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Supporting information

A facile and practical copper diacetate mediated, ligand free C-N cross coupling of trivalent organobismuth compounds with amines and N-Heteroarenes

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1. General information

All reactions and manipulations were conducted under an air atmosphere. Organobismuth (III) compounds were synthesized by literature procedures.[1, 2] Copper acetate and heteroarenes were purchased from commercial sources and used without further purification. Solvents were distilled before use. IR spectra were recorded on a Shimadzu 8400 FT-IR spectrometer. ^{1}H NMR and ^{13}C NMR spectra were measured on a Varian-300MHz spectrometer with $CDCl_3$ as the solvent and tetramethyl silane (TMS) as the internal standard. GCMS data were collected on a Shimadzu Gas chromatograph mass spectrometer QP5050. The reactions were monitored by TLC, and visualized with UV light followed by development in iodine chamber. Preparative column chromatography was carried out on a column 10cm x l.5cm with silica gel 60/120 mesh size. GCMS /CHNS analysis of few representative compounds is provided in characterization section.

2. General procedure for the *N*-arylation

To a solution of $Cu(OAc)_2.H_2O$ (1.5 mmol) inTHF (5 mL) were added organobismuth (III) compound (1.2 mmol), amine or nitrogen-containing heterocycle (1.0 mmol) and Cs_2CO_3 (2 mmol) under air atmosphere. The mixture was stirred at 80°C for 12 h. After cooling to ambient temperature, the mixture was partitioned between water and ethyl acetate. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate. The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography on silica gel. Known compounds exhibited ^{1}H and ^{13}C NMR in agreement with previously reported data cited below.

3. Combined Spectral Data

I) Table 4 N-arylation of Amines with triphenyl bismuthine in THF[a] at 80°C for 12h

1) **N-(Phenyl) aniline (3a)** [3] , m.p. 52°C;
   IR (KBr) cm^{-1}: 696, 732, 878, 1024, 1075, 1166, 1320, 1491, 1594, 1937, 2099, 2548, 3039, 3390 cm^{-1};
   ^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 5.69 (s, 1H), 6.93-6.89 (m, 2H), 7.07-7.04 (d, *J* = 7.2 Hz, 4H), 7.27-7.22 (m, 4H);
   ^{13}CNMR (75 MHz, $CDCl_3$) δ 118.51, 120.90, 129.65, 142.83
2) **N-(4-bromophenyl)aniline(3b)** [4] , m.p. 86°C ;
   IR (KBr) cm^{-1}: 1328, 1584, 1692, 2721, 3024, 3405, cm^{-1};
   ^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 5.69 (s, 1H), 7.08-6.92 (m, 4H), 7.35-7.25 (m, 5H);
   ^{13}C NMR (75 MHz, $CDCl_3$) δ 114.30, 117.57, 126.57, 128.01, 129.48, 129.76, 145.34, 147.23
3) **N-(4-chlorophenyl)aniline (3c)** [4] , m.p. 73°C ;
   IR (KBr) cm^{-1}: 1044, 1207, 1378, 1438, 1476, 1717, 2340, 2910, 3014 cm^{-1}
   ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 3.65 (s, 1H), 7.03-6.91 (m, 4H), 7.27-7.16 (m, 5H);
   ^{13} C NMR (75 MHz, $CDCl_3$) δ 115.4, 119.2, 121.4, 129.7, 132.4, 146.3, 147.3
4) **N-(4-Nitrophenyl)aniline (3d)** [5] , m.p. 134°C ;
   IR (KBr) cm^{-1}: 1209, 1382, 1434, 1476, 1556, 2340, 2910, 3017, 3405, cm^{-1} ;
   ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 6.34 (s, 1H), 6.93 (d, *J* = 7.6 Hz, 2H), 7.20-7.12 (m, 3H), 7.38 (t, *J* = 8.0 Hz, 2H), 8.11 (d, *J* = 9.2 Hz, 2H)
   ^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 114.0, 123.4, 125.7, 127.6, 129.7, 137.6, 138.2, 151.5
5) **N-(4-Methoxyphenyl)aniline (3e)** [6] , m.p. 105°C ;
   IR (KBr): 3402, cm^{-1};
   ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 3.79 (s, 3H), 5.48 (s, 1H) 6.80-6.91 (m, 5H), 7.05-7.08 (m, 2H) 7.18-7.25 (m, 2H). ;
   ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 55.5, 114.6, 115.6, 119.5, 122.2, 129.3, 135.7, 145.1, 155.2.

6) **N-(4-Methylphenyl)aniline (3f)** [6] , m.p. 88°C ;

IR (KBr): 3344 cm^{-1};

^1H NMR (300 MHz, $CDCl_3$, ppm): δ 2.30 (s, 3H), 5.59 (s, 1H), 6.85 (t, J = 7.2 Hz, 1H), 6.99 (m, 4H), 7.07 (m, 2H), 7.20 (m, 2H)

^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 20.7, 116.8, 118.9, 120.3, 129.3, 129.8, 130.9, 140.3, 143.9

7) **1-phenyl-1H-imidazole (3l)** [7] ,Colorless liquid ;

IR (neat) cm^{-1}: 1496, 3408, cm^{-1} ;

^1H NMR (300 MHz, $CDCl_3$, ppm): δ 6.71-7.92 (8H, m, ArH);

^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ 118.3, 121.5, 127.5, 129.9, 130.3, 135.6, 136.7

8) **1-*p*-Tolyl-1*H*-imidazole(3m)** [8] m.p.149°C;

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 2.30 (m, 3 H), 7.01 (s, 1 H), 7.30-7.36 (m, 3 H), 7.46 (m, 2 H), 7.78 (s, 1 H);

^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 118.3, 121.5, 127.5, 129.9, 130.3, 135.6, 136.7

9) **1-phenyl-1H-indole (3n)** (Table 5, entry 9) [9] , Colorless oil;

^1H NMR (300 MHz, $CDCl_3$, ppm) δ 6.58 (s, 1H), 7.30-7.25 (m, 3H), 7.41-7.40 (m, 2H), 7.57-7.56 (m, 3H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H);

^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ103.7, 110.7, 120.5, 121.3, 122.5, 124.5, 126.6, 128.1, 129.5, 129.8, 136.0, 140.0,

10) **N-Phenylbenzamide (3g) [**10] , m.p.163 °C;

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 7.14-7.17 (m, 1 H), 7.37-7.39 (m, 2 H), 7.48-7.51 (m, 2 H), 7.55-7.57 (m, 1 H), 7.64-7.65 (m, 2 H), 7.82 (s, 1 H), 7.87-7.88 (m, H);

^{13}CNMR (100 MHz, $CDCl_3$, ppm) δ 120.23, 124.99, 127.49, 128.53, 129.18, 130.21, 131.99, 135.16, 137.98, 165.77

11) **N-Phenylacetamide (3h)** [11] , m.p.114°C;

IR (neat) cm^{-1} 501, 605, 746, 1019,1328,1531,1657, 1959, 2267, 2625, 2807, 3067, 3298cm^{-1};

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 2.15 (m, 3 H), 7.08-7.11 (m, 2 H), 7.26-7.3 (m, 2 H), 7.49-7.51 (m, 2 H), 7.78 (s, 1 H);

^{13}CNMR (100 MHz, $CDCl_3$, ppm) δ 24.72, 120.28, 124.64, 128.90, 137.91, 169.44

12) **N-Phenyl-4-methylbenzenesulfonamide (3k)** [12] , m.p.101°C;

IR (neat) cm^{-1}: 749.17, 703.29, 808.79, 906.86, 1089.83, 1152.47, 1300, 1524.17, 1615.65, 1664.28, 1931.31, 2317.03, 2477.74, 2597.25, 2926.92, 3039.08, 3270.60, 3362.30;

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.38 (s, 3H), 6.56 (s, 1H), 7.13-7.06 (m, 3H), 7.24-7.21 (m, 4H), 7.72-7.65 (m, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 121.4, 125.2, 127.3, 129.3, 135.9, 136.6, 143.99,

II) Table 5 N-arylation of pthalimide with functionalized bismuthanes (**2**) in THF[a] at 80^0C for 12h

14) **2-phenylisoindoline-1, 3-dione** (**5a**) [13], m.p. 206-208°C;

IR (neat) cm^{-1} 501,517,620,703,756,876,1027,1069,1106,1174,1376,1421, 1461, 1565, 1696, 3046, 3462 cm^{-1};

^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ7.48 (m, 3H), 7.78(m, 4H), 7.94(d, 2H);

^{13}CNMR (75MHz, $CDCl_3$, ppm) δ 123.7, 126.5, 128.1, 129.1, 131.7, 134.4, 167.30

15) **2-o-tolylisoindoline-1, 3-dione (5b)** [14], m.p. 159°C;

IR (neat) cm^{-1} 444.50, 528.57, 626.64, 710.71, 766.75, 886.26, 1096.42, 1229.94, 1384.06, 15.3.37, 1713.73, 3074.37 cm^{-1};

^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 2.22(s, 3H), 7.36(m, 4H), 7.80(dd, 2H, J= 8.8 Hz), 7.96 (dd, 2H, J= 8.4Hz)

^{13}C NMR (75MHz, $CDCl_3$) δ 17.97, 76.68, 77.00, 77.32, 123.68, 126.80, 128.67, 129.37, 130.54, 131.08, 131.95, 134.25, 136.25, 167.26

16) **2-m-tolylisoindoline-1, 3-dione (5c)** [14], m.p 168°C;

IR (neat) cm^{-1} 444.50, 535.16, 533.34, 724.77, 786.16, 872.25, 1069.83,1230, 1370, 1485.56, 1608.04,1706,1762, 2351.64, 2926.92cm^{-1};

^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 2.45(s, 3H), 7.25(dd, 2H) 7.44(dd, 2H, J= 7.8 Hz), 7.81(d, 2H, J= 8.2 Hz), 7.97 (d, 2H, J= 8.7Hz);

^{13}CNMR (75MHz, $CDCl_3$, ppm) δ 21.31, 123.60, 127.18, 128.84, 131.69, 134.26, 139.02, 167.24

17) **2-p-tolylisoindoline-1,3-dione (5d)** [14] , m.p 203-204°C;
IR (neat) cm^{-1} 437,521,535,823,886,1082,1216,1290,1376,1503,1713, 2912, 3041 cm^{-1};
^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 2.43 (s, 3H), 7.53-7.13 (m, 4H), 8.05-7.51 (m, 4H);
^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 21.26, 76.92, 77.17, 77.43, 123.69, 126.21, 126.50, 129.03, 129.56, 129.80, 131.82, 134.36, 134.47, 138.17, 167.44

18) **2-(4-methoxyphenyl)isoindoline-1,3-dione (5e)** [14] , m.p 159-160°C;
IR (neat) cm^{-1} 711, 774, 886, 1110, 1222,1370,1503,1727, 3059, cm^{-1};
^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 3.76 (s, 3H), 6.83 -7.02 (m, 4H), 7.15-7.59 (m, 4H), 8.15-8.21(d, 2H);
^{13}C NMR (75 MHz, $CDCl_3$, ppm) δ 55.7, 76.92, 77.17, 77.43, 123.69, 126.21, 126.50, 129.03, 129.56, 129.80, 130.12, 133.36, 133.47, 158.23, 167.49

19) **2-(4-bromophenyl)isoindoline-1,3-dione (5f)** [14] , m.p 192-193°C;
IR (neat) cm^{-1} 458,517,710, 821, 883, 951, 1009, 1078, 1117, 1174, 1219, 1284, 1380, 1488, 1609, 1704, 2323, 2376, 3060, 3480;
$^{1}HNMR$ (300MHz, $CDCl_3$, ppm) δ 7.37(s, 4H), 7.77(dd, 2H), J= 8.4 Hz), 7.92(dd, 2H, J= 8.3 Hz);
^{13}C NMR (75MHz, $CDCl_3$, ppm) δ 77.04, 77.17, 77.30, 121.74, 123.84, 127.96, 130.75, 131.54, 132.24, 134.61, 166.88

20) **2-(4-chlorophenyl)isoindoline-1,3-dione (5g)** [14], m.p 201-202°C;
IR (neat) cm^{-1} 501, 655, 711, 823, 872, 1005, 1068, 1124, 1222, 1376, 1482, 1706, 1741, 1791, 3059 cm^{-1}
$^{1}HNMR$ (300 MHz, $CDCl_3$, ppm) δ 7.35(d, 2H, J= 8.8 Hz), 7.63 (d, 2H, J=8.8), 7.80(dd, 2H, J= 8.3), 7.95(dd, 2H, J= 8.8 Hz);
^{13}C NMR (75 MHz, $CDCl_3$) δ 76.73, 77.05, 77.37, 123.87, 127.68, 129.32, 130.24, 131.63, 133.81, 134.58, 166.98

21) **Triphenylbismuth acetate** (Intermediate) [15] , m.p.172°C;
IR (neat) cm^{-1} 451, 668, 732, 984, 1054, 1328, 1384, 1580, 3039;
^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 1.87 (s), 7.26 (s), 7.55-7.36 (m), 7.61 (dd, J = 17.2, 9.8 Hz), 7.90 (d, J = 7.9 Hz), 8.15 (d, J = 7.9 Hz), 8.25 (d, J = 8.0 Hz)

III) Spectral data of functionalized Oranibismuthines (2a-g)

1) Triphenyl bismuthine (**2a**) , m.p.78^{0}C

   C, 49.10; H, 3.43; Bi, 47.46;

   IR(KBr) cm^{-1} 3053,1568,1427,728,447;

   ^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 7.7 (m,6H),7.39,7.34 (m,9H);

   ^{13}CNMR (75 MHz, $CDCl_3$, ppm) δ 128 ,131

2) Tri- o tolyl bismuthine(**2b**), m.p. 104^{0}C

   C, 52.29; H, 4.39; Bi, 43.32

   IR(KBr) cm^{-1} 3051, 2924,1578,1446,742,447

   ^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 2.43 (s,9H),7.07(m,3H),7.28 (m,6H),7.54 (d,3H)

   ^{13}CNMR (75 MHz, $CDCl_3$, ppm) δ 26.4, 128.1,128.7,130,138.6,143.7

3) Tri- m- tolyl bismuthine (**2c**), m.p. 64^{0}C

   C, 52.29; H, 4.39; Bi, 43.32

   IR(KBr) cm^{-1} 3051, 2916,1589,1471,772,468

   ^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 2.36 (s,9H),7.10 (m,3H),7.33 (m,6H),7.41 (d,3H)

   ^{13}CNMR (75 MHz, $CDCl_3$, ppm) δ 25.4, 128.7,128.7, 129,132,132.4

4) Tri- *p*- tolyl bismuthine (**2d**) , m.p.118^{0}C

   C, 52.29; H, 4.39; Bi, 43.32

   IR(KBr)cm^{-1} 3026, 2916,1585,1485, 794,480;

   ^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 2. 3 (s,9H),7.1(m,6H),,7.6 (m,6H);

   ^{13}CNMR (75 MHz, $CDCl_3$, ppm) δ 21.4, 128.7,129.3,131.3,137.3

5) Tri- *p*-methoxy bismuthine(2e) , m.p. 184^{0}C

   C, 47.56; H, 3.99; Bi, 39.40; O, 9.05;

   IR(KBr) cm^{-1} 3007, 2928,15731485,823 ,516;

   ^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ 3.76 (s,9H),6.8(d,6H),7.6 (d,6H);

   ^{13}CNMR (75 MHz, $CDCl_3$, ppm) δ 55,116.2,138.6 ,145,159.2

6) Tri- *p*-bromo bismuthine (2f) , m.p 149^{0}C

   C, 61.02; H, 3.58; Bi, 30.69;

   IR(KBr) cm^{-1} 3043,1546,1496,792, 460;

   ^{1}HNMR(300 MHz, $CDCl_3$, ppm) δ 7.2-7.4(dd,9H),7.9 (m,9H);

^{13}CNMR (75 MHz, $CDCl_3$, ppm) δ 126,128.5,128.9-130.9 ,134, 138

7) Tri- *p*-chloro bismuthine (**2f**) , m.p. 117^{0}C

C, 60.69; H, 3.32; Bi, 38.19;

IR(KBr) cm^{-1} 3039,1537,1489,779, 464;

^{1}HNMR (300 MHz, $CDCl_3$, ppm) δ7.2-7.4 (dd,9H),7.9 (m,9H);

^{13}CNMR (75 MHz, $CDCl_3$, ppm) δ 124.6,129.5,127.9-131.9,135,139

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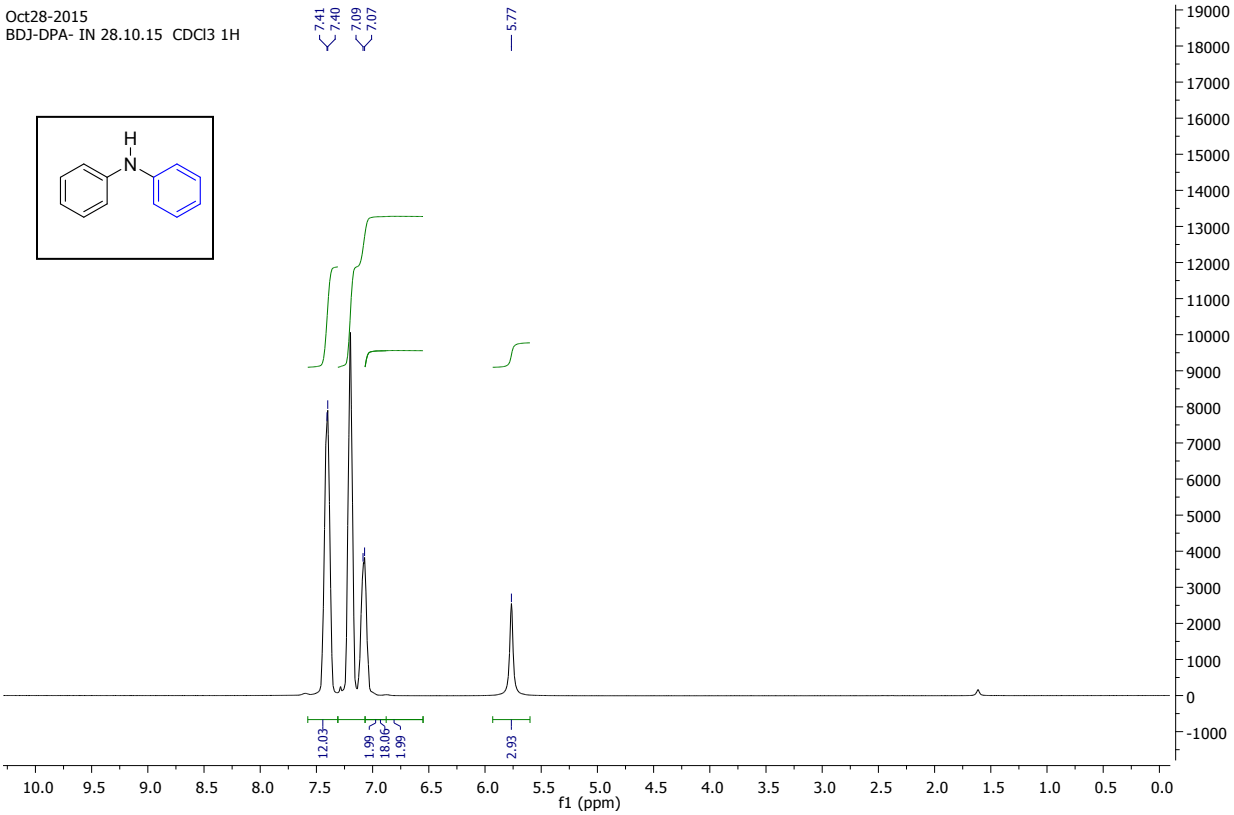
5. Spectra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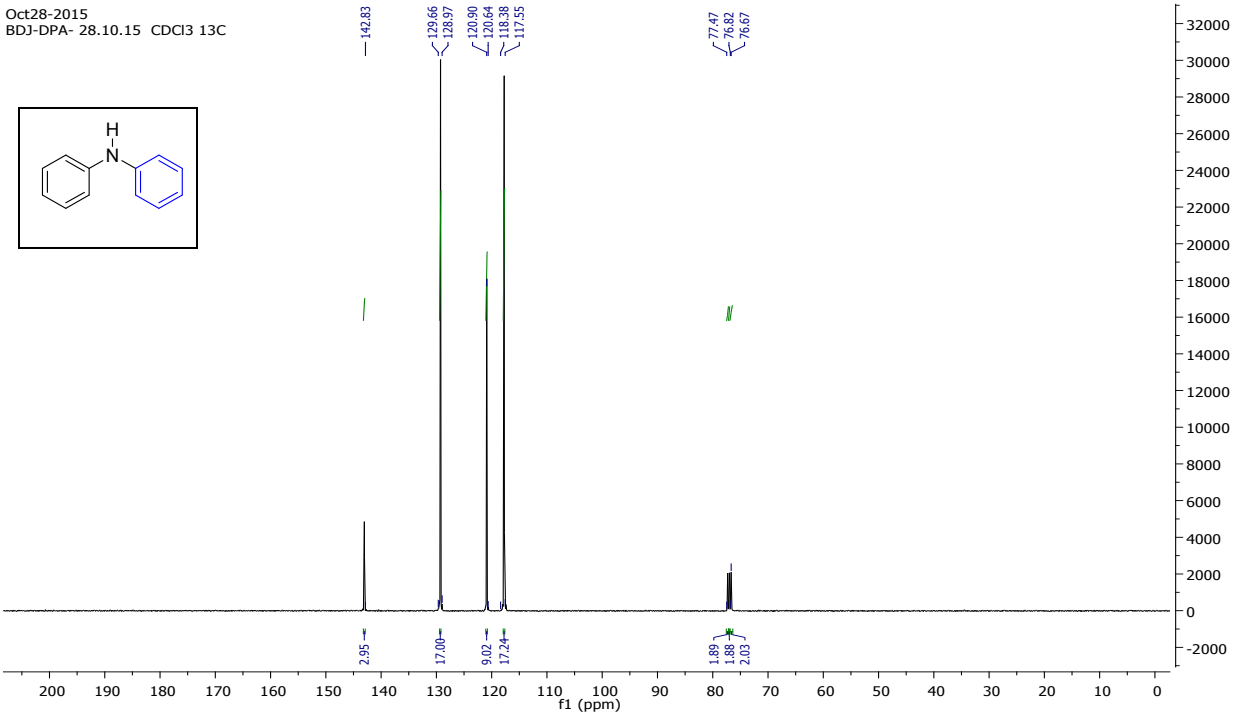
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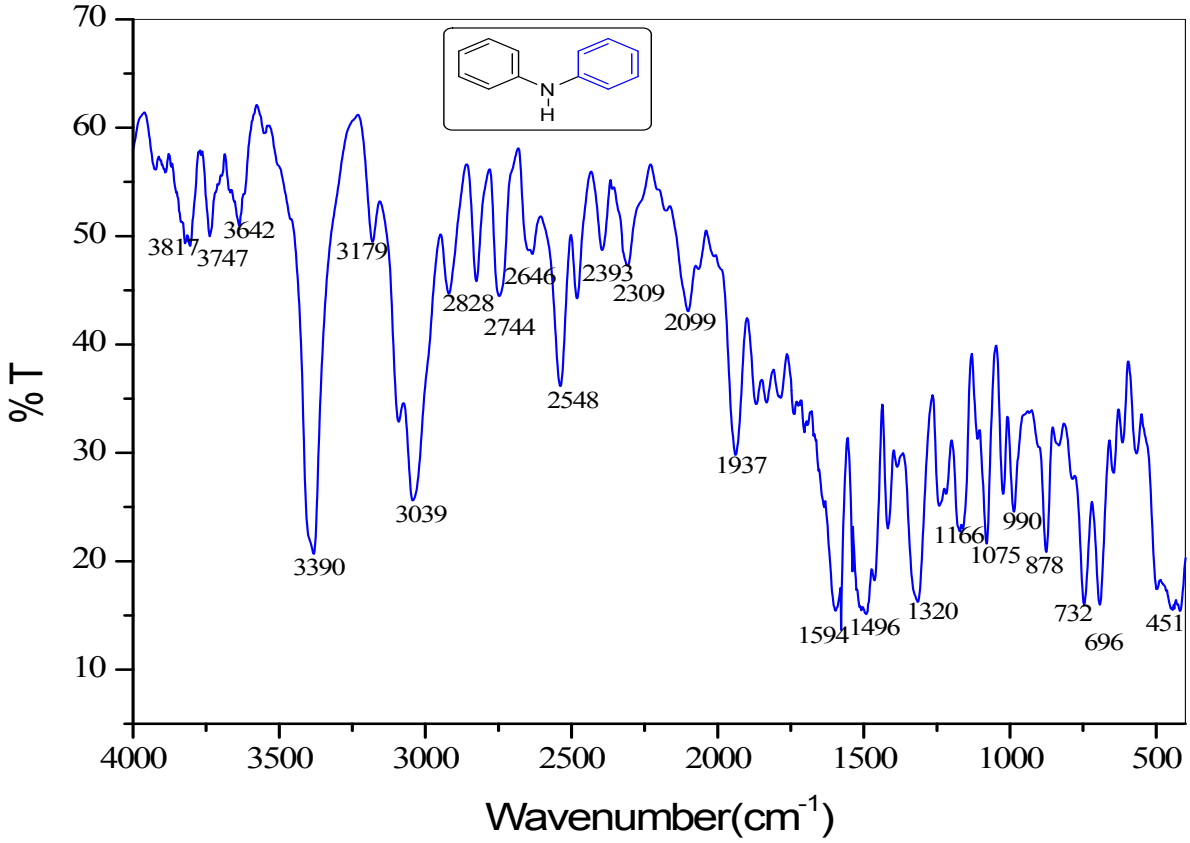
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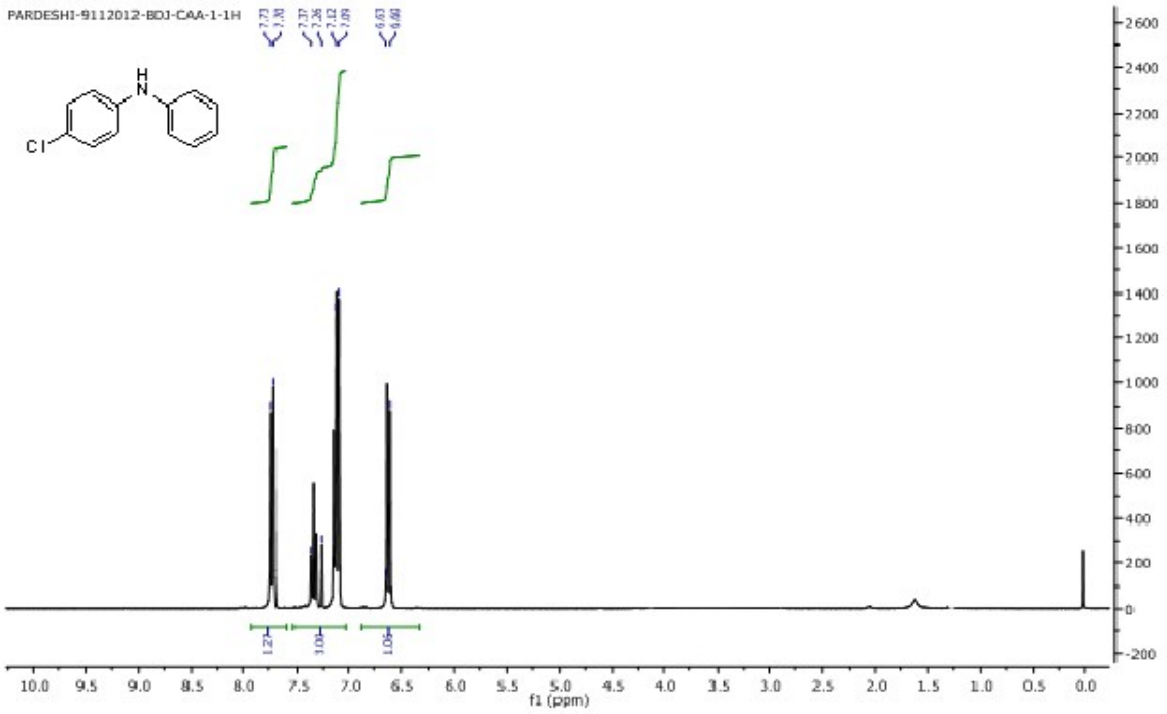
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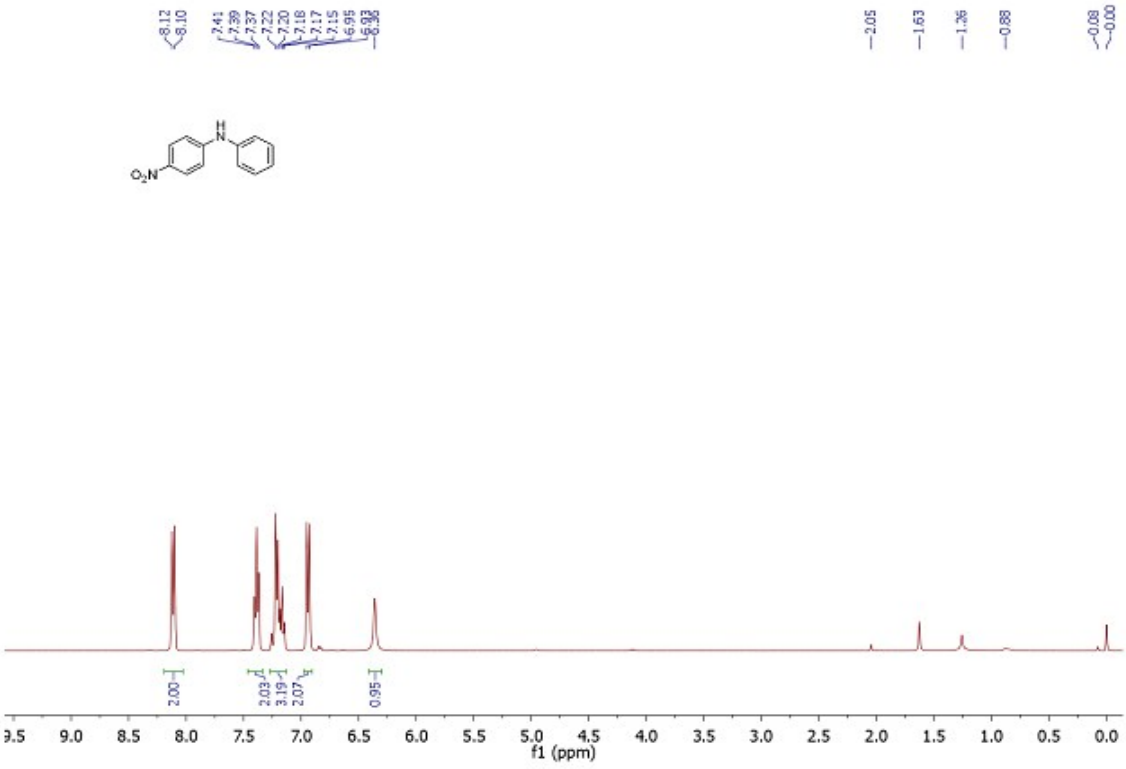
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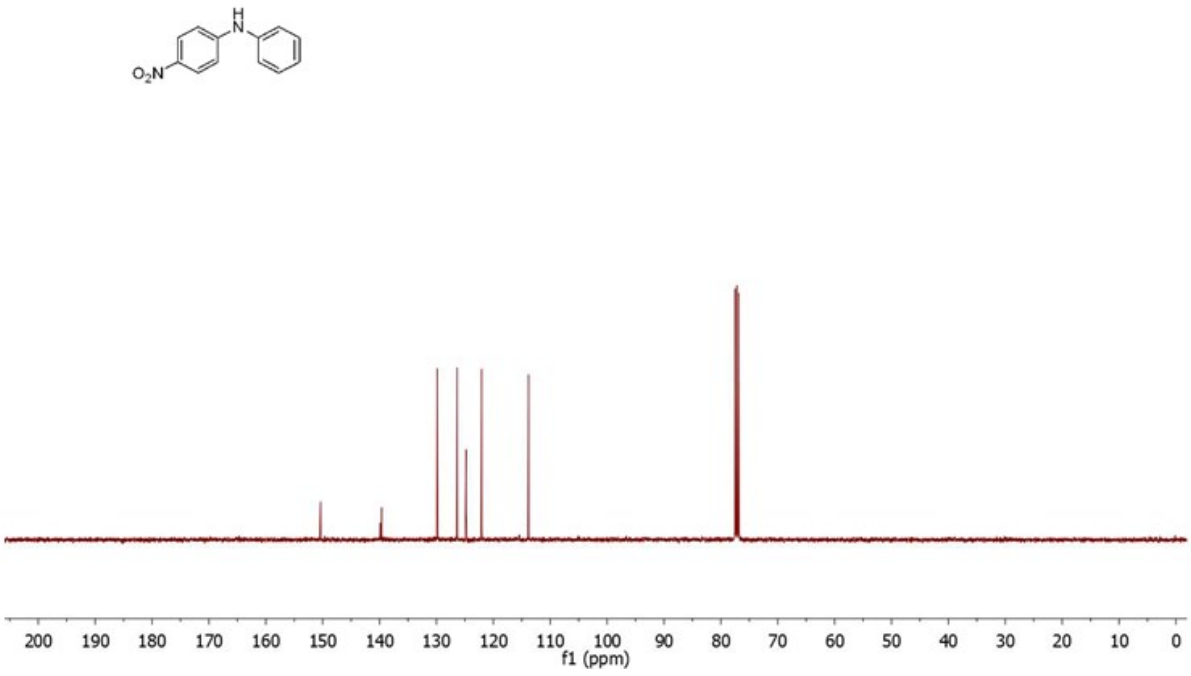
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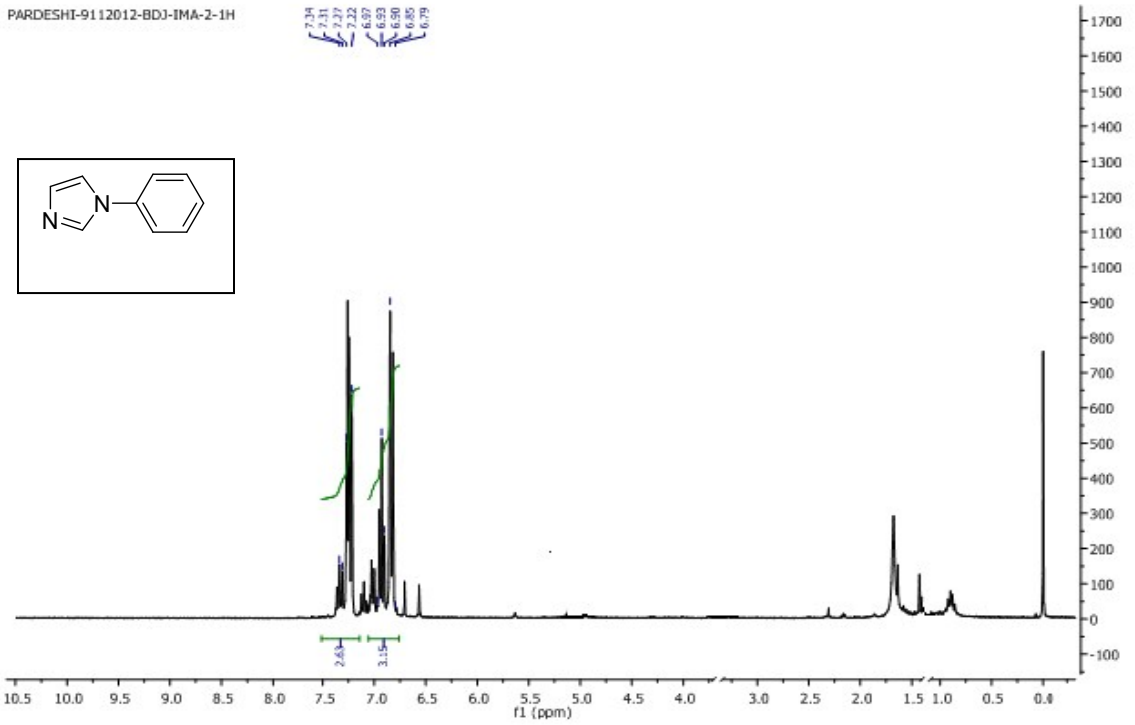
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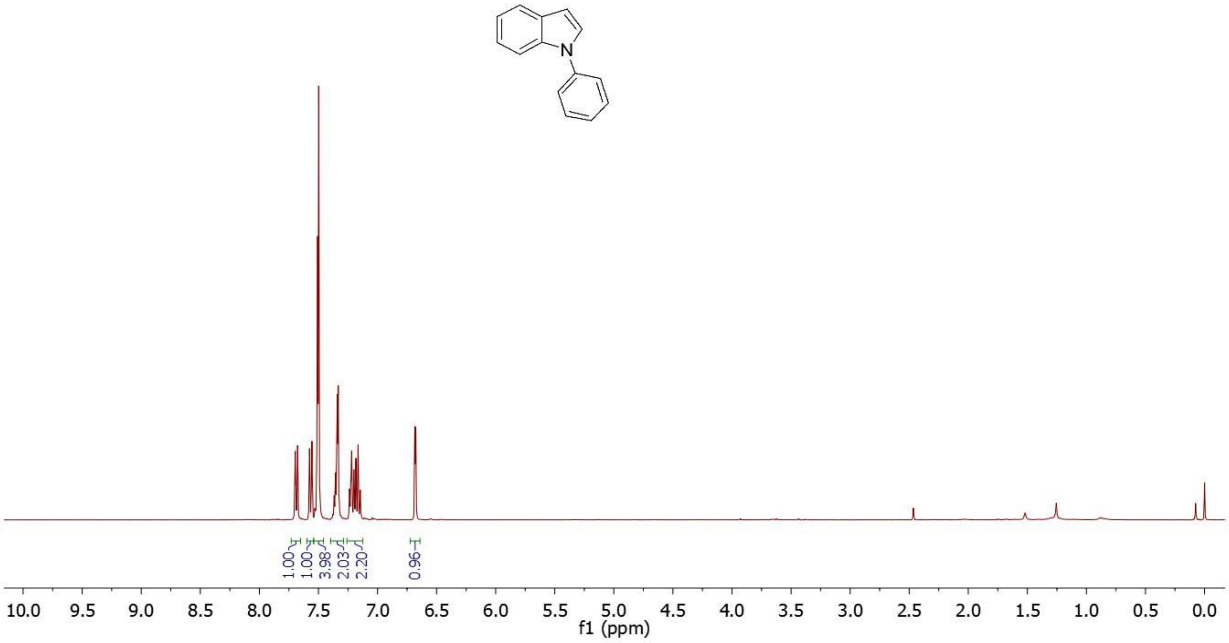
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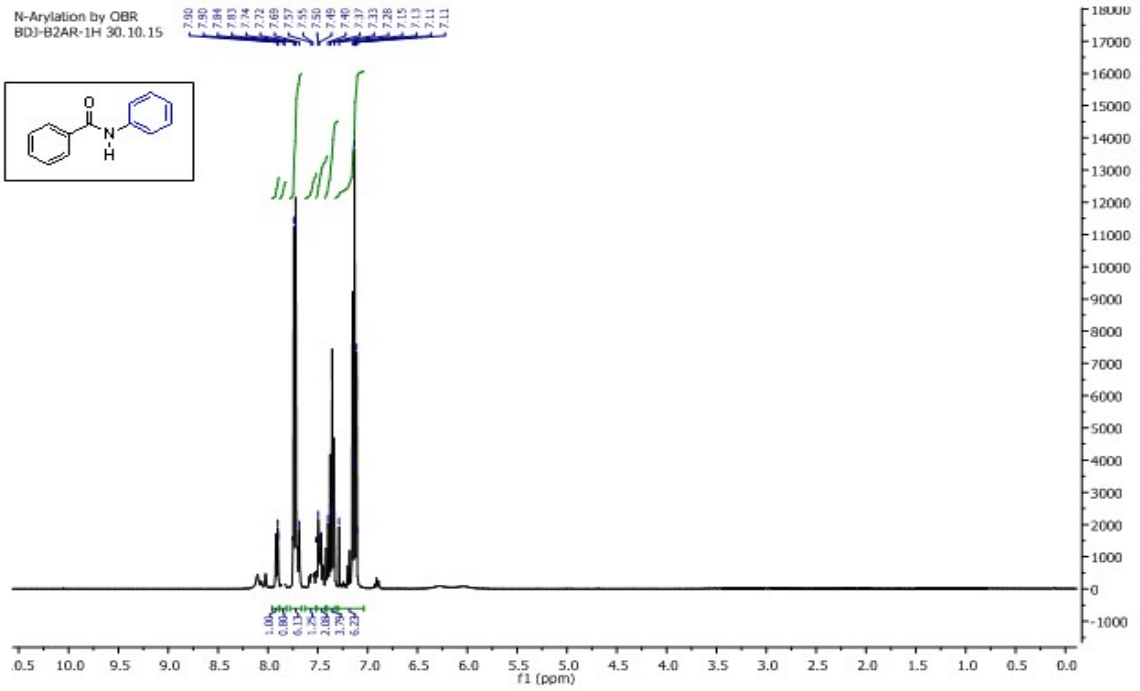
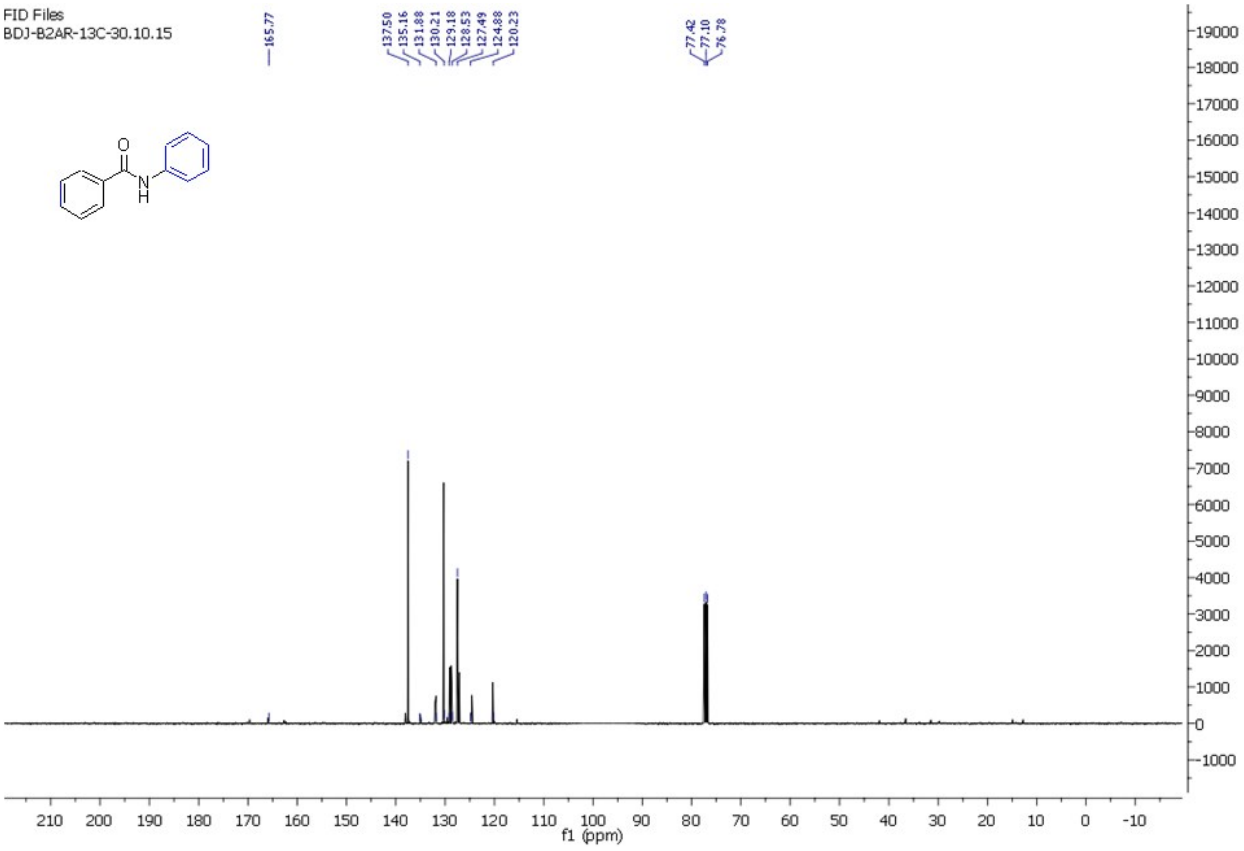
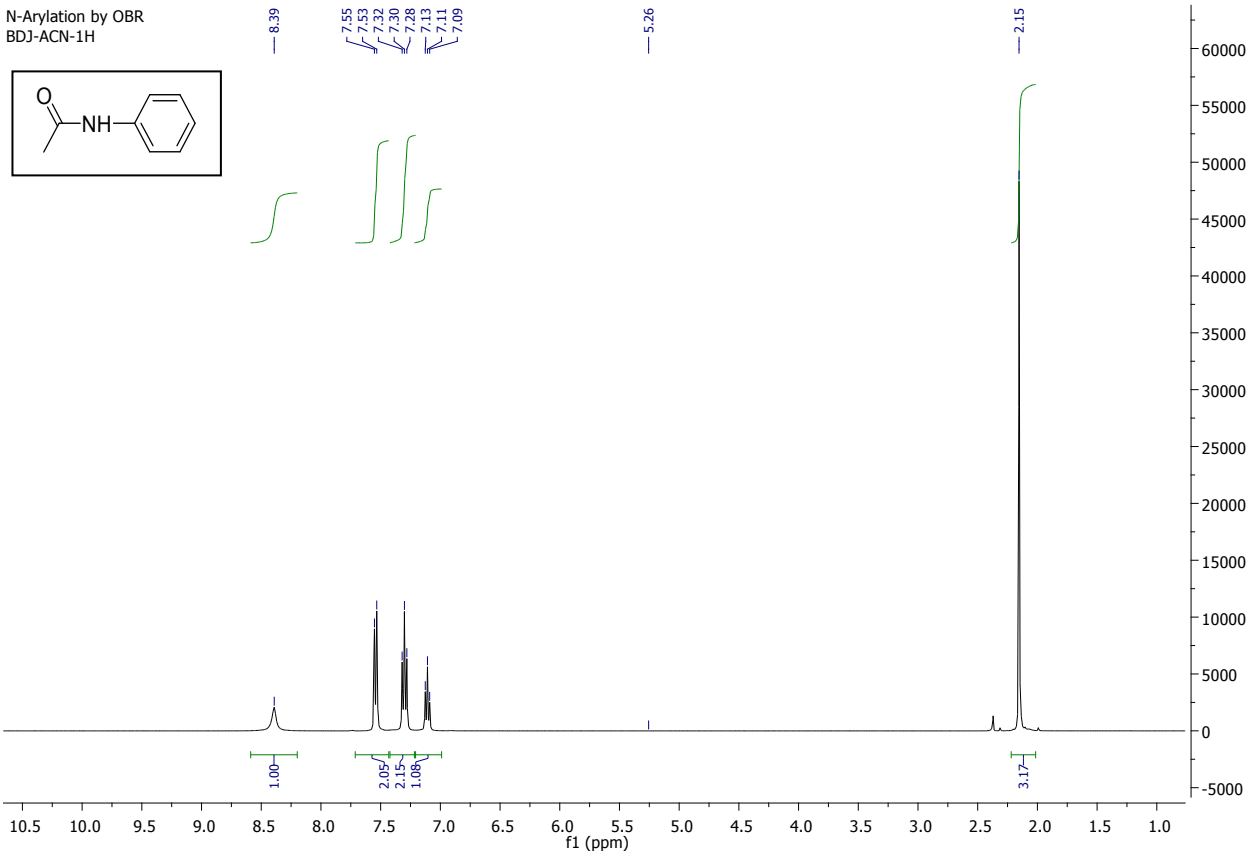
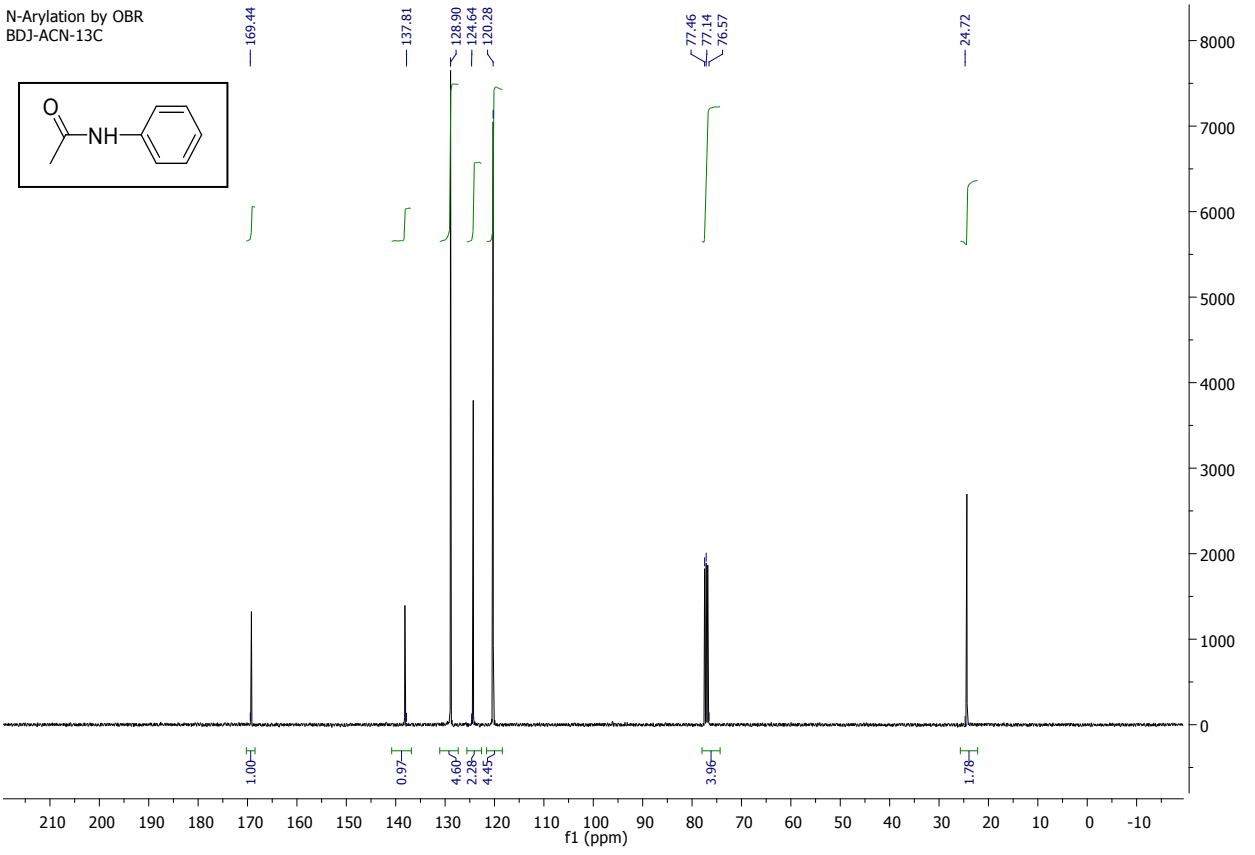
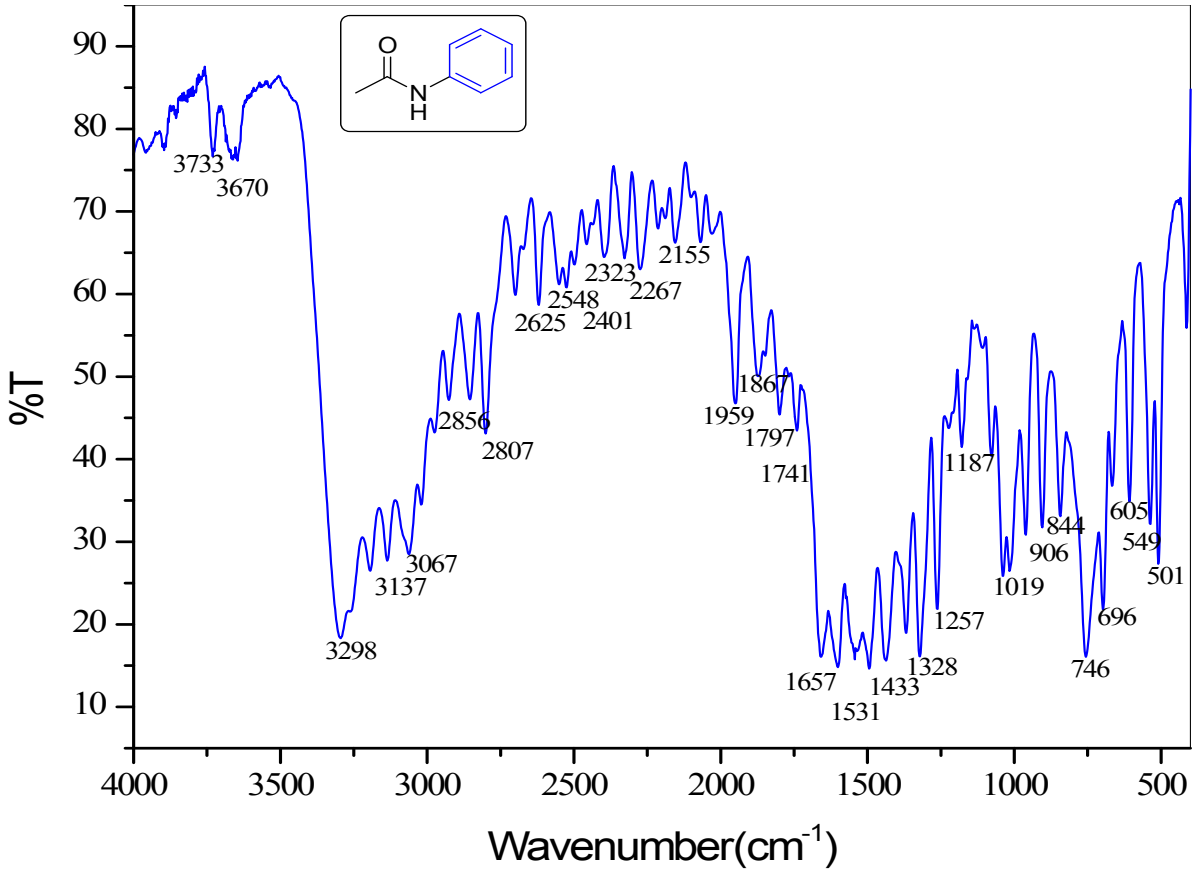
f1 (ppm)

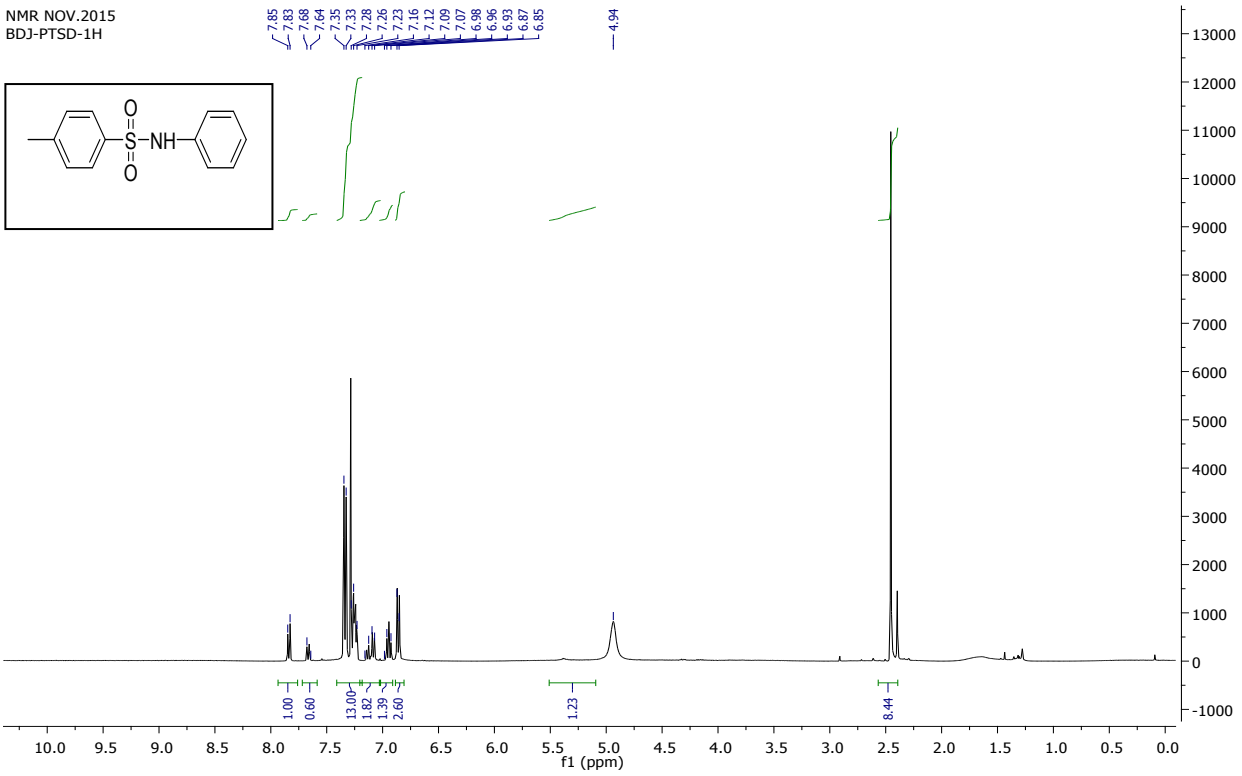

N-Arylation by OBR
BDJ-B2AR-1H 30.10.15
f1 (ppm)

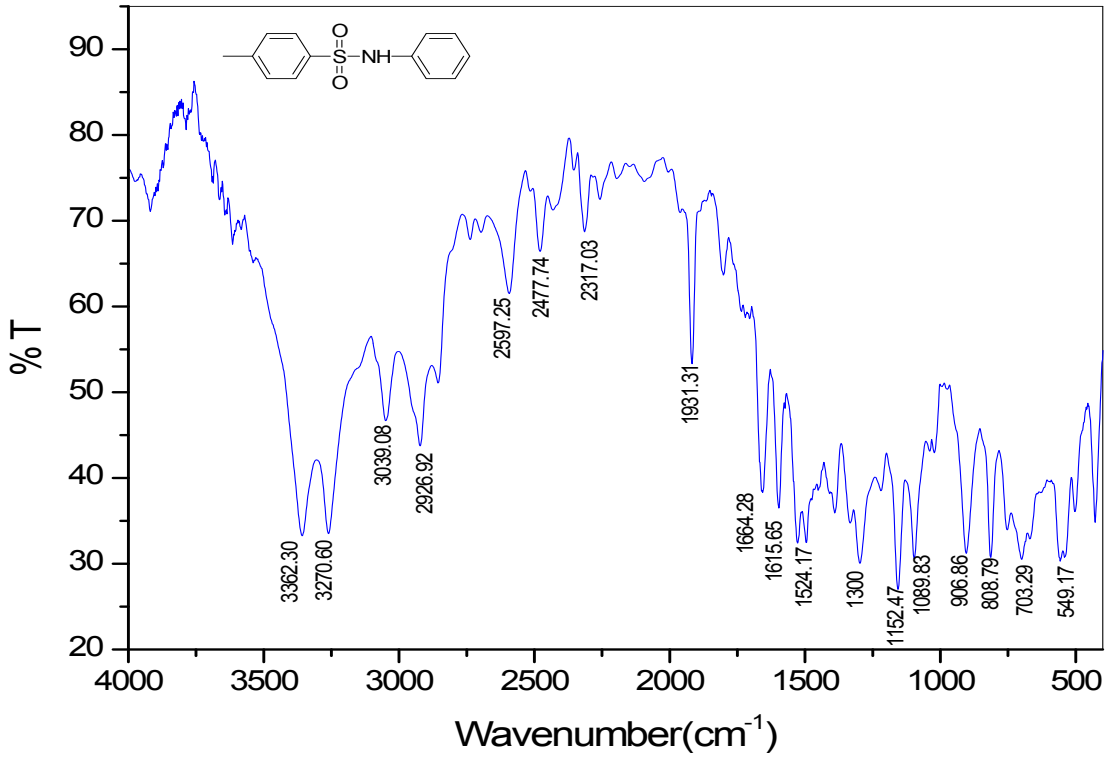

FID Files
BDJ-B2AR-13C-30.10.15
f1 (ppm)

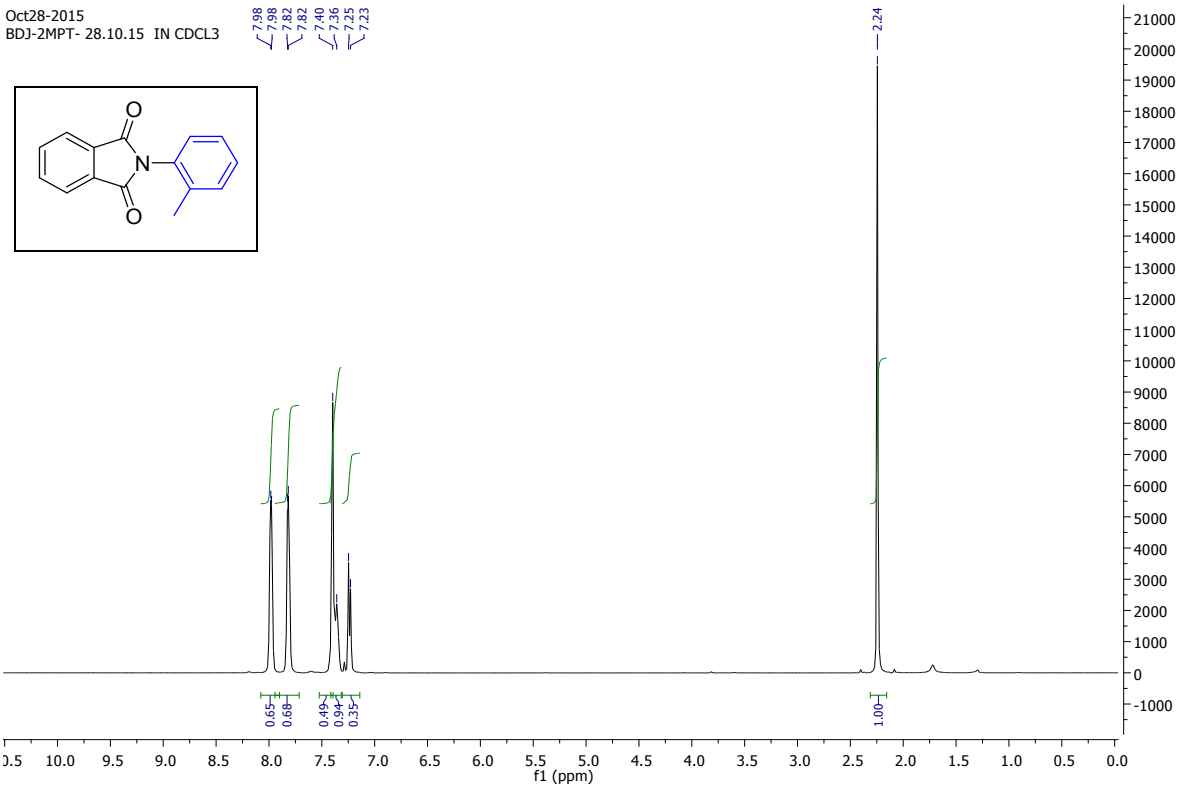

N-Arylation by OBR
BDJ-ACN-1H
8.39
7.55
7.53
7.32
7.30
7.28
7.13
7.11
7.09
5.26
2.15
1.00
2.05
2.15
1.08
3.17
f1 (ppm)

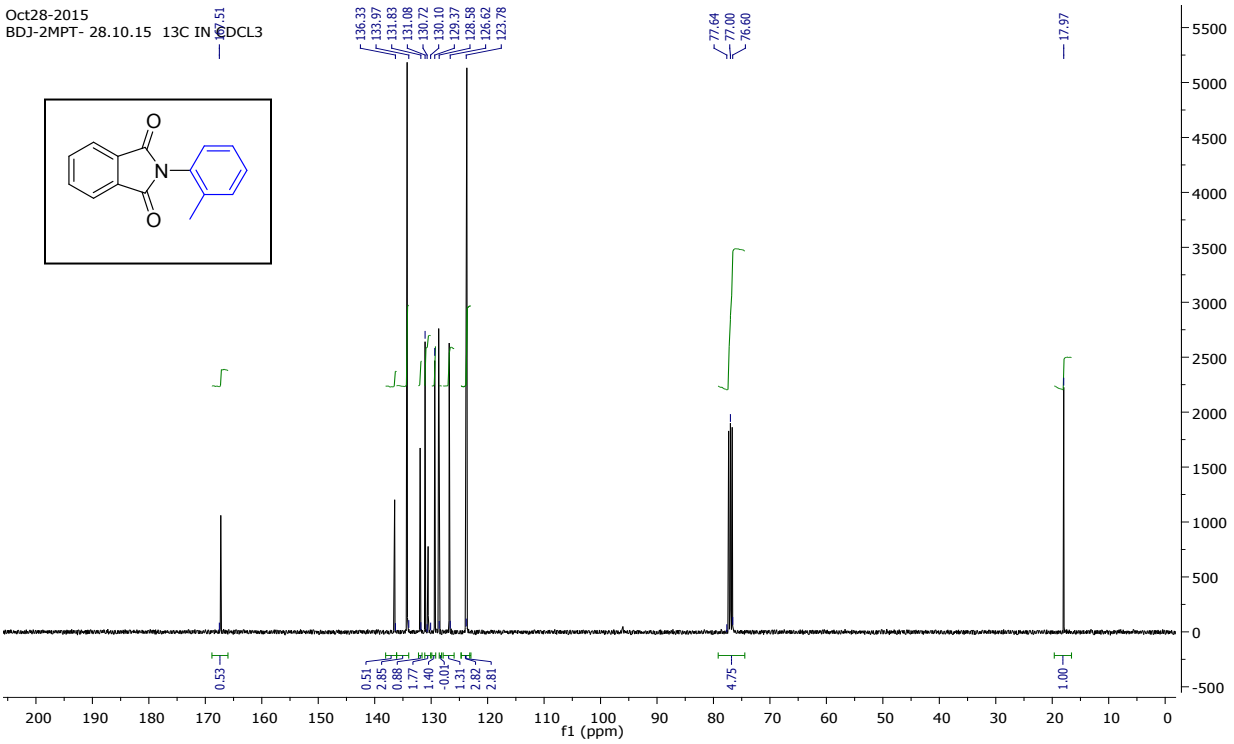

N-Arylation by OBR
BDJ-ACN-13C
169.44
137.81
128.90
124.64
120.28
77.46
77.14
76.57
24.72
1.00
0.97
4.60
2.28
4.45
3.96
1.78
f1 (ppm)

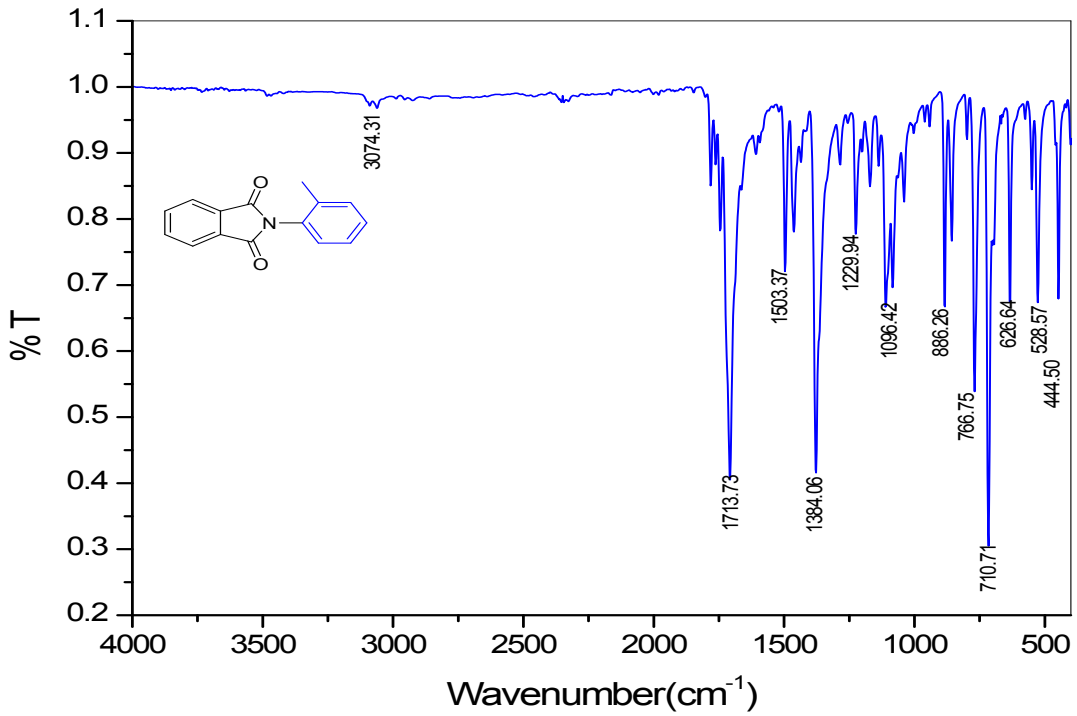

%T
Wavenumber(cm-1)
3733
3670
3298
3137
3067
2856
2807
2625
2548
2401
2323
2267
2155
1959
1867
1797
1741
1657
1531
1433
1328
1257
1187
1019
906
844
746
696
605
549
501

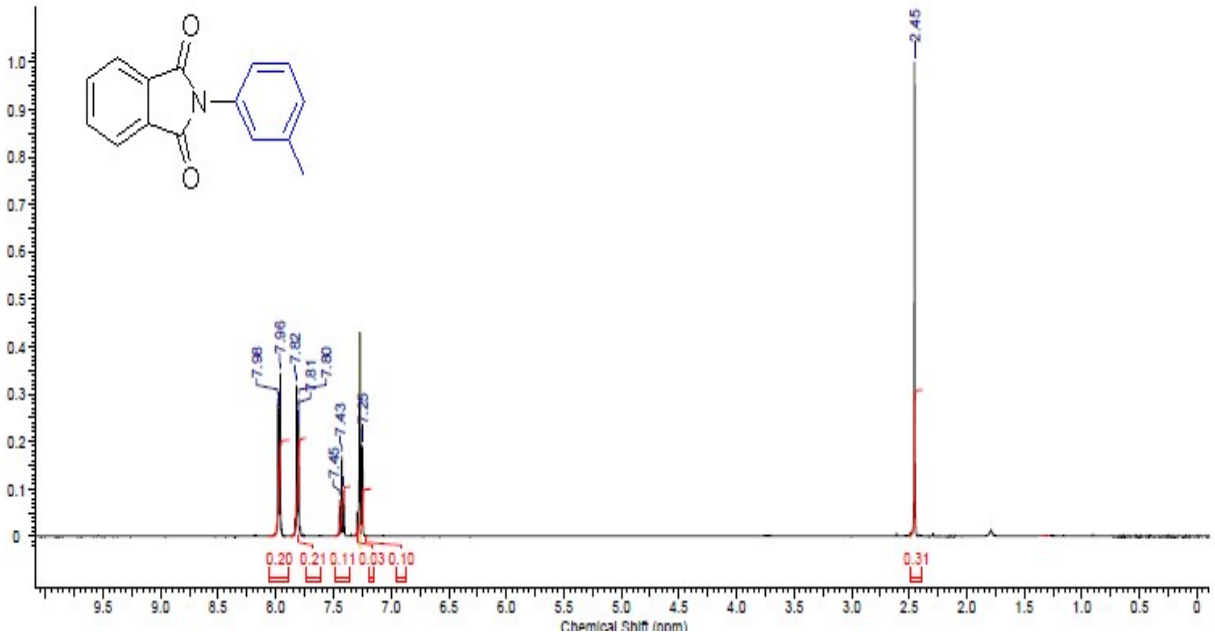

NMR NOV.2015
BDJ-PTSD-1H
f1 (ppm)

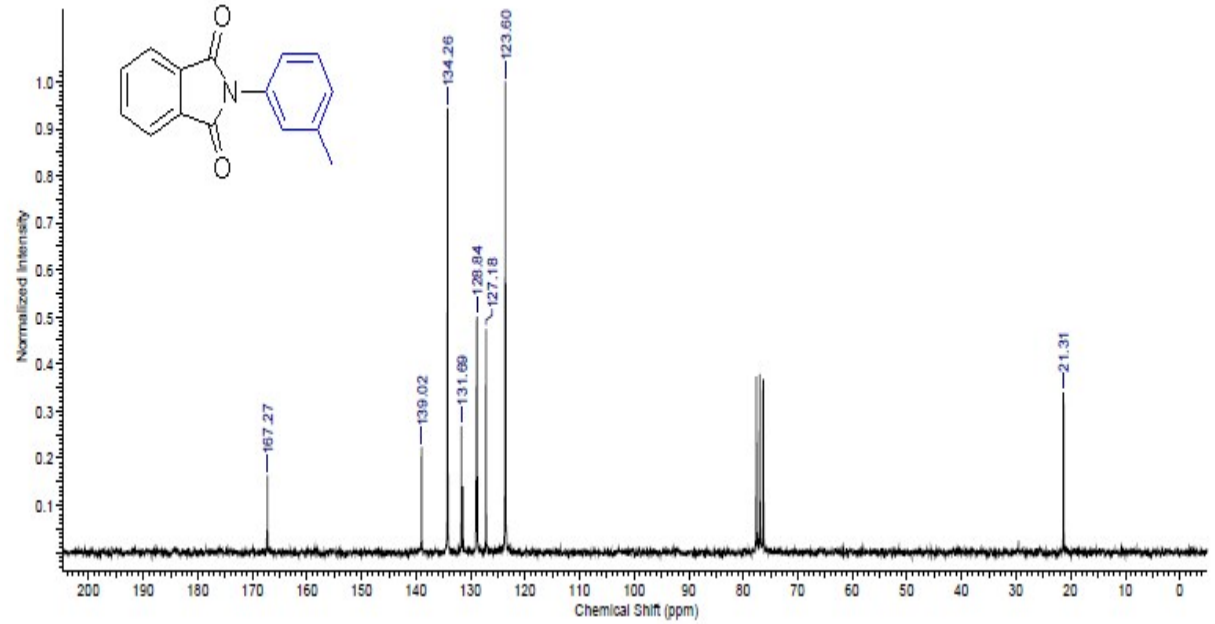

% T
Wavenumber(cm-1)
3362.30
3270.60
3039.08
2926.92
2597.25
2477.74
2317.03
1931.31
1664.28
1615.65
1524.17
1300
1152.47
1089.83
906.86
808.79
703.29
549.17

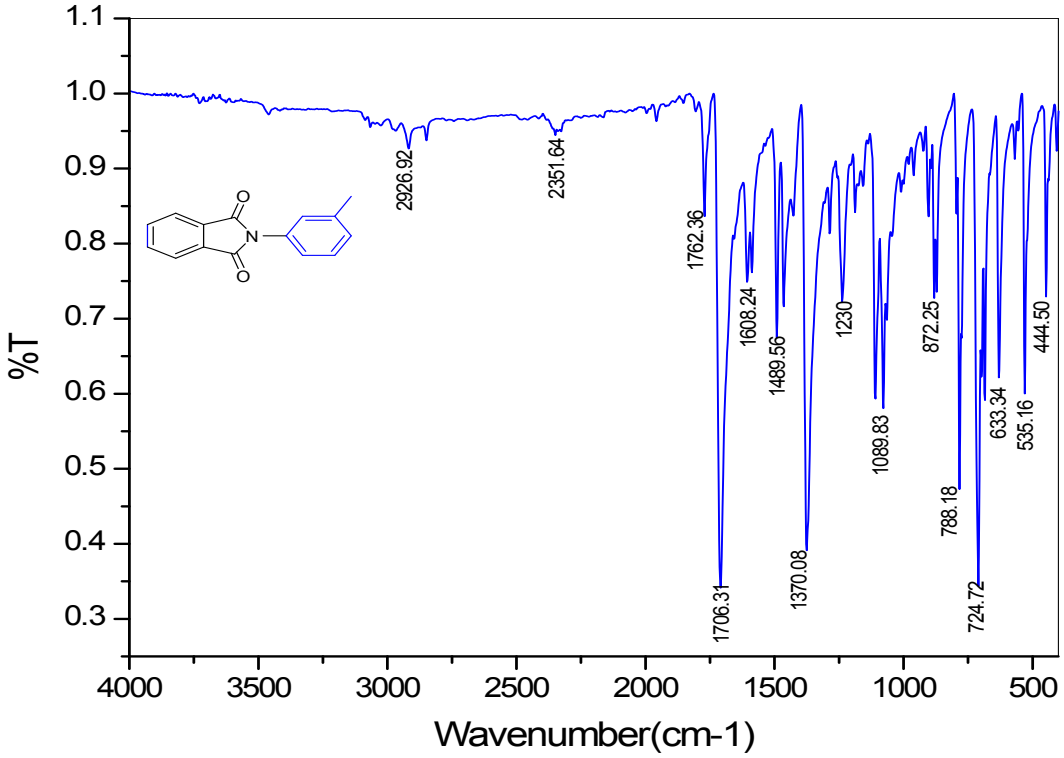

Oct28-2015
BDJ-2MPT- 28.10.15 IN CDCL3
7.98
7.98
7.82
7.82
7.40
7.36
7.25
7.23
2.24
0.65
0.68
0.49
0.94
0.35
1.00
f1 (ppm)

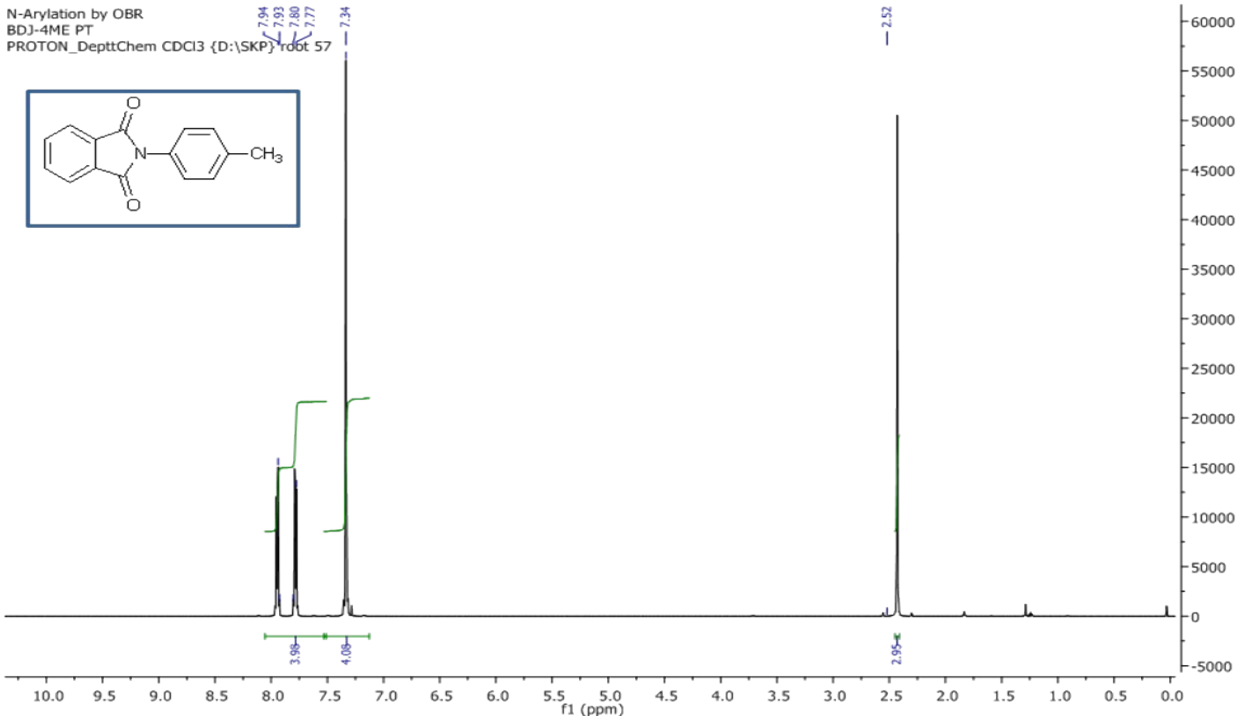

Oct28-2015
BDJ-2MPT- 28.10.15 13C IN CDCL3
167.51
136.33
133.97
131.83
131.08
130.72
130.10
129.37
128.58
126.62
123.78
77.64
77.00
76.60
17.97
0.53
0.51
2.85
0.88
1.77
1.40
-0.01
1.31
2.82
2.81
4.75
1.00
f1 (ppm)

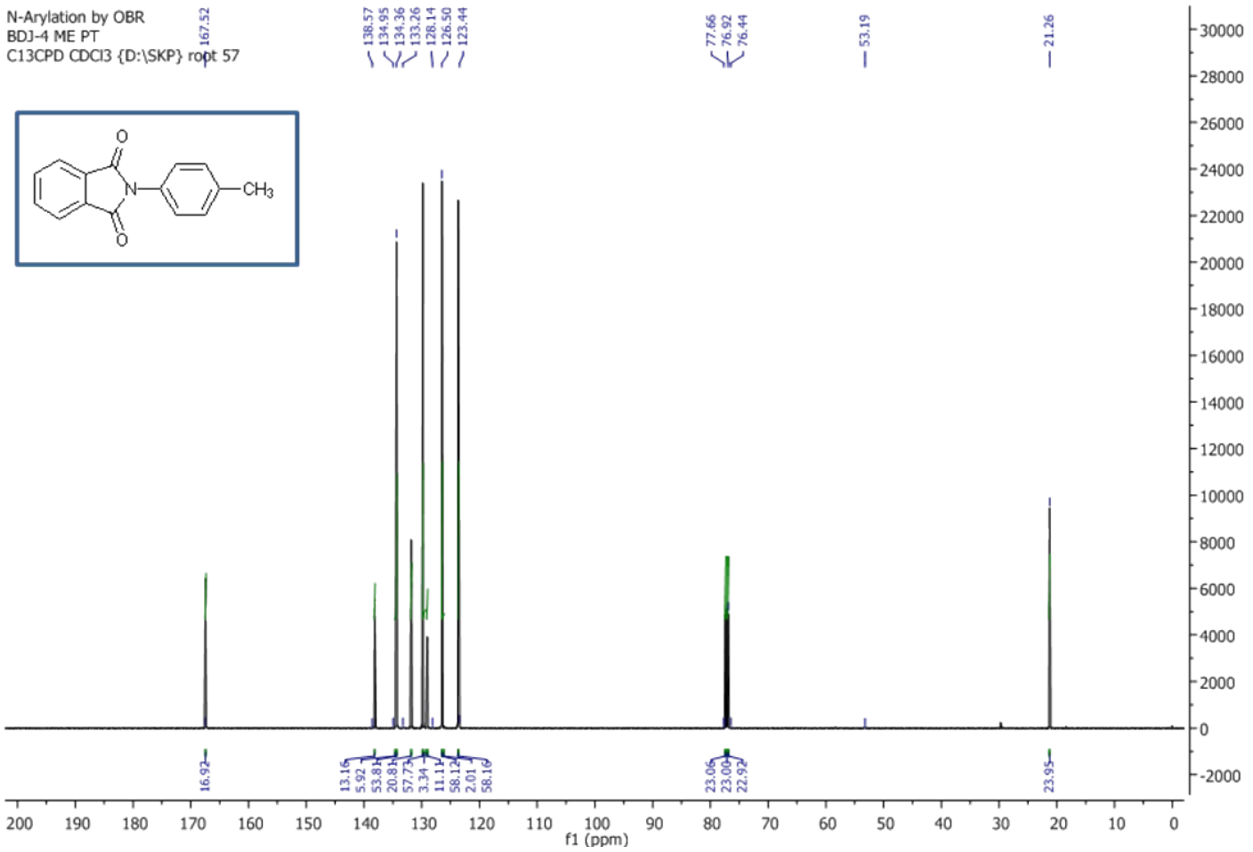

%T
Wavenumber(cm-1)
3074.31
1713.73
1503.37
1384.06
1229.94
1096.42
886.26
766.75
710.71
626.64
528.57
444.50

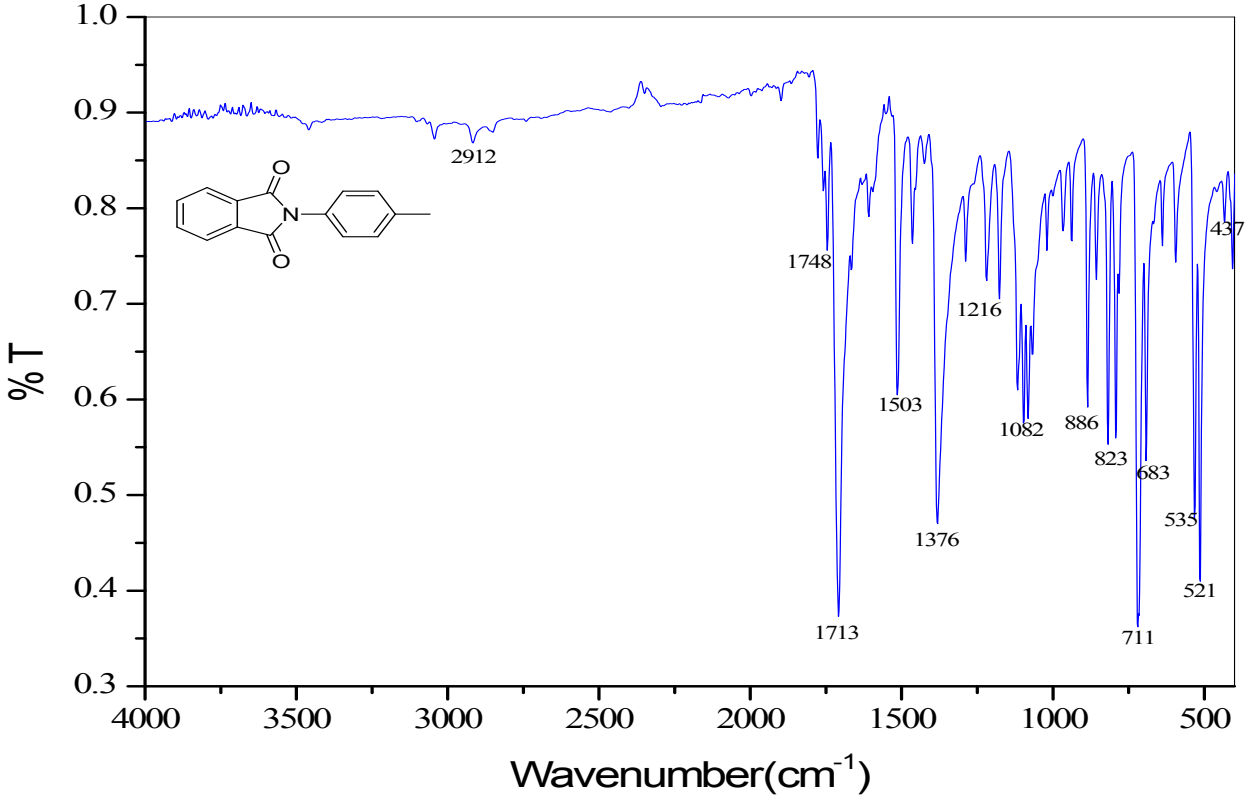

2.45
7.98
7.96
7.82
7.81
7.80
7.43
7.45
7.25
0.20 0.21 0.11 0.03 0.10
0.31
Chemical Shift (ppm)

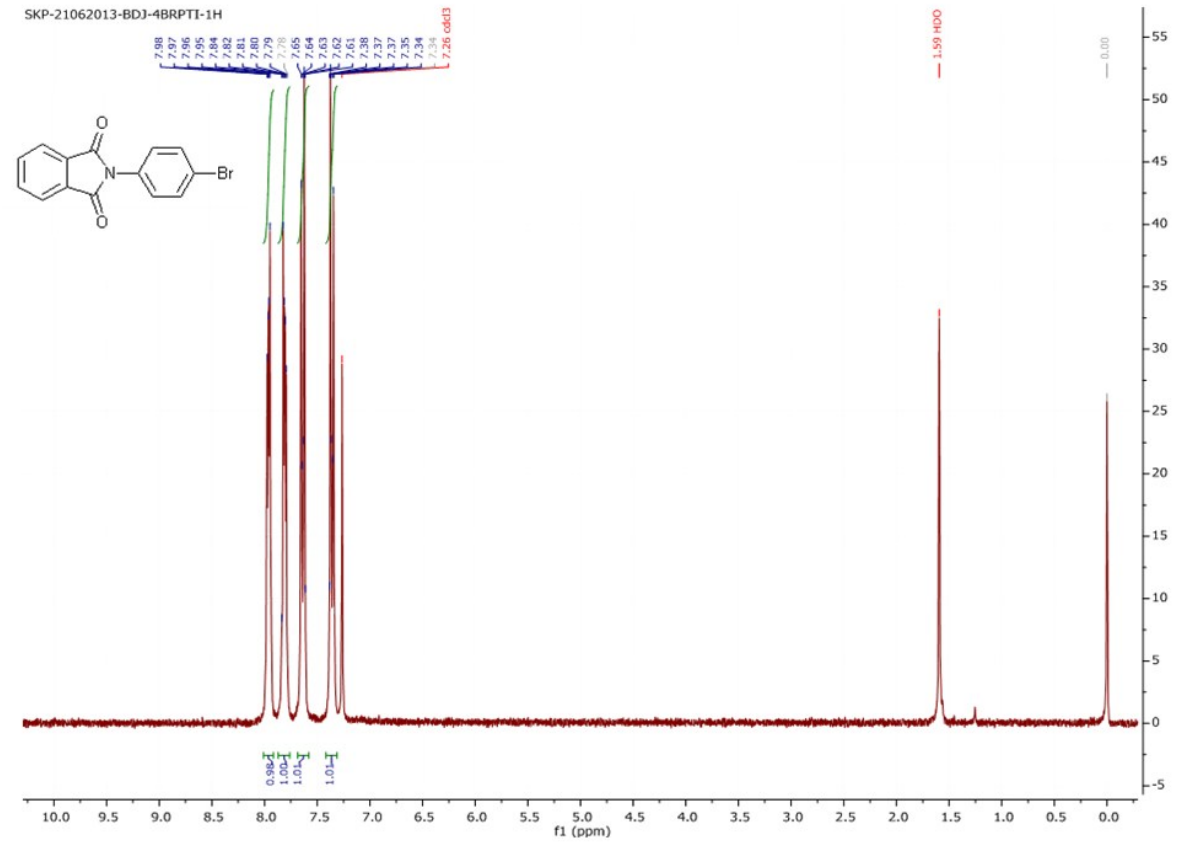

Normalized Intensity
167.27
139.02
134.26
131.69
128.84
127.18
123.60
21.31
Chemical Shift (ppm)

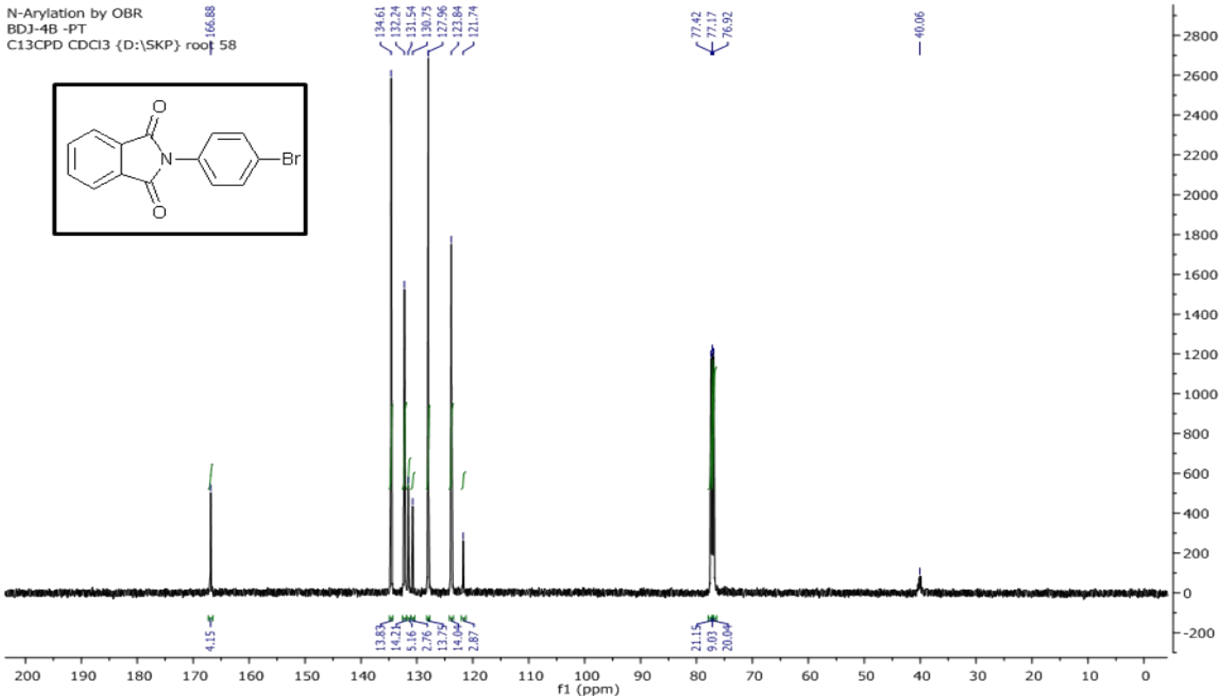

%T
Wavenumber(cm-1)
2926.92
2351.64
1762.36
1608.24
1489.56
1370.08
1230
1089.83
872.25
788.18
724.72
633.34
535.16
444.50
1706.31

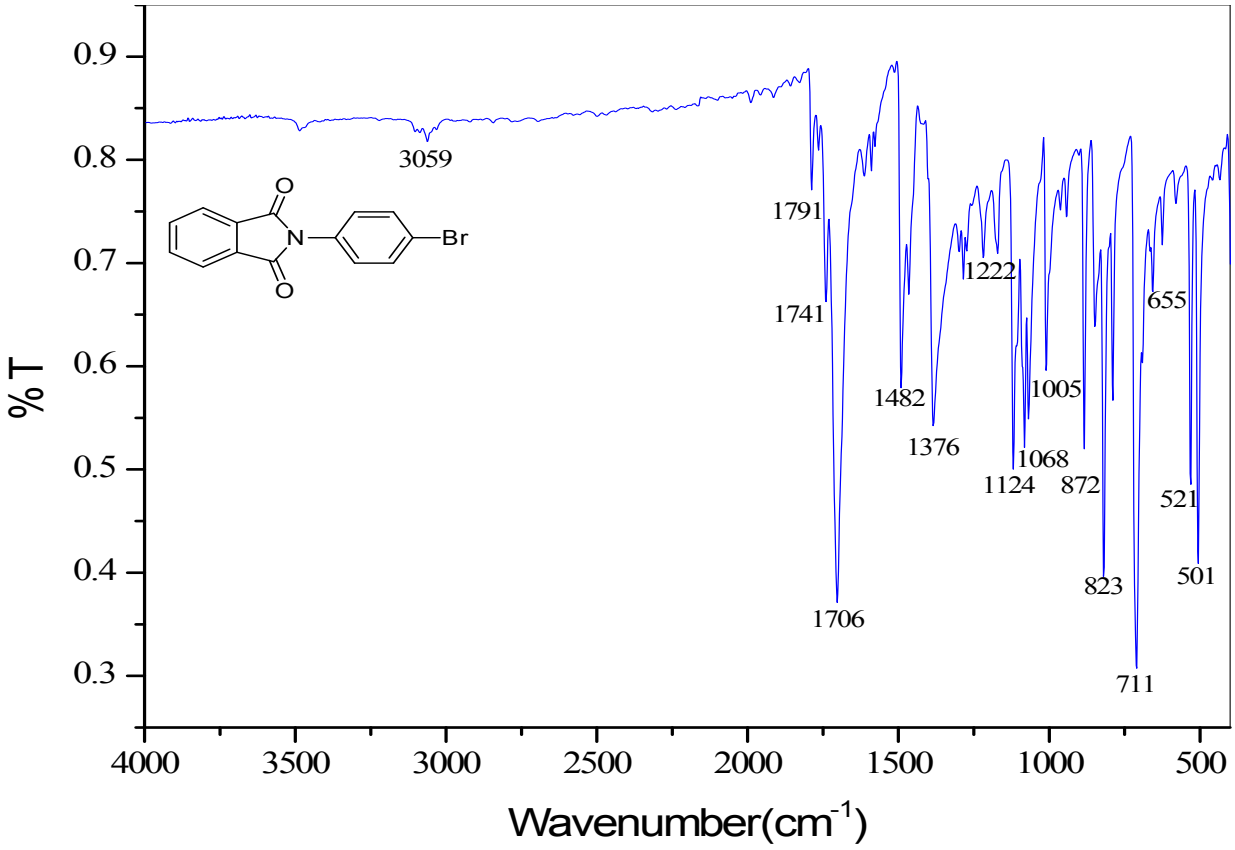

N-Arylation by OBR
BDJ-4ME PT
PROTON_DepttChem CDCl3 {D:\SKP} root 57
7.94
7.93
7.80
7.77
7.34
2.52
CH3
3.88
4.08
2.95
f1 (ppm)

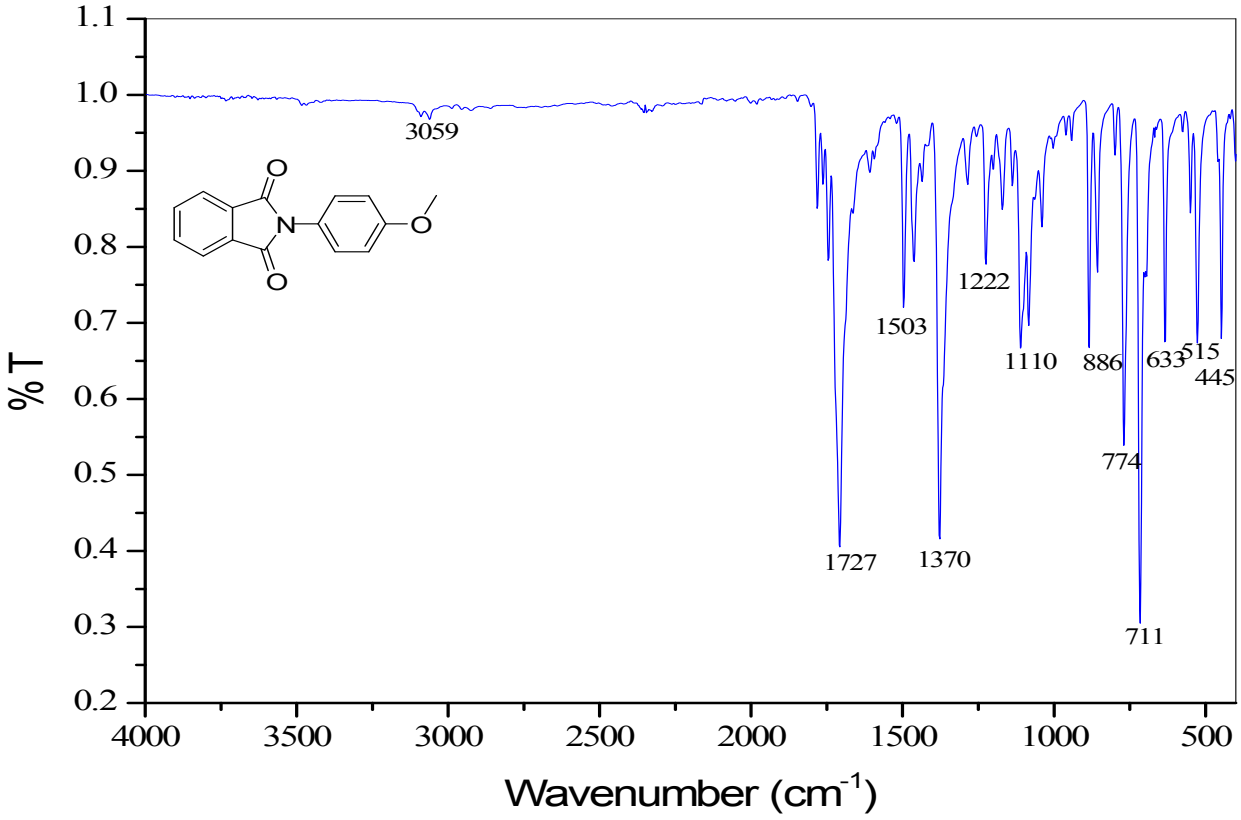

N-Arylation by OBR
BDJ-4 ME PT
C13CPD CDCl3 {D:\SKP} ropt 57
167.52
138.57
134.95
134.36
133.26
128.14
126.50
123.44
77.66
76.92
76.44
53.19
21.26
f1 (ppm)

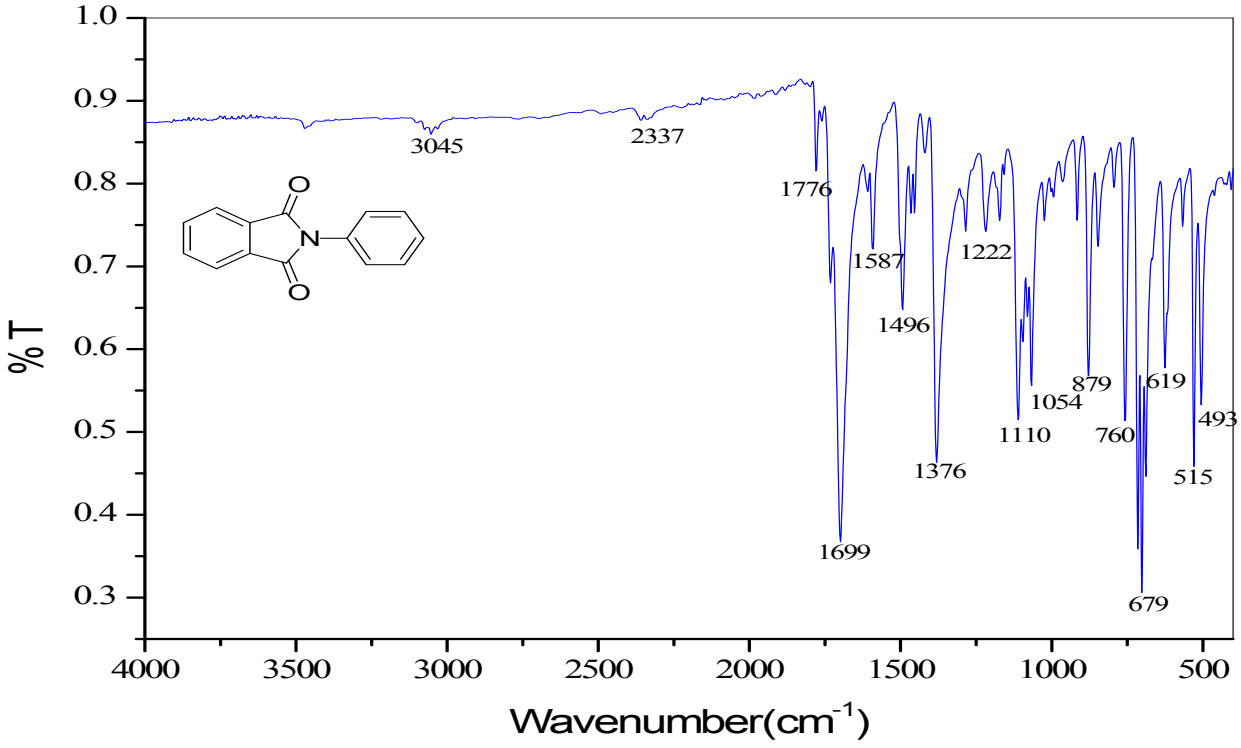

%T
Wavenumber(cm-1)
2912
1748
1713
1503
1376
1216
1082
886
823
711
683
535
521
437

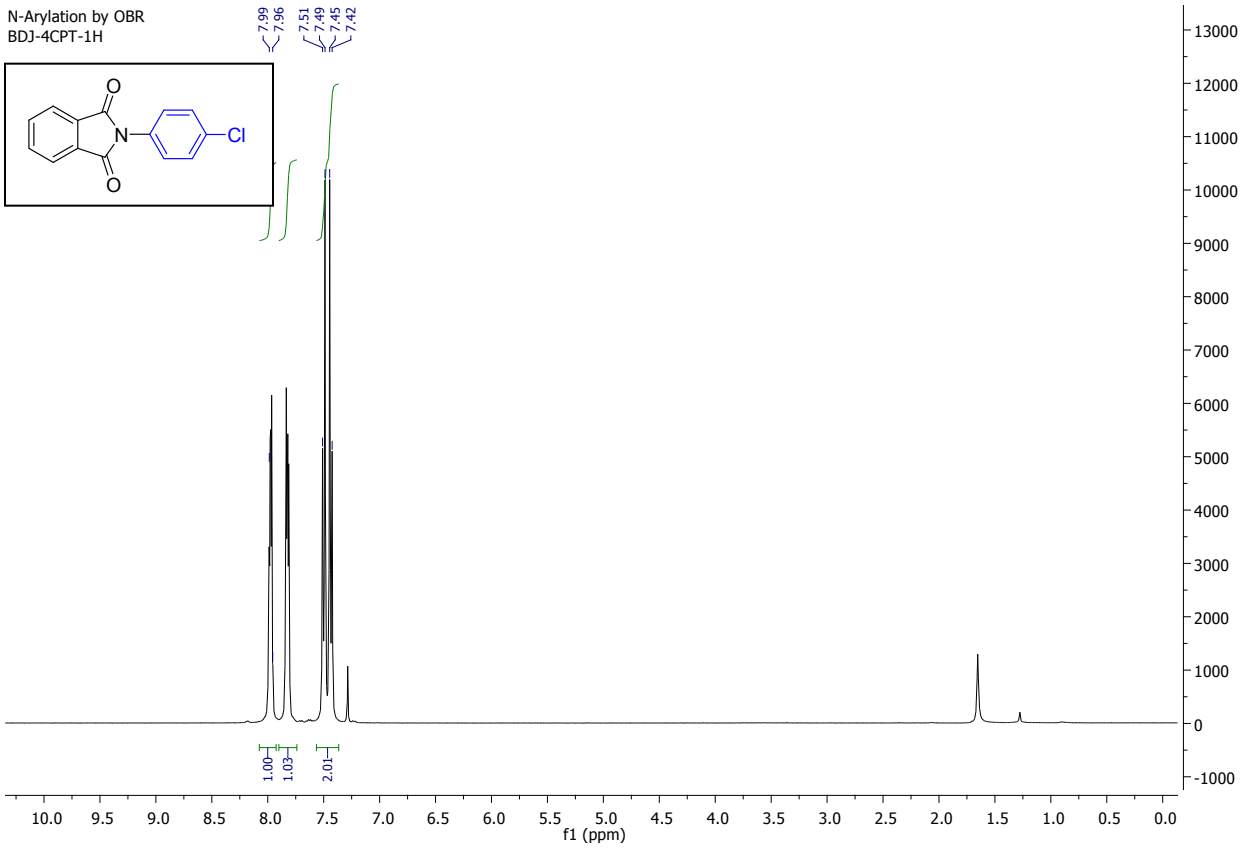

SKP-21062013-BDJ-4BRPTI-1H
7.98
7.97
7.96
7.95
7.84
7.82
7.81
7.80
7.79
7.78
7.65
7.64
7.63
7.62
7.61
7.38
7.37
7.37
7.35
7.34
7.34
7.26 cdcl3
1.59 HDO
0.00
O
N
Br
O
0.98
1.00
1.01
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
55
50
45
40
35
30
25
20
15
10
5
0
-5

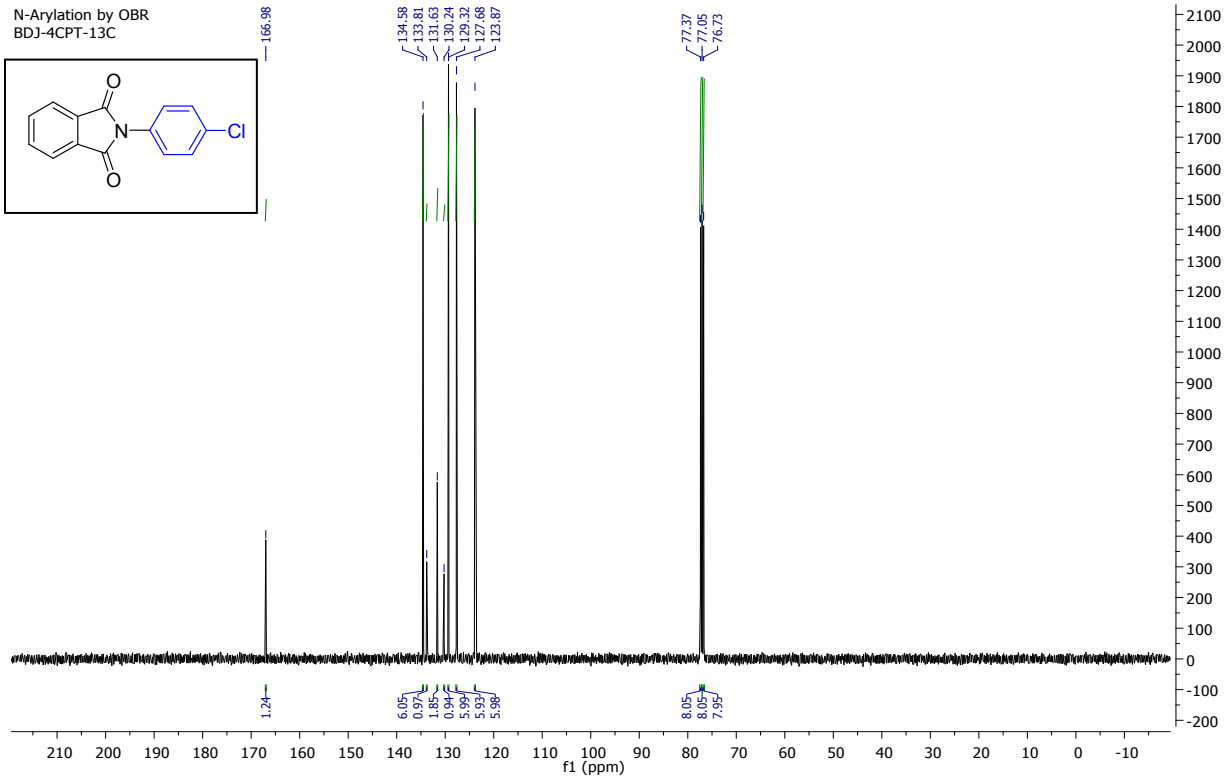

N-Arylation by OBR
BDJ-4B -PT
C13CPD CDCl3 {D:\SKP} roo 58
166.88
134.61
132.24
131.54
130.75
127.96
123.84
121.74
77.42
77.17
76.92
40.06
O
N
Br
O
4.15
13.83
14.21
5.16
2.76
13.79
14.04
2.87
21.15
9.03
20.04
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200

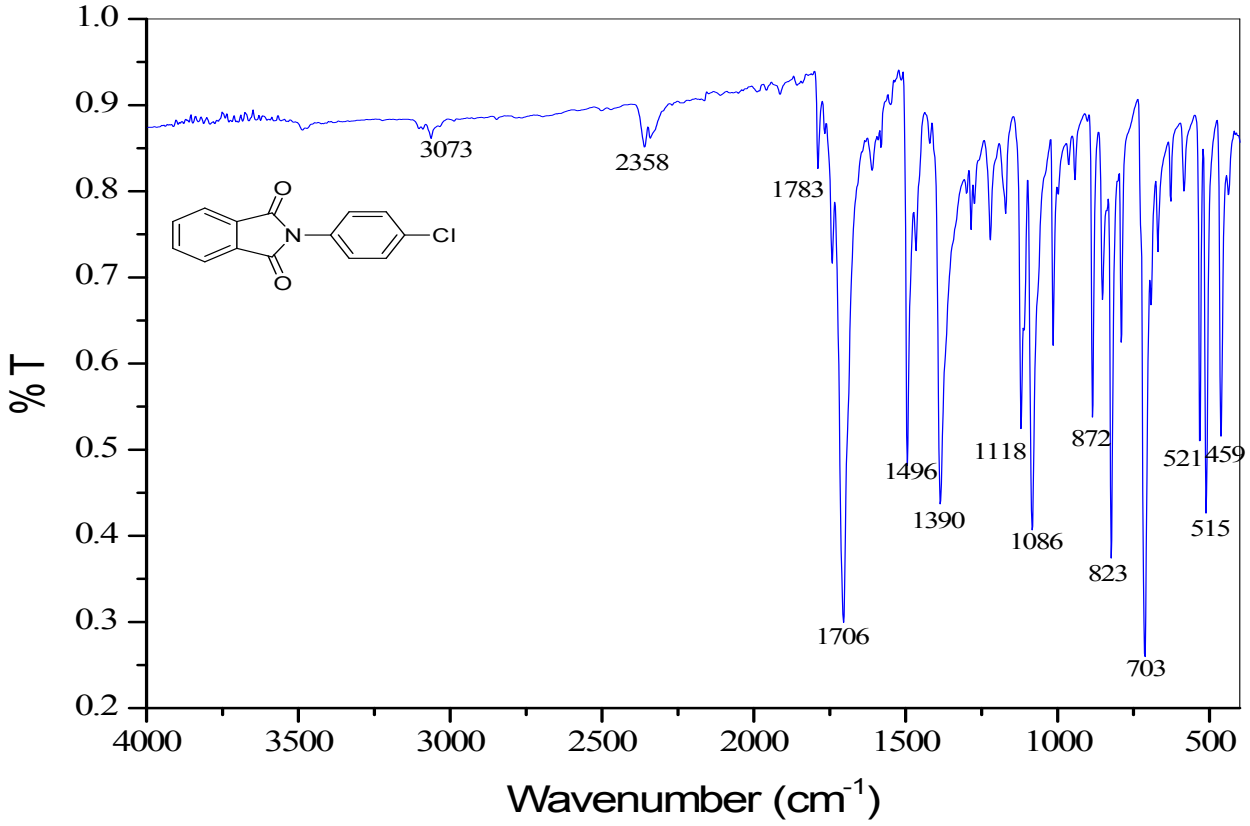

0.9
0.8
0.7
0.6
0.5
0.4
0.3
%T
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber(cm-1)
3059
1791
1741
1706
1482
1376
1222
1124
1068
1005
872
823
711
655
521
501
O
N
Br
O

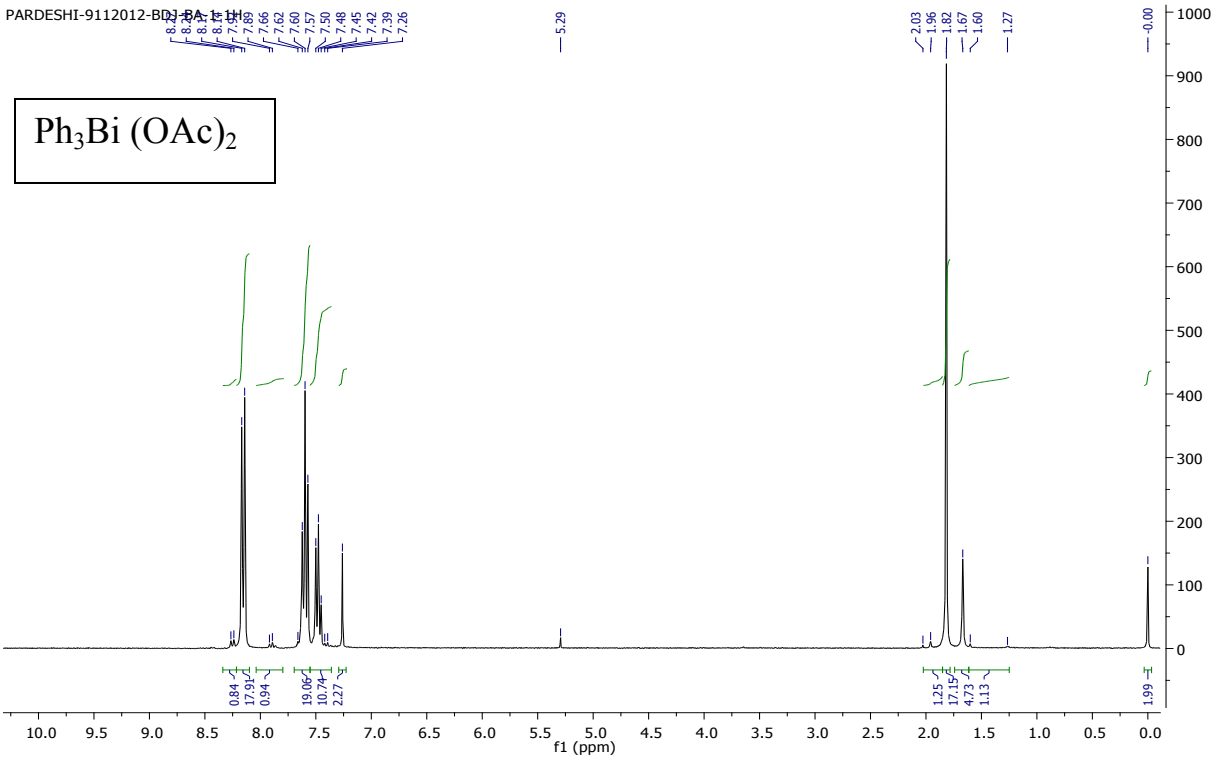

%T
Wavenumber (cm-1)
3059
1727
1503
1370
1222
1110
886
774
711
633
515
445

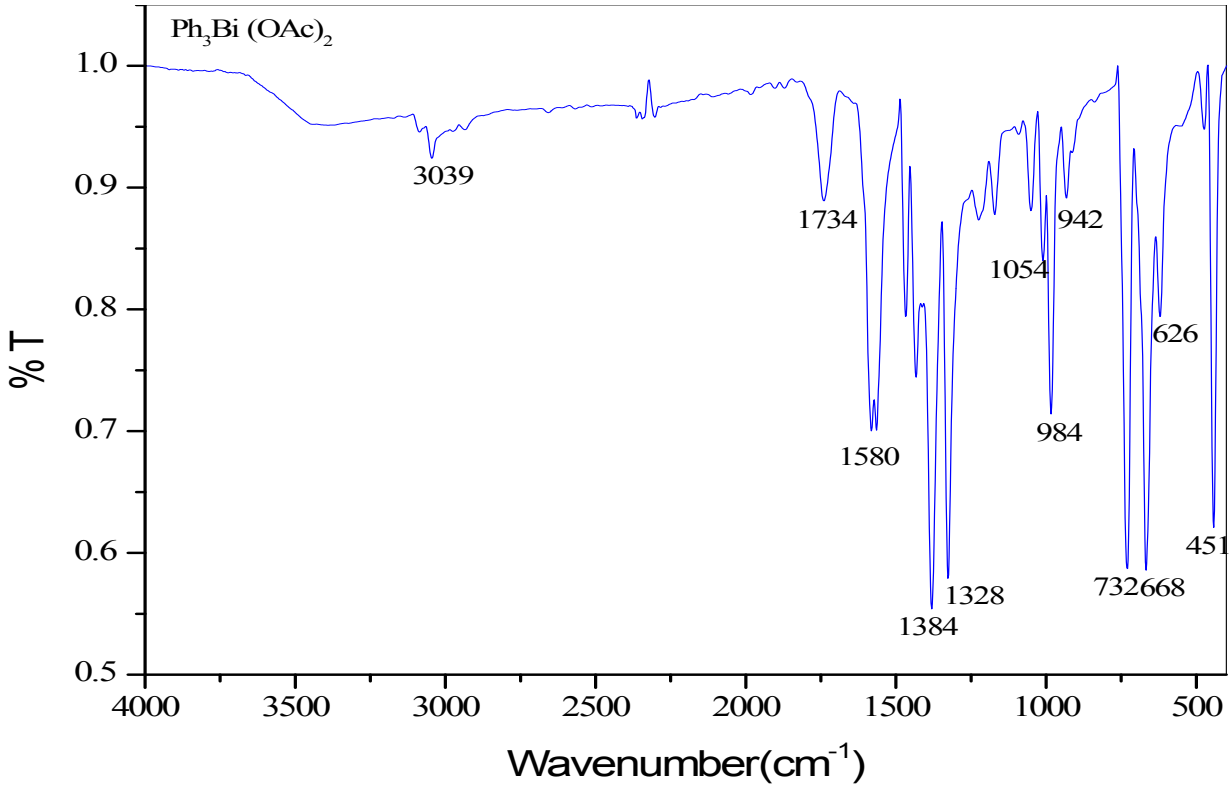

%T
Wavenumber(cm-1)
3045
2337
1776
1699
1587
1496
1376
1222
1110
1054
879
760
679
619
515
493

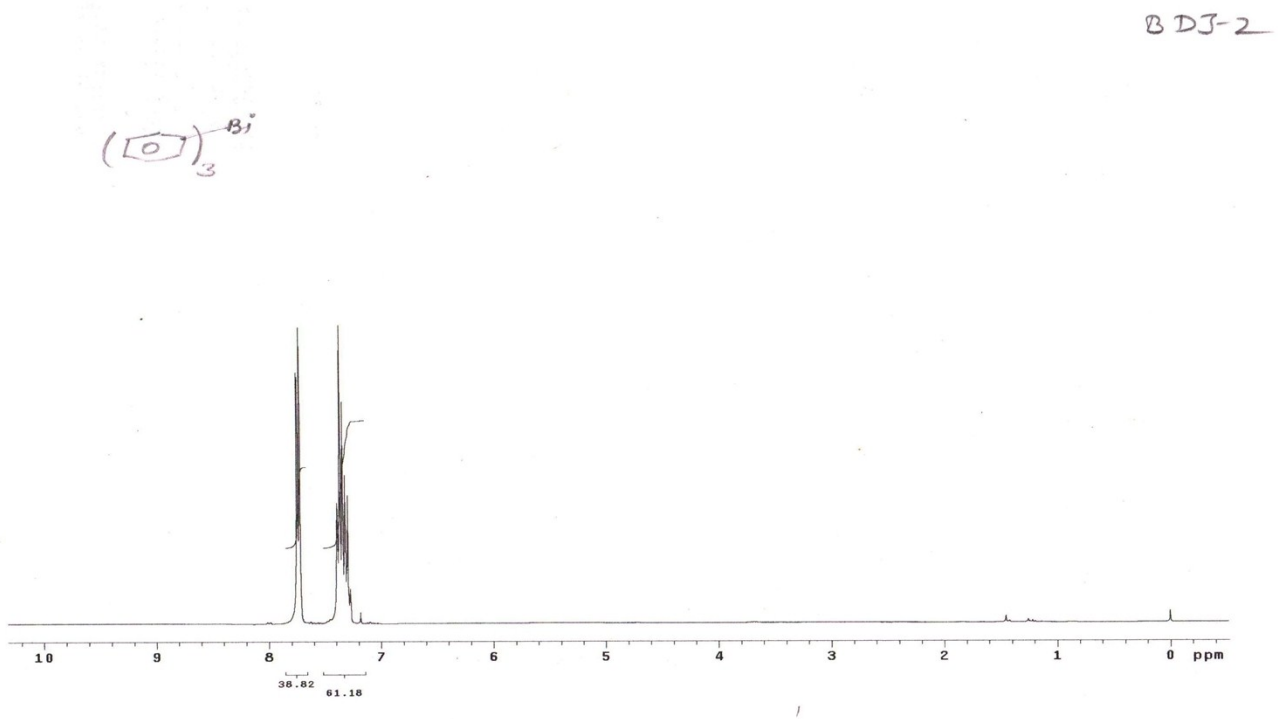

N-Arylation by OBR
BDJ-4CPT-1H
7.99
7.96
7.51
7.49
7.45
7.42
O
N
Cl
O
1.00
1.03
2.01
f1 (ppm)


N-Arylation by OBR
BDJ-4CPT-13C
166.98
134.58
133.81
131.63
130.24
129.32
127.68
123.87
77.37
77.05
76.73
O
N
Cl
O
1.24
6.05
0.97
1.85
0.94
5.99
5.93
5.98
8.05
8.05
7.95
f1 (ppm)

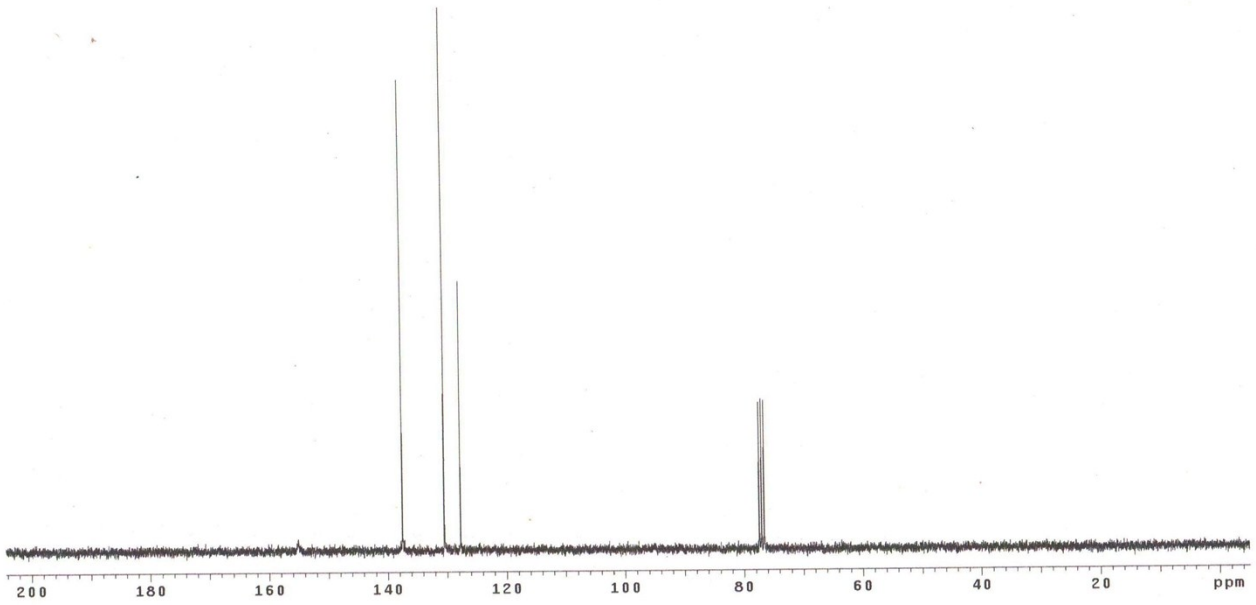

%T
Wavenumber (cm-1)
3073
2358
1783
1706
1496
1390
1118
1086
872
823
703
521
515
459
Cl
N
O


PARDESHI-9112012-BDJ-BA-1-1H
Ph3Bi (OAc)2
f1 (ppm)

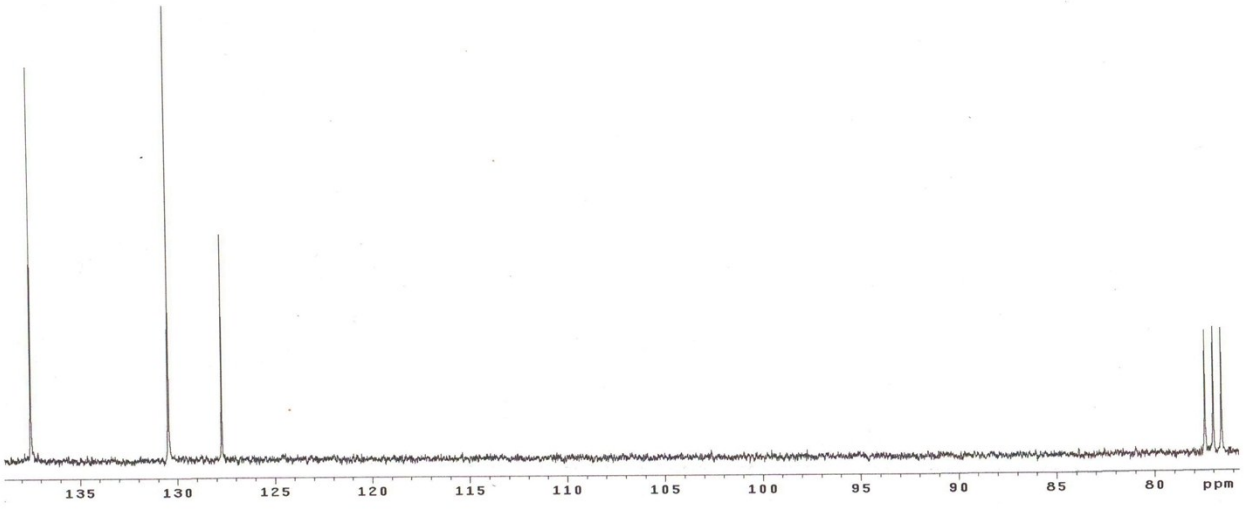

Ph3Bi (OAc)2
%T
Wavenumber(cm-1)
3039
1734
1580
1384
1328
1054
984
942
626
732
668
451

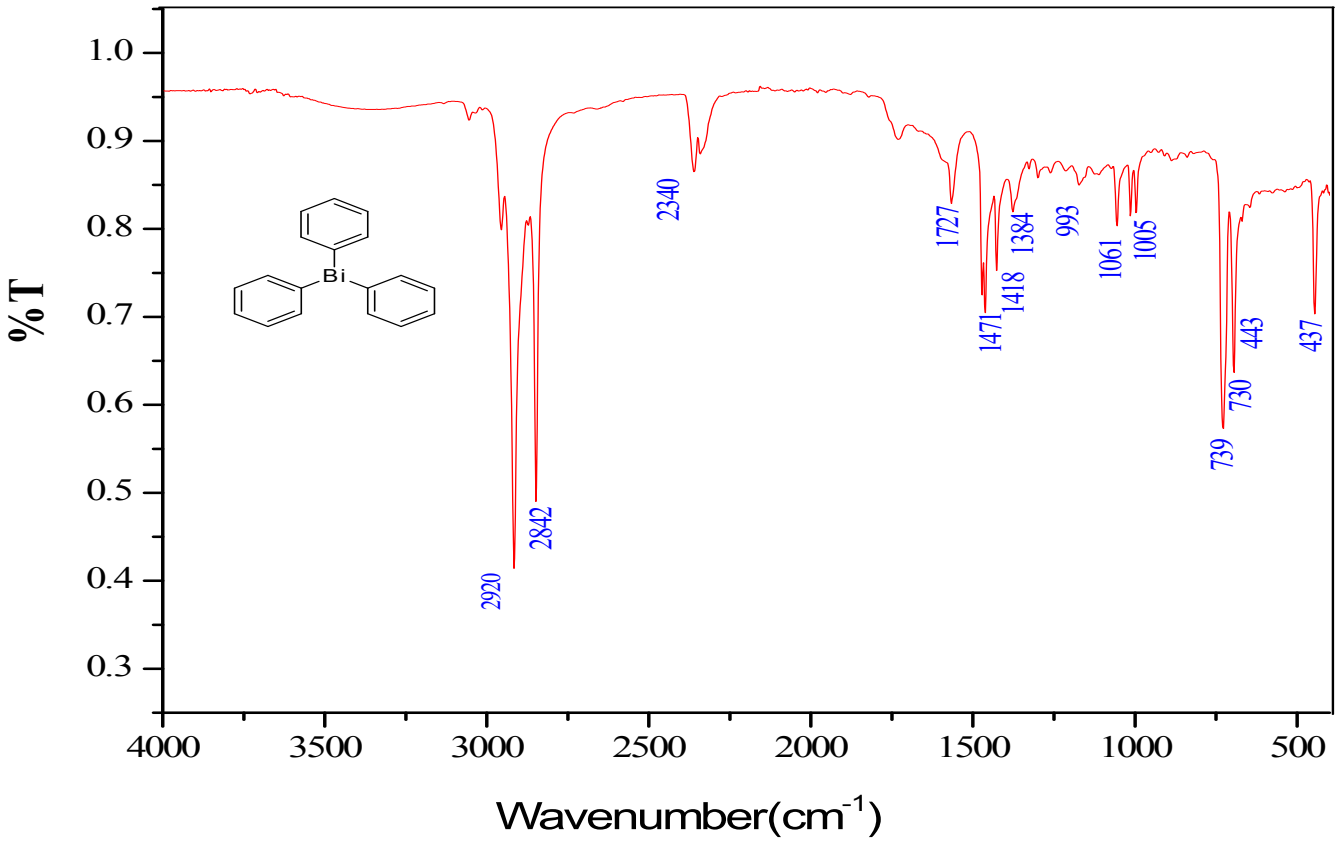

BDJ-2
38.82
61.18
ppm

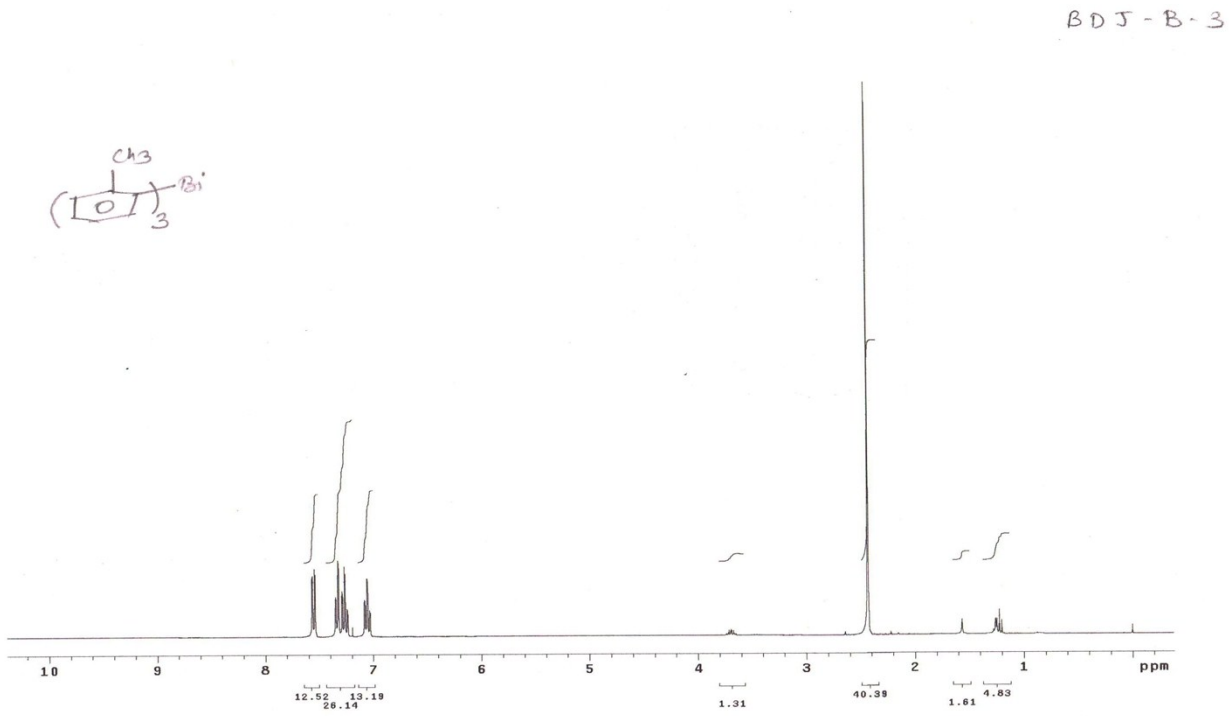
BDJ-2

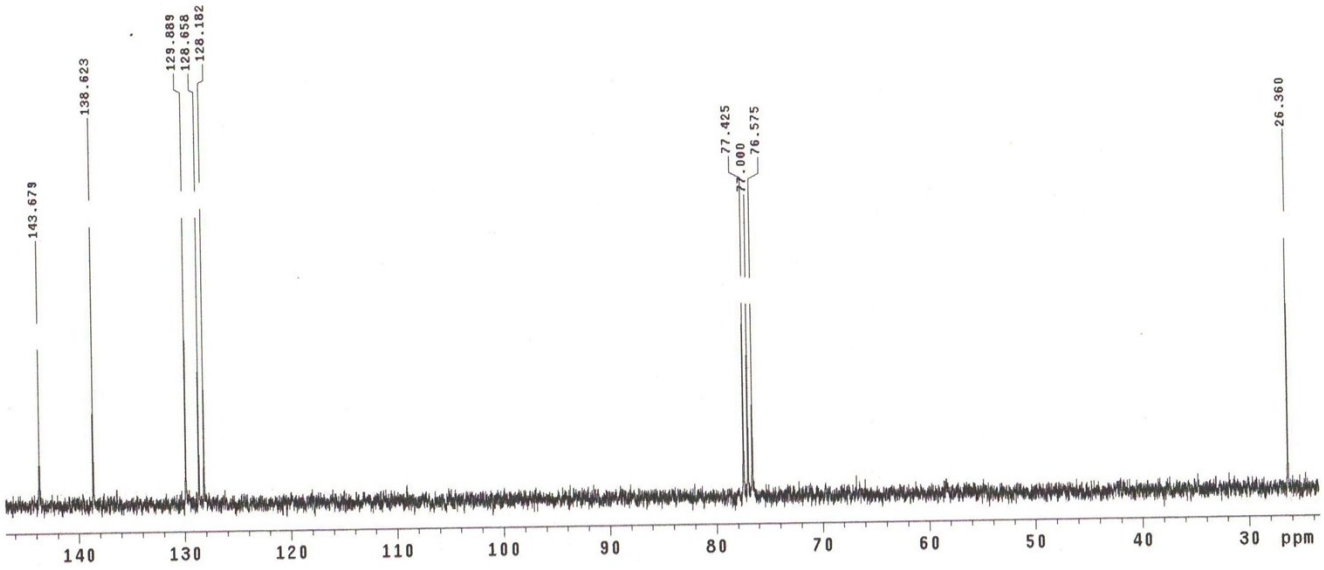


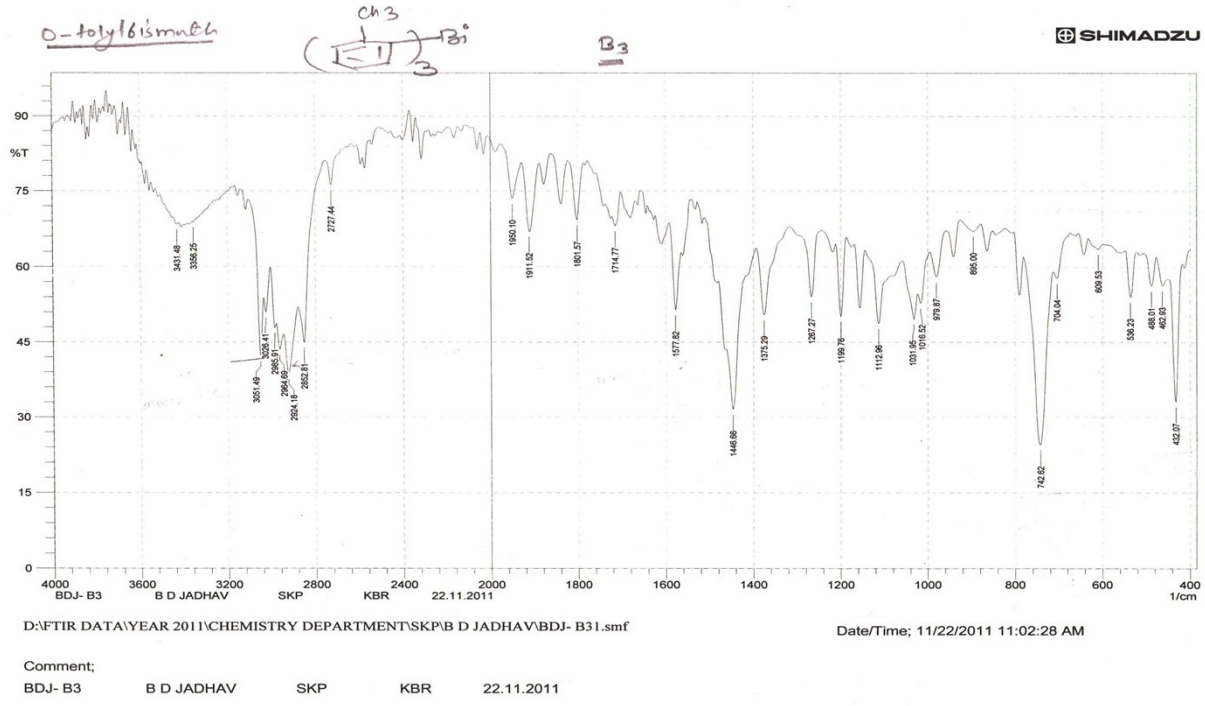
INDEX	FREQUENCY	PPM	HEIGHT	
1	10375.2	137.510	110.7	
2	9843.3	130.461	127.6	
3	9636.0	127.713	63.3	
4	5841.7	77.425	34.3	
5	5809.7	77.000	35.2	$CDCl_3$
6	5777.8	76.575	34.8	




%T
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber(cm-1)
Bi
2920
2842
2340
1727
1471
1418
1384
993
1061
1005
739
730
443
437


BDJ-B-3
CH3
Bi
3
10
9
8
7
6
5
4
3
2
1
ppm
12.52
13.19
20.14
1.31
40.38
1.61
4.83



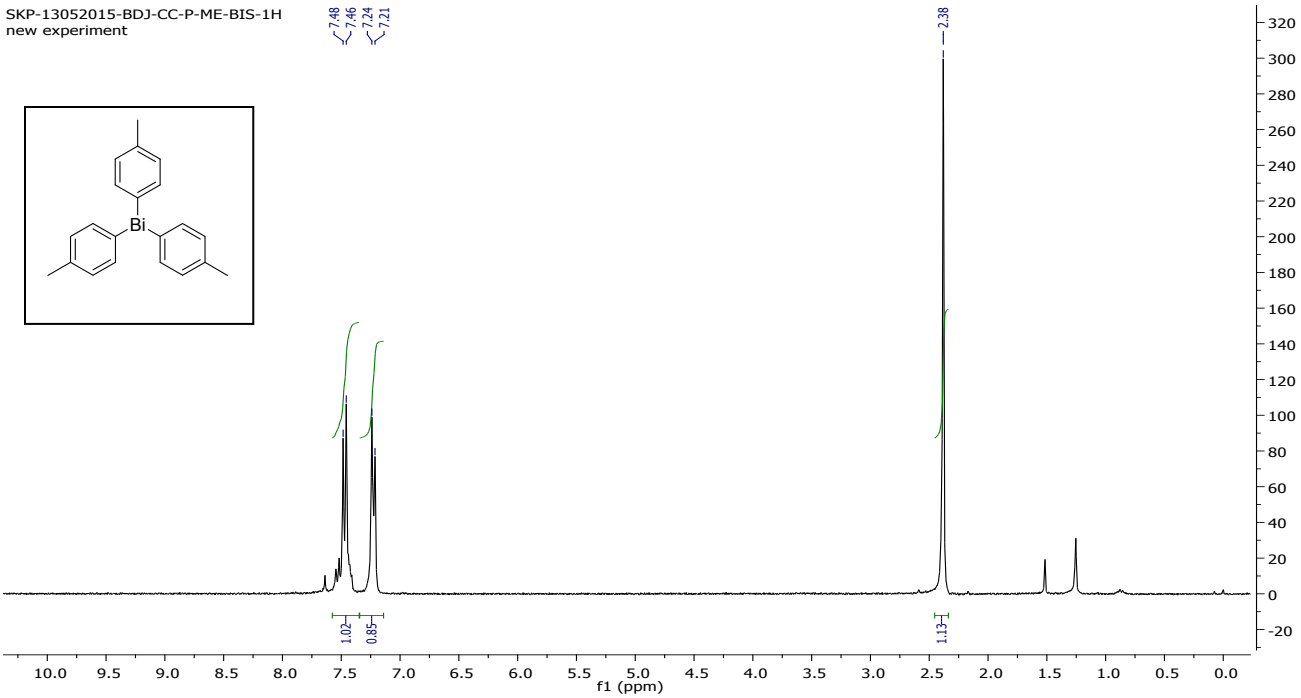


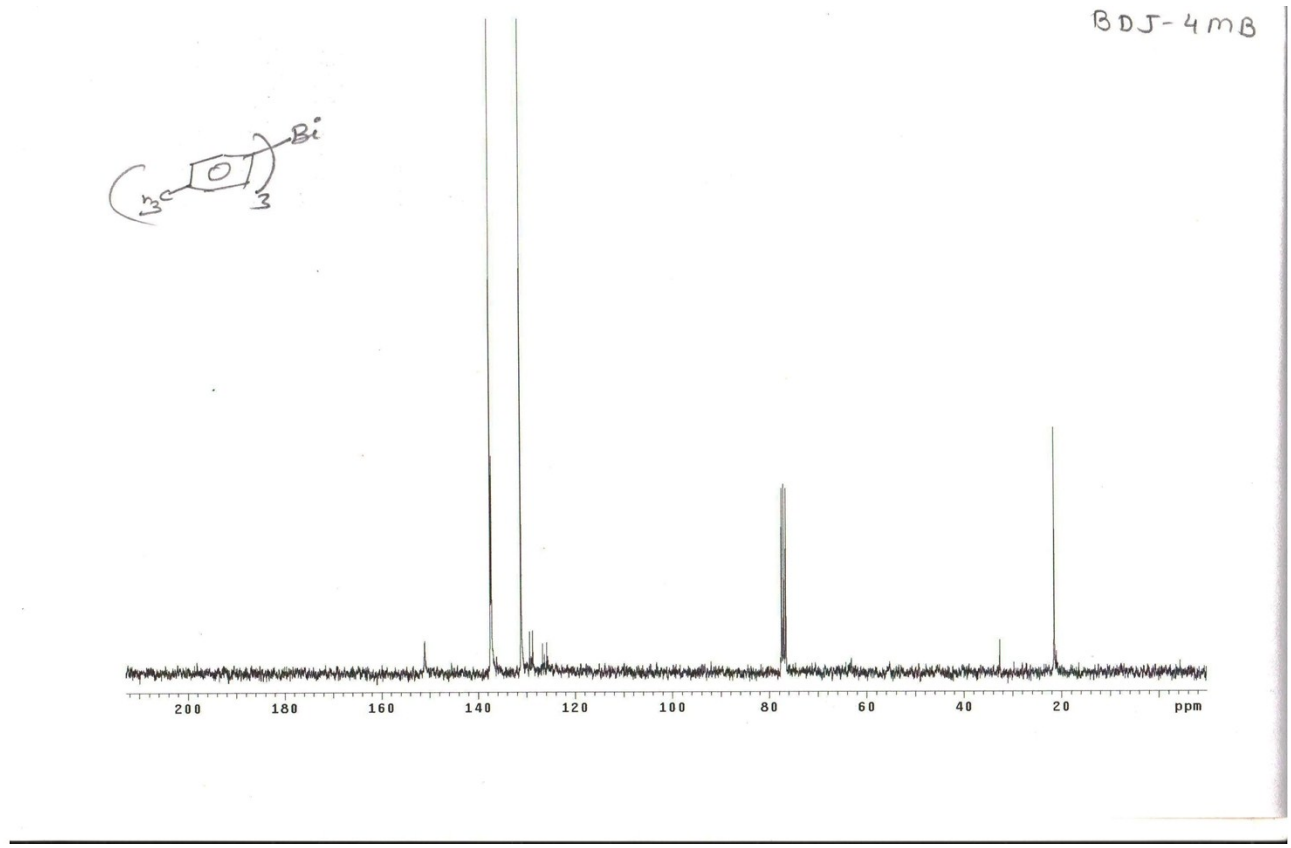
D:\FTIR DATA\YEAR 2011\CHEMISTRY DEPARTMENT\SKP\B D JADHAV\BDJ- B31.smf

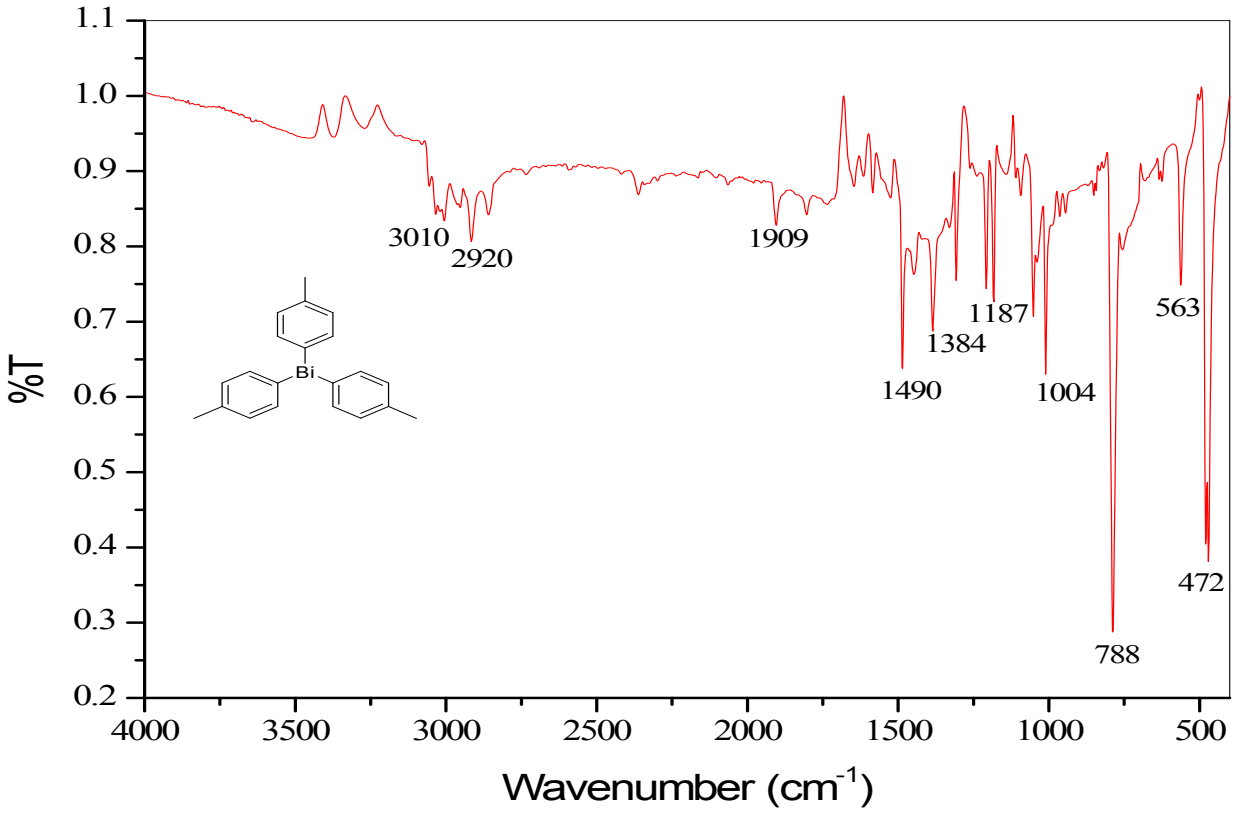
Date/Time; 11/22/2011 11:02:28 AM

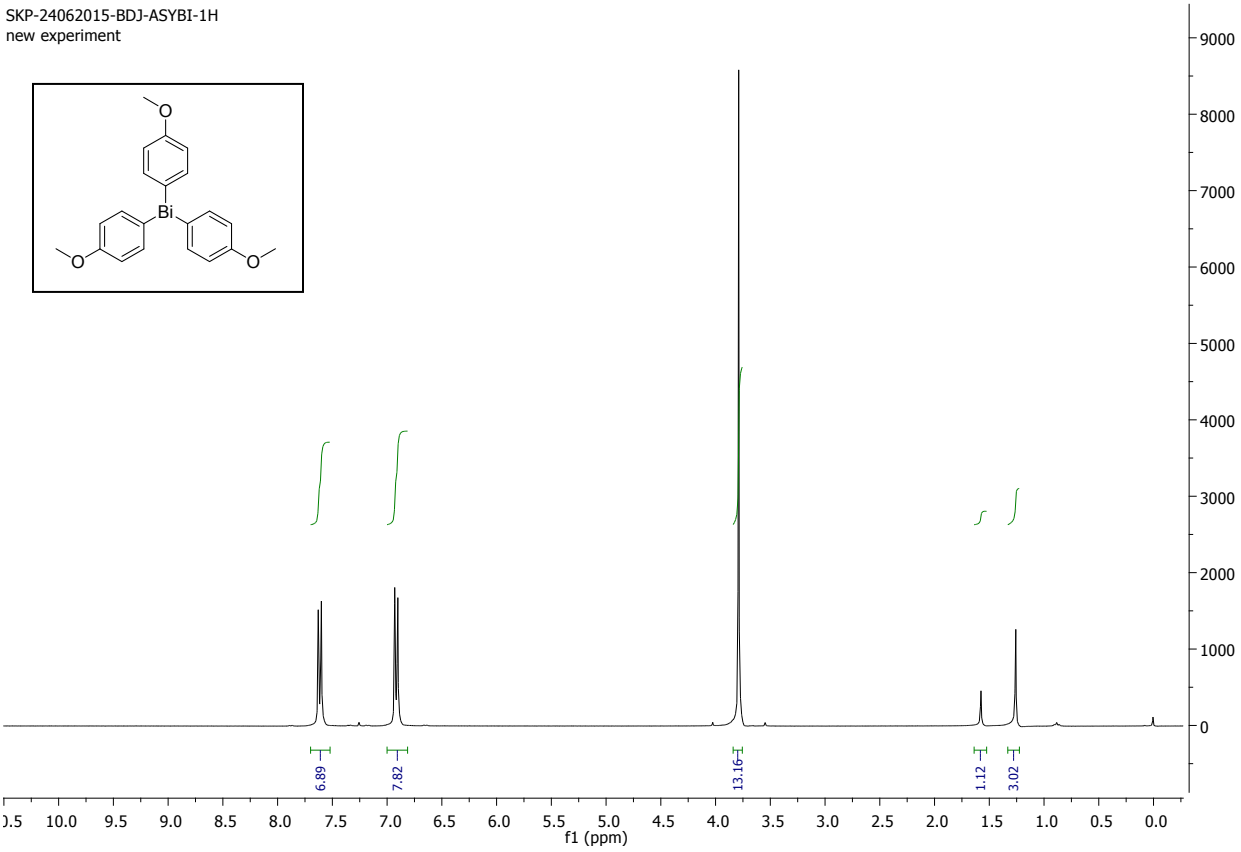
Comment;

BDJ- B3 B D JADHAV SKP KBR 22.11.2011

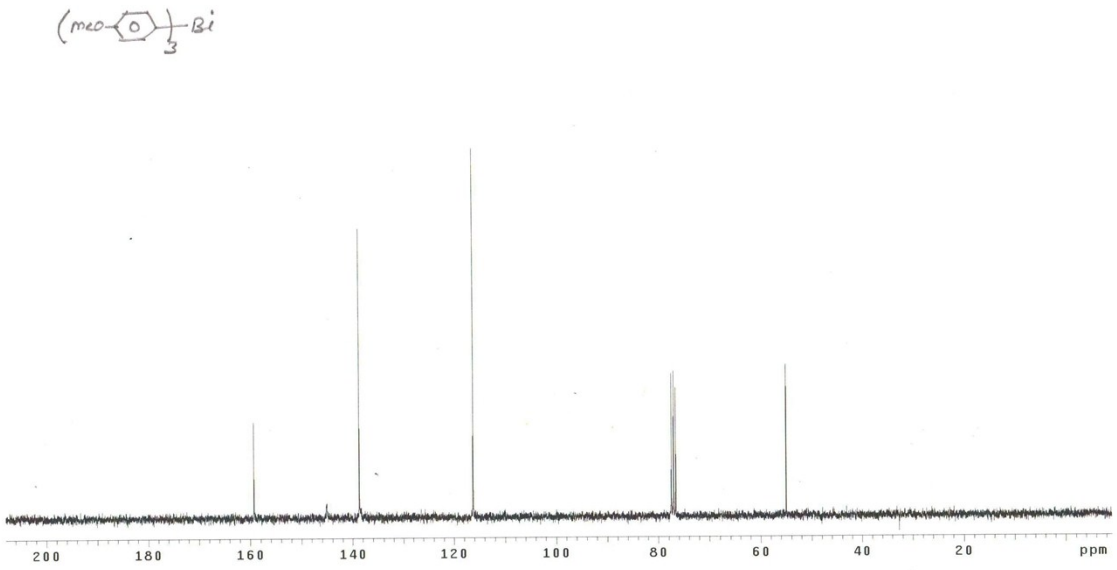

SKP-13052015-BDJ-CC-P-ME-BIS-1H
new experiment
7.48
7.46
7.24
7.21
2.38
Bi
1.02
0.85
1.13
f1 (ppm)

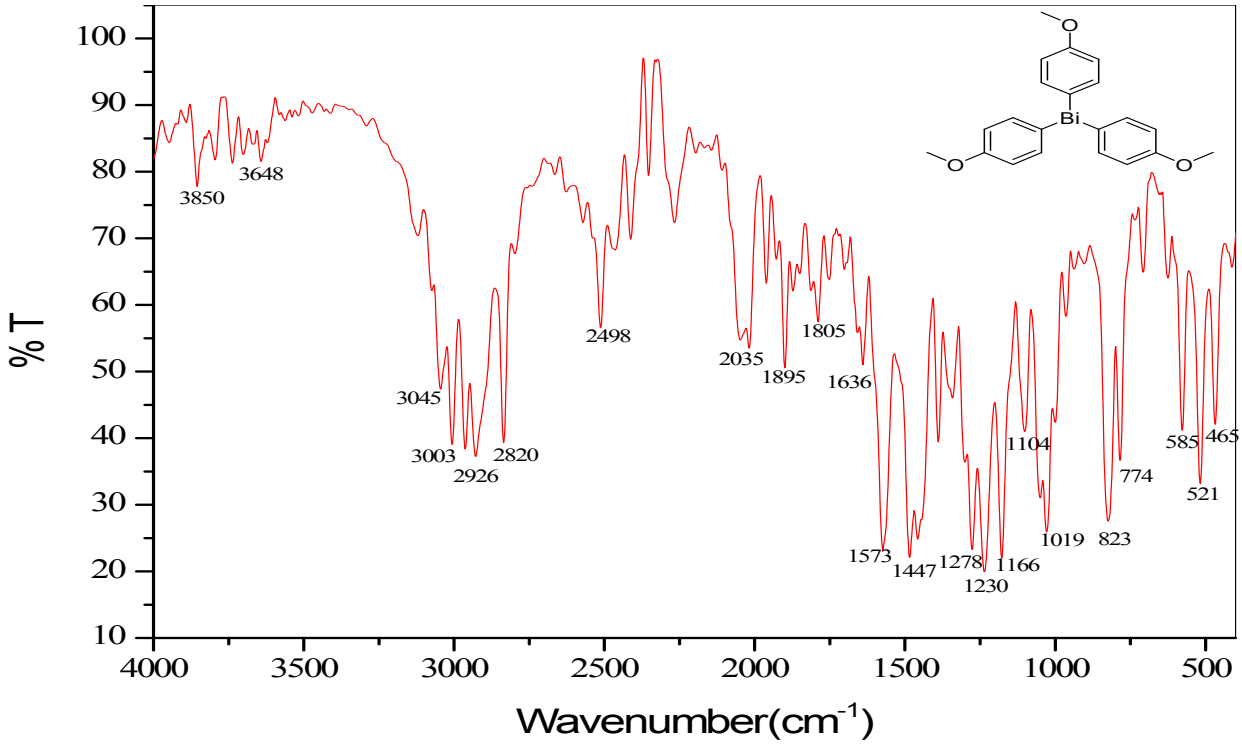

BDJ-4MB
Bi
ppm

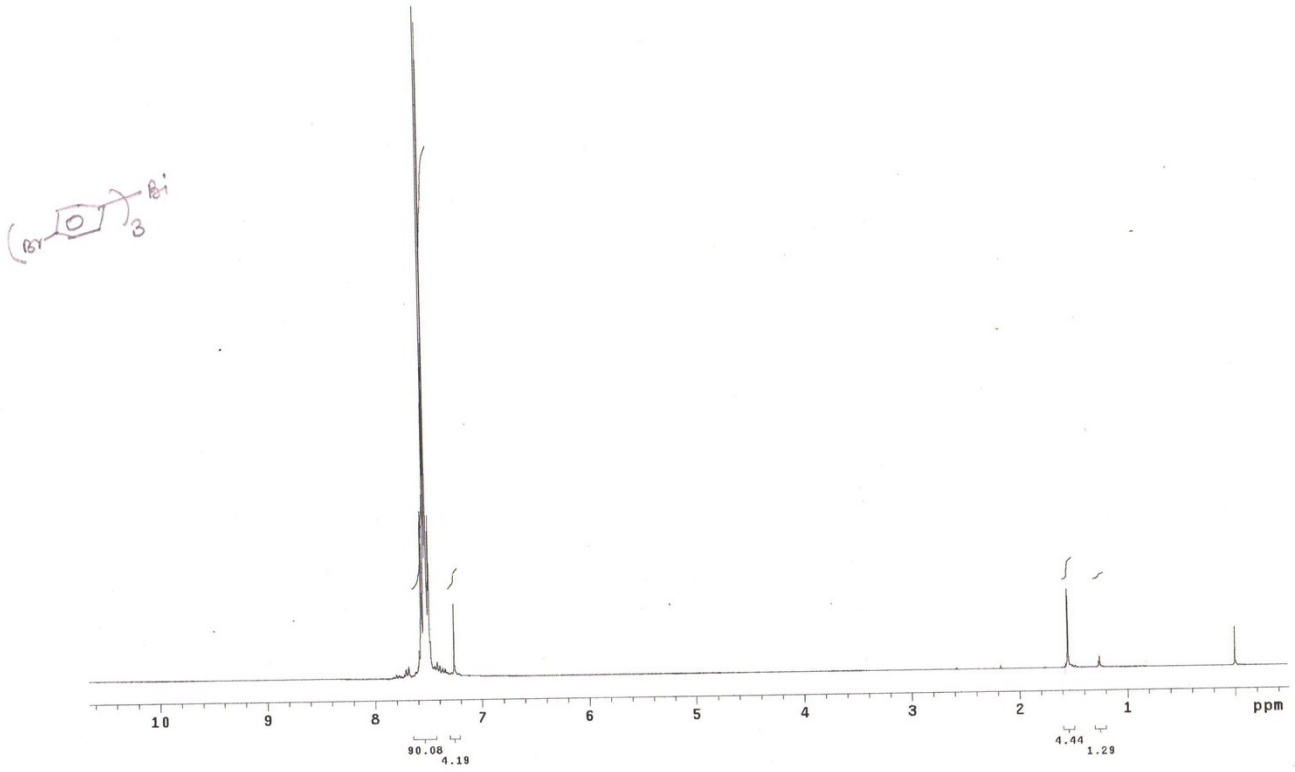

%T
Wavenumber (cm-1)
3010
2920
1909
1490
1384
1187
1004
788
563
472
Bi


SKP-24062015-BDJ-ASYBI-1H
new experiment
Bi
O
f1 (ppm)
6.89
7.82
13.16
1.12
3.02

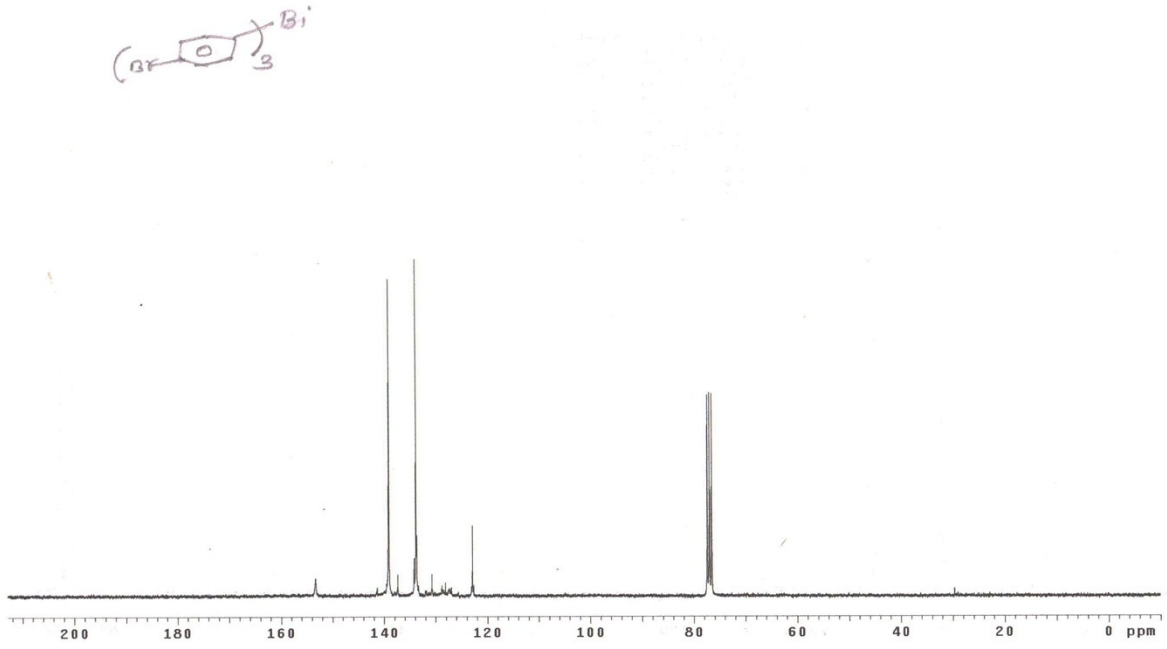
BDT-PAB


200
180
160
140
120
100
80
60
40
20
ppm


%T
Wavenumber(cm-1)
3850
3648
3045
3003
2926
2820
2498
2035
1895
1805
1636
1573
1447
1278
1230
1166
1104
1019
823
774
585
521
465
Bi
O

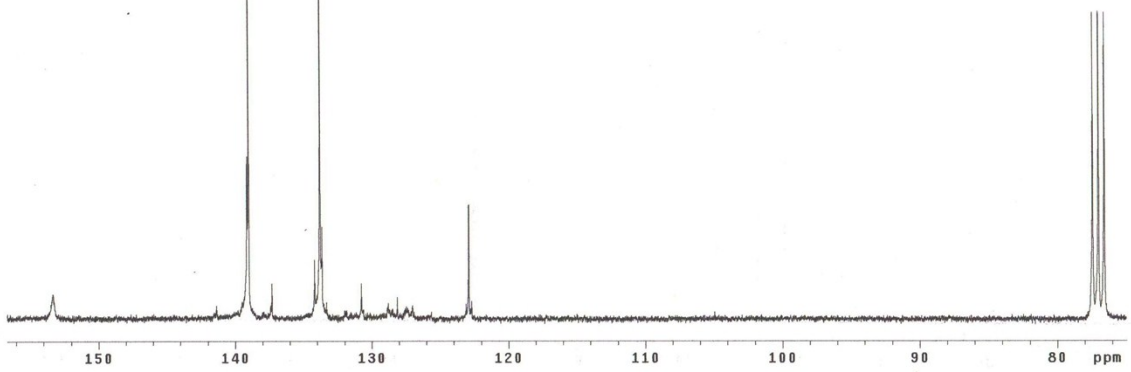

10
9
8
7
6
5
4
3
2
1
ppm
90.08
4.19
4.44
1.29

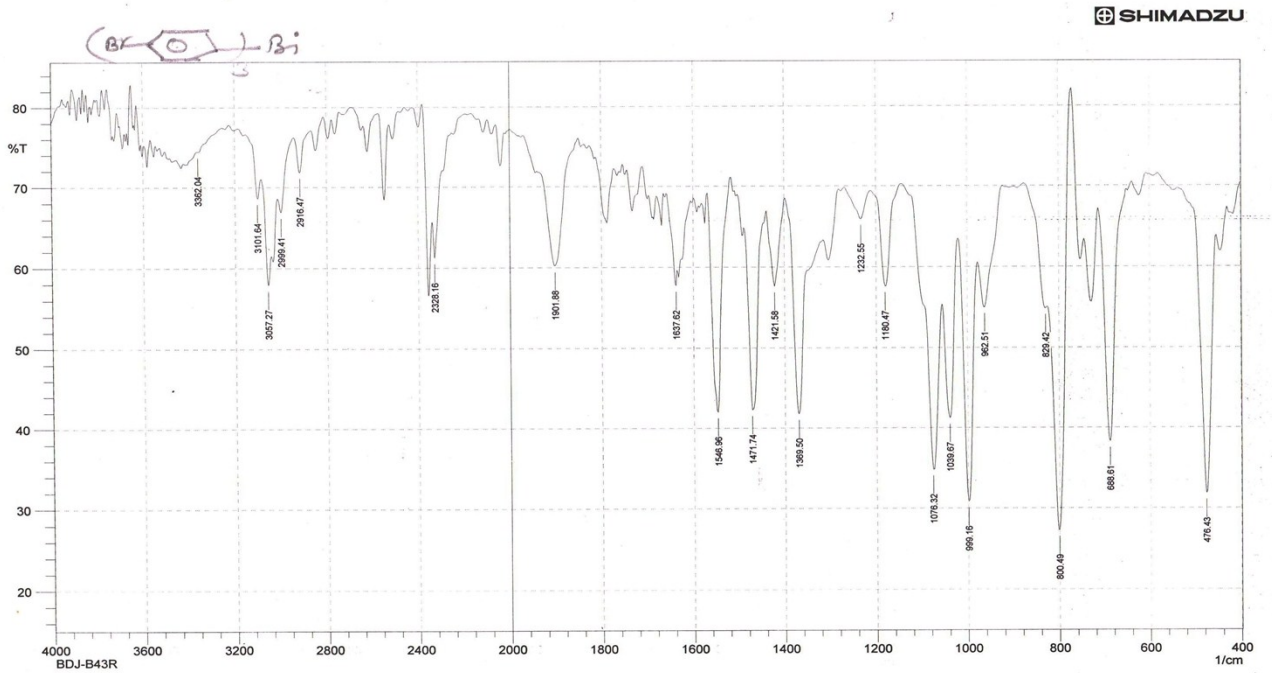
BDJ-B-4


200
180
160
140
120
100
80
60
40
20
0 ppm

INDEX	FREQUENCY	PPM	HEIGHT
1	11568.2	153.322	6.1
2	10497.3	139.129	38.6
3	10489.0	139.019	122.7
4	10360.2	137.312	8.5
5	10124.2	134.183	14.2
6	10094.3	133.787	133.0
7	10083.2	133.641	22.0
8	9864.8	130.746	8.6
9	9666.4	128.116	5.4
10	9272.8	122.899	27.1
11	5841.2	77.418	72.3
12	5809.7	77.000	72.6
13	5777.6	76.575	72.4

CDCl3





D:\FTIR DATA\YEAR 2011- 12\CHEMISTRY DEPARTMENT\BDJ-B43R.smf

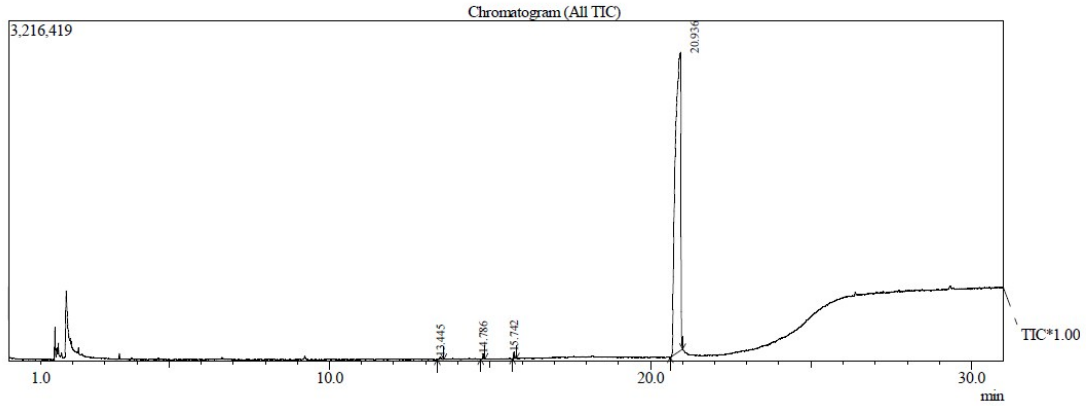
Date/Time; 4/24/2012 4:19:36 PM

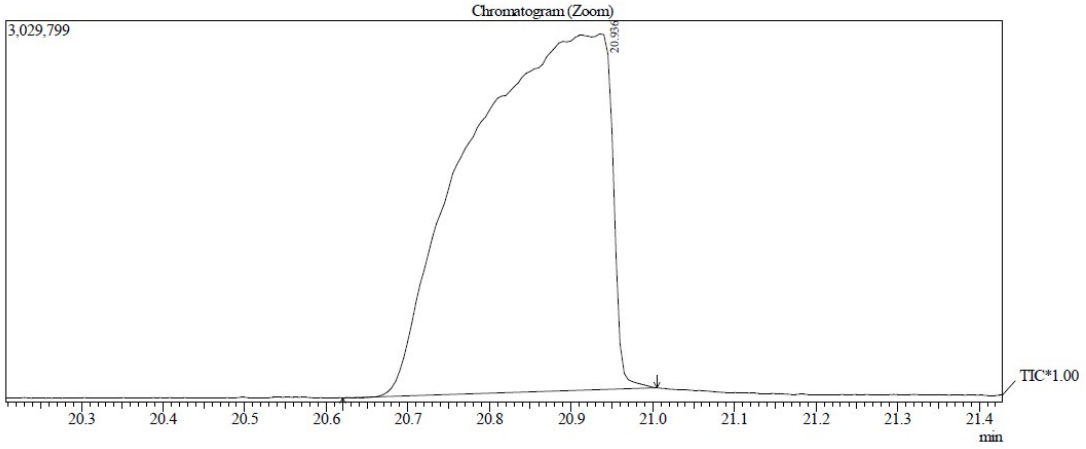
Comment;
BDJ-B43R

UNIVERSITY OF PUNE

2a

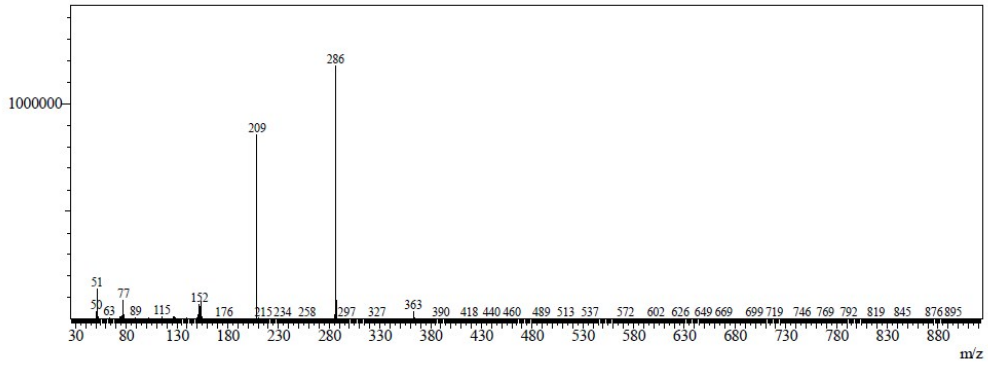
F:\gcms2015\APRIL\DATA\BDJ TYB.qgd





Spectrum

Line#:1 R.Time:20.925(Scan#:4186)
MassPeaks:747
RawMode:Single 20.925(4186) BasePeak:285.85(1175979)
BG Mode:None Group 1 - Event 1 Scan



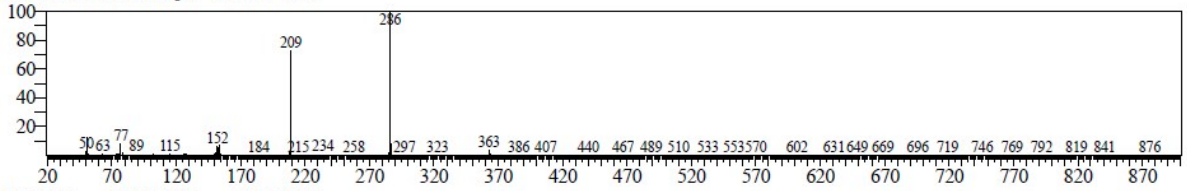
Library Search

<< Target >>

Line#:1 R.Time:20.925(Scan#:4186) MassPeaks:747

RawMode:Single 20.925(4186) BasePeak:285.85(10000)

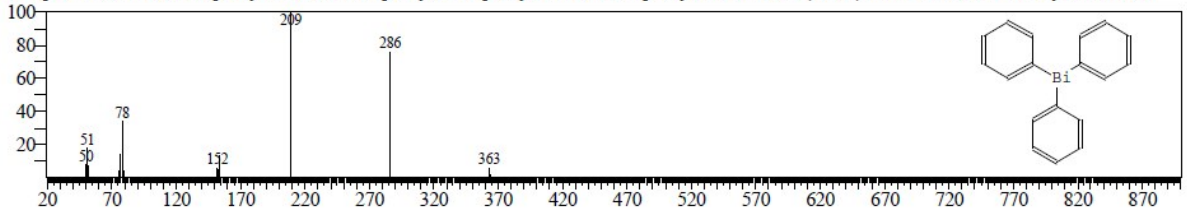
BG Mode:None Group 1 - Event 1 Scan



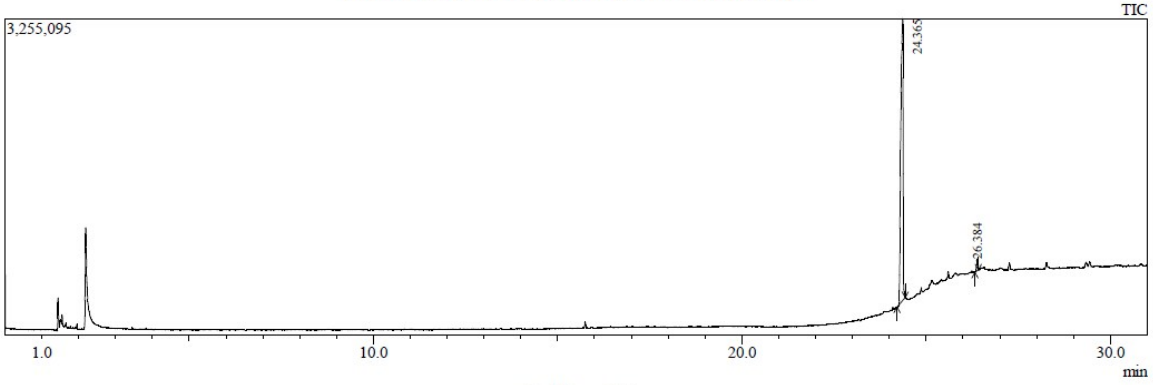
Hit#:1 Entry:194423 Library:NIST11.lib

SI:84 Formula:C18H15Bi CAS:603-33-8 MolWeight:440 RetIndex:0

CompName:Bismuthine, triphenyl- $$ Bismuth triphenyl $$ Triphenylbismuth $$ Triphenylbismuthine $$ (C6H5)3Bi $$ Aerotex $$ Trifenylbismutin $$



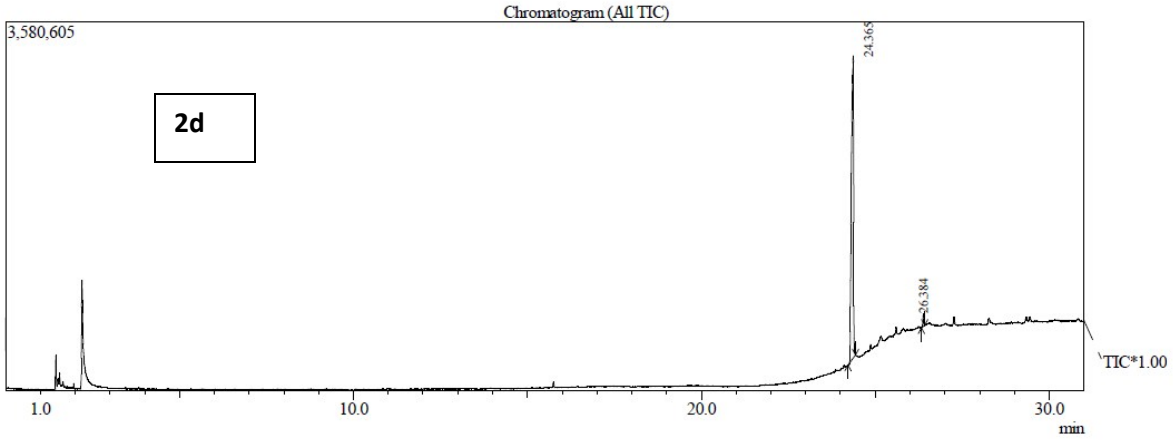
Chromatogram BDJ P tal B F:\gcms2015\APRIL\DATA\BDJ P tal B.qgd

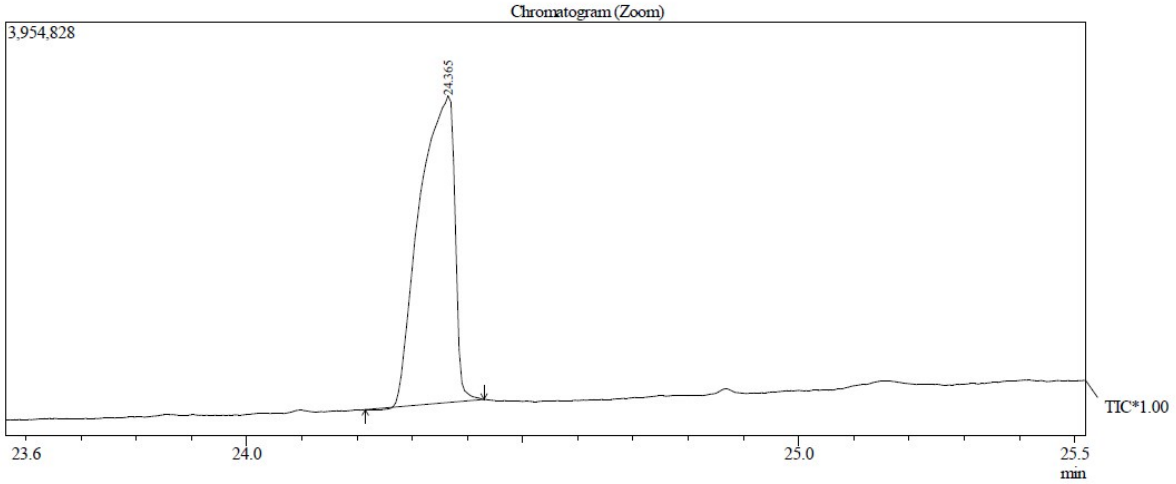


Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	24.365	24.215	24.430	12820965	98.19	2900386	95.97	4.42	MI	
2	26.384	26.325	26.420	236984	1.81	121814	4.03	1.95	MI	
				13057949	100.00	3022200	100.00			

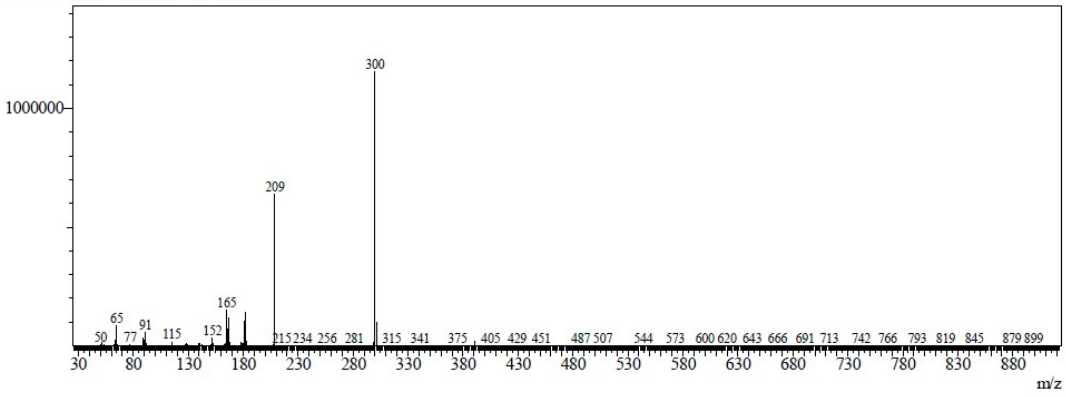
F:\gcms2015\APRIL\DATA\BDJ P tal B.qgd





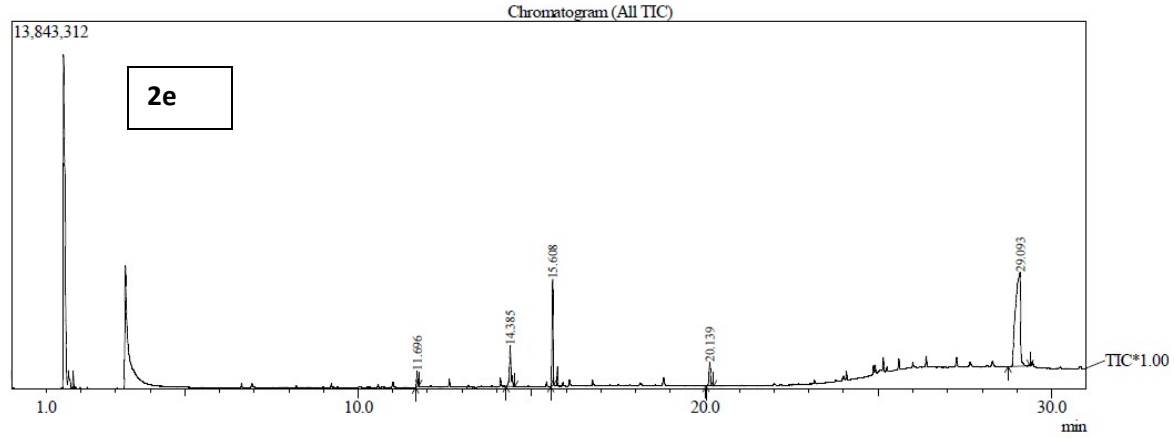
Spectrum

Line#:1 R.Time:24.355(Scan#:4872)
MassPeaks:792
RawMode:Single 24.355(4872) BasePeak:299.95(1155459)
BG Mode:None Group 1 - Event 1 Scan

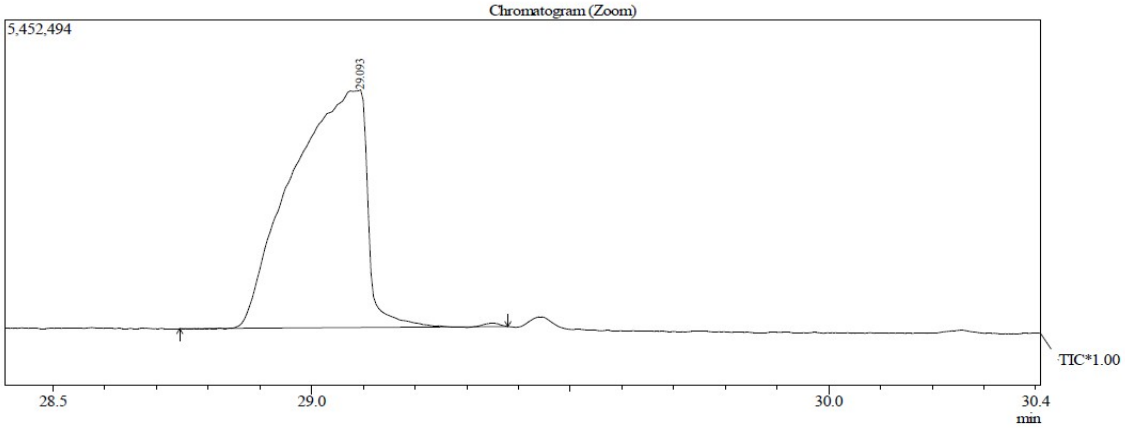


209 peak is due to bismuth and molecular weight matches with p-tolyl bismuthine

F:\gcms2015\APRIL\DATA\BDJ P ansyl B.qgd

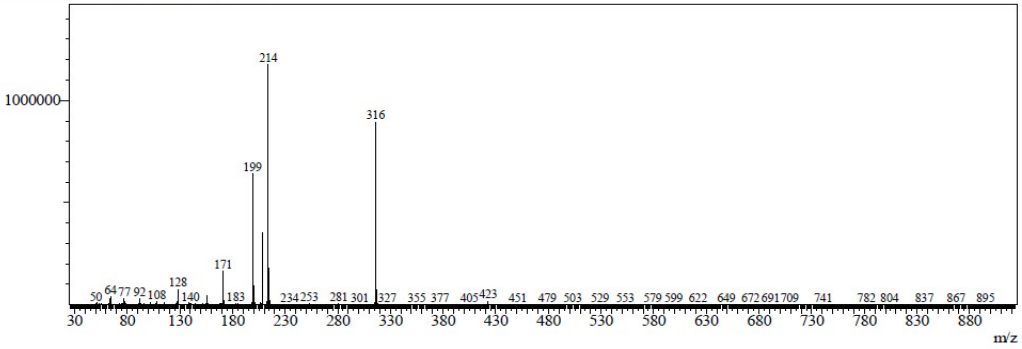


Chromatogram (Zoom)



Spectrum

Line#:1 R.Time:29.080(Scan#:5817)
MassPeaks:754
RawMode:Single 29.080(5817) BasePeak:214.00(1177894)
BG Mode:None Group 1 - Event 1 Scan



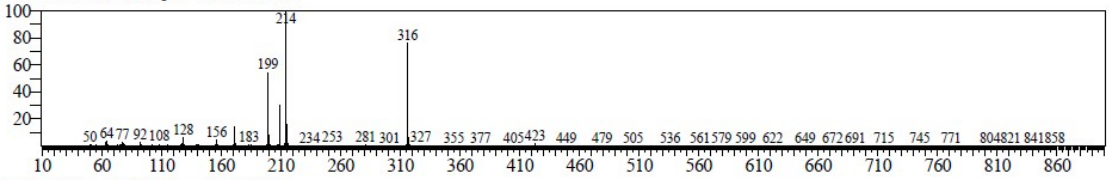
Library Search

<< Target >>

Line#:1 R.Time:29.080(Scan#:5817) MassPeaks:754

RawMode:Single 29.080(5817) BasePeak:214.00(10000)

BG Mode:None Group 1 - Event 1 Scan



Hit#:1 Entry:53691 Library:NIST11.lib

SI:70 Formula:C14H14O2 CAS:84591-12-8 MolWeight:214 RetIndex:1745

CompName:1,1'-Biphenyl, 3,4'-dimethoxy- $$ 3,4'-Dimethoxy-1,1'-biphenyl # $$