Supporting Information

Hydrogen-bonding and acid cooperative catalysis for benzylation of arenes with benzyl alcohols over ionic liquids

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1. Materials and Methods

1.1 Materials

Benzyl alcohol, *p*-tolylmethanol, *m*-tolylmethanol, *o*-tolylmethanol, (4-fluorophenyl)methanol, (4-chlorophenyl)methanol, (4-bromophenyl)methanol, (4-iodophenyl)methanol, (4-(trifluoromethyl)phenyl)methanol, 2-phenylethan-1-ol, 3-phenylprop-2-en-1-ol and methyl 4-(hydroxymethyl)benzoate were purchased from J&K Scientific Ltd. [1,1'-Biphenyl]-4-ylmethanol, naphthalen-2-ylmethanol, (4-nitrophenyl)methanol, 1,4-phenylenedimethanol, toluene, *m*-xylene, *o*-xylene, mesitylene, trifluoromethanesulfonic acid, 1,2-phenylenedimethanol, [1,1'-biphenyl]-2-ylmethanol and [1,1'-biphenyl]-2-carbaldehyde were purchased from Innochem.

The ionic liquids (ILs) were provided by Centre of Green Chemistry and Catalysis, Lanzhou Institute of Chemical Physics (LICP), Chinese Academy of Sciences (CAS), and their chemical structures are shown in Figure S1.

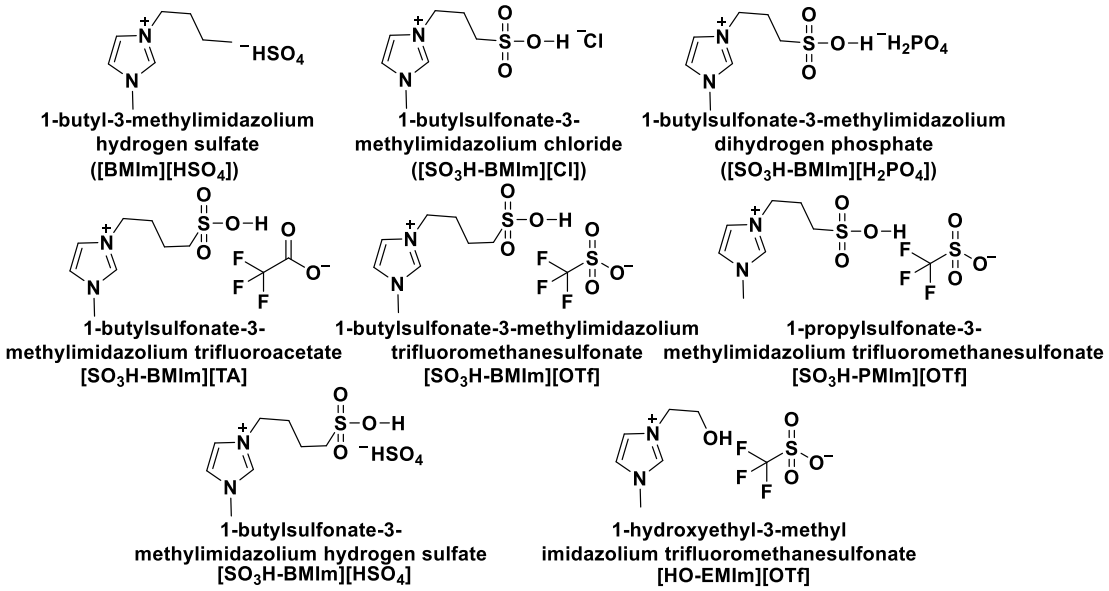


Fig. S1 The ILs used in this study.

1.2 Instrumentation

Column chromatography was performed with silica gel (200-300 mesh) purchased from Qingdao Haiyang Chemical Co. Ltd. Thin-layer chromatography was carried out with Merck silica gel GF_{254} plates. ^{1}H and ^{13}C spectra were recorded on Bruker Avance III 400 HD or 500 WB. Chemical shifts are given in ppm relative to tetramethylsilane (TMS). For the study of reaction mechanism, to eliminate the effect of solvent, wilmad coaxial insert NMR tubes were used for ^{1}H NMR, ^{19}F NMR and ^{17}O NMR at 333.2 K. DMSO-d6 was added in the inner tube, and the sample was added in the outer tube. High-resolution electrospray ionization mass spectrometry (HR-ESI-MS) was performed on Bruker FT-ICR-MS (Solarix 9.4T).

1.3 The General Procedure for the Benzylation of Benzyl Alcohols with Arenes

In a typical reaction, benzyl alcohol (0.5 mmol) and *p*-xylene (1.0 mL) was mixed with [SO_3H-PMIm][OTf] (0.5 mmol) in a 25 mL glass tubular reactor equipped with a magnetic stir bar. And then, the mixture was stirred at 120 °C for 6 h. After the reaction, the mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic phases was washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatograph on silica gel to afford the target product **3a**. Synthesis of other compounds **3b**-**3z**, and **3aa**-**3ac** was performed by an analogous procedure.

1.4 DFT calculations

All calculations were performed with the Gaussian 09 package.[1] Geometry optimizations were carried out at the M06-2X[2]/def2-TZVP[3] level at 298.15 K. The free energy of solvation of gas-phase optimized structures was calculated using the SMD-GIL solvation model.[4, 5] Vibrational frequency analysis was performed to estimate thermochemical data.

Note: DFT calculation was performed to understand the interaction of [SO_3H-BMIm][OTf] with and benzyl alcohol, which can provide the H-bond interaction information between IL and benzyl alcohol. Our DFT data presented have some limitations, which do not include greater numbers of cations and anions to demonstrate the effect of cluster size, nonetheless, support the experimental results as they stand.

2. Additional Schemes and Figures

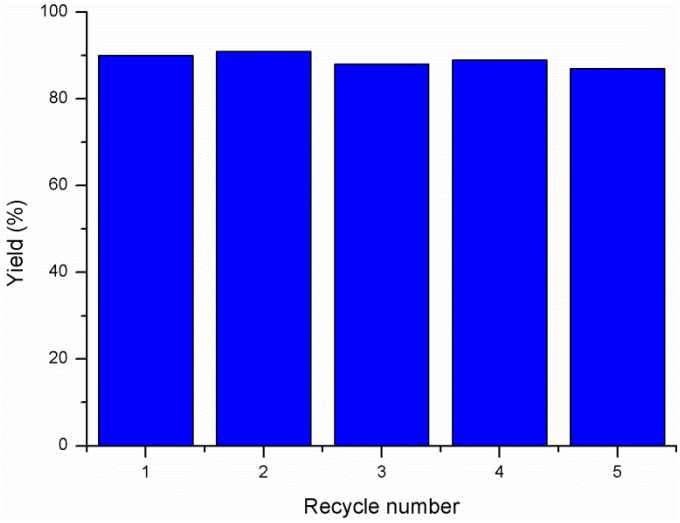


Fig. S2 Recycling experiments of the catalyst (the product yield: recycle 1: 90%; recycle 2: 92%; recycle 3: 87%; recycle 4: 89%; recycle 5: 86%).
Note: after recycling experiment, the IL was dried for 24 h in vacuum oven at 60 °C, and then following the procedure part 1.3.

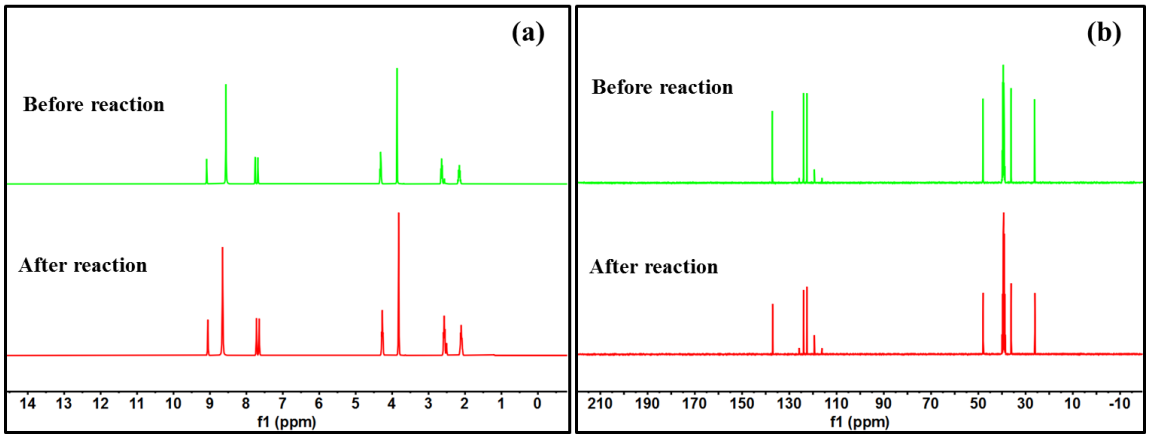


Fig. S3 ^{1}H and ^{13}C NMR spectra of [SO_3H-PMIm][OTf] before and after reaction. a) ^{1}H NMR. b) ^{13}C NMR.
Note: Before the catalyst was used for the next run, it needed to be dried under vacuum at 100 °C for 12 h.

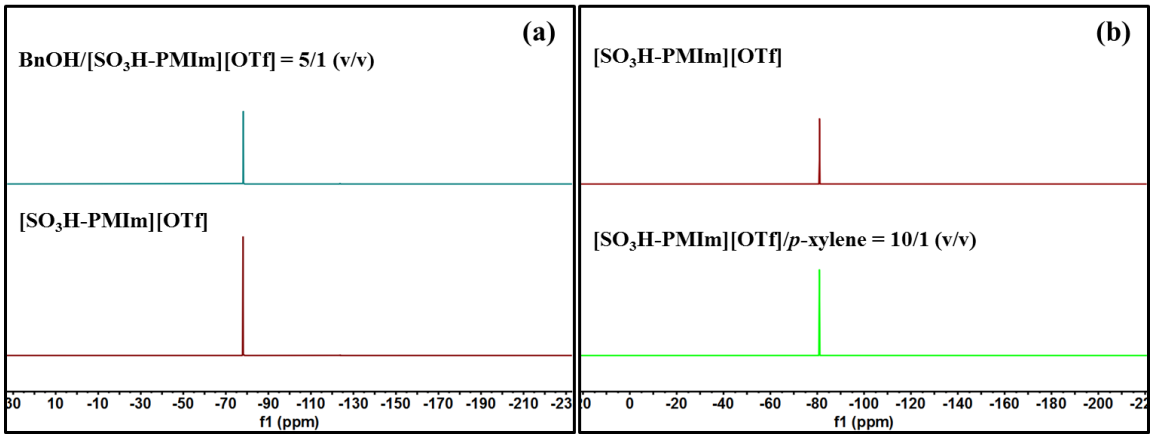


Fig. S4 ^{19}F NMR spectra recorded at 333.2 K. a) The neat IL and its mixture with **1a**. b) The neat IL and its mixture with **2a**.

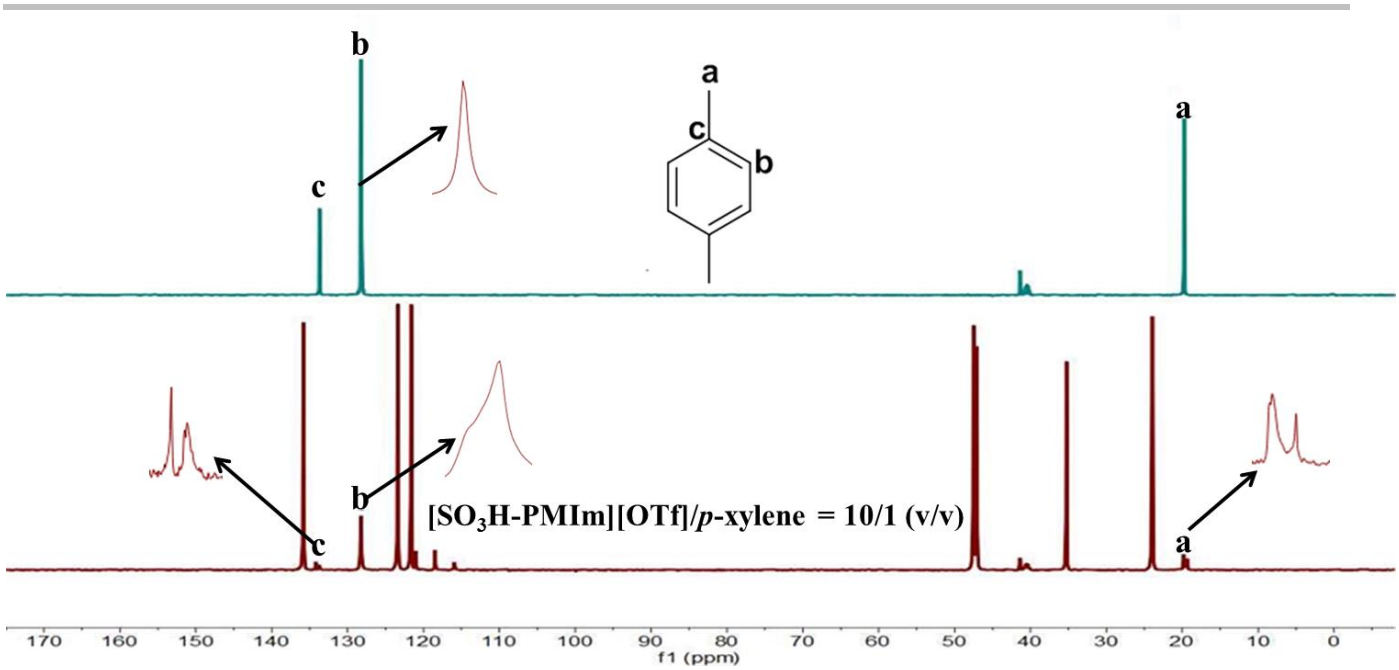


Fig. S5 ^{13}C NMR spectra of the neat **2a** and its mixture with IL recorded at 333.2 K.

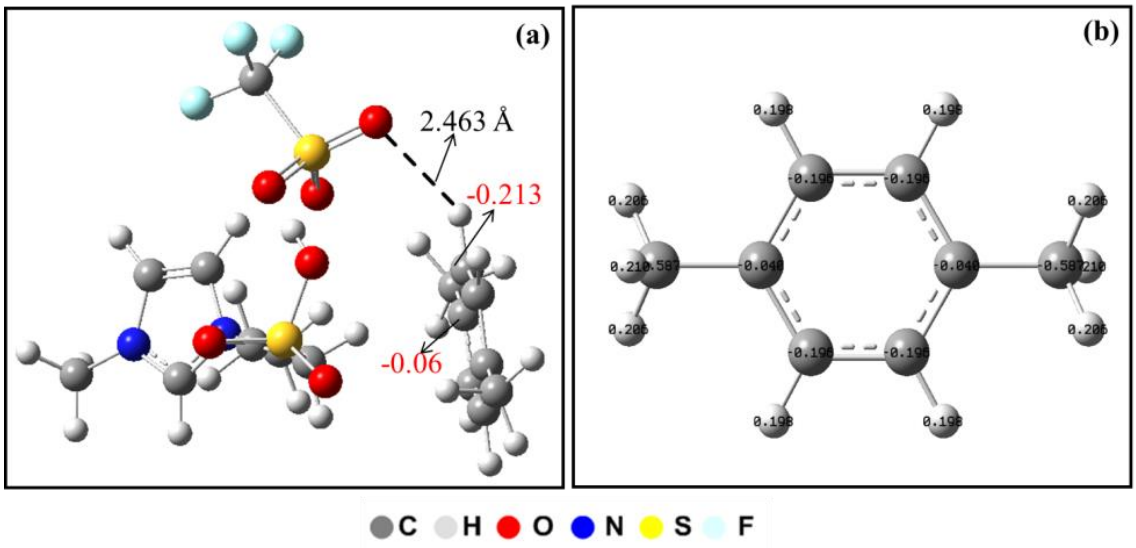
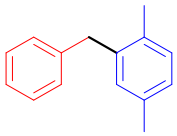


Fig. S6 NBO charges distribution and atom distance. a) Interaction structures of **2a** with [SO_3H-PMIm][OTf] (black font: atom distance; red font: NBO charges). b) NBO charges distribution of **2a**.

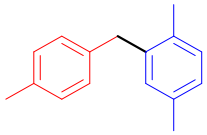
3. ^{1}H NMR and ^{13}C NMR spectra Data of the products

2-Benzyl-1,4-dimethylbenzene[6] (3a)



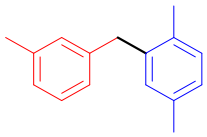
Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.23-7.27 (m, 2H), 7.15-7.18 (m, 1H), 7.10-7.11 (m, 2H), 7.03-7.05 (m, 1H), 6.92-6.96 (m, 2H), 3.94 (s, 2H), 2.28 (s, 3H), 2.18 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 140.8, 138.9, 135.6, 133.7, 131.0, 130.4, 128.9, 128.6, 127.3, 126.1, 39.6, 21.2, 19.4 ppm.

1,4-Dimethyl-2-(4-methylbenzyl)benzene[6] (3b)



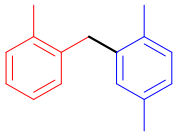
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.02-7.06 (m, 2H), 6.98-7.01 (m, 3H), 6.91-6.94 (m, 2H), 3.89 (s, 2H), 2.29 (s, 3H), 2.26 (s, 3H), 2.18 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 139.1, 137.6, 135.4, 135.3, 133.5, 130.9, 130.3, 129.2, 128.7, 127.2, 39.1, 21.2, 21.1, 19.3 ppm.

1,4-Dimethyl-2-(3-methylbenzyl)benzene[7] (3c)



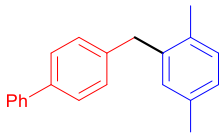
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.12-7.16 (m, 1H), 7.03-7.04 (m, 1H), 6.89-6.99 (m, 5H), 3.90 (s, 2H), 2.29 (s, 3H), 2.28 (s, 3H), 2.19 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 140.5, 138.8, 137.9, 135.4, 133.5, 130.8, 130.2, 129.5, 128.3, 127.1, 126.7, 125.8, 39.4, 21.5, 21.0, 19.3 ppm.

1,4-Dimethyl-2-(2-methylbenzyl)benzene[8] (3d)



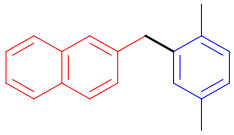
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.05-7.19 (m, 4H), 6.94-6.96 (m, 1H), 6.85-6.87 (m, 1H), 6.72 (s, 1H), 3.87 (s, 2H), 2.27 (s, 3H), 2.23 (s, 3H), 2.20 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 140.5, 138.8, 137.9, 135.4, 133.5, 130.8, 130.2, 129.5, 128.3, 127.1, 126.7, 125.8, 39.4, 21.5, 21.0, 19.3 ppm.

4-(2,5-Dimethylbenzyl)-1,1'-biphenyl[8] (3e)



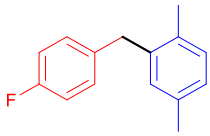
White solid;^{1}H NMR (400 MHz, DMSO-d_6, 25 °C): δ = 7.60-7.62 (m, 2H), 7.54-7.56 (m, 2H), 7.41-7.45 (m, 2H), 7.30-7.34 (m, 1H), 7.19-7.21 (s, 2H), 7.03-7.05 (m, 1H), 6.99 (s, 1H), 6.93-6.95 (m, 1H), 3.94 (s, 2H), 2.23 (s, 3H), 2.17 ppm (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6, 25 °C): δ = 140.5, 140.2, 139.1, 138.2, 135.2, 133.3, 131.0, 130.6, 129.5, 129.3, 127.6, 127.4, 127.1, 126.9, 38.7, 21.1, 19.3 ppm.

2-(2,5-Dimethylbenzyl)naphthalene[7] (3f)



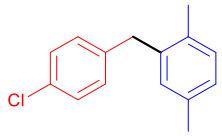
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.77-7.80 (m, 1H), 7.71-7.74 (m, 2H), 7.51 (s, 1H), 7.37-7.42 (m, 2H), 7.27-7.29 (m, 1H), 7.05-7.07 (m, 1H), 6.95-6.98 ppm (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 138.6, 138.2, 135.5, 133.7, 133.6, 132.1, 130.9, 130.3, 128.0, 127.7, 127.6, 127.5, 127.2, 126.9, 125.9, 125.3, 39.7, 21.0, 19.3 ppm.

2-(4-Fluorobenzyl)-1,4-dimethylbenzene[7] (3g)



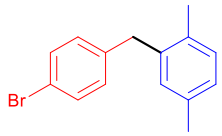
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.13-7.19 (m, 1H), 6.89-7.06 (m, 6H), 3.94 (s, 2H), 2.27 (s, 3H), 2.20 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 162.3, 159.9, 137.4, 135.5, 133.5, 130.7, 130.6, 130.3, 127.7 (d, $J_{C\text{-}F}$ = 18 Hz), 127.5 (d, $J_{C\text{-}F}$ = 15 Hz), 127.3, 124.0 (d, $J_{C\text{-}F}$ = 3 Hz), 115.1 (d, $J_{C\text{-}F}$ = 22 Hz), 31.9 (d, $J_{C\text{-}F}$ = 4 Hz), 21.0, 19.0 ppm; ^{19}F NMR (400 MHz, $CDCl_3$, 25 °C): δ = -117.6 ppm.

2-(4-chlorobenzyl)-1,4-dimethylbenzene[6] (3h)



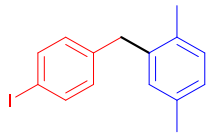
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.18-7.21 (m, 2H), 7.01-7.04 (m, 3H), 6.95-6.96 (m, 1H), 6.88 (m, 1H), 3.88 (s, 2H), 2.27 (s, 3H), 2.15 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 138.0, 137.1, 134.5, 132.3, 130.6, 129.7, 129.3, 129.0, 127.4, 126.3, 37.8, 19.9, 18.1 ppm.

2-(4-Bromobenzyl)-1,4-dimethylbenzene[6] (3i)



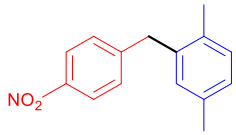
Brown oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.33-7.37 (m, 2H), 7.02-7.04 (m, 1H), 6.94-6.97 (m, 3H), 6.88 (m, 1H), 3.86 (s, 2H), 2.27 (s, 3H), 2.15 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 139.7, 138.1, 135.6, 133.4, 131.5, 130.8, 130.5, 130.4, 127.4, 119.8, 38.9, 21.0, 19.2 ppm.

2-(4-Iodobenzyl)-1,4-dimethylbenzene (3j)



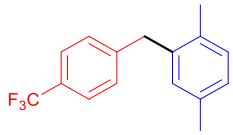
White solid; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.53-7.55 (m, 2H), 7.01-7.03 (m, 1H), 6.94-6.96 (m, 1H), 6.82-6.87 (m, 3H), 3.85 (s, 2H), 2.27 (s, 3H), 2.14 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 140.4, 138.1, 137.5, 135.6, 133.4, 130.9, 130.8, 130.4, 127.5, 91.2, 39.1, 21.1, 19.3 ppm; FTIR (neat): 2999, 2919, 2861, 1615, 1586, 1502, 1482, 1444, 1398, 1377, 1301, 1233, 1187, 1154, 1059, 1036, 1006, 949, 916, 885, 807, 793, 757, 641, 628, 531, 477, 448, 434 cm^{-1}; HR-MS(EI) calc. for $C_{15}H_{15}I$ [M] 322.02184, found 322.02118.

1,4-Dimethyl-2-(4-nitrobenzyl)benzene[9] (3k)



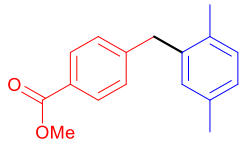
Light yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 8.09-8.12 (m, 2H), 7.23-7.27 (m, 2H), 7.06-7.08 (m, 1H), 6.99-7.01 (m, 1H), 6.91 (m, 1H), 4.03 (s, 2H), 2.30 (s, 3H), 2.15 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 148.6, 146.5, 136.9, 135.8, 133.4, 130.8, 130.6, 129.4, 127.8, 123.7, 39.4, 20.9, 19.1 ppm.

1,4-Dimethyl-2-(4-(trifluoromethyl)benzyl)benzene[7] (3l)



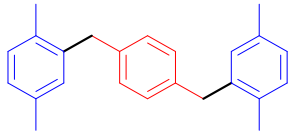
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.48-7.50 (m, 2H), 7.19-7.21 (m, 2H), 7.04-7.06 (m, 1H), 6.96-6.99 (m, 1H), 6.91 (m, 1H), 3.98 (s, 2H), 2.29 (s, 3H), 2.16 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 144.9, 137.6, 135.7, 133.4, 130.9, 130.5, 129.0, 127.6, 125.3 (dd, $J_{C\text{-}F}$ = 4.0, 17 Hz), 39.3, 20.9, 19.1 ppm; ^{19}F NMR (400 MHz, $CDCl_3$, 25 °C): δ = -62.3 ppm.

Methyl 4-(2,5-dimethylbenzyl)benzoate[10] (3m)



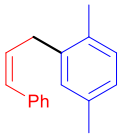
White solid; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.83-7.85 (m, 2H), 7.07-7.09 (m, 2H), 6.95-6.96 (m, 1H), 6.87-6.89 (m, 1H), 6.81 (m, 1H), 3.89 (s, 2H), 3.78 (s, 3H), 2.19 (s, 3H), 2.06 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 167.1, 146.2, 137.8, 135.6, 133.4, 130.8, 130.4, 129.8, 128.7, 128.0, 127.5, 52.0, 39.6, 21.0, 19.2 ppm.

1,4-Bis(2,5-dimethylbenzyl)benzene[11] (3s)



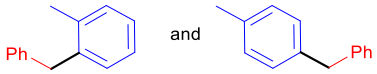
White solid; ^{1}H NMR (400 MHz, DMSO-d_6, 25 °C): δ = 7.00-7.02 (m, 6H), 6.91-6.93 (m, 4H), 3.85 (s, 4H), 2.22 (s, 6H), 2.13 ppm (s, 6H); ^{13}C NMR (101 MHz, DMSO-d_6, 25 °C): δ = 167.1, 146.2, 137.8, 135.6, 133.4, 130.8, 130.4, 129.8, 128.7, 128.0, 127.5, 52.0, 39.6, 21.0, 19.2 ppm.

1,4-Dimethyl-2-(3-phenylallyl)benzene[12] (3t)



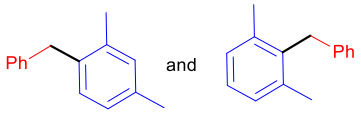
White solid; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.33-7.35 (m, 2H), 7.25-7.29 (m, 2H), 7.15-7.19 (m, 1H), 6.99-7.08 (m, 2H), 6.92-6.96 (m, 1H), 3.48 (d, J = 5.6 Hz, 2H), 2.30 (s, 3H), 2.28 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 137.0, 136.6, 134.5, 132.2, 129.8, 129.1, 129.0, 127.7, 127.4, 126.0, 125.9, 125.1, 35.9, 19.9, 17.9 ppm.

1-Benzyl-2-methylbenzene and 1-benzyl-4-methylbenzene[6] (3u)



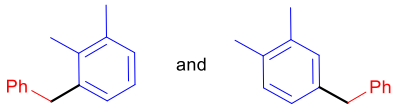
Colourless oi; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.22-7.27 (m, 4H), 7.06-7.17 (m, 14H), 3.96 (s, 2H), 3.92 (s, 2H), 2.29 (s, 3H), 2.22 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 141.5, 140.5, 139.0, 138.2, 136.7, 135.6, 130.4, 130.1, 129.3, 129.0, 128.9, 128.8, 128.5, 128.4, 126.6, 126.2, 126.2, 126.0, 41.6, 39.6, 21.1, 19.7 ppm.

1-Benzyl-2,4-dimethylbenzene and 2-benzyl-1,3-dimethylbenzene[11] (3v)



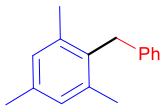
Colourless oi; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.22-7.27 (m, 4H), 7.14-7.18 (m, 4H), 7.09-7.12 (m, 2H), 7.02-7.05 (m, 3H), 6.95-6.98 (m, 2H), 6.90-6.92 (m, 1H), 4.00 (s, 2H), 3.90 (s, 2H), 2.27 (s, 3H), 2.21 (s, 6H), 2.12 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 141.6, 140.9, 138.8, 138.6, 137.0, 136.6, 135.3, 134.2, 130.3, 129.8, 128.9, 128.7, 128.5, 128.4, 128.3, 128.2, 126.4, 126.0, 125.9, 125.5, 41.6, 40.1, 20.7, 19.8, 19.3, 15.4 ppm.

4-Benzyl-1,2-dimethylbenzene and 2-benzyl-1,2-dimethylbenzene[11] (3w)



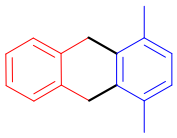
Colourless oi; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.21-7.26 (m, 4H), 7.13-7.20 (m, 3H), 7.05-7.12 (m, 5H), 6.93-7.01 (m, 6H), 4.05 (s, 1H), 3.93 (s, 3H), 2.29 (s, 3H), 2.23 (s, 3H), 2.19 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 140.8, 138.9, 137.2, 136.9, 136.5, 135.9, 131.2, 130.0, 128.8, 128.5, 128.4, 128.2, 127.9, 126.7, 126.4, 125.9, 125.8, 39.1, 35.1, 21.0, 20.3, 19.6 ppm.

2-Benzyl-1,3,5-trimethylbenzene[8] (3x)



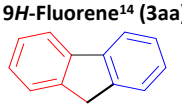
Colourless oi; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.18-7.23 (m, 2H), 7.11-7.15 (m, 1H), 6.99-7.01 (m, 2H), 6.88 (s, 2H), 4.01 (s, 2H), 2.28 (s, 3H), 2.19 ppm (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 140.2, 137.1, 135.7, 133.9, 129.0, 128.4, 127.9, 125.7, 34.8, 21.0, 20.2 ppm.

1,4-Dimethyl-9,10-dihydroanthracene[13] (3z)



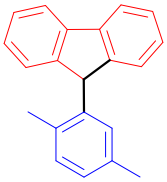
White solid; ^{1}H NMR (400 MHz, DMSO-d_6, 25 °C): δ = 7.11-7.13 (m, 2H), 7.04-7.06 (m, 1H), 6.92-6.94 (m, 1H), 6.85-6.87 (m, 1H), 6.68 (s, 1H), 3.84 (s, 4H), 2.16 (s, 3H), 2.06 ppm (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6, 25 °C): δ = 138.8, 138.4, 135.1, 133.4, 130.3, 130.1, 129.5, 127.2, 126.7, 36.1, 21.1, 19.0 ppm.

9*H*-Fluorene[14] (3aa)



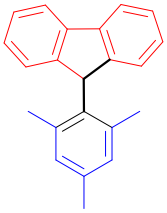
White solid; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.77-7.79 (m, 2H), 7.52-7.54 (m, 2H), 7.35-7.38 (m, 2H), 7.27-7.31 (m, 2H), 3.89 ppm (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 143.2, 141.8, 126.8, 126.7, 125.0, 119.9, 37.0 ppm.

9-(2,5-Dimethylphenyl)-9*H*-fluorene[15] (3ab)



White solid; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.76-7.78 (m, 3H), 7.32-7.38 (m, 4H), 7.12-7.18 (m, 8H), 6.81-6.99 (m, 2H), 6.18 (s, 1H), 5.34 (s, 1H), 4.92 (s, 0.5 H), 2.68 (s, 3H), 2.41 (s, 2H), 1.98 (s, 3H), 1.08 ppm (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 148.7, 147.1, 141.3, 141.0, 139.9, 138.4, 136.0, 135.1, 134.2, 133.6, 133.1, 131.7, 130.4, 130.0, 128.0, 127.6, 127.4, 127.3, 127.2, 125.2, 124.8, 120.0, 58.5, 56.4, 50.1, 21.1, 20.9, 20.1, 18.5, 17.8 ppm.

9-Mesityl-9*H*-fluorene[15] (3ac)



White solid; ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ = 7.78-7.79 (m, 2H), 7.32-7.34 (m, 2H), 7.19-7.20 (m, 4H), 7.00 (m, 1H), 6.62-6.77 (m, 1H), 5.46 (s, 1H), 2.64 (s, 3H), 2.24 (s, 3H), 1.08 ppm (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ = 147.4, 141.0, 138.0, 137.8, 137.7, 136.3, 135.1, 134.0, 130.7, 129.0, 127.3, 127.1, 126.9, 124.3, 120.1, 49.9, 21.8, 21.0, 18.8 ppm.

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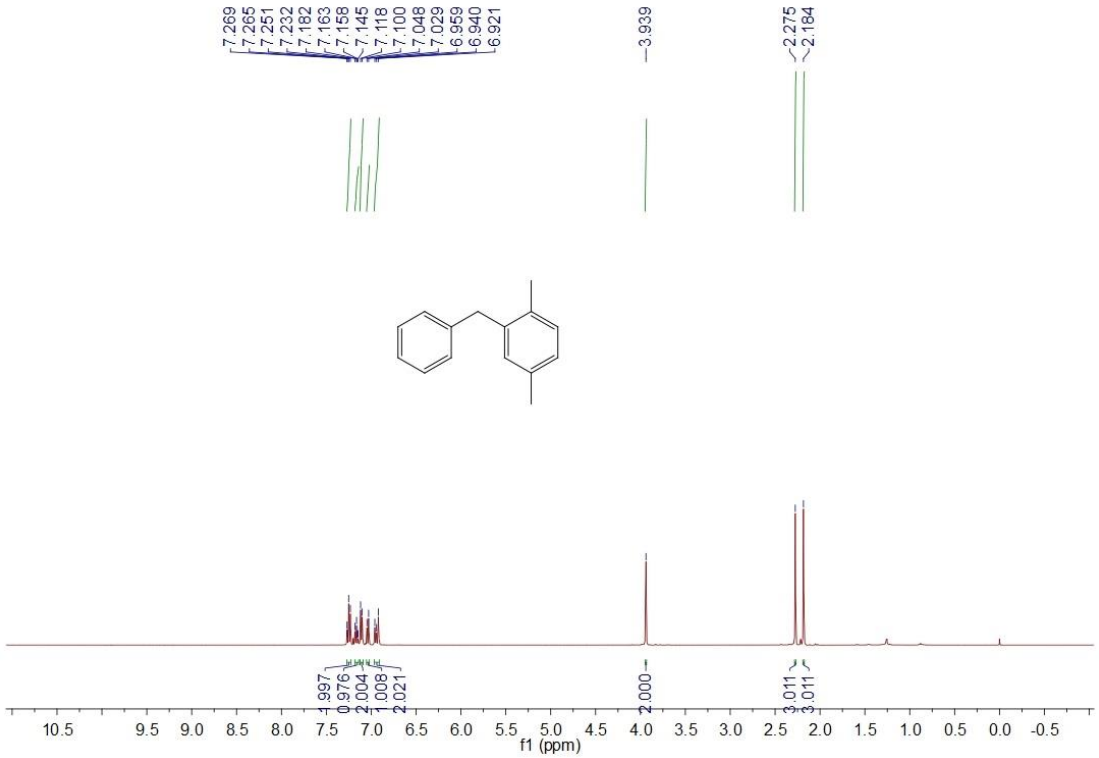
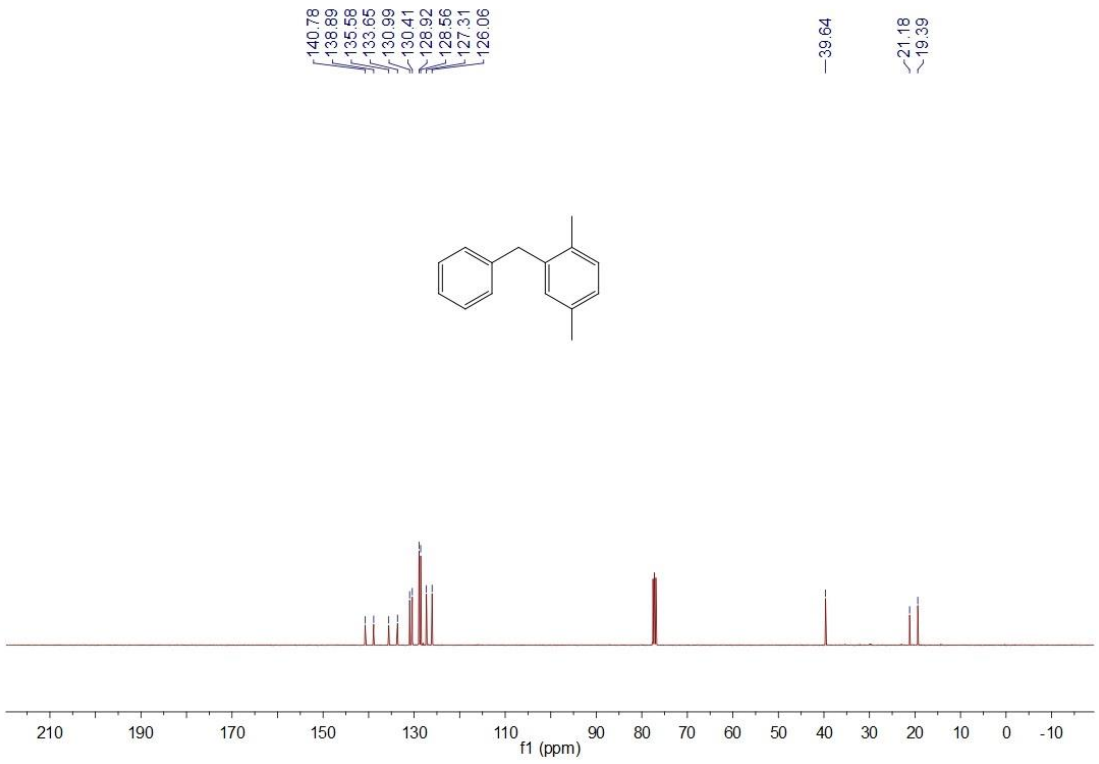
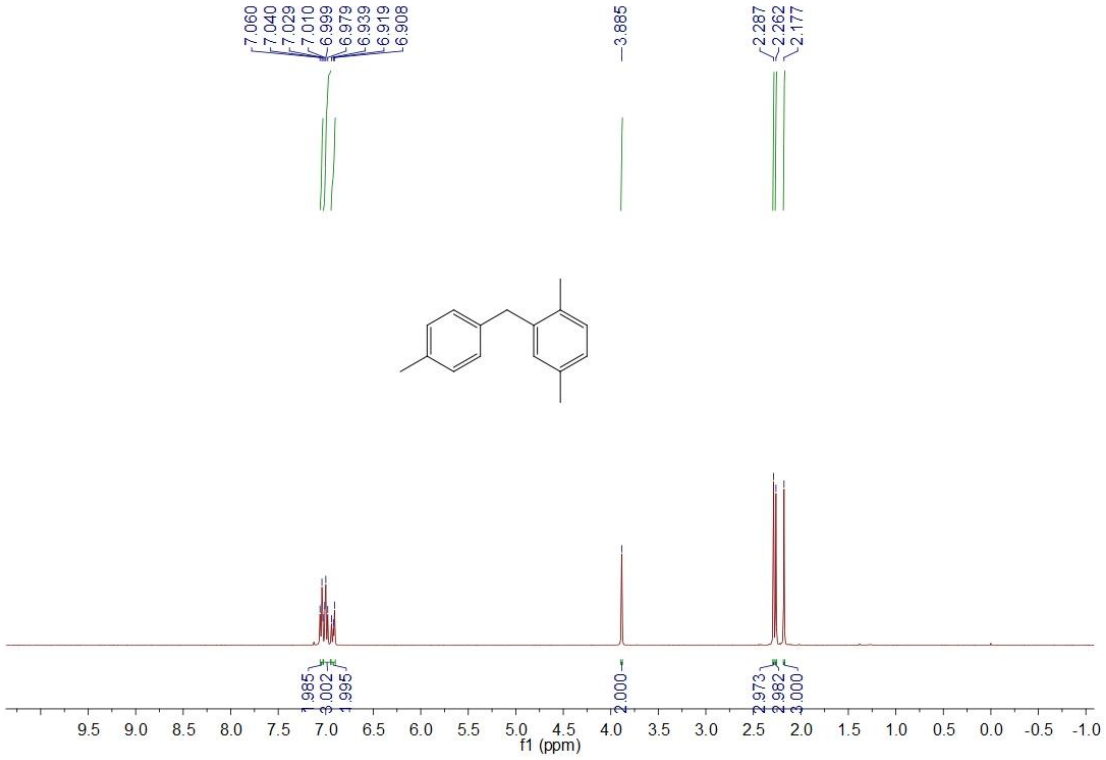
4. ^{1}H and ^{13}C NMR Spectra of products

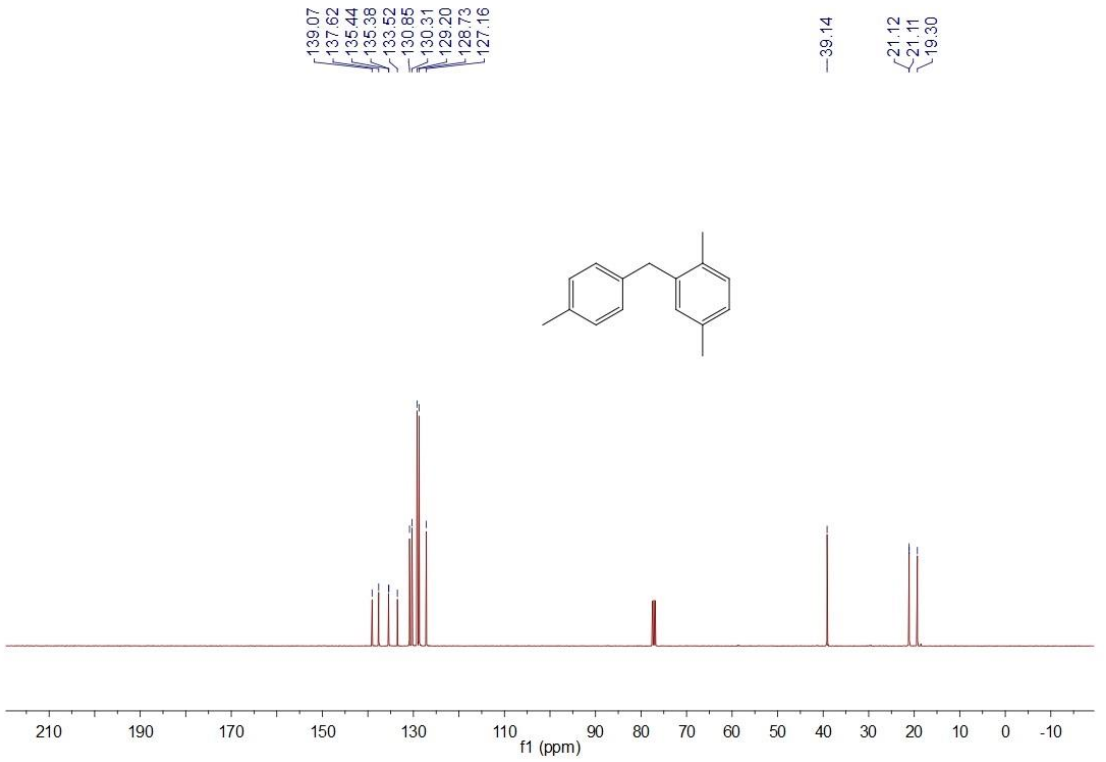
2-Benzyl-1,4-dimethylbenzene (3a)



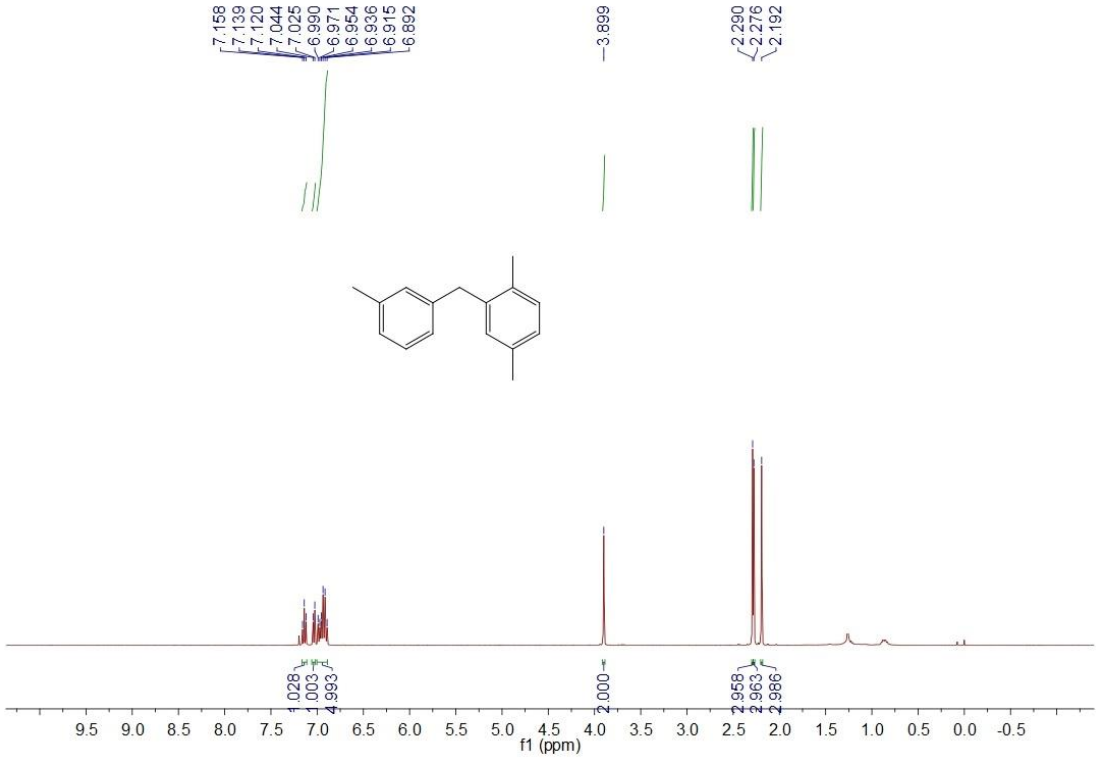


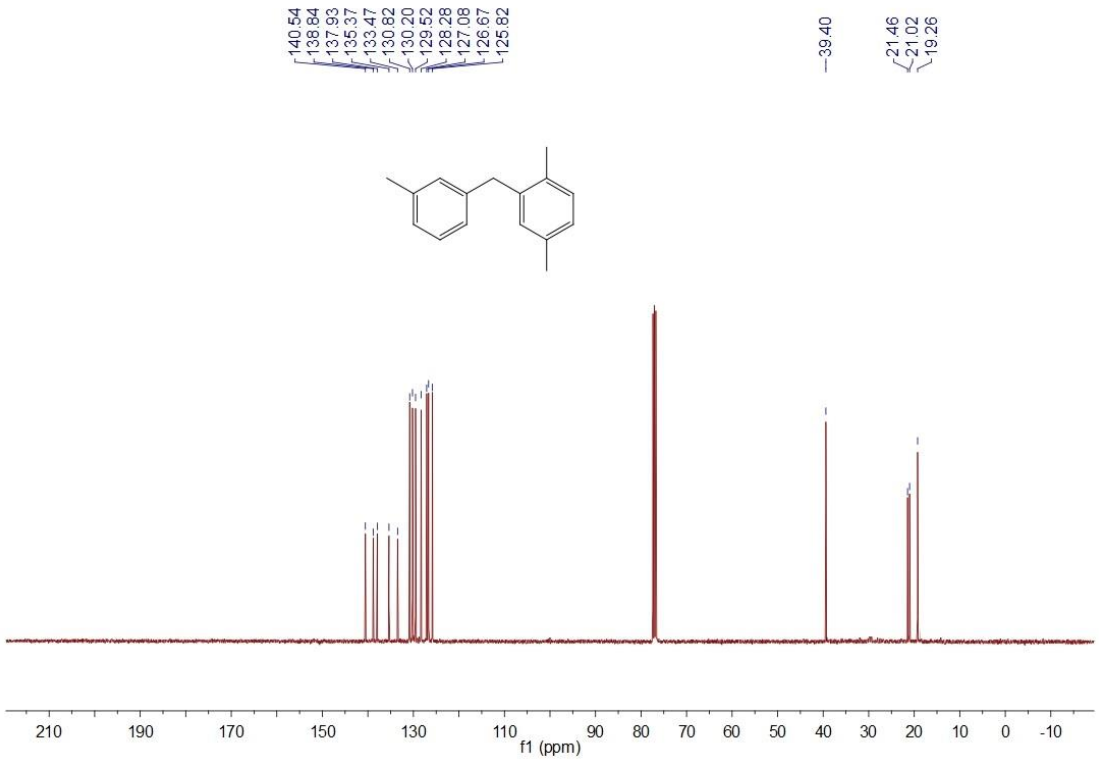
1,4-Dimethyl-2-(4-methylbenzyl)benzene (3b)



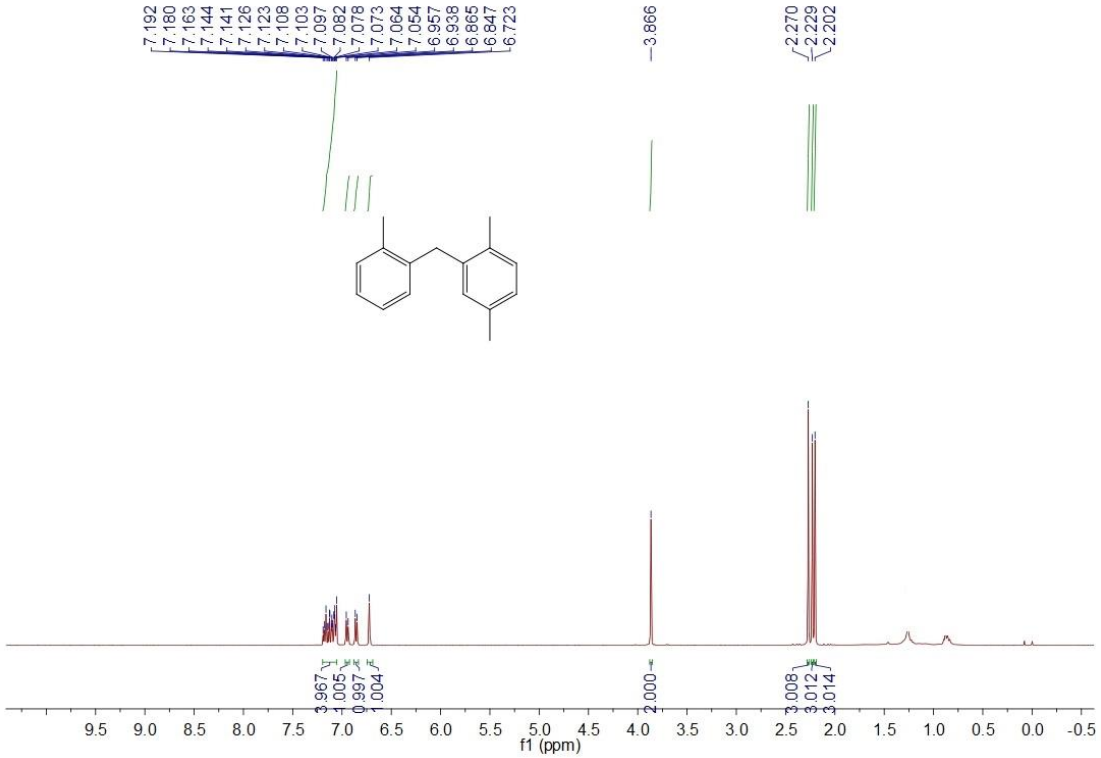


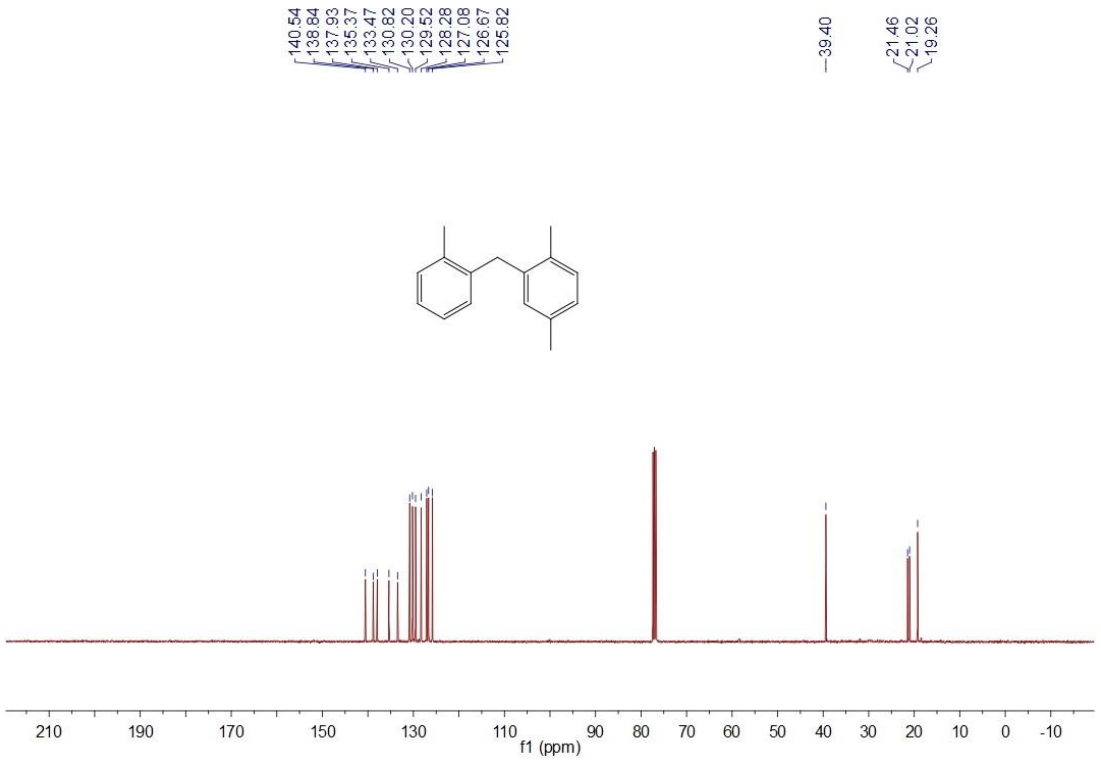
1,4-Dimethyl-2-(3-methylbenzyl)benzene (3c)



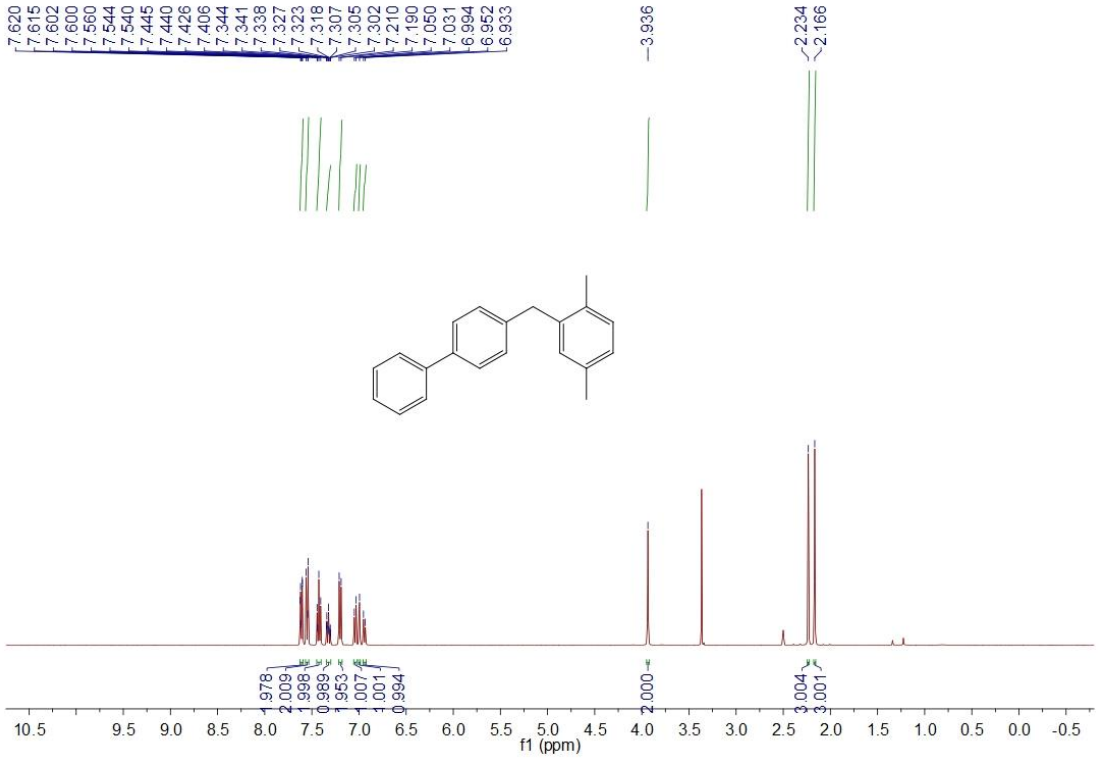


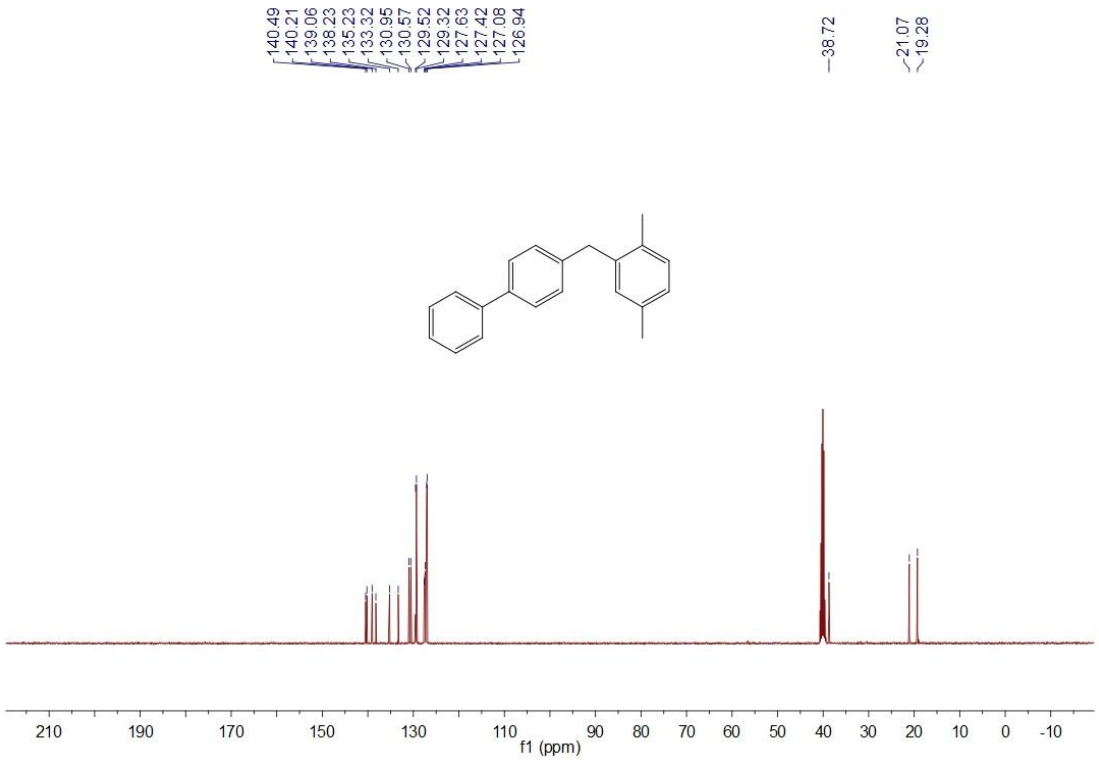
1,4-Dimethyl-2-(2-methylbenzyl)benzene (3d)



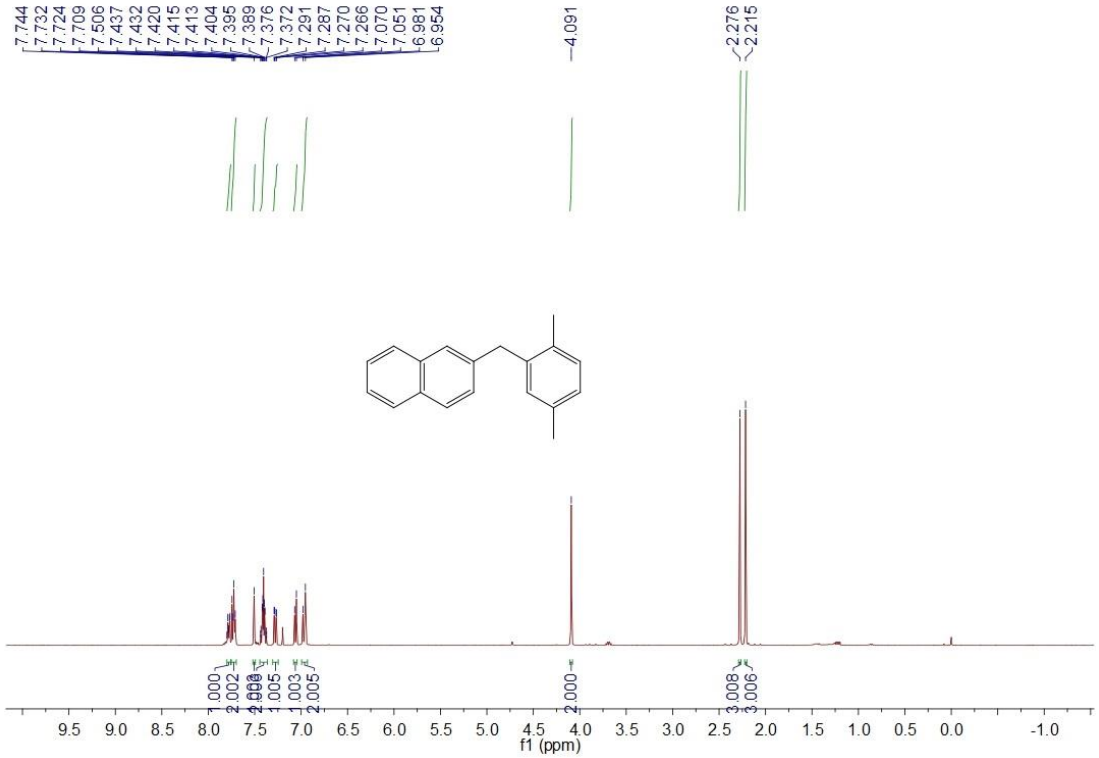


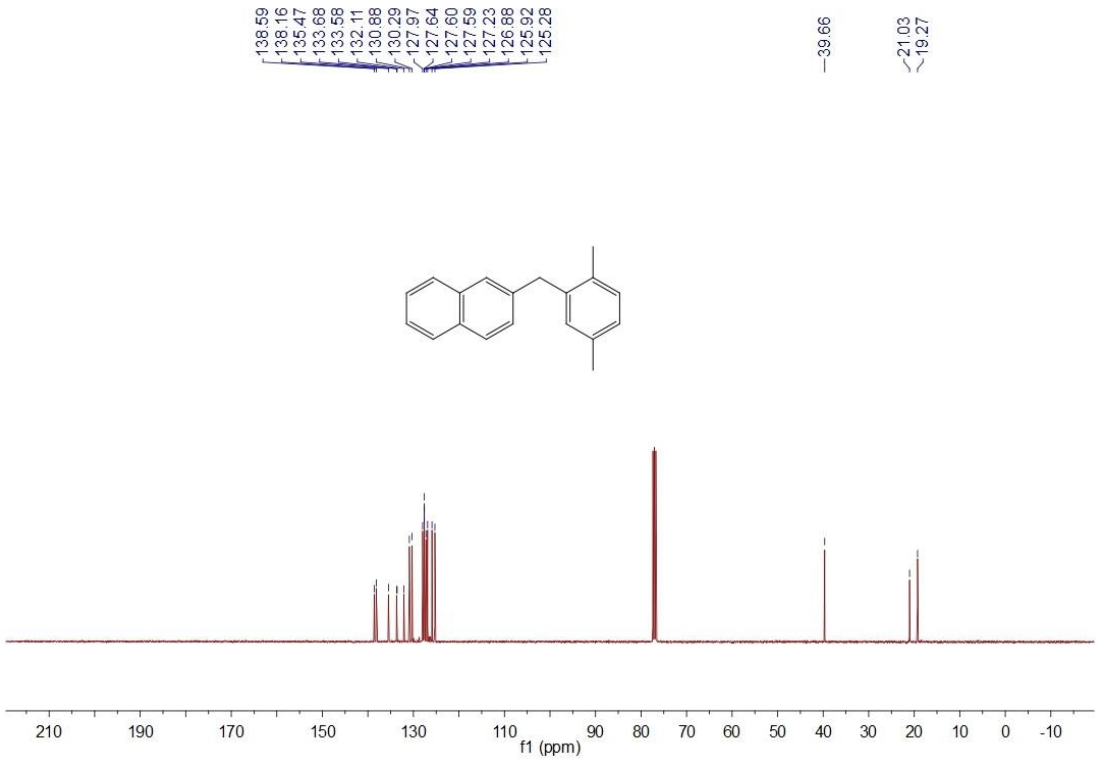
4-(2,5-Dimethylbenzyl)-1,1'-biphenyl (3e)



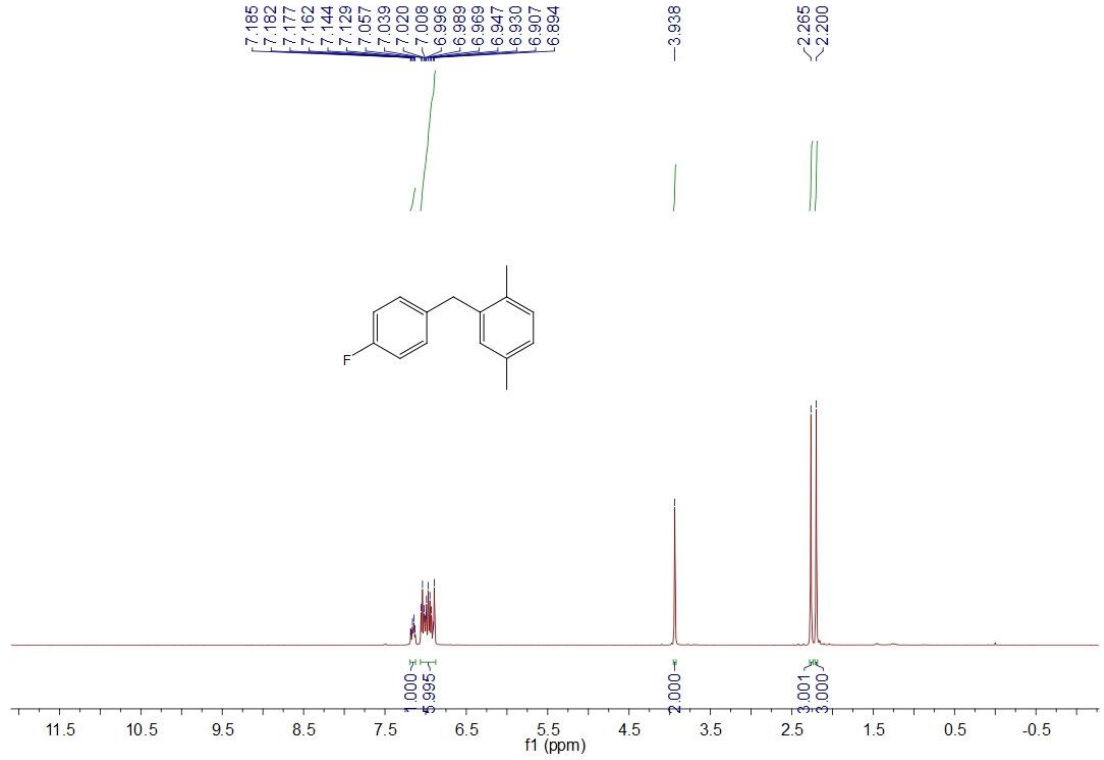


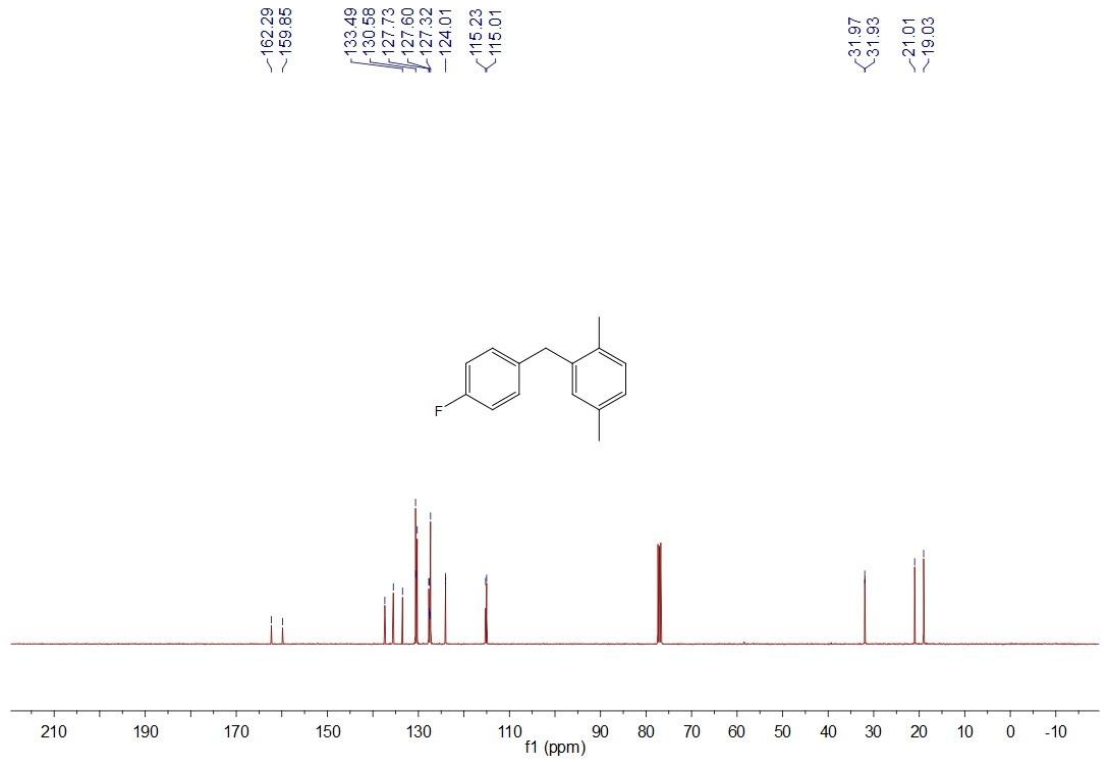
2-(2,5-Dimethylbenzyl)naphthalene (3f)

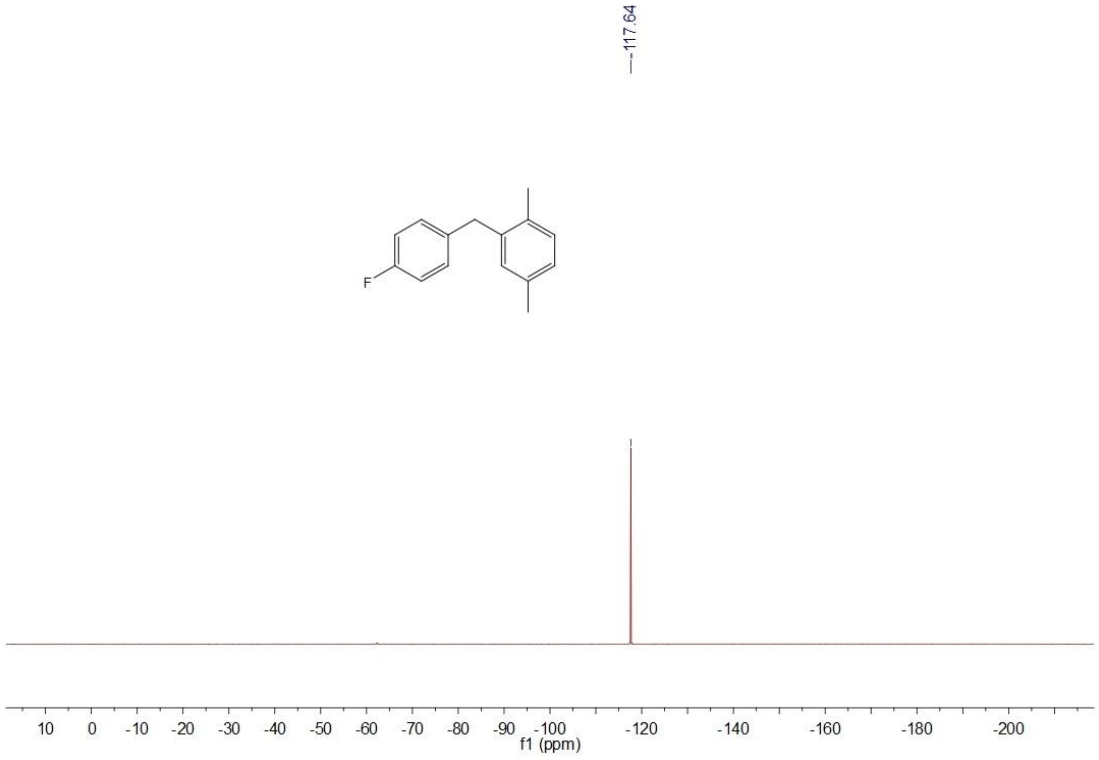




2-(4-Fluorobenzyl)-1,4-dimethylbenzene (3g)



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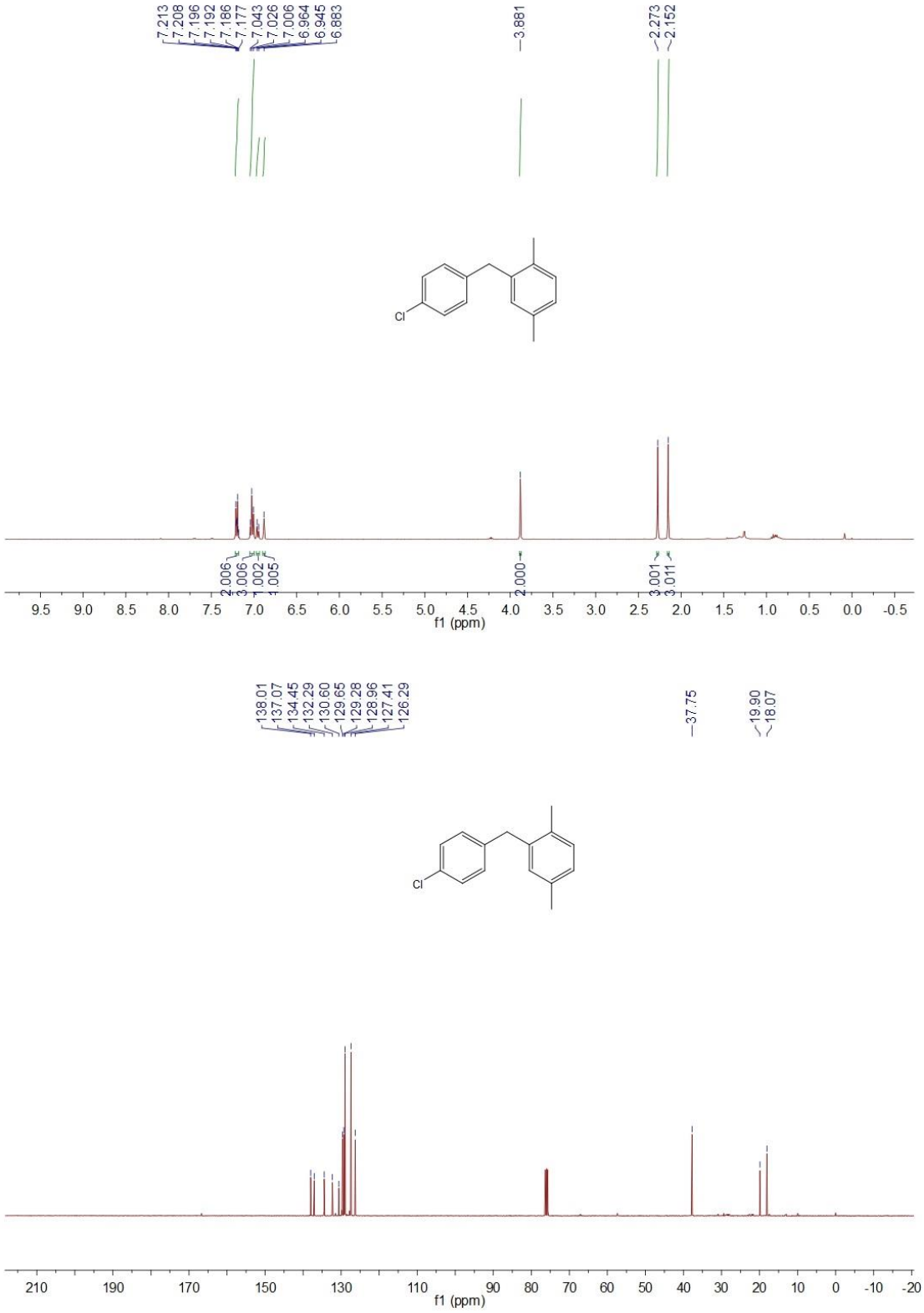
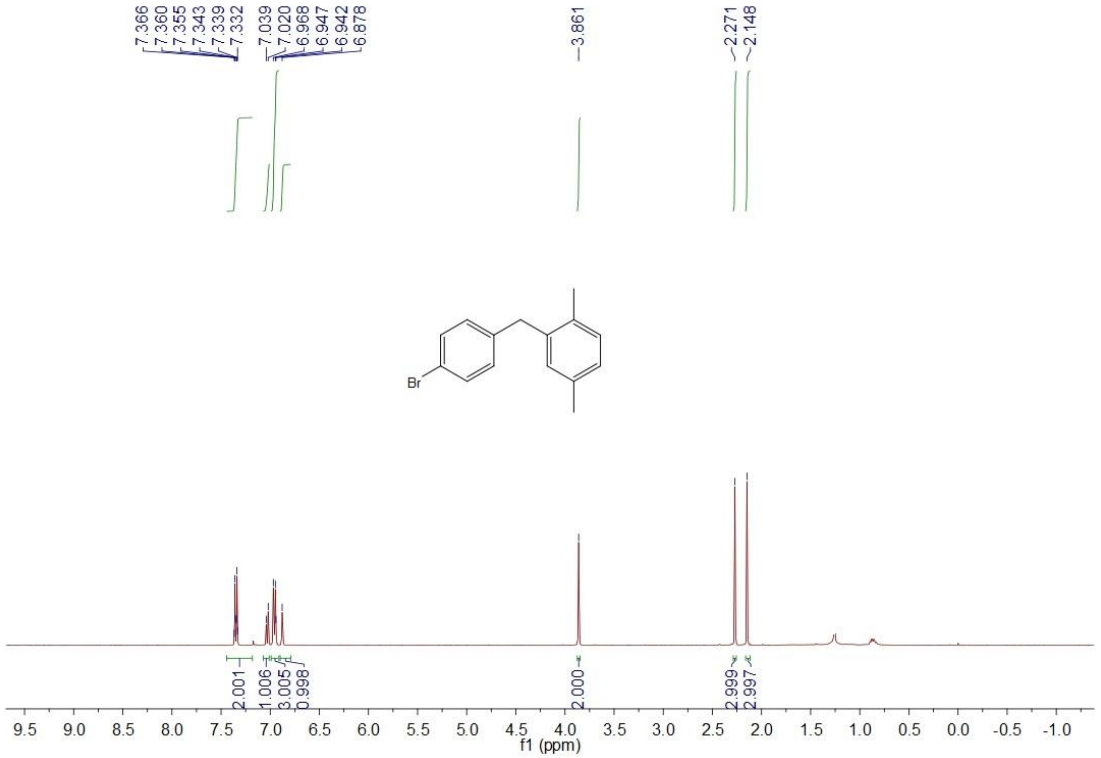
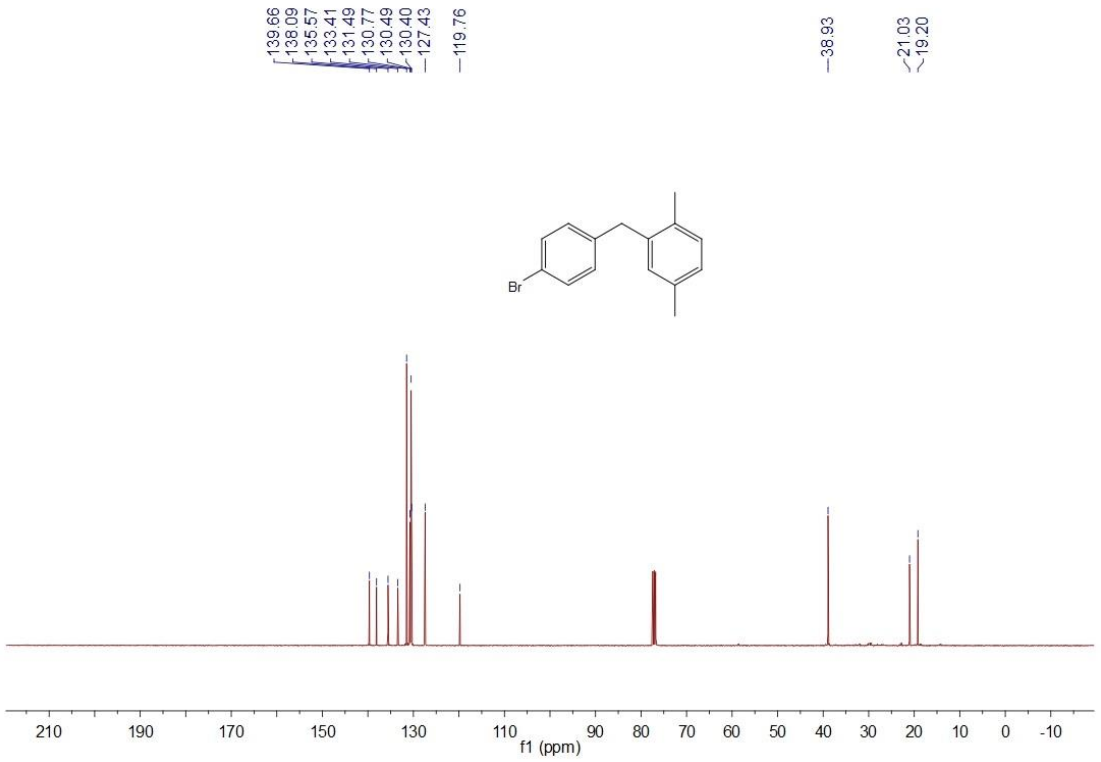
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

2-(4-Chlorobenzyl)-1,4-dimethylbenzene (3h)

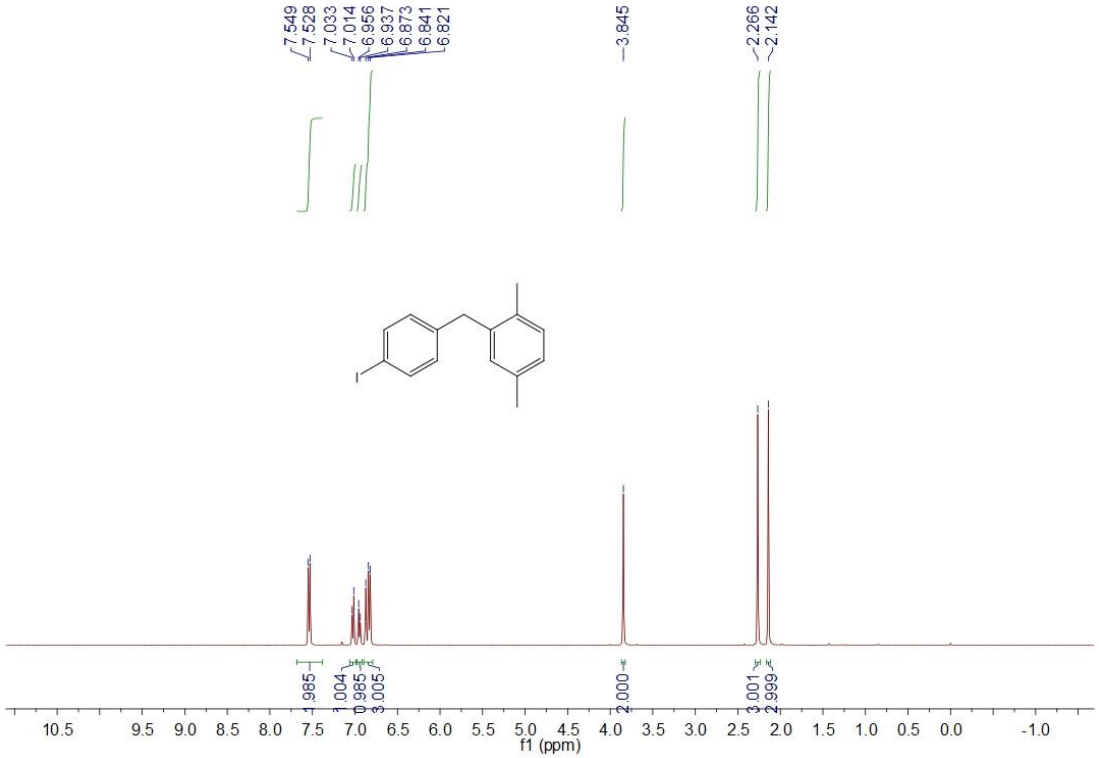


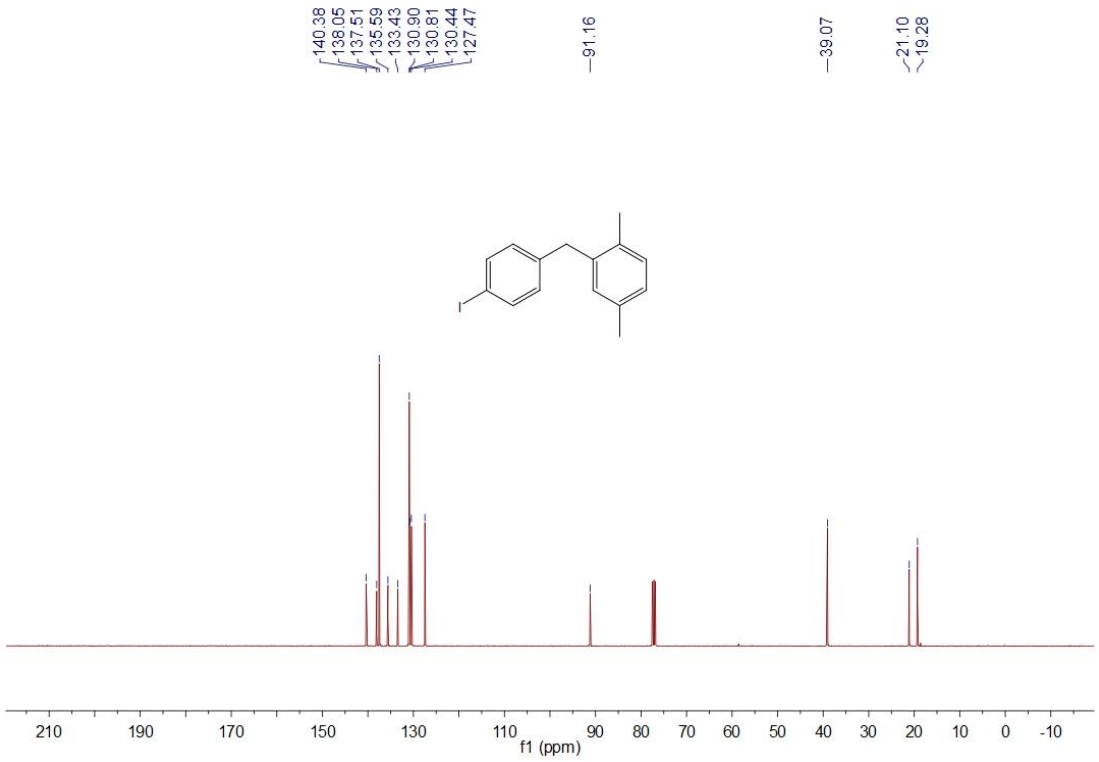
2-(4-Bromobenzyl)-1,4-dimethylbenzene (3i)



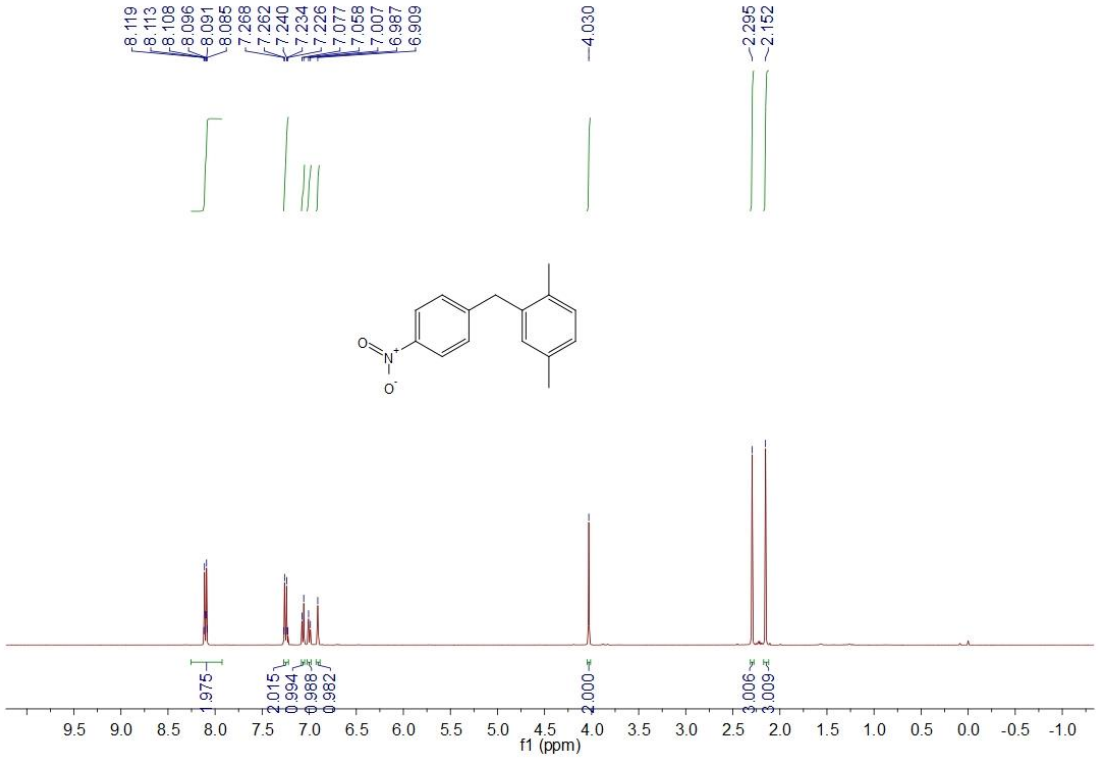


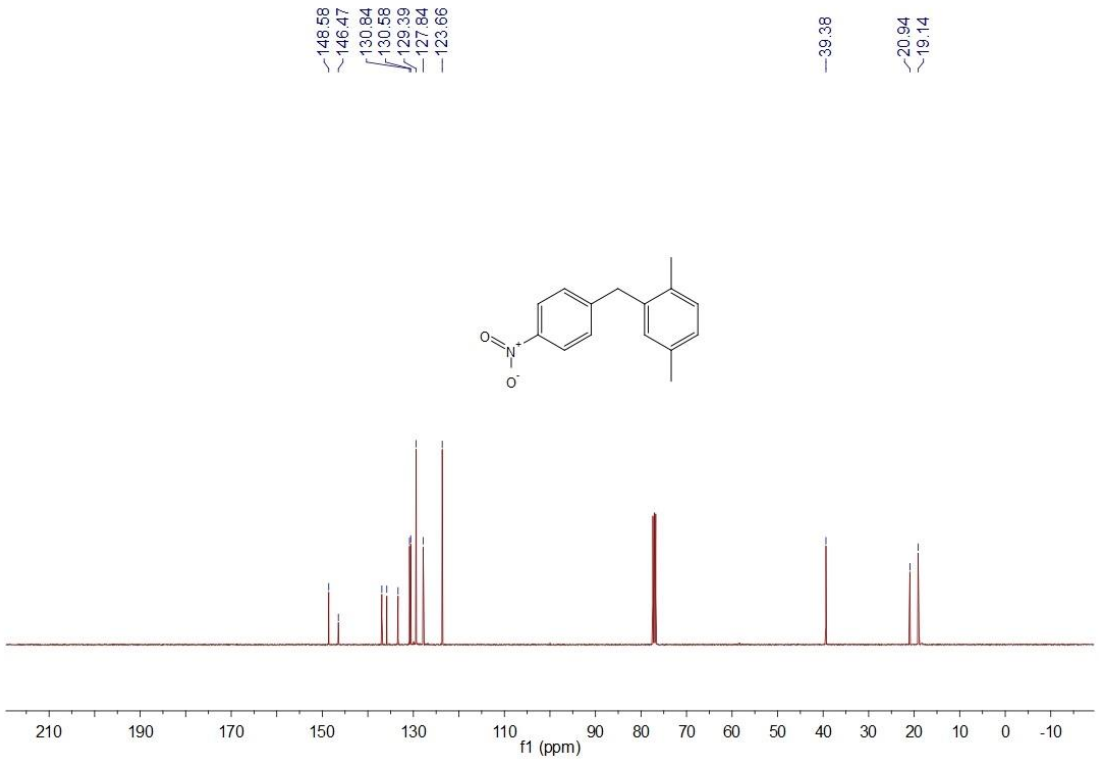
2-(4-Iodobenzyl)-1,4-dimethylbenzene (3j)



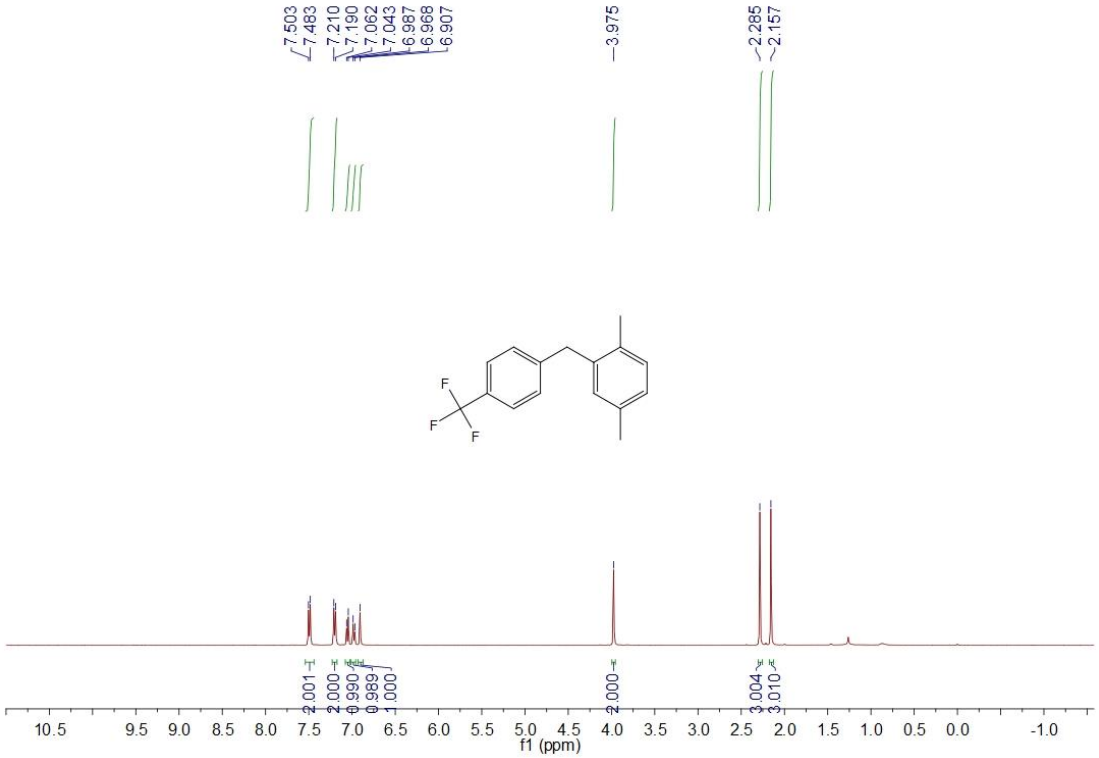


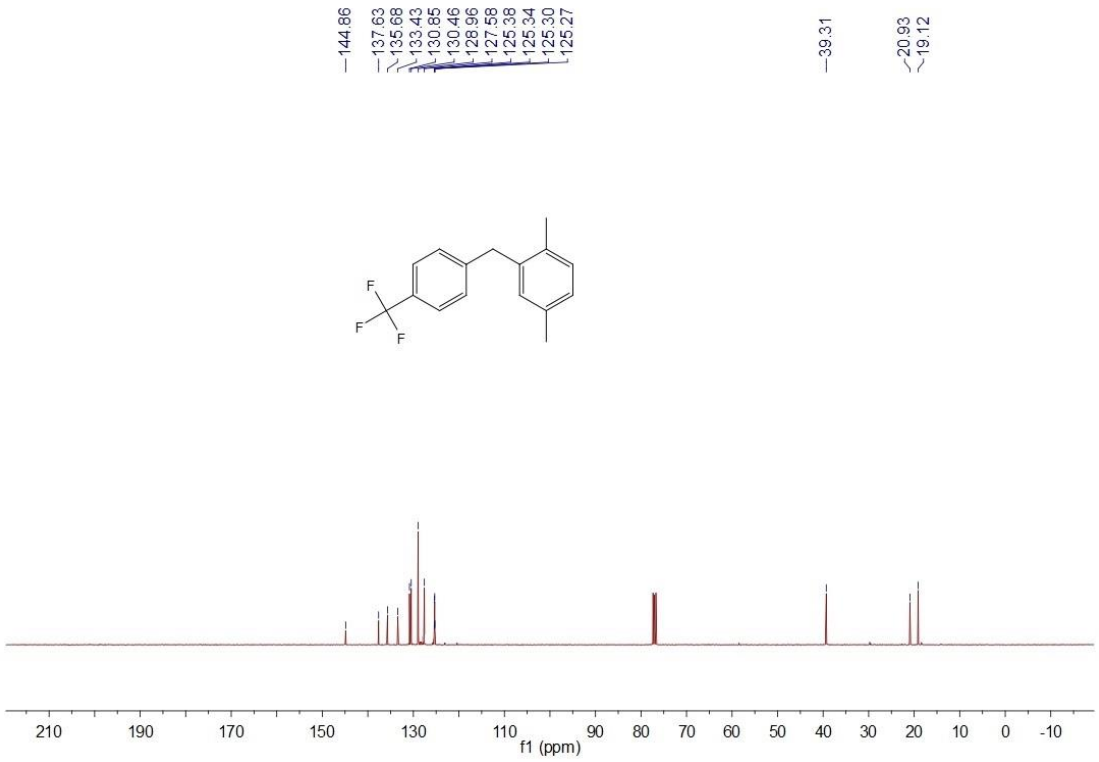
1,4-Dimethyl-2-(4-nitrobenzyl)benzene (3k)

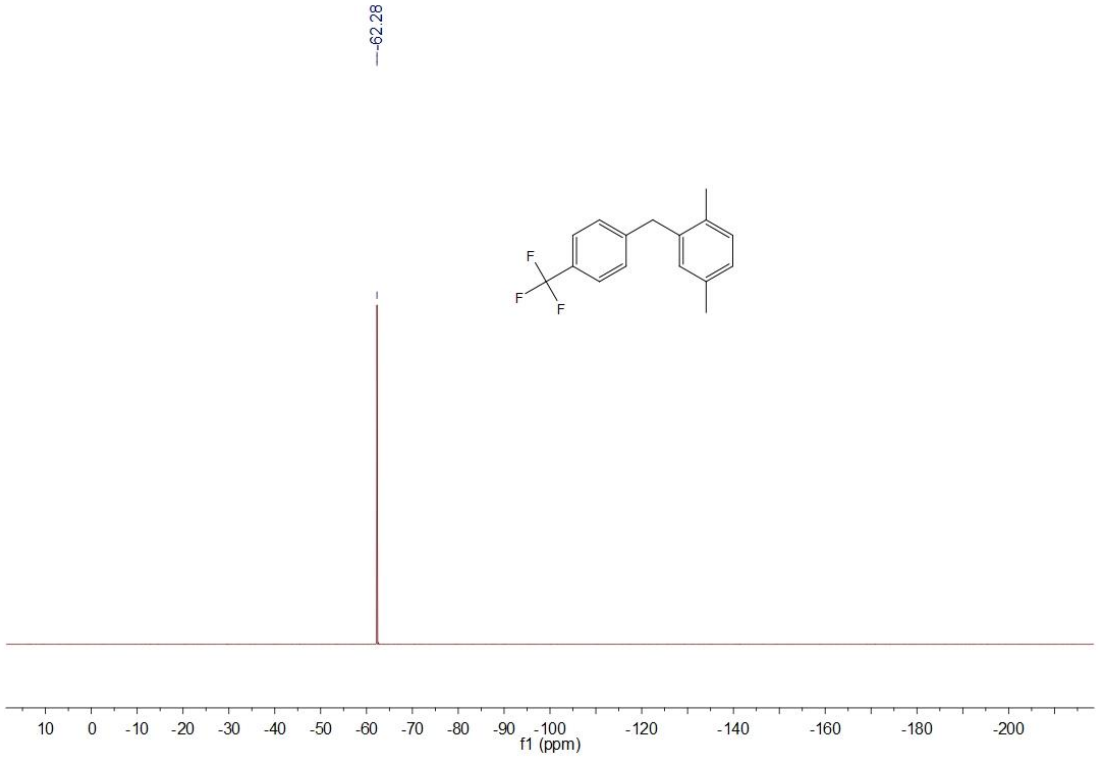




1,4-Dimethyl-2-(4-(trifluoromethyl)benzyl)benzene (3l)






-62.28
F
F
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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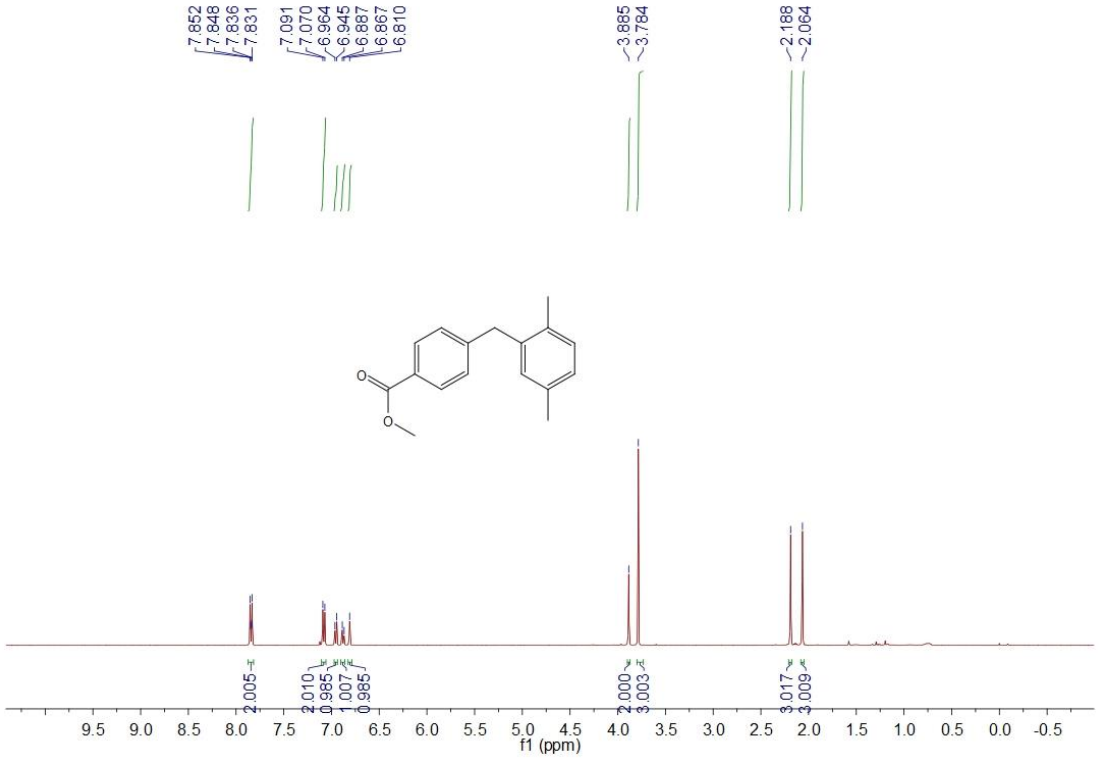
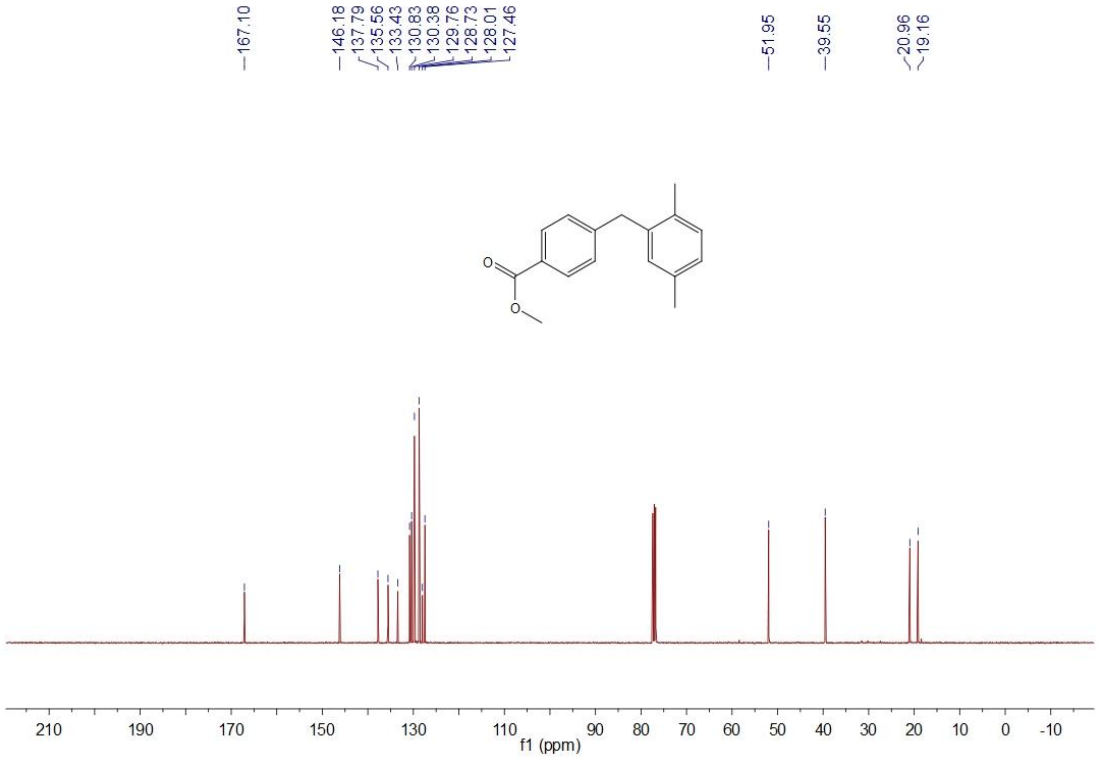
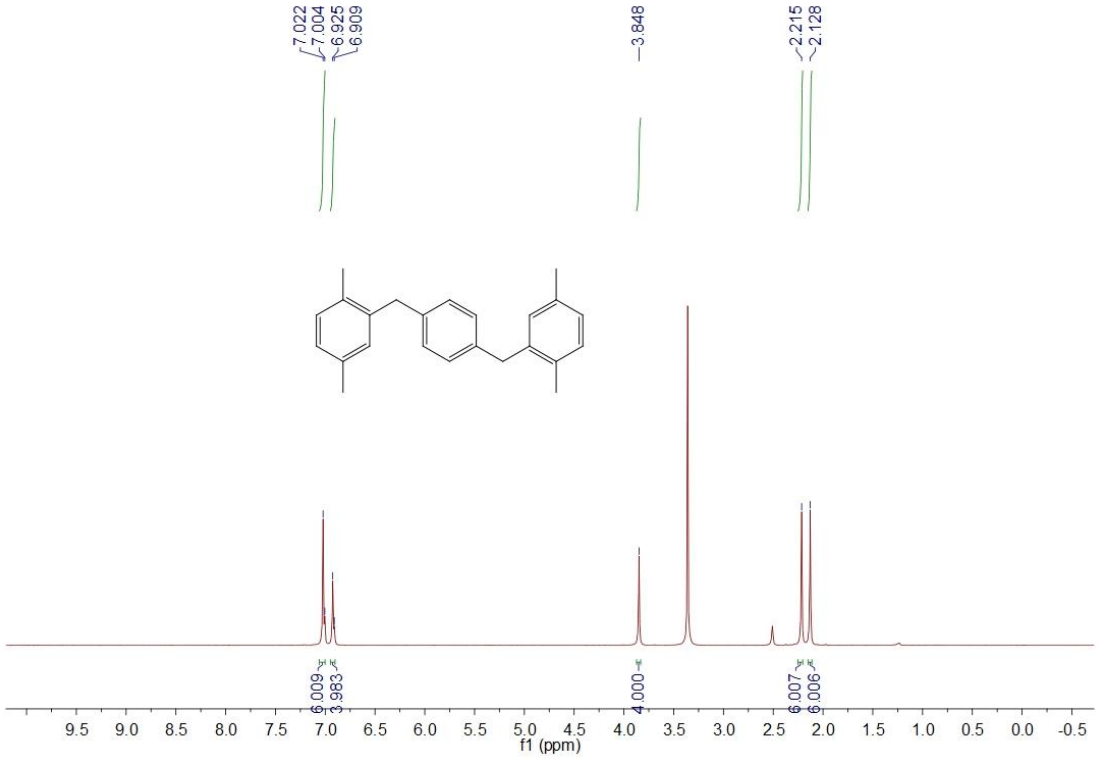
-120
-140
-160
-180
-200
f1 (ppm)

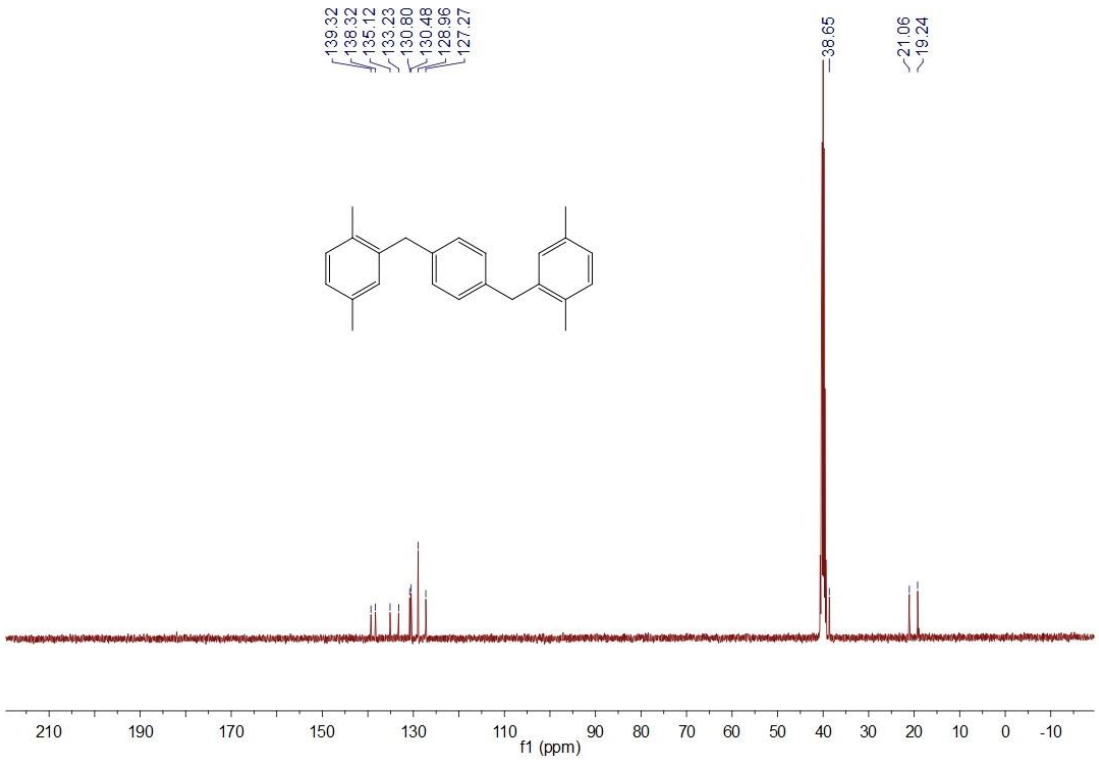
Methyl 4-(2,5-dimethylbenzyl)benzoate (3m)



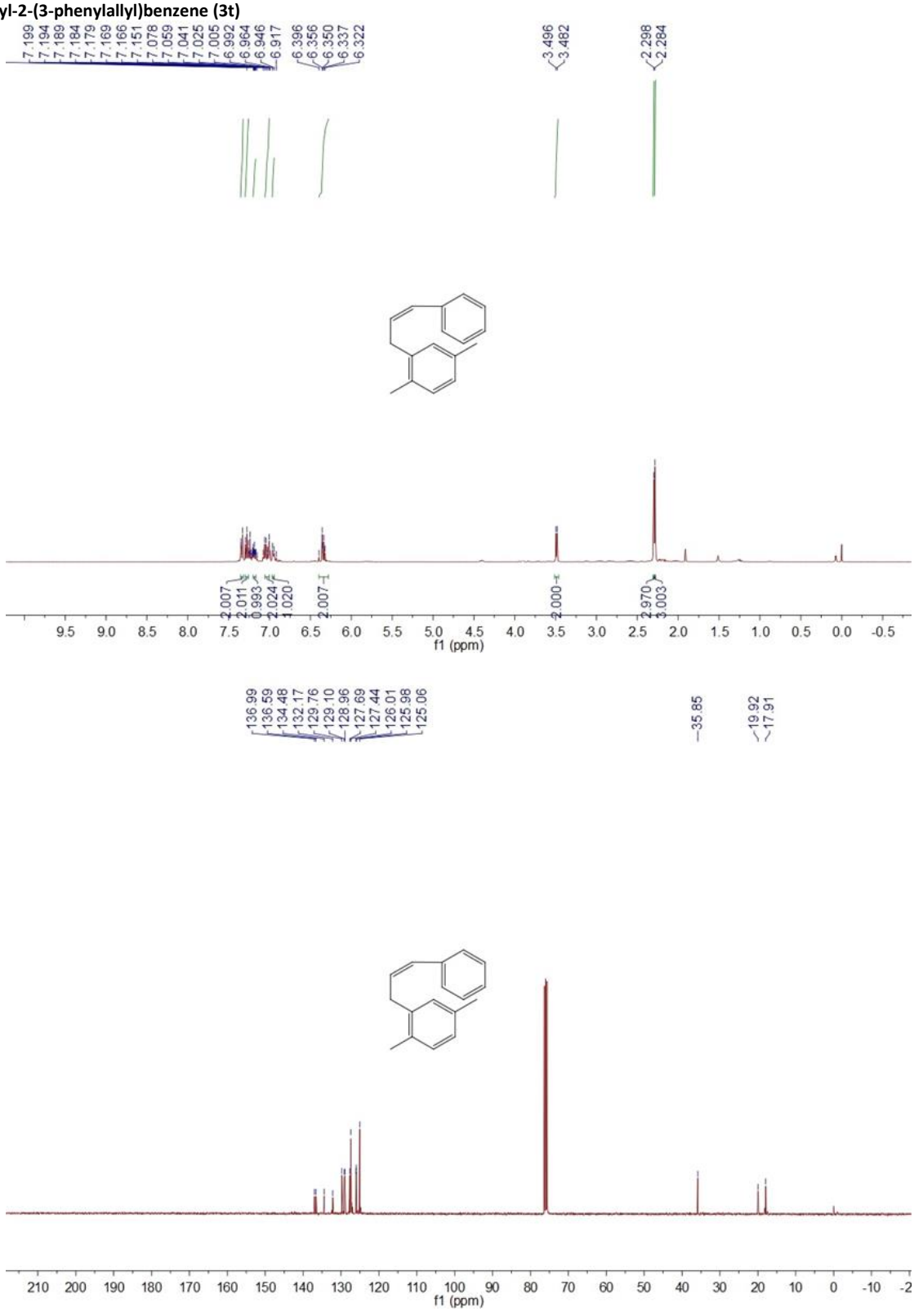


1,4-Bis(2,5-dimethylbenzyl)benzene (3s)

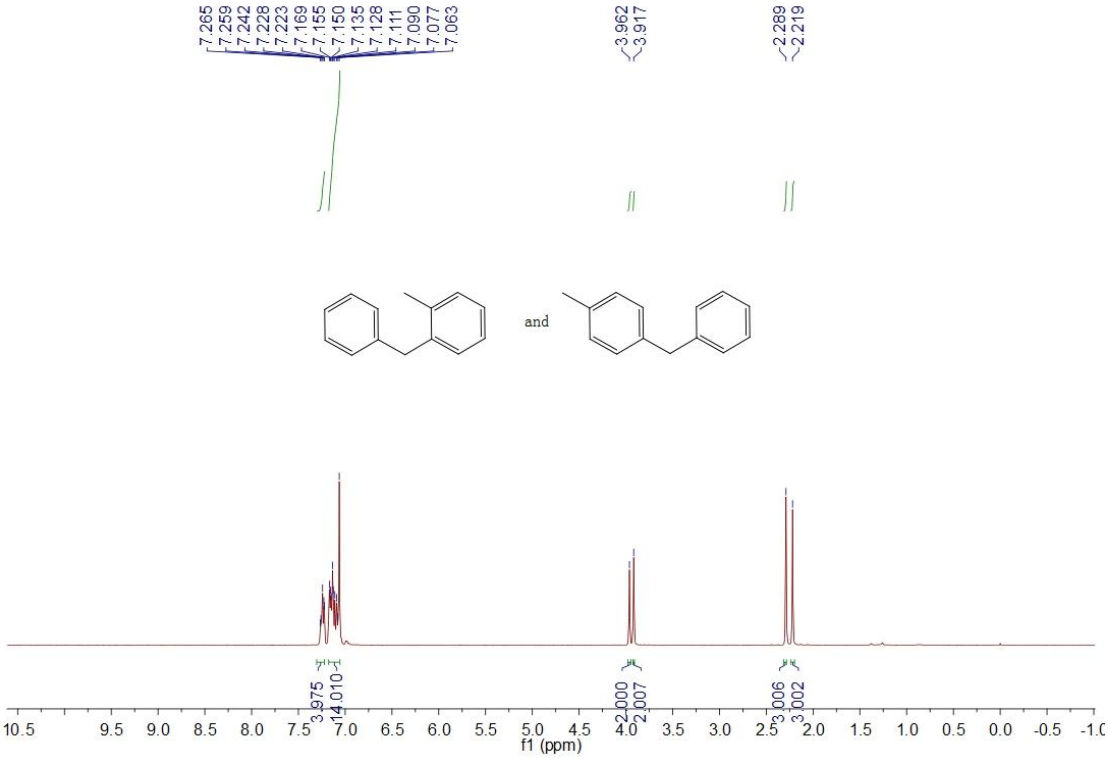


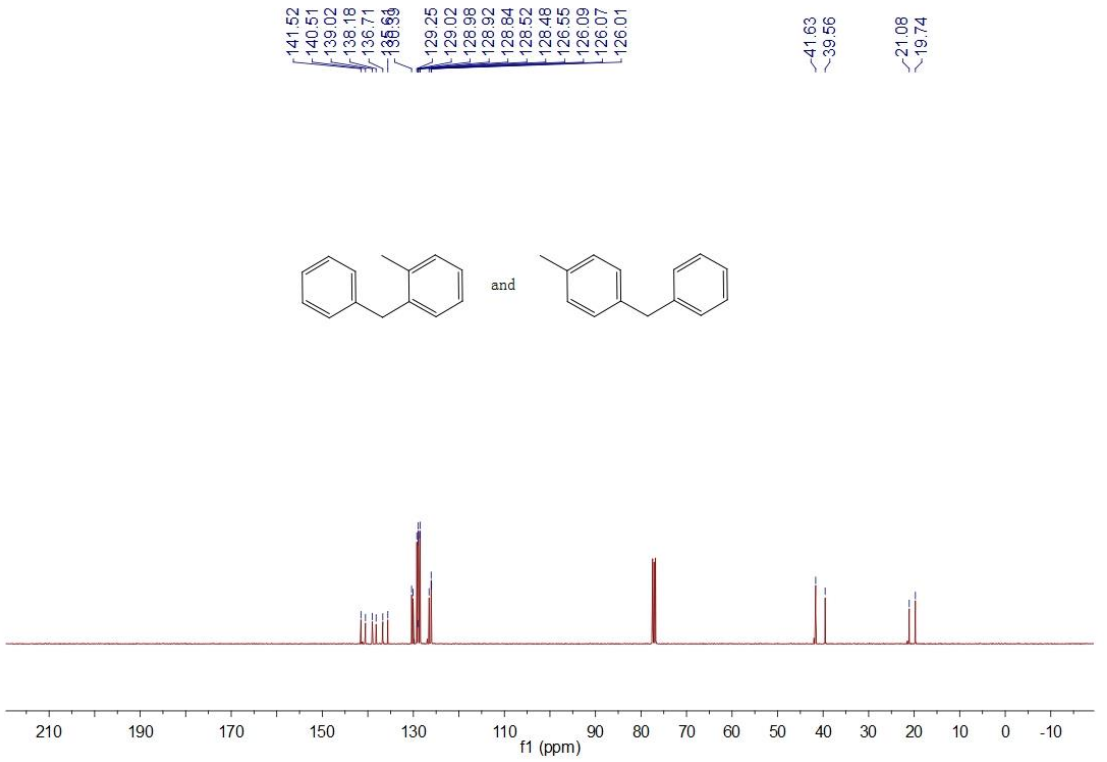


1,4-Dimethyl-2-(3-phenylallyl)benzene (3t)

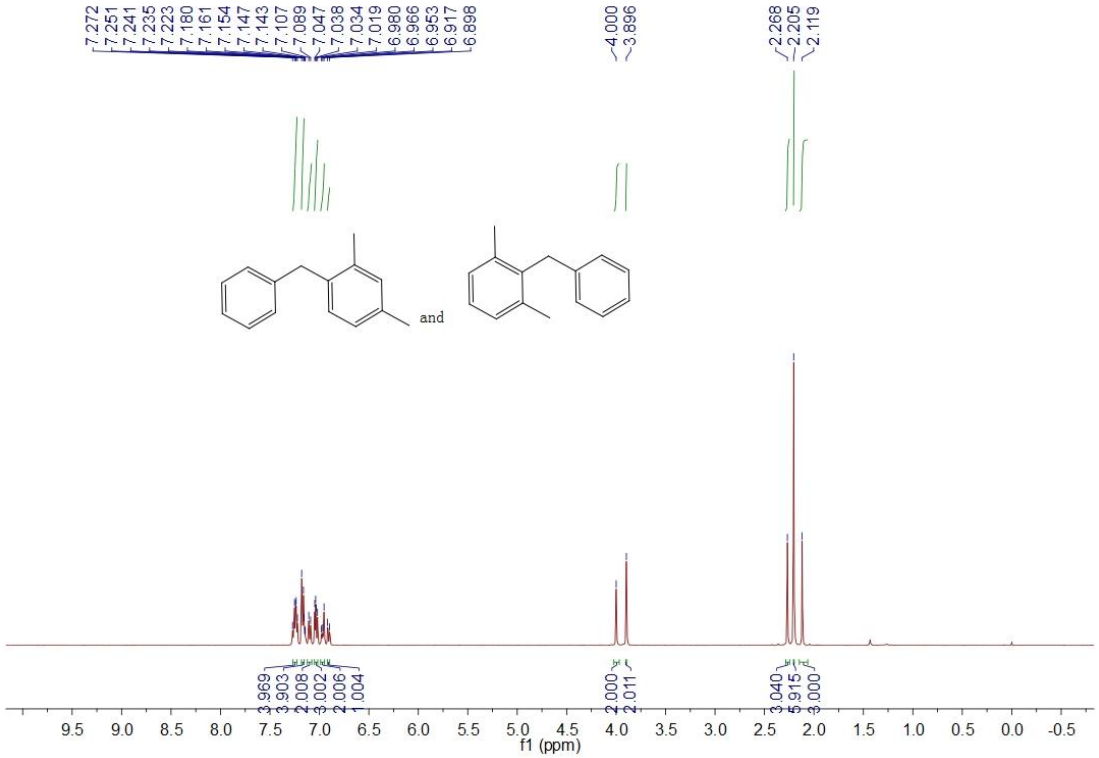


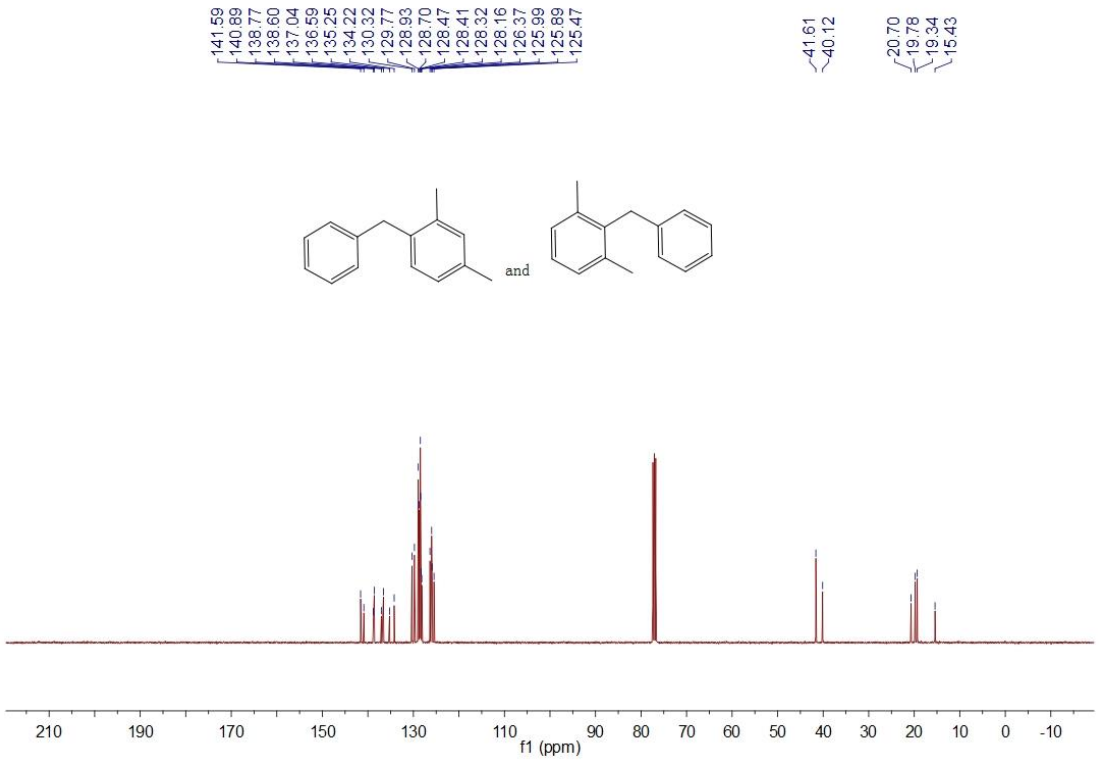
1-Benzyl-2-methylbenzene and 1-benzyl-4-methylbenzene (3u)



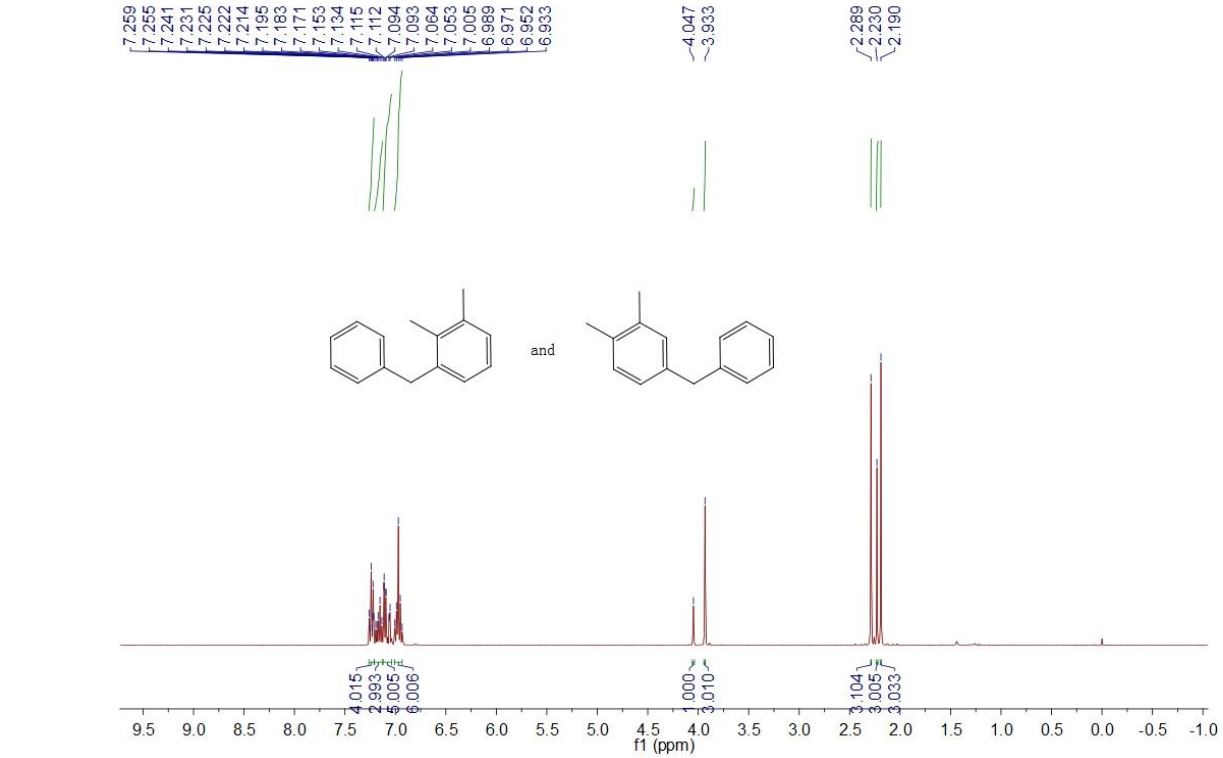


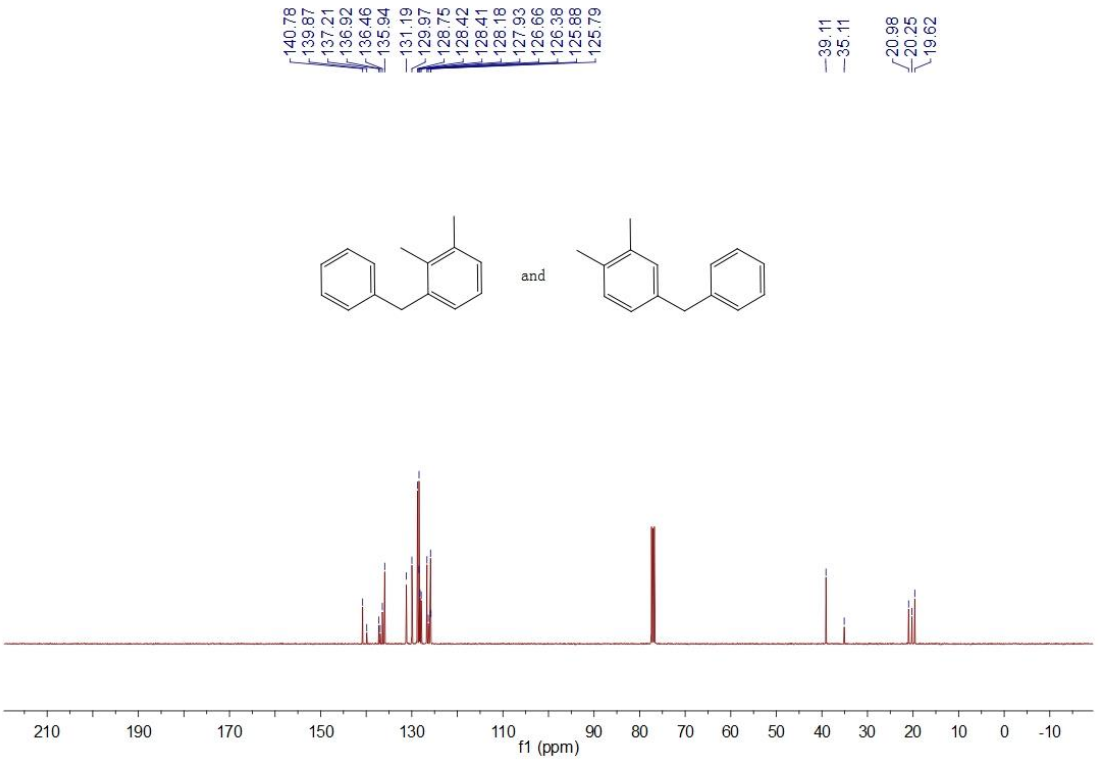
1-Benzyl-2,4-dimethylbenzene and 2-benzyl-1,3-dimethylbenzene (3v)



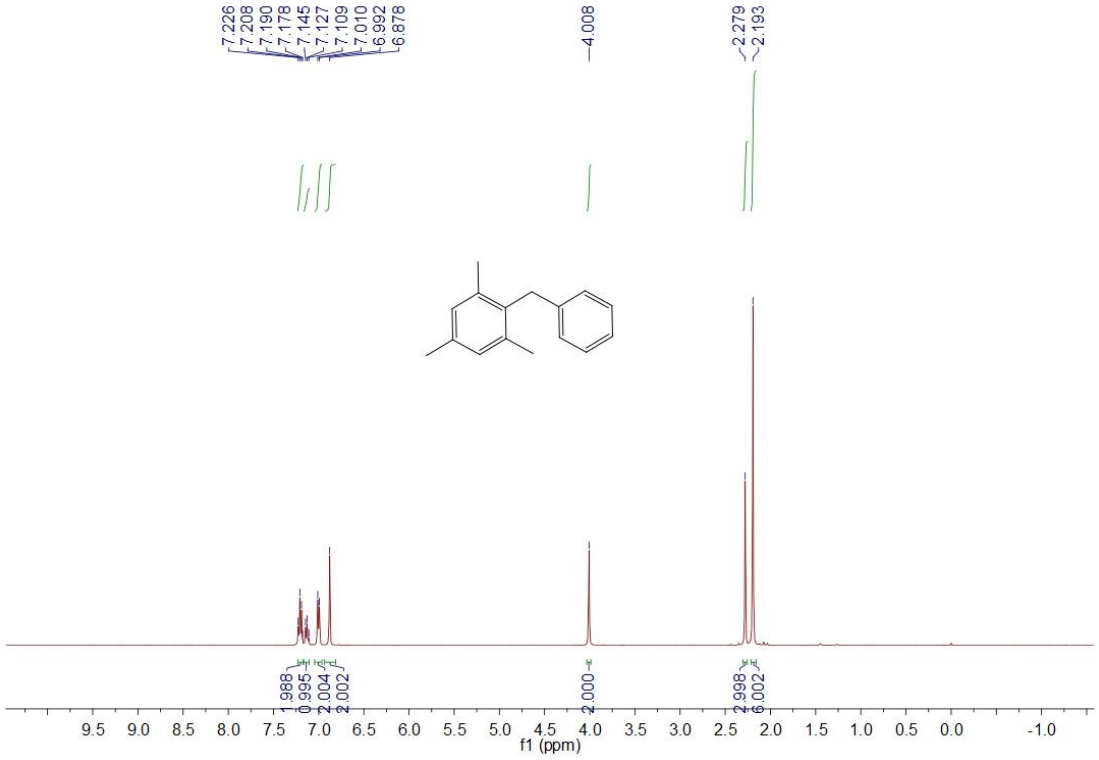


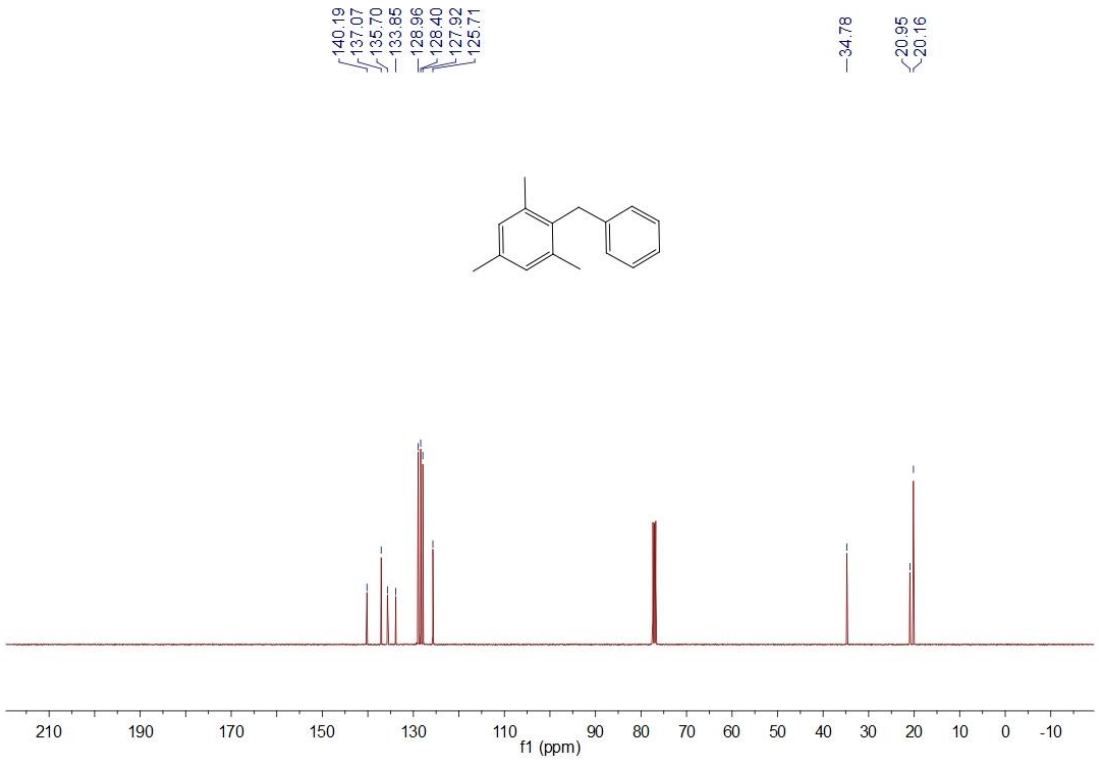
4-Benzyl-1,2-dimethylbenzene and 2-benzyl-1,2-dimethylbenzene (3w)



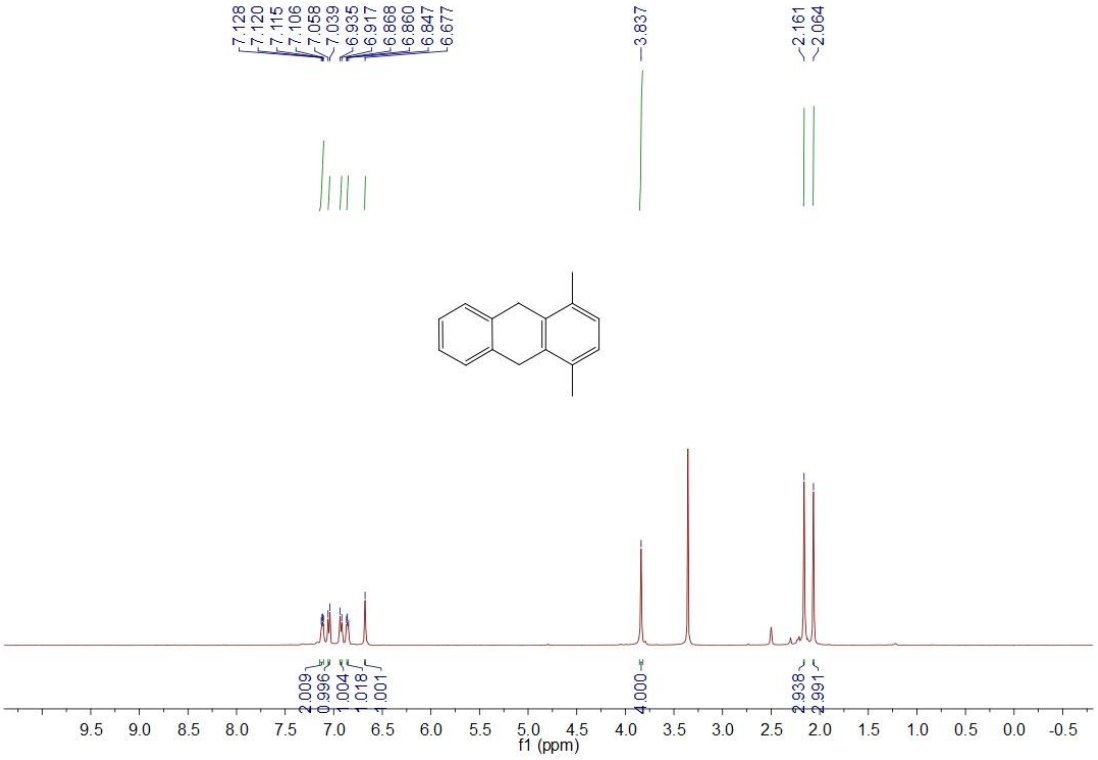


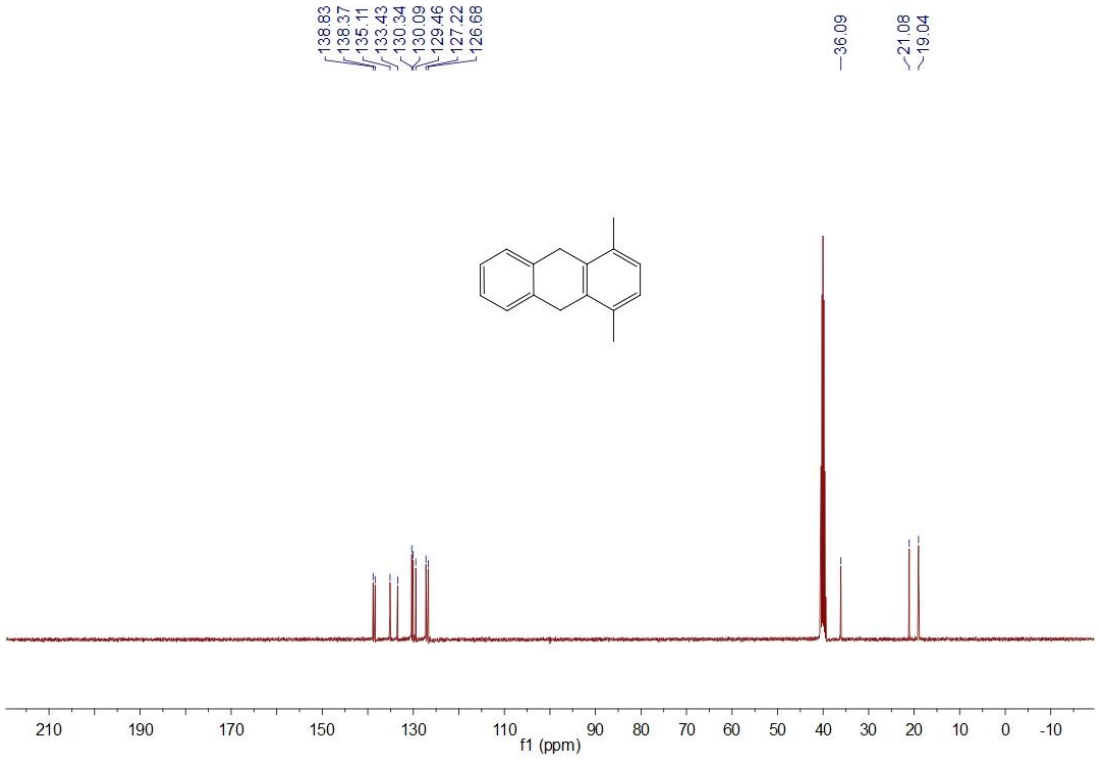
2-Benzyl-1,3,5-trimethylbenzene (3x)



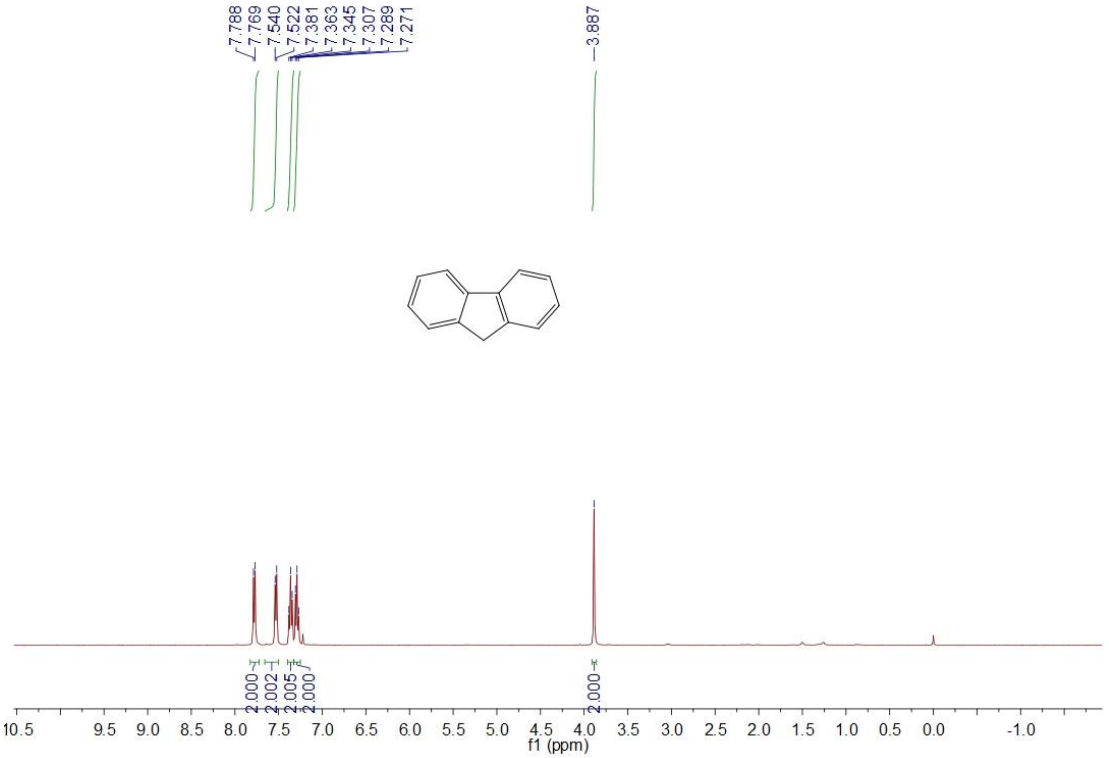


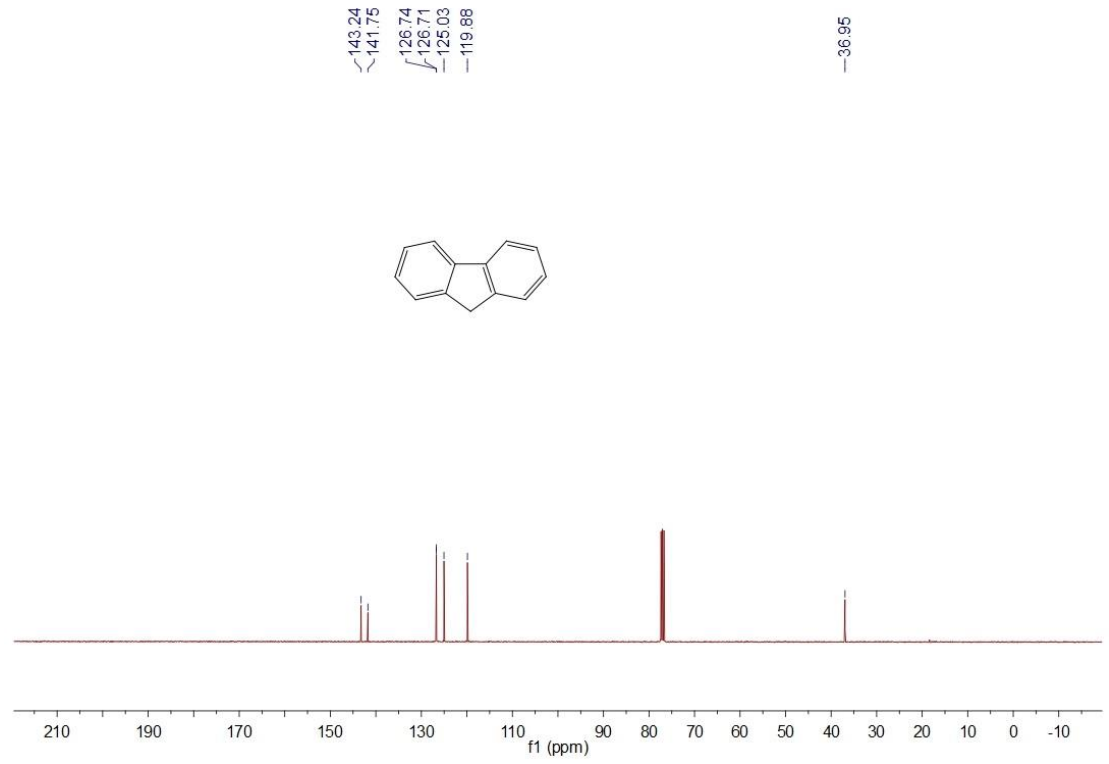
1,4-Dimethyl-9,10-dihydroanthracene (3z)



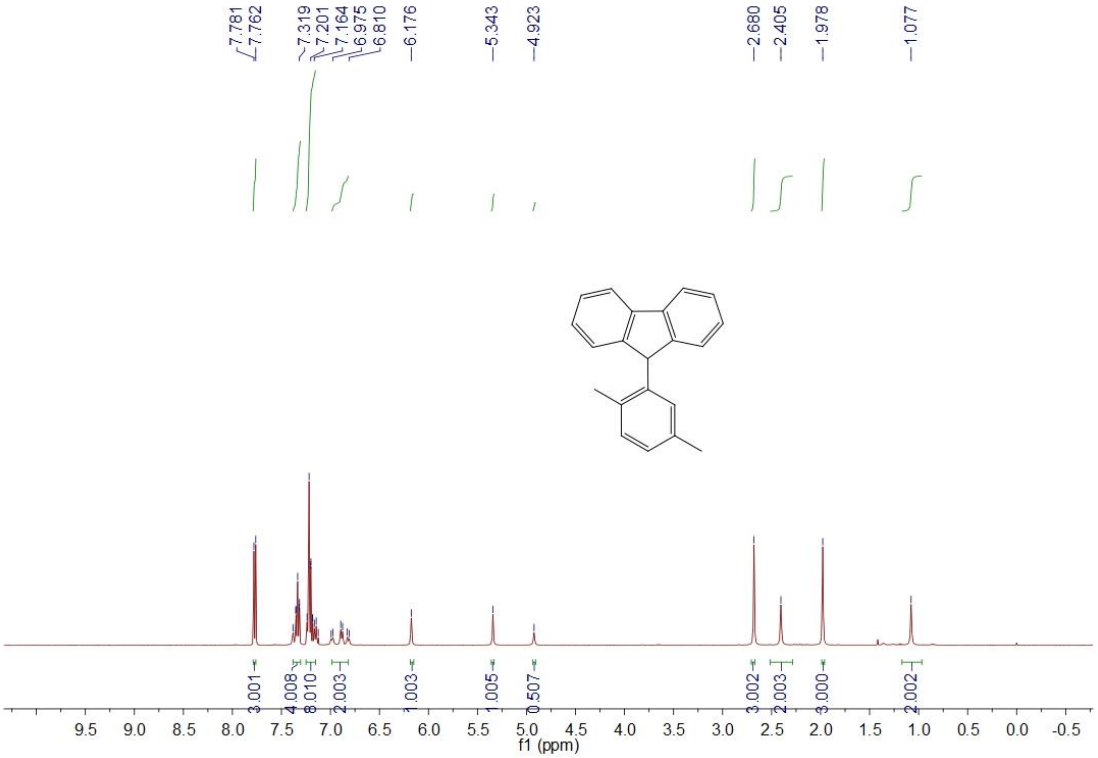


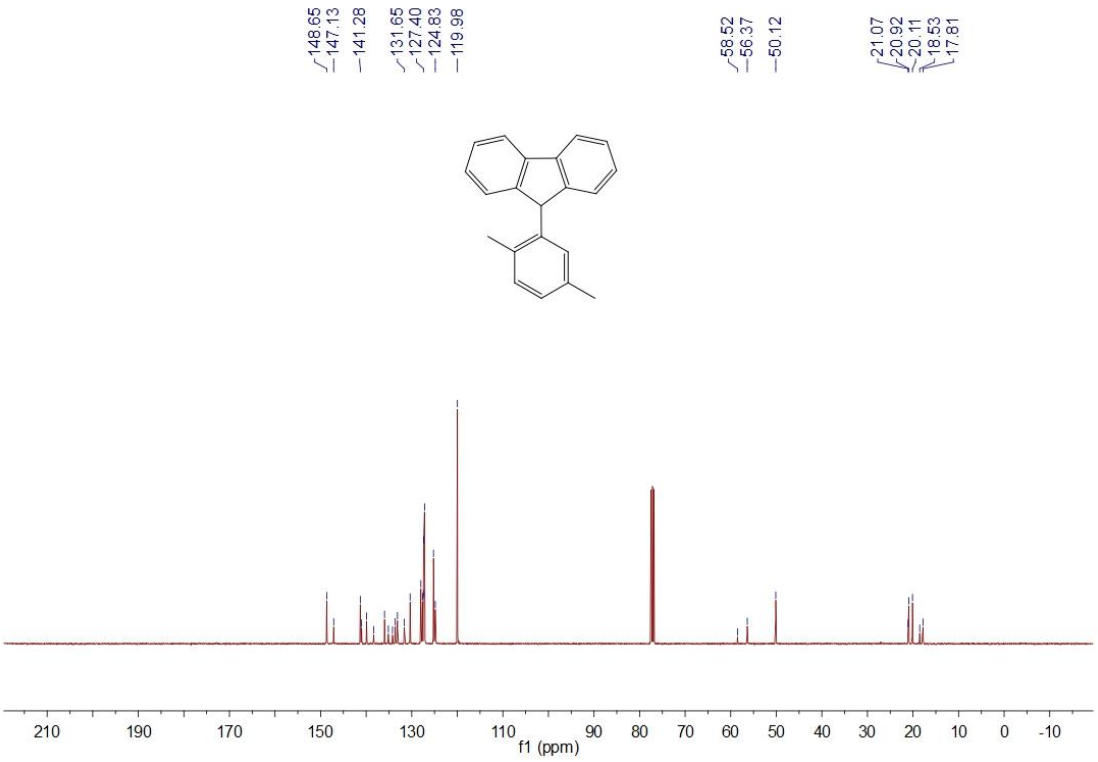
9*H*-Fluorene (3aa)





9-(2,5-Dimethylphenyl)-9*H*-fluorene (3ab)





9-Mesityl-9*H*-fluorene (3ac)