

Supporting Information

Synthesis of diverse β -(nitrooxy)-substituted amines by regioselective ring-opening of aziridines under neat conditions

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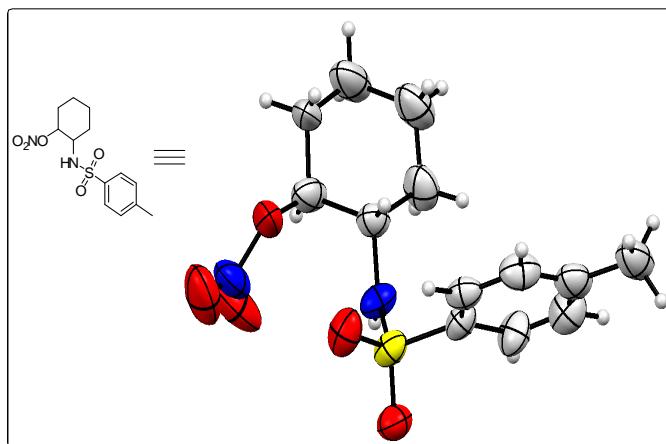
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A. General Information. All reagents were purchased from commercial sources and used without further purification. ^1H NMR spectra were determined on 400 MHz spectrometer as solutions in CDCl_3 . Chemical shifts are expressed in parts per million (δ) and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet), dd (double doublet) and coupling constants (J) were given in Hz. ^{13}C NMR spectra were recorded at 100 MHz in CDCl_3 solution. Chemical shifts as internal standard are referenced to CDCl_3 ($\delta = 7.26$ for ^1H and $\delta = 77.16$ for ^{13}C NMR) as internal standard. TLC was done on silica gel coated glass slide. X-ray single crystal data were collected using Mo K α ($\lambda = 0.71073 \text{ \AA}$) radiation with a CCD area detector. All solvents were dried and distilled before use. All the aziridines were prepared according to the previously reported method.^[1]

B. Typical procedure for the synthesis of *N*-(2-hydroxycyclohexyl)-4-methylbenzenesulfonamide (2o).^[2] A mixture of **2j** (0.25 mmol), Zn dust (6 equiv) and NH_4Cl (10 equiv) in acetic acid (2 mL) were taken in a dry sealed tube and heated at 80 °C for 1 h. After that the reaction mixture was neutralized by the saturated solution of NaHCO_3 . Then it was extracted with dichloromethane (5 mL) and the organic layer was dried over anhydrous Na_2SO_4 . After evaporation of the organic solvent, the crude product was subjected to column chromatography to obtain the pure product.

C. Structure Determination (X-ray crystallographic data of **2j**):

The Colourless crystal of **2j** were obtained by crystallization from a solution in dichloromethane/ hexane. Chemical Formula: **C₁₃H₁₈N₂O₅S**

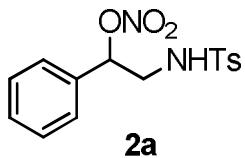


❖ ORTEP (with 50% probability) diagram for the structure 2-(4-Methylphenylsulfonamido)cyclohexyl nitrate (**2j**)

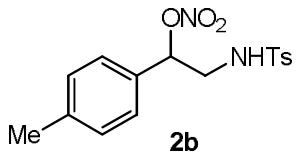
Crystal system	monoclinic	
Formula	C₁₃H₁₈N₂O₅S	
Space group	P 1 c 1	
Wavelength	0.71073 Å	
Unit cell dimensions	a = 8.623(2) Å	α = 90°
	b = 9.268(2) Å	β = 101.362(14)°
	c = 19.565(5) Å	γ = 90°
R-factor (%)	4.87	
Volume	1533.0(7) Å ³	
Z	4	

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication with a CCDC reference number **CCDC 1549293**.

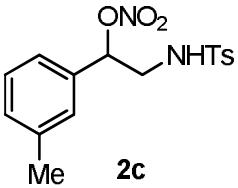
D. Analytical data for 2a-2n and 2o:



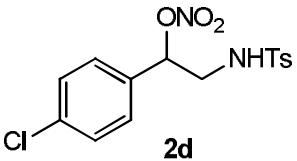
2-(4-Methylphenylsulfonamido)-1-phenylethyl nitrate (2a).^[3] Yellow solid (302 mg, 90%), mp: 85-87 °C; ¹H NMR (CDCl₃, 400 MHz): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.37-7.36 (m, 3H), 7.32-7.26 (m, 4H), 5.83-5.80 (m, 1H), 5.13 (s, 1H), 3.38-3.32 (m, 2H), 2.43 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ 144.1, 136.8, 134.8, 130.1, 129.8, 129.2, 127.1, 126.6, 83.6, 46.0, 21.7.



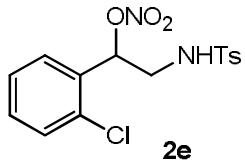
2-(4-Methylphenylsulfonamido)-1-(p-tolyl)ethyl nitrate (2b).^[3] Pale yellow gummy mass, (304 mg, 87%); ¹H NMR (CDCl₃, 400MHz): δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.16 (s, 4H), 5.79-5.75 (m, 1H), 4.97 (t, *J* = 6.4 Hz, 1H), 3.37-3.20 (m, 2H), 2.43 (s, 3H), 2.34 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ 144.1, 139.9, 136.9, 131.7, 130.0, 129.9, 127.1, 126.6, 83.6, 45.9, 21.7, 21.3.



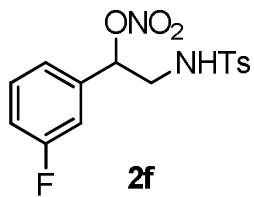
2-(4-Methylphenylsulfonamido)-1-(m-tolyl)ethyl nitrate (2c). White Solid, (322 mg, 92%), mp: 89-91 °C; ^1H NMR (CDCl_3 , 400 MHz): δ 7.78 (d, $J = 8.4$ Hz, 2H), 7.35 (d, $J = 8.0$ Hz, 2H), 7.30-7.27 (m, 1H), 7.20 (d, $J = 7.2$ Hz, 1H), 7.11-7.09 (m, 2H), 5.84-5.80 (m, 1H), 5.24 (s, 1H), 3.45-3.33 (m, 2H), 2.46 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 144.1, 139.0, 136.9, 134.7, 130.5, 130.0, 129.0, 127.2, 127.1, 123.6, 83.7, 46.0, 21.6, 21.4. Anal. Calcd For $\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_5\text{S}$: C, 54.85; H, 5.18; N, 8.00%; Found: C, 54.78; H, 5.12; N, 8.05%.



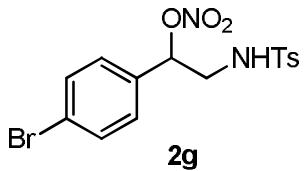
1-(4-Chlorophenyl)-2-(4-methylphenylsulfonamido)ethyl nitrate (2d). Light yellow gummy mass (289 mg, 78%); ^1H NMR (CDCl_3 , 400 MHz): δ 7.71 (d, $J = 8.0$ Hz, 2H), 7.35-7.30 (m, 4H), 7.23-7.21 (m, 2H), 5.81-5.78 (m, 1H), 4.90 (s, 1H), 3.37-3.30 (m, 2H), 2.44 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 144.3, 136.8, 135.9, 133.3, 130.1, 129.5, 128.0, 127.1, 82.9, 45.9, 21.7. Anal. Calcd For $\text{C}_{15}\text{H}_{15}\text{ClN}_2\text{O}_5\text{S}$: C, 48.59; H, 4.08; N, 7.55%; Found: C, 48.51; H, 4.01; N, 7.46%.



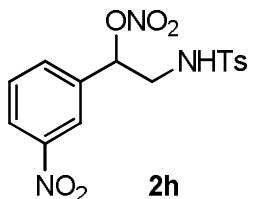
1-(2-Chlorophenyl)-2-(4-methylphenylsulfonamido)ethyl nitrate (2e).^[4] Pale yellow oil (322 mg, 87%) ; ¹H NMR (CDCl₃, 400 MHz): δ 7.76 (d, J = 8.4 Hz, 2H), 7.38-7.36 (m, 1H), 7.32-7.27 (m, 5H), 6.23-6.20 (m, 1H), 5.27-5.23 (m, 1H), 3.57-3.50 (m, 1H), 3.31-3.23 (m, 1H), 2.43 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ 144.1, 137.0, 132.9, 132.5, 130.5, 130.2, 130.0, 127.7, 127.1, 126.7, 79.9, 44.7, 21.6.



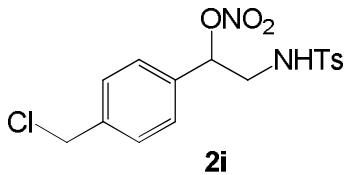
1-(3-Fluorophenyl)-2-(4-methylphenylsulfonamido)ethyl nitrate (2f). Colourless oil (290 mg, 82%); ¹H NMR (CDCl₃, 400 MHz): δ 7.73 (d, J = 8.0 Hz, 2H), 7.37-7.30 (m, 3H), 7.09-6.95 (m, 3H), 5.82-5.79 (m, 1H), 5.21 (s, 1H), 3.38-3.28 (m, 2H), 2.43 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ 163.0 (d, $^1J_{C-F}$ = 246 Hz), 144.3, 137.3 (2C), 136.7, 131.0 (d, $^4J_{C-F}$ = 8 Hz), 130.1, 127.1, 122.3 (d, $^3J_{C-F}$ = 3 Hz), 116.8, 116.6, 113.6 (d, $^2J_{C-F}$ = 22 Hz), 82.7, 45.9, 21.7. Anal. Calcd For C₁₅H₁₅FN₂O₅S: C, 50.84; H, 4.27; N, 7.91%; Found: C, 50.92; H, 4.20; N, 7.98%.



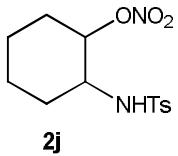
1-(4-Bromophenyl)-2-(4-methylphenylsulfonamido)ethyl nitrate (2g). Pale yellow oil (348 mg, 84%); ^1H NMR (CDCl_3 , 400 MHz): δ 7.71 (d, $J = 8.0$ Hz, 2H), 7.49-7.47 (m, 2H), 7.30 (d, $J = 8.0$ Hz, 2H), 7.15 (d, $J = 8.4$ Hz, 2H), 5.80-5.77 (m, 1H), 5.16 (s, 1H), 3.36-3.30 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 144.2, 136.7, 133.8, 132.4, 130.1, 128.3, 127.0, 123.9, 82.9, 45.8, 21.7. Anal. Calcd For $\text{C}_{15}\text{H}_{15}\text{BrN}_2\text{O}_5\text{S}$: C, 43.39; H, 3.64; N, 6.75%; Found: C, 43.29; H, 3.70; N, 6.68%.



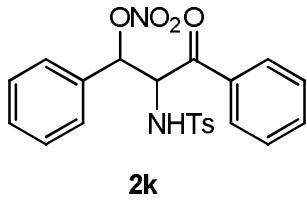
2-(4-Methylphenylsulfonamido)-1-(3-nitrophenyl)ethyl nitrate (2h). White gummy mass (324 mg, 85%); ^1H NMR (CDCl_3 , 400 MHz): δ 8.22-8.19 (m, 1H), 8.13-8.12 (m, 1H), 7.72-7.66 (m, 3H), 7.57 (t, $J = 8.0$ Hz, 1H), 7.30 (d, $J = 8.0$ Hz, 2H), 5.95-5.92 (m, 1H), 5.37 (t, $J = 6.4$ Hz, 1H), 3.43-3.38 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 148.6, 144.4, 137.1, 136.6, 132.8, 130.4, 130.1, 127.0, 124.6, 121.7, 82.1, 45.8, 21.6. Anal. Calcd For $\text{C}_{15}\text{H}_{15}\text{N}_3\text{O}_7\text{S}$: C, 47.24; H, 3.96; N, 11.02%; Found: C, 47.15; H, 3.82; N, 10.94%.



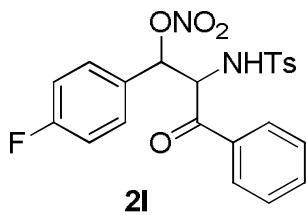
1-(4-(Chloromethyl)phenyl)-2-(4-methylphenylsulfonamido)ethyl nitrate (2i). Light yellow gummy mass (338 mg, 88%); ^1H NMR (CDCl_3 , 400 MHz): δ 7.73 (d, J = 8.0 Hz, 2H), 7.40-7.38 (m, 2H), 7.32-7.27 (m, 4H), 5.85-5.81 (m, 1H), 5.23-5.20 (m, 1H), 4.55 (s, 2H), 3.36-3.31 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 144.2, 139.1, 136.7, 135.0, 130.1, 129.3, 127.1, 127.0, 83.2, 45.9, 45.5, 21.6. Anal. Calcd For $\text{C}_{16}\text{H}_{17}\text{ClN}_2\text{O}_5\text{S}$: C, 49.94; H, 4.45; N, 7.28%; Found: C, 49.84; H, 4.36; N, 7.37%.



2-(4-Methylphenylsulfonamido)cyclohexyl nitrate (2j).^[5] Colourless solid (282 mg, 90%), mp: 116-117 °C; ^1H NMR (CDCl_3 , 400 MHz): δ 7.75 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 5.37 (s, 1H), 4.81-4.75 (m, 1H), 3.29-3.21 (m, 1H), 2.42 (s, 3H), 2.04-1.98 (m, 2H), 1.70-1.61 (m, 2H), 1.42-1.31 (m, 4H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 143.7, 137.6, 129.8, 127.0, 82.9, 54.0, 32.4, 29.0, 23.4, 23.1, 21.6.

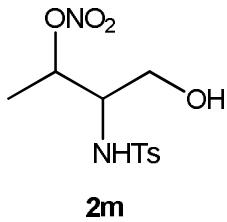


2-(4-Methylphenylsulfonamido)-3-oxo-1,3-diphenylpropyl nitrate (2k). White gummy mass (317 mg, 72%); ^1H NMR (CDCl_3 , 400 MHz): δ 7.81-7.78 (m, 2H), 7.67-7.63 (m, 3H), 7.59-7.57 (m, 1H), 7.51-7.47 (m, 2H), 7.25-7.24 (m, 2H), 7.15 (d, $J = 8.4$ Hz, 2H), 7.03-7.00 (m, 2H), 6.06-6.03 (m, 1H), 5.62 (d, $J = 8.4$ Hz, 1H), 5.57-5.54 (m, 1H), 2.31 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 193.8, 144.0, 134.8, 129.9, 129.8, 129.3 (2C), 128.9, 128.8, 128.6, 127.7, 127.3, 127.2, 83.1, 59.2, 21.6. Anal. Calcd For $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}_6\text{S}$: C, 59.99; H, 4.58; N, 6.36%; Found: C, 59.90; H, 4.47; N, 6.30%.

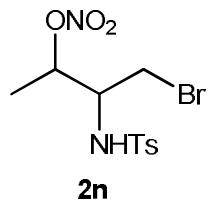


1-(4-Fluorophenyl)-2-(4-methylphenylsulfonamido)-3-oxo-3-phenylpropyl nitrate (2l). Yellow gummy mass (343 mg, 75%); ^1H NMR (CDCl_3 , 400 MHz): δ 7.83-7.80 (m, 2H), 7.70-7.61 (m, 3H), 7.52-7.48 (m, 2H), 7.14 (d, $J = 8.0$ Hz, 2H), 7.05-7.01 (m, 2H), 6.95-6.90 (m, 2H), 6.03 (d, $J = 4.8$ Hz, 1H), 5.73 (d, $J = 8.8$ Hz, 1H), 5.54-5.51 (m, 1H), 2.31 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 194.0, 163.5 (d, $^1J_{C-F} = 248$ Hz), 144.1, 136.7, 135.0, 134.2, 129.8 (d, $^3J_{C-F} = 4$ Hz), 129.4 (d, $^4J_{C-F} = 9$ Hz), 128.8, 128.6, 128.5, 127.1, 115.9 (d, $^2J_{C-F} = 22$ Hz), 82.5, 58.9,

21.6. Anal. Calcd For C₂₂H₁₉FN₂O₆S: C, 57.64; H, 4.18; N, 6.11%; Found: C, 57.54; H, 4.06; N, 6.03%.

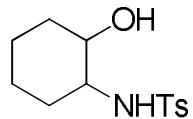


4-Hydroxy-3-(4-methylphenylsulfonamido)butan-2-yl nitrate (2m). Brown gummy mass (234 mg, 77%); ¹H NMR (CDCl₃, 400 MHz): δ 7.74 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 5.22 (d, J = 9.2 Hz, 1H), 5.15-5.08 (m, 1H), 4.48-4.38 (m, 2H), 3.83-3.79 (m, 1H), 2.44 (s, 3H), 1.37 (d, J = 6.4 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ 144.7, 136.7, 130.2, 127.1, 78.9, 69.8, 53.4, 21.7, 15.3. Anal. Calcd For C₁₁H₁₆N₂O₆S: C, 43.42; H, 5.30; N, 9.21%; Found: C, 43.31; H, 5.22; N, 9.26%.



4-Bromo-3-(4-methylphenylsulfonamido)butan-2-yl nitrate (2n). Light yellow oil (308 mg, 84%); ¹H NMR (CDCl₃, 400 MHz): δ 7.74 (d, J = 8.4 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 5.31-5.25 (m, 2H), 4.14-4.10 (m, 1H), 3.42-3.28 (m, 2H), 2.43 (s, 3H), 1.46 (d, J = 6.4 Hz, 3H);

¹³C NMR (CDCl₃, 100 MHz): δ 144.3, 136.5, 130.1, 127.1, 78.8, 52.4, 45.9, 21.7, 16.0. Anal. Calcd For C₁₁H₁₅BrN₂O₅S: C, 35.98; H, 4.12; N, 7.63%; Found: C, 35.87; H, 4.04; N, 7.56%.



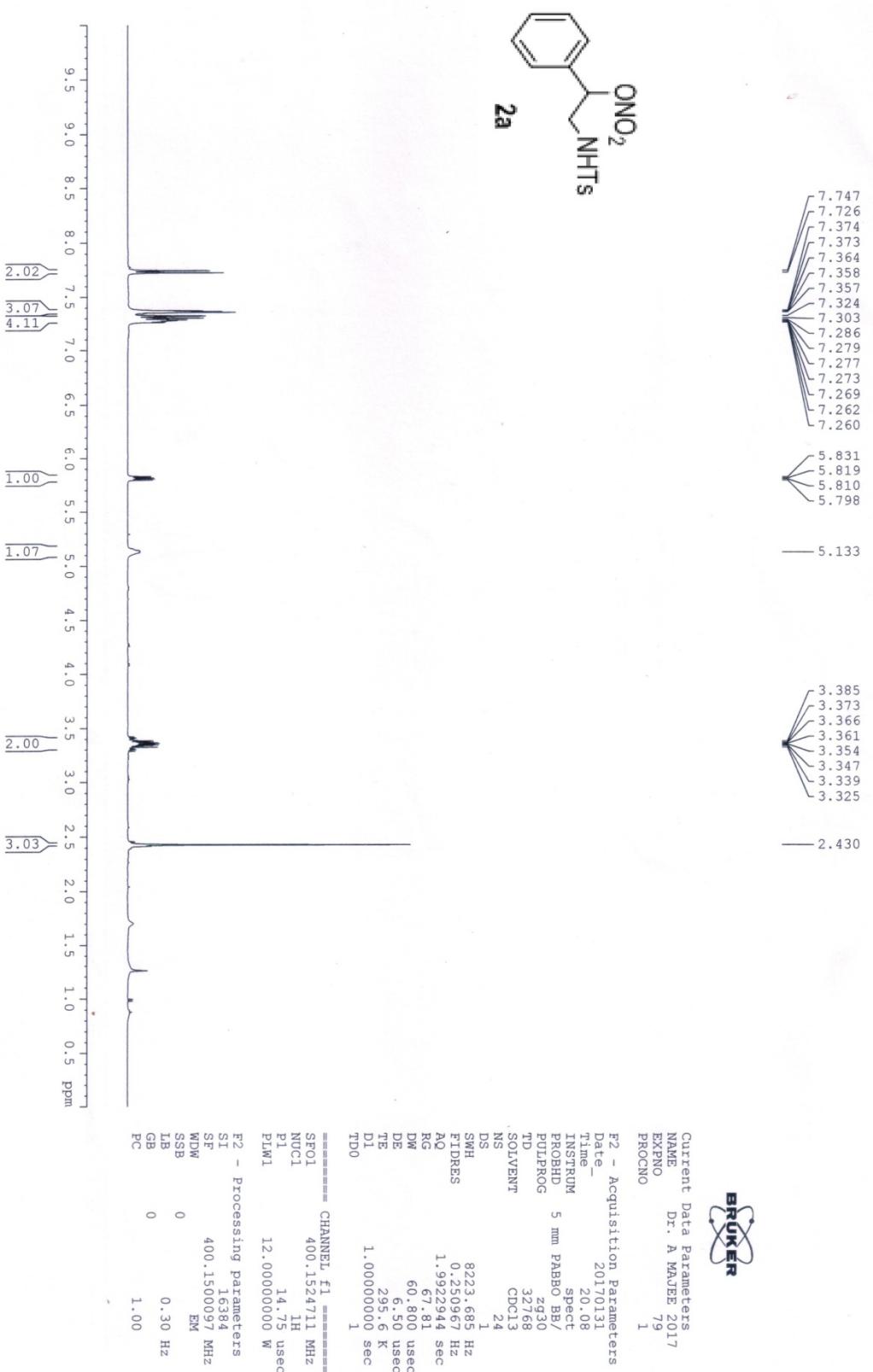
2o

N-(2-hydroxycyclohexyl)-4-methylbenzenesulfonamide (2o).^[2] White solid (50.50 mg, 75%), mp: 128-130 °C; ¹H NMR (400 MHz, CDCl₃): δ 7.79 (d, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 4.96 (d, J = 6.8 Hz, 1H), 3.31-3.26 (m, 1H), 2.89-2.81 (m, 1H), 2.66 (s, 1H), 2.43 (s, 3H), 2.03-1.99 (m, 1H), 1.74-1.58 (m, 3H), 1.25-1.11 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 143.8, 137.5, 129.9, 127.3, 73.5, 59.8, 33.5, 32.0, 24.8, 24.0, 21.7.

E. References:

1. Thakur, V. V.; Sudalai, A. *Tetrahedron Lett.* **2003**, *44*, 989–992.
2. Prasad, B. A. B.; Sanghi, R.; Singh, V. K. *Tetrahedron*. **2002**, *58*, 7355–7363.
3. Das, B.; Krishnaiah, M.; Venkateswarlu, K.; Reddy, V.S. *Helv. Chim. Acta*. **2007**, *90*, 110-113.
4. Volkova, Y.A.; Averina, E.B.; Kuznetsova, T.S.; Zefirov, N.S. *Tetrahedron Lett.* **2010**, *51*, 2254–2257.
5. Liu , Z-Q.; Fan, Y.; Li, R.; Zhou, B.; Wu, L-M. *Tetrahedron Lett.* **2005**, *46*, 1023-1025.

F. NMR spectra for the synthesized compounds:



— 144.15
— 136.84
— 134.78
— 130.06
— 129.76
— 129.21
— 127.09
— 126.58

— 83.65
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— 77.16
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— 45.97

— 21.67

Current Data Parameters

Dr. A MAJEE 2017
EXPTNO 80
PROCNO 1

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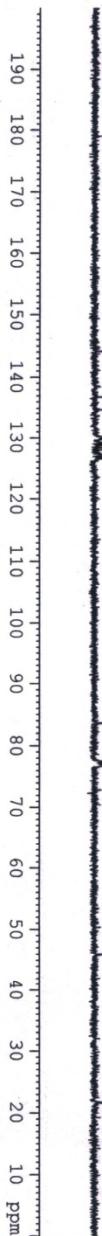
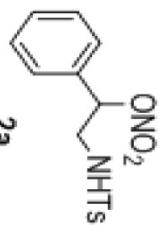
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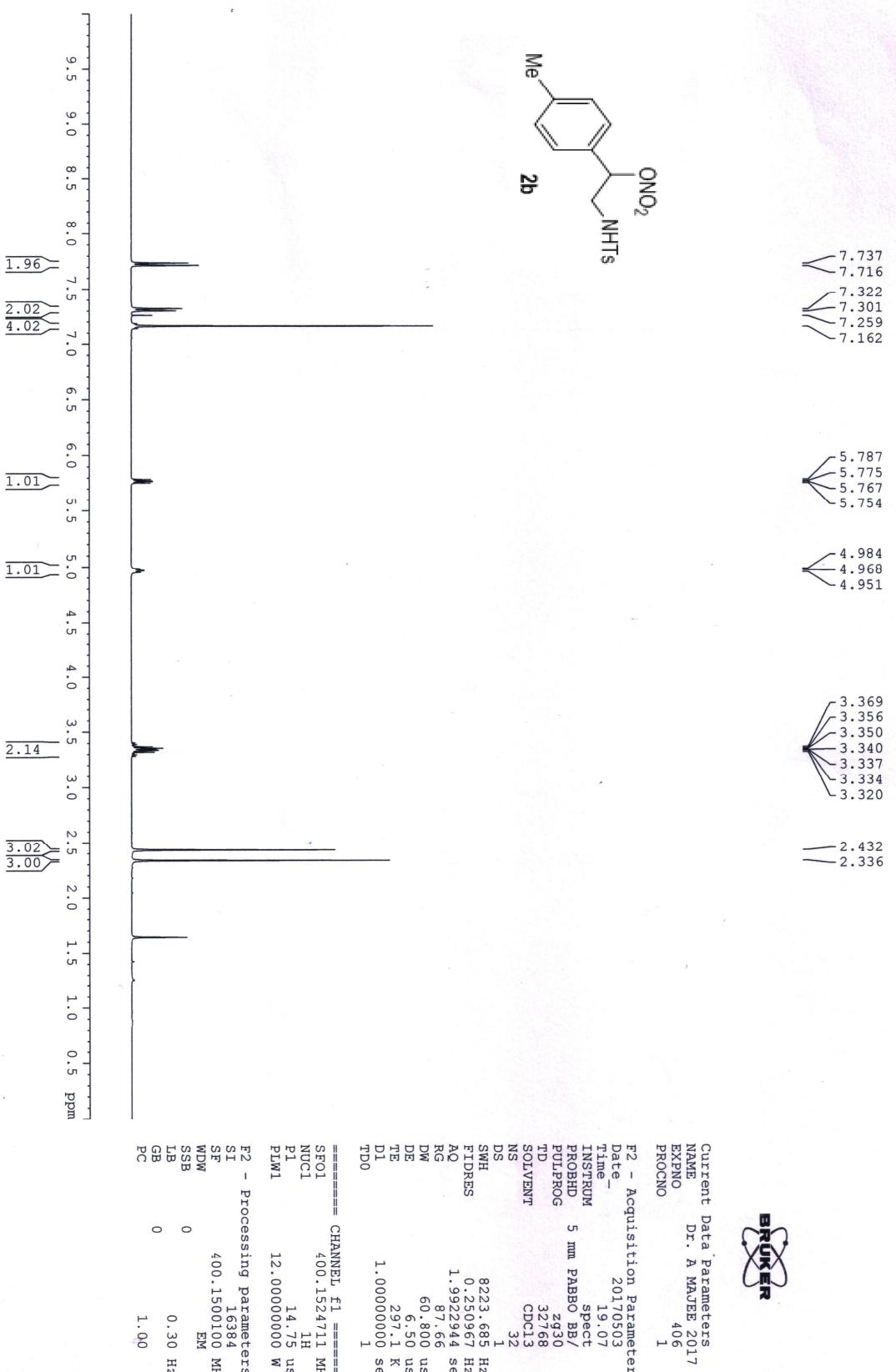
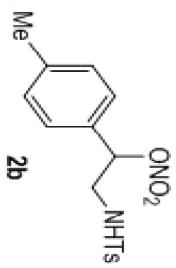
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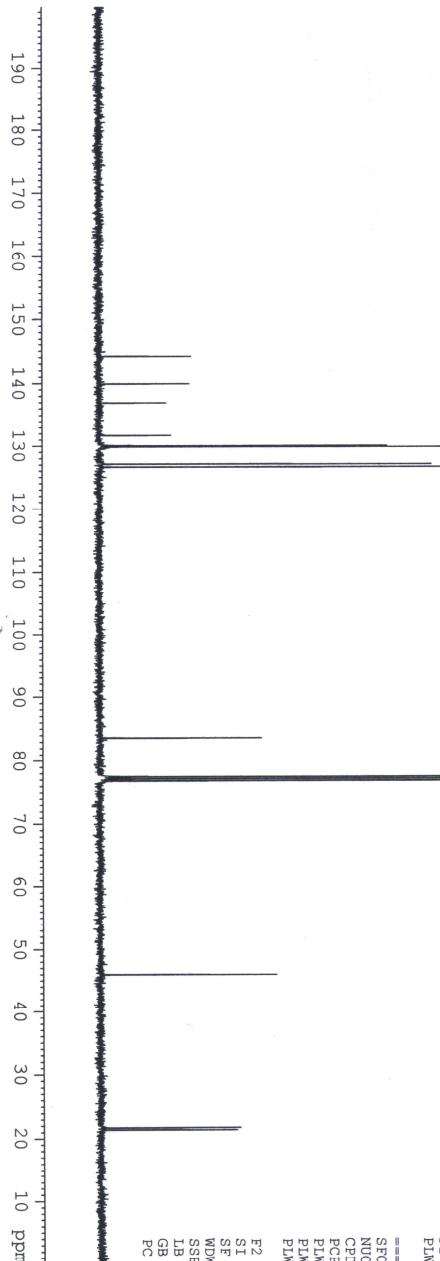
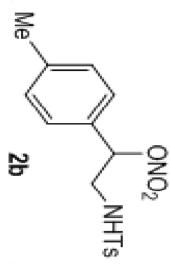
BRUKER

— 144.13
— 139.90
— 136.91
— 131.70
— 130.05
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— 77.15
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— 21.67
— 21.33



Current Data Parameters
NAME Dr. A MAJEE 2017
EXNO 407
PROCNO 1

F2 - Acquisition Parameters

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PULPROG zppg30
TD 3768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.73596 Hz
AQ 0.6815744 sec
RG 47.25
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====

SFO1 100.6270588 MHz
NUCL 13C
P1 8.90 usec
PLW1 54.0000000 W

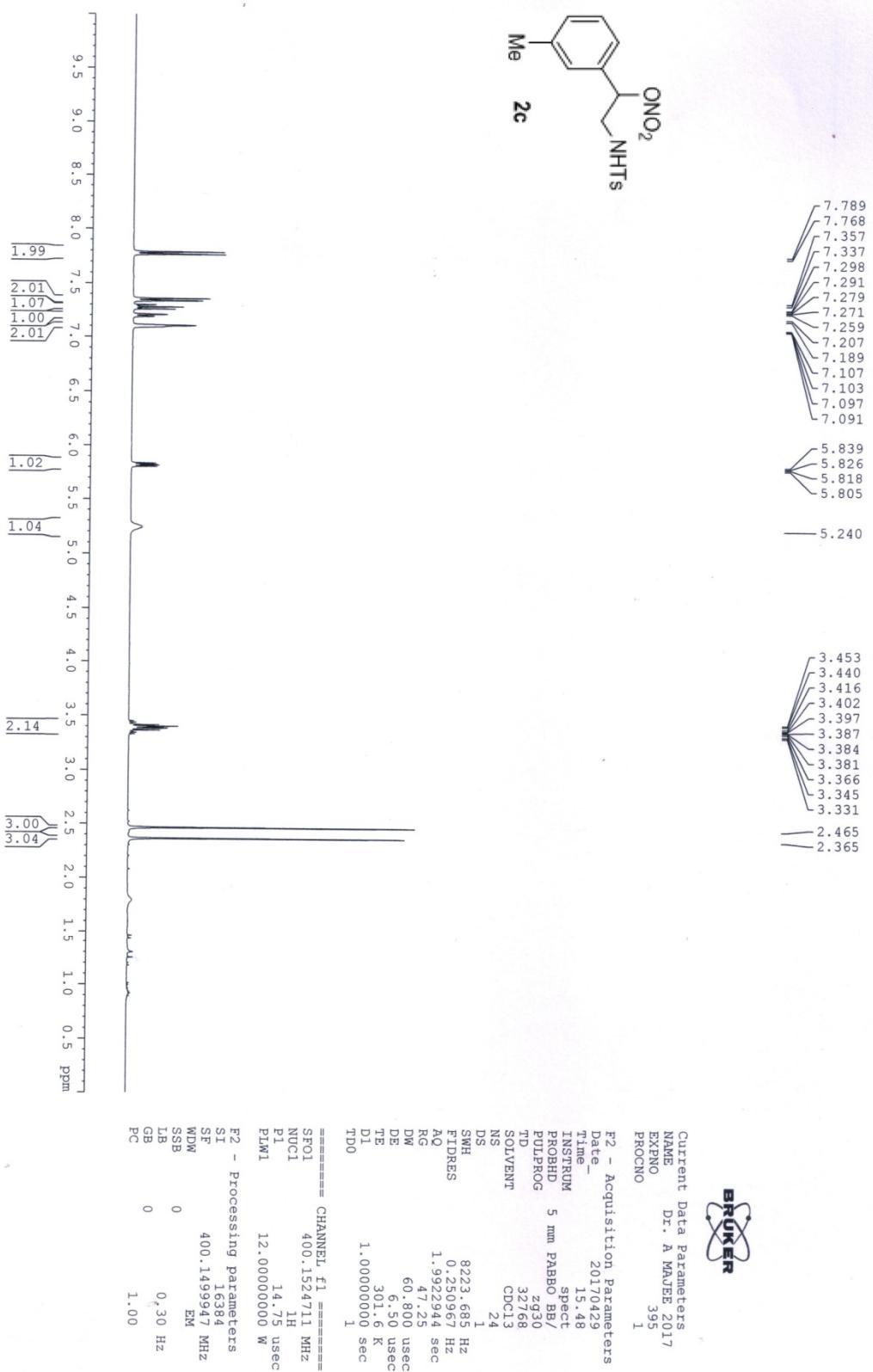
===== CHANNEL f2 =====

SFO2 400.1516006 MHz
NUC2 1H
OPPRG12 waltz16
PCP12 90.00 usec
PLW2 12.0000000 W
PLW12 0.32233000 W
PLW13 0.16212000 W

F2 - Processing parameters

SI	16384
SF	100.6177858 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1H of VBSAS-19A-21



144.06
139.04
136.94
134.72
130.48
130.02
129.05
127.16
127.08
123.60

83.72
77.47
77.15
76.83

46.00

21.61
21.42



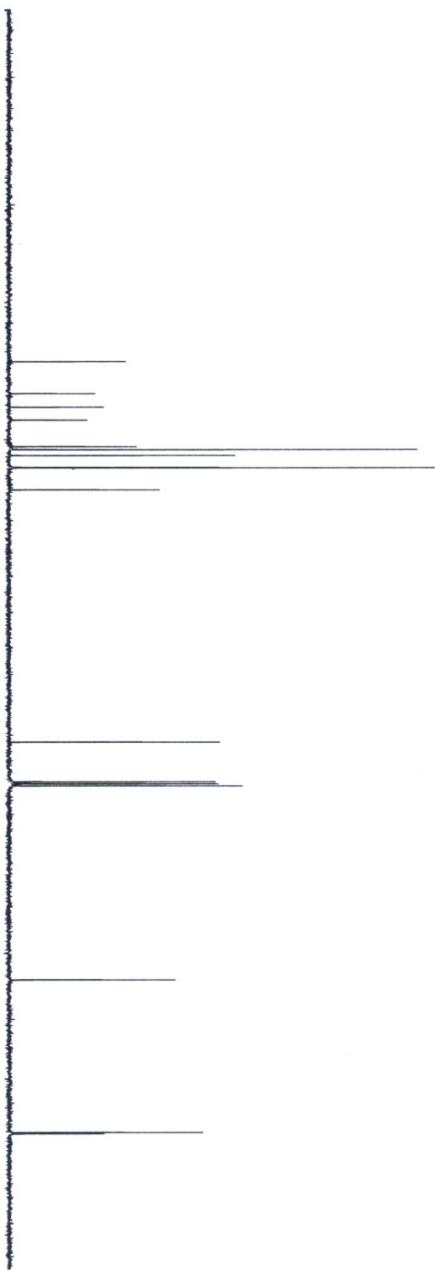
Current Data Parameters
NAME Dr. A Maje 2017
EXPNO 396
PROCNO 1

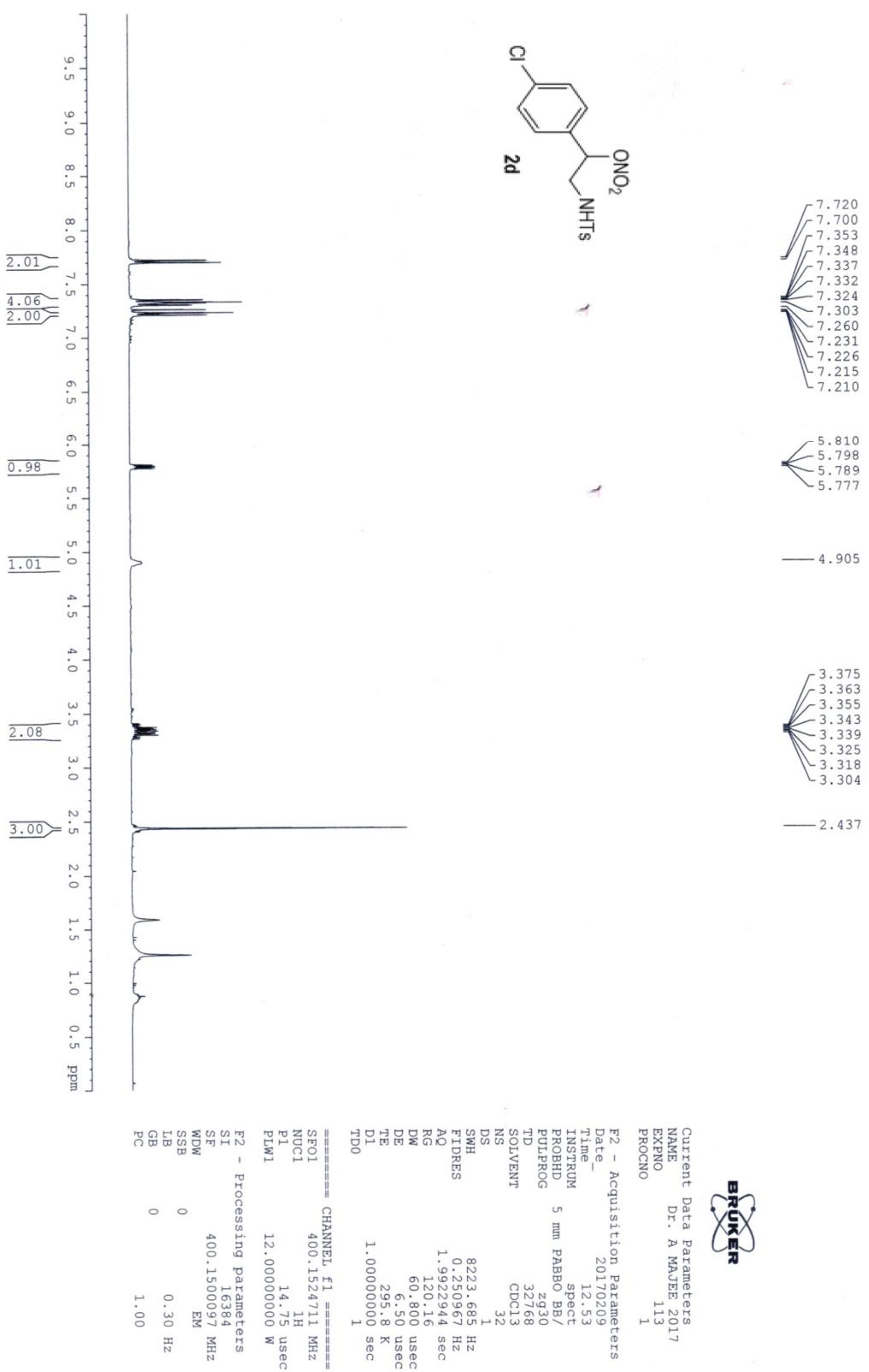
F2 - Acquisition Parameters
Date_ 20110429
Time_ 16.00
INSTRUM spect
PROBID 5 mm PABBO BB/
PULPROG zap930
TD 32768
SOLVENT CDCl3
NS 212
DS 2
SWH 24038.461 Hz
SFDRSS 0.733566 Hz
AO 0.6835744 sec
RG 47.25
DW 20.00 usec
DE 6.50 usec
TE 302.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 100.627858 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

===== CHANNEL f2 =====
SF02 400.1516006 MHz
NUC2 1H
CPDPG[2] waltz16
PPDP2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.617783 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





144.29
136.81
135.87
133.30
130.12
129.52
128.02
127.09

82.86
77.48
77.16
76.85

45.89

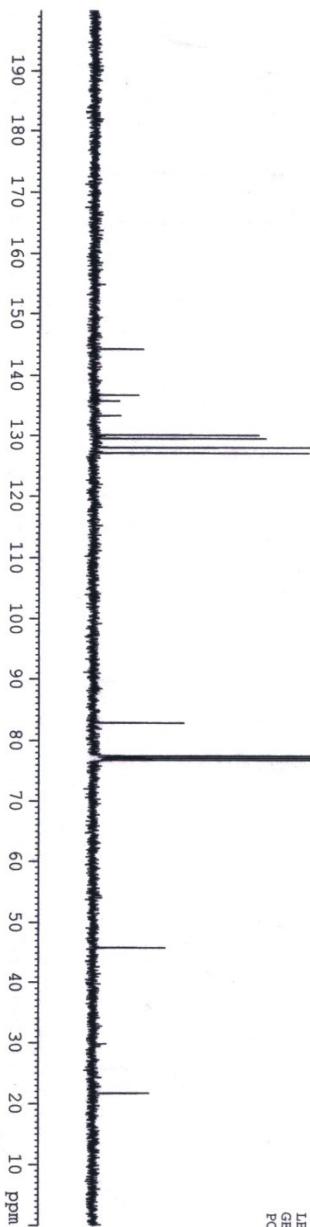
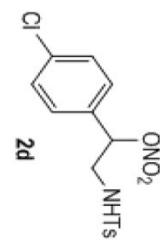
21.72



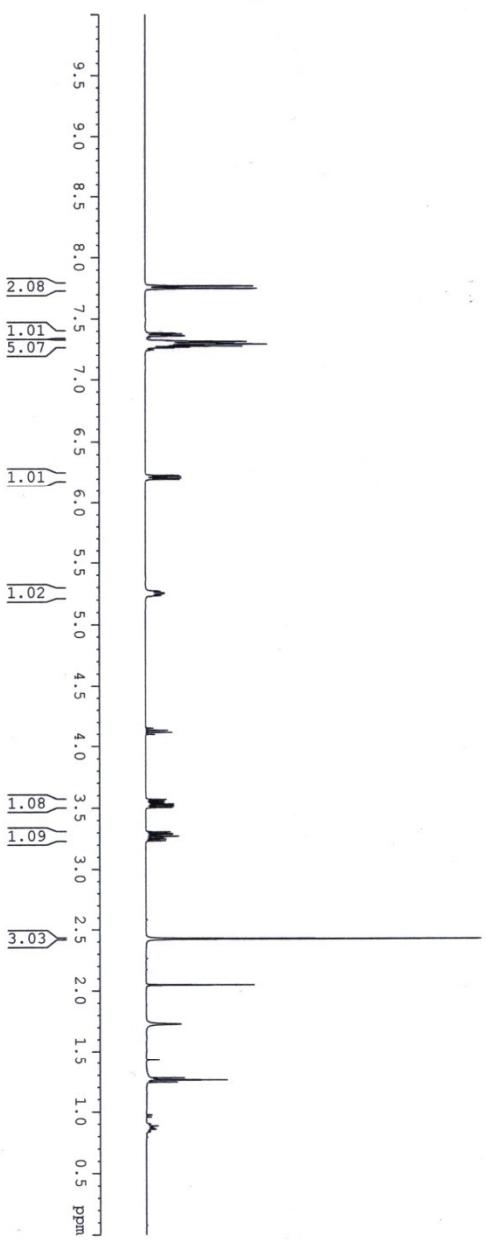
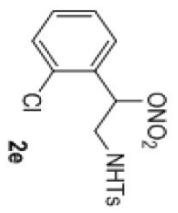
Current Data Parameters^a
NAME DR. A MAJEE 2017
EXPNO 114
PROCNO 1

F2 - Acquisition Parameters

DATE	20170209
TIME	13:19
INSTRUM	spect
PROBID	5 mm PARBO BB/
PULPROG	2ppq30
TD	32768
SOLVENT	CDCl ₃
NS	512
D1	2
SWH	24038.461 Hz
FTDRES	0.733596 Hz
AQ	0.6515744 sec
RQ	120.16
DW	20.800 usec
DE	6.50 usec
TE	296.3 K
D1	2.0000000 sec
D1L	0.0300000 sec
TDD	1
<hr/>	
CHANNEL f1	
SP01	100.6278589 MHz
NUC1	¹³ C
PL	8.90 usec
PW1	54.0000000 W
<hr/>	
CHANNEL f2	
SP02	400.1516006 MHz
NUC2	¹ H
CPDPG12	walt16
PCPD2	
PW2	12.0000000 W
PW12	90.00 usec
PW13	0.3223100 W
	0.1612000 W
<hr/>	
F2 - Processing parameters	
SF	16384
WDW	100.6177837 MHz
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



1H OF VBSAS 19A 14 P



Dendrogram illustrating the hierarchical clustering of 19 samples. The x-axis represents the distance between clusters, ranging from 0 to 7.770. The y-axis lists the sample names.

Merge Step	Clusters Merged	Distance
1	19 individual samples	0
2	18, 19	0.235
3	17, 18, 19	0.235
4	16, 17, 18, 19	0.235
5	15, 16, 17, 18, 19	0.235
6	14, 15, 16, 17, 18, 19	0.235
7	13, 14, 15, 16, 17, 18, 19	0.235
8	12, 13, 14, 15, 16, 17, 18, 19	0.235
9	11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
10	10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
11	9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
12	8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
13	7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
14	6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
15	5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
16	4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
17	3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
18	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
19	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	0.235
20	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19	7.770

3.571
3.562
3.551
3.542
3.534
3.525
3.514
3.505
3.308
3.294
3.285
-3.271
-3.257
-3.248
-3.235
-2.426

Current	Data	Parameters
NAME	Dr.	A MAJEE
EXPNO		2017
PROCNO		287

```

===== CHANNEL f1 ======
SFOL      400.152411 MHz
NUCI      1H
PL       14.75 usec
PLWI     12.0000000 W

F2 - Processing Parameters
SI        1.6384
SF        400.1500067 MHz
WDM      EM
SSB       0
LB       0.30 Hz
GB       0
PC      1.00

```

```

===== CHANNEL f1 ======
SFOL      400.152411 MHz
NUCI      1H
PL       14.75 usec
PLWI     12.0000000 W

F2 - Processing Parameters
SI        1.6384
SF        400.1500067 MHz
WDM      EM
SSB       0
LB       0.30 Hz
GB       0
PC      1.00

```

79.91
77.47
77.15
76.83

44.68

21.63

Current Data Parameters
NAME Dr. A MAJEE 2017
EXPM 288
PROCNO 1

F2 - Acquisition Parameters
Date 20170401
Time 20:33
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 320
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.881744 sec
RG 62.69
DW 20.800 usec
DE 6.50 usec
TE 302.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO

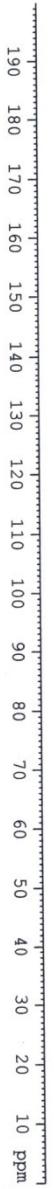
===== CHANNEL f1 =====

SPEC1 100.627589 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.0000000 W

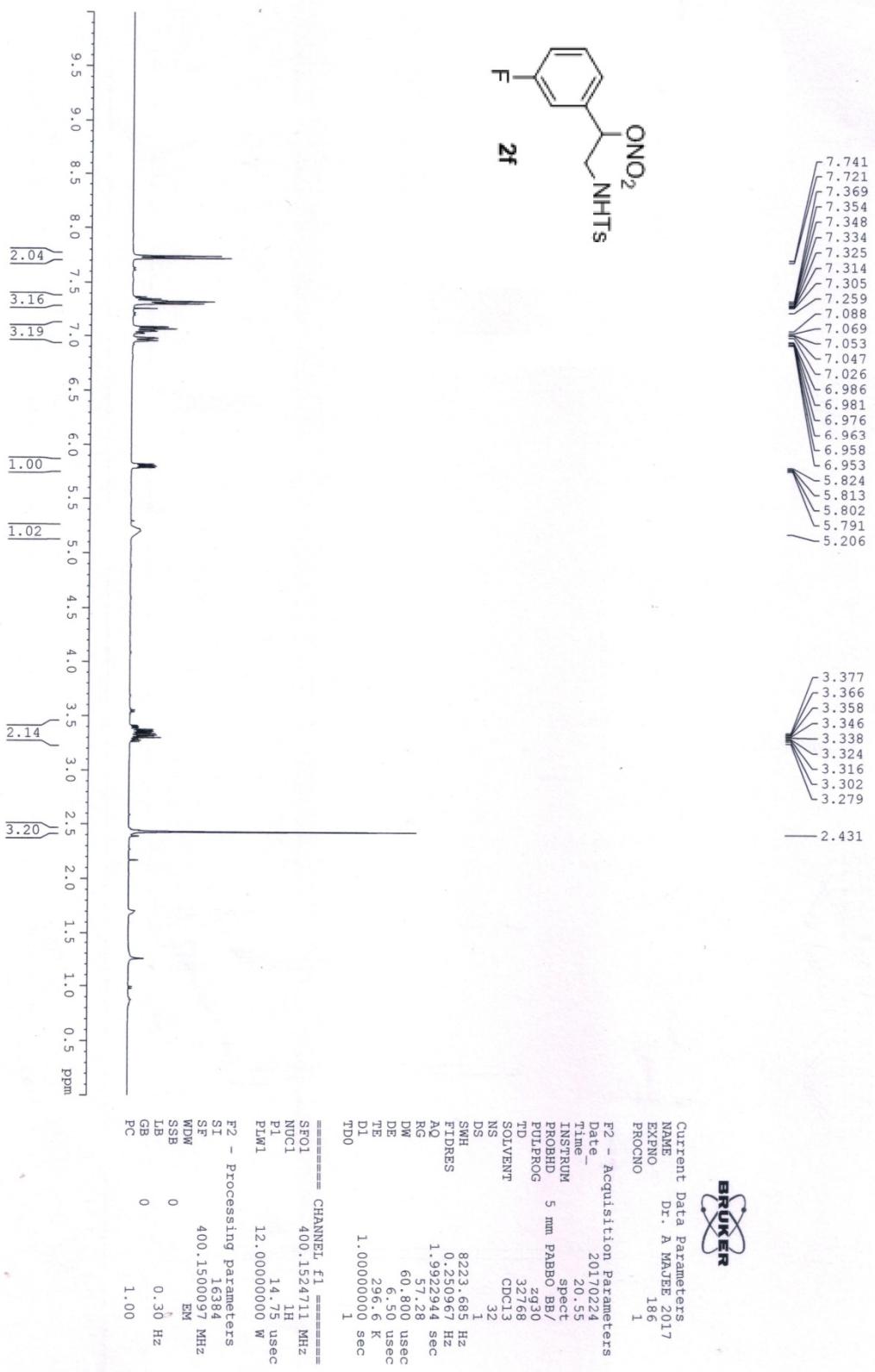
===== CHANNEL f2 =====

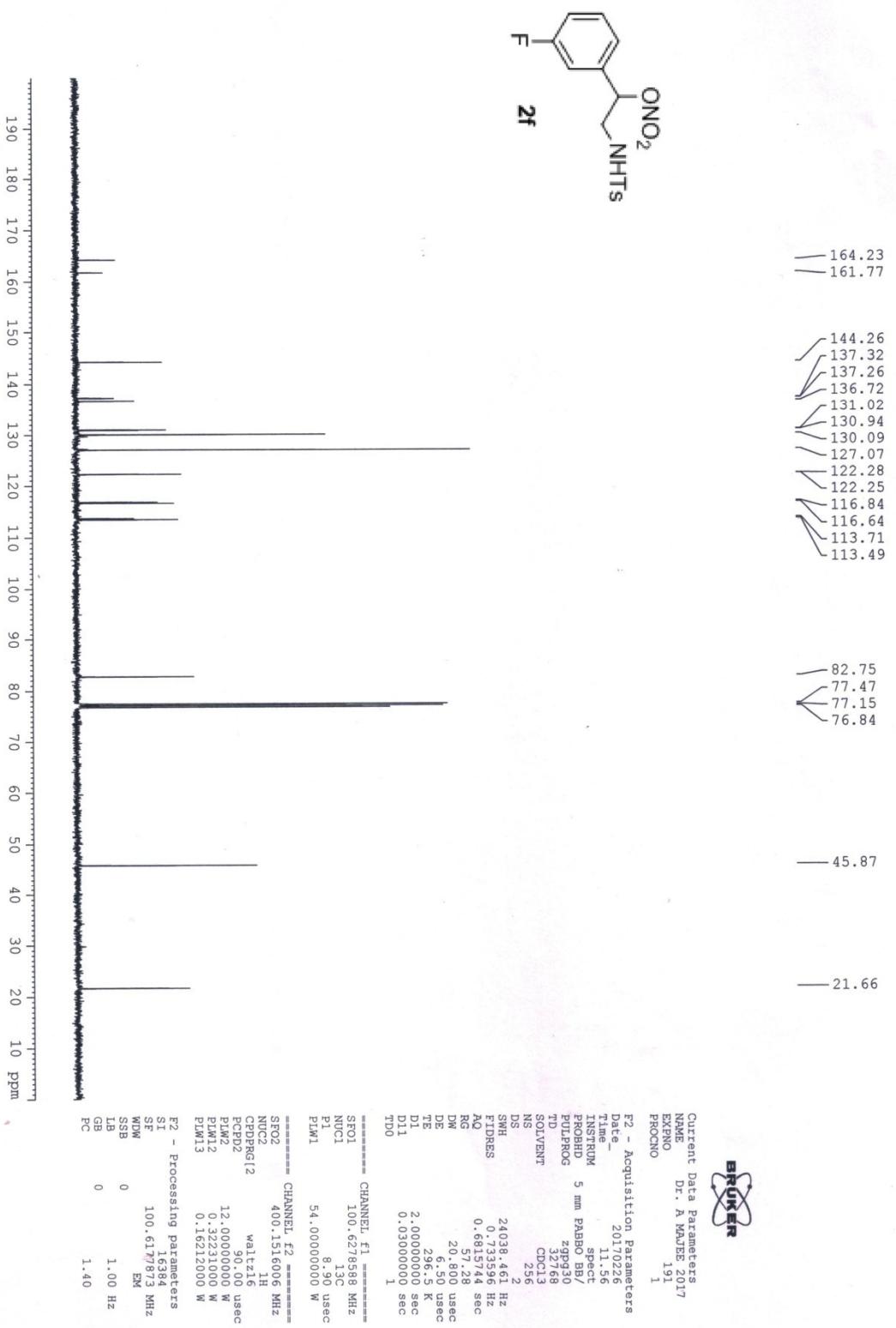
SI 400.131606 MHz
NUC2 1H
CPDPG1 2 waltz16
CPDPG2 90.00 usec
P1W2 12.0000000 W
PLW12 0.32231000 W

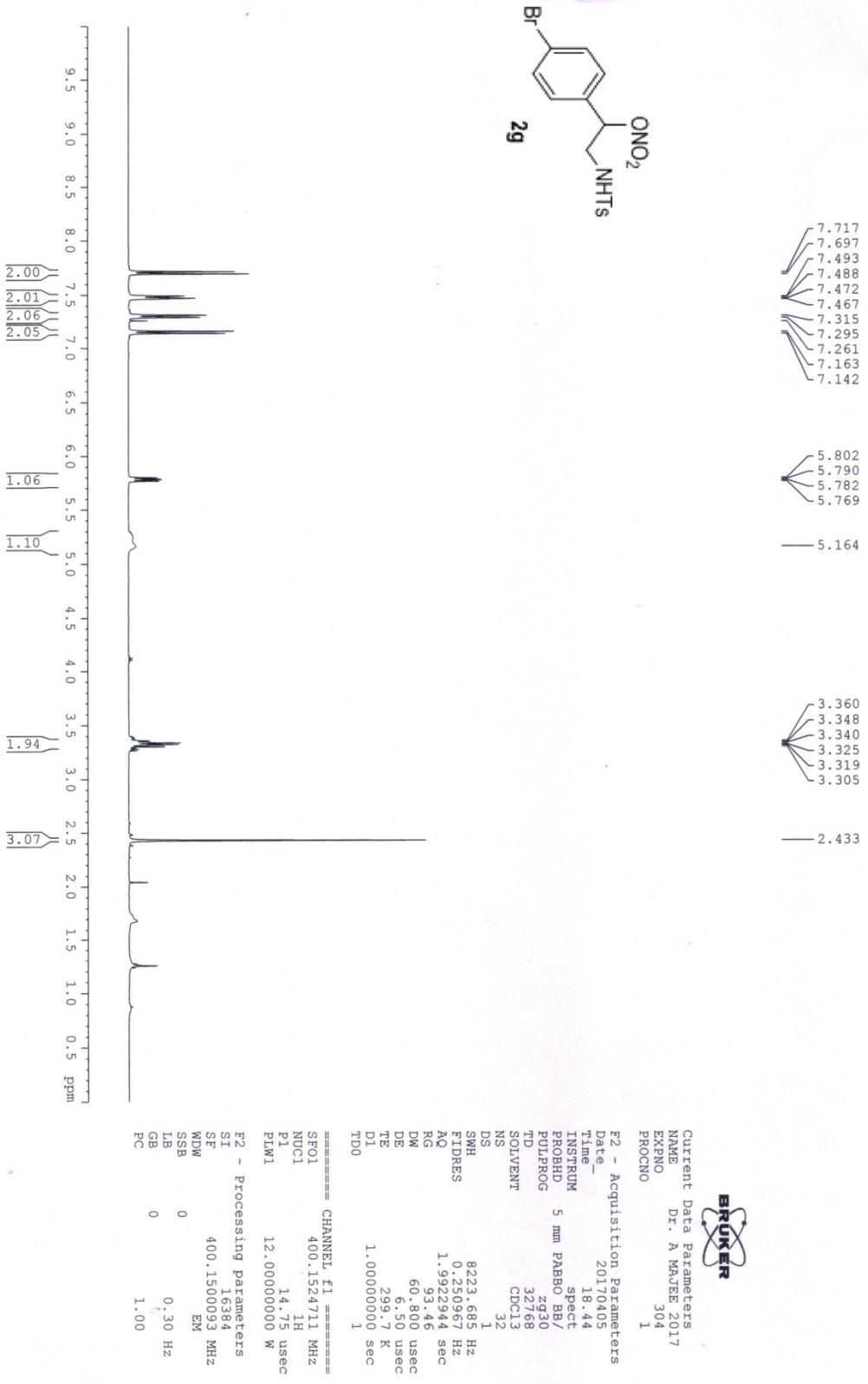
F2 - Processing parameters
SI 1.384
SF 100.6177859 MHz
NMW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

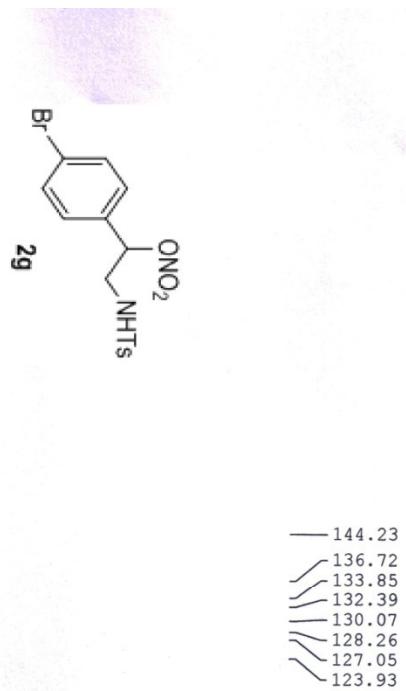


1H of VBSAS-A 9





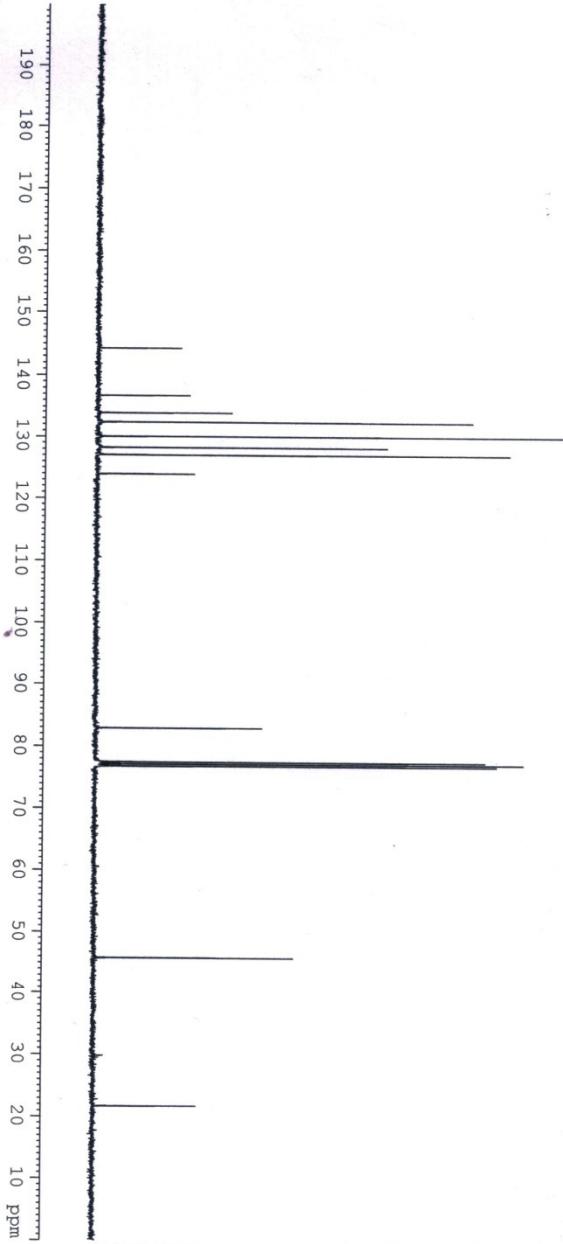




82.87
77.47
77.15
76.83

45.77

21.68



BROUKER

Current Data Parameters
NAME Dr. A MAJEE 2017
EXPNO 305
PROCNO 1

F2 - Acquisition Parameters
Date 20170406
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zppg30
TD 32768
SOLVENT CDCl3
NS 512
DS 2
SWH 0.733566 Hz
FIDRES 0.6815744 sec
RG 93.46
DW 20.800 usec
DE 6.00 usec
TE 298.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SF01 100.627858 MHz
NUC1 13C
P1 8.00 usec
PIW1 54.0000000 W

===== CHANNEL f2 =====
SF02 400.1516006 MHz
NUC2 1H
CPDPG[1,2] waltz16
PCPD2 90.00 usec
PIW2 12.0000000 W
PIW12 0.32221000 W
PIW13 0.162212000 W

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

1H of VBSAS-19A/16

8.218
8.215
8.213
8.210
8.197
8.195
8.193
8.190
8.127
8.124
8.123
8.118
7.719
7.715
7.698
7.694
7.689
7.684
7.681
7.662
7.659
7.594
7.574
7.554
7.312
7.292
7.259
5.949
5.937
5.930
5.917
5.390
5.374
5.357

3.430
3.417
3.412
3.401
3.398
3.382

— 2.426



Current Data Parameters
NAME Dr. A MAJEE 2017
EXPNO 311
PROCNO 1

F2 - Acquisition Parameters

Date 20170406

Time 19.41

INSTRUM spect

PROBID 5 mm PABBO BB/

PULPROG 2930

TD 32768

SOLVENT CDCl3

NS 32

DS 1

SWH 8223.685 Hz

FIDRES 0.350967 Hz

AQ 1.992944 sec

RG 93.46

DW 60.800 usec

DE 6.50 usec

TE 299.3 K

D1 1.0000000 sec

TDO 1

===== CHANNEL f1 ======
SF01 400.1524711 MHz
NUCL 1H
PL 14.75 usec
PIWI 12.0000000 W

F2 - Processing parameters

SI 16384

SF 400.1500097 MHz

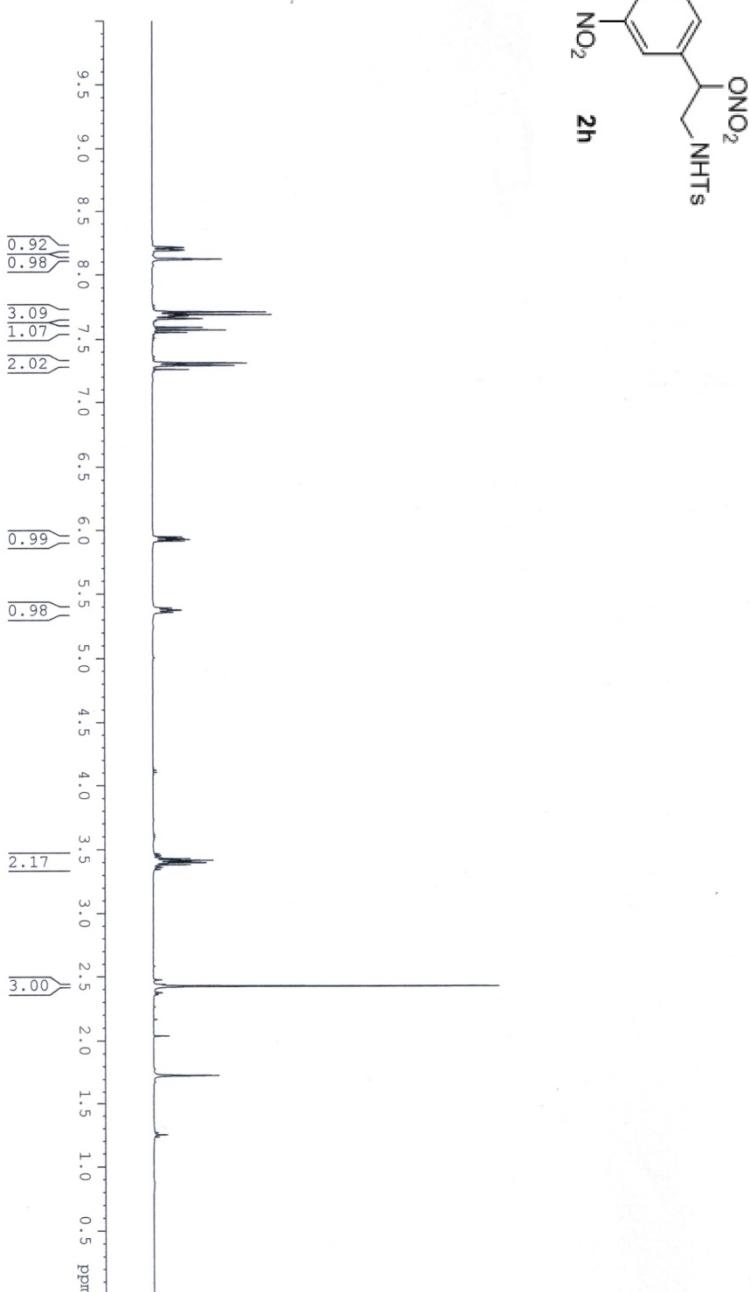
WDW EM

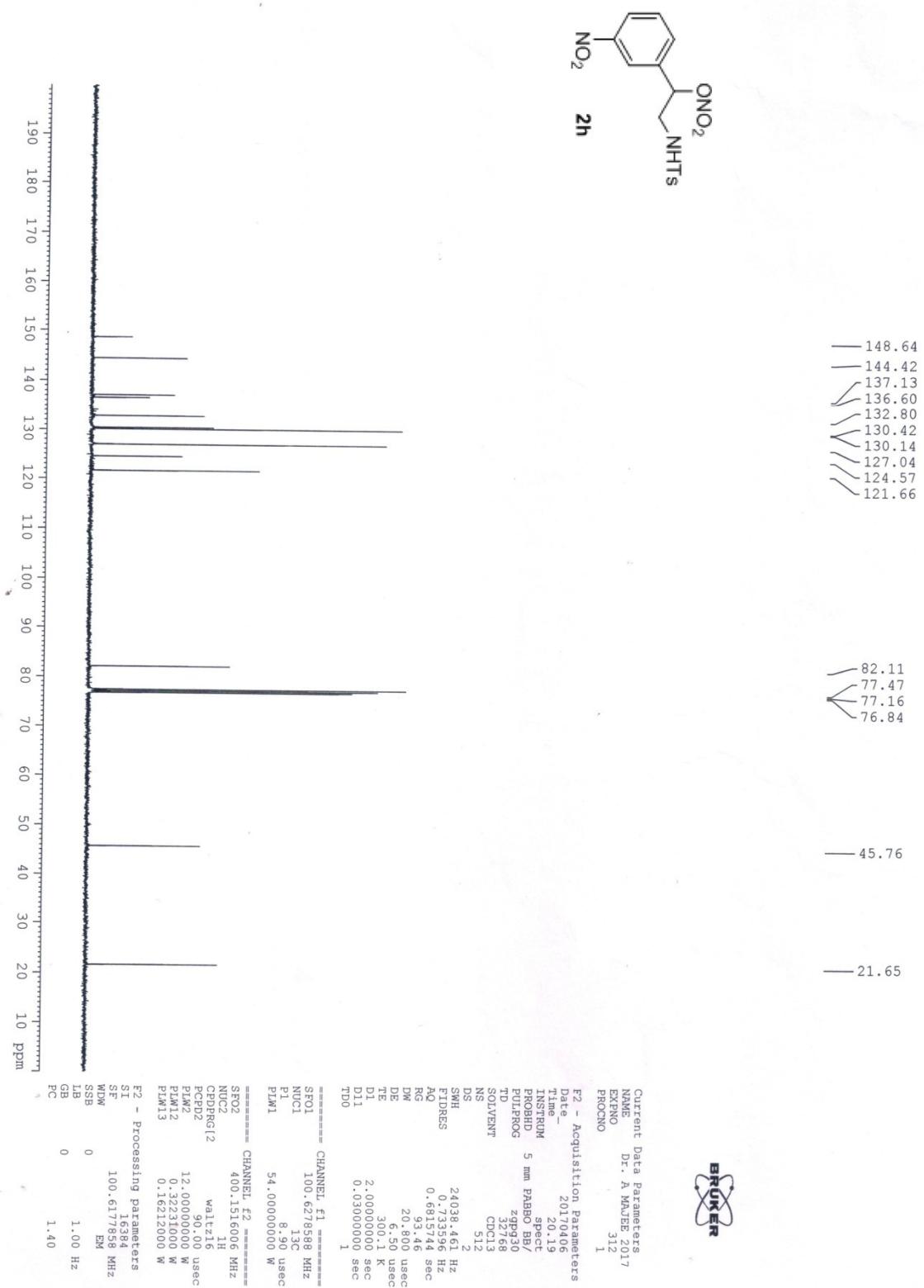
SSB 0

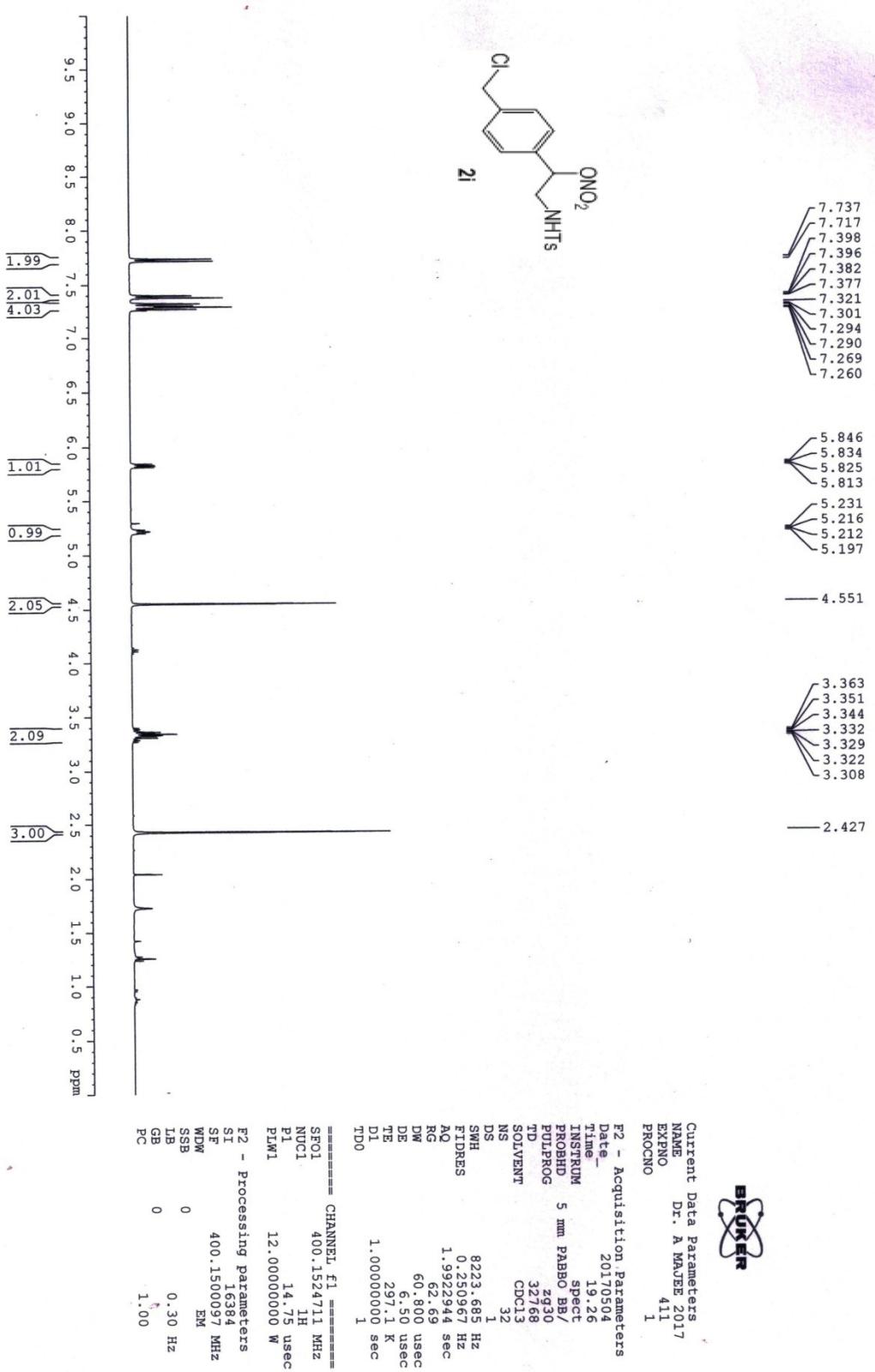
LB 0

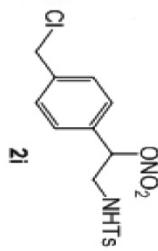
GB 0.30 Hz

PC 1.00









144.18
139.08
136.75
135.00
130.06
129.35
127.07
126.99

83.21
77.47
77.15
76.83

45.89
45.51

21.64

EPIKURE
Current Data Parameters
NAME Dr. A MAJEE 2017
EXPNO 414
PROCNO 1

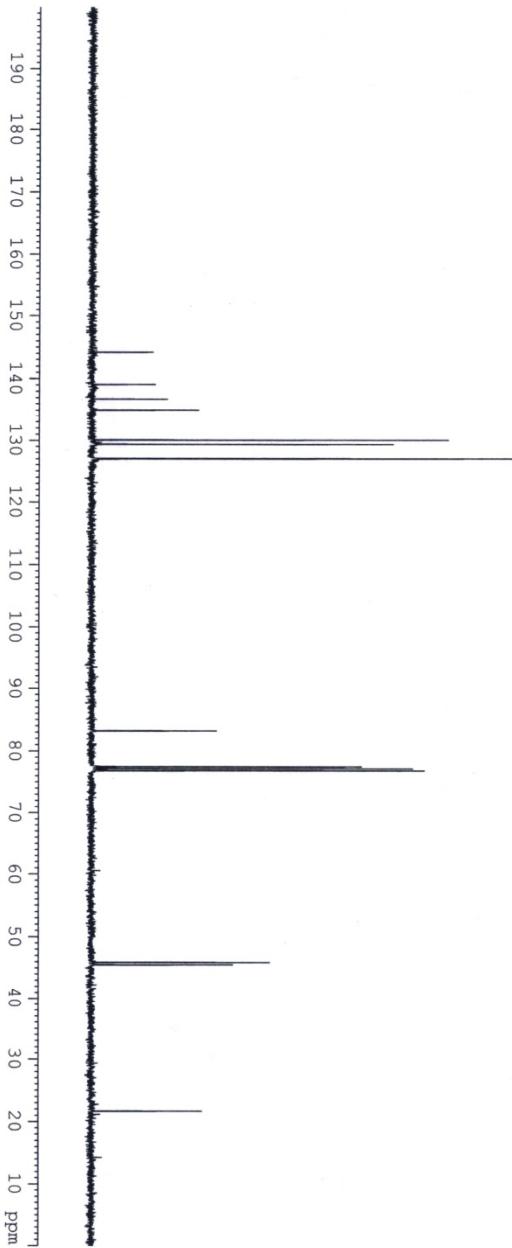
F2 = Acquisition Parameters
Date_ 2017-05-04
Time 19:55
INSTRUM spect
PROBID 5 mm PABCO BB/
PULPROG zgpp30
TD 32768

SOLVENT CDCl3
NS 180
DS 2
SWH 24038.461 Hz
EIDRES 0.733396 Hz
AQ 0.615144 sec
RG 62.69
DW 2.00 usec
DE 6.50 usec
TE 29.7 K
D1 2.000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL F1 =====
SFO1 100.627888 MHz
NUC1 13C
PI 8.90 usec
PLW1 54.0000000 W

===== CHANNEL F2 =====
SFO2 400.1216006 MHz
NUC2 1H
CPDPFG[12] waltz16
PCPD2 90.00 usec
PLW2 12.0000000 W
PLW12 0.3223100 W
PLW13 0.16521200 W

F2 - Processing parameters
SI 6384
SF 100.6177887 MHz
WM EM
SSB 0
LB 1.00 Hz
GB 1.40
PC



7.763
7.743

7.306
7.286
7.259

5.373
4.806
4.796
4.783
4.773
4.760
4.749
3.292
3.281
3.269
3.259
3.246
3.235
3.214
3.214
2.422
2.038
2.034
2.023
2.013
1.978
1.701
1.686
1.676
1.636
1.624
1.609
1.425
1.408
1.401
1.391
1.382
1.367
1.363
1.355
1.330
1.323
1.306

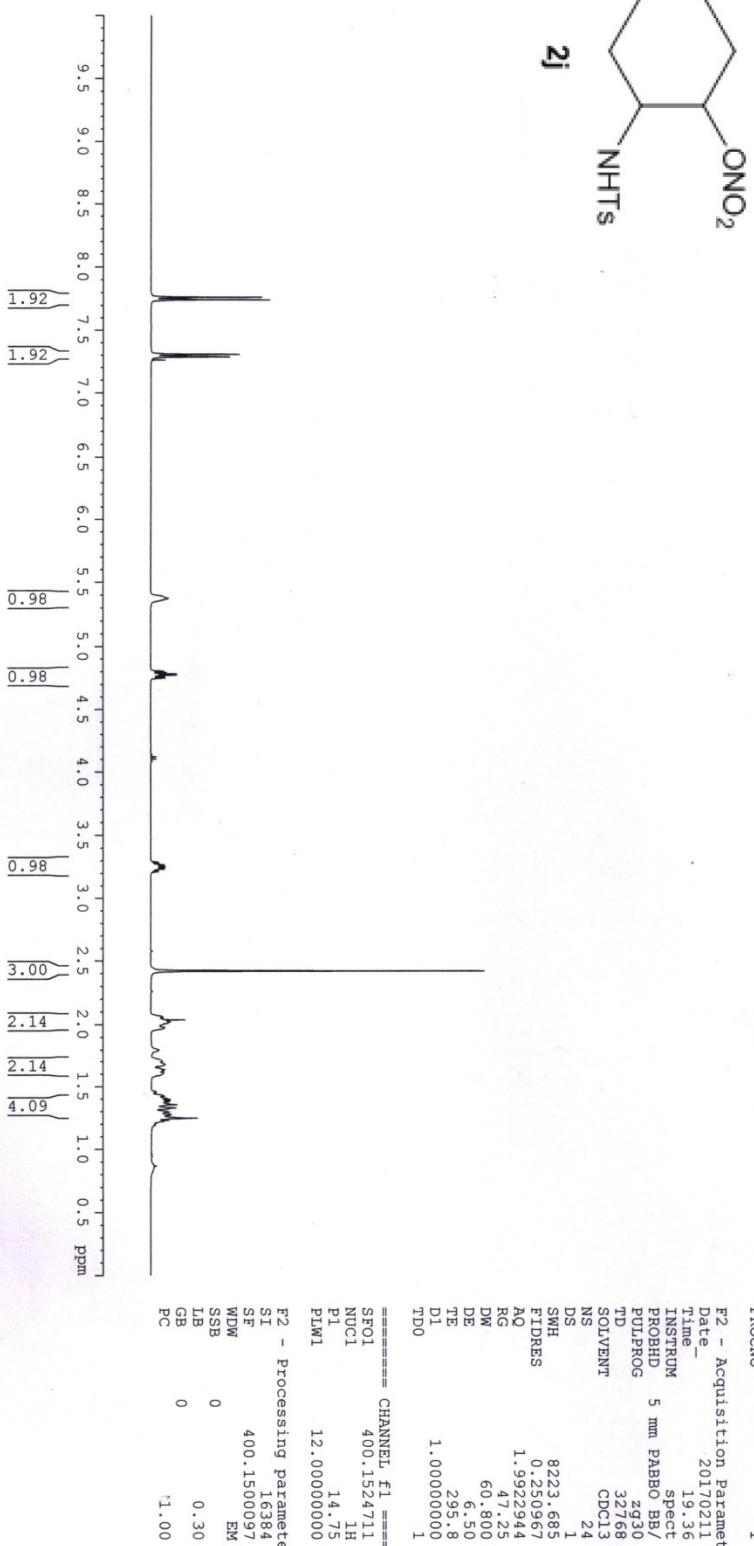
BRUKER

Current Data Parameters
NAME DR. A MAJEE 2017
EXPNO 125
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170211
Time 19.36
INSTRUM spect
PROBODP 5 mm PABBO BB/
PULPROG zg30
TD 29768
SOLVENT CDCl3
NS 24
DS 1
SWH 8223.695 Hz
FIDRES 0.250967 Hz
AQ 1.992294 sec
RG 47.25
DW 60.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.0000000 sec
TDO 1

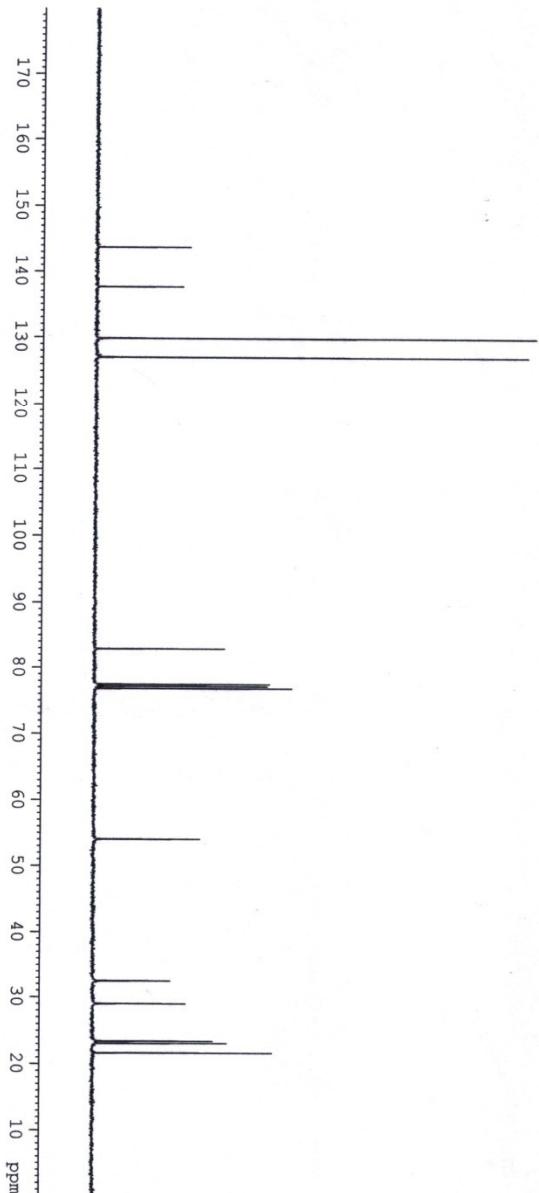
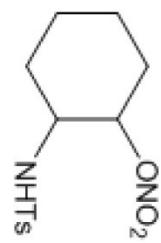
===== CHANNEL f1 =====
SF01 400.1524711 MHz
NUCL 1H
P1 14.75 usec
PLW1 12.0000000 W

F2 - Processing parameters
SI 16384
SF 400.150007 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 1.00
PC



¹³C of SAS-ZnNO₃

143.71
 137.63
 129.84
 127.04
 82.90
 77.47
 77.16
 76.84
 54.04
 32.43
 28.98
 23.41
 23.08
 21.63



Current Data Parameters
 NAME Dr. A MAJEE 2017
 EXPNO 324
 PROCN0 1
 F2 - Acquisition Parameters
 Date 20170412
 Time 17:20
 INSTRUM spect
 PROBHD 5 mm PABO BB/
 PULPROG zpd30
 TD 32768
 SOLVENT CDCl₃
 NS 320
 DSS 2
 SWH 24038.461 Hz
 FIDRES 0.733556 Hz
 AQ 0.681574 sec
 RG 67.81
 DW 20.800 usc
 DE 6.50 usc
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1 sec

===== CHANNEL f1 ======
 SF01 1.00.627858 MHz
 NUC1 13C
 P1 8.90 usec
 PLW1 54.0000000 W

===== CHANNEL f2 ======
 SF02 40.0.1516006 MHz
 NUC2 1H
 CPB2G12 walt:16
 PCP2 90.00 usec
 PLW2 12.0000000 W
 PLW12 0.02221000 W
 PLW13 0.16212000 W

F2 - Processing parameters
 SI 16384
 SF 100.6177880 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

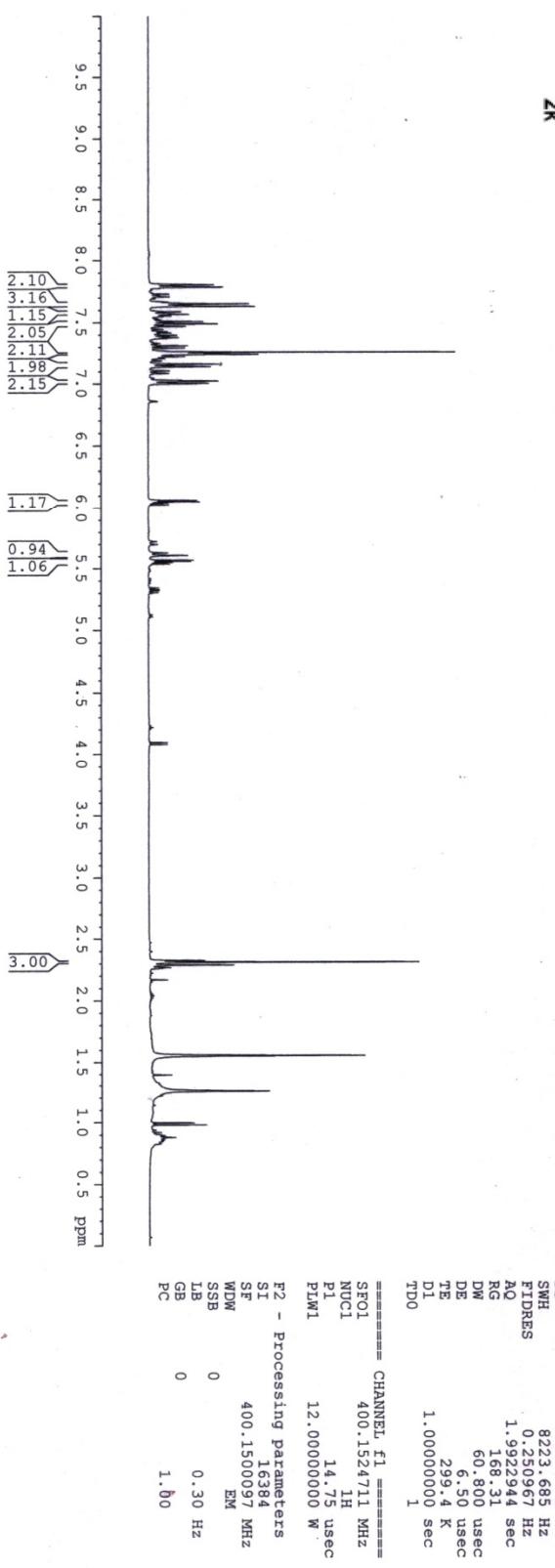
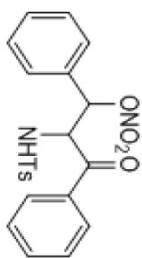
1H of VBSAS 19A/18

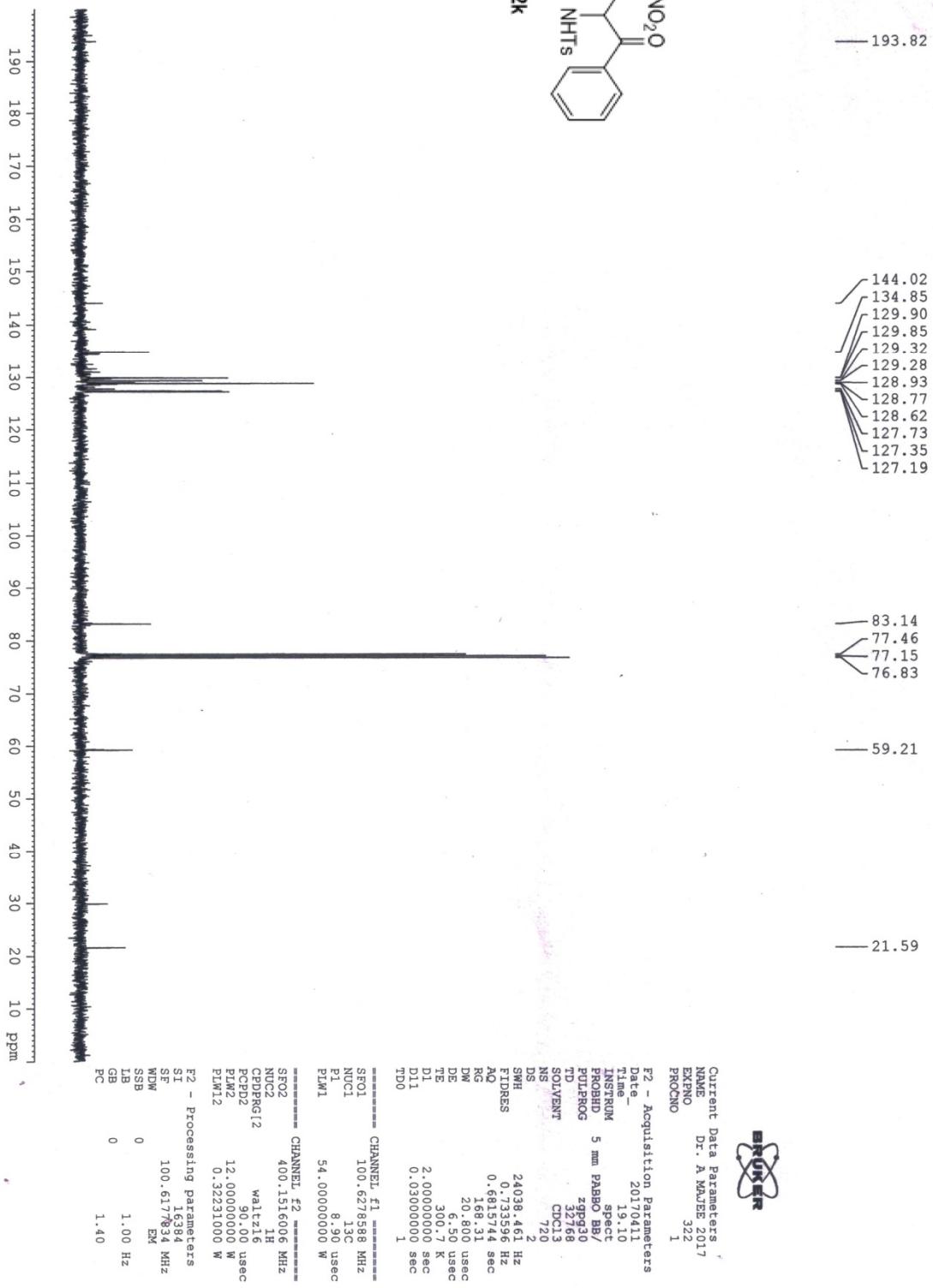
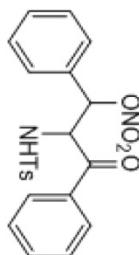
7.809
7.806
7.788
7.785
7.668
7.659
7.653
7.650
7.632
7.629
7.589
7.586
7.575
7.568
7.510
7.502
7.491
7.475
7.471
7.260
7.251
7.250
7.247
7.243
7.162
7.141
7.030
7.024
7.009
7.005
7.002
6.065
6.054
6.043
6.029
5.630
5.609
5.571
5.561
5.550
5.539

— 2.315



Current Data Parameters
NAME Dr. A MAJEE 2017
EXPN 320
PROCNO 1





7.827
7.823
7.805
7.802
7.697
7.684
7.663
7.644
7.632
7.611
7.523
7.503
7.495
7.489
7.484
7.260
7.154
7.134
7.053
7.046
7.040
7.032
7.023
7.016
7.011
6.946
6.940
6.924
6.902
6.036
6.024
5.742
5.720
5.545
5.533
5.523
5.511

2.312



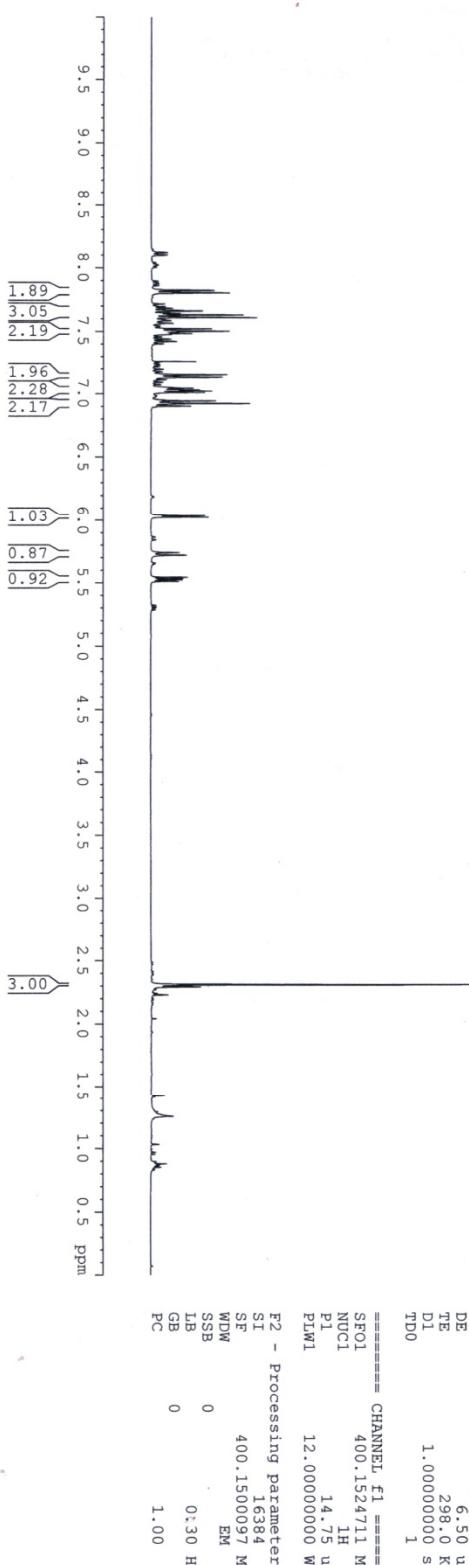
Current Data Parameters
NAME : Dr. A MAJEE 2017
EXPNO : 465
PROCNO : 1

F2 - Acquisition Parameters
Date : 20170518
Time : 18.05

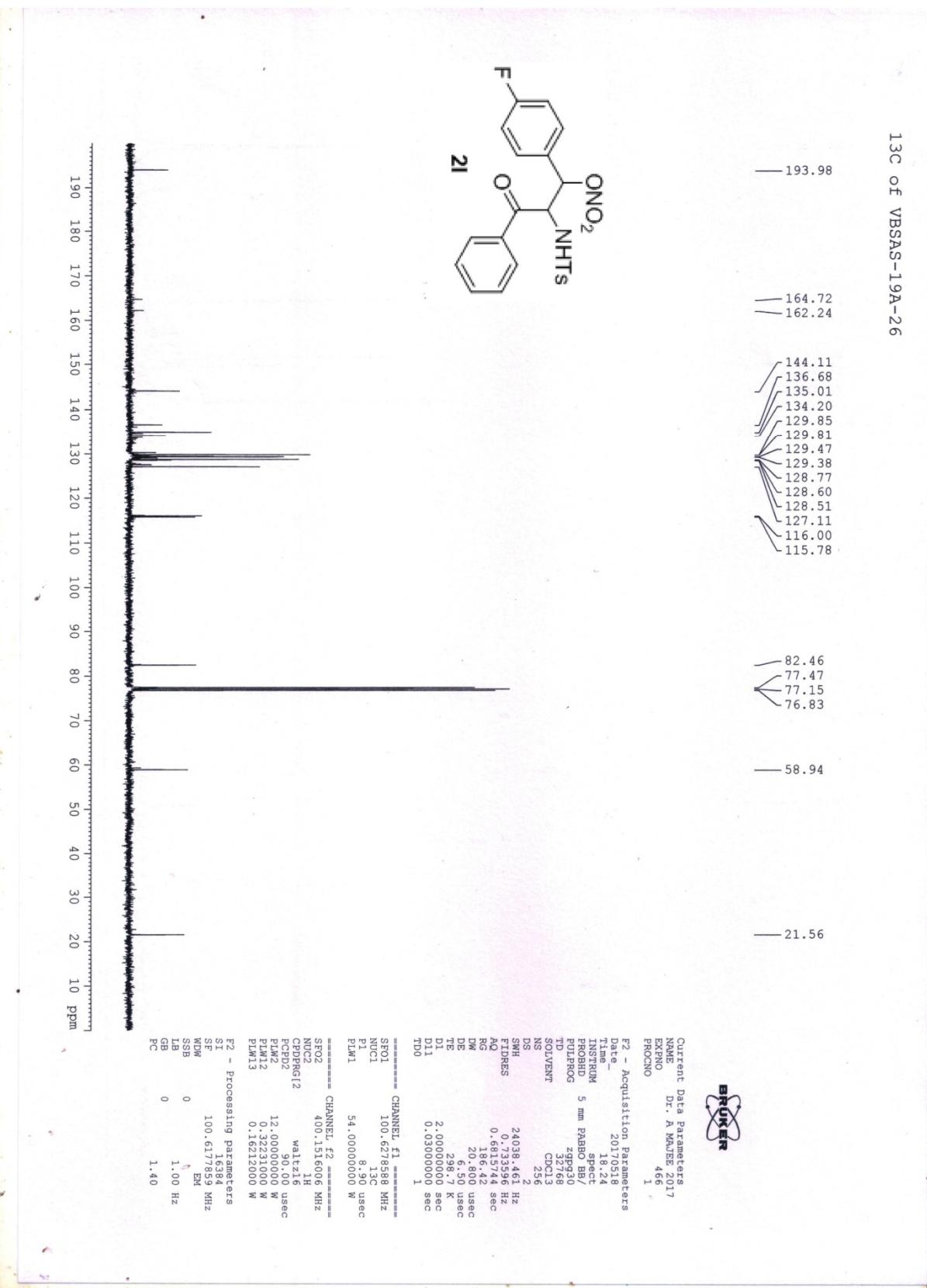
INSTRUM : 5 mm PABBO BB/
PROBHD : 2430
PULPROG : 32268
TD : 32768
SOLVENT : CDCl3
NS : 32
DS : 1
SWH : 8223.685 Hz
FIDRES : 0.250967 Hz
AQ : 1.992294 sec
RG : 62.69
DW : 60.800 usec
DE : 6.50 usec
TE : 298.0 K
D1 : 1.0000000 sec
TDO : 1

===== CHANNEL f1 =====
SFO1 : 400.1524711 MHz
NUC1 : 1H
PLW1 : 14.75 usec
PLW1 : 12.0000000 W

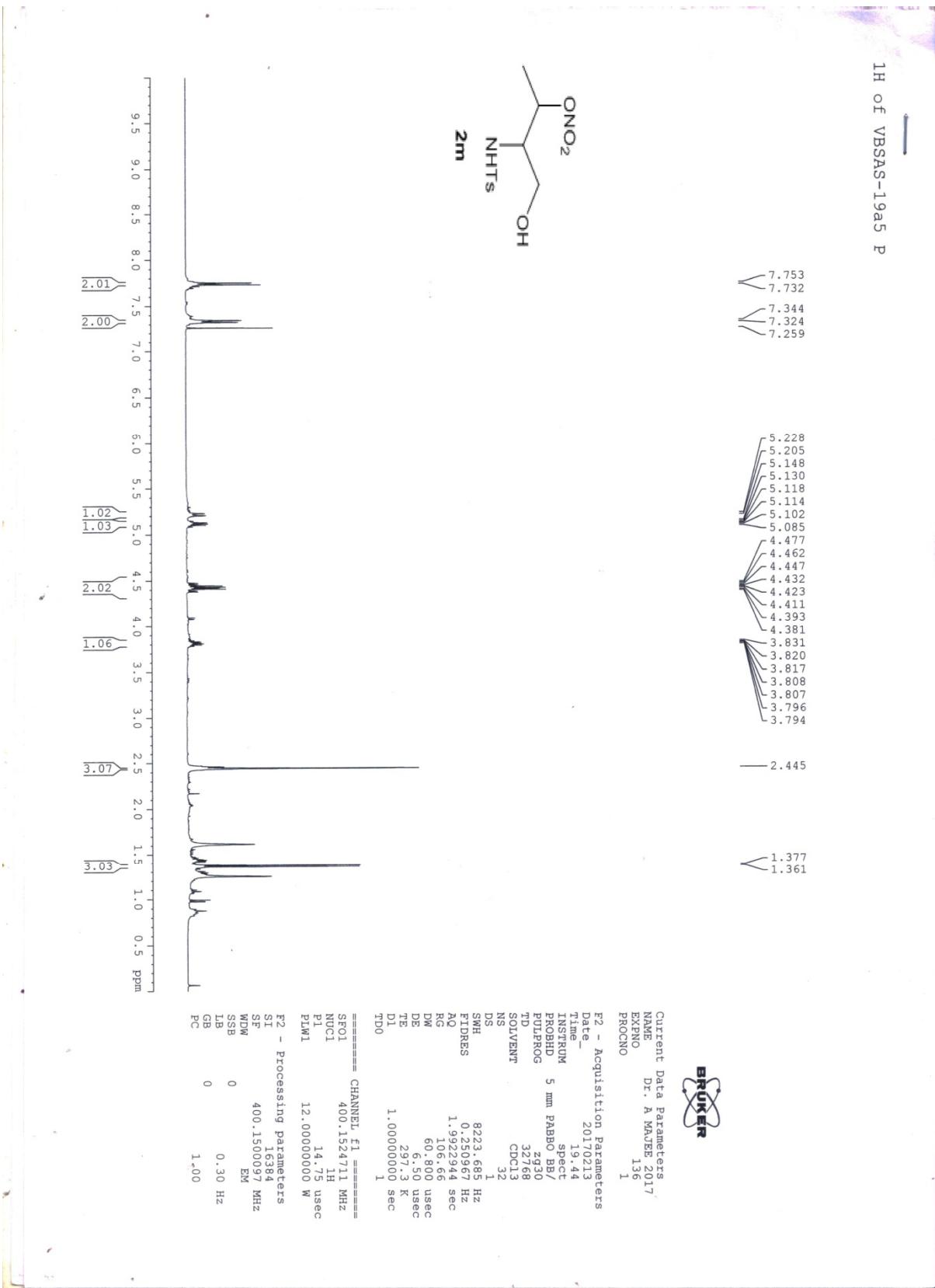
F2 - Processing parameters
SI : 1634
SF : 400.1500037 MHz
WDW : EM
SSB : 0
LB : 0
GB : 0.30 Hz
PC : 1.00



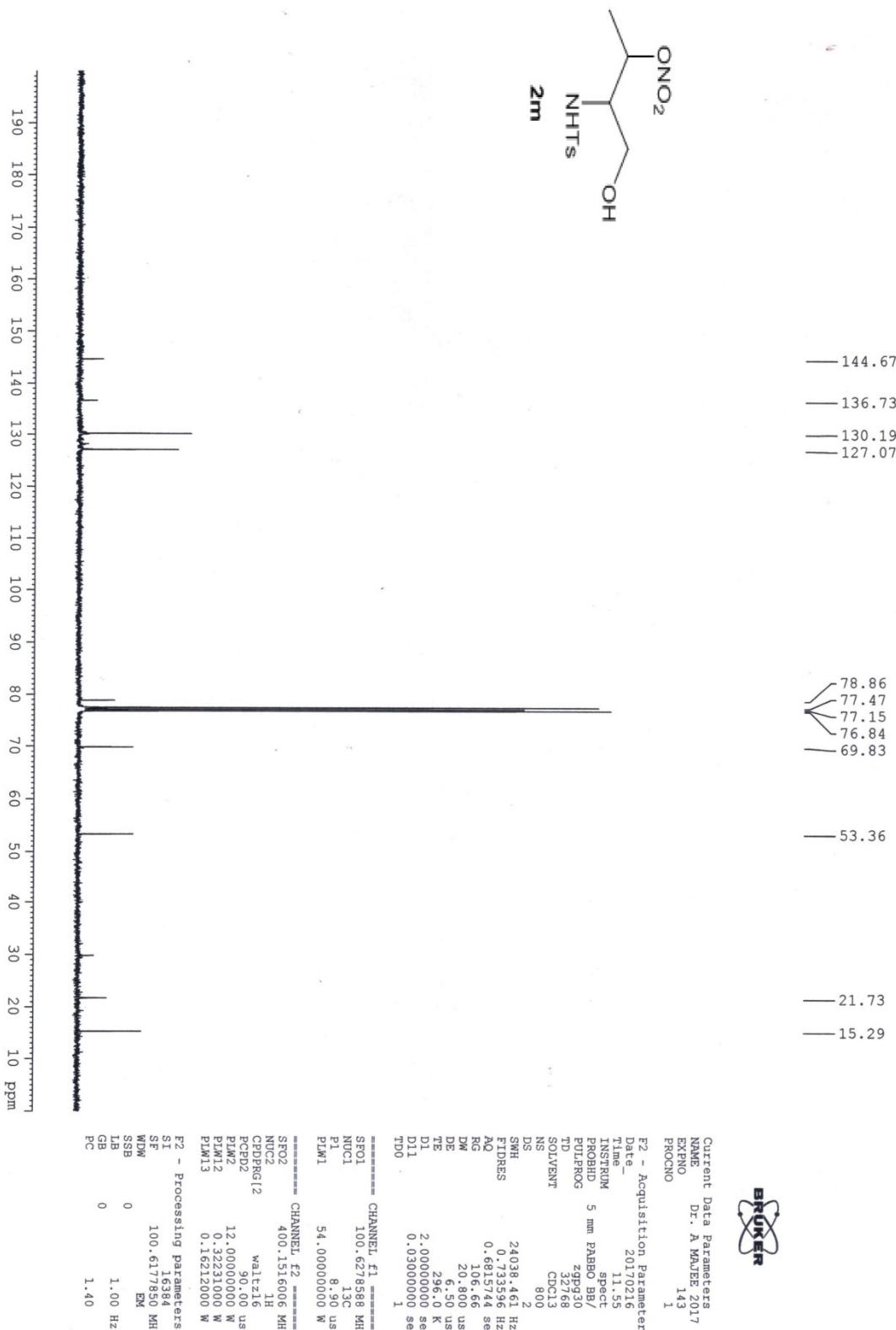
13C of VBSAS-19A-26



1H of VBSAS-19a5 P



13C of VBSAS-19a5p



¹H OF VBSAS-19-A6

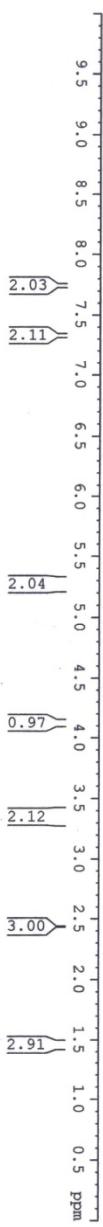
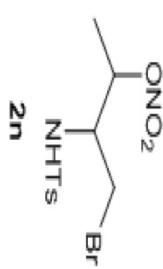
7.753
7.732

7.339
7.319
7.260

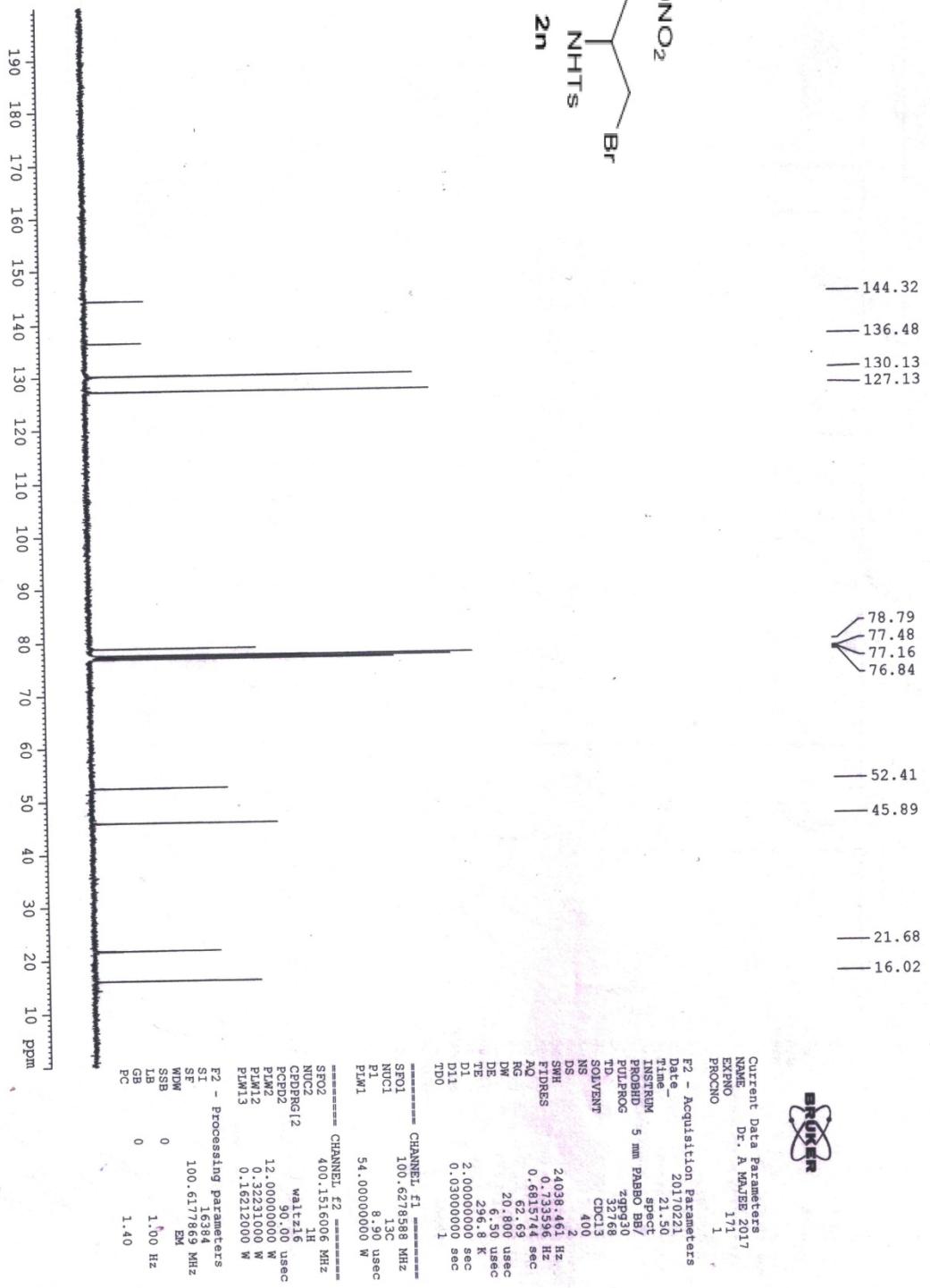
5.310
5.294
5.280
5.264
5.248

4.145
4.132
4.128
4.119
4.115
4.102
3.423
3.387
3.373
3.368
3.355
3.346
3.330
3.314
3.294
3.279
2.435

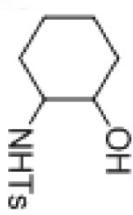
1.464
1.448



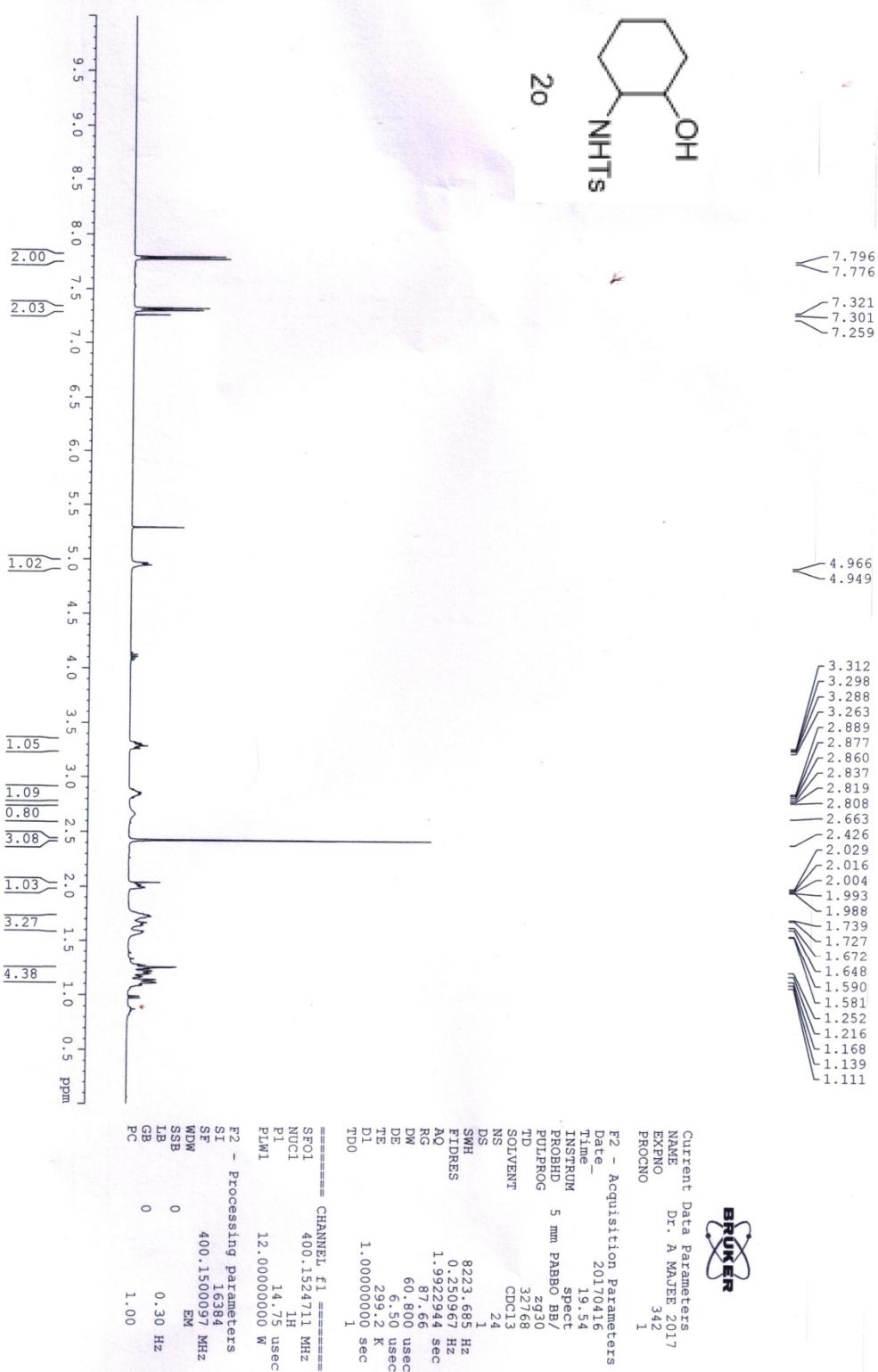
Current Data Parameters
 NAME Dr. A MAJEE 2017
 EXPNO 170
 PROCN 1
 F2 - Acquisition Parameters
 Date 20170221
 Time 21.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 32
 DS 1
 SWH 8223.685 Hz
 FIDRES 0.250987 Hz
 FIDRESS 1.992294 sec
 AQ 62.69
 RG 60.800 usec
 DW 6.50 usec
 DE 296.1 K
 TE 1.0000000 sec
 D1 1
 TDO 1
 ===== CHANNEL f1 ======
 SF01 400.1524711 MHz
 NUC1 1H
 P1 14.75 usec
 PLW1 12.0000000 W
 F2 - Processing parameters
 ST 16384
 SF 400.150005 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

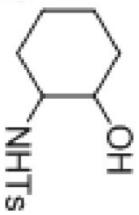


1H of SAS-APP



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— 143.76
— 137.51
— 129.93
— 127.29

77.47
77.15
76.84
73.52

— 59.83

33.52
32.01
24.77
23.96
21.68

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



Current Data Parameters
NAME Dr. A MAUE 2017
EXPM 343
PROCNO 1

F2 - Acquisition Parameters
Date 20170416
Time 20:58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zppg930
TD 32768
SOLVENT CDCl₃
NS 640
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 77.59
DW 20.800
DE 6.50 usec
TE 300.0 K
TEC 0.0000000 sec
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6278388 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.0000000 W

===== CHANNEL f2 =====
SFO2 40.1516006 MHz
NUC2 1H
CPDPG1[2 waltz16
CPDPG2 90.00 usec
PLW2 12.0000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.6177843 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

