Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

for

Visible-light-initiated photo-oxidative cyclization of phenolic amidines using CBr_4 – A metal free approach to 2-aminobenzoxazoles

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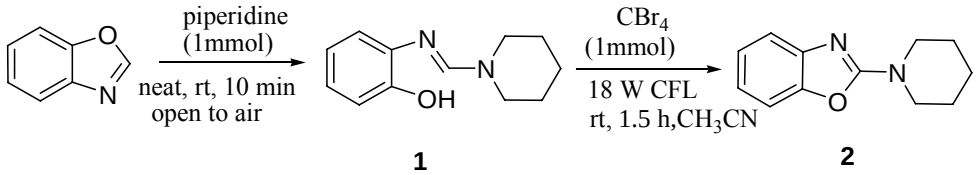
I. General methods

All commercially available reagents were obtained from commercial suppliers and used without further purification. Solvents were purified by the usual methods and stored over molecular sieves. All reactions were performed using oven-dried glass ware. Organic solutions were concentrated using a Buchi rotary evaporator. Flash chromatography was carried out over silica gel (Merck 200–300 mesh) and TLC was performed using silica gel GF254 (Merck) plates. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a Bruker AVII spectrometer in $CDCl_3$ using TMS as internal reference with chemical shift values being reported in ppm. All coupling constants (*J*) are reported in Hertz (Hz). MS (EI) spectra were recorded on double focusing mass spectrometer. 18 W CFL (Compact fluorescent lamp; Philips, 6500 k, 1010 1m, 85 mA) was used as visible light source.

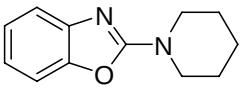
Experimental procedure for the sequential one-pot synthesis of 2-aminobenzoxazoles



A mixture of benzoxazole (1 mmol) and piperidine (2 mmol) was taken in a round bottom flask and stirred under neat condition for 10 min at rt in an air atmosphere. After confirming the completion of the reaction by TLC, the reaction mixture was diluted with acetonitrile (3 mL) and CBr_4 (1 mmol.) was added. Then, the reaction mixture was irradiated with visible light, using 18 W CFL. After completion of the reaction (indicated by TLC), it was quenched with saturated aqueous sodium hydrogen carbonate (5 mL) and extracted with ethyl acetate (3 × 5 mL). The combined organic phases were dried over anhyd. Na_2SO_4, filtered and the solvent was removed under reduced pressure. The resulting crude product was purified by flash chromatography on silica gel (silica: 200~300; eluant: hexane/ ethyl acetate (10:1~5:1)) to afford an analytically pure sample of 2-aminobenzoxazoles **2**. All the products are known compounds and were characterized by comparison of their spectral data with those reported in the literature.[1-6]

II. Experimental Data of Products (2a-2o)

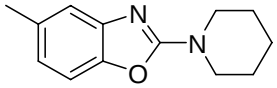
Characterization data of products **2a-2o** with relevant references are given below:



2-(Piperidin-1-yl)benzo[*d*]oxazole (2a)[1,5,6]: ^{1}H NMR (400 MHz,$CDCl_3$): δ 1.66 (s, 6H), 3.63 (s, 4H), 6.94 (t, *J* = 7.6 Hz, 1H), 7.12 (t, *J* = 7.6 Hz, 1H), 7.20 (d, *J* = 8 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 24.1, 25.1, 46.5, 108.5, 115.8, 120.3, 123.8, 143.5, 148.7, 162.5.

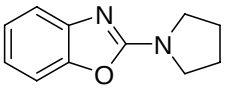
HRMS (EI) m/z: calcd for $C_{12}H_{14}N_2ONa$ (M + H) 203.1184, found (M + H) 203.1182.



5-Methyl-2-(piperidin-1-yl)benzoxazole (2b)[1,4,5]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.68 (s, 6H), 2.39 (s, 3H), 3.61 (s, 4H), 6.80 (d, *J* = 8 Hz, 1H), 7.08 (d, *J* = 8 Hz, 1H), 7.16 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 21.4, 23.9, 25.0, 46.6, 107.9, 116.2, 120.9, 133.2, 143.2, 146.6, 162.3.

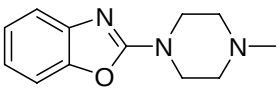
HRMS (EI) m/z: calcd for $C_{13}H_{16}N_2ONa$ (M + H) 217.1341, found (M + H) 217.1348.



2-(Pyrrolidin-1-yl)benzoxazole (2c)[2-4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.87-2.01 (m, 4H), 3.51-3.63 (m, 4H), 6.96 (t, *J* = 7.7 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 25.3, 47.2, 108.4, 115.9, 119.8, 123.7, 143.5, 148.9, 160.7.

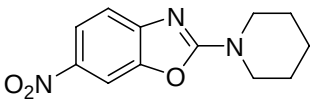
HRMS (EI) m/z: calcd for $C_{11}H_{12}N_2ONa$ (M+H) 189.1028, found (M+H) 189.1025.



2-(4-Methyl-1-piperazinyl)benzoxazole (2d)[5]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.39 (s, 3H), 2.61 (t, *J* = 4.3 Hz, 4H), 3.78 (t, *J* = 4.7 Hz, 4H),7.02 (t, *J* = 7.7 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.25-7.26 (m, 1H), 7.38 (d, *J* = 7.8 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 45.0, 46.0, 53.8, 108.7, 116.4, 120.8, 123.8, 142.7, 148.8, 162.0.

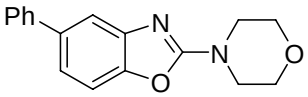
HRMS (EI) m/z: calcd for $C_{12}H_{15}N_3ONa$ (M + H) 218.1293, found (M + H) 218.1296.



6-Nitro-2-(piperidin-1-yl)benzoxazole (2e)[5]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.73 (s, 6H), 3.70 (s, 4H), 7.29 (d, *J* = 8.7 Hz, 1H), 8.07-8.16 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 23.8, 25.6, 46.6, 104.8, 114.6, 121.4, 141.1, 147.7, 150.5, 164.9.

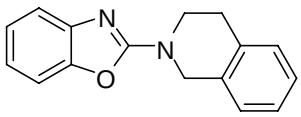
HRMS (EI) m/z: calcd for $C_{12}H_{13}N_3O_3Na$ (M + H) 248.1030, found (M + H) 248.1033.



2-(4-Morpholinyl)-5-phenylbenzoxazole (2f)[3,5]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.68 (t, *J* = 7.9 Hz, 4H), 3.86 (t, *J* = 4.8 Hz, 4H), 7.24-7.37 (m, 3H), 7.38-7.42 (m, 2H), 7.59-7.61 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 45.5, 66.0, 108.8, 115.0, 120.3, 126.7, 127.1, 128.7, 137.8, 141.3, 143.4, 148.2, 162.5.

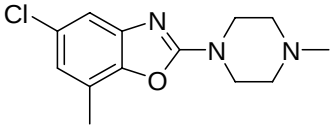
HRMS (EI) m/z: calcd for $C_{17}H_{16}N_2O_2Na$ (M + H) 281.1285, found (M + H) 281.1288.



2-(3,4-Dihydroisoquinolin-2(1*H*)-yl)benzoxazole (2g)[4,5]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.02 (t, *J* = 5.9 Hz, 2H), 3.98 (t, *J* = 5.9 Hz, 2H), 4.87 (s, 2H), 7.05 (t, *J* = 7.7 Hz, 1H), 7.14-7.23 (m, 5H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.40 (d, *J* = 7.7 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 28.2, 42.8, 47.0, 108.4, 116.0, 120.3, 123.9, 126.0, 126.3, 126.7, 128.7, 132.3, 133.7, 143.0, 148.6, 162.0.

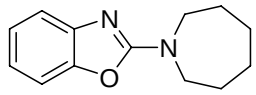
HRMS (EI) m/z: calcd for $C_{16}H_{14}N_2ONa$ (M+H) 251.1184, found (M+H) 251.1182.



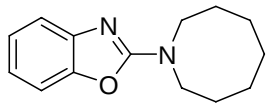
5-Chloro-7-methyl-2-(4-methyl-1-piperazinyl)benzoxazole (2h)[5]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3H), 2.42 (s, 3H), 2.56 (t, *J* = 5.2 Hz, 4H), 3.76 (t, *J* = 5.2 Hz, 4H), 6.78 (s, 1H), 7.12 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 14.9, 45.0, 46.0, 53.9, 113.8, 120.0, 121.9, 128.7, 143.5, 146.2, 162.5.

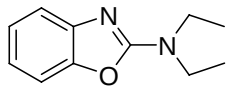
HRMS (EI) m/z: calcd for $C_{13}H_{16}ClN_3ONa$ (M + H) 266.1060, found (M + H) 266.1063.



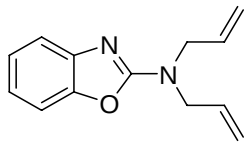
2-(Azepan-1-yl)benzoxazole (2i)[4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.50-1.62 (m, 4H), 1.73-1.90 (m, 4H), 3.55-3.80 (m, 4H), 6.95 (t, *J* = 7.7 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.20 (d, *J*= 7.9 Hz, 1H), 7.36 (d, *J* = 7.7 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 27.2, 28.1, 47.7, 108.2, 115.6, 119.7, 123.5, 143.7, 148.6, 162.4.
HRMS (EI) m/z: calcd for $C_{13}H_{16}N_2ONa$ (M+H) 217.1341, found (M+H) 217.1344.



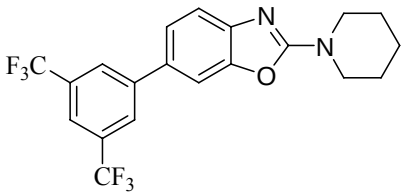
2-(Azocan-1-yl)benzoxazole (2j)[4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.50-1.64 (m, 6H), 1.78-1.88 (m, 4H), 3.65 (t, *J* = 5.7 Hz, 4H), 6.99 (dt, *J* = 7.7 Hz, *J* = 0.7 Hz, 1H), 7.12 (dt, *J* = 7.7 Hz, *J* = 0.7 Hz, 1H), 7.26 (d, *J* = 7.8 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 25.7, 26.3, 26.6, 50.0, 108.4, 115.5, 119.7, 123.6, 143.5, 148.7, 162.0.
HRMS (EI) m/z: calcd for $C_{14}H_{18}N_2ONa$ (M+H) 231.1497, found (M+H) 231.1495.



2-(Diethylamino)benzoxazole(2k)[4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.23 (t, *J* = 7.1 Hz, 6H), 3.61 (q, *J* = 7.1 Hz, 4H), 6.95 (dt, *J* = 7.7 Hz, *J* = 0.7 Hz, 1H), 7.13 (dt, *J* = 7.7 Hz, *J* = 0.7 Hz, 1H), 7.25 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 13.5, 43.1, 108.6, 115.7, 119.9, 123.7, 143.6, 148.8, 162.1.
HRMS (EI) m/z: calcd for $C_{11}H_{14}N_2ONa$ (M+H) 191.1184, found (M+H) 191.1181.



2-(Diallylamino)benzoxazole (2l)[4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.05-4.21 (m, 4H), 5.13-5.30 (m, 4H), 6.00-6.77 (m, 2H), 6.96 (t, *J* = 7.7 Hz, 1H), 7.14 (t, *J* = 7.7 Hz, 1H), 7.20 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 7.8 Hz, 1H).
^{13}C NMR (100 MHz, $CDCl_3$): δ 49.5, 108.3, 115.8, 117.4, 119.8, 123.3, 132.2, 143.0, 148.5, 161.7.
HRMS (EI) m/z: calcd for $C_{13}H_{14}N_2ONa$ (M+H) 215.1184, found (M+H) 215.1186.

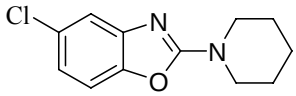


6-(3,5-Bis(trifluoromethyl)phenyl)-2-(piperidin-1-yl)benzoxazole (2m)[4]: ^{1}H NMR (400 MHz,$CDCl_3$): δ 1.71 (s, 6H), 3.65 (br s, 4H), 7.40 (s, 2H), 7.47 (s, 1H), 7.76 (s, 1H), 7.96 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 23.3, 24.5, 45.8, 106.3, 115.4, 118.9-119.3, 122.5, 122.7, 125.8-126.3, 129.8, 131.2, 142.7, 143.6, 148.6, 162.3.

^{19}F NMR (282 MHz, $CDCl_3$): δ -62.7 (s, 6F).

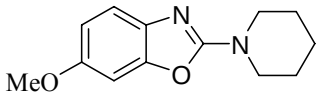
HRMS (EI) m/z: calcd for $C_{20}H_{16}F_6N_2ONa$ (M+H) 415.1245, found (M+H) 415.1243.



5-Chloro-2-(piperidin-1-yl)benzoxazole (2n)[4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.66 (s, 6H), 3.63 (br s, 4H) ,6.90 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 1H), 7.26 (d, *J* = 2.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 23.9, 25.1, 46.5, 108.8, 115.9, 119.9, 129.0, 144.7, 147.2, 163.0.

HRMS (EI) m/z: calcd for $C_{12}H_{13}ClN_2ONa$ (M+H) 237.0795, found (M+H) 237.0792.



6-Methoxy-2-(piperidin-1-yl)benzoxazole (2o)[4]: ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.60 (s, 6H), 3.55 (br s, 4H), 3.78 (s, 3H), 6.70 (dd, *J* = 8.5 Hz, *J* = 2.3 Hz, 1H), 6.86 (d, *J* = 2.3 Hz, 1H), 7.17 (d, *J* = 8.5 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 24.0, 25.1, 46.4, 55.9, 95.6, 109.7, 115.6, 136.9, 149.2, 154.7, 162.0.

HRMS (EI) m/z: calcd for $C_{13}H_{16}N_2O_2Na$ (M+H) 233.1290, found (M+H) 233.1288.

III. References

1 D. Xu, W. Wang, C. Miao, Q. Zhang, C. Xia and W. Sun, *Green Chem.*, 2013, **15**, 2975.
2 J. Joseph, J. Y. Kim and S. Chang, *Chem. Eur.J.*, 2011, **17**, 8294.
3 Y. Xie, B. Qian, P. Xie and H. Huang, *Adv. Synth. Catal.*, 2013, **355**, 1315.
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5 M. Lamani and K. R. Prabhu, *J. Org. Chem.*, 2011, **76**, 7938.
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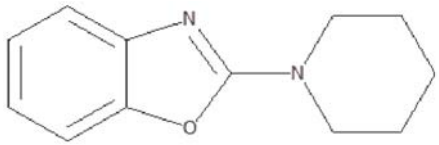
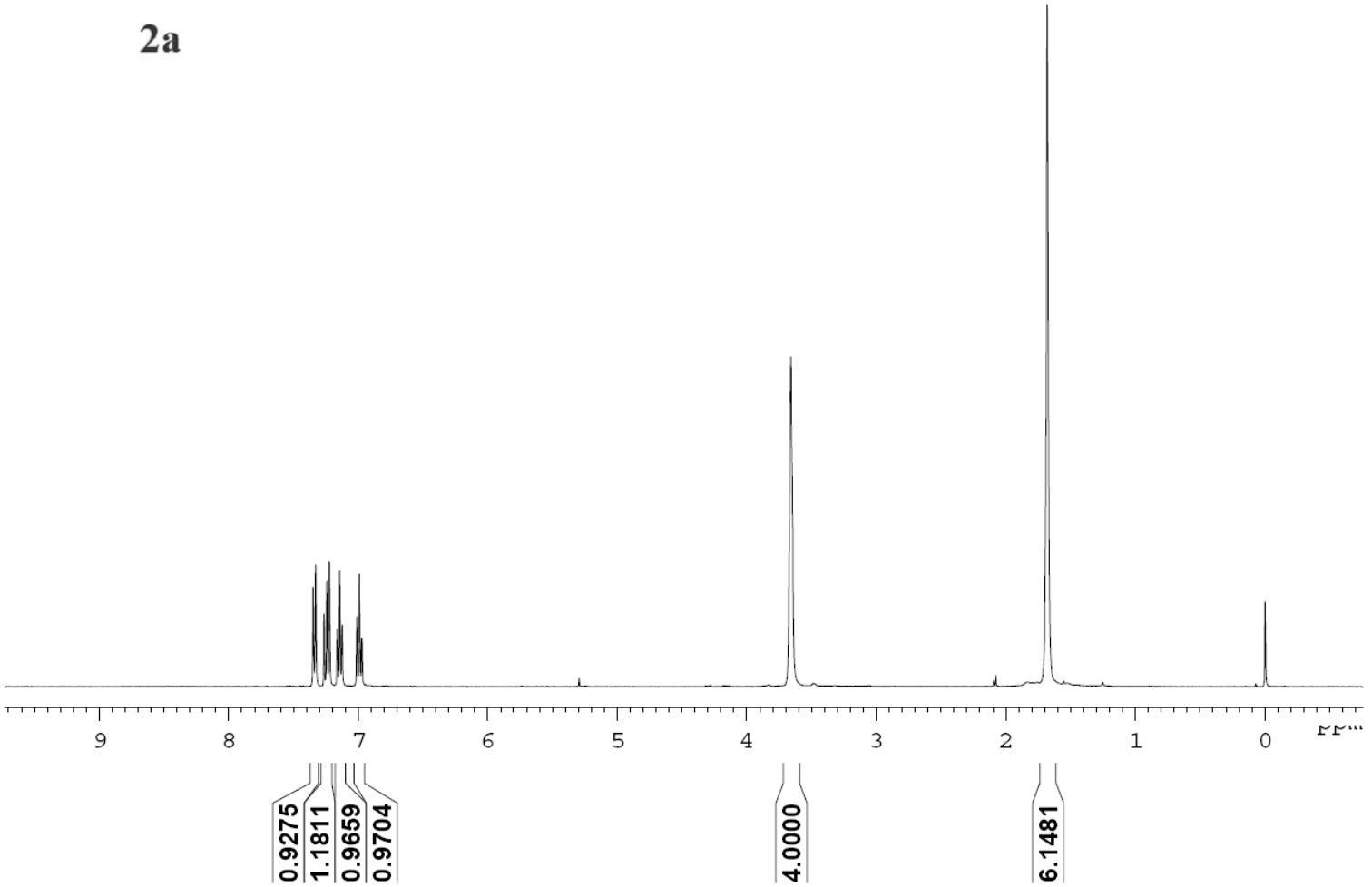
Electronic Supplementary Material (ESI) for RSC Advances

IV. ^{1}H NMR and ^{13}C NMR spectra for the products



2a



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

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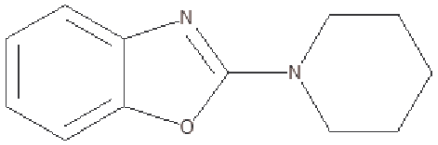
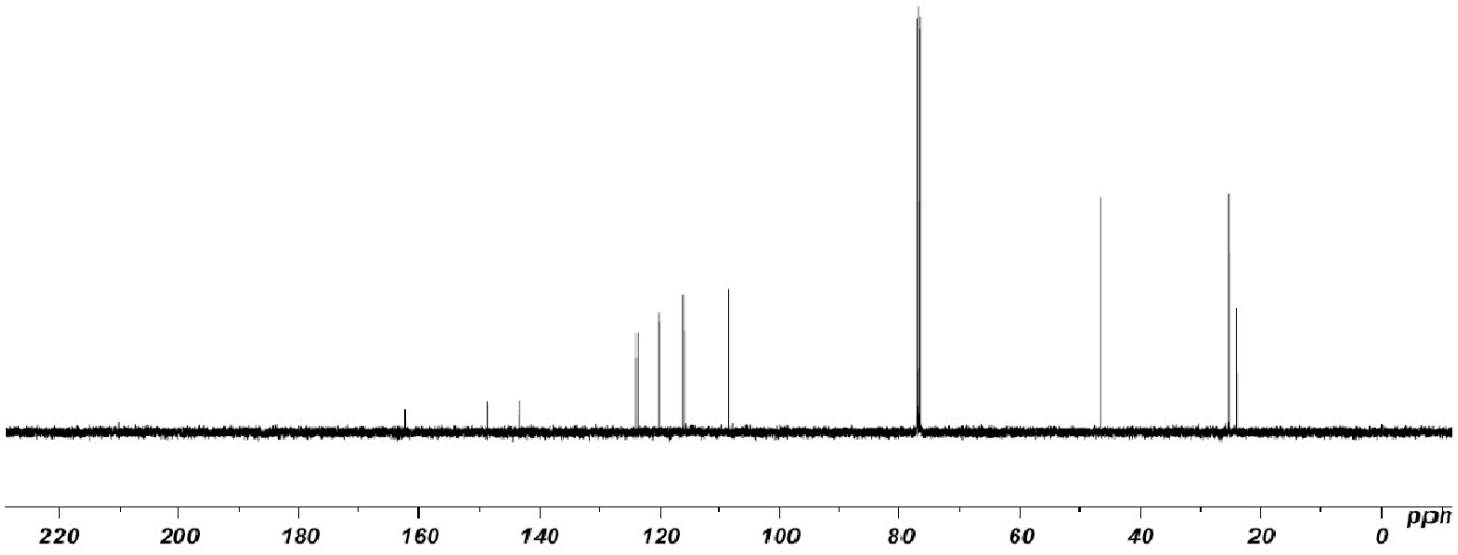


2a



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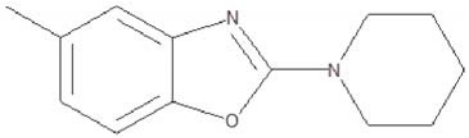
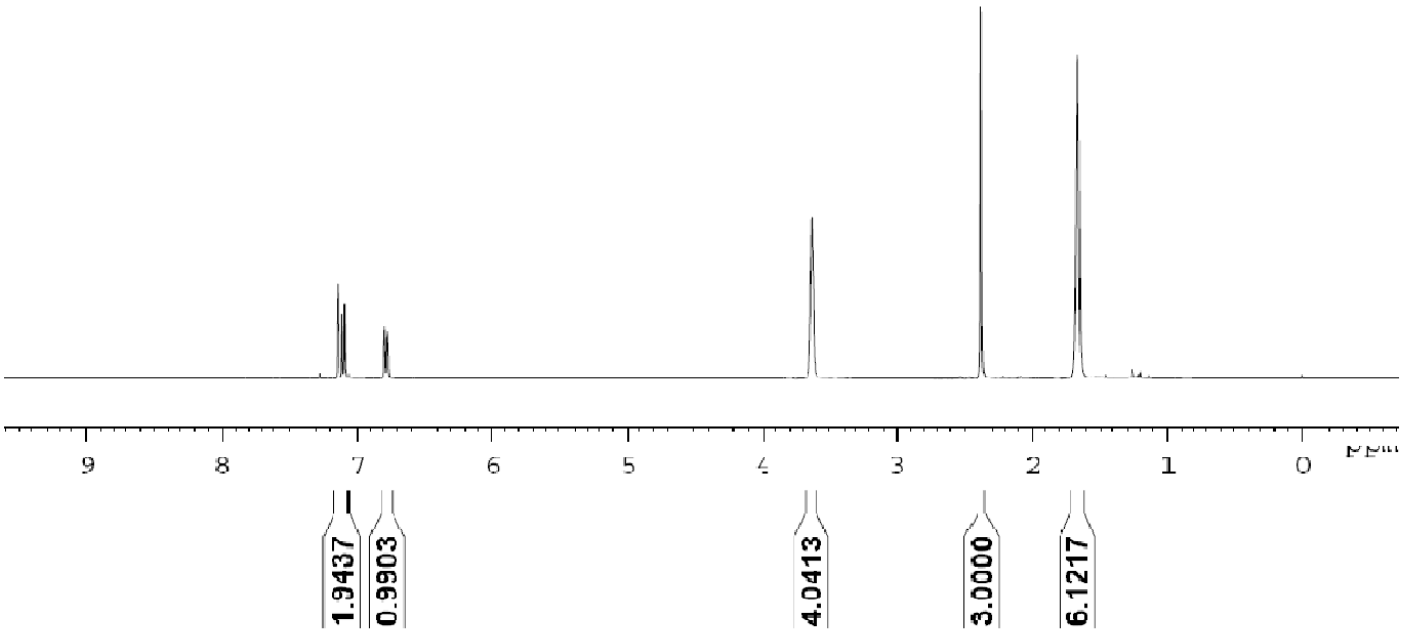
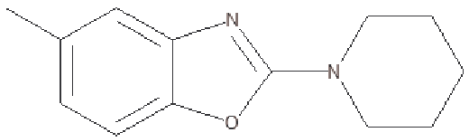


2b



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

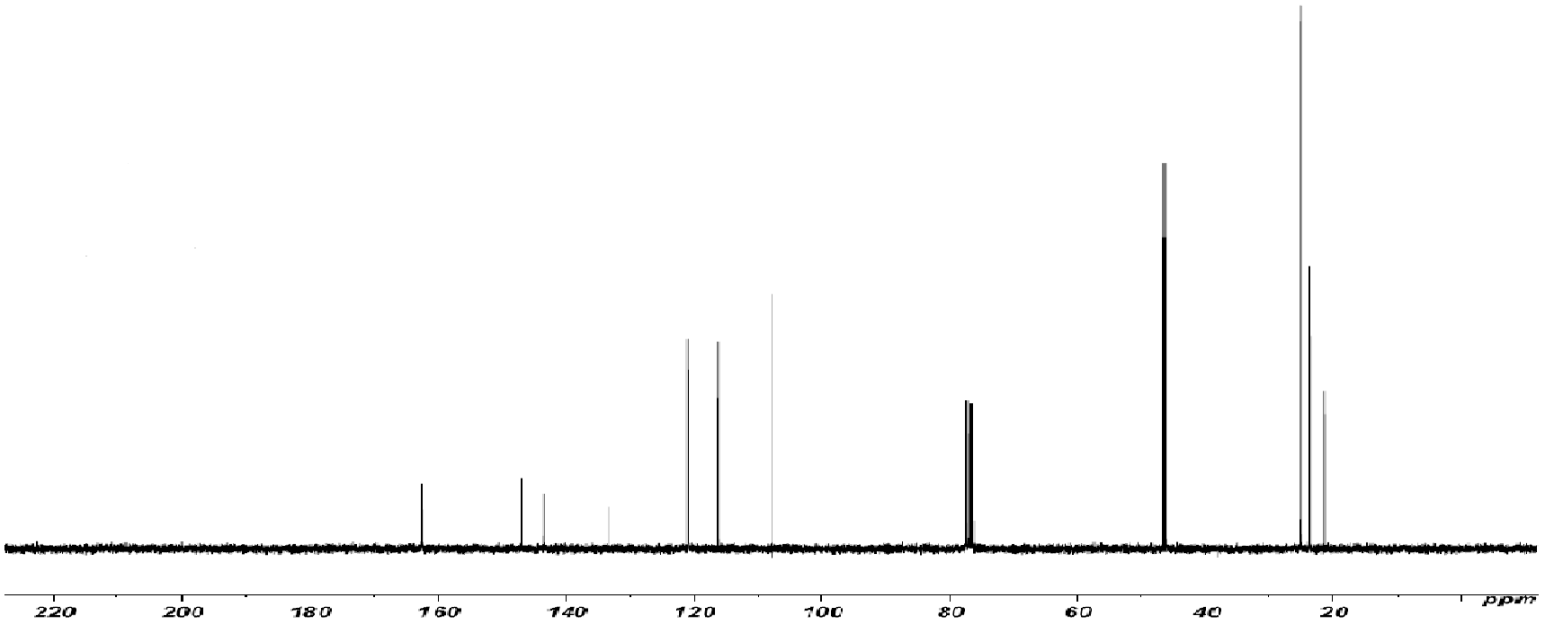
Current Data Parameters
NAME JUN28-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130628
Time 10.29
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

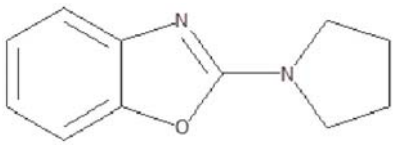


2b

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME JUN28-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130628
Time 10.58
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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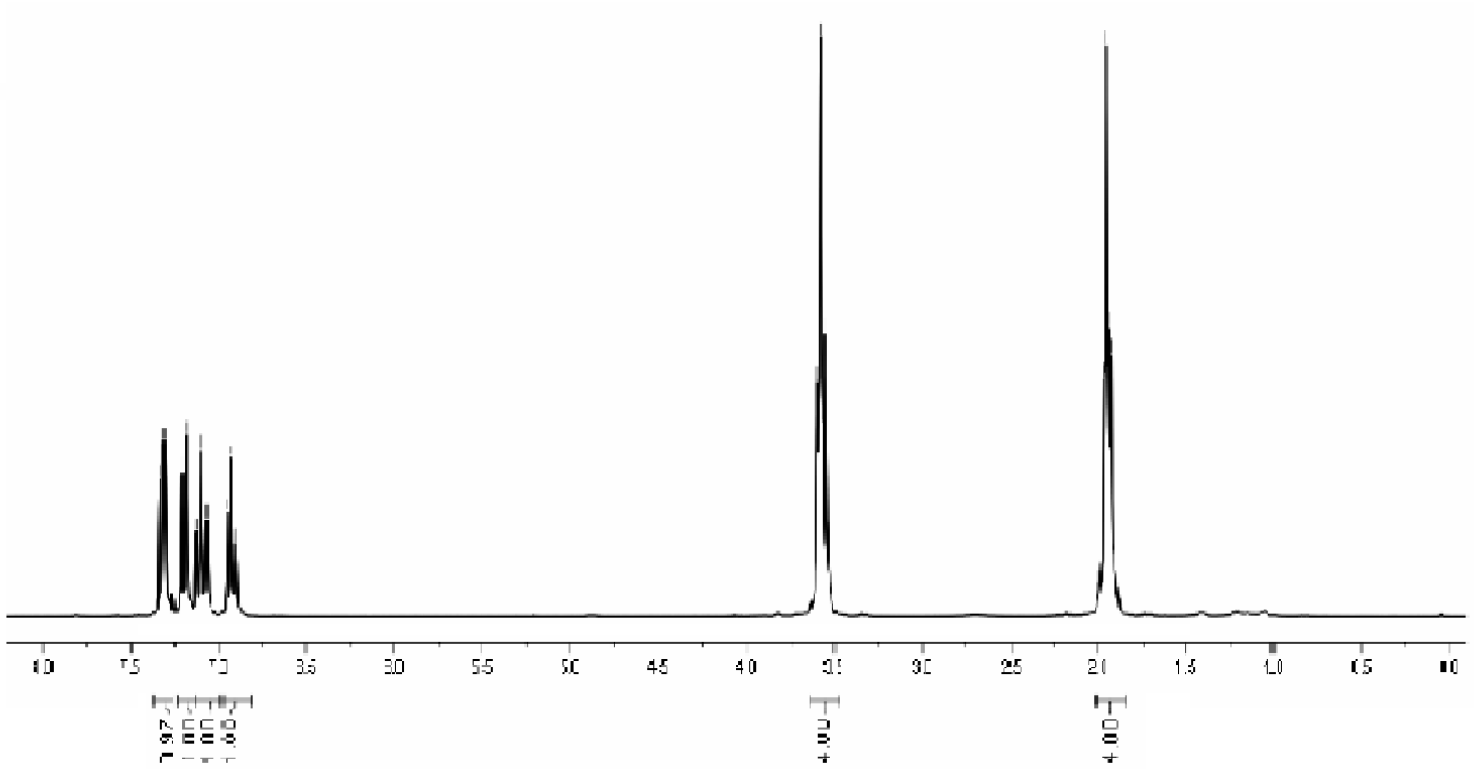

BRUKER
AVANCE II 400 NMR
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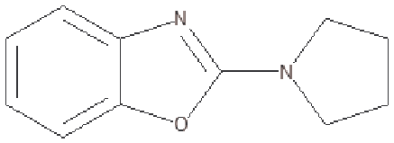
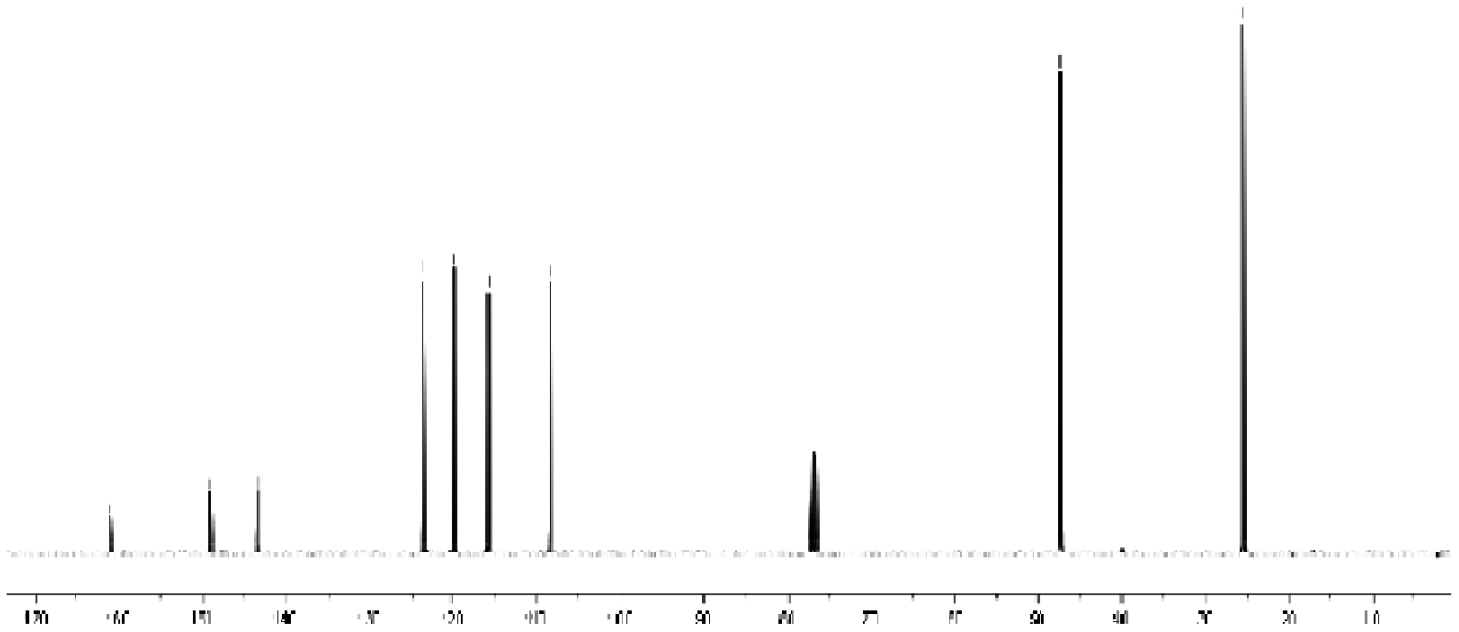
Chandigarh

Current Data Parameters
NAME JULY16-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130716
Time 10.29
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2c



BRUKER
AVANCE II 400 NMR
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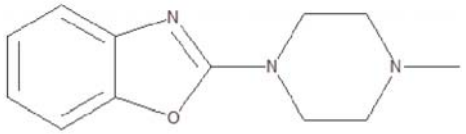
Chandigarh

Current Data Parameters
NAME JULY16-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130716
Time 10.58
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2d

BRUKER
AVANCE II 400 NMR
Spectrometer
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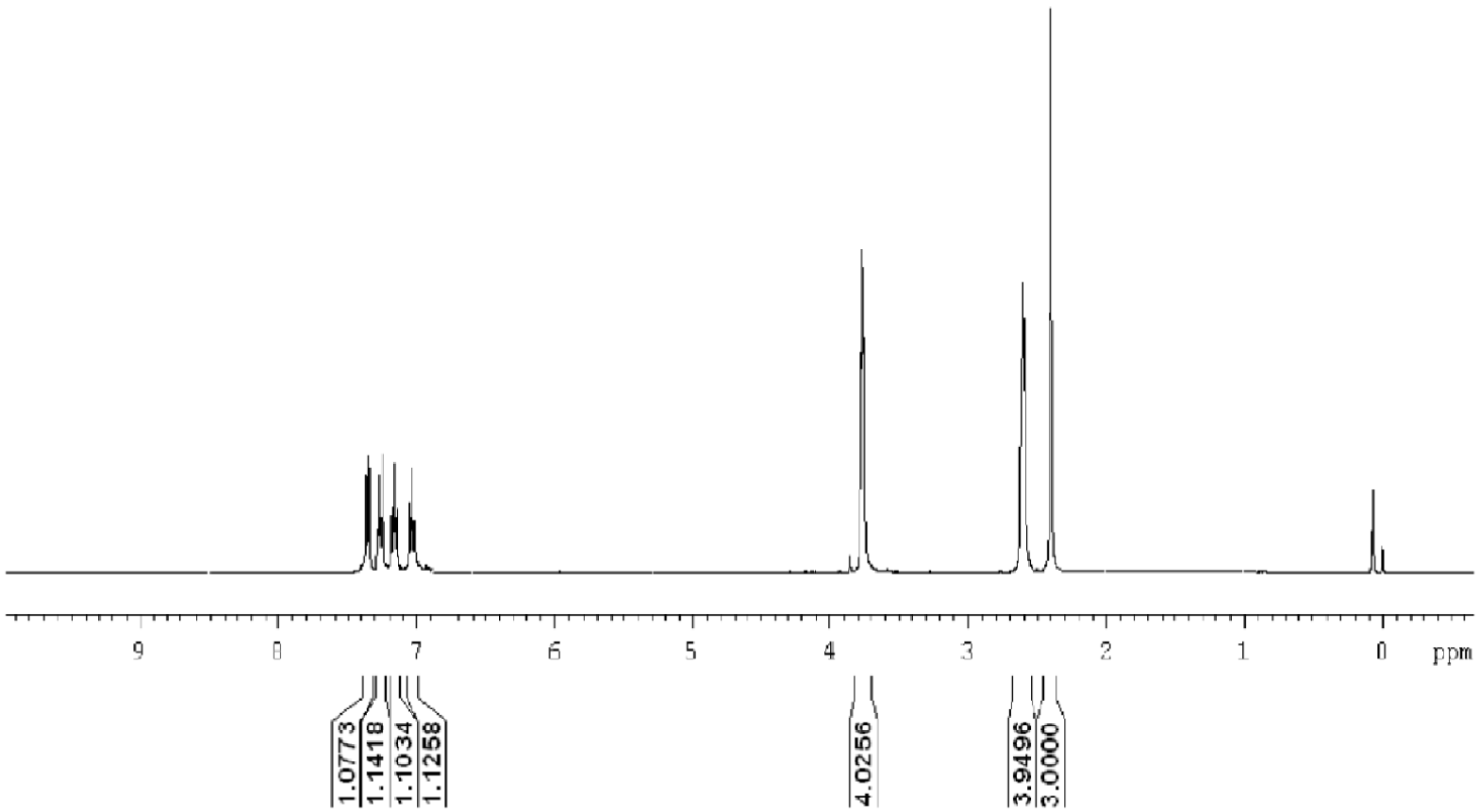
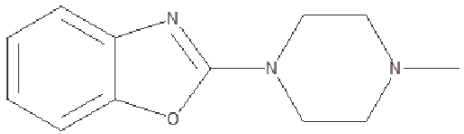
Panjab University
Chandigarh

Current Data Parameters
NAME JULY16-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130716
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

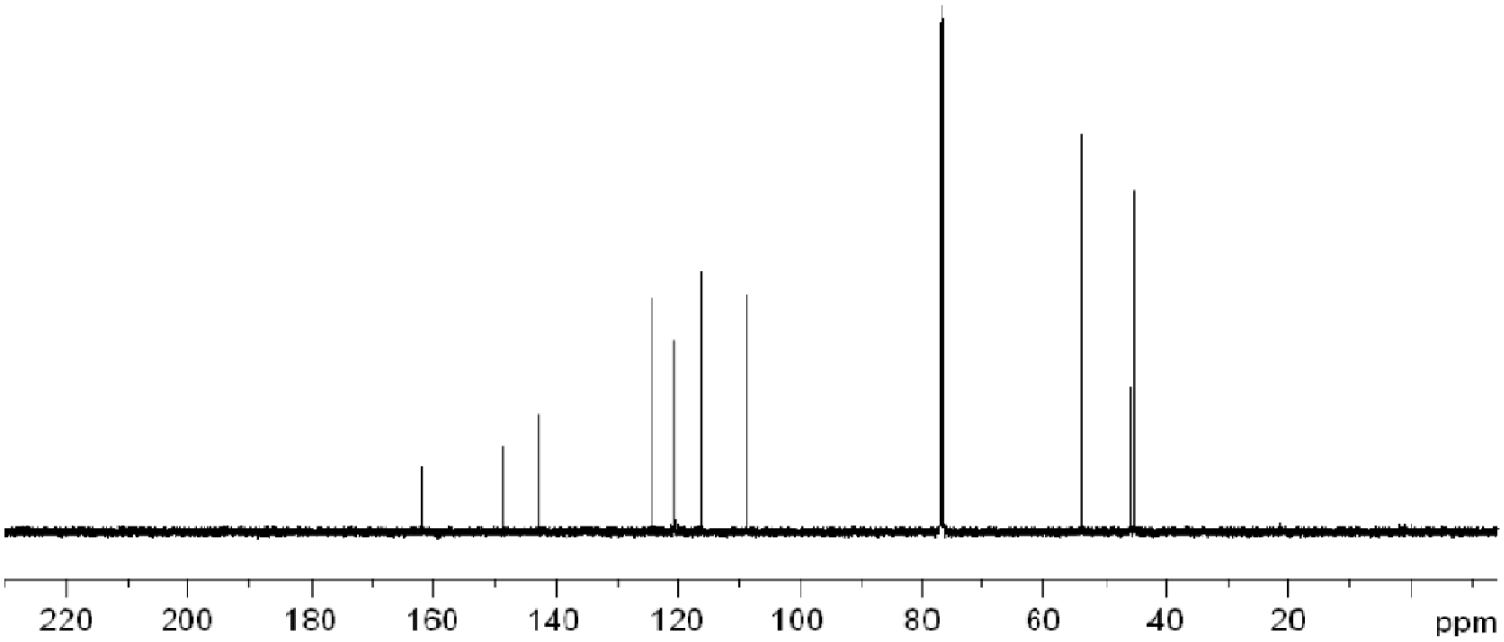


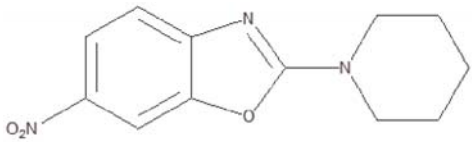


2d

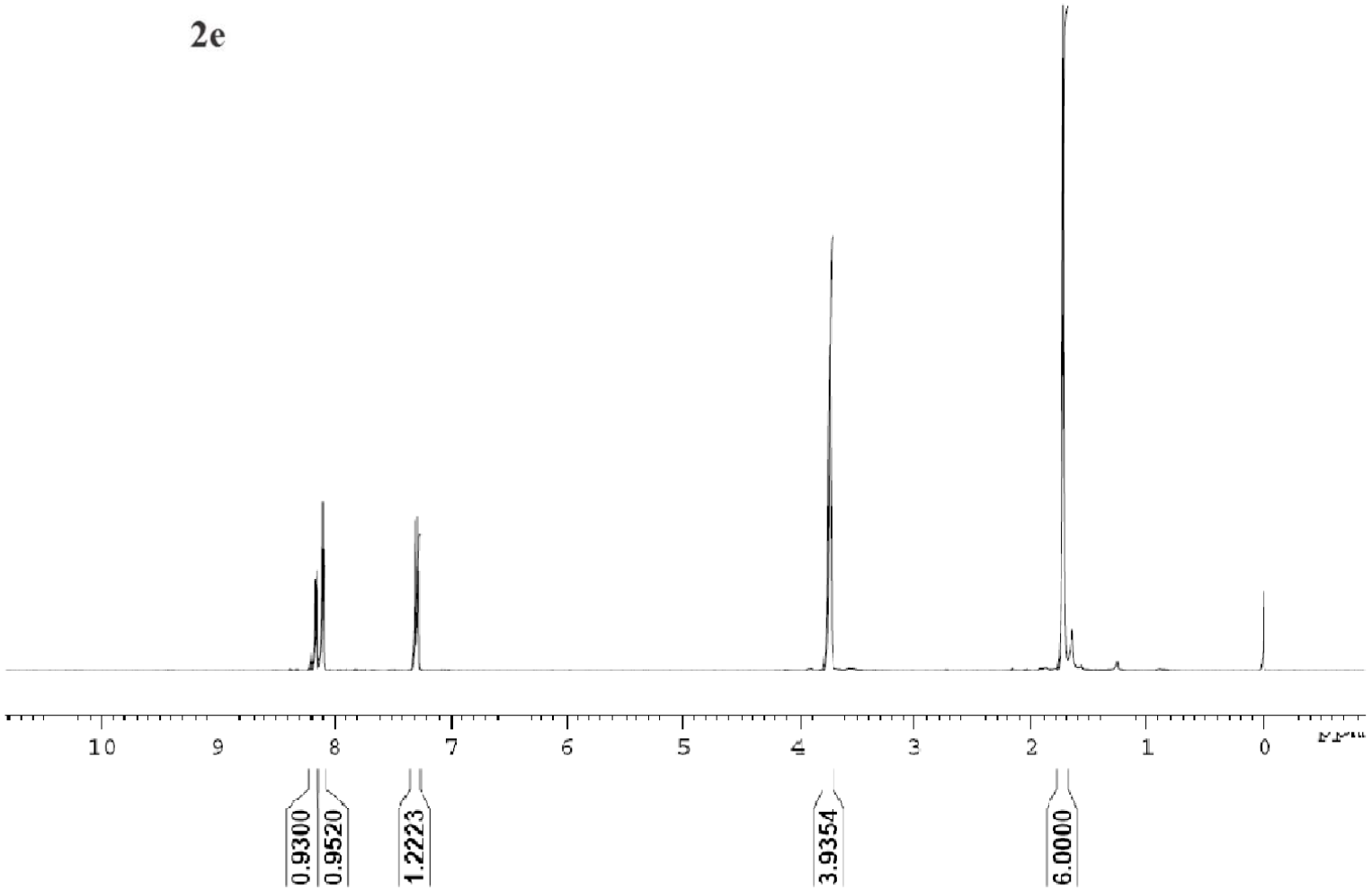
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME JULY16-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130716
Time 10.15
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





2e



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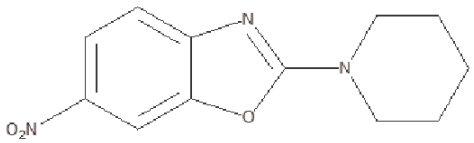
Current Data Parameters
NAME AUG02-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130802
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2e

BRUKER
AVANCE II 400 NMR
Spectrometer
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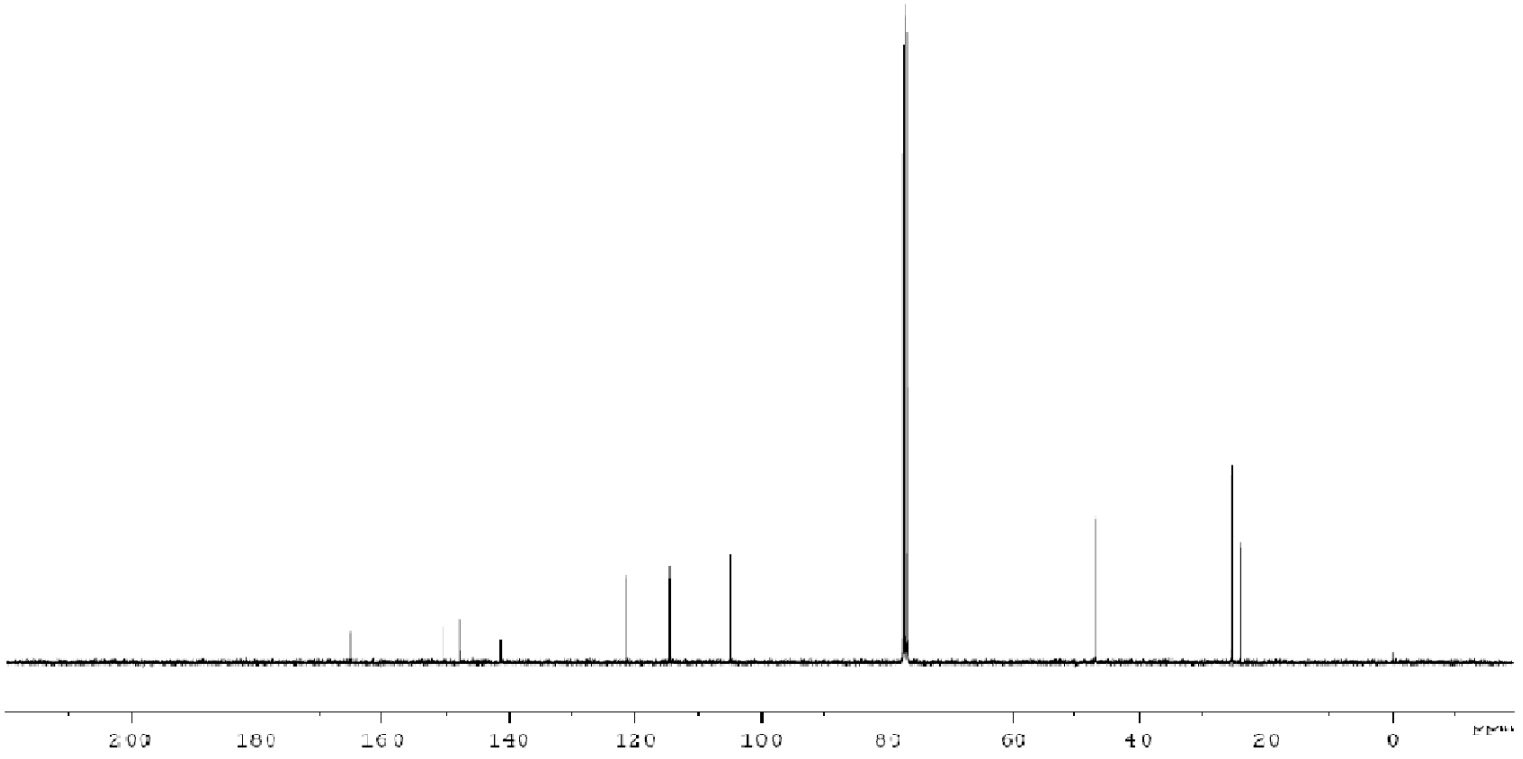
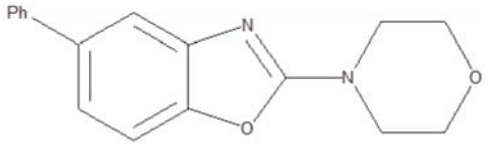
Current Data Parameters
NAME AUG2-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130802
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





2f

BRUKER
AVANCE II 400 NMR
Spectrometer
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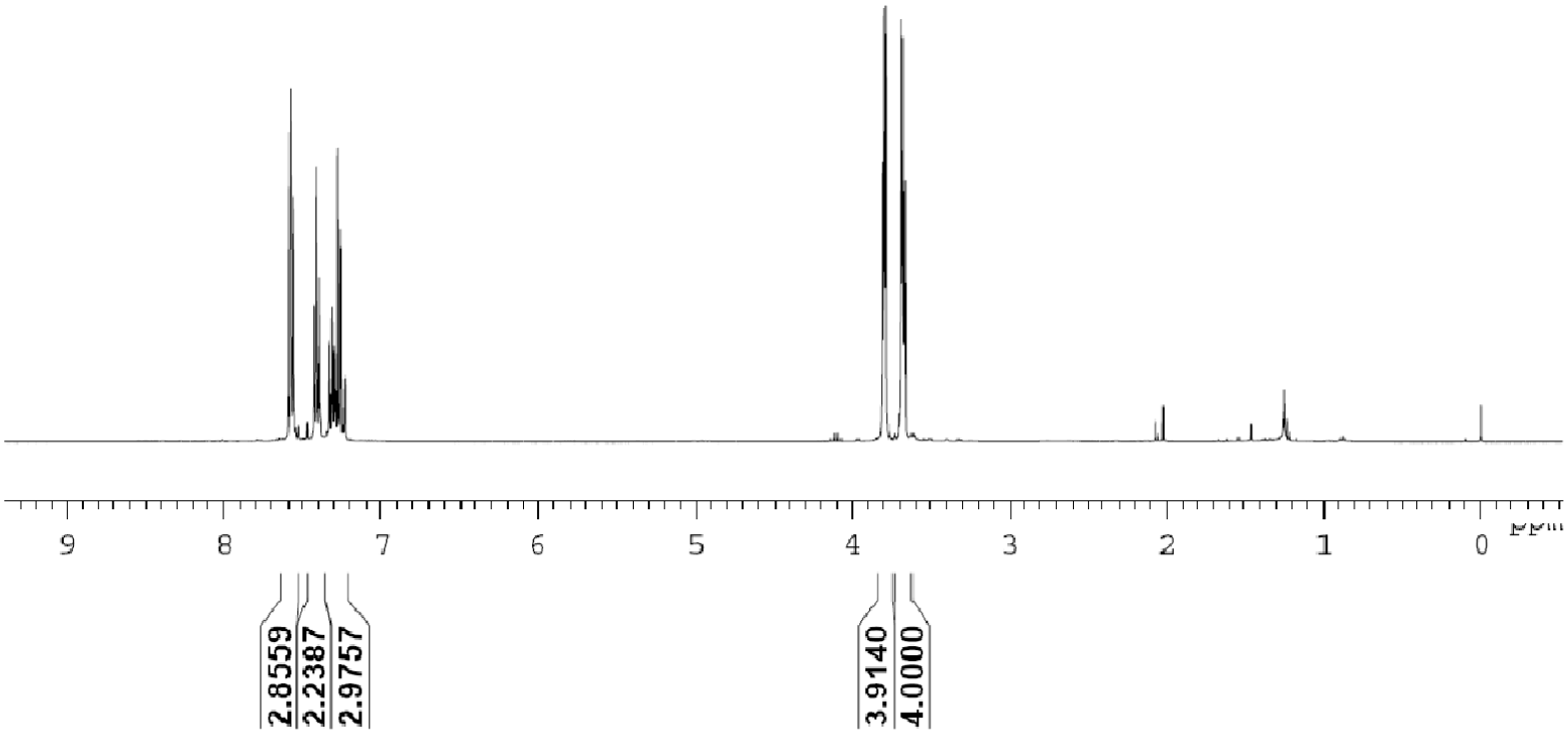
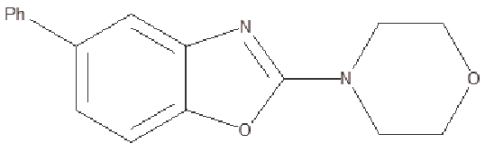
Panjab University
Chandigarh

Current Data Parameters
NAME AUG02-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130802
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

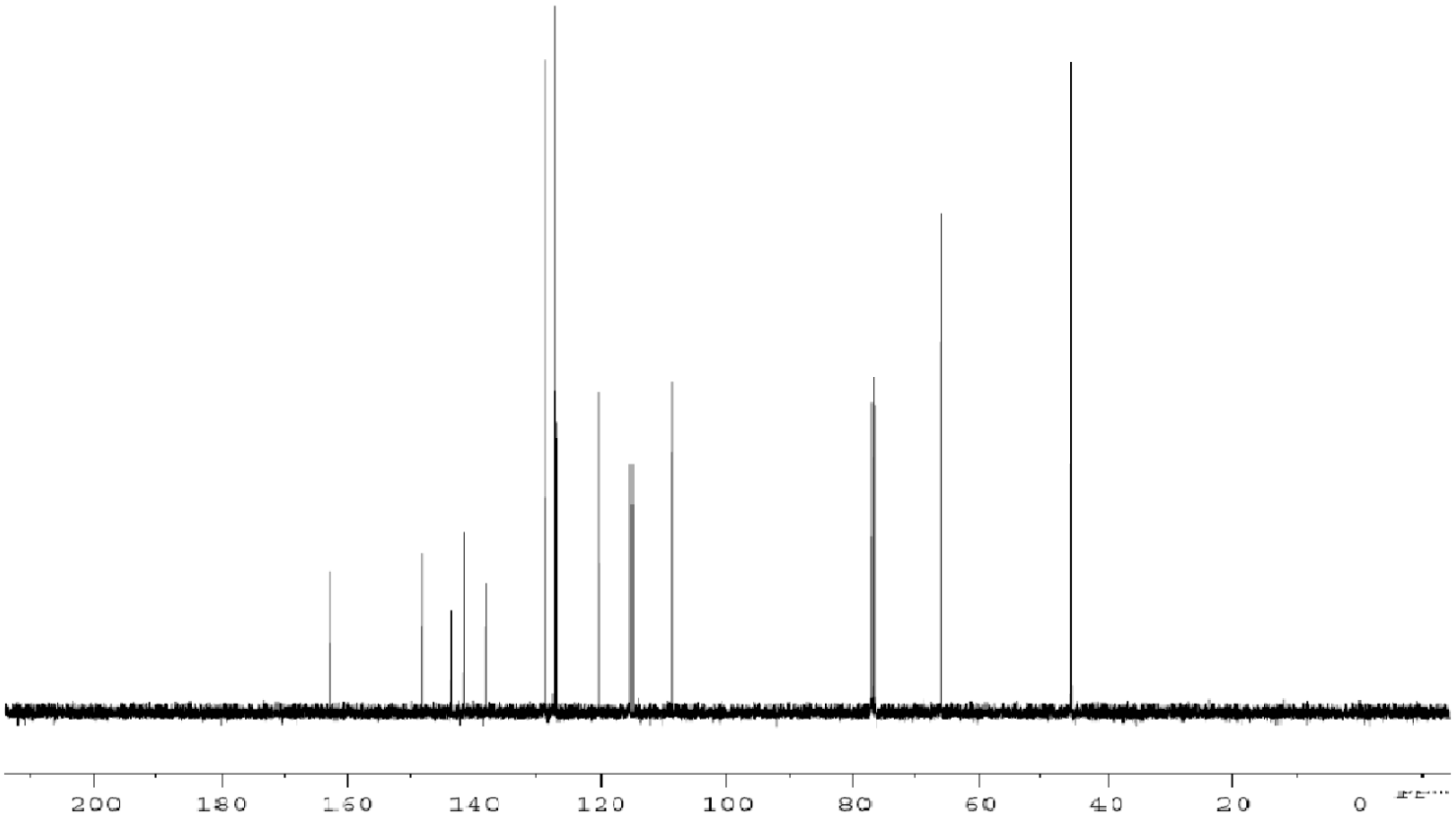


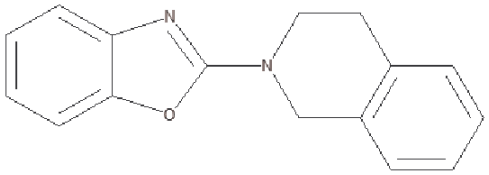


2f

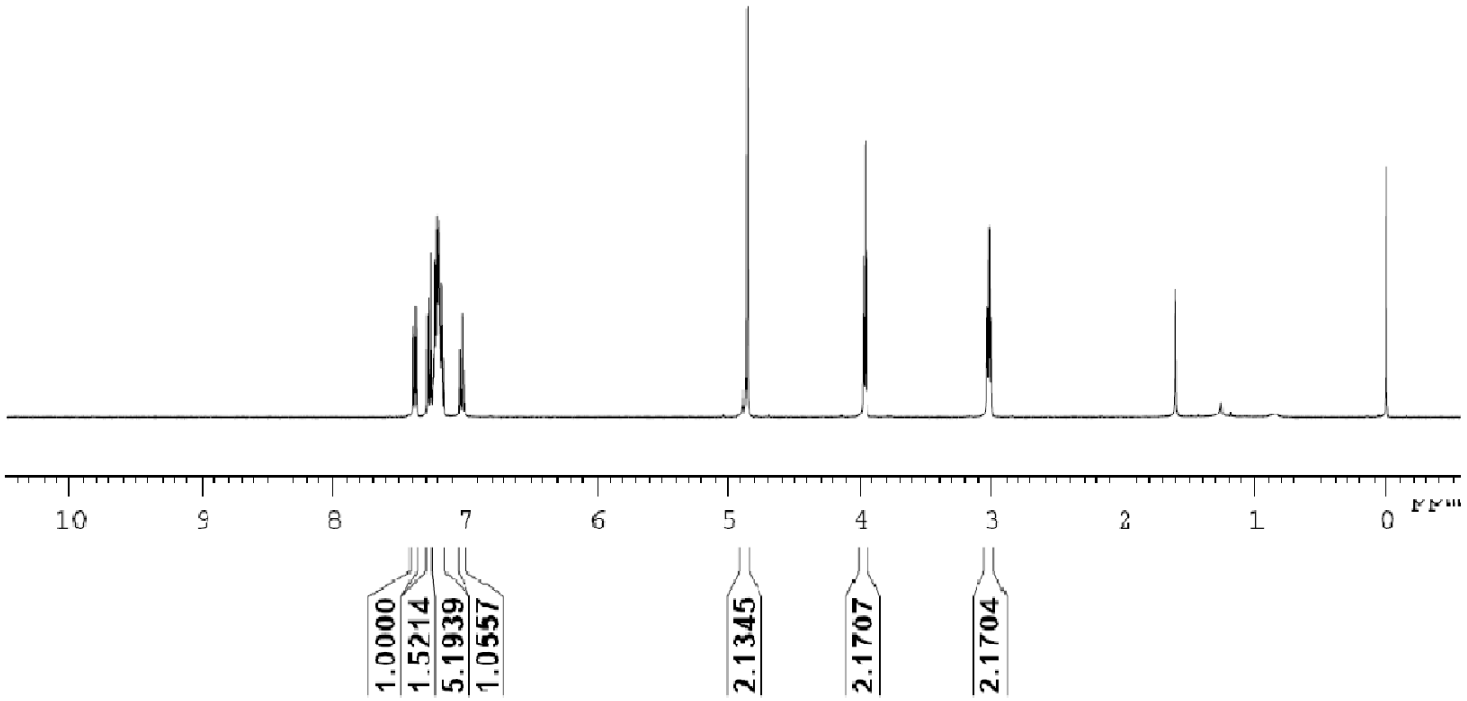
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME AUG2-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130802
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



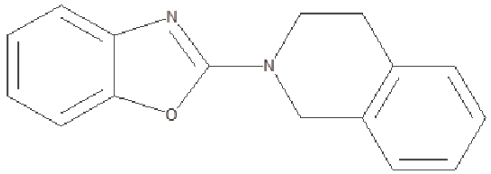


2g



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

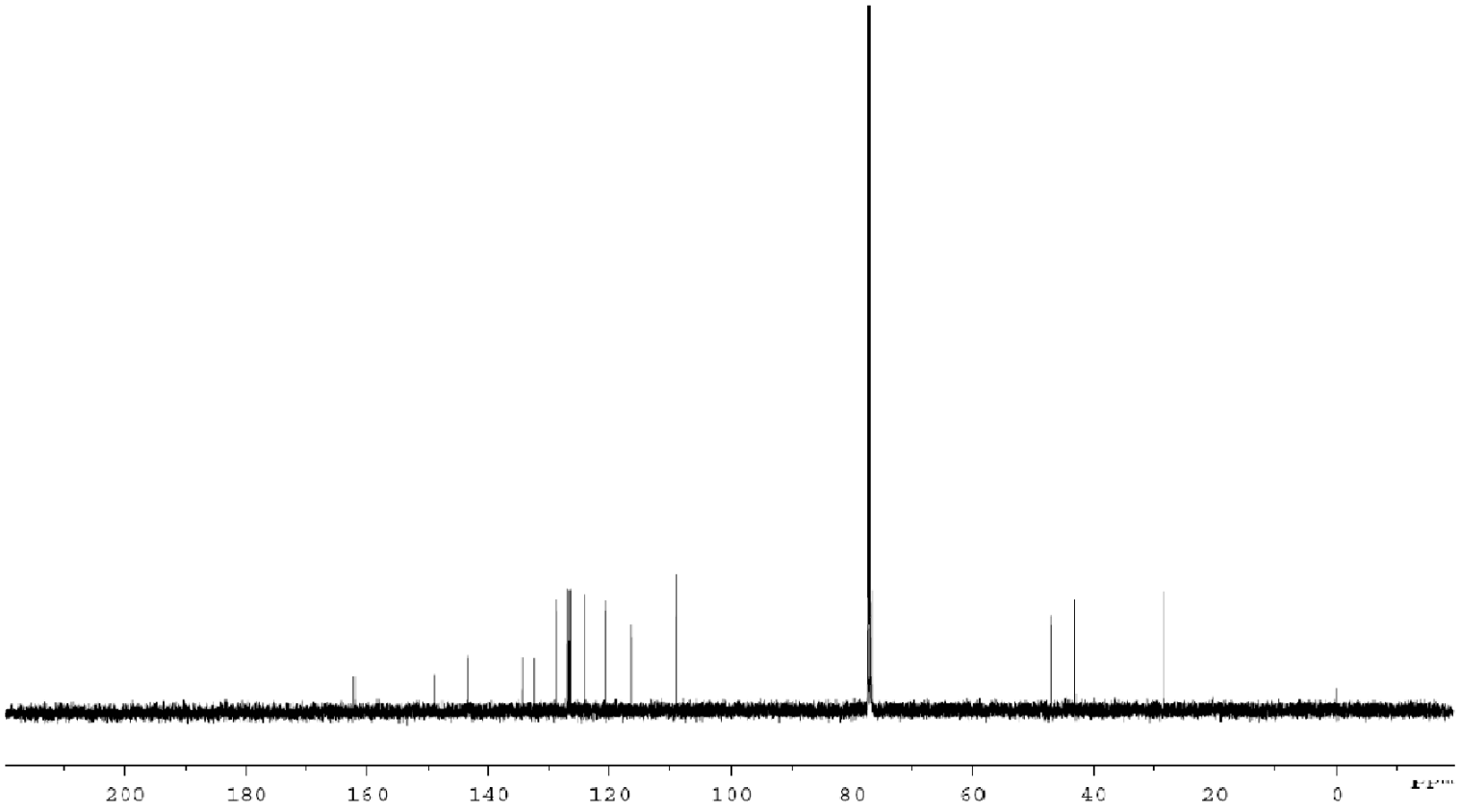
Current Data Parameters
NAME AUG10-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130810
Time 10.15
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

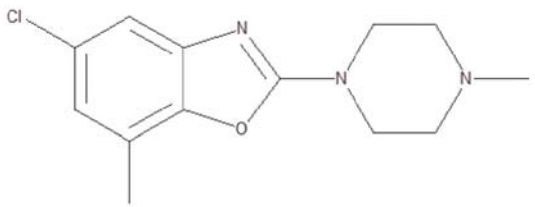


2g

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME AUG10-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130810
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

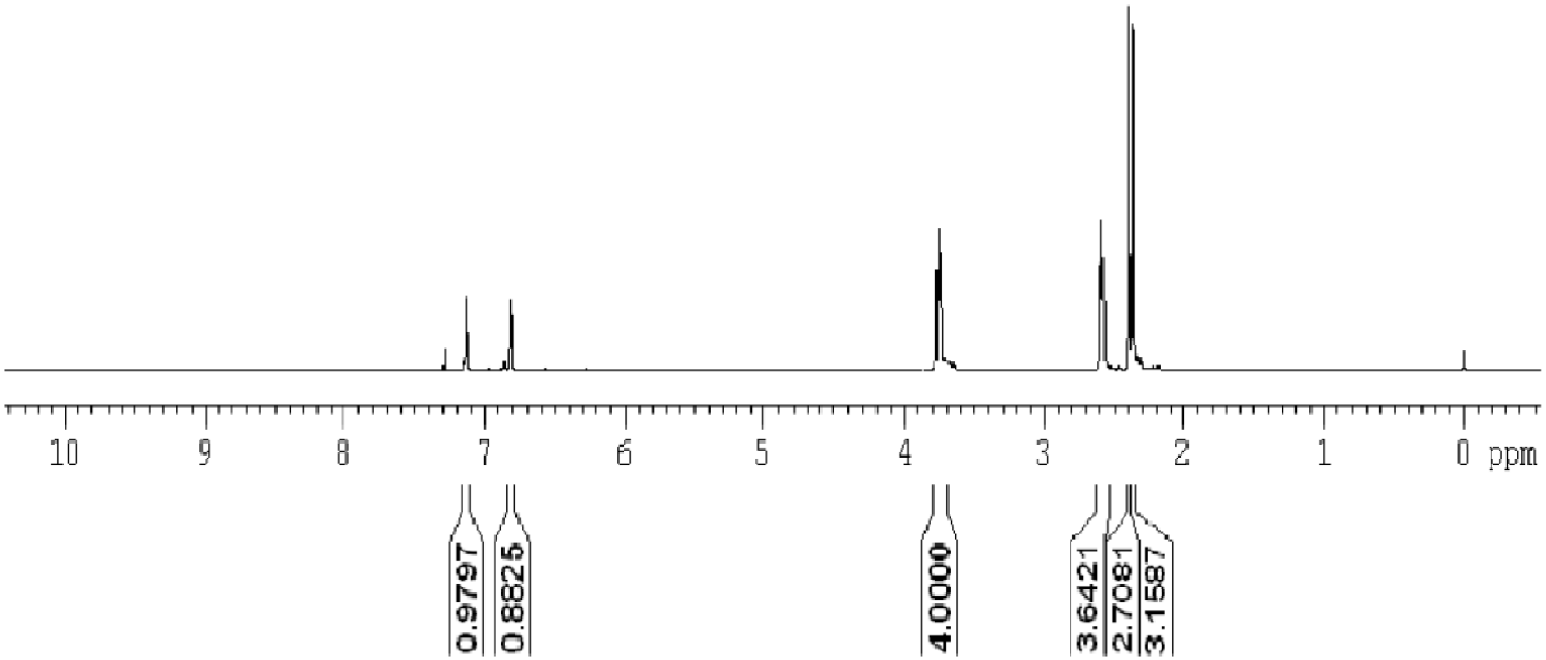


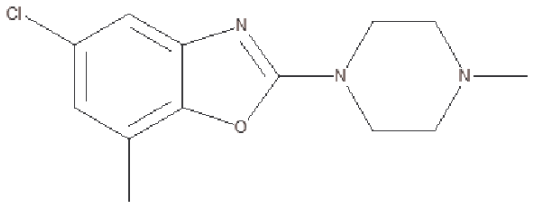


2h

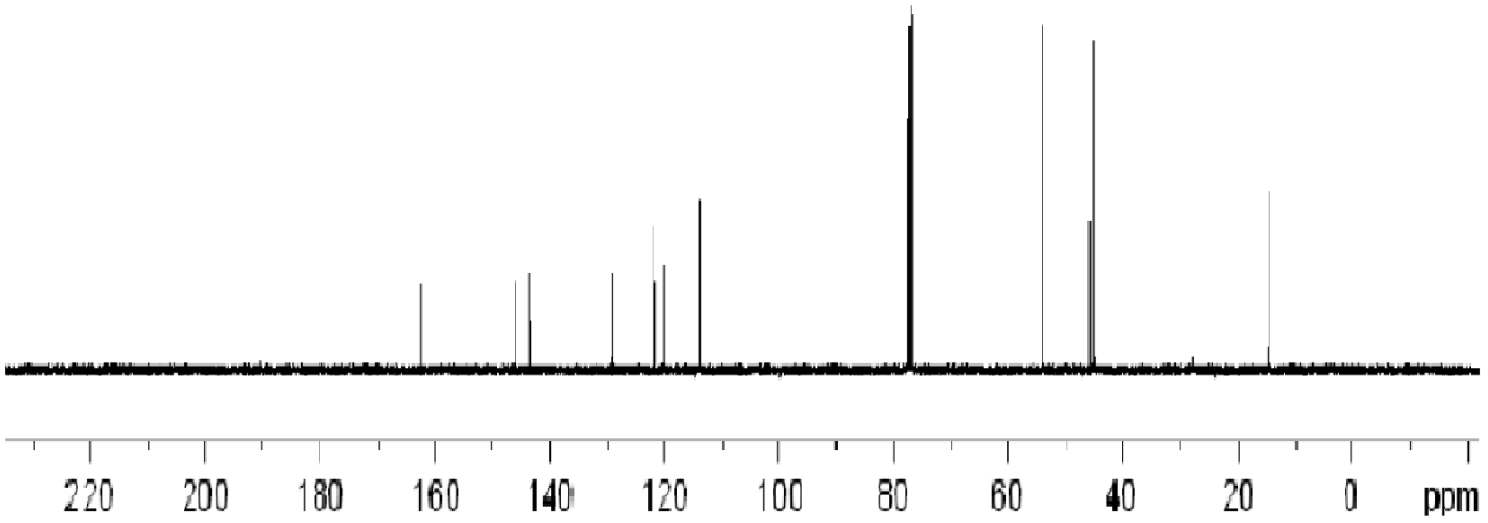
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME AUG22-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130822
Time 11.30
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





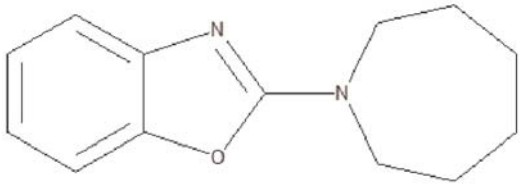
2h



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME AUG22-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130822
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0

PC 1.40



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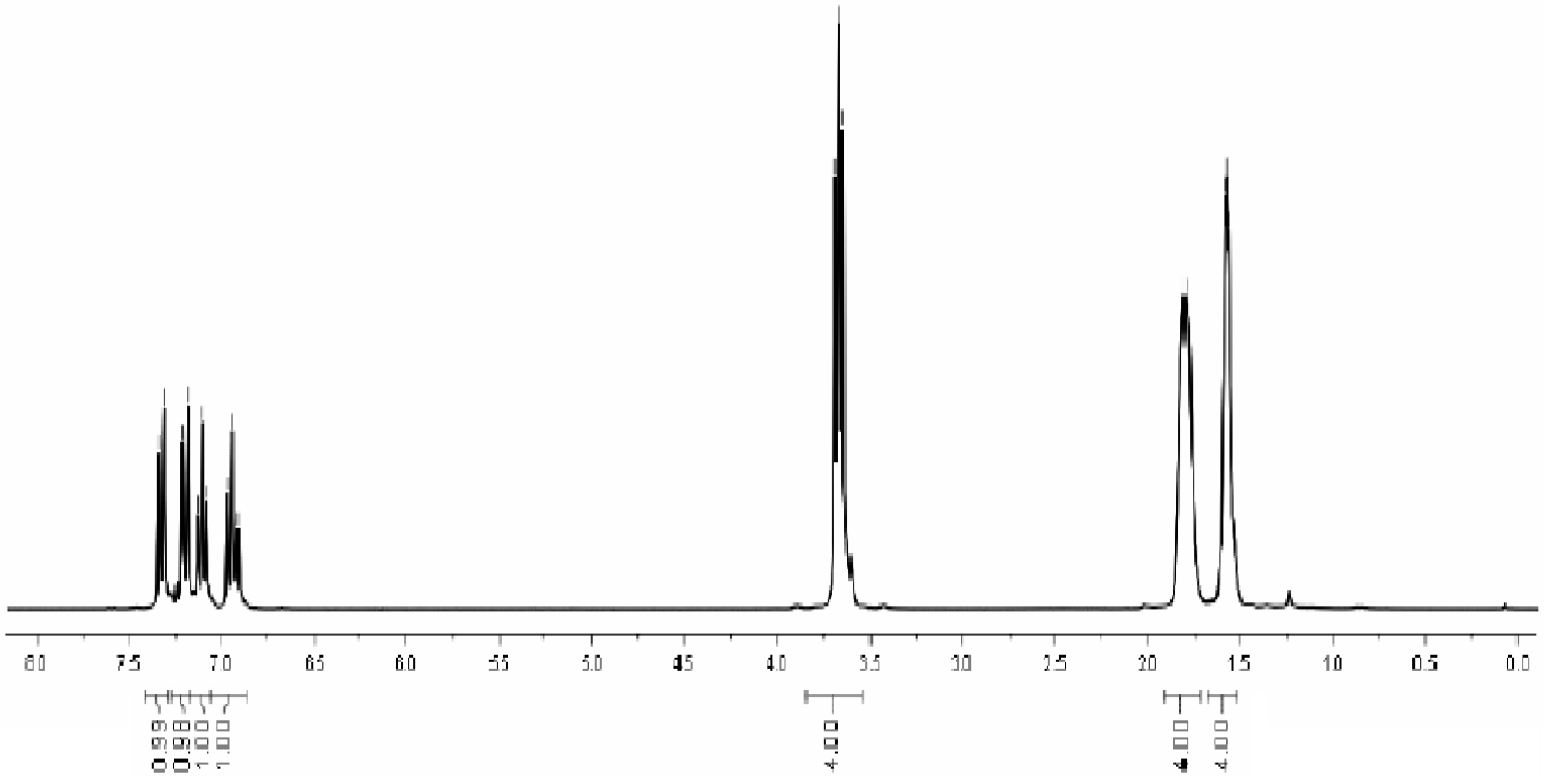

BRUKER
AVANCE II 400 NMR
Spectrometer
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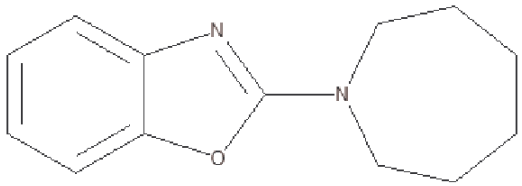
Panjab University
Chandigarh

Current Data Parameters
NAME AUG30-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130830
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2i

BRUKER
AVANCE II 400 NMR
Spectrometer
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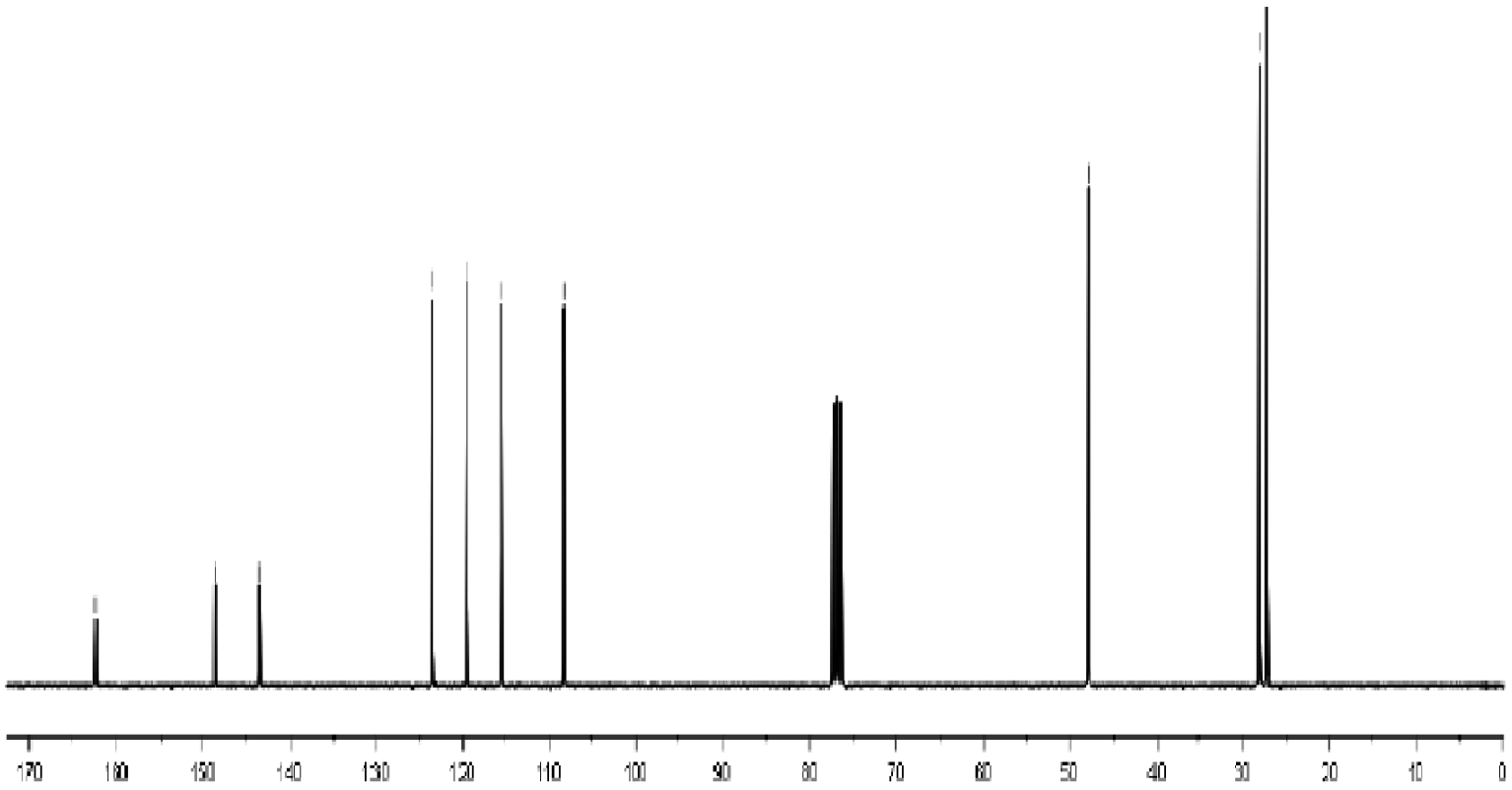
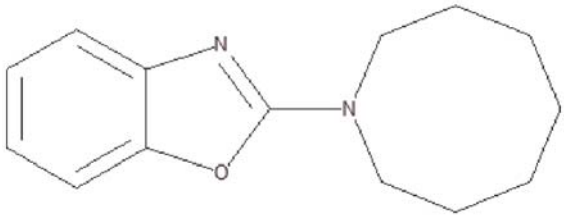
Panjab University
Chandigarh

Current Data Parameters
NAME AUG30-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130830
Time 10.15
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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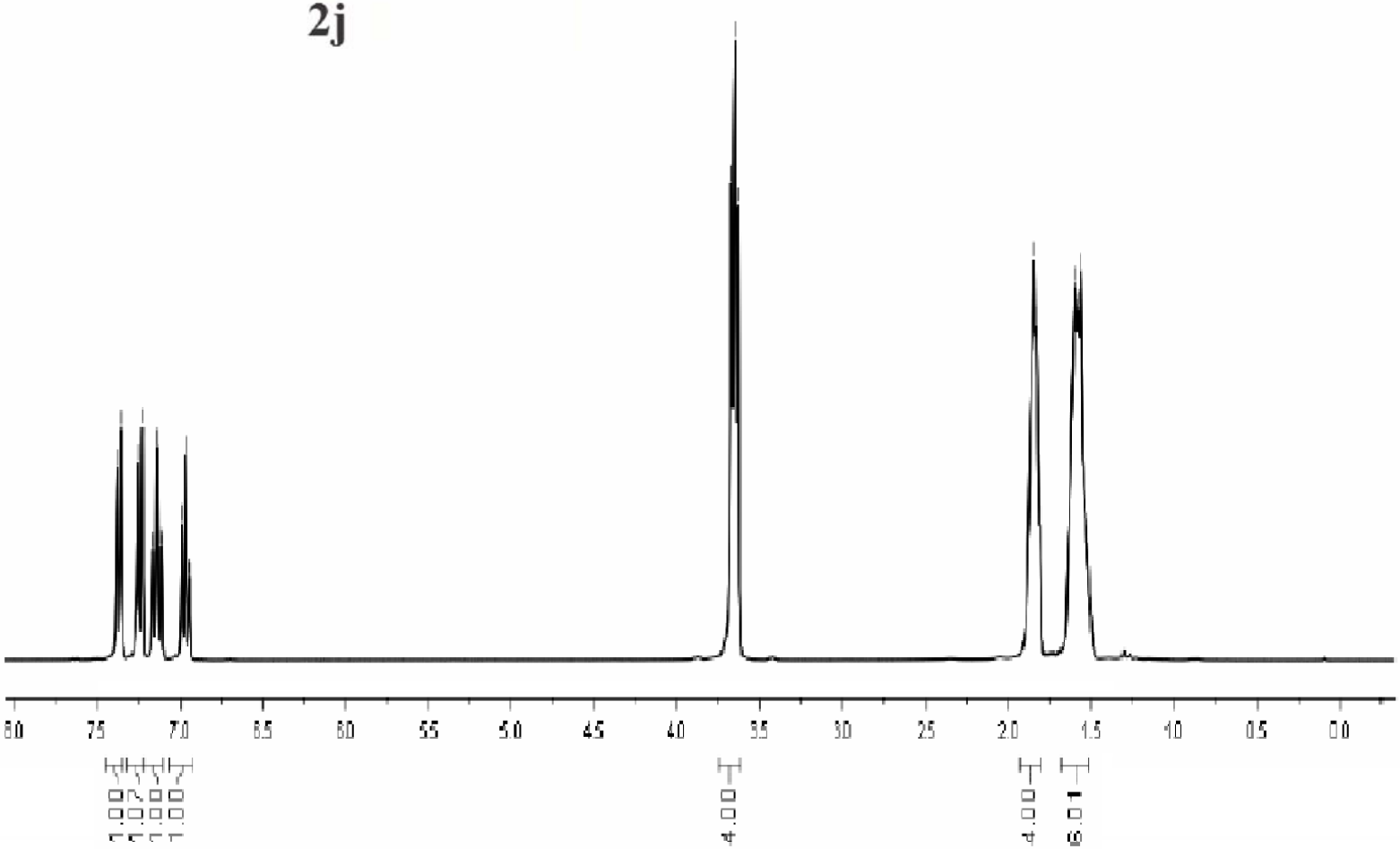

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AVANCE II 400 NMR
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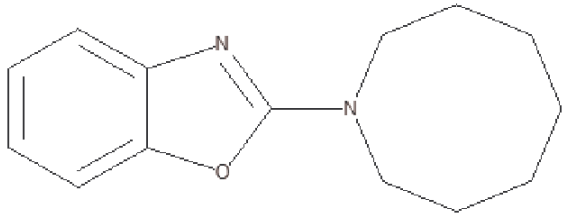
Current Data Parameters
NAME SEP3-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130903
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2j

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AVANCE II 400 NMR
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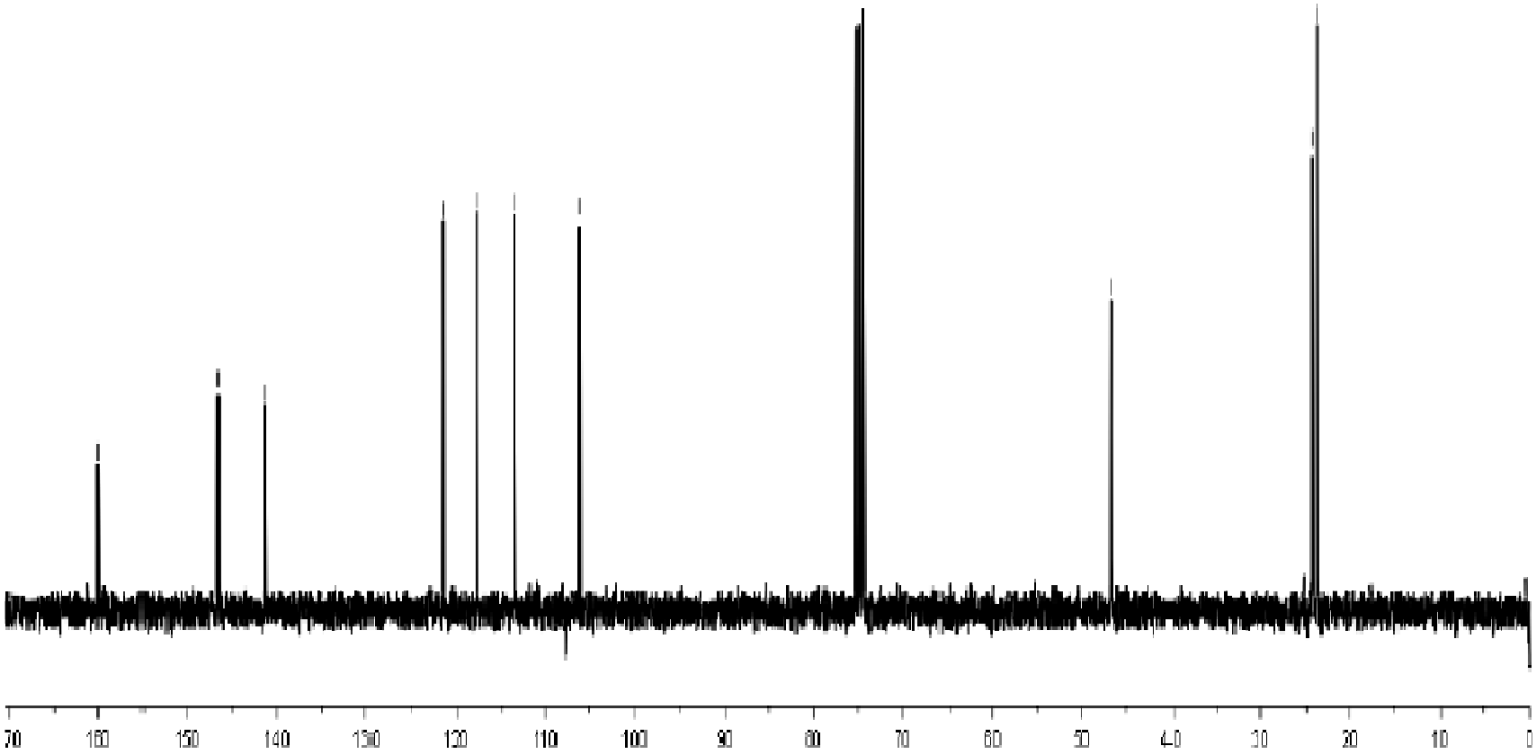
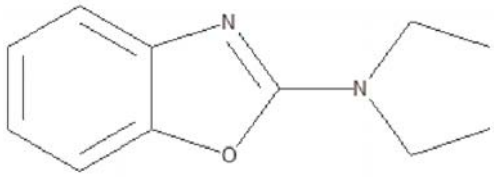
Current Data Parameters
NAME SEP3-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130903
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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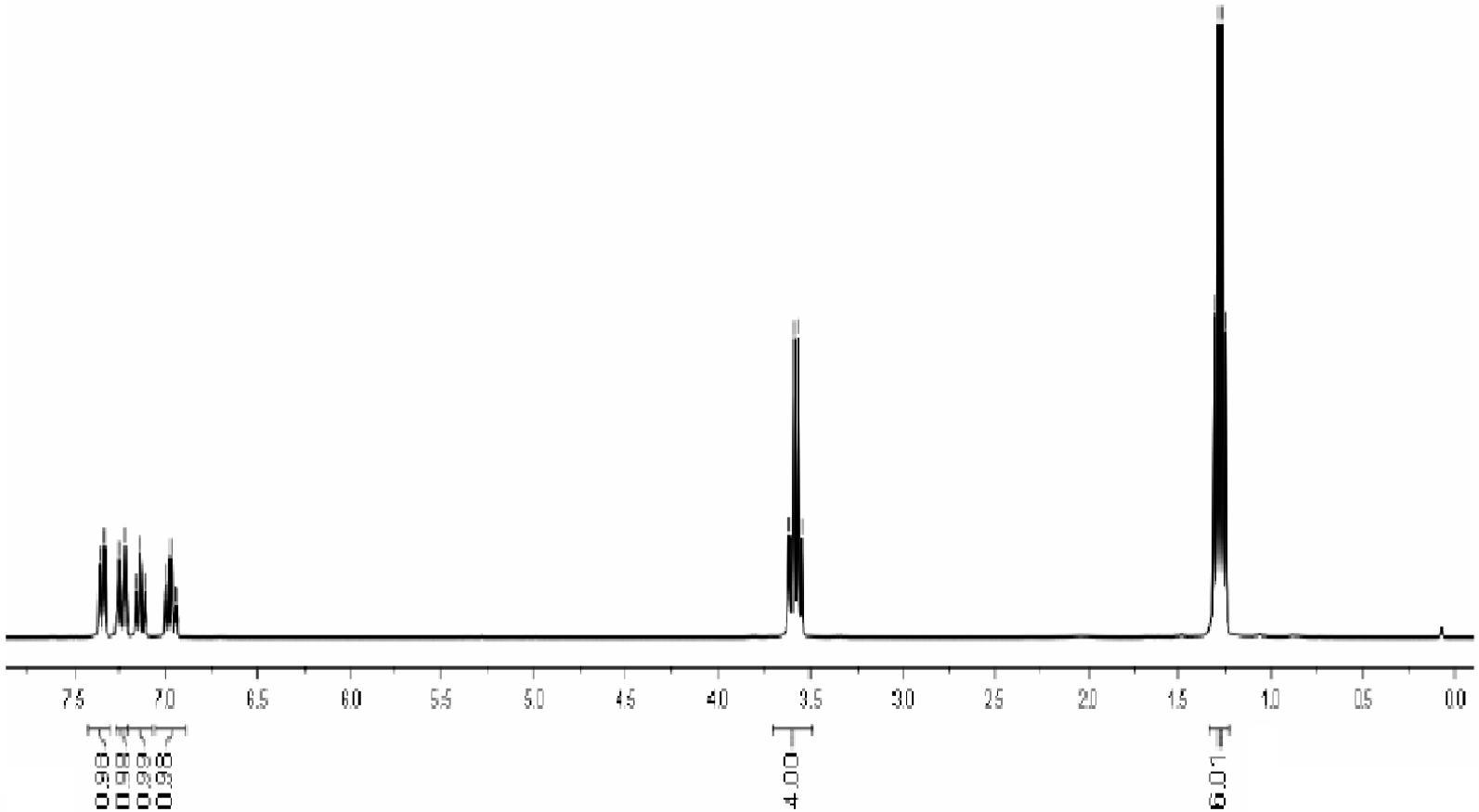

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AVANCE II 400 NMR
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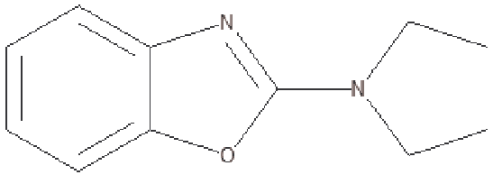
Current Data Parameters
NAME SEP19-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130919
Time 11.30
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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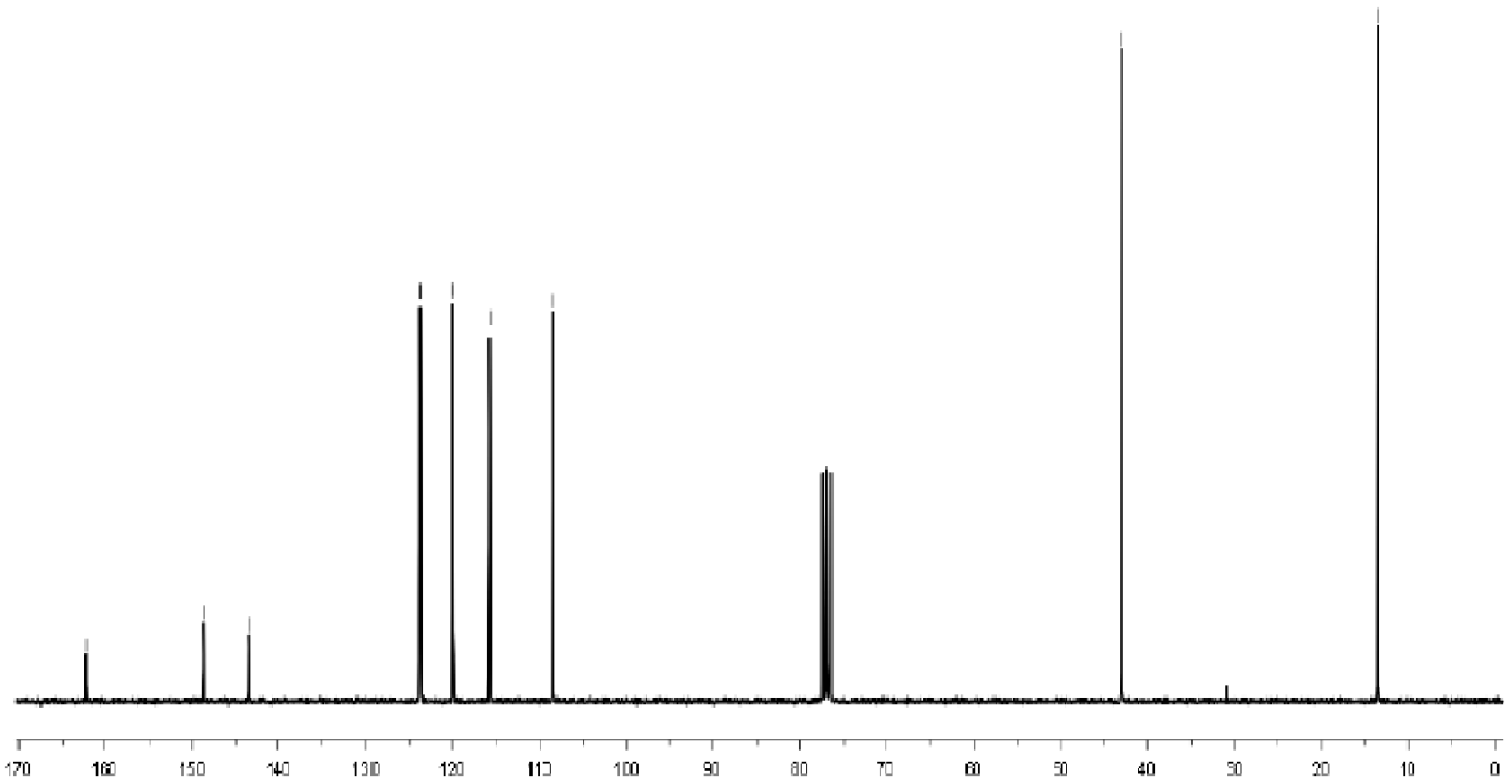

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AVANCE II 400 NMR
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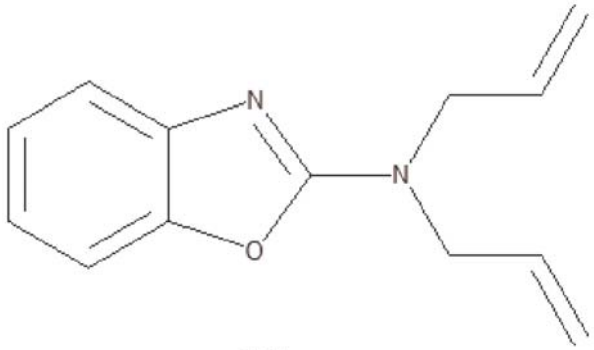
Current Data Parameters
NAME SEP19-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130919
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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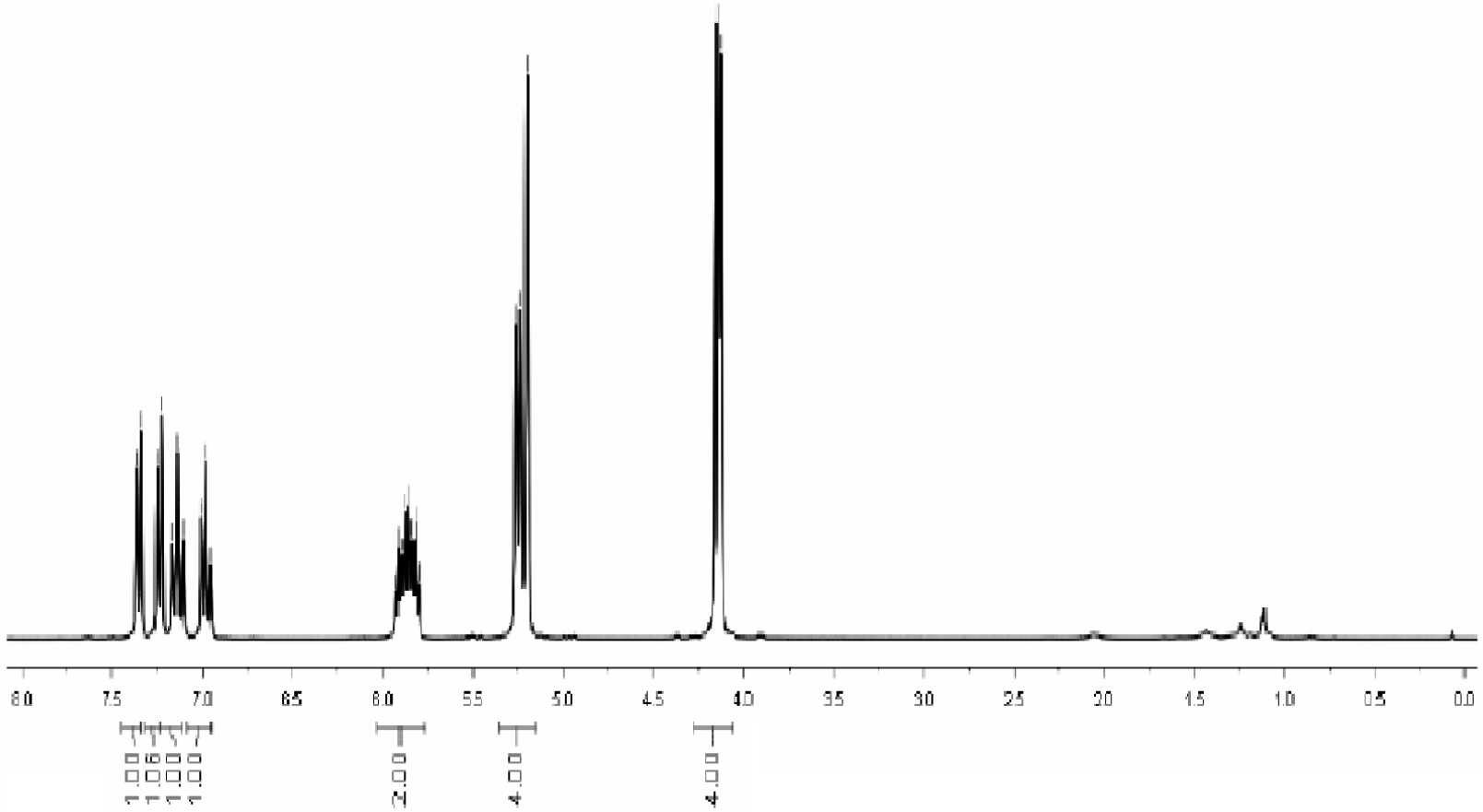

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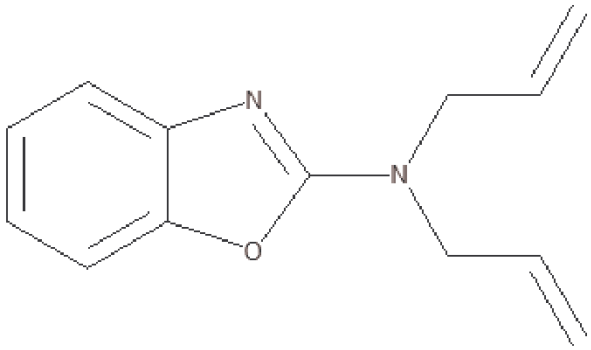
Current Data Parameters
NAME SEP29-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130929
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00



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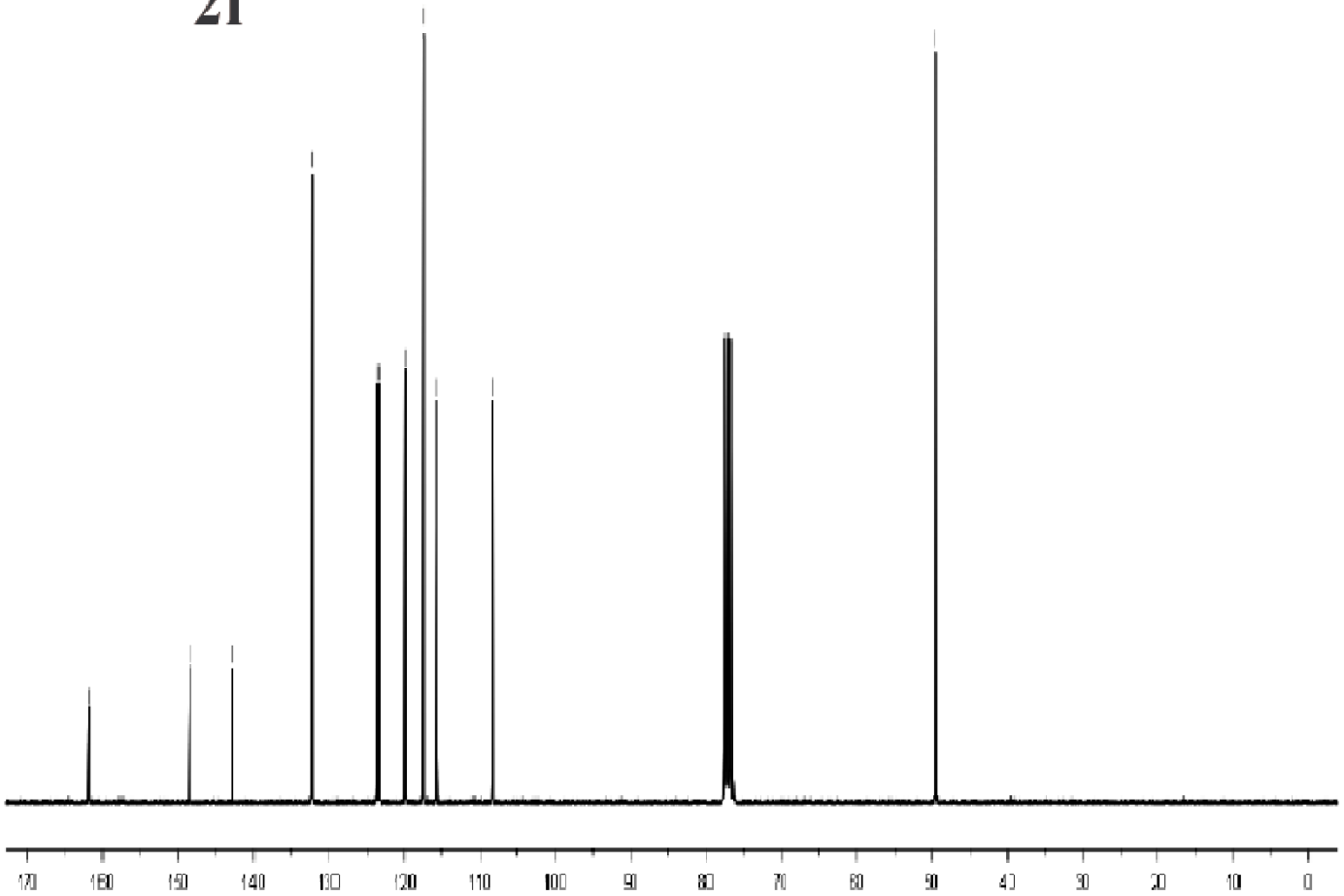
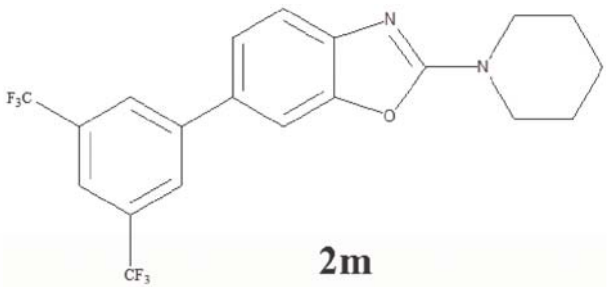


BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME SEP29-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130929
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
========= CHANNEL f1 =========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
========= CHANNEL f2 =========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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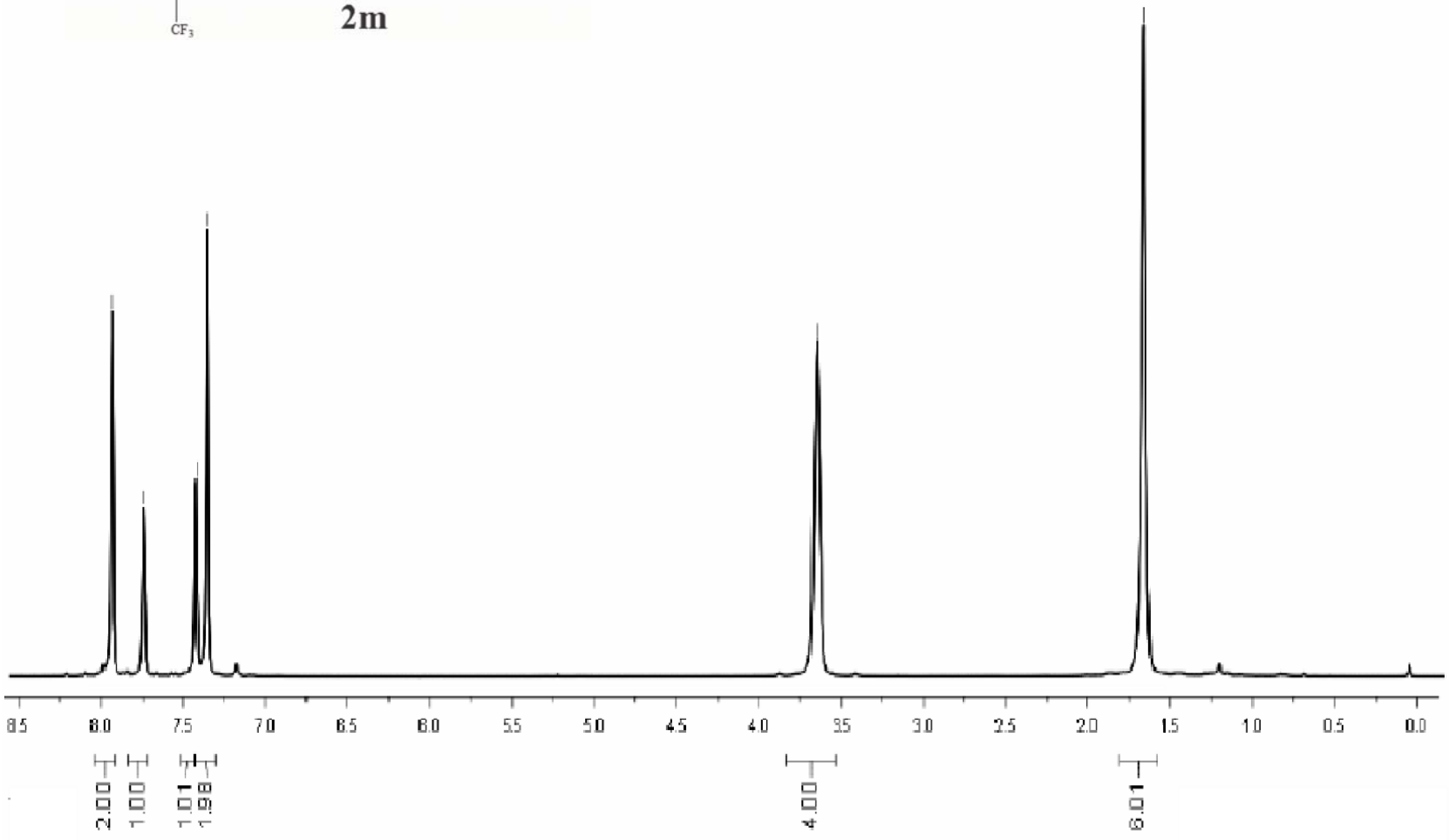

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AVANCE II 400 NMR
Spectrometer
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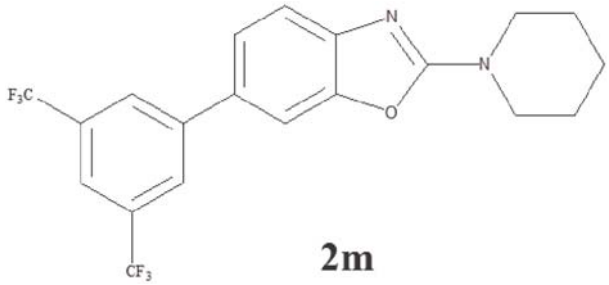
Current Data Parameters
NAME OCT10-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131010
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2m

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
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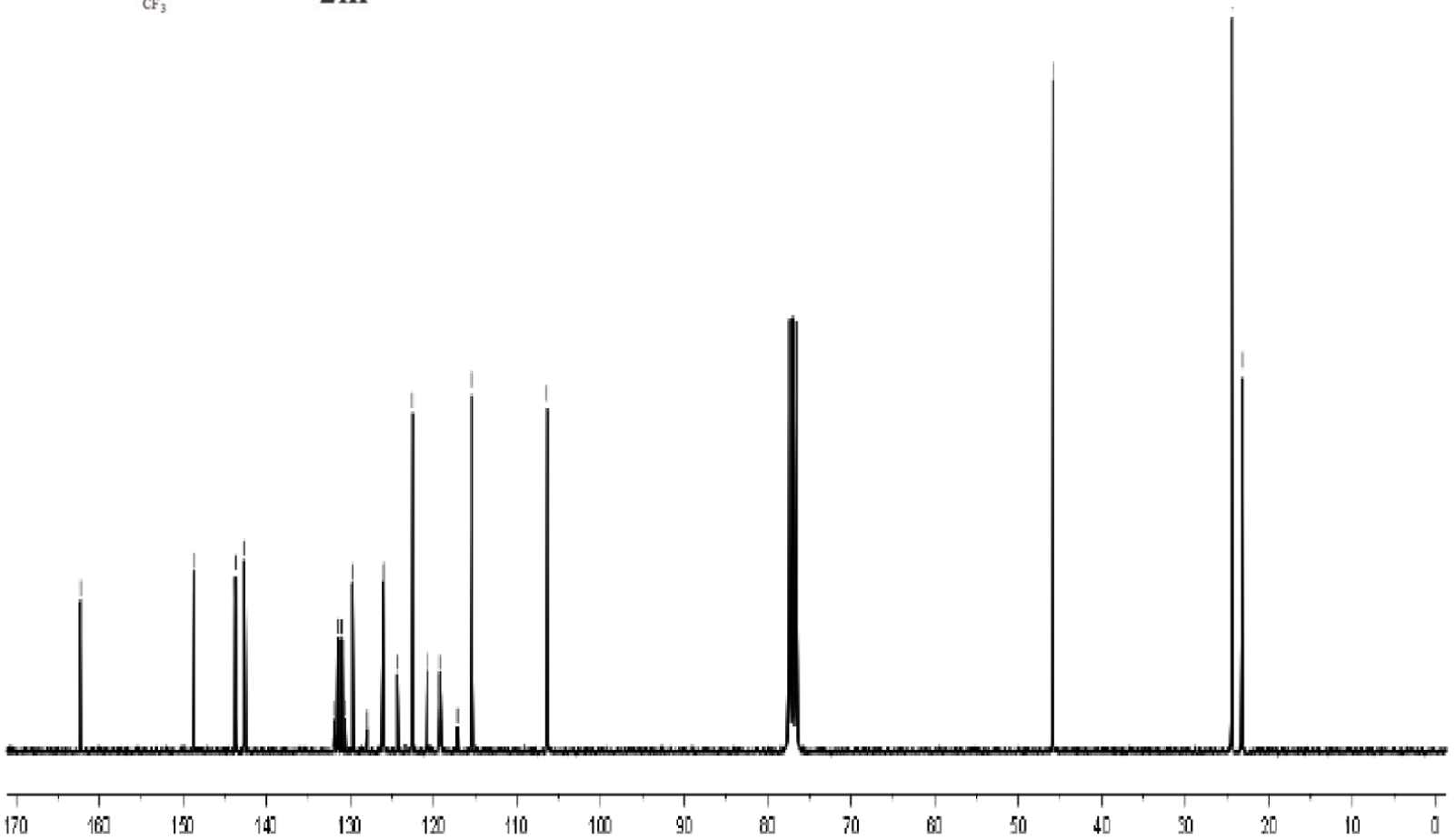
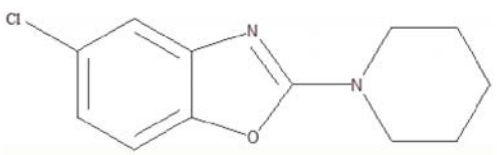
Chandigarh

Current Data Parameters
NAME OCT10-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131010
Time 11.15
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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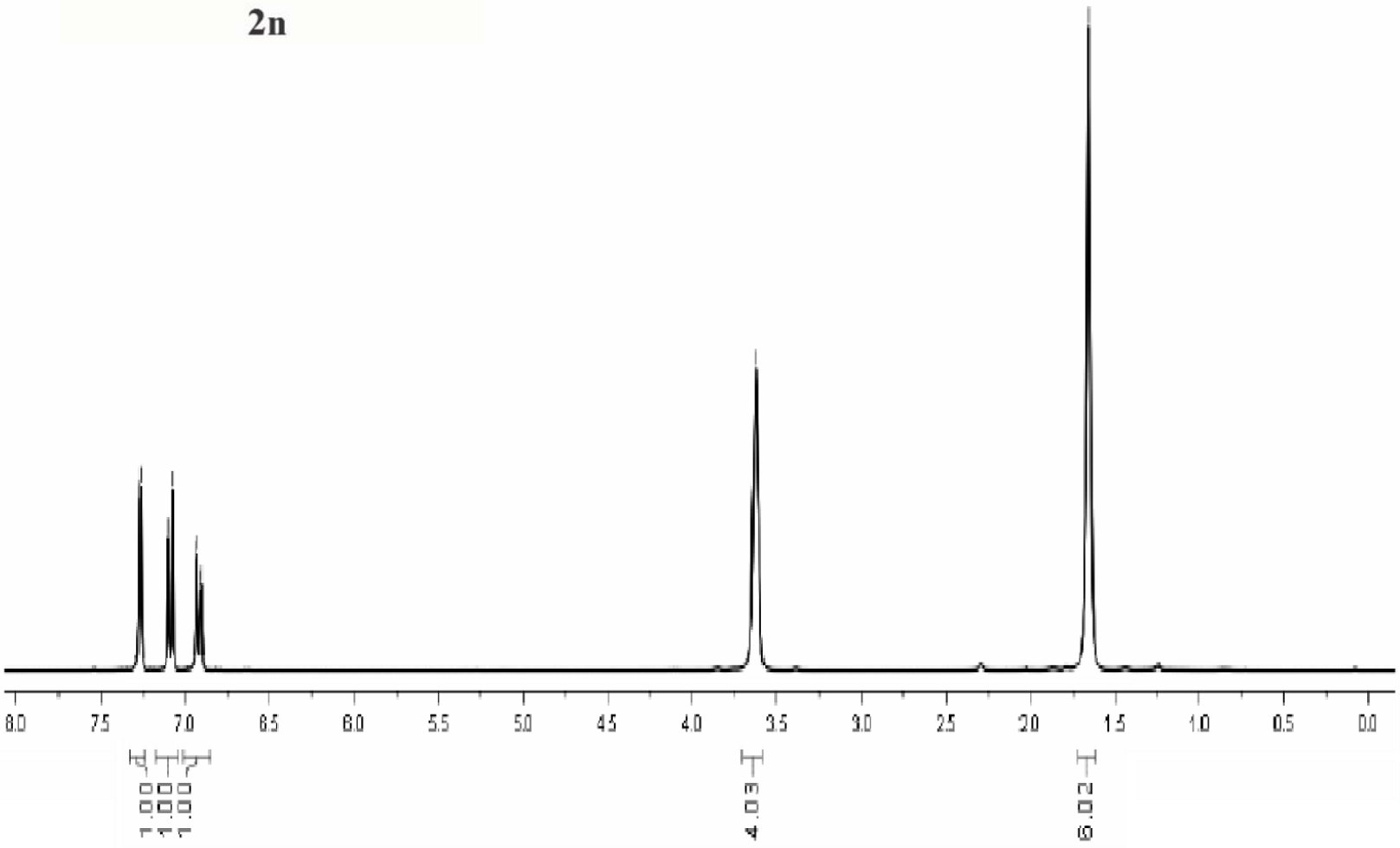

BRUKER
AVANCE II 400 NMR
Spectrometer
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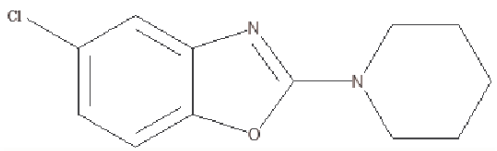
Chandigarh

Current Data Parameters
NAME OCT24-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131024
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0

PC 1.00



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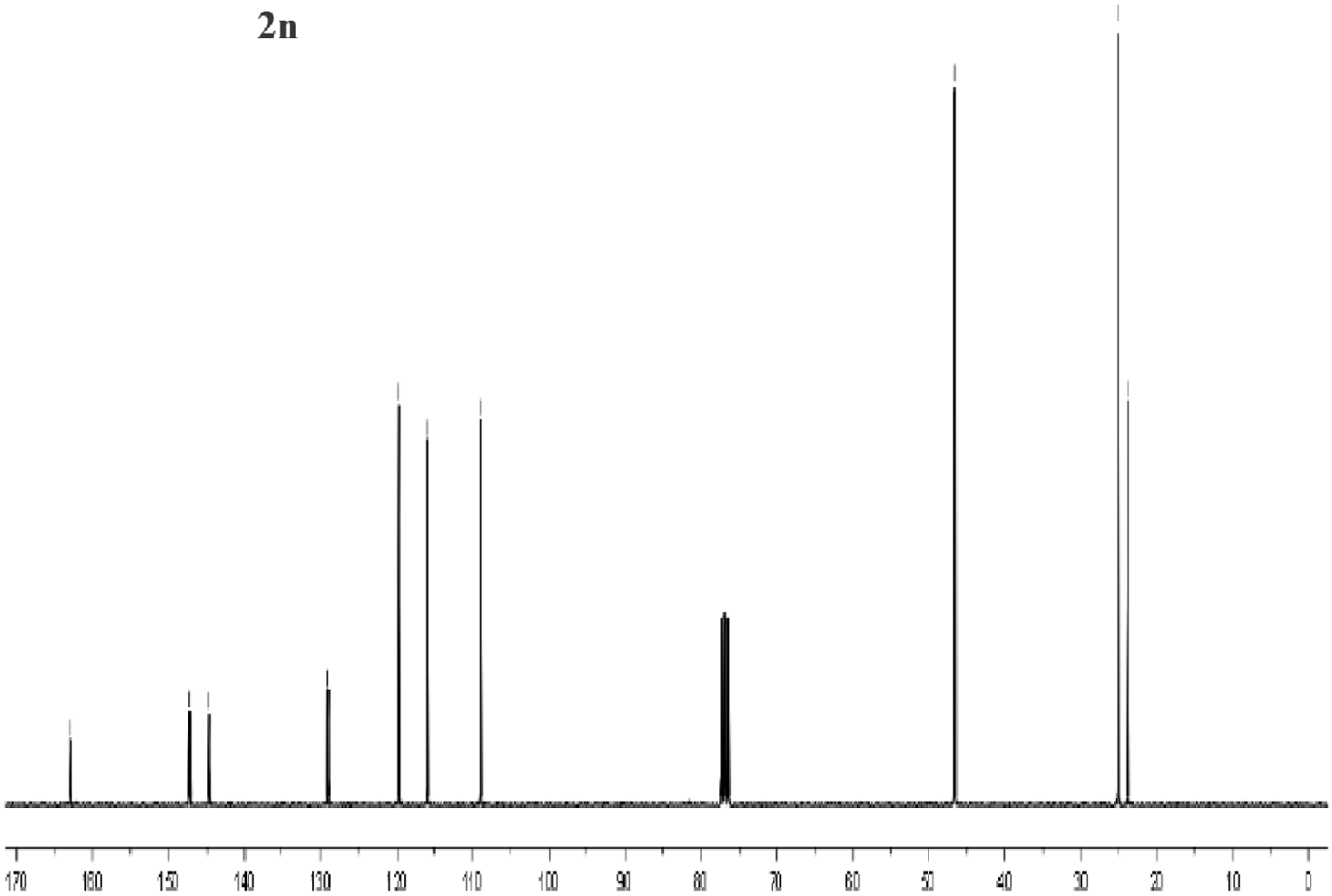

BRUKER
AVANCE II 400 NMR
Spectrometer
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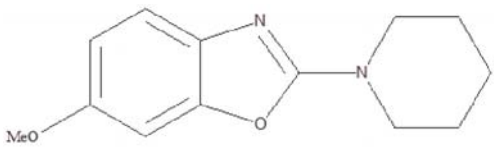
Chandigarh

Current Data Parameters
NAME OCT24-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131024
Time 10.45
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



2o

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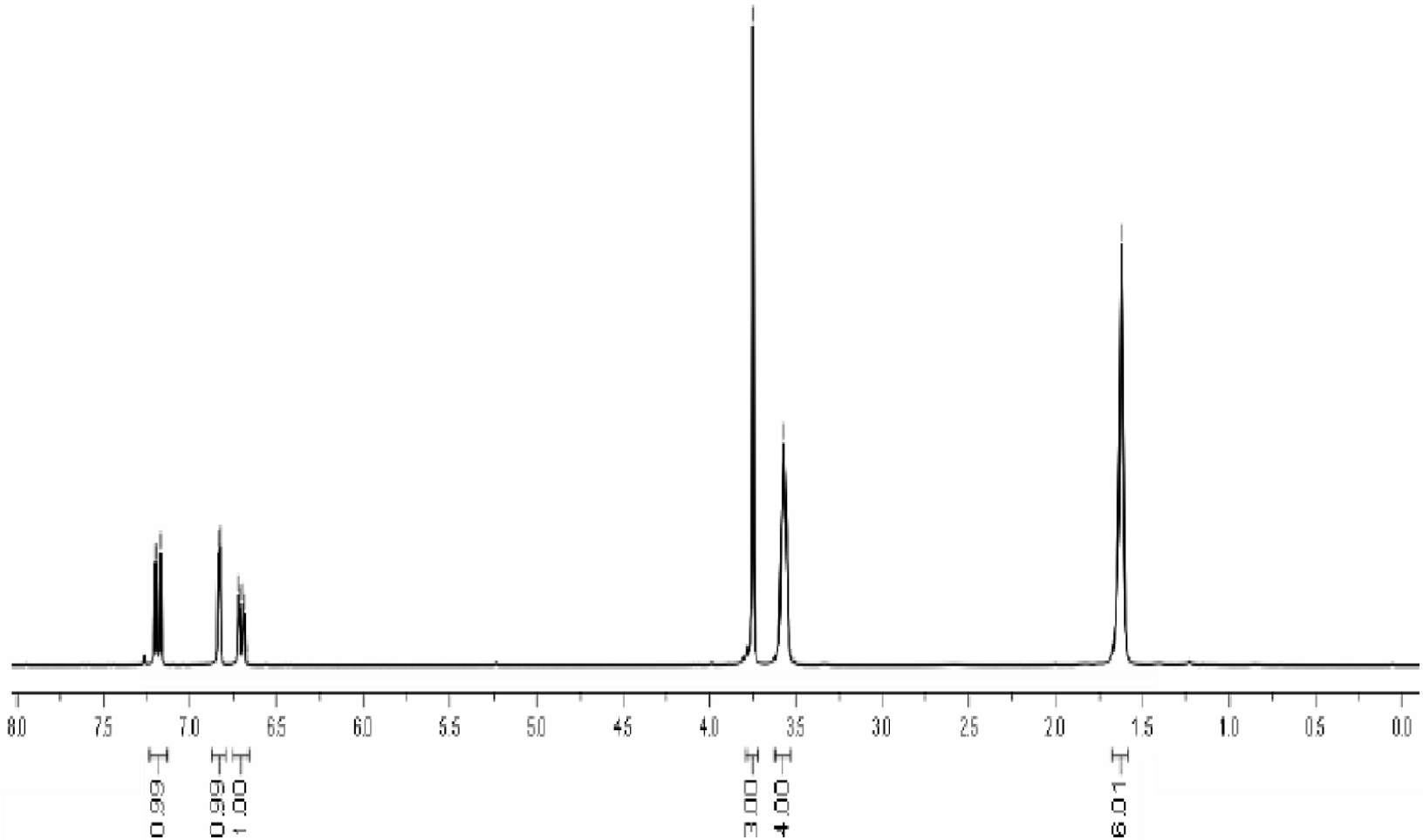
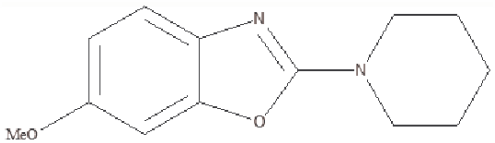
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME OCT26-2013
EXPNO 420
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131026
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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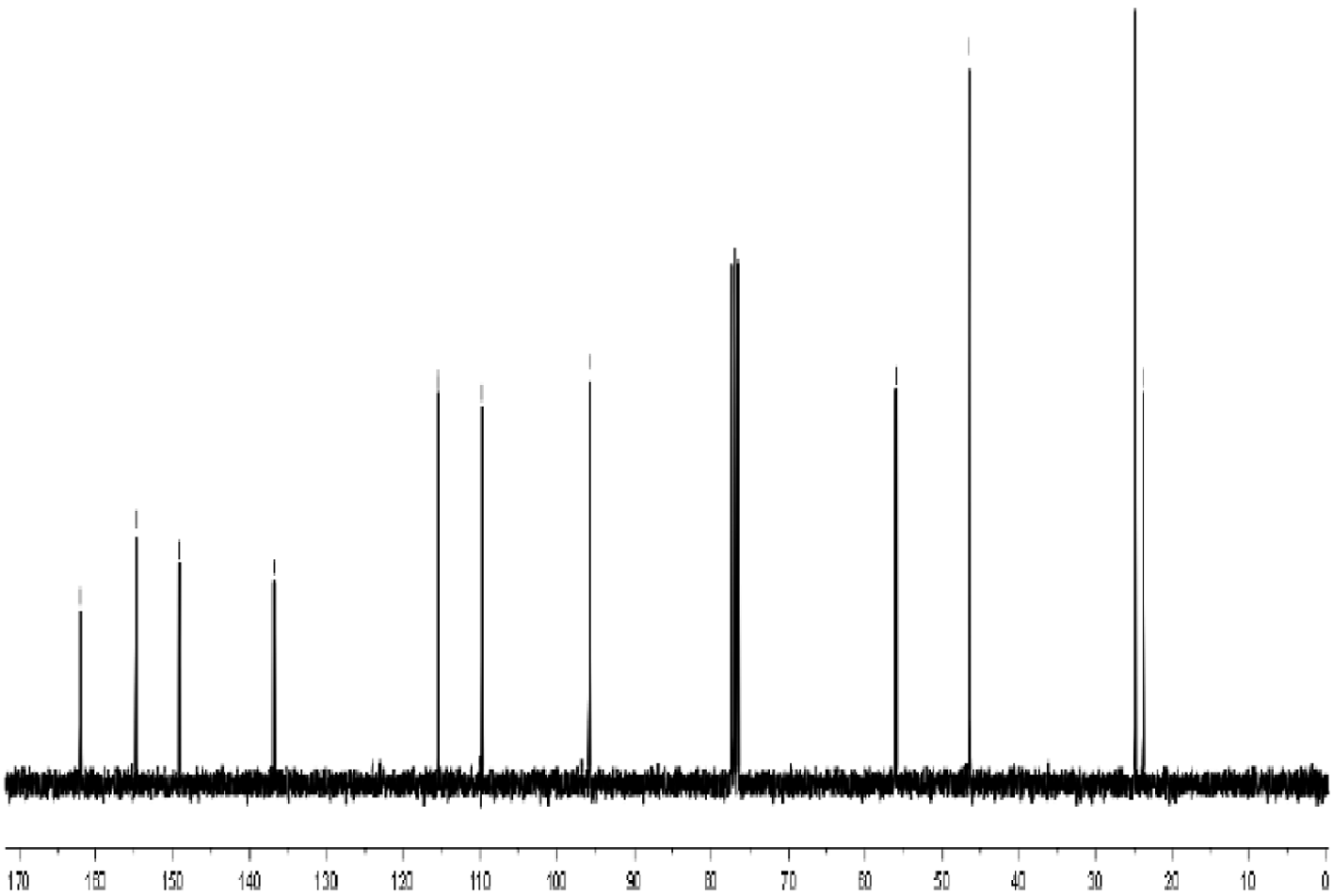

BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME OCT26-2013
EXPNO 421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20131026
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BBPULPROG
zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 36
DW 16.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40