Supporting Information

Metal nano particle in "on-water" organic synthesis: one-pot nano CuO catalyzed synthesis of isoindolo[2,1-*a*]quinazolines

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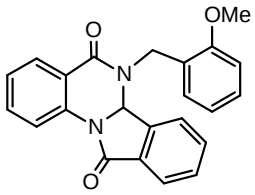
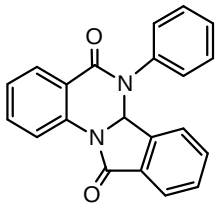
General: ^{1}H NMR spectra were determined on a Bruker 400 (400 MHz) spectrometer as solutions in $CDCl_3$. Chemical shifts are expressed in parts per million (δ) and are referenced to tetramethylsilane (TMS) as internal standard and the signals were reported as s (singlet), d (doublet), t (triplet), m (multiplet) and coupling constants *J* were given in Hz. ^{13}C NMR spectra were recorded at 100 MHz in $CDCl_3$ solution. TLC was done on silica gel coated glass slide (Merck, Silica gel G for TLC). Silica gel (60-120 mesh, SRL, India) was used for column chromatography. Petroleum ether refers to the fraction boiling in the range of 60-80 ºC unless otherwise mentioned. All solvents were dried and distilled before use. Commercially available substrates were freshly distilled before the reaction. Solvents, reagents and chemicals were purchased from Aldrich, Fluka, Merck, SRL, Spectrochem and Process Chemicals.

Typical procedure for synthesis of 6-(2-methoxy-benzyl)-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4h)



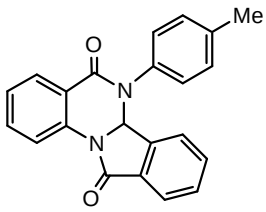
A mixture of isatoic anhydride (163 mg, 1 mmol), 2-carboxybenzaldehyde (150 mg, 1 mmol) and 2-methoxybenzyl amine (130 µL, 137 mg, 1 mmol) was stirred in presence of CuO nano (5 mol%) in water (3 mL) under refluxed conditions for 10h (TLC). After completion, ethyl acetate (10 mL) was added to the reaction mixture. Then the insoluble CuO nanoparticles was filtered by Teflon membrane (PTFE, 0.2 µm pore size) and the filtrate was extracted with ethylacetate (5 mL) followed by washing with brine (5 mL) and dried over Na_2SO_4. After evaporation of solvent the crude product was purified by column chromatography on silica gel using petroleum ether/ethyl acetate (4:1 to 3:1) as eluent. The CuO nanoparticles were thoroughly washed with the ethanol and reused for the next cycle. Yield: 314 mg, 85%; White solid, mp. 160-162 °C; IR (KBr)**:** 3024, 1959, 1716, 1656, 1476 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 7.6 Hz, 1H), 8.15 (d, *J* = 8 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.67-7.51 (m, 3H), 7.42-7.36 (m, 2H), 7.23-7.21 (m, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.92-6.88 (m, 2H), 6.38 (s, 1H), 5.24 (d, *J* = 17.2 Hz, 1H), 4.84 (d, *J* = 17.6 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1, 164.2, 156.5, 138.0, 137.0, 133.6, 132.6, 132.5, 130.5, 129.4, 128.3, 127.1, 125.4, 125.3, 124.8, 124.4, 120.9, 120.5, 120.2, 110.5, 70.9, 55.4, 42.4.

Anal. Calcd. for $C_{23}H_{18}N_2O_3$: C, 74.58; H, 4.90; N, 7.56%;. Found: C, 74.51; H, 4.82; N, 7.52%.



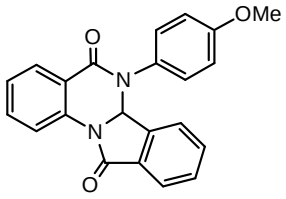
6-phenyl-6,6a-dihydroisoindolo[2,1-*a*]quinazoline-5,11-dione (4a)[1]

Yield: 280 mg, 86%; White solid, mp. 184-186 ^{o}C; IR (KBr)**:** 3029, 1963, 1721, 1658, 1468 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10-8.09 (m, 2H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.63-7.55 (m, 2H), 7.53-7.29 (m, 5H), 7.26-7.22 (m, 1H), 7.16-7.13 (m, 1H), 6.44 (s, 1H), 6.04 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.5, 164.3, 138.8, 138.3, 137.2, 134.0, 132.3, 132.2, 130.4, 129.9, 129.5, 129.3, 125.5, 125.4, 124.6, 120.4, 120.3, 120.2, 72.1.



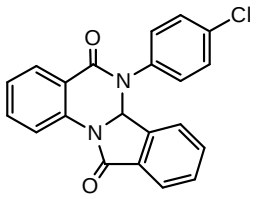
6-*p*-Tolyl-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4b)[2]

Yield: 285 mg, 84%; Gummy mass; IR (KBr)**:** 3015, 1718, 1655, 1472 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12-8.09 (m, 2H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.61-7.41 (m, 4H), 7.28-7.18 (m, 4H), 6.42 (s, 1H), 6.13 (d, *J* = 7.2 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.3, 164.2, 139.0, 138.7, 137.0, 135.3, 134.3, 133.8, 132.1, 132.0, 130.3, 130.1, 129.6, 129.4, 125.4, 125.2, 124.3, 120.2, 72.2, 21.3.



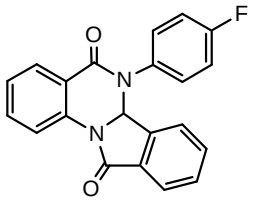
6-(4-Methoxy-phenyl)-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4c)

Yield: 285 mg, 80%; White solid, mp. 141-143 °C; IR (KBr)**:** 3033, 1967, 1717, 1661, 1482 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04-8.01 (m, 2H), 7.80 (d, *J* = 7.2 Hz, 1H), 7.54-7.49 (m, 1H), 7.41-7.32 (m, 2H), 7.20-7.14 (m, 2H), 6.95-6.50 (m, 3H), 6.35 (s, 1H), 6.10 (d, *J* = 8 Hz, 1H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1, 164.2, 159.6, 138.6, 136.9, 133.6, 132.0, 131.9, 130.6, 130.0, 129.2, 125.4, 125.0, 124.2, 120.2, 120.0, 114.9, 114.5, 72.2, 55.4. Anal. Calcd. for $C_{22}H_{16}N_2O_3$: C, 74.15; H, 4.53; N, 7.86%;. Found: C, 74.07; H, 4.42; N, 7.77%.



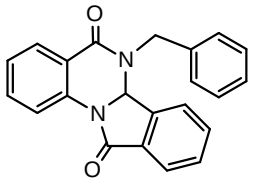
6-(4-Chloro-phenyl)-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4d)[2]

Yield: 280 mg, 78%; White solid, mp. 186-188 °C; IR (KBr)**:** 3021, 1954, 1718, 1656, 1479 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19-8.15 (m, 2H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.70-7.66 (m, 1H), 7.64-7.50 (m, 3H), 7.42-7.32 (m, 4H), 6.51 (s, 1H), 6.28 (d, *J* = 8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.4, 164.4, 138.5, 137.3, 136.8, 135.2, 134.3, 132.5, 132.3, 130.6, 130.1, 129.6, 129.5, 125.5, 124.8, 120.5, 120.2, 120.1, 72.3.



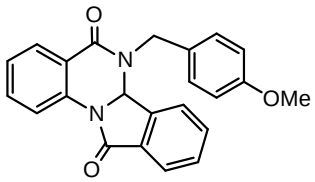
6-(4-Fluoro-phenyl)-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4e)

Yield: 258 mg, 75%; Gummy mass; IR (KBr)**:** 3027, 1951, 1718, 1659, 1477 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18-8.13 (m, 2H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.72-7.68 (m, 1H), 7.59-7.53 (m, 2H), 7.39-7.32 (m, 3H), 7.08-6.74 (m, 2H), 6.51 (s, 1H), 6.24 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.1, 164.2, 162.5 (d, $^{1}J_{C-F}$ = 247 Hz), 138.4, 137.0, 134.0, 133.9 (d, $^{4}J_{C-F}$ = 3 Hz), 132.2, 132.0, 130.3, 129.4, 125.2 (d, $^{3}J_{C-F}$ = 6 Hz), 124.6, 120.3, 120.0, 116.8, 116.5, 115.7 (d, $^{2}J_{C-F}$ = 21 Hz), 72.2; Anal. Calcd. for $C_{21}H_{13}FN_2O_2$: C, 73.25; H, 3.81; N, 8.14%;. Found: C, 73.17; H, 3.76; N, 8.07%.



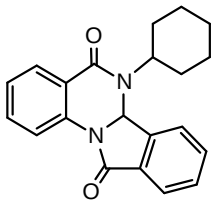
6-Benzyl-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4f).[1]

Yield: 282 mg, 83%; White solid, mp. 154-156 °C; IR (KBr)**:** 3024, 1956, 1715, 1660, 1482 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, *J* = 7.6 Hz, 1H), 8.04 (d, *J* = 8 Hz, 1H), 7.88 (d, *J* = 6.8 Hz, 1H), 7.87-7.44 (m, 3H), 7.34-7.11 (m, 7H), 6.27 (s, 1H), 5.42 (d, *J* = 16.4 Hz, 1H), 4.54 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.8, 164.1, 137.6, 136.8, 136.1, 133.7, 132.6, 132.5, 130.5, 129.4, 129.0, 127.2, 126.2, 125.4, 125.3, 124.9, 120.1, 120.0, 70.6, 46.6.



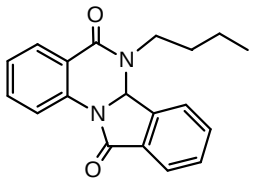
6-(4-Methoxy-benzyl)-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4g).[1]

Yield: 314 mg, 85%; White solid, mp. 143-145 °C; IR (KBr)**:** 3028, 1959, 1718, 1656 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 8.00 (d, J = 8 Hz, 1H), 7.85 (d, J = 6.8 Hz, 1H), 7.56-7.23 (m, 5H), 7.01 (d, J = 8.8 Hz, 2H), 6.76 (d, J = 6.8 Hz, 2H), 6.21 (s, 1H), 5.30 (d, J = 16.4 Hz, 1H), 4.44 (d, J = 16.4 Hz, 1H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.9, 164.2, 158.7, 137.7, 136.8, 133.7, 132.6, 130.6, 129.8, 129.4, 128.0, 127.6, 125.5, 125.3, 125.0, 120.3, 120.2, 114.4, 70.7, 55.3, 46.1.



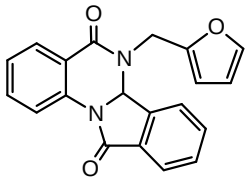
6-Cyclohexyl-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4i).[1]

Yield: 252 mg, 76%; White solid, mp. 150-152 °C; IR (KBr)**:** 3021, 1717, 1659, 1468 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, J = 7.6 Hz, 1H), 7.77-7.62 (m, 2H), 7.48-7.41 (m, 2H), 7.32-7.28 (m, 1H), 6.92-6.83 (m, 2H), 6.02 (d, J = 7.2 Hz, 1H), 3.89-3.82 (m, 1H), 1.99-1.38 (m, 5H), 1.26-1.16 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.4, 168.2, 146.0, 145.4, 134.6, 132.8, 130.6, 127.8, 127.0, 125.6, 123.1, 118.9, 117.7, 114.1, 86.2, 48.5, 33.1, 25.5, 24.8.



6-Butyl-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4j)

Yield: 251 mg, 82%; White solid, mp. 158-160 °C; IR (KBr)**:** 3022, 1965, 1714, 1660, 1452 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14-8.02 (m, 3H), 7.74-7.65 (m, 3H), 7.63-7.59 (m, 1H), 7.34-7.28 (m, 1H), 6.23 (s, 1H), 3.92-3.86 (m, 1H), 3.73-3.67 (m, 1H), 1.59-1.31 (m, 4H), 0.92 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.7, 163.5, 138.1, 136.5, 133.2, 132.8, 132.6, 130.5, 128.9, 125.2, 125.1, 125.0, 120.4, 120.0, 70.4, 42.7, 30.2, 20.0, 13.7. Anal. Calcd. for $C_{19}H_{18}N_2O_2$: C, 74.49; H, 5.92; N, 9.14%;. Found: C, 74.41; H, 5.84; N, 9.08%.



6-Furan-2-ylmethyl-6,6a-dihydro-isoindolo[2,1-*a*]quinazoline-5,11-dione (4k)

Yield: 250 mg, 76%; Gummy mass; IR (KBr)**:** 3023, 1718, 1657, 1474 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02-7.90 (m, 4H), 7.65-7.53 (m, 3H), 7.34 (d, *J* = 1.2 Hz, 1H), 7.24 (t, *J* = 7.2 Hz, 1H), 6.32-6.30 (m, 2H), 6.28 (s, 1H), 5.35 (d, *J* = 16.4 Hz, 1H), 4.37 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.0, 163.8, 150.4, 142.1, 138.1, 136.8, 133.6, 132.8, 132.6, 130.6, 129.2, 126.0, 125.2, 125.0, 120.3, 120.1, 110.8, 108.6, 70.9, 39.6. Anal. Calcd. for $C_{20}H_{14}N_2O_3$: C, 72.72; H, 4.27; N, 8.48%;. Found: C, 72.64; H, 4.21; N, 8.43%.

E-factor Calculations:[3]

Table 1 Three-component coupling of 2-carboxybenzaldehyde, isatoic anhydride and various amines: E-factor value for this protocol.[a]

Entry	Isatoic anhydride (mmol)	2-Carboxy benzaldehyde (mmol)	Amines (mmol)	Product	Isolated yield (%)[b]	Time (h)	E factor (kg waste/kg product)[c]
1	1	1	Aniline (1)	**4a**	86	10	0.45
2	1	1	*p*-Toluidine (1)	**4b**	84	10	0.47

[a] All reactions are performed with CuO nano (5 mol%) in 3 mL of water under reflux.
[b] Isolated yields.
[c] Exclusion of ethyl acetate used for work up procedure, exclusion of the amount of the CuO nano used, and exclusion of ingredients used for chromatography.

Note (Regarding Table 1, SI): When the Authors have not reported the amount of solvent used in the work-up procedure, we have not accounted for solvent and considered that solvent can be recovered. By considering the CuO nano catalyst is recyclable and hence, waste is essentially eliminated.

For Entry 1, Table1 (SI)

E = [0.163 g (isatoic anhydride) + 0.150 g (2-carboxybenzaldehyde) + 0.093 g (aniline) – 0.280 g (product × yield)] / 0.280 g

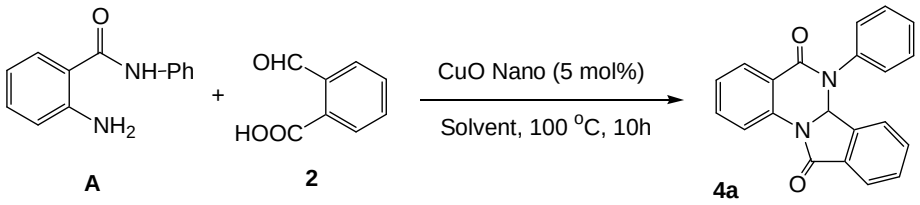
= 0.45

For Entry 1, Table1 (SI)

E = [0.163 g (isatoic anhydride) + 0.150 g (2-carboxybenzaldehyde) + 0.107 g (*p*-toluidine) – 0.285 g (product × yield)] / 0.285 g

= 0.47

Table 2 Effect of solvents on the synthesis of **4a** from compound **A** (Scheme 2 in Manuscript)[a]



A **2** **4a**

Entry	Solvent	Yield (%)[b]
1	EtOH	75
2	MeOH	70
3	MeCN	52
4	THF	50
5	Toluene	57
6	Dioxane	54

[a] Reaction conditions: 1 mmol of **A** and 1 mmol of **2** in the presence of CuO nano (5 mol%) in 3 mL of solvents at 100 °C for 10 h. [b] Isolated yields.

Reusability of the catalyst:

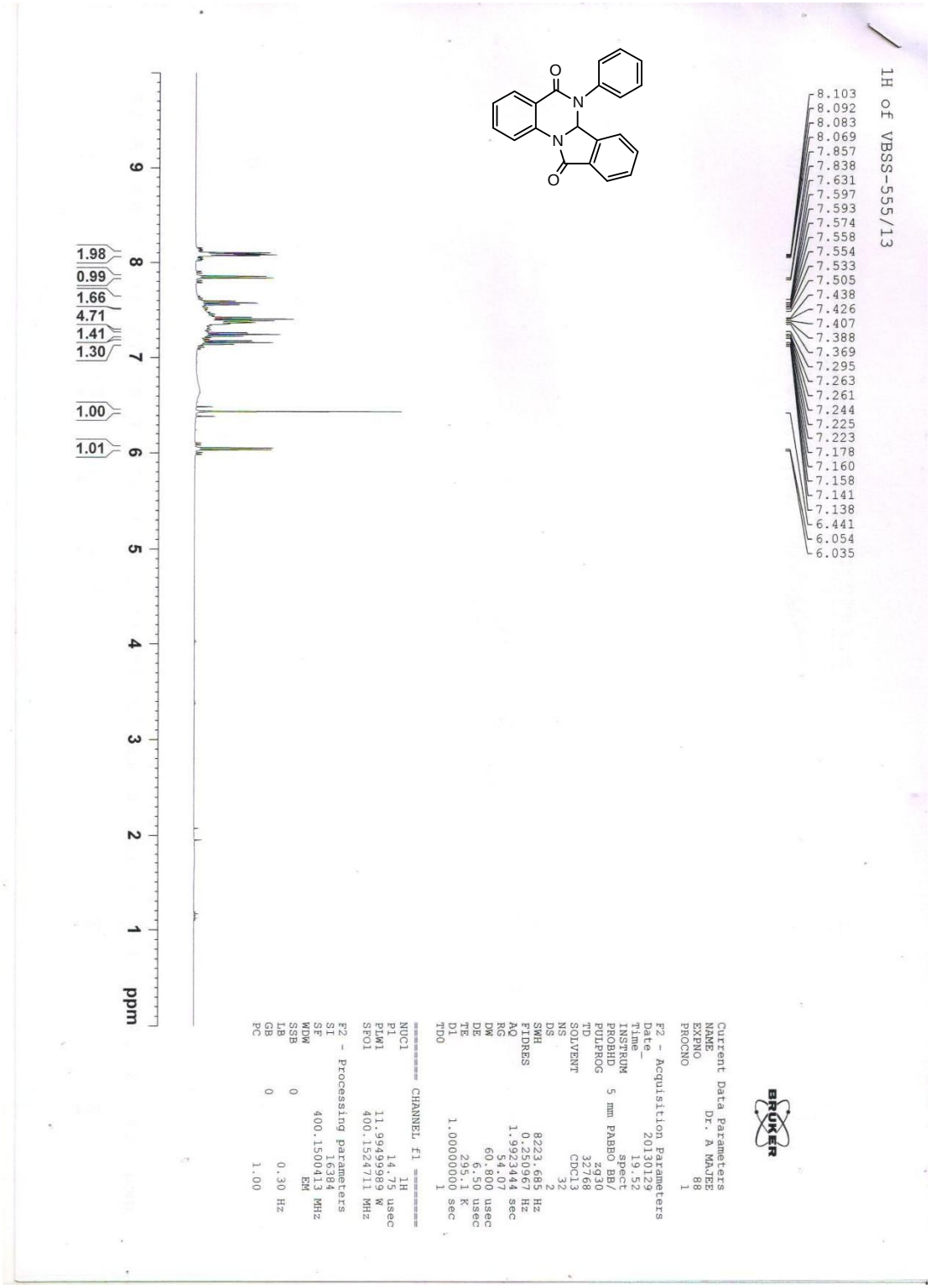
After completion of the reaction, ethylacetate (10 mL) was added to the reaction mixture. Then the insoluble CuO nanoparticles were filtered by Teflon membrane (PTFE, 0.2 µm pore size). The CuO nanoparticles was thoroughly washed with the ethanol, dried and reused for the next cycle. The catalyst was found to be effective upto sixth cycle giving a conversion of 78% in the case of **4a.**

References:

1 K. S. Kumar, P. M. Kumar, K. A. Kumar, M. Sreenivasulu, A. A. Jafar, D. Rambabu, G. R. Krishna, C. M. Reddy, R. Kapavarapu, K. Shivakumar, K. K. Priya, K. V. L. Parsa and M. Pal, *Chem. Commun*., 2011, **47**, 5010.

2 K. V. Sashidhara, G. R. Palnati, R. P. Dodda, S. R. Avula, P. Swami, *Synlett*, 2013, **24**, 105.

3 (*a*) A. Kamal, V. Srinivasulu, B. N. Seshadri, N. Markandeya, A. Alarifi and N. Shankaraiah, *Green Chem*., 2012, **14**, 2513; (*b*) R. A. Sheldon, *Chem. Commun*., 2008, 3352.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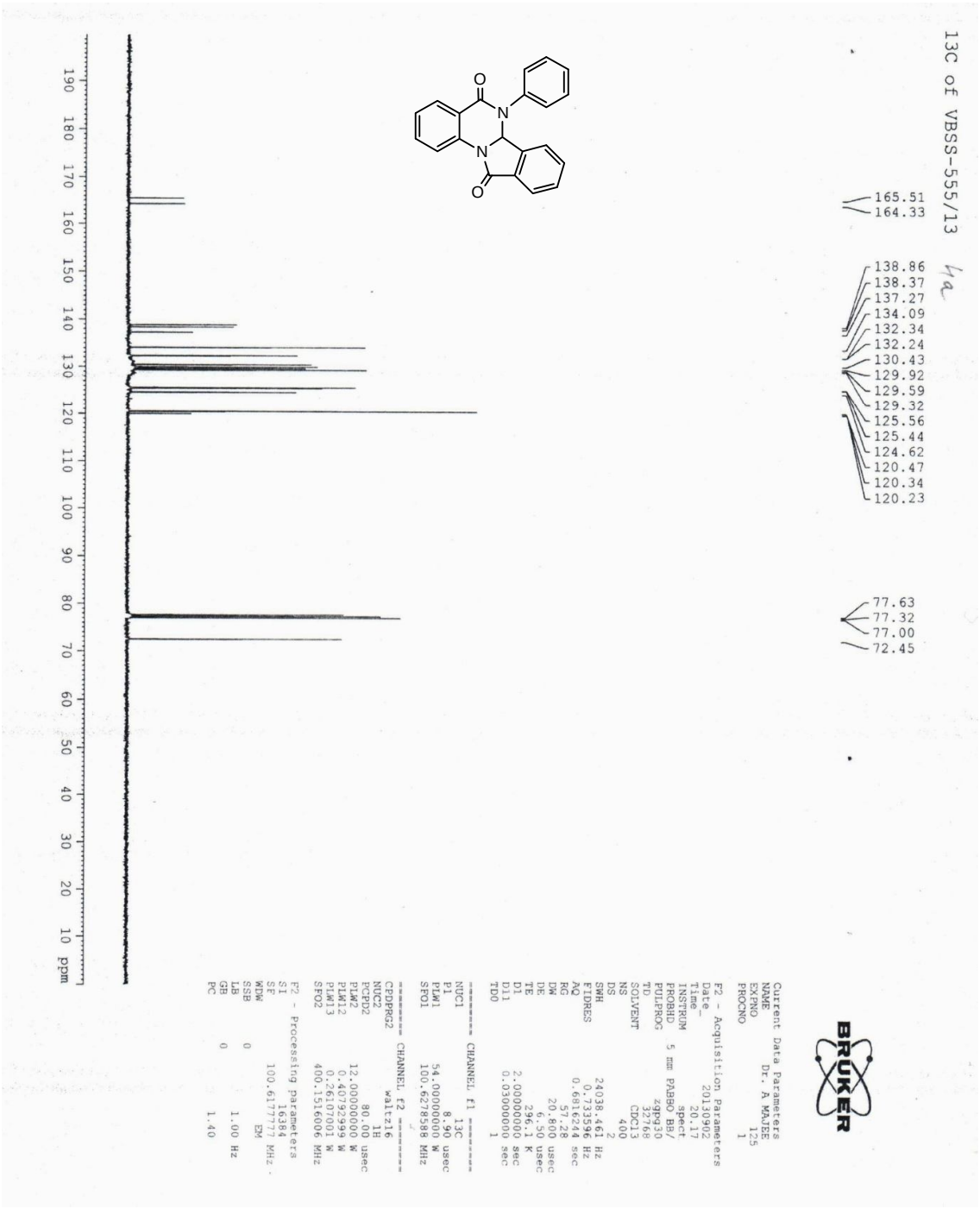
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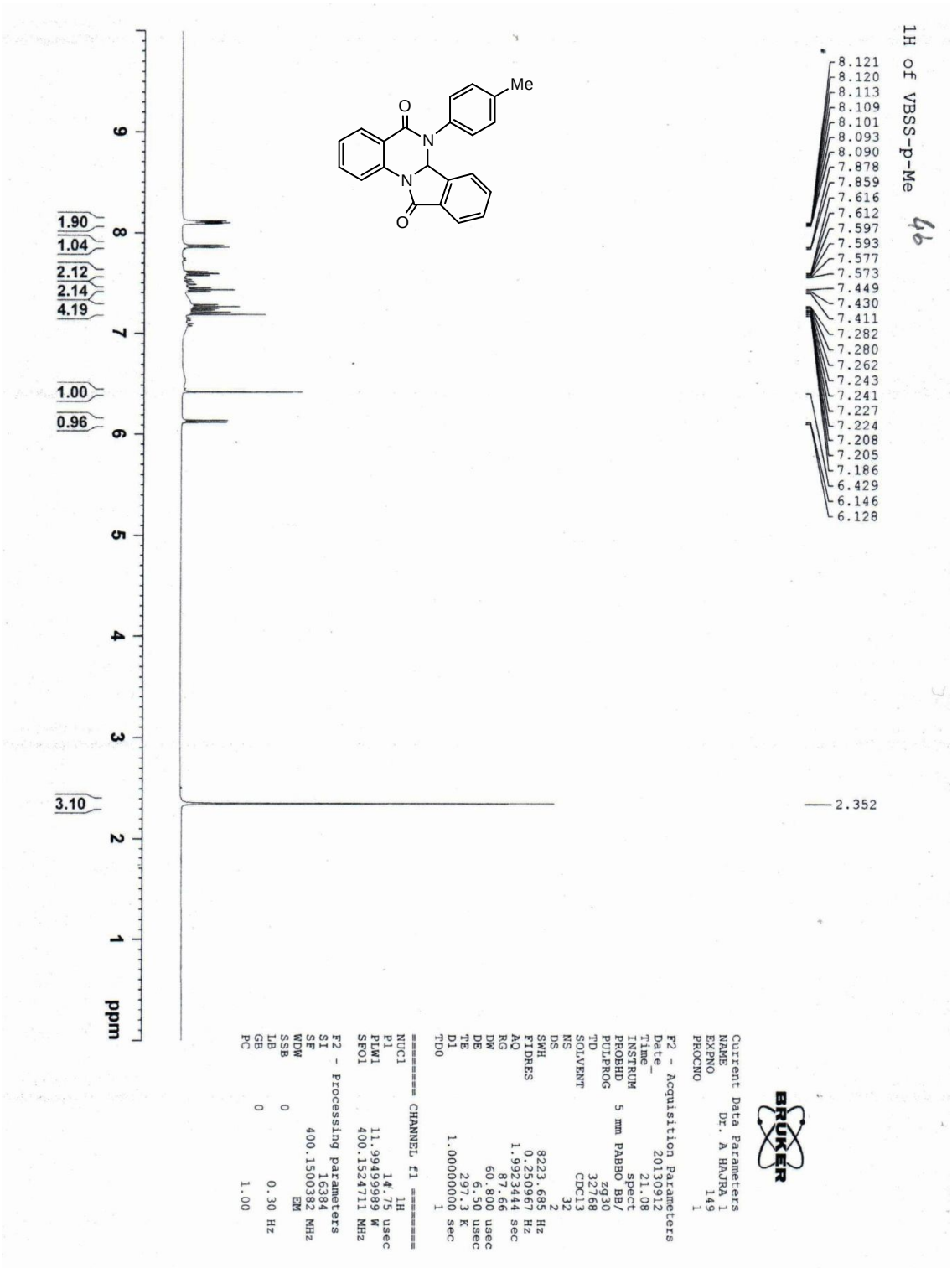
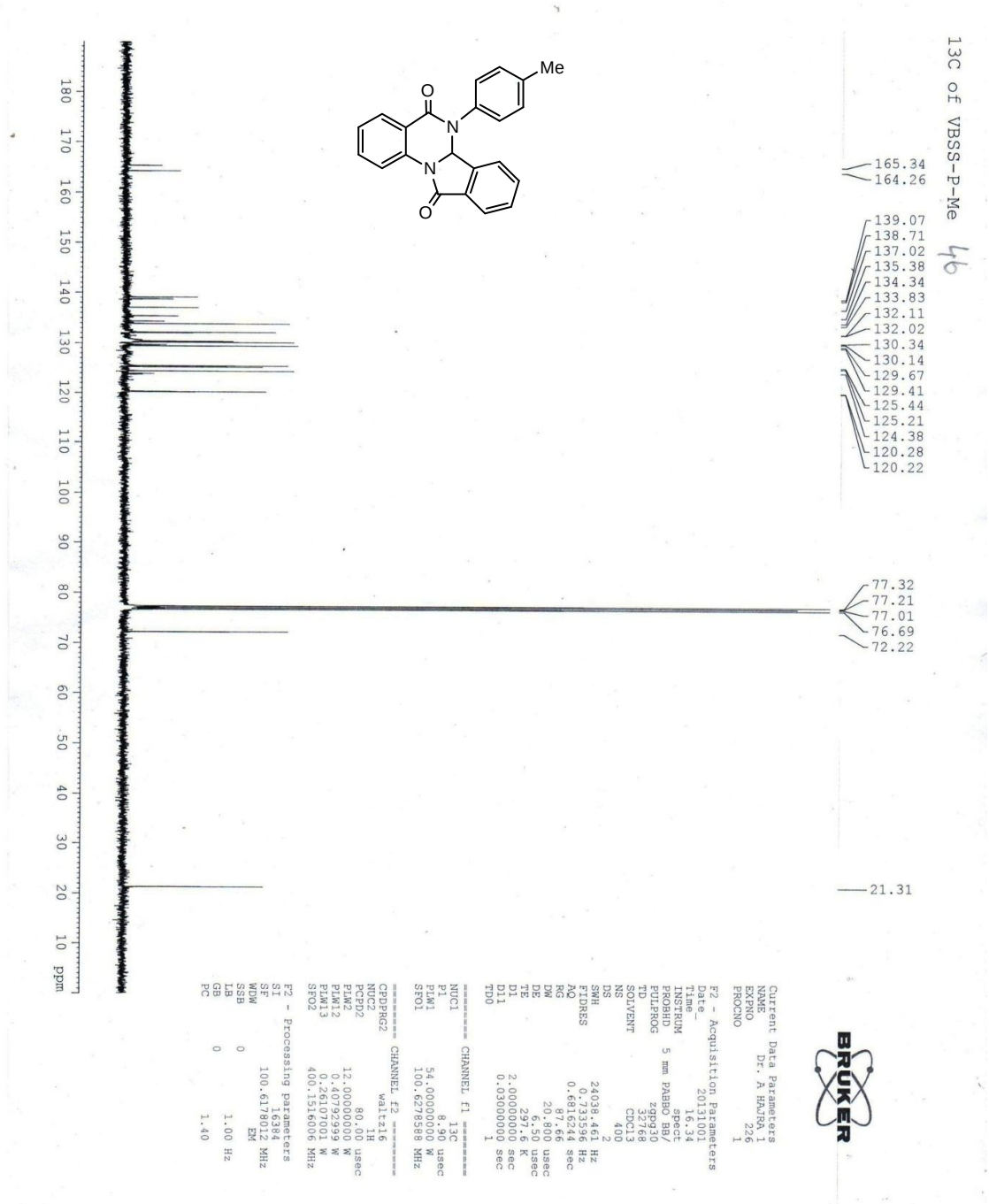
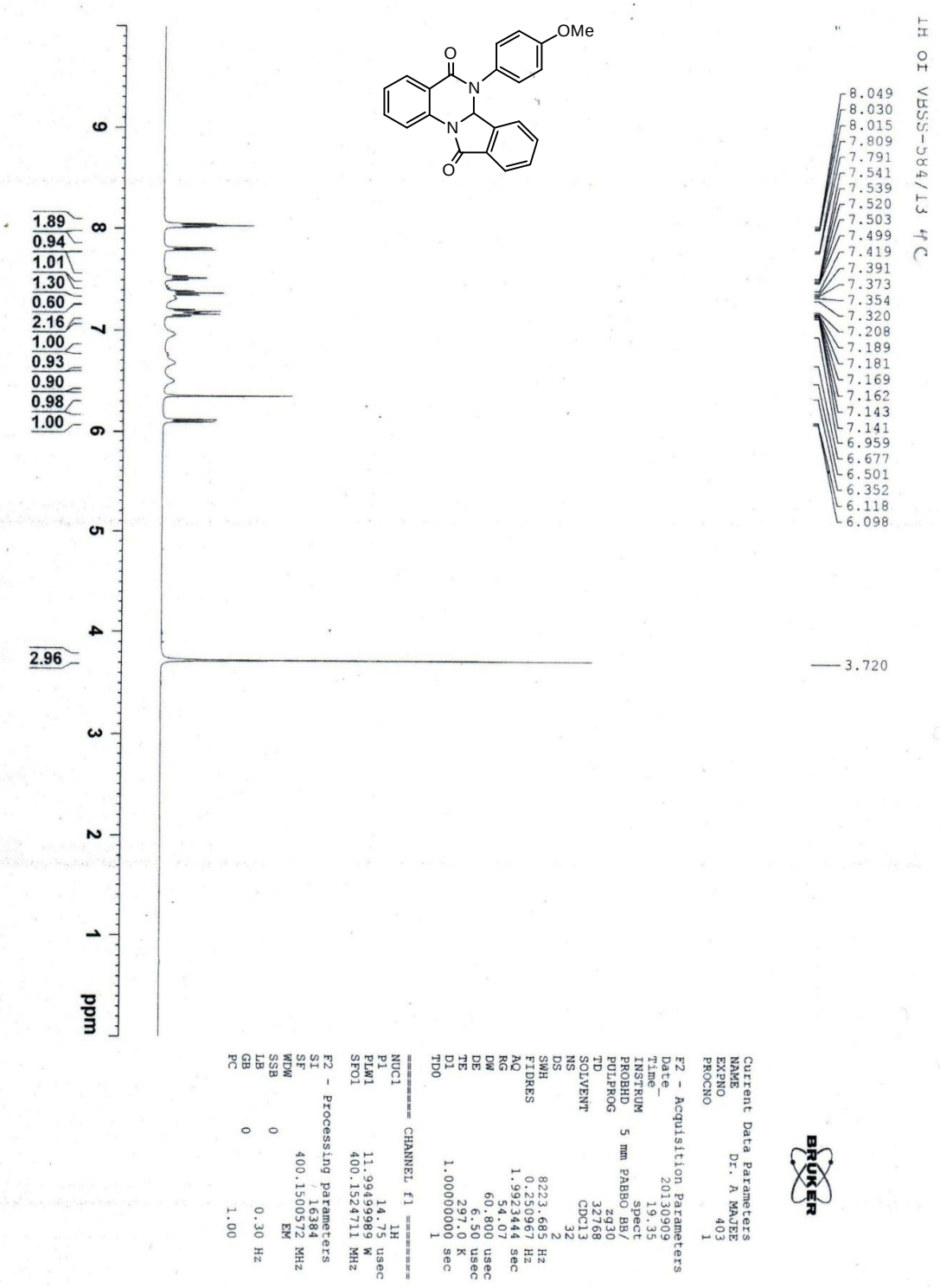
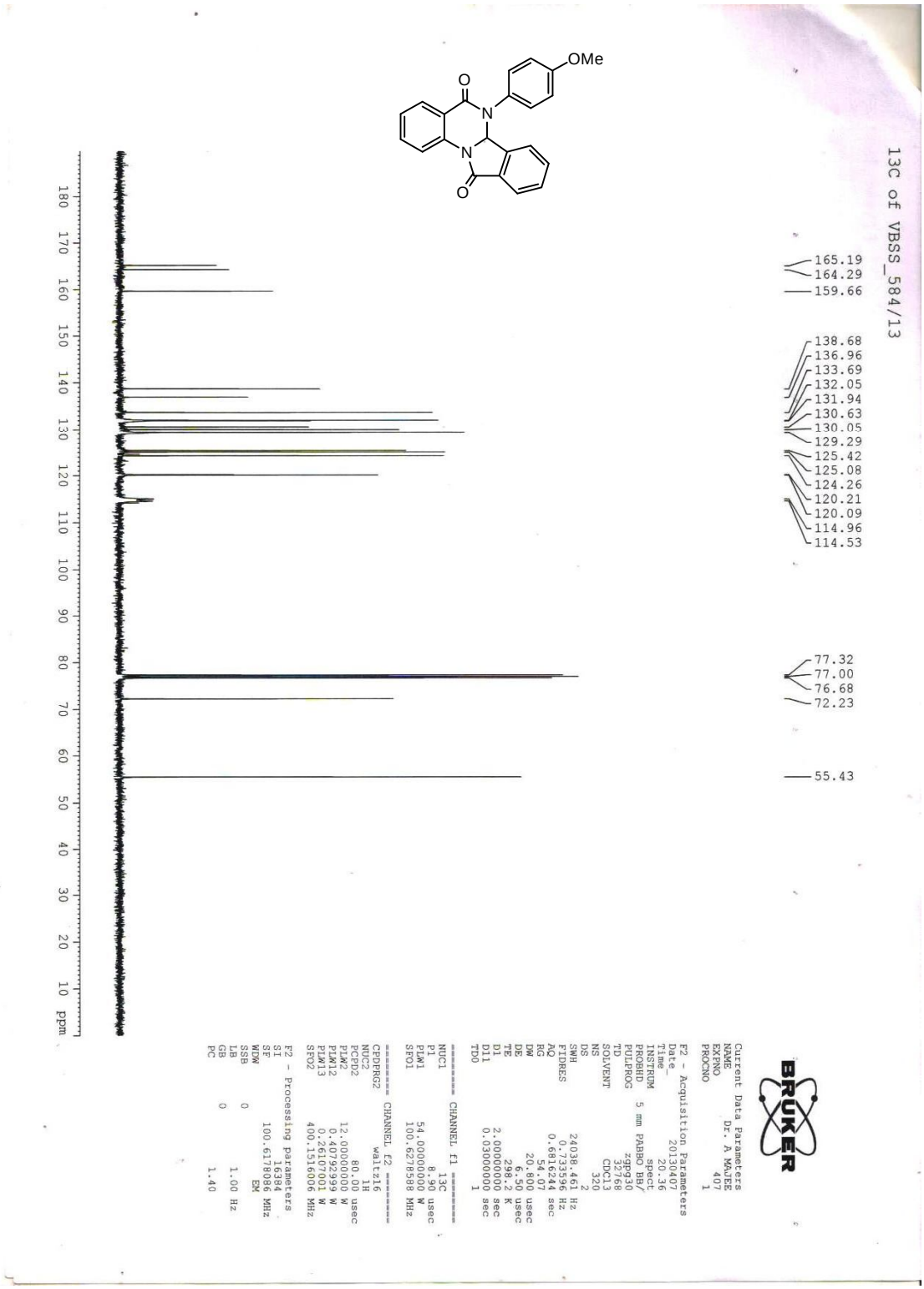
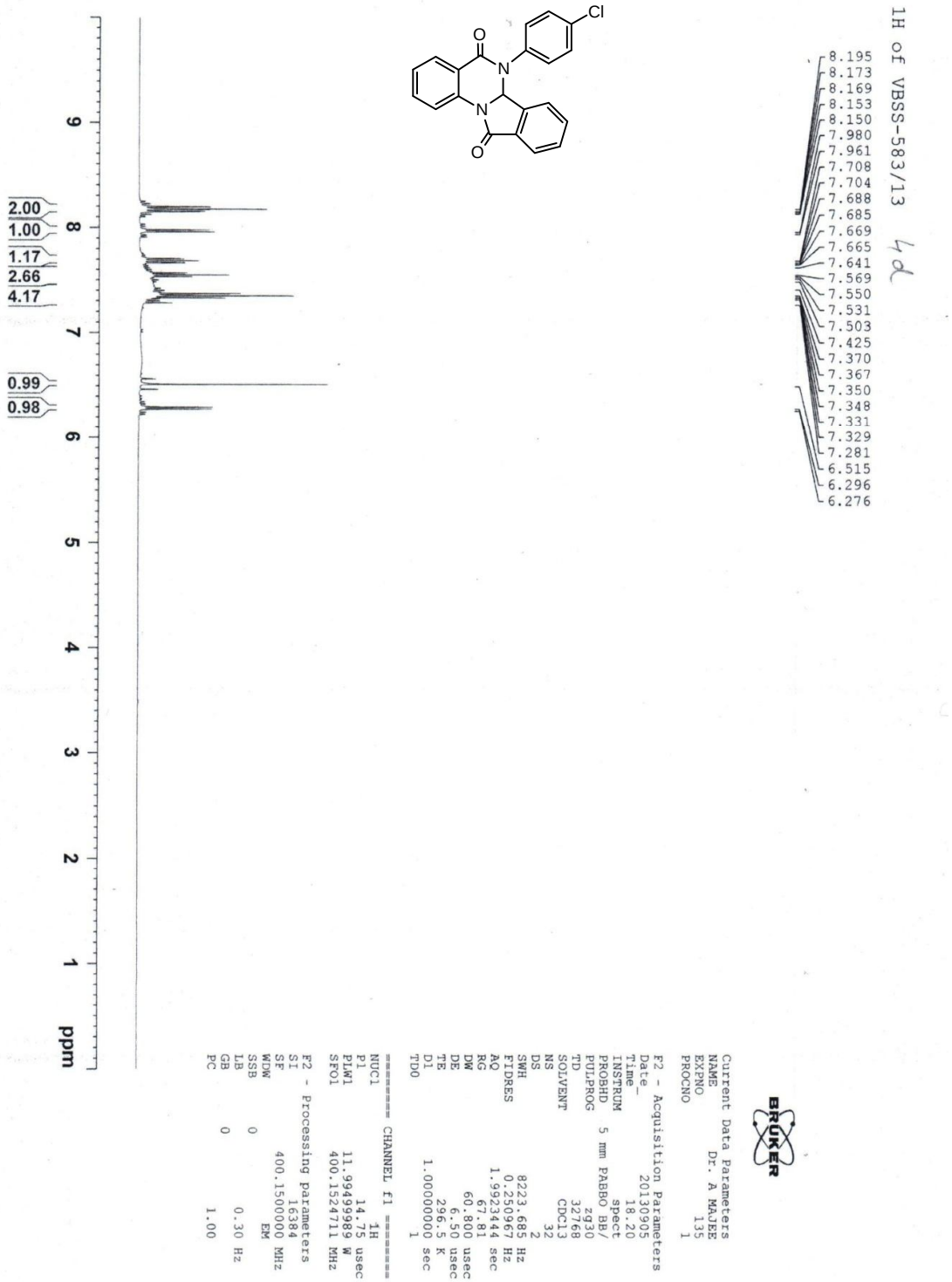
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

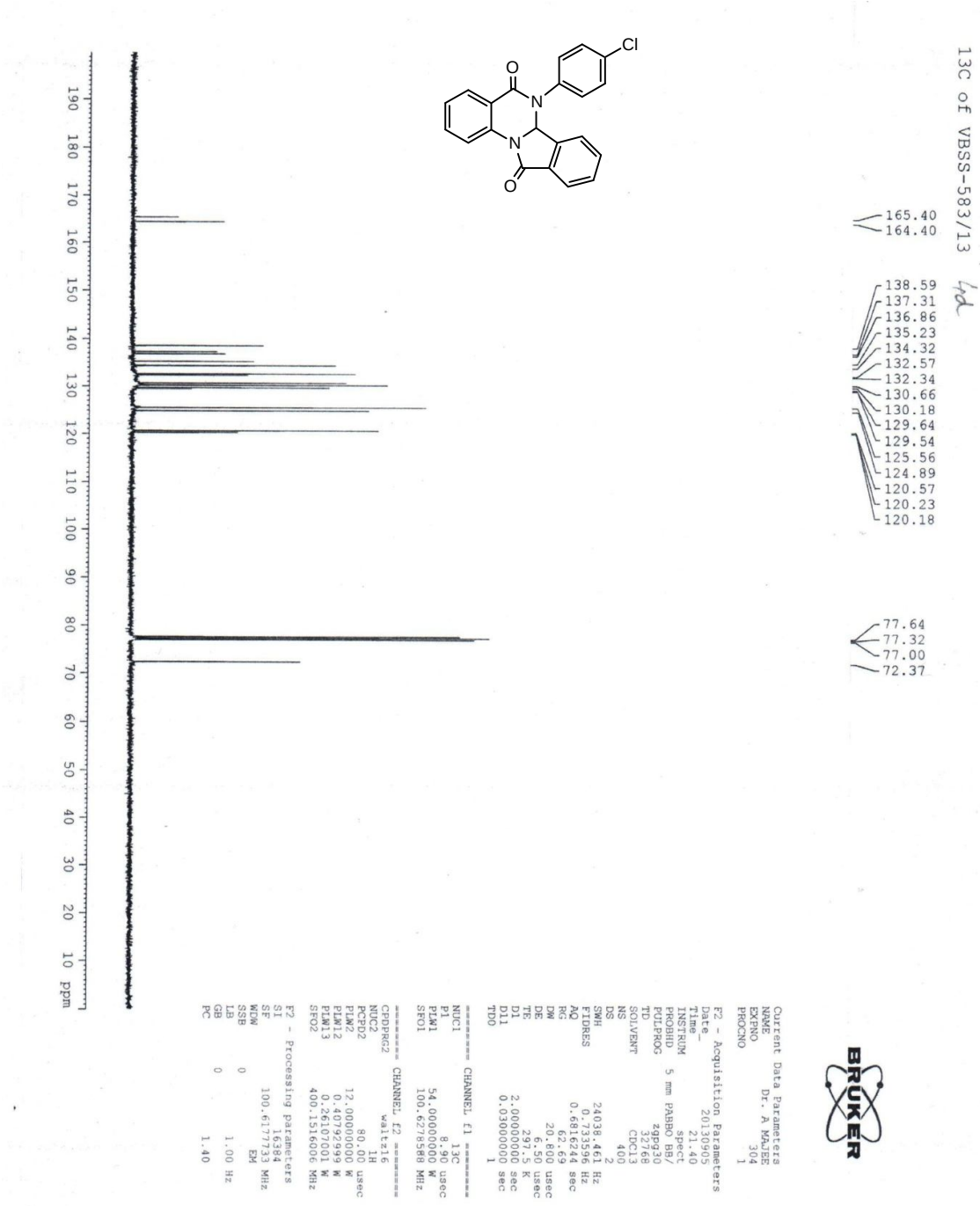

1H of VBSS-p-Me 46
8.121
8.120
8.113
8.109
8.101
8.093
8.090
7.878
7.859
7.616
7.612
7.597
7.593
7.577
7.573
7.449
7.430
7.411
7.282
7.280
7.262
7.243
7.241
7.227
7.224
7.208
7.205
7.186
6.429
6.146
6.128
2.352
Me
O
N
N
O
1.90
1.04
2.12
2.14
4.19
1.00
0.96
3.10
9
8
7
6
5
4
3
2
1
ppm
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 149
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130912
Time_ 21.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 87.66
DW 60.800 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500382 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

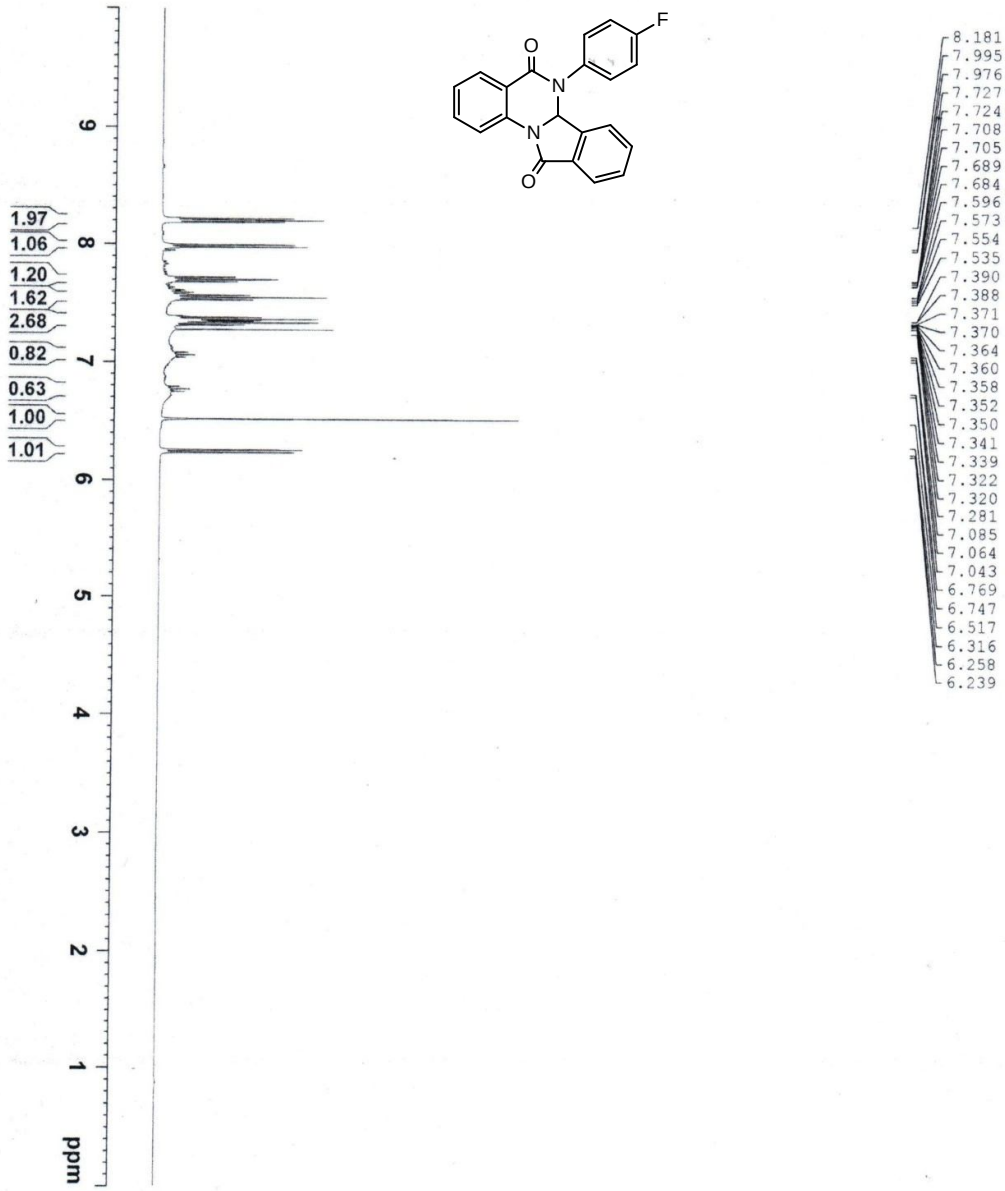

13C of VBSS-P-Me 46
Me
O
N
N
O
165.34
164.26
139.07
138.71
137.02
135.38
134.34
133.83
132.11
132.02
130.34
130.14
129.67
129.41
125.44
125.21
124.38
120.28
120.22
77.32
77.21
77.01
76.69
72.22
21.31
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 226
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131001
Time 16.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 87.66
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178012 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

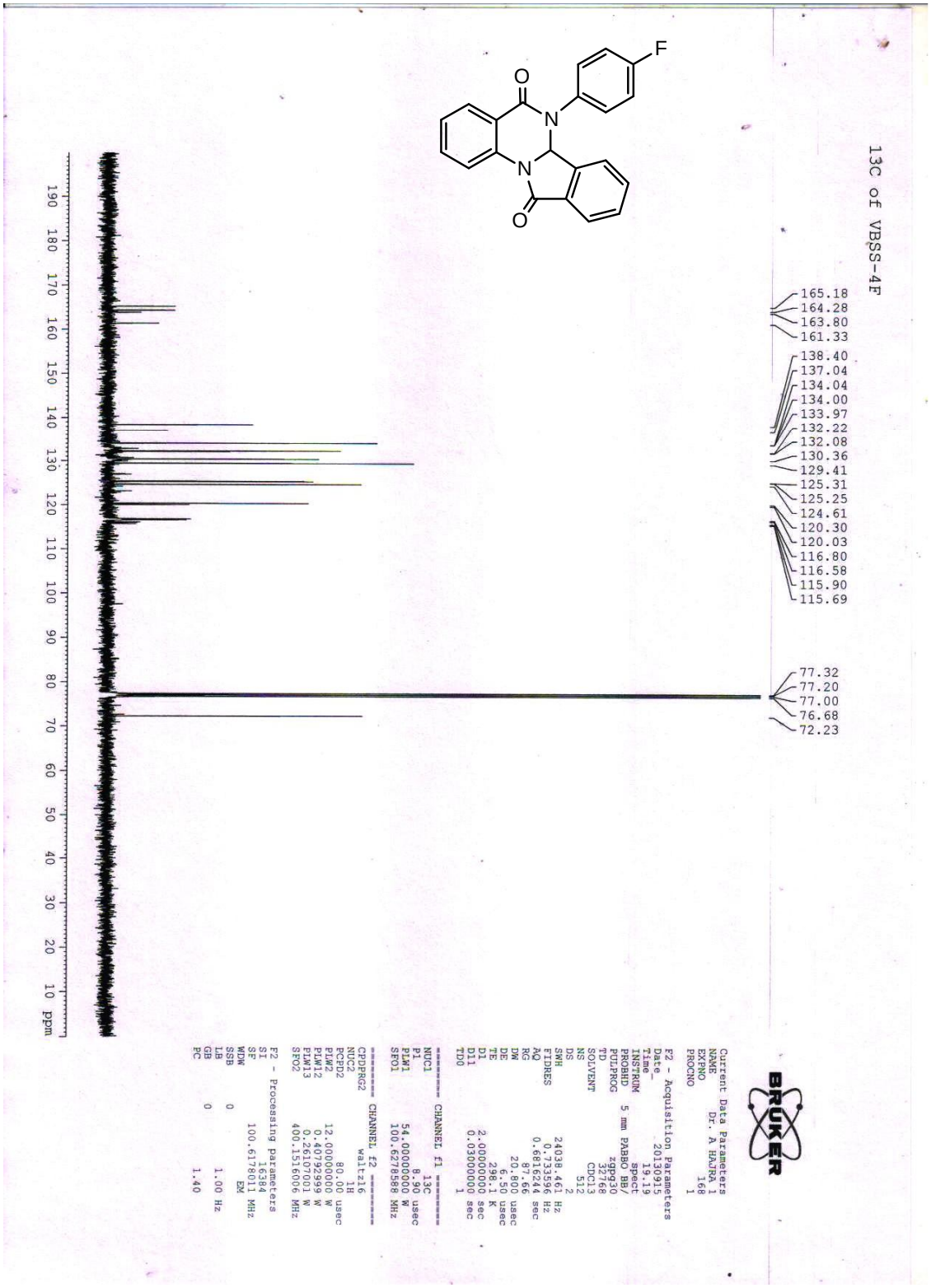

1H of VBSS-584/13 4C
8.049
8.030
8.015
7.809
7.791
7.541
7.539
7.520
7.503
7.499
7.419
7.391
7.373
7.354
7.320
7.208
7.189
7.181
7.169
7.162
7.143
7.141
6.959
6.677
6.501
6.352
6.118
6.098
3.720
OMe
O
N
N
O
1.89
0.94
1.01
1.30
0.60
2.16
1.00
0.93
0.90
0.98
1.00
2.96
9
8
7
6
5
4
3
2
1
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 403
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130909
Time 19.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 54.07
DW 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500572 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
BRUKER

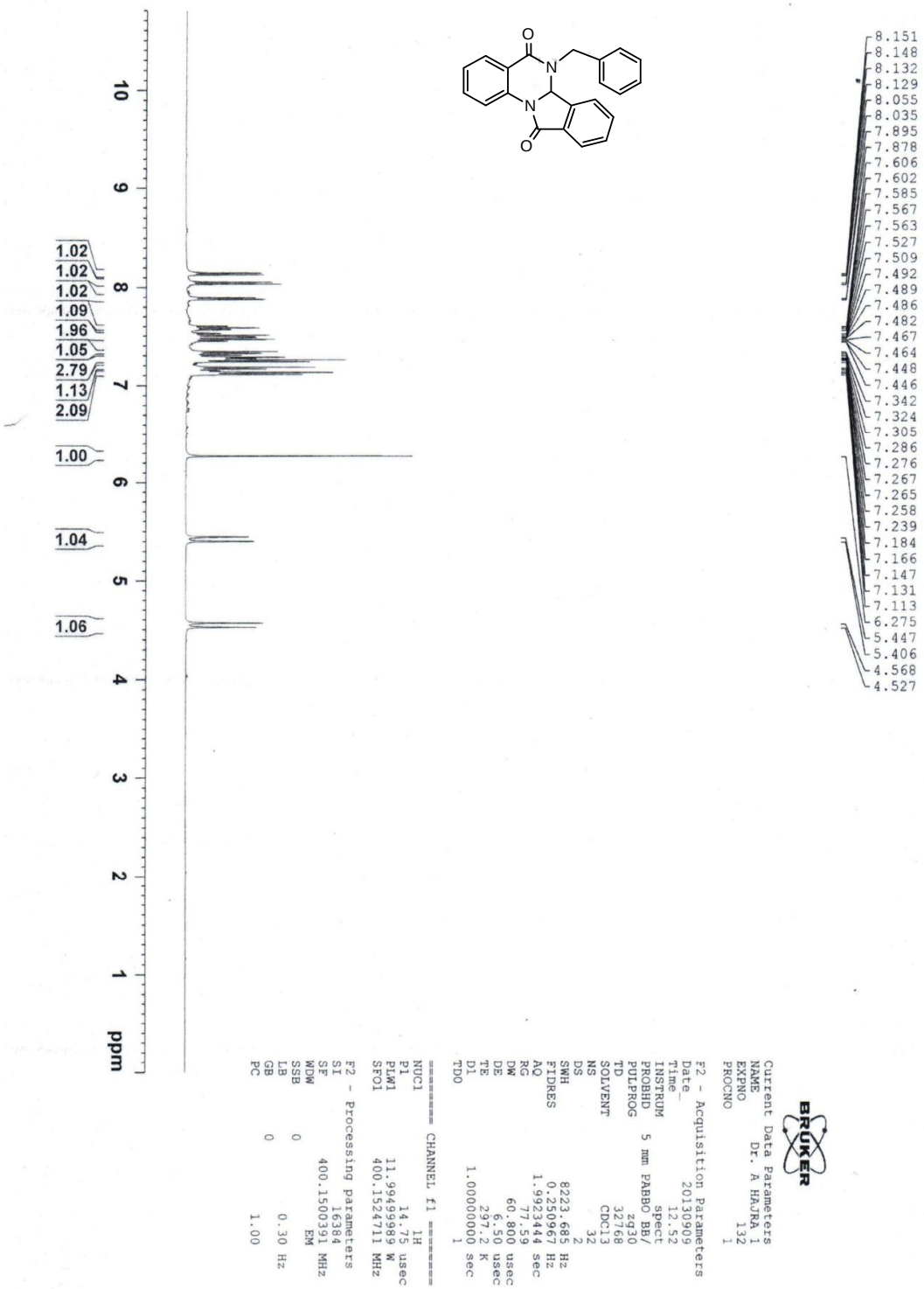

13C of VBSS_584/13
OMe
O
N
N
O
165.19
164.29
159.66
138.68
136.96
133.69
132.05
131.94
130.63
130.05
129.29
125.42
125.08
124.26
120.21
120.09
114.96
114.53
77.32
77.00
76.68
72.23
55.43
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 407
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130717
Time 2.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 320
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816224 sec
RG 54.07
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792599 W
PLW13 0.26107001 W
SFO2 400.1316006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178086 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

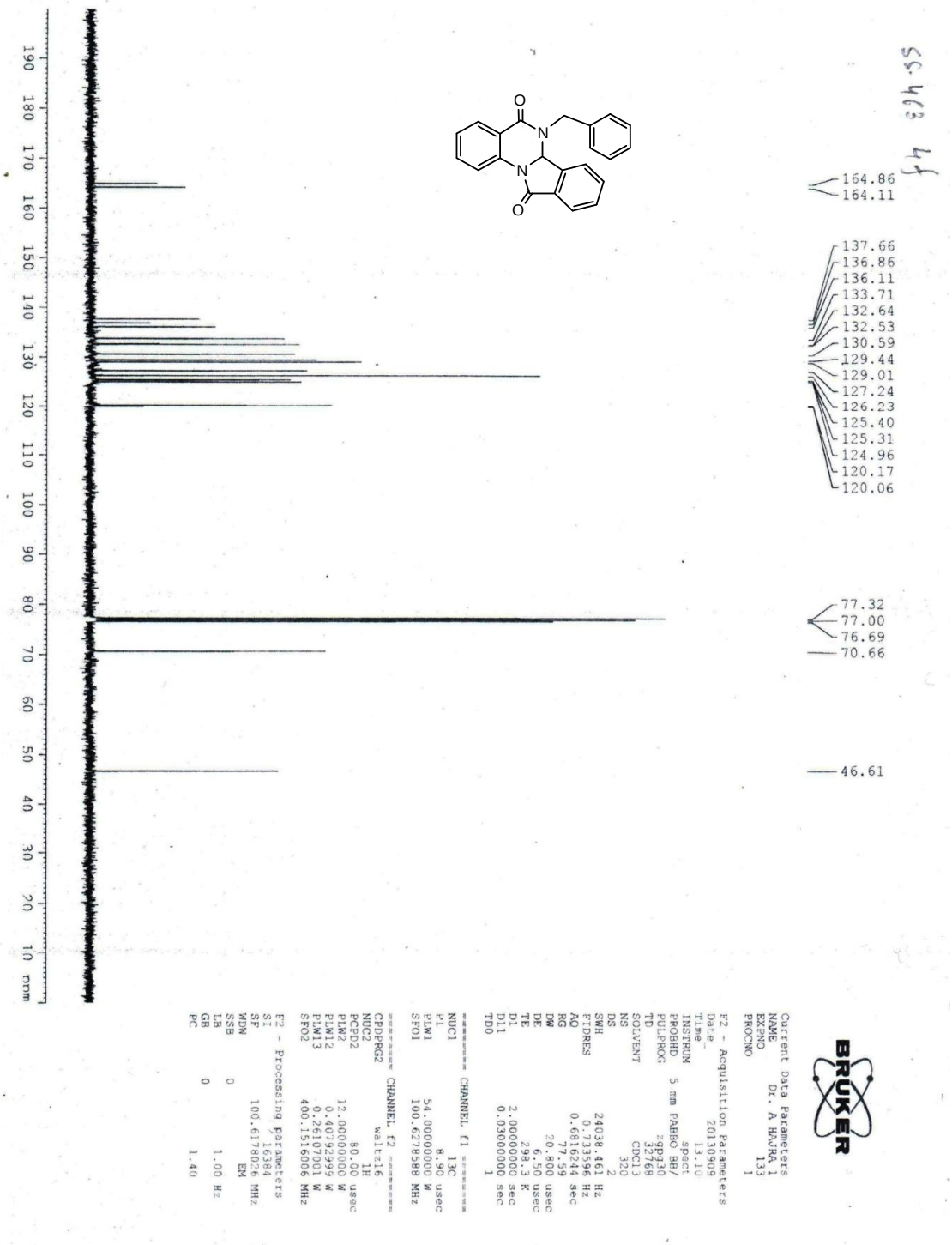

1H of VBSS-583/13 4d
8.195
8.173
8.169
8.153
8.150
7.980
7.961
7.708
7.704
7.688
7.685
7.669
7.665
7.641
7.569
7.550
7.531
7.503
7.425
7.370
7.367
7.350
7.348
7.331
7.329
7.281
6.515
6.296
6.276
Cl
O
N
N
O
2.00
1.00
1.17
2.66
4.17
0.99
0.98
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 135
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130905
Time 18.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 67.81
DW 60.800 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

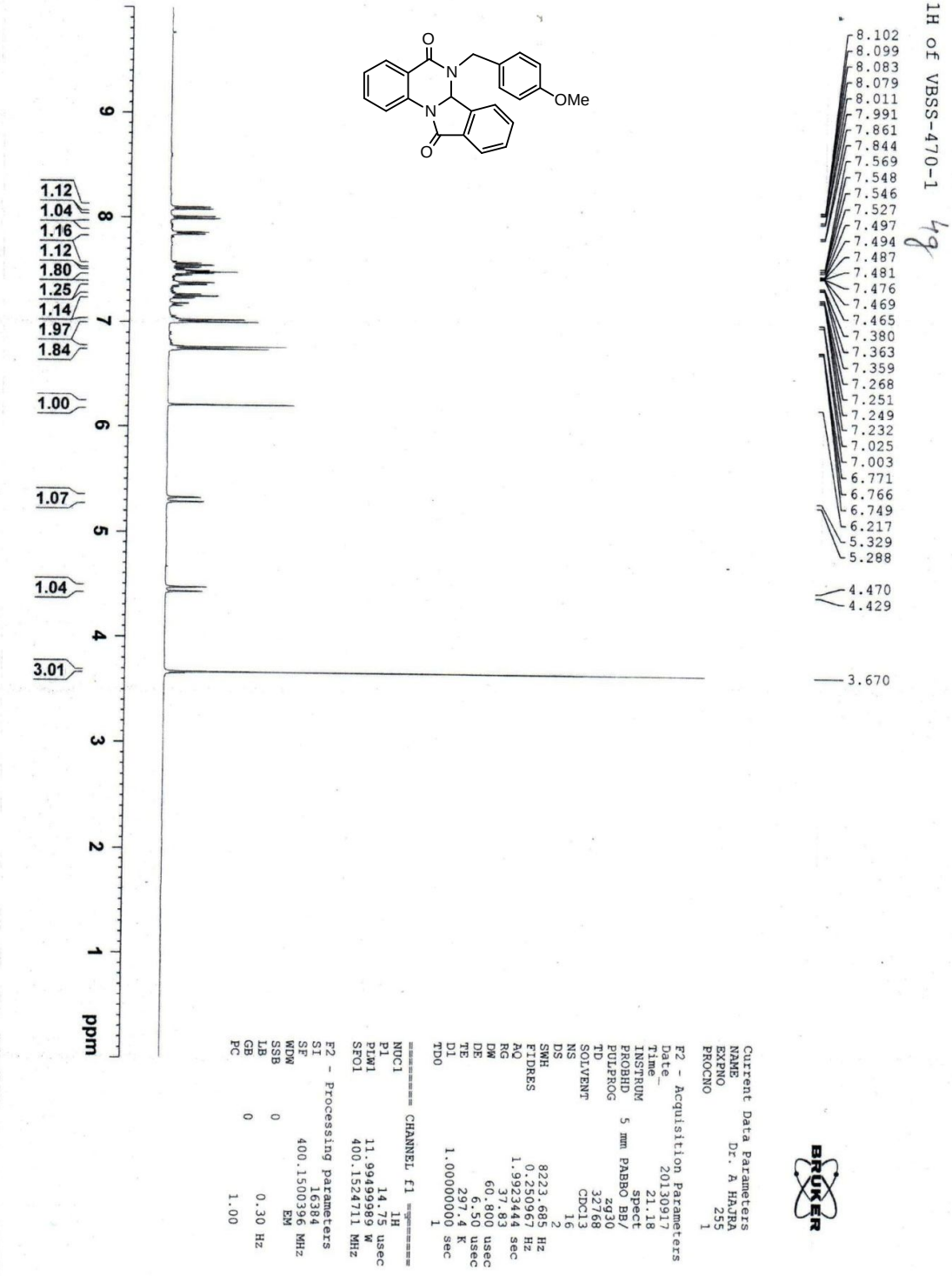

13C of VBSS-583/13 4d
165.40
164.40
138.59
137.31
136.86
135.23
134.32
132.57
132.34
130.66
130.18
129.64
129.54
125.56
124.89
120.57
120.23
120.18
77.64
77.32
77.00
72.37
Cl
O
N
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 304
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130905
Time_ 21.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.68162441 sec
RG 62.69
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278580 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6177733 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

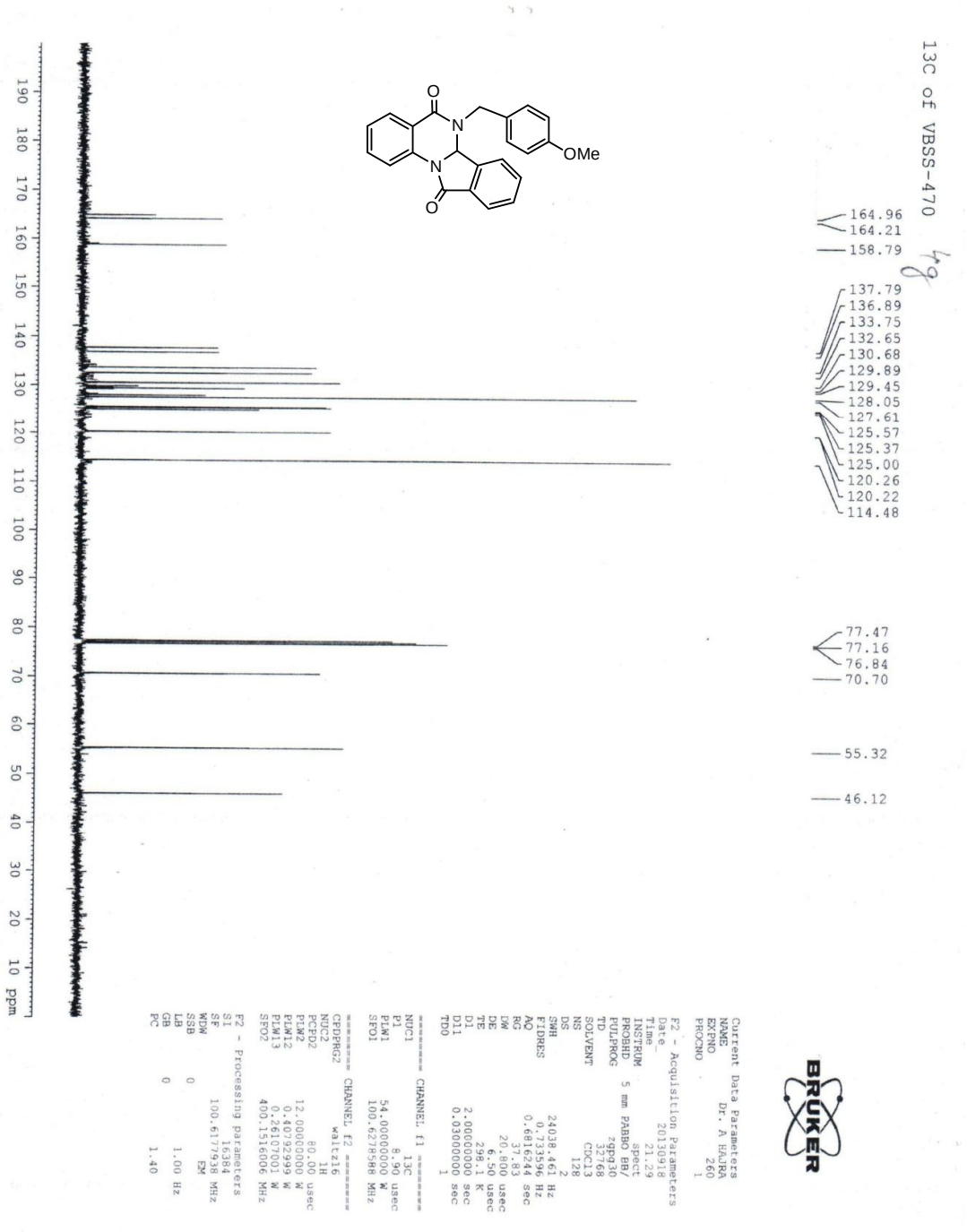

1H of VBSS-4F 4e
8.181
7.995
7.976
7.727
7.724
7.708
7.705
7.689
7.684
7.596
7.573
7.554
7.535
7.390
7.388
7.371
7.370
7.364
7.360
7.358
7.352
7.350
7.341
7.339
7.322
7.320
7.281
7.085
7.064
7.043
6.769
6.747
6.517
6.316
6.258
6.239
F
O
N
N
O
1.97
1.06
1.20
1.62
2.68
0.82
0.63
1.00
1.01
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 167
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130915
Time_ 18.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 93.46
DW 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TDO 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

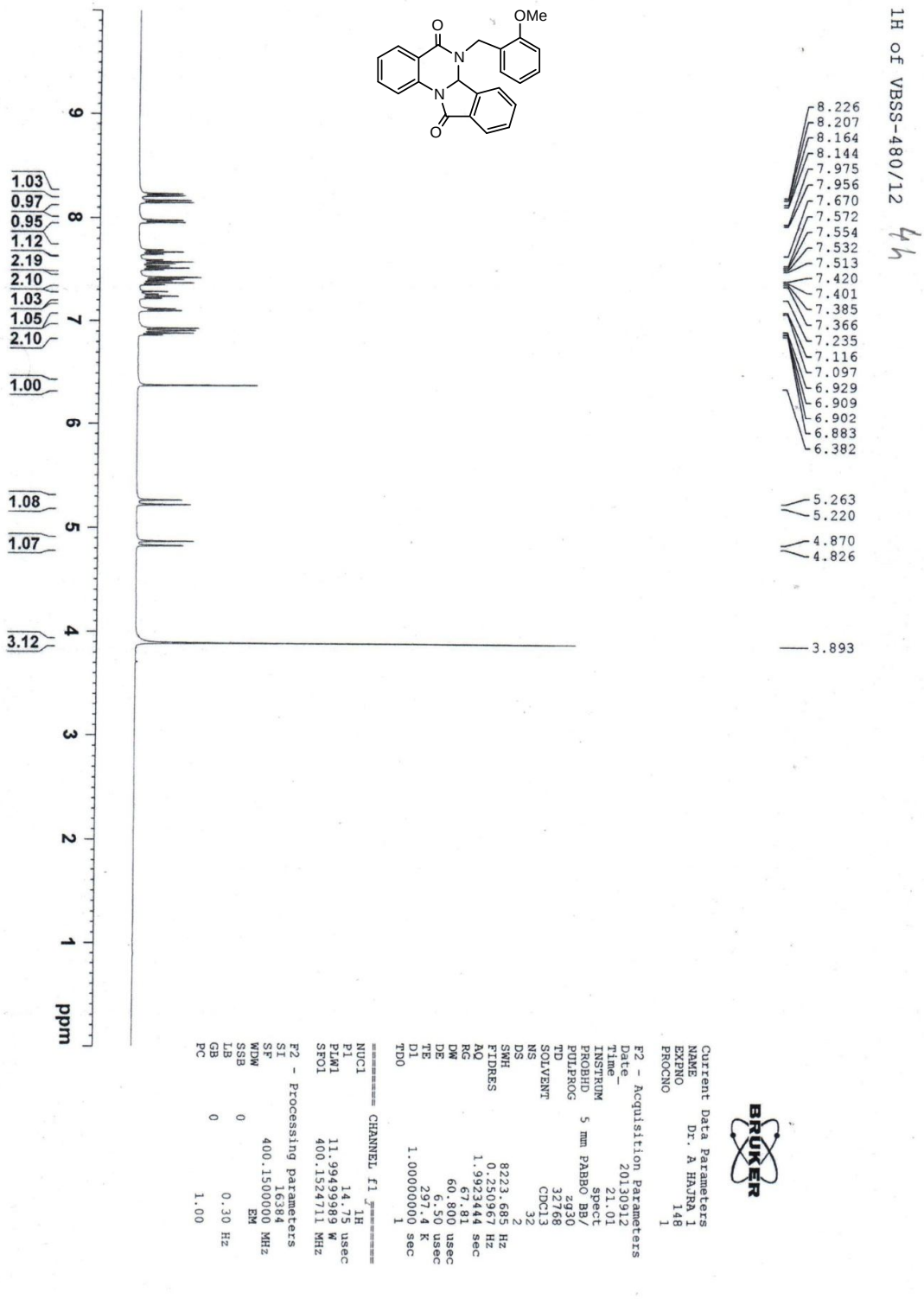

13C of VBSS-4F
F
O
N
N
O
165.18
164.28
163.80
161.33
138.40
137.04
134.04
134.00
133.97
132.22
132.08
130.36
129.41
125.31
125.25
124.61
120.30
120.03
116.80
116.58
115.90
115.69
77.32
77.20
77.00
76.68
72.23
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 168
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130915
Time 19.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 27938
SOLVENT CDCl3
NS 512
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.68116244 sec
RG 87.66
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178011 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

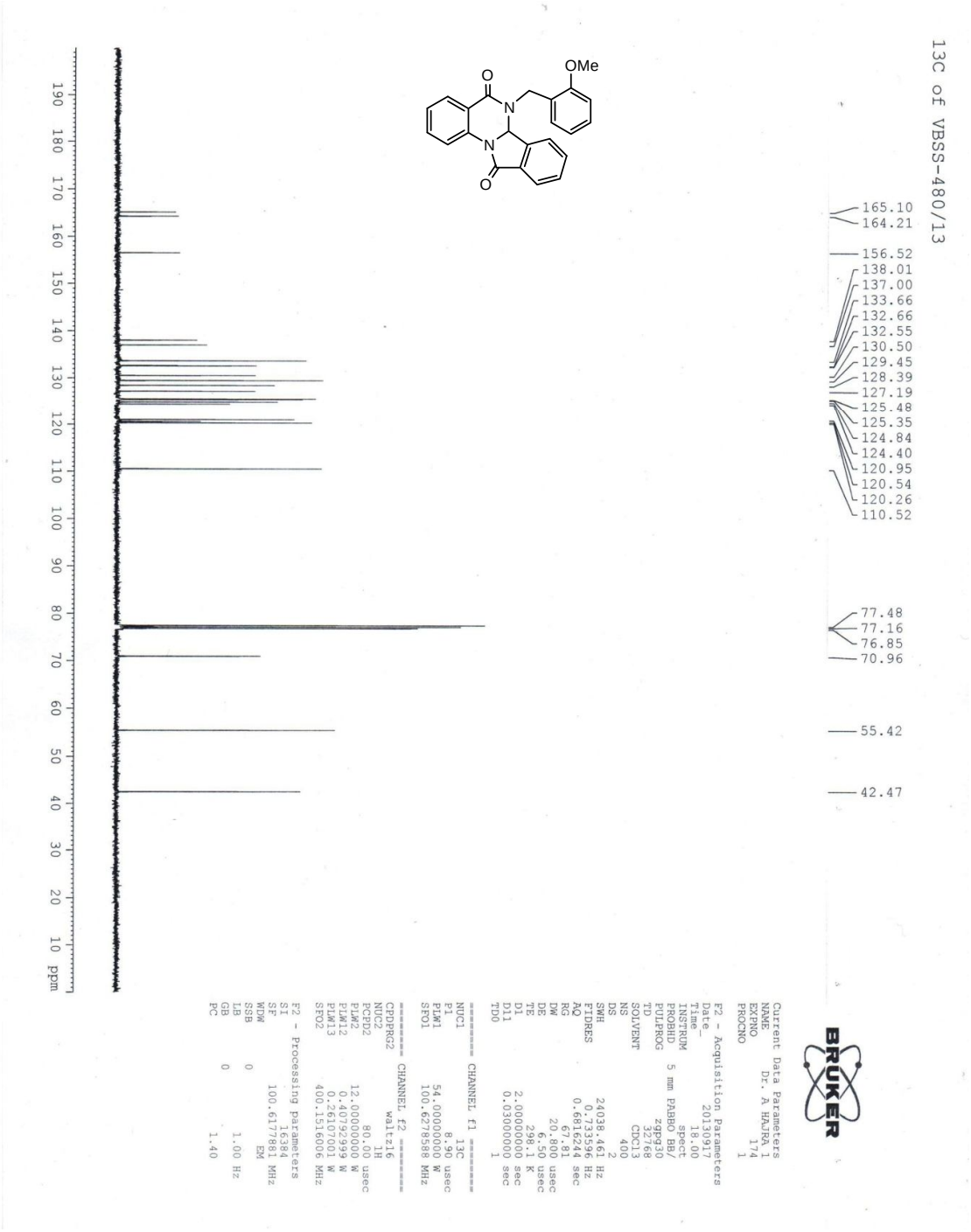

1H of VBSS-463/13
8.151
8.148
8.132
8.129
8.055
8.035
7.895
7.878
7.606
7.602
7.585
7.567
7.563
7.527
7.509
7.492
7.489
7.486
7.482
7.467
7.464
7.448
7.446
7.342
7.324
7.305
7.286
7.276
7.267
7.265
7.258
7.239
7.184
7.166
7.147
7.131
7.113
6.275
5.447
5.406
4.568
4.527
BRUKER
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 132
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130909
Time 12.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 77.59
DW 60.800 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500391 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.02
1.02
1.02
1.09
1.96
1.05
2.79
1.13
2.09
1.00
1.04
1.06
10
9
8
7
6
5
4
3
2
1
ppm

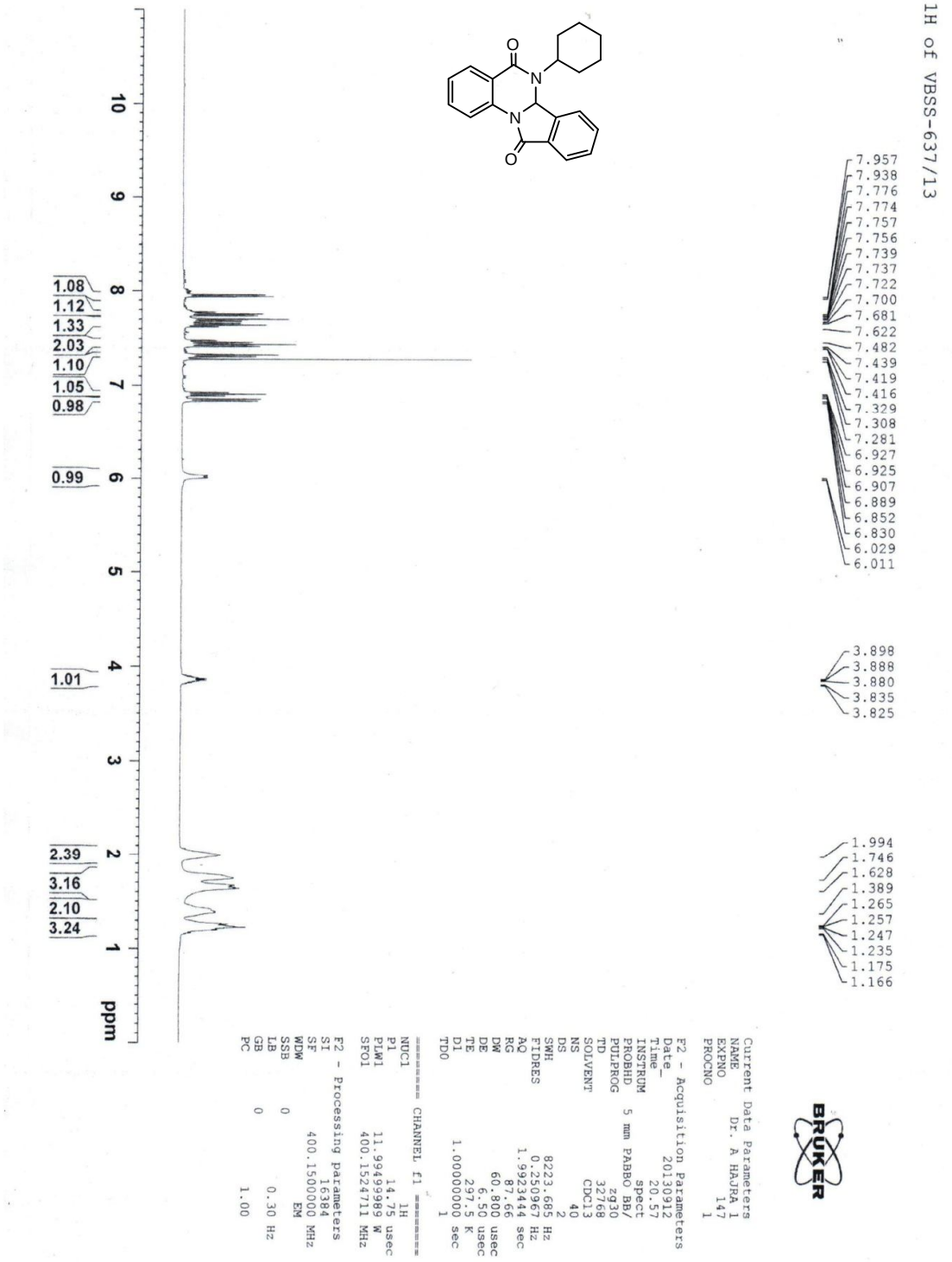

164.86
164.11
137.66
136.86
136.11
133.71
132.64
132.53
130.59
129.44
129.01
127.24
126.23
125.40
125.31
124.96
120.17
120.06
77.32
77.00
76.69
70.66
46.61
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 133
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130909
Time 13.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 320
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 77.59
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6279588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792399 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 131072
SF 100.6176024 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

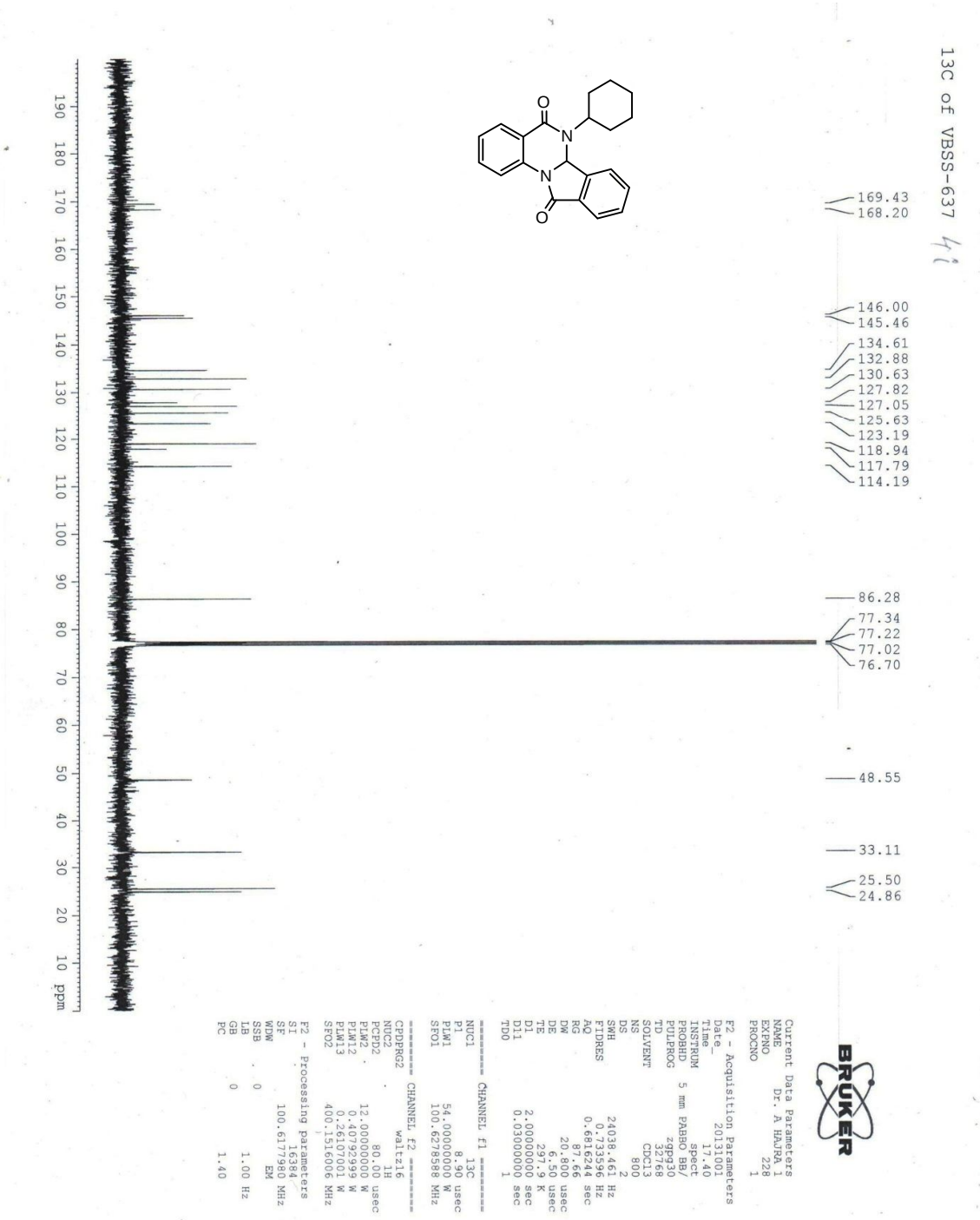

1H of VBSS-470-1 49
8.102
8.099
8.083
8.079
8.011
7.991
7.861
7.844
7.569
7.548
7.546
7.527
7.497
7.494
7.487
7.481
7.476
7.469
7.465
7.380
7.363
7.359
7.268
7.251
7.249
7.232
7.025
7.003
6.771
6.766
6.749
6.217
5.329
5.288
4.470
4.429
3.670
OMe
1.12
1.04
1.16
1.12
1.80
1.25
1.14
1.97
1.84
1.00
1.07
1.04
3.01
ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 255
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130917
Time 21.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 37.83
DW 60.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500396 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

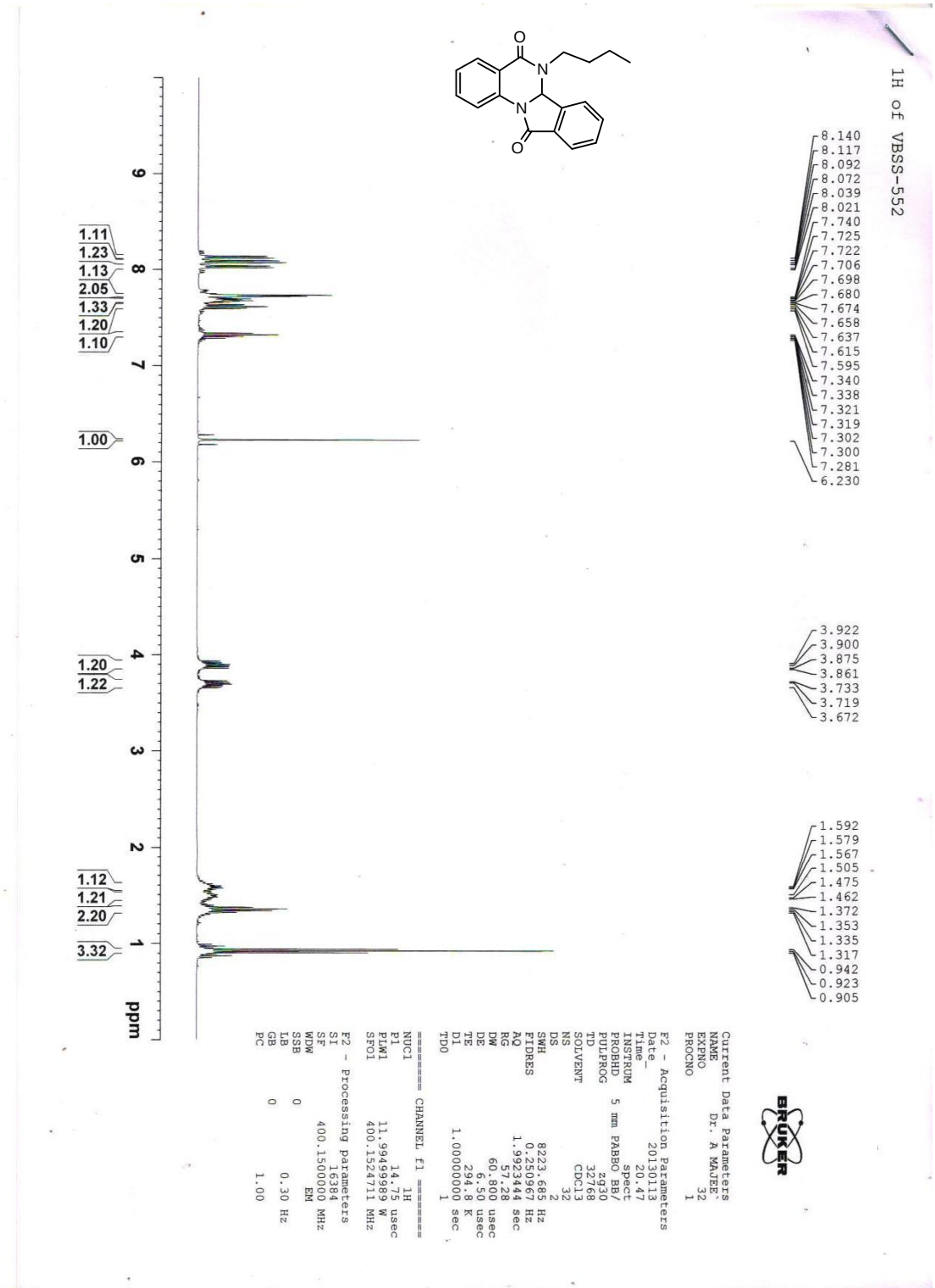

13C of VBSS-470
49
164.96
164.21
158.79
137.79
136.89
133.75
132.65
130.68
129.89
129.45
128.05
127.61
125.57
125.37
125.00
120.26
120.22
114.48
77.47
77.16
76.84
70.70
55.32
46.12
O
N
N
O
OMe
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A HAJRA
EXPNO 260
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130918
Time 21.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 128
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 37.83
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6279588 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792599 W
PLW13 0.26107601 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6177998 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
BRUKER

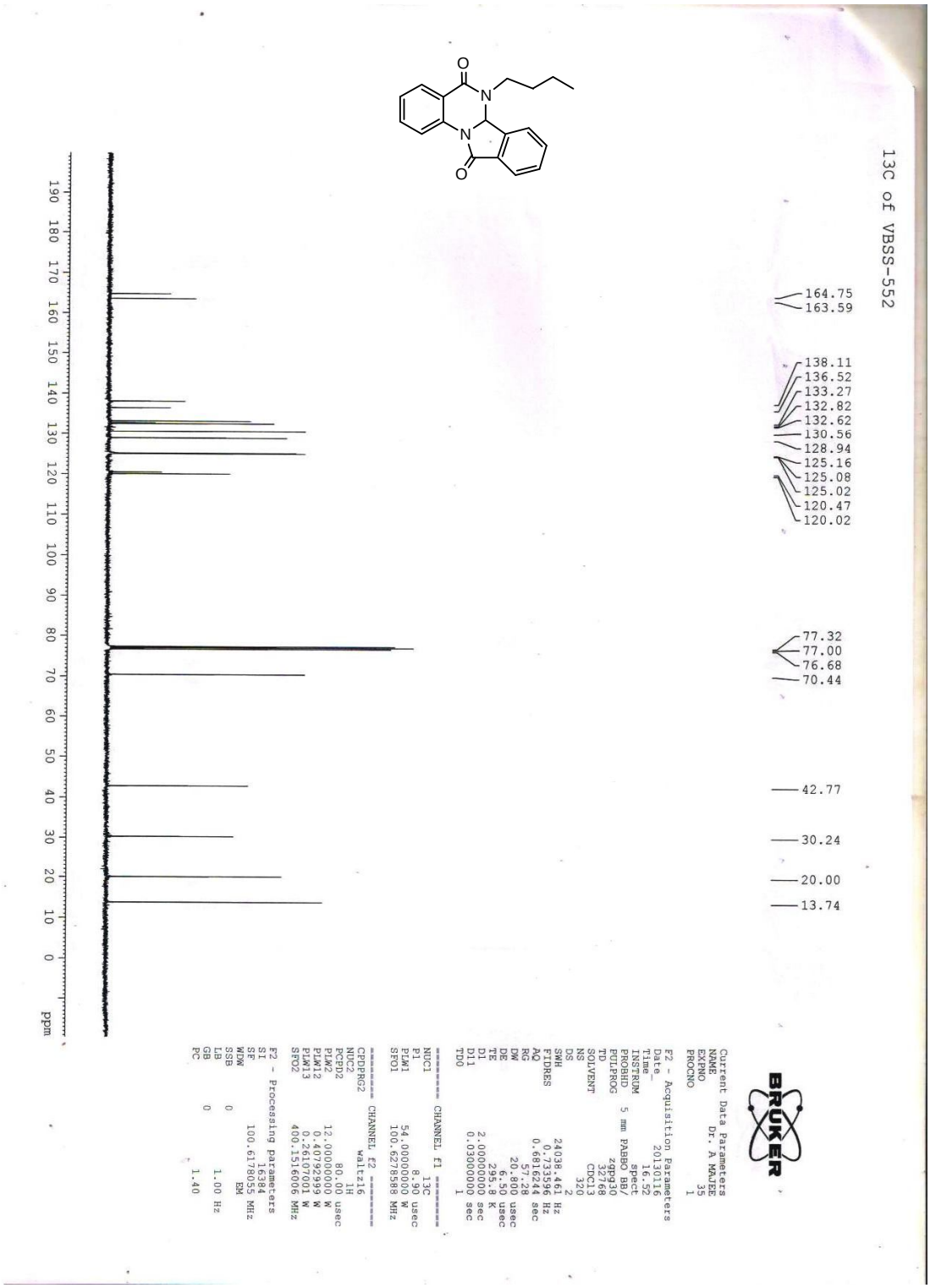

1H of VBSS-480/12 4h
OMe
O
N
N
O
8.226
8.207
8.164
8.144
7.975
7.956
7.670
7.572
7.554
7.532
7.513
7.420
7.401
7.385
7.366
7.235
7.116
7.097
6.929
6.909
6.902
6.883
6.382
5.263
5.220
4.870
4.826
3.893
1.03
0.97
0.95
1.12
2.19
2.10
1.03
1.05
2.10
1.00
1.08
1.07
3.12
9
8
7
6
5
4
3
2
1
ppm
BRUKER
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 148
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130912
Time 21.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.992344 sec
RG 67.81
DW 60.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

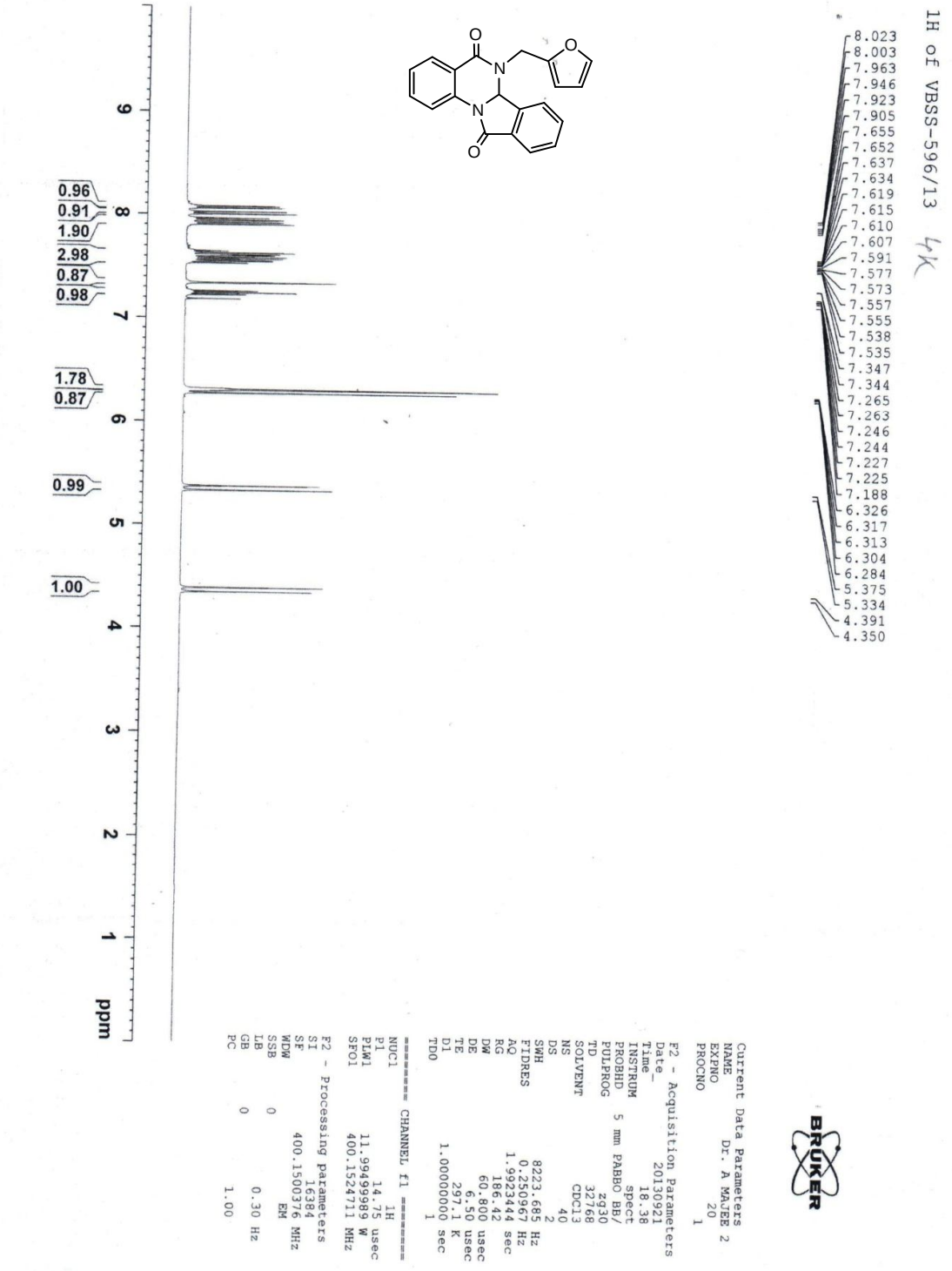

13C of VBSS-480/13
OMe
O
N
N
O
165.10
164.21
156.52
138.01
137.00
133.66
132.66
132.55
130.50
129.45
128.39
127.19
125.48
125.35
124.84
124.40
120.95
120.54
120.26
110.52
77.48
77.16
76.85
70.96
55.42
42.47
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 174
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130917
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 8718.1
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 131581
SF 100.6177881 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
BRUKER

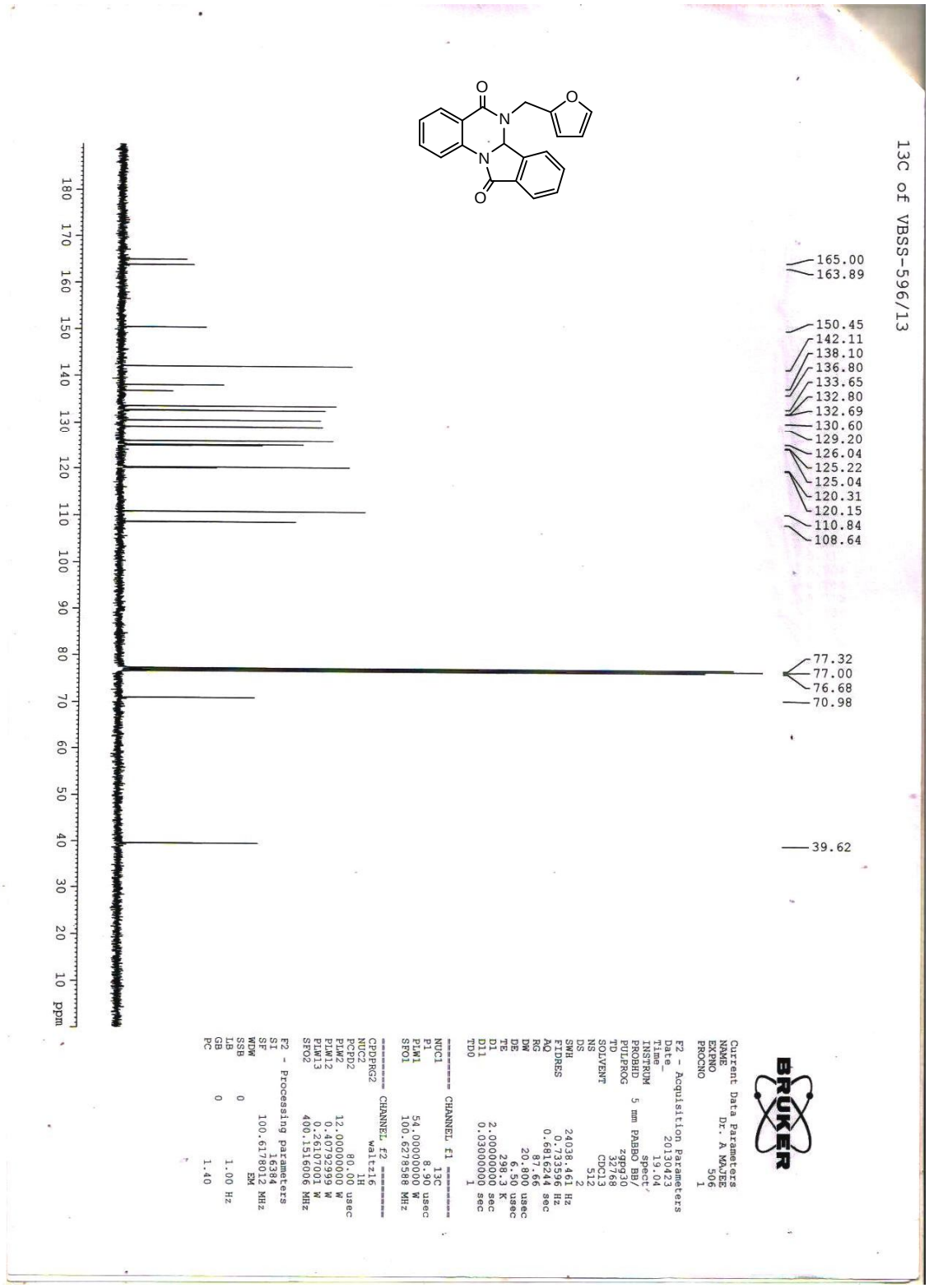

1H of VBSS-637/13
7.957
7.938
7.776
7.774
7.757
7.756
7.739
7.737
7.722
7.700
7.681
7.622
7.482
7.439
7.419
7.416
7.329
7.308
7.281
6.927
6.925
6.907
6.889
6.852
6.830
6.029
6.011
3.898
3.888
3.880
3.835
3.825
1.994
1.746
1.628
1.389
1.265
1.257
1.247
1.235
1.175
1.166
1.08
1.12
1.33
2.03
1.10
1.05
0.98
0.99
1.01
2.39
3.16
2.10
3.24
ppm
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 147
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130912
Time 20.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 40
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 87.66
DW 60.800 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C of VBSS-637
169.43
168.20
146.00
145.46
134.61
132.88
130.63
127.82
127.05
125.63
123.19
118.94
117.79
114.19
86.28
77.34
77.22
77.02
76.70
48.55
33.11
25.50
24.86
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME Dr. A HAJRA 1
EXPNO 228
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131001
Time 17.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 800
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816224 sec
RG 87.66
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 12.00000000 W
PL12 0.40792999 W
PL13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6177980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
BRUKER


1H of VBSS-552
8.140
8.117
8.092
8.072
8.039
8.021
7.740
7.725
7.722
7.706
7.698
7.680
7.674
7.658
7.637
7.615
7.595
7.340
7.338
7.321
7.319
7.302
7.300
7.281
6.230
3.922
3.900
3.875
3.861
3.733
3.719
3.672
1.592
1.579
1.567
1.505
1.475
1.462
1.372
1.353
1.335
1.317
0.942
0.923
0.905
1.11
1.23
1.13
2.05
1.33
1.20
1.10
1.00
1.20
1.22
1.12
1.21
2.20
3.32
ppm
BRUKER
Current Data Parameters
NAME Dr. A MAJEE`
EXPNO 32
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130113
Time_ 20.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 57.28
DW 60.800 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


13C of VBSS-552
164.75
163.59
138.11
136.52
133.27
132.82
132.62
130.56
128.94
125.16
125.08
125.02
120.47
120.02
77.32
77.00
76.68
70.44
42.77
30.24
20.00
13.74
ppm
Current Data Parameters
NAME Dr. A MAJEE
EXPNO 35
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130116
Time 16.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 320
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 57.28
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178055 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


1H of VBSS-596/13 4K
8.023
8.003
7.963
7.946
7.923
7.905
7.655
7.652
7.637
7.634
7.619
7.615
7.610
7.607
7.591
7.577
7.573
7.557
7.555
7.538
7.535
7.347
7.344
7.265
7.263
7.246
7.244
7.227
7.225
7.188
6.326
6.317
6.313
6.304
6.284
5.375
5.334
4.391
4.350
Current Data Parameters
NAME Dr. A MAJEE 2
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130921
Time_ 18.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 40
DS 2
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 186.42
DW 60.800 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.75 usec
PLW1 11.99499989 W
SFO1 400.1524711 MHz
F2 - Processing parameters
SI 16384
SF 400.1500376 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0.96
0.91
1.90
2.98
0.87
0.98
1.78
0.87
0.99
1.00
ppm
1
2
3
4
5
6
7
8
9
O
N
N
O
O
BRUKER


13C of VBSS-596/13
165.00
163.89
150.45
142.11
138.10
136.80
133.65
132.80
132.69
130.60
129.20
126.04
125.22
125.04
120.31
120.15
110.84
108.64
77.32
77.00
76.68
70.98
39.62
O
N
N
O
O
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 MAJEE
EXPNO 506
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130423
Time 19.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.462 Hz
FIDRES 0.733594 Hz
AQ 0.6816244 sec
RG 87.66
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W
SFO1 100.6278588 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.00000000 W
PLW12 0.40792999 W
PLW13 0.26107001 W
SFO2 400.1516006 MHz
F2 - Processing parameters
SI 16384
SF 100.6178012 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40