

## One-pot synthesis of β-O-4 lignin models via the insertion of stable 2-diazo-1,3-dicarbonyls into O-H bonds

Rafael Mafra P. Dias, Gabriela Pilli, Antonio C. B. Burtoloso

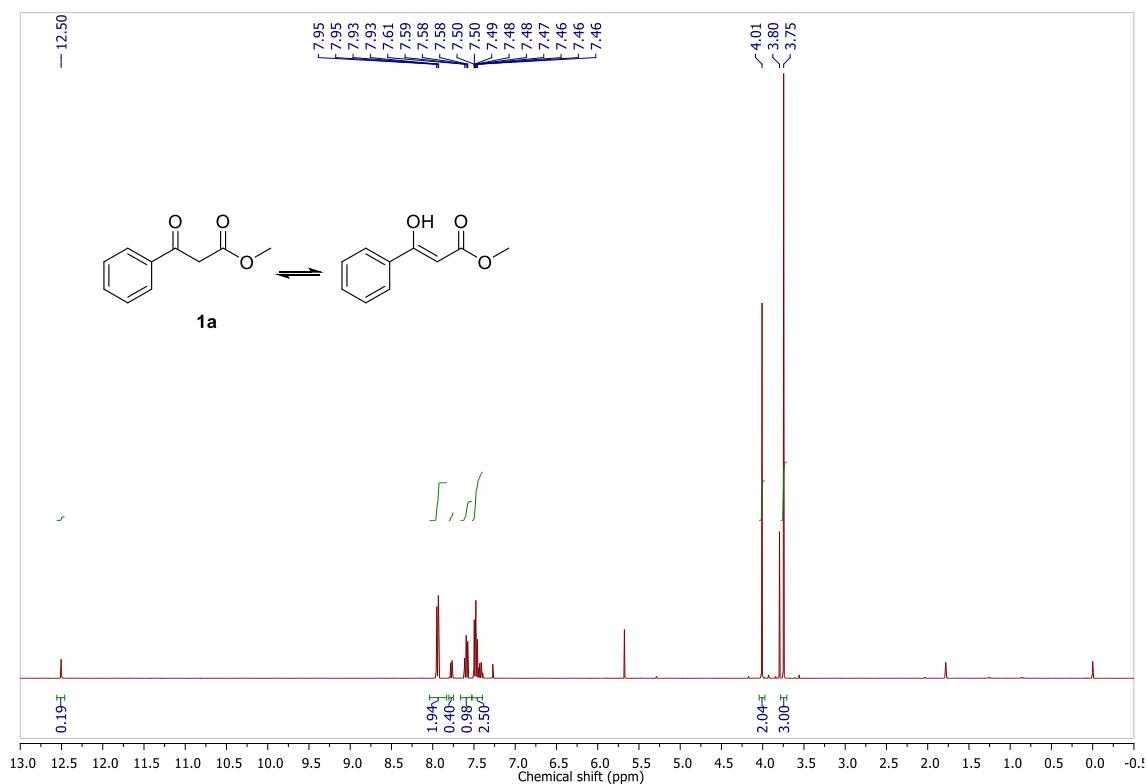
### Spectra data

#### Summary

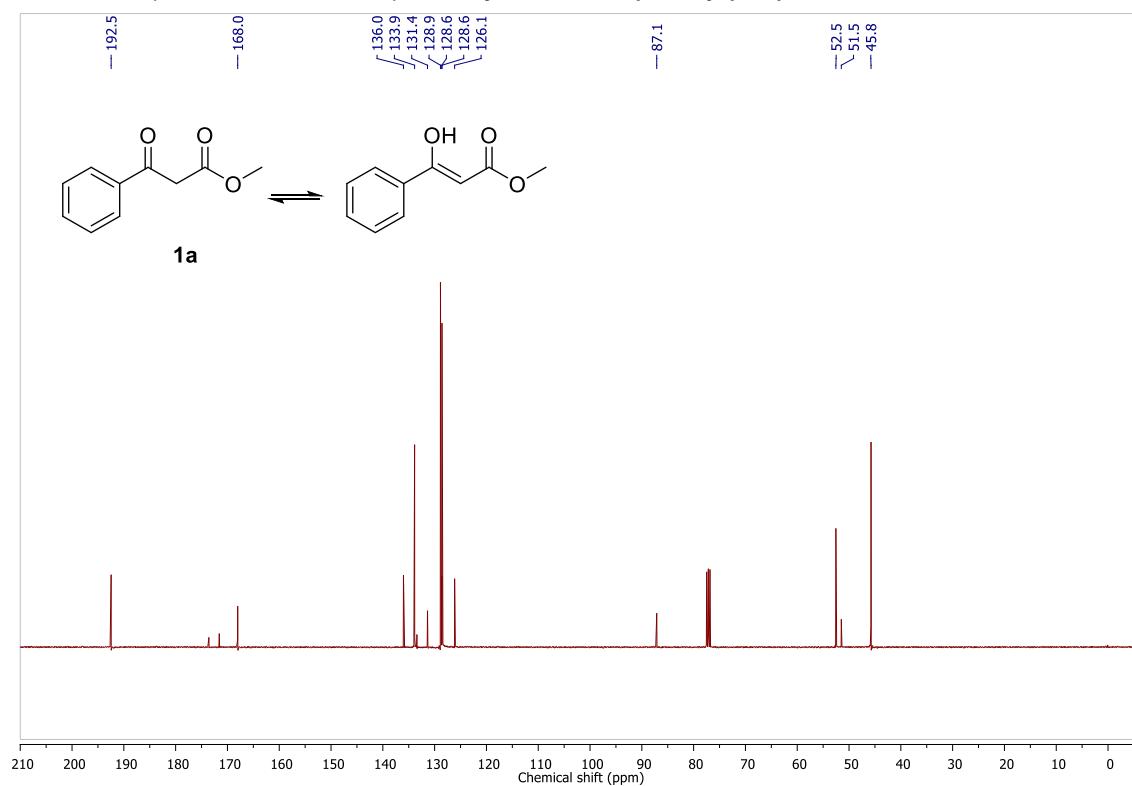
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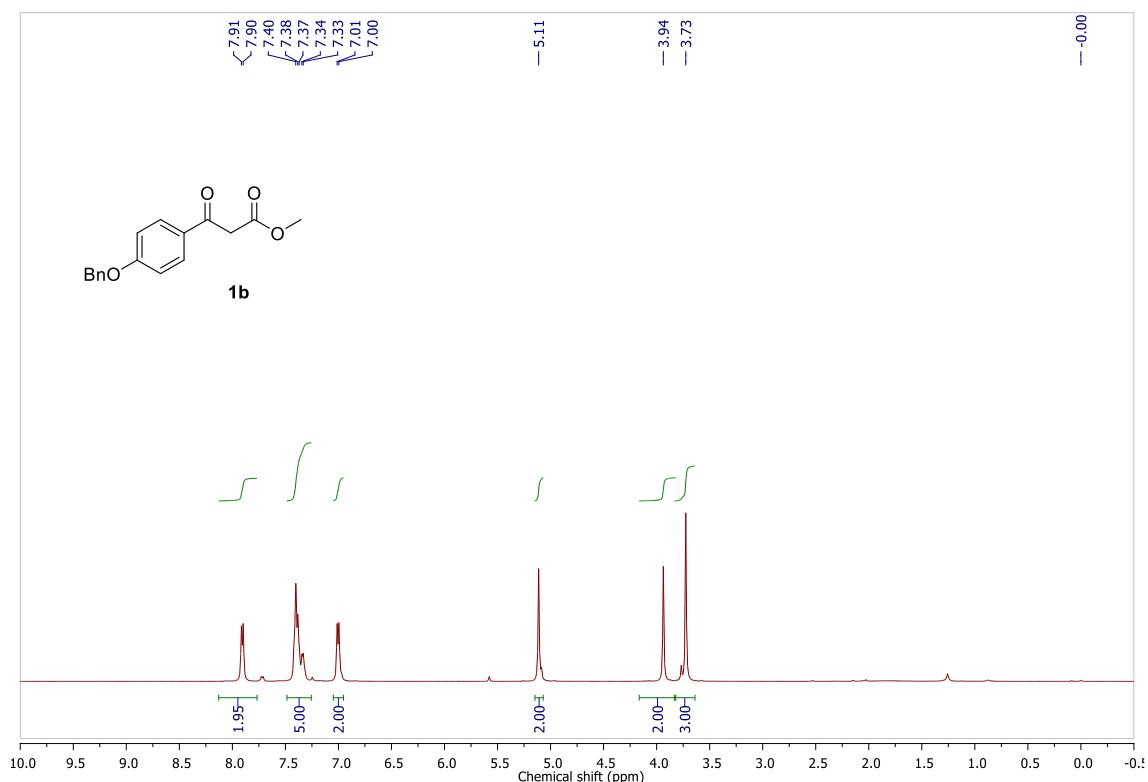
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 3-oxo-3-phenylpropanoate **1a****



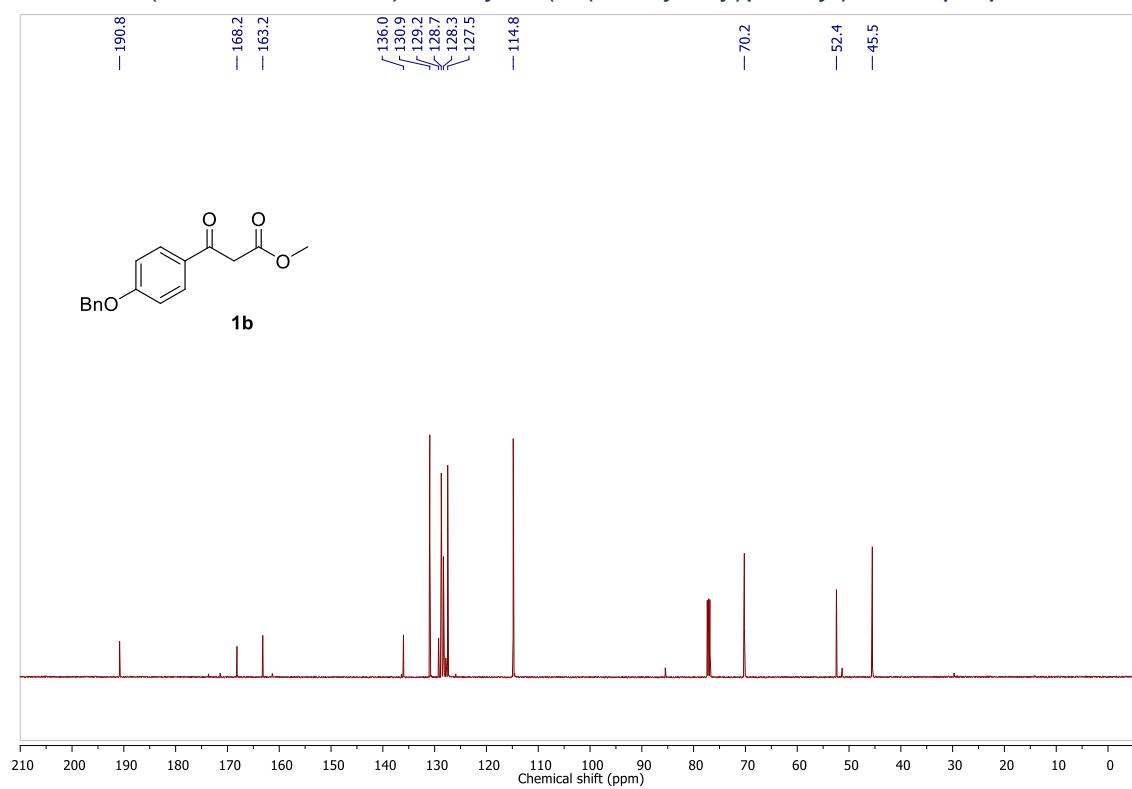
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 3-oxo-3-phenylpropanoate **1a****



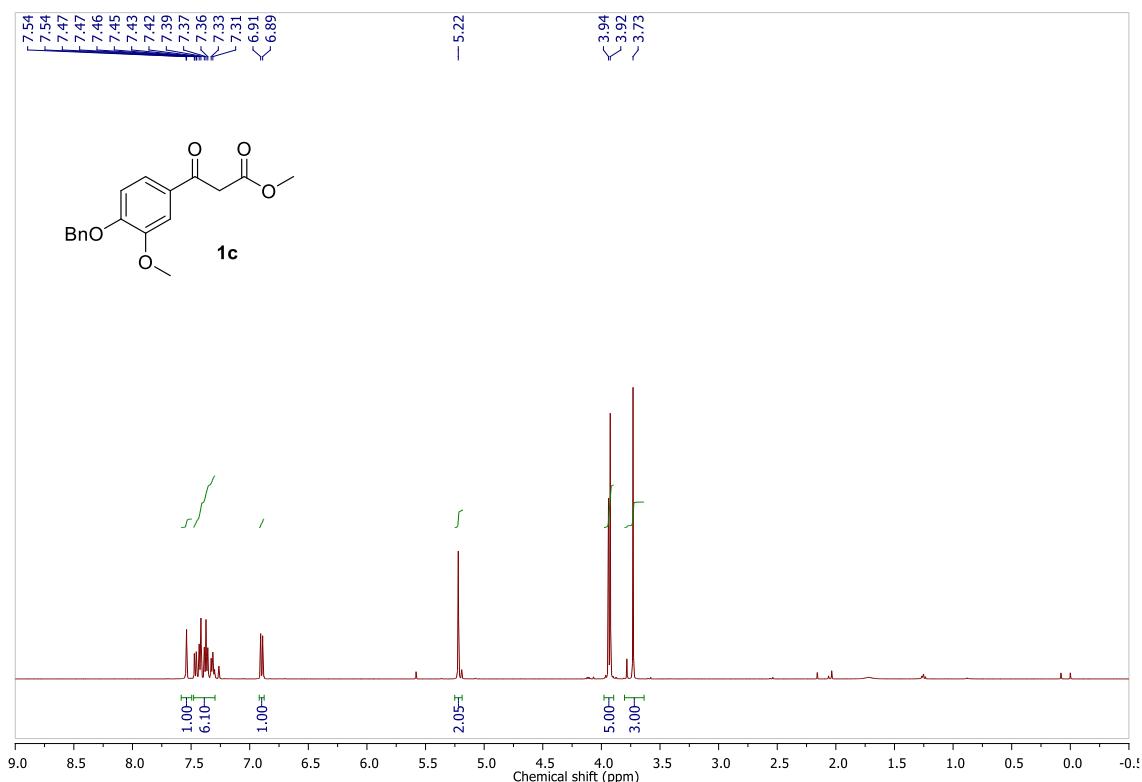
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)phenyl)-3-oxopropanoate **1b****



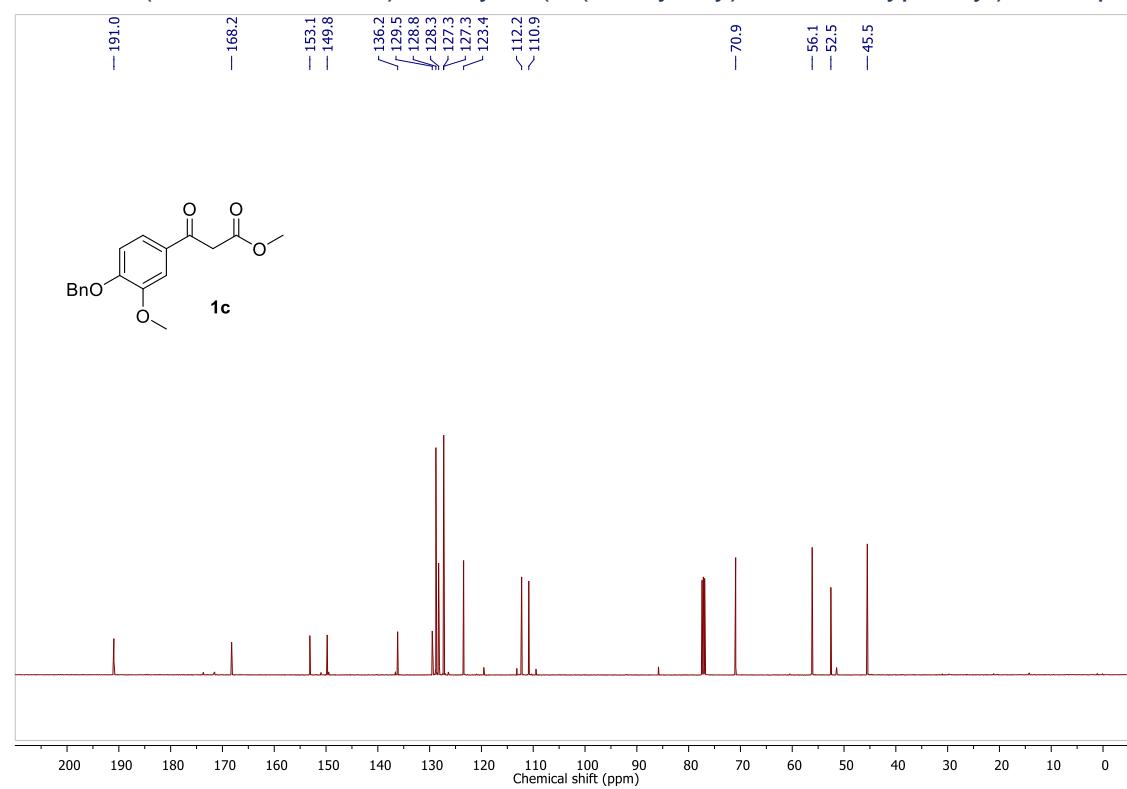
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)phenyl)-3-oxopropanoate **1b****



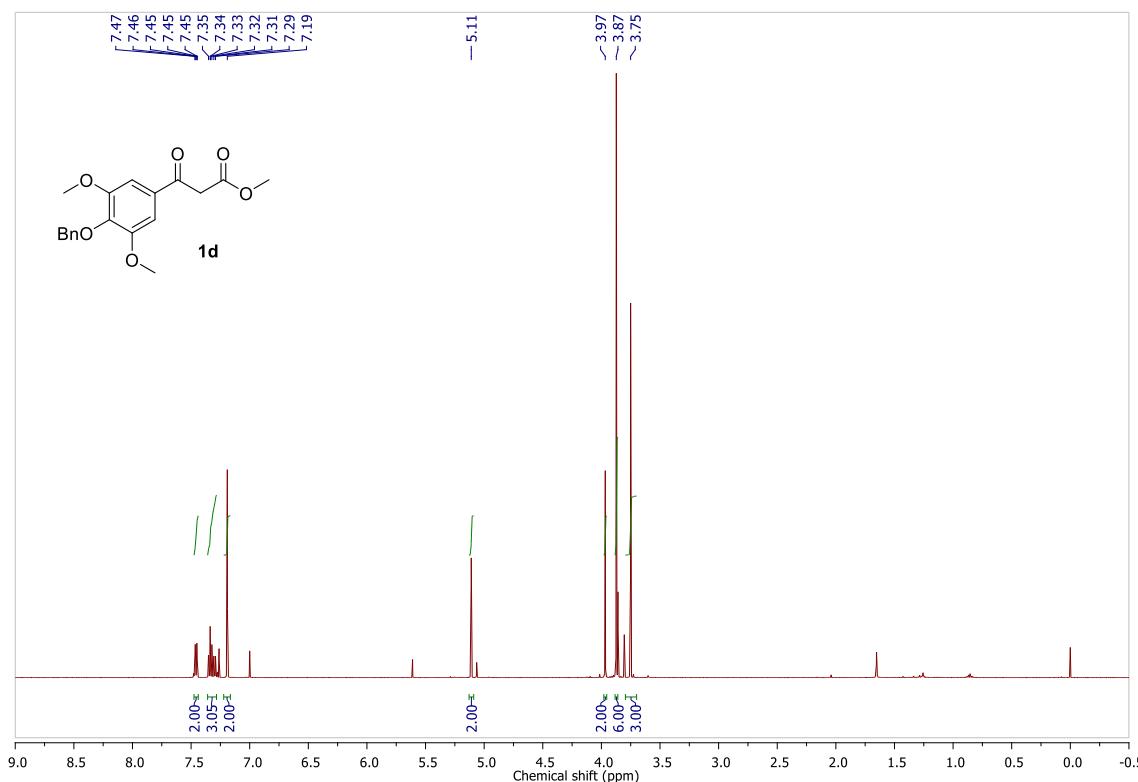
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3-methoxyphenyl)-3-oxopropanoate **1c****



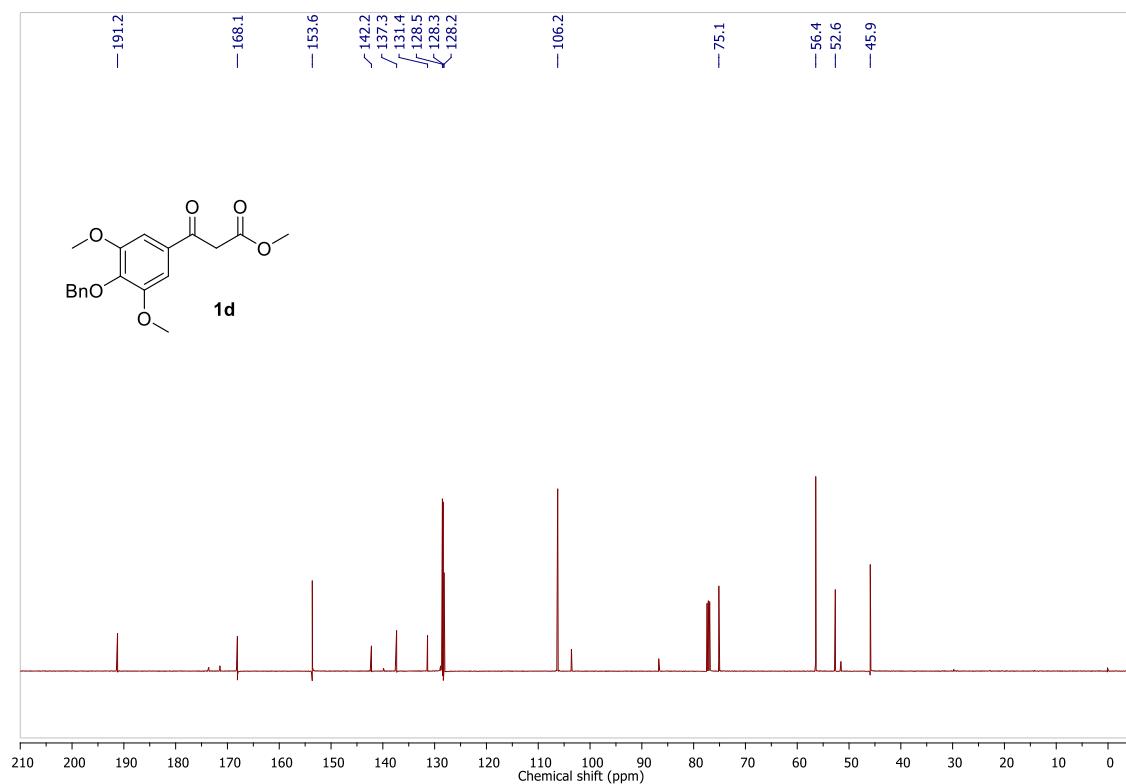
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3-methoxyphenyl)-3-oxopropanoate **1c****



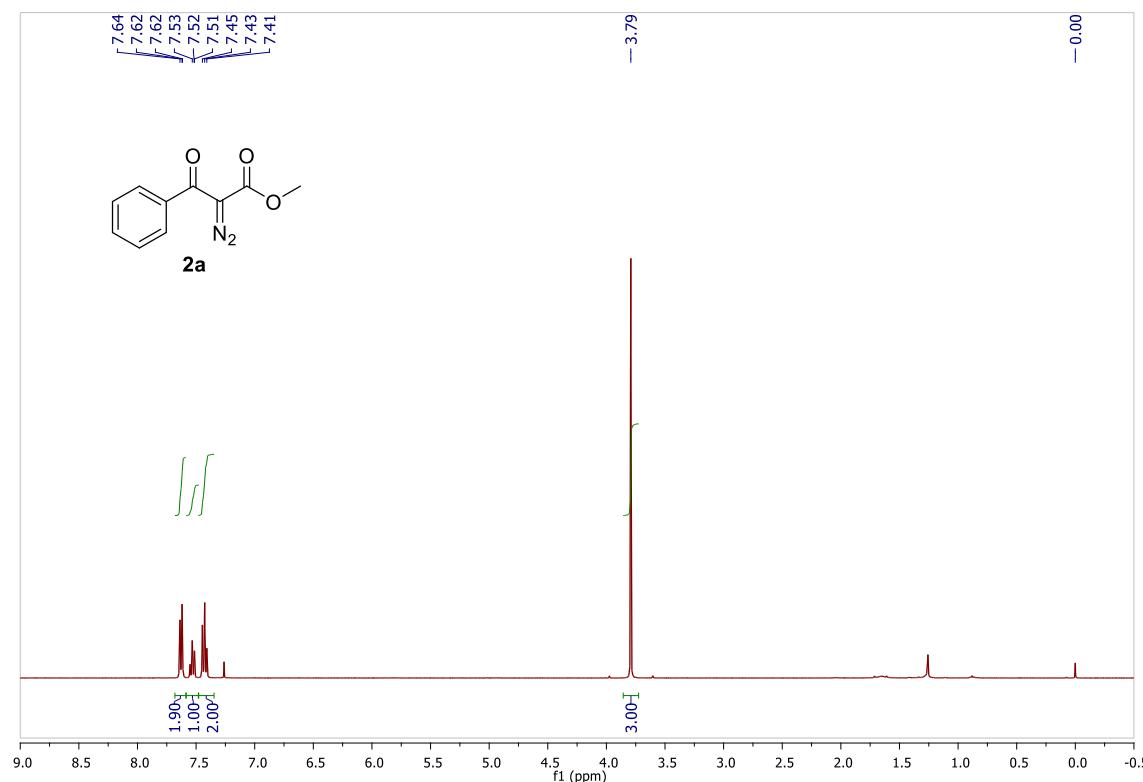
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3,5-dimethoxyphenyl)-3-oxopropanoate **1d****



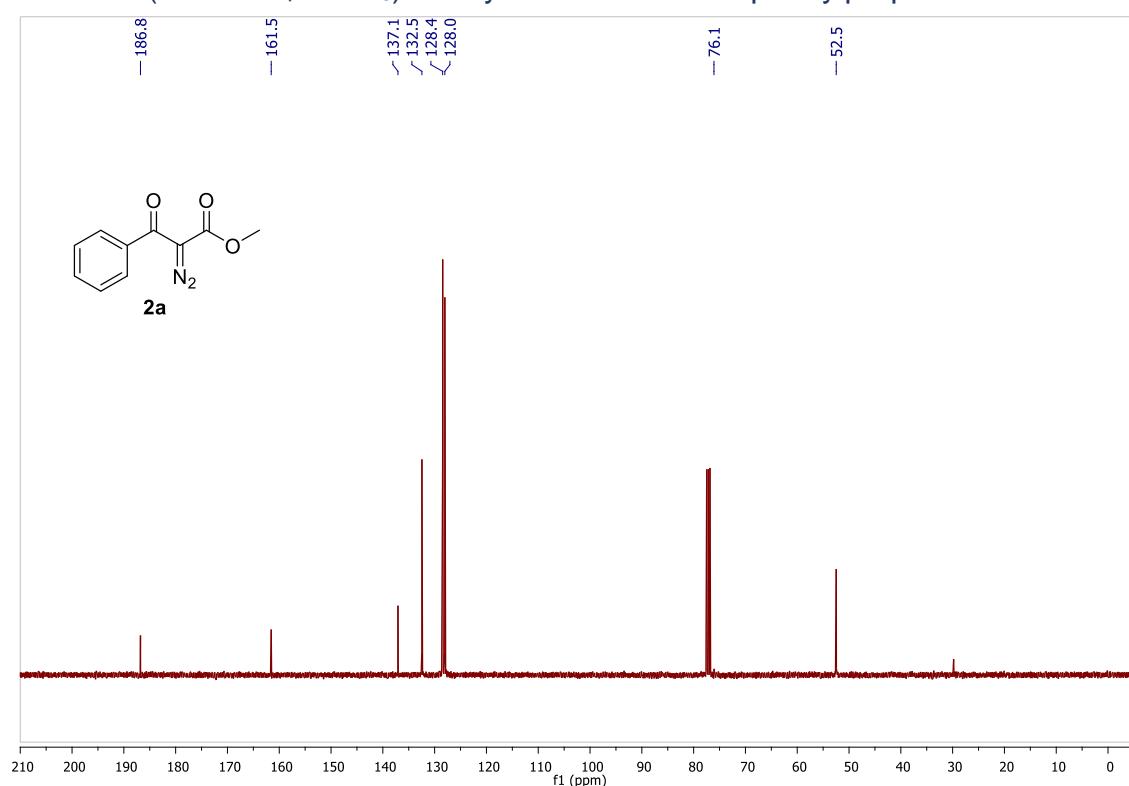
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3,5-dimethoxyphenyl)-3-oxopropanoate **1d****



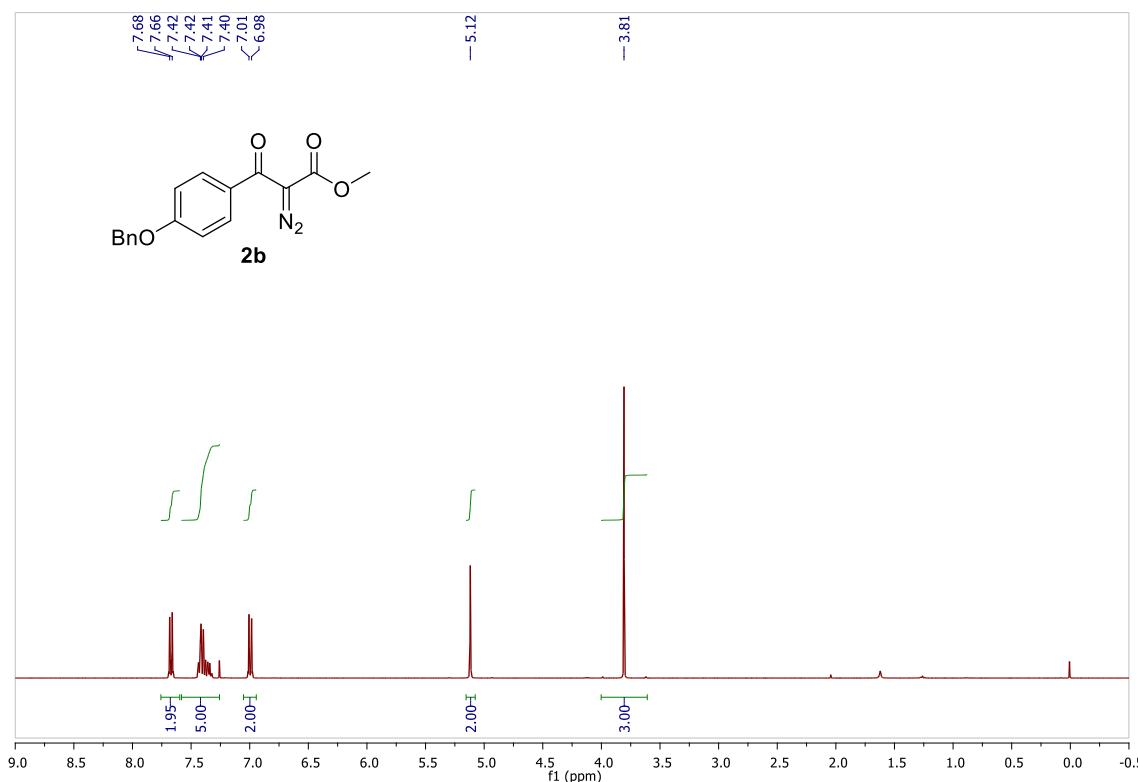
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 2-diazo-3-oxo-3-phenylpropanoate 2a**



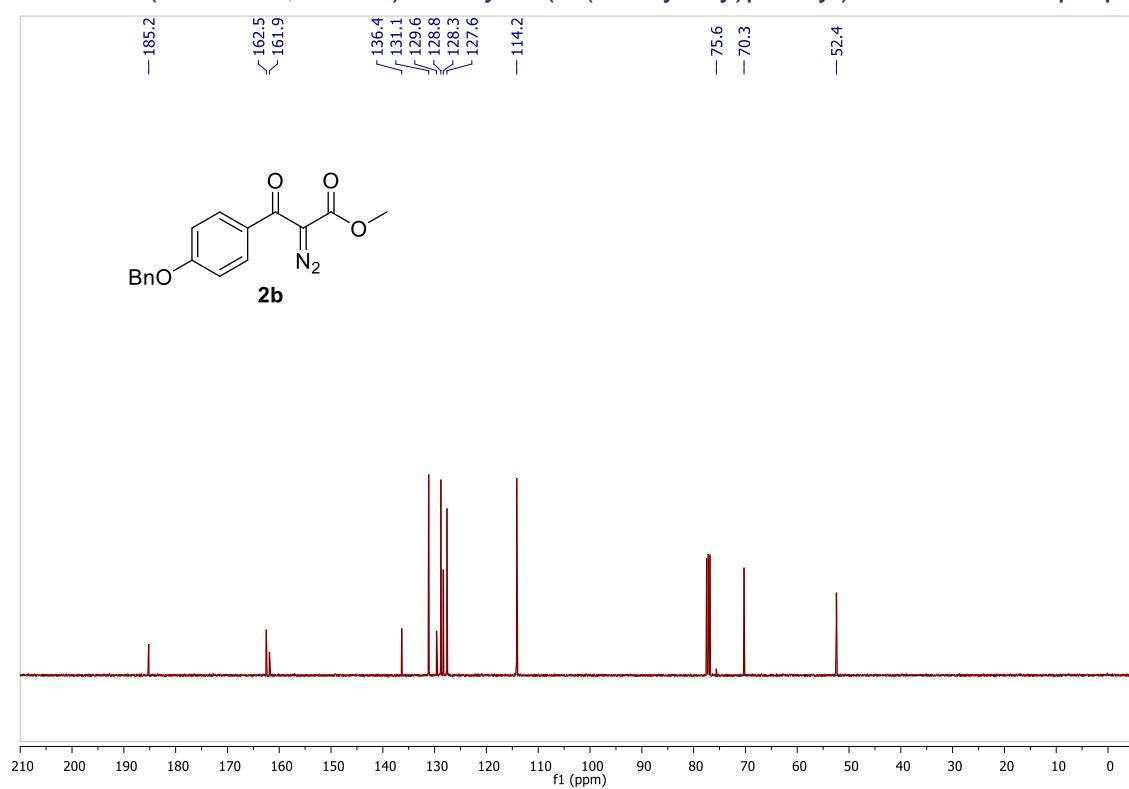
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 2-diazo-3-oxo-3-phenylpropanoate 2a**



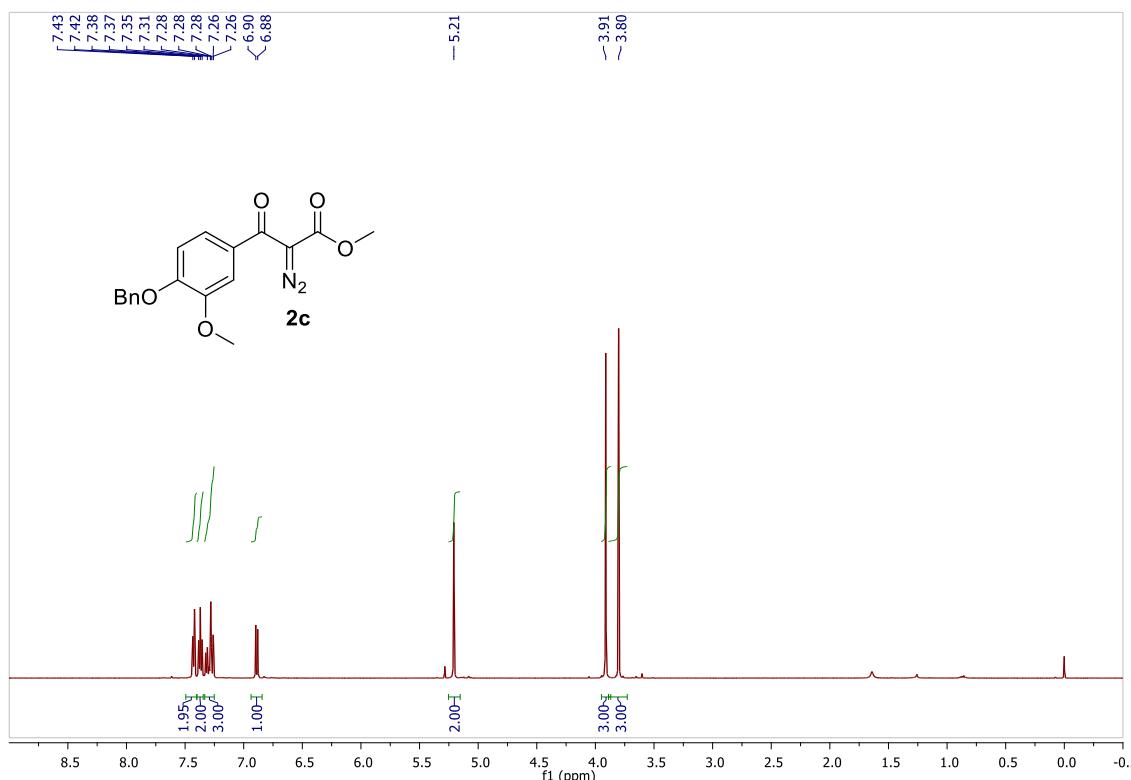
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)phenyl)-2-diazo-3-oxopropanoate 2b**



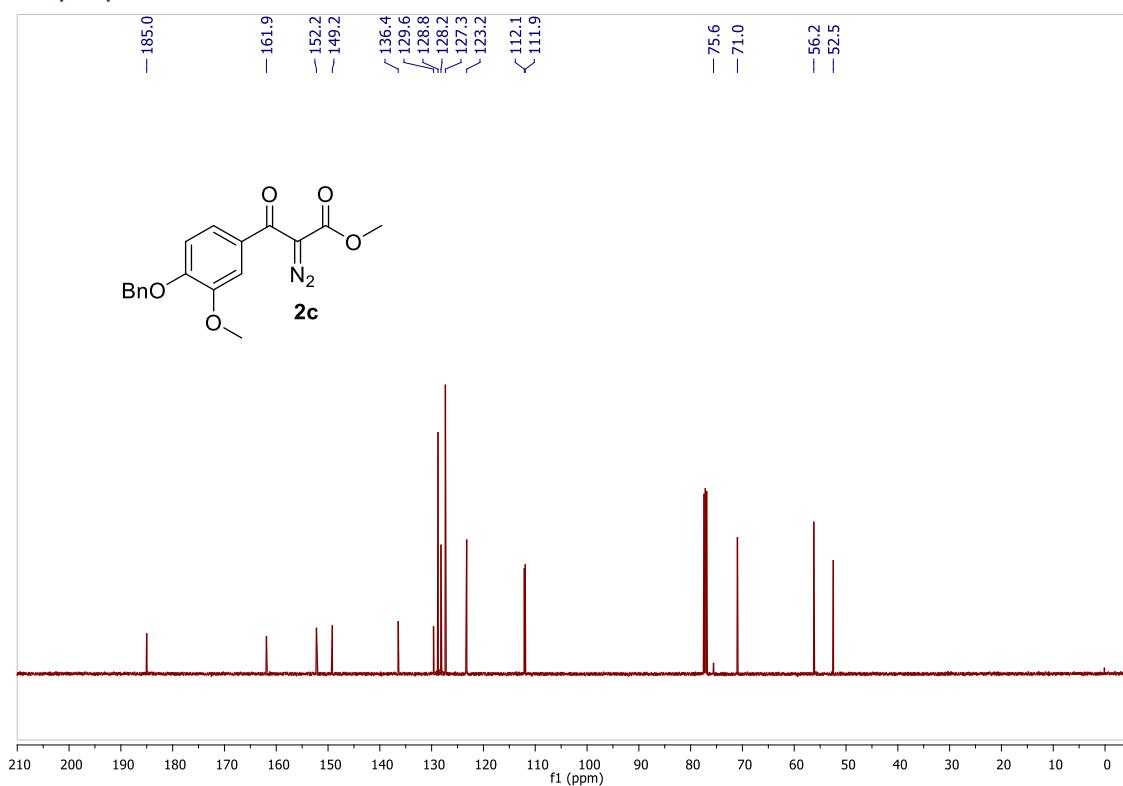
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)phenyl)-2-diazo-3-oxopropanoate 2b**



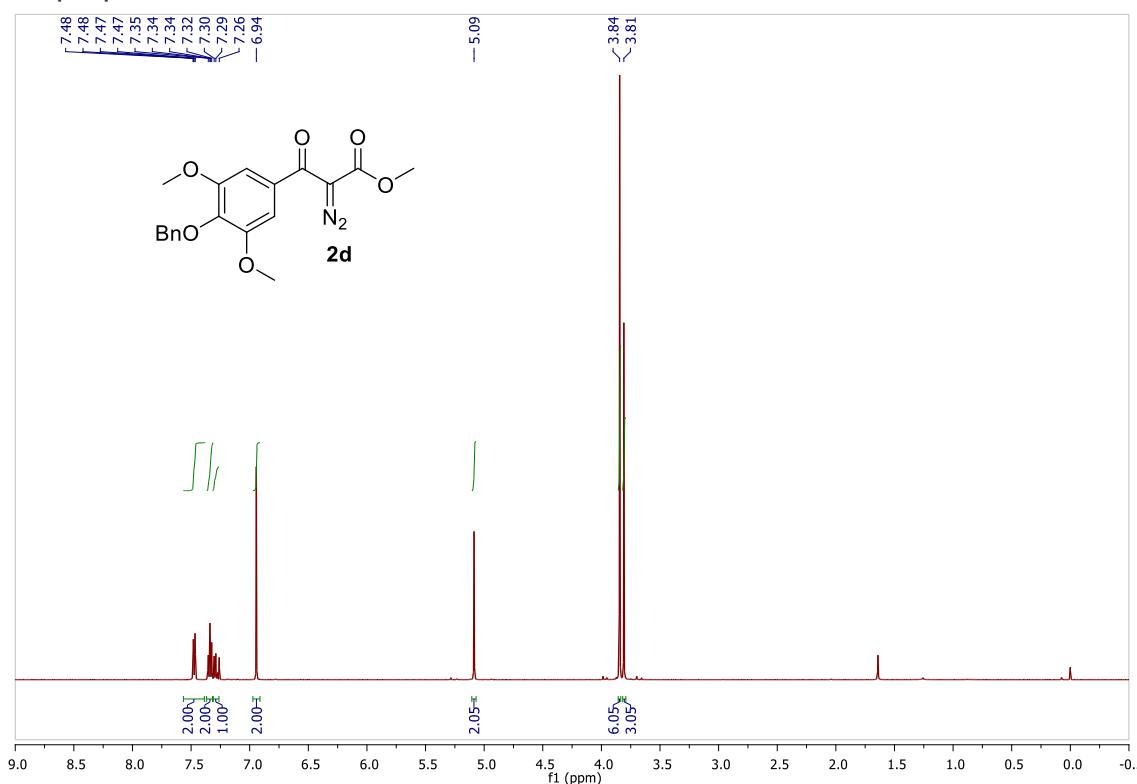
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3-methoxyphenyl)-2-diazo-3-oxopropanoate **2c**



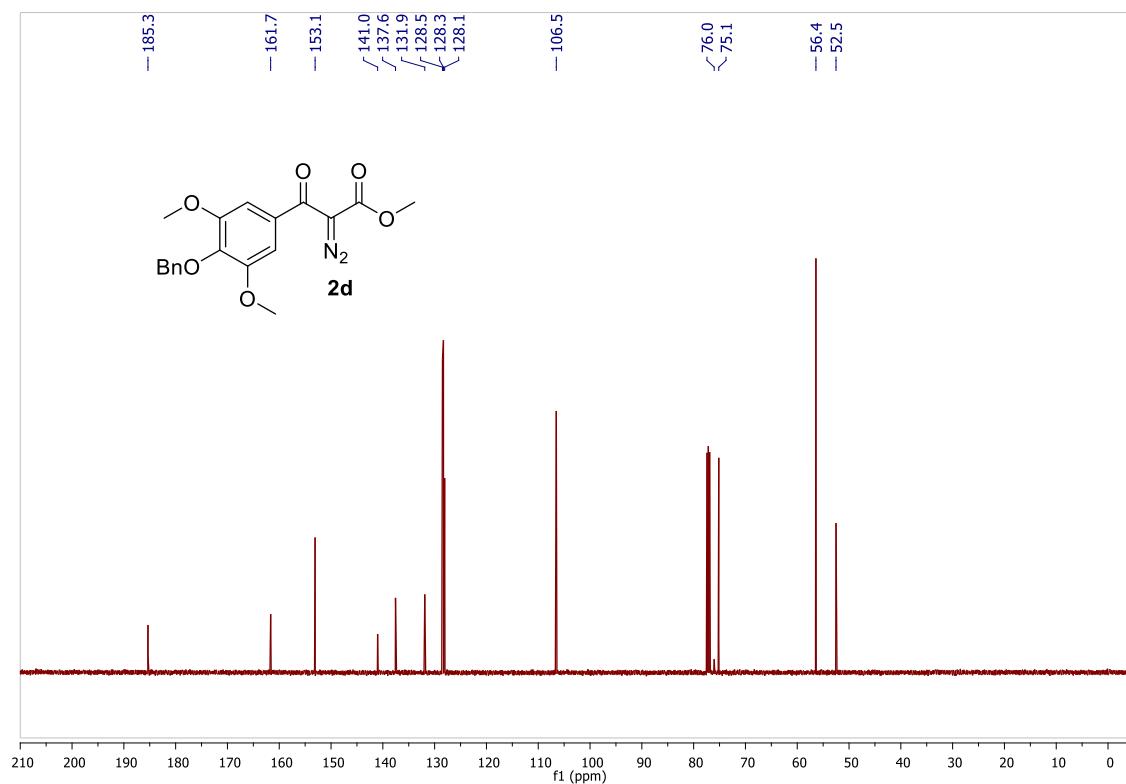
**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3-methoxyphenyl)-2-diazo-3-oxopropanoate **2c**



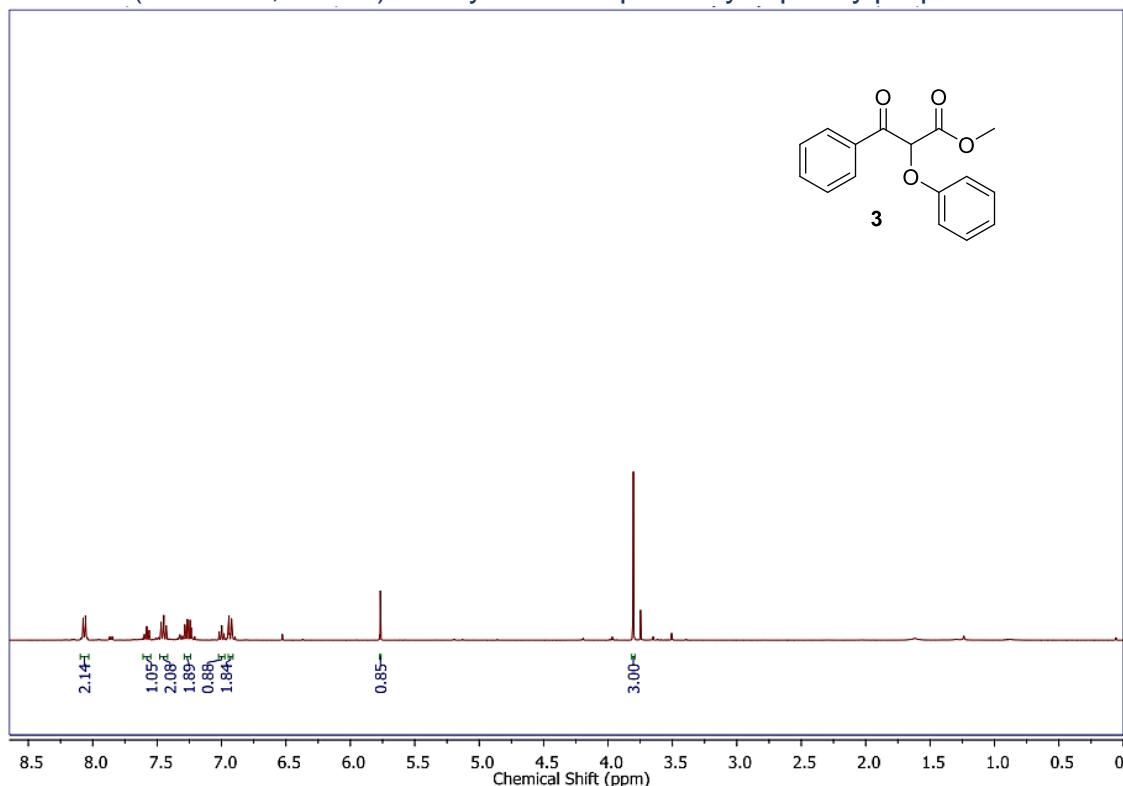
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3,5-dimethoxyphenyl)-2-diazo-3-oxopropanoate **2d****



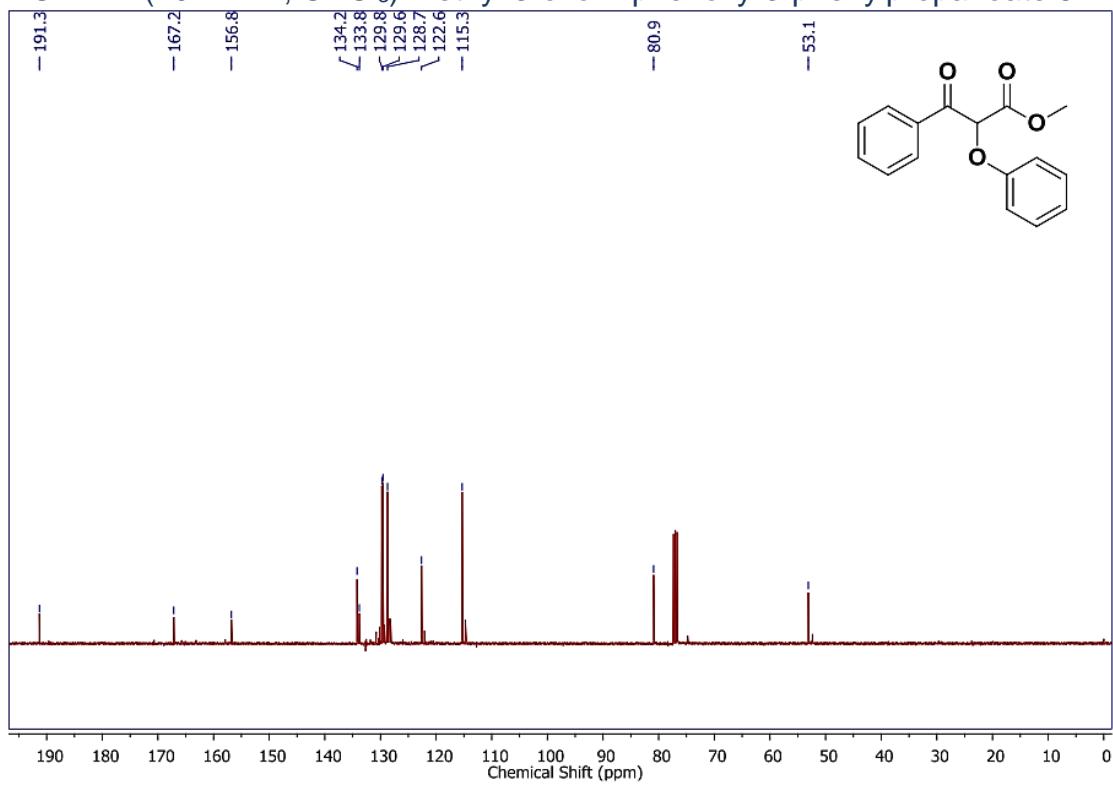
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 3-(4-(benzyloxy)-3,5-dimethoxyphenyl)-2-diazo-3-oxopropanoate **2d****



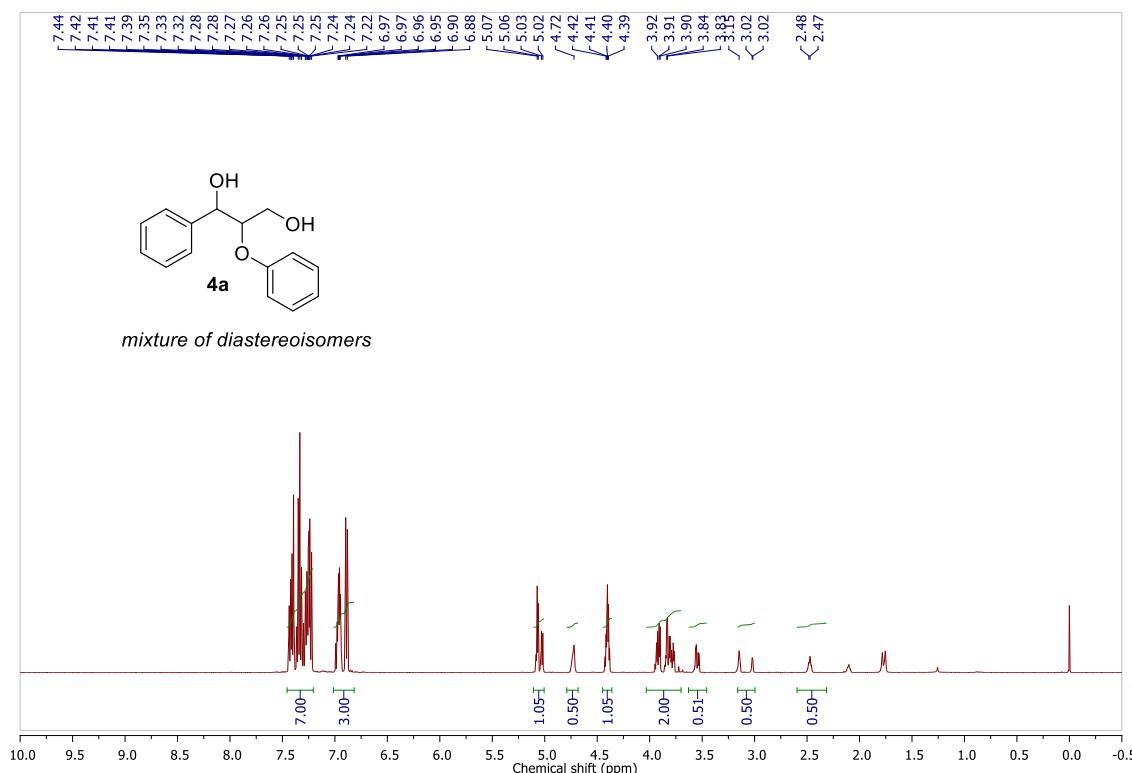
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) methyl 3-oxo-2-phenoxy-3-phenylpropanoate 3**



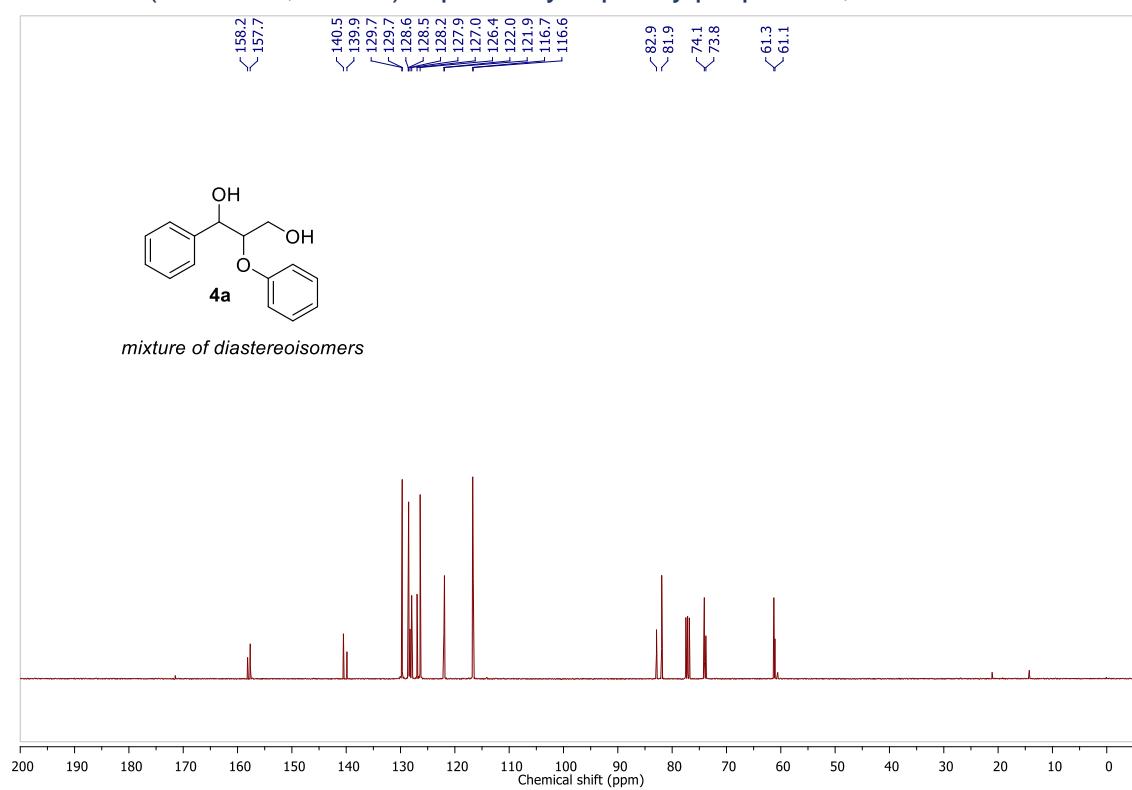
**<sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) methyl 3-oxo-2-phenoxy-3-phenylpropanoate 3**



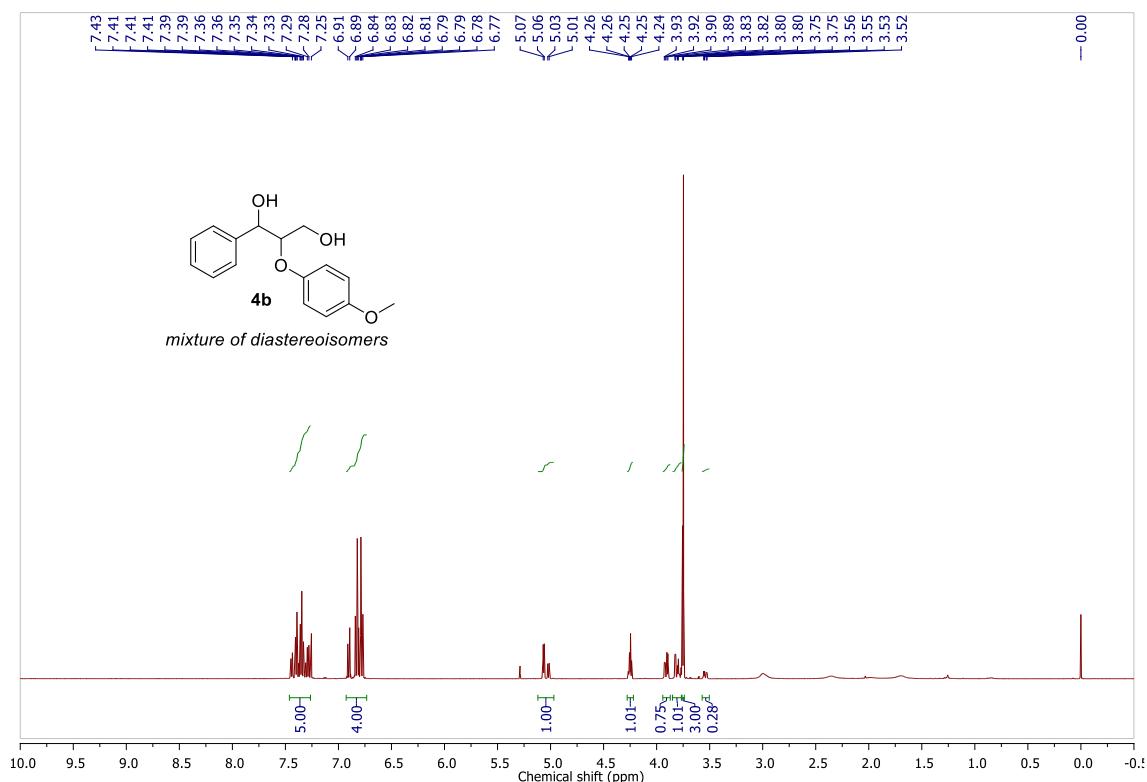
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 2-phenoxy-1-phenylpropane-1,3-diol 4a**



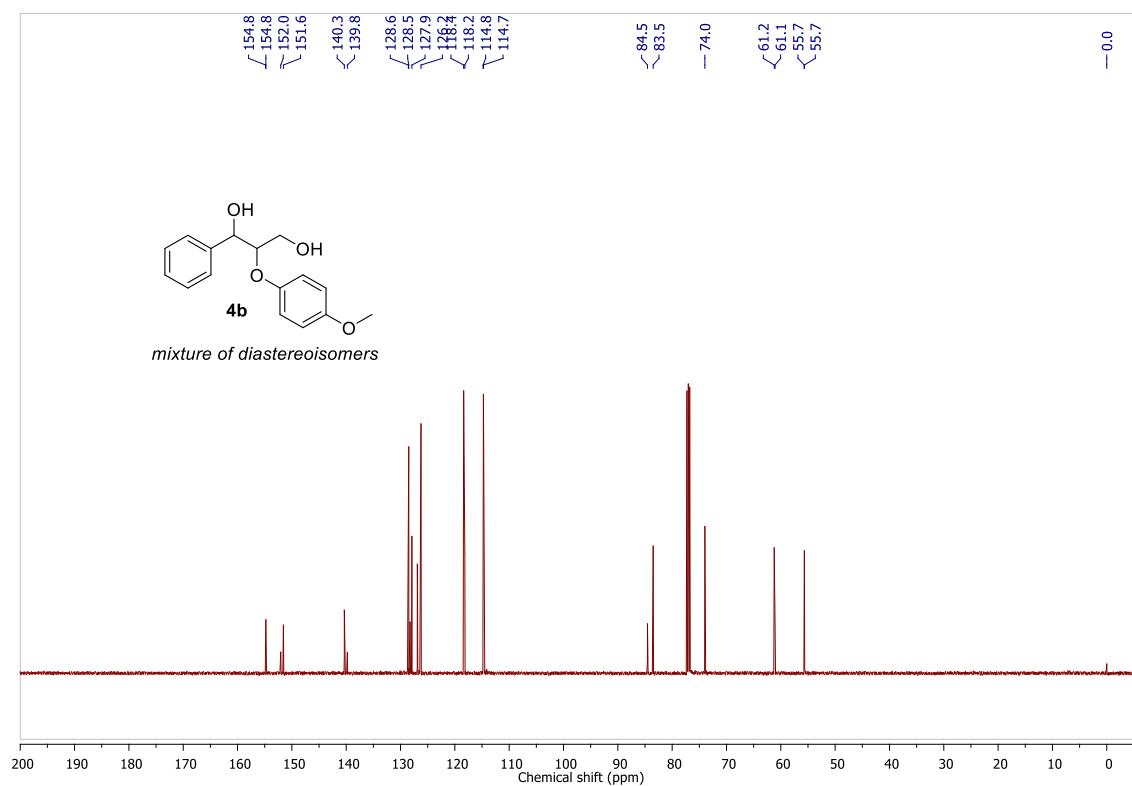
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) 2-phenoxy-1-phenylpropane-1,3-diol 4a**



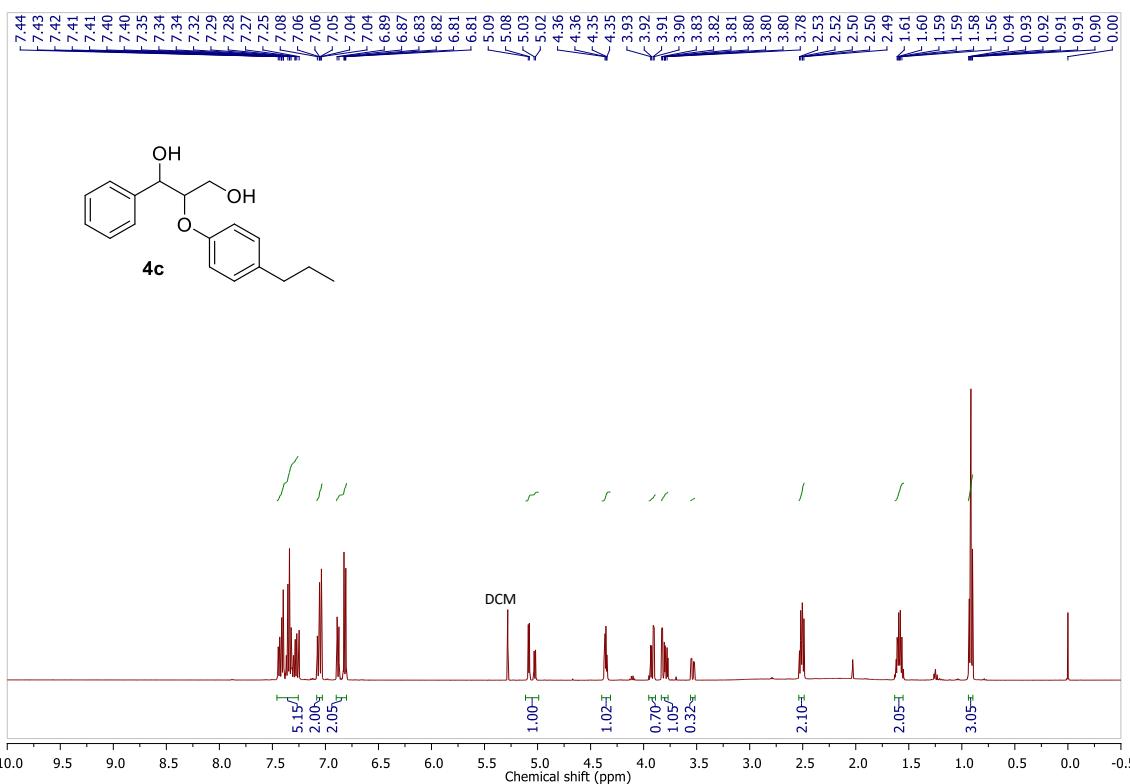
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 2-(4-methoxyphenoxy)-1-phenylpropane-1,3-diol 4b**



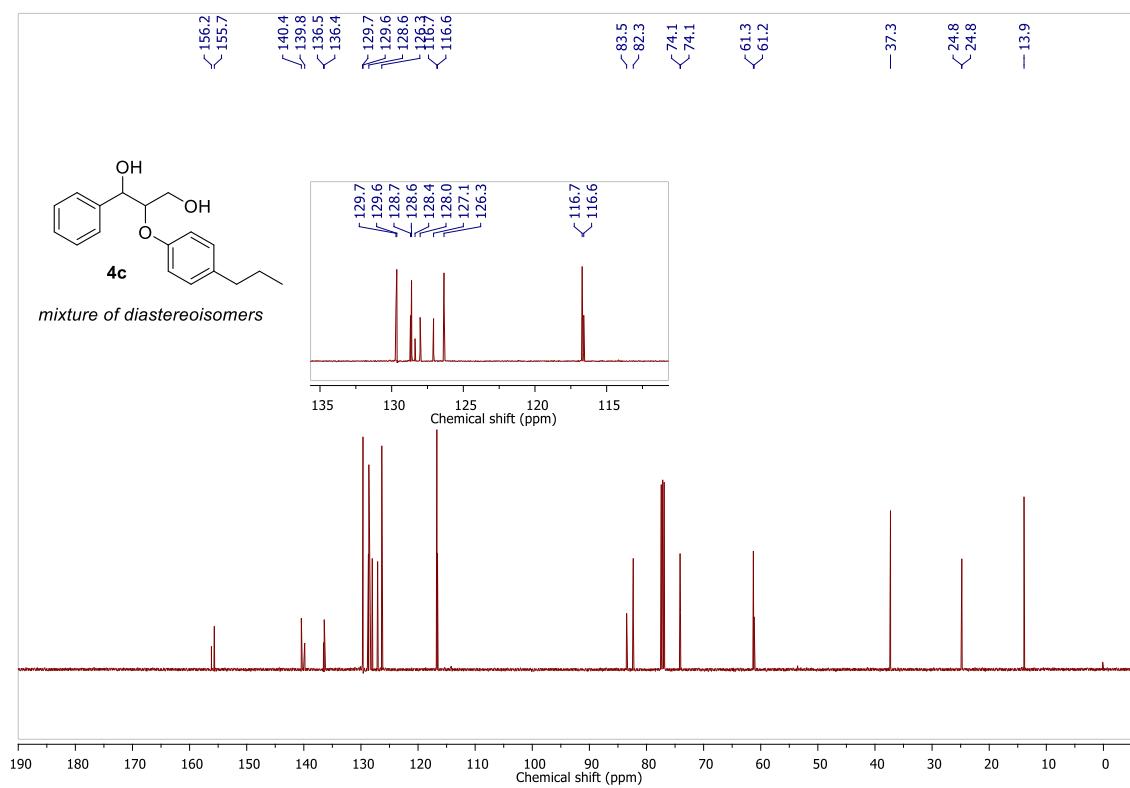
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) 2-(4-methoxyphenoxy)-1-phenylpropane-1,3-diol 4b**



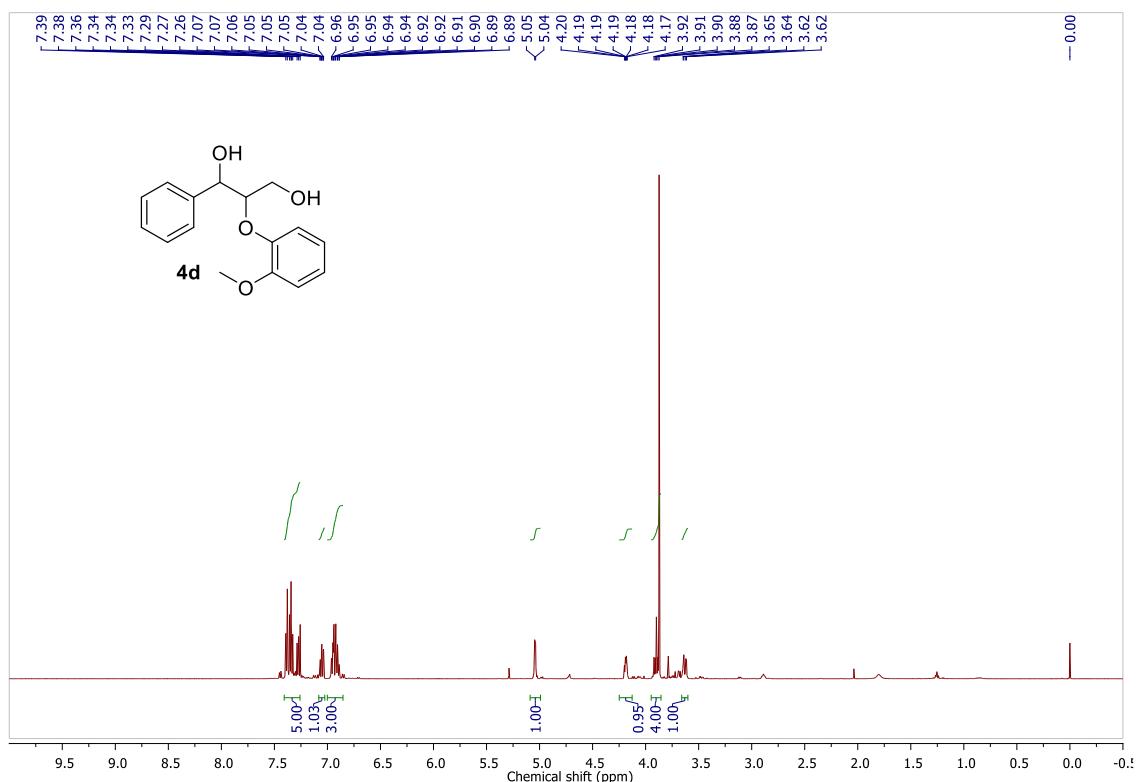
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 1-phenyl-2-(4-propylphenoxy)propane-1,3-diol **4c**



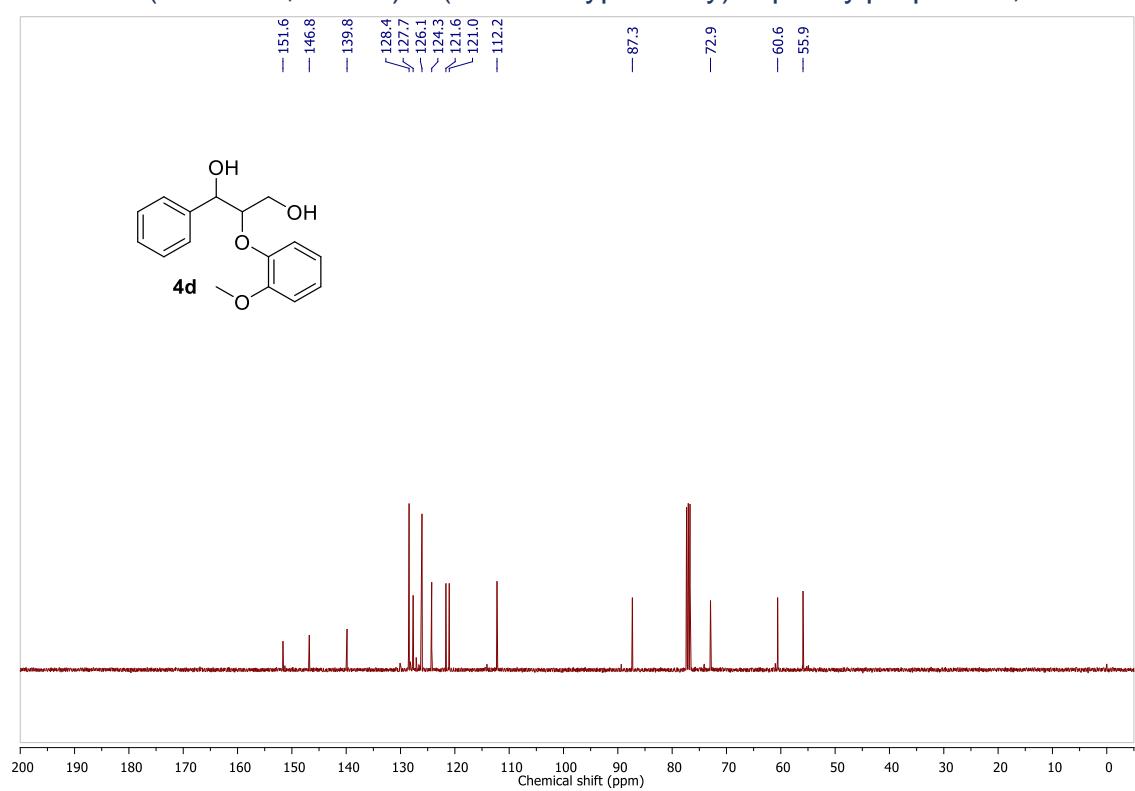
<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) 1-phenyl-2-(4-propylphenoxy)propane-1,3-diol **4c**



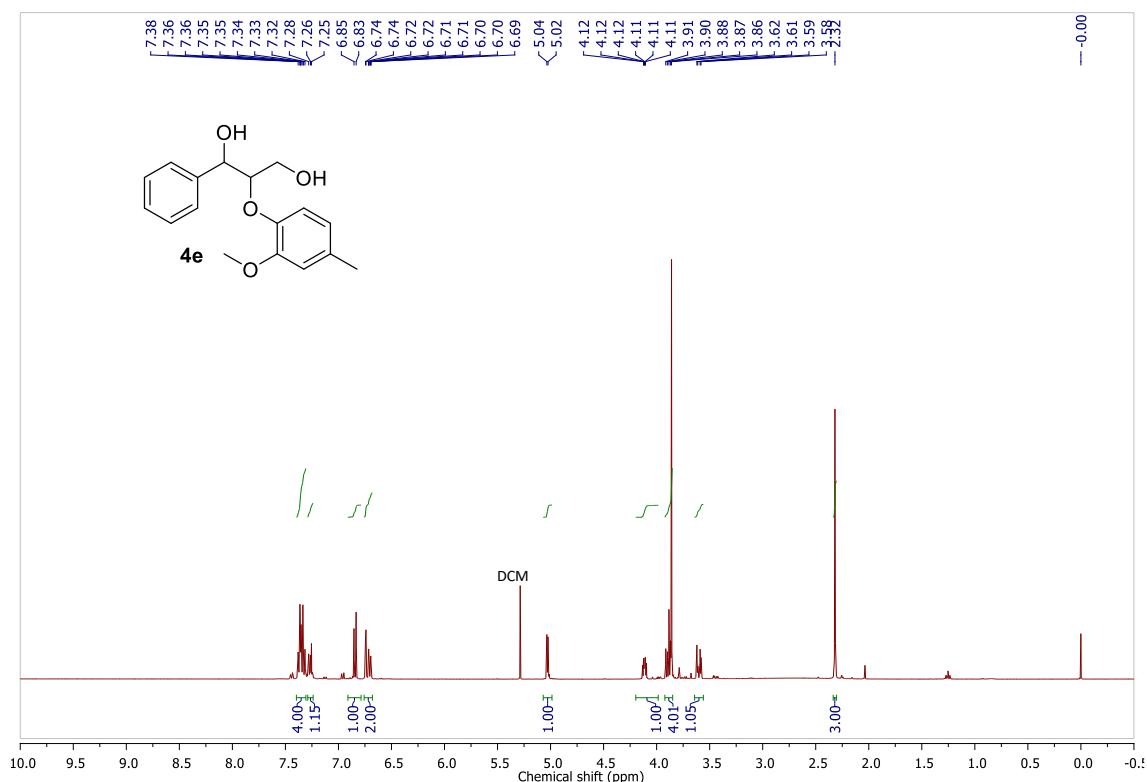
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) 2-(2-methoxyphenoxy)-1-phenylpropane-1,3-diol **4d**



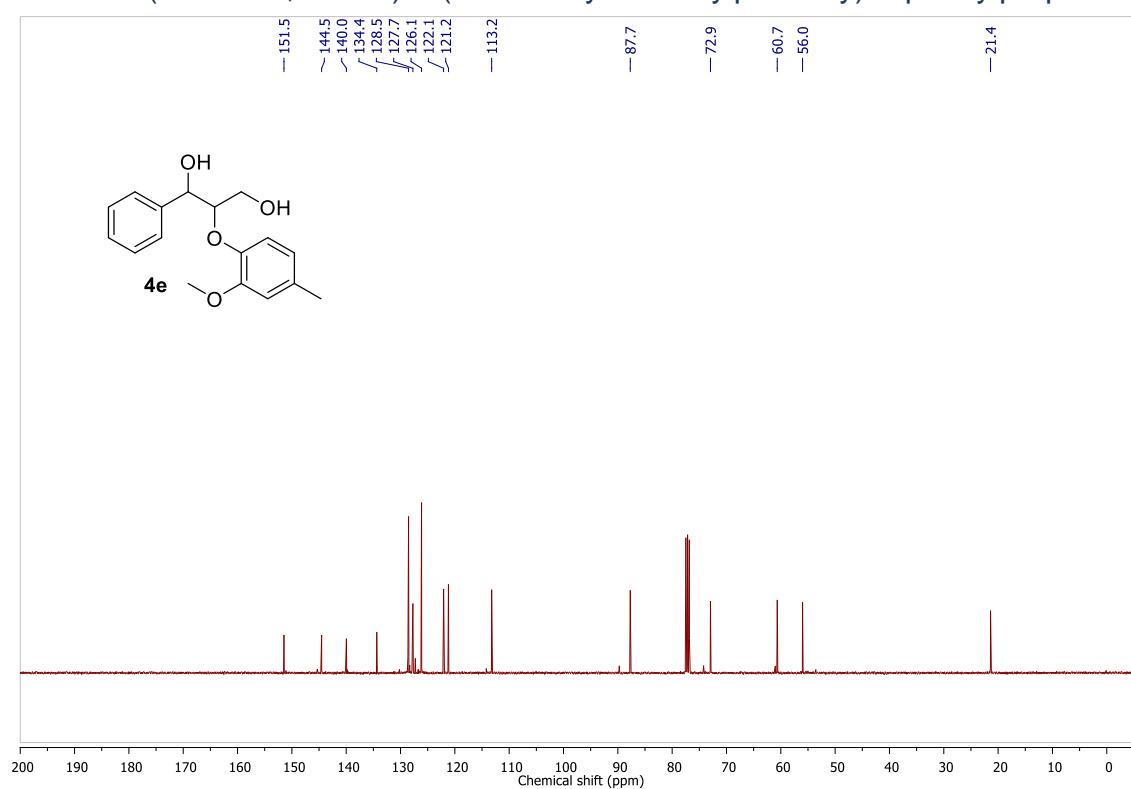
**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) 2-(2-methoxyphenoxy)-1-phenylpropane-1,3-diol **4d**



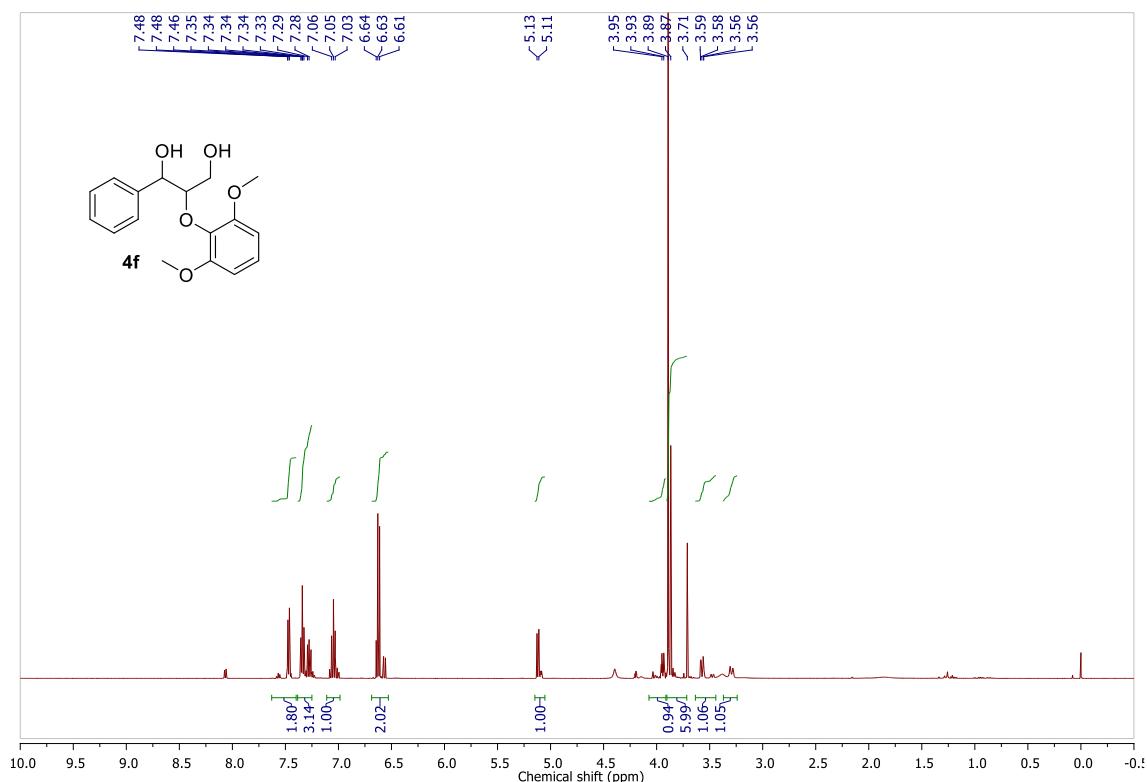
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 2-(2-methoxy-4-methylphenoxy)-1-phenylpropane-1,3-diol 4e**



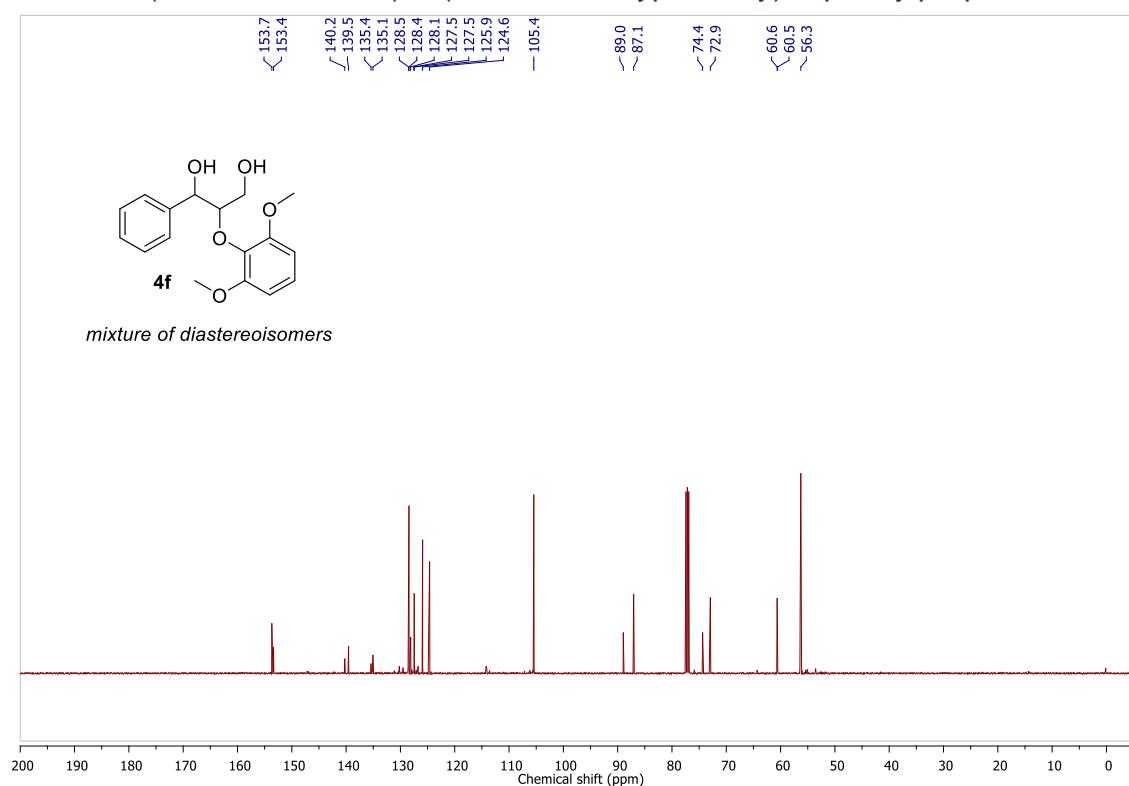
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) 2-(2-methoxy-4-methylphenoxy)-1-phenylpropane-1,3-diol 4e**



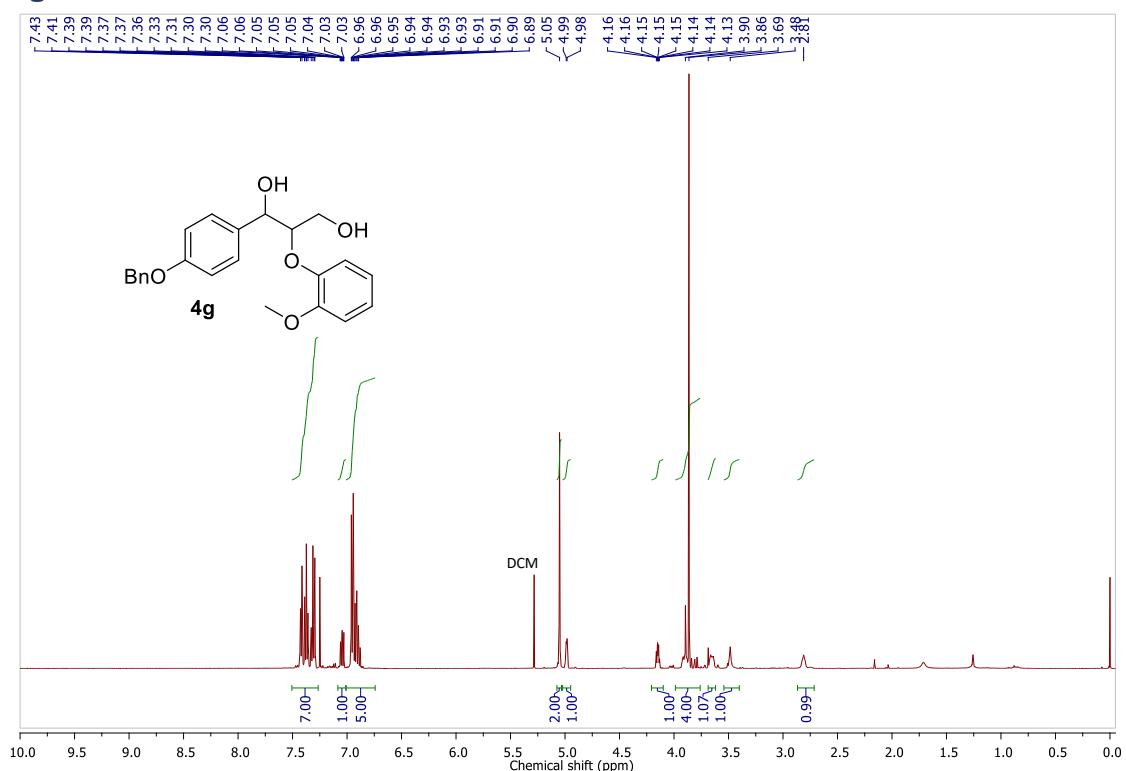
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 2-(2,6-dimethoxyphenoxy)-1-phenylpropane-1,3-diol **4f****



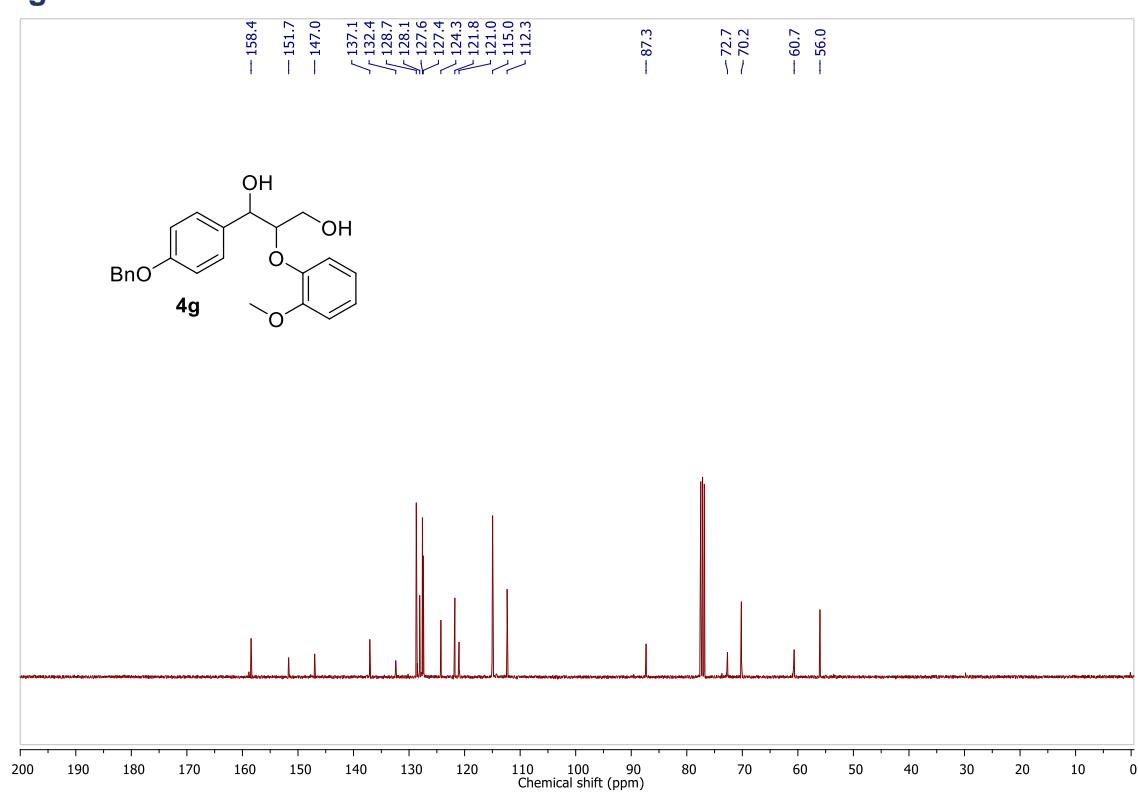
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) 2-(2,6-dimethoxyphenoxy)-1-phenylpropane-1,3-diol **4f****



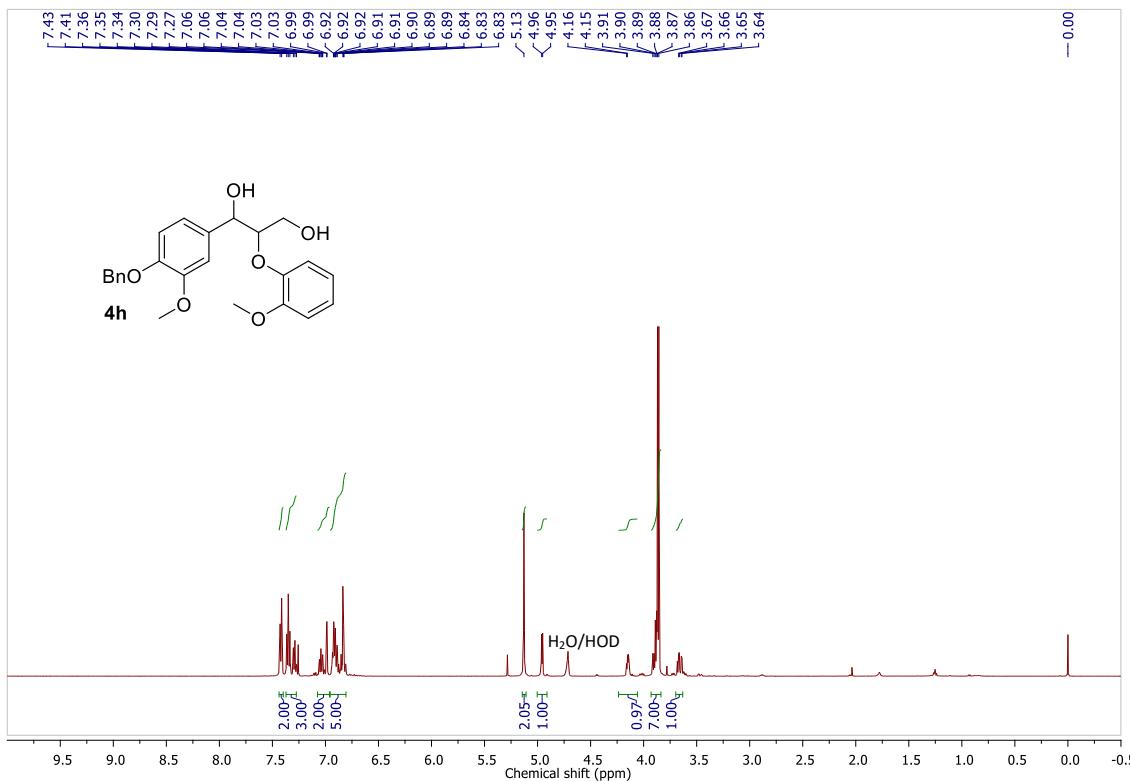
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 1-(4-(benzyloxy)phenyl)-2-(2-methoxyphenoxy)propane-1,3-diol  
4g**



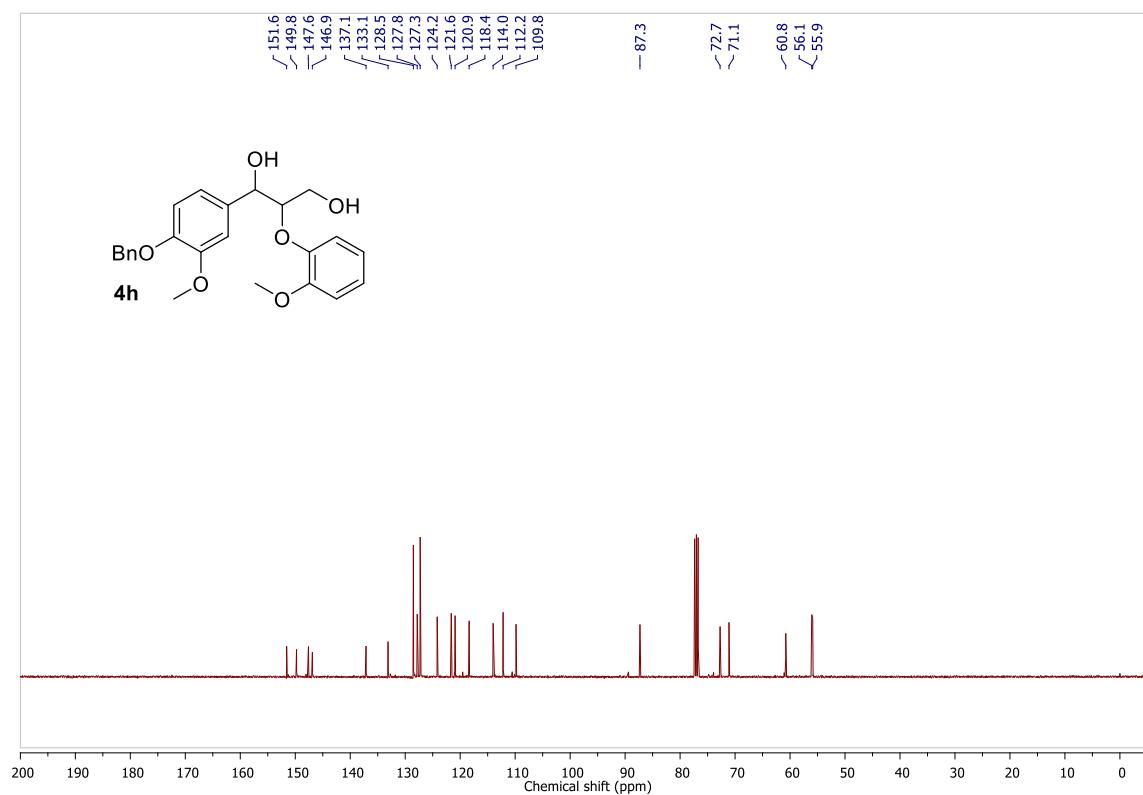
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) 1-(4-(benzyloxy)phenyl)-2-(2-methoxyphenoxy)propane-1,3-diol  
4g**



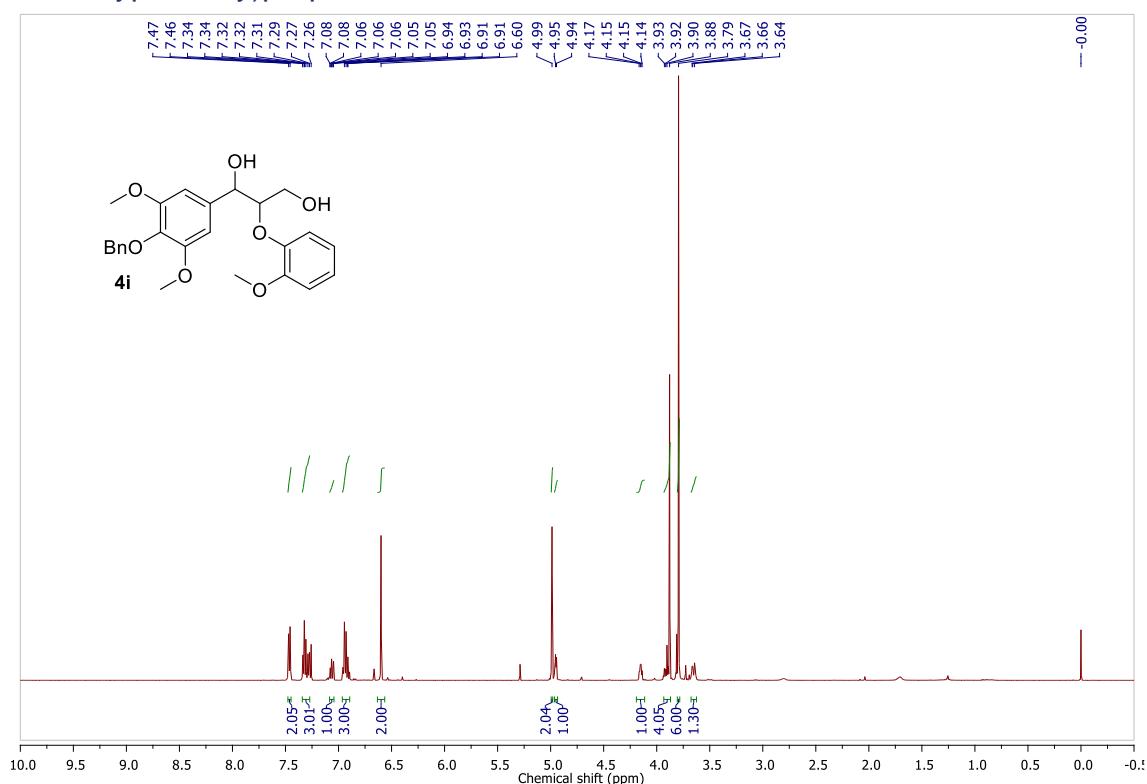
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>+ few drops of D<sub>2</sub>O) 1-(4-(benzyloxy)-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4h**



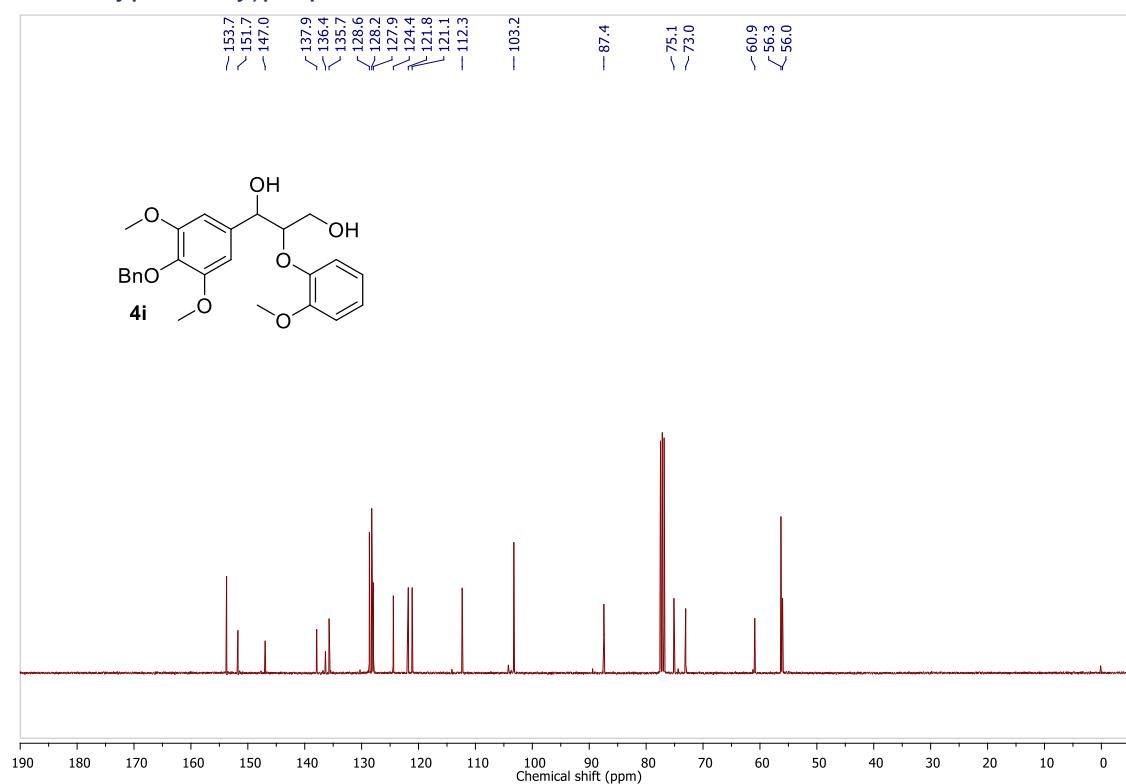
**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) 1-(4-(benzyloxy)-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4h**



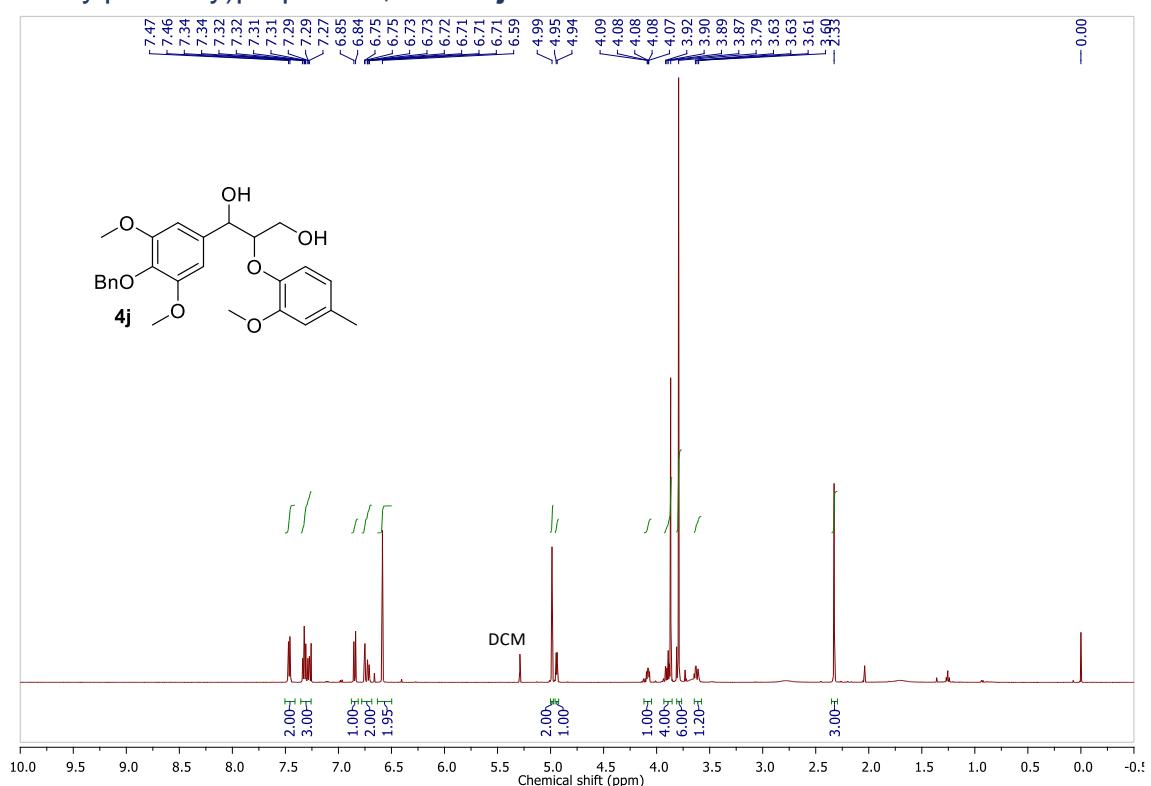
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) 1-(4-(benzyloxy)-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4i**



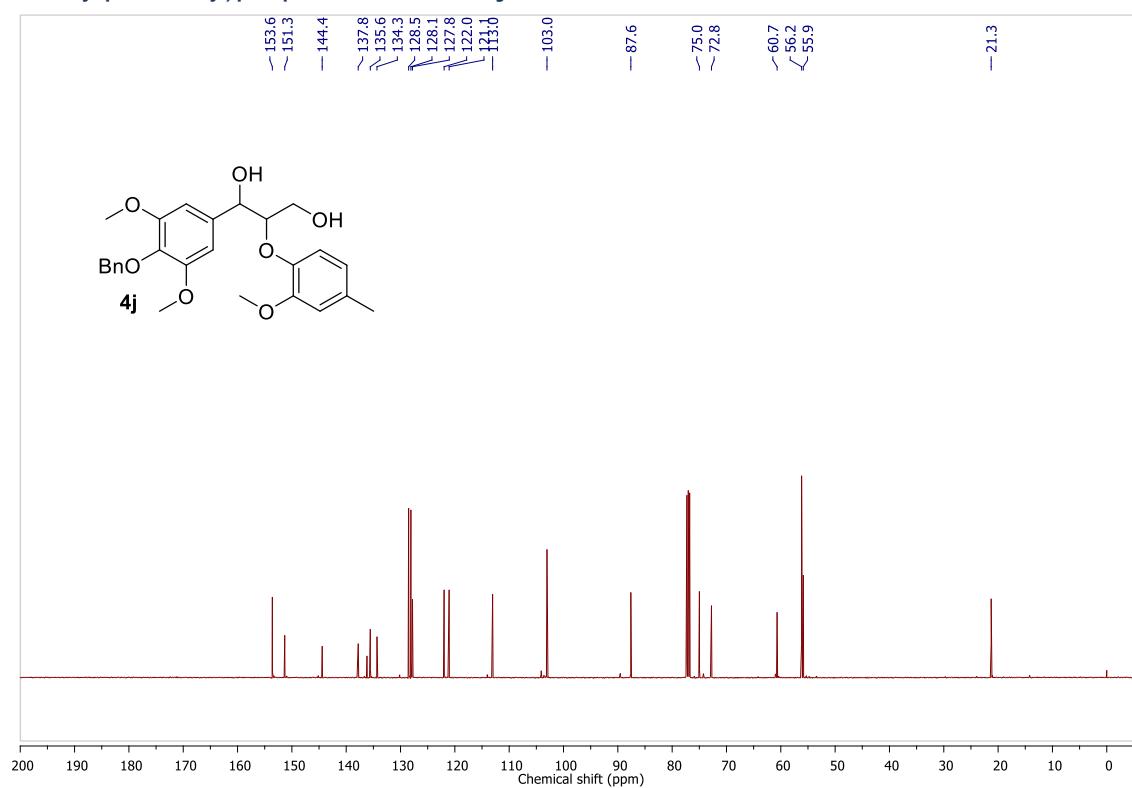
**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) 1-(4-(benzyloxy)-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4i**



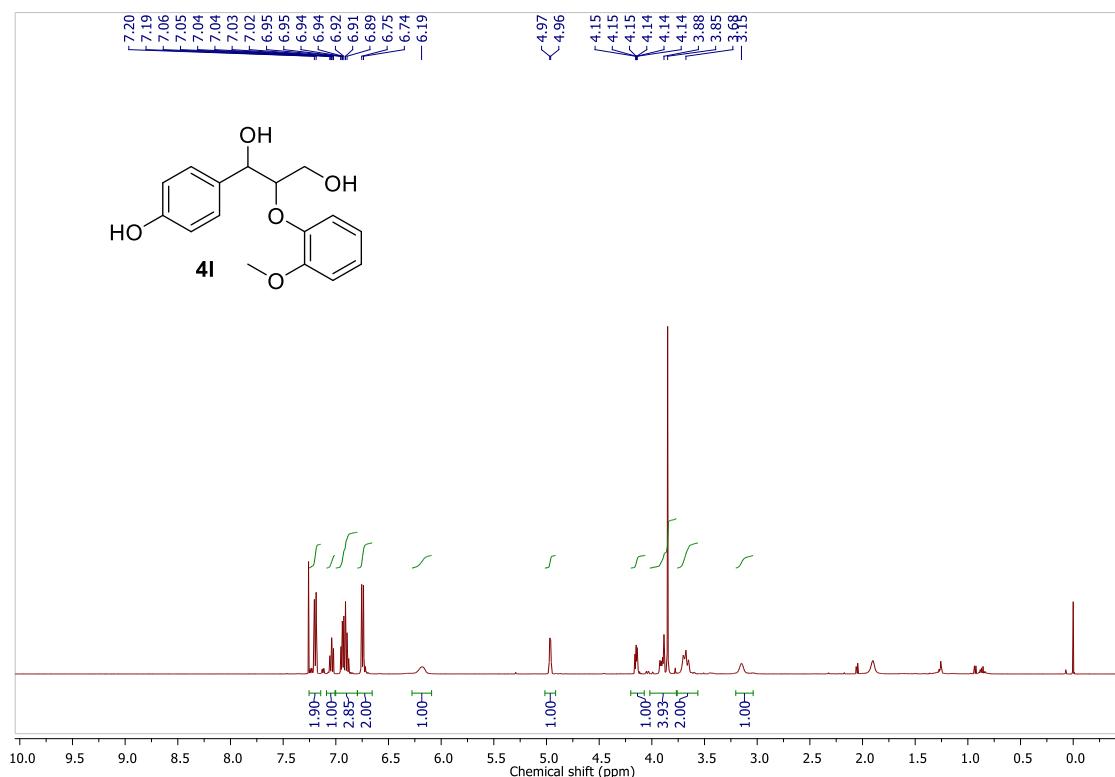
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) 1-(4-(benzyloxy)-3,5-dimethoxyphenyl)-2-(2-methoxy-4-methylphenoxy)propane-1,3-diol **4j**



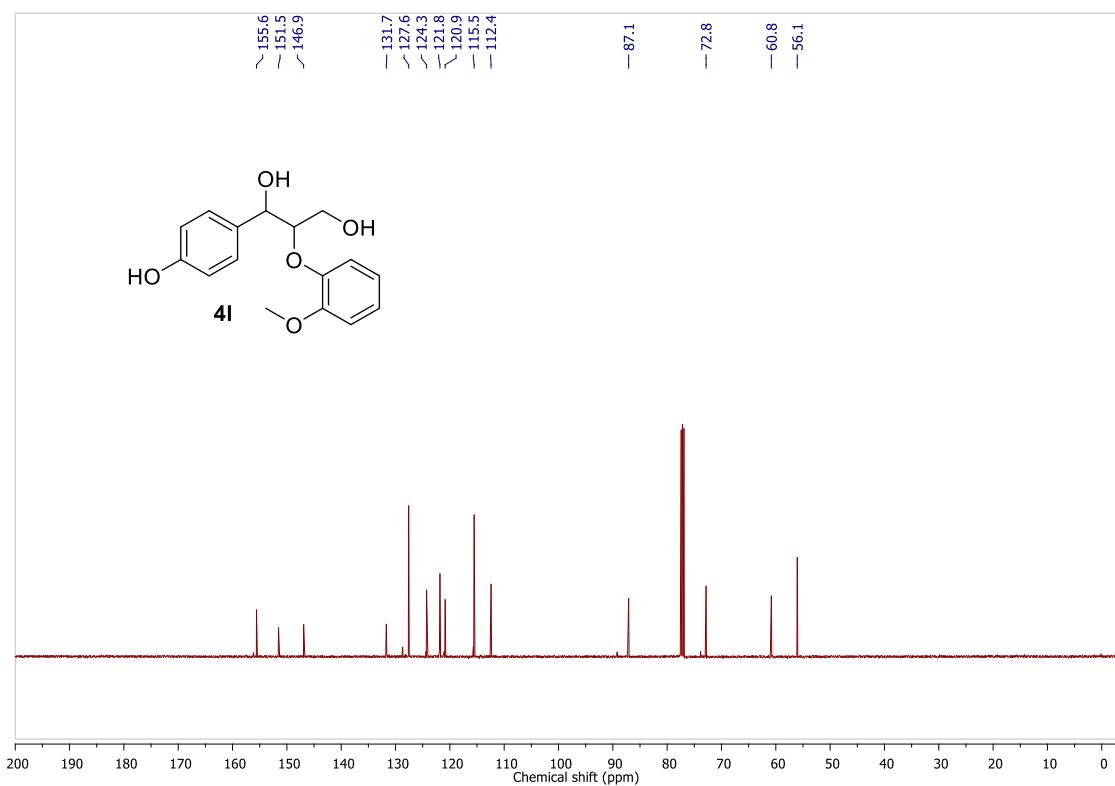
**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) 1-(4-(benzyloxy)-3,5-dimethoxyphenyl)-2-(2-methoxy-4-methylphenoxy)propane-1,3-diol **4j**



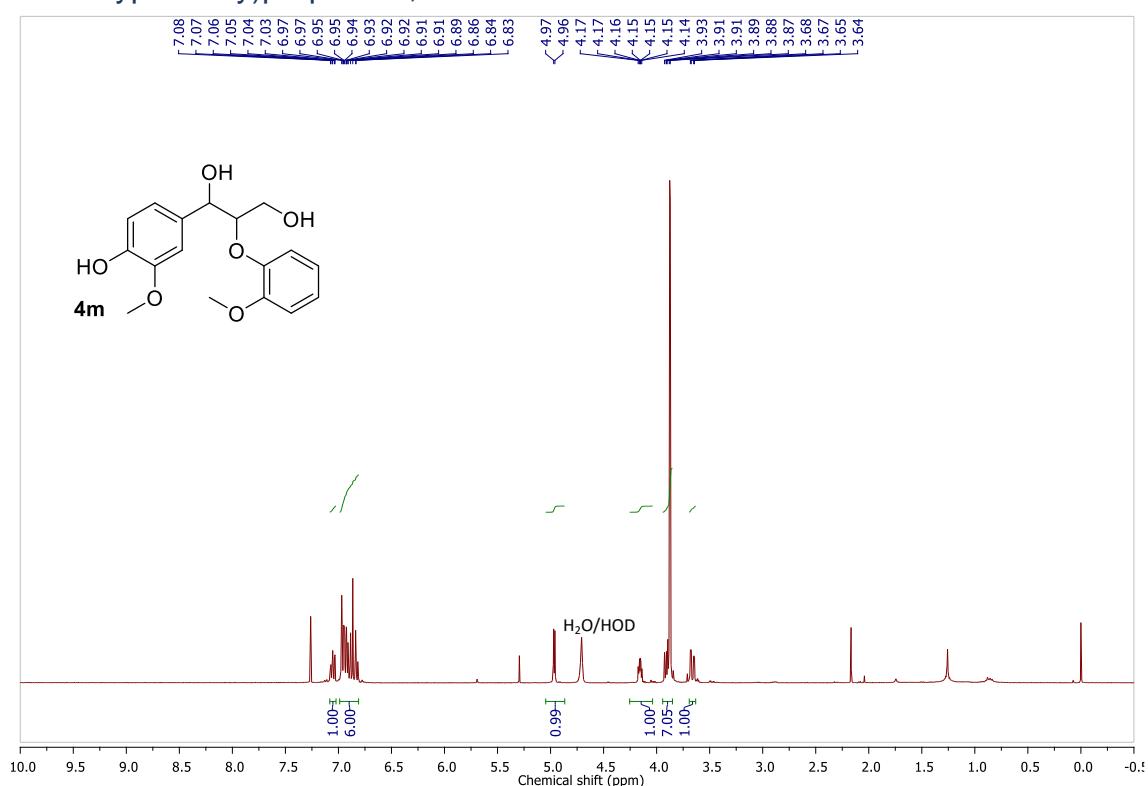
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) 1-(4-hydroxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4I****



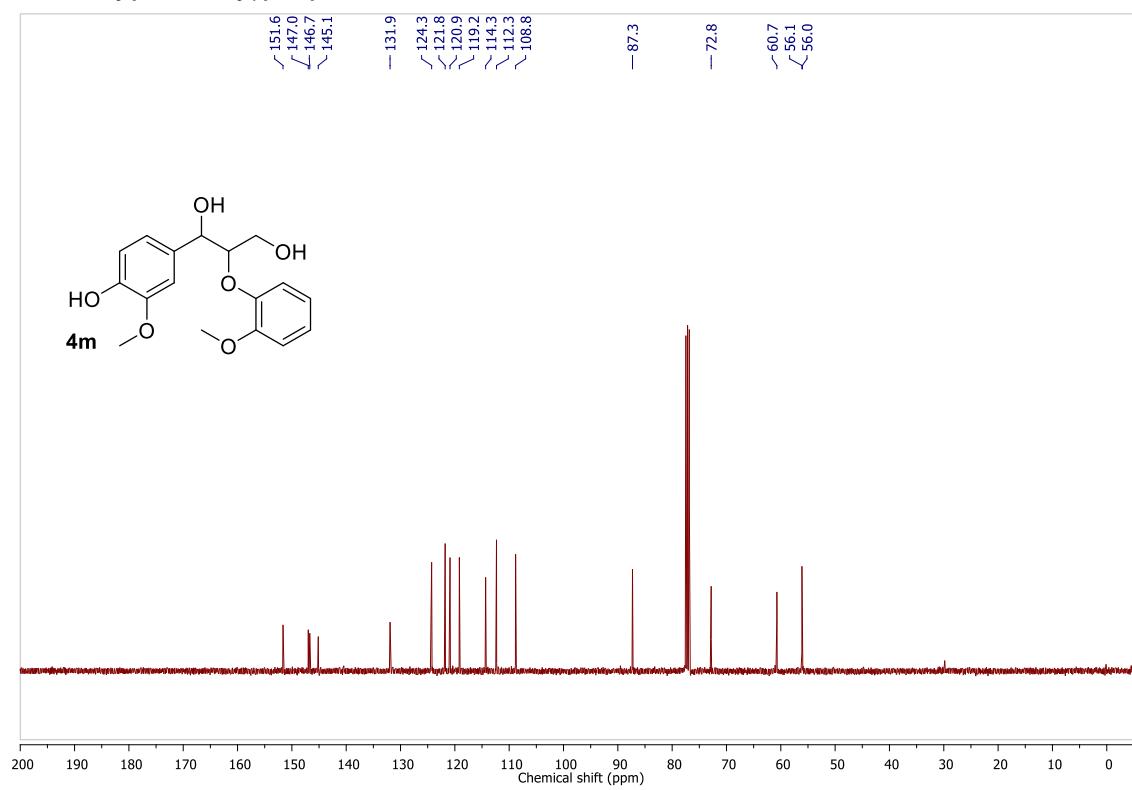
**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) 1-(4-hydroxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4I****



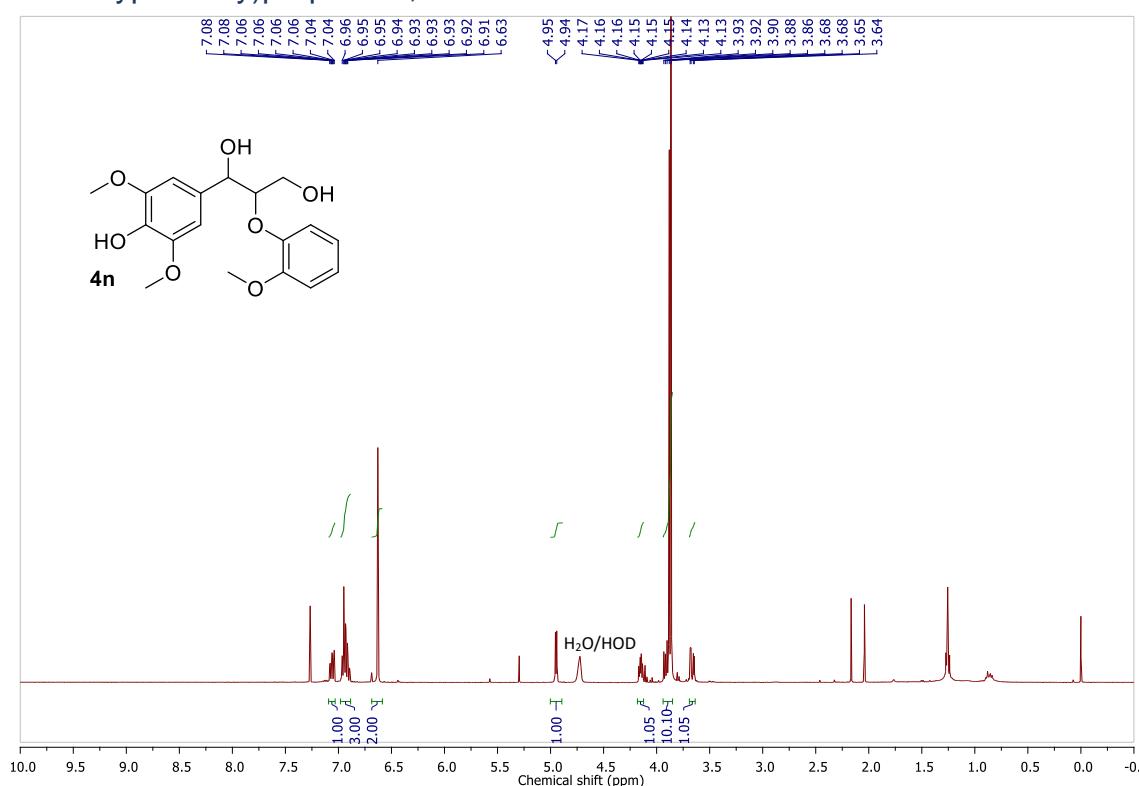
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub> + few drops of D<sub>2</sub>O) 1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **3m**



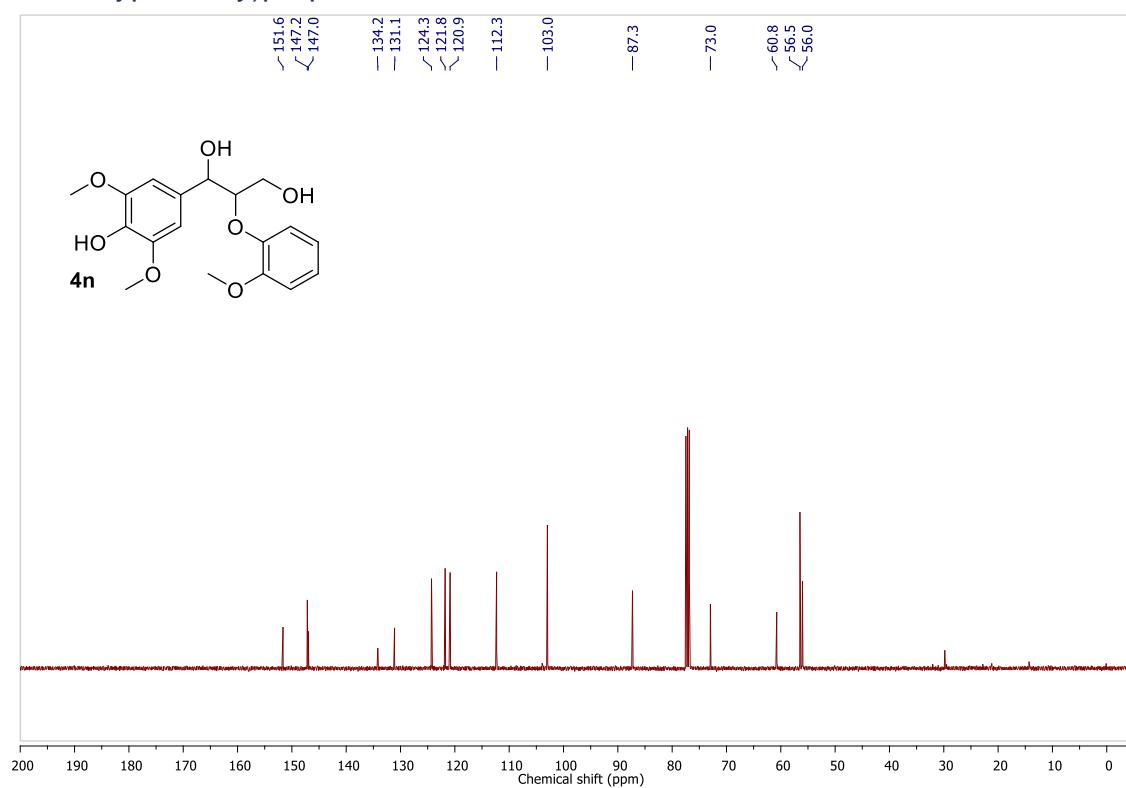
**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) 1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4m**



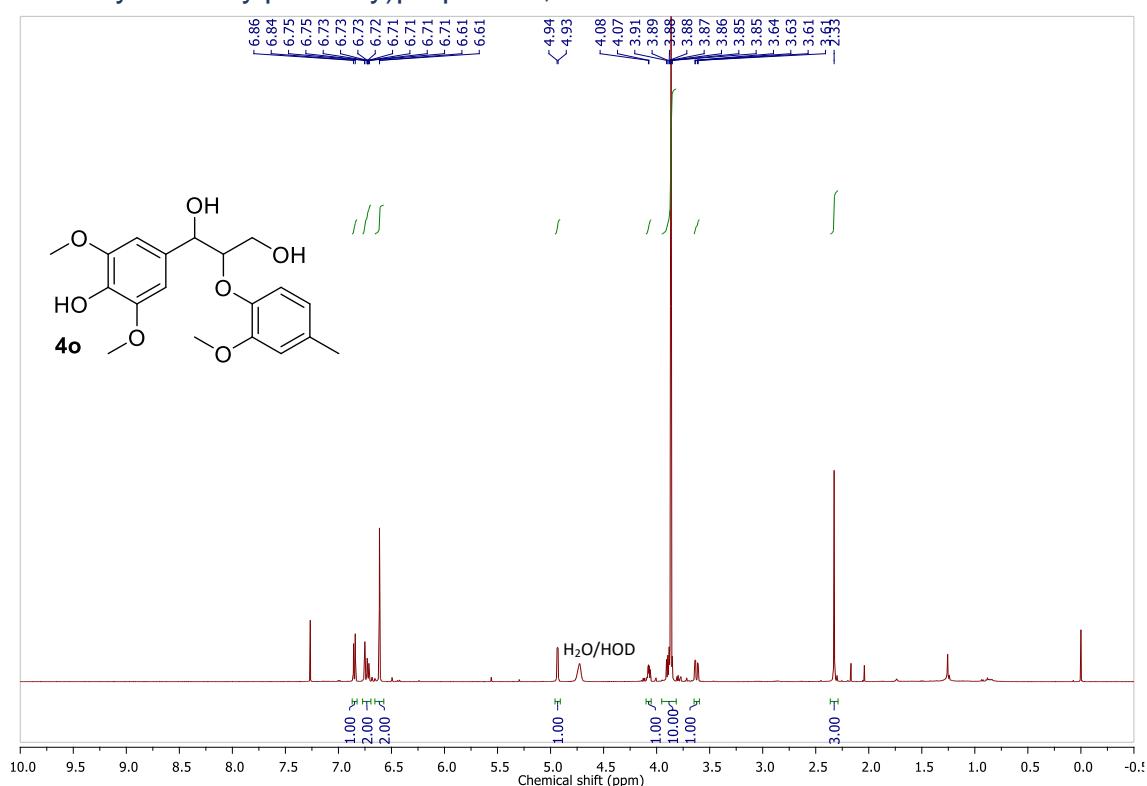
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub> + few drops of D<sub>2</sub>O) 1-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4n**



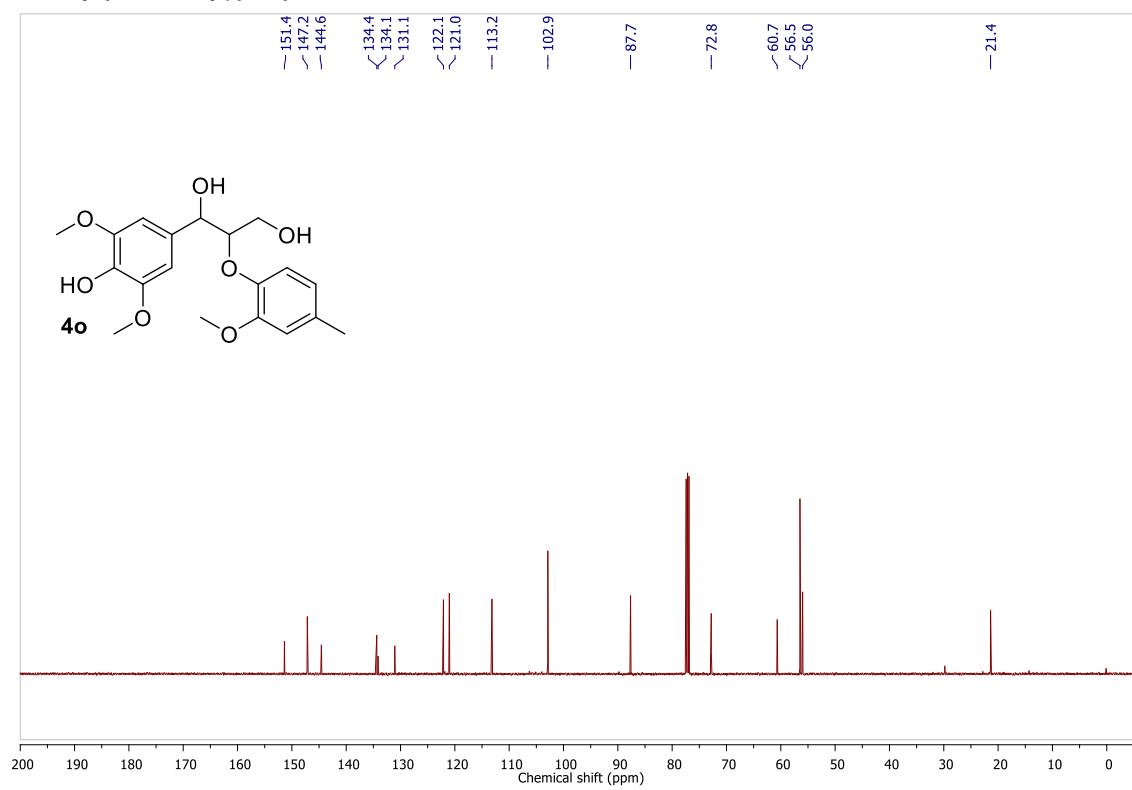
**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) 1-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol **4n**



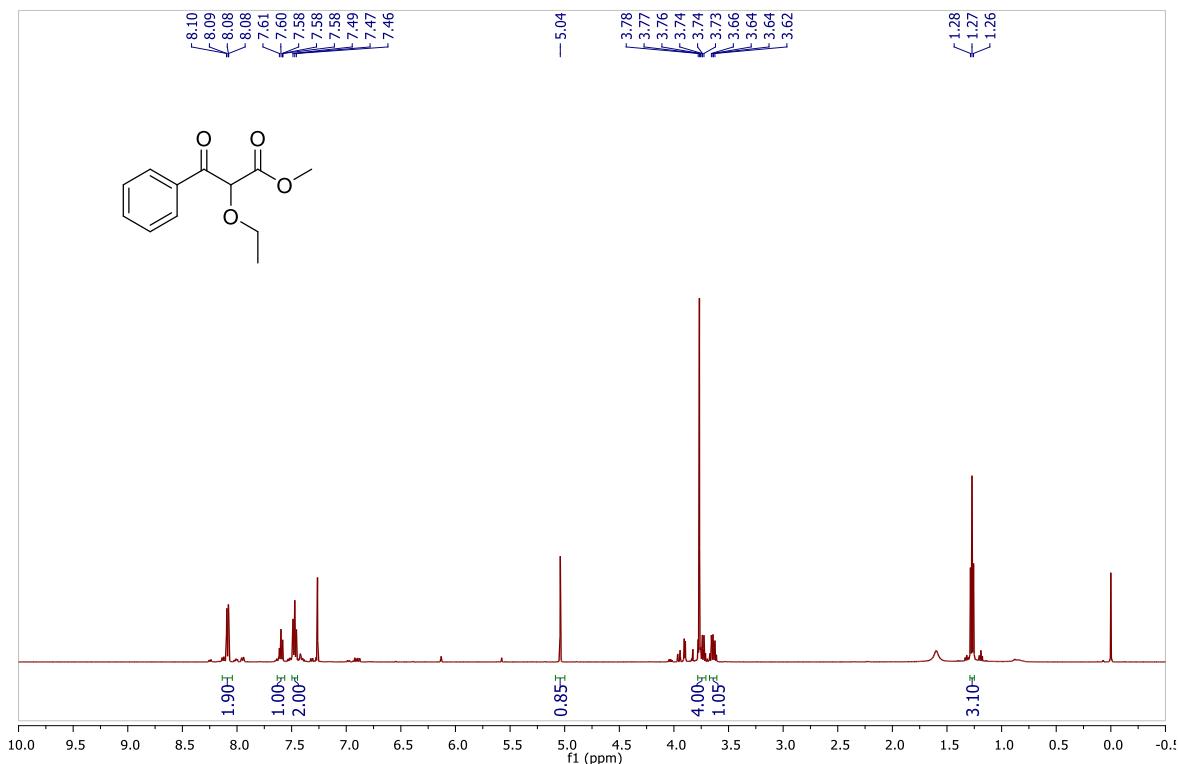
**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub> + few drops of D<sub>2</sub>O) 1-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxy-4-methylphenoxy)propane-1,3-diol **4o**



**<sup>13</sup>C NMR** (126 MHz, CDCl<sub>3</sub>) 1-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxy-4-methylphenoxy)propane-1,3-diol **4o**



**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) methyl 2-ethoxy-3-oxo-3-phenylpropanoate**



**<sup>13</sup>C NMR (126 MHz, CDCl<sub>3</sub>) methyl 2-ethoxy-3-oxo-3-phenylpropanoate**

