

## Supporting Information

### **‘On-water’ organic synthesis: A green, highly efficient, low cost and reusable catalyst system for biaryl synthesis under aerobic conditions at room temperature**

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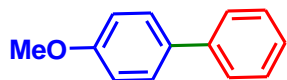
## Materials and Methods

All aryl/heteroaryl bromides and arylboronic acids were used as received (Alfa Aesar, MARC, Sigma-Aldrich). All other chemicals were purchased from commercial sources and used without further purification.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded at 500 MHz using TMS as internal standard. Mass spectroscopy data of the product of Suzuki reaction was collected on a MS-EI instrument.

## General experimental procedure

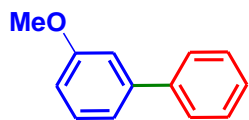
In a round bottomed flask, a mixture of aryl/heteroaryl halide (1 mmol), arylboronic acid (1.2 mmol),  $\text{PdCl}_2$  (0.01 mmol), sucrose (0.005 mmol) and  $\text{K}_2\text{CO}_3$  (1.2 mmol) in  $\text{H}_2\text{O}$  (3 mL) and the mixture was stirred at room temperature for a time period as mentioned in Table 2 in the manuscript. The progress of the reaction was monitored by TLC. After completion of the reaction it was extracted with diethyl ether (3 x 10 mL) and washed with water. The combined ether extract was dried over anhydrous  $\text{Na}_2\text{SO}_4$ . The filtrate was concentrated under reduced pressure. The product was purified by column chromatography over silica gel using *n*-hexane/ethyl acetate (9:1 v/v) to get the desired coupling product. The products were characterized by IR,  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectroscopy.

## Characterization data of the product of the Suzuki reaction<sup>1-22</sup>



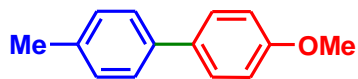
### 4-Methoxybiphenyl

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, TMS): δ 7.54–7.53 (m, 4 H), 7.42 (t, 2 H, *J* = 8 Hz), 7.28 (t, 1 H, *J* = 15 Hz), 6.98 (d, 2 H, *J* = 5 Hz), 3.85 (s, 3 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, TMS): δ 161.5, 139, 129, 128.8, 128.5, 127.6, 127.5, 127.37, 127.34, 127.32, 127.30, 114.7, 57.6; MS (EI): *m/z* (%) = 184 (100) [M<sup>+</sup>].



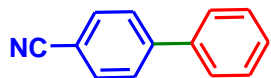
### 3-Methoxybiphenyl

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, TMS): δ 7.62–7.59 (m, 2 H), 7.49–7.45 (m, 2 H), 7.41–7.38 (m, 2 H), 7.19–7.18 (m, 1 H), 7.14–7.12 (m, 1 H), 6.90 (ddd, 1 H, *J* = 10, 7.5, 1.5 Hz), 3.86 (s, 3 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, TMS): δ 161.7, 139, 129, 128.8, 128.5, 127.6, 127.5, 127.37, 127.34, 127.32, 127.2, 113, 57; MS (EI): *m/z* (%) = 184 (100) [M<sup>+</sup>].



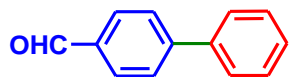
### 4-Methoxy-4'-methylbiphenyl

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  7.51 (d, 2 H,  $J = 8.0$  Hz), 7.45 (d, 2 H,  $J = 8.0$  Hz), 7.22 (d, 2 H,  $J = 8.0$  Hz), 6.97 (d, 2 H,  $J = 8.5$  Hz), 3.84 (s, 3 H), 2.38 (s, 3 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 158.7, 137.8, 136.2, 133.6, 129.3, 127.8, 126.4, 114, 55.2, 20.9; MS (EI):  $m/z$  (%) = 198 (100) [ $\text{M}^+$ ].



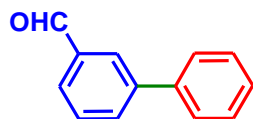
### Biphenyl-4-carbonitrile

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  7.73 (d, 2 H,  $J = 8.4$  Hz), 7.69 (d, 2 H,  $J = 8.5$  Hz), 7.58 (t, 2 H,  $J = 4.5$  Hz), 7.48 (t, 2 H,  $J = 7.5$  Hz), 7.42–7.37 (m, 1 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 145.5, 139.6, 132.5, 129.0, 128.5, 127.6, 127.5, 127.37, 127.34, 127.32, 127.1, 118.8, 110.7; MS (EI):  $m/z$  (%) = 179 (100) [ $\text{M}^+$ ].



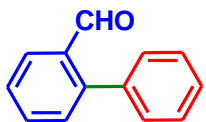
### Biphenyl-4-carbaldehyde

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  1.08 (s, 1 H), 7.95 (d, 2 H,  $J = 1.5$  Hz), 7.79 (d, 2 H,  $J = 1.5$  Hz), 7.65 (d, 2 H,  $J = 1.5$  Hz), 7.49 (t, 2 H,  $J = 1.0$  Hz), 7.43 (t, 1 H,  $J = 1.5$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 192.2, 145.8, 137.6, 133.5, 130.6, 130.3, 129.9, 128.1, 127.9, 127.8, 127.6, 127.5, 127.4; MS (EI):  $m/z$  (%) = 182 (100) [ $\text{M}^+$ ].



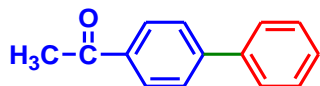
### Biphenyl-3-carbaldehyde

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  9.85 (s, 1 H), 8.04 (s, 1 H), 7.68–7.66 (m, 2 H), 7.58–7.55 (m, 1 H), 7.48 (d, 2 H,  $J = 1.0$  Hz), 7.43–7.37 (m, 3 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 192.4, 145.8, 137.6, 133.57, 133.51, 129.9, 129.8, 129.5, 128.5, 128.3, 127.5, 127.46, 127.43; MS (EI):  $m/z$  (%) = 182 (100) [ $\text{M}^+$ ].



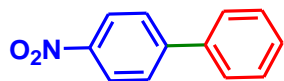
### Biphenyl-2-carbaldehyde

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  9.9 (s, 1 H), 8.02 (d, 1 H,  $J = 1$  Hz), 7.68–7.66 (m, 2 H), 7.50–7.41 (m, 6 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 192.3, 145.8, 137.6, 133.57, 133.50, 130.2, 129.9, 129.5, 127.9, 127.8, 127.6, 127.5, 127.4; MS (EI):  $m/z$  (%) = 182 (100) [ $\text{M}^+$ ].



### 1-Biphenyl-4-yl-ethanone

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  8.04 (d, 2 H,  $J = 7.0$  Hz), 7.69 (d, 2 H,  $J = 5.0$  Hz), 7.63 (t, 2 H,  $J = 5.5$  Hz), 7.49 (t, 2 H,  $J = 7.5$  Hz), 7.42–7.40 (m, 1 H), 2.64 (s, 3 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 197.7, 145.6, 139.7, 135.7, 128.86, 128.82, 128.14, 127.18, 127.13, 26.6; MS (EI):  $m/z$  (%) = 196 (51) [ $\text{M}^+$ ].



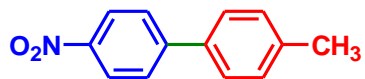
### 4-Nitrobiphenyl

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  8.31 (d, 2 H,  $J = 7.5$  Hz), 7.75 (d, 2 H,  $J = 9.0$  Hz), 7.64 (d, 2 H,  $J = 7.0$  Hz), 7.51 (t, 2 H,  $J = 7.5$  Hz), 7.46 (t, 1 H,  $J = 7.2$  Hz);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 147.6, 142.7, 135.7, 128.86, 128.82, 128.14, 127.92, 127.18; MS (EI):  $m/z$  (%) = 199 (100)  $[\text{M}^+]$ .



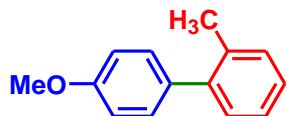
### 4-Methoxy-4'-trifluoromethylbiphenyl

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  7.54 (d, 2 H,  $J = 3.0$  Hz), 7.5 (d, 2 H,  $J = 2.0$  Hz), 7.19 (d, 2 H,  $J = 7.5$  Hz), 6.96 (d, 2 H,  $J = 2$  Hz), 3.84 (s, 3 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 161.3, 139, 129, 128.8, 128.5, 127.6, 127.5, 127.37, 127.34, 127.32, 127.29, 119.06, 114.06, 57.1; MS (EI):  $m/z$  (%) = 252 (100)  $[\text{M}^+]$ .



### 4'-Methyl-4-nitrobiphenyl

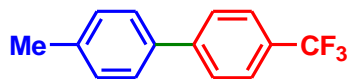
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, TMS): δ 8.29 (d, 2 H, *J* = 2.5 Hz), 7.72 (d, 2 H, *J* = 4.5 Hz), 7.35 (d, 2 H, *J* = 8.5 Hz), 7.29 (d, 2 H, *J* = 11.5 Hz), 2.42 (s, 3 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, TMS): 147.4, 146.7, 138.9, 135.7, 129.7, 127.3, 127.1, 123.9, 21.1; MS (EI): *m/z* (%) = 213 (100) [M<sup>+</sup>].



### 4'-Methoxy-2-methylbiphenyl

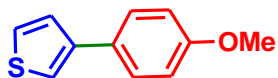
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, TMS): δ 7.30–7.22 (m, 6 H), 6.90 (d, 2 H, *J* = 2.0 Hz), 3.8 (s, 3 H), 2.2 (s, 3 H); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, TMS): 158.3, 141.4, 135.3, 134.2, 130.18, 130.14, 129.7, 126.8, 125.6, 113.3, 55.1, 20.4; MS (EI): *m/z* (%) = 198 (100) [M<sup>+</sup>].





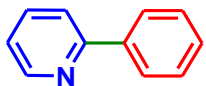
### 4'-Methyl-4-trifluoromethylbiphenyl

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  7.67 (s, 4 H), 7.50 (d, 2 H,  $J = 8.1$  Hz), 7.29 (d, 2 H,  $J = 8.0$  Hz), 2.41 (s, 3 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS): 139, 136.8, 133, 129, 128.8, 128.5, 127.6, 127.5, 127.37, 127.34, 127.32, 127.29, 119, 20; MS (EI):  $m/z$  (%) = 236 (100)  $[\text{M}^+]$ .



### 3-(4-Methoxy-phenyl)-thiophene

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  7.52 (d, 2 H,  $J = 1.5$  Hz), 7.38–7.34 (m, 3 H), 6.94 (d, 2 H,  $J = 7.0$  Hz), 3.84 (s, 3 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  158.7, 141.8, 128.6, 127.4, 125.9, 123.7, 114, 55.2; MS (EI):  $m/z$  (%) = 190 (100)  $[\text{M}^+]$ .



## 2-Phenylpyridine

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  8.3 (s, 1 H), 7.73–7.70 (m, 2 H), 7.48–7.43 (m, 2 H), 7.36–7.12 (m, 3 H), 6.7–6.6 (m, 1 H);  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ , TMS):  $\delta$  157.3, 149.5, 139.2, 136.6, 128.7, 128.5, 126.8, 121.9, 120.4; MS (EI)  $m/z$  155 ( $\text{M}^+$ , 100%); MS (EI):  $m/z$  (%) = 155 (100) [ $\text{M}^+$ ].

## References

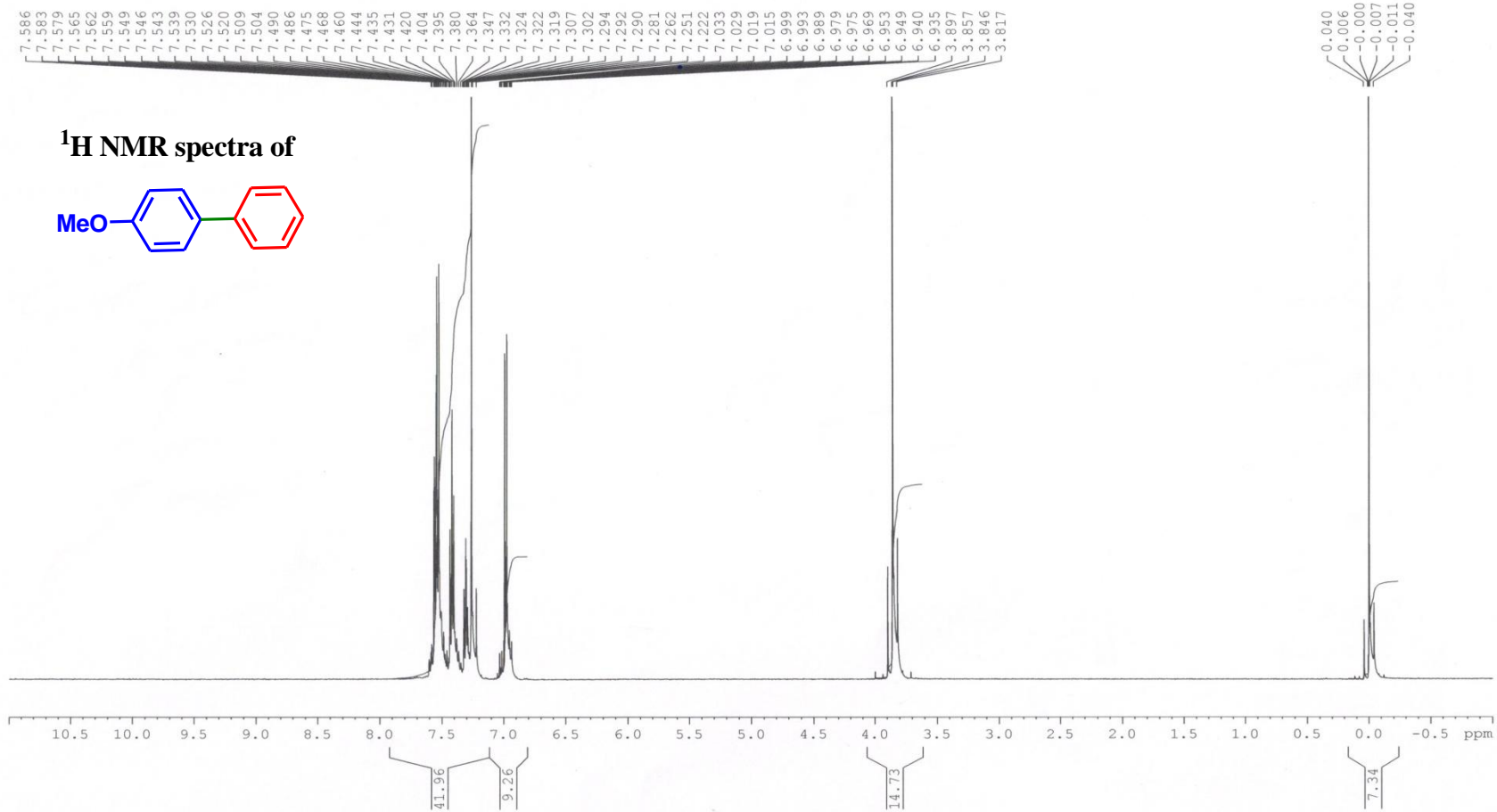
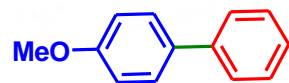
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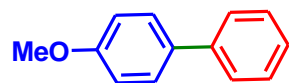
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Name of Sample: SB-1  
Spectrum No: 3570

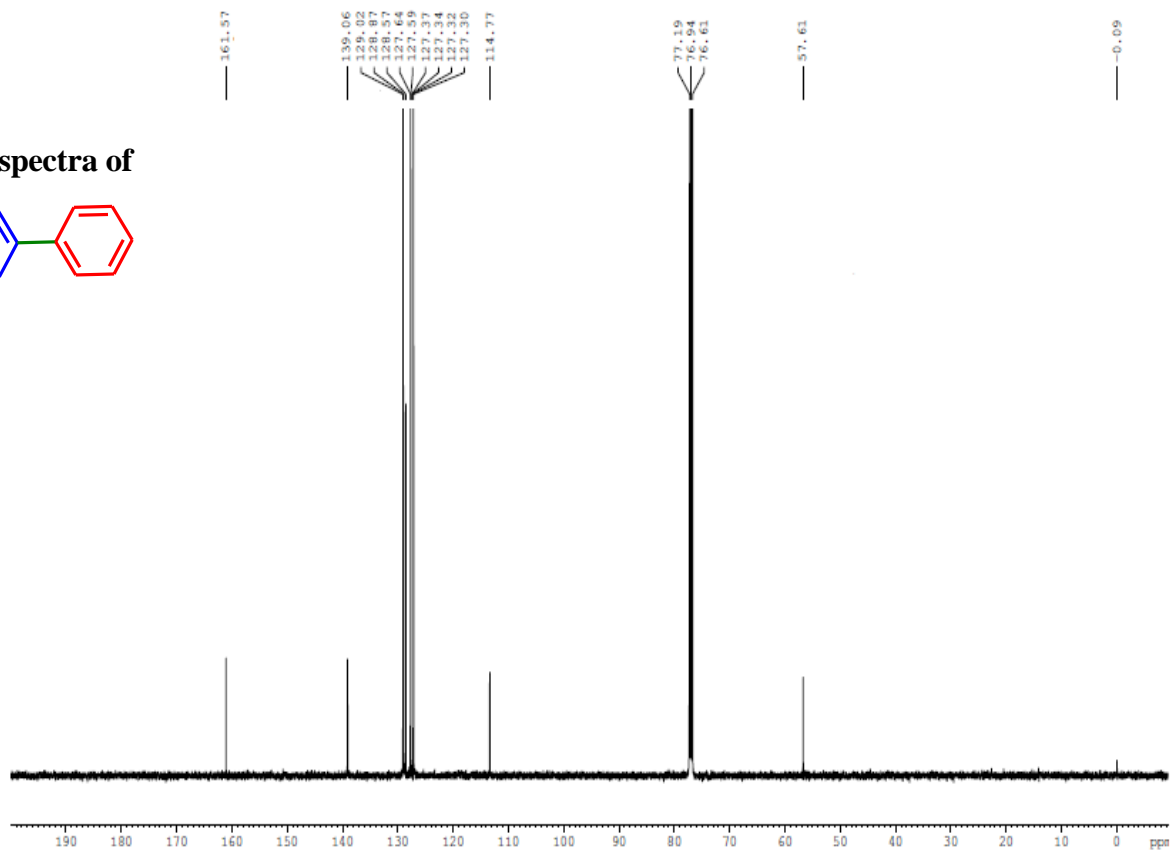
<sup>1</sup>H NMR spectra of



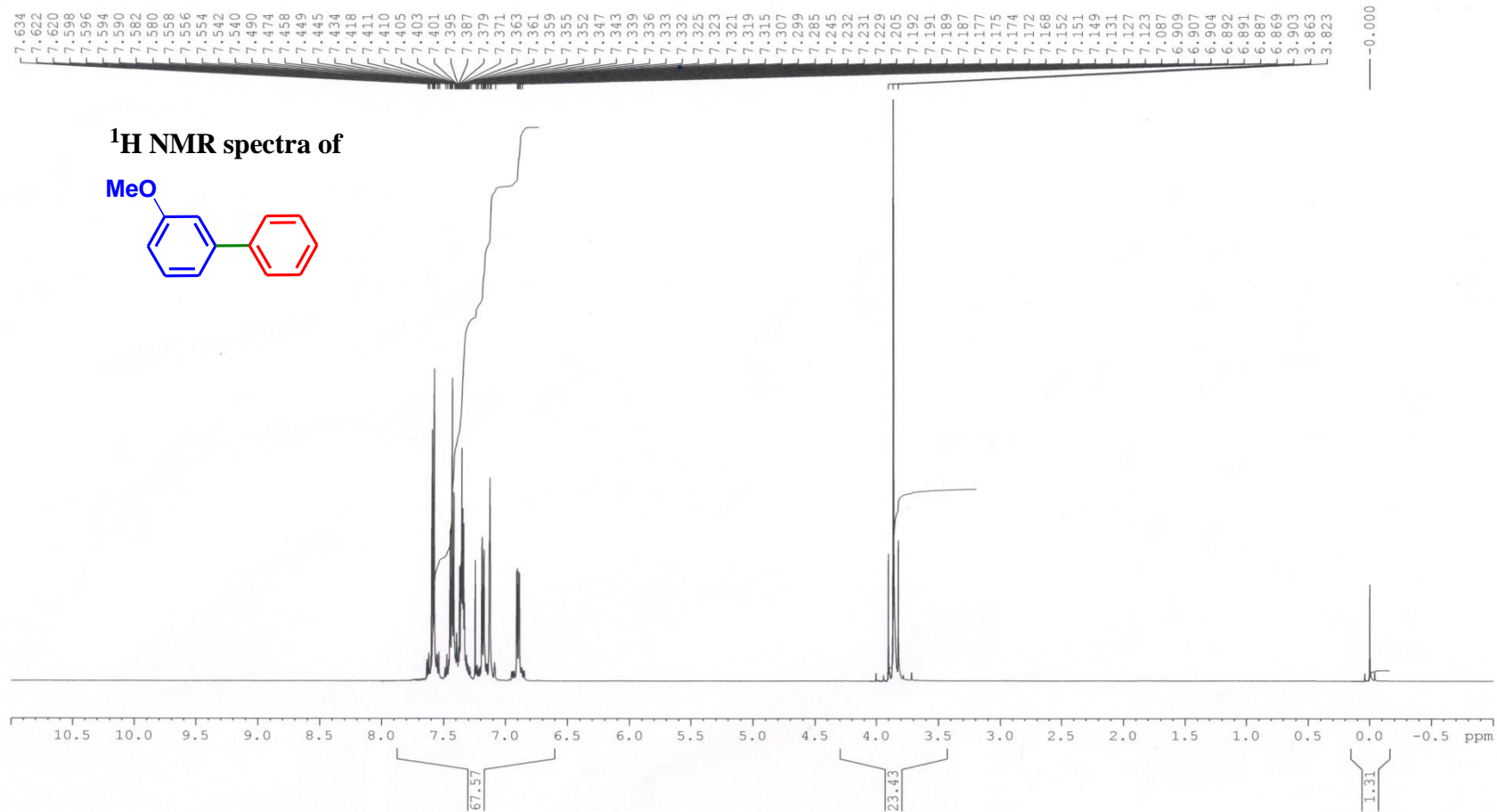
**<sup>13</sup>C NMR spectra of**



Name of Sample: S-2  
Spectrum No : 2522

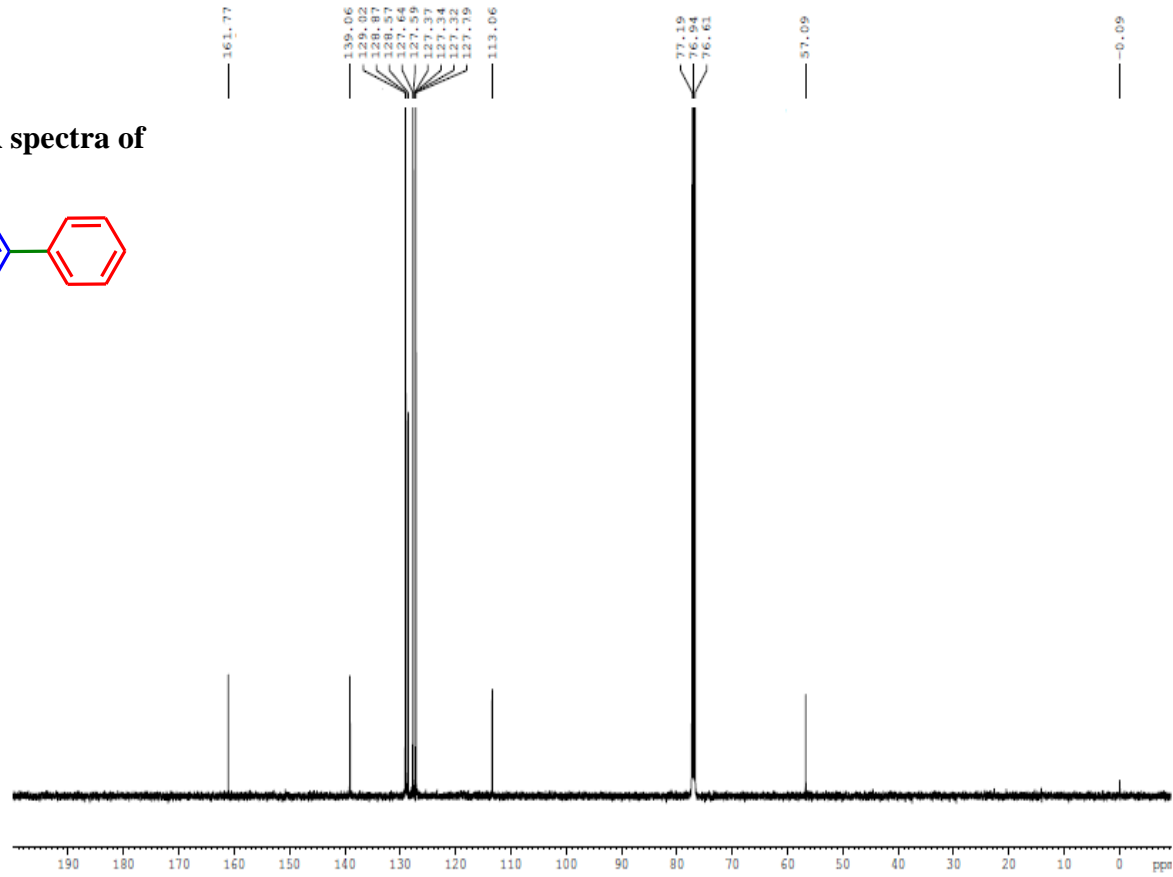
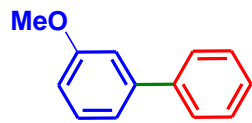


Name of Sample: SB-7  
Spectrum No.: 3757



Name of Sample:S-21  
Spectrum No:2527

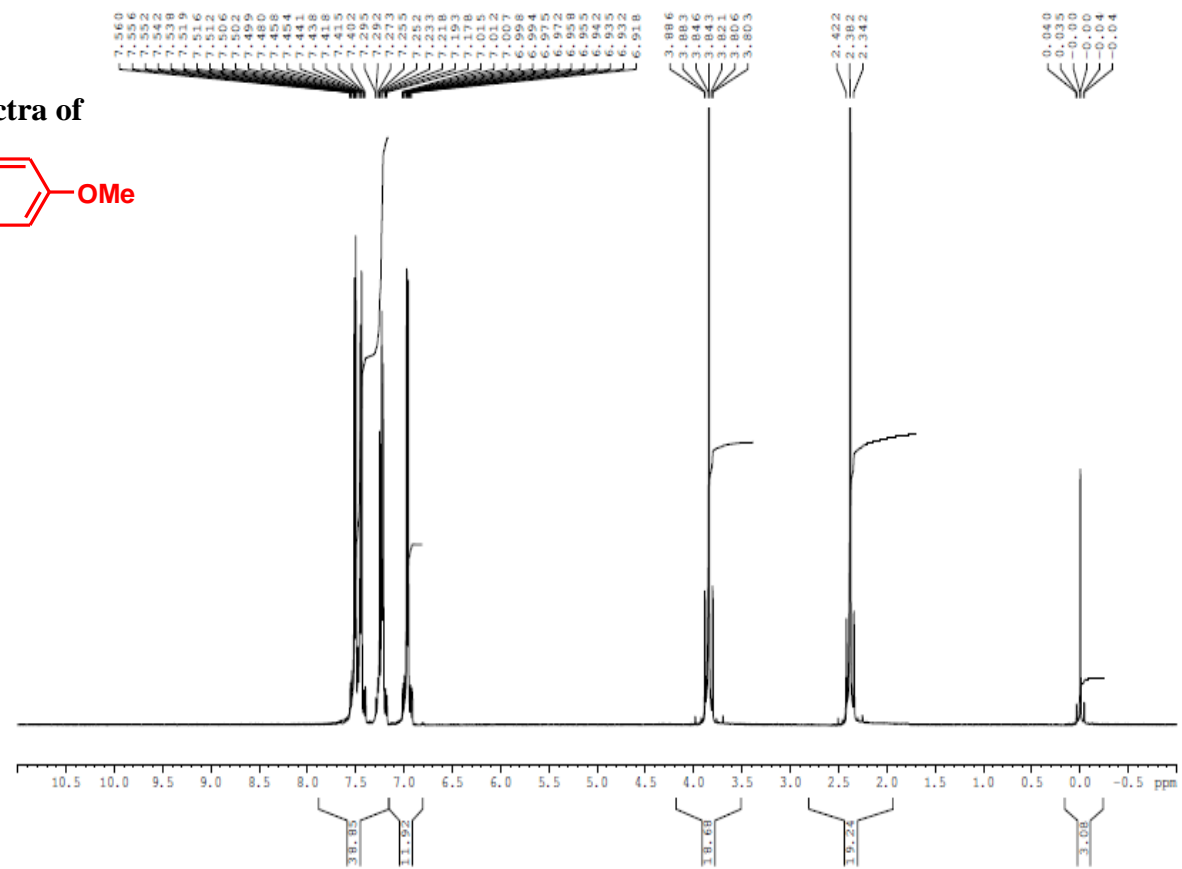
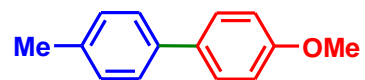
<sup>13</sup>C NMR spectra of





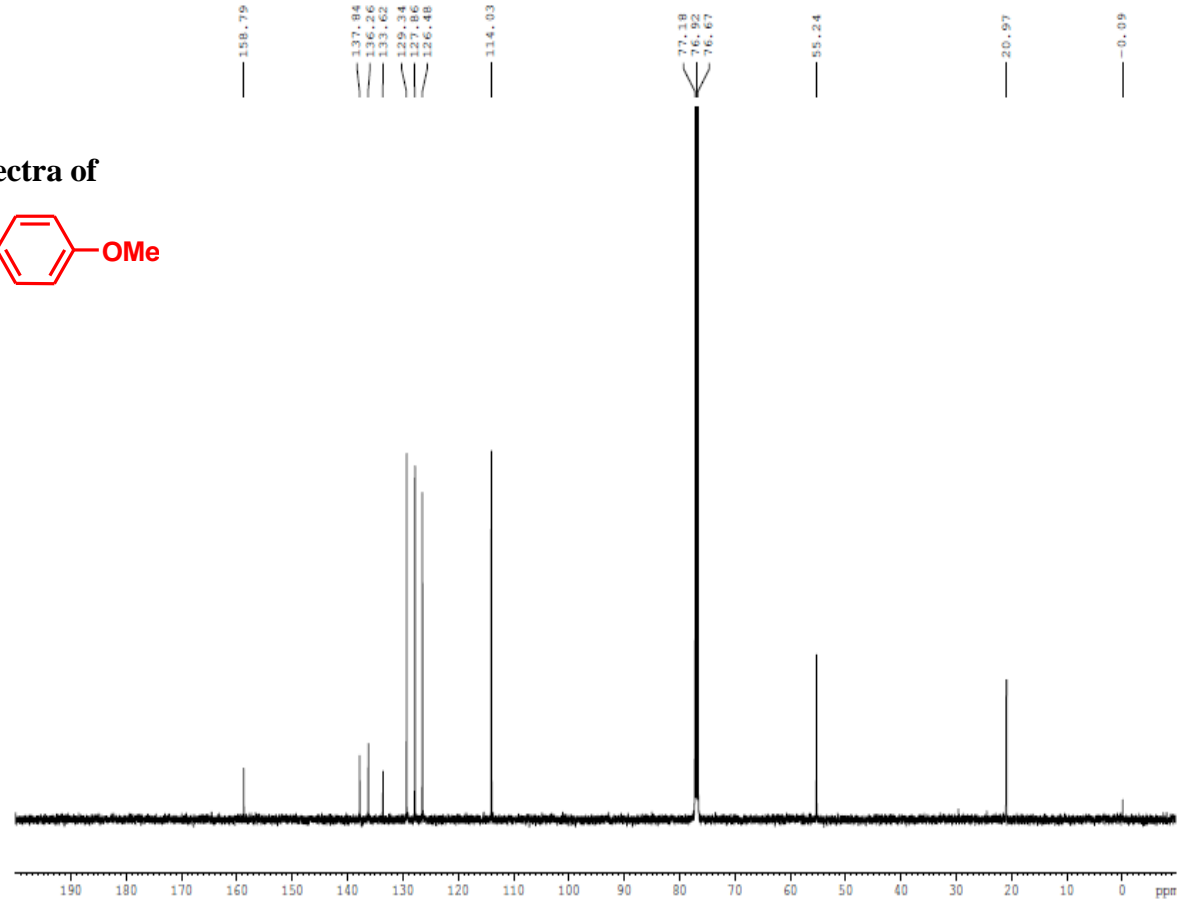
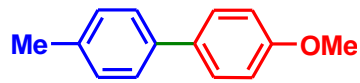
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Spectrum No: 2562

<sup>1</sup>H NMR spectra of



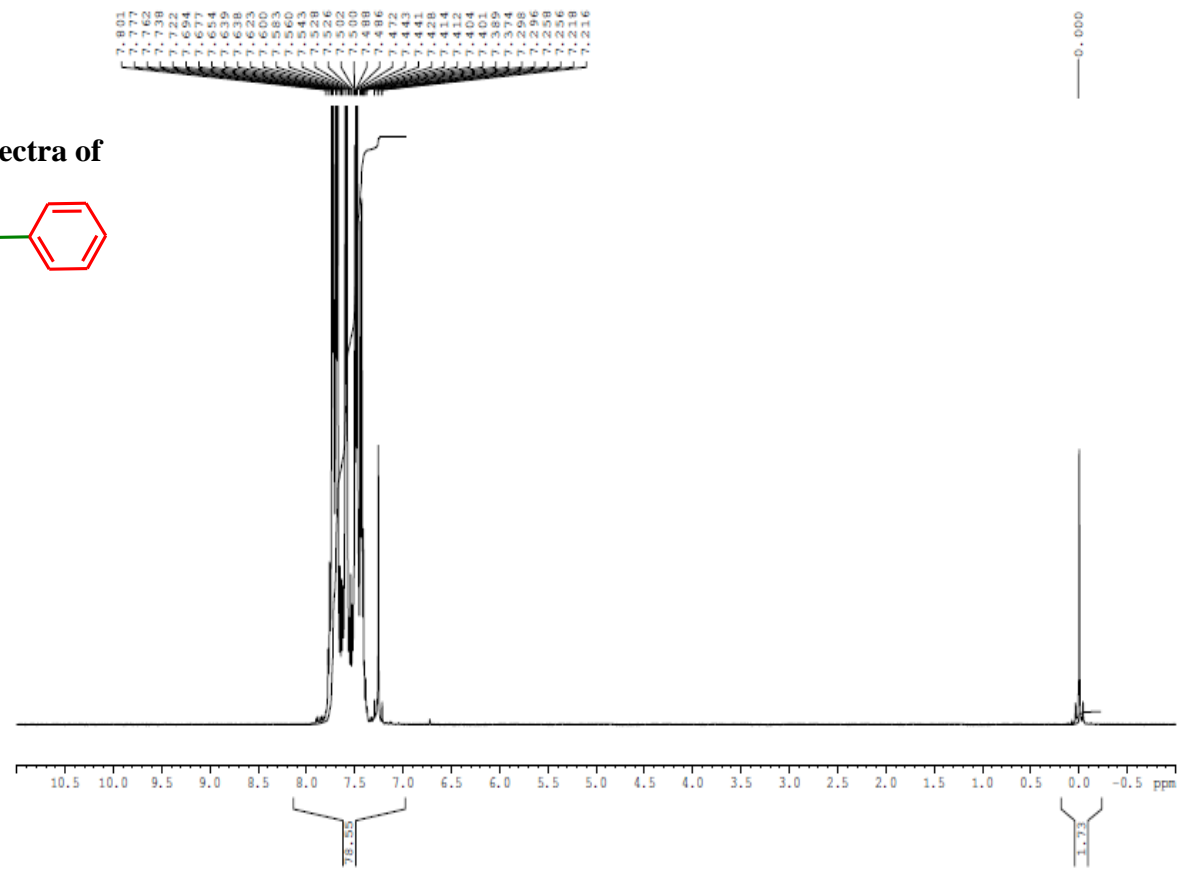
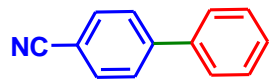
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<sup>13</sup>C NMR spectra of



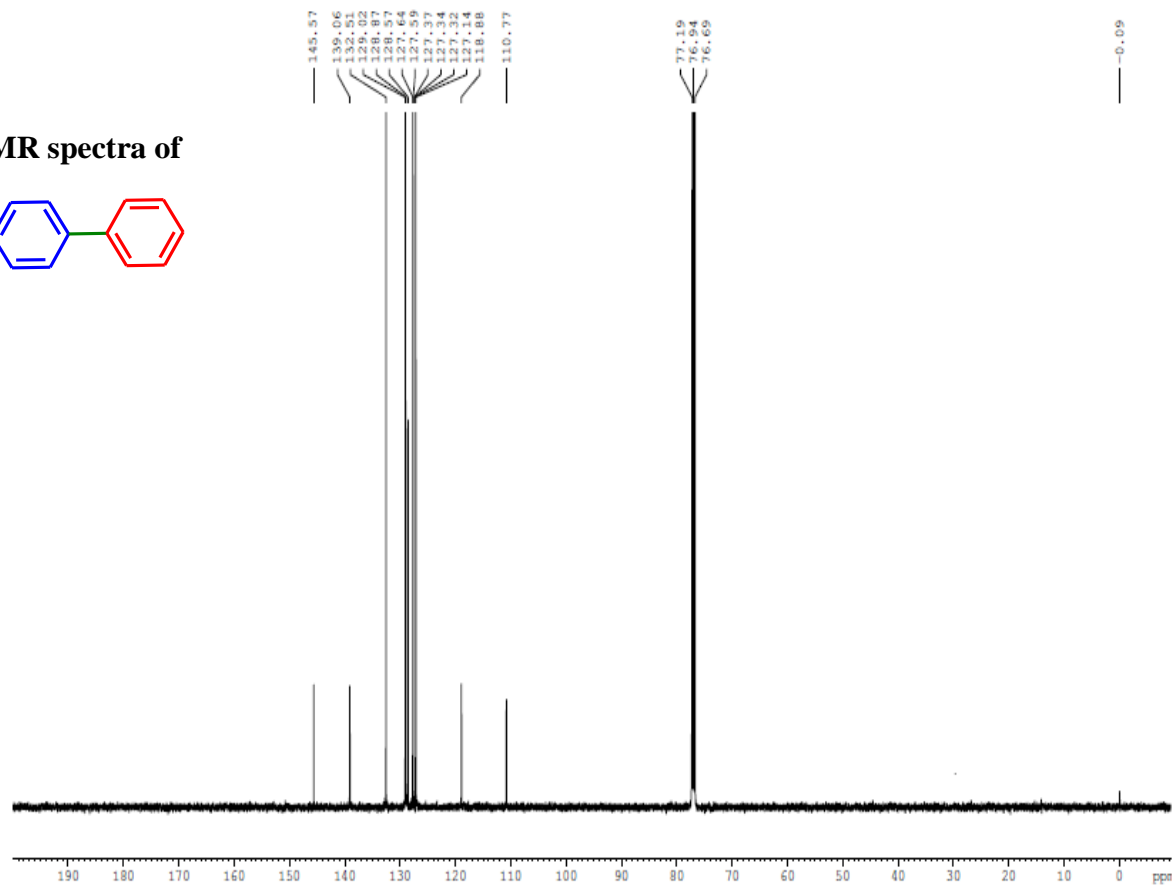
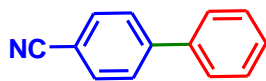
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Spectrum No: 2437

<sup>1</sup>H NMR spectra of

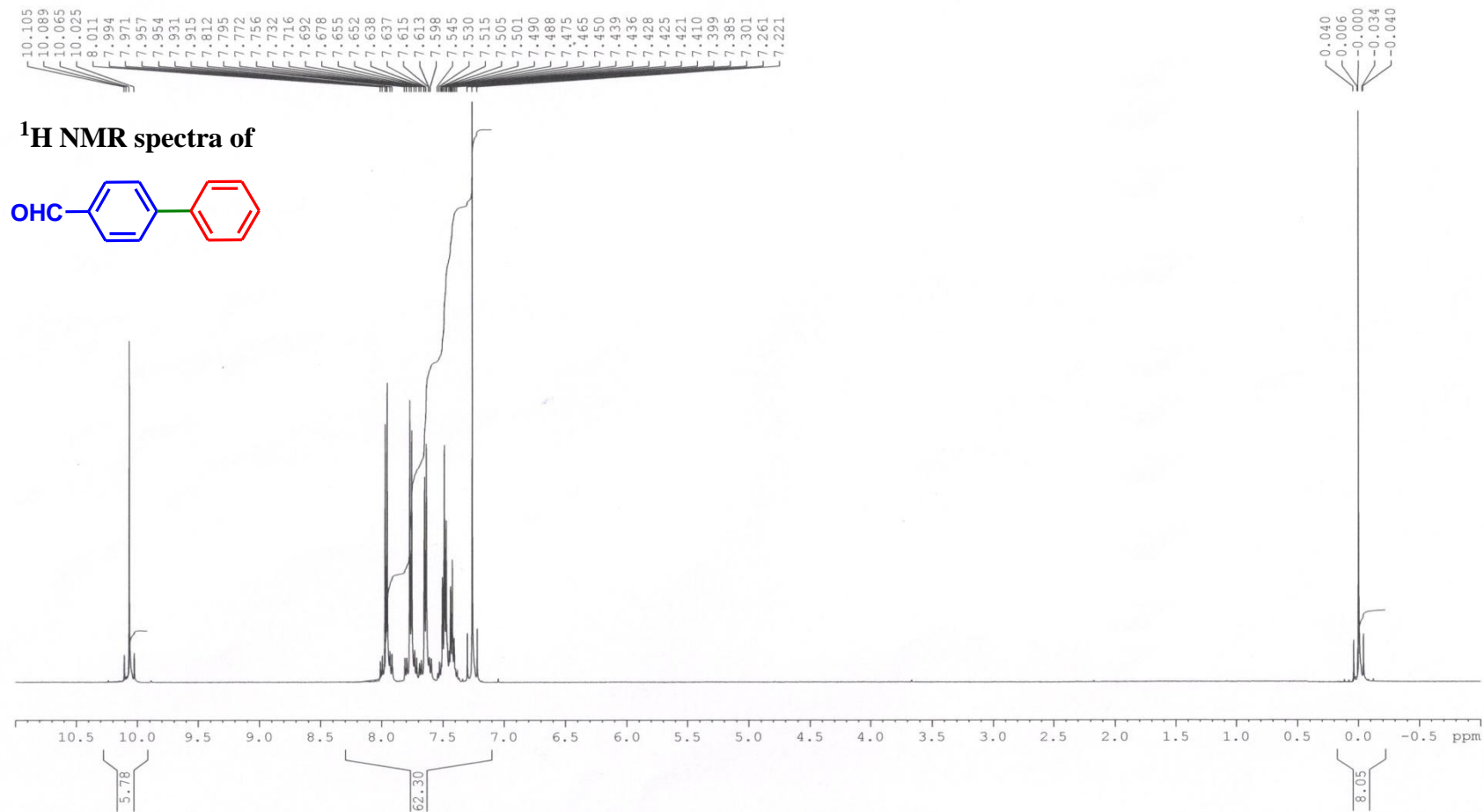


Name of Sample: S-7a  
Spectrum No: 2560

<sup>13</sup>C NMR spectra of

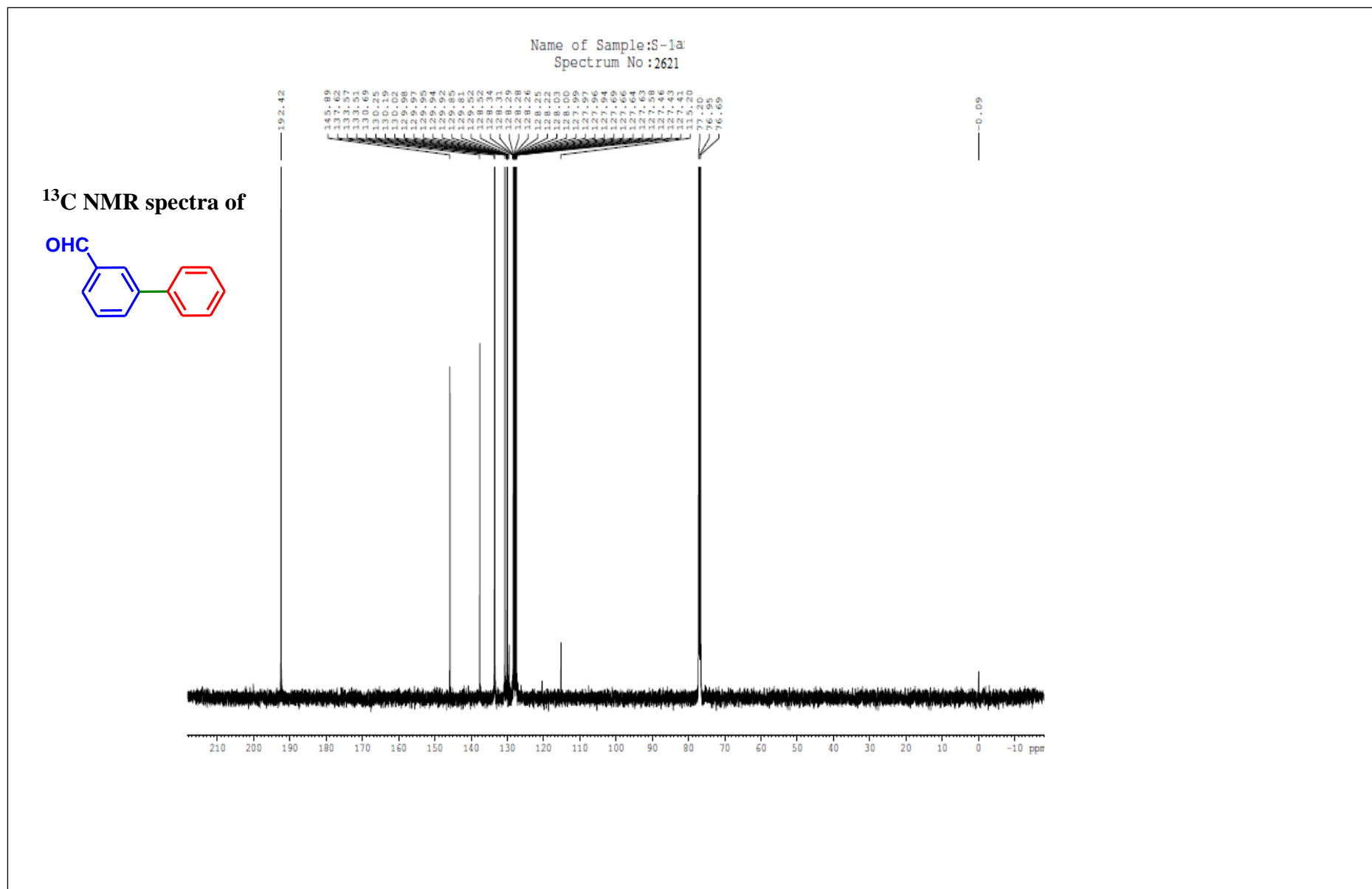


Name of Sample: SB-4  
Spectrum No: 3642





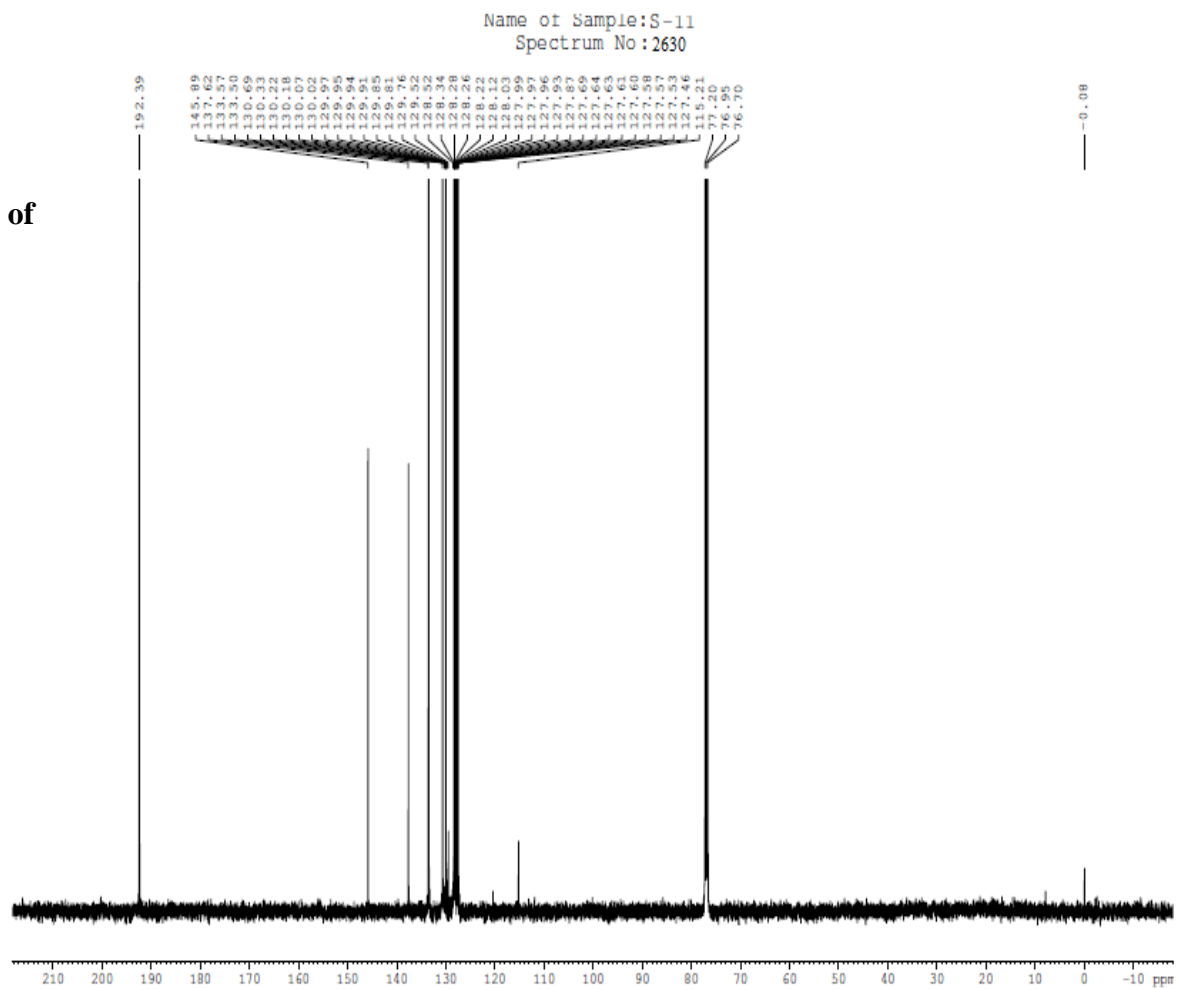
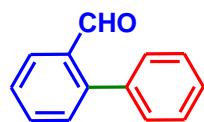






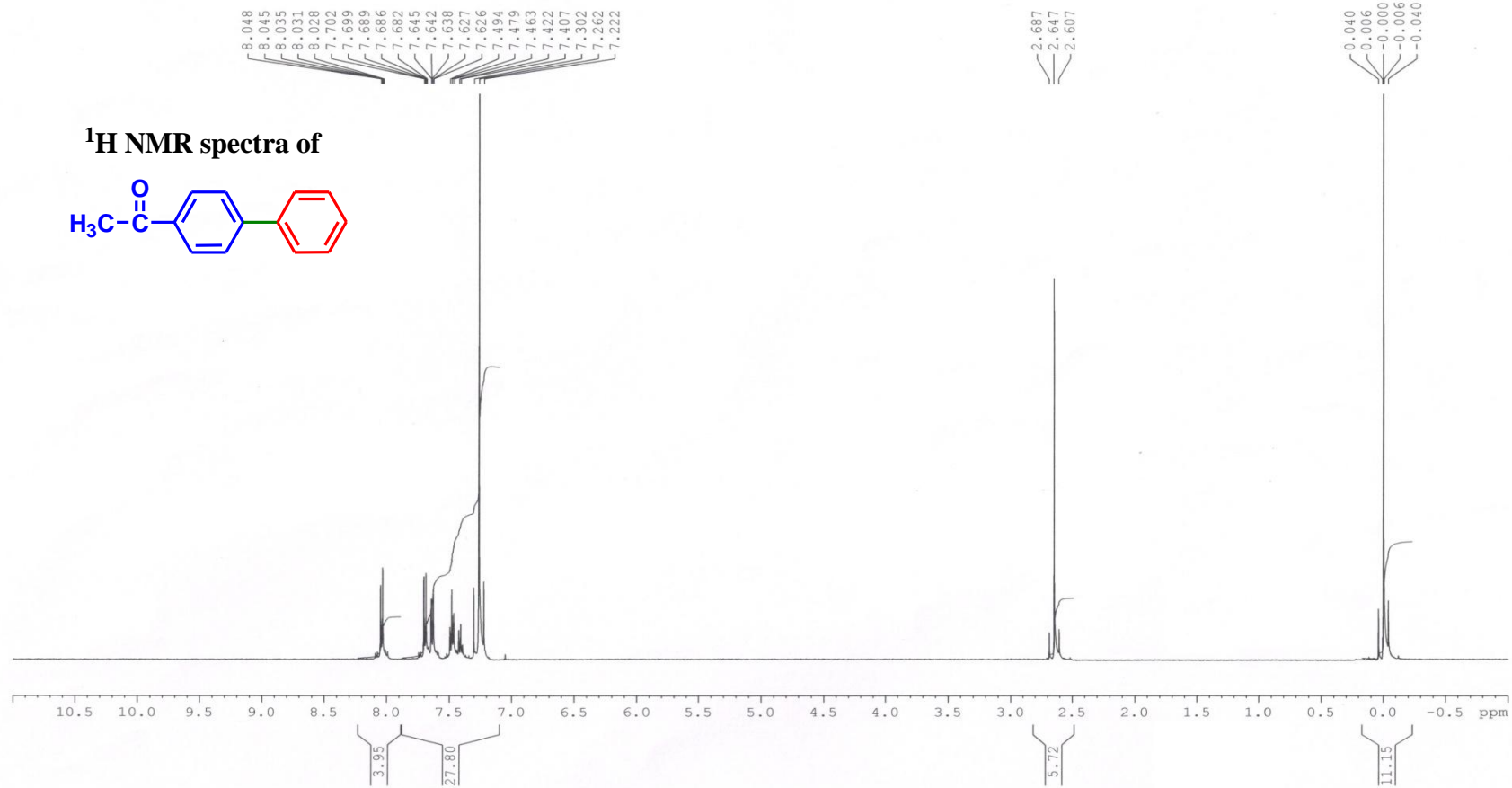
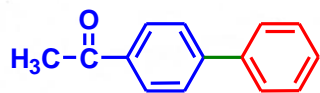


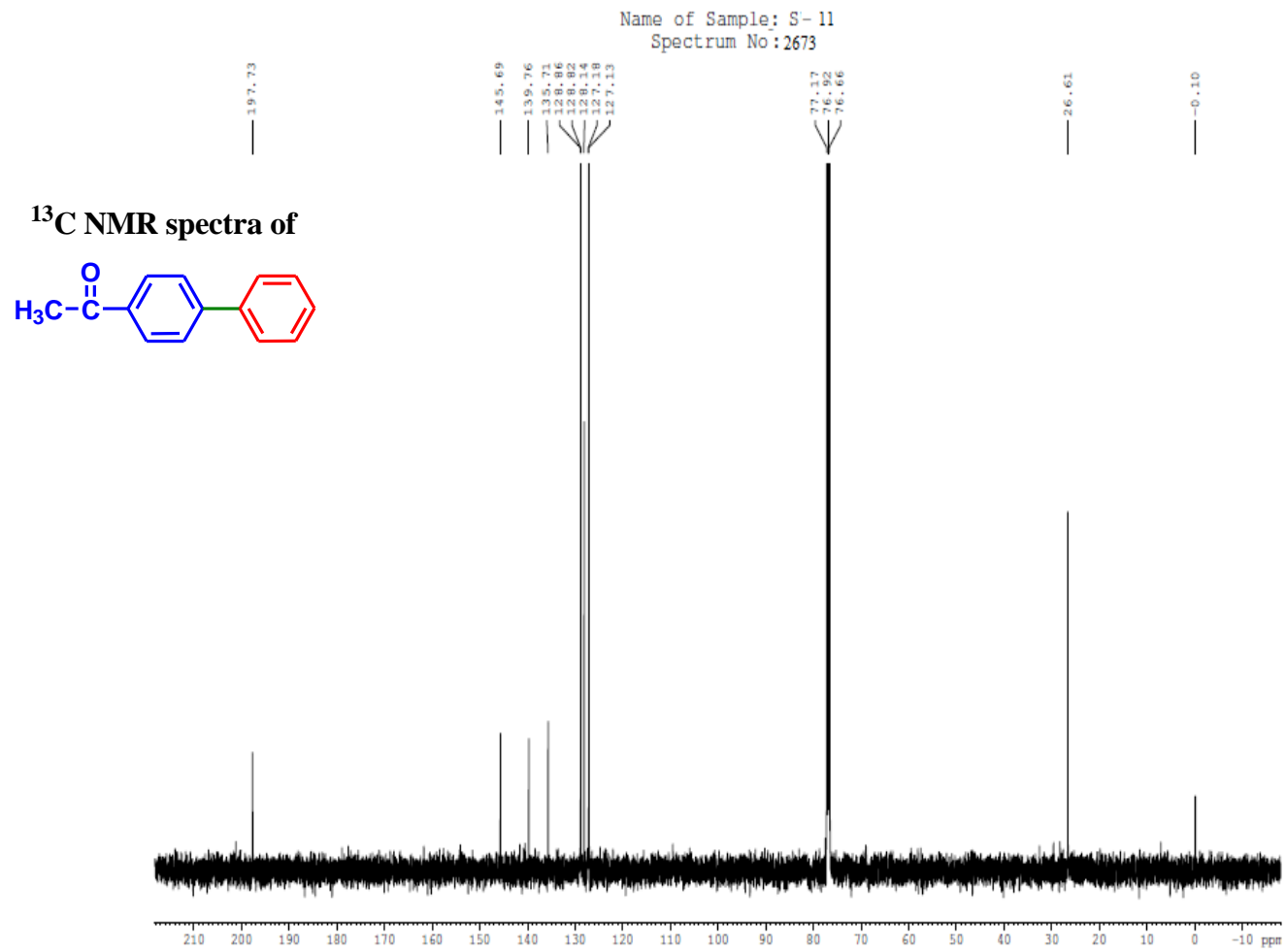
<sup>13</sup>C NMR spectra of



Name of Sample: SB-5  
Spectrum No.: 3745

<sup>1</sup>H NMR spectra of



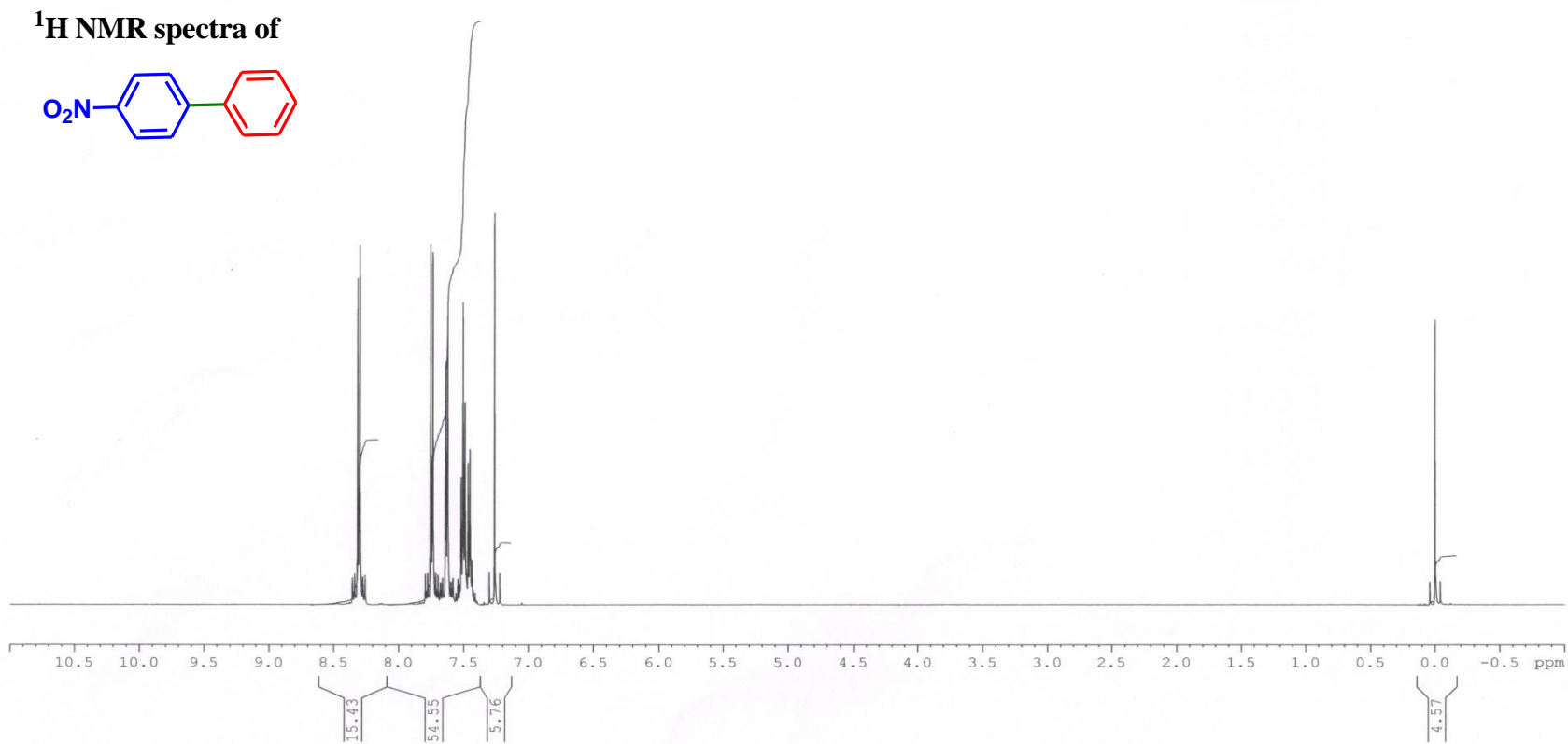
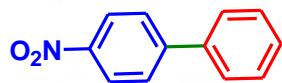


Name of Sample: SB-3  
Spectrum No: 3641

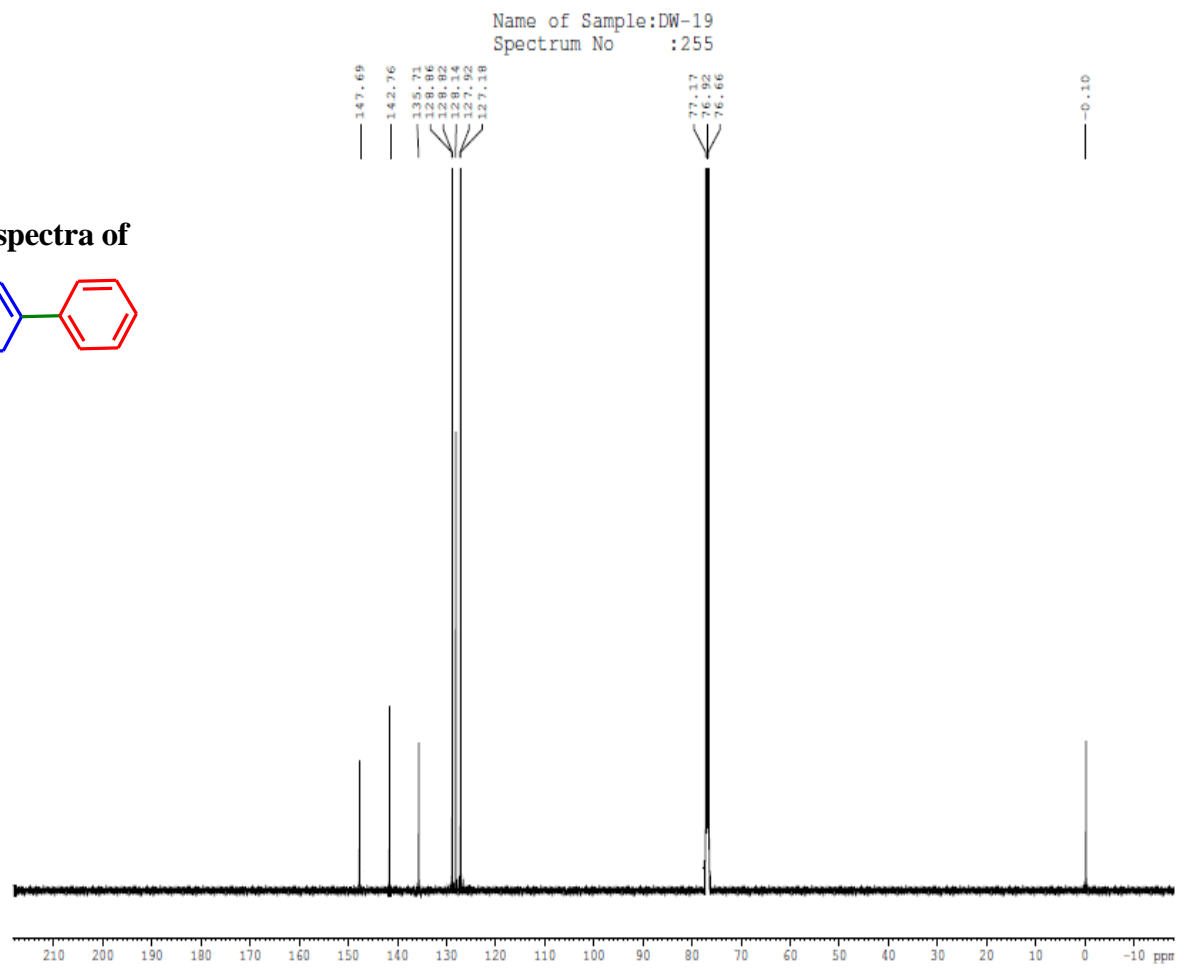
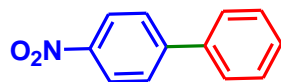
8.312  
8.301  
8.297  
8.293  
8.275  
8.272  
8.258  
7.793  
7.790  
7.779  
7.776  
7.758  
7.753  
7.749  
7.739  
7.736  
7.731  
7.719  
7.713  
7.710  
7.700  
7.696  
7.681  
7.678  
7.662  
7.641  
7.638  
7.623  
7.622  
7.601  
7.598  
7.583  
7.582  
7.559  
7.545  
7.529  
7.519  
7.516  
7.505  
7.503  
7.489  
7.479  
7.465  
7.455  
7.451  
7.446  
7.439  
7.437  
7.426  
7.411  
7.301  
7.261  
7.222

0.040  
0.001  
-0.000  
-0.006  
-0.040

<sup>1</sup>H NMR spectra of

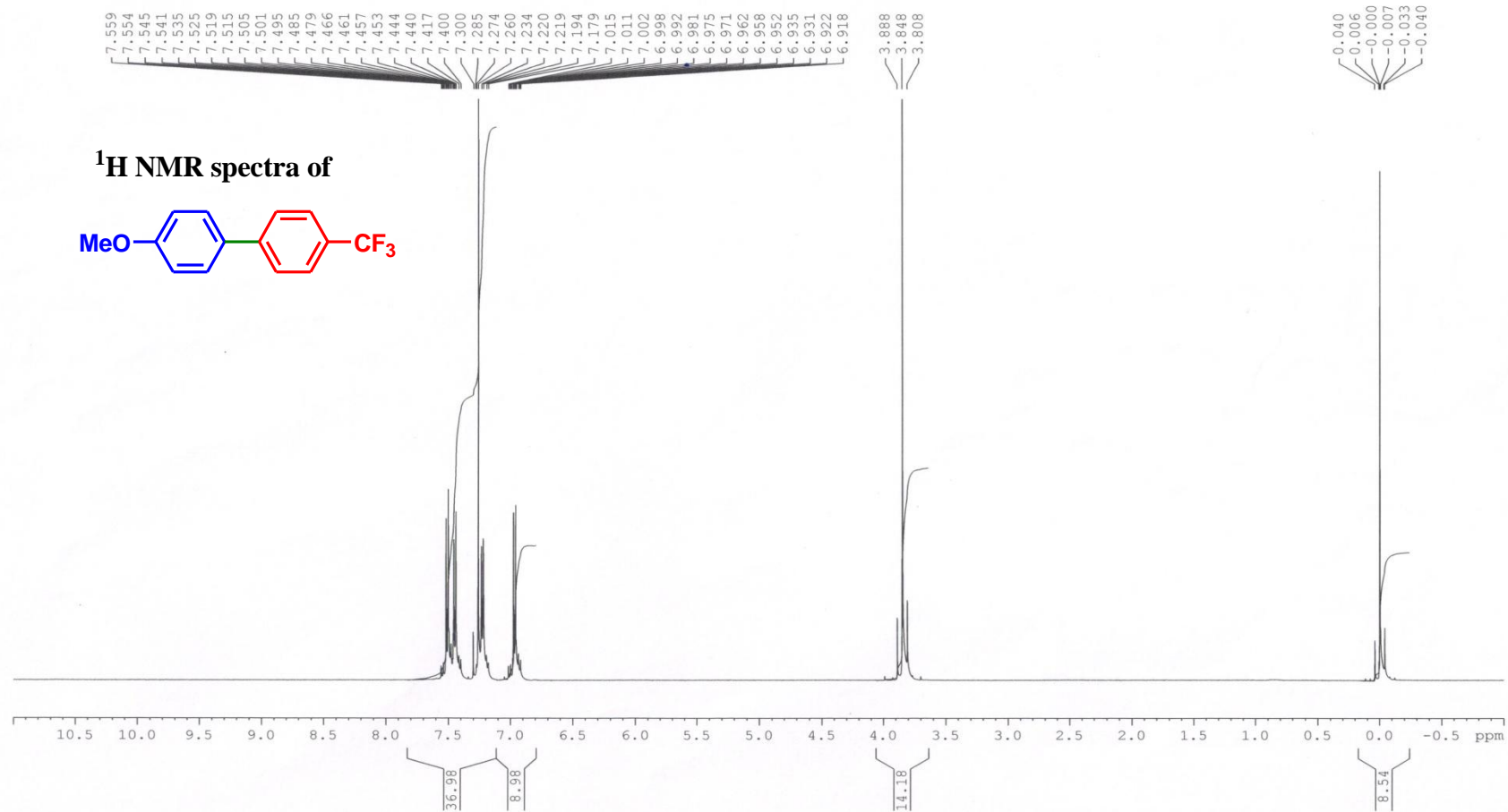
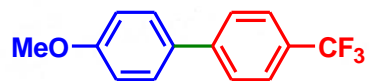


**$^{13}\text{C}$  NMR spectra of**



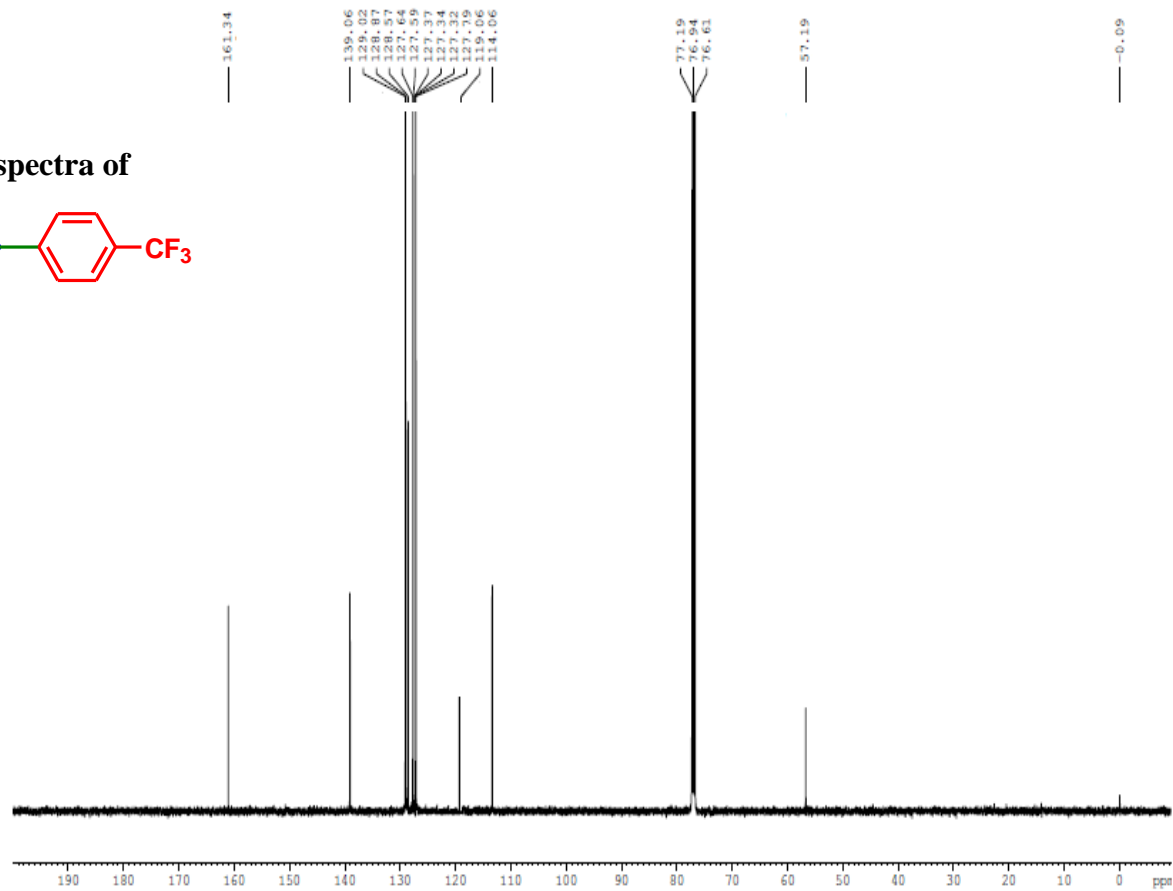
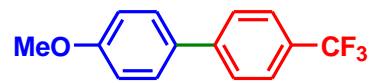
Name of Sample: SB-2  
Spectrum No: 3613

<sup>1</sup>H NMR spectra of



Name of Sample: S-25  
Spectrum No: 2577

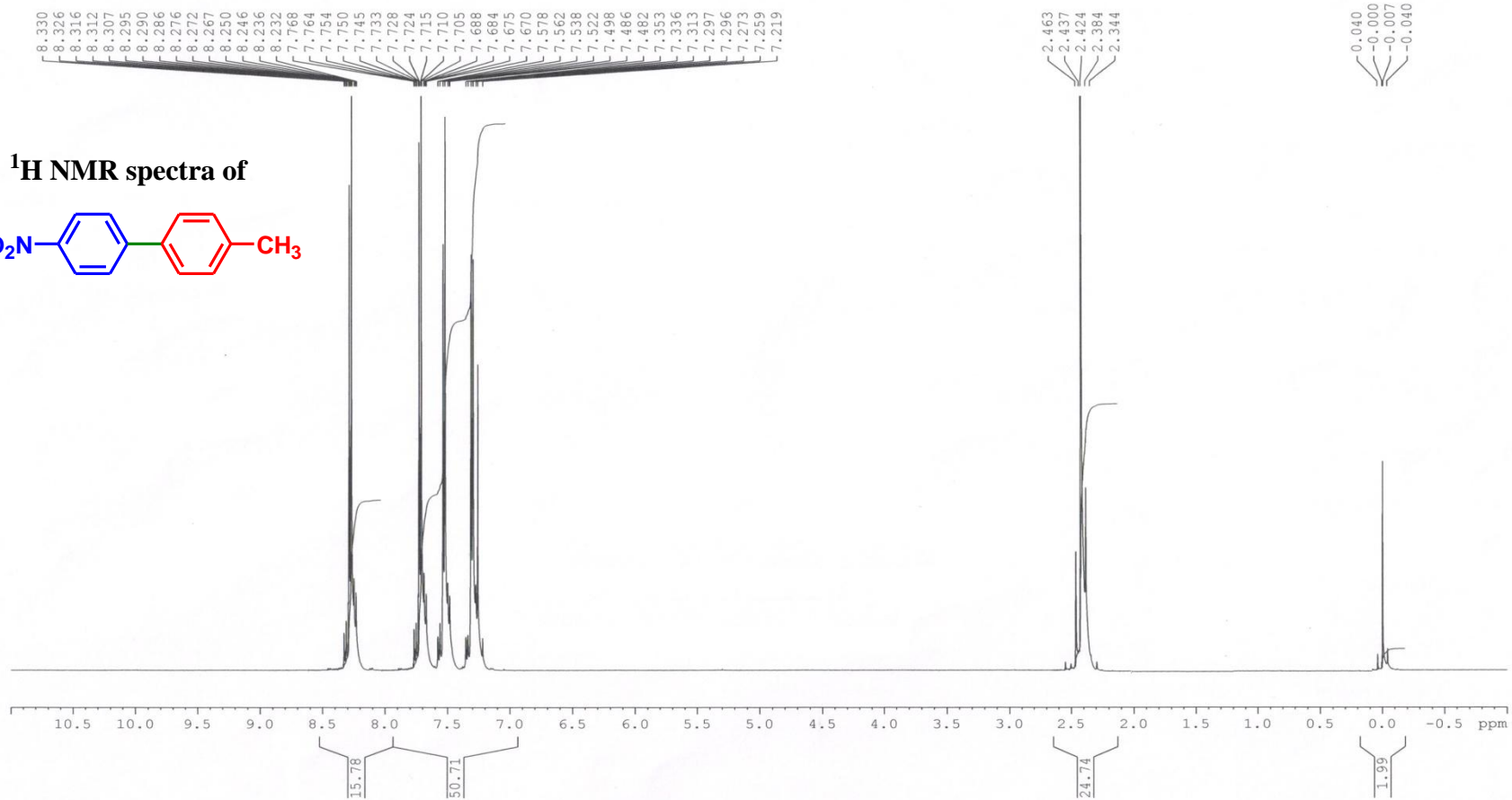
<sup>13</sup>C NMR spectra of





Name of Sample: SB-10  
Spectrum No : 3861

<sup>1</sup>H NMR spectra of



Name of Sample: SB-10  
Spectrum No : 3923

<sup>13</sup>C NMR spectra of



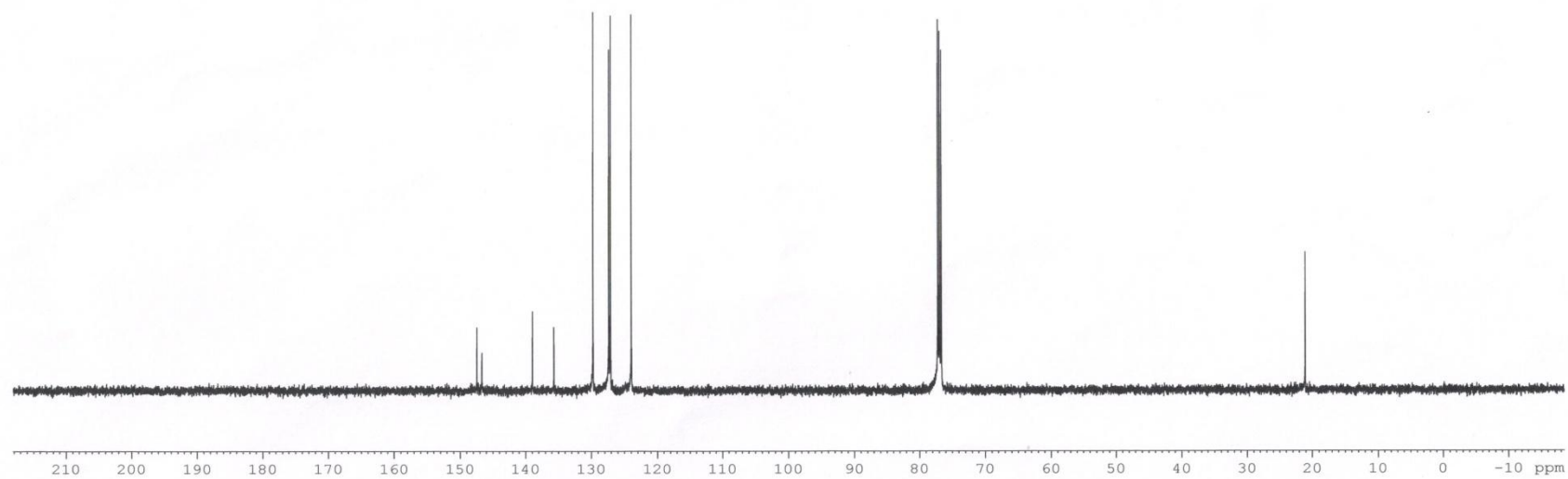
147.47  
146.72

138.99  
135.73

129.78  
127.37  
127.11  
123.99

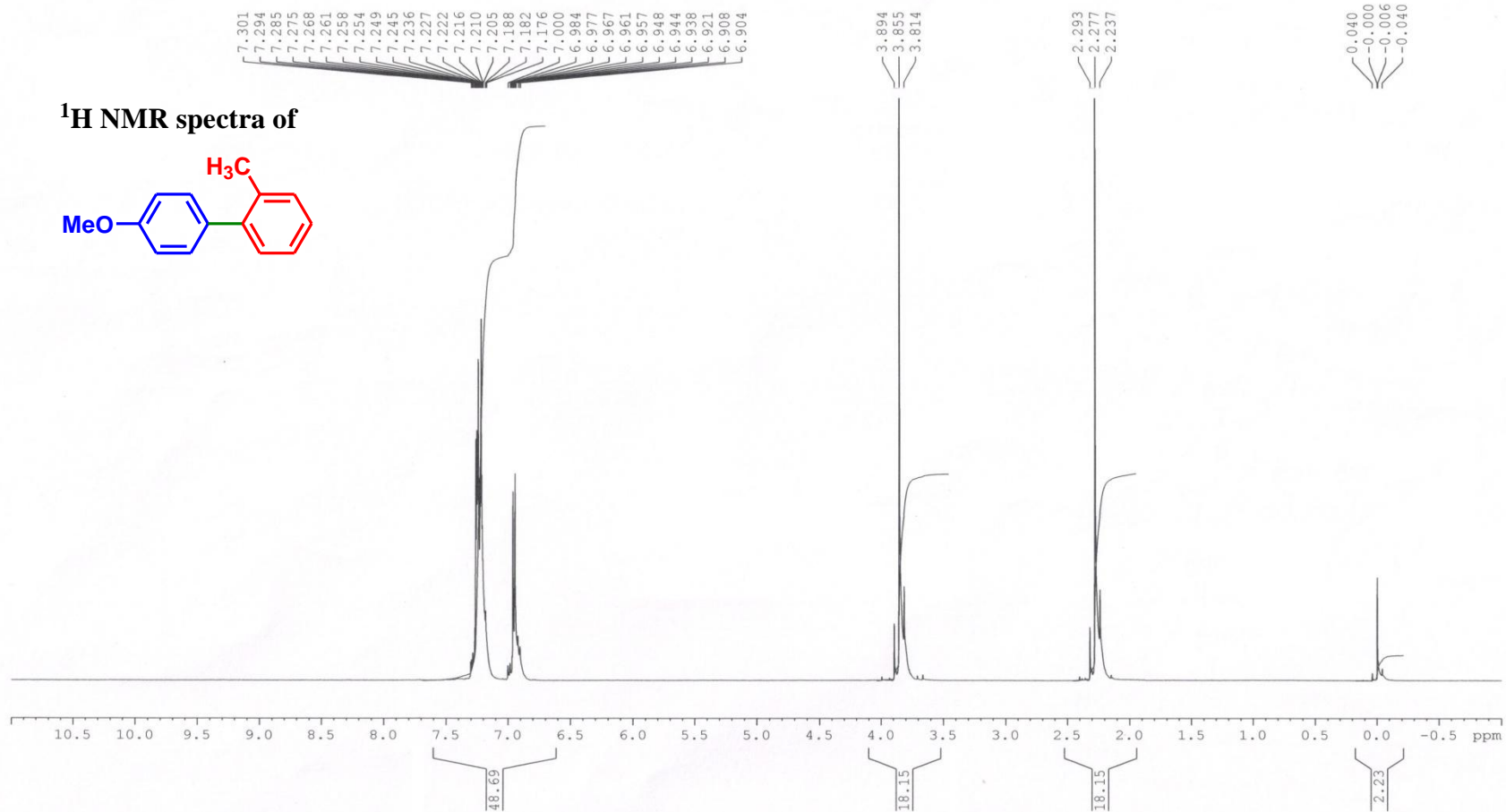
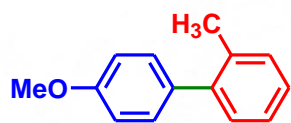
77.18  
76.93  
76.67

21.11



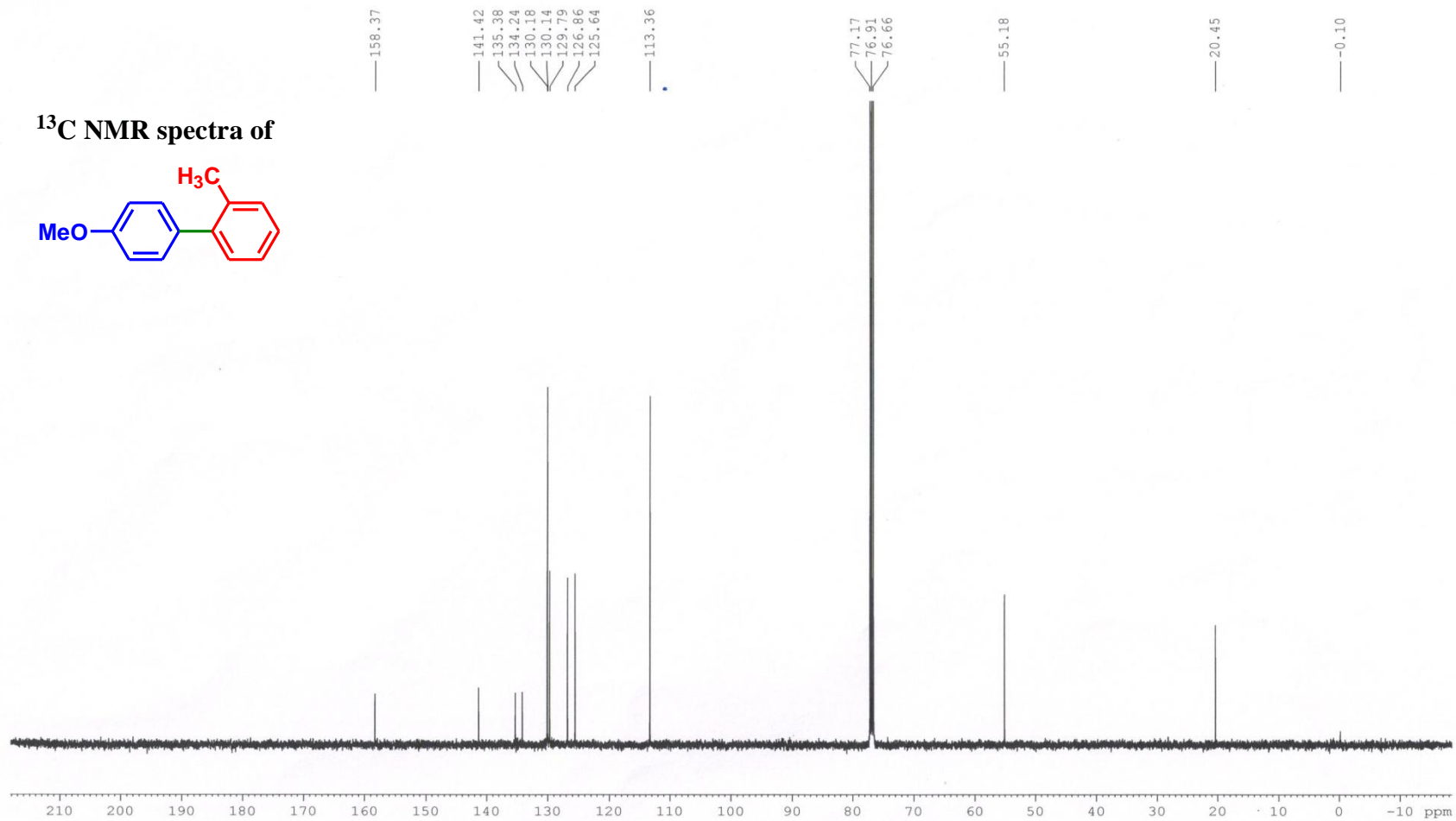
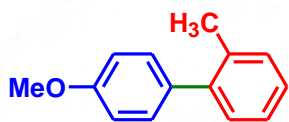
Name of Sample: SB-11  
Spectrum No : 3862

<sup>1</sup>H NMR spectra of

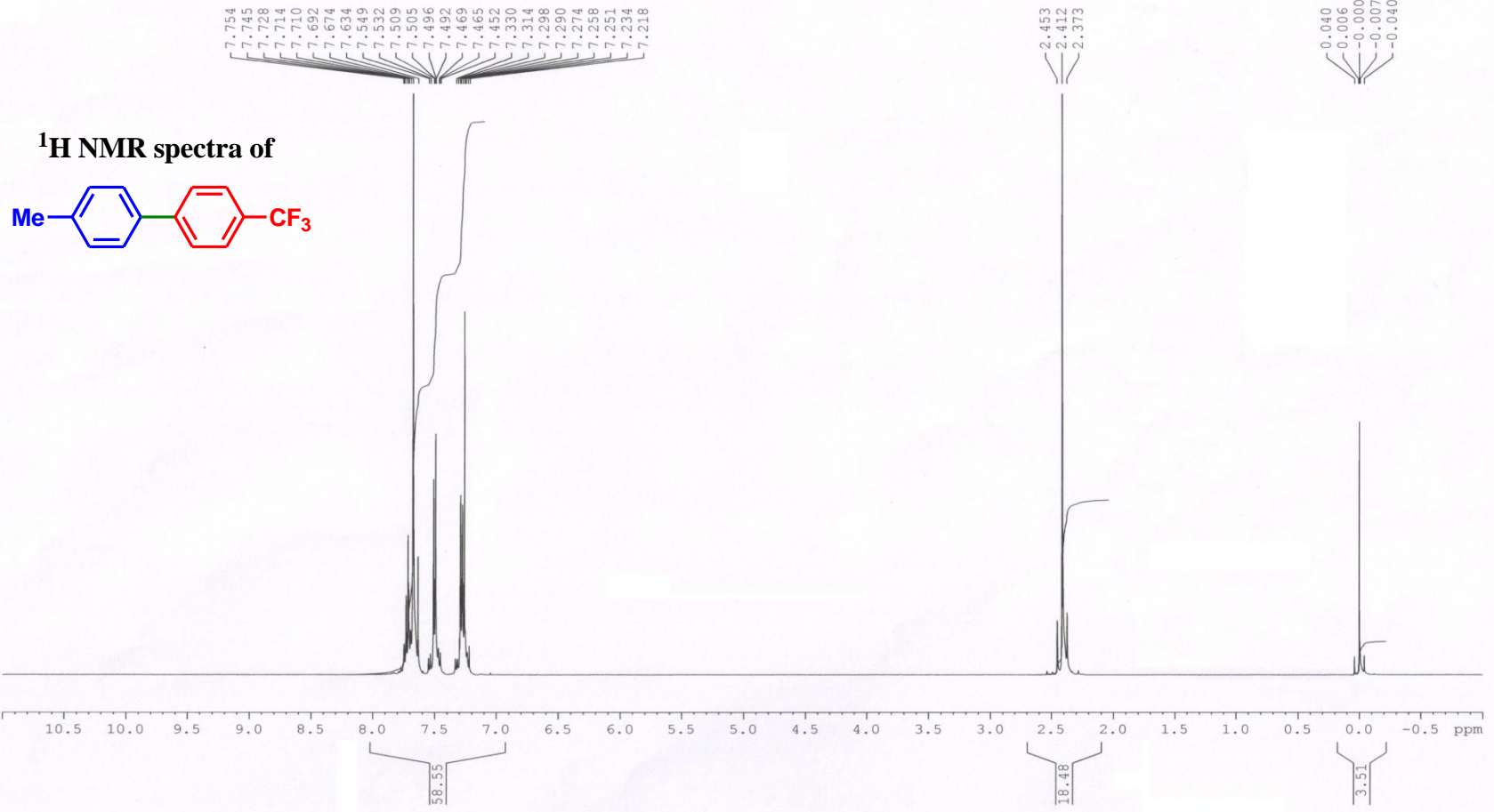


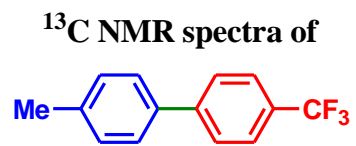
Name of Sample: SB-11  
Spectrum No : 4059

<sup>13</sup>C NMR spectra of

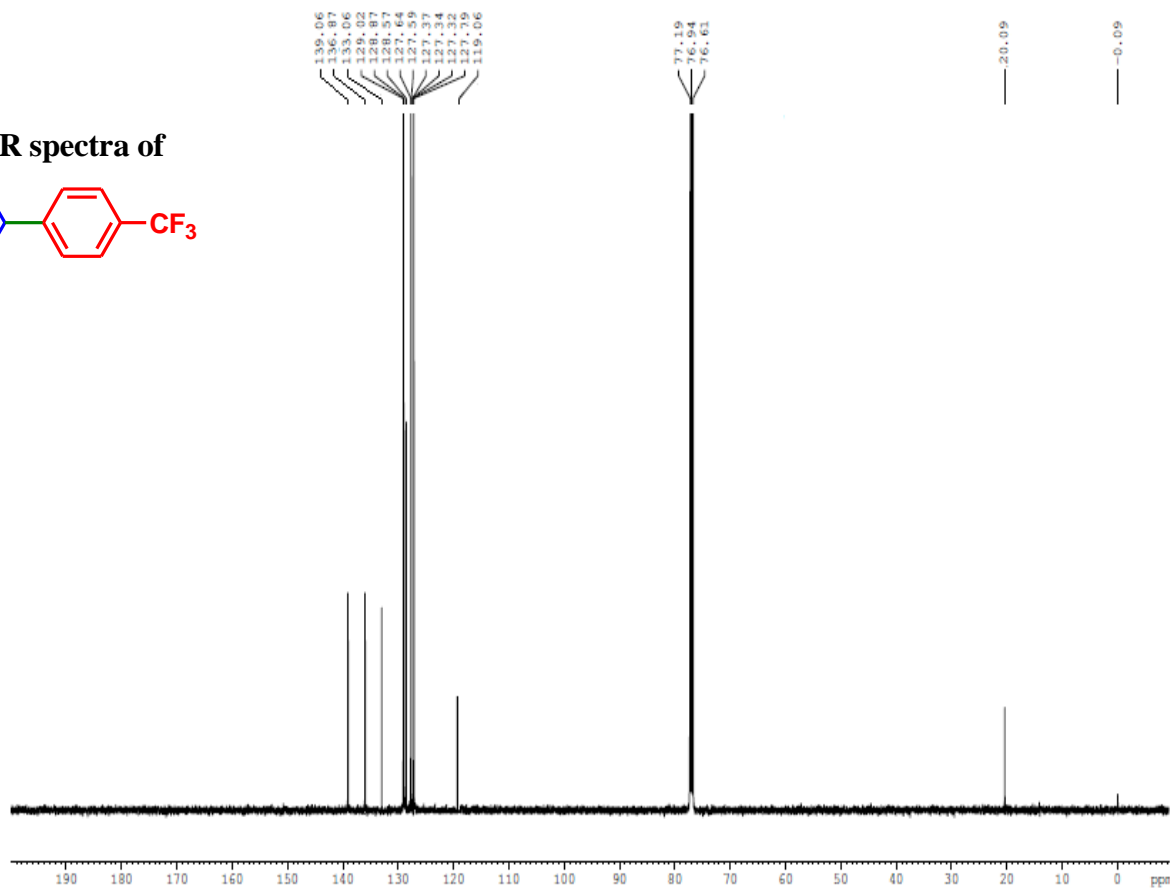


Name of Sample: SB-6  
Spectrum No.: 3746

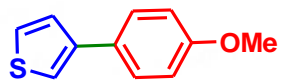




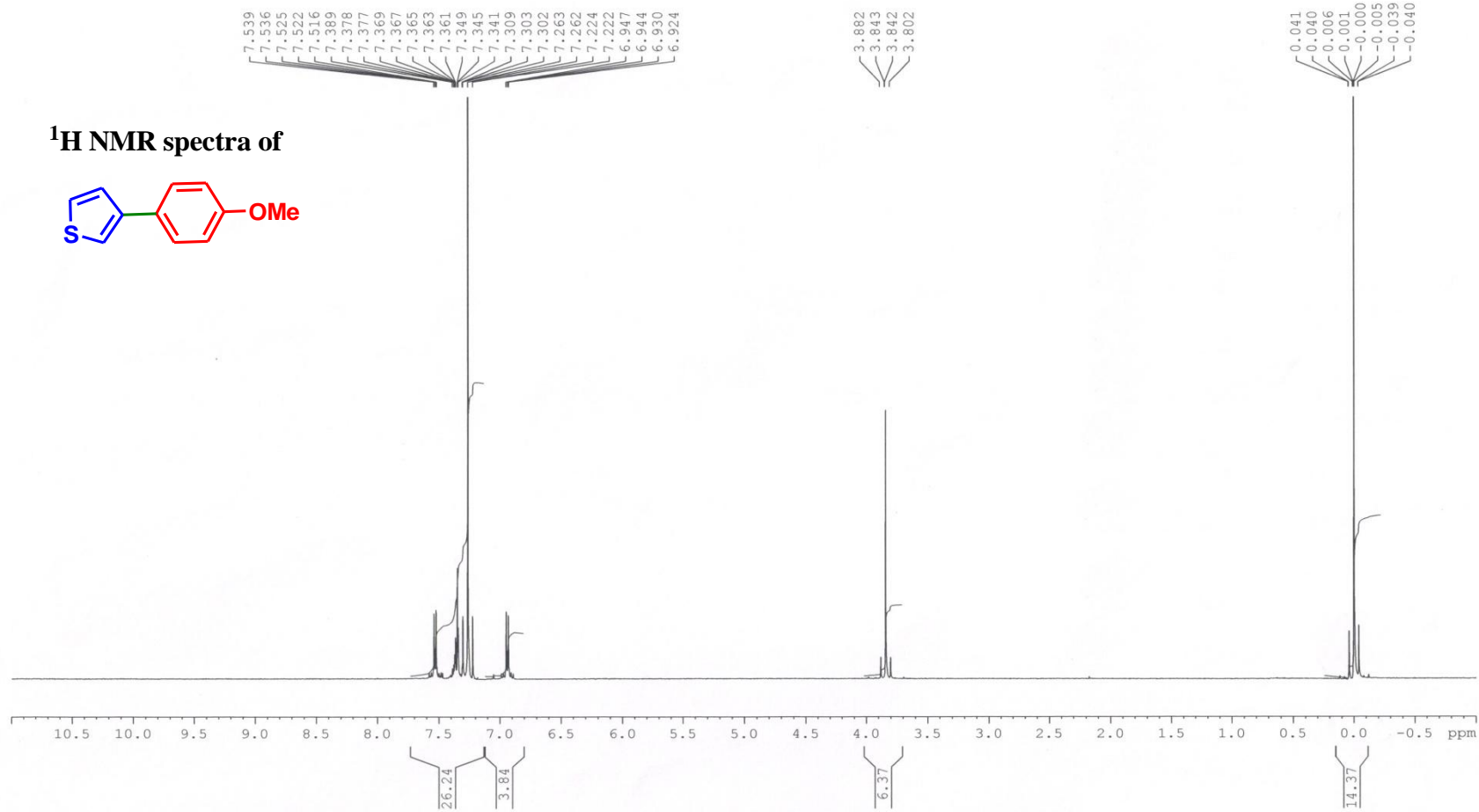
Name of Sample: S-5a  
Spectrum No: 2600



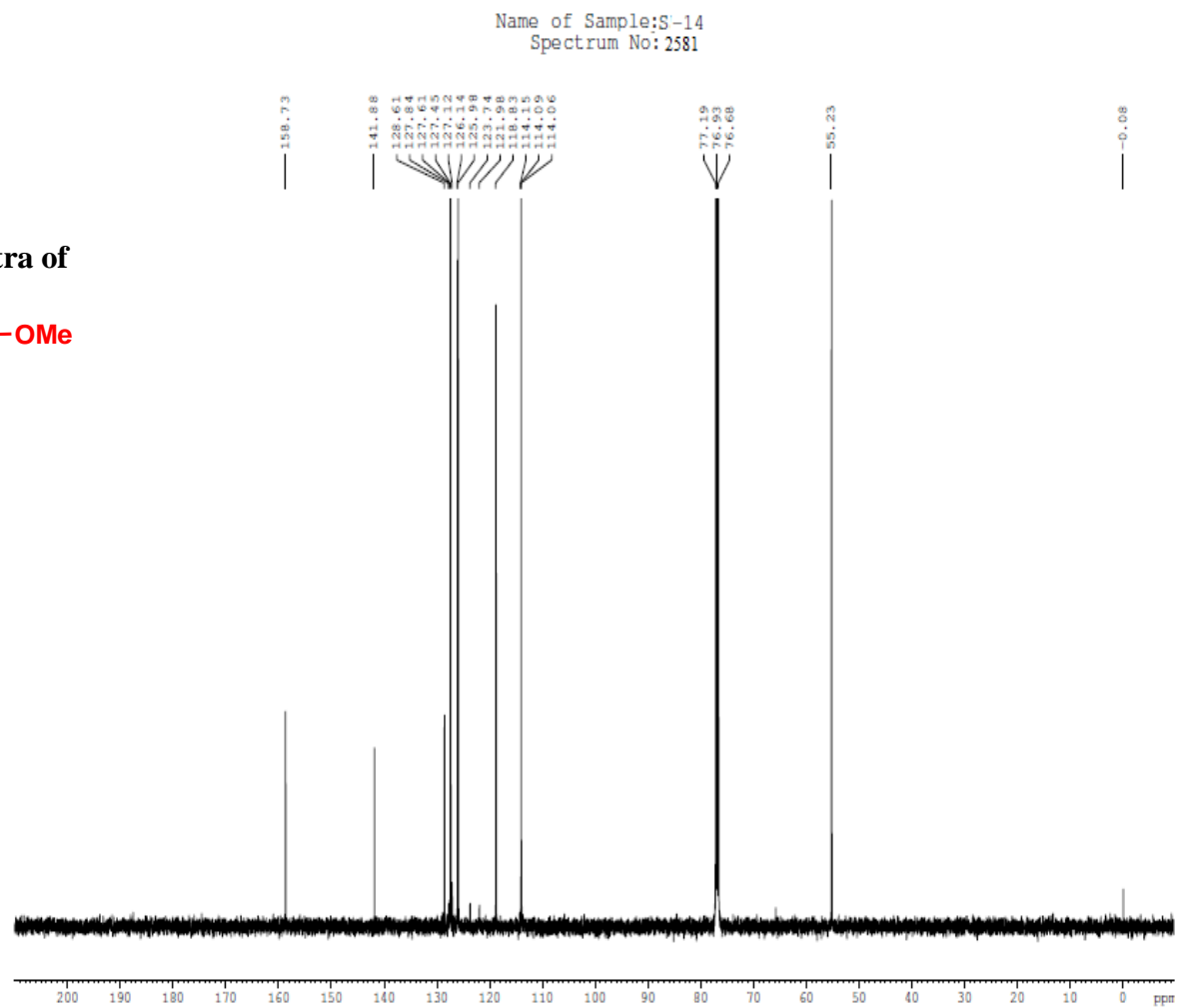
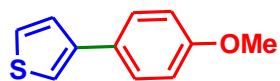
**<sup>1</sup>H NMR spectra of**



Name of Sample: SB-8  
Spectrum No.: 3758



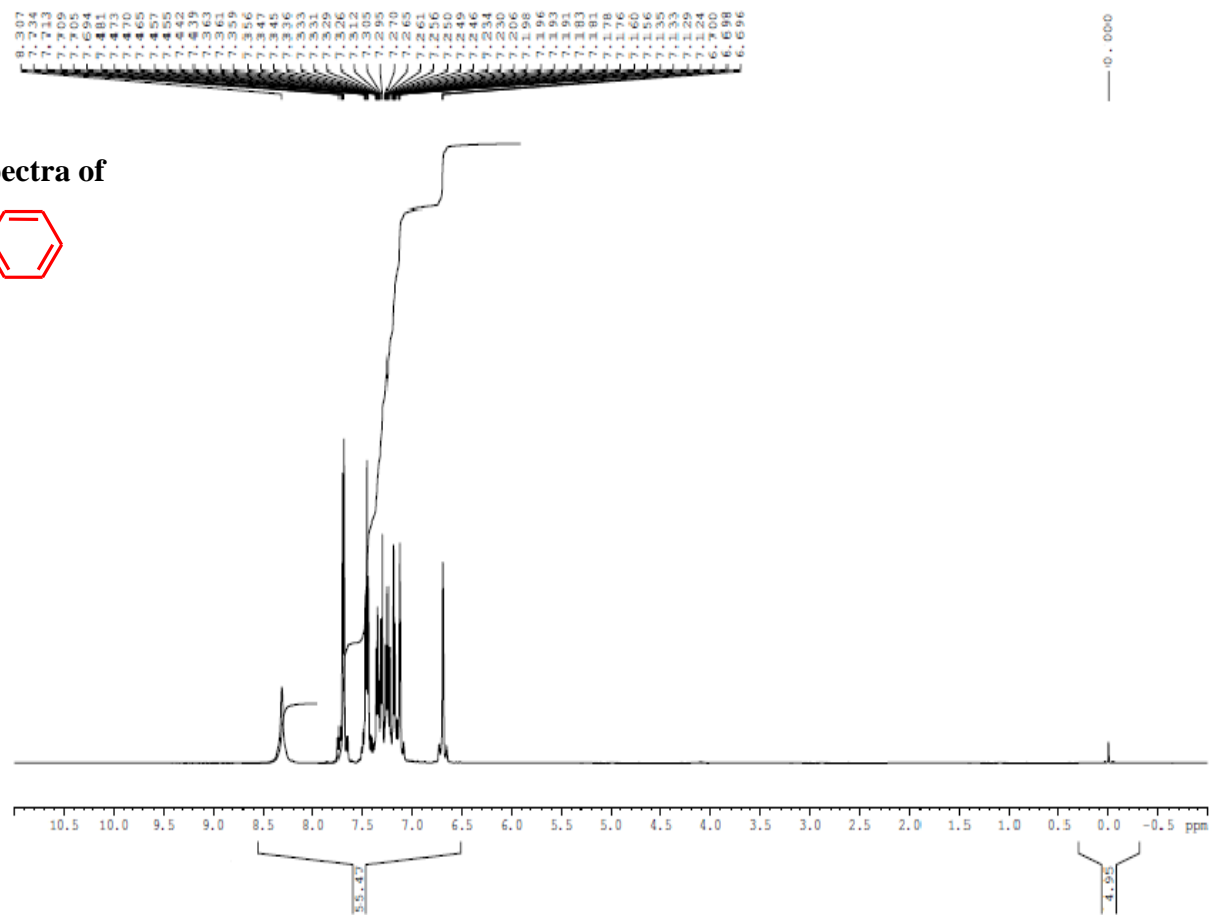
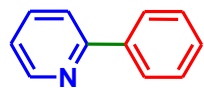
**<sup>13</sup>C NMR spectra of**





Name of Sample: S-17  
Spectrum No: 2263

<sup>1</sup>H NMR spectra of



<sup>13</sup>C NMR spectra of

