Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting information

Nitromethane as a Surrogate Cyanating Agent: 7-*N*,*N*-Dimethylamino-4-Hydroxycoumarin-Catalyzed, Metal-Free Synthesis of α-Iminonitriles

Iddum Satyanarayana,[a] Kiran B. Manjappa,[b]* and Ding-Yah Yang[a,b]*

[a]Department of Chemistry, Tunghai University

[b]Graduate Program for Biomedical and Materials Science, Tunghai University

No. 1727, Sec. 4, Taiwan Boulevard, Xitun District, Taichung 40704, Taiwan

Tel: 886-4-2359-7613; Fax: 886-4-2359-0426;

*Email: *kiran@thu.edu.tw*, *yang@thu.edu.tw*

Table of Contents

Instrumentation ……...…….……S3

X-ray crystallographic data of compounds **7k**, **9** and **11**.....S4-S9

General procedure A&B for the synthesis of α-Iminonitriles and procedure for the gram scale synthesis of compound **7k**……S10

Spectral data of compounds **7a–w**……S10-S16

Spectral data of compound **4c**…….……...…….S17

Spectral data of compound **11**…….S17

Procedure for the synthesis and spectral data of compounds **8** and **9**……..S17-S18

Spectral data of compounds **12** and **4a**……S18

Procedure for the synthesis and spectral data of compound **13**…….S18-S19

References……S20

^{1}H and ^{13}C NMR spectra for synthesized compounds…….……...……...S21-S82

Instrumentation: Melting points were determined on a Mel-Temp melting point apparatus in open capillaries and are uncorrected. Infrared (IR) spectra were recorded using 1725XFT-IR spectrophotometer. High-resolution mass spectra (HRMS) were obtained on a Thermo Fisher Scientific Finnigan MAT95XL spectrometer using a magnetic sector analyzer. ^{1}H NMR (400 MHz) and ^{13}C NMR (100) spectra were recorded on a Bruker 400 spectrometer. Chemical shifts were reported in parts per million on the scale relative to an internal standard (tetramethylsilane, or appropriate solvent peaks) with coupling constants given in hertz. ^{1}H NMR multiplicity data are denoted by s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). Analytical thin-layer chromatography (TLC) was carried out on Merck silica gel 60G-254 plates (25 mm) and developed with the solvents mentioned. Visualization was accomplished by using portable UV light, and iodine chamber. Flash chromatography was performed in columns of various diameters with Merck silica gel (230–400 mesh ASTM 9385 kieselgel 60H) by elution with the solvent systems. Solvents, unless otherwise specified, were reagent grade and distilled once before use. All new compounds exhibited satisfactory spectroscopic and analytical data.

X-ray crystallographic data of compound **7k** (CCDC-2023156)

Single crystal of **7k** was obtained by slow evaporation from dichloromethane and *n*-hexane at 25 ℃. Single-crystal X-ray data were collected at 150 K on a Bruker APEX-II CCD diffractometer using graphite-monochromated Mo KR radiation (λ = 0.71073A°). The crystal structures were solved by using SHELXS-97, and the structures were refined using SHELXL-97 2014. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were fixed at geometrically calculated positions and were refined using riding model.

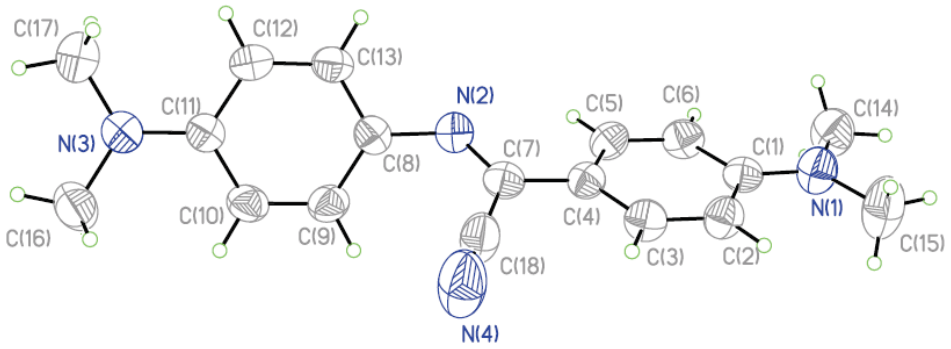


Figure S1: ORTEP diagram of compound **7k**. The ellipsoid contour probability levels: 50%

Table S1. Crystal data and structure refinement for **7k**.

Identification code	bmk4739	
Empirical formula	C18 H20 N4	
Formula weight	292.38	
Temperature	280(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.6739(15) Å	α = 105.074(5)°.
	b = 9.7128(14) Å	β = 113.757(4)°.
	c = 9.8240(13) Å	γ = 94.114(5)°.
Volume	799.3(2) $Å^3$	
Z	2	
Density (calculated)	1.215 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	312	
Crystal size	0.490 x 0.420 x 0.380 mm^3	

Theta range for data collection	2.889 to 25.000°.
Index ranges	-11<=h<=11, -11<=k<=11, -11<=l<=11
Reflections collected	19624
Independent reflections	2659 [R(int) = 0.0374]
Completeness to theta = 25.000°	94.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9281 and 0.8604
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2659 / 0 / 200
Goodness-of-fit on F^2	0.985
Final R indices [I>2sigma(I)]	R1 = 0.0774, wR2 = 0.2251
R indices (all data)	R1 = 0.1051, wR2 = 0.2633
Extinction coefficient	0.023(9)
Largest diff. peak and hole	0.286 and -0.240 e.$Å^{-3}$

X-ray crystallographic data of compound **9** (CCDC-2023155)

Single crystal of **9** was obtained by slow evaporation from dichloromethane and *n*-hexane at 25 ℃. Single-crystal X-ray data were collected at 150 K on a Bruker APEX-II CCD diffractometer using graphite-monochromated Mo KR radiation (λ = 0.71073A°). The crystal structures were solved by using SHELXS-97, and the structures were refined using SHELXL-97 2014. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were fixed at geometrically calculated positions and were refined using riding model.

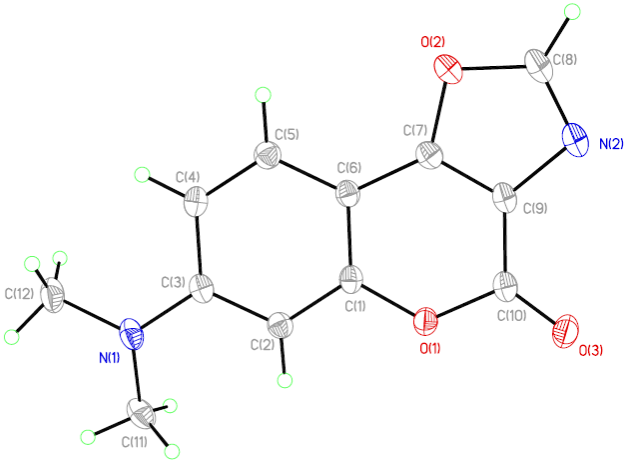


Figure S2: ORTEP diagram of compound **9**. The ellipsoid contour probability levels: 50%

Table S2. Crystal data and structure refinement for **9**.

Identification code	is204a	
Empirical formula	C12 H10 N2 O3	
Formula weight	230.22	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 7.7193(5) Å	α = 90°.
	b = 22.2405(17) Å	β = 90°.
	c = 5.8028(5) Å	γ = 90°.
Volume	996.23(13) $Å^3$	
Z	4	
Density (calculated)	1.535 Mg/m^3	
Absorption coefficient	0.113 mm^{-1}	
F(000)	480	

Crystal size	0.470 x 0.380 x 0.070 mm^3
Theta range for data collection	3.213 to 27.962°.
Index ranges	-10<=h<=10, -29<=k<=29, -7<=l<=7
Reflections collected	14325
Independent reflections	2328 [R(int) = 0.0185]
Completeness to theta = 25.242°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9281 and 0.8268
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2328 / 1 / 154
Goodness-of-fit on F^2	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0302, wR2 = 0.0893
R indices (all data)	R1 = 0.0311, wR2 = 0.0906
Absolute structure parameter	-0.18(19)
Extinction coefficient	n/a
Largest diff. peak and hole	0.259 and -0.205 $e.Å^{-3}$

X-ray crystallographic data of compound **11** (CCDC-2023154)

Single crystal of **11** was obtained by slow evaporation from CH_3CN and *n*-hexane at 25 ℃. Single-crystal X-ray data were collected at 150 K on a Bruker APEX-II CCD diffractometer using graphite-monochromated Mo KR radiation (λ = 0.71073A°). The crystal structures were solved by using SHELXS-97, and the structures were refined using SHELXL-97 2014. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were fixed at geometrically calculated positions and were refined using riding model.

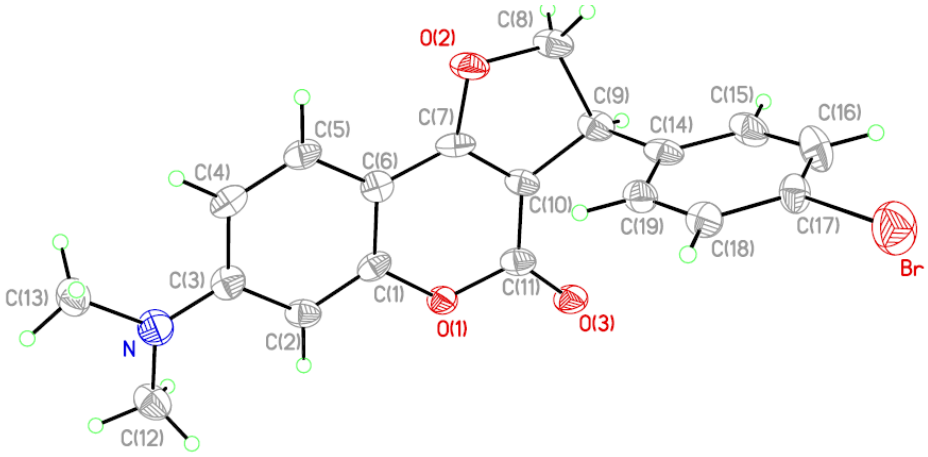


Figure S3: ORTEP diagram of compound **11**. The ellipsoid contour probability levels: 50%

Table S3. Crystal data and structure refinement for **11**.

Identification code	IS243	
Empirical formula	C19 H16 Br N O3	
Formula weight	386.24	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 15.431(2) Å	α = 90°.
	b = 13.4305(19) Å	β = 96.797(6)°.
	c = 7.9796(9) Å	γ = 90°.
Volume	1642.1(4) $Å^3$	
Z	4	
Density (calculated)	1.562 Mg/m^3	
Absorption coefficient	2.520 mm^{-1}	
F(000)	784	

Crystal size	0.560 x 0.270 x 0.050 mm^3
Theta range for data collection	2.985 to 28.072°.
Index ranges	-20<=h<=20, -17<=k<=17, -10<=l<=10
Reflections collected	25833
Independent reflections	3942 [R(int) = 0.1415]
Completeness to theta = 25.242°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.3506
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3942 / 0 / 217
Goodness-of-fit on F^2	1.136
Final R indices [I>2sigma(I)]	R1 = 0.0970, wR2 = 0.1802
R indices (all data)	R1 = 0.1667, wR2 = 0.2155
Extinction coefficient	n/a
Largest diff. peak and hole	1.090 and -0.720 $e.Å^{-3}$

General procedure A for the synthesis of compounds 7a–w.

To a stirred solution of amine **1** (1.0 mmol, 1.0 equiv.), aldehyde **2** (1.1 equiv.) and 7-*N*,*N*-dimethylamino-4-hydroxycoumarin (**3b**, 1.0 equiv.) in CH_3NO_2 (5 mL) was added DABCO (3.0 equiv.) at room temperature. The resulting mixture was heated at 80 □ in oil bath for 2 h. After completion of the reaction, the mixture was cooled to room temperature and was diluted with ethyl acetate (50 mL). The organic phase was washed with water (10 mL), brine (10 mL), dried over anhydrous $MgSO_4$, and evaporated under reduced pressure to provide the crude product. The crude product was purified by column chromatography to obtain the desired compound.

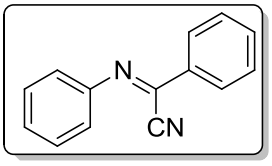
General procedure B for the synthesis of compounds 7a, 7c, 7k and 7l.

To a stirred solution of β-nitrostyrene derivative (1.0 mmol, 1.0 equiv.), amine (1.1 equiv.) and 7-*N*,*N*-dimethylamino-4-hydroxycoumarin (**3b**, 1.0 equiv.) in EtOH (5 mL) was added DABCO (3.0 equiv.) at room temperature. The resulting mixture was heated at 80 □ in oil bath for 0.5 h. After completion of the reaction, the reaction mixture was concentrated under reduced pressure. The crude product was simply passed through a small pad of a silica gel column chromatography to give the corresponding α-iminonitrile.

Procedure for the gram scale synthesis of compound 7k.

To a stirred solution of compound **8** (1.0 g, 5.2 mmol, 1.0 equiv.), amine **5** (779 mg, 5.72 mmol, 1.1 equiv.) and 7-*N*,*N*-dimethylamino-4-hydroxycoumarin (**3b**, 1.1 g, 5.2 mmol, 1.0 equiv.) in EtOH (20 mL) was added DABCO (1.75 g, 15.6 mmol, 3.0 equiv.) at room temperature. The resulting mixture was heated at 80 □ in oil bath for 1.5 h. After cooled down to room temperature, the reaction mixture was concentrated under reduced pressure, and the residue was purified through silica gel column chromatography using 10% EtOAc/hexanes to give the desired product **7k** in 72% yield (1.1 g) along with the catalyst **3b** in 17% yield (182 mg).

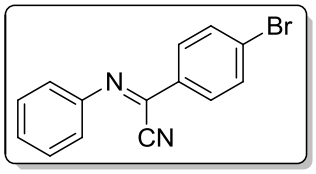
(*Z*)-*N*-Phenylbenzimidoyl cyanide (7a).[1]



Yellow solid (85 mg, 41% yield from general procedure A; 93 mg, 45% yield from general procedure B). R_f = 0.5 (10% EtOAc/hexanes). mp 74−76 ℃ (lit. 74−76 ℃). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, J = 7.6 Hz, 2H), 7.63−7.55 (m, 3H), 7.50 (t, J = 7.6 Hz, 2H), 7.35 (t, J = 7.6 Hz, 1H), 7.22 (d, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.1, 139.8, 133.6, 132.9, 129.3,

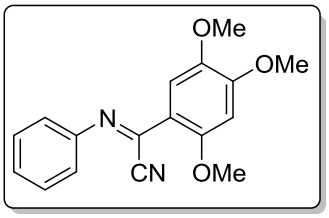
129.1, 128.3, 127.3, 120.3, 110.9. IR (neat) ν_{max}: 2218, 1601, 1588, 1568, 1475, 1452, 1188, 1003 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{14}H_{10}N_2$, 206.0844; found, 206.0837.

(*Z*)-4-Bromo-*N*-phenylbenzimidoyl cyanide (7b).[2]



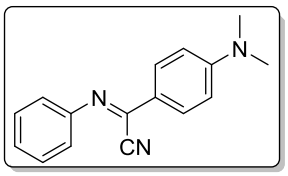
Yellow solid (155 mg, 54% yield). R_f = 0.6 (10% EtOAc/hexanes). mp 102−104 °C (lit. 103.8−104.7 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, J = 8.8 Hz, 2H), 7.71 (d, J = 8.8 Hz, 2H), 7.50 (t, J = 7.6 Hz, 2H), 7.38−7.34 (m, 1H), 7.23 (d, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.8, 138.6, 132.6, 132.4, 129.6, 129.4, 127.9, 127.7, 120.4, 110.7. IR (neat) ν_{max}: 2219, 1896, 1578, 1468, 848, 776, 688 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{14}H_9BrN_2$, 283.9949; found, 283.9953.

(*Z*)-2,4,5-Trimethoxy-*N*-phenylbenzimidoyl cyanide (7c).



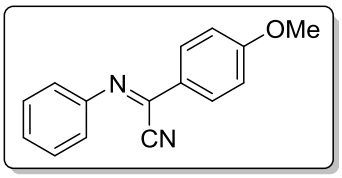
Orange solid (142 mg, 48% yield from general procedure A; 171 mg, 58% yield from general procedure B). R_f = 0.5 (20% EtOAc/hexanes). mp 72−74 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49−7.45 (m, 3H), 7.31−7.27 (m, 1H), 7.15− 7.13 (m, 2H), 6.59 (s, 1H), 4.00 (s, 3H), 3.99 (s, 3H), 3.94 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.8, 154.2, 149.5, 143.9, 137.2, 129.1, 126.4, 120.1, 115.3, 111.8, 111.2, 97.3, 56.9, 56.4, 56.2. IR (neat) ν_{max}: 2216, 1612, 1564, 1542, 1438, 1190, 1002 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{17}H_{16}N_2O_3$, 296.1161; found, 296.1164.

(*Z*)-4-(Dimethylamino)-*N*-phenylbenzimidoyl cyanide (7d).



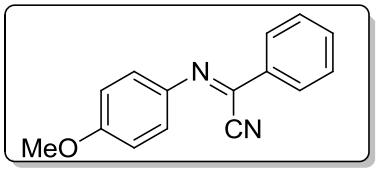
Orange solid (143 mg, 57% yield). R_f = 0.5 (10% EtOAc/hexanes). mp 104−106 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J = 9.2 Hz, 2H), 7.45 (t, J = 8.4 Hz, 2H), 7.30−7.25 (m, 1H), 7.16−7.14 (m, 2H), 6.76 (d, J = 9.2 Hz, 2H), 3.13 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.3, 150.1, 139.5, 130.0, 129.1, 126.1, 121.8, 120.5, 111.40, 111.35, 40.1. IR (neat) ν_{max}: 2212, 1612, 1568, 1448, 1112, 1058 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{16}H_{15}N_3$, 249.1266; found, 249.1272.

(*Z*)-4-Methoxy-*N*-phenylbenzimidoyl cyanide (7e).[2]



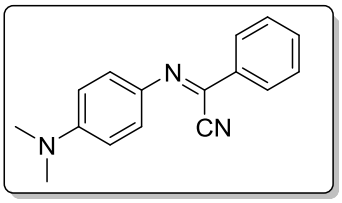
Yellow solid (130 mg, 55% yield). R_f = 0.4 (10% EtOAc/hexanes). mp 82−84 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (d, J = 9.2 Hz, 2H), 7.48 (t, J = 7.6 Hz, 2H), 7.34−7.30 (m, 1H), 7.19−7.17 (m, 2H), 7.05 (d, J = 9.2 Hz, 2H), 3.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.5, 149.4, 139.2, 132.4, 130.2, 129.2, 126.9, 122.2, 120.4, 114.5, 55.6. IR (neat) $_{vmax}$: 2963, 2845, 2219, 1602, 1556, 1489, 1447, 1108, 1026 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{15}H_{12}N_2O$, 236.0950; found, 236.0954.

(*Z*)-*N*-(4-Methoxyphenyl)benzimidoyl cyanide (7f).[1]



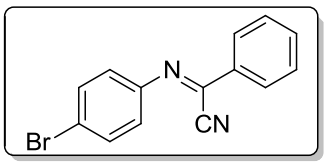
Yellow solid (123 mg, 52% yield). R_f = 0.6 (10% EtOAc/hexanes). mp 76−78 °C (lit. 78 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17−8.15 (m, 2H), 7.59−7.53 (m, 3H), 7.36 (d, J = 8.8 Hz, 2H), 7.03 (d, J = 8.8 Hz, 2H), 3.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 141.8, 136.9, 134.2, 132.4, 129.0, 127.9, 123.1, 114.5, 111.7, 55.5. IR (neat) $_{vmax}$: 2976, 2854, 2211, 1558, 1552, 1465, 1443, 1038 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{15}H_{12}N_2O$, 236.0950; found, 236.0946.

(*Z*)-*N*-(4-(Dimethylamino)phenyl)benzimidoyl cyanide (7g).



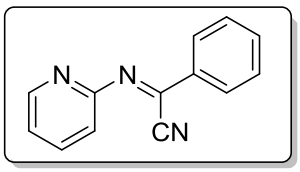
Orange solid (145 mg, 58% yield). R_f = 0.6 (10% EtOAc/hexanes). mp 106−108 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15−8.12 (m, 2H), 7.55−7.51 (m, 5H), 6.79 (d, J = 9.2 Hz, 2H), 3.08 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.8, 137.0, 135.1, 131.4, 131.3, 128.8, 127.4, 124.6, 113.0, 111.9, 40.3. IR (neat) $_{vmax}$: 2217, 1618, 1564, 1452, 1122, 1158 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{16}H_{15}N_3$, 249.1266; found, 249.1269.

(*Z*)-*N*-(4-Bromophenyl)benzimidoyl cyanide (7h).[3]



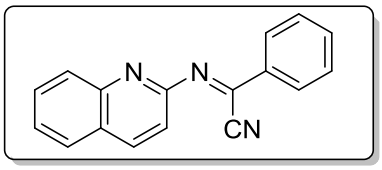
Yellow solid (166 mg, 58% yield). R_f = 0.5 (5% EtOAc/hexanes). mp 113−115 °C (lit. 115 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18−8.16 (m, 2H), 7.64−7.55 (m, 5H), 7.11 (d, J = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 140.3, 133.4, 133.2, 132.5, 129.1, 128.3, 122.1, 120.9, 110.7. IR (neat) $_{vmax}$: 2220, 1894, 1587, 1467, 836, 774, 682 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{14}H_9BrN_2$, 283.9949; found, 283.9952.

(*Z*)-*N*-(Pyridin-2-yl)benzimidoyl cyanide (7i).[4]



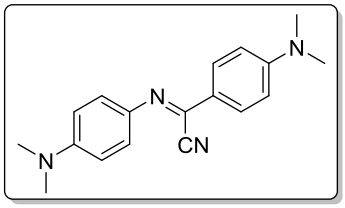
Orange solid (116 mg, 56% yield). R_f = 0.4 (10% EtOAc/hexanes). mp 62−64 °C (lit. 62−64 °C). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.64−8.62 (m, 1H), 8.27−8.24 (m, 2H), 7.89−7.84 (m, 1H), 7.67−7.62 (m, 1H), 7.59−7.55 (m, 2H), 7.32−7.28 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.2, 148.9, 141.2, 138.3, 133.7, 133.4, 129.1, 128.7, 123.0, 118.4, 111.5. IR (neat) ν_{max} : 2917, 2318, 1578, 1522, 1449, 1200, 778 cm^{-1}.

(*Z*)-*N*-(Isoquinolin-3-yl)benzimidoyl cyanide (7j).[4]



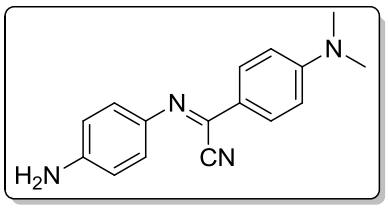
Orange solid (140 mg, 54% yield). R_f = 0.4 (10% EtOAc/hexanes). mp 76−78 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32−8.29 (m, 3H), 8.16 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.81−7.77 (m, 1H), 7.69−7.65 (m, 1H), 7.62−7.57 (m, 3H), 7.39 (d, J = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.8, 147.2, 142.1, 138.7, 133.56, 133.53, 130.4. 129.3, 129.1, 128.9, 127.6, 127.4, 126.8, 116.7, 111.4. IR (neat) ν_{max} : 2921, 2322, 1644, 1576, 1528, 1441, 1190, 788 cm^{-1}.

(*Z*)-4-(Dimethylamino)-*N*-(4-(dimethylamino)phenyl)benzimidoyl cyanide (7k).



Orange solid (217 mg, 74% yield from general procedure A; 240 mg, 82% yield from general procedure B). R_f = 0.5 (10% EtOAc/hexanes). mp 80−82 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, J = 8.8 Hz, 2H), 7.36 (d, J = 8.8 Hz, 2H), 6.79 (d, J = 8.8 Hz, 2H), 6.75 (d, J = 9.2 Hz, 2H), 3.10 (s, 6H), 3.04 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 149.8, 138.6, 133.8, 129.2, 123.4, 123.1, 112.9, 112.3, 111.5, 40.5, 40.1. IR (neat) ν_{max} : 2226, 1648, 1559, 1465, 1139, 1161 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{18}H_{20}N_4$, 292.1688; found, 292.1682.

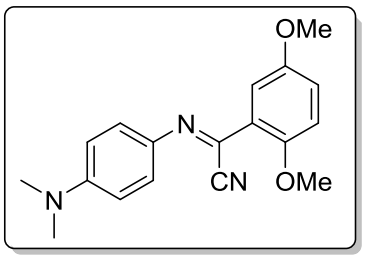
(*Z*)-*N*-(4-Aminophenyl)-4-(dimethylamino)benzimidoyl cyanide (7l).



Yellow solid (127 mg, 48% yield from general procedure A; 148 mg, 56% yield from general procedure B). R_f = 0.6 (30% EtOAc/hexanes). mp 100−102 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, J = 8.8 Hz, 2H), 7.19 (d, J = 8.8 Hz, 2H), 6.77−6.74 (m, 4H), 3.82 (s, 2H), 3.10 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.8, 145.7, 140.9, 135.6, 129.4, 123.1, 122.6, 115.3, 112.4, 111.4, 40.1. IR (neat) ν_{max} : 3427,

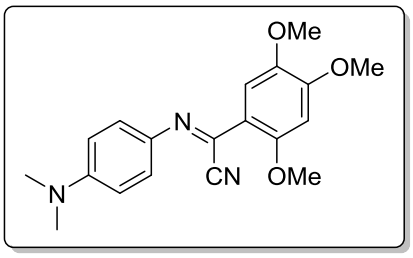
3357, 2221, 1619, 1558, 1449, 1001 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{16}H_{16}N_4$, 264.1375; found, 264.1382.

(*Z*)-*N*-(4-(Dimethylamino)phenyl)-2,5-dimethoxybenzimidoyl cyanide (7m).



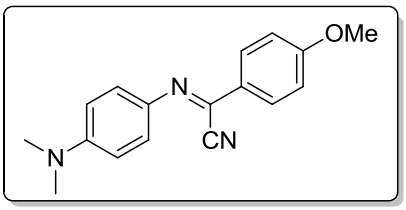
Orange solid (208 mg, 67% yield). R_f = 0.6 (20% EtOAc/hexanes). mp 92−94 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (d, J = 9.2 Hz, 2H), 7.37 (d, J = 3.2 Hz, 1H), 7.06−7.03 (m, 1H), 6.97 (d, J = 9.2 Hz, 1H), 6.78 (d, J = 9.2 Hz, 2H), 3.95 (s, 3H), 3.85 (s, 3H), 3.07 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 152.7, 150.6, 137.2. 130.1, 125.8, 124.4, 119.0, 113.9, 113.6, 111.9, 56.7, 55.9, 40.4. IR (neat) ν_{max}: 2217, 1648, 1572, 1468, 1432, 1114 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{18}H_{19}N_3O_2$, 309.1477; found, 309.1475.

(*Z*)-*N*-(4-(Dimethylamino)phenyl)-2,4,5-trimethoxybenzimidoyl cyanide (7n).



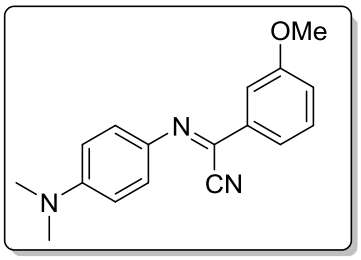
Orange solid (222 mg, 65% yield). R_f = 0.5 (30% EtOAc/hexanes). mp 78−80 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (s, 1H), 7.41 (d, J = 9.2 Hz, 2H), 6.78 (d, J = 8.8 Hz, 2H), 6.59 (s, 1H), 3.984 (s, 3H), 3.981 (s, 3H), 3.93 (s, 3H), 3.05 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9, 153.0, 150.1, 143.8, 137.7, 130.6, 123.8, 116.9, 113.6, 112.0, 111.4, 97.6, 57.0, 56.4, 56.2, 40.5. IR (neat) ν_{max}: 2211, 1624, 1568, 1478, 1432, 1070 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{19}H_{21}N_3O_3$, 339.1583; found, 339.1580.

(*Z*)-*N*-(4-(Dimethylamino)phenyl)-4-methoxybenzimidoyl cyanide (7o).



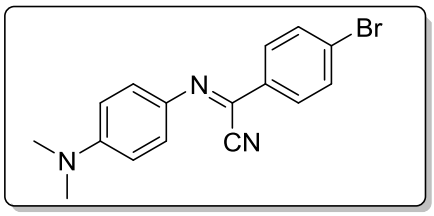
Yellow solid (190 mg, 68% yield). R_f = 0.4 (10% EtOAc/hexanes). mp 84−86 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (d, J = 8.8 Hz, 2H), 7.45 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.8 Hz, 2H), 6.79 (d, J = 8.8 Hz, 2H), 3.91 (s, 3H), 3.06 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.4, 150.4, 137.6, 132.0, 129.2, 128.0, 124.0, 114.2, 112.9, 112.1, 55.5, 40.4. IR (neat) ν_{max}: 2225, 1656, 1578, 1468, 1444, 1108 cm^{-1}. HRMS (EI) m/z: [M^+] calcd for $C_{17}H_{17}N_3O$, 279.1372; found, 279.1368.

(*Z*)-*N*-(4-(Dimethylamino)phenyl)-3-methoxybenzimidoyl cyanide (7p).



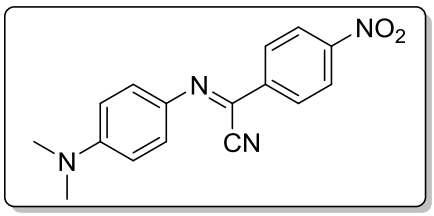
Yellow solid (179 mg, 64% yield). R_f = 0.5 (10% EtOAc/hexanes). mp 70−72 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72−7.68 (m, 2H), 7.54 (d, *J* = 9.2 Hz, 2H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.09−7.06 (m, 1H), 6.79 (d, *J* = 9.2 Hz, 2H), 3.92 (s, 3H), 3.08 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 150.8, 136.9, 136.5, 131.3, 129.8, 124.6, 120.4, 118.1, 113.0, 111.9, 111.2, 55.5, 40.3. IR (neat) $_{vmax}$: 2226, 1658, 1565, 1477, 1445, 1128 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{17}H_{17}N_3O$, 279.1372; found, 279.1367.

(*Z*)-4-Bromo-*N*-(4-(dimethylamino)phenyl)benzimidoyl cyanide (7q).



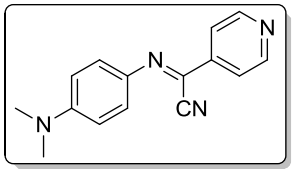
Yellow solid (220 mg, 67% yield). R_f = 0.5 (10% EtOAc/hexanes). mp 64−66 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.8 Hz, 2H), 7.64 (d, *J* = 8.8 Hz, 2H), 7.57 (d, *J* = 9.2 Hz, 2H), 6.78 (d, *J* = 9.2 Hz, 2H), 3.09 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.0, 136.6, 134.2, 132.0, 129.4, 128.6, 125.8, 125.0, 112.9, 111.8, 40.3. IR (neat) $_{vmax}$: 2209, 1678, 1564, 1455, 849, 764, 685 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{16}H_{14}BrN_3$, 327.0371; found, 327.0365.

(*Z*)-*N*-(4-(dimethylamino)phenyl)-4-nitrobenzimidoyl cyanide (7r).



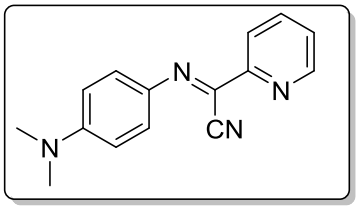
Yellow solid (171 mg, 58% yield). R_f = 0.7 (20% EtOAc/hexanes). mp 96−98 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, *J* = 9.2 Hz, 2H), 8.27 (d, *J* = 9.2 Hz, 2H), 7.74 (d, *J* = 9.2 Hz, 2H), 6.79 (d, *J* = 9.2 Hz, 2H), 3.14 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.9, 148.8, 141.0, 135.8, 127.6, 126.4, 125.6, 124.0, 113.3, 111.7, 40.2. IR (neat) $_{vmax}$: 3219, 2812, 2214, 1614, 1532, 1435, 1441, 989 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{16}H_{14}N_4O_2$, 294.1117; found, 294.1113.

(*Z*)-*N*-(4-(Dimethylamino)phenyl)isonicotinimidoyl cyanide (7s).



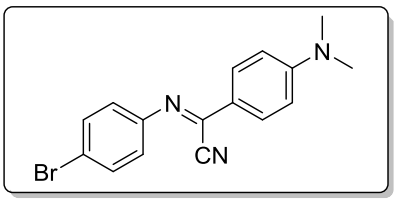
Yellow solid (156 mg, 62% yield). R_f = 0.5 (10% EtOAc/hexanes). mp 78−80 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, *J* = 6.0 Hz, 2H), 7.94 (d, *J* = 6.0 Hz, 2H), 7.73 (d, *J* = 9.2 Hz, 2H), 6.78 (d, *J* = 9.2 Hz, 2H), 3.12 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.9, 150.5, 142.4, 135.7, 126.4, 126.0, 120.5, 113.0, 111.7, 40.2. IR (neat) $_{vmax}$: 2921, 2322, 1642, 1521, 1454, 1202, 771 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{15}H_{14}N_4$, 250.1218; found, 250.1215.

(*Z*)-*N*-(4-(dimethylamino)phenyl)picolinimidoyl cyanide (7t).



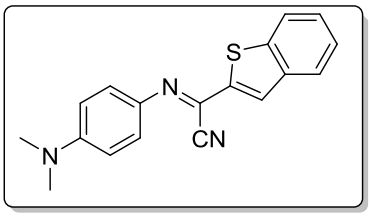
Yellow solid (136 mg, 54% yield). R_f = 0.6 (10% EtOAc/hexanes). mp 88−90 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79−8.77 (m, 1H), 8.24 (d, J = 8.0 Hz, 1H), 7.84−7.80 (m, 1H), 7.74 (d, J = 8.8 Hz, 2H), 7.40−7.37 (m, 1H), 6.78 (d, J = 8.8 Hz, 2H), 3.10 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.8, 151.5, 149.5, 136.6, 135.8, 130.3, 126.0, 124.8, 121.0, 113.6, 111.7, 40.3. IR (neat) ν_{max} : 2929, 2311, 1612, 1558, 1424, 1233, 769 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{15}H_{14}N_4$, 250.1218; found, 250.1215.

(*Z*)-*N*-(4-Bromophenyl)-4-(dimethylamino)benzimidoyl cyanide (7u).



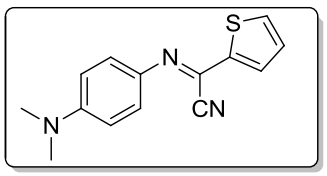
Orange solid (201 mg, 61% yield). R_f = 0.5 (10% EtOAc/hexanes). mp 59−61 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, J = 9.2 Hz, 2H), 7.56 (d, J = 8.8 Hz, 2H), 7.03 (d, J = 8.8 Hz, 2H), 6.75 (d, J = 9.2 Hz, 2H), 3.13 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.4, 149.0, 139.8, 132.2, 130.2, 122.4, 121.5, 119.5, 111.4, 111.2, 40.1. IR (neat) ν_{max} : 2219, 1658, 1528, 1477, 853, 761, 677 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{16}H_{14}BrN_3$, 327.0371; found, 327.0368.

(*E*)-*N*-(4-(Dimethylamino)phenyl)benzo[b]thiophene-2-carbimidoyl cyanide (7v).



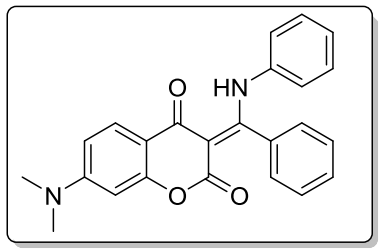
Orange solid (190 mg, 62% yield). R_f = 0.5 (30% EtOAc/hexanes). mp 114−116 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (s, 1H), 7.87−7.83 (m, 2H), 7.64 (d, J = 9.2 Hz, 2H), 7.44−7.41 (m, 2H), 6.77 (d, J = 9.2 Hz, 2H), 3.10 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 143.2, 141.0, 139.5, 136.1, 127.2, 126.6, 125.5, 125.0, 124.9, 124.5, 122.5, 112.6, 111.8, 40.3. IR (neat) ν_{max} : 2922, 2234, 1716, 1648, 1528, 1468, 1201 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{18}H_{15}N_3S$, 305.0987; found, 305.0984.

(*E*)-*N*-(4-(Dimethylamino)phenyl)thiophene-2-carbimidoyl cyanide (7w).



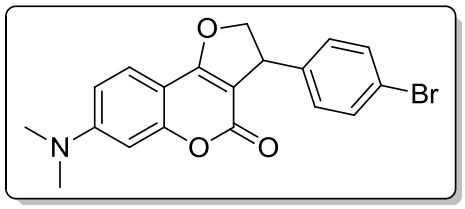
Orange solid (108 mg, 42% yield). R_f = 0.5 (20% EtOAc/hexanes). mp 103−105 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70−7.69 (m, 1H), 7.51 (t, J = 9.2 Hz, 3H), 7.17−7.15 (m, 1H), 6.76 (d, J = 9.2 Hz, 2H), 3.07 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 142.8, 136.45, 136.37, 130.5, 128.0, 125.4, 124.7, 112.5, 111.9, 40.3. IR (neat) ν_{max} : 2912, 2209, 1721, 1658, 1532, 1425 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{14}H_{13}N_3S$, 255.0830; found, 255.0828.

(*E*)-7-(Dimethylamino)-3-(phenyl(phenylamino)methylene)chromane-2,4-dione (4c).



Yellow solid (192 mg, 50% yield). R_f = 0.5 (20% EtOAc/hexanes). mp 216−218 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 15.7 (bs, 1H), 7.96 (d, J = 8.8 Hz, 1H), 7.38−7.36 (m, 2H), 7.27−7.25 (m, 2H), 7.18−7.11 (m 4H), 6.83 (d, J = 7.6 Hz, 2H), 6.63 (dd, J = 8.8, 2.4 Hz, 1H), 6.35 (d, J = 2.4 Hz, 1H), 3.10 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 182.2, 172.2, 162.0, 156.3, 154.9, 137.4, 133.7, 129.5, 128.8, 128.4, 127.7, 127.3, 126.5, 125.0, 109.3, 108.5, 97.2, 96.8, 40.2. IR (neat) ν_{max}: 1721, 1614, 1548, 1442, 1121, 899 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{24}H_{20}N_2O_3$, 384.1474; found, 384.1472.

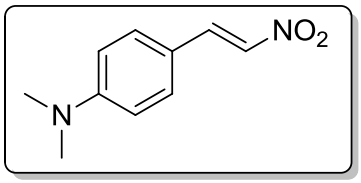
3-(4-Bromophenyl)-7-(dimethylamino)-2,3-dihydro-4*H*-furo[3,2-*c*]chromen-4-one (11).



Yellow solid (66 mg, 17% yield). R_f = 0.5 (20% EtOAc/hexanes). mp 222−224 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, J = 8.8 Hz, 1H), 7.46 (d, J = 8.4 Hz, 2H), 7.17 (d, J = 8.4 Hz, 2H), 6.67 (dd, J = 8.8, 2.4 Hz, 1H), 6.58 (d, J = 2.4 Hz, 1H), 5.12 (t, J = 9.2 Hz, 1H), 4.68−4.60 (m, 2H), 3.09 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 160.8, 157.6, 153.7, 140.7. 132.0, 129.0, 123.6, 121.2, 108.9, 101.0, 100.4, 98.1, 81.7, 45.1, 40.2. IR (neat) ν_{max}: 3442, 3814, 2938, 2844, 1616, 1224, 1158, 1119 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{19}H_{16}BrNO_3$, 385.0314; found, 385.0310.

Synthesis of (*E*)-*N*,*N*-dimethyl-4-(2-nitrovinyl)aniline (8).[6]

To a solution of 4-(*N*,*N*-dimethylamino)benzaldehyde (1.0 mmol, 1.0 equiv.) in nitromethane (10 mL) was refluxed for 0.5 h in oil bath. After completion of the reaction, the cooled reaction mixture was concentrated *in vacuo*. The crude residue was subjected to column chromatography to afford the desired β-nitrostyrene **8**.

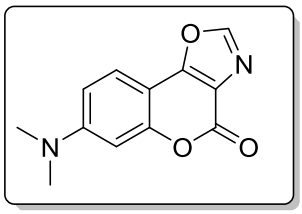


Orange solid (164 mg, 85% yield). R_f = 0.5 (10% EtOAc/hexanes). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (d, J = 13.2 Hz, 1H), 7.53 (d, J = 13.2 Hz, 1H), 7.45 (d, J = 9.2 Hz, 2H), 6.70 (d, J = 9.2 Hz, 2H), 3.10 (s, 6H).

Procedure for the synthesis of 7-(*N*,*N*-dimethylamino)-4*H*-chromeno[3,4-*d*]oxazol-4-one (9).

In a 25 mL round bottom flask, a mixture of 4-hydroxycoumarin **3b** (1.0 mmol, 1.0 equiv.) and DABCO (3.0 equiv.) in nitromethane (10 mL) was refluxed for 3 h in oil bath. After completion

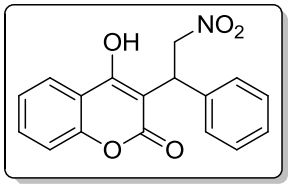
of the reaction, the cooled reaction mixture was concentrated *in vacuo*. The crude residue was subjected to column chromatography to afford the desired oxazole **9**.



Colorless solid (124 mg, 54% yield). R_f = 0.4 (50% EtOAc/hexanes). mp 202−204 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (s, 1H), 7.65 (d, J = 8.8 Hz, 1H), 6.74 (dd, J = 8.8, 2.4 Hz, 1H), 6.68 (d, J = 2.4 Hz, 1H), 3.11 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 156.8, 156.7, 155.5, 153.1, 150.1, 122.3, 120.0, 109.6, 99.9, 98.7, 40.2. IR (neat) $_{vmax}$: 2947, 2917, 1768, 1616, 1224, 1148, 1058 cm^{-1}. HRMS (EI) m/z: [M$^+$] calcd for $C_{12}H_{10}N_2O_3$, 230.0691; found, 230.0697.

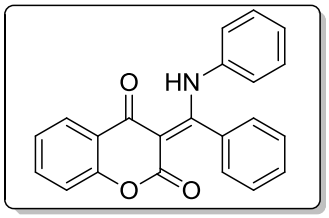
Synthesis of 4-Hydroxy-3-(2-nitro-1-phenylethyl)-2*H*-chromen-2-one (12).[7]

This compound **12** was prepared according to the literature procedure.



^{1}H NMR (400 MHz, DMSO-d_6): δ 8.07−8.04 (m, 1H), 7.66−7.62 (m, 1H), 7.42−7.33 (m, 4H), 7.32 (t, J = 7.2 Hz, 2H), 7.24 (t, J = 7.2 Hz, 2H), 5.45 (d, J = 8.0 Hz, 2H), 5.30 (t, J = 8.0 Hz, 1H).

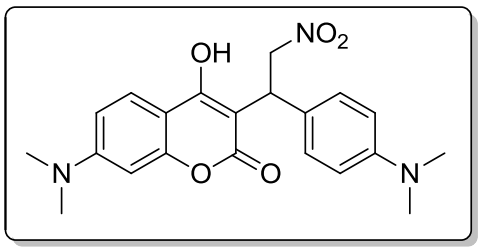
(*E*)-3-(Phenyl(phenylamino)methylene)chroman-2,4-dione (4a).[6]



Colorless solid (213 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 15.7 (s, 1H), 8.15 (d, J = 7.6 Hz, 1H), 7.60 (t, J = 6.8 Hz, 1H), 7.42−7.35 (m, 3H), 7.31 (d, J = 7.6 Hz, 1H), 7.27−7.22 (m, 3H), 7.20−7.16 (m, 3H), 6.87 (d, J = 6.8 Hz, 2H).

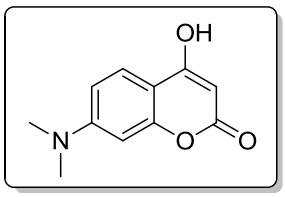
Synthesis of 7-(dimethylamino)-3-(1-(4-(dimethylamino)phenyl)-2-nitroethyl)-4-hydroxy-2*H*-chromen-2-one (13).

In a 25 mL round bottom flask, a mixture of 4-hydroxycoumarin **3b** (1.0 mmol, 1.0 equiv.) and *β*-nitrostyrene **8** (3.0 equiv.) in THF (10 mL) was stirred at 0 °C for 1 h. After that, the cooled reaction mixture was concentrated *in vacuo*. The crude residue was subjected to column chromatography to afford a mixture of **13** and **3b** with the ratio of 1:1.4 (a total of 53 mg).



Yield: 10% (38 mg). ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.81 (d, J = 9.2 Hz, 1H), 7.21 (d, J = 8.8 Hz, 2H), 6.74 (dd, J = 9.2, 2.4 Hz, 1H), 6.65 (d, J = 8.8 Hz, 2H), 6.50 (d, J = 2.4 Hz, 1H), 5.36, 5.30 (ABdq, J = 12.8, 8.0 Hz, 1H each), 5.07 (t, J = 8.0 Hz, 1H), 3.00 (s, 6H), 2.83 (s, 6H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 163.0, 162.9, 154.8, 153.4, 149.8, 128.55, 128.45, 127.6, 124.6, 112.9, 109.2, 104.4, 100.1, 97.4, 77.8, 40.7, 38.3.

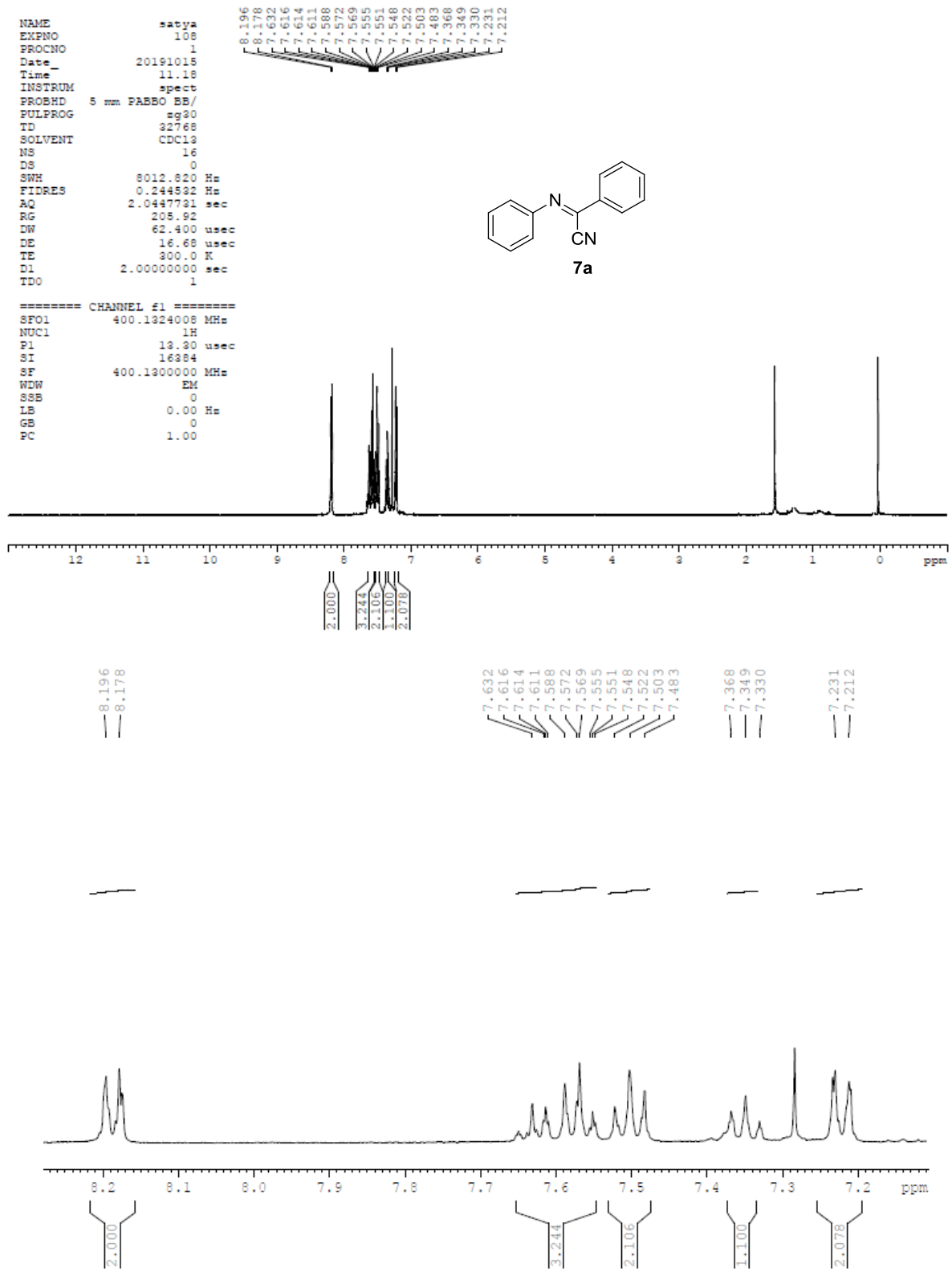
7-*N*,*N*-Dimethylamino-4-hydroxycoumarin (3b).

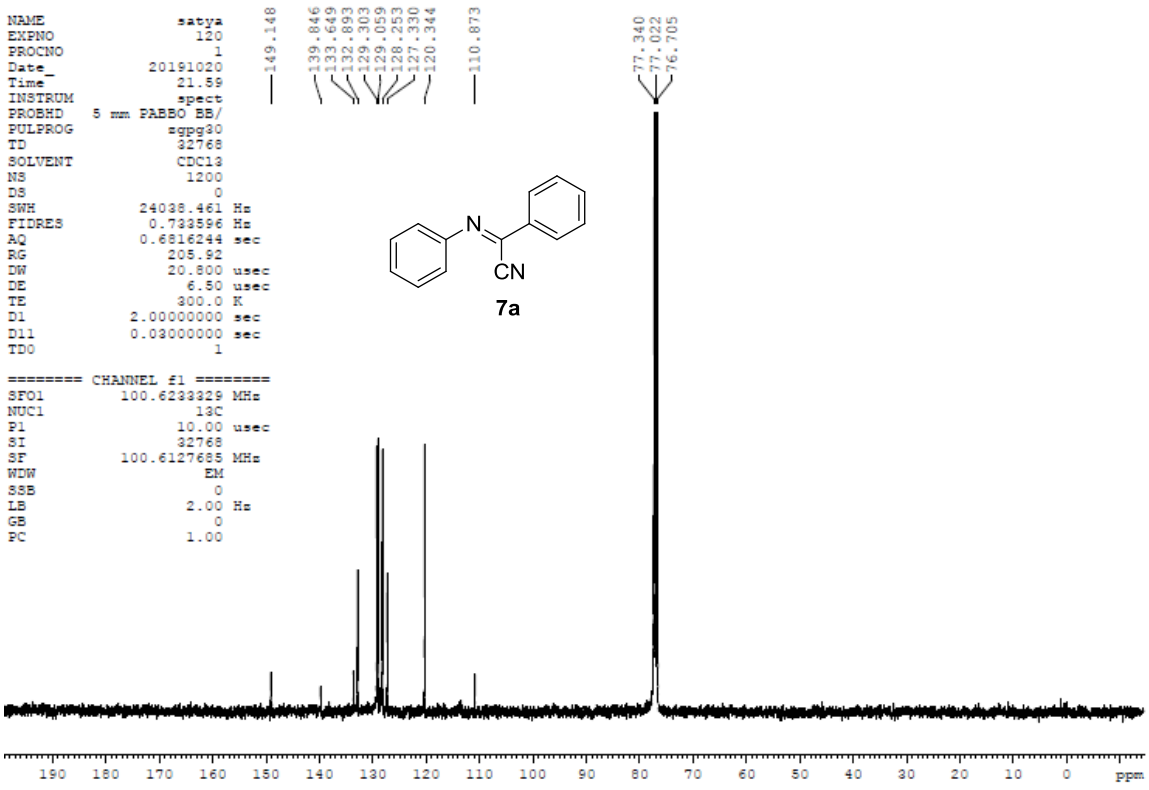


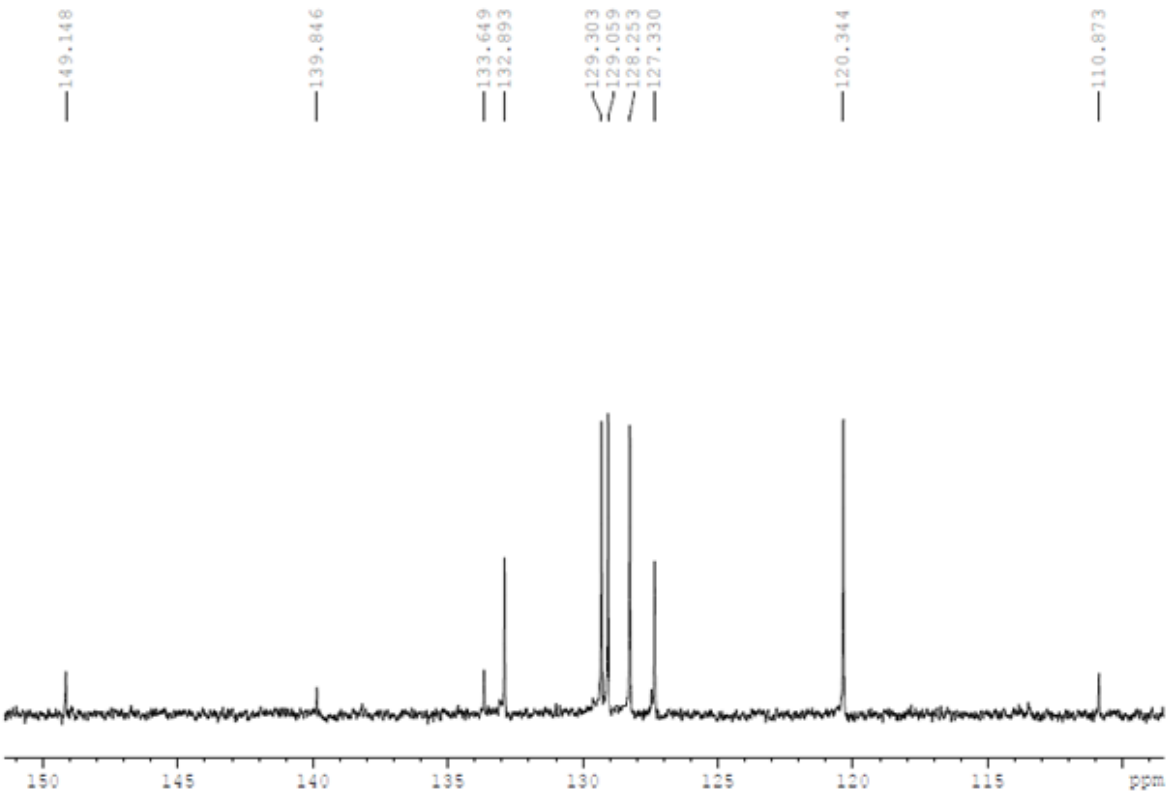
Violet solid (182 mg, 17% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.99 (s, 1H), 7.58 (d, J = 8.8 Hz, 1H), 6.71 (dd, J = 8.8, 2.8 Hz, 1H), 6.50 (d, J = 2.8 Hz, 1H), 5.28 (s, 1H), 3.01 (s, 6H).

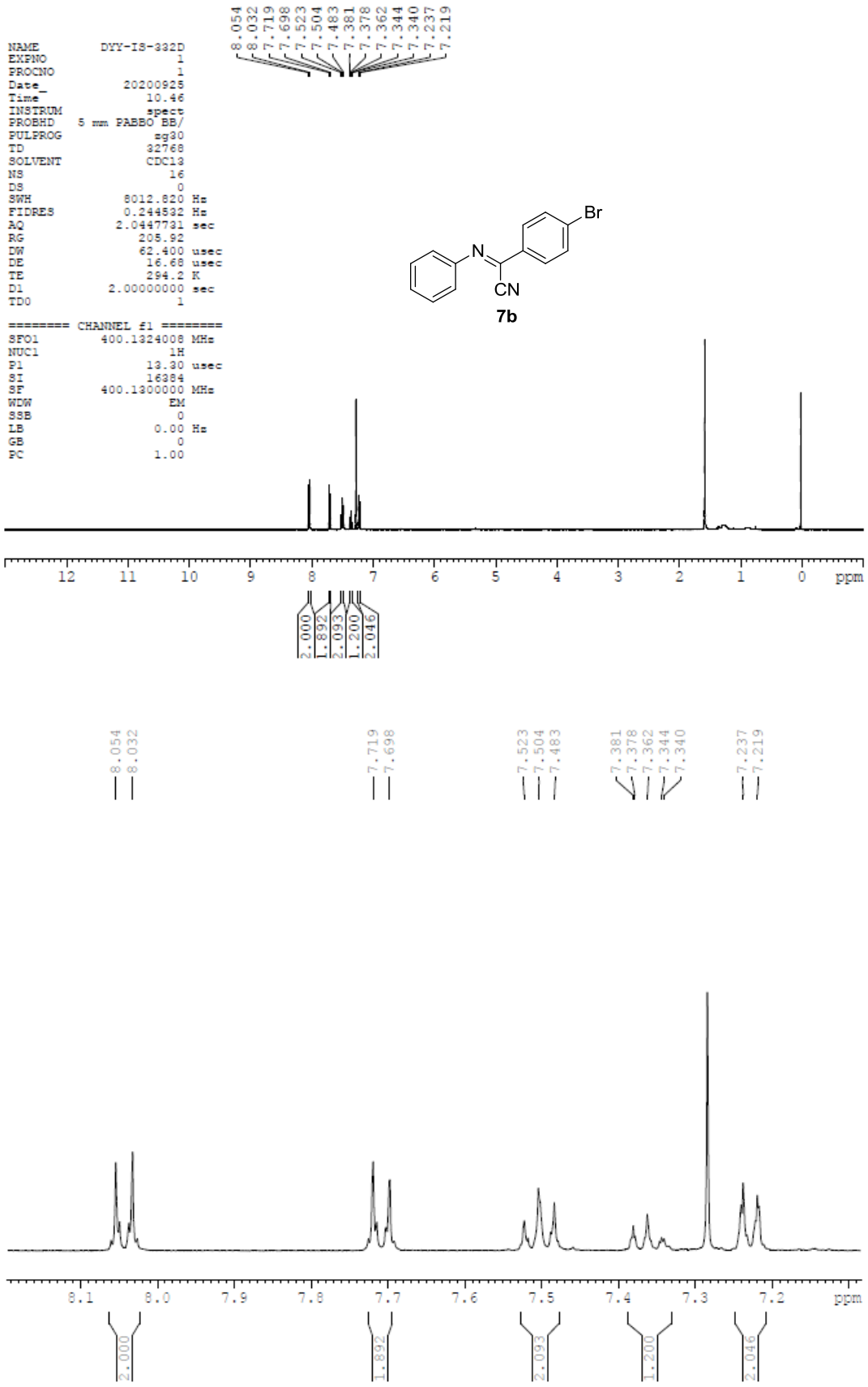
References

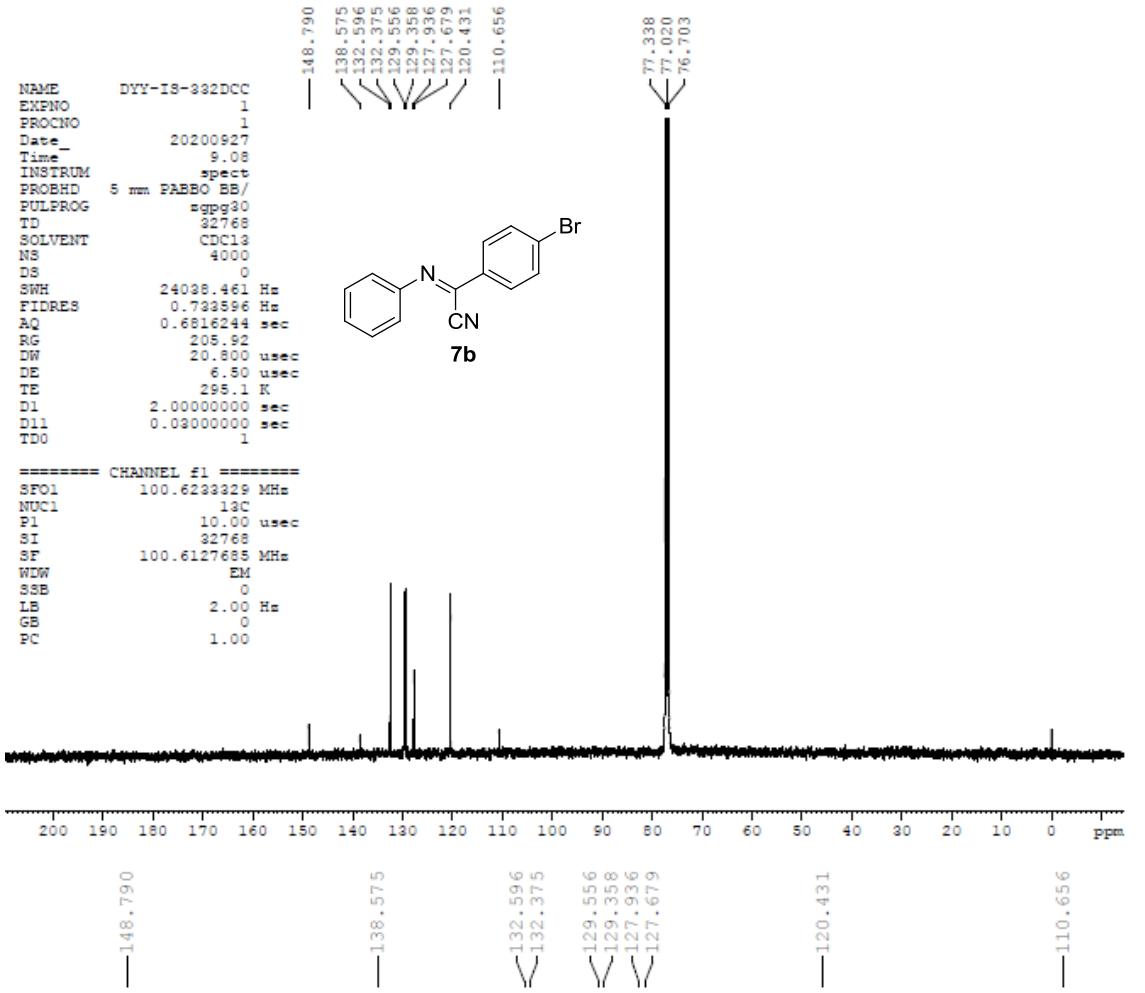
1. P. Fontaine, A. Chiaroni, G. Masson and J. Zhu, *Org. Lett*., 2008, **10**, 1509.
2. Y. Su, J. L. Petersen, T. L. Gregg and X. Shi, *Org. Lett.*, 2015, **17**, 1208.
3. X. You, X. Xie, R. Sun, H. Chen, S. Li and Y. Liu, *Org. Chem. Front*., 2014, **1**, 940.
4. Z. Chen, P. Liang, J. Zheng, Z. Zhou, X. Wen, T. Liu and M. Ye, *ACS Omega*, 2018, **3**, 12520.
5. A. Jarrahpour, P. Shrivani, V. Sinou, C. Latour and J. M. Brunel, *Med. Chem. Res.*, 2016, **25**, 149.
6. W. C. Hsieh, K. B. Manjappa and D. Y. Yang, *RSC Adv*., 2019, **9**, 34088.
7. D. K. Barange, V. Kavala, C. W. Kuo, P. M. Lei and C. F. Yao, *Tetrahedron*, 2011, **67**, 2870.

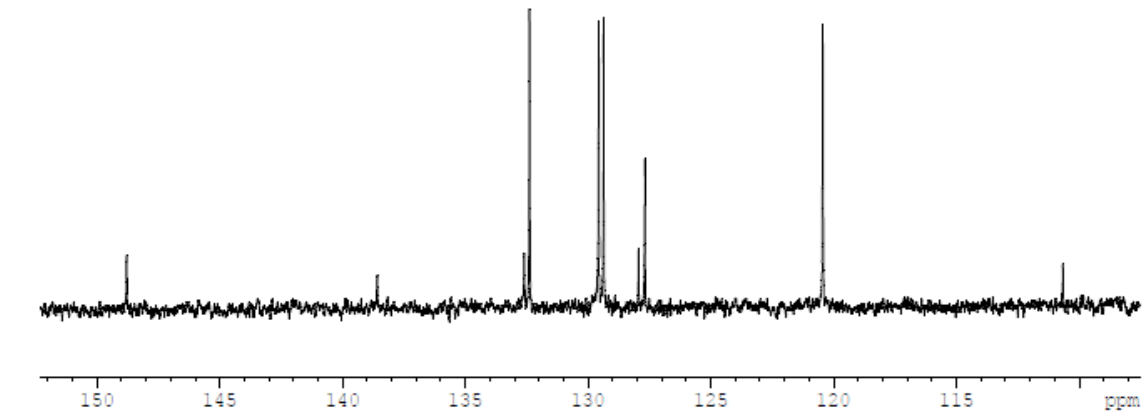

NAME satya
EXPNO 108
PROCNO 1
Date_ 20191015
Time_ 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.196 8.178 7.632 7.616 7.614 7.611 7.588 7.572 7.569 7.555 7.551 7.548 7.522 7.503 7.483 7.368 7.349 7.330 7.231 7.212
N
CN
7a
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.000 3.244 2.106 1.100 2.078
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm

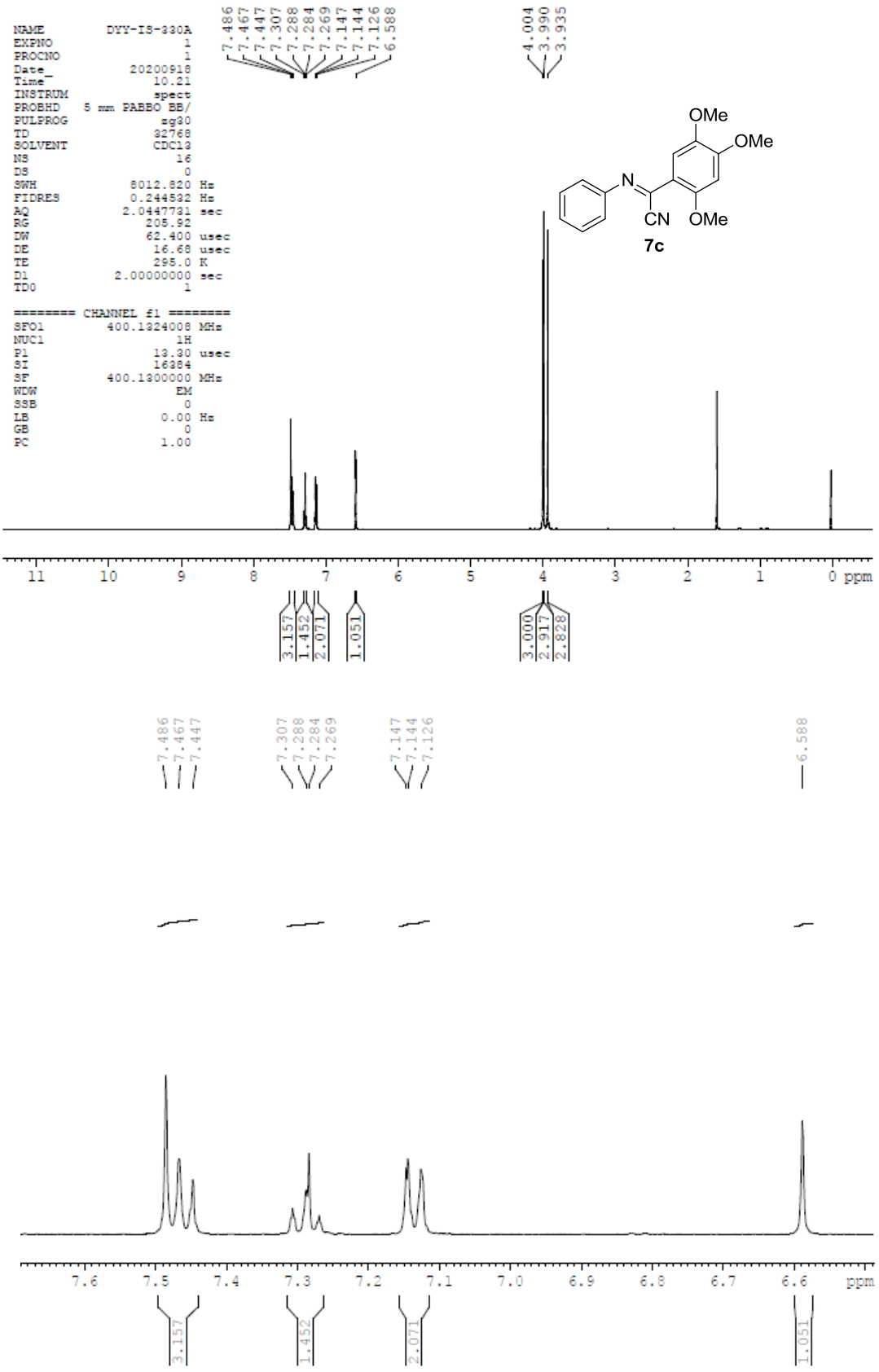

NAME satya
EXPNO 120
PROCNO 1
Date_ 20191020
Time 21.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
149.148
139.846
133.649
132.893
129.303
129.059
128.253
127.330
120.344
110.873
77.340
77.022
76.705
N
CN
7a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

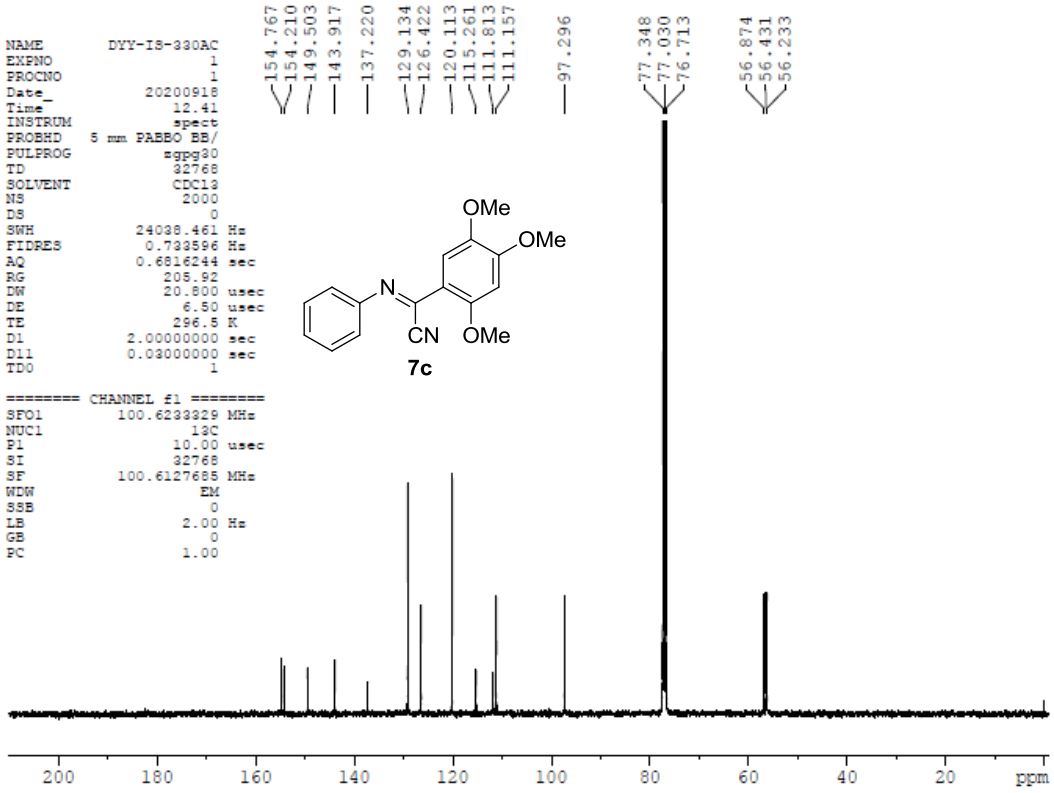

149.148
139.846
133.649
132.893
129.303
129.059
128.253
127.330
120.344
110.873
150 145 140 135 130 125 120 115 ppm

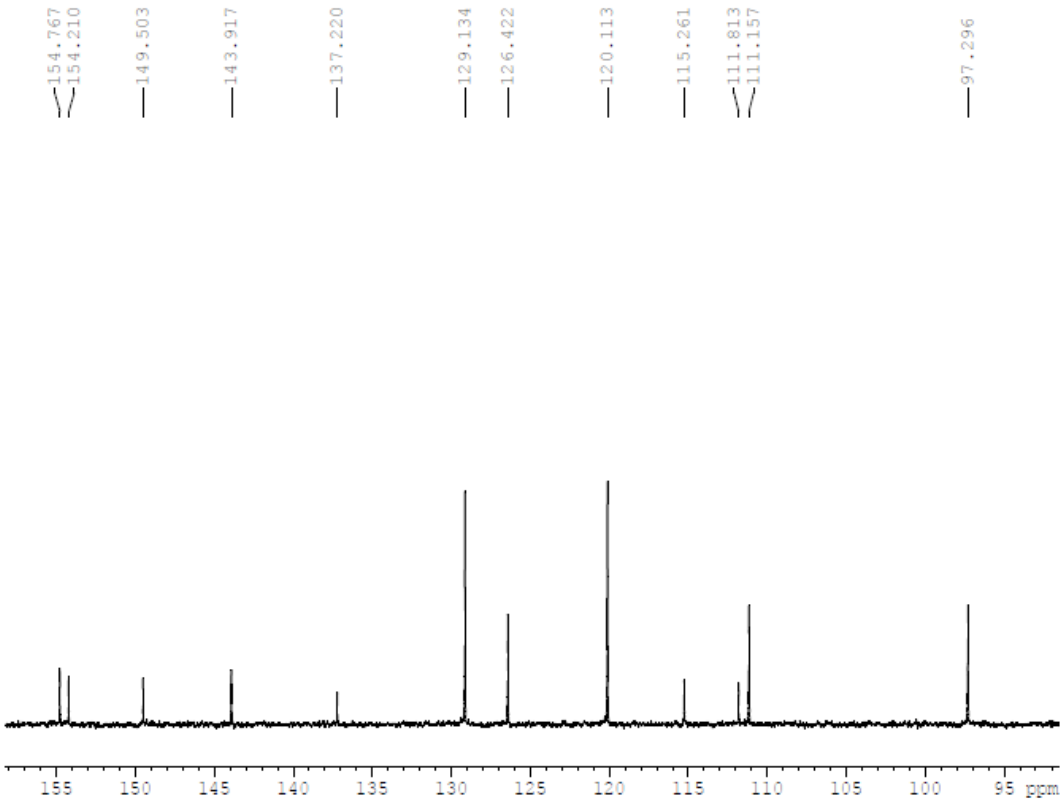

8.054
8.032
7.719
7.698
7.523
7.504
7.483
7.381
7.378
7.362
7.344
7.340
7.237
7.219
NAME DYY-IS-332D
EXPNO 1
PROCNO 1
Date_ 20200925
Time 10.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 294.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Br
N
CN
7b
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.000
1.892
2.093
1.200
2.046
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
2.000
1.892
2.093
1.200
2.046

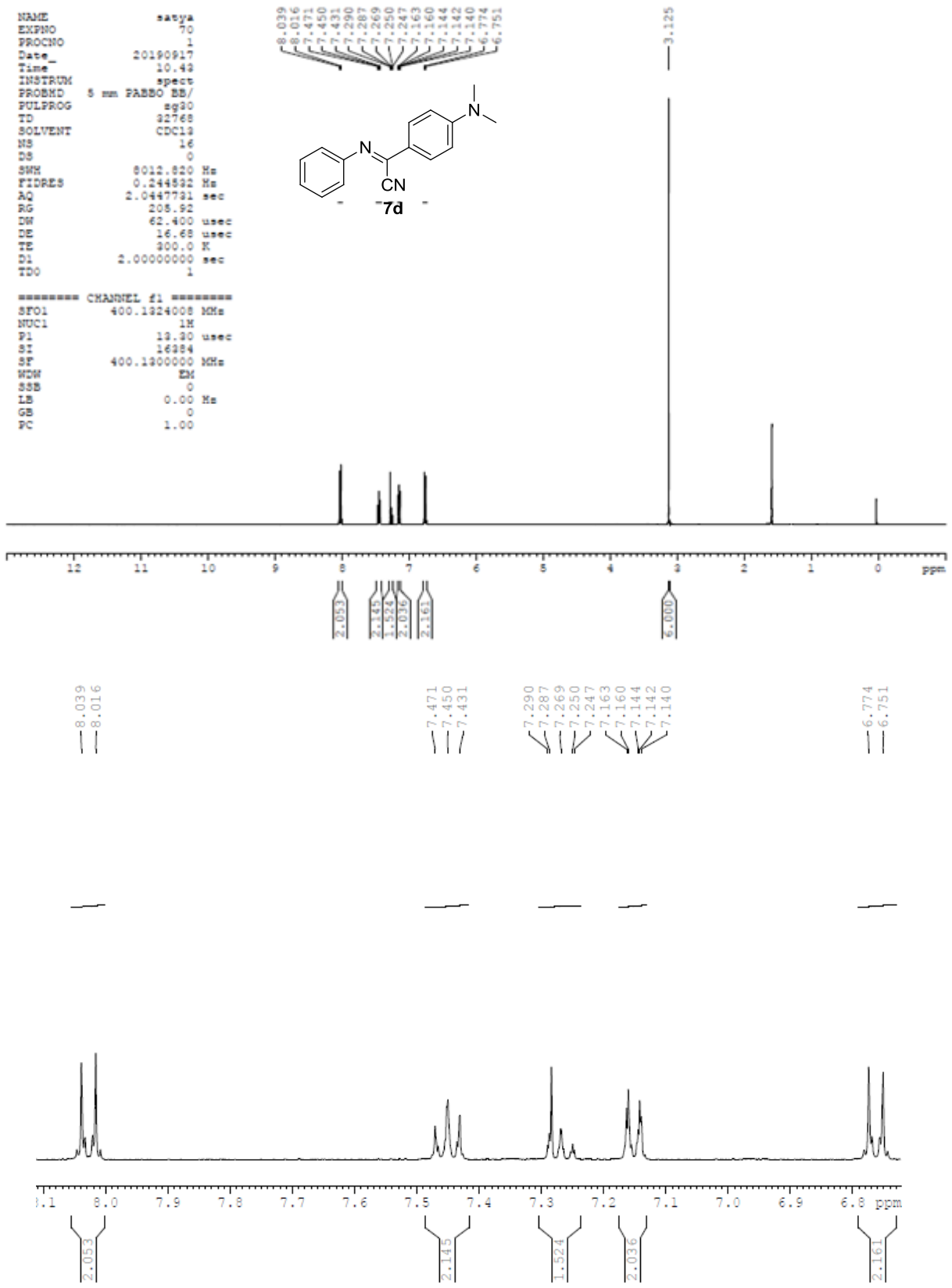

148.790
138.575
132.596
132.375
129.556
129.358
127.936
127.679
120.431
110.656
77.338
77.020
76.703
NAME DYY-IS-332DCC
EXPNO 1
PROCNO 1
Date_ 20200927
Time_ 9.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
Br
N
CN
7b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

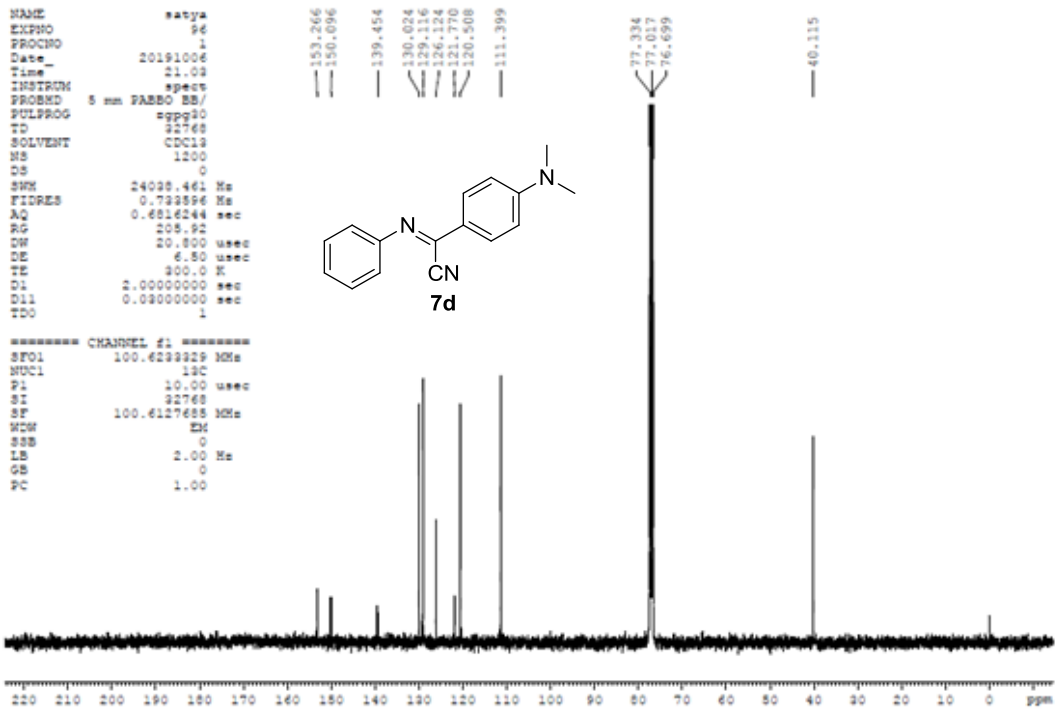

150 145 140 135 130 125 120 115 ppm

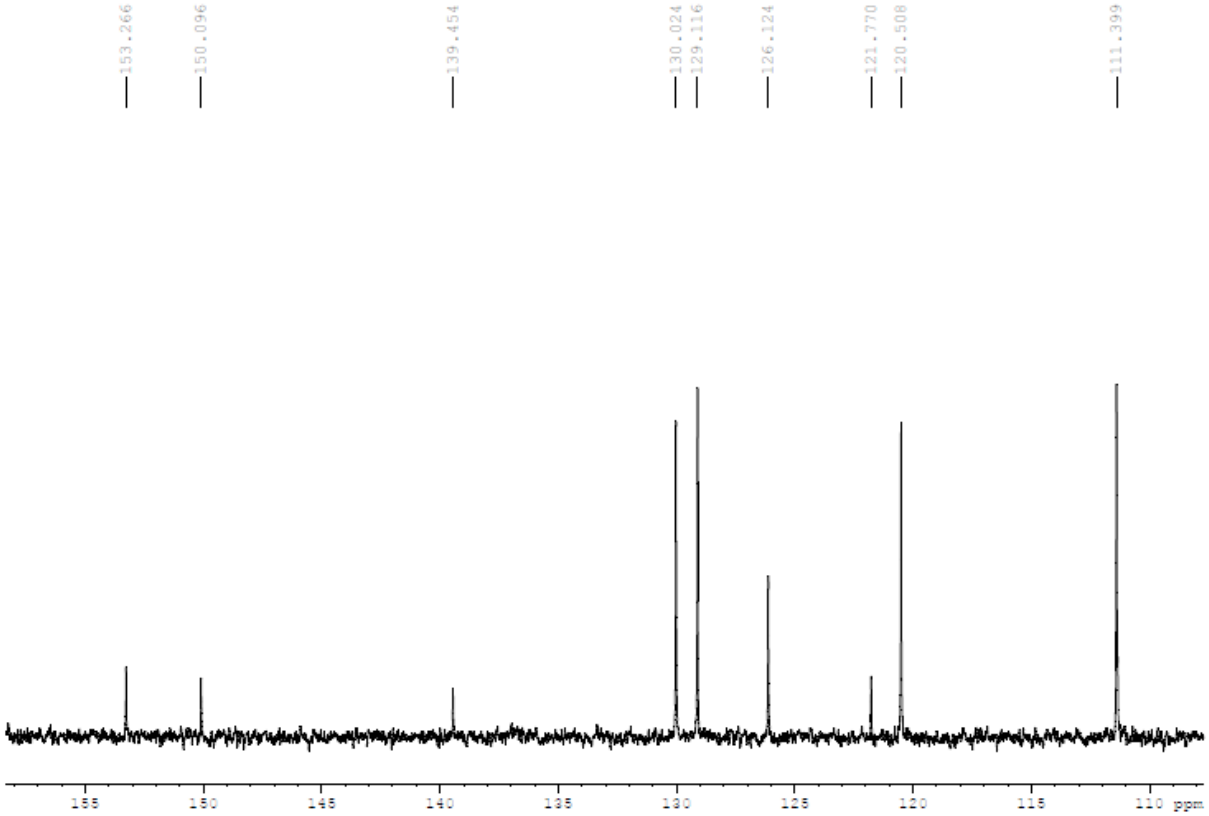

NAME DYY-IS-330A
EXPNO 1
PROCNO 1
Date_ 20200918
Time 10.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.486
7.467
7.447
7.307
7.288
7.284
7.269
7.147
7.144
7.126
6.588
4.004
3.990
3.935
OMe
OMe
N
CN
OMe
7c
11
10
9
8
7
6
5
4
3
2
1
0 ppm
3.157
1.452
2.071
1.051
3.000
2.917
2.828
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
ppm

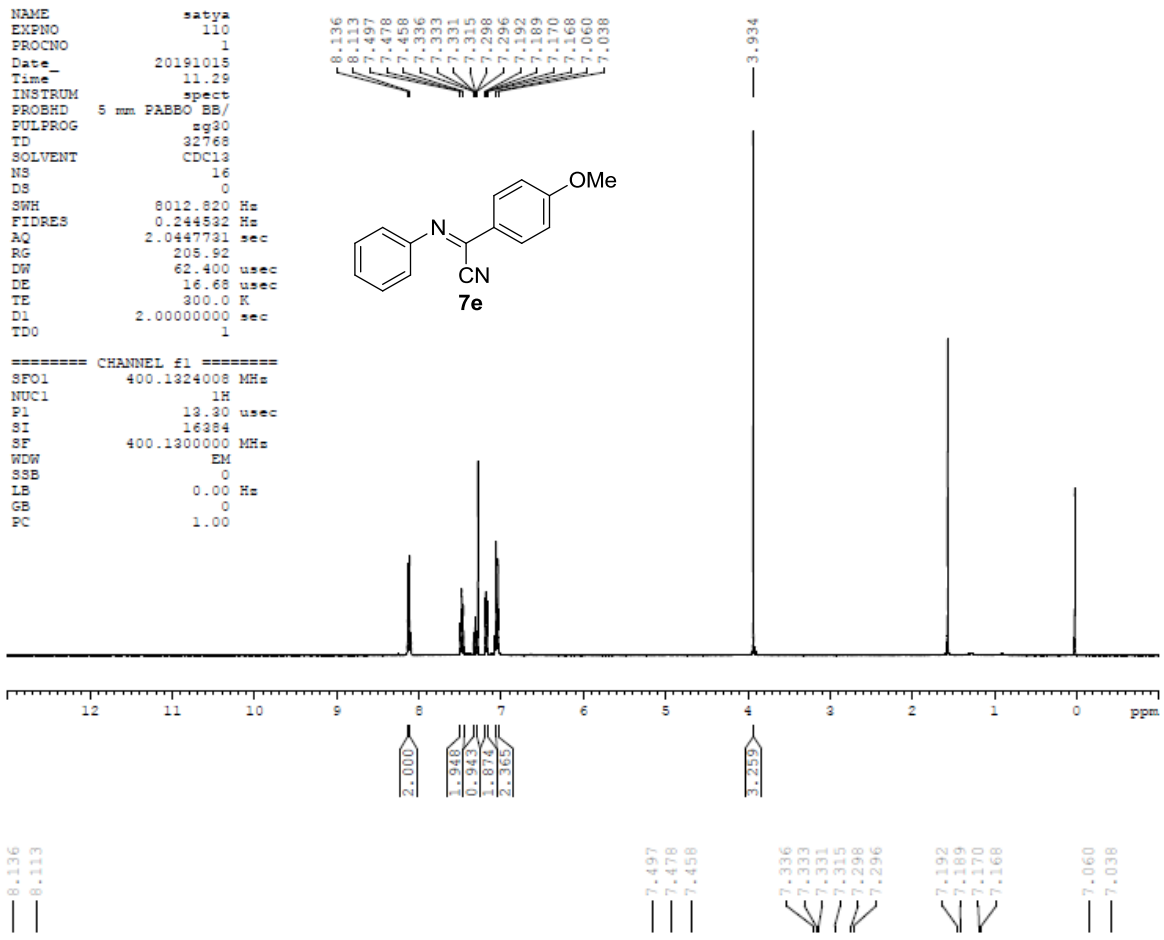

NAME DYY-IS-330AC
EXPNO 1
PROCNO 1
Date_ 20200918
Time 12.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
154.767
154.210
149.503
143.917
137.220
129.134
126.422
120.113
115.261
111.813
111.157
97.296
77.348
77.030
76.713
56.874
56.431
56.233
OMe
OMe
N
CN
OMe
7c
200
180
160
140
120
100
80
60
40
20
ppm

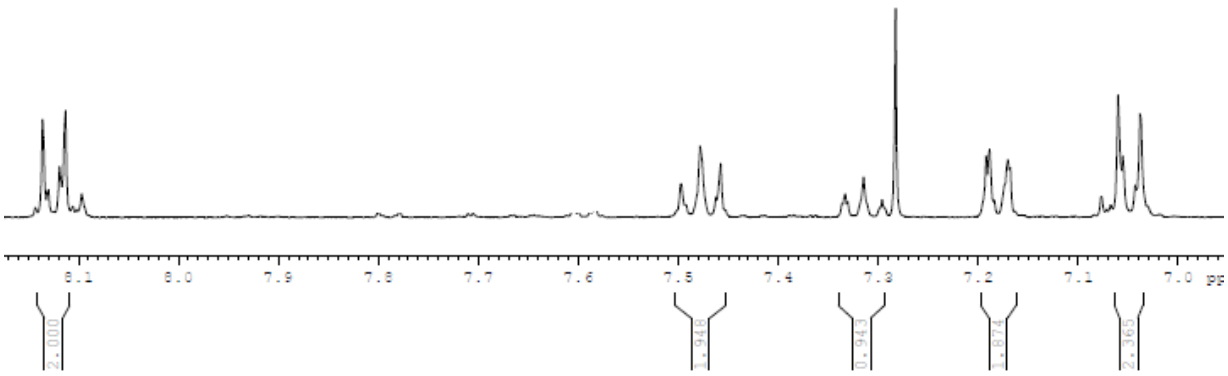

154.767
154.210
149.503
143.917
137.220
129.134
126.422
120.113
115.261
111.813
111.157
97.296
155
150
145
140
135
130
125
120
115
110
105
100
95 ppm

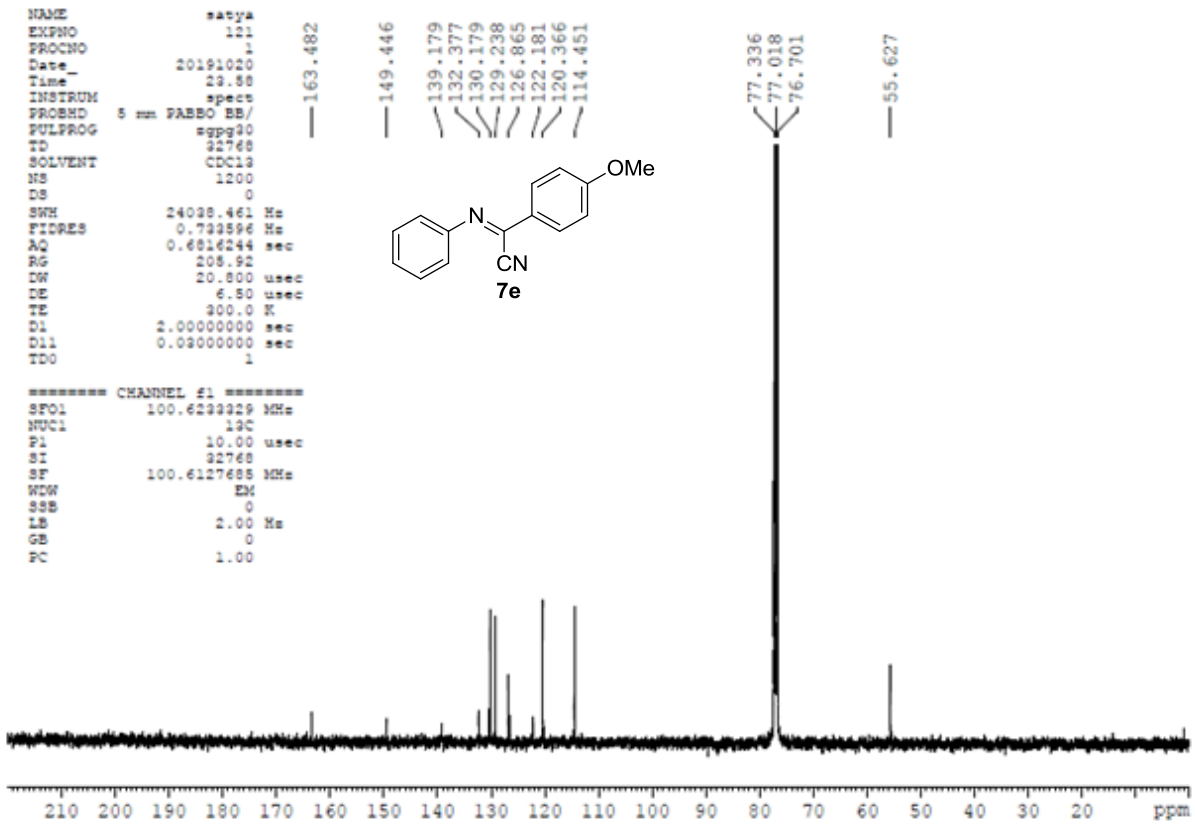

NAME satya
EXPNO 70
PROCNO 1
Date_ 20190917
Time 10.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244832 Hz
AQ 2.0447781 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.039
8.016
7.471
7.450
7.431
7.290
7.287
7.269
7.250
7.247
7.163
7.160
7.144
7.142
7.140
6.774
6.751
3.125
N
N
CN
7d
ppm
2.053
2.145
1.524
2.036
2.161
6.000

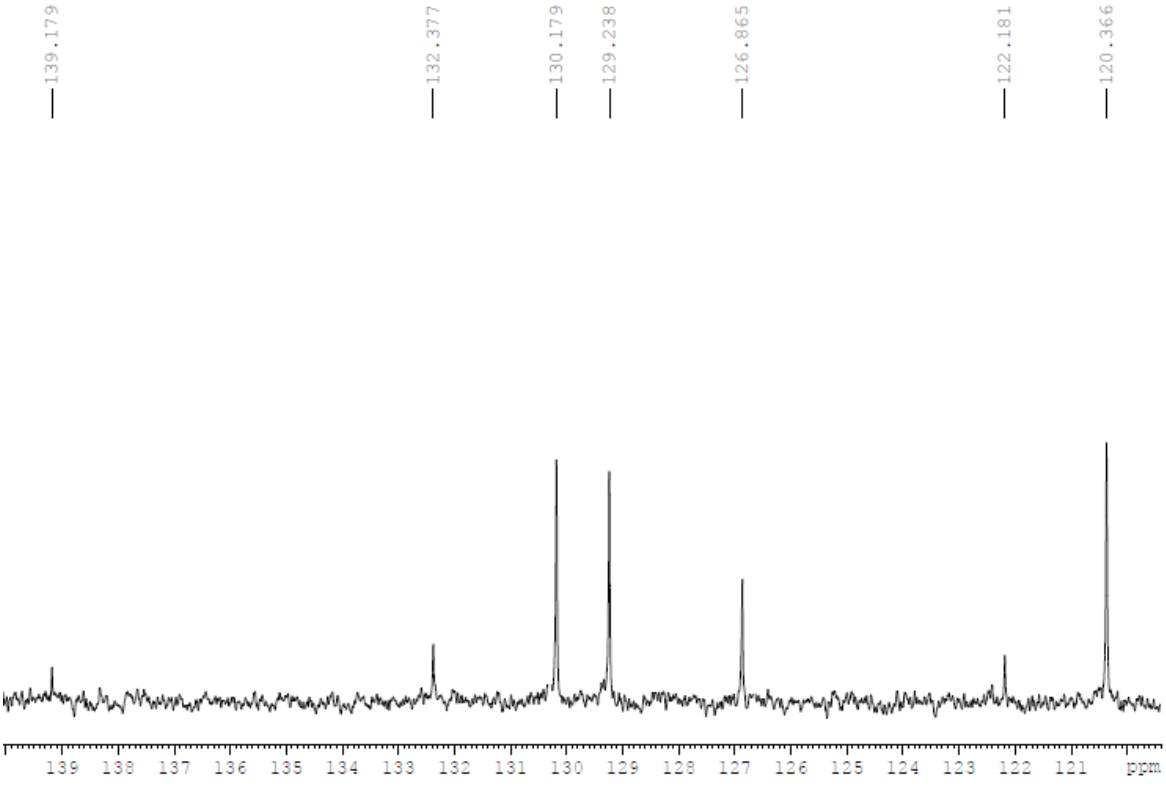

NAME satya
EXPNO 96
PROCNO 1
Date_ 20191006
Time 21.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733856 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6293329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
153.266
150.096
139.454
130.024
129.116
126.124
121.770
120.508
111.399
77.334
77.017
76.699
40.115
N
N
CN
7d
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

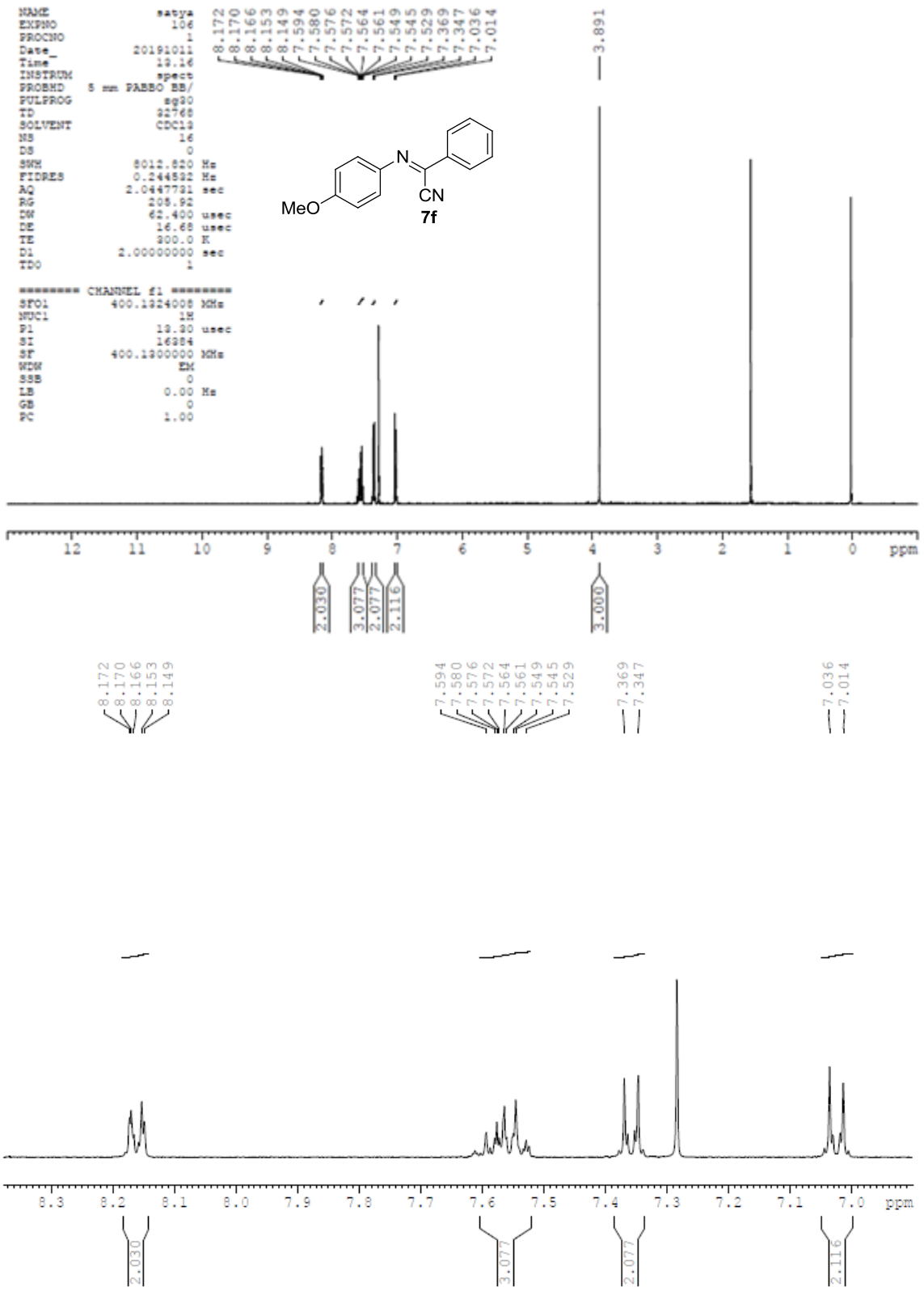

153.266
150.096
139.454
130.024
129.116
126.124
121.770
120.508
111.399
155 150 145 140 135 130 125 120 115 110 ppm

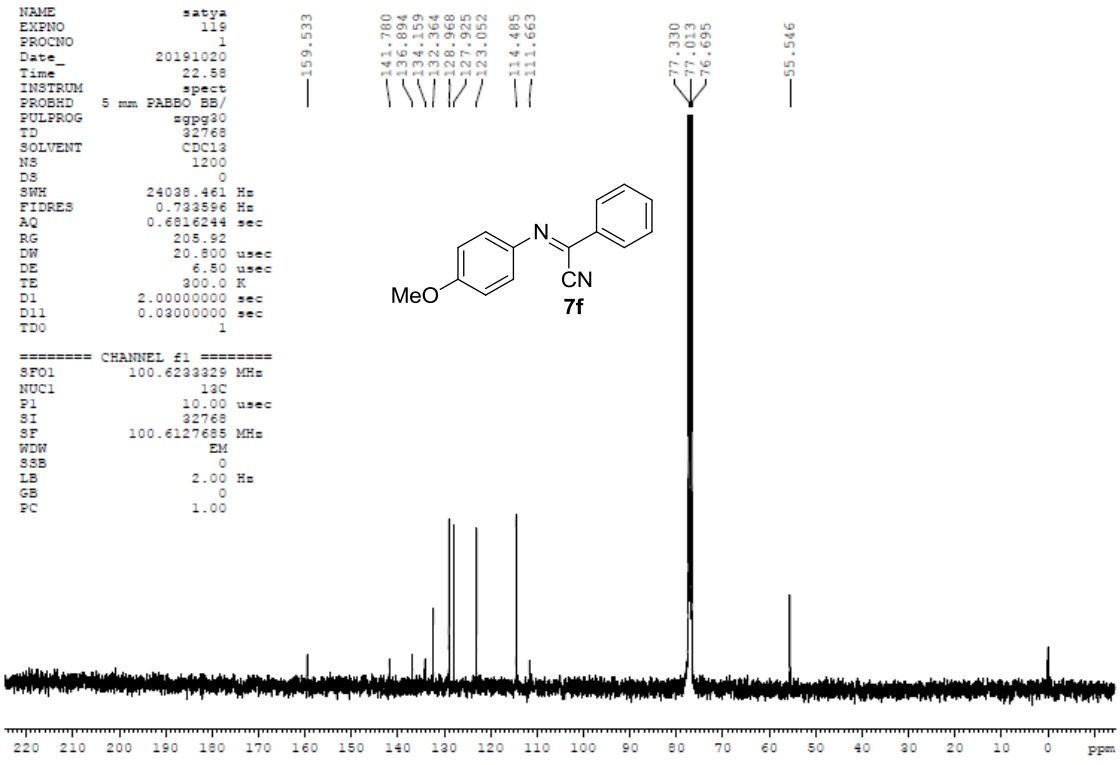

NAME satya
EXPNO 110
PROCNO 1
Date_ 20191015
Time 11.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.136
8.113
7.497
7.478
7.458
7.336
7.333
7.331
7.315
7.298
7.296
7.192
7.189
7.170
7.168
7.060
7.038
3.934
OMe
N
CN
7e
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.000
1.948
0.943
1.874
2.365
3.259

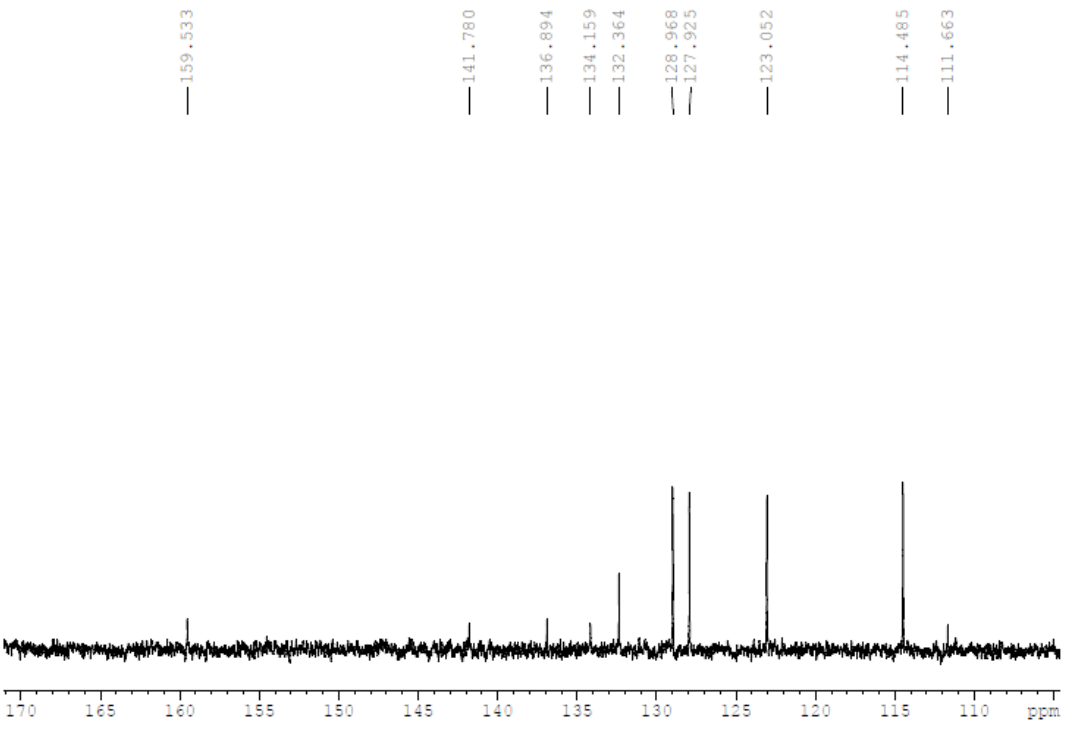

8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
pp
2.000
3.948
0.943
1.874
2.365

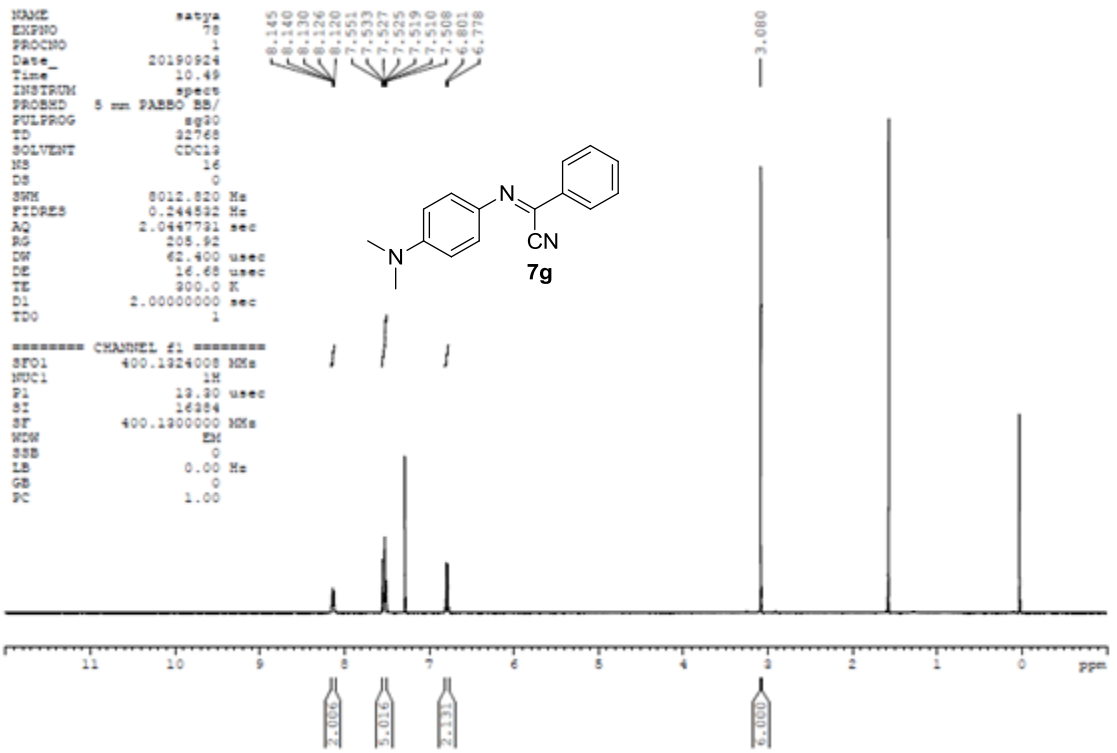

NAME satya
EXPNO 121
PROCNO 1
Date_ 20191020
Time_ 23.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233929 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
163.482
149.446
139.179
132.377
130.179
129.238
126.865
122.181
120.366
114.451
77.336
77.018
76.701
55.627
OMe
N
CN
7e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

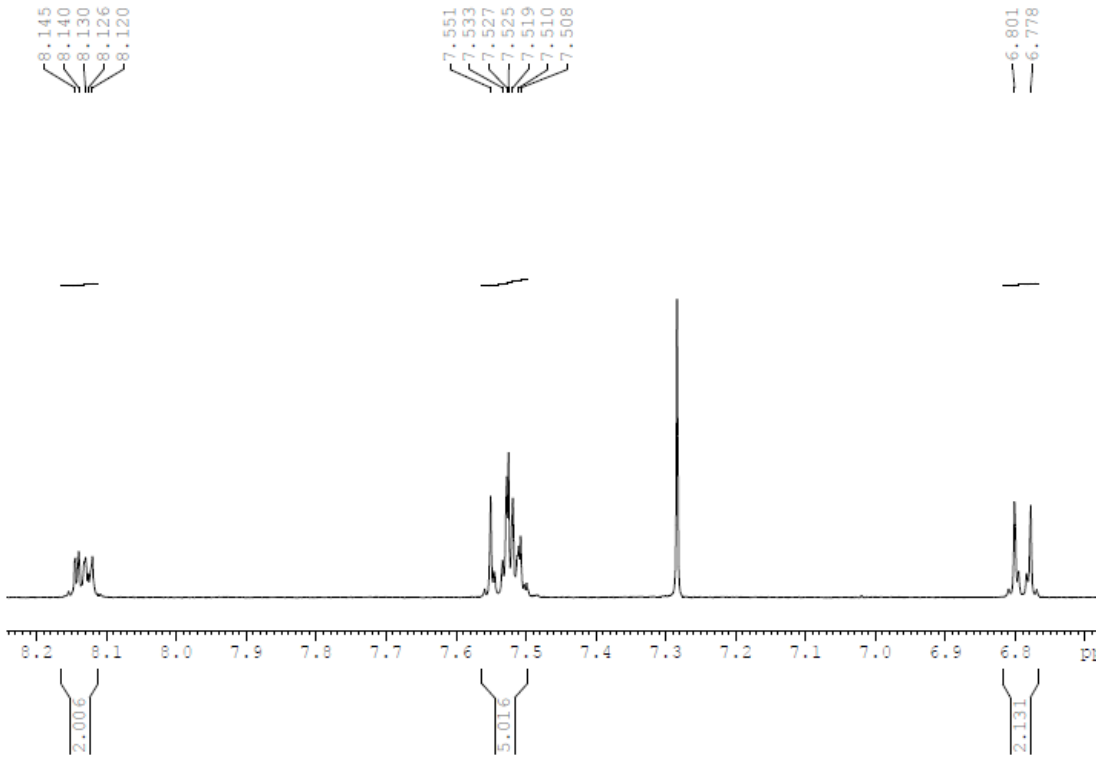

139.179
132.377
130.179
129.238
126.865
122.181
120.366
139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 ppm

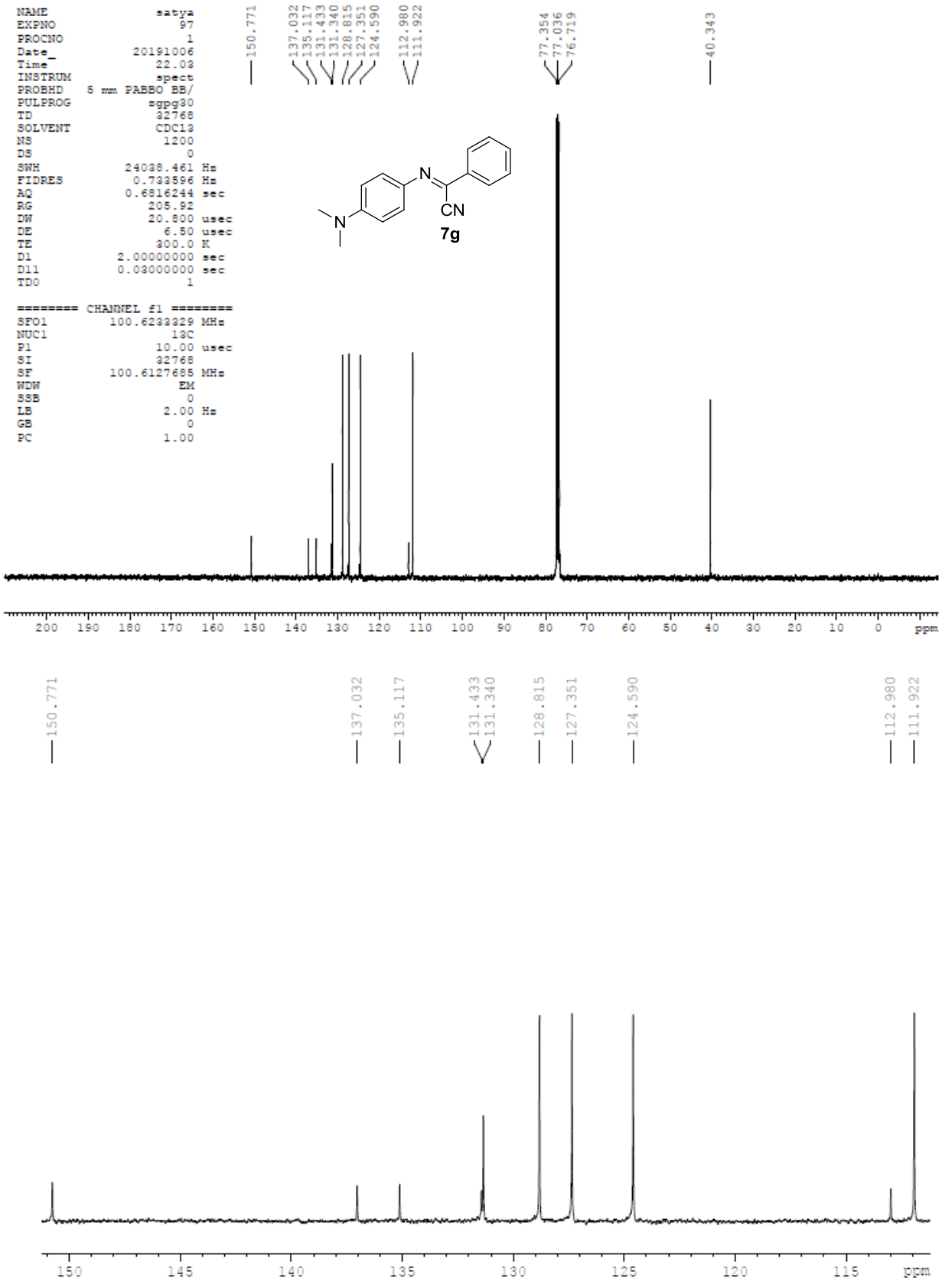

NAME satya
EXPNO 106
PROCNO 1
Date_ 20191011
Time 13.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244592 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.65 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.172
8.170
8.166
8.153
8.149
7.594
7.580
7.576
7.572
7.564
7.561
7.549
7.545
7.529
7.369
7.347
7.036
7.014
3.891
MeO
N
CN
7f
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.030
3.077
2.077
2.116
3.000
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
2.030
3.077
2.077
2.116

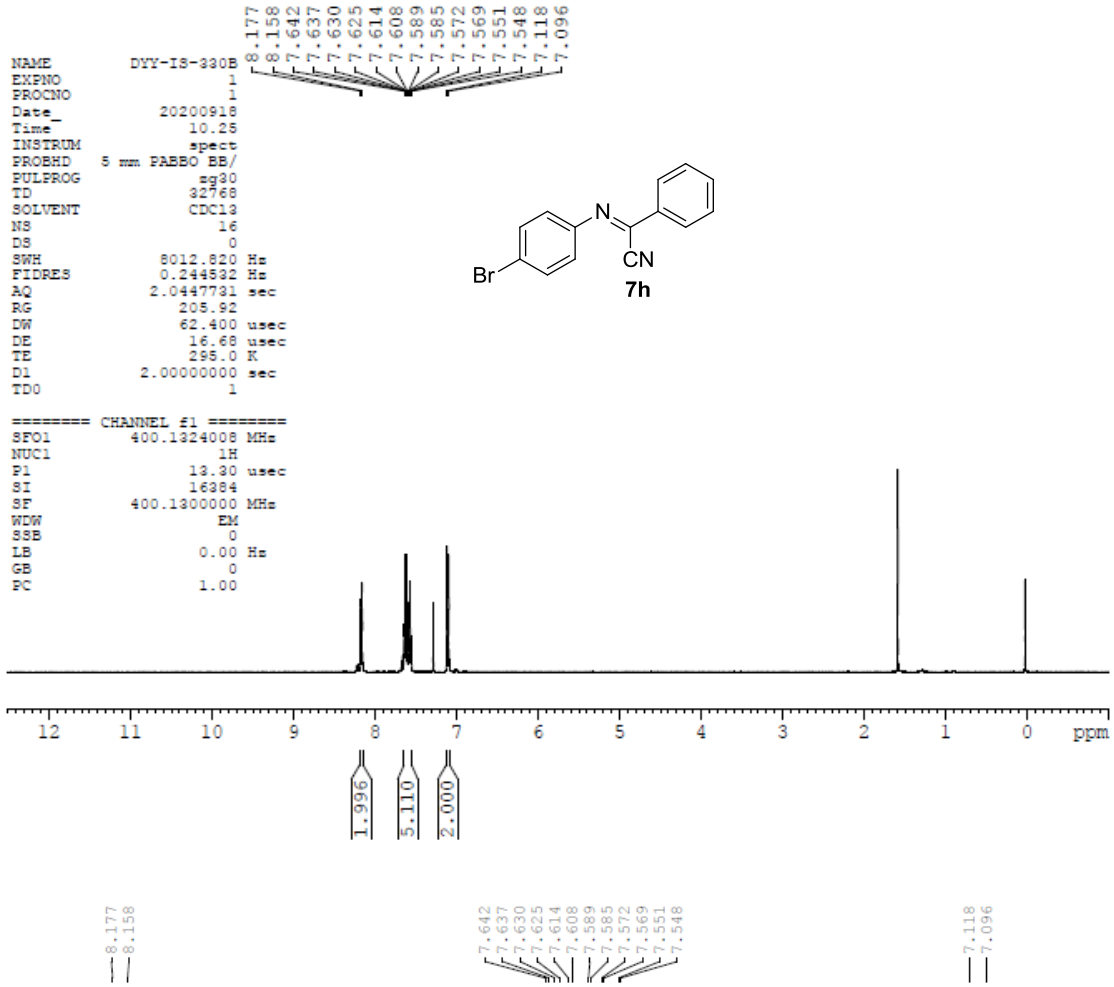

NAME satya
EXPNO 119
PROCNO 1
Date_ 20191020
Time 22.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
159.533
141.780
136.894
134.159
132.364
128.968
127.925
123.052
114.485
111.663
77.330
77.013
76.695
55.546
MeO
N
CN
7f
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

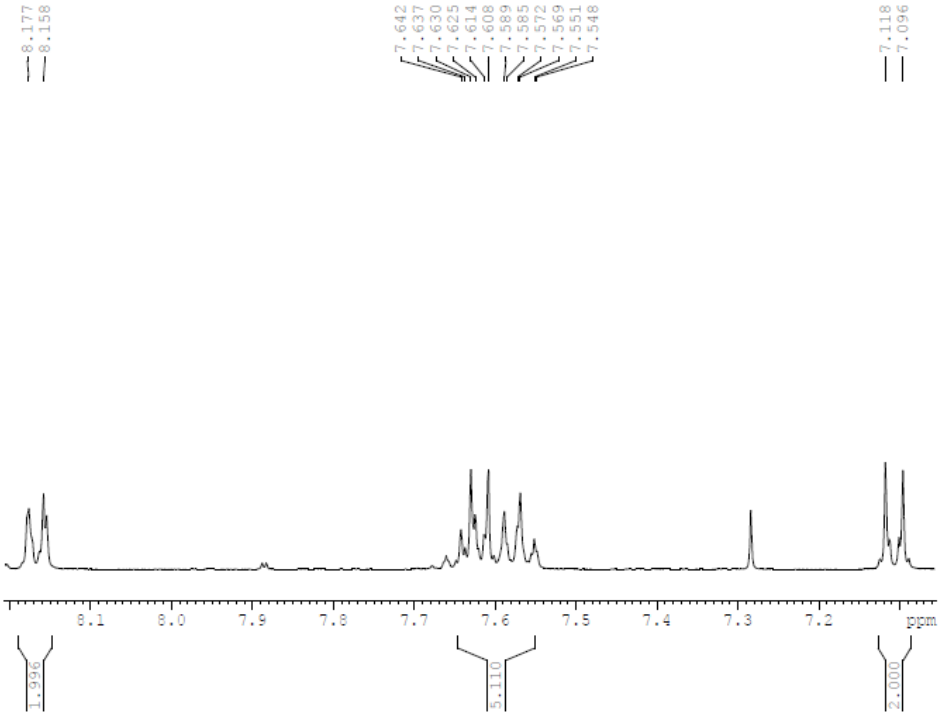

159.533
141.780
136.894
134.159
132.364
128.968
127.925
123.052
114.485
111.663
170 165 160 155 150 145 140 135 130 125 120 115 110 ppm

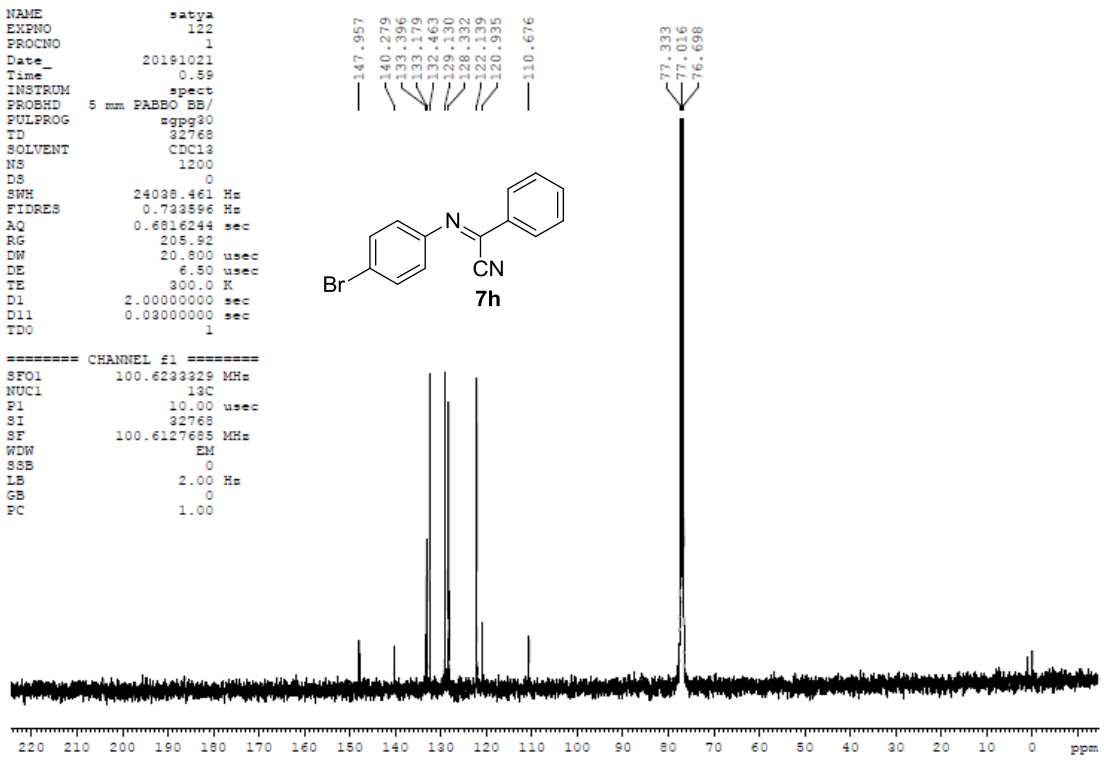

NAME satya
EXPNO 78
PROCNO 1
Date_ 20190924
Time 10.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244592 Hz
AQ 2.0447791 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.145
8.140
8.130
8.126
8.120
7.551
7.533
7.527
7.525
7.519
7.510
7.508
6.801
6.778
3.080
N
CN
N
7g
ppm
2.006
5.016
2.131
6.000

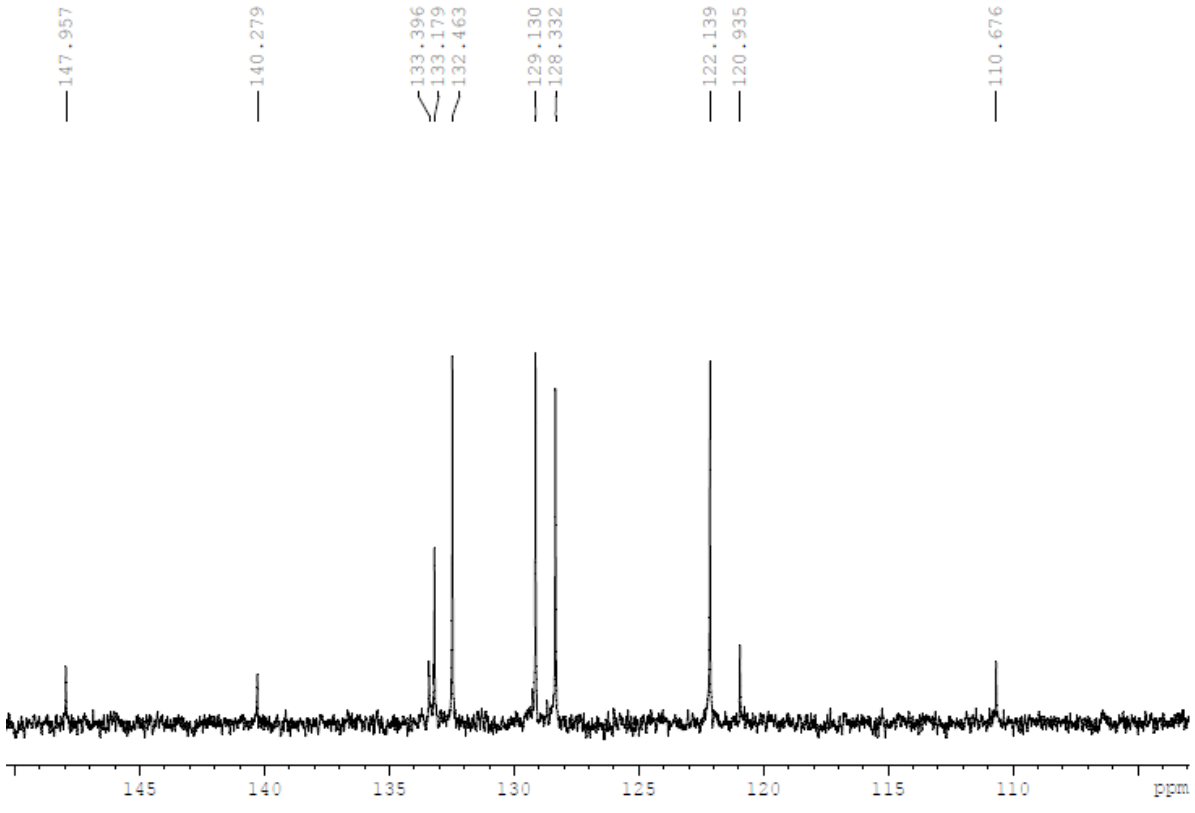

8.145
8.140
8.130
8.126
8.120
7.551
7.533
7.527
7.525
7.519
7.510
7.508
6.801
6.778
2.006
5.016
2.131

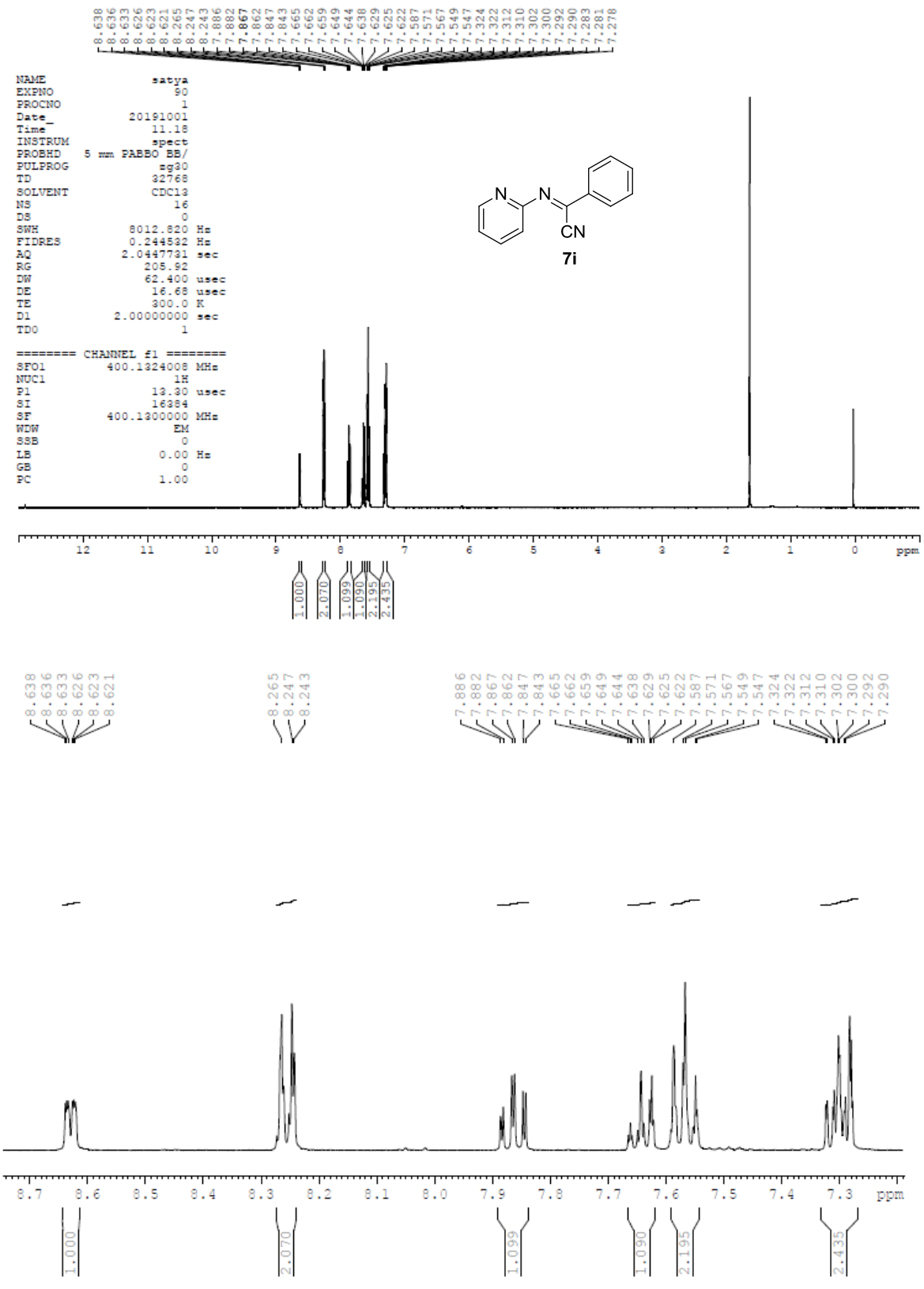

NAME satya
EXPNO 97
PROCNO 1
Date_ 20191006
Time 22.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
150.771
137.032
135.117
131.433
131.340
128.815
127.351
124.590
112.980
111.922
77.354
77.036
76.719
40.343
N
N
CN
7g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
150.771
137.032
135.117
131.433
131.340
128.815
127.351
124.590
112.980
111.922
150 145 140 135 130 125 120 115 ppm

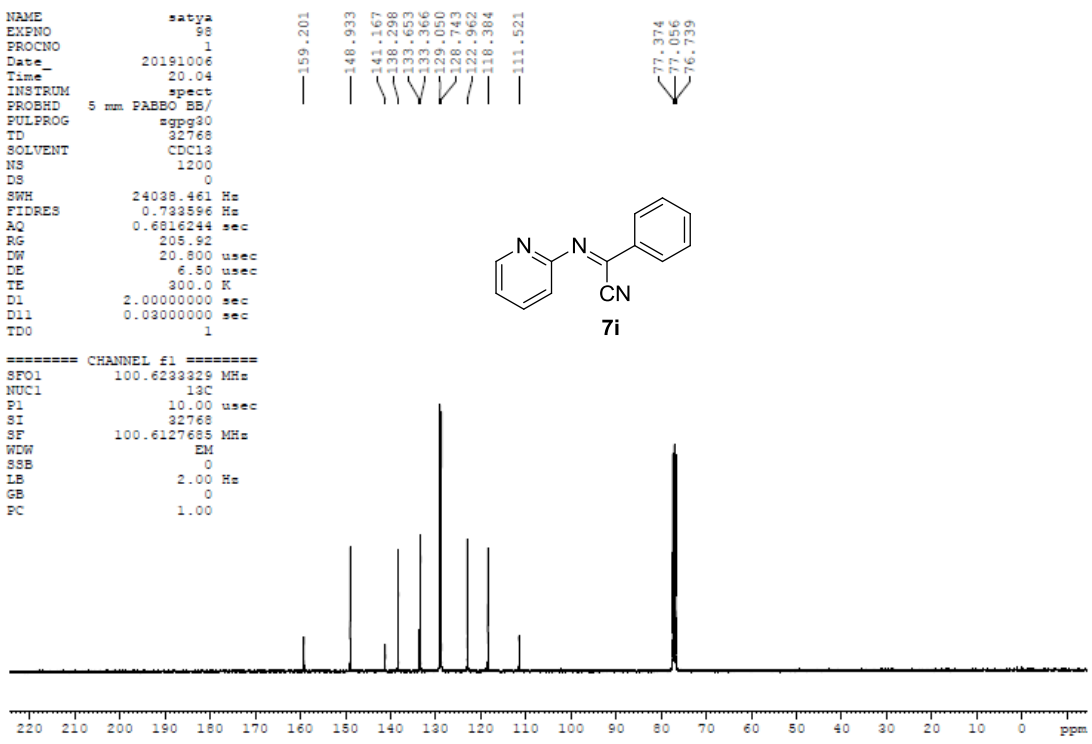

8.177
8.158
7.642
7.637
7.630
7.625
7.614
7.608
7.589
7.585
7.572
7.569
7.551
7.548
7.118
7.096
NAME DYY-I8-330B
EXPNO 1
PROCNO 1
Date_ 20200918
Time 10.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
CN
Br
7h
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.996
5.110
2.000

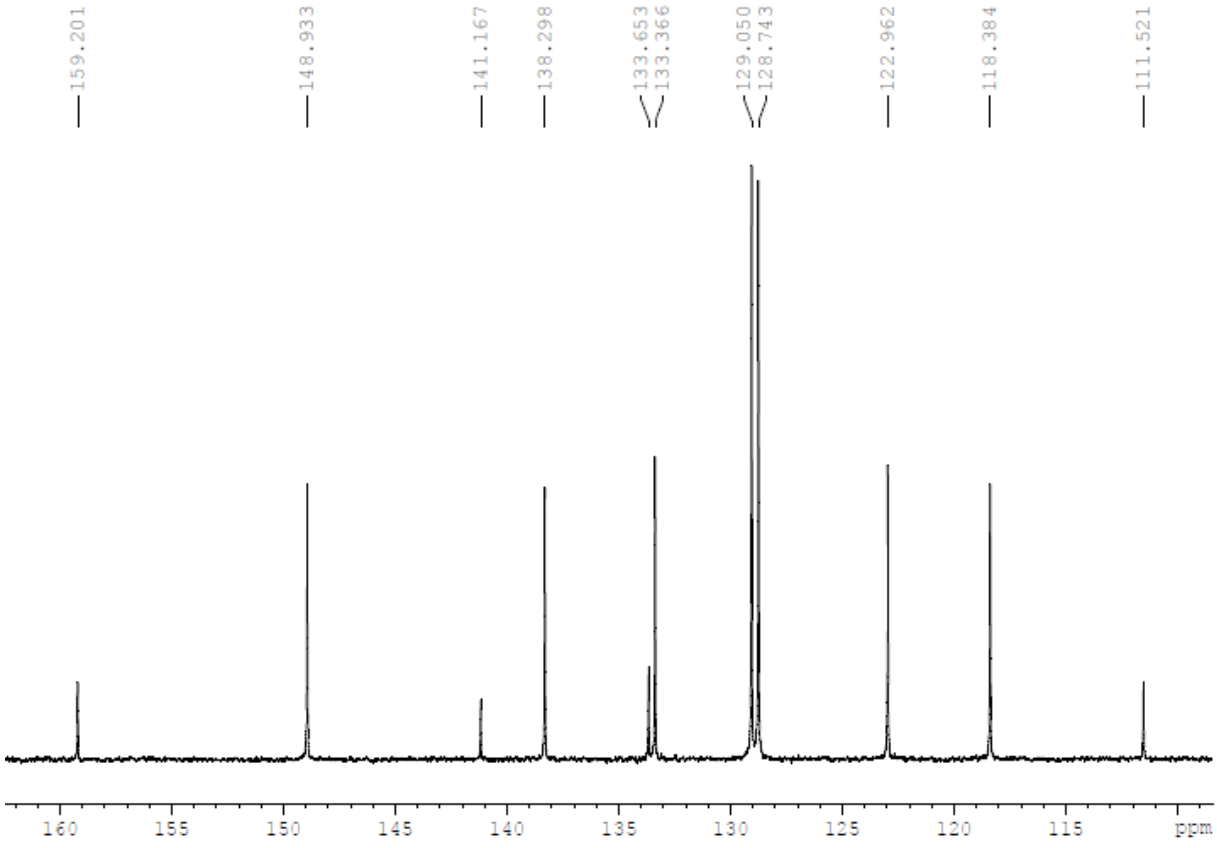

8.177
8.158
7.642
7.637
7.630
7.625
7.614
7.608
7.589
7.585
7.572
7.569
7.551
7.548
7.118
7.096
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
1.996
5.110
2.000

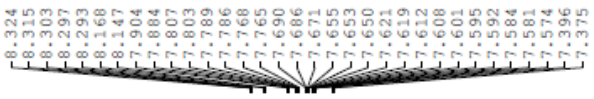

NAME satya
EXPNO 122
PROCNO 1
Date_ 20191021
Time 0.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG sgpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
147.957
140.279
133.396
133.179
132.463
129.130
128.332
122.139
120.935
110.676
77.333
77.016
76.698
N
CN
Br
7h
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


147.957
140.279
133.396
133.179
132.463
129.130
128.332
122.139
120.935
110.676
145 140 135 130 125 120 115 110 ppm


8.638
8.636
8.633
8.626
8.623
8.621
8.265
8.247
8.243
7.886
7.882
7.867
7.862
7.847
7.843
7.665
7.662
7.659
7.649
7.644
7.638
7.629
7.625
7.622
7.587
7.571
7.567
7.549
7.547
7.324
7.322
7.312
7.310
7.302
7.300
7.292
7.290
7.283
7.281
7.278
NAME satya
EXPNO 90
PROCNO 1
Date_ 20191001
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
N
CN
7i
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.070
1.099
1.090
2.195
2.435
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm

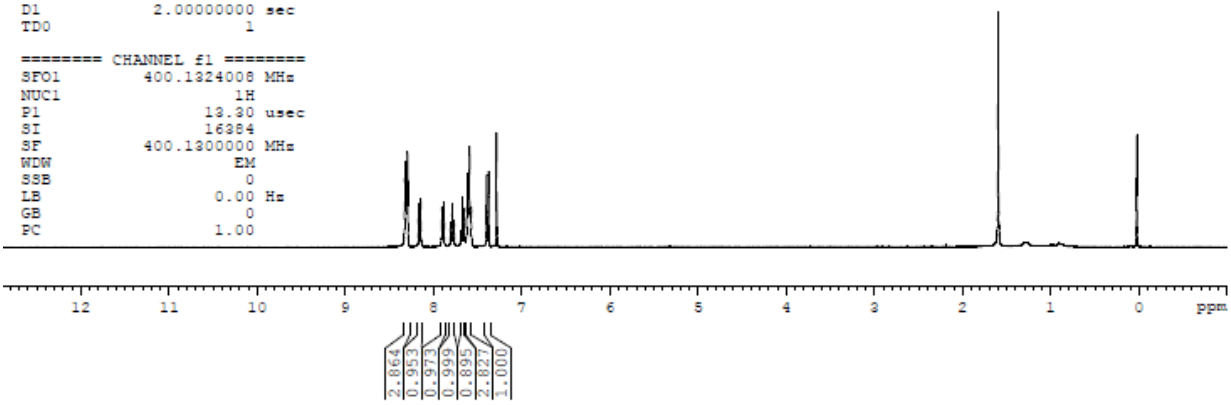

NAME satya
EXPNO 98
PROCNO 1
Date_ 20191006
Time 20.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG sqpg30
TD 32768
SOLVENT CDCl3
NS 1200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
159.201
148.933
141.167
138.298
133.653
133.366
129.050
128.743
122.962
118.384
111.521
77.374
77.056
76.739
N
N
CN
7i
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

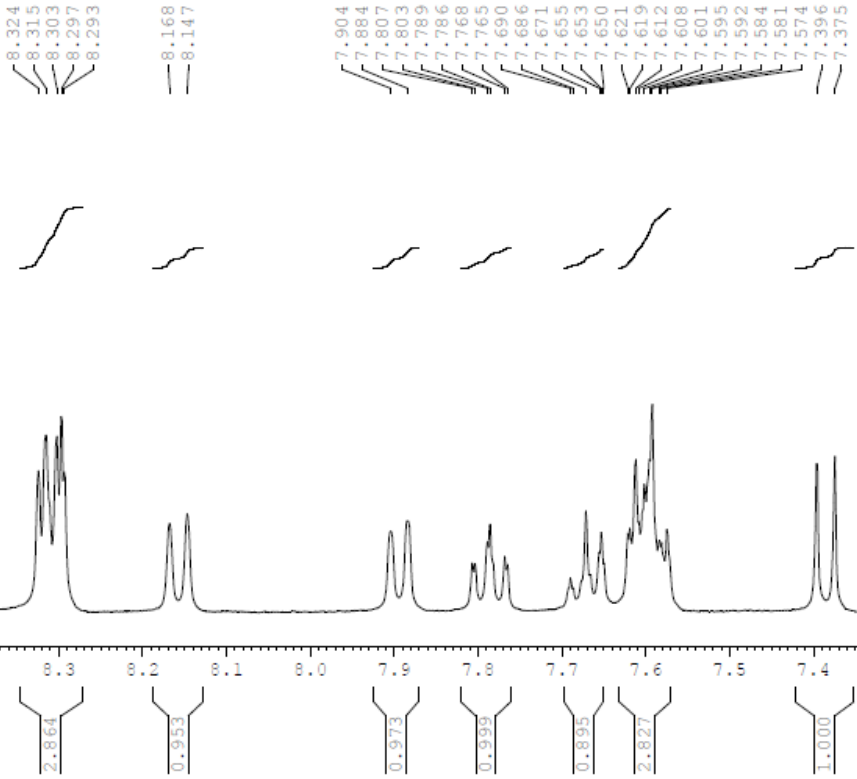

159.201
148.933
141.167
138.298
133.653
133.366
129.050
128.743
122.962
118.384
111.521
160 155 150 145 140 135 130 125 120 115 ppm

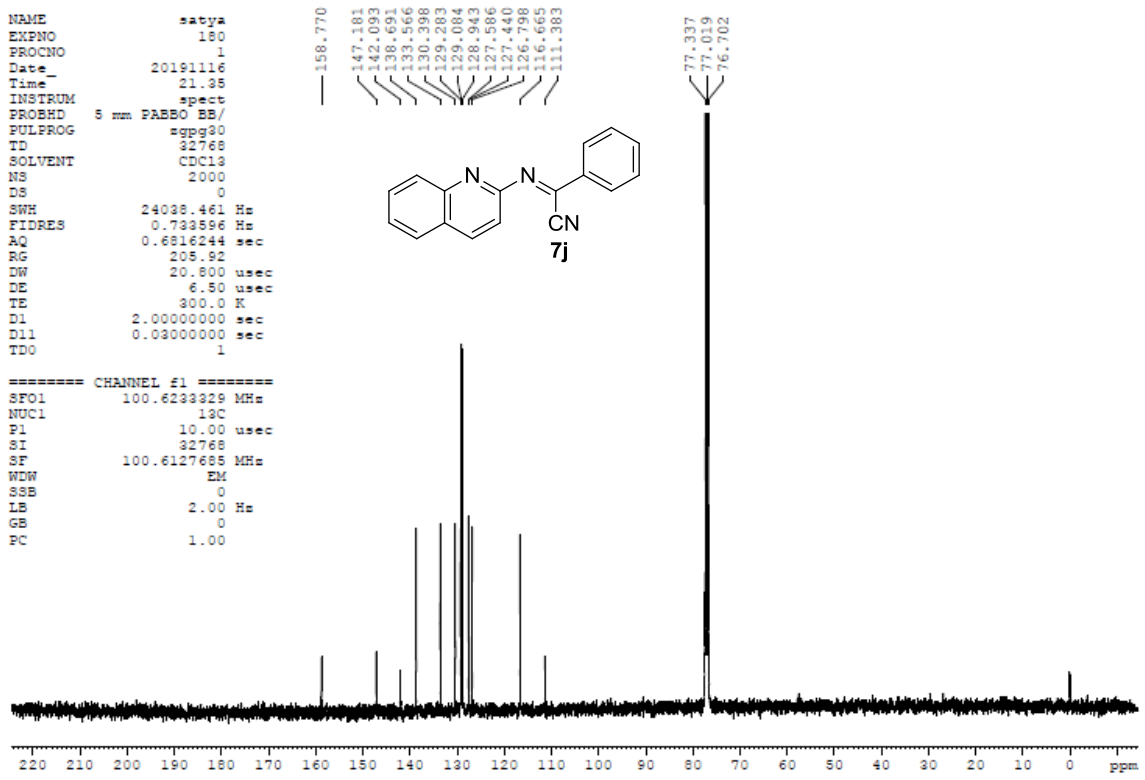


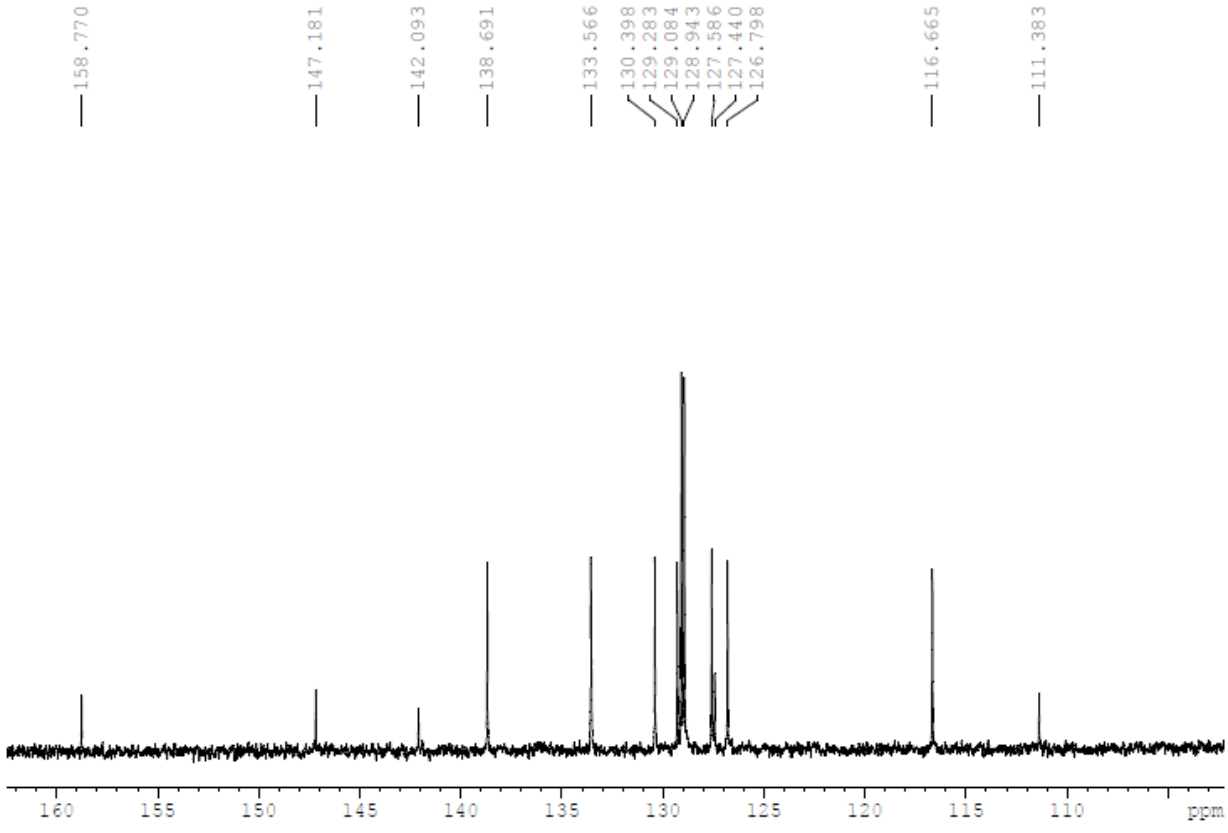

```
NAME                satya
EXPNO                 143
PROCNO                  1
Date_            20191105
Time                10.53
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              2.0447731 sec
RG                 205.92
DW                 62.400 usec
DE                 16.68 usec
TE                 300.0 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                  1H
P1                 13.30 usec
SI                 16384
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

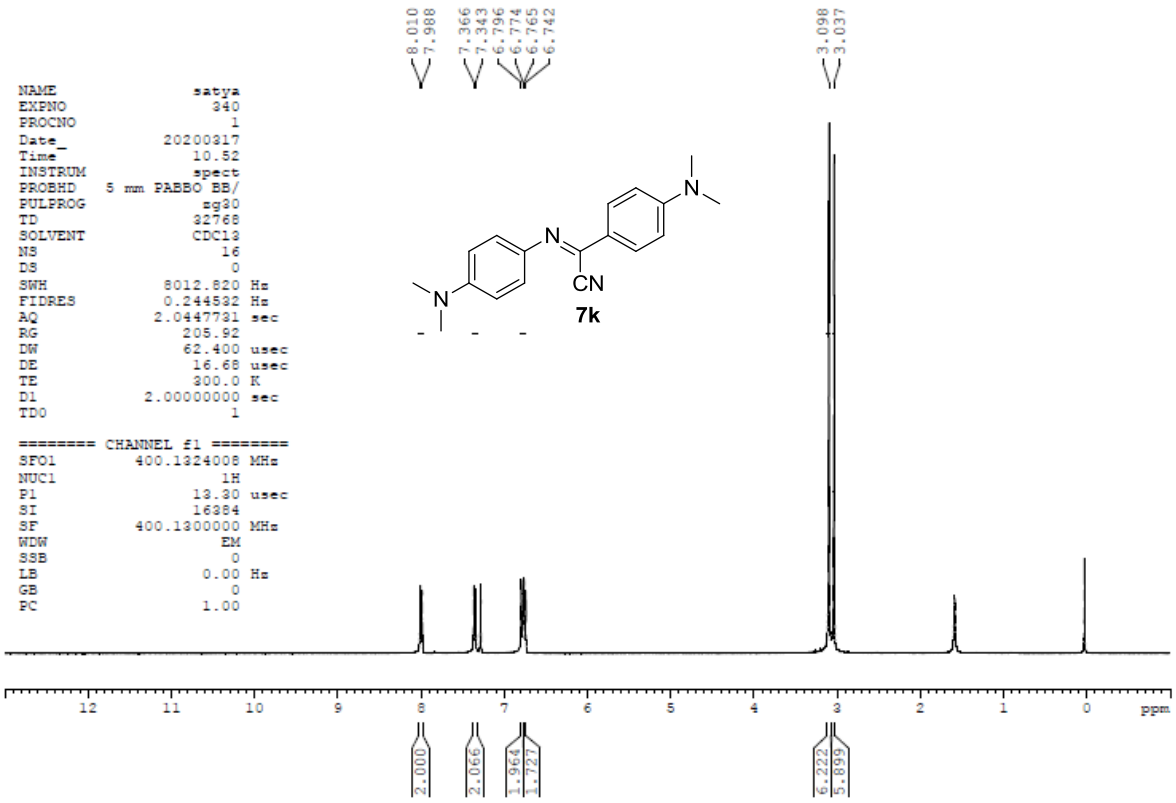
7j

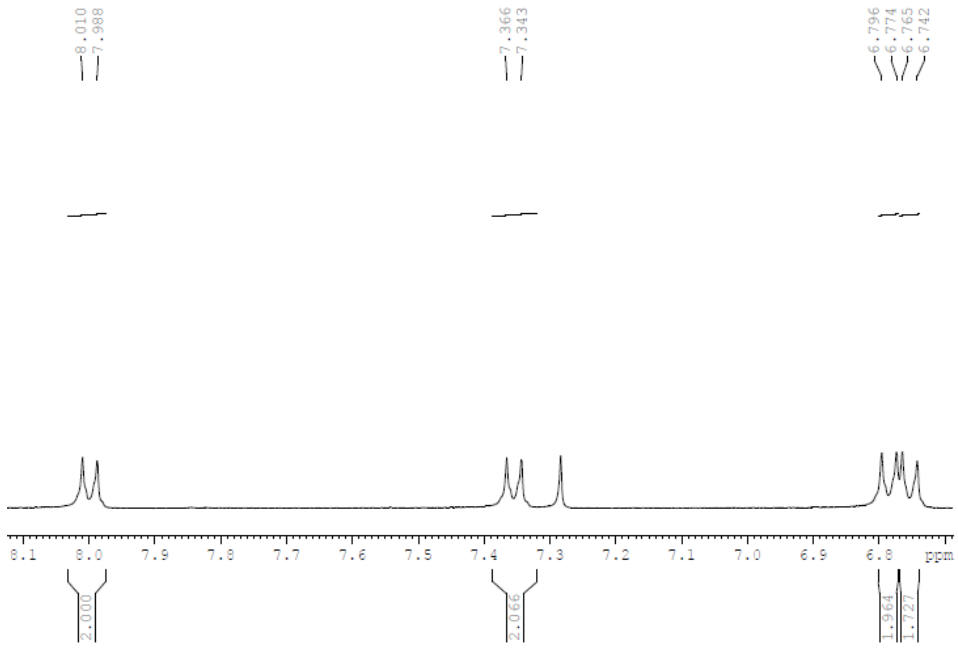


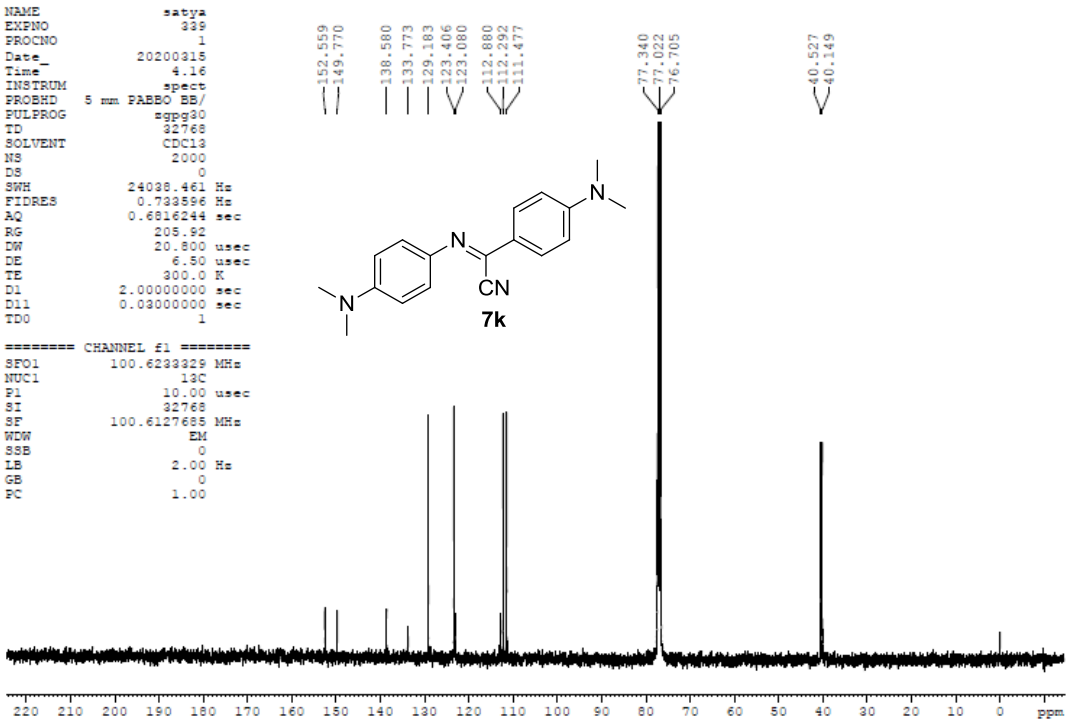


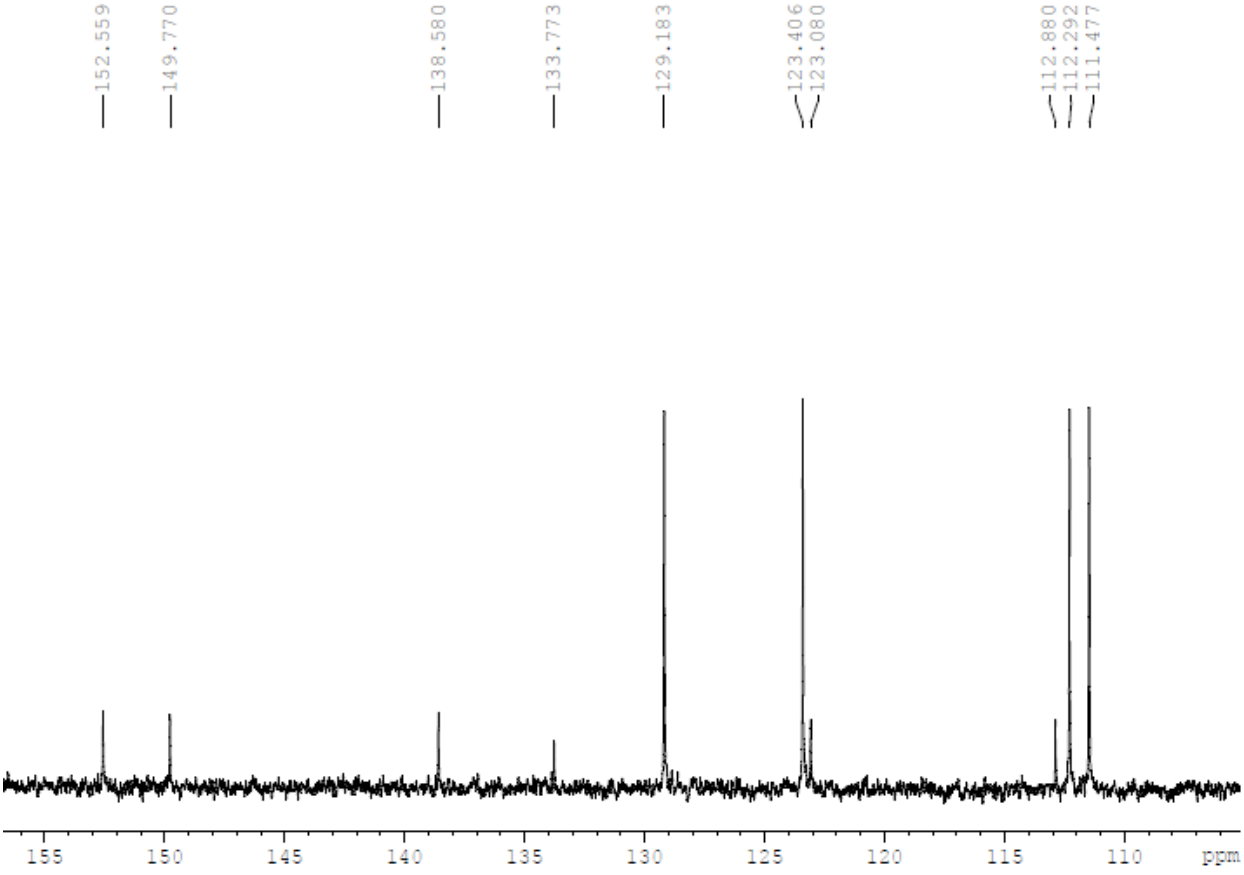

NAME satya
EXPNO 180
PROCNO 1
Date_ 20191116
Time 21.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
158.770
147.181
142.093
138.691
133.566
130.398
129.283
129.084
128.943
127.586
127.440
126.798
116.665
111.383
77.337
77.019
76.702
N
N
CN
7j
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

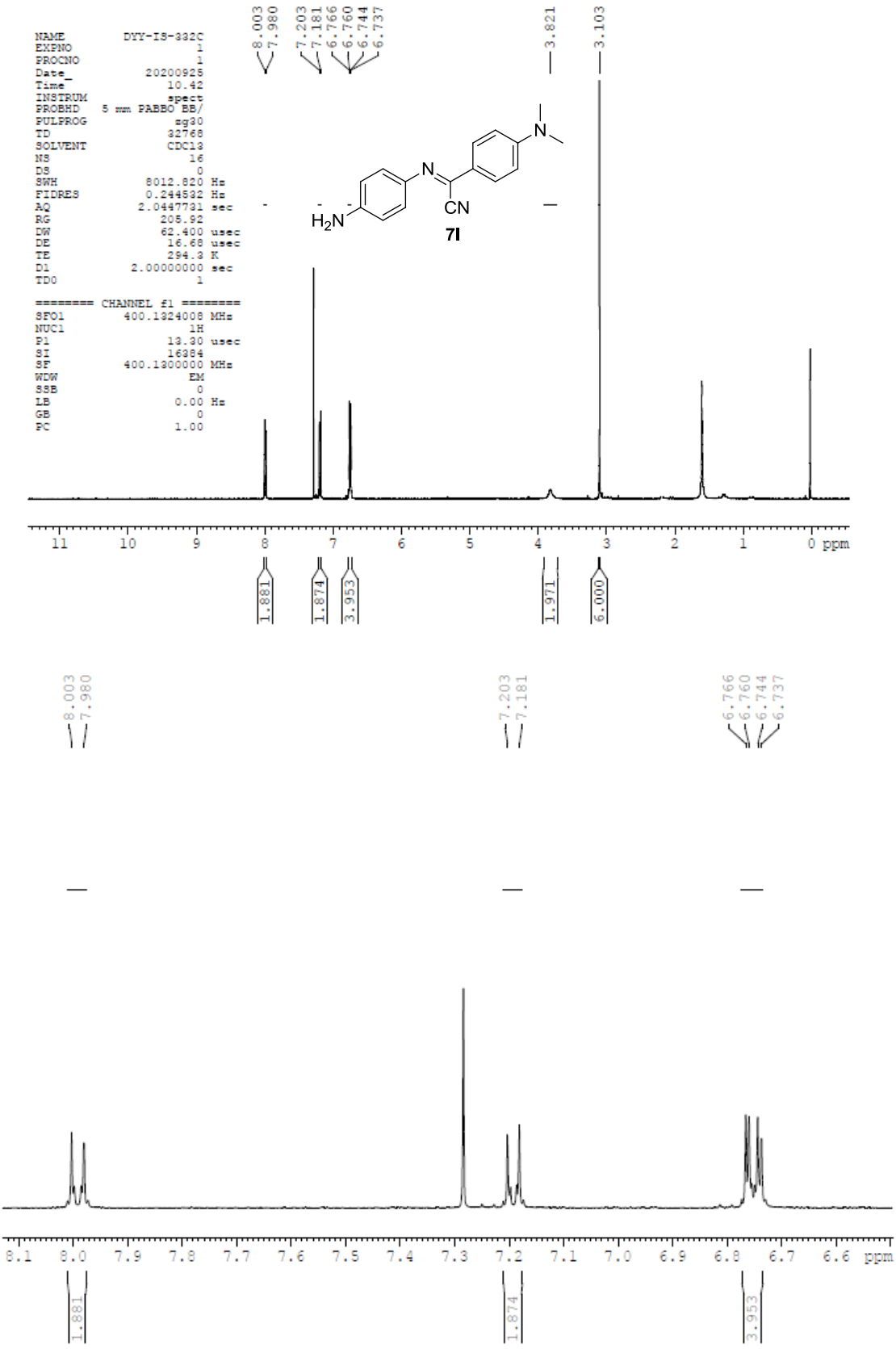

158.770
147.181
142.093
138.691
133.566
130.398
129.283
129.084
128.943
127.586
127.440
126.798
116.665
111.383
160 155 150 145 140 135 130 125 120 115 110 ppm

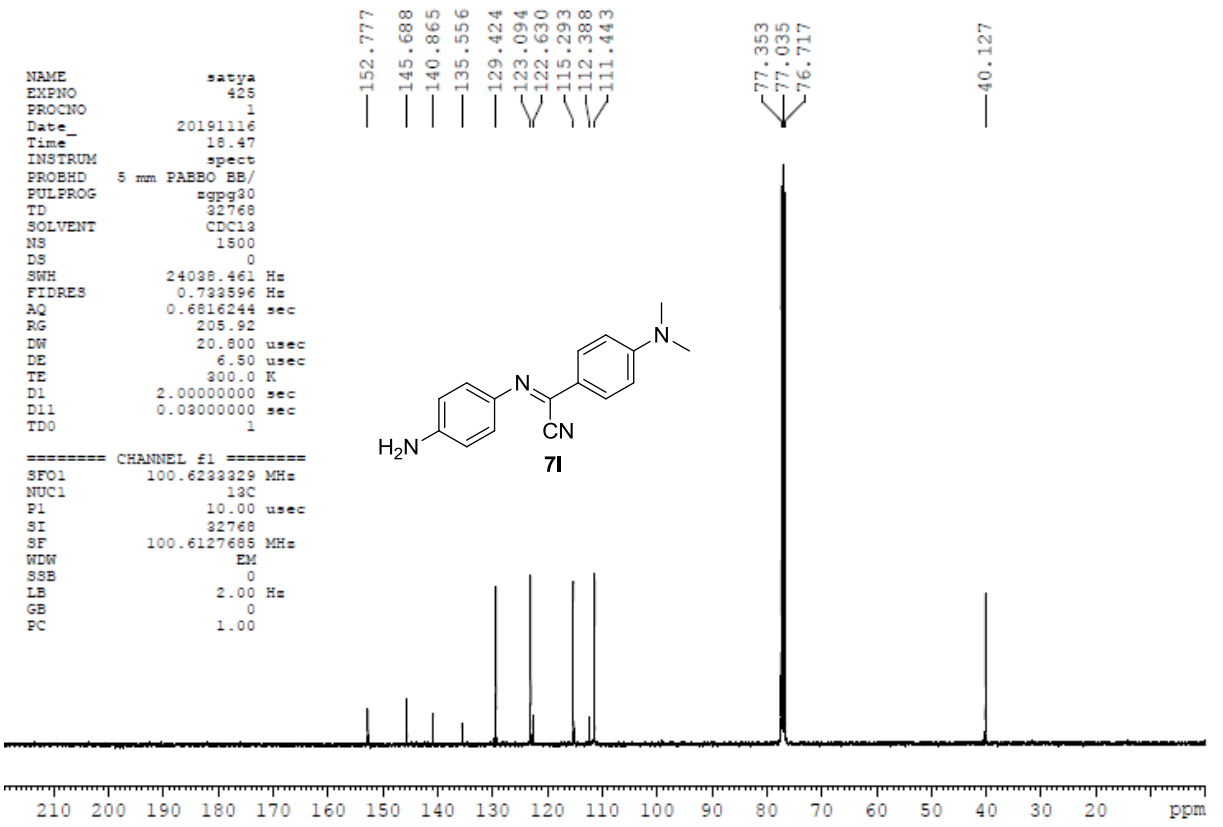

8.010
7.988
7.366
7.343
6.796
6.774
6.765
6.742
3.098
3.037
NAME satya
EXPNO 340
PROCNO 1
Date_ 20200317
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
N
CN
7k
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.000
2.066
1.964
1.727
6.222
5.899

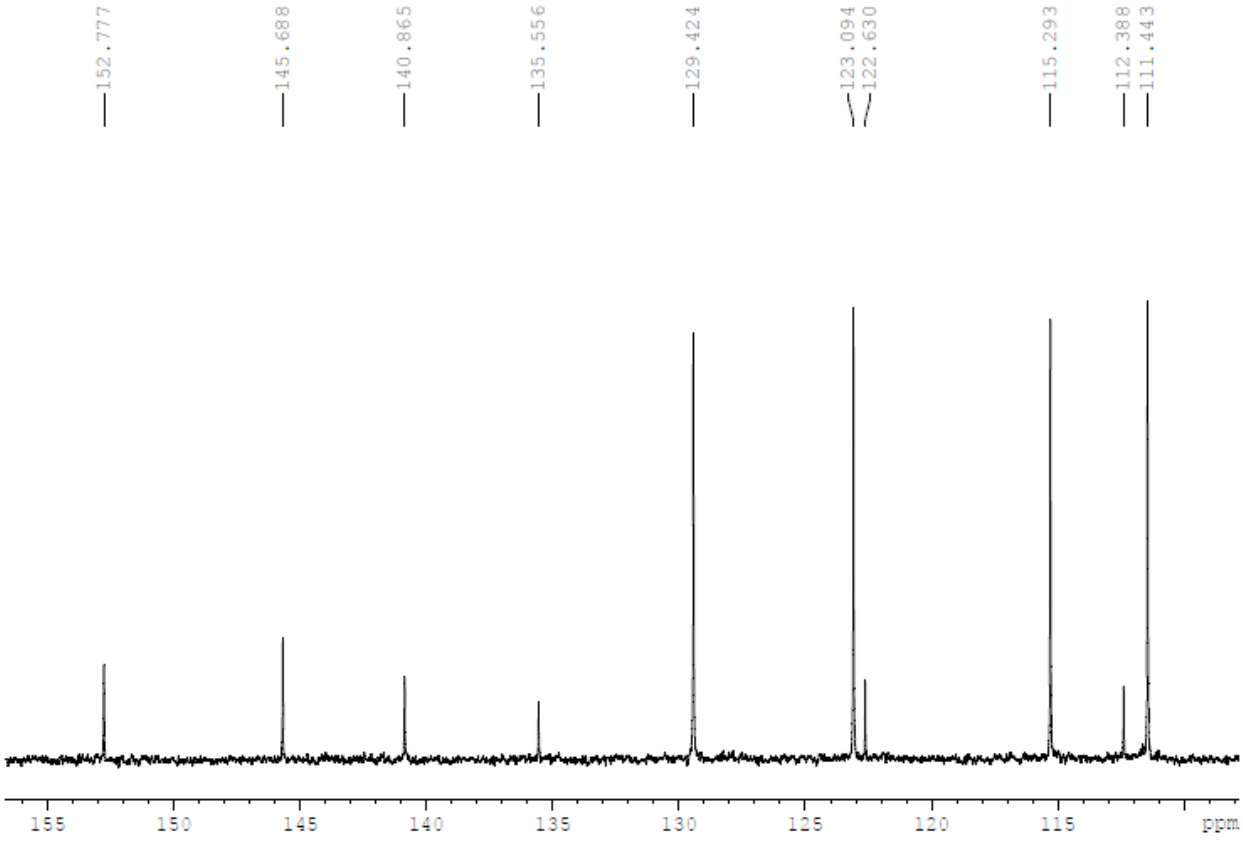

8.010
7.988
7.366
7.343
6.796
6.774
6.765
6.742
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm
2.000
2.066
1.964
1.727

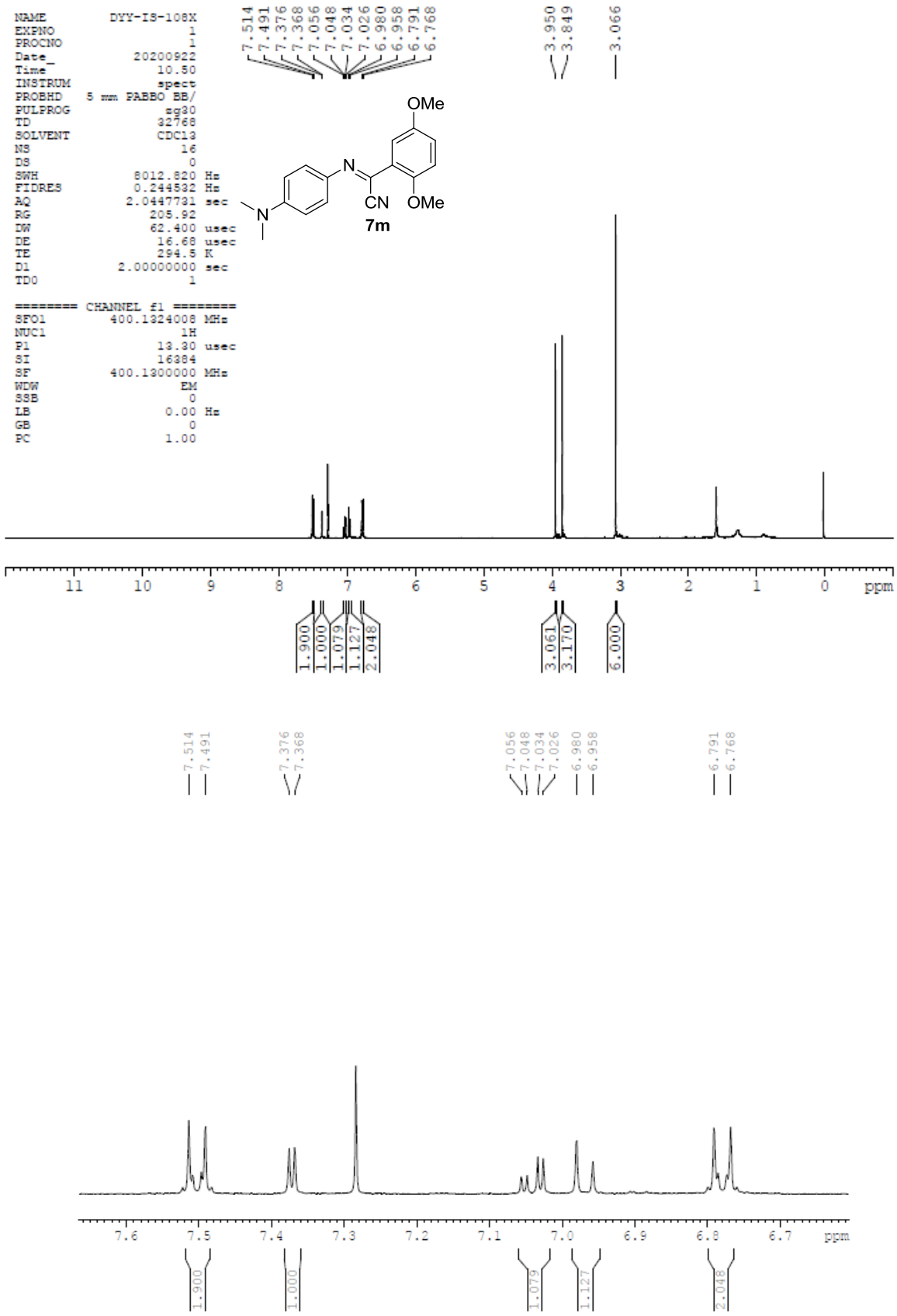

NAME satya
EXPNO 339
PROCNO 1
Date_ 20200315
Time_ 4.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
152.559
149.770
138.580
133.773
129.183
123.406
123.080
112.880
112.292
111.477
77.340
77.022
76.705
40.527
40.149
N
N
N
CN
7k
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

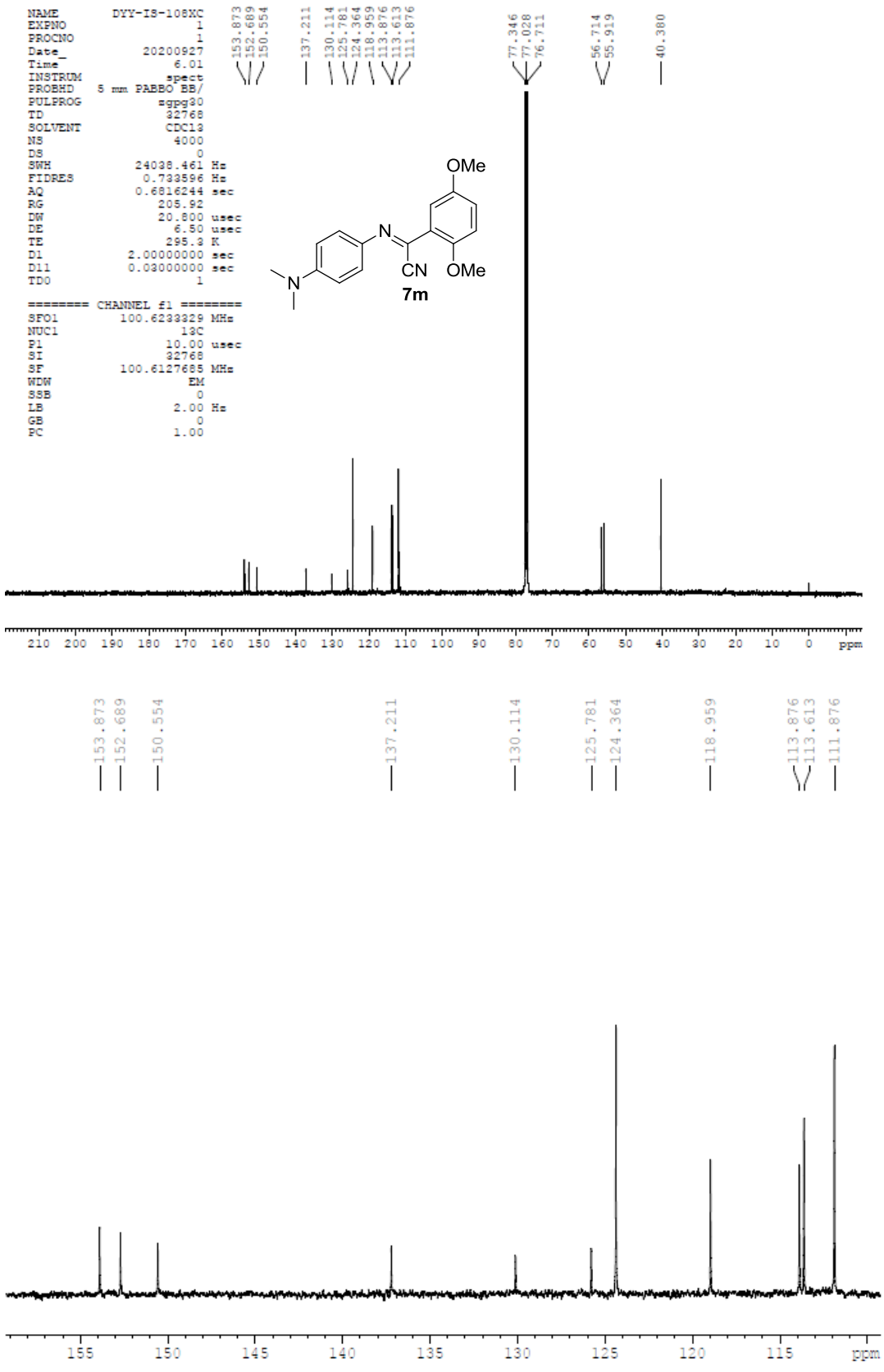

152.559
149.770
138.580
133.773
129.183
123.406
123.080
112.880
112.292
111.477
155 150 145 140 135 130 125 120 115 110 ppm

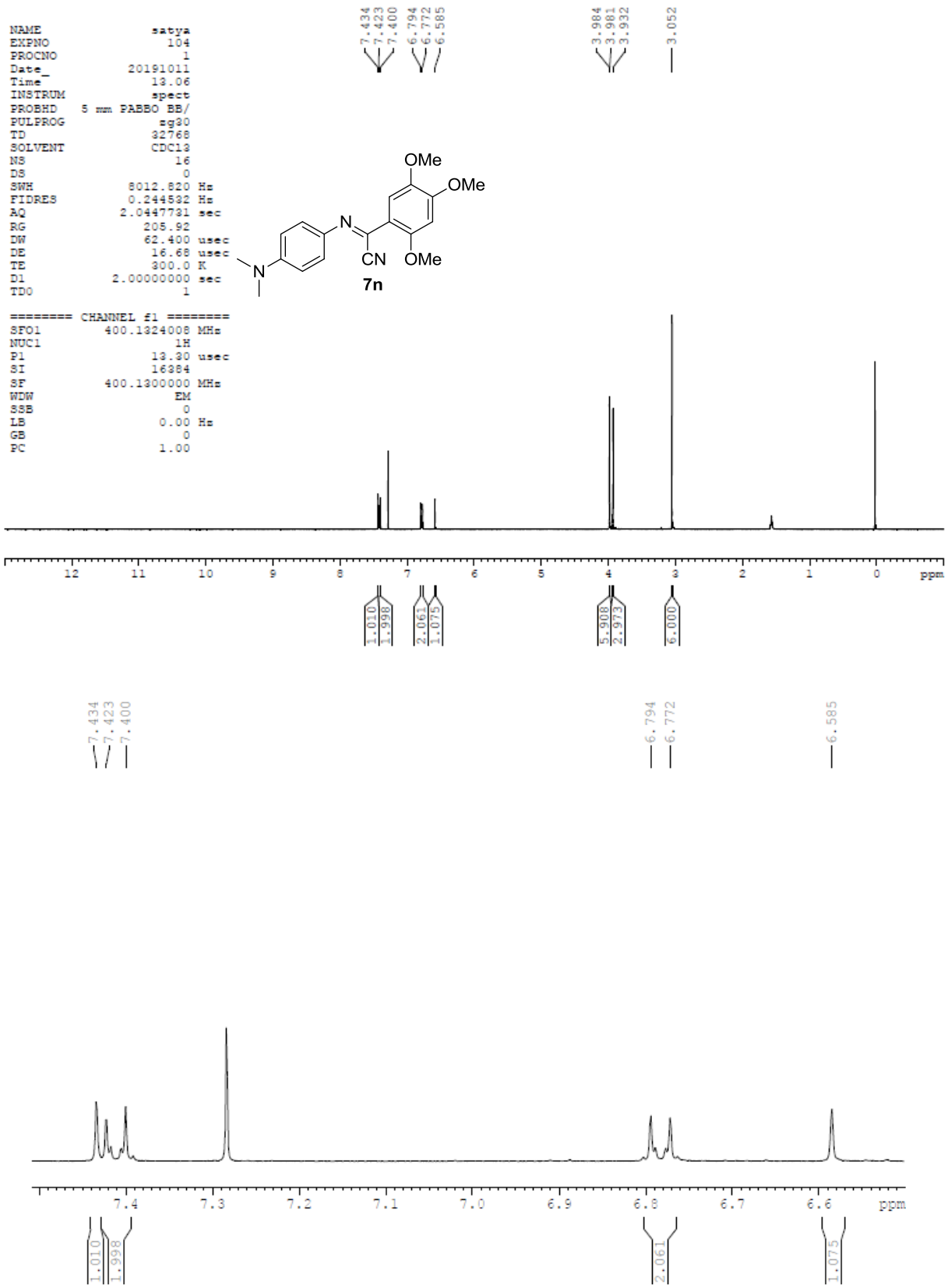

NAME DYY-IS-332C
EXPNO 1
PROCNO 1
Date_ 20200925
Time 10.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 294.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.003
7.980
7.203
7.181
6.766
6.760
6.744
6.737
3.821
3.103
N
N
CN
H2N
7l
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.881
1.874
3.953
1.971
6.000
8.003
7.980
7.203
7.181
6.766
6.760
6.744
6.737
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6 ppm
1.881
1.874
3.953

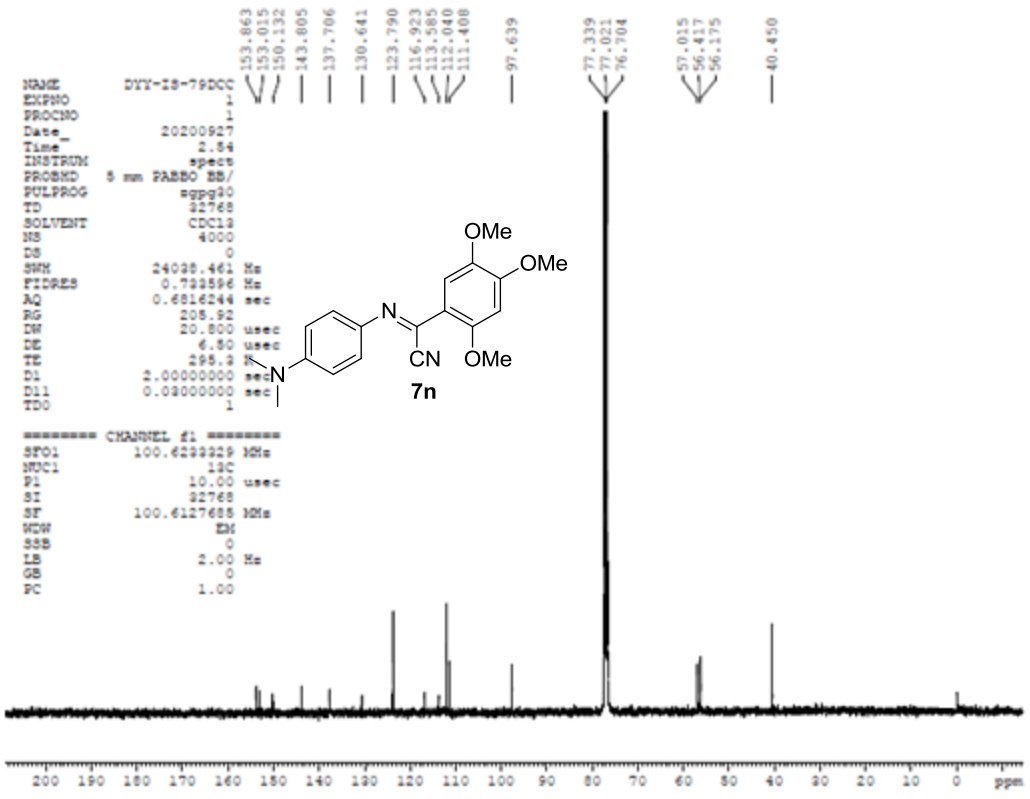

NAME satya
EXPNO 425
PROCNO 1
Date_ 20191116
Time 18.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG sgpg30
TD 32768
SOLVENT CDCl3
NS 1500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
152.777
145.688
140.865
135.556
129.424
123.094
122.630
115.293
112.388
111.443
77.353
77.035
76.717
40.127
N
N
CN
H2N
7l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

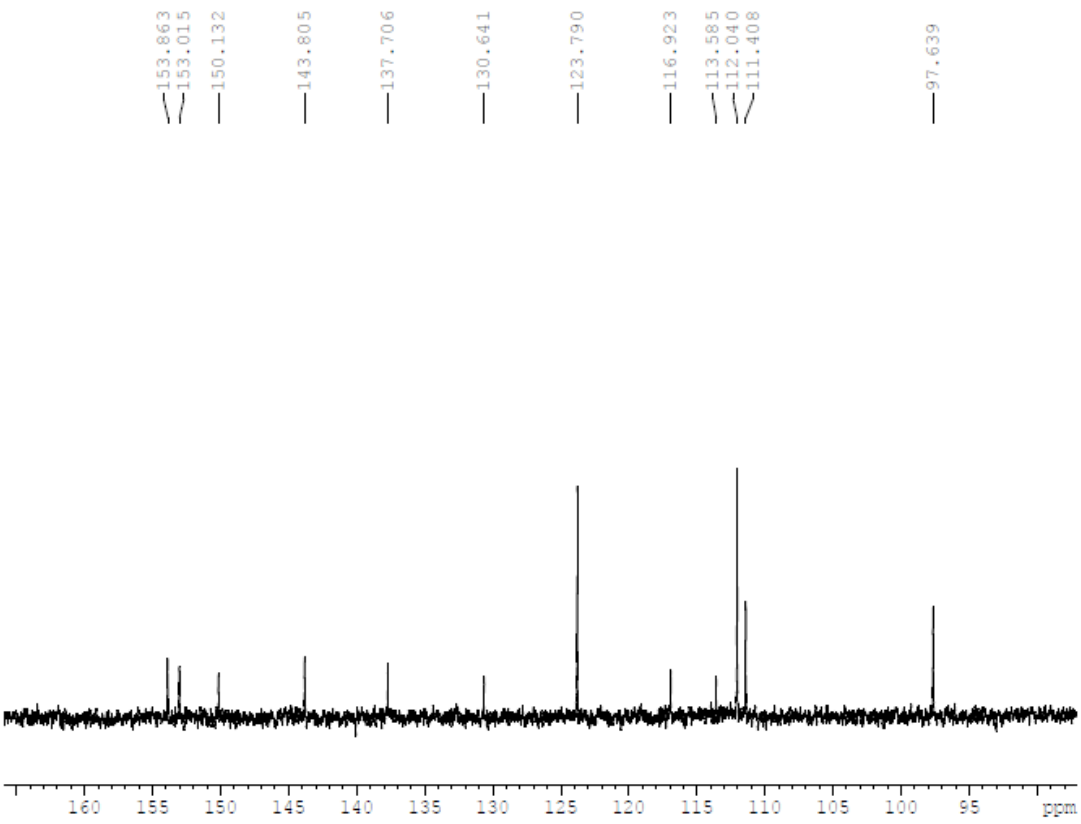

152.777
145.688
140.865
135.556
129.424
123.094
122.630
115.293
112.388
111.443
155 150 145 140 135 130 125 120 115 ppm

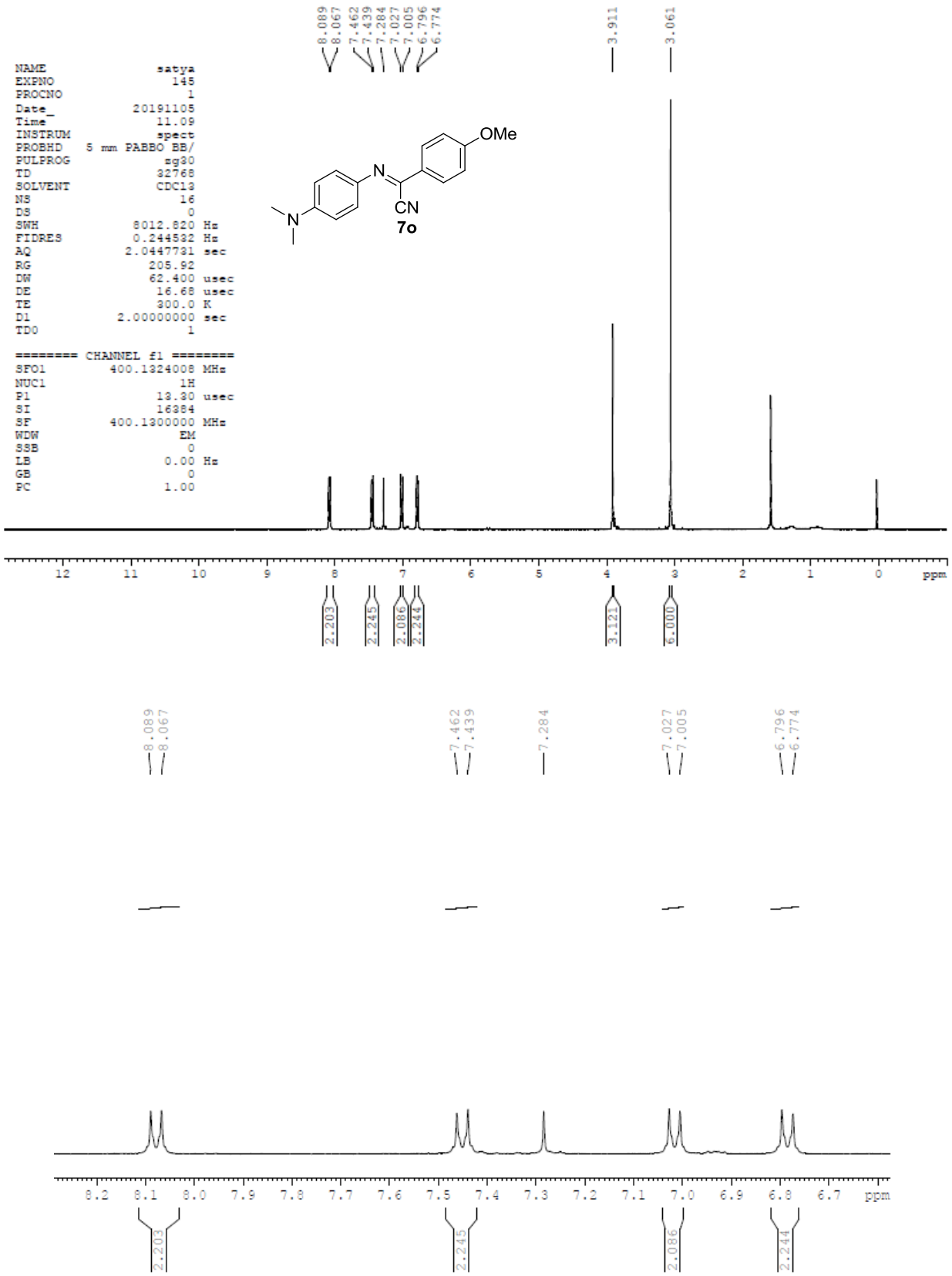

NAME DYY-IS-108X
EXPNO 1
PROCNO 1
Date_ 20200922
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244832 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 294.5 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.514
7.491
7.376
7.368
7.056
7.048
7.034
7.026
6.980
6.958
6.791
6.768
3.950
3.849
3.066
OMe
N
CN
OMe
N
7m
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.900
1.000
1.079
1.127
2.048
3.061
3.170
6.000
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm
1.900
1.000
1.079
1.127
2.048

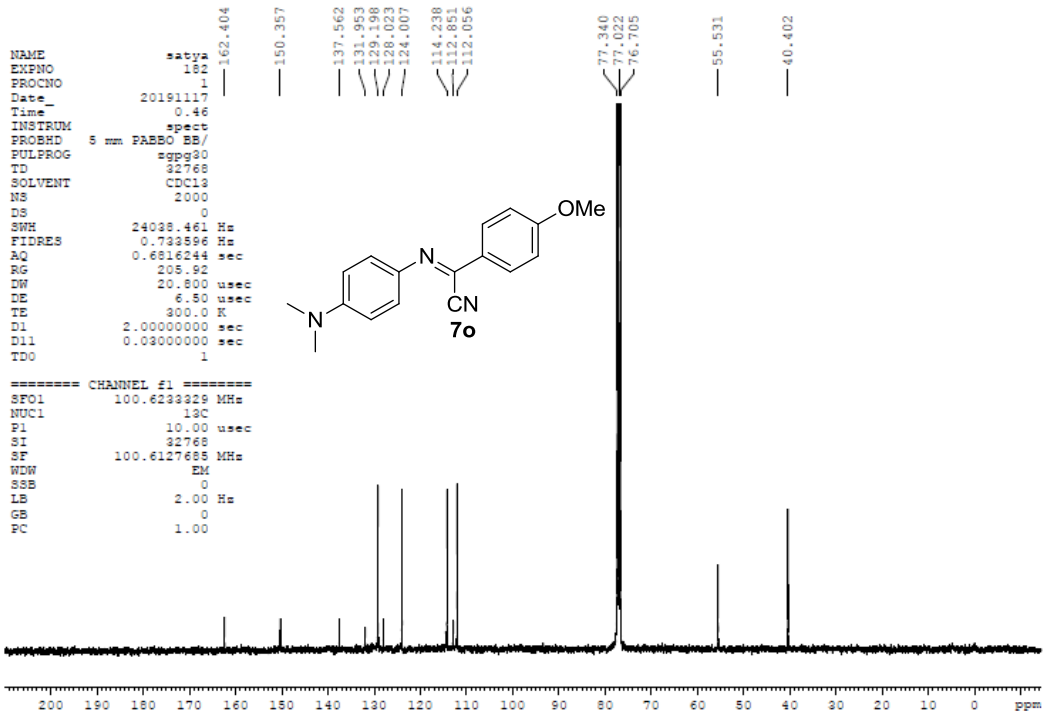

NAME DYY-IS-108XC
EXPNO 1
PROCNO 1
Date_ 20200927
Time 6.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
153.873
152.689
150.554
137.211
130.114
125.781
124.364
118.959
113.876
113.613
111.876
77.346
77.028
76.711
56.714
55.919
40.380
OMe
N
CN
OMe
N
7m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
155 150 145 140 135 130 125 120 115 ppm


NAME satya
EXPNO 104
PROCNO 1
Date_ 20191011
Time 13.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OMe
OMe
N
CN
OMe
N
7n
7.434
7.423
7.400
6.794
6.772
6.585
3.984
3.981
3.932
3.052
ppm
1.010
1.998
2.061
1.075
5.908
2.973
6.000

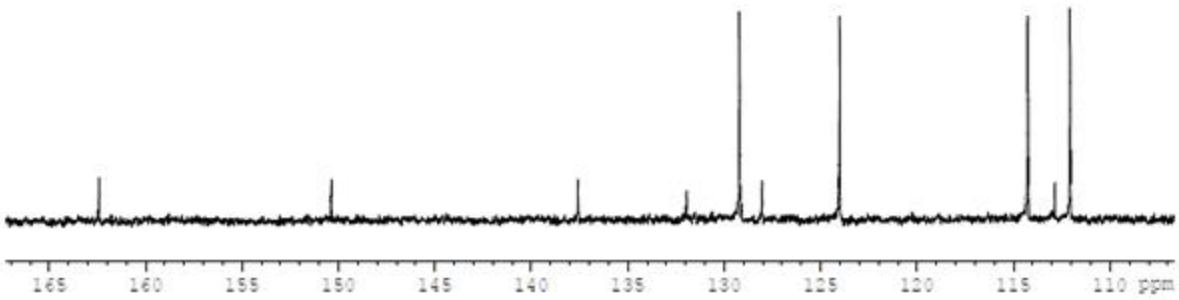

153.863
153.015
150.132
143.805
137.706
130.641
123.790
116.923
113.585
112.040
111.408
97.639
77.339
77.021
76.704
57.015
56.417
56.175
40.450
NAME DYY-28-79DCC
EXPNO 1
PROCNO 1
Date_ 20200927
Time 2.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233929 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
OMe
OMe
OMe
N
CN
N
7n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

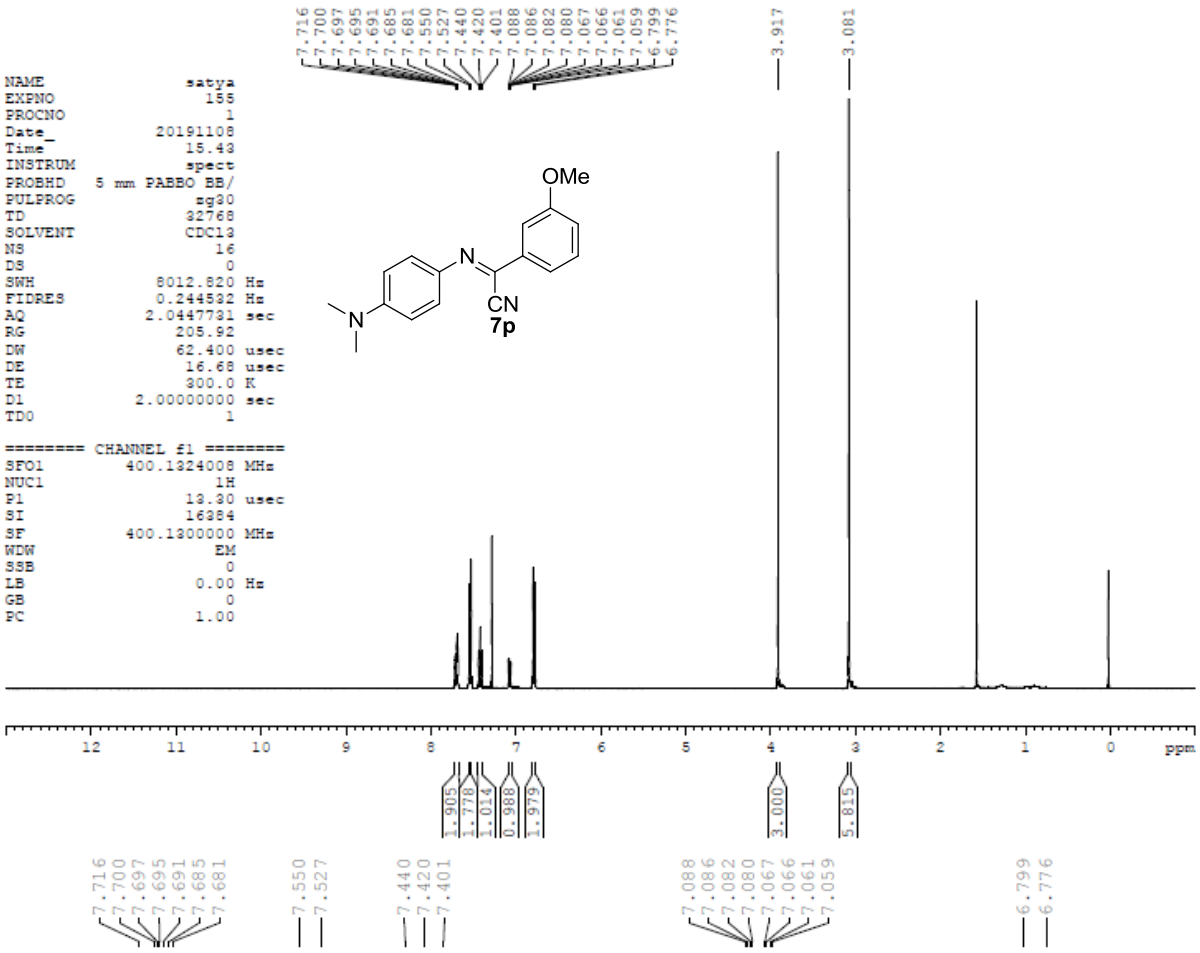

153.863
153.015
150.132
143.805
137.706
130.641
123.790
116.923
113.585
112.040
111.408
97.639
160 155 150 145 140 135 130 125 120 115 110 105 100 95 ppm

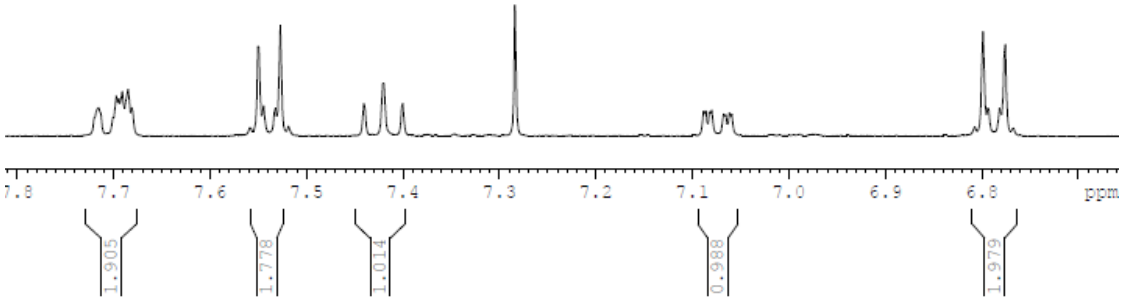

8.089
8.067
7.462
7.439
7.284
7.027
7.005
6.796
6.774
3.911
3.061
NAME satya
EXPNO 145
PROCNO 1
Date_ 20191105
Time 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OMe
N
CN
7o
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.203
2.245
2.086
2.244
3.121
6.000
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm

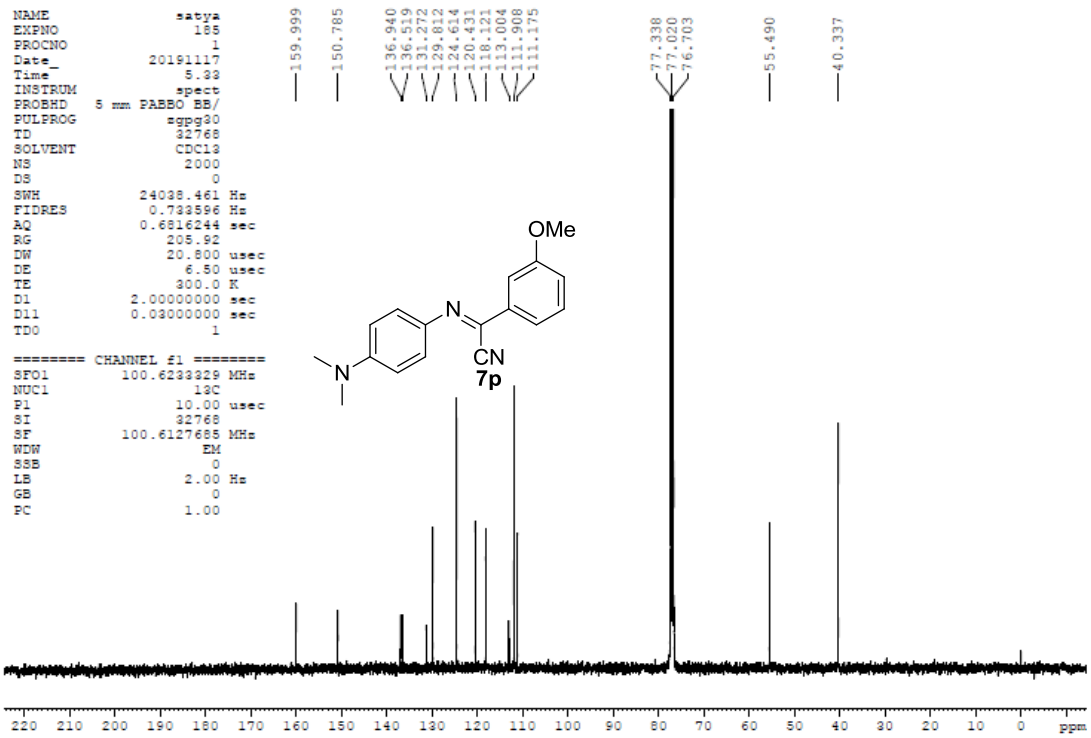

NAME satya
EXPNO 182
PROCNO 1
Date_ 20191117
Time 0.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
162.404
150.357
137.562
131.953
129.198
128.023
124.007
114.238
112.851
112.056
77.340
77.022
76.705
55.531
40.402
OMe
N
CN
N
7o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

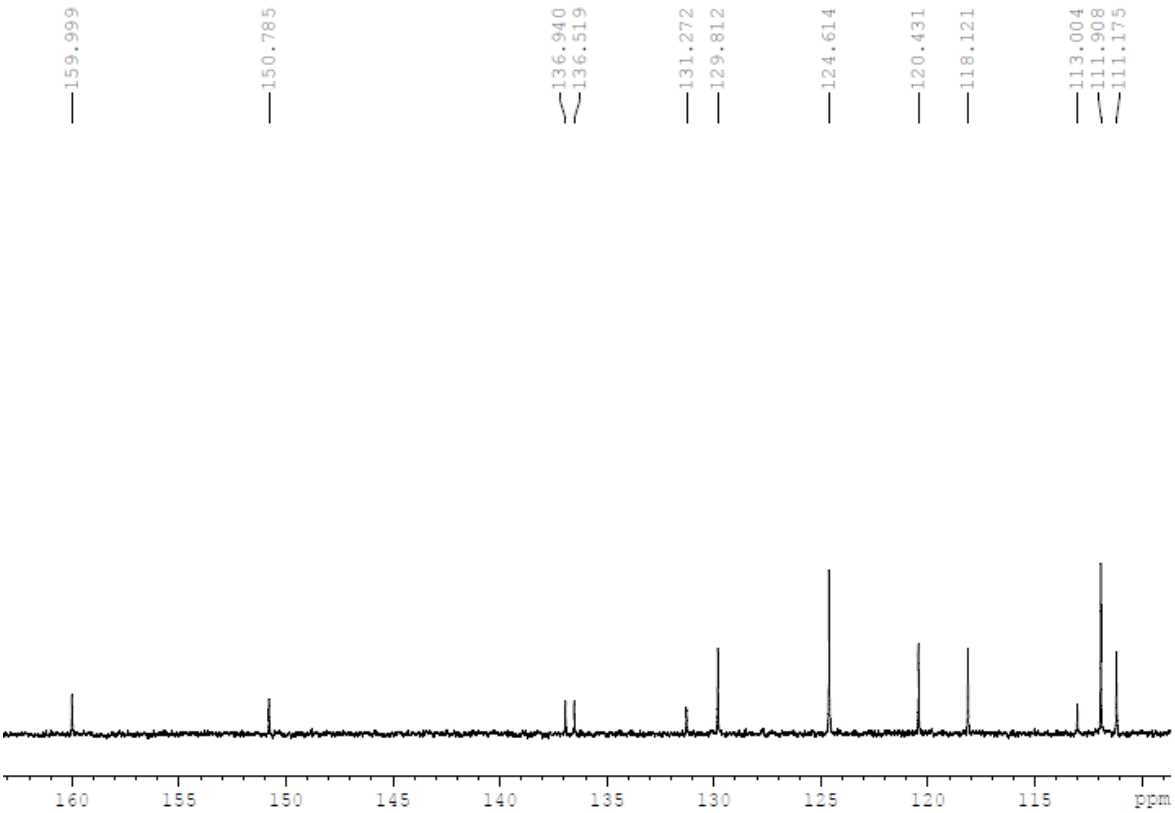

162.404
150.357
137.562
131.953
129.198
128.023
124.007
114.238
112.851
112.056

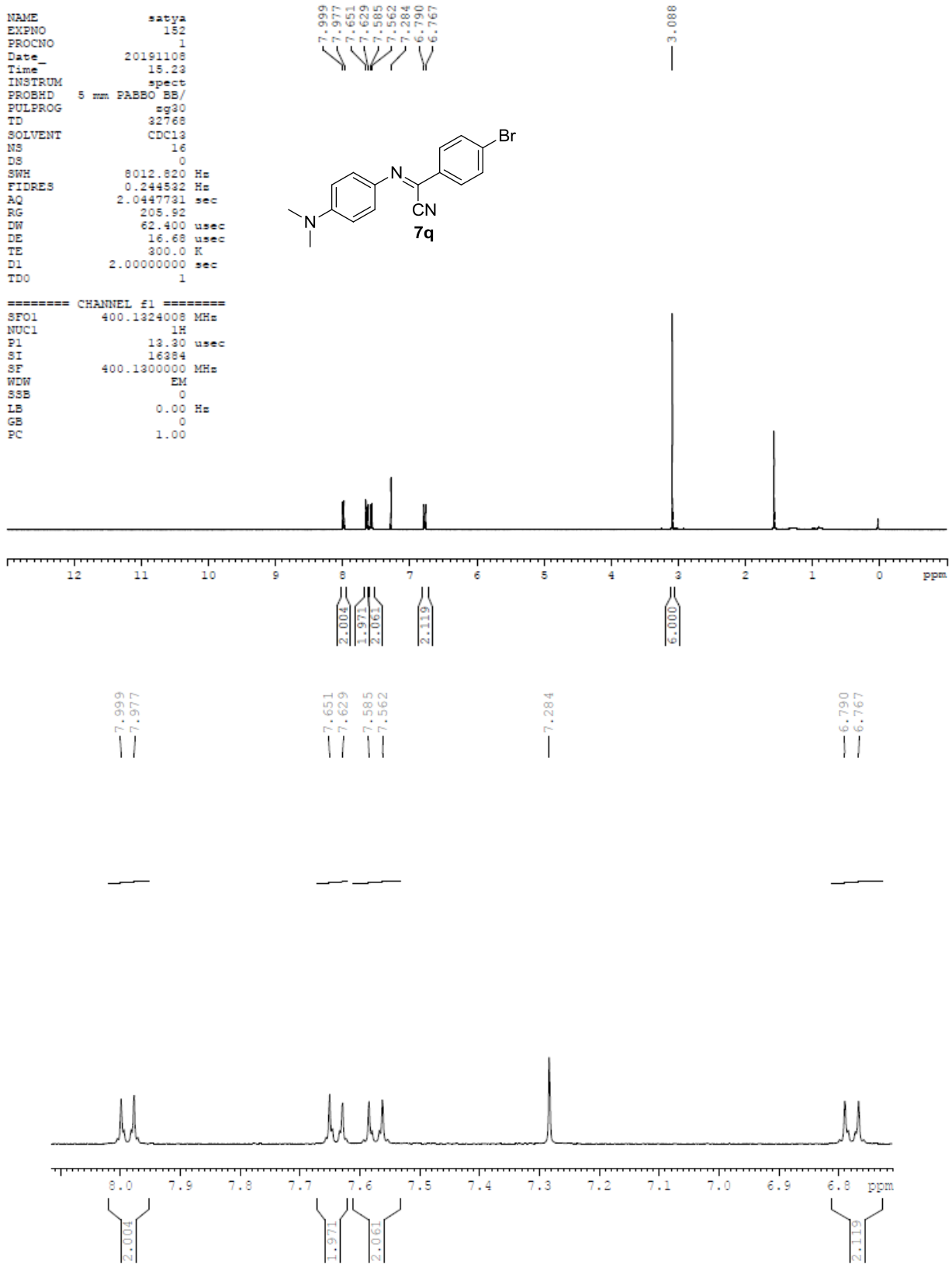

165 160 155 150 145 140 135 130 125 120 115 110 ppm

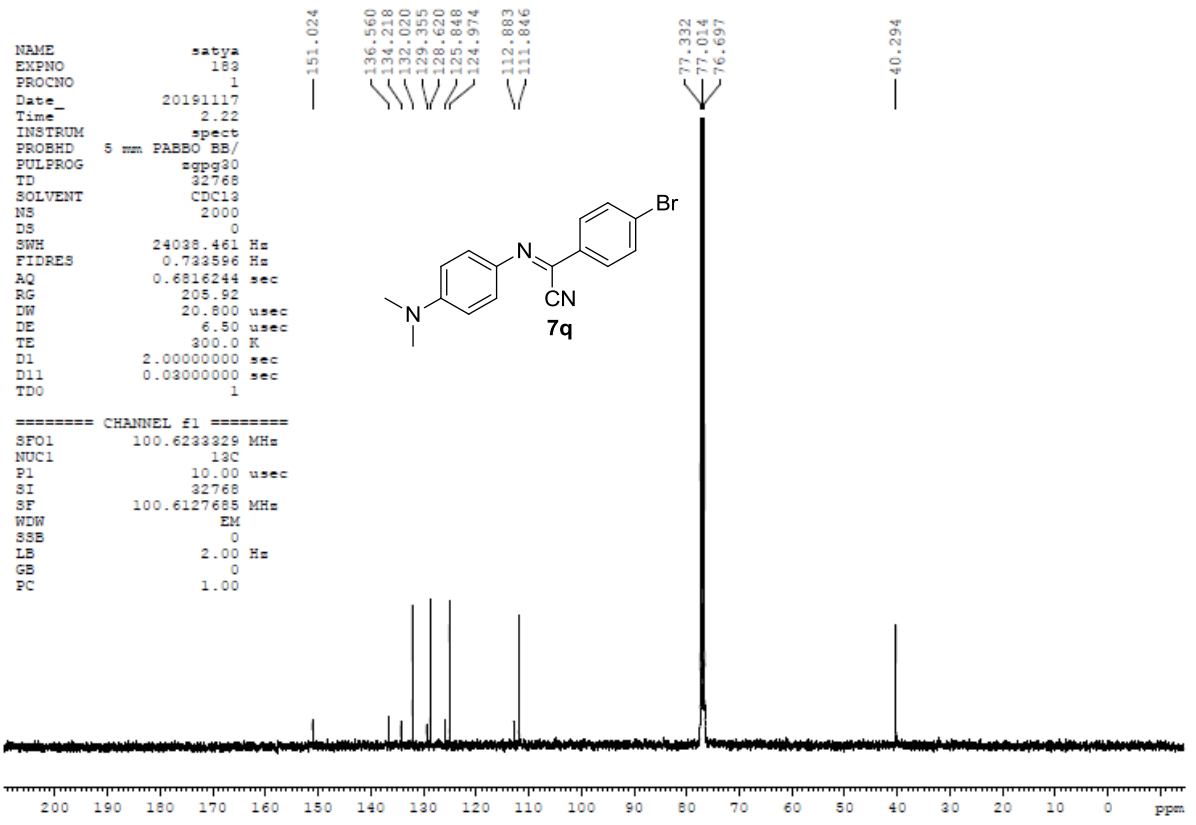

NAME satya
EXPNO 155
PROCNO 1
Date_ 20191108
Time 15.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OMe
N
N
CN
7p
7.716
7.700
7.697
7.695
7.691
7.685
7.681
7.550
7.527
7.440
7.420
7.401
7.088
7.086
7.082
7.080
7.067
7.066
7.061
7.059
6.799
6.776
3.917
3.081
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.905
1.778
1.014
0.988
1.979
3.000
5.815

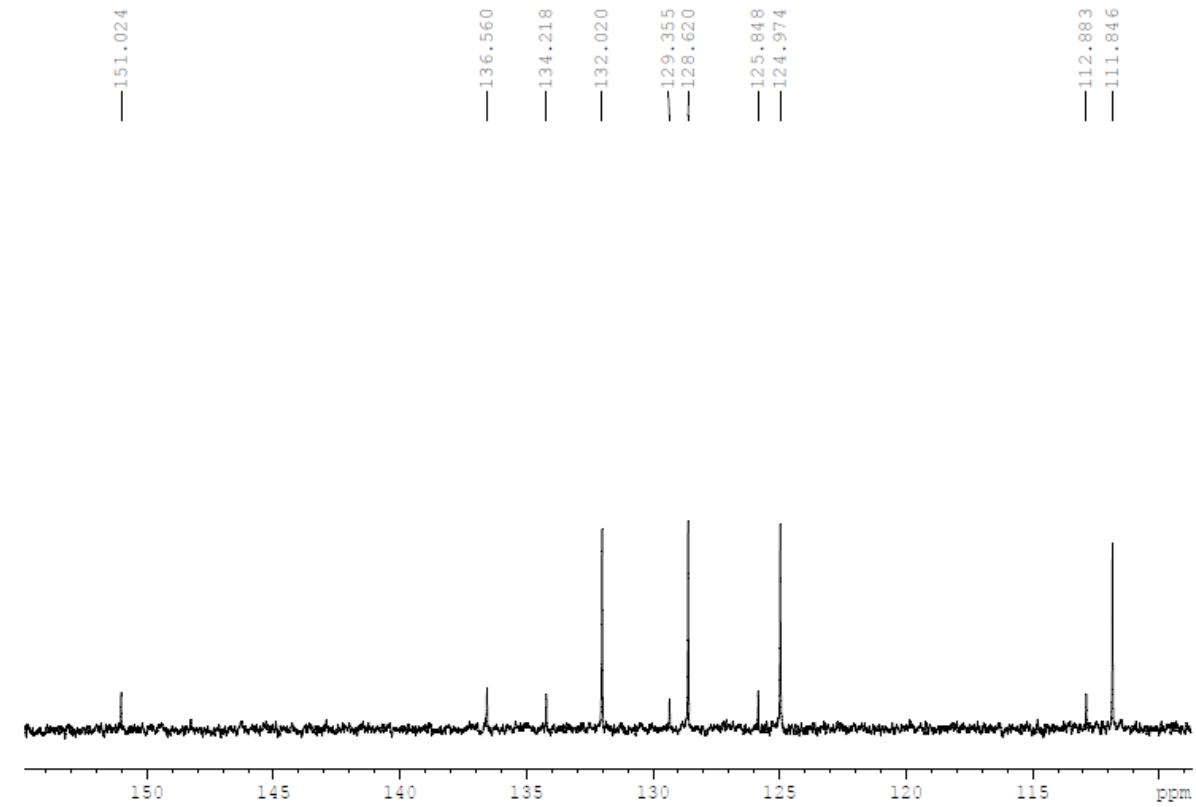

7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm
1.905
1.778
1.014
0.988
1.979

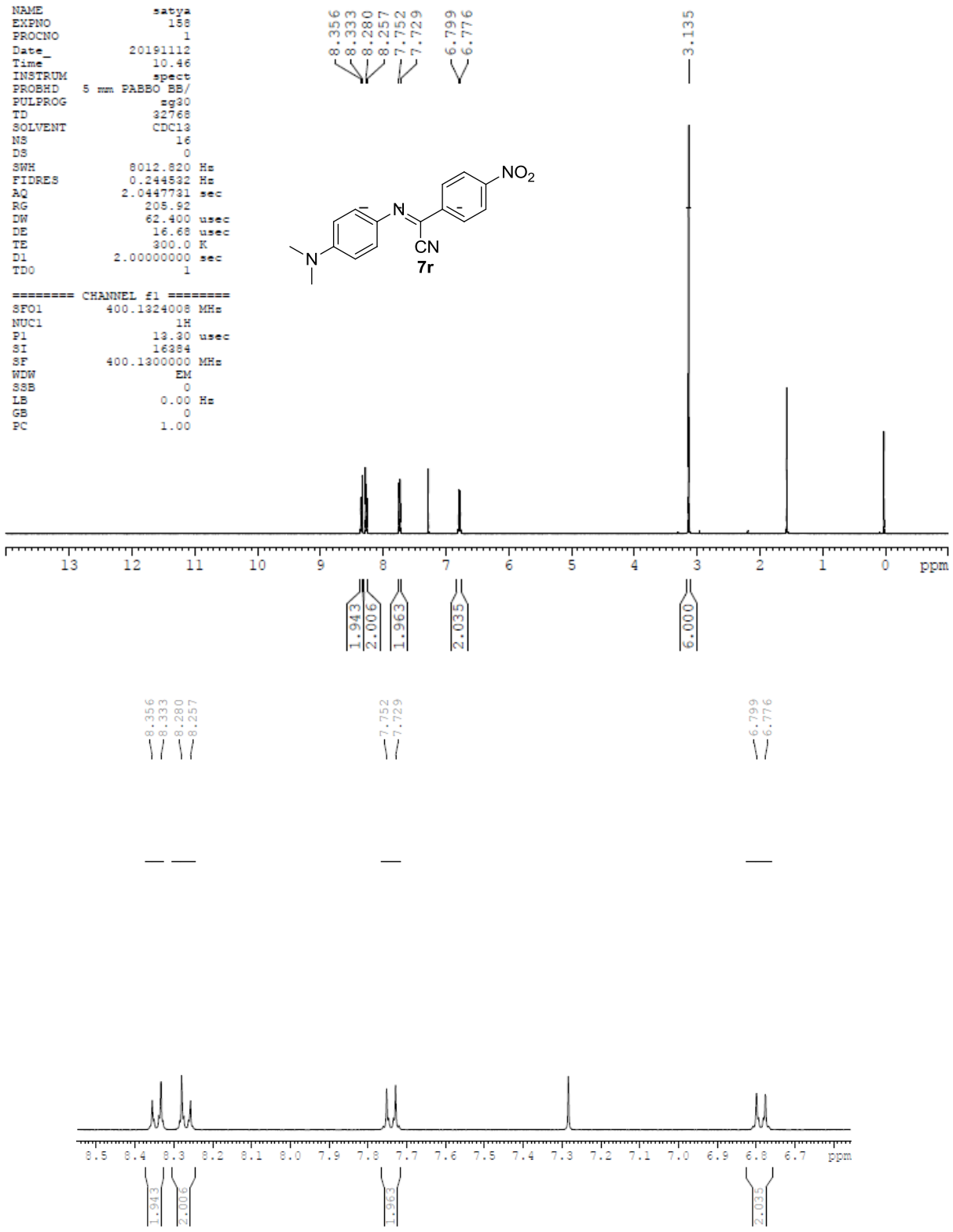

NAME satya
EXPNO 185
PROCNO 1
Date_ 20191117
Time_ 5.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
159.999
150.785
136.940
136.519
131.272
129.812
124.614
120.431
118.121
113.004
111.908
111.175
77.338
77.020
76.703
55.490
40.337
OMe
N
CN
N
7p
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

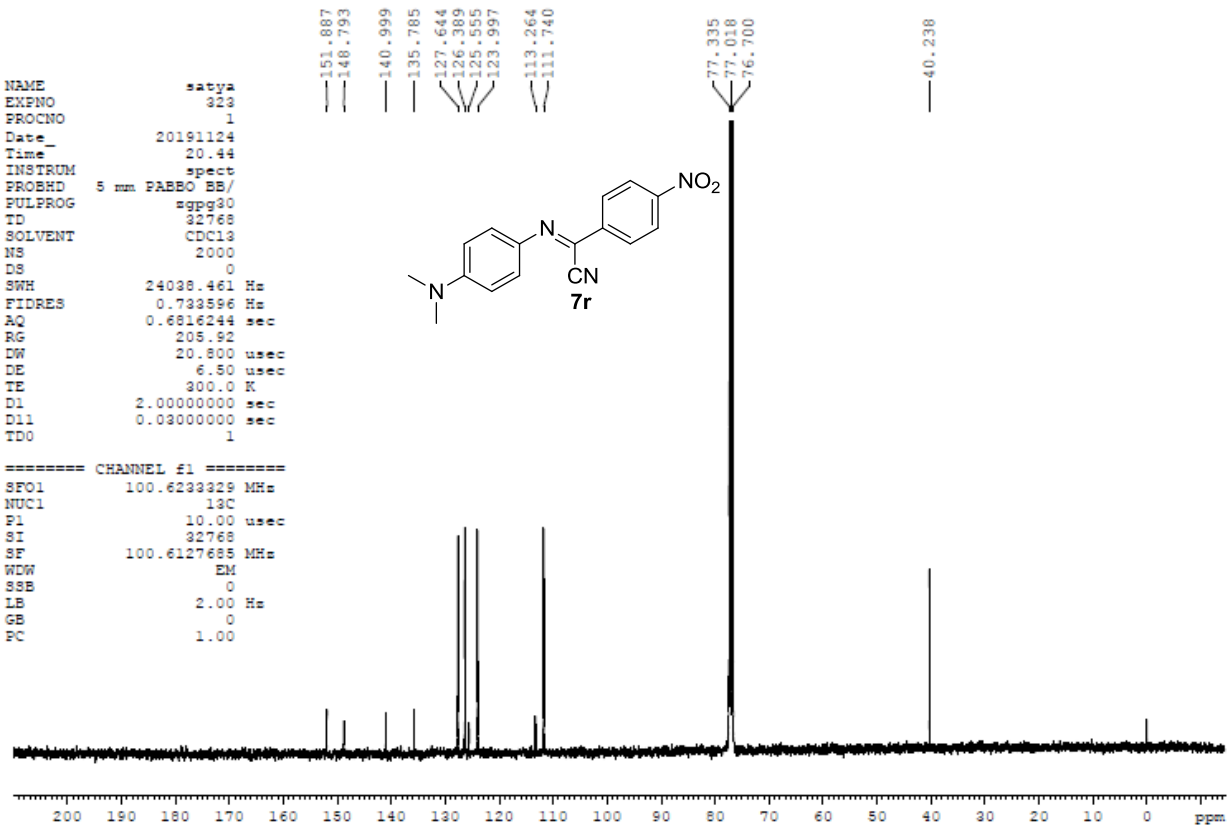

159.999
150.785
136.940
136.519
131.272
129.812
124.614
120.431
118.121
113.004
111.908
111.175
160 155 150 145 140 135 130 125 120 115 ppm

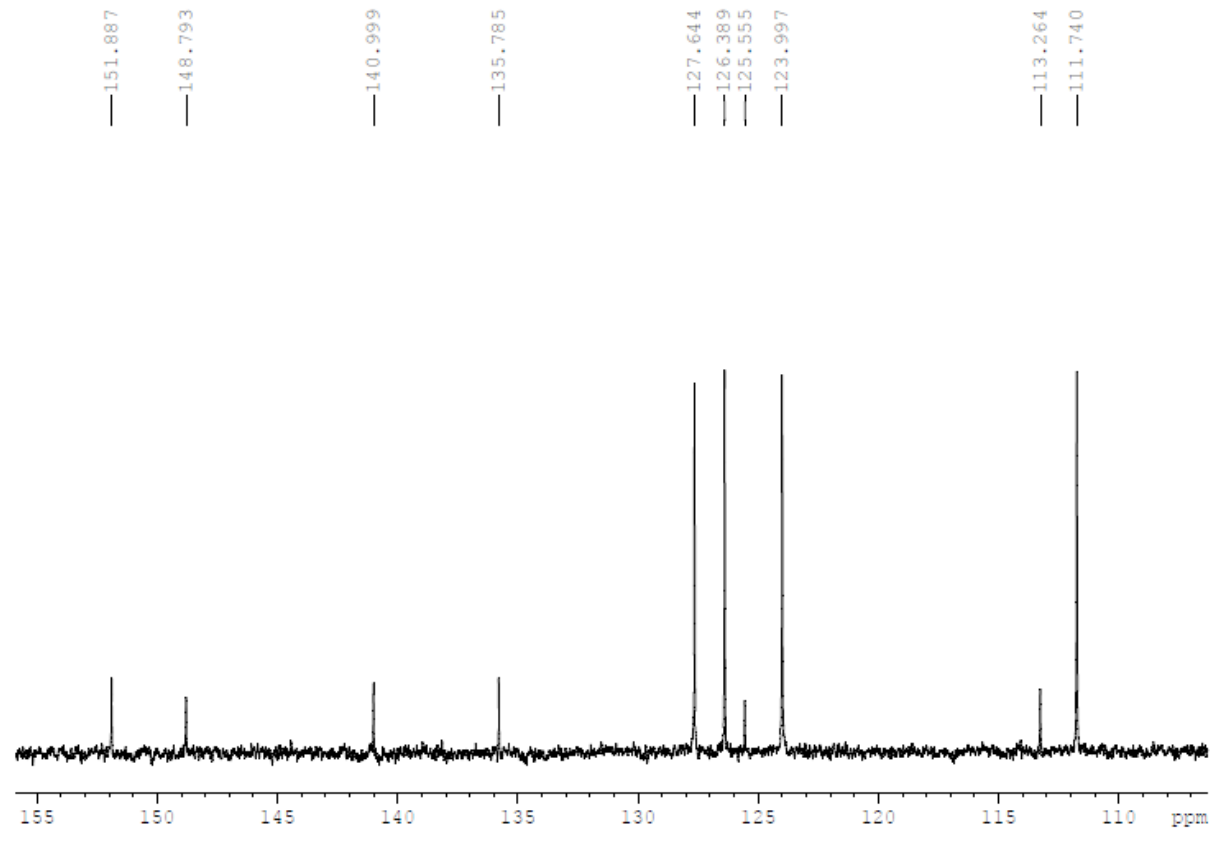

NAME satya
EXPNO 152
PROCNO 1
Date_ 20191108
Time 15.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.999
7.977
7.651
7.629
7.585
7.562
7.284
6.790
6.767
3.088
Br
N
CN
N
7q
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.004
1.971
2.061
2.119
6.000
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm

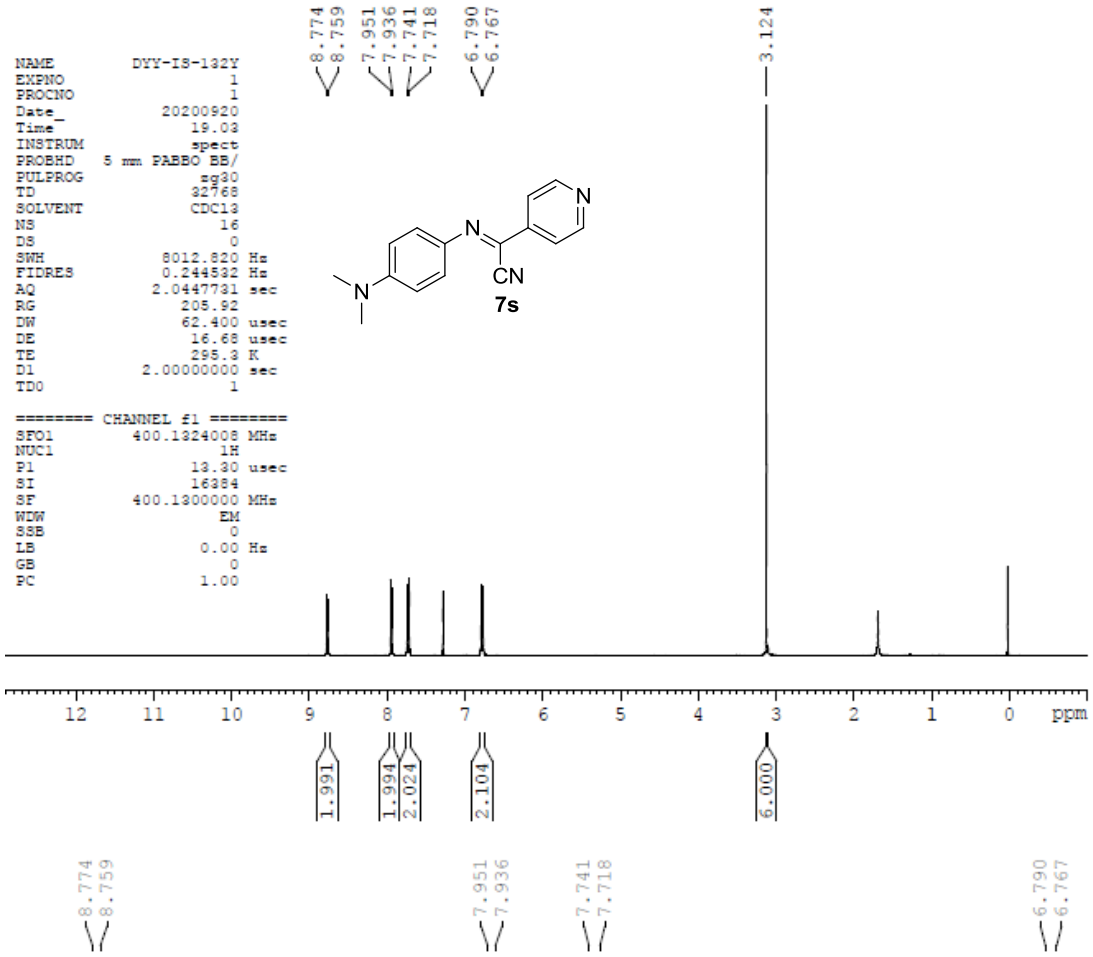

NAME satya
EXPNO 183
PROCNO 1
Date_ 20191117
Time 2.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
151.024
136.560
134.218
132.020
129.355
128.620
125.848
124.974
112.883
111.846
77.332
77.014
76.697
40.294
Br
N
CN
N
7q
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

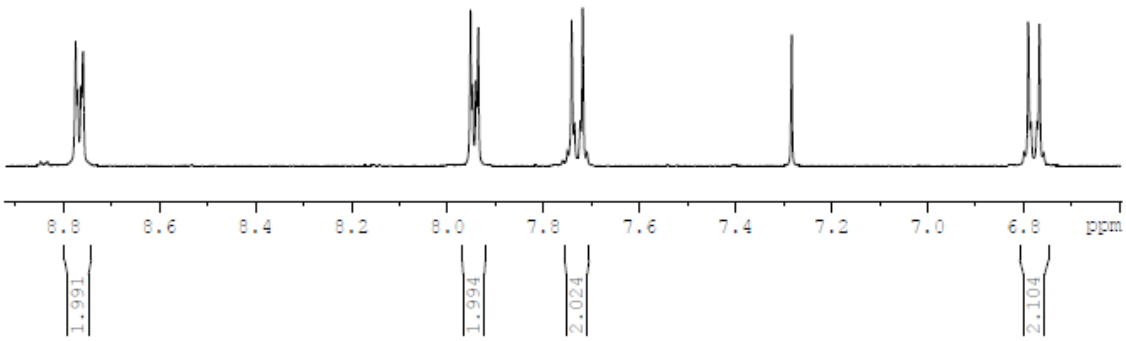

151.024
136.560
134.218
132.020
129.355
128.620
125.848
124.974
112.883
111.846
150 145 140 135 130 125 120 115 ppm

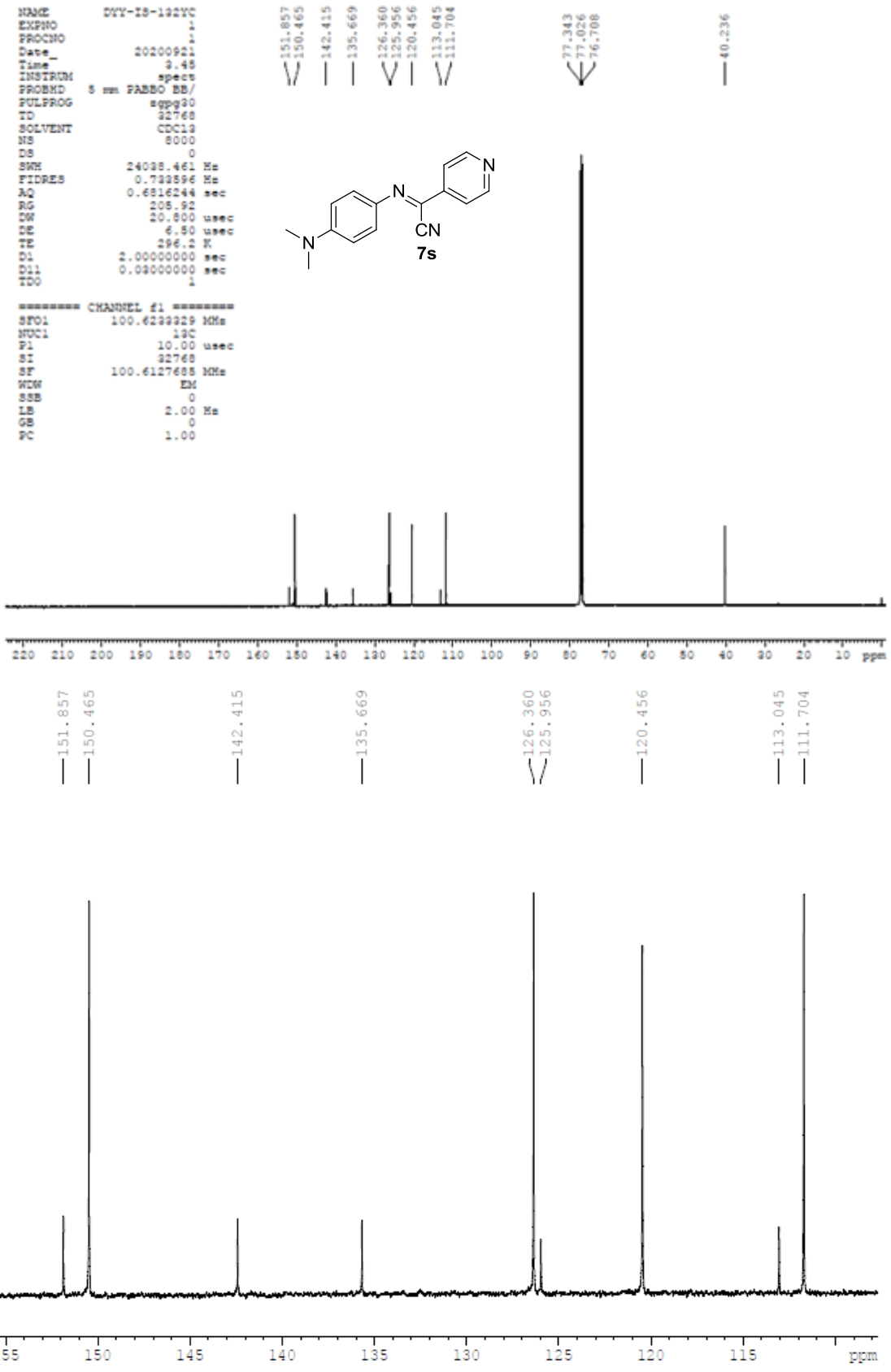

NAME satya
EXPNO 158
PROCNO 1
Date_ 20191112
Time 10.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.356
8.333
8.280
8.257
7.752
7.729
6.799
6.776
3.135
NO2
N
CN
N
7r
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.943
2.006
1.963
2.035
6.000
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm

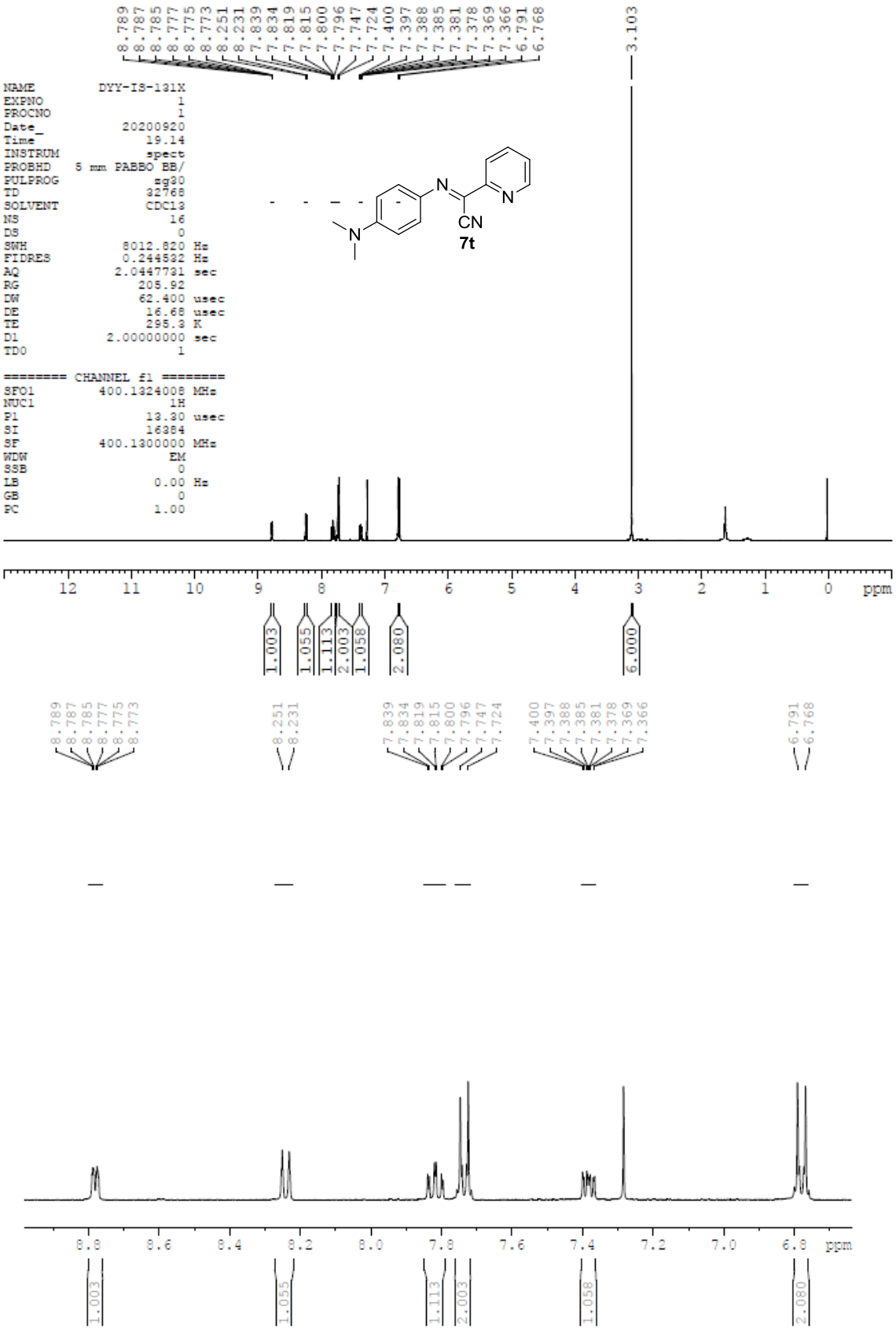

151.887
148.793
140.999
135.785
127.644
126.389
125.555
123.997
113.264
111.740
77.335
77.018
76.700
40.238
NAME satya
EXPNO 323
PROCNO 1
Date_ 20191124
Time_ 20.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
NO2
N
CN
N
7r
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

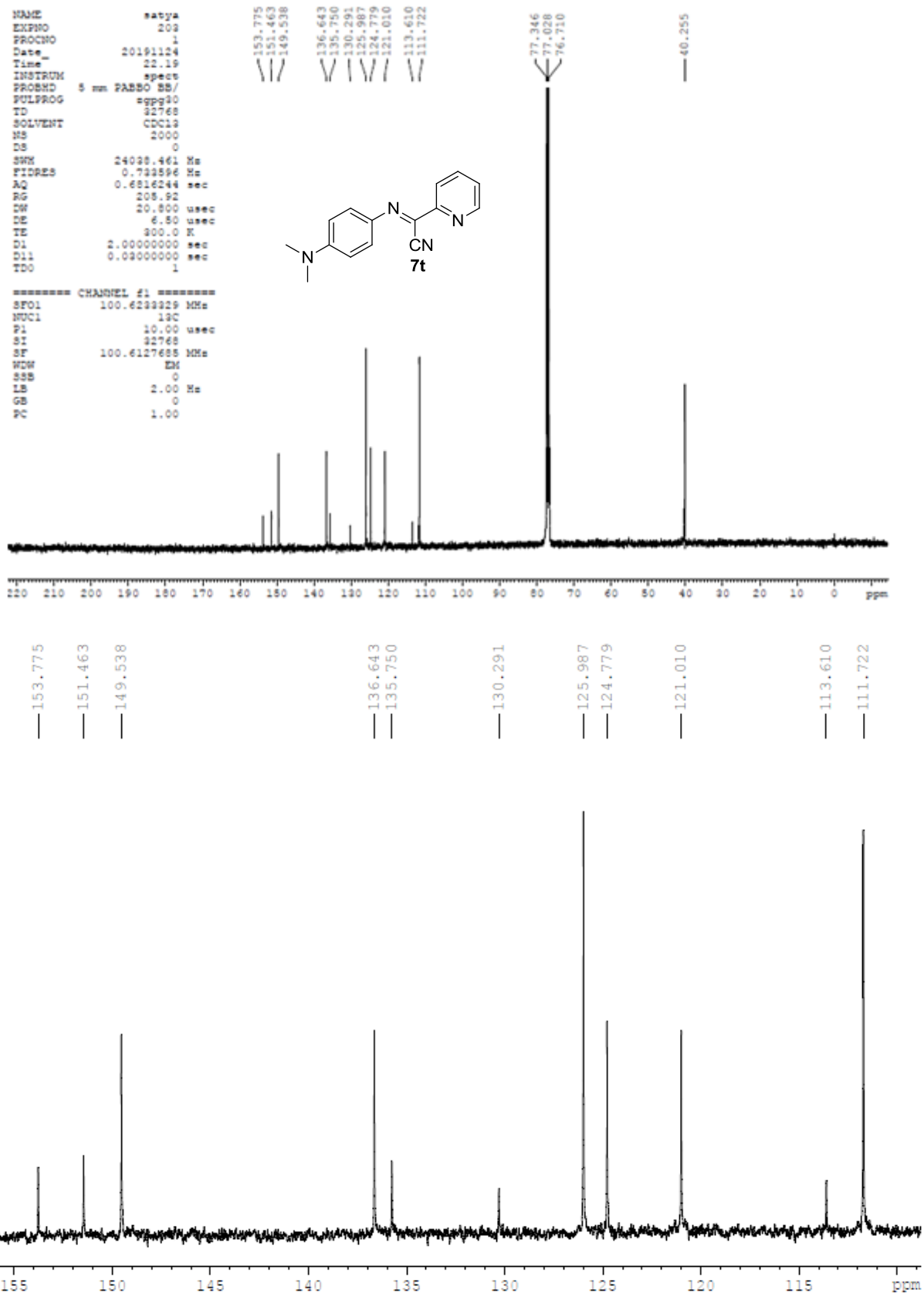

151.887
148.793
140.999
135.785
127.644
126.389
125.555
123.997
113.264
111.740
155 150 145 140 135 130 125 120 115 110 ppm

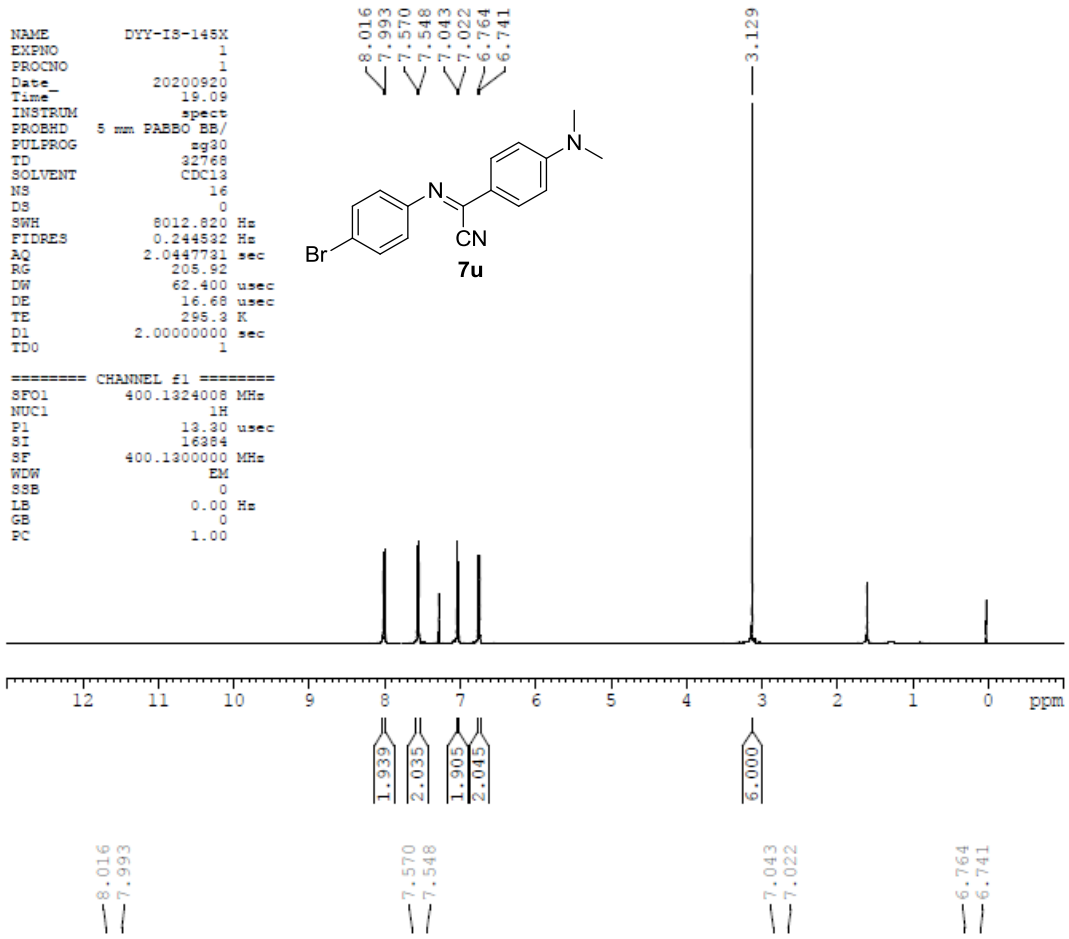

NAME DYY-IS-132Y
EXPNO 1
PROCNO 1
Date_ 20200920
Time 19.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.774
8.759
7.951
7.936
7.741
7.718
6.790
6.767
3.124
N
N
CN
7s
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.991
1.994
2.024
2.104
6.000

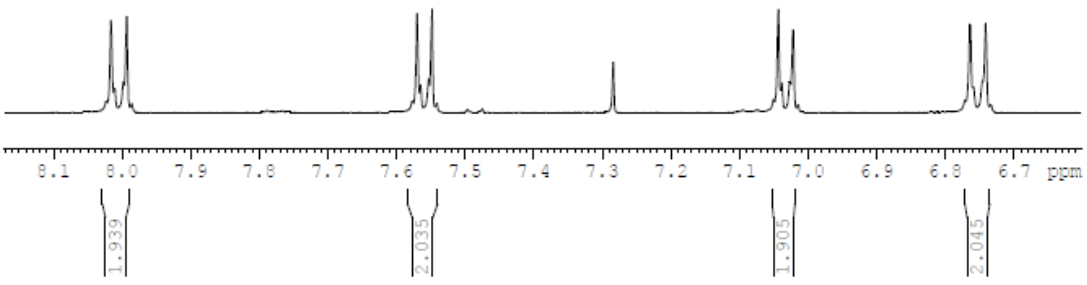

8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
ppm
1.991
1.994
2.024
2.104

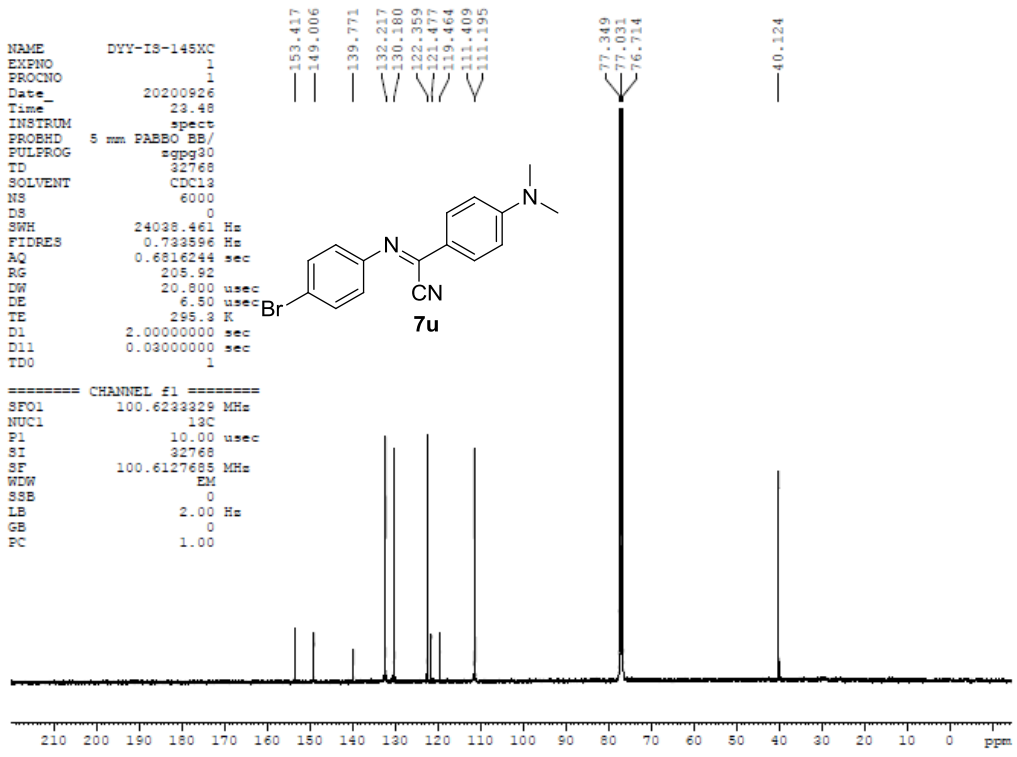

NAME DYY-IS-192YC
EXPNO 1
PROCNO 1
Date_ 20200921
Time 9.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 8000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
151.857
150.465
142.415
135.669
126.360
125.956
120.456
113.045
111.704
77.343
77.026
76.708
40.236
N
N
CN
N
7s
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
151.857
150.465
142.415
135.669
126.360
125.956
120.456
113.045
111.704
155 150 145 140 135 130 125 120 115 ppm


8.789
8.787
8.785
8.777
8.775
8.773
8.251
8.231
7.839
7.834
7.819
7.815
7.800
7.796
7.747
7.724
7.400
7.397
7.388
7.385
7.381
7.378
7.369
7.366
6.791
6.768
3.103
NAME DYY-IS-131X
EXPNO 1
PROCNO 1
Date_ 20200920
Time 19.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
N
N
CN
7t
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.003
1.055
1.113
2.003
1.058
2.080
6.000
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 ppm
1.003
1.055
1.113
2.003
1.058
2.080

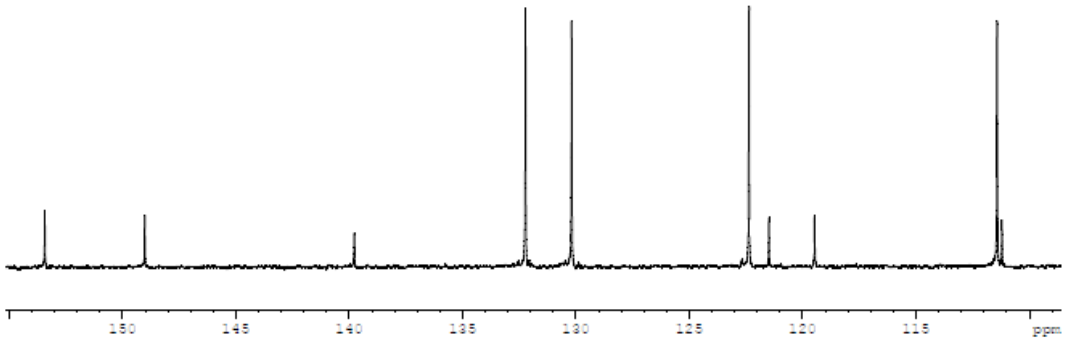

NAME satya
EXPNO 203
PROCNO 1
Date_ 20191124
Time 22.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233929 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
153.775
151.463
149.538
136.643
135.750
130.291
125.987
124.779
121.010
113.610
111.722
77.346
77.028
76.710
40.255
N
N
CN
N
7t
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
153.775
151.463
149.538
136.643
135.750
130.291
125.987
124.779
121.010
113.610
111.722
155 150 145 140 135 130 125 120 115 ppm

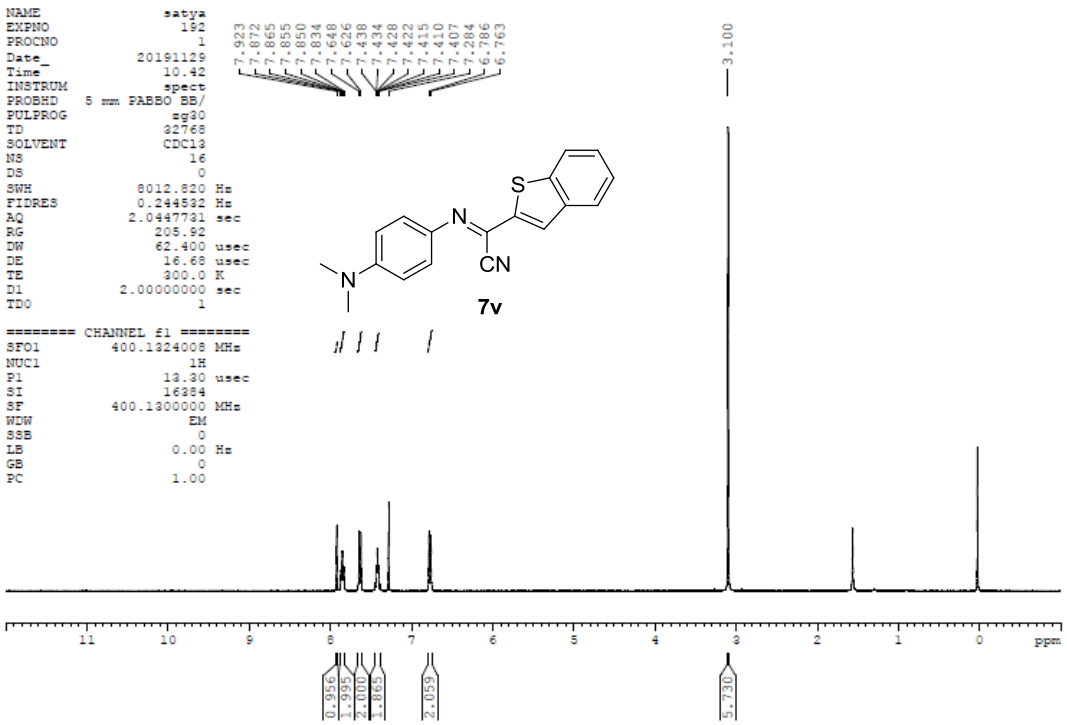

NAME DYY-IS-145X
EXPNO 1
PROCNO 1
Date_ 20200920
Time 19.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.016
7.993
7.570
7.548
7.043
7.022
6.764
6.741
3.129
Br
N
CN
7u
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.939
2.035
1.905
2.045
6.000

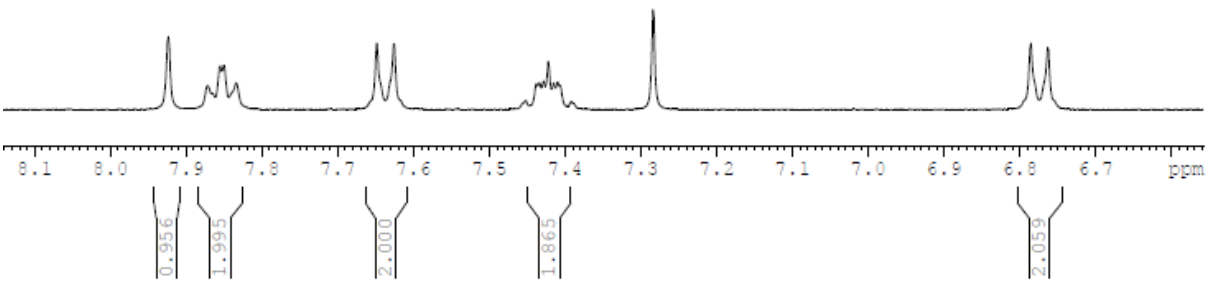

8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm
1.939
2.035
1.905
2.045

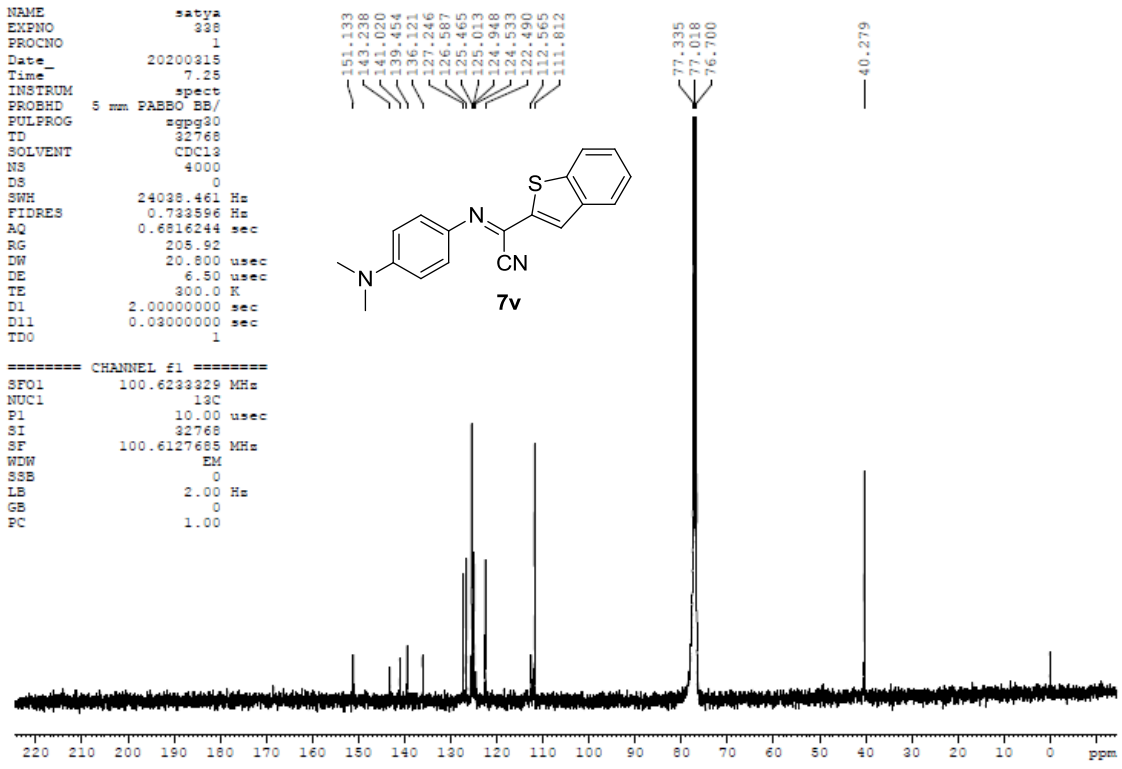

153.417
149.006
139.771
132.217
130.180
122.359
121.477
119.464
111.409
111.195
77.349
77.031
76.714
40.124
NAME DYY-IS-145XC
EXPNO 1
PROCNO 1
Date_ 20200926
Time 23.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 6000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
N
CN
Br
7u
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


153.417
149.006
139.771
132.217
130.180
122.359
121.477
119.464
111.409
111.195

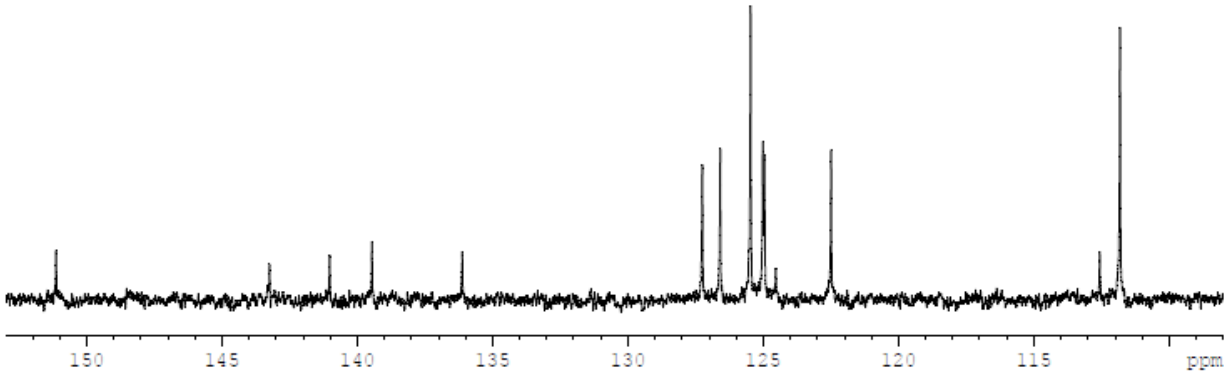

150 145 140 135 130 125 120 115 ppm

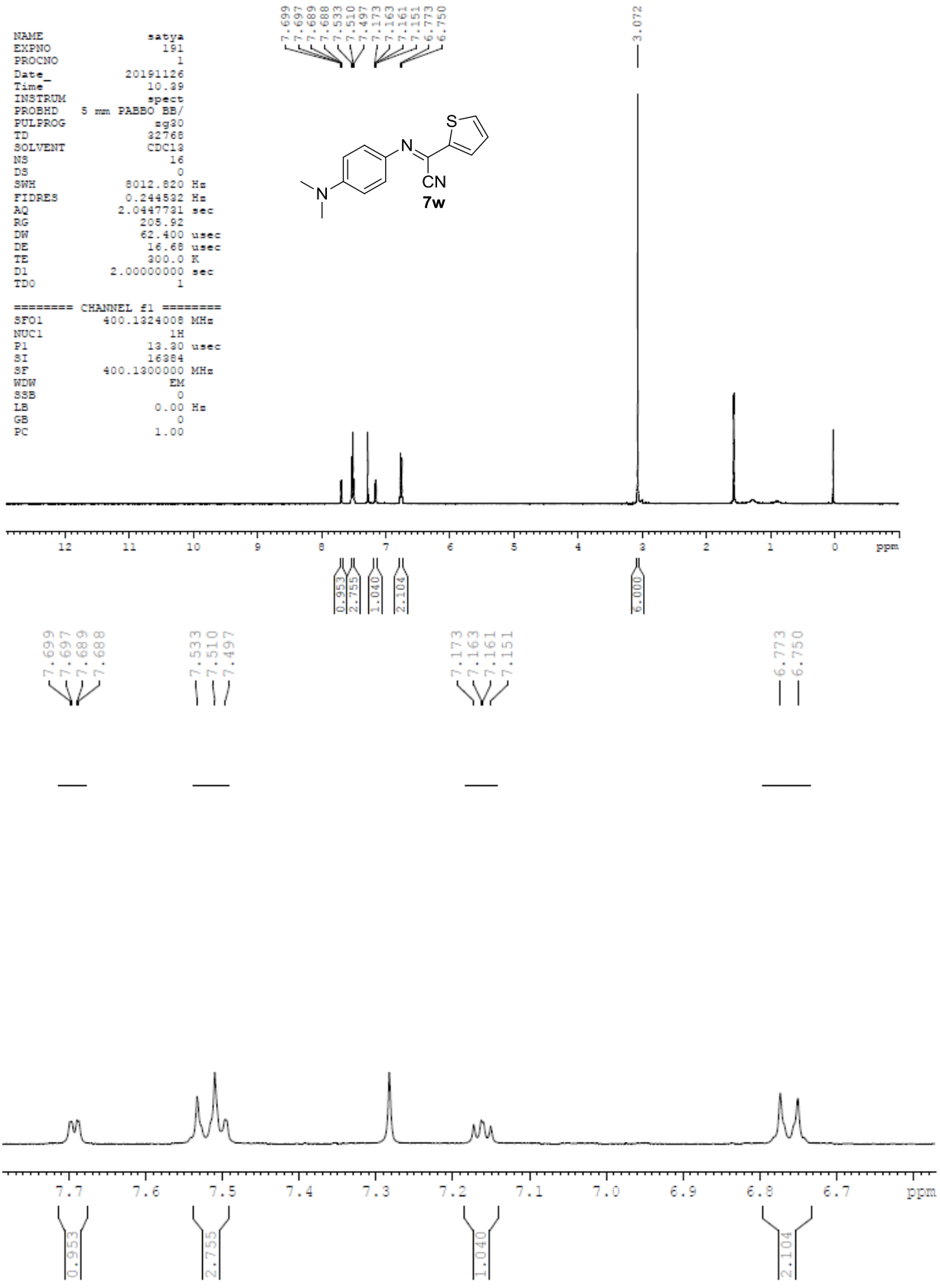

NAME satya
EXPNO 192
PROCNO 1
Date_ 20191129
Time 10.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.923
7.872
7.865
7.855
7.850
7.834
7.648
7.626
7.438
7.434
7.428
7.422
7.415
7.410
7.407
7.284
6.786
6.763
3.100
S
N
CN
N
7v
ppm
0.956
1.995
2.000
1.865
2.059
5.730

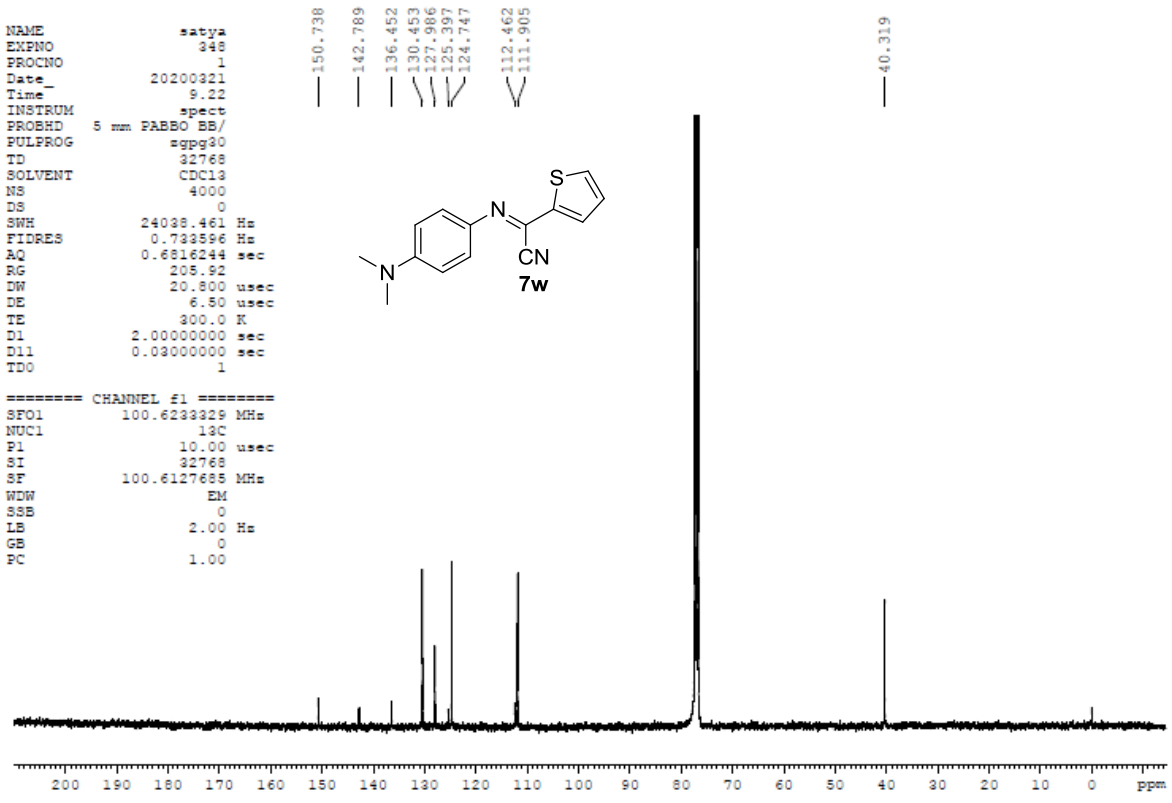

8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
ppm
0.956
1.995
2.000
1.865
2.059

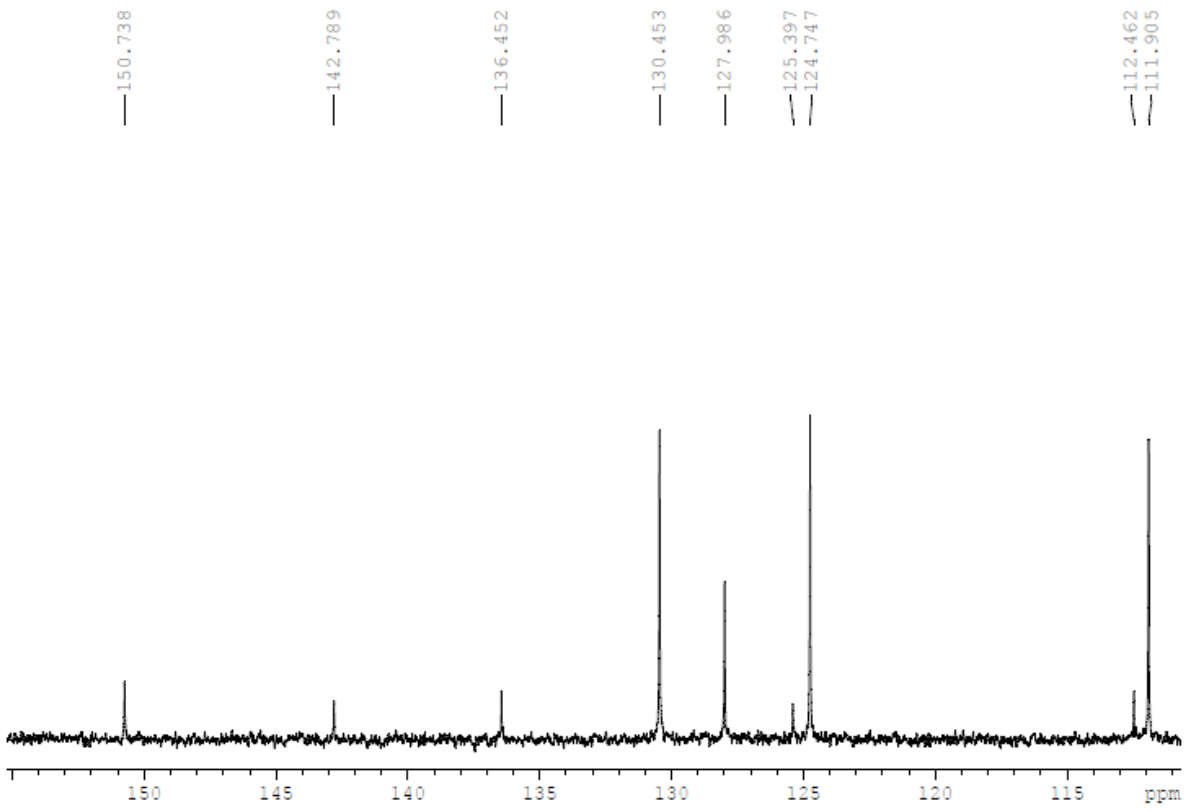

NAME satya
EXPNO 338
PROCNO 1
Date_ 20200315
Time 7.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
151.133
143.238
141.020
139.454
136.121
127.246
126.587
125.465
125.013
124.948
124.533
122.490
112.565
111.812
77.335
77.018
76.700
40.279
S
N
CN
N
7v
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

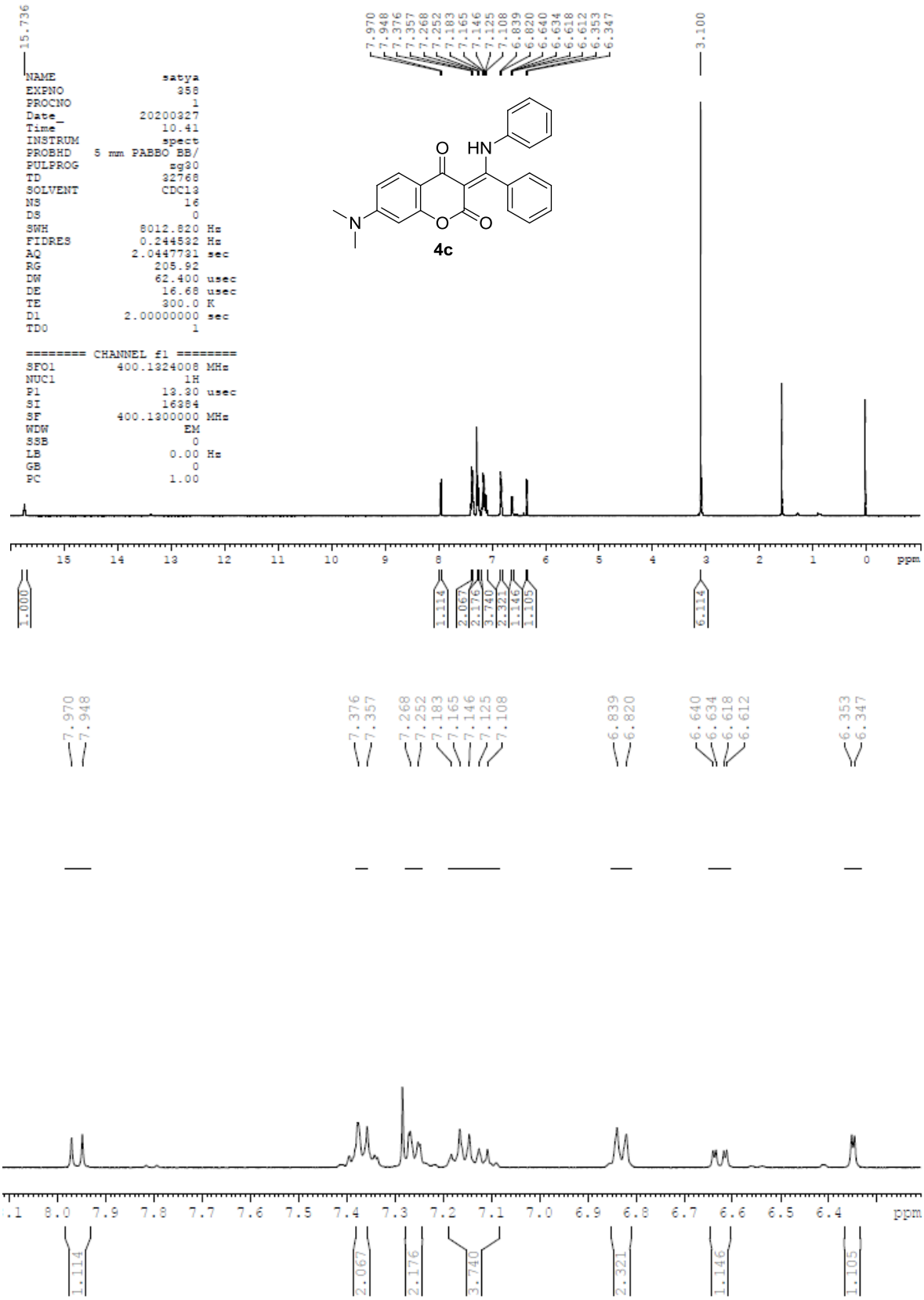

151.133
143.238
141.020
139.454
136.121
127.246
126.587
125.465
125.013
124.948
124.533
122.490
112.565
111.812

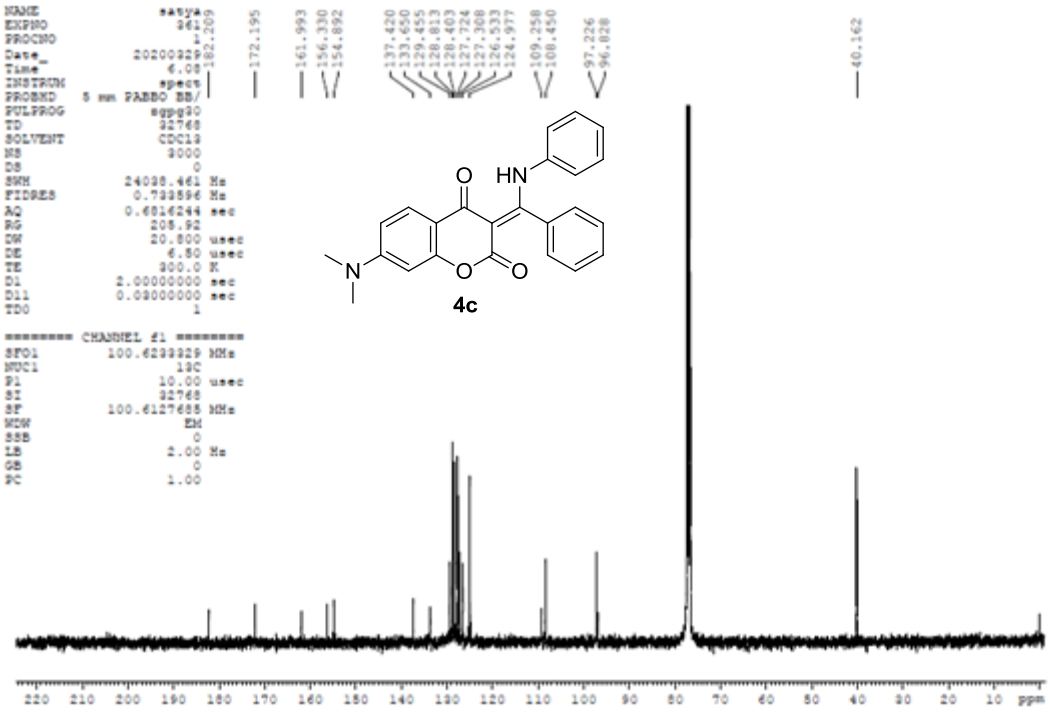

150 145 140 135 130 125 120 115 ppm


NAME satya
EXPNO 191
PROCNO 1
Date_ 20191126
Time 10.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.699
7.697
7.689
7.688
7.533
7.510
7.497
7.173
7.163
7.161
7.151
6.773
6.750
3.072
S
N
CN
N
7w
ppm
0.953
2.755
1.040
2.104
6.000

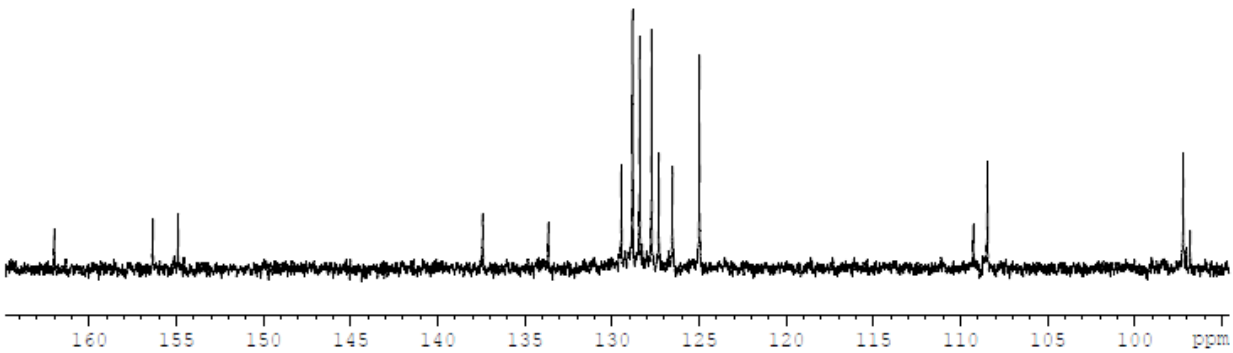

NAME satya
EXPNO 348
PROCNO 1
Date_ 20200321
Time 9.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG sgpg30
TD 32768
SOLVENT CDCl3
NS 4000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
150.738
142.789
136.452
130.453
127.986
125.397
124.747
112.462
111.905
40.319
S
N
CN
N
7w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

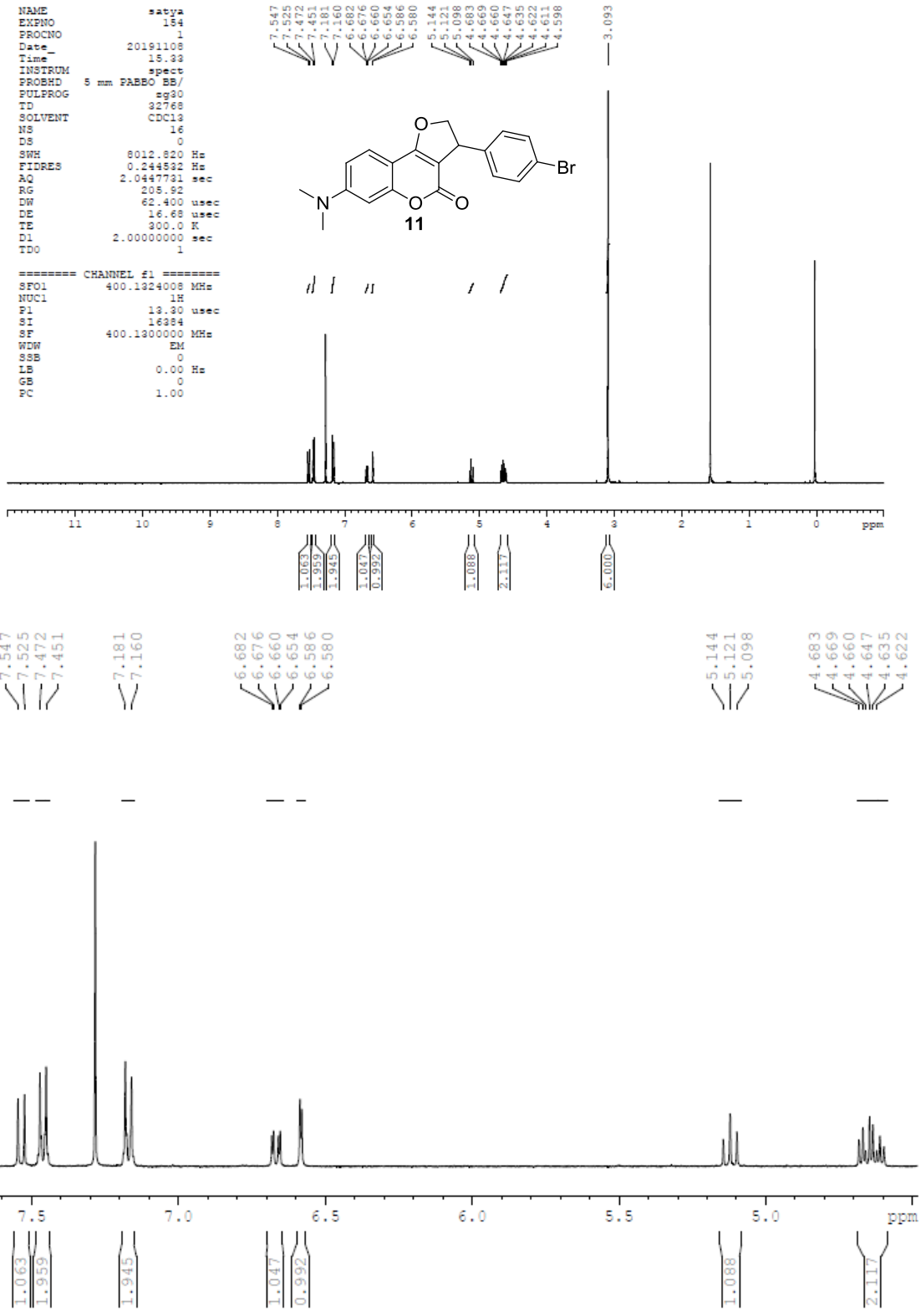

150.738
142.789
136.452
130.453
127.986
125.397
124.747
112.462
111.905
150 145 140 135 130 125 120 115 ppm

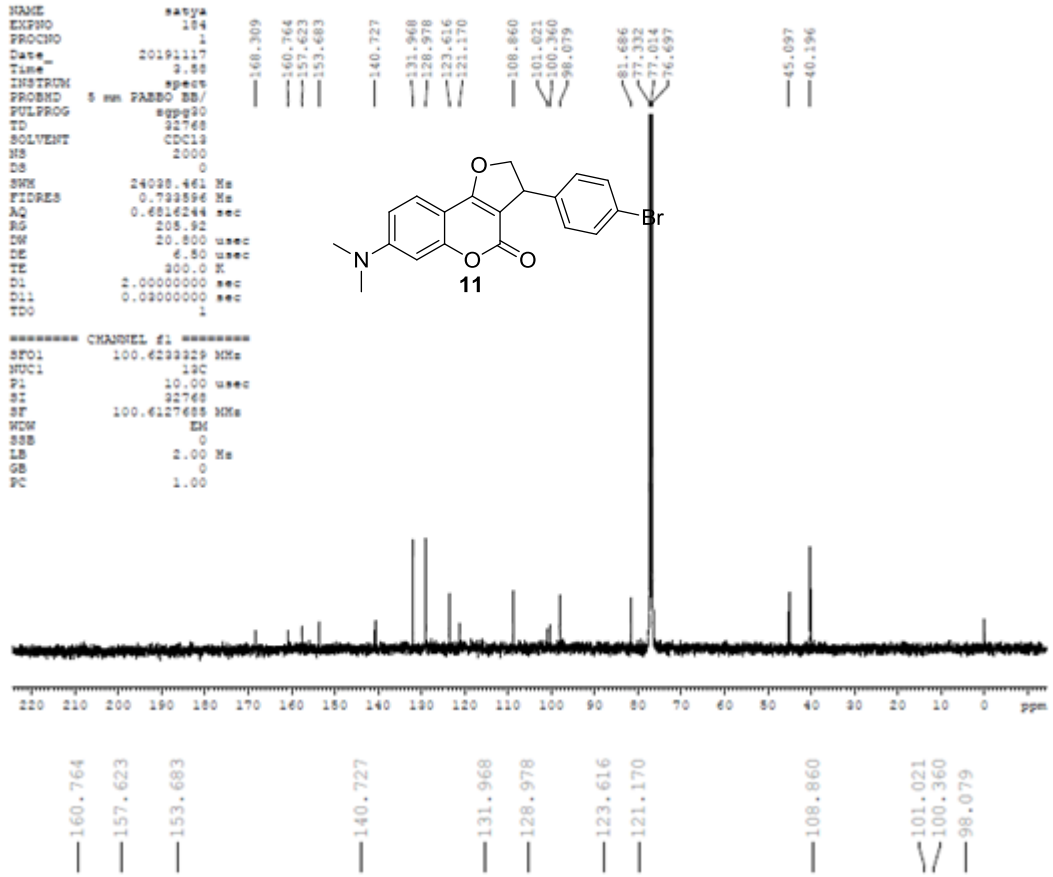

15.736
NAME satya
EXPNO 358
PROCNO 1
Date_ 20200327
Time 10.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.970
7.948
7.376
7.357
7.268
7.252
7.183
7.165
7.146
7.125
7.108
6.839
6.820
6.640
6.634
6.618
6.612
6.353
6.347
3.100
O
HN
N
O
O
4c
ppm
1.000
1.114
2.067
2.176
3.740
2.321
1.146
1.105
6.114


NAME satya
EXPNO 361
PROCNO 1
Date_ 20200321
Time 6.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6239329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
172.195
161.993
156.330
154.892
137.420
133.650
129.455
128.813
128.403
127.724
127.308
126.533
124.977
109.258
108.450
97.226
96.828
40.162
O
HN
N
O
O
4c
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

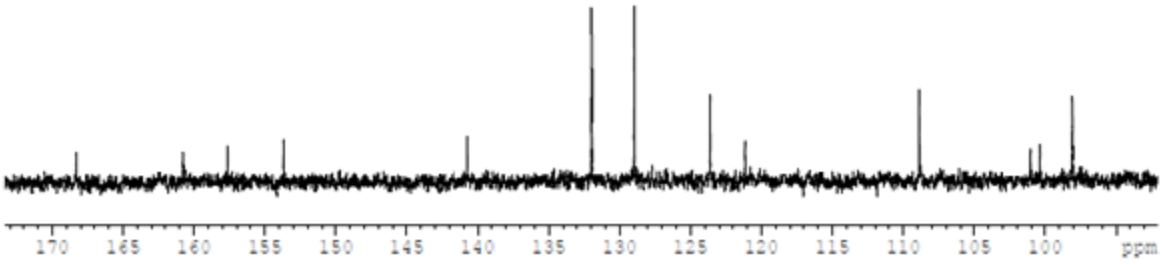

161.993
156.330
154.892
137.420
133.650
129.455
128.813
128.403
127.724
127.308
126.533
124.977
109.258
108.450
97.226
96.828

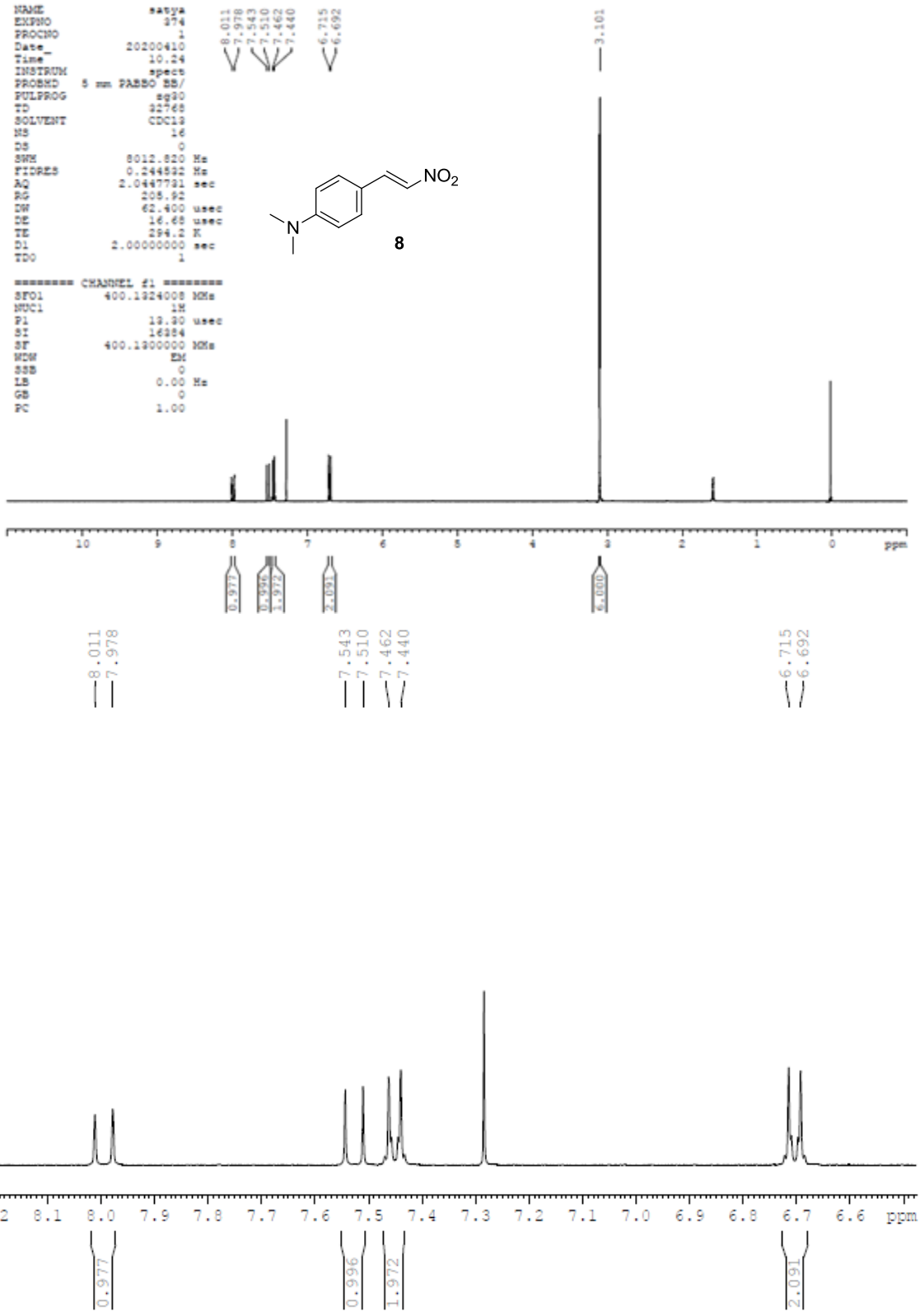

160 155 150 145 140 135 130 125 120 115 110 105 100 ppm


NAME satya
EXPNO 154
PROCNO 1
Date_ 20191108
Time 15.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.547
7.525
7.472
7.451
7.181
7.160
6.682
6.676
6.660
6.654
6.586
6.580
5.144
5.121
5.098
4.683
4.669
4.660
4.647
4.635
4.622
4.611
4.598
3.093
O
Br
N
O
O
11
ppm
1.063
1.959
1.945
1.047
0.992
1.088
2.117
6.000

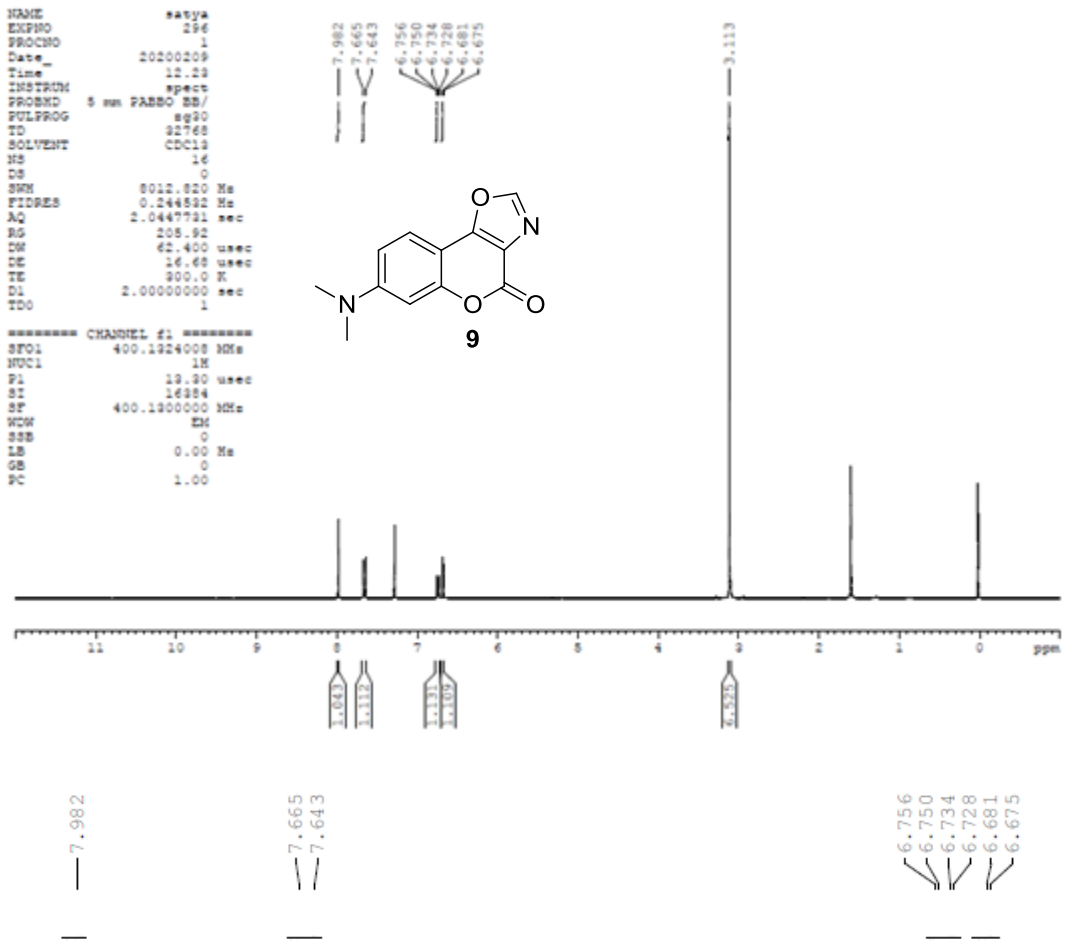

NAME satya
EXPNO 184
PROCNO 1
Date_ 20191117
Time 2.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127688 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
168.309
160.764
157.623
153.683
140.727
131.968
128.978
123.616
121.170
108.860
101.021
100.360
98.079
81.686
77.332
77.014
76.697
45.097
40.196
O
Br
N
O
O
11
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

168.309
160.764
157.623
153.683
140.727
131.968
128.978
123.616
121.170
108.860
101.021
100.360
98.079

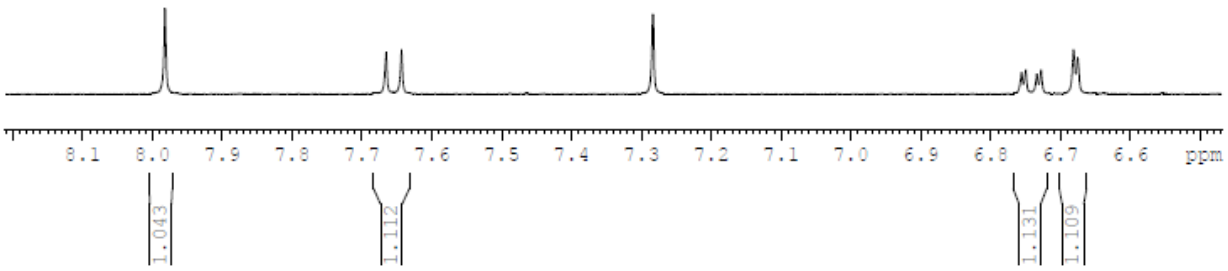

170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 ppm

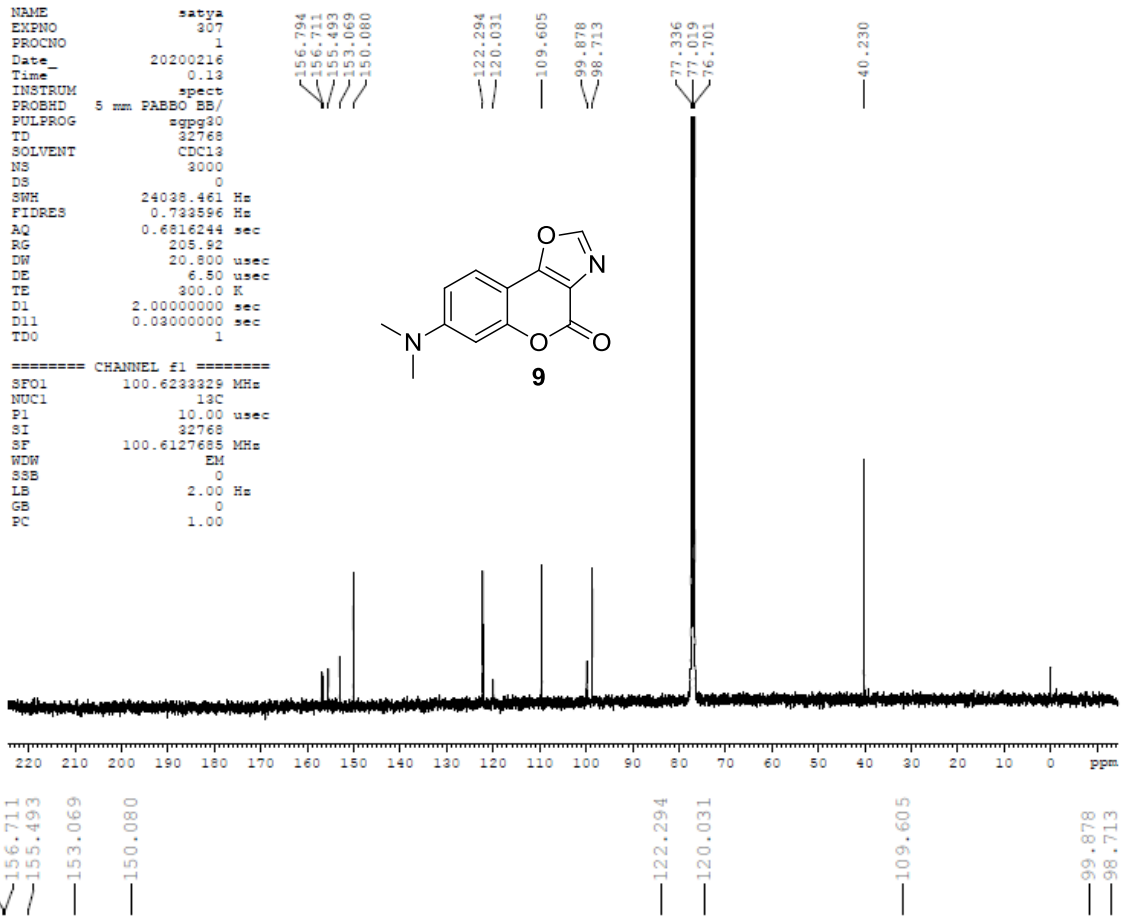

NAME satya
EXPNO 274
PROCNO 1
Date_ 20200410
Time 10.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 294.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1924008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.011
7.978
7.543
7.510
7.462
7.440
6.715
6.692
3.101
NO2
N
8
ppm
0.977
0.996
1.972
2.091
6.000

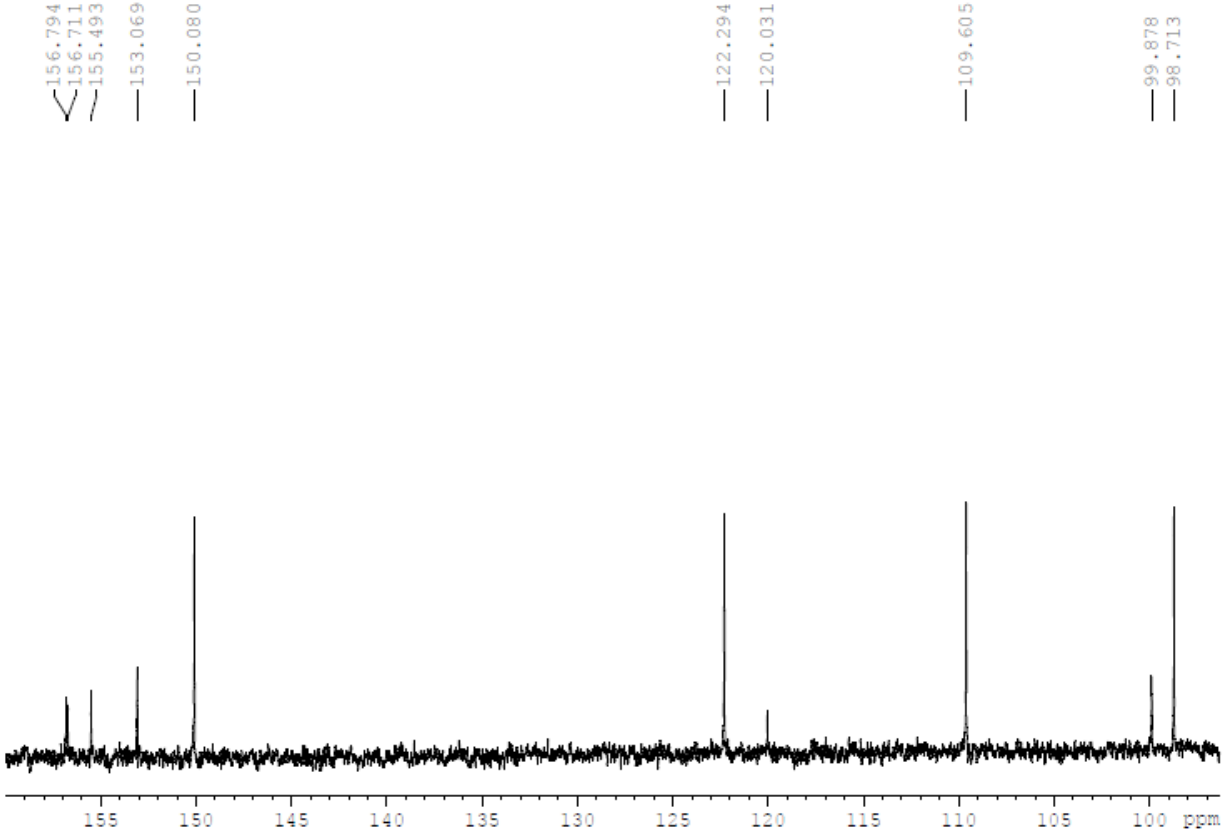
ppm
0.977
0.996
1.972
2.091

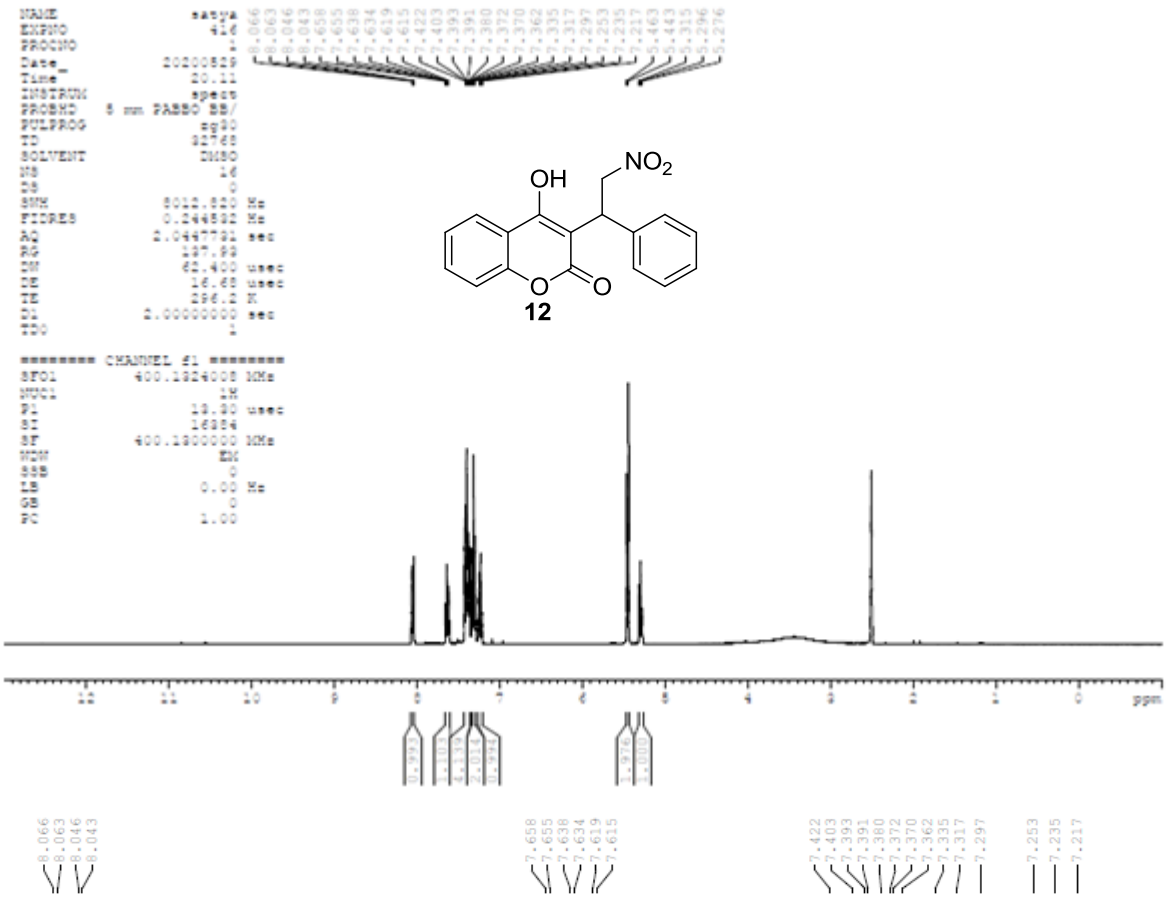

NAME satya
EXPNO 296
PROCNO 1
Date_ 20200209
Time 12.23
INSTRM spect
PROBND 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244592 Hz
AQ 2.0447791 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
7.982
7.665
7.643
6.756
6.750
6.734
6.728
6.681
6.675
3.113
O
N
N
O
O
9
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.043
1.112
1.131
1.109
6.525

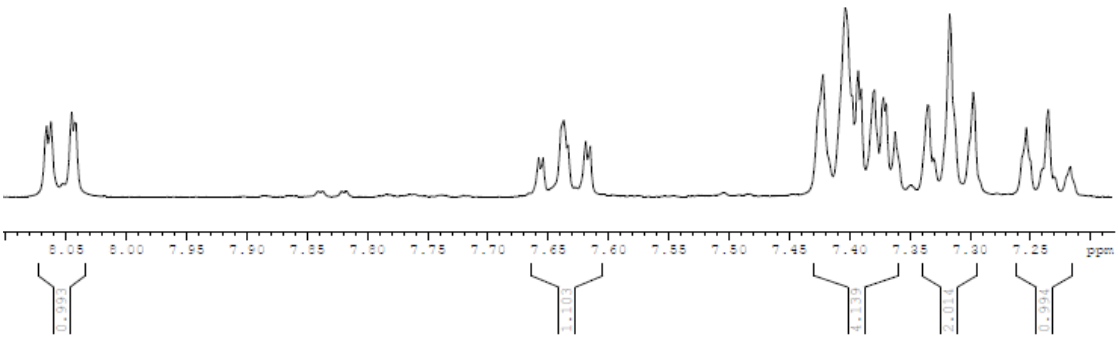
7.982
7.665
7.643
6.756
6.750
6.734
6.728
6.681
6.675

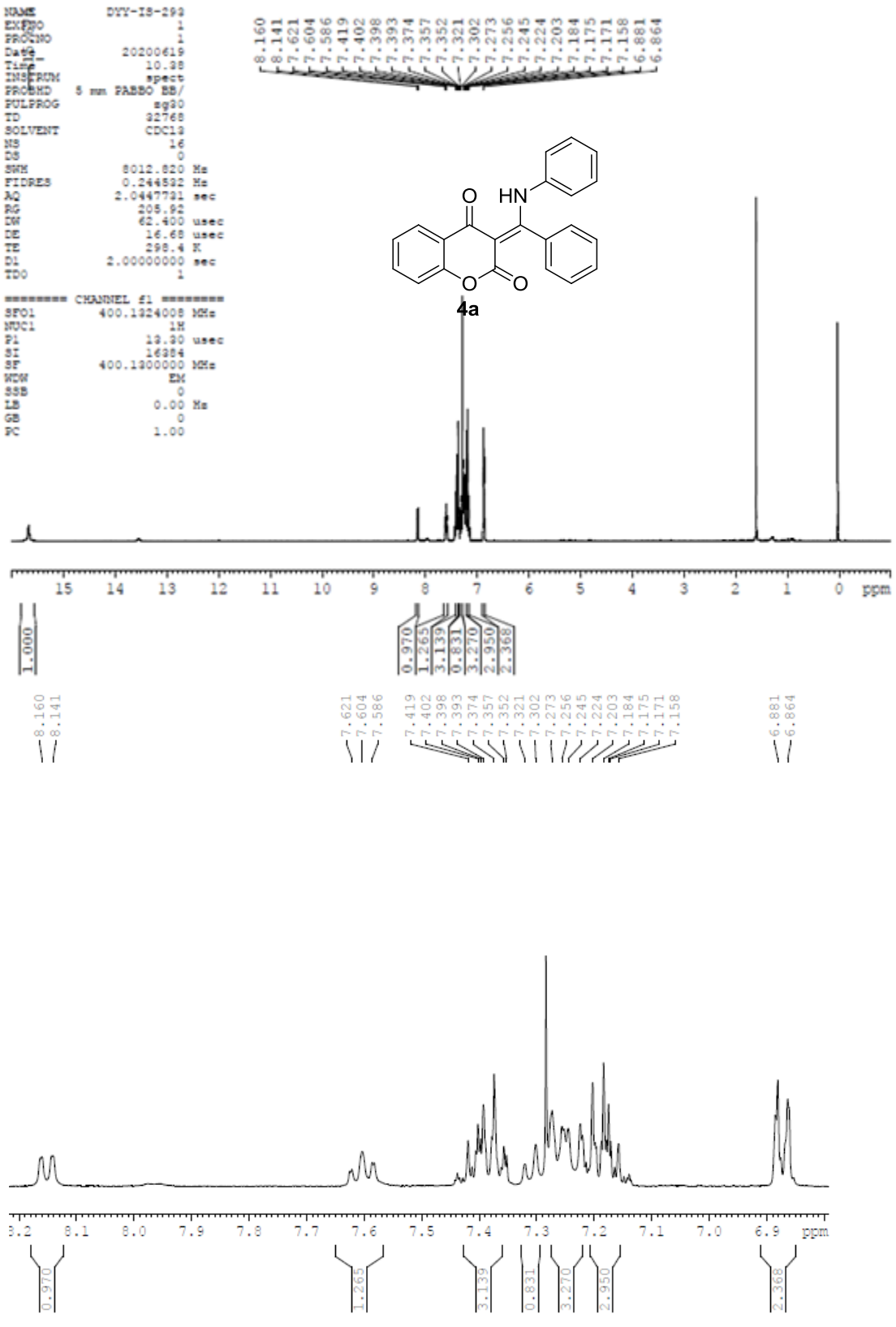

8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
ppm
1.043
1.112
1.131
1.109

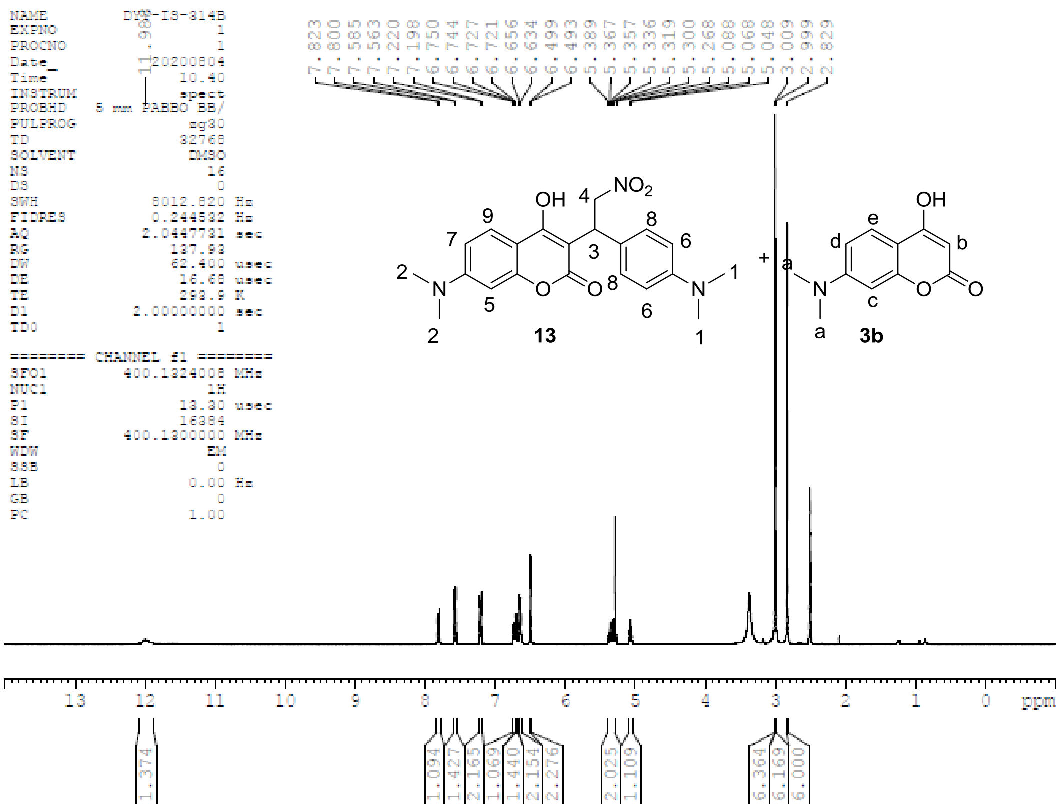

NAME satya
EXPNO 307
PROCNO 1
Date_ 20200216
Time 0.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6233329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
156.794
156.711
155.493
153.069
150.080
122.294
120.031
109.605
99.878
98.713
77.336
77.019
76.701
40.230
9
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

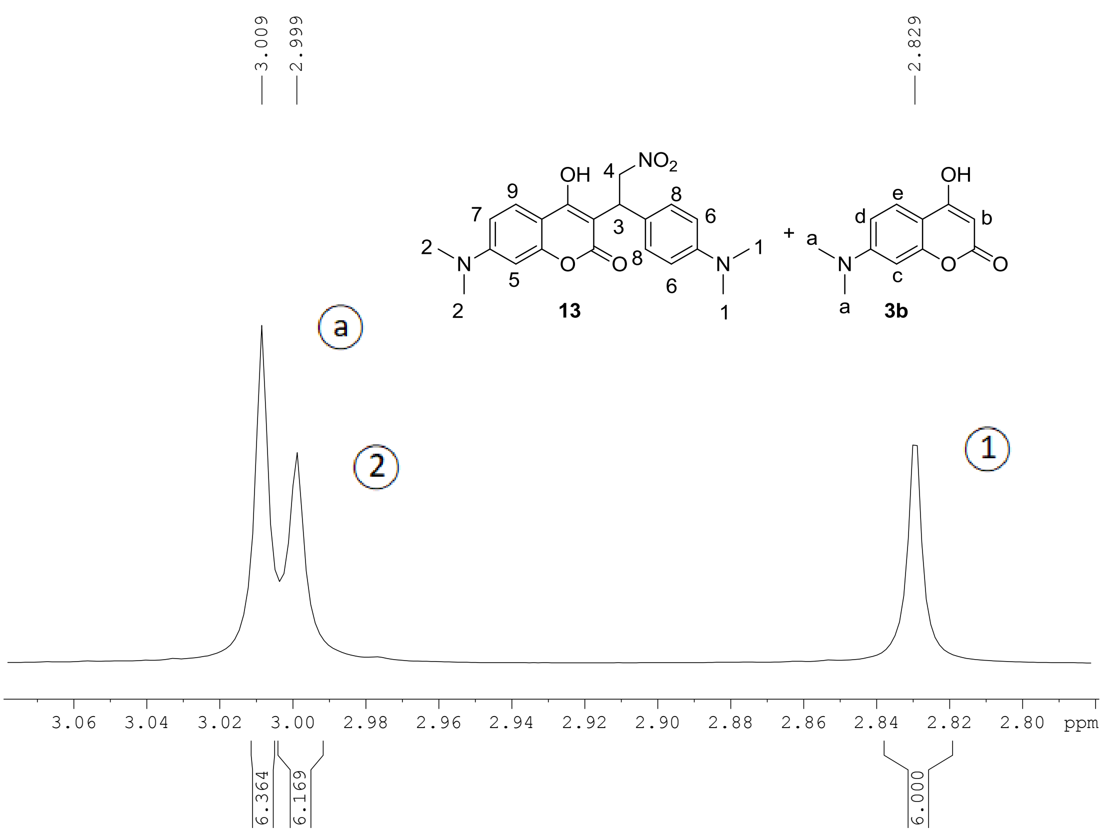

155 150 145 140 135 130 125 120 115 110 105 100 ppm

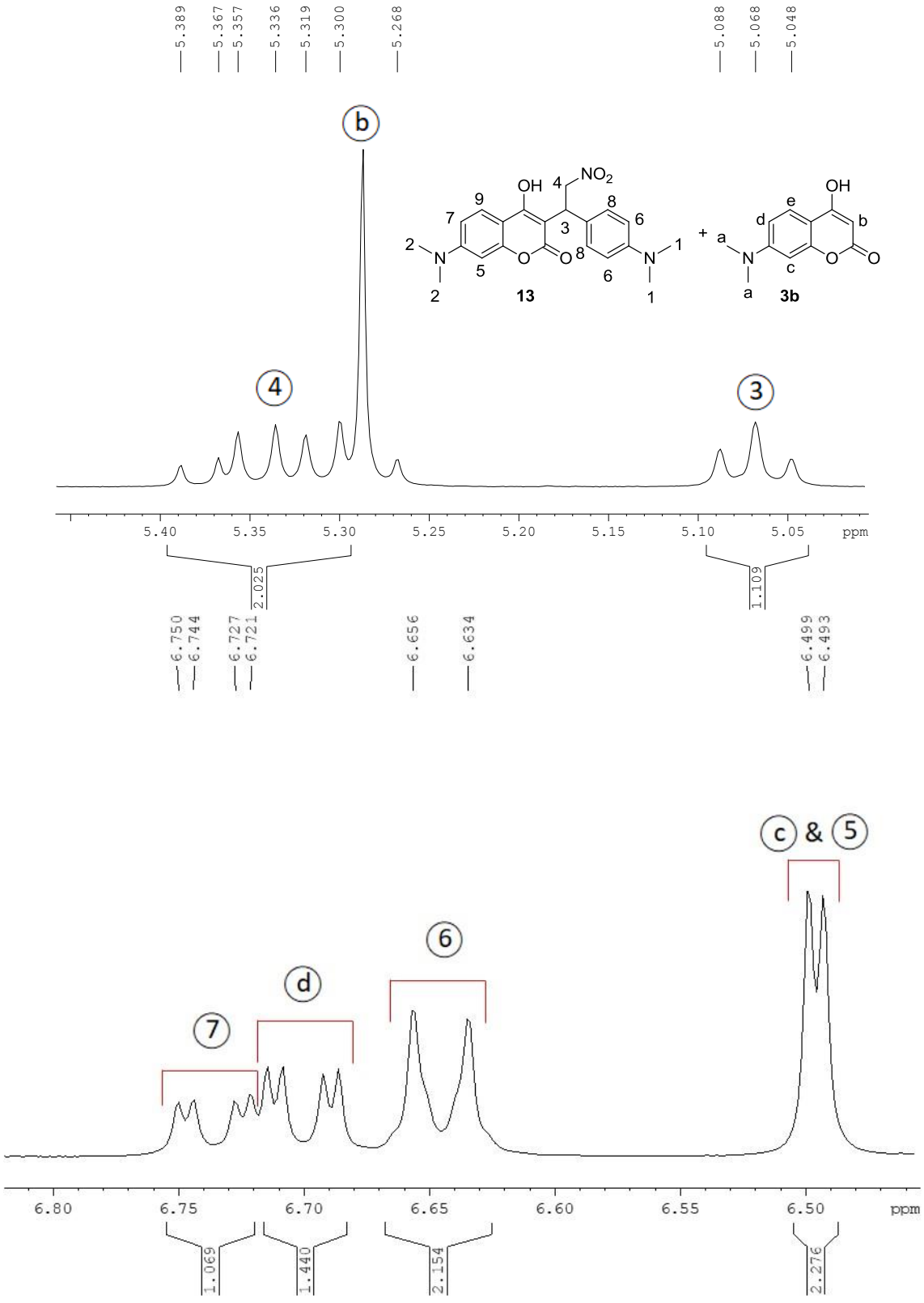

OH
NO2
O
O
12
ppm

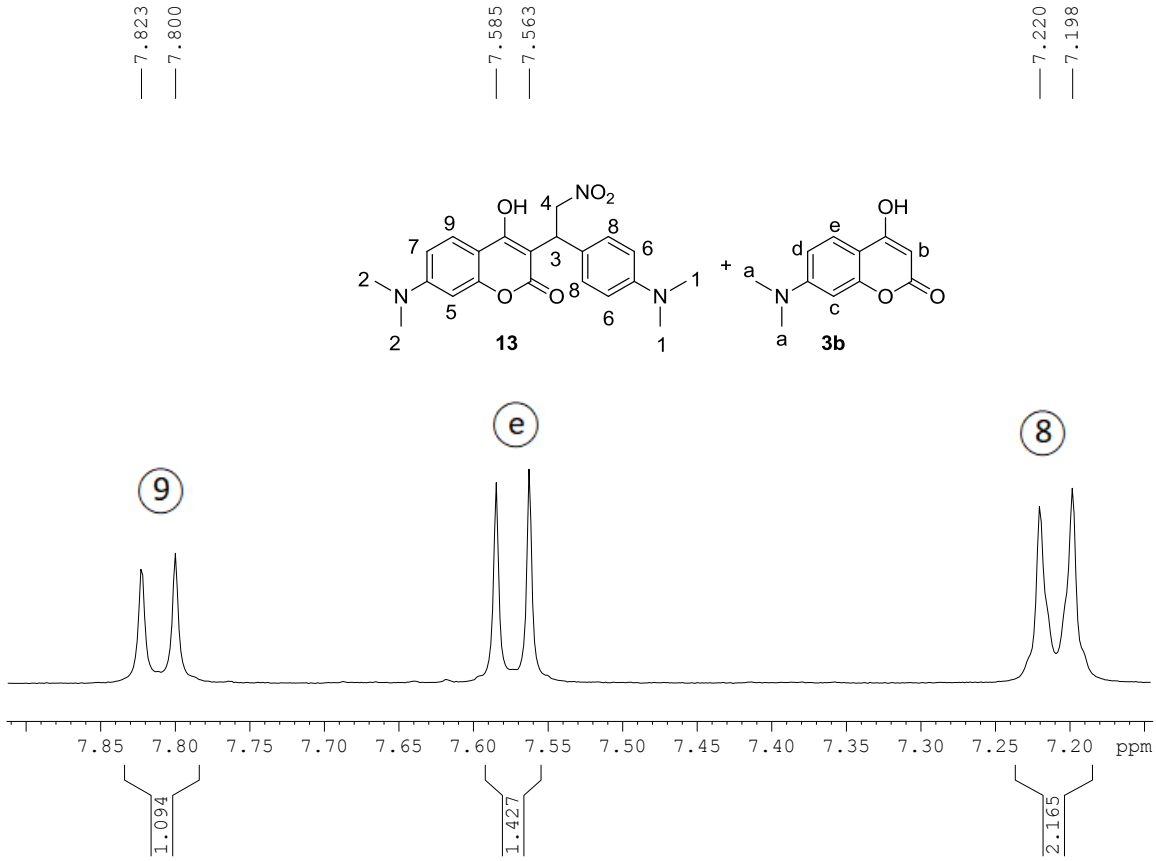

ppm

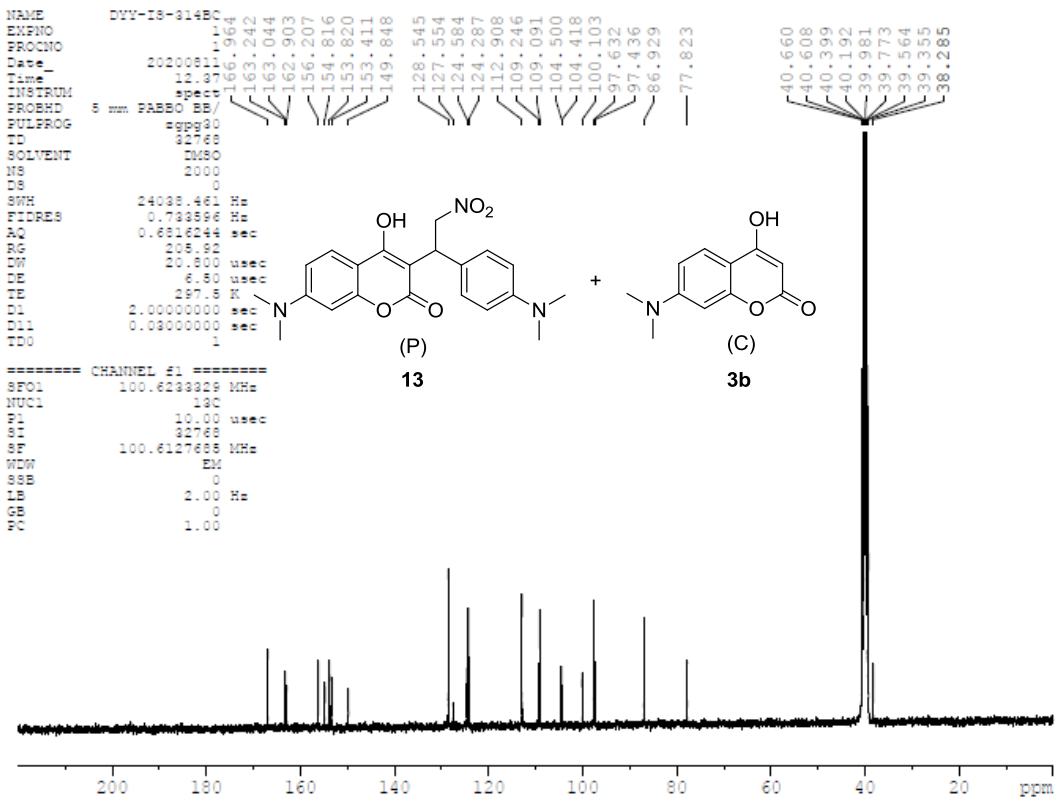

NAME DYY-IS-293
EXPNO 1
PROCNO 1
Date_ 20200619
Time 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244592 Hz
AQ 2.0447791 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
8.160 8.141 7.621 7.604 7.586 7.419 7.402 7.398 7.393 7.374 7.357 7.352 7.321 7.302 7.273 7.256 7.245 7.224 7.203 7.184 7.175 7.171 7.158 6.881 6.864
O HN O O
4a
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000 0.970 1.265 3.139 0.831 3.270 2.950 2.368
8.160 8.141 7.621 7.604 7.586 7.419 7.402 7.398 7.393 7.374 7.357 7.352 7.321 7.302 7.273 7.256 7.245 7.224 7.203 7.184 7.175 7.171 7.158 6.881 6.864
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 ppm
0.970 1.265 3.139 0.831 3.270 2.950 2.368

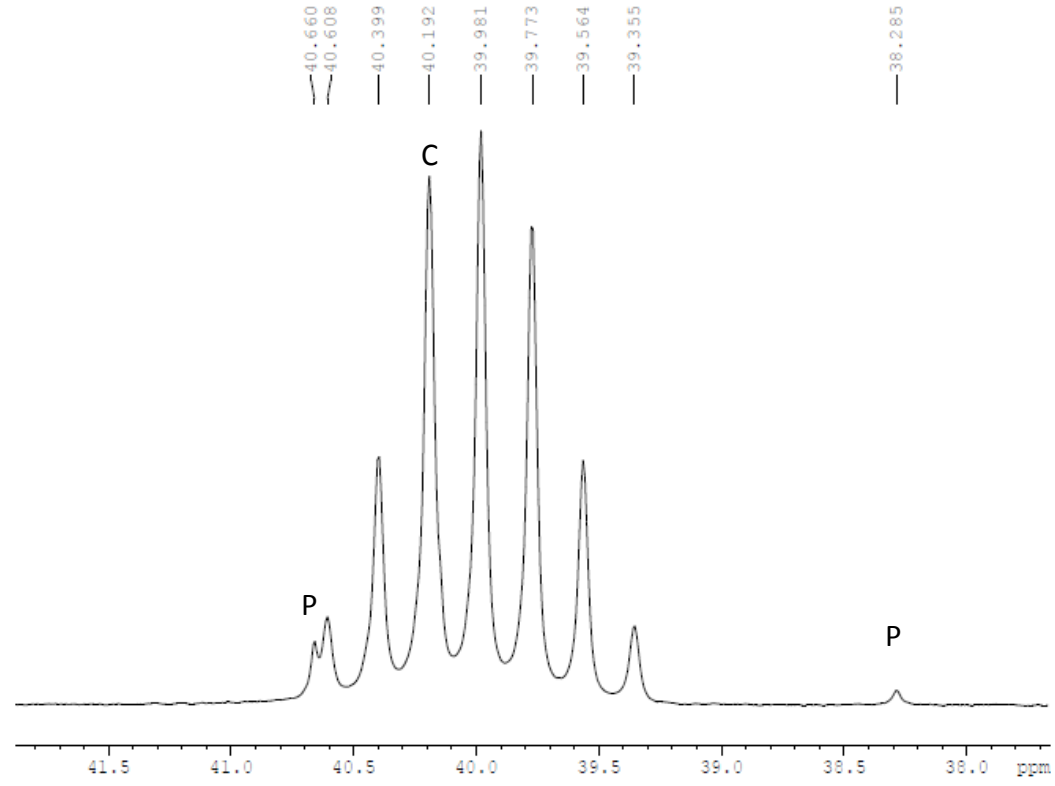

NAME DWN-IS-314B
EXPNO 1
PROCNO 1
Date_ 20200804
Time 10.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 137.93
DW 62.400 usec
DE 16.68 usec
TE 293.9 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1824008 MHz
NUC1 1H
P1 13.80 usec
SI 16384
SF 400.1800000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
13
3b
ppm

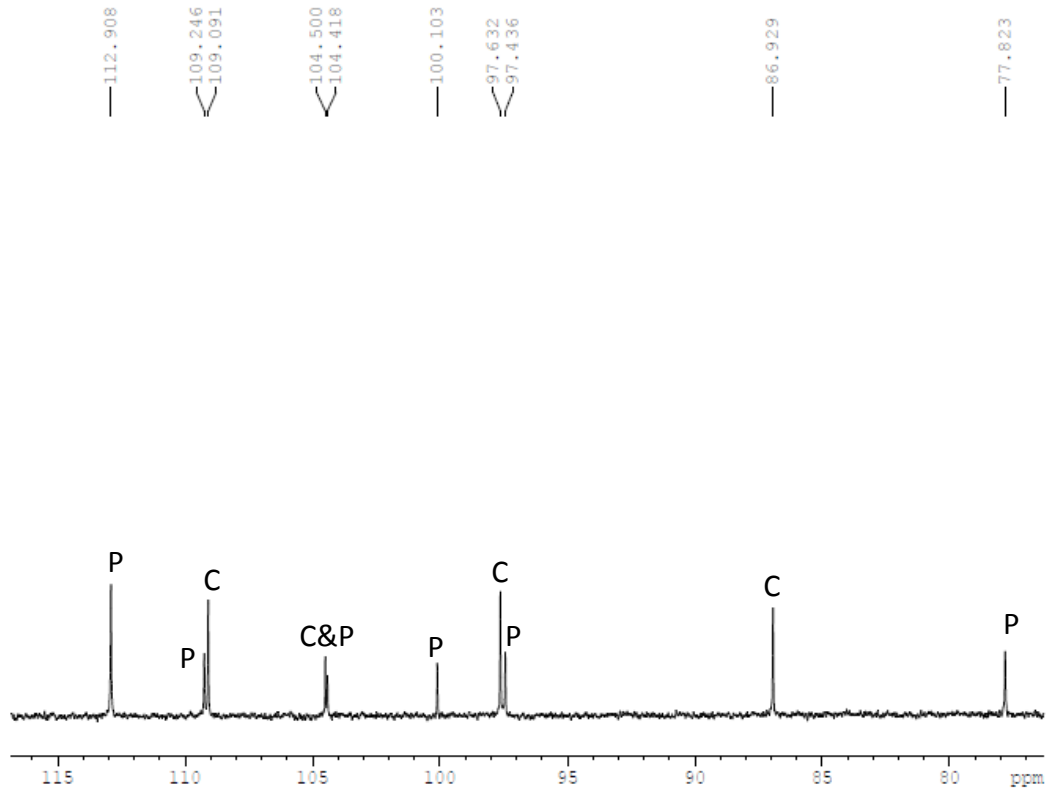

3.009
2.999
2.829
13
3b
a
2
1
ppm
6.364
6.169
6.000

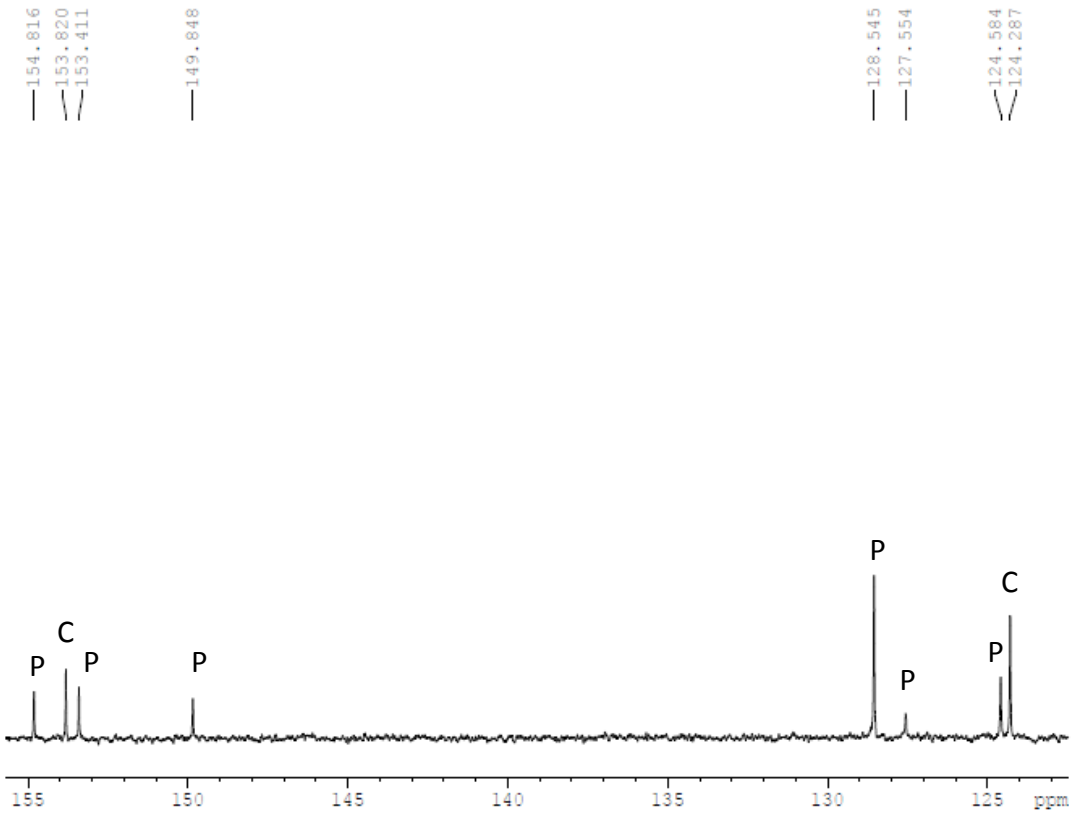

5.389
5.367
5.357
5.336
5.319
5.300
5.268
5.088
5.068
5.048
b
4
3
OH
4
NO2
9
8
7
6
3
2
N
1
5
O
O
8
6
N
2
1
13
+
a
OH
e
d
b
N
c
O
O
a
3b
5.40
5.35
5.30
5.25
5.20
5.15
5.10
5.05
ppm
2.025
1.109
6.750
6.744
6.727
6.721
6.656
6.634
6.499
6.493
c & 5
6
d
7
6.80
6.75
6.70
6.65
6.60
6.55
6.50
ppm
1.069
1.440
2.154
2.276

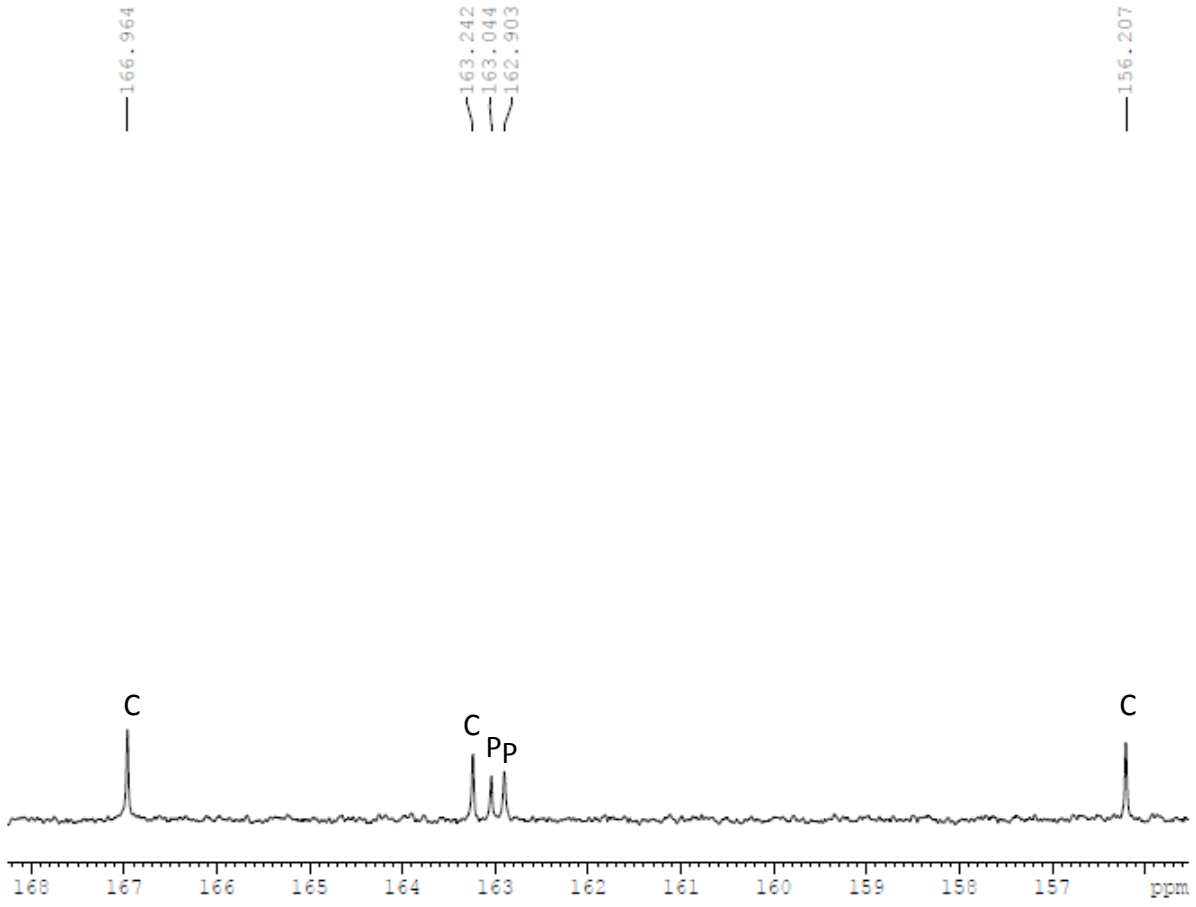

7.823
7.800
7.585
7.563
7.220
7.198
OH
NO2
13
3b
9
e
8
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
ppm
1.094
1.427
2.165

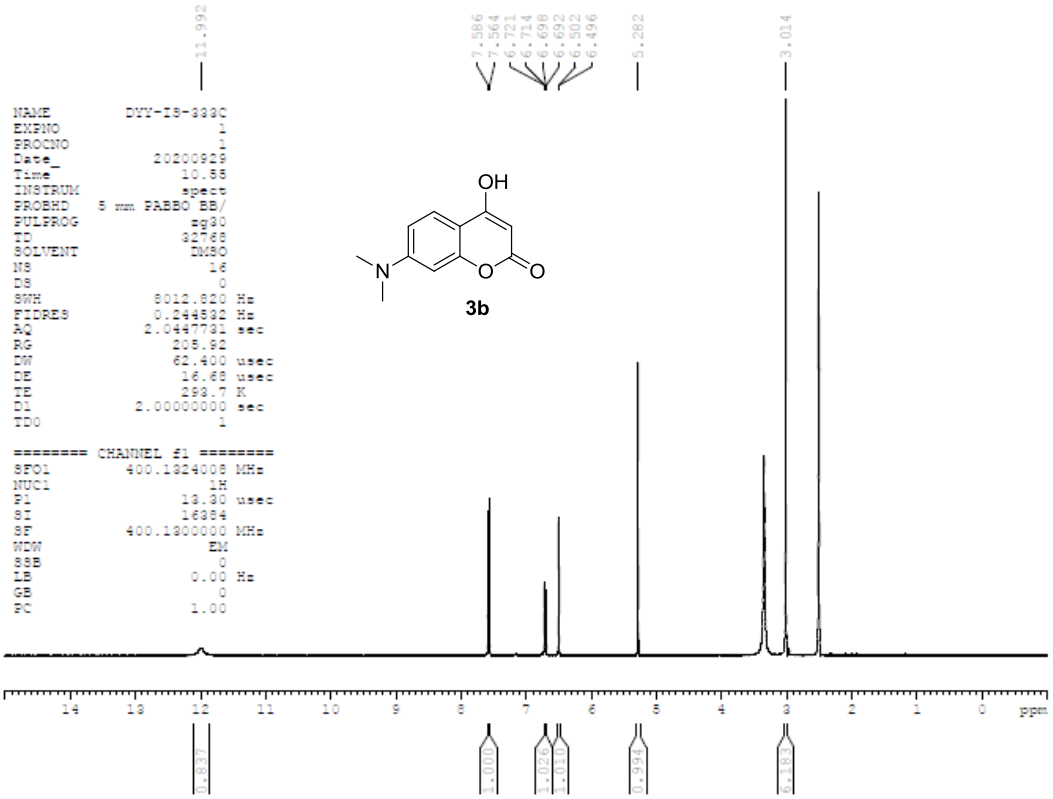

NAME DYY-I8-314BC
EXPNO 1
PROCNO 1
Date_ 20200811
Time 12.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 205.92
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6238329 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
166.964
163.242
163.044
162.903
156.207
154.816
153.820
153.411
149.848
128.545
127.554
124.584
124.287
112.908
109.246
109.091
104.500
104.418
100.103
97.632
97.436
86.929
77.823
40.660
40.608
40.399
40.192
39.981
39.773
39.564
39.355
38.285
OH
NO2
N
O
O
(P)
13
+
OH
N
O
O
(C)
3b
200
180
160
140
120
100
80
60
40
20
ppm

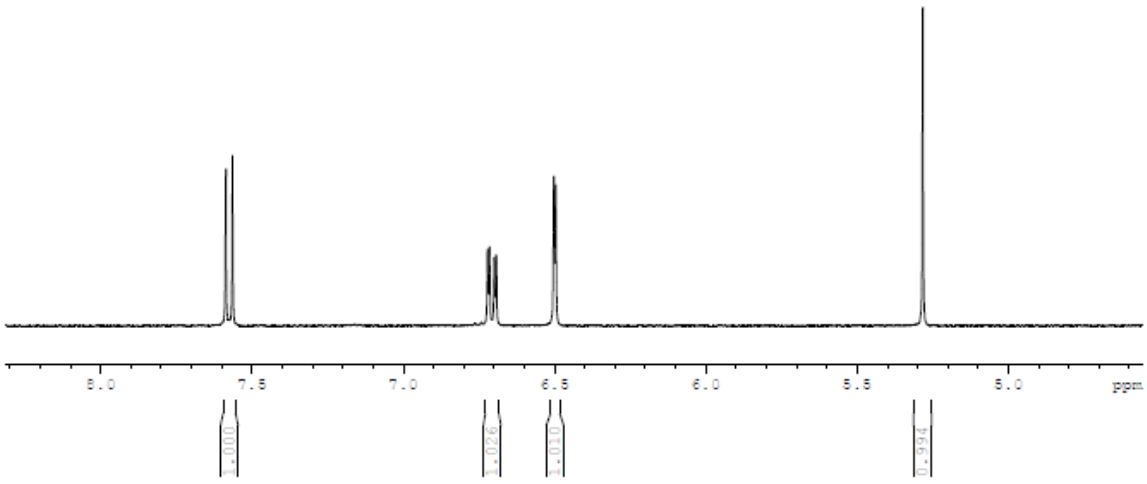

40.660
40.608
40.399
40.192
39.981
39.773
39.564
39.355
38.285
C
P
P
41.5
41.0
40.5
40.0
39.5
39.0
38.5
38.0
ppm


112.908
109.246
109.091
104.500
104.418
100.103
97.632
97.436
86.929
77.823
P
C
P
C&P
P
C
P
C
P
115
110
105
100
95
90
85
80
ppm


154.816
153.820
153.411
149.848
128.545
127.554
124.584
124.287
P
C
P
P
P
P
C
P
155
150
145
140
135
130
125
ppm


166.964
163.242
163.044
162.903
156.207
C
C
P
P
C
168
167
166
165
164
163
162
161
160
159
158
157
ppm


11.992
7.586
7.564
6.721
6.714
6.698
6.692
6.502
6.496
5.282
3.014
NAME DVT-IS-333C
EXPNO 1
PROCNO 1
Date_ 20200929
Time 10.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.244592 Hz
AQ 2.0447791 sec
RG 205.92
DW 62.400 usec
DE 16.68 usec
TE 298.7 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324006 MHz
NUC1 1H
P1 13.30 usec
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OH
N
O
O
3b
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.837
3.000
3.026
3.010
0.994
3.192


7.586
7.564
6.721
6.714
6.698
6.692
6.502
6.496
5.282
8.0
7.5
7.0
6.5
6.0
5.5
5.0
ppm
3.000
3.026
3.010
0.994