Electronic Supporting Information

Site-Selective Direct Nitration of 2*H*-Indazoles: Easy Access to 7-Nitroindazoles

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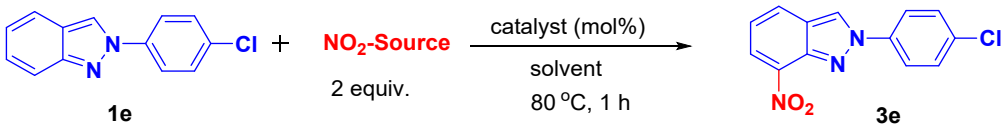
1. General information:

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), m (multiplet), and coupling constants (J) were given in Hz. $^{13}C\{^{1}H\}$ NMR spectra were recorded at 100 MHz in $CDCl_3$ solution. Chemical shifts are referenced to $CDCl_3$ (δ = 7.26 for ^{1}H and δ = 77.16 for $^{13}C\{^{1}H\}$ NMR) and DMSO-d_6 (δ = 2.50 for ^{1}H and δ = 39.52 for $^{13}C\{1H\}$ 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. High-resolution mass spectra (HRMS) were collected using electrospray ionization (ESI) on a time-of-flight (TOF) mass spectrometer. The crystallographic data for the compound **3g** was collected by SCXRD-BRUKER D8QUEST and the crystal data was solved by APEX4 software.

All the 2*H*-indazoles as starting materials were prepared by reported methods.[1,2]

Table S1. Optimization of the Reaction Conditions[a]



1e 3e

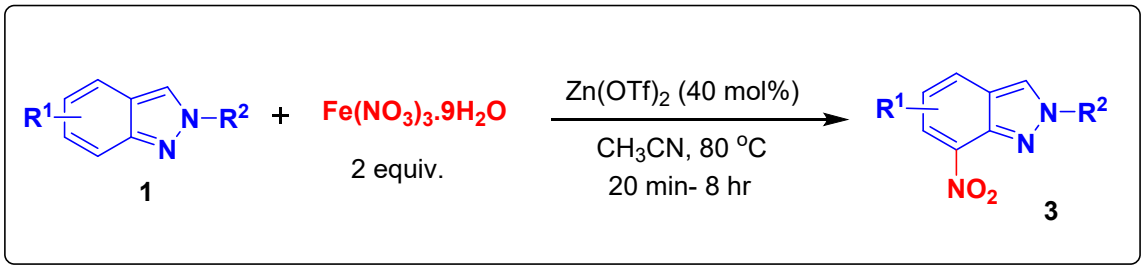
Different nitrating agents (NO_2-source):

$Fe(NO_3)_3.9H_2O$	^tBuONO	$(NH_4)_2Ce(NO_3)_6$	$AgNO_3$	$NaNO_2$	$Zn(NO_3)_2.6H_2O$
I	II	III	IV	V	VI

entry	catalyst (40 mol%)	solvent (2 mL)	[NO_2]	yield (%)
1	**$Zn(OTf)_2$**	**CH_3CN**	**I**	**78,** 69[b]
2	$Zn(OTf)_2$	Toluene	I	18
3	$Zn(OTf)_2$	1,2-DCE	I	trace
4	$Zn(OTf)_2$	MeOH	I	nr
5	$Zn(OTf)_2$	THF	I	nr
6	-	CH_3CN	I	13
7	$Zn(BF_4)_2$	CH_3CN	I	51
8	ZnI_2	CH_3CN	I	nr
9	$Cu(OTf)_2$	CH_3CN	I	56
10	$AlCl_3$	CH_3CN	I	61
11	$Zn(OTf)_2$	CH_3CN	II	trace
12	$Zn(OTf)_2$	CH_3CN	III	10
13	$Zn(OTf)_2$	CH_3CN	IV	12
14	$Zn(OTf)_2$	CH_3CN	V	nr
15	-	CH_3CN	VI	trace
16	$Zn(OTf)_2$	CH_3CN	I	52,[c] 66,[d] 75,[e]
17	$Zn(OTf)_2$	CH_3CN	I	57,[f] 76,[g] 55,[h] 69[i]

[a]Reaction conditions: All reactions were performed using 0.2 mmol of **1e**, 0.4 mmol of NO_2-agents and 40 mol% catalysts in 2 mL of solvent for 1 h at 80 °C under N_2 atmosphere. [b]Under open atmosphere. [c]Using 10 mol% of $Zn(OTf)_2$. [d]Using 20 mol% of $Zn(OTf)_2$. [e]Using 1 equiv. of $Zn(OTf)_2$. [f]Using 1 equiv. of **I**. [g]Using 3 equiv. of **I**. [h]At 50 °C. [i]At 100 °C. nr = no reaction.

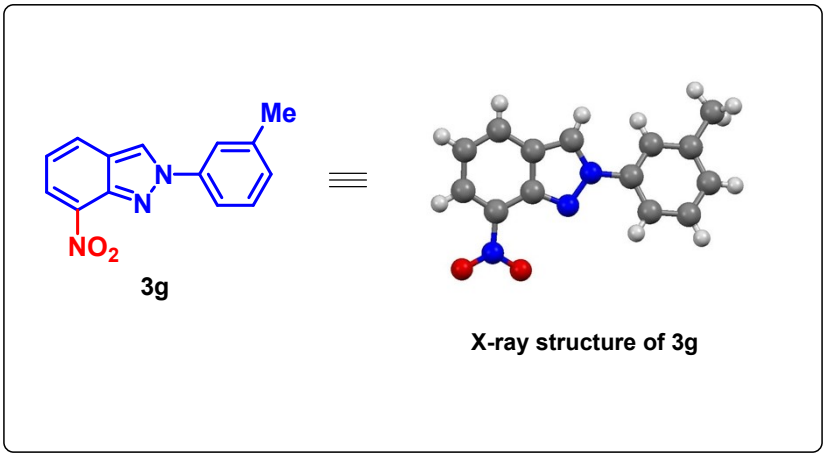
2. General experimental procedure for the synthesis of 3a-3z:

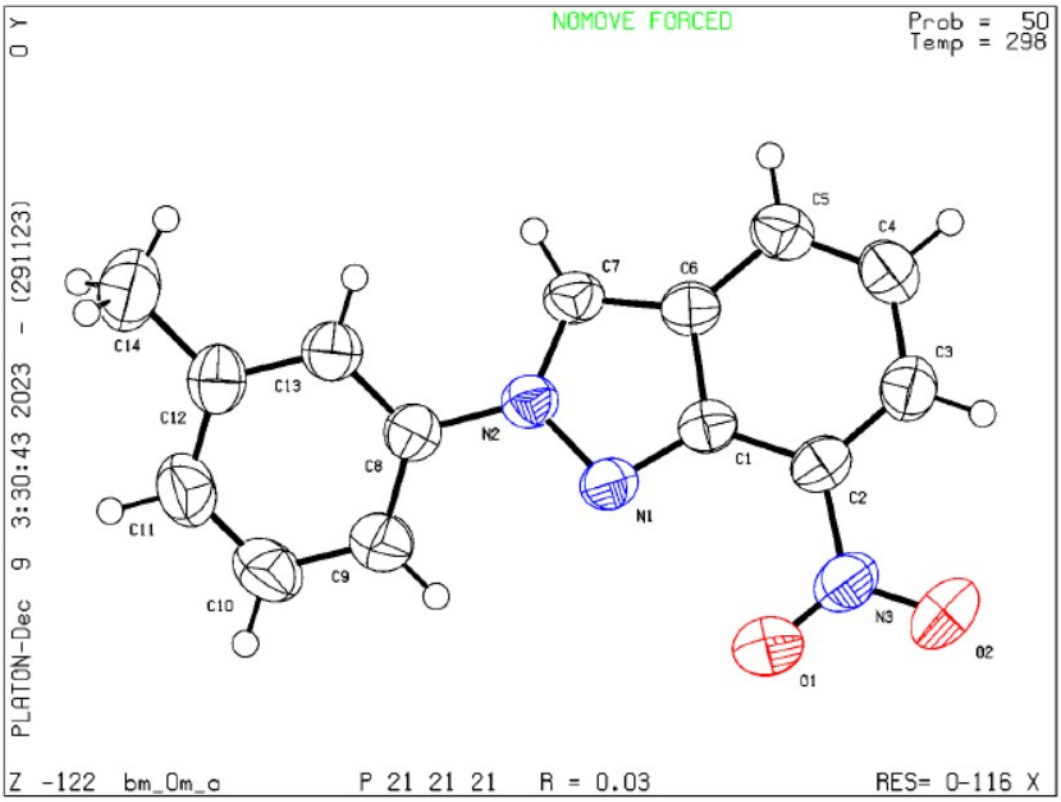


2*H*-indazoles (**1a-1z**, 0.2 mmol), $Fe(NO_3)_3.9H_2O$ (0.4 mmol, 162 mg), $Zn(OTf)_2$ (40 mol%, 29 mg) and 2.0 mL CH_3CN solvent were added to an oven-dried reaction tube, which was equipped with a magnetic stirrer bar. At the last, tube was heated in a preheated oil bath at 80 °C under N_2 atmosphere. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction was cooled to room temperature and extracted with ethyl acetate (10-15 mL). The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude residue which was purified by column chromatography on silica gel (60−120 mesh) using a mixture of petroleum ether and ethyl acetate as an eluent to afford their corresponding 7-nitro-2*H*-indazoles (**3a-3z**).

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

The brown block crystal of **3g** was obtained by crystallization from a solution in dichloromethane/petroleum ether after purification by column chromatography. The chemical formula of compound **3g**: $C_{14}H_{11}N_3O_2$.



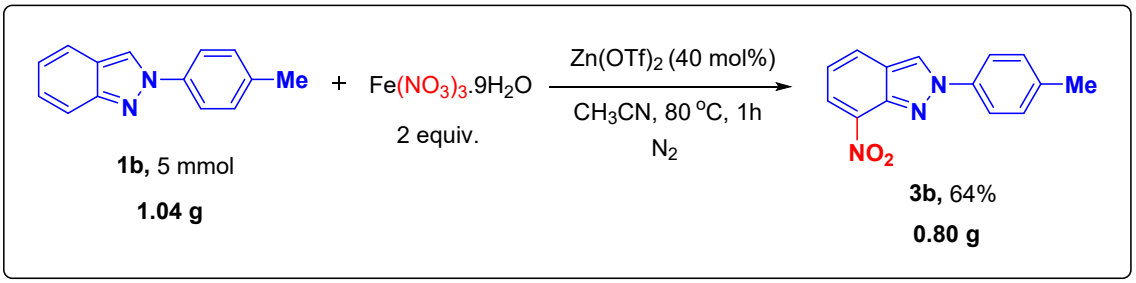


View of ORTEP diagram for the crystal structure of the compound ***7-Nitro-2-(m-tolyl)-2H-indazole*** (**3g**) (Thermal ellipsoid contour at 50% probability level).

Wavelength	0.71073Å	
Formula	$C_{14}\ H_{11}\ N_3\ O_2$	
Crystal system	orthorhombic	
Space group	P 2_1 2_1 2_1	
Unit cell dimensions	a = 8.1213(7) Å	α = 90°
	b = 11.1938(9) Å	β = 90°
	c = 13.6325(11) Å	γ =90°
Volume	1239.31 $Å^3$	
Z	4	
R-factor (%)	3	

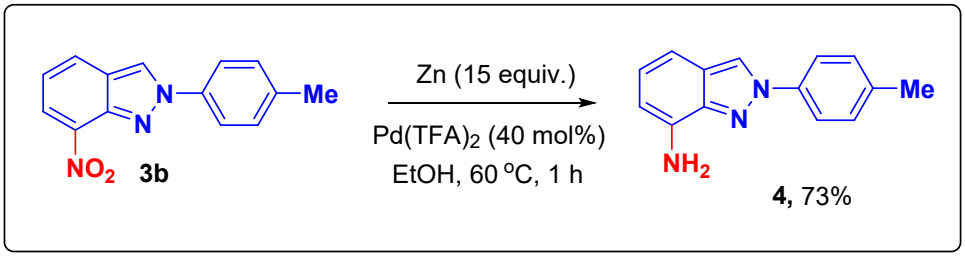
The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication with a CCDC reference number CCDC 2313021.

4. Large scale synthesis of 7-Nitro-2-(*p*-tolyl)-2*H*-indazole (3b):



To an oven dried 50 mL round bottom flask equipped with a magnetic bar were charged with 2-(*p*-tolyl)-2*H*-indazole (**1b**, 5.0 mmol, 1.04 g), $Fe(NO_3)_3.9H_2O$ (2 equiv., 4.04 g) and $Zn(OTf)_2$ (40 mol%, 727 mg) in 20 mL CH_3CN were added. After that, the round bottom flask was heated in an oil bath at 80 °C for 1 hour under N_2 atmosphere. The progress of the reaction was monitored by TLC. After completion of the reaction, the reaction was cooled to room temperature and extracted with 40 mL ethyl acetate. The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to get the crude residue which was purified by column chromatography on silica gel (60−120 mesh) using a mixture of petroleum ether and ethyl acetate (90 : 10) as an eluent to afford the 7-nitro-2-(*p*-tolyl)-2*H*-indazole (**3b**) (64%, 0.80 g) as a yellow solid.

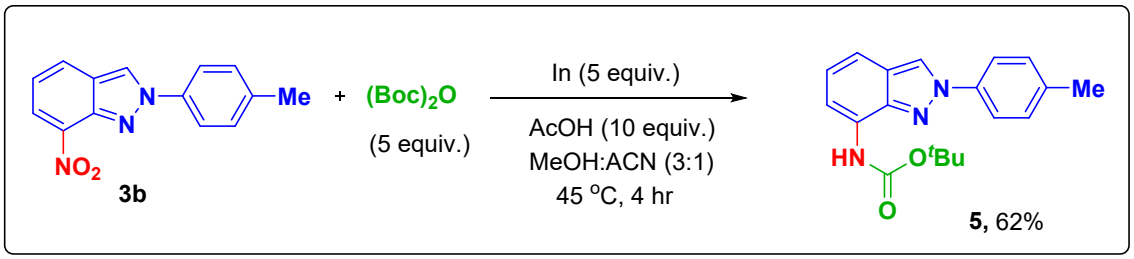
5. Experimental procedure for the synthesis of 2-(*p*-Tolyl)-2*H*-indazol-7-amine (4):



7-Nitro-2-(*p*-tolyl)-2*H*-indazole (**3b**, 0.1 mmol, 25 mg), Zn powder (15 equiv., 98 mg), $Pd(TFA)_2$ (40 mol%, 13 mg) and 2 mL EtOH as a solvent were added in an oven dried reaction tube then the tube was heated at 60 °C in an oil bath for 1 h under open atmosphere. Thereafter, the product formation of the reaction was monitored by TLC. After the reaction

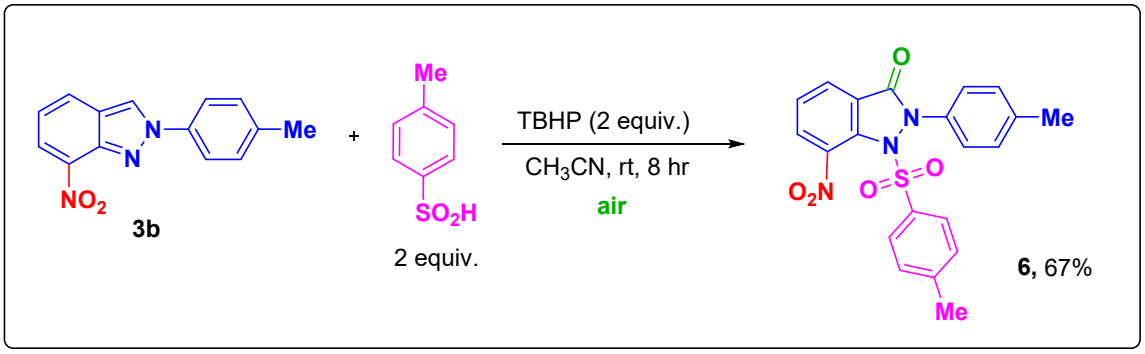
was completed, ethanol was evaporated under vacuum using rotary evaporator. The reaction mixture was diluted with ethyl acetate and washed with brine. The organic layer was dried over anhydrous Na_2SO_4, concentrated and the crude mixture was purified by a flash column chromatography on silica gel (60–120 mesh) using 20% ethyl acetate in hexane on silica gel to afford the corresponding 7-amino-2*H*-indazole (**4**) (16 mg, 73%) as a black gummy mass.

6. Synthetic procedure of *tert*-Butyl (2-(*p*-tolyl)-2*H*-indazol-7-yl)carbamate (5):



7-Nitro-2-(*p*-tolyl)-2*H*-indazole (**3b**, 0.1 mmol, 25 mg), $(Boc)_2O$ (5 equiv., 109 mg), In-metal (5 equiv., 57 mg) and AcOH (10 equiv., 60 mg) in MeOH/ACN (3:1) (2 mL) as solvent were taken in an oven dried reaction tube and stirred at 45 °C for 4 h under open atmosphere. Then the product formation of the reaction was monitored by TLC. After the reaction was completed, the reaction mixture was diluted with ethyl acetate and washed with brine. The organic layer was dried over anhydrous Na_2SO_4, concentrated and the crude mixture was purified by a flash column chromatography on silica gel (100−200 mesh) using 3% ethyl acetate in hexane on silica gel to furnish the corresponding 7-amidated derivative **5** (20 mg, 62%) as a light yellow solid.

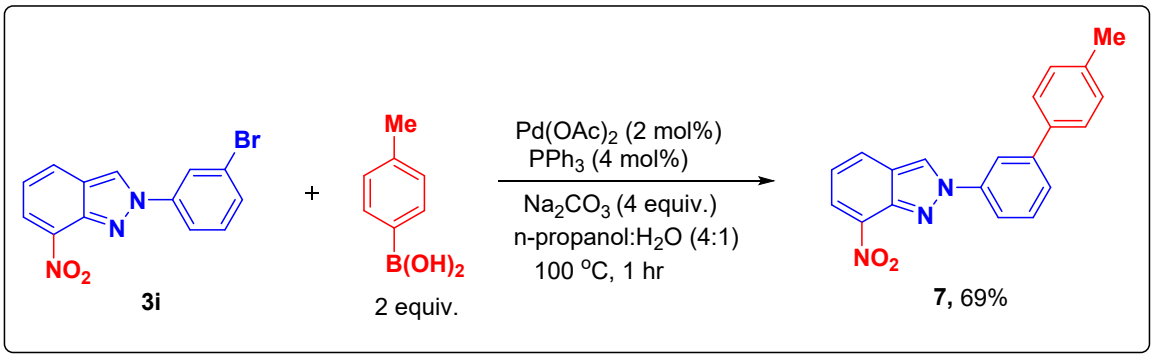
7. Synthesis of 7-Nitro-2-(*p*-tolyl)-1-tosyl-1,2-dihydro-3*H*-indazol-3-one (6):



7-Nitro-2-(*p*-tolyl)-2*H*-indazole (**3b**, 0.1 mmol, 25 mg), 4-methylbenzenesulfinic acid (2 equiv., 31 mg), TBHP (2 equiv., 0.035 mL) in CH_3CN (2 mL) as a solvent were taken in an

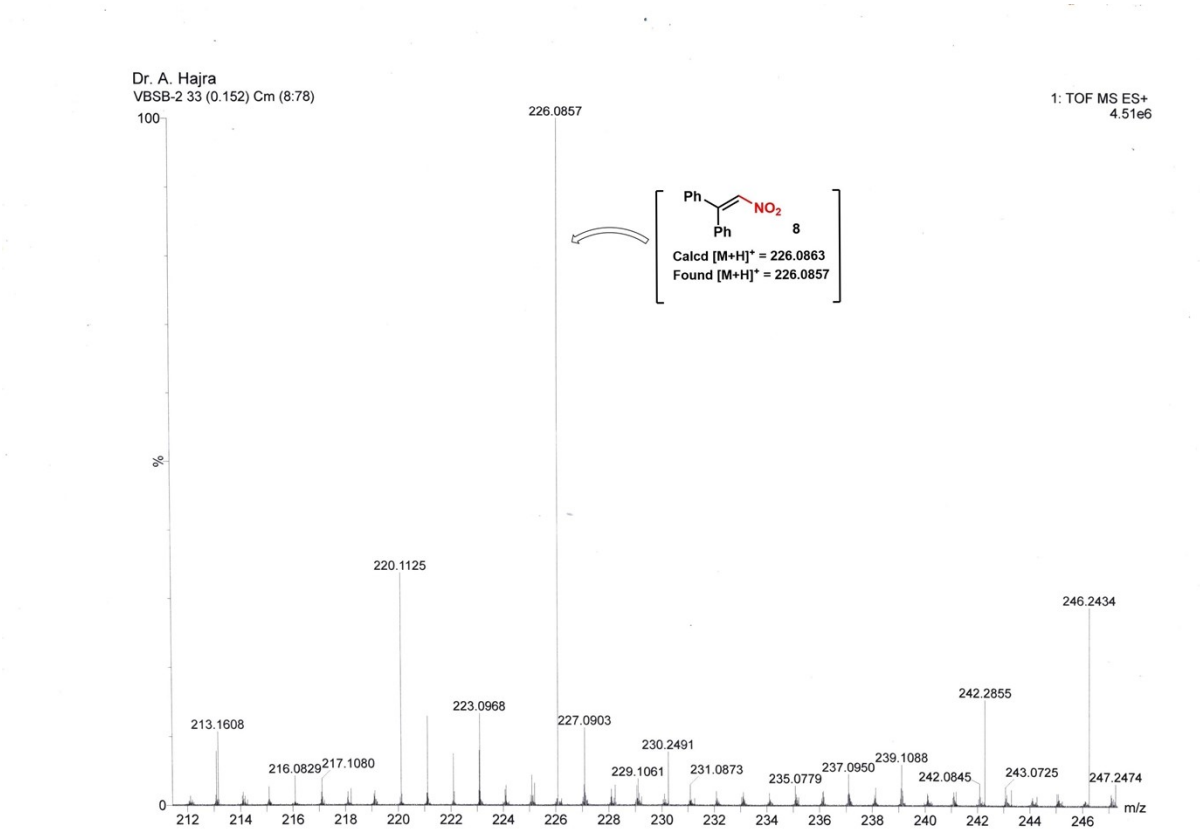
oven dried reaction tube and stirred at room temperature for 8 hr in open atmosphere. Then the product formation of the reaction was monitored by TLC. After the reaction was completed, the reaction mixture was diluted with ethyl acetate and water. The organic layer was dried over anhydrous Na_2SO_4, concentrated and the crude mixture was purified by a flash column chromatography on silica gel (60−120 mesh) using 18% ethyl acetate in hexane on silica gel to furnish the nitro bearing indazolone derived product **6** (28 mg, 67%) as a brown gummy mass.

8. Synthetic procedure of 2-(4'-Methyl-[1,1'-biphenyl]-3-yl)-7-nitro-2*H*-indazole (7):

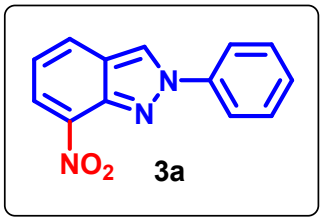


In an oven-dried reaction tube 2-(3-bromophenyl)-7-nitro-2*H*-indazole (**3i**, 0.1 mmol, 32 mg), *p*-tolylphenylboronic acid (2 equiv., 27 mg), $Pd(OAc)_2$ (2.0 mol%, 0.4 mg), PPh_3 (4 mol%, 1.0 mg) and Na_2CO_3 (4.0 equiv., 42.4 mg) were added in 2mL n-propanol:H_2O (4:1) mixed solvent and stirred at 100 °C under open atmosphere for 1 hr. After the completion of the reaction (monitored by TLC), the crude reaction mixture was extracted with ethyl acetate and brine solution. The organic extract was dried over anhydrous Na_2SO_4 and concentrated. The product was subjected to column chromatography (silica gel, 100-200 mesh), eluting with petroleum ether and ethyl acetate (94:6) to afford the product **7** (69%, 23 mg) as a yellow gummy mass.

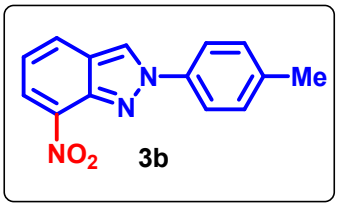
9. HRMS analysis of the NO_2-radical scavenged adduct (8):



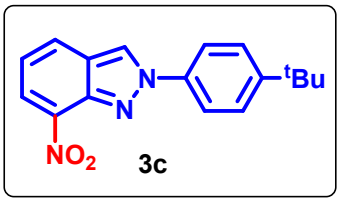
10. Characterization data of the synthesized compounds (3a-7):



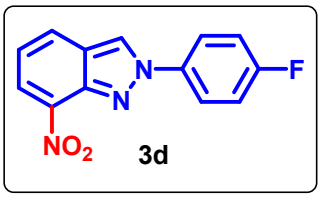
7-Nitro-2-phenyl-2H-indazole (3a): Green solid (32 mg, 67%); M.p. 174–175 °C; R_f = 0.55 (PE : EA = 85 : 15); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.65 (s, 1H), 8.37 (d, J = 7.6 Hz, 1H), 8.11 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 7.6 Hz, 2H), 7.58-7.54 (m, 2H), 7.48-7.45 (m, 1H), 7.22 (d, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.6, 139.9, 138.1, 129.8, 129.1, 129.0, 126.3, 125.9, 122.8, 121.7, 120.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{13}H_{10}N_3O_2]^+$: 240.0768; found: 240.0774.



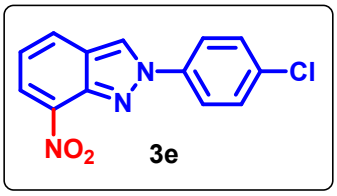
7-Nitro-2-(p-tolyl)-2H-indazole (3b): Yellow solid (38 mg, 75%); M.p. 106–107 °C; R_f = 0.5 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.59 (s, 1H), 8.32 (d, J = 7.6 Hz, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.82 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.4 Hz, 2H), 7.19 (t, J = 8.0 Hz, 1H), 2.41 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.4, 139.2, 138.0, 137.6, 130.3, 128.9, 126.2, 125.6, 122.6, 121.4, 120.6, 21.2; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{14}H_{12}N_3O_2]^+$: 254.0924; found: 254.0923.



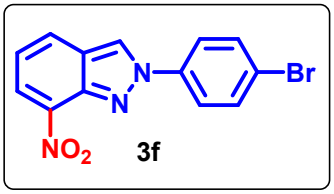
2-(4-(tert-Butyl)phenyl)-7-nitro-2H-indazole (3c): Red gummy mass (37 mg, 63%); R_f = 0.5 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.61 (s, 1H), 8.35 (d, J = 7.6 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.89-7.85 (m, 2H), 7.57-7.53 (m, 2H), 7.21 (t, J = 8.0 Hz, 1H), 1.36 (s, 9H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 152.5, 141.5, 138.0, 137.5, 128.9, 126.7, 125.7, 122.7, 121.4, 120.7, 114.4, 34.9, 31.3; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{17}H_{18}N_3O_2]^+$: 296.1394; found: 296.1391.



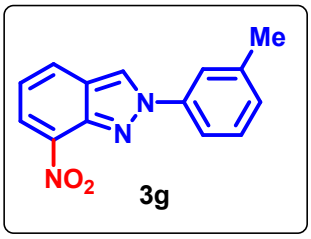
2-(4-Fluorophenyl)-7-nitro-2H-indazole (3d): Yellow solid (36 mg, 71%); M.p. 198–199 °C; R_f = 0.45 (PE : EA = 85 : 15); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.60 (s, 1H), 8.35 (d, J = 7.6 Hz, 1H), 8.10 (d, J = 8.0 Hz, 1H), 7.96-7.92 (m, 2H), 7.25-7.18 (m, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 162.7 ($J_{C\text{-}F}$ = 248.0 Hz), 141.6, 138.0, 136.2, 129.0, 126.3, 126.0, 123.5 ($J_{C\text{-}F}$ = 9.0 Hz), 122.9, 121.0, 116.8 ($J_{C\text{-}F}$ = 23.0 Hz); HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{13}H_9FN_3O_2]^+$: 258.0673; found: 258.0678.



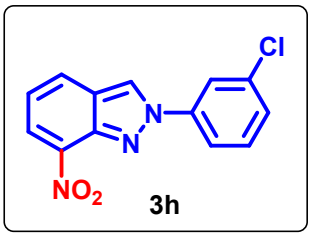
2-(4-Chlorophenyl)-7-nitro-2H-indazole (3e): Yellow solid (43 mg, 78%); M.p. 175-176 °C; R_f = 0.55 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.62 (s, 1H), 8.36 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 7.94-7.91 (m, 2H), 7.53-7.50 (m, 2H), 7.23 (d, J = 7.6 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.7, 138.4, 138.1, 135.0, 130.0, 128.9, 126.3, 126.1, 122.7, 121.2; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{13}H_9{}^{35}ClN_3O_2]^+$: 274.0378; found: 274.0361.



2-(4-Bromophenyl)-7-nitro-2H-indazole (3f): Yellow solid (39 mg, 61%); M.p. 176-177 °C; R_f = 0.55 (PE : EA = 80 : 20); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.50 (s, 1H), 8.38 (d, J = 7.6 Hz, 1H), 8.31 (d, J = 8.4 Hz, 1H), 8.10 (d, J = 8.8 Hz, 2H), 7.83 (d, J = 8.8 Hz, 2H), 7.32 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (DMSO-d_6, 400 MHz): δ 140.6, 138.5, 136.9, 132.7, 130.4, 126.4, 126.0, 124.9, 122.7, 121.6, 121.0; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{13}H_9{}^{81}BrN_3O_2]^+$: 319.9852; found: 319.9845.

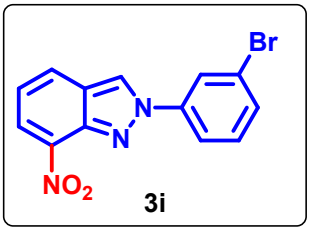


7-Nitro-2-(m-tolyl)-2H-indazole (3g): Yellow solid (37 mg, 74%); M.p. 180-181 °C; R_f = 0.5 (PE : EA = 86 : 14); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.63 (s, 1H), 8.37-8.35 (m, 1H), 8.11-8.09 (m, 1H), 7.83 (s, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.42 (t, J = 8.0 Hz, 1H), 7.28-7.25 (m, 1H), 7.22 (t, J = 8.0 Hz, 1H) 2.47 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.5, 140.1, 139.9, 138.1, 129.9, 129.6, 129.0, 126.2, 125.8, 122.8, 122.4, 120.8, 118.6, 21.5; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{14}H_{12}N_3O_2]^+$: 254.0924; found: 254.0916.



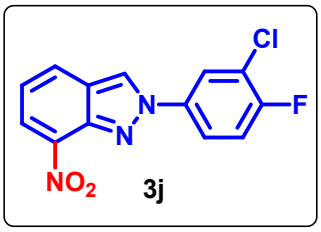
3h

2-(3-Chlorophenyl)-7-nitro-2H-indazole (3h): Yellow solid (38 mg, 69%); M.p. 206-207 °C; R_f = 0.5 (PE : EA = 85 : 15); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.46 (s, 1H), 8.35 (d, J = 7.2 Hz, 1H), 8.28 (d, J = 8.4 Hz, 1H), 8.18 (t, J = 2.0 Hz, 1H), 8.09-8.07 (m, 1H), 7.63 (t, J = 8.4 Hz, 1H), 7.56-7.54 (m, 1H), 7.30 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 140.7, 140.4, 137.0, 134.2, 131.6, 130.5, 128.7, 126.6, 126.0, 125.3, 121.2, 120.7, 119.5; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for [$C_{13}H_9{}^{35}ClN_3O_2$]$^+$: 274.0378; found: 274.0372.



3i

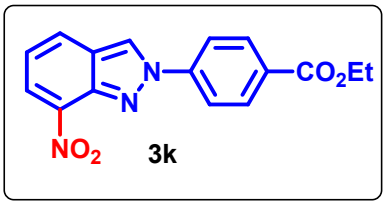
2-(3-Bromophenyl)-7-nitro-2H-indazole (3i): Yellow solid (42 mg, 66%); M.p. 205-206 °C; R_f = 0.45 (PE : EA = 85 : 15); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.50 (s, 1H), 8.38-8.28 (m, 3H), 8.16-8.13 (m, 1H), 7.71-7.69 (m, 1H), 7.58 (t, J = 8.4 Hz, 1H), 7.31 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 140.6, 140.5, 136.9, 131.8, 131.6, 130.4, 126.5, 125.9, 125.2, 123.4, 122.4, 121.1, 119.9; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for [$C_{13}H_9{}^{79}BrN_3O_2$]$^+$: 317.9873; found: 317.9871.



3j

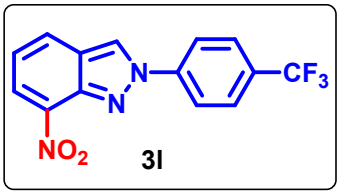
2-(3-Chloro-4-fluorophenyl)-7-nitro-2H-indazole (3j): Yellow solid (42 mg, 72%); M.p. 219-220 °C; R_f = 0.45 (PE : EA = 85 : 15); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.44 (s, 1H), 8.37-8.31 (m, 2H), 8.28 (d, J = 8.4 Hz, 1H), 8.14-8.10 (m, 1H), 7.66 (t, J = 9.2 Hz, 1H), 7.31 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 157.1 ($J_{C\text{-}F}$ = 247.0 Hz), 140.6, 136.9, 136.3, 130.5, 126.5, 126.0, 125.4, 123.0, 121.7, 121.2, 120.8 ($J_{C\text{-}F}$ = 19.0 Hz), 118.1

($J_{C\text{-}F}$ = 23.0 Hz); HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{13}H_8{}^{35}ClFN_3O_2]^+$: 292.0284; found: 292.0299.



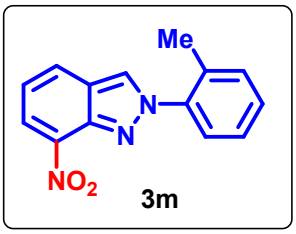
3k

Ethyl 4-(7-nitro-2H-indazol-2-yl)benzoate (3k): Yellow solid (42 mg, 67%); M.p. 162-163 °C; R_f = 0.5 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.72 (s, 1H), 8.37-8.35 (m, 1H), 8.22-8.20 (m, 2H), 8.12-8.09 (m, 1H), 8.07 (d, J = 8.4 Hz, 2H), 7.26-7.22 (m, 1H), 4.42 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 165.6, 142.8, 141.9, 138.2, 131.3, 130.9, 129.1, 126.4, 122.9, 121.3, 121.0, 61.5, 14.4; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{16}H_{14}N_3O_4]^+$: 312.0979; found: 312.0992.



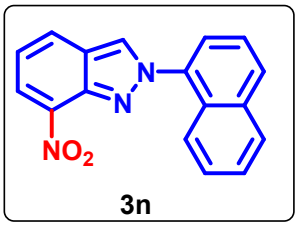
3l

7-Nitro-2-(4-(trifluoromethyl)phenyl)-2H-indazole (3l): Light green solid (38 mg, 62%); M.p. 159-160 °C; R_f = 0.55 (PE : EA = 88 : 12); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.72 (s, 1H), 8.37 (d, J = 7.6 Hz, 1H), 8.13 (t, J = 8.4 Hz, 3H), 7.82 (d, J = 8.8 Hz, 2H), 7.26 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 142.3, 141.9, 138.2, 131.2, 129.1, 127.1 (q, $J_{C\text{-}F}$ = 5 Hz), 126.5, 126.4 (q, $J_{C\text{-}F}$ = 272 Hz), 126.3, 122.9, 121.6, 121.5; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{14}H_9F_3N_3O_2]^+$: 308.0641; found: 308.0644.



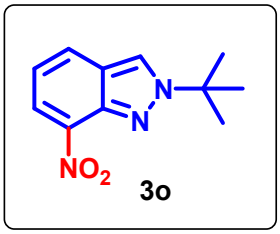
3m

7-Nitro-2-(o-tolyl)-2H-indazole (3m): Yellow solid (35 mg, 70%); M.p. 227-228 °C; R_f = 0.6 (PE : EA = 85 : 15); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.06 (s, 1H), 8.40-8.34 (m, 2H), 7.56-7.49 (m, 3H), 7.46-7.44 (m, 1H), 7.34 (t, J = 8.0 Hz, 1H), 2.19 (s, 3H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 140.1, 139.5, 136.9, 133.3, 131.4, 130.5, 129.8, 128.8, 126.9, 126.6, 125.8, 125.3, 120.6, 17.5; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{14}H_{12}N_3O_2]^+$: 254.0924; found: 254.0922.



3n

2-(Naphthalen-1-yl)-7-nitro-2H-indazole (3n): Brown solid (39 mg, 68%); M.p. 234-235 °C; R_f = 0.40 (PE : EA = 85 : 15); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.24 (s, 1H), 8.46-8.40 (m, 2H), 8.22 (d, J = 8.0 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.84 (d, J = 6.8 Hz, 1H), 7.73 (t, J = 8.0 Hz, 1H), 7.67-7.63 (m, 1H), 7.61-7.56 (m, 2H), 7.39 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 140.5, 137.0, 136.5, 133.7, 130.7, 130.4, 130.1, 128.3, 128.2, 128.1, 127.2, 126.1, 125.48, 125.45, 124.6, 122.5, 120.8; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{17}H_{12}N_3O_2]^+$: 290.0924; found: 290.0940.



3o

2-(tert-Butyl)-7-nitro-2H-indazole (3o): Yellow gummy mass (28 mg, 63%); R_f = 0.55 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.30-8.28 (m, 2H), 8.03-8.01 (m, 1H), 7.14 (t, J = 8.0 Hz, 1H), 1.80 (s, 9H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 140.2, 137.8, 128.9, 125.3, 124.7, 121.8, 119.7, 61.6, 30.3; HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $[C_{11}H_{13}N_3NaO_2]^+$: 242.0900; found: 242.0901.

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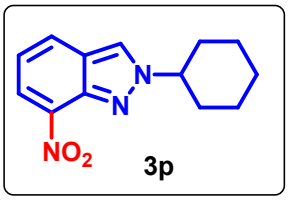
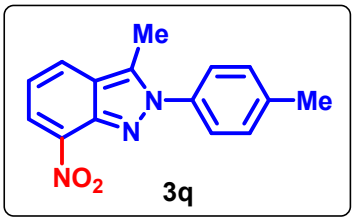
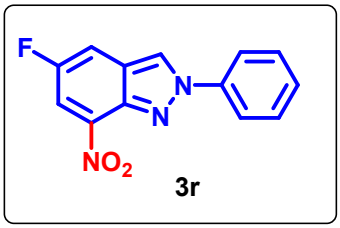


3p

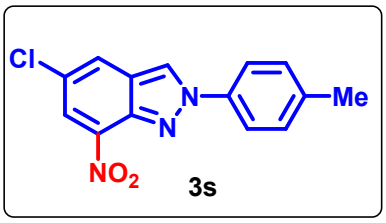
2-Cyclohexyl-7-nitro-2H-indazole (3p): Light orange solid (31 mg, 64%); M.p. 129-130 °C; R_f = 0.6 (PE : EA = 88 : 12); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.29 (d, J = 7.6 Hz, 1H), 8.20 (s, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.14 (t, J = 8.0 Hz, 1H), 4.66-4.58 (m, 1H), 2.36-2.33 (m, 2H), 1.96-1.92 (m, 2H), 1.87-1.76 (m, 3H), 1.55-1.43 (m, 2H), 1.36-1.23 (m, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 139.9, 137.5, 128.9, 125.5, 124.9, 122.2, 119.8, 63.6, 34.1, 25.4, 25.2; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{13}H_{16}N_3O_2]^+$: 246.1237; found: 246.1230.



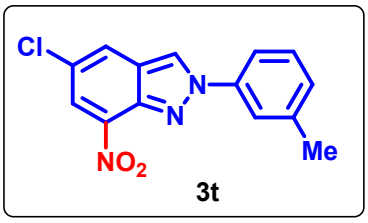
3-Methyl-7-nitro-2-(p-tolyl)-2H-indazole (3q): Yellow solid (39 mg, 73%); M.p. 118-119 °C; R_f = 0.45 (PE : EA = 85 : 15); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.38 (d, J = 7.2 Hz, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.46 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.17 (t, J = 8.0 Hz, 1H), 2.68 (s, 3H), 2.45 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 140.5, 139.8, 137.4, 136.6, 135.1, 130.0, 128.9, 126.2, 125.9, 125.5, 119.2, 21.3, 11.4; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{15}H_{14}N_3O_2]^+$: 268.1081; found: 268.1075.



5-Fluoro-7-nitro-2-phenyl-2H-indazole (3r)*:* Yellow solid (36 mg, 70%); M.p. 185-186 °C; R_f = 0.5 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.63 (s, 1H), 8.17-8.15 (m, 1H), 7.96-7.94 (m, 2H), 7.75-7.72 (m, 1H), 7.58-7.53 (m, 2H), 7.49-7.45 (m, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 156.1 ($J_{C\text{-}F}$ = 242 Hz), 139.8, 139.0, 138.3, 129.9, 129.3, 125.1 ($J_{C\text{-}F}$ = 10 Hz), 122.6 ($J_{C\text{-}F}$ = 8 Hz), 121.6, 116.8 ($J_{C\text{-}F}$ = 32 Hz), 111.9 ($J_{C\text{-}F}$ = 24 Hz); HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{13}H_9FN_3O_2]^+$: 258.0673; found: 258.0687.

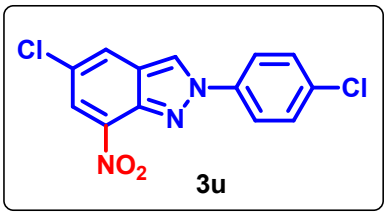


5-Chloro-7-nitro-2-(p-tolyl)-2H-indazole (3s): Yellow solid (41 mg, 71%); M.p. 201-202 °C; R_f = 0.55 (PE : EA = 90 : 10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.56 (s, 1H), 8.29 (d, J = 1.6 Hz, 1H), 8.05 (d, J = 1.6 Hz, 1H), 7.82 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.4 Hz, 2H), 2.44 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 139.9, 139.7, 138.1, 137.4, 130.4, 127.2, 126.4, 126.1, 122.0, 121.4, 21.2; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for $[C_{14}H_{11}{}^{35}ClN_3O_2]^+$: 288.0534; found: 288.0549.



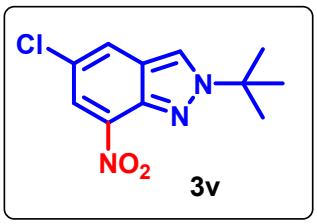
3t

5-Chloro-7-nitro-2-(m-tolyl)-2H-indazole (3t): Yellow solid (37 mg, 65%); M.p. 192-193 °C; R_f = 0.55 (PE : EA = 90 : 10); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.33 (s, 1H), 8.37 (d, J = 1.6 Hz, 1H), 8.25 (d, J = 1.6 Hz, 1H), 7.89 (s, 1H), 7.85 (d, J = 8.8 Hz, 1H), 7.48 (t, J = 8.4 Hz, 1H), 7.32 (d, J = 7.6 Hz, 1H), 2.42 (s, 3H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 139.8, 139.2, 137.4, 130.0, 129.9, 128.8, 126.3, 126.1, 125.1, 124.7, 124.5, 121.5, 118.3, 21.1; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for [$C_{14}H_{11}{}^{35}ClN_3O_2$]$^+$: 288.0534; found: 288.0536.



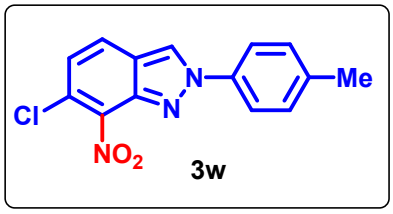
3u

5-Chloro-2-(4-chlorophenyl)-7-nitro-2H-indazole (3u): Yellow solid (41 mg, 66%); M.p. 237-238 °C; R_f = 0.5 (PE : EA = 90 : 10); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.41 (s, 1H), 8.41 (d, J = 2.4 Hz, 1H), 8.29 (d, J = 1.2 Hz, 1H), 8.12 (d, J = 8.8 Hz, 2H), 7.68 (d, J = 9.2 Hz, 2H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 139.1, 137.9, 137.3, 133.6, 129.9, 128.7, 126.3, 126.2, 124.8, 124.6, 122.6; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for [$C_{13}H_8{}^{35}Cl_2N_3O_2$]$^+$: 307.9988; found: 307.9994.



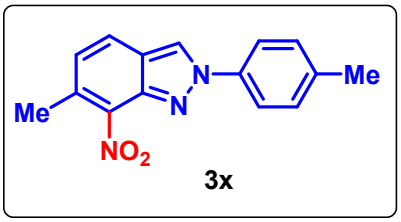
3v

2-(tert-Butyl)-5-chloro-7-nitro-2H-indazole (3v): Yellow solid (31 mg, 62%); M.p. 138-139 °C; R_f = 0.45 (PE : EA = 92 : 08); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.24 (s, 1H), 8.23 (d, J = 2.0 Hz, 1H), 7.98 (d, J = 1.6 Hz, 1H), 1.79 (s, 9H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 138.7, 137.9, 127.2, 125.5, 125.4, 125.0, 121.3, 62.0, 30.2; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for [$C_{11}H_{13}{}^{35}ClN_3O_2$]$^+$: 254.0691; found: 254.0691.



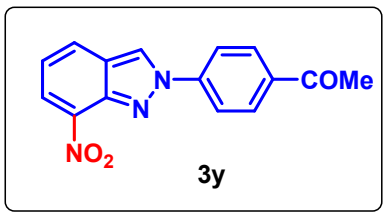
3w

6-Chloro-7-nitro-2-(p-tolyl)-2H-indazole (3w): Brown solid (39 mg, 68%); M.p. 146-147 °C; R_f = 0.55 (PE : EA = 88 : 12); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.49 (s, 1H), 7.79 (d, J = 8.8 Hz, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.4 Hz, 2H), 7.14 (d, J = 8.8 Hz, 1H), 2.42 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.9, 139.3, 137.4, 130.4, 125.1, 124.79, 124.72, 123.9, 123.4, 122.2, 121.2, 21.2; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{14}H_{11}{}^{35}ClN_3O_2]^+$: 288.0534; found: 288.0531.



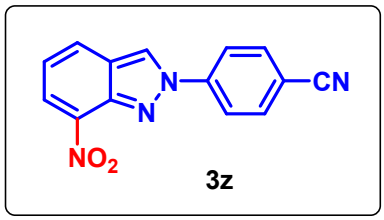
3x

6-Methyl-7-nitro-2-(p-tolyl)-2H-indazole (3x): Yellow solid (37 mg, 70%); M.p. 136-137 °C; R_f = 0.45 (PE : EA = 92 : 08); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.43 (s, 1H), 7.76 (d, J = 8.4 Hz, 3H), 7.29 (d, J = 8.4 Hz, 2H), 6.99 (d, J = 8.4 Hz, 1H), 2.58 (s, 3H), 2.41 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 142.2, 138.8, 138.7, 137.7, 131.7, 130.2, 125.7, 124.5, 123.6, 121.7, 121.1, 21.2, 19.2; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{15}H_{14}N_3O_2]^+$: 268.1081; found: 268.1086.

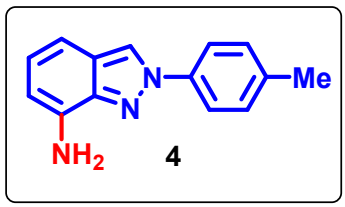


3y

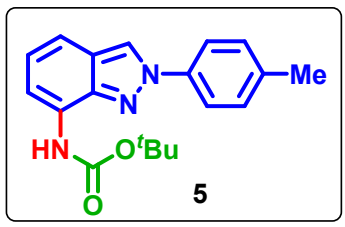
1-(4-(7-Nitro-2H-indazol-2-yl)phenyl)ethan-1-one (3y): Yellow gummy mass (31 mg, 56%); R_f = 0.45 (PE : EA = 70 : 30); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.74 (s, 1H), 8.40-8.38 (m, 1H), 8.17-8.11 (m, 5H), 7.28 (d, J = 7.6 Hz, 1H), 2.68 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 196.8, 142.9, 142.0, 137.1, 132.6, 130.1, 129.1, 126.5, 126.4, 122.9, 121.5, 121.3, 26.9; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{15}H_{12}N_3O_3]^+$: 282.0873; found: 282.0867.



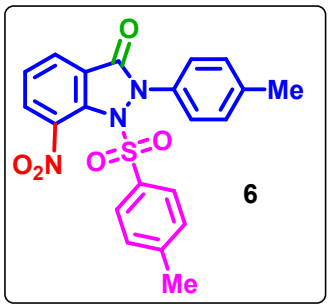
4-(7-Nitro-2H-indazol-2-yl)benzonitrile (3z): Yellow solid (34 mg, 64%); M.p. 166 -167 °C; R_f = 0.5 (PE : EA = 85 : 25); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 9.65 (s, 1H), 8.44-8.34 (m, 4H), 8.15 (d, J = 8.8 Hz, 2H), 7.36 (t, J = 8.0 Hz, 1H); ^{13}C{^{1}H} NMR (DMSO-d_6, 100 MHz): δ 142.3, 140.9, 137.0, 134.2, 130.6, 127.0, 126.1, 125.7, 121.5, 121.4, 118.2, 111.1; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for [$C_{14}H_9N_4O_2$]$^+$: 265.0720; found: 265.0706.



2-(p-Tolyl)-2H-indazol-7-amine (4): Black gummy mass (16 mg, 73%); R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.27 (s, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.31 (d, J = 8.4 Hz, 2H), 7.09 (d, J = 8.0 Hz, 1H), 6.95-6.91 (m, 1H), 6.46 (d, J = 7.2 Hz, 1H), 3.62 (s, 2H), 2.42 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 143.1, 138.4, 137.8, 136.9, 130.1, 123.8, 123.4, 120.9, 120.5, 109.4, 105.9, 21.1; HRMS (ESI-TOF) m/z: [M + H]$^+$ Calcd for [$C_{14}H_{14}N_3$]$^+$: 224.1182; found: 224.1180.

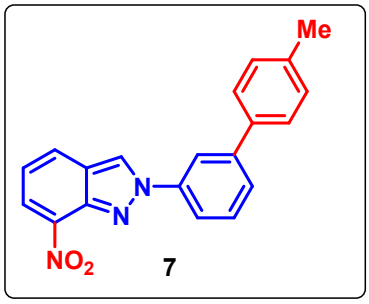


tert-Butyl (2-(p-tolyl)-2H-indazol-7-yl)carbamate (5): Light yellow solid (20 mg, 62%); M.p. 115-116 °C; R_f = 0.5 (PE : EA = 95 : 05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.30 (s, 1H), 7.88-7.86 (m, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.64 (s, 1H), 7.33-7.29 (m, 3H), 7.07 (t, J = 8.0 Hz, 1H), 2.42 (s, 3H), 1.57 (s, 9H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 152.8, 142.6, 138.2, 138.1, 130.2, 128.4, 123.6, 122.9, 120.9, 116.2, 113.5, 111.0, 80.7, 28.5, 21.1; HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for [$C_{19}H_{21}N_3NaO_2$]$^+$: 346.1526; found: 346.1544.



6

7-Nitro-2-(p-tolyl)-1-tosyl-1,2-dihydro-3H-indazol-3-one (6): Brown gummy mass (28 mg, 67%); R_f = 0.45 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.27 (d, J = 8.0 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.60 (t, J = 8.0 Hz, 1H), 7.53 (d, J = 8.4 Hz, 2H), 7.25 (d, J = 8.4 Hz, 2H), 7.14 (q, J = 8.8 Hz, 4H), 2.39 (s, 3H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 160.9, 147.1, 141.2, 137.4, 137.1, 133.8, 129.7, 129.5, 129.3, 129.2, 128.9, 128.2, 127.6, 126.6, 122.8, 21.9, 21.2; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{21}H_{18}N_3O_5S]^+$: 424.0962; found: 424.0951.



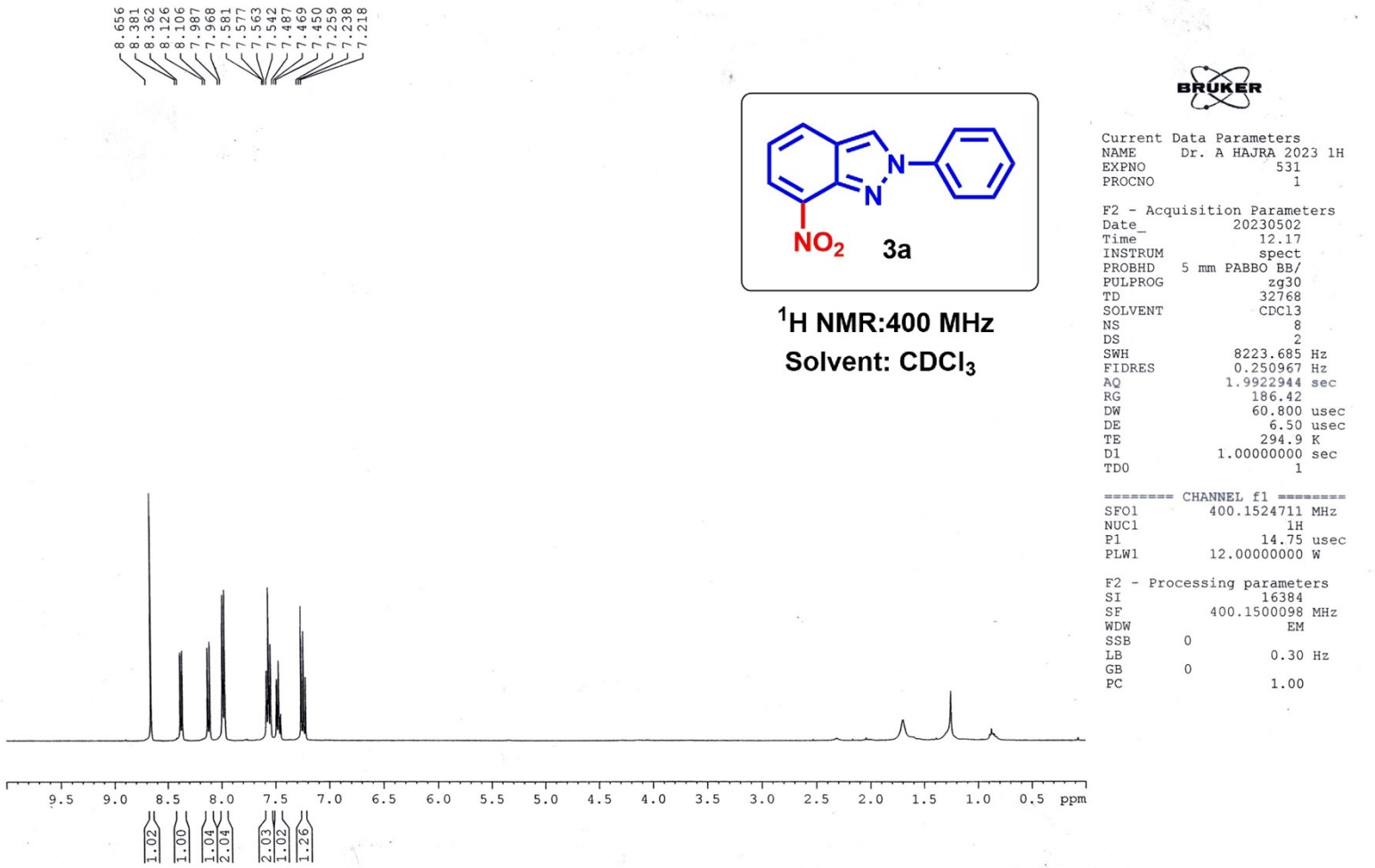
7

2-(4'-Methyl-[1,1'-biphenyl]-3-yl)-7-nitro-2H-indazole (7): Yellow gummy mass (23 mg, 69%); R_f = 0.50 (PE : EA = 80 : 20); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.70 (s, 1H), 8.39 (d, J = 7.2 Hz, 1H), 8.16 (t, J = 1.6 Hz, 1H), 8.13 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 7.6 Hz, 1H), 7.68 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.57 (d, J = 8.0 Hz, 2H), 7.31-7.27 (m, 2H), 7.24 (d, J = 8.0 Hz, 1H), 2.42 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 143.2, 141.6, 140.4, 138.2, 136.9, 130.2, 129.8, 129.0, 127.7, 127.2, 126.3, 126.0, 123.0, 121.0, 120.3, 120.2, 21.3; HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $[C_{20}H_{16}N_3O_2]^+$: 330.1237; found: 330.1227.

11. References:

1. (a) M. R. Kumar, A. Park, N. Park and S. Lee, *Org. Lett*., 2011, **13**, 3542–3545; (b) G. Bogonda, H. Y. Kim and K. Oh, *Org. Lett.,* 2018, **20**, 2711–2715; (c) D. Maiti, K. Mahanty and S. D. Sarkar, *Org. Lett.,* 2021, **23**, 1742–1747.
2. S. Bhattacharjee, S. Laru and A. Hajra, *Chem. Commun.,* 2022, **58**, 981-984.

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



BRUKER

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EXPNO                  531
PROCNO                   1

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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               294.9 K
D1            1.00000000 sec
TD0                   1

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

F2 - Processing parameters
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WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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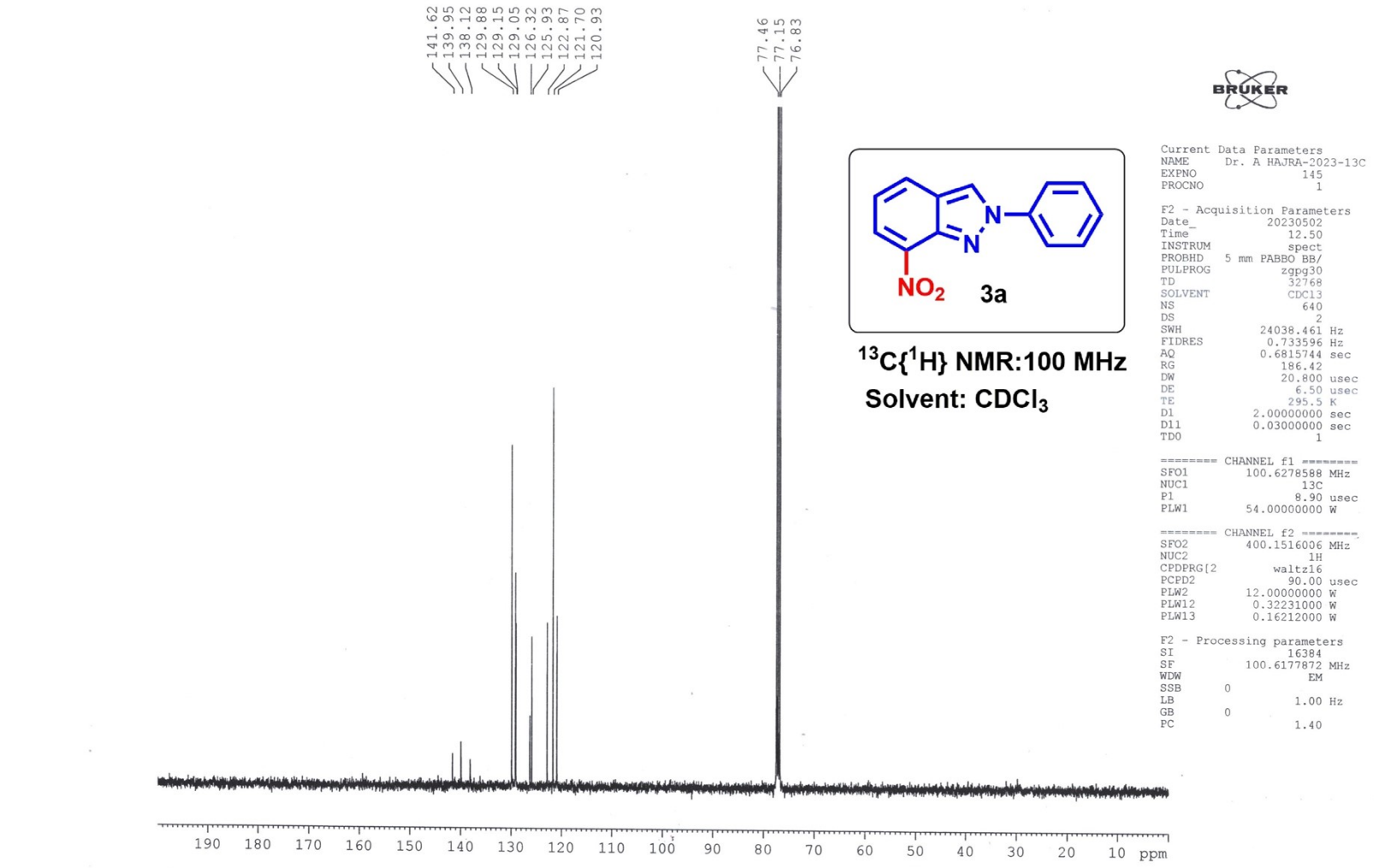


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EXPNO              145
PROCNO               1

F2 - Acquisition Parameters
Date_          20230502
Time              12.50
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               186.42
DW               20.800 usec
DE                6.50 usec
TE               295.5 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
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WDW                EM
SSB       0
LB                1.00 Hz
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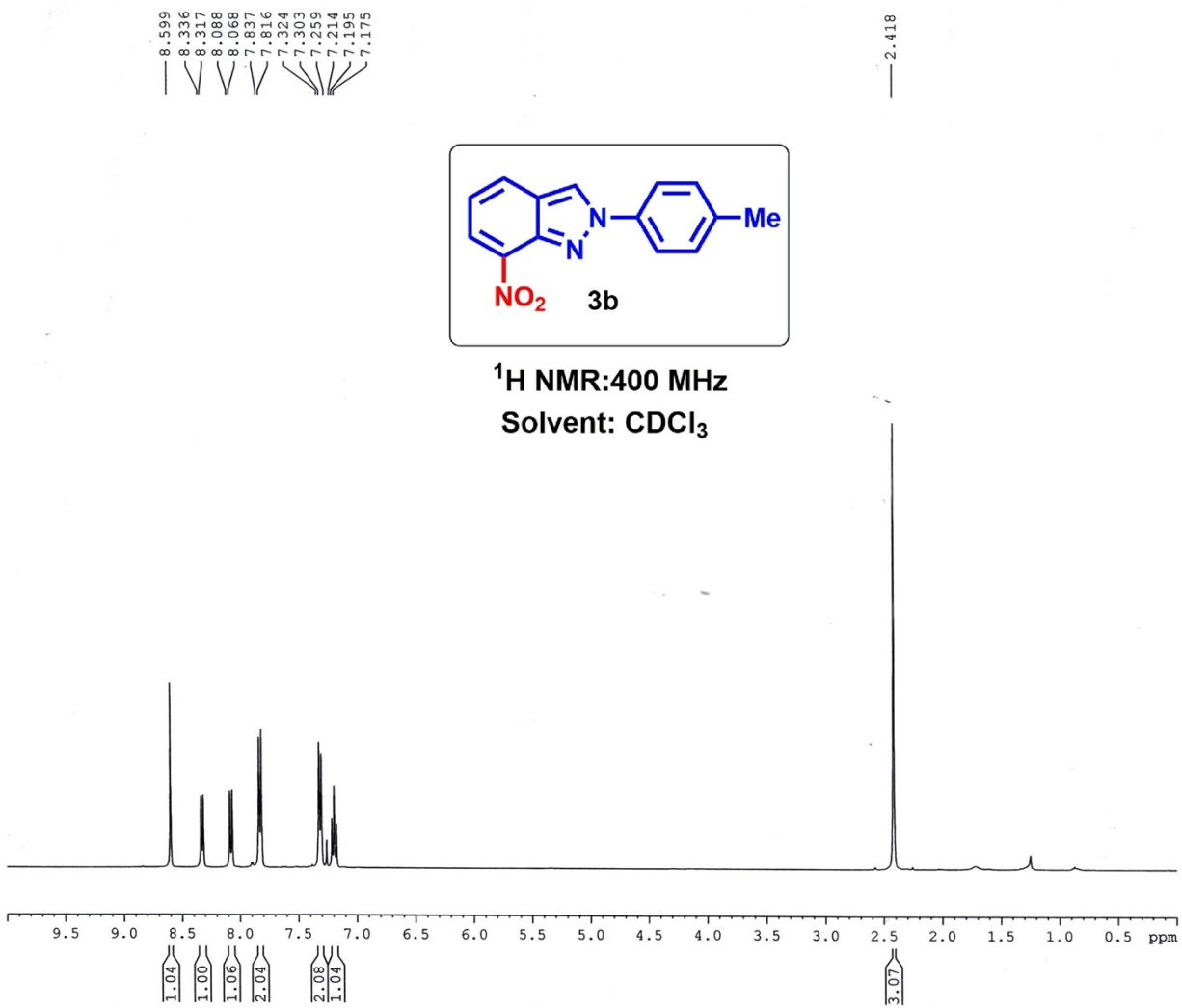

BRUKER

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EXPNO                  579
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230510
Time              12.14
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               301.4 K
D1           1.00000000 sec
TD0                  1

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

F2 - Processing parameters
SI                16384
SF          400.1500097 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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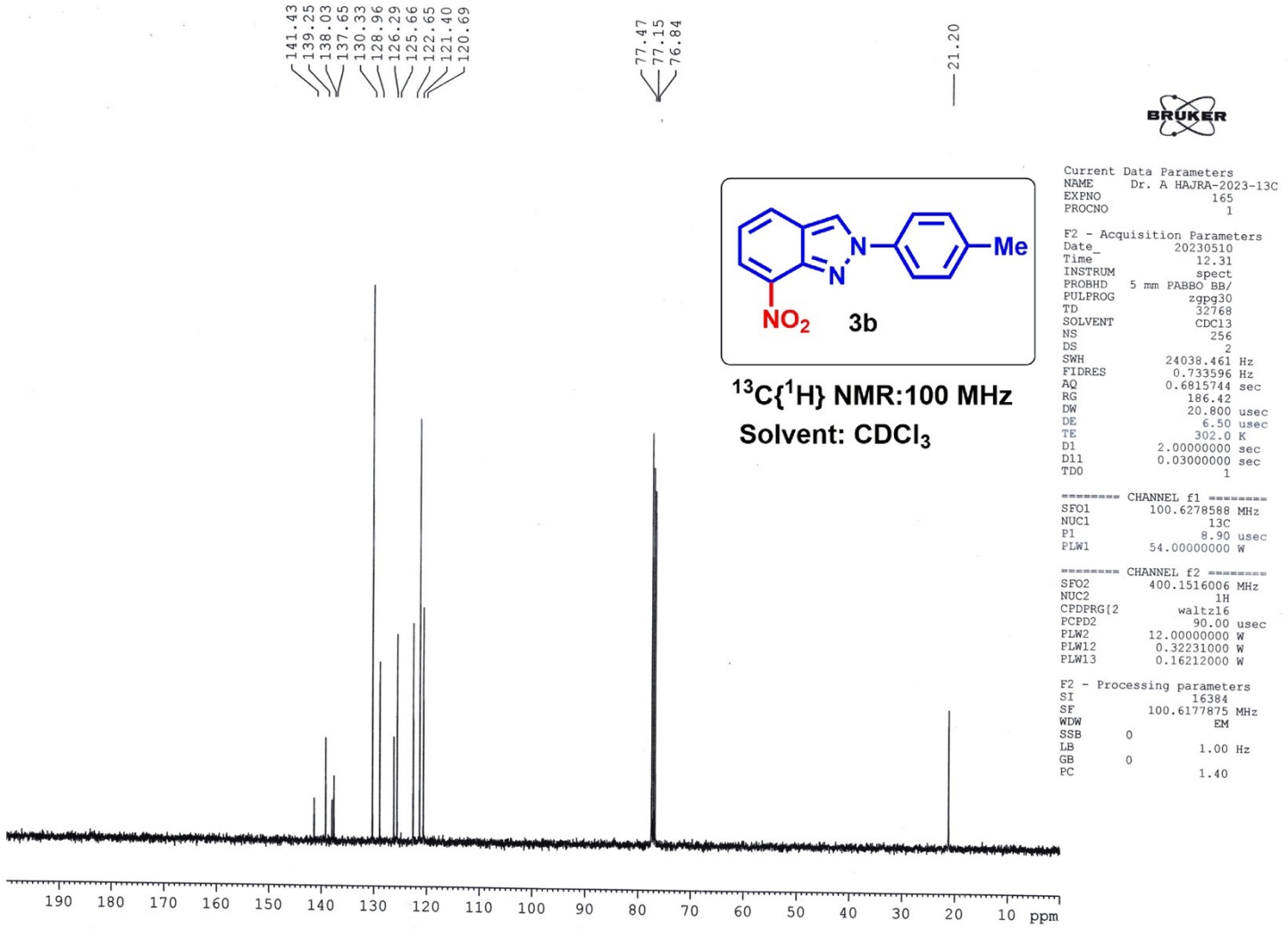

BRUKER

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Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  165
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230510
Time                 12.31
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                    256
DS                      2
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                  186.42
DW                  20.800 usec
DE                   6.50 usec
TE                  302.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

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

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

F2 - Processing parameters
SI                   16384
SF            100.6177875 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
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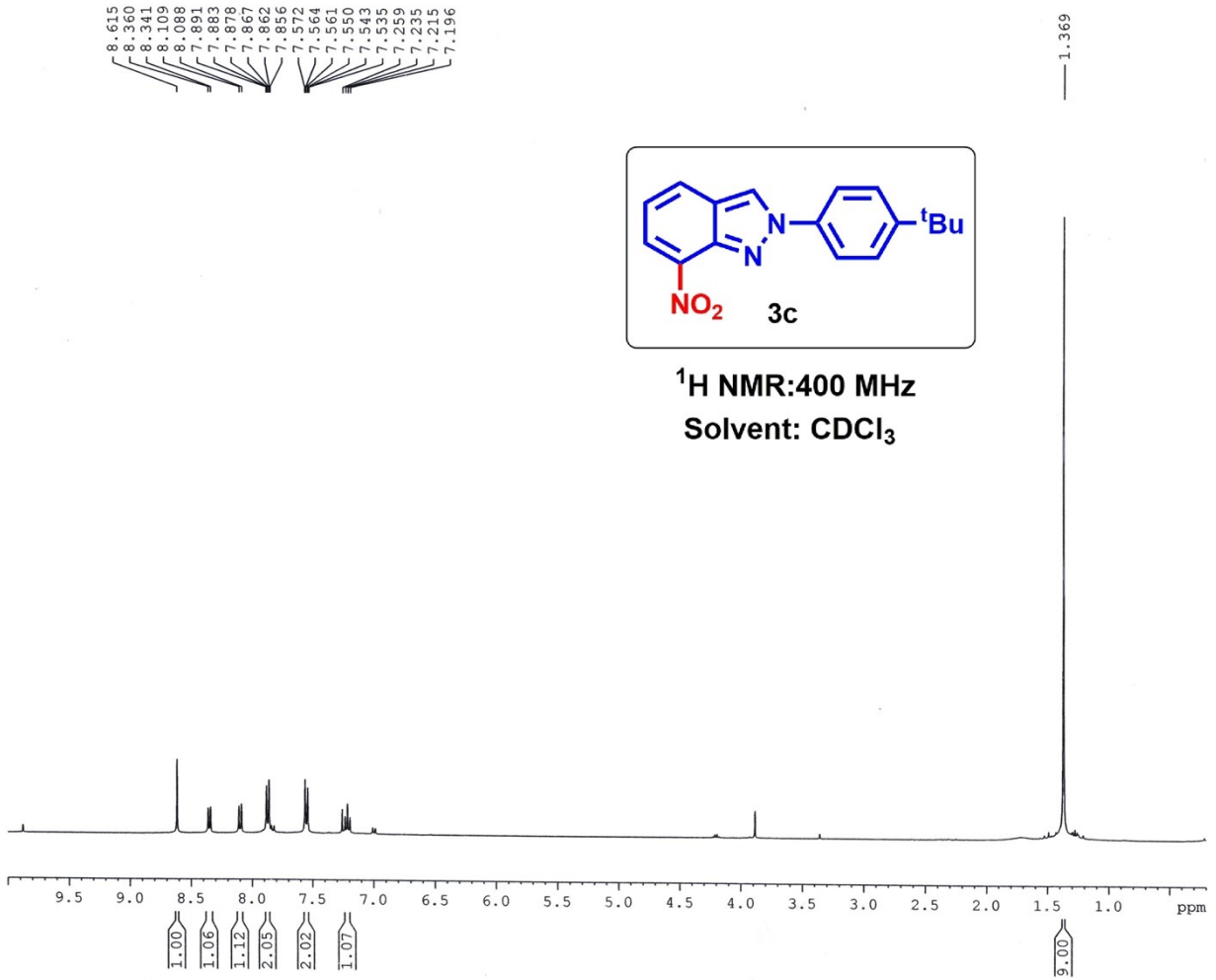


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Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1027
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230815
Time              17.15
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               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          400.1500098 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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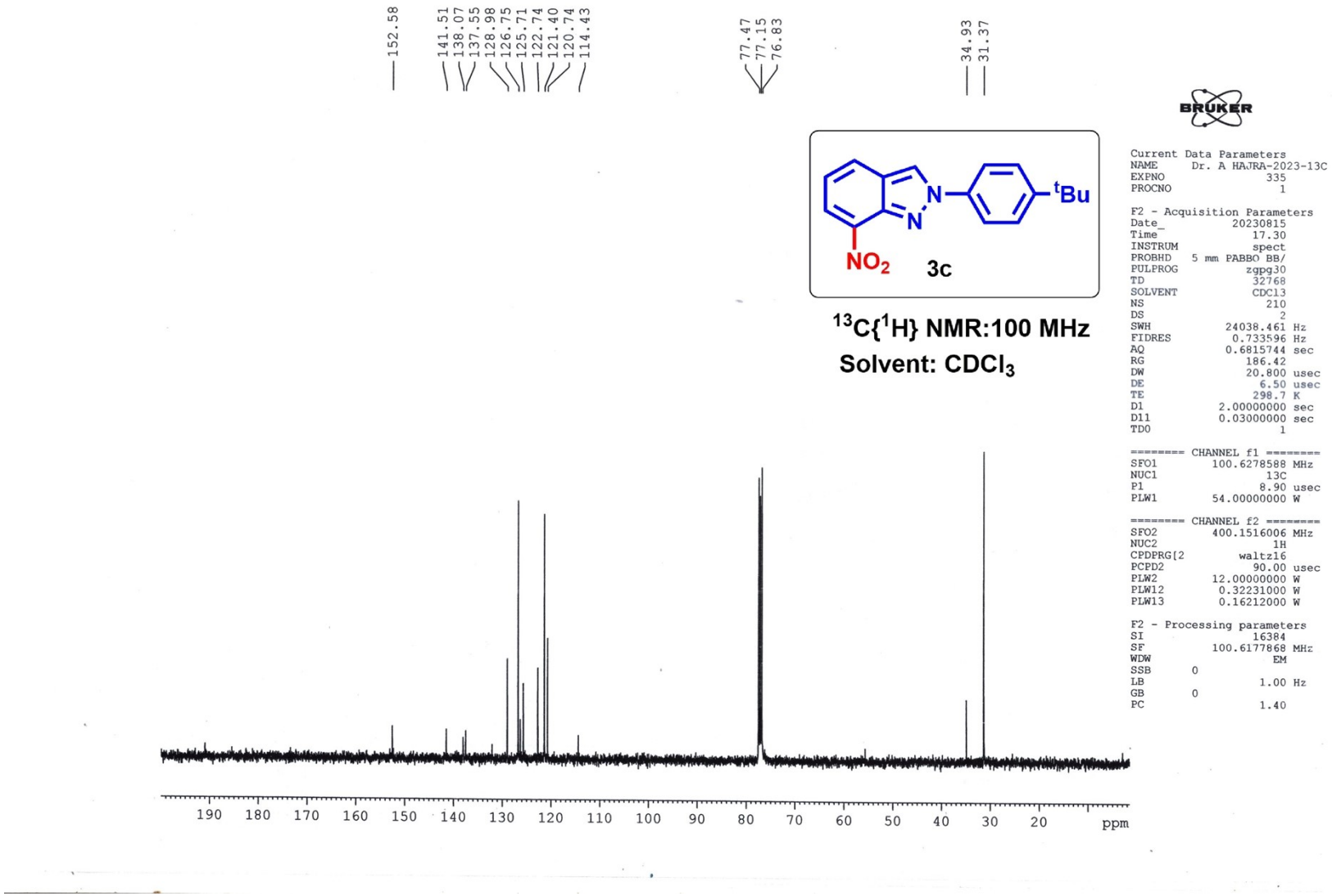

BRUKER

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Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  335
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230815
Time                 17.30
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    210
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                 298.7 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           100.6177868 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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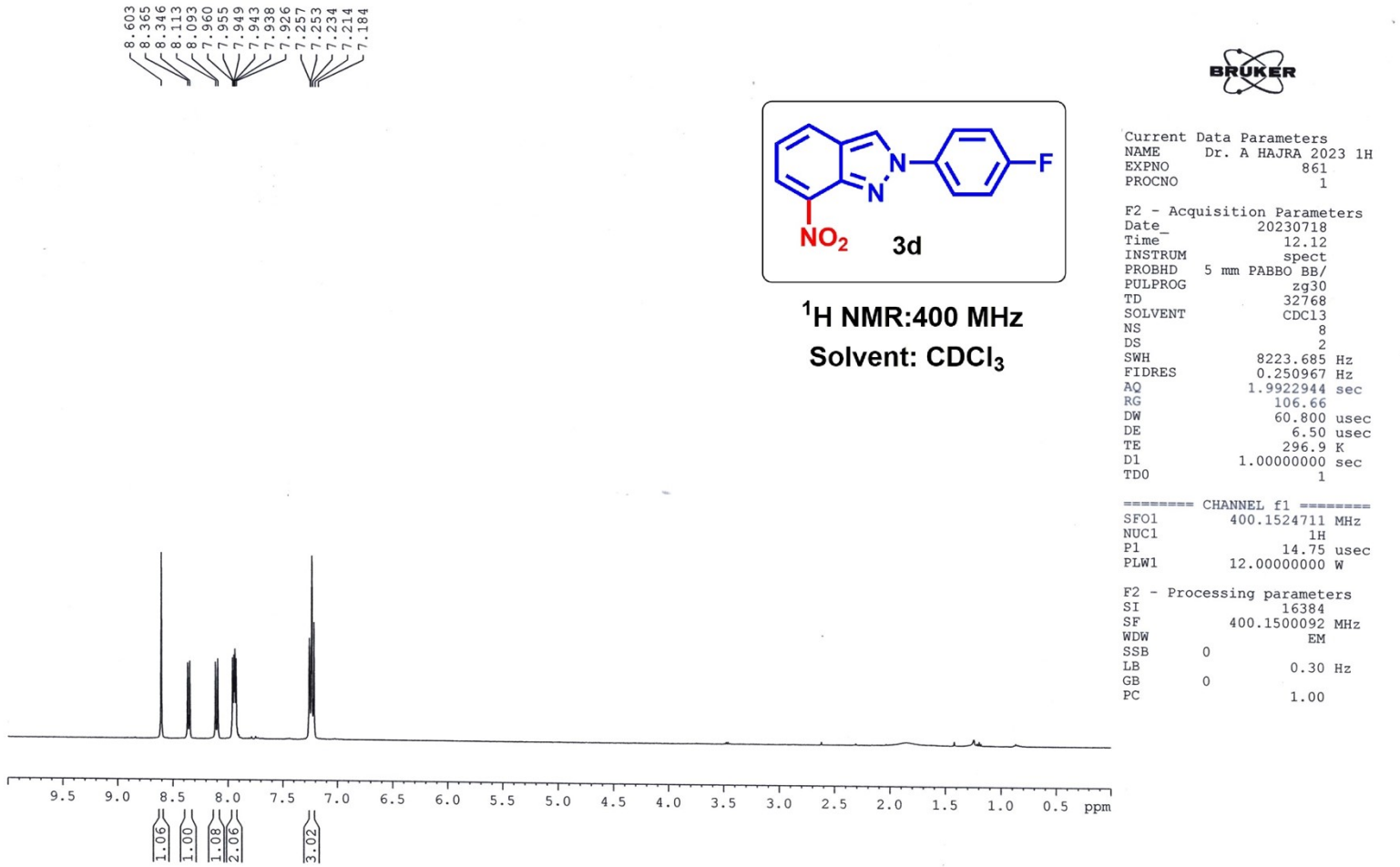

BRUKER

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Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                  861
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230718
Time                 12.12
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                   106.66
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            400.1500092 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
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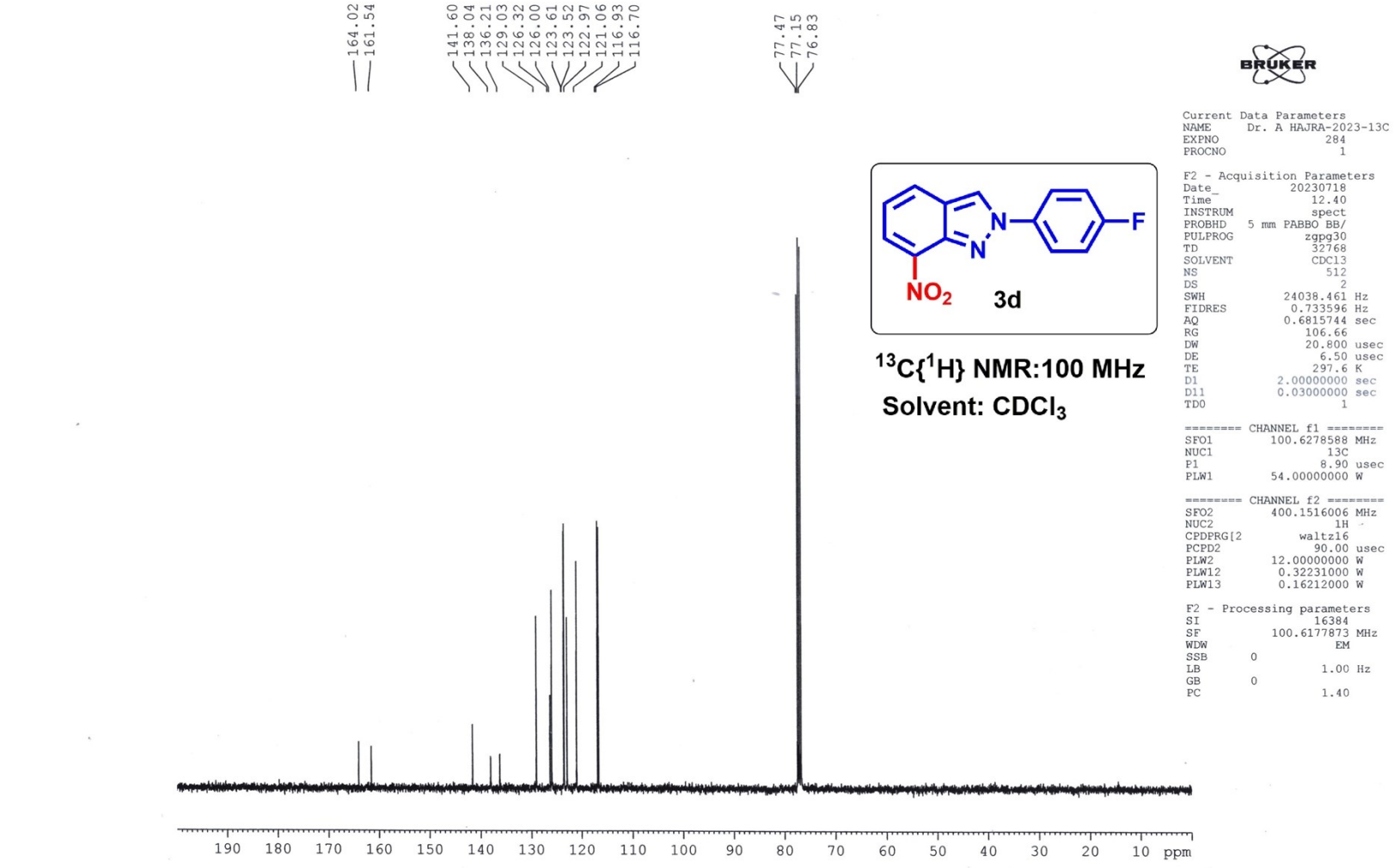


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Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  284
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230718
Time              12.40
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD               32768
SOLVENT          CDCl3
NS                 512
DS                   2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                106.66
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         100.6278588 MHz
NUC1               13C
P1                 8.90 usec
PLW1        54.00000000 W

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

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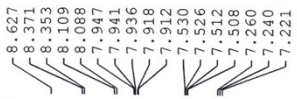

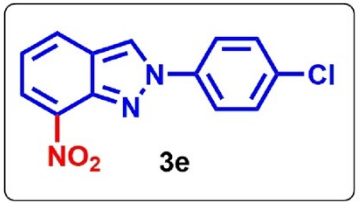

3e

^{1}H NMR:400 MHz

Solvent: $CDCl_3$

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                828
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230711
Time              12.44
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               298.8 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          400.1500097 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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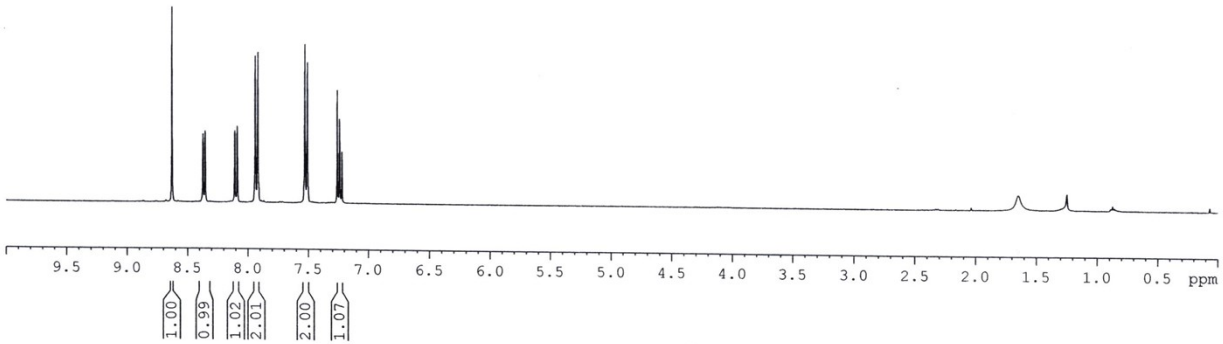

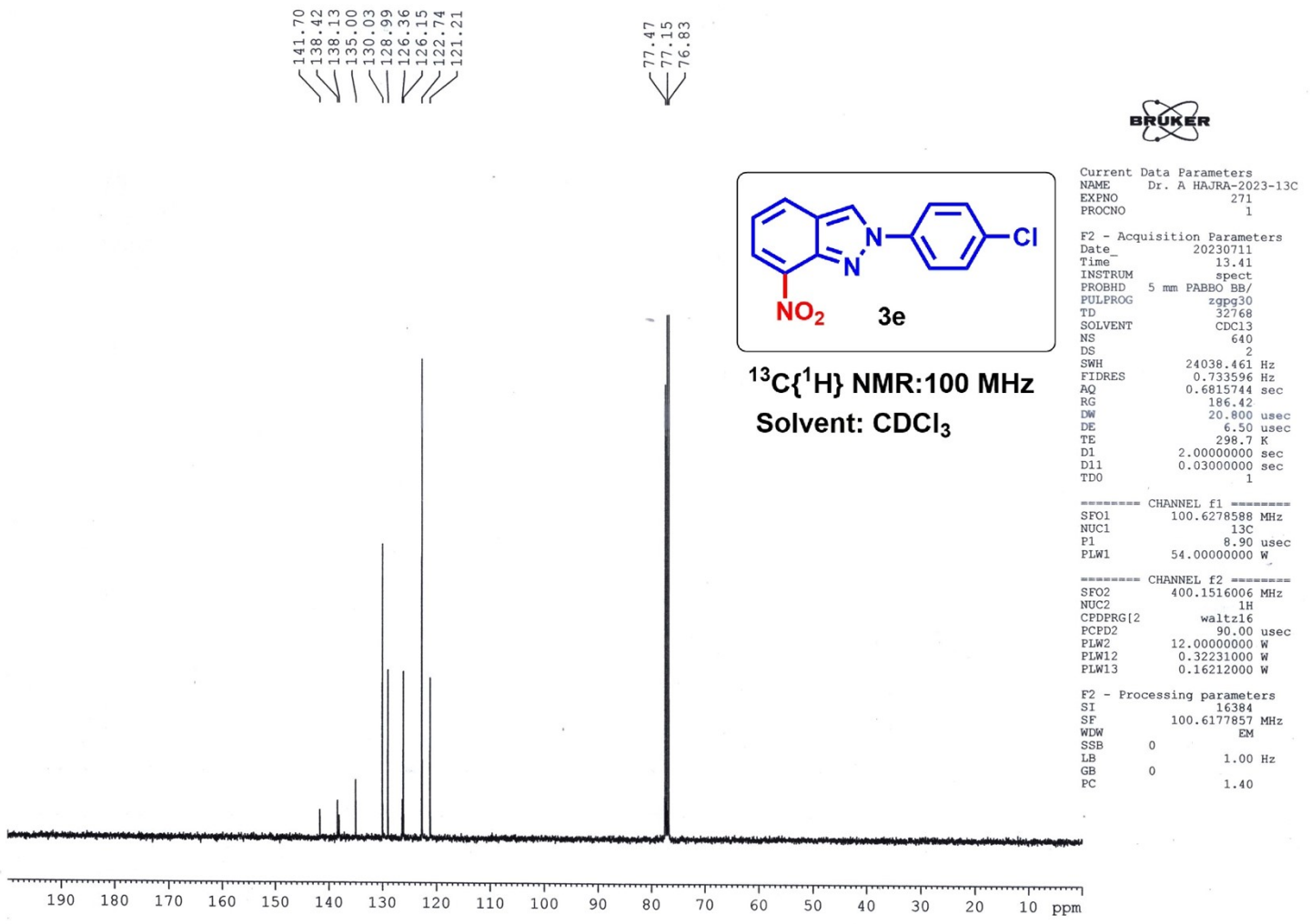

BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  271
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230711
Time                 13.41
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                   186.42
DW                   20.800 usec
DE                    6.50 usec
TE                   298.7 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            100.6177857 MHz
WDW                    EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
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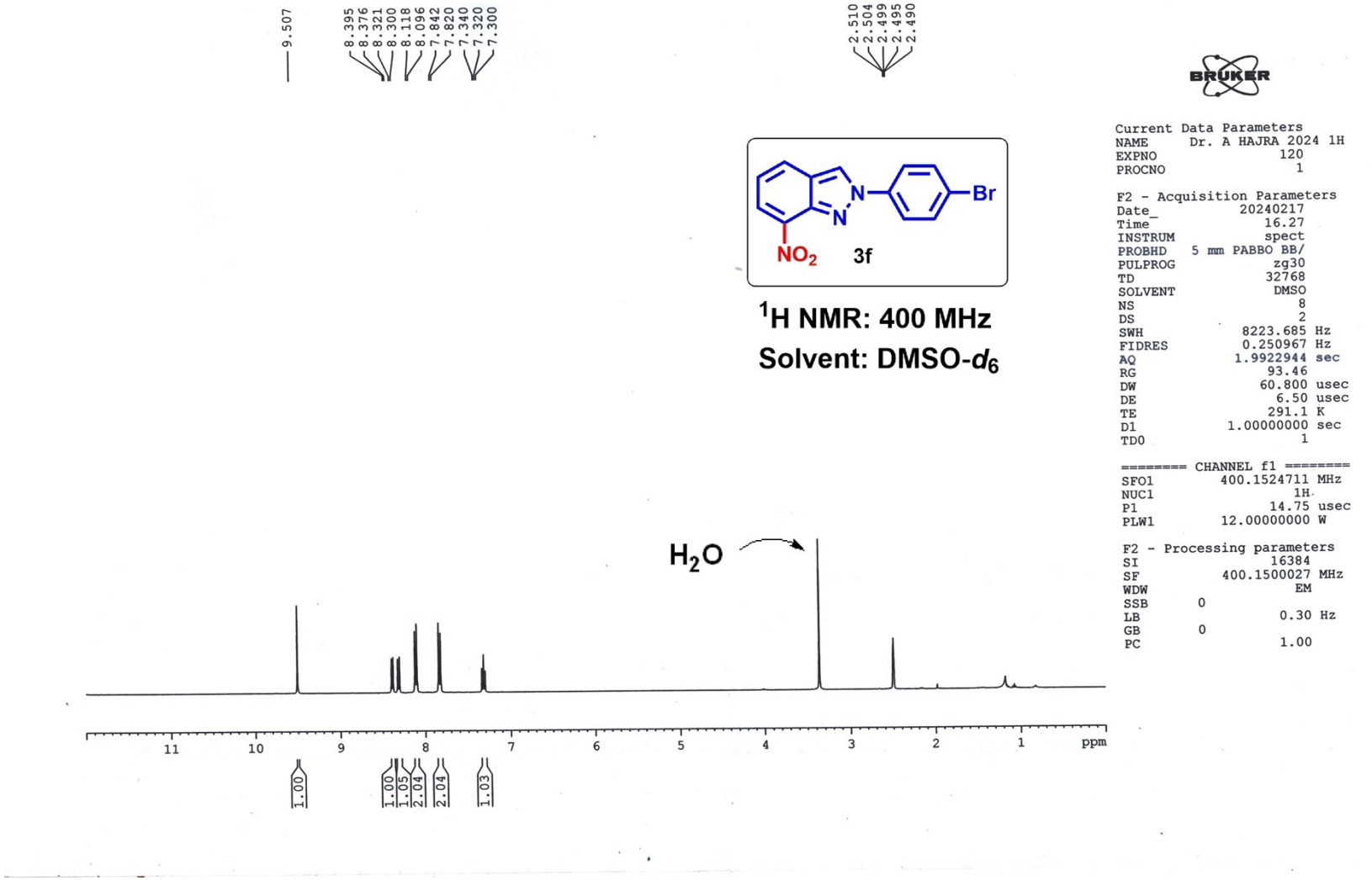

BRUKER

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NAME      Dr. A HAJRA 2024 1H
EXPNO                  120
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240217
Time              16.27
INSTRUM           spect
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PULPROG           zg30
TD               32768
SOLVENT           DMSO
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               291.1 K
D1          1.00000000 sec
TD0                  1

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

F2 - Processing parameters
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SF          400.1500027 MHz
WDW                EM
SSB       0
LB              0.30 Hz
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PC              1.00
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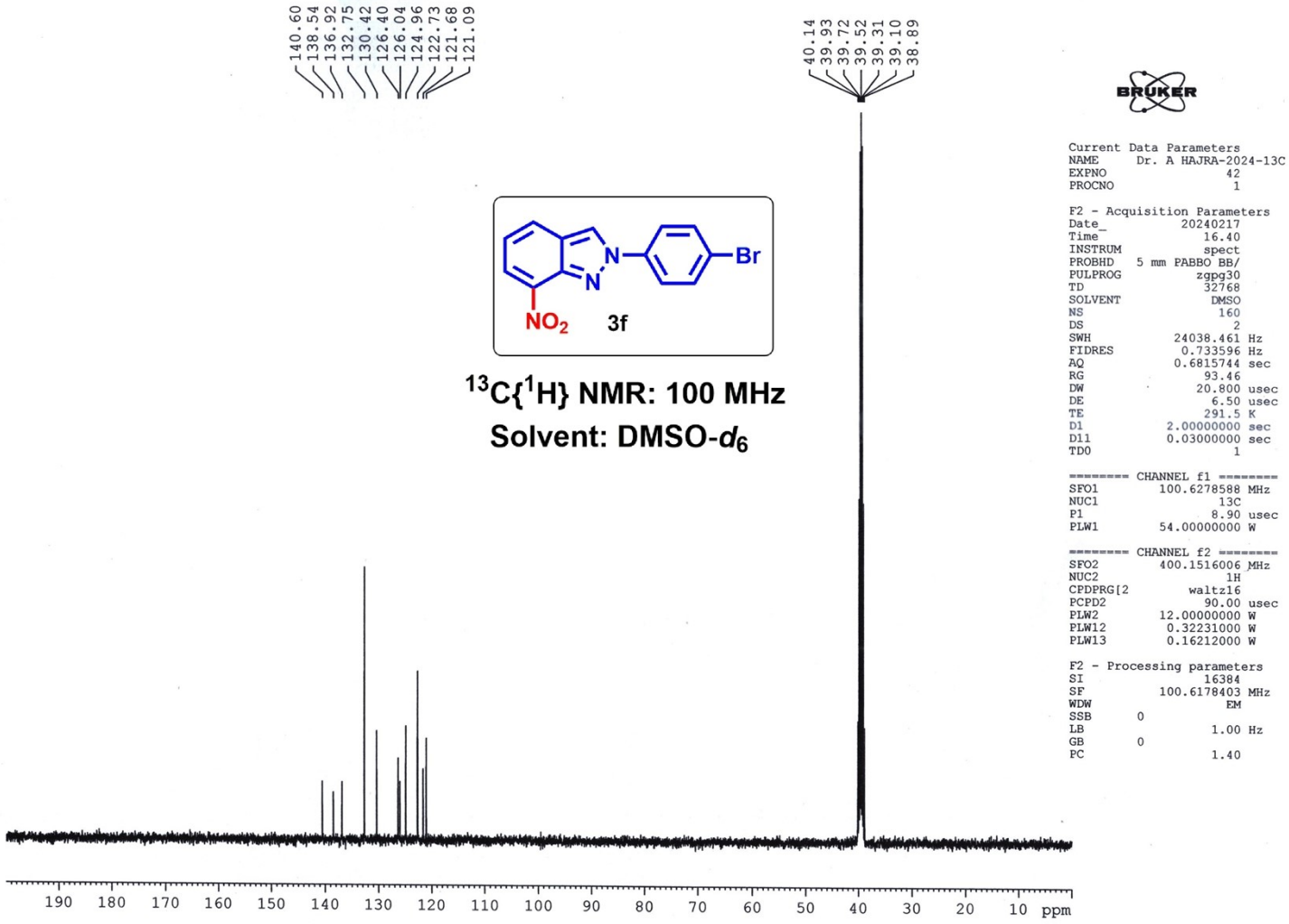


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Current Data Parameters
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EXPNO                  42
PROCNO                  1

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Time                16.40
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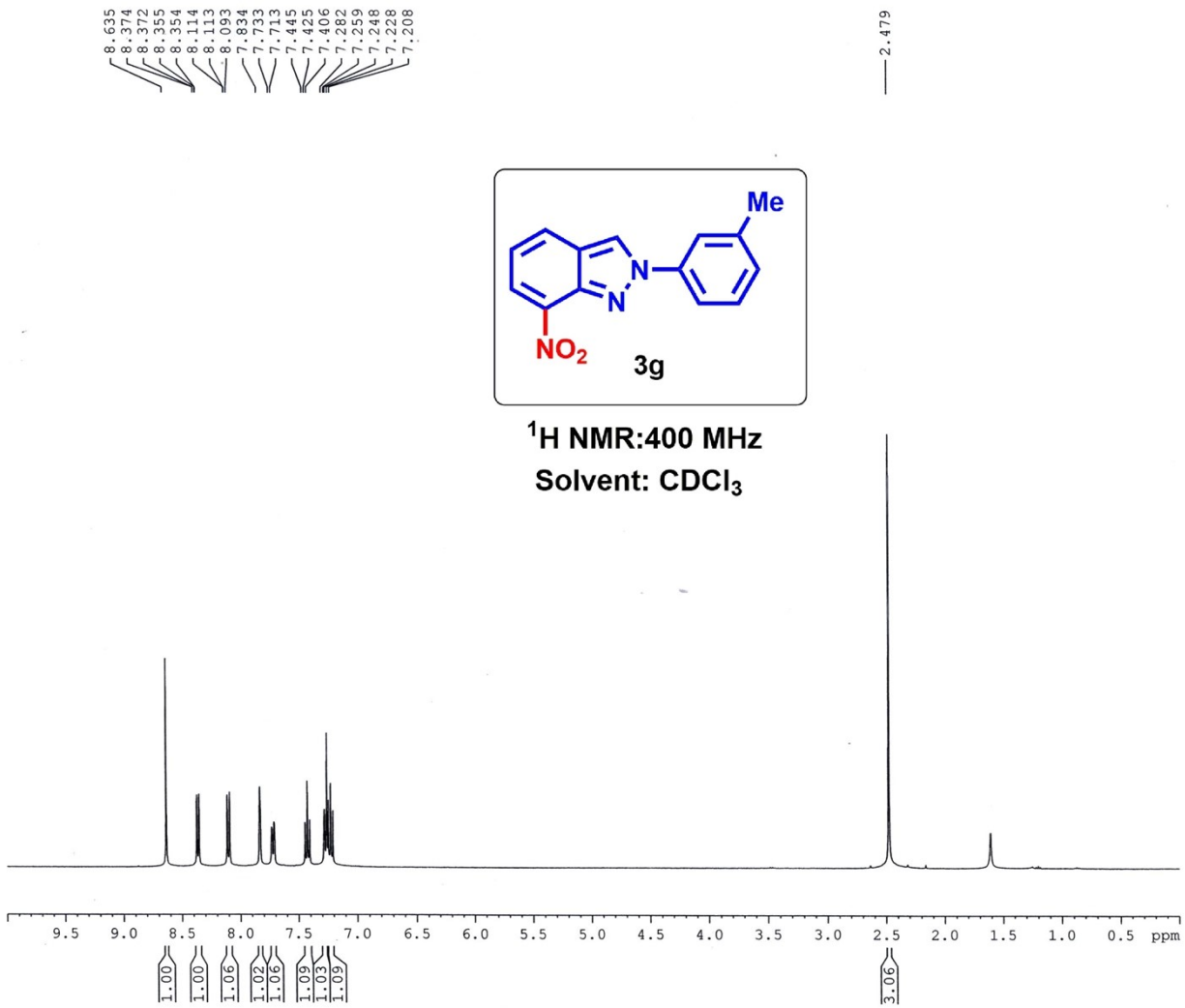
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                   160
DS                     2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 93.46
DW                20.800 usec
DE                 6.50 usec
TE                291.5 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           100.6178403 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

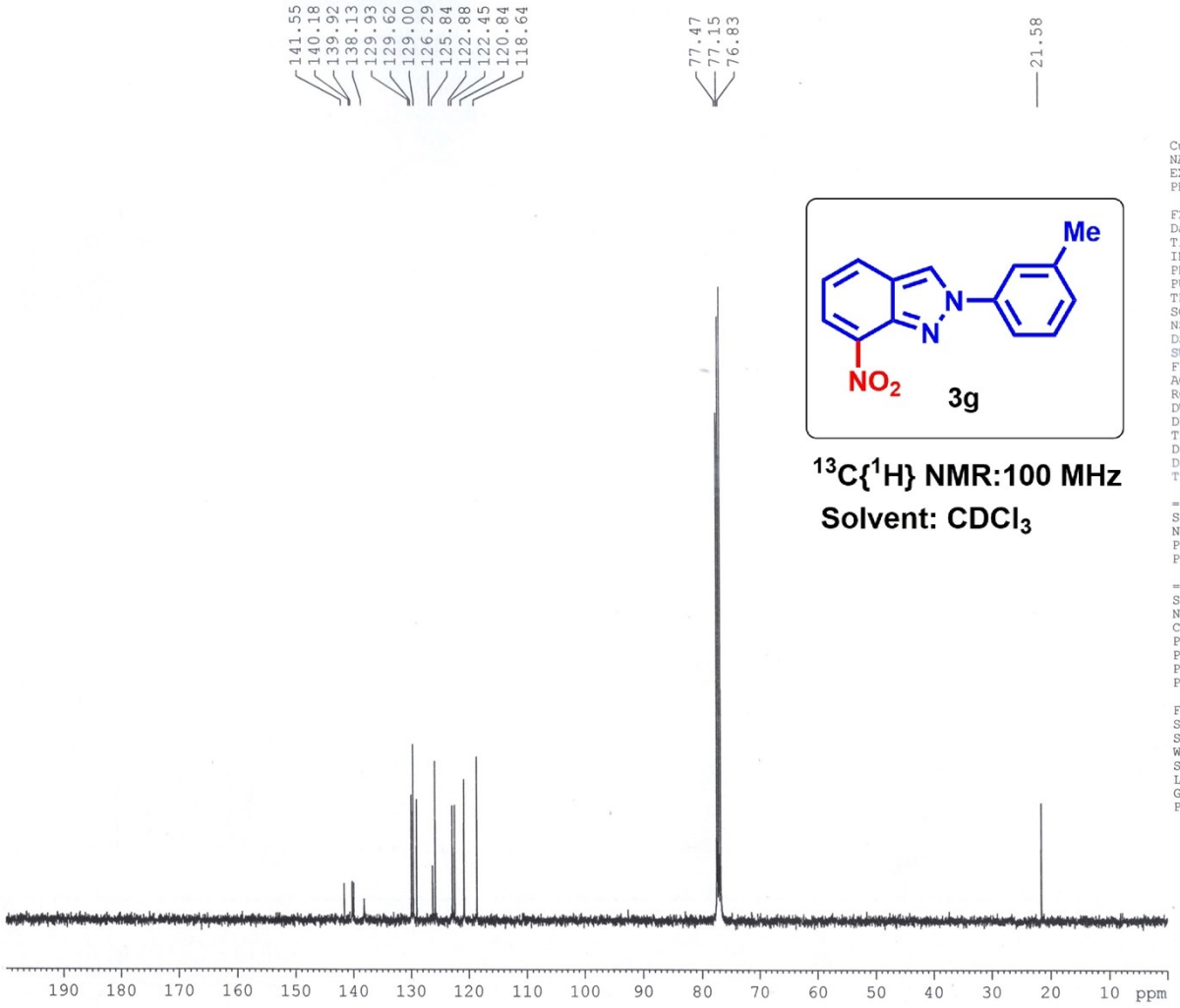



```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                  573
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230508
Time              20.12
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                299.3 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           400.1500097 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



BRUKER

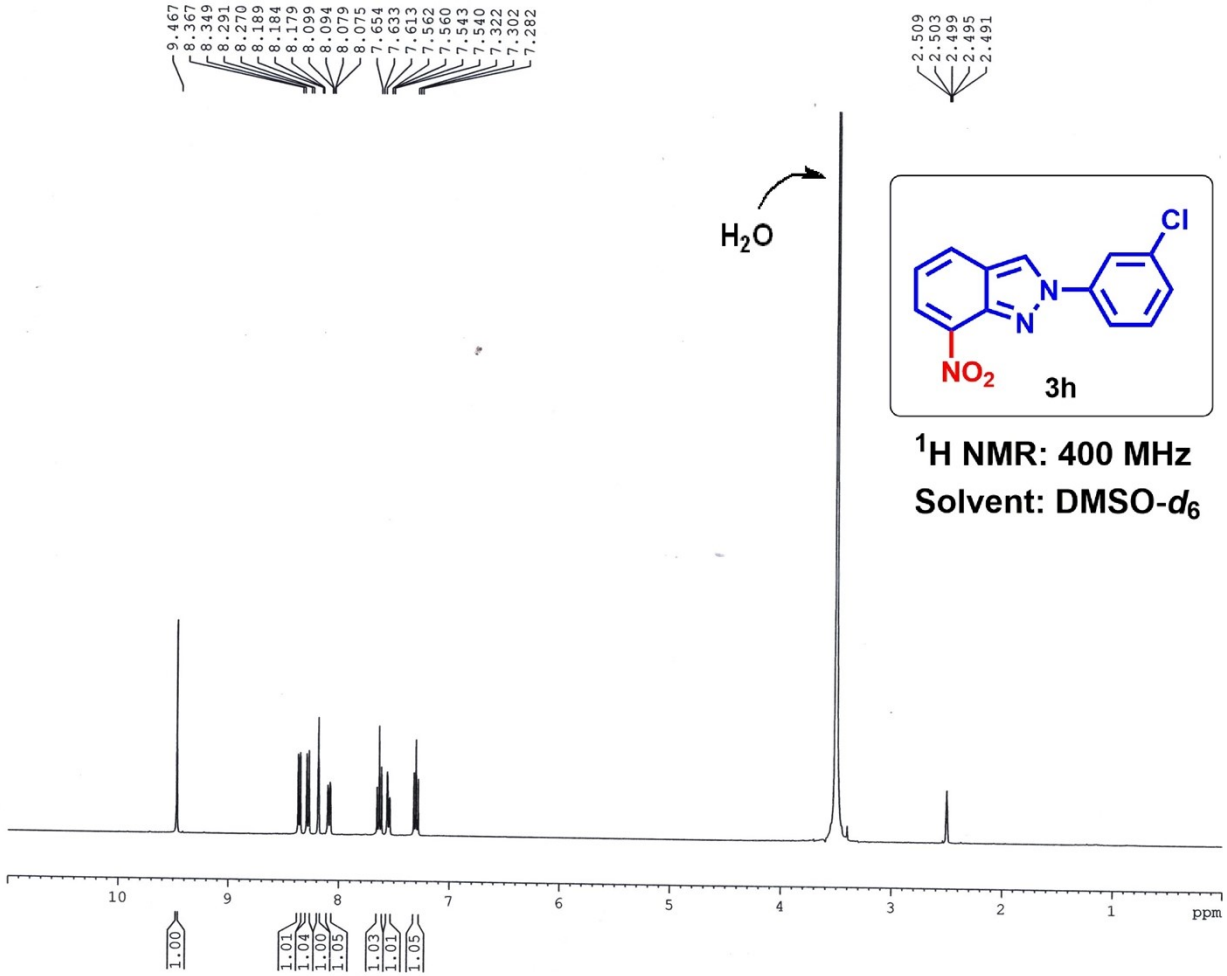
```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  162
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230508
Time                 20.39
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     512
DS                       2
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                   186.42
DW                  20.800 usec
DE                   6.50 usec
TE                  299.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                     16384
SF            100.6177857 MHz
WDW                       EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



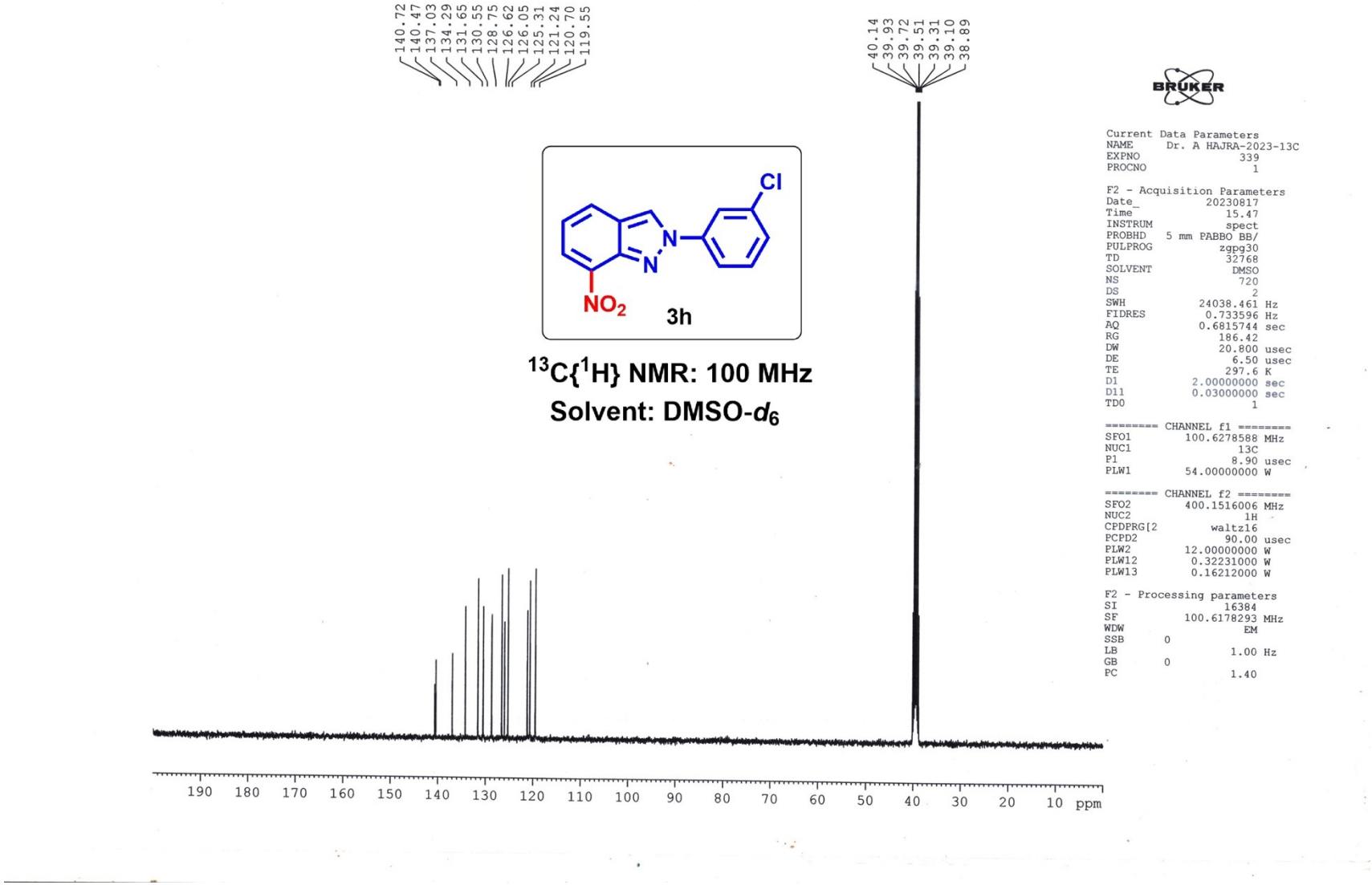
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1039
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230817
Time              15.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           DMSO
NS                   8
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                54.07
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          400.1500036 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



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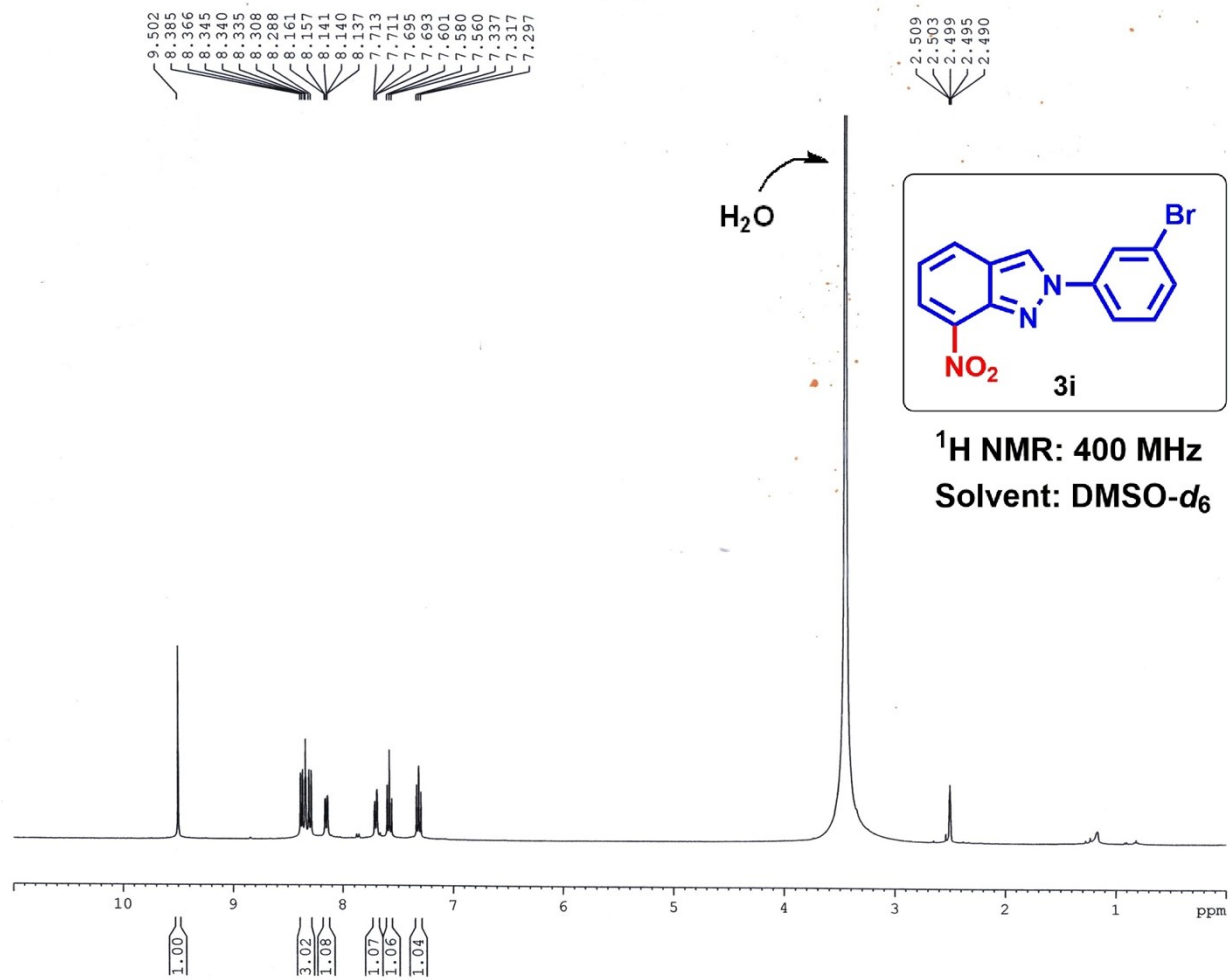
Current Data Parameters
NAME Dr. A HAJRA-2023-13C
EXPNO 339
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230817
Time 15.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
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 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

F2 - Processing parameters
SI 16384
SF 100.6178293 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



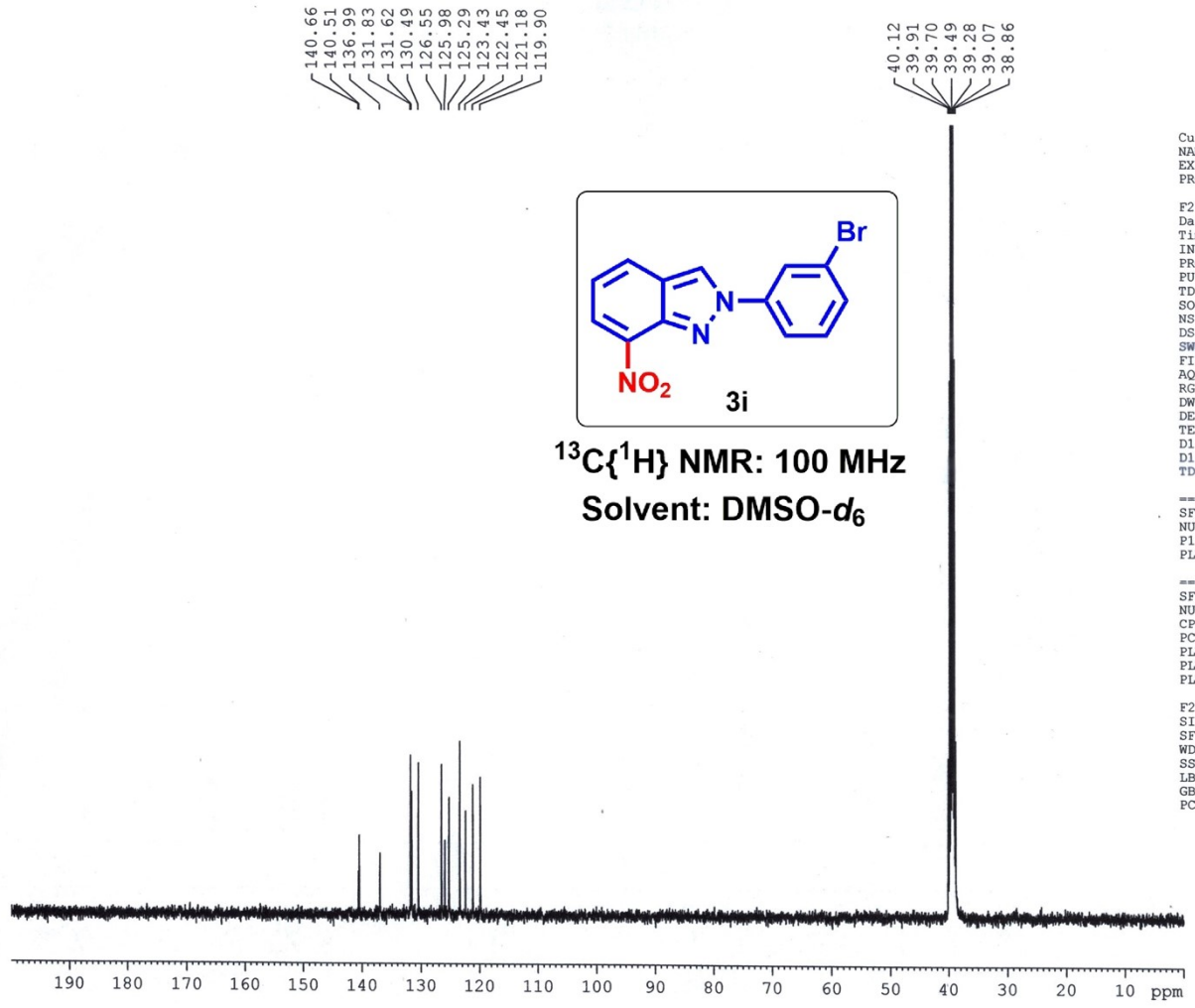
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                870
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230720
Time              12.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           DMSO
NS                   8
DS                   2
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                57.28
DW               60.800 usec
DE                6.50 usec
TE               297.7 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          400.1500034 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



BRUKER

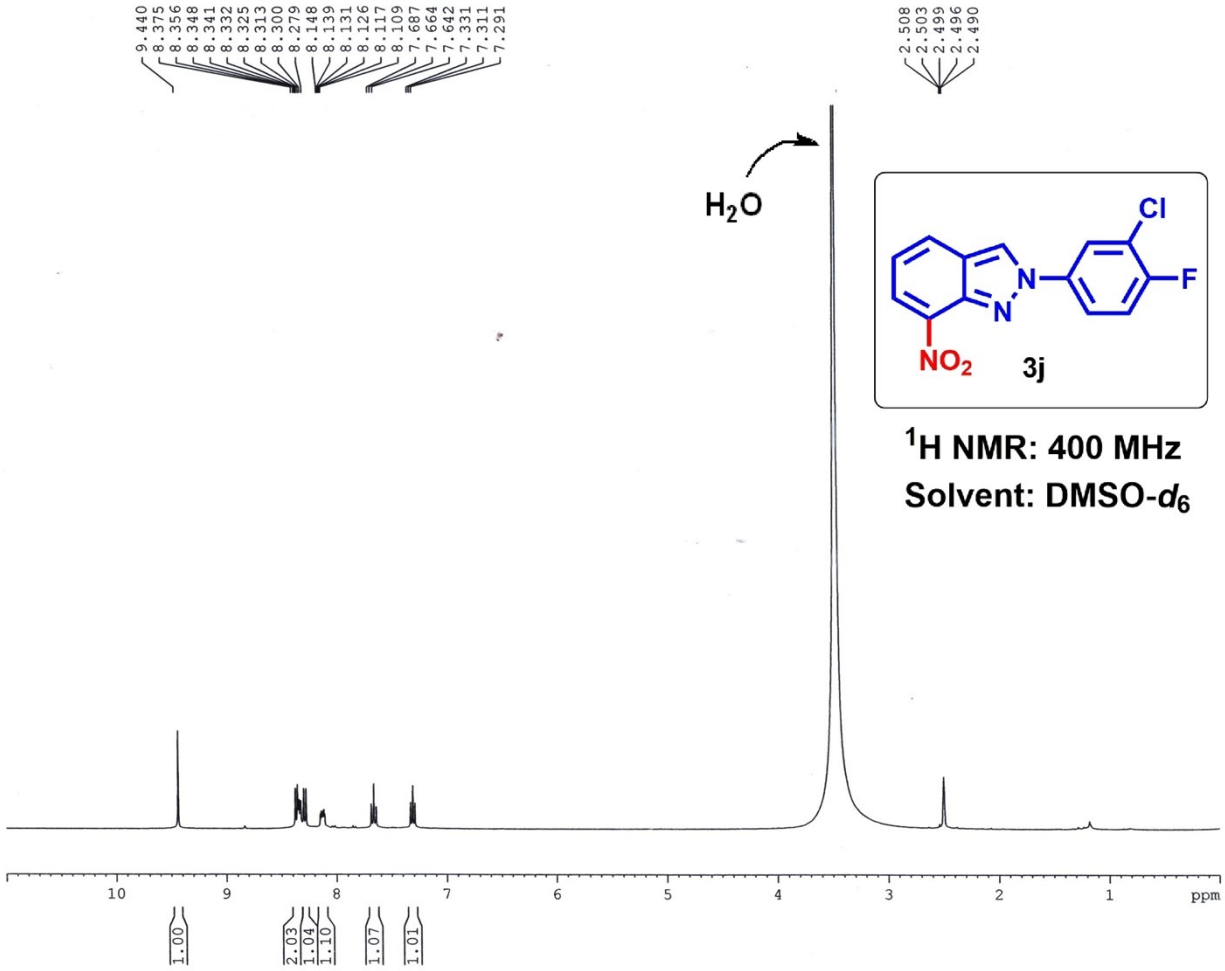
Current Data Parameters
NAME Dr. A HAJRA-2023-13C
EXPNO 287
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230720
Time 12.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 350
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 57.28
DW 20.800 usec
DE 6.50 usec
TE 298.8 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 100.6178376 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



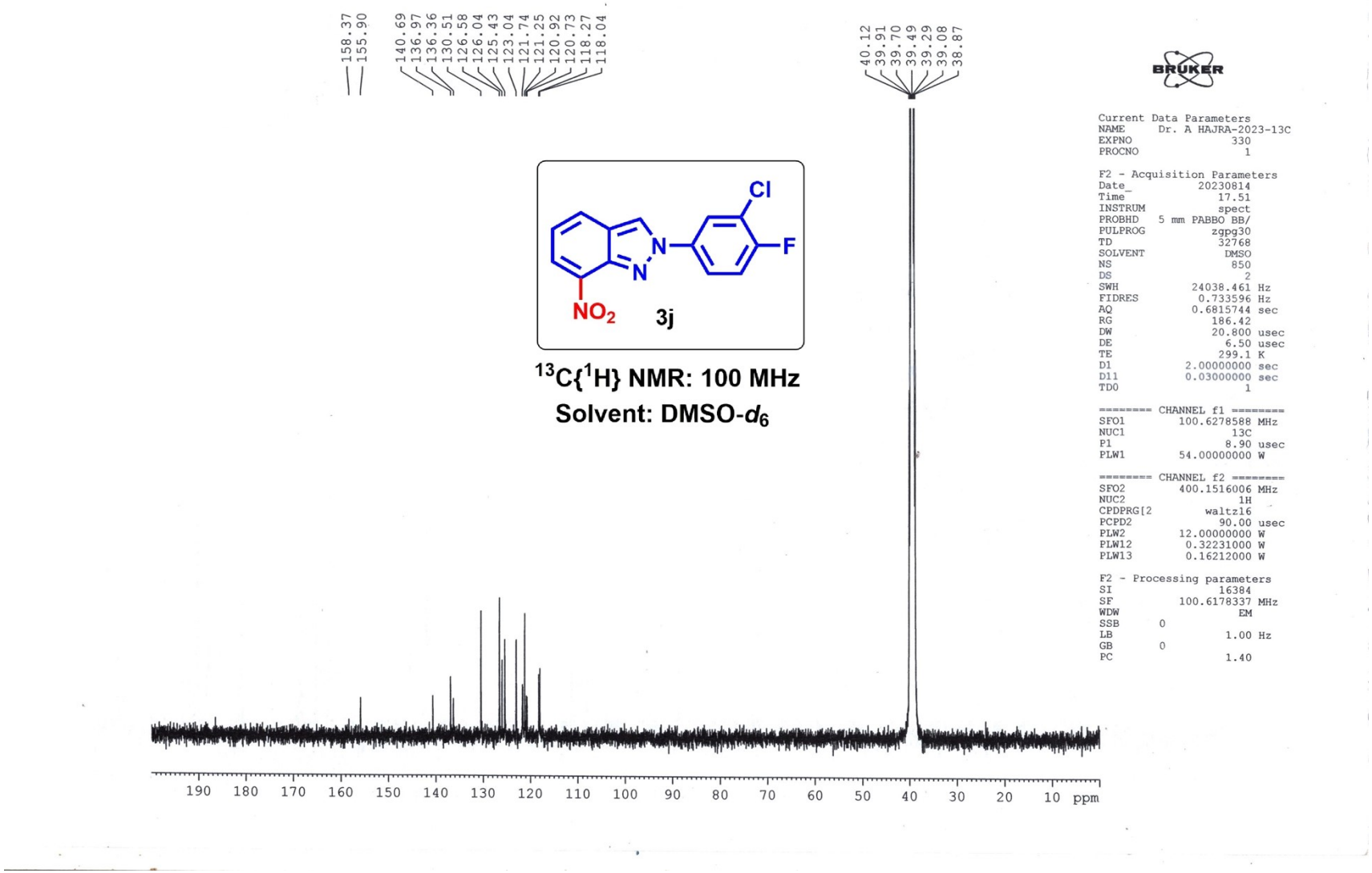
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                 1018
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230814
Time              17.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           DMSO
NS                   8
DS                   2
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                54.07
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          400.1500039 MHz
WDW                EM
SSB       0
LB               0.30 Hz
GB        0
PC               1.00
```



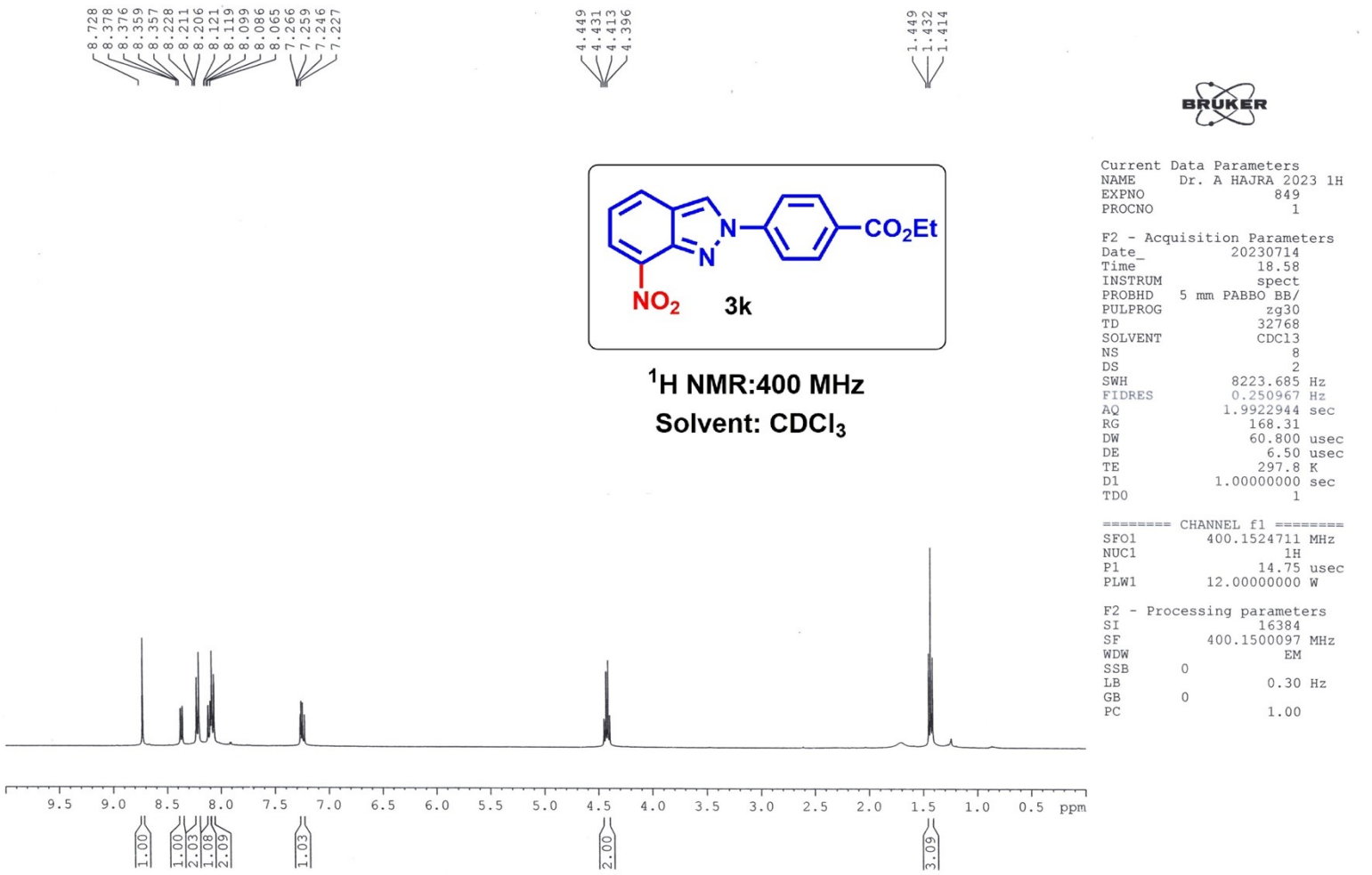

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  330
PROCNO                   1

F2 - Acquisition Parameters
Date_               20230814
Time                   17.51
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    32768
SOLVENT                DMSO
NS                       850
DS                         2
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6815744 sec
RG                     186.42
DW                     20.800 usec
DE                      6.50 usec
TE                     299.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

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

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

F2 - Processing parameters
SI                     16384
SF           100.6178337 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



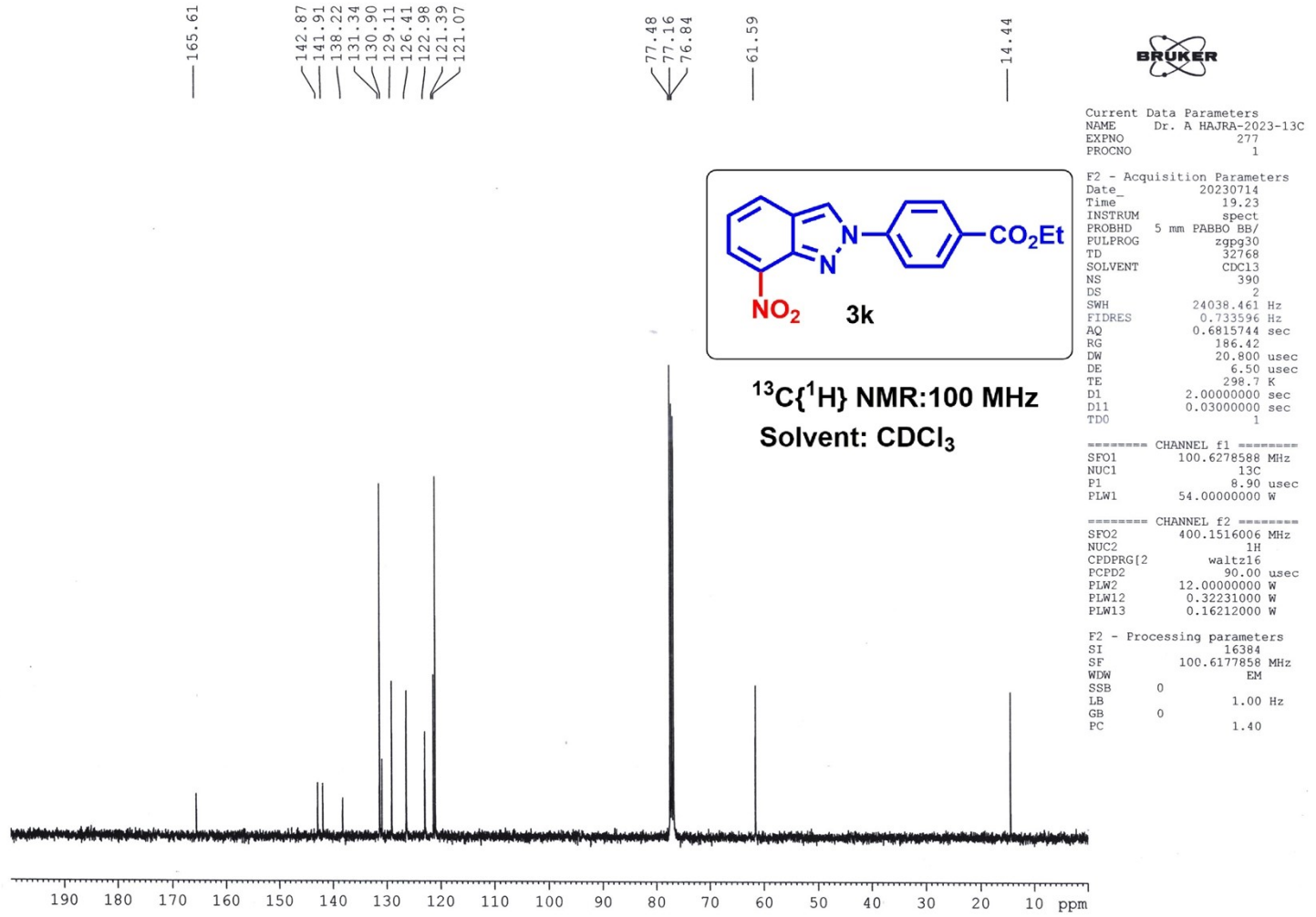
BRUKER

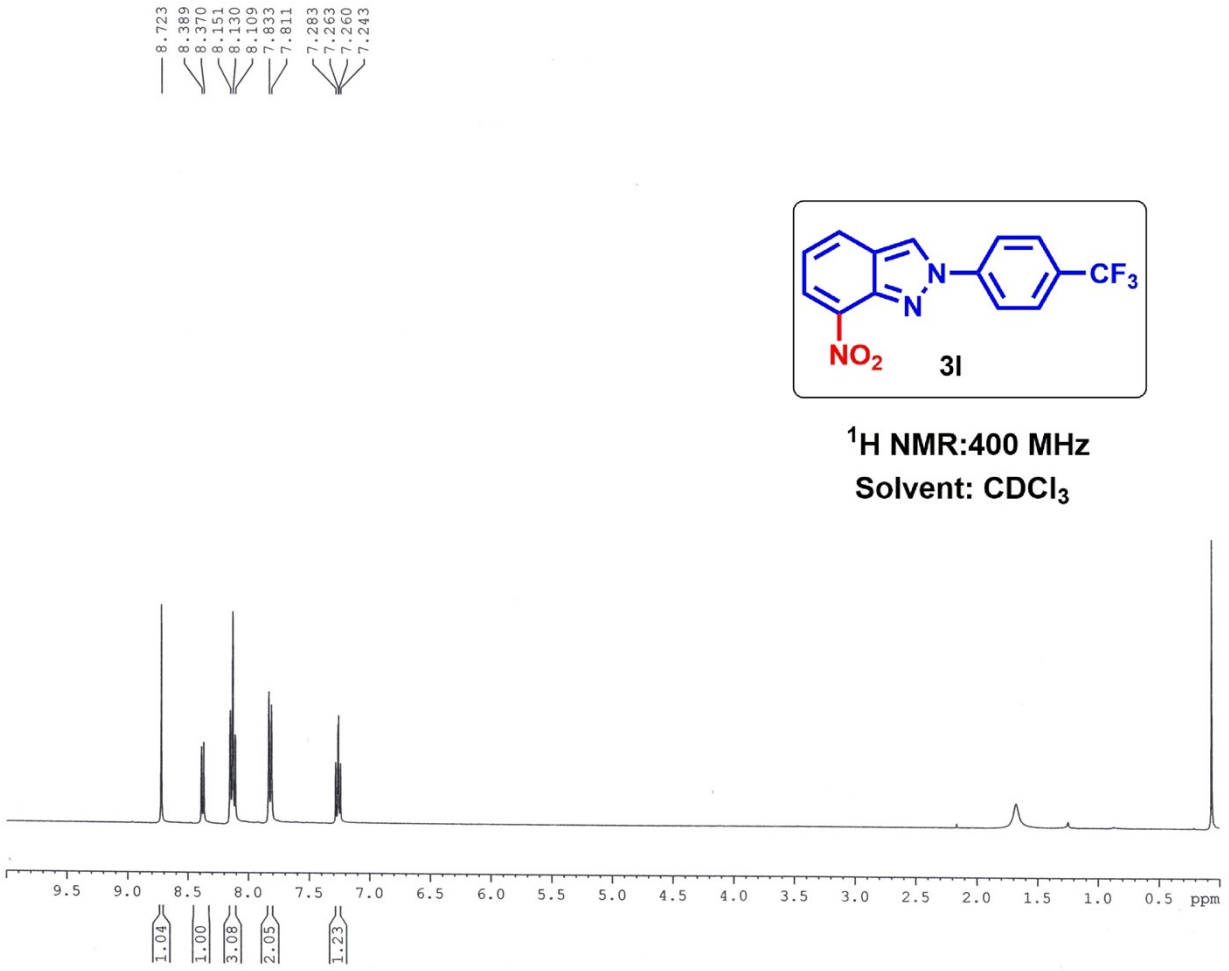
```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                849
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230714
Time               18.58
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                297.8 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           400.1500097 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```


165.61
142.87
141.91
138.22
131.34
130.90
129.11
126.41
122.98
121.39
121.07
77.48
77.16
76.84
61.59
14.44
BRUKER
Current Data Parameters
NAME Dr. A HAJRA-2023-13C
EXPNO 277
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230714
Time 19.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 390
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 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6177858 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
N
CO2Et
NO2
3k
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



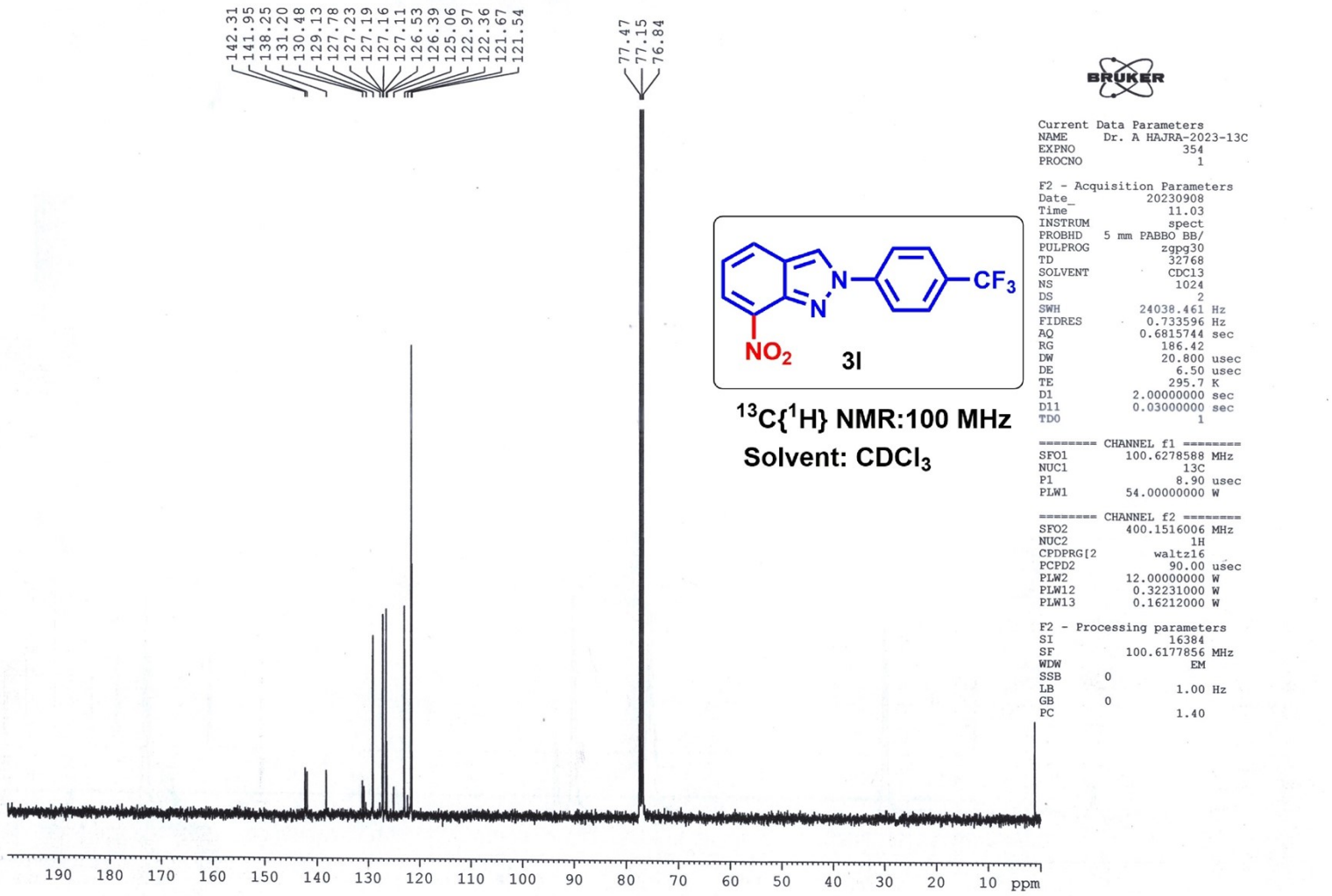
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                 1078
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230908
Time              10.14
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                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           400.1500097 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



BRUKER

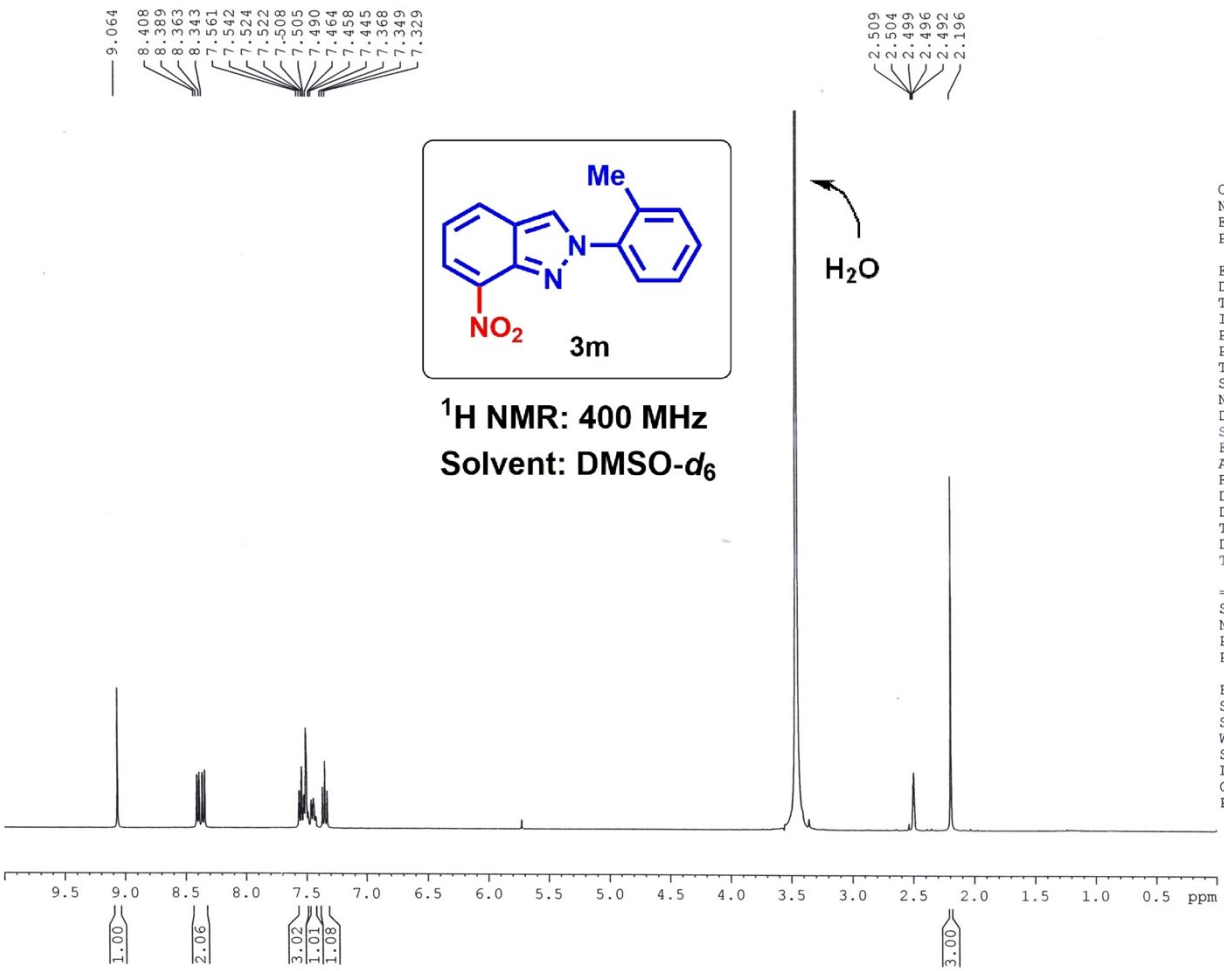
```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                354
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230908
Time              11.03
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                186.42
DW                20.800 usec
DE                 6.50 usec
TE                295.7 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           100.6177856 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



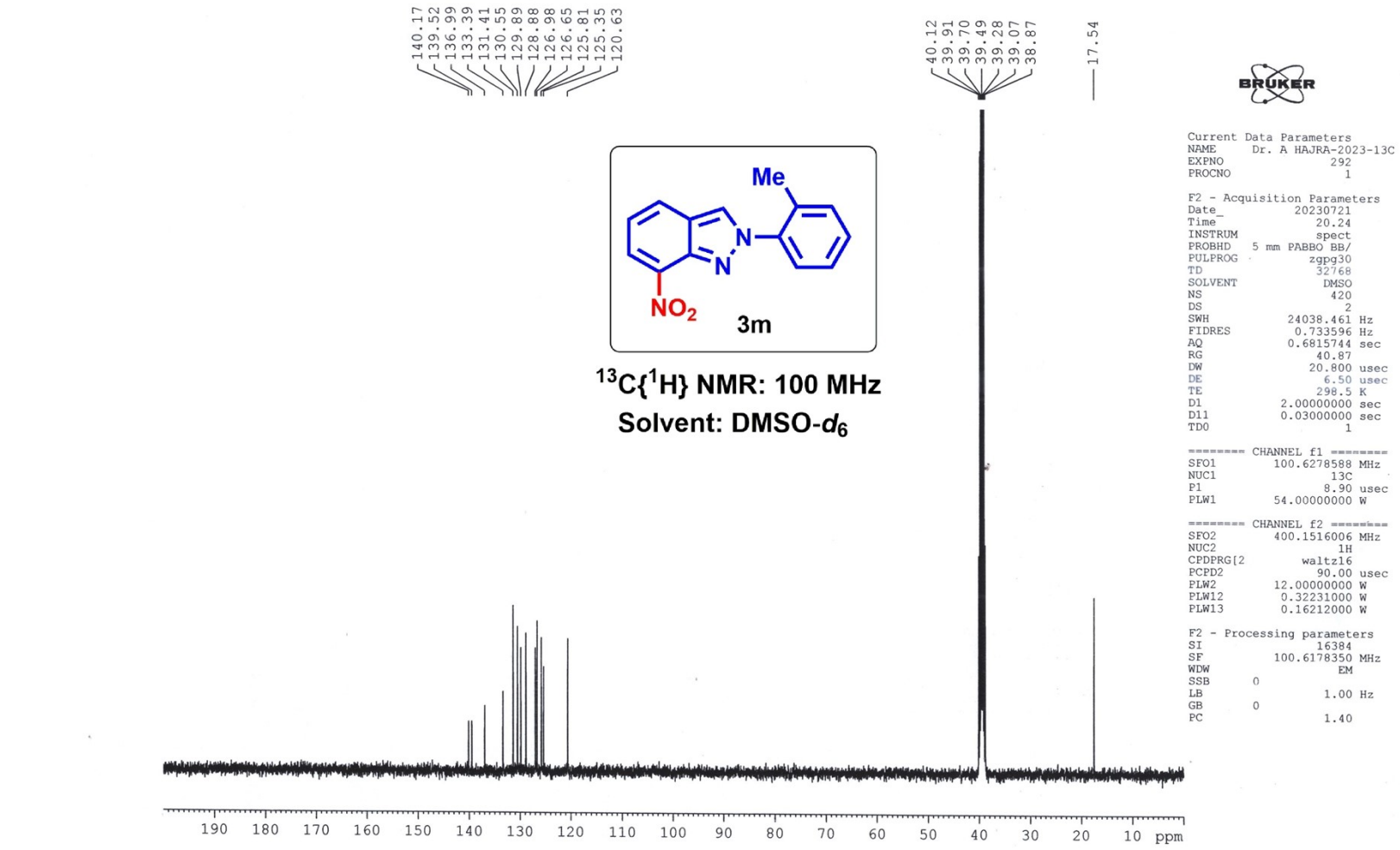
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                  876
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230721
Time              20.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                     8
DS                     2
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                40.87
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           400.1500032 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



BRUKER

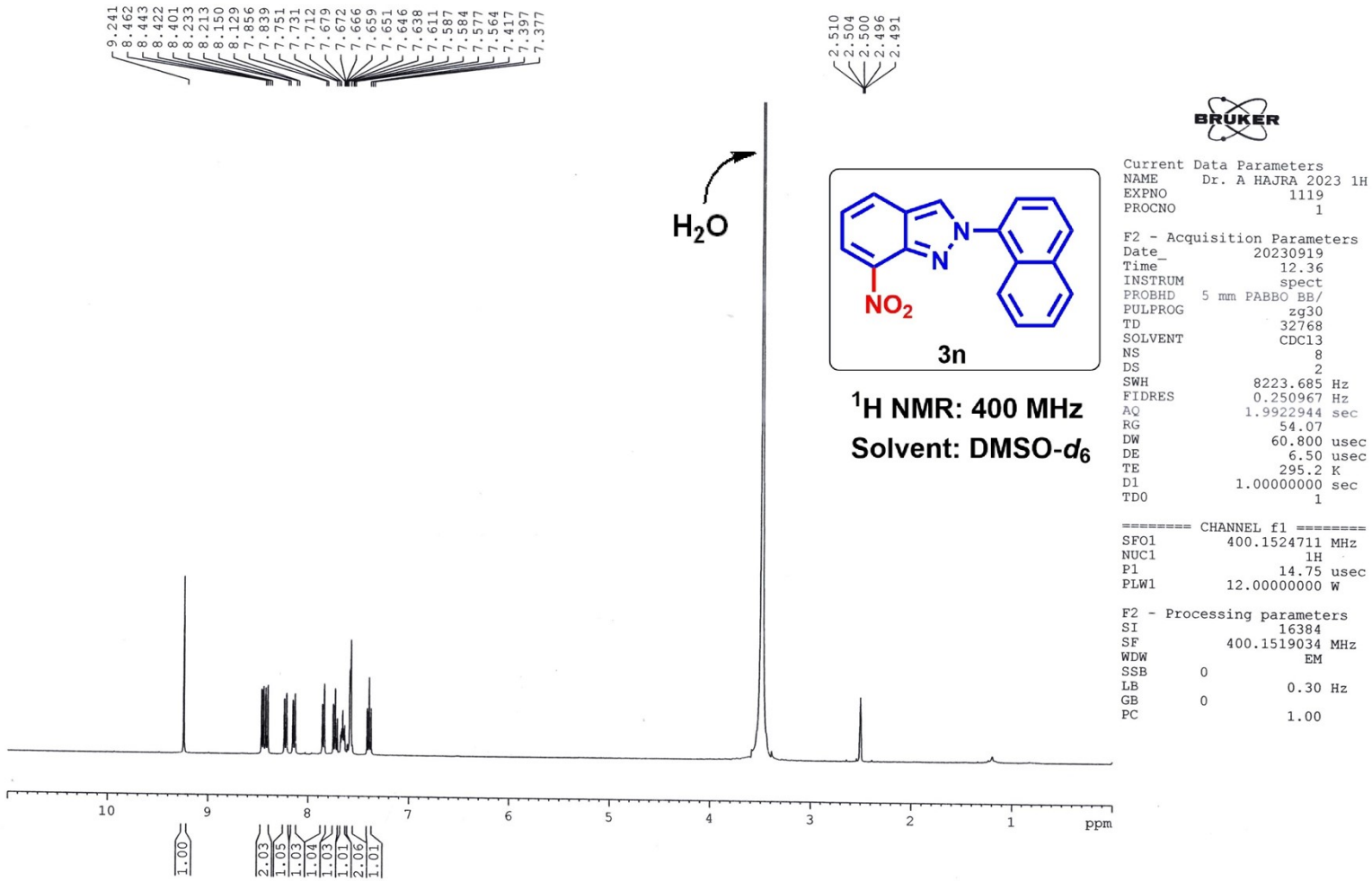
```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  292
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230721
Time              20.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                   420
DS                     2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                40.87
DW               20.800 usec
DE                6.50 usec
TE                298.5 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          100.6178350 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



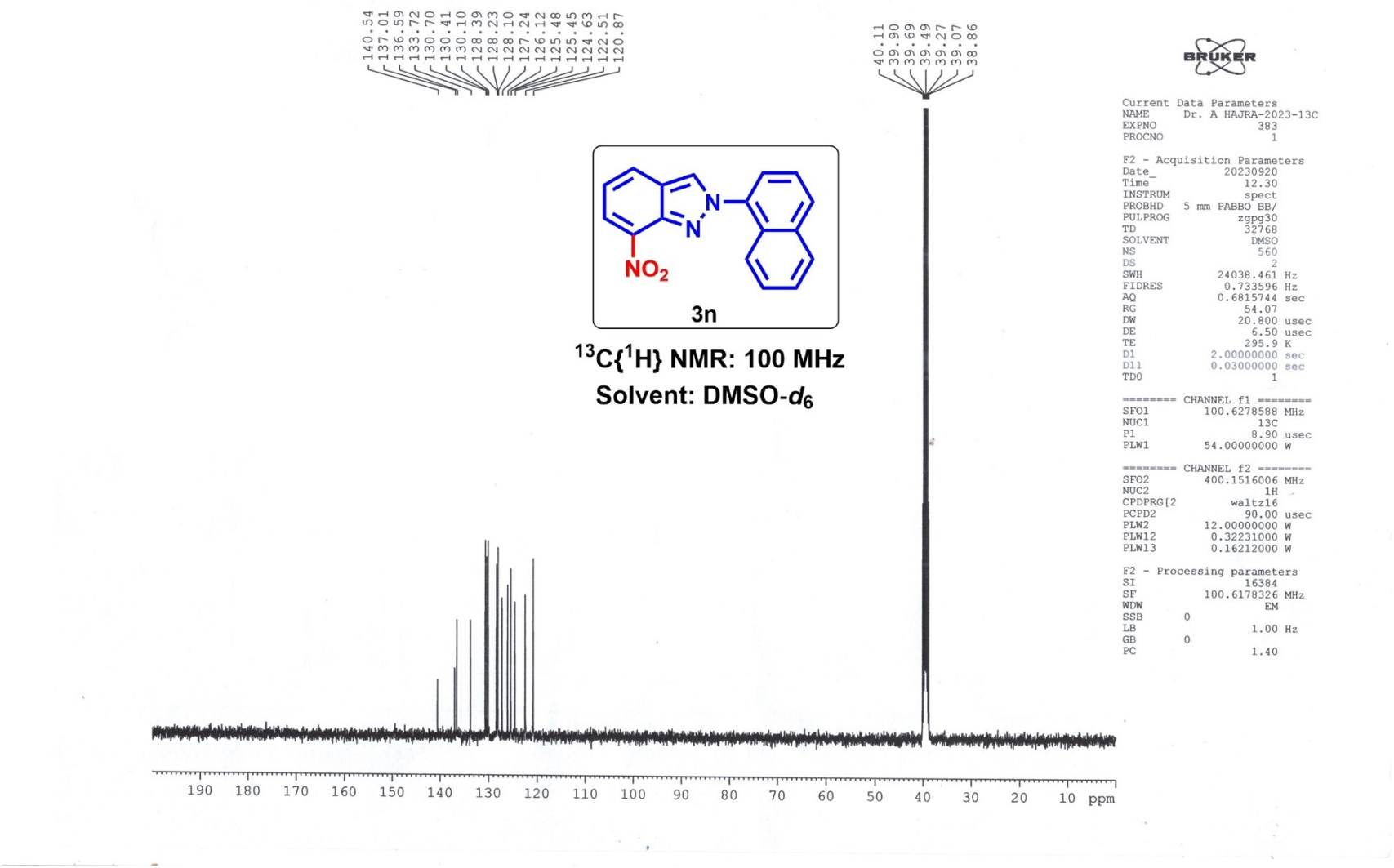
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                 1119
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230919
Time              12.36
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                54.07
DW               60.800 usec
DE                6.50 usec
TE               295.2 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           400.1519034 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



BRUKER

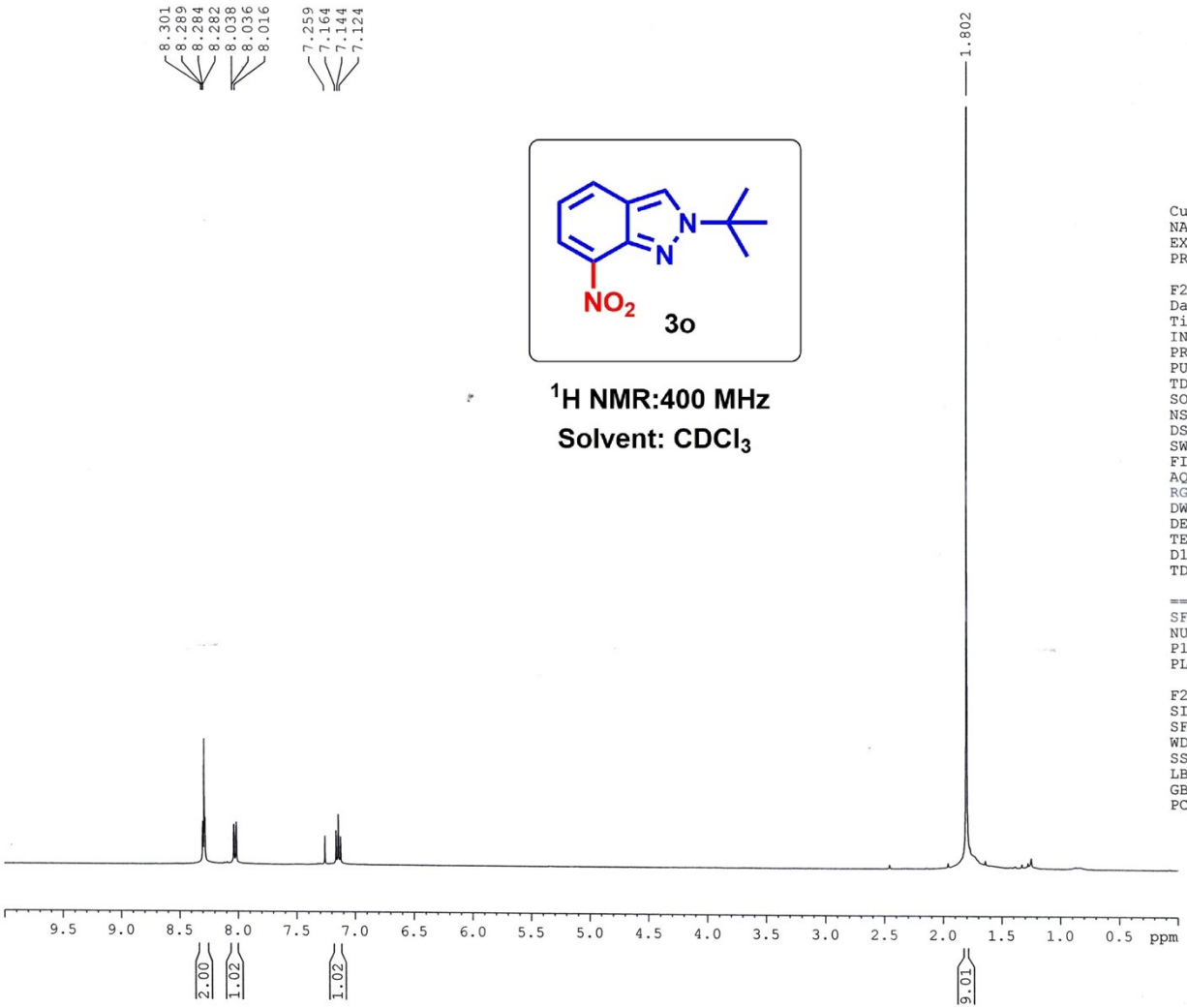
```
Current Data Parameters
NAME       Dr. A HAJRA-2023-13C
EXPNO                       383
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20230920
Time_                     12.30
INSTRUM                   spect
PROBHD     5 mm PABBO BB/
PULPROG                zgpg30
TD                        32768
SOLVENT                   DMSO
NS                          560
DS                            2
SWH                24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                        54.07
DW                       20.800 usec
DE                        6.50 usec
TE                       295.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                           1

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

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

F2 - Processing parameters
SI                        16384
SF               100.6178326 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```



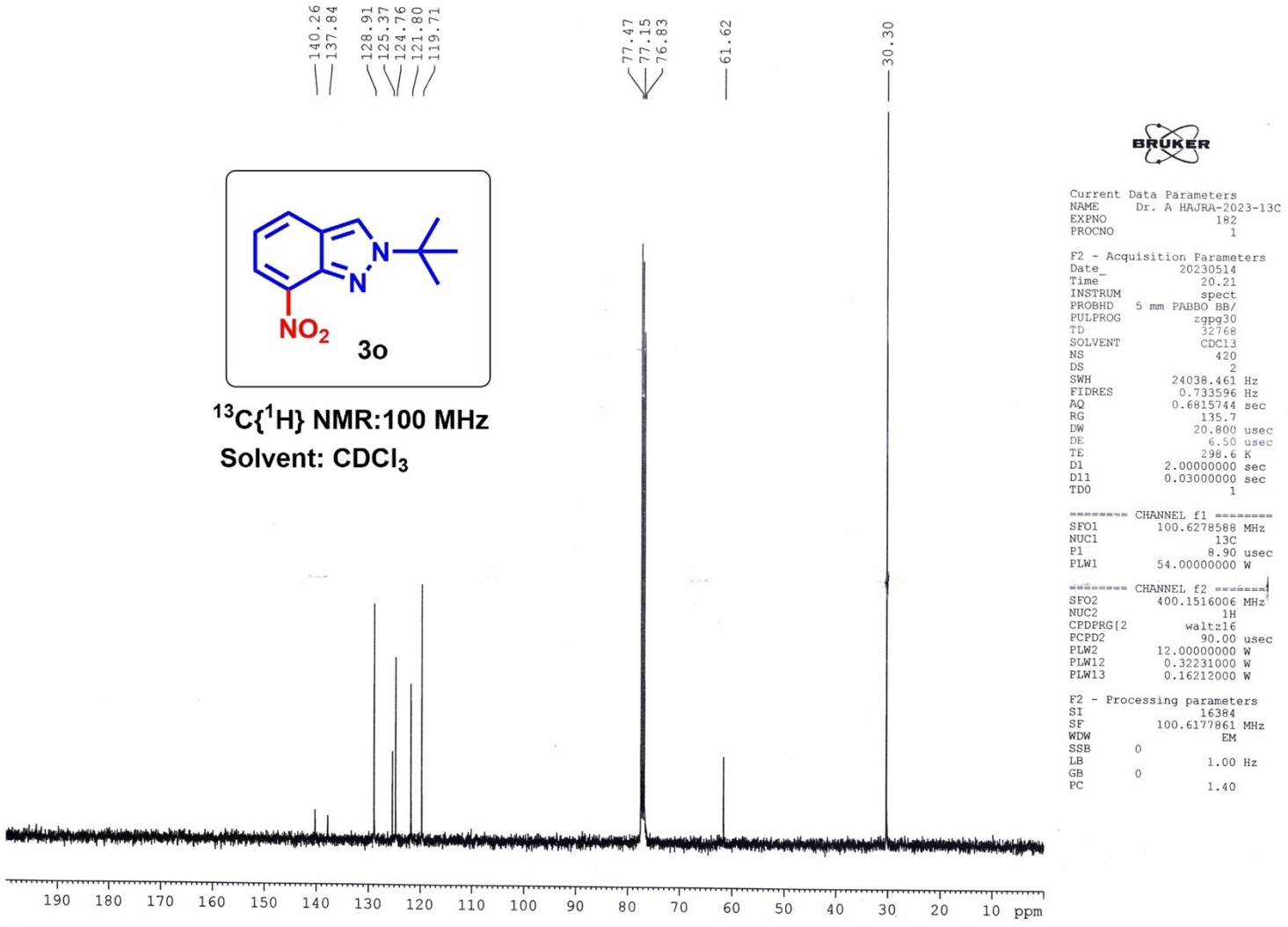
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                  609
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230514
Time              19.56
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               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          400.1500097 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



BRUKER

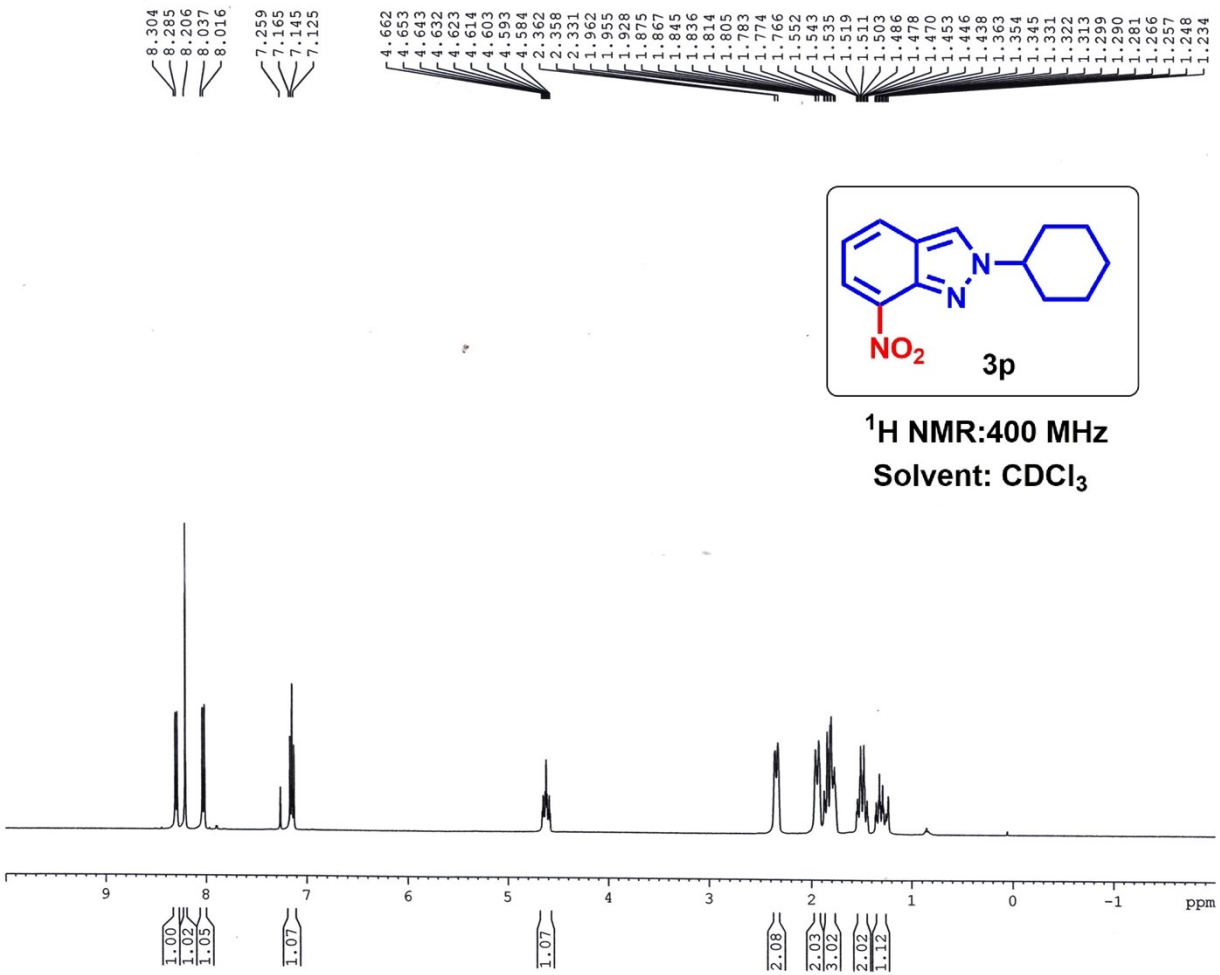
```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  182
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230514
Time                20.21
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    420
DS                      2
SWH             24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                  135.7
DW                 20.800 usec
DE                  6.50 usec
TE                 298.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1

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

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

F2 - Processing parameters
SI                  16384
SF            100.6177861 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



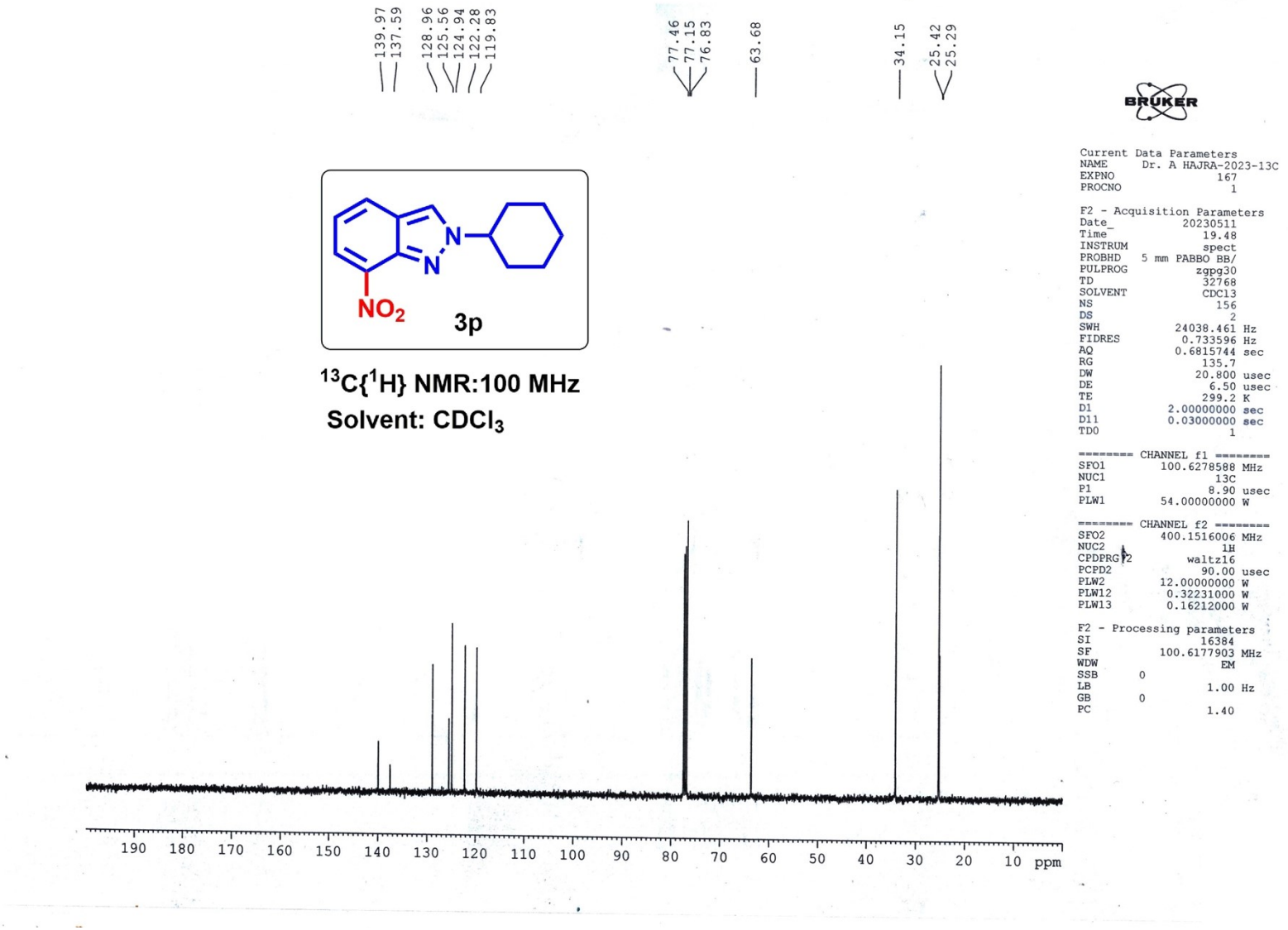
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                  584
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230511
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               62.69
DW               60.800 usec
DE                6.50 usec
TE                298.8 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          400.1500096 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



BRUKER

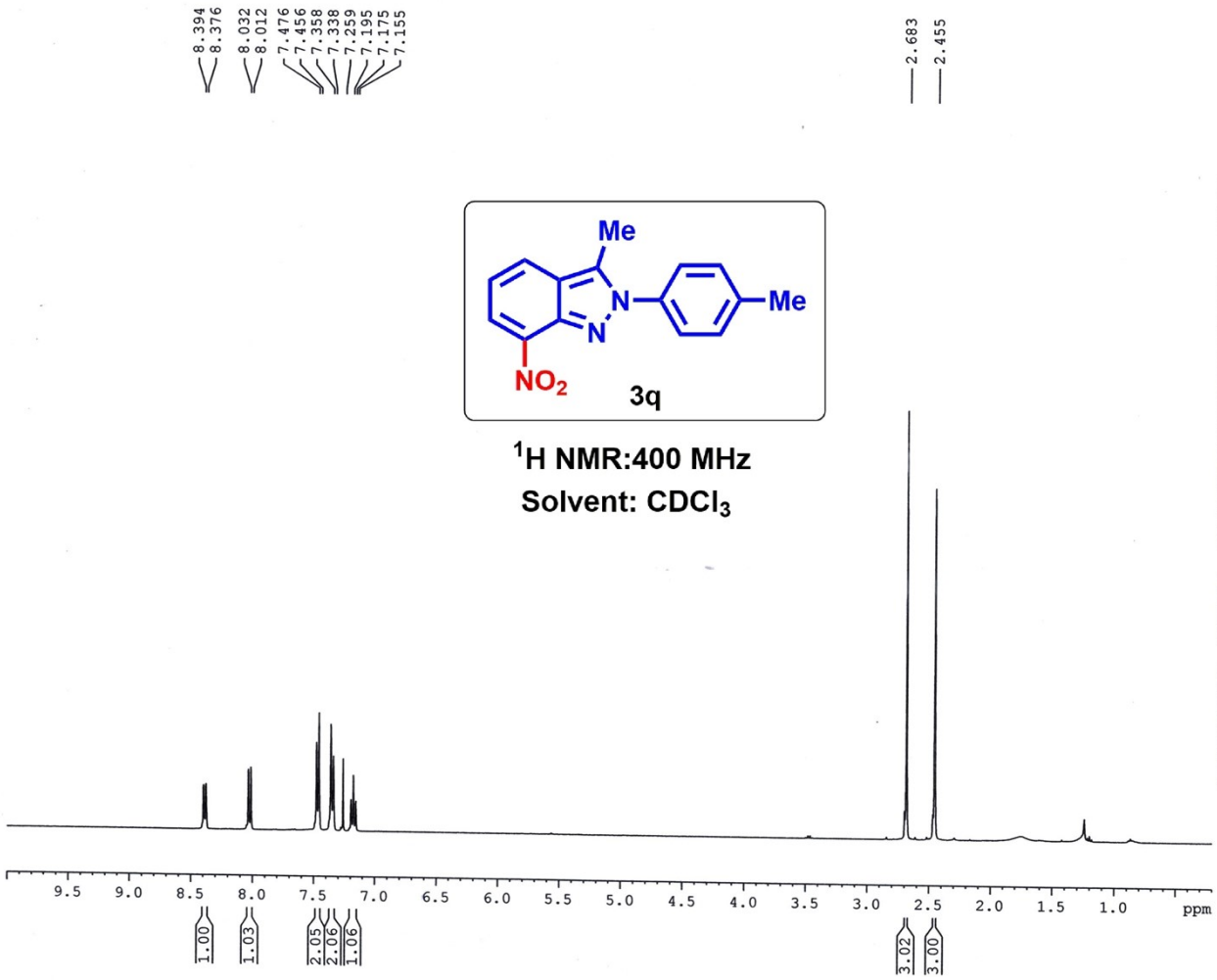
```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  167
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230511
Time                 19.48
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     156
DS                       2
SWH              24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6815744 sec
RG                   135.7
DW                  20.800 usec
DE                   6.50 usec
TE                  299.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                   16384
SF            100.6177903 MHz
WDW                    EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

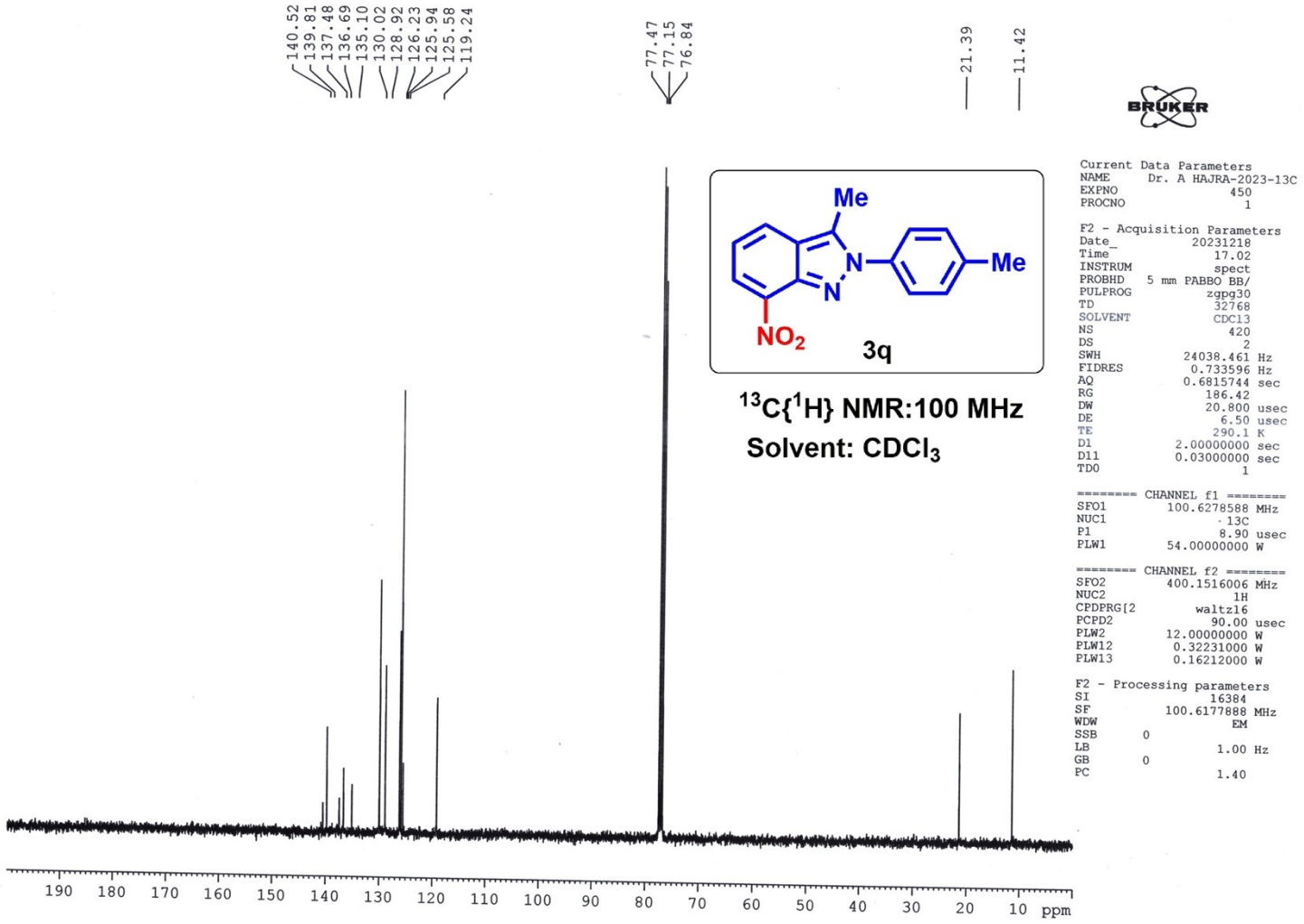



```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1304
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231218
Time              16.38
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               289.6 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          400.1500097 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



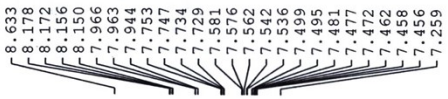

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  450
PROCNO                   1

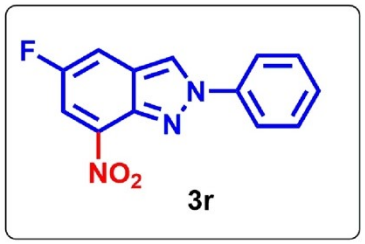
F2 - Acquisition Parameters
Date_           20231218
Time              17.02
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT           CDCl3
NS                  420
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG               186.42
DW              20.800 usec
DE               6.50 usec
TE              290.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

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

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

F2 - Processing parameters
SI                16384
SF           100.6177888 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

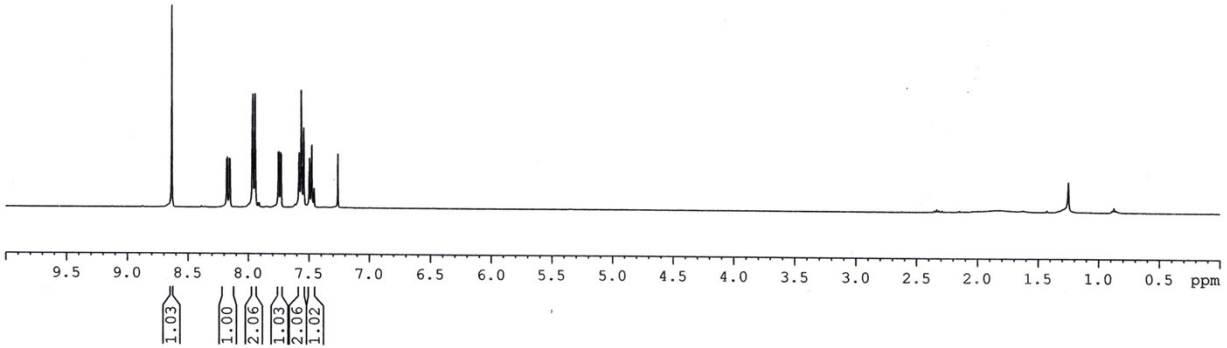




3r

^{1}H NMR:400 MHz

Solvent: $CDCl_3$

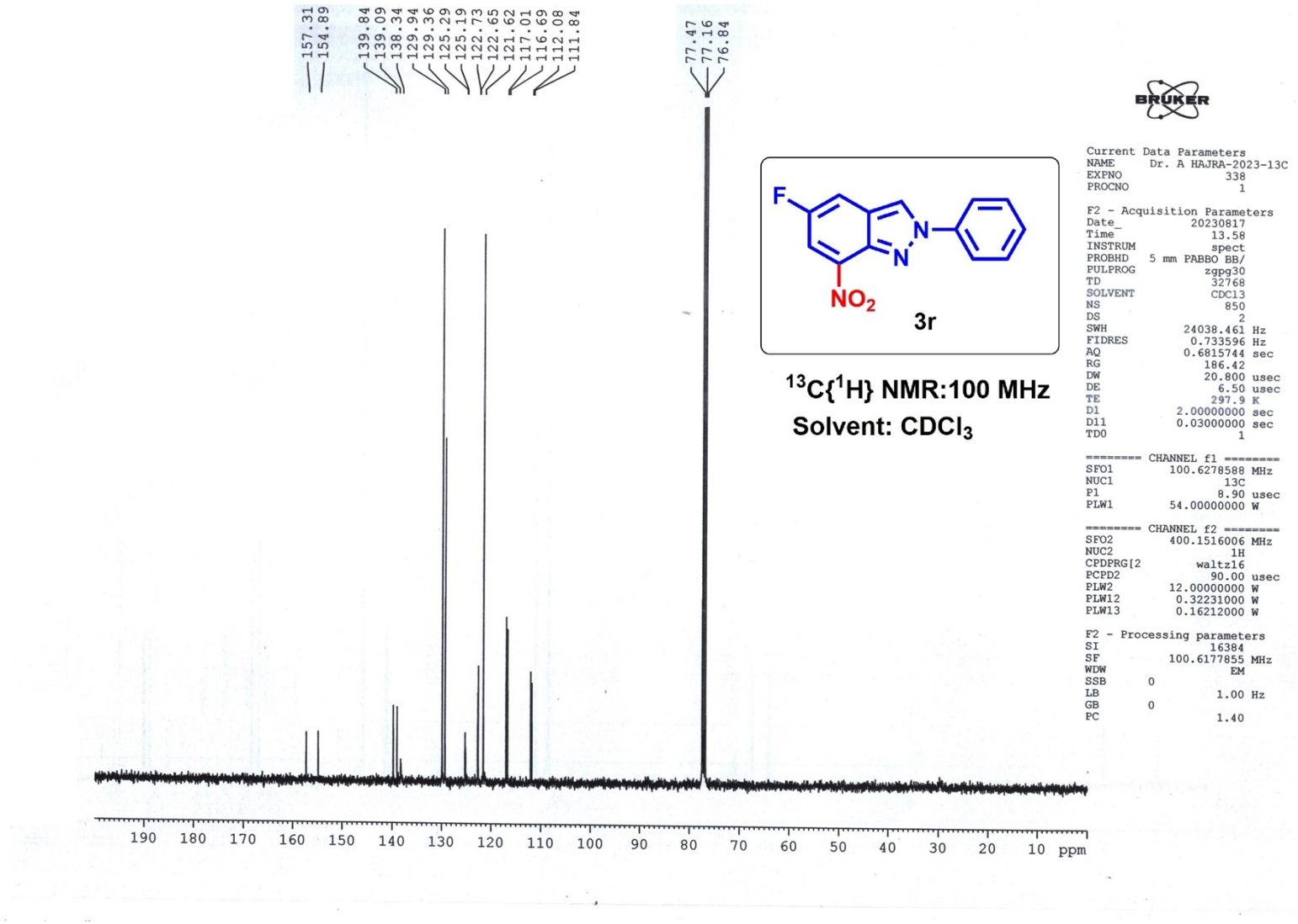



```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1037
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230817
Time              13.16
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              297.5 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          400.1500098 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



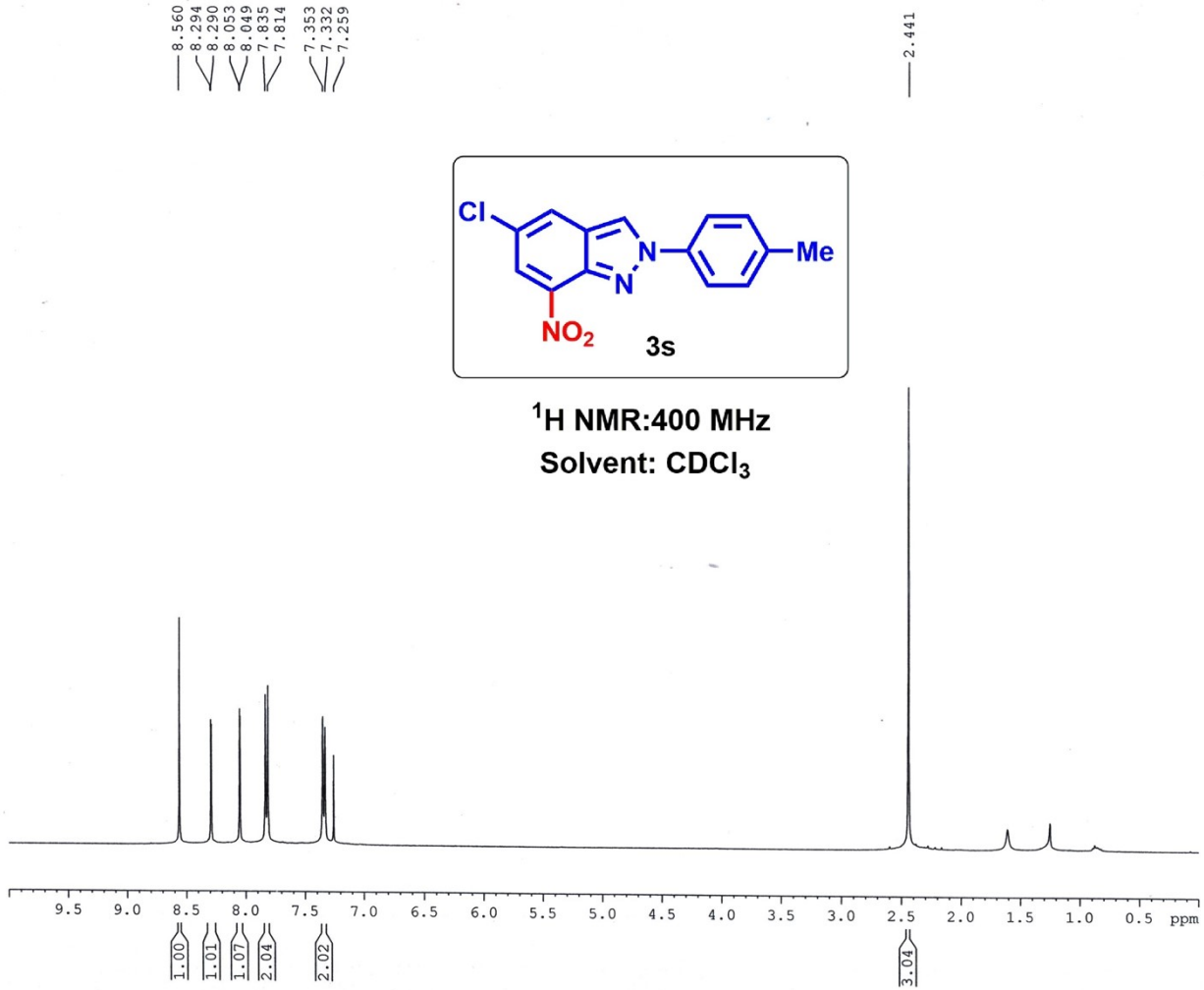

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  338
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230817
Time                 13.58
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     850
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                297.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                   16384
SF            100.6177855 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



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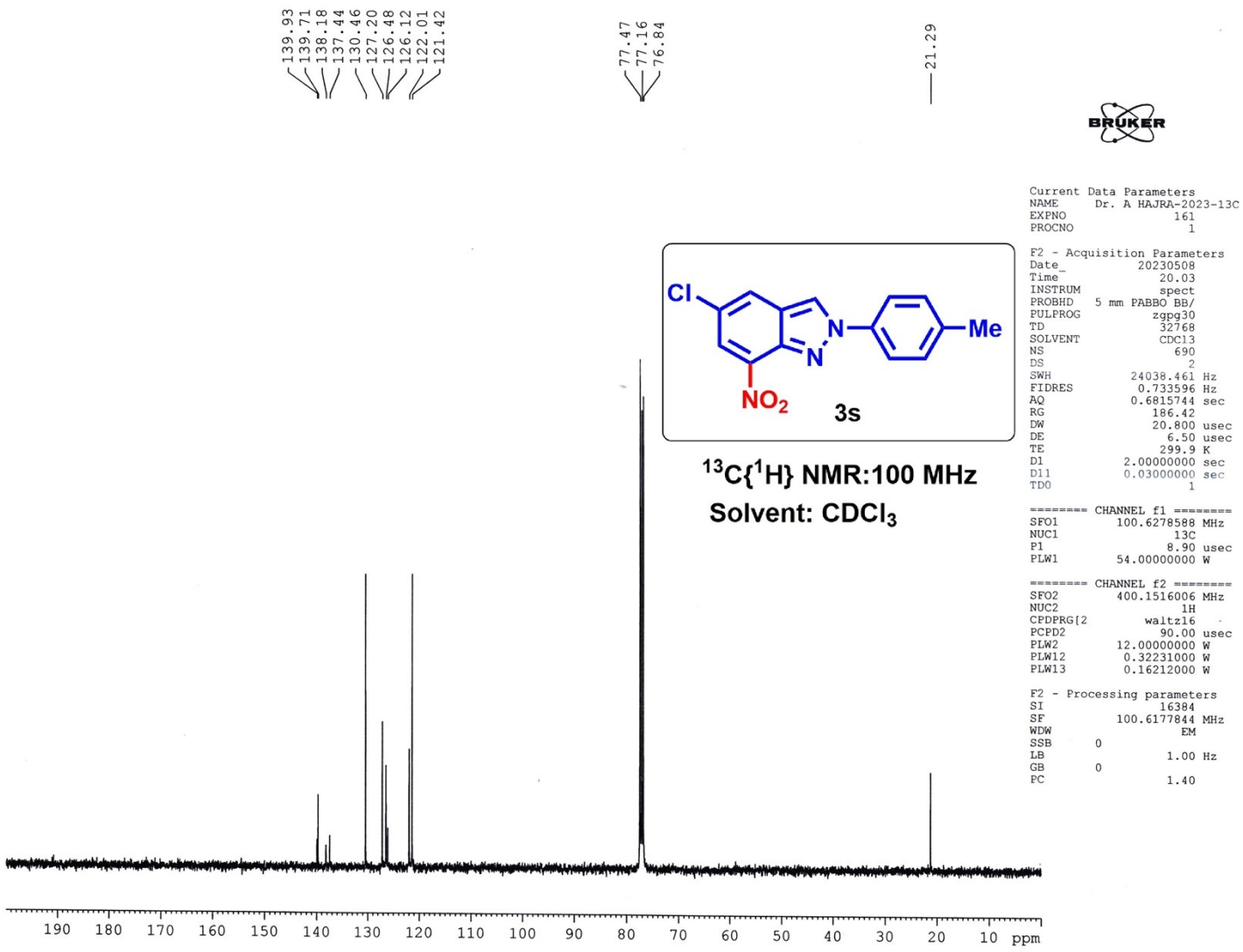
```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                  572
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230508
Time              19.27
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               299.3 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           400.1500097 MHz
WDW                EM
SSB       0
LB              0.30 Hz
GB        0
PC                1.00
```



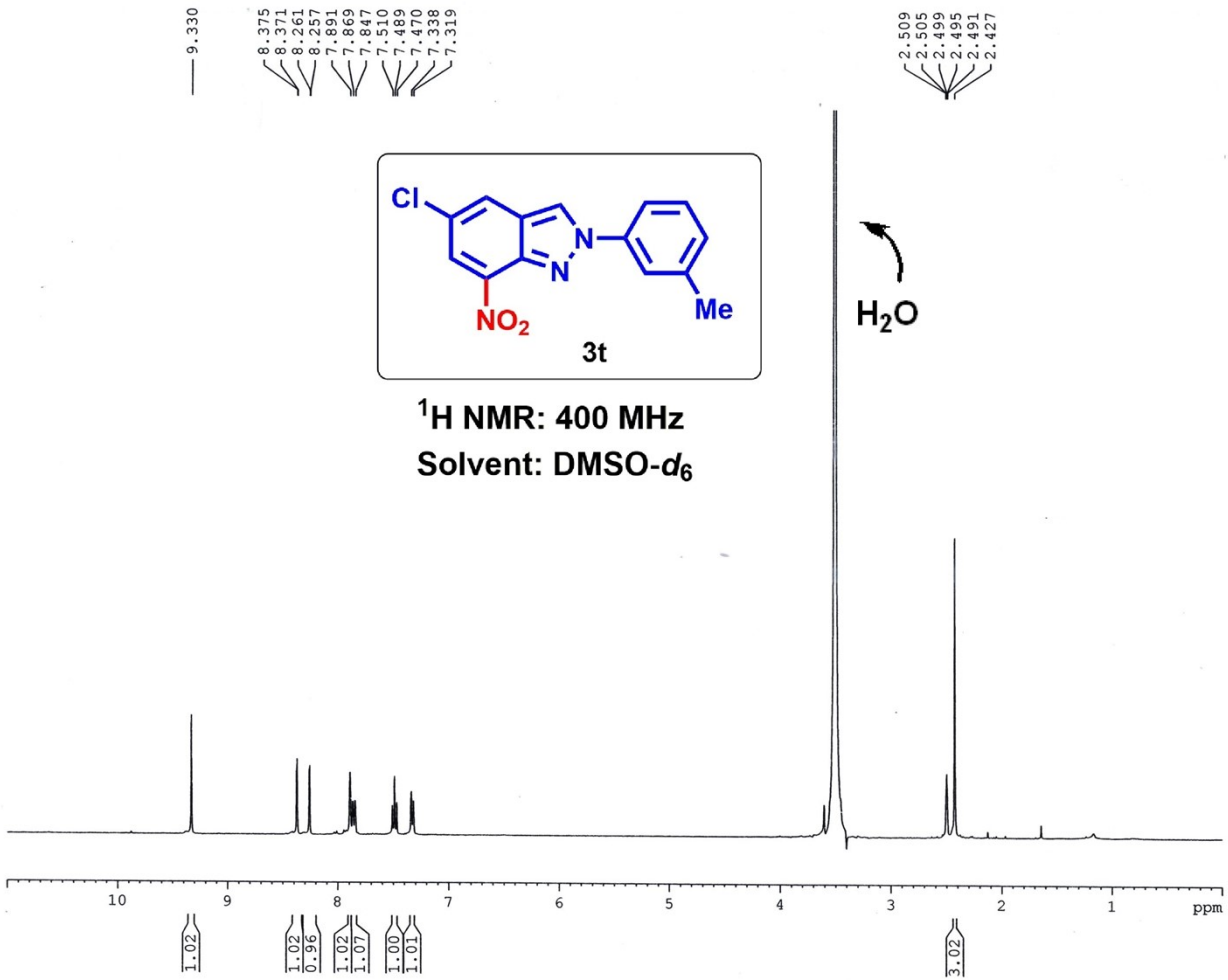

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  161
PROCNO                   1

F2 - Acquisition Parameters
Date_             20230508
Time                20.03
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   690
DS                     2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                186.42
DW                20.800 usec
DE                 6.50 usec
TE                299.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

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

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

F2 - Processing parameters
SI                  16384
SF           100.6177844 MHz
WDW                  EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



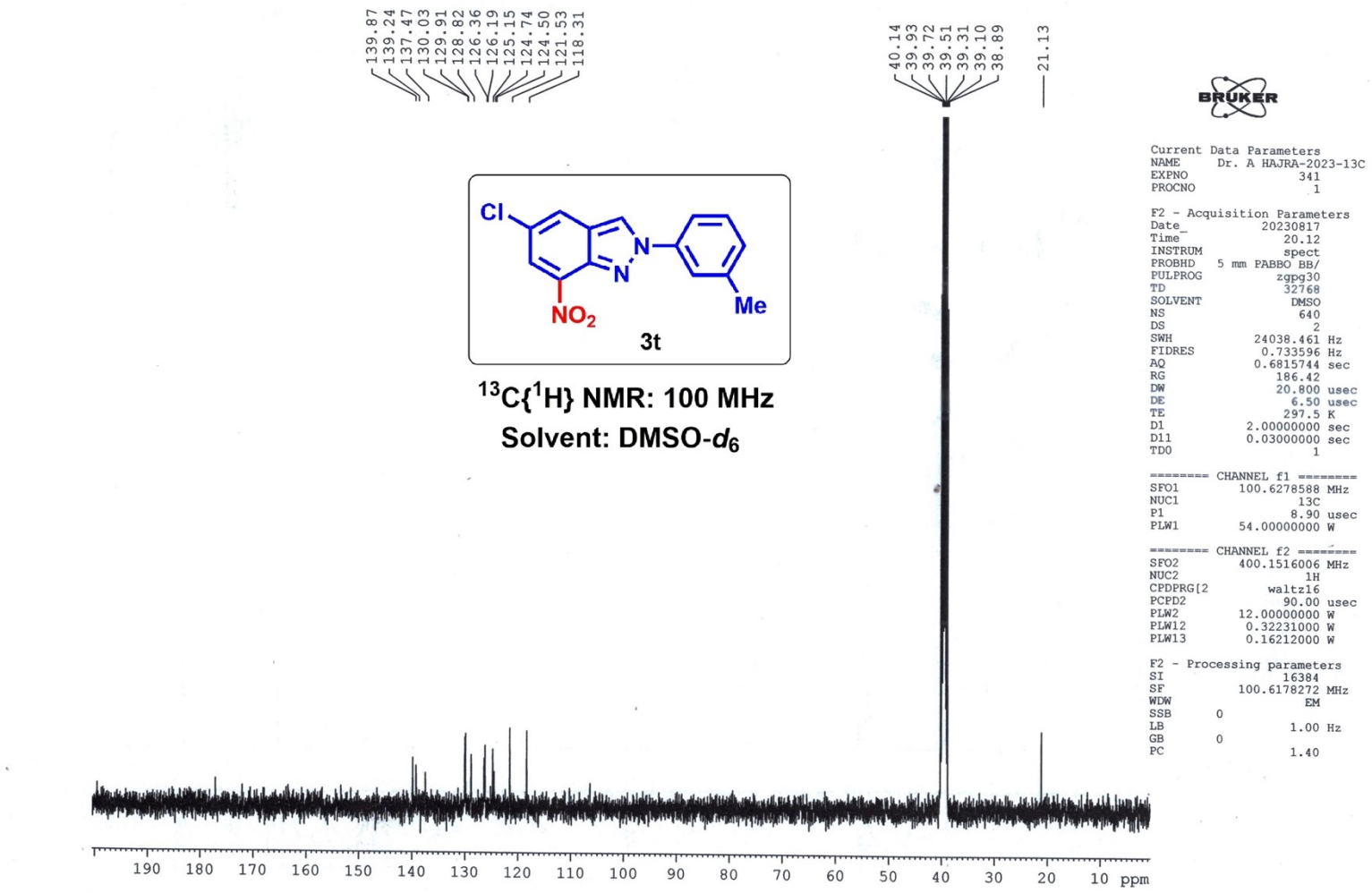
BRUKER

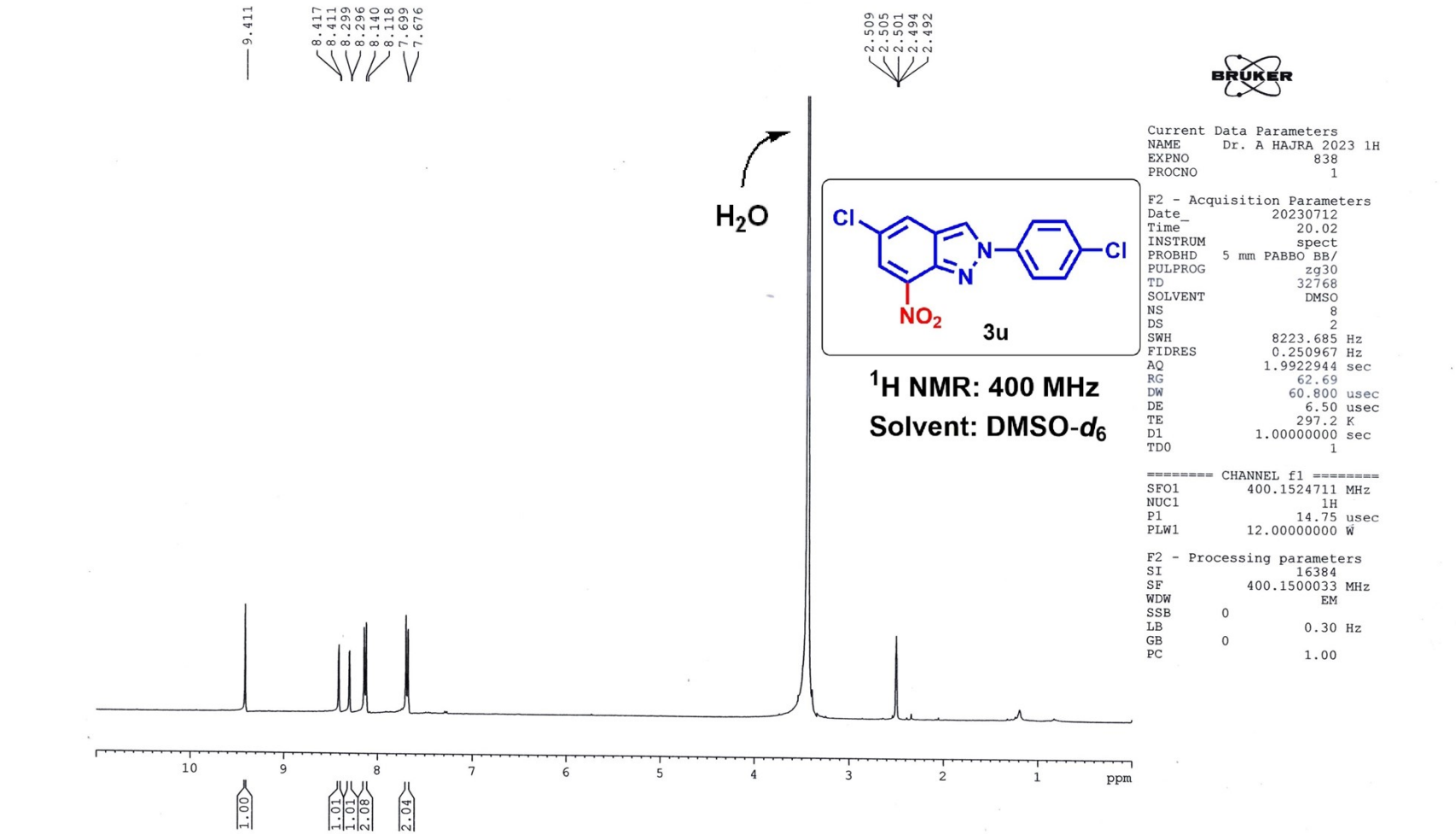
```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1041
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230817
Time              19.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT            DMSO
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                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           400.1500035 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```


139.87
139.24
137.47
130.03
129.91
128.82
126.36
126.19
125.15
124.74
124.50
121.53
118.31
40.14
39.93
39.72
39.51
39.31
39.10
38.89
21.13
Cl
N
N
NO2
Me
3t
13C{1H} NMR: 100 MHz
Solvent: DMSO-d6
BRUKER
Current Data Parameters
NAME Dr. A HAJRA-2023-13C
EXPNO 341
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230817
Time 20.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 640
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 297.5 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 100.6178272 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

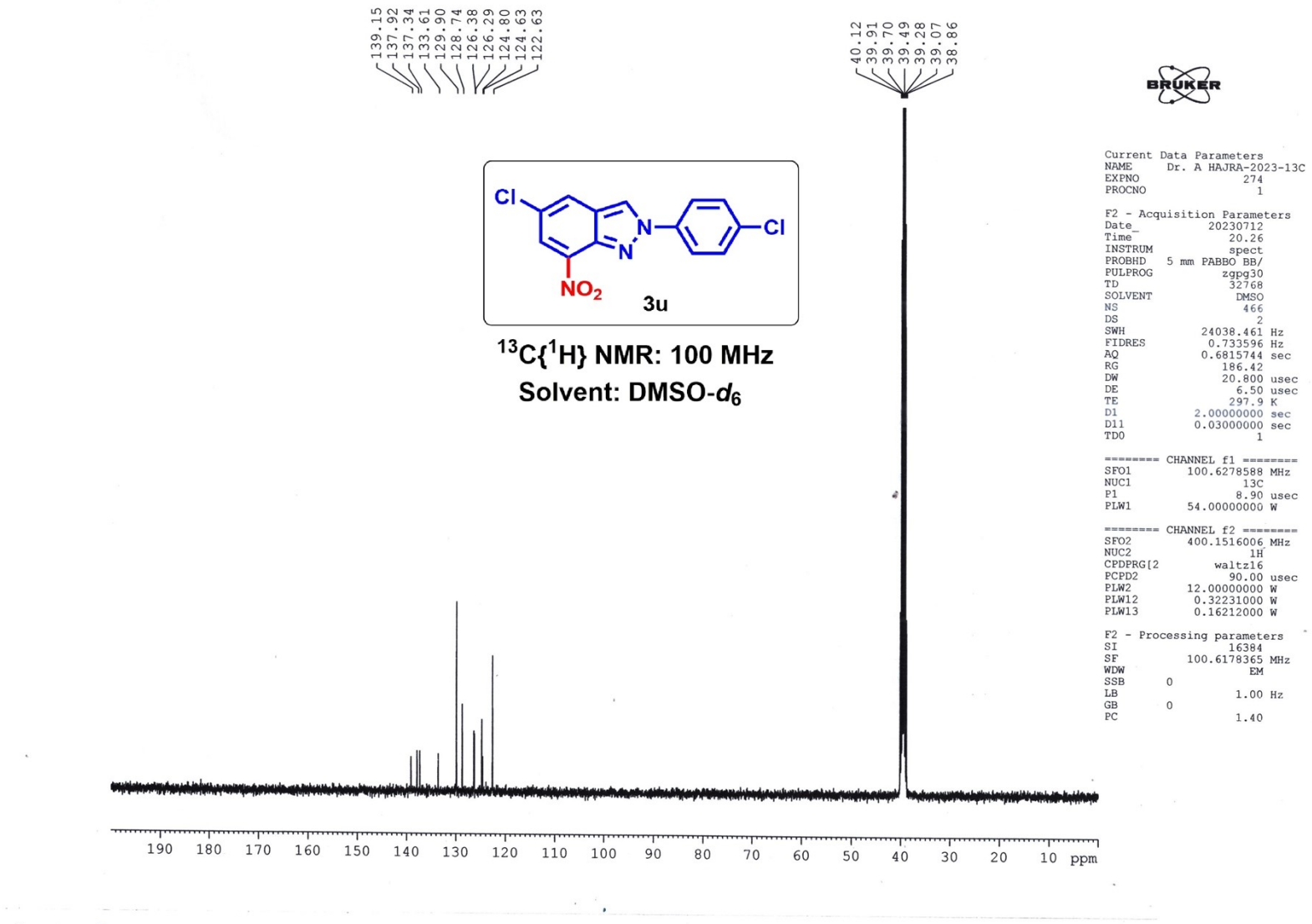


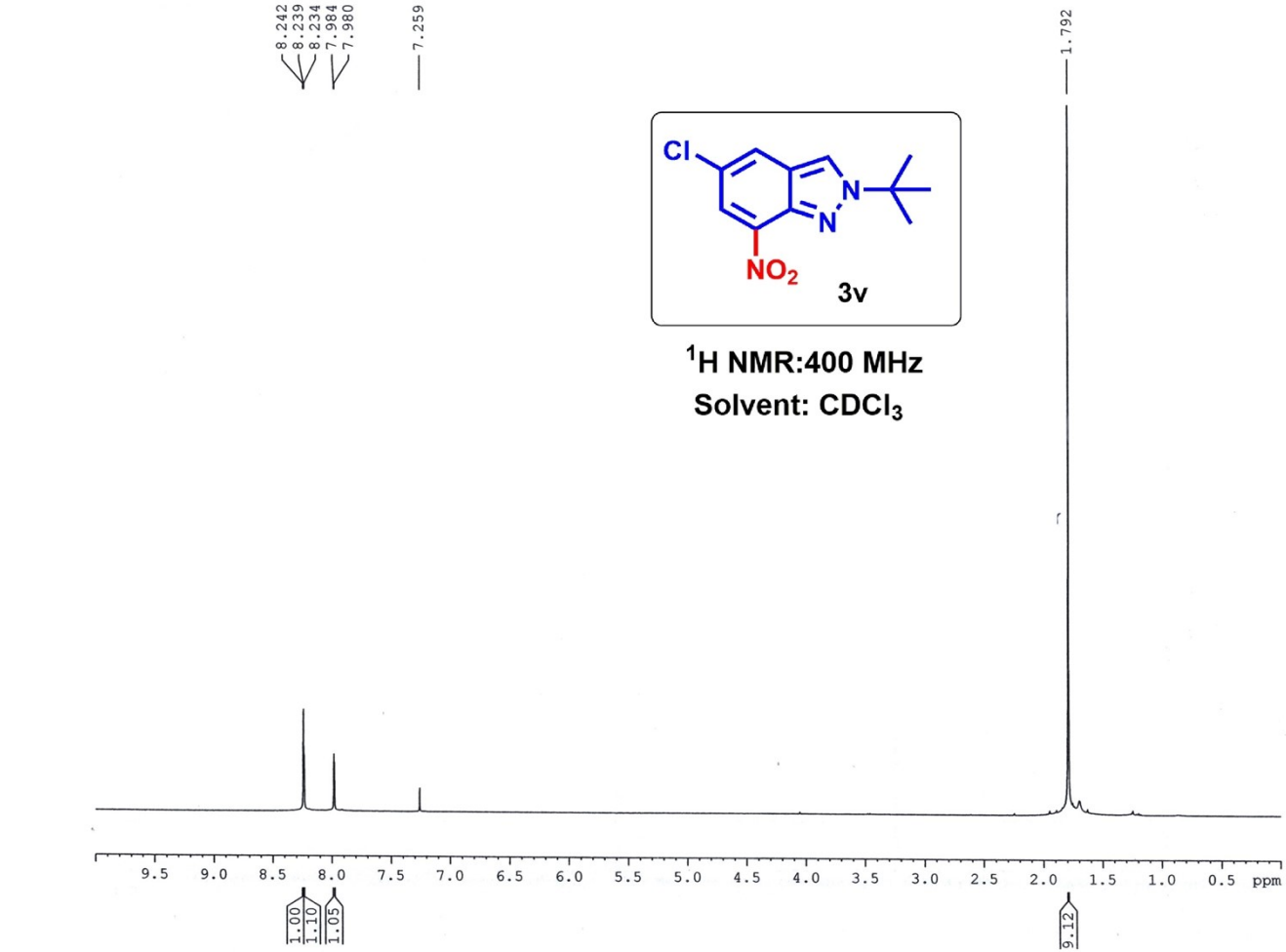

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                838
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230712
Time              20.02
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                     8
DS                     2
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9922944 sec
RG                62.69
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           400.1500033 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```


139.15
137.92
137.34
133.61
129.90
128.74
126.38
126.29
124.80
124.63
122.63
40.12
39.91
39.70
39.49
39.28
39.07
38.86
Cl
N
N
Cl
NO2
3u
13C{1H} NMR: 100 MHz
Solvent: DMSO-d6
BRUKER
Current Data Parameters
NAME Dr. A HAJRA-2023-13C
EXPNO 274
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230712
Time 20.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 466
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 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W
F2 - Processing parameters
SI 16384
SF 100.6178365 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



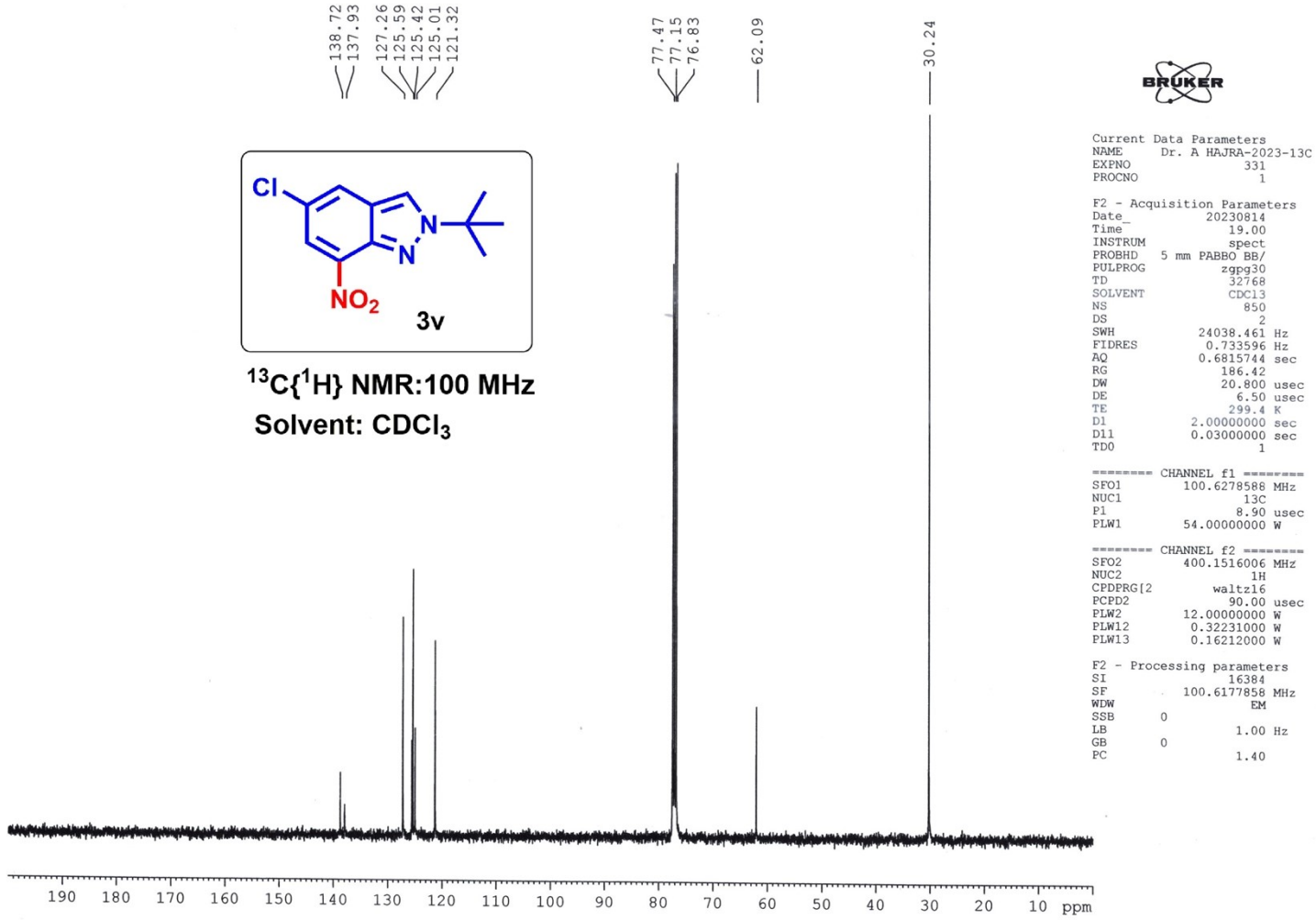
BRUKER

```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1021
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230814
Time              18.18
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               298.9 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           400.1500098 MHz
WDW                  EM
SSB       0
LB              0.30 Hz
GB        0
PC                1.00
```



BRUKER

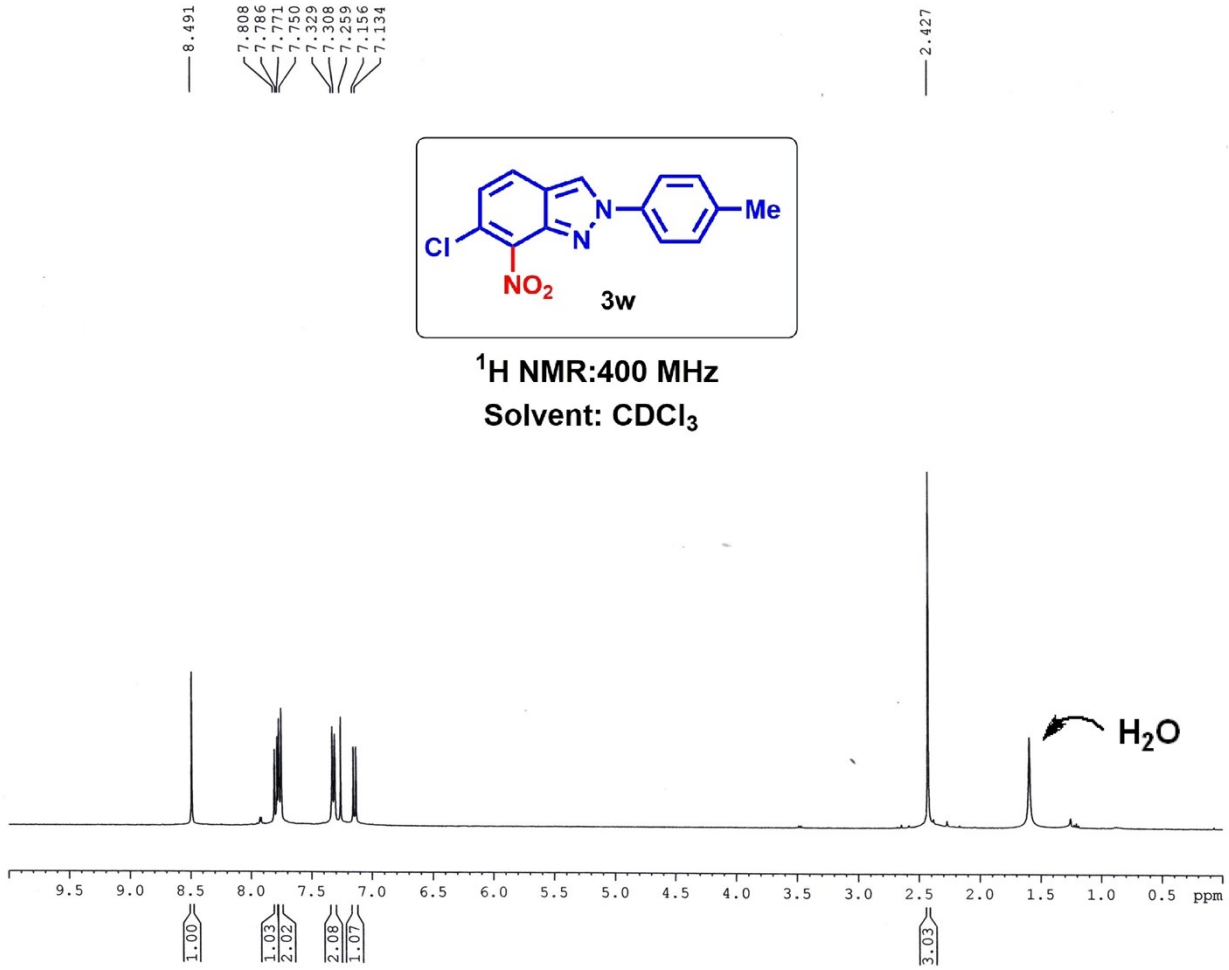
Current Data Parameters
NAME Dr. A HAJRA-2023-13C
EXPNO 331
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230814
Time 19.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 850
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 186.42
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

F2 - Processing parameters
SI 16384
SF 100.6177858 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

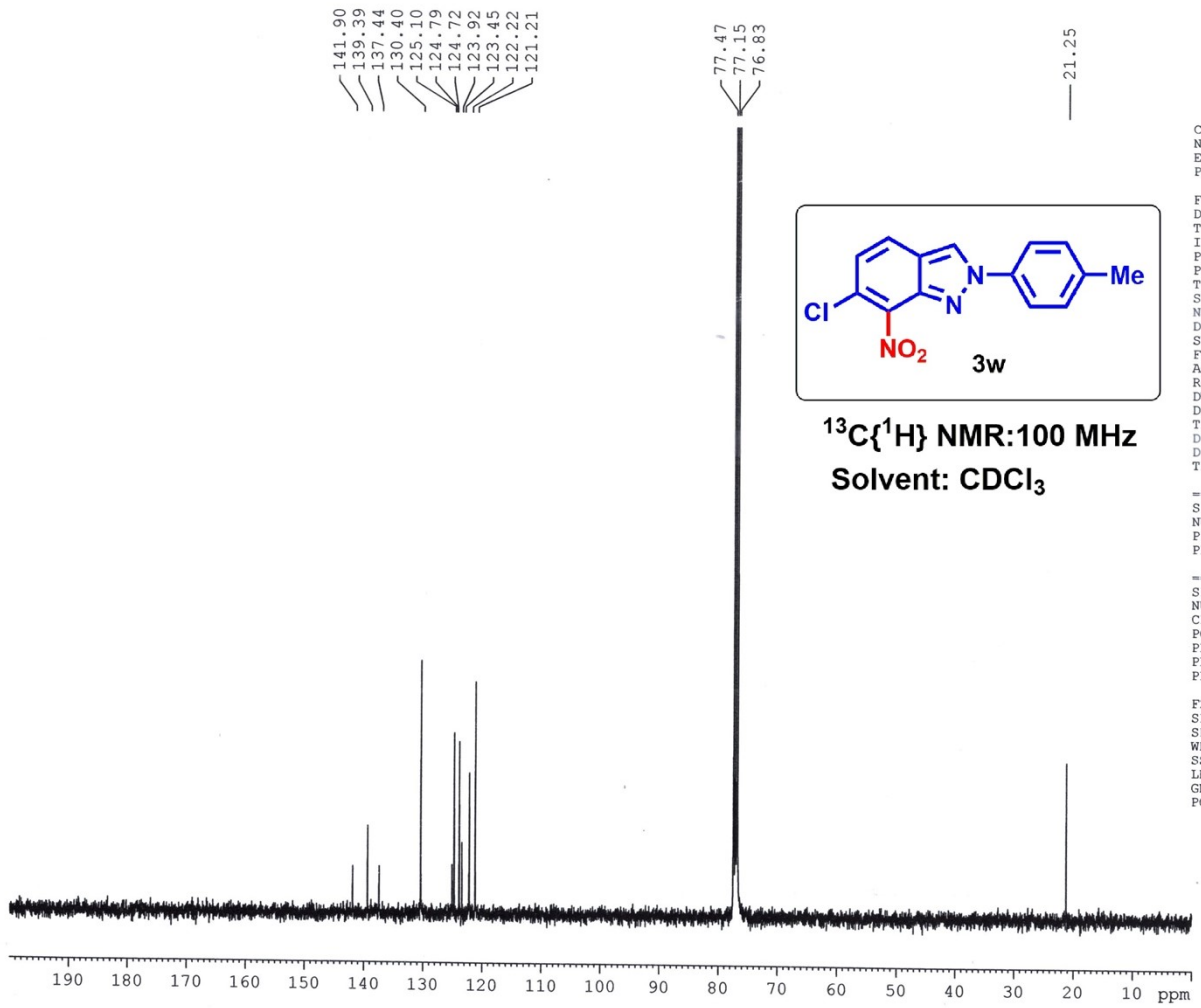



```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1022
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230814
Time              19.51
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               186.42
DW               60.800 usec
DE                6.50 usec
TE               298.7 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           400.1500098 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



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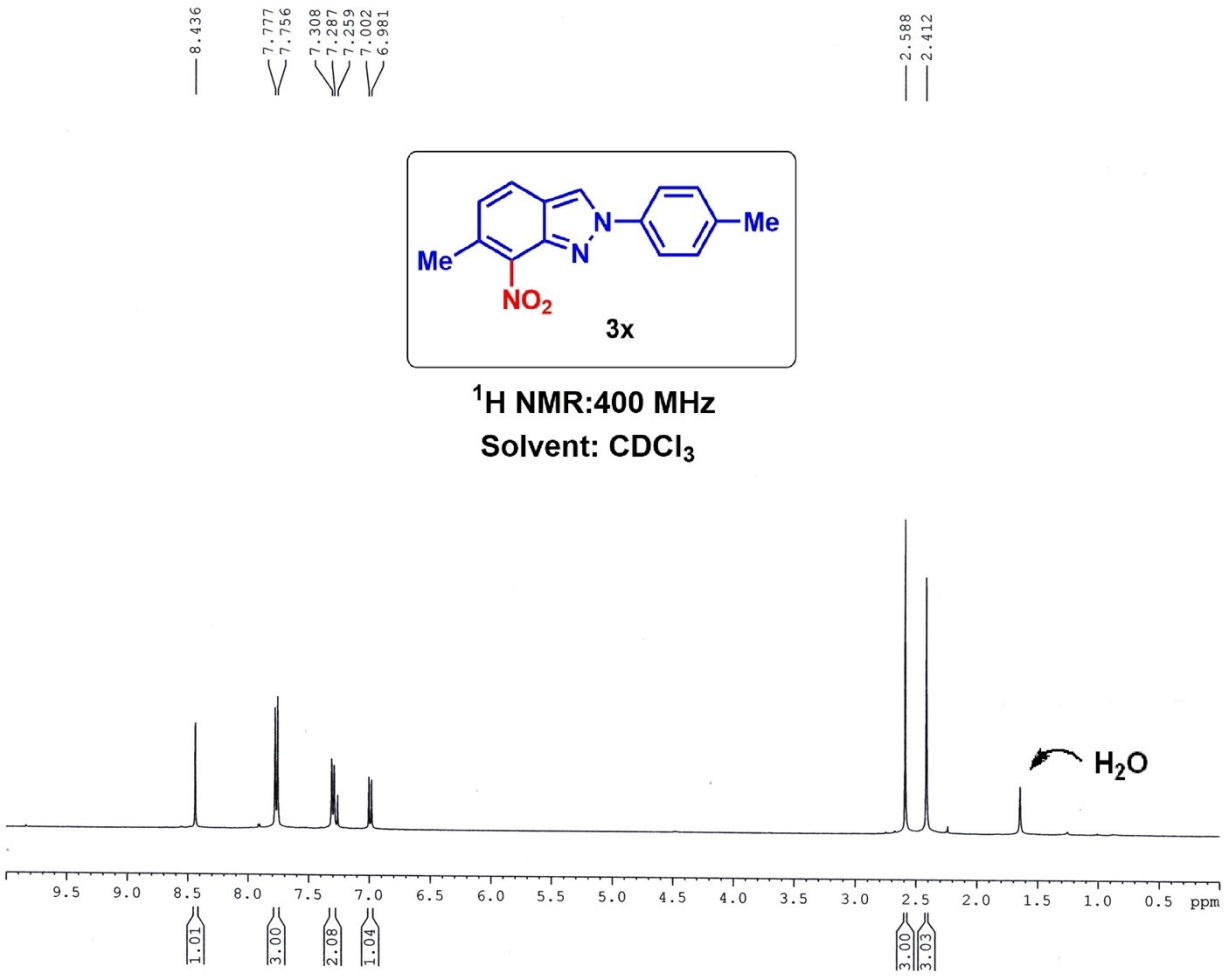
```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                      332
PROCNO                       1

F2 - Acquisition Parameters
Date_              20230814
Time                  20.32
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     850
DS                       2
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                   186.42
DW                   20.800 usec
DE                    6.50 usec
TE                   299.5 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            100.6177843 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

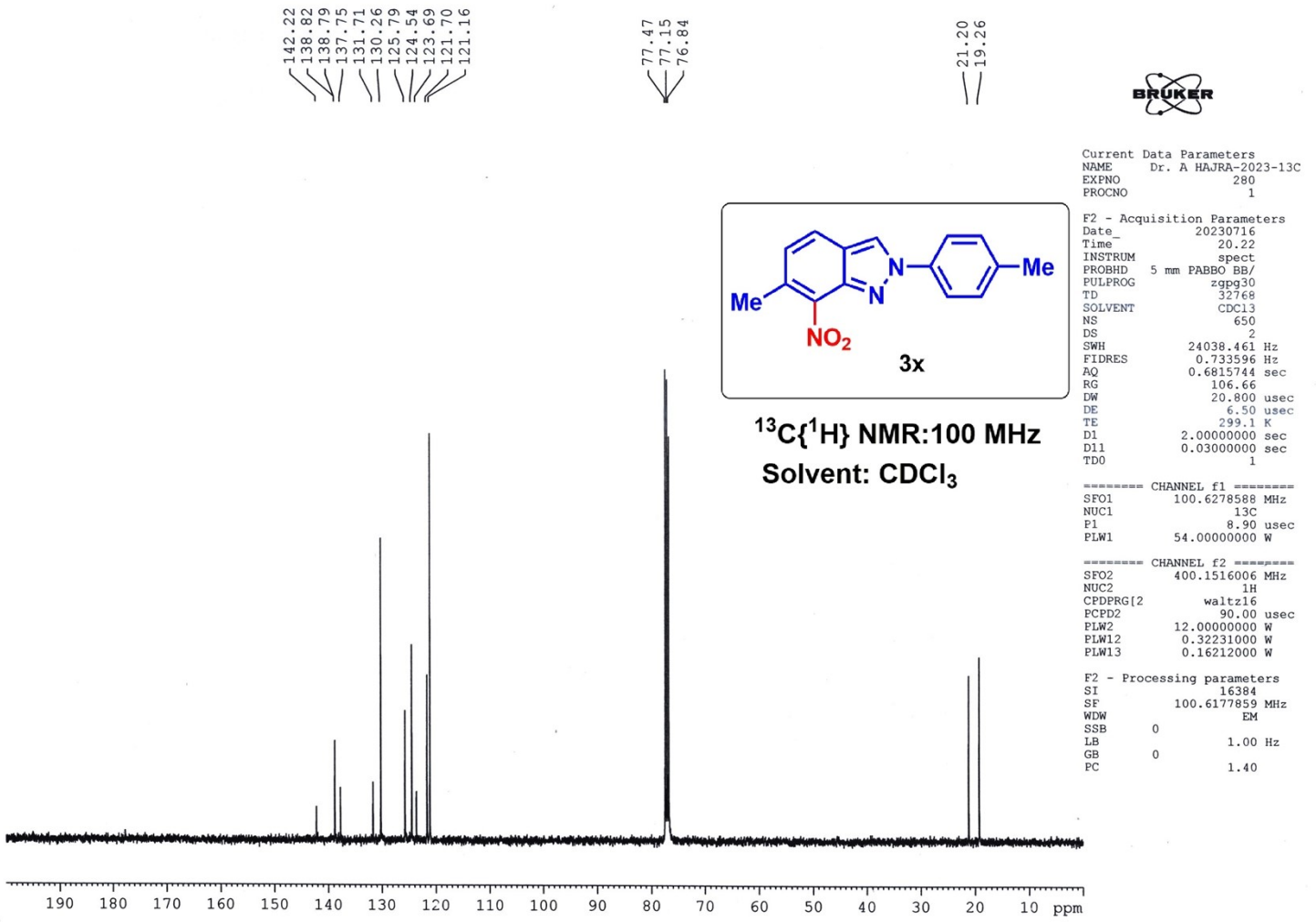



```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO                  855
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230716
Time              19.47
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               298.6 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           400.1500099 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



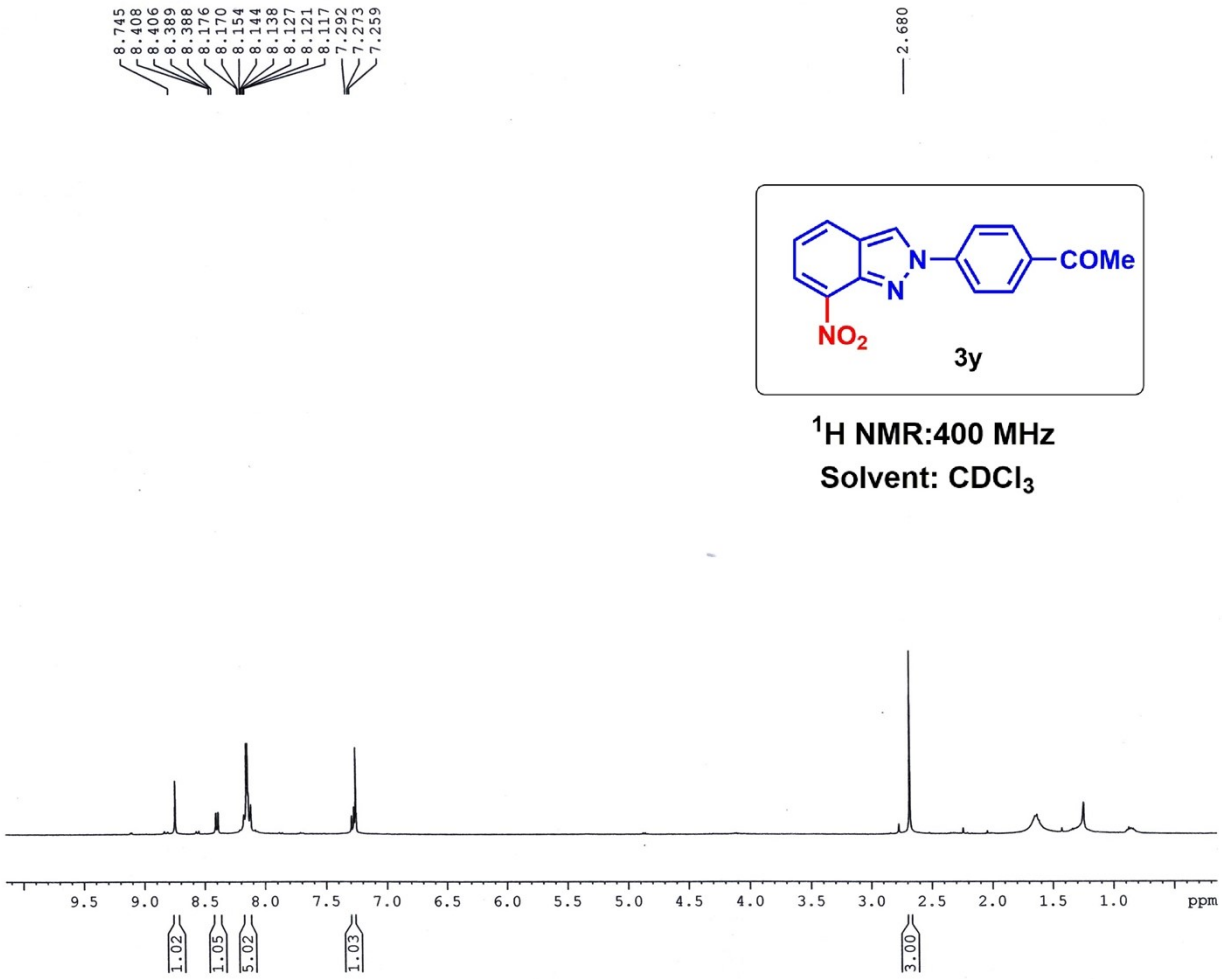

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  280
PROCNO                   1

F2 - Acquisition Parameters
Date_           20230716
Time              20.22
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD              32768
SOLVENT          CDCl3
NS                 650
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               299.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                  1

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

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

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



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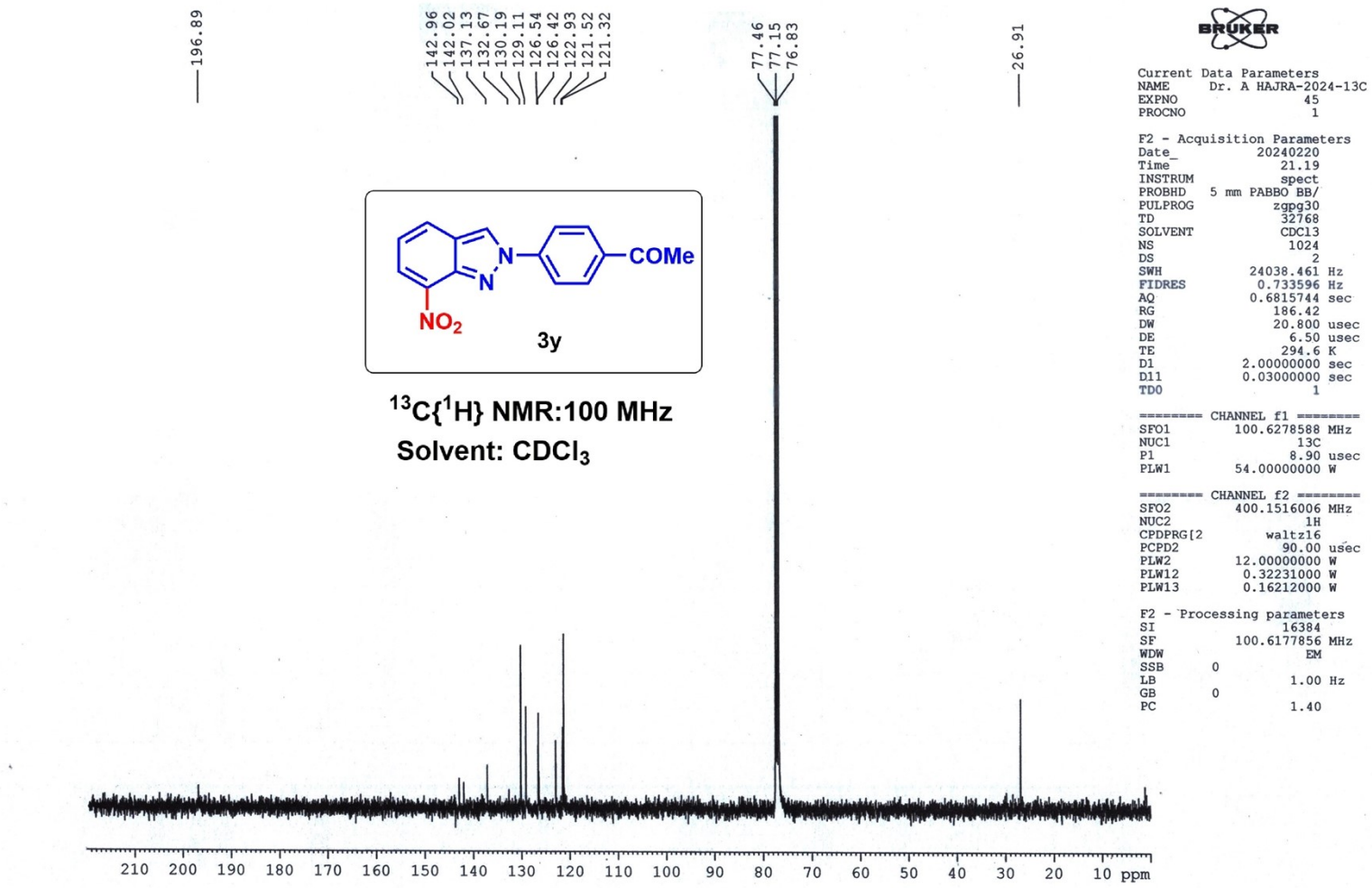
```
Current Data Parameters
NAME      Dr. A HAJRA 2024 1H
EXPNO                  133
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240220
Time              20.27
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               294.4 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          400.1500097 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



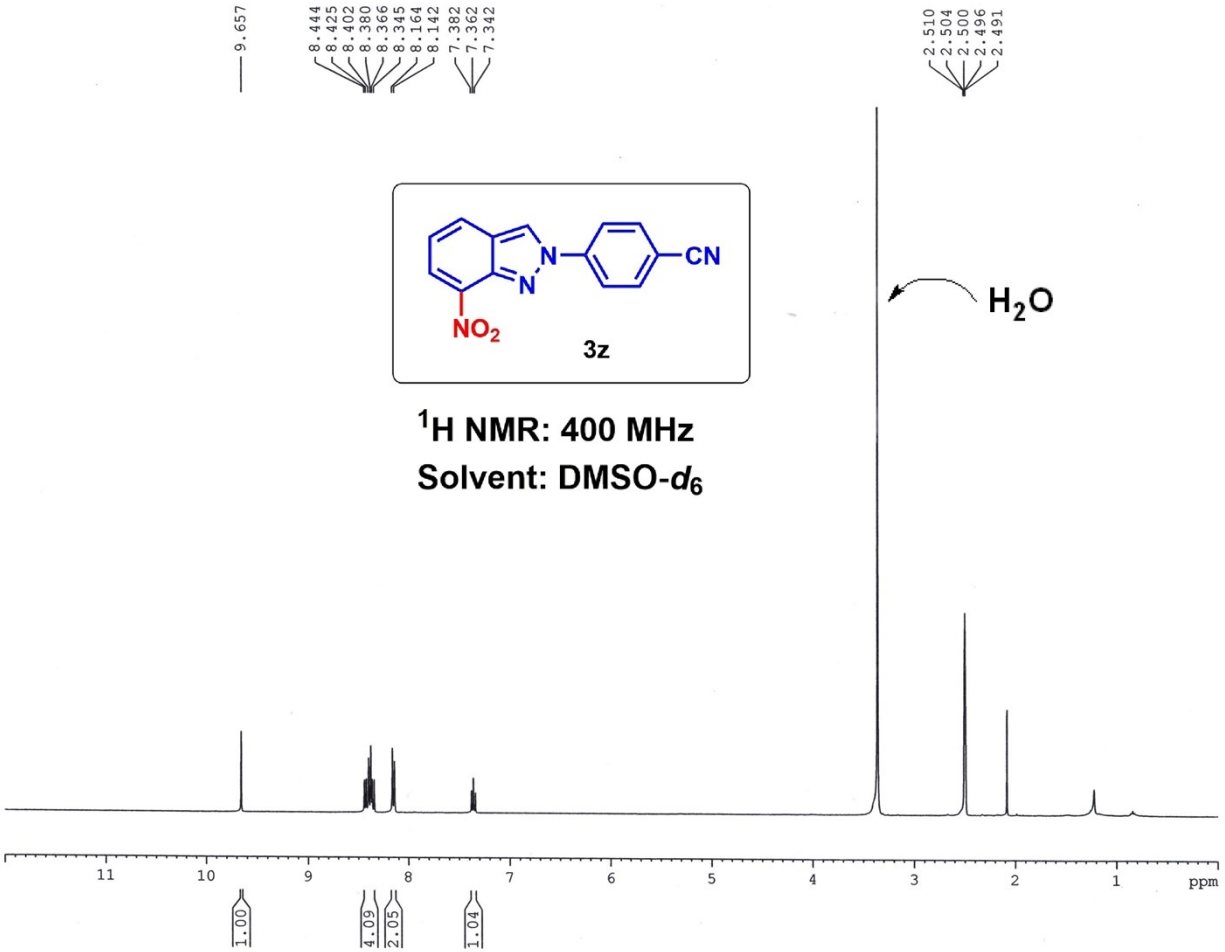

```
Current Data Parameters
NAME      Dr. A HAJRA-2024-13C
EXPNO                   45
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240220
Time                 21.19
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                  294.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                    16384
SF           100.6177856 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

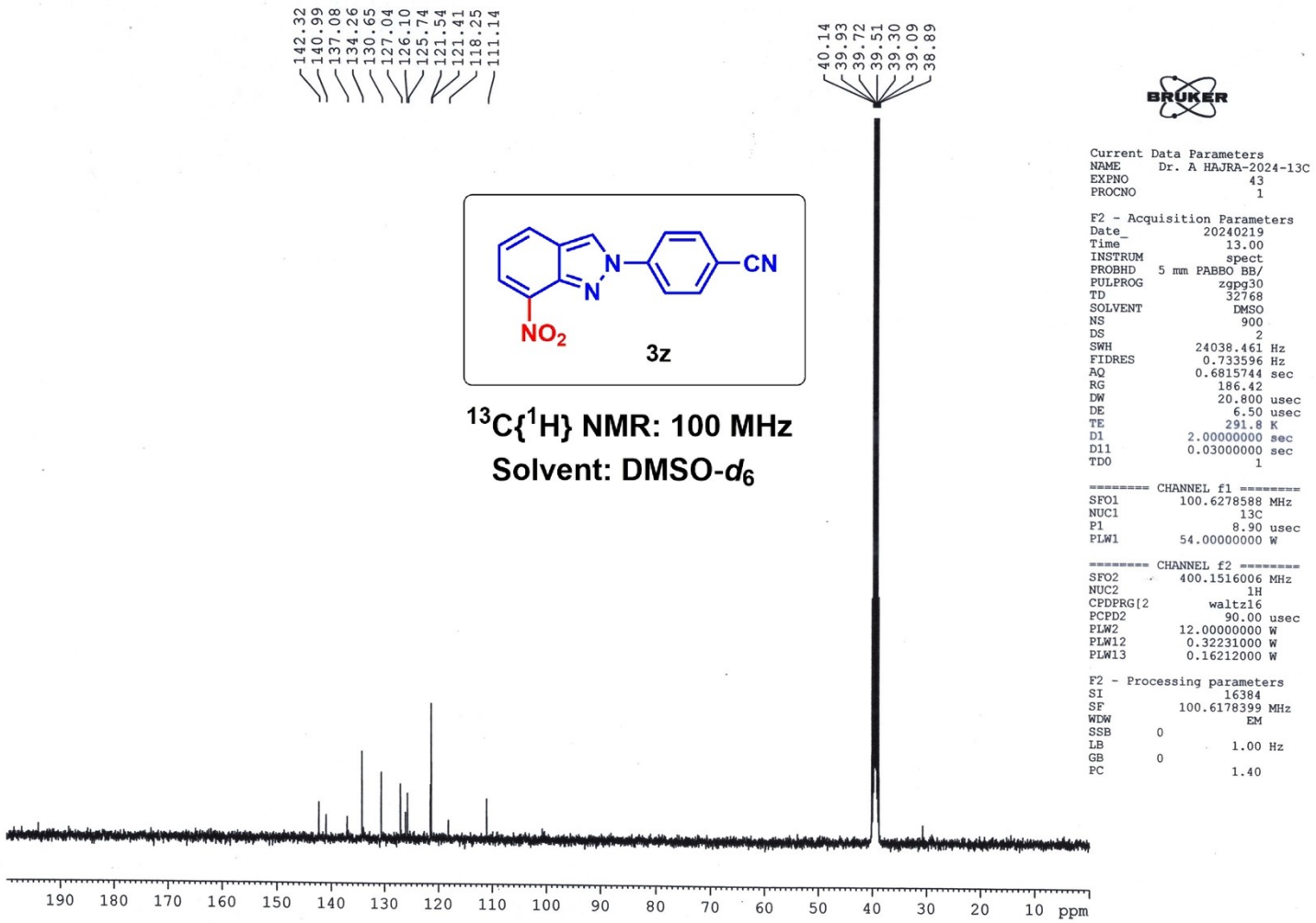



```
Current Data Parameters
NAME      Dr. A HAJRA 2024 1H
EXPNO                  125
PROCNO                   1

F2 - Acquisition Parameters
Date_             20240219
Time                 12.13
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
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                  291.5 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            400.1500021 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



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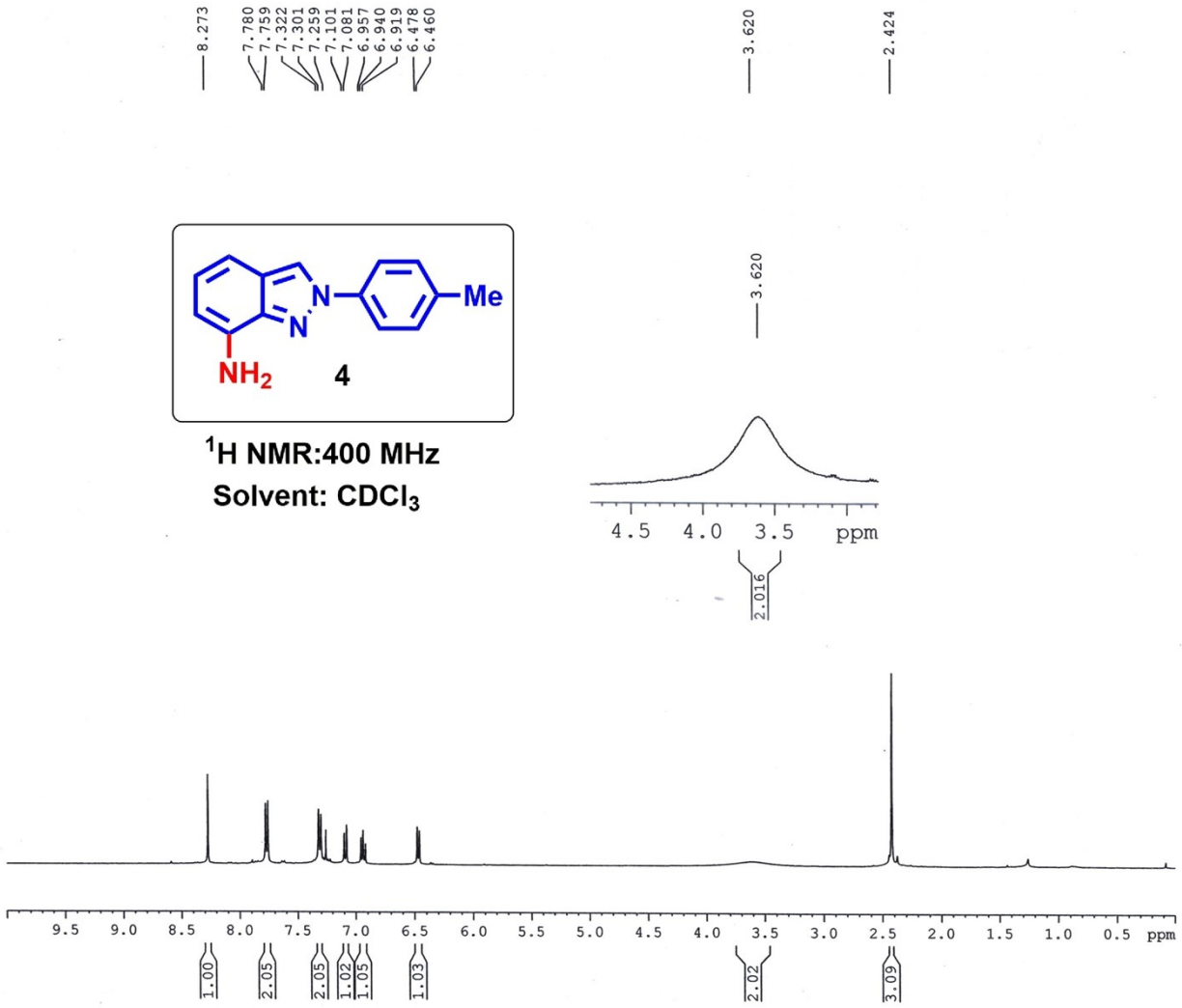
Current Data Parameters
NAME Dr. A HAJRA-2024-13C
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240219
Time 13.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 900
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 186.42
DW 20.800 usec
DE 6.50 usec
TE 291.8 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 100.6178399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

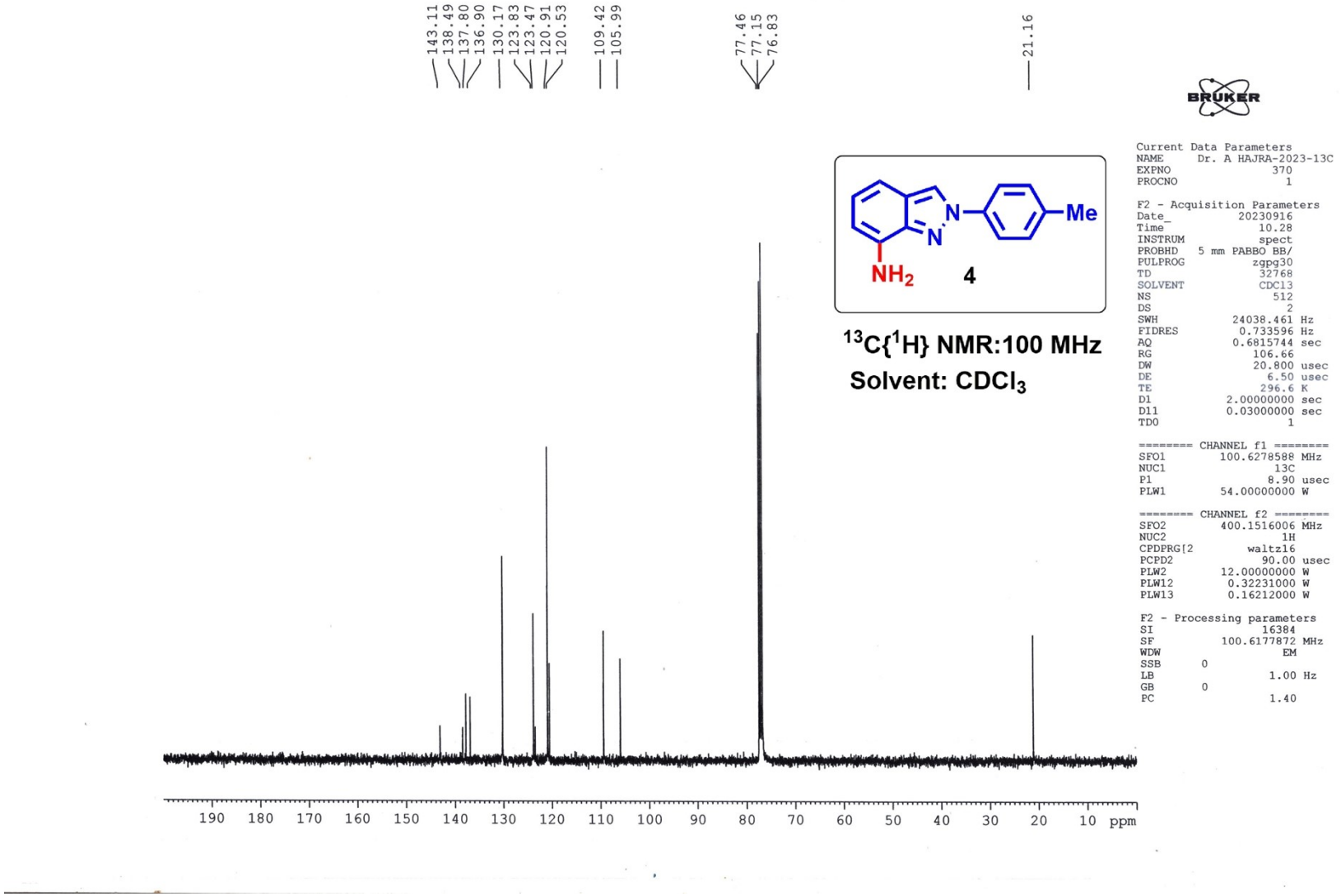



```
Current Data Parameters
NAME      Dr. A HAJRA 2024 1H
EXPNO                163
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240228
Time              19.29
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               292.6 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           400.1500097 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



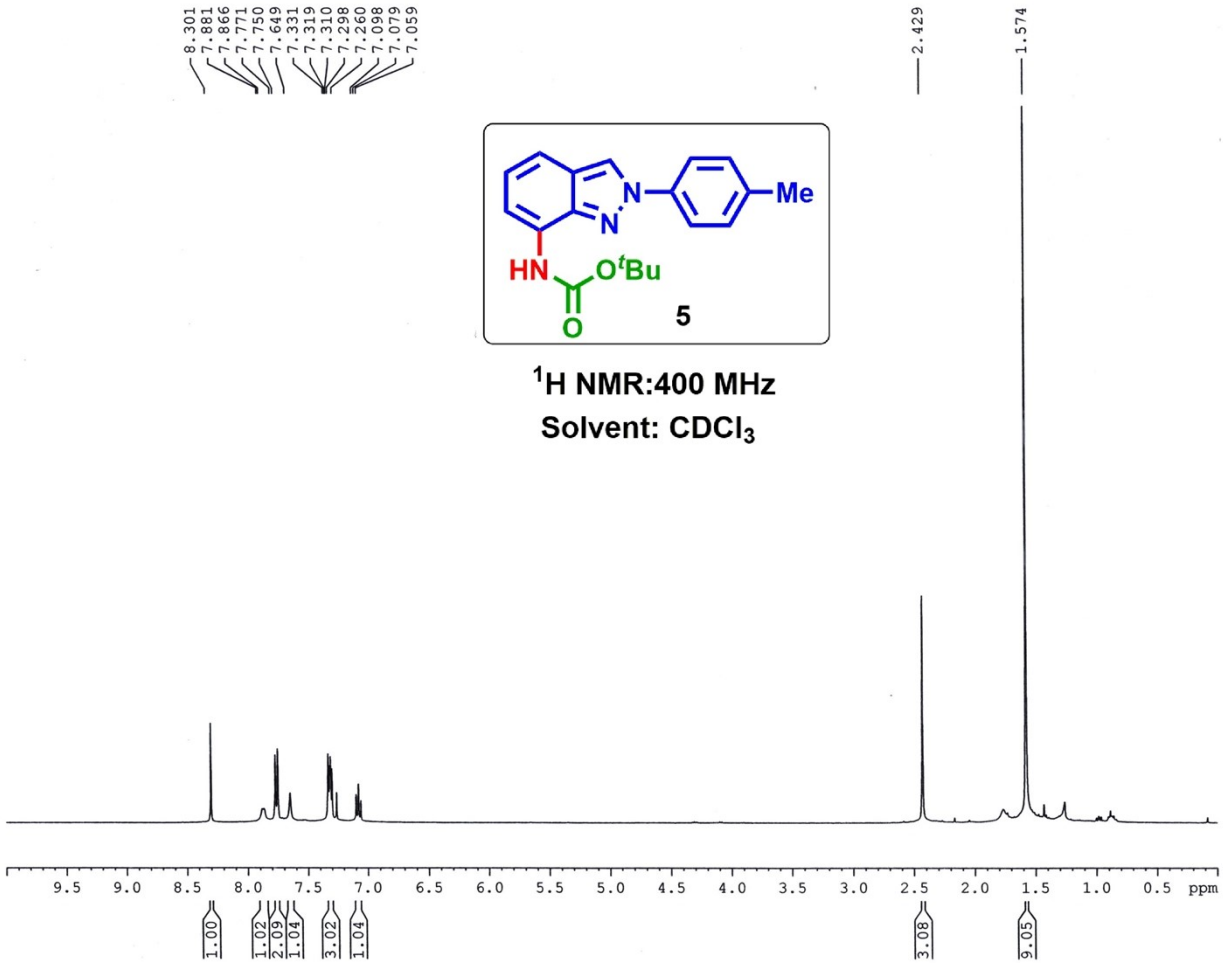

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  370
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230916
Time                 10.28
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     512
DS                       2
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                   106.66
DW                  20.800 usec
DE                   6.50 usec
TE                  296.6 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                   16384
SF            100.6177872 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

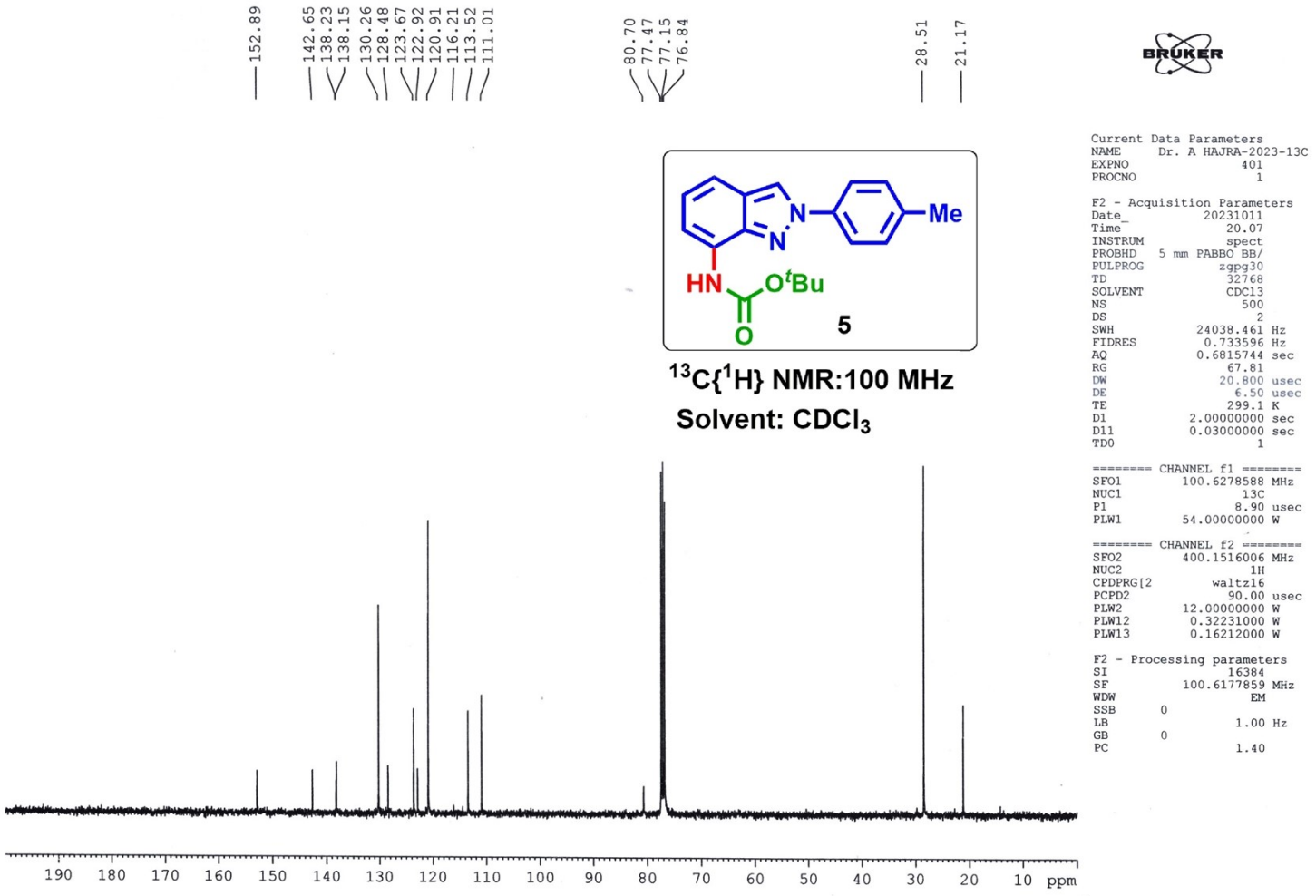



```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1171
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231011
Time              19.41
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                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           400.1500094 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



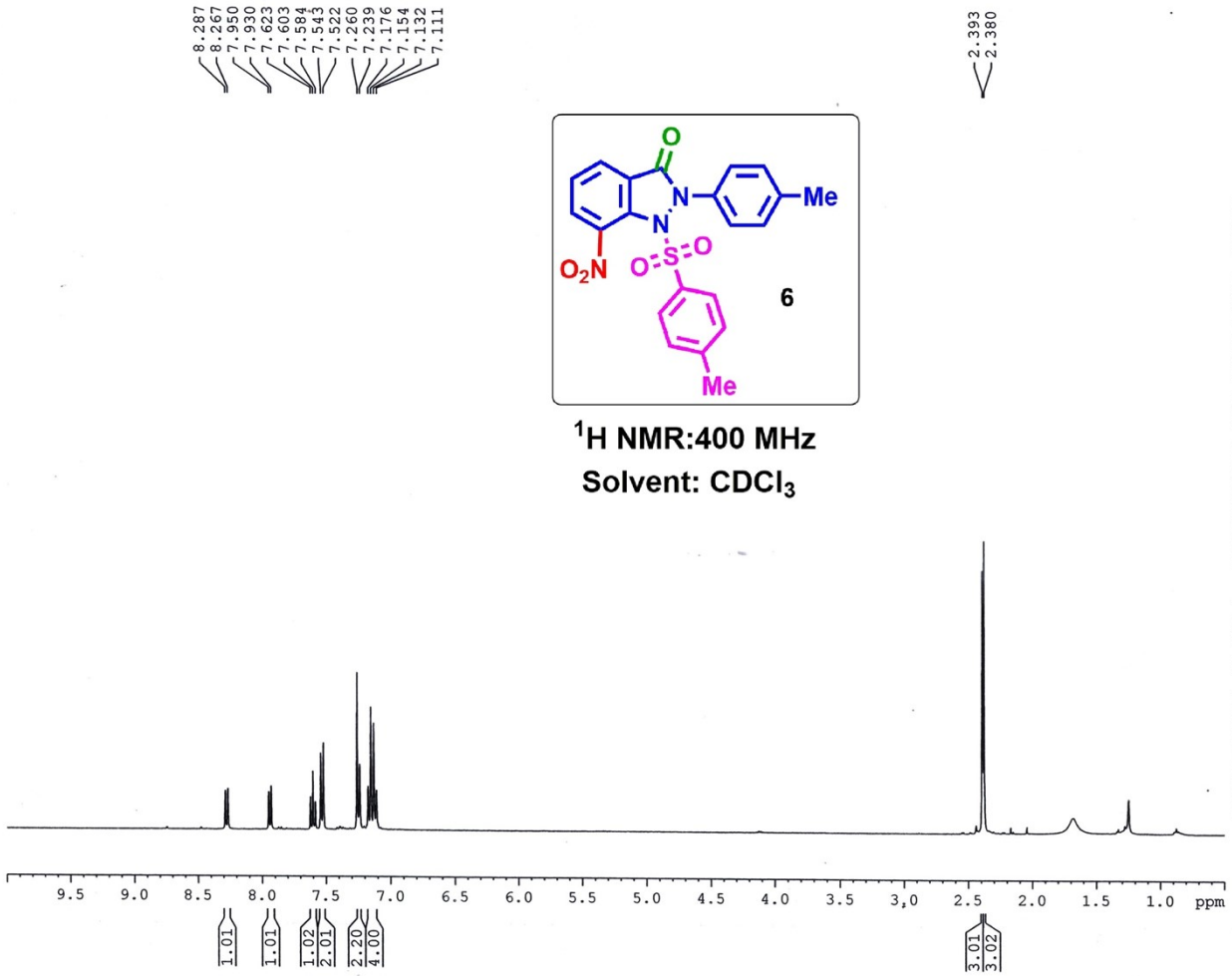

```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  401
PROCNO                   1

F2 - Acquisition Parameters
Date_           20231011
Time              20.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                 500
DS                   2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                67.81
DW               20.800 usec
DE                6.50 usec
TE               299.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

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

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

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

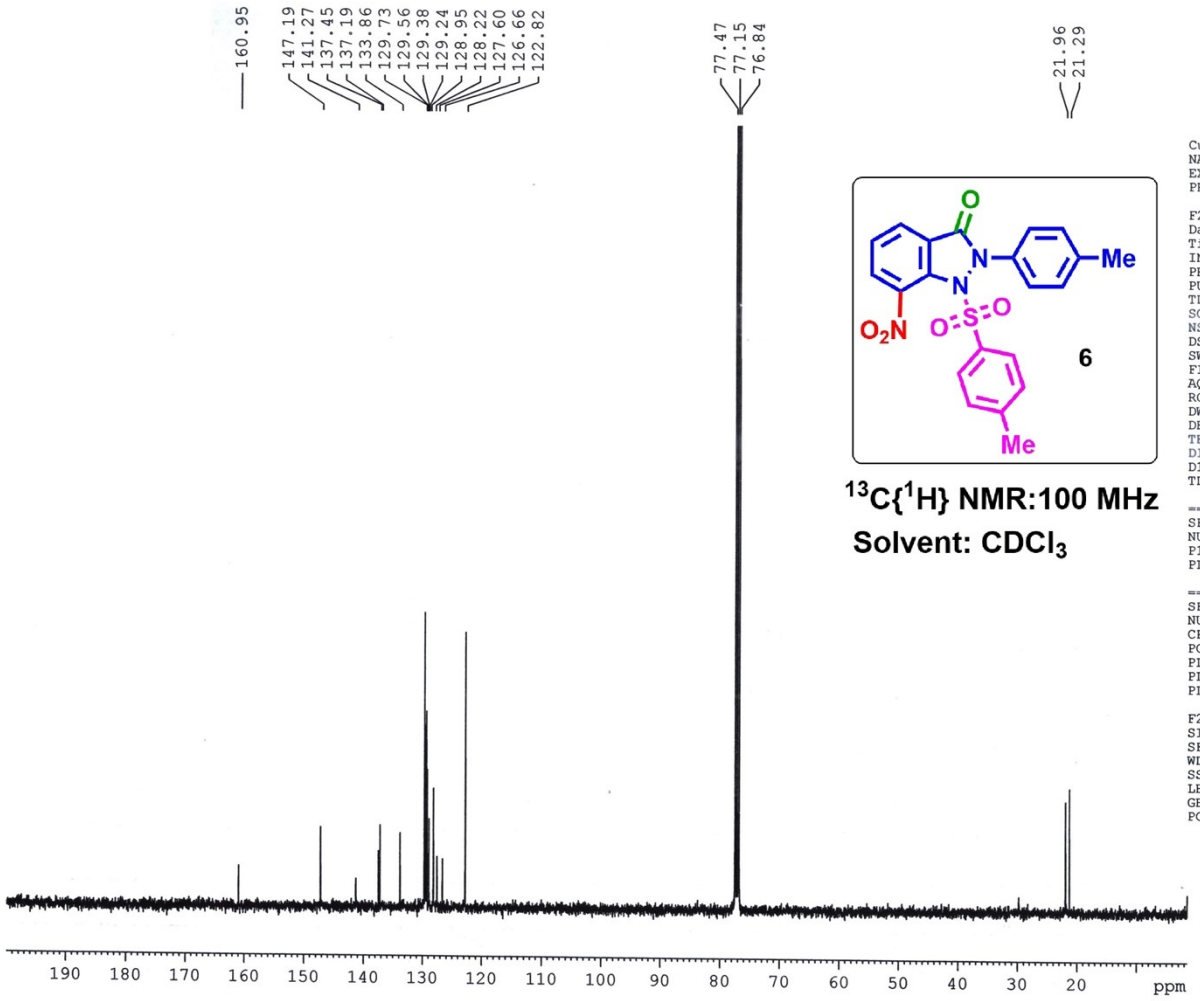



```
Current Data Parameters
NAME      Dr. A HAJRA 2023 1H
EXPNO               1133
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230925
Time              11.55
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              293.1 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          400.1500097 MHz
WDW                EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```



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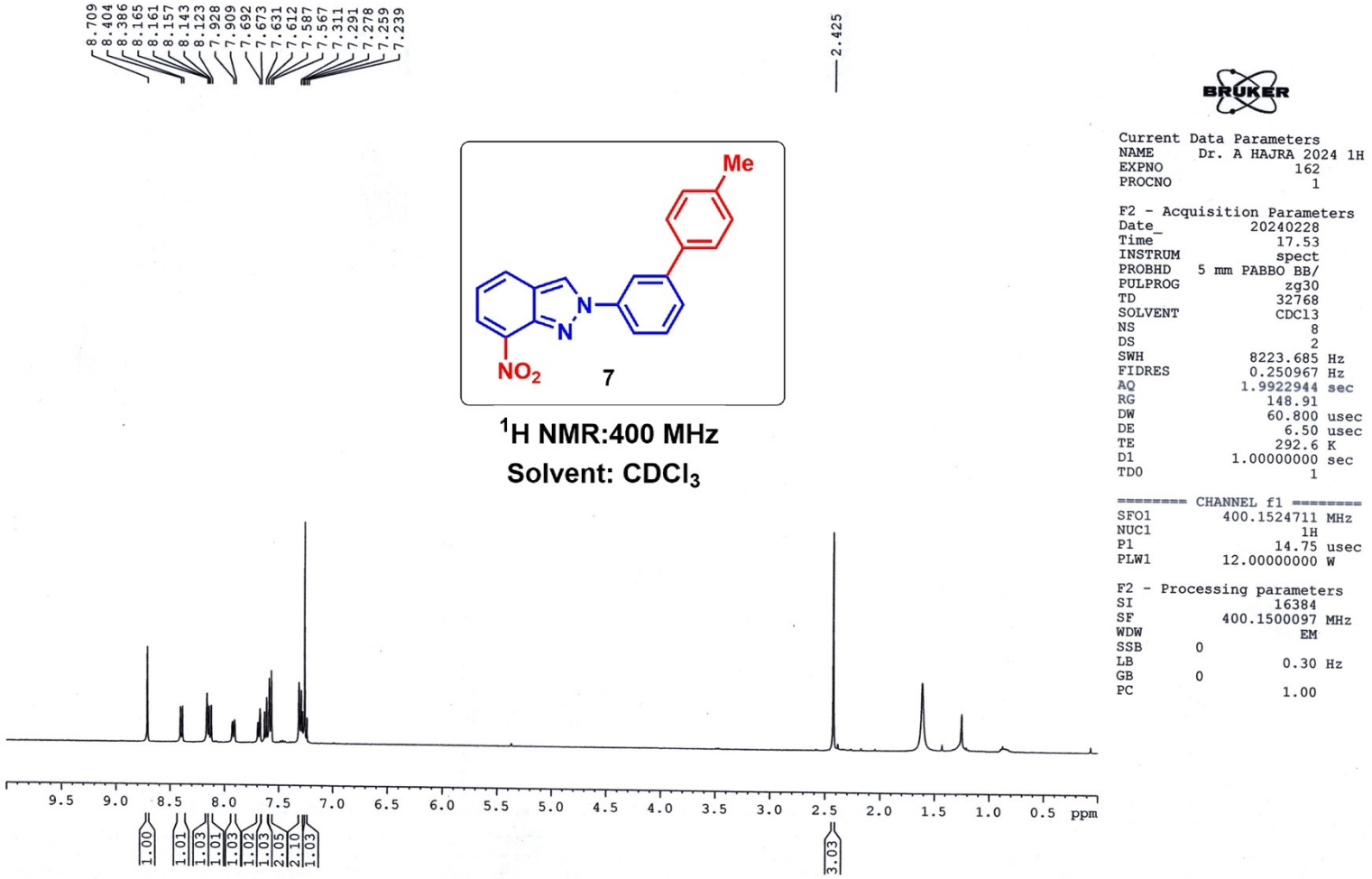
```
Current Data Parameters
NAME      Dr. A HAJRA-2023-13C
EXPNO                  387
PROCNO                   1

F2 - Acquisition Parameters
Date_              20230925
Time                  12.34
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      740
DS                        2
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                    186.42
DW                    20.800 usec
DE                     6.50 usec
TE                   294.4 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            100.6177859 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



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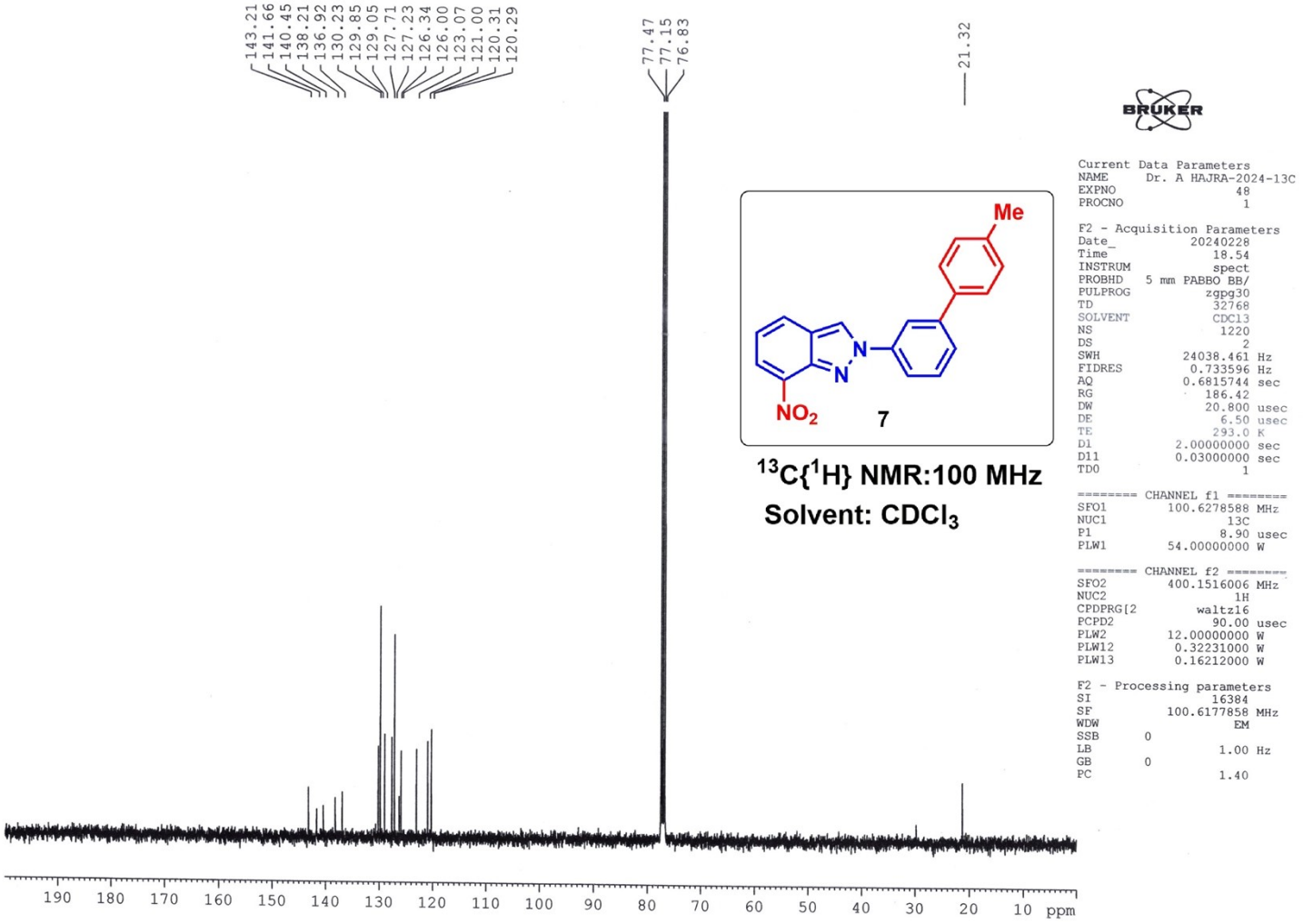
```
Current Data Parameters
NAME      Dr. A HAJRA 2024 1H
EXPNO                  162
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240228
Time              17.53
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              292.6 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          400.1500097 MHz
WDW                EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```




```
Current Data Parameters
NAME      Dr. A HAJRA-2024-13C
EXPNO                   48
PROCNO                   1

F2 - Acquisition Parameters
Date_               20240228
Time                   18.54
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     1220
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                  293.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

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

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

F2 - Processing parameters
SI                    16384
SF            100.6177858 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```