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Electronic Supplementary Information

Selective formation of angular tricyclic compounds by ruthenium-mediated ring-rearrangement metathesis

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General

Reactions were conducted under inert atmosphere (dry N_2). All solvents were distilled before use. Flash chromatography employed silica gel (40-63μm particle size, 230-240 mesh). Melting points are uncorrected. ^{1}H NMR spectra were acquired at 500 MHz and ^{13}C NMR spectra at 125 MHz as $CDCl_3$ solutions. Some ^{13}C NMR shifts are followed in brackets by the number of attached hydrogens based on HSQC, and DEPT spectra.

Synthesis of substrates

(1*R*,4*S*,5*s*)-1,4-Diallylspiro[4.5]dec-7-ene-1,4-diol (7) and (1*R,4*R**)-1,4-diallylspiro[4.5]-dec-7-ene-1,4-diol (16)**

Method 1. A solution of allylmagnesium bromide (0.80 M in ether, 4.8 mL) was added rapidly to a solution of spiro[4.5]dec-7-ene-1,4-dione[6c] (0.105 g, 0.640 mmol) in anhydrous ether (5.0 mL) under argon. The solution was stirred at rt for 4 h. Saturated ammonium chloride solution was added, and the mixture was extracted with ether. The organic layer was dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. Flash chromatography (10% ethyl acetate/hexanes) of the residue provided the diastereomeric diallyl compounds **7** (68 mg, 43%) and **16** (64 mg, 40%) as colourless solids.

Method 2. A solution of allylmagnesium bromide (0.80 M in ether, 1.5 mL) was added dropwise via syringe to a solution of spiro[4.5]dec-7-ene-1,4-dione[6c] (180 mg, 1.10 mmol) in anhydrous ether (5.0 mL) under argon. The solution was stirred at rt for 15 min before TMSOTf (0.30 g, 1.35 mmol) was added. This solution was stirred for 20 min, and more of the allylmagnesium bromide solution (2.5 mL) was added. The solution was stirred at rt for 16 h. Saturated ammonium chloride solution was added, and the mixture was extracted with ether. The organic layer was dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. Flash chromatography (5% ethyl acetate/hexanes) of the residue failed to separate the major monoallyl isomer from a significant amount of unreacted diketone, but the minor monoallyl compound *(4R*,5S*)-4-allyl-4-hydroxyspiro[4.5]dec-7-en-1-one* (28 mg, 12%) was obtained as a colourless solid: mp: 64–67 ^{o}C; ^{1}H NMR δ 5.92 (1H, m), 5.79 (1H, m), 5.73 (1H, m), 5.29–5.21 (2H, m), 2.39–2.33 (4H, m), 2.16–2.02 (4H, m), 1.98–1.90 (2H, m), 1.66 (1H, br), 1.63–1.53 (2H, m); ^{13}C

NMR δ 219.3 (0, C-1), 132.5 (1), 126.0 (1), 125.6 (1), 120.6 (2), 81.3 (0, C-4), 55.1 (0), 40.0 (2), 33.2 (2), 31.8 (2), 25.5 (2), 25.0 (2), 22.3 (2). A solution of allylmagnesium bromide (0.80 M in ether, 3.0 mL) was added rapidly to a solution of the above (21 mg, 0.10 mmol) in anhydrous ether (2.0 mL) under argon at 0 ^{o}C. The solution was warmed to rt, and it was stirred at rt for 4 h. Saturated ammonium chloride solution was added, and the mixture was extracted with ether. The organic layer was dried over anhydrous $MgSO_4$, and it was concentrated under reduced pressure. Flash chromatography (10% ethyl acetate/hexanes) of the residue gave only **16** (19 mg, 73%).

For **7**: mp 50–51 ^{o}C; ^{1}H NMR δ 5.95 (2H, m), 5.74 (1H, m), 5.65 (1H, m), 5.14–5.08 (4H, m), 3.34 (2H, s), 2.36 (2H, dd, J = 13.5, 7.7 Hz), 2.27 (2H, dd, J = 13.5, 6.9 Hz), 2.21 (2H, narrow m), 1.89–1.81 (8H); ^{13}C NMR δ 135.1 (2C, 1), 127.6 (1), 125.9 (1), 118.4 (2C, 2), 86.2 (2C, 0), 51.2 (0), 42.1 (2C, 2), 35.9 (2C, 2), 29.0 (2), 23.2 (2), 20.9 (2).

For **16**: mp 72–73 ^{o}C; ^{1}H NMR δ 5.97 (1H, m), 5.89 (1H, m), 5.83 (1H, m), 5.72 (1H, m), 5.19–5.10 (4H, m), 2.74 (1H, dd, J = 13.9, 7.5 Hz), 2.45–2.37 (2H, m), 2.34–2.16 (4H, m), 2.08–1.93 (3H, m), 1.80 (1H, s), 1.77–1.72 (2H, m), 1.60–1.53 (2H, m), 1.58 (1H, s); ^{13}C NMR δ 135.6 (1), 134.6 (1), 127.6 (1), 126.8 (1), 119.6 (2), 118.5 (2), 84.1 (0), 83.5 (0), 51.7 (0), 43.4 (2), 42.3 (2), 35.8 (2), 34.3 (2), 28.3 (2), 23.9 (2), 23.2 (2).

(1*R*,4*S*,5*s*)-1,4-Diallyl-7-methylspiro[4.5]dec-7-ene-1,4-diol (10) and (1*R,4*R**)-1,4-diallyl-7-methylspiro[4.5]dec-7-ene-1,4-diol (20)**

$ZnCl_2$ (30 μL, 0.03 mmol) of a 1 M solution in ether was added to 3.0 mL of an ether solution of allylmagnesium bromide (0.8 M) followed by 7-methylspiro[4.5]dec-7-ene-1,4-dione[6d,e] (53 mg, 0.30 mmol) in ether (5.0 mL). The solution was stirred for 14 h. Work-up and purification was as for **7** and **16**. This provided **10** (38 mg, 48%) and **20** (18 mg, 23%) as colourless liquids, although **22** was not homogeneous by NMR.

For **10**: ^{1}H NMR δ 5.94 (2H, m), 5.45 (1H, narrow m), 5.15–5.07 (4H, m), 3.30 (2H, s), 2.36 (2H, dd, J = 13.5, 7.8 Hz), 2.22–2.14 (4H, m), 1.90–1.77 (6H), 1.70 (2H, br s), 1.66 (3H, br s); ^{13}C NMR δ 135.1 (2C, 1), 132.4 (0), 122.0 (1), 118.4 (2C, 2), 86.2 (2C, 0), 52.0 (0), 42.0 (2C, 2), 36.0 (2C, 2), 34.0 (2), 24.0 (3), 23.4 (2), 20.7 (2).

For **20**: (impure product) ^{1}H NMR δ 5.97 (1H, m), 5.92 (1H, m), 5.47 (1H, narrow m), 5.23–5.12 (4H, m), 2.78 (1H, dd, J = 13.9, 7.4 Hz), 2.45–2.38 (2H, m), 2.30 (1H, dd, J = 13.4, 8.4 Hz),

2.26 (1H, m), 2.17 (1H, br d, J = 17.3 Hz), 2.12–1.95 (3H, m), 1.89 (1H, br d, J = 17.3 Hz), 1.84–1.53 (9H); ^{13}C NMR δ 135.6 (1), 134.8 (0), 134.7 (1), 120.7 (1), 119.7 (2), 118.5 (2), 84.2 (0), 83.7 (0), 52.5 (0), 43.3 (2), 42.6 (2), 35.9 (2), 34.3 (2), 33.4 (2), 24.1 (2), 24.0 (3), 22.8 (2).

(1*R*,4*S*,5*s*)-1,4-Diallylspiro[4.6]undec-7-ene-1,4-diol (11) and (1*R*,4*S*,5*r*)-1,4-diallylspiro-[4.6]undec-7-ene-1,4-diol (12)

A solution of $ZnCl_2$ (1.0 M in ether, 45 μL) was added to solution of allylmagnesium bromide (0.8 M in ether, 5.0 mL, 4.0 mmol) under argon. This was stirred for 2 h at rt. A solution of spiro[4.6]undec-7-ene-1,4-dione[6d] (80 mg, 0.45 mmol) in ether (5 mL) was added, and the solution was stirred at rt for 16 h. Saturated aqueous NH_4Cl solution was added, and the mixture was extracted with ether. The combined ether extracts were washed with brine and dried over $MgSO_4$. The solution was concentrated under vacuum. Flash chromatography (10% ethyl acetate/hexane) of the residue yielded a 1:1 mixture of **11** and **12** (48 mg, 41%) as a colourless liquid: ^{1}H NMR δ 6.00–5.89 (4H), 5.70 (major isomer 1H, m), 5.53–5.43 (3H, m), 5.18–5.11 (8H), 3.46 (2H, s), 3.42 (2H, s), and other multiplets: 2.51–2.24, 2.09, 1.95–1.75, 1.50; ^{13}C NMR δ 135.0, 129.8, 129.6, 127.0, 126.3, 118.6, 86.7, 86.6, 59.4, 59.1, 42.9, 42.0, 35.5, 35.1, 33.1, 32.8, 30.8, 29.1, 25.0, 22.3, 21.7, 21.5.

(1*R,5*R**)-1,5-Diallylspiro[5.5]undec-8-ene-1,5-diol (18)**

$BF_3.OEt_2$ (18.9 mL, 133 mmol) was added dropwise to a solution of 1,4-dioxaspiro[4.5]dec-7-ene (1.24 g, 8.87 mmol) and 1,2-bis(trimethylsilyloxy)-cyclopent-1-ene (2.80 g, 11.5 mmol) in CH_2Cl_2 (80 mL) at −78 ºC. The resulting yellow solution was stirred at −78 ºC for 2 h, after which time TLC analysis indicated that none of the ketal remained. The solution was warmed to 0 ºC over 15 min and stirred at 0 ºC for an additional 1 h, during which time the solution darkened substantially. The solution was then poured into cold sat. aqueous $NaHCO_3$ solution (150 mL). The aqueous layer was re-extracted thoroughly with CH_2Cl_2, and the combined organic layers were washed with brine and dried over Na_2SO_4. Removal of the solvent under reduced pressure gave a dark oil. Flash column chromatography (10% EtOAc/hexanes) provided *spiro[5.5]undec-8-ene-1,5-dione* (0.815 g, 52%) as a low-melting solid: mp 38–40 °C; ^{1}H NMR

δ 5.75 (1H, m), 5.59 (1H, m), 2.87 (2H, ddd, J = 15.3, 11.1, 6.0 Hz), 2.60 (2H, dt, J = 15.3, 5.0 Hz), 2.45 (2H, narrow m), 2.08 (1H, m), 2.05 (4H, apparent s), 1.78 (1H, m); ^{13}C NMR δ 208.2, 125.1, 124.0, 66.4, 36.9, 30.6, 26.1, 22.5, 18.4; HRMS (ESI-TOF) *m/z* 201.0878, $[C_{11}H_{14}O_2 + Na]^+$ requires 201.0886. A 2 M solution of allylmagnesium chloride in THF (7.2 mL, 14.3 mmol) was added dropwise to a solution of the above compound (0.638 g, 3.58 mmol) in THF (30 mL) at −78 ºC. The solution was stirred at −78 ºC for 2 h. The solution was then warmed to rt, and sat. aqueous NH_4Cl (30 mL) was added. The aqueous layer re-extracted thoroughly with Et_2O. The combined organic layers were washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. Flash chromatography (50% CH_2Cl_2/hexanes) of the residue provided much ring-opened material and **18** (122 mg, 13%) as a colourless solid: mp 98–99 °C; ^{1}H NMR δ 5.92 (2H, m), 5.83 (2H, s), 5.21 (1H, dd, J = 10.2, 2.3 Hz), 5.17–5.14 (2H, m), 5.12 (1H, m), 3.05 (1H, br s), 2.54 (1H, br s), 2.46 (4H, m), 2.23 (3H, m), 1.93 (2H, m), 1.71 (1H, m), 1.62–1.46 (6H, m); ^{13}C NMR δ 135.9 (1), 134.9 (1), 128.2 (1), 127.3 (1), 119.9 (2), 118.6 (2), 77.9 (0), 77.7 (0), 46.4 (0), 42.5 (2), 40.1 (2), 33.5 (2), 33.3 (2), 27.0 (2), 24.5 (2), 22.2 (2), 18.5 (2); HRMS (ESI-TOF) *m/z* 285.1822, $[C_{17}H_{26}O_2 + Na]^+$ requires 285.1825.

(1*R,4*S**,5*R**)-1-Allyl-4-vinylspiro[4.5]dec-7-ene-1,4-diol (21)**

A solution of $ZnCl_2$ (1.0 M in ether, 0.10 mL) was added to solution of vinylmagnesium bromide (1.0 M in THF, 6.0 mL, 6.0 mmol) at rt under argon. The solution was stirred at rt for 2 h. The solution was cooled in an ice bath, and a solution of spiro[4.5]dec-7-ene-1,4-dione[6c] (160 mg, 0.98 mmol) in ether (10 mL) was added, and the mixture was stirred at rt for 15 h. Sat. aqueous NH_4Cl solution was added, and the mixture was extracted thoroughly with ether. The combined ether extracts were washed with brine and dried over $MgSO_4$. The solution was concentrated under vacuum. Flash chromatography (10% ethyl acetate/hexane) of the residue yielded two monovinyl products, *(4R*,5R*)-4-hydroxy-4-vinylspiro[4.5]dec-7-en-1-one* (104 mg, 54%) and *(4R*,5S*)-4-hydroxy-4-vinylspiro[4.5]dec-7-en-1-one* (22 mg, 11%) as liquids. For the major product: ^{1}H NMR δ 6.07 (1H, dd, J = 17.0, 11.0 Hz), 5.71 (1H, m), 5.60 (1H, m), 5.37 (1H, dd, J = 17.0, 0.9 Hz), 5.14 (1H, dd, J = 11.0, 0.9 Hz), 2.52 (1H, m), 2.33 (1H, m), 2.29–1.90 (6H), 1.85 (1H, m), 1.76–1.70 (2H, m); ^{13}C NMR δ 220.1, 140.5, 127.8, 123.5, 113.7, 82.1, 54.7, 34.0, 33.1, 28.9, 22.3, 22.0; HRMS (EI) *m/z* 192.1157, $[C_{12}H_{16}O_2]^+$ requires

192.1150. For the minor product: ^{1}H NMR δ 6.04 (1H, dd, J = 17.2, 10.8 Hz), 5.79–5.66 (2H, m), 5.40 (1H, dd, J = 17.2, 0.9 Hz), 5.30 (1H, dd, J = 10.8, 0.9 Hz), 2.47–2.33 (3H, m), 2.09–1.89 (6H), 1.64 (1H, m), 1.50 (1H, m); ^{13}C NMR δ 218.8, 139.2, 125.9, 125.5, 115.9, 82.8, 55.7, 33.2, 32.4, 25.4, 24.6, 22.1; HRMS (EI) *m/z* 192.1157, $[C_{12}H_{16}O_2]^+$ requires 192.1150. A solution of $ZnCl_2$ (1.0 M in ether, 0.05 mL) was added to solution of allylmagnesium bromide (0.8 M in ether, 3.8 mL, 1.5 mmol) at rt under argon. The solution was stirred at rt for 2 h. Then the solution was cooled in an ice bath, and the major mono-vinyl product, (4*R**,5*R**)-4-hydroxy-4-vinylspiro[4.5]dec-7-en-1-one, (96 mg, 0.5 mmol) in ether (2.0 mL) was added. The mixture was stirred at rt for 15 h. Sat. aqueous NH_4Cl solution was added, and the mixture was extracted thoroughly with ether. The combined ether extracts were washed with brine and dried over $MgSO_4$. The solution was concentrated under vacuum. Flash chromatography (10% ethyl acetate/hexane) of the residue yielded **21** (92 mg, 90%) as a colourless solid: mp 89–90 °C; ^{1}H NMR δ 6.00 (1H, dd, J = 17.2, 10.8 Hz), 5.94 (1H, m), 5.68 (1H, m), 5.62 (1H, m), 5.32 (1H, dd, J = 17.2, 1.6 Hz), 5.16–5.11 (2H, m), 5.05 (1H, dd, J = 10.8, 1.6 Hz), 3.51 (1H, s), 3.20 (1H, s), 2.39 (1H, m), 2.34 (1H, m), 2.19–1.79 (10H); ^{13}C NMR δ 141.2 (1), 134.9 (1), 127.9 (1), 125.5 (1), 118.8 (2), 113.5 (2), 86.7 (0), 86.1 (0, C-1), 52.3 (0), 42.2 (2), 36.6 (2), 36.4 (2), 29.4 (2), 22.8 (2), 20.9 (2); HRMS (EI) *m/z* 216.1516, $[C_{15}H_{22}O_2 - H_2O]^+$ requires 216.1514.

(1*R,5*S**,6*R**)-1-Allyl-5-vinylspiro[5.5]undec-8-ene-1,5-diol (24) and (1*R**,5*R**,6*R**)-1-allyl-5-vinylspiro[5.5]undec-8-ene-1,5-diol (25)**

A 2 M solution of allylmagnesium chloride in THF (0.92 mL, 1.84 mmol) was added dropwise to a solution of spiro[5.5]undec-8-ene-1,5-dione (326 mg, 1.83 mmol) in THF (16 mL) under dry N_2 at −78 ºC. The solution was stirred at −78 ºC for 1 h before it was warmed to rt. Sat. aqueous NH_4Cl solution (20 mL) was added, and the aqueous layer was re-extracted thoroughly with Et_2O. The combined organic layers were washed with brine and dried over Na_2SO_4. Concentration under vacuum gave a colourless residue that was subjected to flash chromatography (60–80% CH_2Cl_2/hexanes), which provided the mono-allyl compound *(5R*,6R*)-5-allyl-5-hydroxyspiro[5.5]undec-8-en-1-one* (110 mg, 41%) as a solid, **18** (14 mg, 3%), recovered diketone (35 mg, 11%) and ring-opened products. For the mono-allyl compound: mp 80–82 °C; IR (film) λ 3476, 3073, 3024, 2934, 1705, 1659, 1638 cm^{-1}; ^{1}H NMR δ 5.83 (1H,

m), 5.72 (1H, m), 5.59 (1H, m), 5.16 (1H, br d, J = 10.2 Hz), 5.09 (1H, dq, J = 17.1, 1.4 Hz), 2.65 (1H, td, J = 13.3, 7.1 Hz), 2.39 (1H, m), 2.26 (3H, m), 2.09 (3H, m), 2.03–1.75 (5H), 1.66 (1H, s), 1.52 (1H, qt, J = 13.4, 5.1 Hz); ^{13}C NMR δ 212.5 (0), 132.9 (1), 126.1 (1), 124.7 (1), 119.2 (2), 77.9 (0), 57.9 (0), 38.6 (2), 36.1 (2), 30.4 (2), 26.4 (2), 25.5 (2), 22.5 (2), 20.0 (2); HRMS (ESI-TOF) *m/z* 243.1364, $[C_{14}H_{20}O_2 + Na]^+$ requires 243.1361. THF (0.3 mL) was added to anhydrous $CeCl_3$ (111 mg, 0.45 mmol), and the resulting suspension was stirred for 30 min at rt. The suspension was then cooled to −78 °C, and a 1 M solution of vinylmagnesium bromide in THF (0.50 mL, 0.50 mmol) was added dropwise. The yellow suspension was stirred at −78 °C for 2 h. A solution of (5*R**,6*R**)-5-allyl-5-hydroxyspiro[5.5]undec-8-en-1-one (50 mg, 0.21 mmol) in THF (1.3 mL) was then added dropwise to the cold suspension, and this was stirred at −78 °C for 1 h. The mixture was warmed to rt, and 5% aqueous citric acid solution (5 mL) was added. The mixture was extracted thoroughly with Et_2O, and the combined organic layers were washed with brine and dried over Na_2SO_4. Evaporation of the solvent and flash chromatography of the residue (5–10% EtOAc/hexanes) gave **24** and **25** (36 mg, 63%) as an inseparable 3:1 mixture; IR (film) λ 3302, 3075, 3022, 2928, 1638 cm^{-1}; HRMS (ESI-TOF) *m/z* 271.1671, $[C_{16}H_{24}O_2 + Na]^+$ requires 271.1669.

For **24** (data from the mixture): ^{1}H NMR δ 6.08 (1H, dd, J = 17.9, 10.1 Hz), 5.87 (1H, m), 5.76 (1H, m), 5.68 (1H, m), 5.29 (1H, dd, J = 17.2, 1.6 Hz), 5.17 (1H, m), 5.09 (1H, m), 5.02 (1H, dd, J = 10.9, 1.6 Hz), 3.85 (1H, s), 3.22 (1H, s), 2.51 (1H, dd, J = 13.7, 7.5 Hz), 2.37 (1H, m), 2.16 (1H, dd, J = 13.7, 7.5 Hz), 2.06–1.78 (6H, m), 1.72–1.44 (4H, m), 1.38 (1H, m); ^{13}C NMR δ 143.5 (1), 134.1 (1) , 127.7 (1), 126.3 (1), 119.2 (2), 112.7 (2), 79.3 (0), 78.5 (0), 44.6 (0), 41.9 (2), 35.3 (2), 32.4 (2), 28.1 (2), 23.9 (2), 21.1 (2), 16.3(2).

For **25** (data from the mixture): ^{1}H NMR δ 6.05 1H, m), 4.05 (1 H, s), 3.32 (1 H, s), other signals overlapped by signals of **24**; ^{13}C NMR δ 143.1 (1), 134.0 (1), 129.4 (1), 126.4 (1), 119.9 (2), 114.4 (2), 79.7 (0), 78.8 (0), 45.5 (0), 42.6 (2), 33.2 (2), 32.1 (2), 26.1 (2), 24.0 (2), 23.6 (2), 16.6 (2).

(1*R,4*R**,5*S**)-1-Allyl-4-(3-butenyl)spiro[4.5]dec-7-ene-1,4-diol (28)**

Following the procedure for **21**, spiro[4.5]dec-7-ene-1,4-dione[6c] (66 mg, 0.40 mmol) with

$ZnCl_2$ (40 μL of a 1 M solution in ether) and but-3-en-1-ylmagnesium bromide (6.0 mL of a 0.67 M solution in ether) yielded *(4R*,5S*)-4-(3-butenyl)-4-hydroxyspiro[4.5]dec-7-en-1-one* (28 mg, 32%) as a colourless liquid: ^{1}H NMR δ 5.87 (1H, m), 5.77 (1H, m), 5.63 (1H, m), 5.08 (1H, d of narrow m, J = 18 Hz), 5.00 (1H, d of narrow m, J = 10 Hz), 2.44 (1H, m), 2.35–1.83 (10H), 1.77–1.60 (4H, m); ^{13}C NMR δ 220.4 (0), 138.9 (1), 127.5 (1), 123.8 (1), 115.3 (2), 82.3 (0), 54.7 (0), 35.2 (2), 33.8 (2), 30.7 (2), 28.2 (2), 28.1 (2), 22.5 (2C, 2). To a mixture of $ZnCl_2$ (8 μL of a 1.0 M solution) and allylmagnesium bromide (0.8 M) 1.0 mL was added the mono-butenyl compound (18 mg, 0.082 mmol), and, after 16 h at rt, workup and flash chromatography provided **28** (18 mg, 84%) as a colourless liquid: ^{1}H NMR δ 5.96–5.82 (2H, m), 5.73 (1H, m), 5.65 (1H, m), 5.16 (1H, d of narrow m, J = 10.3 Hz), 5.13 (1H, d of narrow m, J = 17.0 Hz), 5.03 (1H, d of narrow m, J = 17.1 Hz), 4.94 (1H, d of narrow m, J = 10.2 Hz), 3.63 (1H, s), 2.89 (1H, s), 2.38–2.30 (3H, m), 2.20 (2H, m), 2.09 (1H, m), 1.98–1.79 (8H), 1.70 (1H, ddd, J = 13.4, 11.4, 5.2 Hz), 1.55 (1H, dddd, J = 13.4, 11.3, 4.9, 1.0 Hz); ^{13}C NMR δ 139.9, 134.8, 127.5, 126.1, 119.1, 114.4, 87.1, 86.4, 51.5, 42.4, 36.4, 36.0, 35.6, 29.1, 29.0, 23.3, 20.8; HRMS (EI) *m/z* 244.1834, $[C_{17}H_{26}O_2 - H_2O]^+$ requires 244.1827.

(1*R,4*R**,5*S**)-1-Allyl-4-(4-pentenyl)spiro[4.5]dec-7-ene-1,4-diol (29)**

Following the procedure for **21**, spiro[4.5]dec-7-ene-1,4-dione[6c] (66 mg, 0.40 mmol) with $ZnCl_2$ (40 μL of a 1 M solution in ether) and pent-4-en-1-ylmagnesium bromide (6.0 mL of a 0.67 M solution in ether) yielded *(4R*,5S*)-4-(4-pentenyl)-4-hydroxyspiro[4.5]dec-7-en-1-one* (30 mg, 32%) as a colourless liquid: ^{1}H NMR δ 5.84–5.75 (2H, m), 5.64 (1H, m), 5.02 (1H, d of narrow m, J = 17.2 Hz), 4.98 (1H, d of narrow m, J = 10.4 Hz), 2.42 (1H, m), 2.34–2.21 (2H, m), 2.14–1.94 (6H, m), 1.93–1.83 (2H, m), 1.64–1.45 (5H, m); ^{13}C NMR δ 220.3 (0), 138.5 (1), 127.5 (1), 123.8 (1), 115.2 (2), 82.2 (0), 54.7 (0), 35.5 (2), 34.3 (2), 33.9 (2), 30.6 (2), 28.0 (2), 22.8 (2), 22.6 (2), 22.5 (2);. HRMS (ESI-TOF) *m/z* 257.1497, $[C_{15}H_{22}O_2 + Na]^+$ requires 257.1512. Addition of $ZnCl_2$/allylmagnesium bromide gave **29** as an oil following flash chromatography (5% ethyl acetate/hexane): ^{1}H NMR δ 5.91 (1H, m), 5.81 (1H, m), 5.73 (1H, m), 5.64 (1H, m), 5.13 (2H, m), 5.00 (1H, ddd, J = 17.2, 4.1, 1.8 Hz), 4.93 (1H, d of narrow m, J = 10.5 Hz), 3.60 (1H, br s), 3.00 (1H, br s), 2.33 (2H, m), 2.20 (2H, m), 2.04 (1H, m), 1.96–1.75

(8H, m), 1.67 (1H, m), 1.57 (1H, m), 1.47 (1H, m), 1.39 (1H, m); ^{13}C NMR δ 139.1 (1), 134.9 (1), 127.4 (1), 126.1 (1), 118.9 (2), 114.6 (2), 87.2 (0), 86.3 (0), 51.4 (0), 42.5 (2), 36.4 (2), 36.0 (2), 35.4 (2), 34.7 (2), 29.0 (2), 23.9 (2), 23.2 (2), 20.8 (2); HRMS (ESI-TOF) *m/z* 299.1976, $[C_{18}H_{28}O_2 + Na]^+$ requires 299.1982.

Ring-rearrangement metathesis reactions

RRM of 6: (4a*R**,6a*S**,11a*S**)-4,4a,5,6,6a,7,10,11-octahydro-1*H*-benz[*c*]azulene-4a,6a-diol (8)

Ruthenium catalyst **6** (34 mg, 0.04 mmol) was added to a stirred solution of **7** (100 mg, 0.403 mmol) in dry benzene (30 mL) under argon. The mixture was maintained under gentle reflux for 2 h at which time TLC indicated that **7** had been consumed. Distilled water was added, and the mixture was extracted with ether. The combined ether extracts were washed with brine before being dried over $MgSO_4$. The solution was concentrated under reduced pressure, and flash chromatography (20% EtOAc/hexanes) of the residue afforded **8** (80.0 mg, 90%) as a colourless solid: mp 114–115 ^{o}C; ^{1}H NMR δ 5.87 (1H, m), 5.61–5.47 (3H, m), 4.56 (1H, s), 2.98 (1H, s), 2.45 (1H, d of narrow m, J = 16.6 Hz), 2.34–2.21 (5H), 2.12–1.85 (6H), 1.67 (1H, m), 1.48 (1H, dt, J = 14.7, 4.1 Hz); ^{13}C NMR δ 133.4 (1), 126.0 (1), 125.1 (1), 123.3 (1), 84.9 (0), 83.5 (0), 50.9 (0), 36.3 (2C, 2), 35.6 (2), 34.2 (2), 29.7 (2), 24.2 (2), 22.0 (2); HRMS (EI) *m/z* 202.1362, $[C_{14}H_{20}O_2 - H_2O]^+$ requires 202.1358.

(4a*R**,6a*R**,11a*S**)-4,4a,5,6,6a,7,8,11-Octahydro-1*H*-benz[*c*]azulene-4a,6a-diol (9)

During crystallization of **8** from ethyl acetate-hexanes over 30 days, some double-bond isomerization occurred giving crystals that were a 1:1 mixture of **8** and **9**. The following (partial) NMR data for **9** are from mixtures of **8** and **9**: ^{1}H NMR δ 5.70 (1H, m); ^{13}C NMR δ 130.2, 128.1, 124.6, 123.8, 87.1, 84.1, 49.6, 37.9, 35.4, 34.8, 32.3 (2C), 26.0, 23.6.

RRM of 11 and 12: (4a*R,6a*R**,12a*R**)-1,4,4a,5,6,6a,7,8,11,12-decahydrocyclooct[*c*]-indene-4a,6a-diol (11) and (4a*R**,6a*R**,12a*S**)-1,4,4a,5,6,6a,7,10,11,12-decahydrocyclo-oct[*c*]indene-4a,6a-diol (12)**

Following the procedure for **8**, a mixture of **11** and **12** (44 mg, 0.17 mmol) with **6** (8 mg, 0.009 mmol) in benzene (10 mL) under reflux for 2 h yielded 26 mg of a mixture of containing **13** (*ca.* 45%) with dimeric material, and **14** (8 mg, 20%) after flash chromatography and crystallization from ethyl acetate-hexanes. Further flash chromatography and repeated recrystallization from CH_2Cl_2 provided pale yellow crystals of **13**: mp 136–138 °C; ^{1}H NMR δ 5.82 (2H, m), 5.74 (1H, narrow m), 5.54 (1H, narrow m), 3.88 (1H, br s), 2.66 (1H, m), 2.59 (1H, br s), 2.53–2.37 (3H, m), 2.31–2.21 (2H, m), 2.16–2.02 (4H, m), 1.85 (1H, m), 1.76–1.62 (2H, m), 1.54 (1H, m), 1.43 (1H, m), 1.25 (1H, m); ^{13}C NMR δ 132.0, 130.2, 127.4, 123.4, 87.5, 85.5, 51.5, 39.9, 37.7, 36.6, 33.7, 32.4, 27.8, 27.3, 26.2; HRMS (ESI-TOF) *m/z* 257.1508, $[C_{15}H_{22}O_2 + Na]^+$ requires 257.1512.

For **14**: mp 132–134 °C; ^{1}H NMR δ 6.00 (2H, m), 5.58 (1H, m), 5.52 (1H, m), 4.29 (1H, br s), 3.36 (1H, br s), 2.56–2.44 (2H, m), 2.38 (1H, m), 2.24–2.15 (2H, m), 2.10–1.89 (7H), 1.86–1.71 (3H, m), 1.59 (1H, ddd, J = 14.9, 7.8, 2.2 Hz); ^{13}C NMR δ 135.5 (1), 132.4 (1), 124.9 (1), 123.6 (1), 88.6 (0), 83.8 (0), 52.0 (0), 40.3 (2), 40.2 (2), 35.8 (2), 33.7 (2), 30.0 (2), 26.7 (2), 23.8 (2), 22.4 (2); HRMS (EI) *m/z* 216.1515, $[C_{15}H_{22}O_2 - H_2O]^+$ requires 216.1514.

RRM of 16: (4a*R,6a*R**,11a*S**)-4,4a,5,6,6a,7,10,11-octahydro-1*H*-benz[*c*]azulene-4a,6a-diol (17)**

Following the procedure for **8**, **16** (100 mg, 0.403 mmol) with **6** (34 mg, 0.04 mmol) in dry benzene (10 mL) under reflux for 2 h provided **17** (76 mg, 85%) as a colourless liquid: ^{1}H NMR δ 5.75 (1H, m), 5.57 (1H, m), 5.51 (1H, m), 5.44 (1H, m), 3.49 (1H, d of narrow m, J = 17.0 Hz), 2.49 (1H, s), 2.48 (1H, overlapped), 2.30 (1H, dd, J = 17.0, 8.3 Hz), 2.27–2.20 (3H, m), 2.21–2.11 (2H, m), 2.08–1.90 (4H, m), 1.47 (1H, m), 1.39 (1H, br dd, J = 14.2, 6.1 Hz), 1.25 (1H, br s); ^{13}C NMR δ 132.2 (1), 126.2 (1), 125.4 (1), 123.4 (1), 86.4 (0), 83.0 (0), 50.7 (0), 43.0 (2), 38.0 (2), 36.6 (2), 35.2 (2), 30.1 (2), 25.5 (2), 24.9 (2); HRMS (EI) *m/z* 202.1356, $[C_{14}H_{20}O_2 - H_2O]^+$ requires 202.1358.

RRM of 18: (4a*R,7a*R**,12a*R**)-1,4,4a,5,6,7,7a,8,11,12-decahydrocyclohepta[*d*]naphthalene-4a,7a-diol (19)**

Ruthenium catalyst **6** (16 mg, 0.019 mmol) was added to a solution of **18** (100 mg, 0.382 mmol) in benzene (32 mL) under dry N_2, and this mixture was heated under reflux for 1 h. The solution was cooled to rt, and the solvent was removed under reduced pressure. Flash chromatography (15% EtOAc/hexanes) of the residue provided **19** (55 mg, 61%) as a solid: mp 97–98 °C; ^{1}H NMR δ 5.90 (1H, m), 5.56 (3H, m), 3.83 (1H, m), 2.60 (1H, s), 2.49 (1H, m), 2.32 (2H, m), 2.17 (2H, m), 2.03-1.74 (3H, m), 1.62 (1H, m), 1.48 (1H, m), 1.22 (1H, m); ^{13}C NMR δ 132.2 (1), 127.2 (1), 125.7 (1), 123.5 (1), 77.2 (0), 74.5 (0), 45.9 (0), 41.1 (2), 40.3 (2), 39.8 (2), 35.2 (2), 31.2 (2), 29.4 (2), 25.1 (2), 18.3 (2); HRMS (ESI-TOF) *m/z* 257.1502, $[C_{15}H_{22}O_2 + Na]^+$ requires 257.1512.

RRM of 23: (4a*R,6a*S**,10a*S**)-1,2,5,6,7,10-hexahydrobenz[*c*]indene-4a,6a-diol (22) and (3a*R**,5a*S**, 10a*S**)-1,3a,4,5,5a,6,9,10-octahydrocyclopent[*c*]azulene-3a,5a-diol (23)**

Following the procedure for **8**, **21** (94 mg, 0.403 mmol) with **6** (34 mg, 0.04 mmol) in benzene (30 mL) under reflux for 2 h provided **22** (33 mg, 40%) and **23** (35 mg, 43%) as solids.

For **22**: mp 132–133 °C; ^{1}H NMR δ 6.08 (1H, dt, J = 9.7, 2.2 Hz), 5.79 (1H, dt, J = 9.7, 3.3 Hz), 5.58 (1H, m), 5.49 (1H, m), 4.81 (1H, s), 2.37–1.92 (10H), 2.23 (1H, s), 1.63–1.53 (2H, m); ^{13}C NMR δ 132.2 (1), 130.9 (1), 124.6 (1), 124.4 (1), 83.4 (0), 80.9 (0), 47.4 (0), 37.6 (2), 34.2 (2), 32.7 (2), 32.3 (2), 23.0 (2), 18.9 (2); HRMS (EI) *m/z* 188.1196, $[C_{13}H_{18}O_2 - H_2O]^+$ requires 188.1201.

For **23**: mp 61–62 °C; ^{1}H NMR δ 5.96 (1H, br m), 5.68 (1H, narrow m), 5.60 (1H, narrow m), 5.55 (1H, br m), 2,48 (1H, d of narrow m, J = 17.1 Hz), 2.40 (1H, dd, J = 15.9, 7.9 Hz), 2.37–2.19 (4H), 2.14 (1H, d of narrow m, J = 17.1 Hz), 2.11–2.00 (2H, m), 1.87 (1H, s), 1.84 (1H, s), 1.76–1.63 (2H, m), 1.38 (1H, dt, J = 14.4, 4.0 Hz); ^{13}C NMR δ 136.7 (1), 133.9 (1), 128.0 (1), 126.1 (1), 95.5 (0), 81.4 (0), 62.0 (0), 41.3 (2), 39.4 (2), 36.7 (2), 36.2 (2), 26.1 (2), 24.3 (2); HRMS (EI) *m/z* 188.1194, $[C_{13}H_{18}O_2 - H_2O]^+$ requires 188.1201.

RRM of 26 and 27: (4a*R,7a*R**,11a*R**)-2,4a,5,6,7,7a,8,11-octahydro-1*H*-benz[*d*]naphthalene-4a,7a-diol (26) and (4a*R**,7a*S**,11a*S**)-2,4a,5,6,7,7a,8,11-octahydro-1*H*-benz[*d*]-naphthalene-4a,7a-diol (27)**

Catalyst **6** (6 mg, 7 μmol) was added to a solution of **24** and **25** (3:1, respectively) (35 mg, 0.14 mmol) in benzene (20 mL). The solution was heated under reflux for 30 min. The solution was cooled, and the solvent removed under vacuum. Flash chromatography (15% EtOAc/hexanes) of the residue gave **26** (21 mg, 90% from **24**) and **27** (7 mg, 90% from **25**) as solids.

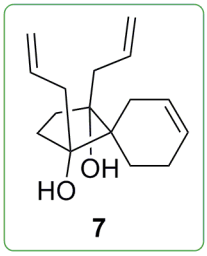
For **26**: mp 118–120 °C; ^{1}H NMR δ 5.76 (1H, dt, J = 9.8, 3.6 Hz), 5.60 (1H, dt, J = 9.8, 2.3 Hz), 5.55 (1H, m), 5.47 (1H, m), 4.98 (1H, s), 2.33 (1H, s), 2.29 (1H, m), 2.25 (1H, m), 2.21 (1H, m), 2.17–2.02 (4H, m), 2.00 (1H, m), 1.96 (1H, m), 1.93 (1H, m), 1.88 (1H, dt, J = 13.5, 4.8 Hz), 1.56 (1H, m), 1.40 (1H, m); ^{13}C NMR δ 132.5 (1), 131.0 (1), 124.6 (1), 123.6 (1), 73.7 (0), 73.5 (0), 40.3 (0), 38.1 (2), 34.2 (2), 32.5 (2), 30.1 (2), 23.0 (2), 18.2 (2), 16.7 (2); HRMS (ESI-TOF) *m/z* 243.1351, $[C_{14}H_{20}O_2 + Na]^+$ requires 243.1356.

For **27**: mp 115–116 °C; ^{1}H NMR δ 5.79 (1H, m), 5.54 (1H, m), 5.50 (1H, dt, J = 10.2, 3.6 Hz), 5.45 (1H, dt, J = 10.2, 2.2 Hz), 3.78 (1H, s), 2.85 (1H, s), 2.57 (1H, m), 2.22 (1H, m), 2.06 (2H, m), 1.96 (1H, m), 1.87 (1H, m), 1.80–1.63 (5H, m), 1.60–1.45 (3H, m); ^{13}C NMR δ 134.5 (1), 127.3 (1), 124.7 (1), 122.4 (1), 74.5 (0), 73.4 (0), 40.7 (0), 38.1 (2), 37.3 (2), 33.5 (2), 24.4 (2), 23.9 (2), 22.7 (2), 16.6 (2); HRMS (ESI-TOF) *m/z* 243.1357, $[C_{14}H_{20}O_2 + Na]^+$ requires 243.1356.

RRM of 28 and 29

Following the procedure for **8**, **28** (18 mg, 0.069 mmol) with **6** (6 mg, 0.007 mmol) in dry benzene (5 mL) under reflux for 2 h yielded **14** (11 mg, 69%). Similarly, **29** (90 mg, 0.33 mmol) with **6** (28 mg, 0.033 mmol) yielded **14** (15 mg, 21%).

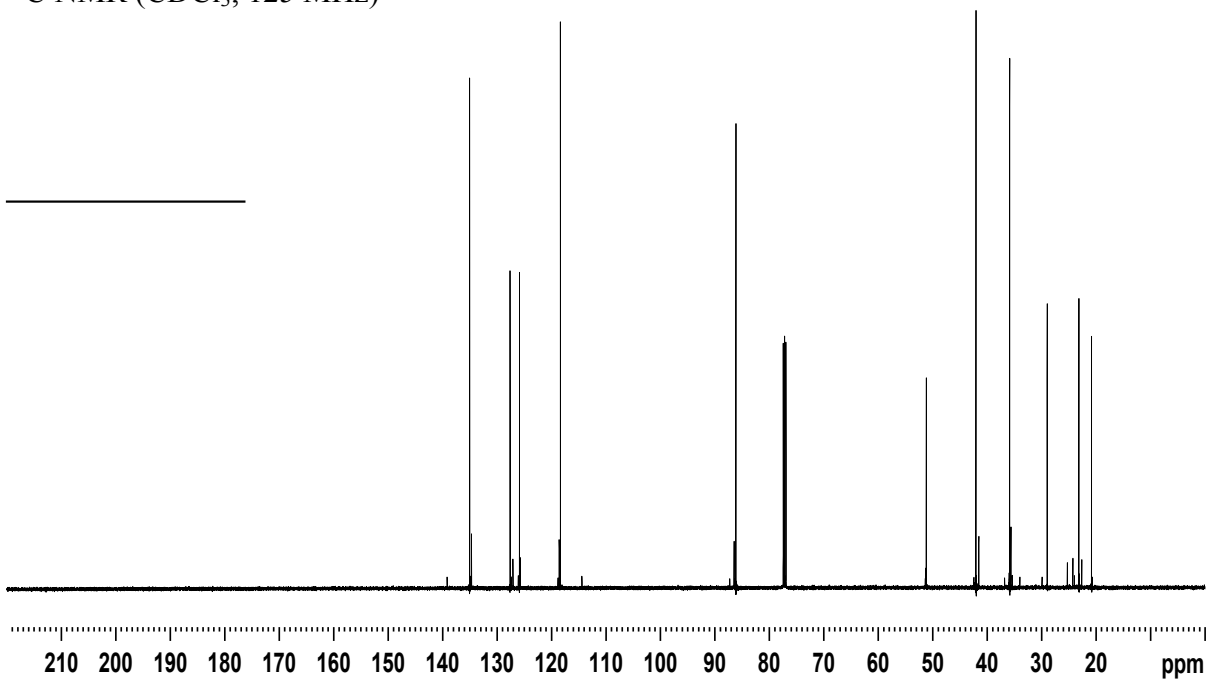
NMR spectra of (1*R*,4*S*,5*s*)-1,4-diallylspiro[4.5]dec-7-ene-1,4-diol (6)



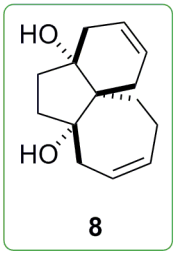
7

^{1}H NMR ($CDCl_3$, 500 MHz)

^{13}C NMR ($CDCl_3$, 125 MHz)

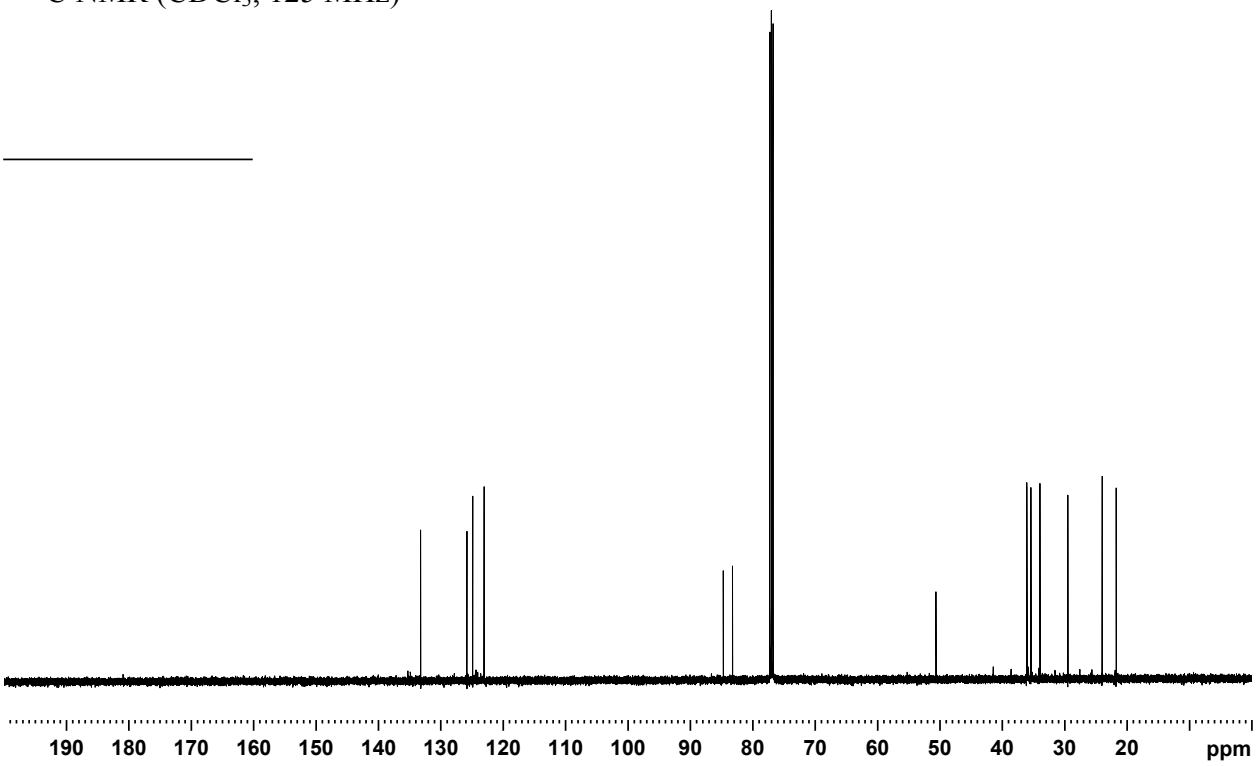


NMR spectra of (4a*R,6a*S**,10a*S**)-4,4a,5,6,6a,7,10,11-octahydro-1*H*-benz[*c*]azulene-4a,6a-diol (8)**



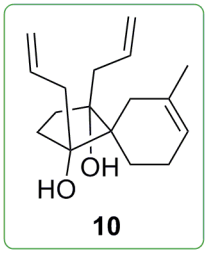
^{1}H NMR ($CDCl_3$, 500 MHz)

^{13}C NMR ($CDCl_3$, 125 MHz)



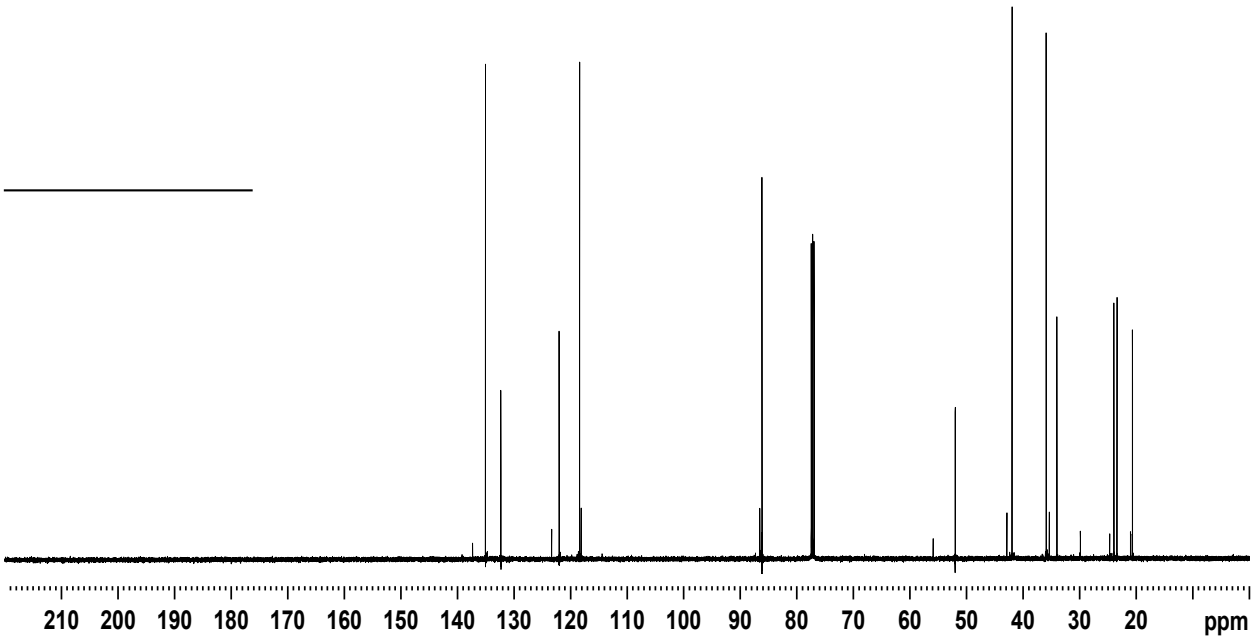
NMR spectra of (1*R*,4*S*,5*s*)-1,4-diallyl-7-methylspiro[4.5]dec-7-ene-1,4-diol 10)

^{1}H NMR ($CDCl_3$, 500 MHz)

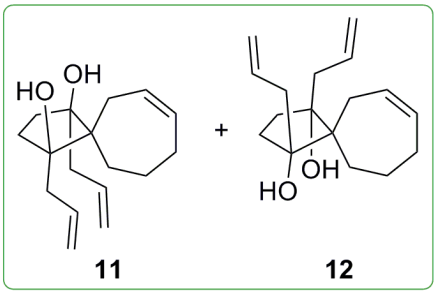


10

^{13}C NMR ($CDCl_3$, 125 MHz)

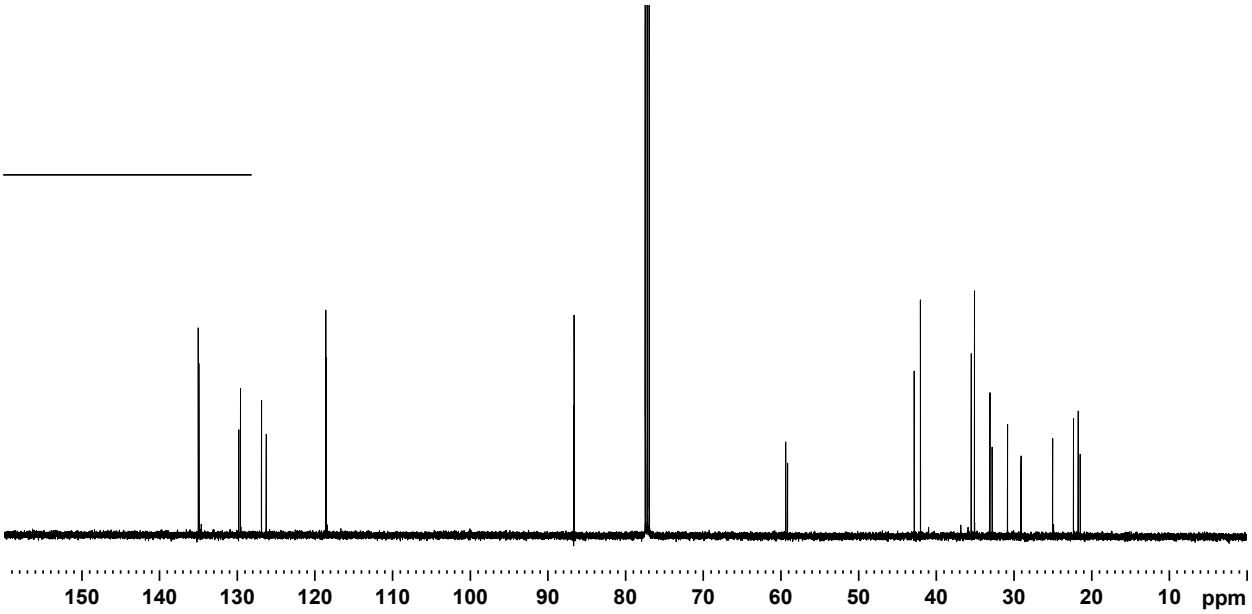


NMR spectra of 1*R*,4*S*,5*s*)-1,4-diallylspiro[4.6]undec-7-ene-1,4-diol (11) and (1*R*,4*S*,5*r*)-1,4-diallylspiro[4.6]undec-7-ene-1,4-diol (12) (1:1 mixture)

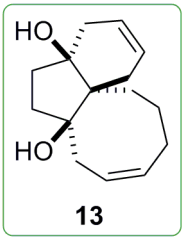


^{1}H NMR ($CDCl_3$, 500 MHz)

^{13}C NMR ($CDCl_3$, 125 MHz)

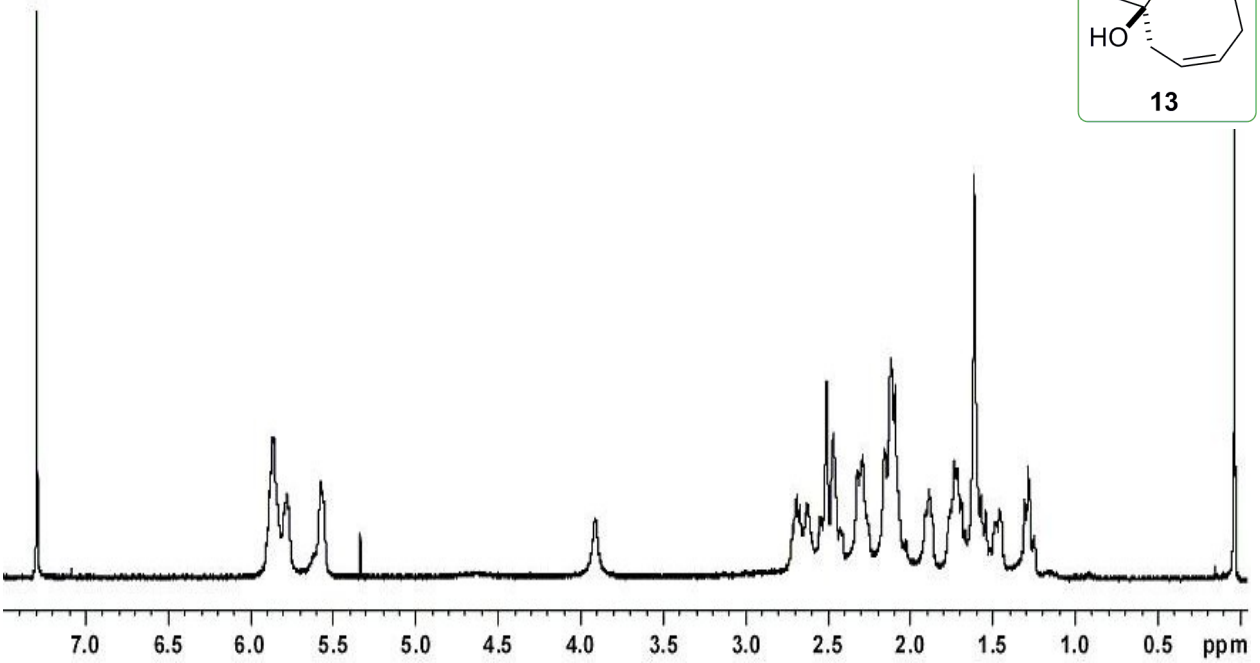


NMR spectra of (4a*R,6a*R**,12a*R**)-1,4,4a,5,6,6a,7,8,11,12-decahydrocyclooct[*c*]indene-4a,6a-diol (13)**

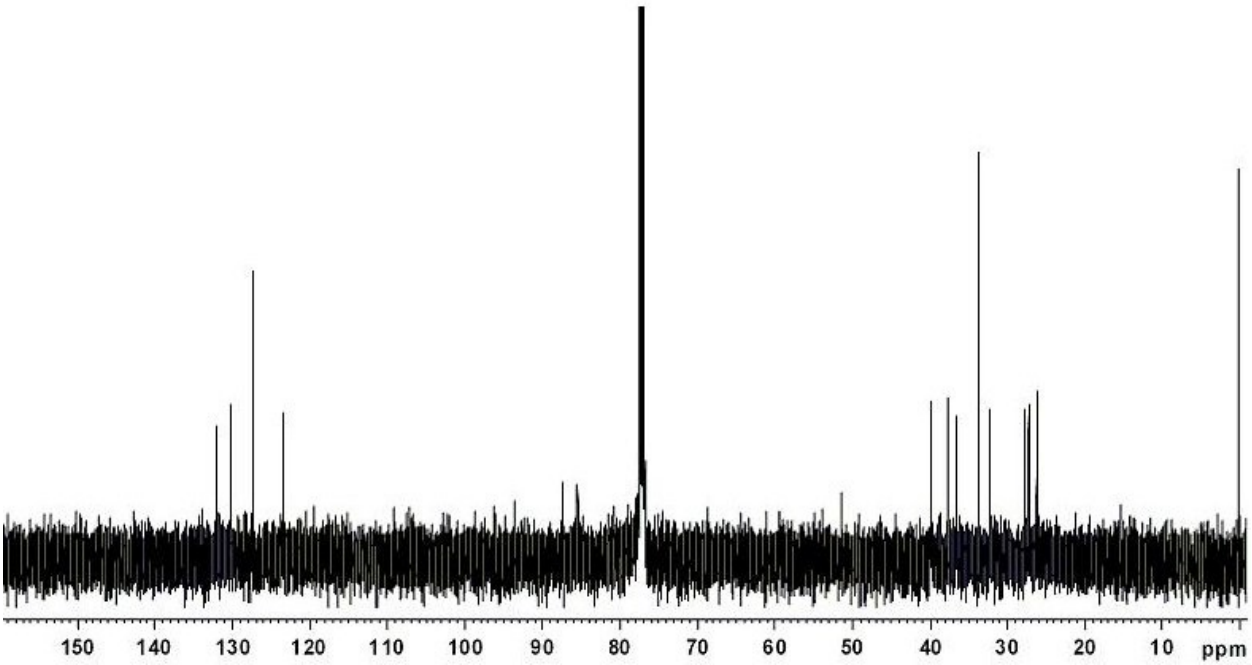


13

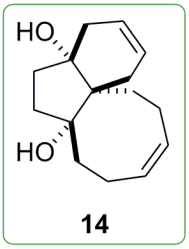
^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C NMR ($CDCl_3$, 125 MHz)

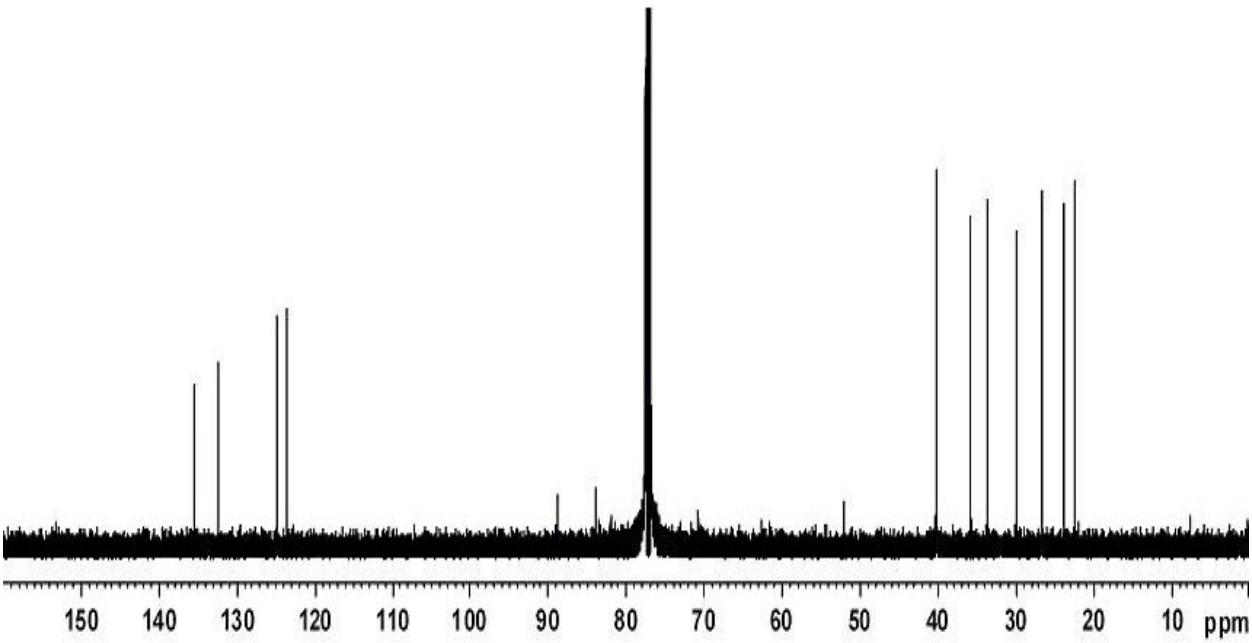


NMR spectra of (4a*R,6a*R**,12a*S**)-1,4,4a,5,6,6a,7,10,11,12-decahydrocyclooct[*c*]indene-4a,6a-diol (14)**



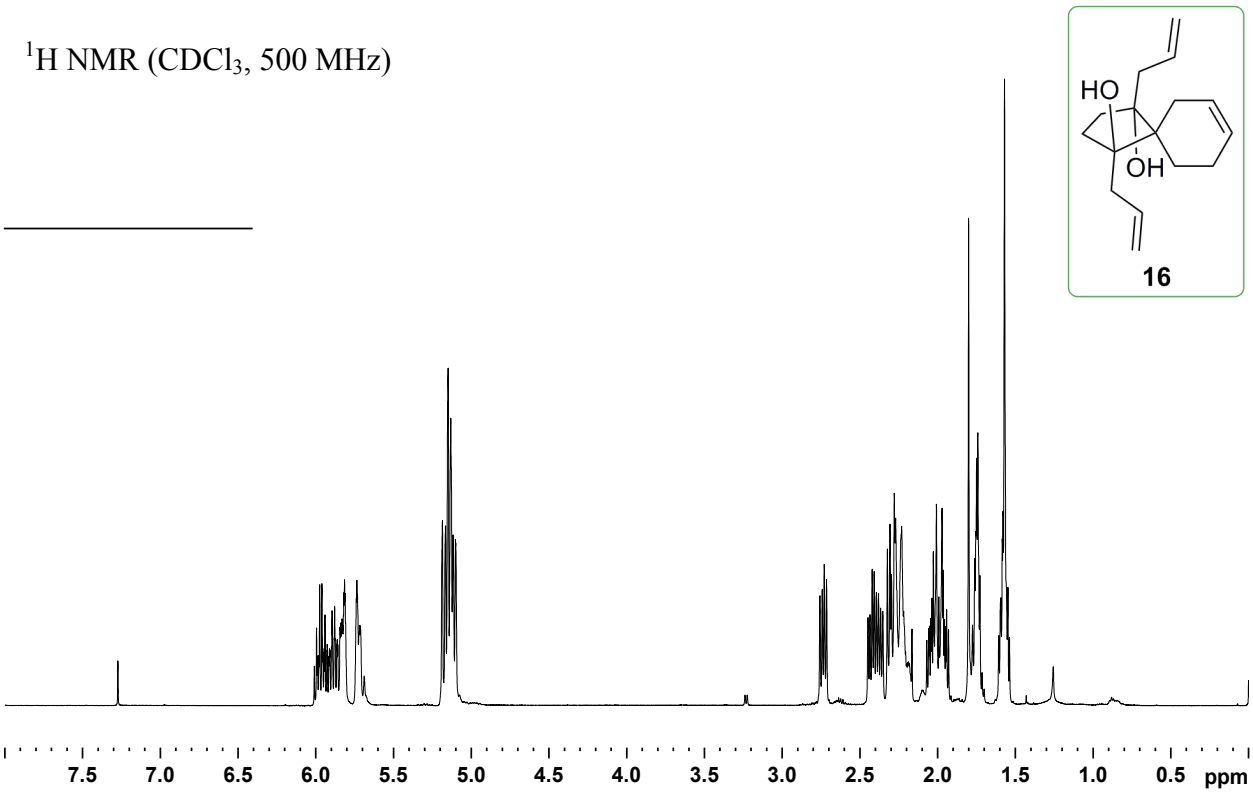
^{1}H NMR ($CDCl_3$, 500 MHz)

^{13}C NMR ($CDCl_3$, 125 MHz)

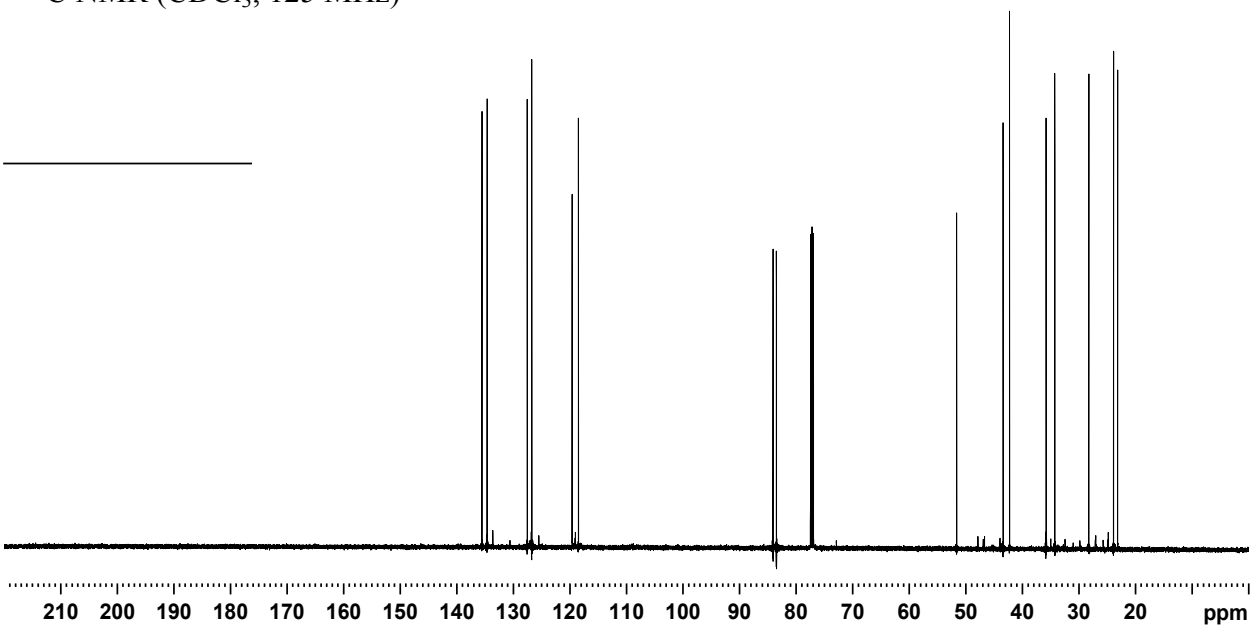


NMR spectra of (1*R,4*R**)-1,4-diallylspiro[4.5]dec-7-ene-1,4-diol (16)**

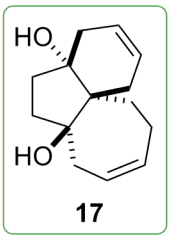
^{1}H NMR ($CDCl_3$, 500 MHz)



^{13}C NMR ($CDCl_3$, 125 MHz)

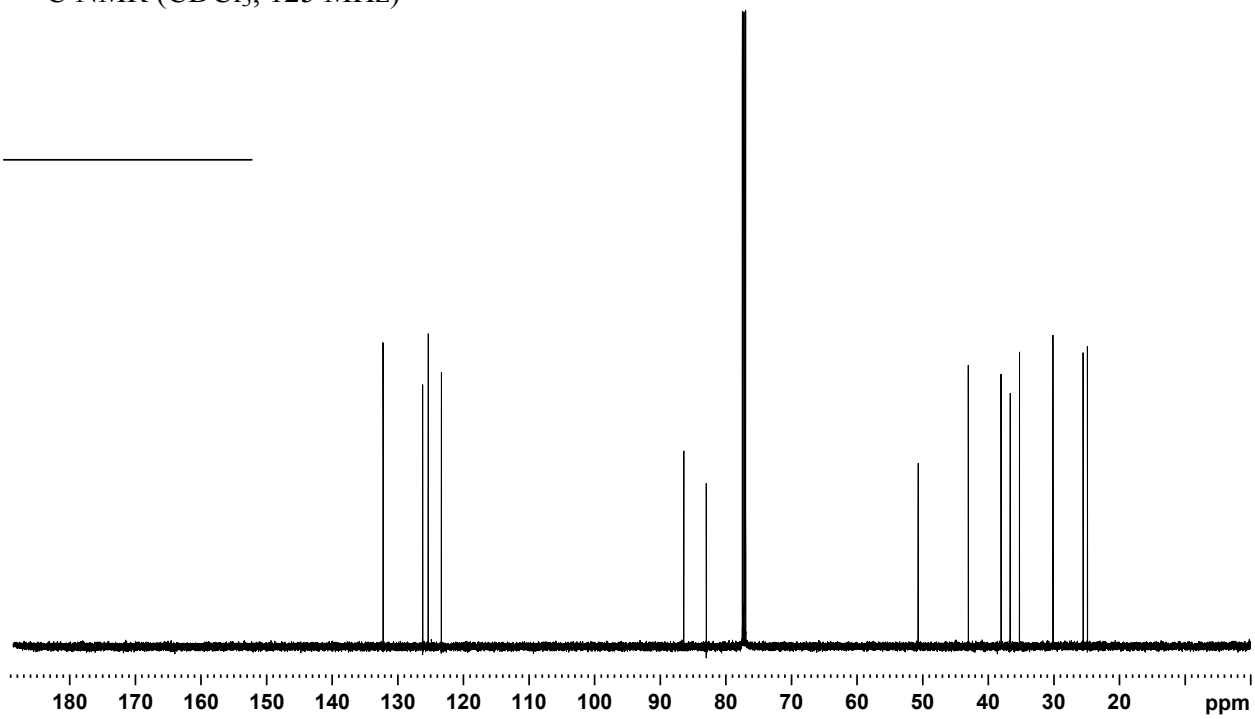


NMR spectra of (4a*R,6a*R**,10a*S**)-4,4a,5,6,6a,7,10,11-octahydro-1*H*-benz[*c*]azulene-4a,6a-diol (17)**



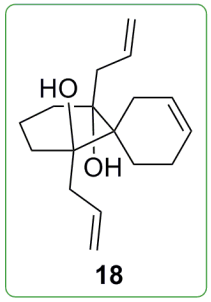
^{1}H NMR ($CDCl_3$, 500 MHz)

^{13}C NMR ($CDCl_3$, 125 MHz)



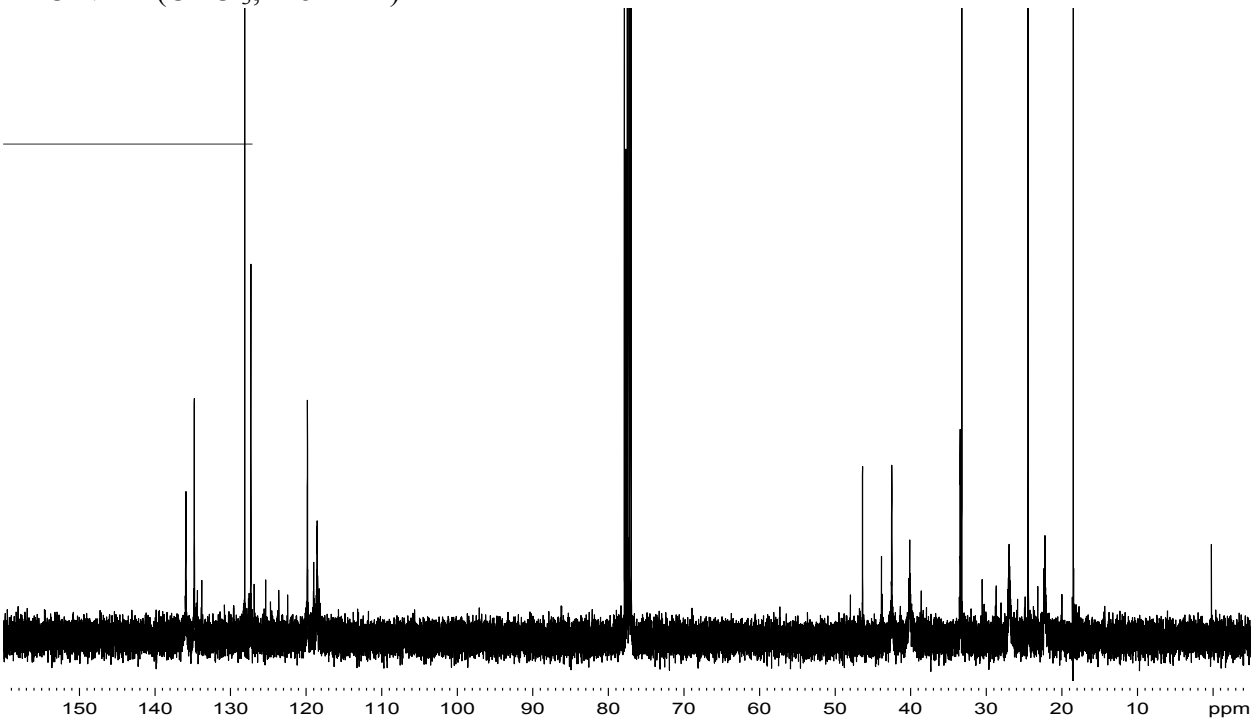
NMR spectra of (1*R,5*R**)-1,5-diallylspiro[5.5]undec-8-ene-1,5-diol (18)**

^{1}H NMR ($CDCl_3$, 500 MHz)

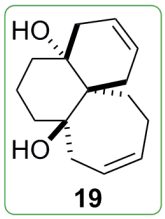


18

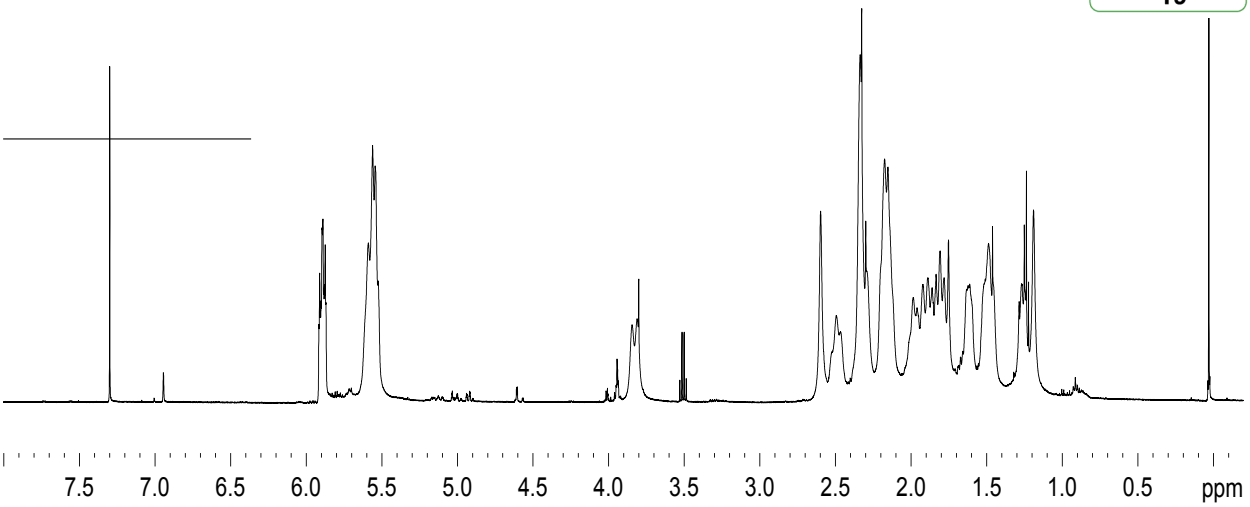
^{13}C NMR ($CDCl_3$, 125 MHz)



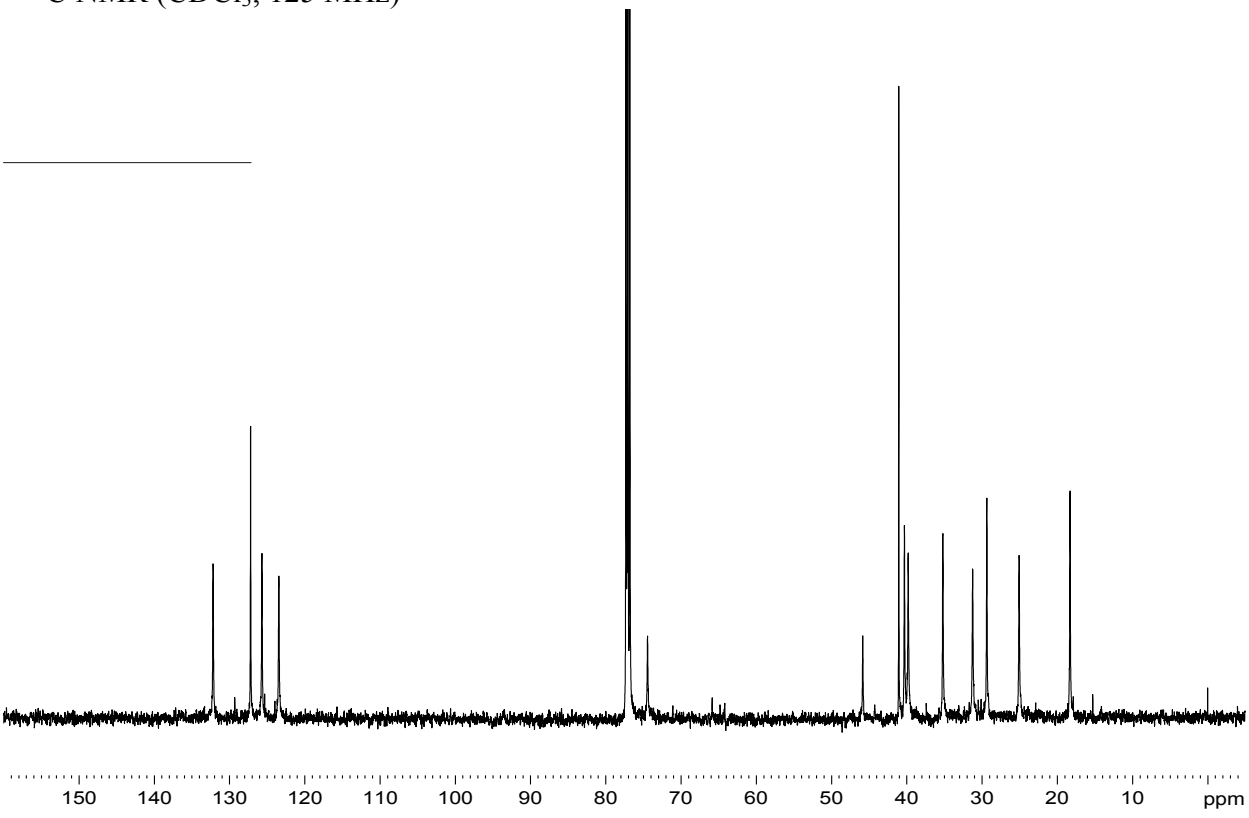
NMR spectra of (4a*R,7a*R**,12a*R**)-1,4,4a,5,6,7,7a,8,11,12-decahydrocyclohepta[*d*]-naphthalene-4a,7a-diol (19)**



^{1}H NMR ($CDCl_3$, 500 MHz)

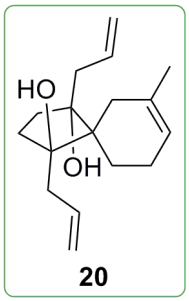


^{13}C NMR ($CDCl_3$, 125 MHz)



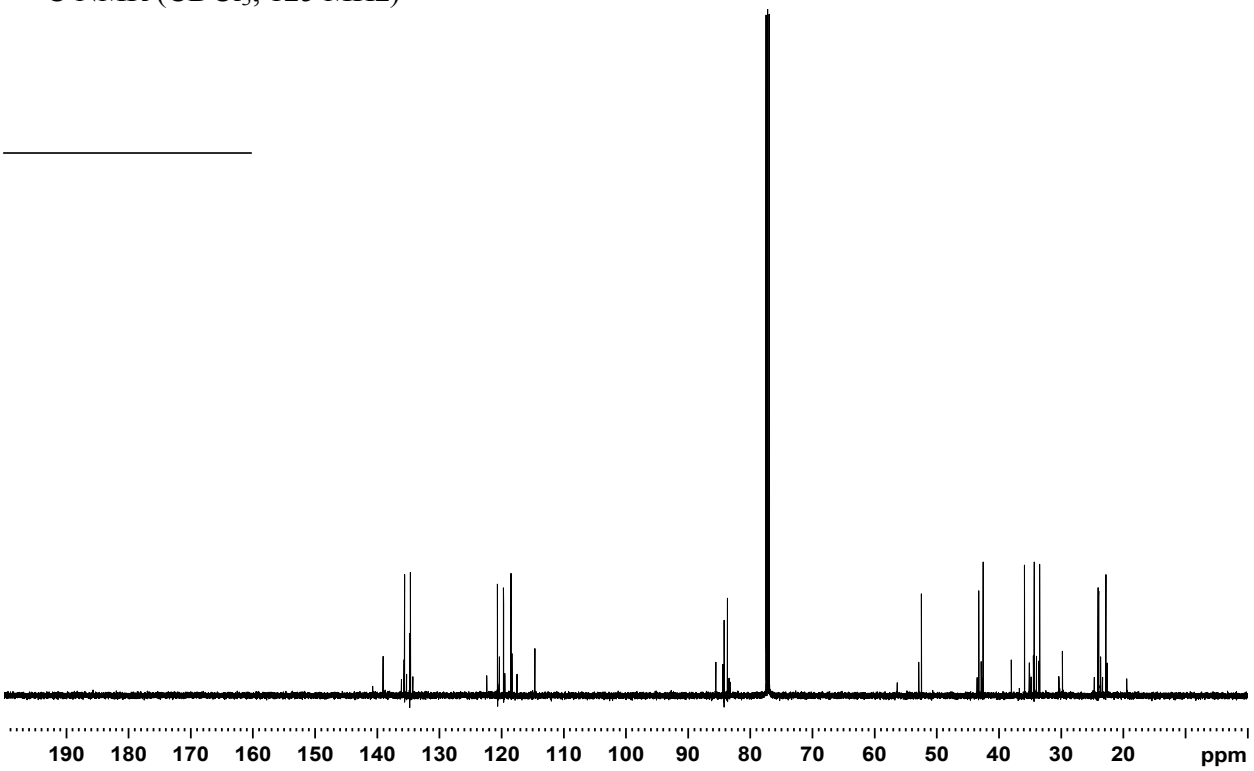
NMR spectra of (1*R,4*R**)-1,4-diallyl-7-methylspiro[4.5]dec-7-ene-1,4-diol (20)** (impure: may include some **10**)

^{1}H NMR ($CDCl_3$, 500 MHz)



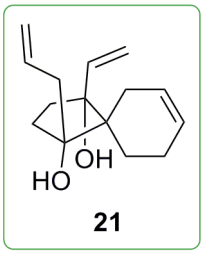
20

^{13}C NMR ($CDCl_3$, 125 MHz)



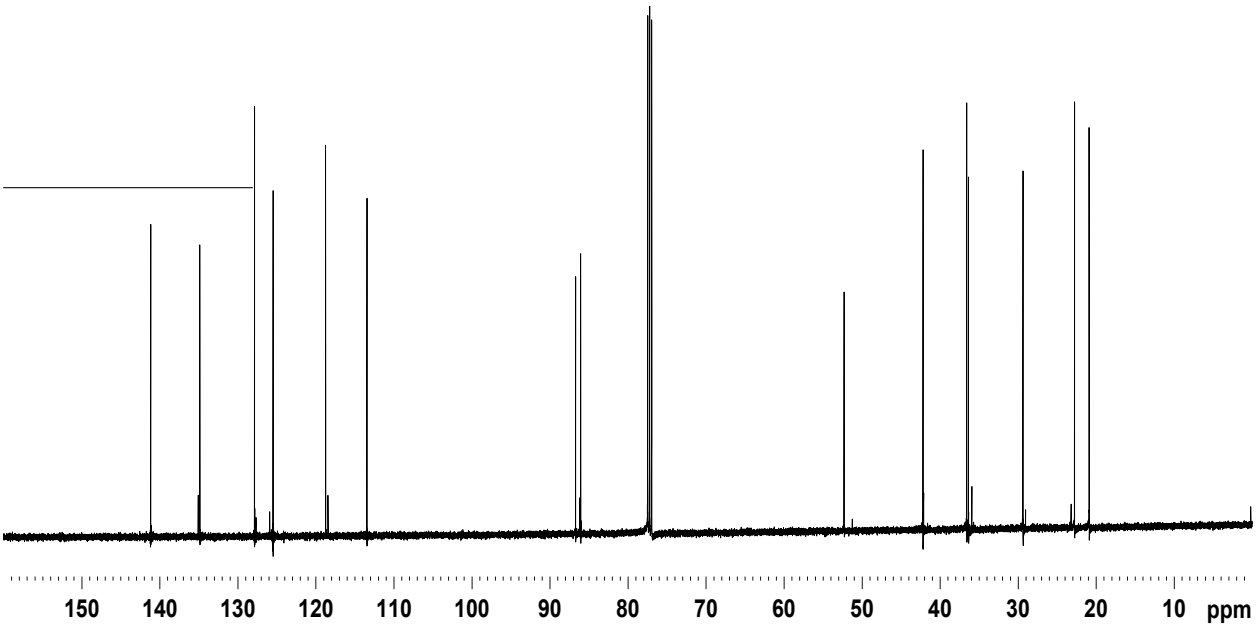
NMR spectra of (1*R,4*S**,5*R**)-1-allyl-4-vinylspiro[4.5]dec-7-ene-1,4-diol (21)**

^{1}H NMR ($CDCl_3$, 500 MHz)



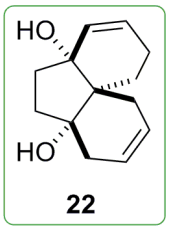
21

^{13}C NMR ($CDCl_3$, 125 MHz)



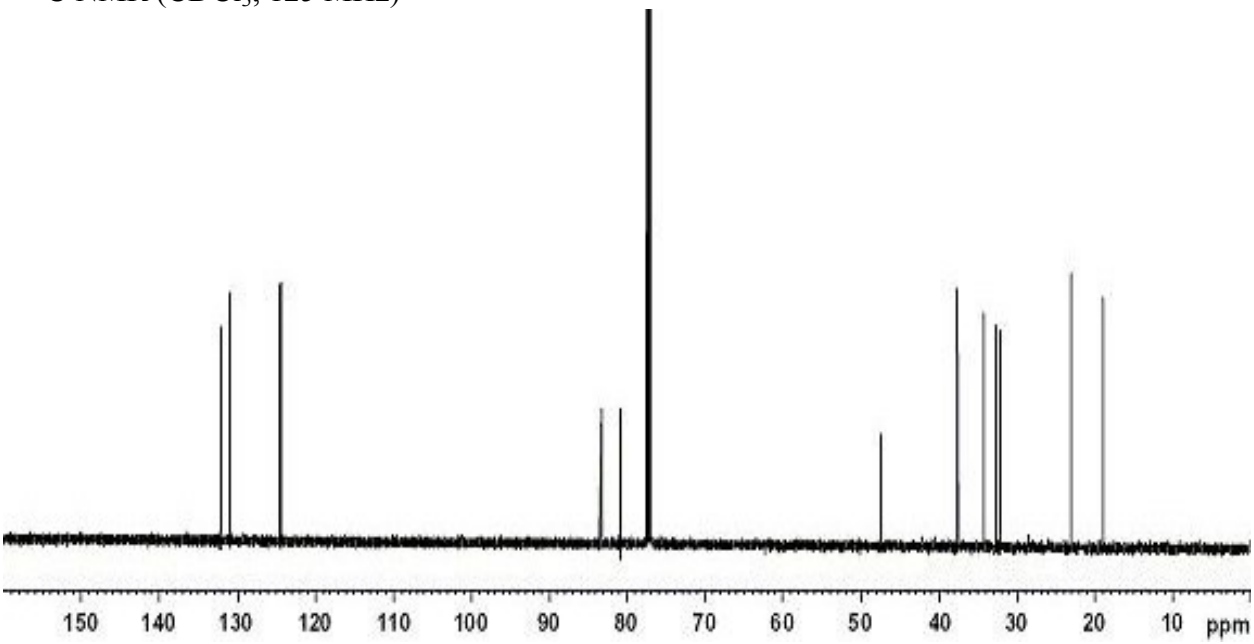
NMR spectra of (4a*R,6a*S**,10a*S**)-1,2,5,6,7,10-hexahydrobenz[*c*]indene-4a,6a-diol (22)**

^{1}H NMR ($CDCl_3$, 500 MHz)

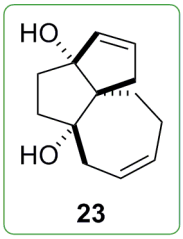


22

^{13}C NMR ($CDCl_3$, 125 MHz)



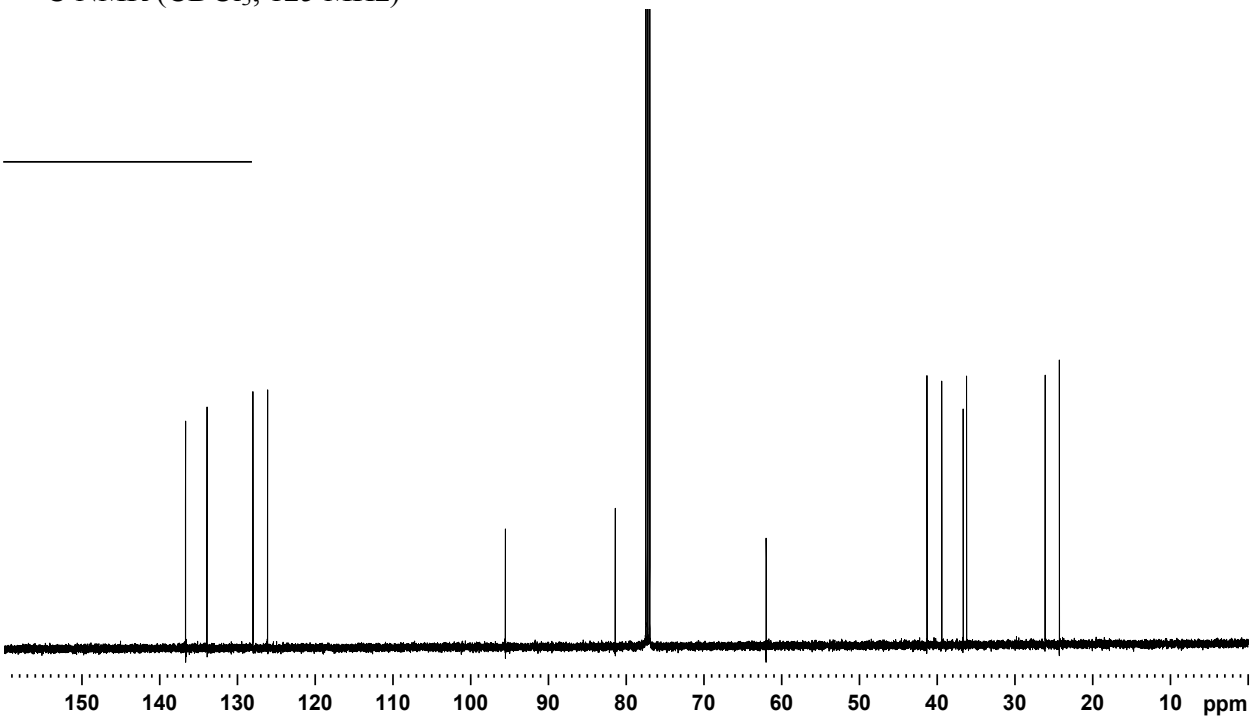
NMR spectra of (3a*R,5a*S**,10a*S**)-1,3a,4,5,5a,6,9,10-octahydrocyclopent[*c*]azulene-3a,5a-diol (23)**



23

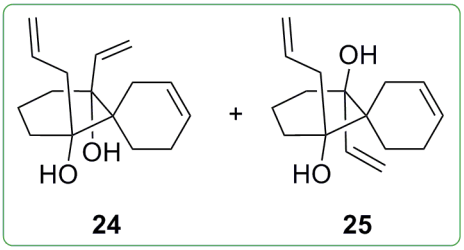
^{1}H NMR ($CDCl_3$, 500 MHz)

^{13}C NMR ($CDCl_3$, 125 MHz)

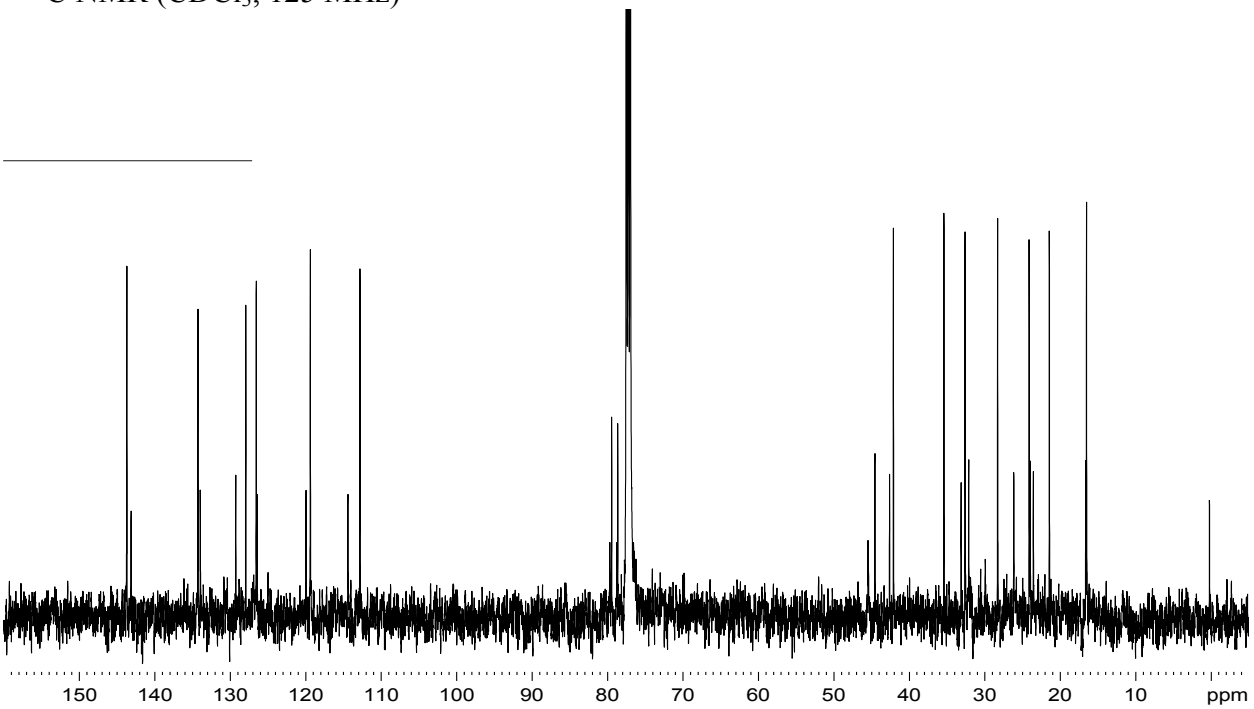


NMR spectra of (1*R,5*S**,6*R**)-1-allyl-5-vinylspiro[5.5]undec-8-ene-1,5-diol (24) and (1*R**,5*R**,6*R**)-1-allyl-5-vinylspiro[5.5]undec-8-ene-1,5-diol (25)** (3:1 mixture)

^{1}H NMR ($CDCl_3$, 500 MHz)

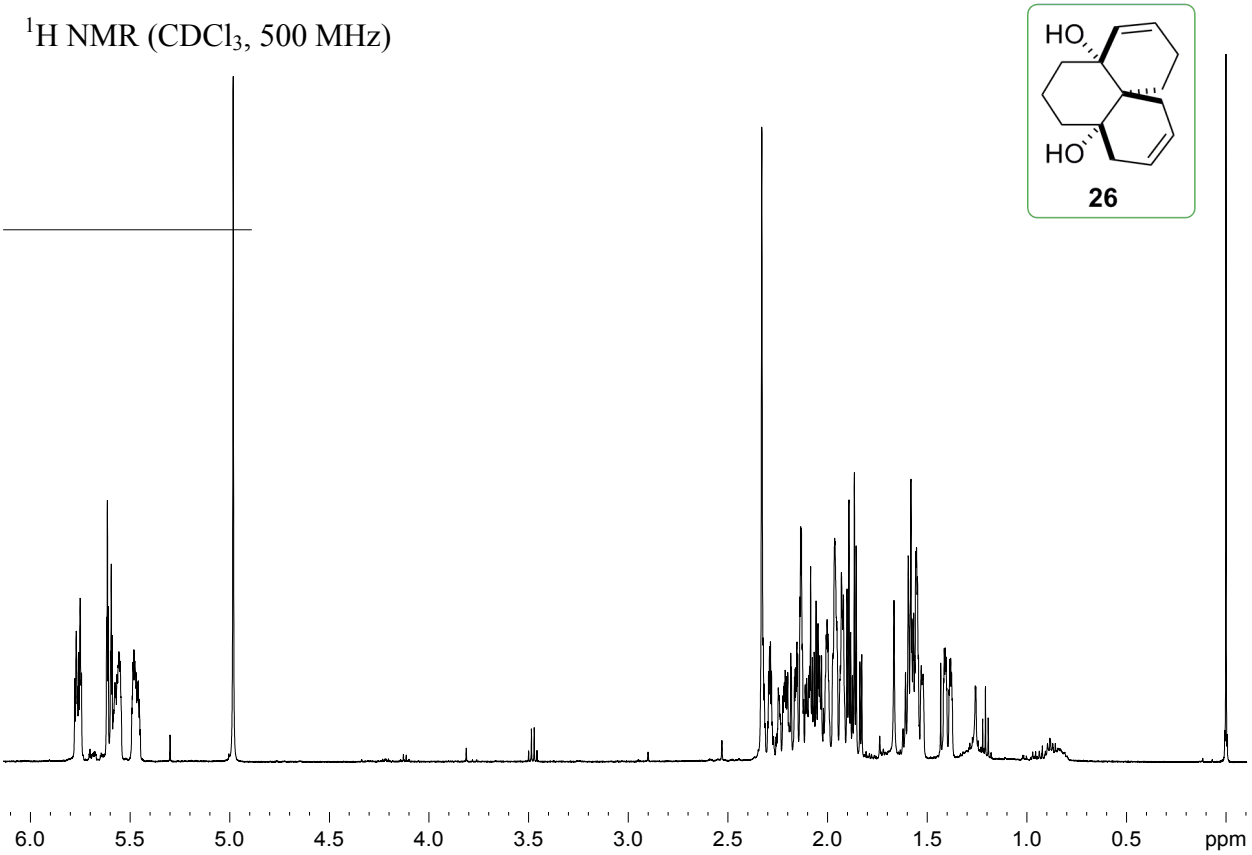


^{13}C NMR ($CDCl_3$, 125 MHz)

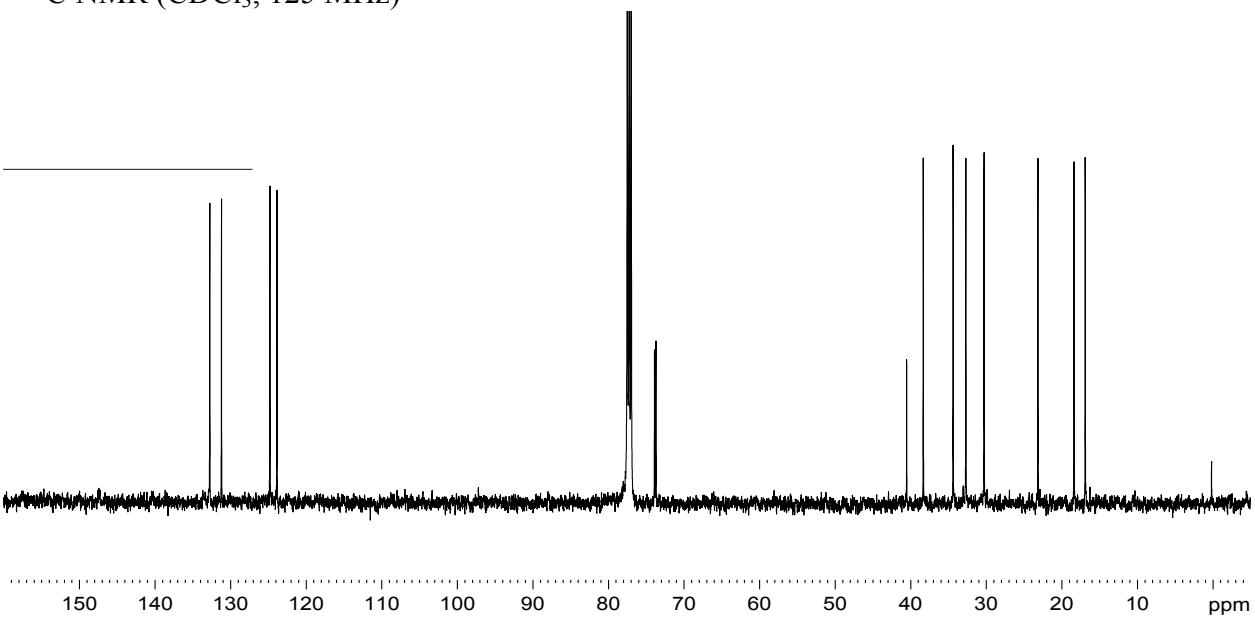


NMR spectra of (4a*R,7a*R**,11a*R**)-2,4a,5,6,7,7a,8,11-octahydro-1*H*-benz[*d*]naphthalene-4a,7a-diol (26)**

^{1}H NMR ($CDCl_3$, 500 MHz)

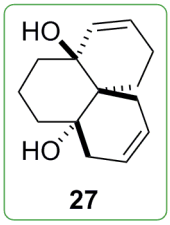


^{13}C NMR ($CDCl_3$, 125 MHz)



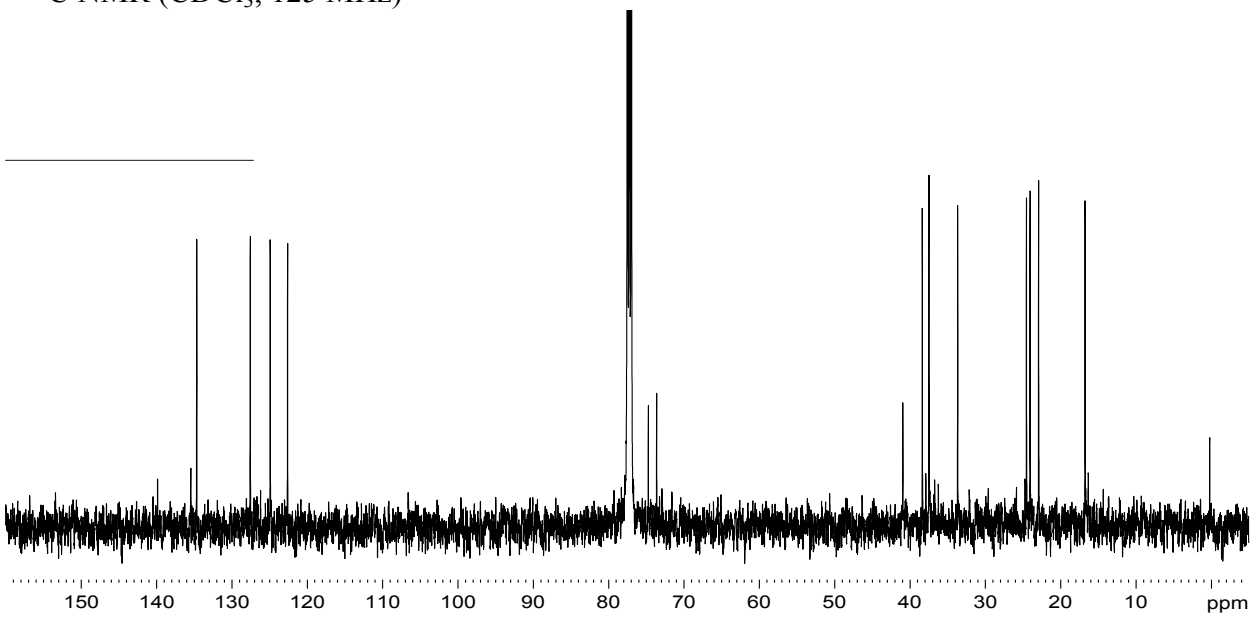
NMR spectra of (4a*R,7a*S**,11a*S**)-2,4a,5,6,7,7a,8,11-octahydro-1*H*-benz[*d*]naphthalene-4a,7a-diol (27)**

^{1}H NMR ($CDCl_3$, 500 MHz)



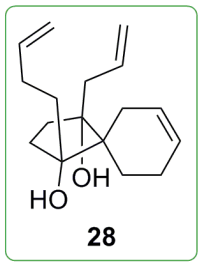
27

^{13}C NMR ($CDCl_3$, 125 MHz)

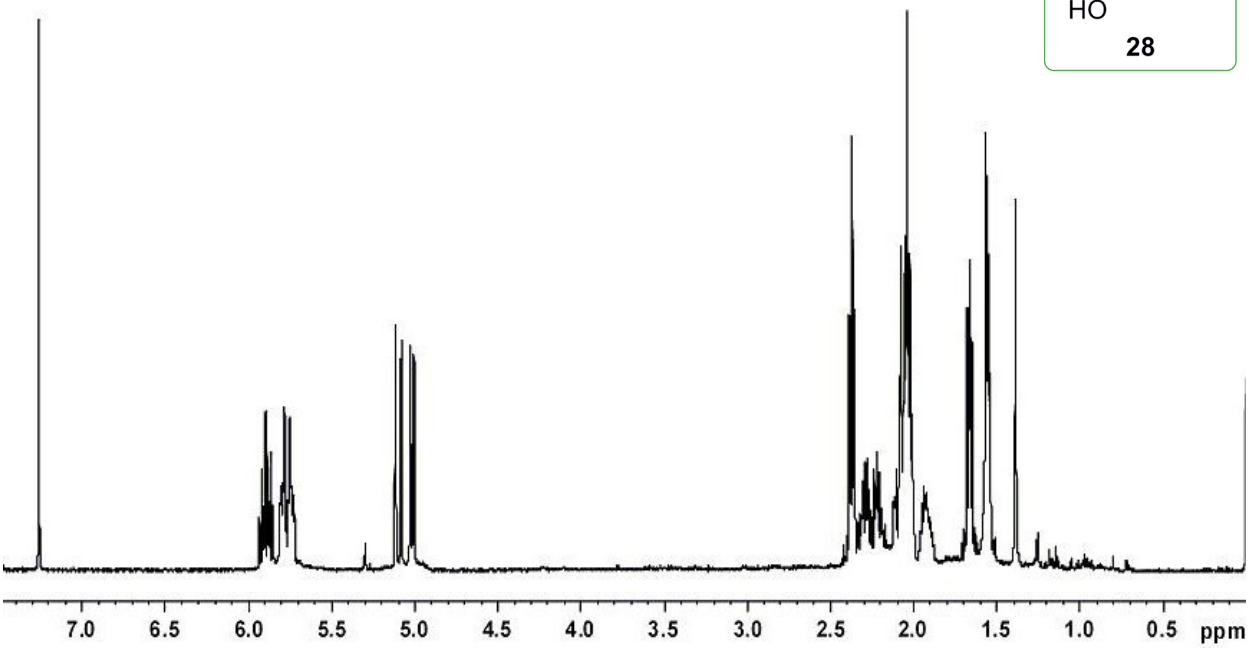


NMR spectra of (1*R,4*R**,5*S**)-1-allyl-4-(3-butenyl)spiro[4.5]dec-7-ene-1,4-diol (28)**

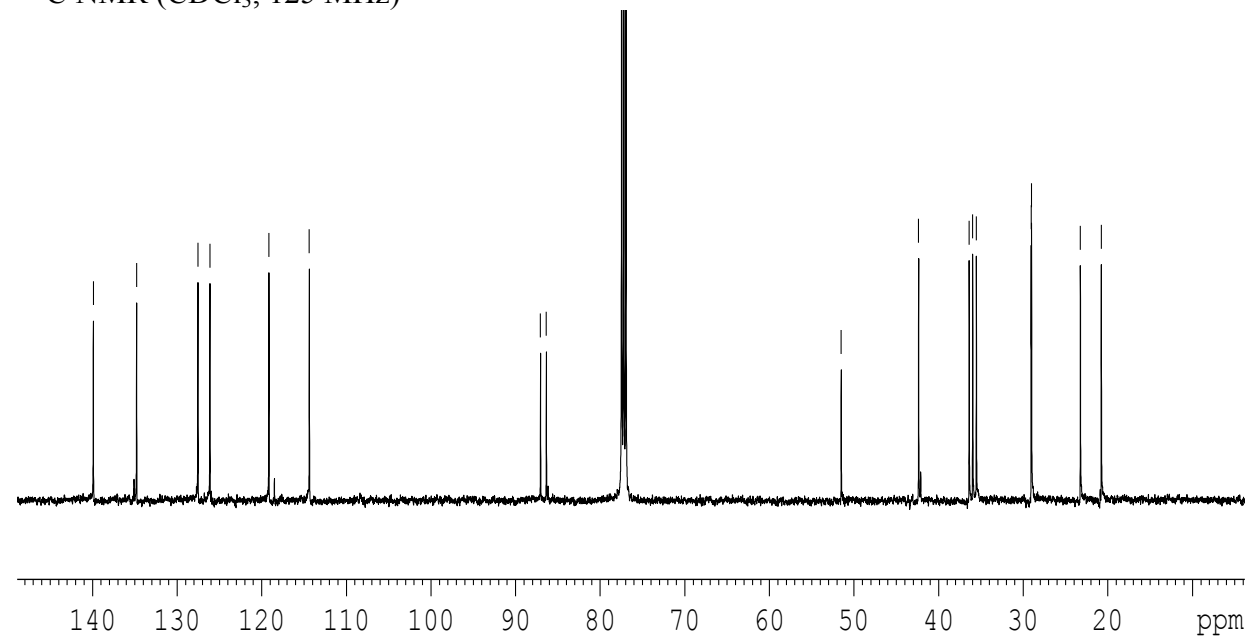
^{1}H NMR ($CDCl_3$, 500 MHz)



28

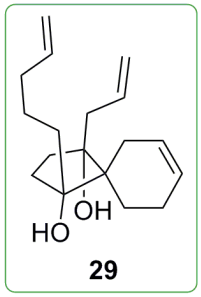


^{13}C NMR ($CDCl_3$, 125 MHz)



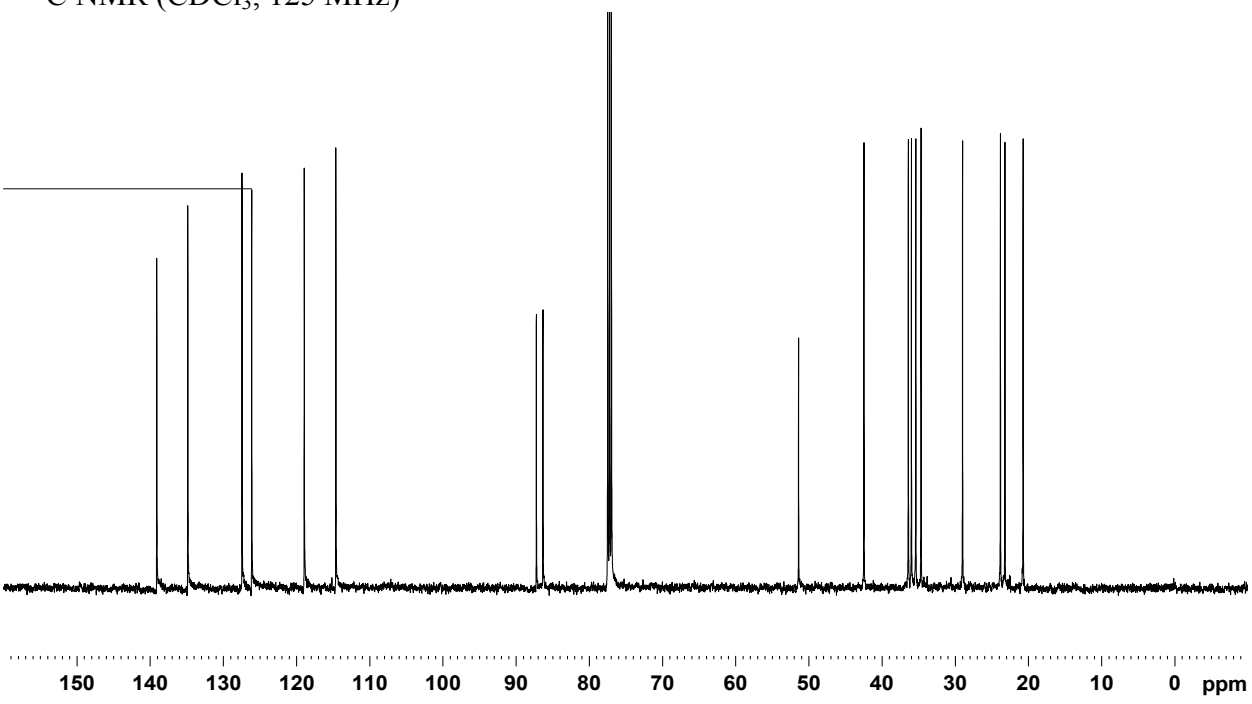
NMR spectra of (1*R,4*R**,5*S**)-1-allyl-4-(4-pentenyl)spiro[4.5]dec-7-ene-1,4-diol (29)**

^{1}H NMR ($CDCl_3$, 500 MHz)



29

^{13}C NMR ($CDCl_3$, 125 MHz)



Computational data for compound 8 with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1243.4011556556 Energy -695.646083
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-3.066960	0.119887	-0.478343
6	-2.933313	1.188805	0.321372
6	-1.714275	1.851251	0.925396
6	-2.041820	-0.820138	-1.072065
6	-0.457682	1.013304	1.220216
6	-0.763072	-1.093660	-0.274031
6	0.110705	0.170828	0.060620
1	-4.086179	-0.105426	-0.795962
1	-3.860851	1.714070	0.557100
1	-1.448737	2.713720	0.292000
1	-0.673861	0.347169	2.057955
1	-1.778767	-0.463979	-2.078450
1	-2.022912	2.303172	1.878535
1	-2.522418	-1.795649	-1.225409
1	0.319382	1.707254	1.567412
6	0.232572	-2.024143	-1.044903
6	1.665437	-1.534092	-0.700615
6	1.489123	-0.476182	0.410409
1	2.152734	-1.077949	-1.569881
1	2.324471	-2.343903	-0.362225
1	0.055973	-3.055216	-0.725441
1	0.057107	-1.991909	-2.126350
6	2.648392	0.520993	0.553801
6	2.610338	1.647837	-0.443011
6	1.549799	1.887457	-1.221067
6	0.309889	1.030132	-1.224231
1	2.621711	0.932808	1.573565
1	3.605418	-0.019803	0.474672
1	3.486447	2.292762	-0.498027
1	1.573427	2.721375	-1.922142
1	0.350191	0.384497	-2.113210
1	-0.573703	1.657125	-1.380051
8	-1.215871	-1.750221	0.916970
8	1.326406	-1.161201	1.686534
1	2.139133	-1.658167	1.873401
1	-0.437650	-1.864251	1.493183

Computational data for compound 8 with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1242.7854326030 Energy -695.646776
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.084855	-0.133396	-0.460722
6	2.939882	-1.203804	0.335054
6	1.702540	-1.890296	0.870902
6	2.045644	0.765723	-1.094075
6	0.446124	-1.057172	1.182138
6	0.762787	1.050641	-0.303105
6	-0.127452	-0.182942	0.049101
1	4.108629	0.120746	-0.738634
1	3.867623	-1.706275	0.614598
1	1.448797	-2.711906	0.181603
1	0.653390	-0.419251	2.043401
1	1.775919	0.366489	-2.082152
1	1.984925	-2.397823	1.803412
1	2.516554	1.737943	-1.311810
1	-0.335821	-1.758261	1.500593
6	-0.209716	2.010251	-1.052026
6	-1.647133	1.594938	-0.633641
6	-1.482034	0.507833	0.460880
1	-2.196057	1.189196	-1.491491
1	-2.234427	2.426610	-0.233182
1	0.018793	3.047327	-0.779610
1	-0.071746	1.937425	-2.136895
6	-2.672641	-0.454413	0.574060
6	-2.673875	-1.569962	-0.431823
6	-1.634405	-1.837535	-1.228993
6	-0.370213	-1.016159	-1.245868
1	-2.669569	-0.872879	1.590720
1	-3.604270	0.125798	0.503869
1	-3.567409	-2.191690	-0.480885
1	-1.691337	-2.665063	-1.935691
1	-0.409405	-0.357229	-2.125200
1	0.490583	-1.669162	-1.428909
8	1.130466	1.659237	0.967672
8	-1.405793	1.122142	1.755369
1	-0.566857	1.618425	1.799885
1	1.698119	2.426307	0.790744

Computational data for compound 9 with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1241.8974433991 Energy -695.649787
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.162286	-0.094814	-0.409013
6	2.851028	-1.360120	0.361909
6	1.733997	-1.777886	0.981902
6	2.028742	0.629307	-1.154317
6	0.364725	-1.151825	1.140471
6	0.783627	0.975906	-0.328261
6	-0.161391	-0.219701	0.033401
6	-0.155126	1.983423	-1.042448
6	-1.605175	1.621555	-0.623327
6	-1.472072	0.535308	0.473045
6	-2.703316	-0.366590	0.620194
6	-2.794483	-1.460090	-0.405237
6	-1.786963	-1.779800	-1.224096
6	-0.462972	-1.058644	-1.246478
8	1.207271	1.670885	0.884235
8	-1.329632	1.152601	1.761482
1	1.760095	1.071929	1.413022
1	3.938490	-0.333717	-1.148281
1	3.654546	0.614853	0.276221
1	2.438721	1.569872	-1.546307
1	3.716908	-2.015616	0.469268
1	1.827793	-2.726147	1.513755
1	-0.359027	-1.970350	1.250344
1	0.325022	-0.627125	2.105829
1	0.345537	-1.786788	-1.390399
1	-0.438452	-0.423996	-2.143737
1	1.730583	0.036778	-2.025768
1	-1.911558	-2.588101	-1.944384
1	-3.728476	-2.019149	-0.453045
1	-3.605418	0.261503	0.593485
1	-2.685201	-0.802212	1.629873
1	-0.502668	1.672101	1.745826
1	-2.169798	1.227727	-1.476530
1	-2.163318	2.475373	-0.227319
1	-0.024241	1.921858	-2.128220
1	0.131903	2.997141	-0.745834

Computational data for compound 2 with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1243.0507312734 Energy -695.649572
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-3.154118	0.056525	-0.283001
6	-2.824045	1.402039	0.327081
6	-1.706043	1.816360	0.944637
6	-2.062276	-0.657079	-1.099411
6	-0.413509	1.071810	1.210431
6	-0.790218	-1.012138	-0.321218
6	0.134979	0.202266	0.059061
6	0.171419	-1.944936	-1.123876
6	1.618703	-1.557193	-0.714042
6	1.473367	-0.518948	0.422211
6	2.679760	0.411473	0.611234
6	2.739732	1.534694	-0.386795
6	1.708336	1.844966	-1.178304
6	0.402811	1.091825	-1.195089
8	-1.263686	-1.692359	0.851252
8	1.257673	-1.223468	1.680646
1	-0.491618	-1.851120	1.425420
1	-4.025960	0.183937	-0.938137
1	-3.476617	-0.619875	0.520067
1	-2.488429	-1.600214	-1.468564
1	-3.645810	2.119670	0.300982
1	-1.730063	2.828379	1.351237
1	0.353967	1.811797	1.471610
1	-0.541766	0.446465	2.101398
1	-0.423979	1.803379	-1.296344
1	0.372757	0.489752	-2.114212
1	-1.807499	-0.065520	-1.985979
1	1.799793	2.673606	-1.880238
1	3.660281	2.115151	-0.431692
1	3.606055	-0.184113	0.566163
1	2.638497	0.823130	1.630610
1	2.044237	-1.760086	1.869990
1	2.164718	-1.109943	-1.552238
1	2.211736	-2.416697	-0.376488
1	0.026732	-1.827365	-2.204092
1	-0.072313	-2.983705	-0.882186

Computational data for compound 14 with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1373.4176534756 Energy -734.926405
Formula C15H22O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.472803	-2.068246	-0.244865
6	-1.724375	0.710340	1.355475
6	-0.151822	-1.426691	-0.753364
6	-0.574388	0.960321	0.330597
6	0.408701	-0.245696	0.072887
6	0.384698	2.100937	0.764502
6	1.778951	1.769220	0.170854
6	1.597987	0.478815	-0.670837
6	2.872983	-0.363365	-0.798014
6	3.188261	-1.189019	0.415151
6	2.314646	-1.384405	1.407816
6	0.932254	-0.782591	1.443795
8	-1.126571	1.437679	-0.927699
8	1.262688	0.812995	-2.023940
6	-3.152550	0.572322	0.786971
6	-3.429121	-0.384094	-0.353825
6	-2.741123	-1.451698	-0.793403
1	0.426641	2.171423	1.856176
1	-0.021077	3.050389	0.400564
1	2.509110	1.598774	0.970513
1	2.173571	2.565190	-0.468018
1	-1.736493	0.759494	-1.271888
1	0.410552	1.290828	-1.992432
1	3.712013	0.306266	-1.035506
1	2.764439	-1.014659	-1.677502
1	4.173196	-1.652540	0.462312
1	2.597255	-1.995440	2.265017
1	0.237620	-1.540357	1.828170
1	0.922784	0.010107	2.204780
1	0.623721	-2.203330	-0.759811
1	-0.272436	-1.122561	-1.798748
1	-1.497873	-2.078560	0.849941
1	-1.469835	-3.122555	-0.546662
1	-3.147372	-1.953967	-1.672647
1	-4.339699	-0.139820	-0.904216
1	-3.820932	0.317848	1.624788
1	-1.484246	-0.155910	1.978084
1	-1.760157	1.563420	2.045112
1	-3.483513	1.563676	0.452650

Computational data for compound 14 with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1370.5335362510 Energy -734.920278
Formula C15H22O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.485255	2.066457	0.272243
6	-1.735552	-0.760474	-1.313578
6	-0.210539	1.363757	0.818950
6	-0.566107	-1.003057	-0.318253
6	0.384664	0.232929	-0.052608
6	0.438014	-2.088445	-0.825995
6	1.831128	-1.719295	-0.249587
6	1.618211	-0.459237	0.623077
6	2.860252	0.429775	0.776978
6	3.139974	1.287936	-0.424236
6	2.239375	1.468048	-1.394543
6	0.878968	0.818643	-1.416375
8	-1.173453	-1.467204	0.892525
8	1.209706	-0.866841	1.962172
6	-3.143919	-0.642923	-0.699830
6	-3.469468	0.412757	0.328595
6	-2.809684	1.502642	0.742253
1	0.470779	-2.121895	-1.920702
1	0.082009	-3.066626	-0.488889
1	2.544529	-1.495062	-1.050620
1	2.274051	-2.526690	0.347320
1	-0.480451	-1.485367	1.578609
1	1.921761	-1.400864	2.349775
1	3.732315	-0.207394	0.996670
1	2.721977	1.064456	1.664548
1	4.108705	1.783088	-0.474942
1	2.484468	2.102979	-2.245793
1	0.154094	1.557078	-1.774928
1	0.885789	0.042972	-2.194198
1	0.573543	2.124414	0.935697
1	-0.421453	0.980833	1.821135
1	-1.462583	2.107912	-0.822326
1	-1.445478	3.114045	0.595163
1	-3.283645	2.072090	1.543106
1	-4.421958	0.218803	0.826696
1	-3.852883	-0.531126	-1.537172
1	-1.523400	0.106148	-1.947059
1	-1.781260	-1.616241	-2.000619
1	-3.391298	-1.608283	-0.241615

Computational data for compound 15 with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1368.5089517235 Energy -734.925032
Formula C15H22O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.541191	2.025424	0.202725
6	-1.685895	-0.917743	-1.312598
6	-0.287739	1.315443	0.774184
6	-0.486911	-1.077927	-0.329394
6	0.381460	0.207195	-0.069734
6	0.560896	-2.116318	-0.806757
6	1.917864	-1.685629	-0.187971
6	1.631119	-0.417922	0.665763
6	2.835330	0.523446	0.793890
6	3.072143	1.392749	-0.405805
6	2.180984	1.523538	-1.393336
6	0.862570	0.792229	-1.437033
8	-0.973352	-1.623272	0.925681
8	1.335110	-0.783035	2.019964
6	-3.046461	-0.716086	-0.668633
6	-3.510093	0.247214	0.147896
6	-2.912611	1.525170	0.685526
1	0.610404	-2.138764	-1.900589
1	0.237525	-3.109803	-0.481806
1	2.647577	-1.455791	-0.973126
1	2.357370	-2.456598	0.452049
1	-1.828460	-1.206032	1.132984
1	0.502510	-1.293572	2.004013
1	3.727619	-0.080680	1.013018
1	2.684289	1.148482	1.685829
1	4.010339	1.945401	-0.446045
1	2.402829	2.170899	-2.241685
1	0.102665	1.476125	-1.832699
1	0.938763	0.000637	-2.194747
1	0.480667	2.080414	0.942018
1	-0.518084	0.918969	1.769439
1	-1.532760	2.046727	-0.893304
1	-1.484231	3.078483	0.506698
1	-3.650938	2.313131	0.469078
1	-2.902731	1.460288	1.786527
1	-4.536792	0.102630	0.491873
1	-3.751241	-1.521459	-0.873738
1	-1.468255	-0.117188	-2.027258
1	-1.751918	-1.836546	-1.906027

Computational data for compound 15 with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1371.6603183552 Energy -734.922567
Formula C15H22O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.555391	-1.916038	0.880093
6	1.662819	1.266647	-1.146098
6	0.209144	-1.191339	1.052122
6	0.503796	1.187629	-0.132532
6	-0.306427	-0.170298	0.004853
6	-0.588116	2.233616	-0.579389
6	-1.967627	1.558835	-0.448216
6	-1.721450	0.354304	0.463164
6	-2.833198	-0.704072	0.443464
6	-2.749153	-1.650583	-0.724023
6	-1.680642	-1.725539	-1.524850
6	-0.466347	-0.843215	-1.387608
8	1.048098	1.582002	1.136564
8	-1.645510	0.935556	1.796514
6	2.874268	0.365375	-1.166546
6	3.365488	-0.548353	-0.319033
6	2.814318	-1.021499	1.002789
1	-0.411776	2.588278	-1.600497
1	-0.502834	3.107291	0.073987
1	-2.341704	1.213084	-1.417947
1	-2.729961	2.214129	-0.014840
1	0.291220	1.642834	1.748350
1	-1.636049	0.218902	2.450712
1	-3.806918	-0.194016	0.458963
1	-2.800804	-1.289793	1.378111
1	-3.603316	-2.305477	-0.891691
1	-1.680307	-2.433810	-2.353085
1	0.439516	-1.415541	-1.617859
1	-0.520563	-0.079112	-2.175914
1	-0.559299	-1.973843	1.128522
1	0.248990	-0.698636	2.030542
1	1.585492	-2.477523	-0.062722
1	1.588583	-2.673546	1.675605
1	3.601031	-1.594559	1.508147
1	2.581069	-0.162238	1.640876
1	4.285689	-1.039688	-0.639194
1	3.459068	0.526984	-2.075259
1	1.226816	1.211177	-2.151887
1	2.031774	2.301823	-1.066681

Computational data for compound 22 with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1116.6763053973 Energy -656.359945
Formula C13H18O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.536163	-1.699135	0.627079
8	-1.030914	-1.593561	1.443834
6	0.233949	-1.626818	-1.435887
6	-1.238923	-1.514782	-0.927456
6	-1.213082	-0.641880	0.355815
6	0.054797	0.240933	0.123556
6	1.077914	-0.814447	-0.420009
6	0.686102	0.955388	1.328890
6	2.047496	1.604263	0.939325
6	2.775178	0.950677	-0.216705
6	2.334322	-0.122921	-0.883753
6	-2.509147	0.130079	0.638013
6	-2.664637	1.381025	-0.179922
6	-1.661694	1.898785	-0.895357
6	-0.287316	1.288845	-0.988798
1	0.739537	-2.074223	1.051402
1	-0.985114	-1.104188	2.281735
1	0.330347	-1.231798	-2.453116
1	0.592551	-2.659949	-1.458594
1	-1.681351	-2.487320	-0.690491
1	-1.878875	-1.040588	-1.678711
1	0.866447	0.229945	2.128858
1	0.014329	1.728023	1.726201
1	2.709488	1.609872	1.816949
1	1.901490	2.666960	0.691991
1	3.714701	1.419782	-0.510204
1	2.909981	-0.556628	-1.699626
1	-2.540862	0.395532	1.708385
1	-3.362793	-0.545332	0.484530
1	-3.637282	1.871135	-0.163896
1	-1.827790	2.806640	-1.475228
1	-0.172197	0.846886	-1.987470
1	0.455644	2.091937	-0.966290

Computational data for compound 22 with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1116.4866825354 Energy -656.363780
Formula C13H18O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	1.452773	-1.766705	0.593426
8	-1.032611	-1.469412	1.571581
6	0.238362	-1.631435	-1.428321
6	-1.225051	-1.558994	-0.885648
6	-1.201781	-0.665031	0.397163
6	0.038660	0.247393	0.113206
6	1.068303	-0.787419	-0.440111
6	0.657239	1.001734	1.299945
6	2.000012	1.674917	0.898268
6	2.768095	0.977870	-0.205675
6	2.339686	-0.107361	-0.870405
6	-2.512160	0.087776	0.656706
6	-2.693143	1.325569	-0.172066
6	-1.711925	1.857292	-0.907609
6	-0.329872	1.265711	-1.018377
1	2.144151	-1.368942	1.146284
1	-0.172030	-1.922786	1.485089
1	0.310565	-1.234089	-2.445263
1	0.630319	-2.652053	-1.452820
1	-1.624780	-2.543783	-0.625631
1	-1.893367	-1.122727	-1.636820
1	0.814716	0.305039	2.130447
1	-0.035991	1.764718	1.674463
1	2.647871	1.770516	1.781951
1	1.823278	2.712256	0.575801
1	3.724673	1.425438	-0.476611
1	2.944545	-0.561944	-1.653665
1	-2.542220	0.346009	1.725099
1	-3.352512	-0.604582	0.502925
1	-3.671603	1.804267	-0.146038
1	-1.900076	2.759009	-1.490326
1	-0.229749	0.804497	-2.009857
1	0.402364	2.079962	-1.027543

Computational data for compound 23 with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1109.0363634915 Energy -656.352449
Formula C13H18O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.885347	-0.888315	0.047249
6	1.730237	1.177993	-0.962633
6	0.431212	1.057778	-0.137513
6	-0.177615	-0.363735	0.007890
6	-0.725257	1.880521	-0.749407
6	-1.962983	1.424209	0.031332
6	-1.724977	-0.085701	0.345298
1	-2.897773	1.584593	-0.516309
1	-2.039930	1.977422	0.974397
1	-0.540602	2.961038	-0.678113
1	-0.830313	1.643746	-1.815330
6	-2.465542	-1.004722	-0.591953
6	-1.669660	-1.552464	-1.511876
6	-0.231941	-1.124441	-1.365248
8	0.640359	1.515440	1.223650
8	-2.141557	-0.398286	1.675127
1	-1.738214	0.248134	2.277687
1	0.935783	2.439746	1.194644
1	-3.539429	-1.144894	-0.501820
1	-2.000626	-2.216347	-2.307218
6	2.771505	0.087219	-0.864489
1	1.455689	1.272946	-2.022279
1	2.196325	2.148901	-0.717919
1	3.508956	0.113254	-1.668342
6	2.029865	-1.080854	1.278467
6	0.504777	-1.253300	1.077337
1	3.712117	-1.587392	-0.082870
1	2.392350	-1.957842	1.828484
1	2.184951	-0.218728	1.937358
1	0.280364	-2.297567	0.825501
1	0.036917	-1.085961	2.050070
1	0.061367	-0.490526	-2.212530
1	0.461843	-1.972882	-1.382342

Computational data for compound 23 with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1109.6741895260 Energy -656.350637
Formula C13H18O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.870146	-0.894498	0.040011
6	1.742173	1.203338	-0.929283
6	0.430731	1.076799	-0.129020
6	-0.173936	-0.354901	0.014264
6	-0.718031	1.882313	-0.778950
6	-1.978029	1.412679	-0.037439
6	-1.717084	-0.085368	0.317779
1	-2.890558	1.544174	-0.630241
1	-2.107400	1.980894	0.892482
1	-0.539843	2.959503	-0.693034
1	-0.794256	1.639636	-1.846222
6	-2.443109	-1.046943	-0.591443
6	-1.630993	-1.604916	-1.491703
6	-0.205906	-1.136205	-1.348378
8	0.705684	1.634573	1.176906
8	-2.005479	-0.322147	1.711805
1	-2.941094	-0.116918	1.868466
1	-0.007530	1.383407	1.787365
1	-3.517737	-1.204791	-0.518330
1	-1.942972	-2.298022	-2.269707
6	2.756553	0.084462	-0.867691
1	1.487233	1.354685	-1.986651
1	2.213845	2.146293	-0.612229
1	3.474528	0.095895	-1.689388
6	2.030866	-1.053901	1.286864
6	0.503299	-1.230908	1.102883
1	3.674422	-1.616471	-0.104715
1	2.396327	-1.916331	1.857642
1	2.195453	-0.172849	1.917807
1	0.275524	-2.278969	0.869283
1	0.038738	-1.044158	2.073861
1	0.072049	-0.503412	-2.201689
1	0.511552	-1.963672	-1.351751

Computational data for compound 26 with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1253.3944032196 Energy -695.654112
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.411172	-1.933081	-1.289078
6	2.348071	-0.791499	0.712648
6	0.172864	-1.074522	-1.293482
6	1.270882	0.294355	0.515027
6	-0.096471	-0.316737	0.046400
1	-0.693882	-1.695775	-1.536486
1	0.247396	-0.371178	-2.132697
6	-0.661596	1.900008	-1.155687
6	-1.162504	0.830698	-0.162023
1	-0.605195	1.486407	-2.170841
1	-1.411205	2.700276	-1.184182
6	-2.484404	0.230152	-0.598296
6	-2.880165	-0.985455	-0.208421
6	-2.031655	-1.915556	0.620762
6	-0.687433	-1.307092	1.082436
1	-0.836462	-0.777031	2.025816
1	0.021657	-2.119428	1.277121
8	1.048573	0.919750	1.811649
8	-1.471625	1.490556	1.086909
1	-0.637383	1.607501	1.579894
1	1.870390	1.356979	2.088216
1	-3.143633	0.864346	-1.190138
1	-3.860480	-1.355739	-0.509730
1	-1.858736	-2.838160	0.043497
1	-2.603878	-2.239158	1.502036
6	2.400300	-1.802867	-0.399200
1	3.328690	-0.301177	0.820825
1	2.160121	-1.295999	1.671459
1	3.274114	-2.451267	-0.448997
1	1.489591	-2.680254	-2.078633
6	0.701829	2.473648	-0.740079
6	1.747405	1.376870	-0.479989
1	1.073797	3.156127	-1.514859
1	0.574568	3.078665	0.166079
1	2.035118	0.891274	-1.420391
1	2.670051	1.827628	-0.082565

Computational data for compound 26 with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1253.2612965570 Energy -695.658134
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.505971	-1.881221	-1.279466
6	2.378009	-0.702567	0.738809
6	0.245602	-1.054383	-1.315174
6	1.259547	0.341482	0.555687
6	-0.069632	-0.324699	0.029038
1	-0.598830	-1.693085	-1.596207
1	0.331742	-0.335479	-2.139122
6	-0.699442	1.877513	-1.167986
6	-1.166163	0.782636	-0.196553
1	-0.605641	1.461577	-2.177582
1	-1.482745	2.644226	-1.214851
6	-2.489505	0.165529	-0.588803
6	-2.851653	-1.066742	-0.205553
6	-1.954438	-2.002934	0.562470
6	-0.636454	-1.354945	1.038370
1	-0.790458	-0.860382	2.003578
1	0.102093	-2.142085	1.221339
8	1.092811	0.905330	1.864753
8	-1.407926	1.525230	1.055838
1	-2.064435	1.033577	1.573717
1	0.254497	1.405926	1.858531
1	-3.181903	0.798485	-1.143399
1	-3.838423	-1.441981	-0.477722
1	-1.747362	-2.879129	-0.071694
1	-2.502001	-2.408476	1.425466
6	2.470299	-1.713918	-0.368018
1	3.332952	-0.170109	0.850176
1	2.218106	-1.209729	1.701175
1	3.362035	-2.339377	-0.400625
1	1.622516	-2.629194	-2.063536
6	0.631329	2.502149	-0.715986
6	1.713901	1.448493	-0.429708
1	0.989242	3.199799	-1.483893
1	0.456812	3.101614	0.185373
1	2.045627	0.985816	-1.368527
1	2.592870	1.935180	0.010312

Computational data for unobserved [7.6.5] compound with hydrogen-bonding pattern A[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1244.2180179361 Energy -695.634193
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.151661	-0.664676	0.098027
6	1.773026	1.259002	-0.900685
6	0.465782	1.051839	-0.094294
6	-0.076807	-0.410057	-0.117677
6	-2.500459	0.634502	-0.190936
6	-1.596489	-0.505304	0.351697
1	-2.651032	0.494729	-1.269341
1	-3.481033	0.524284	0.287123
6	-2.030250	-1.797823	-0.310811
6	-1.281140	-2.052996	-1.387980
6	-0.173305	-1.029199	-1.549713
8	0.655594	1.342176	1.317035
8	-1.756552	-0.574915	1.773141
1	-1.250988	0.161321	2.159247
1	0.974283	2.255091	1.406575
1	-2.902339	-2.351582	0.025445
1	-1.440074	-2.868096	-2.089220
6	2.955892	0.334655	-0.769171
1	1.492430	1.282010	-1.963952
1	2.116701	2.288044	-0.692587
1	3.744526	0.540748	-1.495134
6	2.206533	-1.081317	1.195168
6	0.759975	-1.410623	0.774272
1	4.093403	-1.209737	0.025872
1	2.601685	-1.984663	1.677470
1	2.191289	-0.303585	1.966535
1	0.777227	-2.369064	0.244747
1	0.204279	-1.596538	1.695705
1	-0.453598	-0.282999	-2.309646
1	0.779443	-1.464617	-1.872292
6	-0.546265	2.093369	-0.640680
6	-1.911535	2.024659	0.040445
1	-0.676987	1.948978	-1.721582
1	-0.096777	3.090987	-0.521277
1	-2.577638	2.792468	-0.373820
1	-1.816846	2.237942	1.112757

Computational data for unobserved [7.6.5] compound with hydrogen-bonding pattern B[16,17]

Basis set B3LYP/6-31+G(d)
Nuclear repulsion 1244.9752451807 Energy -695.633645
Formula C14H20O2 Point group C1
Number of imaginary frequencies 0

Cartesian:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	3.133551	-0.653959	0.059040
6	1.771075	1.328451	-0.832346
6	0.448440	1.081355	-0.062811
6	-0.053778	-0.401227	-0.087392
6	-2.501614	0.573824	-0.279722
6	-1.586679	-0.531275	0.305112
1	-2.604214	0.413533	-1.360090
1	-3.511480	0.441870	0.140097
6	-1.959518	-1.854829	-0.342533
6	-1.150940	-2.113086	-1.375039
6	-0.061455	-1.066492	-1.501781
8	0.677988	1.480113	1.307560
8	-1.695990	-0.492495	1.745522
1	-2.634317	-0.432563	1.985447
1	-0.040448	1.115748	1.853570
1	-2.834556	-2.428099	-0.044649
1	-1.251877	-2.949785	-2.061778
6	2.922083	0.354942	-0.792779
1	1.510260	1.470461	-1.890280
1	2.132070	2.313142	-0.495295
1	3.667452	0.532054	-1.570287
6	2.236834	-1.005492	1.217960
6	0.768978	-1.342762	0.878189
1	4.040176	-1.245737	-0.070006
1	2.646367	-1.880632	1.738533
1	2.256721	-0.178416	1.935971
1	0.739861	-2.347259	0.442168
1	0.242940	-1.422515	1.831302
1	-0.312932	-0.346732	-2.296169
1	0.916236	-1.487535	-1.756599
6	-0.576186	2.081360	-0.664569
6	-1.963475	1.982474	-0.035225
1	-0.670634	1.913399	-1.746824
1	-0.157151	3.086072	-0.532406
1	-2.636089	2.725882	-0.481942
1	-1.918264	2.206467	1.037956

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