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Supporting Information

A Practical and General *Ipso* Iodination of Arylboronic Acids Using *N*–Iodomorpholinium Iodide (NIMI) as a Novel Iodinating Agent: Mild and Regioselective Synthesis of Aryliodides

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Contents:

1 General consideration

All the solvents were redistilled before used. Analytical TLCs were performed on Merck silica gel 60F254 plates. The boronic acids were purchased from Johnson Matthey Chem. Ltd. and other chemicals were purchased from Sigma Aldrich Chem. Ltd. The ^{1}H and ^{13}C NMR spectra (in $CDCl_3$) were recorded on Agilent 400 or Bruker Avance II 400 MHz spectrometer. The Chemical shift values are on a δ scale and TMS was used as a internal standard. The ^{19}F NMR spectra were recorded in DMSO-d6 on Bruker Avance II 400 MHz spectrometer using $CFCl_3$ as internal standard. Abbreviations used are: s (singlet), d (doublet), t (triplet), dd (double doublet), dt (doublet triplet), m (multiplet). The high-resolution mass spectra analysis was performed on Micromass Q-Tof (ESI-HRMS) and GCMS was recorded on Shimadzu gas chromatograph.

2 Optimization of reaction conditions:

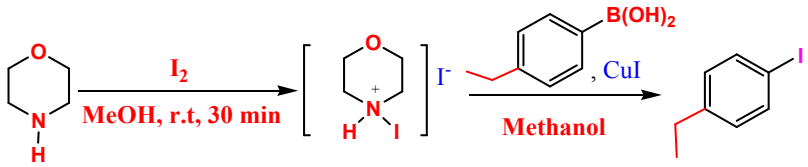


Table-1. Optimising the reaction conditions for the ipso iodination of 4-ethylphenyl boronic acid[a]

Entry	Morpholine (equiv.)	I_2 (equiv.)	CuI (mol %)	Temp. (^{0}C)	Time (h)	Yield (%)[b]
1	None	1.2	None	rt	24	0
2	None	1.2	None	65	10	Trace
3	1.0	1.2	none	rt	24	32
4	1.0	1.2	5	rt	24	40
5	1.0	1.2	5	65	10	68
6	1.0	1.0	10	65	4	39
7	1.0	2.4	10	40	24	68
8	1.0	2.4	5	65	4	50
9	2.0	2.4	None	rt	24	67
10	2.0	2.4	5	rt	24	75
11	2.0	2.4	5	65	4	74
12	2.0	2.4	5	rt	24	62[c]
13	2.0	2.4	100	rt	1	65
14	0.2	1.0	None	40	24	12
15	0.2	2.4	None	40	24	28
16	0.2	2.4	5	40	24	30
17	None	2.4	5	40	24	29
18	None	None	100	rt	5	nd[d]
19	None	None	5	rt	24	0[e]

[a] Reaction conditions: 0.2 mmol of 4-ethylphenyl boronic acid in 1.5 ml of methanol for the time indicated in table. [b] Isolate yields by column chromatography. [c] Under N2 atmosphere. [d] The boronic acid was completely consumed but no iodoproduct was detected. [e] 2.0 equiv. of KI or NaI was used as iodinating agent.

Table-2. Effect of copper salts on the *ipso* iodination of 4-ethylphenylboronic acid[a]

Entry	Copper Salt	Yield (%)[b]
1	None	67
2	CuI	75
3	CuCl	71
4	CuCN	72
5	$Cu(OAc)_2$	65
6	$CuSO_4.5H_2O$	55
7	Cu_2O	71

[a] Reaction conditions: 0.2 mmol of 4-ethylphenyl boronic acid, 0.4 mmol of morpholine, 0.48 mmol of I2 in the presence of 5 mol% of Copper salt in 1.5 ml of methanol at room temperature for 24h. [b] Isolated yield by column chromatography.

Table 3. Effect of solvent on *ipso* iodination of 4-ethylphenyl boronic acid[a]

Entry	Solvent	Yield (%)[b]
1	MeOH	75
2	DCM	72
3	MeCN	58
4	DMF	36
5	Acetone	5
6	THF	---[C]

[a] Reaction conditions: 0.2 mmol of 4-ethylphenyl boronic acid, 0.4 mmol of morpholine, 0.48 mmol of I2 in the presence of 5 mol% of CuI in 1.5 ml of methanol at room temperature for 24h. [b] Isolated yields by column chromatography. [c] A complex reaction mixture was formed

Table 4. Optimising the reaction conditions for the *ipso* iodination of 3-nitrophenyl boronic acid[a]

Entry	Morpholine (equiv.)	I2 (equiv.)	CuI (mol %)	Temp. (^{0}C)	Time (h)	Yield (%)[b]
1	0.2	2.4	5	rt	24	21
2	0.2	2.4	5	40	24	26
3	2.0	2.4	None	rt	24	20
4	2.0	2.4	None	40	24	41
5	1.0	2.4	5.0	40	24	63
6	2.0	2.0	5.0	65	4	92
7	2.0	2.4	5.0	rt	24	94
8	2.0	2.4	5.0	40	24	>99[c]
9	None	2.4	5.0	40	24	15.

[a] Reaction conditions: 0.2 mmol of 3-nitrophenyl boronic acid in 1.5 ml of methanol for the time indicated in table. [b] Isolate yields by column chromatography. [c] reaction time was not optimised and reaction was continued for 24 h

Table-5. Effect of different solvents and copper salts on *ipso* iodination of 3-nitrophenylboronic acid[a]

Entry	Solvent	Copper Salt (CuX)	Yield (%)[b]
1	MeOH	CuI	>99
2	MeOH	CuCl	99
3	MeOH	Cu_2O	80
4	MeOH	$CuSO_4.H_2O$	94
5	MeOH	$Cu(OAc)_2$	89
6	DCM	CuI	10
7	MeCN	CuI	59
8	DMF	CuI	Trace
9	Acetone	CuI	6

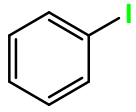
[a] Reaction conditions: 0.2 mmol of 3-nitrolphenyl boronic acid, 0.4 mmol of morpholine, 0.48 mmol of I2 in the presence of 5 mol% of CuX in 1.5 ml of solvent at 40^{0}C for 24h. [b] Isolated yields by column chromatography

3 Experimental procedure.

To a 10 ml round bottomed flask charged with morpholine (0.4 mmol, 2 equiv.) and I_2 (0.48 mmol, 2.4 equiv.) was added methanol (1.5 ml) and the reaction mixture was stirred for 30 minutes at room temperature. Then the appropriate arylboronic acid (0.2 mmol) and CuI (2 mg, 0.01 mmol) was added to it and the mixture was stirred vigorously at room temperature for 24 h. After completion of the reaction (monitored by TLC), the reaction mixture was quenched with 10 % sodium thiosulphate solution (to remove excess of iodine) and extracted with ethyl acetate (3* 10 ml) and the combined organic extract was washed with water and brine. The evaporation of solvent under vaccu after drying over anhy. Na_2SO_4 followed by column chromatography (petroleum ether (100 %) or petroleum ether: ethyl acetate, 9:1) gave the analytically pure product. (Note: direct column chromatography of crude product adsorbed on silica followed by washing the effluent with Na_2SO_4 solution, drying and evaporation of residue gave exactly similar results).

4 Analytical Data

4.1 Iodobenzene (2a):

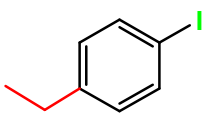


Colourless liquid, yield 39%

^{1}HNMR: δ 7.26 (s, 5H), ^{13}C NMR ($CDCl_3$, 400 MHz): δ 94.5, 127.5, 130.3, 137.5

EI-MS $[M]^+ = 204$

4.2 4-Ethyliodobenzene (2b):

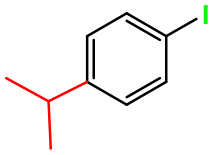


Yellow liquid, 75%

^{1}HNMR: δ 1.18 (t, *J*=7.6 Hz, 3H), 2.57 (q, *J*= 7.6 Hz, 2H), 6.93 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.57 (dd, *J*=8.4, 2 Hz, 2H), ^{13}C NMR ($CDCl_3$, 400 MHz): δ 15.1, 28.4, 90.5, 130.0, 137.3, 143.8

EI-MS $[M]^+$ = 232

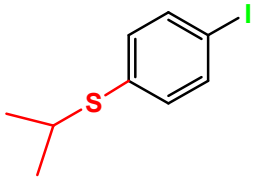
4.3 4-Isopropyl iodobenzene (2c):



Yellow liquid, 90%

^{1}HNMR: ($CDCl_3$, 400 MHz) δ 1.23 (d, *J*=6.8 Hz, 6H), 2.68 (septet, 1H), 6.98 (dd, *J*= 8, 1.6 Hz, 2H), 7.61(dd, *J*= 8.4, 2 Hz, 2H); EI-MS $[M]^+$ = 246

4.4 Isopropyl-4-iodophenyl sulfide (2e):



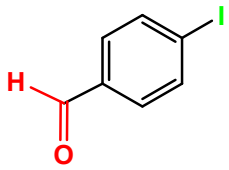
Yellow liquid, Yield 95%

IR (ATR, cm^{-1}) 720 (m), 801 (s), 1001 (s), 1050 (m), 1090 (s), 1154 (m), 1240 (m), 1365 (m), 1469 (s), 1737 (w), 2923 (m), 2959 (m)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 1.27 (d, 6H), 3.35 (septet, 1H), 7.10 (dd, J= 8.4, 1.6 Hz 2H), 7.58 (dd, *J* = 8.4, 2 Hz, 2H). ^{13} C NMR ($CDCl_3$, 400 MHz): δ 23.00, 36.12, 91.71, 133.25, 135.70,

137.76; GC-MS RT= 11.01, [m/e] = 278; HRMS; Calcd. for: $C_9H_{11}IS$, 277.9626; Found 277.9626

4.5 4-iodobenzaldehyde (2g):



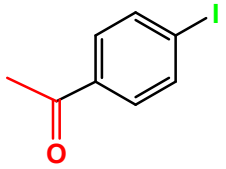
While solid, yield 85 %

IR (ATR, cm^{-1}) 671 (w), 800 (s), 825 (m), 1003 (m), 1048(m), 1158 (m), 1200 (m), 1271 (w), 1376 (w), 1579 (w), 1681 (m), 2822 (w), 2920 (w)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 7.58 (d, *J* = 8 Hz, 2H), 7.90 (d, *J* = 8 Hz, 2H) 9.96 (s, 1H) , ^{13}C NMR ($CDCl_3$, 400 MHz): δ 102.8, 130.8, 131.0, 135.5, 137.7, 138.4, 191.4

HRMS; Calcd. for: C_7H_5IO 231.9385; Found: 231.9385

4.6 4-Iodoacetophenone (2h):

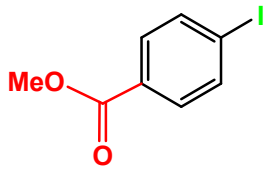


Light orange solid, Yield 53 %

IR (ATR, cm^{-1}) 602 (m), 740 (m), 816 (s), 955 (m), 1003 (m), 1178 (m), 1259 (m), 1355 (m), 1388 (m), 1579 (m), 1670 (m)

^{1}HNMR: ($CDCl_3$, 400 MHz) δ 2.57 (s, 3H), 7.65 (dt, *J*= 4.0, 1.6 Hz, 2H), 7.81 (dt, *J* = 4.0, 2.0 Hz, 2H). ^{13}C NMR ($CDCl_3$, 400 MHz): δ 26.19, 101.15, 129.73, 136.29, 137.90, 197.38

4.7 4-Carbomethoxyiodbenzene (2i):



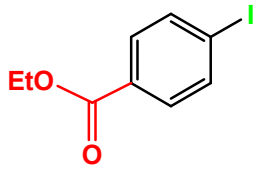
White solid, Yield 82%

IR (ATR, cm^{-1}) 683 (m), 752 (s), 824 (m), 843 (m), 1004 (m), 1105(m), 1177 (m), 1270 (m), 1390 (m), 1434 (m), 1582 (m), 1707 (m)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 3.09 (s, 3H), 7.71 (dt, *J*= 6.8, 2 Hz, 2H), 7.76 (dt, *J* = 6.4, 1.6 Hz, 2H), ^{13}CNMR ($CDCl_3$, 400 MHz): δ 52.30 100.76, 129.57, 131.02, 137.70 166.57

HRMS; Calcd. for: $C_8H_7IO_2$, 261.9491; Found: 261.9491

4.8 4-Carboethoxyiodobezene (2j):

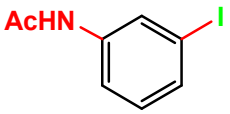


Yellow liquid, Yield 92 %

IR (ATR, cm^{-1}) 626 (m), 681 (s), 749 (s), 844 (s), 1005 (s), 1098 (s), 1174 (s), 1263 (s), 1366 (m), 1392 (s), 1476 (m), 1585 (s), 1713 (s), 2980 (w)

^{1}H NMR (400 M Hz, $CDCl_3$): δ 1.37 (t, *J* =7.2 Hz, 3H), 4.34 (q, *J* =7.2 Hz, 2H), 7.73 (dt, *J*= 3.6, 2 Hz, 2H), 7.78 (dt, *J* = 3.6, 1.8 Hz, 2H). ^{13}C NMR (400 M Hz, $CDCl_3$): δ 14.29, 61.24, 101.56, 129.98, 131.01, 137.67, 166.13; HRMS; Calcd. for: $C_9H_9IO_2$, 275.9647; Found: 275.9647

4.9 *N*-(3-iodophenyl)acetamide (2k):



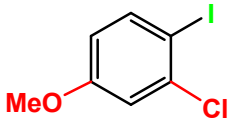
While solid, Yield 85 %

IR (ATR, cm^{-1}) 605 (s), 649 (m), 674 (s), 750 (s), 774 (s), 868 (m), 992 (m), 1166 (m), 1281 (s), 1366 (s), 1409 (s), 1467 (s), 1536 (s), 1585 (s), 1666 (s), 3247 (w), 3289 (w)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 2.17 (s, 3H), 7.01 (t, *J* =8 Hz, 1H), 7.42 (q, *J* =8 Hz, 2H), 7.90 (s, 1H); ^{13}C NMR (400 M Hz, $CDCl_3$): δ 24.3, 94.1, 119.1, 128.5, 130.4, 133.3, 139.0, 168.6

HRMS; Calcd. for: C_8H_8NOINa, 283.9548; Found 283.9547

4.10 2-Chloro-1-iodo-4-methoxybenzene (2l):

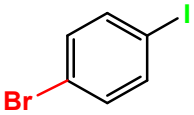


Faint Yellow oil, Yield 93 %

IR (ATR, cm^{-1}) 588 (s), 679 (s), 796 (s), 837 (s), 856 (s), 1003 (s), 1032 (s), 1097 (s), 1181 (m), 1222 (s), 1260 (s), 1282 (s), 1433 (s), 1463 (s), 1580 (s), 2835 (w), 2935 (w)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 3.77 (s, 3H), 6.54 (dd, *J*= 2.93 Hz, 1H), 7.01 (d, *J*= 2.88 Hz, 1H), 7.66 (d, *J*= 8.8 Hz, 1H), ^{13}C NMR (400 M Hz, $CDCl_3$): δ 55.6, 86.4, 114.8, 115.1, 138.9, 140.2, 160.5

4.11 1-Bromo-4-iodobenzene (2m):

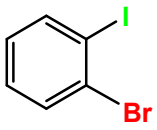


Brown Solid, Yield 90%

IR (ATR, cm^{-1}) 797 (s), 995 (s), 1058 (s), 1372 (m), 1463 (m), 1882 (w), 2850 (w), 2922 (w)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 7.21 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J*= 8.4 Hz, 2H); ^{13}C NMR (400 M Hz, $CDCl_3$): δ 92.0 122.1, 133.4, 139.0

4.12 1-Bromo-2-iodobenzene (2n):

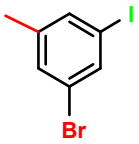


Yellow liquid, Yield 78%

IR (ATR, cm^{-1}) 632 (s), 685 (s), 739 (s), 999 (s), 1030 (m), 1092 (m), 1252 (m), 1421(m), 1437(m), 1560 (m), 2923 (w)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 6.98 (t, *J* = 7.6 Hz, 1H), 7.21 (q, *J* = 7.6 Hz, 1H), 7.62 (d, *J*= 7.6 Hz, 1H), 7.81 (d, J = 4 Hz, 1H); ^{13}C NMR (400 M Hz, $CDCl_3$): δ 101.2, 128.4, 129.4, 129.7, 132.7, 140.3; EI-MS $[M]^+$ = 284

4.13 1-Bromo-3-iodo-5-methylbenzene (2o):

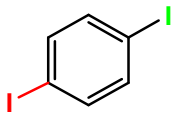


Light Yellow liquid, Yield 96 %

IR (ATR, cm^{-1}) 666 (s), 723 (s), 840 (s), 1103 (s), 1208 (m), 1422 (s), 1546 (s), 1578 (s), 1729 (w), 2852 (m), 2921 (m)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 2.27 (s, 3H), 7.28 (s, 1H), 7.46 (s, 1H), 7.65 (s, 1H), ^{13}C NMR (400 M Hz, $CDCl_3$): δ 20.3, 93.9, 122.2, 131.2, 136.2, 136.4, 141.5, HRMS; Calcd. for: C_7H_6BrI, 295.8698; Found 295.8698

4.14 1,4-Diiodobenzene (2p):

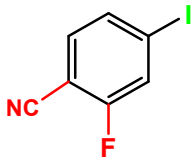


White solid, Yield 95%

IR (ATR, cm^{-1}) 794 (m), 990 (m), 1063 (m), 1368 (w), 1453 (w), 2850 (w), 2920(w)

^{1}H NMR (400 M Hz, $CDCl_3$): δ 7.40 (s, 4H), ^{13}C NMR (400 M Hz, $CDCl_3$): δ 93.36, 139.34

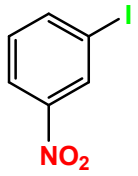
4.15 2-Fluoro-4-iodobenzonitrile (2q):



White solid, Yield 81 %

IR (ATR, cm^{-1}) 582 (s), 813 (s), 863 (s), 1219 (m), 1392 (m), 1556 (m), 1587 (m), 1733 (m), 2848 (m), 2919 (m), ^{1}HNMR ($CDCl_3$, 400 MHz): δ 7.31 (t, J = 7.6 Hz, 1H), 7.63 (d, J = 8 Hz, 2H), ^{13}C NMR ($CDCl_3$, 400 MHz): δ 100.4, 113.4, 126, 133.9, 134.3, 160.7,163.4, ^{19}F NMR (DMSO-d_6, 400 MHz) -106.92 (d, 1F)

4.16 1-Iodo-3-nitrobenzene (2r):



Yellow liquid, Yield 94 %

IR (ATR, cm^{-1}) 640 (s), 660 (s), 709 (s), 725 (s), 797 (s), 862 (s), 886 (m), 997 (m), 1054 (m), 1104 (m), 1271 (m), 1340 (s) 1460 (m), 1518 (s), 2855 (w) 2921 (w)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 7.26 (t, J = 8.4 Hz, 1H), 8.01 (tt, J = 1.6 Hz, 1H), 8.19-8.22 (m, 1 H), 8.57 (d, 1H); ^{13}C NMR ($CDCl_3$, 400 MHz): δ 93.48, 122.75, 130.70, 132.43, 143.46

HRMS; Calcd. for: $C_6H_4INO_2$, 248.9287; Found 248.9287

4.17 1-iodo-4-(methylsulfonyl)benzene (2s):

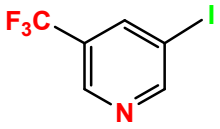
While solid, Yield 83 %

IR (ATR cm^{-1}) 709 (s), 821 (s), 963 (s), 1003 (m), 1074 (m), 1082 (m), 1141 (s), 1264 (m), 1304 (s), 1380 (m), 1462 (m), 1563 (s), 2918 (m), 3001 (m)

^{1}HNMR ($CDCl_3$, 400 MHz): δ 3.03 (s, 3H), 7.63 (dd, J = 8.4, 1.6 Hz, 2H), 7.91 (dd, J = 8.8, 2 Hz, 2H), ^{13}C NMR ($CDCl_3$, 400 MHz): δ 44.47, 101.60, 128.77, 138.67, 140.16

HRMS; Calcd. for: $C_7H_7IO_2S$, 281.9211; Found 281.9211

4.18 3-(trifluoromethyl)-5-iodopyridine (2t)

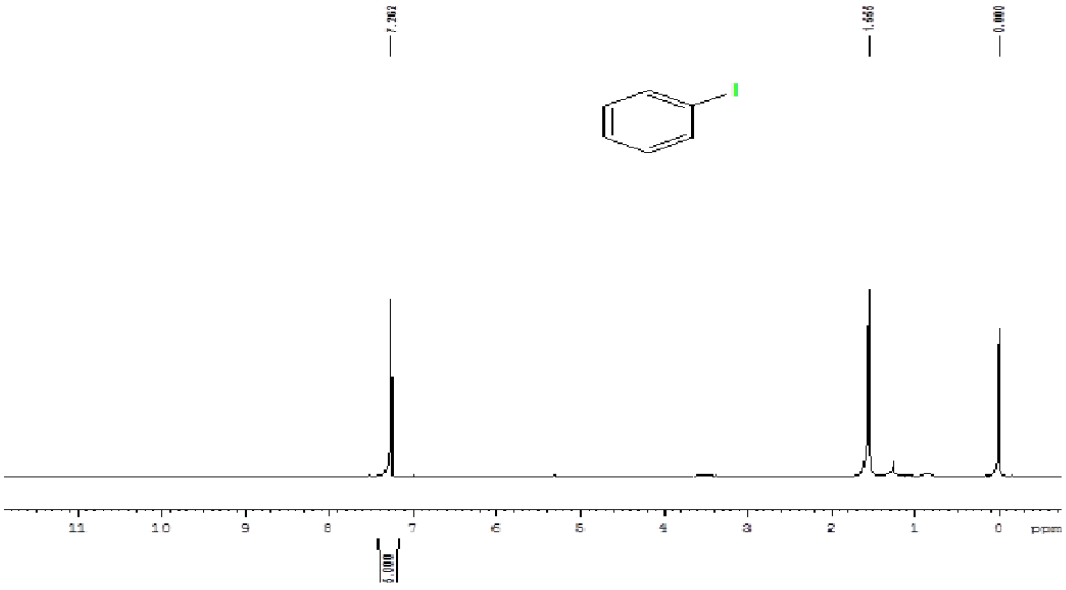


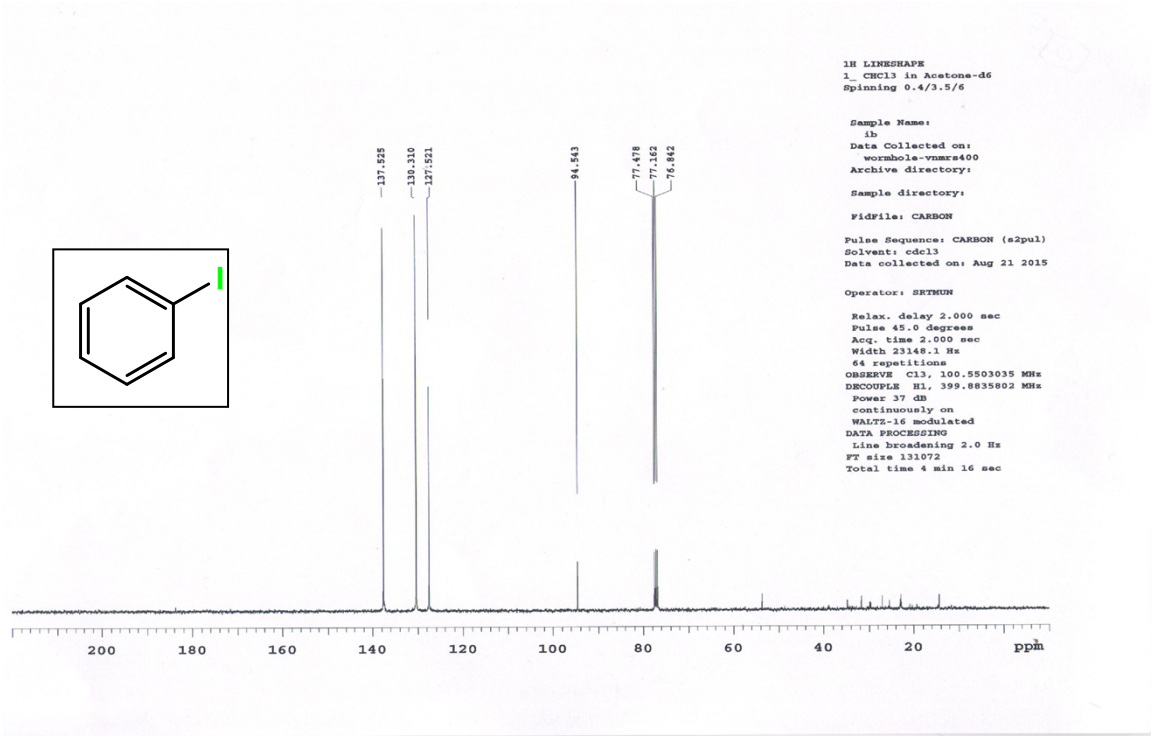
White Solid, Yield 28 % (isolated by column chromatography using **trimethyl amine** pretreated silca gel)

IR (ATR, cm^{-1}) 640 (m), 698 (s), 800 (m), 896 (s), 959 (m), 1009 (m), 1068 (m), 1104 (m), 1127 (m), 1184 (m), 1308 (m), 1335 (m), 1428 (m), 1588 (m), 1915 (w), 3026 (w)

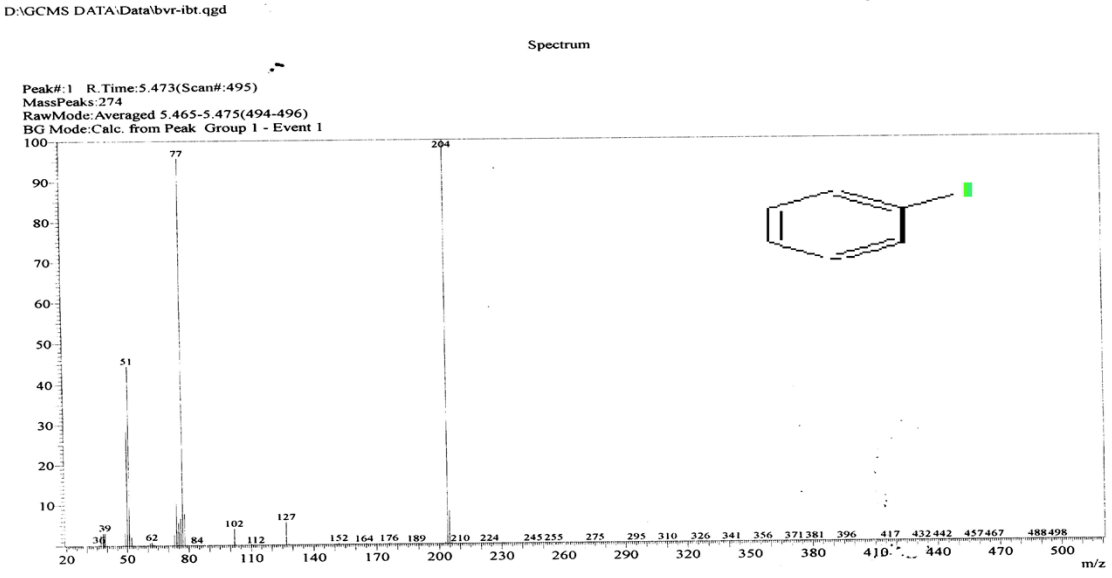
^{1}HNMR ($CDCl_3$, 400 MHz): δ 8.24-8.25 (m, 1H), 8.83 (s, 1H), 9.03 (s, 1H), ^{13}C NMR ($CDCl_3$, 400 MHz): δ 92.7, 120.4, 141.2, 145, 159.1, 161.8 , ^{19}F NMR (DMSO-d_6 400 MHz) -61.03 (t, 3F), HRMS (Calculated for C_6H_3NIH= 272.9271); Found = 273.9341 $(M+H)^+$

4.1 Iodobenzene (2a)

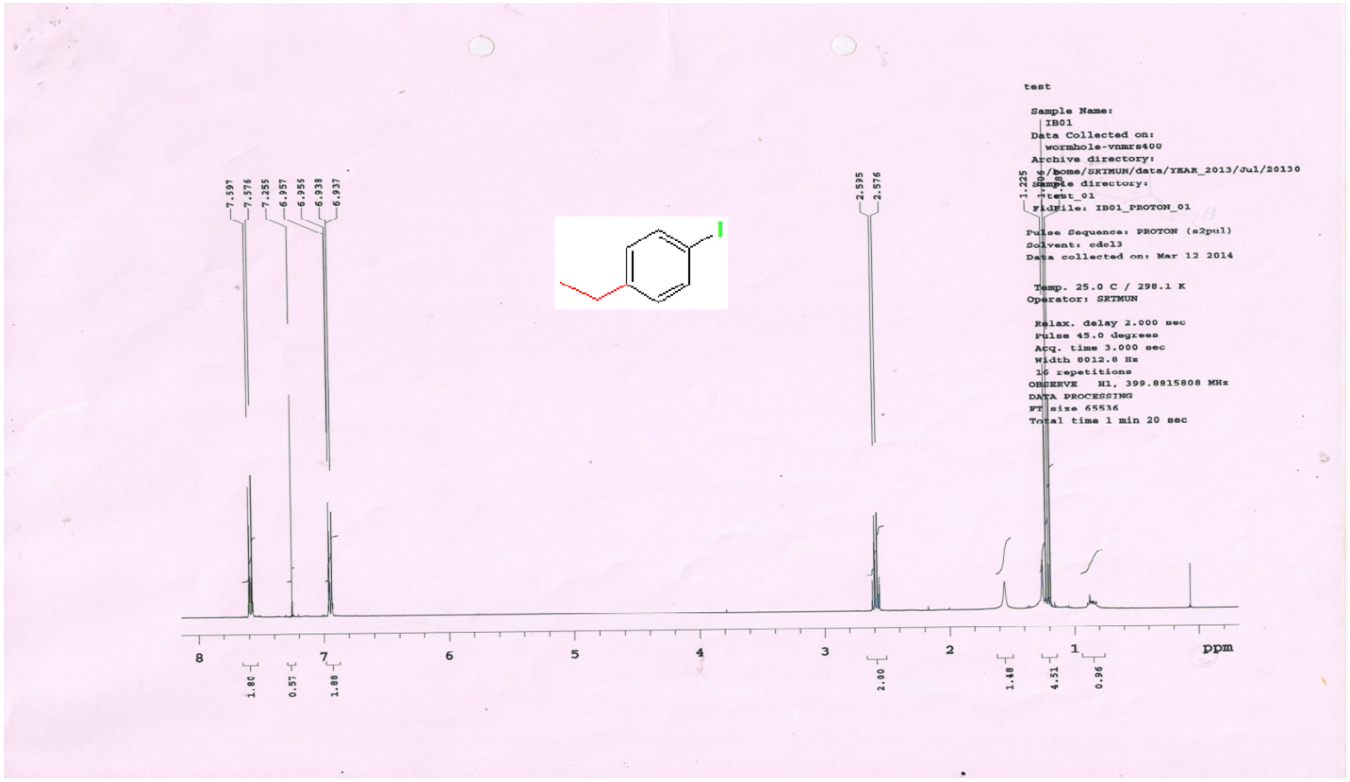


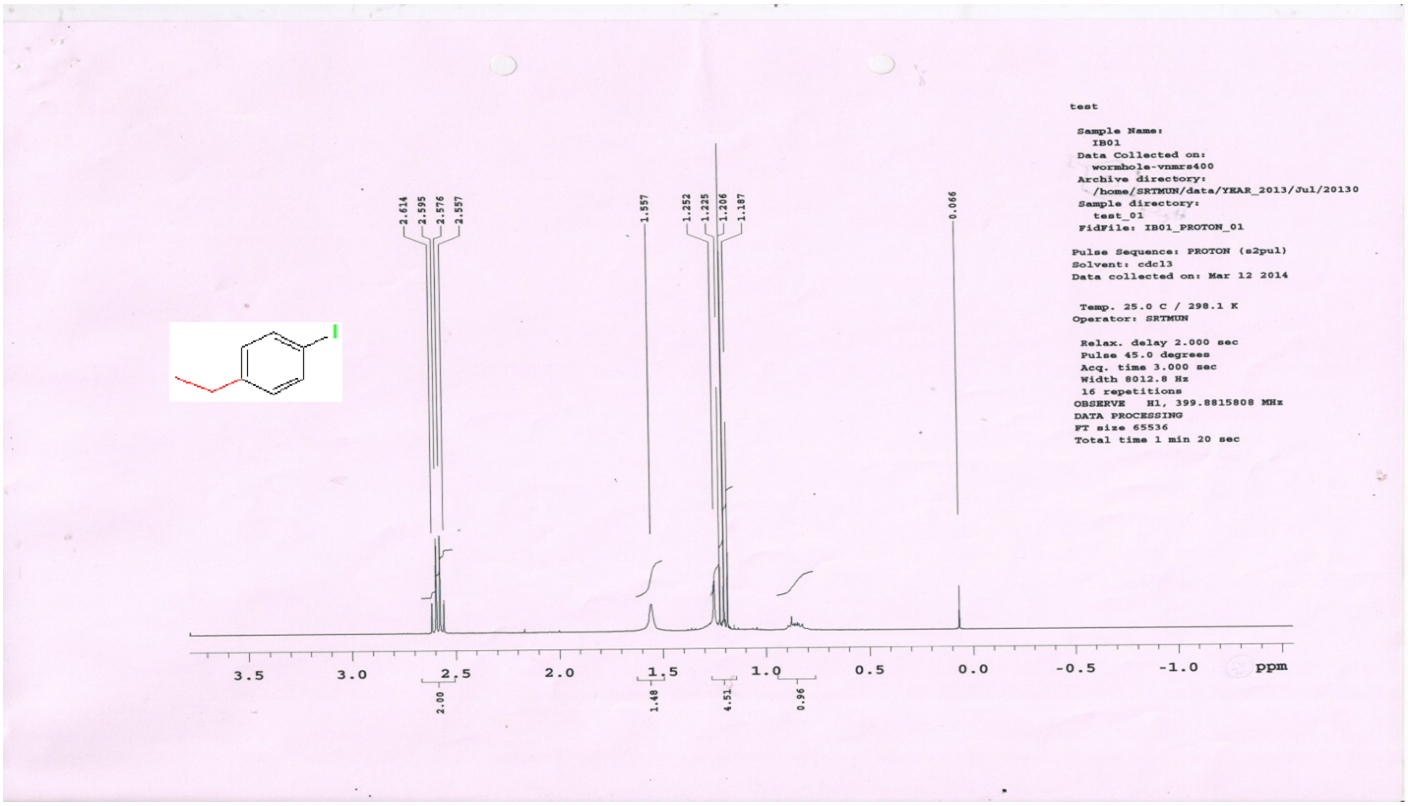


24-11-2014 17:04:35

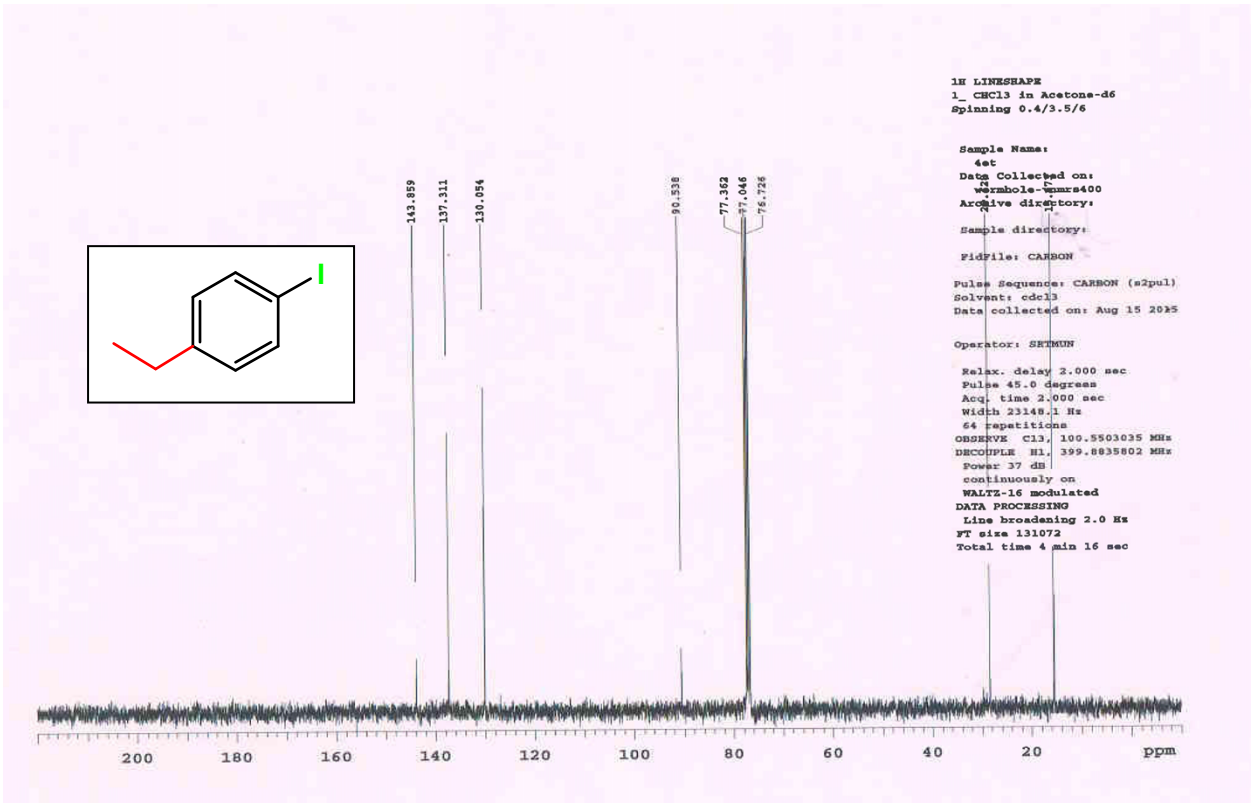


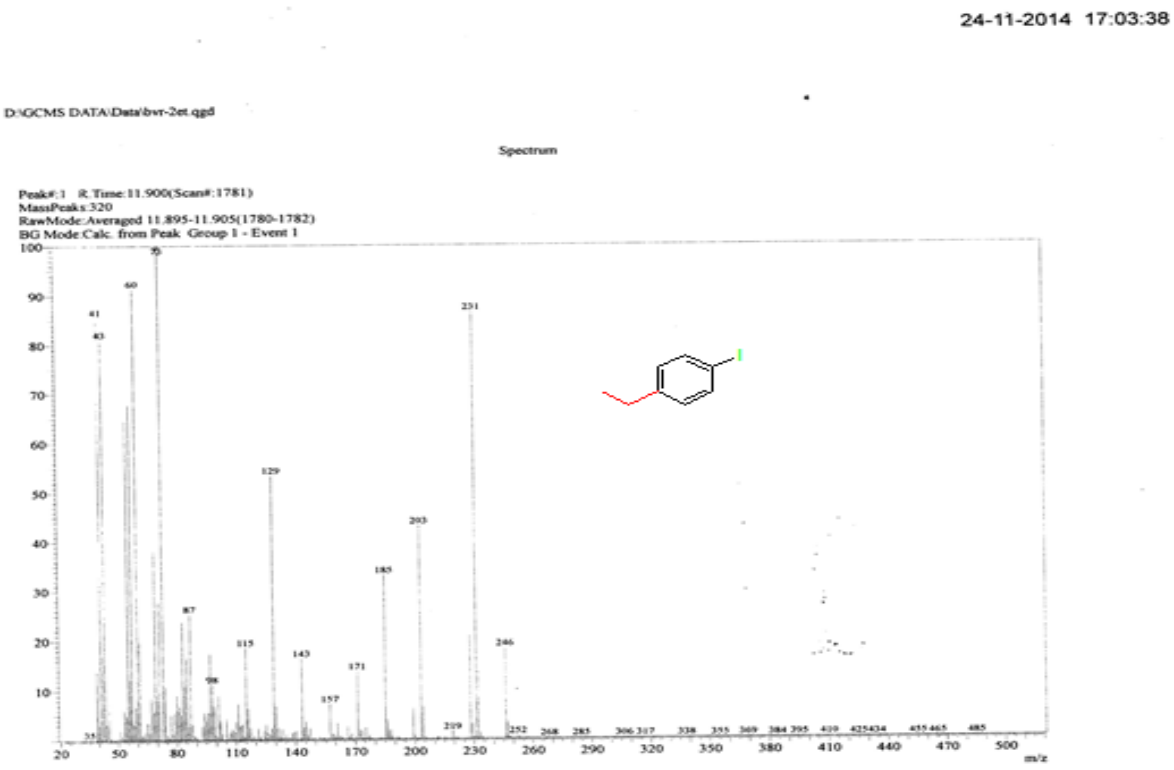
4.2 4-Ethyliodobenzene (2b)



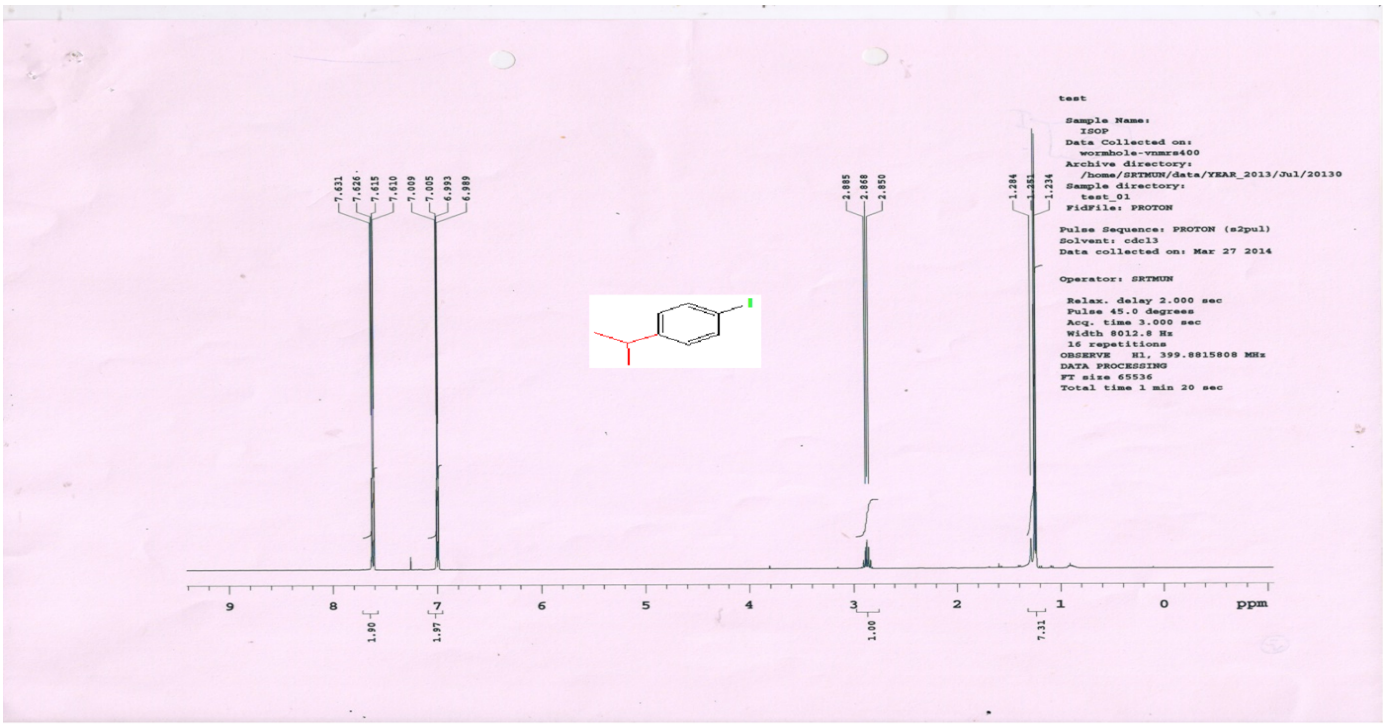


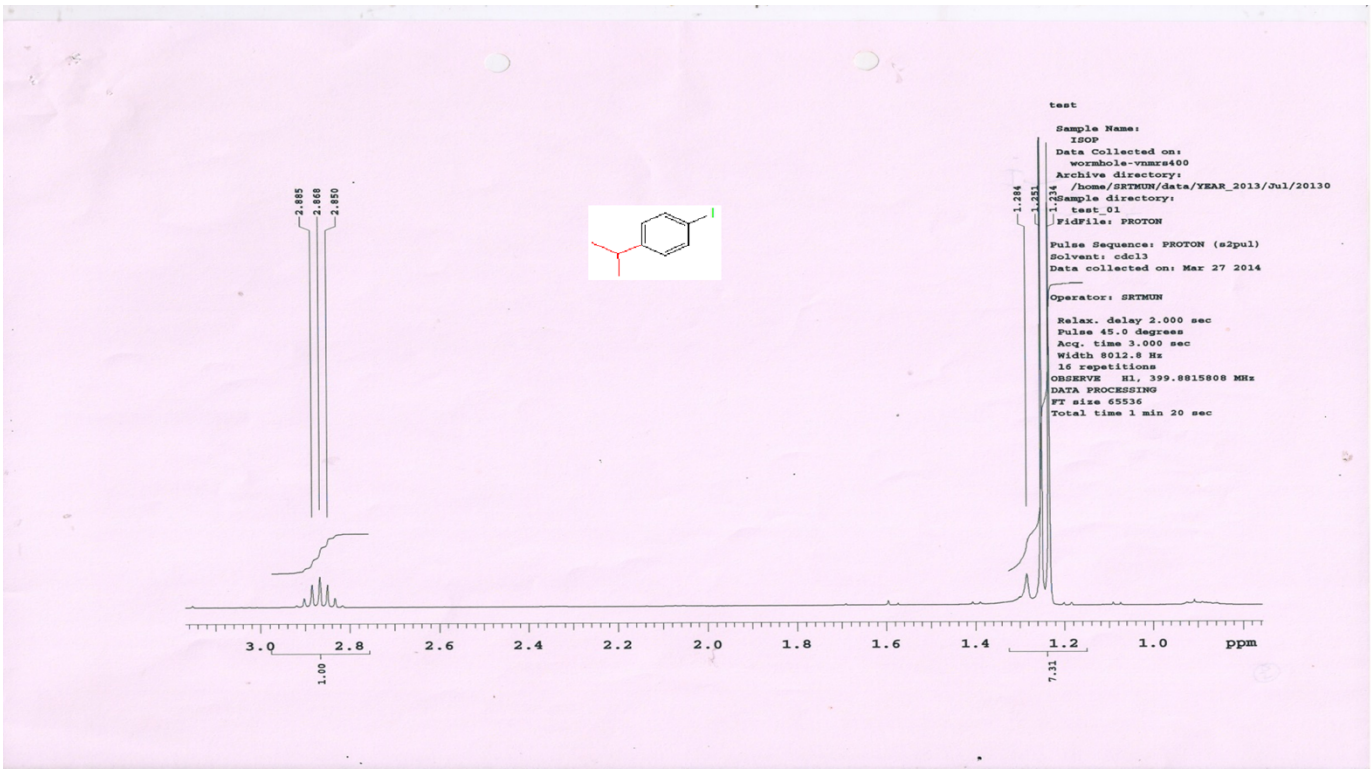

7.597
7.593
7.581
7.576
7.255
6.957
6.956
6.953
6.942
6.938
6.937
I
test
Sample Name:
IB01
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: IB01_PROTON_01
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 12 2014
Temp. 25.0 C / 298.1 K
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 20 sec
8
7
6
5
4
3
ppm
1.80
0.57
1.88
2.00

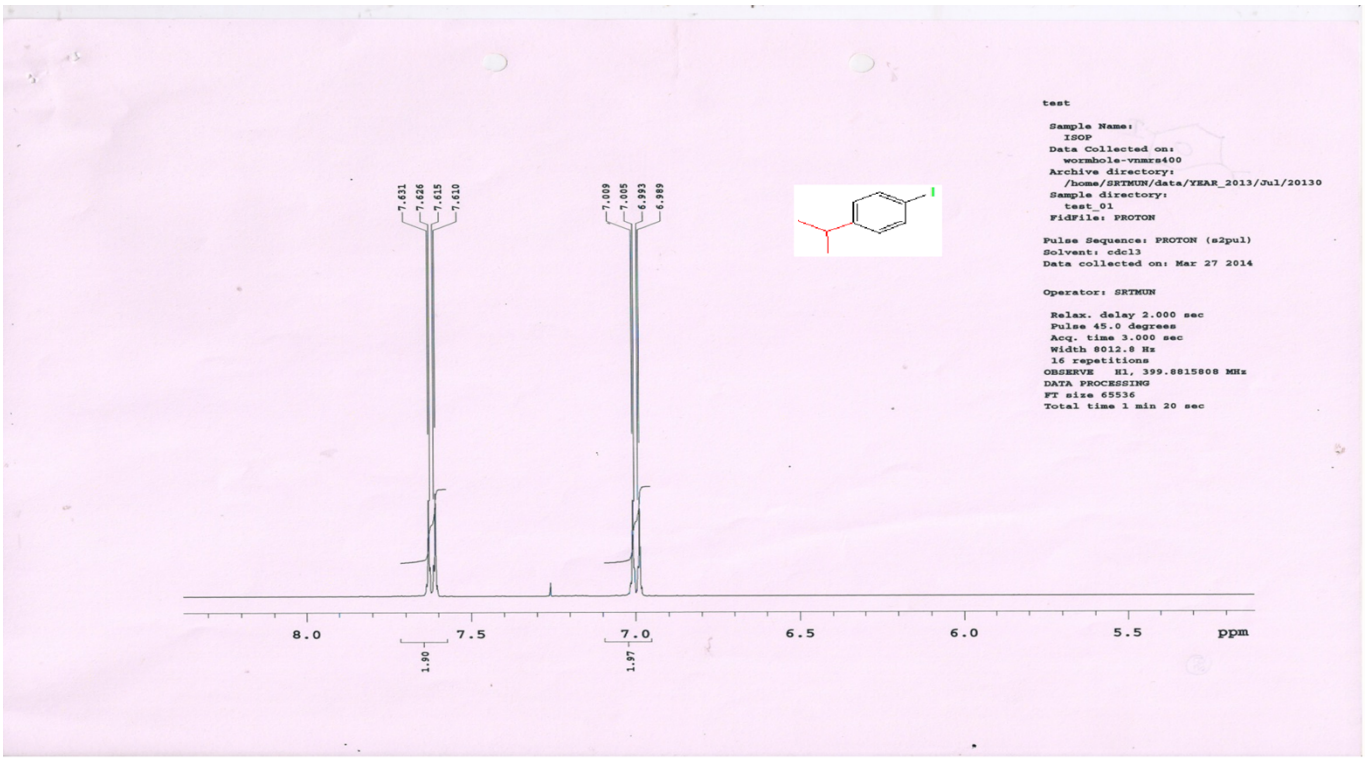

I
143.859
137.311
130.054
90.538
77.362
77.046
76.726
1H LINESHAPE
1_ CHCl3 in Acetone-d6
Spinning 0.4/3.5/6
Sample Name:
4et
Data Collected on:
wormhole-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 15 2015
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec
200
180
160
140
120
100
80
60
40
20
ppm



4.3 4-Isopropyl iodobenzene (2c)

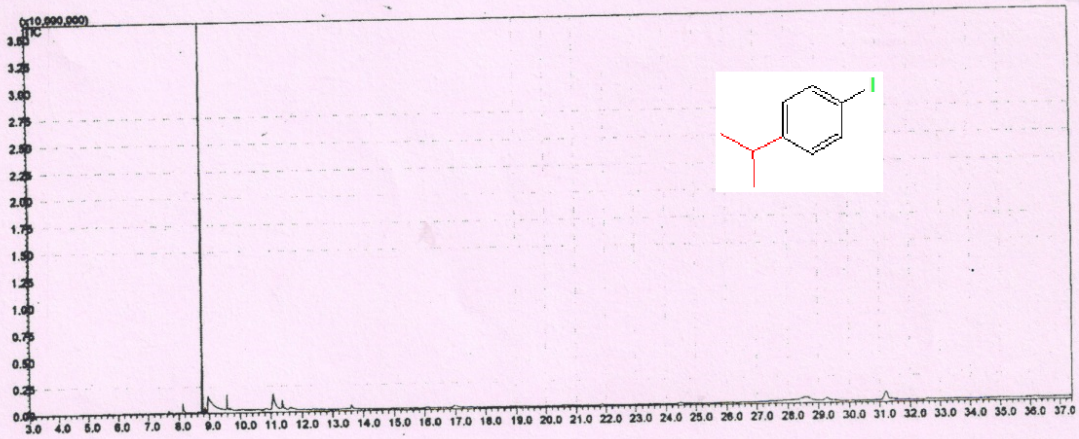



test
Sample Name:
ISOP
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 27 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 20 sec
2.885
2.868
2.850
1.284
1.251
1.234
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ppm
1.00
7.31


test
Sample Name:
ISOP
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 27 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 20 sec
7.631
7.626
7.615
7.610
7.009
7.005
6.993
6.989
8.0
7.5
7.0
6.5
6.0
5.5
ppm
1.90
1.97

30-04-2014 16:38:41

D:\GCMS DATA\Data\bvr-4dibt.QGD

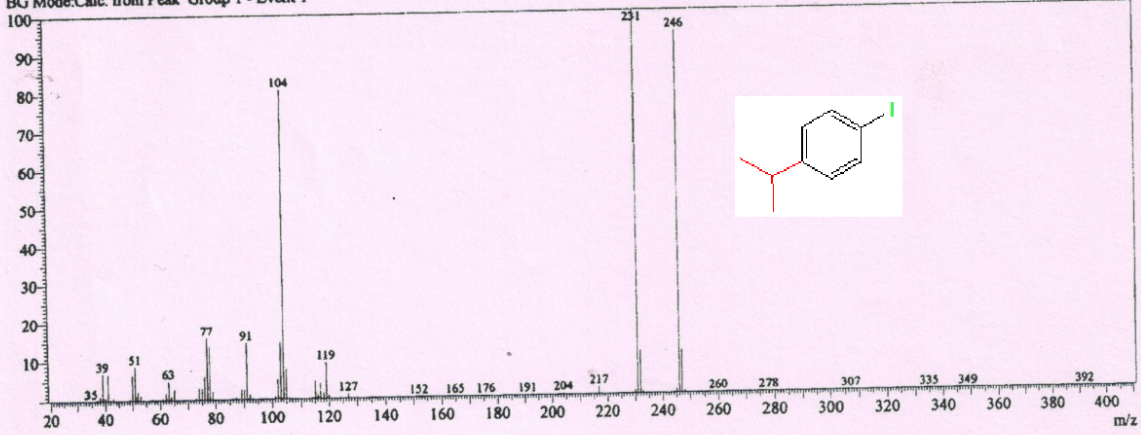


Peak Report TIC

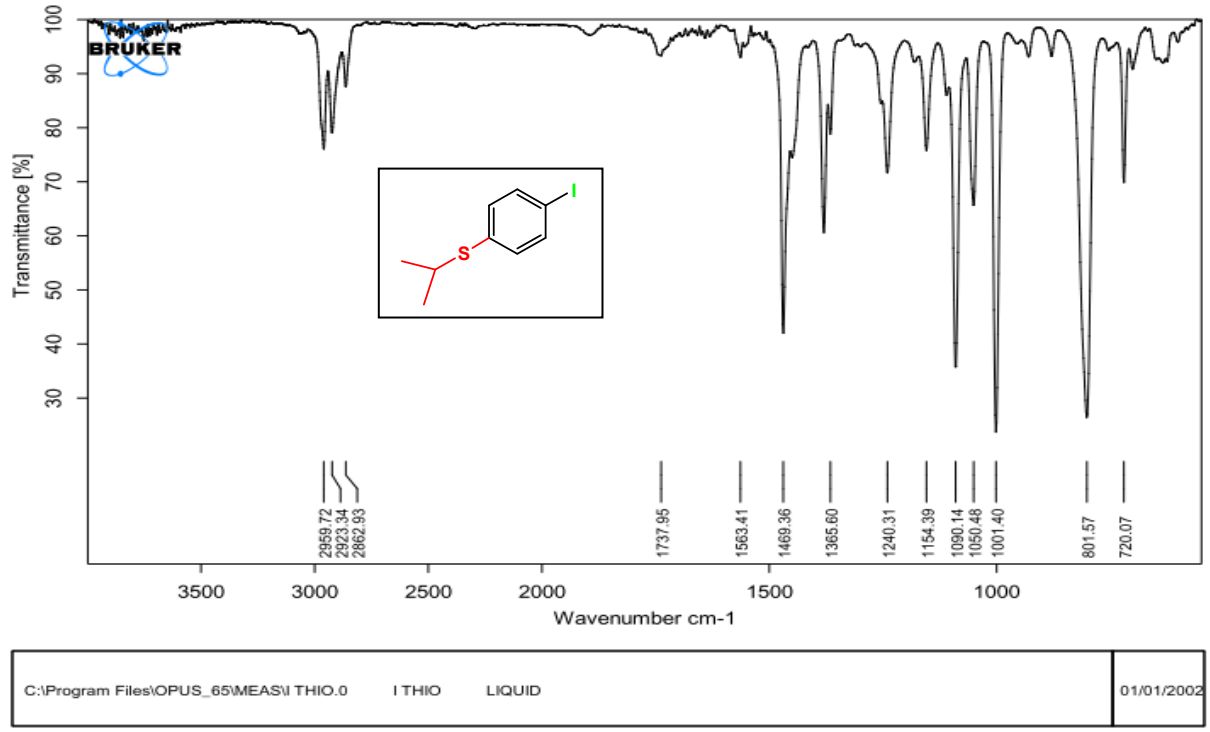
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	8.765	8.630	8.845	43622772	100.00	36209388	100.00	1.20	MI	
				43622772	100.00	36209388	100.00			

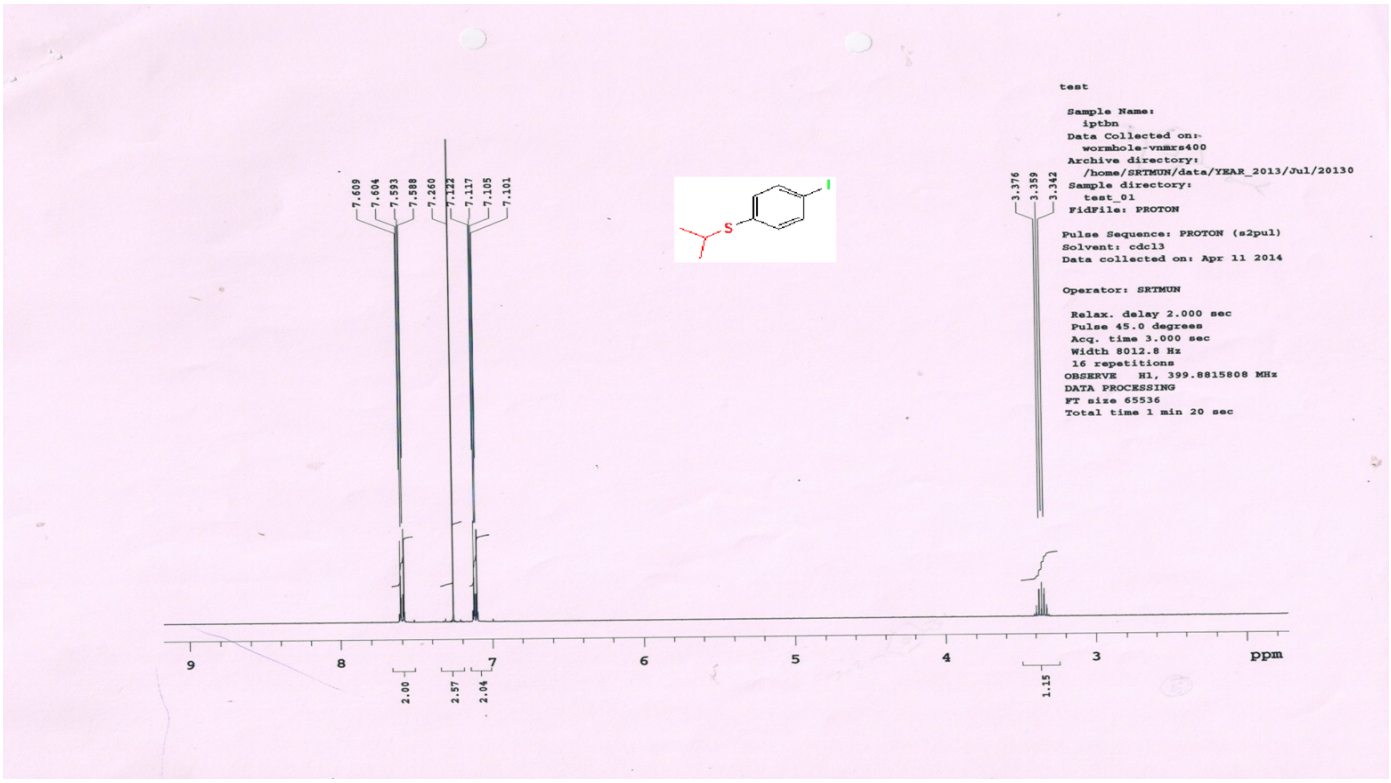
Spectrum

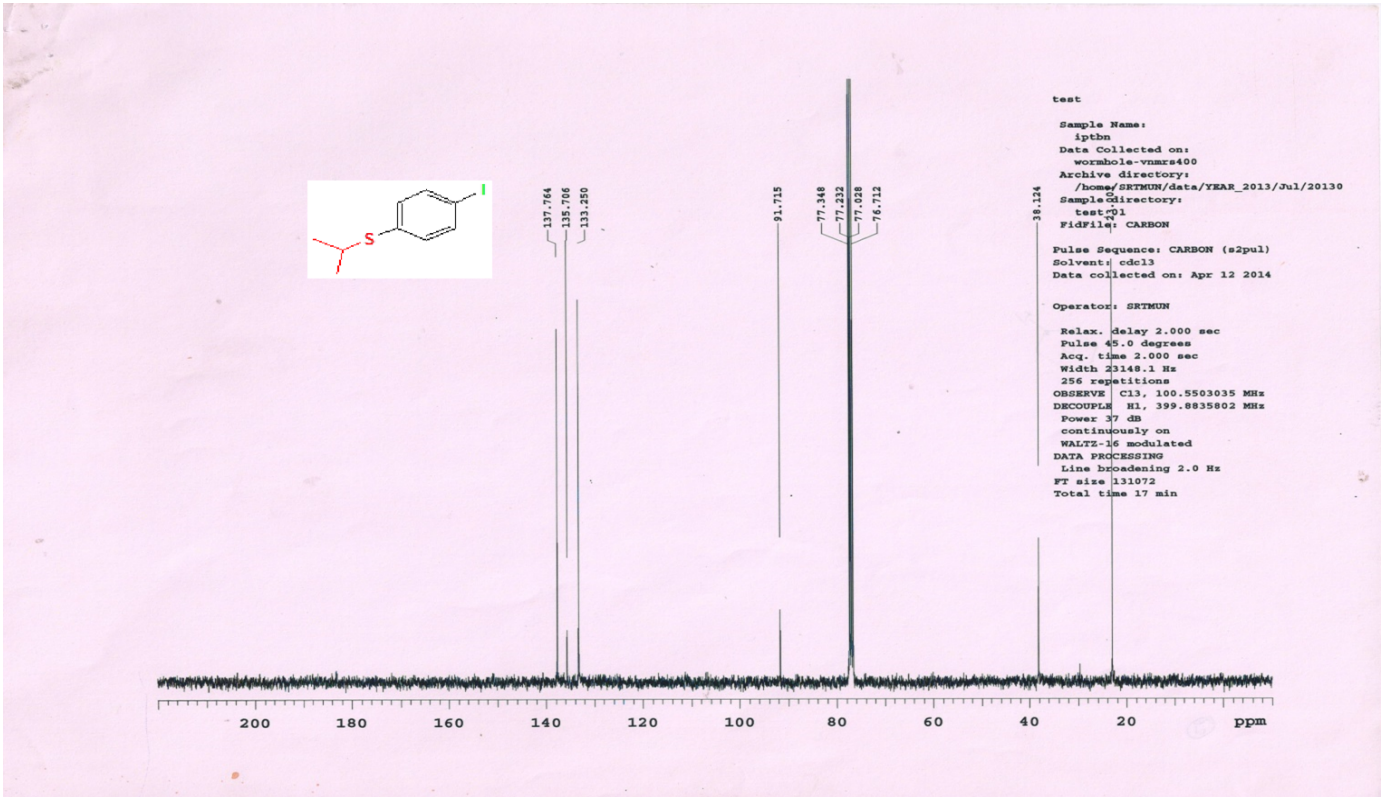
Peak#:1 R.Time:8.765(Scan#:1154)
MassPeaks:224
RawMode:Averaged 8.760-8.770(1153-1155)
BG Mode:Calc. from Peak Group 1 - Event 1

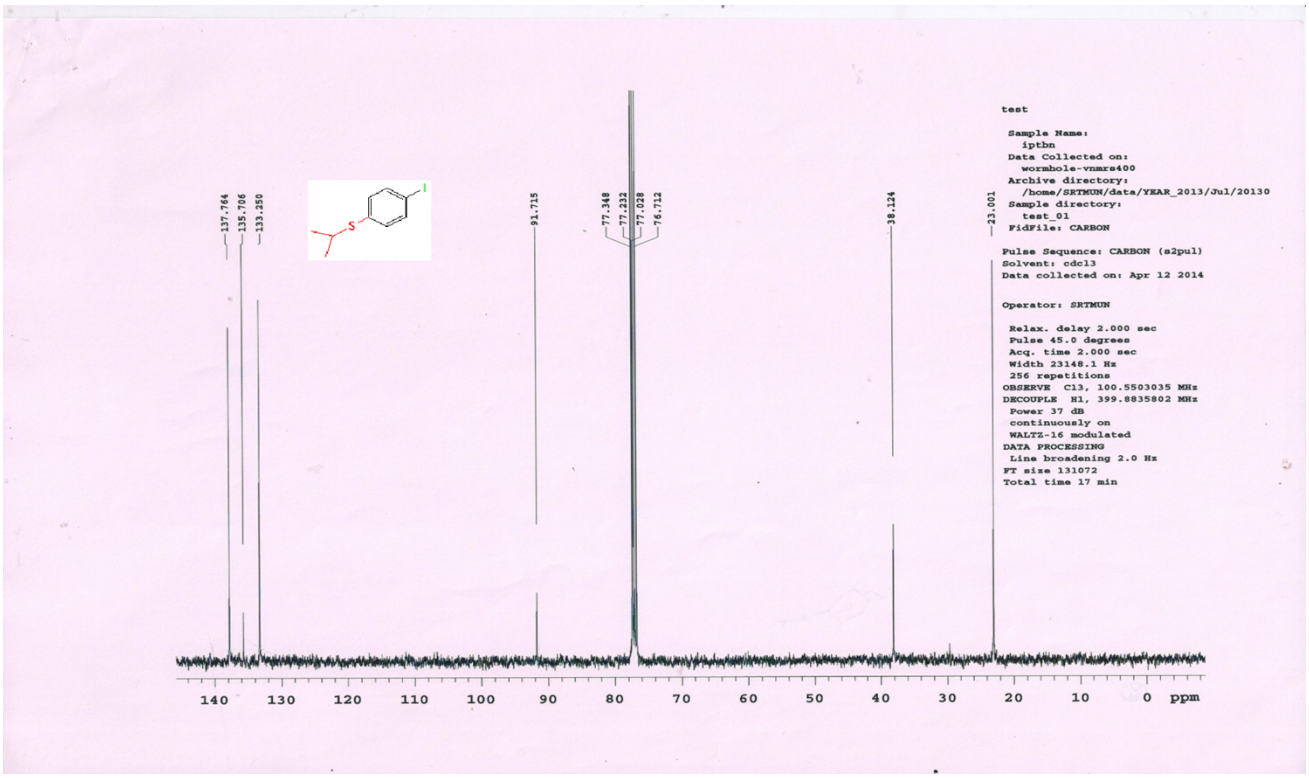


4.4 Isopropyl-4-iodophenyl sulfide (2e)

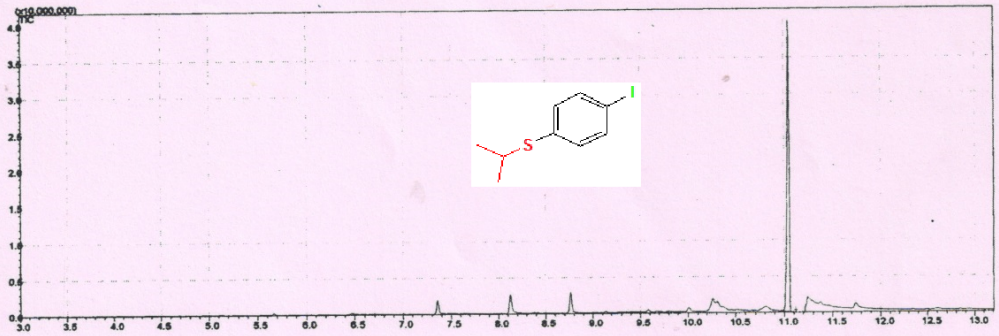



7.609
7.604
7.593
7.588
7.260
7.122
7.117
7.105
7.101
3.376
3.359
3.342
I
S
test
Sample Name:
iptbn
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 11 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 20 sec
9
8
7
6
5
4
3
ppm
2.00
2.57
2.04
1.15


137.764
135.706
133.250
91.715
77.348
77.232
77.028
76.712
38.124
I
S
test
Sample Name:
iptbn
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 12 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
256 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 17 min
200
180
160
140
120
100
80
60
40
20
ppm


137.764
135.706
133.250
91.715
77.348
77.232
77.028
76.712
38.124
23.001
I
S
test
Sample Name:
iptbn
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 12 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
256 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 17 min
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

D:\GCMS DATA\Data\bvr-4ipt.QGD

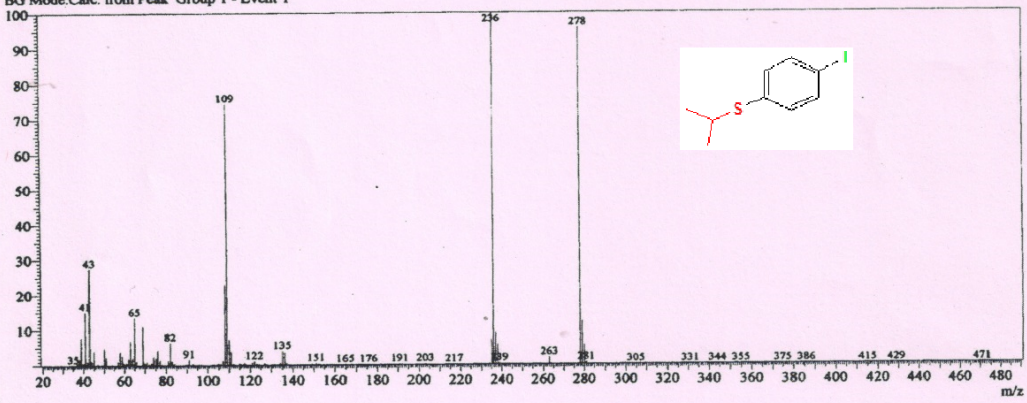


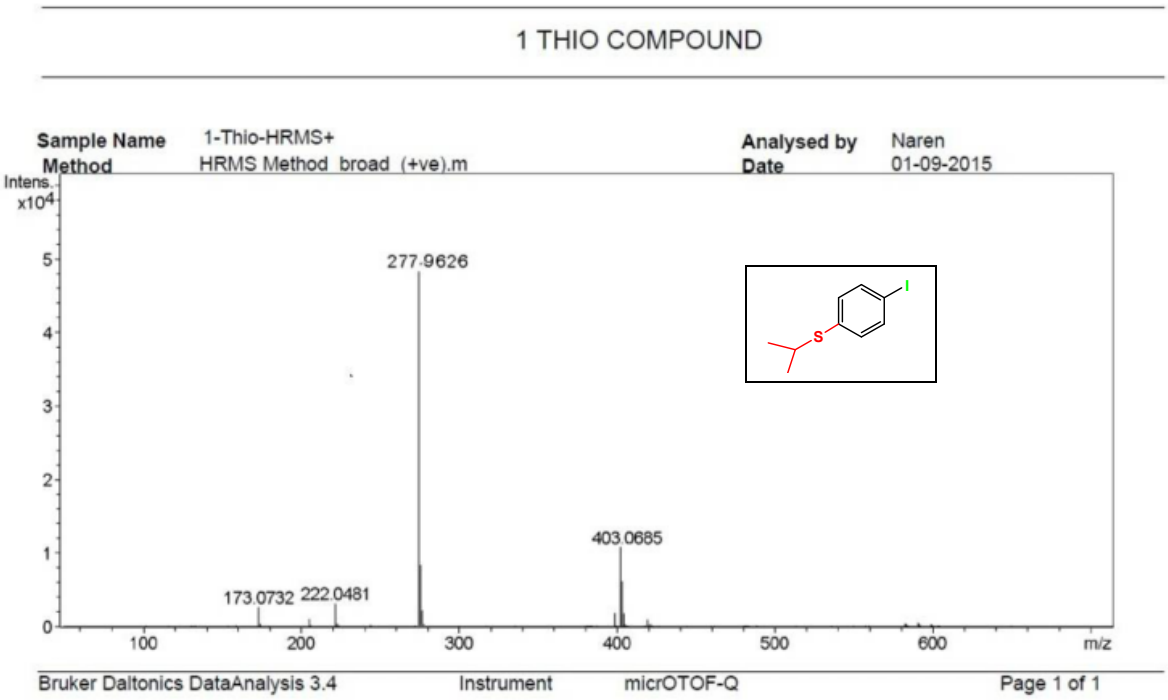
Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	11.049	10.950	11.120	61712963	100.00	39927128	100.00	1.55	MI	
				61712963	100.00	39927128	100.00			

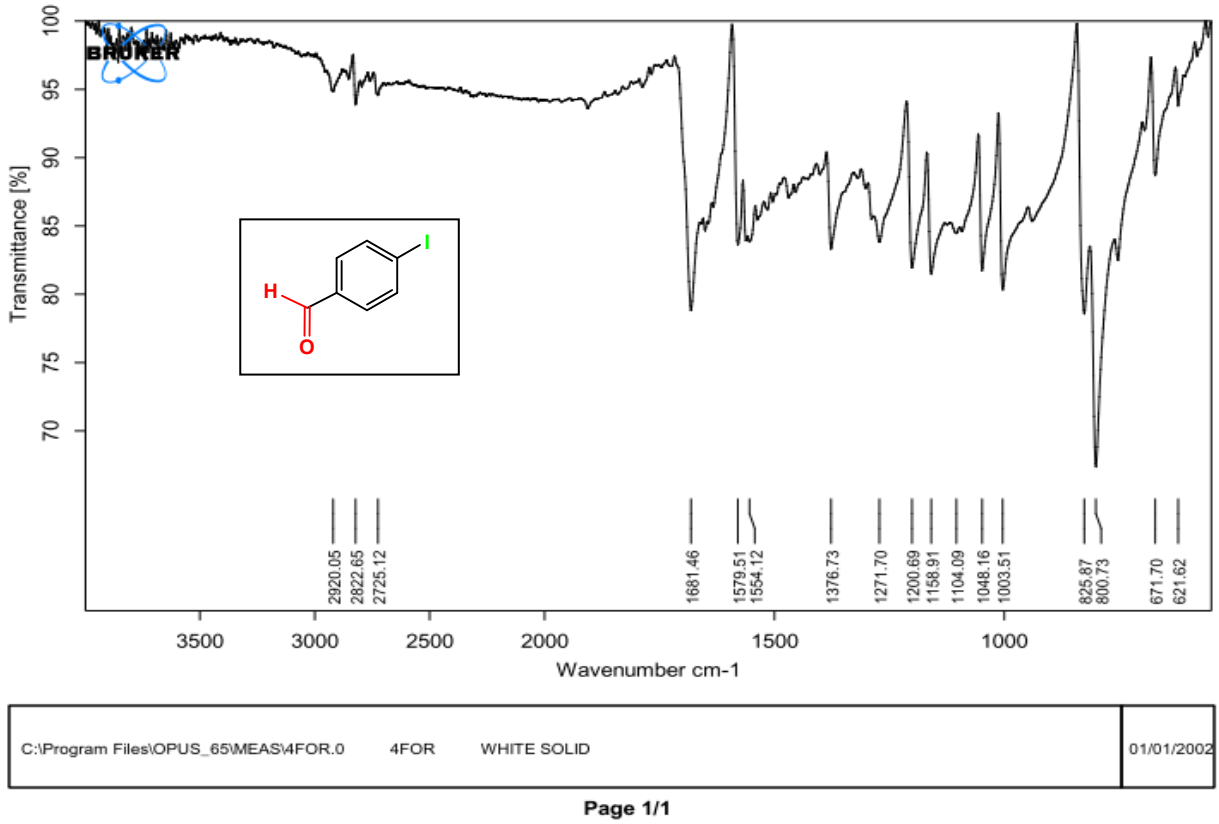
Spectrum

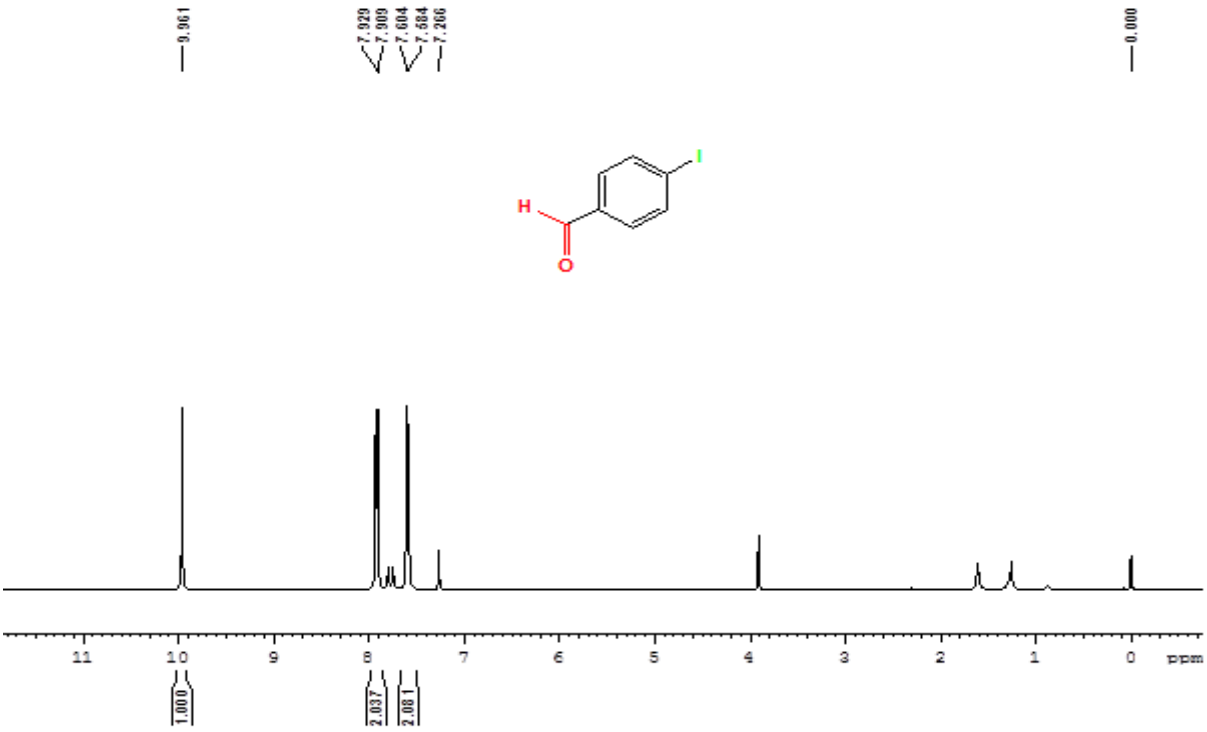
Peak#:1 R.Time:11.049(Scan#:1611)
MassPeaks:256
RawMode:Averaged 11.045-11.055(1610-1612)
BG Mode:Calc. from Peak Group 1 - Event 1

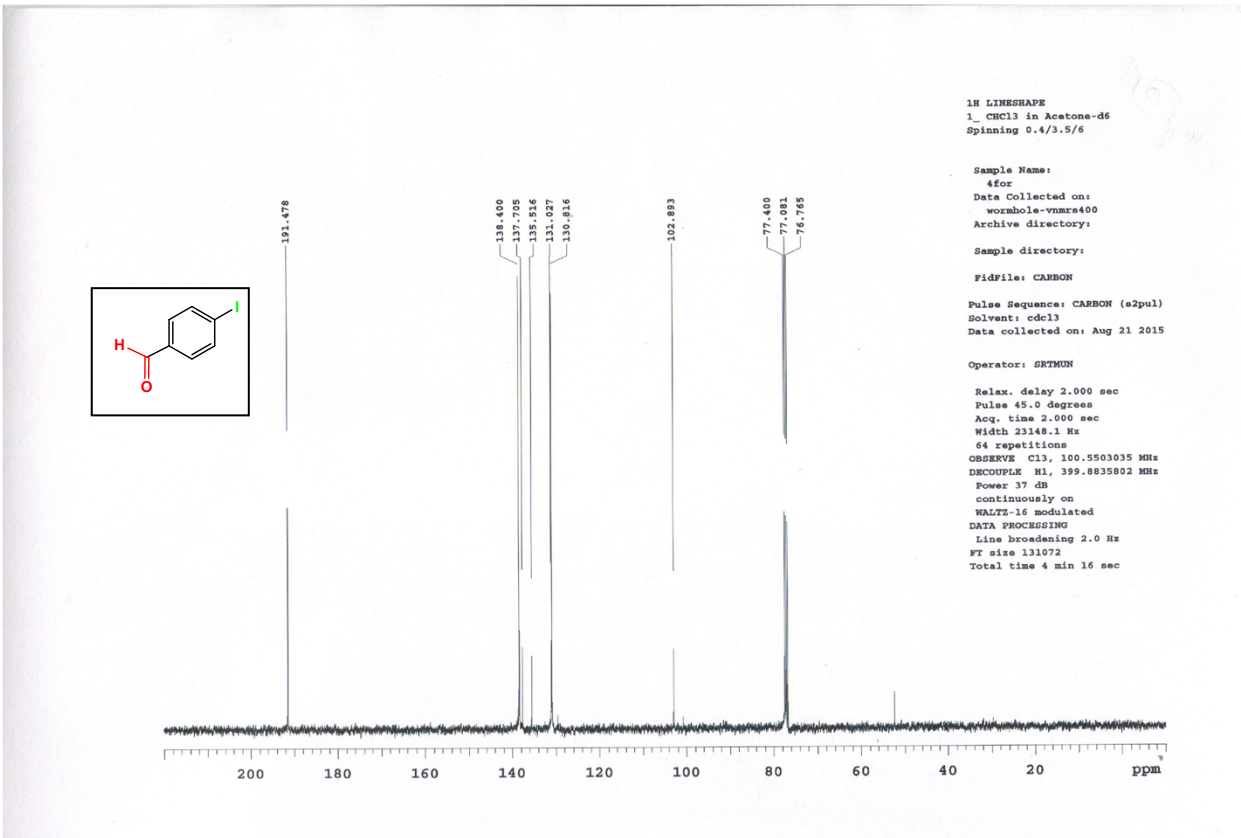


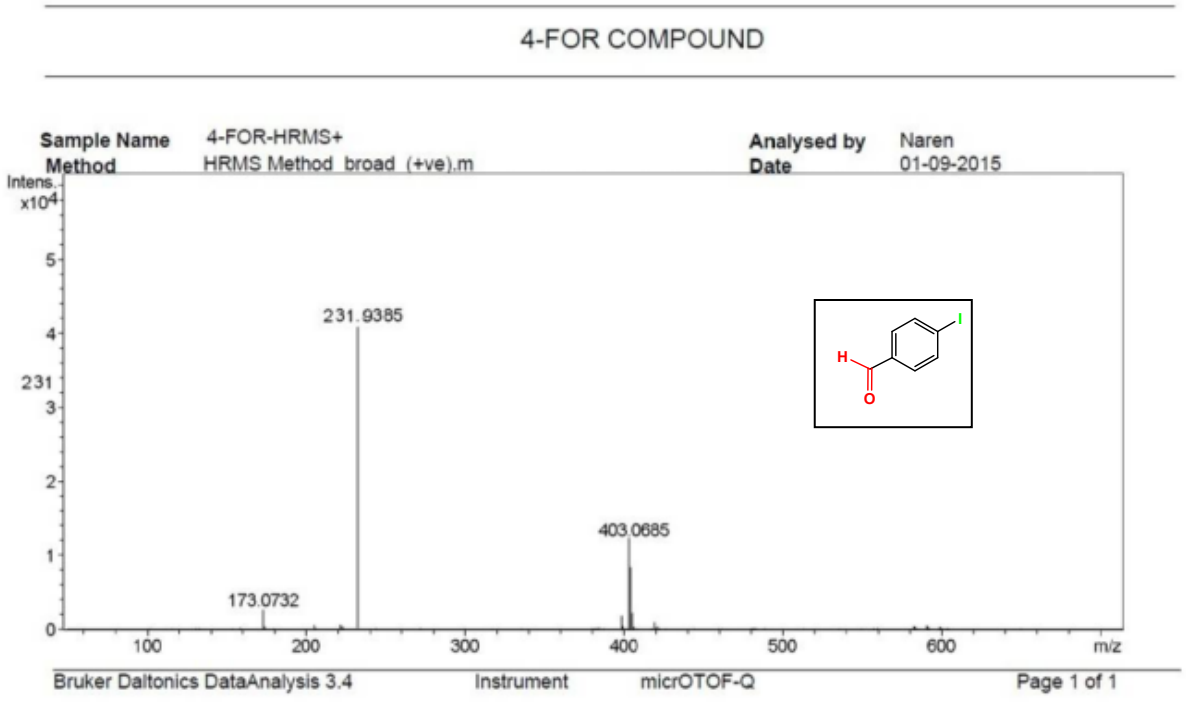


4.5 4-iodobenzaldehyde (2g)

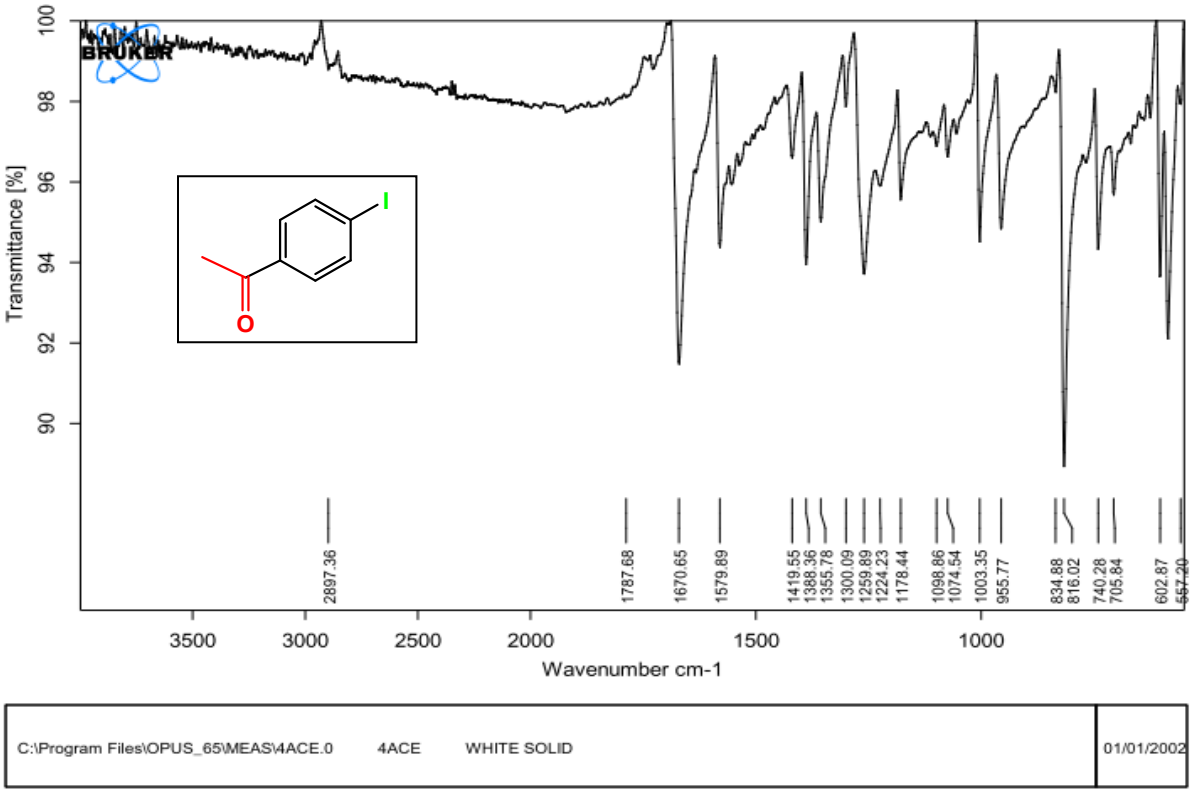


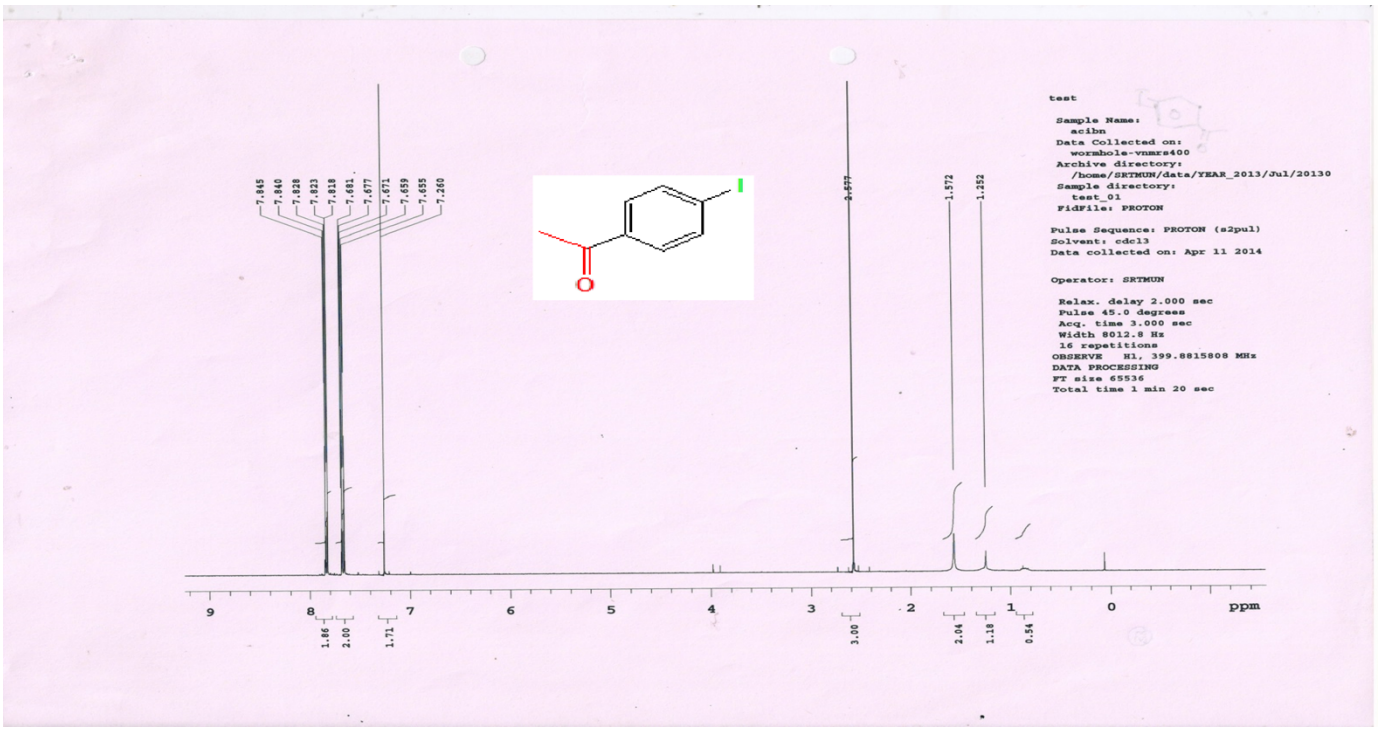

9.961
7.929
7.909
7.604
7.584
7.266
0.000
H
O
I
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.037
2.081

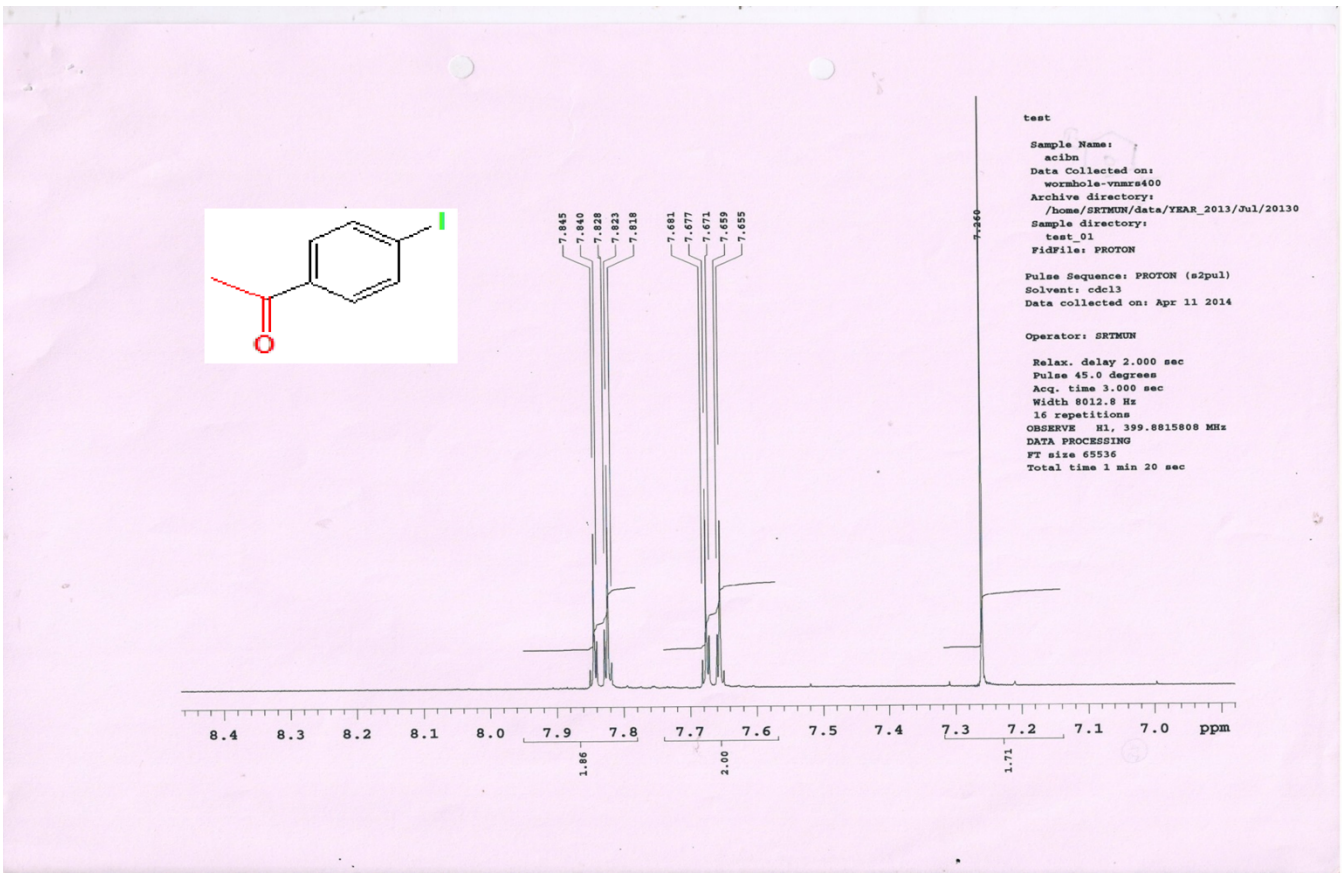

1H LINESHAPE
1_ CHCl3 in Acetone-d6
Spinning 0.4/3.5/6
Sample Name:
4for
Data Collected on:
wormhole-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 21 2015
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec
191.478
138.400
137.705
135.516
131.027
130.816
102.893
77.400
77.081
76.765
H
O
I
200
180
160
140
120
100
80
60
40
20
ppm

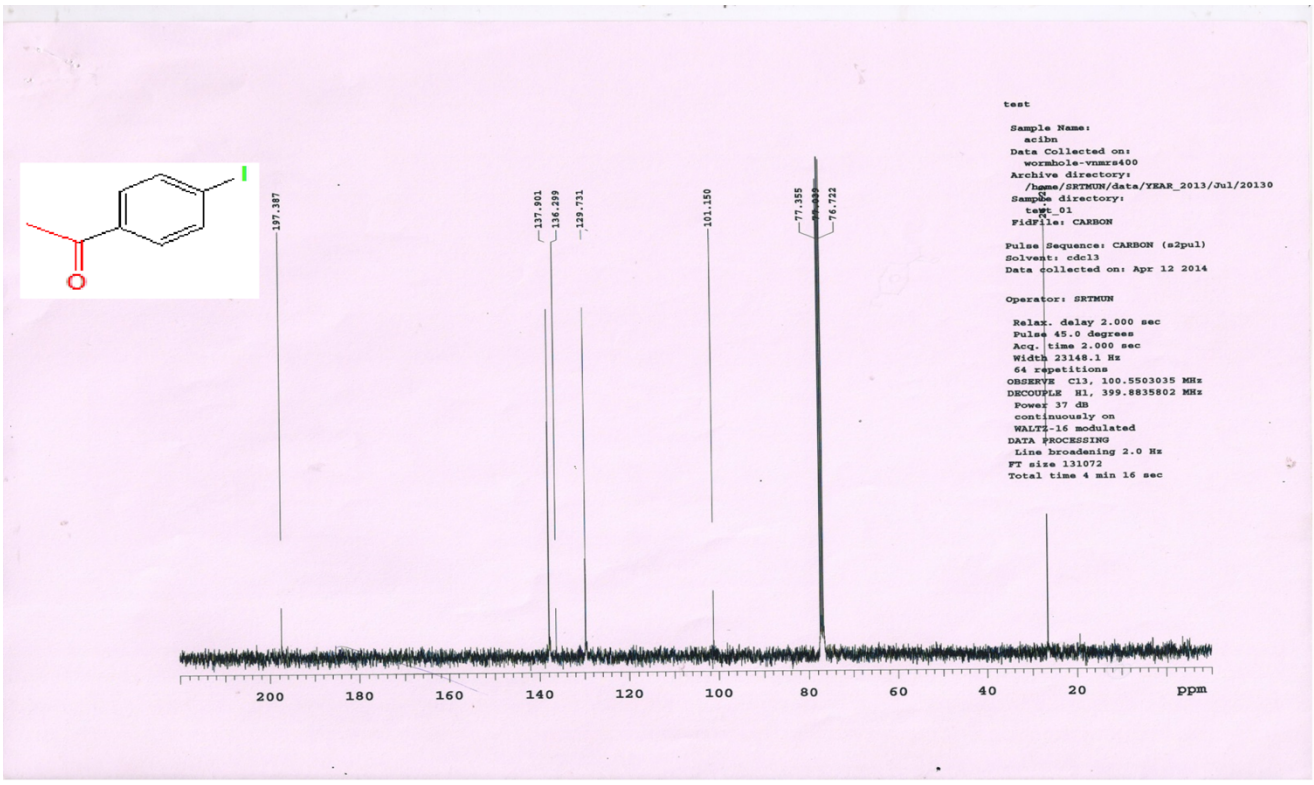


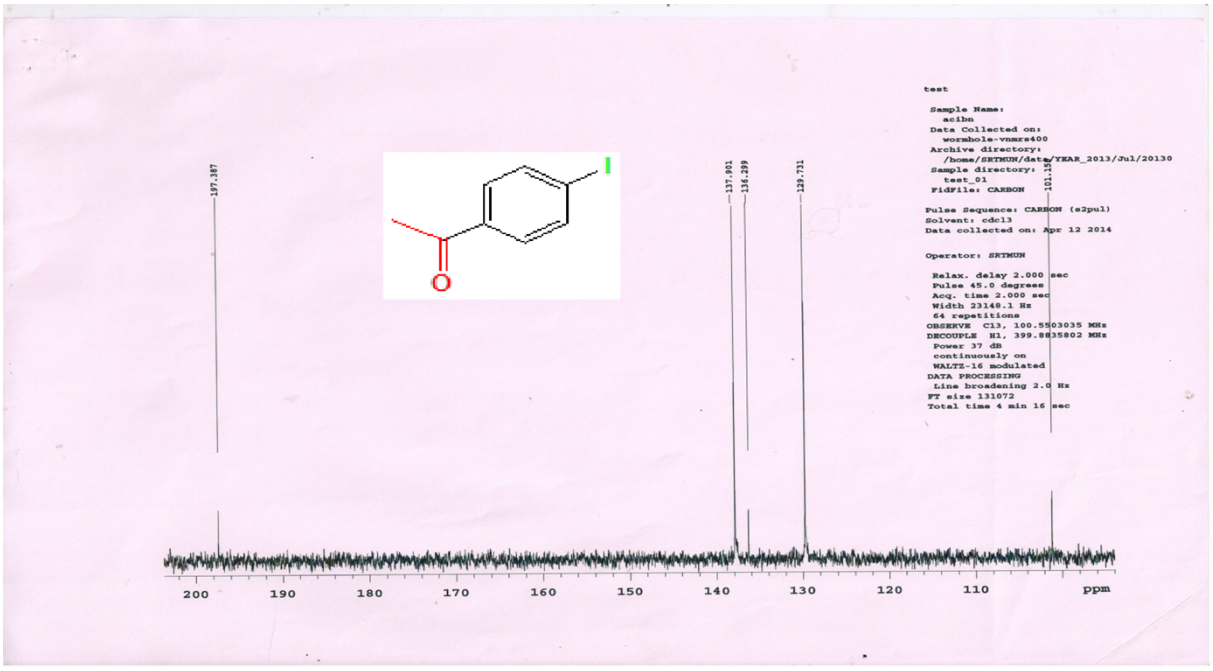
4.6 4-Iodoacetophenone (2h)



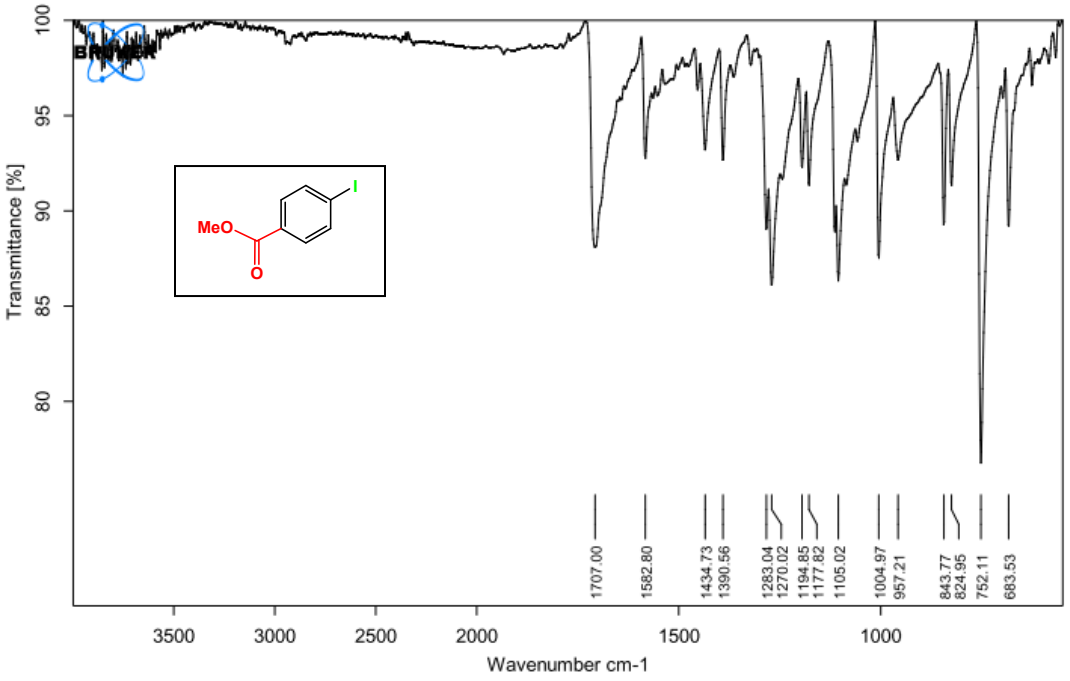

test
Sample Name:
acibn
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 11 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 20 sec
7.845
7.840
7.828
7.823
7.818
7.681
7.677
7.671
7.659
7.655
7.260
2.573
1.572
1.252
O
I
9
8
7
6
5
4
3
2
1
0
ppm
1.86
2.00
1.71
3.00
2.04
1.18
0.54

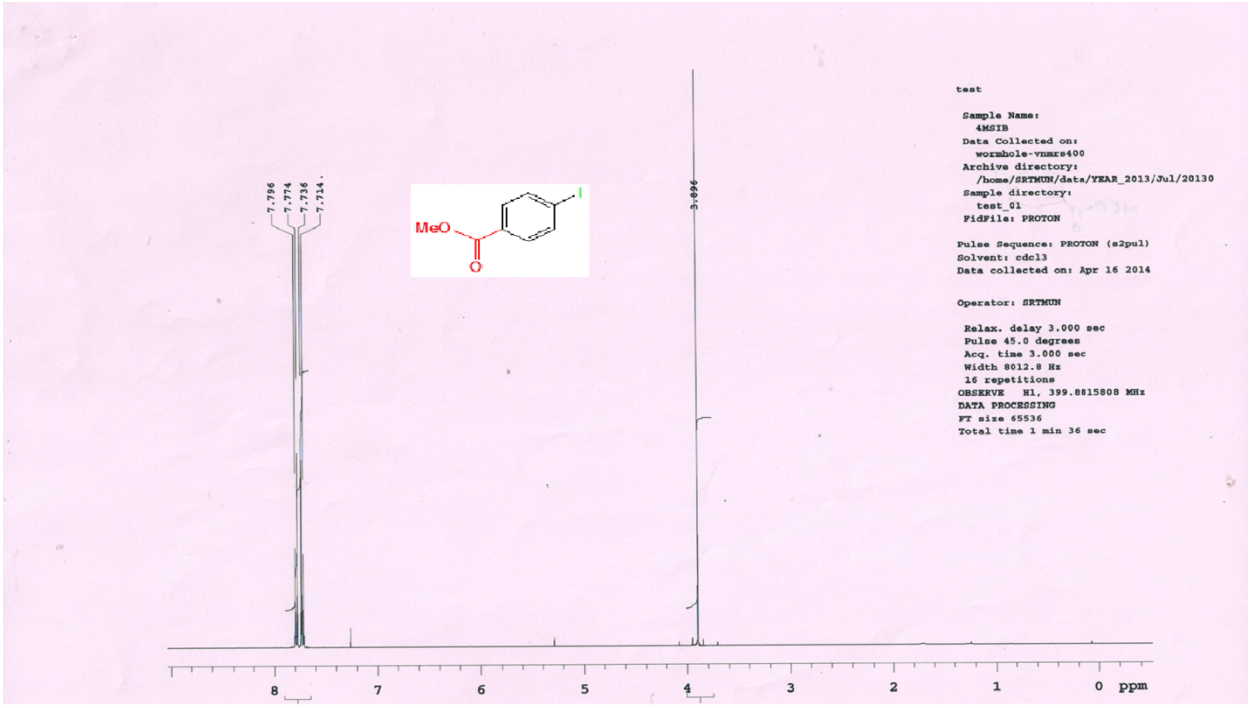

test
Sample Name:
acibn
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 11 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 20 sec
7.845
7.840
7.828
7.823
7.818
7.681
7.677
7.671
7.659
7.655
7.260
O
I
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
1.86
2.00
1.71

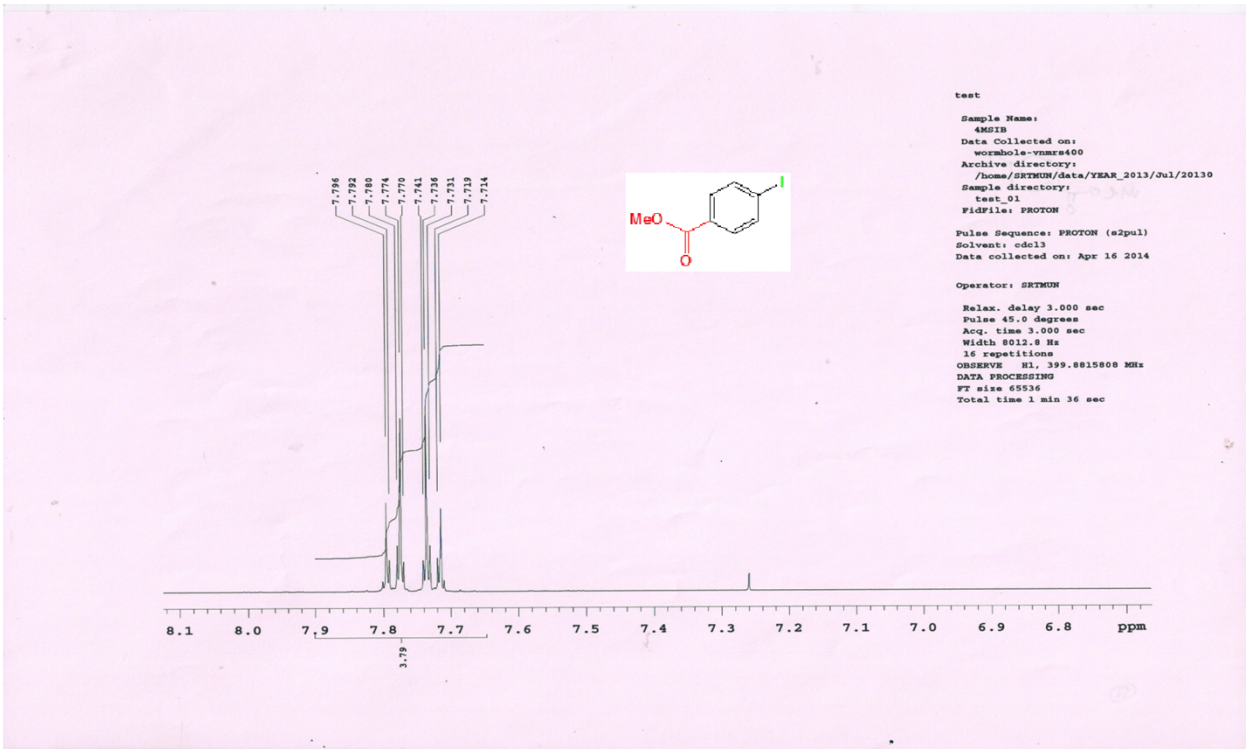

197.387
137.901
136.299
129.731
101.150
77.355
76.722
200
180
160
140
120
100
80
60
40
20
ppm
test
Sample Name:
acibn
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 12 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec

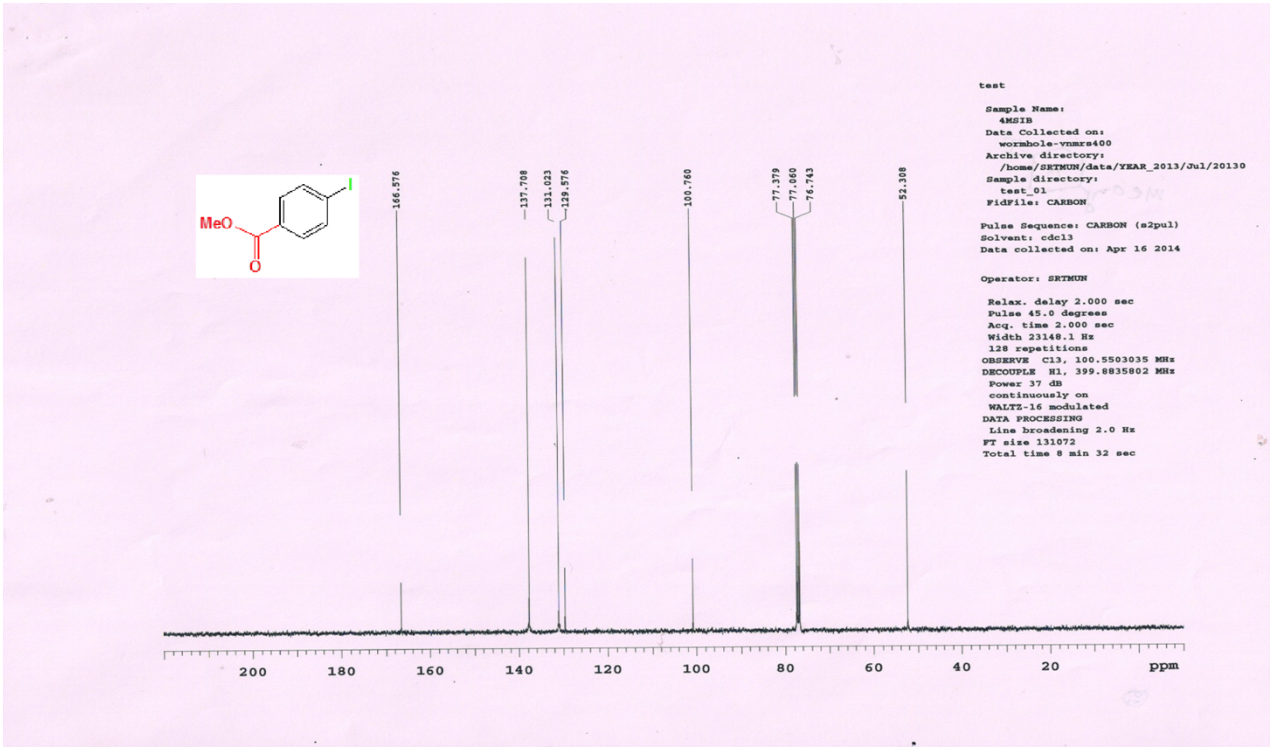

197.387
137.901
136.299
129.731
101.150
200
190
180
170
160
150
140
130
120
110
ppm
test
Sample Name:
acibn
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 12 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec

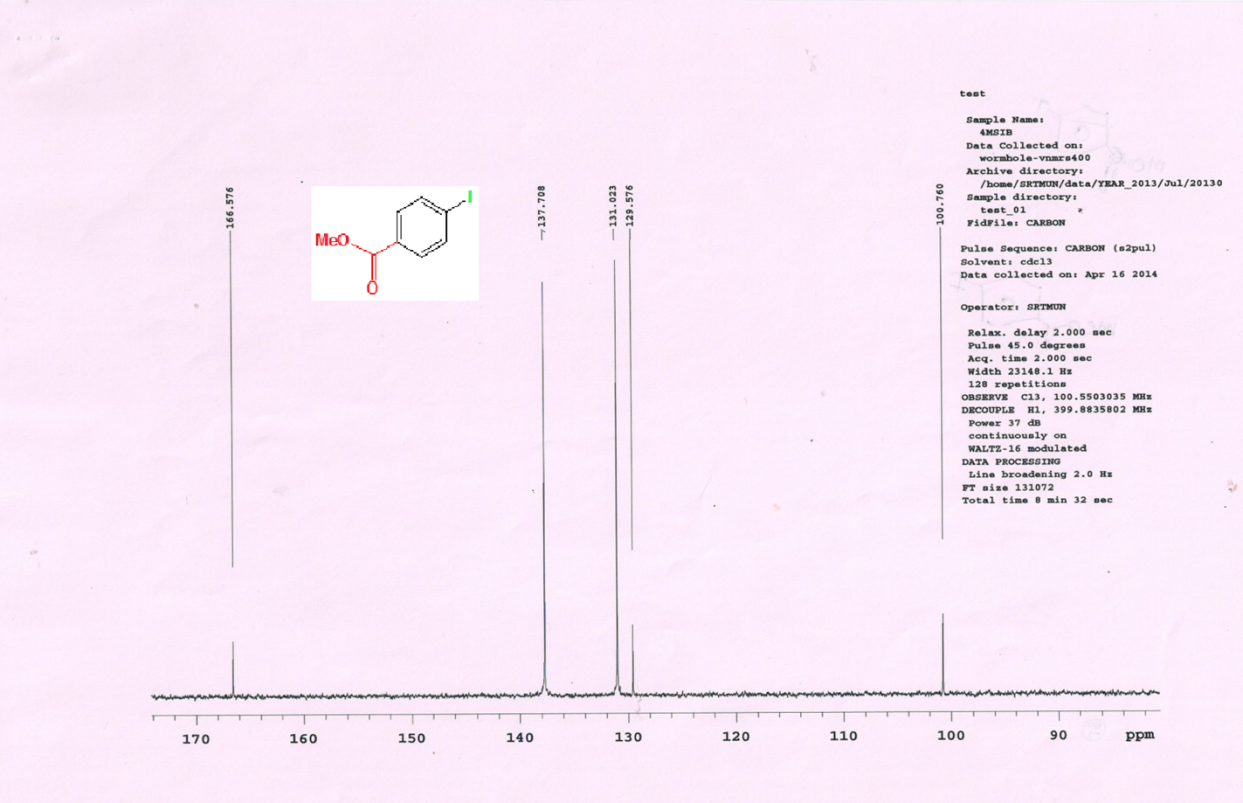
4.7 4-Carbomethoxyiodbezene (2i)



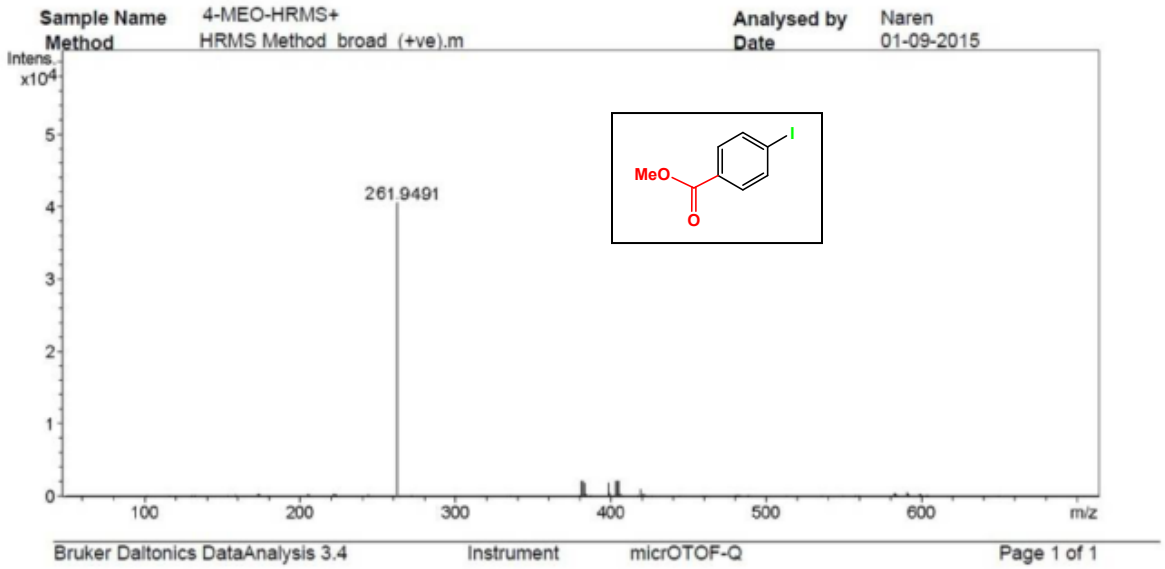



7.796
7.792
7.780
7.774
7.770
7.741
7.736
7.731
7.719
7.714
MeO
O
I
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
ppm
3.79
test
Sample Name:
4MSIB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 36 sec

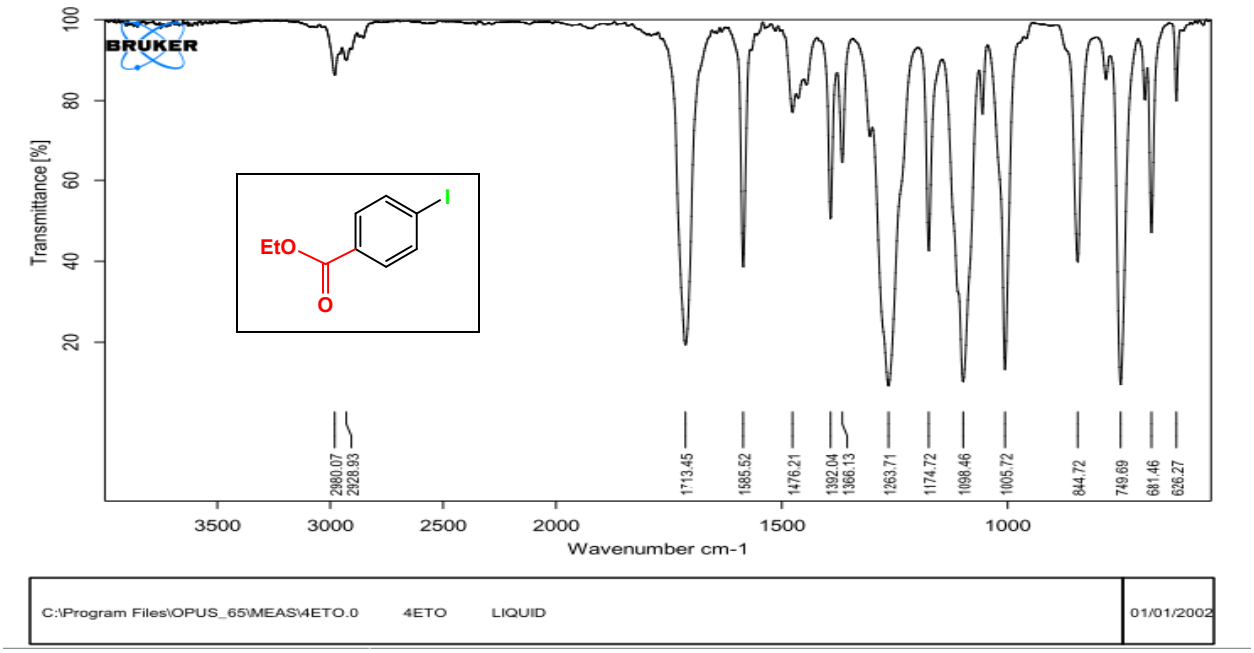

MeO
O
I
166.576
137.708
131.023
129.576
100.760
77.379
77.060
76.743
52.308
200
180
160
140
120
100
80
60
40
20
ppm
test
Sample Name:
4MSIB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
128 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 8 min 32 sec

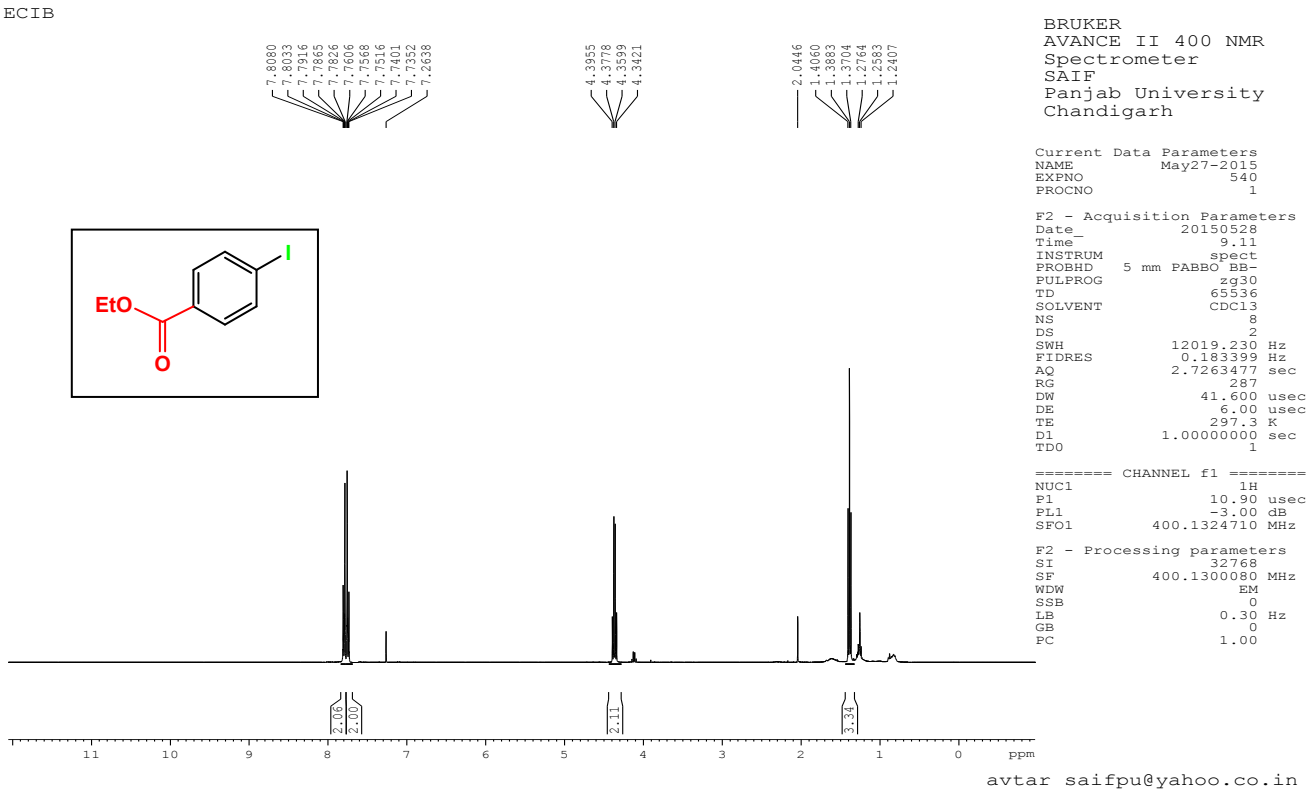


4-MEO COMPOUND

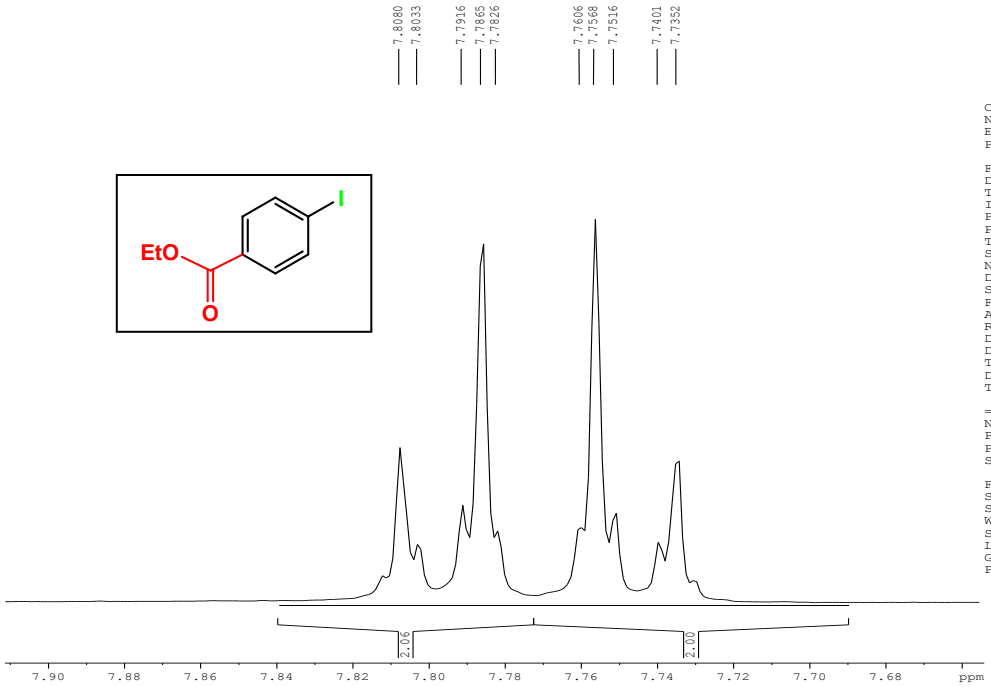


4.8 4-Carboethoxyiodbezene (2j)





ECIB



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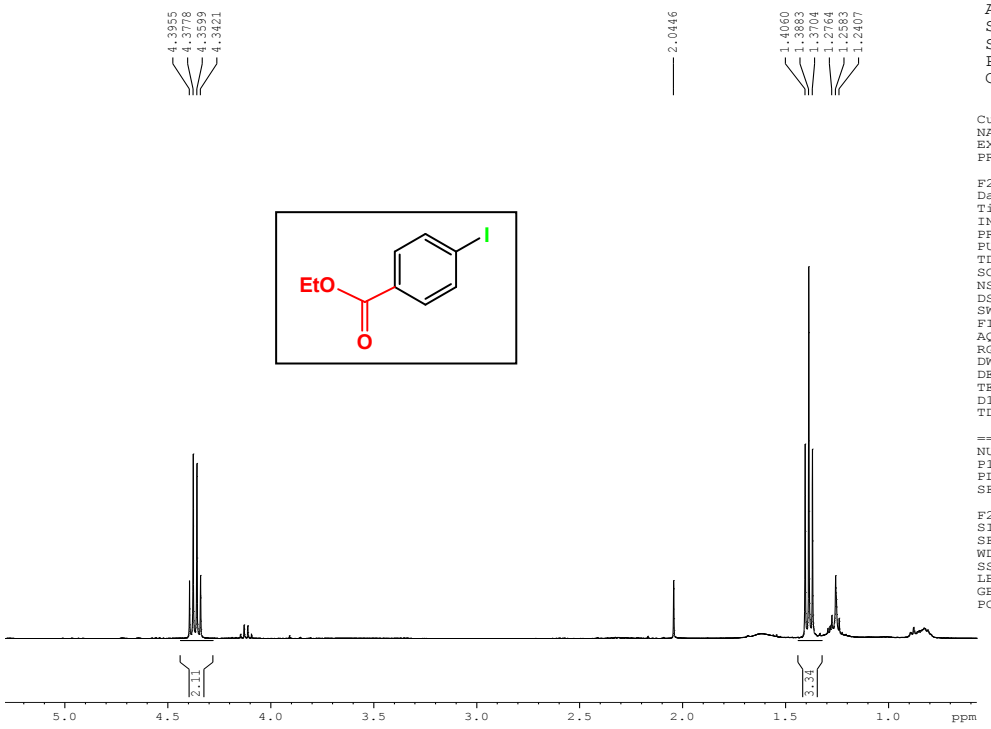
Chandigarh

Current Data Parameters	
NAME	May27-2015
EXPNO	540
PROCNO	1
F2 - Acquisition Parameters	
Date_	20150528
Time	9.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	287
DW	41.600 usec
DE	6.00 usec
TE	297.3 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	400.1300080 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

avtar_saifpu@yahoo.co.in

ECIB



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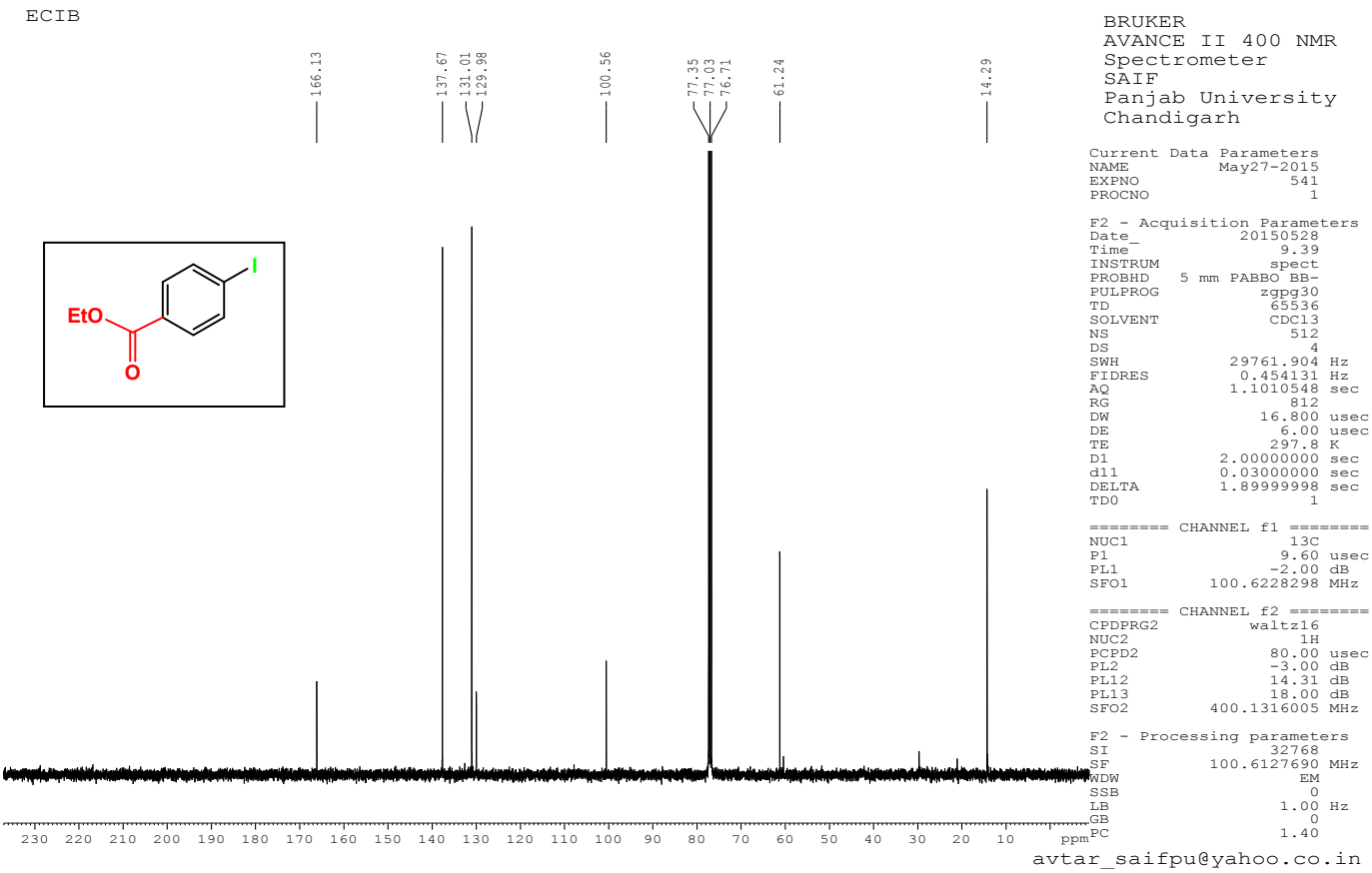
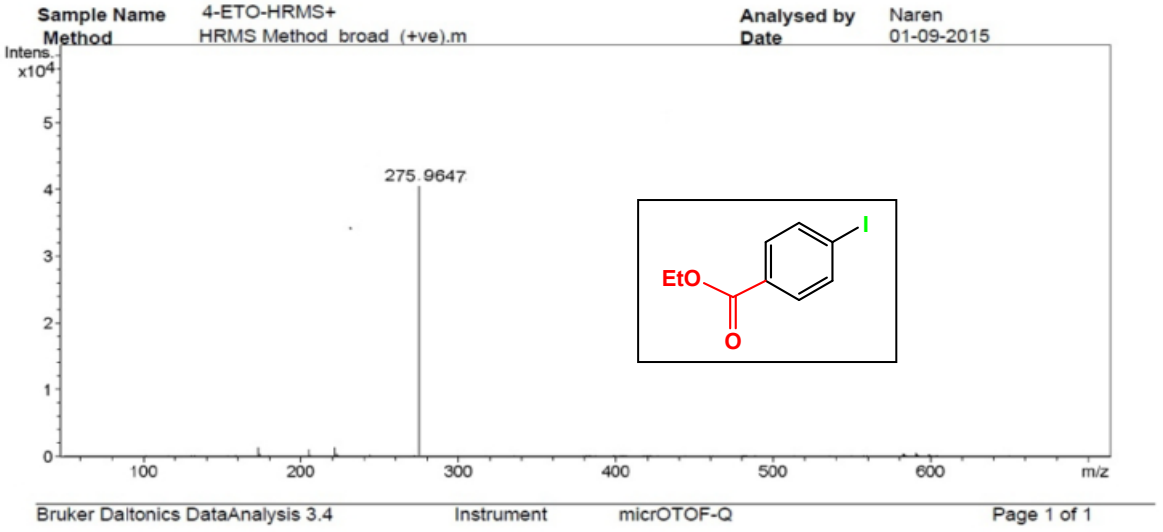
Current Data Parameters	
NAME	May27-2015
EXPNO	540
PROCNO	1
F2 - Acquisition Parameters	
Date_	20150528
Time	9.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	287
DW	41.600 usec
DE	6.00 usec
TE	297.3 K
D1	1.00000000 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	400.1300080 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

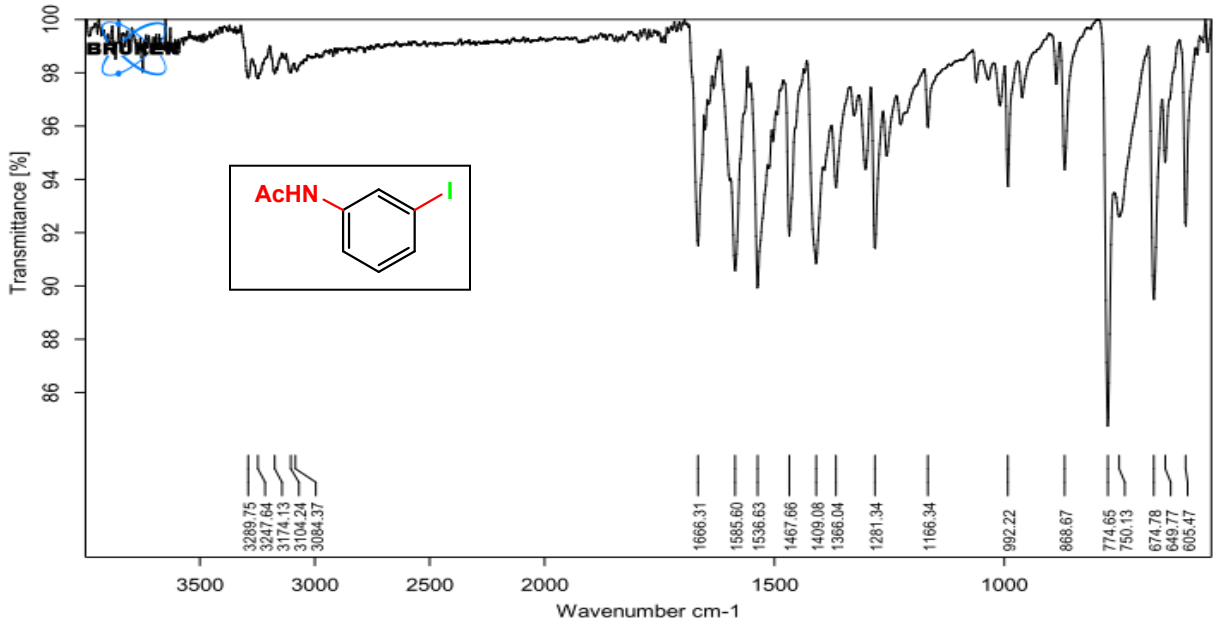
avtar_saifpu@yahoo.co.in



4-ETO COMPOUND

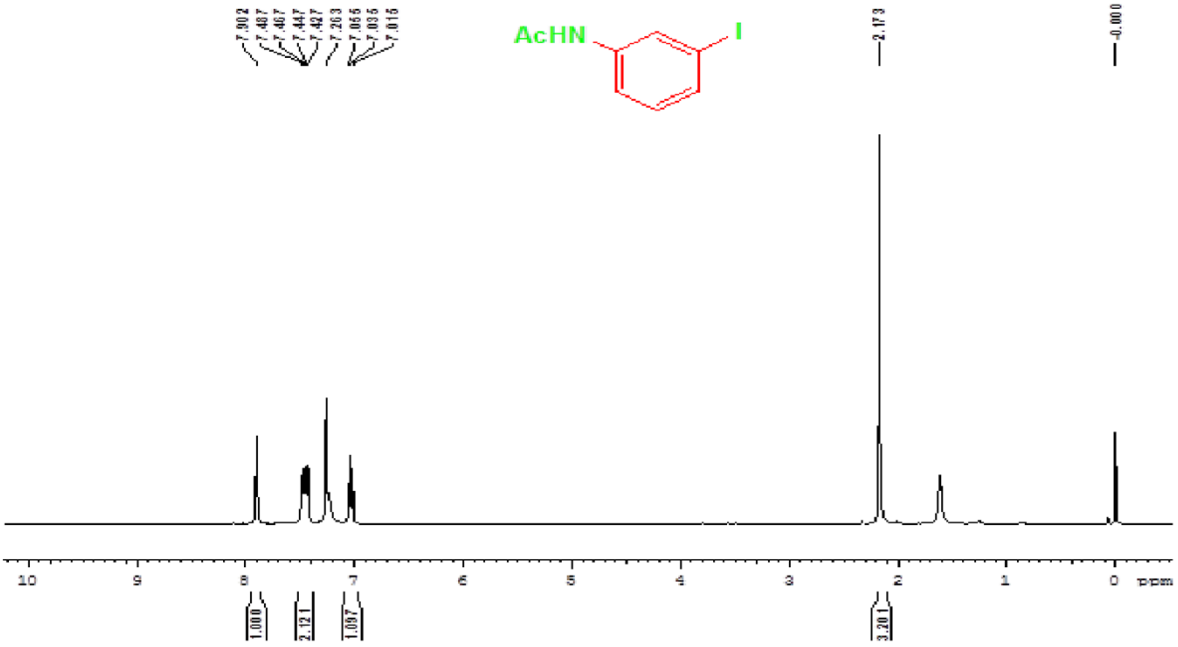


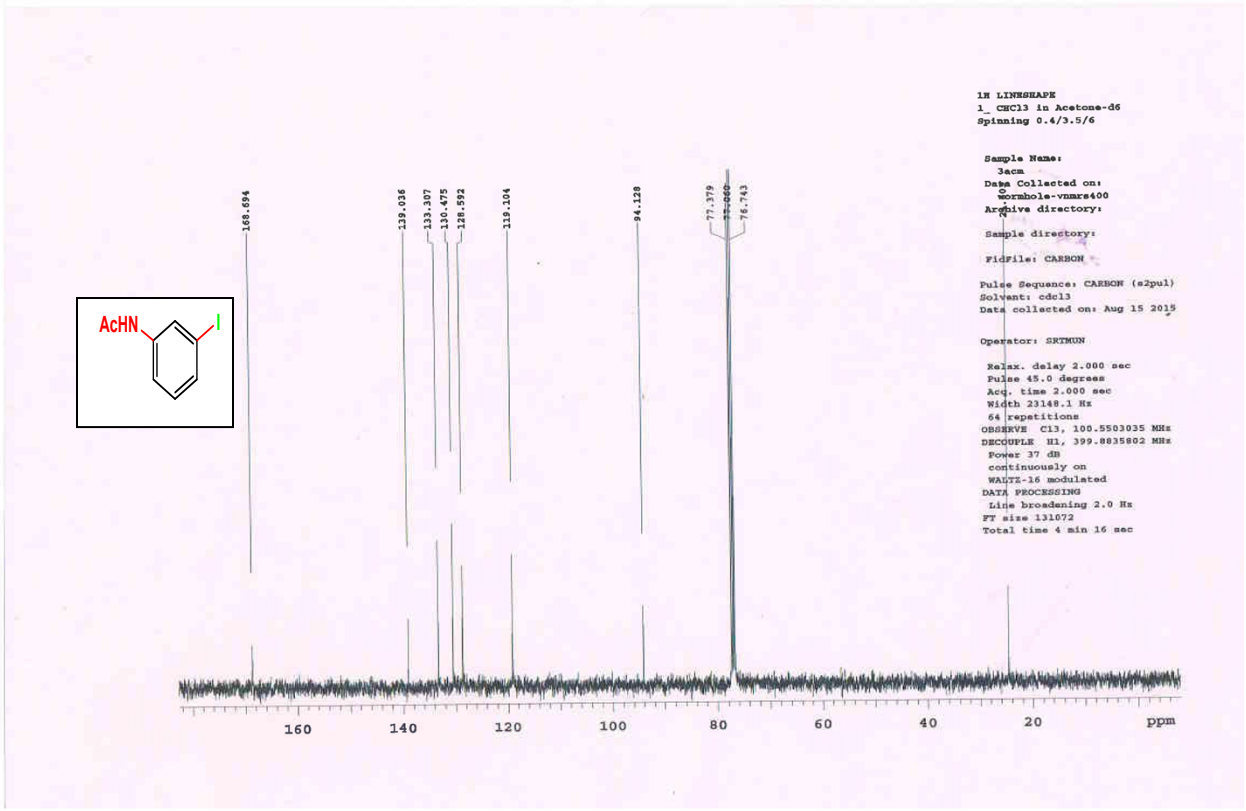
4.9 *N*-(3-iodophenyl)acetamide (2k):

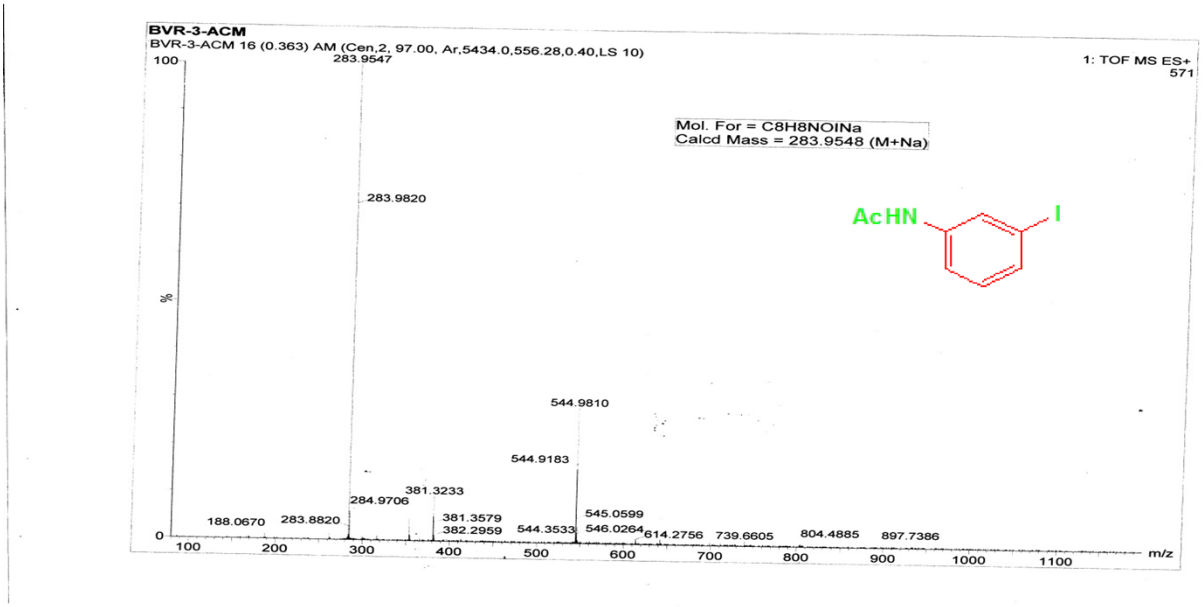


C:\Program Files\OPUS_65\MEAS\3ACM.0 3ACM OFF-WHITE 01/01/2002

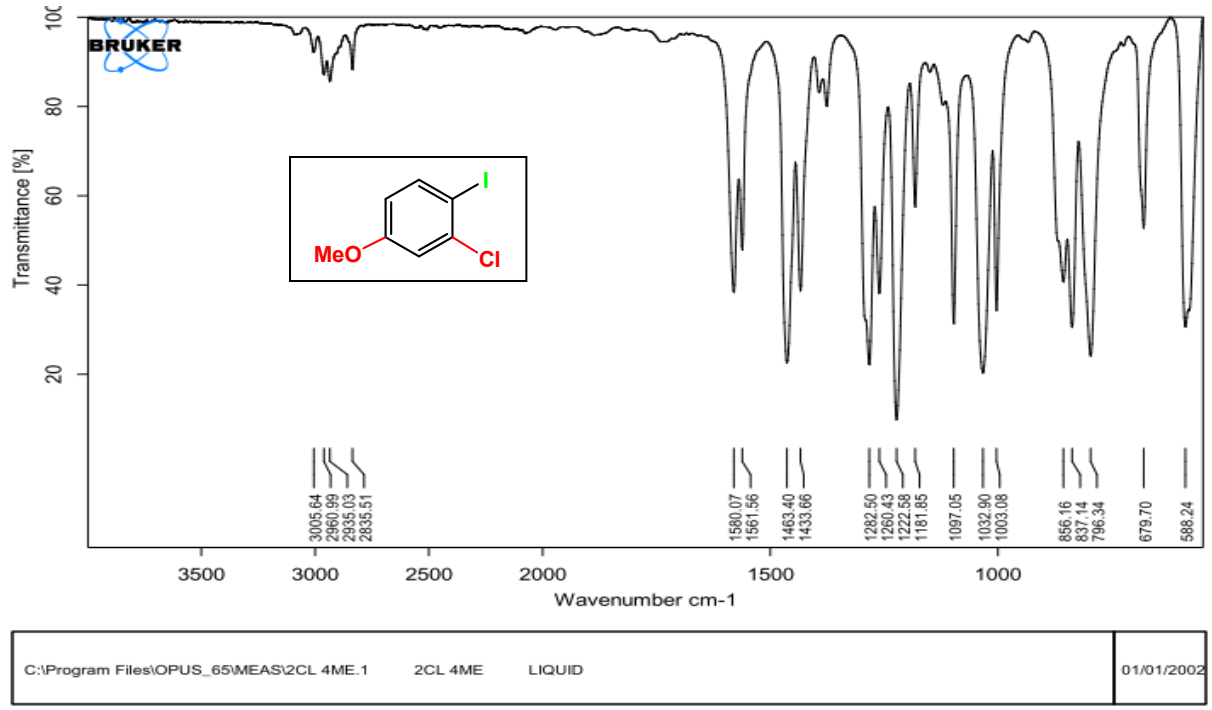
Page 1/1

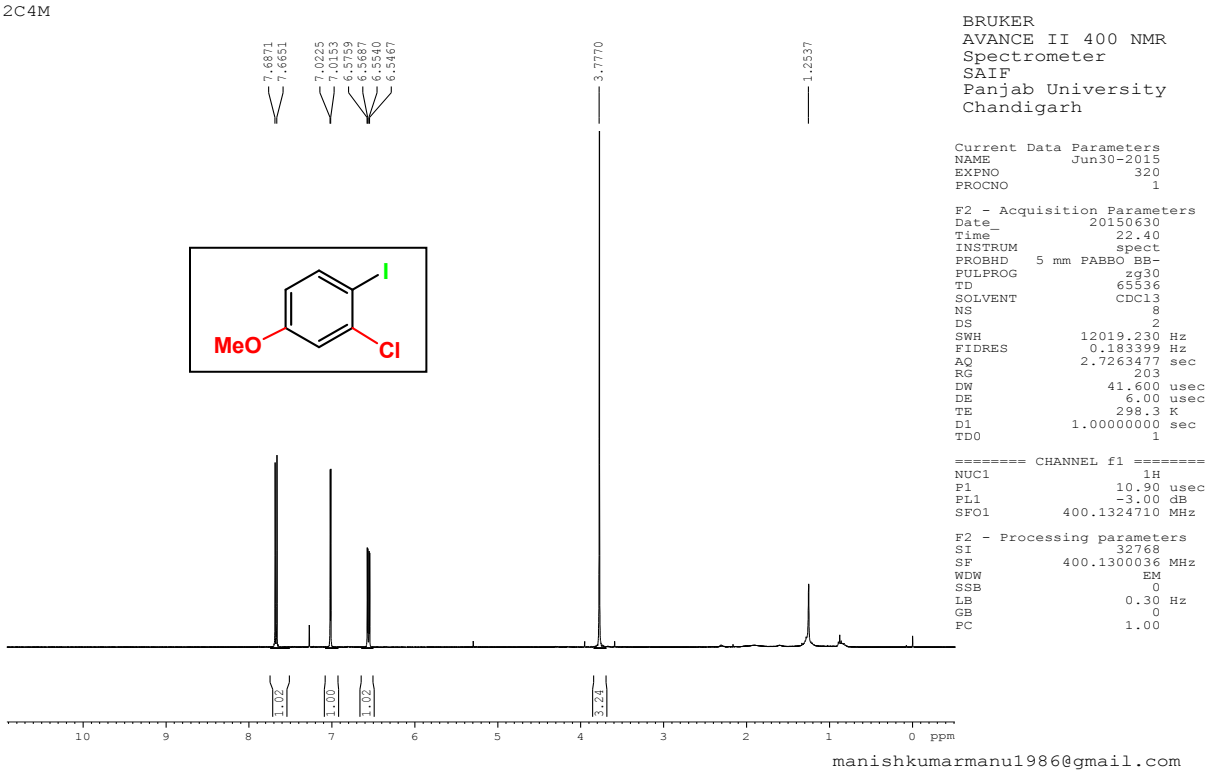



AcHN
I
168.694
139.036
133.307
130.475
128.592
119.104
94.128
77.379
76.743
160
140
120
100
80
60
40
20
ppm
1H LINESHAPE
1_ CHCl3 in Acetone-d6
Spinning 0.4/3.5/6
Sample Name:
3acm
Data Collected on:
wormhole-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 15 2015
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec

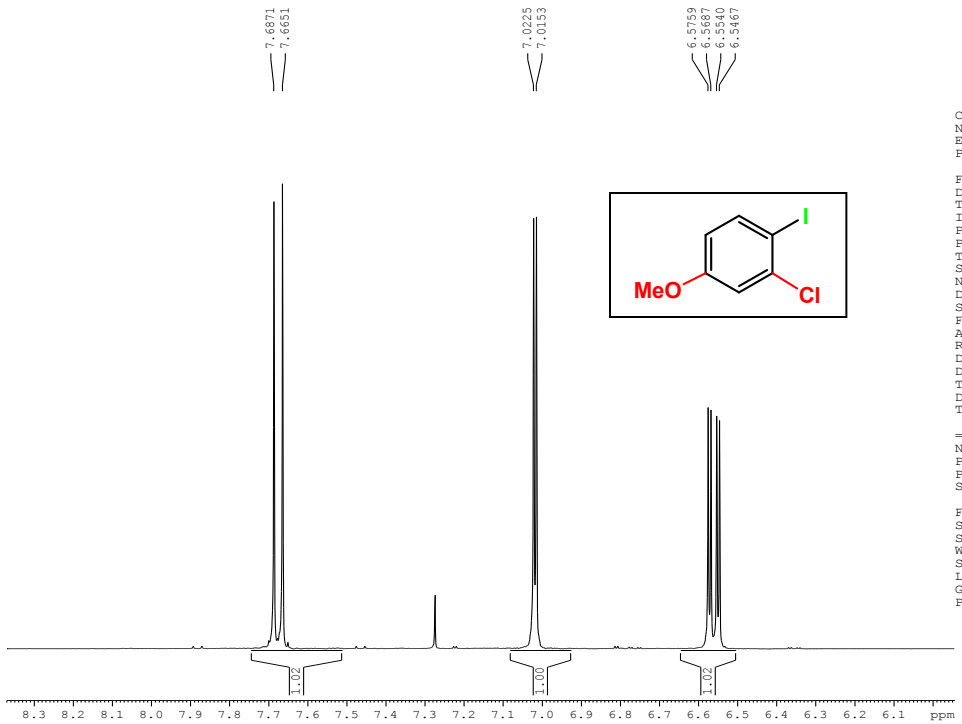

BVR-3-ACM
BVR-3-ACM 16 (0.363) AM (Cen,2, 97.00, Ar,5434.0,556.28,0.40,LS 10)
1: TOF MS ES+
571
Mol. For = C8H8NOINa
Calcd Mass = 283.9548 (M+Na)
AcHN
I
283.9547
283.9820
544.9810
544.9183
381.3233
284.9706
188.0670
283.8820
381.3579
382.2959
544.3533
545.0599
546.0264
614.2756
739.6605
804.4885
897.7386
%
m/z

4.10 2-Chloro-1-iodo-4-methoxybenzene (2l)





2C4M



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Current Data Parameters
NAME Jun30-2015
EXPNO 320
PROCNO 1

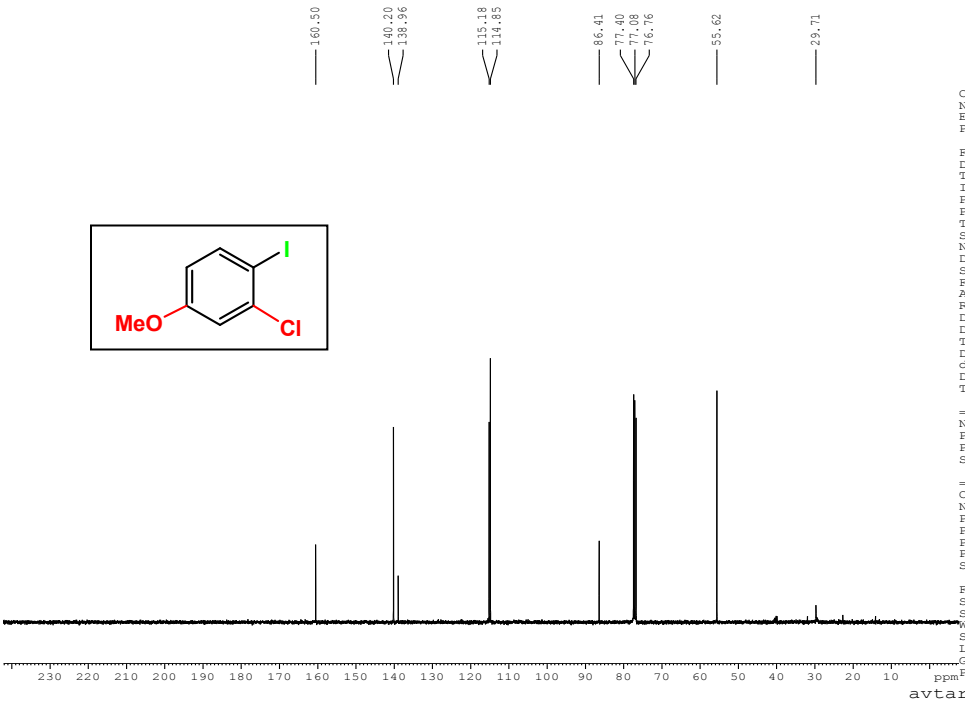
F2 - Acquisition Parameters
Date_ 20150630
Time 22.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 203
DW 41.600 usec
DE 6.00 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

manishkumarmanu1986@gmail.com

2C4M



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Current Data Parameters
NAME Jun30-2015
EXPNO 321
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150630
Time 23.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 406
DW 16.800 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

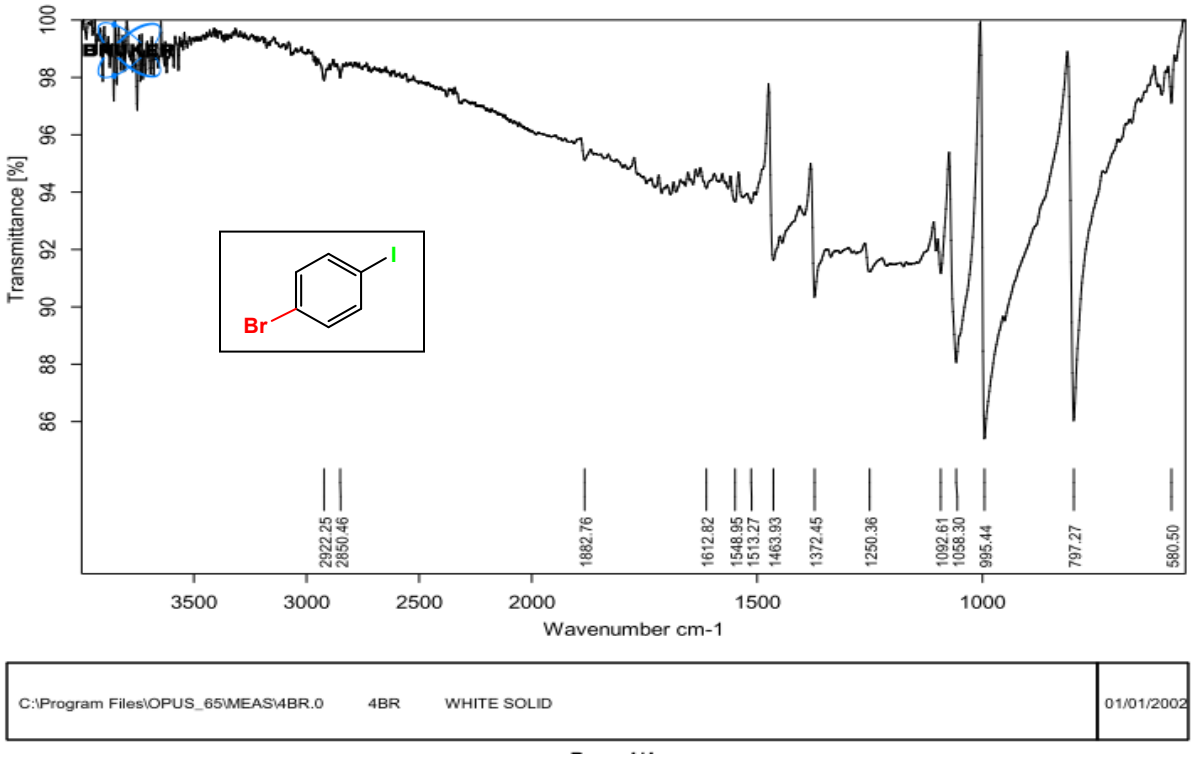
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

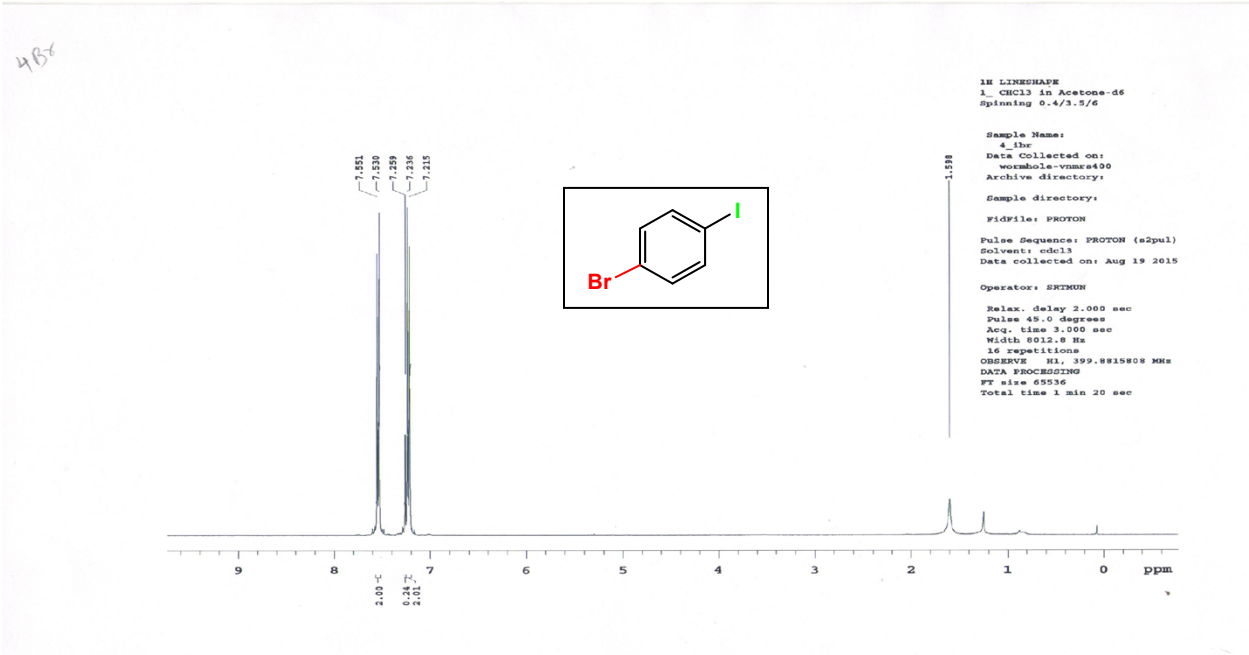
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

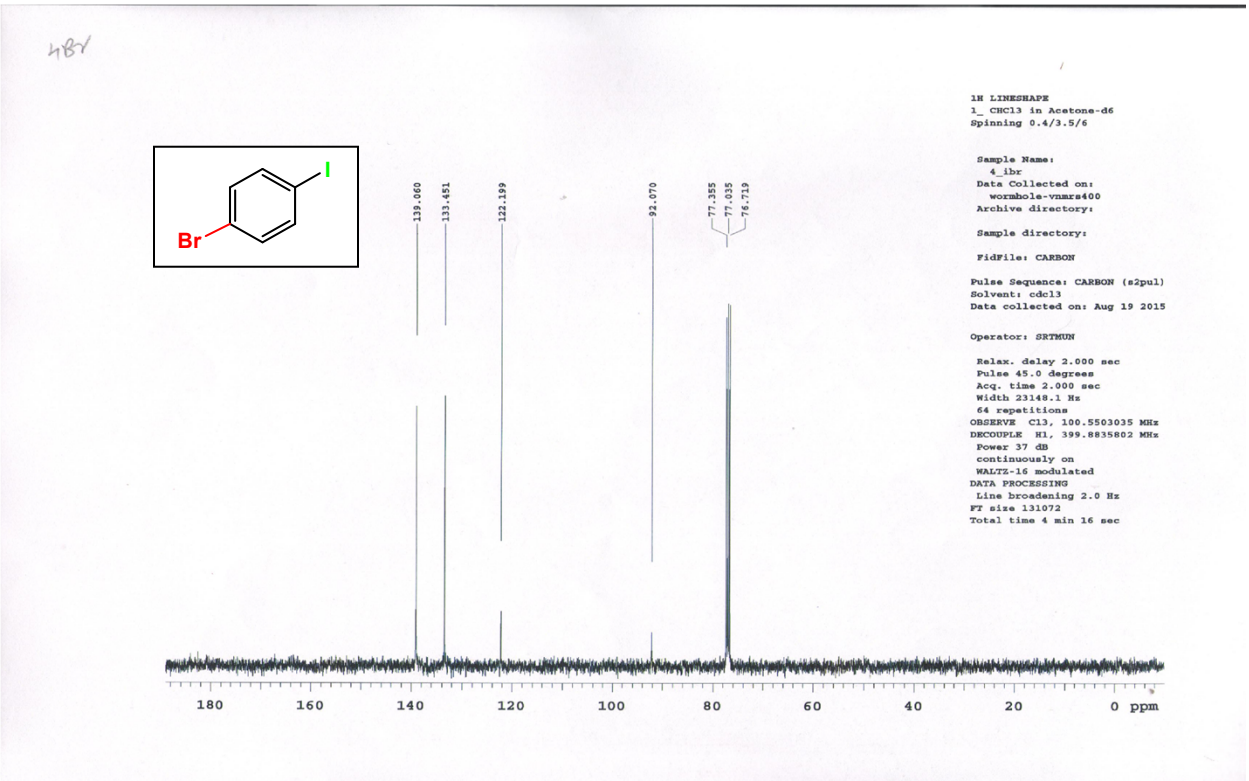
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

avtar_saifpu@yahoo.co.in

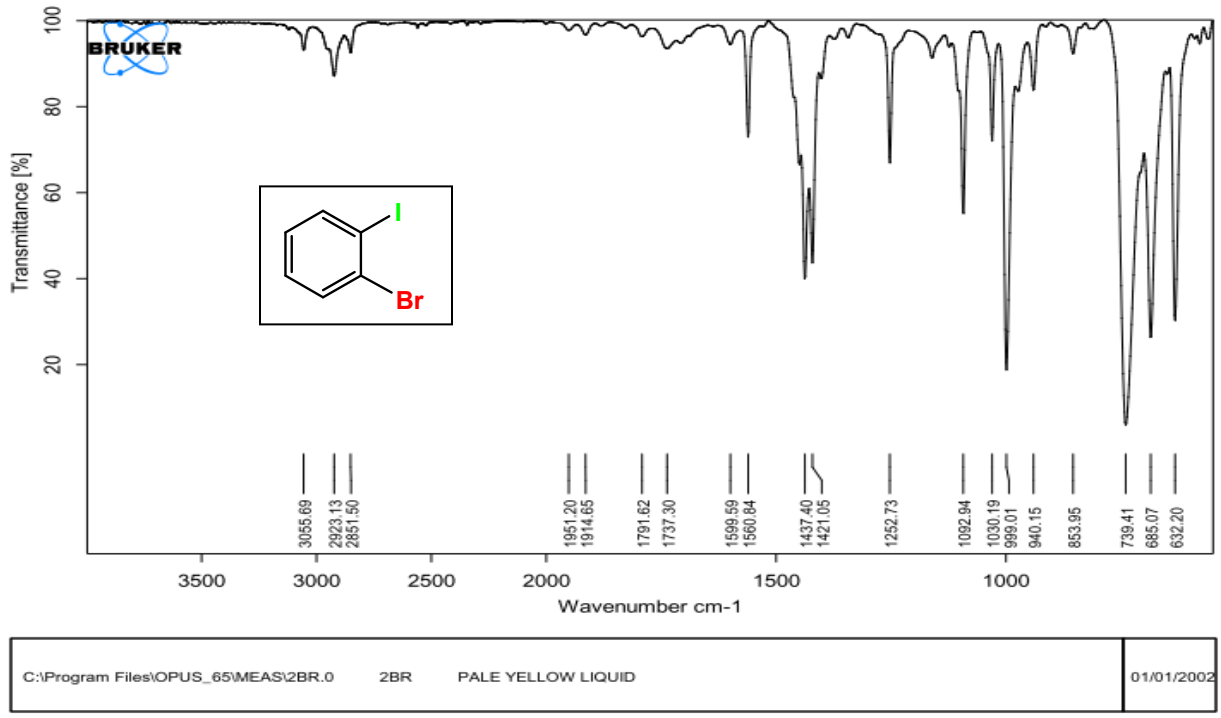
4.11 1-Bromo-4-iodobenzene (2m):

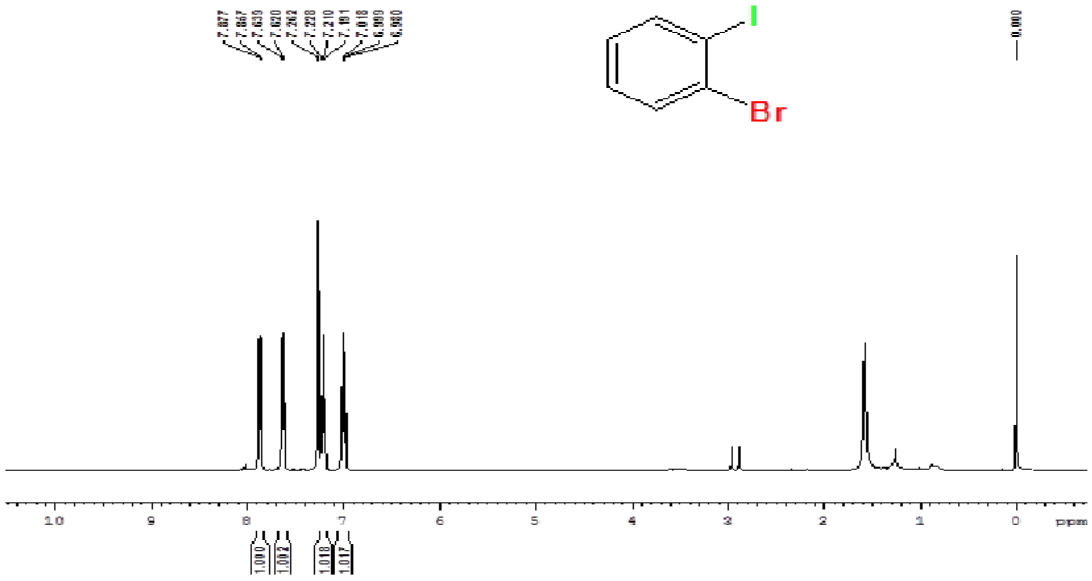


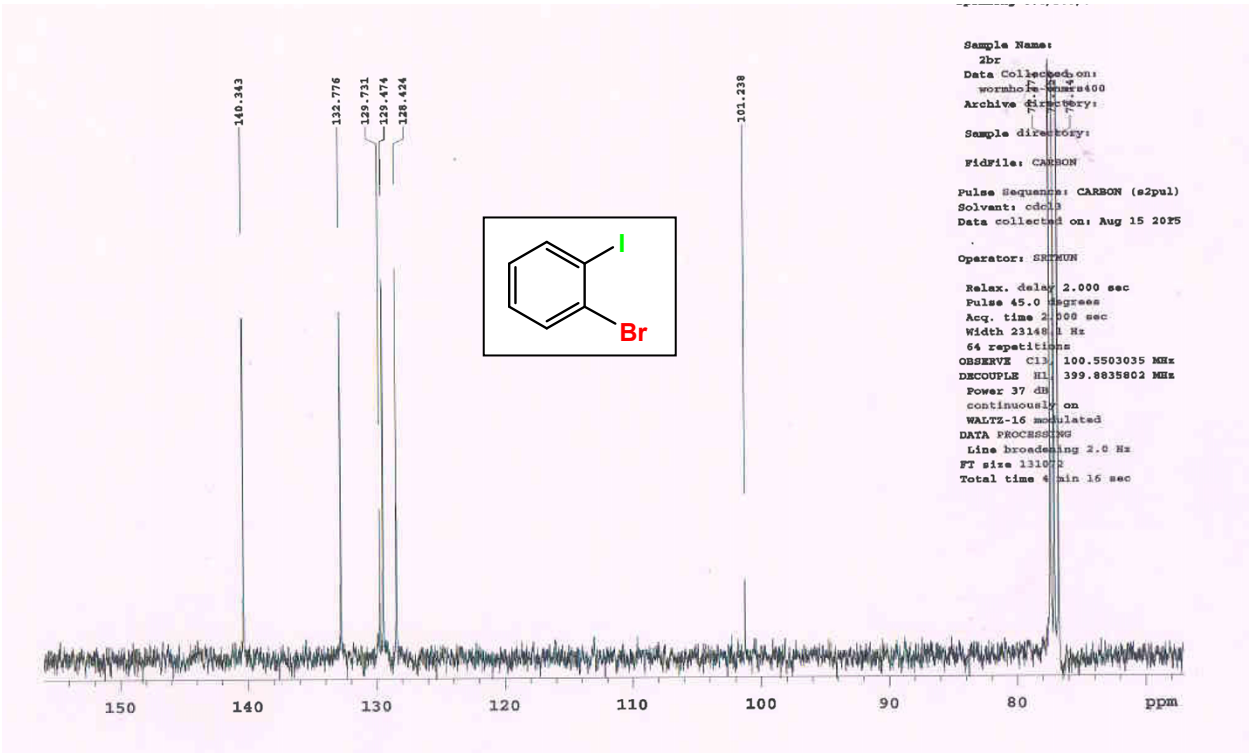


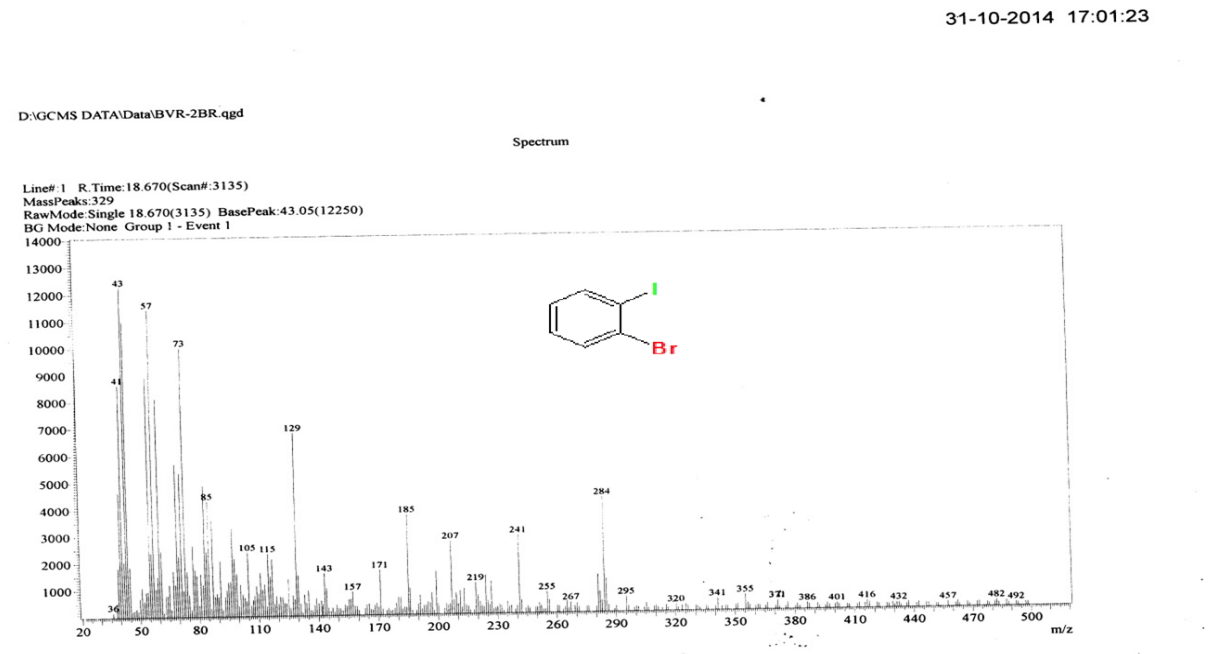


4.12 1-Bromo-2-iodobenzene (2n):

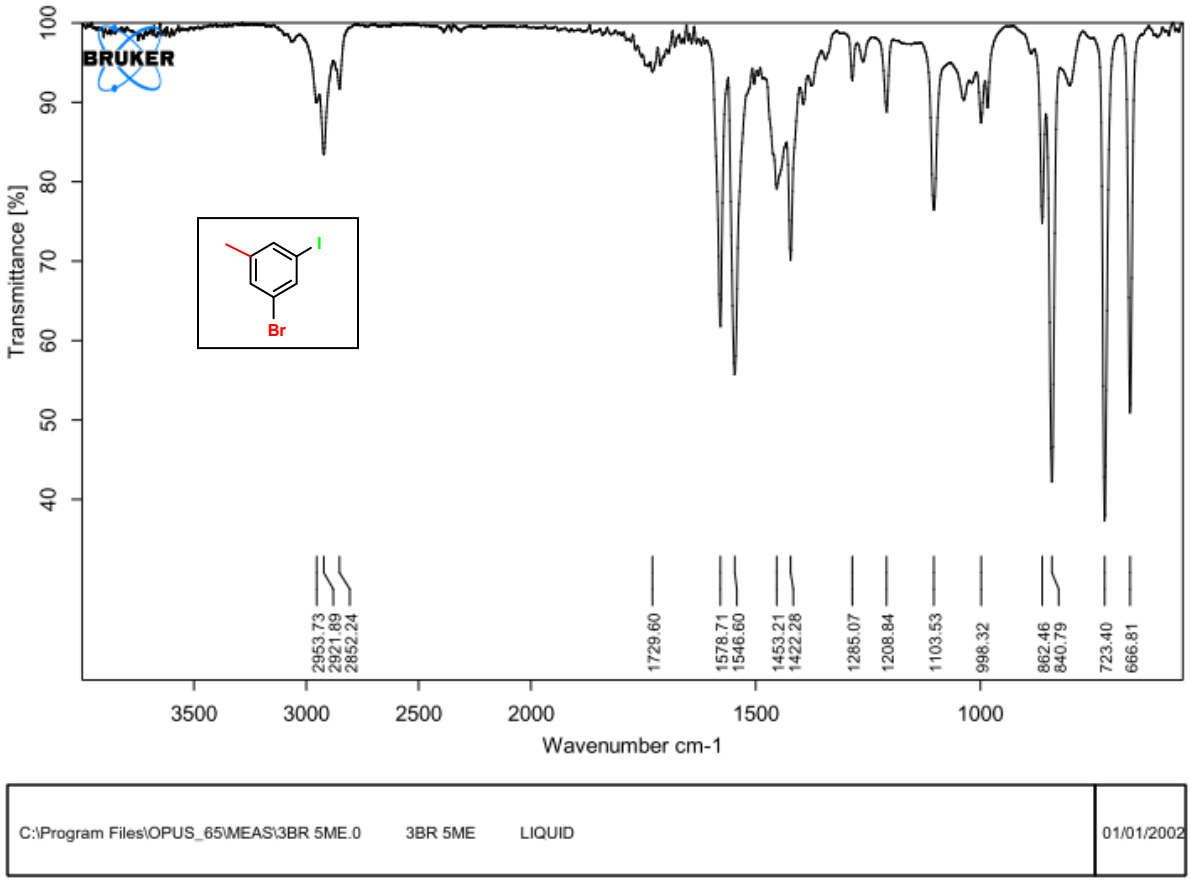


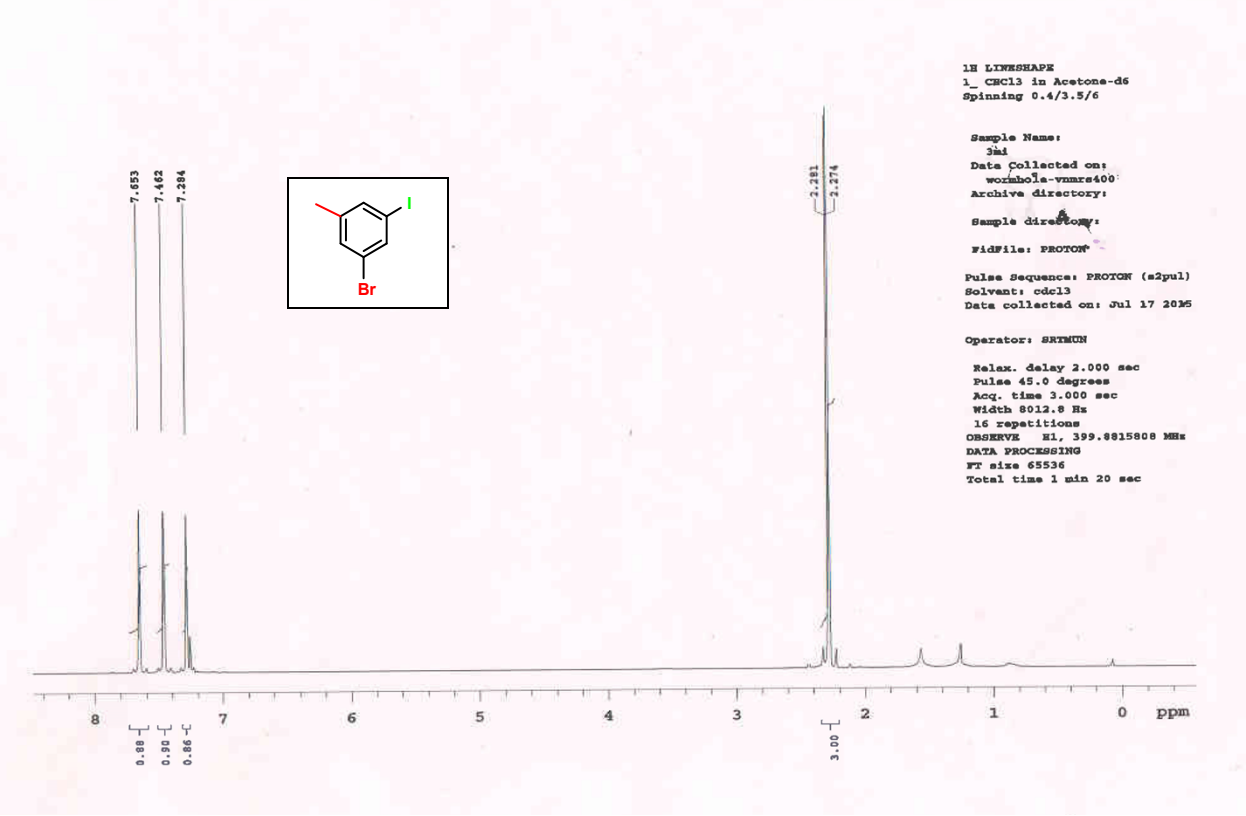

7.877
7.867
7.639
7.620
7.342
7.328
7.210
7.191
7.018
6.999
6.980
0.000
I
Br
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.042
4.018
4.017

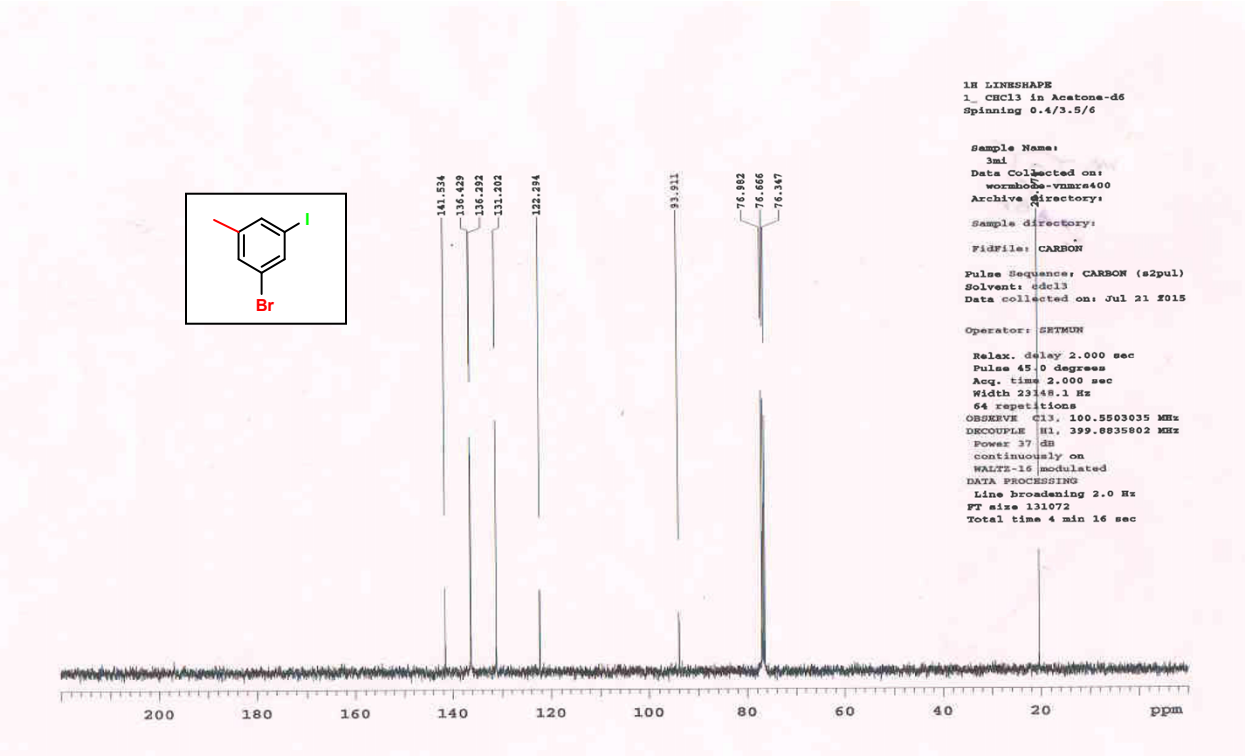

140.343
132.776
129.731
129.474
128.424
101.238
Sample Name:
2br
Data Collected on:
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 15 2025
Operator: SRIMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec
I
Br
150
140
130
120
110
100
90
80
ppm



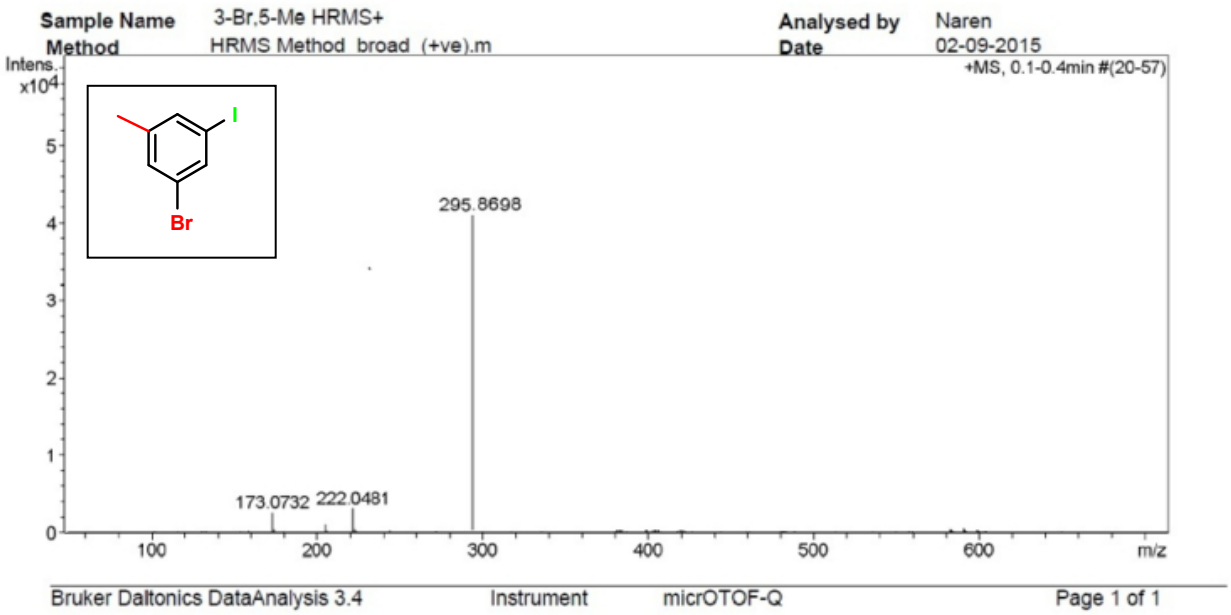
4.13 1-Bromo-3-iodo-5-methylbenzene (2o):



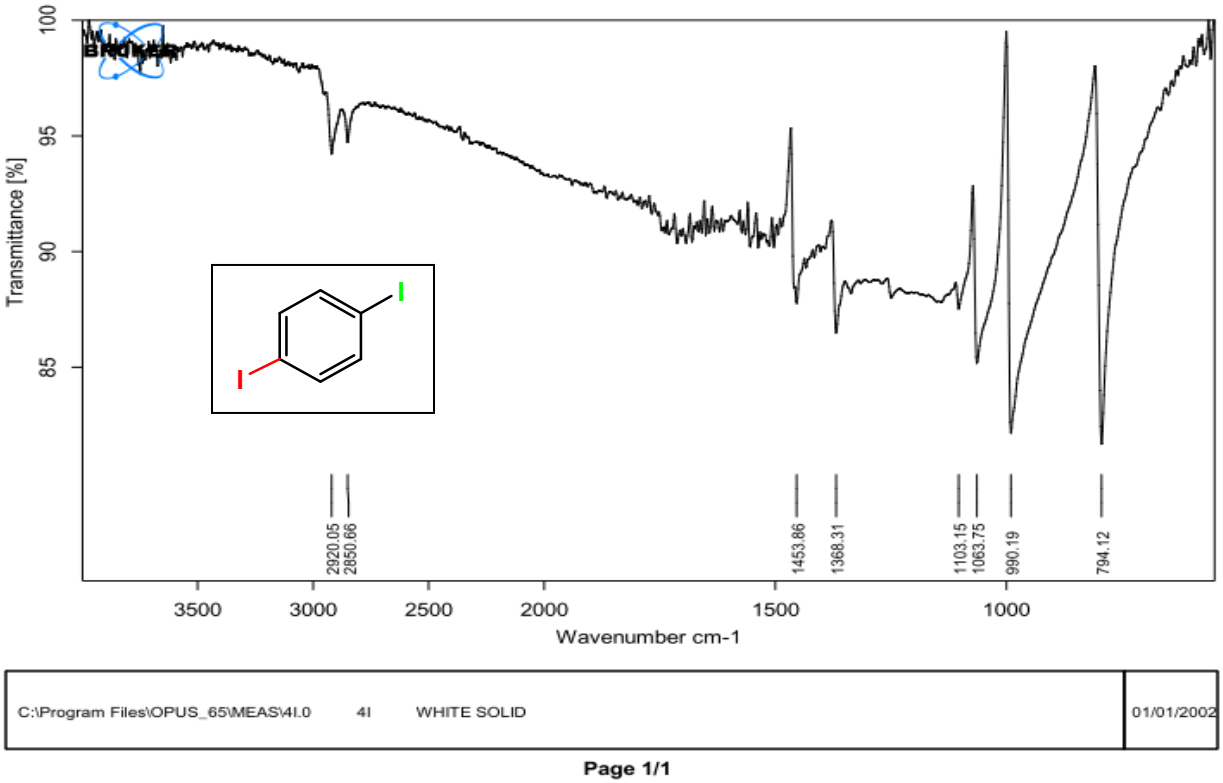

1H LINESHAPE
1_ CHCl3 in Acetone-d6
Spinning 0.4/3.5/6
Sample Name:
3mi
Data Collected on:
wormhole-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 17 2015
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 20 sec
7.653
7.462
7.284
2.281
2.274
I
Br
0.88
0.90
0.86
3.00
8
7
6
5
4
3
2
1
0
ppm

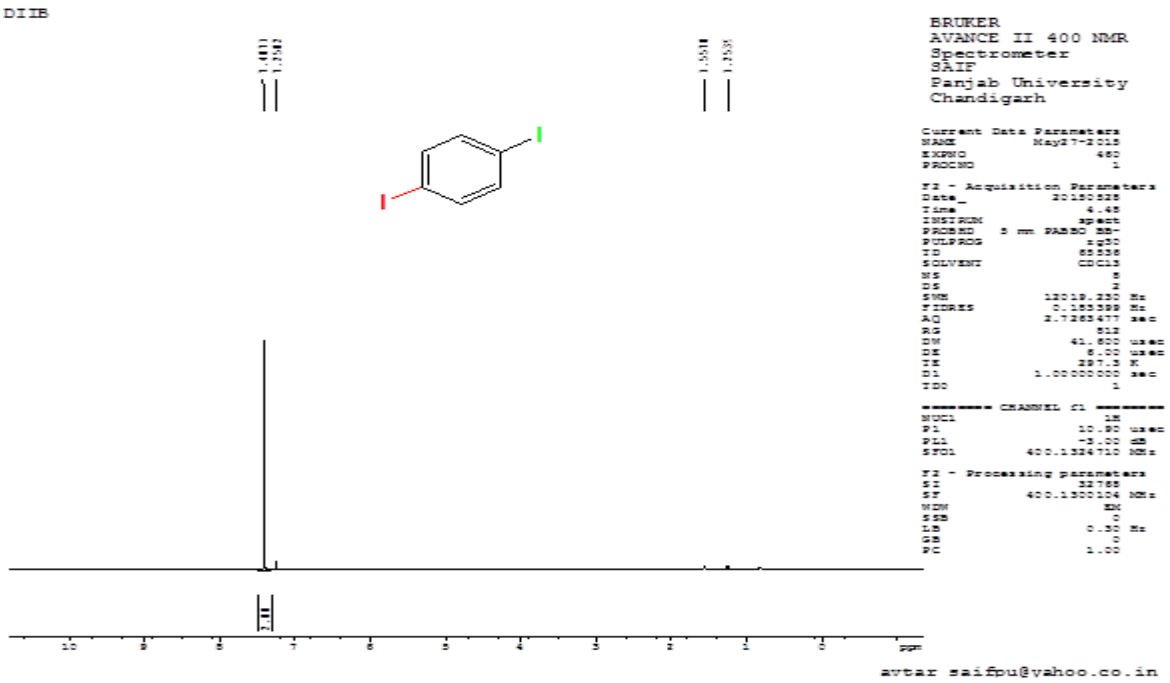

1H LINESHAPE
1_ CHCl3 in Acetone-d6
Spinning 0.4/3.5/6
Sample Name:
3mi
Data Collected on:
wormhole-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 21 2015
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec
141.534
136.429
136.292
131.202
122.294
93.911
76.982
76.666
76.347
29.925
I
Br
200
180
160
140
120
100
80
60
40
20
ppm

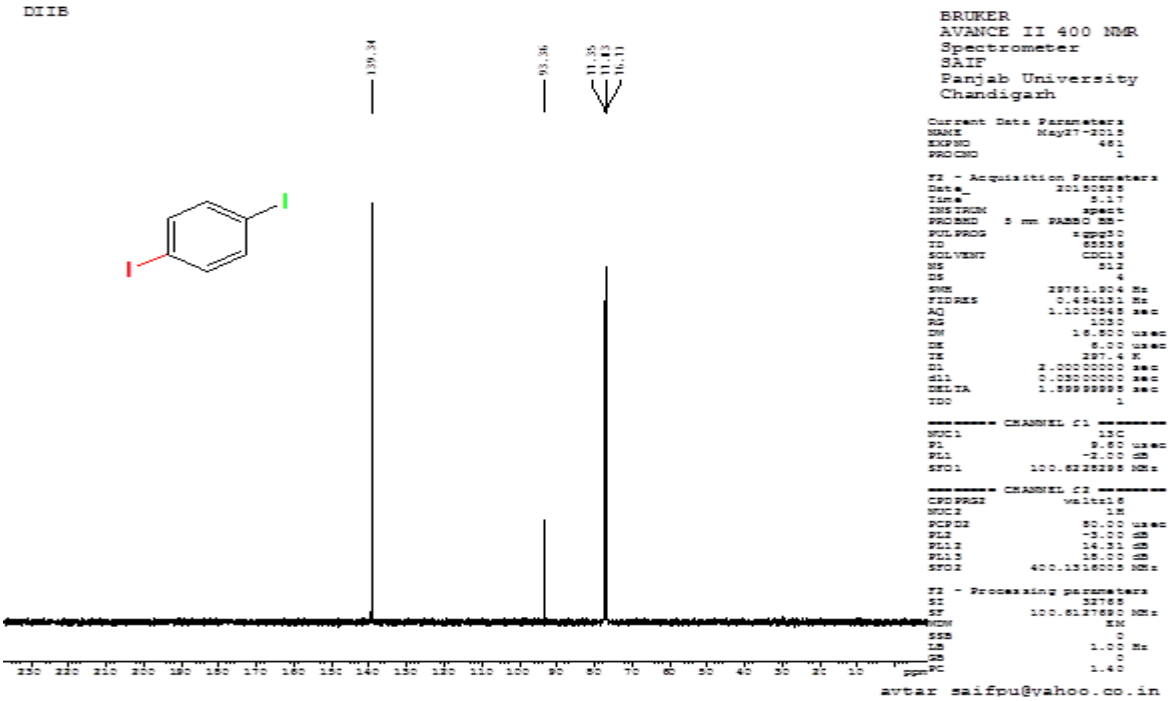
3-Br 5-Me COMPOUND



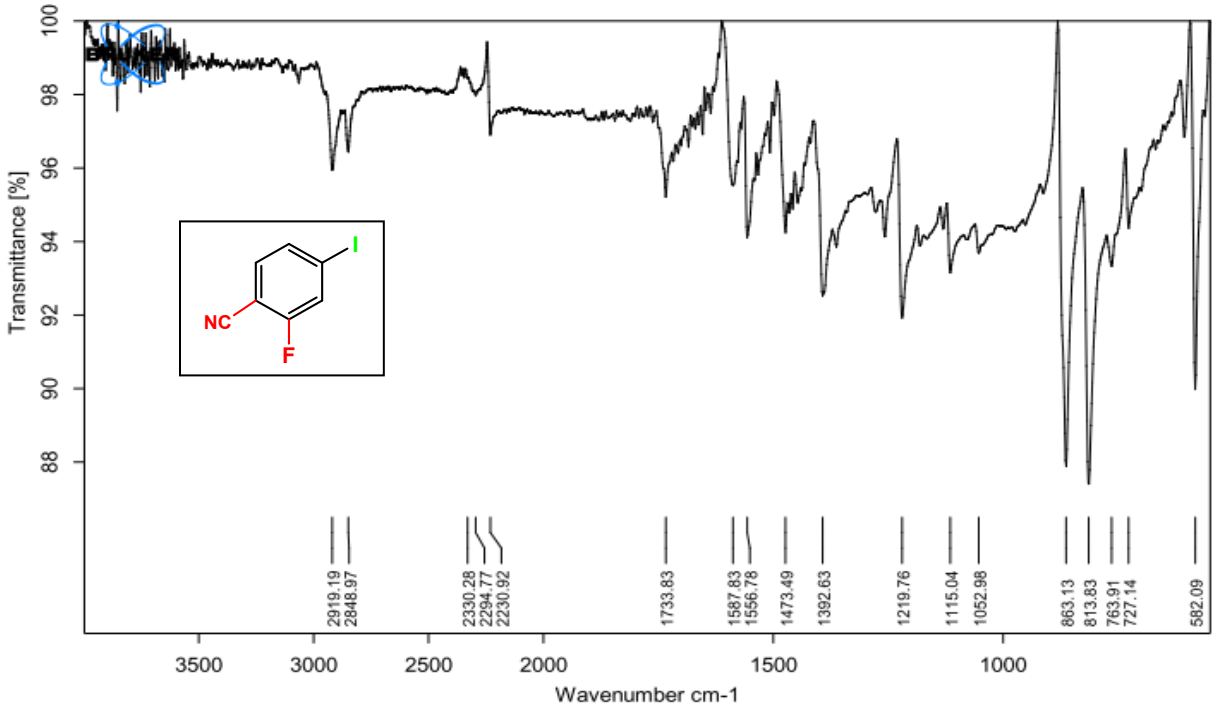
4.14 1,4-Diiodobenzane (2p):



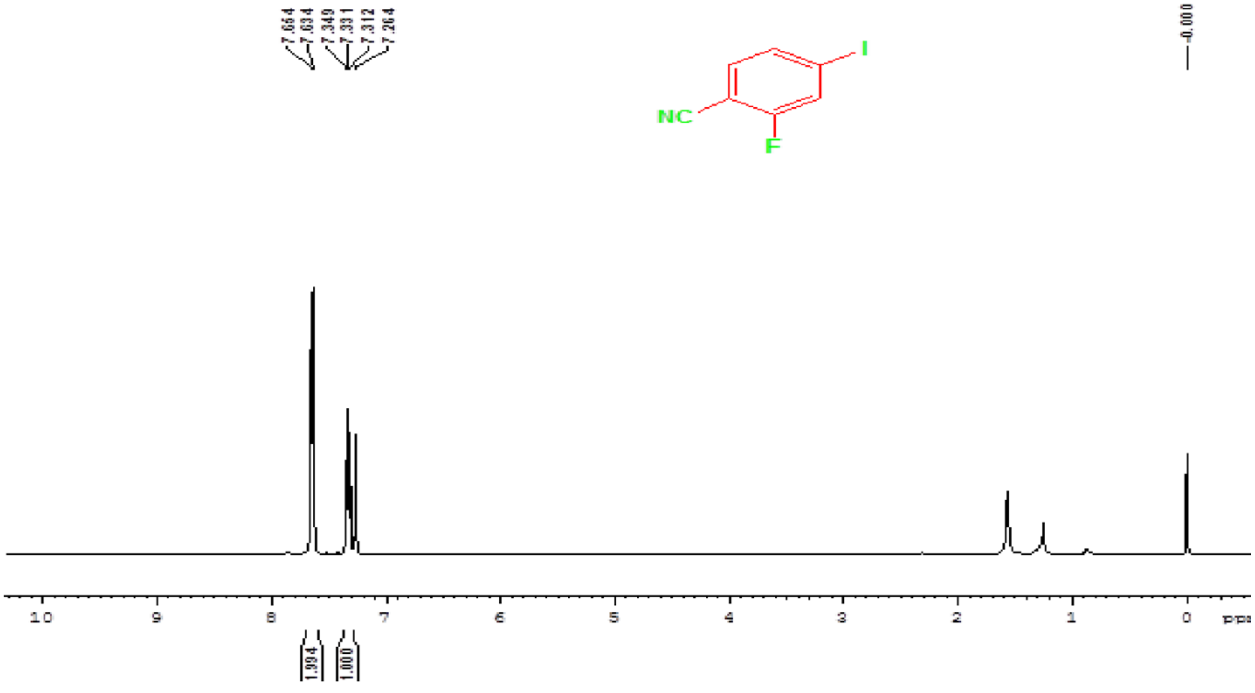


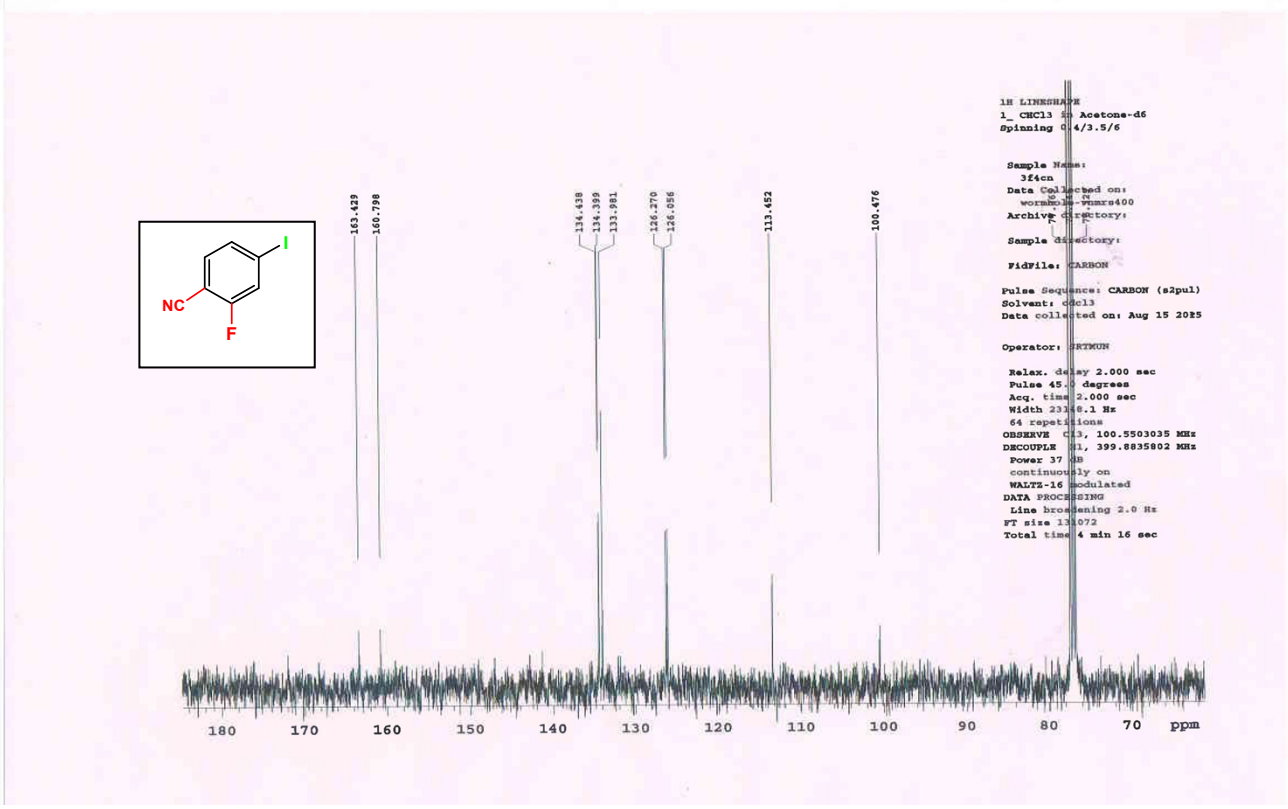


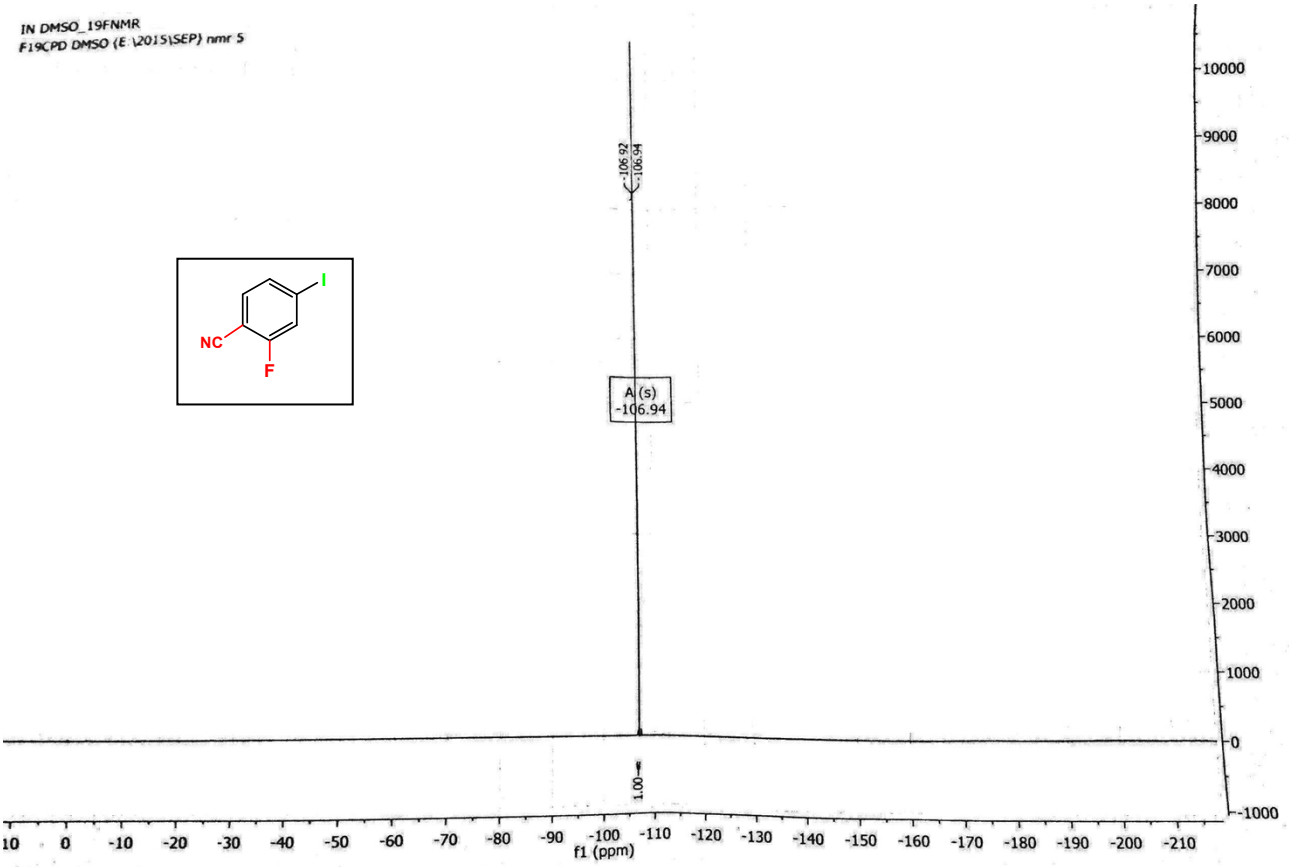
4.12 2-Fluoro-4-iodobenzonitrile (2q):



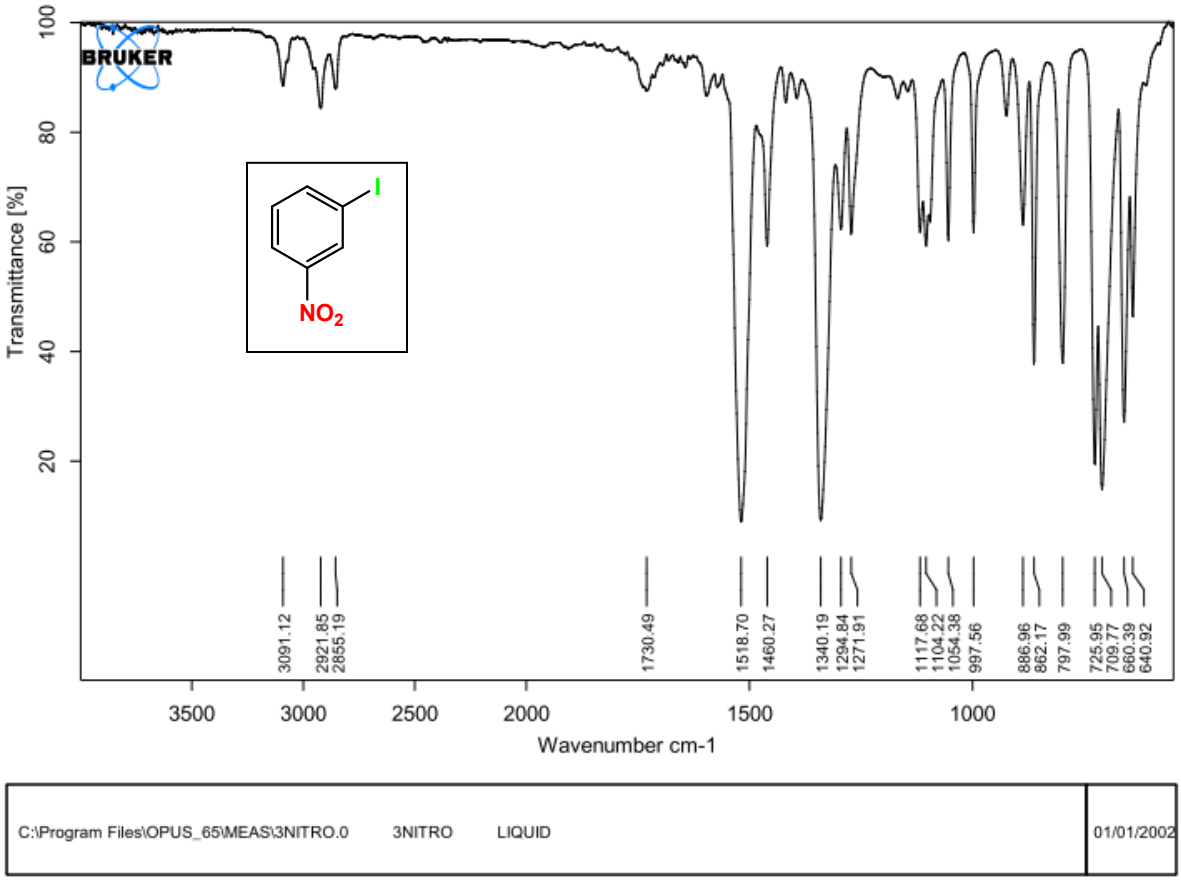
C:\Program Files\OPUS_65\MEAS\3F4CN.0	3F4CN	PALE YELLOW SOLID	01/01/2002



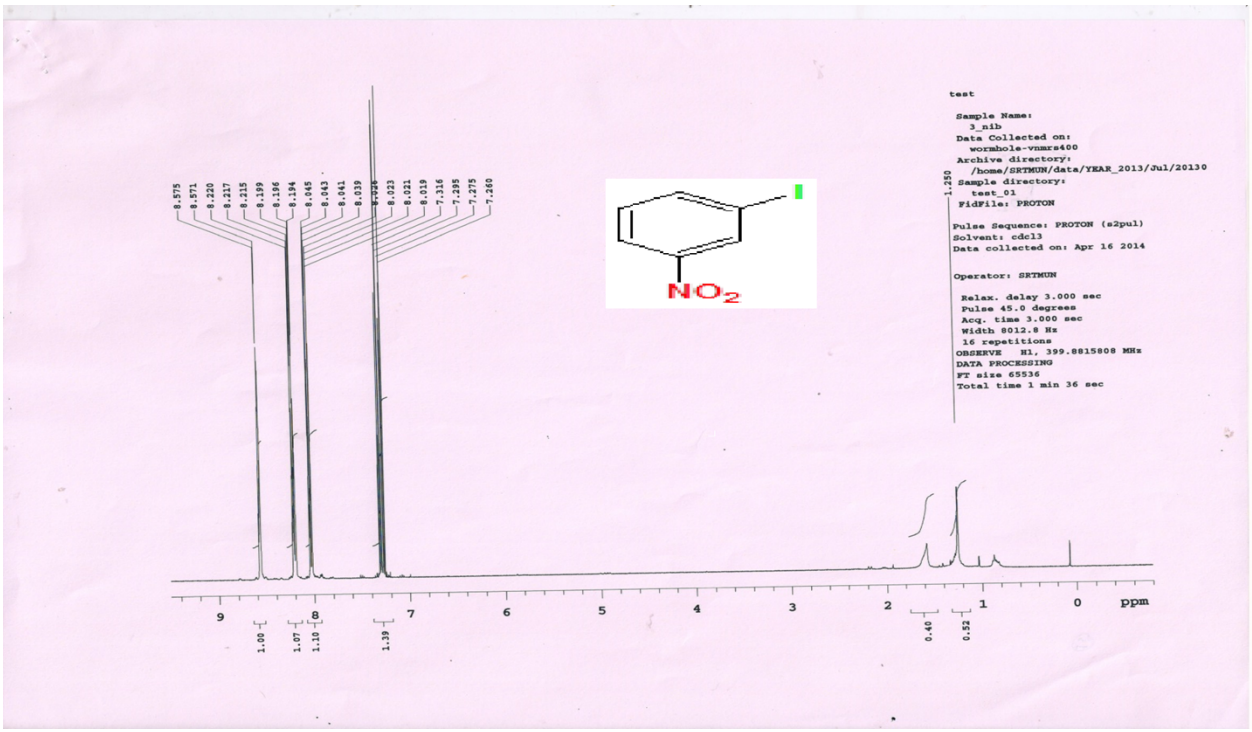

I
NC
F
163.429
160.798
134.438
134.399
133.981
126.270
126.056
113.452
100.476
1H LINESHAPE
1_ CHCl3 in Acetone-d6
Spinning
Sample Name:
3f4cn
Data Collected on:
wormhole-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 15 2025
Operator:
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec
180
170
160
150
140
130
120
110
100
90
80
70
ppm

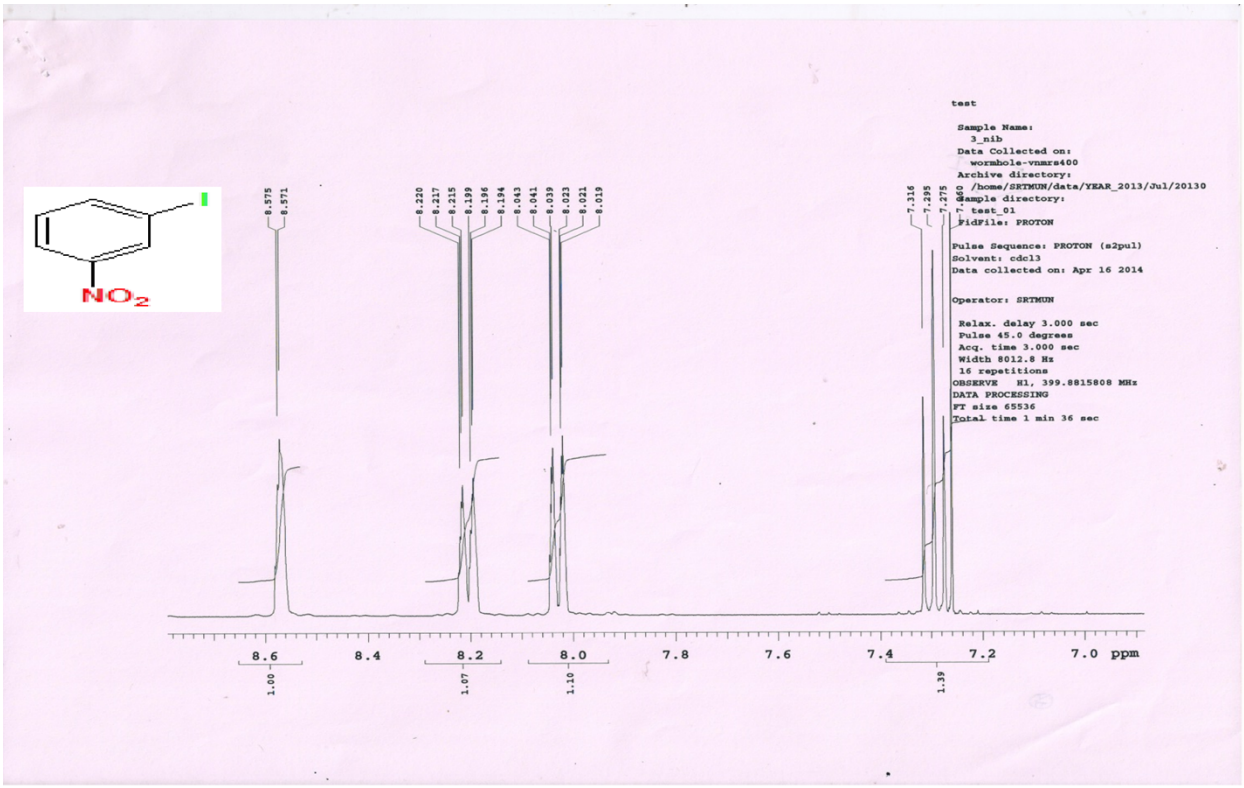


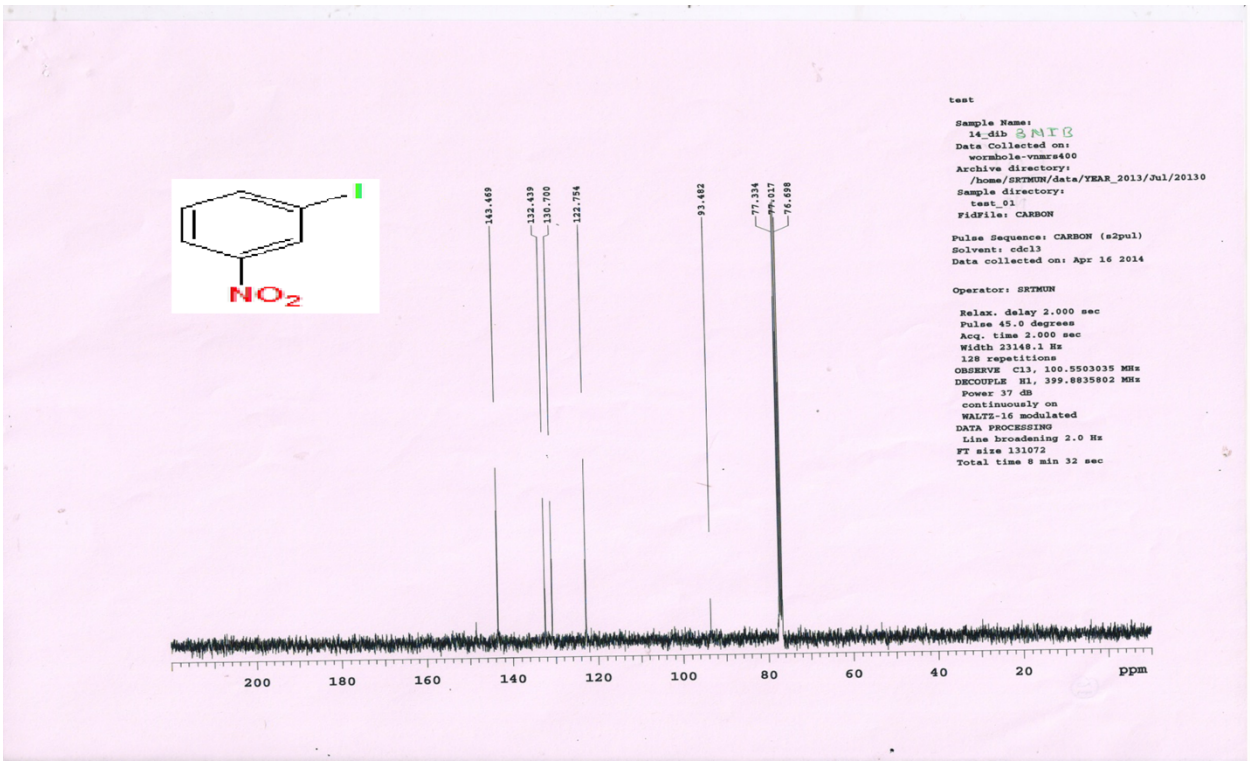
4.13 1-Iodo-3-nitrobenzene (2r):

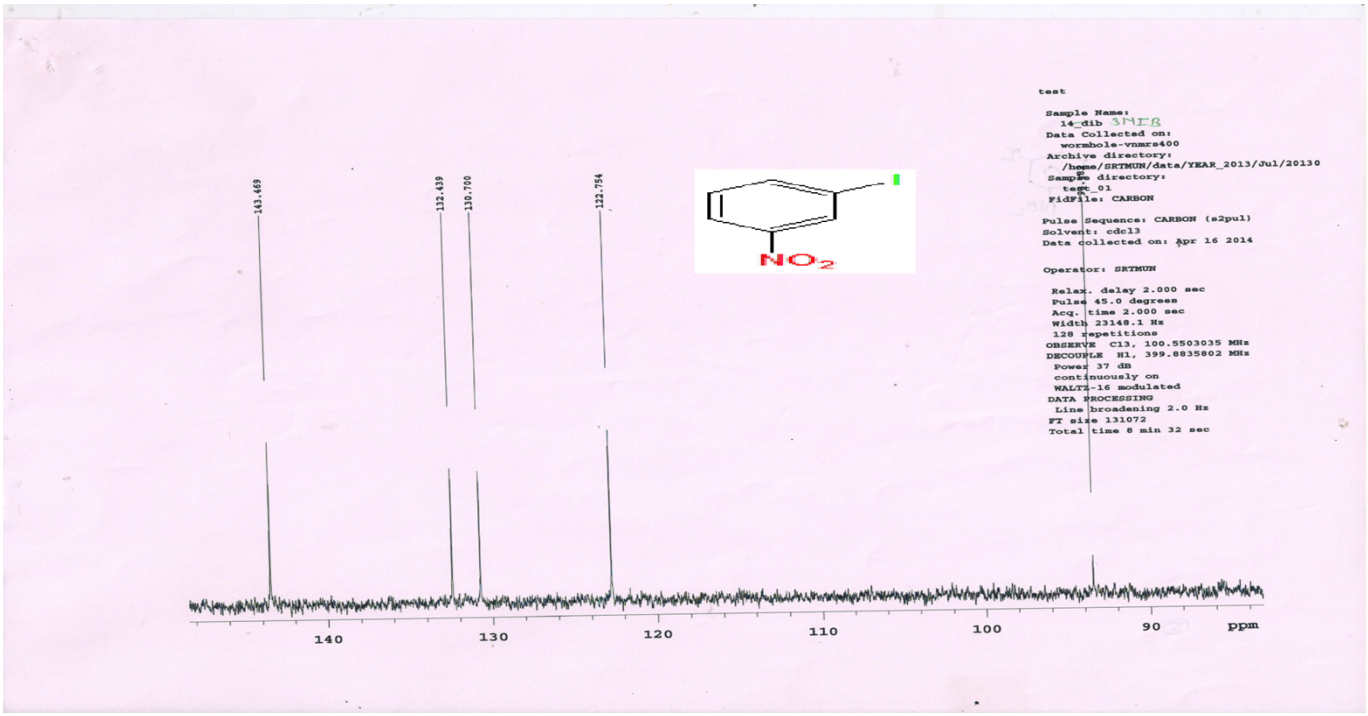


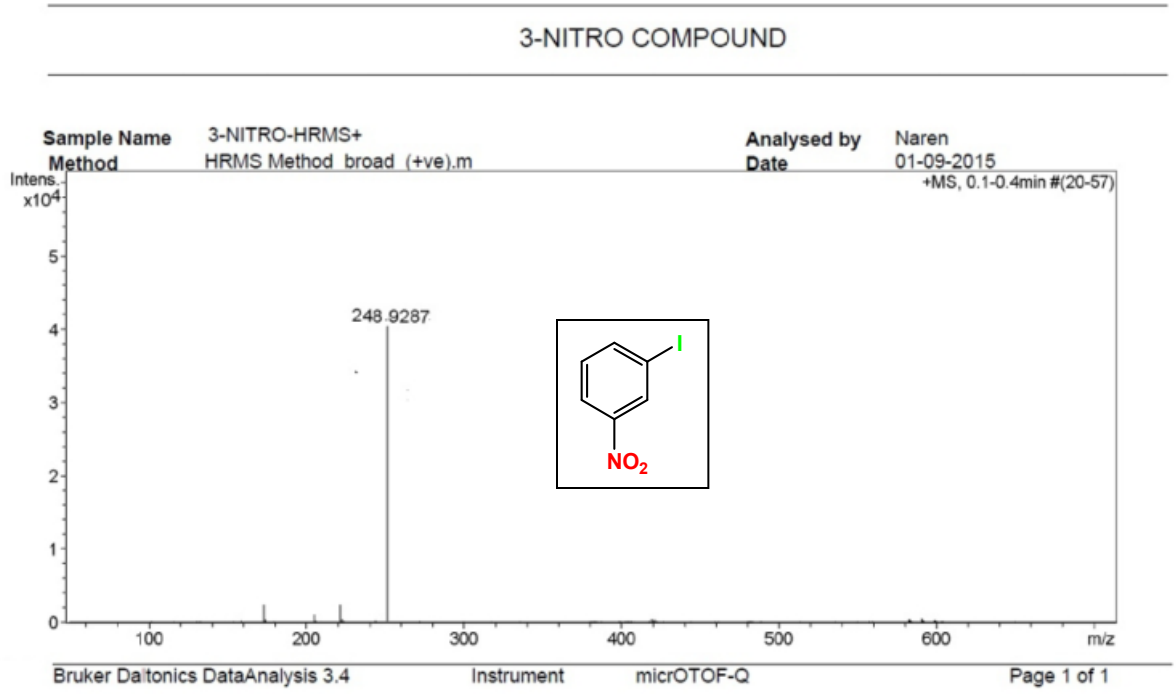
C:\Program Files\OPUS_65\MEAS\3NITRO.0	3NITRO	LIQUID	01/01/2002


test
Sample Name:
3_nib
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 36 sec
NO2
ppm

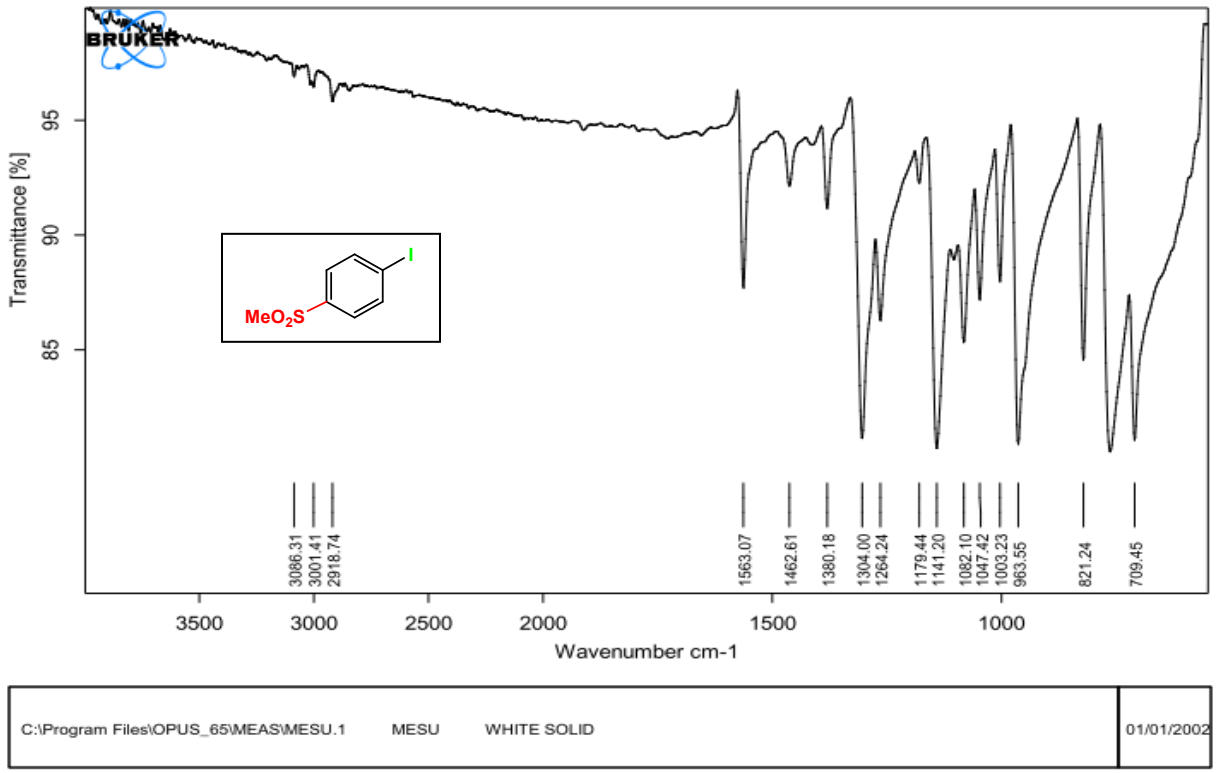

test
Sample Name:
3_nib
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 36 sec
NO2
ppm

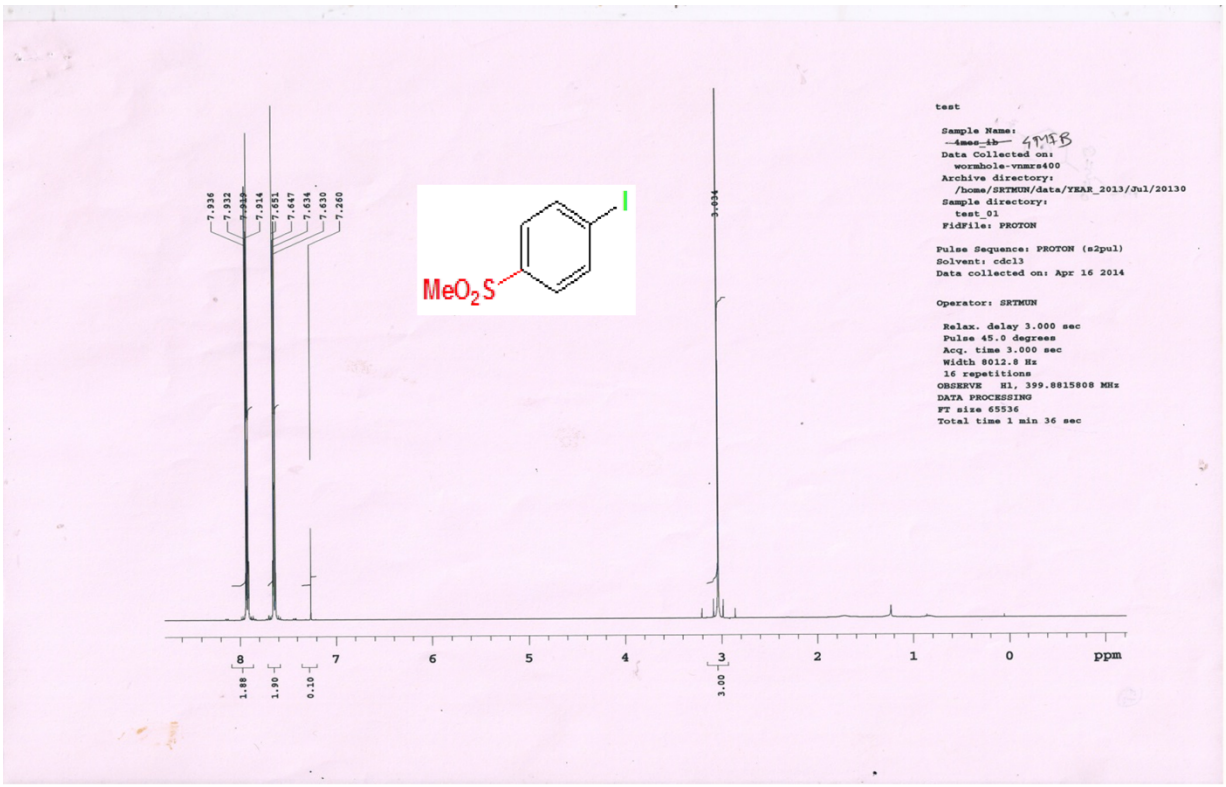

NO2
143.469
132.439
130.700
122.754
93.482
77.334
77.017
76.698
200
180
160
140
120
100
80
60
40
20
ppm
test
Sample Name:
14_dib 3MIB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
128 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 8 min 32 sec

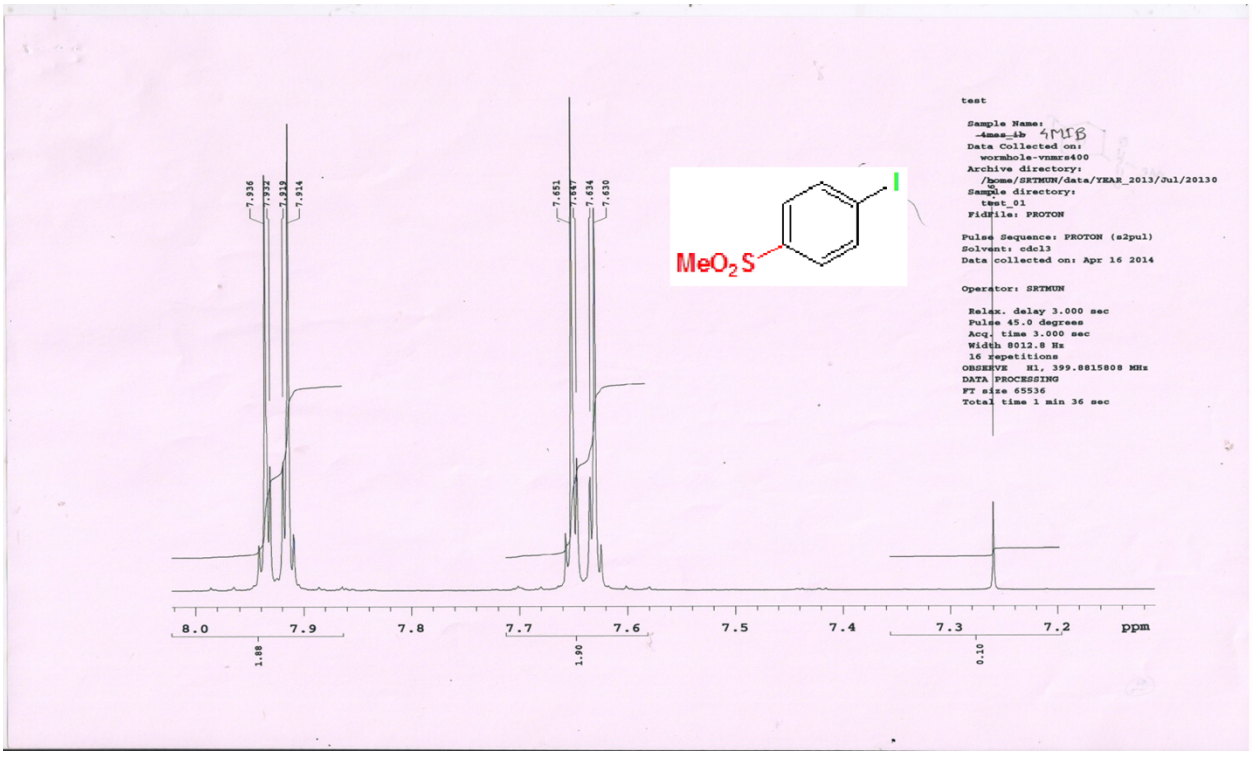

NO2
143.469
132.439
130.700
122.754
140
130
120
110
100
90
ppm
test
Sample Name:
14_dib 3MIB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
128 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 8 min 32 sec

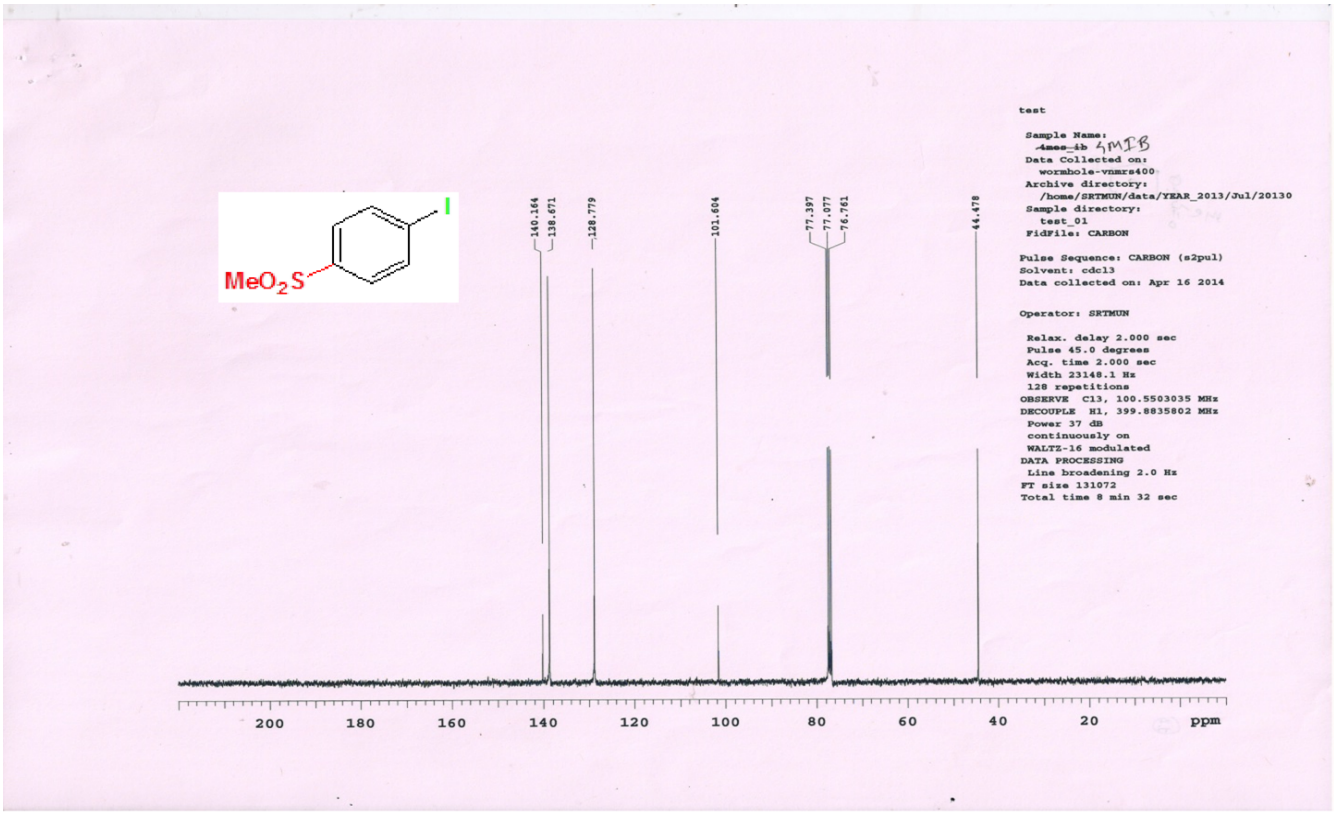


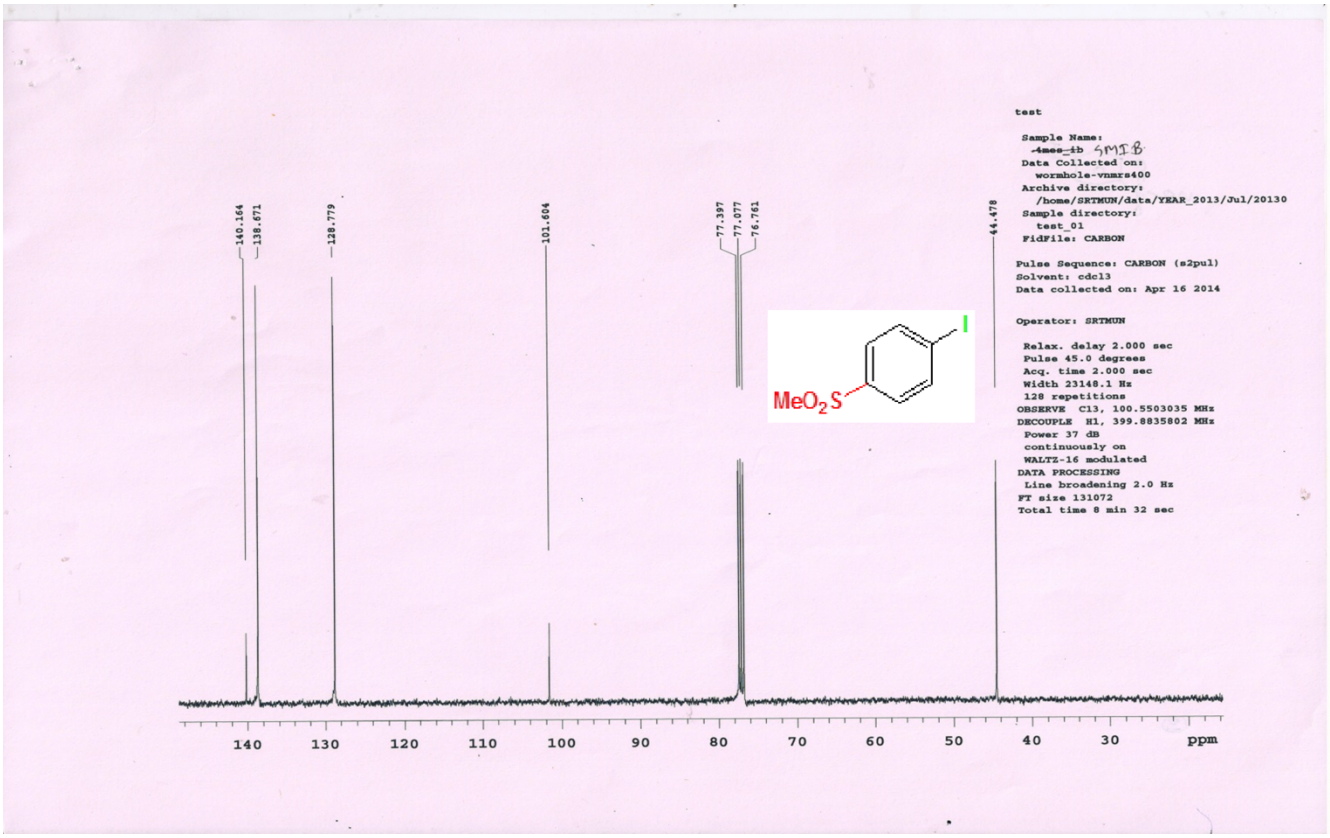
4.14 1-iodo-4-(methylsulfonyl)benzene (2s):

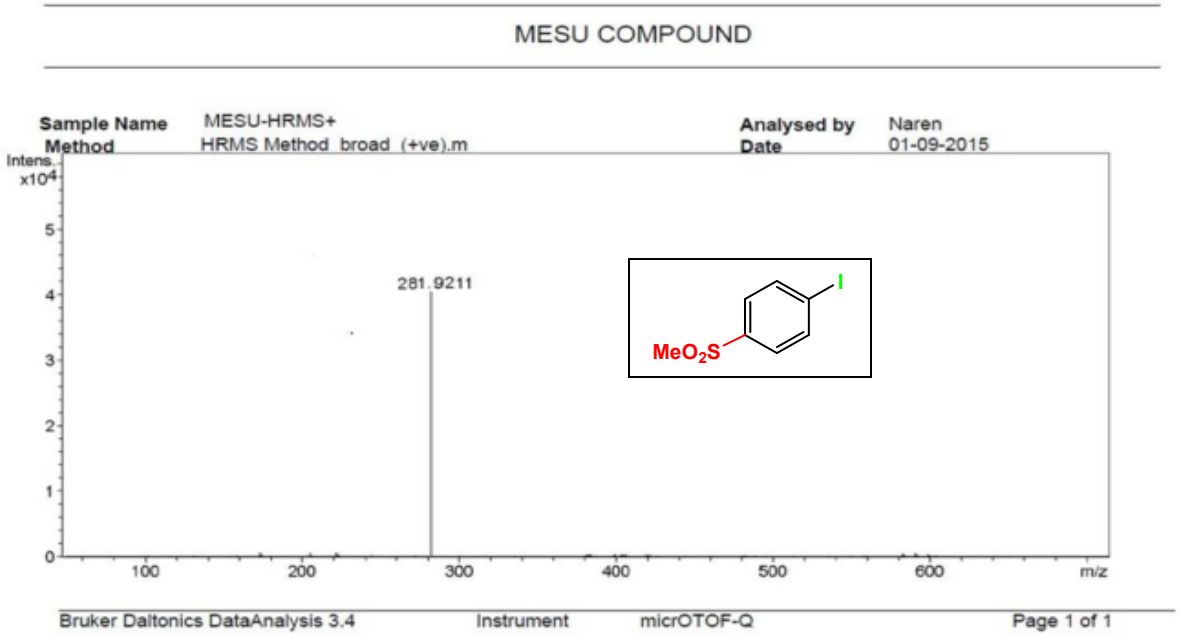



7.936
7.932
7.914
7.651
7.647
7.634
7.630
7.260
3.034
MeO2S
I
test
Sample Name:
4mes_ib
SRTMB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 36 sec
8
7
6
5
4
3
2
1
0
ppm
1.88
1.90
0.10
3.00

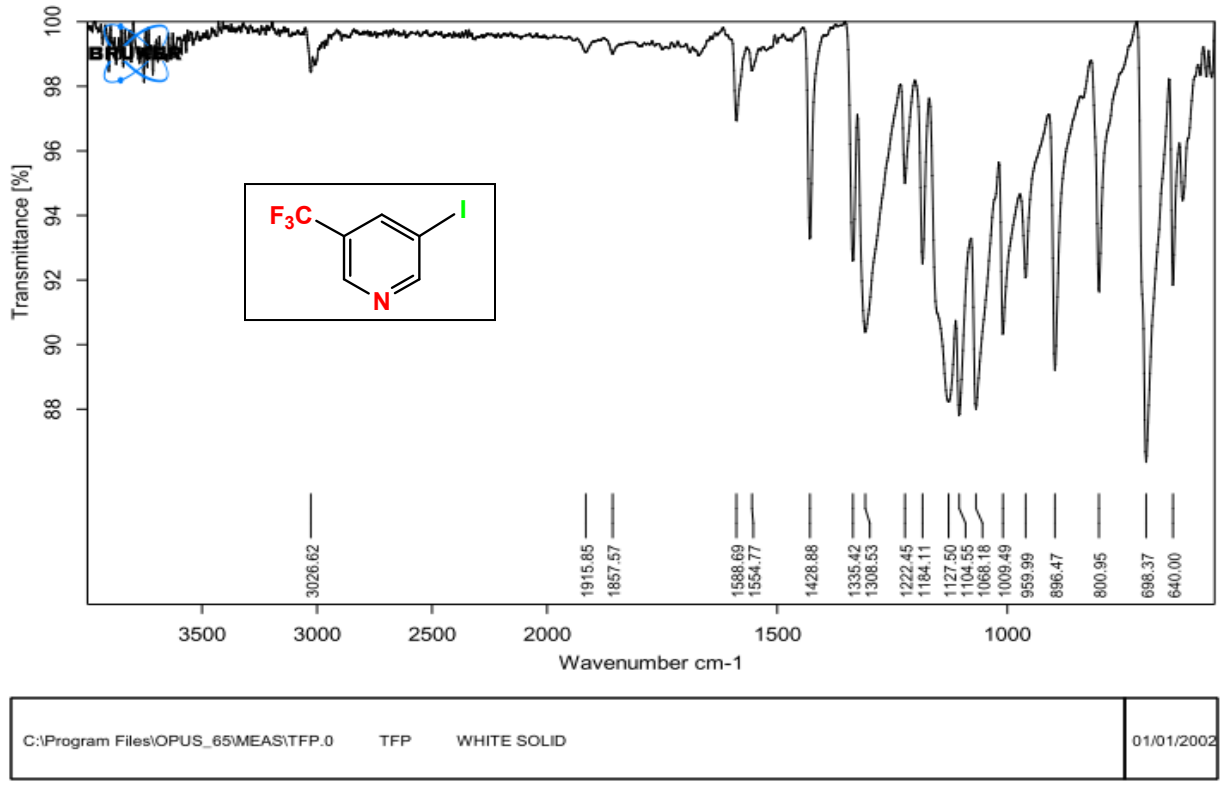

7.936
7.932
7.919
7.914
7.651
7.647
7.634
7.630
MeO2S
I
test
Sample Name:
4mes_ib
SRTMB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 36 sec
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
1.88
1.90
0.10

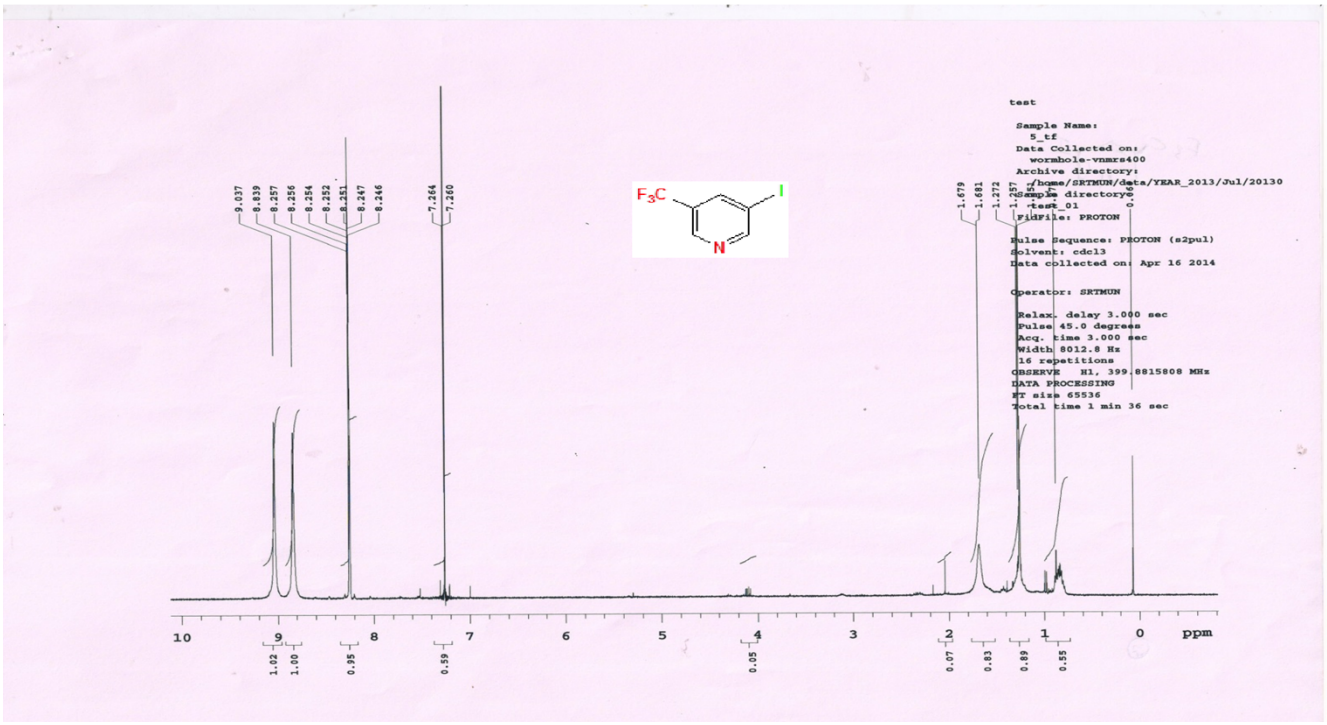

I
MeO2S
140.164
138.671
128.779
101.604
77.397
77.077
76.761
44.478
200
180
160
140
120
100
80
60
40
20
ppm
test
Sample Name:
4mes_ib 4MIB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
128 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 8 min 32 sec

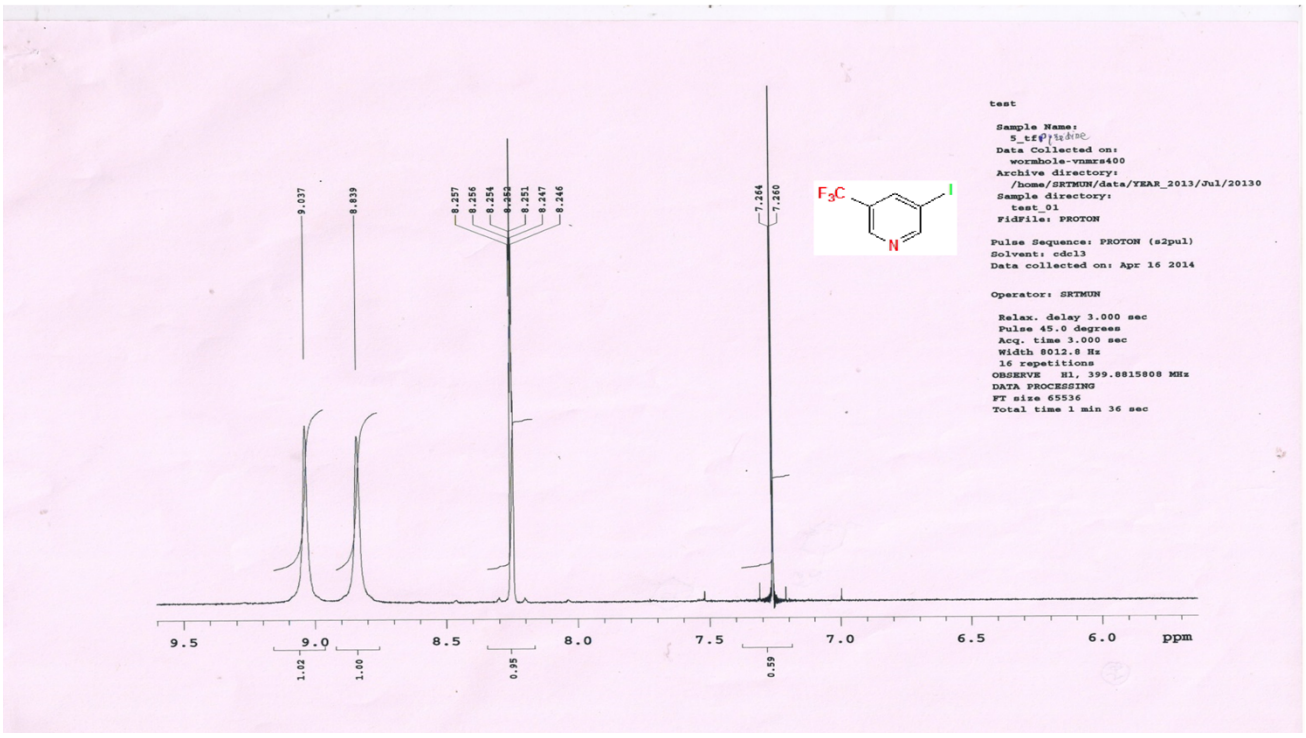

140.164
138.671
128.779
101.604
77.397
77.077
76.761
44.478
I
MeO2S
140
130
120
110
100
90
80
70
60
50
40
30
ppm
test
Sample Name:
4mes_ib 4MIB
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
128 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 8 min 32 sec

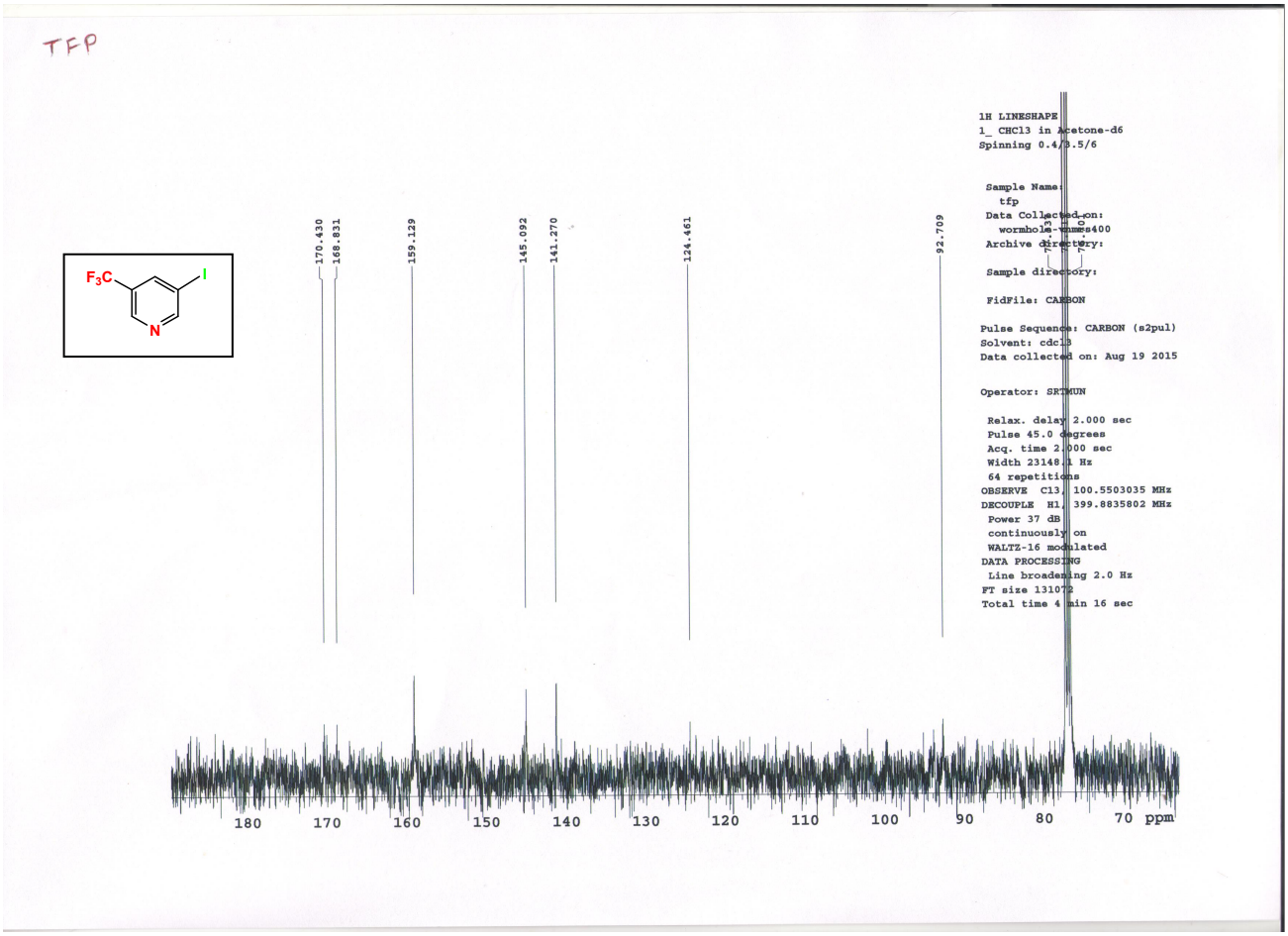


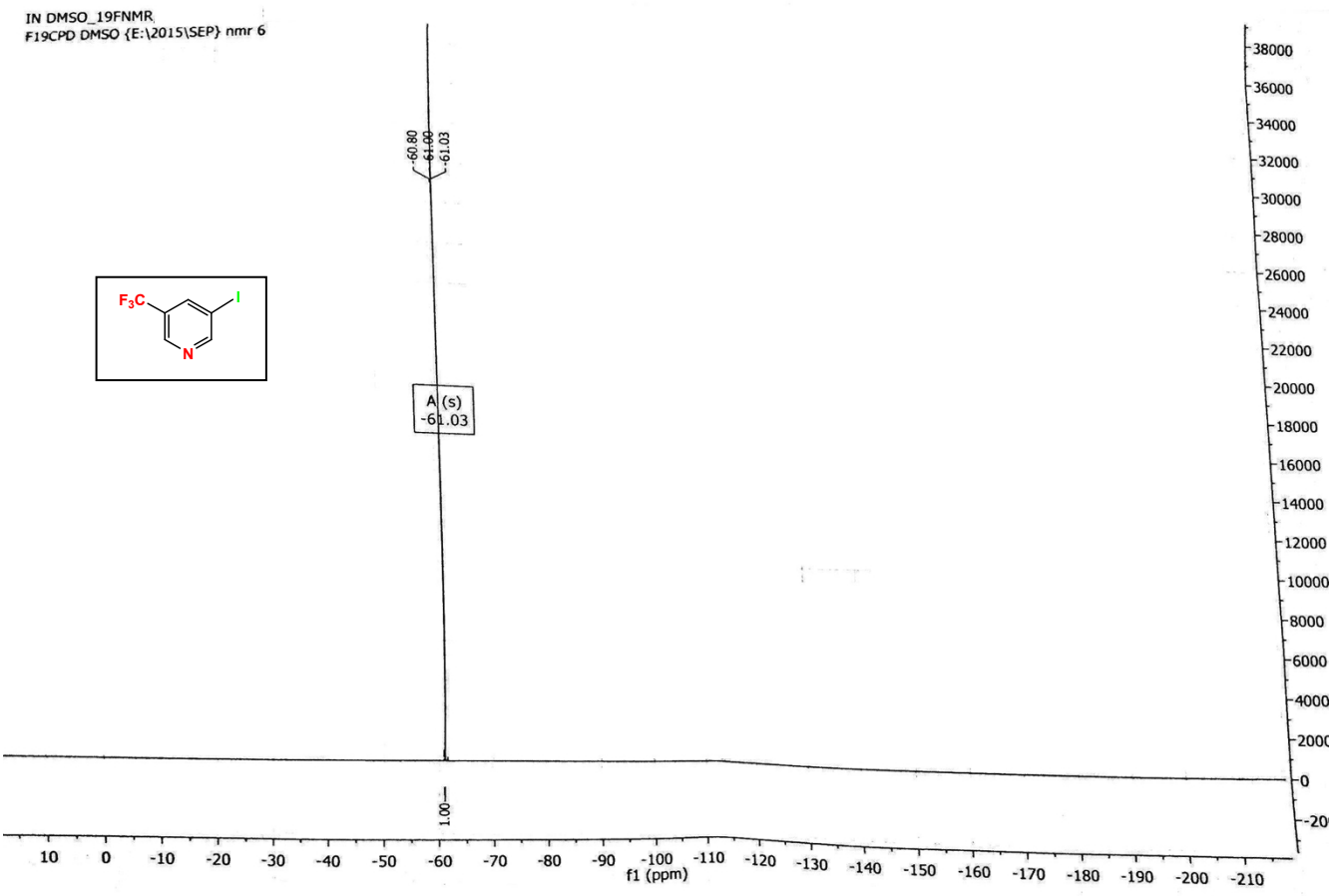
4.15 3-(trifluoromethyl)-5-iodopyridine (2t)

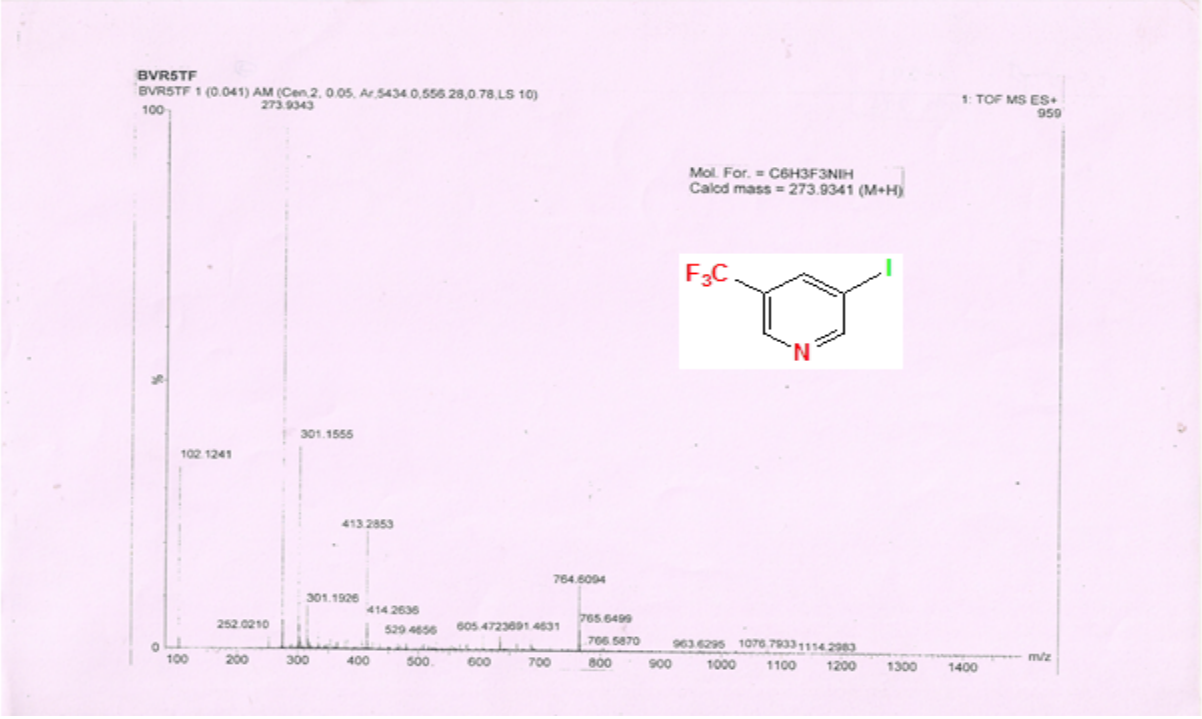



test
Sample Name:
5_tf
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 36 sec
F3C
I
N
ppm


test
Sample Name:
5_tf
Data Collected on:
wormhole-vnmrs400
Archive directory:
/home/SRTMUN/data/YEAR_2013/Jul/20130
Sample directory:
test_01
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2014
Operator: SRTMUN
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 399.8815808 MHz
DATA PROCESSING
FT size 65536
Total time 1 min 36 sec
F3C
I
N
ppm


TFP
F3C
I
N
170.430
168.831
159.129
145.092
141.270
124.461
92.709
77.160
1H LINESHAPE
1_ CHCl3 in Acetone-d6
Spinning 0.4/3.5/6
Sample Name:
tfp
Data Collected on:
wormhole-nmrs400
Archive directory:
Sample directory:
FidFile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 19 2015
Operator: SRTMUN
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 23148.1 Hz
64 repetitions
OBSERVE C13, 100.5503035 MHz
DECOUPLE H1, 399.8835802 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 131072
Total time 4 min 16 sec
180
170
160
150
140
130
120
110
100
90
80
70 ppm


IN DMSO_19FNMR
F19CPD DMSO {E:\2015\SEP} nmr 6
-60.80
-61.00
-61.03
A (s)
-61.03
1.00
f1 (ppm)


BVR5TF
BVR5TF 1 (0.041) AM (Cen,2, 0.05, Ar,5434.0,556.28,0.78,LS 10)
273.9343
1: TOF MS ES+
959
Mol. For. = C6H3F3NIH
Calcd mass = 273.9341 (M+H)
301.1555
102.1241
413.2853
764.6094
301.1926
414.2636
252.0210
529.4656
605.4723691.4631
765.6499
766.5870
963.6295
1076.7933
1114.2983
m/z