Supplementary Information of

Reactions of *p*-Coumaryl Alcohol Model Compounds with Dimethyl Carbonate. Towards the Upgrading of Lignin Building Blocks

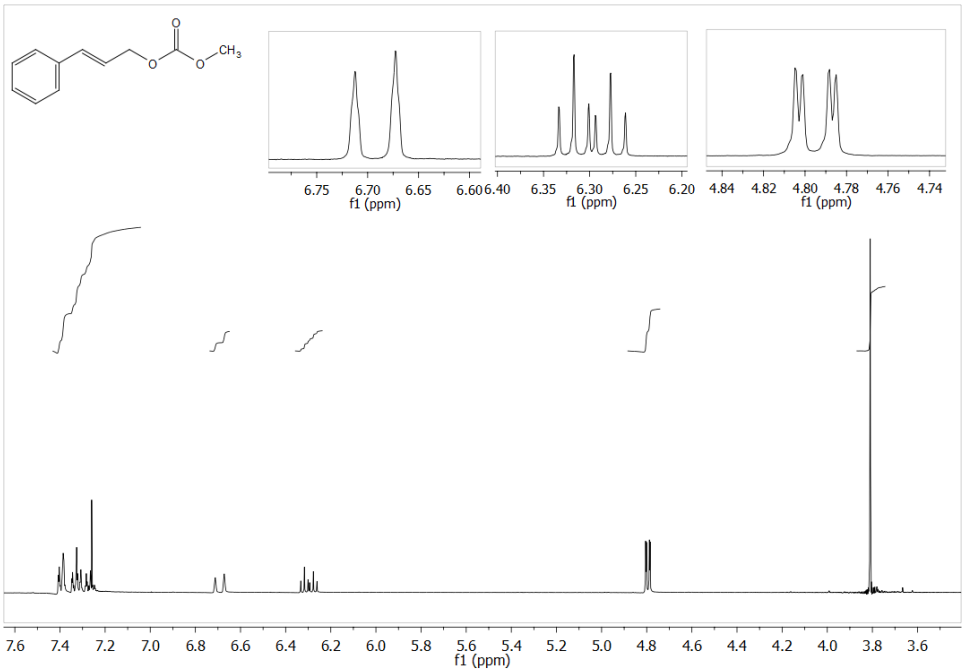
Jessica N.G. Stanley,[a,b] Maurizio Selva,[a] Anthony F. Masters,[b] Thomas Maschmeyer,[b] and Alvise Perosa*[a]

[a] Department of molecular sciences and nanosystems, Centre for sustainable chemical technologies, Università Ca' Foscari, Venezia, Italia. Fax: +39 041 234 8584; Tel: +39 041 234 8958; E-mail: alvise@unive.it

[b] Laboratory of Advanced Catalysis for Sustainability, School of Chemistry F11, The University of Sydney, Sydney, NSW 2006, Australia. Fax: +61 2 9351 3329; Tel: +61 2 9351 4504; E-mail: thomas.maschmeyer@sydney.edu.au

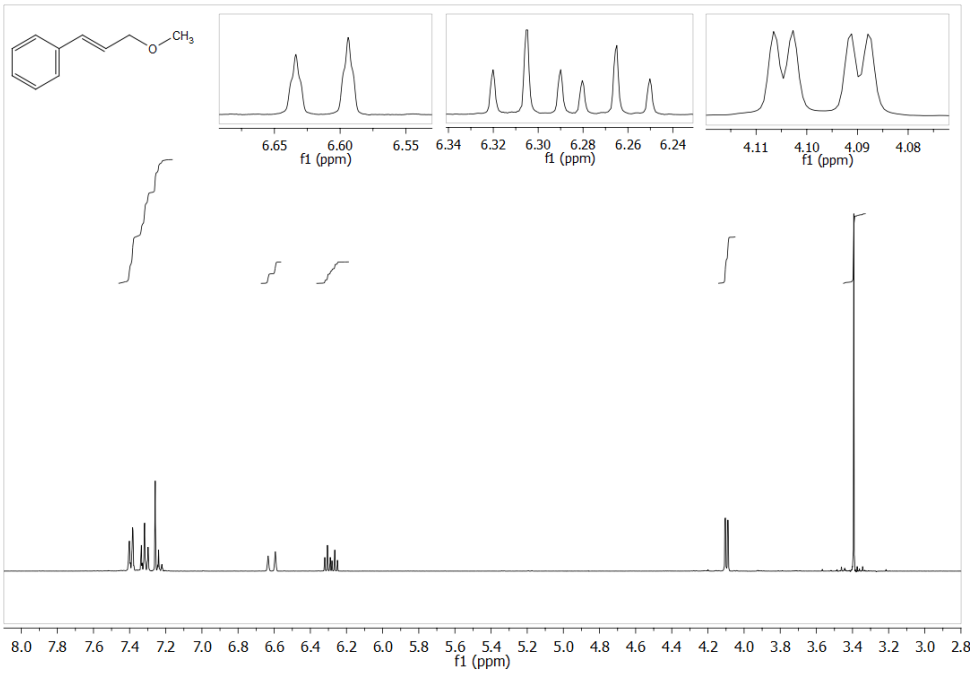
^{1}H NMR and MS spectra of all reported compounds and ^{13}C NMR spectra of new compounds.

cinnamyl methyl carbonate (1a), clear, pale yellow liquid. GC/MS (relative intensity, 70 eV) m/z: 192 (M^{+}, 16%), 133 (19), 103 (67), 102 (68), 91 (26), 79 (11), 78 (10), 77 (27), 50 (12), 43 (19).



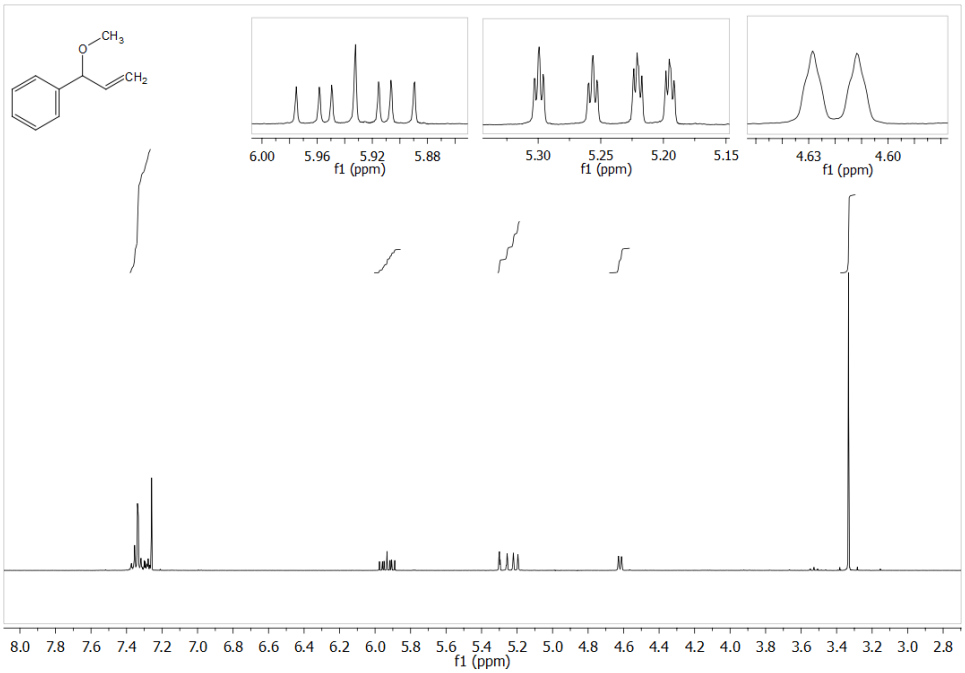
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42–7.24 (m, 5H), 6.69 (d, J = 15.9 Hz, 1H), 6.29 (dt, J = 15.9, 6.5 Hz, 1H), 4.80 (dd, J = 6.5, 1.3 Hz, 2H), 3.81 (s, 3H).

cinnamyl methyl ether (1b), clear, colourless liquid. GC/MS (relative intensity, 70 eV) m/z: 148 (M^+, 55%), 147 (30), 133 (13), 121 (13), 118 (18), 117 (69), 115 (100), 105 (42), 103 (24), 91 (38), 89 (12), 79 (20), 78 (15), 77 (42), 65 (15), 63 (19), 55 (12), 51 (34), 50 (16), 45 (15), 41 (13).



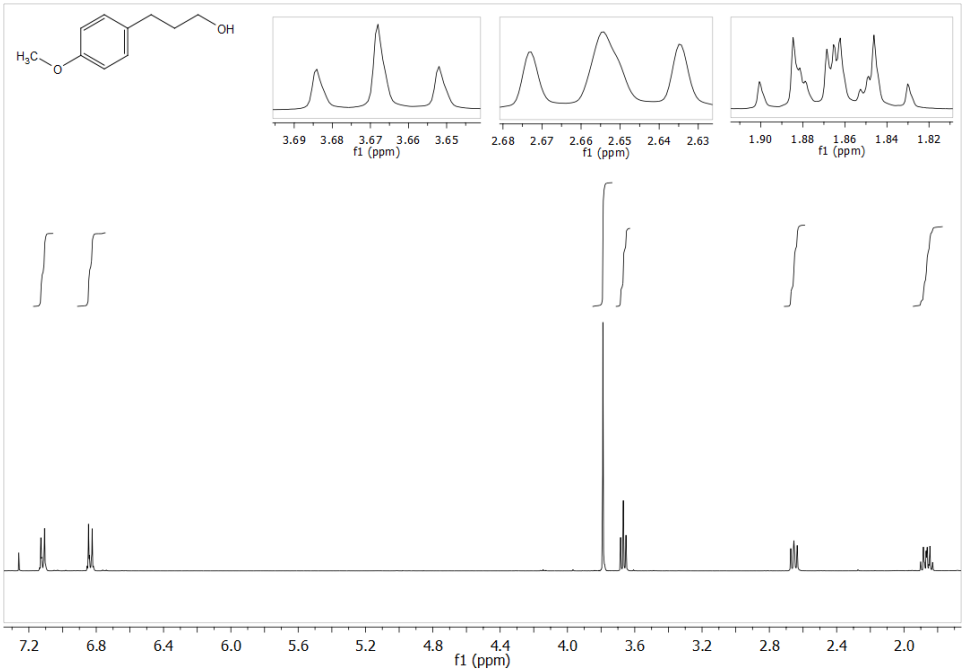
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42–7.21 (m, 5H), 6.61 (d, J = 16.0 Hz, 1H), 6.29 (dt, J = 16.0, 6.0 Hz, 1H), 4.10 (dd, J = 6.0, 1.4 Hz, 2H), 3.39 (s, 3H).

3-methoxy-3-phenylpropene (1c), clear, colourless liquid. GC/MS (relative intensity, 70 eV) m/z: 148 (M^+, 55%), 147 (48), 133 (11), 121 (62), 118 (21), 117 (86), 116 (72), 115 (100), 105 (47), 103 (11), 91 (68), 89 (16), 79 (11), 78 (17), 77 (92), 71 (12), 65 (20), 63 (24), 55 (29), 52 (11), 51 (52), 50 (26), 41 (25).



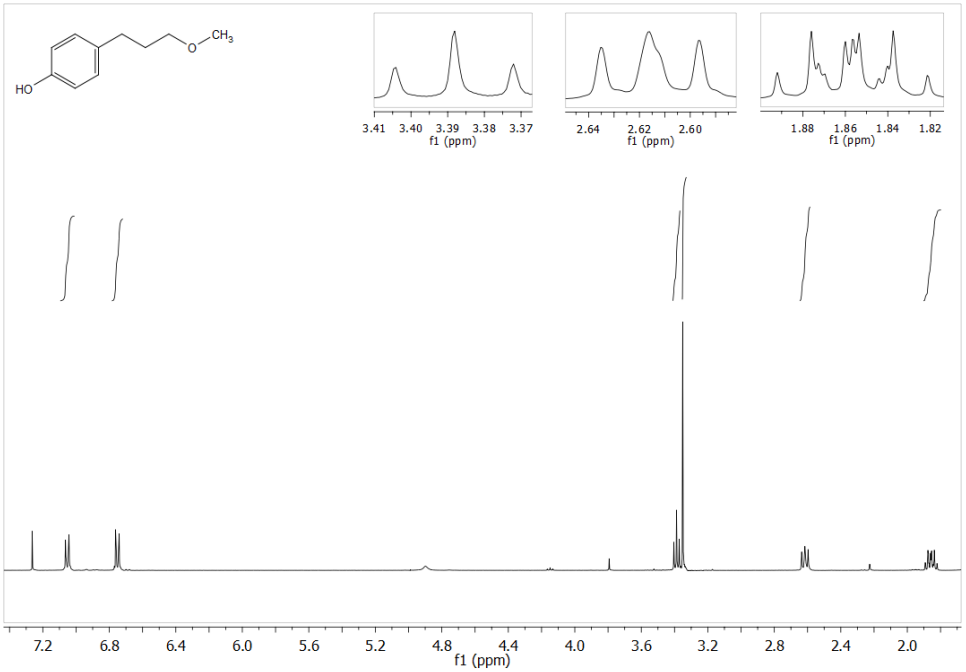
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.38–7.25 (m, 5H), 5.93 (ddd, J = 17.1, 10.4, 6.7 Hz, 1H), 5.25 (m, 2H), 4.62 (d, J = 6.7 Hz, 1H), 3.33 (s, 3H).

3-(4-methoxyphenyl)-1-propanol (2a) clear, colourless liquid. GC/MS (relative intensity, 70eV) m/z: 166 (M^+, 19%), 122 (11), 121 (100), 91 (13), 78 (10), 77 (17).

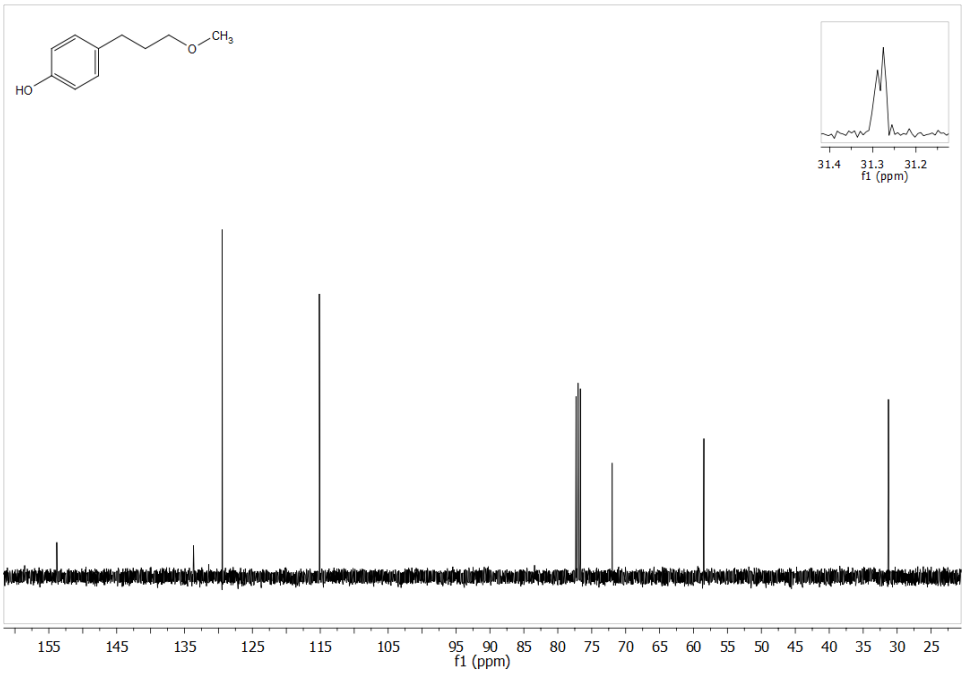


^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.12 (d, J = 8.5 Hz, 2H), 6.83 (d, J = 8.5 Hz, 2H), 3.79 (s, 3H), 3.67 (t, J = 6.5 Hz, 2H), 2.65 (t, J = 7.5 Hz, 2H), 1.90–1.82 (m, 2H).

4-(3-methoxypropyl)phenol (2b), clear, colourless liquid. GC/MS (relative intensity, 70eV) m/z: 166 (M^+, 19%), 134 (73), 133 (75), 108 (13), 107 (100), 105 (11), 91 (17), 78 (10), 77 (38), 65 (10), 51 (11), 45 (35).

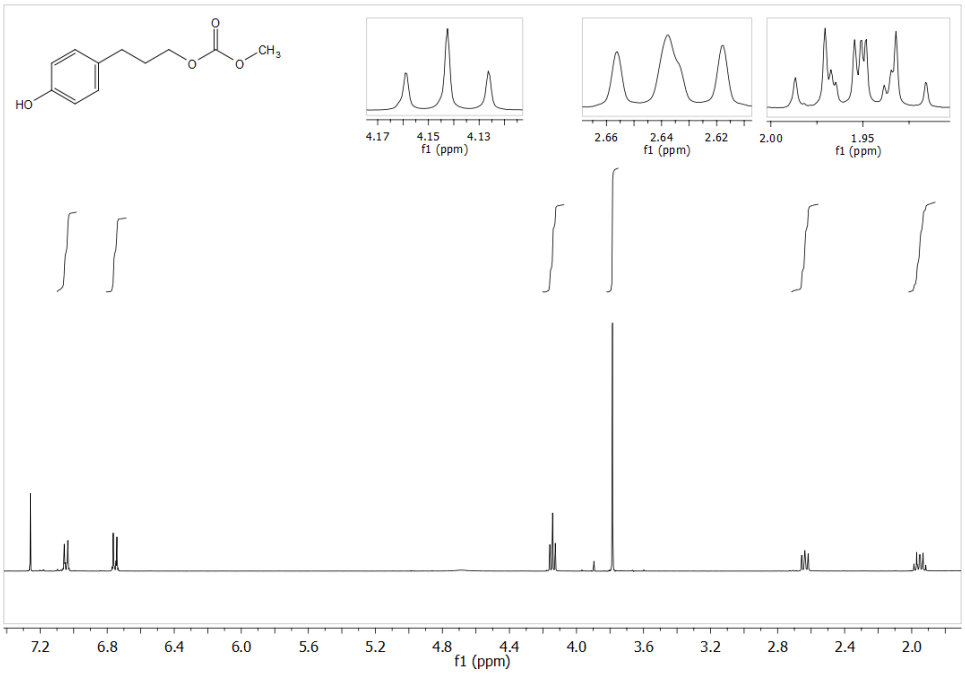


^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.05 (d, J = 8.5Hz, 2H), 6.75 (d, J = 8.5Hz, 2H), 3.39 (t, J = 6.5Hz, 2H), 3.35 (s, 3H), 2.62 (t, J = 7.4 Hz, 2H), 1.90–1.81 (m, 2H).



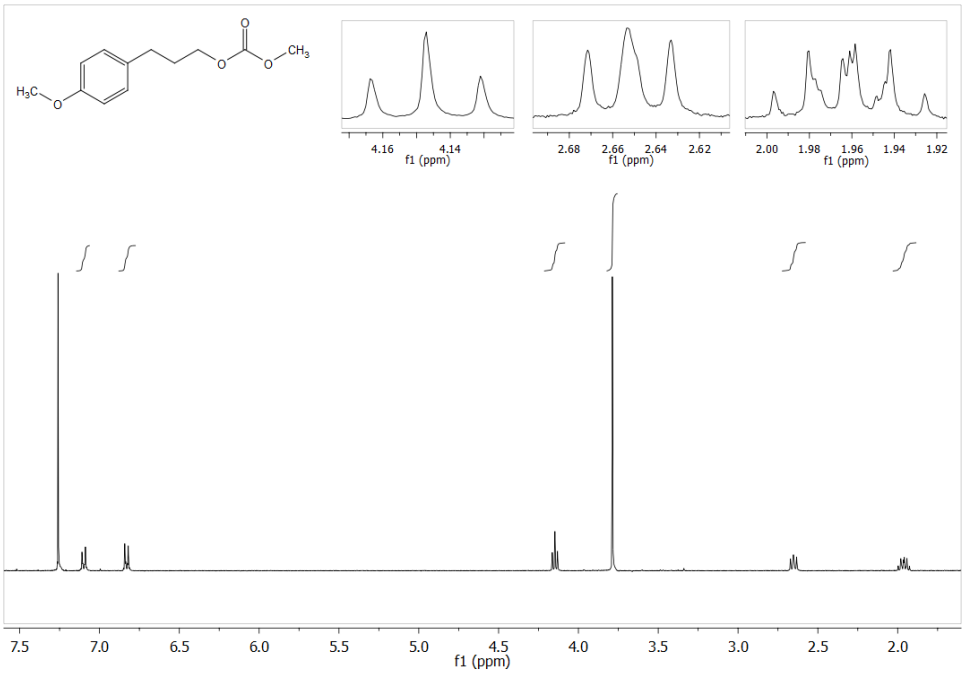
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.8, 133.7, 129.5, 115.1, 72.0, 58.5, 31.3, 31.3.

3-(4-hydroxyphenyl)propyl methyl carbonate (2c), clear, colourless liquid. GC/MS (relative intensity, 70eV) m/z 210 (M^+, 7%), 135 (15), 134 (90), 133 (87), 119 (10), 107 (100), 91 (16), 78 (11), 77 (35), 59 (13).

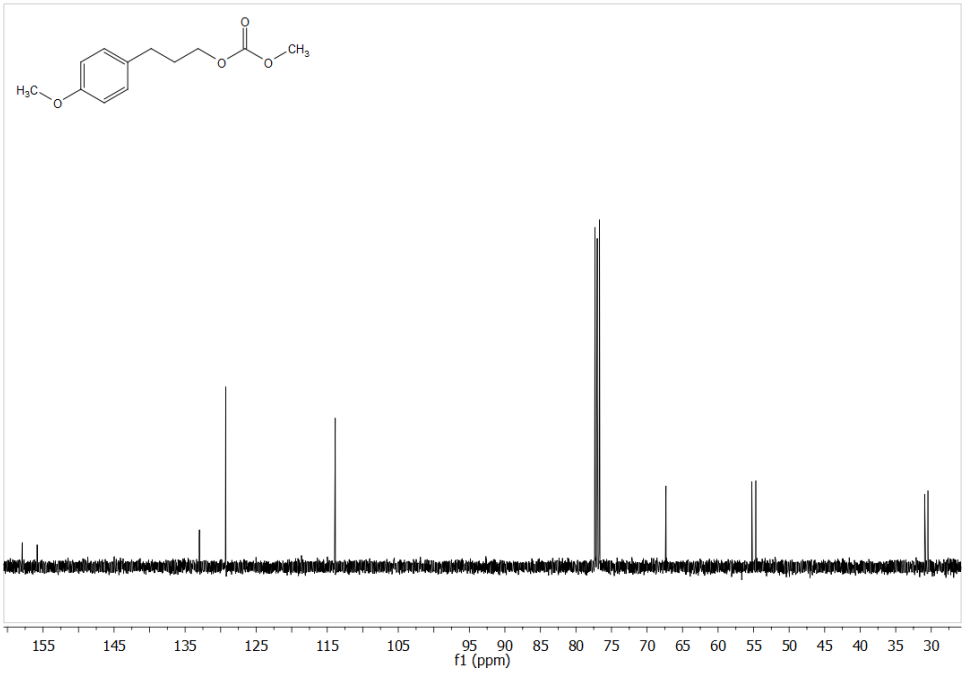


^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.05 (d, J = 8.5, 2H), 6.75 (d, J = 8.5, 2H), 4.14 (t, J = 6.5Hz, 2H), 3.79 (s, 3H), 2.64 (t, J = 7.5Hz, 2H), 1.99–1.91 (m, 2H).

3-(4-methoxyphenyl)propyl methyl carbonate (2d), clear, colourless liquid. GC/MS (relative intensity, 70eV) m/z: 224 (M^+, 12%), 149 (14), 148 (72), 147 (47), 133 (14), 121 (100), 117 (21), 105 (11), 91 (23), 78 (18), 77 (24), 65 (10), 59 (12).

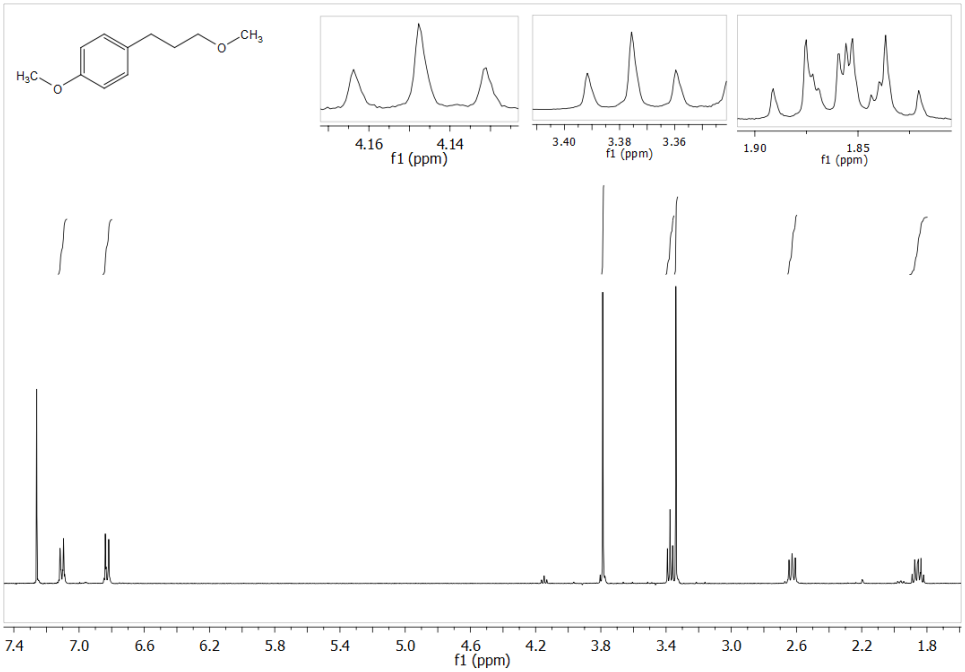


^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.10 (d, J = 8.6 Hz, 2H), 6.83 (d, J = 8.6Hz, 2H), 4.15 (t, J = 6.5Hz, 2H), 3.79 (s, 3H), 2.65 (t, J = 7.4Hz, 2H), 2.00–1.92 (m, 2H).



^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 157.9, 155.7, 132.9, 129.2, 113.8, 67.3, 55.1, 54.7, 30.8, 30.3.

1-methoxy-4-(3-methoxypropyl)benzene (2e),clear, colourless liquid. GC/MS (relative intensity, 70 eV) m/z: 180 (M^+, 22%), 122 (14), 121 (100), 117 (16), 94 (11), 91 (24), 77 (25), 78 (19), 65 (11).



^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.11 (d, J = 8.6 Hz, 2H), 6.83 (d, J = 8.6Hz, 2H), 3.79 (s, 3H), 3.38 (t, J = 6.4 Hz, 2H), 3.34 (s, 3H), 2.63 (t, J = 7.5 Hz, 2H), 1.90–1.81 (m, 2H).