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SUPPLEMENTARY MATERIAL TO

Synthetic study on the angular triquinanes

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1. PHYSICAL DATA

1.1. 5,5,8-Trimethyl-4,5,5a,6-tetrahydrocyclopenta[c]pentalen-2(1H)-one (7):

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.96 (s, 1H), 5.42 (s, 1H), 2.53 - 2.43 (m, 1H), 2.42 (s, 3H), 2.42 (s, 2H), 2.01 (dd, J_1 = 7.8 Hz, J_2 = 1.6 Hz, 1H), 1.43 – 1.41 (m, 3H), 1.11 (s, 3H), 0.91 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 210.5, 188.8, 140.9, 126.8, 125.3, 70.0, 56.0, 48.2, 43.2, 33.5, 32.5, 26.6, 11.4. **IR** (ATR) ν_{max}: 3404, 3038, 2956, 2924, 2860, 1710, 1636, 1441, 1410, 1382, 1365, 1167, 1018, 826, 802. **HRMS** (m/z) $[M+H]^+$ calcd. for $C_{14}H_{18}O$: 203.14304, found: 203.14204.

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*1.2. 3,3,6-Trimethyl-6a-(2-oxopropyl)-3,3a,4,6a-tetrahydropentalen-1(2H)-one (**8**):*

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.40 (s, 1H), 2.90 (d, J = 17.6 Hz, 1H), 2.67 (d, J = 17.6 Hz, 1H), 2.58 (dd, J_1 = 7.30 Hz, J_2 = 2.25 Hz, 1H), 2.47 (d, J = 17 Hz, 1H), 2.41 – 2.31 (m, 2H), 2.19 (d, J = 17 Hz), 2.08 (s, 3H), 1.61 (s, 3H), 1.12 (s, 3H), 0.93 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 218.8, 207.1, 140.0, 128.3, 66.4, 53.9, 53.0, 47.7, 36.1, 32.0, 30.7, 30.7, 25.1, 12.5. **IR** (ATR) ν_{max}: 3037, 2957, 2867, 1732, 1444, 1387, 1360, 1274, 1274, 1214, 1160, 795, 569. **HRMS** (m/z) $[M+H]^+$ calcd. for $C_{14}H_{20}O_2$: 221.15361, found: 221.15257.

*1.3. 3,3,6-Trimethyl-3,3a,4,6a-tetrahydropentalen-1(2H)-one (**9**):*

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.37 – 5.33 (m, 1H), 3.11 (d, J = 8.30 Hz, 1H), 2.76 – 2.69 (m, 1H), 2.49 – 2.33 (m, 2H), 2.23 (d, J = 16.65 Hz, 1H), 1.98 (dt, J_1 = 16.65 Hz, J_2 = 1.25 Hz, 1H), 1.76 (s, 3H), 1.08 (s, 3H), 1.04 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 217.2, 136.9, 127.0, 62.7, 51.9, 51.0, 37.0, 34.0, 30.4, 24.4, 15.3. **IR** (ATR) ν_{max}: 3039, 2956, 2928, 2867, 1736, 1453, 1410, 1370, 1287, 1261, 1219, 1180, 1154, 1124, 1018, 964, 802. **HRMS** (m/z) $[M+H]^+$ calcd. for $C_{11}H_{16}O$: 165.12739, found: 165.12660.

*1.4. 3,3-Dimethyl-4-(3-oxobutyl)cyclopentan-1-one (**10**):*

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.52 – 2.34 (m, 3H), 2.15 (s, 3H), 2.12 (s, 2H), 1.96 – 1.80 (m, 3H), 1.45 – 1.35 (m, 1H), 1.17 (s, 3H), 0.91 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 217.8, 208.4, 55.5, 46.0, 42.8, 42.6, 38.8, 30.1, 27.5, 23.5, 21.7. **IR** (ATR) ν_{max}: 3467, 2956, 2871, 1741, 1716, 1464, 1406, 1368, 1273, 1219, 1183, 1164, 1164, 530. **HRMS** (m/z) $[M+H]^+$ calcd. for $C_{11}H_{18}O_2$: 183.13796, found: 183.13705.

*1.5. 4-(But-3-en-1-yl)-3,3-dimethylcyclopentan-1-one (**12**):*

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.85 – 5.75 (ddt, J_1 = 17.05 Hz, J_2 = 10.22 Hz, J_3 = 6.50 Hz, 1H), 5.05 – 5.00 (dd, J_1 = 17.16 Hz, J_2 = 1.50 Hz, 1H), 4.99 – 4.96 (dd, J_1 = 10.18 Hz, J_2 = 0.7 Hz, 1H), 2.49 – 2.38 (m, 1H), 2.18 – 2.09 (m, 1H), 2.11 (s, 2H), 2.04 – 1.88 (m, 3H), 1.70 – 1.63 (m, 1H), 1.31 – 1.22 (m, 1H), 1.15 (s, 3H), 0.89 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 218.6, 138.5, 115.0, 55.6, 45.9, 42.8, 38.7, 33.0, 28.9, 27.5, 21.8.

*1.6. 6a-Allyl-3,3,6-trimethyl-3,3a,4,6a-tetrahydropentalen-1(2H)-one (**14**):*

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.65 – 5.55 (m, 1H), 5.39 (s, 1H), 5.10 – 5.02 (m, 2H), 2.61 (dd, J_1 = 14.25 Hz, J_2 = 6.50 Hz, 1H), 2.45- 2.42 (m, 1H), 2.39 – 2.35 (m, 1H), 2.28 (d, J = 16.10, 1H), 2.13 (dd, J_1 = 14.20 Hz, J_2 = 7.90 Hz, 1H), 2.01 (d, J = 16.10 Hz, 1H), 1.64 – 1.62 (m, 3H), 1.06 (s, 3H), 1.00 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 218.3, 139.5, 134.4, 128.1, 117.8, 68.9, 53.6, 52.4, 38.5, 36.2, 32.8, 30.5, 24.7, 12.5. **IR** (ATR) ν_{max}: 3076, 3037, 2959, 2926, 2858, 1731, 1640, 1440, 1413, 1380, 1369, 1161, 993, 914, 805. **HRMS** (m/z) $[M+H]^+$ calcd. for $C_{14}H_{20}O$: 205.15869, found: 205.15773.

2. COPIES OF ^{1}H AND ^{13}C NMR SPECTRA FOR SYNTHESIZED COMPOUNDS

*2.1. 5,5,8-Trimethyl-4,5,5a,6-tetrahydrocyclopenta[c]pentalen-2(1H)-one (**7**):*

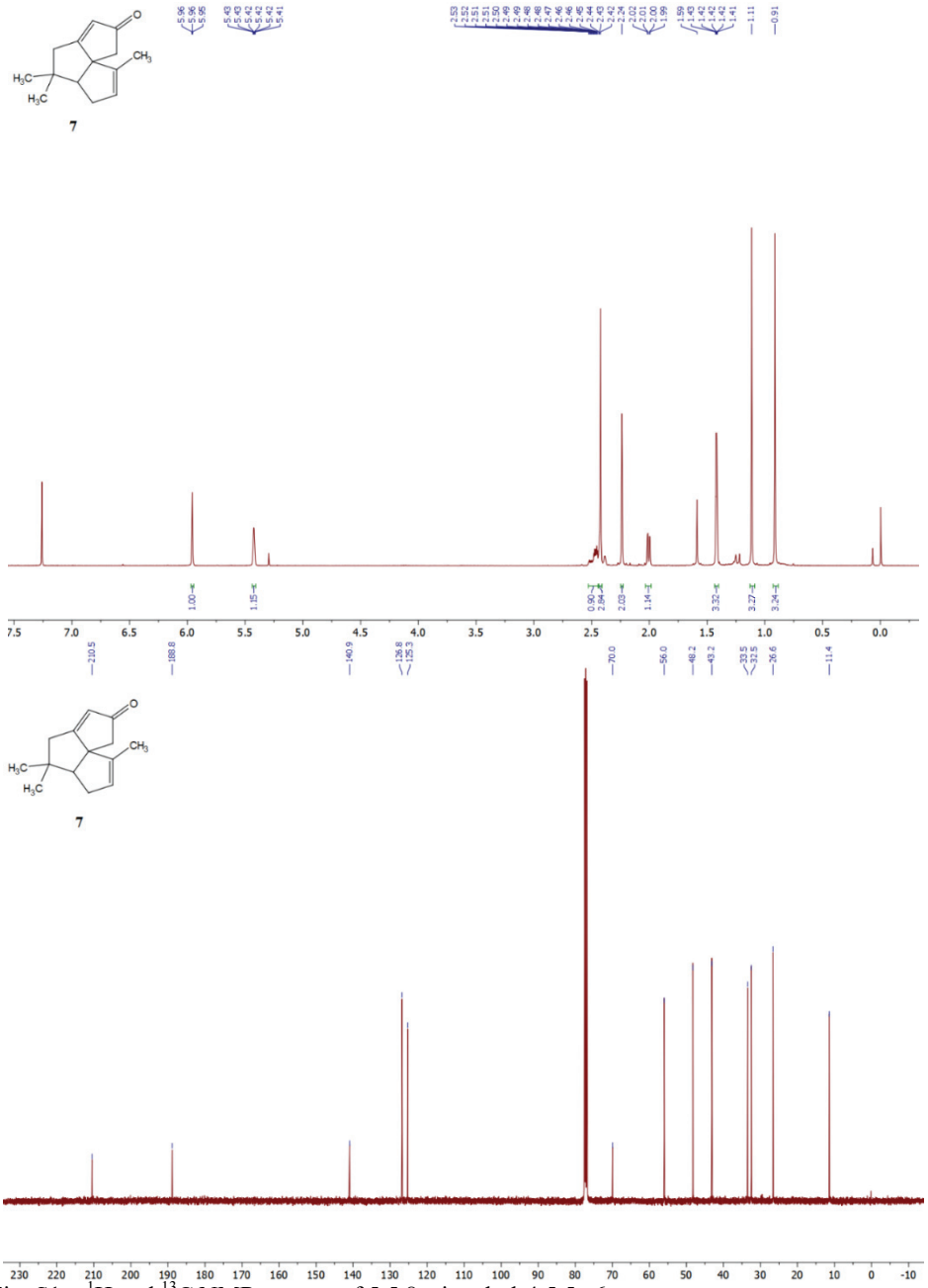

Fig. S1 – ^{1}H and ^{13}C NMR spectra of 5,5,8-trimethyl-4,5,5a,6-tetrahydrocyclopenta[c]pentalen-2(1*H*)-one (**7**)

*2.2. 3,3,6-Trimethyl-6a-(2-oxopropyl)-3,3a,4,6a-tetrahydropentalen-1(2H)-one (**8**):*

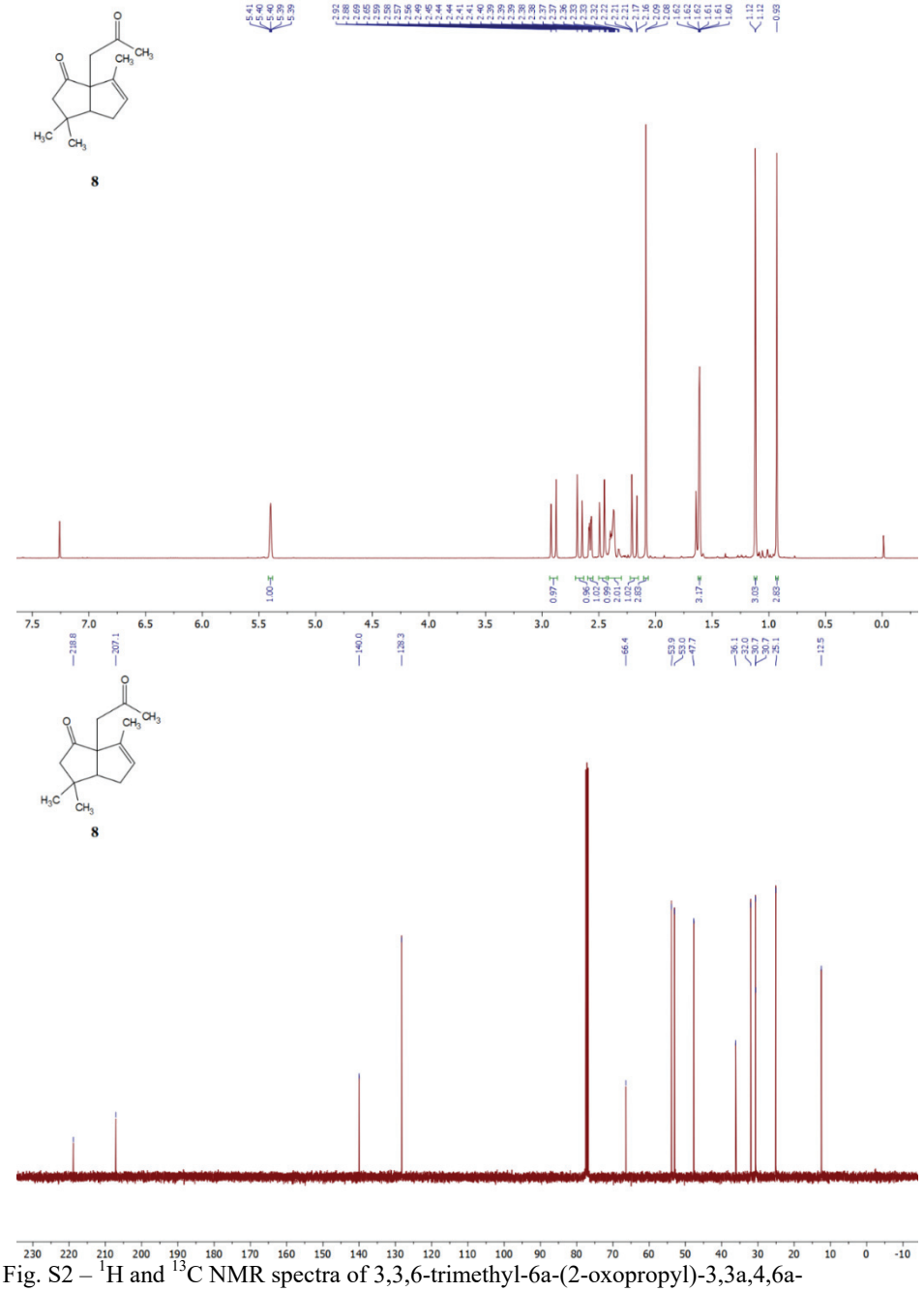

Fig. S2 – ^{1}H and ^{13}C NMR spectra of 3,3,6-trimethyl-6a-(2-oxopropyl)-3,3a,4,6a-tetrahydropentalen-1(2*H*)-one (**8**)

*2.3. 3,3,6-Trimethyl-3,3a,4,6a-tetrahydropentalen-1(2H)-one (**9**):*

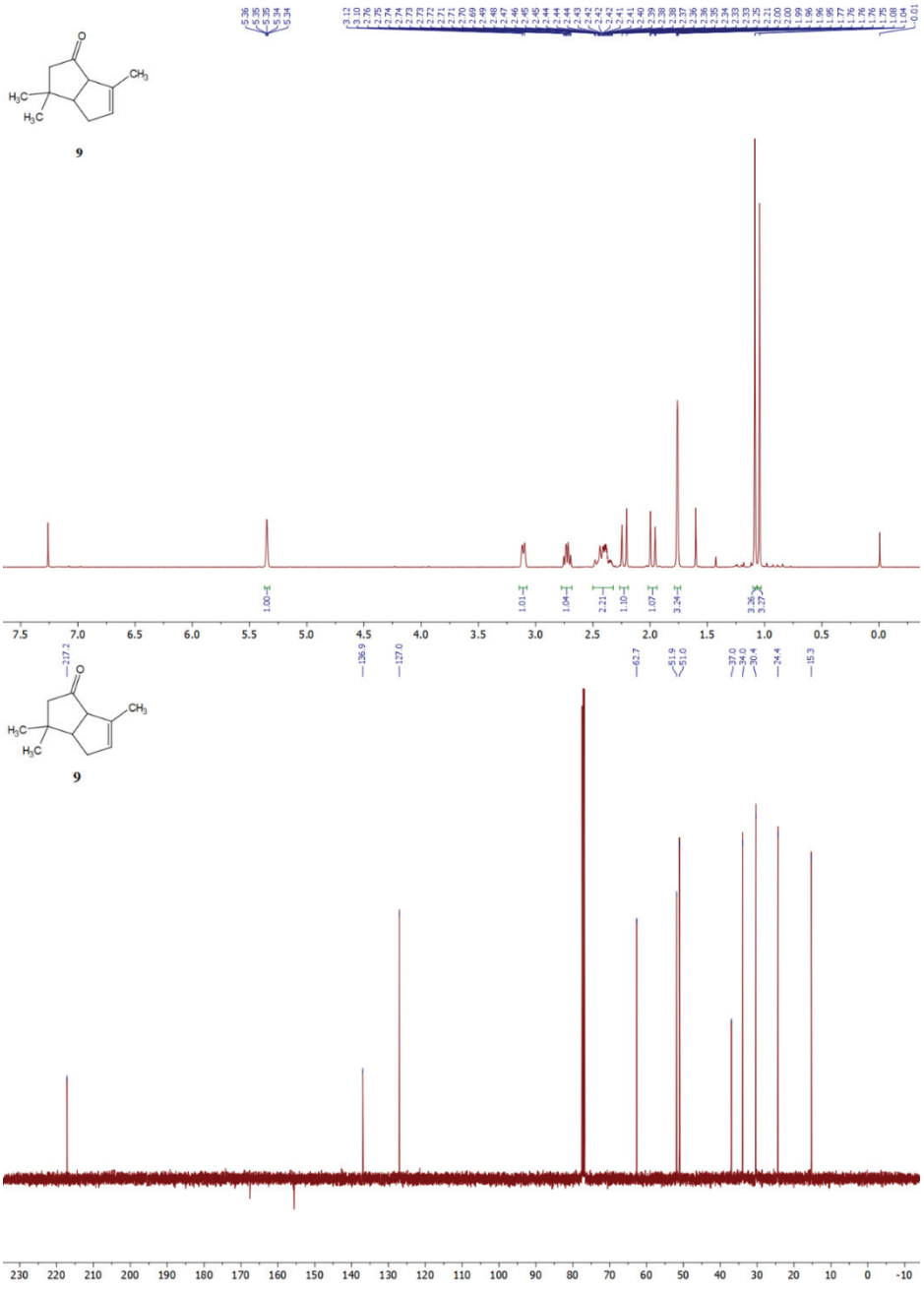

Fig. S3 – ^{1}H and ^{13}C NMR spectra of 3,3,6-trimethyl-3,3a,4,6a-tetrahydropentalen-1(2*H*)-one (**9**)

*2.4. 3,3-Dimethyl-4-(3-oxobutyl)cyclopentan-1-one (**10**):*

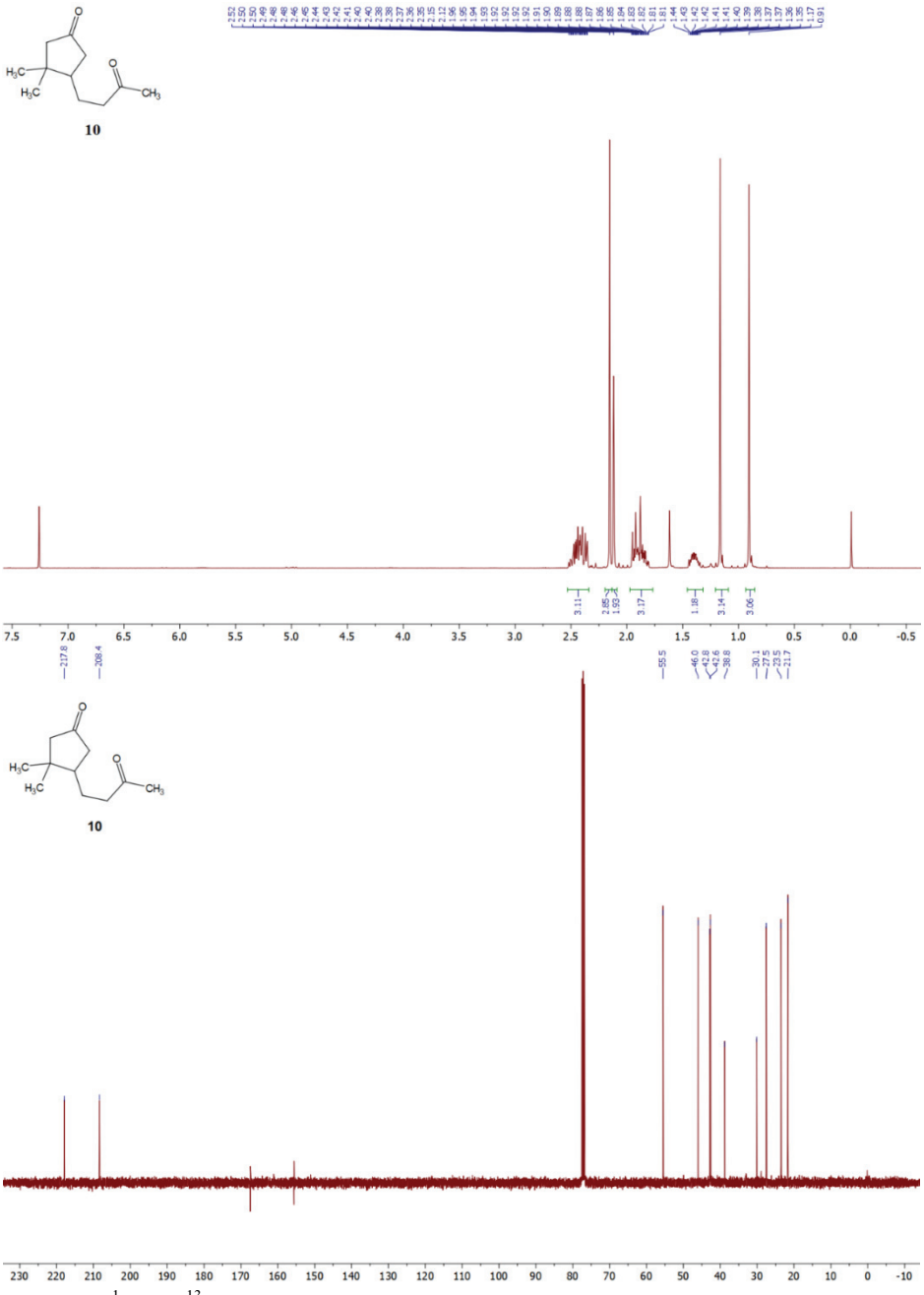

Fig. S4 – ^{1}H and ^{13}C NMR spectra of 3,3-dimethyl-4-(3-oxobutyl)cyclopentan-1-one (**10**)

*2.5. 4-(But-3-en-1-yl)-3,3-dimethylcyclopentan-1-one (**12**):*

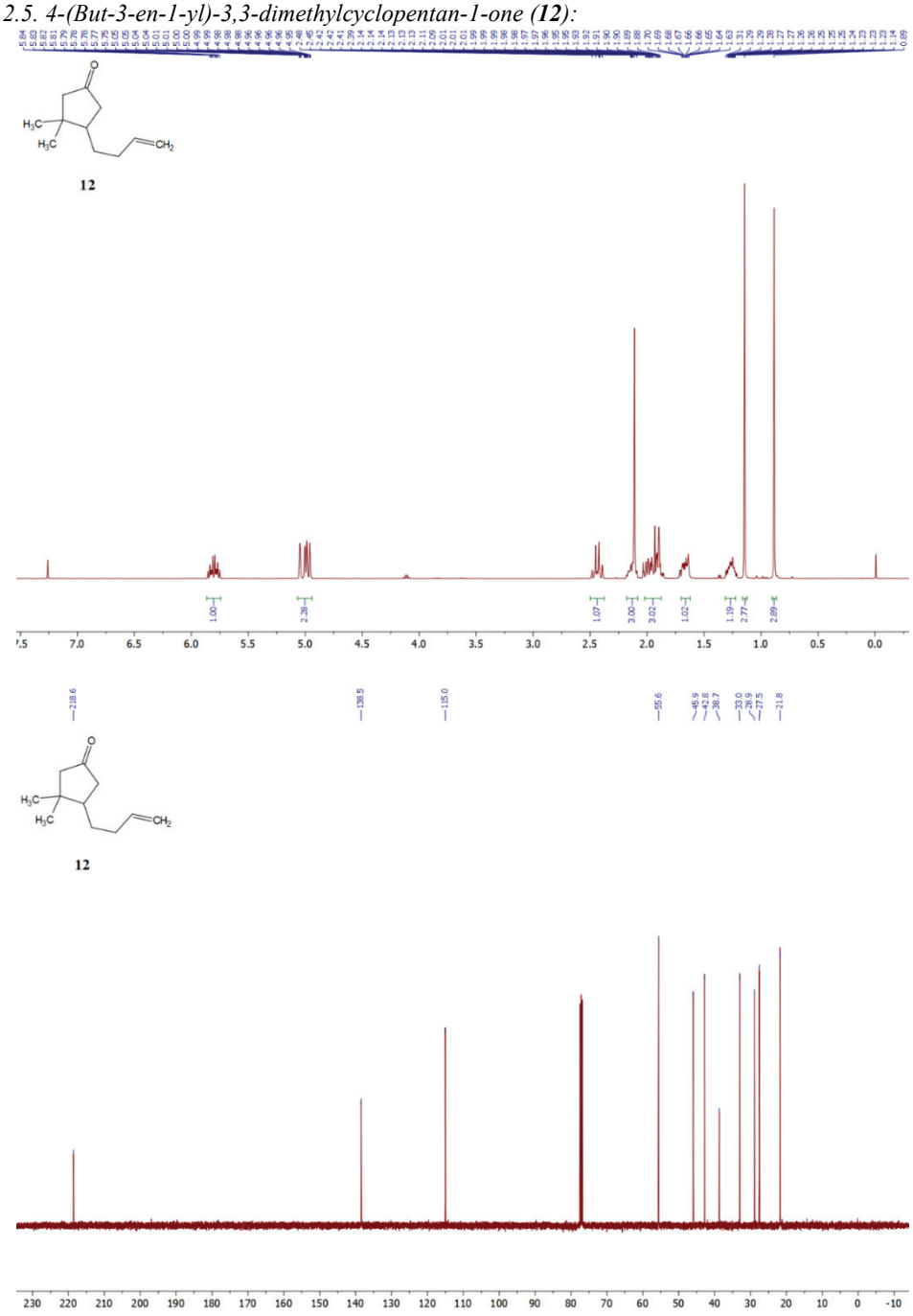

Fig. S5 – ^{1}H and ^{13}C NMR spectra of 4-(but-3-en-1-yl)-3,3-dimethylcyclopentan-1-one (**12**)

*2.6. 6a-Allyl-3,3,6-trimethyl-3,3a,4,6a-tetrahydropentalen-1(2H)-one (**14**):0*

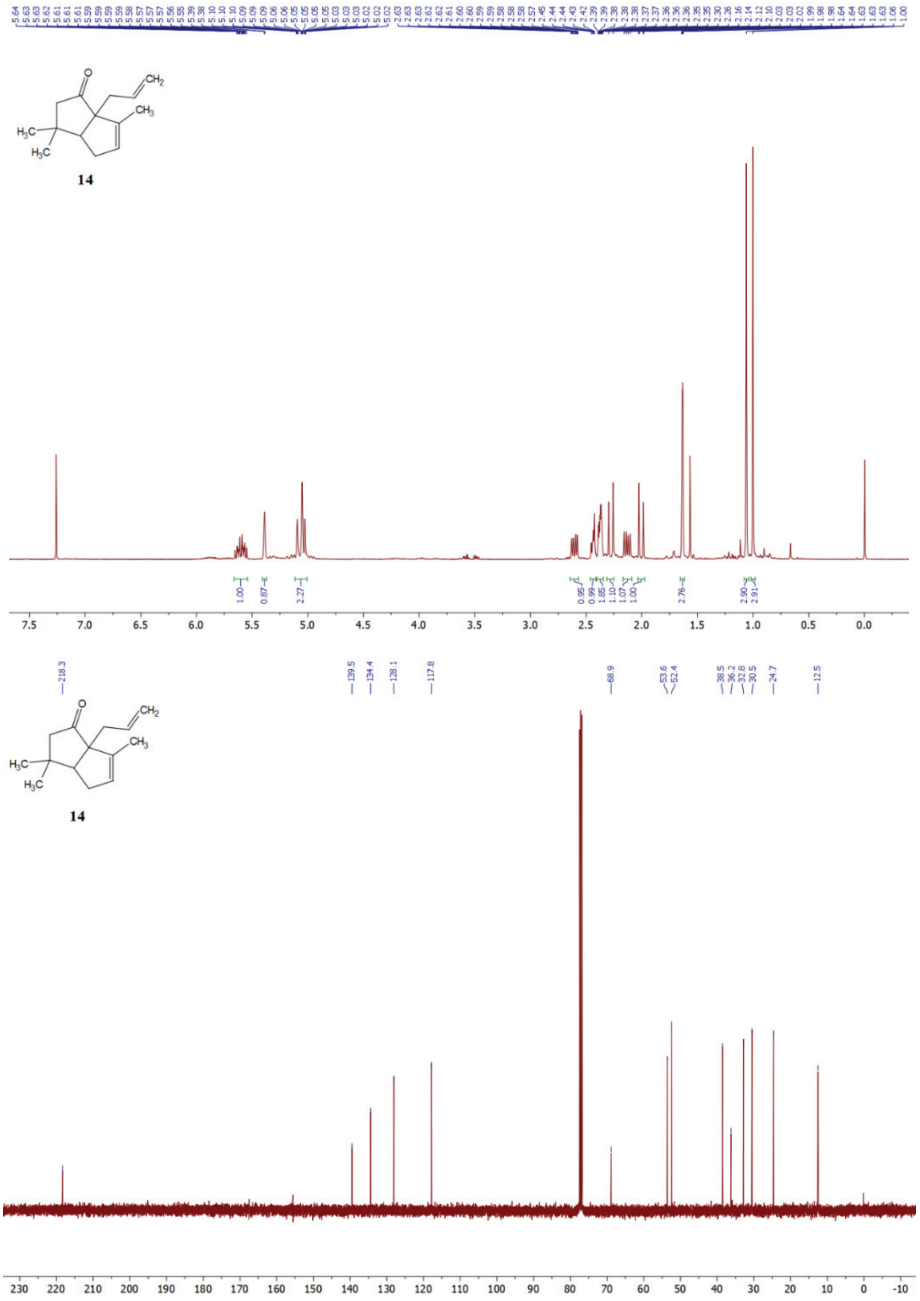

Fig. S6 – ^{1}H and ^{13}C NMR spectra of 6a-allyl-3,3,6-trimethyl-3,3a,4,6a-tetrahydropentalen-1(2*H*)-one (**14**).