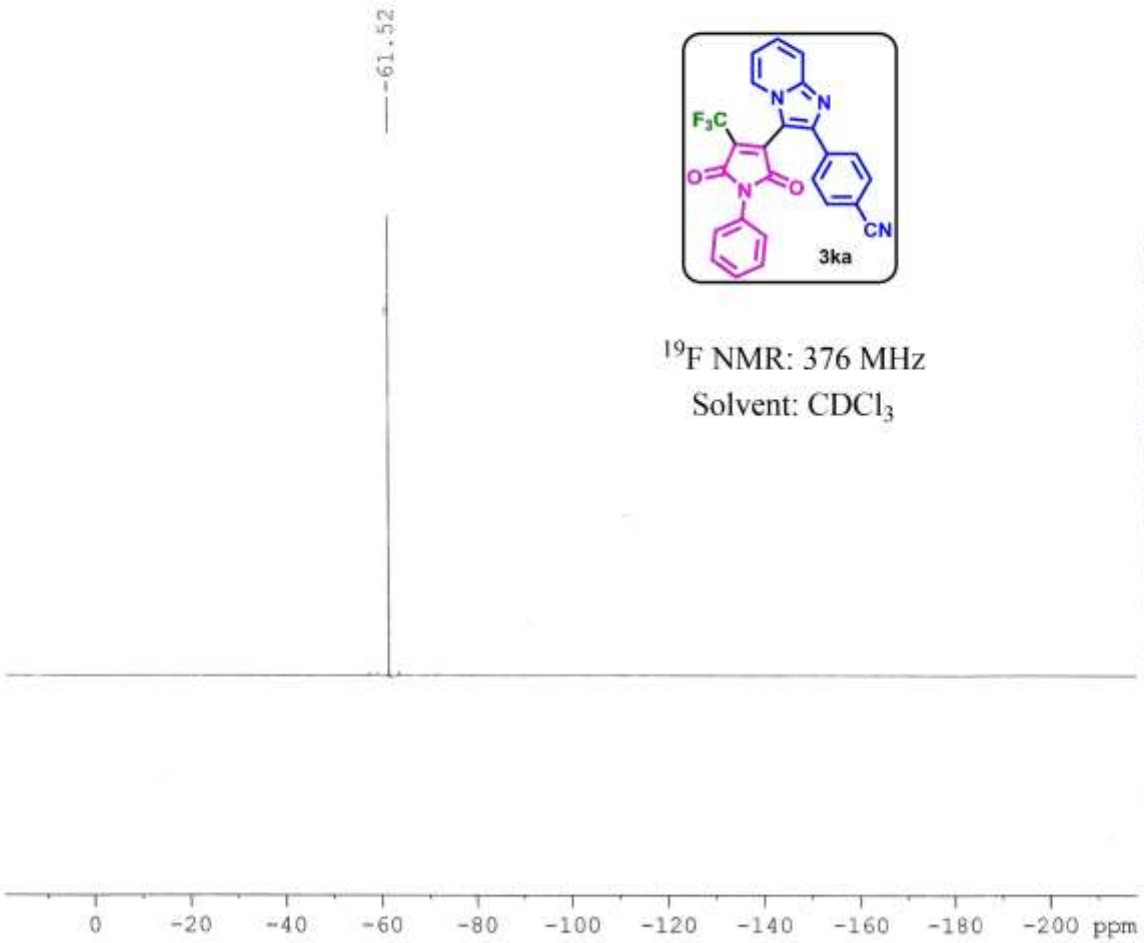

```
Current Data Parameters
NAME        Dr. A MAJRA-2022-13C
EXPNO                         9E
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20230301
Time                       18.03
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                        184.42
DW                        20.800 usec
DE                         6.50 usec
TE                          295.1 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                 100.6276588 MHz
NUC1                         13C
P1                         8.90 usec
PLW1                 58.70000000 W

======== CHANNEL f2 ========
SFO2                 400.1516006 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                     90.00 usec
PLW2                 12.00000000 W
PLW12                 0.32731000 W
PLW13                 0.14212000 W

F2 - Processing parameters
SI                         16384
SF                   100.6127685 MHz
WDW                           EM
SSB                    0
LB                         1.00 Hz
GB                     0
PC                         1.40
```



^{19}F NMR: 376 MHz

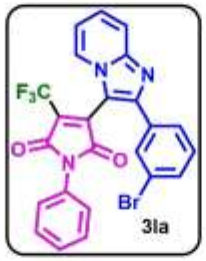
Solvent: $CDCl_3$

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

F2 - Acquisition Parameters
Date_           20220303
Time               6.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD               32768
SOLVENT          CDCl3
NS                   4
DS                   2
SWH           89285.711 Hz
FIDRES        2.724784 Hz
AQ            0.1835008 sec
RG              186.42
DW                5.600 usec
DE                6.50 usec
TE              297.0 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

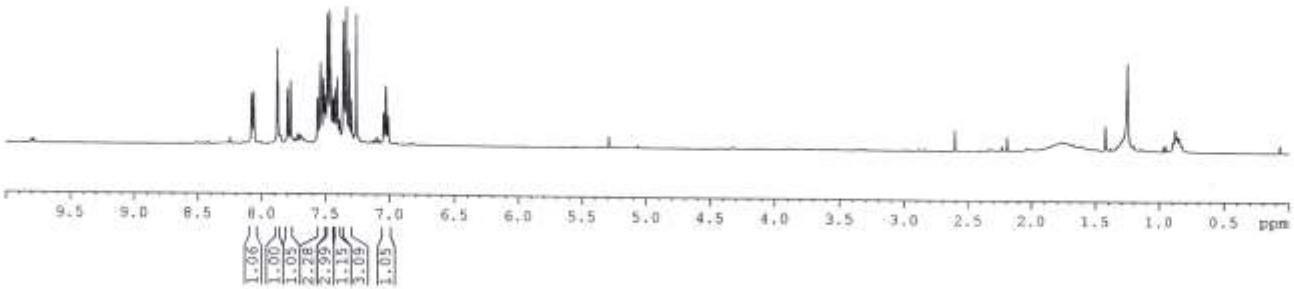
Solvent: $CDCl_3$

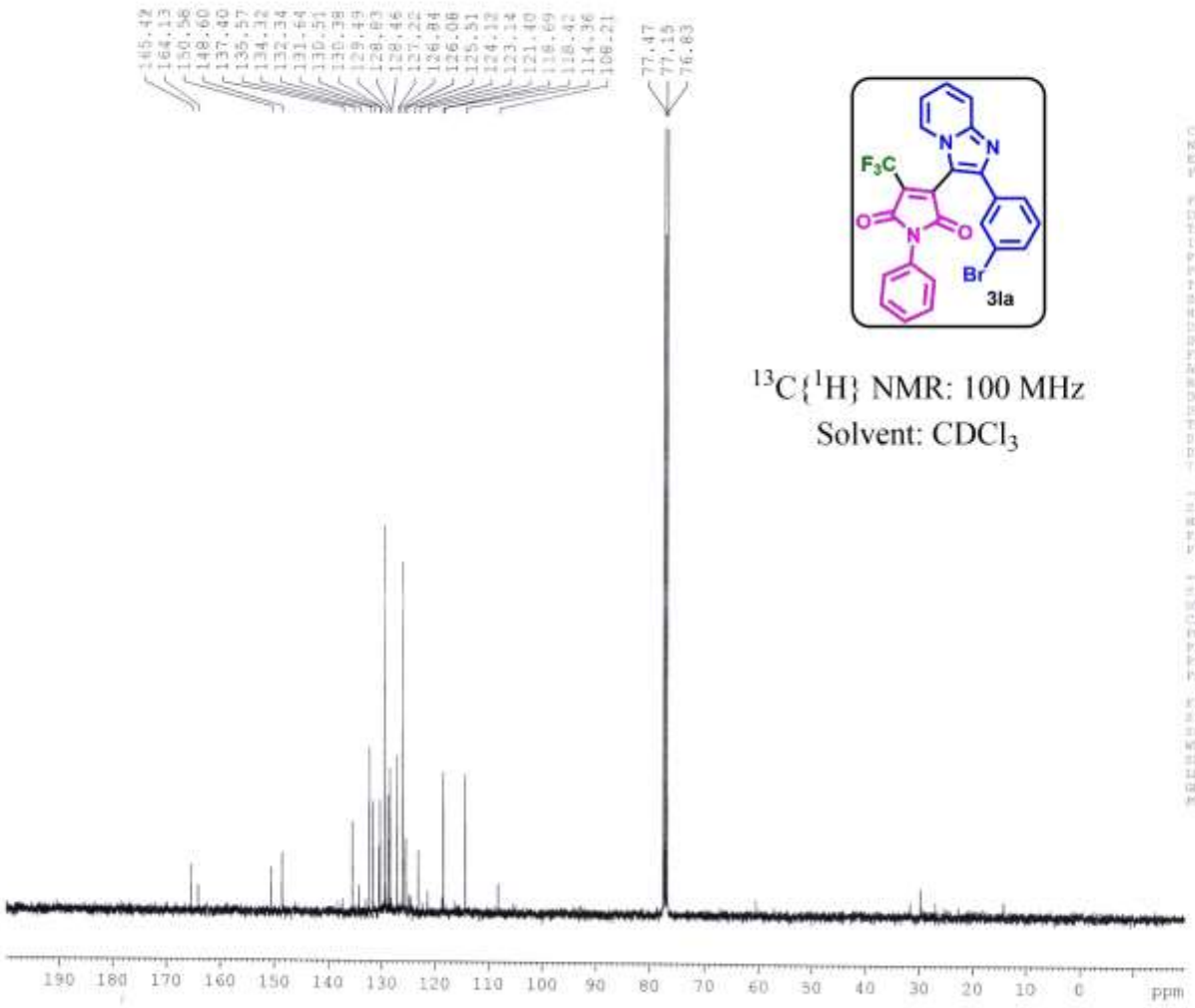
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  857
PROCNO                   1

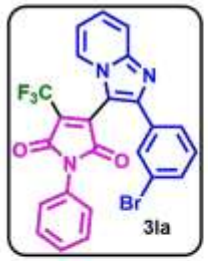
F2 - Acquisition Parameters
Date_           20220927
Time              16.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              168.31
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         400.1500086 MHz
WDW                EM
SSB       0
LB               0.30 Hz
GB        0
PC               1.00
```




145.42
164.13
150.56
148.60
137.40
135.57
134.32
132.34
131.64
130.51
130.38
129.49
128.83
128.46
127.22
126.84
126.08
125.51
124.32
123.14
121.40
118.69
118.42
114.36
106.21
77.47
77.15
76.83
F3C
O
O
N
N
N
Br
3la
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



^{19}F NMR: 376 MHz

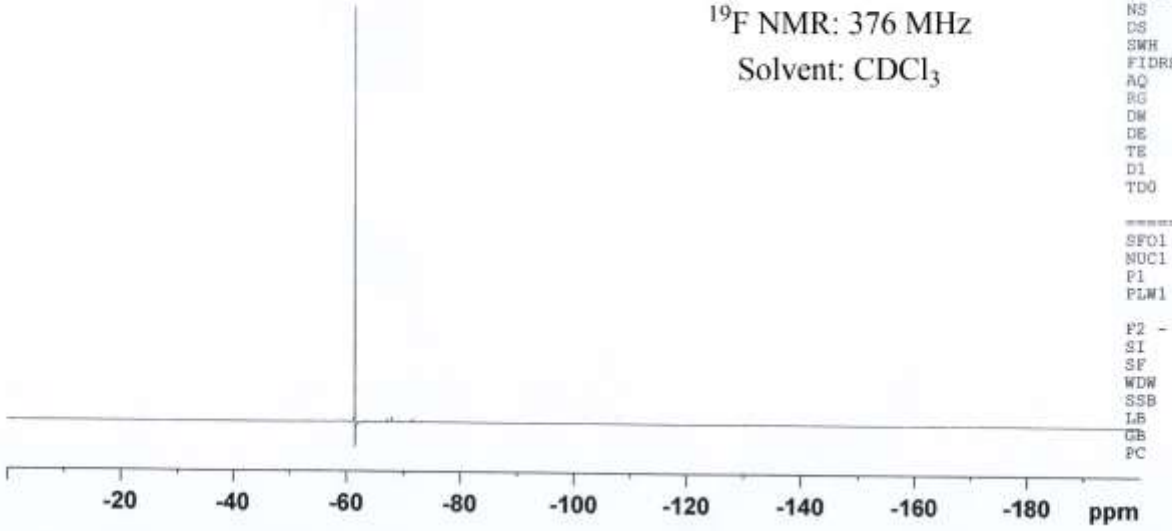
Solvent: $CDCl_3$

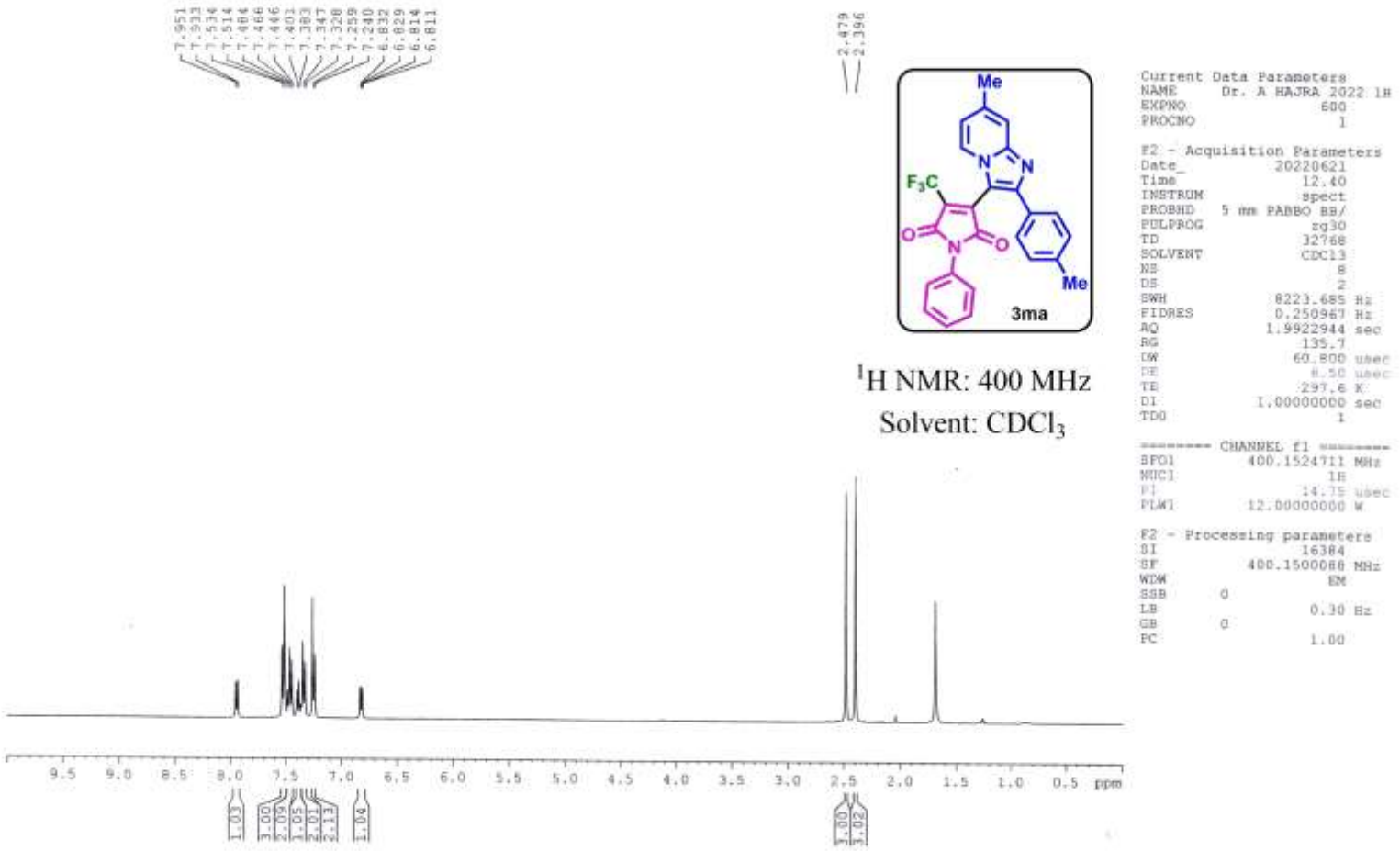
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  676
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220719
Time              18.33
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ            0.1835008 sec
RG               186.42
DW                5.600 usec
DE                6.50 usec
TE                296.5 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
```



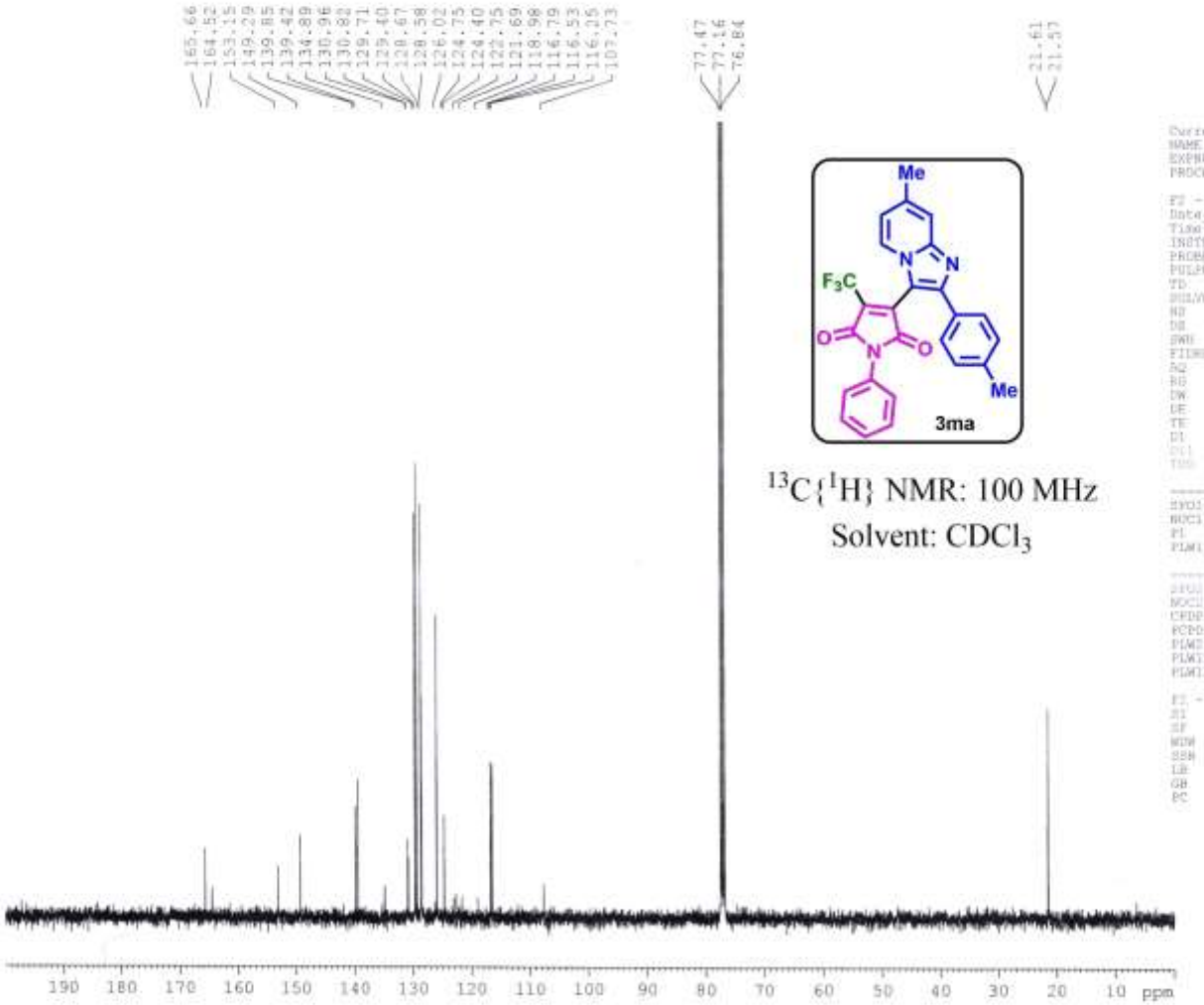



```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  600
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220621
Time                 12.40
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                       8
DS                       2
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9922944 sec
RG                     135.7
DW                    60.800 usec
DE                     6.50 usec
TE                    297.6 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               400.1500068 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



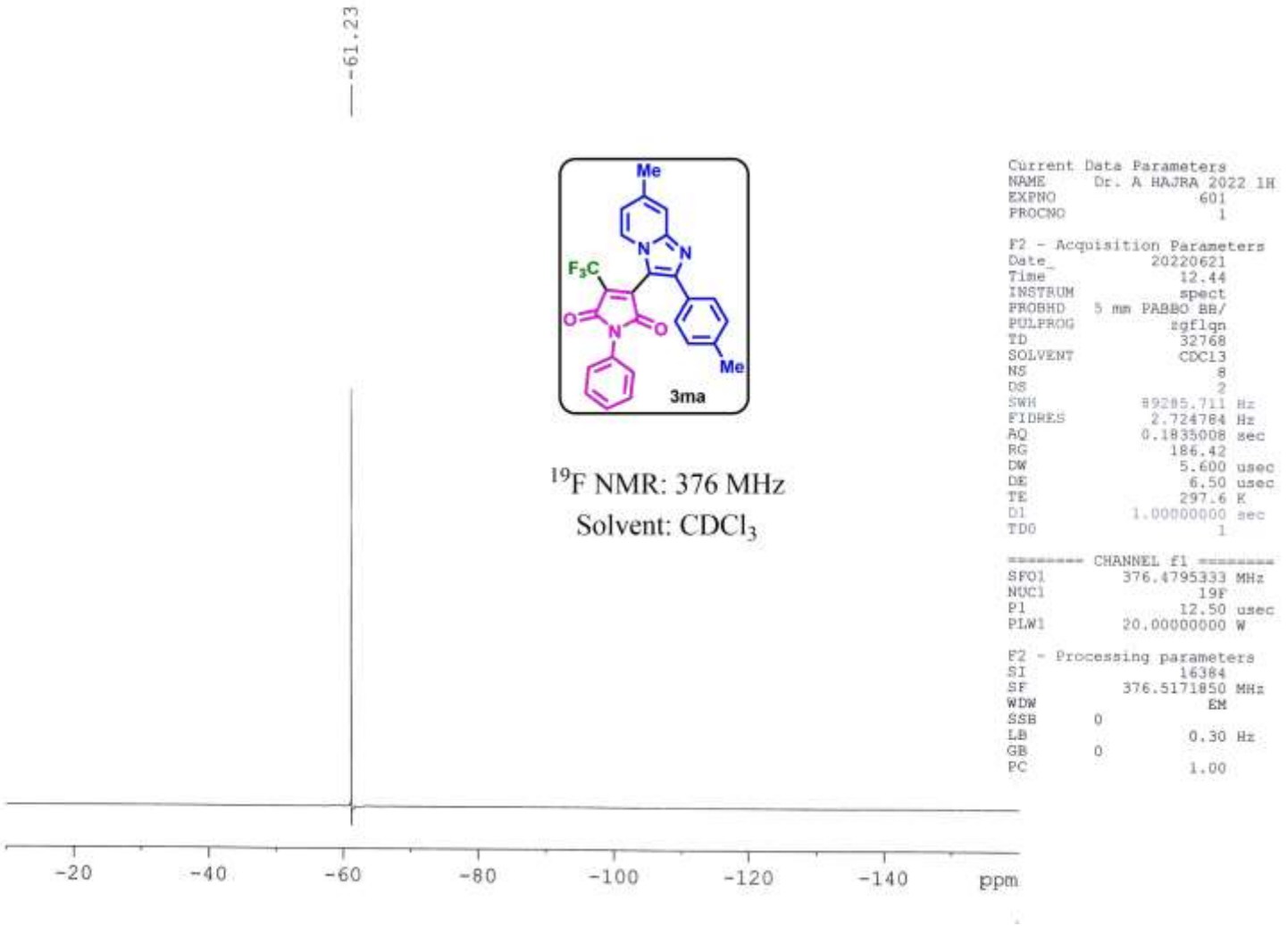
Current Data Parameters
NAME Dr. A MAJRA-2022-13C
EXPNO 231
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220621
Time 13.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 720
DS 2
SWH 26038.461 Hz
FIDRES 0.794596 Hz
AQ 0.6815744 sec
RG 186.42
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6278589 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316006 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 100.6177843 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

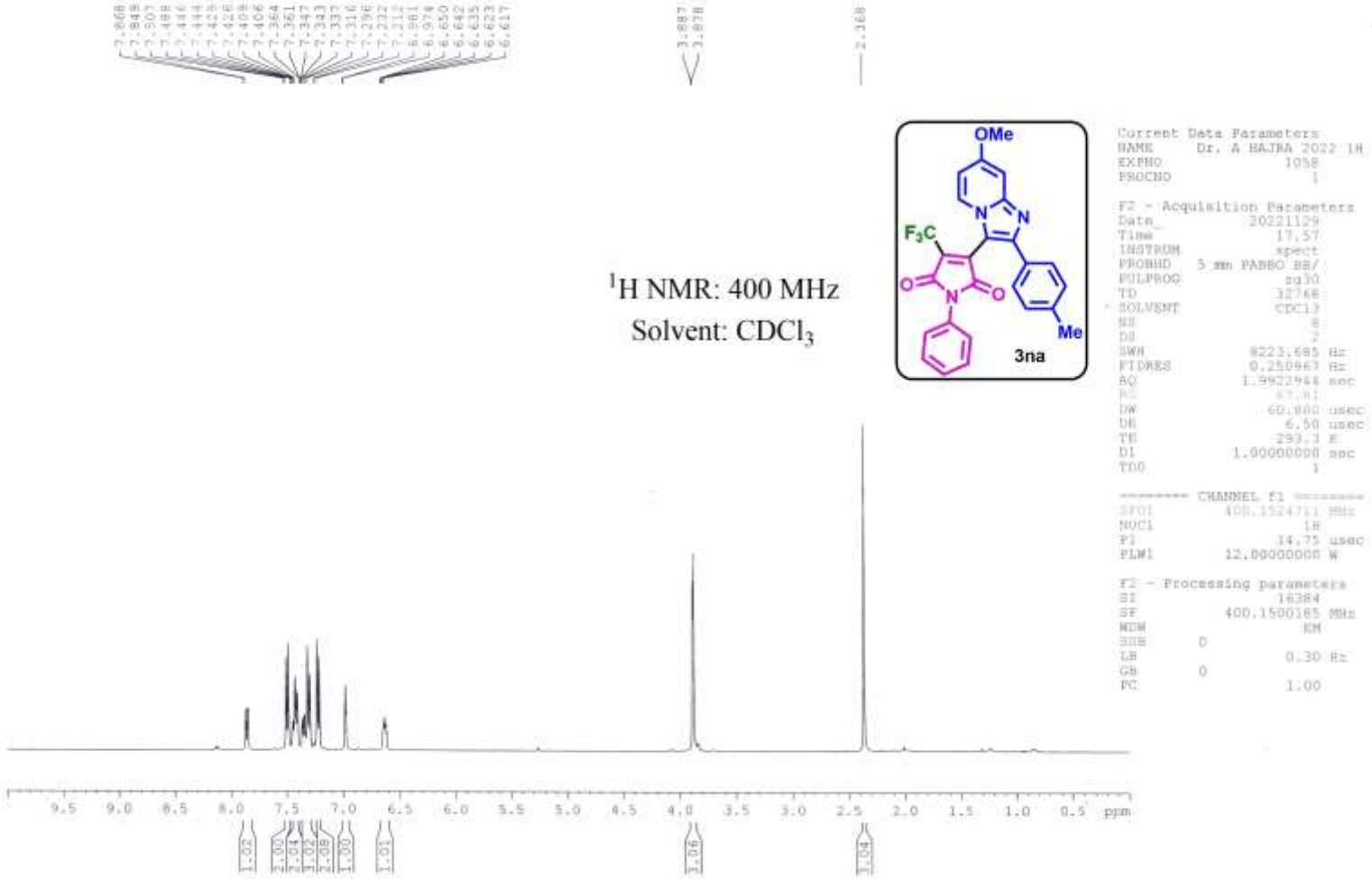


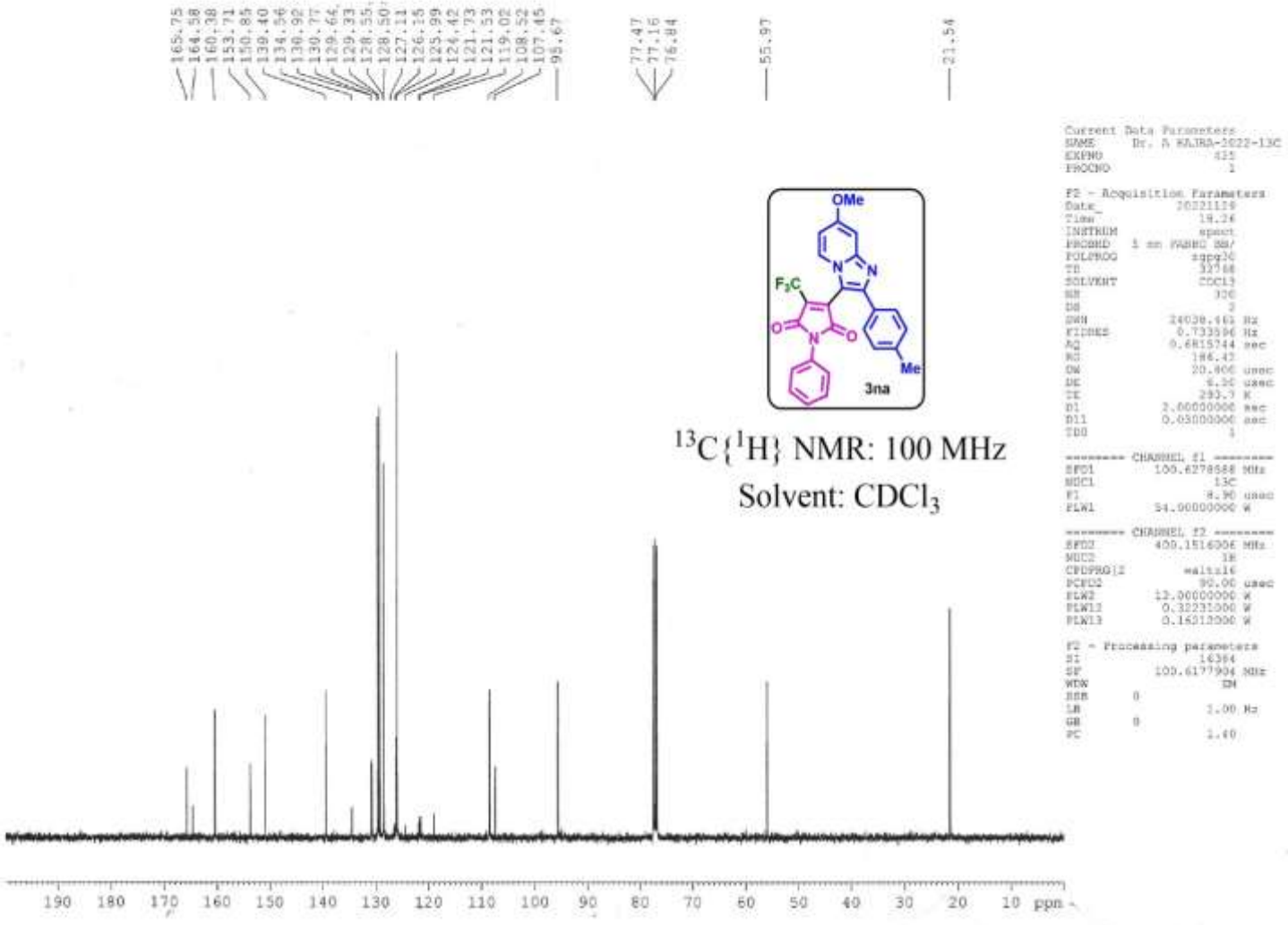

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  601
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220621
Time_              12.44
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ            0.1835008 sec
RG               186.42
DW                5.600 usec
DE                6.50 usec
TE               297.6 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
```


7.868
7.848
7.507
7.488
7.446
7.444
7.426
7.426
7.409
7.406
7.364
7.361
7.347
7.343
7.333
7.316
7.296
7.232
7.211
6.981
6.974
6.650
6.642
6.635
6.623
6.617
3.887
3.878
2.568
OMe
F3C
N
N
O
O
N
Me
3na
1H NMR: 400 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A HAJRA 2022 1H
EXPNO 1058
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221129
Time 17.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 67.61
DW 60.800 usec
DE 6.50 usec
TE 293.3 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 400.1500185 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
1.02
2.00
2.04
1.02
2.08
1.00
1.01
3.06
3.04



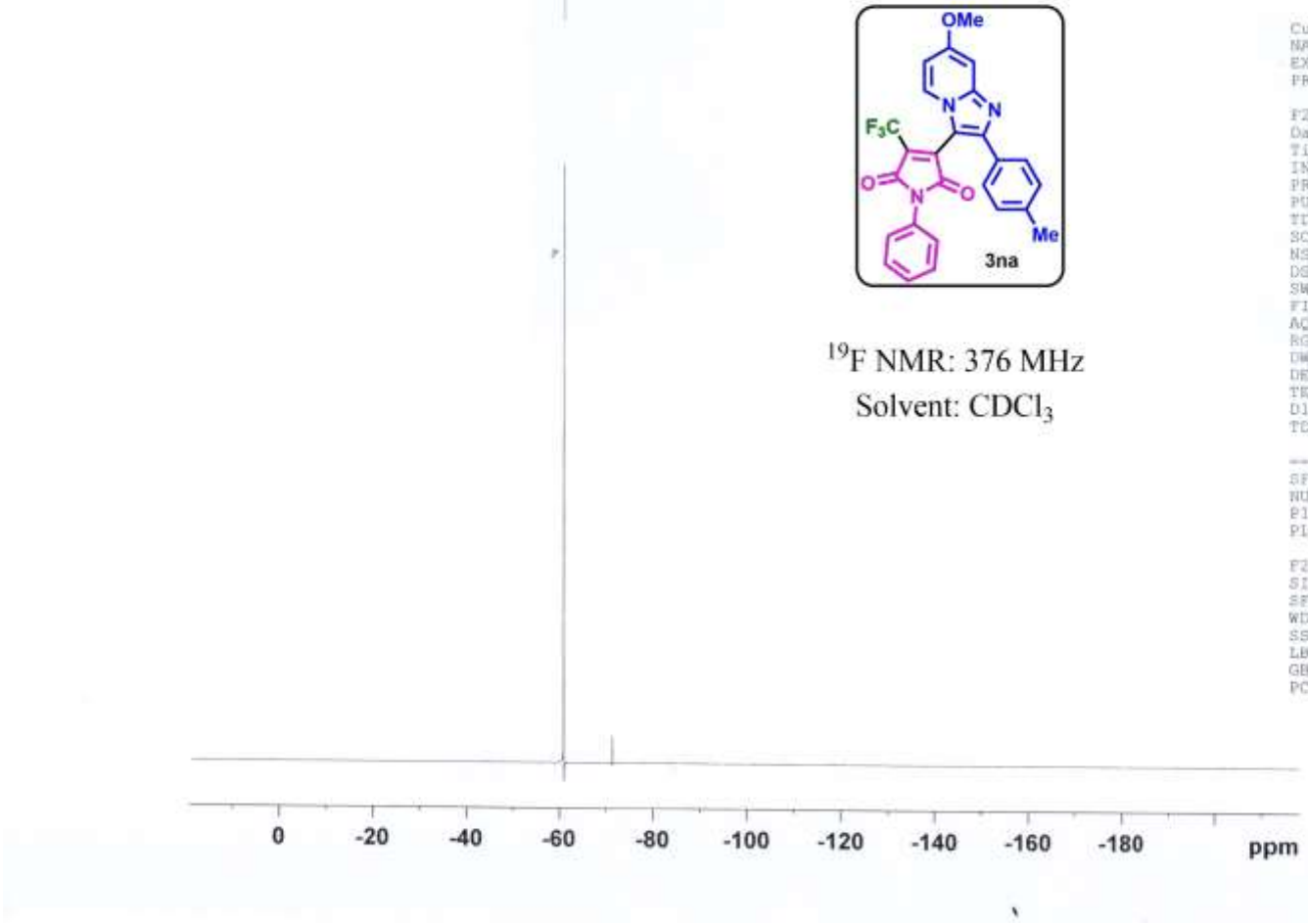

```
Current Data Parameters
NAME       Dr. A KAIRA-2022-13C
EXPNO                 425
PROCNO                  1

F2 - Acquisition Parameters
Date_           20221129
Time              19.26
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              186.43
DW             20.800 usec
DE              6.50 usec
TE             293.3 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          100.6177904 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



^{19}F NMR: 376 MHz

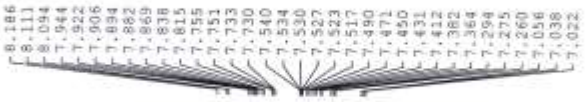
Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO              1059
PROCNO                1

F2 - Acquisition Parameters
Date_          20221129
Time               18.07
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ            0.1835008 sec
RG               186.42
DW               5.600 usec
DE               6.50 usec
TE               293.2 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

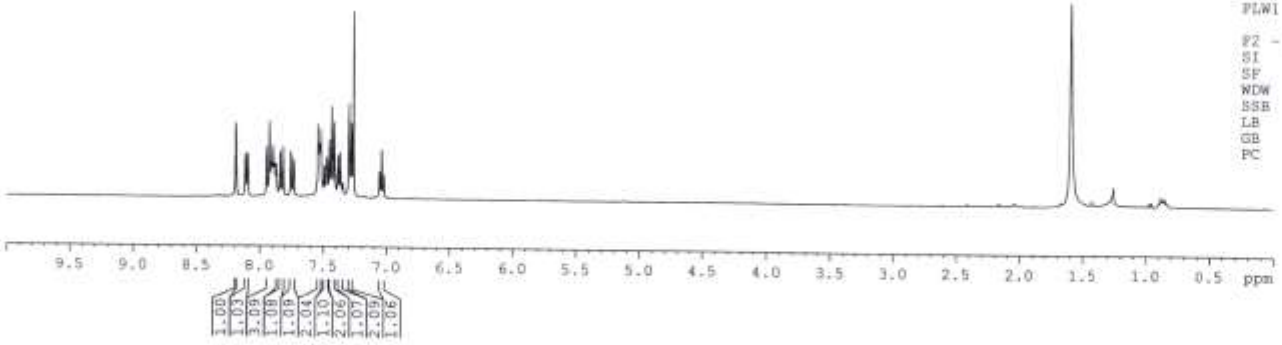
Solvent: $CDCl_3$

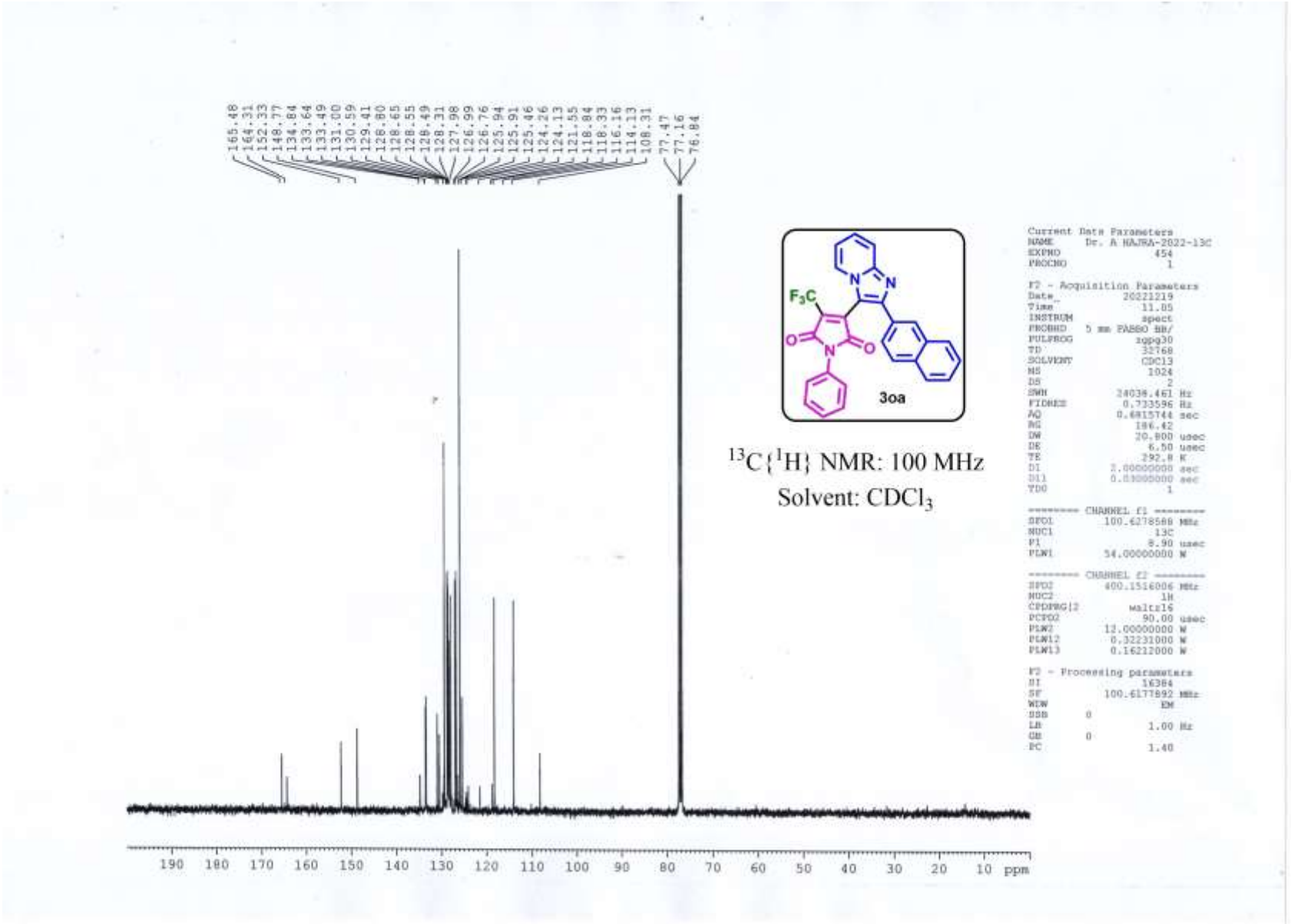
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO              568
PROCNO               1

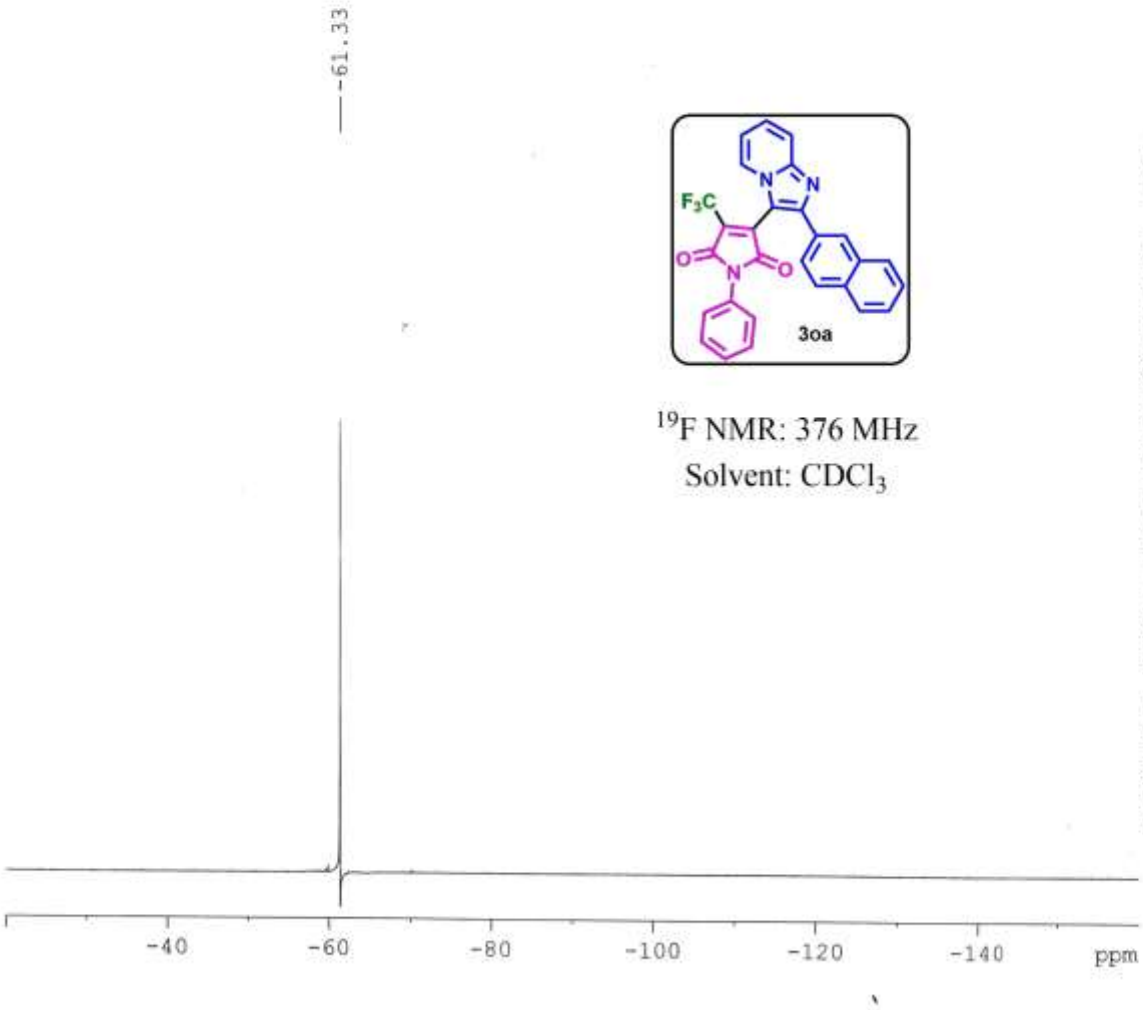
F2 - Acquisition Parameters
Date_          20220618
Time              19.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              186.42
DW             60.800 usec
DE              6.50 usec
TE             296.9 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                1.00
```




165.48
164.31
152.33
148.77
134.84
133.64
133.49
131.00
130.59
129.41
128.80
128.65
128.55
128.49
128.31
127.98
126.99
126.76
125.94
125.91
125.46
124.26
124.13
121.55
118.84
118.33
116.16
114.13
108.31
77.47
77.16
76.84
F3C
O
O
N
N
N
3oa
13C{1H} NMR: 100 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A HAJRA-2022-13C
EXPNO 454
PROCNO 1
F2 - Acquisition Parameters
Date_ 20221219
Time 11.05
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 186.42
DW 20.800 usec
DE 6.50 usec
TE 292.8 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 100.6177892 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



^{19}F NMR: 376 MHz

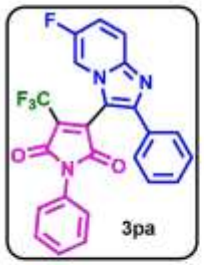
Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  574
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220617
Time              16.09
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ            0.1835008 sec
RG               186.42
DW                5.600 usec
DE                6.50 usec
TE                297.7 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

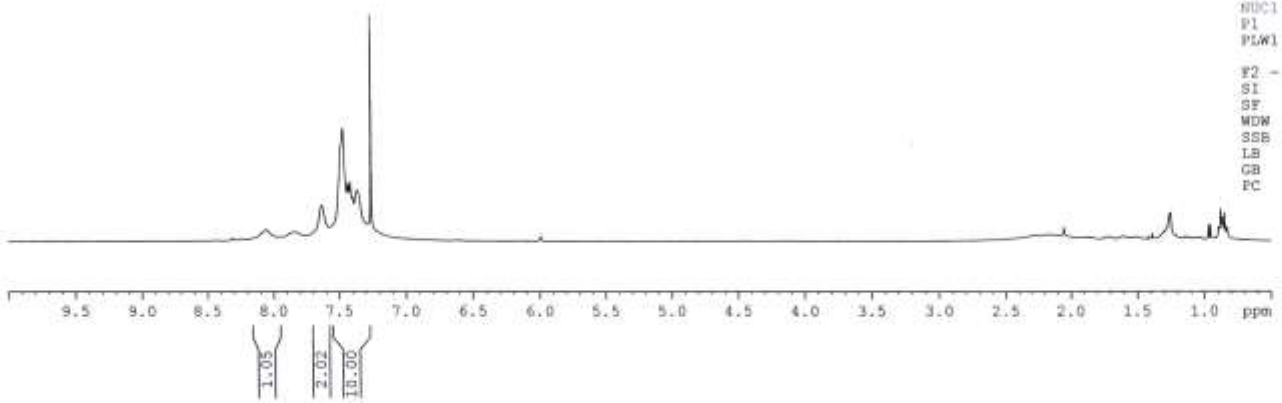
Solvent: $CDCl_3$

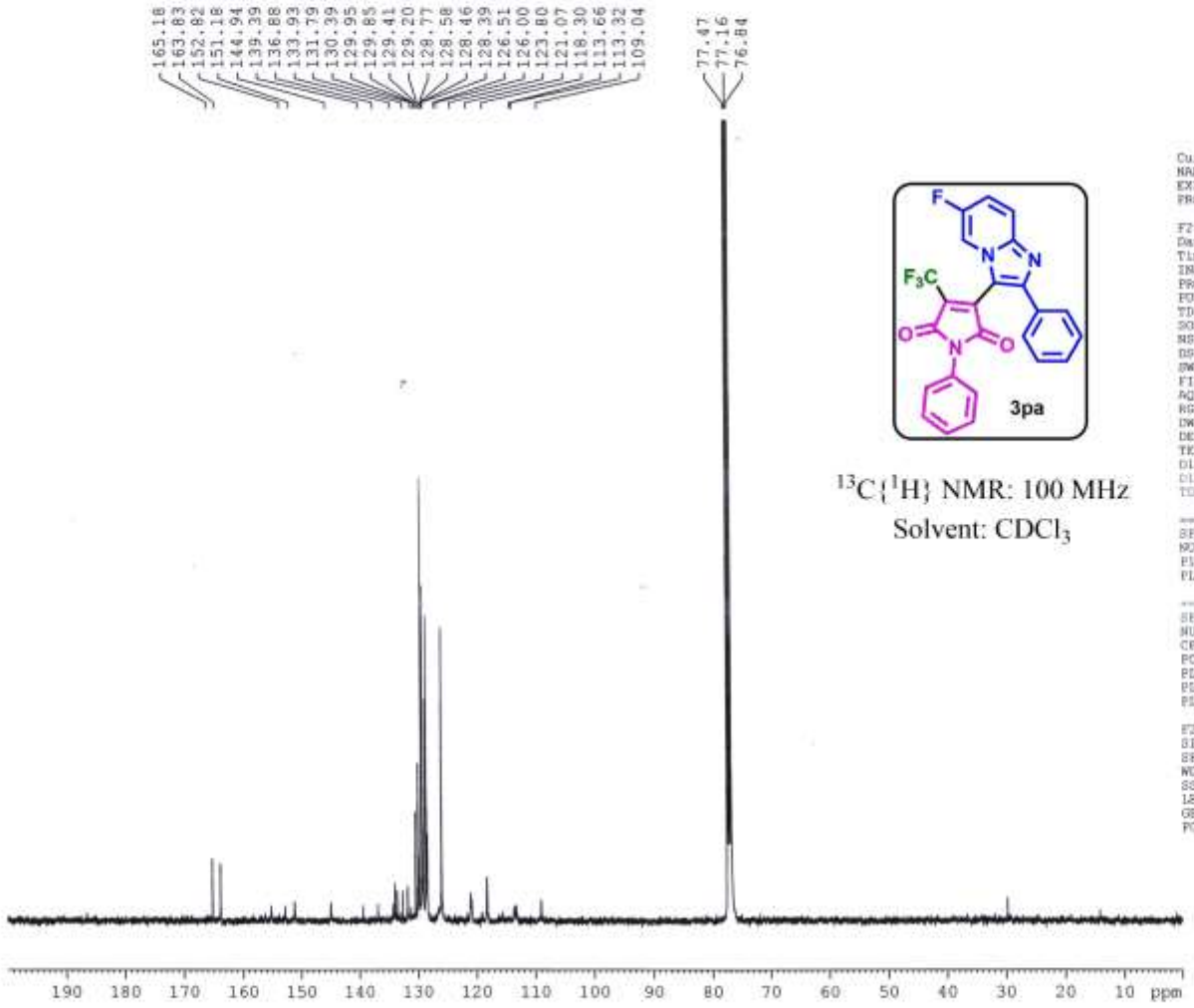
```
Current Data Parameters
NAME      Dr. A HAJRA 2024 1H
EXPNO                 18
PROCNO                 1

F2 - Acquisition Parameters
Date_              20240105
Time                 12.21
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      2
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9922944 sec
RG                   148.91
DW                  60.800 usec
DE                   6.50 usec
TE                  290.7 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              400.1500096 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```





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

Solvent: $CDCl_3$

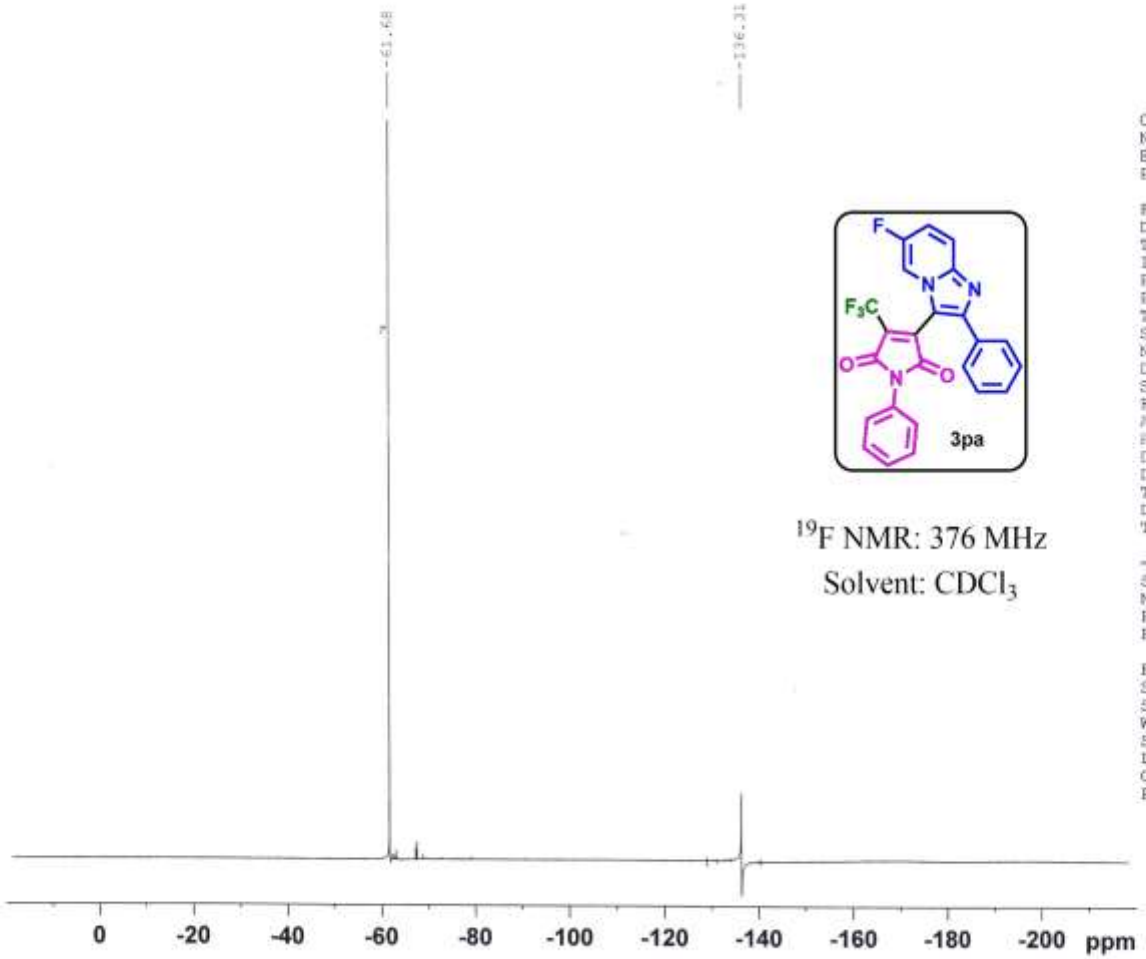
```
Current Data Parameters
NAME      Dr. A HAJRA-2024-13C
EXPNO              11
PROCNO              1

F2 - Acquisition Parameters
Date_          20240113
Time              21.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                2024
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              292.3 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       400.1316006 MHz
NUC2               1H
CPDPRG2        waltz16
PCPD2            90.00 usec
PLW2       12.00000000 W
PLW12       0.32231000 W
PLW13       0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177946 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

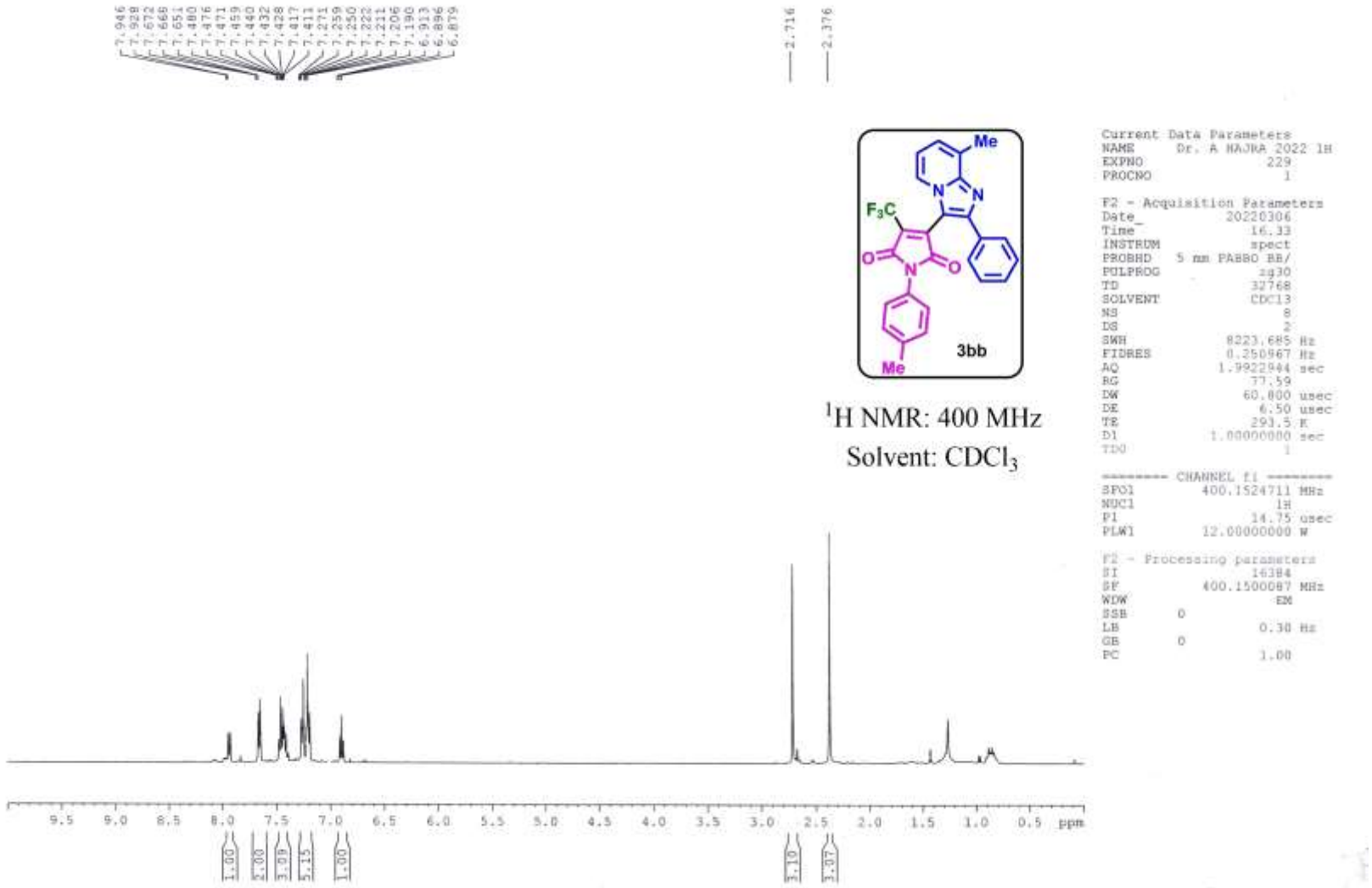


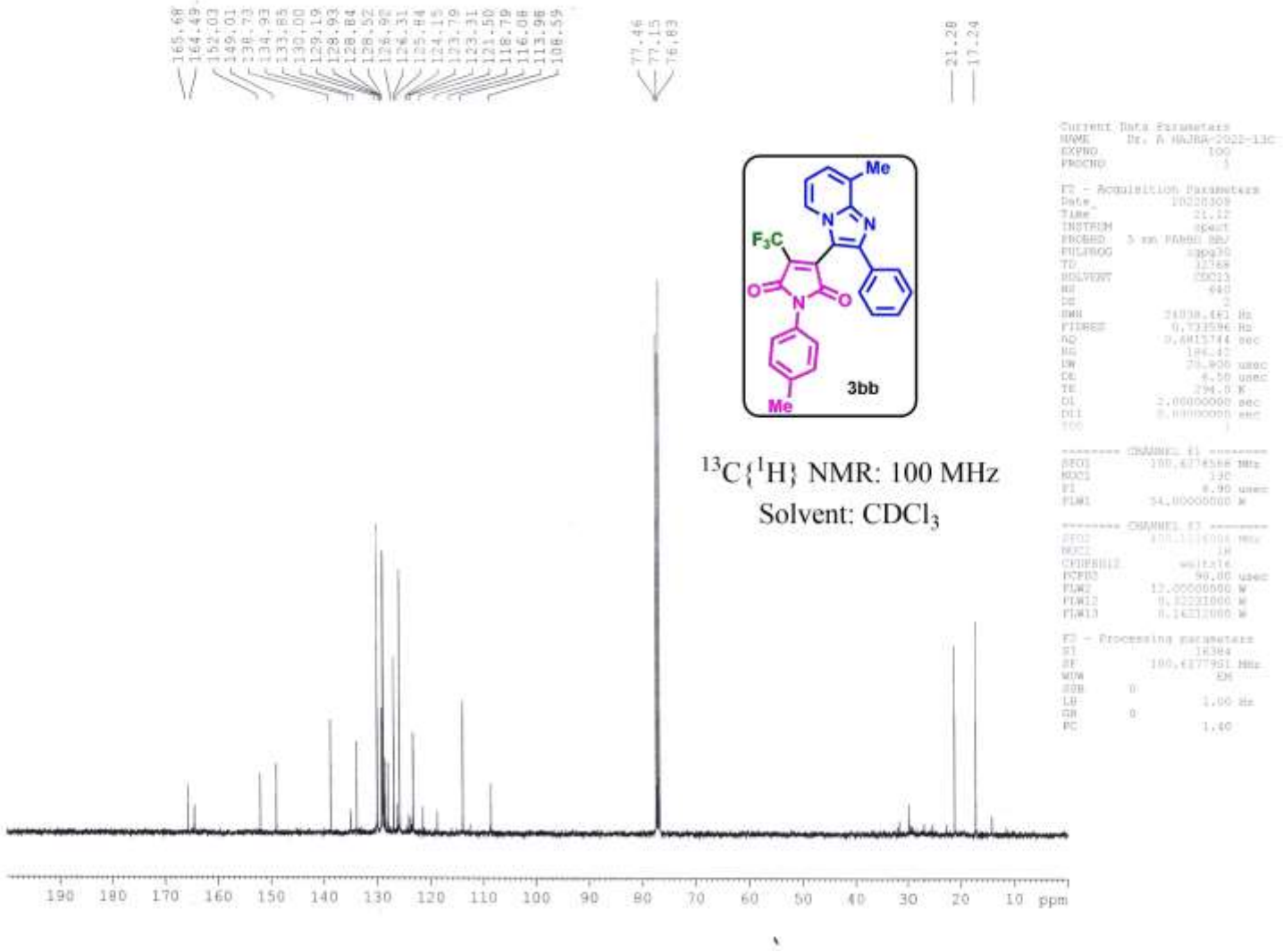

```
Current Data Parameters
NAME      Dr. A HAJRA 2024 1H
EXPNO                 14
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240103
Time              17.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD              32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG               186.42
DW                5.600 usec
DE                6.50 usec
TE              290.0 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
```


7.946
7.928
7.672
7.666
7.651
7.480
7.476
7.471
7.459
7.440
7.432
7.428
7.417
7.411
7.271
7.259
7.250
7.222
7.211
7.206
7.190
6.913
6.896
6.879
2.716
2.376
Me
F3C
N
N
O
O
N
Me
3bb
1H NMR: 400 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A HAJRA 2022 1H
EXPNO 229
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220306
Time 16.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 77.59
DW 60.800 usec
DE 6.50 usec
TE 293.5 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 400.1500087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
1.00
2.00
3.09
5.15
1.00
3.10
3.07



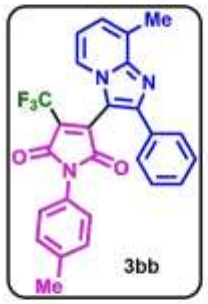
Current Data Parameters
NAME Dr. A HAJBA-2022-13C
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220309
Time 21.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 196.42
DW 20.800 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6274566 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.32231000 W
PLW13 0.16231000 W

F2 - Processing parameters
SI 16384
SF 100.6277901 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^{19}F NMR: 376 MHz

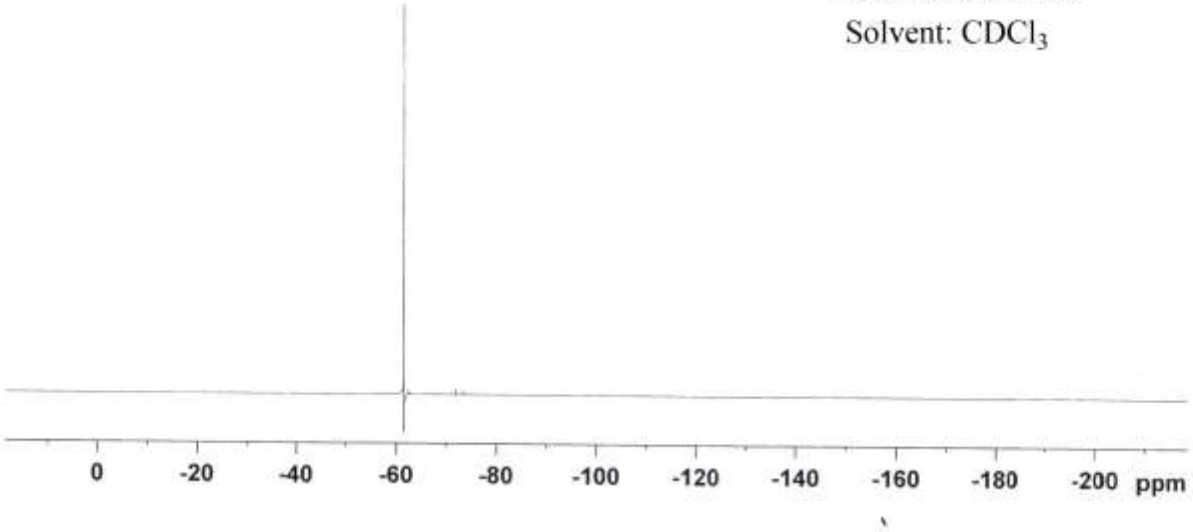
Solvent: $CDCl_3$

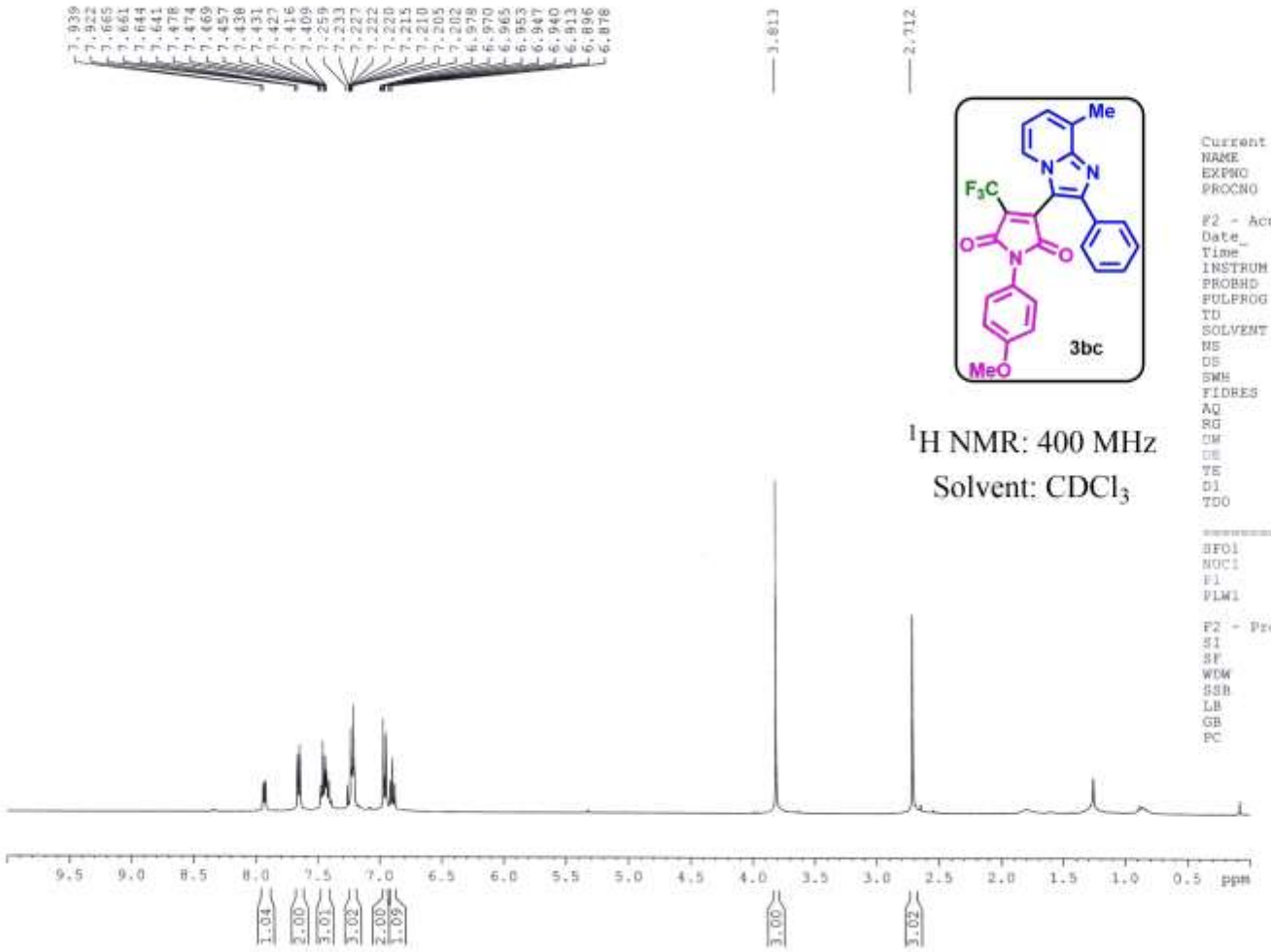
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1
EXPNO              230
PROCNO               1

F2 - Acquisition Parameters
Date_          20220306
Time               16.38
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    4
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG                77.59
DW                5.600 use
DE                6.50 use
TE                293.5 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        376.4795333 MHz
NUC1               19F
P1                12.50 use
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
```



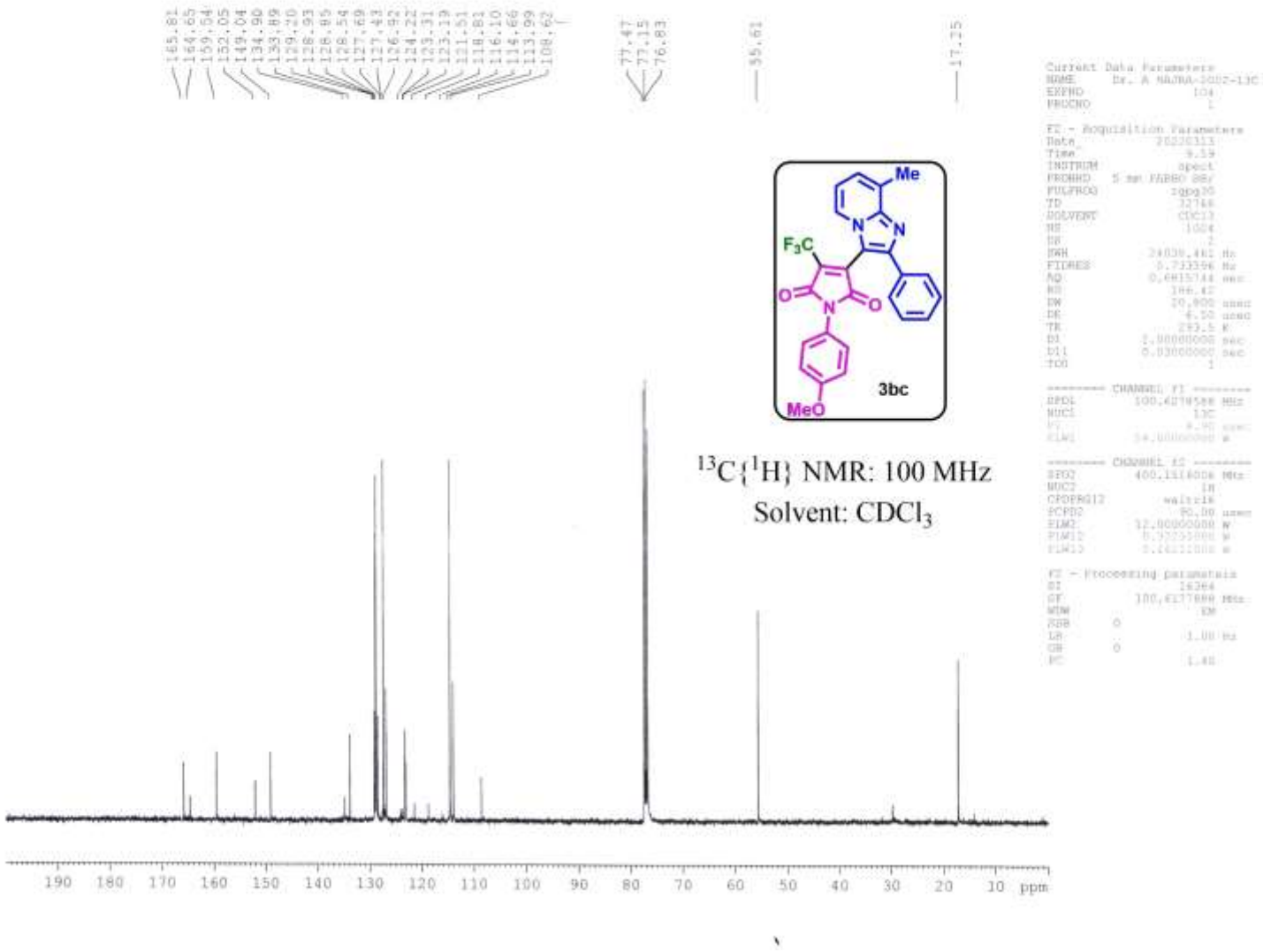


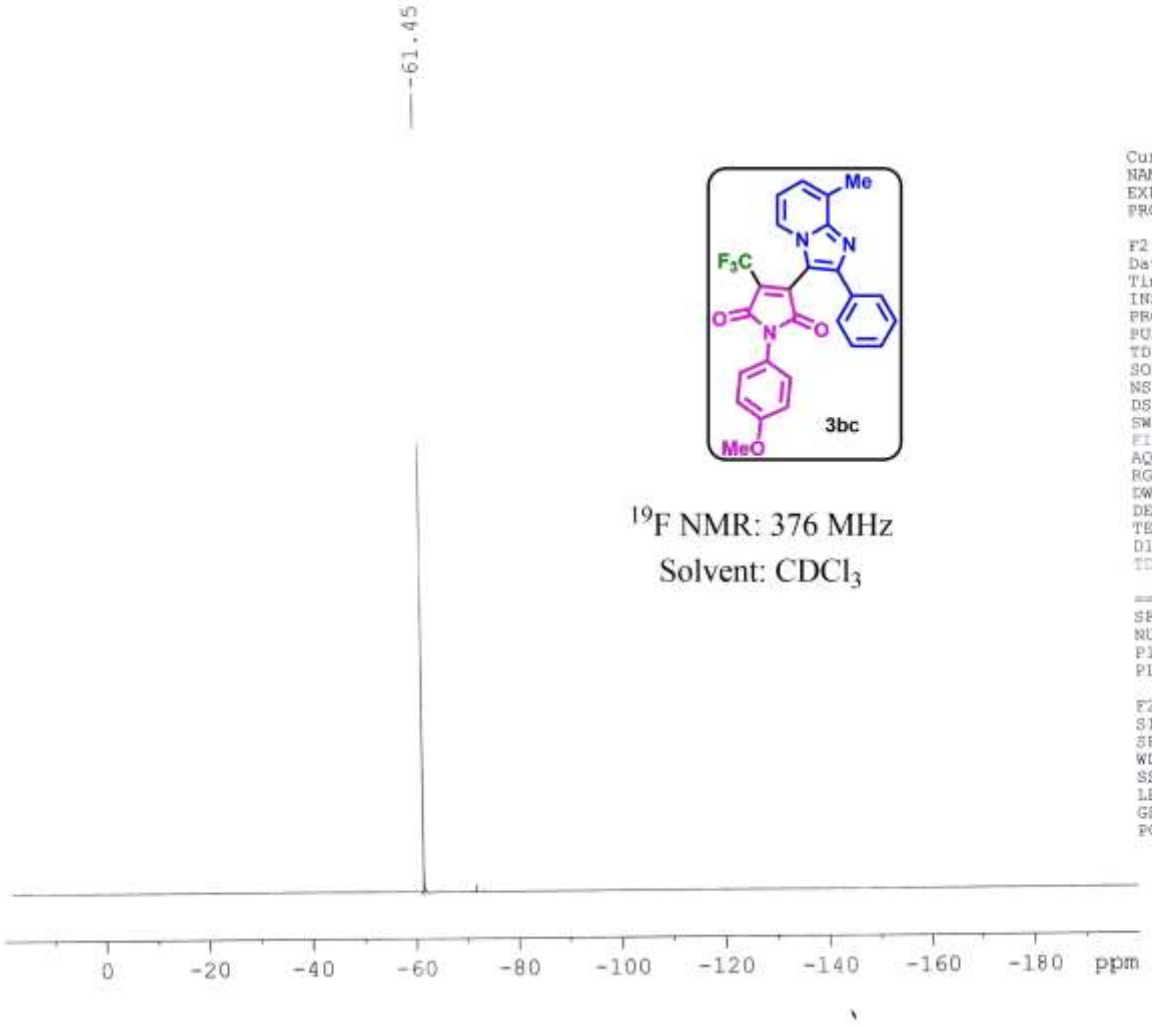

```
Current Data Parameters
NAME      Dr. A MAJRA 2022 1H
EXPNO              251
PROCNO               1

F2 - Acquisition Parameters
Date_          20220313
Time               9.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               67.81
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         400.1500092 MHz
WDW                EM
SSB      0
LB               0.30 Hz
GB       0
PC               1.00
```


165.81
164.65
159.54
152.05
149.04
134.90
133.89
129.70
128.93
128.85
128.54
127.69
127.43
126.92
124.22
123.31
123.19
121.51
118.81
116.10
114.66
113.99
108.62
77.47
77.15
76.83
55.61
17.75
Me
F3C
N
N
O
O
N
O
MeO
3bc
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

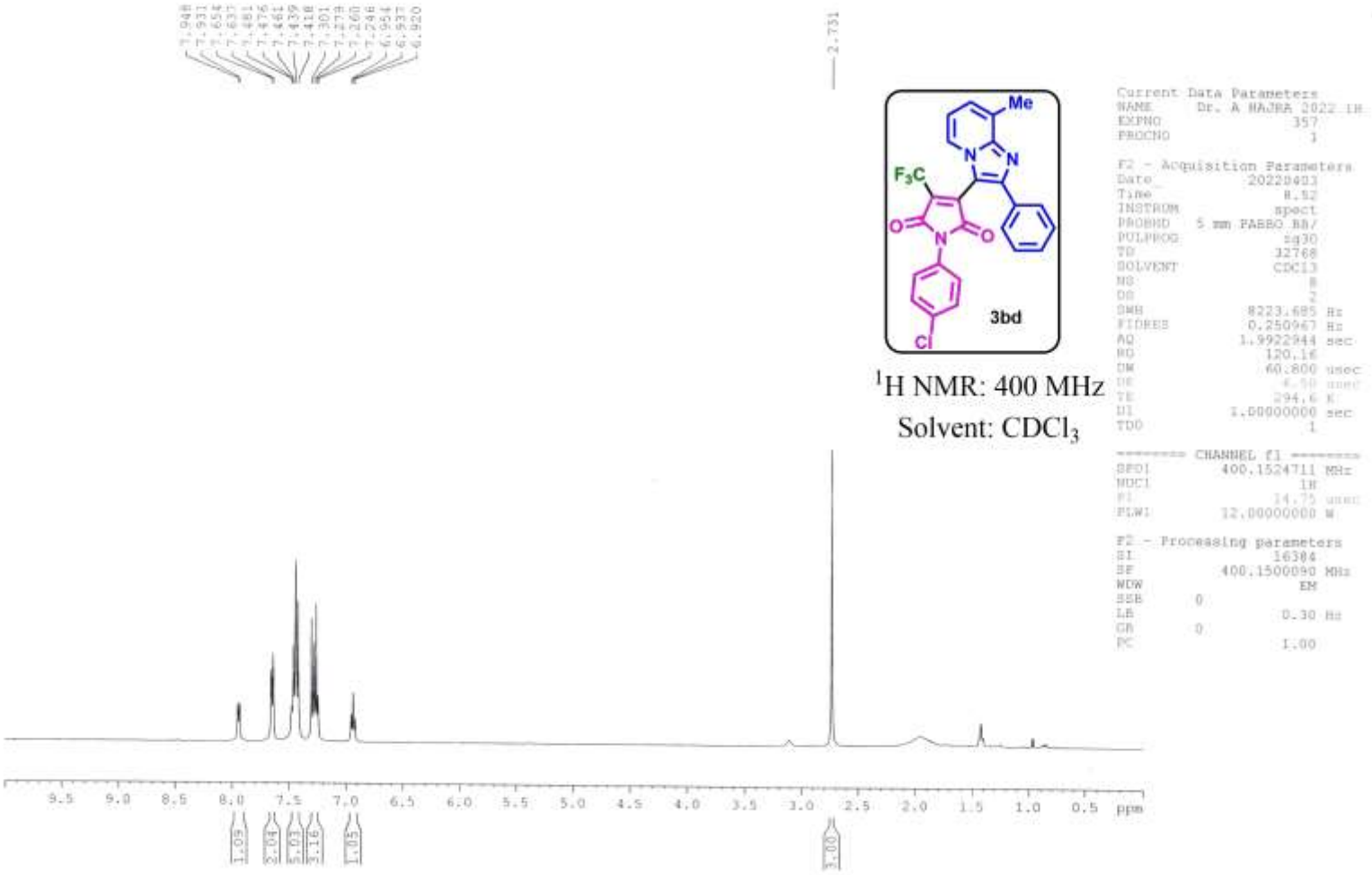


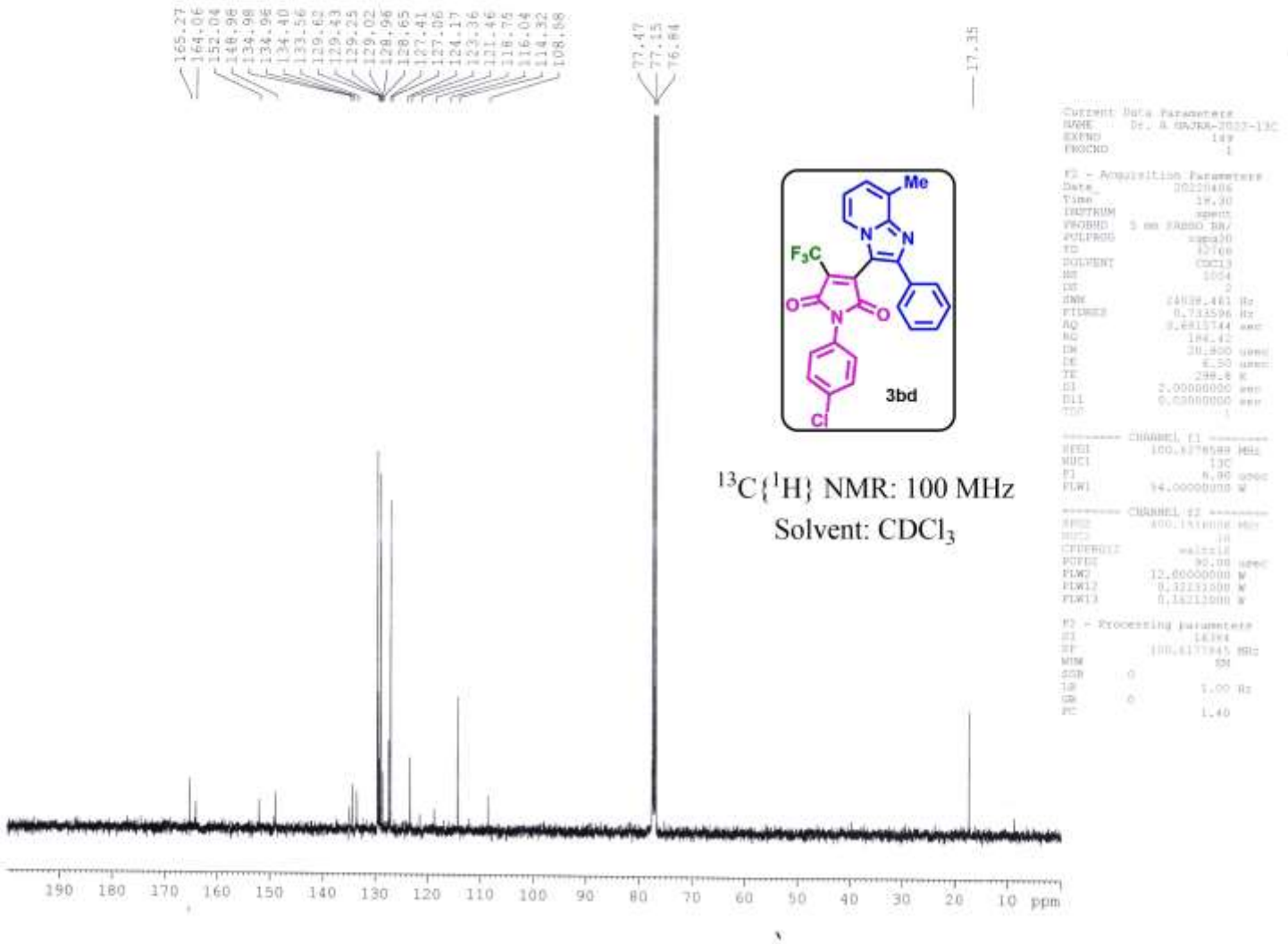

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                252
PROCNO                 1

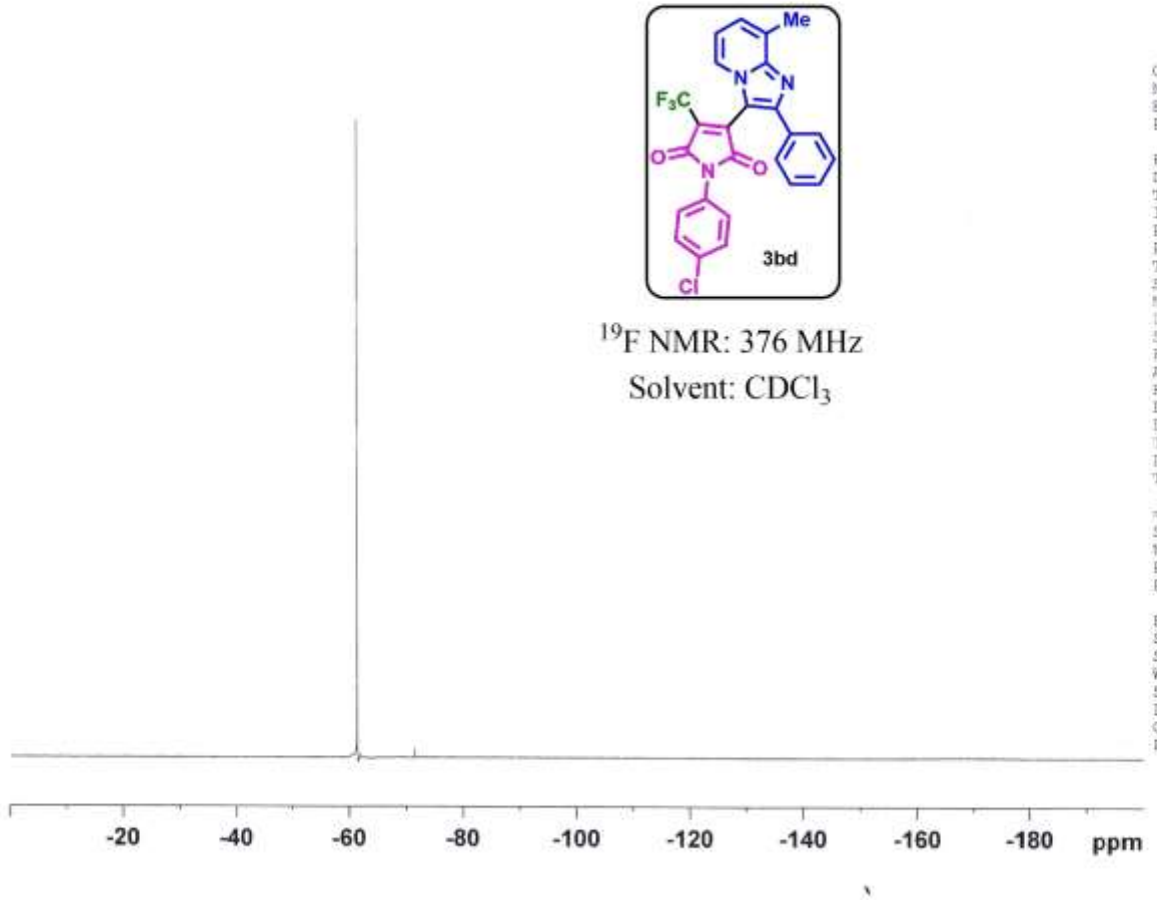
F2 - Acquisition Parameters
Date_           20220313
Time               9.09
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD              32768
SOLVENT          CDCl3
NS                   4
DS                   2
SWH          89285.711 Hz
FIDRES        2.724784 Hz
AQ           0.1835008 sec
RG              186.42
DW              5.600 usec
DE               6.50 usec
TE              291.5 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
```


7.948
7.931
7.658
7.637
7.481
7.476
7.461
7.439
7.418
7.301
7.273
7.260
7.248
6.954
6.937
6.920
2.731
Me
N
N
F3C
O
O
N
O
Cl
3bd
1H NMR: 400 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A HAJRA 2022 1H
EXPNO 357
PROCNO 1
F2 - Acquisition Parameters
Date 20220403
Time 8.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 120.16
DW 60.800 usec
DE 6.50 usec
TE 294.6 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 400.1500090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
1.09
2.04
5.03
3.16
1.05
3.00


165.27
164.06
152.04
140.98
134.98
134.96
134.40
133.56
129.62
129.43
129.25
129.02
128.96
128.65
127.41
127.06
124.17
123.36
121.46
118.75
116.04
114.32
108.88
77.47
77.15
76.84
17.35
Me
N
N
F3C
O
N
O
Cl
3bd
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



^{19}F NMR: 376 MHz

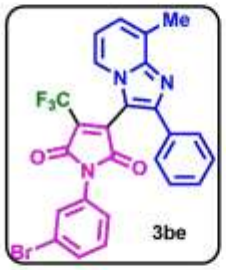
Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A RAJRA 2022 1H
EXPNO                  358
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220403
Time                8.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES        2.724784 Hz
AQ            0.1835008 sec
RG               120.16
DW                5.600 usec
DE                6.50 usec
TE                294.7 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

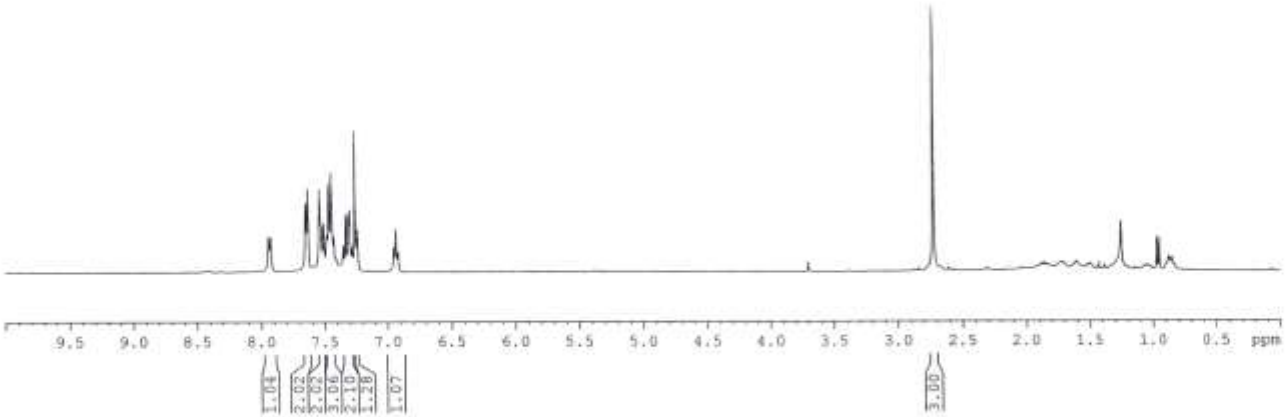
Solvent: $CDCl_3$

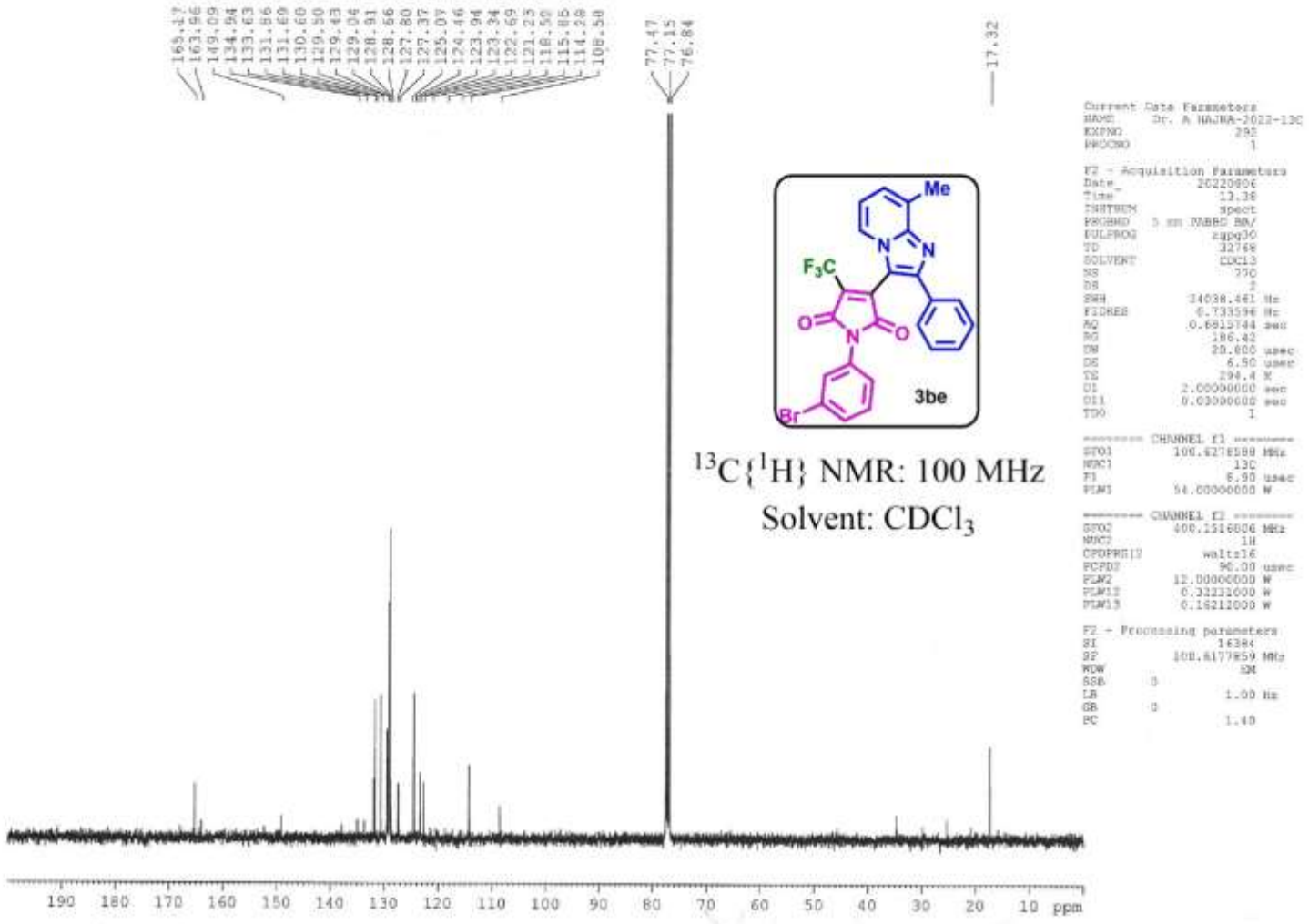
```
Current Data Parameters
NAME       Dr. A HAJBA 2022 1H
EXPNO                  700
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220806
Time               12.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               186.42
DW               60.800 usec
DE                6.50 usec
TE               293.6 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                1.00
```





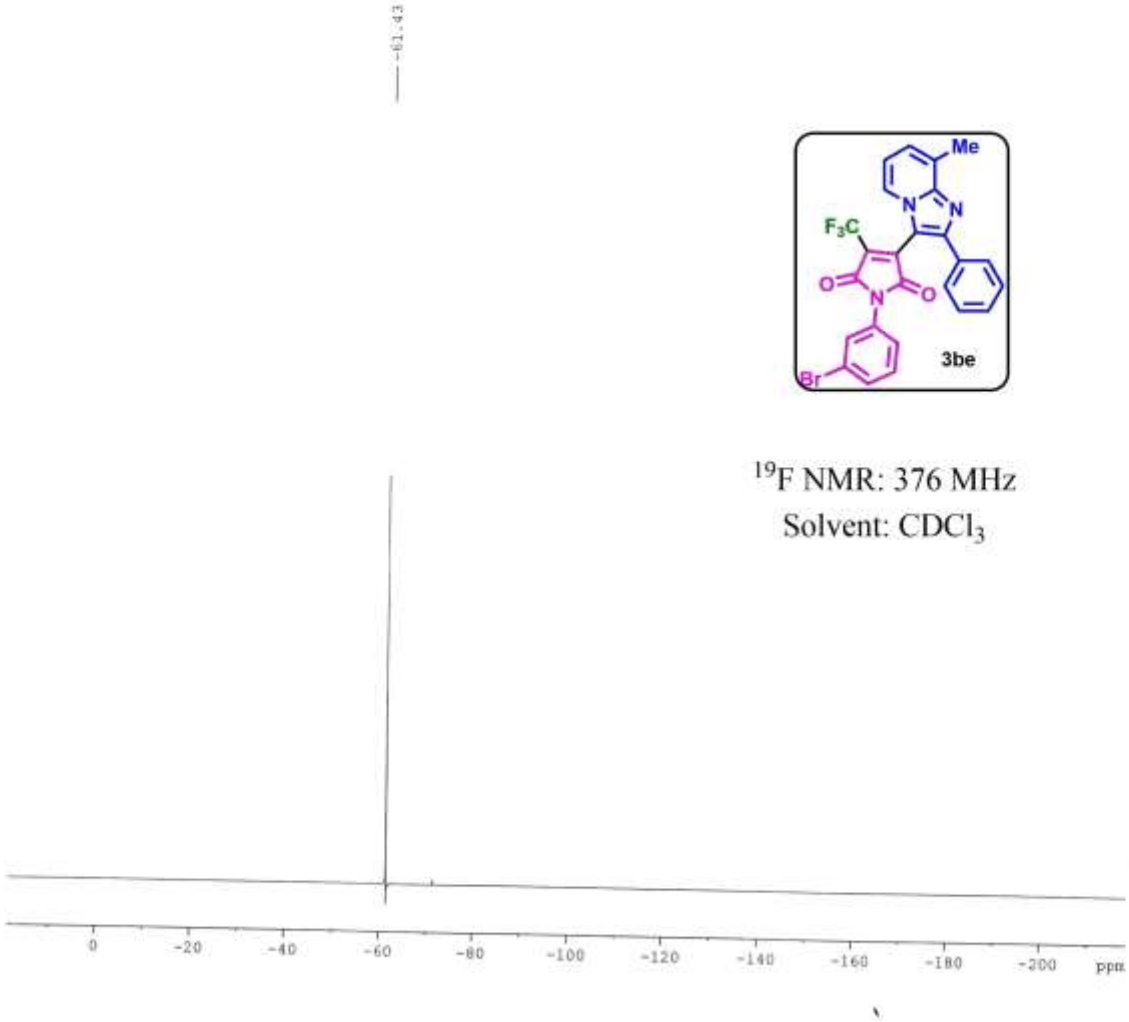

```
Current Data Parameters
NAME       Dr. A NAJNA-2022-13C
EXPNO                       295
PROCNO                        1

F2 - Acquisition Parameters
Date_                20220906
Time                    13.36
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       32768
SOLVENT                 CDCl3
NS                        750
DS                          2
SWH                 34038.441 Hz
FIDRES               0.733596 Hz
AQ                   0.6815744 sec
RG                      186.42
DW                      20.600 usec
DE                        6.50 usec
TE                       294.4 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

======== CHANNEL f2 ========
SFO2            400.1516006 MHz
NUC2                      1H
CPDPRG[2                  waltz16
PCPD2                    96.00 usec
PLW2            12.00000000 W
PLW12            0.32231000 W
PLW13            0.16212000 W

F2 - Processing parameters
SI                        16384
SF              100.6177859 MHz
WDW                         EM
SSB                       0
LB                        1.00 Hz
GB                        0
PC                        1.40
```

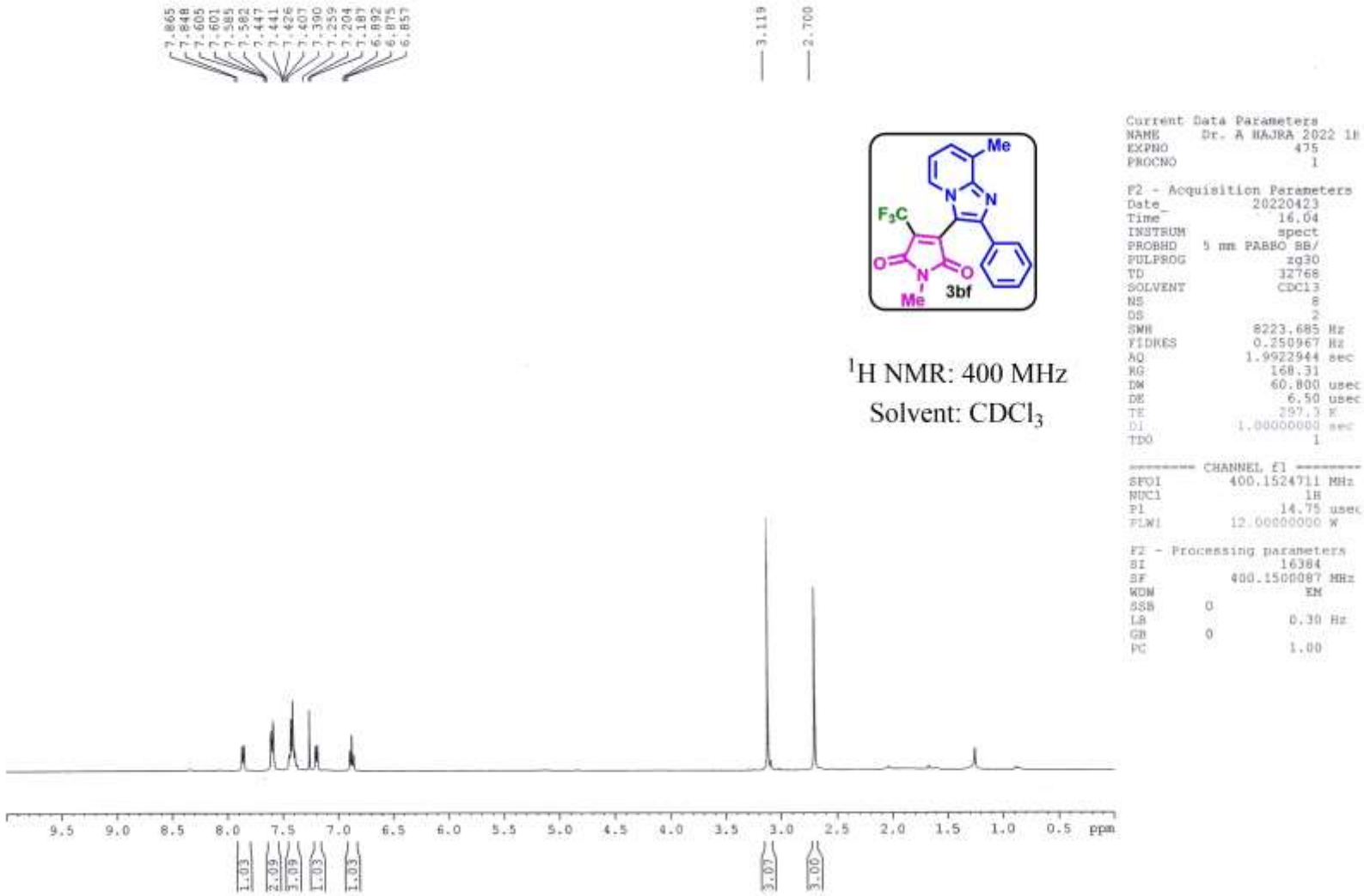


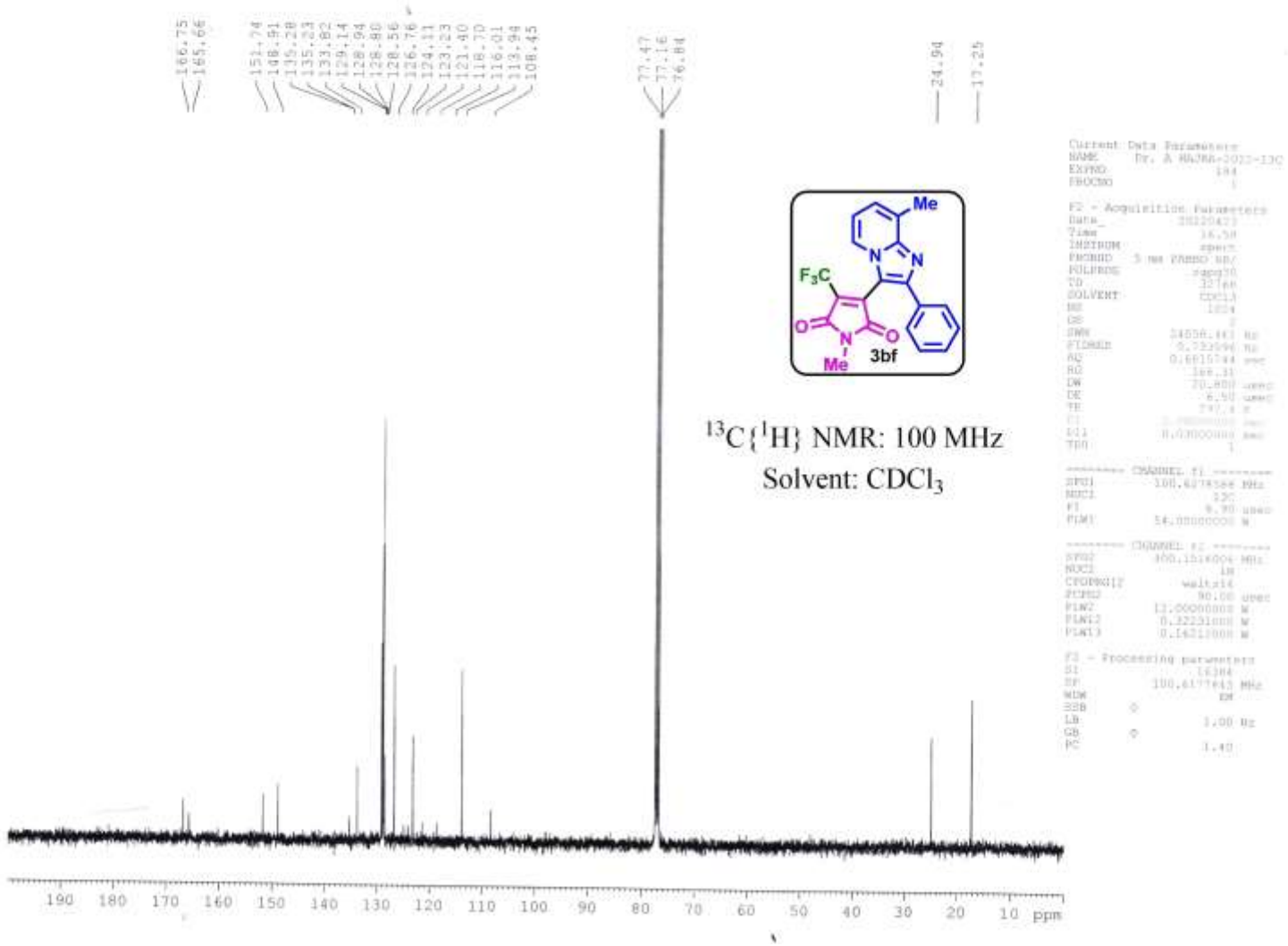

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  701
PROCNO                   1

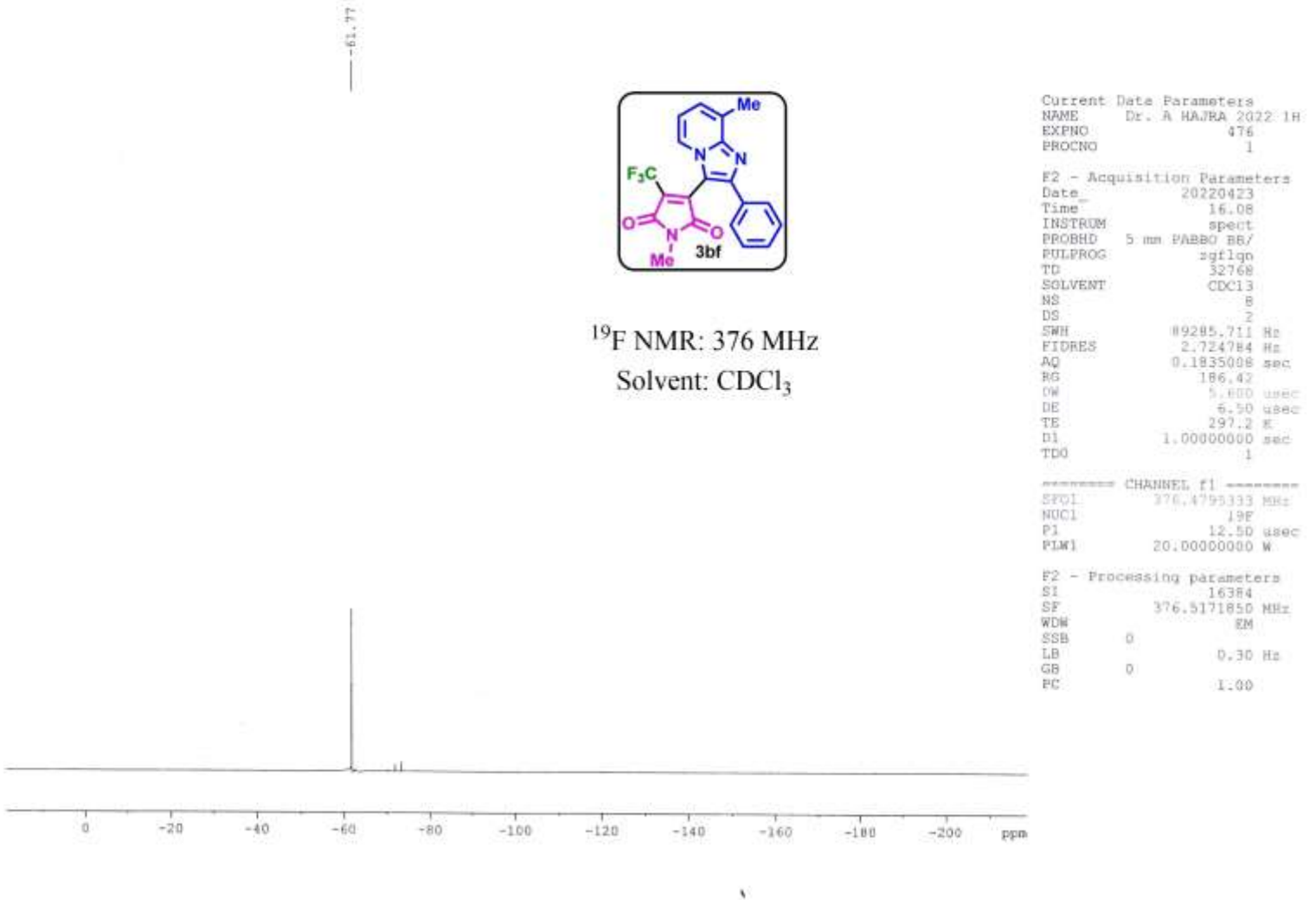
F2 - Acquisition Parameters
Date_           20220806
Time              12.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG                186.42
DW                5.600 usec
DE                6.50 usec
TE                293.6 K
D1            1.00000000 sec
TD0                   1

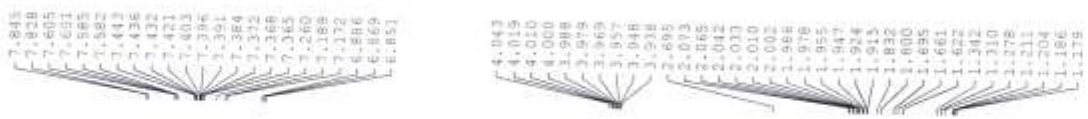
======== CHANNEL f1 ========
SFO1        376.4795333 MHz
NUC1               19F
P1                12.50 usec
PLW1        20.00000000 W

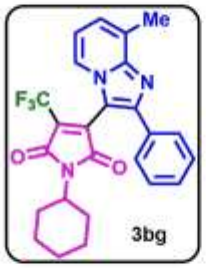
F2 - Processing parameters
SI                16384
SF          376.5171850 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```


7.865
7.848
7.605
7.601
7.585
7.582
7.447
7.441
7.426
7.407
7.390
7.259
7.204
7.187
6.892
6.875
6.857
3.119
2.700
Me
F3C
N
N
O
O
N
Me
3bf
1H NMR: 400 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A BAJRA 2022 18
EXPNO 475
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220423
Time 16.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 168.31
DW 60.800 usec
DE 6.50 usec
TE 297.3 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 1.00
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
1.03
2.09
3.09
1.03
1.03
3.07
3.00


166.75
165.66
151.74
148.91
135.28
135.23
133.82
129.14
128.94
128.80
128.56
126.76
124.11
123.23
121.40
118.70
116.01
113.94
108.45
77.47
77.16
76.84
24.94
17.25
Me
F3C
O
N
O
N
Me
3bf
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

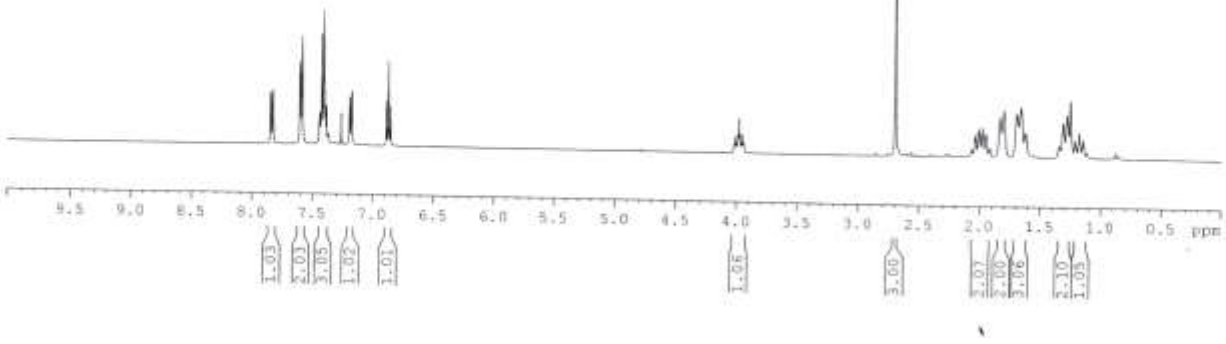

-61.77
Me
F3C
O
N
O
Me
3bf
19F NMR: 376 MHz
Solvent: CDCl3
Current Date Parameters
NAME Dr. A HAJRA 2022 1H
EXPNO 476
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220423
Time 16.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 89285.711 Hz
FIDRES 2.724784 Hz
AQ 0.1835008 sec
RG 186.42
DW 5.600 usec
DE 6.50 usec
TE 297.2 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
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm





^{1}H NMR: 400 MHz

Solvent: $CDCl_3$

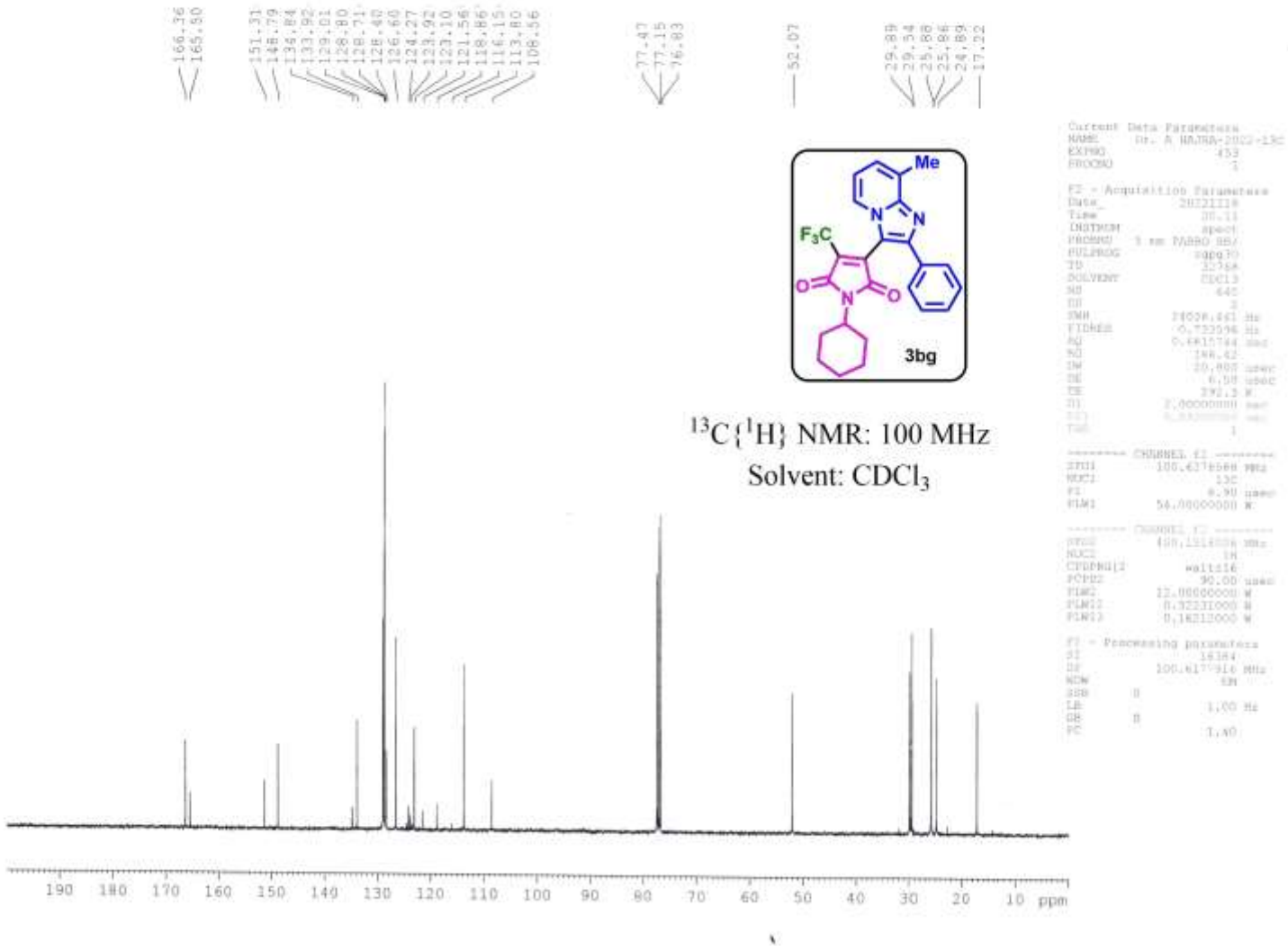


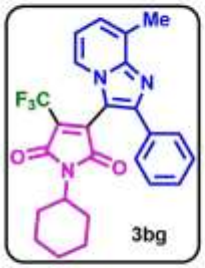

```
Current Data Parameters
NAME       Dr. A HAJRA 2022 1H
EXPNO                 1134
PROCNO                   1

F2 - Acquisition Parameters
Date_           20221218
Time                19.36
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     2
SWH              8223.685 Hz
FIDRES           0.250967 Hz
AQ               1.9922944 sec
RG                  47.25
DW                 60.800 usec
DE                  6.50 usec
TE                 291.7 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           400.1500095 MHz
WDW                   EM
SSB          0
LB                  0.30 Hz
GB           0
PC                  1.00
```


166.36
165.50
151.31
148.79
136.84
133.92
129.01
128.80
128.71
128.40
126.60
124.27
123.92
123.10
121.56
118.86
116.15
113.80
108.56
77.47
77.15
76.83
52.07
29.89
29.54
25.88
25.86
24.89
17.22
Me
N
N
F3C
O
O
N
3bg
13C{1H} NMR: 100 MHz
Solvent: CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



^{19}F NMR: 376 MHz

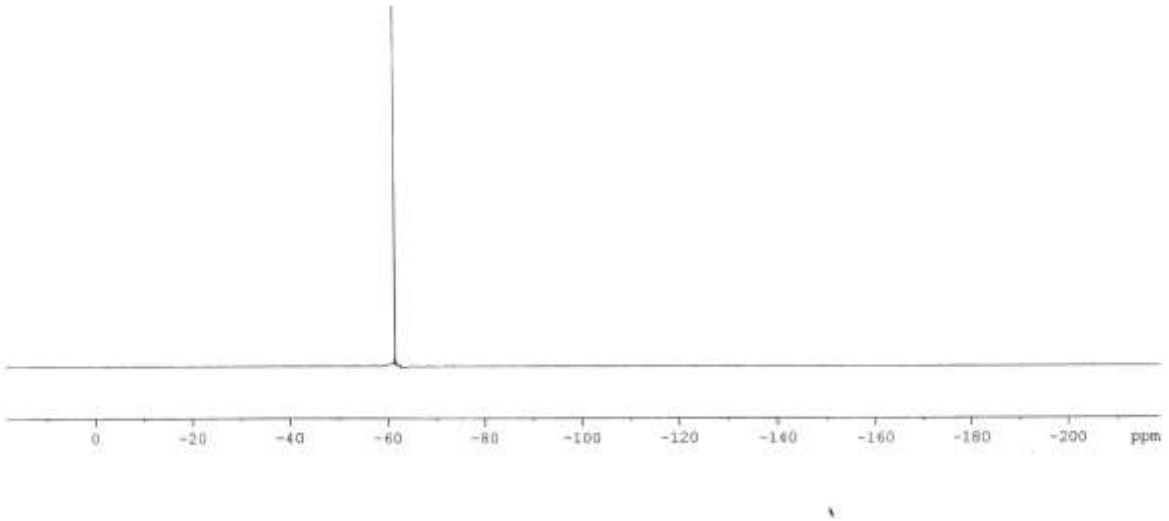
Solvent: $CDCl_3$

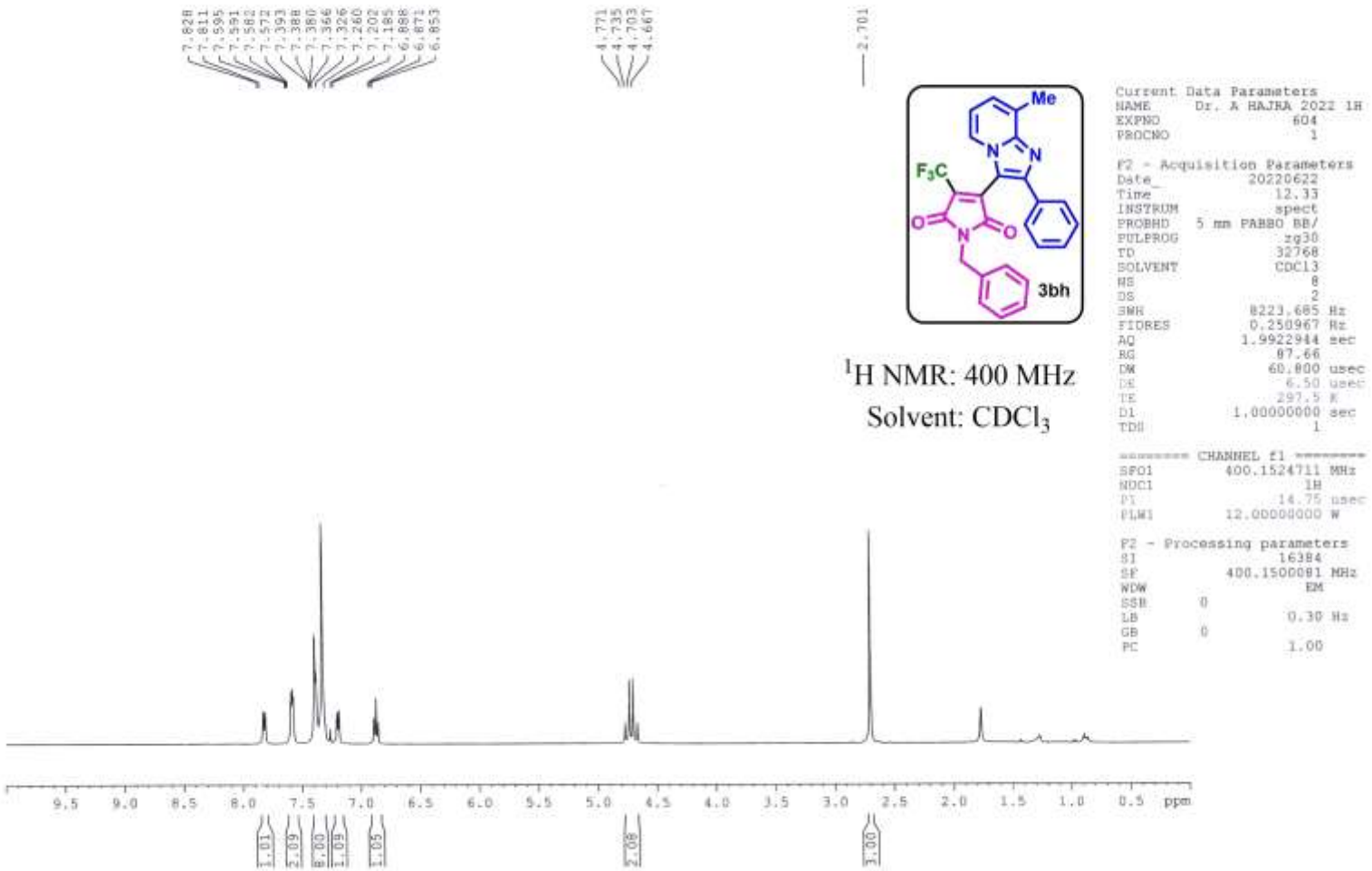
```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  #09
PROCNO                   1

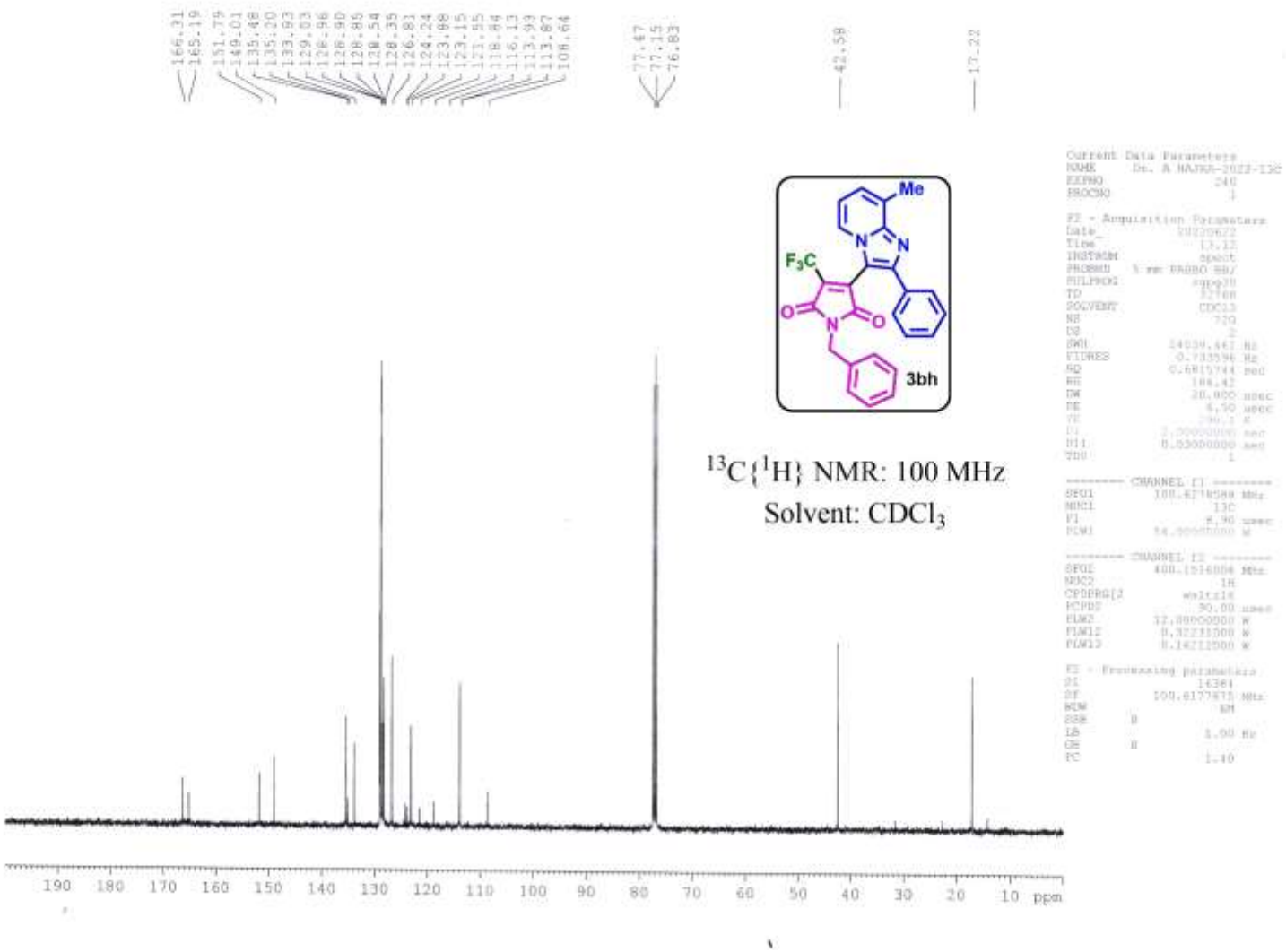
F2 - Acquisition Parameters
Date_           20220917
Time               20.14
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG                62.69
DW                5.600 usec
DE                6.50 usec
TE               295.5 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
```




7.828
7.811
7.595
7.591
7.582
7.572
7.393
7.388
7.380
7.366
7.326
7.260
7.202
7.185
6.888
6.871
6.853
4.771
4.735
4.703
4.667
2.701
Me
F3C
3bh
1H NMR: 400 MHz
Solvent: CDCl3
Current Data Parameters
NAME Dr. A HAJRA 2022 1H
EXPNO 604
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220622
Time 12.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 87.66
DW 60.800 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1524711 MHz
NDC1 1H
P1 14.75 usec
PLW1 12.00000000 W
F2 - Processing parameters
SI 16384
SF 400.1500081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
1.01
2.09
8.00
1.09
1.05
2.08
3.00



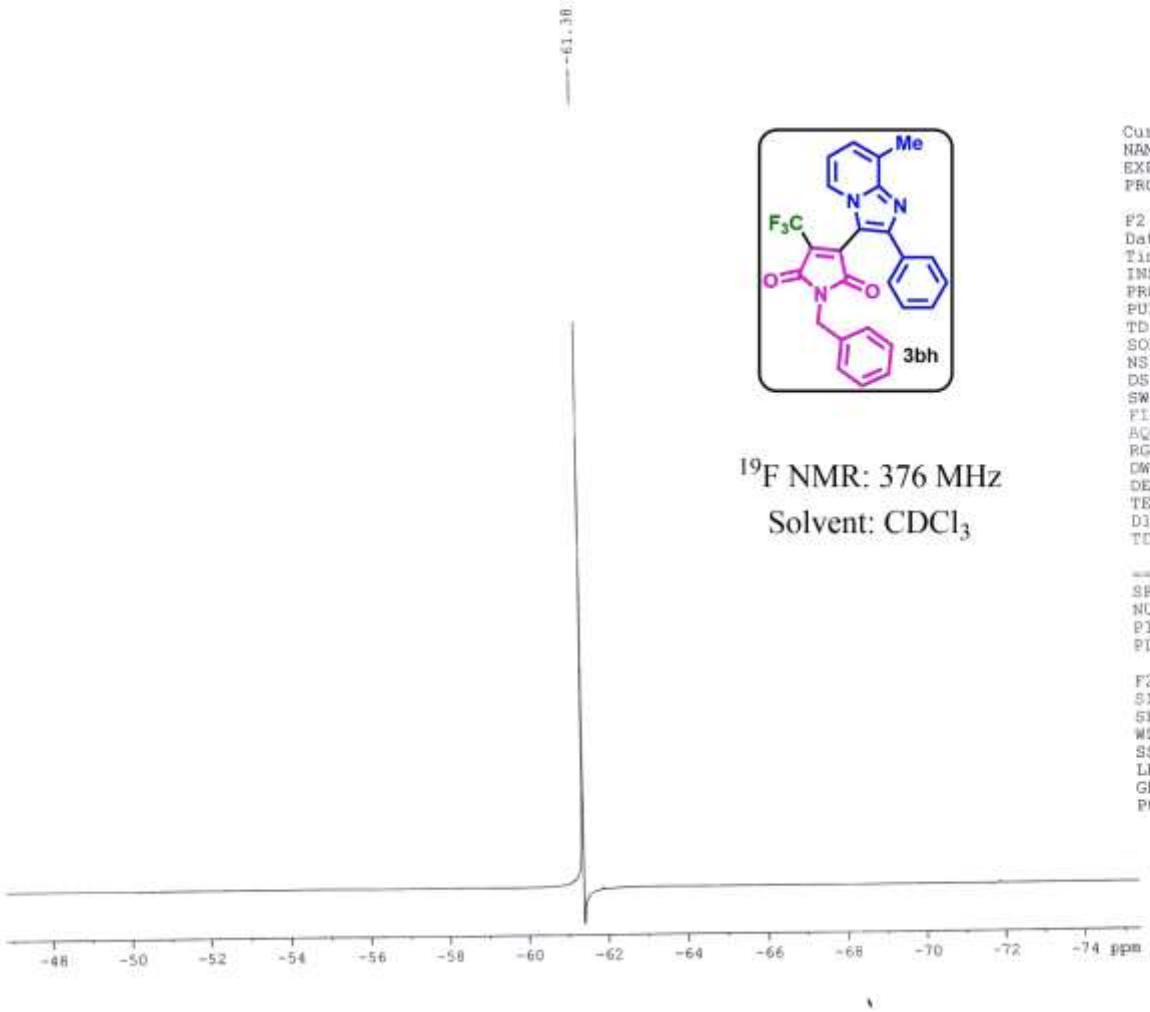
Current Data Parameters
NAME Dr. A NAJMA-2022-13C
EXPNO 240
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220622
Time 13.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 720
DS 2
SWH 24038.447 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 186.42
DW 20.800 usec
DE 6.50 usec
TE 296.1 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 400.1516004 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.80000000 W
PLW12 0.32231500 W
PLW13 0.14211500 W

F2 - Processing parameters
SI 16384
SF 100.6177815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



^{19}F NMR: 376 MHz

Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2022 1H
EXPNO                  605
PROCNO                   1

F2 - Acquisition Parameters
Date_              20220622
Time                  12.37
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zgflqn
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         2
SWH                89285.711 Hz
FIDRES              2.724784 Hz
AQ                  0.1835008 sec
RG                     186.42
DW                    5.600 usec
DE                    6.50 usec
TE                    297.5 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
```