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Supporting Information

## Functionalisation of Chromane by Deprotonative Metallation

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## General Information, Preparation and Analyses of the compounds

**General synthetic and analytical details.** All reactions were carried out in Schlenk tubes under a dry argon atmosphere. Tetrahydrofuran (THF) and toluene were freshly distilled under argon from sodium-benzophenone. All alkyllithiums were titrated before use.<sup>1</sup> Diethylamine and *N,N,N,N*-tetramethylethylenediamine (TMEDA) were distilled under argon over CaH<sub>2</sub>. 2,2,6,6-Tetramethylpiperidine (H-TMP) was distilled under vacuum over CaH<sub>2</sub>. ZnCl<sub>2</sub>-TMEDA was prepared as reported previously.<sup>2</sup> Room temperature (rt) refers to 25 °C. All Thin Layer Chromatographies (TLC) were performed on aluminium backed plates pre-coated with silica gel (Merck, Silica Gel 60 F254); they were visualized by exposure to UV light. Column chromatography separations were achieved on silica gel (40-63 μm). Melting points were measured on a Kofler apparatus. IR spectra were taken on a Perkin-Elmer Spectrum 100 spectrometer. <sup>1</sup>H and <sup>13</sup>C{<sup>1</sup>H} Nuclear Magnetic Resonance (NMR) spectra were recorded at 300 K either on a Bruker Avance III spectrometer fitted with a BBFO probe at 400 MHz and 100 MHz, respectively, or on a Bruker Avance III spectrometer fitted with a BBFO probe at 300 MHz and 75 MHz, respectively. The <sup>1</sup>H chemical shifts (δ) are given relative to the solvent residual peak, and <sup>13</sup>C chemical shifts are relative to the central peak of the solvent signal.<sup>3</sup> When given below, signal assignment was based on 2D NMR experiments (COSY, HSQC, HMBC) and comparison with other spectra; the numbering corresponds to that used in the name of the product and is given, for the new products, on the molecules which appear on the spectra.

**General crystallographic details.** The samples were studied with monochromatized Mo-Kα radiation (λ = 0.71073 Å; multilayer monochromator). The X-ray diffraction data of *racemic* 4,4'-bichromane, **5d** and **5e** were collected at *T* = 150(2) K on a D8 VENTURE Bruker AXS diffractometer equipped with a (CMOS) PHOTON 70 detector. The crystal structures were solved by dual-space algorithm using *SHELXT* program,<sup>4</sup> and then refined with full-matrix least-square methods based on *F*<sup>2</sup> (*SHELXL* program).<sup>5</sup> All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions and treated as riding on their parent atom with constrained thermal parameters. The molecular diagrams of *racemic* 4,4'-bichromane, **5d** and **5e** were generated by ORTEP-3 (version 2020.1).<sup>6</sup>

**7-Methyl-2,3-dihydrobenzofuran (3a).** It was prepared by slightly modifying a described procedure.<sup>7</sup> To a stirred solution of 2,3-dihydrobenzofuran (**1**; 0.23 mL, 2.0 mmol) and TMEDA (0.66 mL, 4.4 mmol) in hexane (7 mL) at rt, was added dropwise a 1.4 M solution of *n*BuLi in hexane (3.1 mL, 4.4 mmol). After 1 h at rt, Mel (0.27 mL, 4.4 mmol) was added dropwise, and the mixture was stirred for 2 h before addition of water (10 mL). Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude. Purification by column chromatography over silica gel (eluent: 98:2 petroleum ether-AcOEt) afforded the title product (Rf 0.8) in 65% yield (0.17 g) as an orange oil: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.22 (s, 3H, Me), 3.21 (t, 2H, *J* = 8.7 Hz, CH<sub>2</sub>CH<sub>2</sub>O), 4.56 (t, 2H, *J* = 8.7 Hz, CH<sub>2</sub>O), 6.76 (t, 1H, *J* = 7.4 Hz, H5), 6.94 (d, 1H, *J* = 7.4 Hz, H4 or H6), 7.03 (d, 1H, *J* = 7.3 Hz, H4 or H6) ppm. These data are in accordance with those reported.<sup>8</sup> A similar procedure was employed in the case of *n*BuLi-TMEDA (1.2 equiv) at 0 °C.

**2-Vinylphenol (4).** To a stirred solution of *t*BuOK (0.33 g, 2.5 mmol) and H-TMP (0.45 mL, 2.5 mmol) in THF (4 mL) at -70°C, was added dropwise a 1.3 M solution of *n*BuLi in hexane (1.8 mL, 2.4 mmol). After 5 min at -50 °C, 2,3-dihydrobenzofuran (**1**; 0.11 mL, 1.0 mmol) was added, and the mixture was stirred at this temperature for 1 h. The mixture was next cooled to -70 °C before addition of Mel (0.15 mL, 2.4 mmol). After stirring for 1 h, water (5 mL) and, after warming the reaction mixture to rt, aqueous 2 M HCl were added until pH < 6. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude. Purification by column chromatography over silica gel (eluent: 98:2 petroleum ether-AcOEt) afforded the title product (Rf 0.2) in a quantitative yield (0.12 g) as a yellow oil: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 5.05 (s, 1H, OH), 5.36 (dd, 1H, *J* = 11.2 and 1.4 Hz, CH=CHH), 5.75 (dd, 1H, *J* = 17.7 and 1.4 Hz, CH=CHH), 6.79 (dd, 1H, *J* = 8.0 and 1.2 Hz, H6), 6.91 (td, 1H, *J* = 7.5 and 1.2 Hz, H4 or H5), 6.95 (dd, 1H, *J* = 17.6 and 11.2 Hz, CH=CH<sub>2</sub>), 7.15 (td, 1H, *J* = 7.7 and 1.7 Hz, H4 or H5), 7.39 (dd, 1H, *J* = 7.7 and 1.7 Hz, H3) ppm. These data are in accordance with those reported.<sup>9</sup>

**Typical procedure for the deprotometallation of 2,3-dihydrobenzofuran (1) using alkyllithiums in THF followed by interception with iodomethane.** To a stirred solution of 2,3-dihydrobenzofuran (**1**; 0.11 mL, 1.0 mmol) in THF (3.5 mL) at 0 °C, was added dropwise a 1.4 M solution of *n*BuLi in hexane (0.85 mL, 1.2 mmol). After 1 h at 0 °C, Mel (75 μL, 1.2 mmol) was added dropwise, and the mixture was stirred for 2 h before addition of aqueous 2 M HCl until pH < 6. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude for which the **1:3a:4** ratio was determined by <sup>1</sup>H NMR. A similar procedure was employed in the case of *s*BuLi and *t*BuLi.

**Typical procedure for the deprotometallation of 2,3-dihydrobenzofuran (1) using lithium dialkylamides in THF followed by interception with iodomethane.** To a stirred solution of H-TMP (0.23 mL, 1.3 mmol) in THF (3.5 mL) at -15 °C were successively added a 1.3 M solution of *n*BuLi in hexane (0.90 mL, 1.2 mmol) and, 5 min later, 2,3-dihydrobenzofuran (**1**; 0.11 mL, 1.0 mmol). After 1 h at this temperature, Mel (75 μL, 1.2 mmol) was added dropwise, and the mixture was stirred for 2 h before addition of aqueous 2 M HCl until pH < 6. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude for which the **1:3a:4** ratio was determined by <sup>1</sup>H NMR. Similar procedures were employed in the case of LiNEt<sub>2</sub>.

**Typical procedure for the deprotometallation of 2,3-dihydrobenzofuran (1) in the presence of ZnCl<sub>2</sub>-TMEDA, using lithium dialkylamides in THF, followed by interception with iodomethane.** To a stirred solution of diethylamine (0.31 mL, 3.0 mmol) in THF (2 mL) at -15 °C was added a 1.3 M solution of *n*BuLi in hexane (2.3 mL, 3.0 mmol). After stirring for 5 min, this solution was added dropwise to a solution of 2,3-dihydrobenzofuran (**1**; 0.11 mL, 1.0 mmol) and ZnCl<sub>2</sub>-TMEDA (0.25 g, 1.0 mmol) in THF at -15 °C. After 1 h at this temperature, Mel (0.19 mL, 3.0 mmol) was added dropwise, and the mixture was stirred for 2 h before addition of aqueous 2 M HCl until pH < 6. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude for which the **1:3a:4** ratio was determined by <sup>1</sup>H NMR.

**Chromane (2).** It was prepared by slightly modifying a described procedure.<sup>10</sup> To 4-chromanone (2.2 g, 15 mmol) in MeOH (45 mL) was added 10% palladium on charcoal (0.16 g, 0.15 mmol), chlorobenzene (46 μL, 0.75 mmol) and, in 1 h, polymethylhydrosiloxane (2.5 mL, 42 mmol). The reaction mixture was then stirred at rt for 15 min and filtered over Celite® (washing using AcOEt). Extraction using AcOEt (3 x 20 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude. Purification by column chromatography over

silica gel (eluent: 98:2 petroleum ether-AcOEt) afforded the title product (Rf 0.6) in 95% yield (1.9 g) as a pale yellow oil: IR (ATR)  $\nu$  711, 726, 750 (s), 815, 846, 881, 929, 1007, 1063 (s), 1115, 1150, 1188, 1225 (s), 1266, 1303, 1338, 1456, 1488 (s), 1581, 1608, 2863, 2936  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  1.97-2.05 (m, 2H,  $\text{CH}_2\text{CH}_2\text{O}$ ), 2.79 (t, 2H,  $J = 6.5$  Hz,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 4.17-4.20 (m, 2H,  $\text{CH}_2\text{O}$ ), 6.79 (dd, 1H,  $J = 8.3$  and 1.4 Hz, H8), 6.83 (td, 1H,  $J = 7.5$  and 1.3 Hz, H6), 7.01-7.11 (m, 2H, H5 and H7) ppm;  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  22.5 ( $\text{CH}_2$ ,  $\text{CH}_2\text{CH}_2\text{O}$ ), 25.0 ( $\text{CH}_2$ ,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 66.6 ( $\text{CH}_2$ ,  $\text{CH}_2\text{O}$ ), 116.8 (CH, C8), 120.2 (CH, C6), 122.3 (C, Cb), 127.3 (CH, C7), 129.9 (CH, C5), 155.0 (C, Ca) ppm. These data are in accordance with those reported.<sup>10</sup>

**Typical procedure for the deprotonation of chromane (2) using *n*BuLi-TMEDA in hexane followed by interception with an electrophile.** To a stirred solution of chromane (**2**; 0.25 mL, 2.0 mmol) and TMEDA (0.66 mL, 4.4 mmol) in hexane (5 mL) at rt, was added dropwise a 1.4 M solution of *n*BuLi in hexane (3.1 mL, 4.4 mmol). Unless stated otherwise, after 2 h at rt, the electrophile (4.4 mmol; either pure for liquids, or in THF for solids) was introduced, and the mixture was stirred for 2 h before addition of water (10 mL). Extraction using AcOEt (3 x 10 mL), drying over  $\text{MgSO}_4$  and concentration under reduced pressure led to the crude which was purified by column chromatography over silica gel.

**8-Methylchromane (5a).**<sup>11</sup> The title product was prepared according to the typical procedure using MeI (0.27 mL) as the electrophile. Purification (eluent: 98:2 petroleum ether-AcOEt) afforded the title product (Rf 0.8) in 75% yield (0.22 g) as a yellow oil: IR (ATR)  $\nu$  659, 730, 760 (s), 804, 850, 875, 897, 953, 998, 1043, 1060, 1090, 1193 (s), 1216 (s), 1262, 1308, 1378, 1430, 1460, 1475 (s), 1594, 1693, 2071, 2929  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  2.00 (tdd, 2H,  $J = 6.5, 5.3$  and 4.5 Hz,  $\text{CH}_2\text{CH}_2\text{O}$ ), 2.18 (s, 3H, Me), 2.79 (t, 2H,  $J = 6.6$  Hz,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 4.20-4.24 (m, 2H,  $\text{CH}_2\text{O}$ ), 6.74 (t, 1H,  $J = 7.4$  Hz, H6), 6.89 (ddd, 1H,  $J = 7.6, 1.7$  and 0.8 Hz, H5 or H7), 6.95 (ddd, 1H,  $J = 7.3, 1.8$  and 0.8 Hz, H5 or H7) ppm;  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  16.1 ( $\text{CH}_3$ ), 22.7 ( $\text{CH}_2$ ,  $\text{CH}_2\text{CH}_2\text{O}$ ), 25.2 ( $\text{CH}_2$ ,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 66.7 ( $\text{CH}_2$ ,  $\text{CH}_2\text{O}$ ), 119.6 (CH, C6), 121.7 (C, Cb), 126.0 (C, C8), 127.5 (CH, C7), 128.5 (CH, C5), 153.2 (C, Ca) ppm; HRMS (ASAP; source at 40 °C),  $m/z$ : 149.0960 (1 ppm) found (calcd for  $\text{C}_{10}\text{H}_{13}\text{O}$ ,  $[\text{M}+\text{H}]^+$ , requires 149.09609).

**(4-Anisyl)(8-chromanyl)methanol (racemic mixture; 5b).** The title product was prepared according to the typical procedure, but from 1.0 mmol of **2** (0.13 mL), using 4-anisaldehyde (0.27 mL) as the electrophile. Purification (eluent: 85:15 petroleum ether-AcOEt) afforded the title product (Rf 0.2) in 57% yield (0.16 g) as an orange oil: IR (ATR)  $\nu$  730, 763, 787, 805, 831, 878, 909, 956, 1033 (s), 1171, 1217, 1243 (s), 1301, 1456, 1471, 1508, 1591, 1610, 2930, 3478  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  1.96-2.04 (m, 2H,  $\text{CH}_2\text{CH}_2\text{O}$ ), 2.79 (t, 2H,  $J = 6.6$  Hz,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 3.11 (d, 1H,  $J = 5.4$  Hz, OH), 3.80 (s, 3H, OMe), 4.20 (t, 2H,  $J = 5.4$  Hz,  $\text{CH}_2\text{O}$ ), 5.96 (d, 1H,  $J = 4.7$  Hz,  $\text{CH}(\text{OH})$ ), 6.80 (dd, 1H,  $J = 7.8$  and 7.2 Hz, H6), 6.84-6.89 (m, 2H, H3' and H5'), 6.97 (dd, 2H,  $J = 7.9$  and 0.9 Hz, H5 and H7), 7.29-7.34 (m, 2H, H2' and H6') ppm;  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  22.4 ( $\text{CH}_2$ ,  $\text{CH}_2\text{CH}_2\text{O}$ ), 25.0 ( $\text{CH}_2$ ,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 55.4 ( $\text{CH}_3$ , OMe), 66.7 ( $\text{CH}_2$ ,  $\text{CH}_2\text{O}$ ), 72.2 (CH,  $\text{CH}(\text{OH})$ ), 113.7 (2CH, C3' and C5'), 120.1 (CH, C6), 122.5 (C, Cb), 125.8 (CH, C5 or C7), 128.0 (2CH, C2' and C6'), 129.3 (CH, C5 or C7), 131.6 (C, C8 or C1'), 135.7 (C, C8 or C1'), 152.4 (C, Ca), 158.9 (C, C4') ppm; HRMS (ASAP; source at 120 °C),  $m/z$ : 270.1249 (1 ppm) found (calcd for  $\text{C}_{17}\text{H}_{18}\text{O}_3$ ,  $\text{M}^+$ , requires 270.12504).

**8-Chromancarboxaldehyde (5c).** The title product was prepared according to the typical procedure, but from 1.0 mmol of **2** (0.13 mL), using *N,N*-dimethylformamide (DMF; 0.17 mL) as the electrophile. Purification (eluent: 60:40 petroleum ether-AcOEt) afforded the title product (Rf 0.2) in 51% yield (83 mg) as an orange oil: IR (ATR)  $\nu$  732, 750, 776, 808, 855, 877, 908, 960, 981, 1018, 1075, 1092, 1189 (s), 1226 (s), 1254, 1276, 1301, 1331, 1379, 1397, 1454, 1474, 1589 (s), 1679 (s), 1724, 2874, 2932  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  2.03-2.09 (m, 2H,  $\text{CH}_2\text{CH}_2\text{O}$ ), 2.83 (t, 2H,  $J = 6.5$  Hz,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 4.29-4.32 (m, 2H,  $\text{CH}_2\text{O}$ ), 6.89 (td, 1H,  $J = 7.6$  and 0.8 Hz, H6), 7.24 (ddt, 1H,  $J = 7.4, 2.0$  and 1.1 Hz, H5), 7.63 (ddd, 1H,  $J = 7.7, 1.7$  and 0.8 Hz, H7), 10.41 (d, 1H,  $J = 0.8$  Hz, CHO) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  21.7 ( $\text{CH}_2$ ,  $\text{CH}_2\text{CH}_2\text{O}$ ), 24.7 ( $\text{CH}_2$ ,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 66.9 ( $\text{CH}_2$ ,  $\text{CH}_2\text{O}$ ), 119.8 (CH, C6), 123.5 (C, C8 or Cb), 124.3 (C, C8 or Cb), 126.5 (CH, C5 or C7), 136.0 (CH, C5 or C7), 157.7 (C, Ca), 190.0 (CH, CHO) ppm. These data are as reported previously.<sup>12</sup>

**8-Iodochromane (5d).** The title product was prepared according to the typical procedure, but from 5.0 mmol of **2** (0.63 mL), using  $\text{I}_2$  (2.8 g) in THF (14 mL) as the electrophile. In this case, saturated aqueous  $\text{Na}_2\text{S}_2\text{O}_3$  (25 mL) was added instead of water. Purification (eluent: 98:2 petroleum ether-AcOEt) afforded the title product (Rf 0.7) in 58% yield (0.75 g) as a white solid: mp 74 °C; IR (ATR)  $\nu$  720, 777 (s), 818, 872, 886, 936, 1001, 1047, 1073, 1128, 1170, 1190, 1202, 1230 (s), 1277, 1293, 1328, 1343, 1379, 1426, 1438 (s), 1468, 1559, 1594, 1693, 1883, 1934, 2883, 2923, 2983  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  2.01 (tdd, 2H,  $J = 6.5, 5.1$  and 4.1 Hz,  $\text{CH}_2\text{CH}_2\text{O}$ ), 2.79 (t, 2H,  $J = 6.5$  Hz,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 4.27-4.30 (m, 2H,  $\text{CH}_2\text{O}$ ), 6.59 (t, 1H,  $J = 7.6$  Hz, H6), 7.00 (ddt, 1H,  $J = 7.5, 1.8$  and 1.0 Hz, H5), 7.57 (ddt, 1H,  $J = 7.8, 1.6$  and 0.8 Hz, H7) ppm;  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  22.4 ( $\text{CH}_2$ ,  $\text{CH}_2\text{CH}_2\text{O}$ ), 25.4 ( $\text{CH}_2$ ,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 67.7 ( $\text{CH}_2$ ,  $\text{CH}_2\text{O}$ ), 85.5 (C, C8), 121.8 (CH, C6), 123.3 (C, Cb), 130.1 (CH, C5), 137.2 (CH, C7), 153.8 (C, Ca) ppm. These data are as reported previously.<sup>13</sup> HRMS (ASAP; source at 40 °C),  $m/z$ : 260.9774 (1 ppm) found (calcd for  $\text{C}_9\text{H}_9\text{OI}$ ,  $[\text{M}+\text{H}]^+$ , requires 260.97709). **Crystal data for 5d.**  $\text{C}_9\text{H}_9\text{OI}$ ,  $M = 260.06$ , orthorhombic,  $Pn a 2_1$ ,  $a = 8.0255(7)$ ,  $b = 9.0271(8)$ ,  $c = 12.0553(12)$  Å,  $V = 873.37(14)$  Å<sup>3</sup>,  $Z = 4$ ,  $d = 1.978$  g  $\text{cm}^{-3}$ ,  $\mu = 3.605$  mm<sup>-1</sup>. A final refinement on  $F^2$  with 1966 unique intensities and 100 parameters converged at  $\omega R(F^2) = 0.0416$  ( $R(F) = 0.0182$ ) for 1952 observed reflections with  $I > 2\sigma(I)$ . CCDC 2352994.

**8-(2-Pyridyl)chromane (5e).** The title product was prepared by adapting a reported procedure.<sup>14</sup> To a stirred solution of chromane (**2**; 0.13 mL, 1.0 mmol) and TMEDA (0.33 mL, 2.2 mmol) in hexane (3 mL) at rt, was added dropwise a 1.4 M solution of *n*BuLi in hexane (1.5 mL, 2.1 mmol). After 2 h at rt, the reaction mixture was cooled to -20 °C before addition of THF (2 mL) and  $\text{ZnCl}_2$ -TMEDA (0.56 g, 2.2 mmol). The mixture was then warmed to rt before addition of  $\text{PdCl}_2$  (14 mg, 80  $\mu\text{mol}$ ), 1,1'-bis(diphenylphosphino)ferrocene (dppf; 44 mg, 80  $\mu\text{mol}$ ) and 2-chloropyridine (0.23 mL, 2.4 mmol). The mixture was heated at 80 °C for 8 h. After filtration over Celite®, brine (5 mL) was added. Extraction using AcOEt (3 x 10 mL), drying over  $\text{MgSO}_4$  and concentration under reduced pressure led to the crude, which was purified by chromatography over silica gel (neutralized using  $\text{NEt}_3$ ; eluent: 80:20 petroleum ether-AcOEt) to afford the title product (Rf 0.3) as a beige oil in 36% yield (77 mg): IR (ATR)  $\nu$  688, 741, 751, 767 (s), 803, 836, 875, 897, 943, 990, 1012, 1053, 1079, 1118, 1157, 1203, 1225 (s), 1273, 1297, 1339, 1381, 1423, 1439, 1474, 1561, 1590, 1693, 2868, 2945  $\text{cm}^{-1}$ ;  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )  $\delta$  1.98-2.06 (m, 2H,  $\text{CH}_2\text{CH}_2\text{O}$ ), 2.85 (t, 2H,  $J = 6.5$  Hz,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 4.19-4.22 (m, 2H,  $\text{CH}_2\text{O}$ ), 6.95 (t, 1H,  $J = 7.5$  Hz, H6), 7.08 (ddt, 1H,  $J = 7.5, 1.9$  and 1.0 Hz, H5), 7.16 (ddd, 1H,  $J = 7.5, 4.9$  and 1.2 Hz, H5'), 7.58 (ddd, 1H,  $J = 7.6, 1.8$  and 0.9 Hz, H7), 7.66 (td, 1H,  $J = 7.7$  and 1.9 Hz, H4'), 7.81 (dt, 1H,  $J = 8.0$  and 1.1 Hz, H3'), 8.69 (ddd, 1H,  $J = 4.9, 1.9$  and 1.0 Hz, H6') ppm;  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )  $\delta$  22.3 ( $\text{CH}_2$ ,  $\text{CH}_2\text{CH}_2\text{O}$ ), 25.4 ( $\text{CH}_2$ ,  $\text{CH}_2(\text{CH}_2)_2\text{O}$ ), 66.8 ( $\text{CH}_2$ ,  $\text{CH}_2\text{O}$ ), 120.3 (CH, C6), 121.7 (CH, C5'), 122.8 (C, Cb), 125.3 (CH, C3'), 128.6 (C, C8), 129.1 (CH, C7), 130.6 (CH, C5), 135.7 (CH, C4'), 149.4 (CH, C6'), 152.6 (C, Ca), 156.5 (C, C2') ppm; HRMS (ESI; 90:10 MeOH- $\text{CH}_2\text{Cl}_2$ ),  $m/z$ : 234.0888 (1 ppm) found (calcd for  $\text{C}_{14}\text{H}_{13}\text{NNaO}$ ,  $[\text{M}+\text{Na}]^+$ , requires 234.08893). **Crystal data for 5e.**

C<sub>14</sub>H<sub>13</sub>NO, *M* = 211.25, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 7.9764(9), *b* = 12.8773(13), *c* = 10.5675(11) Å, β = 90.246(4)°, *V* = 1085.4(2) Å<sup>3</sup>, *Z* = 4, *d* = 1.293 g cm<sup>-3</sup>, μ = 0.082 mm<sup>-1</sup>. A final refinement on *F*<sup>2</sup> with 2482 unique intensities and 146 parameters converged at ω(*R*<sup>2</sup>) = 0.1023 (*R*/*F*) = 0.0400 for 2198 observed reflections with *I* > 2σ(*I*). CCDC 2352995.

**8-Benzoylchromane (5f).** The title product was prepared by adapting a reported procedure.<sup>15</sup> To a stirred solution of chromane (**2**; 0.13 mL, 1.0 mmol) and TMEDA (0.30 mL, 2.0 mmol) in hexane (3 mL) at rt, was added dropwise a 1.4 M solution of *n*BuLi in hexane (1.4 mL, 2.0 mmol). After 2 h at rt, the reaction mixture was cooled to -20 °C before addition of THF (3 mL) and ZnCl<sub>2</sub>:TMEDA (0.50 g, 2.0 mmol). The mixture was then warmed to rt before addition of *N*-(benzoyloxy)piperidine<sup>15</sup> (0.41 g, 2.0 mmol) and Cu(OAc)<sub>2</sub> (15 mg, 75 μmol). After 18 h at rt, water (5 mL) was added. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude, which was purified by chromatography over silica gel (eluent: 95:5 petroleum ether-AcOEt) to afford the title product (Rf 0.15) in 45% yield (0.11 g) as a beige solid: mp 144 °C, IR (ATR) ν 671, 690, 707 (s), 744, 768, 806, 829, 874, 927, 980, 1001, 1022, 1075, 1090, 1155, 1175, 1189, 1230 (s), 1285, 1315, 1381, 1431, 1450, 1471, 1595, 1660 (s), 2872, 2936, 3057 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 1.99 (tdd, 2H, *J* = 6.6, 5.1 and 4.1 Hz, CH<sub>2</sub>CH<sub>2</sub>O), 2.85 (t, 2H, *J* = 6.5 Hz, CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>O), 4.05-4.09 (m, 2H, CH<sub>2</sub>O), 6.90 (t, 1H, *J* = 7.5 Hz, H<sub>6</sub>), 7.16-7.18 (m, 2H, H<sub>5</sub> and H<sub>7</sub>), 7.42 (tt, 2H, *J* = 6.8 and 1.4 Hz, H<sub>3</sub>' and H<sub>5</sub>'), 7.51-7.57 (m, 1H, H<sub>4</sub>'), 7.82-7.86 (m, 2H, H<sub>2</sub>' and H<sub>6</sub>') ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 22.1 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 25.1 (CH<sub>2</sub>, CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>O), 66.6 (CH<sub>2</sub>, CH<sub>2</sub>O), 119.7 (CH, C<sub>6</sub>), 123.1 (C, C<sub>b</sub>), 127.5 (CH, C<sub>5</sub> or C<sub>7</sub>), 128.1 (C, C<sub>8</sub> or C<sub>1</sub>'), 128.2 (2CH, C<sub>3</sub>' and C<sub>5</sub>'), 129.9 (2CH, C<sub>2</sub>' and C<sub>6</sub>'), 132.2 (CH, C<sub>5</sub> or C<sub>7</sub>), 132.9 (CH, C<sub>4</sub>'), 138.0 (C, C<sub>1</sub>' or C<sub>8</sub>), 153.0 (C, C<sub>a</sub>), 196.6 (C, C=O) ppm; HRMS (ASAP; source at 60 °C), *m/z*: 239.1065 (1 ppm) found (calcd for C<sub>16</sub>H<sub>15</sub>O<sub>2</sub>, [M+H]<sup>+</sup>, requires 239.10665). **α-*n*-Butyl-α-phenyl-8-chromanemethanol (racemic mixture; 5'f)** was similarly obtained (Rf 0.3) in 31% yield (93 mg) as a grey solid: mp > 260 °C; IR (ATR) ν 701, 744, 767, 821, 878, 971, 1028 (s), 1053 (s) 1188, 1216, 1330, 1379, 1454, 1470, 1589, 2871, 2954, 3513 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 0.89 (t, 3H, *J* = 7.1 Hz, Me), 1.23-1.39 (m, 3H, CH<sub>2</sub>Me and CHCH<sub>2</sub>Me), 1.44-1.58 (m, 1H, CHHCH<sub>2</sub>Me), 1.78-2.10 (m, 3H, CH<sub>2</sub>CH<sub>2</sub>O and CHH-C(OH)), 2.20-2.30 (m, 1H, CHH-C(OH)), 2.67-2.83 (m, 2H, CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>O), 3.83-3.90 (m, 1H, CHHO), 4.07-4.14 (m, 1H, CHHO), 4.89 (t, 1H, *J* = 1.1 Hz, OH), 6.88 (t, 1H, *J* = 7.6 Hz, H<sub>6</sub>), 6.98 (ddt, 1H, *J* = 7.5, 1.8 and 0.9 Hz, H<sub>5</sub> or H<sub>7</sub>), 7.14-7.33 (m, 6H, H<sub>5</sub> or H<sub>7</sub>, H<sub>2</sub>', H<sub>3</sub>', H<sub>4</sub>', H<sub>5</sub>' and H<sub>6</sub>') ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 14.2 (CH<sub>3</sub>), 22.1 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 23.3 (CH<sub>2</sub>Me), 24.5 (CH<sub>2</sub>, CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>O), 26.1 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>Me), 41.7 (CH<sub>2</sub>, CH<sub>2</sub>-C(OH)), 66.4 (CH<sub>2</sub>, CH<sub>2</sub>O), 78.5 (C, C-OH), 119.9 (CH, C<sub>6</sub>), 123.2 (C, C<sub>b</sub>), 125.3 (CH, C<sub>5</sub> or C<sub>7</sub>), 125.6 (2CH, C<sub>3</sub>'/C<sub>5</sub>' or C<sub>2</sub>'/C<sub>6</sub>'), 126.1 (CH, C<sub>4</sub>'), 127.6 (2CH, C<sub>3</sub>'/C<sub>5</sub>' or C<sub>2</sub>'/C<sub>6</sub>'), 129.2 (CH, C<sub>5</sub> or C<sub>7</sub>), 134.0 (C, C<sub>8</sub>), 148.6 (C, C<sub>1</sub>'), 152.7 (C, C<sub>a</sub>) ppm; HRMS (ESI; 90:10 MeOH-CH<sub>2</sub>Cl<sub>2</sub>), *m/z*: 319.1668 (0 ppm) found (calcd for C<sub>20</sub>H<sub>24</sub>O<sub>2</sub>Na, [M+Na]<sup>+</sup>, requires 319.16685).

**Typical procedure for the deprotometallation of chromane (2) using lithium dialkylamides in THF followed by interception with iodomethane.** To a stirred solution of diethylamine (0.23 mL, 2.3 mmol) in THF (3.5 mL) at -15 °C were successively added a 1.3 M solution of *n*BuLi in hexane (1.8 mL, 2.2 mmol) and, 5 min later, chromane (**2**; 0.13 mL, 1.0 mmol). After 1 h at this temperature, Mel (0.14 mL, 2.2 mmol) was added dropwise, and the mixture was stirred for 2 h before addition of aqueous 2 M HCl until pH < 6. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude for which the **2.5a:6a** ratio was determined by <sup>1</sup>H NMR. Similar procedures were employed in the case of LiTMP.

**Typical procedure for the deprotometallation of chromane (2) using LiTMP in THF containing tBuOK.** To a stirred solution of *t*BuOK (0.67 g, 5.0 mmol) and H-TMP (0.90 mL, 5.0 mmol) in THF (6 mL) at -70°C, was added dropwise a 1.3 M solution of *n*BuLi in hexane (3.6 mL, 4.8 mmol). After 5 min at -50 °C, chromane (**2**; 0.25 mL, 2.0 mmol) was added, and the mixture was stirred at this temperature for 1 h. The mixture was next cooled to -70 °C before the electrophile (either pure for liquids, or in THF for solids) was introduced, and the mixture was stirred for 1 h before addition of saturated aqueous NH<sub>4</sub>Cl (10 mL). Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude which was purified by column chromatography over silica gel.

**4-Methylchromane (racemic mixture; 6a).** The title product was prepared according to the typical procedure using Mel (0.30 mL, 4.8 mmol) as the electrophile. Purification (eluent: 95:5 petroleum ether-AcOEt) afforded the title product (Rf 0.7) in 71% yield (0.25 g) as a pale yellow oil: IR (ATR) ν 709, 750 (s), 816, 852, 879, 890, 935, 966, 989, 1007, 1049, 1059, 1096, 1118, 1223 (s), 1253, 1268, 1308, 1376, 1447, 1488 (s), 1580, 1608, 1713, 2874, 2960 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 1.34 (d, 3H, *J* = 7.0 Hz, Me), 1.73 (dtd, 1H, *J* = 13.9, 6.5 and 3.7 Hz, CHHCH<sub>2</sub>O), 2.04-2.14 (m, 1H, CHHCH<sub>2</sub>O), 2.96 (hex, 1H, *J* = 6.6 Hz, CHMe), 4.19 (ddd, 2H, *J* = 6.5, 6.1 and 3.6 Hz, CH<sub>2</sub>O), 6.79 (dd, 1H, *J* = 8.1 and 1.2 Hz, H<sub>8</sub>), 6.86 (td, 1H, *J* = 7.4 and 1.3 Hz, H<sub>6</sub>), 7.08 (dddd, 1H, *J* = 8.0, 7.3, 1.7 and 0.6 Hz, H<sub>7</sub>), 7.16 (ddd, 1H, *J* = 7.6, 1.4 and 0.9 Hz, H<sub>5</sub>) ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 22.3 (CH<sub>3</sub>), 28.6 (CH, CHMe), 30.4 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 64.0 (CH<sub>2</sub>, CH<sub>2</sub>O), 116.8 (CH, C<sub>8</sub>), 120.3 (CH, C<sub>6</sub>), 127.3 (CH, C<sub>7</sub>), 127.8 (C, C<sub>b</sub>), 128.8 (CH, C<sub>5</sub>), 154.5 (C, C<sub>a</sub>) ppm. These data are as reported previously.<sup>16</sup>

**(4-Anisyl)(4-chromanyl)methanol (mixture of stereoisomers; 6b).** The title product was prepared according to the typical procedure, but from 1.0 mmol of **2** (0.13 mL), using 4-anisaldehyde (0.29 mL, 2.4 mmol) as the electrophile. Purification (eluent: 75:25 petroleum ether-AcOEt) afforded the title product (Rf 0.4) in 65% yield (0.18 g) as an orange oil: IR (ATR) ν 727 (s), 755, 831, 907, 1033, 1079, 1118, 1173, 1222, 1246 (s), 1303, 1452, 1489, 1510, 1581, 1609, 1682, 2250, 2930, 3445 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.66 (dq, 1H, *J* = 14.3 and 3.3 Hz, CH<sub>2</sub>CH<sub>2</sub>O), 1.72-1.80 (m, 1H, CH<sub>2</sub>CH<sub>2</sub>O), 1.88 (dddd, 1H, *J* = 14.3, 11.5, 5.8 and 4.5 Hz, CH<sub>2</sub>CH<sub>2</sub>O), 2.23 (dtd, 1H, *J* = 14.3, 5.7 and 3.1 Hz, CH<sub>2</sub>CH<sub>2</sub>O), 3.09 (q, 2H, *J* = 5.7 Hz, CH(CH<sub>2</sub>)<sub>2</sub>O), 3.82 (s, 3H, OMe), 3.83 (s, 3H, OMe), 4.00 (td, 1H, *J* = 11.3 and 2.8 Hz, CH<sub>2</sub>O), 4.09-4.15 (m, 2H, CH<sub>2</sub>O), 4.32 (ddd, 1H, *J* = 10.9, 9.3 and 3.1 Hz, CH<sub>2</sub>O), 4.72 (d, 1H, *J* = 8.2 Hz, CH(OH)), 5.09 (d, 1H, *J* = 5.6 Hz, CH(OH)), 6.78 (td, 1H, *J* = 7.4 and 1.3 Hz, H<sub>6</sub>), 6.83-6.93 (m, 8H, H<sub>5</sub>, H<sub>6</sub>, H<sub>8</sub>, H<sub>3</sub>' and H<sub>5</sub>'), 7.12 (ddd, 1H, *J* = 8.4, 6.9 and 1.7 Hz, H<sub>7</sub>), 7.18 (ddd, 1H, *J* = 8.5, 7.2 and 1.7 Hz, H<sub>7</sub>), 7.24-7.27 (m, 4H, H<sub>2</sub>', H<sub>2</sub>', H<sub>6</sub>', H<sub>6</sub>'), 7.39 (dd, 1H, *J* = 7.8 and 1.7 Hz, H<sub>5</sub>) ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 22.4 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 24.4 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 40.8 (CH-CH(OH)), 41.3 (CH-CH(OH)), 55.4 (CH<sub>3</sub>, OMe), 63.2 (CH<sub>2</sub>, CH<sub>2</sub>O), 64.3 (CH<sub>2</sub>, CH<sub>2</sub>O), 75.5 (CH(OH)), 77.2 (CH(OH)), 113.7 (2CH, C<sub>3</sub>' and C<sub>5</sub>'), 114.0 (2CH, C<sub>3</sub>' and C<sub>5</sub>'), 117.1 (CH, C<sub>8</sub>), 117.2 (CH, C<sub>8</sub>), 120.0 (CH, C<sub>6</sub>), 120.1 (CH, C<sub>6</sub>), 122.1 (C, C<sub>b</sub>), 122.6 (C, C<sub>b</sub>), 127.6 (2CH, C<sub>2</sub>' and C<sub>6</sub>'), 128.0 (2CH, C<sub>2</sub>' and C<sub>6</sub>'), 128.1 (CH, C<sub>7</sub>), 128.3 (CH, C<sub>7</sub>), 129.4 (CH, C<sub>5</sub>), 131.4 (CH, C<sub>5</sub>), 134.3 (C, C<sub>1</sub>'), 134.4 (C, C<sub>1</sub>'), 154.8 (C, C<sub>a</sub>), 155.8 (C, C<sub>a</sub>), 159.1 (C, C<sub>4</sub>'), 159.4 (C, C<sub>4</sub>') ppm; HRMS (ESI; 90:10 MeOH-CH<sub>2</sub>Cl<sub>2</sub>), *m/z*: 293.1148 (0 ppm) found (calcd for C<sub>17</sub>H<sub>18</sub>O<sub>3</sub>Na, [M+Na]<sup>+</sup>, requires 293.11481).

**4-Chromanecarboxaldehyde (racemic mixture; 6c).** The title product was prepared according to the typical procedure, but from 1.0 mmol of **2** (0.13 mL), using *N,N*-dimethylformamide (DMF; 0.19 mL, 2.4 mmol) as the electrophile. Purification (eluent: 94:6 petroleum

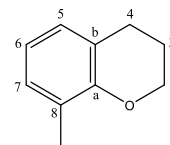
ether-Et<sub>2</sub>O) afforded the title product (Rf 0.15) in 22% yield (35 mg) as a pale yellow oil: IR (ATR)  $\nu$  670, 754 (s), 817, 869, 925, 975, 1019, 1037, 1061, 1094, 1118, 1148, 1186, 1216, 1254, 1299, 1327, 1382, 1402, 1456, 1467, 1478, 1489, 1580, 1604, 1684, 2884, 3426 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  2.04-2.15 (m, 1H, CHHCH<sub>2</sub>O), 2.43 (dddd, 1H, *J* = 14.0, 5.1, 4.3 and 2.7 Hz, CHHCH<sub>2</sub>O), 3.60 (t, 1H, *J* = 5.4 Hz, CHCHO), 4.00 (ddd, 1H, *J* = 11.2, 10.0 and 2.7 Hz, CHHO), 4.23 (dddd, 1H, *J* = 11.2, 4.9, 3.6 and 1.1 Hz, CHHO), 6.89 (d, 1H, *J* = 8.2 Hz, H8), 6.96 (ddd, 1H, *J* = 8.3, 7.5 and 1.3 Hz, H7), 7.17-7.24 (m, 2H, H5 and H6), 9.74 (t, 1H, *J* = 1.2 Hz, CHO) ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  21.9 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 47.2 (CH, CHCHO), 63.9 (CH<sub>2</sub>, CH<sub>2</sub>O), 117.8 (CH, C8), 121.1 (CH, C6), 129.0 (CH, C7), 130.0 (CH, C5), 155.5 (C, Ca), 200.4 (CH, CHO) ppm (Cb not seen). These data are as reported previously.<sup>17</sup> 4-Chromanone was similarly isolated in 19% yield.

**4-Chromanecarboxylic acid (racemic mixture; 6d).** The title product was prepared according to the typical procedure, but from 5.0 mmol of **2** (0.63 mL), using gaseous CO<sub>2</sub> in excess as the electrophile. In this case, after addition of water (10 mL) and washing using AcOEt (3 x 10 mL), the aqueous phase was acidified by addition of aqueous 2 M HCl until pH 1. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the tautomeric form **6d'** of the expected product: Rf (eluent: 70:30 petroleum ether-Et<sub>2</sub>O) 0.0; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  2.58-2.62 (m, 2H, CH<sub>2</sub>CH<sub>2</sub>O), 4.22-4.25 (m, 2H, CH<sub>2</sub>O), 6.85 (dd, 1H, *J* = 8.3 and 1.3 Hz, H8), 6.93 (ddd, 1H, *J* = 7.9, 7.2 and 1.3 Hz, H6), 7.23 (ddd, 1H, *J* = 8.2, 7.2 and 1.6 Hz, H7), 7.47 (dd, 1H, *J* = 7.9 and 1.6 Hz, H5), 8.16 (br s, 2H, OH) ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  29.9 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 54.5 (C, C=C(OH)<sub>2</sub>), 63.1 (CH<sub>2</sub>, CH<sub>2</sub>O), 116.6 (C, Cb), 117.8 (CH, C8), 120.7 (CH, C6), 130.1 (CH, C7), 131.1 (CH, C5), 154.7 (C, Ca), 175.9 (C, C(OH)<sub>2</sub>) ppm). However, after a few days, the title product (acid form) was obtained in 77% yield (0.69 g) as a yellow oil: IR (ATR)  $\nu$  690, 711, 747, 809, 849, 929, 1018, 1054, 1115, 1224, 1259, 1402, 1453, 1489, 1583, 1609, 1699, 2610, 2954 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  2.09 (dddd, 1H, *J* = 13.8, 9.7, 6.1 and 3.6 Hz, CHHCH<sub>2</sub>O), 2.29 (dtd, 1H, *J* = 13.9, 5.0 and 2.8 Hz, CHHCH<sub>2</sub>O), 3.71 (t, 1H, *J* = 5.3 Hz, CHCO<sub>2</sub>H), 4.14-4.20 (m, 1H, CHHO), 4.30 (ddd, 1H, *J* = 10.8, 9.8 and 2.8 Hz, CHHO), 6.77 (dd, 1H, *J* = 8.2 and 1.3 Hz, H8), 6.80 (td, 1H, *J* = 7.5 and 1.3 Hz, H6), 7.07 (ddd, 1H, *J* = 8.6, 7.4 and 1.7 Hz, H7), 7.26 (dd, 1H, *J* = 7.8 and 1.7 Hz, H5), 8.93 (br s, 1H, CO<sub>2</sub>H) ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  24.8 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 39.6 (CH, CHCO<sub>2</sub>H), 63.6 (CH<sub>2</sub>, CH<sub>2</sub>O), 117.5 (CH, C8), 117.8 (C, Cb), 120.6 (CH, C6), 128.9 (CH, C7), 130.6 (CH, C5), 154.7 (C, Ca), 179.6 (C, CO<sub>2</sub>H) ppm. These data are as reported previously.<sup>18</sup>

**4-(Trimethylsilyl)chromane (racemic mixture; 6e).** The title product was prepared according to the typical procedure, but from 1.0 mmol of **2** (0.13 mL) using ClSiMe<sub>3</sub> (0.31 mL, 2.4 mmol) as the electrophile. Purification (eluent: 98:2 petroleum ether-AcOEt) afforded the title product (Rf 0.7) in 87% yield (0.18 g) as a yellow oil: IR (ATR)  $\nu$  689, 749 (s), 831 (s), 880, 940, 1012, 1030, 1050, 1072, 1115, 1151, 1221 (s), 1248, 1267, 1300, 1338, 1450, 1486, 1578, 1604, 1699 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  0.06 (s, 9H, SiMe<sub>3</sub>), 2.01 (dtd, 1H, *J* = 13.8, 4.9 and 3.8 Hz, CHHCH<sub>2</sub>O), 2.18 (dddd, 1H, *J* = 14.2, 7.9, 6.5 and 4.9 Hz, CHHCH<sub>2</sub>O), 2.33 (dd, 1H, *J* = 6.5 and 5.0 Hz, CHSiMe<sub>3</sub>), 4.13-4.17 (m, 2H, CH<sub>2</sub>O), 6.77-6.83 (m, 2H, H6 and H8), 6.96-7.04 (m, 2H, H5 and H7) ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  -1.7 (CH<sub>3</sub>, SiMe<sub>3</sub>), 24.5 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 25.2 (CH, CHSiMe<sub>3</sub>), 65.6 (CH<sub>2</sub>, CH<sub>2</sub>O), 117.0 (CH, C8), 120.1 (CH, C6), 125.2 (C, Cb), 125.9 (CH, C7), 128.9 (CH, C5), 154.3 (C, Ca) ppm; HRMS (ASAP; source at 40 °C), *m/z* 207.1199 (0 ppm) found (calcd for C<sub>12</sub>H<sub>19</sub>OSi, [M+H]<sup>+</sup>, requires 207.11997).

**Unsuccessful attempt to prepare 4-(2-pyridyl)chromane.** To a stirred solution of *t*BuOK (0.33 g, 2.5 mmol) and H-TMP (0.45 mL, 2.5 mmol) in THF (3.5 mL) at -70 °C, was added dropwise a 1.4 M solution of *n*BuLi in hexane (1.7 mL, 2.4 mmol). After 5 min at -50 °C, chromane (**2**; 0.13 mL, 1.0 mmol) and, 1 h later, ZnCl<sub>2</sub>-TMEDA (0.61 g, 2.4 mmol) were introduced, and the mixture was slowly (1 h) warmed to -20 °C under stirring. To the stirred mixture were next added PdCl<sub>2</sub> (14 mg, 80  $\mu$ mol), 1,1'-bis(diphenylphosphino)ferrocene (dppf; 44 mg, 80  $\mu$ mol) and 2-chloropyridine (0.23 mL, 2.4 mmol) at -20 °C, and the mixture was heated at 80 °C for 8 h. After filtration over Celite®, water (5 mL) was added. Extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure led to the crude (complex mixture). Purification by column chromatography over silica gel (eluent: 95:5 petroleum ether-AcOEt) furnished (Rf 0.6) **racemic 4,4'-bichromane** as a white solid in 18% yield (24 mg): IR (ATR)  $\nu$  707, 749 (s), 806, 861, 889, 920, 1012, 1064, 1119, 1213 (s), 1255, 1276, 1445, 1487 (s), 1578, 1603, 2879, 2952 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  1.68-1.86 (m, 4H, CH<sub>2</sub>CH<sub>2</sub>O), 3.60 (quint, 2H, *J* = 6.2 Hz, H4 and H4'), 4.04 (ddd, 2H, *J* = 11.0, 8.8 and 3.7 Hz, CHHO), 4.24 (ddd, 2H, *J* = 11.0, 5.0 and 4.0 Hz, CHHO), 6.83-6.90 (m, 4H, H6/6' and H8/8'), 7.09-7.15 (m, 4H, H5/5' and H7/7') ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  23.7 (2CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 36.8 (2CH, C4 and C4'), 65.6 (2CH<sub>2</sub>, CH<sub>2</sub>O), 117.3 (2CH, C8/8'), 120.6 (2CH, C6/6'), 124.0 (2C, Cb and Cb'), 127.6 (2CH, C7/7'), 128.1 (2CH, C5/5'), 156.1 (Ca and Ca') ppm. **Crystal data for racemic 4,4'-bichromane.** C<sub>18</sub>H<sub>18</sub>O<sub>2</sub>, *M* = 266.32, monoclinic, *P* 2<sub>1</sub>, *a* = 8.9424(7), *b* = 17.3271(13), *c* = 9.0928(6) Å,  $\beta$  = 95.118(3) °, *V* = 1403.27(18) Å<sup>3</sup>, *Z* = 4, *d* = 1.261 g cm<sup>-3</sup>,  $\mu$  = 0.081 mm<sup>-1</sup>. A final refinement on *F*<sup>2</sup> with 6183 unique intensities and 361 parameters converged at  $\omega R(F^2)$  = 0.1261 (*R*(*F*) = 0.0492) for 5719 observed reflections with *I* > 2 $\sigma$ (*I*). CCDC 2352996. **Meso 4,4'-bichromane** was similarly isolated (Rf 0.5) as a beige solid in 9% yield (12 mg) and identified by NMR: <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  1.95-2.13 (m, 4H, CH<sub>2</sub>CH<sub>2</sub>O), 3.42 (t, 2H, *J* = 5.8 Hz, H4 and H4'), 4.16 (ddd, 2H, *J* = 10.9, 7.9 and 3.9 Hz, CHHO), 4.30 (ddd, 2H, *J* = 10.9, 6.1 and 4.1 Hz, CHHO), 6.79 (td, 2H, *J* = 7.7 and 1.3 Hz, H6/6'), 6.83 (dd, 2H, *J* = 8.3 and 1.4 Hz, H8/8'), 6.96 (dd, 2H, *J* = 7.7 and 1.6 Hz, H5/5'), 7.08-7.14 (m, 2H, H7/7') ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  26.2 (2CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 37.4 (2CH, C4 and C4'), 65.1 (2CH<sub>2</sub>, CH<sub>2</sub>O), 117.4 (2CH, C8/8'), 120.5 (2CH, C6/6'), 124.6 (2C, Cb and Cb'), 127.8 (2CH, C7/7'), 129.1 (2CH, C5/5'), 155.5 (Ca and Ca') ppm.

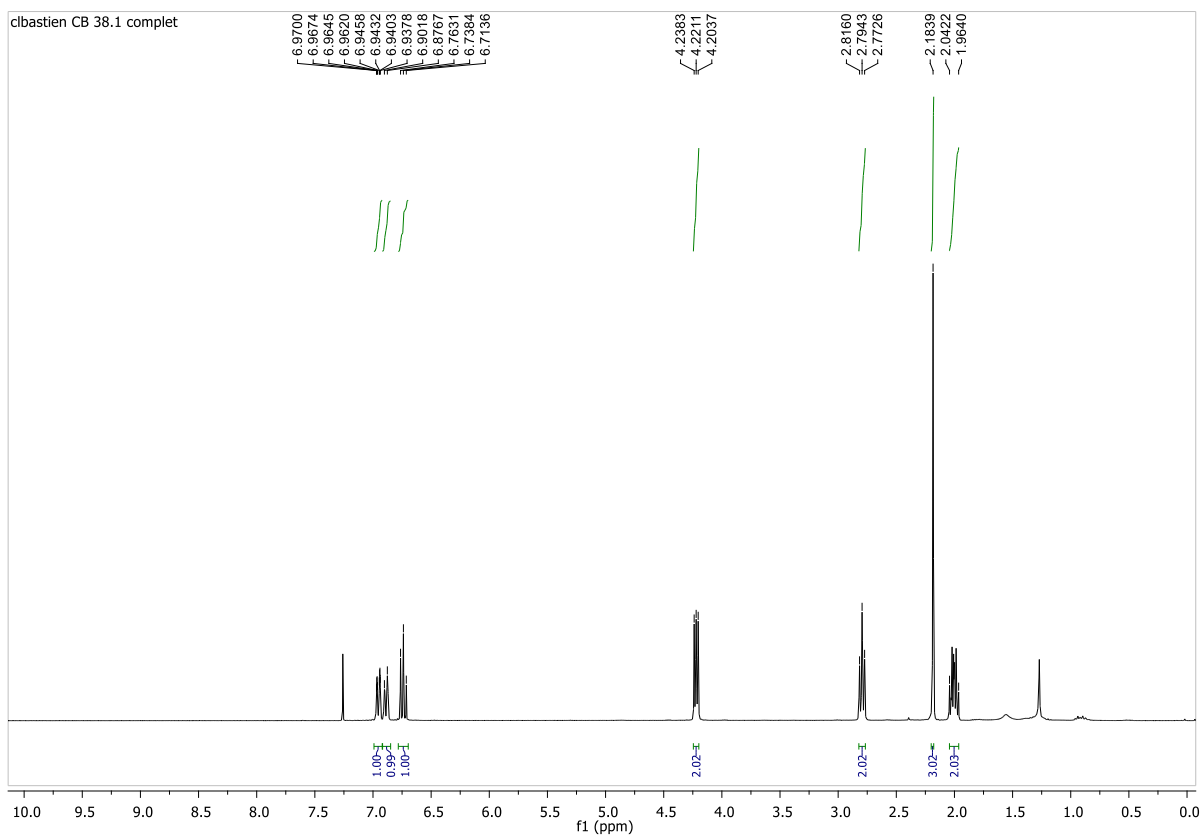
**8-(*N*-Piperidino)chromane (7).** The title product was prepared by adapting a reported procedure.<sup>19</sup> To a stirred solution of 8-iodochromane (**5d**; 0.63 g, 2.4 mmol) in toluene (4 mL) were added piperidine (0.35 mL, 3.6 mmol) and, 2 min later, *t*BuONa (0.35 g, 3.6 mmol), tris(dibenzylideneacetone)dipalladium(0) (Pd<sub>2</sub>(dba)<sub>3</sub>; 48 mg, 53  $\mu$ mol) and 4,5-bis(diphenylphosphino)-9,9-dimethylxanthene (Xantphos; 0.145 g, 0.25 mmol). The mixture was then heated to 100 °C and stirred at this temperature for 12 h. After cooling, water (4 mL) was added before extraction using AcOEt (3 x 10 mL), drying over MgSO<sub>4</sub> and concentration under reduced pressure. Purification by column chromatography over silica gel (eluent: 95:5 petroleum ether-AcOEt) afforded the title product (Rf 0.3) in 47% yield (0.25 g) as a red oil: IR (ATR)  $\nu$  679, 730 (s), 769, 817, 860, 870, 885, 909, 978 (s), 1018, 1034, 1049, 1082, 1095, 1118, 1141, 1153, 1193, 1213 (s), 1241, 1249, 1273, 1300, 1340, 1384, 1450, 1460, 1477, 1581, 2224, 2750, 2801, 2851, 2931 cm<sup>-1</sup>; <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  1.52-1.60 (m, 2H, H4'), 1.76 (p, 4H, *J* = 5.9 Hz, H3' and H5'), 1.96-2.04 (m, 2H, CH<sub>2</sub>CH<sub>2</sub>O), 2.79 (t, 2H, *J* = 6.5 Hz, CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>O), 2.94-2.98 (m, 4H, H2' and H6'), 4.24-4.28 (m, 2H, CH<sub>2</sub>O), 6.69-6.72 (m, 1H, H5), 6.75-6.79 (m, 2H, H6 and H7) ppm; <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)  $\delta$  22.1 (CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>O), 24.3 (CH<sub>2</sub>, C4'), 25.1 (CH<sub>2</sub>, CH<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>O), 26.2 (2CH<sub>2</sub>, C3' and C5'), 52.3 (2CH<sub>2</sub>, C2' and C6'), 66.4 (CH<sub>2</sub>, CH<sub>2</sub>O), 116.0 (CH, C6 or C7), 119.7 (CH, C6 or C7), 122.3 (C, Cb), 123.5 (CH, C5), 142.1 (C8), 147.6 (Ca) ppm; HRMS (ASAP; source at 50 °C), *m/z*: 218.1541 (1 ppm) found (calcd for C<sub>14</sub>H<sub>20</sub>NO, [M+H]<sup>+</sup>, requires 218.15394).



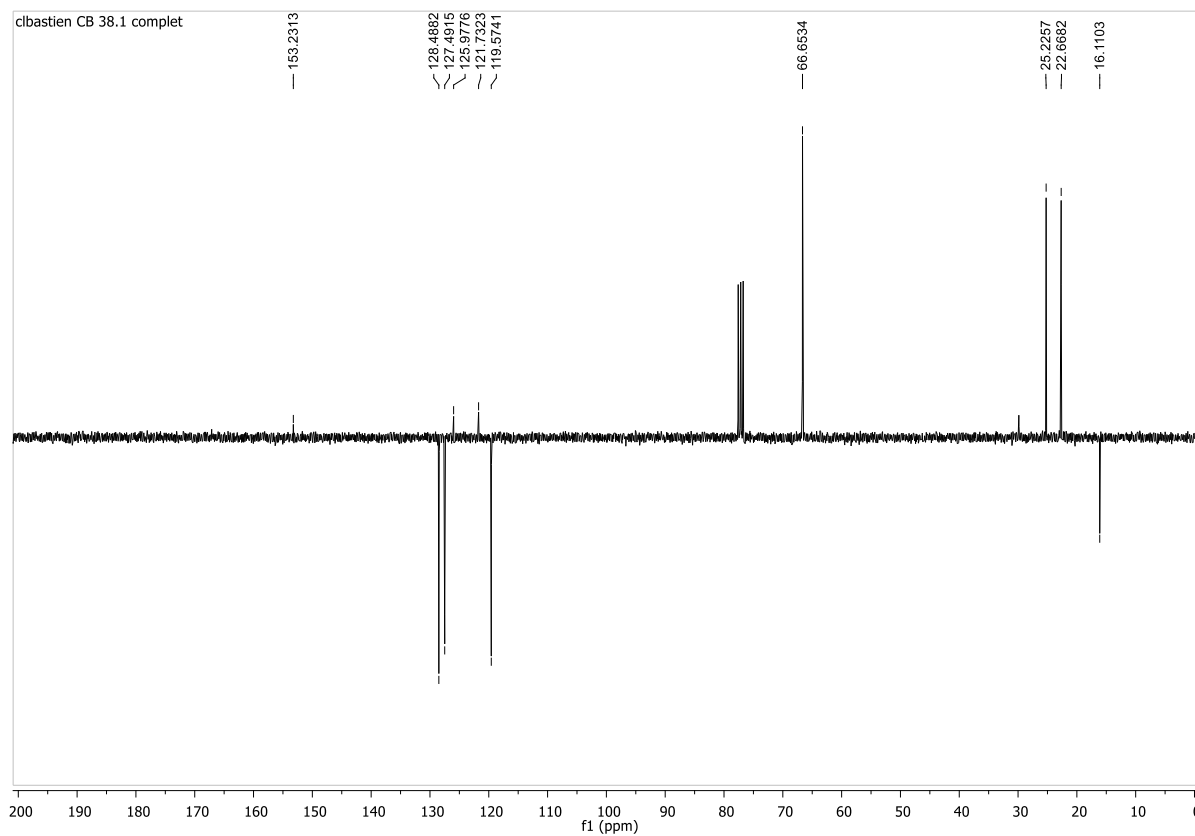
## NMR Spectra

### 8-Methylchromane (5a)

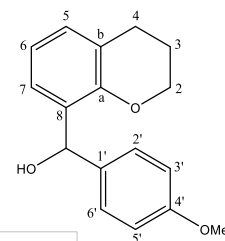
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



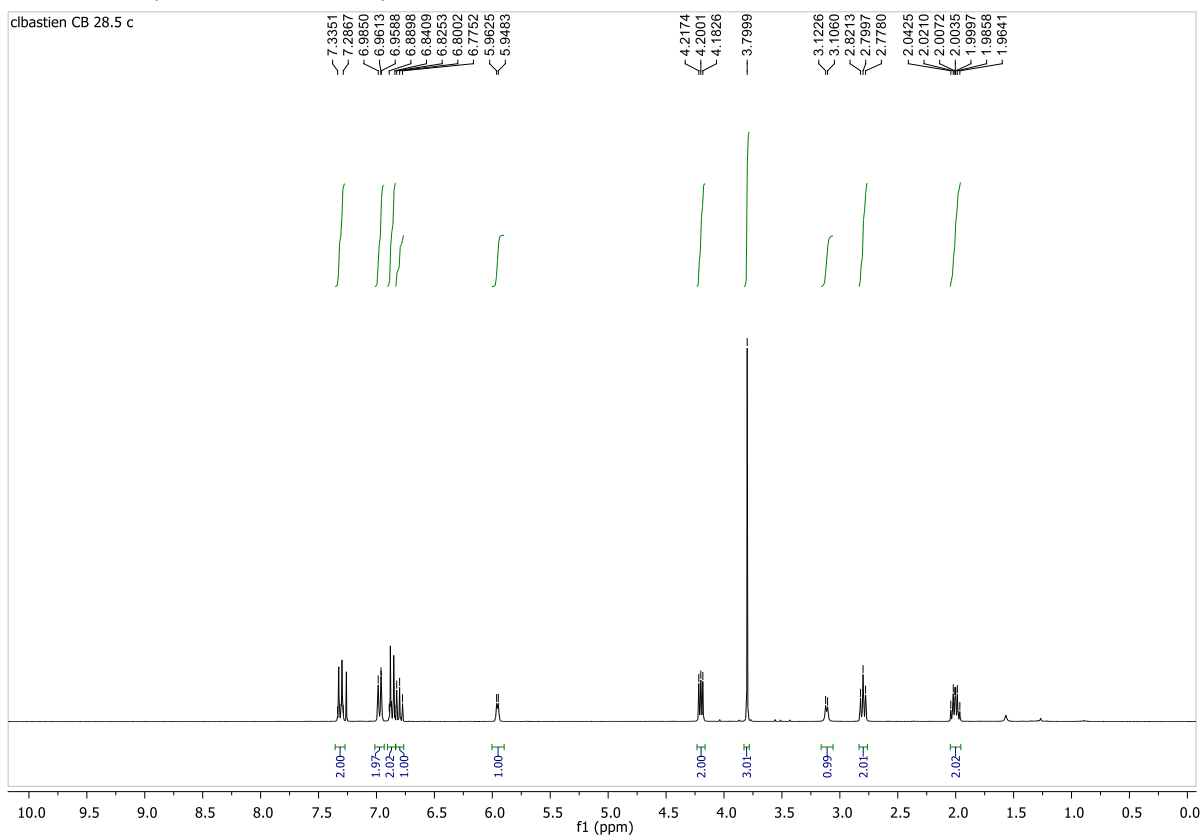
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



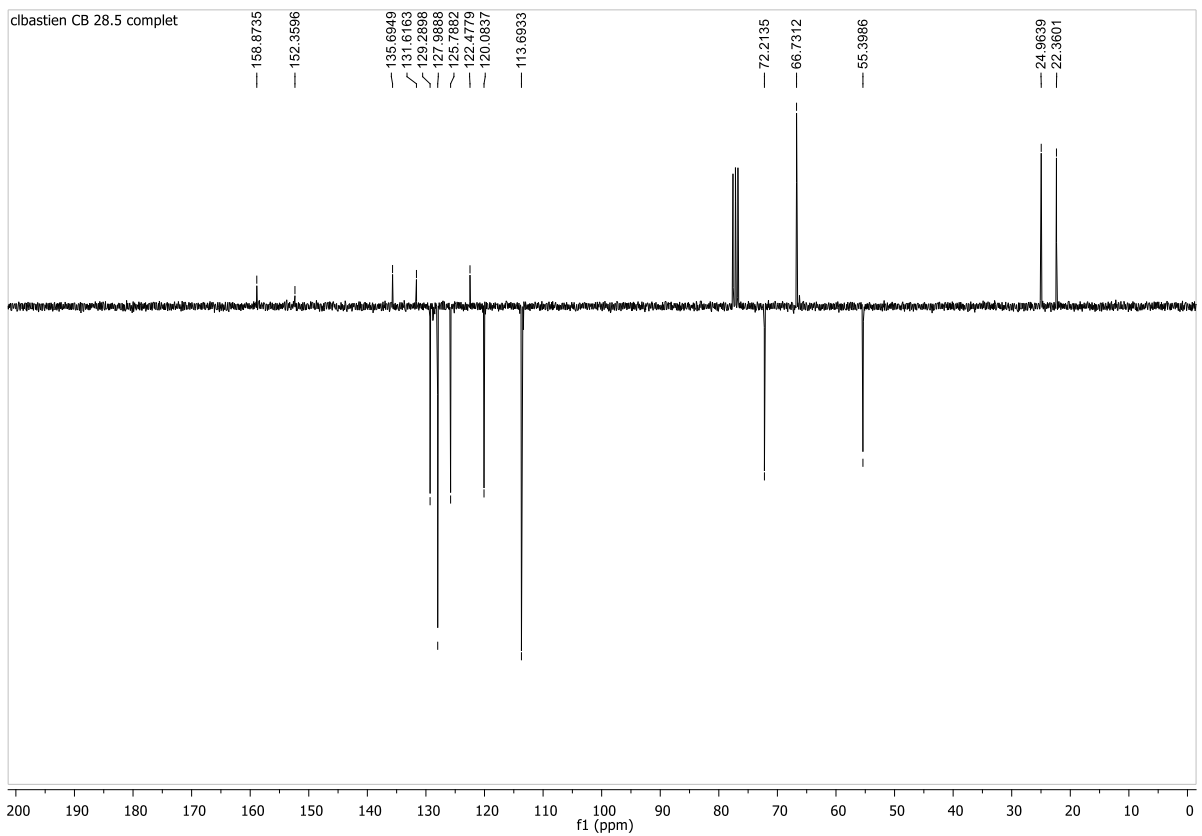
(4-Anisyl)(8-chromanyl)methanol (racemic mixture; 5b)



<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

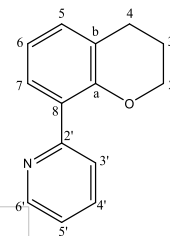


<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

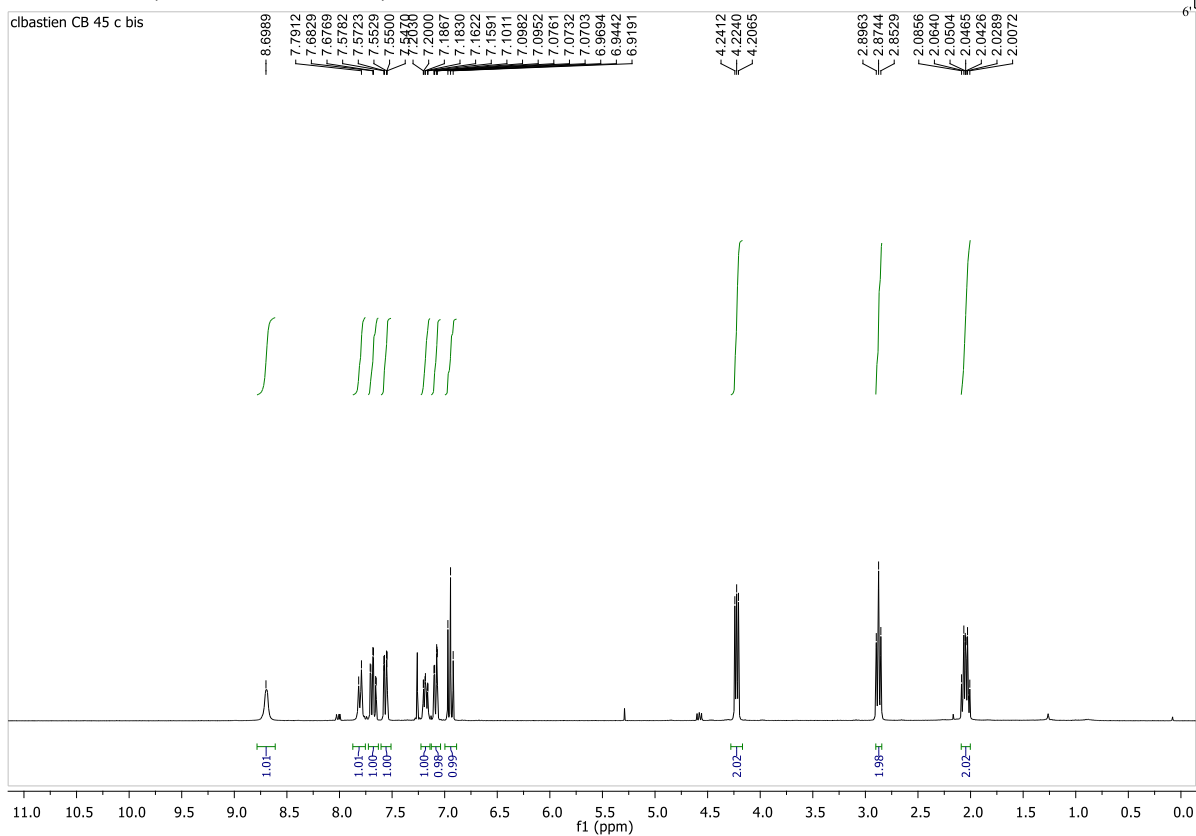




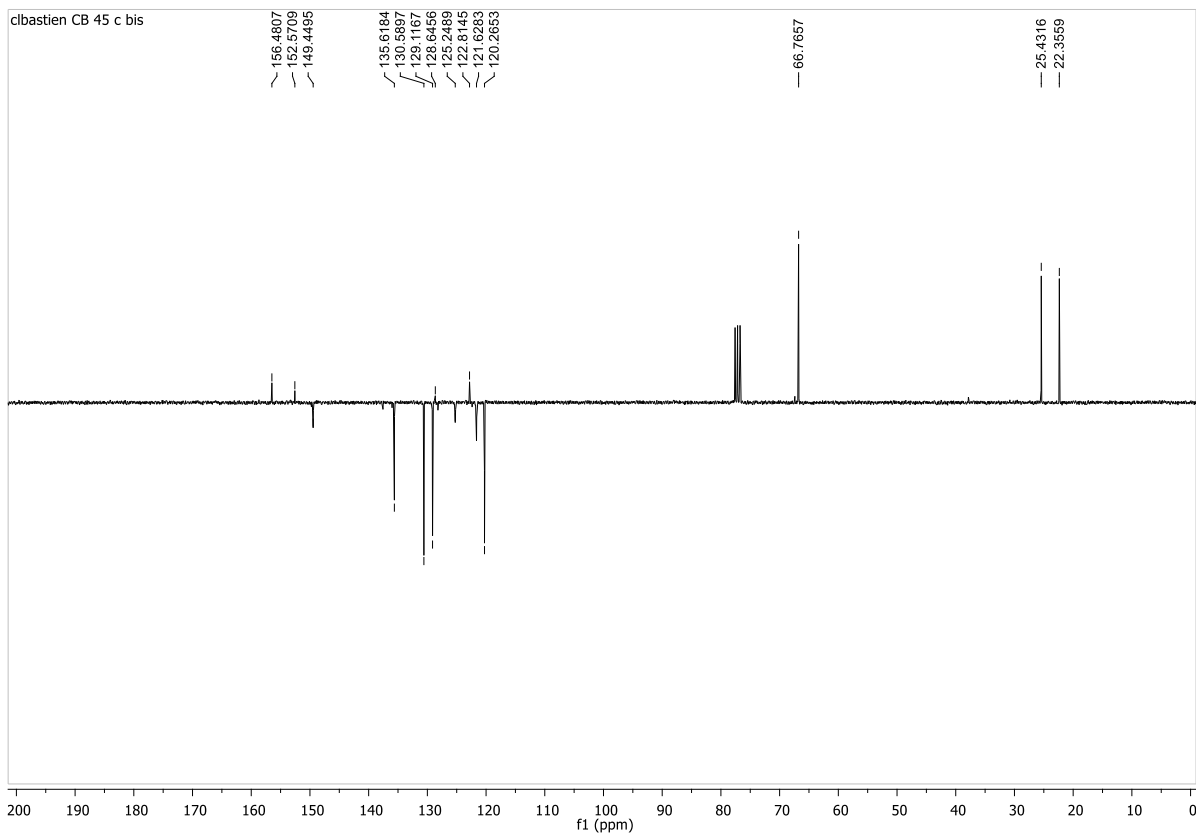
# 8-(2-Pyridyl)chromane (5e)



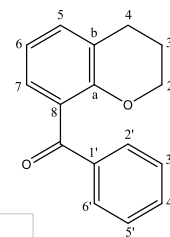
## <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



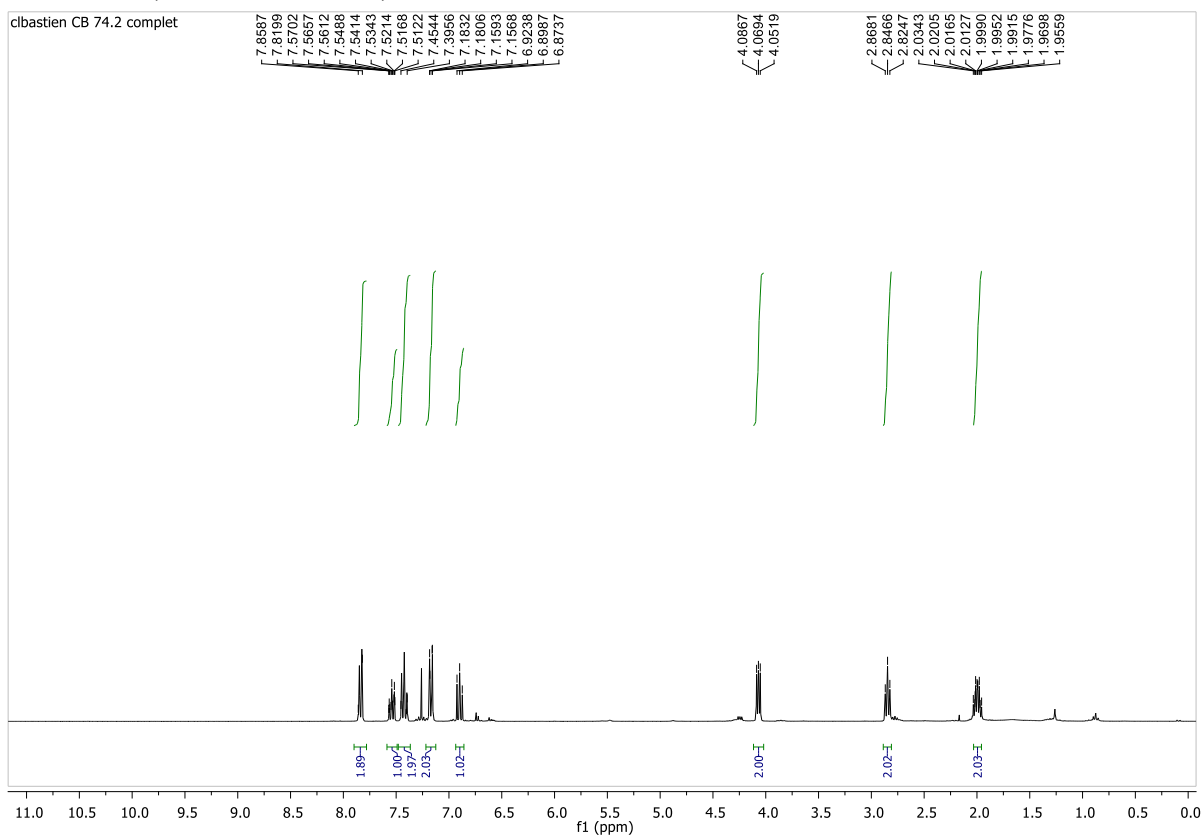
## <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



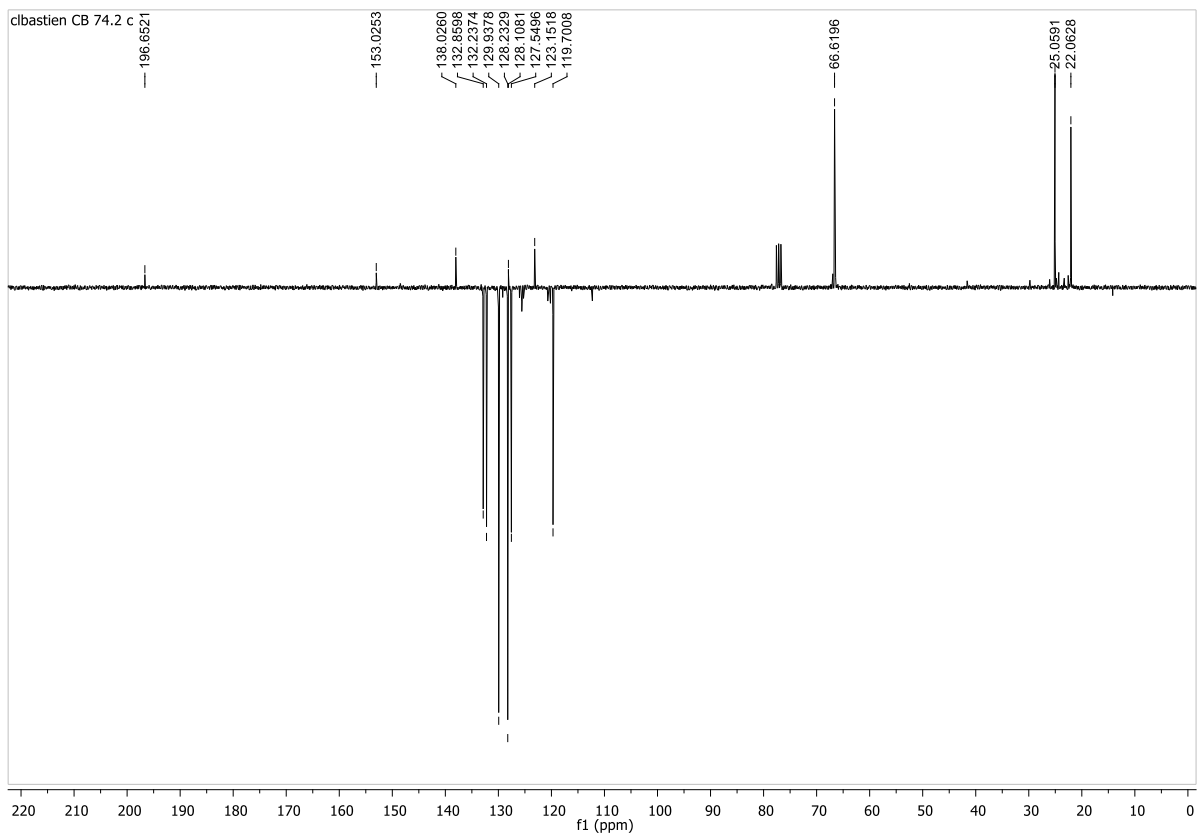
# 8-Benzoylchromane (5f)



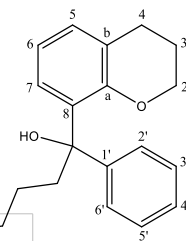
## <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



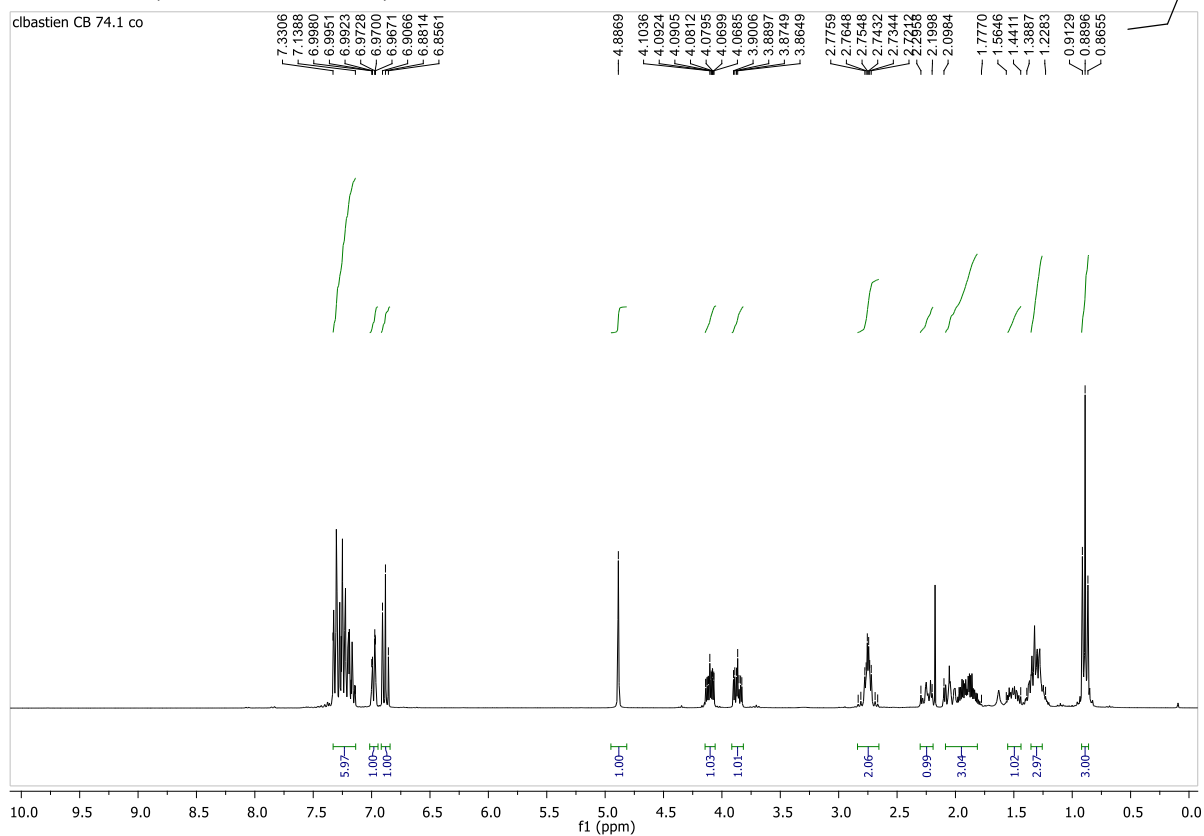
## <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



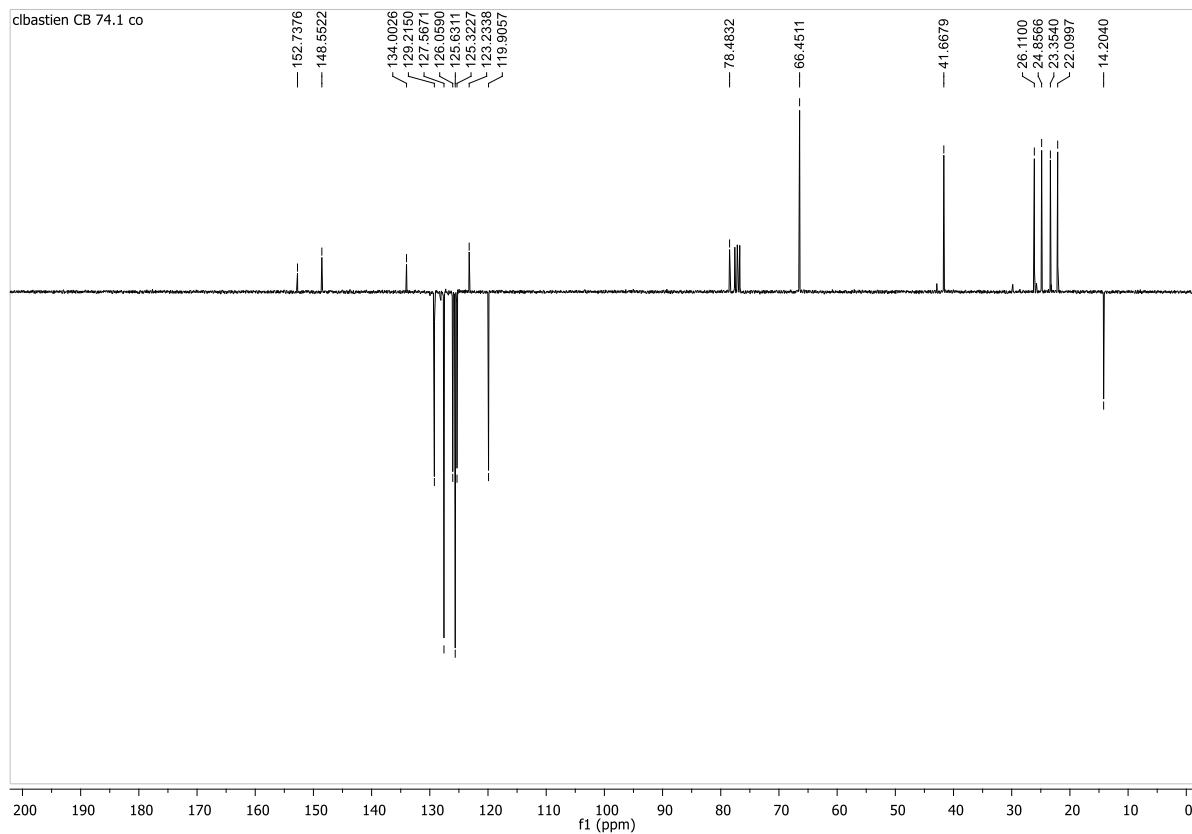
$\alpha$ -*n*-Butyl- $\alpha$ -phenyl-8-chromanemethanol (racemic mixture; 5'f)

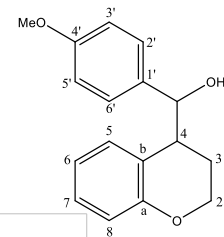


$^1\text{H NMR}$  (300 MHz,  $\text{CDCl}_3$ )



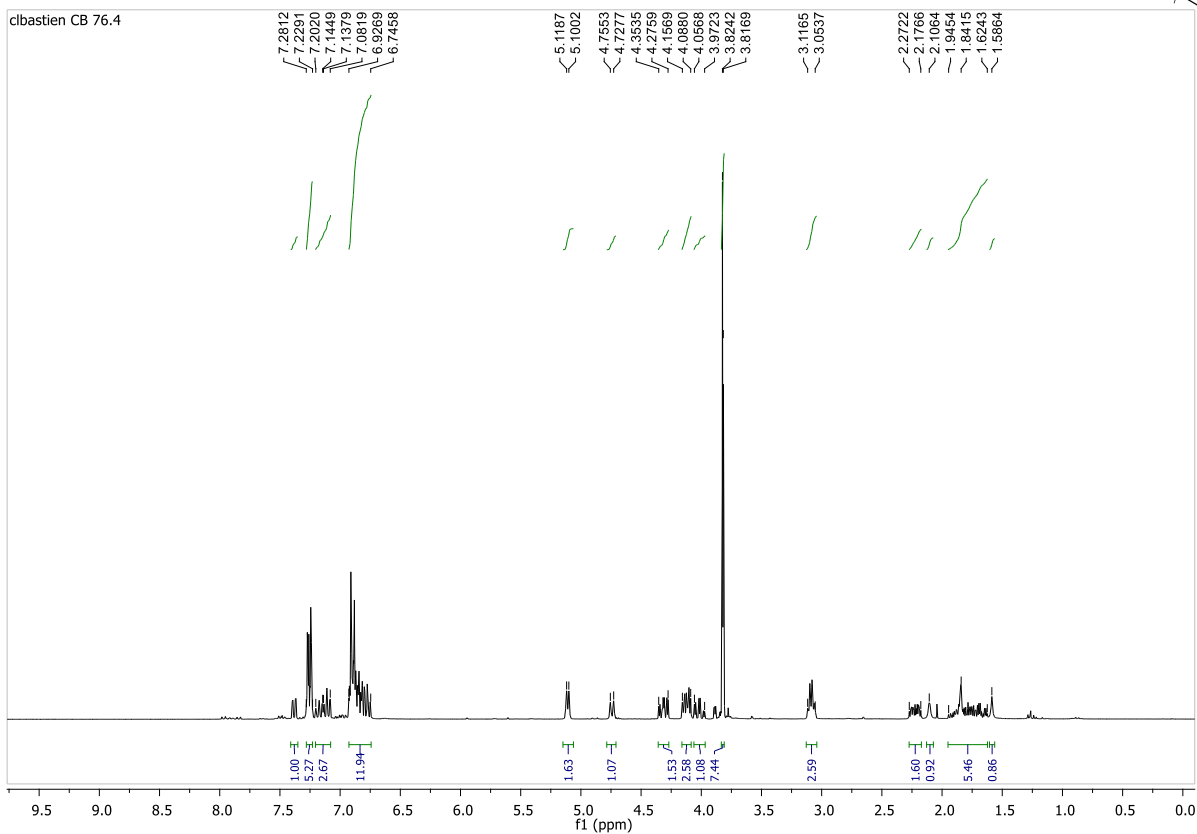
$^{13}\text{C NMR}$  (75 MHz,  $\text{CDCl}_3$ )



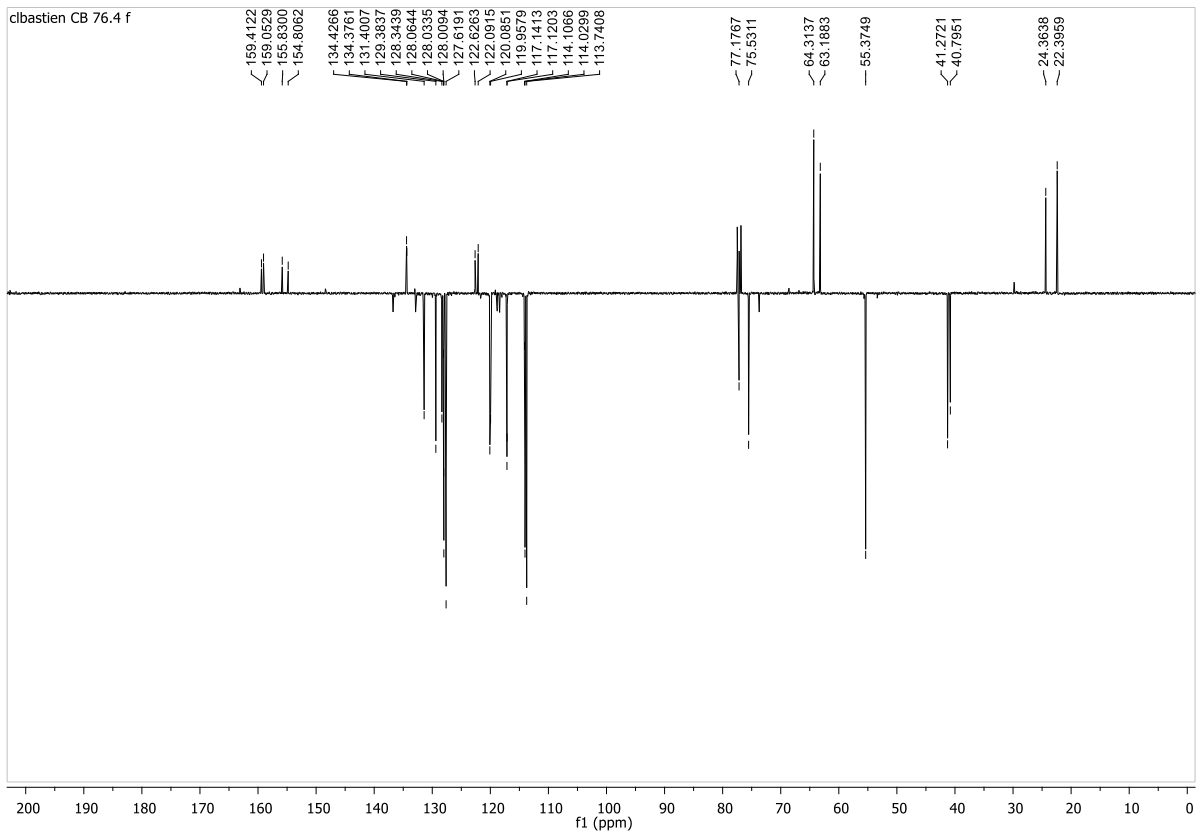


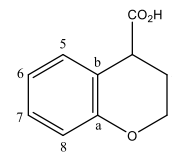
**(4-Anisyl)(4-chromanyl)methanol (mixture of stereoisomers; 6b)**

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)



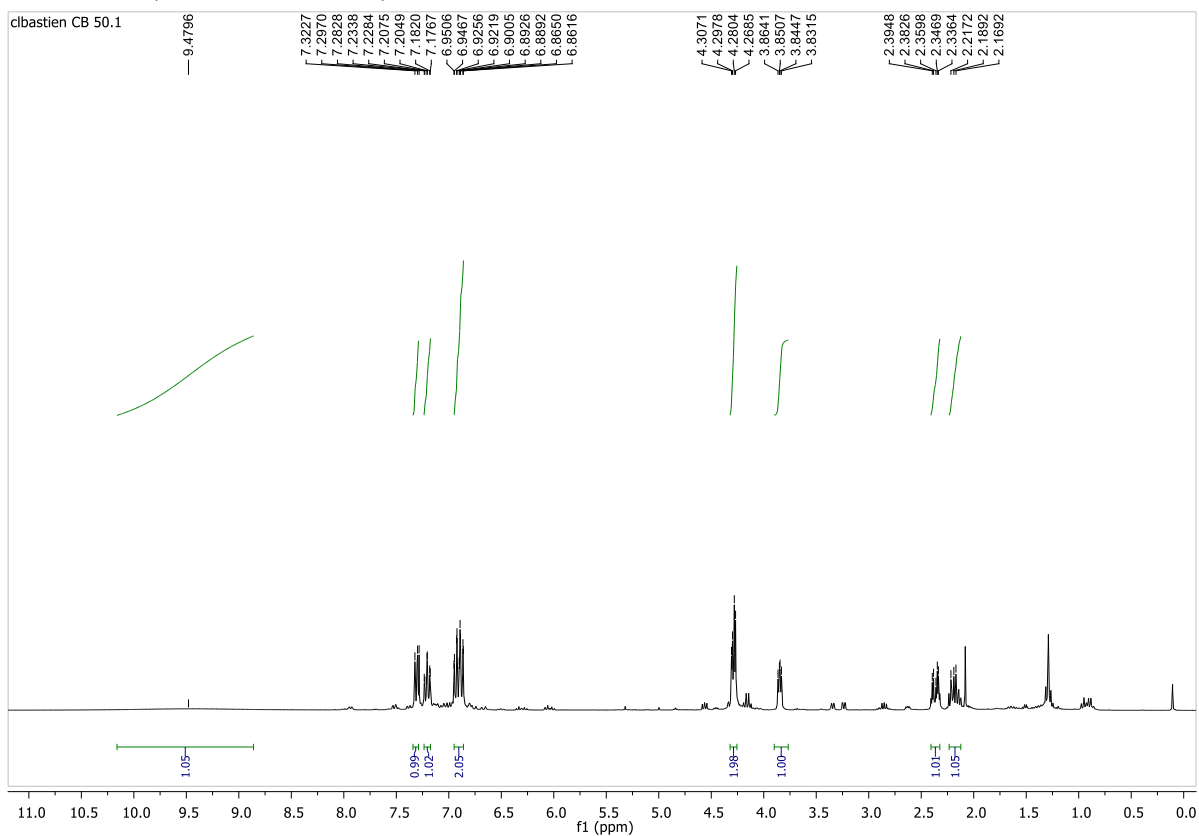
<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)



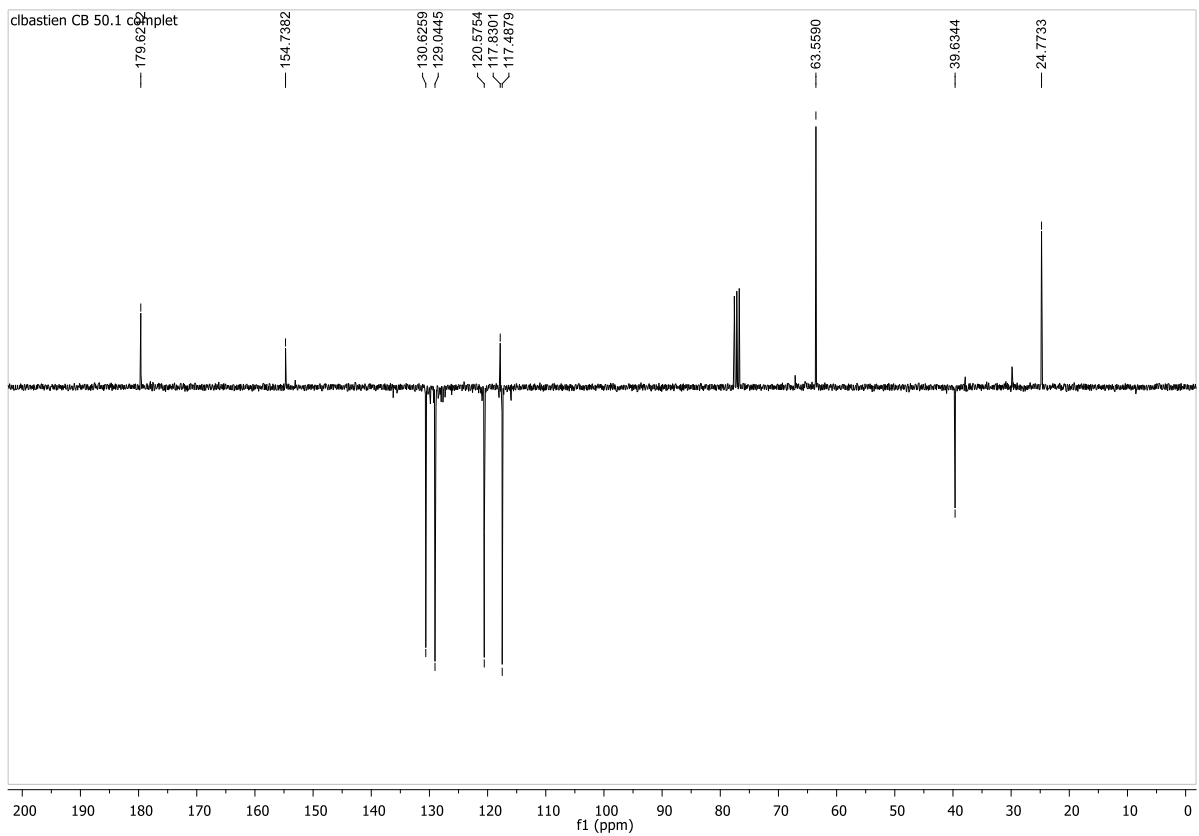


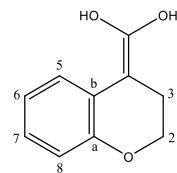
#### 4-Chromanecarboxylic acid (racemic mixture; 6d)

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ )



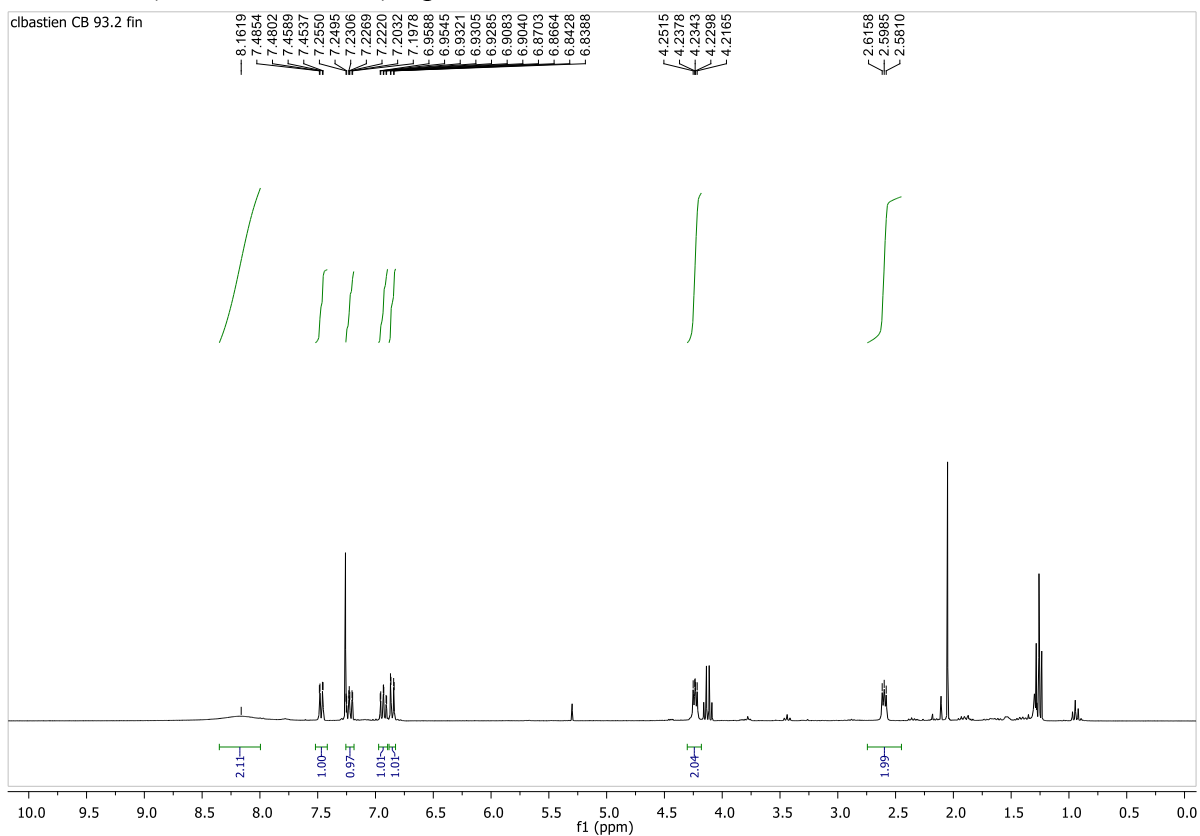
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



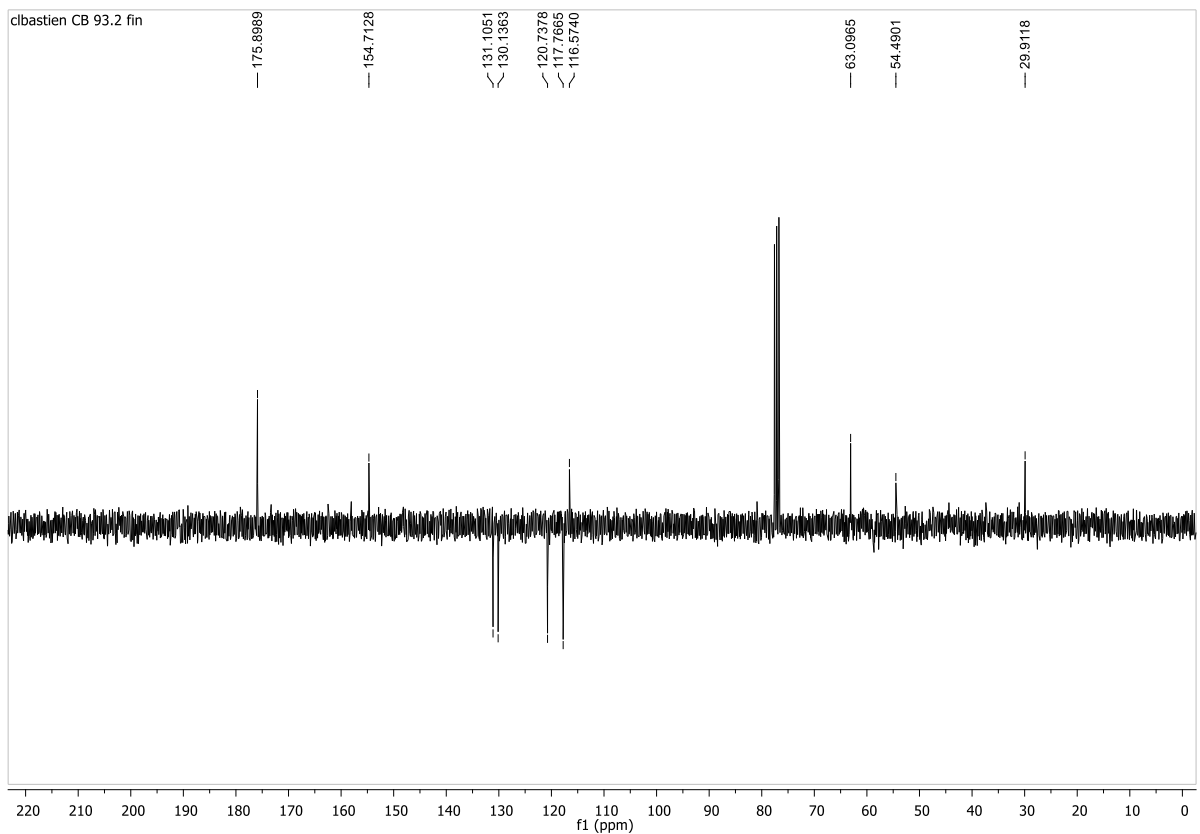


Tautomer form of 4-chromanecarboxylic acid (6d')

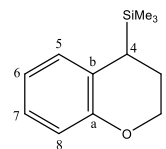
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) – presence of AcOEt



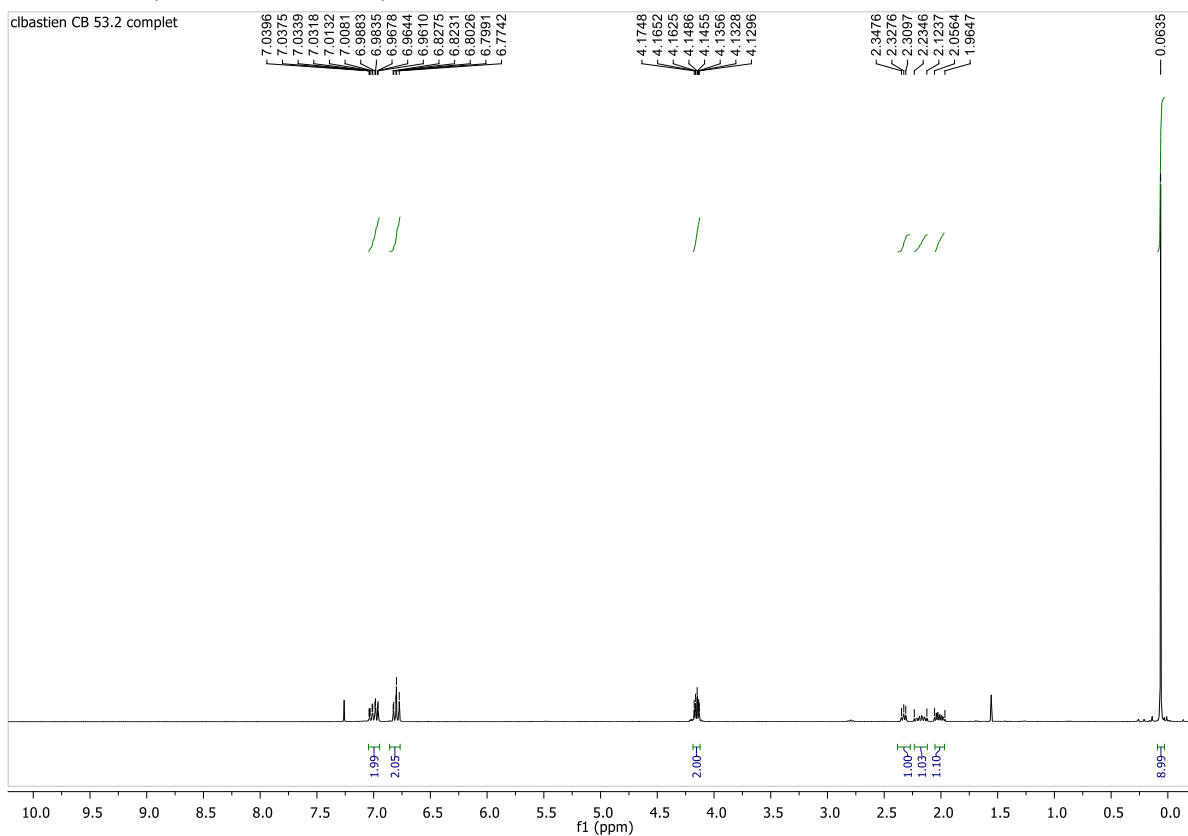
$^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ )



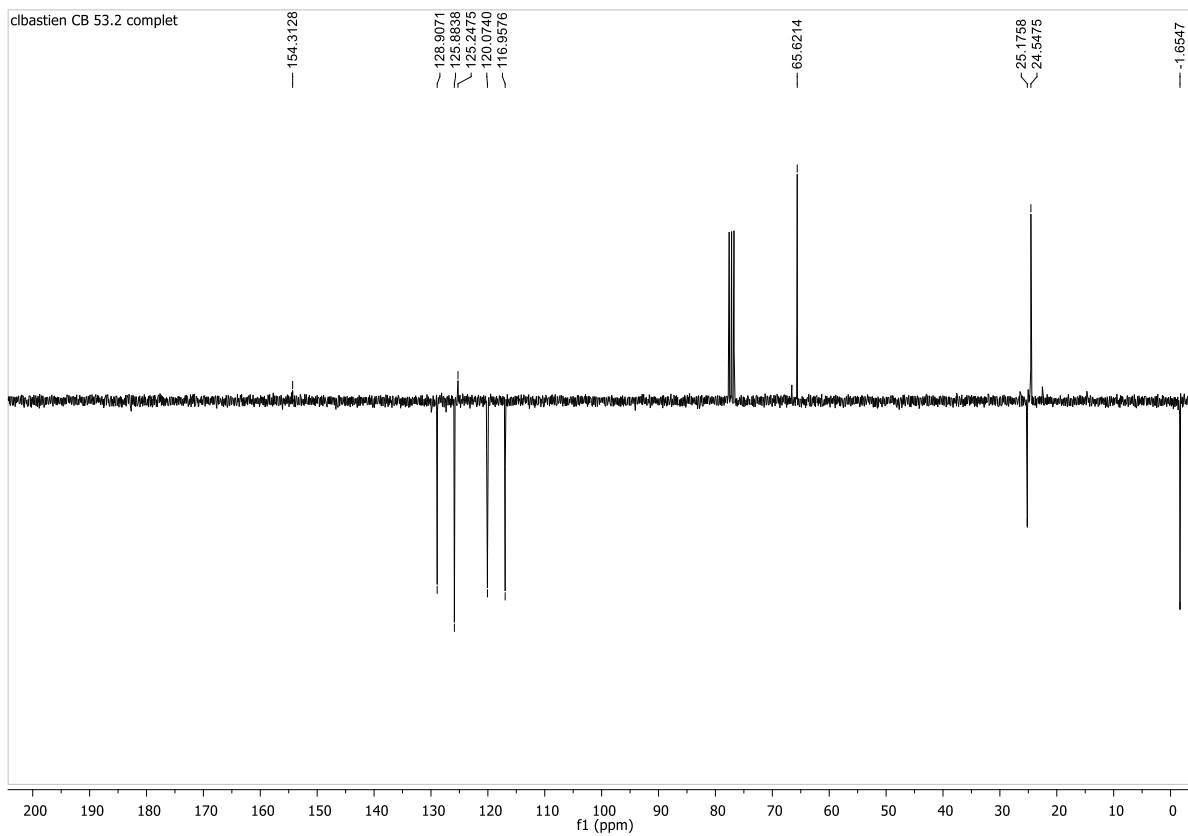
### 4-(Trimethylsilyl)chromane (racemic mixture; 6e)



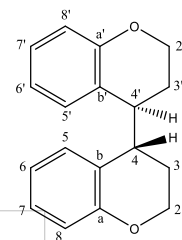
### $^1\text{H NMR}$ (300 MHz, $\text{CDCl}_3$ )



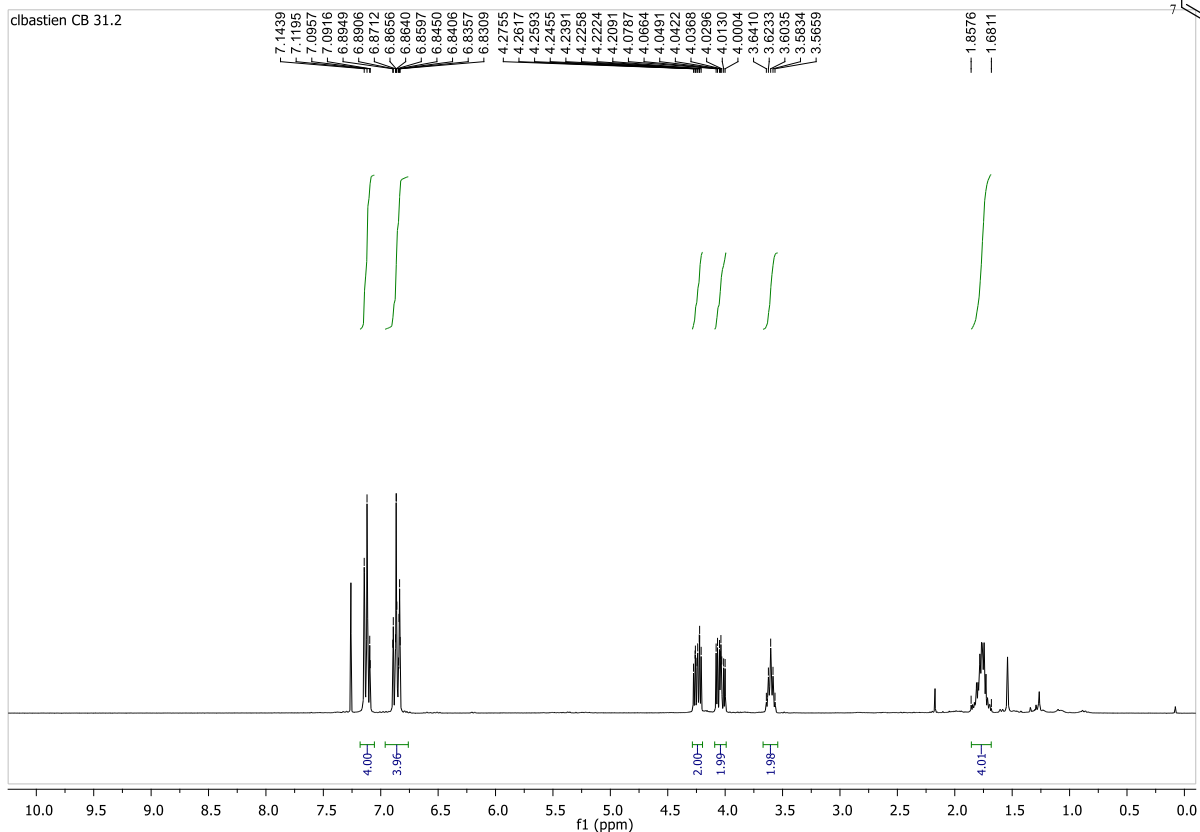
### $^{13}\text{C NMR}$ (75 MHz, $\text{CDCl}_3$ )



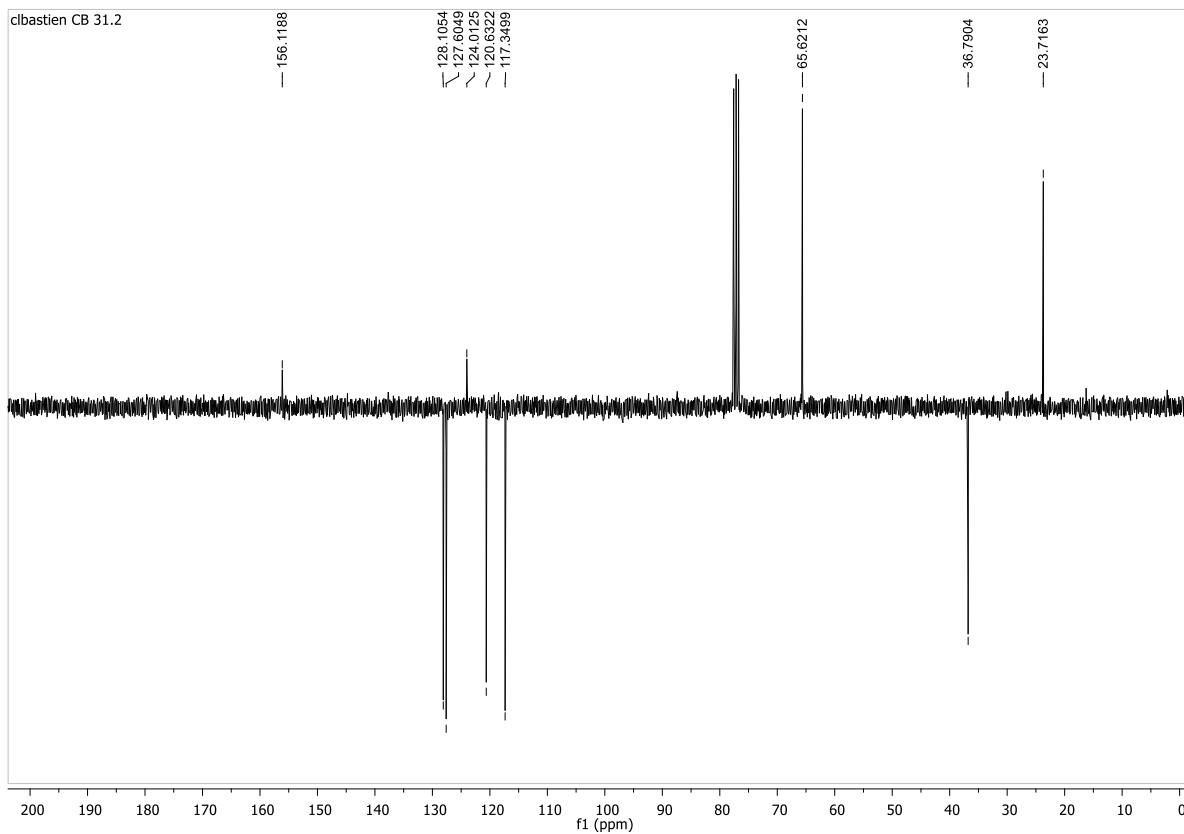
**racemic-4,4'-Bichromane**



**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)**

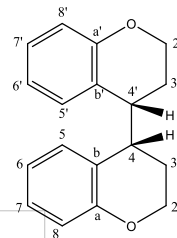


**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**

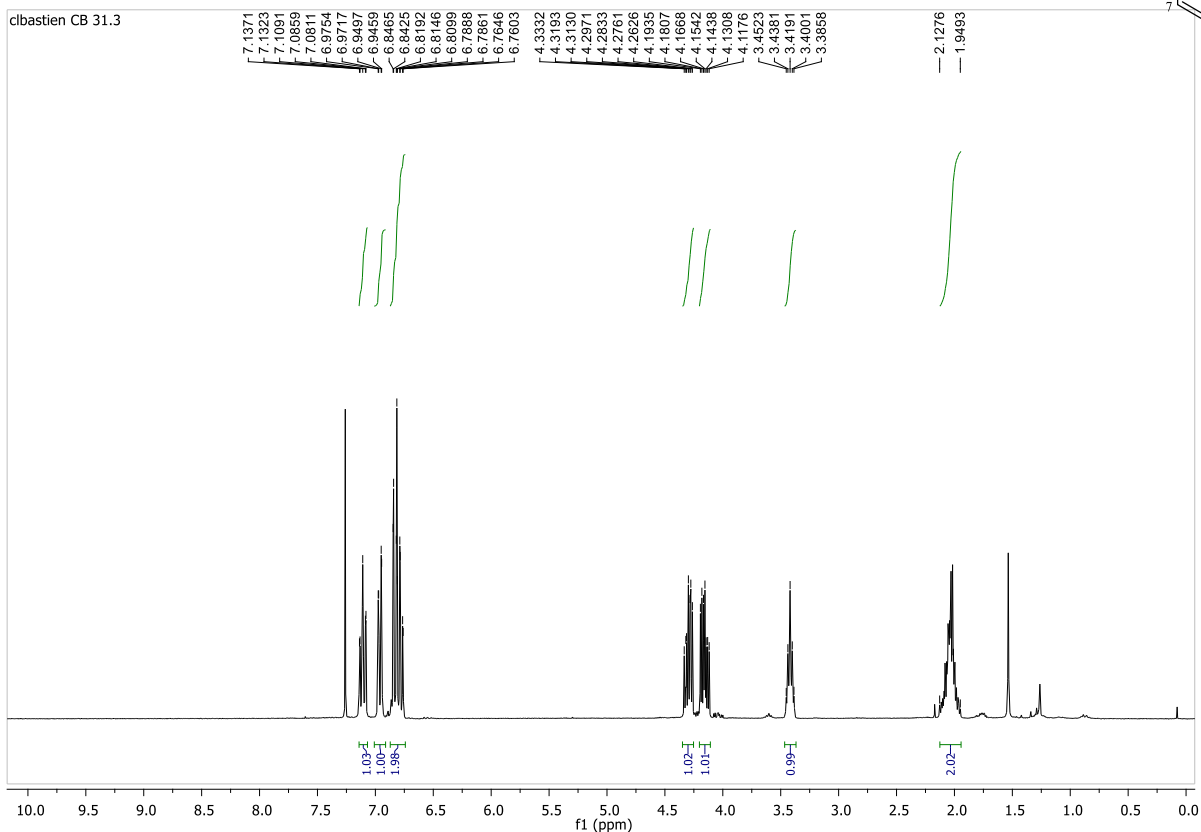




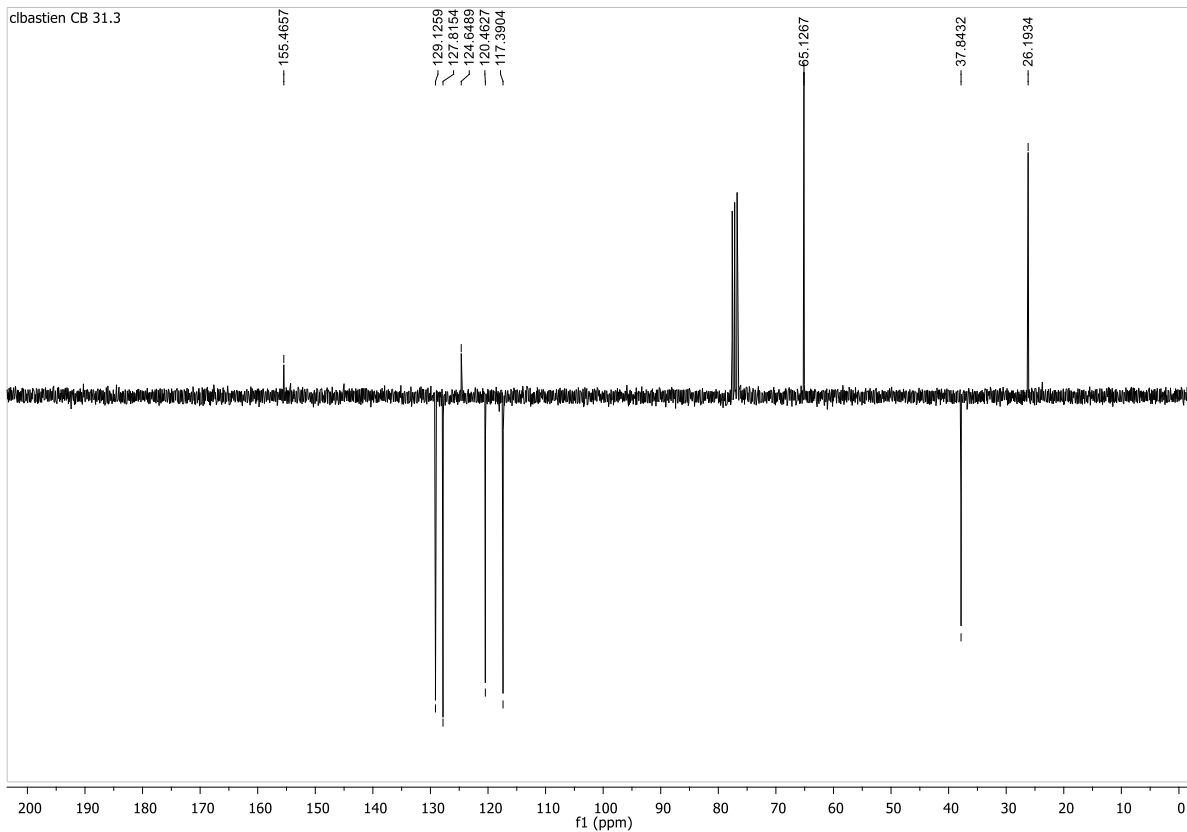
**meso-4,4'-Bichromane**



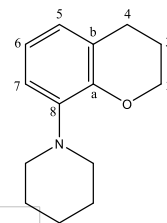
**<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)**



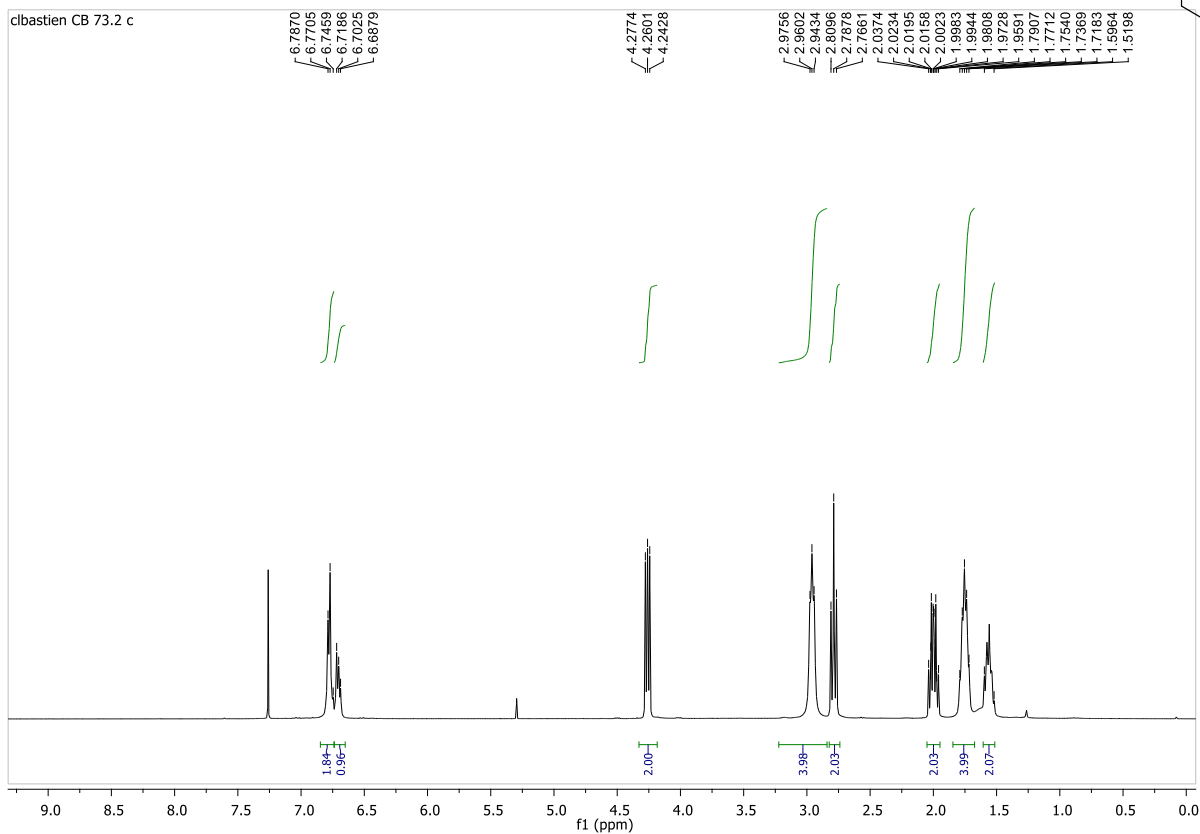
**<sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)**



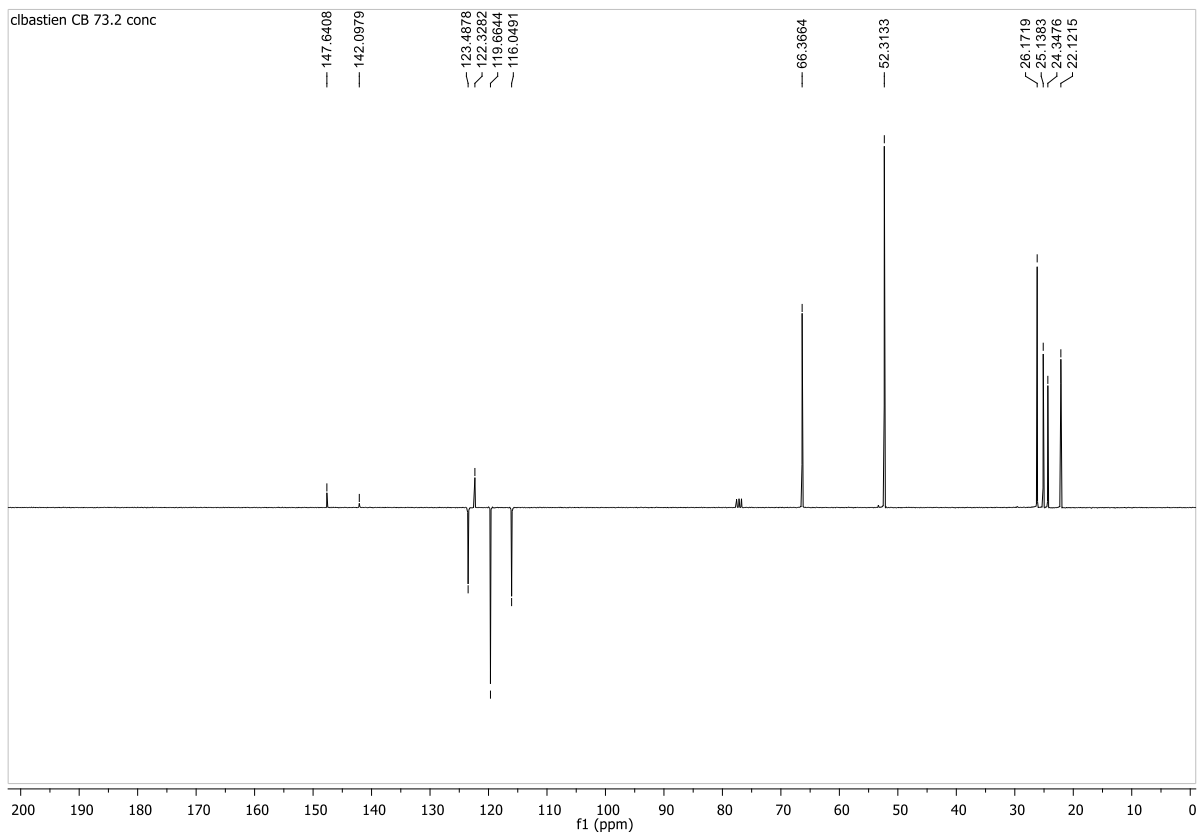
# 8-(N-Piperidino)chromane (7)



## <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)

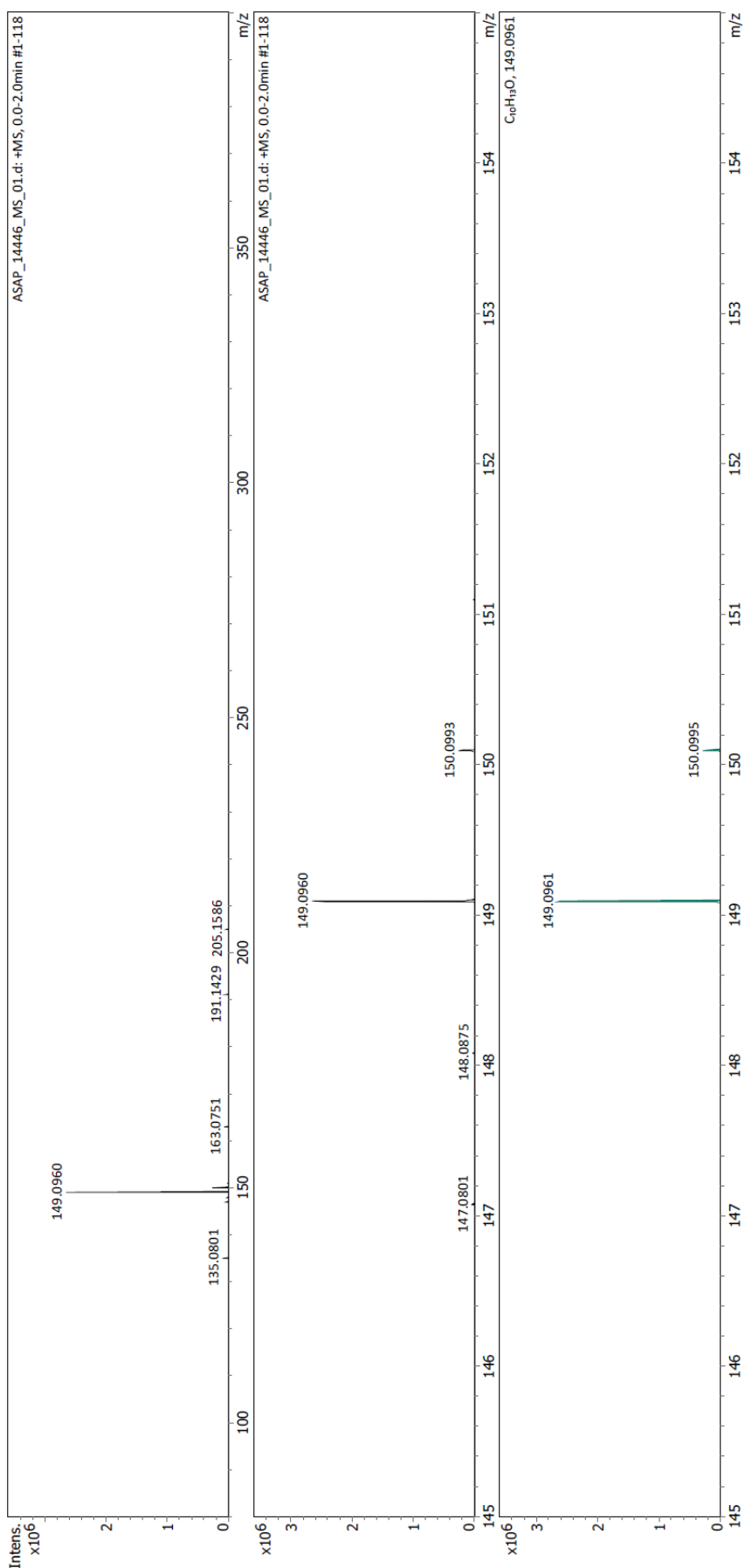


## <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>)

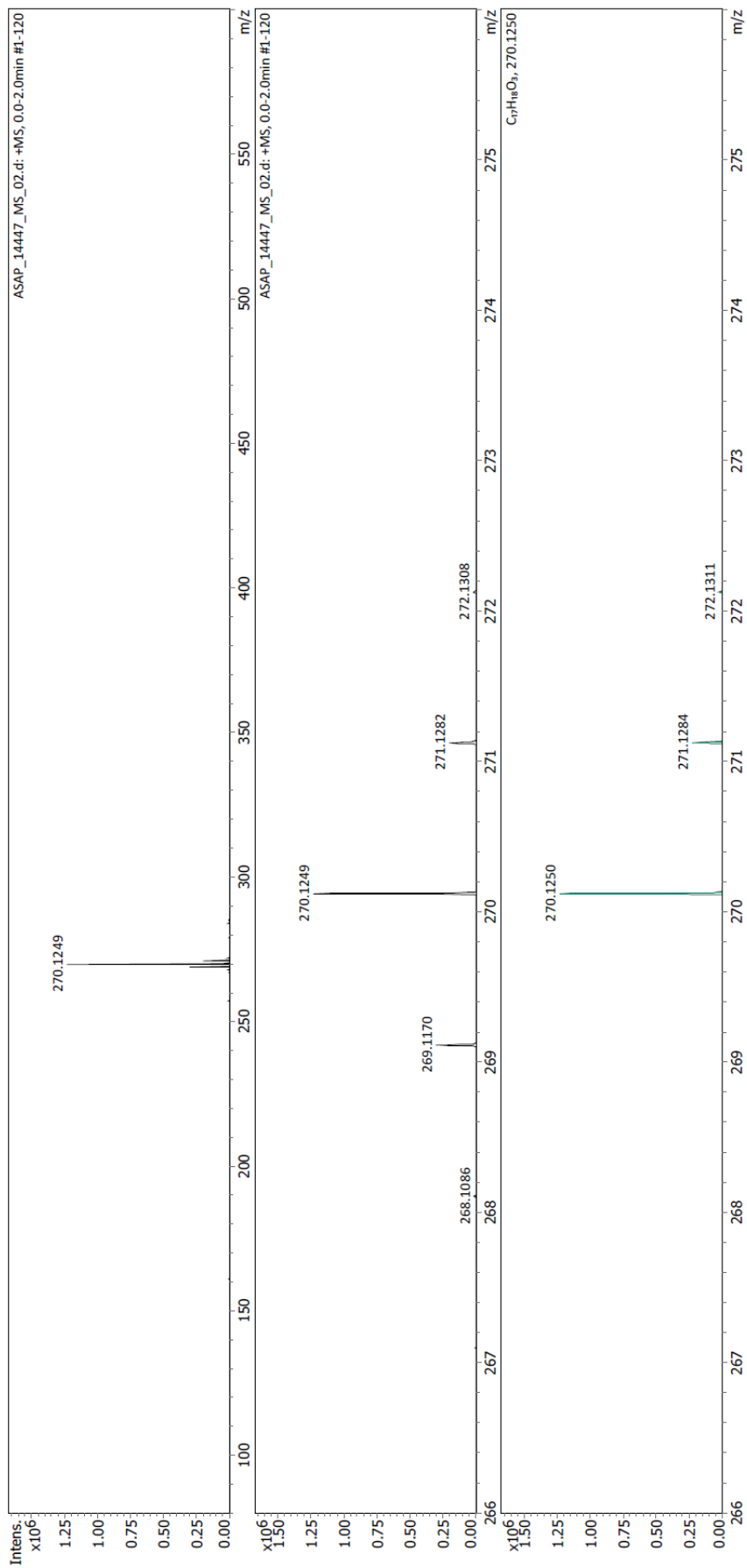


# HRMS Spectra

## 8-Methylchromane (5a)



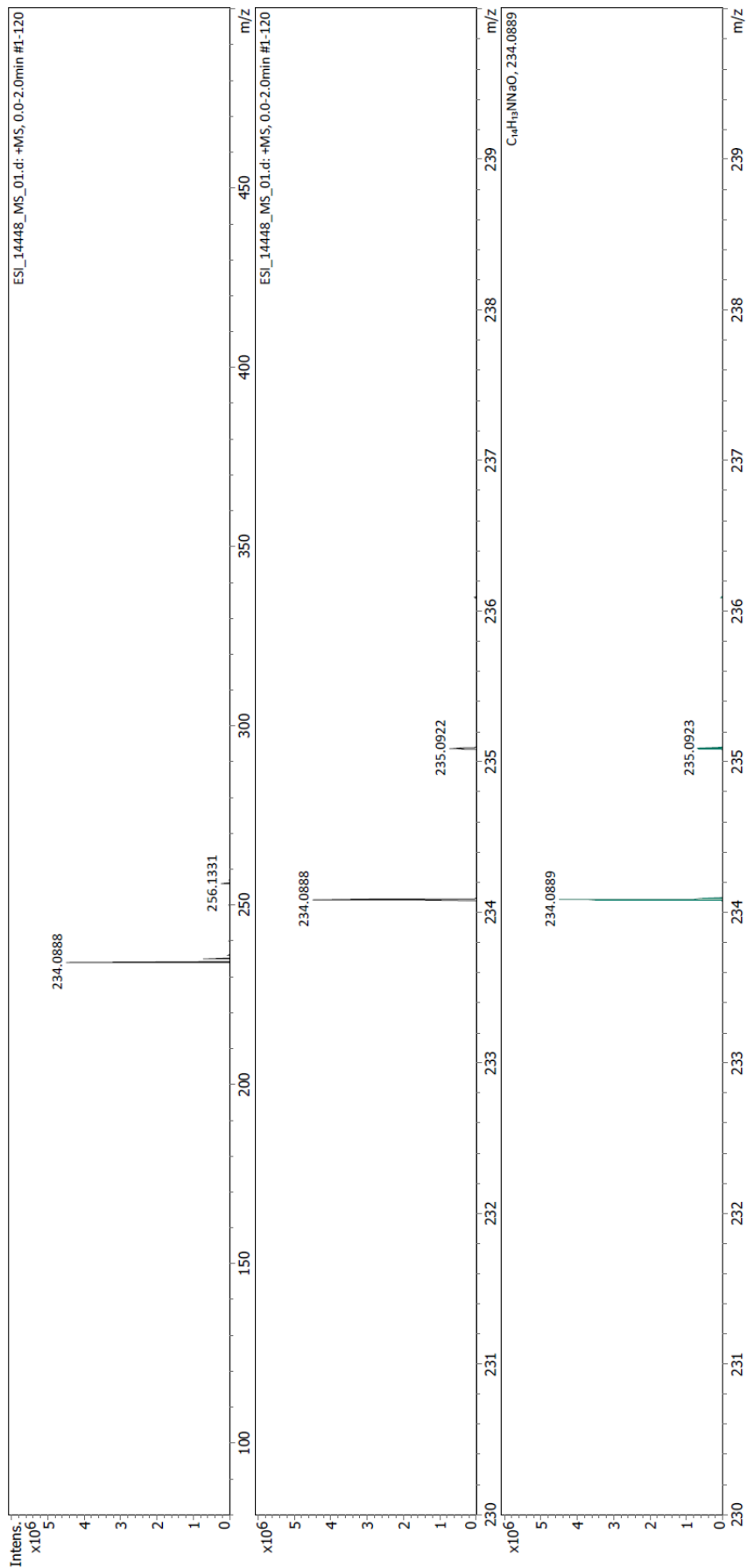
(4-Anisyl)(8-chromanyl)methanol (5b)



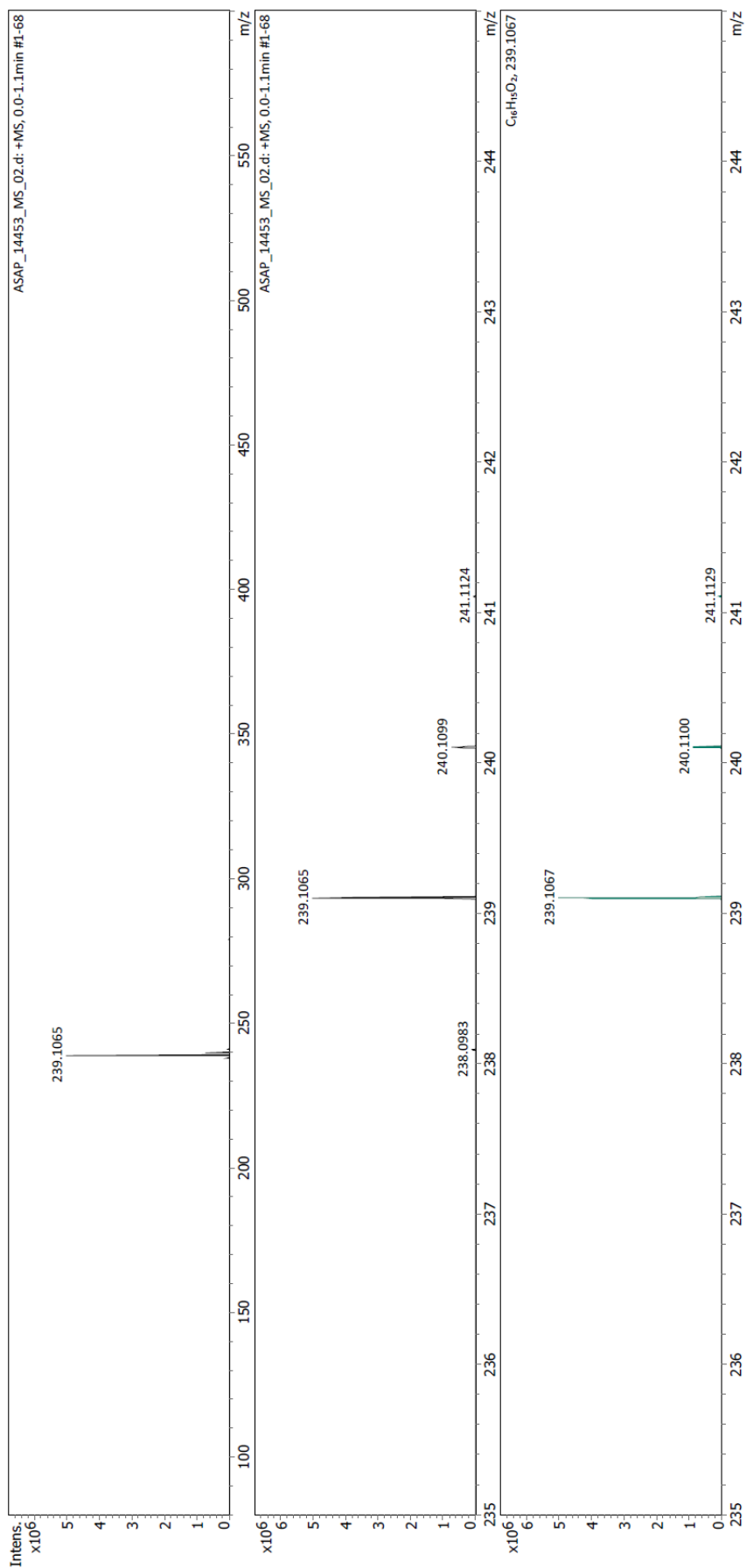
# 8-Iodochromane (5d)



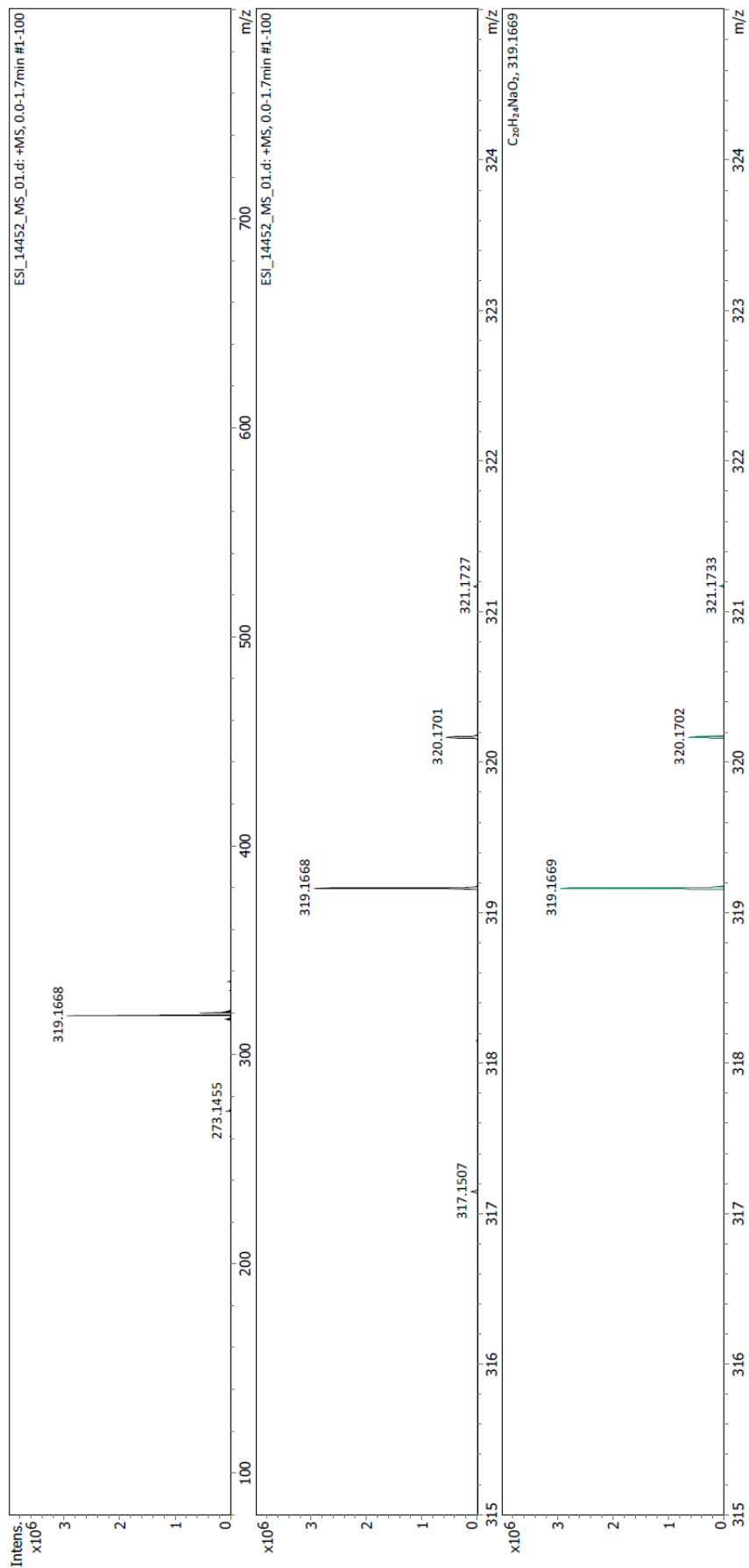
# 8-(2-Pyridyl)chromane (5e)



# 8-Benzoylchromane (5f)



$\alpha$ -*n*-Butyl- $\alpha$ -phenyl-8-chromanemethanol (5'f)

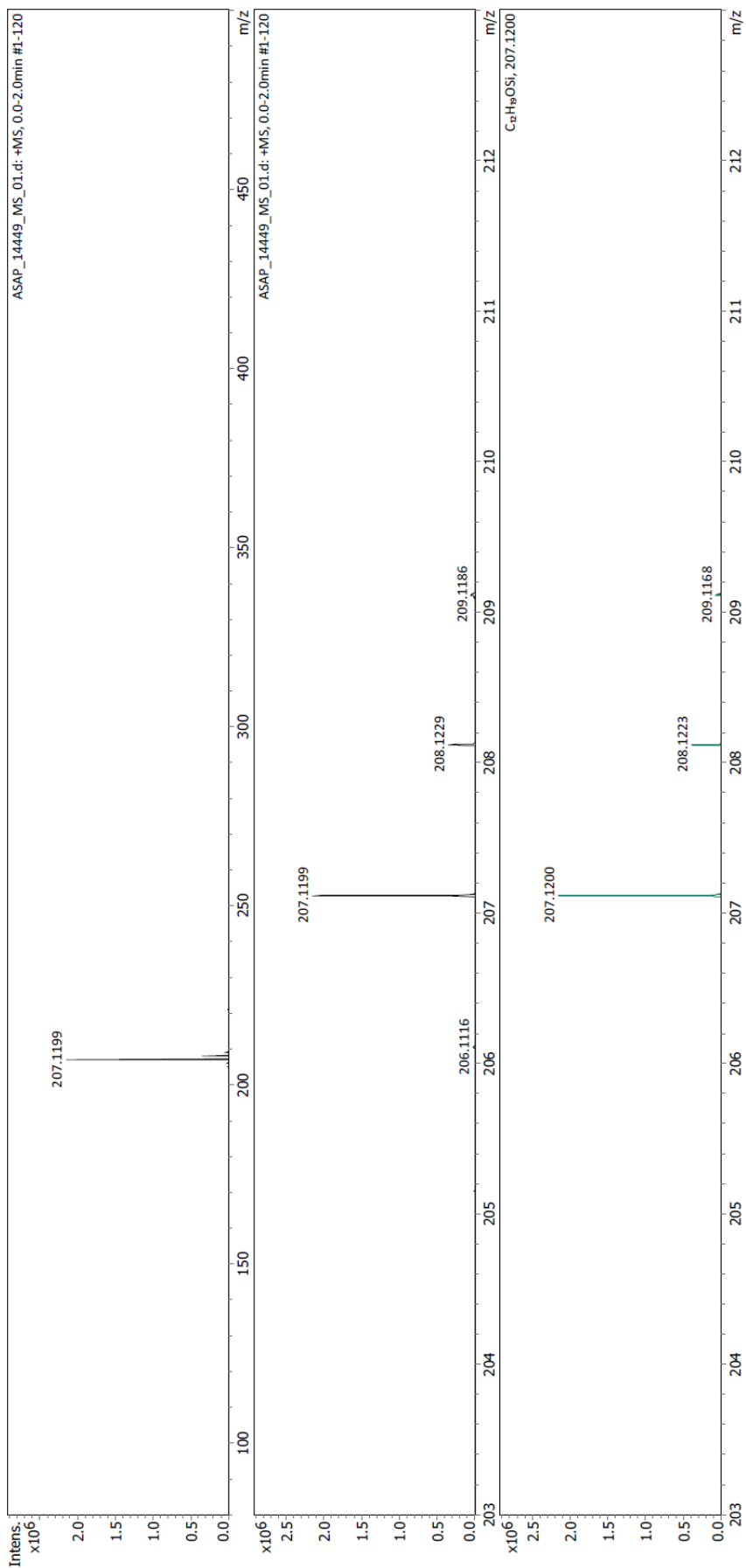




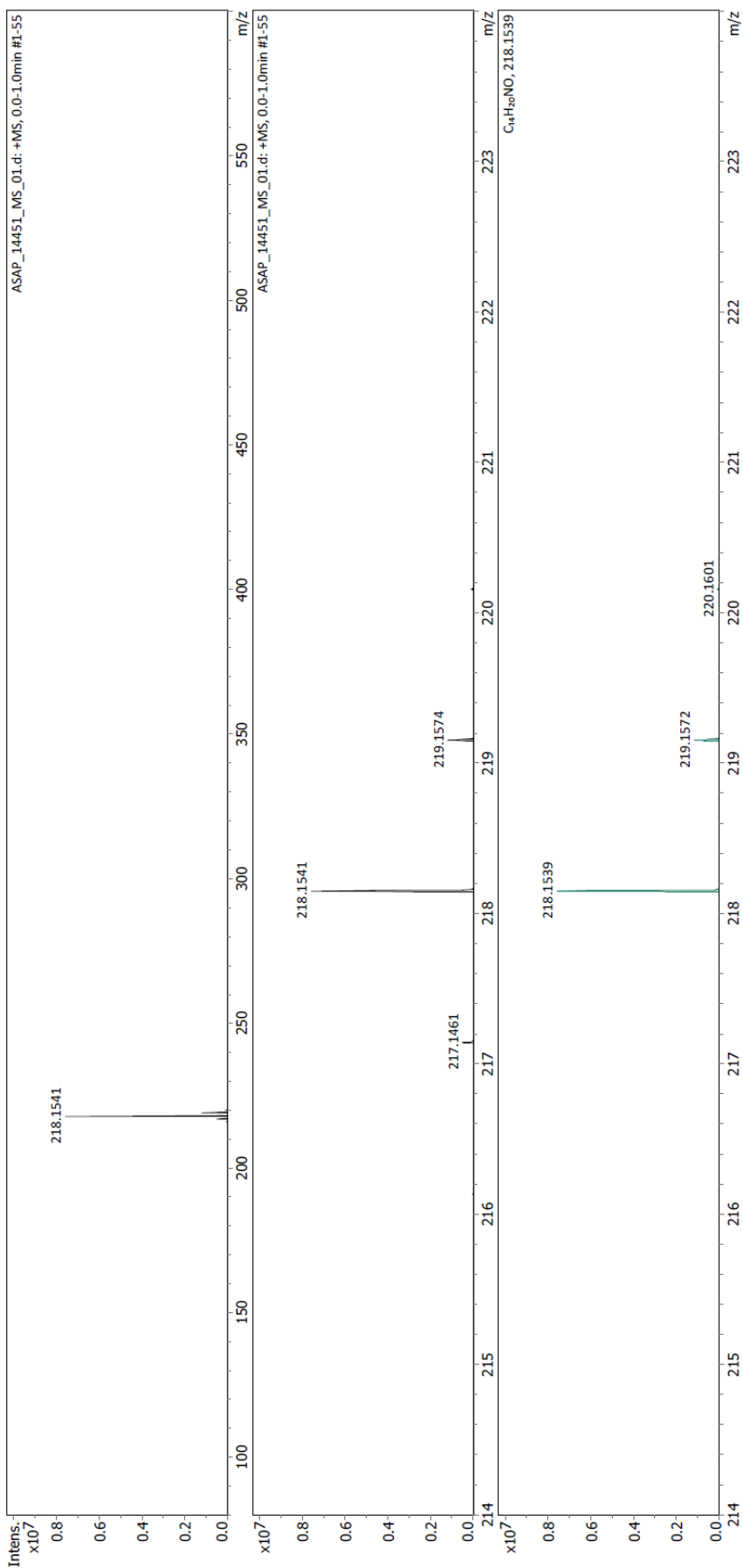
(4-Anisyl)(4-chromanyl)methanol (6b)



4-(Trimethylsilyl)chromane (6e)



8-(*N*-Piperidino)chromane (7)



## Computational Details

Electronic structure calculations were carried out using standard DFT methods implemented in Gaussian 16 package.<sup>20</sup> We used the CAM-B3LYP hybrid functional.<sup>21</sup> The structures of stable conformers for each substance were obtained by full geometry optimization without any symmetry constraints from different initial starting points (including XRD structures where available) using 6-31G(d) basis set.<sup>22</sup> All discussed data correspond to the most stable conformers. Vibrational frequencies were calculated in order to characterize stationary points and calculate zero-point vibrational energies (ZPVE) and thermal corrections. The total energies ( $E$ ) and NPA charges were computed at the CAM-B3LYP/6-311+G(d,p) level.

The gas-phase Gibbs free energies ( $G_{298}^0$ ) were calculated using the equation:

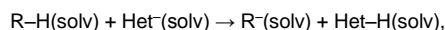
$$G_{298}^0 = E + \text{ZPVE} + H_{0 \rightarrow 298}^0 - TS_{298}^0.$$

The solvent effect for the  $pK_a$  and  $\Delta_rG$  calculations was simulated within the polarized continuum model (IEF-PCM)<sup>23</sup> with the default parameters for THF, *n*-hexane or diethyl ether. The PCM energies ( $E_{\text{PCM}}$ ) were calculated at the CAM-B3LYP/6-311+G(d,p) level using geometries optimized for isolated structures. The solvation Gibbs free energies ( $\Delta_{\text{solv}}G$ ) and Gibbs free energies in solution ( $G_s$ ) were calculated for each species using the equations:

$$\Delta_{\text{solv}}G = E_{\text{PCM}} - E$$

$$G_s = G_{298}^0 + \Delta_{\text{solv}}G$$

In order to study the C-H acidity of 2,3-dihydrobenzofuran and chromane or the corresponding *O*-lithiated species, we used the approach developed earlier.<sup>24</sup> The  $pK_a$  values were obtained from the Gibbs free energy of the isodesmic reaction between the studied (R-H) and a reference compound (Het-H):



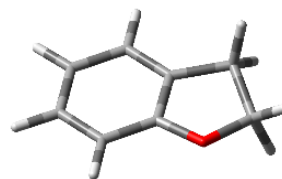
here benzofuran with  $pK_a(\text{THF})$  of 33.2<sup>25</sup> was used as the reference compound due to its structural similarity and since its  $pK_a$  value was expected to be close to the substrates under consideration. When considering the influence of coordination we used complexes of **1** or **2** with LiNMe<sub>2</sub>·2THF in THF or MeLi·TMEDA in hexane to emulate the experimental conditions.

In order to investigate the possibility of 2,3-dihydrobenzofuran to compete with diethyl ether or tetrahydrofuran in the ability to coordinate the metal of the base, we calculated the Gibbs free energy of the substitution ( $\Delta_rG$ ) of the weakest bounded solvent molecule (Et<sub>2</sub>O or THF) in tetrasolvated tetramers [BuLi]<sub>4</sub> by molecule of 2,3-dihydrobenzofuran. The initial structure of [BuLi]<sub>4</sub>·4THF for geometry optimization was taken from the work,<sup>26</sup> but a zigzag conformation was given for all butyl moieties. Other structures were obtained by replacing THF molecules with diethyl ether or 2,3-dihydrobenzofuran molecules. Similarly, the Gibbs free energy ( $\Delta_rG$ ) of the ring opening reaction was calculated as difference of  $G_s$  in THF between the open (phenolate) and cyclic (carbanion) form.

## Cartesian Coordinates of DFT Optimized Structures

1

atom	X	Y	Z
O	-1.41771	-1.21205	-0.08027
C	-2.35988	-0.14942	0.15624
C	-1.61601	1.17625	-0.10168
C	-0.17930	0.72400	-0.01888
C	-0.17031	-0.66737	-0.03684
C	1.01667	1.41820	0.01681
C	2.21525	0.70258	0.03920
C	2.20197	-0.68914	0.01676
C	1.00351	-1.40062	-0.02113
H	-3.21554	-0.31201	-0.50107
H	-2.69590	-0.22013	1.19709
H	-1.87956	1.93930	0.63585
H	-1.84575	1.58302	-1.09347
H	1.02603	2.50449	0.02773
H	3.16078	1.23383	0.07315
H	3.14058	-1.23469	0.03404
H	0.97962	-2.48437	-0.03409



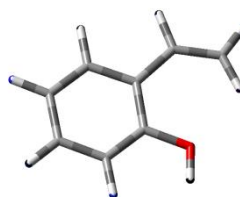
2

atom	X	Y	Z
C	2.24234	-0.77724	0.30351
C	2.36280	0.57397	-0.37949
C	1.21731	1.47073	0.08556
C	-0.09357	0.71870	0.05245
C	-1.31890	1.38518	0.06636
C	-2.52362	0.69947	0.01828
C	-2.51440	-0.69166	-0.05399
C	-1.31180	-1.37845	-0.06849
C	-0.10739	-0.67806	-0.01008
O	1.03007	-1.43319	-0.04437
H	3.03817	-1.46156	0.00253
H	2.28682	-0.65634	1.39555
H	3.33450	1.02251	-0.14951
H	2.31535	0.42537	-1.46397
H	1.14898	2.36761	-0.53919
H	1.42091	1.82146	1.10609
H	-1.31728	2.47185	0.10912
H	-3.46240	1.24358	0.02980
H	-3.44833	-1.24361	-0.09751
H	-1.27395	-2.46116	-0.12256

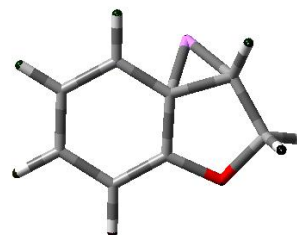


4

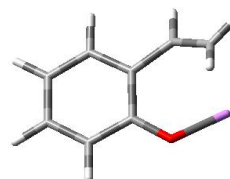
atom	X	Y	Z
O	-0.95535	1.79594	-0.00021
C	-0.36606	-0.52222	0.00001
C	0.02254	0.83837	0.00001
C	0.66917	-1.47544	-0.00004
C	2.01669	-1.12558	0.00006
C	2.36993	0.22349	0.00009
C	1.37301	1.19754	0.00003
H	0.39140	-2.52693	-0.00013
H	2.78110	-1.89684	0.00008
H	3.41420	0.52330	0.00010
H	1.64024	2.25359	-0.00006
C	-1.75183	-1.00886	-0.00016
C	-2.90572	-0.32477	0.00027
H	-1.81681	-2.09758	-0.00081
H	-3.84957	-0.86328	0.00000
H	-2.95122	0.75591	0.00093
H	-0.53288	2.66915	-0.00011

Li salt of **1** deprotonated at benzylic position

atom	X	Y	Z
O	-1.435644	-1.257109	0.116262
C	-2.390453	-0.184484	-0.171864
C	-1.589858	1.111552	-0.053076
C	-0.214156	0.67041	-0.207244
C	-0.180374	-0.741304	-0.011281
C	1.01768	1.360671	-0.210483
C	2.230001	0.631282	-0.1196
C	2.218756	-0.748102	0.023272
C	0.993596	-1.457083	0.085092
H	-2.79221	-0.36854	-1.184387
H	-3.21484	-0.303839	0.539105
H	-1.938024	1.947757	-0.662855
H	1.045811	2.435034	-0.406885
H	3.1754	1.164862	-0.174398
H	3.153552	-1.297186	0.090206
H	0.971524	-2.535653	0.208912
Li	-0.475739	1.718928	1.550437

Li salt of **4**

atom	X	Y	Z
O	-0.90468	1.76754	-0.08840
C	-0.22897	-0.54679	-0.06121
C	0.04017	0.87106	0.00276
C	0.85103	-1.45714	-0.11399
C	2.16764	-1.04018	-0.01395
C	2.43062	0.33591	0.11068
C	1.40174	1.26308	0.11306
H	0.62752	-2.51923	-0.20516
H	2.97979	-1.76060	-0.03482



H	3.45956	0.68111	0.19040
H	1.60473	2.32824	0.17955
C	-1.57213	-1.10200	-0.10189
C	-2.75367	-0.60923	0.36941
H	-1.62869	-2.08993	-0.56584
H	-3.65839	-1.20716	0.31325
H	-2.78167	0.25172	1.04156
Li	-2.46134	1.29575	-0.68034

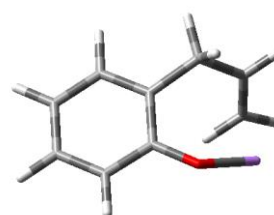
Li salt of **2** deprotonated at position 3

atom	X	Y	Z
C	-2.21180	-0.59559	-0.56665
C	-2.33891	0.60569	0.32414
C	-1.18022	1.53507	-0.05304
C	0.12951	0.75356	-0.04769
C	1.37738	1.39373	-0.03501
C	2.57568	0.68320	-0.00221
C	2.55193	-0.71448	0.01758
C	1.33281	-1.38597	-0.00385
C	0.13757	-0.65831	-0.04186
O	-1.04395	-1.40273	-0.03900
H	-3.05389	-1.29239	-0.52443
H	-1.94364	-0.42599	-1.62825
H	-3.31758	1.08397	0.22773
H	-1.08570	2.37857	0.64339
H	-1.29254	1.99053	-1.06100
H	1.39646	2.48179	-0.04228
H	3.52318	1.21481	0.01108
H	3.47912	-1.28067	0.04068
H	1.28264	-2.47119	-0.01044
Li	-1.62669	-0.71966	1.70235



Li phenolate corresponding to open form of **2** deprotonated at position 3

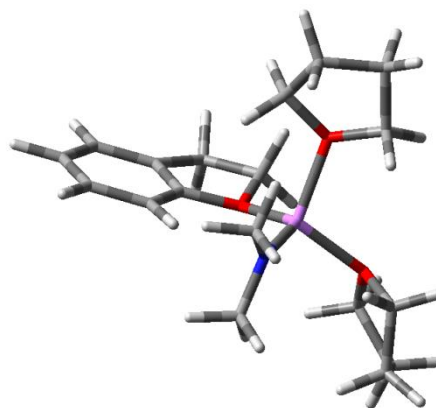
atom	X	Y	Z
C	1.29160	-0.90882	-0.88585
C	-0.07538	-0.50020	-0.38765
C	-1.05078	-1.46519	-0.11289
C	-2.34232	-1.11217	0.27614
C	-2.66453	0.24519	0.38367
C	-1.71487	1.22420	0.11389
C	-0.39423	0.88801	-0.27066
O	0.50731	1.82263	-0.50630
H	1.30236	-1.98873	-1.09862
H	1.49888	-0.42615	-1.85514
H	-0.79012	-2.51839	-0.21430
H	-3.08370	-1.87841	0.48439
H	-3.66898	0.54178	0.67955
H	-1.96134	2.28022	0.18991
C	2.48572	-0.64020	0.00716
C	2.46335	-0.21010	1.28144



H	3.45697	-0.84946	-0.44971
H	3.37798	-0.10884	1.86210
H	1.51715	-0.03556	1.79287
Li	2.10036	1.75941	0.07593

1 with LiNMe<sub>2</sub>·2THF

atom	X	Y	Z
O	-0.87808	-0.85000	-0.65926
C	-1.13885	-0.89386	-2.08066
C	-2.58746	-1.38688	-2.23744
C	-3.15710	-1.05535	-0.88073
C	-2.10350	-0.77105	-0.02458
C	-4.45240	-1.03187	-0.39015
C	-4.65683	-0.71394	0.95283
C	-3.57661	-0.42666	1.78518
C	-2.26569	-0.44752	1.30967
Li	0.75857	0.09283	0.14267
N	0.90935	0.26157	2.00417
C	3.49106	-2.93345	-0.75972
C	3.86511	-2.18547	0.52160
C	3.46711	-0.75680	0.18156
O	2.30897	-0.88163	-0.67395
C	2.21093	-2.21819	-1.18713
C	1.28010	3.98025	-1.24213
C	0.09000	4.01013	-0.28031
C	-0.51754	2.61993	-0.46105
O	0.55579	1.77030	-0.91477
C	1.75284	2.54099	-1.09518
C	0.83687	1.40682	2.86121
C	1.00553	-0.91644	2.81803
H	-1.00771	0.12026	-2.47121
H	-0.39295	-1.54859	-2.53163
H	-2.62733	-2.46543	-2.43103
H	-3.09696	-0.88404	-3.06386
H	-5.29536	-1.25387	-1.03831
H	-5.66629	-0.68666	1.35064
H	-3.75460	-0.17453	2.82602
H	-1.38863	-0.20046	1.90664
H	3.33662	-4.00497	-0.61093
H	4.27164	-2.80539	-1.51710
H	4.92311	-2.27483	0.78011
H	3.27225	-2.54604	1.36725
H	3.14815	-0.16220	1.04185
H	4.25902	-0.24077	-0.37675
H	2.09169	-2.16948	-2.27421
H	1.31931	-2.68893	-0.75748
H	2.05799	4.70523	-0.99077
H	0.95226	4.17044	-2.26970

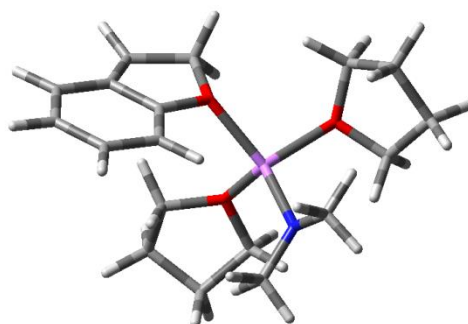




H	-0.62548	4.80645	-0.49876
H	0.43944	4.13935	0.74833
H	-0.92197	2.20158	0.46339
H	-1.30016	2.61261	-1.22826
H	2.27506	2.14905	-1.97069
H	2.39420	2.41832	-0.21371
H	0.79295	2.33731	2.27497
H	-0.05465	1.41715	3.53361
H	1.70636	1.51307	3.54863
H	1.05860	-1.82301	2.19403
H	1.89844	-0.93669	3.48433
H	0.13892	-1.06768	3.50535

1 with LiNMe<sub>2</sub>·2THF deprotonated at benzylic position

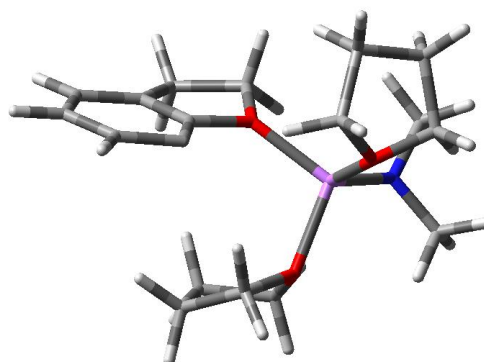
atom	X	Y	Z
O	0.60896	-1.09285	-0.64424
C	0.91165	-1.15267	-2.06891
C	2.39860	-0.96903	-2.14563
C	2.90456	-1.19825	-0.86371
C	1.81237	-1.25457	0.05131
C	4.18463	-1.34955	-0.27795
C	4.30786	-1.49666	1.10739
C	3.21171	-1.51086	1.95937
C	1.91337	-1.38377	1.40393
Li	-0.76011	0.12209	0.12965
N	-1.41327	0.45654	1.91313
C	1.44938	3.54620	-0.90814
C	0.19721	4.09981	-0.22122
C	-0.84064	3.00681	-0.49585
O	-0.10193	1.80524	-0.73566
C	1.31361	2.05587	-0.63553
C	-4.45235	-1.29515	-0.13250
C	-3.49019	-2.41919	-0.54676
C	-2.57775	-1.71092	-1.53939
O	-2.40537	-0.41216	-0.99048
C	-3.63457	-0.00797	-0.36516
C	-1.97566	-0.57818	2.72519
C	-0.72659	1.36669	2.77895
H	0.52731	-2.13386	-2.43993
H	0.29314	-0.37772	-2.54864
H	5.07386	-1.33777	-0.90457
H	5.30715	-1.60567	1.52918
H	3.33590	-1.62162	3.03225
H	1.02013	-1.37283	2.02362
H	2.38007	3.96192	-0.51245
H	1.41670	3.74140	-1.98638
H	-0.11706	5.07745	-0.59915
H	0.37226	4.19304	0.85545



H	-1.52183	2.83408	0.34228
H	-1.43009	3.22903	-1.39456
H	1.82240	1.39505	-1.34419
H	1.65102	1.80402	0.37694
H	-4.77194	-1.38823	0.90801
H	-5.34989	-1.30620	-0.76047
H	-3.99977	-3.28614	-0.97765
H	-2.90000	-2.75493	0.31031
H	-1.58967	-2.15946	-1.64344
H	-3.04961	-1.64166	-2.53270
H	-4.16280	0.68626	-1.03221
H	-3.33525	0.50227	0.55579
H	-2.51530	-1.31749	2.11248
H	-1.22290	-1.15678	3.31620
H	-2.70649	-0.21369	3.48965
H	-0.25128	2.17781	2.20674
H	-1.38643	1.86151	3.53396
H	0.08633	0.89521	3.38218
H	2.94089	-1.14055	-3.06911

1 with LiNMe<sub>2</sub>·2THF deprotonated at aryllic position

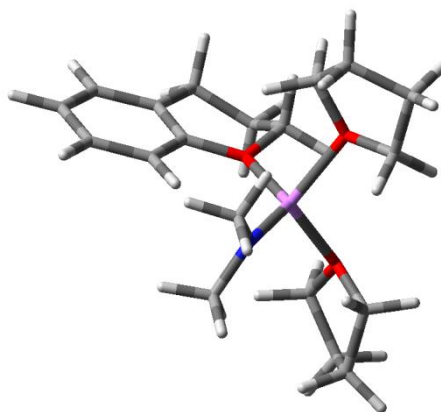
atom	X	Y	Z
O	-0.38200	-0.42637	0.83758
C	-0.44889	-0.36613	2.26529
C	-1.93265	-0.17028	2.62360
C	-2.59910	-0.69578	1.37853
C	-1.66614	-0.80673	0.35206
C	-3.92302	-1.01181	1.10368
C	-4.22943	-1.42024	-0.19367
C	-3.22664	-1.49017	-1.17184
C	-1.86381	-1.18522	-0.96520
Li	1.14730	0.44557	-0.10020
N	2.46443	1.19853	1.10240
C	1.70427	-3.08583	-0.62615
C	3.05760	-2.53885	-0.11126
C	3.26708	-1.25368	-0.92771
O	1.97023	-0.89063	-1.39236
C	1.31055	-2.11117	-1.73996
C	-1.51646	2.89208	-0.22876
C	-1.93357	2.41095	-1.62731
C	-0.66947	1.71430	-2.16573
O	0.36985	1.94110	-1.19805
C	-0.00723	3.03732	-0.36969
C	3.09060	0.57427	2.22357
C	3.35707	2.19242	0.59026
H	-0.08244	-1.31952	2.67144
H	0.21304	0.43726	2.59079
H	-2.16695	0.89120	2.78846



H	-2.20157	-0.70651	3.54067
H	-4.69116	-0.94180	1.87176
H	-5.25735	-1.68305	-0.44412
H	-3.55101	-1.81295	-2.16708
H	0.94815	-3.05424	0.16228
H	1.77144	-4.11648	-0.98814
H	3.88196	-3.24460	-0.25566
H	3.00429	-2.30126	0.95389
H	3.63535	-0.41183	-0.34114
H	3.92110	-1.43852	-1.79434
H	1.68984	-2.45132	-2.71733
H	0.23353	-1.90321	-1.78577
H	-1.74226	2.12129	0.51240
H	-2.00860	3.82221	0.07253
H	-2.21693	3.25829	-2.26177
H	-2.77236	1.71278	-1.58555
H	-0.81099	0.63247	-2.23941
H	-0.35162	2.13019	-3.13095
H	0.25608	3.98679	-0.86362
H	0.56157	2.93635	0.55746
H	2.44157	-0.19502	2.66818
H	4.06144	0.06284	1.98336
H	3.35584	1.27762	3.05075
H	2.92174	2.70112	-0.28193
H	3.62467	2.98937	1.32646
H	4.34952	1.78861	0.25465

2 with LiNMe<sub>2</sub>·2THF

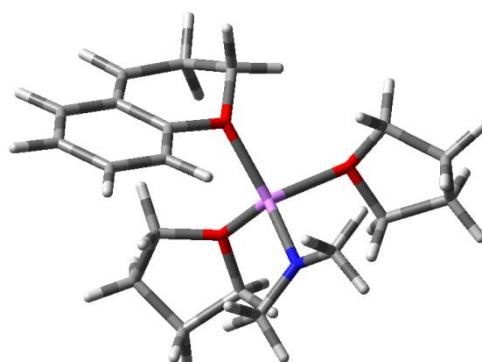
atom	X	Y	Z
O	-0.99768	-0.28651	-0.60039
C	-1.12583	-0.34936	-2.02168
C	-2.24191	-1.29590	-2.42109
C	-3.42287	-0.31094	-0.44579
C	-2.16575	-0.09505	0.11935
C	-4.53893	-0.10327	0.36672
C	-4.41035	0.29814	1.68766
C	-3.14000	0.49329	2.22611
C	-2.01009	0.29754	1.44691
Li	0.88394	0.05851	0.14388
N	1.29276	0.33969	1.95056
C	2.29010	-3.85274	-0.40557
C	3.24784	-3.08187	0.50536
C	3.13081	-1.65668	-0.02627
O	1.80501	-1.55646	-0.59706
C	1.16784	-2.84129	-0.59935
C	2.66919	3.48707	-1.35256
C	1.38229	3.95572	-0.66905
C	0.44759	2.76012	-0.85815



O	1.29389	1.60959	-1.04196
C	2.67481	2.00489	-1.00804
C	1.41677	1.57215	2.67022
C	1.18263	-0.73162	2.89874
H	-1.32203	0.66113	-2.40461
H	-0.14810	-0.67045	-2.38268
H	-2.02997	-2.28710	-2.00405
H	-2.27086	-1.39597	-3.51083
H	-5.52694	-0.27047	-0.05565
H	-5.29495	0.45053	2.29788
H	-3.02507	0.79914	3.26118
H	-0.99291	0.42973	1.82467
H	1.93575	-4.79059	0.02922
H	2.76883	-4.07896	-1.36440
H	4.27406	-3.45551	0.46883
H	2.90519	-3.12529	1.54315
H	3.20133	-0.89054	0.75067
H	3.85681	-1.46020	-0.82419
H	0.63278	-2.95751	-1.54592
H	0.44178	-2.88424	0.22113
H	3.56136	4.00482	-0.99234
H	2.60500	3.62609	-2.43700
H	0.97214	4.87266	-1.09902
H	1.56336	4.13091	0.39514
H	-0.20197	2.58456	0.00327
H	-0.17378	2.86635	-1.75459
H	3.21534	1.38398	-1.72647
H	3.07009	1.82028	-0.00237
H	1.53570	2.42228	1.98162
H	0.53694	1.81313	3.31532
H	2.28859	1.60532	3.36100
H	1.08609	-1.70257	2.38792
H	2.05474	-0.82001	3.58500
H	0.29746	-0.65100	3.57469
C	-3.56720	-0.76220	-1.88150
H	-4.34984	-1.52454	-1.95539
H	-3.89936	0.07959	-2.50356

**2** with LiNMe<sub>2</sub>·2THF deprotonated at benzylic position

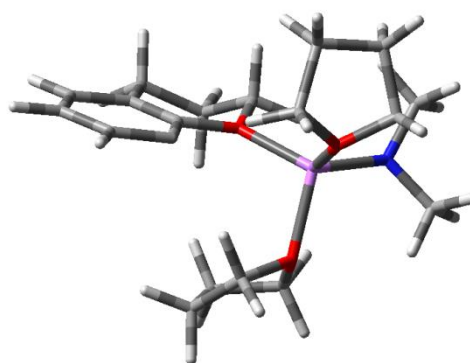
atom	X	Y	Z
O	0.61382	-1.33249	-0.26249
C	0.65591	-2.11999	-1.45539
C	1.52969	-1.46483	-2.51647
C	3.01368	-1.04887	-0.54548
C	1.88080	-1.15479	0.33231
C	4.24834	-0.85172	0.16016
C	4.30848	-0.72745	1.53582
C	3.16782	-0.80910	2.33994



C	1.94100	-1.04063	1.69930
Li	-0.73865	0.02280	0.23593
N	-1.51921	0.59421	1.90875
C	1.35561	3.36260	-1.27123
C	0.08956	3.95311	-0.64533
C	-0.90970	2.80316	-0.78797
O	-0.13304	1.60310	-0.84812
C	1.27631	1.91416	-0.81332
C	-4.73434	-0.62498	-0.70208
C	-4.26987	-1.89469	0.01373
C	-2.83482	-2.04666	-0.49299
O	-2.38665	-0.73318	-0.84444
C	-3.46131	0.21131	-0.69061
C	-2.06591	-0.34889	2.83419
C	-0.91948	1.64939	2.66865
H	1.04927	-3.11327	-1.20049
H	-0.38372	-2.21652	-1.77751
H	0.96367	-0.60682	-2.93061
H	1.62011	-2.18027	-3.35256
H	5.16107	-0.77507	-0.42909
H	5.28053	-0.56227	2.00148
H	3.22065	-0.70504	3.41882
H	1.01193	-1.10385	2.26241
H	2.27402	3.85454	-0.93983
H	1.30911	3.42255	-2.36491
H	-0.25791	4.87003	-1.13103
H	0.26299	4.17329	0.41301
H	-1.60510	2.72342	0.05184
H	-1.48356	2.88830	-1.72071
H	1.80349	1.19408	-1.44412
H	1.64075	1.79777	0.21332
H	-5.56641	-0.12595	-0.19749
H	-5.04177	-0.85269	-1.72967
H	-4.88371	-2.77271	-0.20750
H	-4.27313	-1.73418	1.09519
H	-2.15553	-2.46106	0.25689
H	-2.79098	-2.67943	-1.38883
H	-3.39869	0.92187	-1.51988
H	-3.30238	0.73124	0.26313
H	-2.50890	-1.21197	2.31295
H	-1.31740	-0.77378	3.54879
H	-2.87091	0.06428	3.49245
H	-0.44631	2.39440	2.01117
H	-1.63895	2.21283	3.31337
H	-0.12206	1.30608	3.37061
C	2.86264	-1.11469	-1.92269
H	3.74078	-1.08593	-2.56305

2 with LiNMe<sub>2</sub>·2THF deprotonated at arylc position

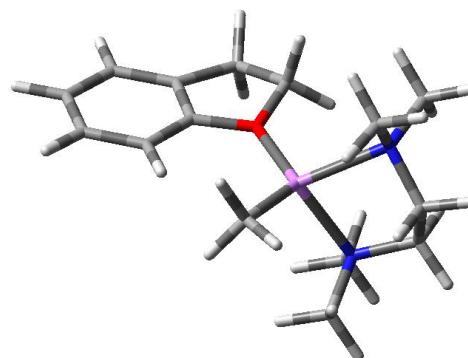
atom	X	Y	Z
O	-0.59443	0.02264	0.87274
C	-0.62187	0.34976	2.25362
C	-1.93849	0.99826	2.64381
C	-2.91755	-0.66014	1.04504
C	-1.71660	-0.65168	0.32565
C	-4.00802	-1.31101	0.45908
C	-3.87665	-1.90917	-0.78357
C	-2.64497	-1.84576	-1.44755
C	-1.50346	-1.21455	-0.93401
Li	1.16972	0.38933	-0.07316
N	2.39689	1.22480	1.20144
C	2.01051	-3.27426	-0.32576
C	3.19935	-2.57198	0.37418
C	3.45111	-1.33587	-0.49630
O	2.19246	-1.05974	-1.09882
C	1.63458	-2.32089	-1.47049
C	-1.32171	2.83483	-1.13643
C	-1.38480	2.20691	-2.53454
C	-0.10206	1.36174	-2.60171
O	0.71800	1.76724	-1.48955
C	0.17896	2.95048	-0.90896
C	2.91590	0.67848	2.41471
C	3.33163	2.19248	0.71562
H	-0.47427	-0.56611	2.84869
H	0.23666	1.00854	2.39811
H	-2.08197	1.89954	2.03553
H	-1.90250	1.31383	3.69371
H	-4.95858	-1.33283	0.99169
H	-4.73044	-2.41397	-1.23651
H	-2.59302	-2.32659	-2.43028
H	1.16544	-3.38776	0.35841
H	2.27170	-4.26935	-0.69973
H	4.08732	-3.20741	0.45122
H	2.92371	-2.25660	1.38350
H	3.73031	-0.44388	0.06373
H	4.19157	-1.55069	-1.28374
H	2.08998	-2.64525	-2.41980
H	0.55624	-2.15682	-1.57966
H	-1.74944	2.14852	-0.40236
H	-1.83983	3.79691	-1.07007
H	-1.38883	2.98463	-3.30720
H	-2.27257	1.58397	-2.66686
H	-0.32034	0.29939	-2.45832
H	0.45588	1.52651	-3.53200
H	0.59065	3.83803	-1.41627
H	0.49109	2.95955	0.13773



H	2.22360	-0.05795	2.85073
H	3.90067	0.15039	2.30006
H	3.11113	1.43713	3.21249
H	2.98445	2.63682	-0.22756
H	3.52151	3.03822	1.42127
H	4.35495	1.77902	0.50784
C	-3.06790	0.00399	2.39838
H	-4.04655	0.49612	2.46972
H	-3.05181	-0.75425	3.19561

1 with MeLi-TMEDA

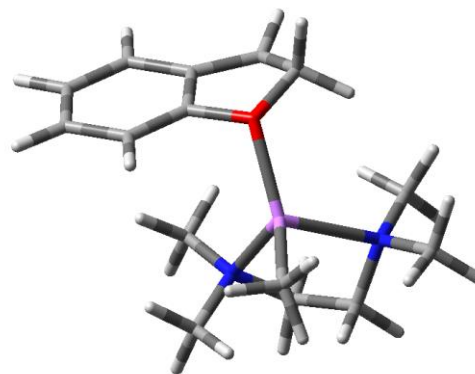
atom	X	Y	Z
O	-0.84899	-0.48659	-0.01588
C	-0.98142	-1.90241	0.23185
C	-2.39838	-2.11401	0.78882
C	-3.09461	-0.87564	0.28332
C	-2.12828	0.02249	-0.14602
C	-4.43030	-0.51323	0.23114
C	-4.76498	0.74921	-0.25835
C	-3.77135	1.62970	-0.68060
C	-2.42186	1.28139	-0.63365
Li	0.84090	0.59230	-0.40565
C	0.79133	2.40226	-1.37089
C	3.19934	-0.13297	1.13270
C	3.50380	-0.08357	-0.36160
N	1.98964	0.61946	1.47538
N	2.44306	-0.68905	-1.17292
C	2.58136	-0.29232	-2.57502
C	2.43916	-2.14237	-1.06813
C	2.27023	2.04830	1.62148
C	1.36319	0.11056	2.68842
H	-0.84865	-2.42436	-0.72207
H	-0.18338	-2.19649	0.91423
H	-5.20437	-1.19892	0.56352
H	-5.80739	1.04629	-0.31195
H	-4.04847	2.60753	-1.06194
H	-1.62446	1.94006	-0.96213
H	0.29444	2.40085	-2.35964
H	0.30148	3.21961	-0.80720
H	1.80744	2.79609	-1.57844
H	4.07438	0.23904	1.69221
H	3.05521	-1.17137	1.44519
H	4.47699	-0.57081	-0.55139
H	3.59618	0.95870	-0.67779
H	3.54551	-0.61906	-3.00101
H	2.48410	0.79124	-2.65207
H	1.77508	-0.74359	-3.15933
H	1.62411	-2.54728	-1.67378



H	3.38496	-2.58742	-1.42319
H	2.27973	-2.46149	-0.03550
H	2.68500	2.44934	0.69716
H	1.33689	2.58420	1.80409
H	2.96715	2.23769	2.45660
H	0.43489	0.65698	2.87399
H	2.01006	0.21694	3.57615
H	1.11747	-0.94860	2.56871
H	-2.83797	-3.04714	0.42673
H	-2.39950	-2.14942	1.88483

1 with MeLi-TMEDA deprotonated at benzylic position

atom	X	Y	Z
O	0.63621	-1.15993	1.21639
C	0.57424	-2.43310	0.51344
C	1.39605	-2.20684	-0.72598
C	2.27494	-1.16458	-0.40466
C	1.80713	-0.53691	0.78920
C	3.43950	-0.59138	-0.96846
C	4.02835	0.52866	-0.37376
C	3.52187	1.11785	0.77879
C	2.37021	0.55283	1.38339
Li	-0.92172	0.10807	1.06818
C	-1.86728	1.07631	2.65265
C	-1.82661	1.20924	-1.54269
C	-2.95922	0.59057	-0.73355
N	-0.64592	1.50998	-0.73807
N	-2.61998	-0.72274	-0.18993
C	-3.64884	-1.15167	0.74762
C	-2.40464	-1.71557	-1.23515
C	-0.76818	2.79790	-0.06609
C	0.56218	1.47220	-1.55920
H	0.97027	-3.20280	1.21595
H	-0.48997	-2.65577	0.37278
H	3.87040	-1.01346	-1.87374
H	4.92297	0.94901	-0.83284
H	4.00926	1.97740	1.22900
H	1.93607	0.96797	2.28936
H	-2.14573	0.36414	3.45471
H	-1.15354	1.77439	3.13288
H	-2.78177	1.68500	2.48561
H	-2.20453	2.11742	-2.04898
H	-1.52788	0.51846	-2.33546
H	-3.86081	0.52467	-1.37569
H	-3.19672	1.23495	0.11696
H	-4.64055	-1.25109	0.26590
H	-3.69888	-0.42914	1.56431
H	-3.37316	-2.12195	1.17072

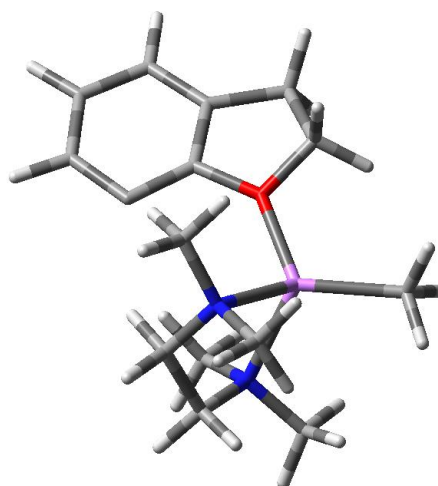




H	-2.37585	-2.70913	-0.78221
H	-3.21491	-1.70932	-1.98861
H	-1.44034	-1.56342	-1.72731
H	-1.62205	2.79046	0.61292
H	0.12445	2.96699	0.54034
H	-0.86881	3.62824	-0.79198
H	1.43251	1.71294	-0.94708
H	0.50477	2.19148	-2.39859
H	0.70389	0.46195	-1.94876
H	1.65945	-3.03790	-1.37327

1 with MeLi-TMEDA deprotonated at aryllic position

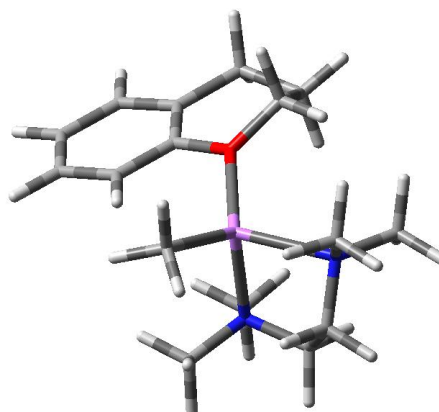
atom	X	Y	Z
O	0.78718	0.96915	-0.20861
C	1.41091	2.19137	-0.61226
C	3.04921	0.64411	0.01369
C	1.81730	-0.00144	-0.05174
C	4.19288	-0.12569	0.17418
C	4.03008	-1.50819	0.25808
C	2.75037	-2.07596	0.19323
C	1.54573	-1.35780	0.03401
Li	-1.21709	1.02060	-0.22073
C	-2.13158	2.86087	-0.53314
C	-1.96877	-1.74221	-0.33625
C	-2.67078	-1.22631	0.91571
N	-1.86911	-0.71748	-1.37569
N	-1.95715	-0.11031	1.53345
C	-2.84741	0.74171	2.30380
C	-0.83526	-0.56892	2.34563
C	-3.14519	-0.37732	-1.97972
C	-0.90620	-1.11851	-2.39410
H	1.42930	2.22708	-1.71091
H	0.79939	3.01690	-0.24740
H	5.17865	0.33310	0.22963
H	4.90694	-2.14554	0.37488
H	2.70708	-3.16792	0.27144
H	-1.86219	3.62078	0.22890
H	-1.88967	3.33971	-1.50323
H	-3.24056	2.82799	-0.50919
H	-2.51024	-2.63613	-0.70647
H	-0.93856	-2.03289	-0.09412
H	-2.79668	-2.06241	1.62897
H	-3.67919	-0.88153	0.66545
H	-3.32716	0.20342	3.14428
H	-3.61819	1.15728	1.65082
H	-2.27820	1.58130	2.71045
H	-0.30351	0.30033	2.74320
H	-1.17904	-1.18936	3.19619



H	-0.12622	-1.13340	1.73084
H	-3.83345	0.02812	-1.23593
H	-2.98954	0.40532	-2.72621
H	-3.61847	-1.25064	-2.47039
H	-0.74120	-0.28601	-3.08584
H	-1.26568	-1.98774	-2.97839
H	0.03624	-1.37387	-1.90026
C	2.84469	2.13525	-0.06326
H	3.55152	2.65806	-0.71741
H	2.91036	2.60177	0.93035

2 with MeLi-TMEDA

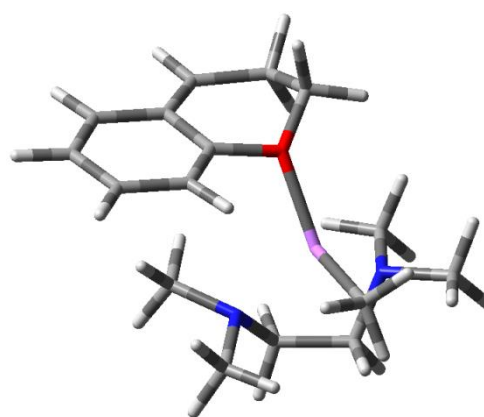
atom	X	Y	Z
O	-0.67742	0.76417	0.63941
C	-0.77145	2.18772	0.61478
C	-2.98032	0.67478	-0.11891
C	-1.87132	0.08340	0.48694
C	-4.12886	-0.10525	-0.26416
C	-4.17375	-1.42058	0.17271
C	-3.05133	-1.98255	0.77743
C	-1.89655	-1.23274	0.94103
Li	1.06910	-0.32817	0.81657
C	1.42058	-1.61823	2.37513
C	2.62321	-0.70771	-1.59532
C	3.48315	-0.27510	-0.41262
N	1.32901	-1.25270	-1.17453
N	2.88259	0.82201	0.35626
C	3.57525	0.97345	1.63745
C	2.92071	2.08020	-0.37936
C	1.43583	-2.67064	-0.82792
C	0.31199	-1.06595	-2.20292
H	-1.28353	2.52333	1.52608
H	0.25731	2.54753	0.64132
H	-5.00181	0.33849	-0.73681
H	-5.07936	-2.00498	0.04560
H	-3.07696	-3.00768	1.13351
H	-1.00724	-1.63079	1.42546
H	1.32925	-1.13715	3.36706
H	0.76926	-2.51107	2.44017
H	2.44636	-2.04189	2.36643
H	3.18533	-1.43963	-2.19944
H	2.43737	0.14890	-2.24934
H	4.48758	0.00573	-0.77720
H	3.60645	-1.11705	0.27338
H	4.64431	1.20970	1.50016
H	3.46592	0.05363	2.21306
H	3.11318	1.78513	2.20595
H	2.51393	2.87950	0.24588



H	3.94869	2.36411	-0.66411
H	2.31580	2.02442	-1.28741
H	2.14110	-2.80712	-0.00824
H	0.46686	-3.02963	-0.47545
H	1.74838	-3.27495	-1.69742
H	-0.64632	-1.44324	-1.83862
H	0.56000	-1.59127	-3.14116
H	0.19556	-0.00094	-2.42335
C	-2.94343	2.11249	-0.58722
C	-1.51340	2.64993	-0.62581
H	-1.50608	3.74314	-0.68128
H	-0.98410	2.27259	-1.50845
H	-3.54465	2.73041	0.09238
H	-3.41351	2.19742	-1.57264

2 with MeLi-TMEDA deprotonated at benzylic position

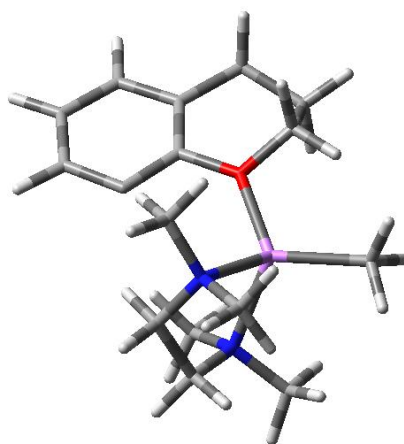
atom	X	Y	Z
O	-0.56783	0.95611	1.05914
C	-0.70904	2.37592	1.03542
C	-2.53719	0.85629	-0.34919
C	-1.74900	0.28093	0.70674
C	-3.66841	0.04412	-0.70483
C	-3.93099	-1.17099	-0.09960
C	-3.12518	-1.68628	0.92193
C	-2.02548	-0.91018	1.32807
Li	0.98738	-0.27332	0.98732
C	1.84584	-1.37748	2.53439
C	2.03170	-1.08239	-1.65676
C	3.13328	-0.54672	-0.74727
N	0.83078	-1.47736	-0.92695
N	2.75632	0.68619	-0.05783
C	3.70756	0.98374	1.00489
C	2.63237	1.81704	-0.96175
C	0.94612	-2.82900	-0.39059
C	-0.36001	-1.36461	-1.76781
H	-1.50226	2.65525	1.74154
H	0.24274	2.77254	1.40388
H	-4.31916	0.40129	-1.50156
H	-4.79966	-1.73991	-0.43234
H	-3.35184	-2.63030	1.40693
H	-1.35190	-1.24861	2.11325
H	2.07014	-0.77233	3.43517
H	1.10827	-2.12925	2.87704
H	2.77273	-1.96219	2.34882
H	2.43726	-1.92648	-2.24565
H	1.74841	-0.31543	-2.38275
H	4.05473	-0.39803	-1.34503
H	3.35297	-1.28573	0.02761



H	4.73255	1.13387	0.61475
H	3.69049	0.16729	1.72832
H	3.40028	1.89865	1.52014
H	2.35251	2.70600	-0.39106
H	3.57789	2.03001	-1.49717
H	1.84495	1.64599	-1.69714
H	1.78257	-2.88948	0.30714
H	0.03877	-3.06370	0.16982
H	1.07321	-3.57674	-1.19721
H	-1.23520	-1.69625	-1.20787
H	-0.26767	-1.97608	-2.68533
H	-0.52947	-0.32014	-2.04254
C	-2.17390	2.05608	-0.93379
C	-1.05182	2.87477	-0.36372
H	-1.32091	3.94238	-0.26727
H	-0.12622	2.87031	-0.96995
H	-2.80048	2.48891	-1.70987

**2** with MeLi-TMEDA deprotonated at arylc position

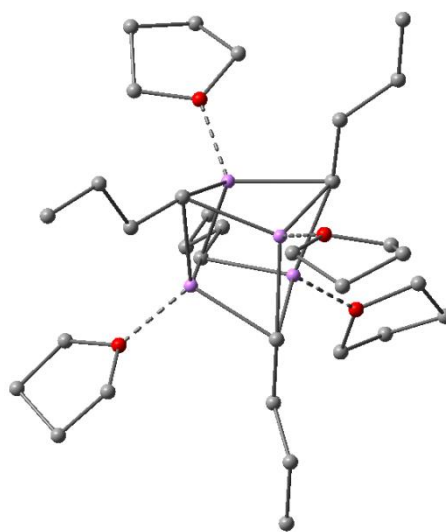
atom	X	Y	Z
O	0.79743	0.83495	-0.35953
C	1.31768	2.07104	-0.82523
C	3.08702	0.12781	0.01168
C	1.73859	-0.21140	-0.15547
C	3.99059	-0.92096	0.21231
C	3.54187	-2.23104	0.24678
C	2.17435	-2.48898	0.09269
C	1.20194	-1.50044	-0.11151
Li	-1.24325	0.96404	-0.23909
C	-2.07876	2.85466	-0.54924
C	-2.32353	-1.66325	-0.25879
C	-2.89264	-1.06011	1.02143
N	-2.18339	-0.67205	-1.32476
N	-2.02704	-0.02439	1.58380
C	-2.77809	0.93902	2.37120
C	-0.93037	-0.59606	2.35677
C	-3.45138	-0.20221	-1.85341
C	-1.33543	-1.19122	-2.39098
H	1.69349	1.94260	-1.85370
H	0.46539	2.75271	-0.84214
H	5.04729	-0.68908	0.34560
H	4.25101	-3.04475	0.40285
H	1.86582	-3.53915	0.14011
H	-1.72975	3.64821	0.14284
H	-1.93076	3.28079	-1.56241
H	-3.18084	2.84010	-0.41652
H	-2.97140	-2.50511	-0.57677
H	-1.31273	-2.04510	-0.07094



H	-3.06990	-1.86986	1.75382
H	-3.86918	-0.60826	0.82109
H	-3.28245	0.47466	3.24080
H	-3.51990	1.43278	1.73991
H	-2.09763	1.71142	2.73828
H	-0.29469	0.21334	2.72730
H	-1.30282	-1.17538	3.22402
H	-0.30927	-1.22771	1.71431
H	-4.04121	0.28705	-1.07645
H	-3.25998	0.54875	-2.62364
H	-4.04775	-1.02452	-2.29559
H	-1.15062	-0.39944	-3.12441
H	-1.81016	-2.04378	-2.91467
H	-0.38486	-1.50511	-1.94655
C	3.59331	1.55680	-0.01475
C	2.44221	2.55301	0.07344
H	2.76068	3.56089	-0.22000
H	2.05946	2.61318	1.09925
H	4.31253	1.71650	0.79935
H	4.14935	1.73763	-0.94692

[*n*BuLi]<sub>4</sub>·4THF

atom	X	Y	Z
Li	-0.56380	-0.58397	-1.14597
Li	0.98056	-0.72553	0.75370
Li	0.83942	1.32098	-0.57761
Li	-1.01950	0.68458	0.90477
O	-1.50007	-1.48768	-2.63997
O	2.06969	-2.10410	1.65868
O	1.95200	2.68798	-1.43581
O	-2.43328	1.30343	2.14609
C	1.69029	-0.59587	-1.36651
C	1.86022	-2.05363	-1.82476
C	3.11488	-2.36091	-2.65291
C	3.22660	-3.82232	-3.08263
C	-1.12073	-1.56462	0.80510
C	-2.63974	-1.75616	0.65994
C	-3.21466	-3.06910	1.20802
C	-4.72737	-3.19763	1.04074
C	-1.29866	1.56370	-1.12921
C	-1.42252	3.05530	-0.76655
C	-2.45590	3.85997	-1.56488
C	-2.53344	5.33144	-1.16278
C	0.99992	1.37739	1.64247
C	2.31414	1.10374	2.39495
C	2.77315	2.19724	3.36746
C	4.07717	1.87047	4.09224
C	-1.76260	-2.89786	-2.68629

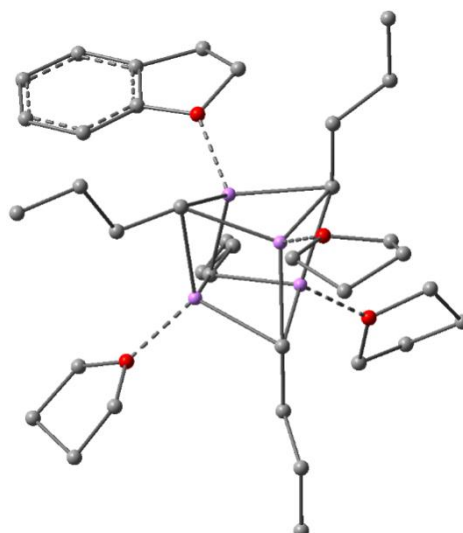


C	-3.10279	-3.02539	-3.39420
C	-3.01723	-1.88953	-4.41568
C	-2.28398	-0.80076	-3.63344
C	1.60478	-2.92307	2.74584
C	2.83847	-3.64886	3.28697
C	3.78932	-3.63080	2.08792
C	3.48132	-2.27131	1.47981
C	3.29288	2.93735	-0.98058
C	4.09806	3.26950	-2.23322
C	3.03461	3.88735	-3.14376
C	1.81856	3.02797	-2.82316
C	-2.46508	0.80331	3.49252
C	-3.75907	1.33785	4.09535
C	-4.67500	1.39374	2.87102
C	-3.71216	1.84642	1.77966
H	2.36587	-4.11892	-3.69357
H	4.13108	-4.01097	-3.67103
H	3.25169	-4.48834	-2.21193
H	4.00532	-2.07805	-2.07314
H	3.11968	-1.71276	-3.53968
H	1.85202	-2.73178	-0.95611
H	0.98957	-2.35567	-2.42578
H	2.64332	-0.30050	-0.87629
H	1.68768	0.02084	-2.28734
H	-5.01333	-3.14558	-0.01671
H	-5.10756	-4.14395	1.44022
H	-5.25192	-2.38526	1.55816
H	-2.95151	-3.15430	2.27135
H	-2.71580	-3.91289	0.71076
H	-2.93694	-1.67442	-0.39808
H	-3.16841	-0.92898	1.15769
H	-0.63876	-2.47140	0.38364
H	-0.89824	-1.65114	1.88837
H	-2.97278	-0.12759	-3.11528
H	-1.61377	-0.19986	-4.25323
H	-1.75958	-3.27335	-1.66168
H	-0.96269	-3.39520	-3.24871
H	1.81112	2.10501	-3.41548
H	0.86293	3.54010	-2.95472
H	2.84975	4.93026	-2.86532
H	3.29959	3.85776	-4.20335
H	4.49604	2.35430	-2.68333
H	4.93537	3.93952	-2.02393
H	3.64984	2.04851	-0.45549
H	3.26678	3.77570	-0.27584
H	3.69178	-2.19868	0.41184
H	4.01133	-1.46653	2.00471

H	3.53515	-4.42684	1.38024
H	4.84019	-3.73986	2.36673
H	2.60320	-4.65558	3.64025
H	3.27613	-3.09215	4.12191
H	1.12620	-2.28129	3.49112
H	0.85459	-3.61215	2.34860
H	-3.27830	5.88008	-1.74945
H	-2.80031	5.43669	-0.10457
H	-1.56677	5.82896	-1.30335
H	-2.21786	3.78076	-2.63486
H	-3.44276	3.39140	-1.44412
H	-0.44718	3.55321	-0.88118
H	-1.65934	3.17086	0.30293
H	-2.31996	1.13244	-1.07236
H	-1.07169	1.51985	-2.21388
H	3.97994	0.95171	4.68302
H	4.89617	1.71544	3.37971
H	4.38028	2.67149	4.77513
H	1.97557	2.37361	4.10173
H	2.88363	3.13986	2.81408
H	3.13622	0.93083	1.67861
H	2.23513	0.16334	2.96341
H	1.10055	2.39670	1.21296
H	0.23397	1.54092	2.42668
H	-3.96645	1.47794	0.78340
H	-3.63096	2.93837	1.73906
H	-5.06769	0.39690	2.64430
H	-5.52051	2.07562	2.98945
H	-4.14073	0.69931	4.89558
H	-3.60509	2.34239	4.50322
H	-2.45753	-0.29249	3.45719
H	-1.56356	1.14658	4.00483
H	-2.42727	-2.20510	-5.28249
H	-3.99248	-1.55338	-4.77557
H	-3.24629	-4.00881	-3.84834
H	-3.92097	-2.84829	-2.68812

[*n*BuLi]<sub>4</sub>·3THF·1

atom	X	Y	Z
Li	-0.91214	-1.16114	-0.76623
Li	-0.59313	1.25744	-0.42702
Li	-1.43465	-0.16498	1.38725
Li	0.91141	-0.32951	0.63790
O	-1.39158	-2.66921	-1.95525
O	-0.71870	2.90634	-1.50675
O	-2.81718	-0.29293	2.77885
O	2.85727	-0.63236	1.15119
C	-2.62131	0.29122	-0.44732



C	-3.08990	0.39926	-1.90765
C	-4.55954	0.78596	-2.11961
C	-4.96610	0.87753	-3.58898
C	0.85180	-0.04573	-1.58298
C	1.78185	-1.18263	-2.04088
C	2.49692	-0.97315	-3.38195
C	3.41470	-2.12816	-3.77717
C	-0.32491	-2.08273	1.23637
C	0.07307	-2.19209	2.72034
C	0.21850	-3.61402	3.27706
C	0.61111	-3.65997	4.75234
C	0.07290	1.42991	1.76409
C	0.10816	2.96477	1.65220
C	0.55623	3.71992	2.90978
C	0.56196	5.23832	2.74672
C	-1.27562	-2.62764	-3.38559
C	-0.87399	-4.03807	-3.78845
C	-1.65254	-4.87823	-2.77404
C	-1.56477	-4.02702	-1.50801
C	0.31427	3.39772	-2.38022
C	-0.18191	4.74685	-2.90276
C	-1.70049	4.62025	-2.76230
C	-1.81791	3.82424	-1.47172
C	-3.50355	0.88913	3.22514
C	-4.96319	0.47881	3.38374
C	-4.83752	-0.99841	3.76249
C	-3.66887	-1.44332	2.89160
C	3.89168	0.21972	0.83764
C	4.83125	-1.93116	0.79006
C	3.43666	-1.93102	1.43709
H	-4.81561	-0.08137	-4.09873
H	-6.01901	1.15474	-3.70872
H	-4.36350	1.62498	-4.11873
H	-4.75221	1.74800	-1.62336
H	-5.19535	0.05313	-1.60456
H	-2.46613	1.12225	-2.45734
H	-2.92690	-0.56055	-2.42022
H	-2.91495	1.23909	0.05409
H	-3.28199	-0.45552	0.03636
H	2.85563	-3.06843	-3.85788
H	3.90704	-1.95221	-4.73959
H	4.20034	-2.27967	-3.02730
H	3.07648	-0.04216	-3.32991
H	1.74489	-0.81439	-4.16809
H	1.22857	-2.13448	-2.09836
H	2.55687	-1.35774	-1.28002
H	0.16995	0.17303	-2.43172

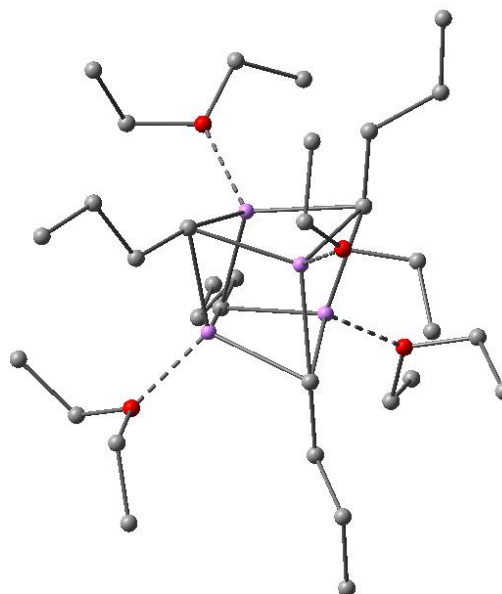


H	1.48144	0.86431	-1.53302
H	-0.70269	-4.29224	-0.88949
H	-2.46403	-4.07906	-0.88900
H	-0.54041	-1.86261	-3.64020
H	-2.24432	-2.34726	-3.81750
H	-4.00229	-1.73318	1.88804
H	-3.08196	-2.25994	3.31772
H	-4.58594	-1.10185	4.82332
H	-5.74494	-1.57538	3.56887
H	-5.49172	0.58258	2.43067
H	-5.48551	1.07818	4.13326
H	-3.34802	1.67621	2.48380
H	-3.06328	1.20748	4.17679
H	-2.73633	3.24118	-1.38674
H	-1.72203	4.47225	-0.59115
H	-2.12006	4.04871	-3.59687
H	-2.21340	5.58375	-2.71168
H	0.14547	4.93802	-3.92739
H	0.18731	5.56253	-2.27267
H	1.24686	3.47389	-1.81467
H	0.45306	2.66511	-3.17978
H	0.70589	-4.68703	5.12116
H	1.57022	-3.15625	4.92075
H	-0.13469	-3.15053	5.37345
H	-0.72883	-4.15104	3.12910
H	0.96377	-4.15749	2.67894
H	-0.65927	-1.65920	3.34621
H	1.01979	-1.65972	2.90550
H	0.39824	-2.69564	0.65872
H	-1.27175	-2.64794	1.12071
H	1.23674	5.54557	1.93872
H	-0.43837	5.61165	2.49691
H	0.88672	5.74837	3.65996
H	1.55994	3.37392	3.19176
H	-0.10161	3.43930	3.74337
H	-0.88892	3.34430	1.37398
H	0.76600	3.27811	0.82349
H	-0.57559	1.21636	2.63953
H	1.06486	1.12970	2.15798
H	2.75495	-2.68388	1.04324
H	3.49602	-2.03061	2.52497
H	4.82177	-2.43194	-0.18506
H	5.56600	-2.44052	1.41925
H	-2.69405	-4.98687	-3.09404
H	-1.23832	-5.87861	-2.62817
H	-1.12622	-4.26638	-4.82678
H	0.20447	-4.17526	-3.65678

C	5.08861	-0.45346	0.63558
C	6.22623	0.26359	0.30718
C	3.77126	1.59223	0.72428
C	6.13999	1.65119	0.18993
H	7.17196	-0.24457	0.14267
C	4.92602	2.30120	0.39404
H	2.82112	2.08615	0.89158
H	7.02501	2.22680	-0.06080
H	4.87364	3.38173	0.30324

[nBuLi]<sub>4</sub>·4Et<sub>2</sub>O

atom	X	Y	Z
Li	1.29467	0.25068	0.71803
Li	0.08848	-1.14505	-0.93474
Li	-1.12387	-0.30999	1.00496
Li	-0.33336	1.34188	-0.72305
O	2.98524	0.75539	1.70615
O	0.46011	-2.72755	-2.15559
O	-2.51608	-0.82963	2.35412
O	-0.72372	2.97942	-1.91386
C	0.51418	-1.82816	1.15950
C	1.86414	-2.56180	1.09777
C	1.98118	-3.83138	1.95110
C	3.34149	-4.51873	1.84995
C	1.58796	0.42782	-1.49816
C	2.43427	1.68494	-1.75907
C	3.58908	1.52467	-2.75606
C	4.37096	2.81269	-3.00673
C	-0.26068	1.68374	1.51071
C	-1.53049	2.52154	1.73865
C	-1.46703	3.54990	2.87542
C	-2.75814	4.34485	3.05865
C	-2.00312	-0.23633	-1.02345
C	-2.72826	-1.48743	-1.55027
C	-4.15173	-1.27013	-2.07986
C	-4.81812	-2.54266	-2.59861
C	4.26871	0.38183	1.20186
C	2.94047	1.05929	3.10289
C	1.04847	-2.56749	-3.44818
C	-0.20244	-3.97612	-1.94671
C	-3.86350	-1.18489	2.03909
C	-2.21355	-0.78917	3.74893
C	-1.04950	2.66482	-3.26633
C	-0.85765	4.36429	-1.58702
H	4.14652	-3.84735	2.17162
H	3.39422	-5.41974	2.47050
H	3.55945	-4.81389	0.81669
H	1.18878	-4.53345	1.65655

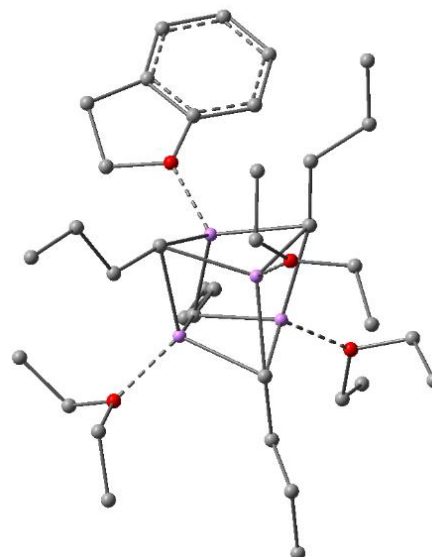


H	1.77525	-3.57394	2.99924
H	2.10060	-2.82644	0.05592
H	2.67546	-1.88587	1.40683
H	-0.26797	-2.58287	0.93188
H	0.32555	-1.60808	2.22998
H	4.80837	3.19721	-2.07783
H	5.18849	2.66482	-3.72052
H	3.71842	3.59704	-3.40784
H	3.18611	1.14784	-3.70628
H	4.27193	0.74434	-2.39088
H	2.85205	2.06825	-0.81503
H	1.78402	2.49230	-2.12364
H	2.29970	-0.40516	-1.31068
H	1.14486	0.15281	-2.47721
H	2.05230	1.68035	3.23097
H	4.07191	-0.06620	0.22585
H	-1.32709	-0.15670	3.83539
H	-4.18829	-1.99798	2.69905
H	-3.83370	-1.57685	1.02163
H	-0.86200	-3.81506	-1.09236
H	-0.83561	-4.20424	-2.81331
H	1.85579	-1.84541	-3.31518
H	-2.68285	5.06730	3.87841
H	-3.01035	4.90148	2.14840
H	-3.60219	3.68043	3.27770
H	-1.21866	3.02727	3.80963
H	-0.63235	4.23957	2.68859
H	-2.38255	1.85552	1.93871
H	-1.81100	3.05689	0.81703
H	0.58754	2.38945	1.41314
H	-0.04583	1.18217	2.47791
H	-4.24302	-2.98009	-3.42319
H	-4.88689	-3.30168	-1.81037
H	-5.83242	-2.35445	-2.96647
H	-4.11901	-0.51759	-2.87937
H	-4.76640	-0.83016	-1.28196
H	-2.77755	-2.26443	-0.76813
H	-2.14066	-1.94476	-2.35953
H	-2.71580	0.27527	-0.34191
H	-1.96708	0.46186	-1.88079
H	-1.84622	4.53833	-1.14590
H	-0.44081	3.29543	-3.92935
H	-0.73016	1.62986	-3.40682
H	-3.02831	-0.28788	4.28560
H	3.81217	1.66574	3.37230
H	-0.79826	4.94924	-2.51357
H	1.49520	-3.51635	-3.76564

C	-1.94272	-2.16769	4.32724
H	-1.11789	-2.64635	3.79362
H	-1.67308	-2.07954	5.38484
H	-2.82006	-2.81797	4.26173
C	-4.81528	-0.00403	2.12240
H	-4.51651	0.77847	1.42058
H	-5.82975	-0.32797	1.86789
H	-4.84463	0.42771	3.12734
C	2.85221	-0.18364	3.97205
H	2.78122	0.10763	5.02528
H	1.96743	-0.77091	3.71275
H	3.73110	-0.82578	3.86276
C	5.21911	1.55832	1.05318
H	5.46966	2.01678	2.01388
H	6.15364	1.21557	0.59756
H	4.78246	2.32443	0.40785
H	4.70511	-0.39517	1.84177
C	0.05107	-2.06498	-4.47765
H	-0.36565	-1.10316	-4.16582
H	0.54804	-1.93006	-5.44385
H	-0.77716	-2.76543	-4.62017
C	0.75903	-5.11691	-1.66006
H	0.19225	-6.03603	-1.47894
H	1.43716	-5.30648	-2.49717
H	1.35787	-4.90036	-0.77272
C	0.24171	4.78987	-0.63690
H	0.11162	5.84446	-0.37290
H	0.21802	4.20168	0.28205
H	1.22360	4.66377	-1.10013
C	-2.52737	2.81795	-3.58119
H	-2.86035	3.85364	-3.46496
H	-2.71834	2.52010	-4.61721
H	-3.12621	2.18345	-2.92261

[*n*BuLi]<sub>4</sub>·3Et<sub>2</sub>O·1

atom	X	Y	Z
Li	-0.58938	1.24875	-0.81733
Li	-1.31558	0.04562	1.21842
Li	-0.99441	-1.20890	-0.87262
Li	0.96745	-0.24251	0.30286
O	-0.57804	2.91559	-1.96124
O	-2.44120	0.39616	2.86652
O	-1.76373	-2.68335	-1.98766
O	2.87738	-0.46933	1.02964
C	-2.62986	0.27903	-0.57810
C	-3.44582	1.56224	-0.35179
C	-4.93073	1.49134	-0.73066
C	-5.69090	2.79447	-0.49173



C	0.25160	1.67278	1.22178
C	1.45137	2.59144	0.93176
C	1.64784	3.76748	1.89727
C	2.87829	4.61887	1.59051
C	0.72296	-0.22953	-1.92075
C	1.54016	-1.47124	-2.32063
C	2.26462	-1.39659	-3.67060
C	3.07107	-2.64968	-4.00422
C	-0.25731	-1.99405	1.06786
C	-1.24795	-2.73962	1.97902
C	-0.82016	-4.14019	2.43602
C	-1.83624	-4.83020	3.34366
C	-0.96420	4.17796	-1.41432
C	-0.66503	2.81134	-3.38474
C	-1.90097	1.04401	4.02044
C	-3.64902	-0.33220	3.09548
C	-1.96050	-4.02404	-1.53509
C	-2.06713	-2.45596	-3.36393
C	3.04116	-0.55656	2.46873
H	-5.25649	3.61589	-1.07378
H	-6.74640	2.71215	-0.77239
H	-5.65016	3.08871	0.56380
H	-5.40475	0.67710	-0.16510
H	-5.01251	1.20536	-1.78832
H	-3.37608	1.87358	0.70190
H	-3.00346	2.39313	-0.92082
H	-3.18694	-0.54293	-0.07954
H	-2.74492	0.02151	-1.65026
H	2.82128	5.04913	0.58380
H	2.99059	5.44744	2.29808
H	3.79342	4.01718	1.63359
H	1.71748	3.37617	2.92198
H	0.74758	4.39797	1.88006
H	1.38334	2.99747	-0.08857
H	2.38054	2.00289	0.93033
H	-0.63525	2.33046	1.34266
H	0.40623	1.27942	2.24738
H	0.01568	2.00190	-3.65410
H	-1.09422	3.99687	-0.34534
H	-1.52960	-1.54327	-3.63134
H	-2.89762	-4.41390	-1.94971
H	-2.08270	-3.95182	-0.45326
H	-3.73843	-1.01860	2.25175
H	-3.54441	-0.93856	4.00393
H	-1.31306	1.88027	3.63882
H	3.56744	-2.57125	-4.97748
H	3.84500	-2.82883	-3.24921

H	2.42774	-3.53707	-4.03003
H	1.52305	-1.20956	-4.45990
H	2.92880	-0.52108	-3.67362
H	0.88570	-2.35519	-2.34256
H	2.29121	-1.70444	-1.54911
H	1.39588	0.64882	-1.99919
H	0.00288	-0.05381	-2.74694
H	-2.01156	-4.24577	4.25461
H	-2.80271	-4.94486	2.83874
H	-1.50241	-5.82729	3.64999
H	0.14565	-4.06179	2.95339
H	-0.63249	-4.76316	1.55040
H	-2.22911	-2.83491	1.48262
H	-1.44883	-2.14386	2.88141
H	0.01821	-2.70640	0.26171
H	0.68791	-1.93840	1.64199
H	2.83708	0.43729	2.88047
H	2.30163	-1.26500	2.83835
H	-1.65234	-3.27026	-3.97030
H	-0.28491	3.73135	-3.84206
H	-2.71817	1.45485	4.62376
C	-3.55638	-2.29024	-3.61539
H	-3.95371	-1.46819	-3.01481
H	-3.73063	-2.06864	-4.67343
H	-4.11647	-3.19738	-3.37027
C	-0.79374	-4.93539	-1.87505
H	0.12700	-4.56527	-1.41748
H	-0.98886	-5.94296	-1.49358
H	-0.63511	-5.01267	-2.95479
C	-2.07370	2.50619	-3.86476
H	-2.07690	2.39695	-4.95433
H	-2.43700	1.57583	-3.42025
H	-2.77724	3.30344	-3.60763
C	0.06945	5.26962	-1.63639
H	0.20763	5.50451	-2.69543
H	-0.25750	6.18648	-1.13551
H	1.03522	4.97513	-1.21879
H	-1.93912	4.47389	-1.82127
C	-1.02809	0.11589	4.84739
H	-0.19909	-0.26392	4.24367
H	-0.61368	0.65843	5.70339
H	-1.59077	-0.73991	5.23200
C	-4.87379	0.56295	3.17624
H	-5.76805	-0.05240	3.31900
H	-4.81842	1.26483	4.01341
H	-4.99241	1.13491	2.25330
C	4.49863	-0.97780	2.70232

H	4.91669	-0.50549	3.59502
H	4.58804	-2.06383	2.82447
C	4.13270	-0.25746	0.49965
C	4.38498	0.16243	-0.79234
C	6.46411	-0.37648	1.03787
C	5.72271	0.30483	-1.16072
H	3.57655	0.37494	-1.48120
C	6.75202	0.04037	-0.26222
H	7.26647	-0.58136	1.74063
H	5.95915	0.63472	-2.16744
H	7.78446	0.16379	-0.57245
C	5.14107	-0.52137	1.41728

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