

## Supporting Information

### **Efficient Aerobic Oxidation of Benzyl Alcohols Using a Magnetically Recoverable Ni/Nitrogen-Containing Carbon Nanocomposite**

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## 1. XPS spectra

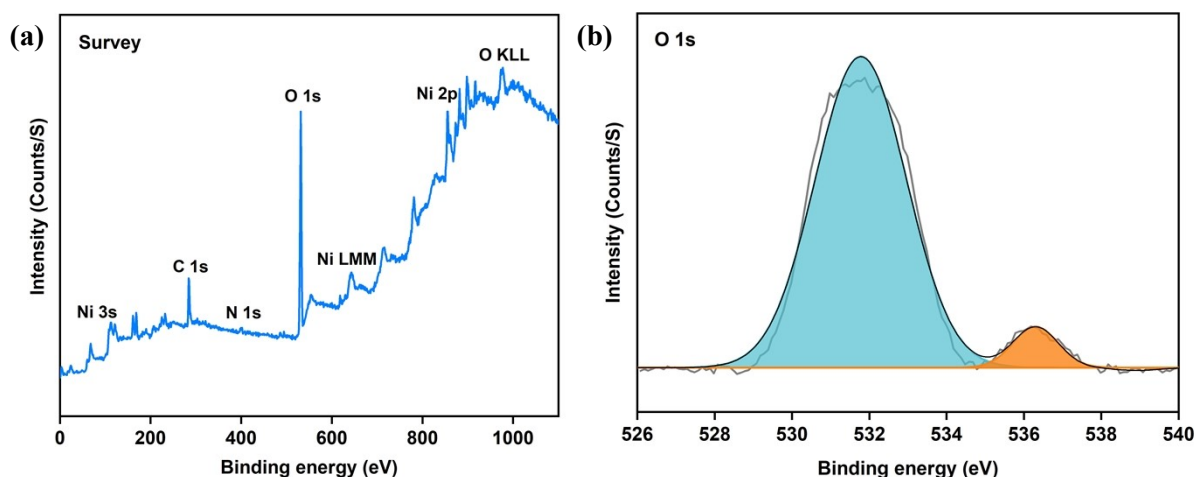
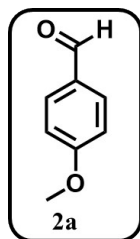
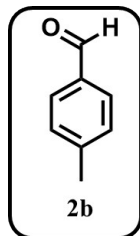


Fig. S1 (a) XPS survey and (b) O1s of Ni/PDC catalyst.

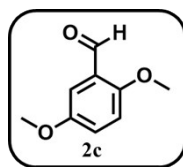
## 1. NMR Spectral data



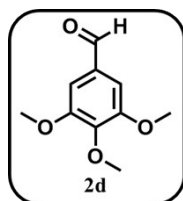
**4-methoxybenzaldehyde (2a):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.89 (s, 1H), 7.85 (d,  $J = 8.4$  Hz, 2H), 7.01 (d,  $J = 8.4$  Hz, 2H), 3.90 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.87, 164.63, 132.02, 129.98, 114.33, 55.61.<sup>1</sup>



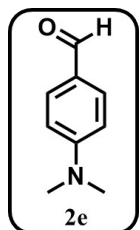
**4-methylbenzaldehyde (2b):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.96 (s, 1H), 7.78 (d,  $J = 8.0$  Hz, 2H), 7.33 (d,  $J = 7.8$  Hz, 2H), 2.44 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.94, 145.56, 134.08, 129.12, 129.05, 129.00, 128.94, 128.89, 22.53.<sup>1</sup>



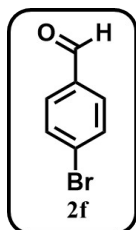
**2,5-dimethoxybenzaldehyde (2c):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  10.45 (s, 1H), 7.33 (d,  $J = 3.3$  Hz, 1H), 7.14 (dd,  $J = 9.1, 3.3$  Hz, 1H), 6.95 (d,  $J = 9.0$  Hz, 1H), 3.90 (s, 3H), 3.81 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  189.63, 156.74, 153.61, 124.93, 123.54, 113.36, 110.40, 56.18, 55.84.<sup>2</sup>



**3,4,5-trimethoxybenzaldehyde (2d):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.88 (t,  $J = 1.9$  Hz, 1H), 7.14 (d,  $J = 2.1$  Hz, 2H), 3.94 (d,  $J = 2.6$  Hz, 9H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.08, 153.66, 143.60, 131.72, 106.71, 61.01, 56.28.

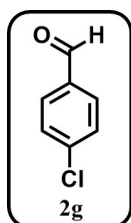


**4-(dimethylamino)benzaldehyde (2e):**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.74 (s, 1H), 7.73 (d,  $J = 8.9$  Hz, 2H), 6.70 (d,  $J = 8.7$  Hz, 2H), 3.08 (s, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.4, 154.4, 132.0, 125.1, 111.1, 40.1.<sup>3</sup>

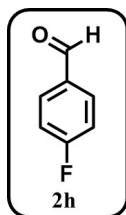


**4-bromobenzaldehyde (2f):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.98 (s, 1H), 7.76 (d,  $J = 8.5$  Hz, 2H), 7.69 (d,  $J = 8.5$  Hz, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.14, 135.07, 132.47, 131.00, 129.82.<sup>3</sup>

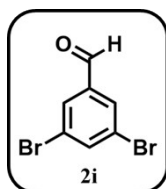
1H), 7.83  
 $\text{CDCl}_3$ )  $\delta$



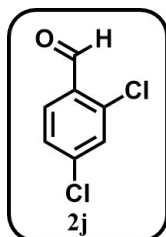
**4-chlorobenzaldehyde (2g):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.99 (s, 1H), 7.83 (d,  $J = 8.4$  Hz, 2H), 7.53 (d,  $J = 8.2$  Hz, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.93, 141.00, 134.71, 130.94, 129.49.<sup>1</sup>



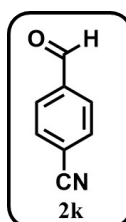
**4-fluorobenzaldehyde (2h):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.94 (s, 1H), 7.89 (dd,  $J = 8.8, 5.4$  Hz, 2H), 7.18 (t,  $J = 8.6$  Hz, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.60, 167.78, 165.23, 132.28, 132.19, 116.43, 116.21.<sup>4</sup>



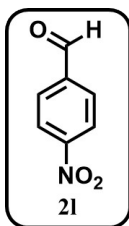
**3,5-dibromobenzaldehyde (2i):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.91 (s, 1H), 7.94 (d,  $J = 1.8$  Hz, 2H), 7.93 – 7.91 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  189.22, 139.60, 138.89, 131.89, 131.22, 123.95, 123.16.



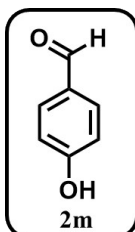
**2,4-dichlorobenzaldehyde (2j):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  10.43 (s, 1H), 7.89 (d,  $J = 8.3$  Hz, 1H), 7.50 (s, 1H), 7.40 (ddd,  $J = 8.3, 2.0, 0.9$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  188.55, 141.13, 138.56, 130.94, 130.48, 130.34, 127.98.



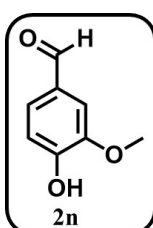
**4-formylbenzonitrile (2k):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  10.12 (s, 1H), 8.03 – 8.00 (m, 2H), 7.89 – 7.82 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.65, 138.75, 132.92, 129.91, 117.73, 117.62.<sup>4</sup>



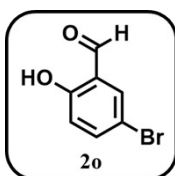
**4-nitrobenzaldehyde (2l):** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.17 (s, 1H), 8.41 (d, *J* = 8.3 Hz, 2H), 8.09 (d, *J* = 8.3 Hz, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 190.32, 140.05, 130.51, 124.34.<sup>3</sup>



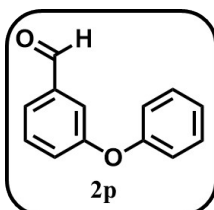
**4-hydroxybenzaldehyde (2m):** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.89 (s, 1H), 7.87 – 7.83 (m, 2H), 7.03 – 6.99 (m, 2H), 6.46 (s, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 191.36, 161.68, 132.58, 129.82, 116.05.<sup>5</sup>



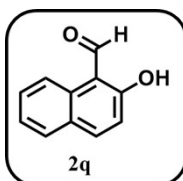
**4-hydroxy-3-methoxybenzaldehyde (2n):** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 9.84 (s, 1H), 7.44 (dt, *J* = 6.8, 0.9 Hz, 2H), 7.06 (dd, *J* = 8.6, 1.1 Hz, 1H), 6.50 – 6.34 (m, 1H), 3.97 (d, *J* = 1.9 Hz, 3H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 191.02, 151.78, 147.21, 129.84, 127.59, 114.45, 108.82, 56.13.<sup>6</sup>



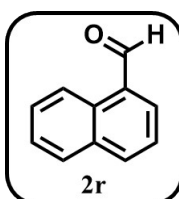
**5-bromo-2-hydroxybenzaldehyde (2o):** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 10.94 (s, 1H), 9.85 (s, 1H), 7.68 (d, *J* = 2.2 Hz, 1H), 7.61 (dd, *J* = 8.9, 2.4 Hz, 1H), 6.91 (d, *J* = 8.9 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 195.47, 160.58, 139.73, 135.66, 121.75, 119.84, 111.39.



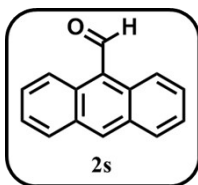
**3-phenoxybenzaldehyde (2p):** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.97 (s, 1H), 7.62 (d, *J* = 7.5 Hz, 1H), 7.55 – 7.46 (m, 2H), 7.42 – 7.37 (m, 2H), 7.31 (dt, *J* = 8.0, 1.3 Hz, 1H), 7.22 – 7.16 (m, 1H), 7.07 (d, *J* = 8.2 Hz, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 191.66, 158.43, 156.22, 138.09, 130.46, 130.07, 124.72, 124.60, 124.21, 119.51, 118.15.



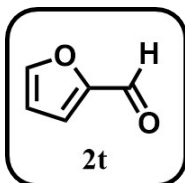
**2-hydroxy-1-naphthaldehyde (2q):** <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 13.16 (s, 1H), 10.80 (s, 1H), 8.33 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 9.1 Hz, 1H), 7.79 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.13 (d, *J* = 9.1 Hz, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 193.31, 164.97, 139.19, 132.91, 129.51, 129.15, 127.83, 124.53, 119.21, 118.62, 111.30.



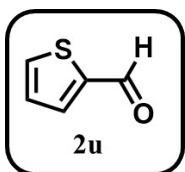
**1-naphthaldehyde (2r):** <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 10.32 (s, 1H), 9.26 (d, *J* = 8.6 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.88 – 7.81 (m, 2H), 7.67 – 7.61 (m, 1H), 7.56 – 7.47 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 193.60, 136.71, 135.33, 133.74, 131.41, 130.55, 129.10, 128.51, 126.99, 124.90.<sup>1</sup>



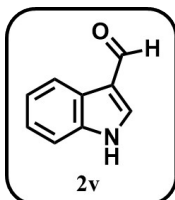
**anthracene-9-carbaldehyde (2s):**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  11.48 (s, 1H), 8.96 (d,  $J = 9.0$  Hz, 2H), 8.61 (s, 1H), 8.02 (d,  $J = 8.5$  Hz, 2H), 7.69 – 7.64 (m, 2H), 7.56 – 7.51 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.99, 135.22, 132.11, 131.04, 129.28, 129.11, 125.67, 124.66, 123.52.<sup>3</sup>



**furan-2-carbaldehyde (2t):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.67 (s, 1H), 7.71 (s, 1H), 7.27 (d,  $J = 3.6$  Hz, 1H), 6.66 – 6.58 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  177.94, 152.97, 148.13, 121.12, 112.62.<sup>3</sup>



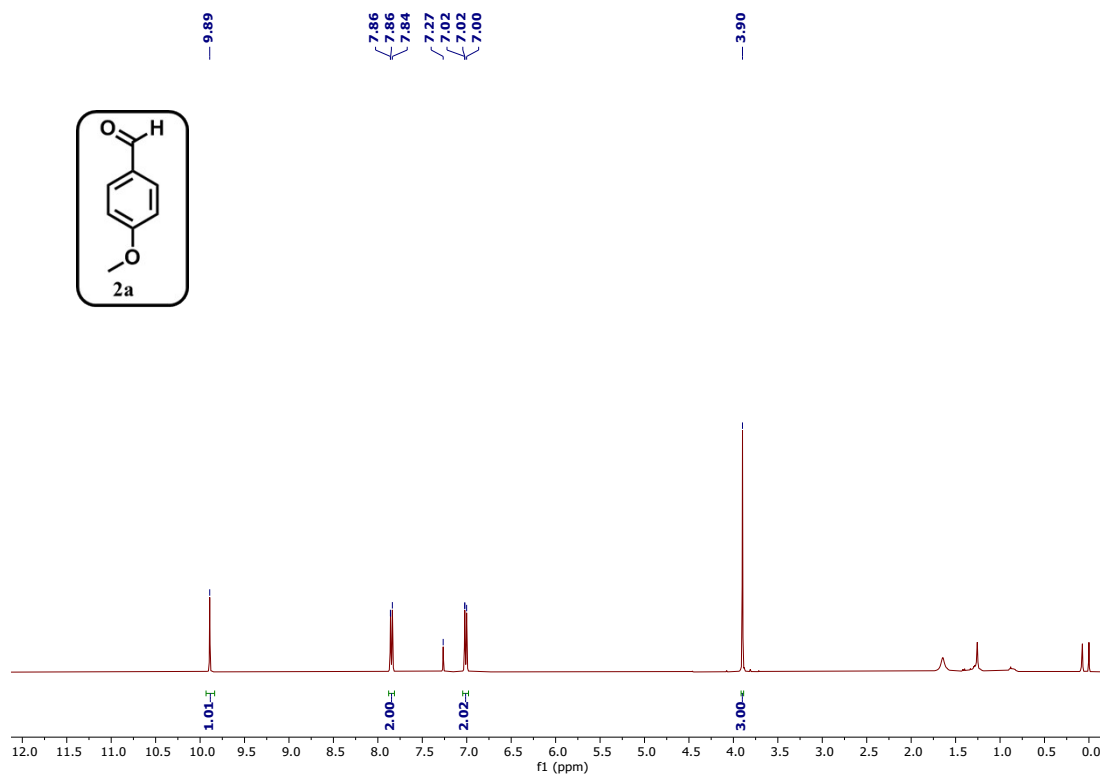
**thiophene-2-carbaldehyde (2u):**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  9.95 (s, 1H), 7.82 – 7.75 (m, 2H), 7.25 – 7.20 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  183.09, 144.01, 136.43, 135.20, 128.37.<sup>1</sup>



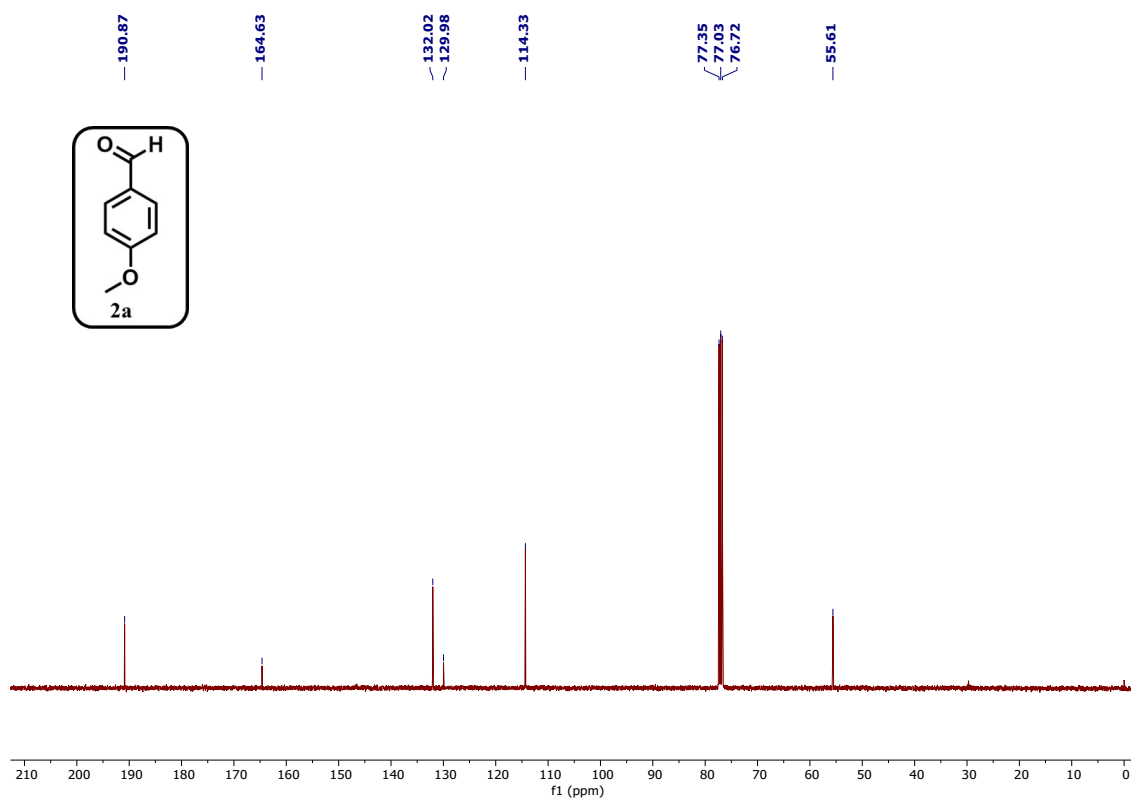
**1H-indole-3-carbaldehyde (2v):**  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  9.94 (s, 1H), 8.29 (s, 1H), 8.10 (d,  $J = 7.9$  Hz, 1H), 7.52 (d,  $J = 8.3$  Hz, 1H), 7.29 – 7.20 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz, DMSO)  $\delta$  185.39, 139.00, 137.62, 124.63, 123.89, 122.56, 121.28, 118.63, 112.93.

## 2. NMR Spectra of synthesized compounds

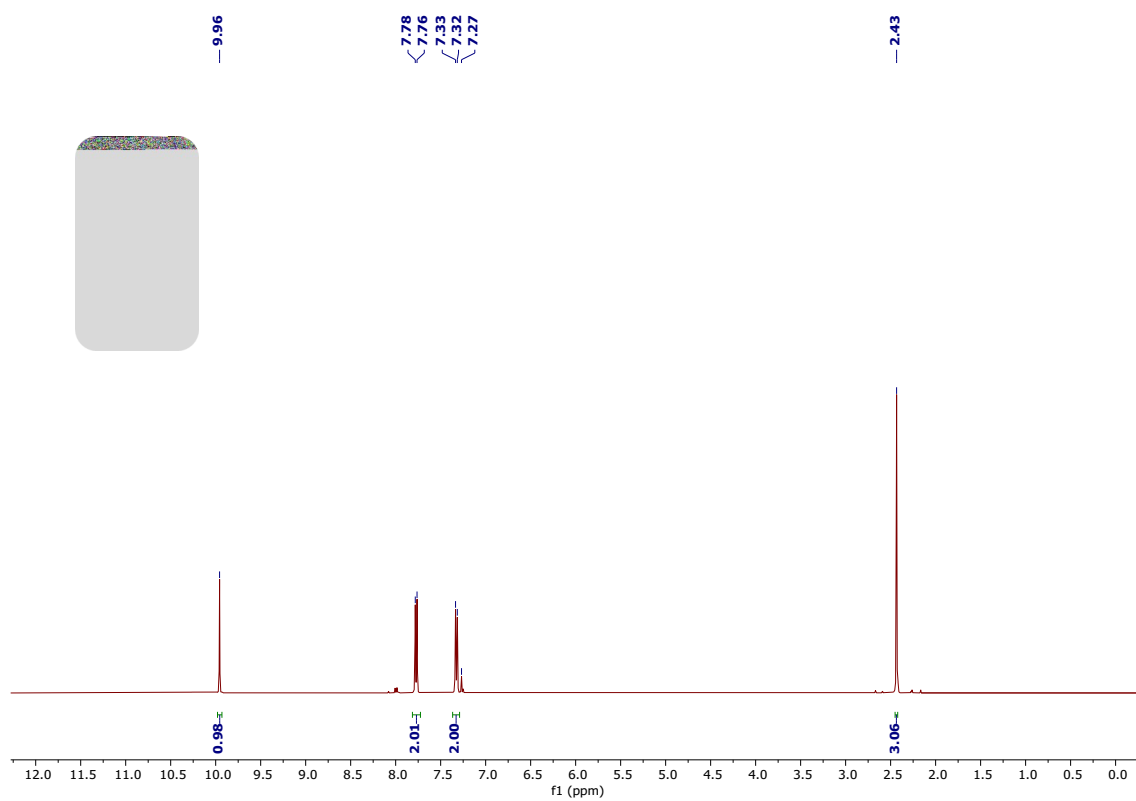
### <sup>1</sup>H NMR spectra of product 2a



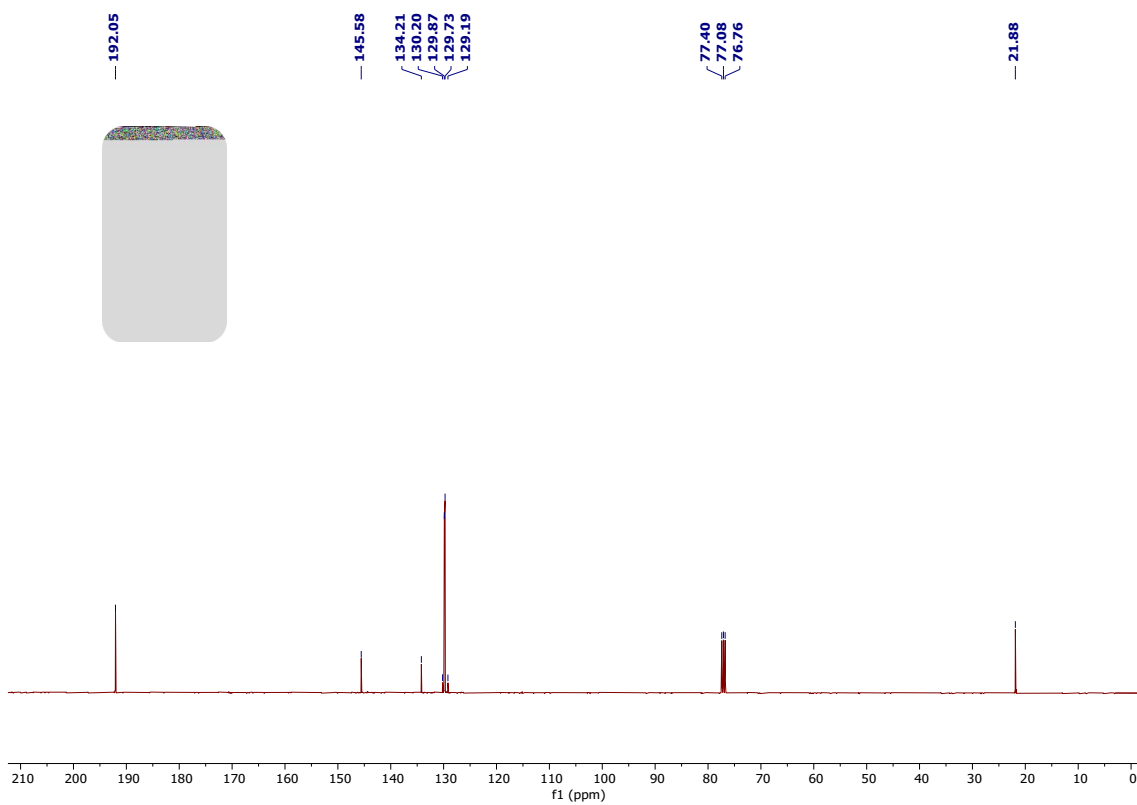
### <sup>13</sup>C NMR spectra of product 2a



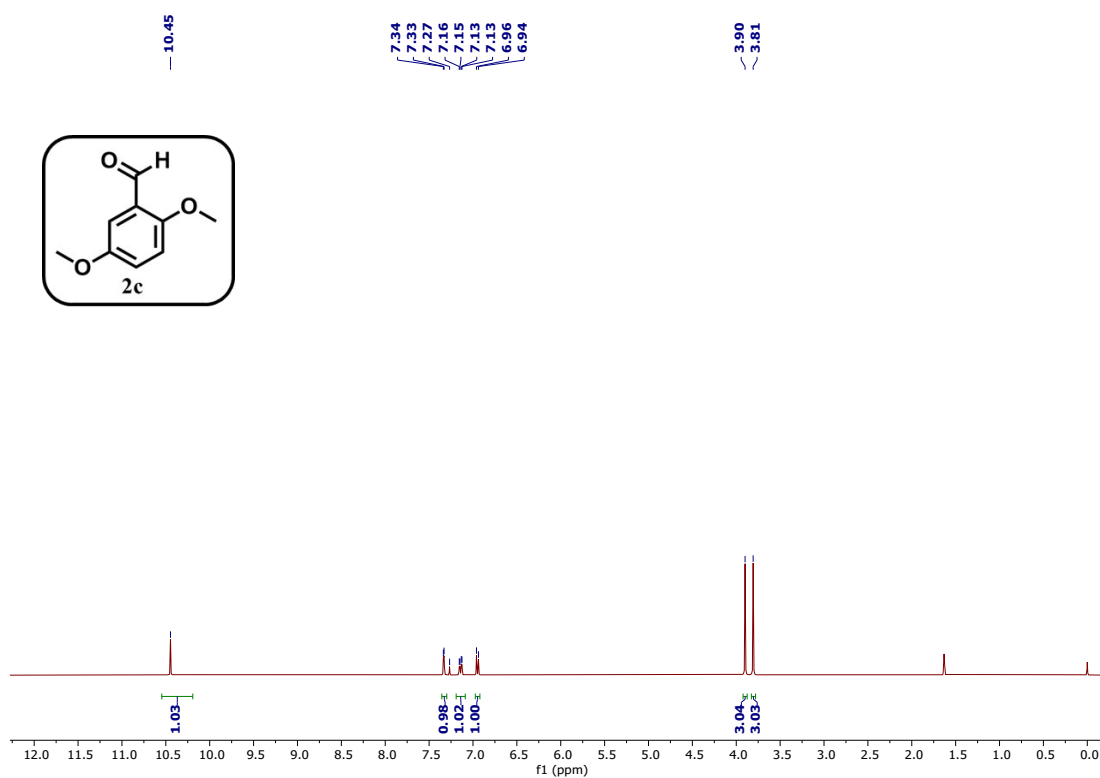
## $^1\text{H}$ NMR spectra of product 2b



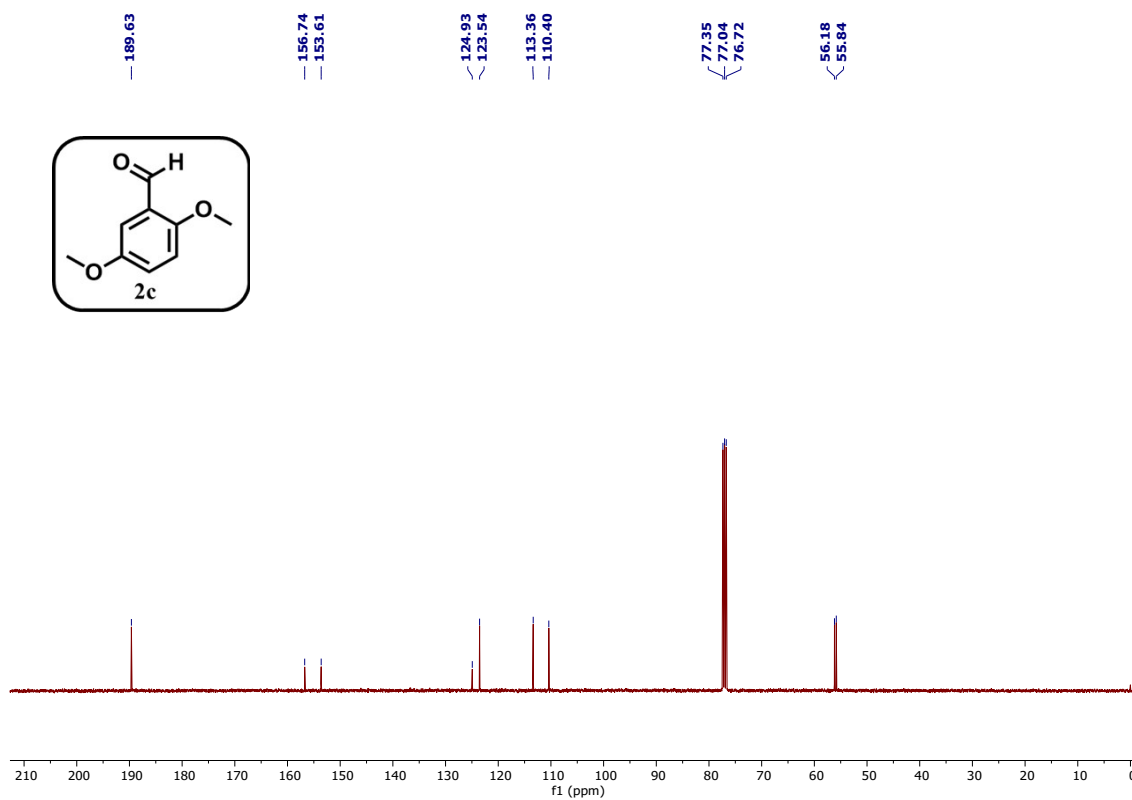
## $^{13}\text{C}$ NMR spectra of product 2b



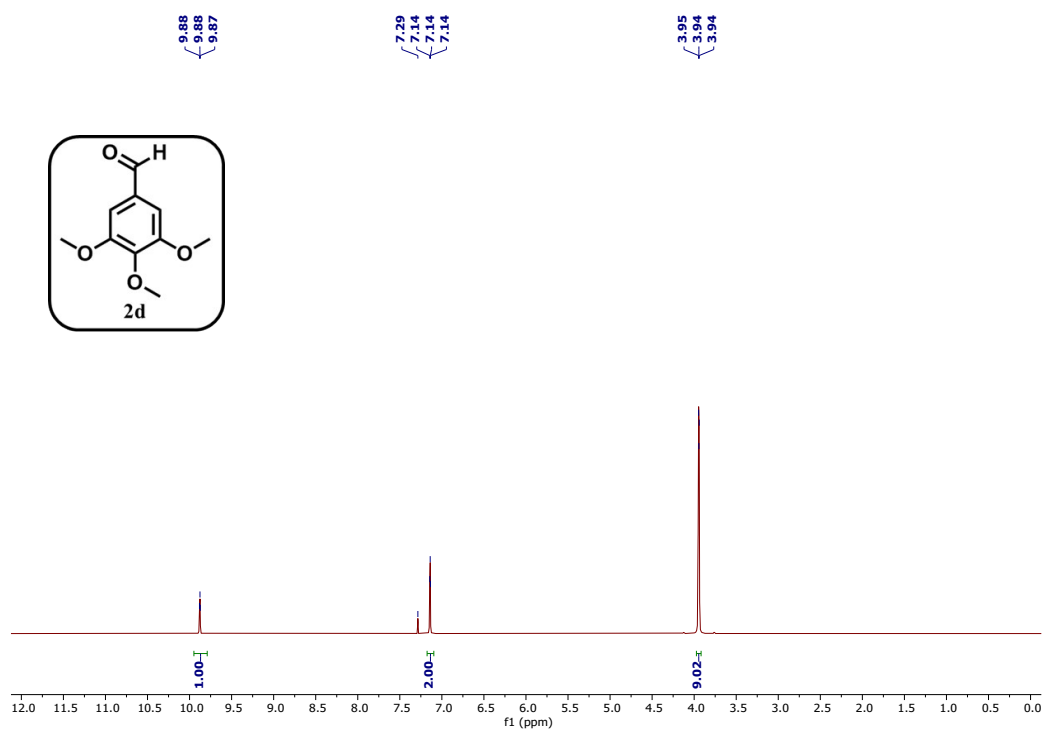
## <sup>1</sup>H NMR spectra of product 2c



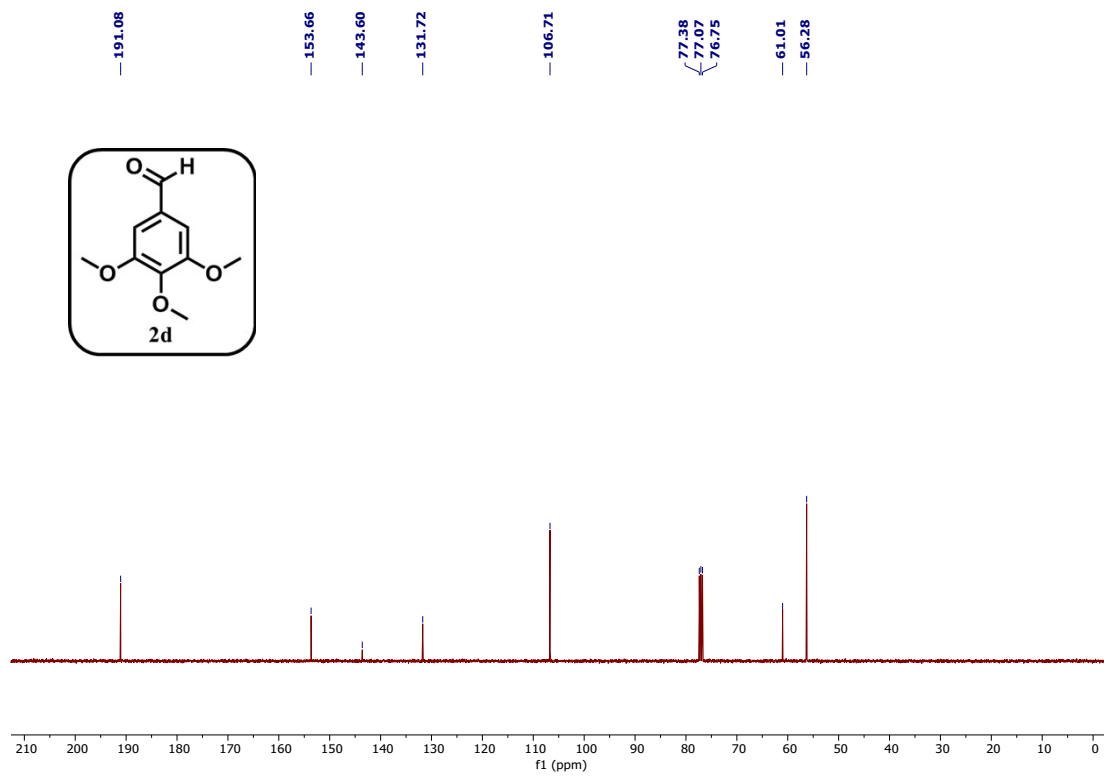
## <sup>13</sup>C NMR spectra of product 2c



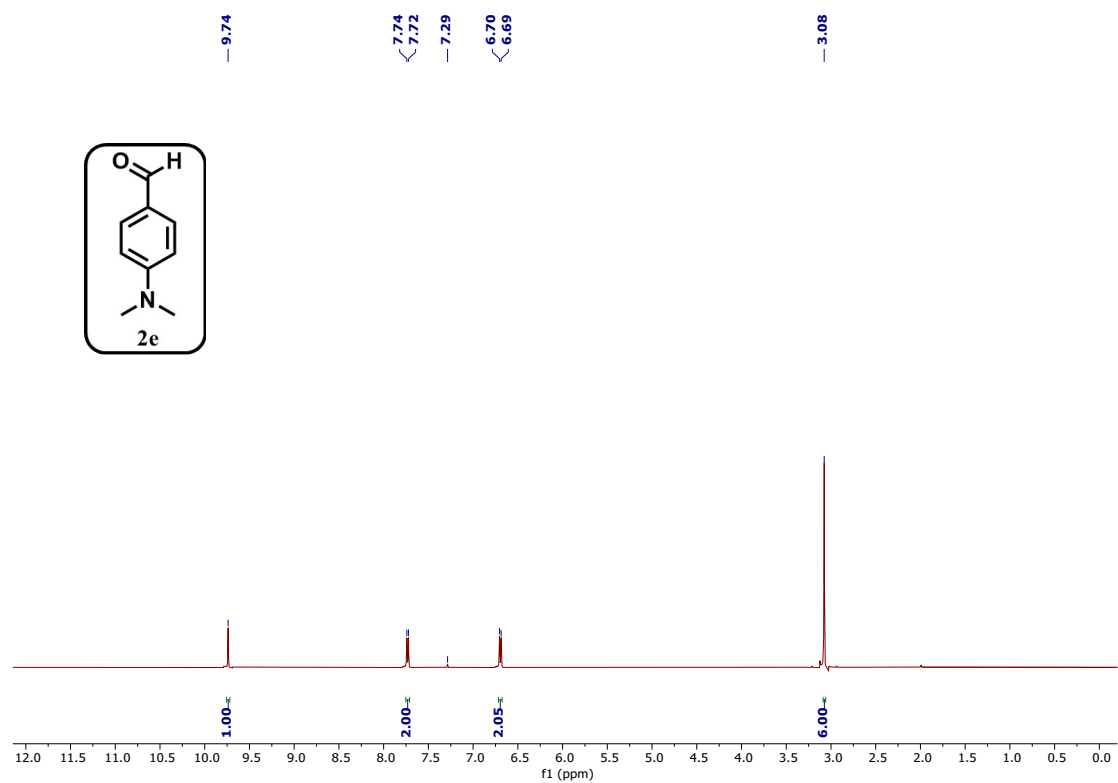
## <sup>1</sup>H NMR spectra of product 2d



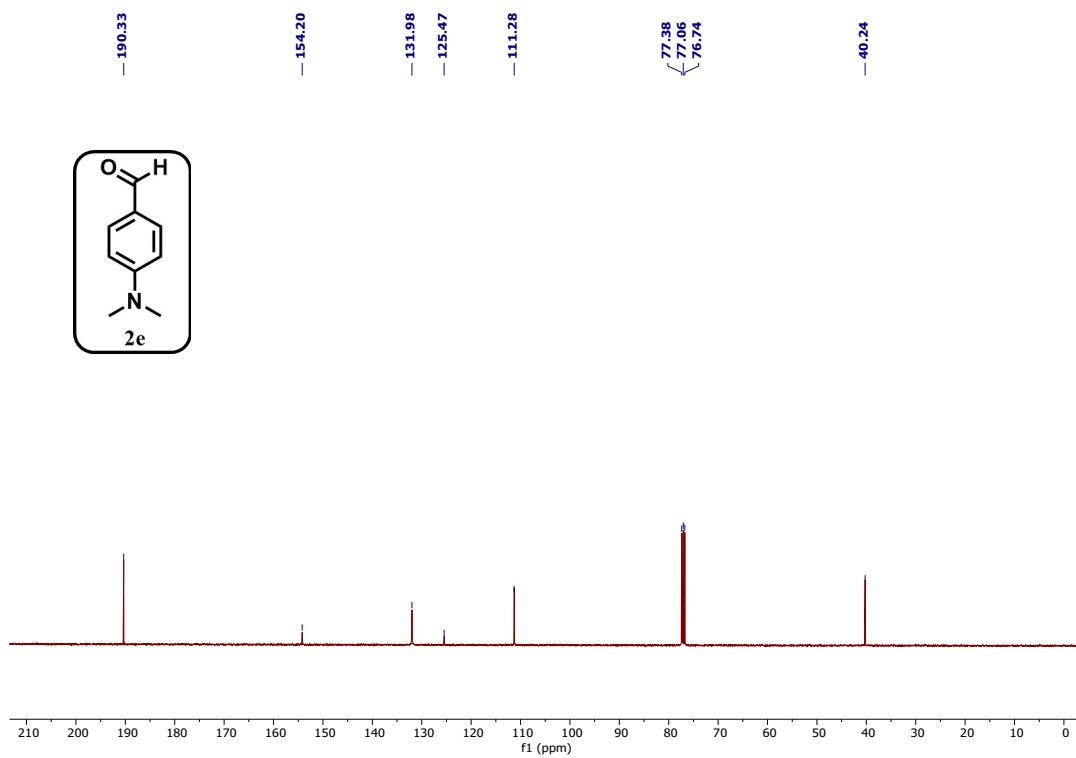
## <sup>13</sup>C NMR spectra of product 2d



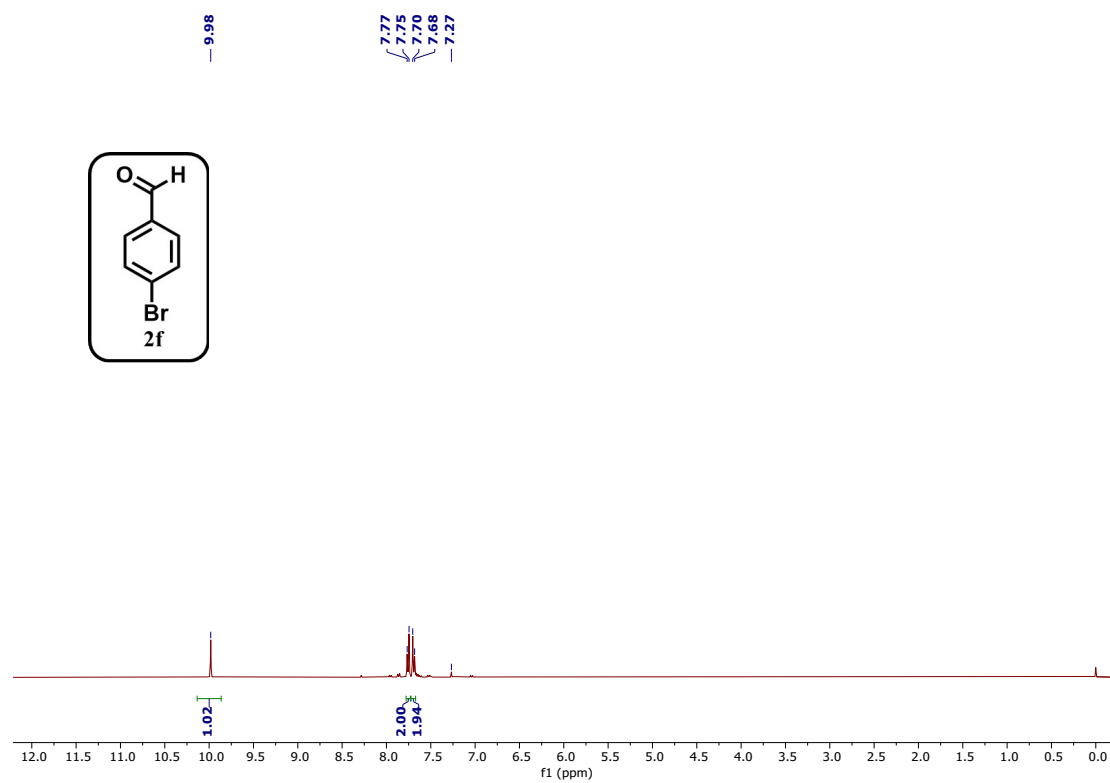
### <sup>1</sup>H NMR spectra of product 2e



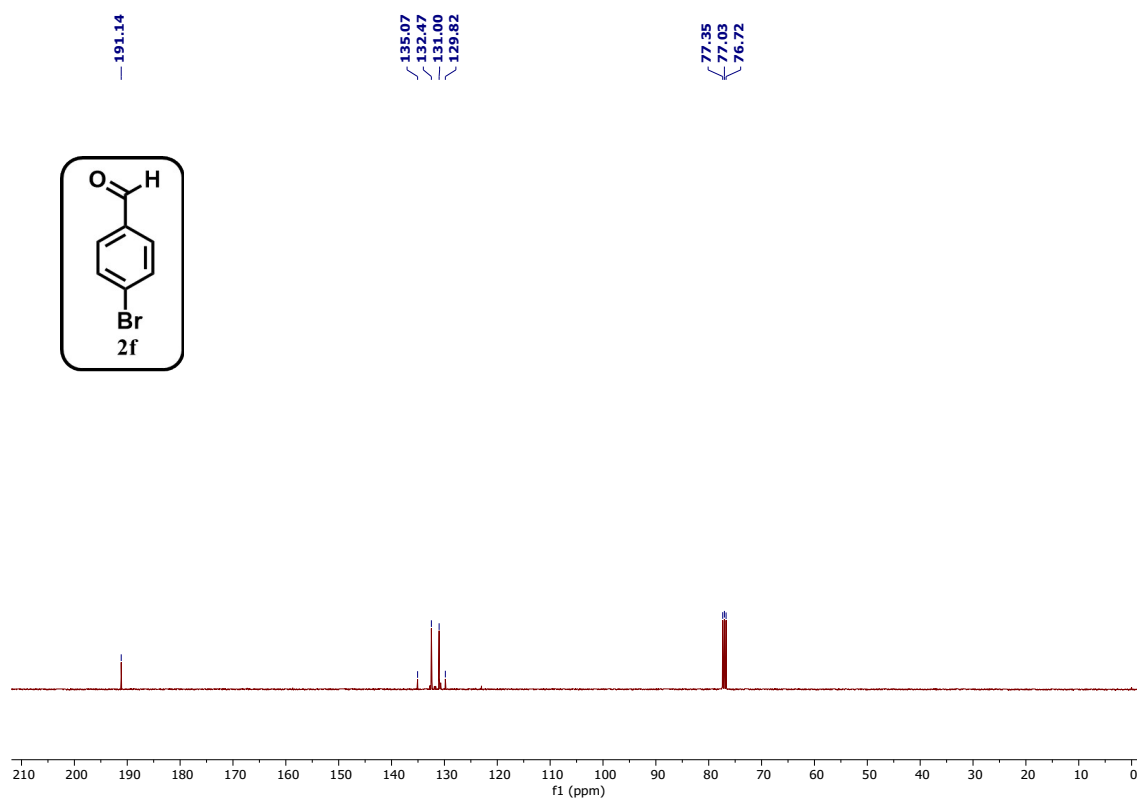
### <sup>13</sup>C NMR spectra of product 2e



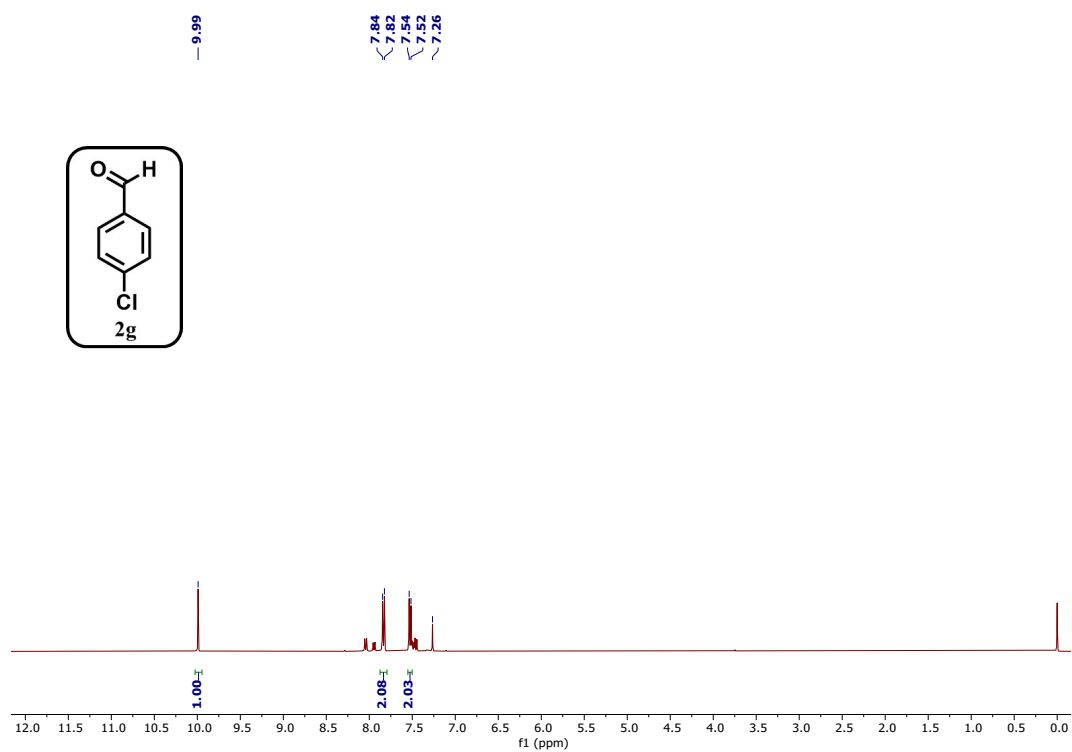
### <sup>1</sup>H NMR spectra of product 2f



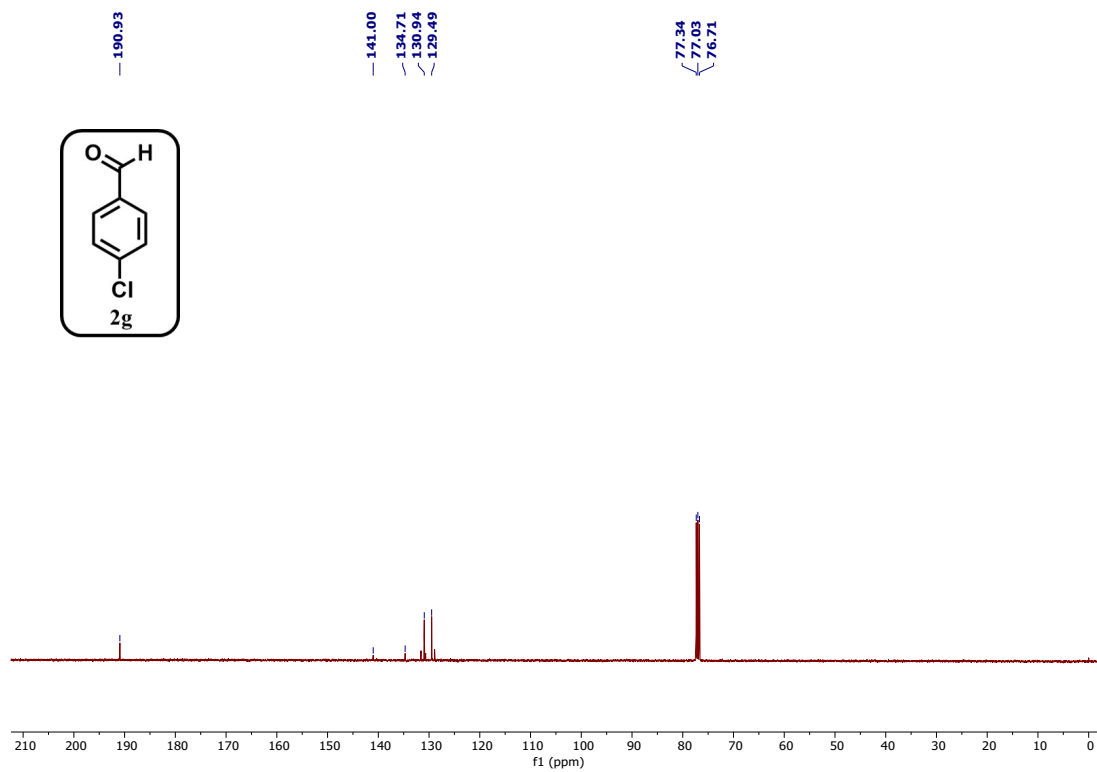
### <sup>13</sup>C NMR spectra of product 2f



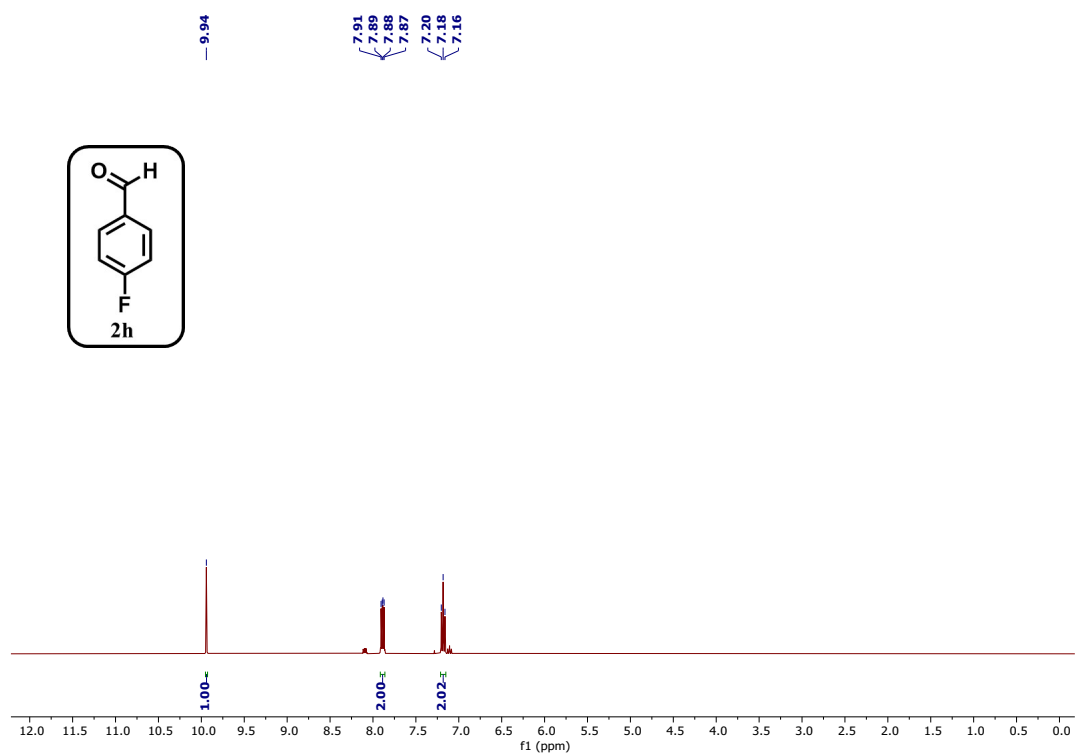
### <sup>1</sup>H NMR spectra of product 2g



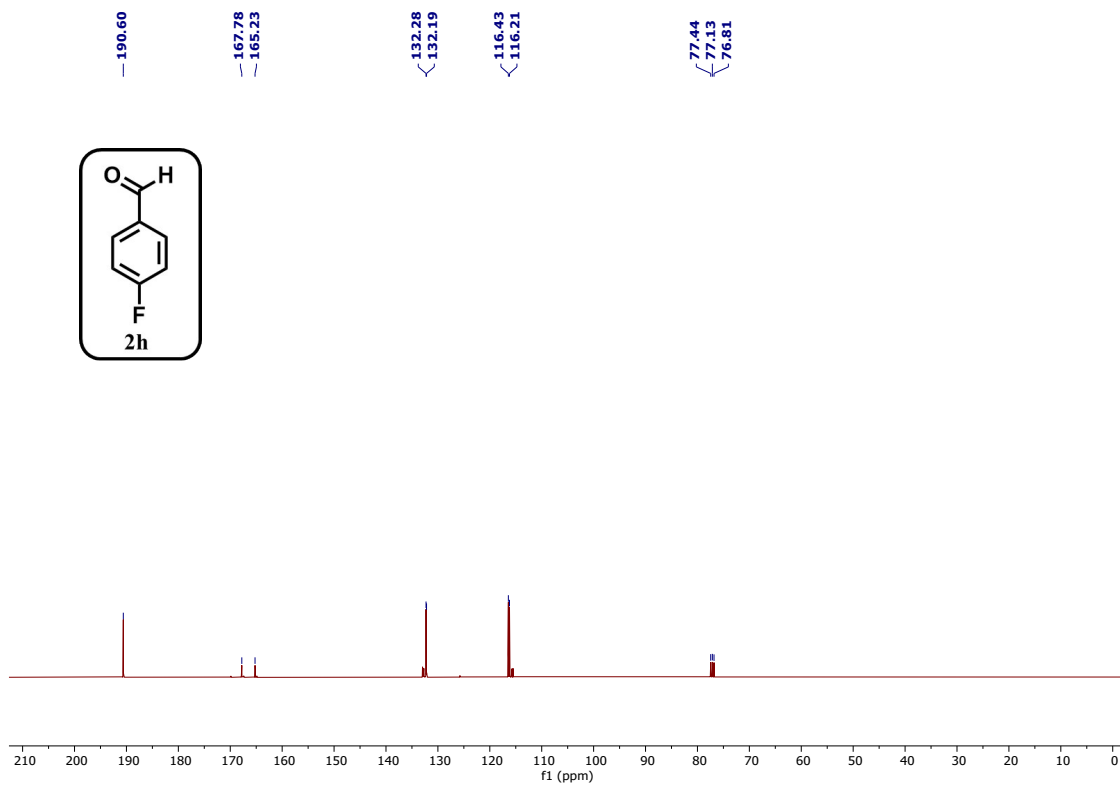
### <sup>13</sup>C NMR spectra of product 2g



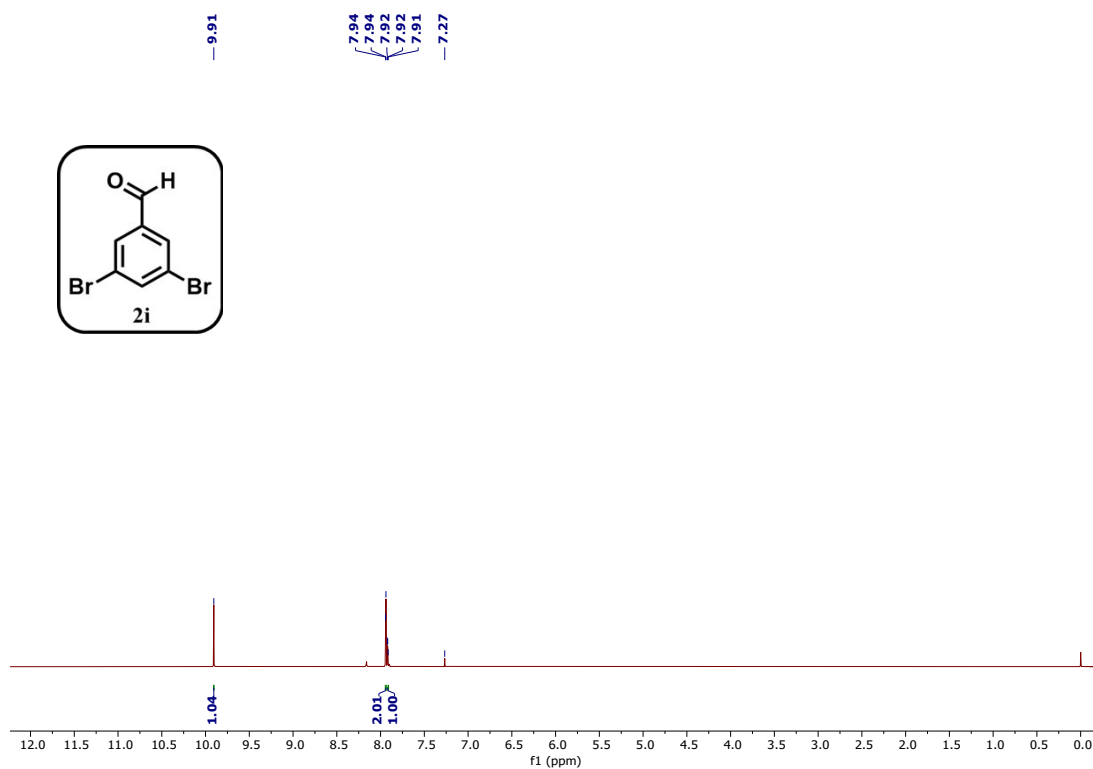
## <sup>1</sup>H NMR spectra of product 2h



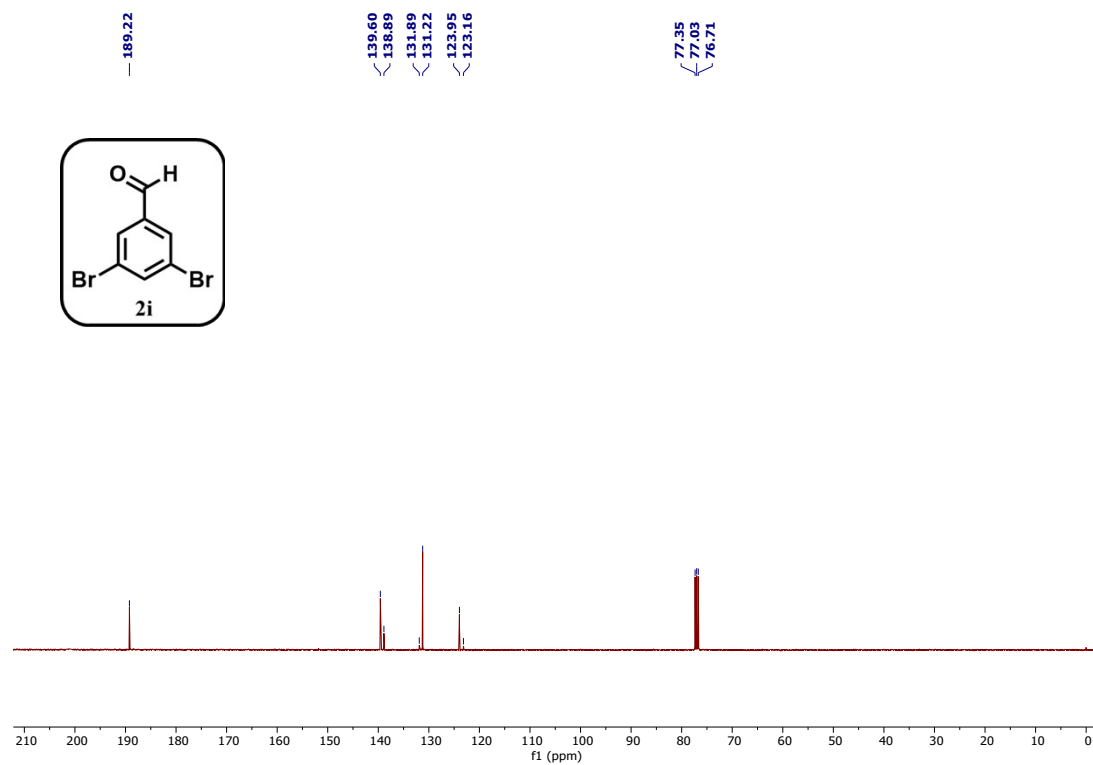
## <sup>13</sup>C NMR spectra of product 2h



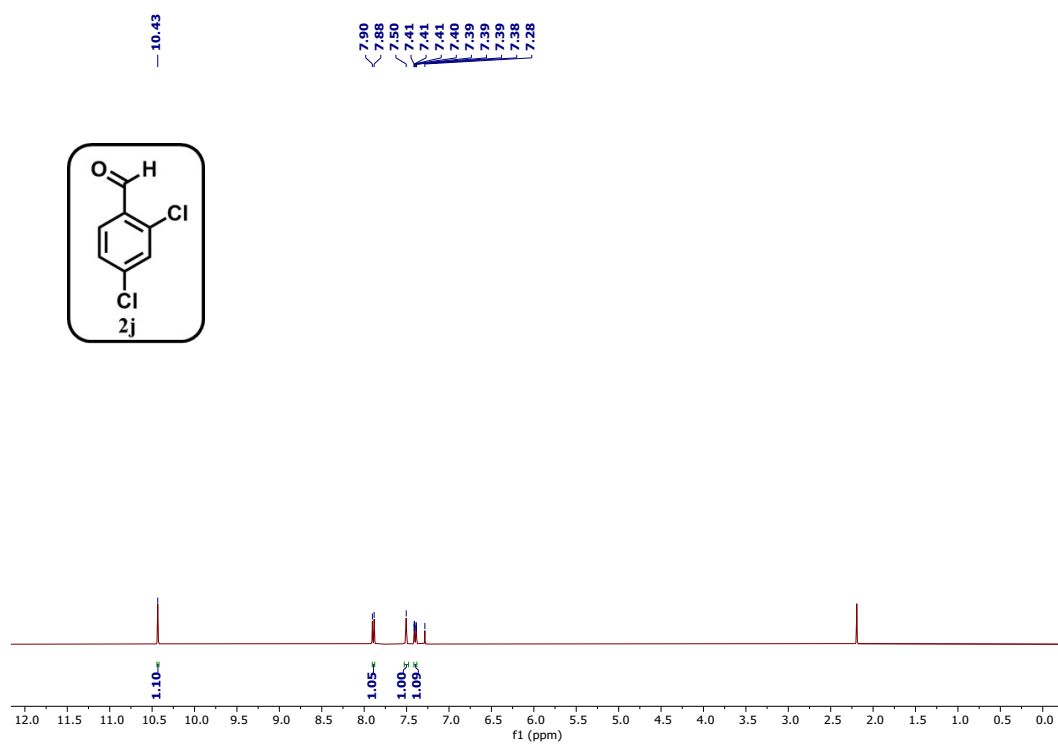
## <sup>1</sup>H NMR spectra of product 2i



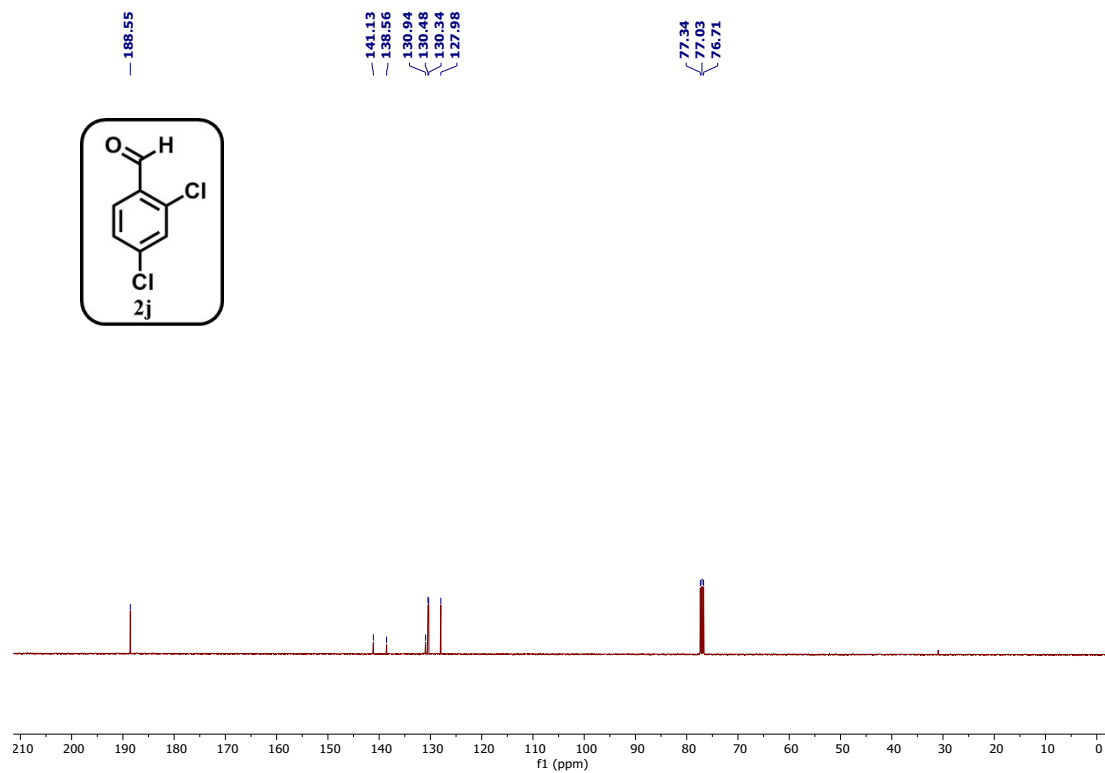
## <sup>13</sup>C NMR spectra of product 2i



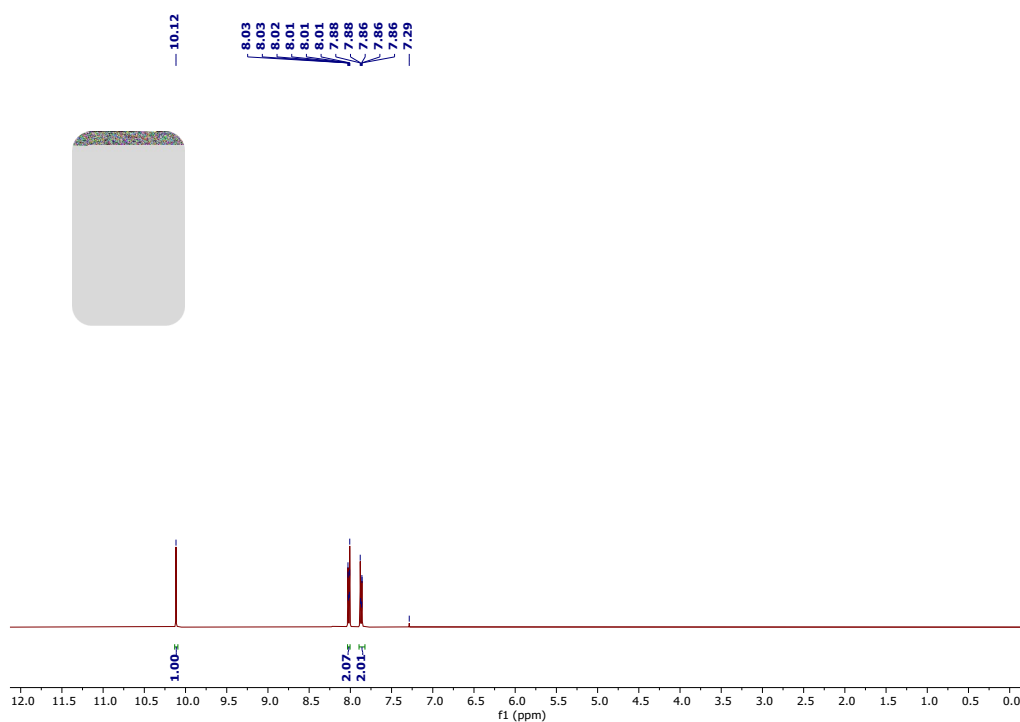
## <sup>1</sup>H NMR spectra of product 2j



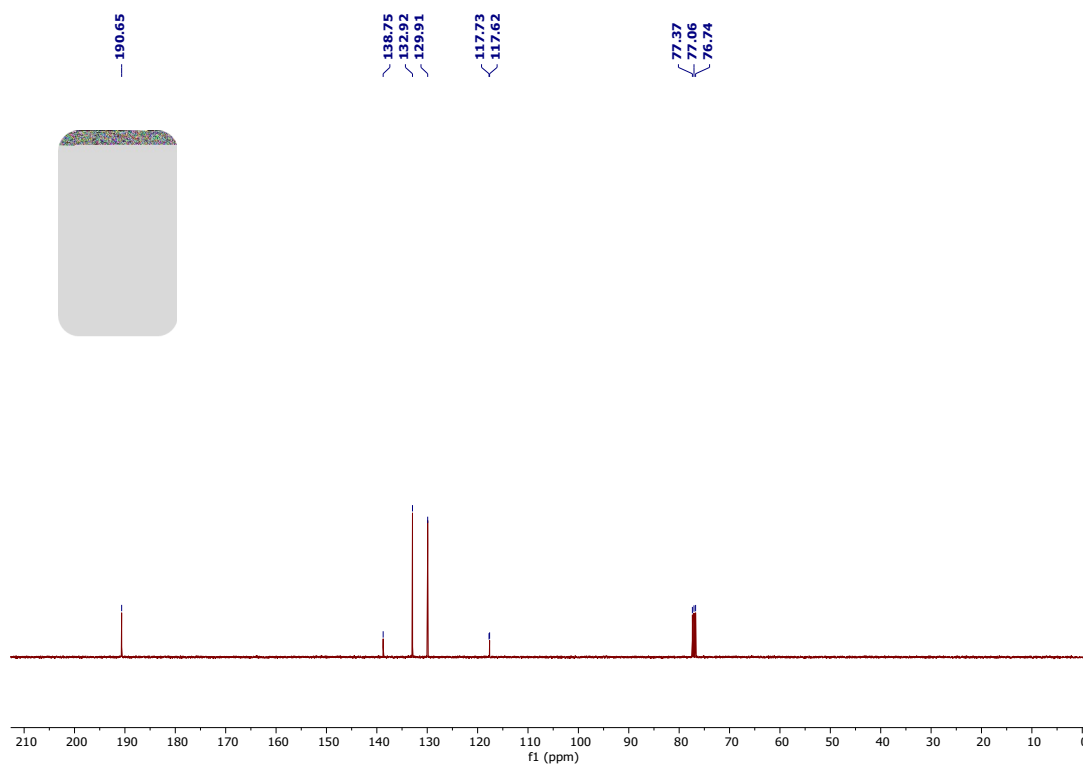
## <sup>13</sup>C NMR spectra of product 2j



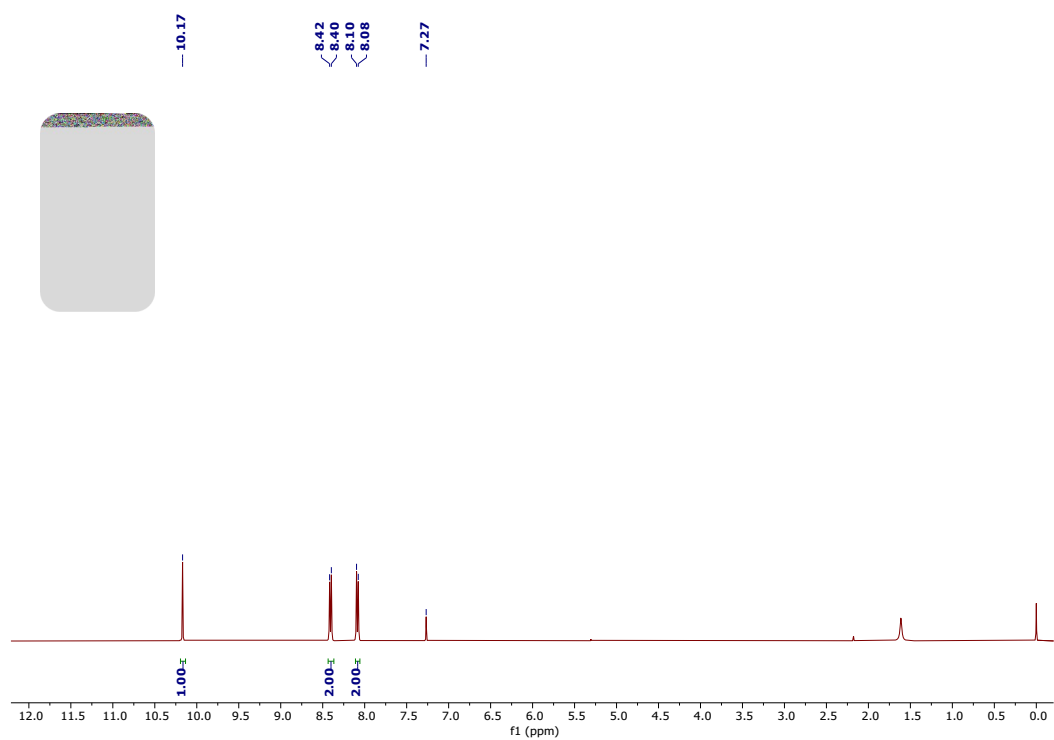
### <sup>1</sup>H NMR spectra of product 2k



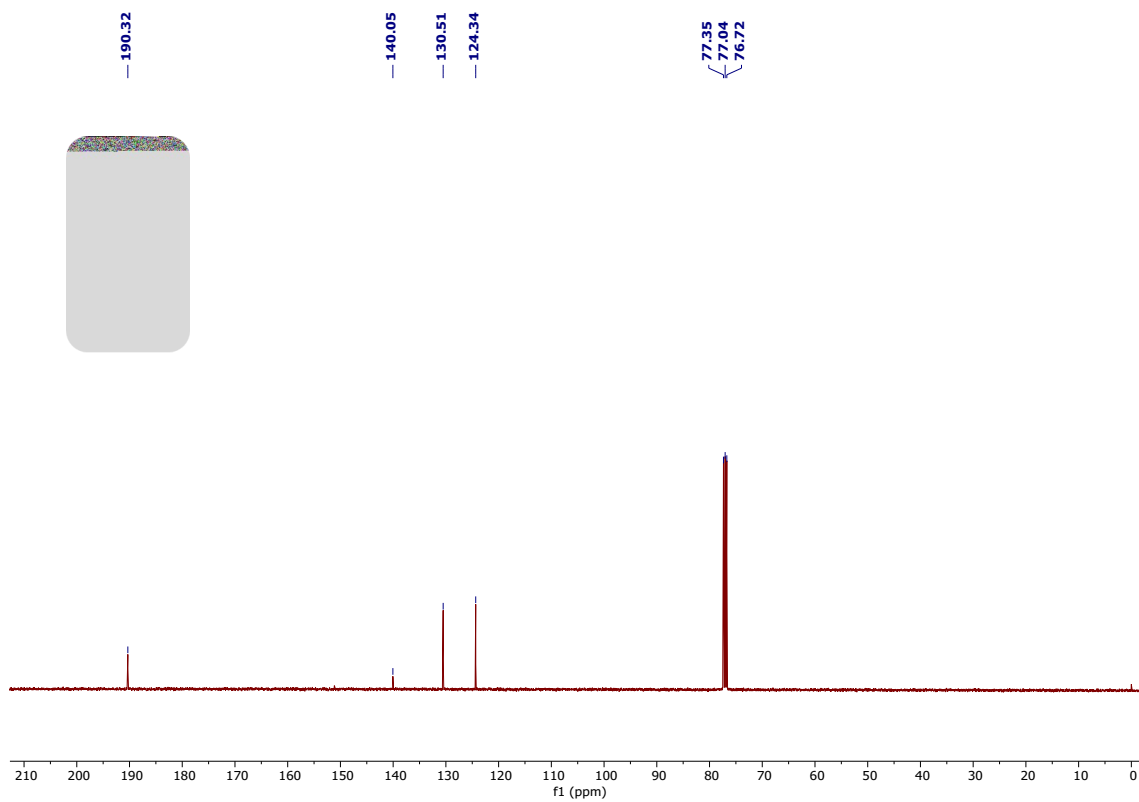
### <sup>13</sup>C NMR spectra of product 2k



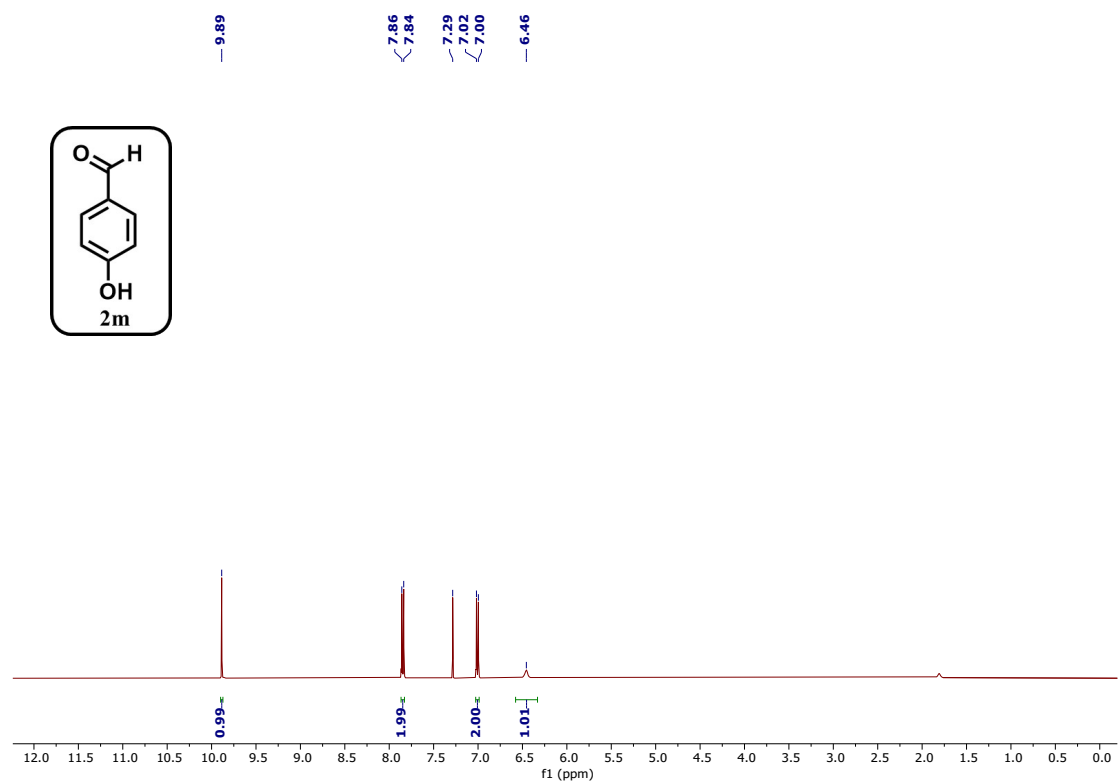
### <sup>1</sup>H NMR spectra of product 2l



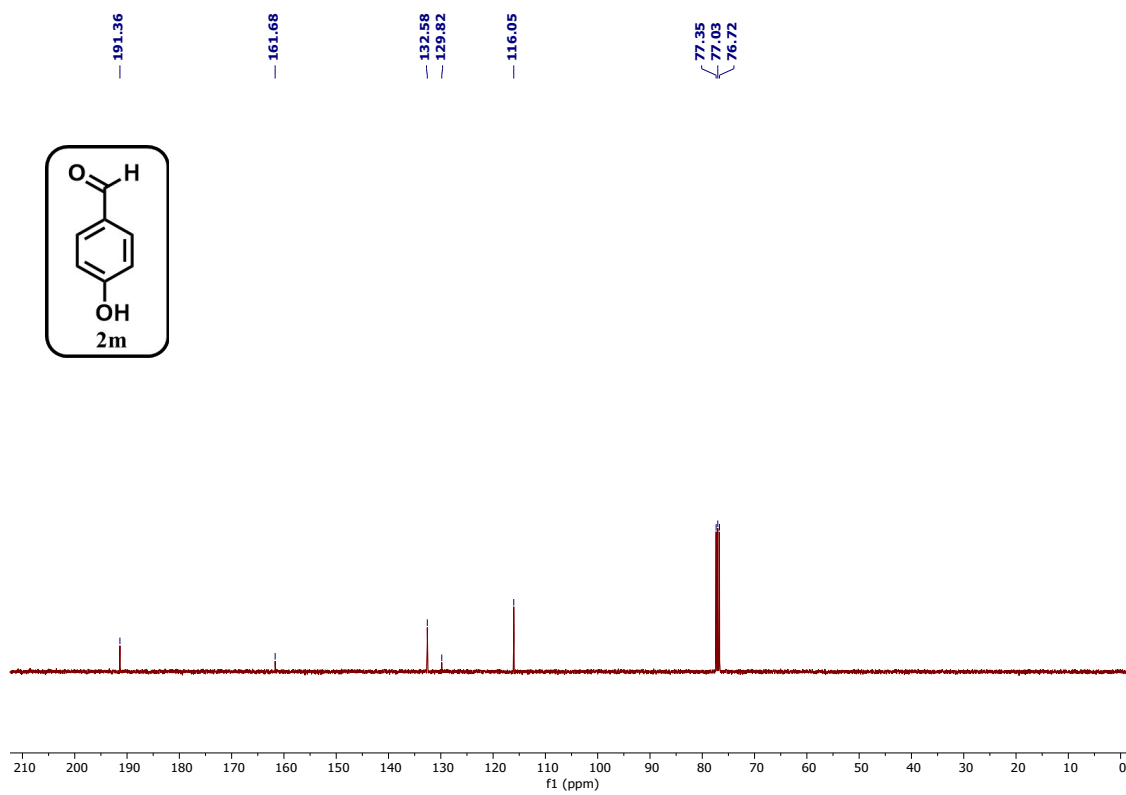
### <sup>13</sup>C NMR spectra of product 2l



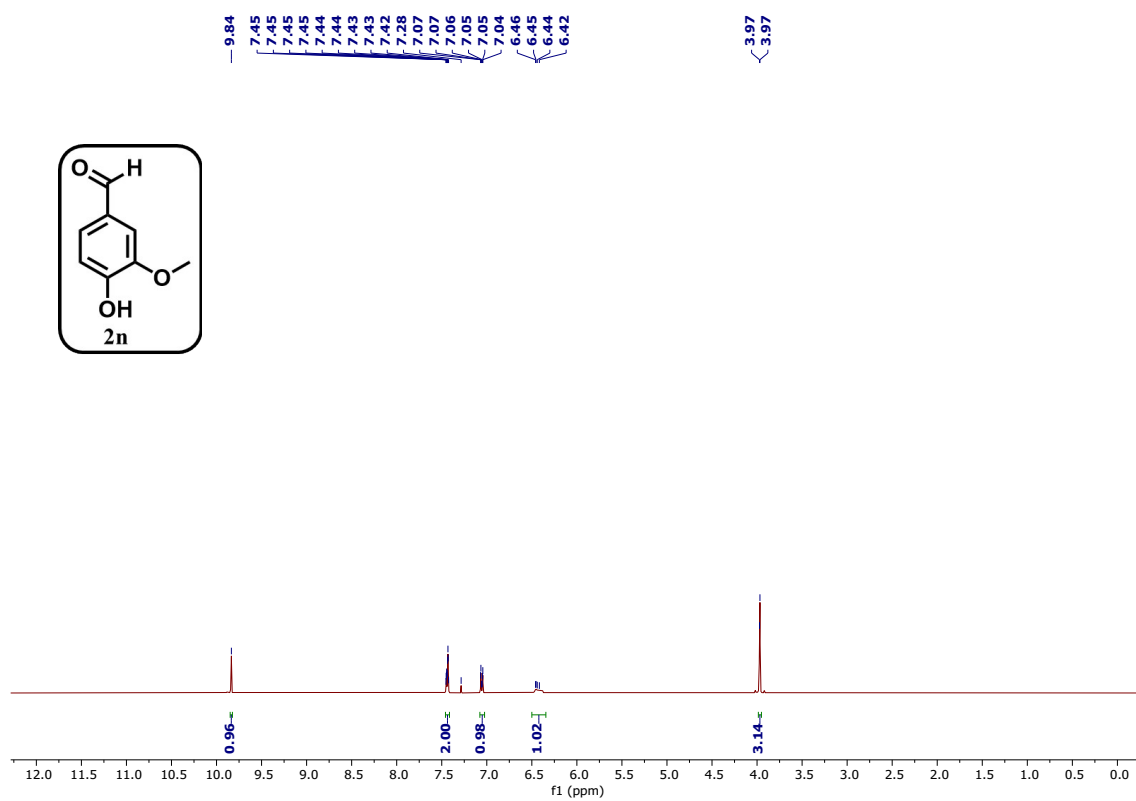
### <sup>1</sup>H NMR spectra of product 2m



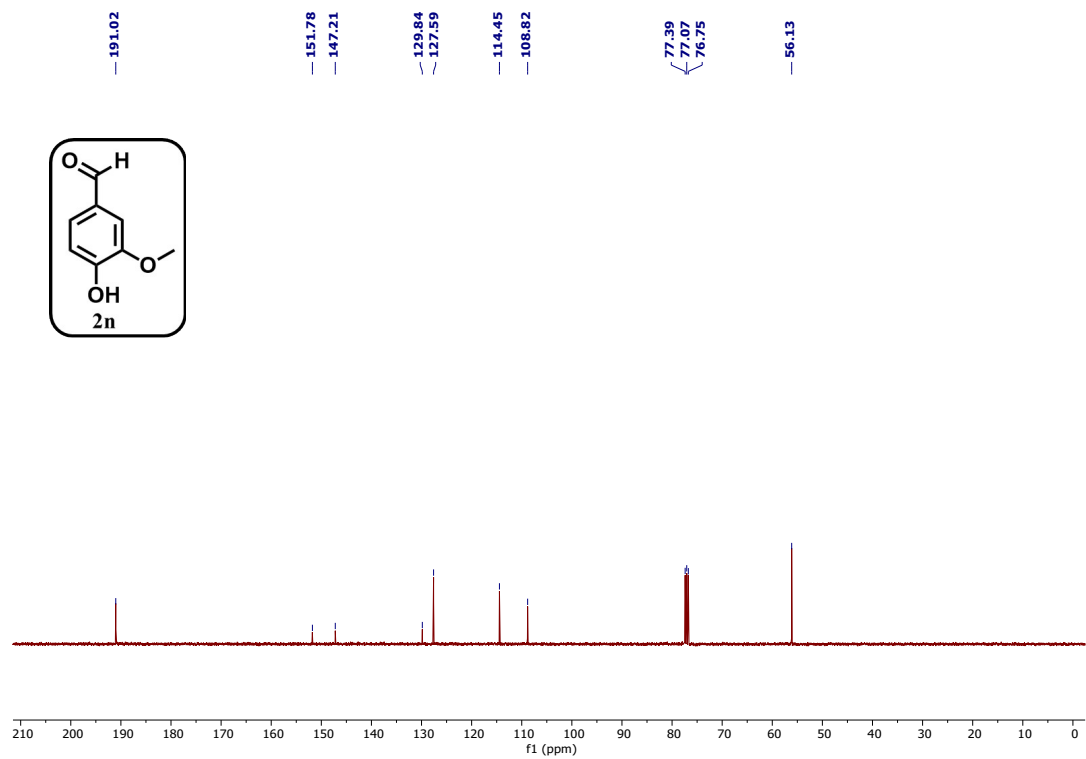
### <sup>13</sup>C NMR spectra of product 2m



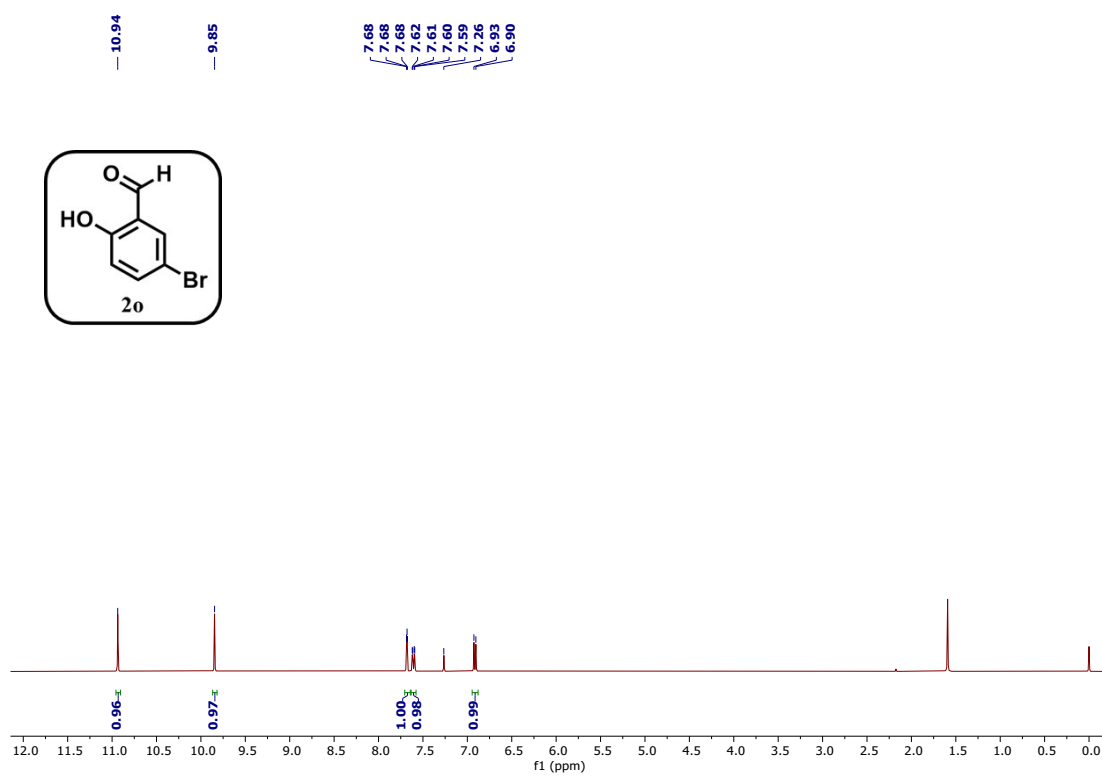
## <sup>1</sup>H NMR spectra of product 2n



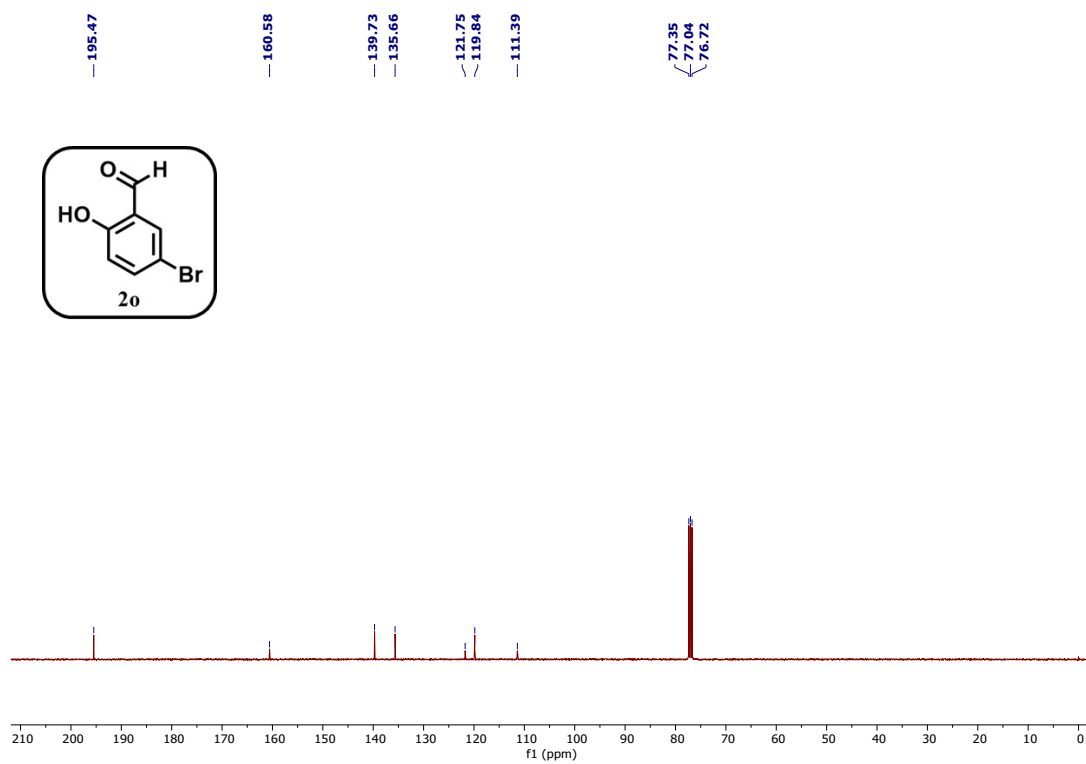
## <sup>13</sup>C NMR spectra of product 2n



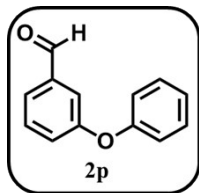
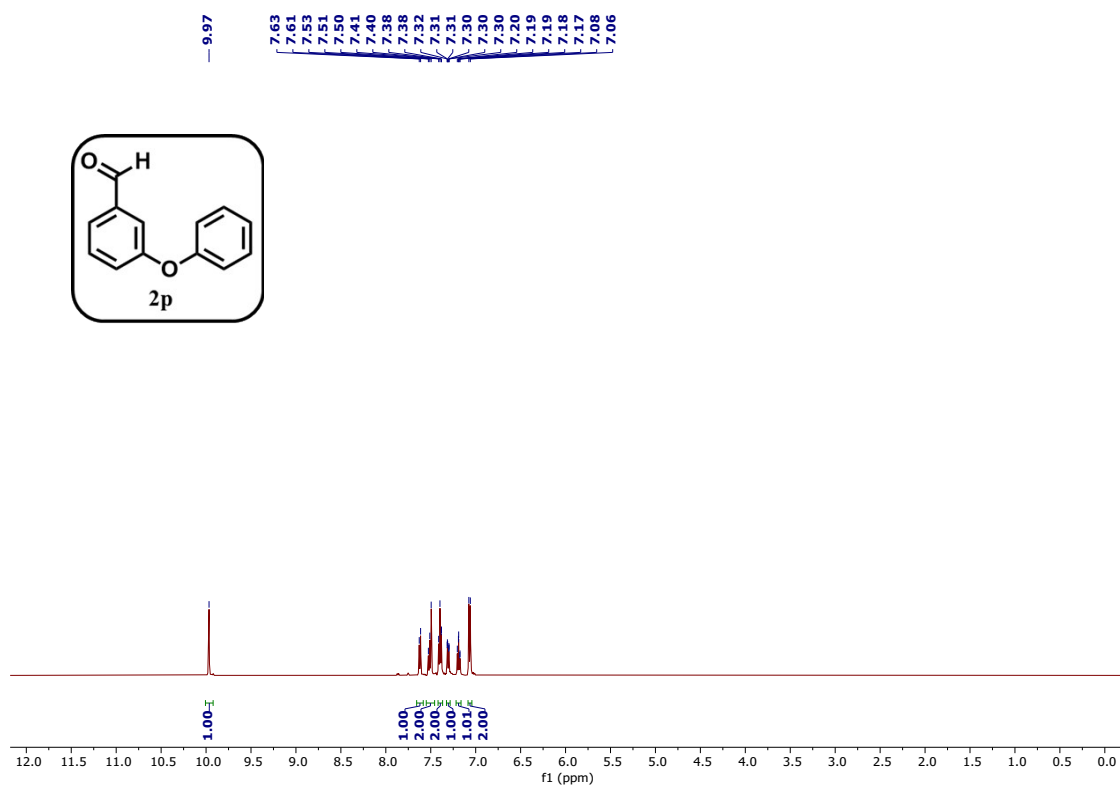
## <sup>1</sup>H NMR spectra of product 2o



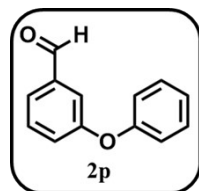
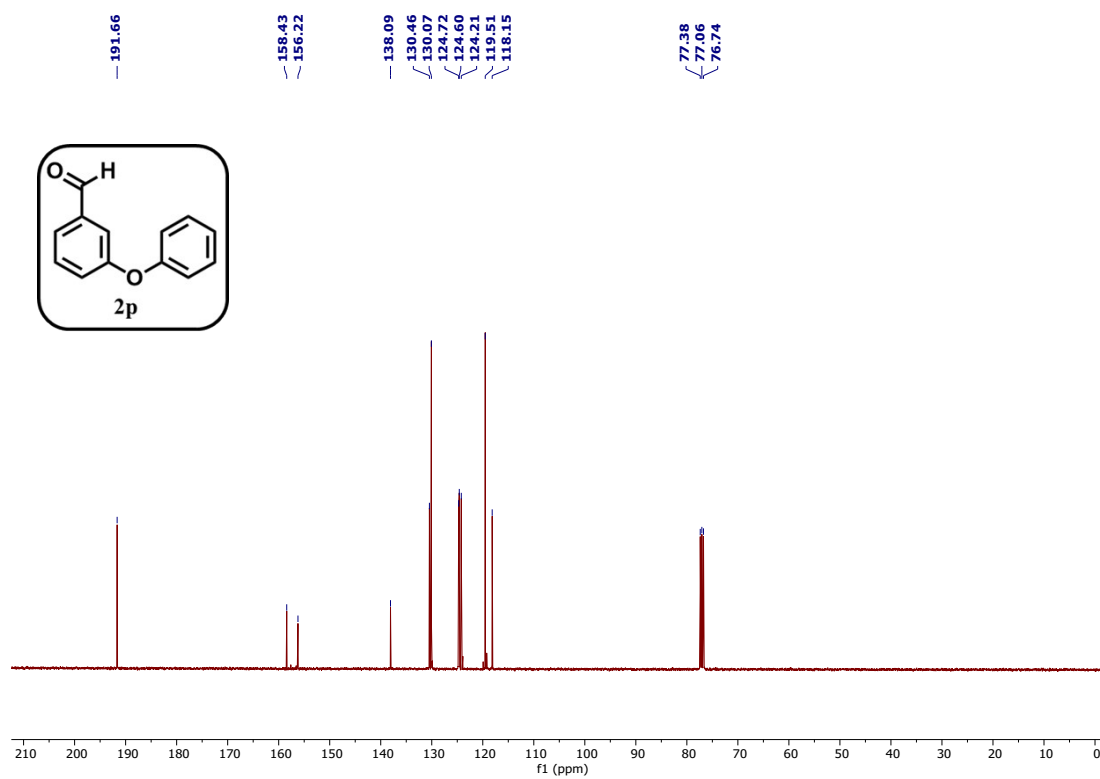
## <sup>13</sup>C NMR spectra of product 2o



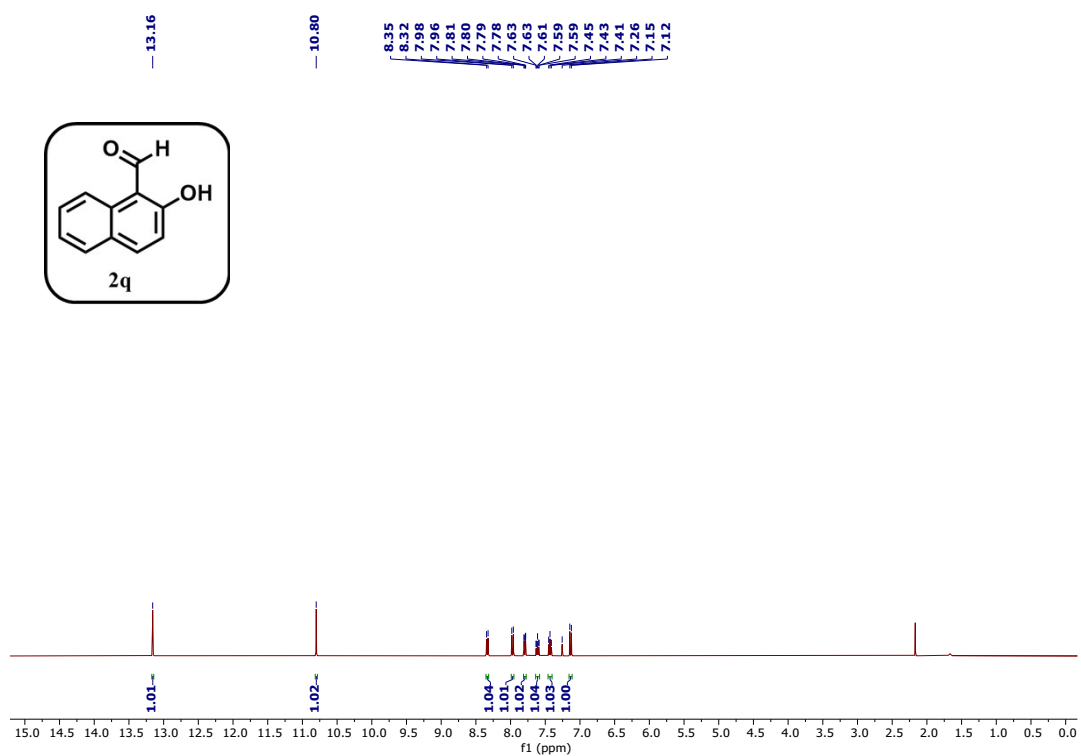
### <sup>1</sup>H NMR spectra of product 2p



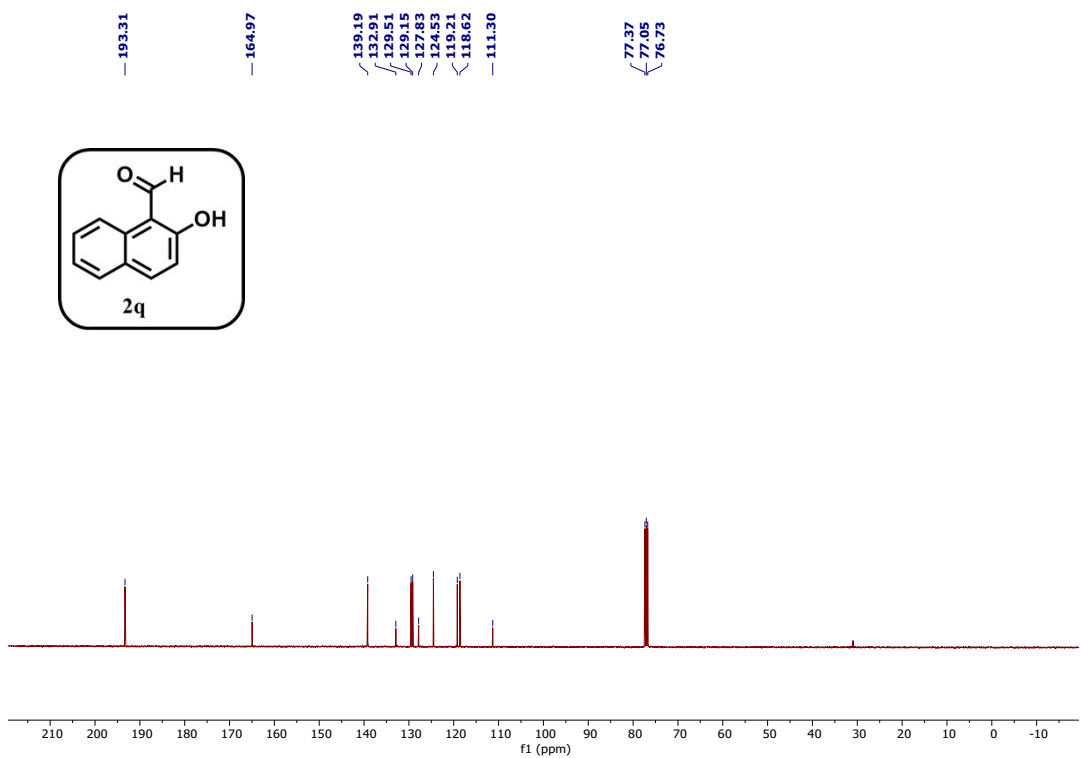
### <sup>13</sup>C NMR spectra of product 2p



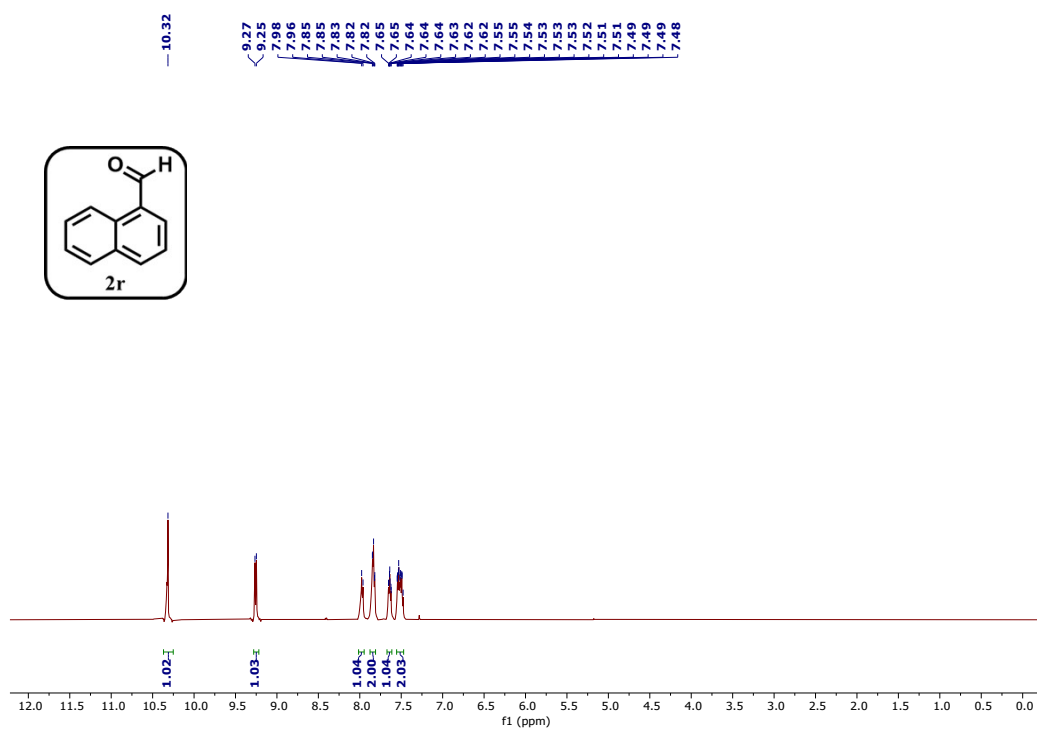
## <sup>1</sup>H NMR spectra of product 2q



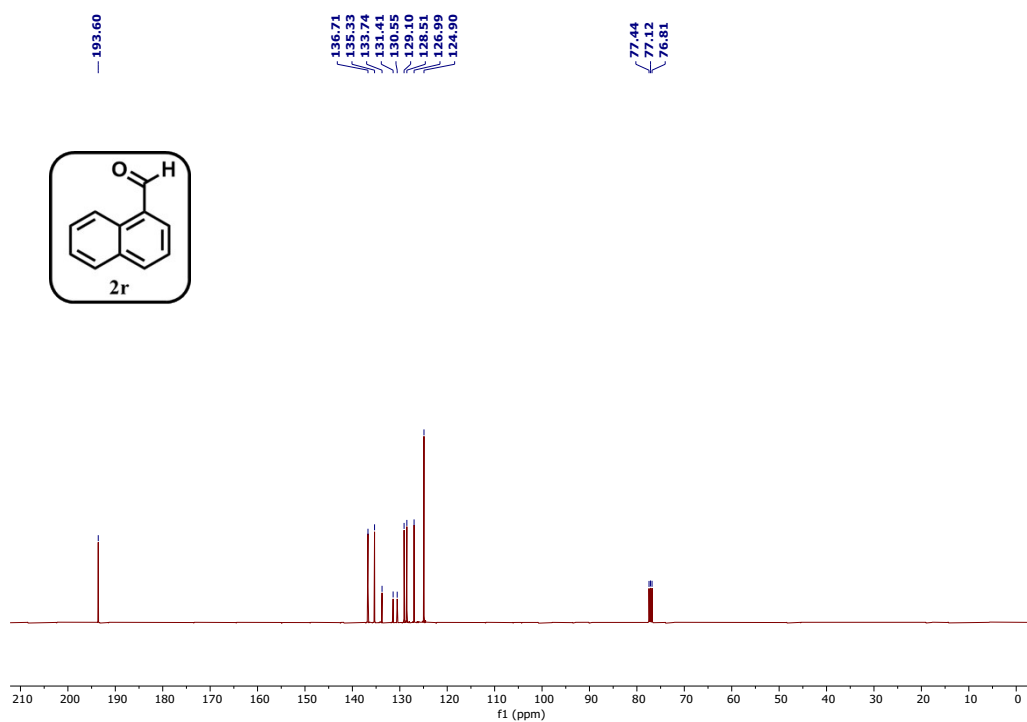
## <sup>13</sup>C NMR spectra of product 2q



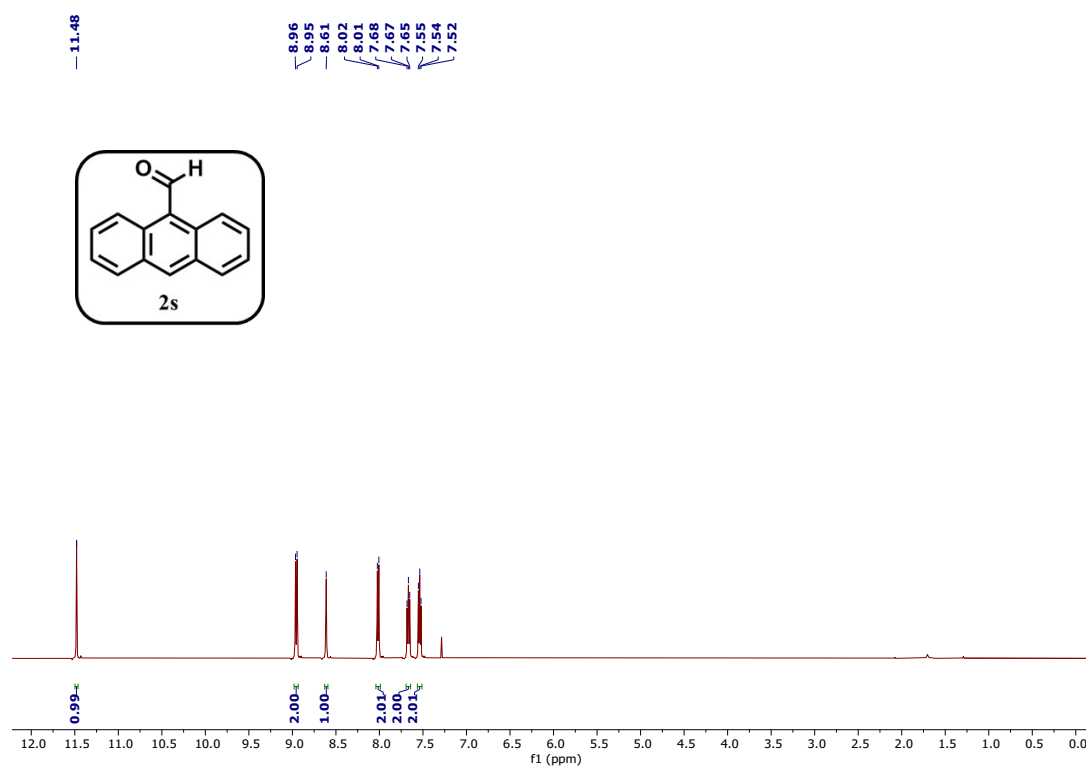
## <sup>1</sup>H NMR spectra of product 2r



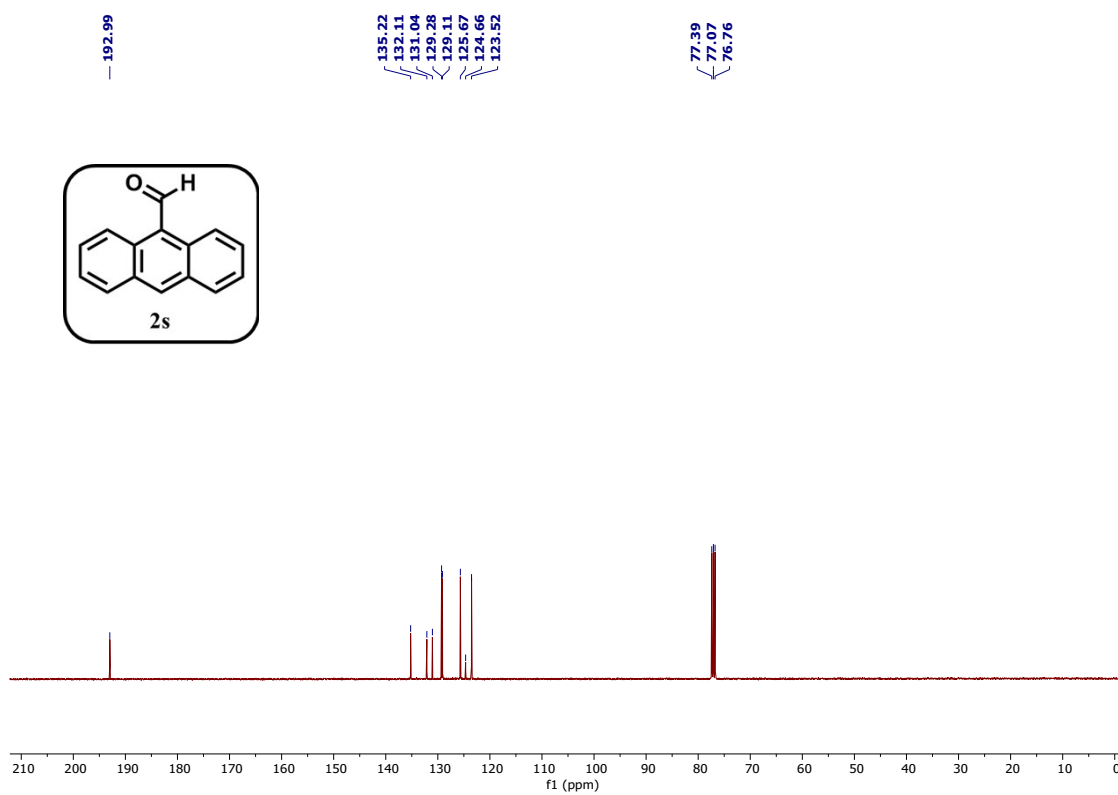
## <sup>13</sup>C NMR spectra of product 2r



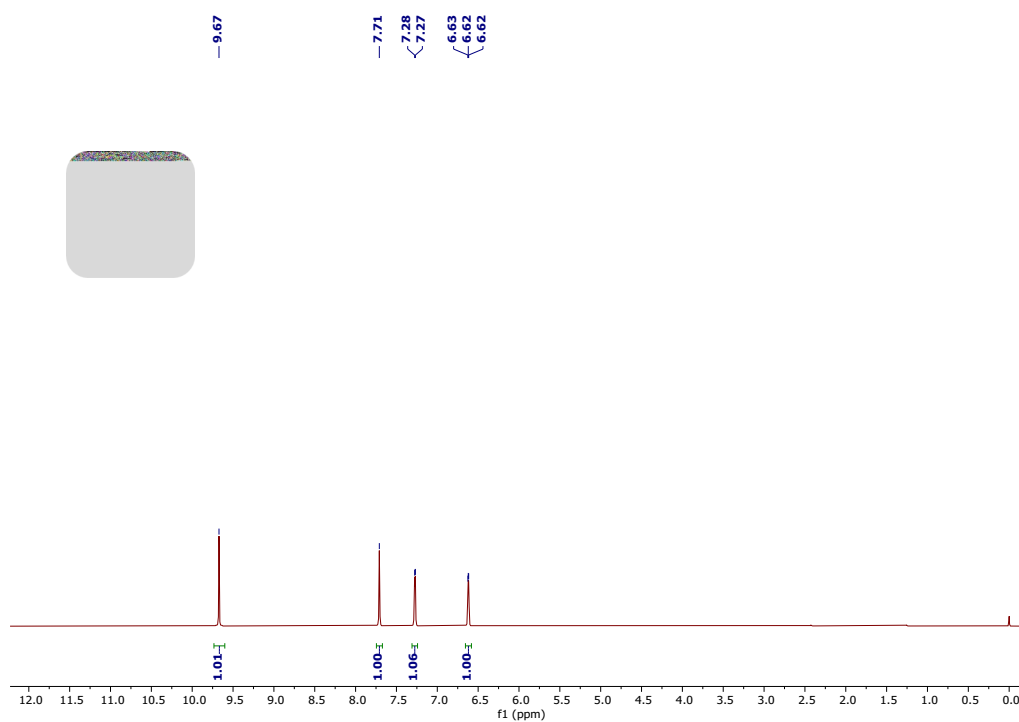
## <sup>1</sup>H NMR spectra of product 2s



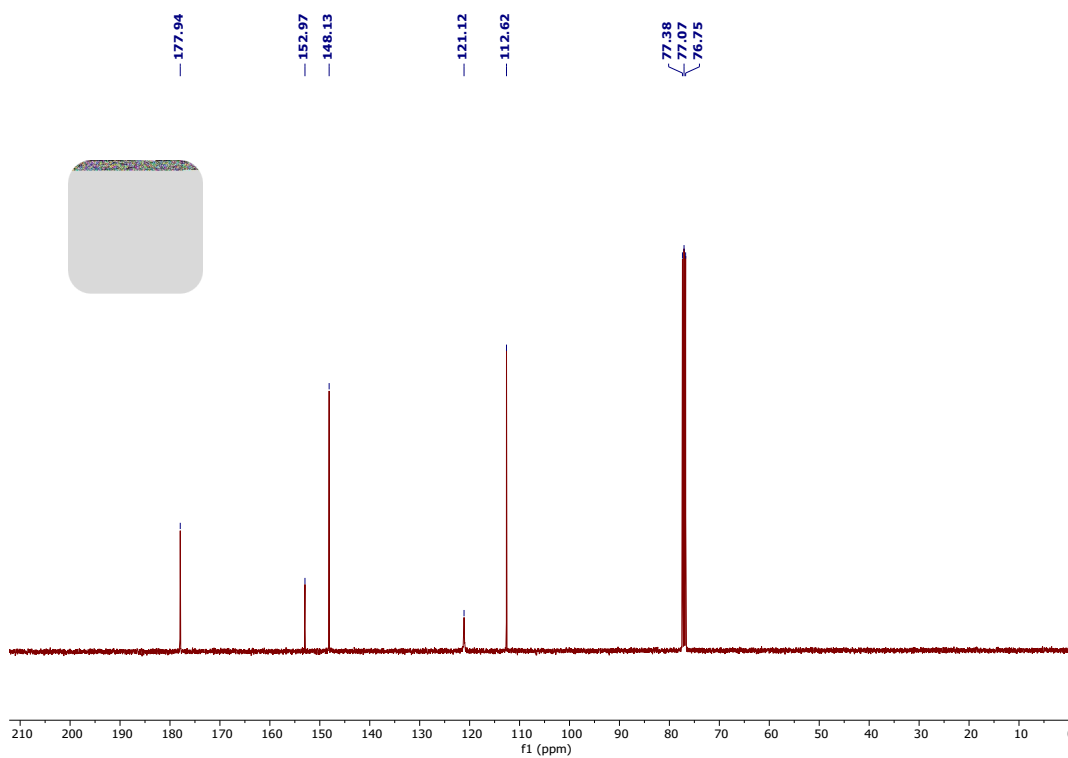
## <sup>13</sup>C NMR spectra of product 2s



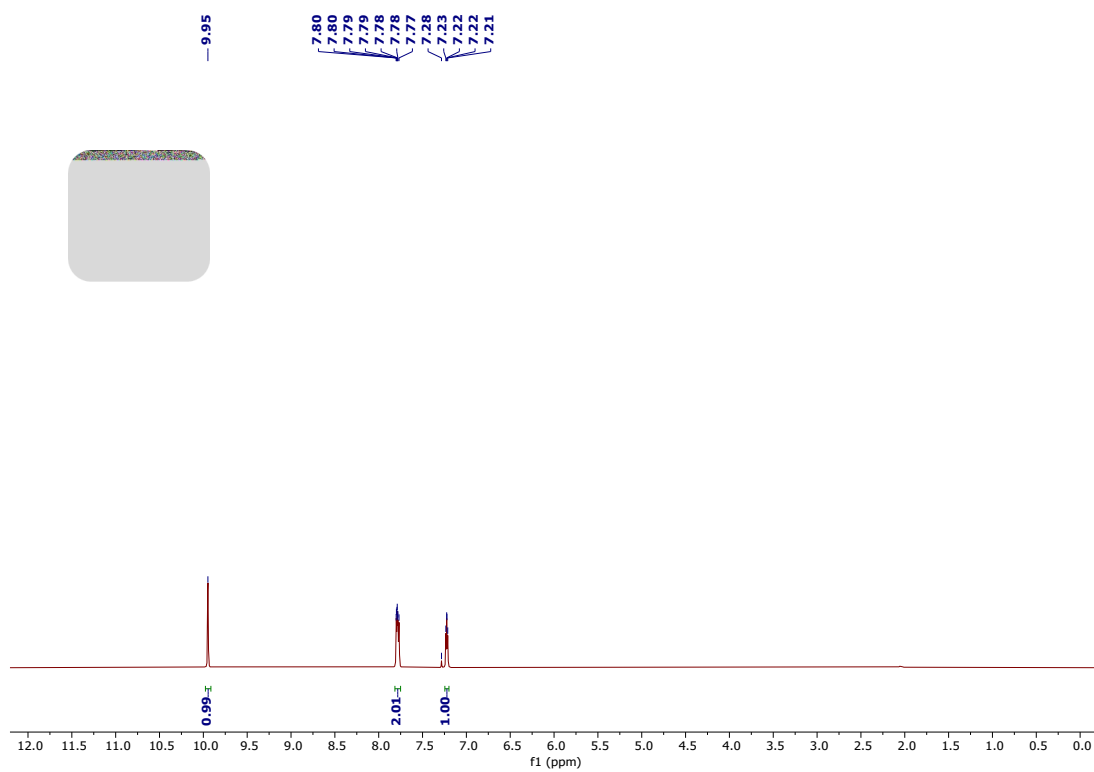
### <sup>1</sup>H NMR spectra of product 2t



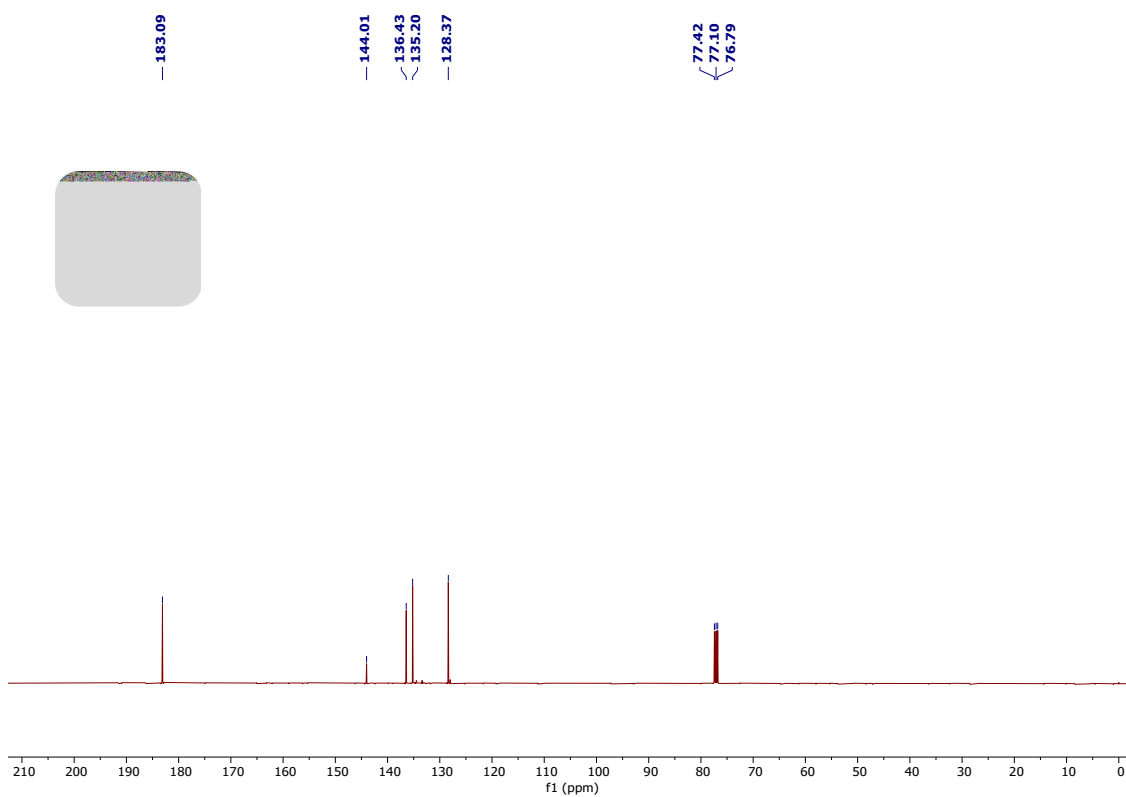
### <sup>13</sup>C NMR spectra of product 2t



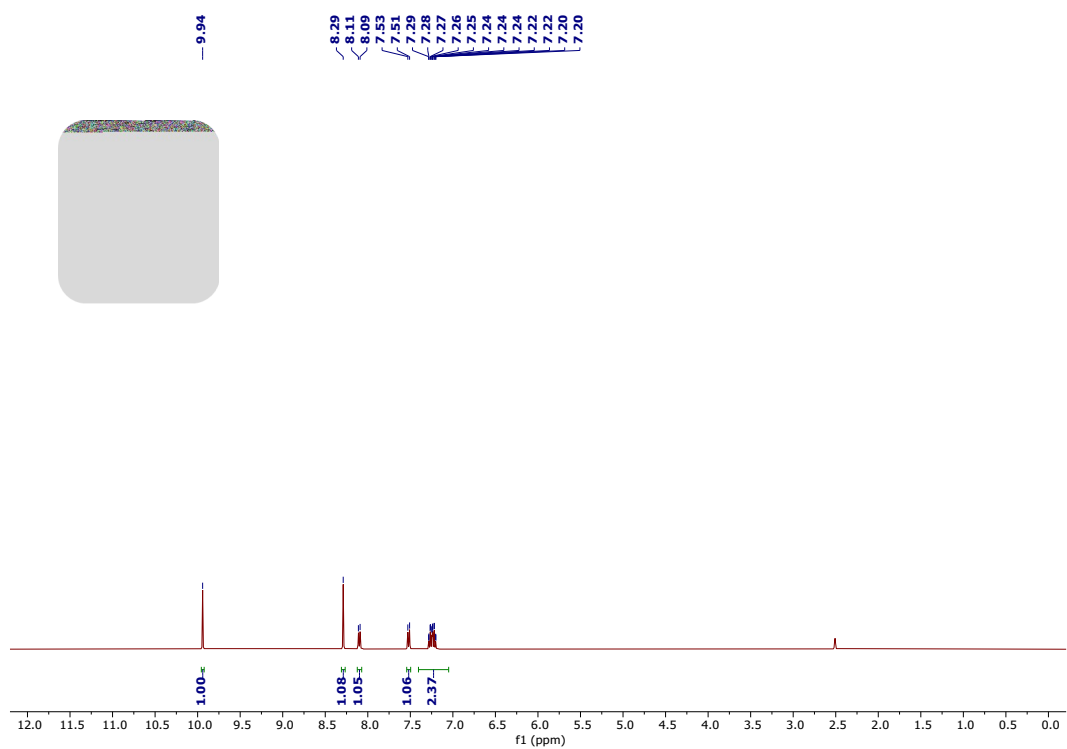
## <sup>1</sup>H NMR spectra of product 2u



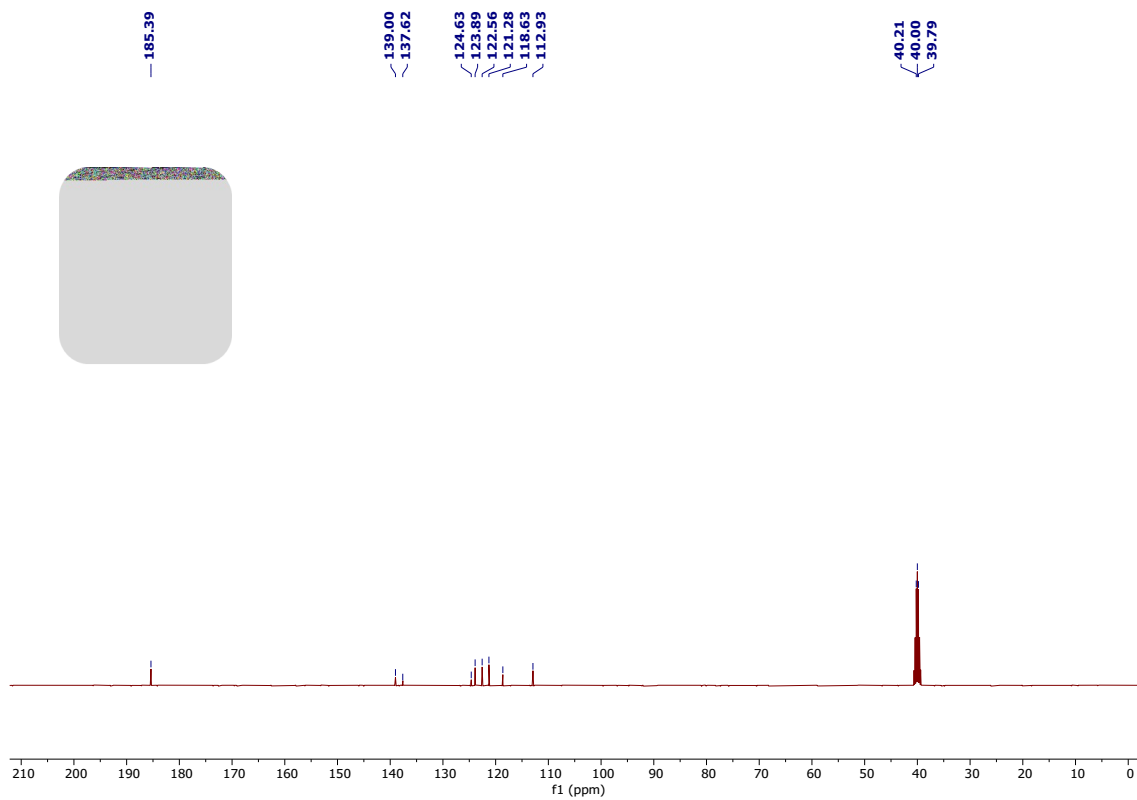
## <sup>13</sup>C NMR spectra of product 2u



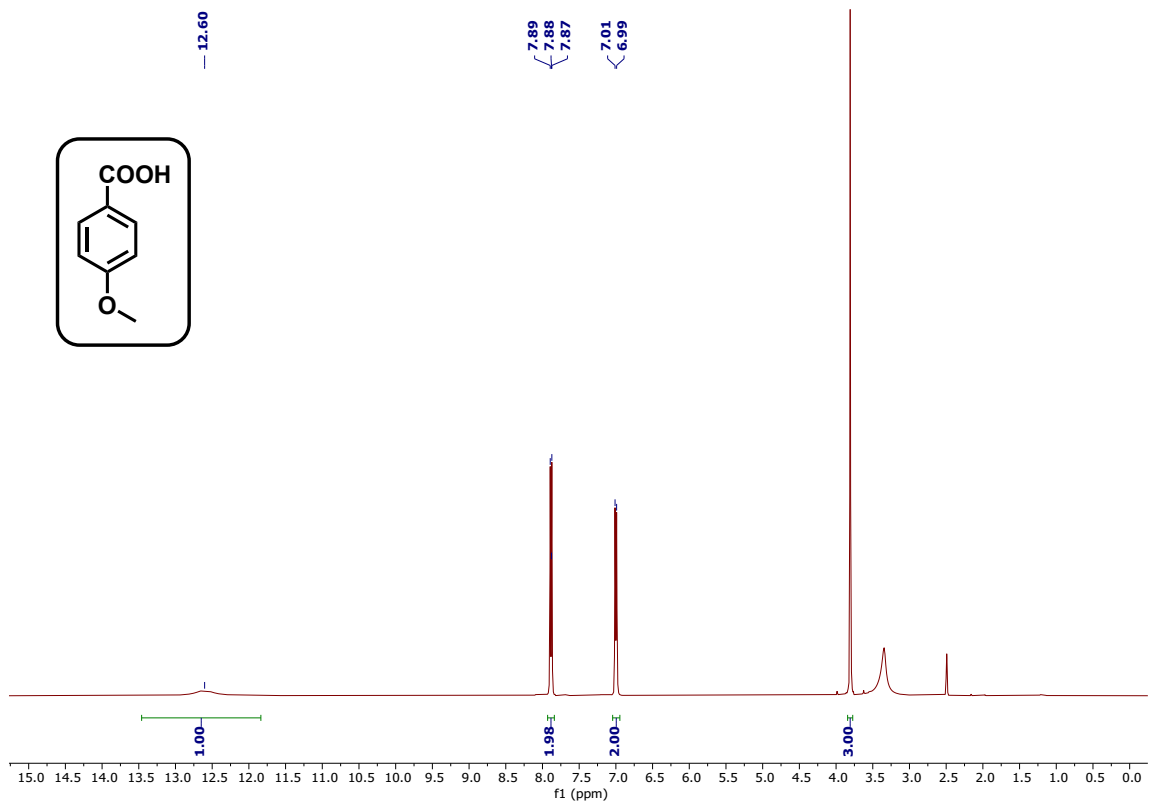
### <sup>1</sup>H NMR spectra of product 2v



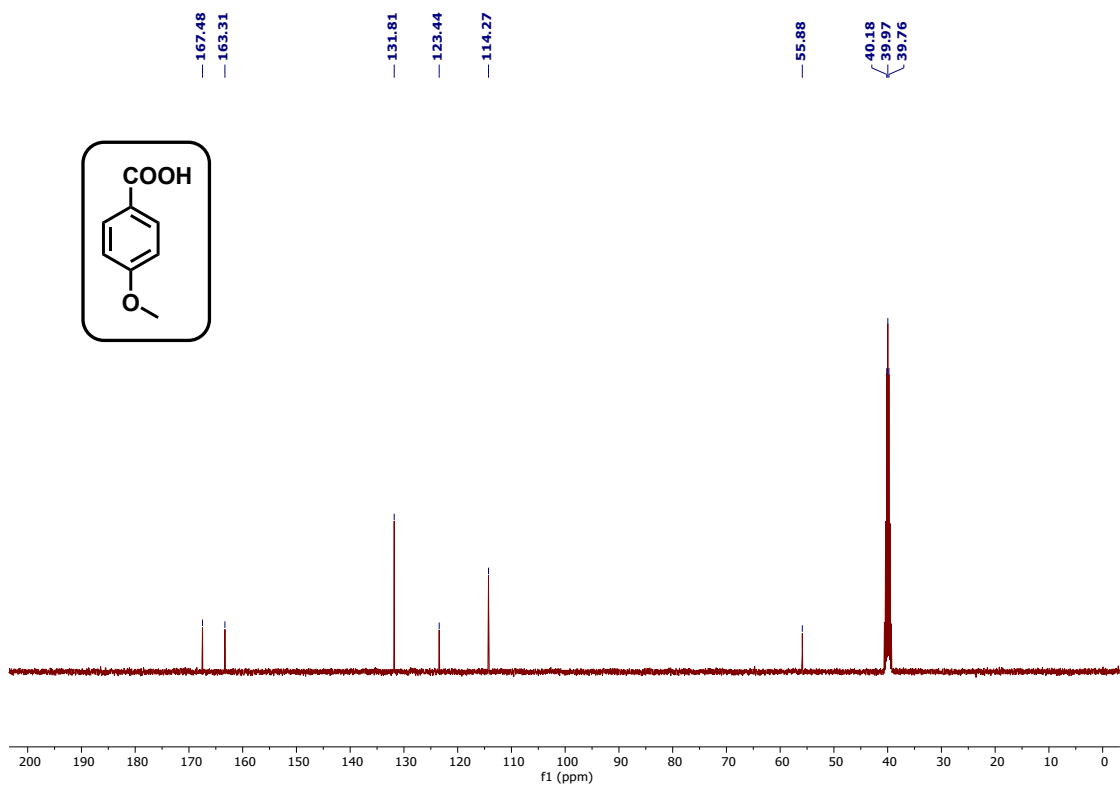
### <sup>13</sup>C NMR spectra of product 2v



## <sup>1</sup>H NMR spectra of 4-methoxy benzoic acid



## <sup>13</sup>C NMR spectra of 4-methoxy benzoic acid



### 3. Zero Pass CHEM21 green metrics toolkit

Supplementary Information: Appendix 2				Summary of Zero Pass Metrics Toolkit														
Yield, conversion, selectivity, AE, RME																		
Reactant (Limiting Reactant First)	Mass (g)	MW	Mol	Catalyst	Mass (g)	Reagent	Mass (g)	Reaction solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	Work up chemical	Mass (g)	Workup solvent	Volume (cm <sup>3</sup> )	Density (g ml <sup>-1</sup> )	Mass (g)	
4-methoxy benzyl alcoho	0.050	138.16	0.00	Ni	0.02			Isopropanol	2.00	0.79	1.57						0.00	
Oxygen		32.00	0.00								0.00						0.00	
<b>Total</b>	<b>0.05</b>	<b>170.16</b>			<b>0.02</b>		<b>0.00</b>				<b>1.57</b>		<b>0.00</b>				<b>0.00</b>	
						Flag												
$AE = \frac{\text{molecular weight of product}}{\text{total molecular weight of reactants}} \times 100$						Yield	93.0	●	93.0									
						Conversion	94.0	●	94.0									
						Selectivity	98.9	●	98.9									
$RME = \frac{\text{mass of isolated product}}{\text{total mass of reactants}} \times 100$						AE	80.0						Product	mass	mw	mol		
						RME	91.6							0.046	136.150	0.0003364		
														Unreacted limiting reactant	mass			
															0.003			
<b>Solvents (Zero Pass)</b>																		
<b>Highly hazardous solvents (Red flag for any of the following)</b>								<b>List Highly Hazardous Solvents Below</b>										
Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA								None										
<b>Health and Safety (Zero Pass)</b>																		
<b>Health &amp; safety (Red flag for any of the following)</b>								<b>List substances plus the red flagged H-codes below</b>										
Highly explosive				H200, H201, H202, H203				None										
Explosive thermal runaway				H240				None										
Fatally toxic				H300, H310, H330				None										
Mutagenic				H350				None										
Repro-toxic				H360				None										
Serious environmental implications				H420				None										

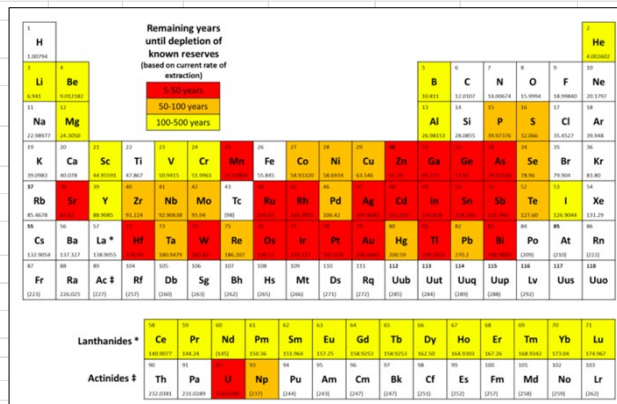
## 4. First Pass CHEM21 green metrics toolkit

Supplementary Information: Appendix 2				Summary of First Pass Metrics Toolkit																																																																																																																																																																																																																																																							
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<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td colspan="18" style="text-align: center;">Flag</td> </tr> <tr> <td>Yield</td> <td>93.0</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Conversion</td> <td>94.0</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>Selectivity</td> <td>98.9</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>AE</td> <td>80.0</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>RME</td> <td>91.6</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td>114.5</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>PMI total</td> <td>35.7</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>PMI Reaction</td> <td>35.7</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>PMI reactants, reagents, catalyst</td> <td>1.4</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>PMI reaction solvents</td> <td>34.3</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>PMI Workup</td> <td>0.0</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>PMI Workup chemical</td> <td>0.0</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> <tr> <td>PMI workup solvents</td> <td>0.0</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> </tr> </table>																		Flag																		Yield	93.0																	Conversion	94.0																	Selectivity	98.9																	AE	80.0																	RME	91.6									114.5								PMI total	35.7																	PMI Reaction	35.7																	PMI reactants, reagents, catalyst	1.4																	PMI reaction solvents	34.3																	PMI Workup	0.0																	PMI Workup chemical	0.0																	PMI workup solvents	0.0																
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List solvents below																																																																																																																																																																																																																																																											
Preferred solvents		water, EtOH, nBuOH, AcOipr, AcOnBu, PhOMe, MeOH, tBuOH, BnOH, ethylene glycol, acetone, MEK, MIBK, AcOEt, sulfolane														i-PrOH																																																																																																																																																																																																																																											
Problematic solvents: (acceptable only if substitution does not offer advantages)		DMSO, cyclohexanone, DMPU, AcOH, Ac <sub>2</sub> O, Acetonitrile, AcOMe, THF, heptane, Me-cyclohexane, toluene, xylene, MTBE, cyclohexane, chlorobenzene, formic acid, pyridine, Me-THF																																																																																																																																																																																																																																																									
Hazardous solvents: These solvents have significant health and/or safety concerns.		dioxane, pentane, TEA, diisopropyl ether, DME, DCM, DMF, DMA, NMP, methoxyethanol, hexane																																																																																																																																																																																																																																																									
Highly hazardous solvents: The solvents which are agreed not to be used, even in screening		Et <sub>2</sub> O, Benzene, CCl <sub>4</sub> , chloroform, DCE, nitromethane, CS <sub>2</sub> , HMPA																																																																																																																																																																																																																																																									

Catalyst/enzyme (First Pass)		Tick			Tick
Catalyst or enzyme used, or reaction takes place without any catalyst/reagents.	Green Flag	*	Facile recovery of catalyst/enzyme	Green Flag	*
Use of stoichiometric quantities of reagents	Amber Flag		catalyst/enzyme not recovered	Amber Flag	
Use of reagents in excess	Red Flag				

### Critical elements

Supply remaining	Flag colour	Note element
5-50 years	Red Flag	
50-500 years	Amber Flag	Ni
+500 years	Green Flag	



Energy (First Pass)		Tick
Reaction run between 0 to 70°C	Green Flag	*
Reaction run between -20 to 0 or 70 to 140°C	Amber Flag	
Reaction run below -20 or above 140°C	Red Flag	

Reaction run at reflux	Red Flag	Tick
Reaction run 5°C or more below the solvent boiling point	Green Flag	*

Batch/flow		Tick
Flow	Green Flag	
Batch	Amber Flag	*

Work Up		List
quenching filtration	Green Flag	
centrifugation crystallisation		
Low temperature distillation/evaporation/ sublimation (< 140 °C at atmospheric solvent exchange, quenching into aqueous solvent		Amber Flag
chromatography/ion exchange high temperature multiple recrystallisation	Red Flag	Column Chromatography

Health & safety	Red Flag	Amber Flag	Green Flag	List substances and H-codes	List substances and H-codes	List substances and H-codes
Highly explosive	H200, H201, H202, H203	H205, H220, H224	If no red or amber flagged H codes present then green flag	None	None	Methoxy benzyl alcohol: H315, H-317, H319
Explosive thermal runaway	H230, H240, H250	H241				
Toxic	H300, H310, H330	H301, H311, H331				
Long Term toxicity	H340, H350, H360, H370, H372	H341, H351, H361, H371, H373				
Environmental implications	H400, H410, H411, H420	H401, H412	None	None		

Use of chemicals of environmental concern		List substances of very high concern
Chemical identified as Substances of Very High Concern by ChemSec which are utilised	Red Flag	None

## 5. Reference

1. Liang, D.; Yan, J.; Yin, X.; Wang, Y.; Du, J.; Qian, J.; He, M.; Zhou, W. J. C. S.; Technology, Effects of doping metal on the catalytic performance of manganese-based layered double hydroxides in the aerobic oxidation of alcohols. *Catal. Sci. Technol.* **2025**, *15* (19), 5876-5885.
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