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Electronic Supplementary Information

A discrete self-assembled palladium nano-cage catalyses Suzuki-Miyaura coupling heterogeneously and Heck-Mizoroki coupling homogeneously

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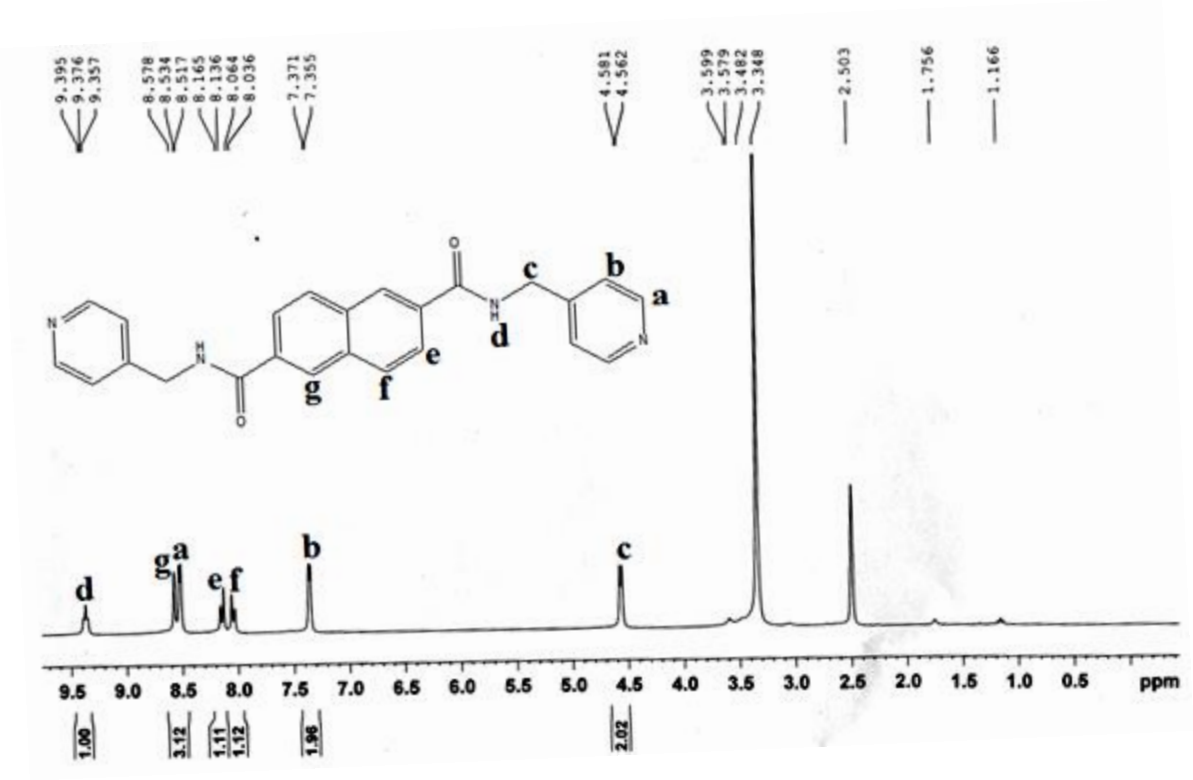


Figure S1: [1]H NMR spectrum of the ligand **L** in DMSO-d_6

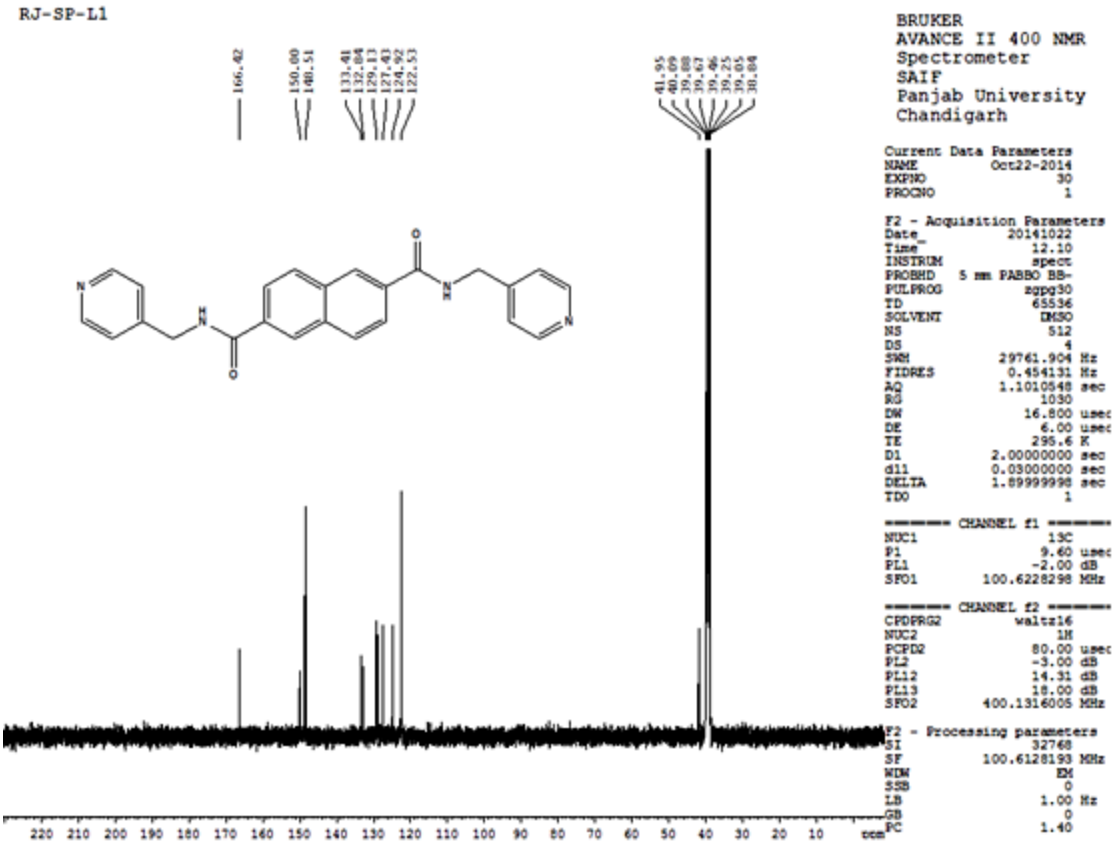


Figure S2: [13]C-NMR spectrum of the ligand **L** in DMSO-d_6

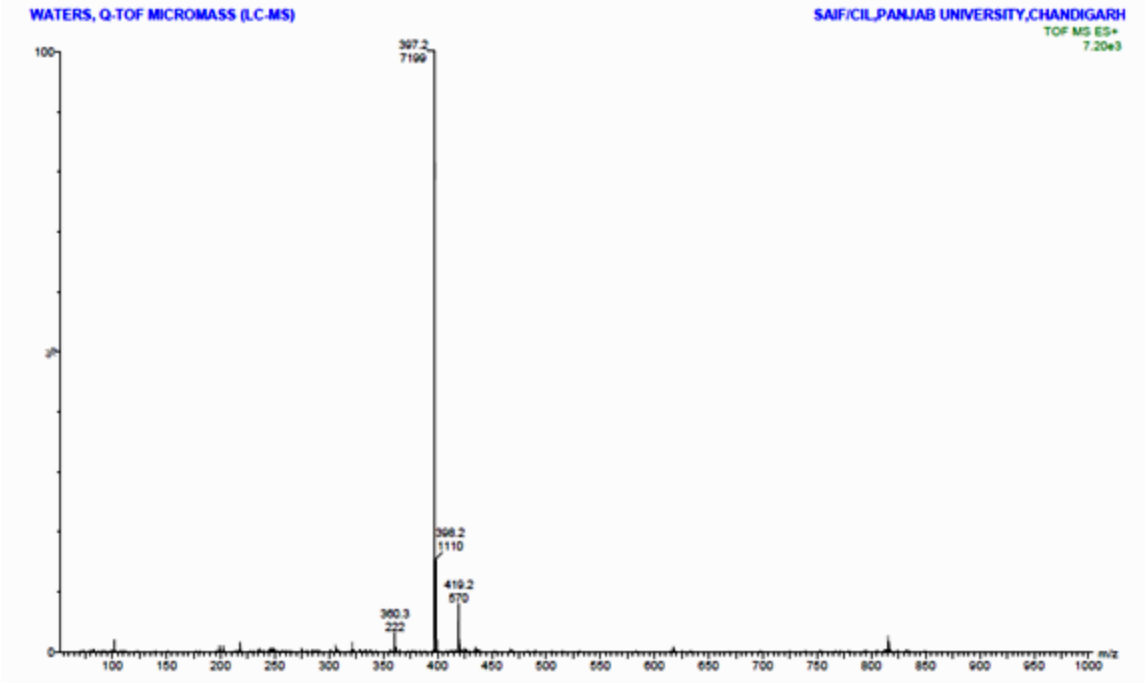


Figure S3: ESI-MS of **L** in DMSO

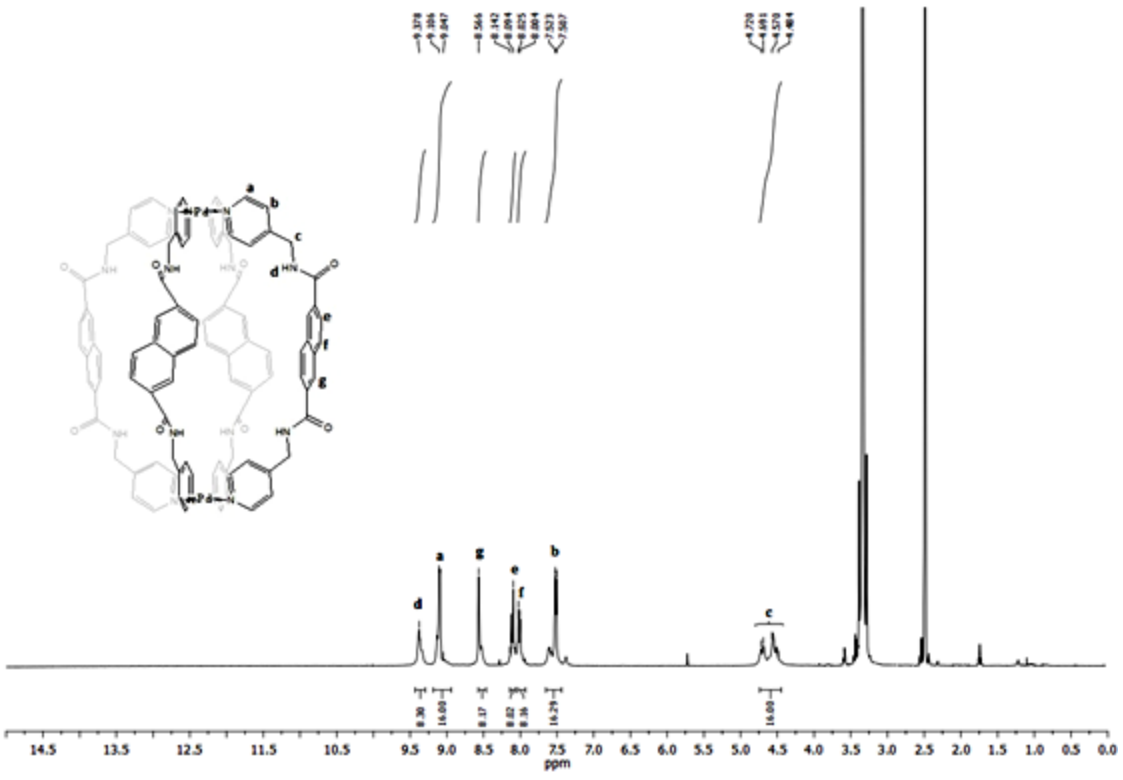


Figure S4: ^{1}H NMR spectrum of **1** in DMSO-d_6

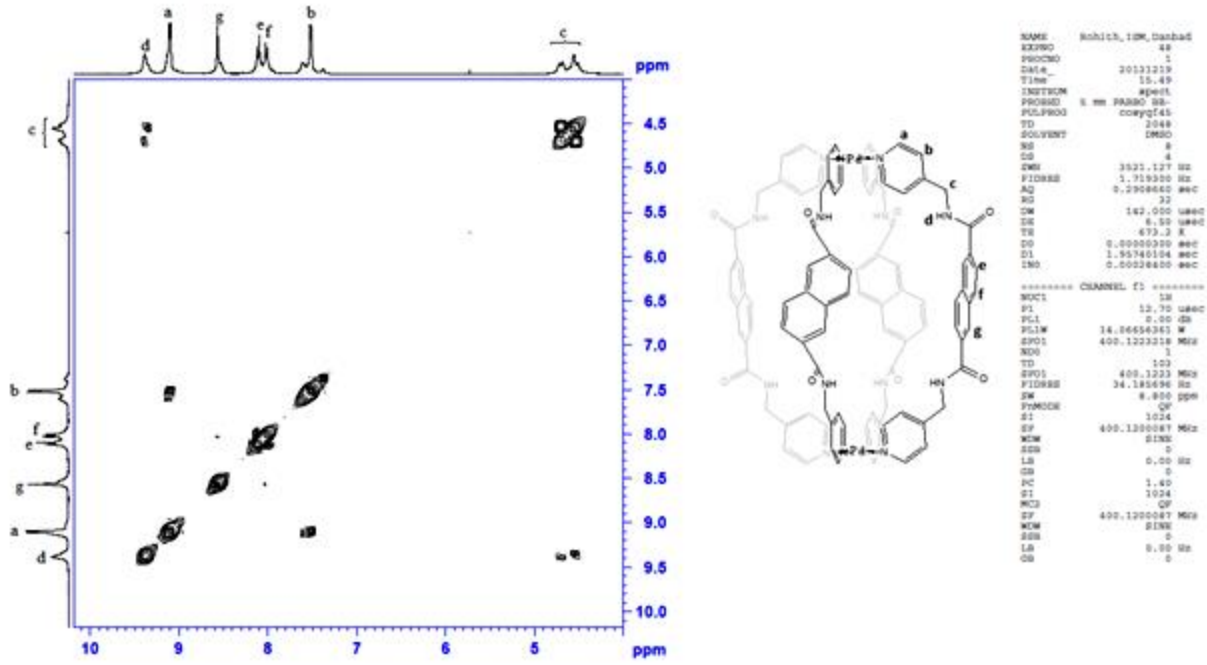


Figure S5: ^{1}H-^{1}H COSY spectrum of **1** in DMSO-d_6

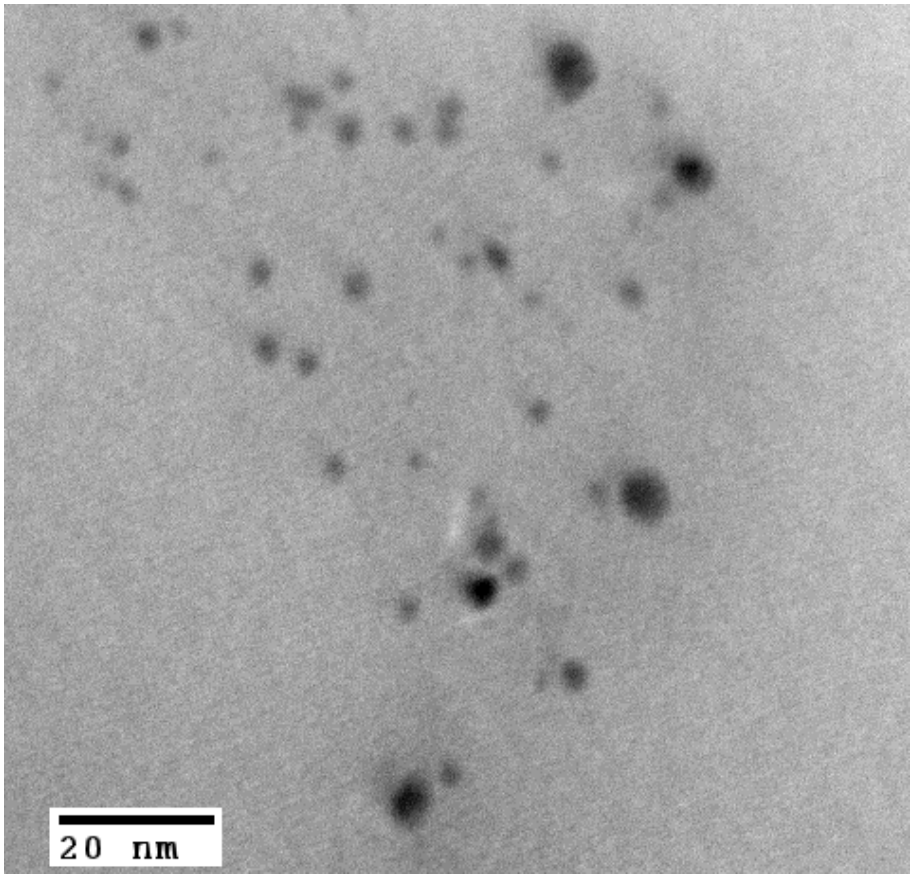


Figure S6. TEM image of the catalyst **1** after second cycle

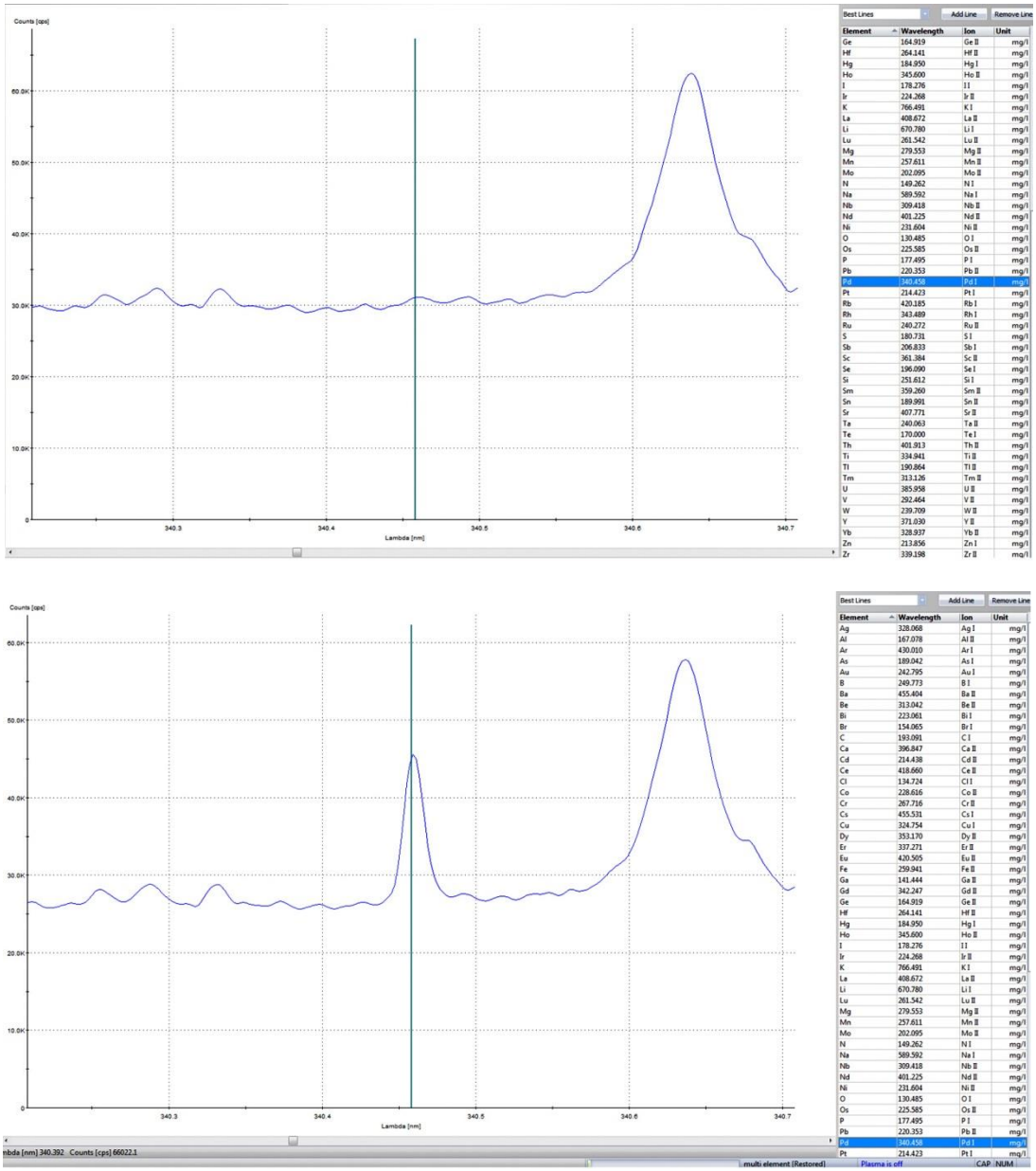


Figure S7: ICP-AES of the reaction mixture filtrate from Suzuki-Miyaura, Table 1, Entry 13 (top) and Heck, Table 2, Entry 1 (bottom) coupling reactions catalysed by **1**.

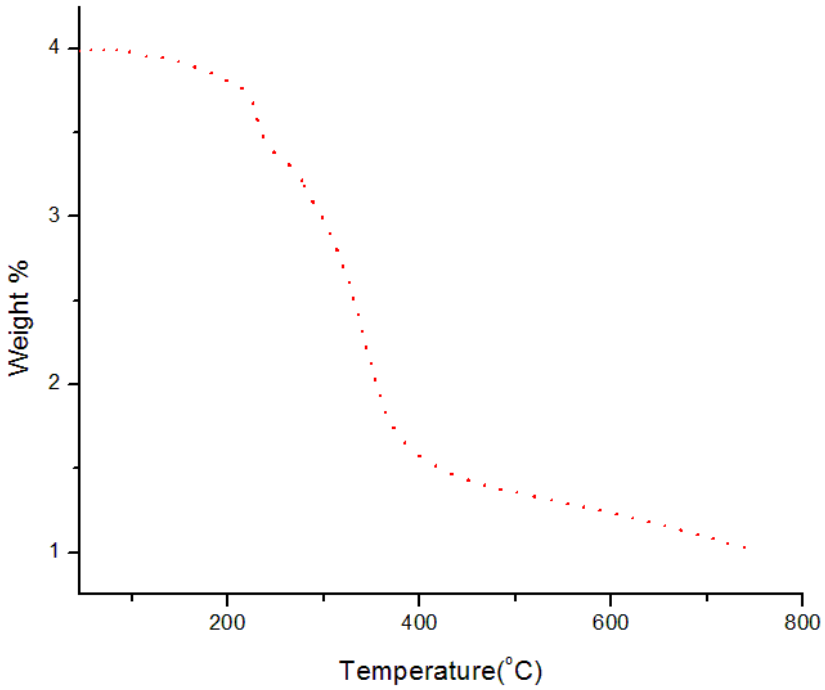
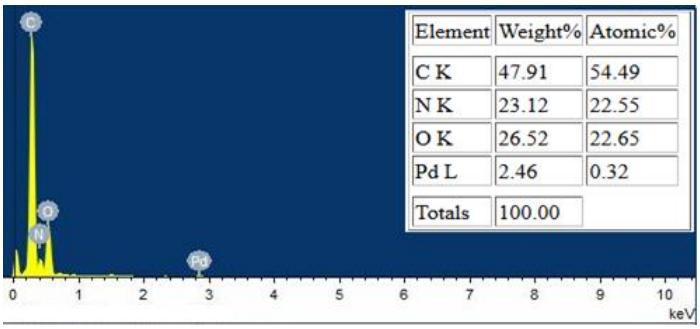


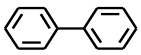
Figure S8: TGA thermogram of catalyst **1.**



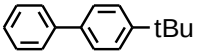
Element	Weight%	Atomic%
C K	47.91	54.49
N K	23.12	22.55
O K	26.52	22.65
Pd L	2.46	0.32
Totals	100.00	

Figure S9: EDX spectra of the catalyst **1**, recovered from filtrate of Heck coupling reaction Table 2, Entry 1.

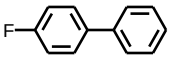
4. Products of Suzuki-Miyaura coupling and their characterization data:



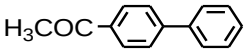
Biphenyl (1):[1] White solid. m.p. 68–70°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.59 (d, J=7.3Hz, 4H), 7.44 (t, J=7.5, 4H), 7.34 (t, J=7.3Hz, 2H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 141.29, 128.81, 127.31, 127.22. Elemental data for $C_{12}H_{10}$Calc: C, 93.46; H, 6.54, Found: C, 93.21; H, 6.79.



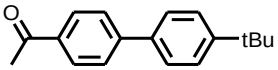
4-tert-Butyl-biphenyl (2):[2] White solid. m.p. 51–53°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$ 25°C, TMS) 7.58 (d, J= 7.88Hz, 2H), 7.54 (d, J=8.44Hz, 2H), 7.47 (d, J=8.48Hz, 2H), 7.42(t, J=6.78Hz, 2H), 7.34-7.7.30(m, 1H), 1.36(s, 9H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 150.30, 141.13, 138.39, 128.77, 127.10, 126.86, 125.79, 125.71, 34.60, 31.45. Elemental data for $C_{16}H_{18}$Calc: C, 91.37; H, 8.63, Found: C, 91.32; H, 8.68.



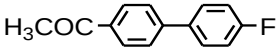
4-Fluorobiphenyl (3):[3] White solid. m.p. 74–76°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.55 (m, 4H), 7.43 (t, J=7.62Hz, 2H), 7.34 (t, J=8.02Hz, 1H), 7.13(t, J=7.65Hz) 2H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 163.73, 161.28, 140.29, 137.37, 128.77, 127.30, 127.06, 115.65. Elemental data for $C_{12}H_9F$ Calc: C, 83.70; H, 5.27, Found: C, 83.52; H, 5.30.



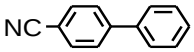
4-Acetylbiphenyl (4):[1] White solid. m.p. 119–121°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 8.04 (d, J=8.5Hz, 2H), 7.69 (d, J=8.4Hz, 2H), 7.63 (d, J=8Hz, 2H), 7.47(t, J=8Hz, 2H), 7.42-7.38 (m, 1H), 2.64(s, 3H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 197.77, 145.76, 139.84, 135.82, 128.95, 128.91, 128.23, 127.26, 127.21, 26.67. Elemental data for $C_{14}H_{12}O$ Calc: C, 85.68; H, 6.16, Found: C, 85.46; H, 5.96.



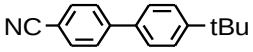
1-(4'-tert-Butyl-biphenyl-4-yl)-ethanone (5):[2] White solid. m.p. 127–129 °C. Eluent: Petether/ethyl acetate. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.95 (d, J=6.62Hz, 2H), 7.61 (d, J=7.52Hz, 2H), 7.51 (d, J=7.78Hz, 2H), 7.43(d, J=7.52Hz, 2H), 2.56(s, 3H), 1.29(s, 9H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 197.74, 151.43, 145.49, 136.87, 135.58, 128.89, 126.97, 126.90, 125.92, 34.62, 31.29, 26.63.Elemental data for $C_{18}H_{20}O$ Calc: C, 85.67; H, 7.99, Found: C, 85.61; H, 7.74.



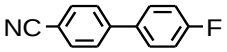
4-Acetyl-4'-fluorobiphenyl (6):[4] White solid. m.p. 103–105 °C. Eluent: Petether/ethyl acetate. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 8.03 (d, J=6.6Hz, 2H), 7.64 (d, J=5.16Hz, 2H), 7.61-7.57 (m, 2H), 7.16(t, J=8.2Hz, 2H), 2.64(s, 3H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 197.7, 164.23, 161.76, 144.72, 135.97, 128.90, 127.07, 116.04, 115.82, 26.67.Elemental data for $C_{14}H_{11}OF$ Calc: C, 78.49; H, 5.18, Found: C, 78.32; H, 5.33.



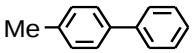
4-Cyanobiphenyl (7):[1] White solid. m.p. 85–87°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.73 (d, J=6.5Hz, 2H), 7.69 (d, J=6.5Hz, 2H), 7.59 (d, J=7.5Hz, 2H), 7.48 (t, J=7Hz, 2H) 7.44-7.42 (m, 2H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 145.68, 139.18, 132.62, 129.15, 128.70, 127.75, 127.25, 118.98, 110.92.Elemental data for $C_{13}H_9N$ Calc: C, 87.12; H, 5.06; N, 7.82, Found: C, 86.93; H, 5.12; N, 7.95.



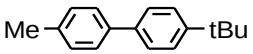
4'-tert-Butyl-biphenyl-4-carbonitrile (8):[2] White solid. m.p. 132–134°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.71 (d, J=8Hz, 2H), 7.67 (d, J=8Hz, 2H), 7.54 (d, J=8Hz, 2H), 7.50 (d, J=8Hz, 2H), 1.36 (s, 9H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 151.98, 145.51, 136.22, 132.59, 127.52, 126.92, 126.13, 119.08, 110.58, 34.71, 31.31. . Elemental data for $C_{17}H_{17}N$ Calc: C, 86.77; H, 7.28; N, 5.95, Found: C, 86.55; H, 7.34; N, 6.11.



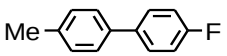
4'-Fluoro-biphenyl-4-carbonitrile (9):[4] White solid. m.p. 105–107°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.72 (d, J=8.44, 2H), 7.63 (d, J=7.48, 2H), 7.58-7.53 (m, 2H), 7.17 (t, J=8Hz, 2H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 161.95, 144.61, 135.3, 132.66, 129.01, 127.56, 118.85, 116.13, 110.95.Elemental data for $C_{13}H_{18}NF$ Calc: C, 79.17; H, 4.09; N, 7.10, Found C, 79.31; H, 4.14; N, 6.96.



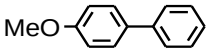
4-Methylbiphenyl (10):[5] White solid. m.p. 45–47°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.58(d, J=8.2Hz, 2H), 7.49 (d, J=7.3Hz, 2H), 7.43 (t, J=7.3Hz, 2H), 7.34 (t, J=7.3Hz, 1H), 7.25(d, J=6.7Hz, 2H), 2.40(s, 3H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 141.22, 138.41, 137.07, 129.53, 128.76, 127.05, 127.03, 21.15.Elemental data for $C_{13}H_{12}$ Calc: C, 92.81; H, 7.19, Found C, 92.69; H, 7.31.



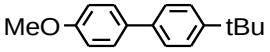
4'-tert-Butyl-4-methyl-biphenyl (11):[6] White solid. m.p. 75–77°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.54(t, J=7.08Hz, 3H), 7.50-7.46 (m, 3H), 7.27 (t, J=6.08Hz, 2H), 2.41 (s, 3H), 1.38(s, 9H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 149.99, 138.28, 136.75, 129.49, 126.92, 126.72, 126.66, 125.73, 34.57, 31.45, 21.17.Elemental data for $C_{17}H_{20}$ Calc: C, 91.01; H, 8.99, Found C, 91.23; H, 8.77.



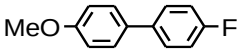
4'-Fluoro-4-methyl-biphenyl (12):[4] White solid. m.p. 74–76°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.46-7.43 (m, 2H), 7.36 (d, J=7.32Hz, 2H), 7.17 (d, J=8Hz, 2H), 7.03(t, J=7.62Hz, 2H), 2.32(s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 163.57, 161.13, 137.34, 129.59, 128.55, 126.91, 115.71, 115.49, 21.13.Elemental data for $C_{13}H_{11}F$Calc: C, 83.84; H, 5.95, Found C, 83.62; H, 6.07.



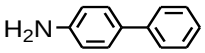
4-Methoxybiphenyl (13):[1] White solid. m.p. 88–90°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.49-7.45 (m, 4H), 7.34 (t, J=7.7Hz, 2H), 7.23 (t, J=7.3Hz, 1H), 6.91(d, J=6.7Hz, 2H), 3.78(s, 3H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 159.14, 140.82, 133.77, 128.71, 128.15, 126.73, 126.65, 114.19, 55.33.Elemental data for $C_{13}H_{12}O$Calc: C, 84.75; H, 6.57, Found: C, 84.55; H, 6.73.



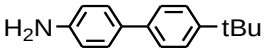
4'-tert-Butyl-4-methoxy-biphenyl (14):[2] White solid. m.p. 136-138°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.51 (t, J=5.64Hz, 4H), 7.44 (d, J=8.5Hz, 2H), 6.96 (d, J=8.76Hz, 2H), 3.84(s, 3H), 1.35(s, 9H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 158.99, 149.65, 137.98, 133.68, 128.05, 126.42, 125.72, 114.19, 55.35, 34.52, 31.44. Elemental data for $C_{17}H_{20}O$Calc: C, 84.96; H, 8.39, Found: C, 84.75; H, 8.63.



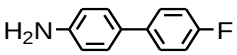
4'-Fluoro-4-methoxy-biphenyl (15):[4] White solid. m.p. 89–91°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.50-7.45 (m, 4H), 7.09 (d, J=7.66Hz, 2H), 6.97 (d, J=8.8Hz, 2H), 3.85(s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 163.31, 160.87, 159.11, 136.96, 132.82, 128.17, 115.42, 114.24, 55.34. Elemental data for $C_{13}H_{11}FO$Calc: C, 77.21; H, 5.48, Found: C, 77.44; H, 5.31.



4-Aminobiphenyl (16):[7] White solid. m.p. 52–54°C. Eluent: Petether/ethylacetate. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.53(d, J=8Hz, 2H), 7.43-7.36 (m, 4H), 7.28-7.24 (m, 1H), 6.75(d, J=8.4Hz, 2H), 3.72(brs,2H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 145.89, 141.20, 131.59, 128.72, 128.05, 126.45, 126.31, 115.44. Elemental data for $C_{12}H_{11}N$Calc: C, 85.17; H, 6.55; N, 8.28, Found: C, 85.43; H, 6.23; N, 8.34.

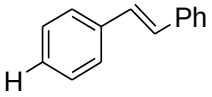


4'-tert-Butyl-biphenyl-4-ylamine (17):[8] White solid. m.p. 82–84°C. Eluent: Petether/ethylacetate. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.47(d, J=8.52, 2H), 7.42-7.39 (m, 4H), 6.75(d, J=8.52Hz, 2H), 3.47(brs, 2H), 1.34 (s, 9H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 149.21, 145.61, 138.31, 131.53, 127.91, 126.07, 125.65, 115.45, 34.48, 31.44. Elemental data for $C_{16}H_{19}N$Calc: C, 85.28; H, 8.50; N, 6.22, Found: C, 85.11; H, 8.63; N, 6.26.

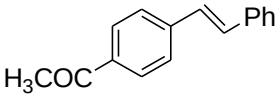


4'-Fluoro-biphenyl-4-ylamine (18):[9] White solid. m.p. 120–122°C. Eluent: Petether/ethylacetate. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.47(t, J=7.06Hz, 2H), 7.35(d, J=8.48Hz, 2H), 7.07 (t, J=8.74Hz, 2H), 6.74 (d, J=8.48Hz, 2H), 3.71(brs, 2H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 163.09, 160.66, 145.82, 137.32, 130.65, 127.90, 127.82, 115.42.Elemental data for $C_{12}H_{10}NF$Calc: C, 76.99; H, 5.38; N, 7.48, Found: C, 77.63; H, 5.51; N, 7.22.

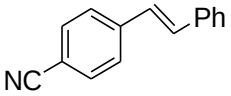
5. Products of Heck-Mizoroki coupling and their characterization data:



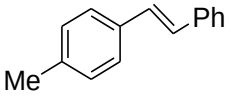
(E)-1, 2-Diphenylethene (1):[10] White solid. m.p. 122–124°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.51(d, J=8Hz, 4H), 7.36 (t, J=7.2Hz, 4H), 7.28-7.23 (m, 2H), 7.11(s, 2H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 137.35, 128.72, 127.66, 126.55. Elemental data for $C_{14}H_{12}$Calc: C, 93.29; H, 6.71, Found: C, 93.52; H, 6.48.



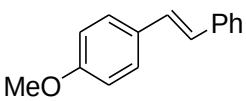
(E)-1-(4-Styrylphenyl) ethanone(2):[10] White solid. m.p. 138–140°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.95(d, J=8Hz, 2H), 7.59 (d, J=8.4Hz, 2H), 7.54 (d,J=8Hz, 2H), 7.38(t,J=8Hz, 2H), 7.31-7.30(m, 1H), 7.23(d, J=16Hz, 1H), 7.13(d, J=16Hz, 1H) ,2.61(s,3H).^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 197.53, 142.01, 136.70, 135.94, 131.47, 128.91, 128.84, 128.36, 127.45, 126.85, 126.53, 26.63.Elemental data for $C_{16}H_{14}O$ Calc: C, 86.45; H, 6.35,Found: C, 86.72; H, 6.11.



(E)-4-Styrylbenzonitrile (3):[10] White solid. m.p 117–119°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.63(d, J=4Hz, 2H), 7.58 (d, J=8Hz, 2H), 7.53 (d, J=8Hz, 2H), 7.39(t, J=8Hz, 1H), 7.31(t, J=8Hz, 1H), 7.22(d, J=16Hz, 1H),7.08(d, J=16Hz, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 141.85, 136.30, 132.51, 132.42, 128.89, 128.68, 126.95, 126.89, 126.73, 119.09, 110.57.Elemental data for $C_{15}H_{11}N$ Calc: C, 87.77; H, 5.40; N, 6.82 Found: C, 87.49; H, 5.76; N, 6.75.

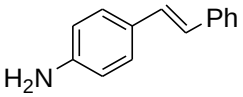


(E)-1-Methyl-4-styryl-benzene (4):[10] White solid. m.p. 118–120°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS)7.50(d, J=7.3 Hz, 2H), 7.41 (d, J=8Hz, 2H), 7.34 (t, J=8Hz, 2H), 7.24-7.22(m, 1H), 7.16(d, J=8Hz, 2H), 7.12-7.03(m, 2H), 2.36 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 137.57, 137.55, 134.58, 129.45, 128.70, 128.66, 127.73, 127.46, 126.48, 126.45, 21.32. Elemental data for $C_{15}H_{14}$Calc: C, 92.74; H, 7.26, Found: C, 92.52; H, 7.48.

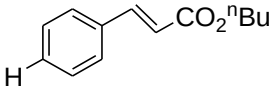


(E)-1-Methoxy-4-styryl-benzene (5):[10] White solid. m.p. 136–138°C. Eluent: Petether/dichloromethane^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS)7.49-7.44(m, 4H), 7.34 (t, J=8Hz,

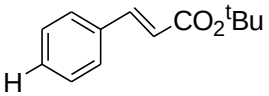
2H), 7.25-7.22 (m, 1H), 7.06 (d, J=16Hz, 1H), 6.97(d, J=16Hz, 1H), 6.90(d, J= 7Hz, 2H), 3.83 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 159.32, 137.67, 130.16, 128.68, 128.23, 127.76, 127.25, 126.63, 126.29, 114.16, 55.35.Elemental data for $C_{15}H_{11}O$ Calc: C, 85.68; H, 6.71, Found: C, 85.37; H, 6.56.



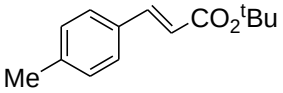
(E)-4-Styryl-phenylamine (6):[11] White solid. m.p. 150–152°C. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.46(d, J=8Hz, 2H), 7.32 (t, J=8Hz, 4H), 7.20(t, J=8Hz, 1H), 7.02 (d, J=16Hz, 1H), 6.91(d, J=16Hz, 1H), 6.67(d, J= 8Hz, 2H), 3.73 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 146.21, 137.98, 128.73, 128.66, 128.03, 127.81, 126.95, 126.16, 125.12, 115.25. Elemental data for $C_{14}H_{13}N$ Calc: C, 86.12; H, 6.71; N, 7.17, Found: C, 85.32; H, 6.92; N, 7.26.



(E)-*n*-Butyl cinnamate (7):[12] Colourless liquid. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.68(d, J=16Hz, 1H), 7.54-7.51 (m, 2H), 7.39-7.36 (m, 3H), 6.44(d, J=16Hz, 1H), 4.21(t, J= 8Hz, 2H), 1.73-1.65 (m, 2H), 1.48-1.39 (m, 2H), 0.96 (t, 7.2Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 166.11, 143.54, 133.44, 129.19, 127.85, 127.03, 117.26, 63.43, 29.75, 18.18, 12.74.Elemental data for $C_{13}H_{16}O_2$ Calc: C, 76.44; H, 7.90, Found: C, 76.12; H, 8.02.

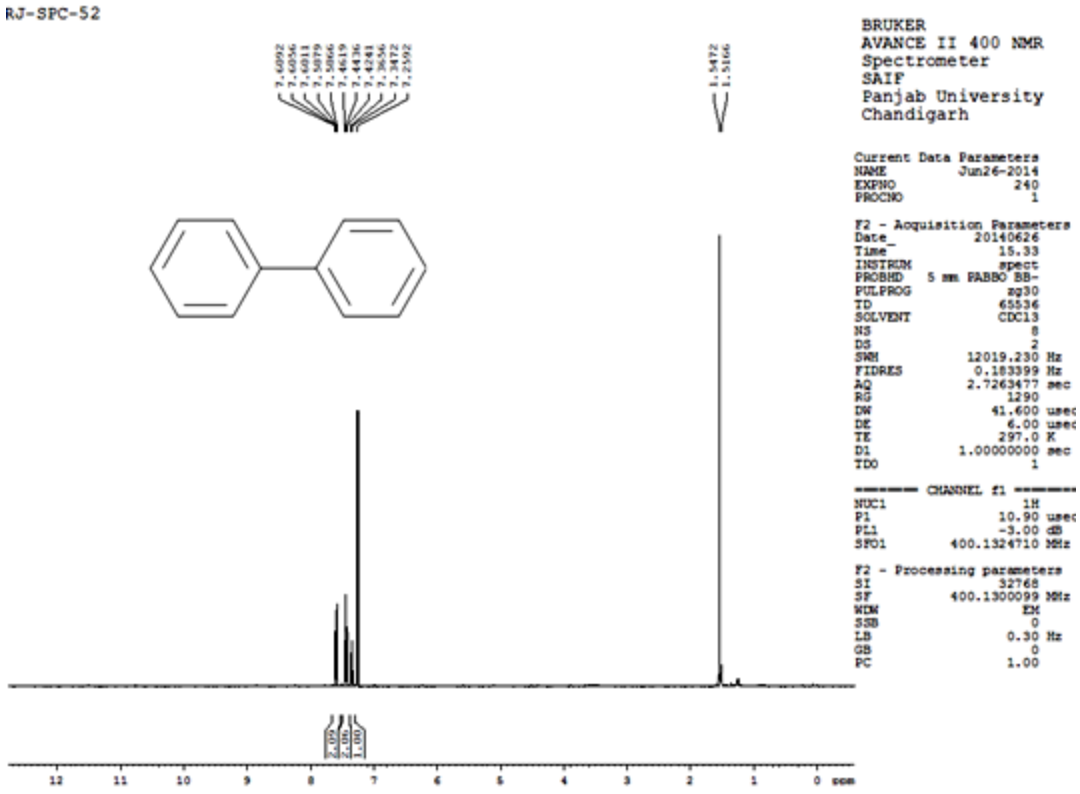


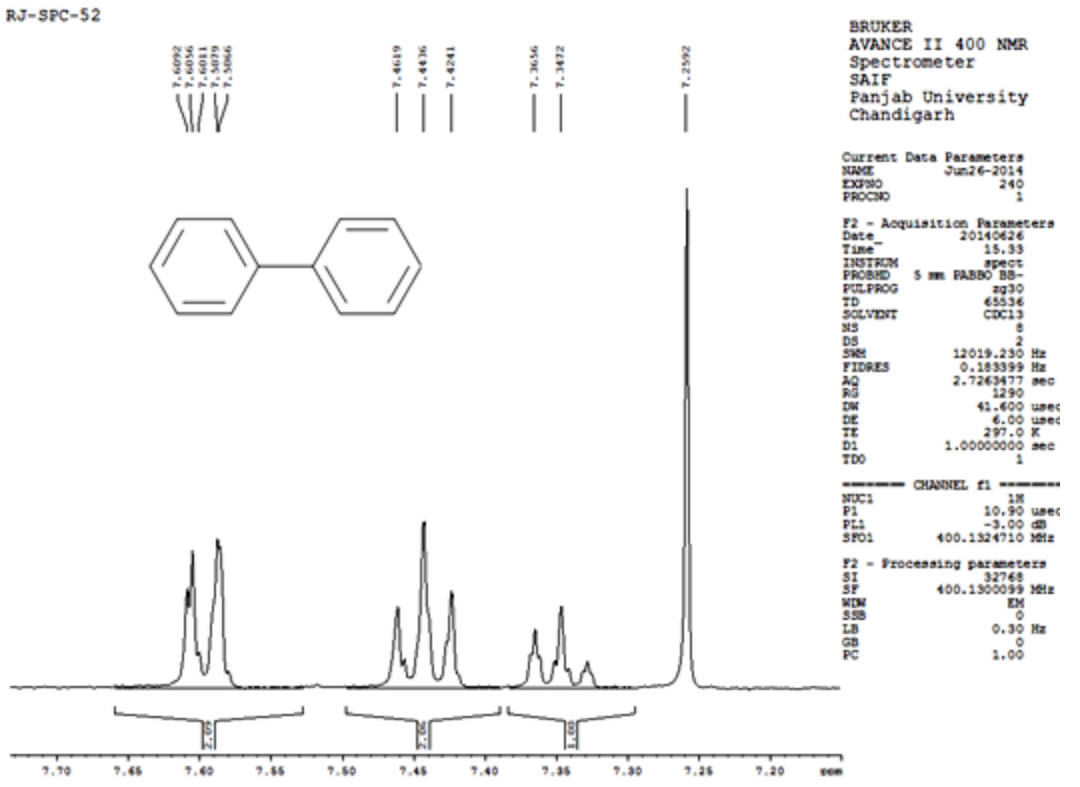
(E)-*t*-Butyl cinnamate (8):[12] Colourless liquid. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.58(d, J=16Hz, 1H), 7.52-7.49 (m, 2H), 7.38-7.35 (m, 3H), 6.37(d, J=16Hz, 1H), 1.53(s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 166.35, 143.56, 134.67, 129.97, 128.83, 127.97, 120.19, 80.51, 28.22.Elemental data for $C_{13}H_{16}O_2$ Calc: C, 76.44; H, 7.90, Found: C, 76.32; H, 7.85.

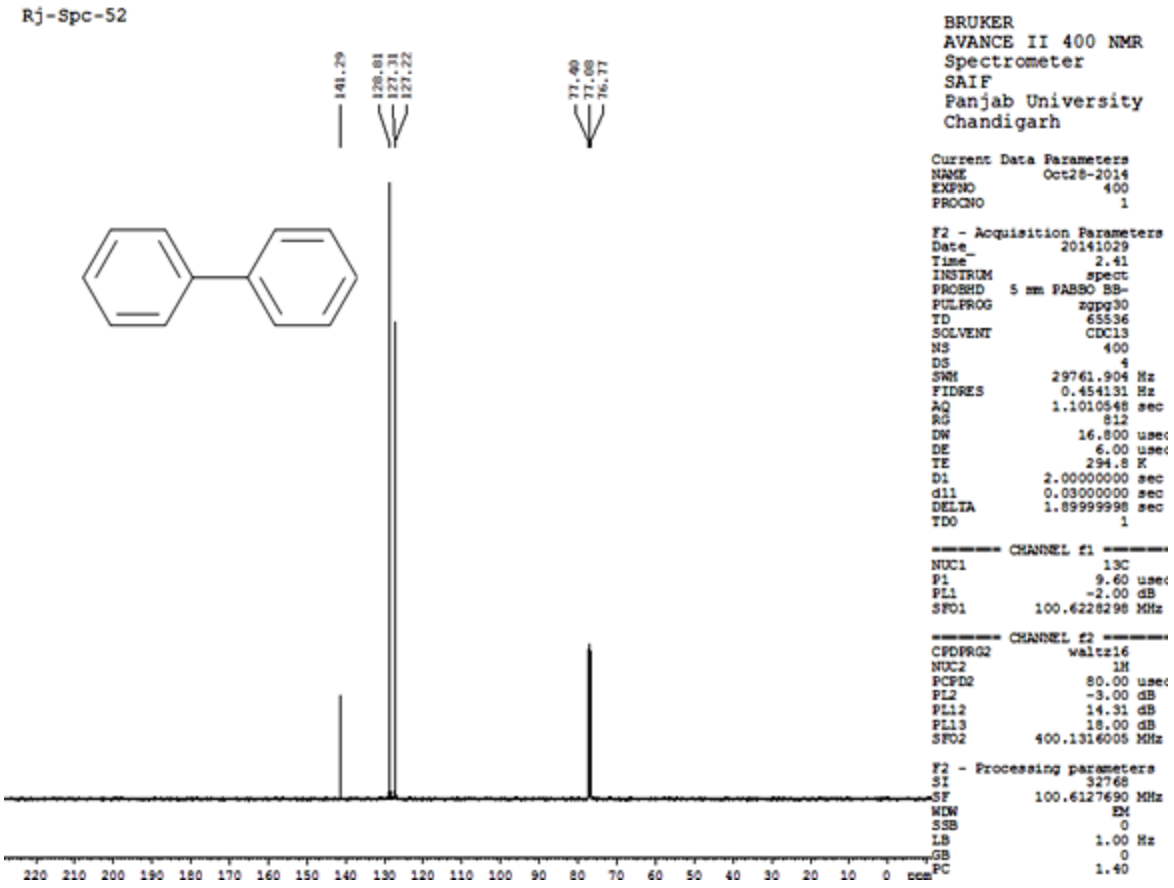


(E)-*t*-butyl 3-*p*-tolylacrylate (9):[13] Colourless liquid. Eluent: Petether/dichloromethane. ^{1}H-NMR (400 MHz, $CDCl_3$, 25°C, TMS) 7.49(d, J=16Hz, 1H), 7.33 (d, J=8Hz, 2H), 7.10 (d, J=8Hz, 2H), 6.25(d, J=16Hz, 1H), 2.29(s, 3H), 1.46(s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$, 25°C, TMS) 166.58, 143.56, 140.32, 131.92, 129.50, 127.96, 119.09, 80.38, 28.23, 21.46. Elemental data for $C_{14}H_{18}O_2$ Calc: C, 77.03; H, 8.31, Found: C, 77.33; H, 8.51.

Table 1, Entry 1:







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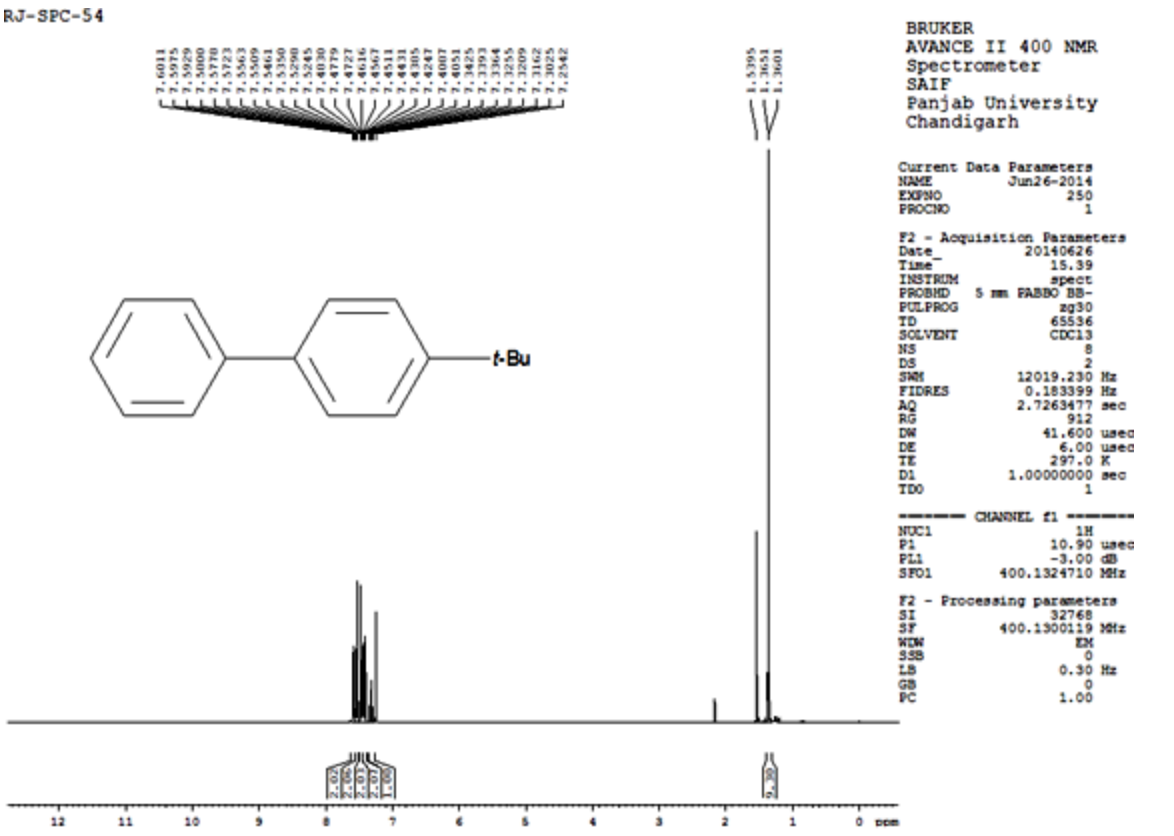
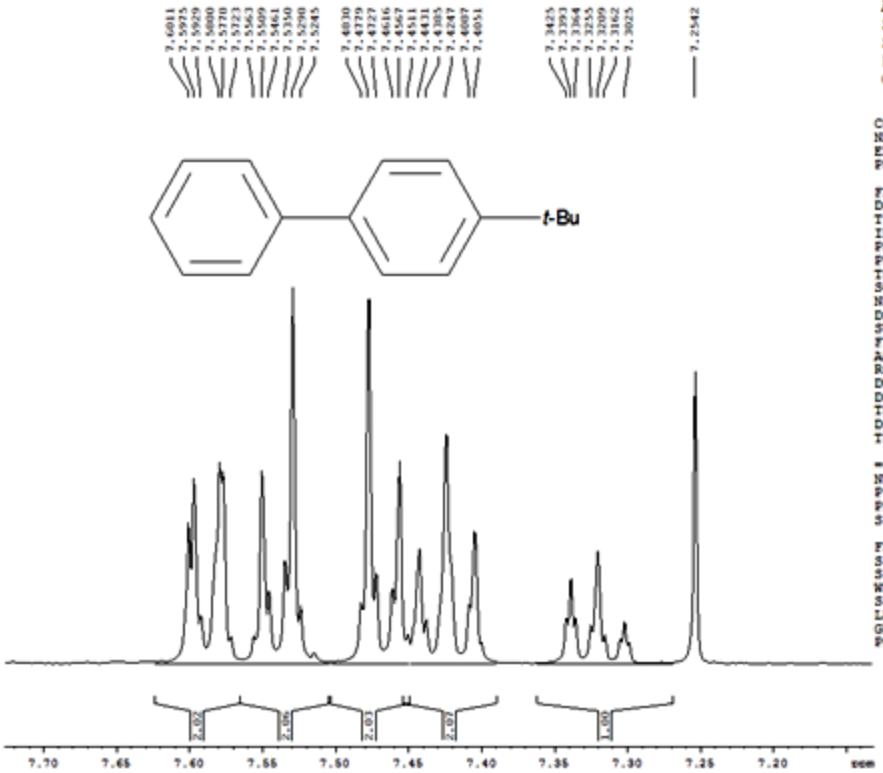


RJ-SPC-54



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Current Data Parameters	
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EXPNO	250
PROCNO	1
F2 - Acquisition Parameters	
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PULPROG	zg30
TD	65536
SOLVENT	CDCl3
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RG	912
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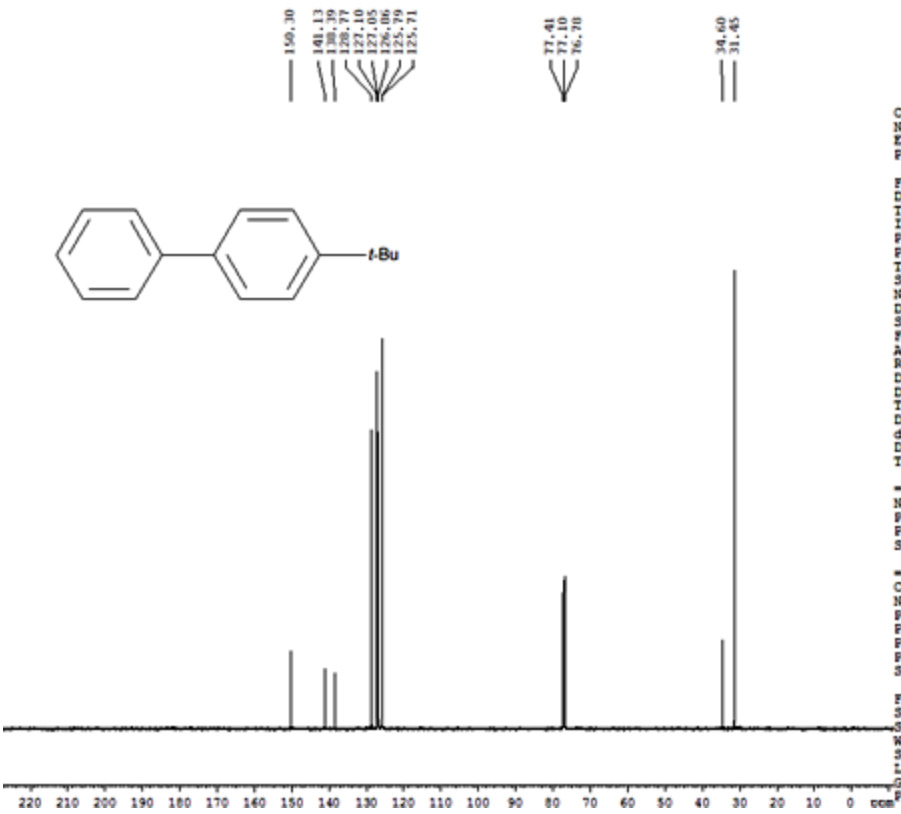
Rj-Spc-54



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Current Data Parameters	
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PROCNO	1
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RG	812
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P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
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NUC2	1H
PCPD2	80.00 usec
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PL12	14.31 dB
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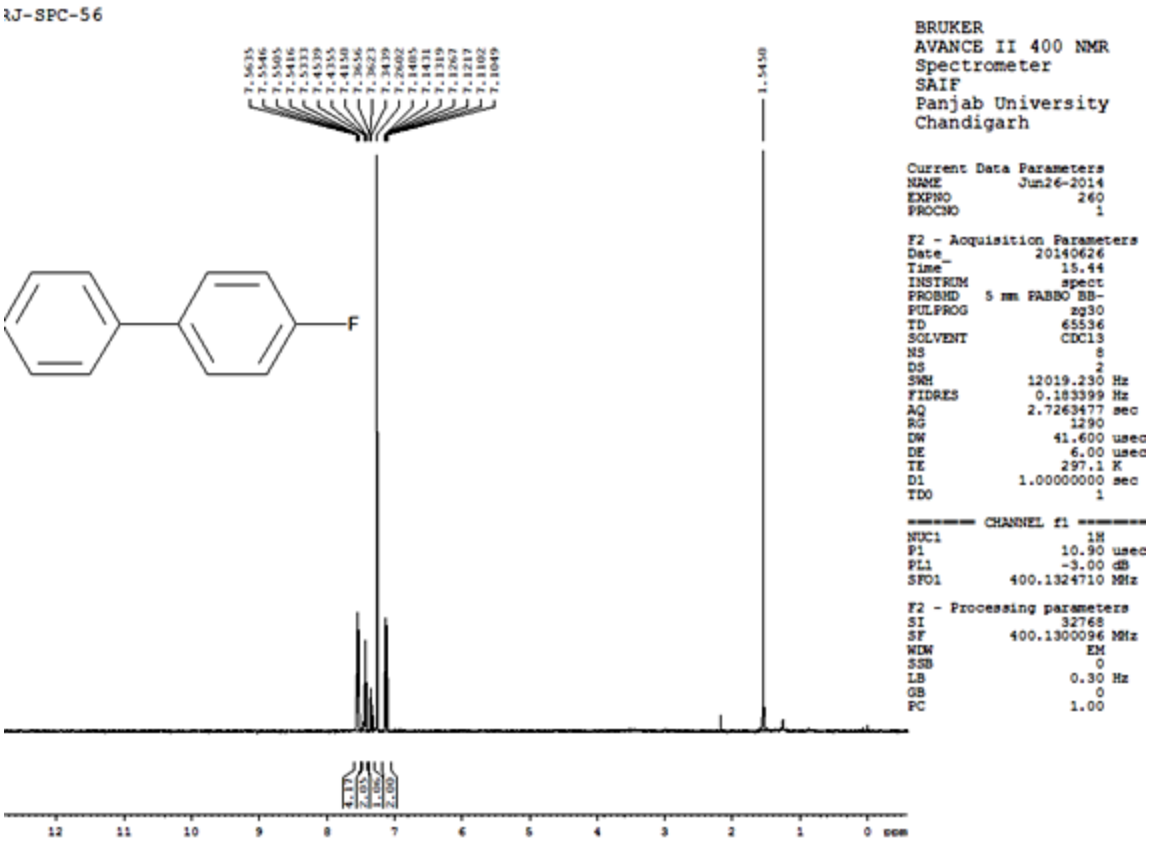

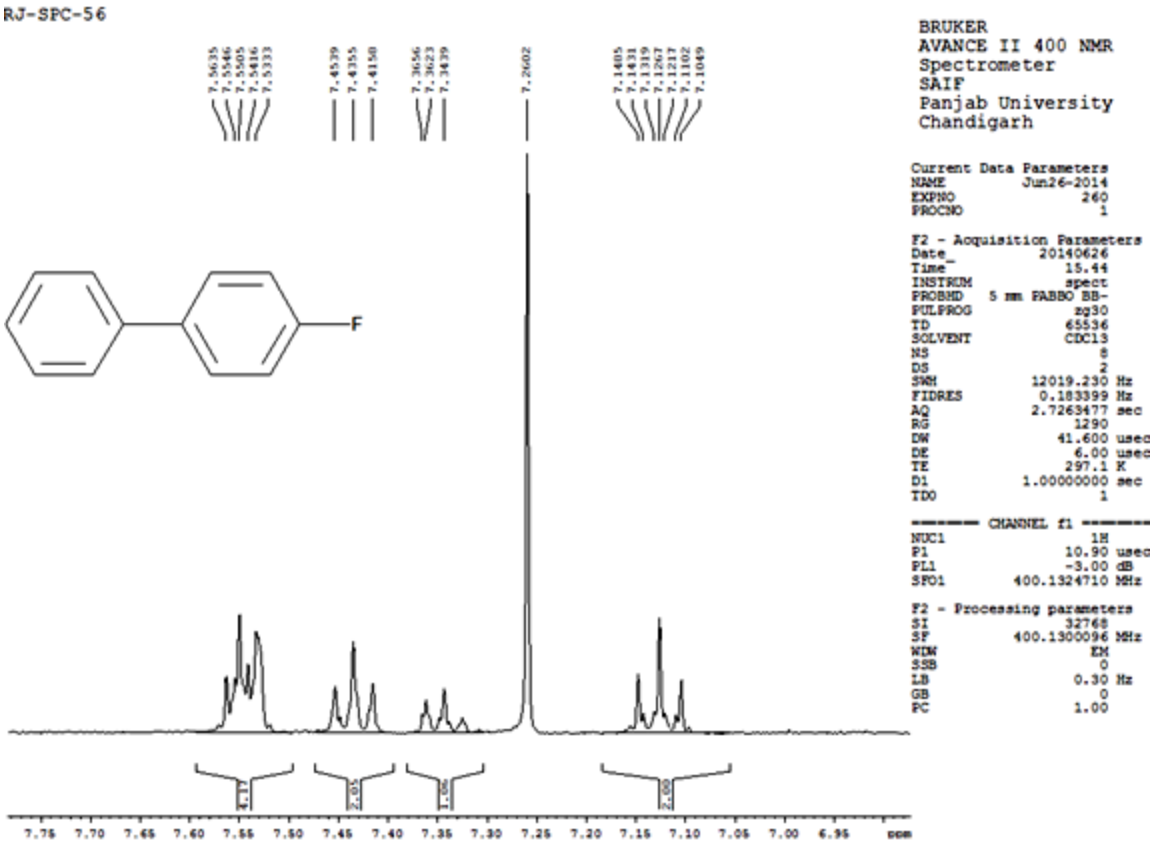

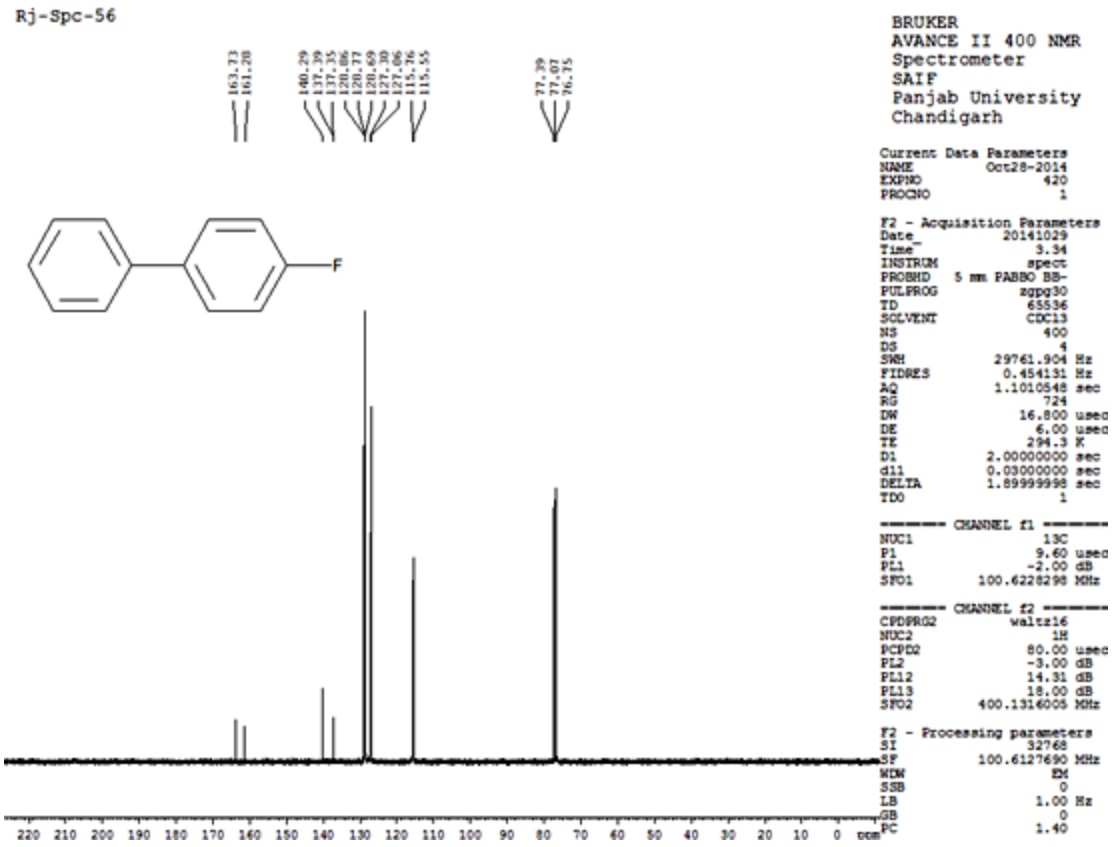

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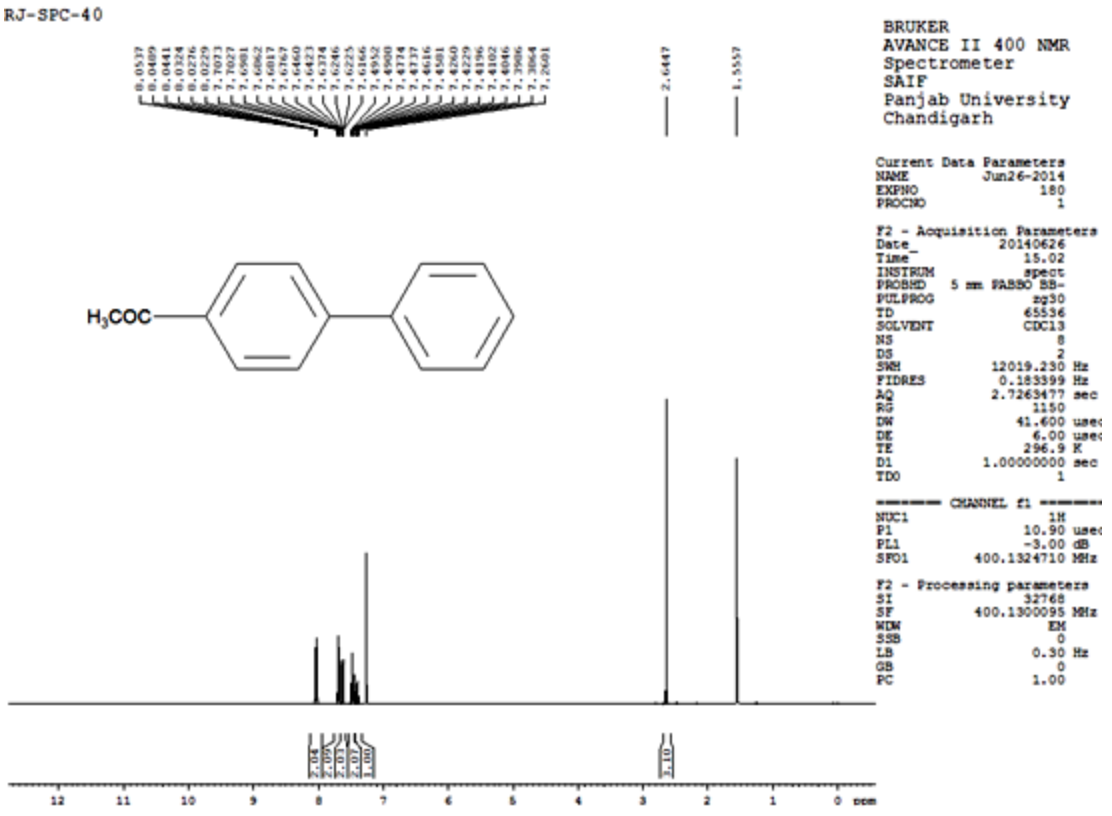
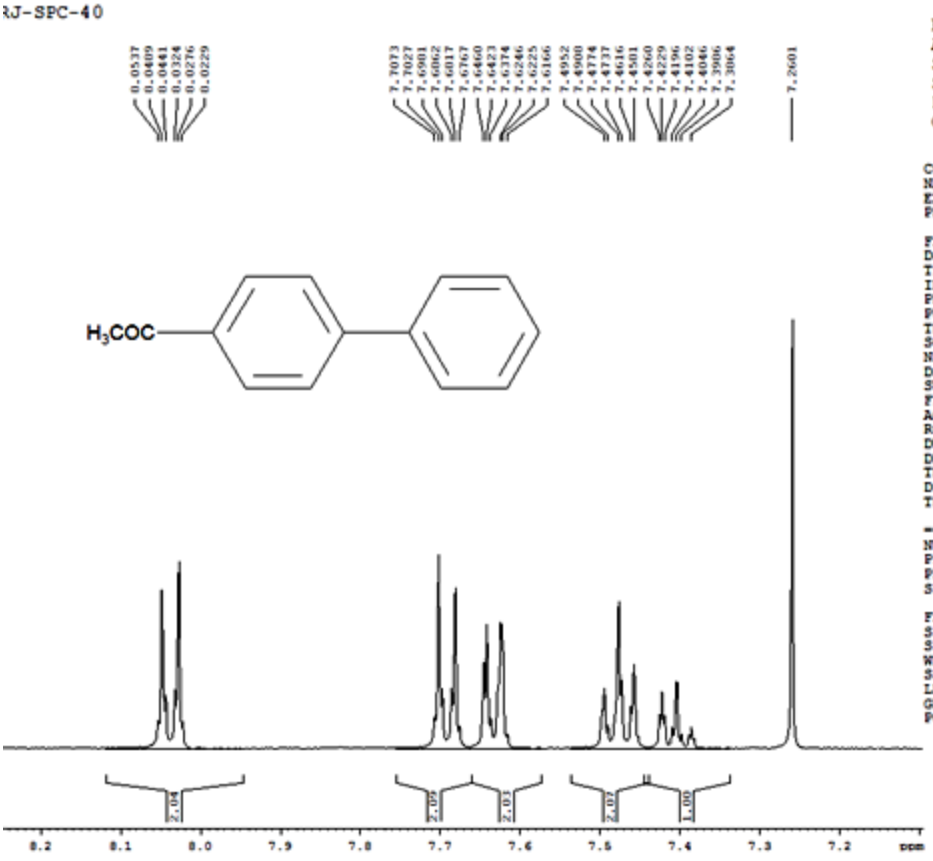


RJ-SPC-40



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Current Data Parameters	
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PROCNO	1
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AQ	2.7263477 sec
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TE	296.9 K
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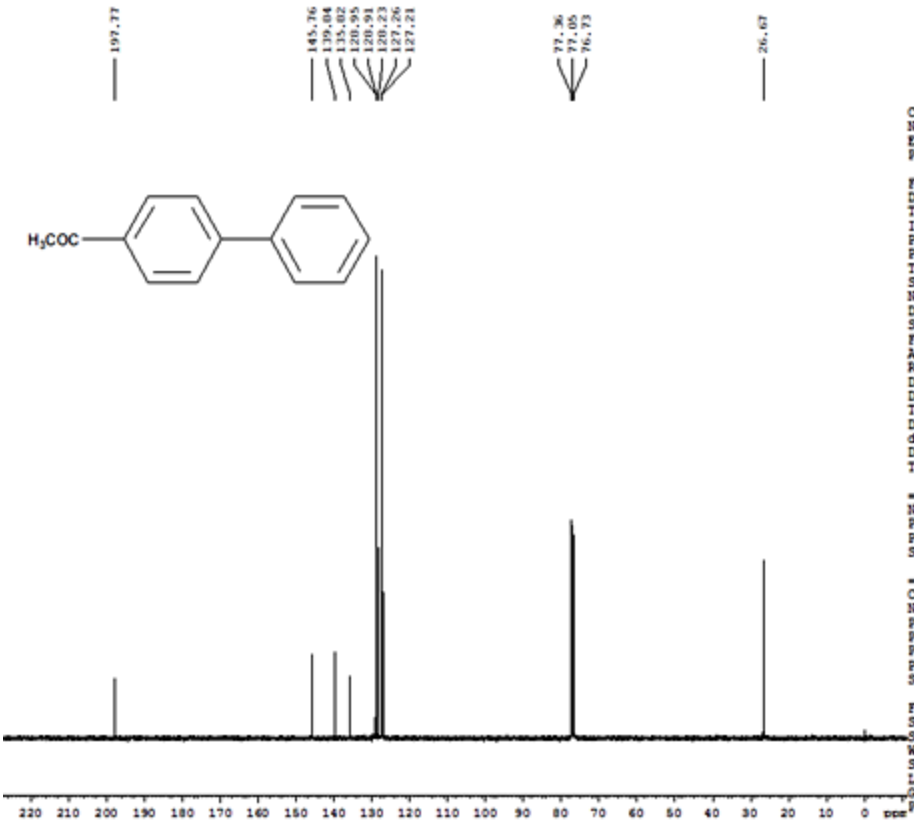
Rj-Spc-40



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Current Data Parameters	
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PROCNO	1
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INSTRUM	spect
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FIDRES	0.454131 Hz
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RG	575
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TE	295.6 K
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DELTA	1.89999998 sec
TD0	1
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P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
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NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
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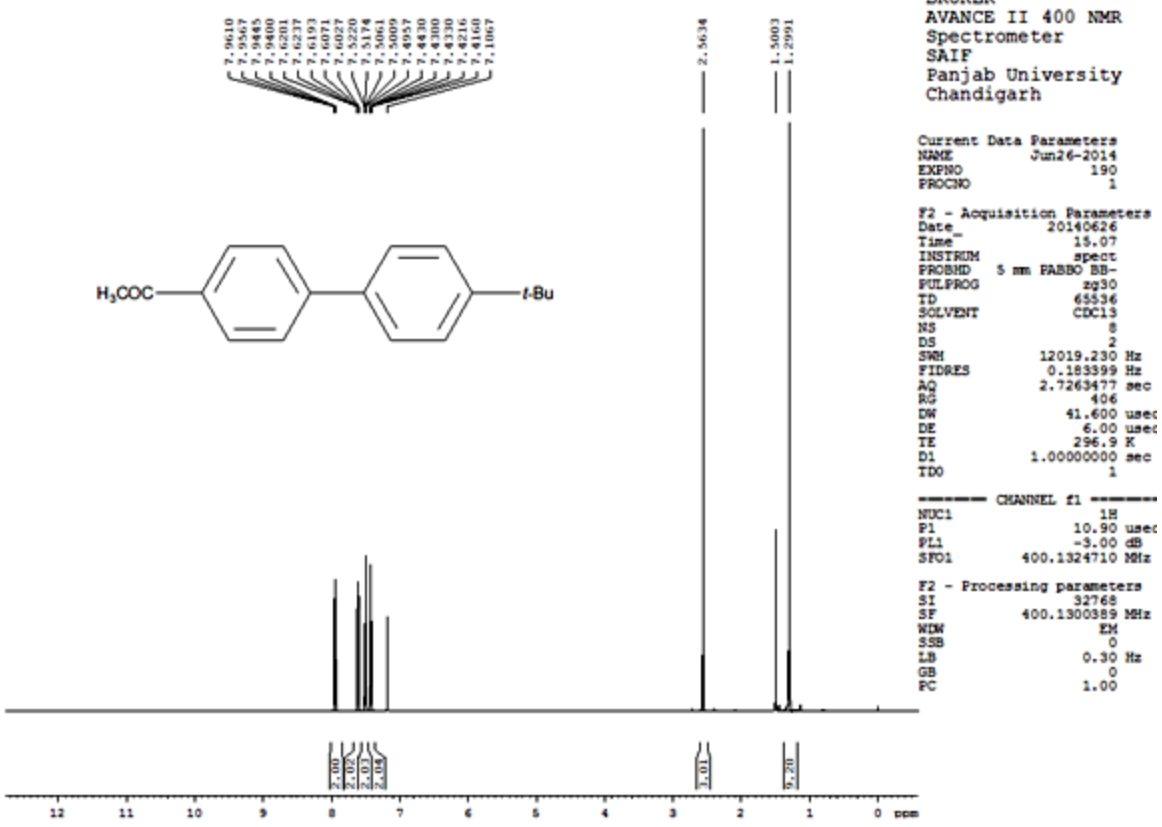
Table 1, Entry 5:

RJ-SPC-42



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Current Data Parameters	
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PROCNO	1
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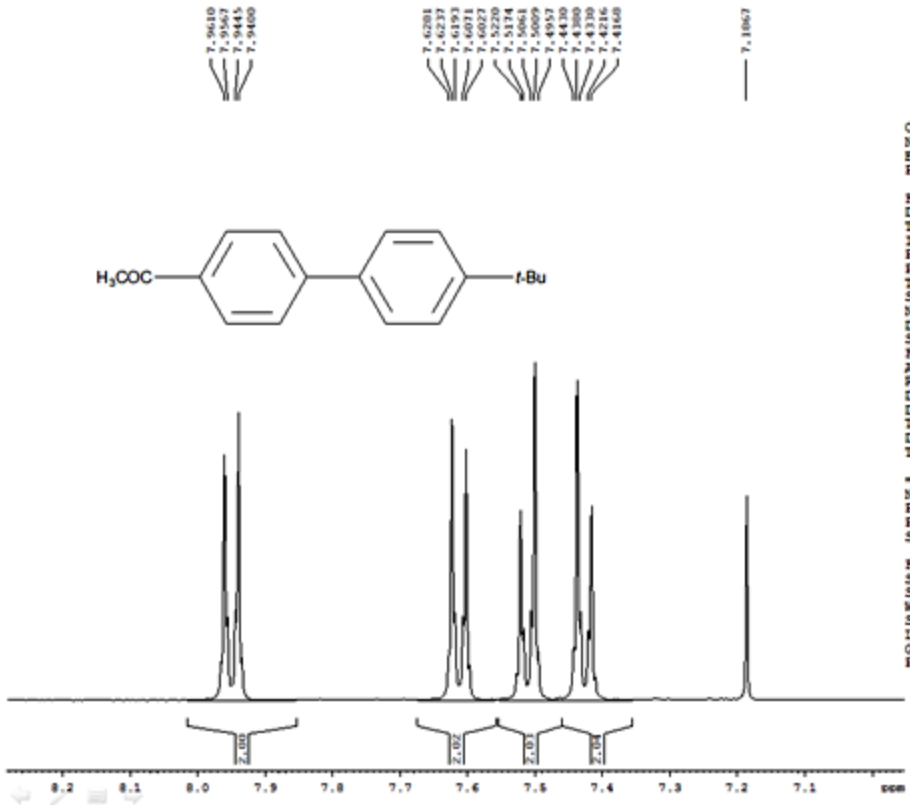
RJ-SPC-42



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Current Data Parameters	
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PROCNO	1
F2 - Acquisition Parameters	
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NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	406
DW	41.600 usec
DE	6.00 usec
TE	296.9 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	400.1300389 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

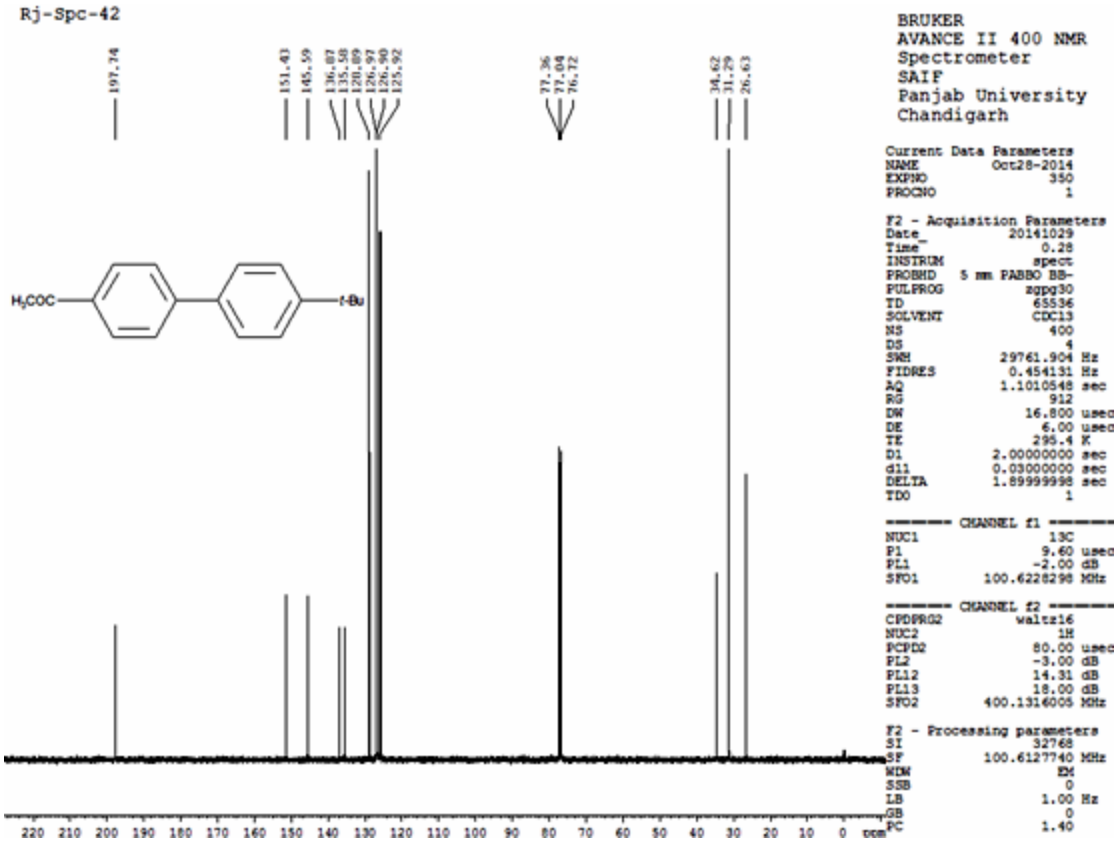
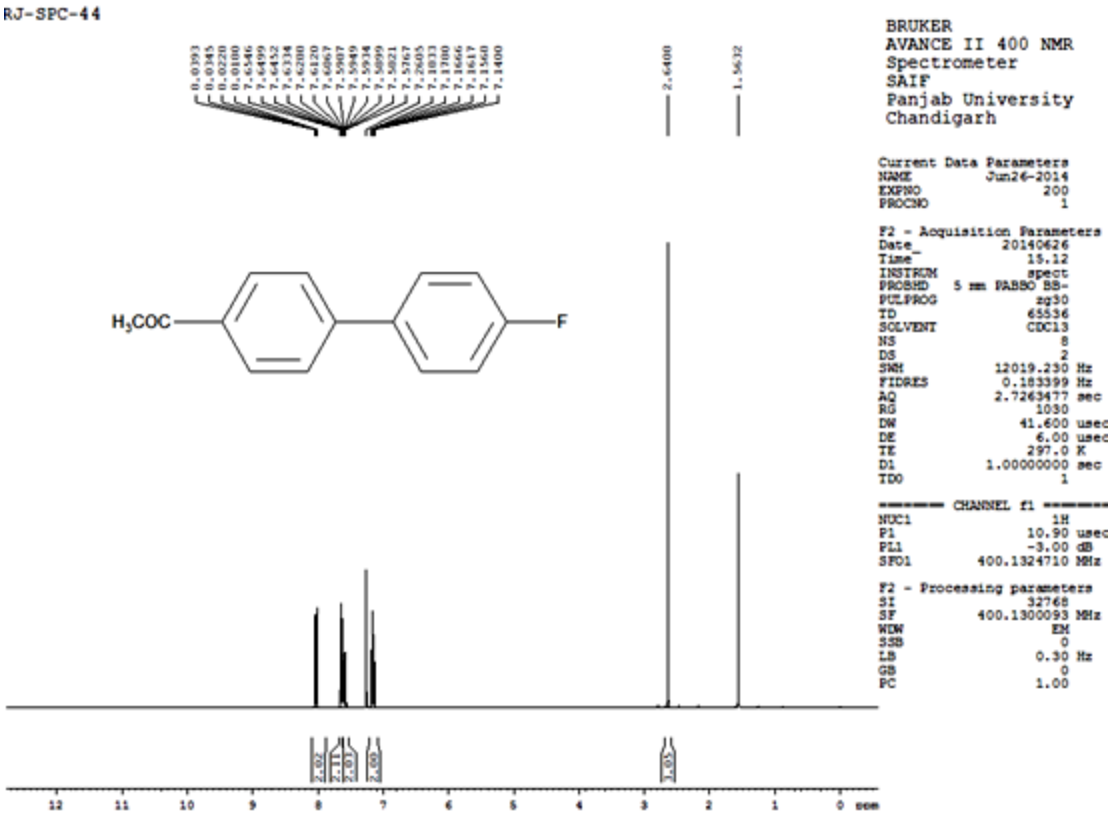
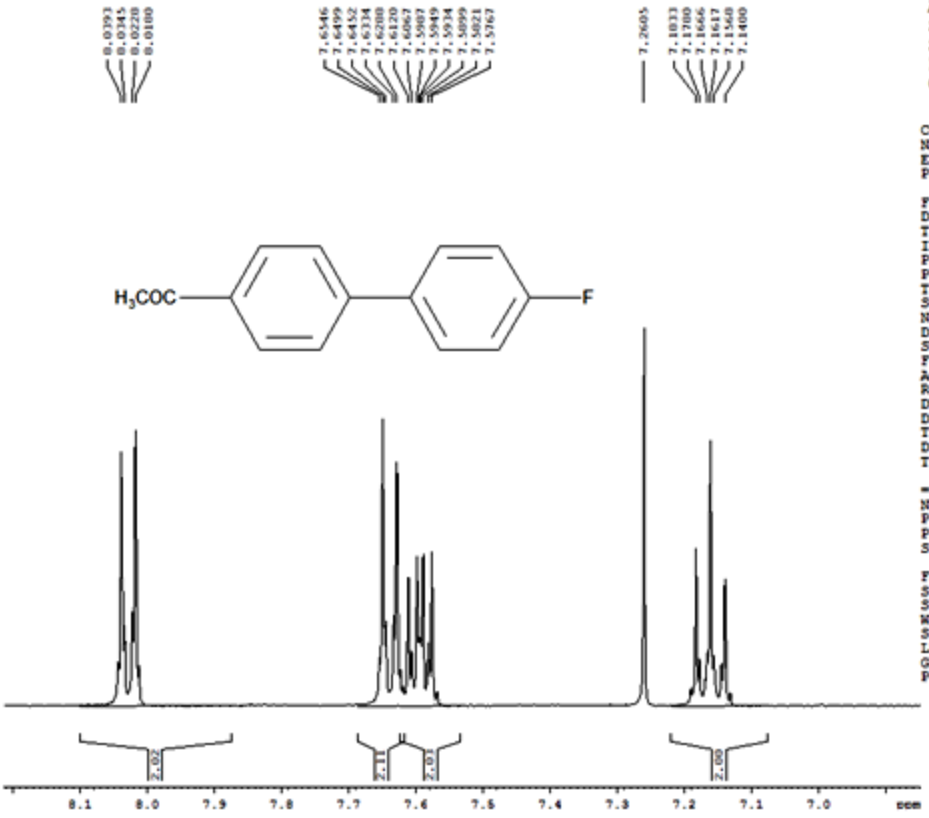


Table 1, Entry6:



RJ-SPC-44



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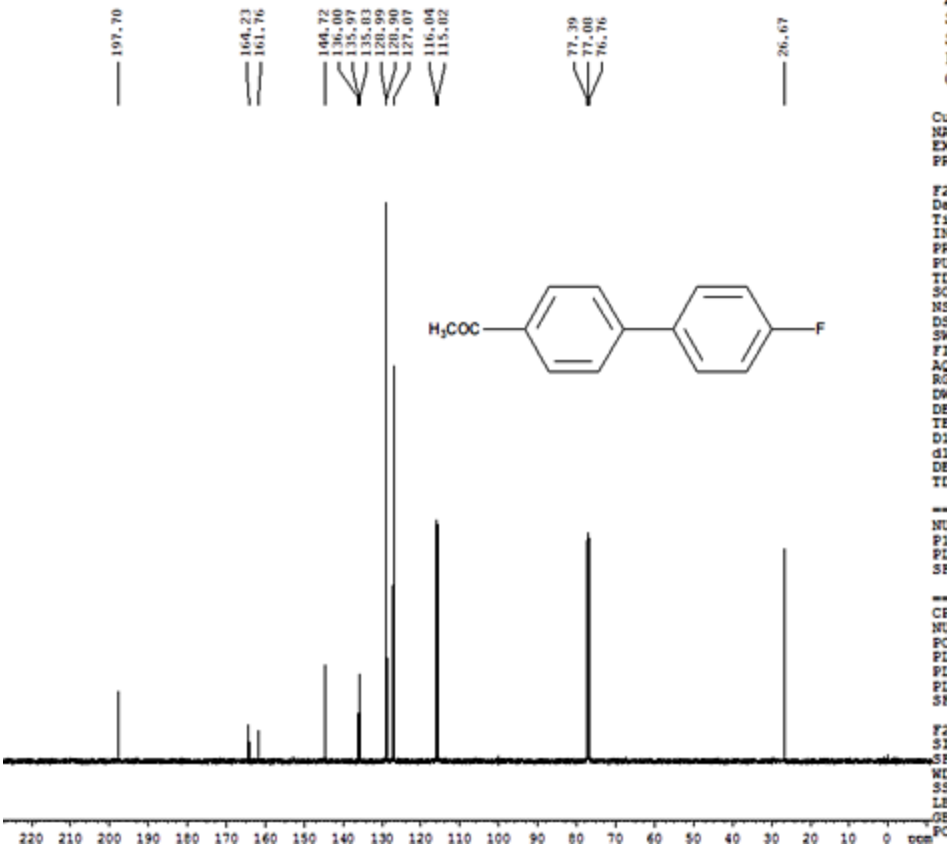
Current Data Parameters	
NAME	Jun26-2014
EXPNO	200
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140626
Time	15.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	1030
DW	41.600 usec
DE	6.00 usec
TE	297.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300093 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Rj-Spc-44



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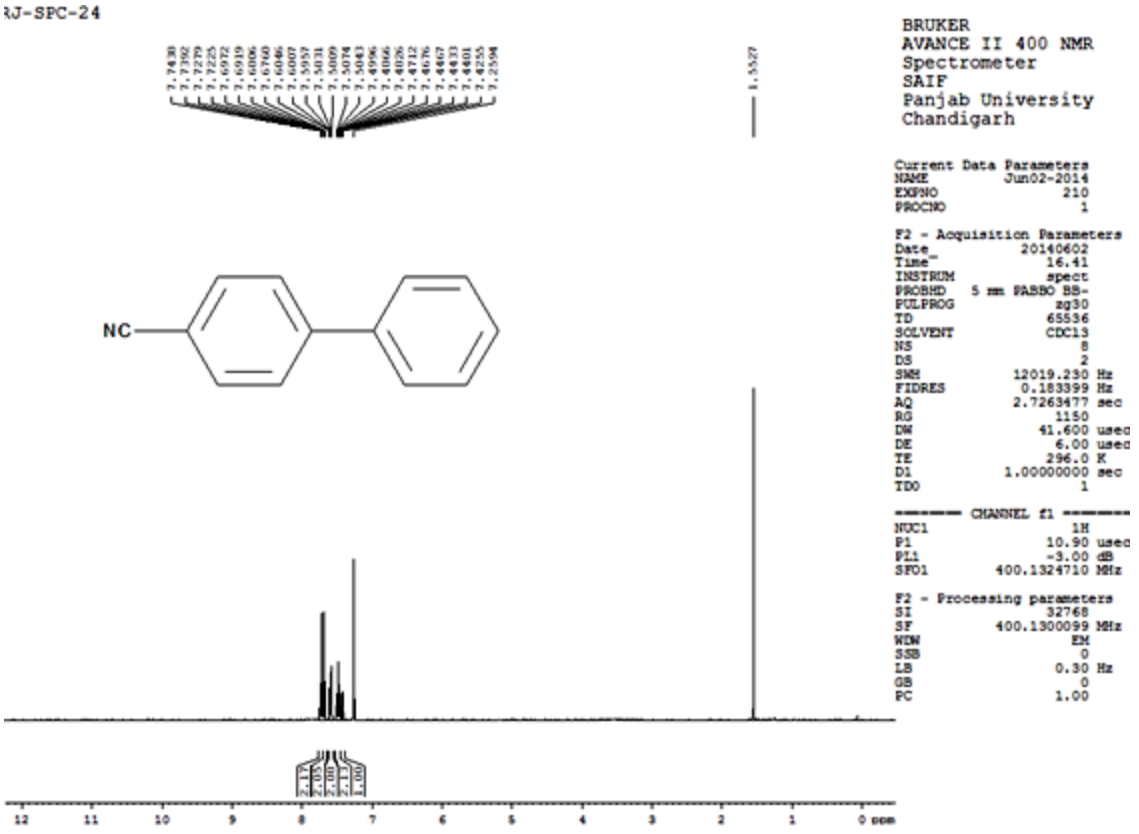
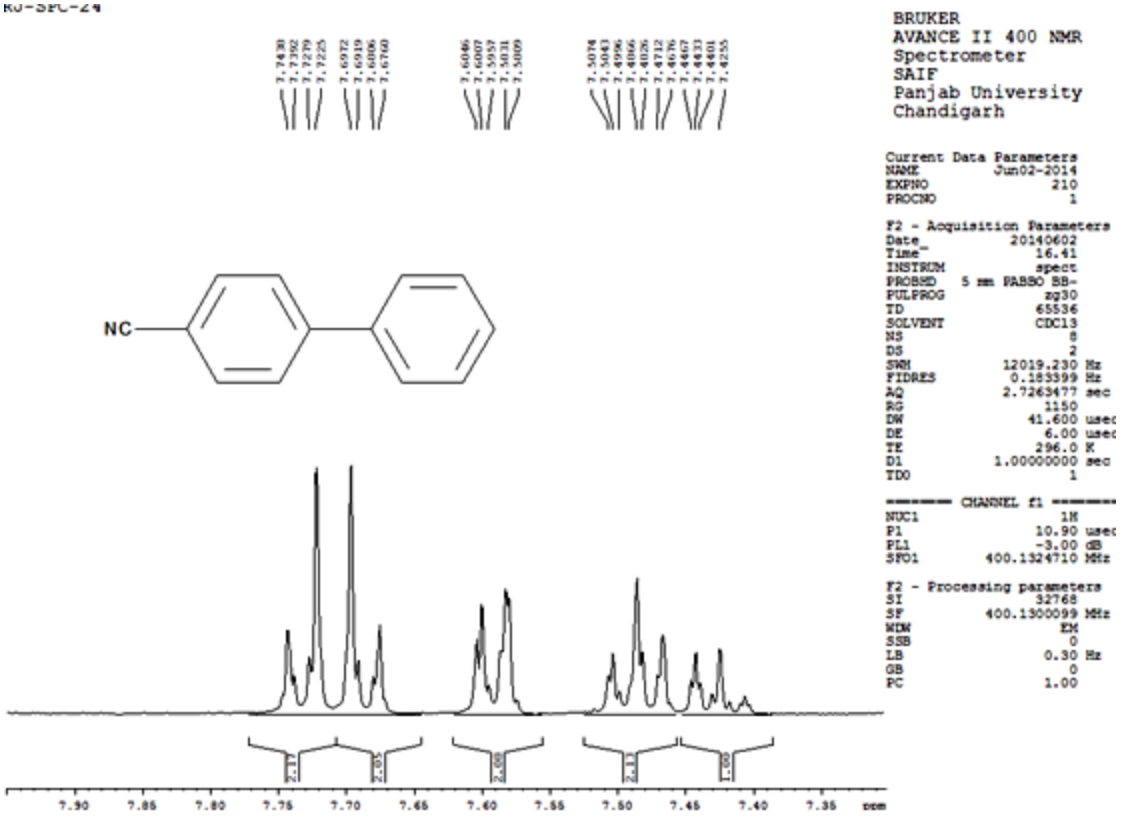
Current Data Parameters	
NAME	Oct28-2014
EXPNO	360
PROCNO	1
F2 - Acquisition Parameters	
Date_	20141029
Time	11.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	400
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	36
DW	16.800 usec
DE	6.00 usec
TE	295.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.60 usec
PL1	-2.00 dB
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-3.00 dB
PL12	14.31 dB
PL13	18.00 dB
SFO2	400.1316005 MHz
F2 - Processing parameters	
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Table 1, Entry7:





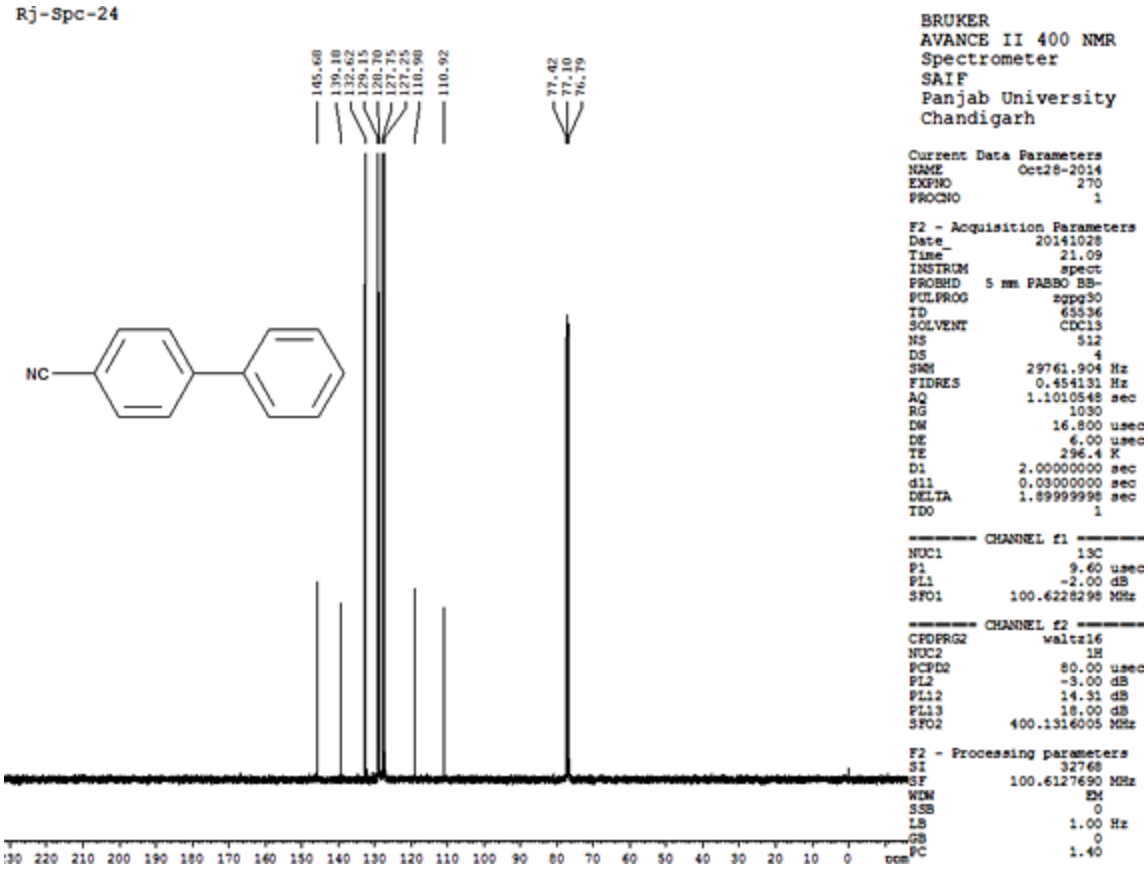
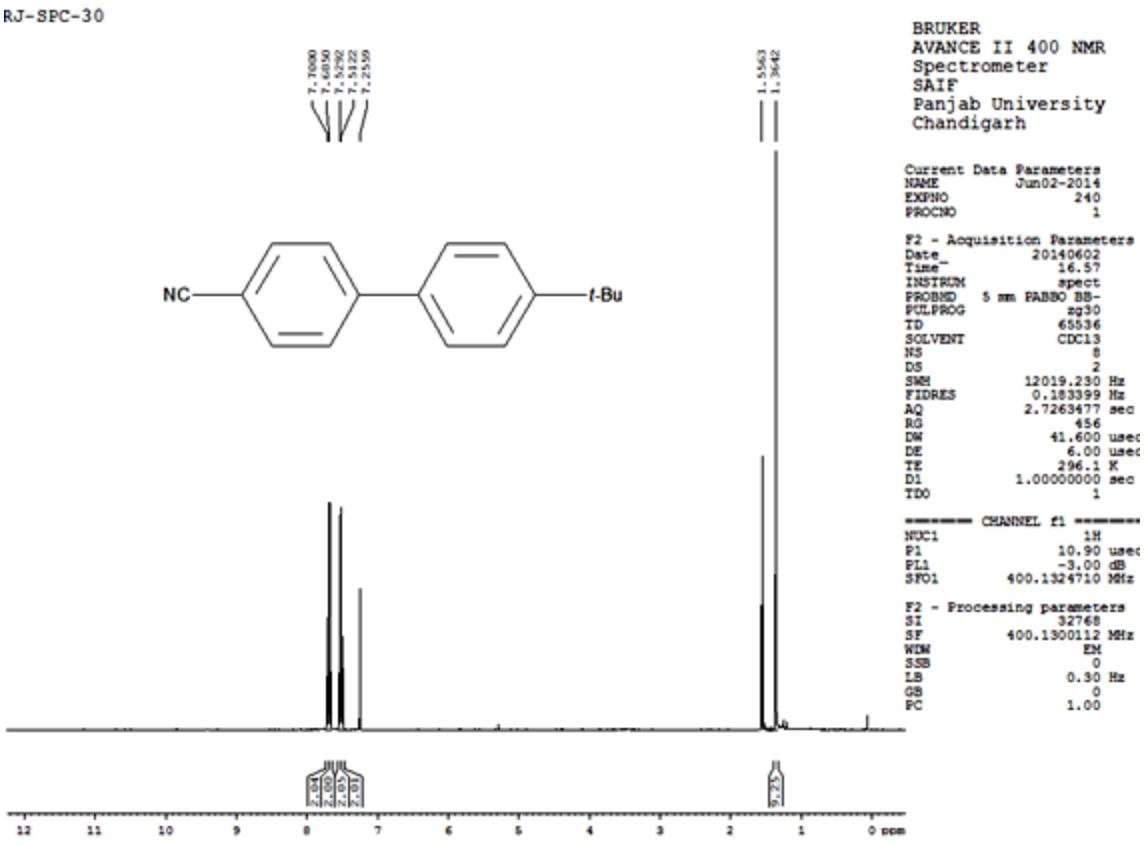
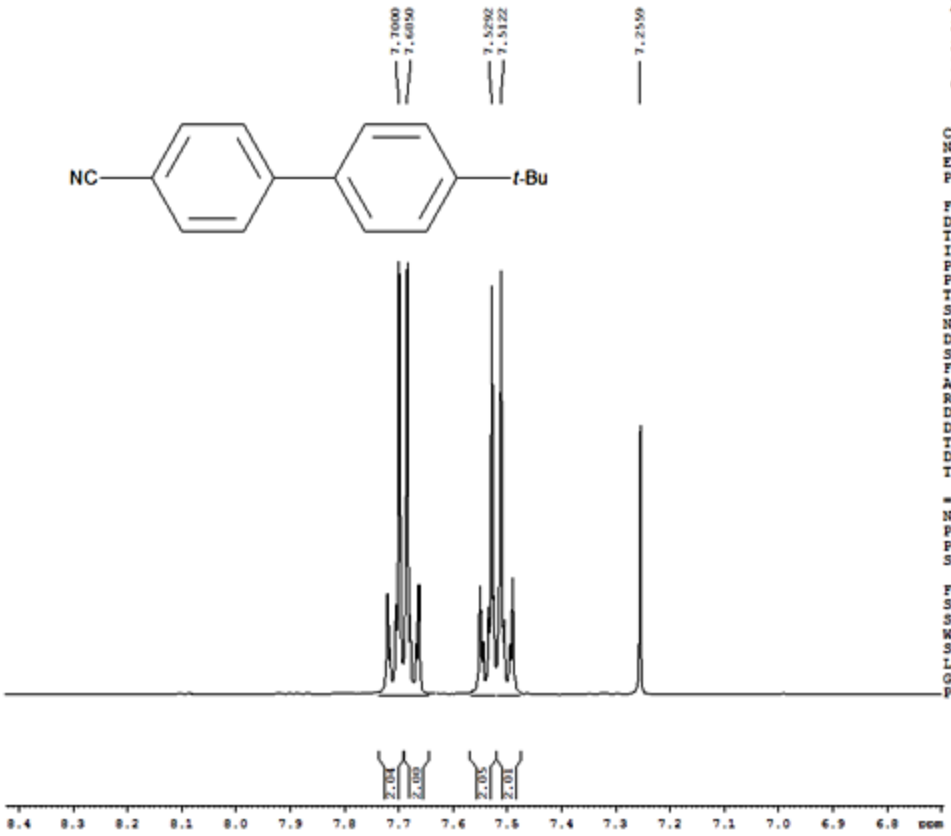


Table 1, Entry 8:



RJ-SPC-30



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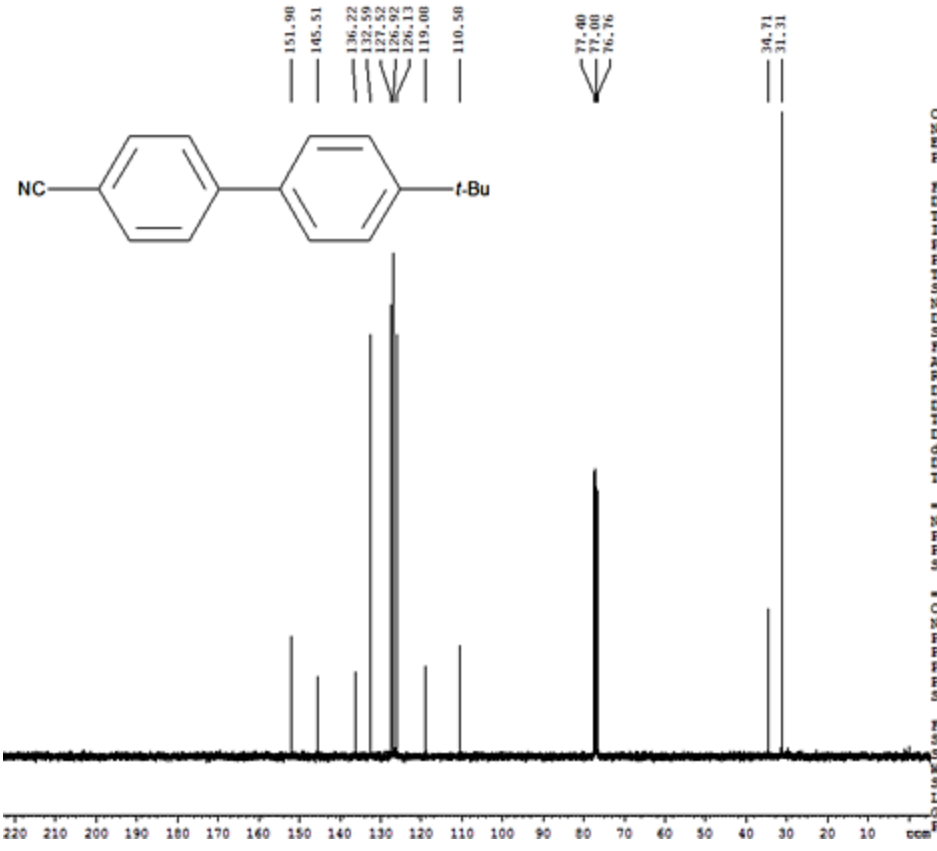
Current Data Parameters	
NAME	Jun02-2014
EXPNO	240
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140602
Time	16.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	456
DW	41.600 usec
DE	6.00 usec
TE	296.1 K
D1	1.00000000 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	400.1300112 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Rj-Spc-30



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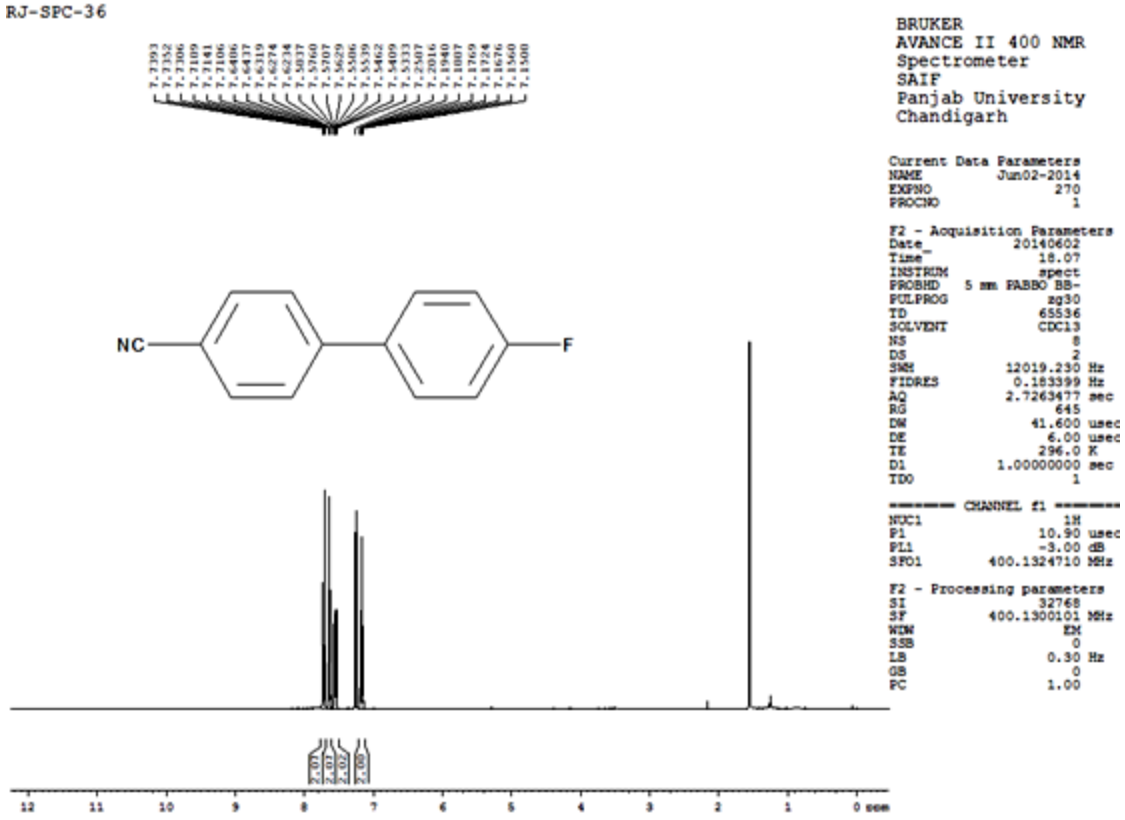
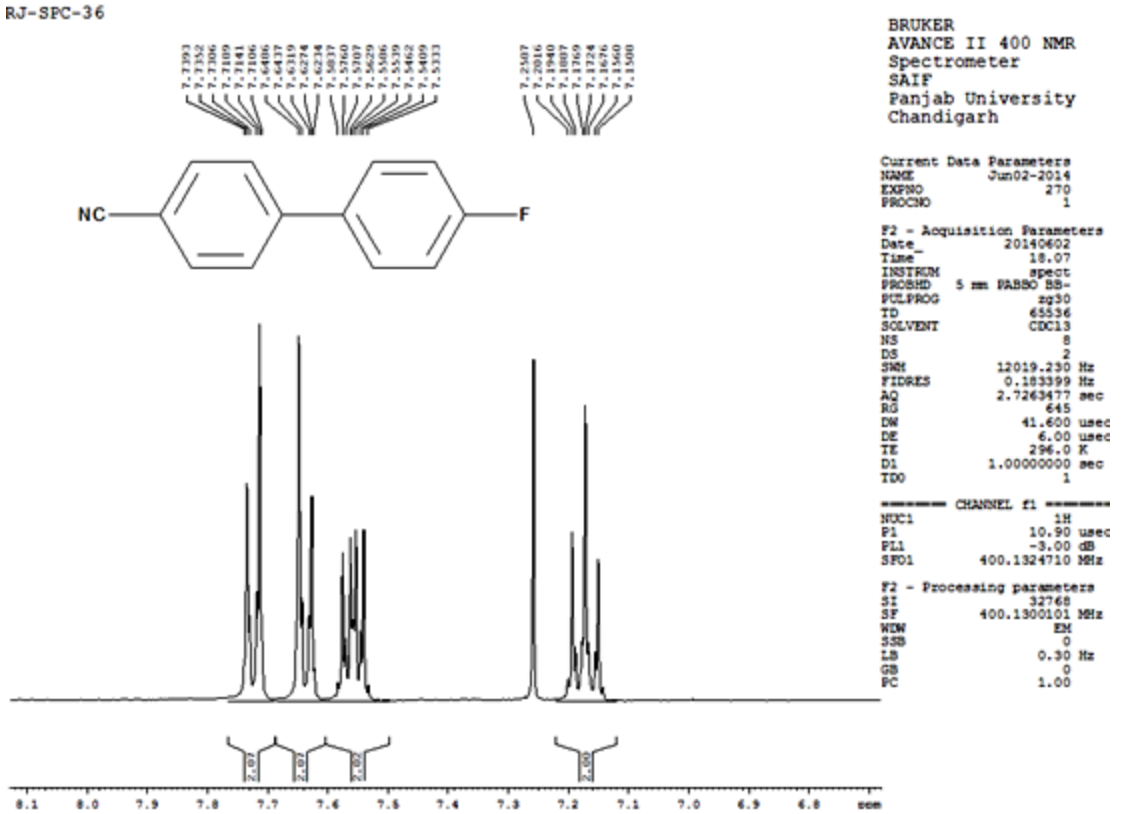
Current Data Parameters	
NAME	Oct28-2014
EXPNO	300
PROCNO	1
F2 - Acquisition Parameters	
Date_	20141028
Time	22.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	176
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	912
DW	16.800 usec
DE	6.00 usec
TE	296.2 K
D1	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

Table 1, Entry 9:





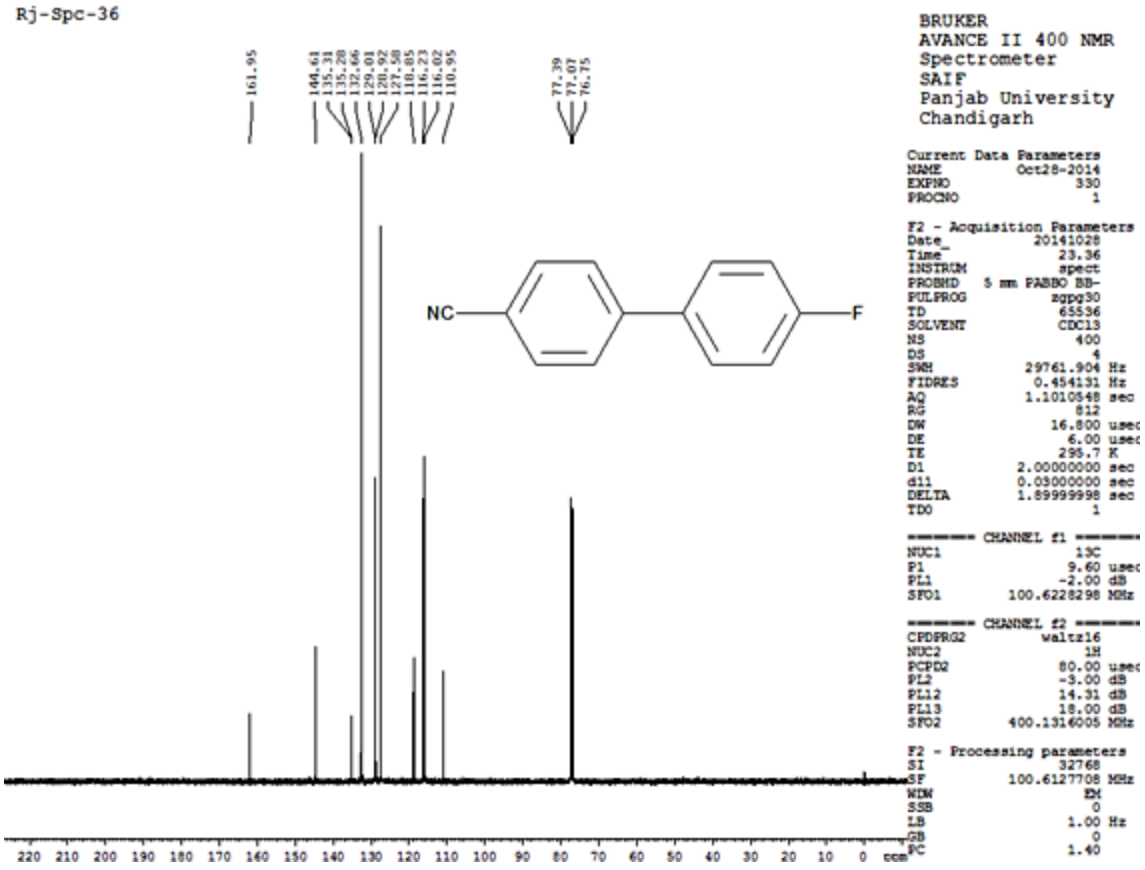
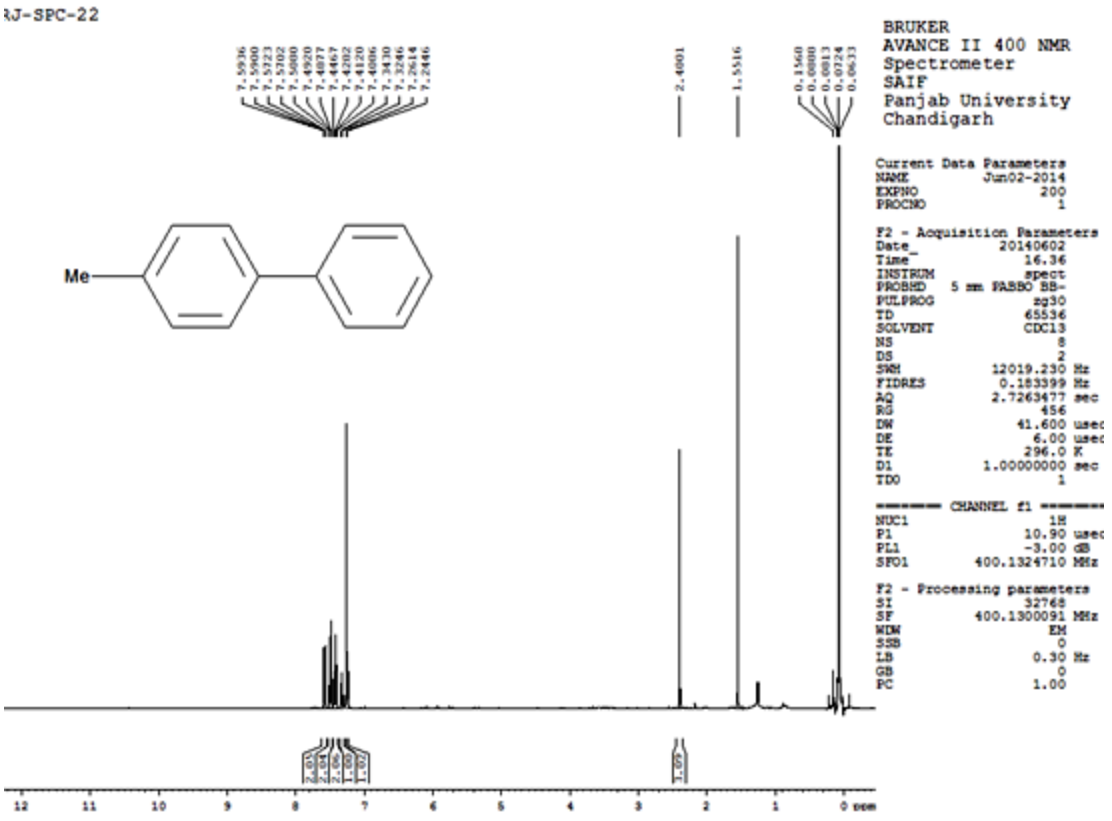
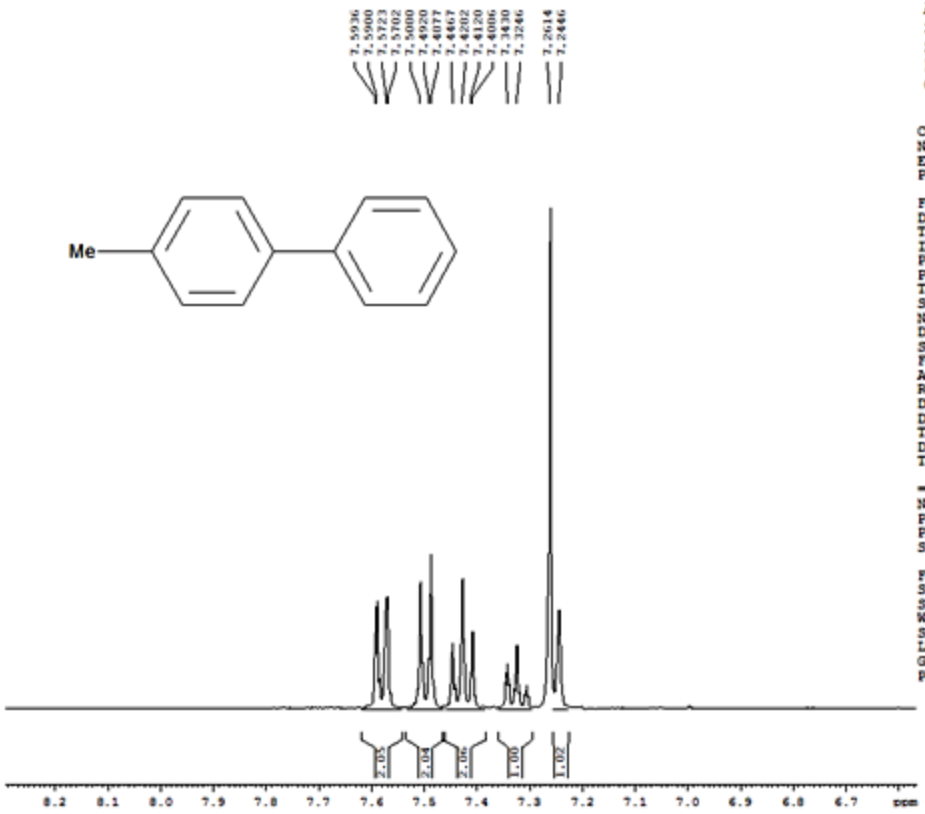


Table1, Entry10:



RJ-SPC-22



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Current Data Parameters	
NAME	Jun02-2014
EXPNO	200
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140602
Time	16.36
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	456
DW	41.600 usec
DE	6.00 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

avtar saifpu@yahoo.co.in

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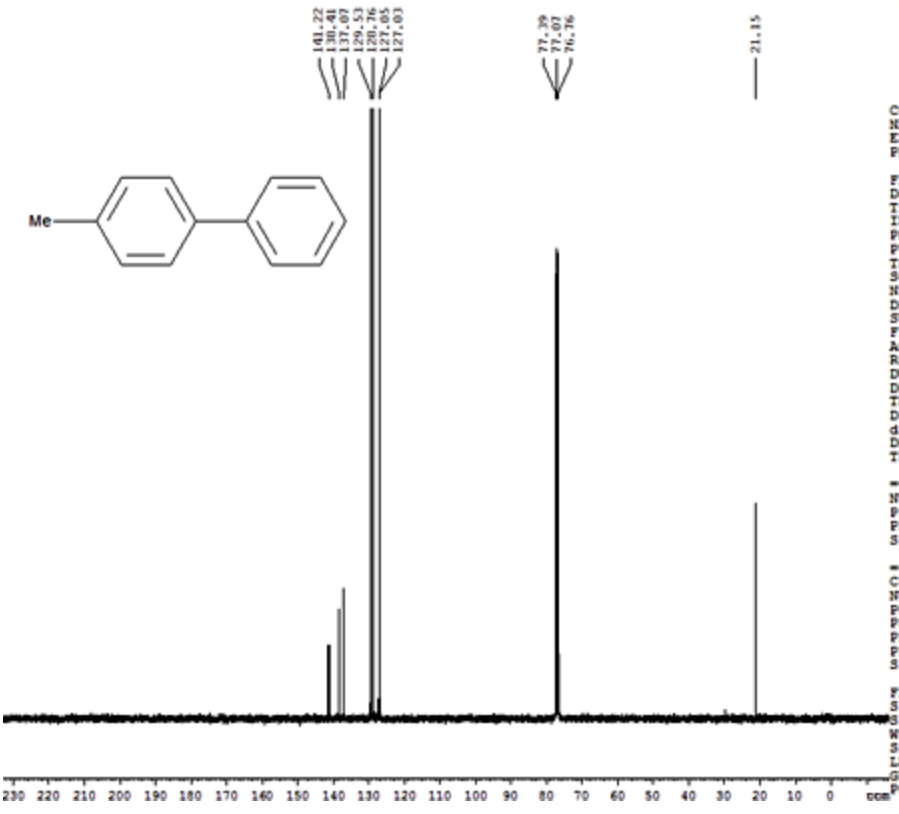

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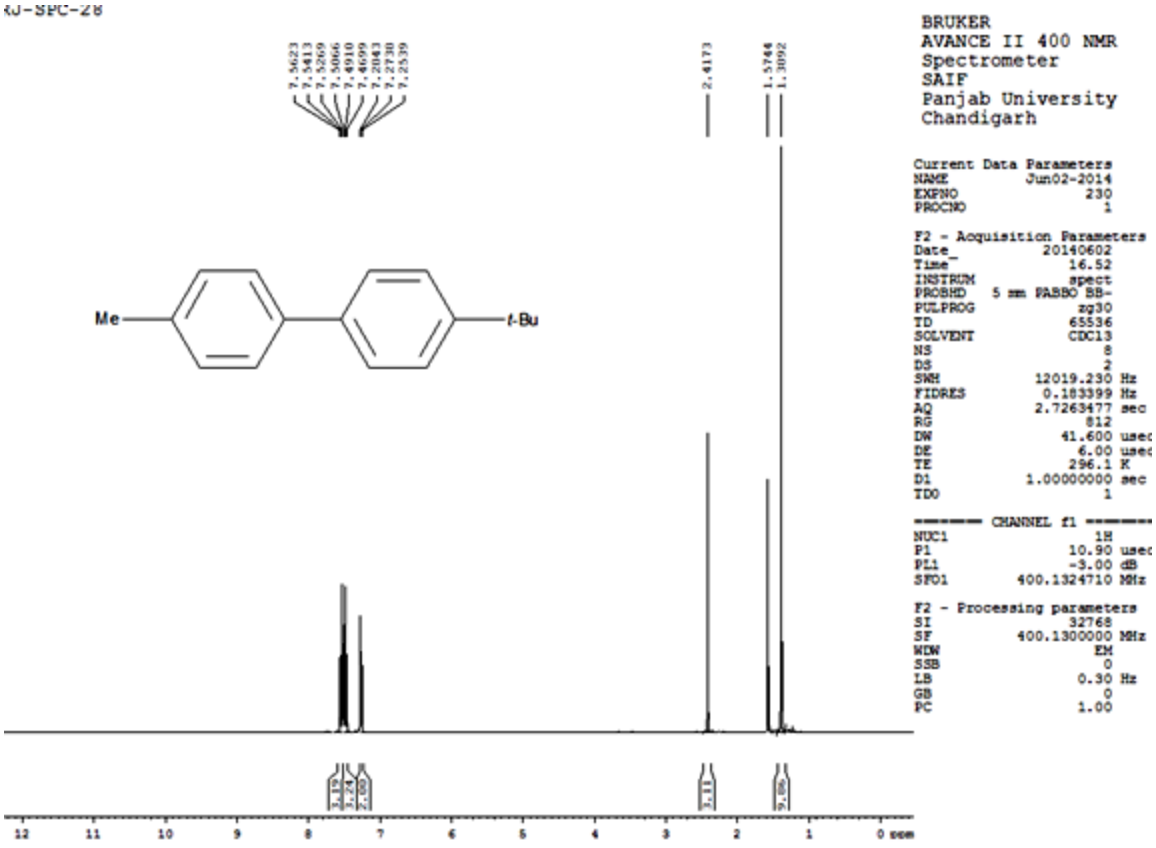
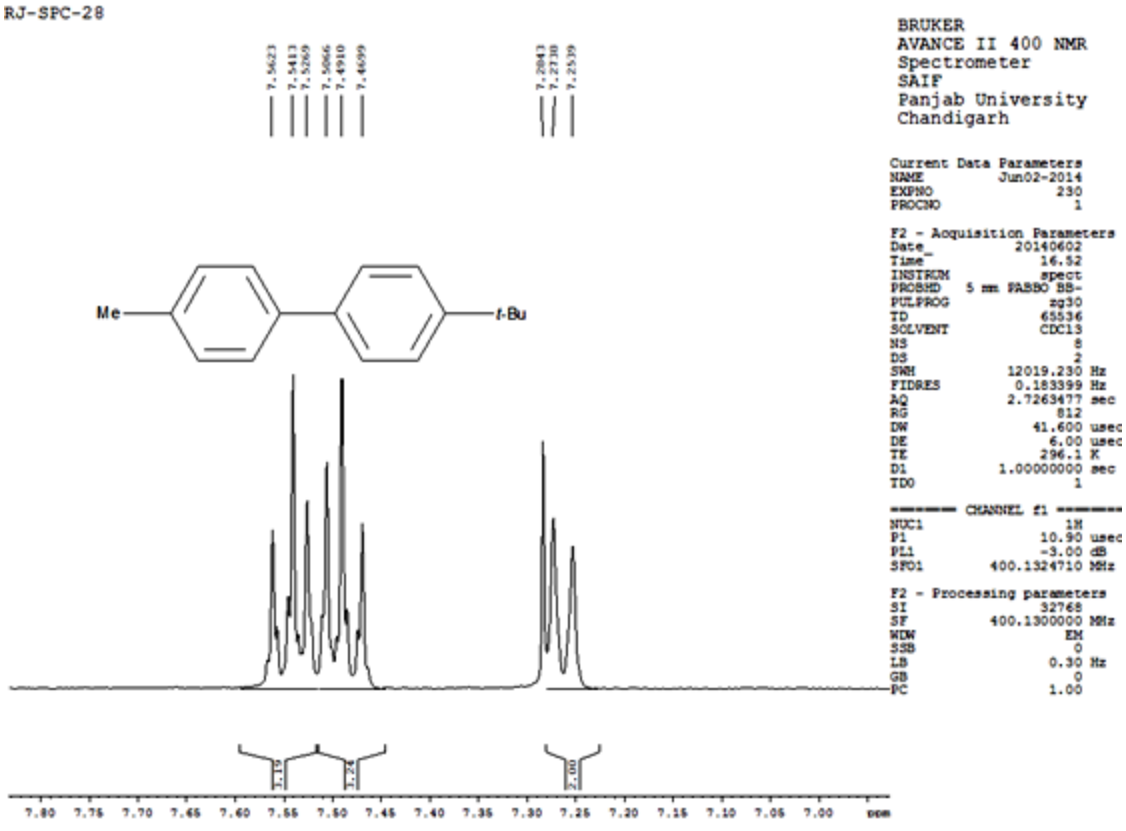
Current Data Parameters	
NAME	Oct28-2014
EXPNO	260
PROCNO	1
F2 - Acquisition Parameters	
Date_	20141028
Time	20.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	296.7 K
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	100.6127674 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Table 1, Entry 11:





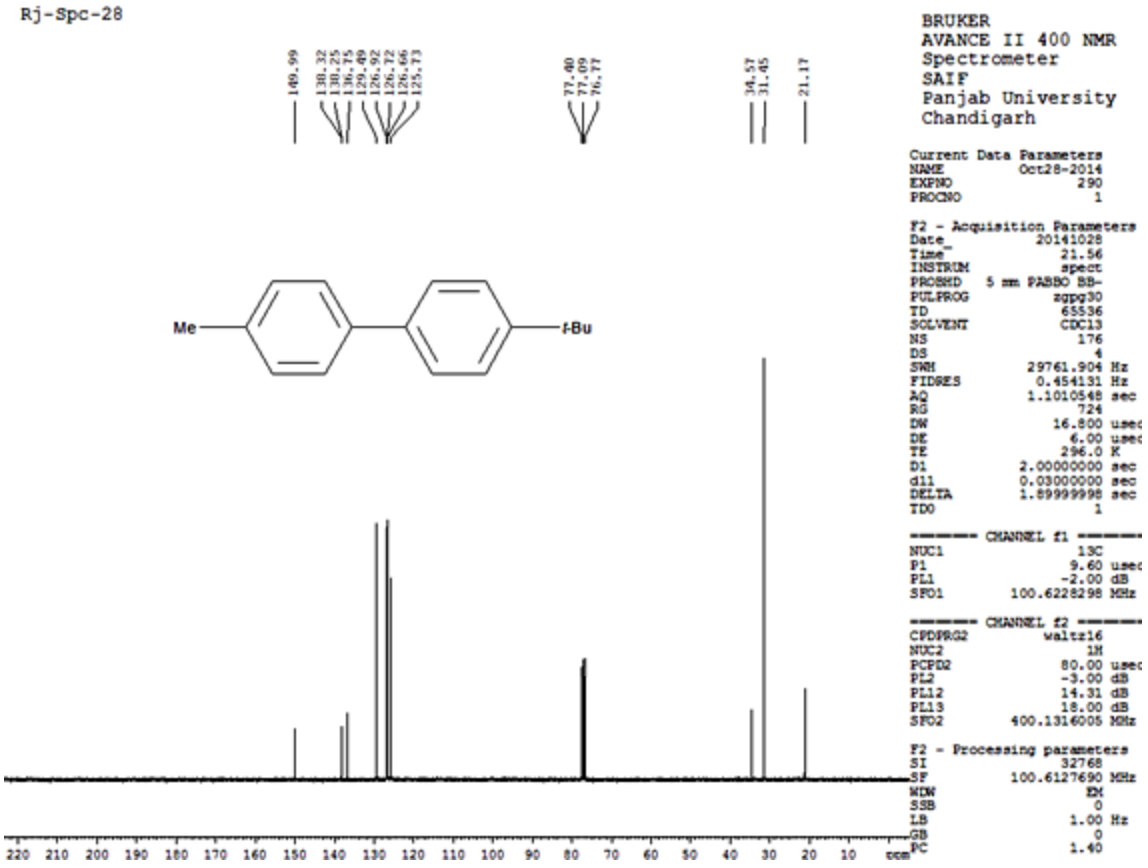
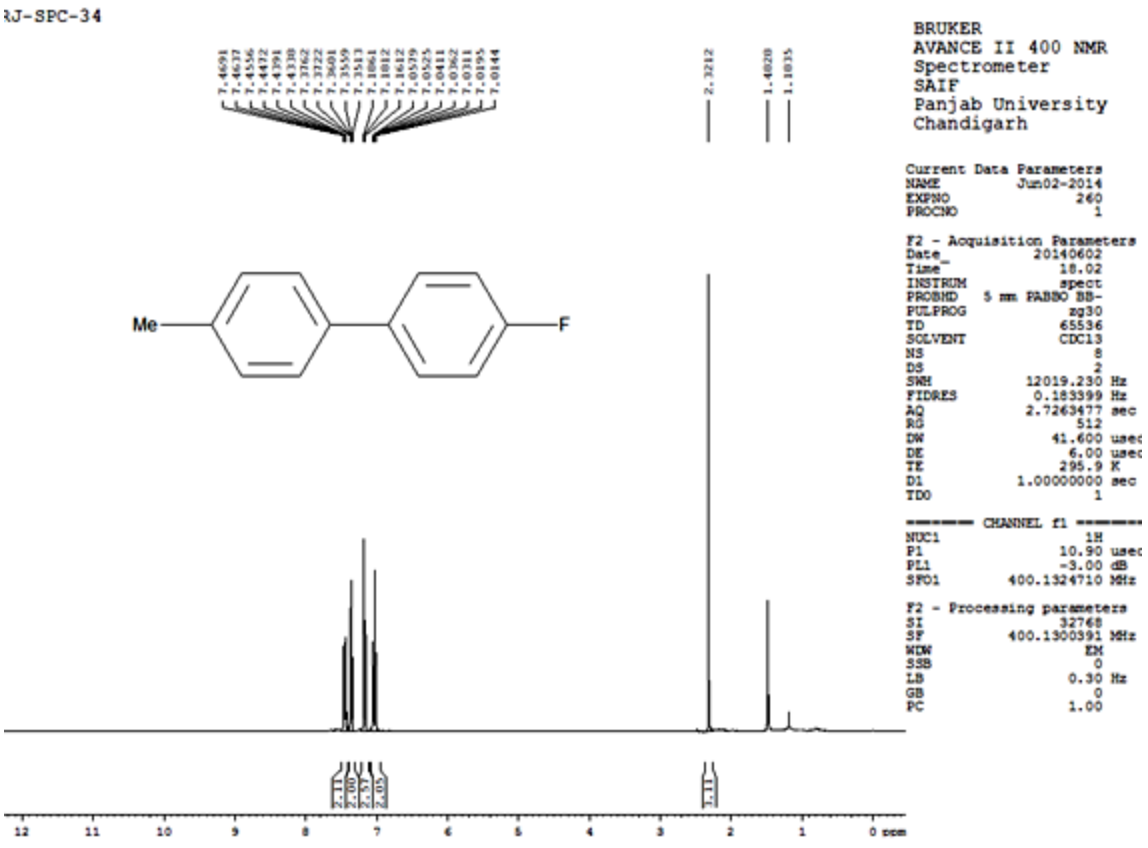


Table 1, Entry 12:



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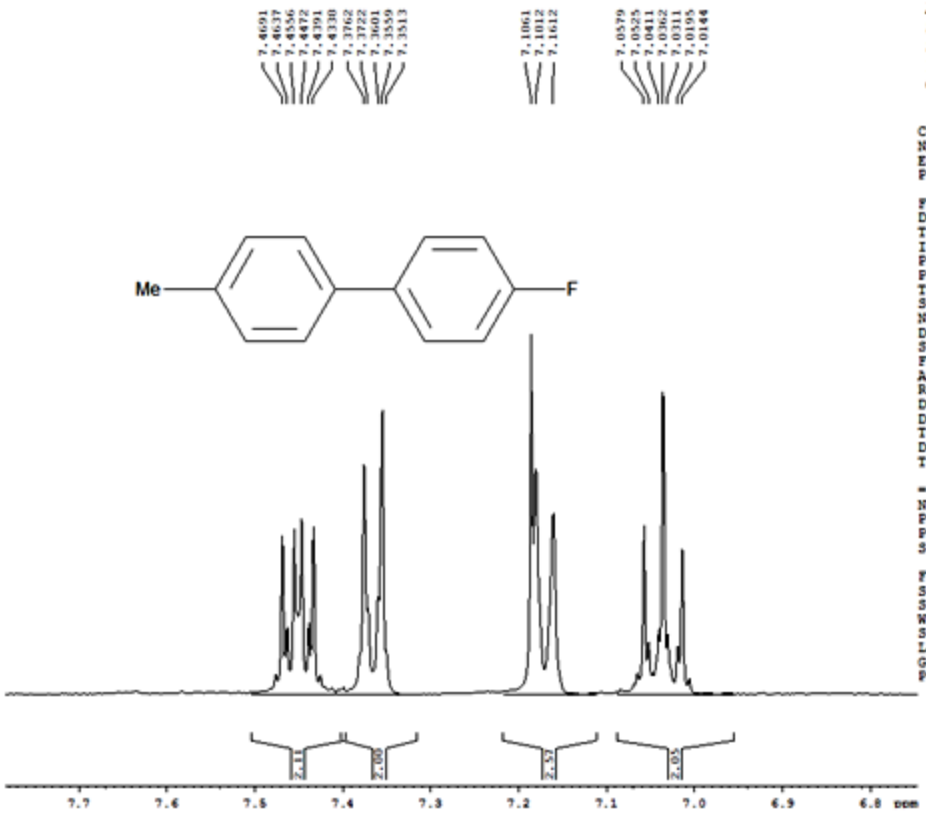

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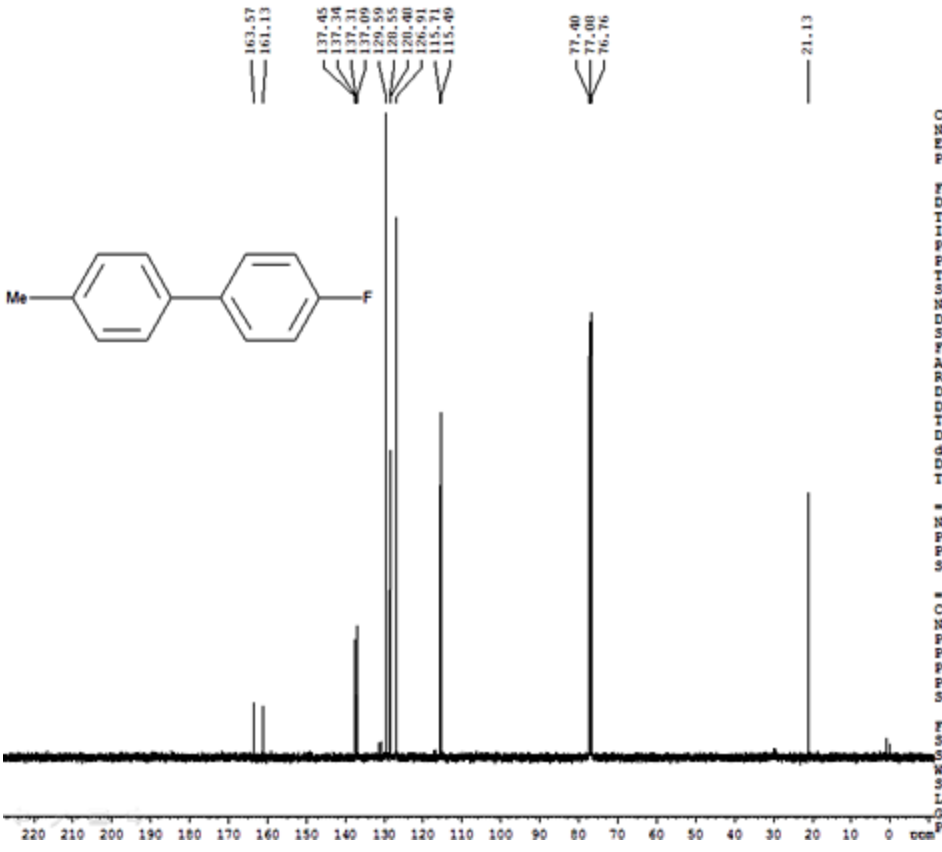
Current Data Parameters	
NAME	Jun02-2014
EXPNO	260
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140602
Time	18.02
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	512
DW	41.600 usec
DE	6.00 usec
TE	298.9 K
D1	1.00000000 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	400.1300391 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Rj-Spc-34



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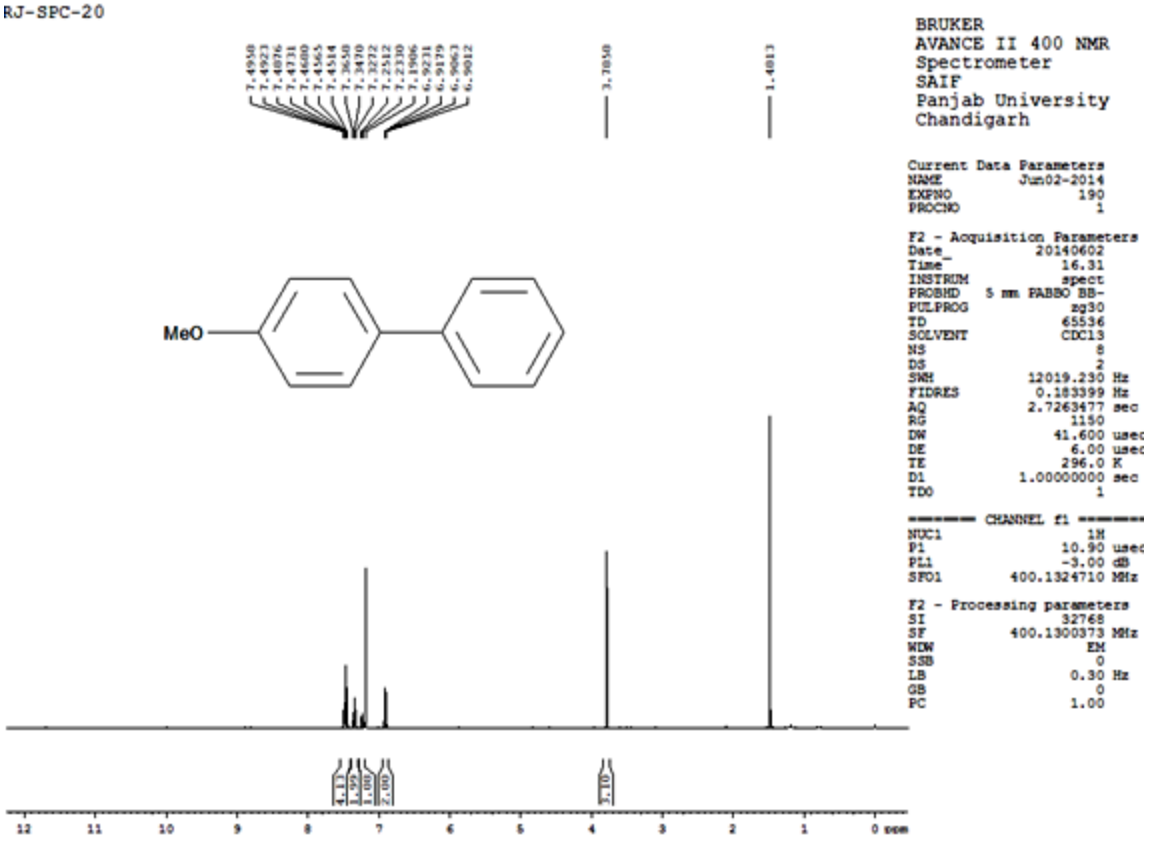
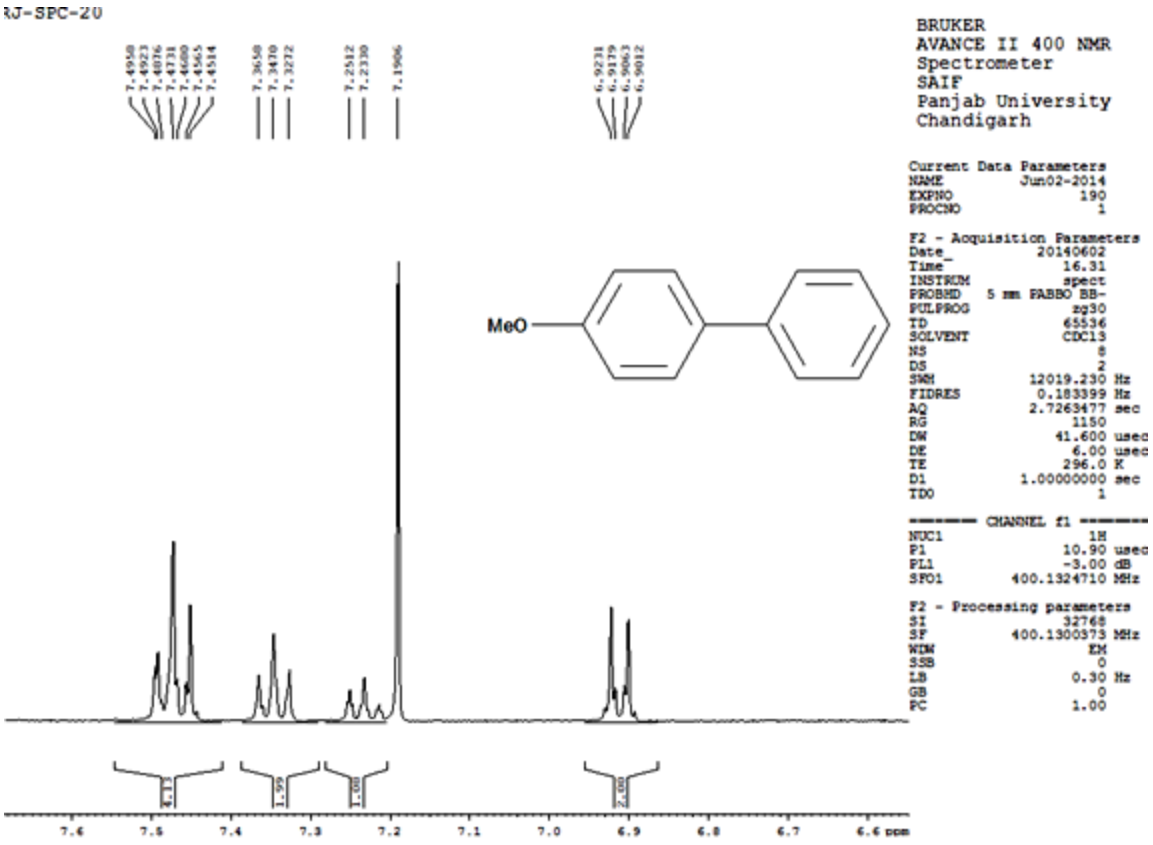
Current Data Parameters	
NAME	Oct28-2014
EXPNO	320
PROCNO	1
F2 - Acquisition Parameters	
Date_	20141028
Time	23.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	400
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	575
DW	16.800 usec
DE	6.00 usec
TE	298.9 K
D1	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	100.6127658 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Table 1, Entry 13:





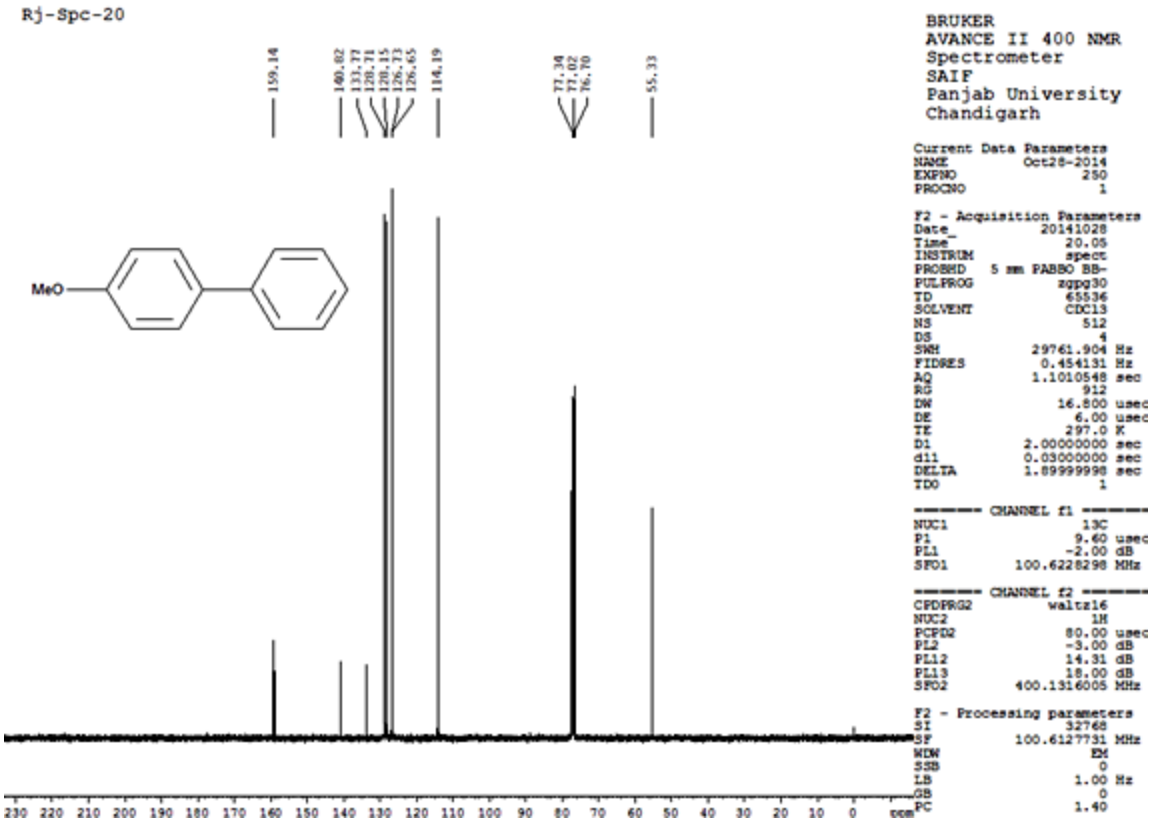
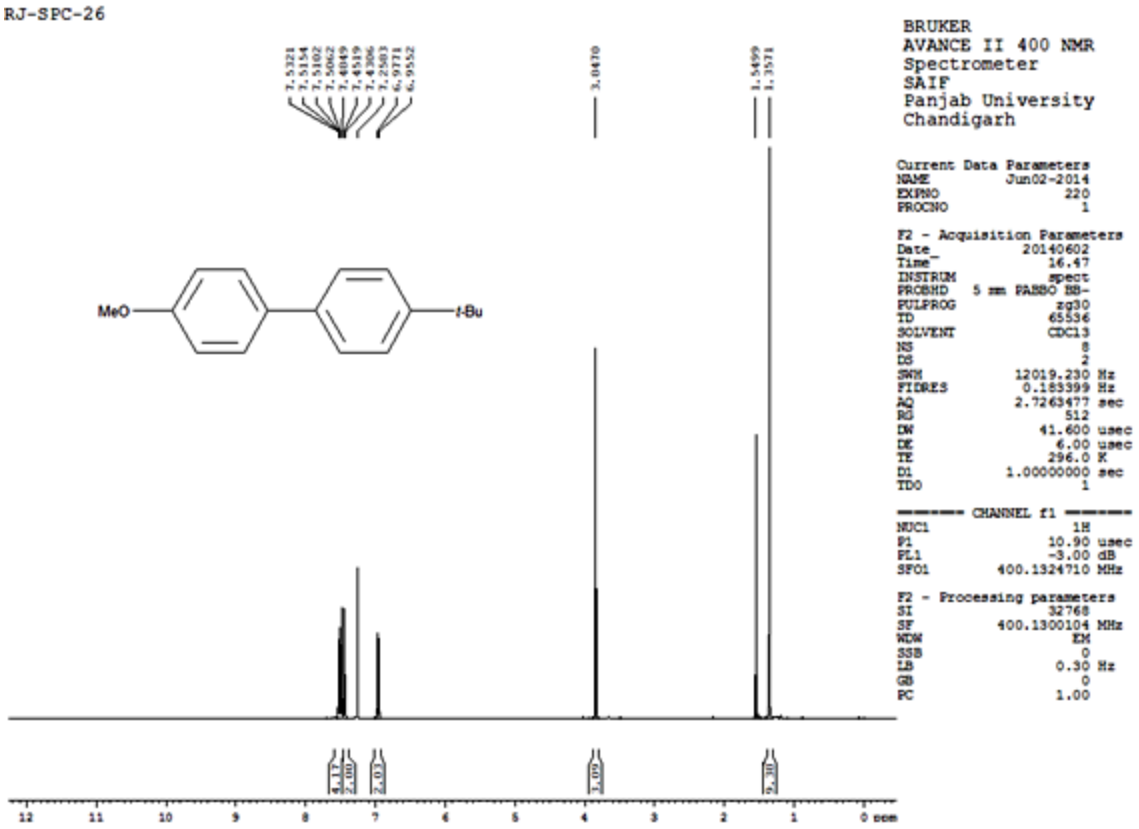
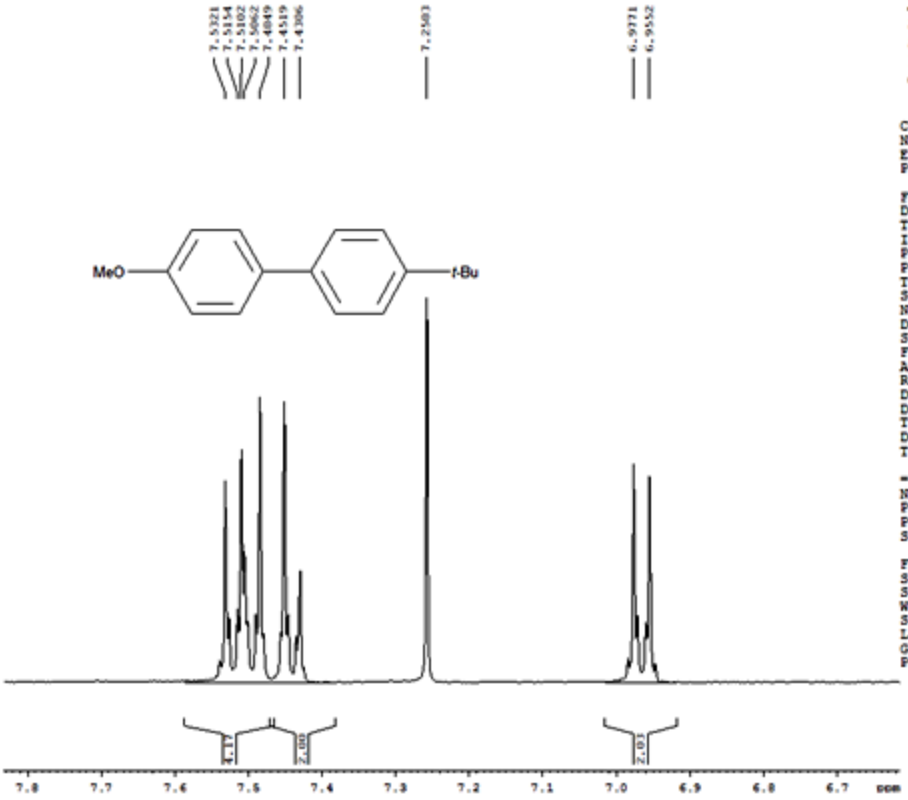


Table 1, Entry14:



RJ-SPC-26



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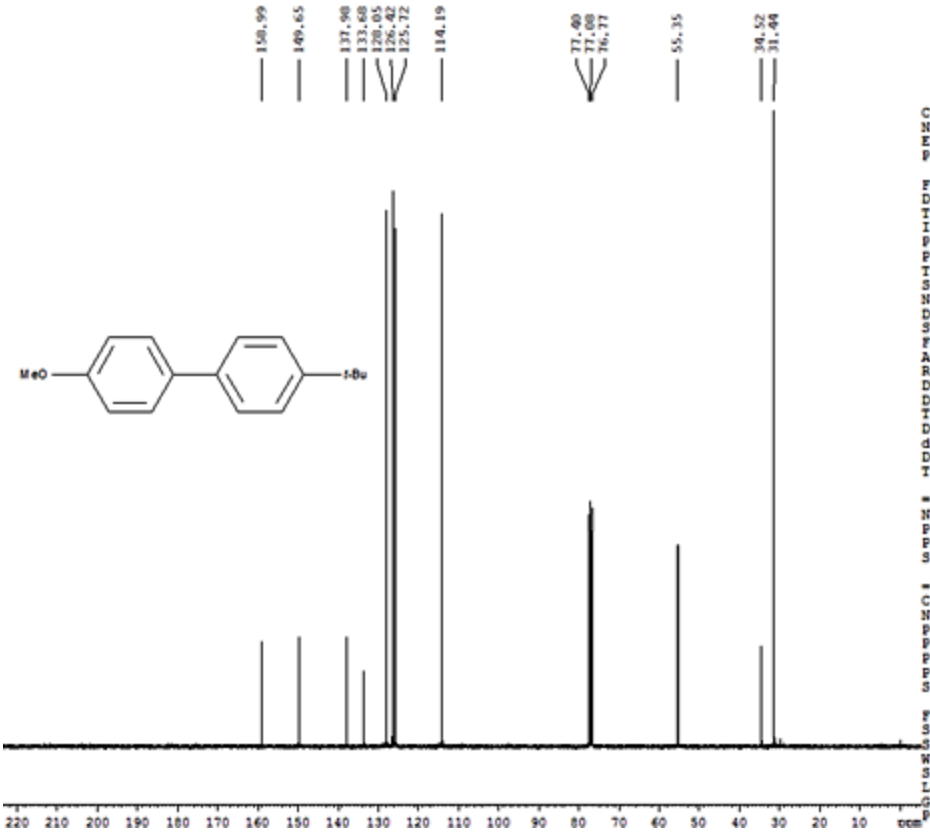
Current Data Parameters	
NAME	Jun02-2014
EXPNO	220
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140602
Time	16.47
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	512
DW	41.600 usec
DE	6.00 usec
TE	296.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300104 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Rj-Spc-26



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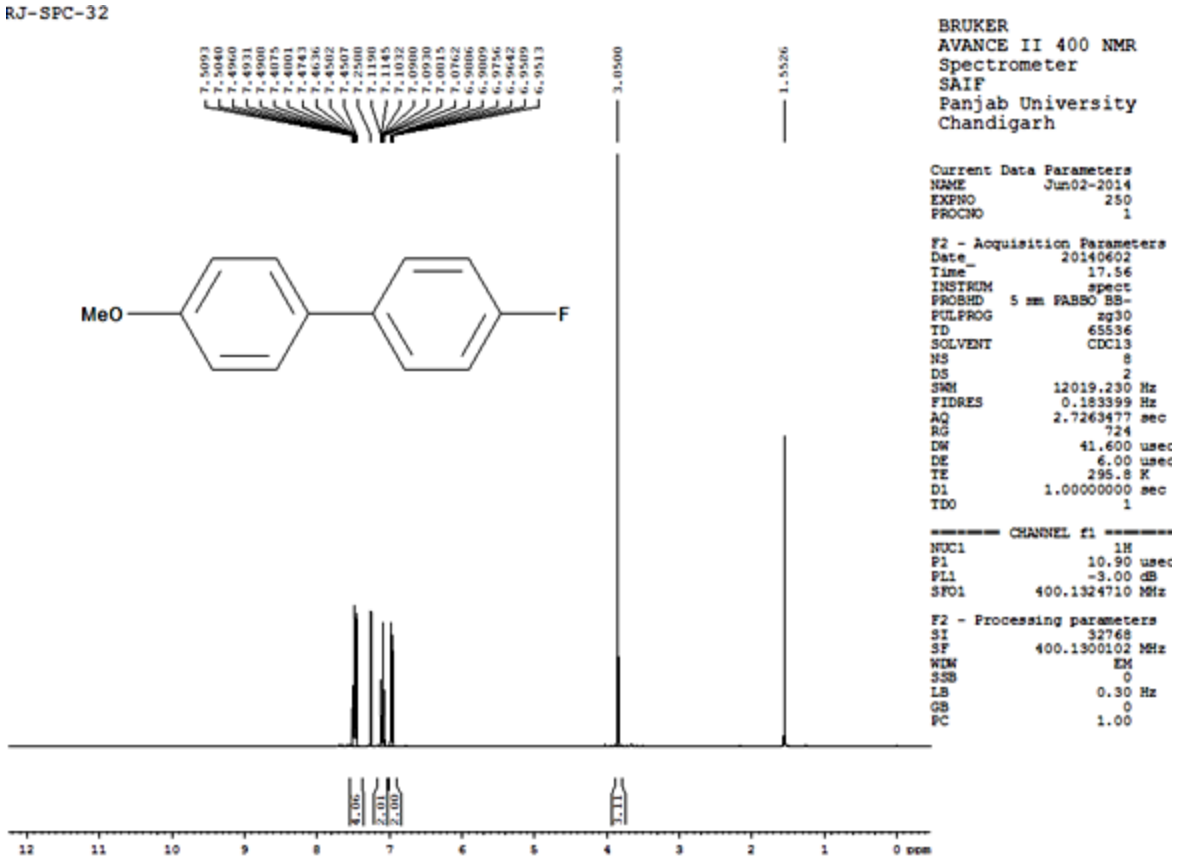
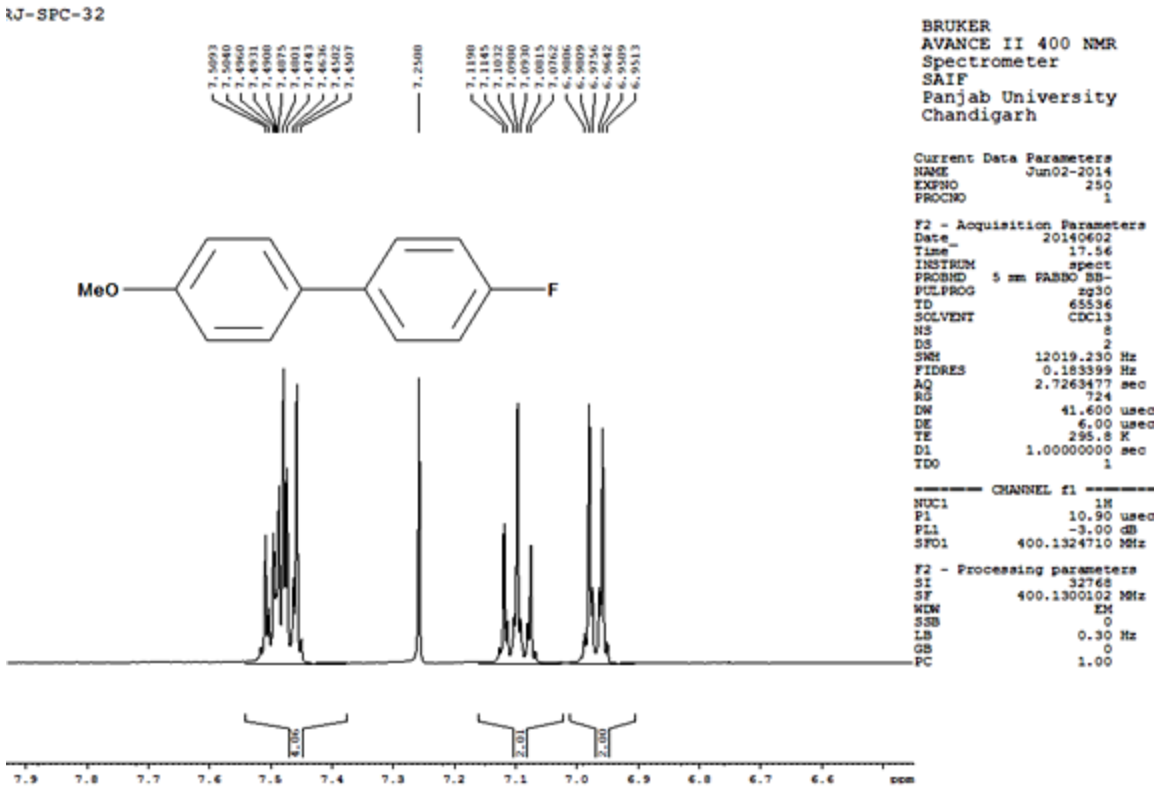
Current Data Parameters	
NAME	Oct28-2014
EXPNO	280
PROCNO	1
F2 - Acquisition Parameters	
Date_	20141028
Time	21.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	1030
DW	16.800 usec
DE	6.00 usec
TE	296.0 K
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

Table 1, Entry 15:





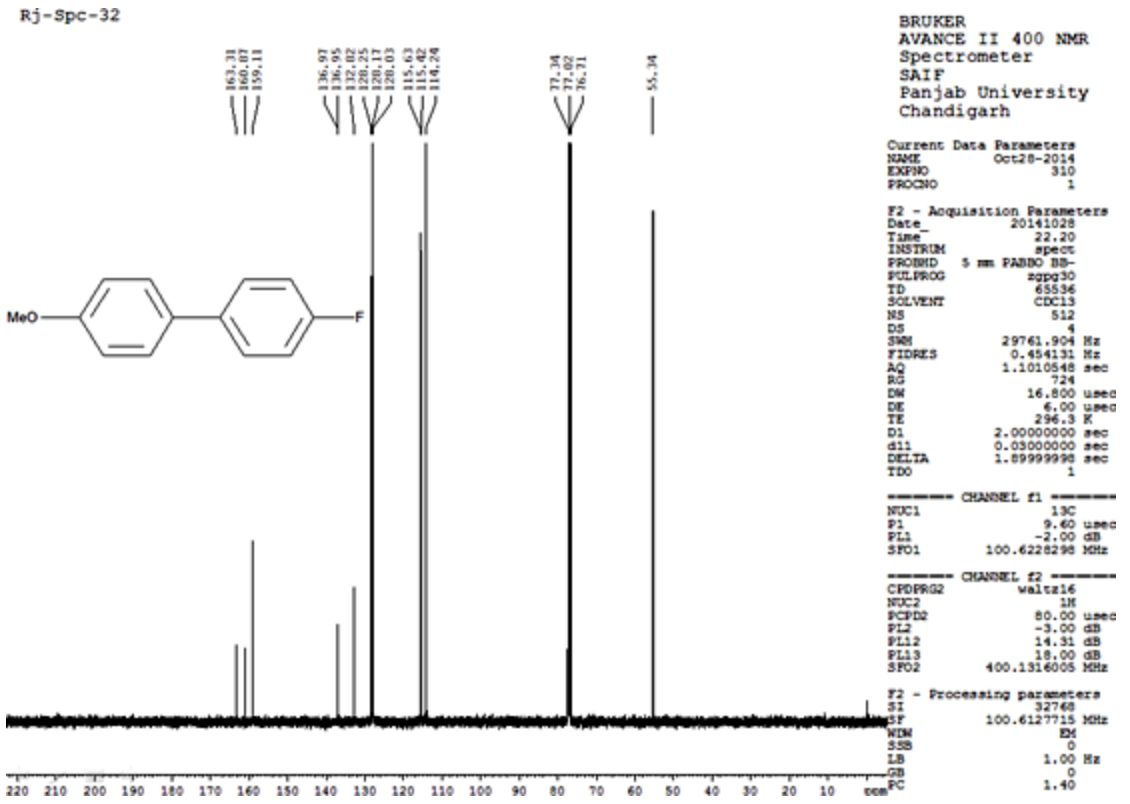
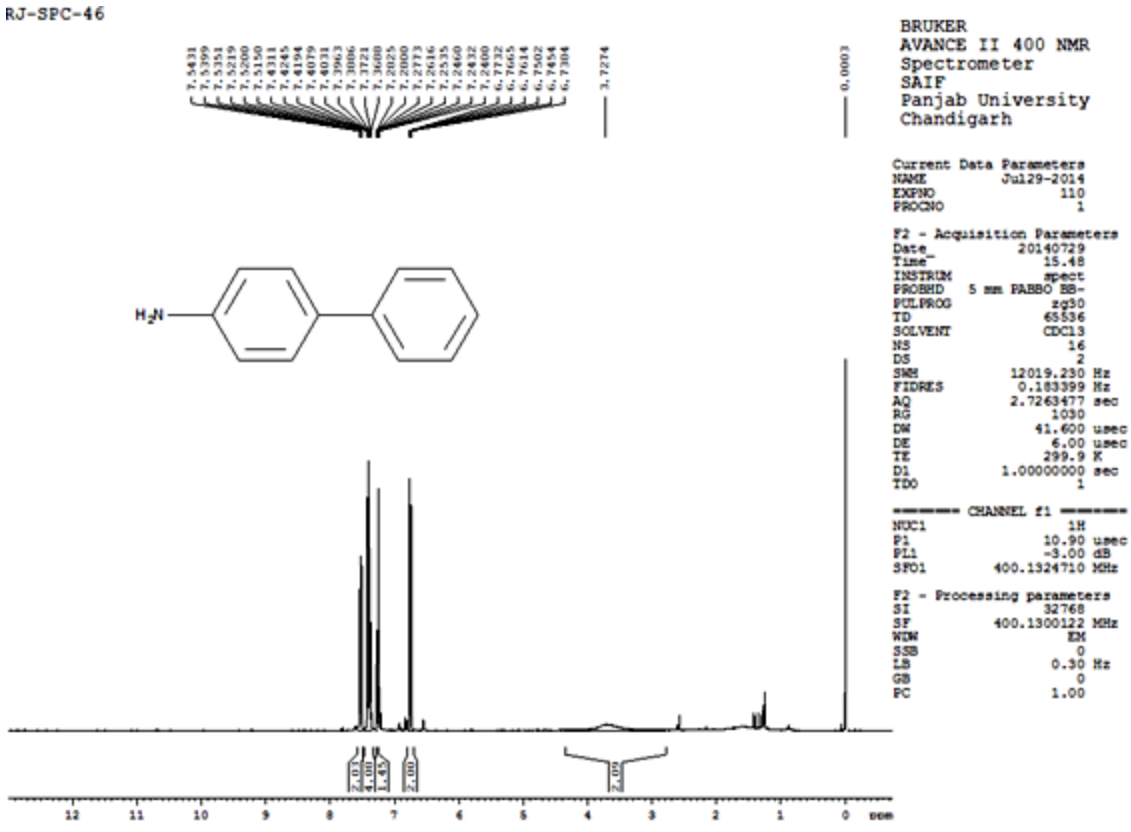
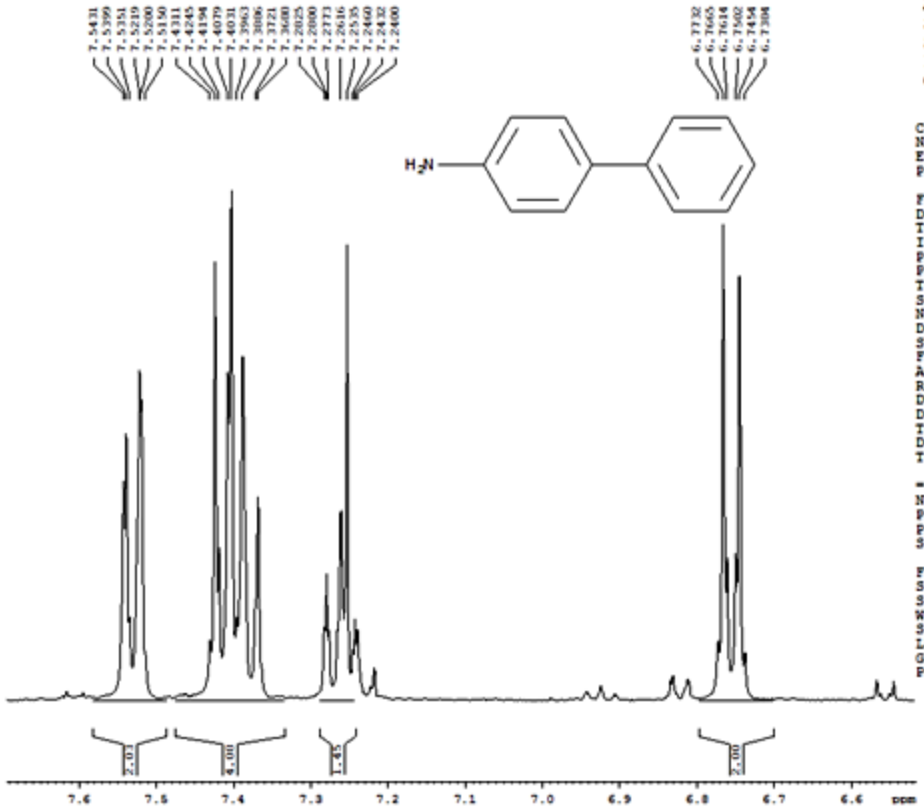


Table 1, Entry 16:



RJ-SPC-46




```
BRUKER
AVANCE II 400 NMR
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Current Data Parameters
NAME                  Jul29-2014
EXPNO                        110
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140729
Time                       15.48
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                   12019.230 Hz
FIDRES                0.183399 Hz
AQ                    2.7263477 sec
RG                         1030
DW                       41.600 usec
DE                        6.00 usec
TE                       299.9 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                  400.1300122 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```
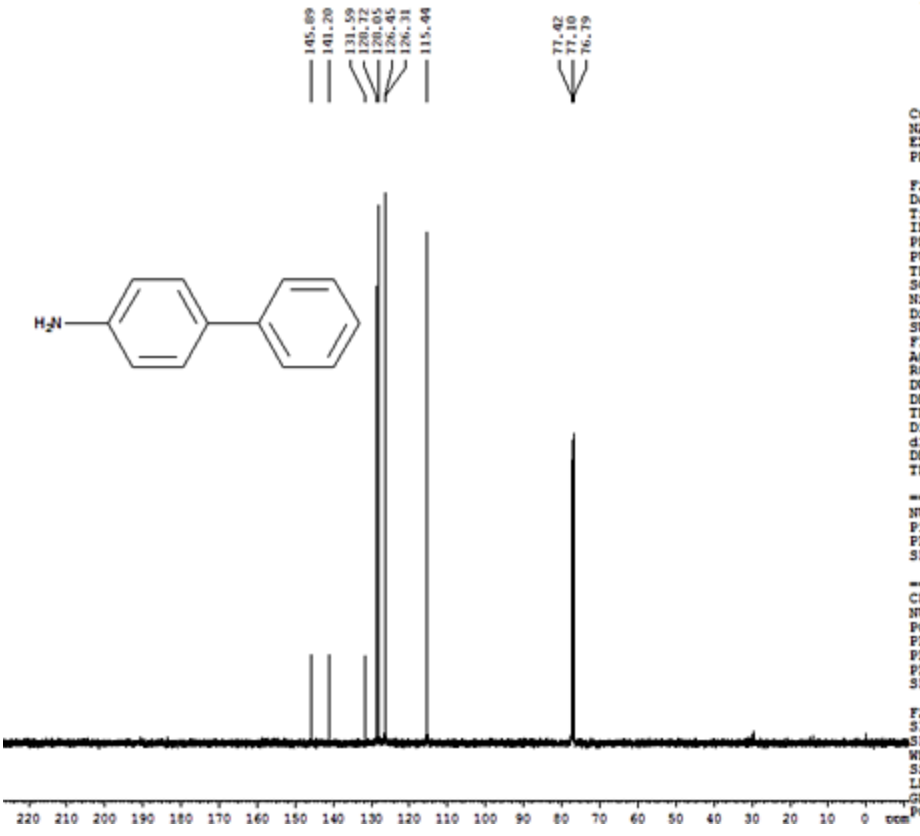

Rj-Spc-46




```
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Current Data Parameters
NAME                  Oct28-2014
EXPNO                        370
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20141029
Time                        9.40
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                           219
DS                             4
SWH                   29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010548 sec
RG                           724
DW                       16.800 usec
DE                        6.00 usec
TE                       294.9 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
```
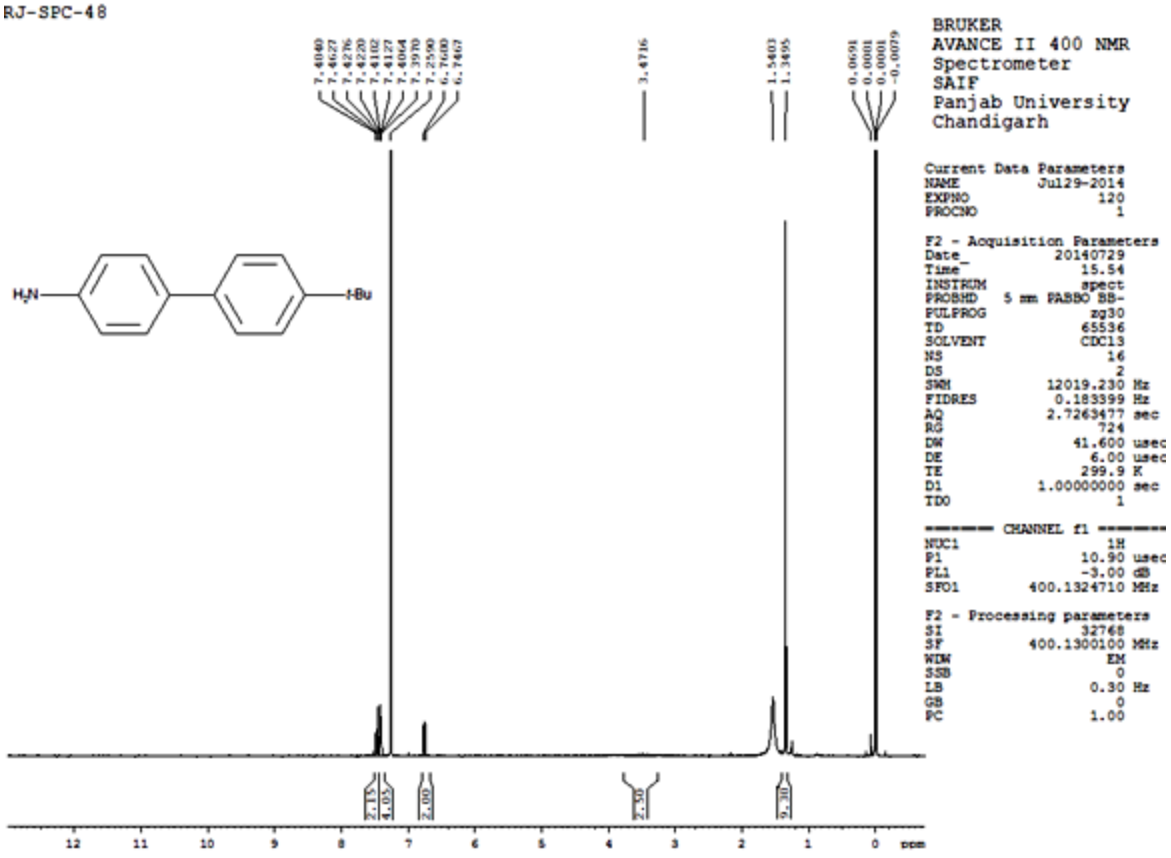
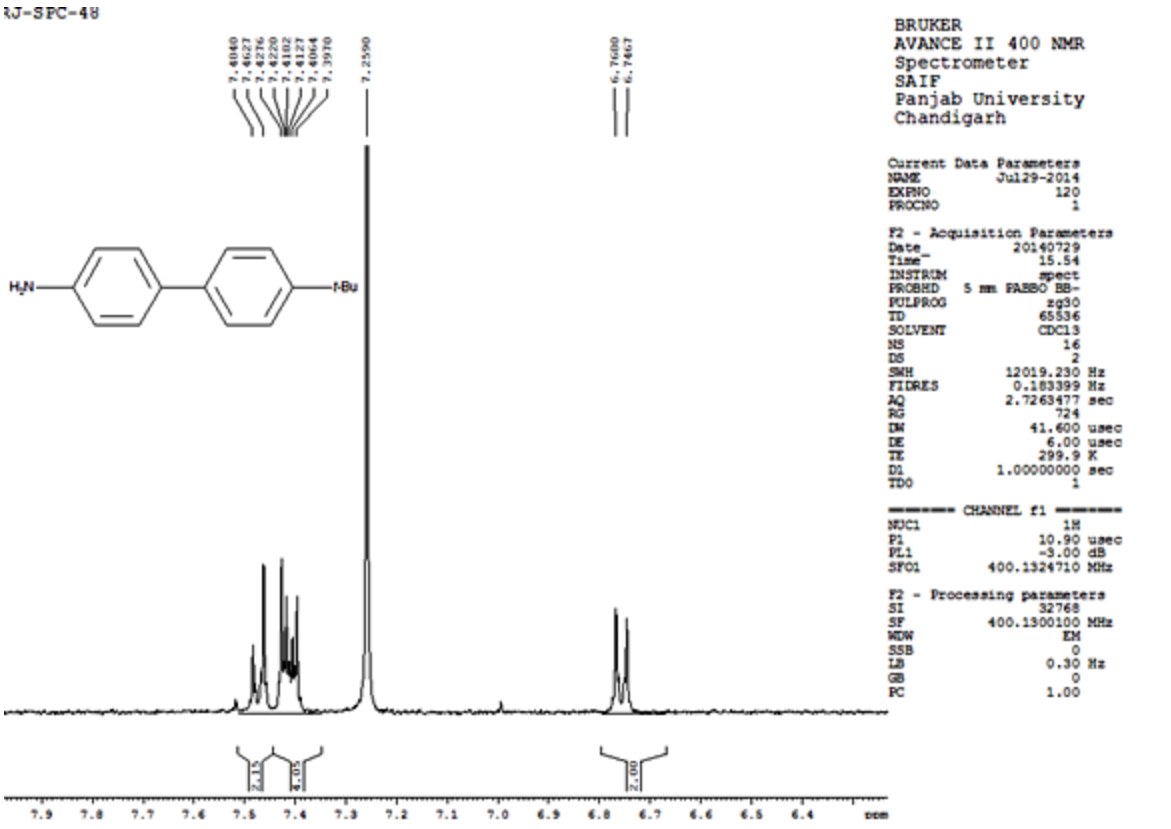

Table 1, Entry17:





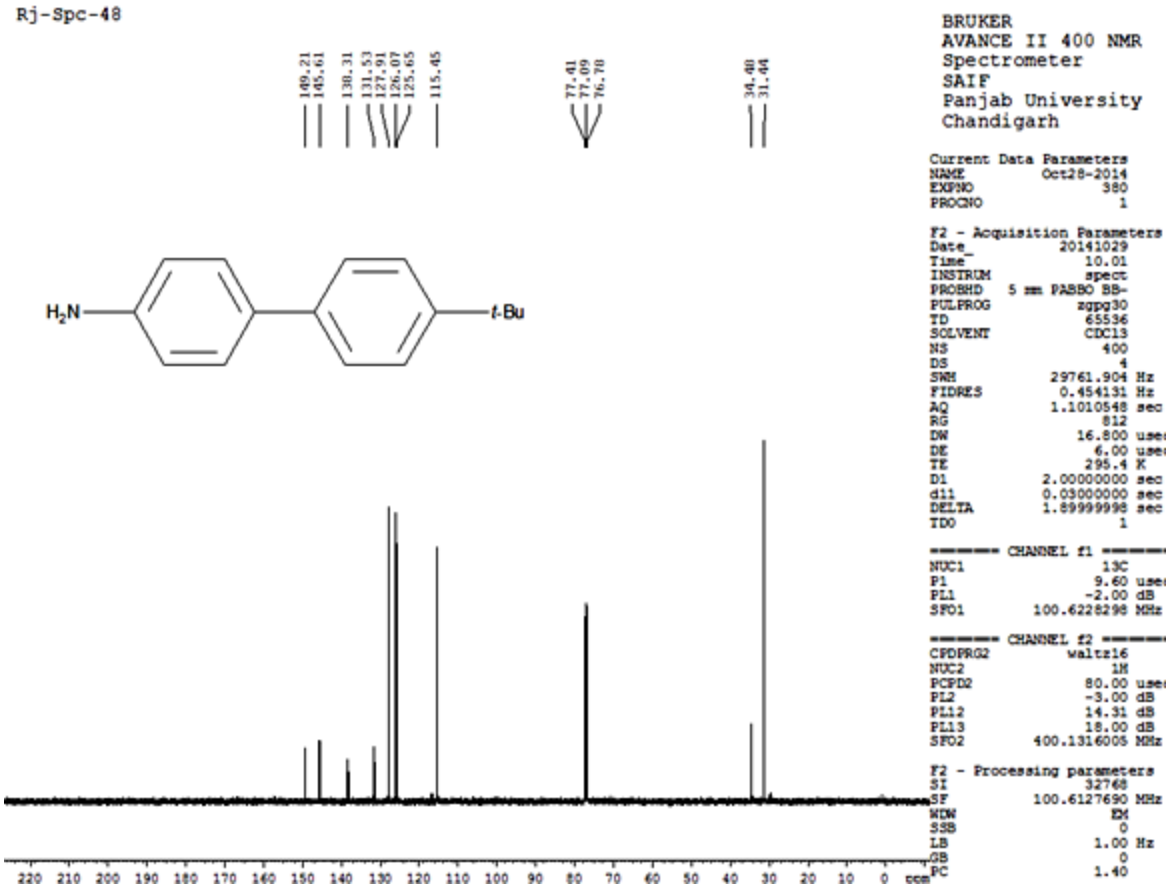
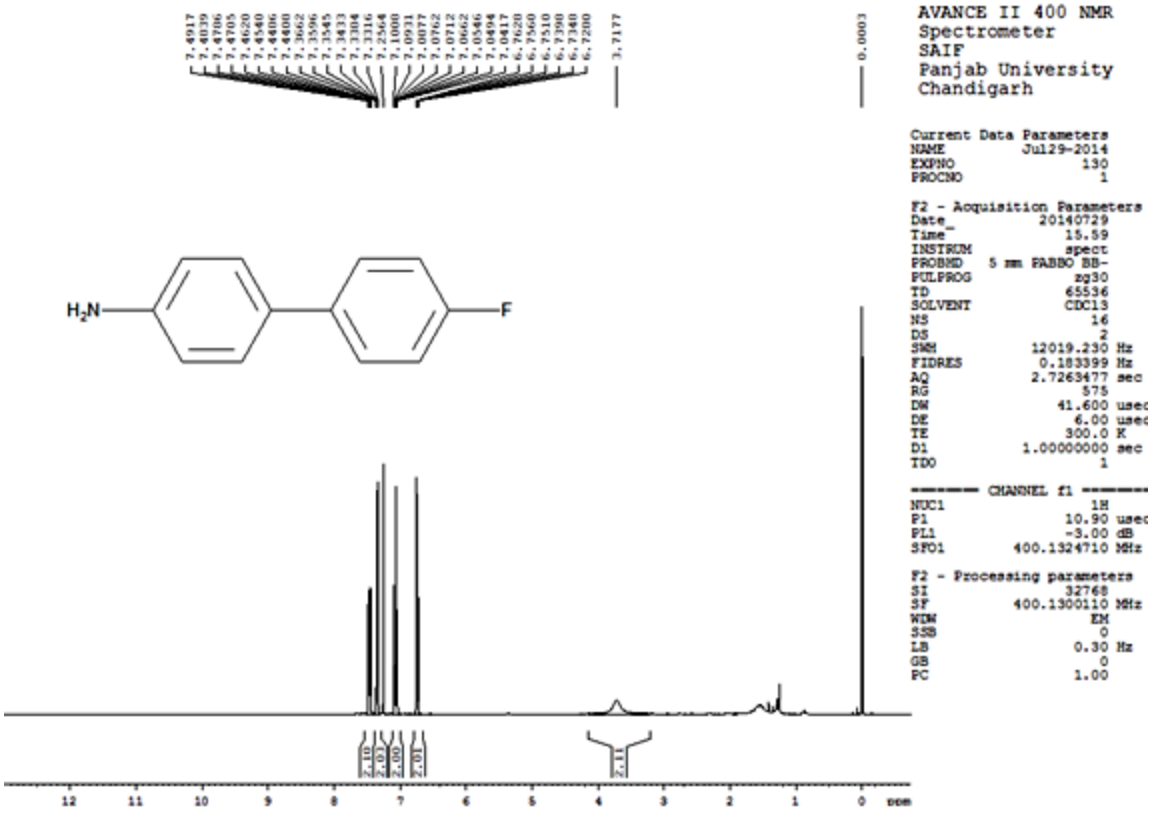
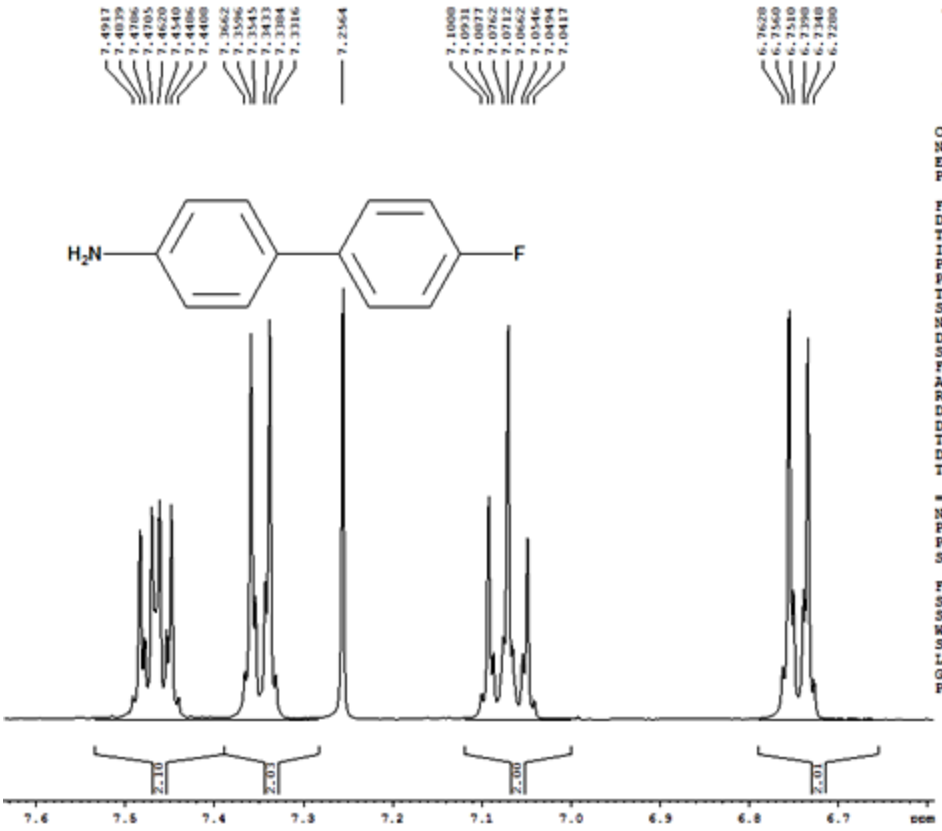


Table 1, Entry 18:



RJ-SPC-50



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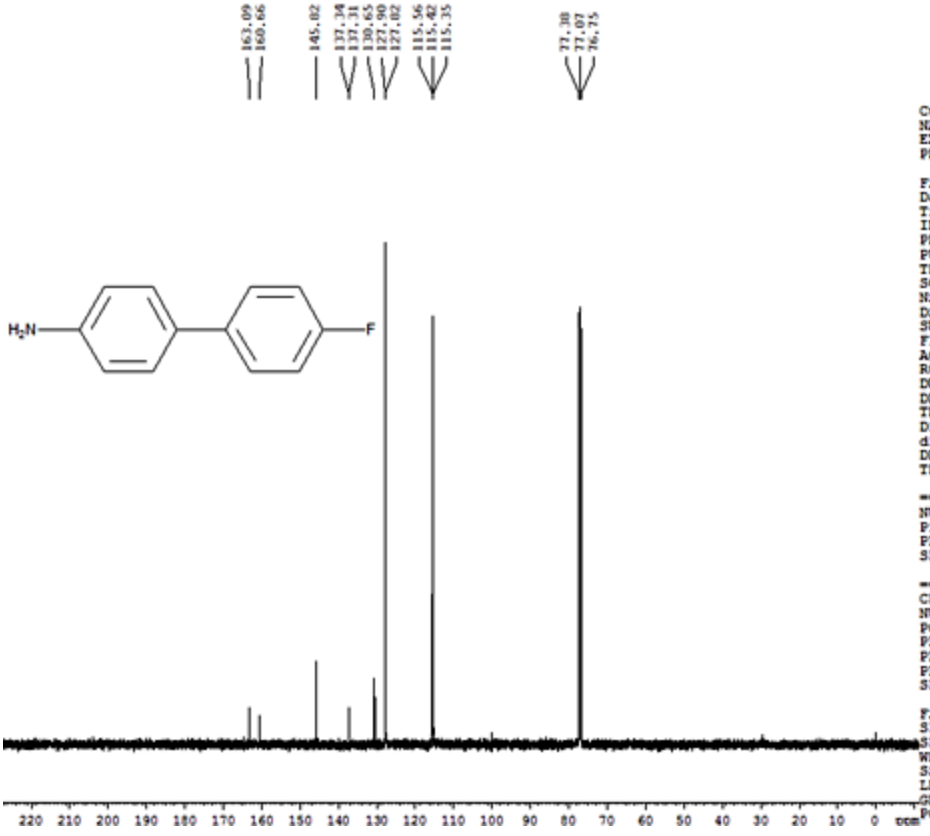
Current Data Parameters	
NAME	Jul29-2014
EXPNO	130
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140729
Time	15.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	575
DW	41.600 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.90 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz
F2 - Processing parameters	
SI	32768
SF	400.1300110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Rj-Spc-50



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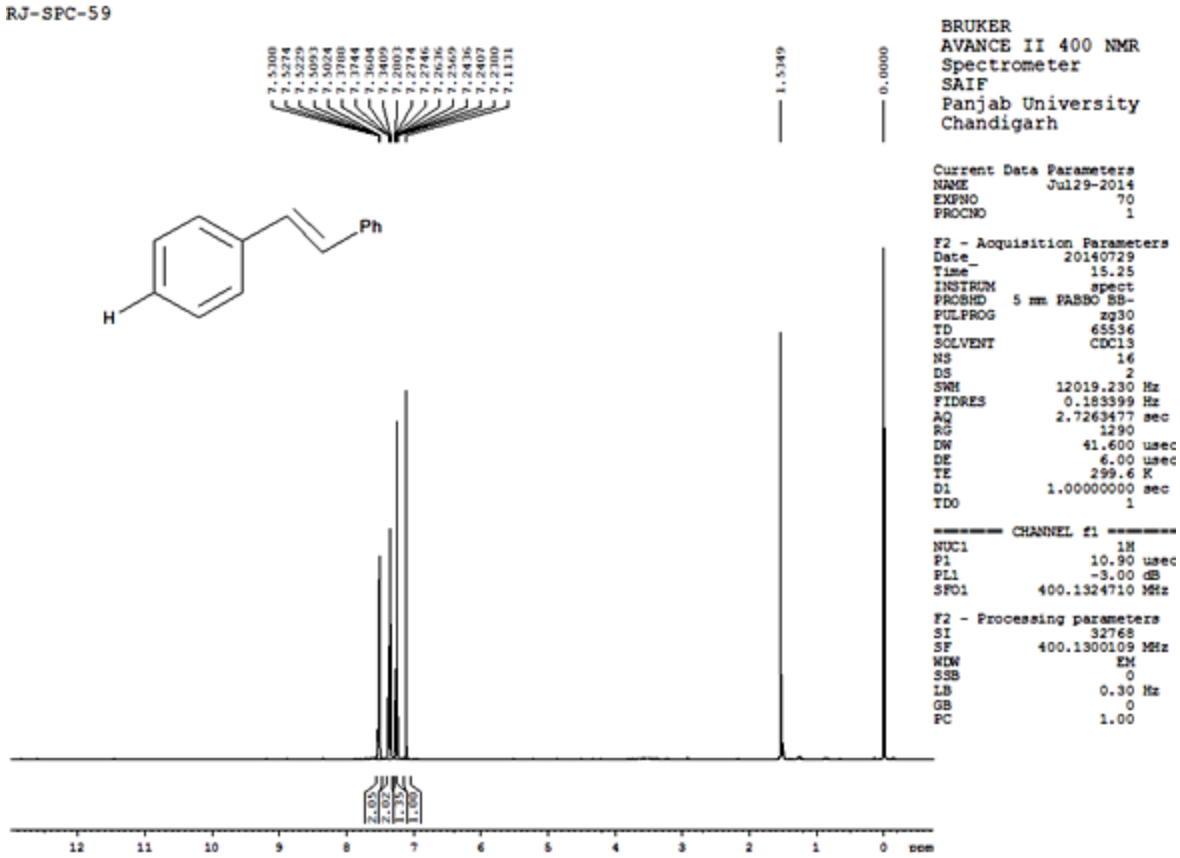
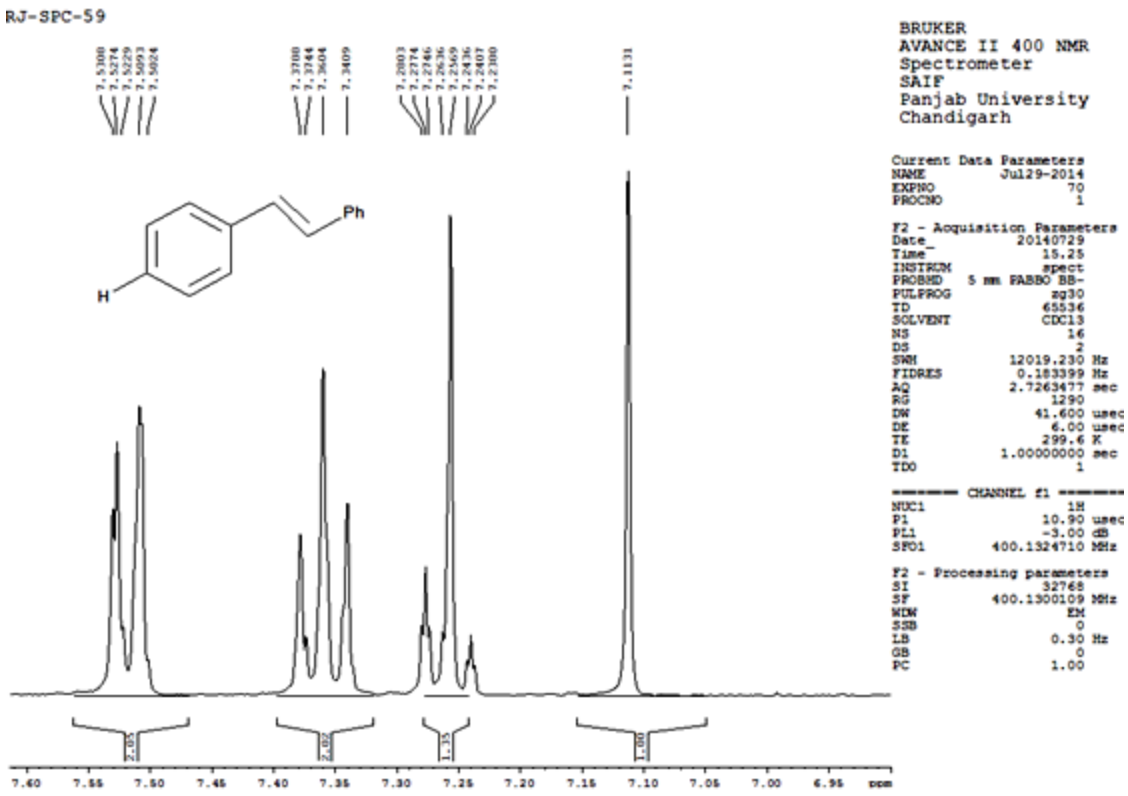
Current Data Parameters	
NAME	Oct28-2014
EXPNO	390
PROCNO	1
F2 - Acquisition Parameters	
Date_	20141029
Time	2.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	400
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	36
DW	16.800 usec
DE	6.00 usec
TE	294.8 K
D1	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

Table 2, Entry 1:





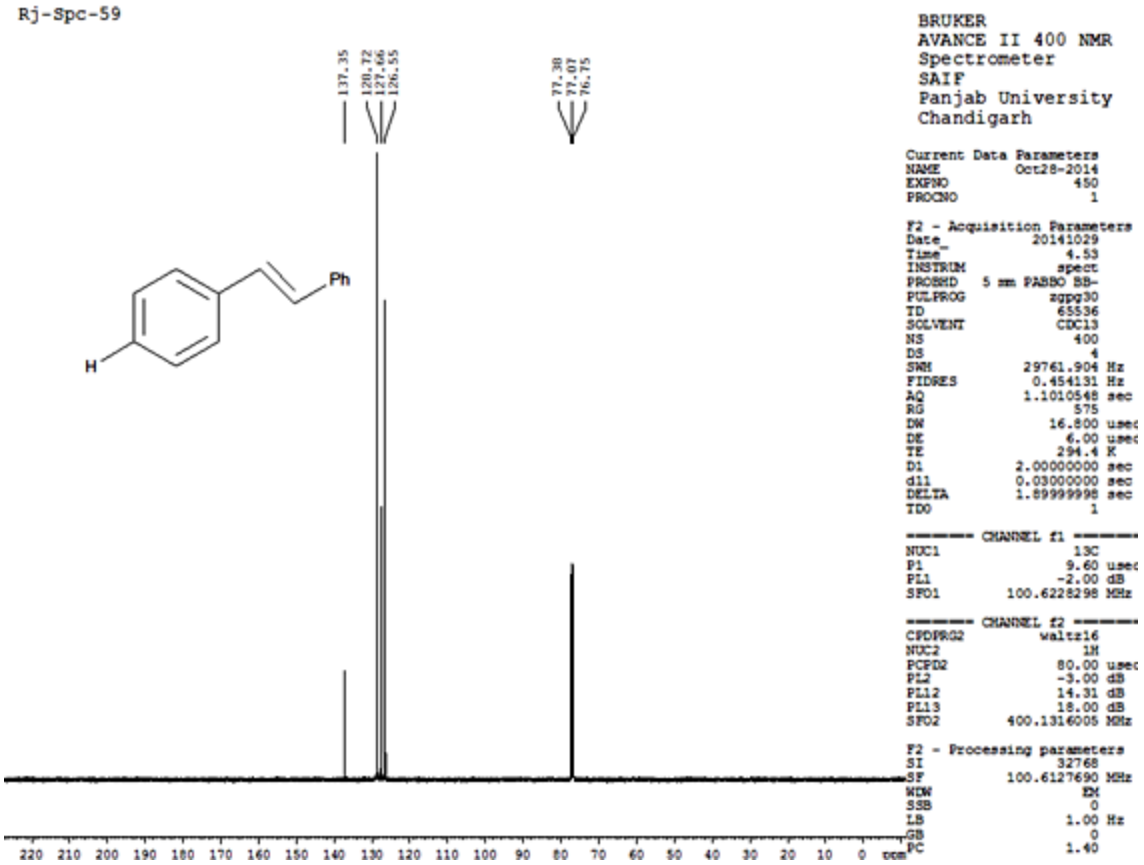
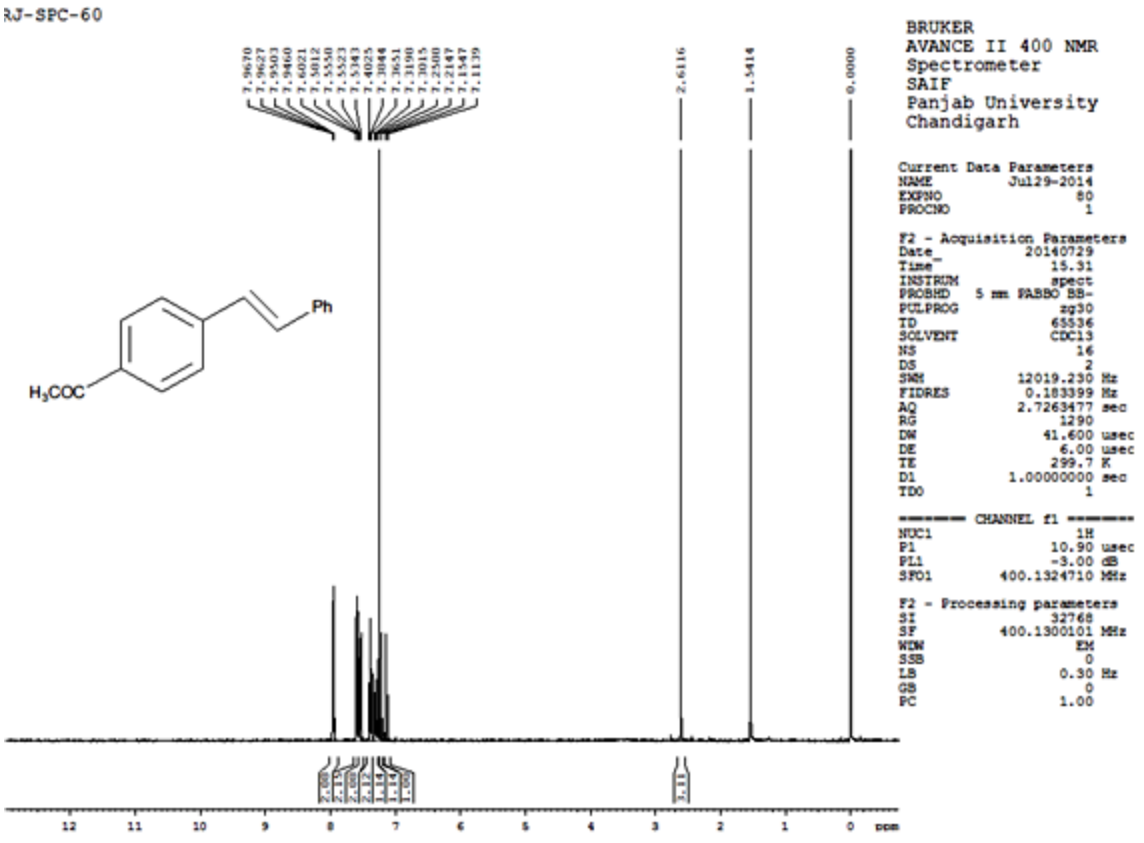
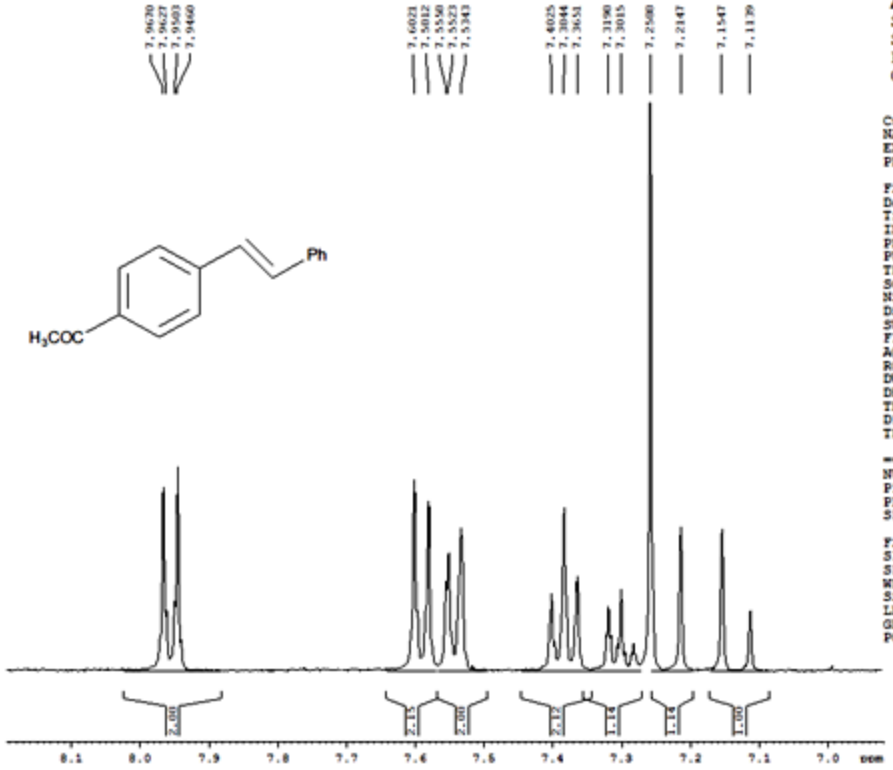


Table 2, Entry2:



RJ-SPC-60

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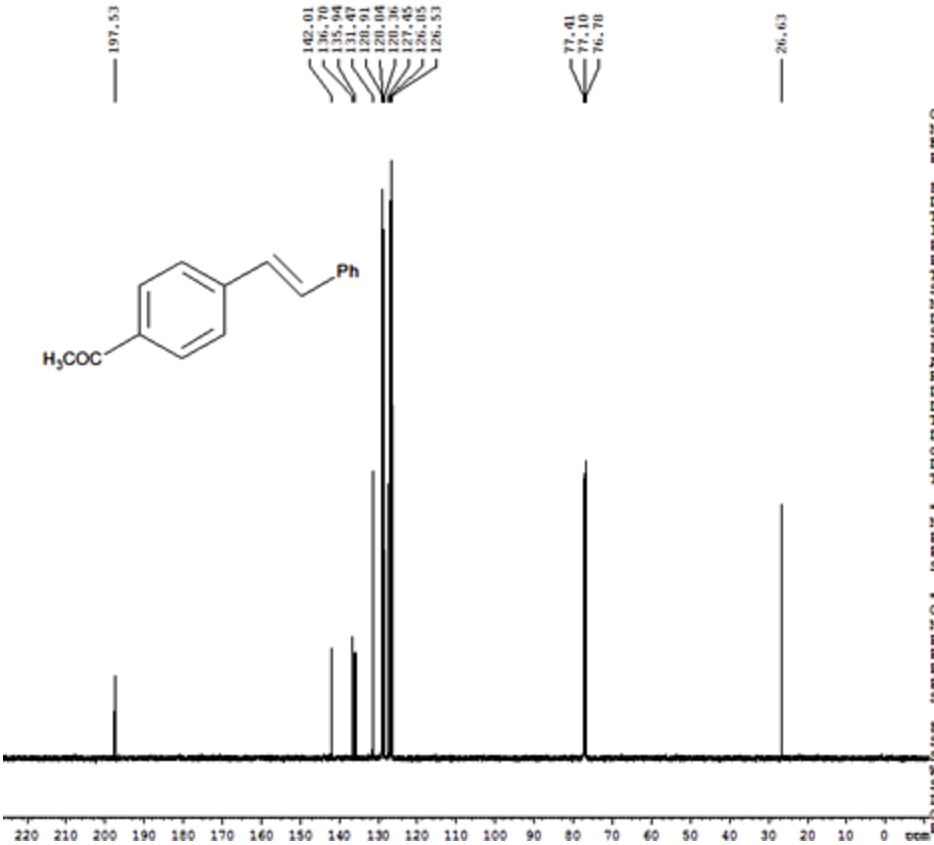
Current Data Parameters
NAME          Jul29-2014
EXPNO                 80
PROCNO                 1

F2 - Acquisition Parameters
Date_          20140729
Time              15.31
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          12019.230 Hz
FIDRES        0.183399 Hz
AQ            2.7263477 sec
RG                1290
DW              41.600 usec
DE               6.00 usec
TE              299.7 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          400.1300101 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

Rj-Spc-60

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Current Data Parameters
NAME          Oct28-2014
EXPNO                460
PROCNO                 1

F2 - Acquisition Parameters
Date_          20141029
Time               5.19
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 400
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG                 724
DW              16.800 usec
DE               6.00 usec
TE              294.3 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
```
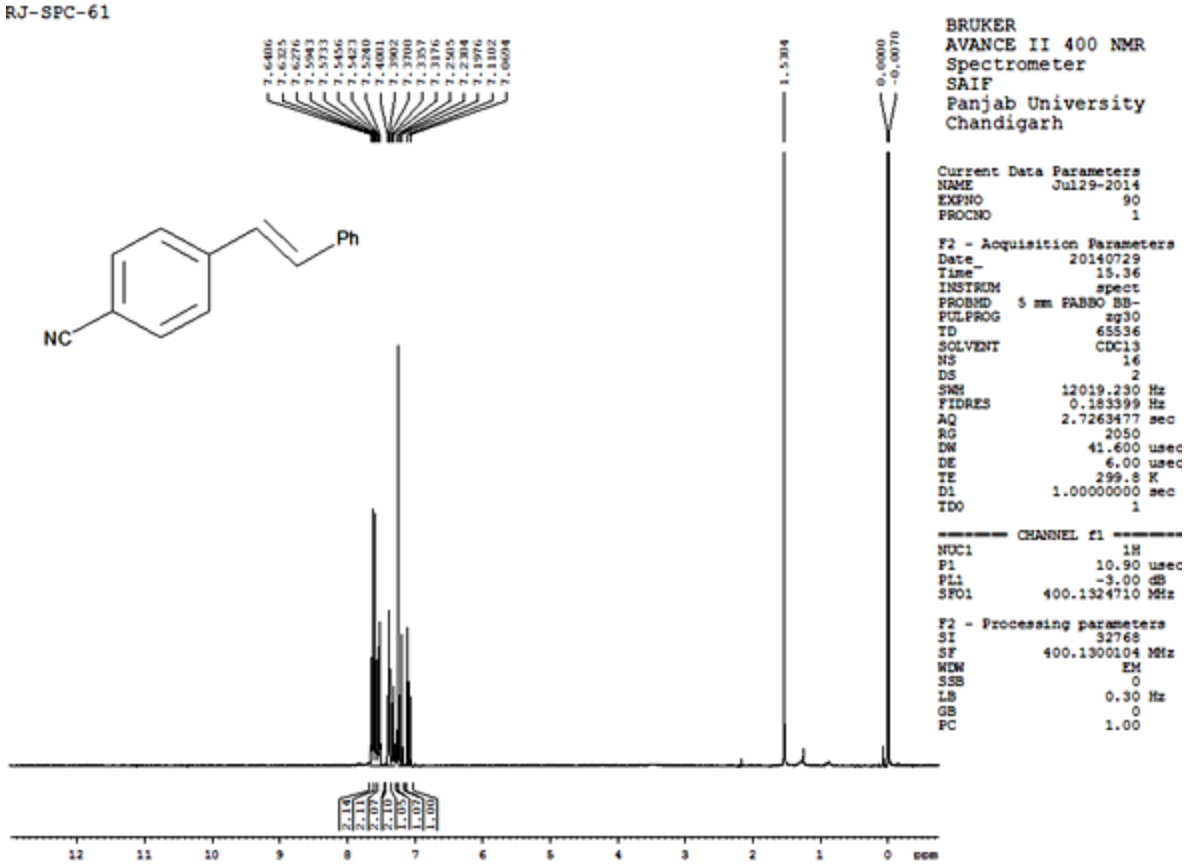
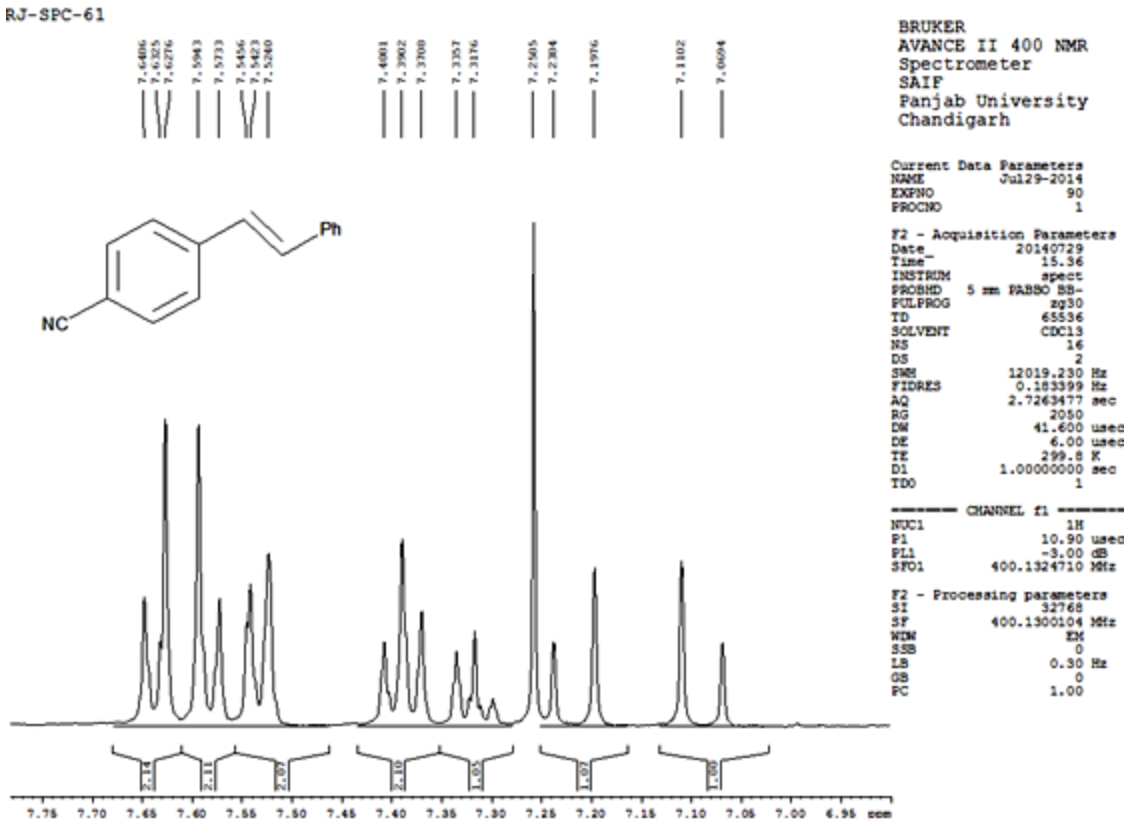

Table 2, Entry3:





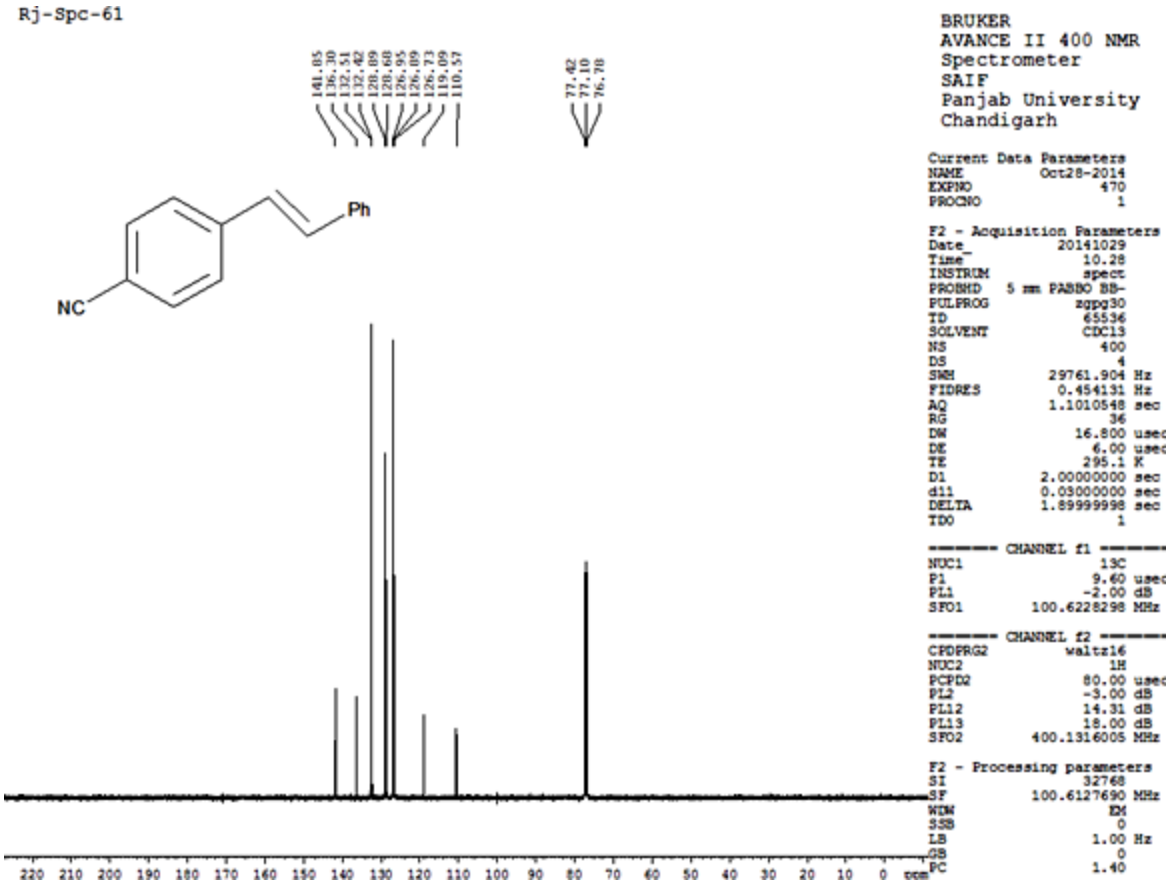
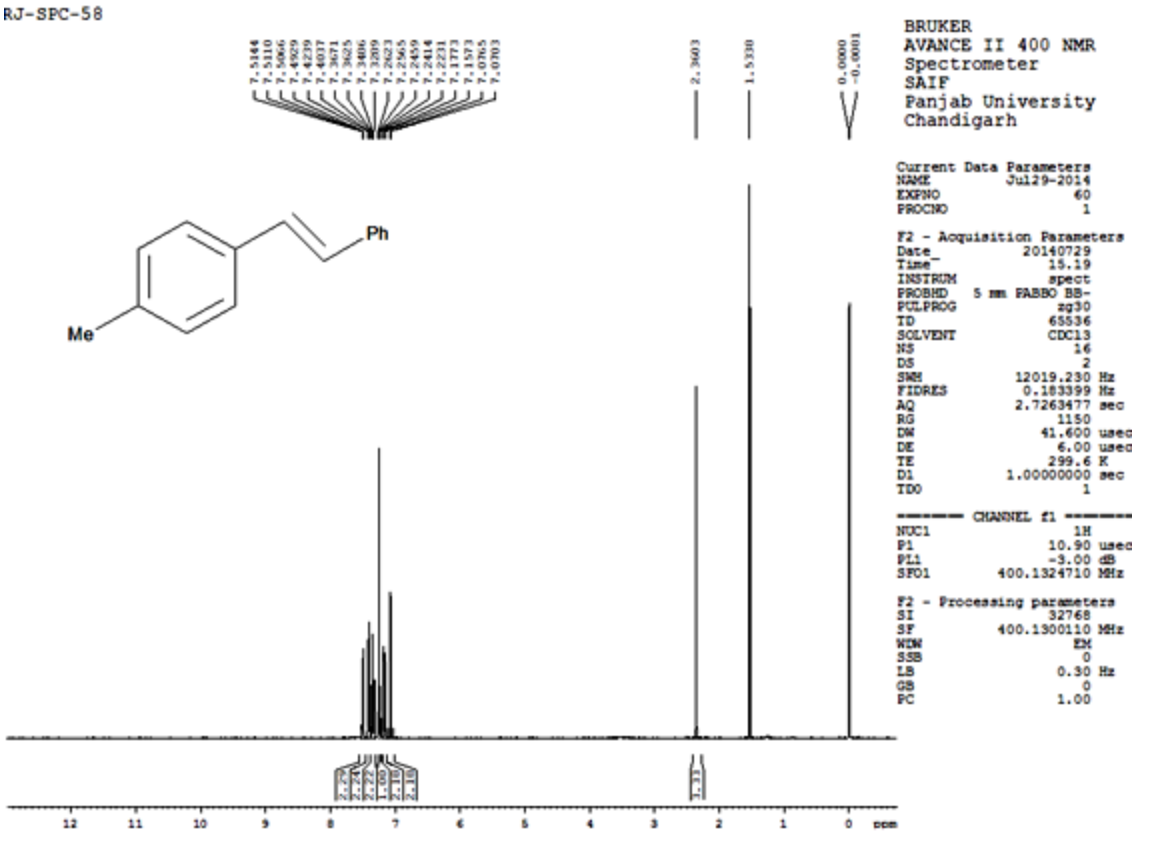
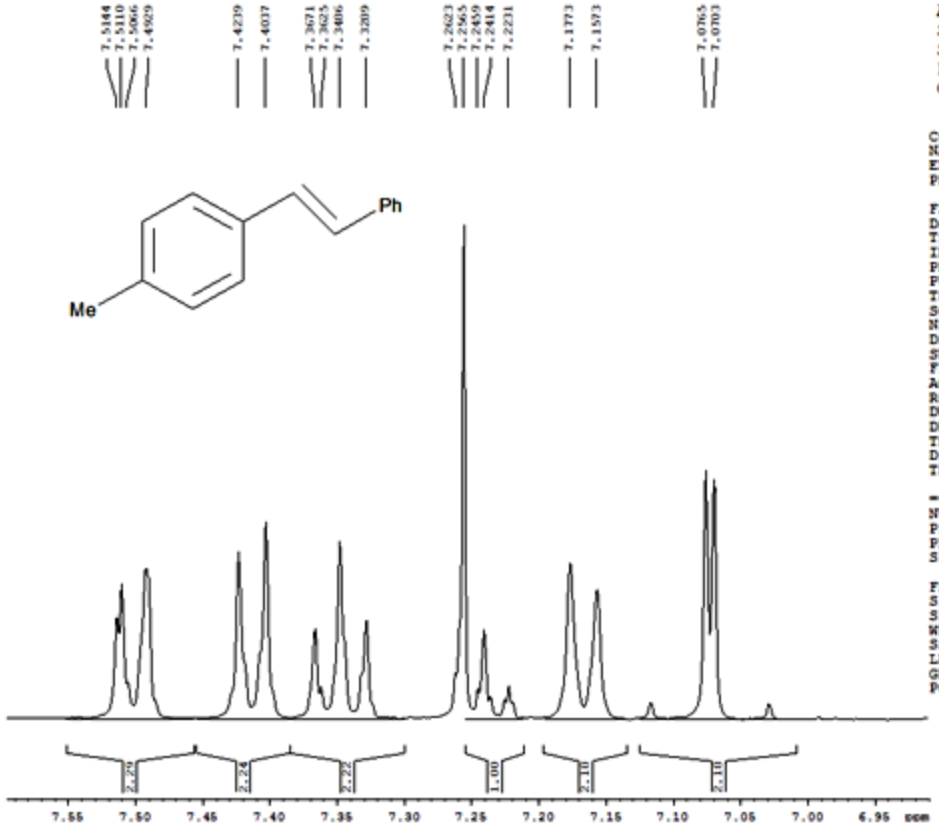


Table 2, Entry 4:



RJ-SPC-58



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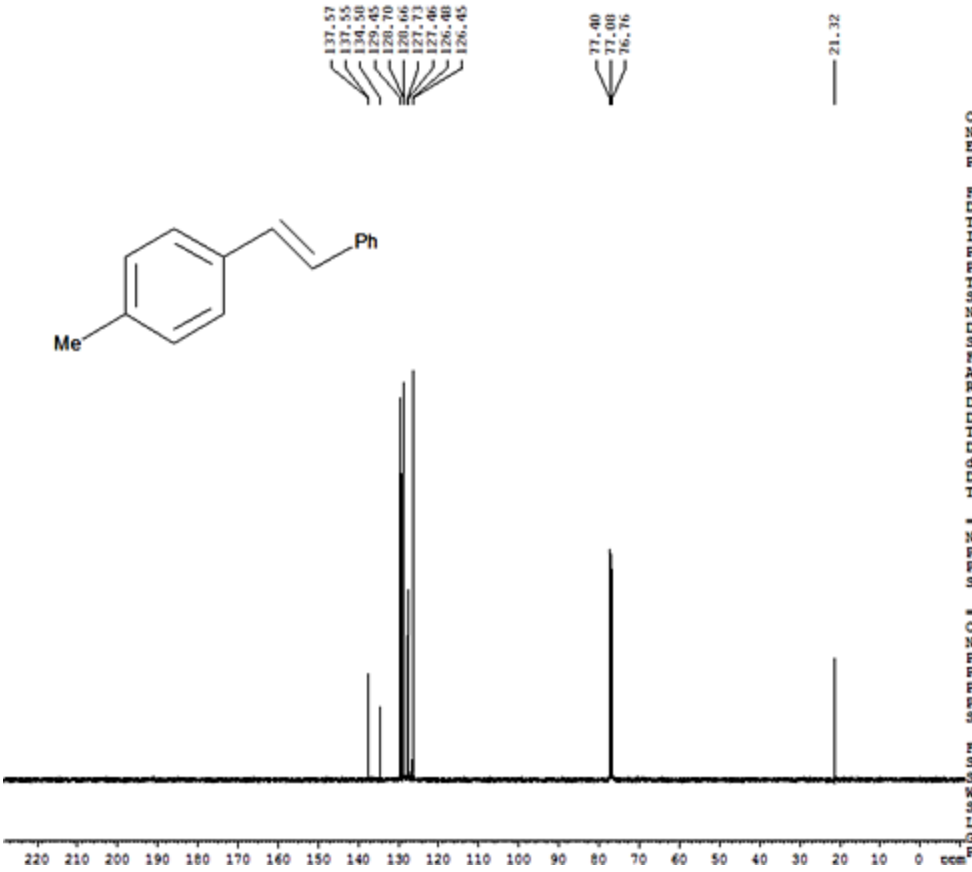
Current Data Parameters	
NAME	Jul29-2014
EXPNO	60
PROCNO	1
F2 - Acquisition Parameters	
Date_	20140729
Time	15.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	12019.230 Hz
FIDRES	0.183399 Hz
AQ	2.7263477 sec
RG	1150
DW	41.600 usec
DE	6.00 usec
TE	299.6 K
D1	1.00000000 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	400.1300110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Rj-Spc-58



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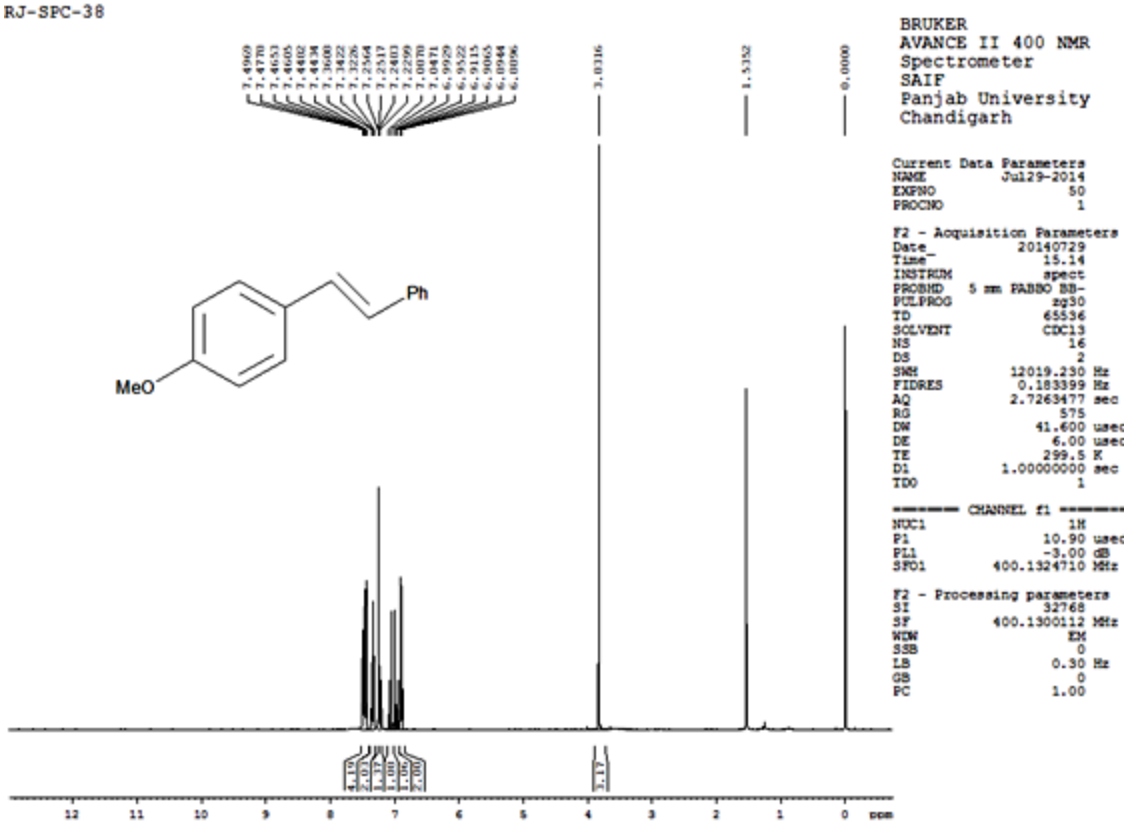
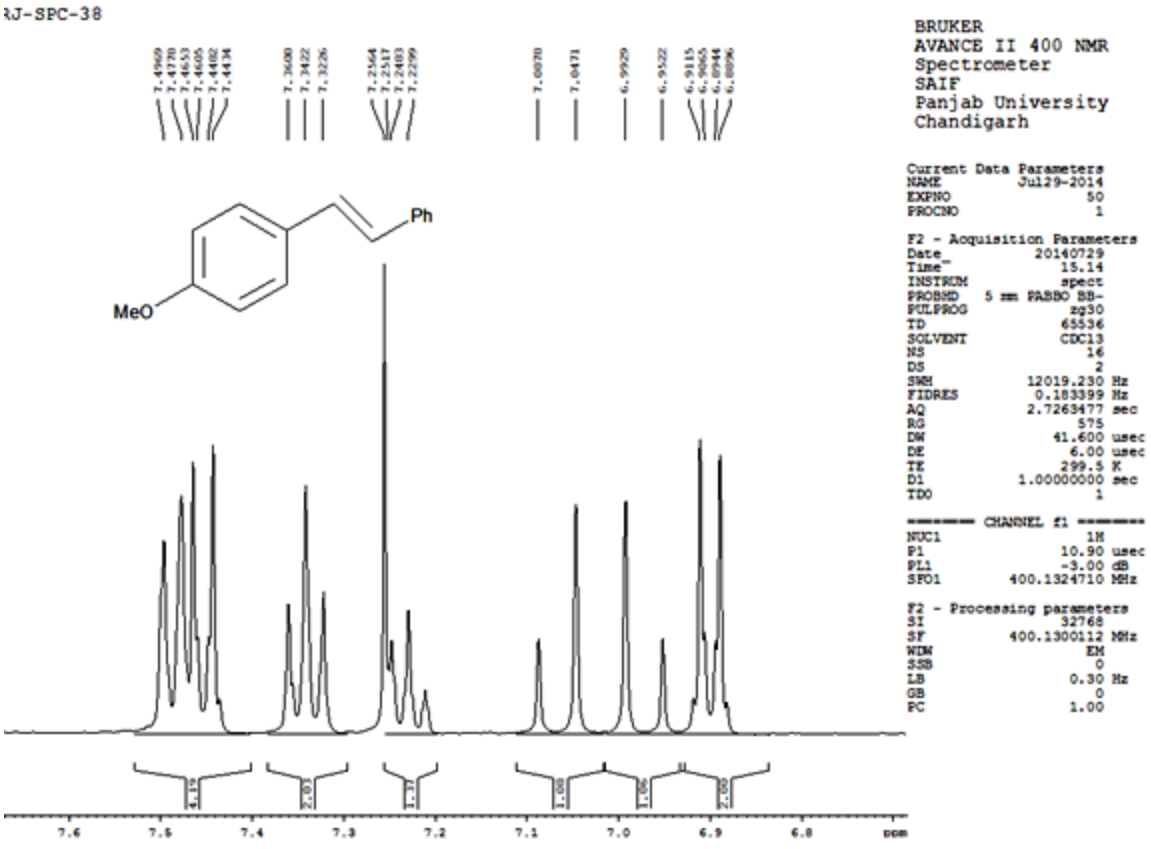
Current Data Parameters	
NAME	Oct28-2014
EXPNO	440
PROCNO	1
F2 - Acquisition Parameters	
Date_	20141029
Time	4.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	400
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	575
DW	16.800 use
DE	6.00 use
TE	294.4 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
====== CHANNEL f1 ======	
NUC1	13C
P1	9.60 use
PL1	-2.00 dB
SFO1	100.6228298 MHz
====== CHANNEL f2 ======	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 use
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

Table 2, Entry 5:





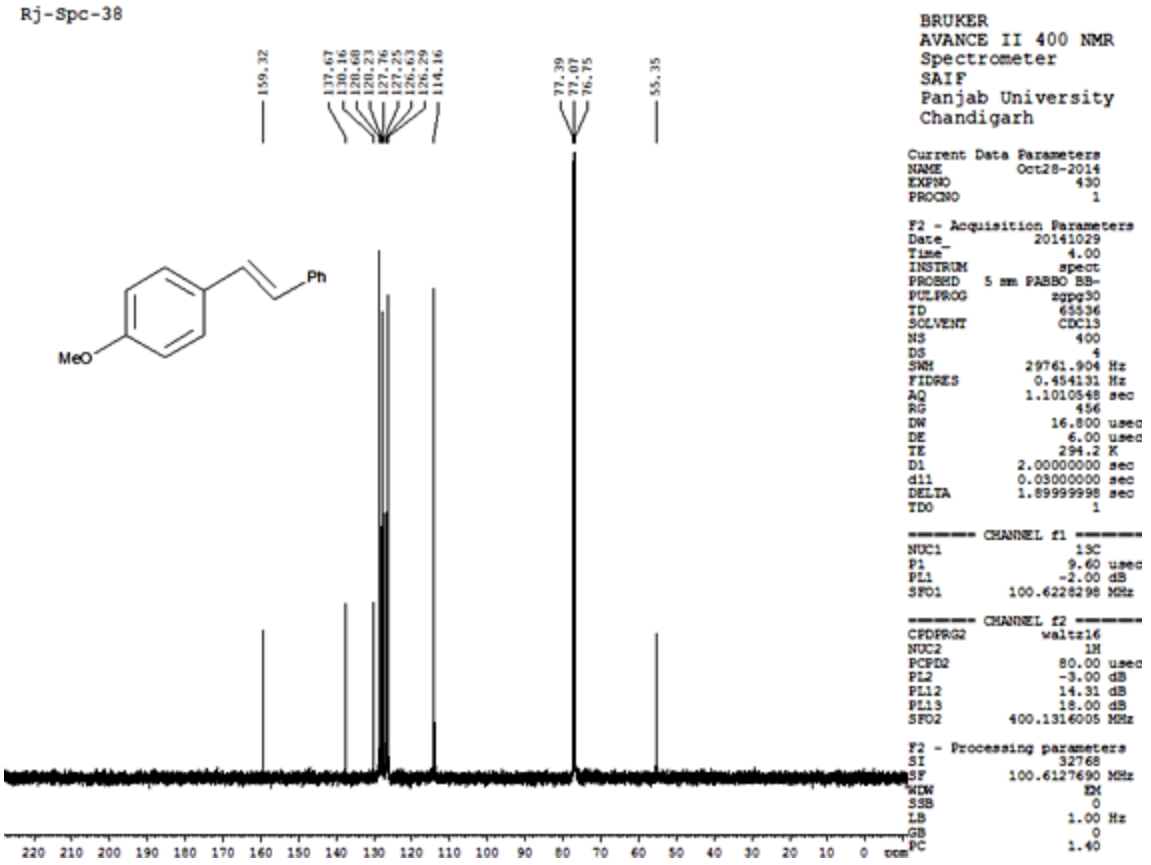
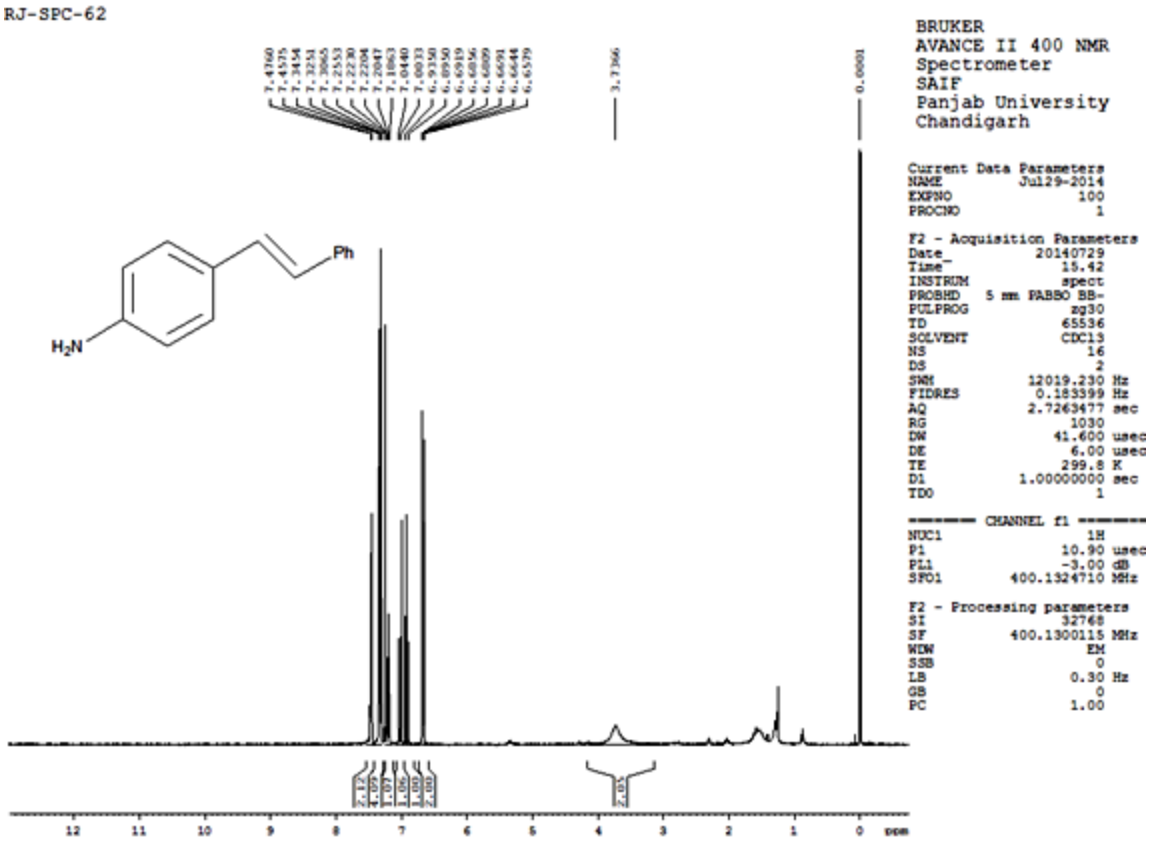
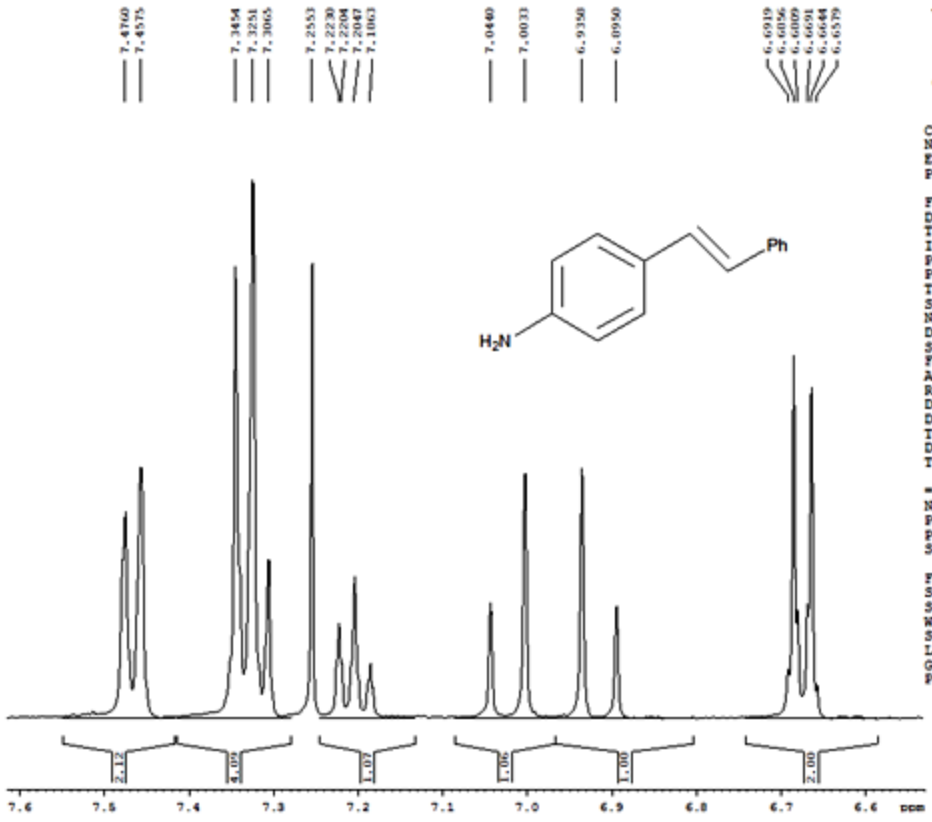


Table 2, Entry 6:



RJ-SPC-62



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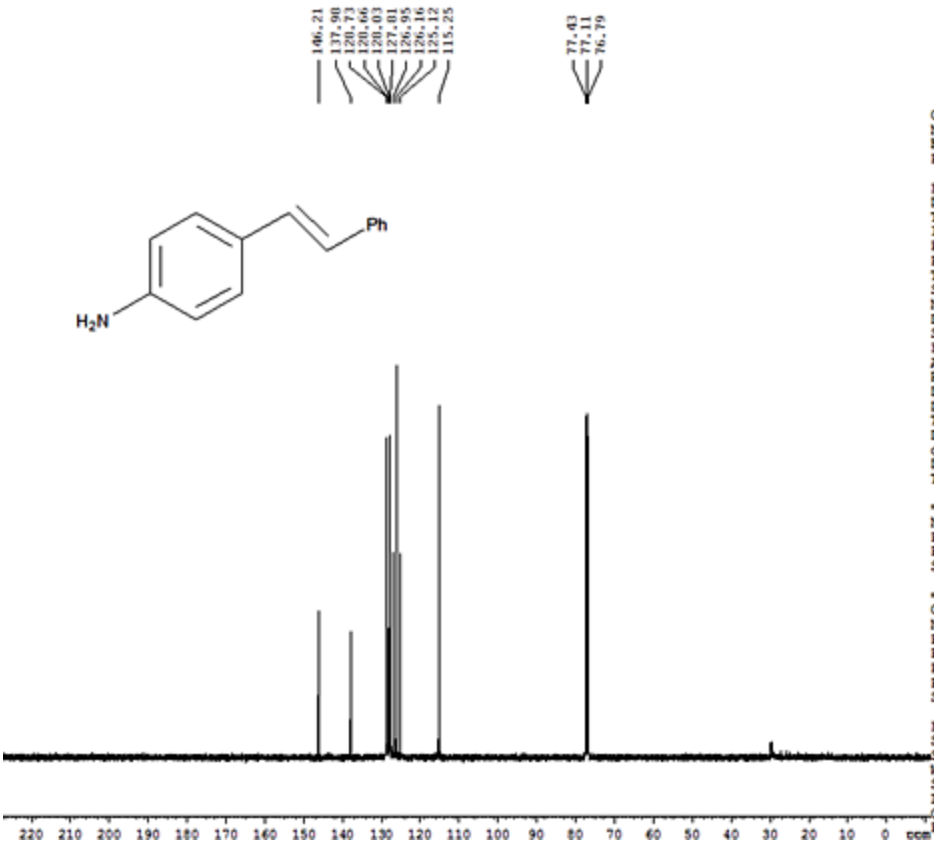
Current Data Parameters
NAME Jul29-2014
EXPNO 100
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140729
Time 15.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 1030
DW 41.600 usec
DE 6.00 usec
TE 299.8 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 400.1300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Rj-Spc-62



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Current Data Parameters
NAME Oct28-2014
EXPNO 480
PROCNO 1

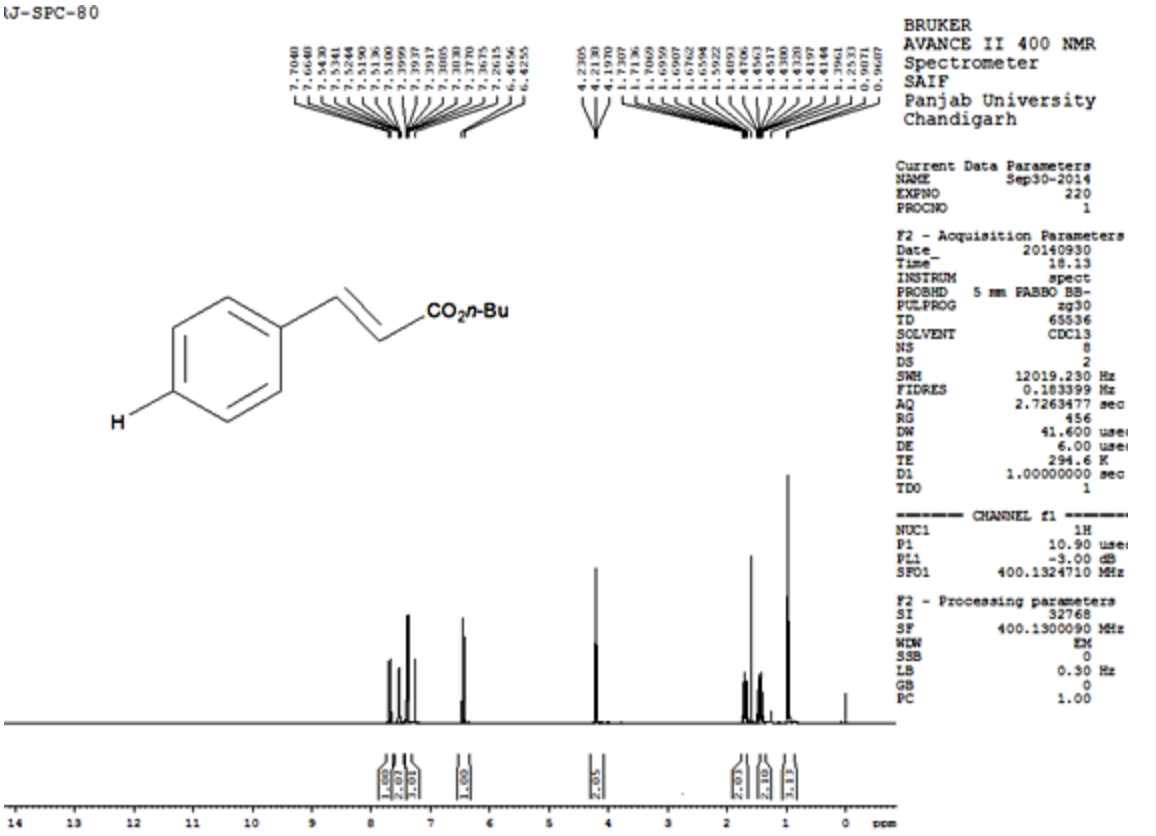
F2 - Acquisition Parameters
Date_ 20141029
Time 6.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 912
DW 16.800 usec
DE 6.00 usec
TE 293.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

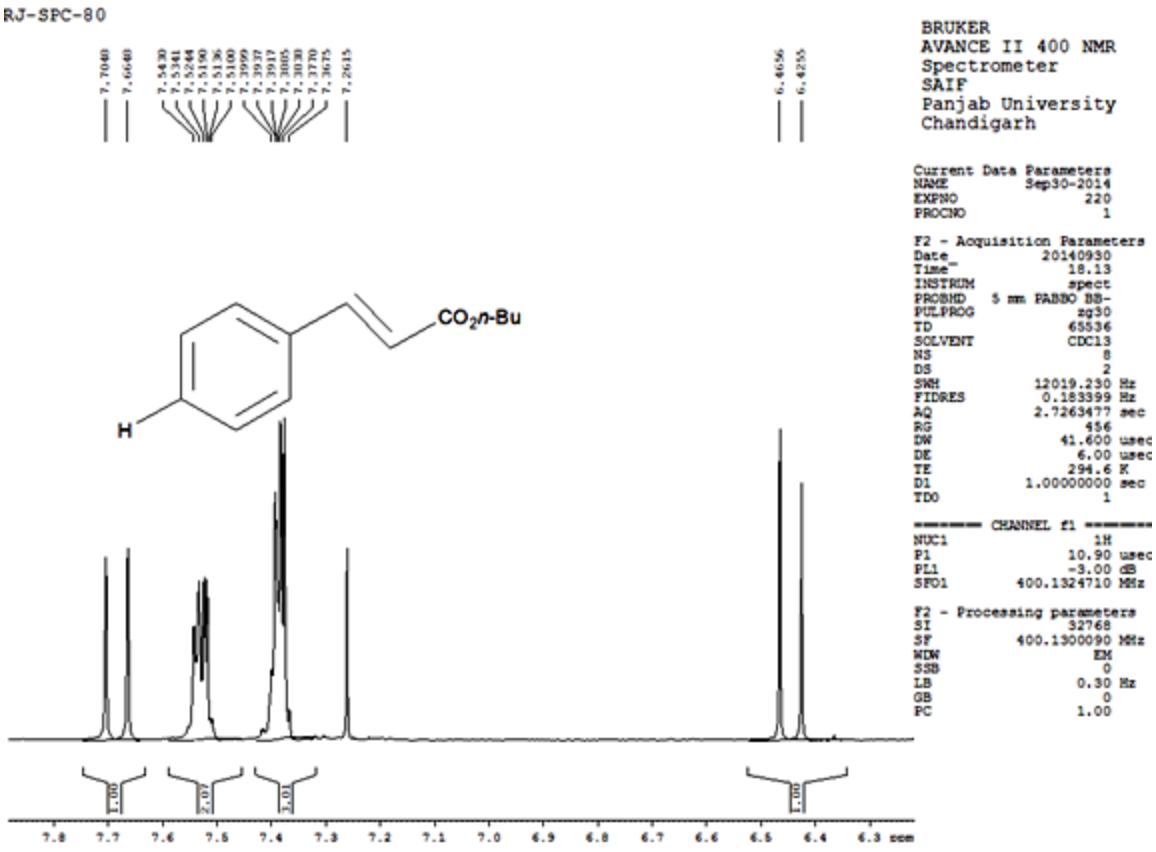
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz

======== 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

Table 2, Entry7:





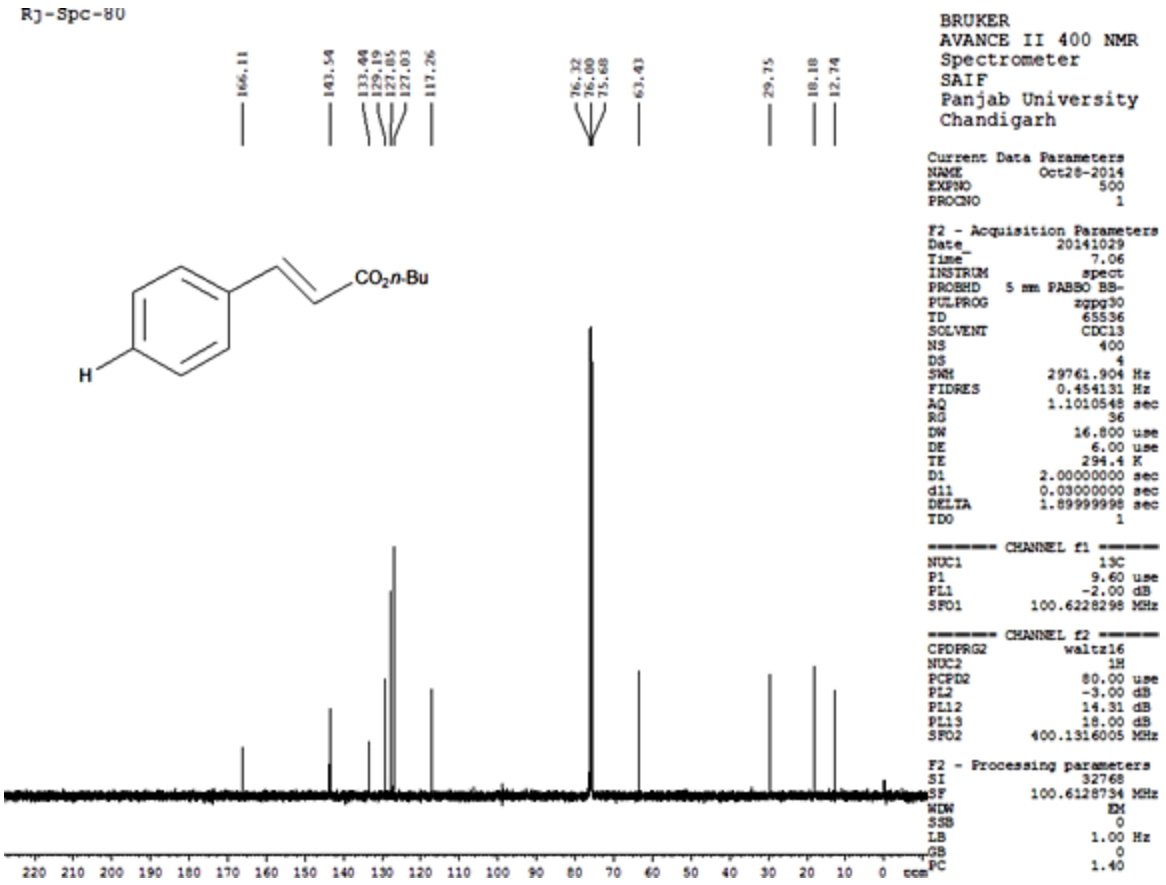
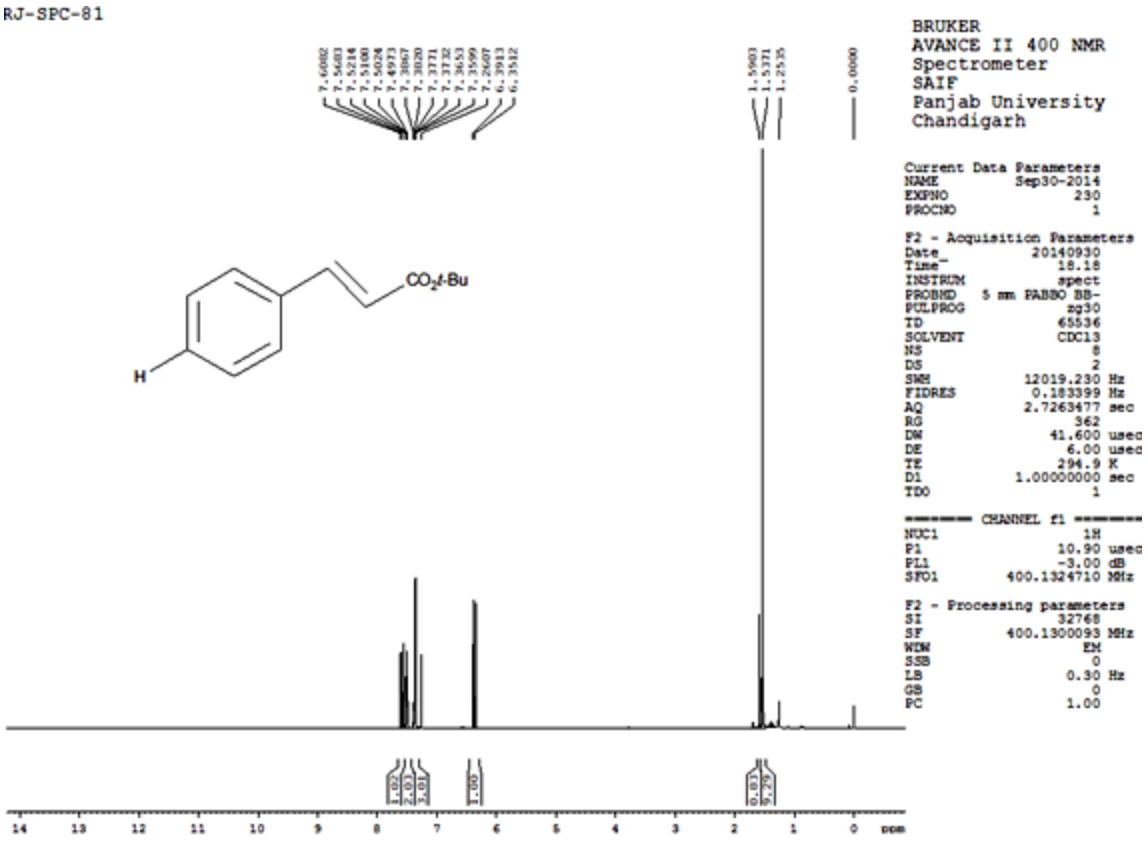
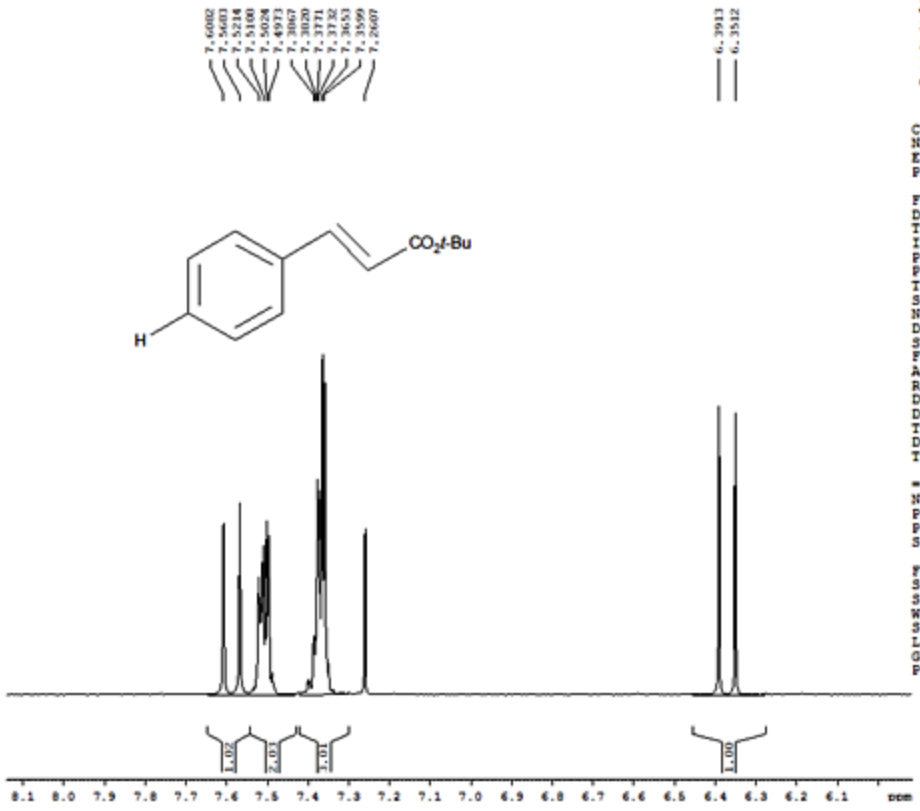


Table 2, Entry 8:



RJ-SPC-81

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BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME                  Sep30-2014
EXPNO                        230
PROCNO                         1

F2 - Acquisition Parameters
Date_                 20140930
Time                         18.18
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                           362
DW                        41.600 usec
DE                         6.00 usec
TE                         294.9 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                  400.1300093 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
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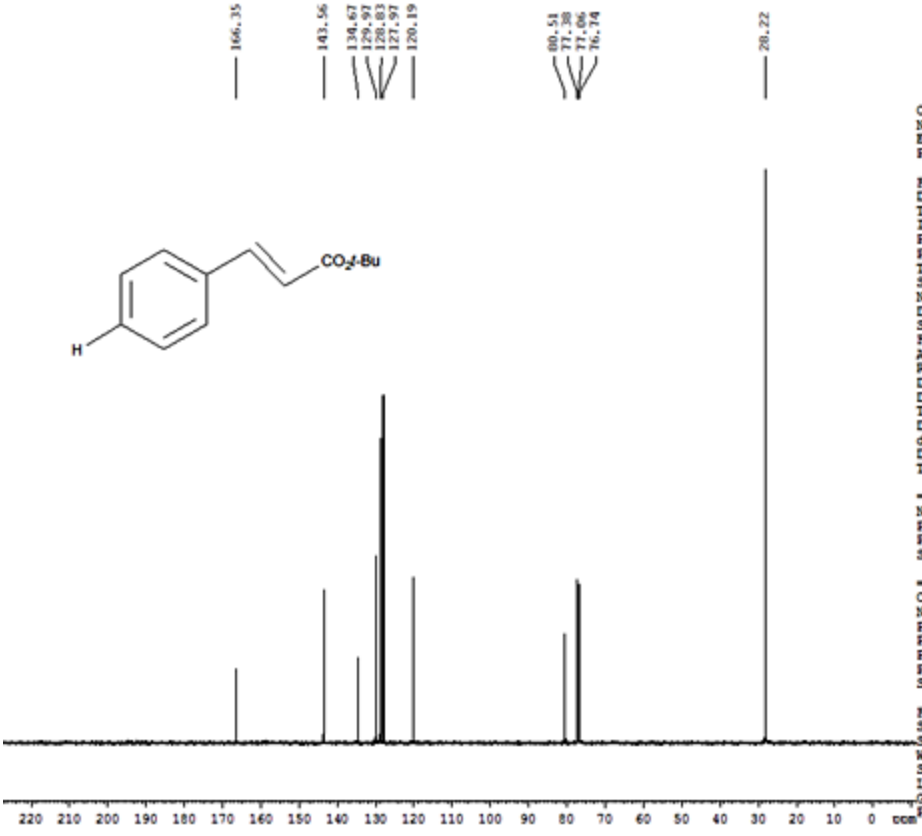
Rj-Spc-81

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BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME                  Oct28-2014
EXPNO                        510
PROCNO                         1

F2 - Acquisition Parameters
Date_                 20141029
Time                          7.32
INSTRUM                      spect
PROBHD     5 mm PABBO BB-
PULPROG                    zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                           400
DS                             4
SWH                    29761.904 Hz
FIDRES                 0.454131 Hz
AQ                     1.1010548 sec
RG                           912
DW                        16.800 use
DE                         6.00 use
TE                         294.6 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                            1

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

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

F2 - Processing parameters
SI                         32768
SF                  100.6127690 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
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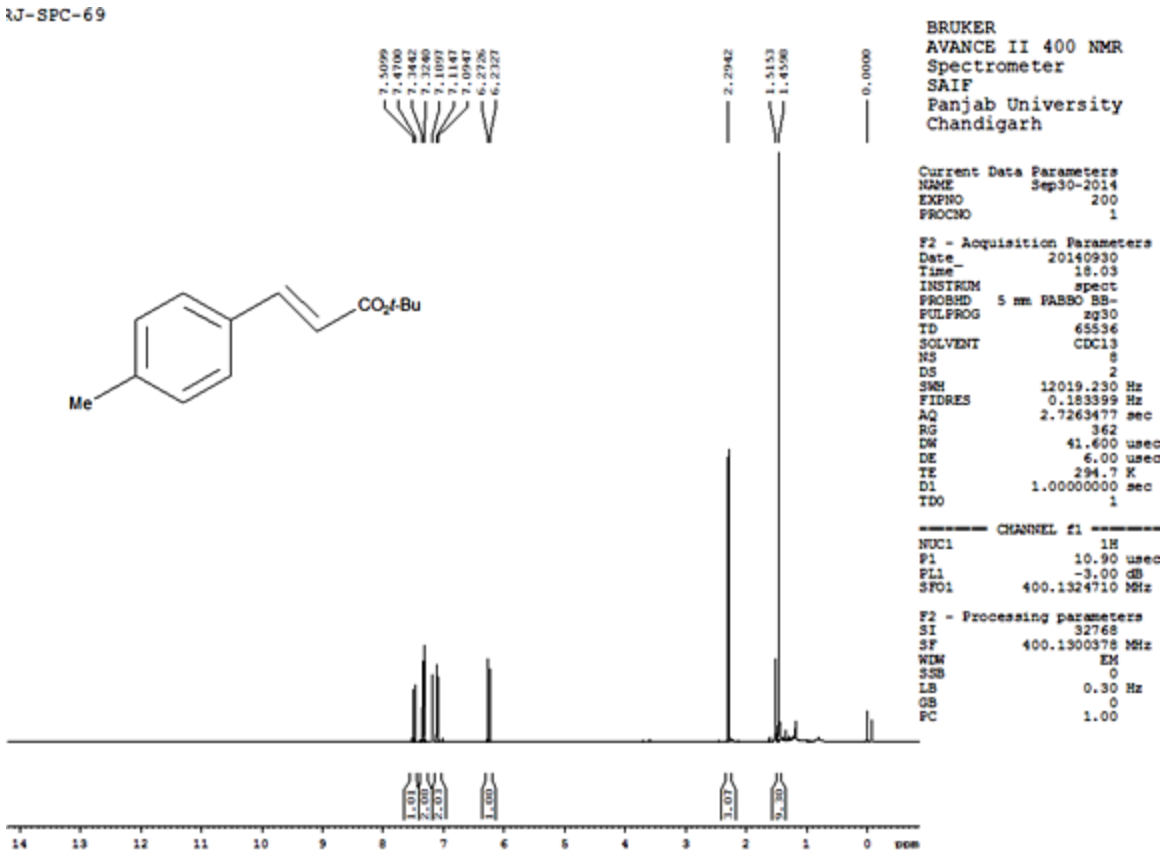
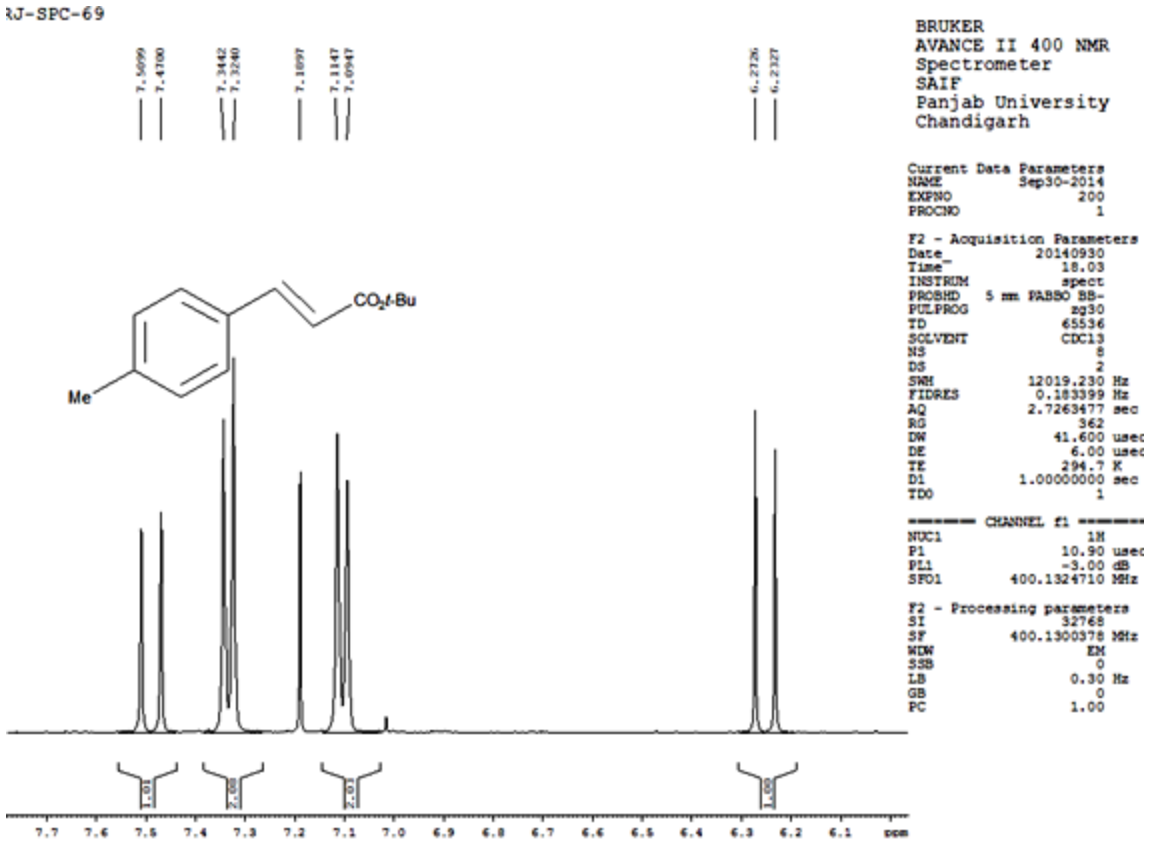
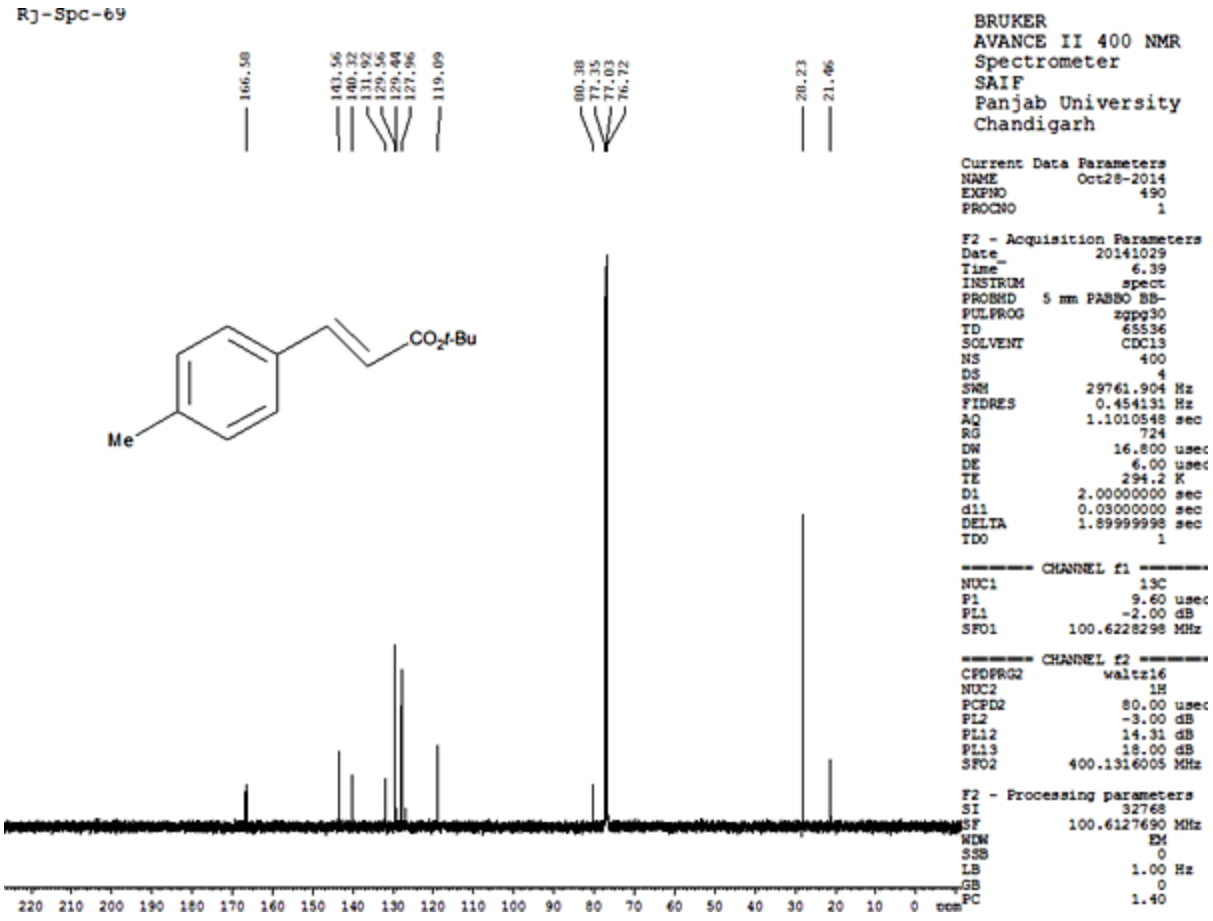
Table 2, Entry 9:







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