Supplementary Materials

Cyclic Monoterpene–Aromatic Hybrids from Chiral Pool Terpenoid Ketones: Practical Synthetic Methodology for Accessing Them and In Silico Assessment as Cannabinoid Receptor CB1/CB2 Ligands

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I. Synthesized (Isolated) Compound Inventory

Compound	Known/New	Compound	Known/New
(-)-1	known	**(+)-1**	known
(-)-2	known	**(+)-2**	known
3	known	**ent-3**	known
4	known	**ent-4**	new
6a	new	**ent-6a**	new
6b	new	**ent-6b**	new
6c	new	**ent-6c**	new
6d	new	**ent-6d**	new
6e	new	**ent-6e**	new
6f	new	**ent-6f**	new
7a	new	**ent-7a**	new
7b	new	**ent-7b**	new
7c	new	**ent-7c**	new
7d	new	**ent-7d**	new
7e	new	**ent-7e**	new
7f	new	**ent-7f**	new
8a	new	**ent-8a***	new
8b**	new	**ent-8b**	new
8c	new	**ent-8c**	new
8d	new	**ent-8d**	new
8e	new	**ent-8e**	new
8f	new	**ent-8f**	new
9a	new	**ent-9a**	new
9b	new	**ent-9b**	new
9c	new	**ent-9c**	new
9d	new	**ent-9d**	new
9e	new	**ent-9e**	new
9f	new	**ent-9f**	new

***** (1*S*,2*R*,5*S*) diastereomer known

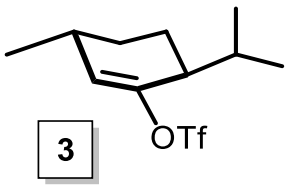
****** (1*R*,2*S*,5*R*) diastereomer known

Notes:

- Enantiomers are formed in independent reactions, each starting from an optically pure precursor.
- Only the major diastereomer was isolated from each hydrogenation reaction (series **8**, **ent-8**, **9**, **ent-9**). The minor diastereomer could not be isolated or characterized.

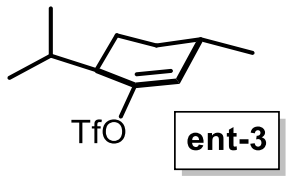
II. Compound Characterization Data

• (3*R*,6*S*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl trifluoromethanesulfonate (3):



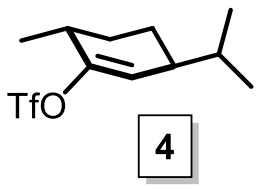
Produced from substrate **(-)-1**. Colorless oil. Yield: 76%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 5.64 (bs, 1H), 2.48 (m, 1H), 2.33 (m, 1H), 2.15 (m, 1H), 1.81 (m, 2H, 2 signals overlapping), 1.42 (m, 1H), 1.13 (m, 1H), 1.04 (d, 3H, *J* = 7.2 Hz), 0.95 (d, 3H, *J* = 6.9 Hz), 0.82 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 151.8, 125.9, 118.6 (q, CF_3, *J* = 319.9 Hz), 43.1, 30.6, 29.9, 27.3, 22.5, 21.3, 19.9, 16.3. FT-IR: v (cm^{-1}) 2962 (m), 2932 (m), 2875 (m), 1674 (w), 1415 (s), 1246 (s), 1203 (s), 1142 (s), 1045 (w), 974 (m), 944 (m), 893 (s), 873 (m), 817 (m). $[a]^{23}_D$ +4.8 (*c* 0.7, CH_2Cl_2).

• (3*S*,6*R*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl trifluoromethanesulfonate (ent-3):



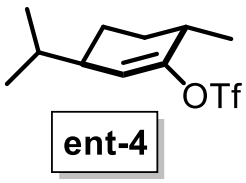
Produced from substrate **(+)-1**. Colorless oil. Yield: 75%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 5.64 (bs, 1H), 2.48 (m, 1H), 2.33 (m, 1H), 2.15 (m, 1H), 1.81 (m, 2H, 2 signals overlapping), 1.42 (m, 1H), 1.13 (m, 1H), 1.04 (d, 3H, *J* = 7.2 Hz), 0.95 (d, 3H, *J* = 6.9 Hz), 0.82 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 151.8, 125.9, 118.6 (q, CF_3, *J* = 319.9 Hz), 43.1, 30.6, 29.9, 27.3, 22.5, 21.3, 19.9, 16.3. FT-IR: v (cm^{-1}) 2962 (m), 2932 (m), 2875 (m), 1674 (w), 1415 (s), 1246 (s), 1203 (s), 1142 (s), 1045 (w), 974 (m), 944 (m), 893 (s), 873 (m), 817 (m). $[a]^{23}_D$ -5.3 (*c* 0.8, CH_2Cl_2).

• (3*S*,6*R*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl trifluoromethanesulfonate (4):



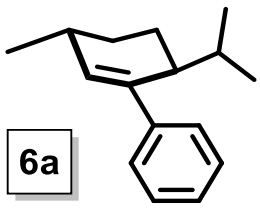
Produced from substrate **(+)-2**. Colorless oil. Yield: 76%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 5.64 (d, 1H, *J* = 2.7 Hz), 2.49 (m, 1H), 2.15 (m, 1H), 1.84 (ddt, 1H, J_1 = 12.7 Hz, J_2 = 5.9 Hz, J_3 = 3.1 Hz), 1.60-1.70 (m, 2H, 2 signals overlapping), 1.56 (m, 1H), 1.39 (m, 1H), 1.14 (d, 3H, *J* = 7.0 Hz), 0.92 (d, 3H, *J* = 6.6 Hz), 0.90 (d, 3H, *J* = 6.6 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 153.7, 121.2, 118.5 (q, CF_3, *J* = 319.2 Hz), 42.0, 31.9, 31.7, 29.5, 20.3, 19.6, 19.4, 17.9. FT-IR: v (cm^{-1}) 2963 (w), 2875 (w), 1652 (w), 1576 (w), 1560 (w), 1541 (w), 1508 (w), 1457 (w), 1414 (w), 1246 (w), 1203 (m), 1141 (m), 1038 (w), 1004 (w), 938 (w), 882 (m), 863 (w), 811 (w). $[a]^{23}_D$ -29.7 (*c* 1.4, CH_2Cl_2).

• **(3*R*,6*S*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl trifluoromethanesulfonate (ent-4):**



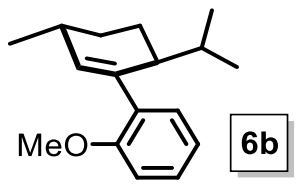
Produced from substrate **(-)-2**. Colorless oil. Yield: 74%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 5.64 (d, 1H, *J* = 2.7 Hz), 2.49 (m, 1H), 2.15 (m, 1H), 1.84 (ddt, 1H, J_1 = 12.7 Hz, J_2 = 5.9 Hz, J_3 = 3.1 Hz), 1.60-1.70 (m, 2H, 2 signals overlapping), 1.56 (m, 1H), 1.39 (m, 1H), 1.14 (d, 3H, *J* = 7.0 Hz), 0.92 (d, 3H, *J* = 6.6 Hz), 0.90 (d, 3H, *J* = 6.6 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 153.7, 121.2, 118.5 (q, CF_3, *J* = 319.2 Hz), 42.0, 31.9, 31.7, 29.5, 20.3, 19.6, 19.4, 17.9. FT-IR: ν (cm^{-1}) 2963 (w), 2875 (w), 1652 (w), 1576 (w), 1560 (w), 1541 (w), 1508 (w), 1457 (w), 1414 (w), 1246 (w), 1203 (m), 1141 (m), 1038 (w), 1004 (w), 938 (w), 882 (m), 863 (w), 811 (w). $[a]^{23}_D$ +26.5 (*c* 1.2, CH_2Cl_2).

• **(2*S*,5*R*)-2-Isopropyl-5-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (6a):**



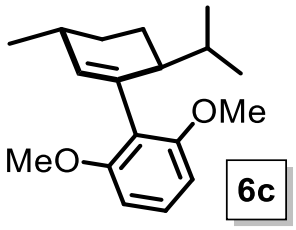
Produced from substrates **3** and **5a**. Colorless oil. Yield: 52%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.24-7.32 (m, 4H, 2 signals overlapping), 7.20 (tt, 1H, J_1 = 7.1 Hz, J_2 = 1.9 Hz), 5.67 (bs, 1H), 2.71 (m, 1H), 2.22 (m, 1H), 1.80-1.90 (m, 3H, 3 signals overlapping), 1.47 (m, 1H), 1.17 (m, 1H), 1.01 (d, 3H, *J* = 7.1 Hz), 0.88 (d, 3H, *J* = 6.9 Hz), 0.58 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 143.5, 141.6, 135.0, 128.0, 126.6, 126.1, 41.6, 31.3, 31.0, 28.4, 22.1, 21.6, 20.7, 15.6. FT-IR: ν (cm^{-1}) 2954 (m), 2918 (s), 2850 (m), 2360 (m), 2344 (w), 2162 (w), 2032 (w), 1738 (w), 1647 (w), 1639 (w), 1563 (w), 1048 (w). $[a]^{23}_D$ +16.5 (*c* 0.3, CH_2Cl_2).

• **(2*S*,5*R*)-2-Isopropyl-2'-methoxy-5-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (6b):**



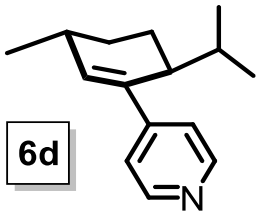
Produced from substrates **3** and **5b**. Colorless oil. Yield: 90%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.20 (dt, 1H, J_1 = 7.9 Hz, J_2 = 1.8 Hz), 7.13 (dd, 1H, J_1 = 7.3 Hz, J_2 = 1.8 Hz), 6.90 (t, 1H, *J* = 7.5 Hz), 6.82 (d, 1H, *J* = 8.1 Hz), 5.56 (bs, 1H), 3.80 (s, 3H), 2.86 (m, 1H), 2.24 (m, 1H), 1.87 (m, 1H), 1.77 (m, 1H), 1.58 (m, 1H), 1.38 (m, 1H), 1.22 (m, 1H), 1.01 (d, 3H, *J* = 7.2 Hz), 0.85 (d, 3H, *J* = 6.9 Hz), 0.57 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 156.7, 141.1, 135.4, 132.9, 130.3, 127.4, 120.6, 110.5, 55.4, 42.2, 31.7, 31.5, 28.7, 22.1, 21.9, 21.0, 15.8. FT-IR: ν (cm^{-1}) 2953 (s), 2926 (s), 2867 (m), 2834 (w), 1597 (w), 1577 (w), 1488 (m), 1460 (m), 1434 (m), 1383 (w), 1365 (w), 1290 (w), 1246 (s), 1230 (m), 1179 (w), 1115 (m), 1052 (w), 1029 (m), 863 (w), 780 (w), 748 (s). $[a]^{23}_D$ +3.5 (*c* 0.6, CH_2Cl_2).

• (2*S*,5*R*)-2-Isopropyl-2',6'-dimethoxy-5-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (6c):



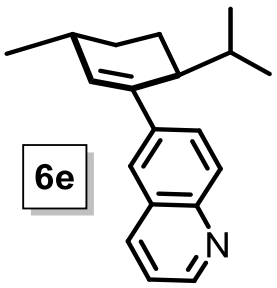
Produced from substrates **3** and **5c**. Colorless oil. Yield 65%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.13 (t, 1H, *J* = 8.3 Hz), 6.54 (bd, 2H, *J* = 8.3 Hz), 5.47 (bs, 1H), 3.76 (s, 6H), 2.68 (m, 1H), 2.32 (m, 1H), 1.88 (m, 1H), 1.75 (m, 1H), 1.50 (m, 1H), 1.46 (m, 1H), 1.25 (m, 1H), 0.99 (d, 3H, *J* = 7.1 Hz), 0.82 (m, 3H, *J* = 6.9 Hz), 0.67 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 158.0, 135.9, 134.3, 127.1, 121.3, 104.4 (app. d), 55.9 (app. d), 43.0, 31.6, 31.4, 29.0, 22.1, 21.9, 21.5, 16.3. FT-IR: v (cm^{-1}) 2952 (m), 2932 (m), 2869 (m), 2836 (m), 1587 (s), 1465 (s), 1442 (m), 1431 (s), 1382 (w), 1280 (w), 1240 (s), 1117 (w), 1102 (s), 1035 (m), 956 (w), 862 (w), 782 (s), 756 (w), 732 (s). $[a]^{23}_{D}$ +3.2 (*c* 1.1, CH_2Cl_2).

• 4-((3*R*,6*S*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl)pyridine (6d):



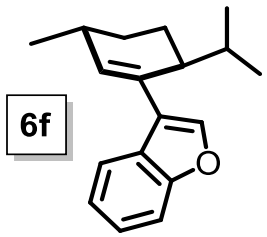
Produced from substrates **3** and **5d**. Colorless oil. Yield: 63%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.50 (d, 2H, *J* = 5.2 Hz), 7.20 (d, 2H, *J* = 5.2 Hz), 5.85 (bs, 1H), 2.69 (m, 1H), 2.24 (m, 1H), 1.78-1.88 (m, 3H, 3 signals overlapping), 1.47 (m, 1H), 1.15 (m, 1H), 1.03 (d, 3H, *J* = 7.1 Hz), 0.88 (d, 3H, *J* = 6.9 Hz), 0.56 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 152.1, 148.5, 139.6, 138.3, 121.8, 41.0, 31.4, 30.5, 28.4, 21.7, 21.3, 20.6, 15.7. FT-IR: v (cm^{-1}) 2959 (s), 2936 (s), 2872 (m), 2850 (m), 1715 (w), 1597 (s), 1544 (w), 1465 (m), 1412 (m), 1366 (m), 1219 (w), 1108 (w), 1062 (w), 992 (w), 819 (m). $[a]^{23}_{D}$ +8.5 (*c* 0.9, CH_2Cl_2).

• 6-((3*R*,6*S*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl)quinoline (6e):



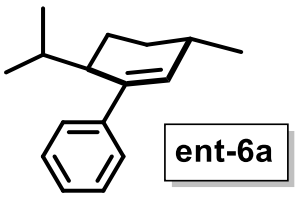
Produced from substrates **3** and **5e**. White crystals. Yield: 99%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.86 (d, 1H, *J* = 4.3 Hz), 8.16 (d, 1H, *J* = 8.4 Hz), 8.08 (d, 1H, *J* = 8.4 Hz), 7.65-7.71 (m, 2H, 2 peaks overlapping), 7.40 (dd, 1H, J_1 = 8.4 Hz, J_2 = 4.3 Hz), 5.83 (bs, 1H), 2.82 (m, 1H), 2.28 (m, 1H), 1.80-1.94 (m, 3H, 3 signals overlapping), 1.51 (m, 1H), 1.21 (m, 1H), 1.04 (d, 3H, *J* = 7.1 Hz), 0.89 (d, 3H, *J* = 6.9 Hz), 0.59 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.0, 146.6, 142.2, 141.0, 136.7, 136.5, 129.7, 128.4, 128.3, 124.4, 121.1, 41.6, 31.5, 30.9, 28.6, 22.0, 21.6, 20.7, 15.7. FT-IR: v (cm^{-1}) 2956 (m), 2923 (m), 2885 (m), 2867 (m), 2846 (m), 2831 (m), 1720 (w), 1589 (m), 1494 (m), 1385 (m), 1366 (m), 1120 (w), 945 (w), 883 (w), 875 (m), 840 (s), 794 (m), 777 (m). $[a]^{23}_{D}$ +2.6 (*c* 0.4, CH_2Cl_2).

• **3-((3*R*,6*S*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl)benzofuran (6f):**



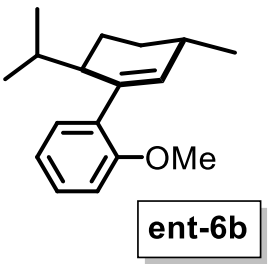
Produced from substrates **3** and **5f**. Colorless oil. Yield: 81%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.66 (d, 1H, *J* = 7.7 Hz), 7.48 (s, 1H), 7.47 (d, 1H, *J* = 7.5 Hz), 7.28 (t, 1H, *J* = 7.4 Hz), 7.24 (t, 1H, *J* = 7.5 Hz), 5.90 (bs, 1H), 2.66 (m, 1H), 2.29 (m, 1H), 1.80-2.00 (m, 3H, 3 signals overlapping), 1.50 (m, 1H), 1.24 (m, 1H), 1.02 (d, 3H, *J* = 7.1 Hz), 0.88 (d, 3H, *J* = 6.9 Hz), 0.64 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.3, 140.7, 135.4, 132.2, 127.4, 124.0, 122.9, 122.5, 120.7, 111.5, 42.4, 31.0, 30.9, 28.9, 22.0, 21.6, 20.8, 16.1. FT-IR: ν (cm^{-1}) 2961 (s), 2928 (s), 2870 (s), 1763 (m), 1604 (m), 1460 (s), 1382 (w), 1329 (w), 1242 (w), 1077 (s), 1047 (s), 879 (m), 746 (s). $[a]^{23}_{D}$ +5.7 (*c* 0.2, CH_2Cl_2).

• **(2*R*,5*S*)-2-Isopropyl-5-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (ent-6a):**



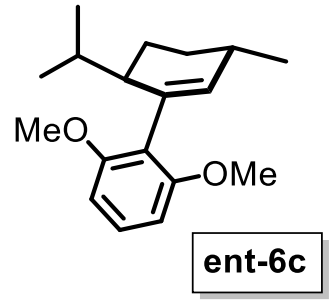
Produced from substrates **ent-3** and **5a**. Colorless oil. Yield: 60%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.24-7.32 (m, 4H, 2 signals overlapping), 7.20 (tt, 1H, J_1 = 7.1 Hz, J_2 = 1.9 Hz), 5.67 (bs, 1H), 2.71 (m, 1H), 2.22 (m, 1H), 1.80-1.90 (m, 3H, 3 signals overlapping), 1.47 (m, 1H), 1.17 (m, 1H), 1.01 (d, 3H, *J* = 7.1 Hz), 0.88 (d, 3H, *J* = 6.9 Hz), 0.58 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 143.5, 141.6, 135.0, 128.0, 126.6, 126.1, 41.6, 31.3, 31.0, 28.4, 22.1, 21.6, 20.7, 15.6. FT-IR: ν (cm^{-1}) 2954 (m), 2918 (s), 2850 (m), 2360 (m), 2344 (w), 2162 (w), 2032 (w), 1738 (w), 1647 (w), 1639 (w), 1563 (w), 1048 (w). $[a]^{23}_{D}$ -17.2 (*c* 1.01, CH_2Cl_2).

• **(2*R*,5*S*)-2-Isopropyl-2'-methoxy-5-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (ent-6b):**



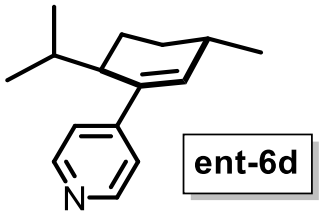
Produced from substrate **ent-3** and **5b**. Yellow oil. Yield: 80%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.20 (dt, 1H, J_1 = 7.9 Hz, J_2 = 1.9 Hz), 7.13 (dd, 1H, J_1 = 7.4 Hz, J_2= 1.7 Hz), 6.90 (t, 1H, *J* = 7.5 Hz), 6.82 (d, 1H, *J* = 8.1 Hz), 5.56 (bs, 1H), 3.80 (s, 3H), 2.86 (m, 1H), 2.24 (m, 1H), 1.87 (m, 1H), 1.77 (m, 1H), 1.58 (m, 1H), 1.38 (m, 1H), 1.22 (m, 1H), 1.01 (d, 3H, *J* = 7.2 Hz), 0.85 (d, 3H, *J* = 6.9 Hz), 0.57 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 156.7, 141.1, 135.4, 132.9, 130.3, 127.4, 120.6, 110.5, 55.4, 42.2, 31.7, 31.5, 28.7, 22.1, 21.9, 21.0, 15.8. FT-IR: ν (cm^{-1}) 2955 (s), 2923 (s), 2869 (m), 2850 (m), 1597 (w), 1488 (m), 1461 (s), 1434 (m), 1378 (m), 1247 (s), 1230 (m), 1178 (w), 1115 (m), 1097 (w), 1049 (m), 1029 (s), 803 (m) 748 (s). $[a]^{23}_{D}$ -4.0 (*c* 0.5, CH_2Cl_2).

• **(2*R*,5*S*)-2-Isopropyl-2',6'-dimethoxy-5-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (ent-6c):**



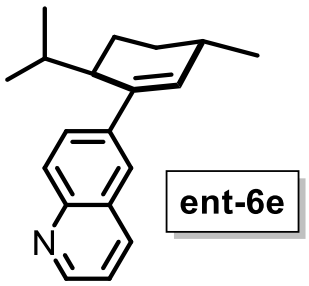
Produced from substrates **ent-3** and **5c**. White solid. Yield: 56%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.13 (t, 1H, *J* = 8.3 Hz), 6.54 (bd, 2H, *J* = 8.3 Hz), 5.47 (bs, 1H), 3.76 (s, 6H), 2.68 (m, 1H), 2.32 (m, 1H), 1.88 (m, 1H), 1.75 (m, 1H), 1.50 (m, 1H), 1.46 (m, 1H), 1.25 (m, 1H), 0.99 (d, 3H, *J* = 7.1 Hz), 0.82 (m, 3H, *J* = 6.9 Hz), 0.67 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 158.0, 135.9, 134.3, 127.1, 121.3, 104.4 (app. d), 55.9 (app. d), 43.0, 31.6, 31.4, 29.0, 22.1, 21.9, 21.5, 16.3. FT-IR: v (cm^{-1}) 2952 (m), 2934 (m), 2870 (w), 2836 (w), 1589 (s), 1465 (s), 1442 (m), 1431 (s), 1382 (w), 1280 (w), 1240 (s), 1171 (w), 1128 (w), 1103 (s), 1037 (m), 958 (w), 863 (w). 783 (s), 733 (s). $[a]^{23}_{D}$ -3.9 (*c* 0.7, CH_2Cl_2).

• **4-((3*S*,6*R*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl)pyridine (ent-6d):**



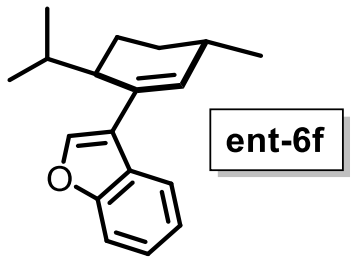
Produced from substrates **ent-3** and **5d**. Colorless oil. Yield 70%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.50 (d, 2H, *J* = 5.2 Hz), 7.20 (d, 2H, *J* = 5.2 Hz), 5.85 (bs, 1H), 2.69 (m, 1H), 2.24 (m, 1H), 1.78-1.88 (m, 3H, 3 signals overlapping), 1.47 (m, 1H), 1.15 (m, 1H), 1.03 (d, 3H, *J* = 7.1 Hz), 0.88 (d, 3H, *J* = 6.9 Hz), 0.56 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 152.1, 148.5, 139.6, 138.3, 121.8, 41.0, 31.4, 30.5, 28.4, 21.7, 21.3, 20.6, 15.7. FT-IR: v (cm^{-1}) 2960 (s), 2933 (s), 2871 (s), 1713 (m), 1687 (m), 1597 (s), 1544 (w), 1465 (m), 1411 (s), 1386 (w), 1366 (s), 1219 (m), 1065 (m), 994 (m), 819 (m). $[a]^{23}_{D}$ -7.6 (*c* 1, CH_2Cl_2).

• **6-((3*S*,6*R*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl)quinoline (ent-6e):**



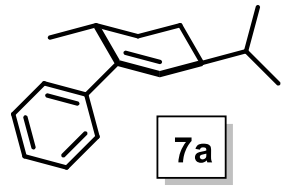
Produced from substrates **ent-3** and **5e**. White crystals. Yield: 95%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.86 (d, 1H, *J* = 4.3 Hz), 8.16 (d, 1H, *J* = 8.4 Hz), 8.08 (d, 1H, *J* = 8.4 Hz), 7.65-7.71 (m, 2H, 2 peaks overlapping), 7.40 (dd, 1H, J_1 = 8.4 Hz, J_2 = 4.3 Hz), 5.83 (bs, 1H), 2.82 (m, 1H), 2.28 (m, 1H), 1.80-1.94 (m, 3H, 3 signals overlapping), 1.51 (m, 1H), 1.21 (m, 1H), 1.04 (d, 3H, *J* = 7.1 Hz), 0.89 (d, 3H, *J* = 6.9 Hz), 0.59 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.0, 146.6, 142.2, 141.0, 136.7, 136.5, 129.7, 128.4, 128.3, 124.4, 121.1, 41.6, 31.5, 30.9, 28.6, 22.0, 21.6, 20.7, 15.7. FT-IR: v (cm^{-1}) 2956 (s), 2925 (s), 2867 (m), 2832 (w), 1656 (w), 1629 (w), 1588 (w), 1494 (m), 1460 (m), 1451 (w), 1386 (m), 1366 (m), 1322 (w), 1181 (m), 883 (w) 875 (m), 840 (s), 794 (m), 777 (m). $[a]^{23}_{D}$ -3.0 (*c* 0.7, CH_2Cl_2).

• **3-((3*S*,6*R*)-6-Isopropyl-3-methylcyclohex-1-en-1-yl)benzofuran (ent-6f):**



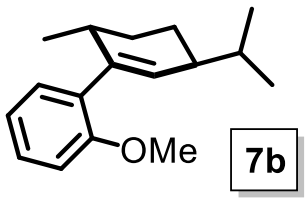
Produced from substrates **ent-3** and **5f**. Yellow oil. Yield: 86%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.66 (d, 1H, *J* = 7.7 Hz), 7.48 (s, 1H), 7.47 (d, 1H, *J* = 7.5 Hz), 7.28 (t, 1H, *J* = 7.4 Hz), 7.24 (t, 1H, *J* = 7.5 Hz), 5.90 (bs, 1H), 2.66 (m, 1H), 2.29 (m, 1H), 1.80-2.00 (m, 3H, 3 signals overlapping), 1.50 (m, 1H), 1.24 (m, 1H), 1.02 (d, 3H, *J* = 7.1 Hz), 0.88 (d, 3H, *J* = 6.9 Hz), 0.64 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.3, 140.7, 135.4, 132.2, 127.4, 124.0, 122.9, 122.5, 120.7, 111.5, 42.4, 31.0, 30.9, 28.9, 22.0, 21.6, 20.8, 16.1. FT-IR: v (cm^{-1}) 2956 (s), 2923 (s), 2869 (m), 1765 (m), 1614 (m), 1460 (s), 1382 (w), 1329 (w), 1242 (w), 1127 (w), 1068 (m), 1029 (m), 936 (w), 791 (w), 746 (s). $[a]^{23}_{D}$ -6.3 (*c* 0.6, CH_2Cl_2).

• **(2*R*,5*S*)-5-Isopropyl-2-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (7a):**



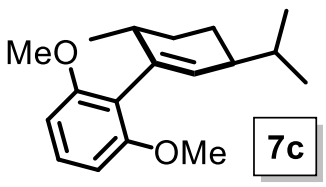
Produced from substrates **4** and **5a**. Colourless oil. Yield: 88%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.34 (d, 2H, *J* = 7.9 Hz), 7.30 (app. t, 2H, *J* = 7.6 Hz), 7.22 (tt, 1H, J_1 = 7.3 Hz, J_2 = 1.8 Hz), 5.79 (bs, 1H), 2.84 (m, 1H), 2.12 (m, 1H), 1.84 (m, 1H), 1.68-1.76 (m, 2H, 2 signals overlapping), 1.58 (m, 1H), 1.44 (m, 1H), 0.98 (d, 3H, *J* = 6.9 Hz), 0.94(9) (d, 3H, *J* = 6.9 Hz), 0.94(6) (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 143.2, 129.0, 128.1, 127.9, 126.5, 126.2, 42.7, 32.3, 30.3, 29.9, 20.0, 19.9, 19.8, 19.3. FT-IR: v (cm^{-1}) 2961 (s), 2929 (s), 2873 (m), 1705 (w), 1682 (m), 1599 (w), 1493 (w), 1458 (m), 1448 (m), 1366 (m), 973 (w), 761 (s). $[a]^{23}_{D}$ +4.3 (*c* 0.5, CH_2Cl_2).

• **(2*R*,5*S*)-5-Isopropyl-2'-methoxy-2-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (7b):**



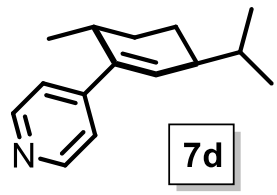
Produced from substrates **4** and **5b**. Colorless oil. Yield: 35%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.22 (dt, 1H, J_1 = 7.8 Hz, J_2 = 1.7 Hz), 7.06 (dd, 1H, J_1 = 7.4 Hz, J_2 = 1.7 Hz), 6.90 (dt, 1H, J_1 = 7.4 Hz, J_2 = 1.0 Hz), 6.85 (dd, 1H, J_1 = 8.2 Hz, J_2 = 1.0 Hz), 5.51 (bs, 1H), 3.80 (s, 3H), 2.80 (m, 1H), 2.13 (m, 1H), 1.88 (m, 1H), 1.69 (m, 1H), 1.54-1.62 (m, 2H, 2 signals overlapping), 1.49 (m, 1H), 0.96 (d, 3H, *J* = 6.8 Hz), 0.94 (d, 3H, *J* = 6.8 Hz), 0.84 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 156.7, 143.1, 133.2, 130.8, 129.7, 127.7, 120.3, 110.5, 55.5, 42.0, 32.3, 31.0, 29.6, 20.6, 19.8, 19.7, 19.4. FT-IR: v (cm^{-1}) 2956 (m), 2920 (m), 2869 (m), 2831 (w), 1726 (w), 1597 (m), 1579 (w), 1488 (m), 1462 (m), 1435 (m), 1378 (w), 1365 (w), 1289 (m), 1244 (s), 1179 (w), 1115 (m), 1052 (m), 1028 (m), 751 (s). $[a]^{23}_{D}$ +5.3 (*c* 0.6, CH_2Cl_2).

• **(2*R*,5*S*)-5-Isopropyl-2',6'-dimethoxy-2-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (7c):**



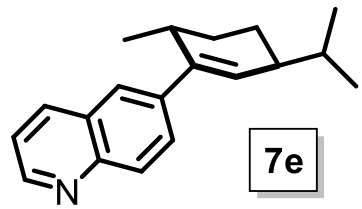
Produced from substrates **4** and **5c**. Colorless oil. Yield: 31%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.16 (t, 1H, *J* = 8.3 Hz), 6.55 (d, 2H, *J* = 8.3 Hz), 5.37 (bs, 1H), 3.76 (s, 6H), 2.52 (m, 1H), 2.18 (m, 1H), 1.88 (m, 1H), 1.71 (m, 1H), 1.59 (m, 1H), 1.52-1.58 (m, 2H, 2 signals overlapping), 0.95 (d, 3H, *J* = 6.9 Hz), 0.94 (d, 3H, *J* = 6.9 Hz), 0.84 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 158.1, 136.2, 130.5, 127.4, 121.8, 104.0, 55.8, 42.0, 32.3, 31.8, 29.7, 20.2, 19.5, 19.3, 19.1. FT-IR: ν (cm^{-1}) 2958 (m), 2932 (m), 2870 (w), 2834 (w), 1709 (w), 1585 (m), 1468 (s), 1432 (m), 1245 (s), 1107 (s), 778 (w), 726 (m). $[a]^{23}_{D}$ -14.3 (*c* 0.3, CH_2Cl_2).

• **4-((3*S*,6*R*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl)pyridine (7d):**



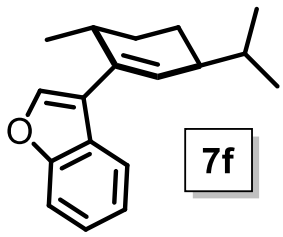
Produced from substrates **4** and **5d**. Yellow oil. Yield: 99%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.51 (d, 2H, *J* = 5.5 Hz), 7.27 (d, 2H, *J* = 5.5 Hz), 6.05 (bs, 1H), 2.82 (m, 1H), 2.14 (m, 1H), 1.81 (ddt, 1H, J_1 = 12.9 Hz, J_2 = 5.5 Hz, J_3 = 3.2 Hz), 1.69-1.79 (m, 2H, 2 signals overlapping), 1.60 (m, 1H), 1.45 (m, 1H), 0.98 (d, 3H, *J* = 6.7 Hz), 0.96 (d, 3H, *J* = 6.7 Hz), 0.94 (d, 3H, *J* = 6.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 150.1, 149.2, 140.8, 132.8, 120.9, 42.8, 32.2, 29.6, 29.3, 19.7(9), 19.7(7), 19.7(0), 19.2. FT-IR: ν (cm^{-1}) 2960 (m), 2930 (m), 2872 (m), 1601 (m), 1458 (m), 1418 (w), 1382 (w), 1364 (w), 1220 (w), 1197 (w), 1069 (w), 1028 (w), 1006 (w), 852 (w), 827 (m). $[a]^{23}_{D}$ +8.3 (*c* 0.7, CH_2Cl_2).

• **6-((3*S*,6*R*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl)quinoline (7e):**



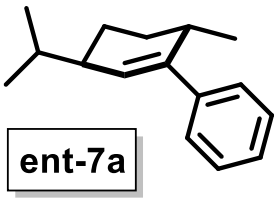
Produced from substrates **4** and **5e**. Colorless oil. Yield: 92%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.86 (dd, 1H, J_1 = 4.3 Hz, J_2 = 1.5 Hz), 8.19 (d, 1H, *J* = 8.2 Hz), 8.10 (d, 1H, *J* = 8.8 Hz), 7.79 (dd, 1H, J_1 = 8.8 Hz, J_2 = 2.0 Hz), 7.73 (d, 1H, *J* = 2.0 Hz), 7.42 (dd, 1H, J_1 = 8.2 Hz, J_2= 4.3 Hz), 5.98 (bs, 1H), 2.97 (m, 1H), 2.18 (m, 1H), 1.88 (ddt, 1H, J_1 = 13.0 Hz, J_2 = 5.5 Hz, J_3 = 3.1 Hz), 1.73-1.83 (m, 2H, 2 signals overlapping), 1.63 (m, 1H), 1.48 (m, 1H), 1.02 (d, 3H, *J* = 6.9 Hz), 0.99 (d, 6H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.0, 142.4, 141.1, 136.9, 131.1, 129.3, 128.4, 128.3, 126.5, 124.0, 121.1, 42.9, 32.3, 30.2, 29.9, 20.0, 19.9, 19.8, 19.3. FT-IR: ν (cm^{-1}) 2962 (m), 2871 (m), 1706 (s), 1677 (s), 1654 (m), 1620 (m), 1591 (w), 1577 (w), 1560 (w), 1498 (m), 1460 (s), 1368 (w), 1322 (w), 1167 (w), 1116 (w), 982 (w), 898 (w), 839 (m), 800 (w), 771 (w). $[a]^{23}_{D}$ +16.7 (*c* 0.6, CH_2Cl_2).

• **3-((3*S*,6*R*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl)benzofuran (7f):**



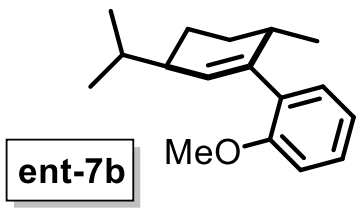
Produced from substrates **4** and **5f**. Colorless oil. Yield: 67%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.75 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.3 Hz), 7.57 (s, 1H), 7.48 (d, 1H, J = 8.0 Hz), 7.30 (dt, 1H, J_1 = 7.4 Hz, J_2 = 1.3 Hz), 7.26 (dt, 1H, J_1 = 7.6 Hz, J_2 = 1.3 Hz), 6.08 (bs, 1H), 2.68 (m, 1H), 2.19 (m, 1H), 1.88 (ddd, 1H, J_1 = 13.0 Hz, J_2 = 5.4 Hz, J_3 = 3.2 Hz), 1.77 (m, 1H), 1.71 (m, 1H), 1.63 (m, 1H), 1.52 (m, 1H), 1.09 (d, 3H, J = 6.8 Hz) 1.03 (d, 3H, J = 6.8 Hz), 1.00 (d, 3H, J = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.7, 140.9, 134.3, 129.1, 126.9, 124.1, 122.5, 122.2, 121.2, 111.6, 42.8, 32.3, 31.4, 29.7, 20.2, 19.9, 19.8, 19.4. FT-IR: ν (cm^{-1}) 2956 (m), 2928 (m), 2869 (m), 1814 (w), 1613 (w), 1475 (w), 1461 (s), 1451 (s), 1384 (w), 1366 (w), 1067 (w), 744 (s). $[a]^{23}_D$ +8.5 (*c* 1.5, CH_2Cl_2).

• **(2*S*,5*R*)-5-Isopropyl-2-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (ent-7a):**



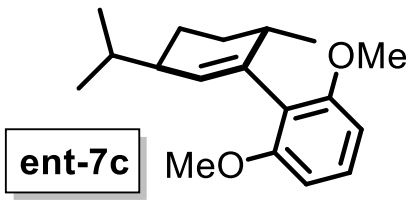
Produced from substrates **ent-4** and **5a**. Colourless oil. Yield: 78%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.34 (d, 2H, J = 7.9 Hz), 7.30 (app. t, 2H, J = 7.6 Hz), 7.22 (tt, 1H, J_1 = 7.3 Hz, J_2 = 1.8 Hz), 5.79 (bs, 1H), 2.84 (m, 1H), 2.12 (m, 1H), 1.84 (m, 1H), 1.68-1.76 (m, 2H, 2 signals overlapping), 1.58 (m, 1H), 1.44 (m, 1H), 0.98 (d, 3H, J = 6.9 Hz), 0.94(9) (d, 3H, J = 6.9 Hz), 0.94(5) (d, 3H, J = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 143.2, 129.0, 128.1, 127.9, 126.5, 126.2, 42.7, 32.3, 30.3, 29.9, 20.0, 19.9, 19.8, 19.3. FT-IR: ν (cm^{-1}) 2965 (m), 2933 (m), 2875 (w), 1709 (s), 1680 (s), 1649 (w), 1597 (w), 1578 (w), 1459 (m), 1448 (m), 1382 (w), 1368 (w), 973 (w), 762 (m). $[a]^{23}_D$ -4.8 (*c* 0.6, CH_2Cl_2).

• **(2*S*,5*R*)-5-Isopropyl-2'-methoxy-2-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (ent-7b):**



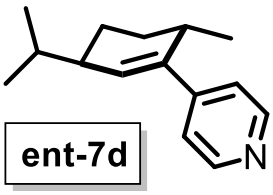
Produced from substrates **ent-4** and **5b**. Colorless oil. Yield: 35%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.22 (dt, 1H, J_1 = 7.8 Hz, J_2 = 1.7 Hz), 7.06 (dd, 1H, J_1 = 7.4 Hz, J_2 = 1.7 Hz), 6.90 (dt, 1H, J_1 = 7.4 Hz, J_2 = 1.0 Hz), 6.85 (dd, 1H, J_1 = 8.2 Hz, J_2 = 1.0 Hz), 5.51 (bs, 1H), 3.80 (s, 3H), 2.80 (m, 1H), 2.13 (m, 1H), 1.88 (m, 1H), 1.69 (m, 1H), 1.54-1.62 (m, 2H, 2 signals overlapping), 1.49 (m, 1H), 0.96 (d, 3H, J = 6.8 Hz), 0.94 (d, 3H, J = 6.8 Hz), 0.84 (d, 3H, J = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 156.7, 143.1, 133.2, 130.8, 129.7, 127.7, 120.3, 110.5, 55.5, 42.0, 32.3, 31.0, 29.6, 20.6, 19.8, 19.7, 19.4. FT-IR: ν (cm^{-1}) 2959 (m), 2918 (m), 2872 (m), 2829 (m), 1729 (w), 1597 (m), 1580 (w), 1488 (m), 1464 (m), 1436 (m), 1378 (w), 1366 (w), 1286 (m), 1243 (m), 1179 (m), 1115 (w), 1052 (m), 1027 (m), 753 (s). $[a]^{23}_D$ -5.8 (*c* 0.2, CH_2Cl_2).

• **(2*S*,5*R*)-5-Isopropyl-2',6'-dimethoxy-2-methyl-2,3,4,5-tetrahydro-1,1'-biphenyl (ent-7c):**



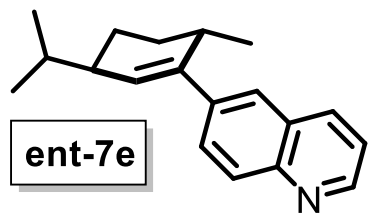
Produced from substrates **ent-4** and **5c**. Colorless oil. Yield: 35%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.16 (t, 1H, *J* = 8.3 Hz), 6.55 (d, 2H, *J* = 8.3 Hz), 5.37 (bs, 1H), 3.76 (s, 6H), 2.52 (m, 1H), 2.18 (m, 1H), 1.88 (m, 1H), 1.71 (m, 1H), 1.59 (m, 1H), 1.52-1.58 (m, 2H, 2 signals overlapping), 0.95 (d, 3H, *J* = 6.9 Hz), 0.94 (d, 3H, *J* = 6.9 Hz), 0.84 (d, 3H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 158.1, 136.2, 130.5, 127.4, 121.8, 104.0, 55.8, 42.0, 32.3, 31.8, 29.7, 20.2, 19.5, 19.3, 19.1. FT-IR: ν (cm^{-1}) 2956 (m), 2931 (m), 2869 (w), 2834 (w), 1708 (w), 1586 (m), 1468 (s), 1432 (m), 1244 (s), 1107 (s), 778 (w), 725 (m). $[a]^{23}_D$ +13.8 (*c* 0.3, CH_2Cl_2).

• **4-((3*R*,6*S*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl)pyridine (ent-7d):**



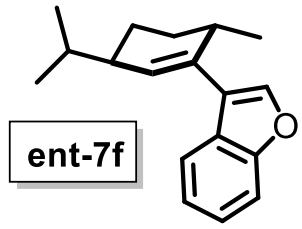
Produced from substrates **ent-4** and **5d**. Yellow oil. Yield: 90%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.51 (d, 2H, *J* = 5.5 Hz), 7.27 (d, 2H, *J* = 5.5 Hz), 6.05 (bs, 1H), 2.82 (m, 1H), 2.14 (m, 1H), 1.81 (ddt, 1H, J_1 = 12.9 Hz, J_2 = 5.5 Hz, J_3 = 3.2 Hz), 1.69-1.79 (m, 2H, 2 signals overlapping), 1.60 (m, 1H), 1.45 (m, 1H), 0.98 (d, 3H, *J* = 6.7 Hz), 0.96 (d, 3H, *J* = 6.7 Hz), 0.94 (d, 3H, *J* = 6.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 150.1, 149.2, 140.8, 132.8, 120.9, 42.8, 32.2, 29.6, 29.3, 19.7(9), 19.7(7), 19.7(0), 19.2. FT-IR: ν (cm^{-1}) 2959 (m), 2932 (m), 2872 (m), 1600 (m), 1458 (m), 1418 (w), 1382 (w), 1363 (w), 1220 (w), 1197 (w), 1068 (w), 1028 (w), 1006 (w), 850 (w), 827 (m). $[a]^{23}_D$ -9.0 (*c* 0.4, CH_2Cl_2).

• **6-((3*R*,6*S*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl)quinoline (ent-7e):**



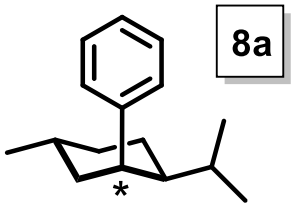
Produced from substrates **ent-4** and **5e**. Colorless oil. Yield: 96%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.86 (dd, 1H, J_1 = 4.3 Hz, J_2 = 1.5 Hz), 8.19 (d, 1H, *J* = 8.2 Hz), 8.10 (d, 1H, *J* = 8.8 Hz), 7.79 (dd, 1H, J_1 = 8.8 Hz, J_2 = 2.0 Hz), 7.73 (d, 1H, *J* = 2.0 Hz), 7.42 (dd, 1H, J_1 = 8.2 Hz, J_2= 4.3 Hz), 5.98 (bs, 1H), 2.97 (m, 1H), 2.18 (m, 1H), 1.88 (ddt, 1H, J_1 = 13.0 Hz, J_2 = 5.5 Hz, J_3 = 3.1 Hz), 1.73-1.83 (m, 2H, 2 signals overlapping), 1.63 (m, 1H), 1.48 (m, 1H), 1.02 (d, 3H, *J* = 6.9 Hz), 0.99 (d, 6H, *J* = 6.9 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.0, 142.4, 141.1, 136.9, 131.1, 129.3, 128.4, 128.3, 126.5, 124.0, 121.1, 42.9, 32.3, 30.2, 29.9, 20.0, 19.9, 19.8, 19.3. FT-IR: ν (cm^{-1}) 2963 (m), 2872 (m), 1706 (s), 1676 (s), 1654 (m), 1619 (m), 1591 (w), 1577 (w), 1560 (w), 1498 (m), 1459 (s), 1368 (w), 1320 (w), 1167 (w), 1118 (w), 982 (w), 897 (w), 839 (m), 800 (w), 772 (w). $[a]^{23}_D$ - 17.4 (*c* 0.4, CH_2Cl_2).

• **3-((3*R*,6*S*)-3-Isopropyl-6-methylcyclohex-1-en-1-yl)benzofuran (ent-7f):**



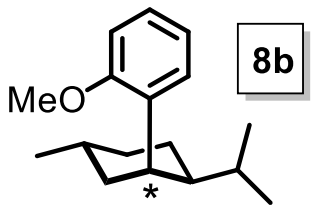
Produced from substrates **ent-4** and **5f**. Colorless oil. Yield: 82%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.75 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.3 Hz), 7.57 (s, 1H), 7.48 (d, 1H, J = 8.0 Hz), 7.30 (dt, 1H, J_1 = 7.4 Hz, J_2 = 1.3 Hz), 7.26 (dt, 1H, J_1 = 7.6 Hz, J_2 = 1.3 Hz), 6.08 (bs, 1H), 2.68 (m, 1H), 2.19 (m, 1H), 1.88 (ddd, 1H, J_1 = 13.0 Hz, J_2 = 5.4 Hz, J_3 = 3.2 Hz), 1.77 (m, 1H), 1.71 (m, 1H), 1.63 (m, 1H), 1.52 (m, 1H), 1.09 (d, 3H, J = 6.8 Hz) 1.03 (d, 3H, J = 6.8 Hz), 1.00 (d, 3H, J = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.7, 140.9, 134.3, 129.1, 126.9, 124.1, 122.5, 122.2, 121.2, 111.6, 42.8, 32.3, 31.4, 29.7, 20.2, 19.9, 19.8, 19.4. FT-IR: ν (cm^{-1}) 2958 (m), 2929 (m), 2870 (m), 1814 (m), 1610 (w), 1475 (m), 1461 (s), 1452 (s), 1385 (w), 1368 (w), 1230 (w), 1137 (w), 1065 (w), 747 (s). $[a]^{23}_{D}$ -9.4 (*c* 0.5, CH_2Cl_2).

• **((1*S*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)benzene (8a):**



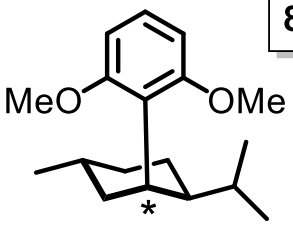
Produced from substrate **6a**. Colorless oil. Yield: 93%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.36 (d, 2H, J = 7.7 Hz), 7.26 (app. t, 2H, J = 7.5 Hz), 7.18 (t, 1H, J = 7.3 Hz), 3.18 (bs, 1H), 1.84-1.94 (m, 2H, 2 signals overlapping), 1.60-1.76 (m, 3H, 3 signals overlapping), 1.27-1.43 (m, 3H, 3 signals overlapping), 1.01 (ddd, 1H, J_1 = 26.0 Hz, J_2 = 12.0 Hz, J_3 = 4.5 Hz), 0.83 (d, 3H, J = 6.3 Hz), 0.81 (d, 3H, J = 6.3 Hz), 0.77 (d, 3H, J = 6.3 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 145.7, 130.1, 127.8, 125.4, 47.2, 43.1, 43.0, 35.4, 30.1, 26.6, 25.8, 22.8, 21.3, 21.2. FT-IR: ν (cm^{-1}) 2922 (s), 2853 (s), 2358 (w), 1742 (w), 1458 (m), 1378 (w), 767 (w). $[a]^{23}_{D}$ +5.9 (*c* 0.8, CH_2Cl_2).

• **1-((1*S*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)-2-methoxybenzene (8b):**



Produced from substrate **6b**. Yellow oil. Yield: 84%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.49 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.5 Hz), 7.16 (dt, 1H, J_1 = 7.7 Hz, J_2 = 1.5 Hz), 6.88 (d, 1H, J = 8.8 Hz), 6.85 (t, 1H, J = 7.2 Hz), 3.82 (s, 3H), 3.73 (bs, 1H), 1.80-1.96 (m, 2H, 2 signals overlapping), 1.67 (m, 2H, 2 signals overlapping), 1.54 (m, 1H), 1.44 (m, 1H), 1.28 (m, 2H, 2 signals overlapping), 1.00 (m, 1H), 0.87 (d, 3H, J = 6.6 Hz), 0.79 (d, 3H, J = 6.6 Hz), 0.68 (d, 3H, J = 6.6 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 157.3, 133.7, 130.2, 126.1, 119.2, 110.6, 55.5, 46.8, 41.2, 35.4, 32.3, 29.9, 27.4, 25.9, 22.7, 21.4, 21.2. FT-IR: ν (cm^{-1}) 2945 (s), 2923 (s), 2867 (m), 1600 (w), 1490 (m), 1453 (m), 1438 (w), 1259 (m), 1236 (s), 1107 (m), 1032 (w), 799 (m), 747 (s). $[a]^{23}_{D}$ +14.4 (*c* 0.6, CH_2Cl_2).

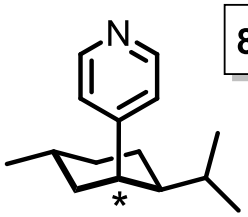
• 2-((1*S*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)-1,3-dimethoxybenzene (8c):



8c

Produced from substrate **6c**. Colorless oil. Yield: 81%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.10 (t, 1H, *J* = 8.2 Hz), 6.53 (app. t, 2H, 2 signals overlapping, *J* = 8.6 Hz), 3.79 (s, 3H), 3.78 (s, 3H), 3.21 (dt, 1H, J_1 = 11.5 Hz, J_2 = 3.4 Hz), 2.11 (tt, 1H, J_1 = 11.4 Hz, J_2 = 2.8 Hz), 1.77 (m, 1H), 1.63-1.71 (m, 2H, 2 signals overlapping), 1.54 (m, 1H), 1.49 (m, 1H), 1.34 (m, 1H), 1.05 (m, 2H, 2 signals overlapping), 0.89 (d, 3H, *J* = 6.4 Hz), 0.80 (d, 3H, *J* = 7.0 Hz), 0.64 (d, 3H, *J* = 7.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 159.7, 158.2, 126.4, 122.2, 104.7, 104.2, 56.0, 55.3, 43.9, 39.9, 38.0, 35.6, 33.6, 28.7, 25.4, 22.6, 21.7, 15.7. FT-IR: ν (cm^{-1}) 2949 (s), 2921 (s), 2853 (s), 2838 (m), 1590 (s), 1470 (s), 1433 (m), 1249 (m), 1220 (w), 1140 (w), 1105 (s), 1093 (s), 780 (w), 724 (m). $[a]^{23}_{D}$ +3.7 (*c* 1.3, CH_2Cl_2).

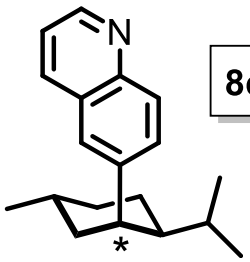
• 4-((1*S*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)pyridine (8d):



8d

Produced from substrate **6d**. Colorless oil. Yield: 38%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.47 (d, 2H, *J* = 5.3 Hz), 7.32 (d, 2H, *J* = 5.3 Hz), 3.18 (bs, 1H), 1.86-1.96 (m, 2H, 2 signals overlapping), 1.69 (ddd, 1H, J_1 = 13.1 Hz, J_2 = 6.4 Hz, J_3 = 2.5 Hz), 1.57 (m, 2H, 2 signals overlapping), 1.42 (dt, 1H, J_1 = 12.8 Hz, J_2 = 5.6 Hz), 1.31 (m, 2H, 2 signals overlapping), 1.01 (ddd, 1H, J_1 = 25.4 Hz, J_2 = 13.0 Hz, J_3 = 4.8 Hz), 0.86 (d, 3H, *J* = 6.1 Hz), 0.81 (d, 3H, *J* = 6.3 Hz), 0.74 (d, 3H, *J* = 6.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.9, 148.2, 125.8, 46.8, 42.8, 42.3, 35.0, 30.0, 26.7, 25.9, 22.6, 21.2, 21.1. FT-IR: ν (cm^{-1}) 2953 (s), 2923 (s), 2869 (s), 2852 (s), 1719 (m), 1639 (w), 1585 (m), 1459 (m), 1414 (w), 1377 (w), 1366 (w), 820 (m). $[a]^{23}_{D}$ +20.2 (*c* 0.5, CH_2Cl_2).

• 6-((1*S*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)quinoline (8e):

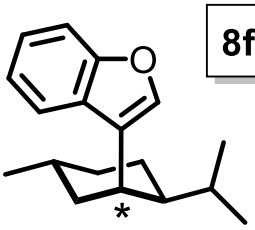


8e

Produced from substrate **6e**. Yellow oil. Yield: 60%. ^{1}H NMR ($CDCl_3$): δ (500 MHz, ppm) 8.85 (dd, 1H, J_1 = 4.2 Hz, J_2 = 1.4 Hz), 8.14 (d, 1H, *J* = 8.0 Hz), 8.04 (d, 1H, *J* = 8.7 Hz), 7.80 (d, 1H, *J* = 2.0 Hz), 7.74 (dd, 1H, J_1 = 8.7 Hz, J_2 = 2.0 Hz), 7.39 (dd, 1H, J_1 = 8.2 Hz, J_2 = 4.2 Hz), 3.38 (bs, 1H), 1.90-2.00 (m, 2H, 2 signals overlapping), 1.72-1.84 (m, 2H, 2 signals overlapping), 1.69 (m, 1H), 1.32-1.52 (m, 3H, 3 signals overlapping), 1.06 (m, 1H), 0.87 (d, 3H, *J* = 6.3 Hz), 0.81 (d, 3H, *J* = 6.3 Hz), 0.77 (d, 3H, *J* = 6.3 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.2, 146.3, 144.4, 136.3, 133.2, 128.3, 128.0, 127.6, 120.9, 47.2, 43.0, 42.9, 35.3, 30.1, 26.8,

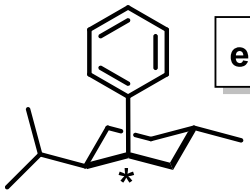
25.9, 22.7, 21.3, 21.2. FT-IR: v (cm^{-1}) 2924 (s), 2866 (m), 2839 (m), 2089 (w), 1613 (w), 1508 (s), 1454 (m), 836 (s), 799 (m), 775 (m). $[a]^{23}_{D}$ +2.2 (*c* 2.0, CH_2Cl_2).

• 3-((1*S*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)benzofuran (8f):



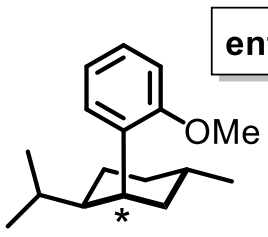
Produced from substrate **6f**. Colorless oil. Yield: 50%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.56 (dd, 1H, J_1 = 7.8 Hz, J_2 = 1.1 Hz), 7.54 (bs, 1H), 7.47 (d, 1H, J = 8.0 Hz), 7.29 (dt, 1H, J_1 = 7.4 Hz, J_2 = 1.4 Hz), 7.24 (dt, 1H, J_1 = 7.5 Hz, J_2 = 1.1 Hz), 3.51 (bs, 1H), 1.96 (m, 1H), 1.77-1.85 (m, 2H, 2 signals overlapping), 1.42-1.52 (m, 2H, 2 signals overlapping), 1.23-1.39 (m, 3H, 3 signals overlapping), 1.00 (ddd, J_1 = 26.6 Hz, J_2 = 12.5 Hz, J_3 = 4.0 Hz), 0.89 (d, 3H, J = 6.5 Hz), 0.80 (d, 3H, J = 6.5 Hz), 0.74 (d, 3H, J = 6.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 154.3, 141.4, 129.1, 124.0, 122.1, 120.9, 119.4, 111.2, 47.3, 40.5, 35.3, 32.5, 30.2, 27.2, 26.8, 22.3, 21.3, 21.2. FT-IR: v (cm^{-1}) 2922 (s), 2867 (m), 2843 (m), 1454 (s), 1272 (w), 1179 (w), 1098 (w), 1085 (m), 859 (w), 743 (s). $[a]^{23}_{D}$ +10.2 (*c* 0.1, CH_2Cl_2).

• ((1*R*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl)benzene (ent-8a):



Produced from substrate **ent-6a**. Colorless oil. Yield: 99%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.36 (d, 2H, J = 7.7 Hz), 7.26 (app. t, 2H, J = 7.5 Hz), 7.18 (t, 1H, J = 7.3 Hz), 3.18 (bs, 1H), 1.84-1.94 (m, 2H, 2 signals overlapping), 1.60-1.76 (m, 3H, 3 signals overlapping), 1.27-1.43 (m, 3H, 3 signals overlapping), 1.01 (ddd, 1H, J_1 = 26.0 Hz, J_2 = 12.0 Hz, J_3 = 4.5 Hz), 0.83 (d, 3H, J = 6.3 Hz), 0.81 (d, 3H, J = 6.3 Hz), 0.77 (d, 3H, J = 6.3 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 145.7, 130.1, 127.8, 125.4, 47.2, 43.1, 43.0, 35.4, 30.1, 26.6, 25.8, 22.8, 21.3, 21.2. FT-IR: v (cm^{-1}) 2922 (s), 2853 (s), 2358 (w), 1742 (w), 1458 (m), 1378 (w), 767 (w). $[a]^{23}_{D}$ -5.4 (*c* 1.4, CH_2Cl_2).

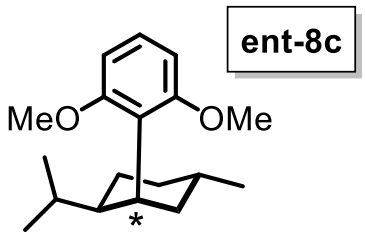
• 1-((1*R*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl)-2-methoxybenzene (ent-8b):



Produced from substrate **ent-6b**. Colorless oil. Yield: 81%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.49 (dd, 1H, J_1 = 7.6 Hz, J_2 = 1.5 Hz), 7.16 (dt, 1H, J_1 = 7.7 Hz, J_2 = 1.5 Hz), 6.88 (d, 1H, J = 8.8 Hz), 6.85 (t, 1H, J = 7.2 Hz), 3.82 (s, 3H), 3.73 (bs, 1H), 1.80-1.96 (m, 2H, 2 signals overlapping), 1.67 (m, 2H, 2 signals overlapping), 1.54 (m, 1H), 1.44 (m, 1H), 1.28 (m, 2H, 2 signals overlapping), 1.00 (m, 1H), 0.87 (d, 3H, J = 6.6 Hz), 0.79 (d, 3H, J = 6.6 Hz), 0.68

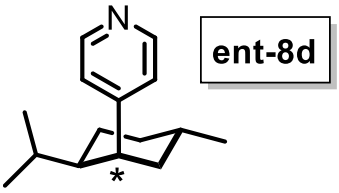
(d, 3H, *J* = 6.6 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 157.3, 133.7, 130.2, 126.1, 119.2, 110.6, 55.5, 46.8, 41.2, 35.4, 32.3, 29.9, 27.4, 25.9, 22.7, 21.4, 21.2. FT-IR: ν (cm^{-1}) 2946 (s), 2923 (s), 2866 (m), 1600 (w), 1491 (m), 1450 (m), 1438 (m), 1258 (m), 1235 (s), 1107 (m), 1034 (m), 800 (m), 748 (s). $[a]^{23}_D$ -14.9 (*c* 0.3, CH_2Cl_2).

• 2-((1*R*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl)-1,3-dimethoxybenzene (ent-8c):



Produced from substrate **ent-6c**. White solid. Yield: 76%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.10 (t, 1H, *J* = 8.2 Hz), 6.53 (app. t, 2H, 2 signals overlapping, *J* = 8.6 Hz), 3.79 (s, 3H), 3.78 (s, 3H), 3.21 (dt, 1H, J_1 = 11.5 Hz, J_2 = 3.4 Hz), 2.11 (tt, 1H, J_1 = 11.4 Hz, J_2 = 2.8 Hz), 1.77 (m, 1H), 1.63-1.71 (m, 2H, 2 signals overlapping), 1.54 (m, 1H), 1.49 (m, 1H), 1.34 (m, 1H), 1.05 (m, 2H, 2 signals overlapping), 0.89 (d, 3H, *J* = 6.4 Hz), 0.80 (d, 3H, *J* = 7.0 Hz), 0.64 (d, 3H, *J* = 7.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 159.7, 158.2, 126.4, 122.2, 104.7, 104.2, 56.0, 55.3, 43.9, 39.9, 38.0, 35.6, 33.6, 28.7, 25.4, 22.6, 21.7, 15.7. FT-IR: ν (cm^{-1}) 2949 (m), 2923 (m), 2857 (s), 2836 (m), 1590 (s), 1470 (s), 1435 (m), 1249 (m), 1220 (m), 1140 (m), 1104 (s), 1094 (s), 780 (m), 725 (s). $[a]^{23}_D$ -3.4 (*c* 1.1, CH_2Cl_2).

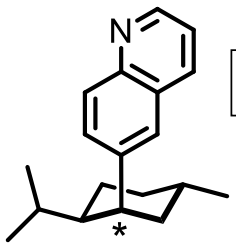
• 4-((1*R*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl)pyridine (ent-8d):



Produced from substrate **ent-6d**. Yellow oil. Yield: 33%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.47 (d, 2H, *J* = 5.3 Hz), 7.32 (d, 2H, *J* = 5.3 Hz), 3.18 (bs, 1H), 1.86-1.96 (m, 2H, 2 signals overlapping), 1.69 (ddd, 1H, J_1 = 13.1 Hz, J_2 = 6.4 Hz, J_3 = 2.5 Hz), 1.57 (m, 2H, 2 signals overlapping), 1.42 (dt, 1H, J_1 = 12.8 Hz, J_2 = 5.6 Hz), 1.31 (m, 2H, 2 signals overlapping), 1.01 (ddd, 1H, J_1 = 25.4 Hz, J_2 = 13.0 Hz, J_3 = 4.8 Hz), 0.86 (d, 3H, *J* = 6.1 Hz), 0.81 (d, 3H, *J* = 6.3 Hz), 0.74 (d, 3H, *J* = 6.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.9, 148.2, 125.8, 46.8, 42.8, 42.3, 35.0, 30.0, 26.7, 25.9, 22.6, 21.2, 21.1. FT-IR: ν (cm^{-1}) 2953 (s), 2924 (s), 2869 (m), 2854 (m), 1719 (m), 1639 (w), 1587 (m), 1459 (m), 1414 (w), 1378 (w), 1366 (w), 821 (m). $[a]^{23}_D$ -21.3 (*c* 0.3, CH_2Cl_2).

• 6-((1*R*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl)quinoline (ent-8e):

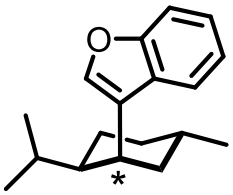
Produced from substrate **ent-6e**. Yellow crystals. Yield: 65%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.85 (dd, 1H, J_1 = 4.2 Hz, J_2 = 1.4 Hz), 8.14 (d, 1H, *J* = 8.0 Hz), 8.04 (d, 1H, *J* = 8.7 Hz), 7.80 (d, 1H, *J* = 2.0 Hz), 7.74 (dd, 1H, J_1 = 8.7 Hz, J_2 = 2.0 Hz), 7.39 (dd, 1H, J_1 = 8.2 Hz, J_2 = 4.2 Hz), 3.38 (bs, 1H), 1.90-2.00 (m, 2H, 2 signals overlapping), 1.72-1.84 (m, 2H, 2 signals overlapping), 1.69 (m, 1H), 1.32-1.52 (m, 3H, 3 signals overlapping), 1.06 (m, 1H), 0.87 (d,



ent-8e

3H, *J* = 6.3 Hz), 0.81 (d, 3H, *J* = 6.3 Hz), 0.77 (d, 3H, *J* = 6.3 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.2, 146.3, 144.4, 136.3, 133.2, 128.3, 128.0, 127.6, 120.9, 47.2, 43.0, 42.9, 35.3, 30.1, 26.8, 25.9, 22.7, 21.3, 21.2. FT-IR: v (cm^{-1}) 2922 (s), 2867 (s), 2840 (m), 1592 (w), 1505 (m), 1455 (m), 836 (s), 796 (m), 773 (m). [a]$^{23}_D$ -2.5 (*c* 1.1, CH_2Cl_2).

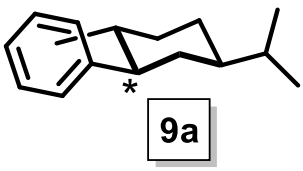
• 3-((1*R*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl)benzofuran (ent-8f):



ent-8f

Produced from substrate **ent-6f**. Colorless oil. Yield: 54%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.56 (dd, 1H, J_1 = 7.8 Hz, J_2 = 1.1 Hz), 7.54 (bs, 1H), 7.47 (d, 1H, *J* = 8.0 Hz), 7.29 (dt, 1H, J_1 = 7.4 Hz, J_2 = 1.4 Hz), 7.24 (dt, 1H, J_1 = 7.5 Hz, J_2 = 1.1 Hz), 3.51 (bs, 1H), 1.96 (m, 1H), 1.77-1.85 (m, 2H, 2 signals overlapping), 1.42-1.52 (m, 2H, 2 signals overlapping), 1.23-1.39 (m, 3H, 3 signals overlapping), 1.00 (ddd, J_1 = 26.6 Hz, J_2 = 12.5 Hz, J_3 = 4.0 Hz), 0.89 (d, 3H, *J* = 6.5 Hz), 0.80 (d, 3H, *J* = 6.5 Hz), 0.74 (d, 3H, *J* = 6.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 154.3, 141.4, 129.1, 124.0, 122.1, 120.9, 119.4, 111.2, 47.3, 40.5, 35.3, 32.5, 30.2, 27.2, 26.8, 22.3, 21.3, 21.2. FT-IR: v (cm^{-1}) 2920 (s), 2867 (m), 2843 (m), 1452 (s), 1383 (w), 1271 (w), 1179 (w), 1098 (m), 1085 (m), 1011 (w), 859 (m), 741 (s). [a]$^{23}_D$ -9.3 (*c* 0.7, CH_2Cl_2).

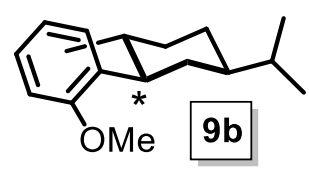
• ((1*R*,2*R*,5*R*)-5-Isopropyl-2-methylcyclohexyl)benzene (9a):



9a

Produced from substrate **7a**. Colorless oil. Yield: 81%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.37 (d, 2H, *J* = 8.1 Hz), 7.22-7.28 (m, 3H, 2 signals overlapping), 2.92 (td, 1H, J_1 = 12.7 Hz, J_2 = 4.0 Hz), 2.16 (m, 1H), 1.75-1.85 (m, 2H, 2 signals overlapping), 1.72 (m, 1H), 1.66 (m, 1H), 1.56-1.62 (m, 2H, 2 signals overlapping), 1.27-1.33 (m, 2H, 2 signals overlapping), 1.00 (d, 6H, *J* = 6.9 Hz), 0.72 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 146.3, 127.9, 127.6, 125.5, 46.6, 44.8, 34.3, 33.6, 33.1, 27.6, 23.3, 19.9, 19.8(5), 12.1. FT-IR: v (cm^{-1}) 1646 (w), 1060 (s), 1032 (w), 871 (w). [a]$^{23}_D$ +3.5 (*c* 1.0, CH_2Cl_2).

• 1-((1*R*,2*R*,5*R*)-5-Isopropyl-2-methylcyclohexyl)-2-methoxybenzene (9b):

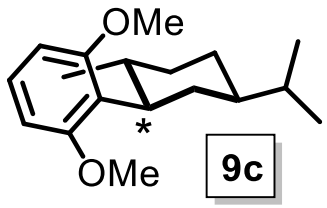


9b

Produced from substrate **7b**. Colorless oil. Yield: 54%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.17 (td, 1H, J_1 = 7.5 Hz, J_2 = 1.7 Hz), 7.10 (dd, 1H, J_1 = 7.7 Hz, J_2 = 1.5 Hz), 6.92 (td, 1H, J_1 = 7.4, J_2 = 0.9 Hz), 6.84 (dd, 1H, J_1 = 8.3 Hz, J_2 = 0.9 Hz), 3.82 (s, 3H), 3.23 (td, 1H, J_1 = 13.1 Hz, J_2 = 3.5 Hz), 2.18 (m, 1H), 1.75 (m, 1H), 1.66 (m, 1H), 1.60 (m, 1H), 1.47-1.53 (m, 3H, 3 signals overlapping), 1.26 (m, 2H, 2 signals overlapping), 0.92 (d, 6H, *J* =

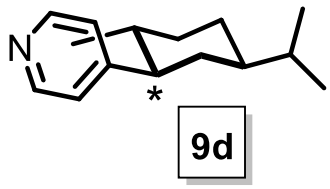
6.9 Hz), 0.64 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 156.8, 134.5, 127.8, 126.3, 119.9, 110.0, 55.2, 45.1, 39.5, 33.4, 33.2, 30.7, 27.8, 23.6, 20.0, 19.8, 12.6. FT-IR: v (cm^{-1}) 2962 (m), 2925 (m), 2870 (m), 1601 (s), 1489 (m), 1459 (m), 1419 (m), 1230 (m), 1088 (m), 1068 (m), 1040 (s), 748 (s), 727 (m). [a]$^{23}_D$ +11.6 (*c* 0.4 CH_2Cl_2).

• 2-((1*R*,2*R*,5*R*)-5-Isopropyl-2-methylcyclohexyl)-1,3-dimethoxybenzene (9c):



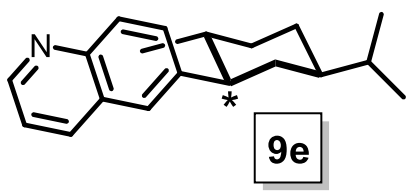
Produced from substrate **7c**. Yellow oil. Yield: 36%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.11 (t, 1H, *J* = 8.3 Hz), 6.54 (d, 2H, *J* = 8.3 Hz), 3.77 (s, 6H), 3.39 (dt, 1H, J_1 = 13.0 Hz, J_2 = 3.3 Hz), 2.26 (q, 1H, *J* = 12.8 Hz), 1.96 (m, 1H), 1.72 (tt, 1H, J_1 = 13.3 Hz, J_2 = 4.4 Hz), 1.60 (dq, 1H, J_1 = 13.0 Hz, J_2 = 3.0 Hz), 1.48 (m, 3H, 3 signals overlapping), 1.27 (qd, 1H, J_1 = 12.8 Hz, J_2 = 3.7 Hz), 1.12 (m, 1H), 0.90 (d, 3H, *J* = 6.9 Hz), 0.89 (d, 3H, *J* = 6.9 Hz), 0.83 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 159.2, 126.5, 122.6, 104.5, 55.7, 46.1, 39.7, 34.0, 33.2, 33.1, 28.5, 24.1, 20.0(4), 20.0(0), 14.0. FT-IR: v (cm^{-1}) 2955 (m), 2925 (m), 2869 (m), 2834 (m), 1587 (s), 1468 (s), 1434 (m), 1376 (m), 1273 (w), 1260 (m), 1246 (s), 1230 (s), 1167 (w), 1141 (s), 1101 (s), 1041 (w), 806 (w), 784 (m), 760 (m), 724 (s), 708 (w). [a]$^{23}_D$ +6.1 (*c* 0.5, CH_2Cl_2).

• 4-((1*R*,2*R*,5*R*)-5-Isopropyl-2-methylcyclohexyl)pyridine (9d):



Produced from substrate **7d**. Yellow oil. Yield: 89%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.48 (d, 2H, *J* = 6.1 Hz), 7.10 (d, 2H, *J* = 6.1 Hz), 2.81 (dt, 1H, J_1 = 12.7 Hz, J_2 = 3.8 Hz), 2.10 (oct, 1H, *J* = 3.7 Hz), 1.70-1.76 (m, 2H, 2 signals overlapping), 1.63 (m, 1H), 1.47-1.57 (m, 3H, 3 signals overlapping), 1.16-1.28 (m, 2H, 2 signals overlapping), 0.92 (d, 6H, *J* = 6.9 Hz), 0.61 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.4, 149.2, 123.1, 45.9, 44.4, 33.7, 33.4, 33.0, 26.7, 23.1, 19.8, 12.0. FT-IR: v (cm^{-1}) 2956 (s), 2928 (s), 2856 (s), 1597 (s), 1558 (m), 1508 (m), 1466 (s), 1418 (m), 1365 (m), 1288 (m), 1069 (w), 990 (w), 822 (m), 764 (w). [a]$^{23}_D$ +2.0 (*c* 1.3, CH_2Cl_2).

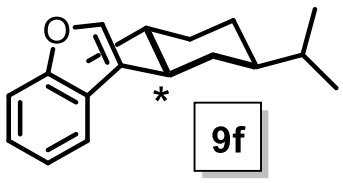
• 6-((1*R*,2*R*,5*R*)-5-Isopropyl-2-methylcyclohexyl)quinoline (9e):



Produced from substrate **7e**. Yellow oil. Yield: 46%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.86 (dd, 1H, J_1 = 4.4 Hz, J_2 = 1.6 Hz), 8.16 (d, 1H, *J* = 8.3 Hz), 8.07 (d, 1H, *J* = 8.7 Hz), 7.61 (dd, 1H, J_1 = 8.8 Hz, J_2 = 1.9 Hz), 7.55 (s, 1H), 7.40 (dd, 1H, J_1 = 8.1 Hz, J_2 = 4.1 Hz), 3.02 (td, 1H, J_1 = 12.6, J_2 = 3.7 Hz), 2.21 (m, 1H), 1.72-1.82 (m, 3H, 3 signals overlapping), 1.68 (q, 1H, *J*

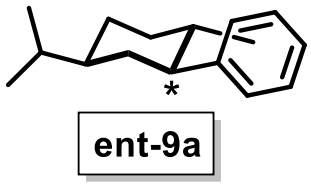
= 11.7 Hz), 1.51-1.61 (m, 2H, 2 signals overlapping), 1.24-1.30 (m, 2H, 2 signals overlapping), 0.96 (d, 3H, *J* = 6.9 Hz), 0.96 (d, 3H, *J* = 6.9 Hz), 0.63 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.1, 146.5, 145.1, 136.3, 130.9, 128.3, 128.2, 124.9, 120.9, 46.4, 44.7, 34.0, 33.6, 33.1, 27.6, 23.2, 19.8(9), 19.8(7), 12.1. FT-IR: ν (cm^{-1}) 2955 (m), 2919 (s), 2867 (m), 1593 (w), 1571 (w), 1498 (s), 1464 (m), 1439 (w), 1378 (m), 1366 (m), 1170 (w), 1117 (w), 883 (m), 834 (s), 796 (m), 777 (m). [a]$^{23}_{D}$ +15.8 (*c* 1.1, CH_2Cl_2).

• 3-((1*R*,2*R*,5*R*)-5-Isopropyl-2-methylcyclohexyl)benzofuran (9f):



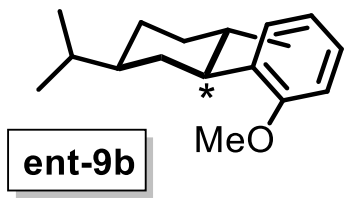
Produced from substrate **7f**. Colorless oil. Yield: 35%. ^{1}H NMR (500 MHz, C_6D_6): δ (ppm) 7.47-7.43 (m, 2H, 2 signals overlapping), 7.13-7.10 (m, 2H, 2 signals overlapping), 7.05 (d, 1H, *J* = 1.18 Hz), 2.85 (dt, 1H, J_1 = 12.6 Hz, J_2 = 4.3 Hz), 2.29 (m, 1H), 1.64-1.59 (m, 2H, 2 signals overlapping), 1.57 (m, 1H), 1.38 (m, 1H), 1.33 (m, 2H, 2 signals overlapping), 1.14 (m, 1H), 1.08 (m, 1H), 0.90 (d, 6H, *J* = 6.8 Hz), 0.62 (d, 3H, *J* = 7.2 Hz). ^{13}C NMR (125 MHz, C_6D_6): δ (ppm) 155.9, 154.8, 140.8, 124.1, 122.1, 120.2, 119.6, 111.6, 44.5, 37.5, 32.9, 32.7, 31.1, 27.8, 23.2, 19.7, 19.6, 12.3. FT-IR: ν (cm^{-1}) 2956 (m), 2925 (m), 1726 (m), 1452 (s), 1382 (w), 1366 (w), 1277 (m), 1190 (w), 1120 (w), 1090 (m), 1072 (w), 857 (m), 741 (s). [a]$^{23}_{D}$ +31.6 (*c* 0.2, CH_2Cl_2).

• ((1*S*,2*S*,5*S*)-5-Isopropyl-2-methylcyclohexyl)benzene (ent-9a):



Produced from substrate **ent-7a**. Colorless oil. Yield: 99%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.37 (d, 2H, *J* = 8.1 Hz), 7.22-7.28 (m, 3H, 2 signals overlapping), 2.92 (td, 1H, J_1 = 12.7 Hz, J_2 = 4.0 Hz), 2.16 (m, 1H), 1.75-1.85 (m, 2H, 2 signals overlapping), 1.72 (m, 1H), 1.66 (m, 1H), 1.56-1.62 (m, 2H, 2 signals overlapping), 1.27-1.33 (m, 2H, 2 signals overlapping), 1.00 (d, 6H, *J* = 6.9 Hz), 0.72 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 146.3, 127.9, 127.6, 125.5, 46.6, 44.8, 34.3, 33.6, 33.1, 27.6, 23.3, 19.9, 19.8(5), 12.1. FT-IR: ν (cm^{-1}) 1646 (w), 1061 (s), 1034 (w), 870 (w). [a]$^{23}_{D}$ -3.1 (*c* 0.5, CH_2Cl_2).

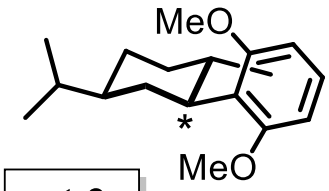
• 1-((1*S*,2*S*,5*S*)-5-Isopropyl-2-methylcyclohexyl)-2-methoxybenzene (ent-9b):



Produced from substrate **ent-7b**. Colorless oil. Yield: 87%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.17 (td, 1H, J_1 = 7.5 Hz, J_2 = 1.7 Hz), 7.10 (dd, 1H, J_1 = 7.7 Hz, J_2 = 1.5 Hz), 6.92 (td, 1H, J_1 = 7.4, J_2 = 0.9 Hz), 6.84 (dd, 1H, J_1 = 8.3 Hz, J_2 = 0.9 Hz), 3.82 (s, 3H), 3.23 (td, 1H, J_1 = 13.1 Hz, J_2 = 3.5 Hz), 2.18 (m, 1H), 1.75 (m, 1H), 1.66 (m, 1H), 1.60 (m, 1H), 1.47-1.53 (m, 3H, 3 signals overlapping), 1.26 (m, 2H, 2 signals overlapping), 0.92 (d, 6H, *J* = 6.9 Hz), 0.64 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ

(ppm) 156.8, 134.5, 127.8, 126.3, 119.9, 110.0, 55.2, 45.1, 39.5, 33.4, 33.2, 30.7, 27.8, 23.6, 20.0, 19.8, 12.6. FT-IR: v (cm^{-1}) 2965 (m), 2923 (s), 2869 (m), 1600 (m), 1491 (s), 1462 (m), 1418 (w), 1233 (s), 1086 (m), 1069 (m), 1038 (s), 748 (s), 727 (m). $[a]^{23}_D$ -12.9 (*c* 0.6, CH_2Cl_2).

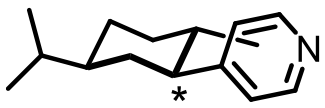
• 2-((1*S*,2*S*,5*S*)-5-Isopropyl-2-methylcyclohexyl)-1,3-dimethoxybenzene (ent-9c):



ent-9c

Produced from substrate **ent-7c**. Yellow oil. Yield: 86%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 7.11 (t, 1H, *J* = 8.3 Hz), 6.54 (d, 2H, *J* = 8.3 Hz), 3.77 (s, 6H), 3.39 (dt, 1H, J_1 = 13.0 Hz, J_2 = 3.3 Hz), 2.26 (q, 1H, *J* = 12.8 Hz), 1.96 (m, 1H), 1.72 (tt, 1H, J_1 = 13.3 Hz, J_2 = 4.4 Hz), 1.60 (dq, 1H, J_1 = 13.0 Hz, J_2 = 3.0 Hz), 1.48 (m, 3H, 3 signals overlapping), 1.27 (qd, 1H, J_1 = 12.8 Hz, J_2 = 3.7 Hz), 1.12 (m, 1H), 0.90 (d, 3H, *J* = 6.9 Hz), 0.89 (d, 3H, *J* = 6.9 Hz), 0.83 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 159.2, 126.5, 122.6, 104.5, 55.7, 46.1, 39.7, 34.0, 33.2, 33.1, 28.5, 24.1, 20.0(4), 20.0(0), 14.0. FT-IR: v (cm^{-1}) 2955 (m), 2924 (s), 2869 (m), 2834 (m), 1587 (s), 1491 (w), 1468 (s), 1434 (m), 1376 (w), 1244 (s), 1232 (s), 1141 (s), 1102 (s), 785 (m), 751 (m), 724 (m). $[a]^{23}_D$ -5.6 (*c* 0.6, CH_2Cl_2).

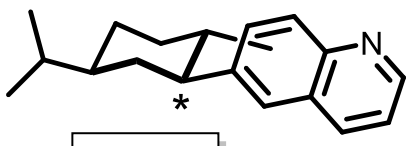
• 4-((1*S*,2*S*,5*S*)-5-Isopropyl-2-methylcyclohexyl)pyridine (ent-9d):



ent-9d

Produced from substrate **ent-7d**. Yellow oil. Yield: 95%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.48 (d, 2H, *J* = 6.1 Hz), 7.10 (d, 2H, *J* = 6.1 Hz), 2.81 (dt, 1H, J_1 = 12.7 Hz, J_2 = 3.8 Hz), 2.10 (oct, 1H, *J* = 3.7 Hz), 1.70-1.76 (m, 2H, 2 signals overlapping), 1.63 (m, 1H), 1.47-1.57 (m, 3H, 3 signals overlapping), 1.16-1.28 (m, 2H, 2 signals overlapping), 0.92 (d, 6H, *J* = 6.9 Hz), 0.61 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 155.4, 149.2, 123.1, 45.9, 44.4, 33.7, 33.4, 33.0, 26.7, 23.1, 19.8, 12.0. FT-IR: v (cm^{-1}) 2956 (s), 2929 (s), 2859 (s), 1597 (s), 1557 (w), 1465 (m), 1415 (m), 1381 (w), 1368 (w), 1287 (m), 1071 (w), 994 (w), 824 (m), 763 (w). $[a]^{23}_D$ -1.5 (*c* 1.1, CH_2Cl_2).

• 6-((1*S*,2*S*,5*S*)-5-Isopropyl-2-methylcyclohexyl)quinoline (ent-9e):

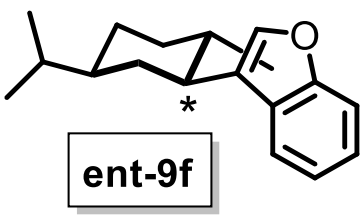


ent-9e

Produced from substrate **ent-7e**. Yellow oil. Yield: 25%. ^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) 8.86 (dd, 1H, J_1 = 4.4 Hz, J_2 = 1.6 Hz), 8.16 (d, 1H, *J* = 8.3 Hz), 8.07 (d, 1H, *J* = 8.7 Hz), 7.61 (dd, 1H, J_1 = 8.8 Hz, J_2 = 1.9 Hz), 7.55 (s, 1H), 7.40 (dd, 1H, J_1 = 8.1 Hz, J_2 = 4.1 Hz), 3.02 (td, 1H, J_1 = 12.6, J_2 = 3.7 Hz), 2.21 (m, 1H), 1.72-1.82 (m, 3H, 3 signals overlapping), 1.68 (q, 1H, *J* = 11.7 Hz), 1.51-1.61 (m, 2H, 2 signals overlapping), 1.24-1.30 (m, 2H, 2 signals

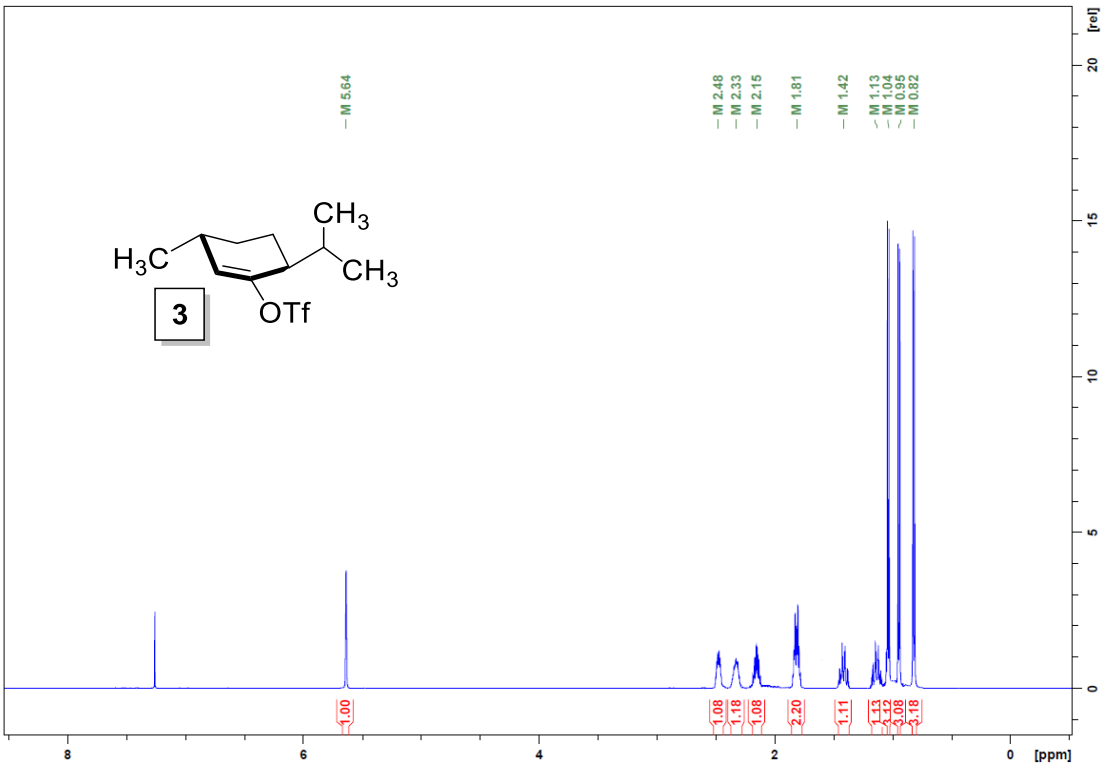
overlapping), 0.96 (d, 3H, *J* = 6.9 Hz), 0.96 (d, 3H, *J* = 6.9 Hz), 0.63 (d, 3H, *J* = 7.1 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) 149.1, 146.5, 145.1, 136.3, 130.9, 128.3, 128.2, 124.9, 120.9, 46.4, 44.7, 34.0, 33.6, 33.1, 27.6, 23.2, 19.8(9), 19.8(7), 12.1. FT-IR: v (cm^{-1}) 2954 (m), 2918 (s), 2867 (m), 1593 (w), 1571 (w), 1498 (s), 1464 (m), 1439 (w), 1378 (m), 1366 (m), 1171 (w), 1115 (w), 883 (m), 834 (s), 796 (m), 778 (m). $[a]^{23}_D$ -16.6 (*c* 0.5, CH_2Cl_2).

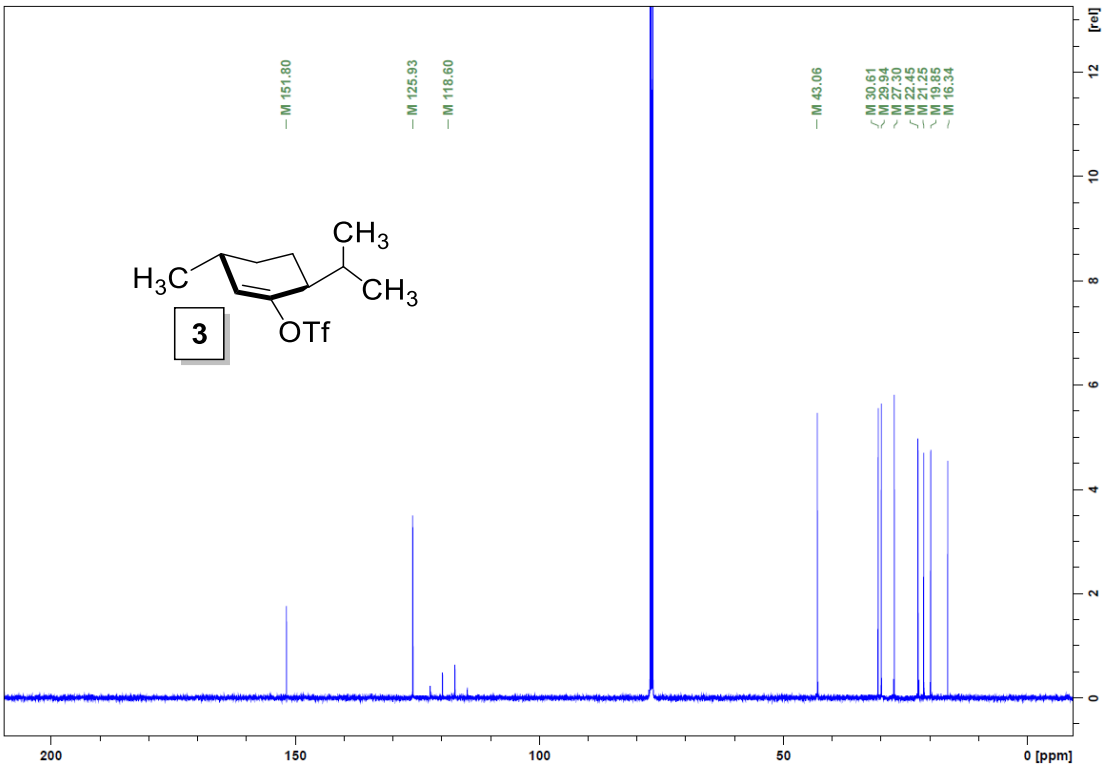
• 3-((1*S*,2*S*,5*S*)-5-Isopropyl-2-methylcyclohexyl)benzofuran (ent-9f):

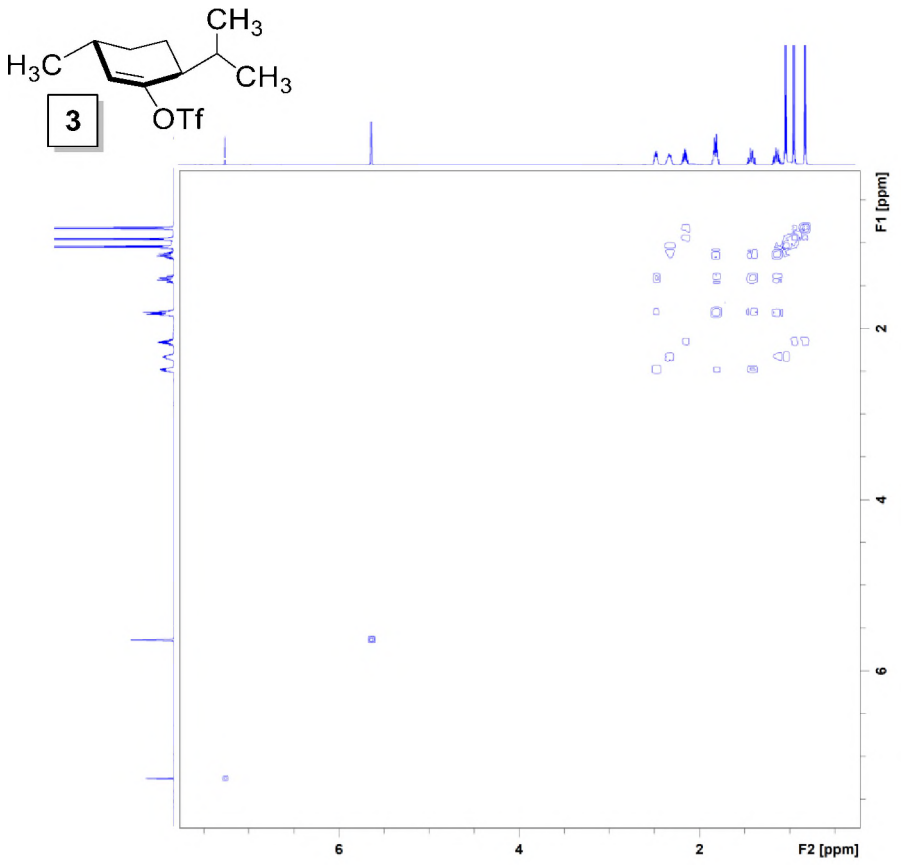


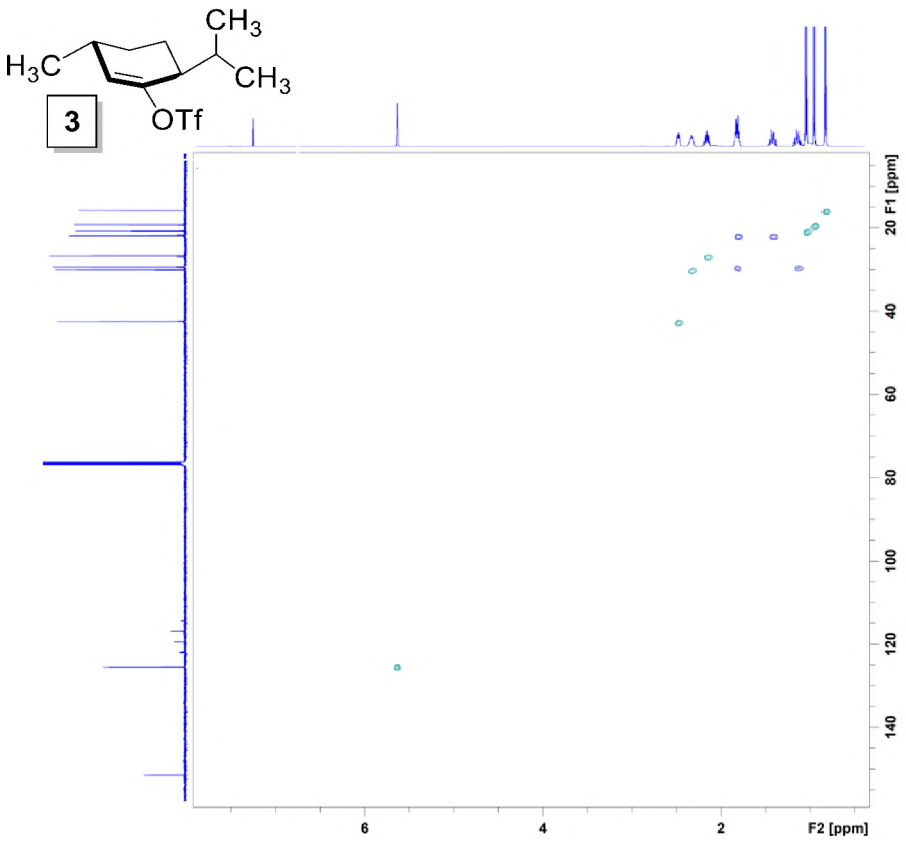
Produced from substrate **ent-7f**. Colorless oil. Yield: 39%. ^{1}H NMR (500 MHz, C_6D_6): δ (ppm) 7.47-7.43 (m, 2H, 2 signals overlapping), 7.13-7.10 (m, 2H, 2 signals overlapping), 7.05 (d, 1H, *J* = 1.18 Hz), 2.85 (dt, 1H, J_1 = 12.6 Hz, J_2 = 4.3 Hz), 2.29 (m, 1H), 1.64-1.59 (m, 2H, 2 signals overlapping), 1.57 (m, 1H), 1.38 (m, 1H), 1.33 (m, 2H, 2 signals overlapping), 1.14 (m, 1H), 1.08 (m, 1H), 0.90 (d, 6H, *J* = 6.8 Hz), 0.62 (d, 3H, *J* = 7.2 Hz). ^{13}C NMR (125 MHz, C_6D_6): δ (ppm) 155.9, 154.8, 140.8, 124.1, 122.1, 120.2, 119.6, 111.6, 44.5, 37.5, 32.9, 32.7, 31.1, 27.8, 23.2, 19.7, 19.6, 12.3. FT-IR: v (cm^{-1}) 2954 (m), 2923 (m), 1726 (m), 1450 (s), 1382 (w), 1366 (w), 1277 (m), 1190 (w), 1121 (w), 1090 (m), 1072 (w), 857 (m), 740 (s). $[a]^{23}_D$ -32.8 (*c* 0.3, CH_2Cl_2).

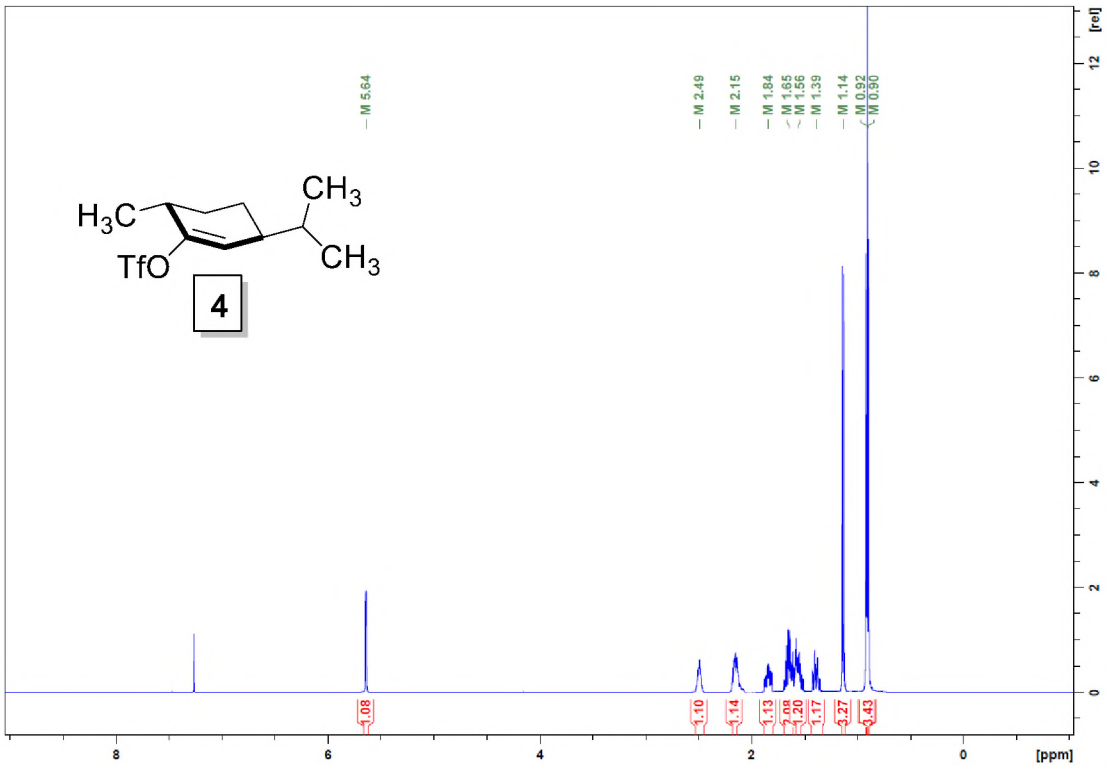
III. Compound 1D and 2D NMR Spectra

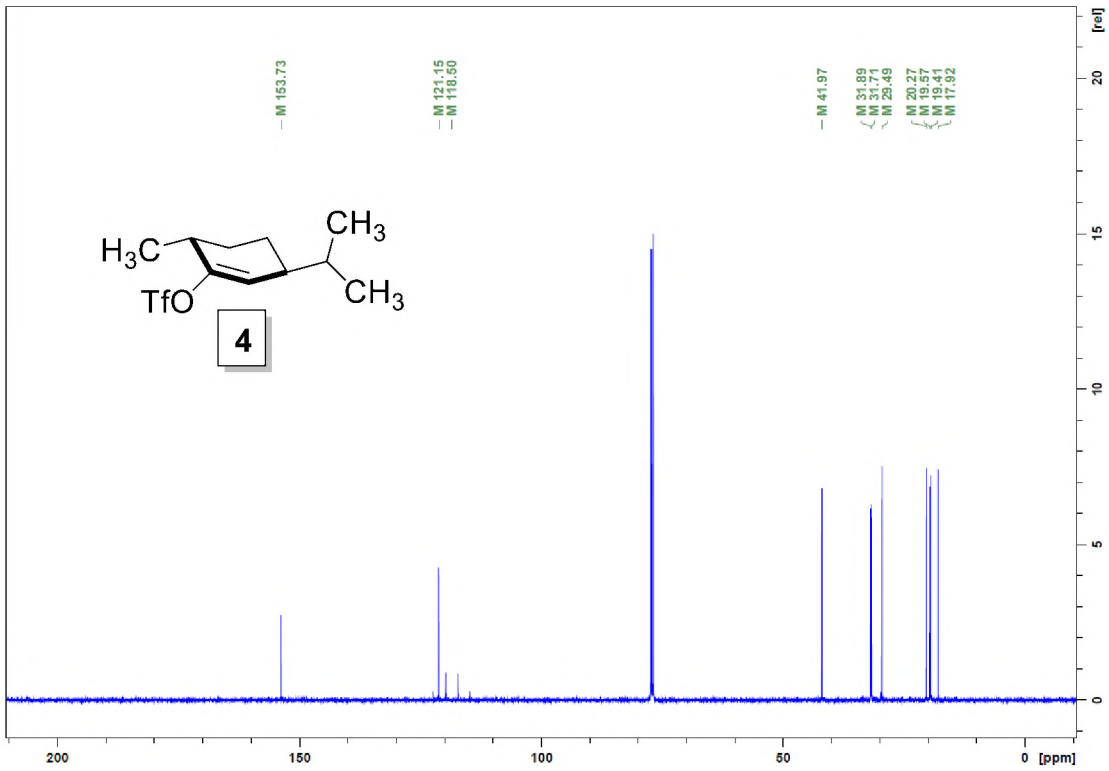


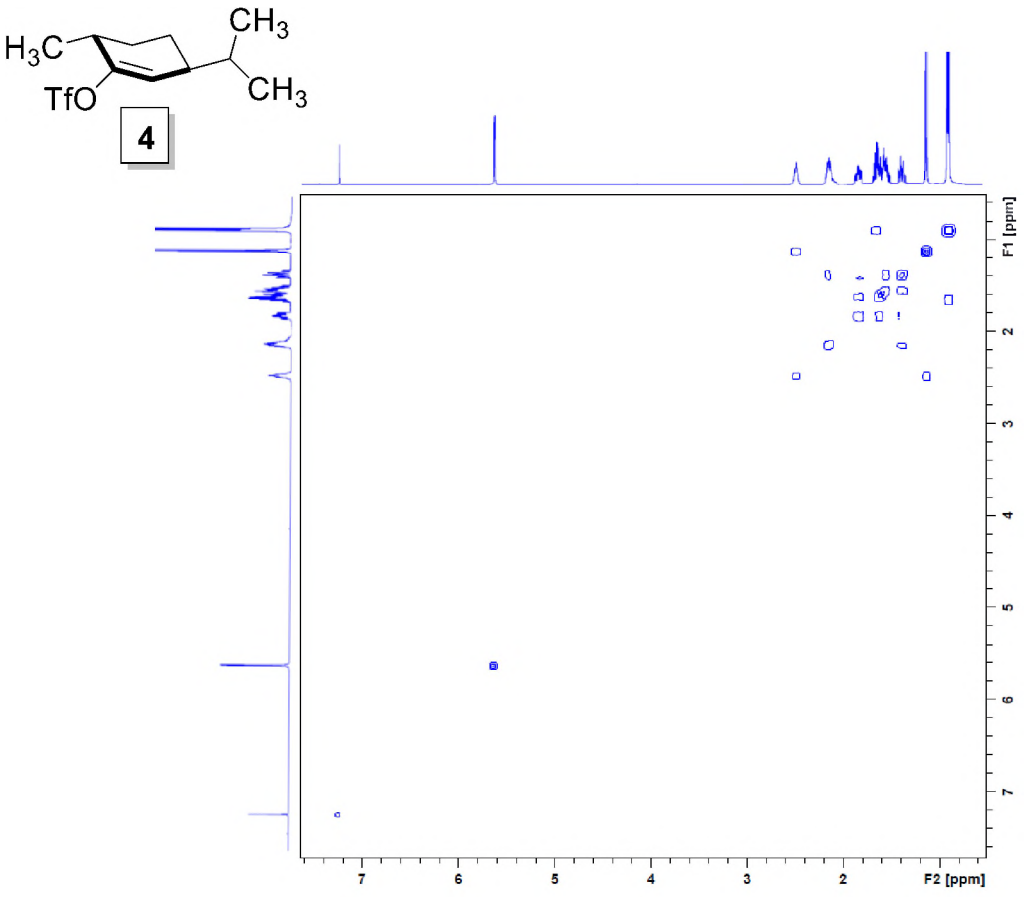


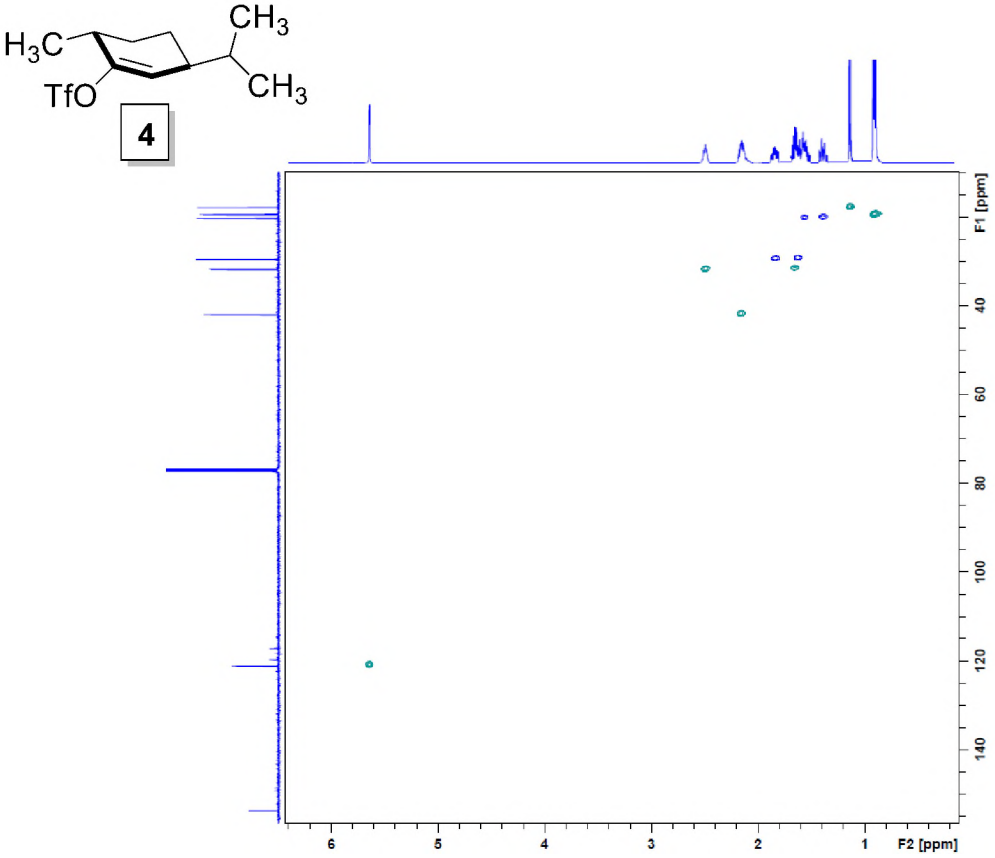

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H3C
CH3
OTf
3
F1 [ppm]
2
4
6
6
4
2
F2 [ppm]

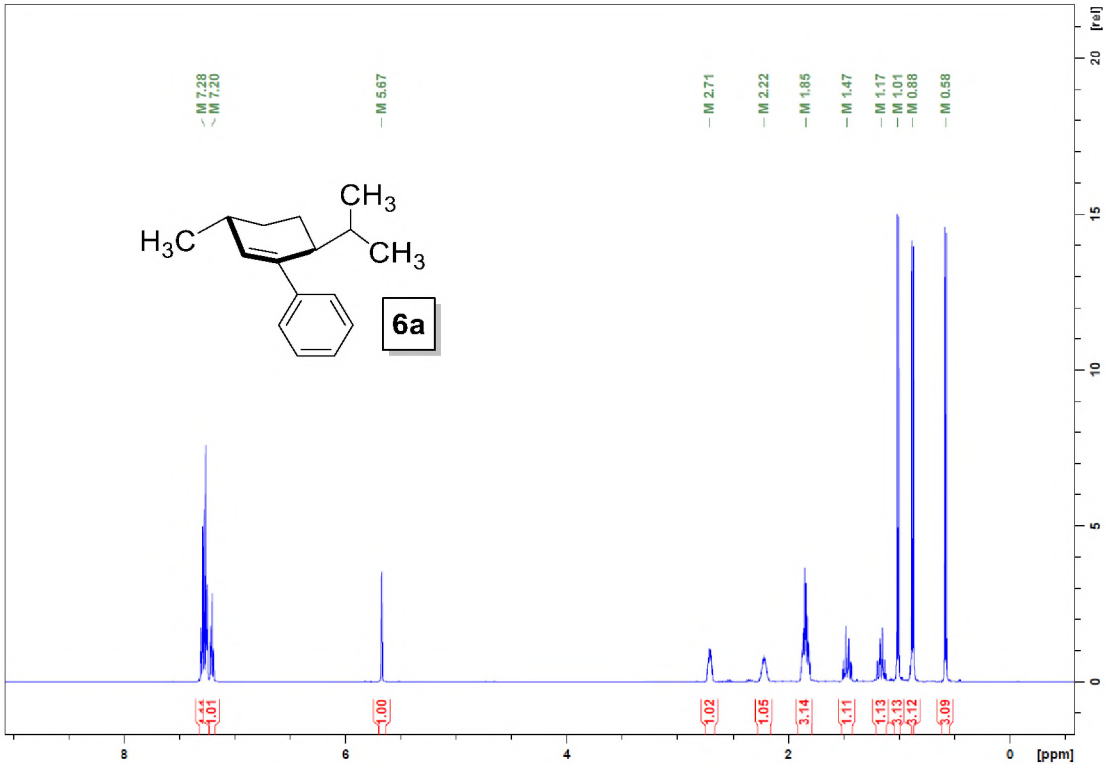

CH3
H3C
CH3
OTf
3
20 F1 [ppm]
40
60
80
100
120
140
6
4
2
F2 [ppm]

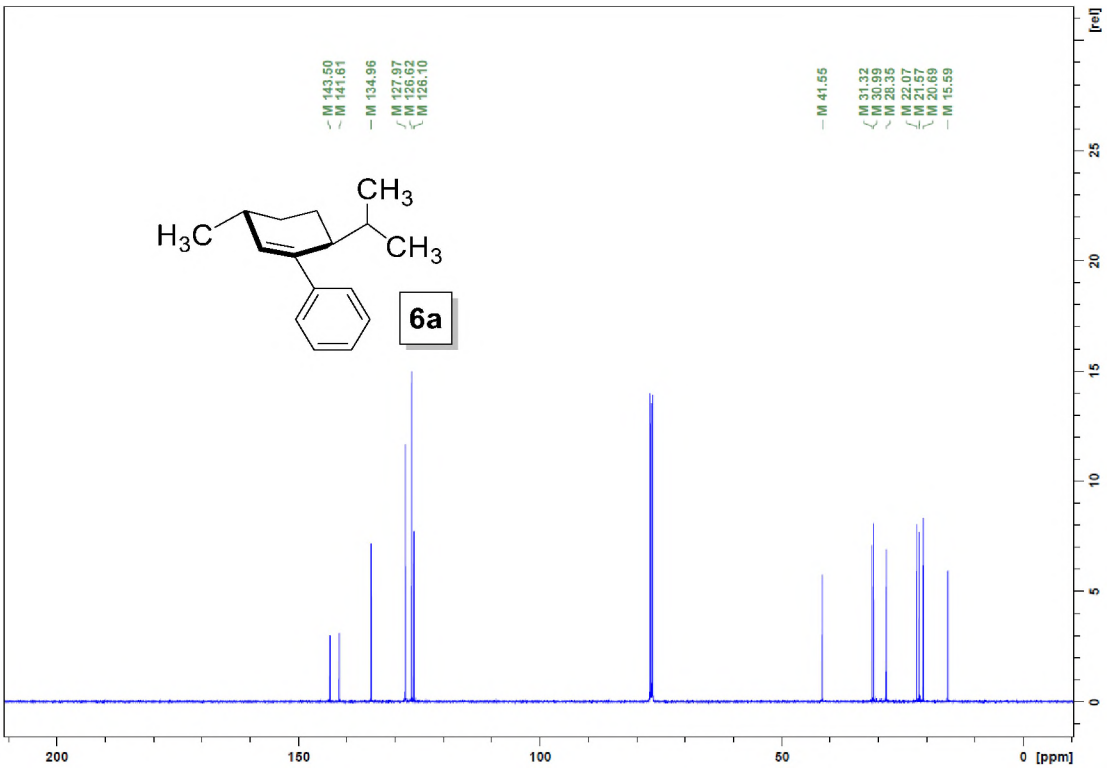

M 5.64
M 2.49
M 2.15
M 1.84
M 1.65
M 1.56
M 1.39
M 1.14
M 0.92
M 0.90
H3C
CH3
TfO
CH3
4
1.08
1.10
1.14
1.13
2.08
1.20
1.17
3.27
6.43
[rel]
[ppm]

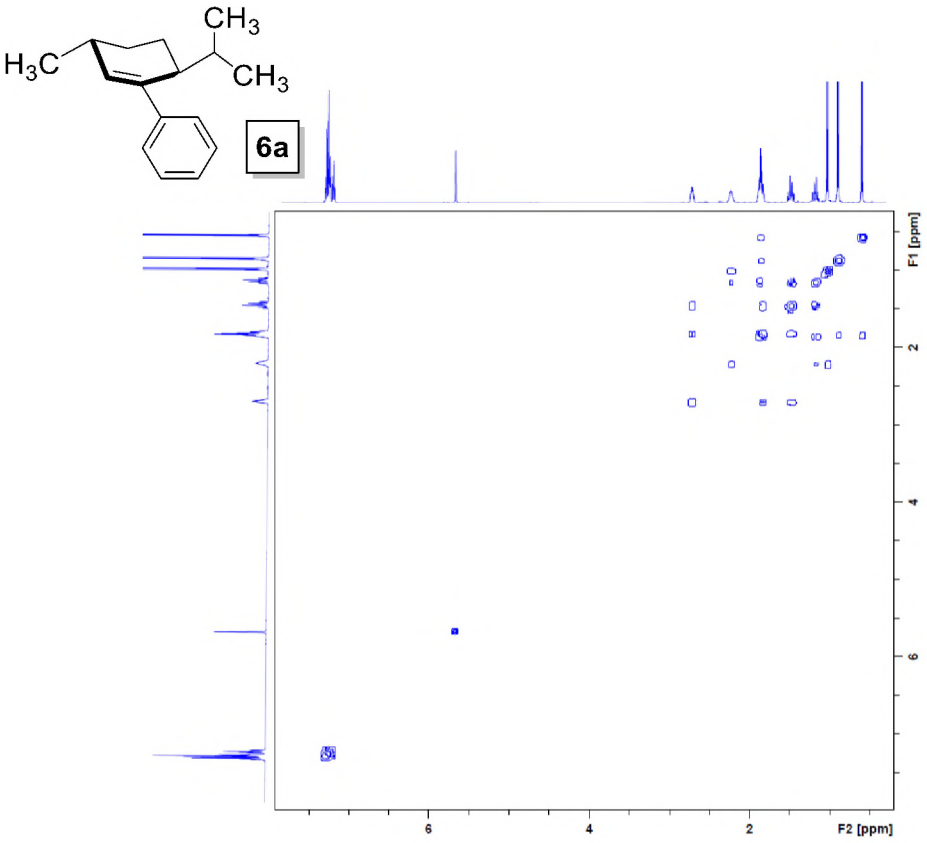

M 153.73
M 121.15
M 118.50
M 41.97
M 31.89
M 31.71
M 29.49
M 20.27
M 19.57
M 19.41
M 17.92
H3C
CH3
TfO
CH3
4
[rel]
[ppm]

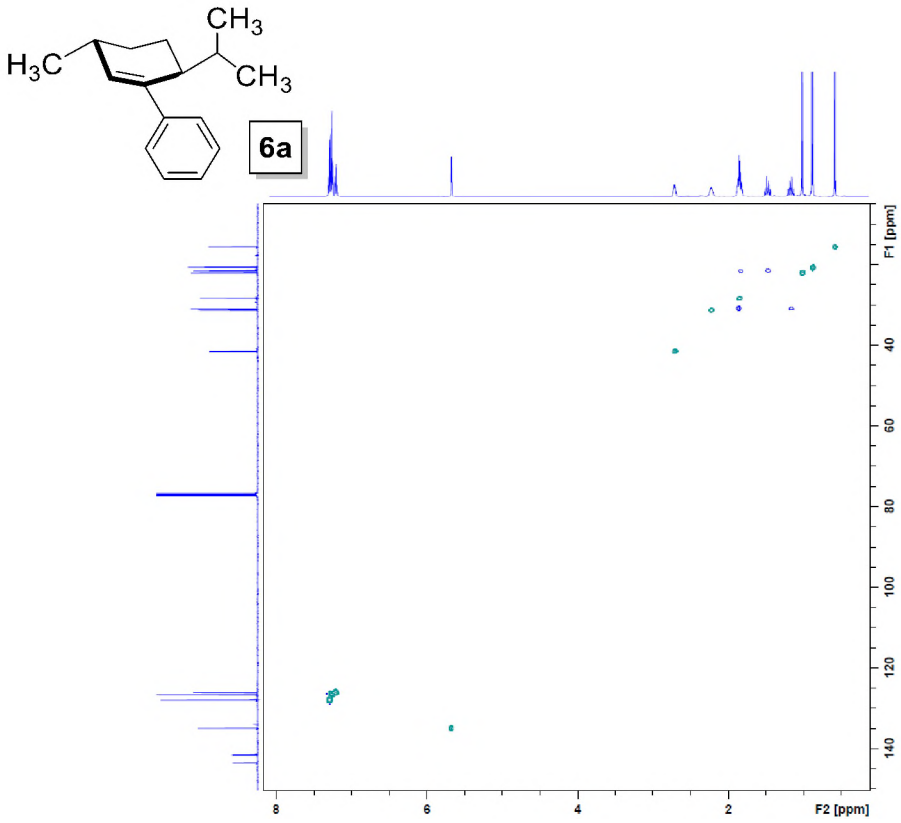

H3C
CH3
TfO
CH3
4
F1 [ppm]
F2 [ppm]

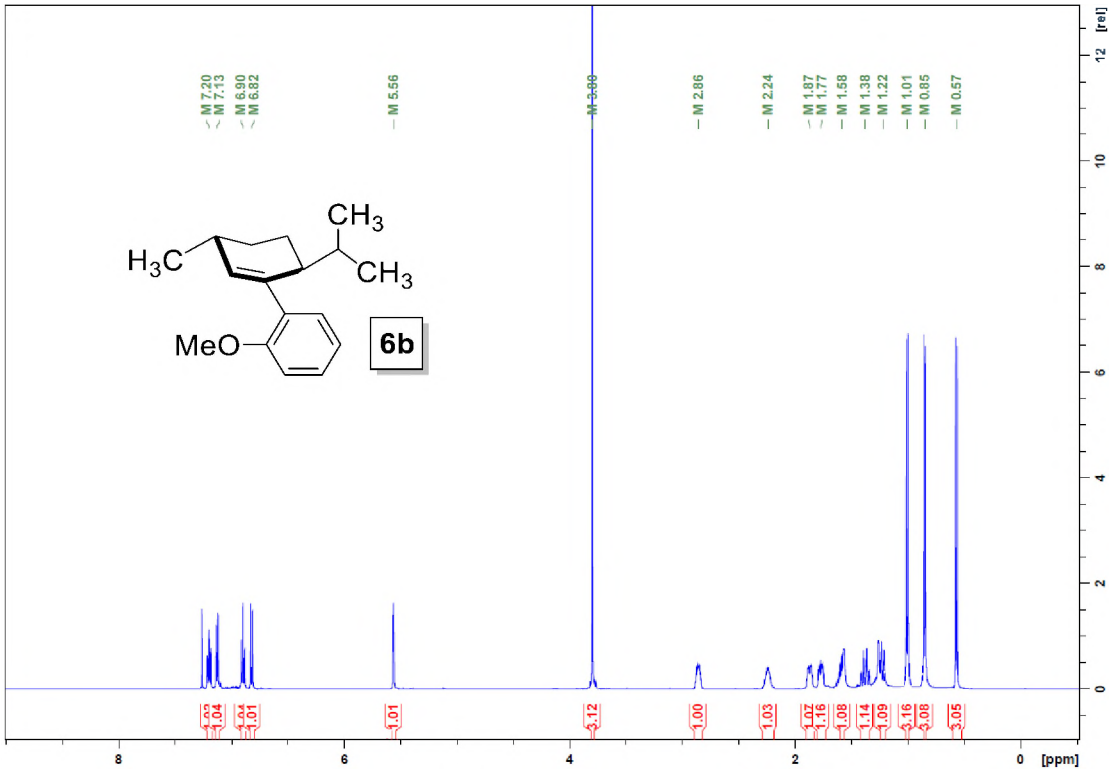

H3C
CH3
TfO
CH3
4
F1 [ppm]
F2 [ppm]

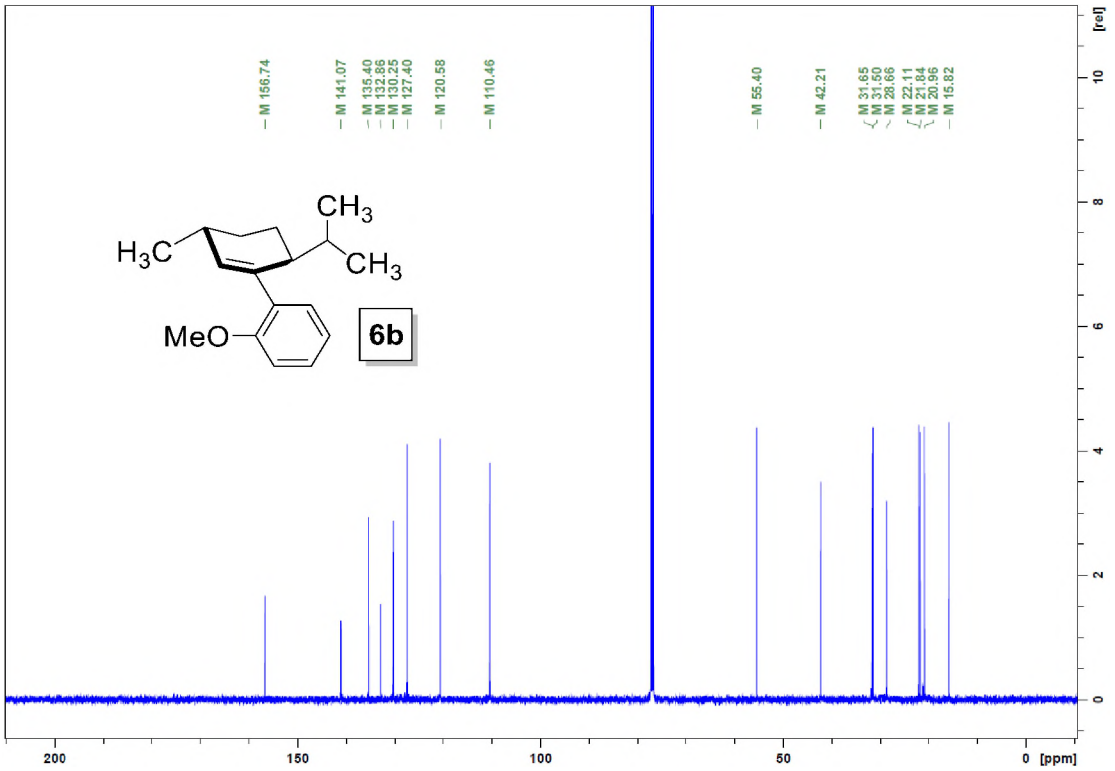

M 7.28
M 7.20
M 5.67
M 2.71
M 2.22
M 1.85
M 1.47
M 1.17
M 1.01
M 0.88
M 0.58
CH3
H3C
CH3
6a
1.01
1.00
1.02
1.05
3.14
1.11
1.13
3.13
3.12
3.09
8
6
4
2
0
[ppm]
[rel]

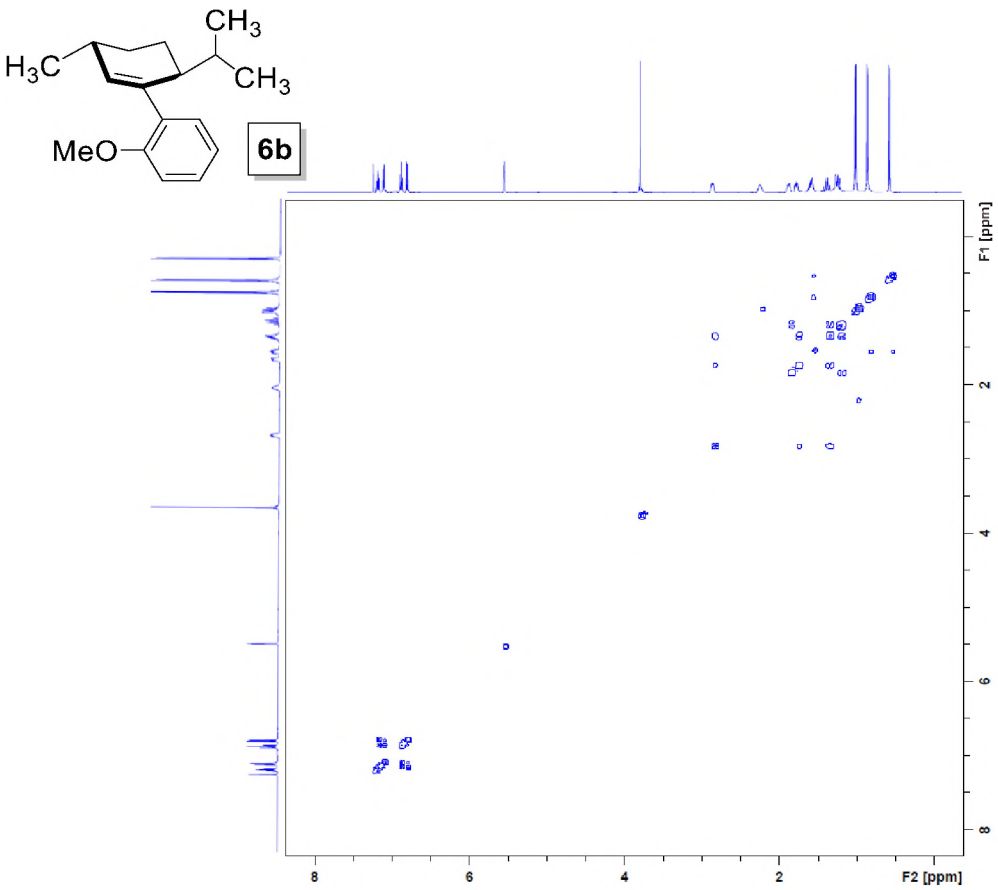

M 143.50
M 141.61
M 134.96
M 127.97
M 126.62
M 126.10
M 41.55
M 31.32
M 30.99
M 28.35
M 22.07
M 21.57
M 20.69
M 15.59
CH3
H3C
CH3
6a
200
150
100
50
0
[ppm]
[rel]

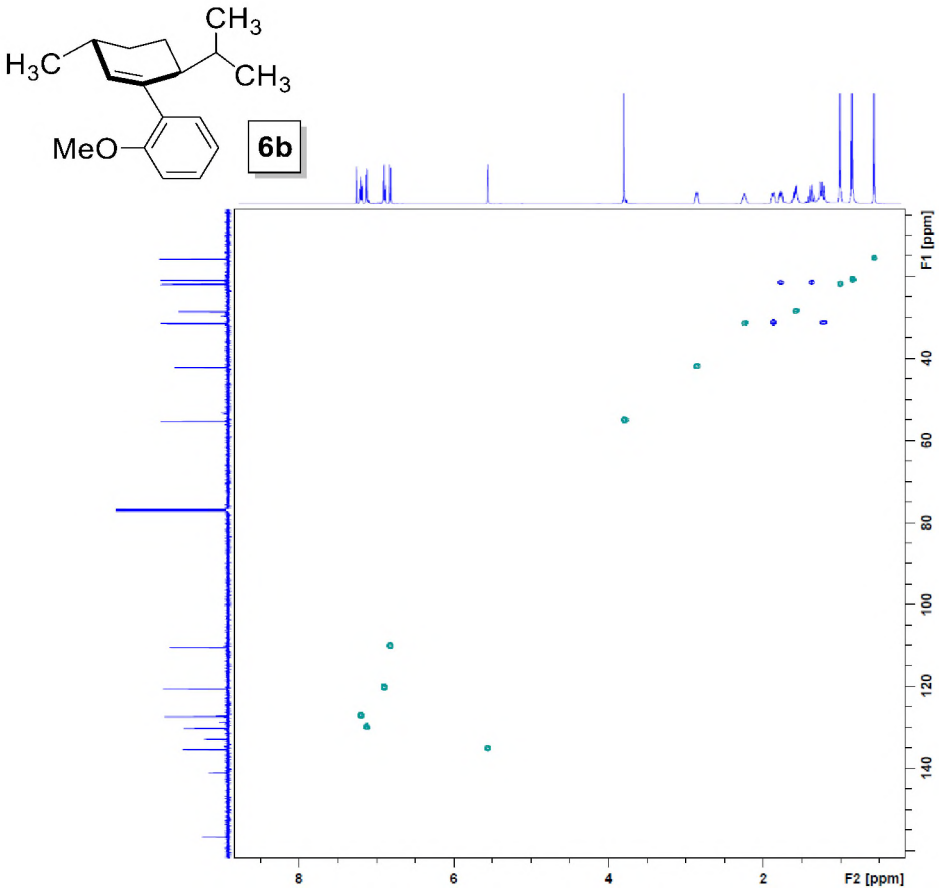

CH3
H3C
CH3
6a
F1 [ppm]
F2 [ppm]

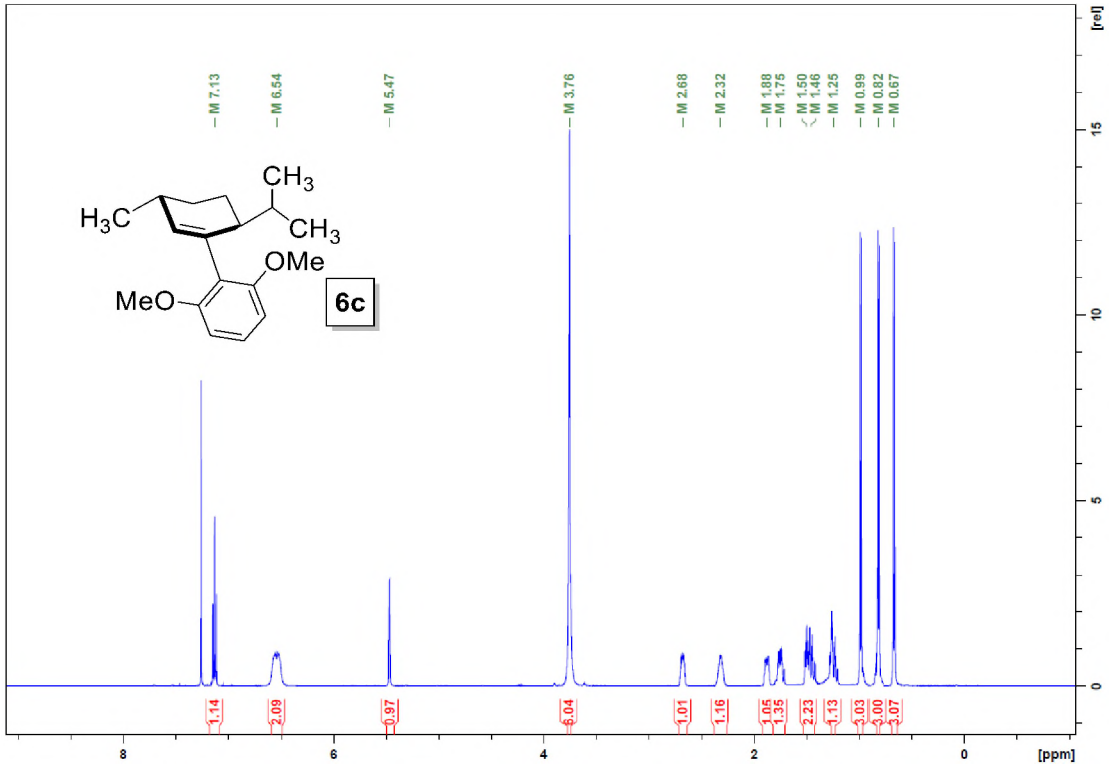

CH3
H3C
CH3
6a
F1 [ppm]
F2 [ppm]

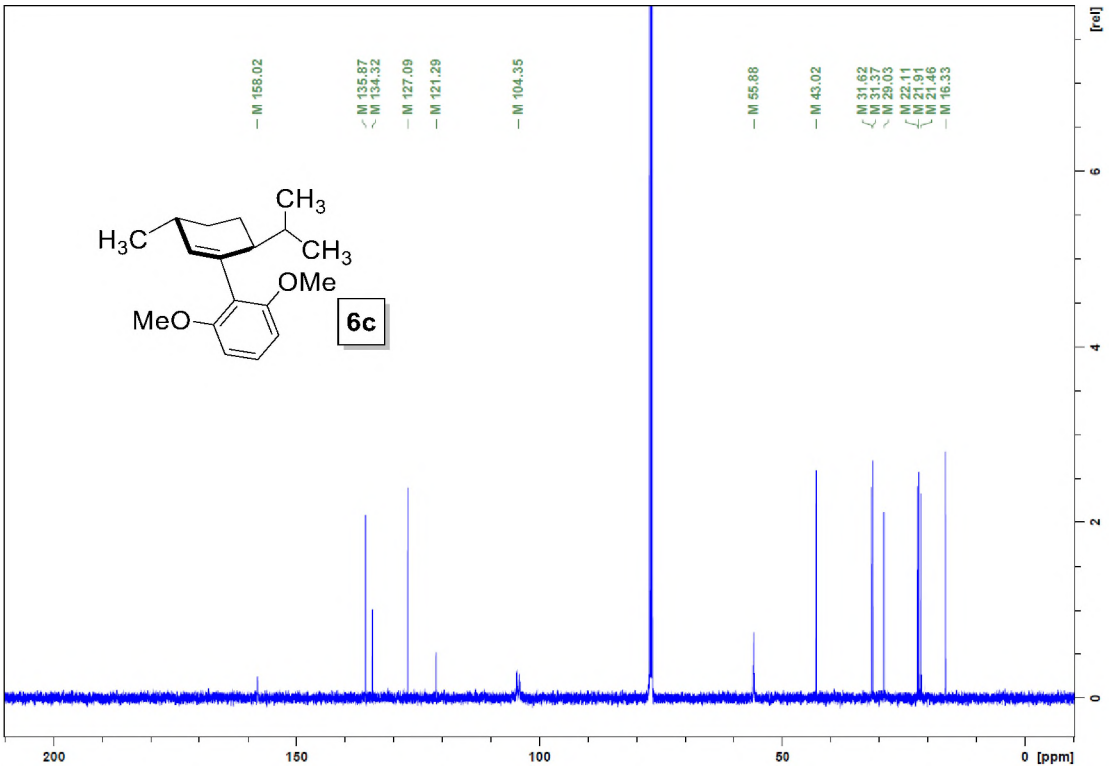

M 7.20
M 7.13
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M 6.82
M 5.56
M 3.80
M 2.86
M 2.24
M 1.87
M 1.77
M 1.58
M 1.38
M 1.22
M 1.01
M 0.85
M 0.57
CH3
H3C
CH3
MeO
6b
[rel]
[ppm]

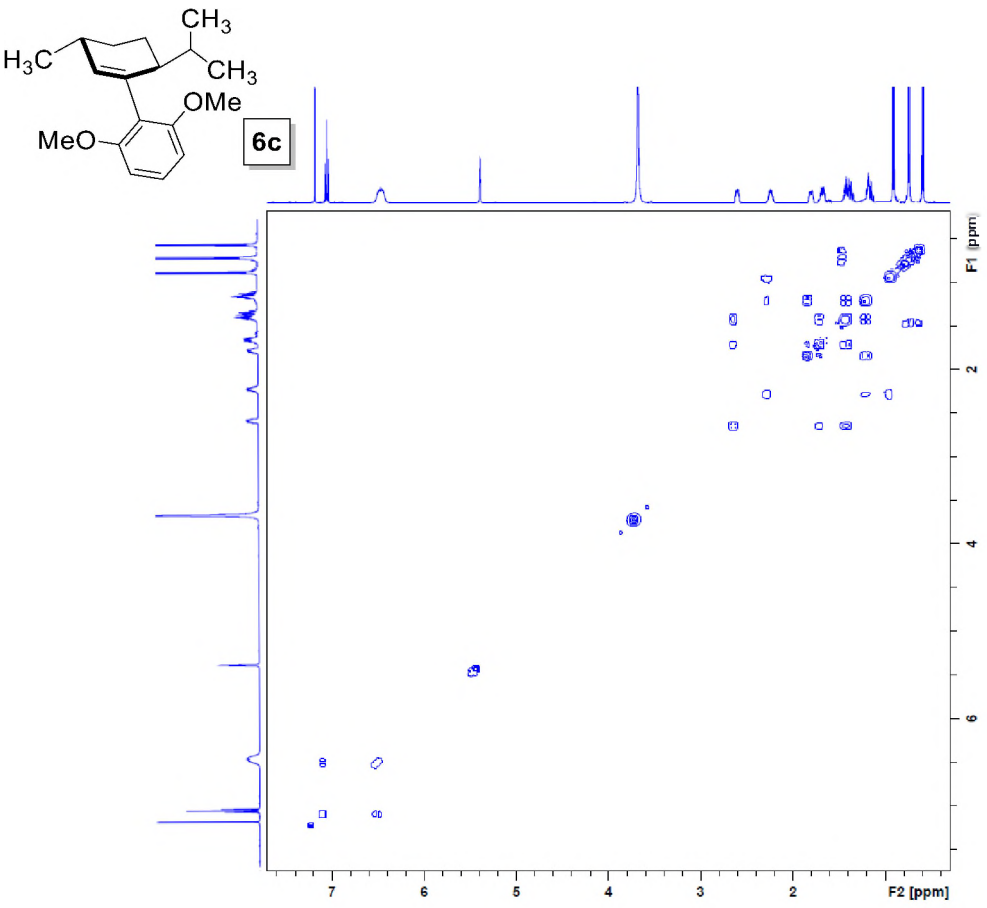

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M 135.40
M 132.86
M 130.25
M 127.40
M 120.58
M 110.46
M 55.40
M 42.21
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M 31.50
M 28.66
M 22.11
M 21.84
M 20.96
M 15.82
CH3
H3C
CH3
MeO
6b
[rel]
[ppm]

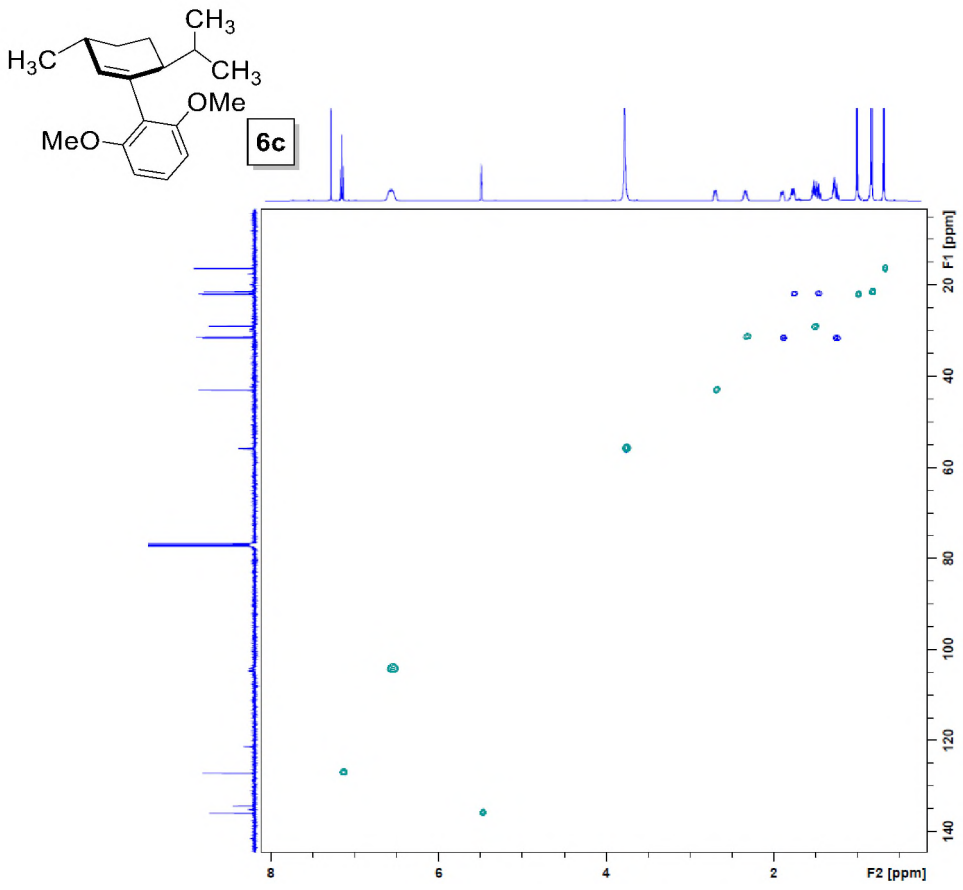

CH3
H3C
CH3
MeO
6b
F1 [ppm]
F2 [ppm]
2
4
6
8

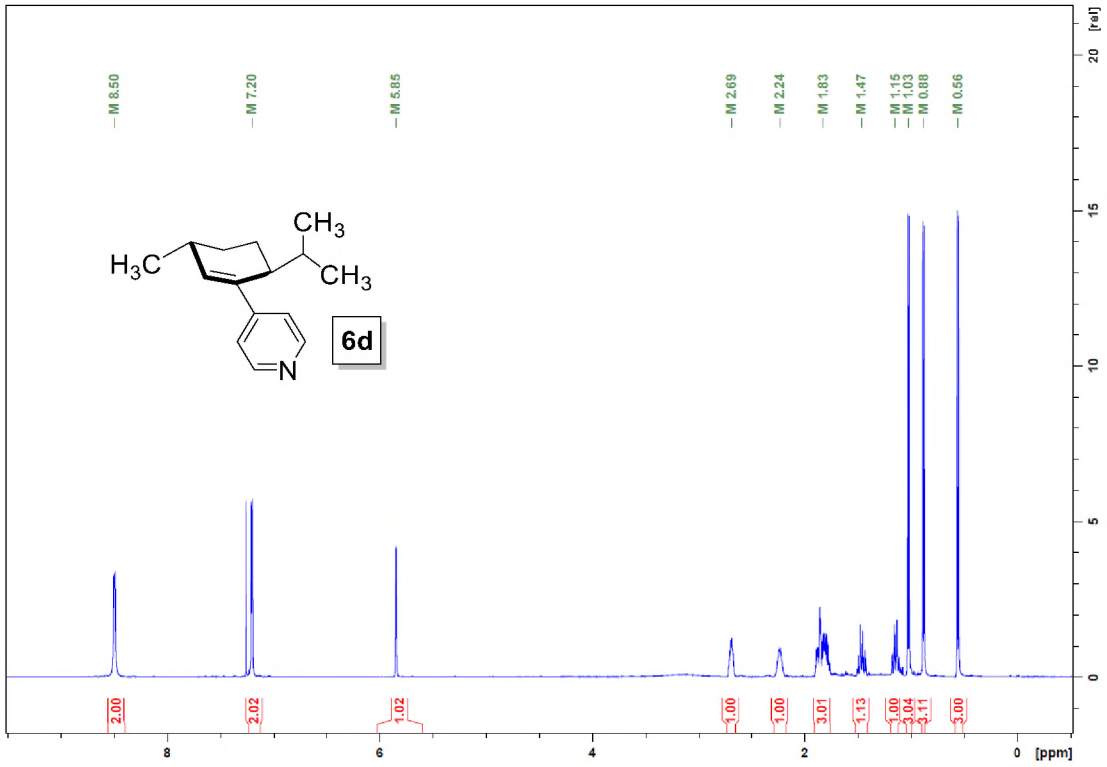

CH3
H3C
CH3
MeO
6b
F1 [ppm]
F2 [ppm]
40
60
80
100
120
140
2
4
6
8

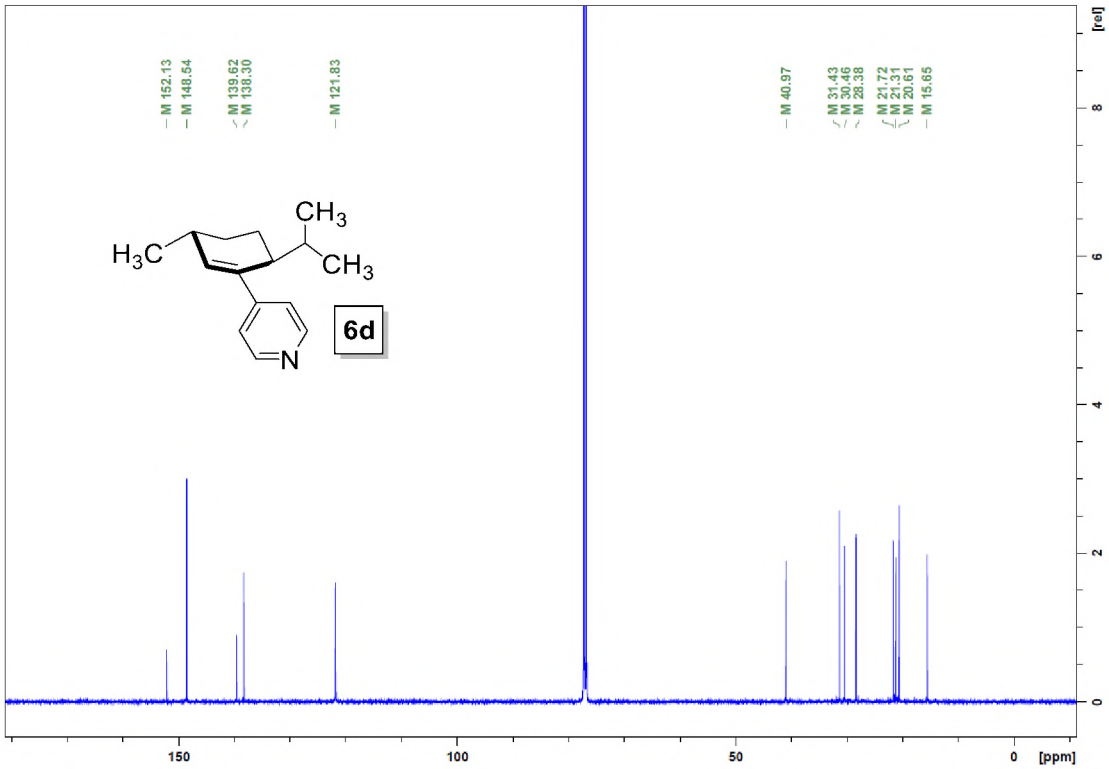

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M 5.47
M 3.76
M 2.68
M 2.32
M 1.88
M 1.75
M 1.50
M 1.46
M 1.25
M 0.99
M 0.82
M 0.67
CH3
H3C
CH3
OMe
MeO
6c
1.14
2.09
0.97
6.04
1.01
1.16
1.05
1.35
2.23
1.13
3.03
3.00
3.07
[rel]
[ppm]

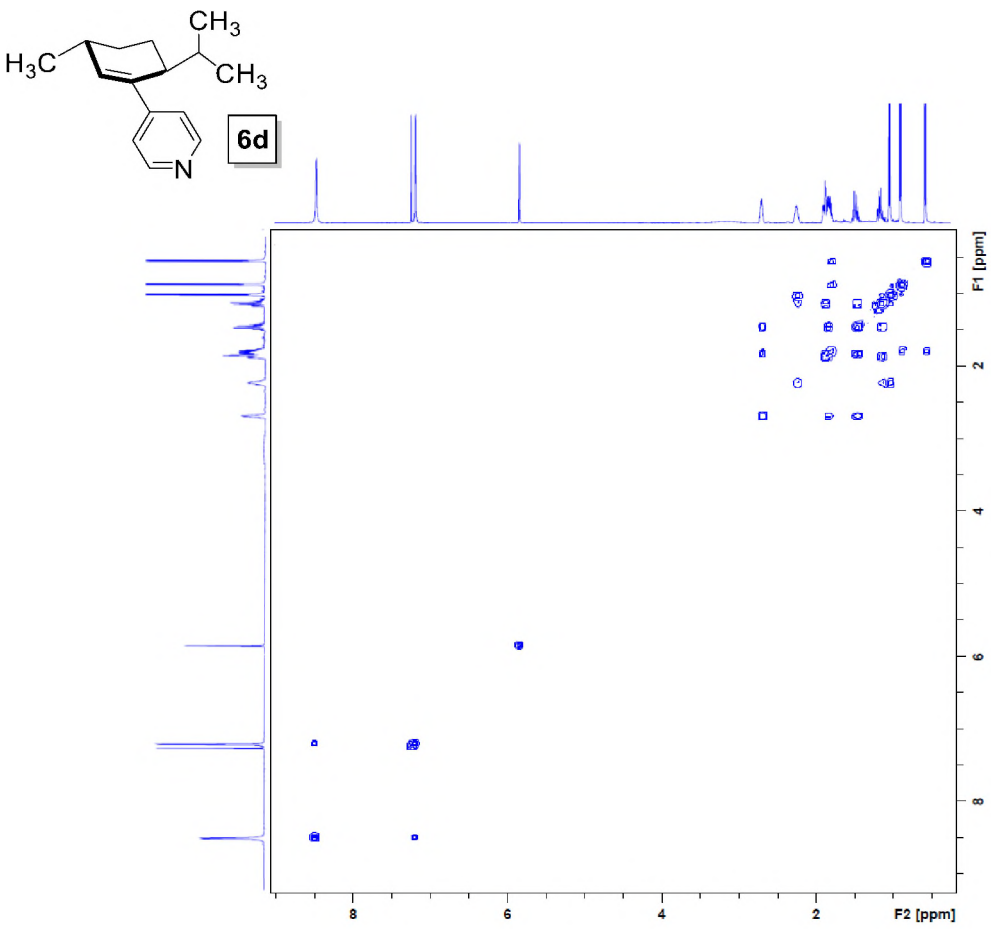

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M 55.88
M 43.02
M 31.62
M 31.37
M 29.03
M 22.11
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M 21.46
M 16.33
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H3C
CH3
OMe
MeO
6c
[rel]
[ppm]

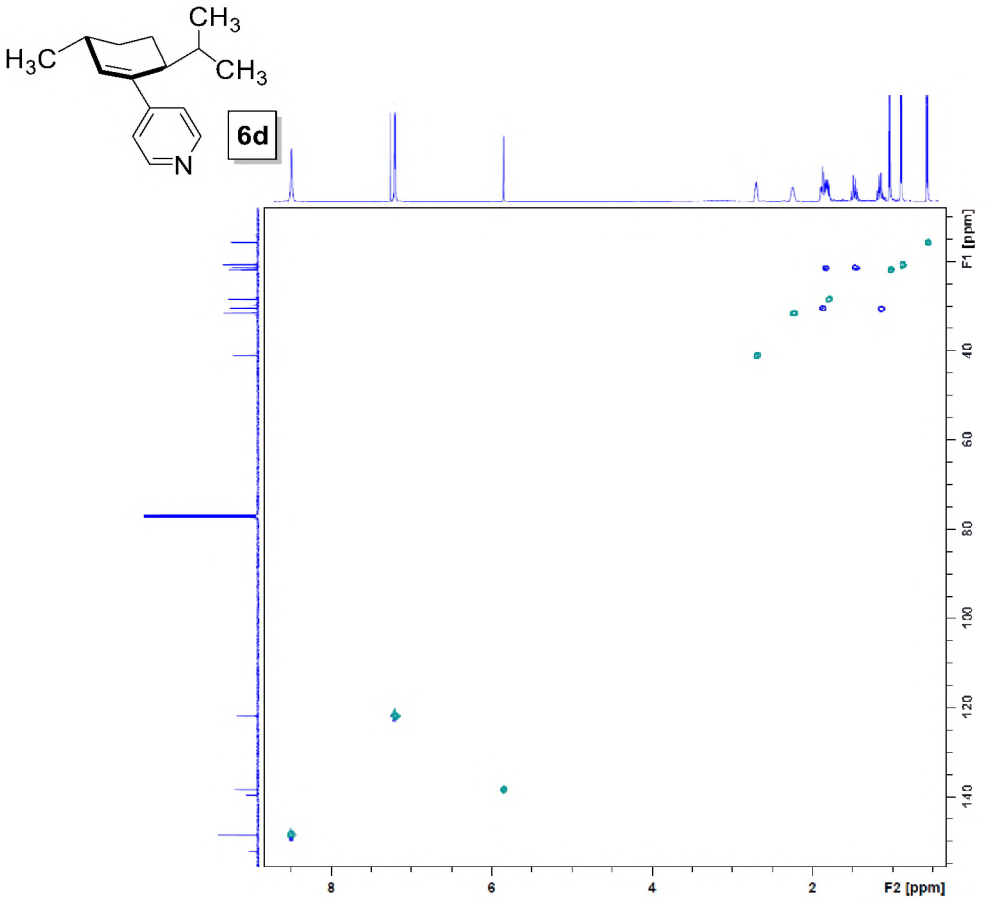

CH3
H3C
CH3
OMe
MeO
6c
F1 [ppm]
F2 [ppm]

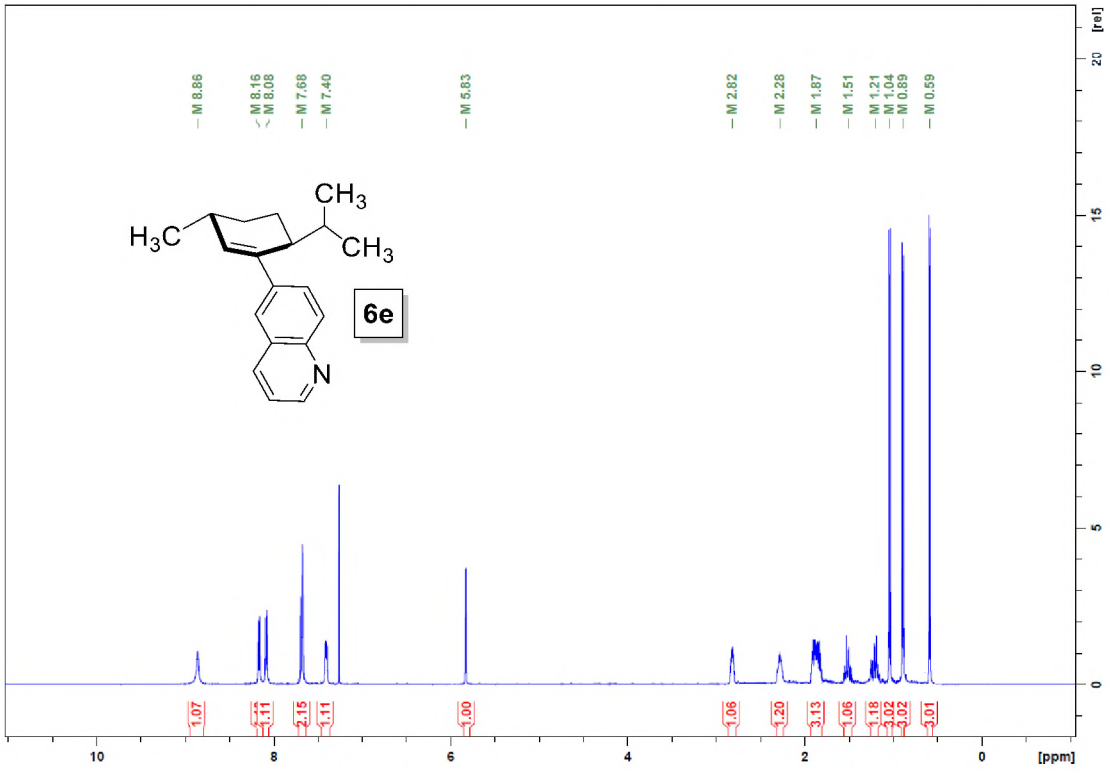

CH3
H3C
CH3
OMe
MeO
6c
F1 [ppm]
F2 [ppm]

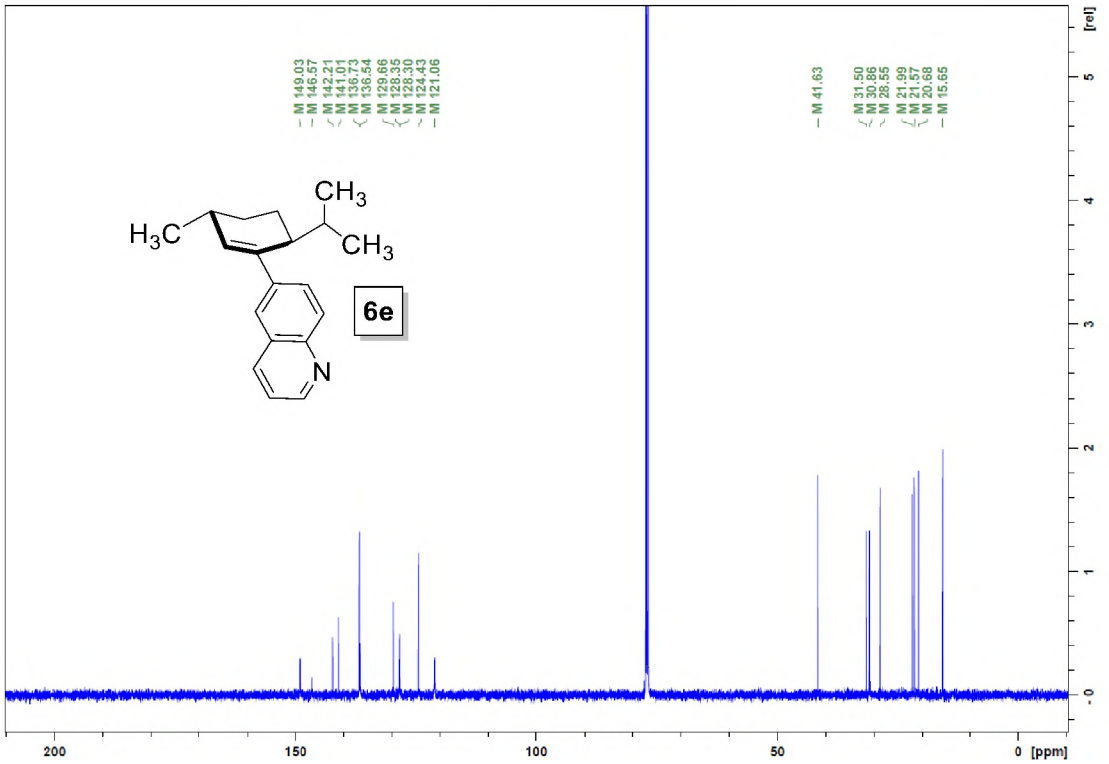

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M 2.69
M 2.24
M 1.83
M 1.47
M 1.15
M 1.03
M 0.88
M 0.56
CH3
H3C
CH3
N
6d
2.00
2.02
1.02
1.00
1.00
3.01
1.13
1.00
3.04
3.11
3.00
[rel]
[ppm]

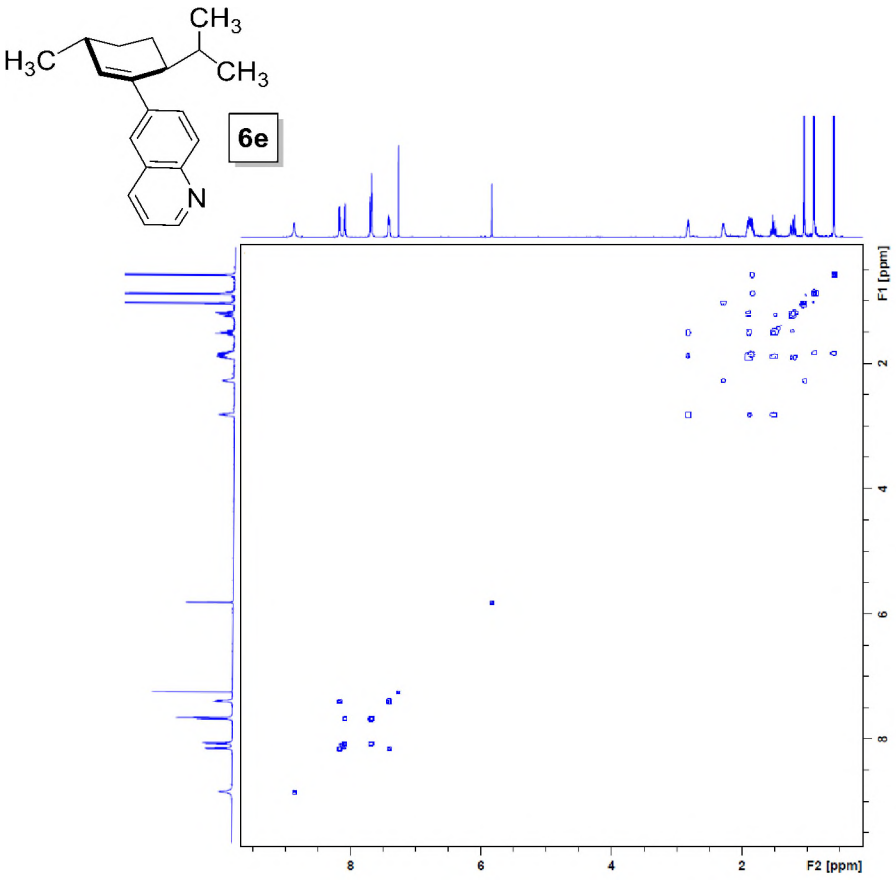

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M 138.30
M 121.83
M 40.97
M 31.43
M 30.46
M 28.38
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M 21.31
M 20.61
M 15.65
CH3
H3C
CH3
N
6d
[rel]
[ppm]

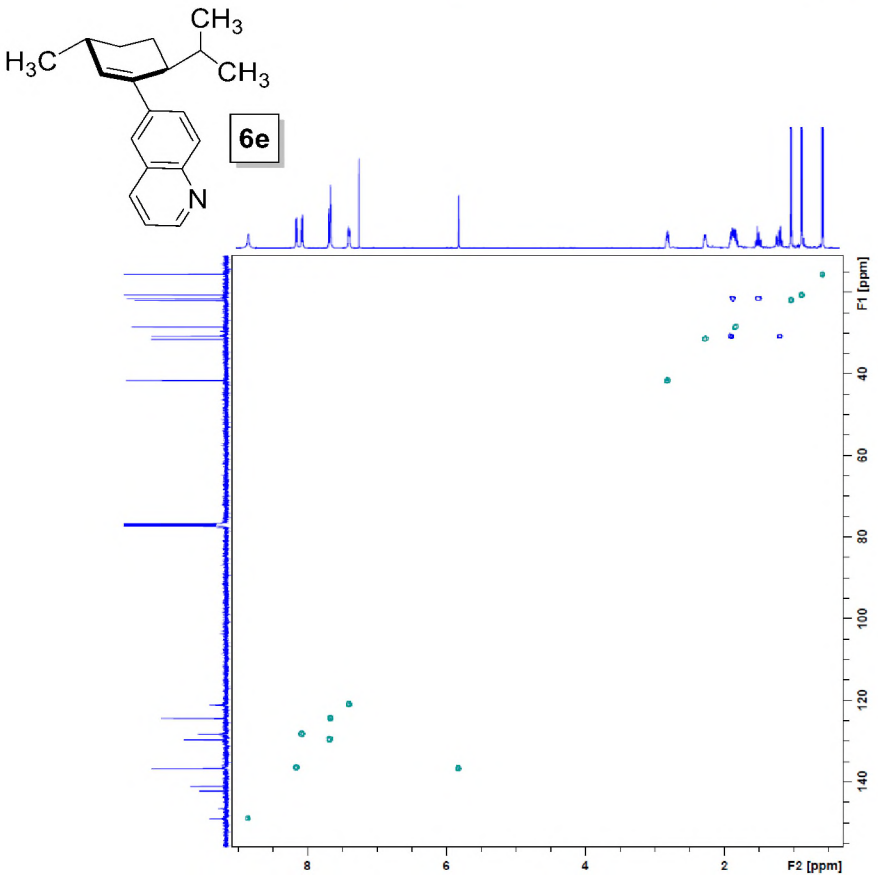

CH3
H3C
CH3
N
6d
F1 [ppm]
F2 [ppm]
8
6
4
2

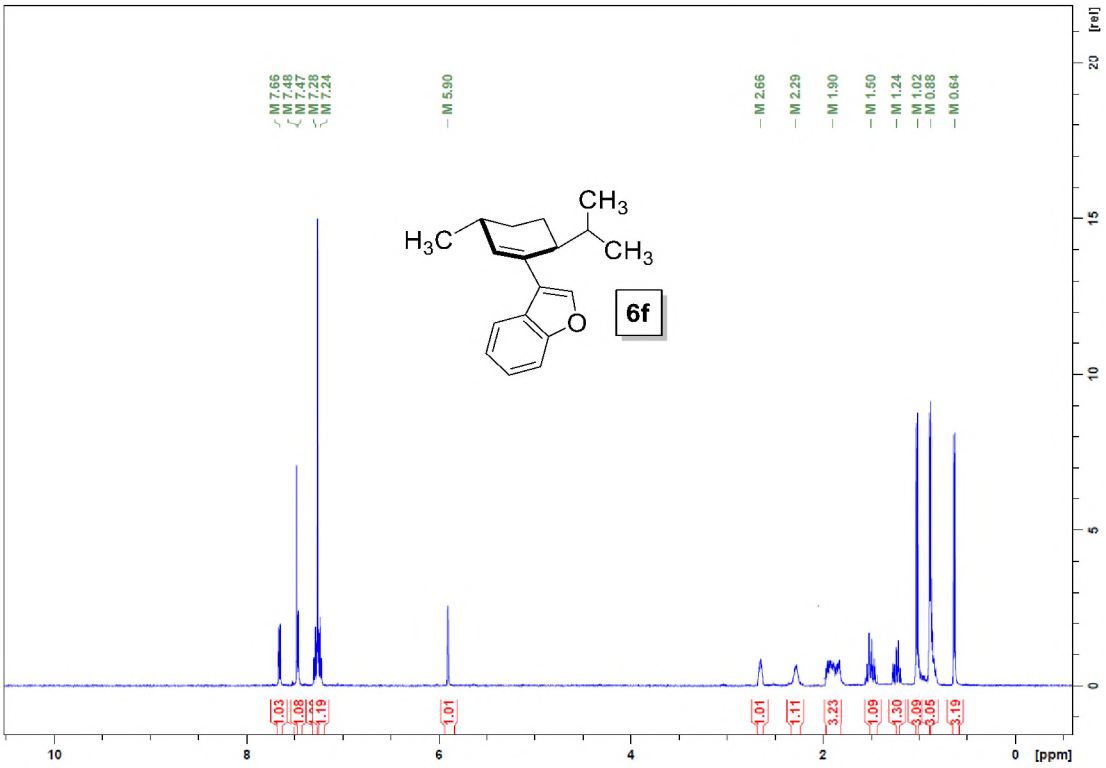

CH3
H3C
CH3
N
6d
F1 [ppm]
F2 [ppm]
8
6
4
2
40
60
80
100
120
140

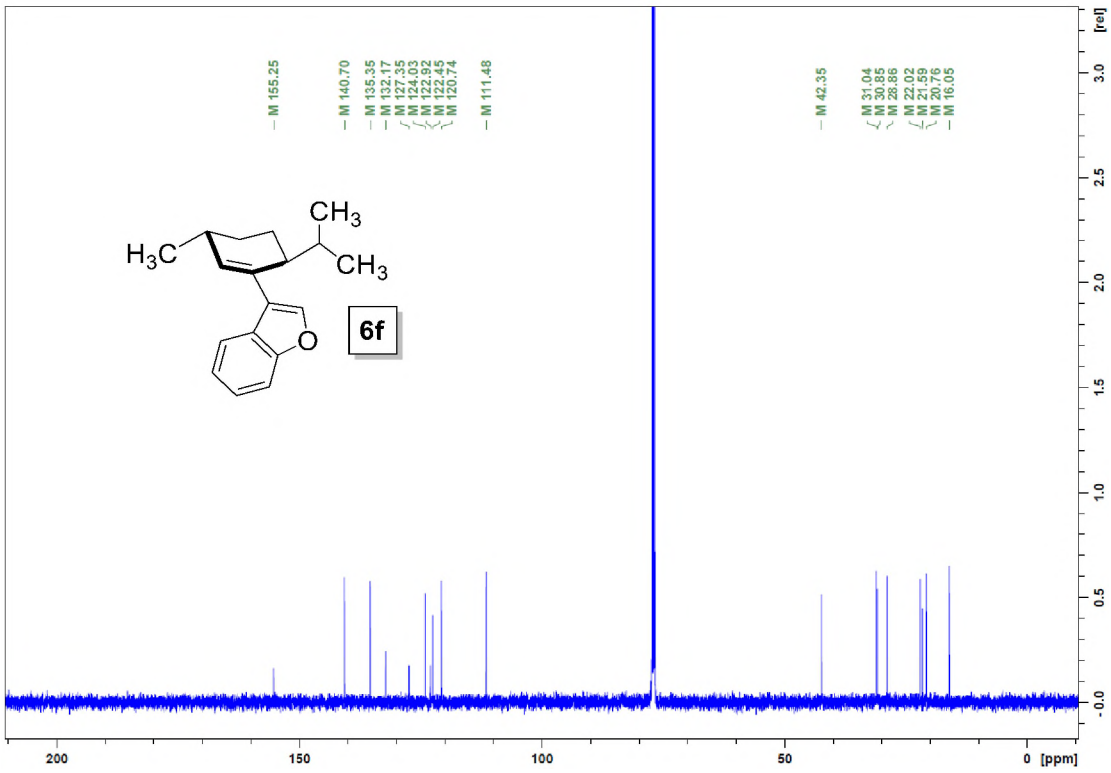

M 8.86
M 8.16
M 8.08
M 7.68
M 7.40
M 5.83
M 2.82
M 2.28
M 1.87
M 1.51
M 1.21
M 1.04
M 0.89
M 0.59
CH3
H3C
CH3
6e
N
1.07
1.11
2.15
1.11
1.00
1.06
1.20
3.13
1.06
1.18
3.02
3.02
3.01
10
8
6
4
2
0
[ppm]
[rel]

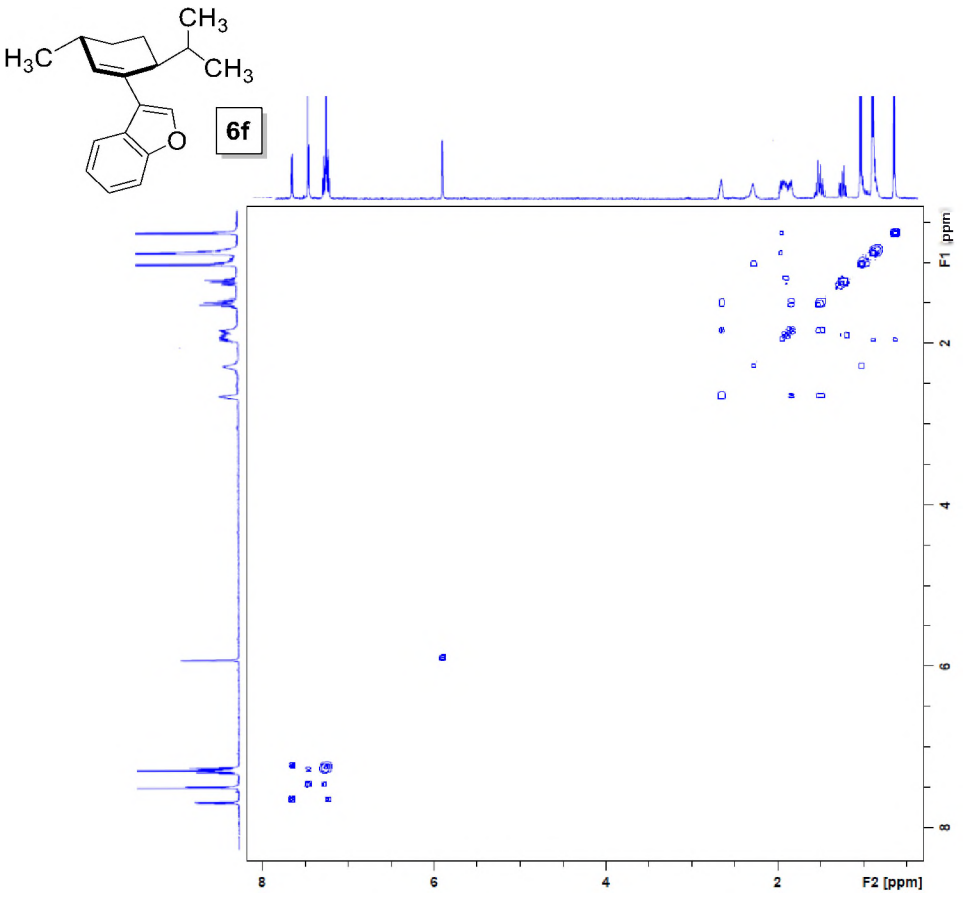

M 149.03
M 146.57
M 142.21
M 141.01
M 136.73
M 136.54
M 129.66
M 128.35
M 126.30
M 124.43
M 121.06
M 41.63
M 31.50
M 30.86
M 28.55
M 21.99
M 21.57
M 20.68
M 15.65
CH3
H3C
CH3
6e
N
200
150
100
50
0 [ppm]
[rel]

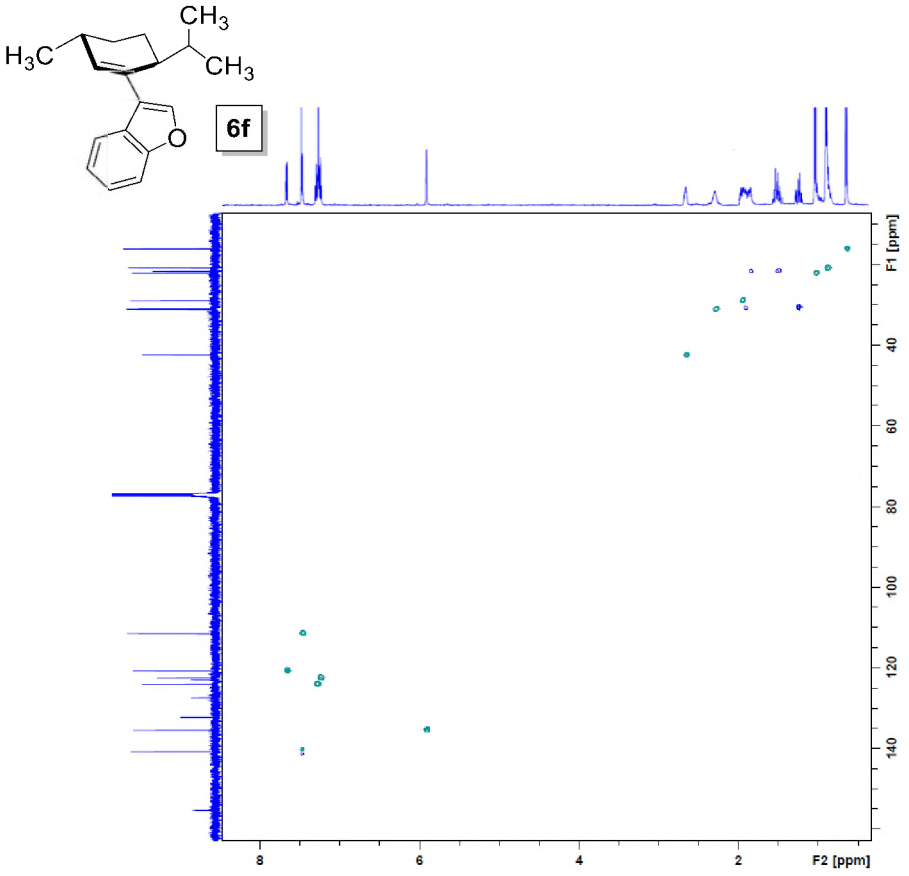

CH3
H3C
CH3
6e
N
F1 [ppm]
F2 [ppm]
8
6
4
2

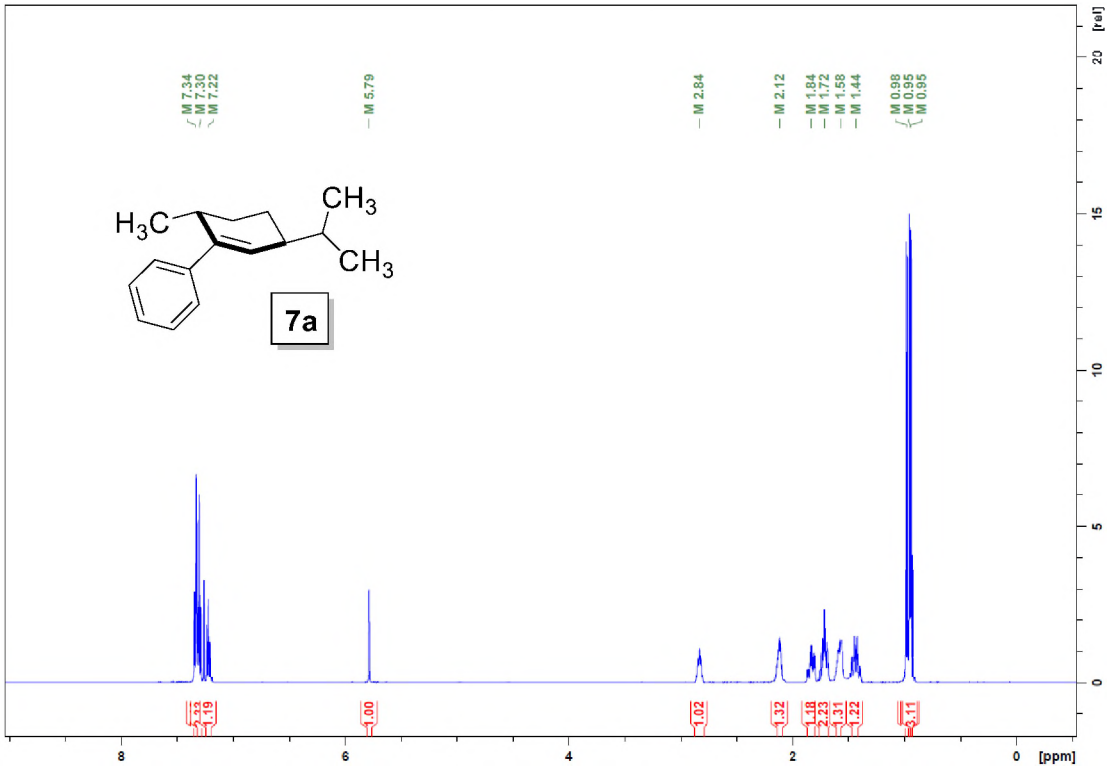

CH3
H3C
CH3
6e
N
F1 [ppm]
F2 [ppm]
8
6
4
2
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60
80
100
120
140

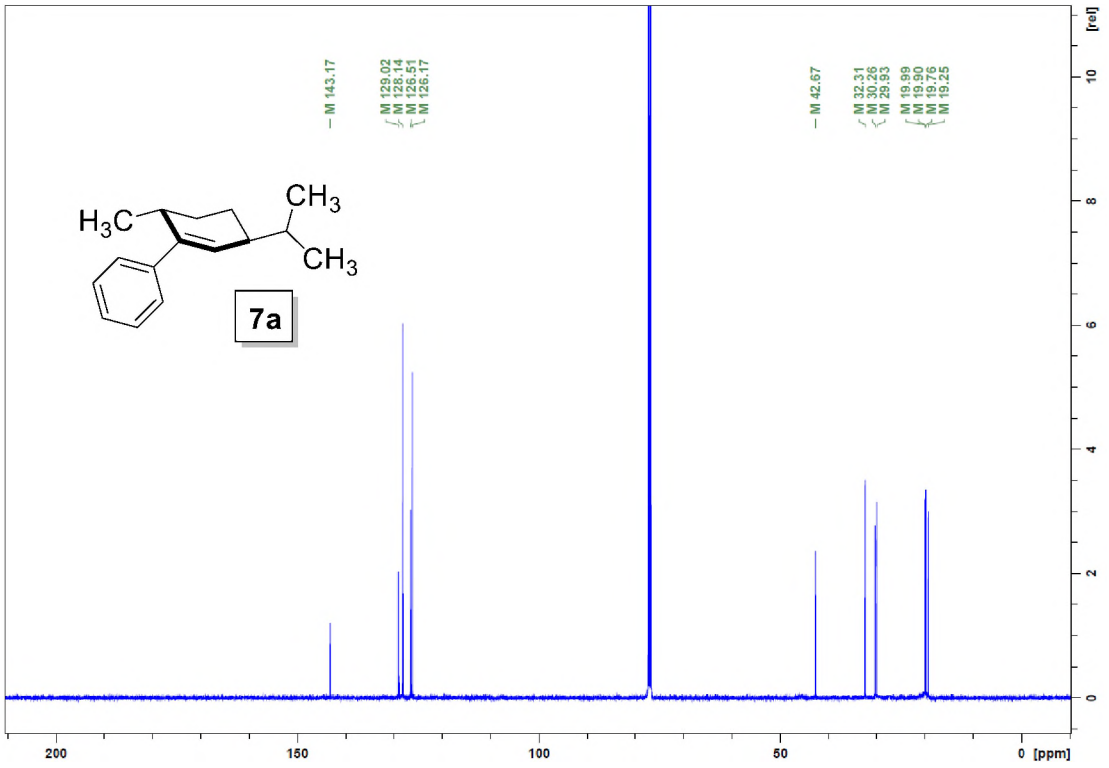

M 7.66
M 7.48
M 7.47
M 7.28
M 7.24
M 5.90
M 2.66
M 2.29
M 1.90
M 1.50
M 1.24
M 1.02
M 0.88
M 0.64
CH3
H3C
CH3
O
6f
1.03
1.08
1.19
1.01
1.01
1.11
3.23
1.09
1.30
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3.05
3.19
10
8
6
4
2
0 [ppm]
20 [rel]
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10
5
0

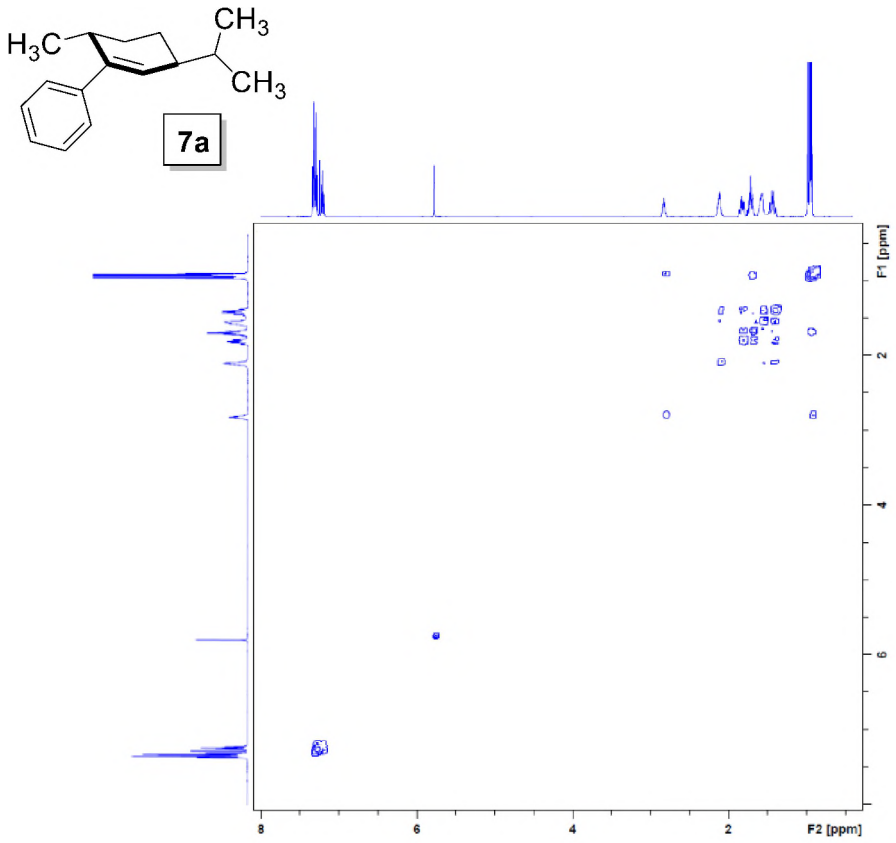

M 155.25
M 140.70
M 135.35
M 132.17
M 127.35
M 124.03
M 122.92
M 122.45
M 120.74
M 111.48
M 42.35
M 31.04
M 30.85
M 28.86
M 22.02
M 21.69
M 20.76
M 16.05
CH3
H3C
CH3
O
6f
200
150
100
50
0 [ppm]
3.0 [rel]
2.5
2.0
1.5
1.0
0.5
-0.0

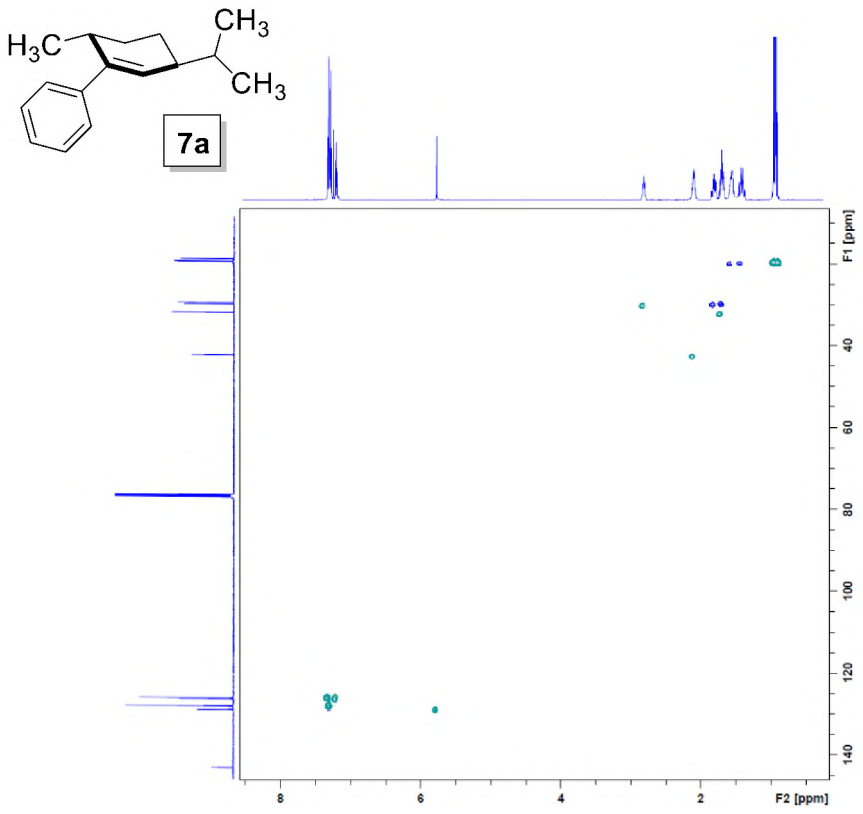

CH3
H3C
CH3
O
6f
F1 [ppm]
F2 [ppm]

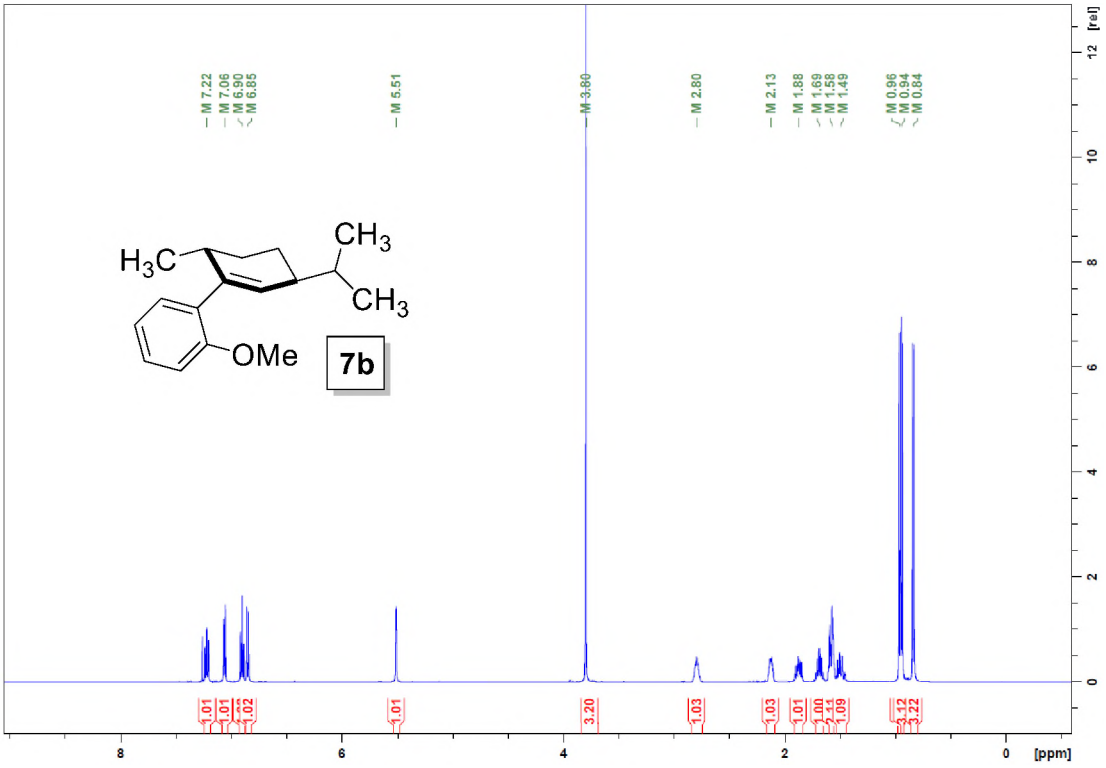

CH3
H3C
CH3
O
6f
F1 [ppm]
F2 [ppm]

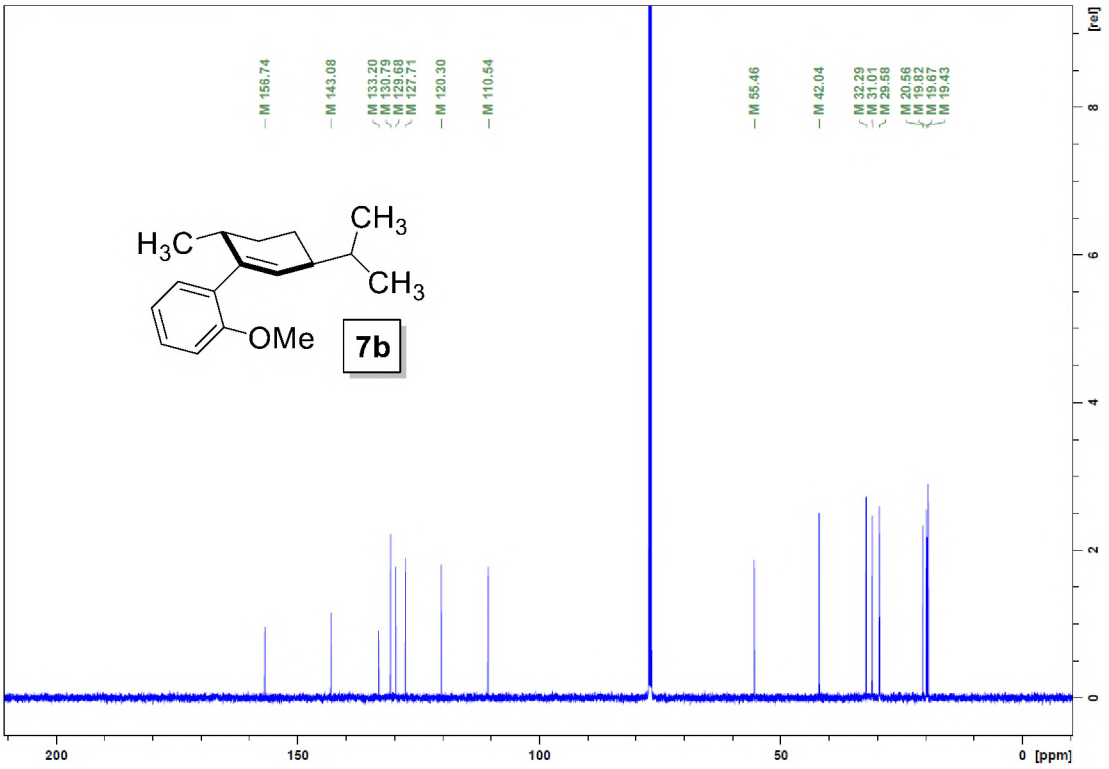

M 7.34
M 7.30
M 7.22
M 5.79
M 2.84
M 2.12
M 1.84
M 1.72
M 1.58
M 1.44
M 0.98
M 0.95
M 0.95
H3C
CH3
CH3
7a
2.33
1.19
1.00
1.02
1.32
1.18
2.23
1.31
1.22
3.11
8
6
4
2
0
[ppm]
[rel]

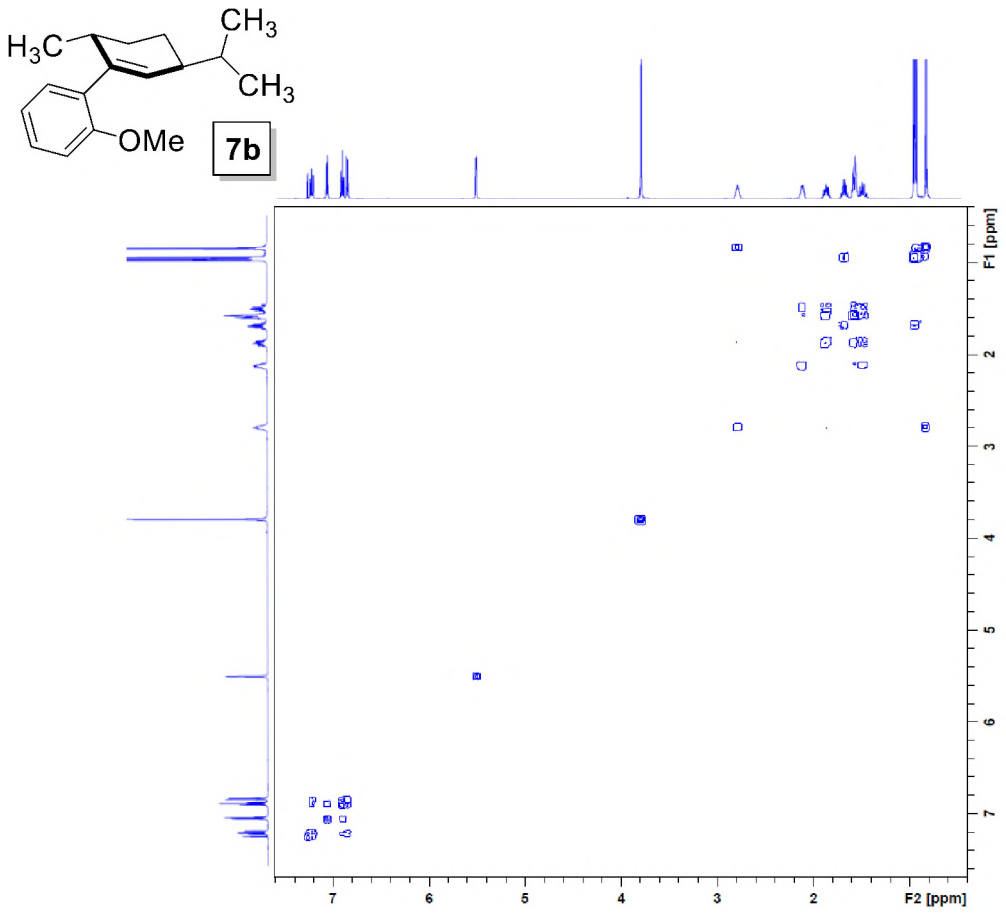

M 143.17
M 129.02
M 128.14
M 126.51
M 126.17
M 42.67
M 32.31
M 30.26
M 29.93
M 19.99
M 19.90
M 19.76
M 19.25
H3C
CH3
CH3
7a
200
150
100
50
0
[ppm]
[rel]

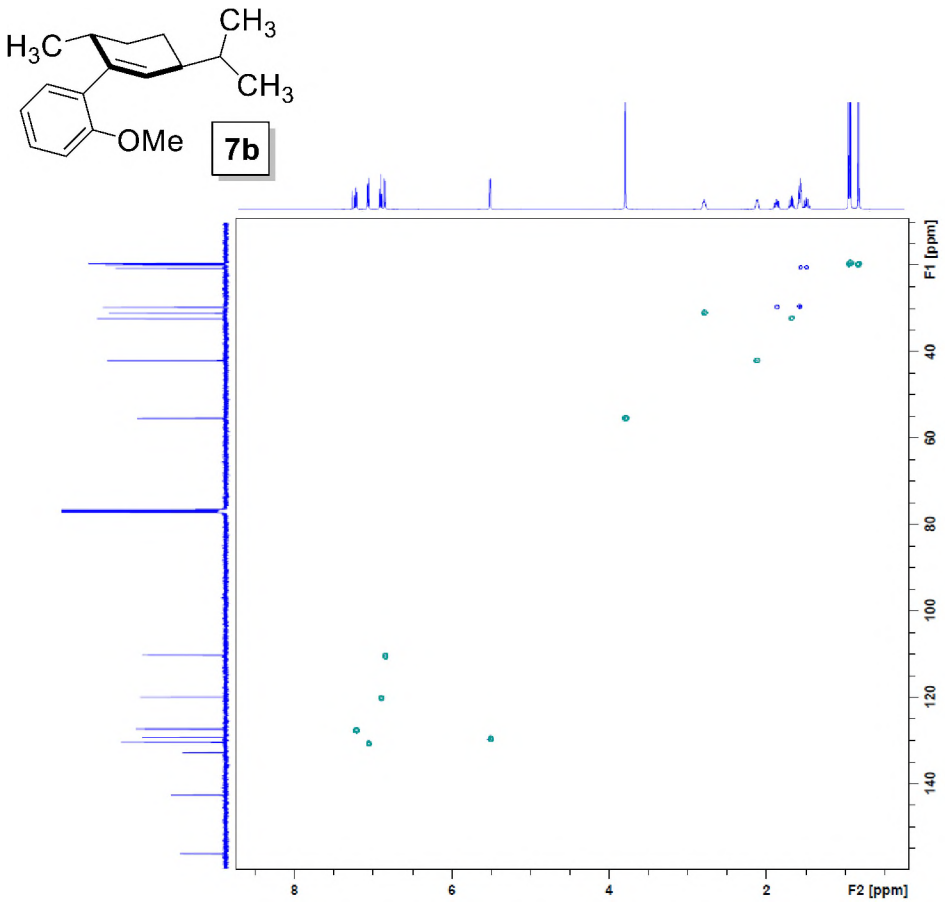

H3C
CH3
CH3
7a
F1 [ppm]
F2 [ppm]

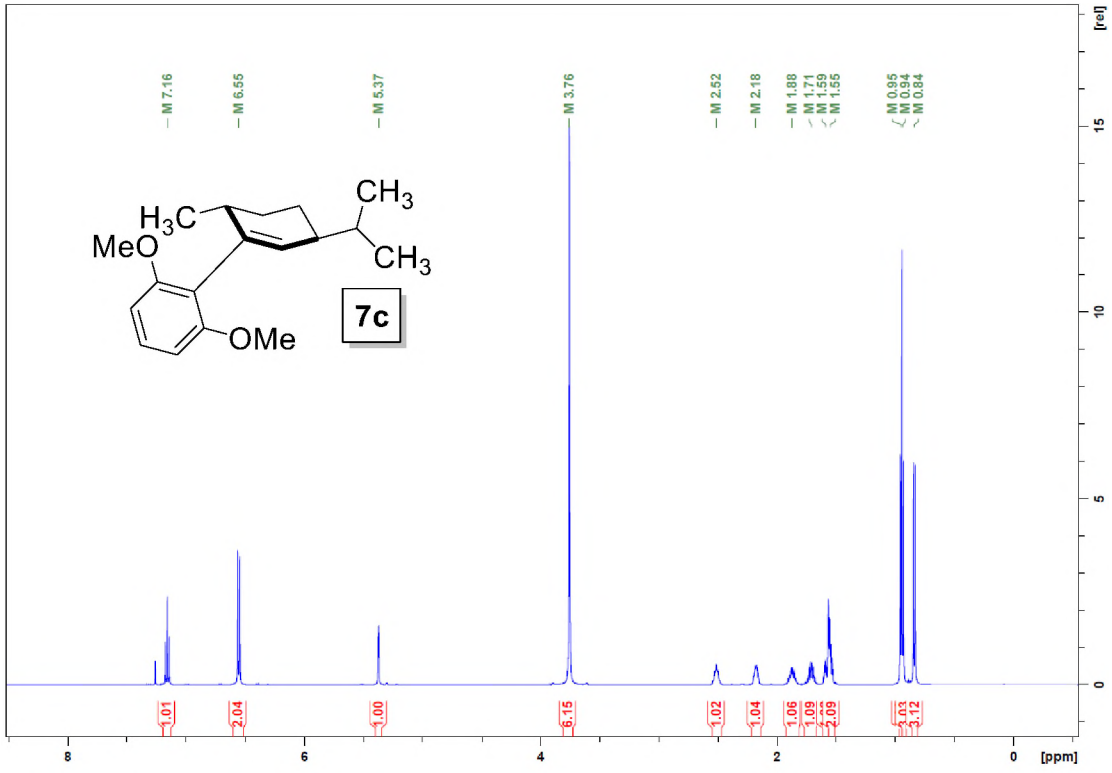

H3C
CH3
CH3
7a
F1 [ppm]
F2 [ppm]

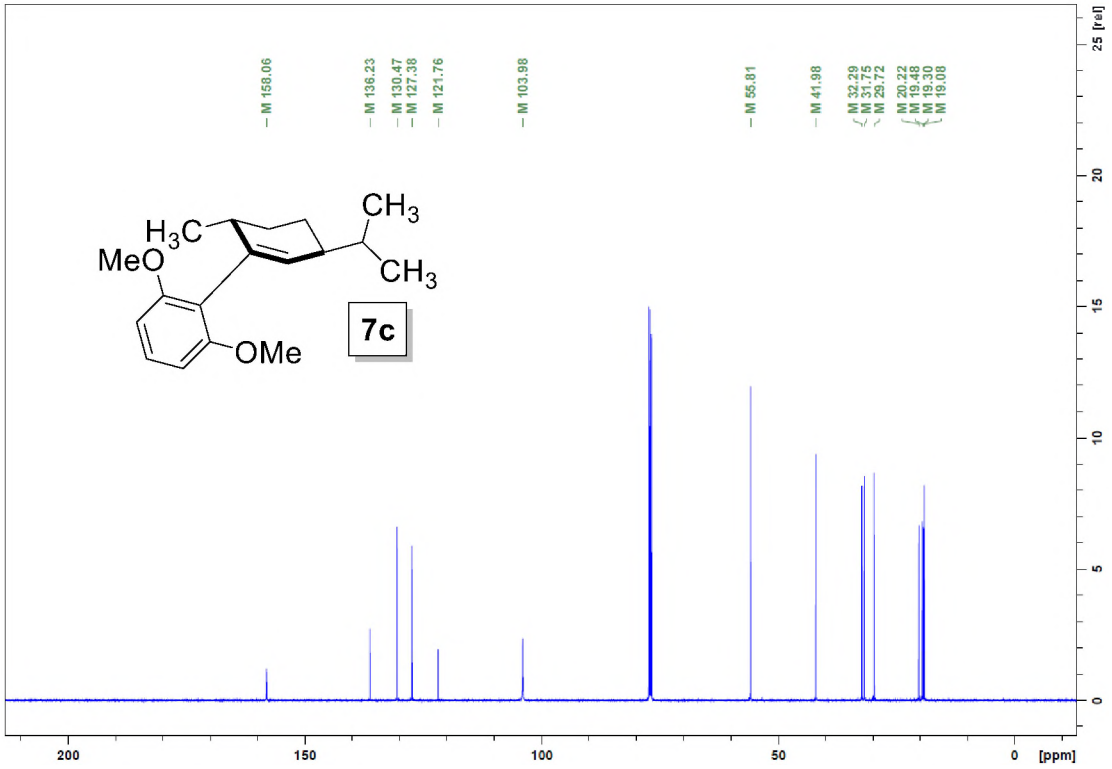

M 7.22
M 7.06
M 6.90
M 6.85
M 5.51
M 3.80
M 2.80
M 2.13
M 1.88
M 1.69
M 1.58
M 1.49
M 0.96
M 0.94
M 0.84
1.01
1.01
2.02
1.01
3.20
1.03
1.03
1.01
1.00
2.11
1.09
3.12
3.22
H3C
CH3
CH3
OMe
7b
[rel]
[ppm]

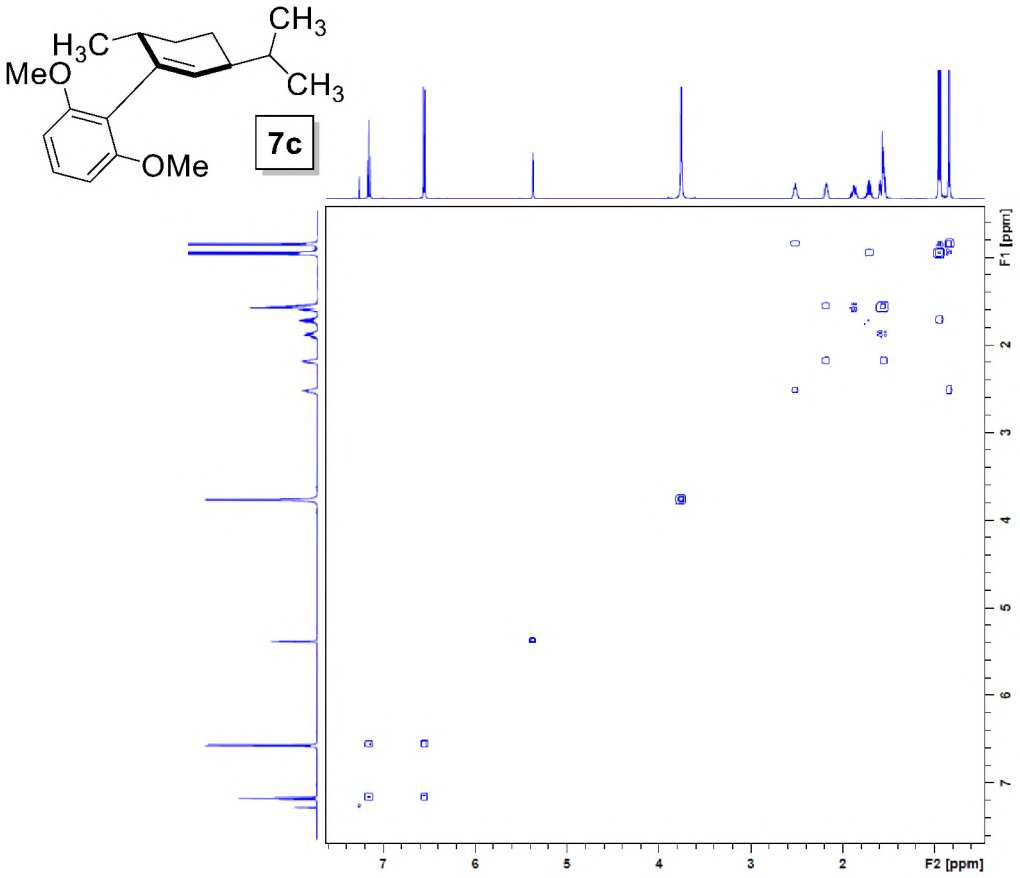

M 156.74
M 143.08
M 133.20
M 130.79
M 129.68
M 127.71
M 120.30
M 110.54
M 55.46
M 42.04
M 32.29
M 31.01
M 29.58
M 20.56
M 19.82
M 19.67
M 19.43
H3C
CH3
CH3
OMe
7b
[rel]
[ppm]

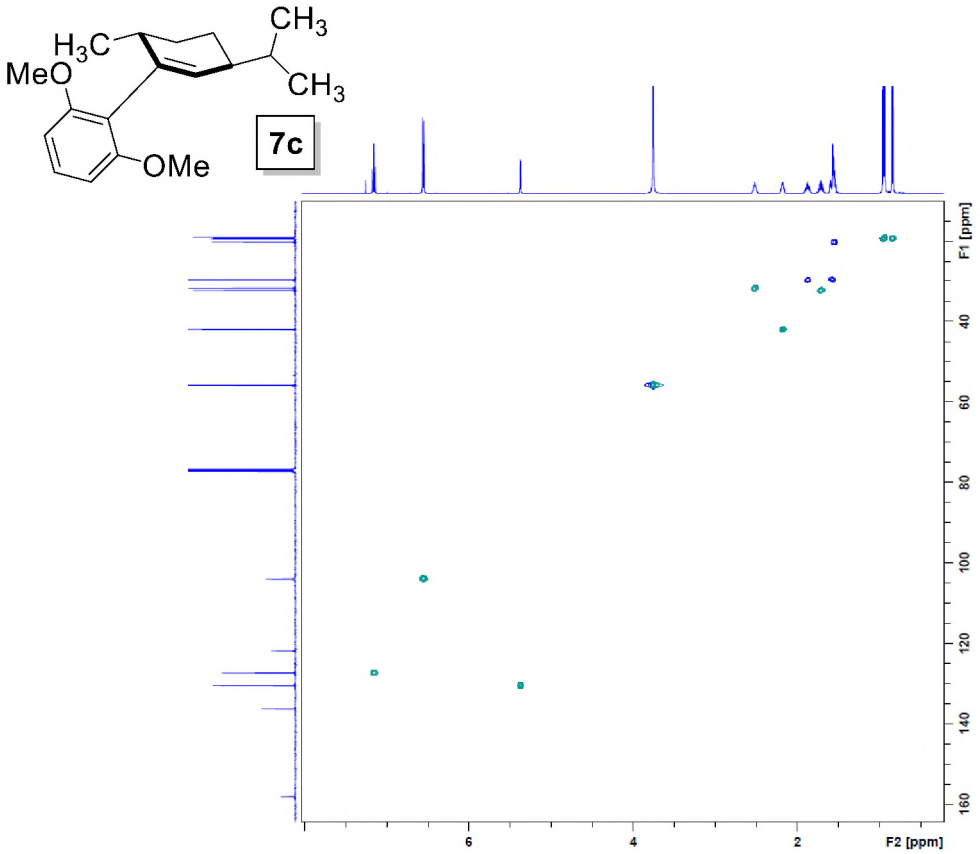

H3C
CH3
CH3
OMe
7b
F1 [ppm]
F2 [ppm]

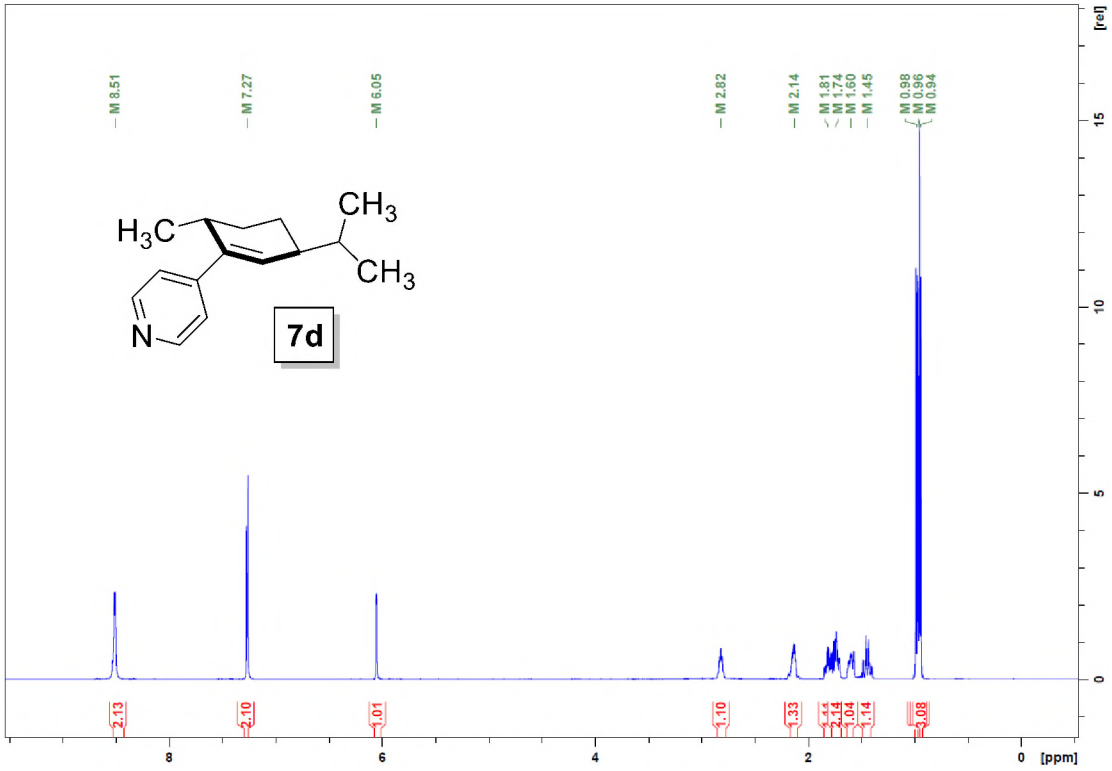

H3C
CH3
CH3
OMe
7b
F1 [ppm]
F2 [ppm]

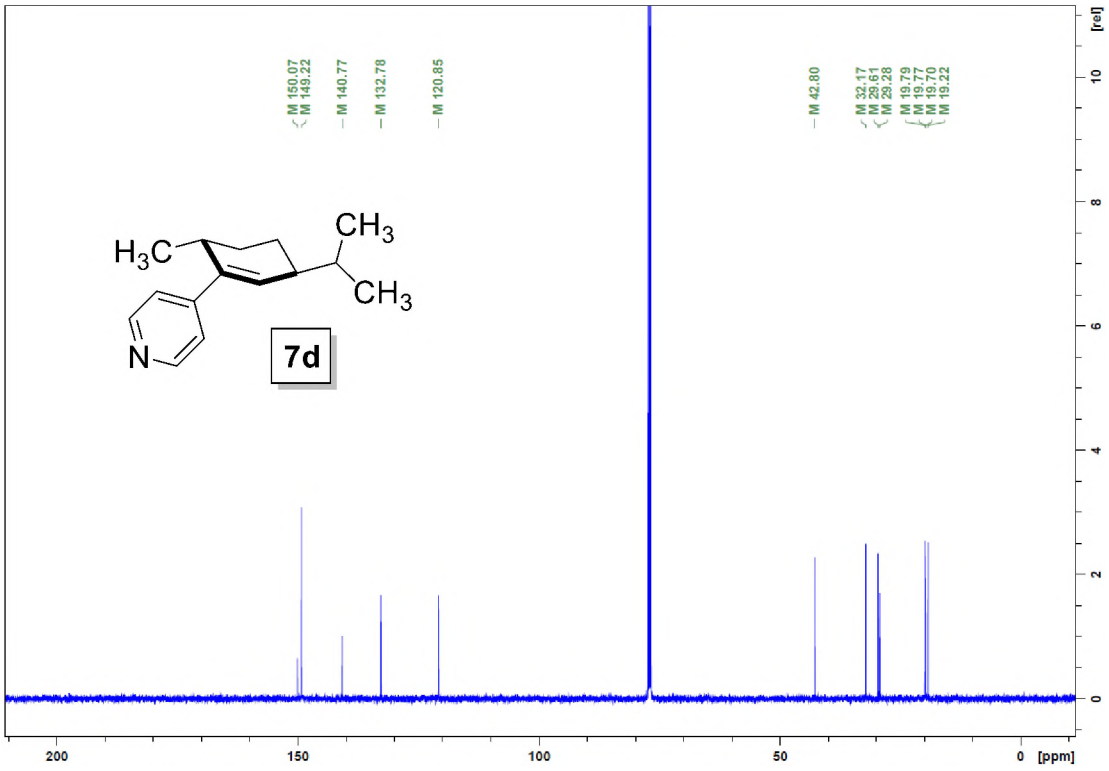

M 7.16
M 6.55
M 5.37
M 3.76
M 2.52
M 2.18
M 1.88
M 1.71
M 1.59
M 1.55
M 0.95
M 0.94
M 0.84
1.01
2.04
1.00
6.15
1.02
1.04
1.06
1.09
2.09
3.03
3.12
[rel]
[ppm]
H3C
MeO
CH3
CH3
OMe
7c

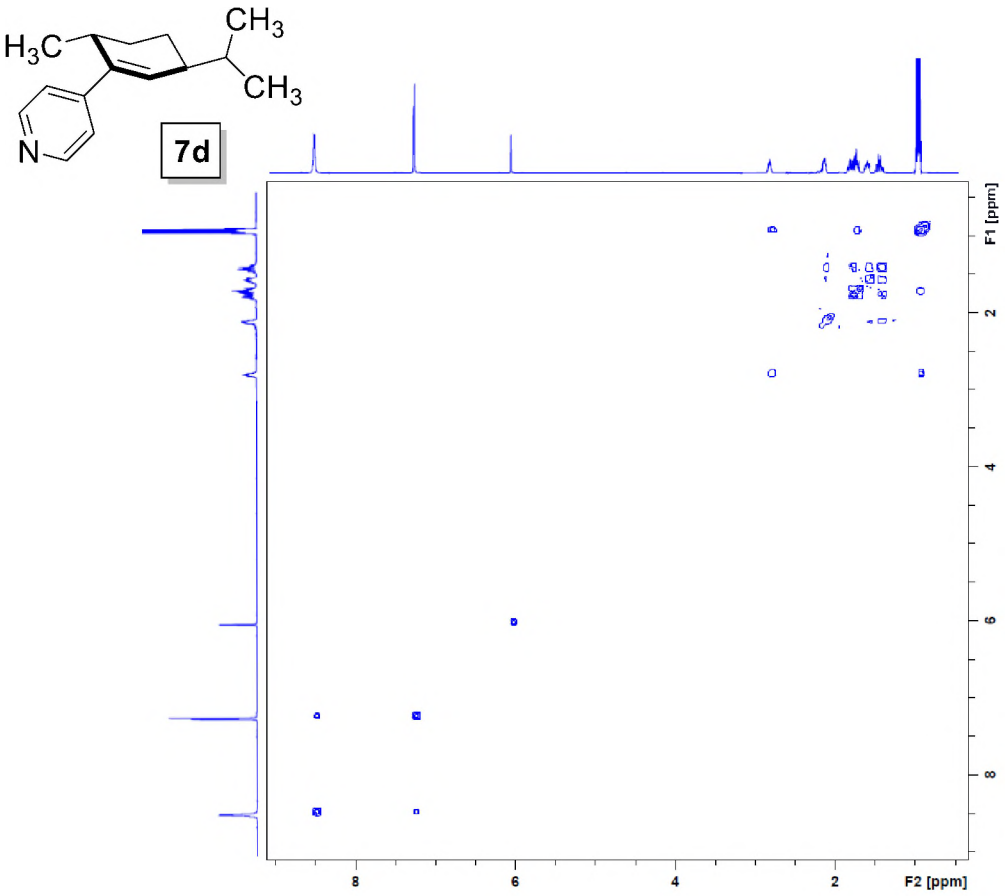

M 158.06
M 136.23
M 130.47
M 127.38
M 121.76
M 103.98
M 55.81
M 41.98
M 32.29
M 31.75
M 29.72
M 20.22
M 19.48
M 19.30
M 19.08
[rel]
[ppm]
H3C
MeO
CH3
CH3
OMe
7c

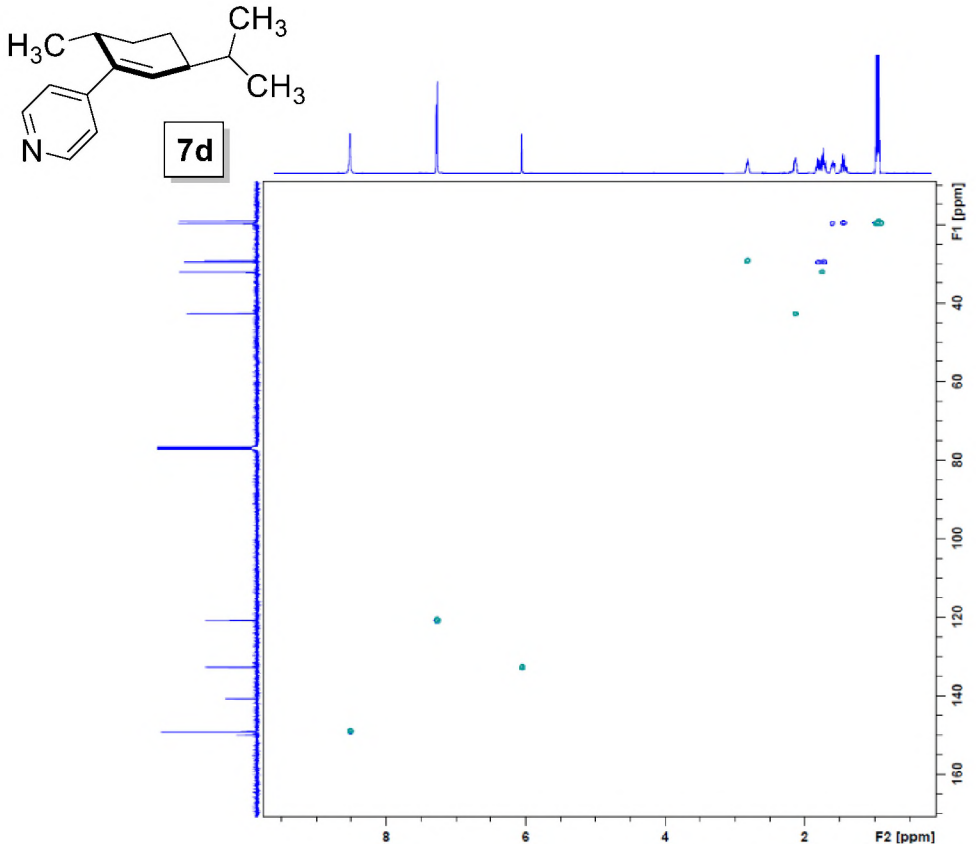

H3C
MeO
CH3
CH3
OMe
7c
F1 [ppm]
F2 [ppm]

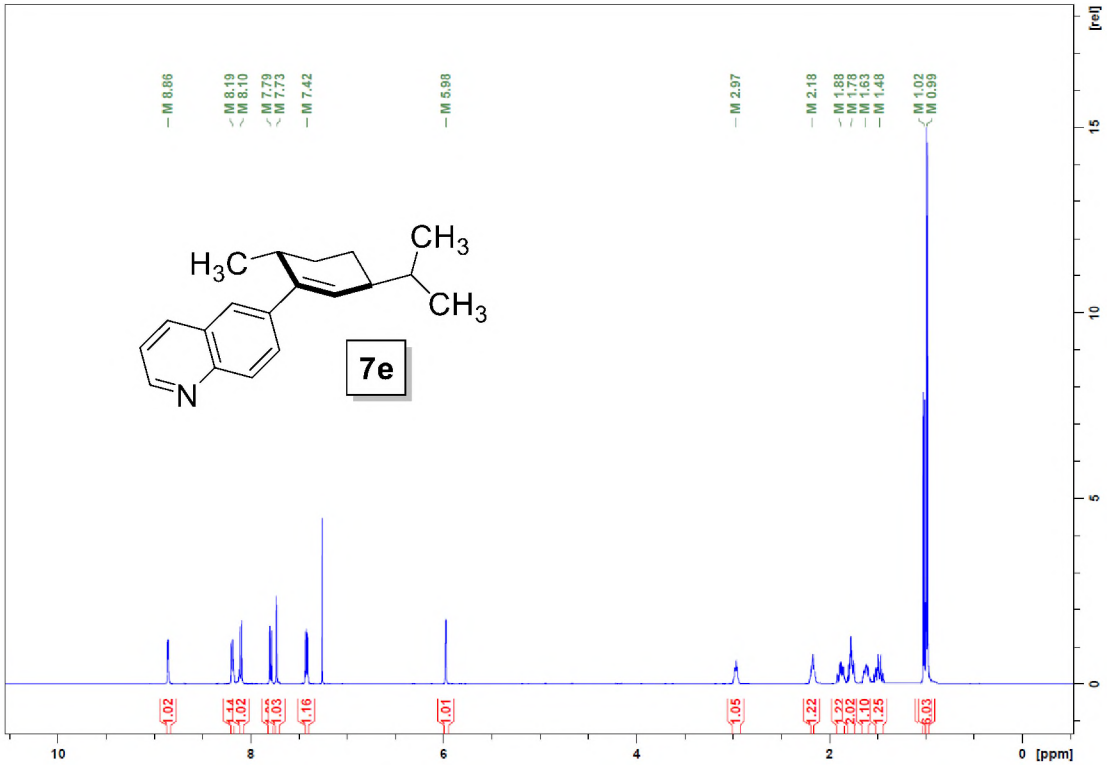

H3C
MeO
CH3
CH3
OMe
7c
F1 [ppm]
F2 [ppm]

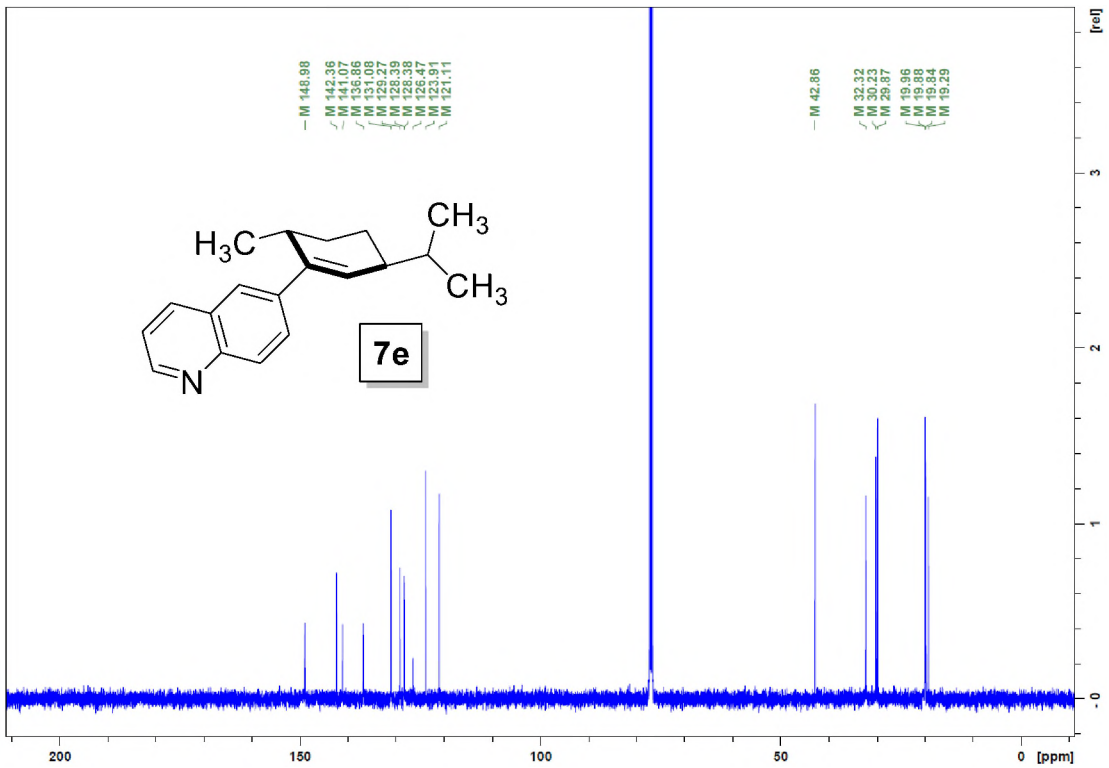

M 8.51
M 7.27
M 6.05
M 2.82
M 2.14
M 1.81
M 1.74
M 1.60
M 1.45
M 0.98
M 0.96
M 0.94
H3C
CH3
CH3
N
7d
2.13
2.10
1.01
1.10
1.33
2.14
1.04
1.14
3.08
8
6
4
2
0
[ppm]
[rel]

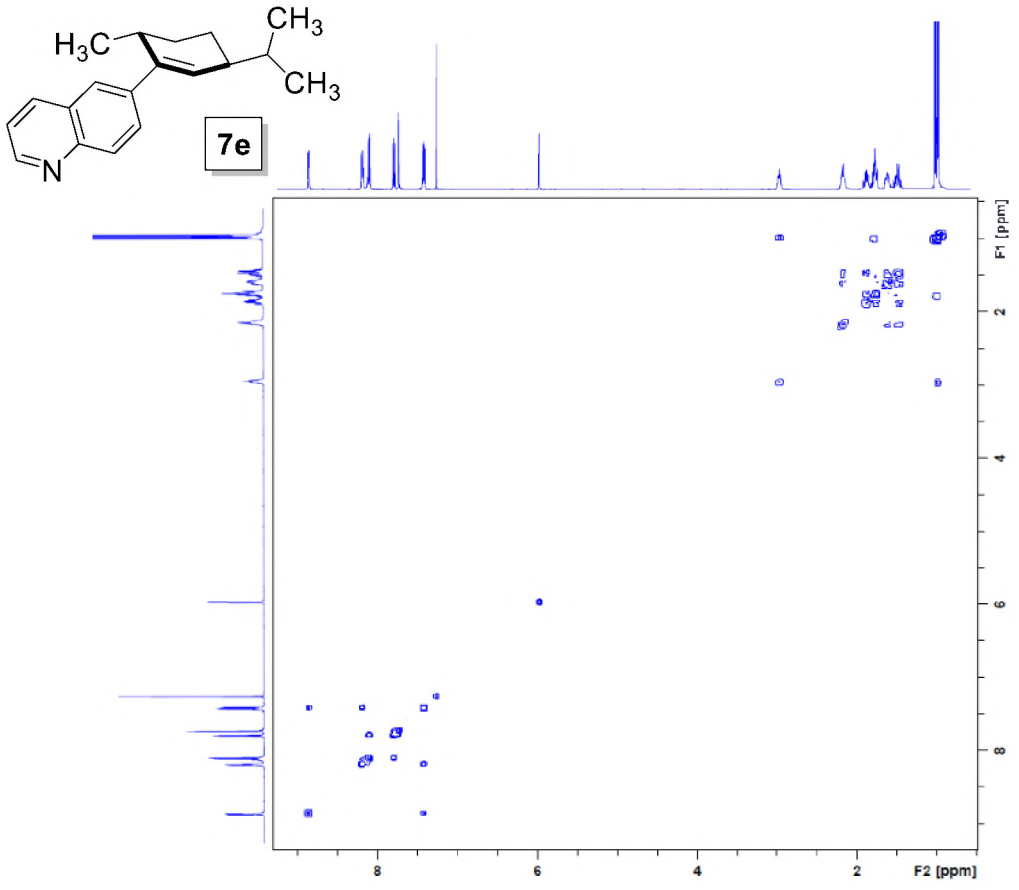

M 150.07
M 149.22
M 140.77
M 132.78
M 120.85
M 42.80
M 32.17
M 29.61
M 29.28
M 19.79
M 19.77
M 19.70
M 19.22
H3C
CH3
CH3
N
7d
200
150
100
50
0
[ppm]
[rel]

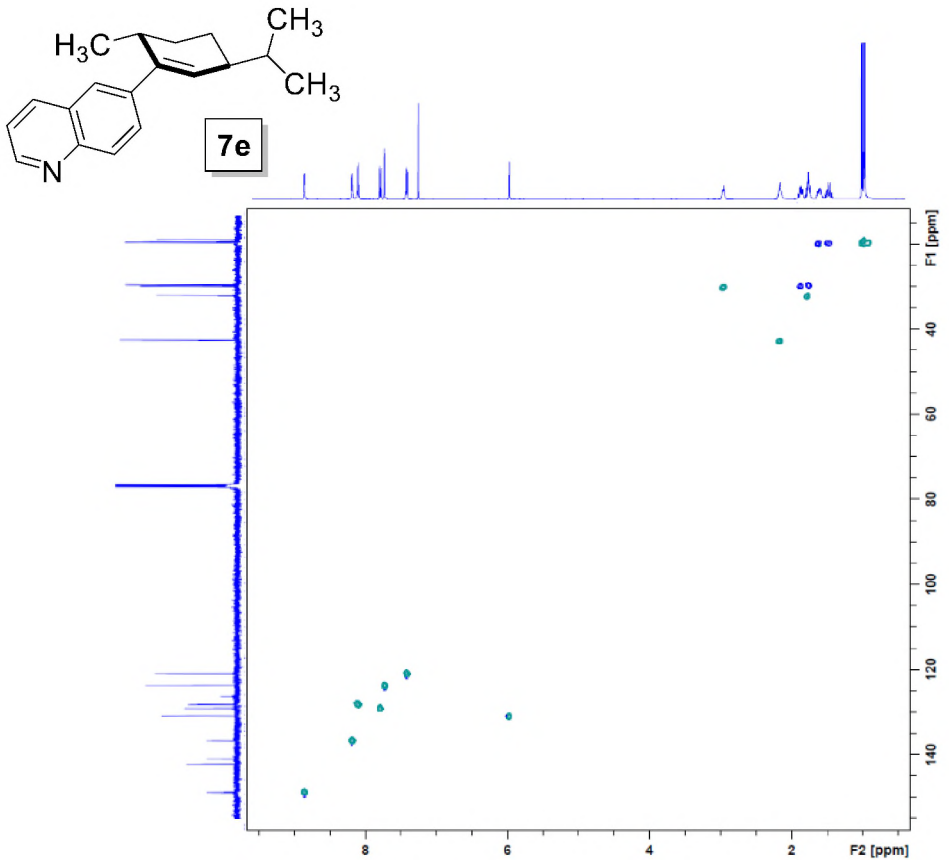

H3C
CH3
CH3
N
7d
F1 [ppm]
F2 [ppm]

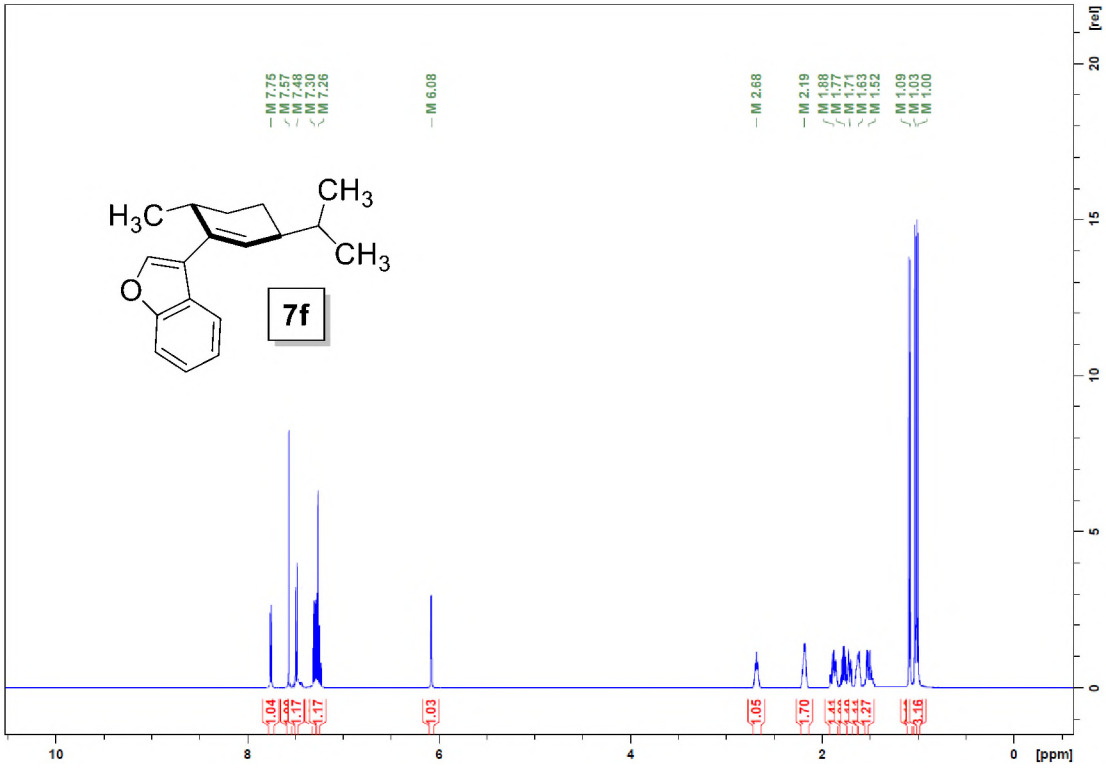

H3C
CH3
CH3
N
7d
F1 [ppm]
F2 [ppm]

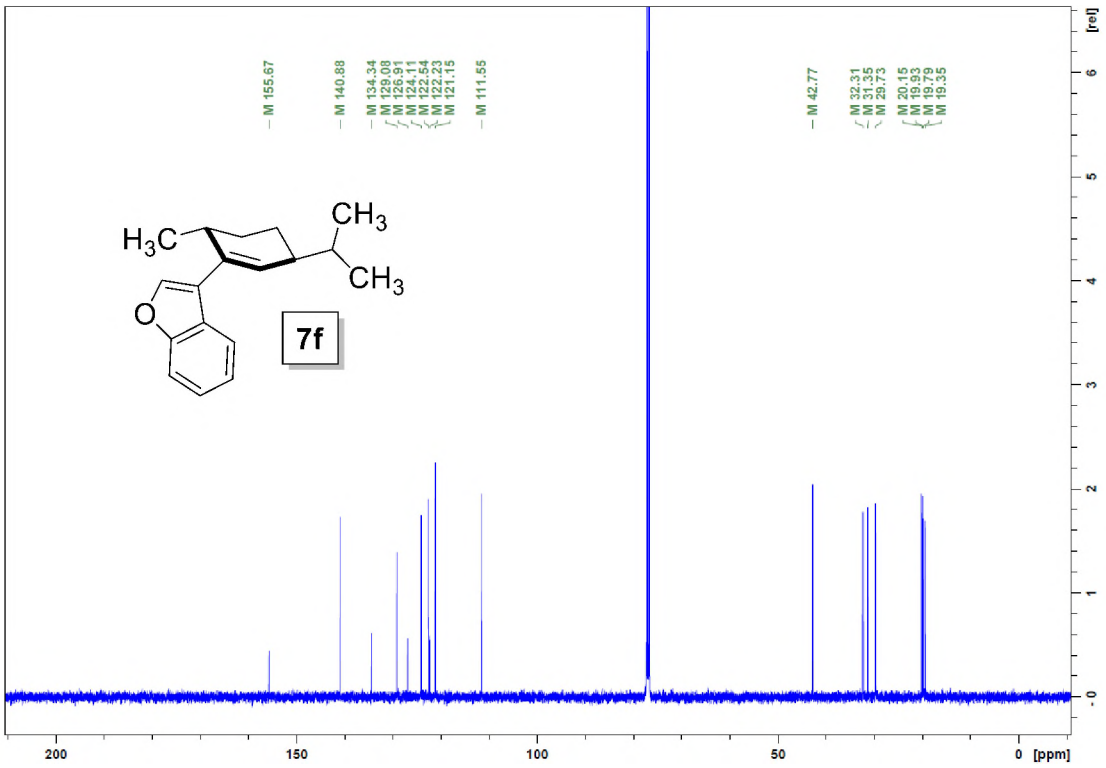

M 8.86
M 8.19
M 8.10
M 7.79
M 7.73
M 7.42
M 5.98
M 2.97
M 2.18
M 1.88
M 1.73
M 1.53
M 1.48
M 1.02
M 0.99
H3C
CH3
CH3
N
7e
[rel]
[ppm]

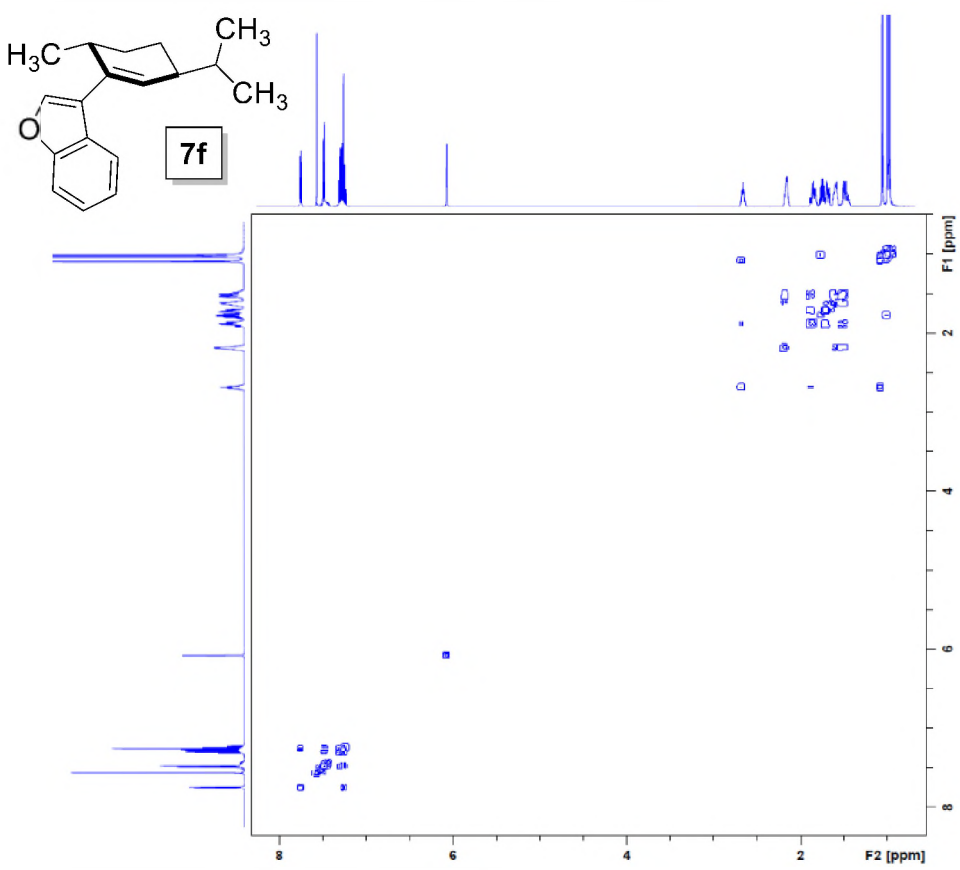

M 148.98
M 142.36
M 141.07
M 136.86
M 131.08
M 129.27
M 128.39
M 128.38
M 126.47
M 123.91
M 121.11
M 42.86
M 32.32
M 30.23
M 29.87
M 19.96
M 19.88
M 19.84
M 19.29
H3C
CH3
CH3
N
7e
[rel]
[ppm]

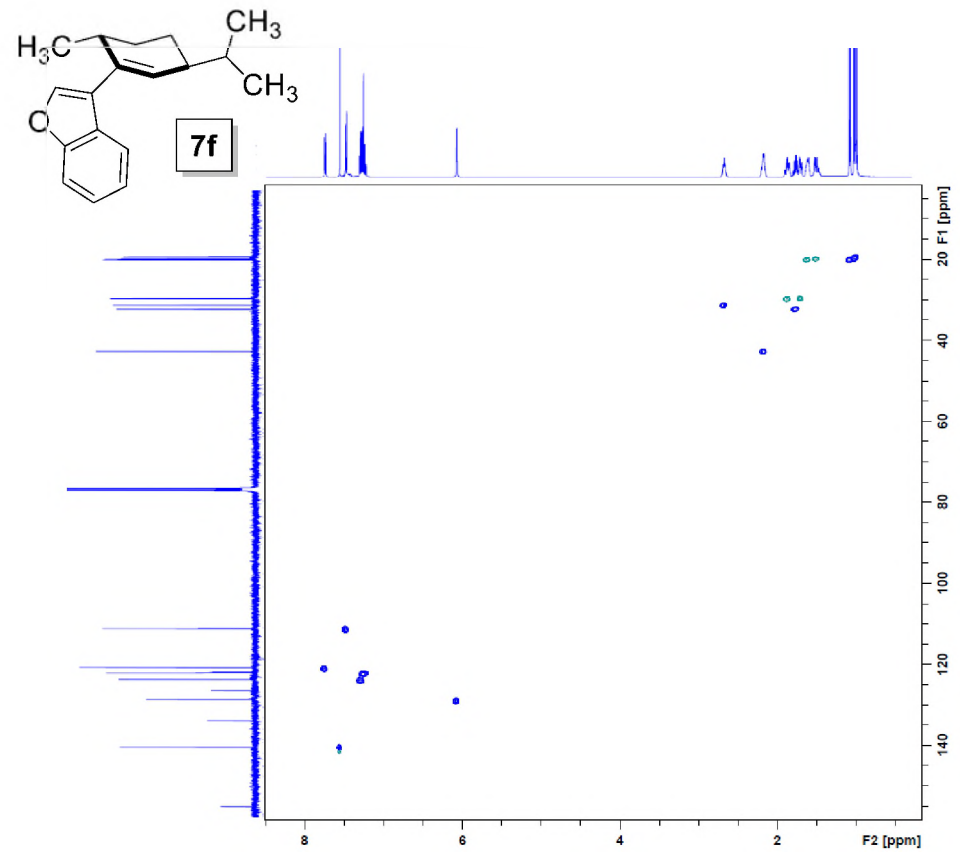

H3C
CH3
CH3
N
7e
F1 [ppm]
F2 [ppm]

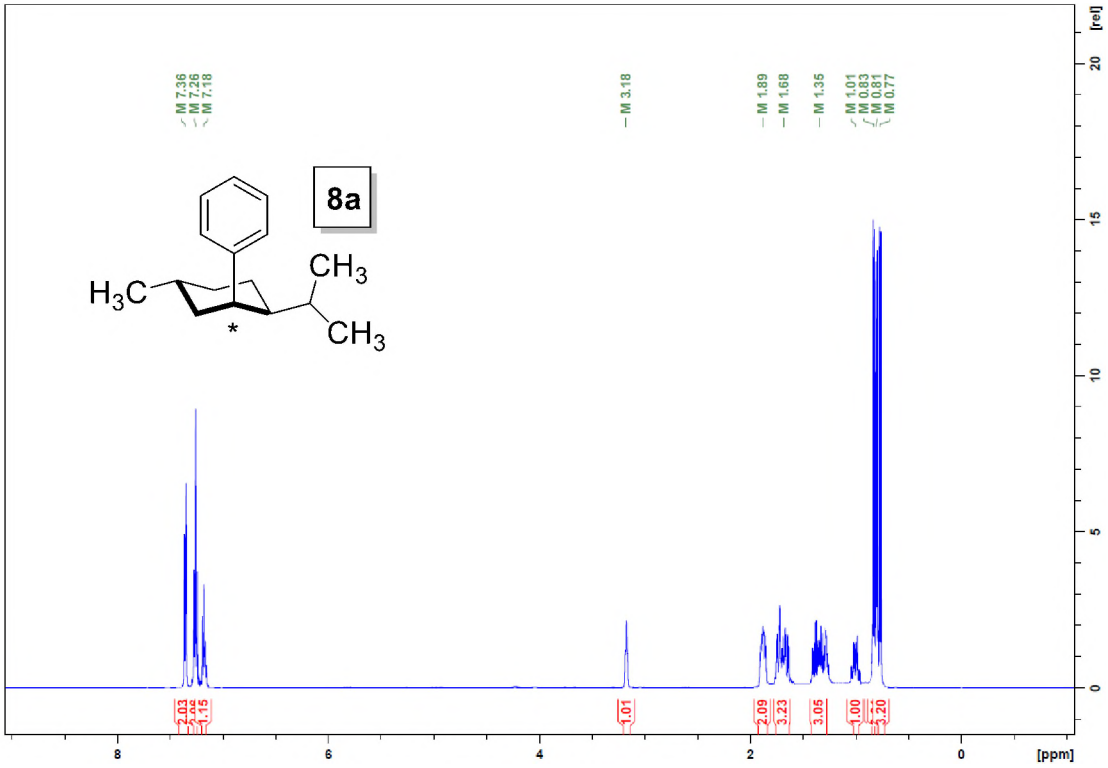

H3C
CH3
CH3
N
7e
F1 [ppm]
F2 [ppm]

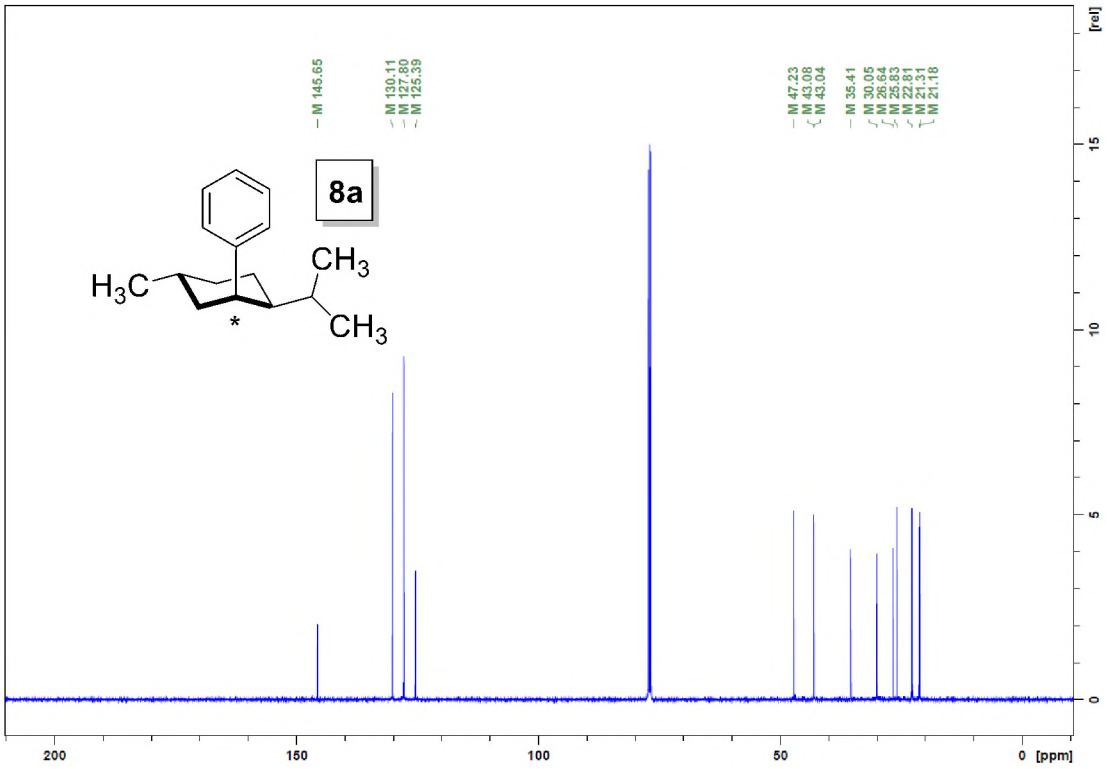

M 7.75
M 7.57
M 7.48
M 7.30
M 7.26
M 6.08
M 2.68
M 2.19
M 1.88
M 1.77
M 1.71
M 1.63
M 1.52
M 1.09
M 1.03
M 1.00
H3C
CH3
CH3
O
7f
1.04
1.17
1.17
1.03
1.05
1.70
1.27
3.16
10
8
6
4
2
0
[ppm]
[rel]

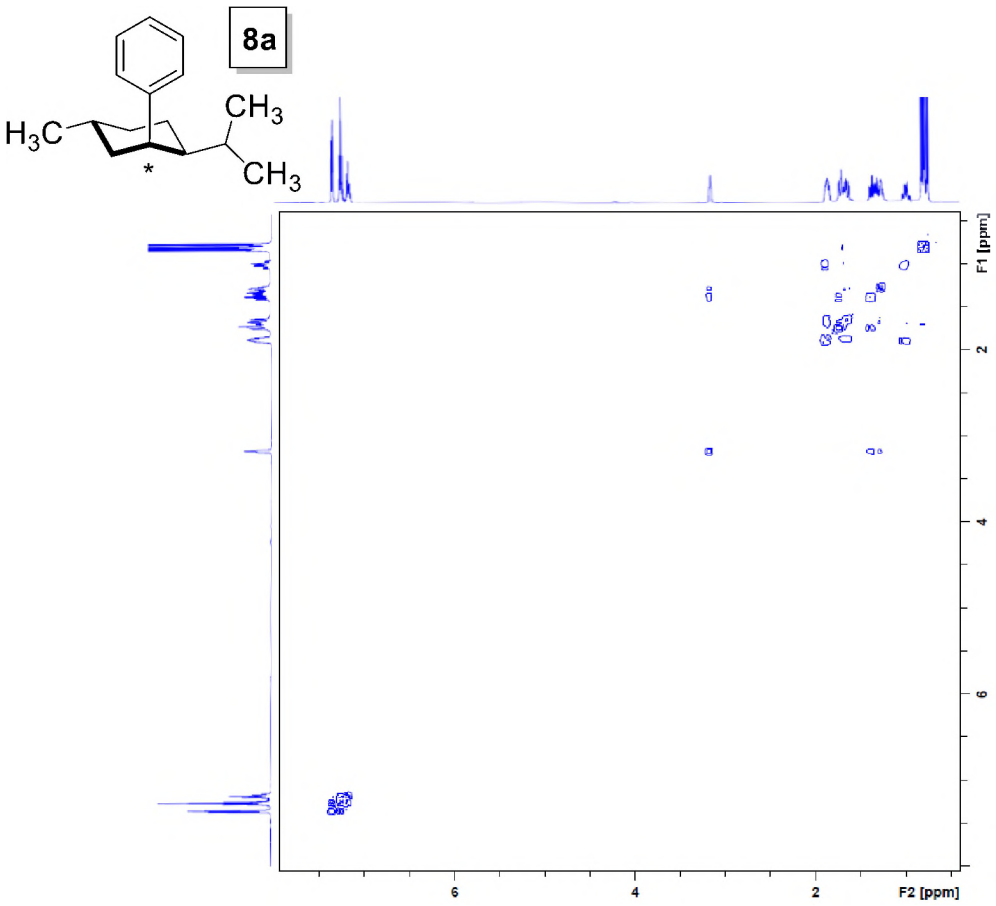

M 155.67
M 140.88
M 134.34
M 129.08
M 126.91
M 124.11
M 122.54
M 122.23
M 121.15
M 111.55
M 42.77
M 32.31
M 31.35
M 29.73
M 20.15
M 19.93
M 19.79
M 19.35
H3C
CH3
CH3
O
7f
200
150
100
50
0
[ppm]
[rel]

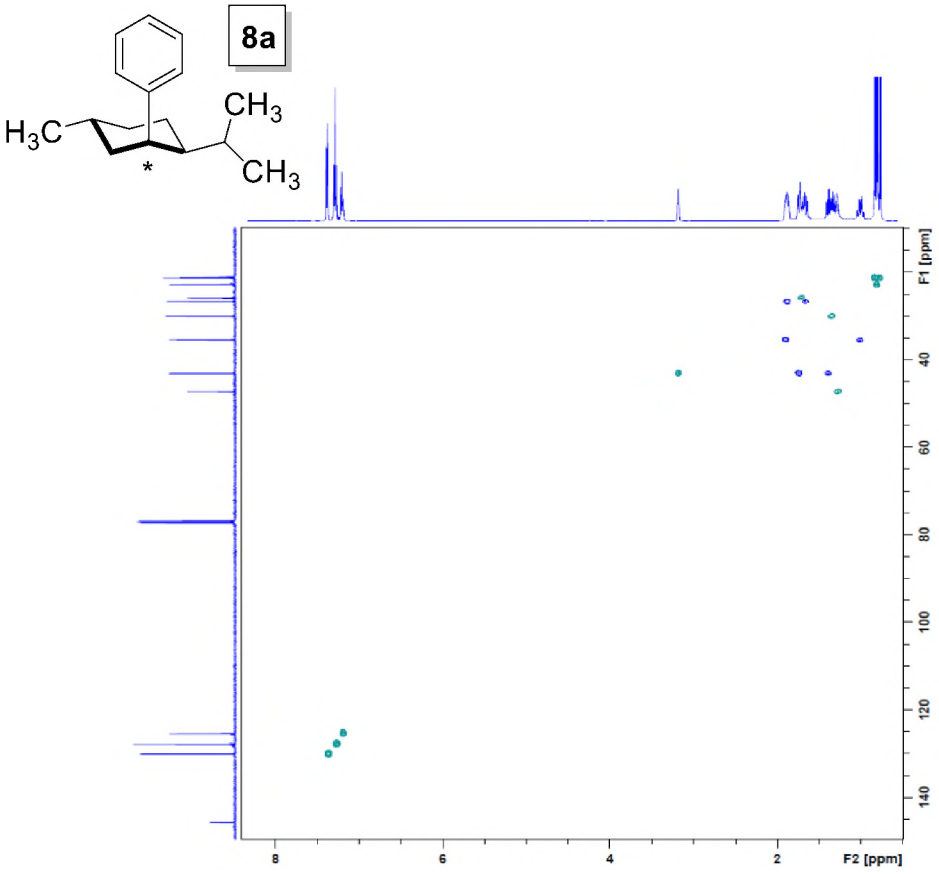

H3C
CH3
CH3
O
7f
F1 [ppm]
F2 [ppm]

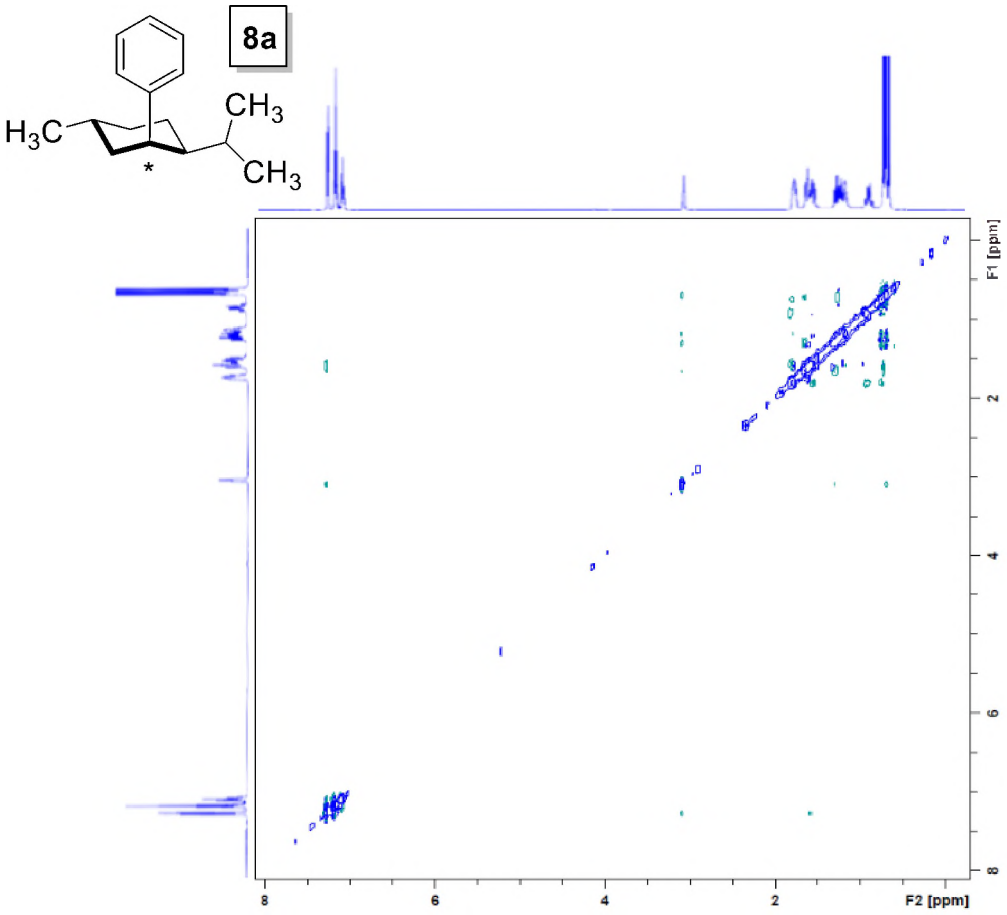

H3C
CH3
CH3
O
7f
F1 [ppm]
F2 [ppm]

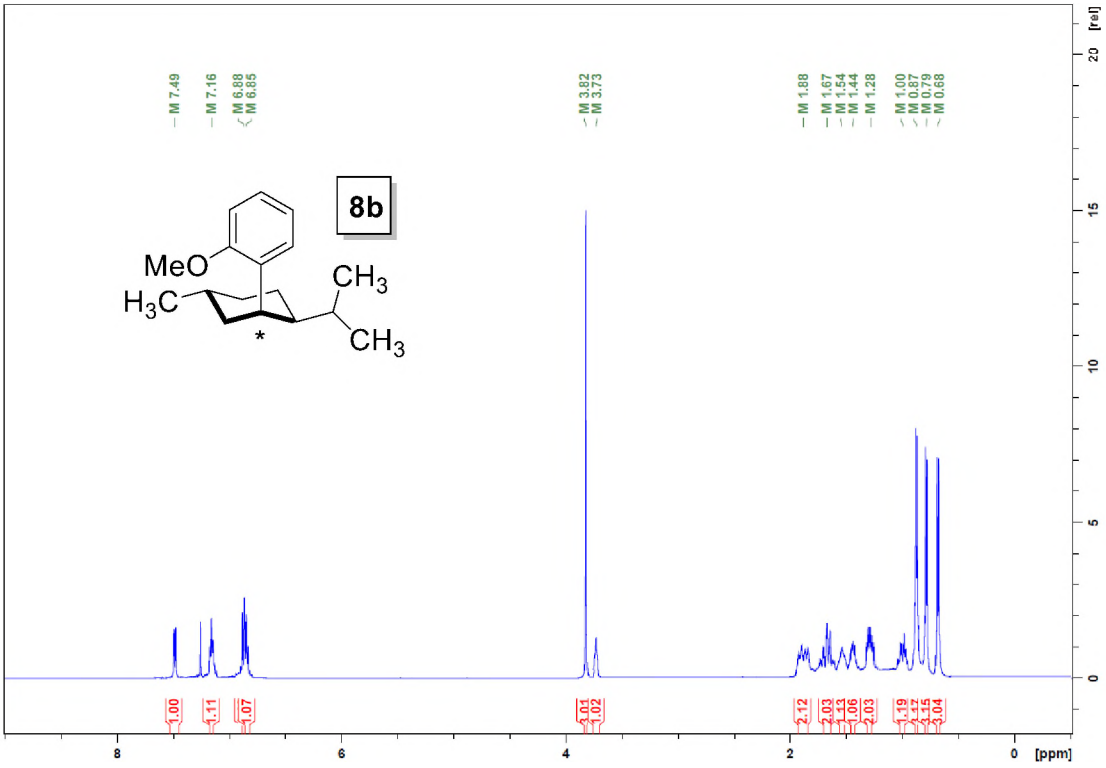

M 7.36
M 7.26
M 7.18
M 3.18
M 1.89
M 1.68
M 1.35
M 1.01
M 0.93
M 0.91
M 0.77
8a
H3C
CH3
CH3
*
2.03
2.04
1.15
1.01
2.09
3.23
3.06
1.00
3.20
[rel]
[ppm]

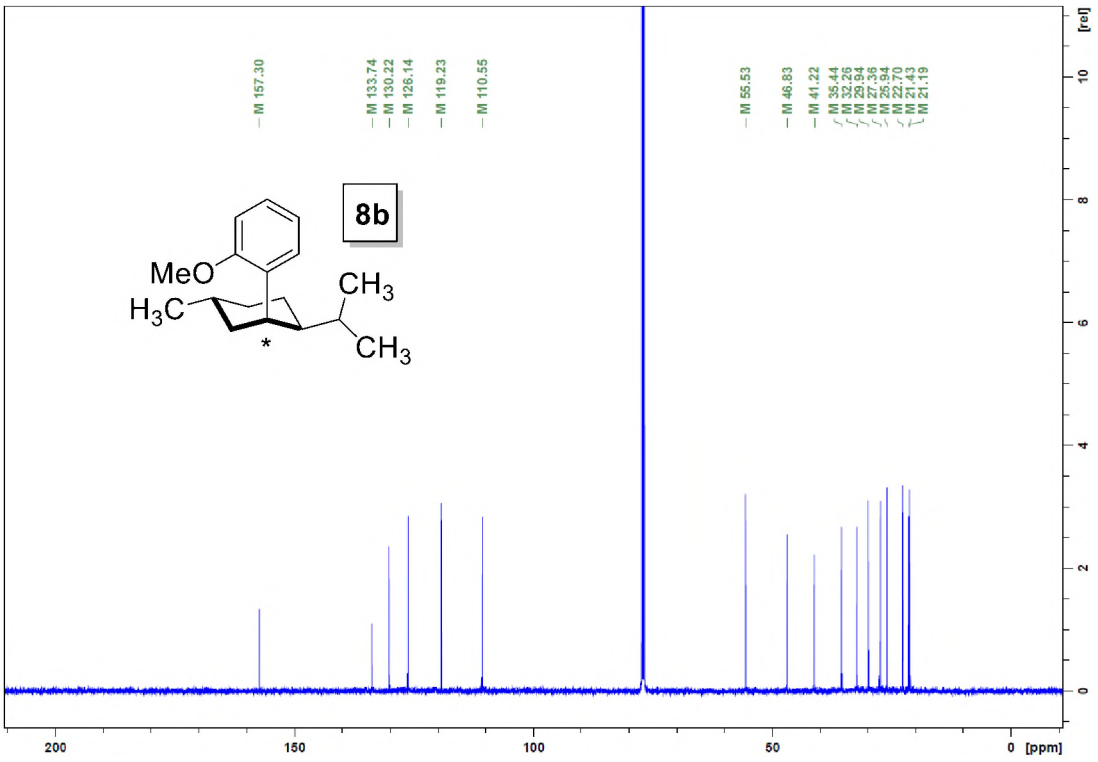

M 145.65
M 130.11
M 127.80
M 125.39
M 47.23
M 43.08
M 43.04
M 35.41
M 30.05
M 26.64
M 25.83
M 22.81
M 21.31
M 21.18
8a
H3C
CH3
CH3
*
[rel]
[ppm]

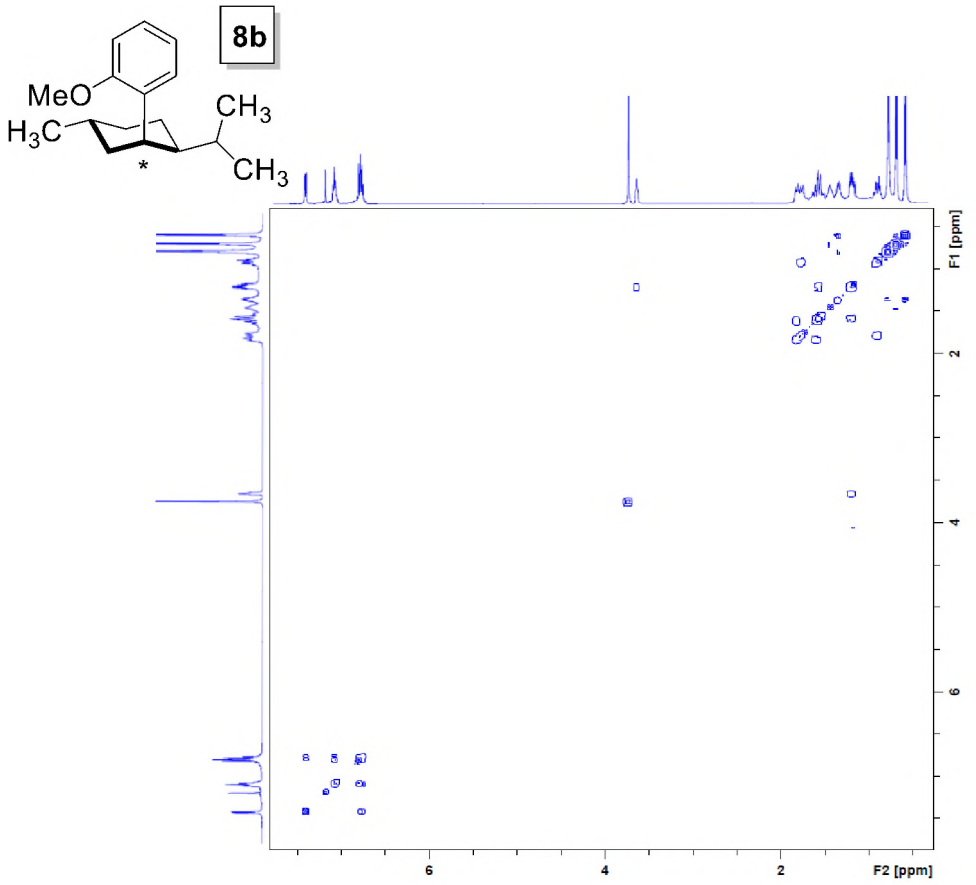

8a
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
2
4
6
6
4
2

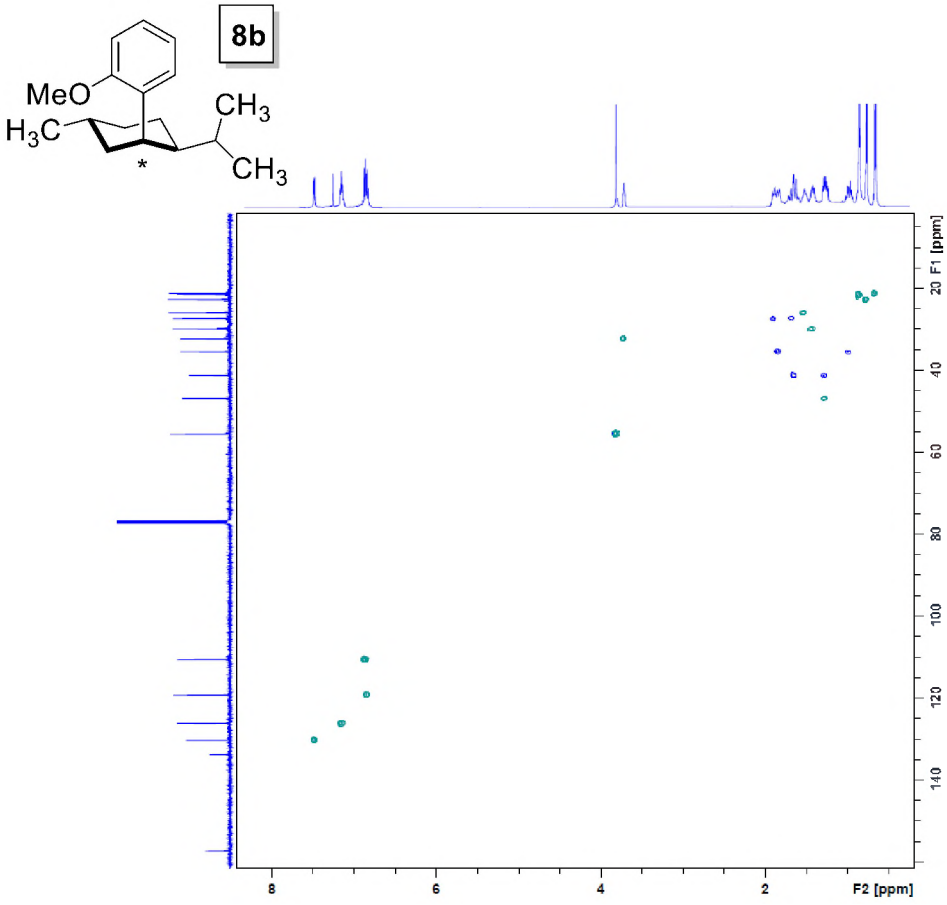

8a
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
40
60
80
100
120
140
8
6
4
2

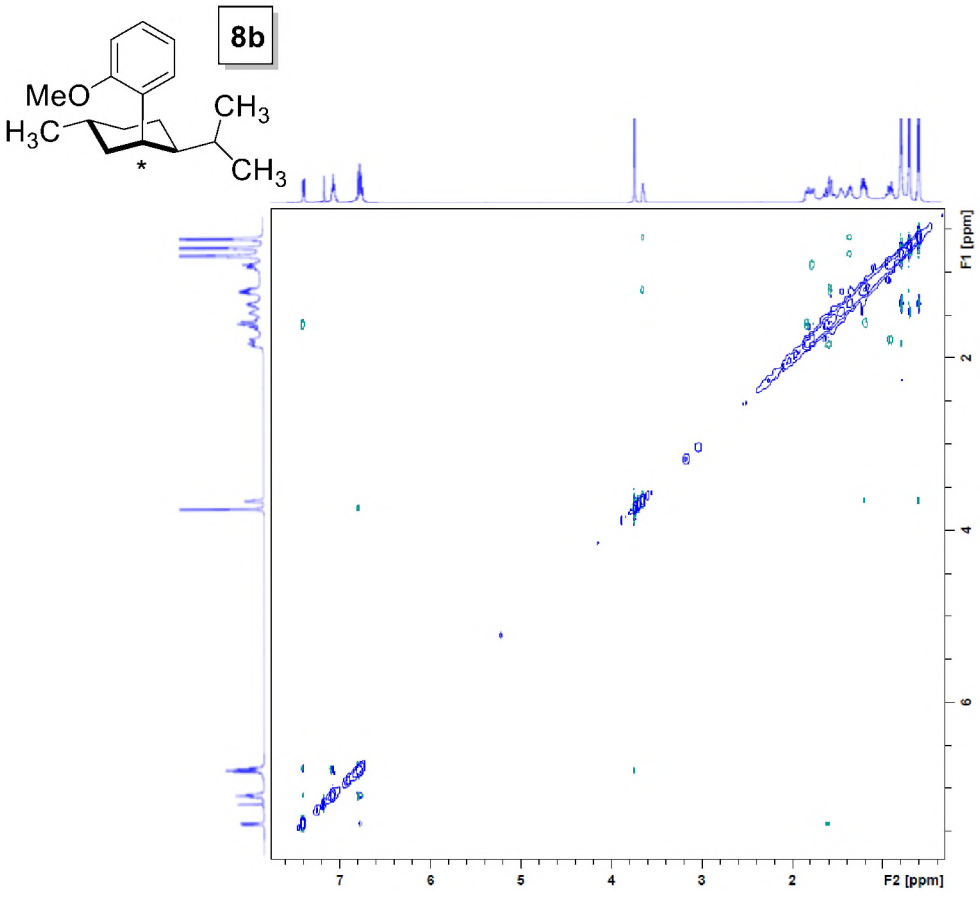

8a
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
2
4
6
8

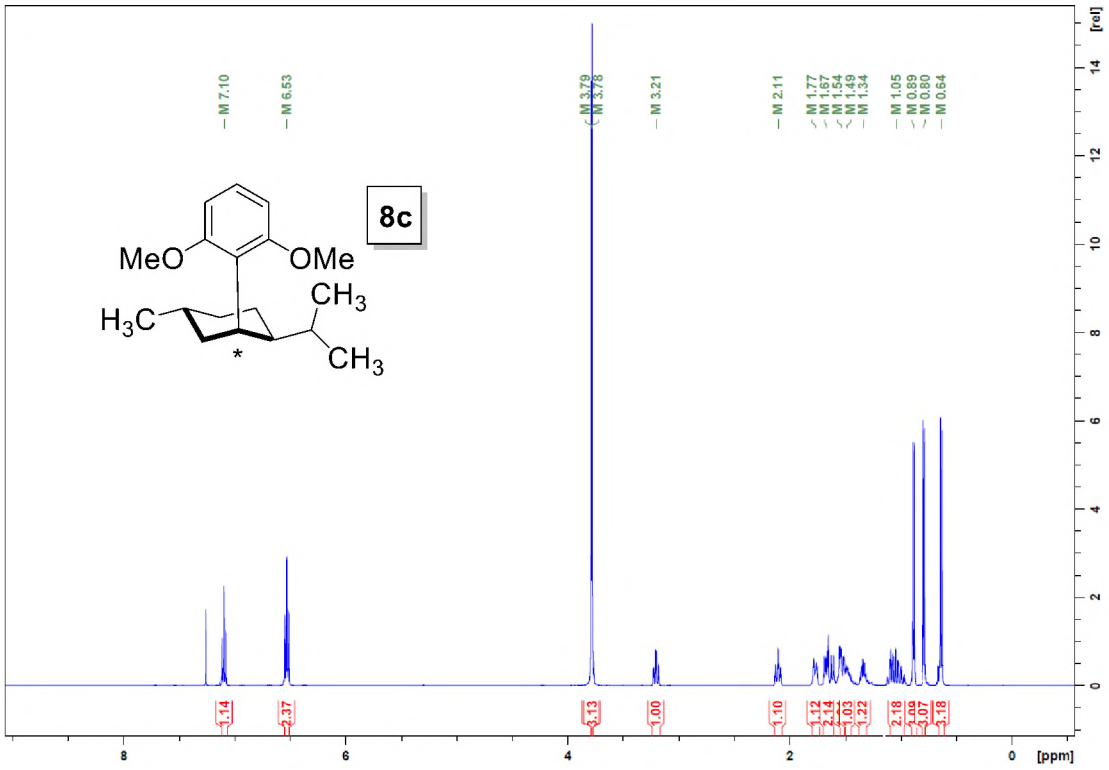

M 7.49
M 7.16
M 6.88
M 6.85
M 3.82
M 3.73
M 1.88
M 1.67
M 1.54
M 1.44
M 1.28
M 1.00
M 0.87
M 0.79
M 0.68
8b
MeO
H3C
CH3
CH3
*
1.00
1.11
1.07
2.01
1.02
2.12
2.03
1.13
1.06
2.03
1.19
0.17
0.15
3.04
8
6
4
2
0
[ppm]
20
15
10
5
0
[rel]

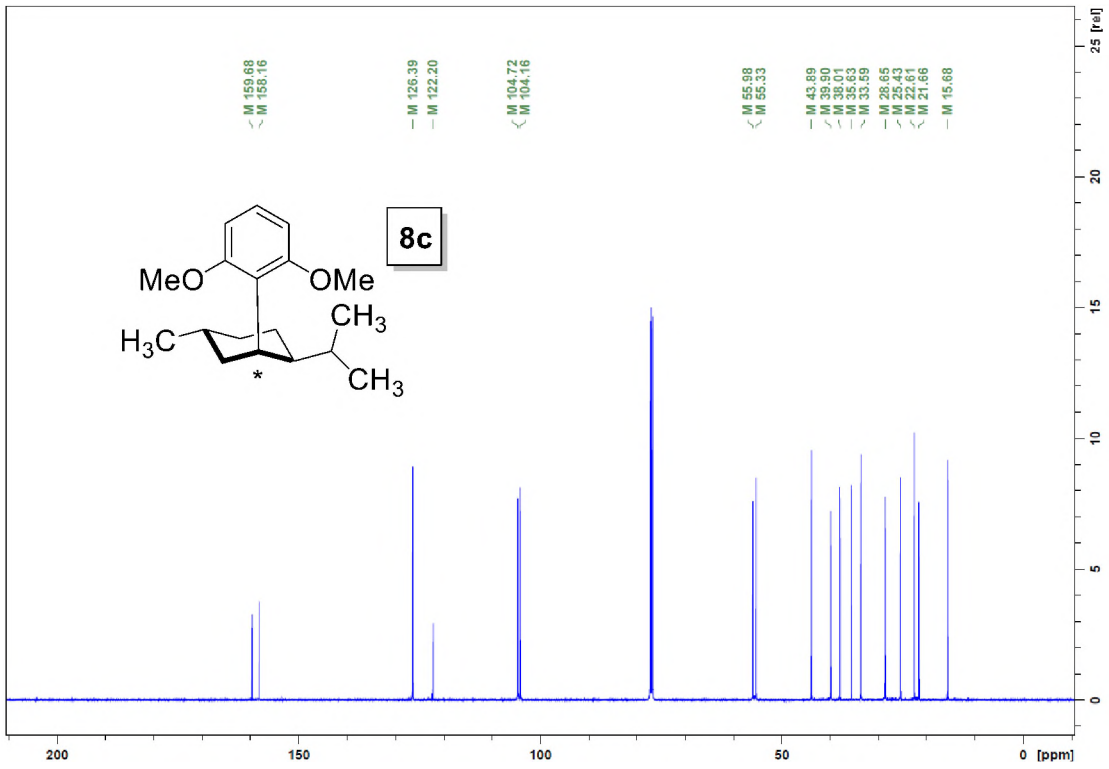

M 157.30
M 133.74
M 130.22
M 126.14
M 119.23
M 110.55
M 55.53
M 46.83
M 41.22
M 35.44
M 32.26
M 29.94
M 27.36
M 25.54
M 23.70
M 21.43
M 21.19
8b
MeO
H3C
CH3
CH3
*
200
150
100
50
0
[ppm]
10
8
6
4
2
0
[rel]

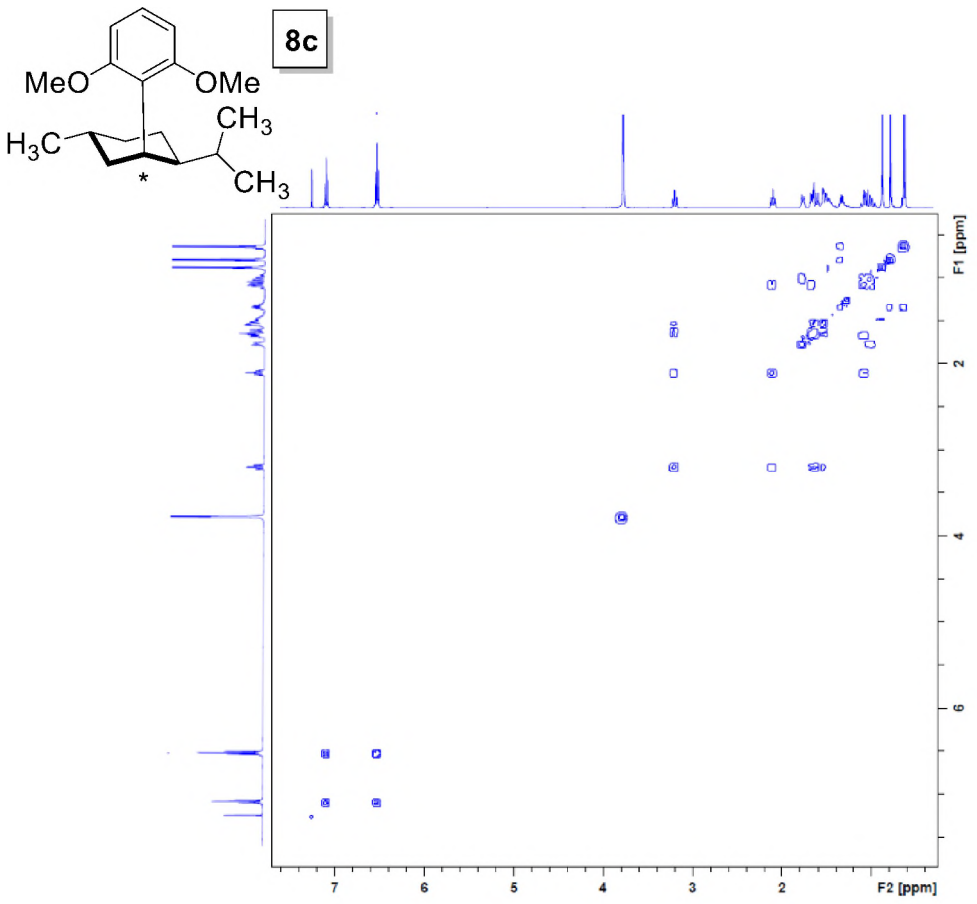

8b
MeO
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]

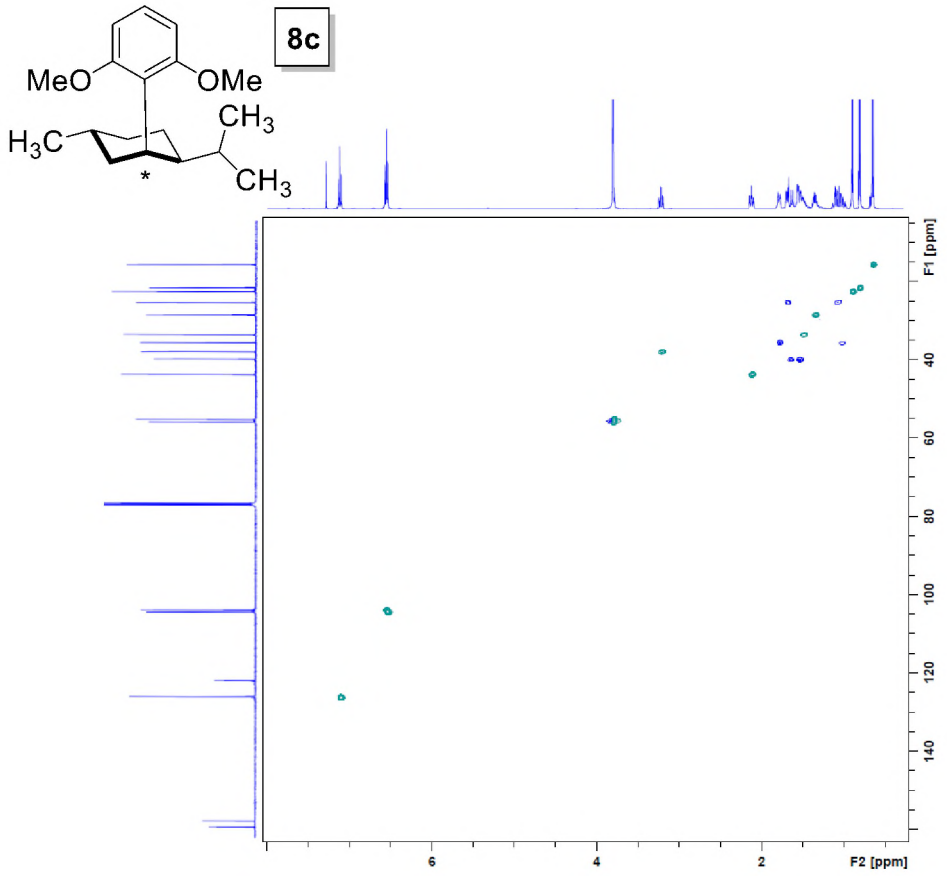

8b
MeO
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]

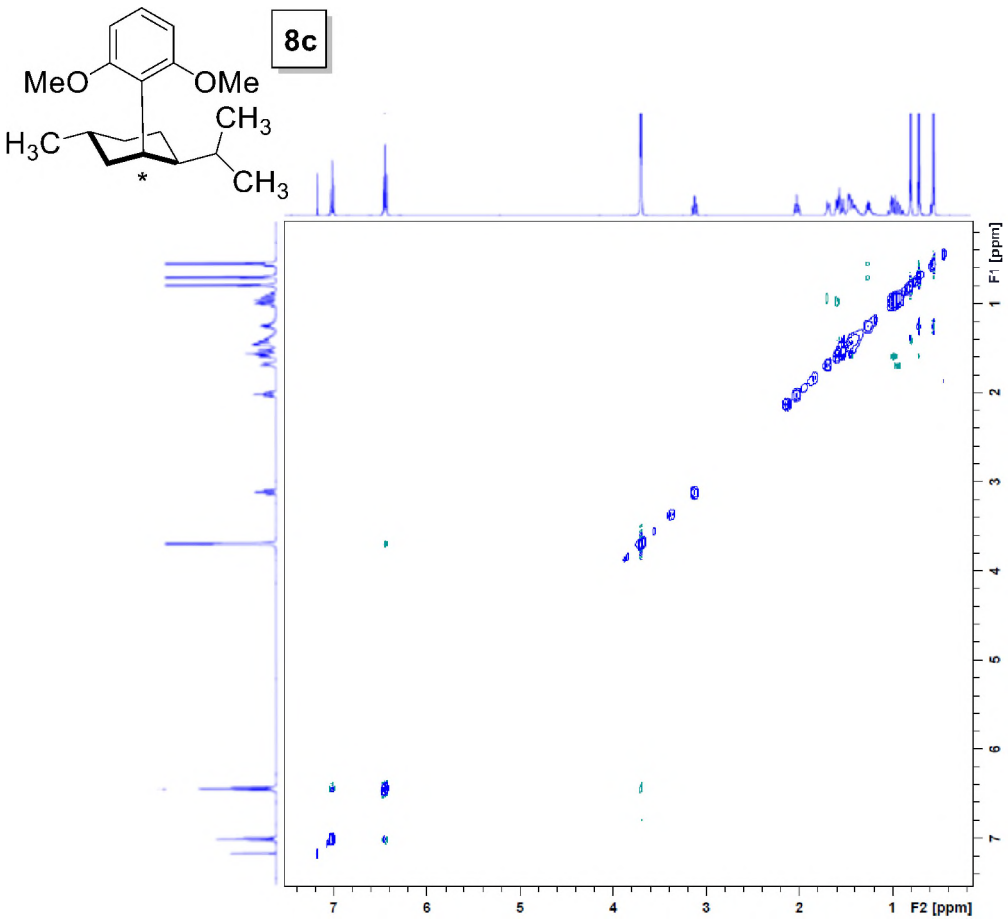

8b
MeO
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
2
4
6
7
6
5
4
3
2

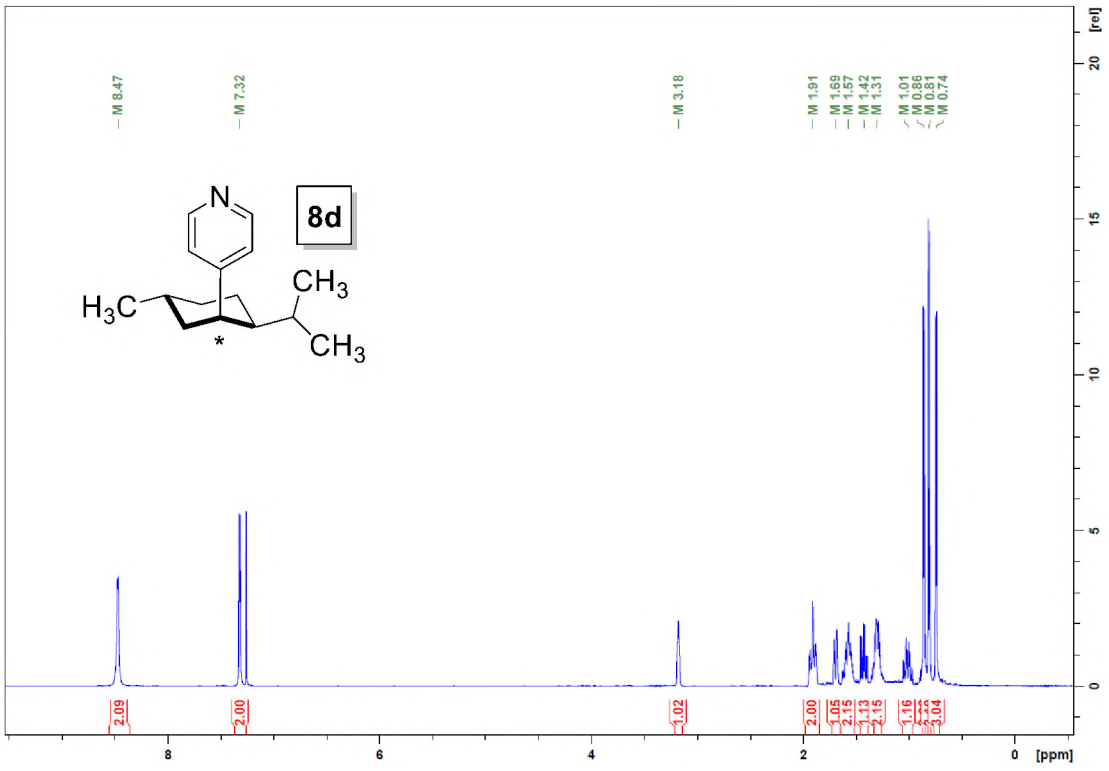

8c
MeO
OMe
H3C
CH3
CH3
*
M 7.10
M 6.53
M 3.79
M 3.78
M 3.21
M 2.11
M 1.77
M 1.67
M 1.54
M 1.49
M 1.34
M 1.05
M 0.89
M 0.80
M 0.64
1.14
2.37
3.13
1.00
1.10
1.12
2.14
2.11
1.03
1.22
2.18
3.09
3.07
3.18
[ppm]
[rel]

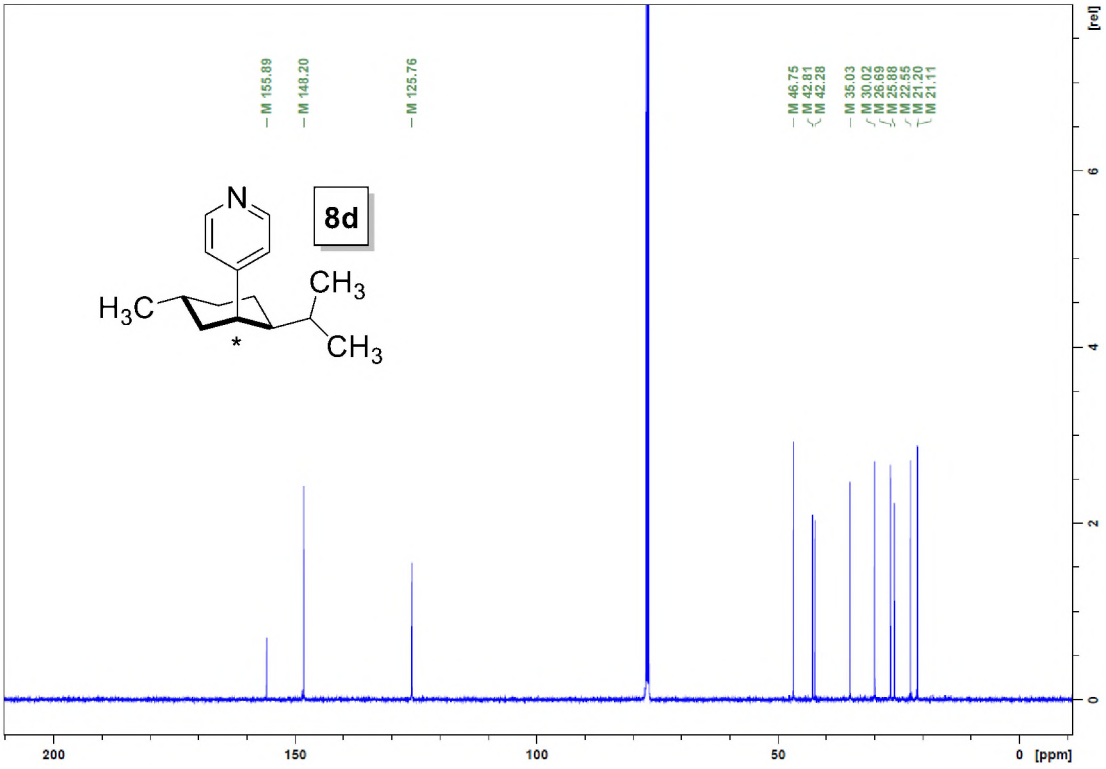

8c
MeO
OMe
H3C
CH3
CH3
*
M 159.68
M 158.16
M 126.39
M 122.20
M 104.72
M 104.16
M 55.88
M 55.33
M 43.89
M 39.90
M 39.01
M 35.63
M 33.59
M 28.65
M 25.43
M 24.61
M 21.66
M 15.68
[ppm]
[rel]

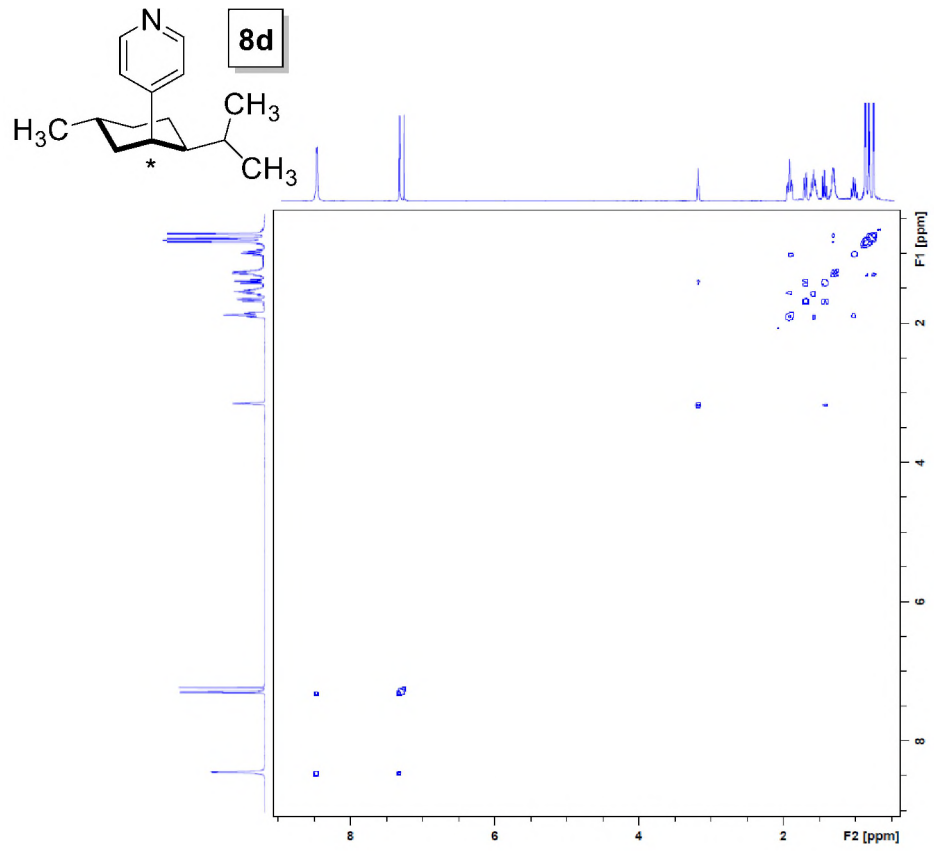

8c
MeO
OMe
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]

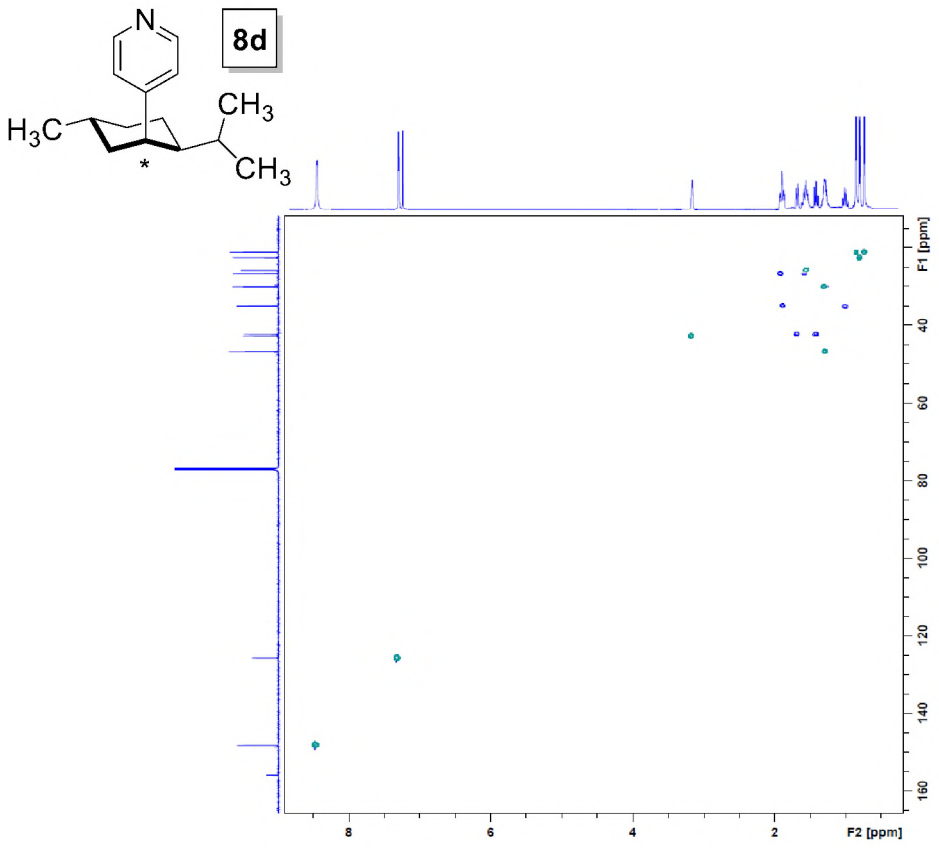

8c
MeO
OMe
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]

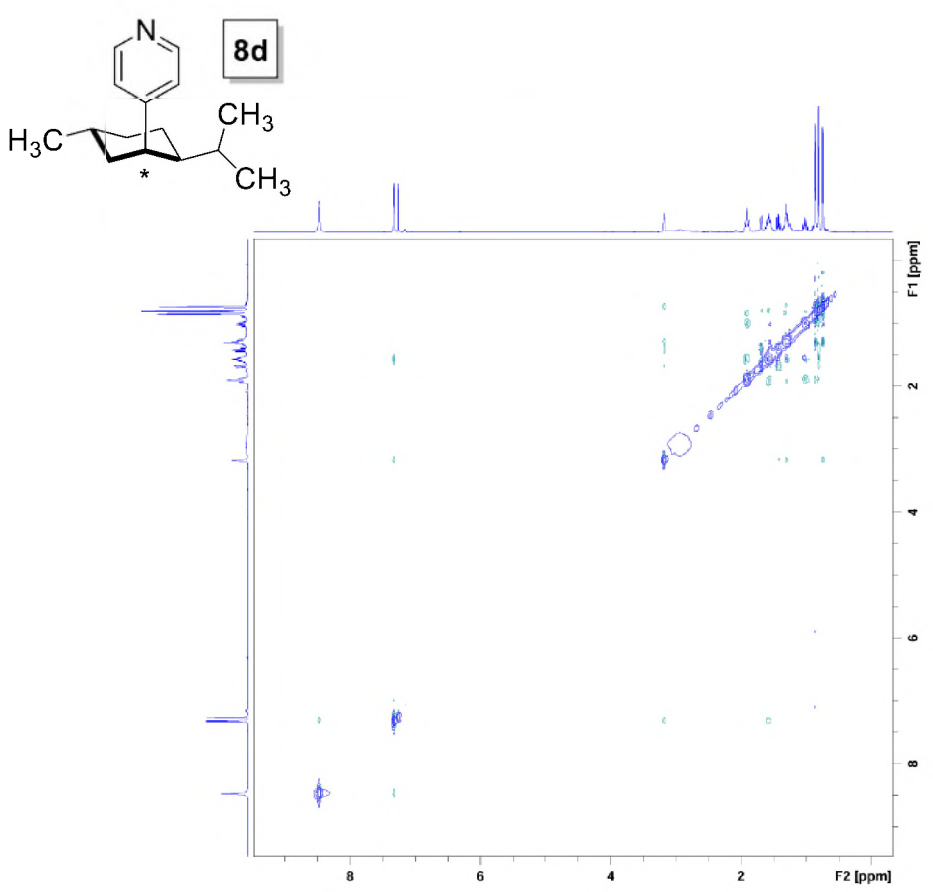

8c
MeO
OMe
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]

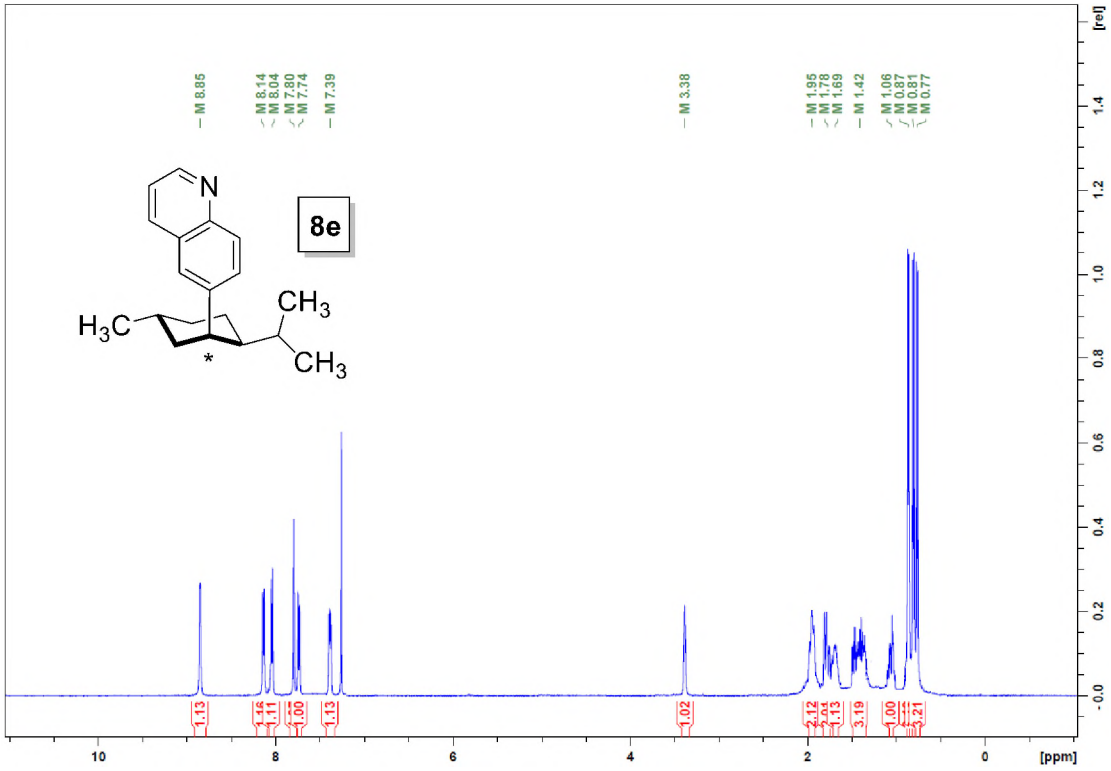

M 8.47
M 7.32
M 3.18
M 1.91
M 1.69
M 1.57
M 1.42
M 1.31
M 1.01
M 0.86
M 0.81
M 0.74
8d
N
H3C
CH3
CH3
*
2.09
2.00
1.02
2.00
1.05
2.15
3.13
2.15
1.16
3.04
[rel]
[ppm]

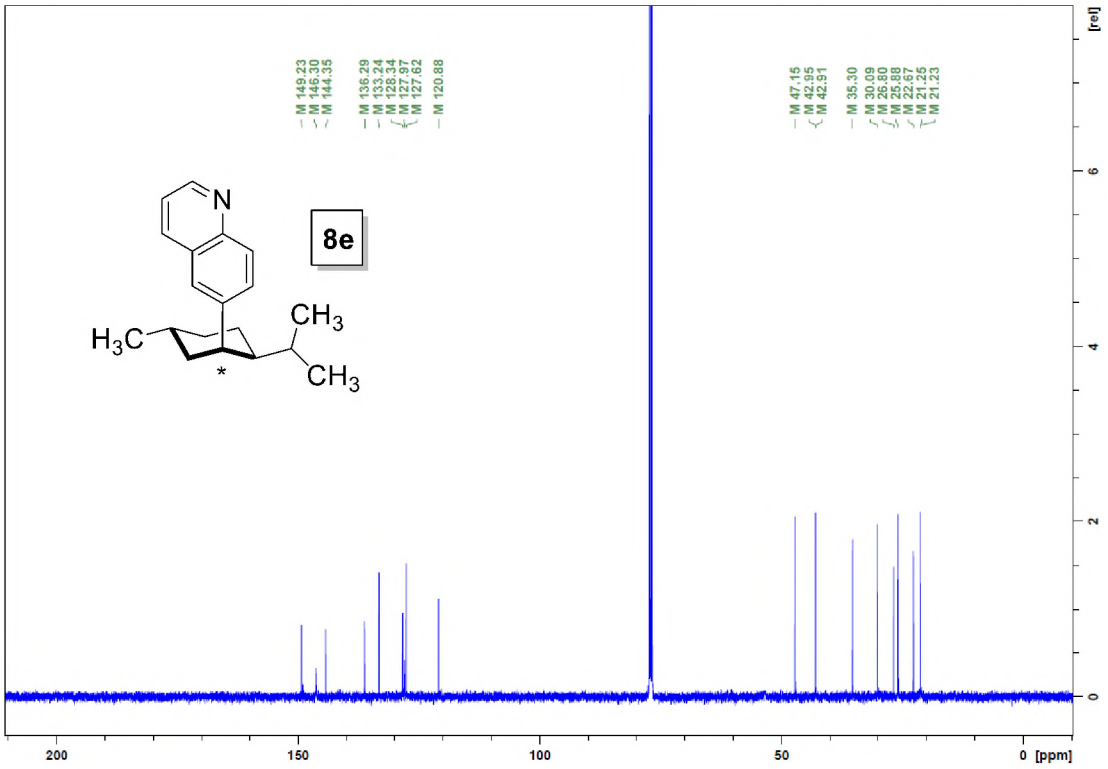

M 155.89
M 148.20
M 125.76
M 46.75
M 42.81
M 42.28
M 35.03
M 30.02
M 28.69
M 25.88
M 22.55
M 21.20
M 21.11
8d
N
H3C
CH3
CH3
*
[rel]
[ppm]

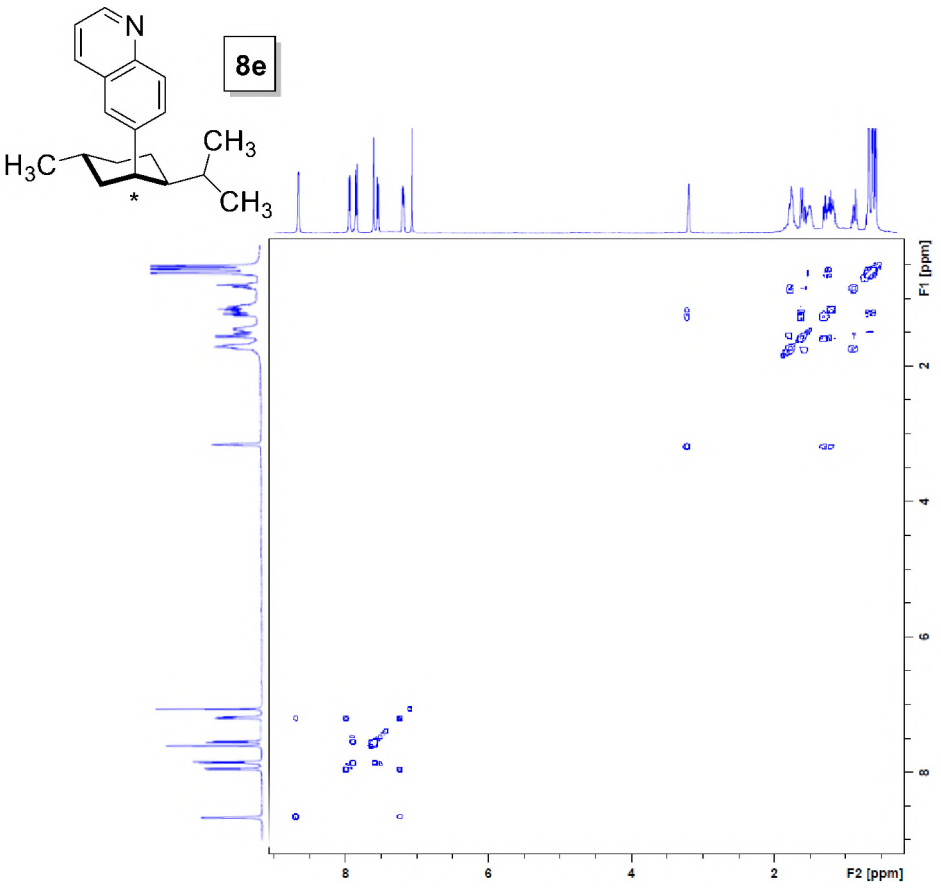

8d
N
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
8
6
4
2

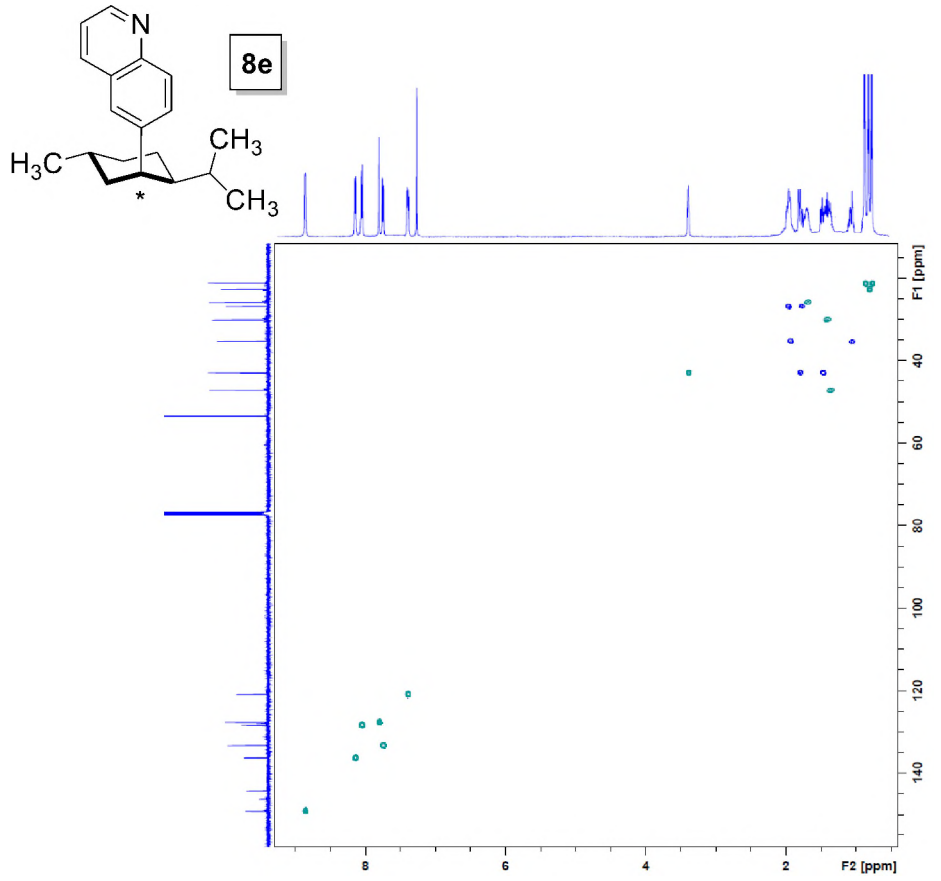

8d
N
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
8
6
4
2
40
60
80
100
120
140
160

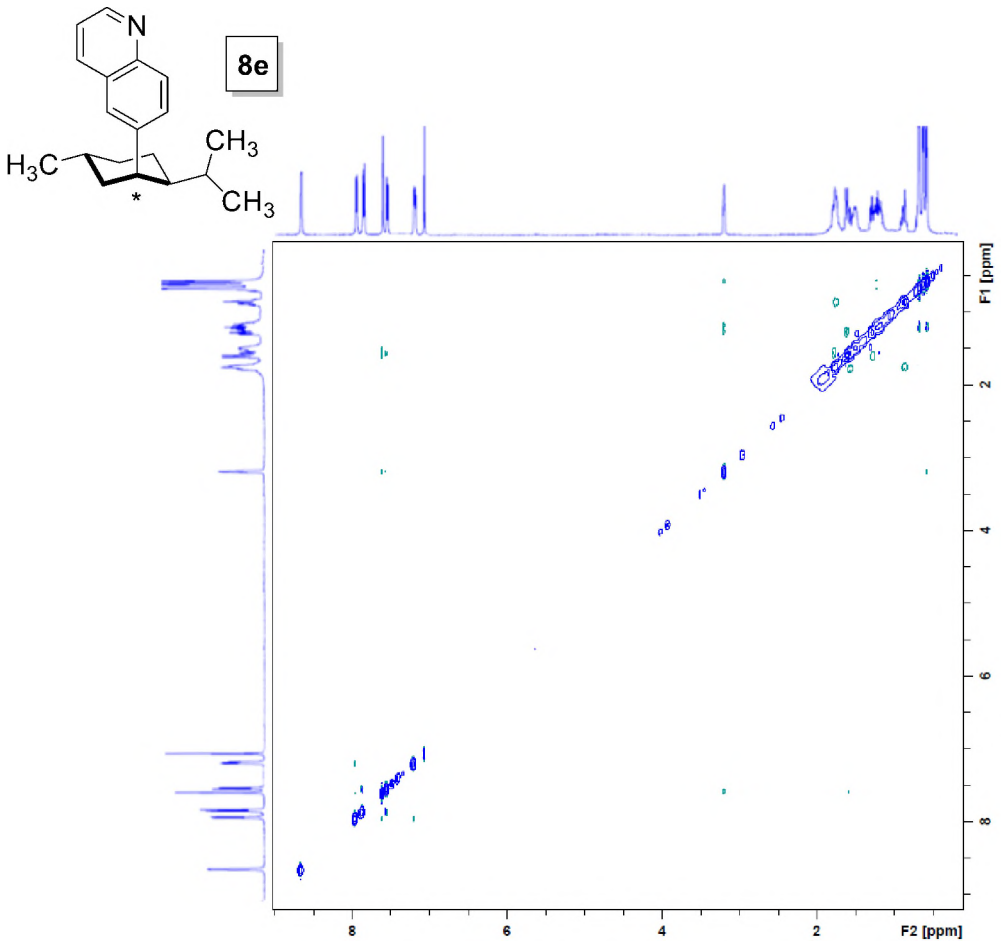

8d
N
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
2
4
6
8

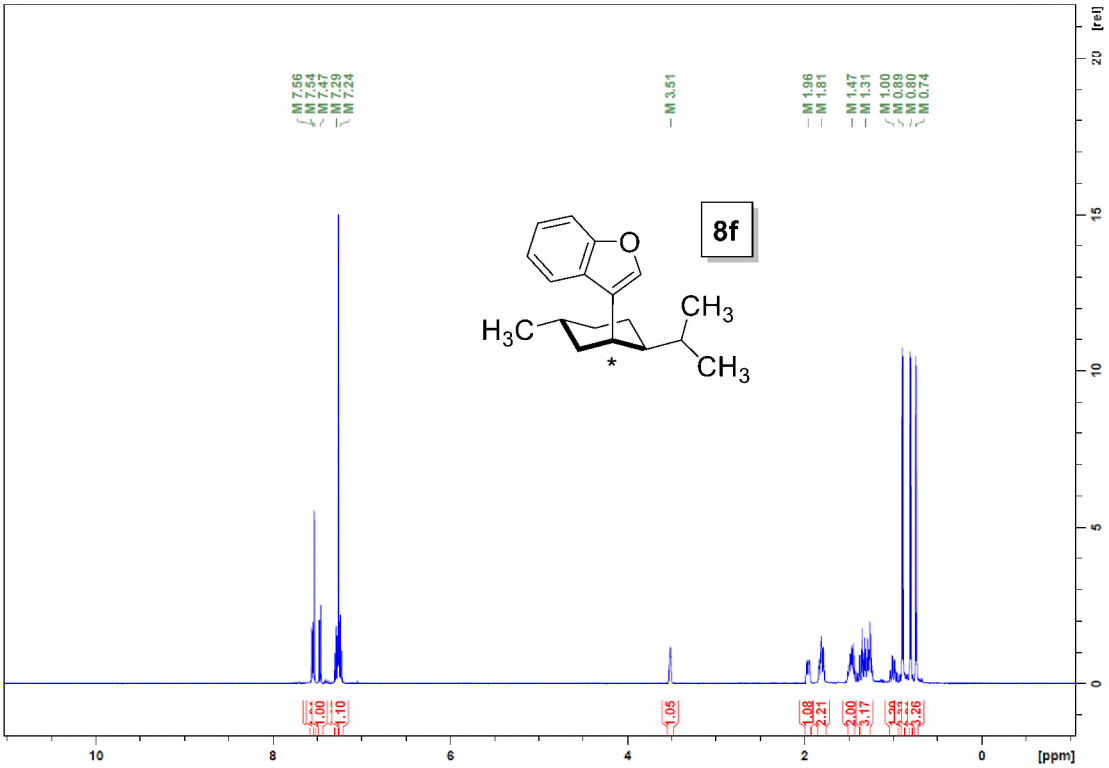

M 8.85
M 8.14
M 8.04
M 7.80
M 7.74
M 7.39
M 3.38
M 1.95
M 1.78
M 1.69
M 1.42
M 1.06
M 0.87
M 0.81
M 0.77
8e
N
H3C
CH3
CH3
*
[rel]
[ppm]

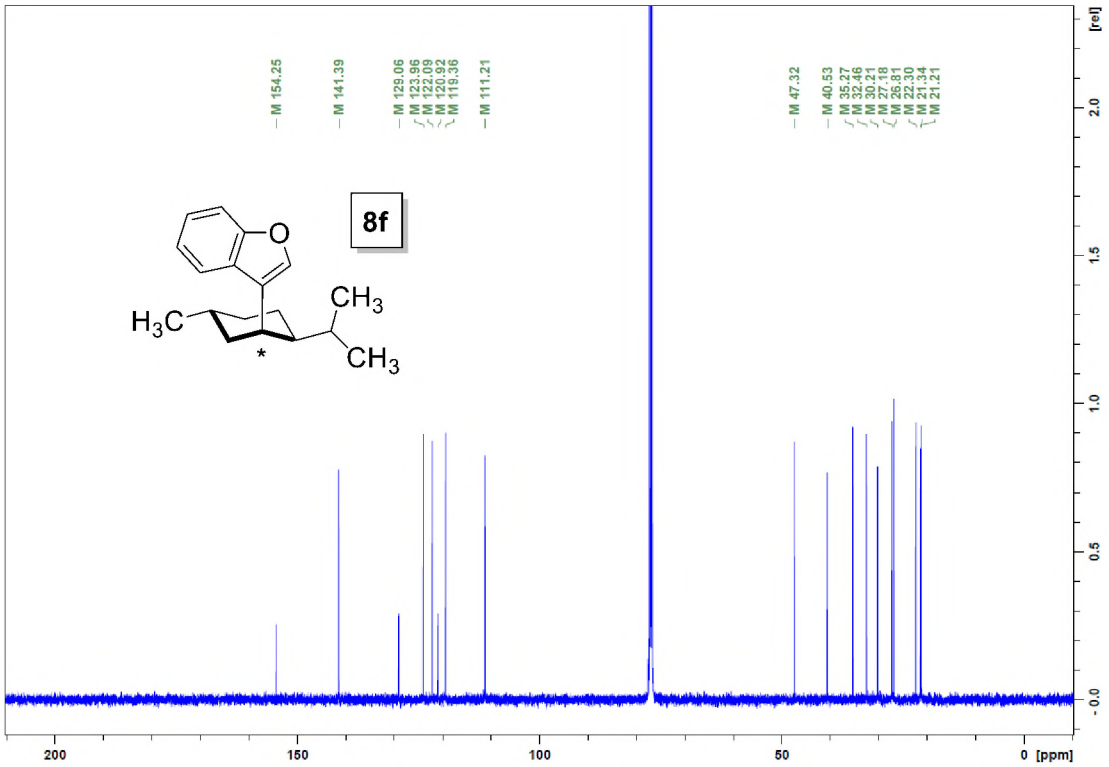

M 149.23
M 146.30
M 144.35
M 136.29
M 133.24
M 128.34
M 127.97
M 127.62
M 120.88
M 47.15
M 42.95
M 42.91
M 35.30
M 30.09
M 26.80
M 25.88
M 22.67
M 21.25
M 21.23
8e
N
H3C
CH3
CH3
*
[rel]
[ppm]

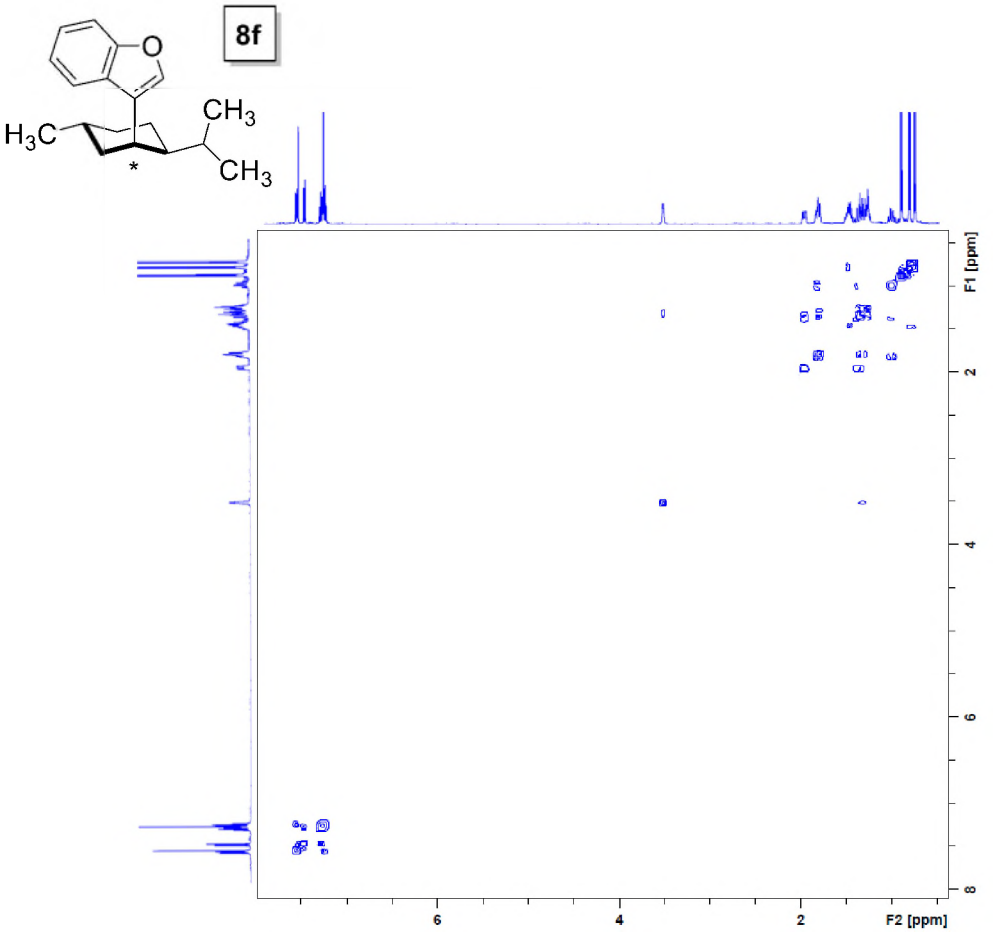

N
8e
H_3C
CH_3
CH_3
*
F1 [ppm]
F2 [ppm]
2
4
6
8
2
4
6
8

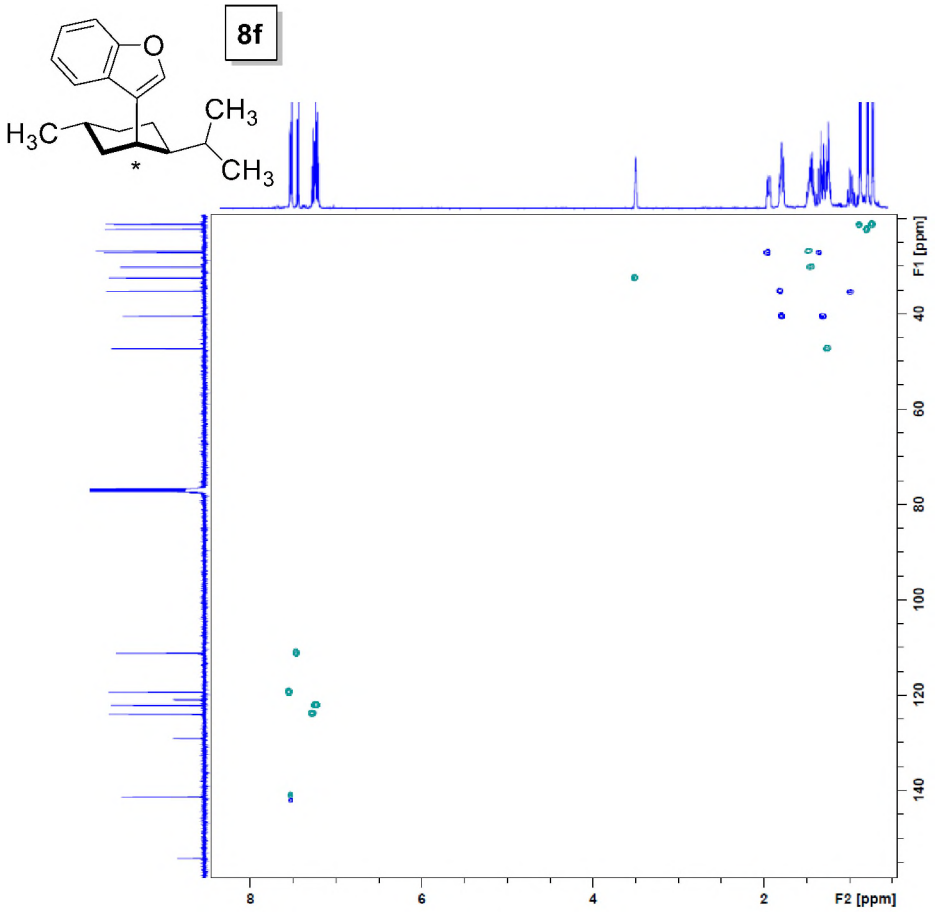

N
8e
H_3C
CH_3
CH_3
*
F1 [ppm]
F2 [ppm]
40
60
80
100
120
140
2
4
6
8

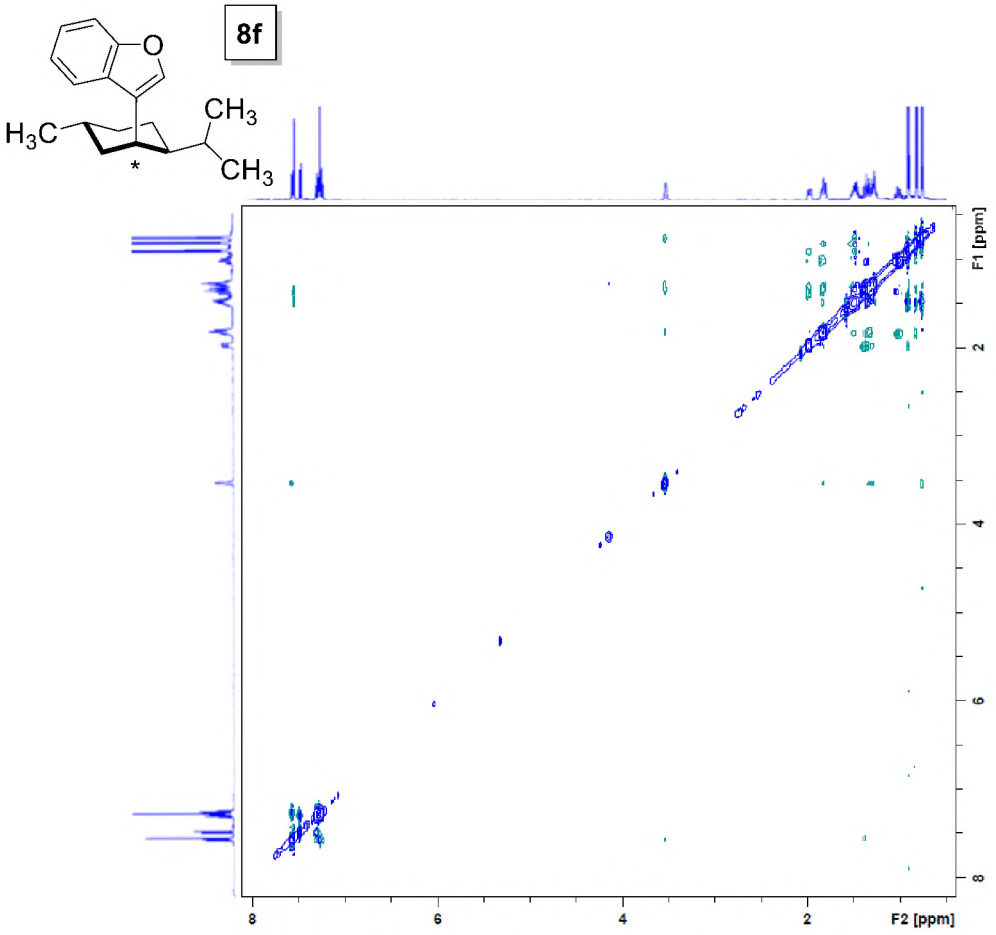

N
8e
H_3C
CH_3
CH_3
*
F1 [ppm]
2
4
6
8
8
6
4
2
F2 [ppm]

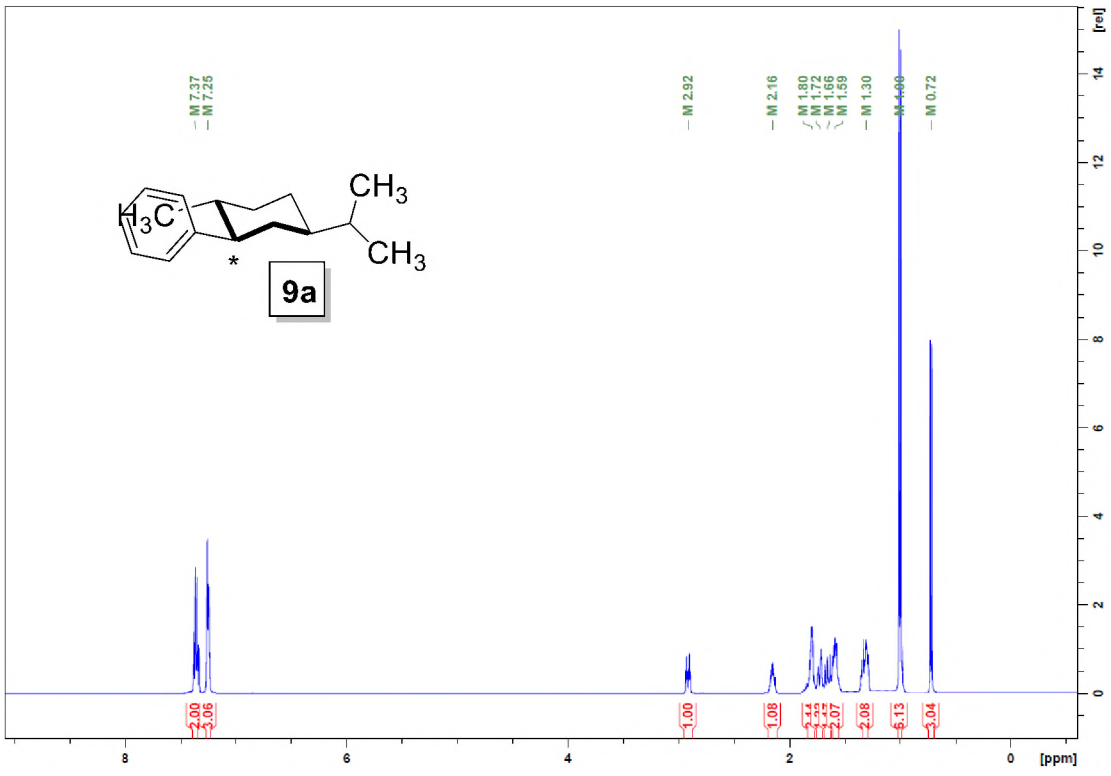

M 7.56
M 7.54
M 7.47
M 7.29
M 7.24
M 3.51
M 1.96
M 1.81
M 1.47
M 1.31
M 1.00
M 0.89
M 0.80
M 0.74
8f
O
H3C
CH3
CH3
*
[rel]
[ppm]

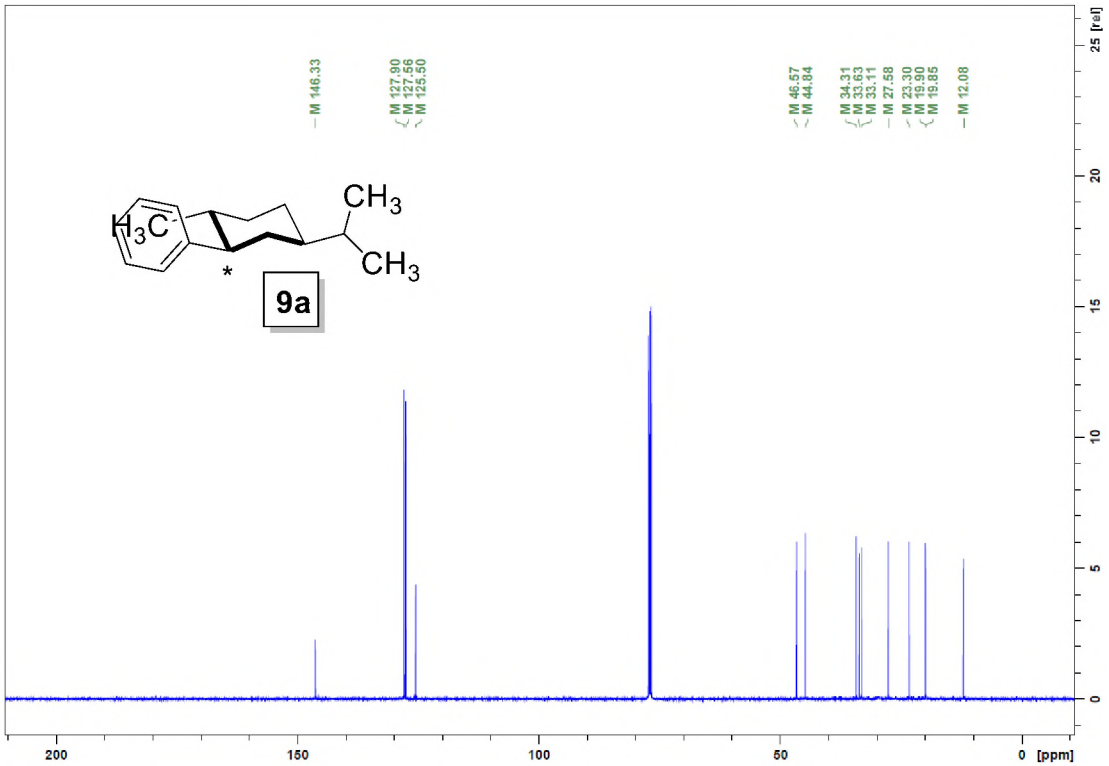

M 154.25
M 141.39
M 129.06
M 123.96
M 122.09
M 120.92
M 119.36
M 111.21
M 47.32
M 40.53
M 35.27
M 32.46
M 30.21
M 27.18
M 26.81
M 22.30
M 21.34
M 21.21
8f
O
H3C
CH3
CH3
*
[rel]
[ppm]

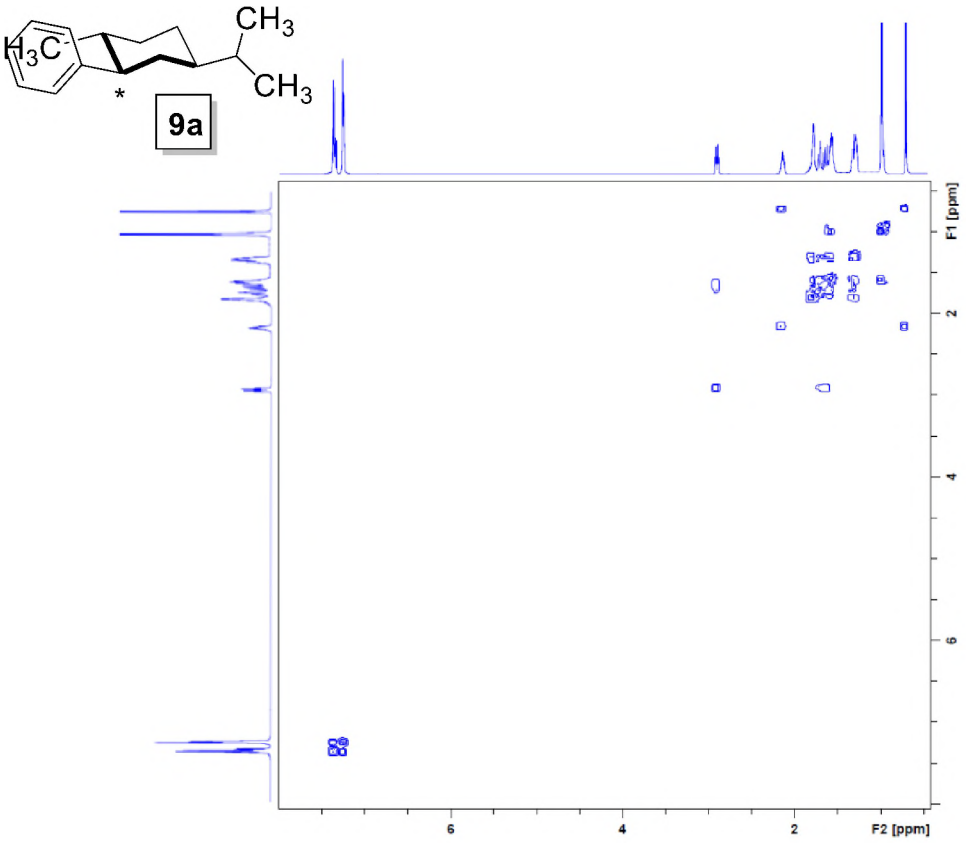

8f
O
CH3
H3C
CH3
*
F1 [ppm]
F2 [ppm]
2
4
6
8
6
4
2

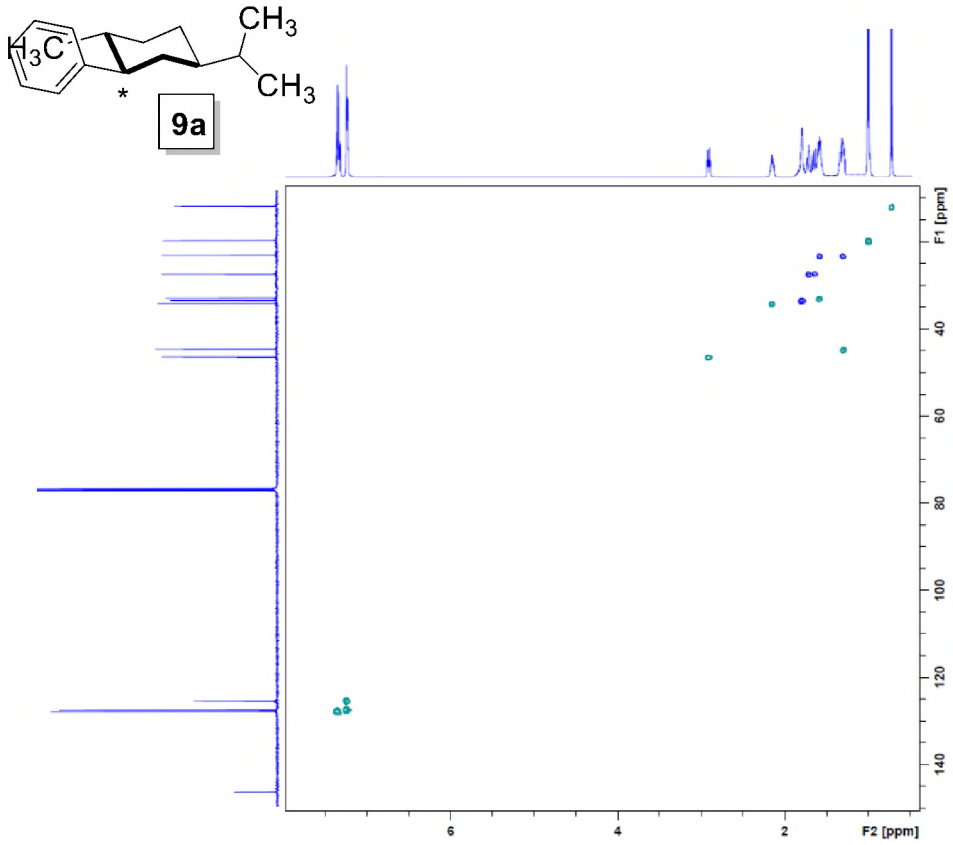

8f
O
CH3
H3C
CH3
*
F1 [ppm]
F2 [ppm]
40
60
80
100
120
140
8
6
4
2

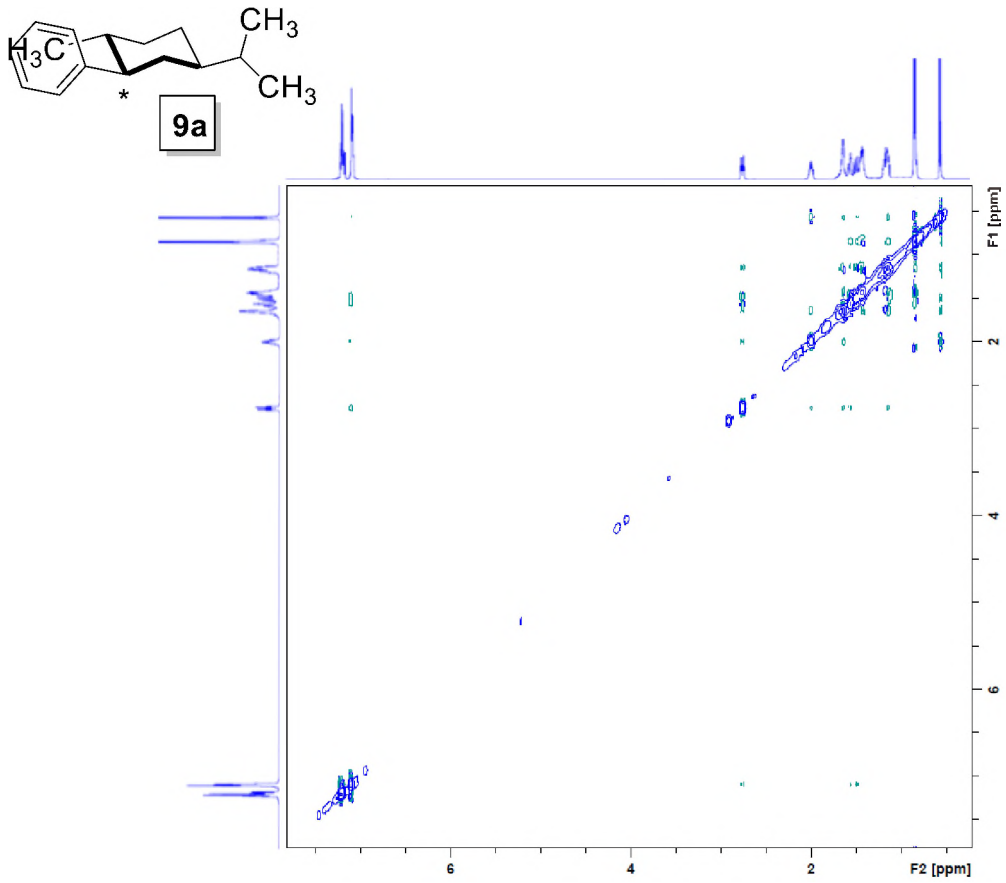

8f
O
H3C
CH3
CH3
*
F1 [ppm]
F2 [ppm]
8
6
4
2
2
4
6
8

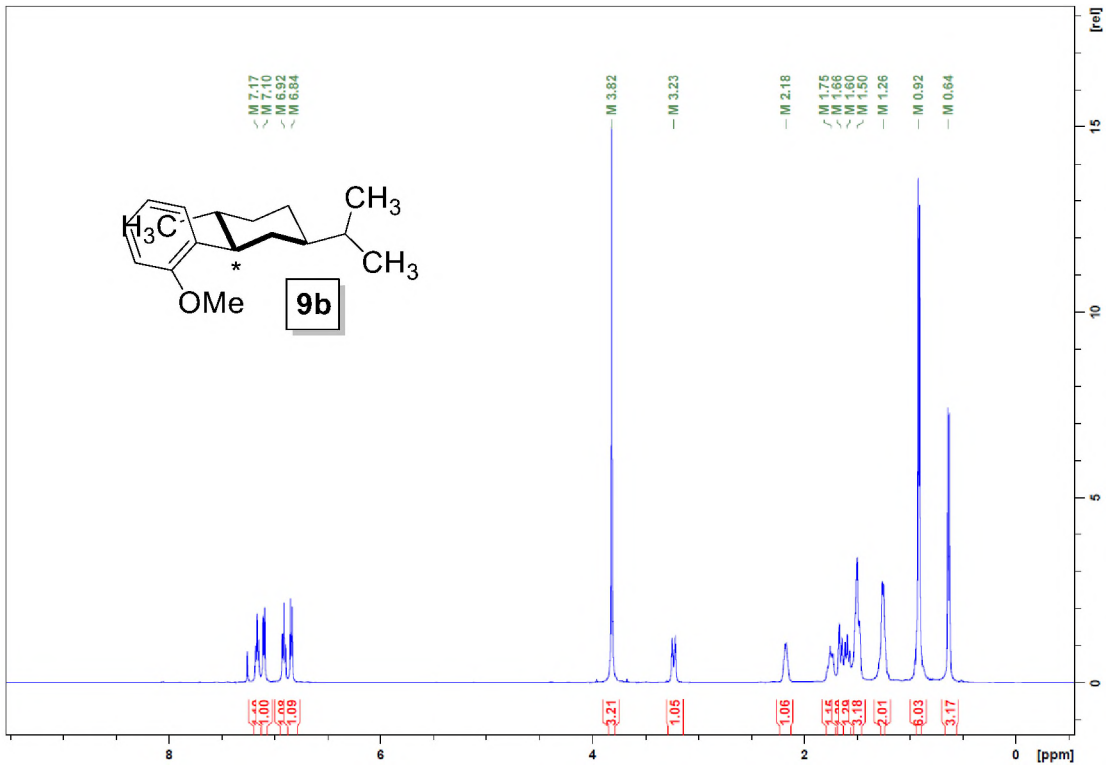

M 7.37
M 7.25
M 2.92
M 2.16
M 1.80
M 1.72
M 1.66
M 1.59
M 1.30
M 1.00
M 0.72
CH3
H3C
CH3
*
9a
2.00
2.06
1.00
1.08
2.07
2.08
6.13
3.04
[rel]
[ppm]

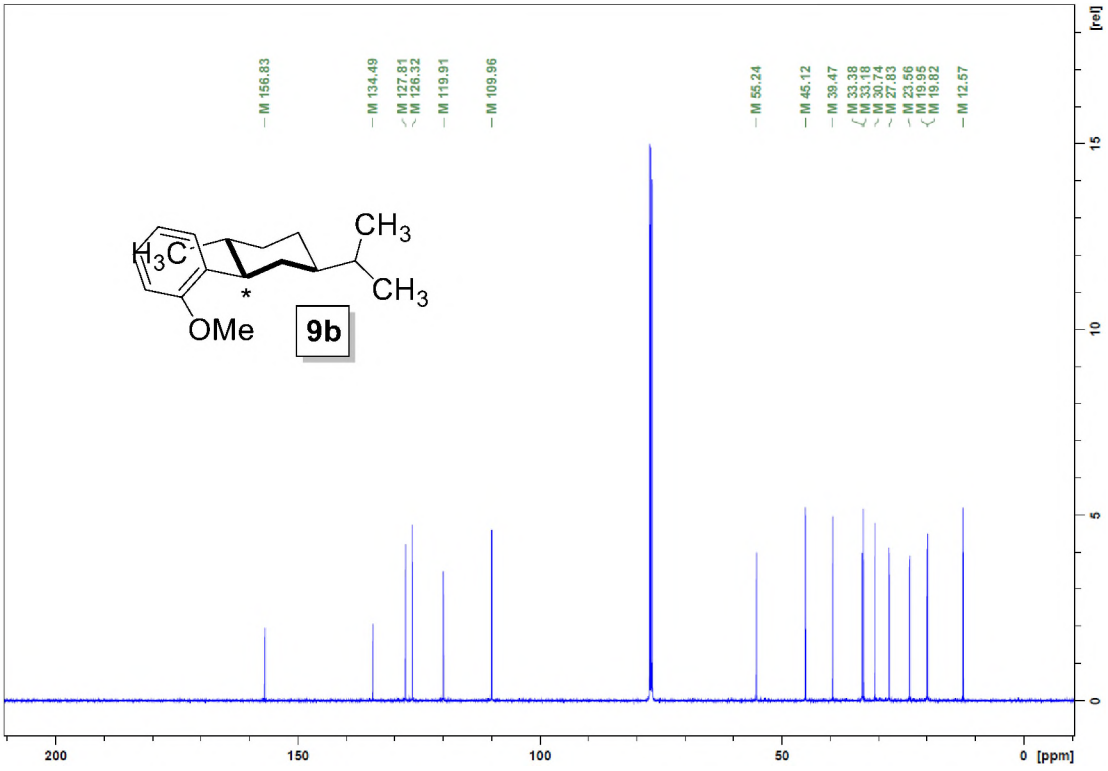

M 146.33
M 127.90
M 127.56
M 125.50
M 46.57
M 44.84
M 34.31
M 33.63
M 33.11
M 27.58
M 23.30
M 19.90
M 19.85
M 12.08
CH3
H3C
CH3
*
9a
[rel]
[ppm]

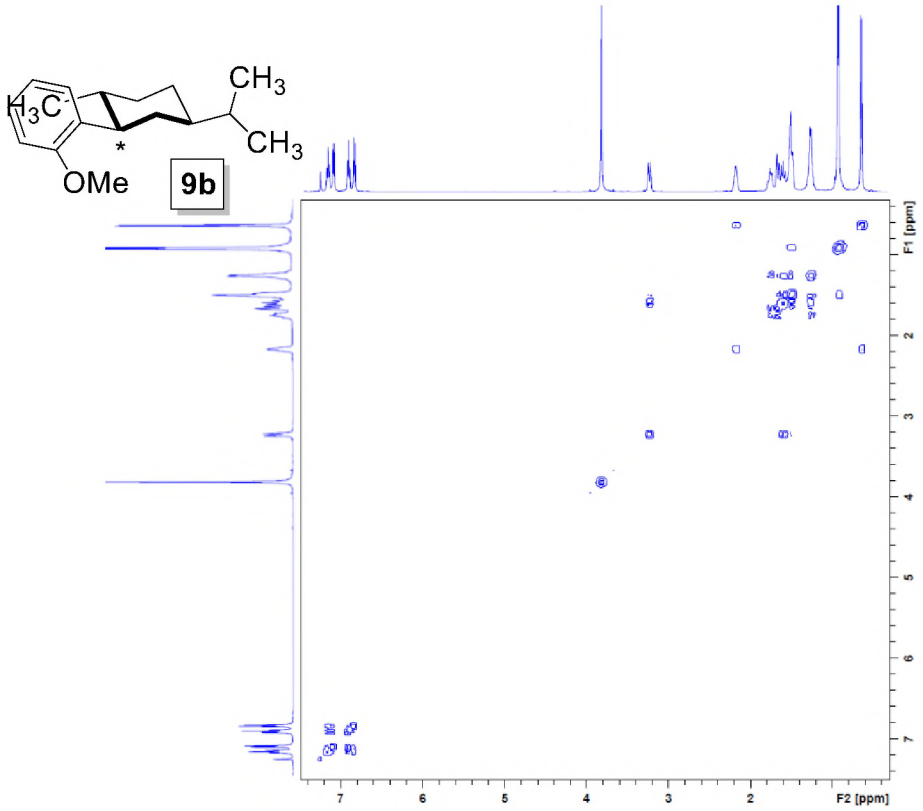

CH3
H3C
CH3
*
9a
F1 [ppm]
F2 [ppm]

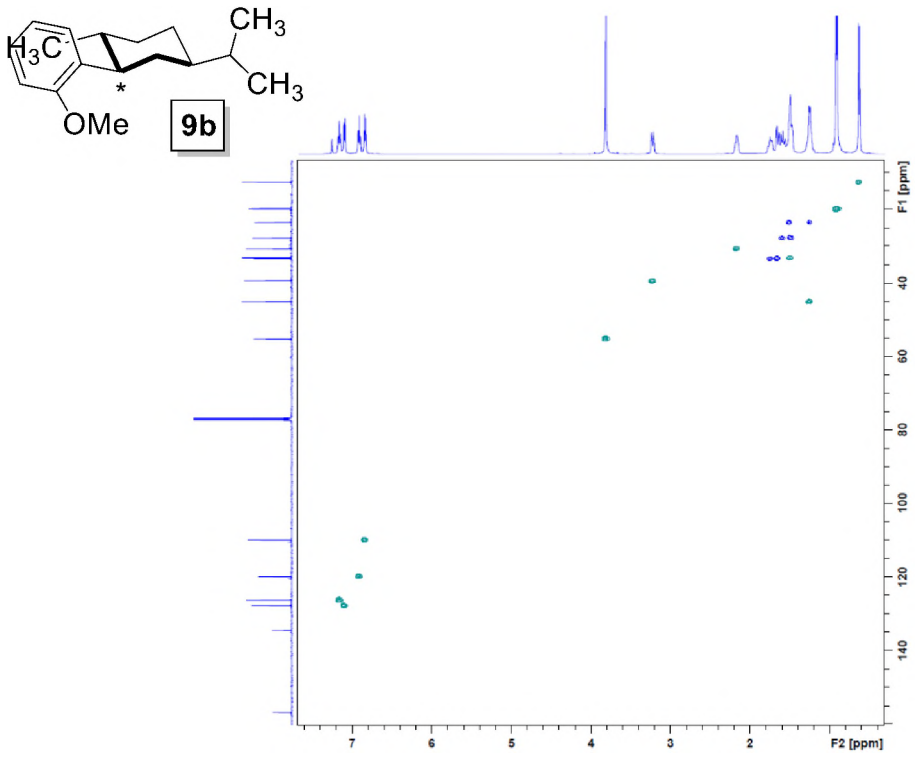

CH3
H3C
CH3
*
9a
F1 [ppm]
F2 [ppm]

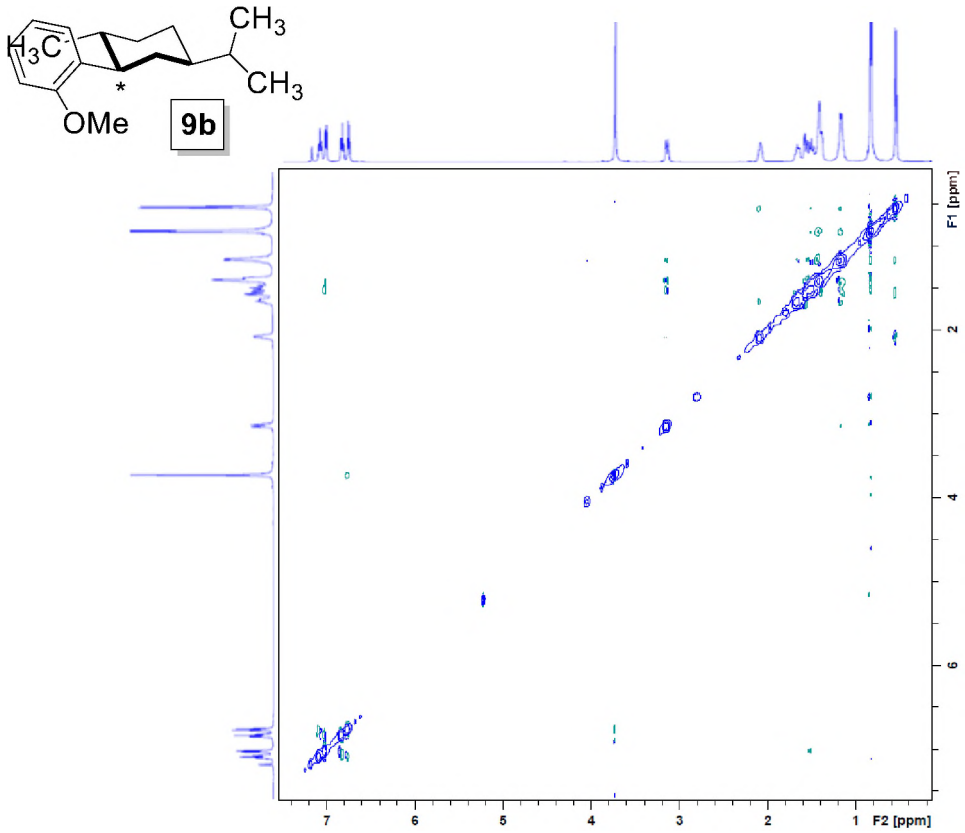

CH3
H3C
CH3
*
9a
F1 [ppm]
2
4
6
6
4
2
F2 [ppm]

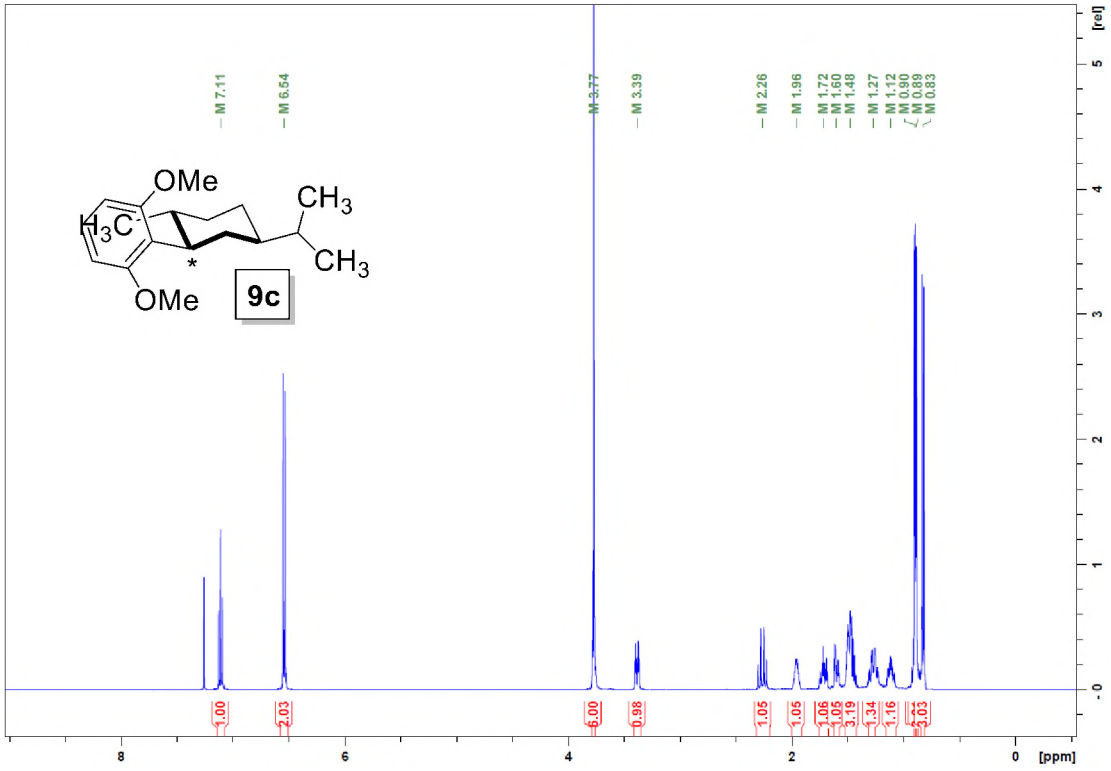

M 7.17
M 7.10
M 6.92
M 6.84
M 3.82
M 3.23
M 2.18
M 1.75
M 1.66
M 1.60
M 1.50
M 1.26
M 0.92
M 0.64
CH3
H3C
CH3
*
OMe
9b
[rel]
[ppm]

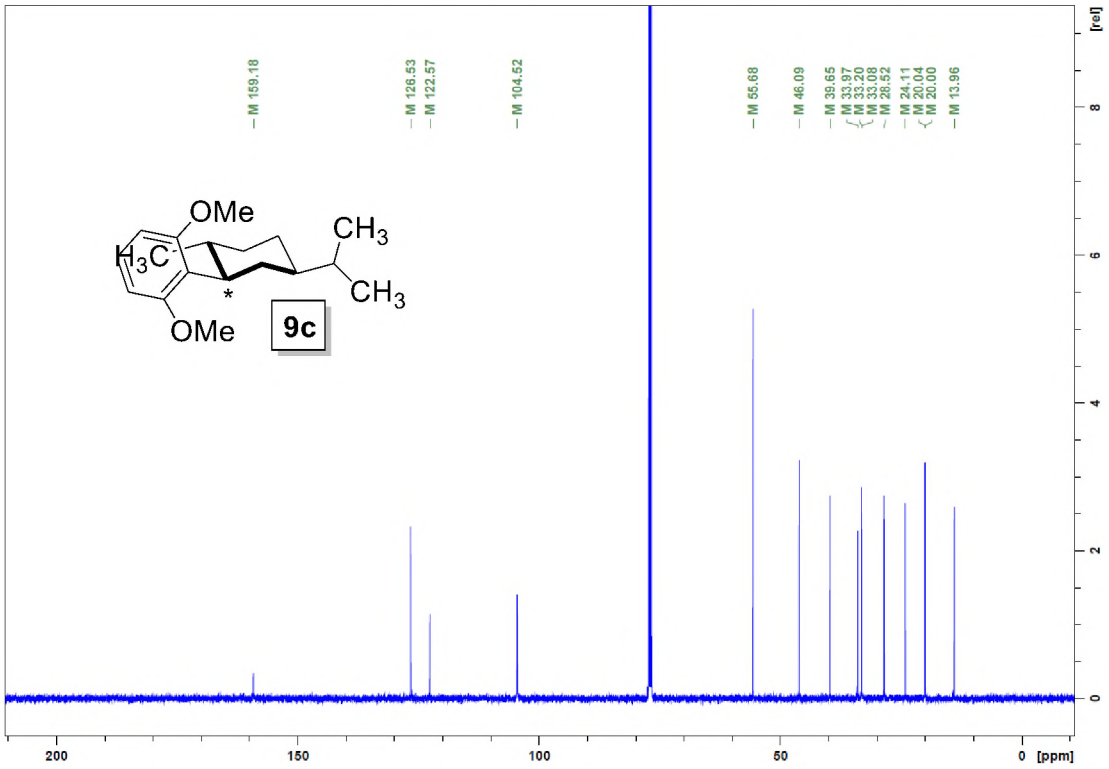

M 156.83
M 134.49
M 127.81
M 126.32
M 119.91
M 109.96
M 55.24
M 45.12
M 39.47
M 33.38
M 33.18
M 30.14
M 27.83
M 23.56
M 19.95
M 19.82
M 12.57
CH3
H3C
CH3
*
OMe
9b
[rel]
[ppm]

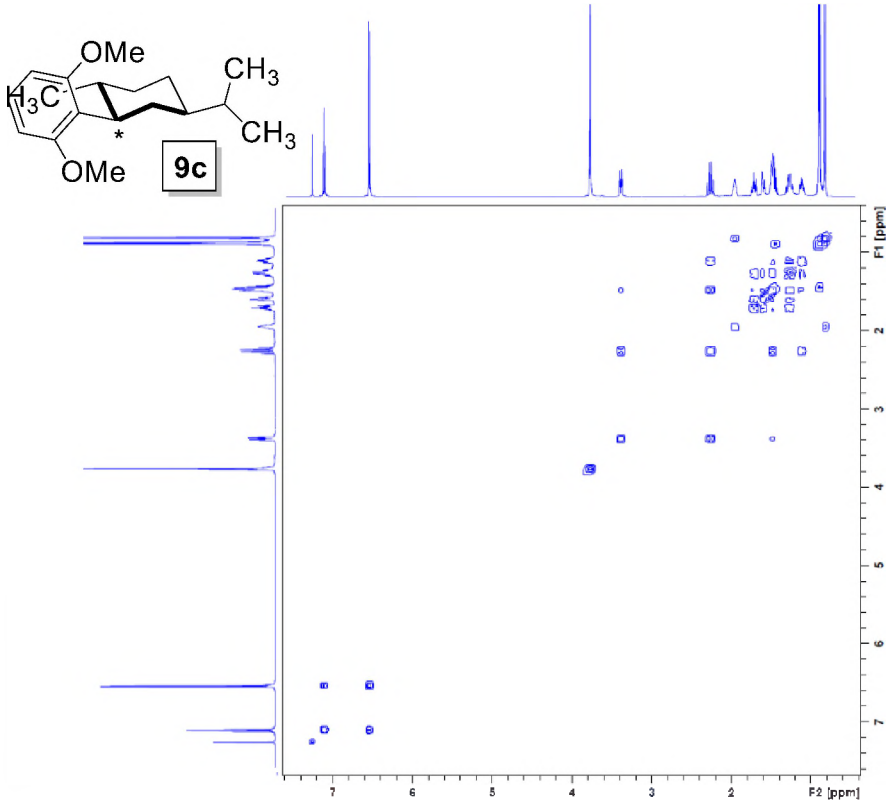

CH3
H3C
CH3
*
OMe
9b
F1 [ppm]
F2 [ppm]

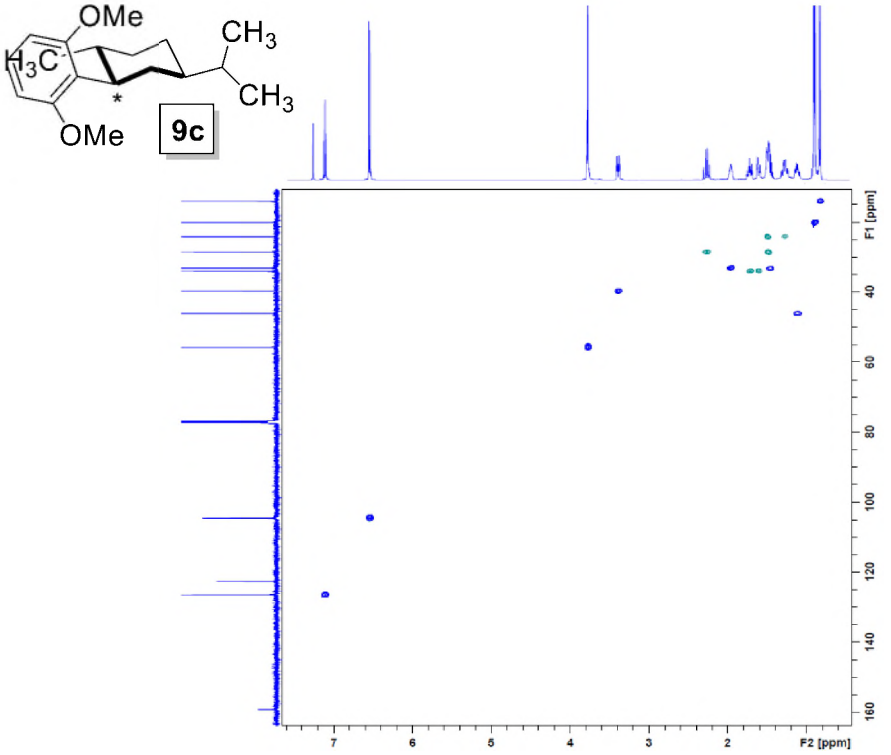

CH3
H3C
CH3
*
OMe
9b
F1 [ppm]
F2 [ppm]

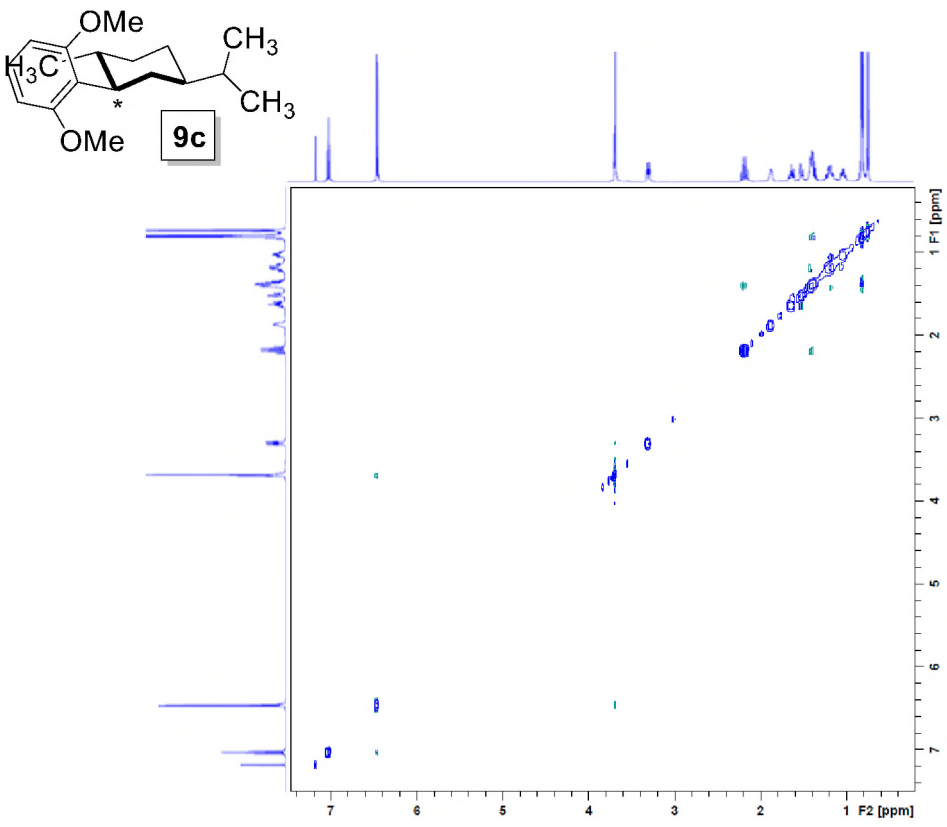

CH3
H3C
CH3
*
OMe
9b
F1 [ppm]
2
4
6
7
6
5
4
3
2
1
F2 [ppm]

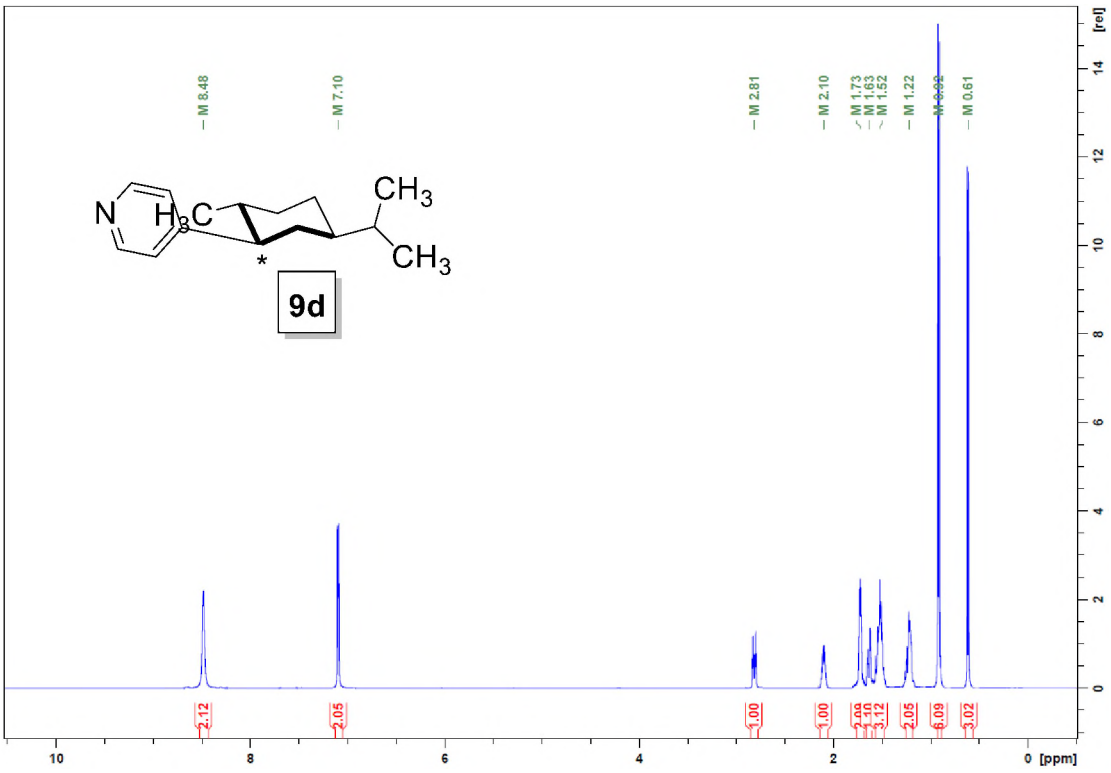

M 7.11
M 6.64
M 3.77
M 3.39
M 2.26
M 1.96
M 1.72
M 1.60
M 1.48
M 1.27
M 1.12
M 0.90
M 0.89
M 0.83
OMe
H3C
CH3
CH3
OMe
9c
1.00
2.03
6.00
0.98
1.05
1.05
1.06
1.06
3.19
1.34
1.16
2.03
[rel]
[ppm]

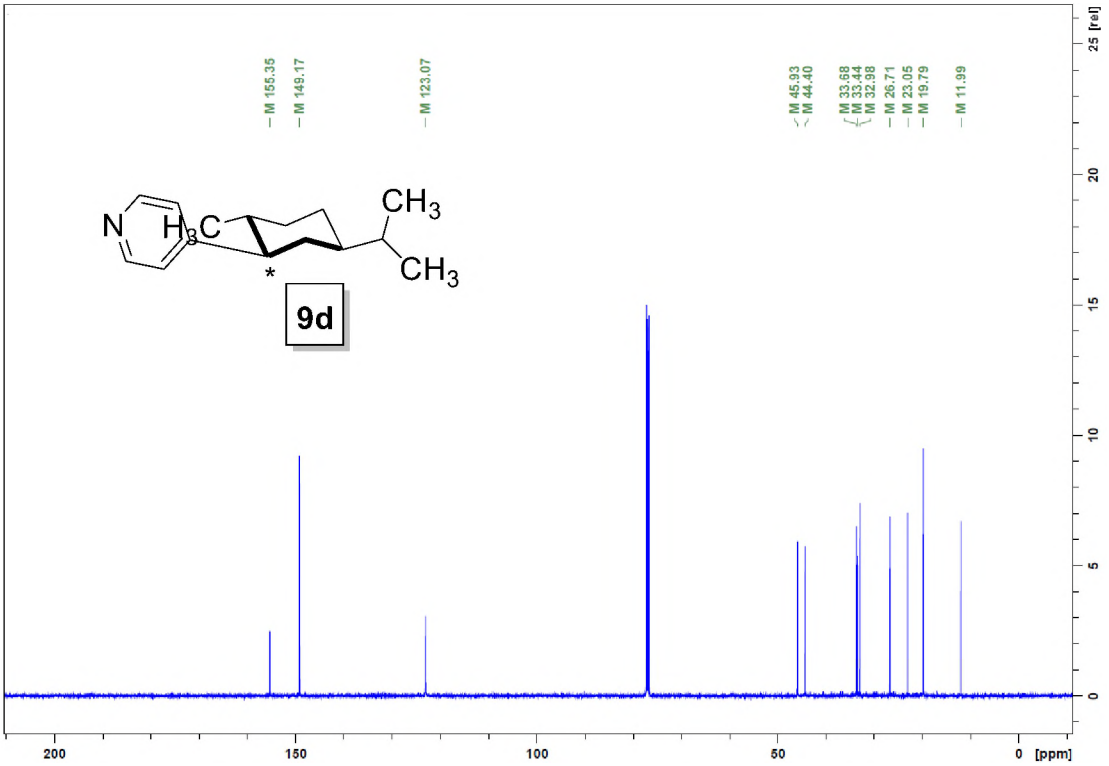

M 159.18
M 126.53
M 122.57
M 104.52
M 55.68
M 46.09
M 39.65
M 33.97
M 33.20
M 33.08
M 28.52
M 24.11
M 20.04
M 20.00
M 13.96
OMe
H3C
CH3
CH3
OMe
9c
[rel]
[ppm]

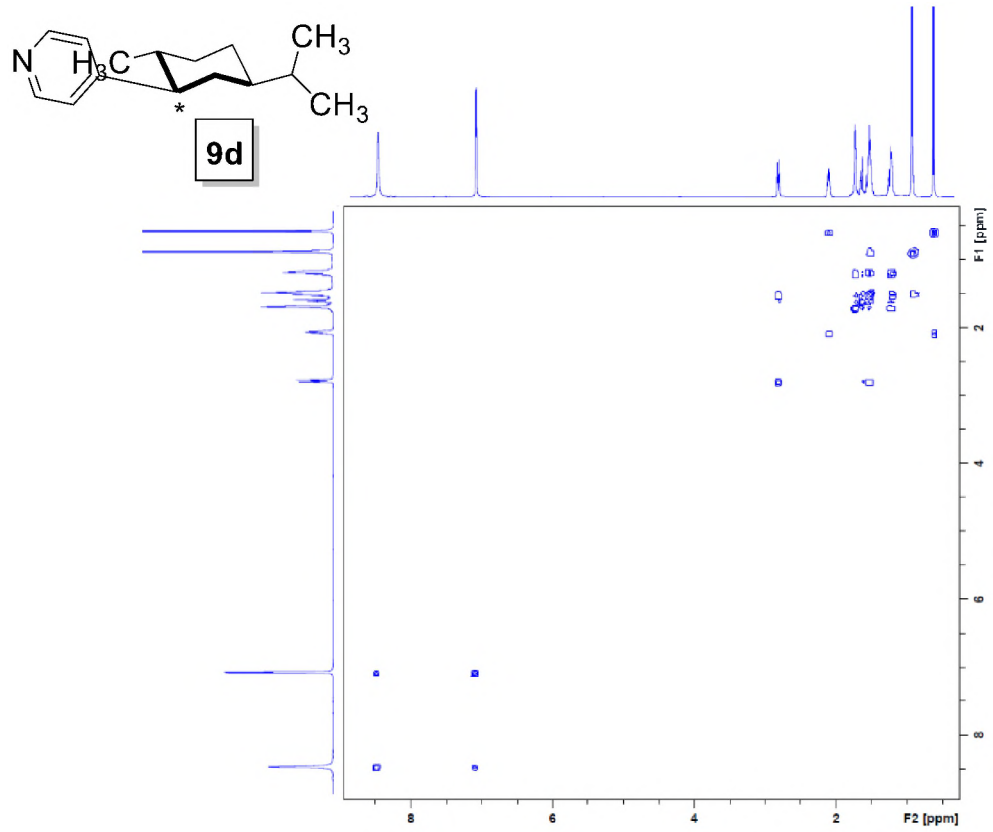

OMe
CH3
H3C
CH3
*
OMe
9c
F1 [ppm]
F2 [ppm]

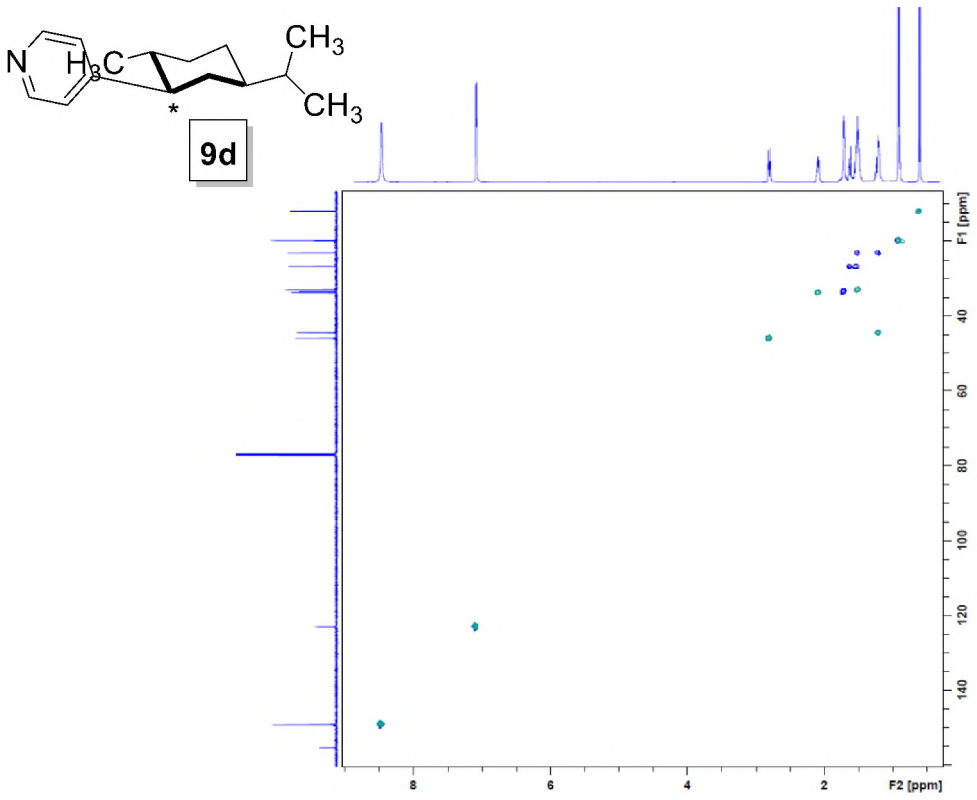

OMe
CH3
H3C
CH3
*
OMe
9c
F1 [ppm]
F2 [ppm]

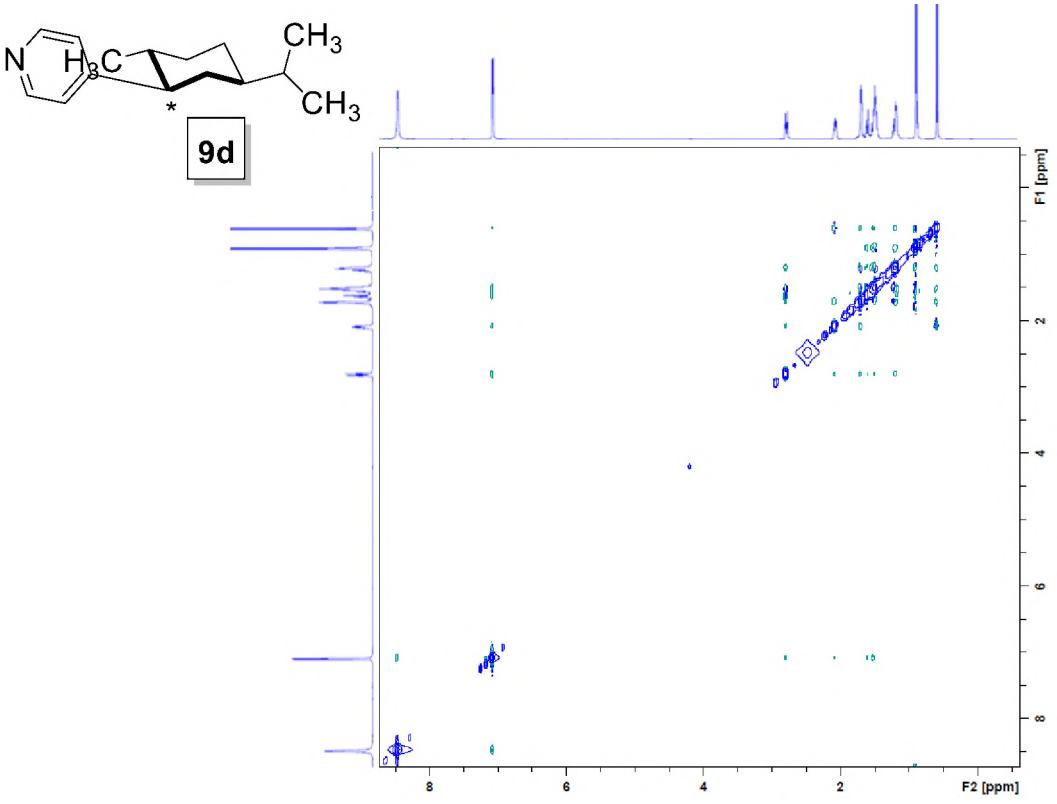

OMe
H3C
CH3
CH3
*
OMe
9c
F1 [ppm]
F2 [ppm]

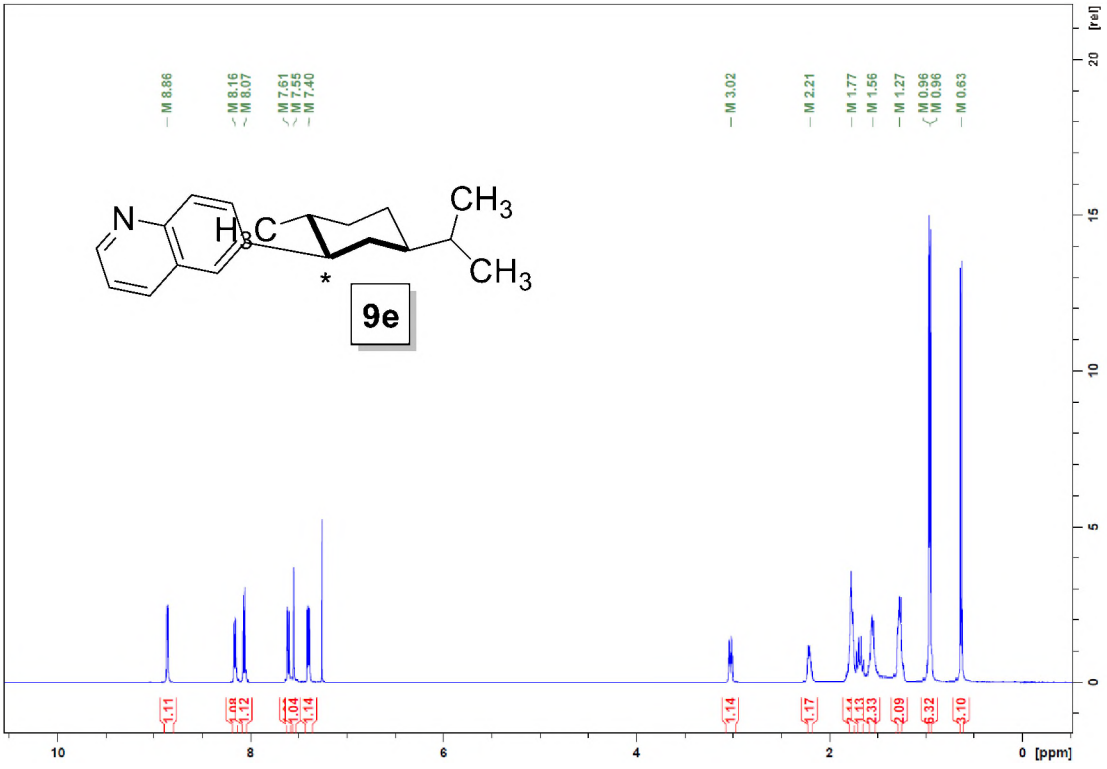

M 8.48
M 7.10
M 2.81
M 2.10
M 1.73
M 1.63
M 1.52
M 1.22
M 0.61
CH3
H3C
CH3
N
*
9d
2.12
2.05
1.00
1.00
2.00
4.10
3.12
2.05
6.09
3.02
[rel]
[ppm]

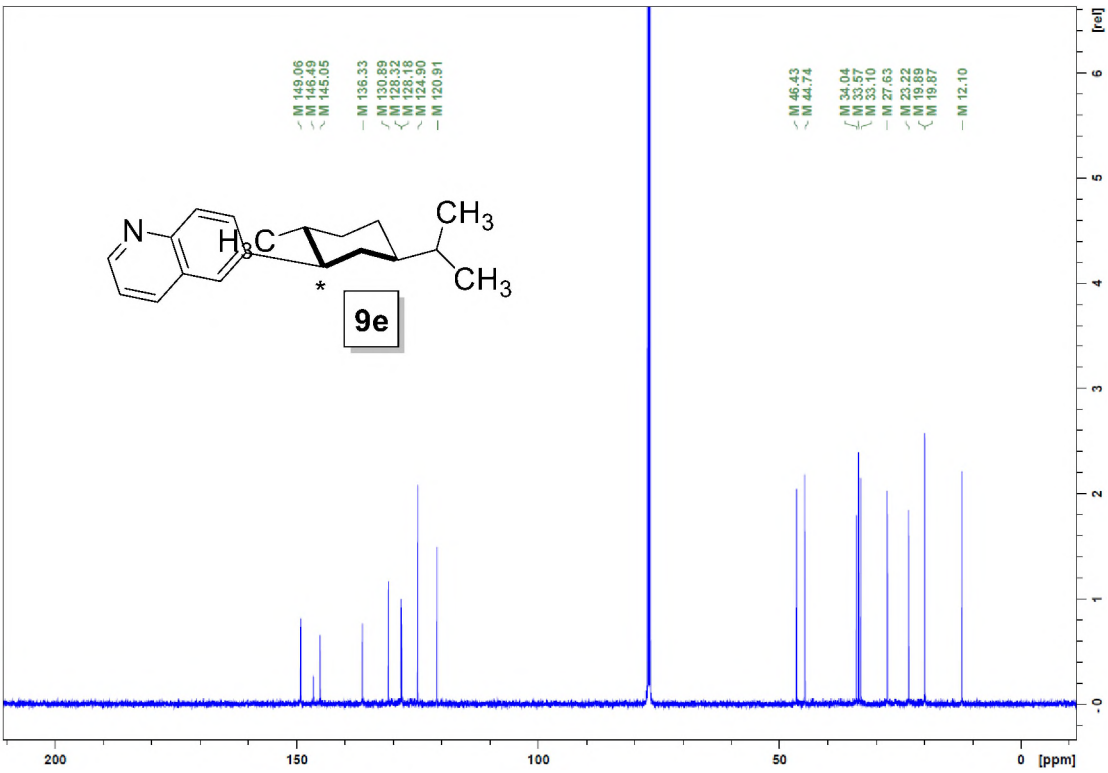

M 156.35
M 149.17
M 123.07
M 45.93
M 44.40
M 33.68
M 33.44
M 32.98
M 26.71
M 23.05
M 19.79
M 11.99
CH3
H3C
CH3
N
*
9d
[rel]
[ppm]

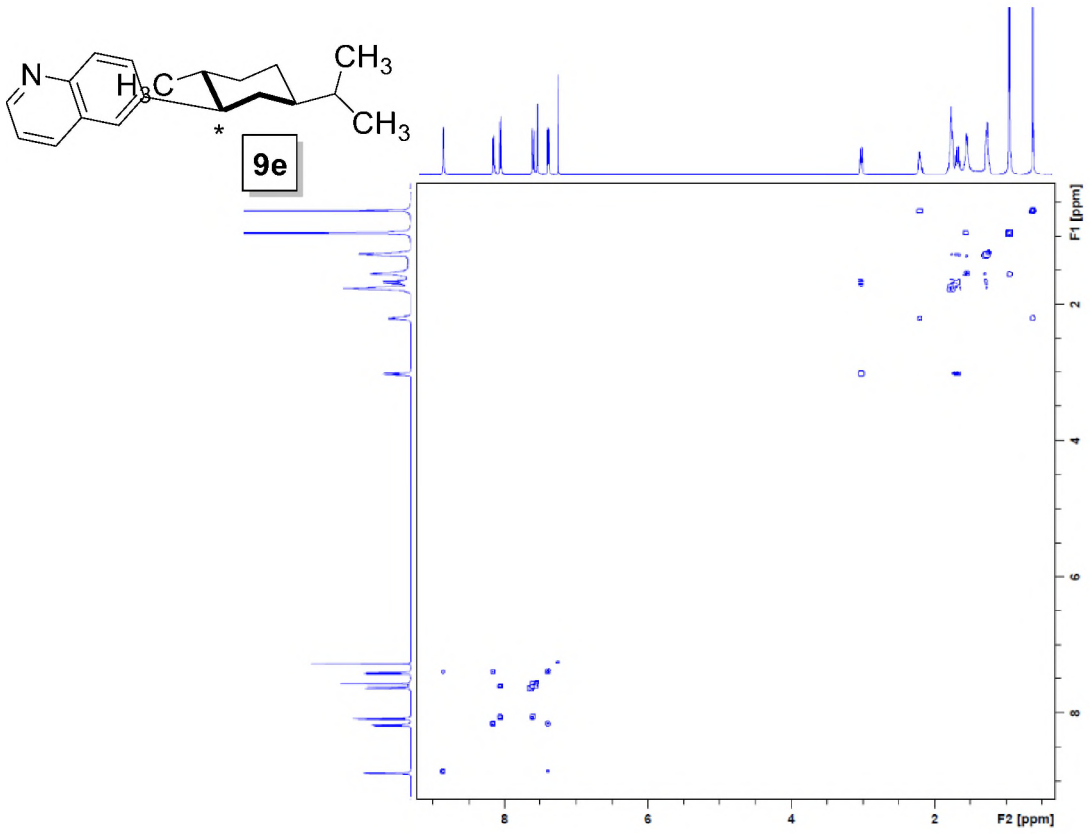

N
H3C
CH3
CH3
*
9d
F1 [ppm]
F2 [ppm]

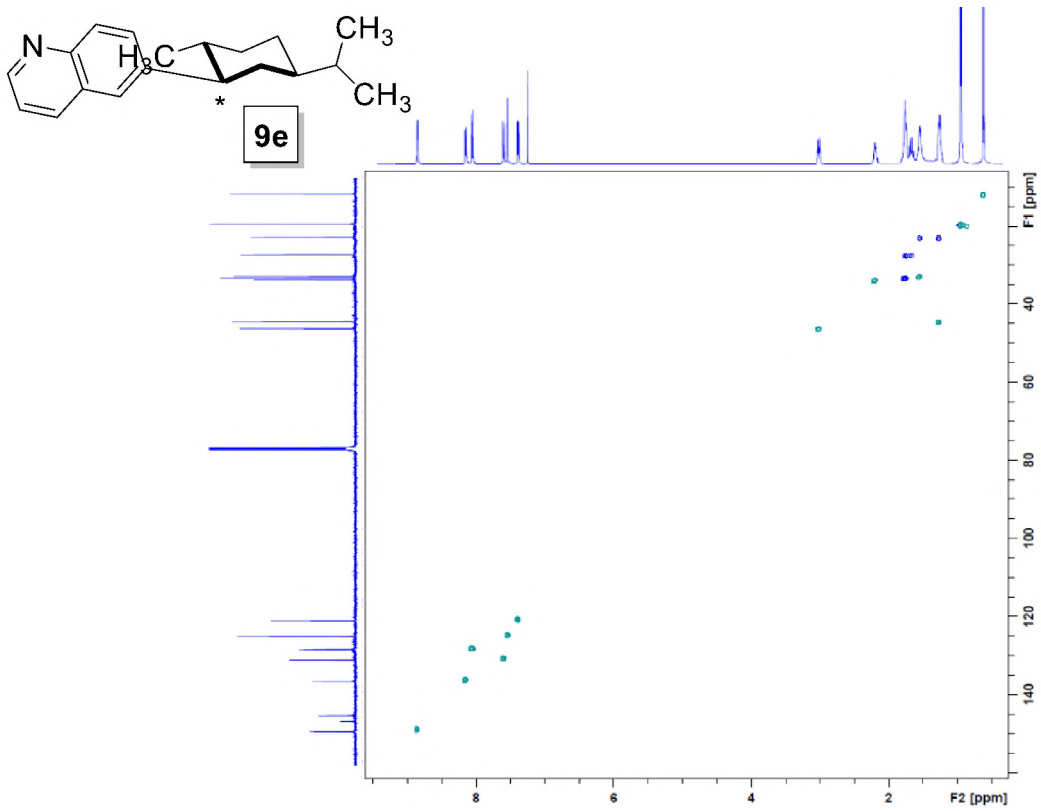

N
H3C
CH3
CH3
*
9d
F1 [ppm]
F2 [ppm]

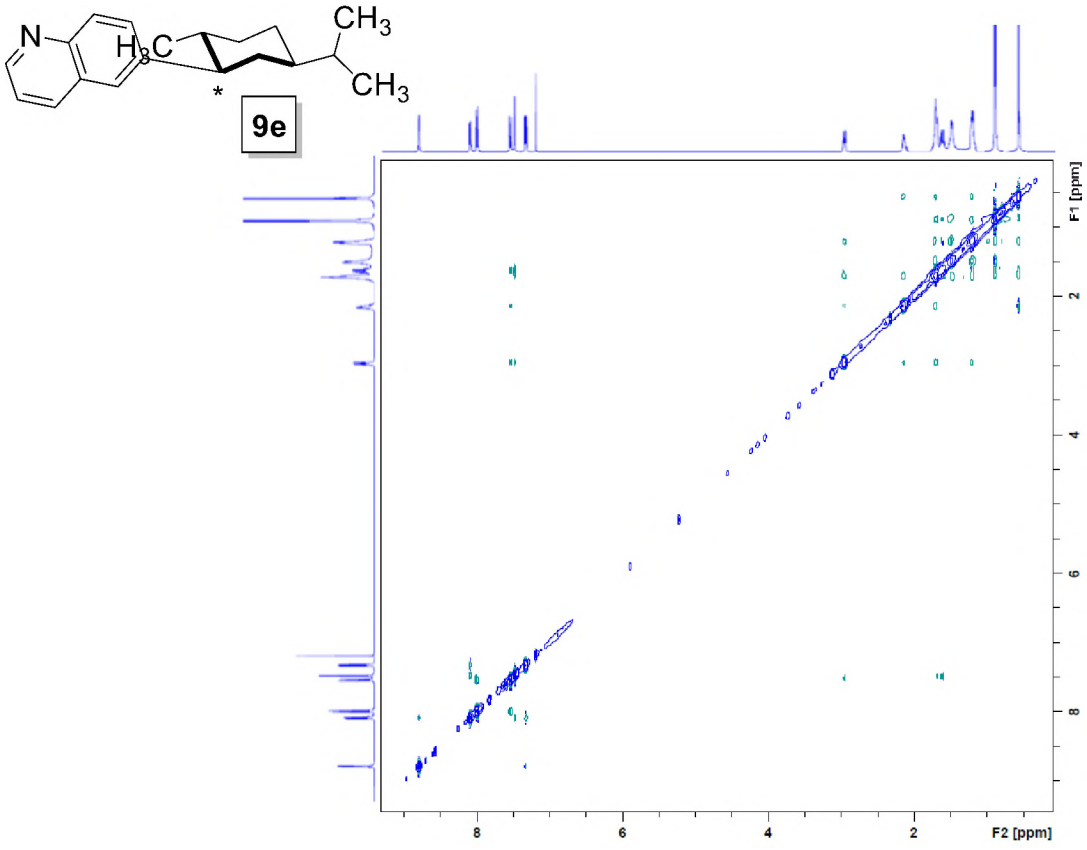

N
H3C
CH3
CH3
*
9d
F1 [ppm]
F2 [ppm]
2
4
6
8
8
6
4
2

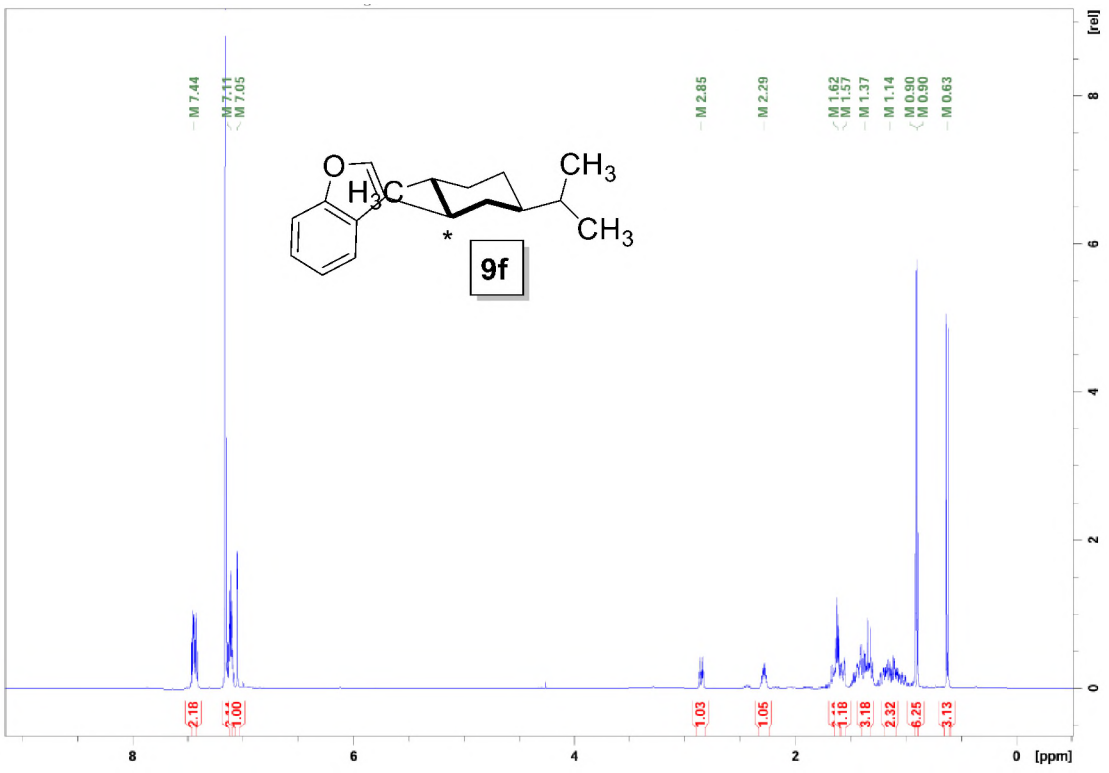

M 8.86
M 8.16
M 8.07
M 7.61
M 7.55
M 7.40
M 3.02
M 2.21
M 1.77
M 1.56
M 1.27
M 0.96
M 0.96
M 0.63
N
H3C
CH3
CH3
*
9e
1.11
1.12
1.04
1.14
1.14
4.17
2.13
2.33
2.09
6.32
5.10
10
8
6
4
2
0 [ppm]
20 [rel]
15
10
5
0

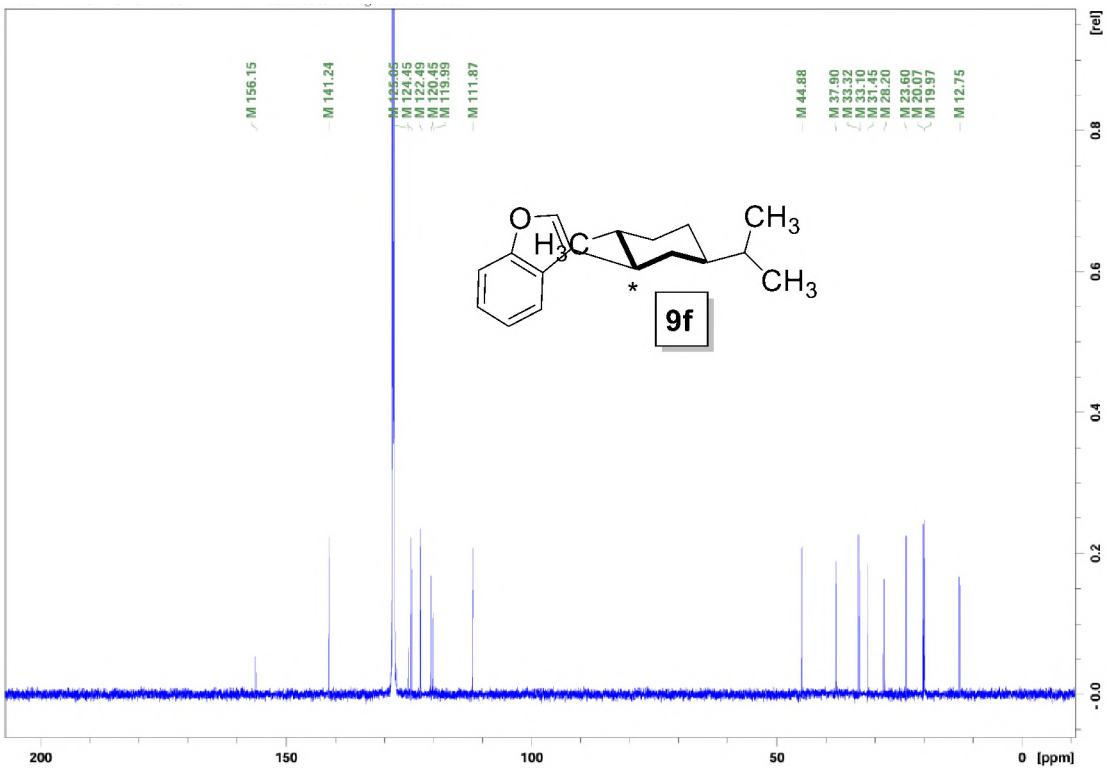

M 149.06
M 146.49
M 145.05
M 136.33
M 130.89
M 128.32
M 128.18
M 124.90
M 120.91
M 46.43
M 44.74
M 34.04
M 33.57
M 33.10
M 27.63
M 23.22
M 19.85
M 19.87
M 12.10
N
H3C
CH3
CH3
*
9e
200
150
100
50
0 [ppm]
[rel]
6
5
4
3
2
1
-0

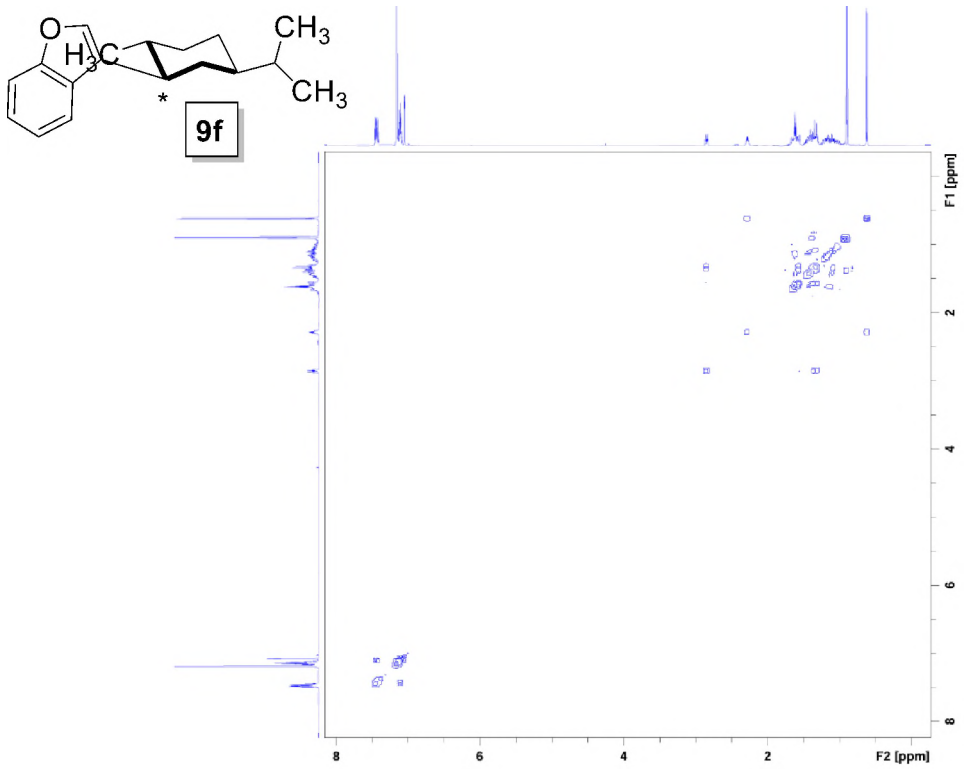

N
H3C
CH3
CH3
*
9e
F1 [ppm]
F2 [ppm]

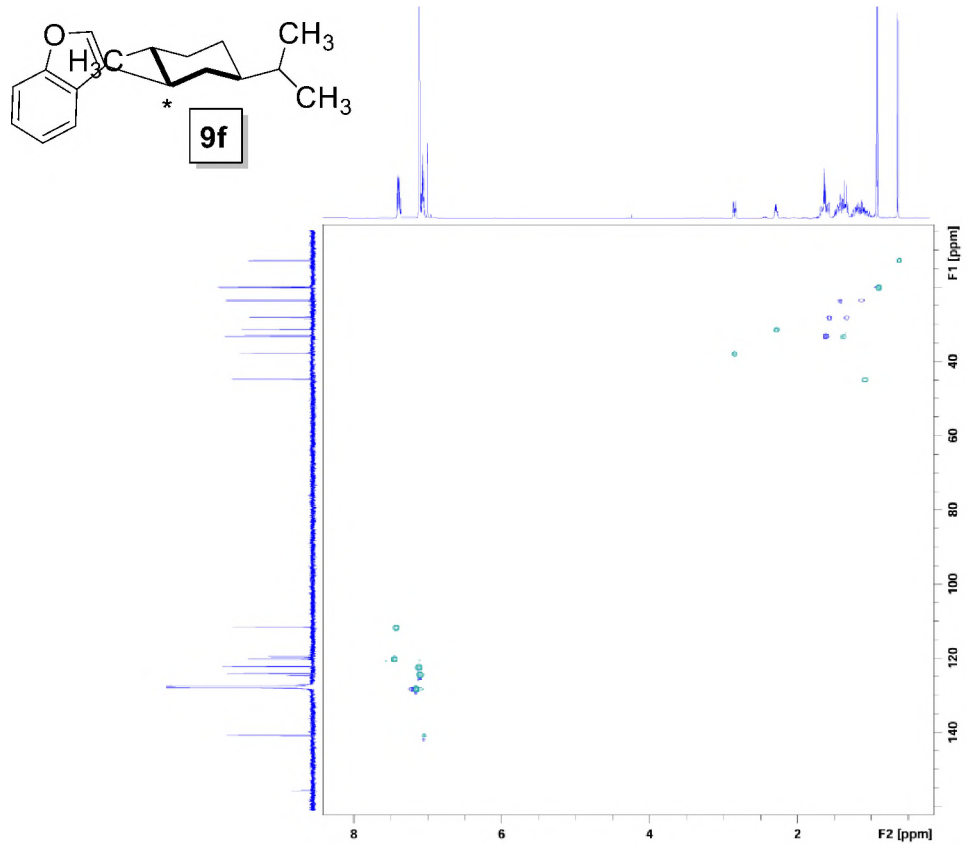

N
H3C
CH3
CH3
*
9e
F1 [ppm]
F2 [ppm]


N
H3C
CH3
CH3
*
9e
F1 [ppm]
F2 [ppm]
2
4
6
8


M 7.44
M 7.11
M 7.05
M 2.85
M 2.29
M 1.62
M 1.57
M 1.37
M 1.14
M 0.90
M 0.90
M 0.63
O
H3C
CH3
CH3
*
9f
2.18
2.00
1.03
1.05
1.18
3.18
2.32
6.25
3.13
[rel]
[ppm]


M 156.15
M 141.24
M 124.45
M 122.49
M 120.45
M 119.99
M 111.87
M 44.88
M 37.90
M 33.32
M 33.10
M 31.45
M 28.20
M 23.60
M 20.07
M 19.97
M 12.75
O
H3C
CH3
CH3
*
9f
[rel]
[ppm]

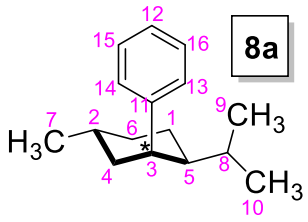

O
H3C
CH3
CH3
*
9f
F1 [ppm]
F2 [ppm]
8
6
4
2


O
H3C
CH3
CH3
*
9f
F1 [ppm]
F2 [ppm]
8
6
4
2
40
60
80
100
120
140

IV. Calculated ^{1}H and ^{13}C NMR Spectra

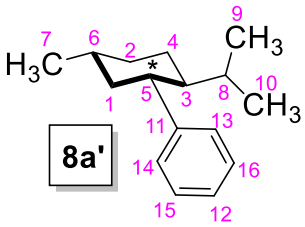
The calculations to obtain NMR spectra computationally for two model compounds, **8a** and **9a**, and their diastereomers, **8a'** and **9a'**, believed to be the corresponding minor products in the hydrogenation (not isolated), were conducted using SPARTAN'24 Quantum Mechanics Driver (Win/64), Release 1.3.0, single-point job type, method RWB97X-D, basis set 6-31G(D), number of basis functions 288, number of electrons 120. A SCF model was applied to perform a restricted hybrid HF-DFT SCF calculation, using Pulay DIIS + Geometric Direct Minimization.

- Compound **8a** (isolated) – Calculated NMR chemical shifts



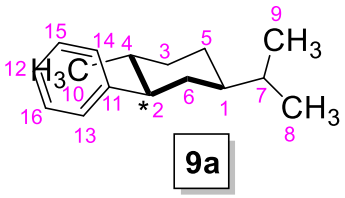
position	δ_C	mult	δ_H	splitting (Hz)	HMBC(H→C) (2,3-bond)
1	28.0	CH_2	1.93	dd (12.9, 12.3)	2, 3, 5, 6, 8
.			2.01	dd (4.3, 4.1)	2, 3, 5, 6, 8
2	24.3	CH	2.07	m (12.5, 12.4, 6.4$_{x3}$, 2.7)	1, 3, 4, 6, 7
3	43.6	CH	3.26	ddd (5.3, 5.3, 1.7)	1, 2, 4, 5, 8, 11, 13, 14
4	41.5	CH_2	1.80	ddd (-13.1, 2.7, 1.7)	2, 3, 5, 6, 7, 11
.			1.57	ddd (-13.1, 12.5, 5.3)	2, 3, 5, 6, 7, 11
5	44.9	CH	1.57	ddd (12.3, 5.3, 4.1)	1, 3, 4, 6, 8, 9, 10, 11
6	33.6	CH_2	1.98	d (-13.0)	1, 2, 4, 5, 7
.			1.29	m (-13.0, 12.9, 12.4, 4.3)	1, 2, 4, 5, 7
7	22.7	CH_3	0.86	d (6.4)	2, 4, 6
8	29.8	CH	1.63	m (6.4$_{x6}$)	1, 3, 5, 9, 10
9	21.3	CH_3	0.94	d (6.4)	5, 8, 10
10	20.9	CH_3	0.82	d (6.4)	5, 8, 9
11	144.1	C			...
12	125.3	CH	7.26	s	13, 14, 15, 16
13	129.5	CH	7.42	s	3, 11, 12, 14, 16
14	129.5	CH	7.42	s	3, 11, 12, 13, 15
15	127.7	CH	7.34	s	11, 12, 14, 16
16	127.7	CH	7.34	s	11, 12, 13, 15

- Diastereomer **8a'** (not isolated) – Calculated NMR chemical shifts



position	δ_C	mult	δ_H	splitting (Hz)	HMBC(H→C) (2,3-bond)
1	43.7	CH_2	1.46	ddd (-13.7, 12.8, 12.4)	2, 3, 5, 6, 7, 11
.			1.93	ddd (-13.7, 3.0, 2.7)	2, 3, 5, 6, 7, 11
2	33.9	CH_2	1.91	ddd (-12.9, 3.4, 3.0)	1, 3, 4, 6, 7
.			1.31	m (13.3, -12.9, 12.4, 3.3)	1, 3, 4, 6, 7
3	47.0	CH	1.85	ddd (12.7, 12.0, 2.9)	1, 2, 4, 5, 8, 9, 10, 11
4	24.4	CH_2	1.87	dd (-13.0, 3.3)	2, 3, 5, 6, 8
.			1.47	m (13.3, -13.0, 12.7, 3.4)	2, 3, 5, 6, 8
5	48.1	CH	2.71	ddd (12.8, 12.0, 2.7)	1, 3, 4, 6, 8, 11, 13, 14
6	32.0	CH	1.79	m (12.4, 12.4, 6.4_{x3}, 3.0, 3.0)	1, 2, 4, 5, 7
7	22.5	CH_3	0.98	d (6.4)	1, 2, 6
8	27.3	CH	1.57	m (6.4_{x3}, 6.4_{x3}, 2.9)	3, 4, 5, 9, 10
9	21.5	CH_3	0.87	d (6.4)	3, 8, 10
10	14.9	CH_3	0.78	d (6.4)	3, 8, 9
11	144.7	C			...
12	125.5	CH	7.24	s	13, 14, 15, 16
13	127.0	CH	7.27	s	5, 11, 12, 14, 16
14	127.0	CH	7.27	s	5, 11, 12, 13, 15
15	128.0	CH	7.33	s	11, 12, 14, 16
16	128.0	CH	7.33	s	11, 12, 13, 15

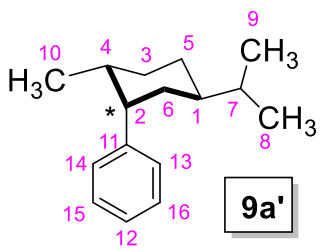
- Compound **9a** (isolated) – Calculated NMR chemical shifts



9a

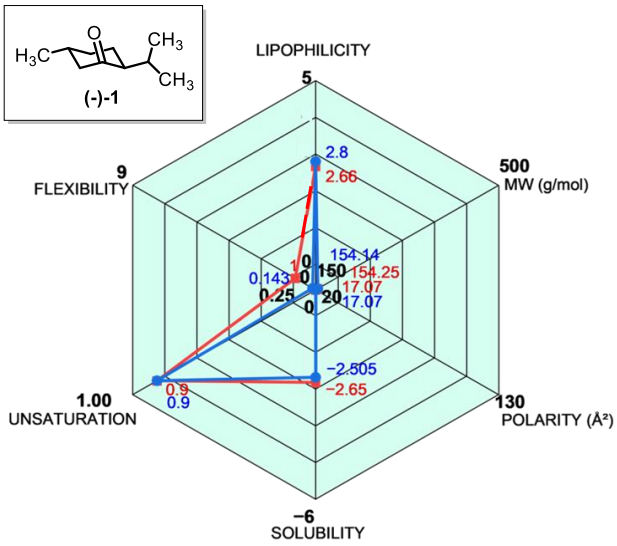
position	δ_C	mult	δ_H	splitting (Hz)	HMBC(H→C) (2,3-bond)
1	42.7	CH	1.70	ddd (12.7, 2.6, 2.2)	2, 3, 5, 6, 7, 8, 9
2	51.7	CH	2.25	ddd (12.8, 11.8, 2.7)	1, 3, 4, 6, 10, 11, 13, 14
3	34.5	CH_2	1.92	ddd (-13.1, 3.4, 3.1)	1, 2, 4, 5, 10
.			1.41	m (13.3, -13.1, 12.4, 3.4)	1, 2, 4, 5, 10
4	37.5	CH	1.91	m (12.4, 11.8, 6.4_{x3})	2, 3, 5, 6, 10, 11
5	31.8	CH_2	1.61	ddd (-12.5, 3.4, 3.1)	1, 3, 4, 6, 7
.			1.75	ddd (13.3, -12.5, 3.4)	1, 3, 4, 6, 7
6	33.9	CH_2	1.89	ddd (-13.3, 2.7, 2.6)	1, 2, 4, 5, 7, 11
.			1.54	ddd (-13.3, 12.8, 12.7)	1, 2, 4, 5, 7, 11
7	32.4	CH	1.85	m (6.4_{x3}, 6.4_{x3}, 2.2)	1, 5, 6, 8, 9
8	21.9	CH_3	1.01	d (6.4)	1, 7, 9
9	15.7	CH_3	0.92	d (6.4)	1, 7, 8
10	20.7	CH_3	0.68	d (6.4)	2, 3, 4
11	145.3	C			...
12	125.5	CH	7.24	s	13, 14, 15, 16
13	127.0	CH	7.24	s	2, 11, 12, 14, 16
14	127.0	CH	7.24	s	2, 11, 12, 13, 15
15	128.0	CH	7.32	s	11, 12, 14, 16
16	128.0	CH	7.32	s	11, 12, 13, 15

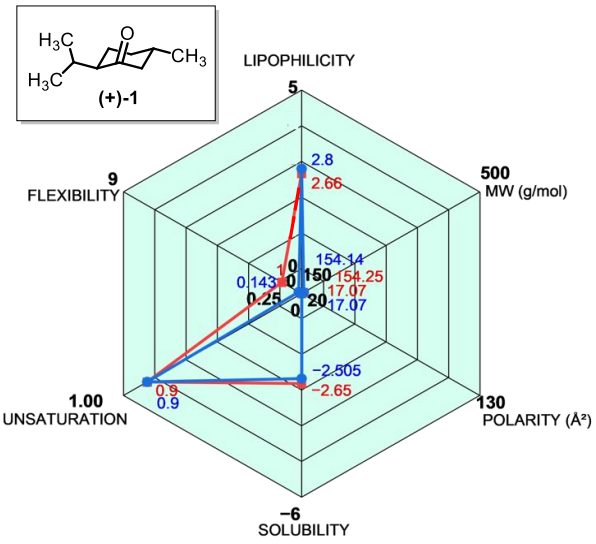
- Diastereomer **9a'** (not isolated) – Calculated NMR chemical shifts



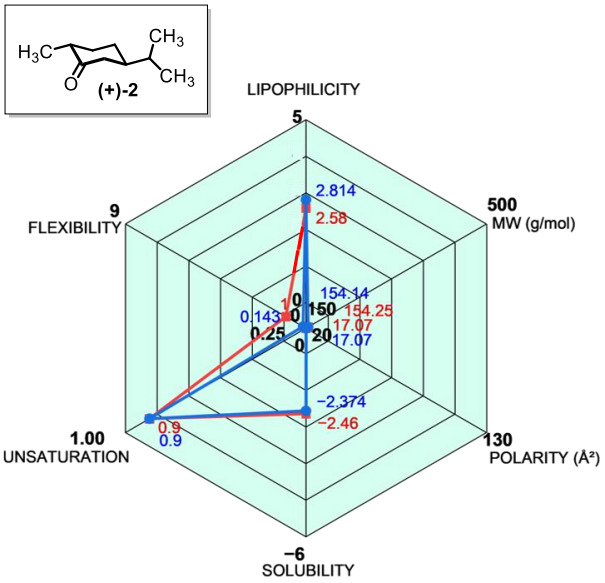
position	δ_C	mult	δ_H	splitting (Hz)	HMBC(H→C) (2,3-bond)
1	37.8	CH	1.92	m (12.4, 12.4, 11.6, 3.9_{x2})	2, 3, 5, 6, 7, 8, 9
2	46.5	CH	2.96	ddd (5.9, 4.7, 1.4)	1, 3, 4, 6, 10, 11, 13, 14
3	28.4	CH_2	1.57	m (-14.7, 3.8, 3.0, 2.9)	1, 2, 4, 5, 10
.			1.90	ddd (-14.7, 13.1, 3.8)	1, 2, 4, 5, 10
4	34.1	CH	1.98	m (6.4_{x3}, 4.7, 3.0)	2, 3, 5, 6, 10, 11
5	30.3	CH_2	2.28	m (-12.8, 3.9, 3.8, 2.9)	1, 3, 4, 6, 7
.			1.24	m (13.1, -12.8, 12.4, 3.8)	1, 3, 4, 6, 7
6	36.4	CH_2	2.28	ddd (-13.2, 3.9, 1.4)	1, 2, 4, 5, 7, 11
.			1.50	ddd (-13.2, 12.4, 5.9)	1, 2, 4, 5, 7, 11
7	34.7	CH	1.40	m ($11.6, 6.4_{x6}$)	1, 5, 6, 8, 9
8	21.1	CH_3	0.91	d (6.4)	1, 7, 9
9	21.2	CH_3	1.05	d (6.4)	1, 7, 8
10	20.6	CH_3	0.65	d (6.4)	2, 3, 4
11	143.5	C			...
12	125.6	CH	7.27	s	13, 14, 15, 16
13	129.2	CH	7.42	d (7.7)	2, 11, 12, 14, 16
14	129.2	CH	7.42	d (7.3)	2, 11, 12, 13, 15
15	127.6	CH	7.32	d (7.3)	11, 12, 14, 16
16	127.6	CH	7.32	d (7.7)	11, 12, 13, 15

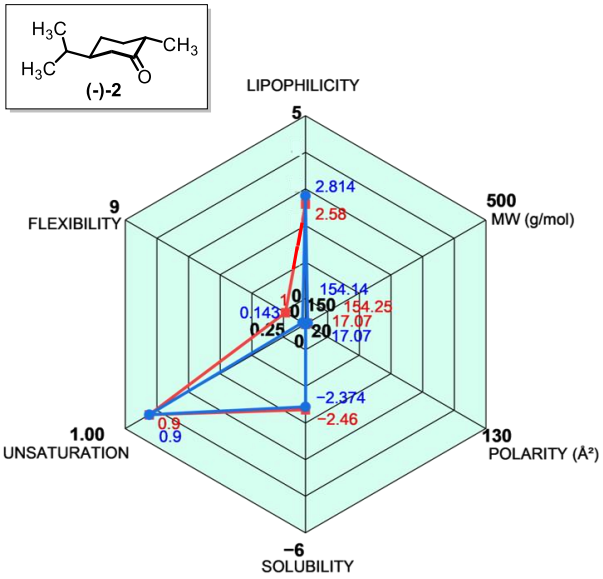
V. ADMET Computational Study of Synthesized Compounds and Known CB1/2 Ligands



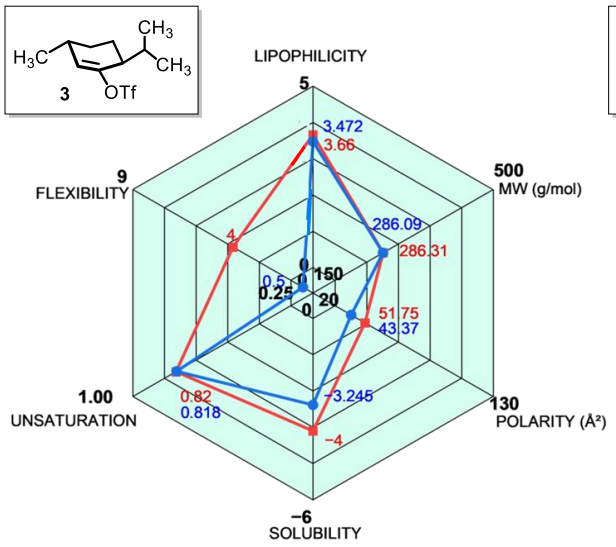


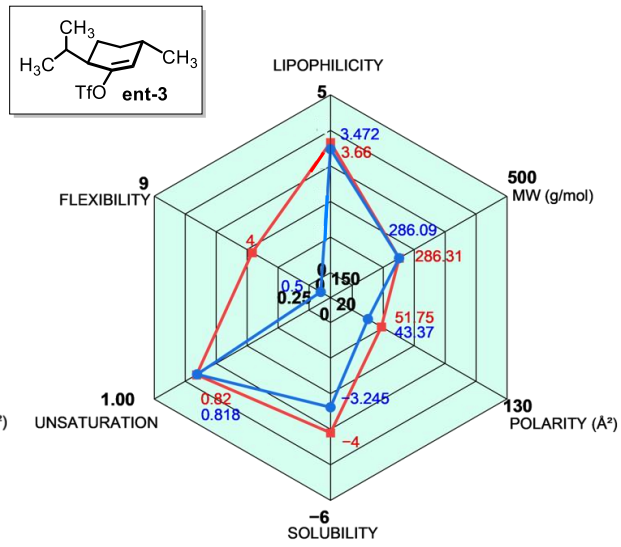
Compound	(-)-1	(+)-1
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-5.08/-1.909	-5.08/-1.909
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



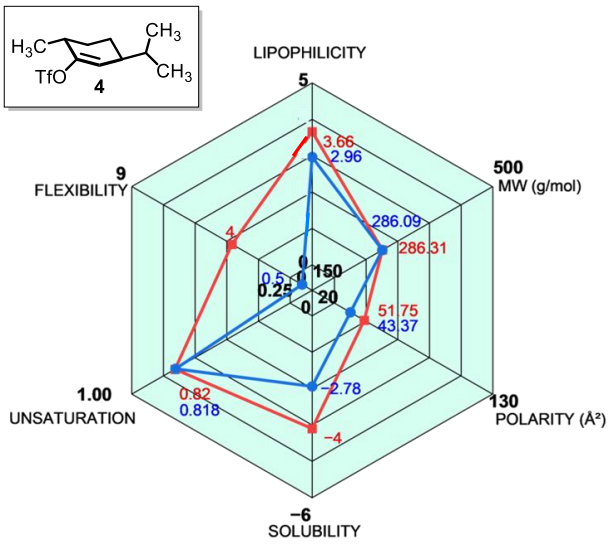


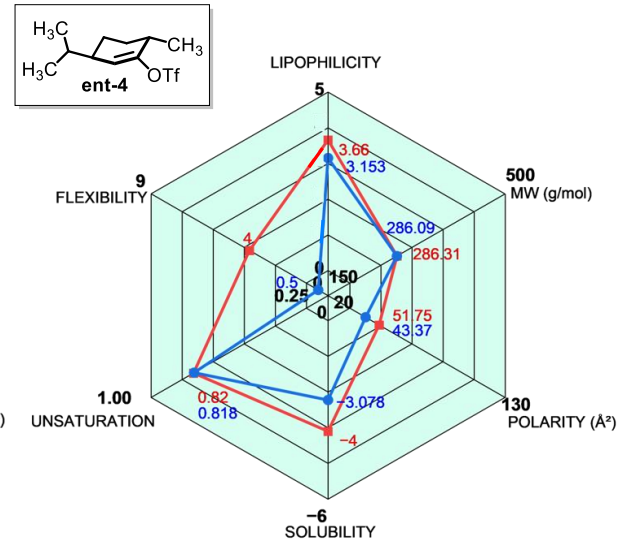
Compound	(+)-2	(-)-2
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-5.30/-1.909	-5.30/-1.909
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



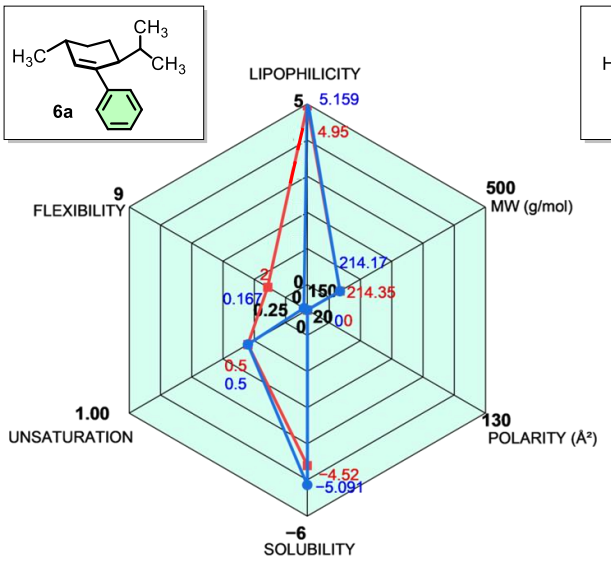


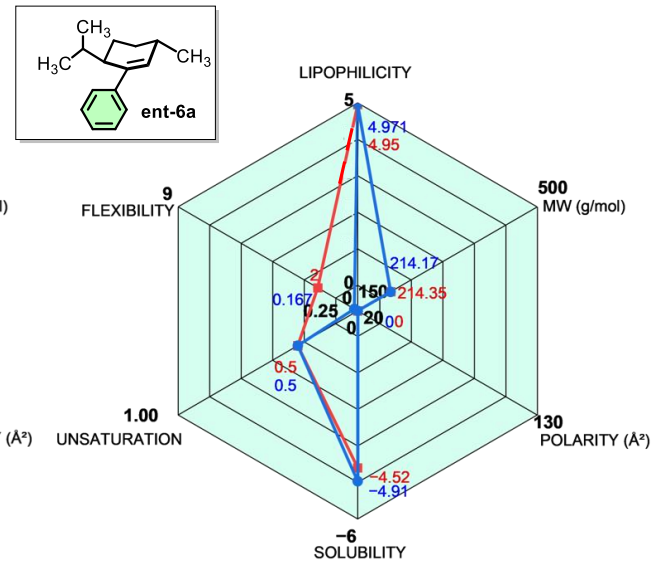
Compound	3	ent-3
BBB permeability	No/Yes	No/Yes
Skin permeability (cm.s^{-1})	-5.06/-2.343	-5.06/-2.343
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



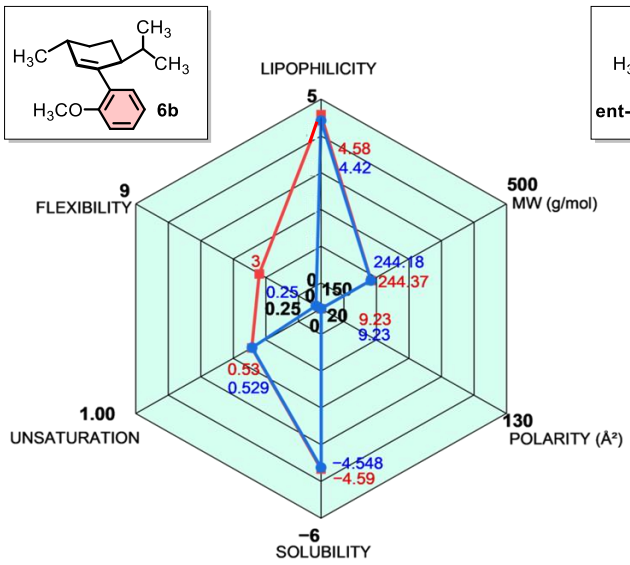


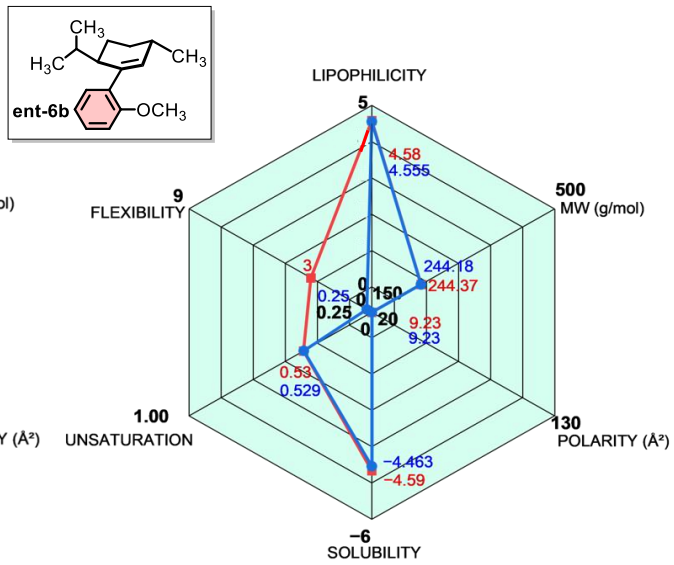
Compound	4	ent-4
BBB permeability	No/Yes	No/Yes
Skin permeability (cm.s^{-1})	-5.06/-2.339	-5.06/-2.339
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



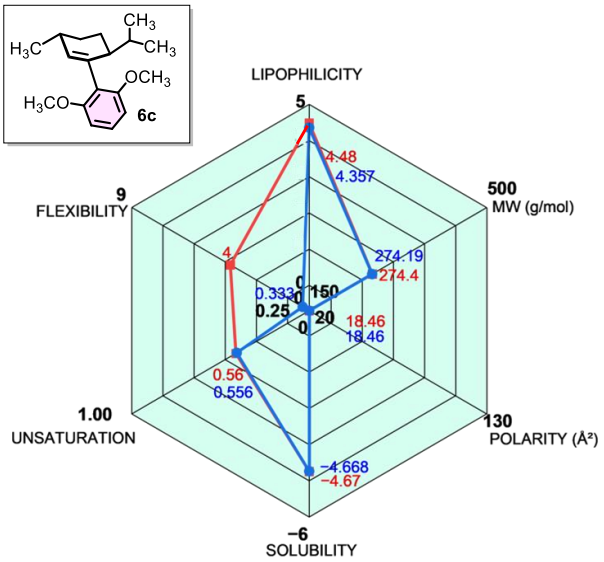


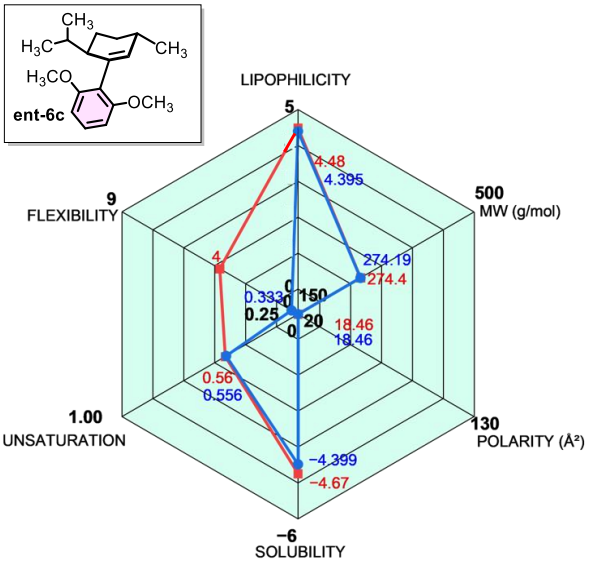
Compound	6a	ent-6a
BBB permeability	No/Yes	No/Yes
Skin permeability (cm.s^{-1})	-3.99/-1.506	-3.99/-1.506
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



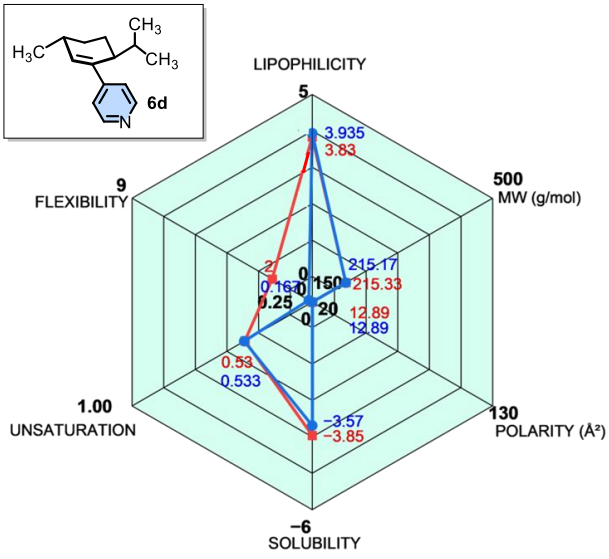


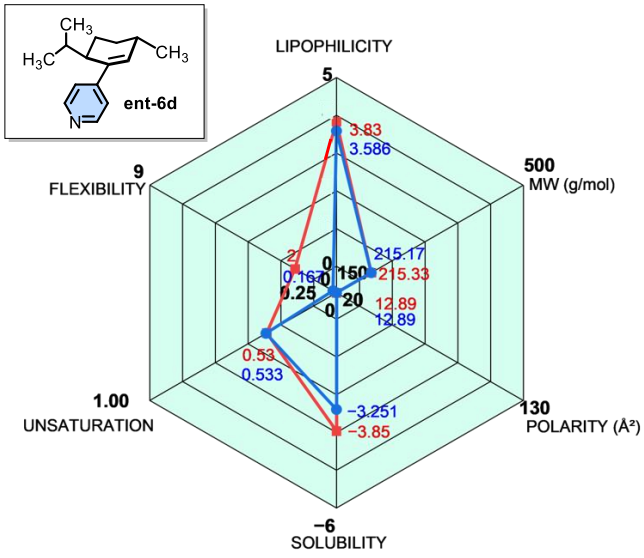
Compound	6b	ent-6b
BBB permeability	Yes/No	Yes/No
Skin permeability (cm.s^{-1})	-4.2/-1.7	-4.2/-1.7
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



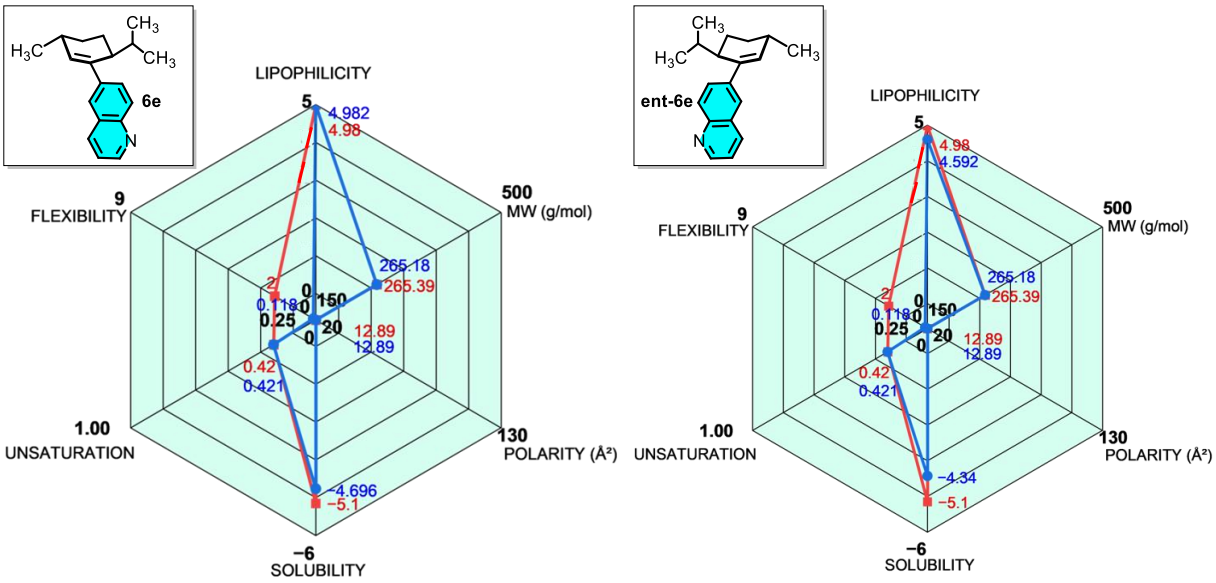


Compound	6c	ent-6c
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.4/-2.146	-4.4/-2.146
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes

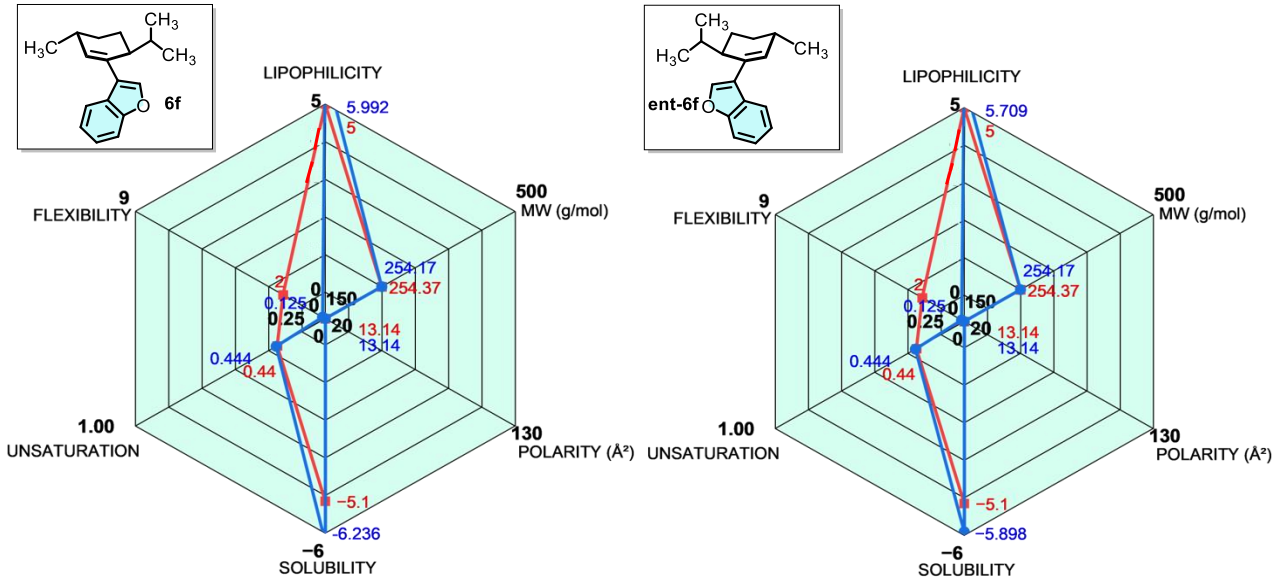




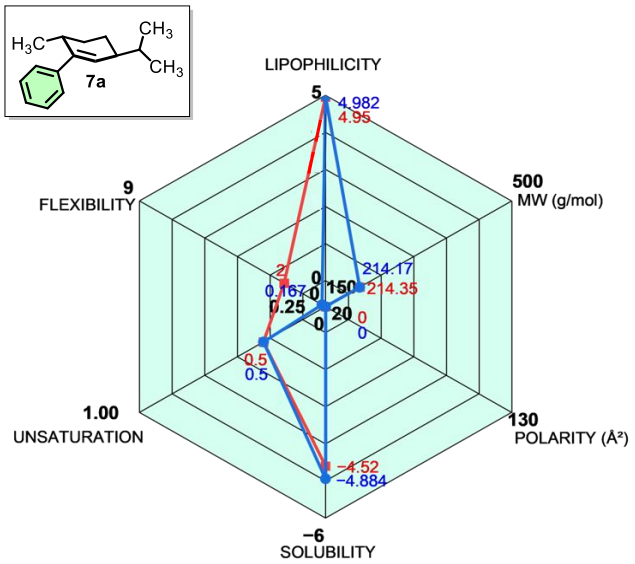
Compound	6d	ent-6d
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.76/-1.513	-4.76/-1.513
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes

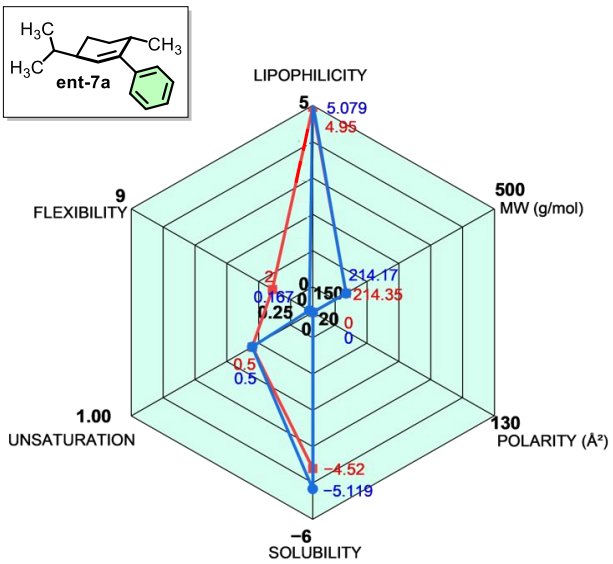


Compound	6e	ent-6e
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.11/-1.95	-4.11/-1.95
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes

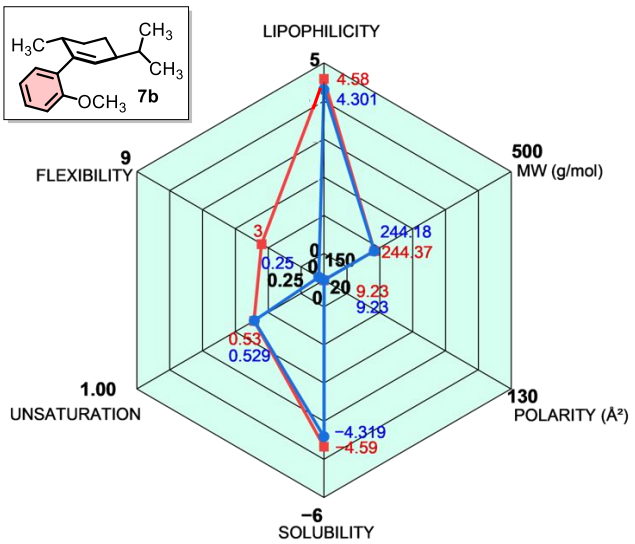


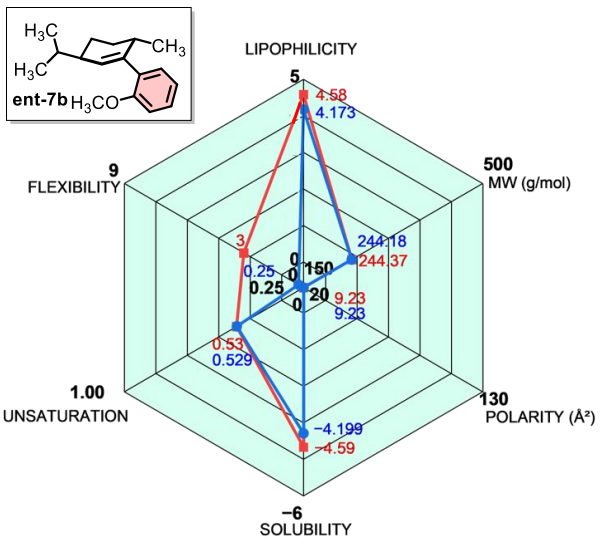
Compound	6f	ent-6f
BBB permeability	No/Yes	No/Yes
Skin permeability (cm.s^{-1})	-3.95/-1.854	-3.95/-1.854
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



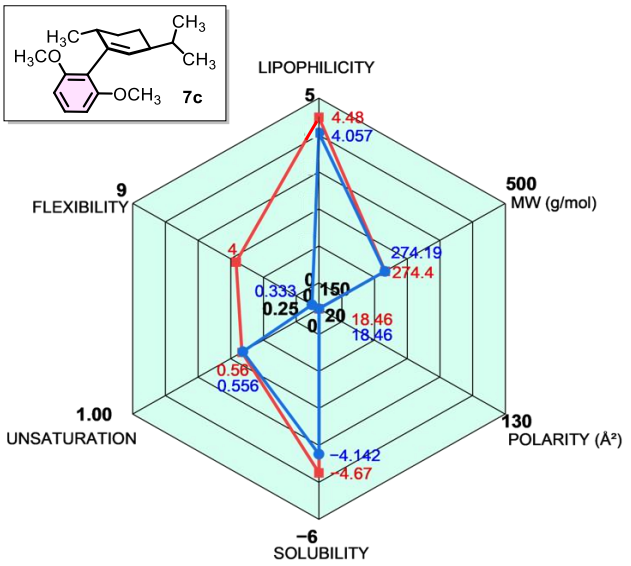


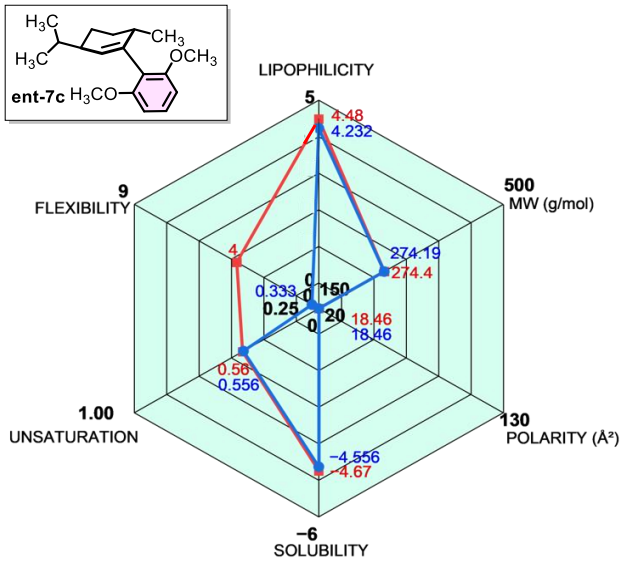
Compound	7a	ent-7a
BBB permeability	No/Maybe	No/Maybe
Skin permeability (cm.s^{-1})	-3.99/-1.456	-3.99/-1.456
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



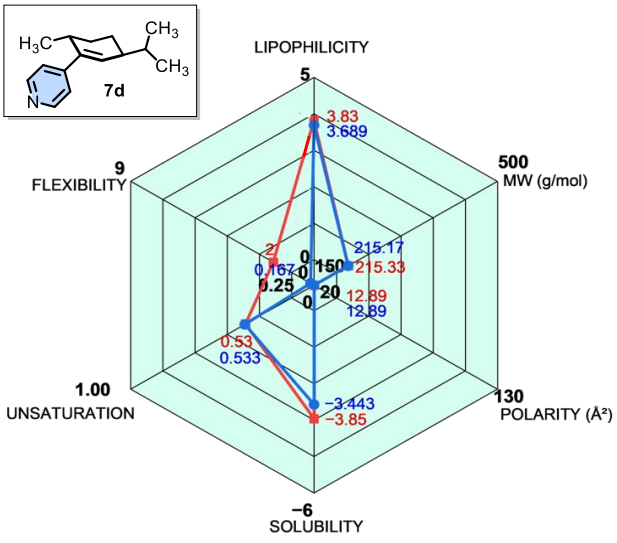


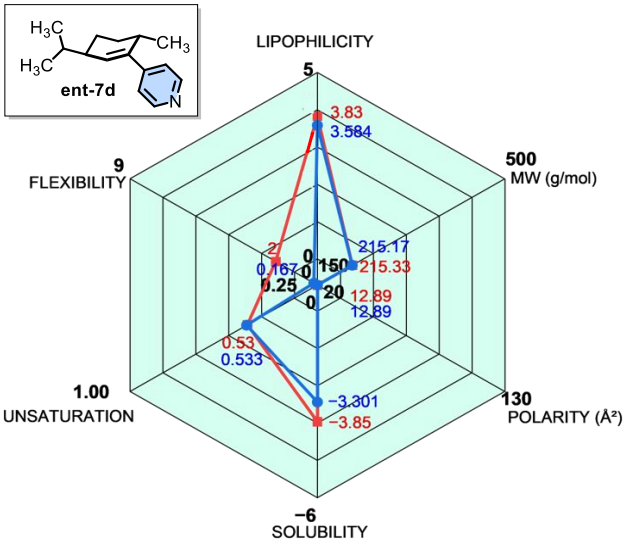
Compound	7b	ent-7b
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.2/-1.992	-4.2/-1.992
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



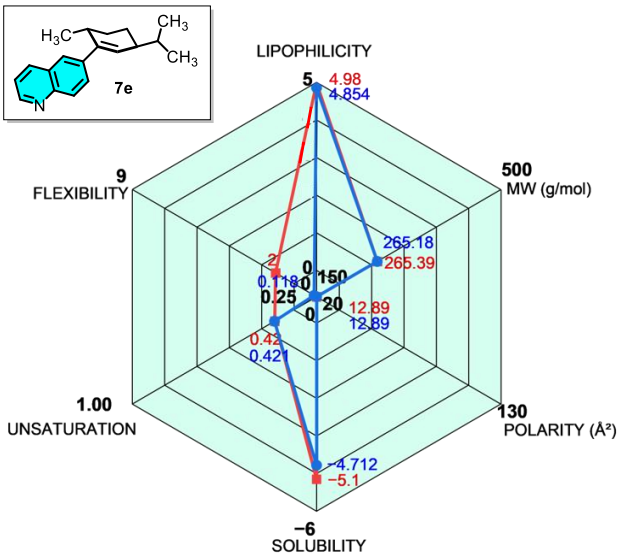


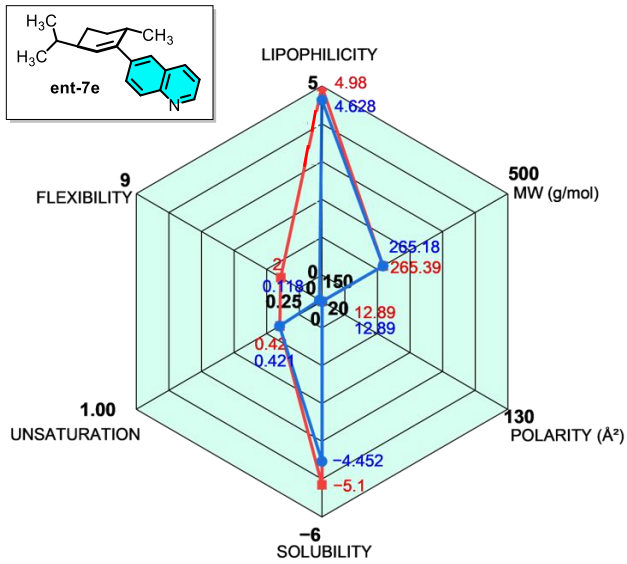
Compound	7c	ent-7c
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.4/-2.263	-4.4/-2.263
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



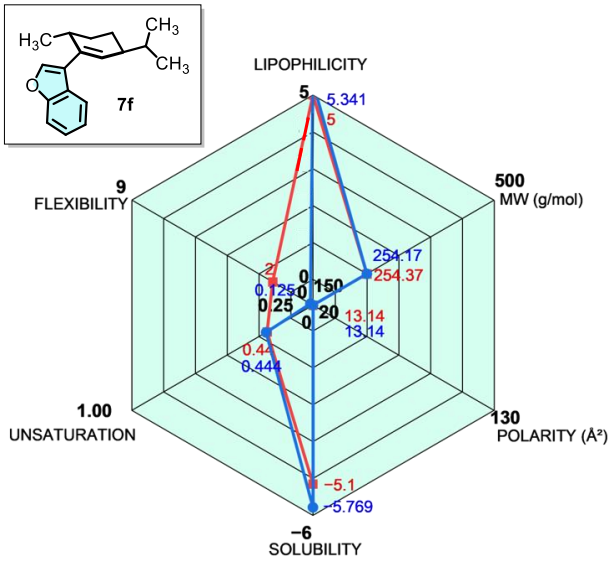


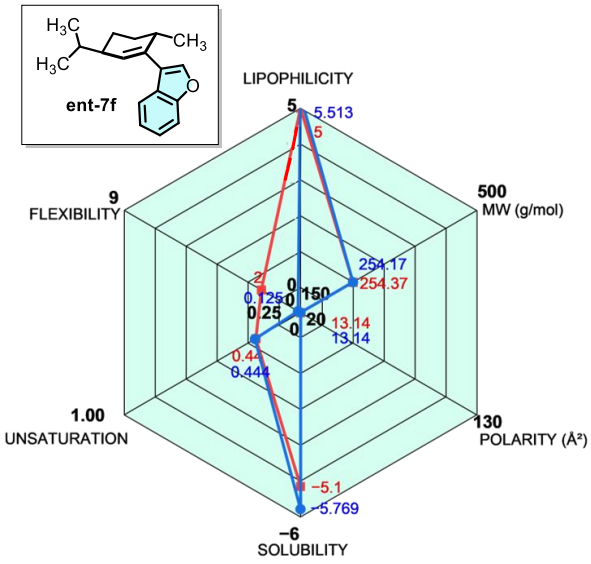
Compound	7d	ent-7d
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.76/-1.545	-4.76/-1.545
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



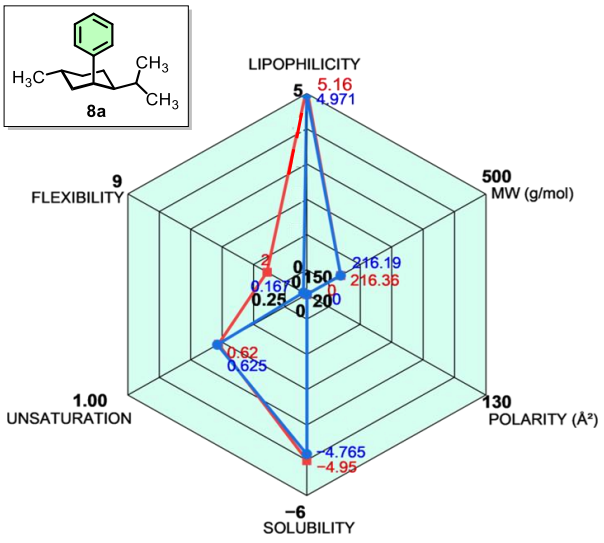


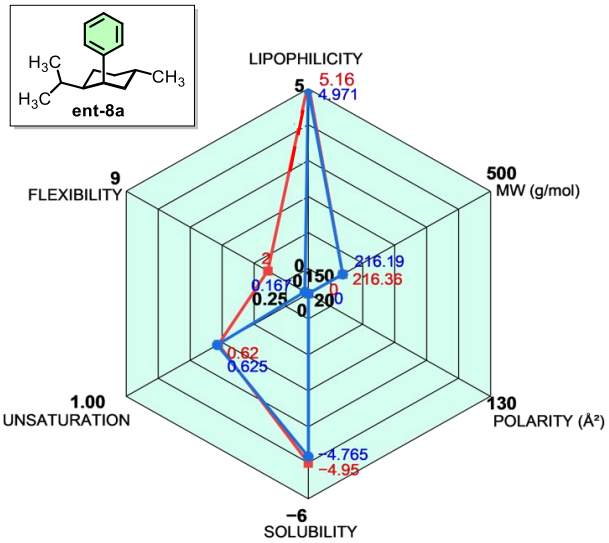
Compound	7e	ent-7e
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.11/-1.919	-4.11/-1.919
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



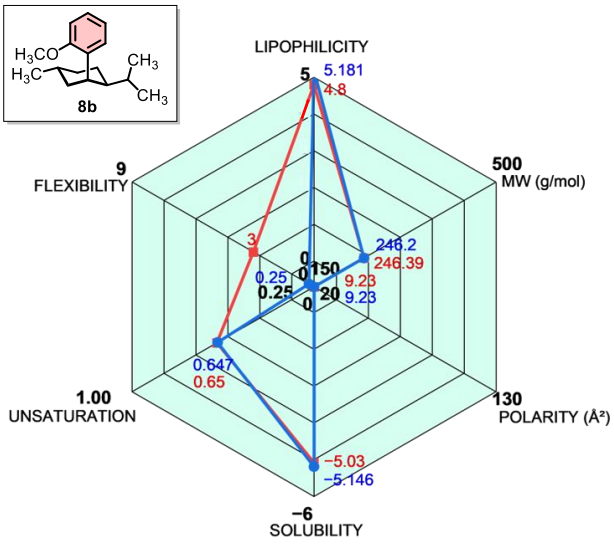


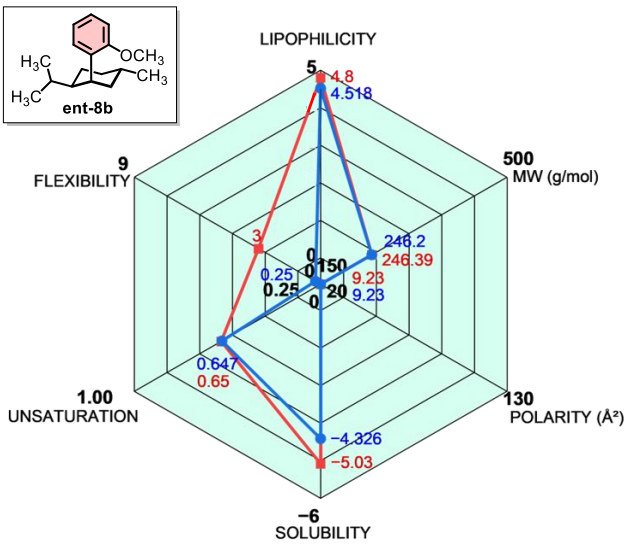
Compound	7f	ent-7f
BBB permeability	No/Maybe	No/Maybe
Skin permeability (cm.s^{-1})	-3.95/-1.897	-3.95/-1.897
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



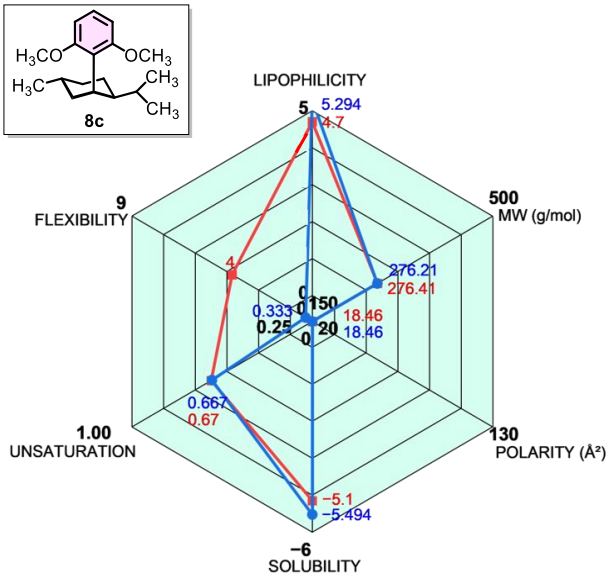


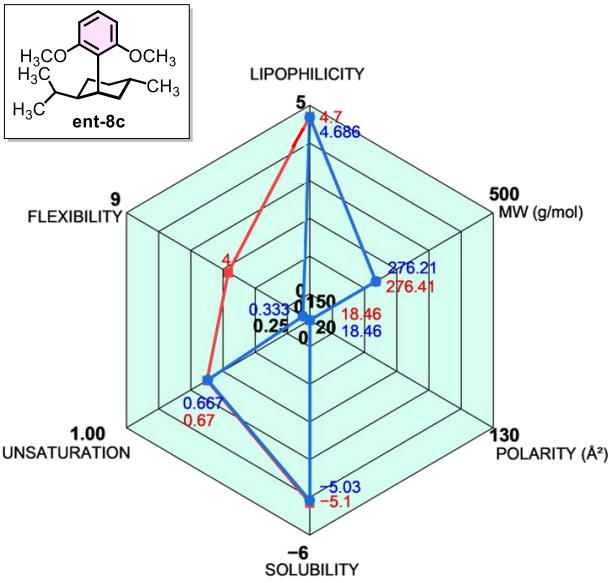
Compound	8a	ent-8a
BBB permeability	No/Maybe	No/Maybe
Skin permeability (cm.s^{-1})	-3.54/-2.165	-3.54/-2.165
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



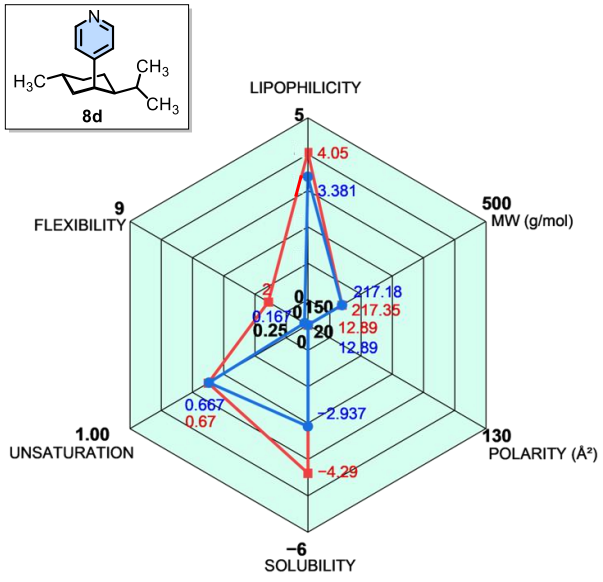


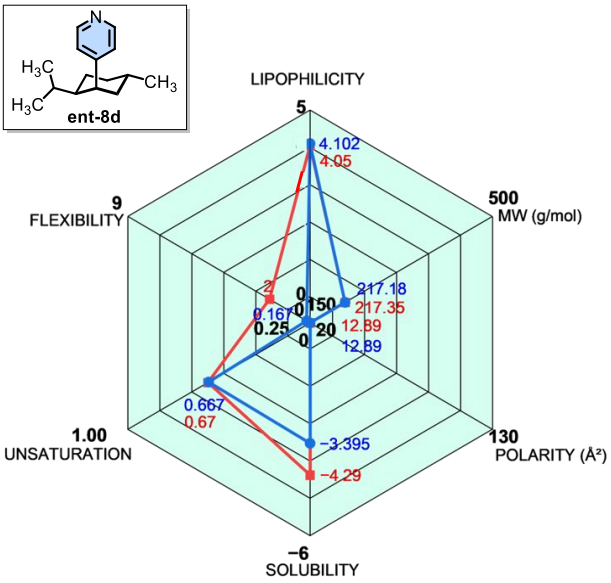
Compound	8b	ent-8b
BBB permeability	Yes/No	Yes/No
Skin permeability (cm.s^{-1})	-3.73/-2.069	-3.73/-2.069
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



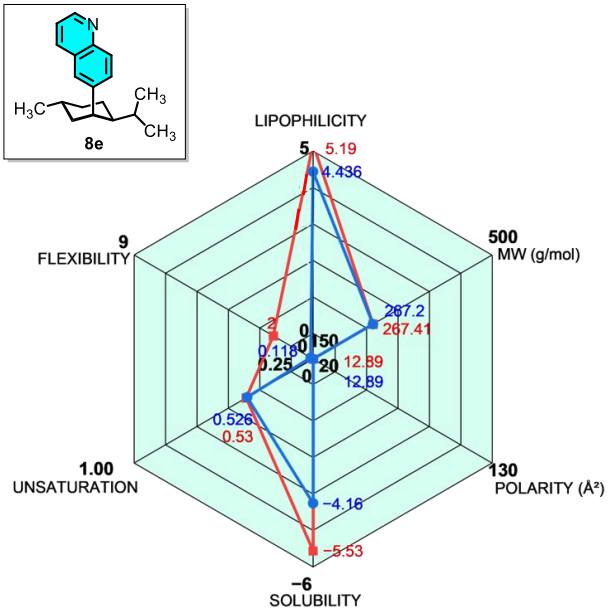


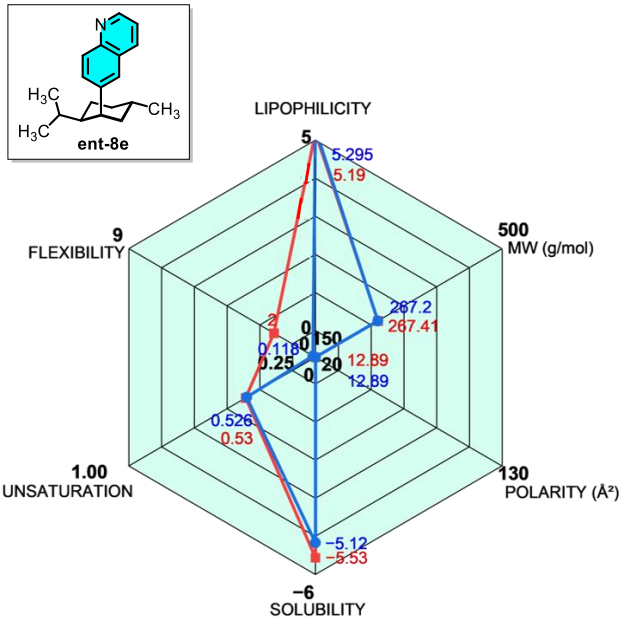
Compound	8c	ent-8c
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-3.94/-2.182	-3.94/-2.182
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



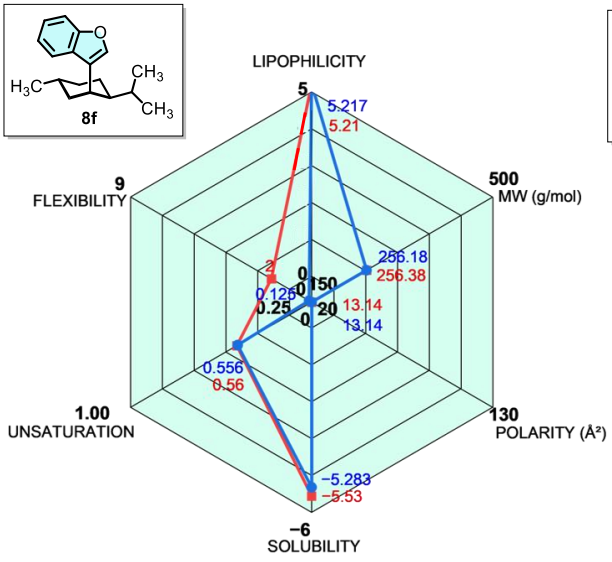


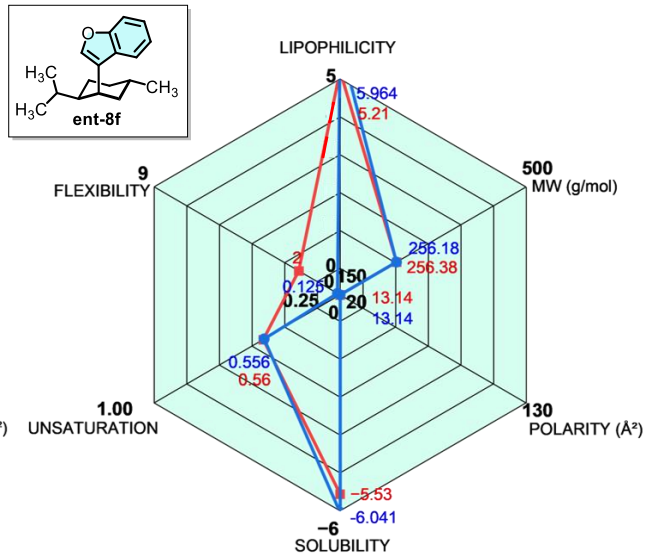
Compound	8d	ent-8d
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.3/-1.489	-4.3/-1.489
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



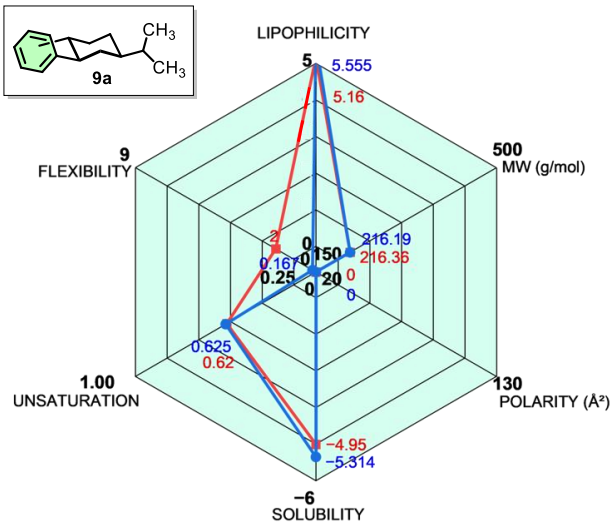


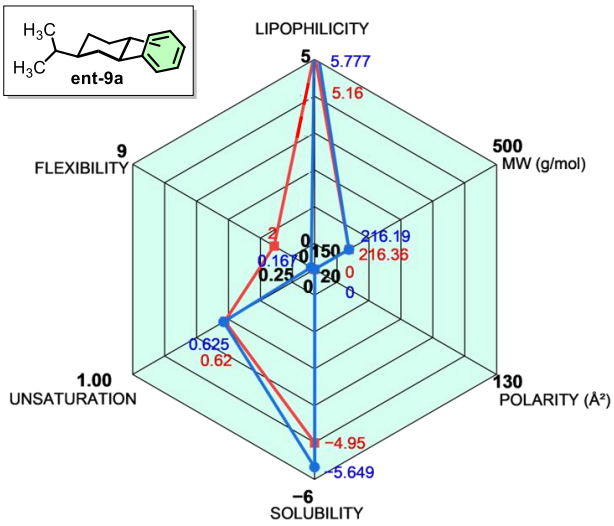
Compound	8e	ent-8e
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-3.66/-2.237	-3.66/-2.237
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



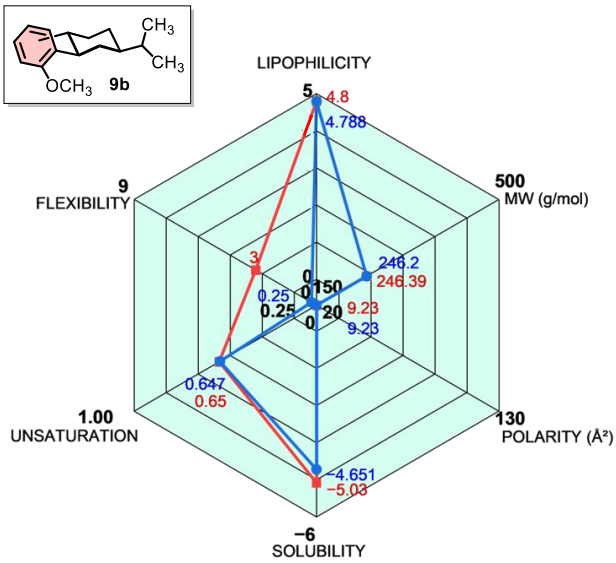


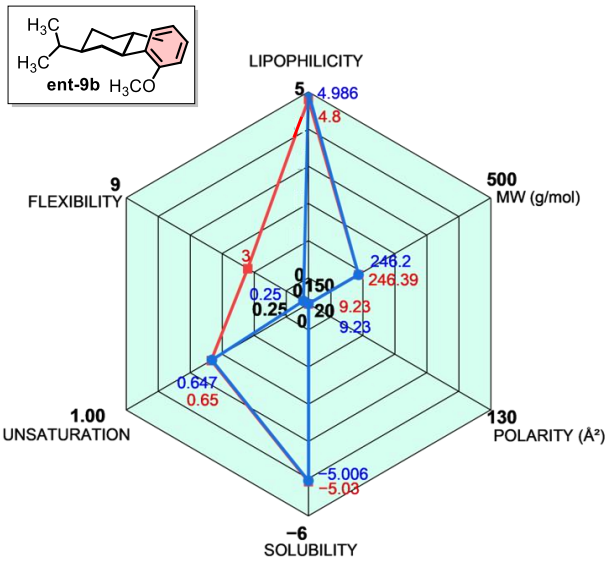
Compound	8f	ent-8f
BBB permeability	No/Yes	No/Yes
Skin permeability (cm.s^{-1})	-3.49/-2.173	-3.49/-2.173
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



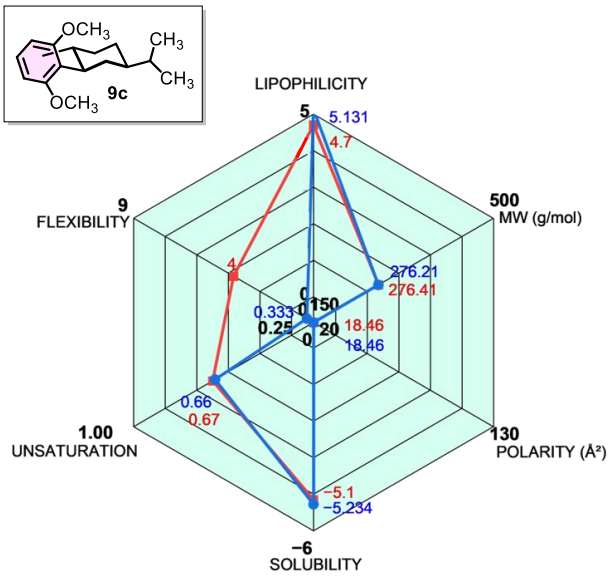


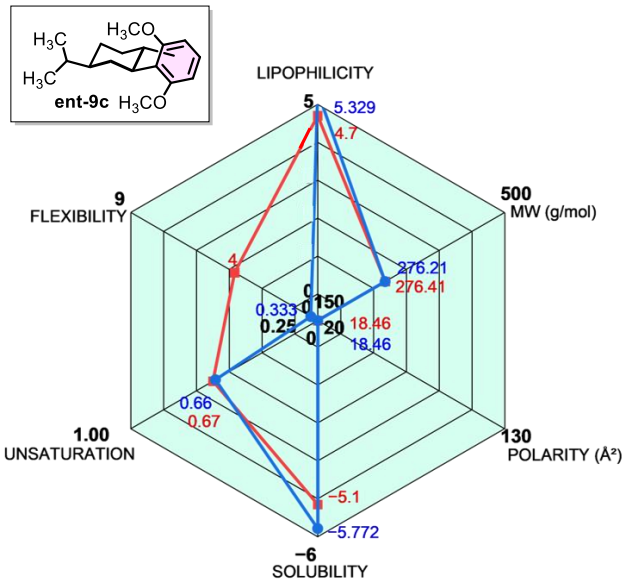
Compound	9a	ent-9a
BBB permeability	No/Maybe	No/Maybe
Skin permeability (cm.s^{-1})	-3.54/-1.975	-3.54/-1.975
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



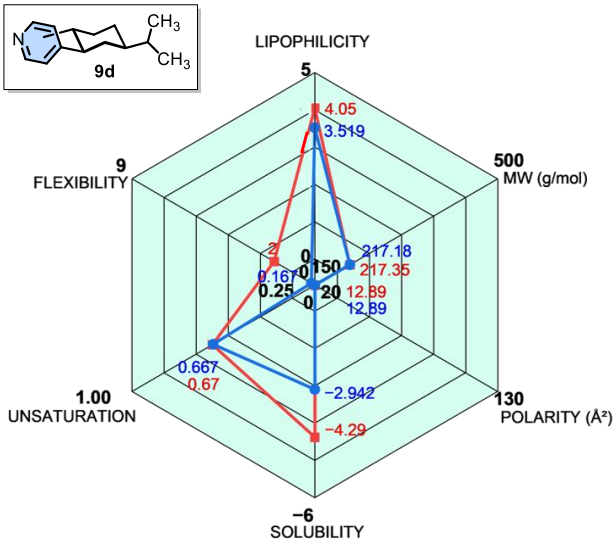


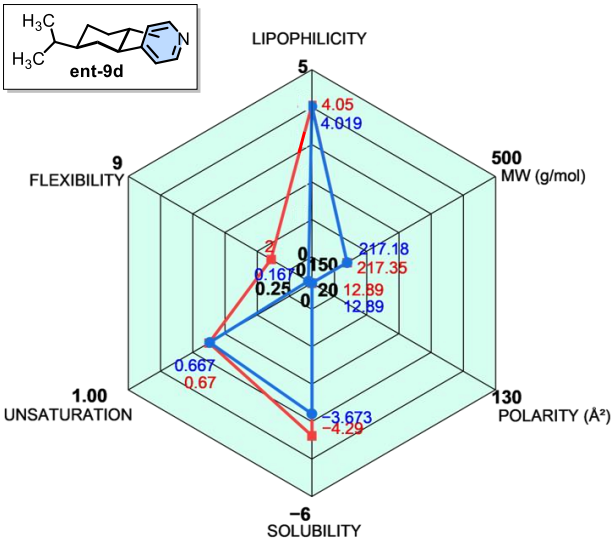
Compound	9b	ent-9b
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-3.73/-2.061	-3.73/-2.061
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



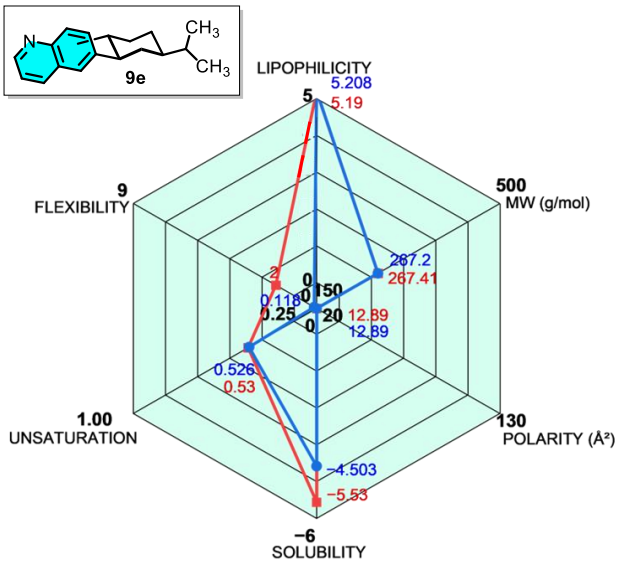


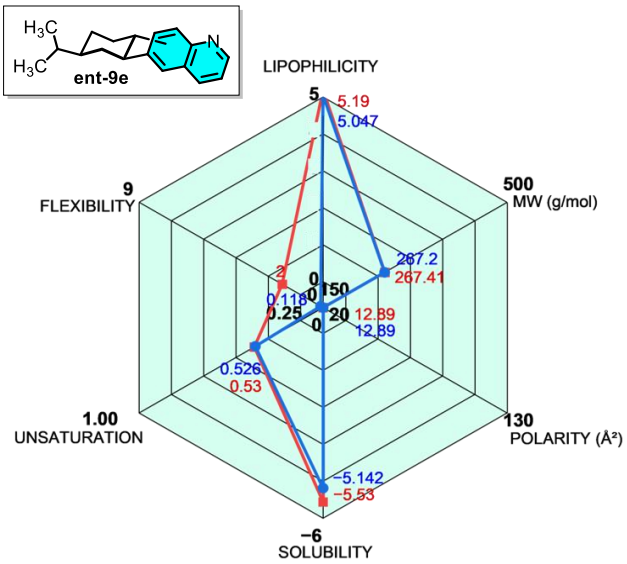
Compound	9c	ent-9c
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-3.94/-2.201	-3.94/-2.201
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



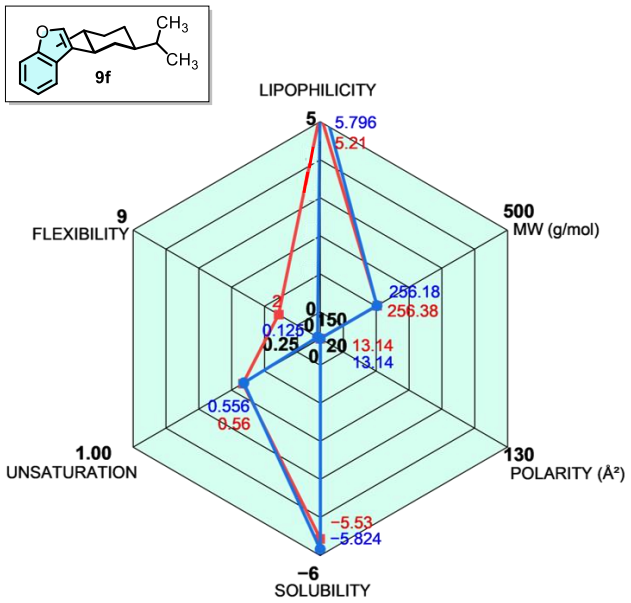


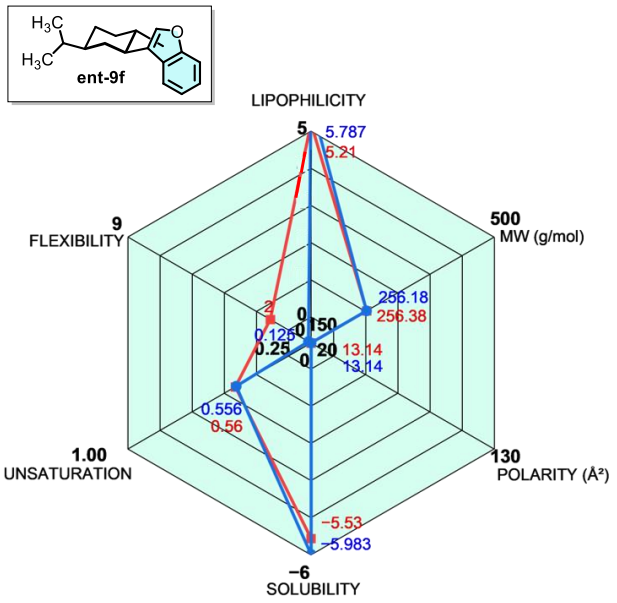
Compound	9d	ent-9d
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-4.3/-1.477	-4.3/-1.477
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes



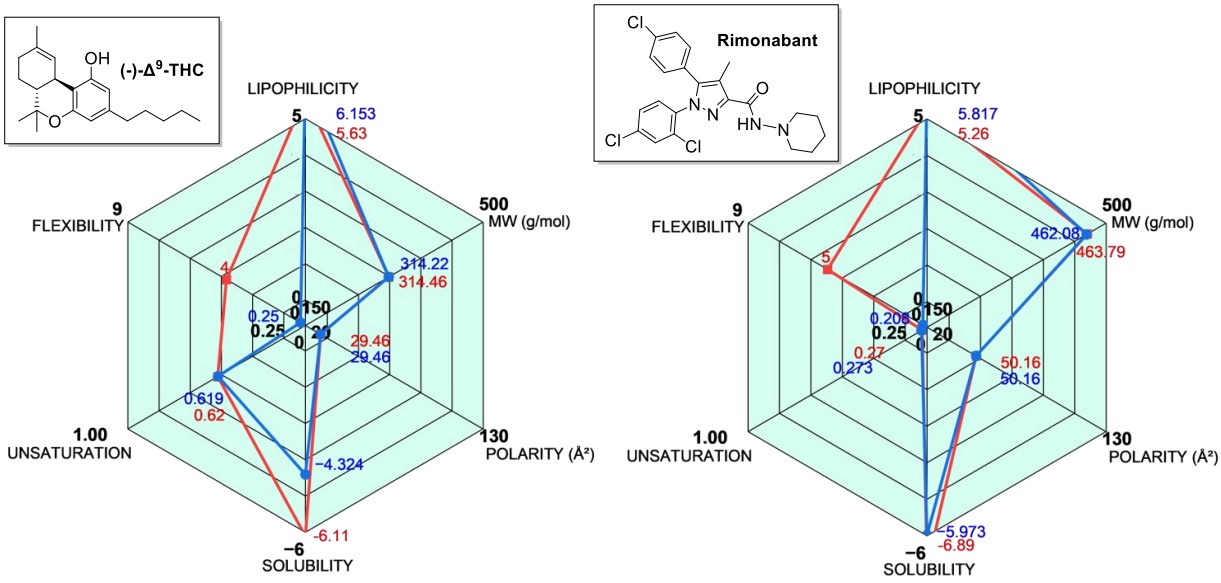


Compound	9e	ent-9e
BBB permeability	Yes/Yes	Yes/Yes
Skin permeability (cm.s^{-1})	-3.66/-2.128	-3.66/-2.128
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes





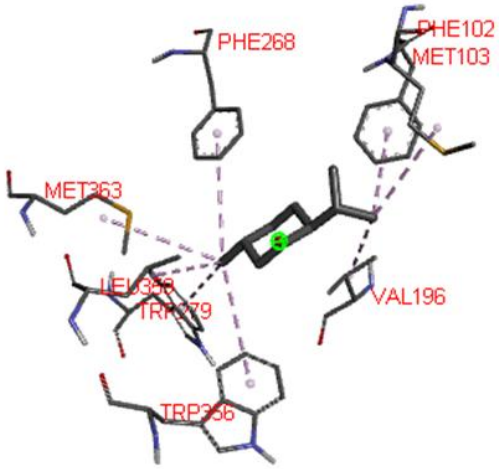
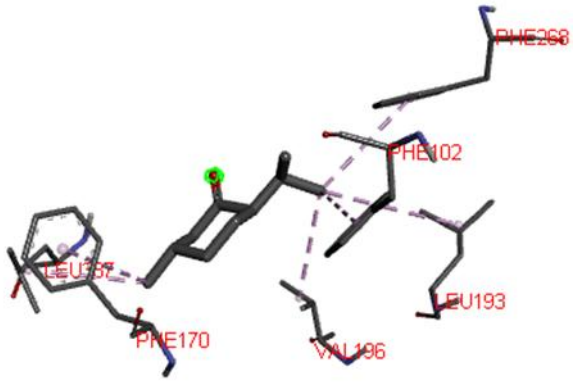
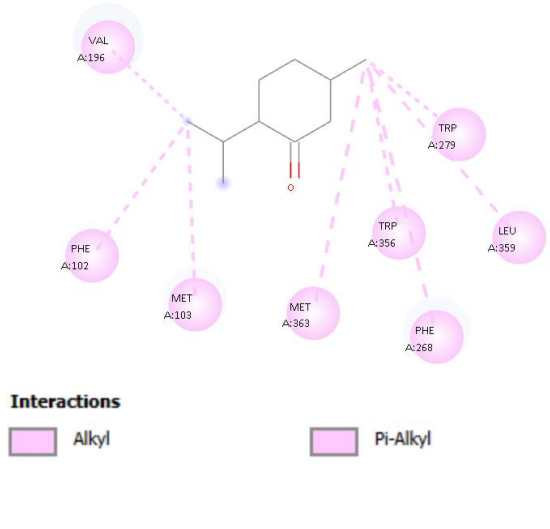
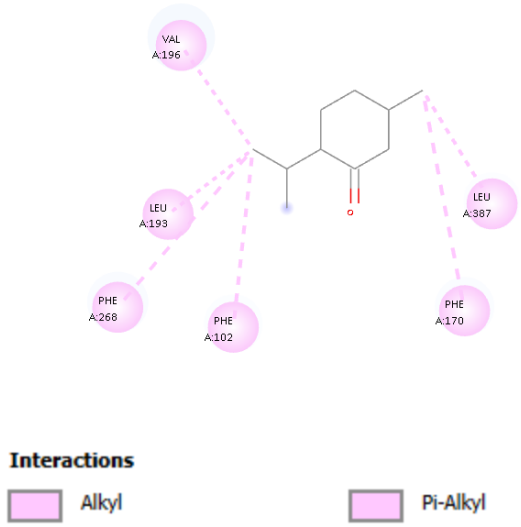
Compound	9f	ent-9f
BBB permeability	No/Yes	No/Yes
Skin permeability (cm.s^{-1})	-3.49/-2.151	-3.49/-2.151
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/No
Lipinski's rule of five	Yes/Yes	Yes/Yes

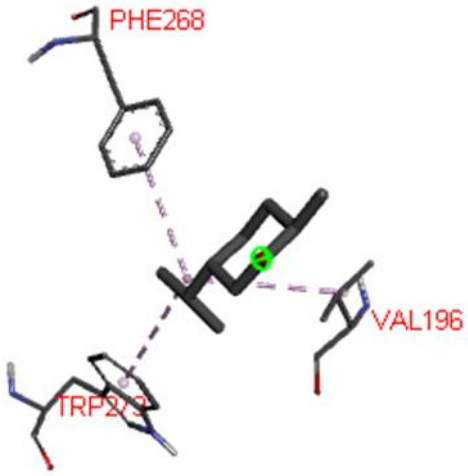
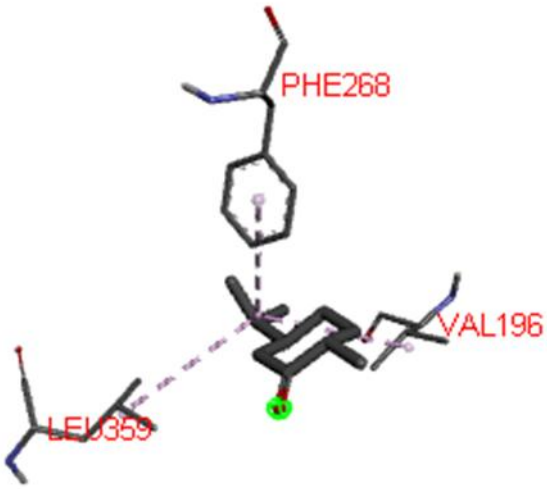
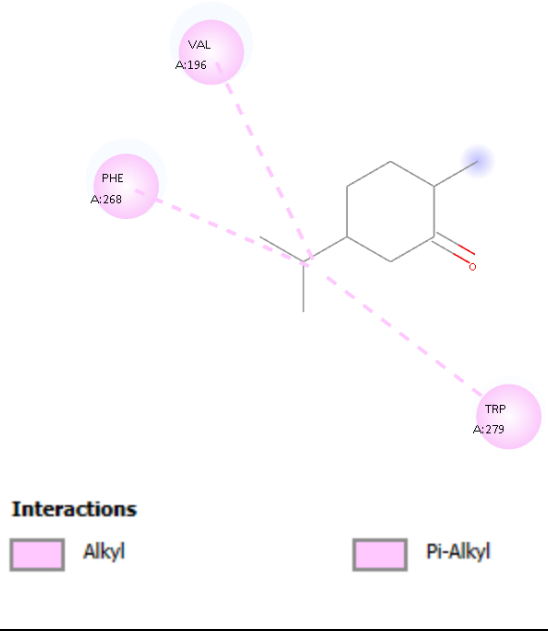
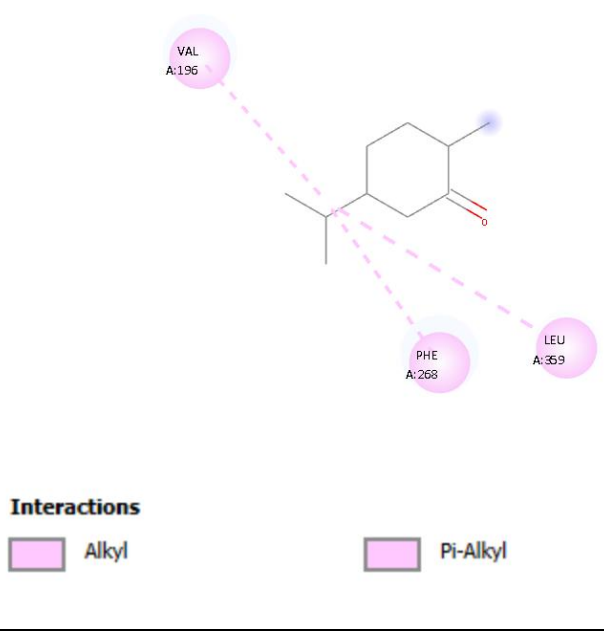


Compound	(-)-Δ⁹-THC	Rimonabant
BBB permeability	Yes/No	Yes/No
Skin permeability (cm.s^{-1})	-3.27/-2.696	-4.52/-2.671
Intestinal absorption	Yes/Yes/Yes	Yes/Yes/Yes
P-gp substrate	No/No	No/Yes
Lipinski's rule of five	Yes/Yes	Yes/Yes

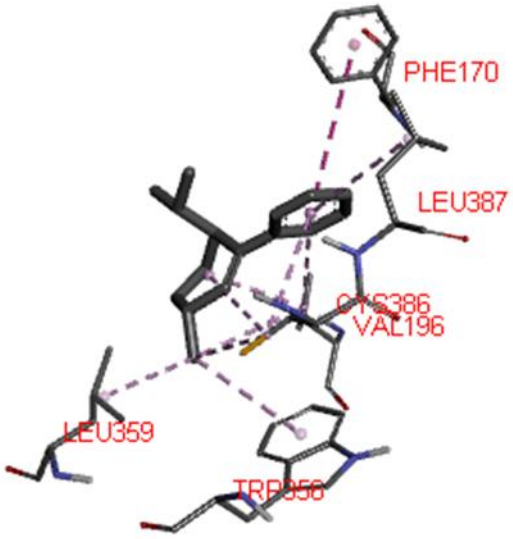
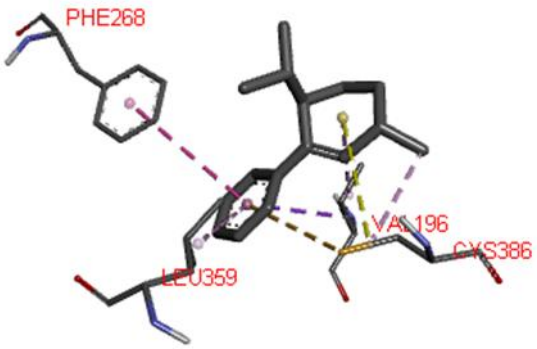
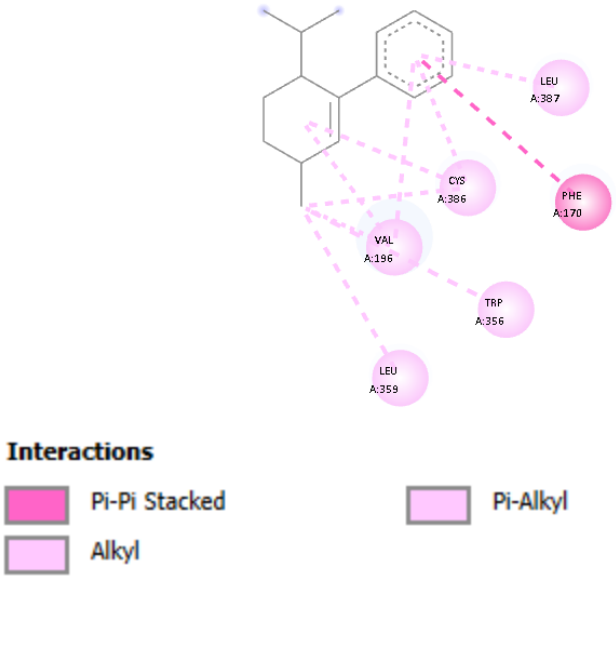
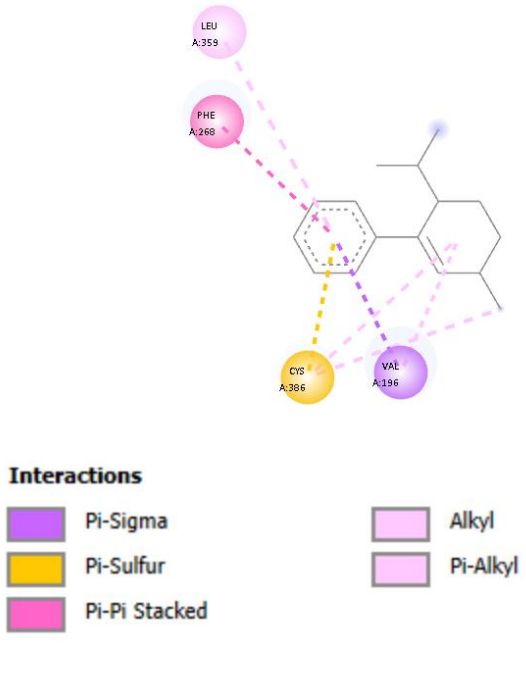
VI. Molecular Docking of Ketone Precursors and Synthesized Compounds Against Cannabinoid Receptors CB1 and CB2: Optimal Complex Poses and Intermolecular Interactions

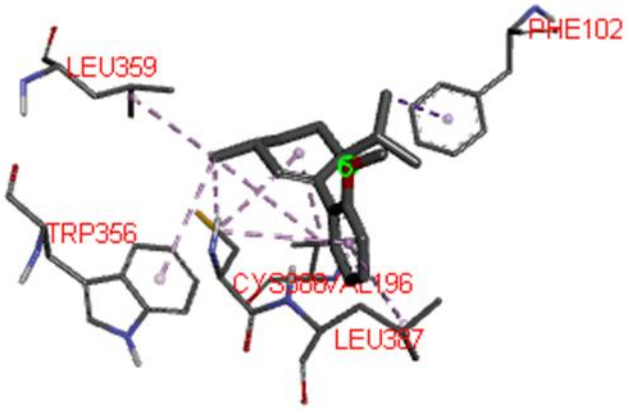
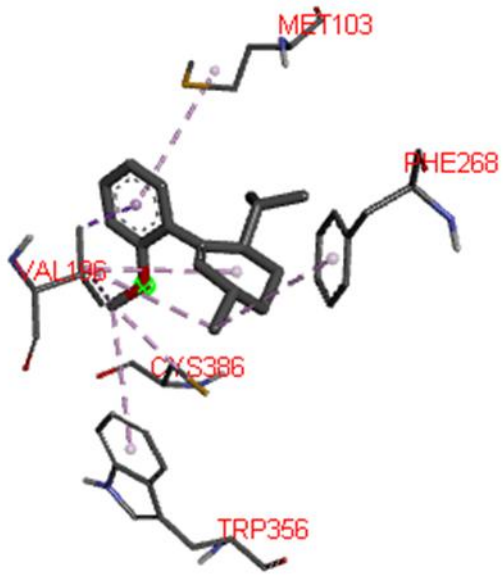
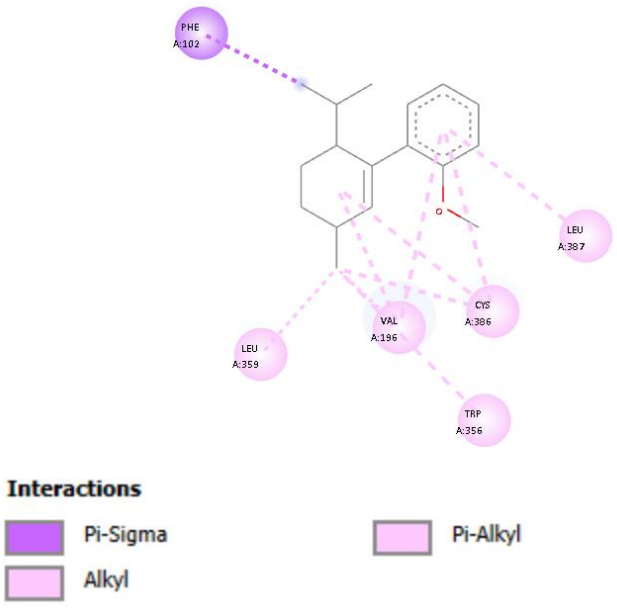
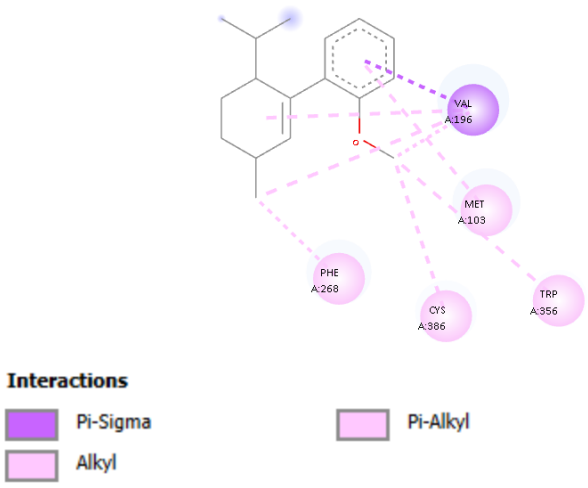
• *Ketone Precursors with CB1 Receptor*

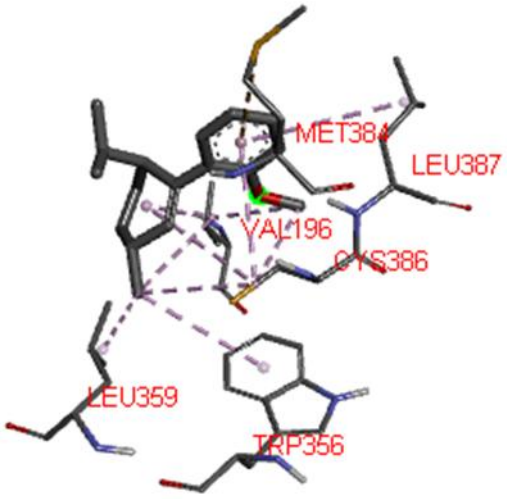
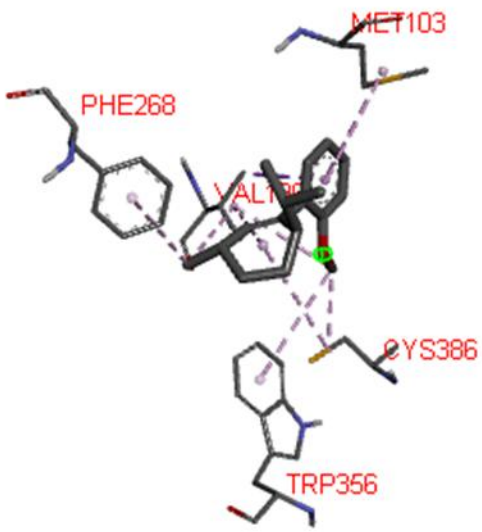
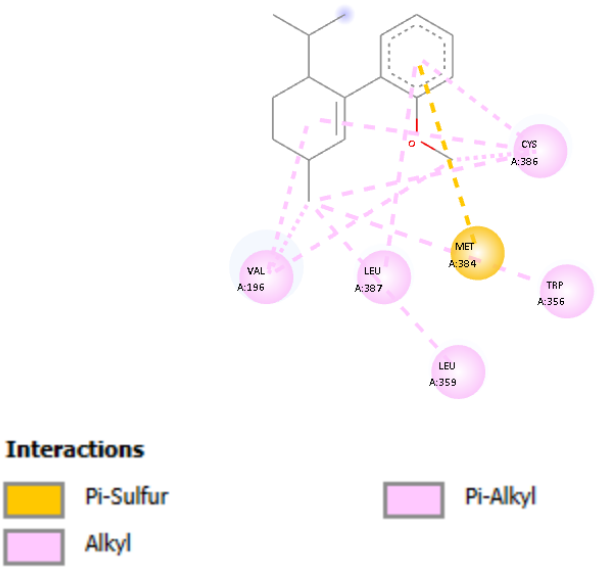
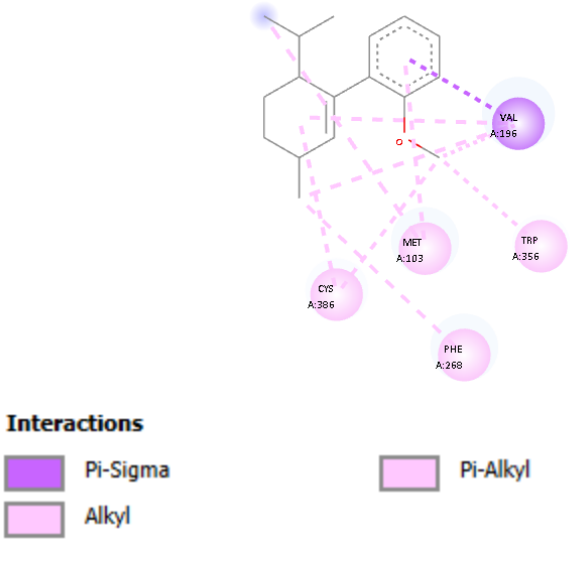
(-)-1	(+)-1
	
	
Binding energy: -6.3	**Binding energy: -6.2**

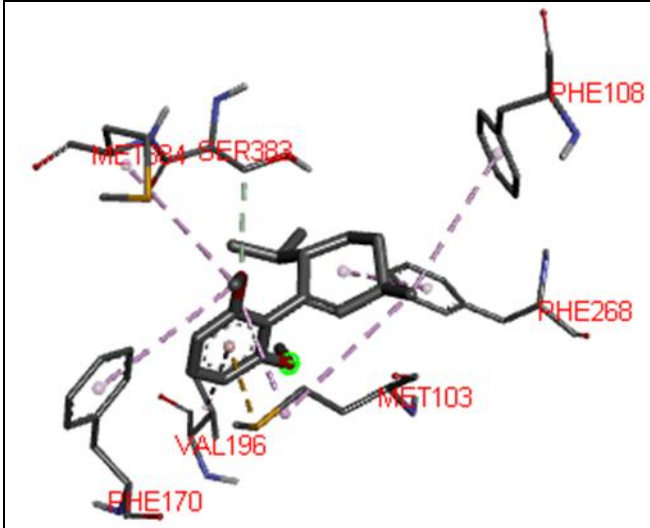
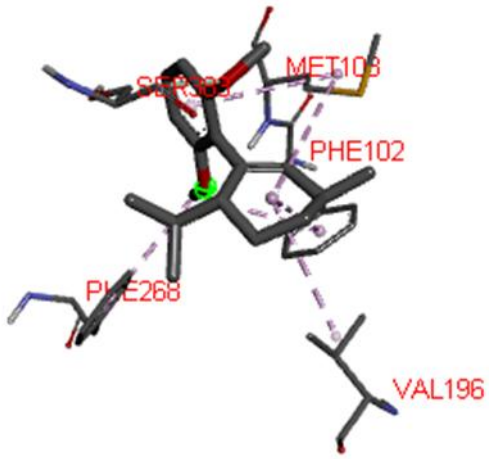
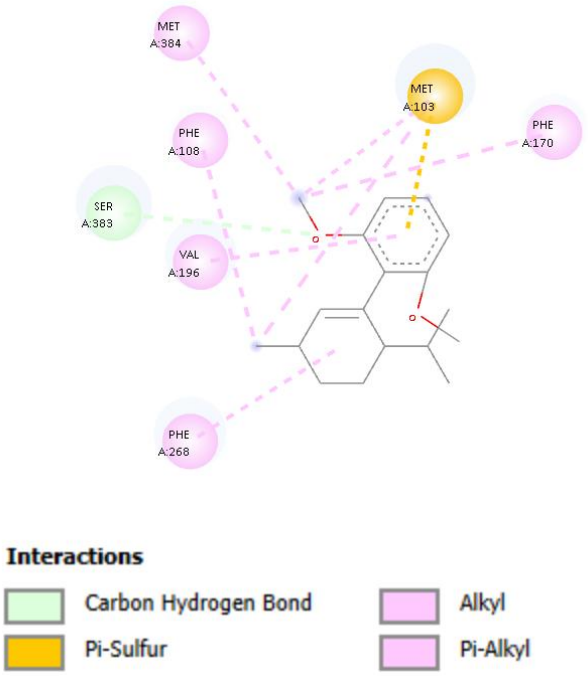
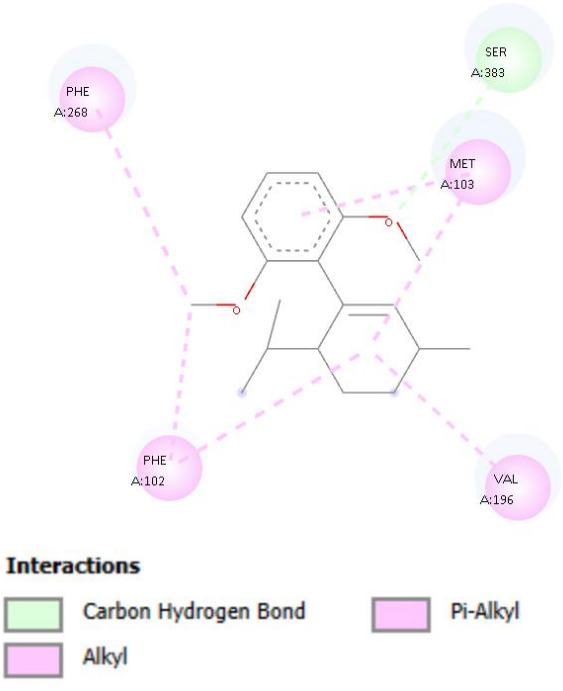
(+)-2	(-)-2
	
	
Binding energy: -6.3	**Binding energy: -6.2**

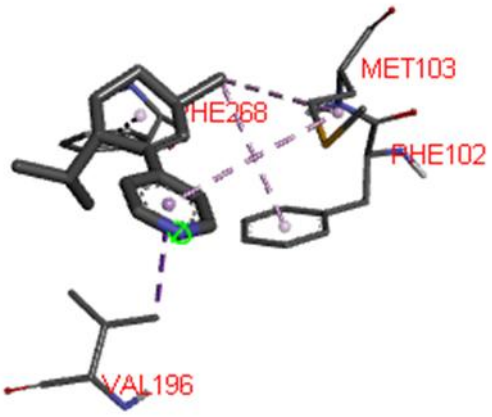
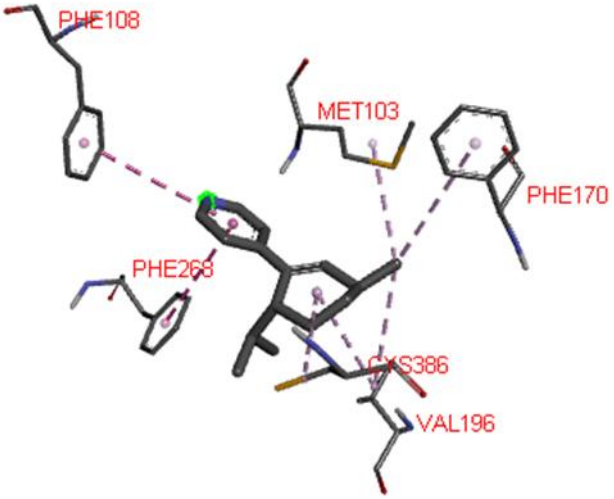
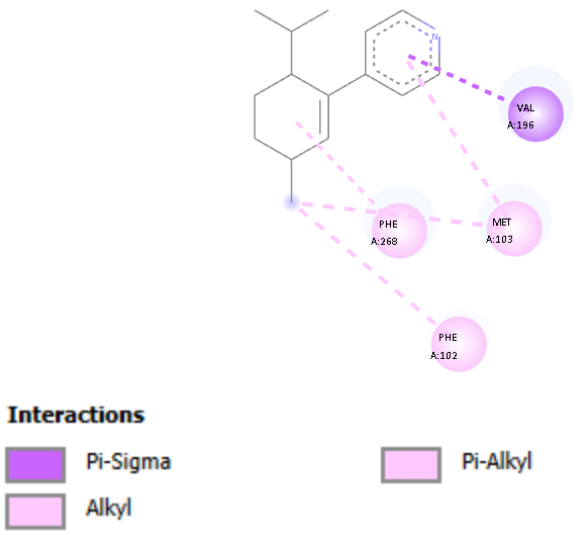
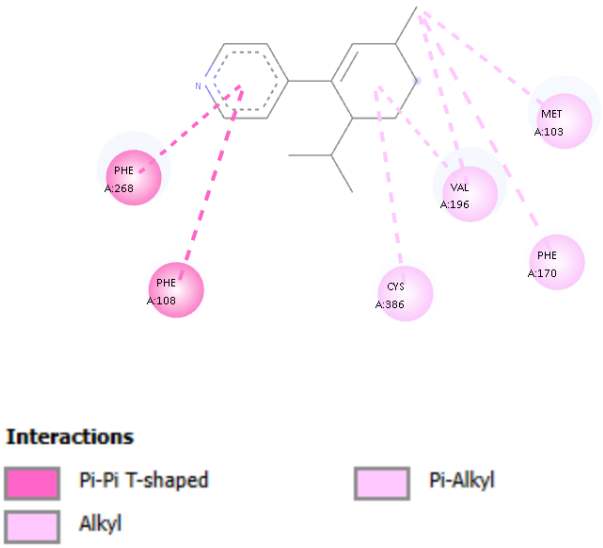
• *Synthesized Ligands of Series **6**/ent-**6** with CB1 Receptor*

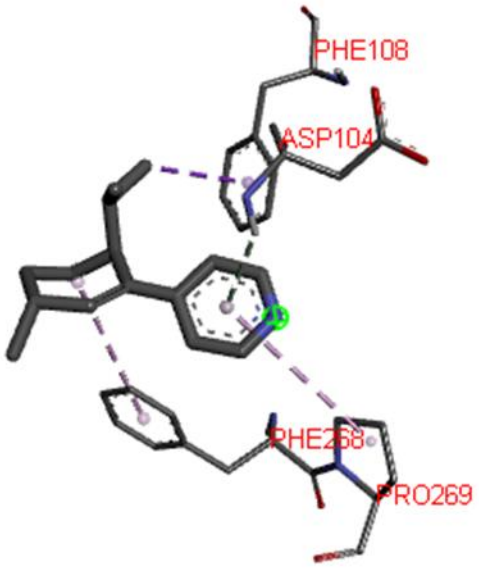
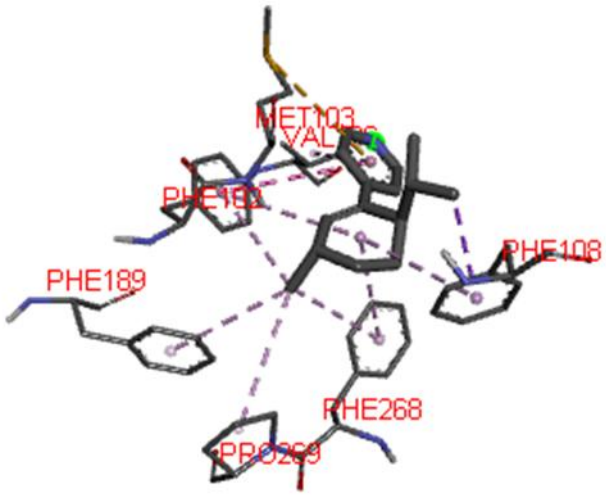
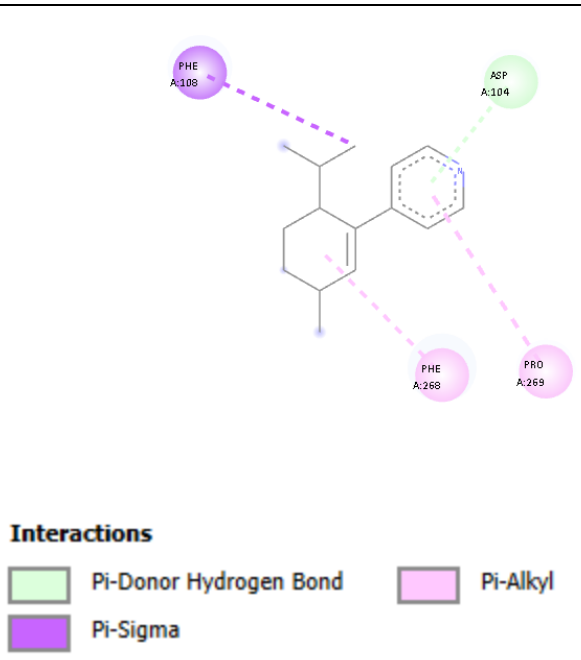
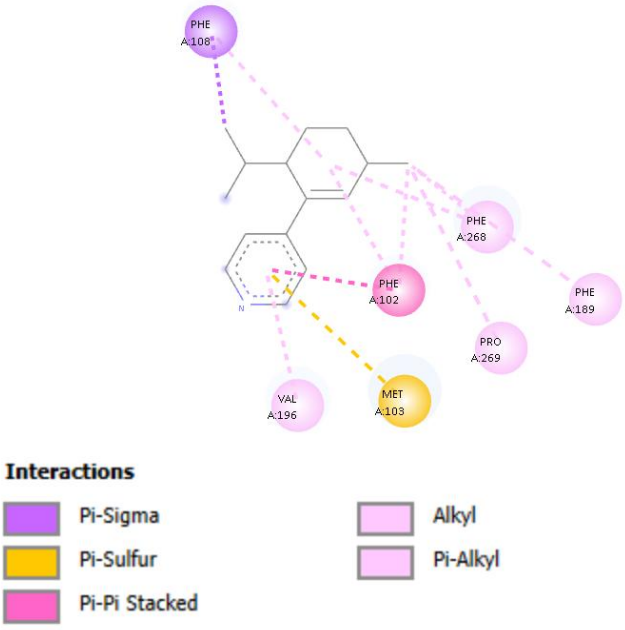
6a (II)	**ent-6a (II)**
	
	
Binding energy: -8.0	**Binding energy: -7.7**

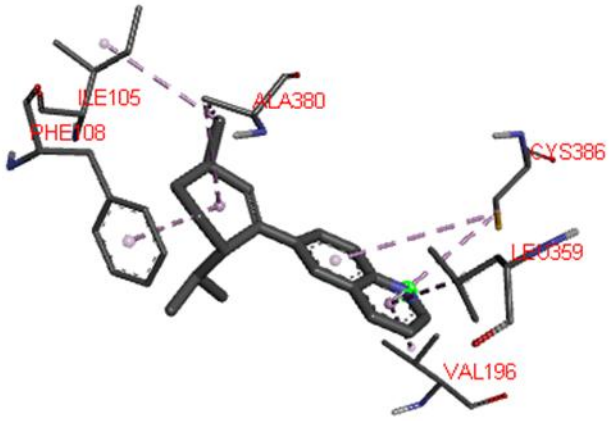
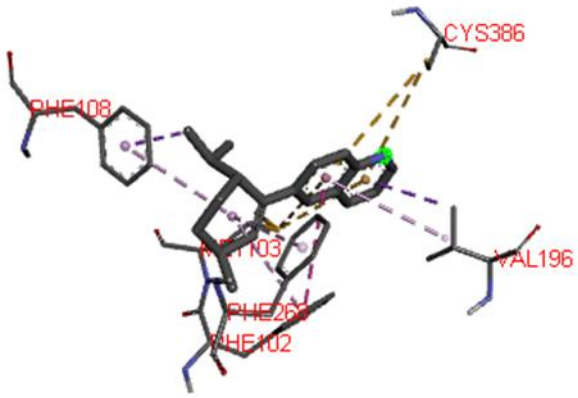
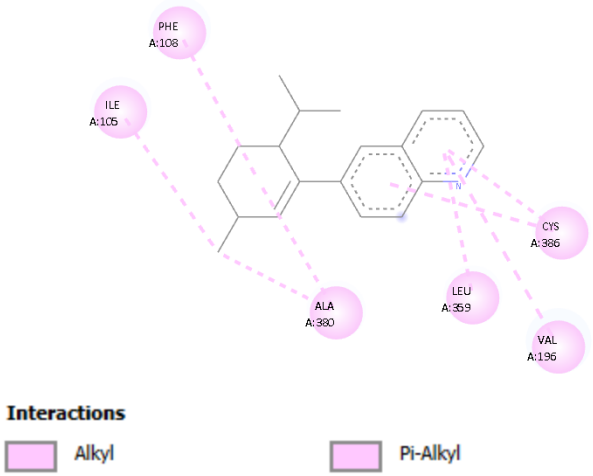
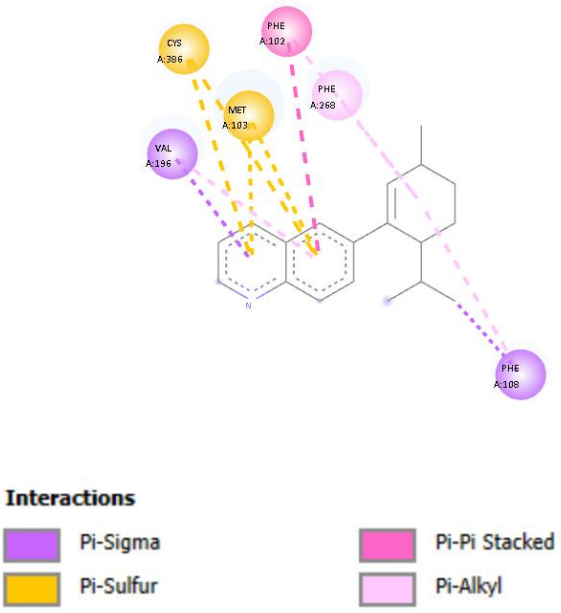
6b (l)	ent-6b (l)
	
	
Binding energy: -7.1	**Binding energy: -7.1**

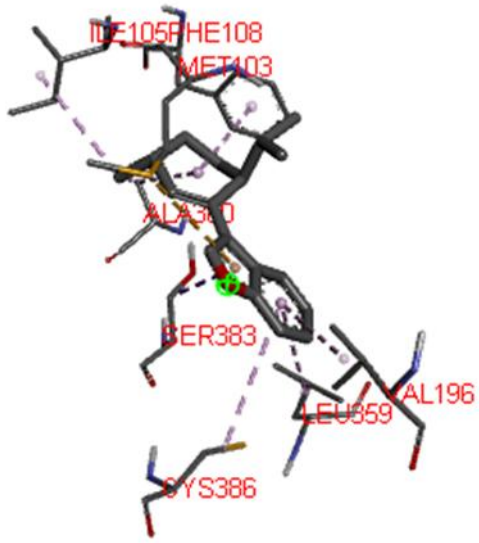
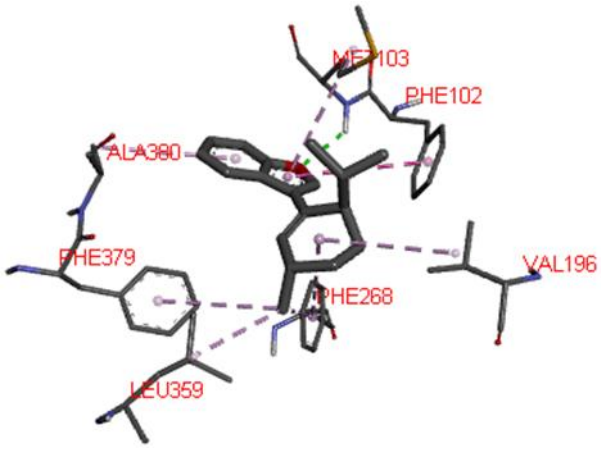
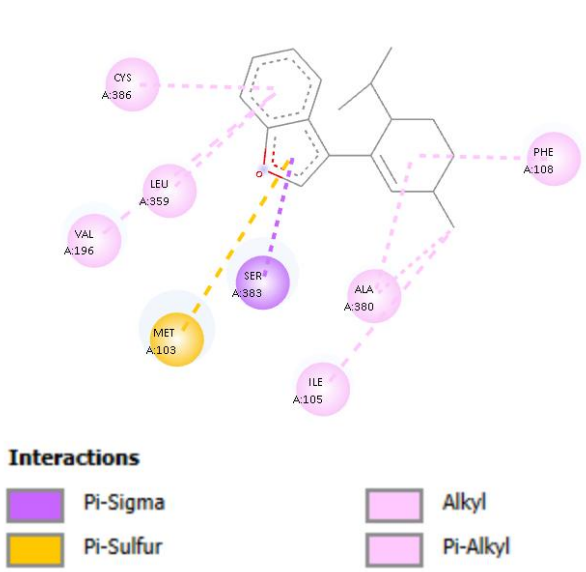
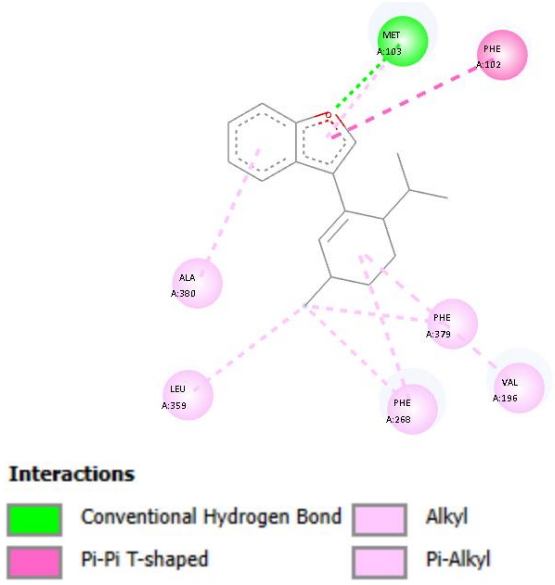
6b (II)	ent-6b (II)
	
	
Binding energy: -8.0	**Binding energy: -7.1**

6c (I)	ent-6c (I)
	
	
Binding energy: -6.1	**Binding energy: -5.8**

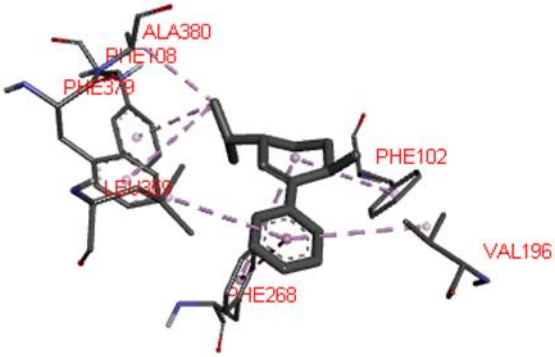
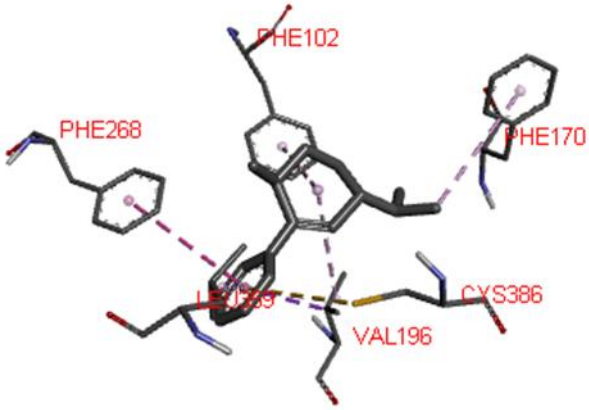
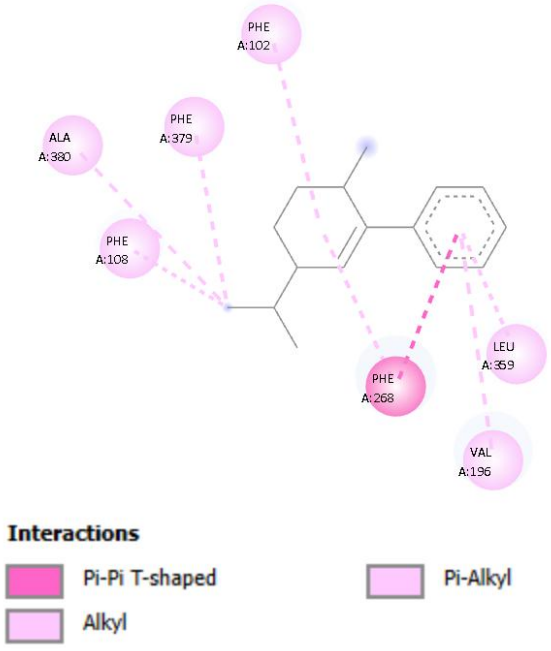
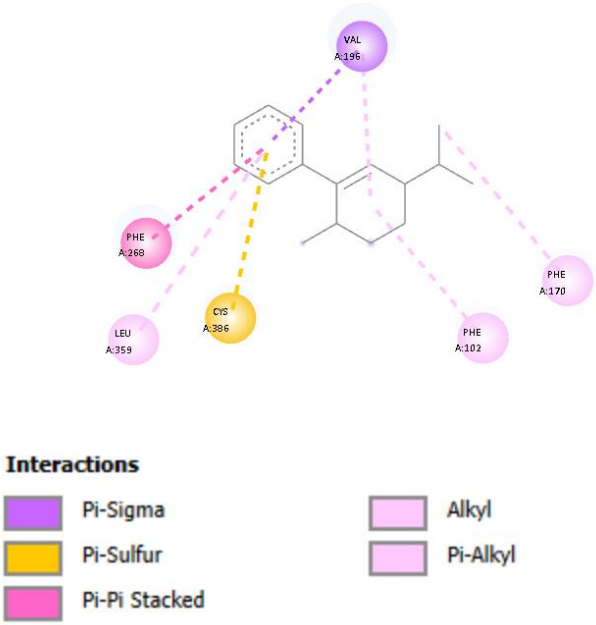
6d (l)	ent-6d (l)
	
	
Binding energy: -8.0	**Binding energy: -7.8**

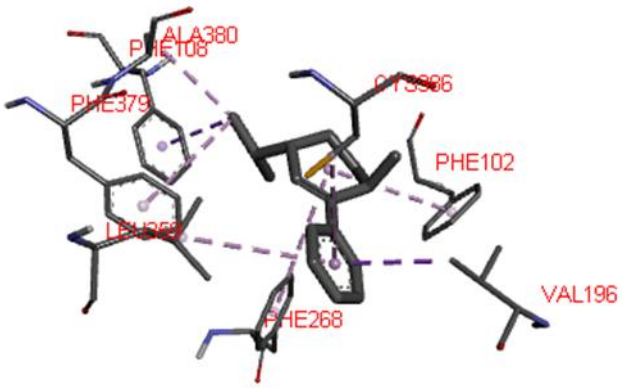
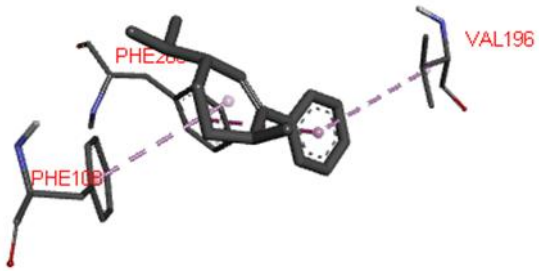
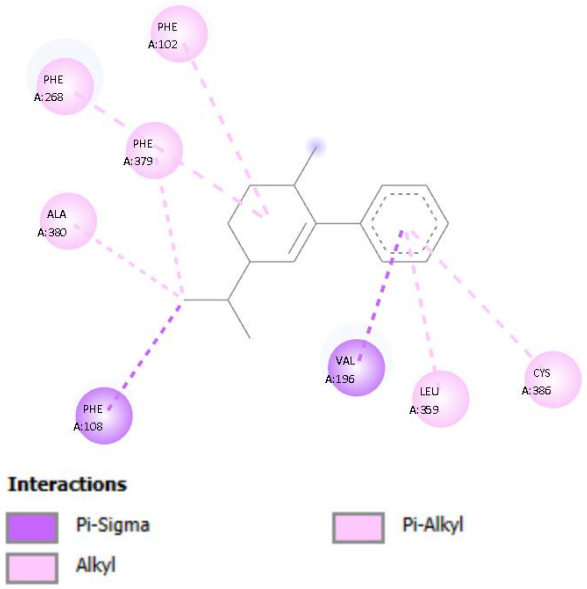
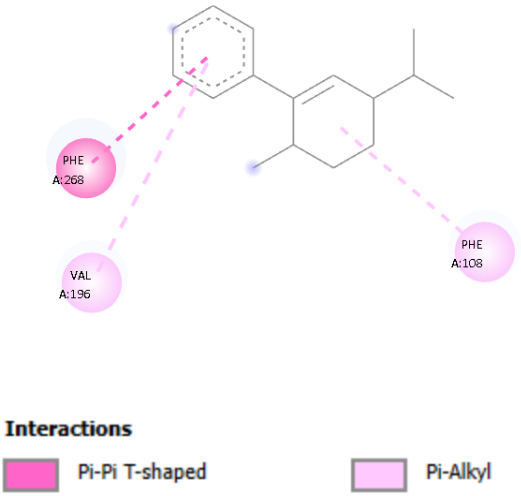
6d (II)	ent-6d (II)
	
	
Binding energy: -8.4	**Binding energy: -7.7**

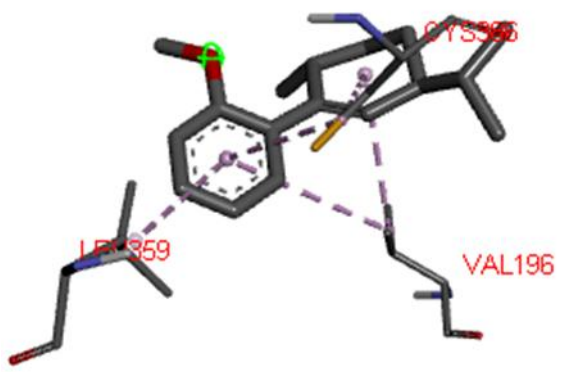
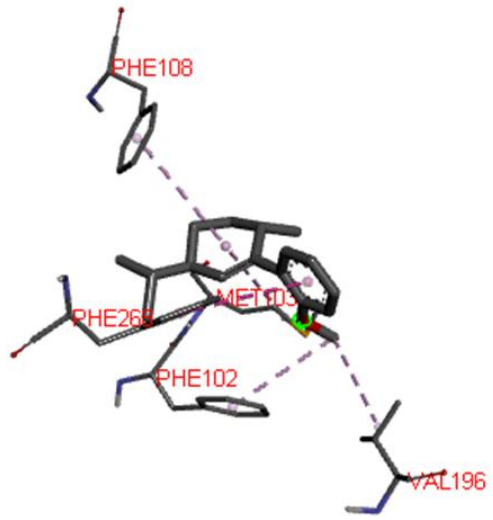
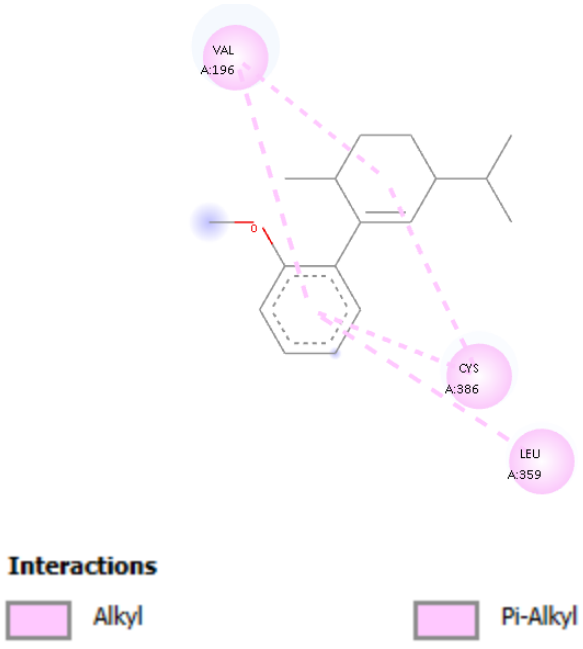
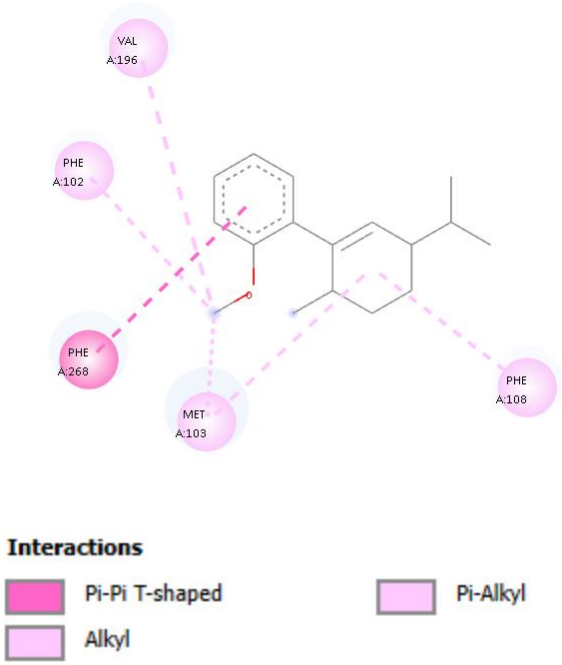
6e (II)	ent-6e (II)
	
	
Binding energy: -9.6	**Binding energy: -9.6**

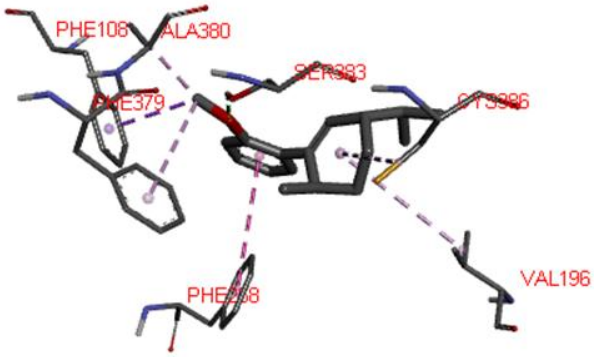
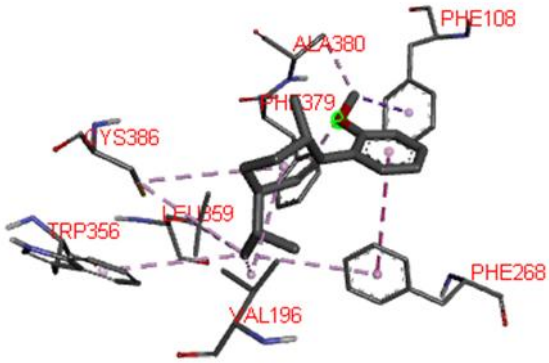
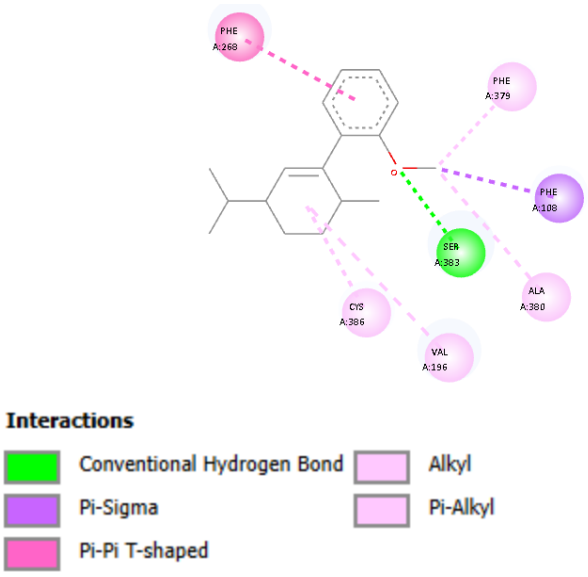
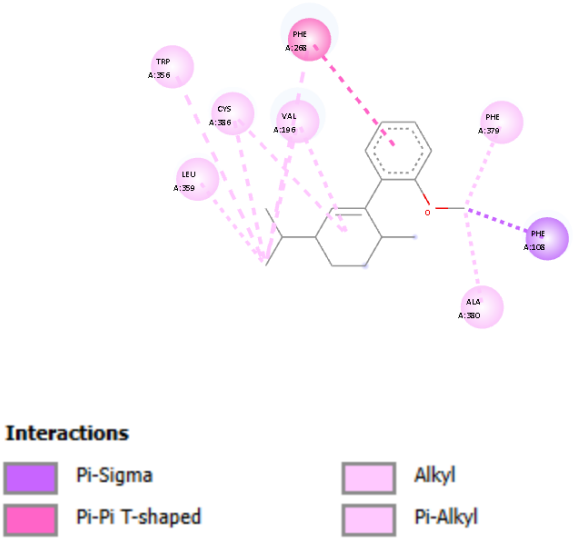
6f (II)	ent-6f (II)
	
	
Binding energy: -9.5	**Binding energy: -9.2**

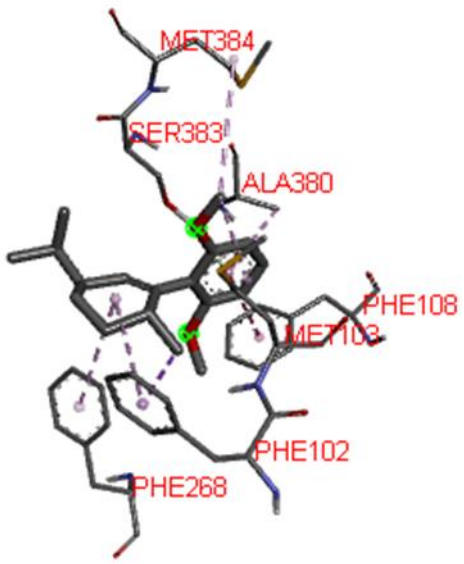
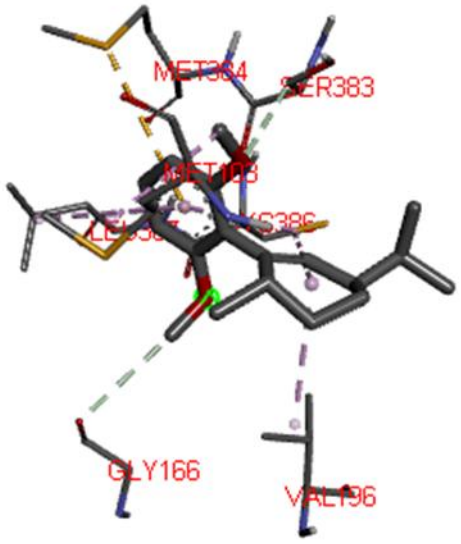
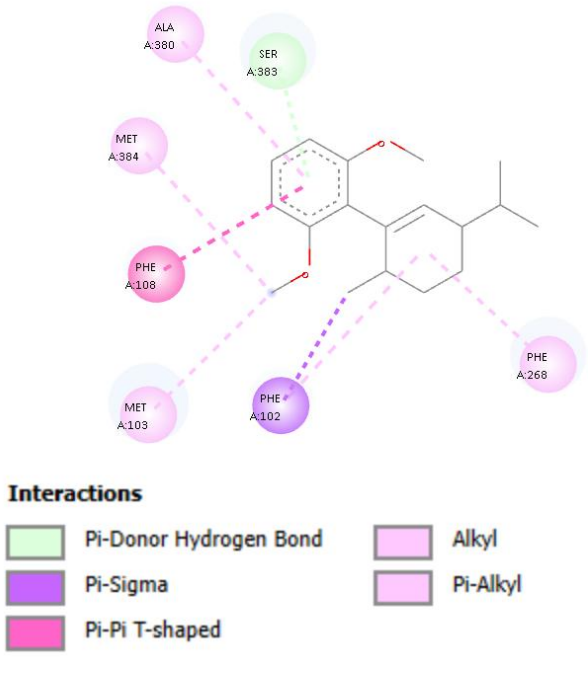
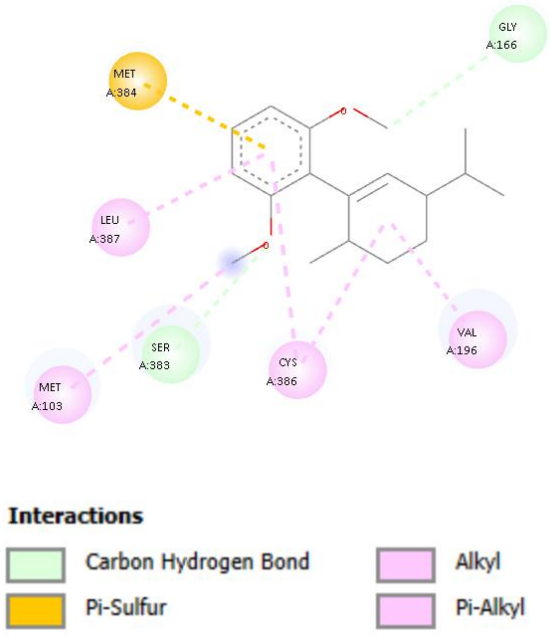
• *Synthesized Ligands of Series **7**/ent-**7** with CB1 Receptor*

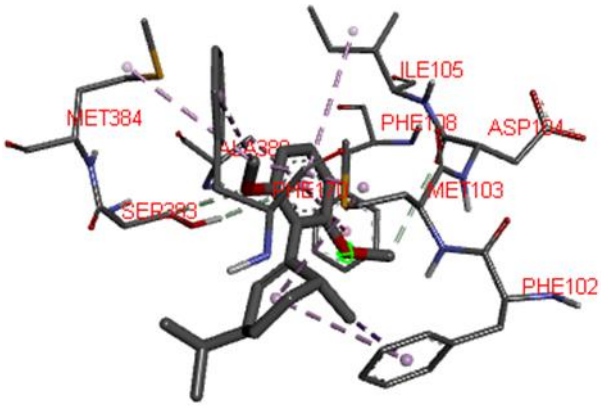
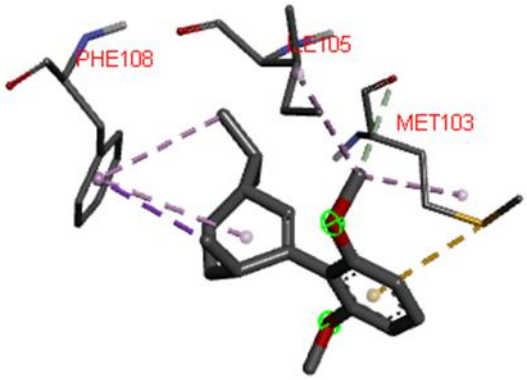
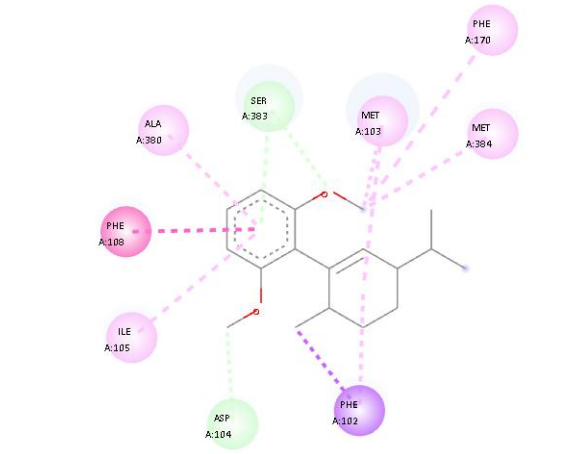
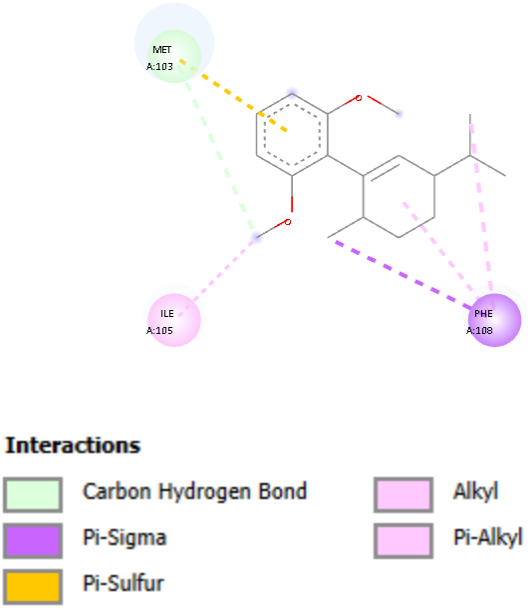
7a (I)	**ent-7a (I)**
	
	
Binding energy: -8.8	**Binding energy: -8.4**

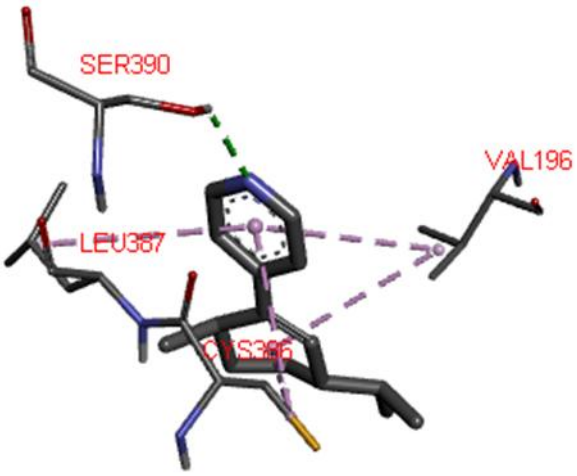
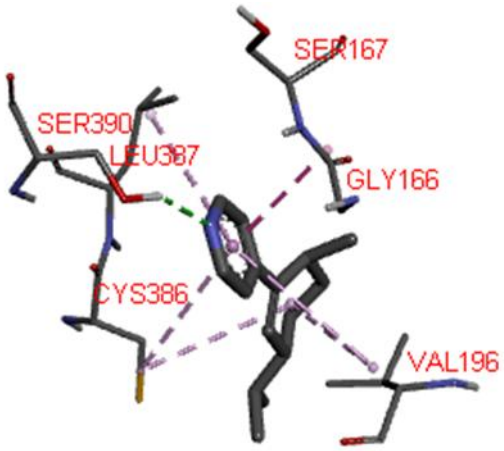
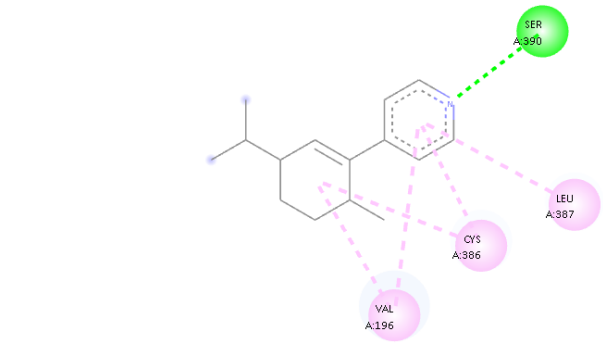
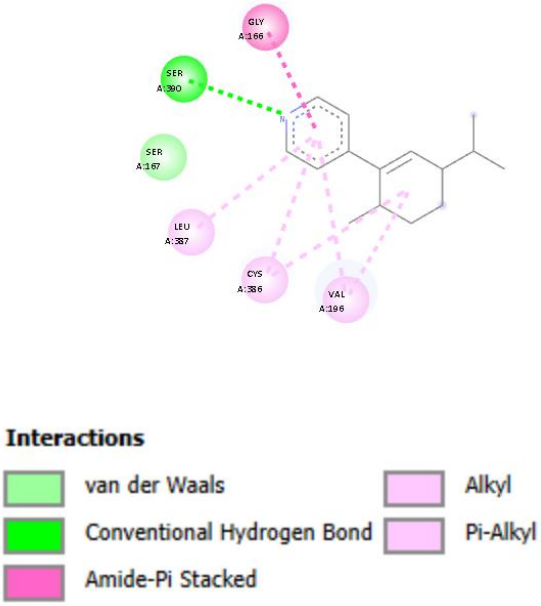
7a (II)	ent-7a (II)
	
	
Binding energy: -8.8	**Binding energy: -8.7**

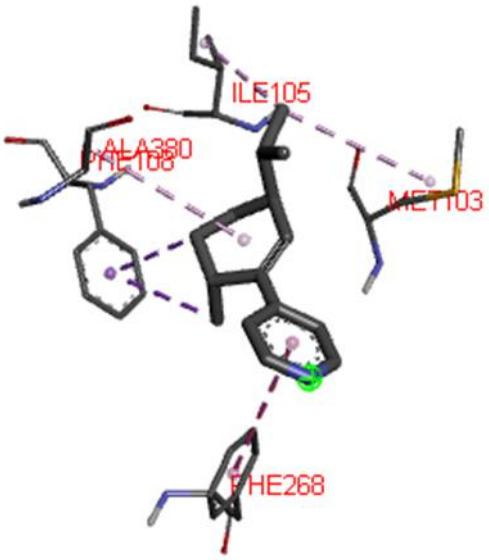
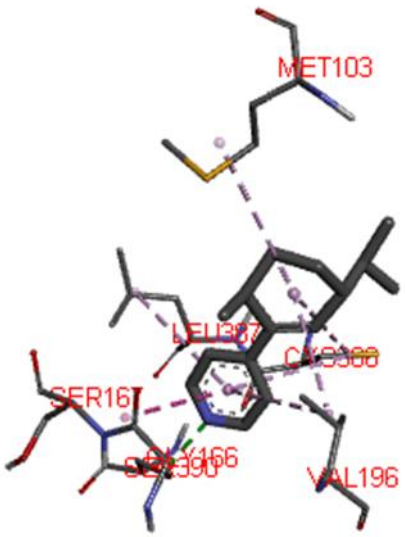
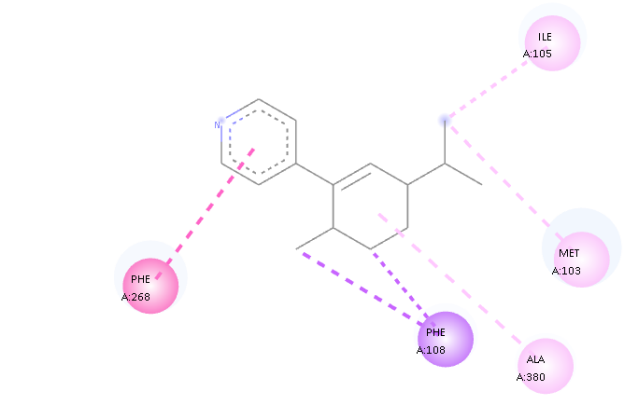
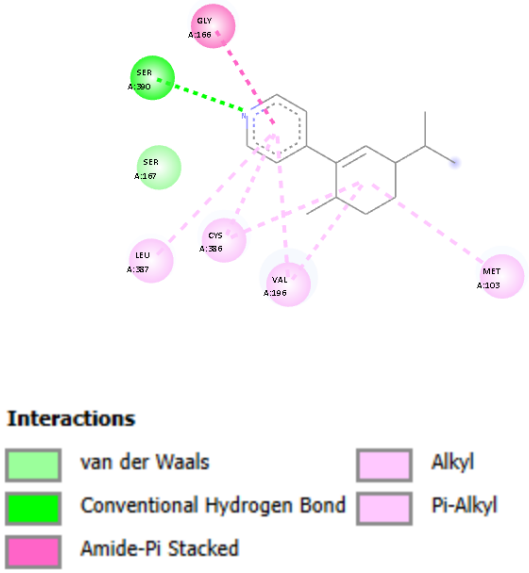
7b (I)	ent-7b (I)
	
	
Binding energy: -8.4	**Binding energy: -8.1**

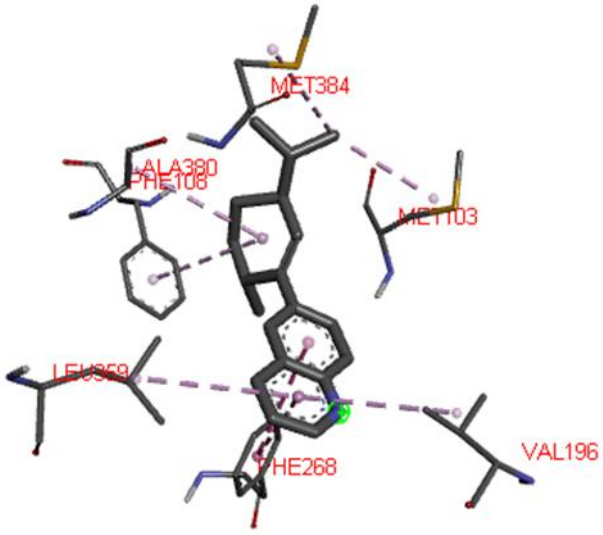
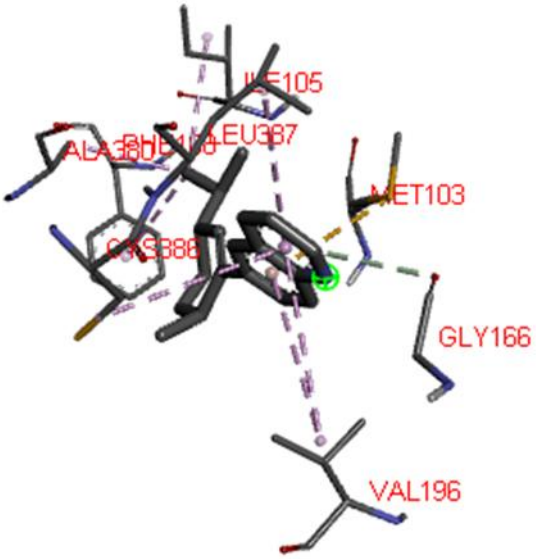
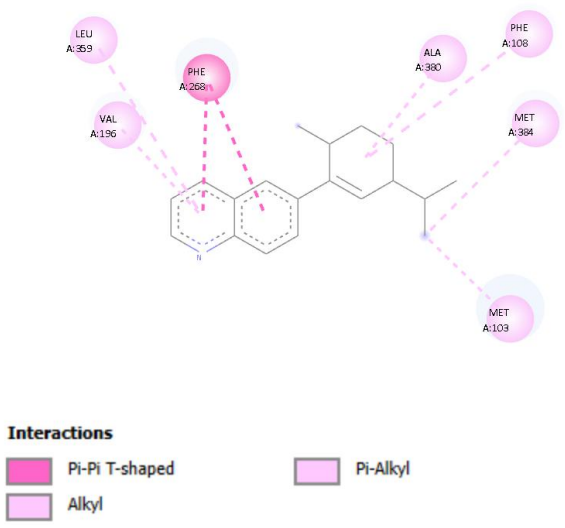
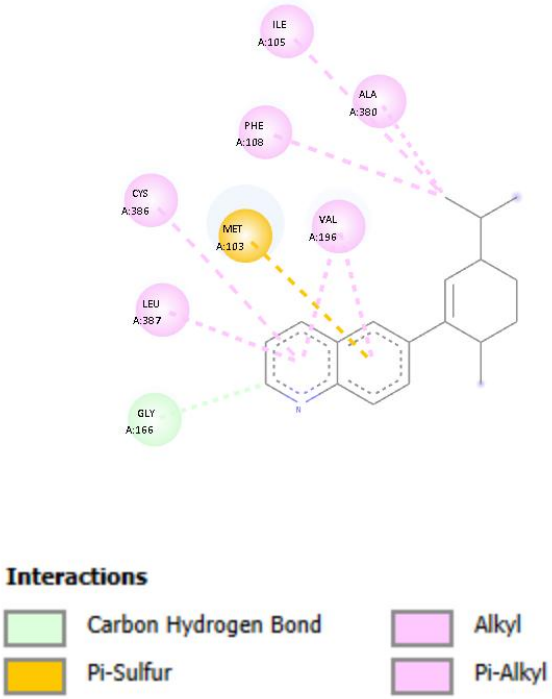
7b (II)	ent-7b (II)
	
	
Binding energy: -8.3	**Binding energy: -8.3**

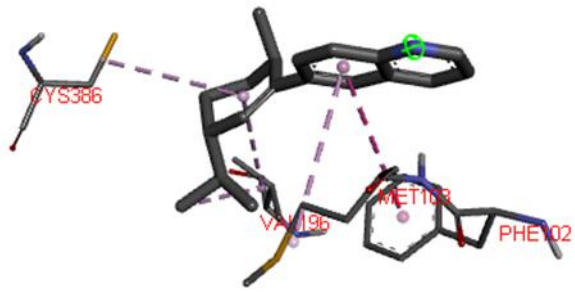
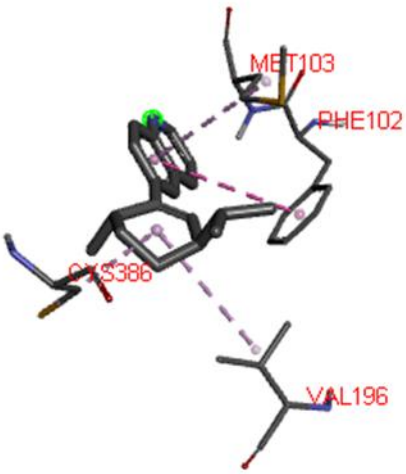
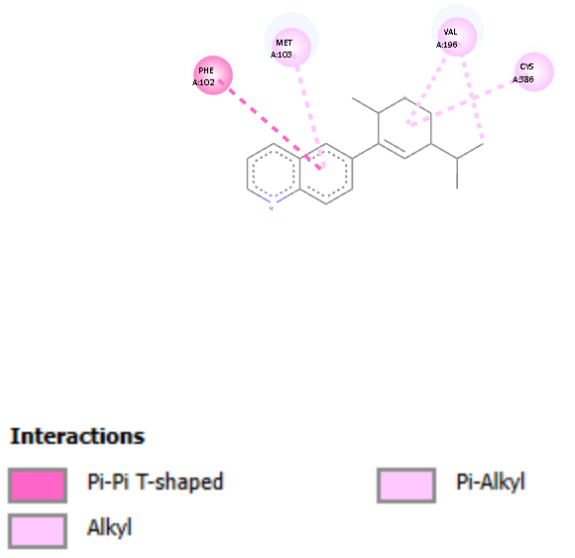
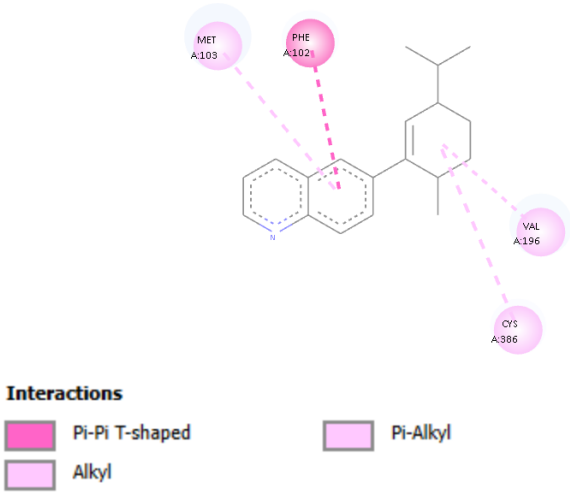
7c (I)	ent-7c (I)
	
	
Binding energy: -7.6	**Binding energy: -7.4**

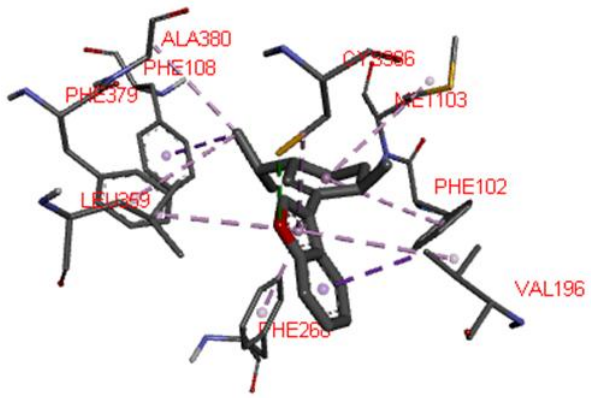
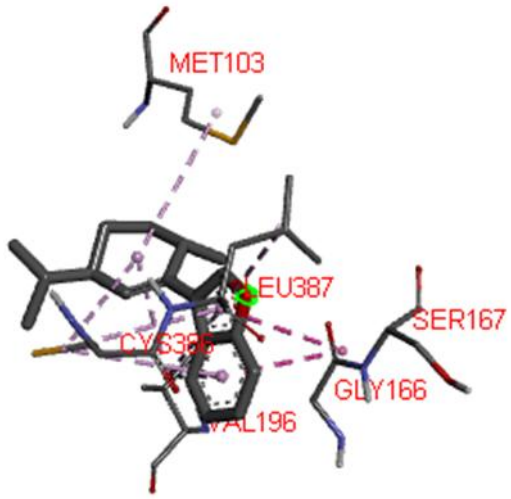
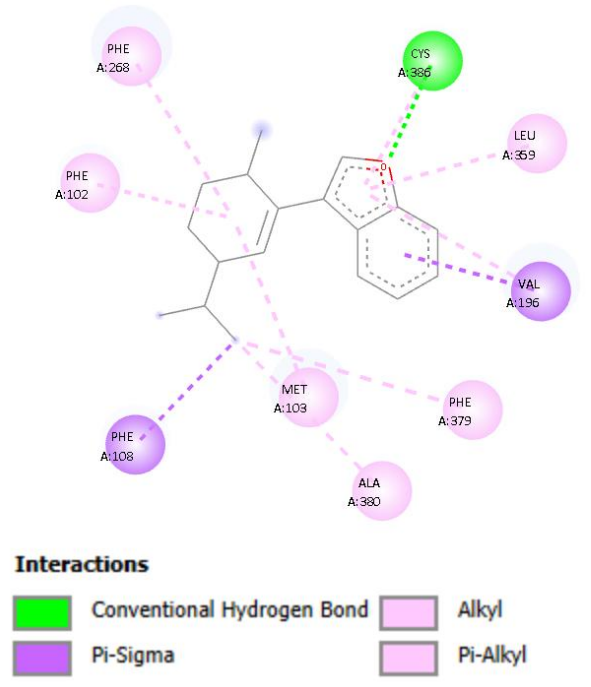
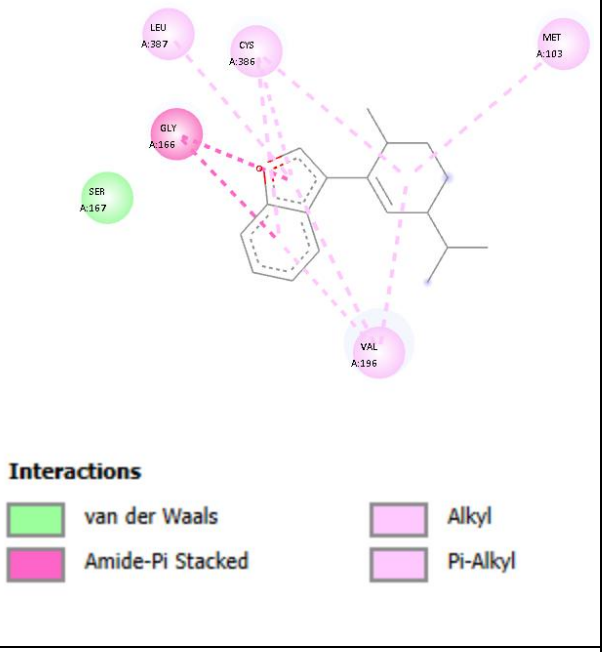
7c (II)	ent-7c (II)
	
	
Binding energy: -7.6	**Binding energy: -7.6**

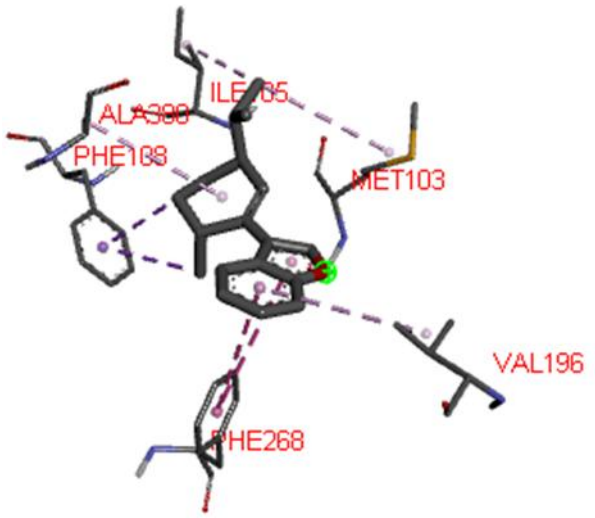
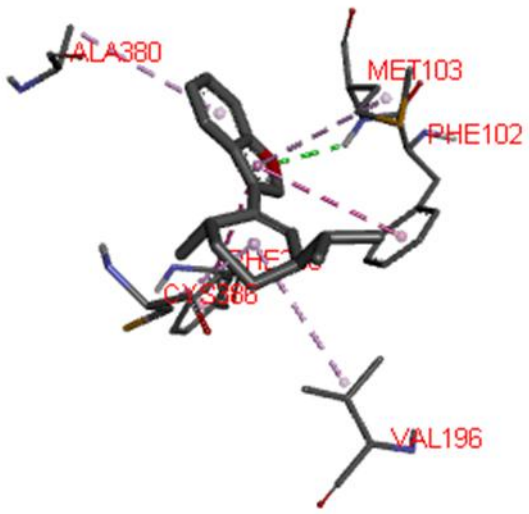
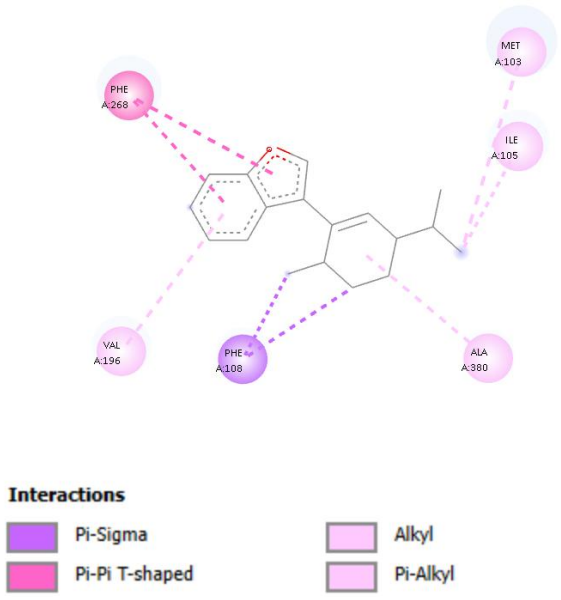
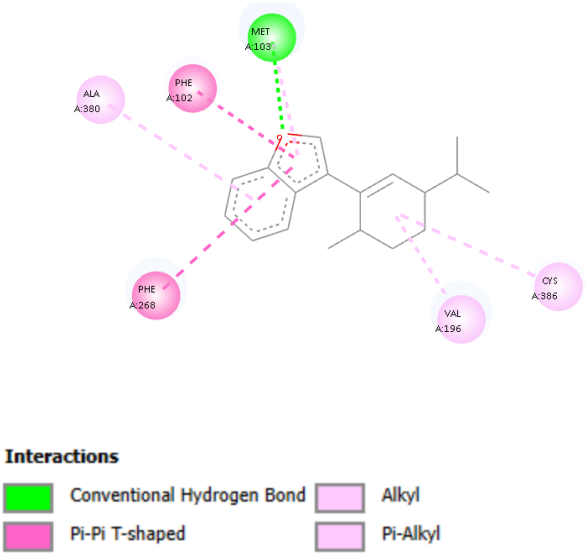
7d (I)	ent-7d (I)
	
	
Binding energy: -8.5	**Binding energy: -8.3**

7d (II)	ent-7d (II)
	
	
Binding energy: -7.6	**Binding energy: -7.9**

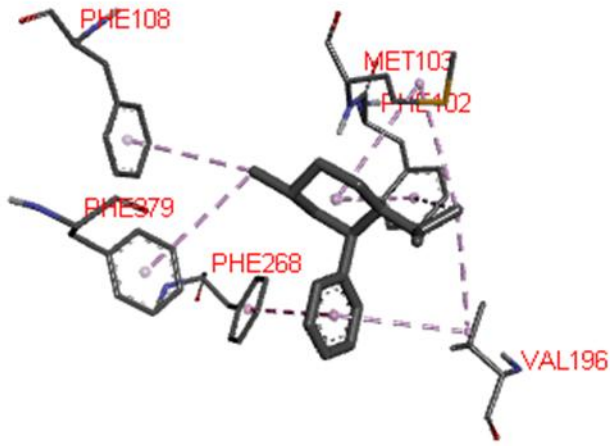
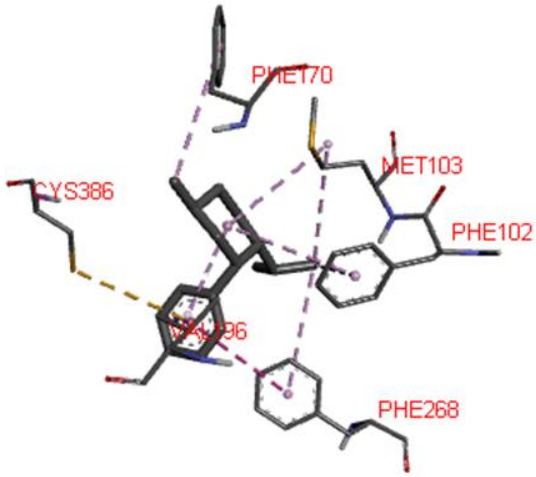
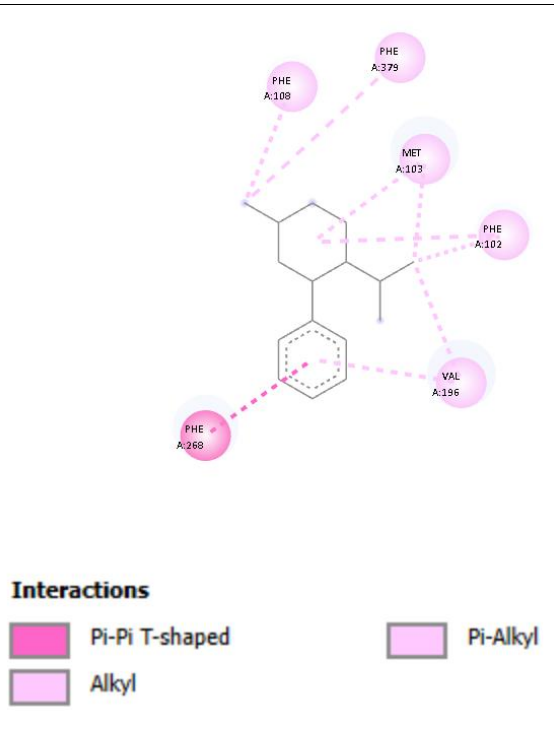
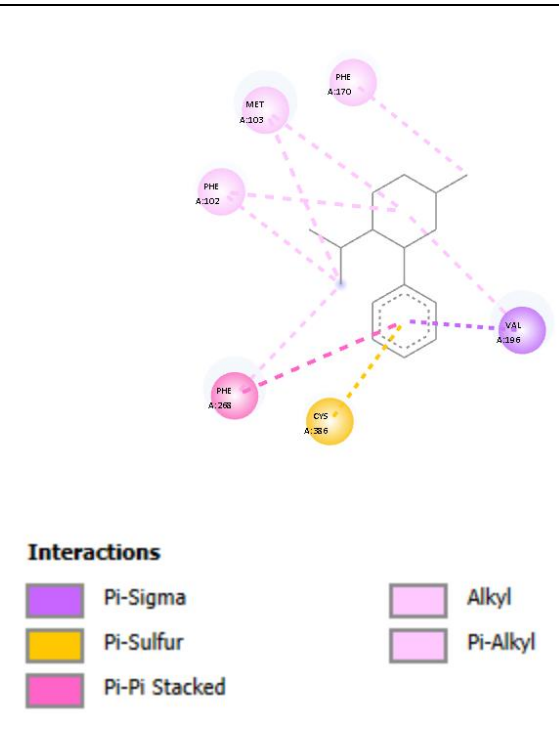
7e (I)	ent-7e (I)
	
	
Binding energy: -9.8	**Binding energy: -9.5**

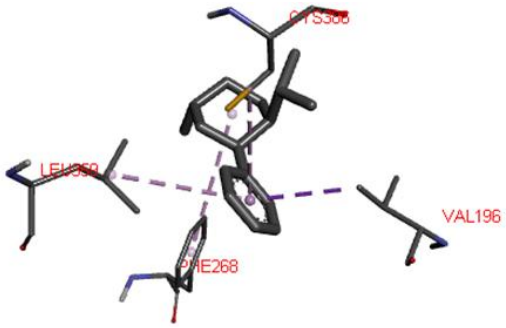
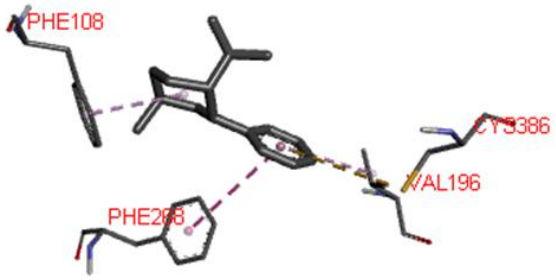
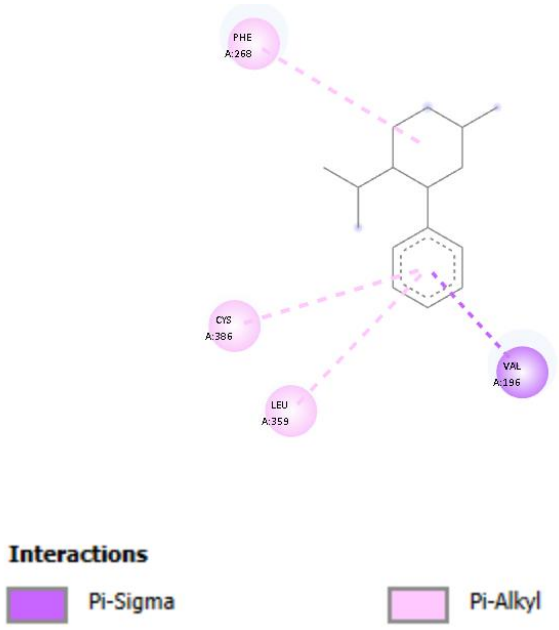
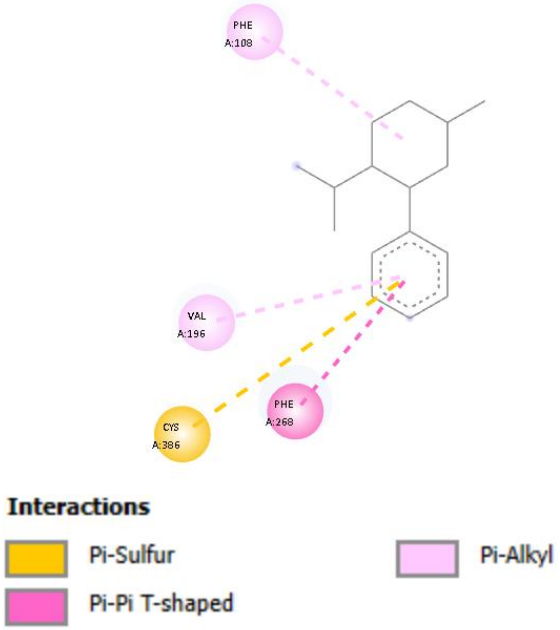
7e (II)	ent-7e (II)
	
	
Binding energy: -9.5	**Binding energy: -9.9**

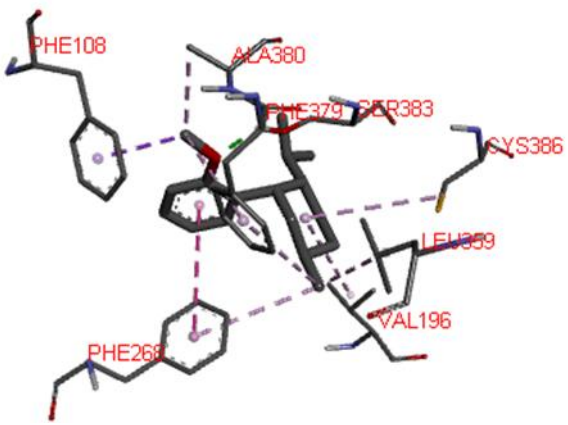
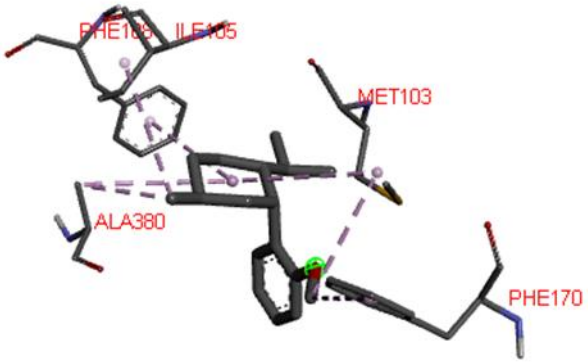
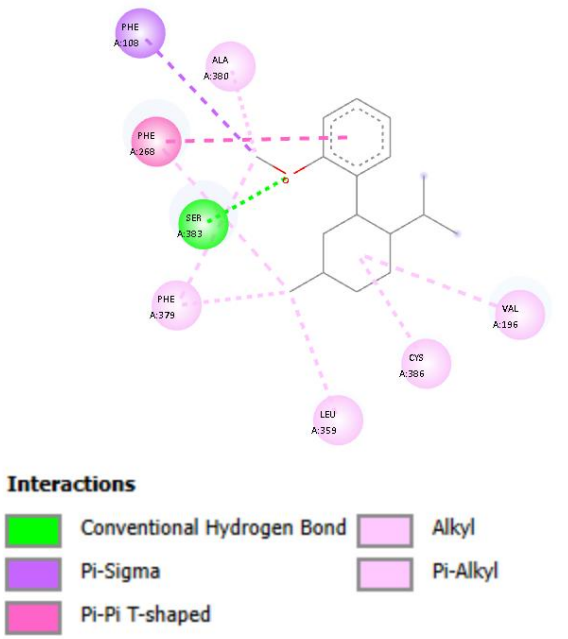
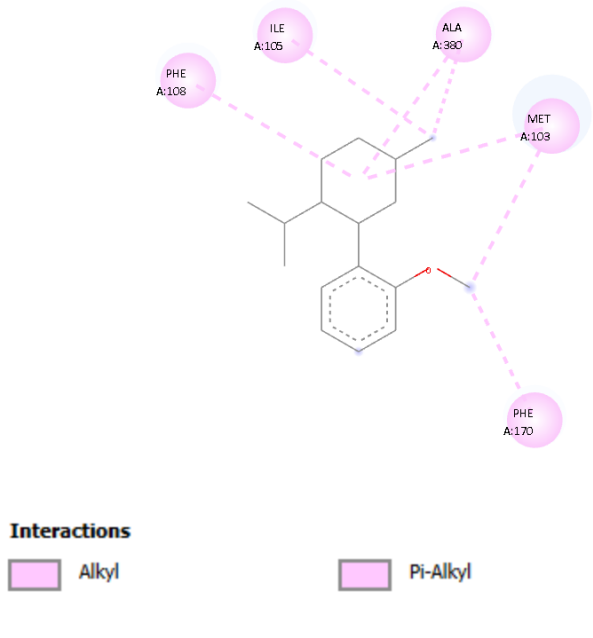
7f (l)	ent-7f (l)
	
	
Binding energy: -9.5	**Binding energy: -9.5**

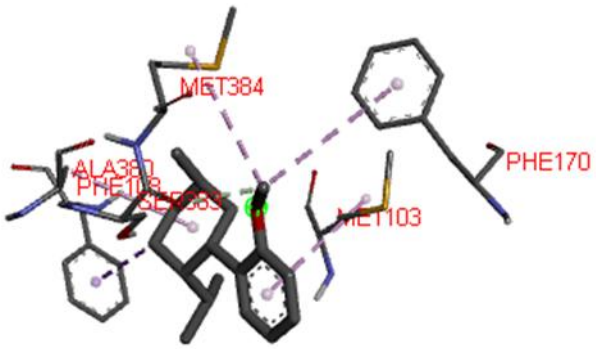
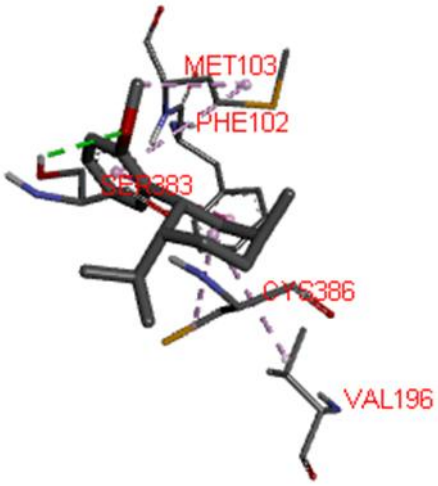
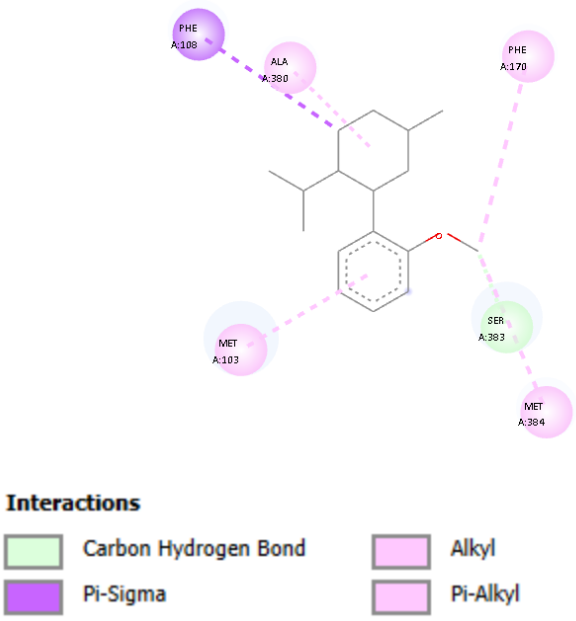
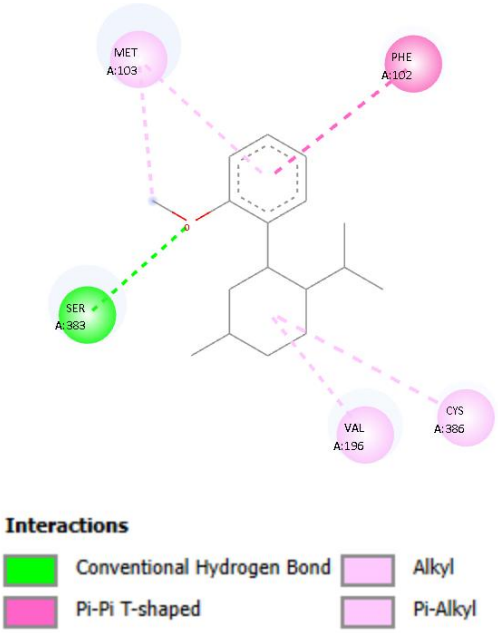
7f (II)	ent-7f (II)
	
	
Binding energy: -9.0	**Binding energy: -9.1**

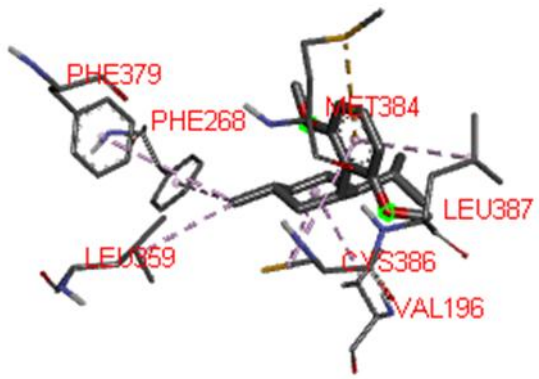
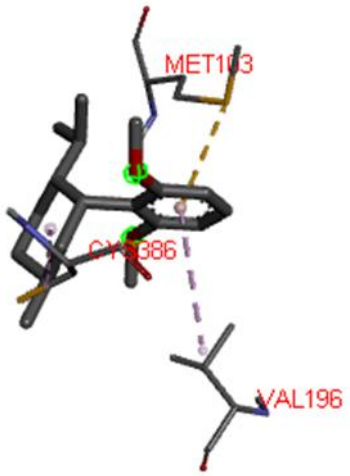
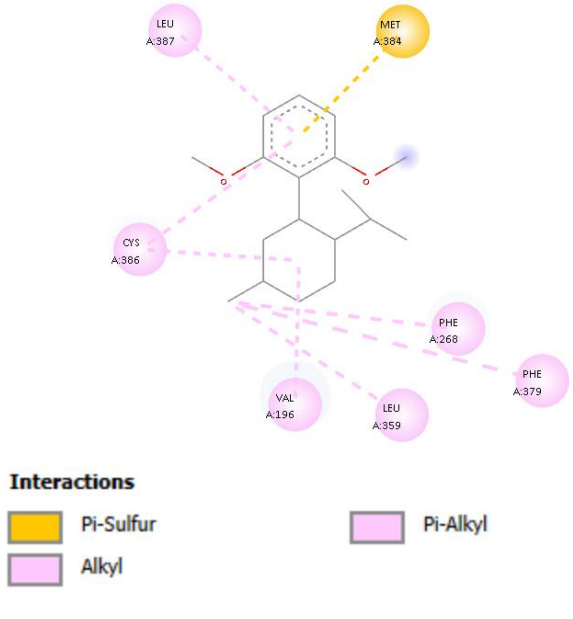
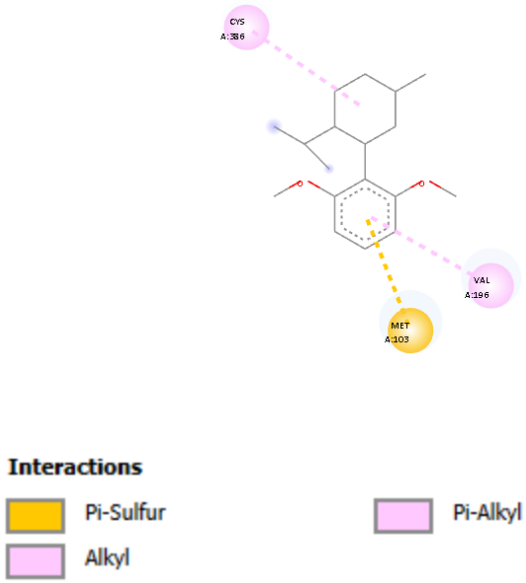
• *Synthesized Ligands of Series **8**/ent-**8** with CB1 Receptor*

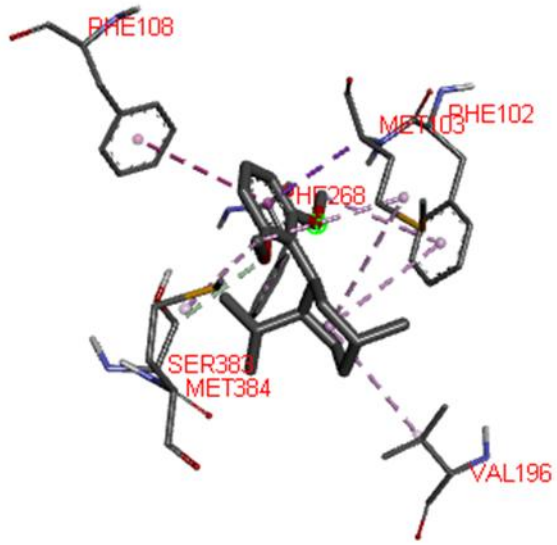
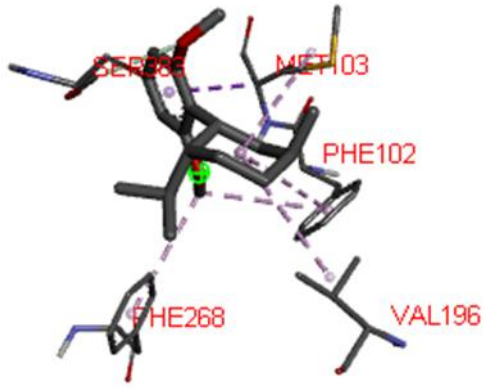
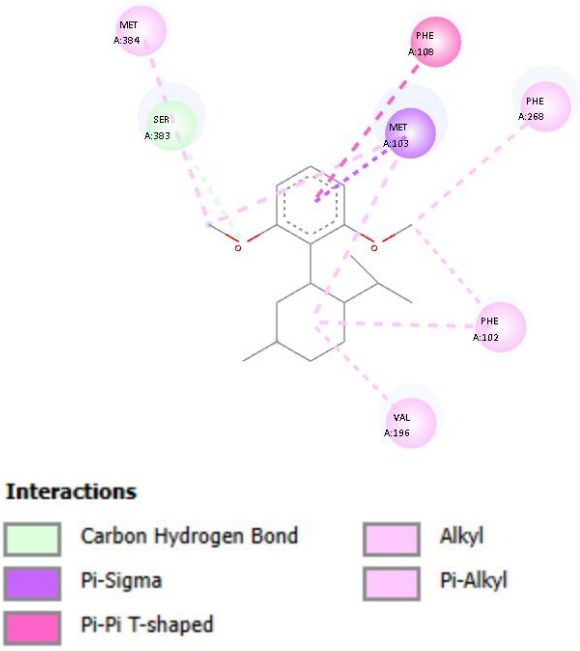
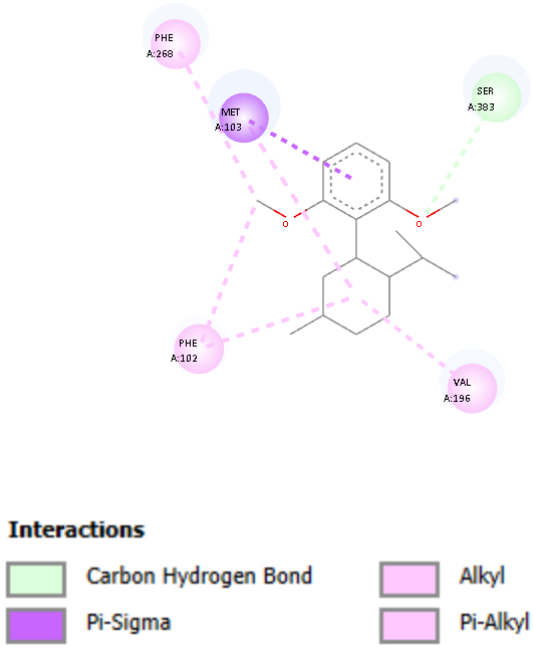
8a (I)	**ent-8a (I)**
	
	
Binding energy: -8.3	**Binding energy: -8.2**

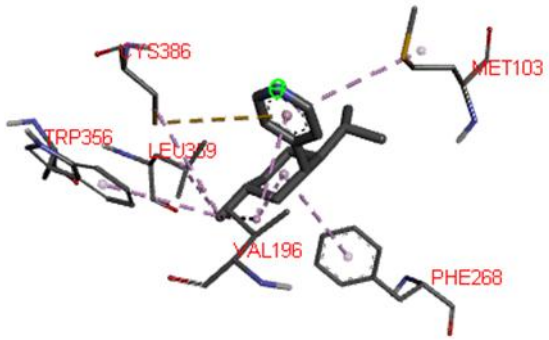
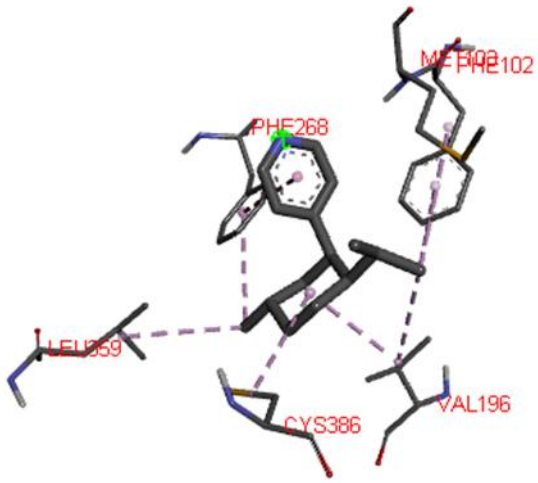
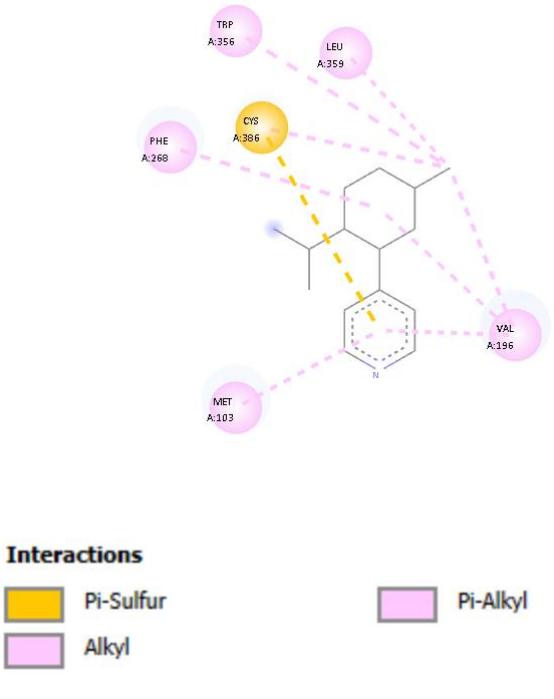
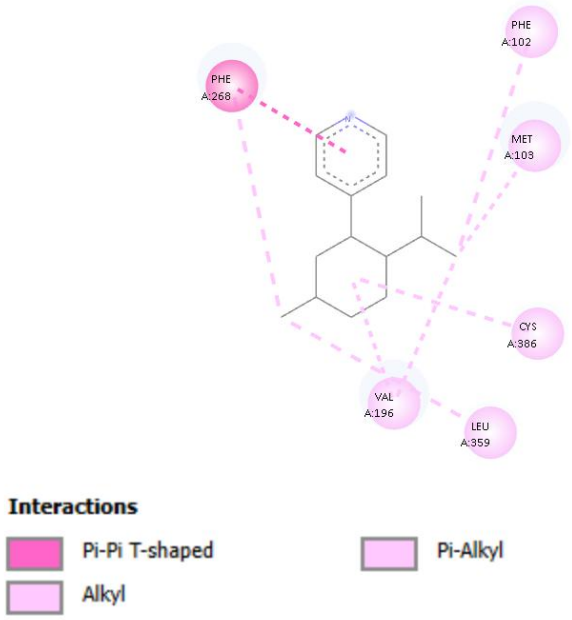
8a (II)	ent-8a (II)
	
	
Binding energy: -7.6	**Binding energy: -7.8**

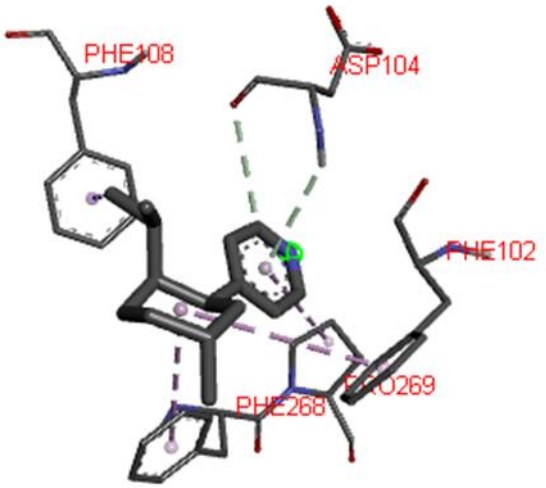
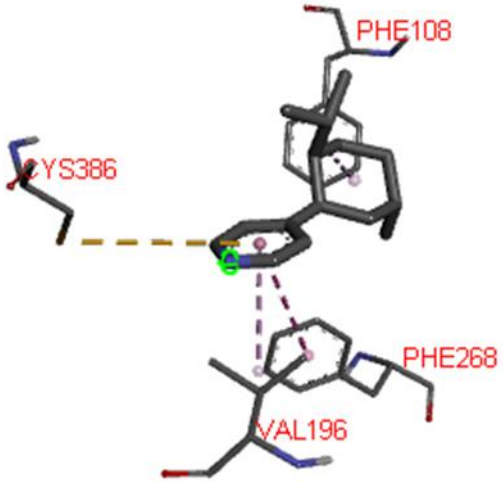
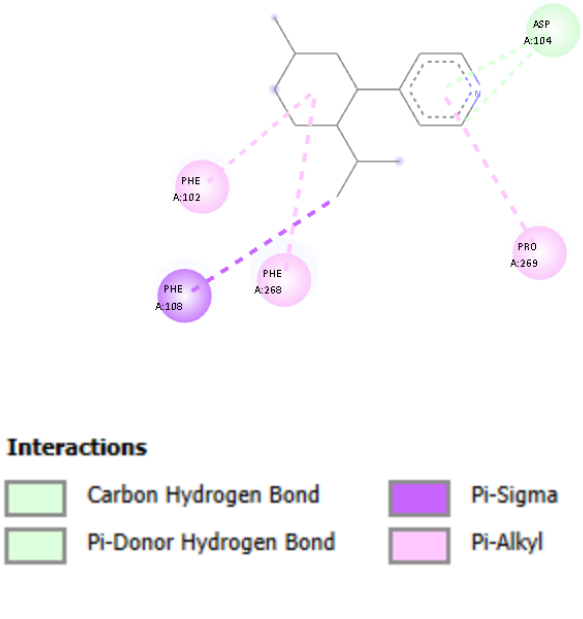
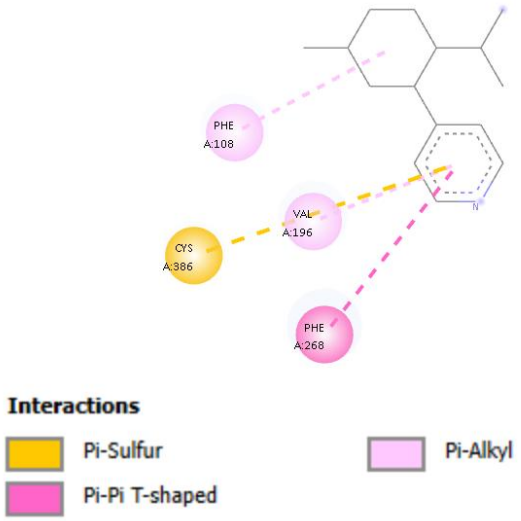
8b (I)	ent-8b (I)
	
	
Binding energy: -7.6	**Binding energy: -7.8**

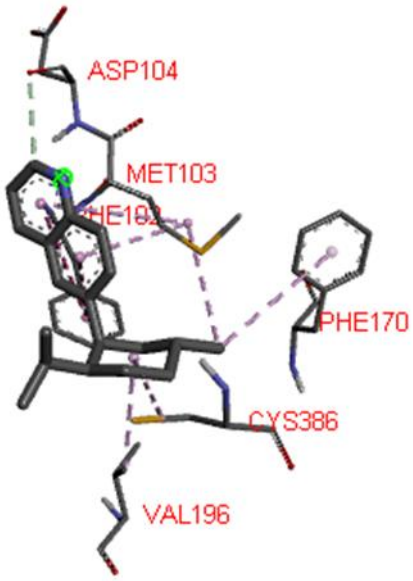
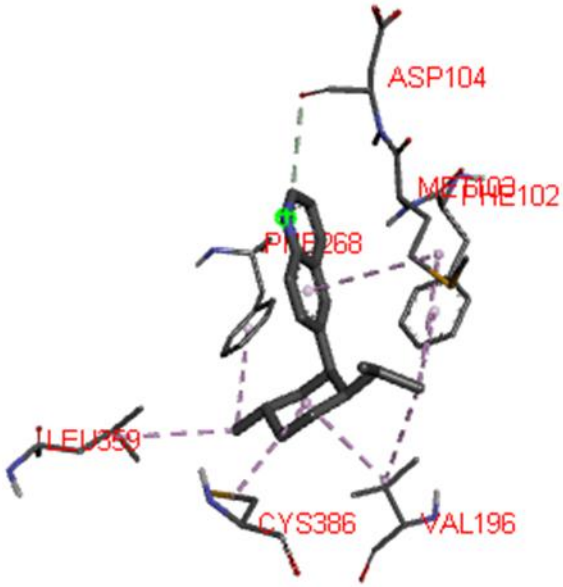
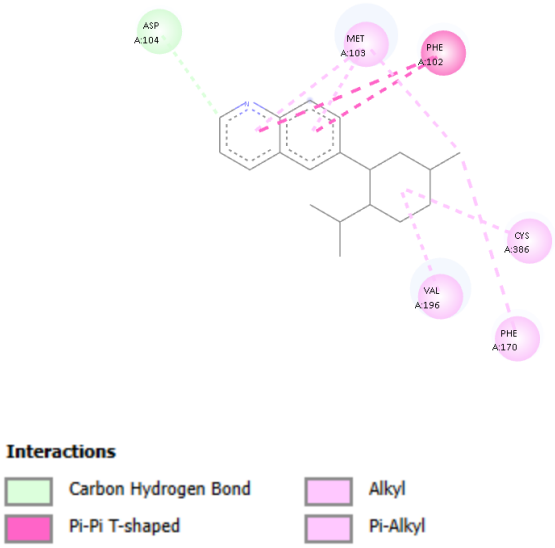
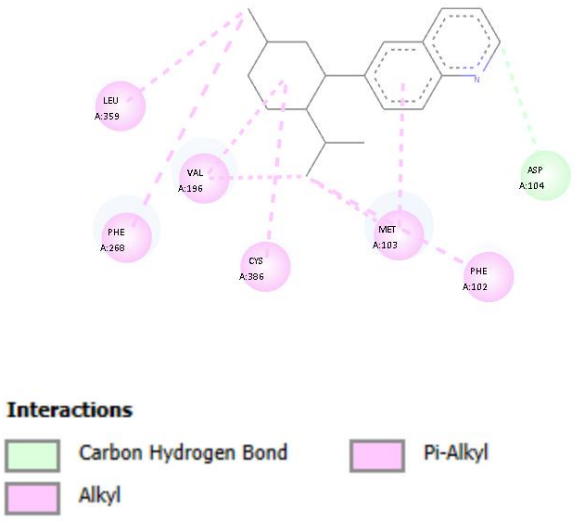
8b (II)	ent-8b (II)
	
	
Binding energy: -8.4	**Binding energy: -7.6**

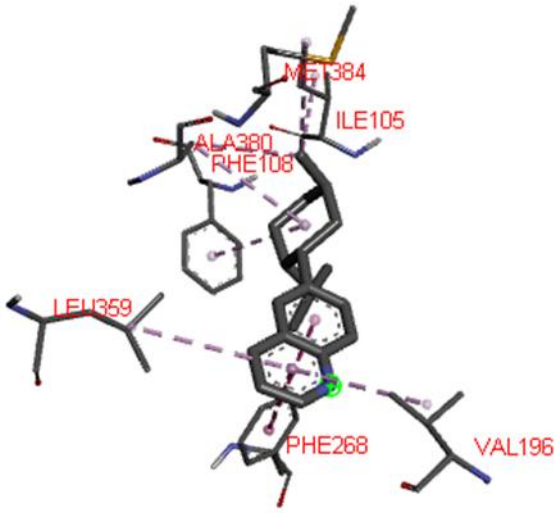
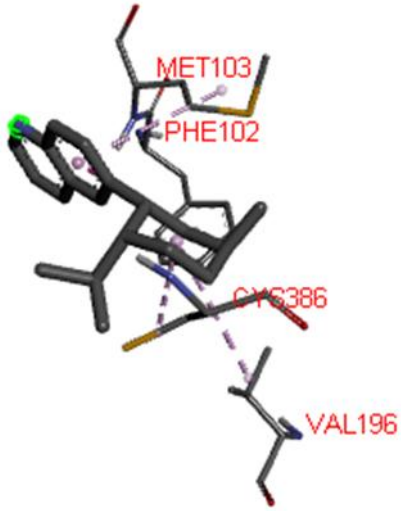
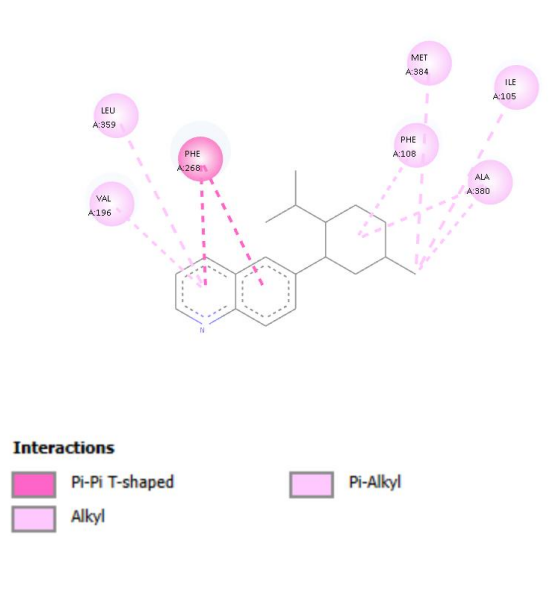
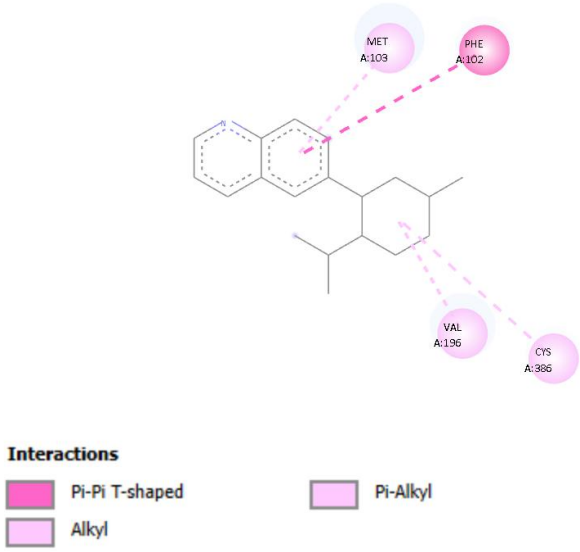
8c (I)	ent-8c (I)
	
	
Binding energy: -7.1	**Binding energy: -6.8**

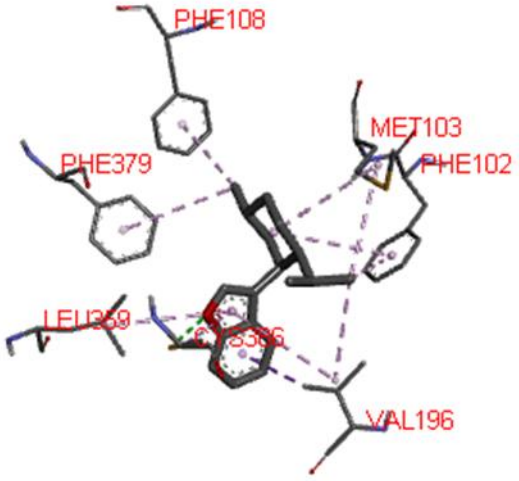
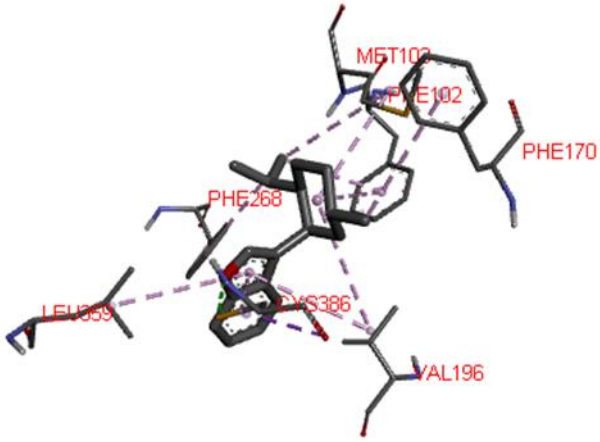
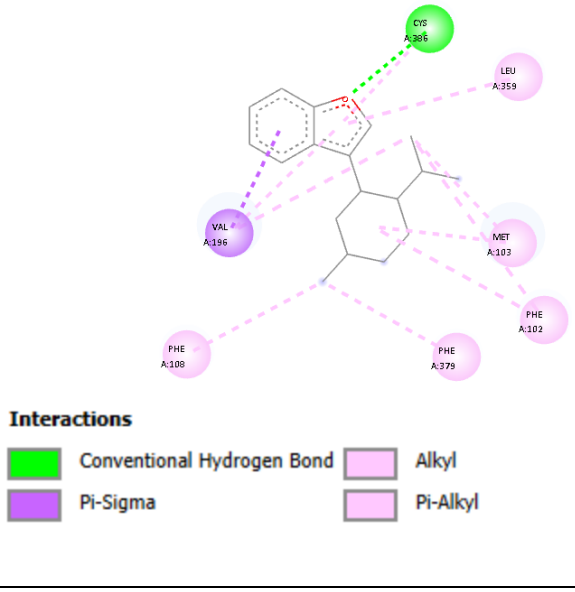
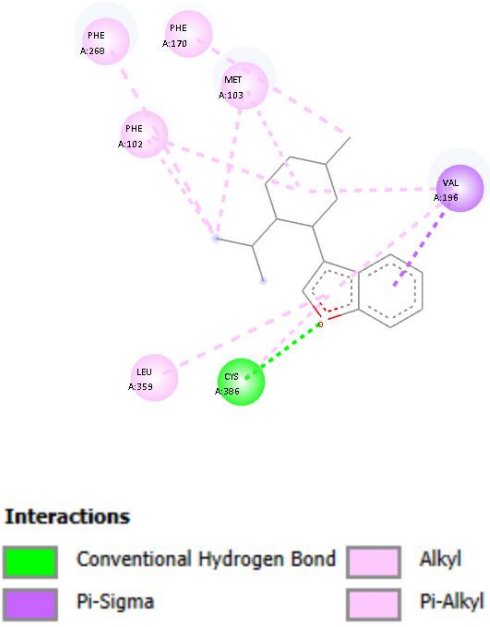
8c (II)	ent-8c (II)
	
	
Binding energy: -6.7	**Binding energy: -6.3**

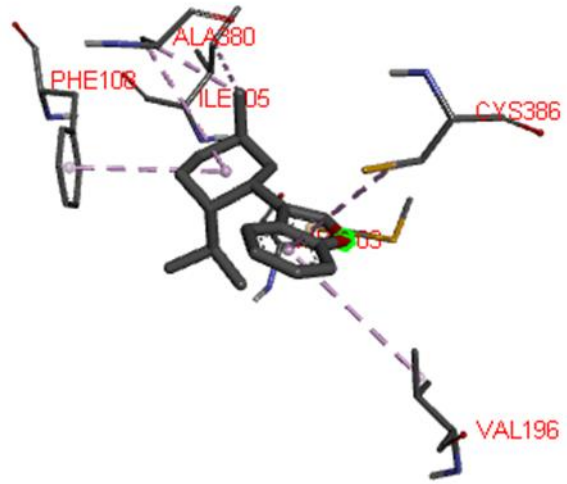
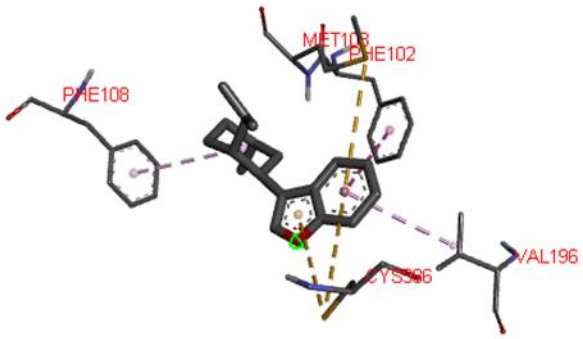
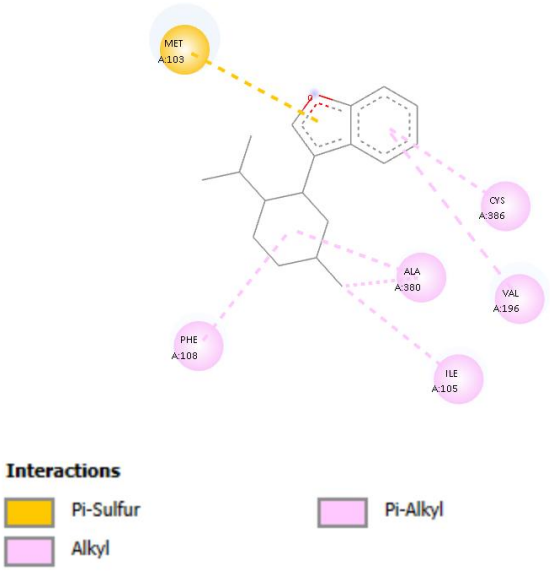
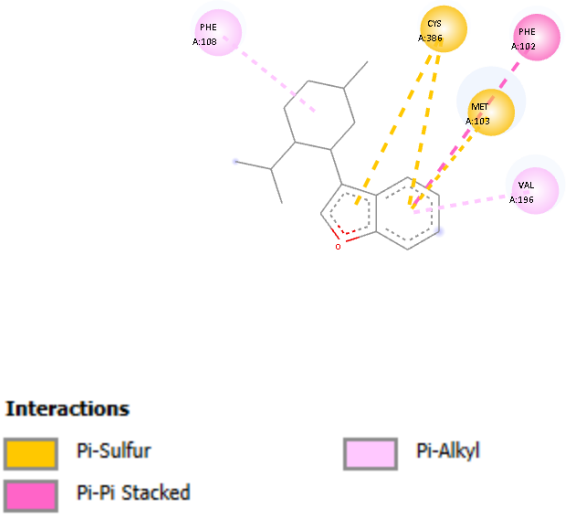
8d (l)	ent-8d (l)
	
	
Binding energy: -7.9	**Binding energy: -7.7**

8d (II)	ent-8d (II)
	
	
Binding energy: -8.2	**Binding energy: -7.4**

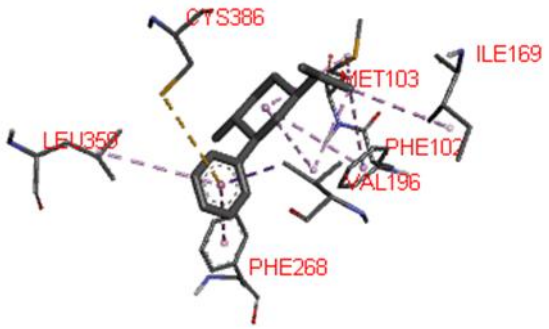
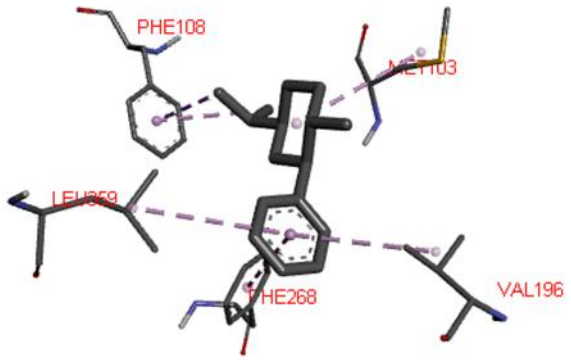
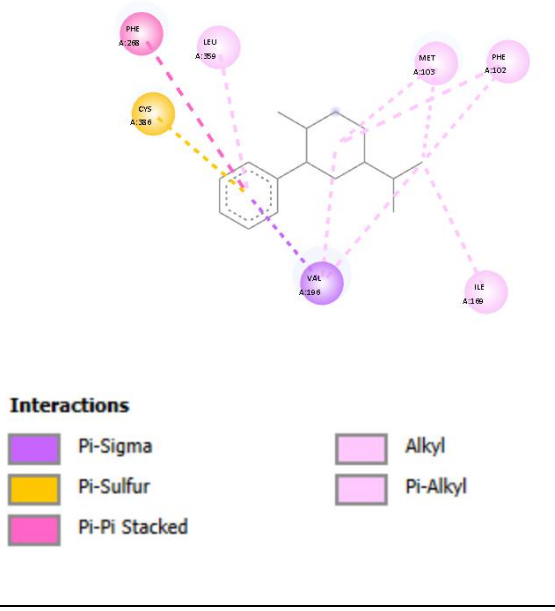
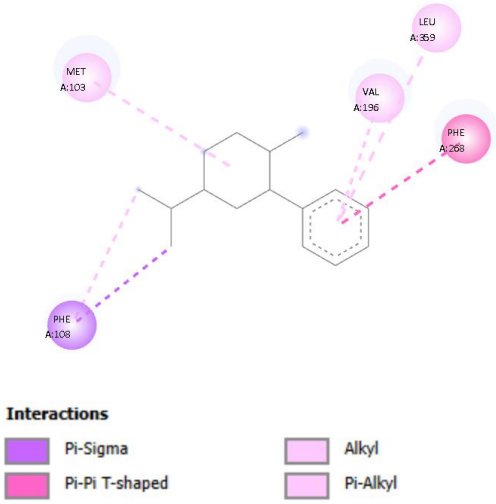
8e (l)	ent-8e (l)
	
	
Binding energy: -9.6	**Binding energy: -9.6**

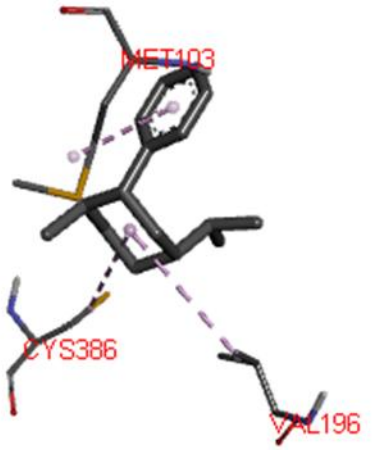
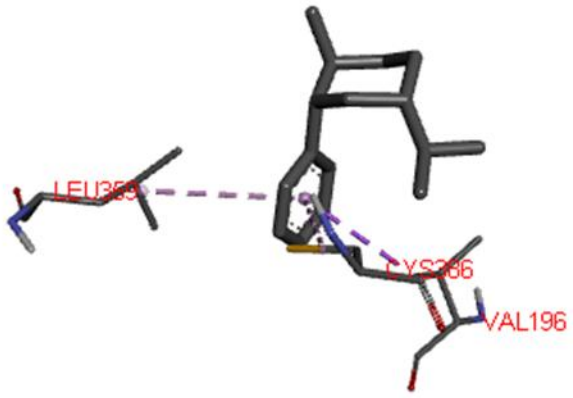
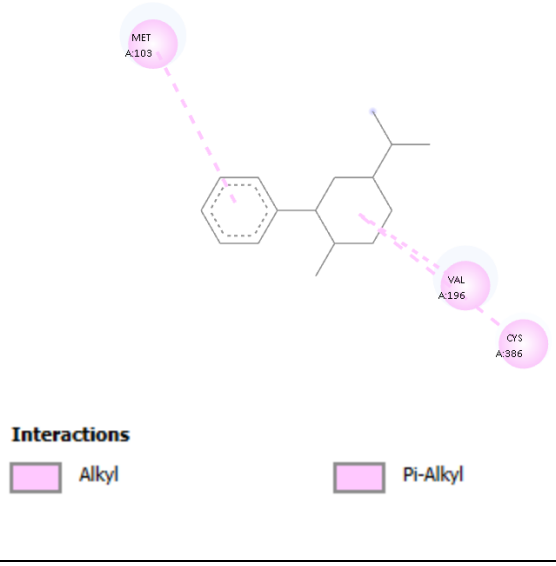
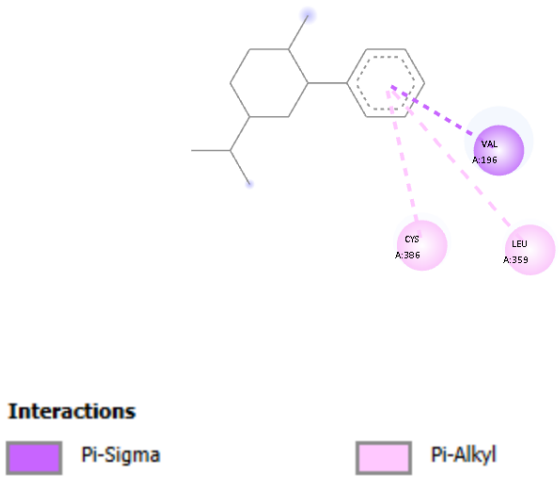
8e (II)	ent-8e (II)
	
	
Binding energy: -9.6	**Binding energy: -9.2**

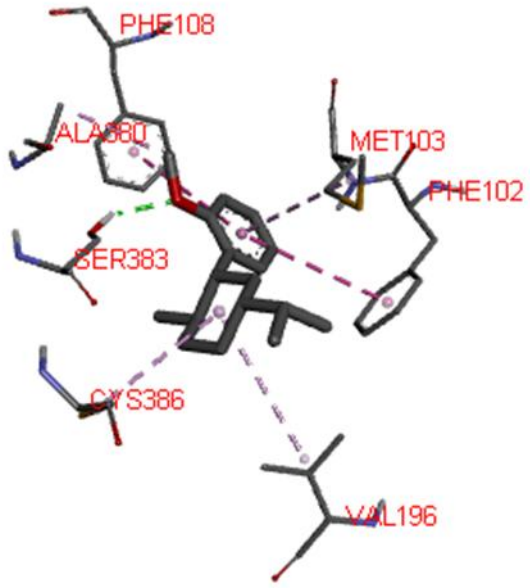
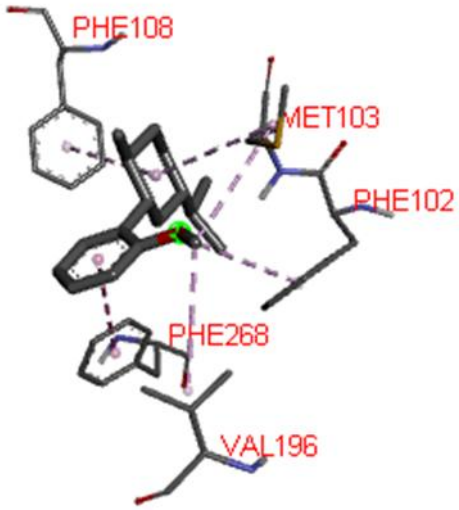
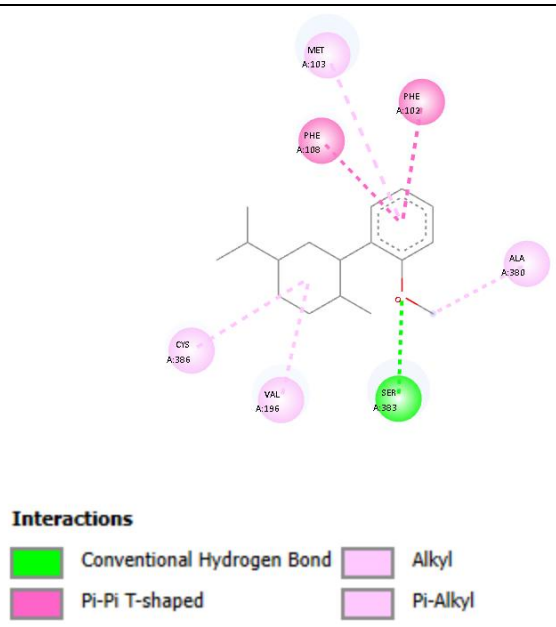
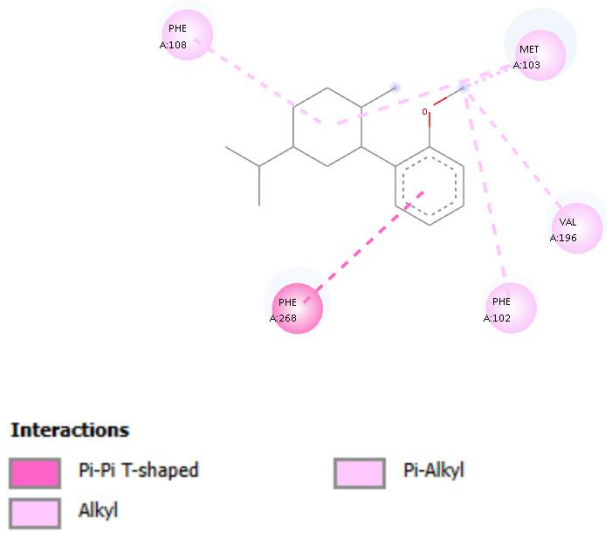
8f (I)	ent-8f (I)
	
	
Binding energy: -8.9	**Binding energy: -9.0**

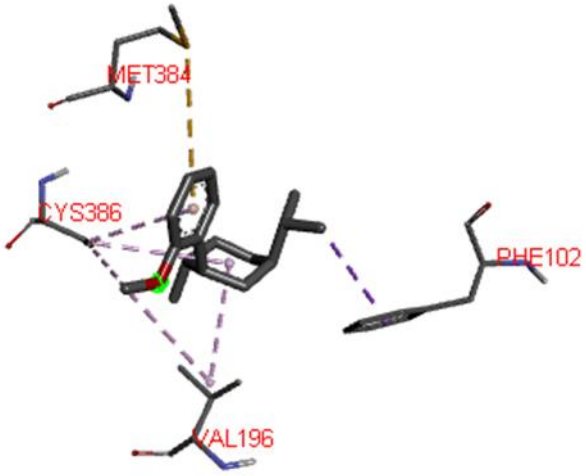
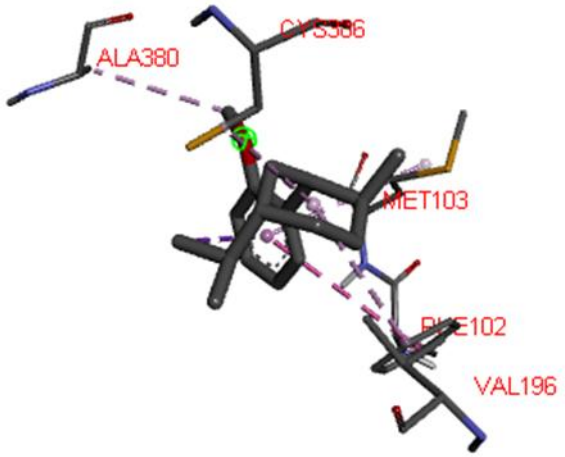
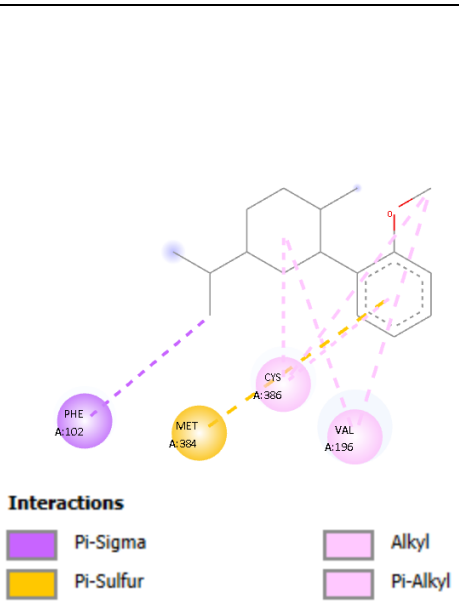
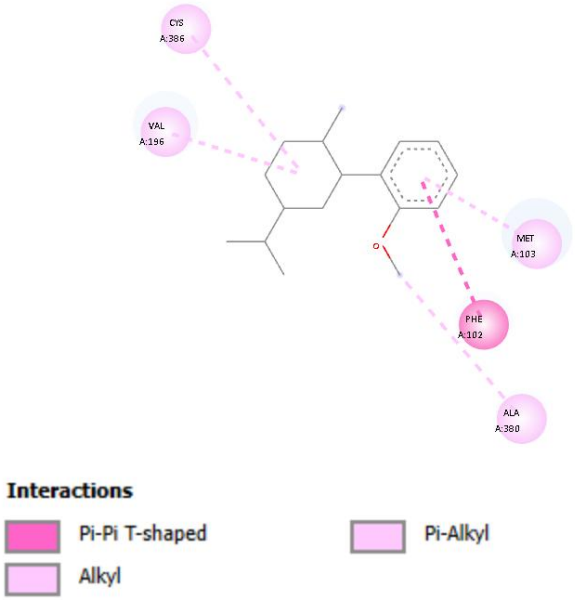
8f (II)	ent-8f (II)
	
	
Binding energy: -9.0	**Binding energy: -8.7**

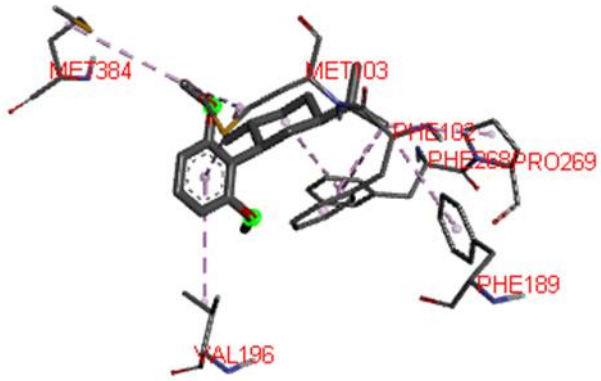
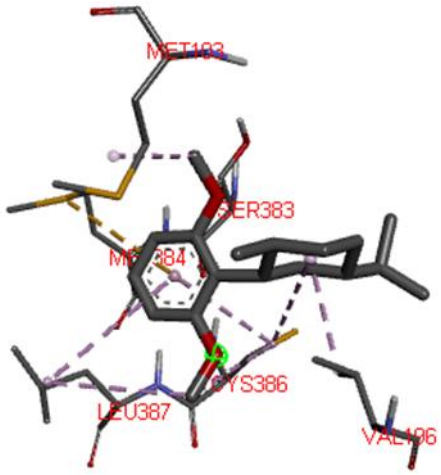
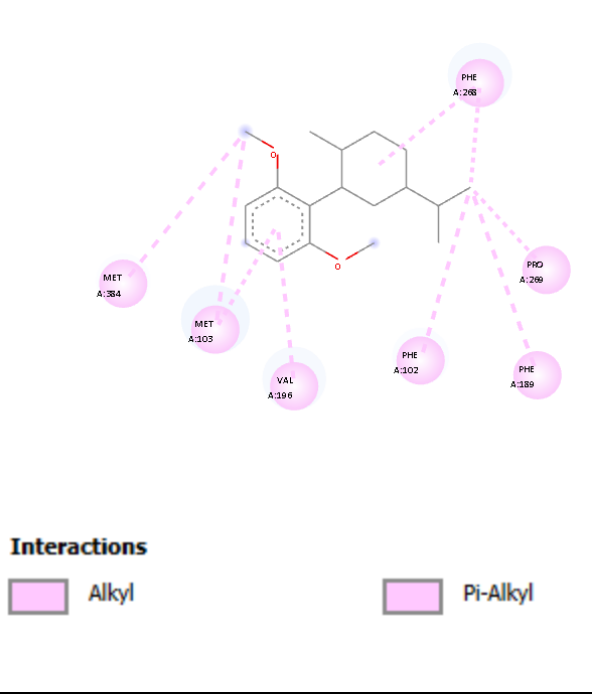
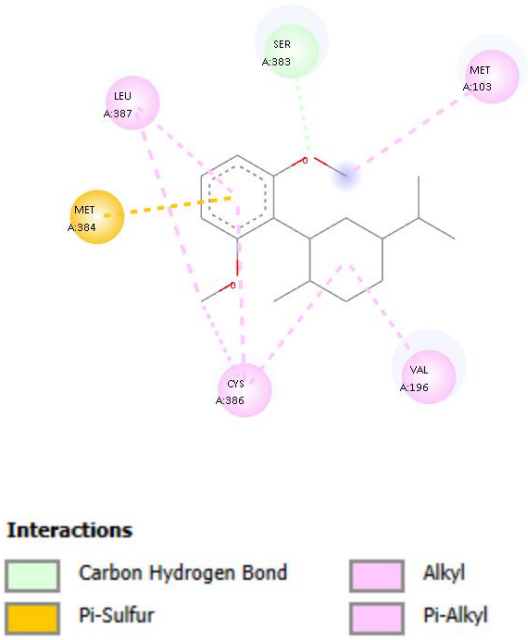
• *Synthesized Ligands of Series* ***9****/ent-****9*** *with CB1 Receptor*

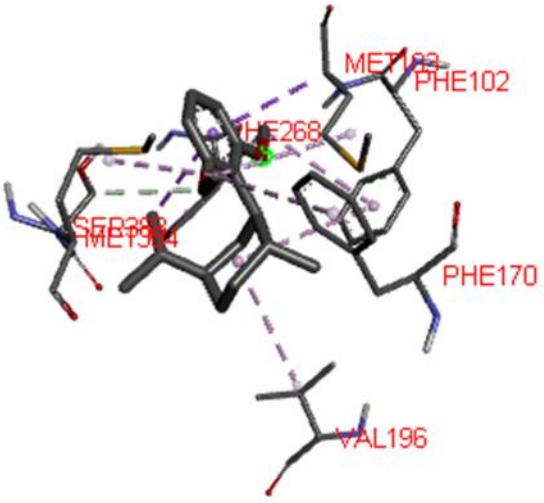
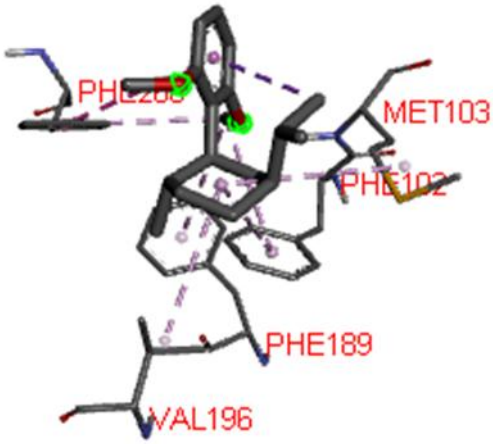
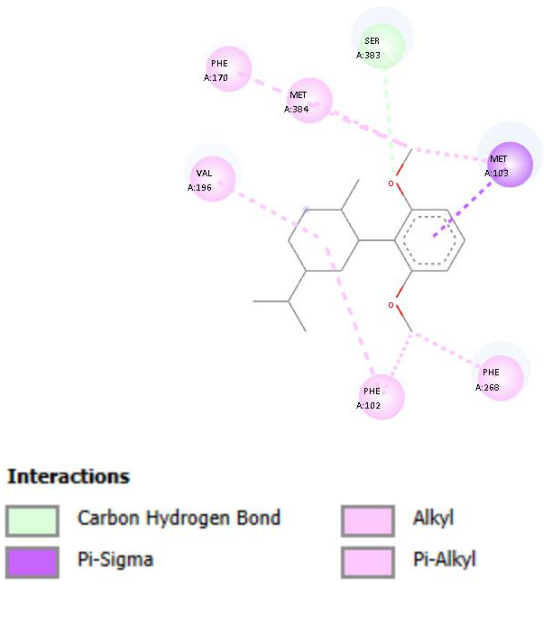
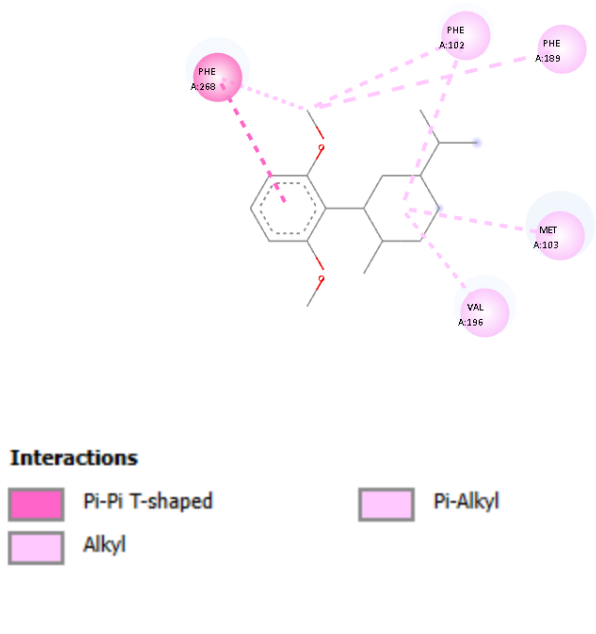
9a (I)	**ent-9a (I)**
	
	
Binding energy: -8.5	**Binding energy: -8.2**

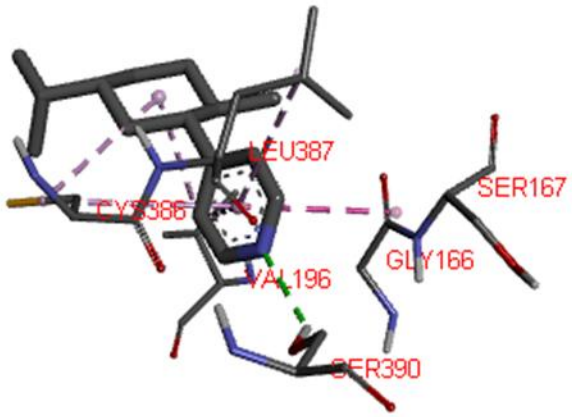
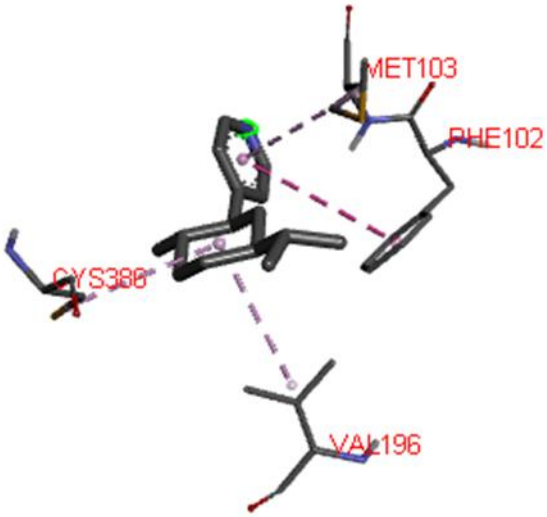
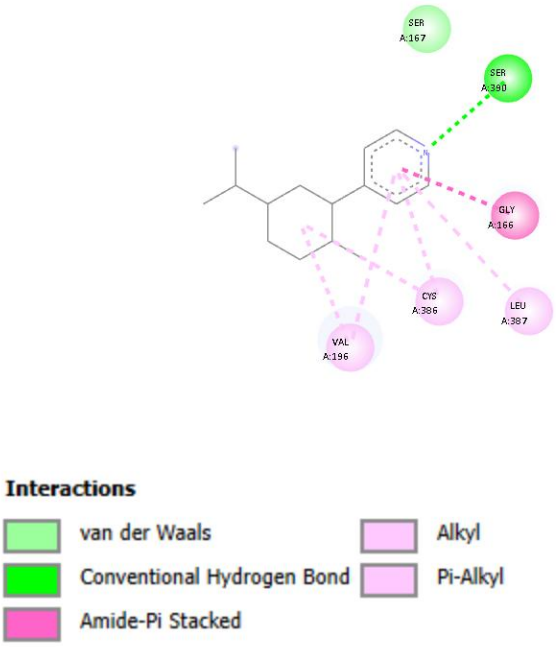
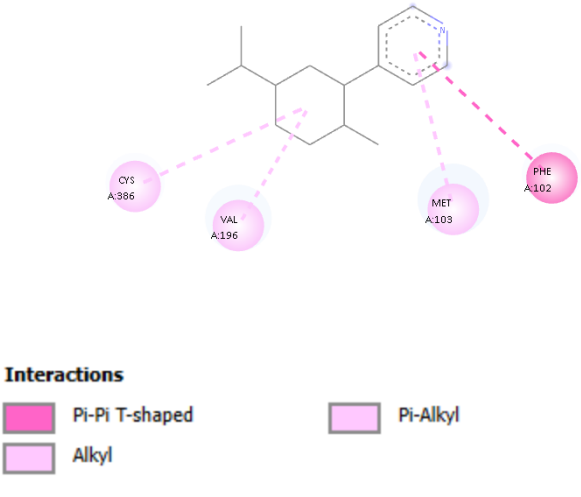
9a (II)	ent-9a (II)
	
	
Binding energy: -7.3	**Binding energy: -7.2**

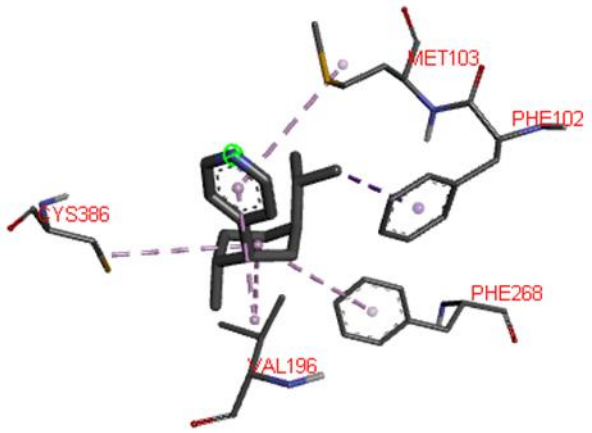
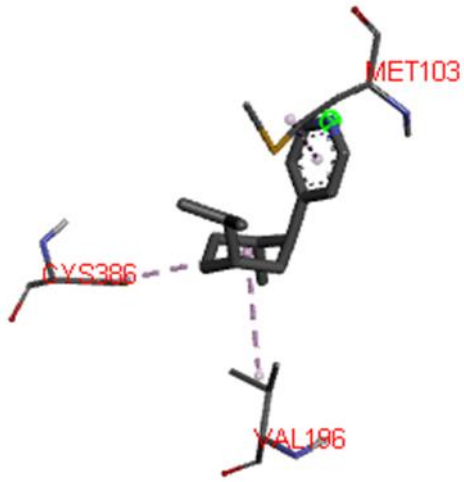
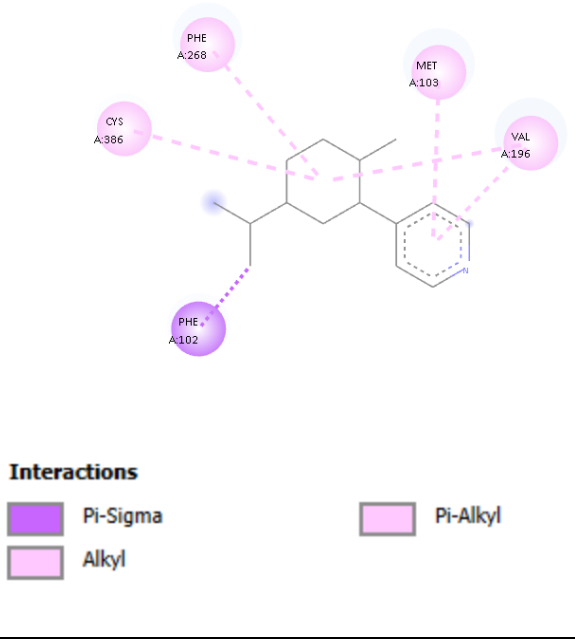
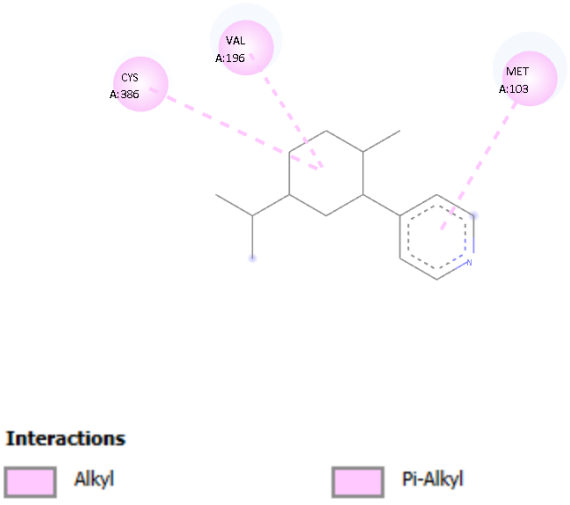
9b (I)	ent-9b (I)
	
	
Binding energy: -8.2	**Binding energy: -8.0**

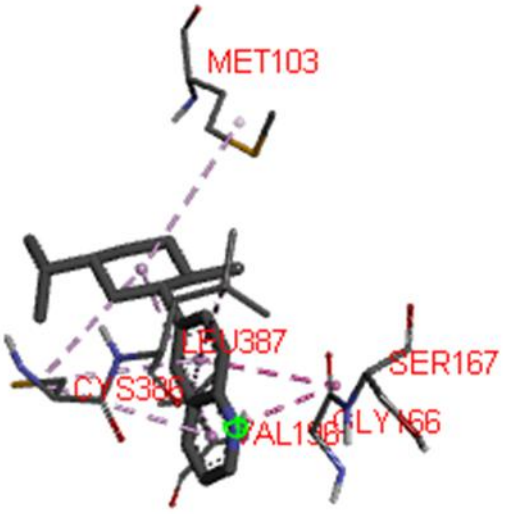
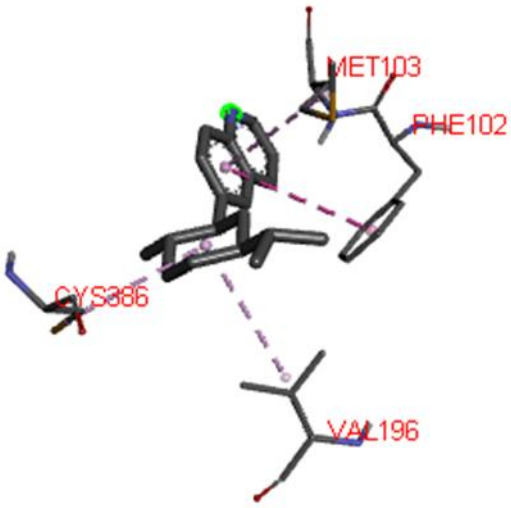
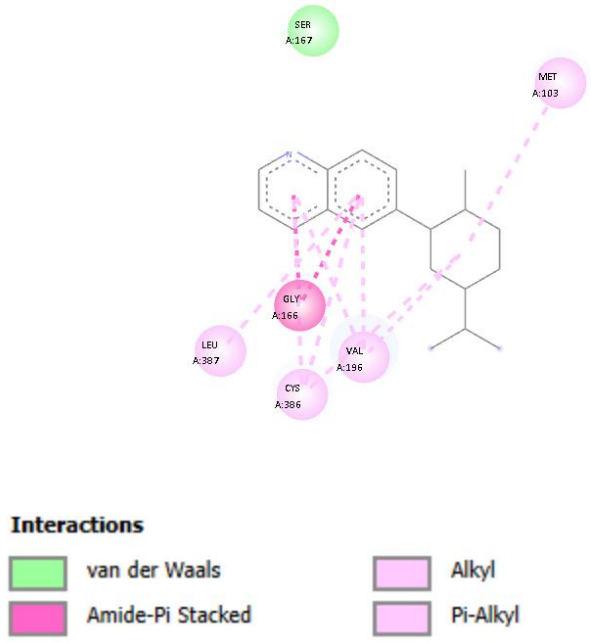
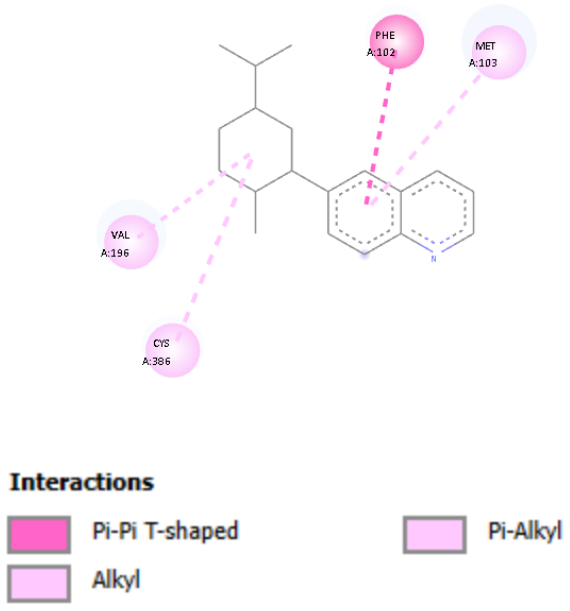
9b (II)	ent-9b (II)
	
	
Binding energy: -7.0	**Binding energy: -7.2**

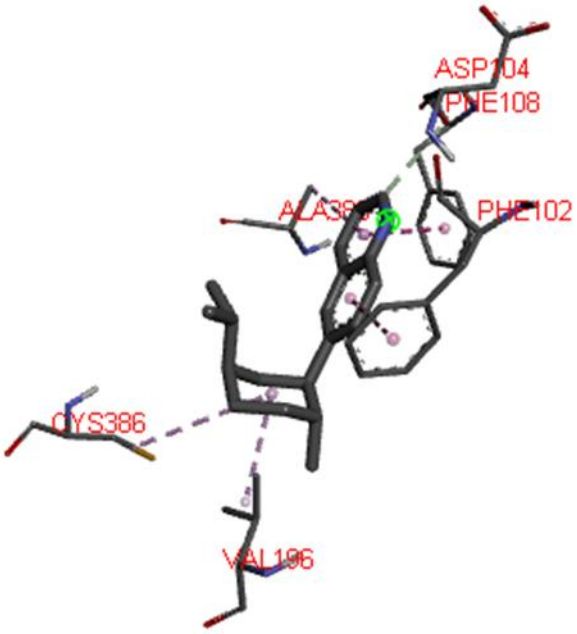
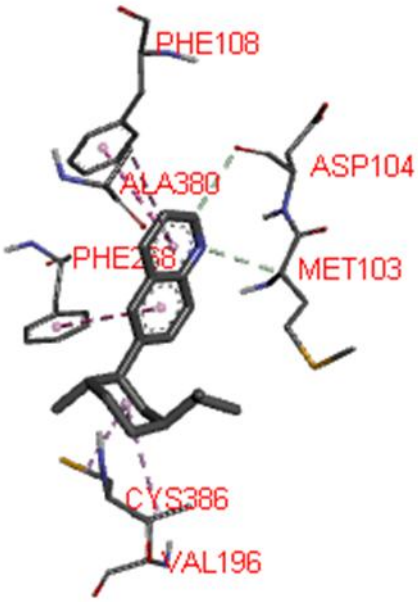
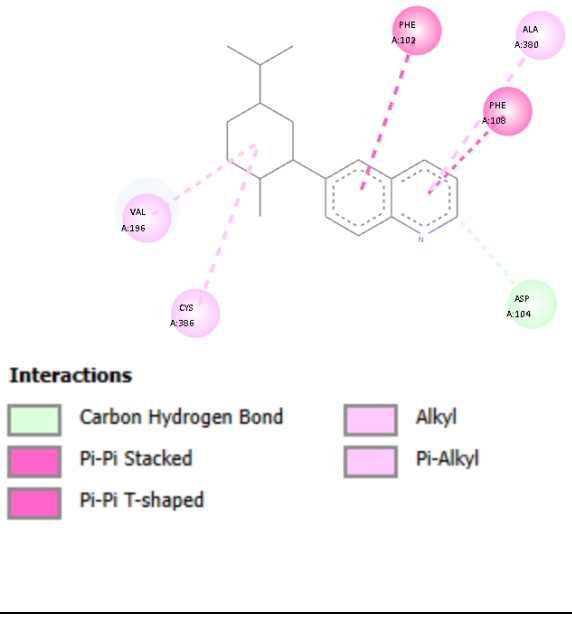
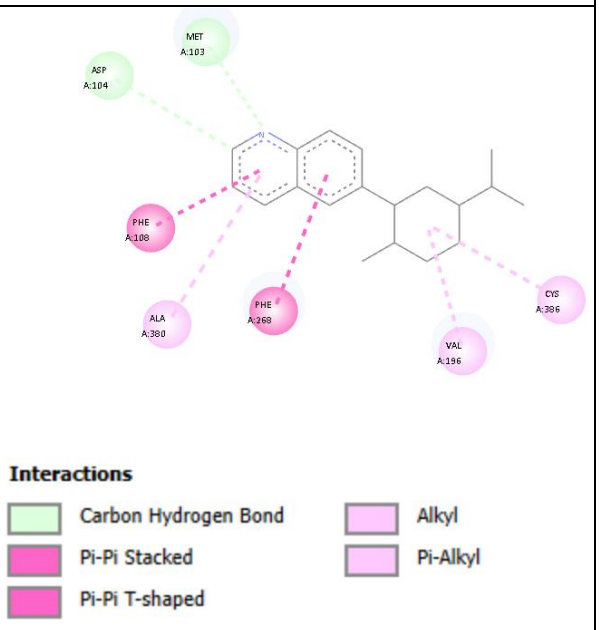
9c (l)	ent-9c (l)
	
	
Binding energy: -7.5	**Binding energy: -7.7**

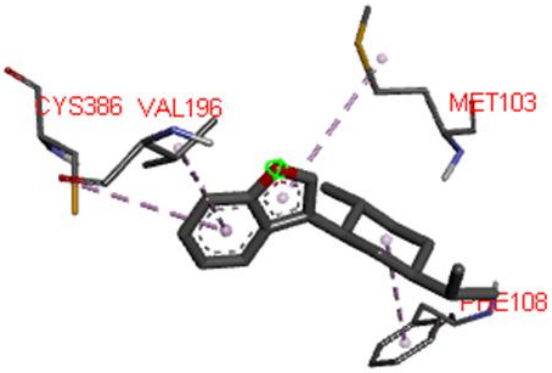
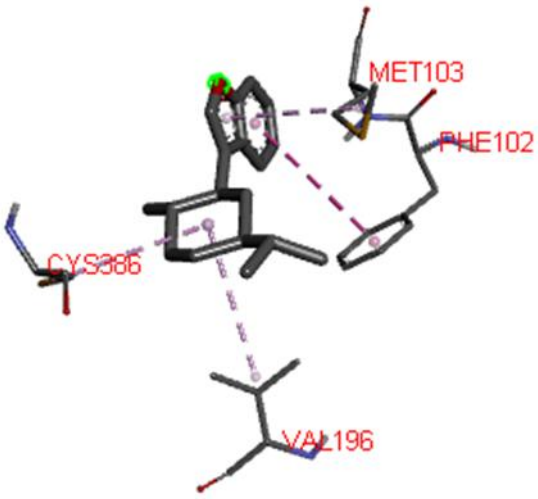
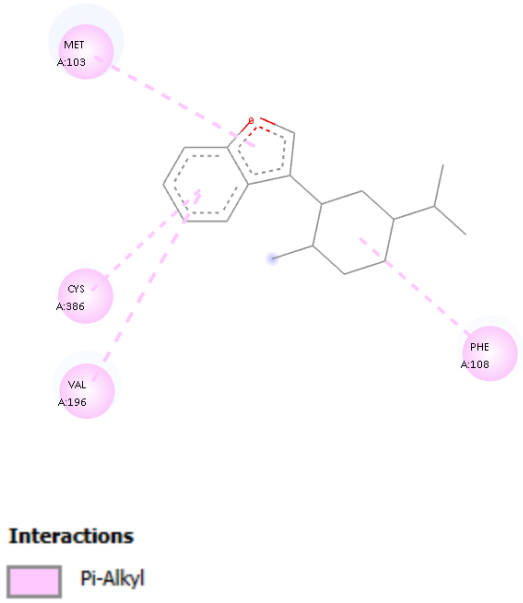
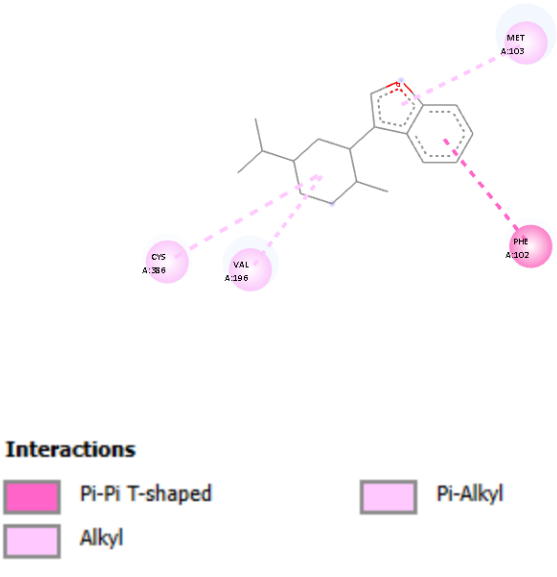
9c (II)	ent-9c (II)
	
	
Binding energy: -6.2	**Binding energy: -6.5**

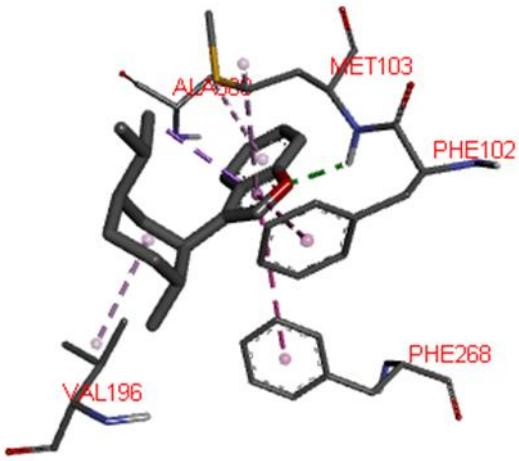
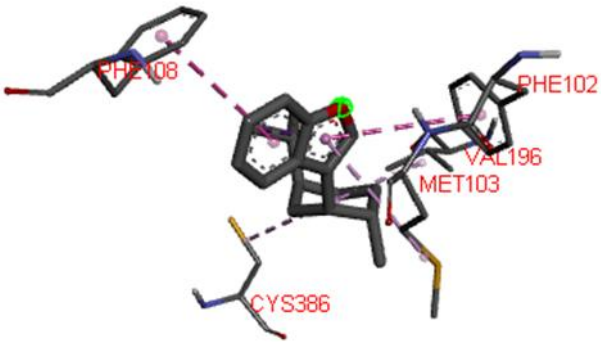
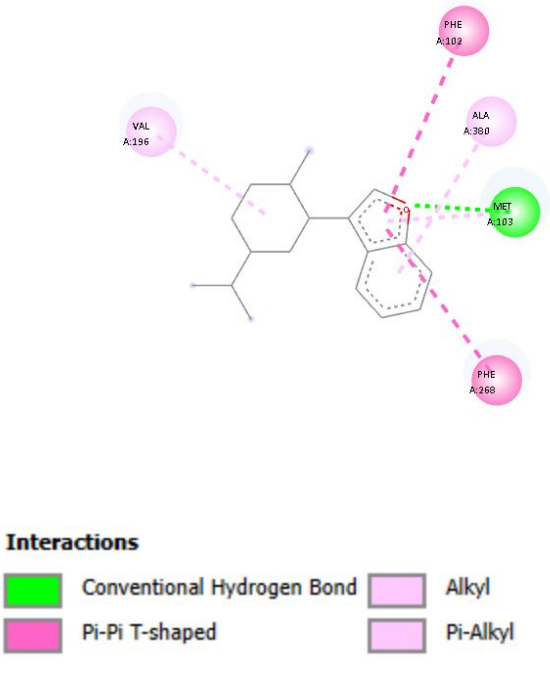
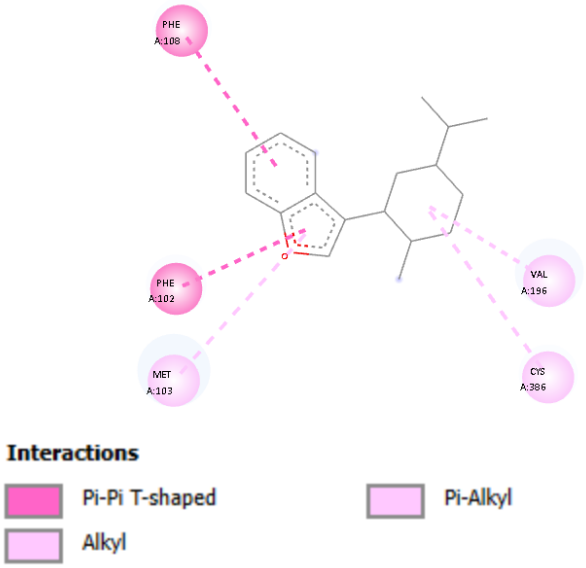
9d (I)	ent-9d (I)
	
	
Binding energy: -8.5	**Binding energy: -7.6**

9d (II)	ent-9d (II)
	
	
Binding energy: -6.9	**Binding energy: -6.9**

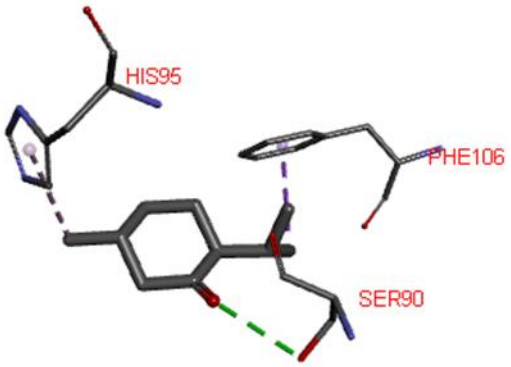
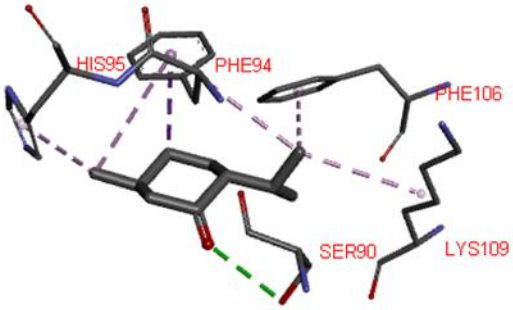
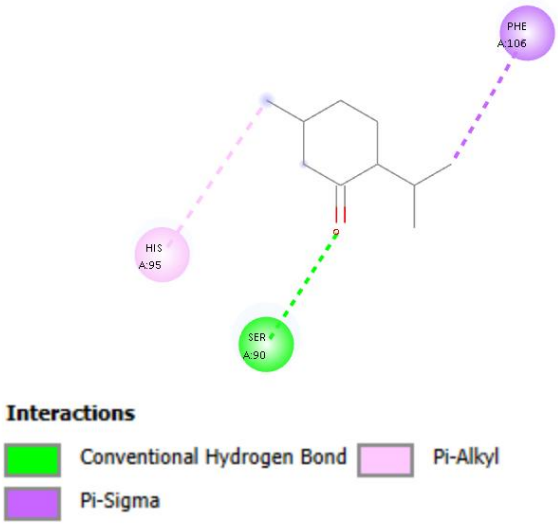
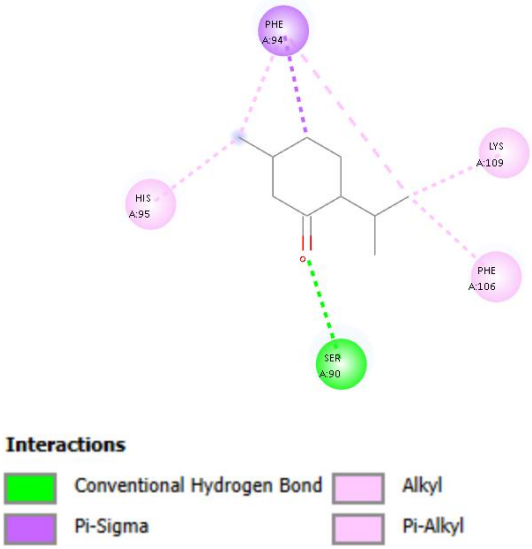
9e (I)	ent-9e (I)
	
	
Binding energy: -9.8	**Binding energy: -10.1**

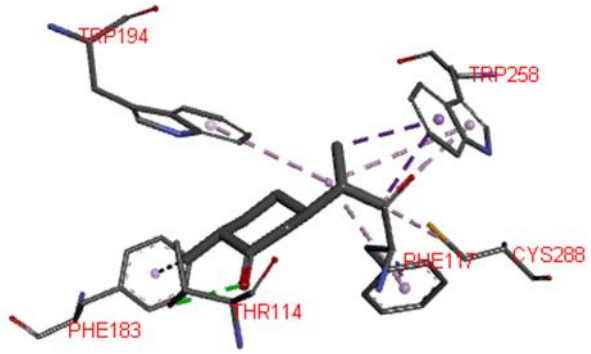
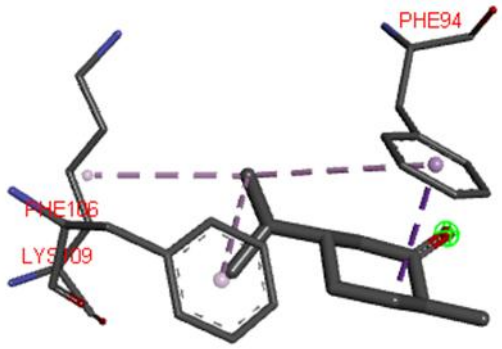
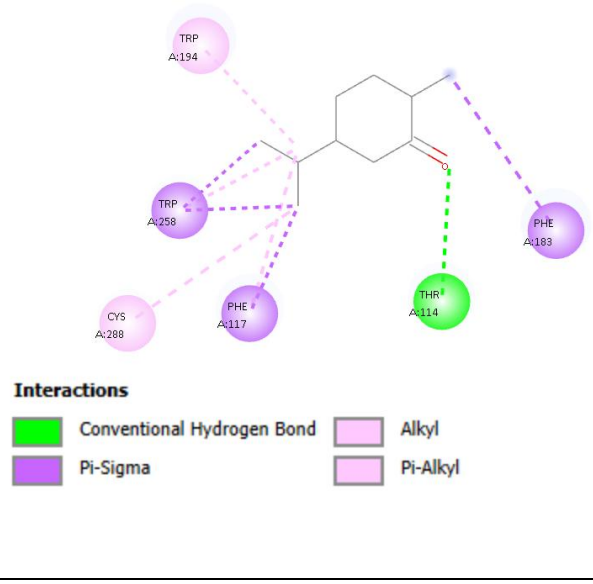
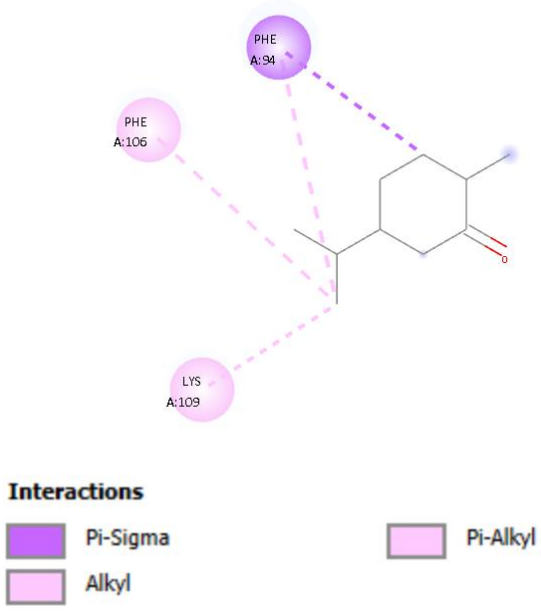
9e (II)	ent-9e (II)
	
	
Binding energy: -8.6	**Binding energy: -9.4**

9f (I)	ent-9f (I)
	
	
Binding energy: -9.1	**Binding energy: -9.2**

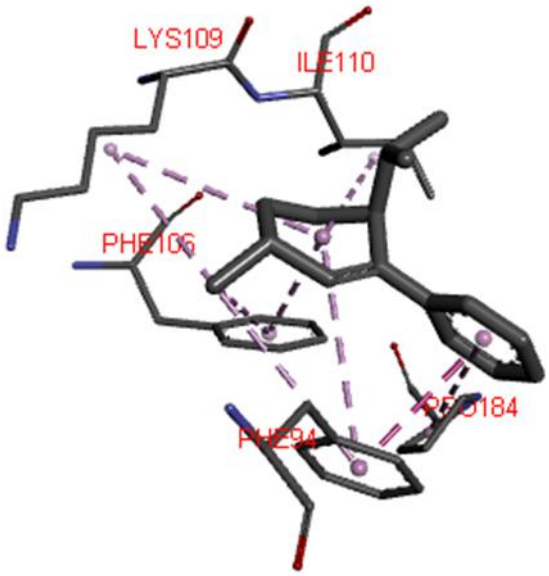
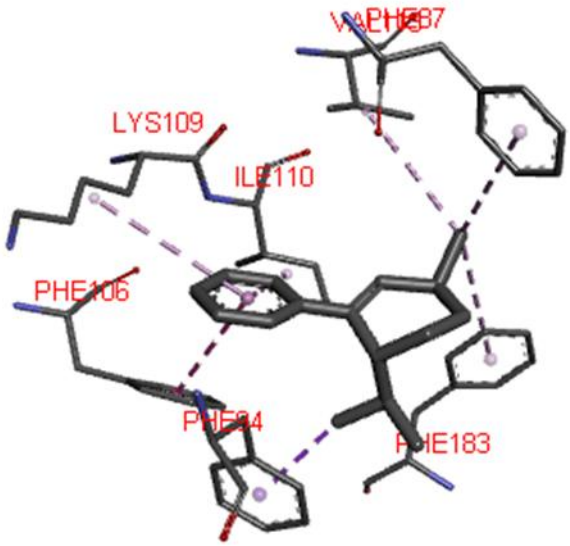
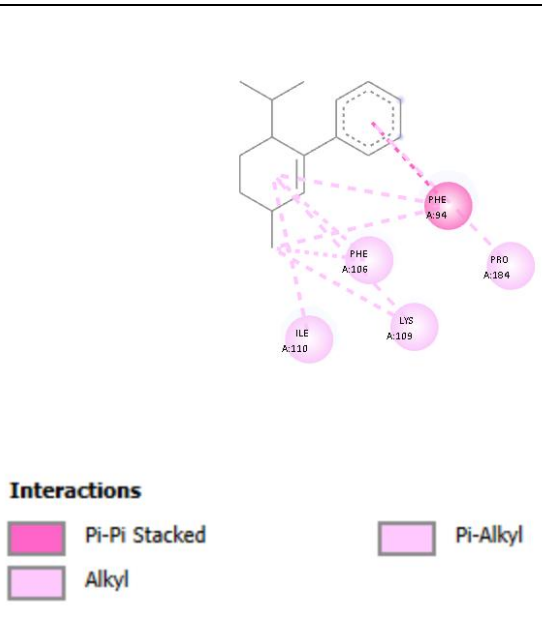
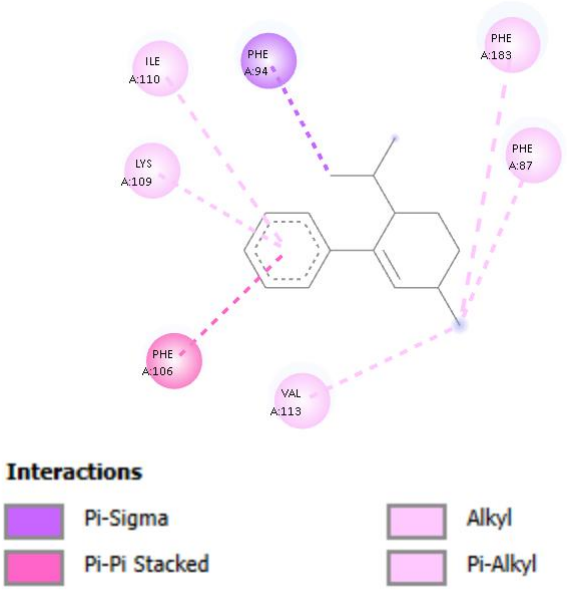
9f (II)	ent-9f (II)
	
	
Binding energy: -8.4	**Binding energy: -7.9**

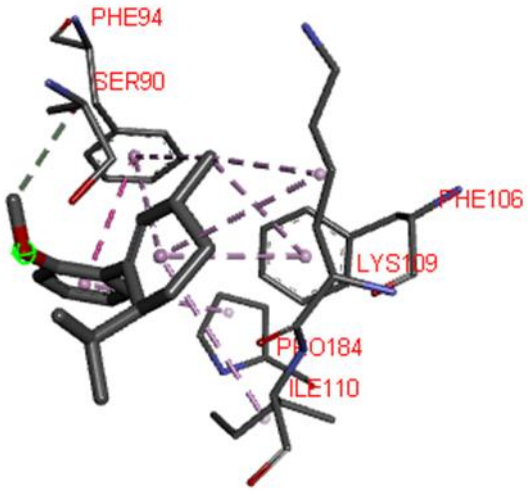
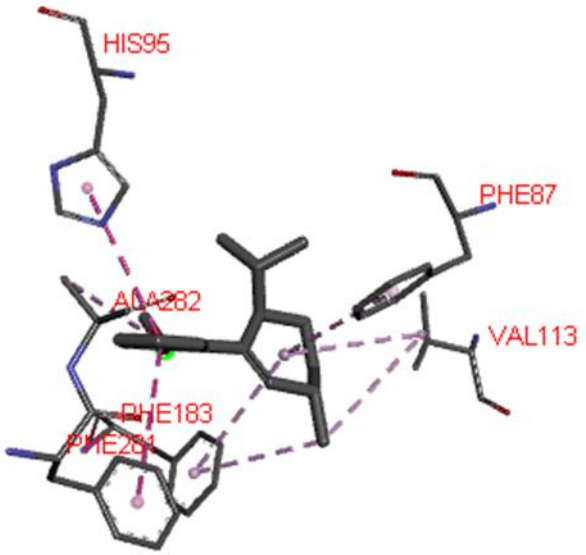
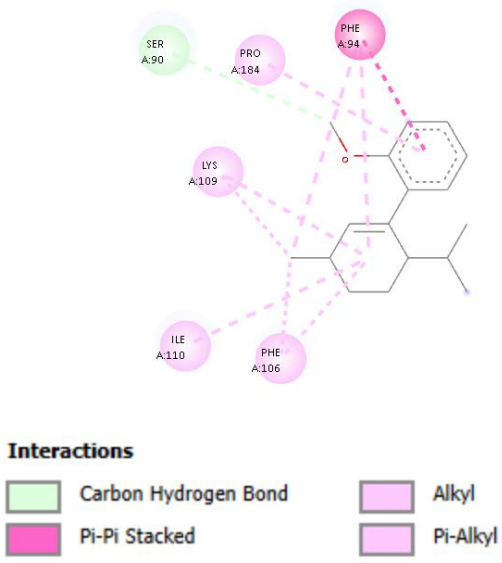
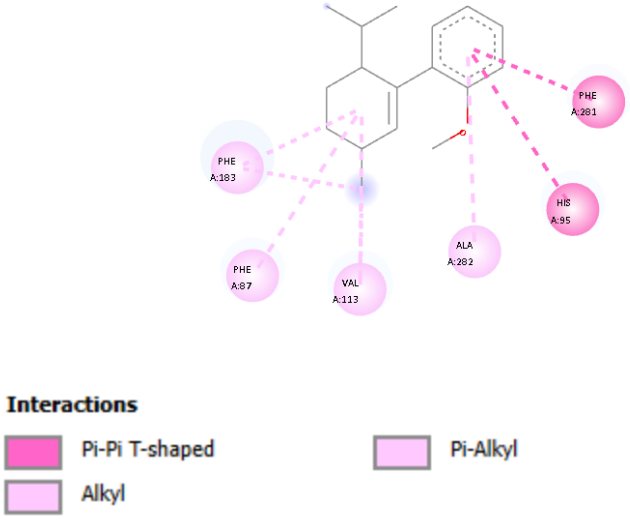
• *Ketone Precursors with CB2 Receptor*

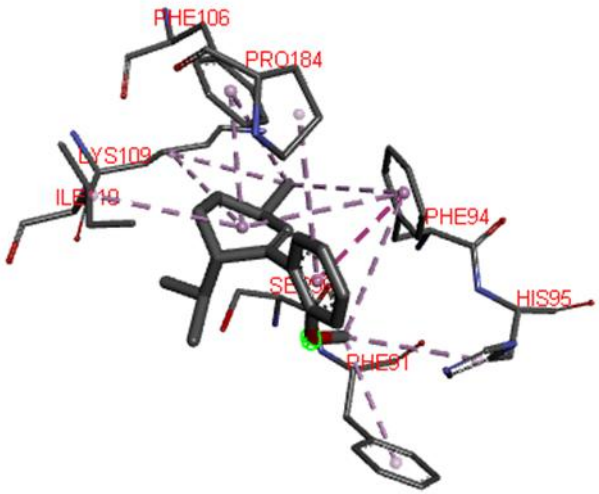
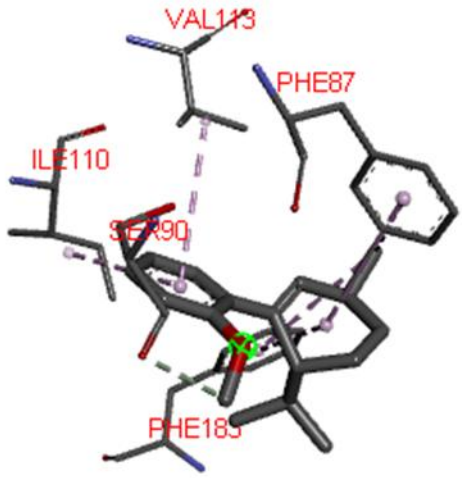
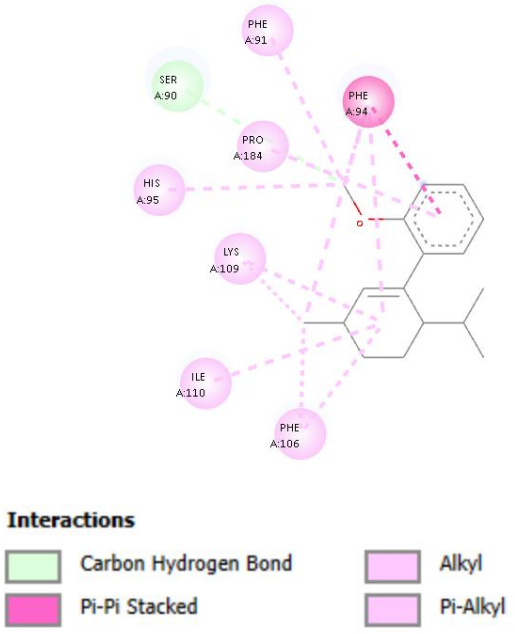
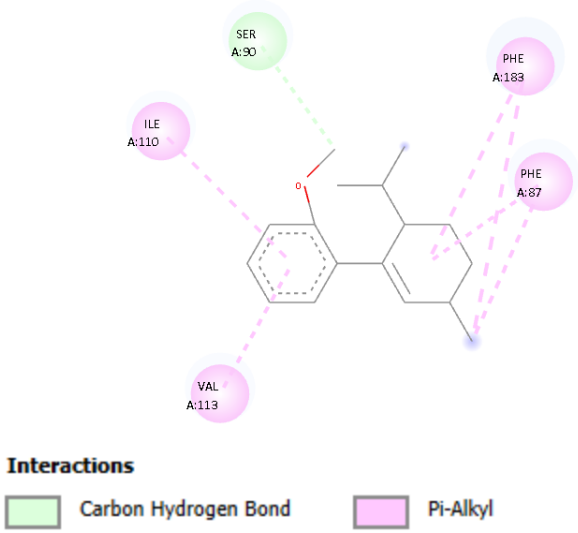
(-)-1	(+)-1
	
	
Binding energy: -6.6	**Binding energy: -7.0**

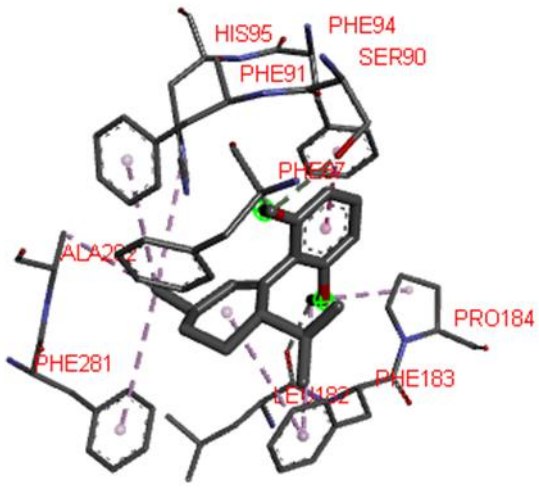
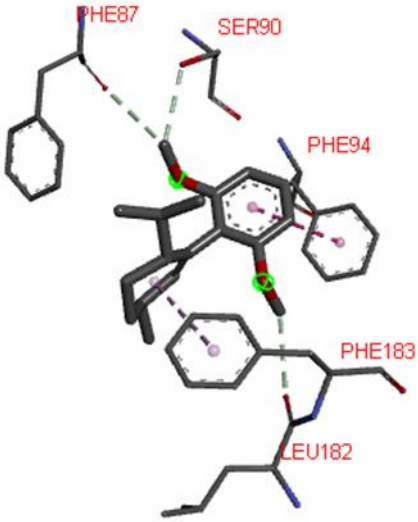
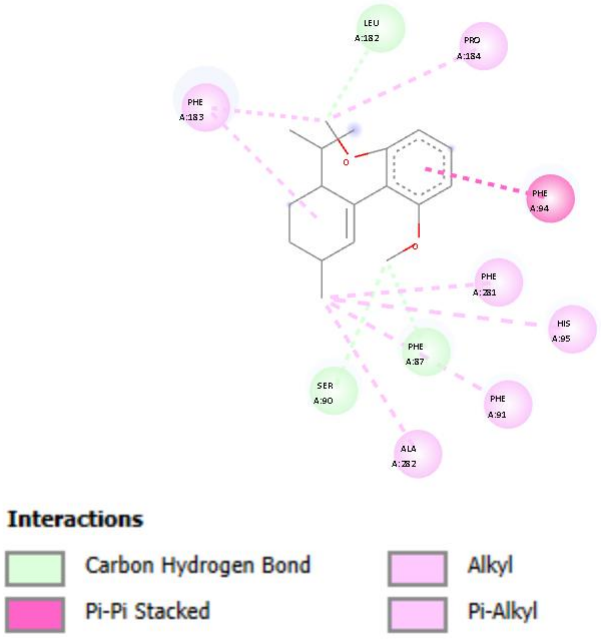
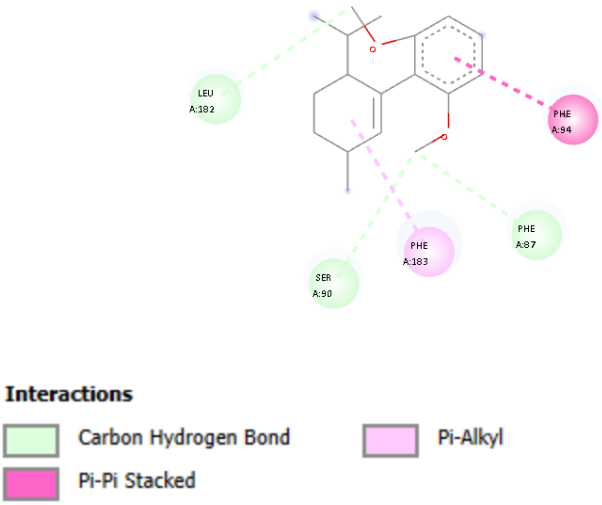
(+)-2	(-)-2
	
	
Binding energy: -6.7	**Binding energy: -6.8**

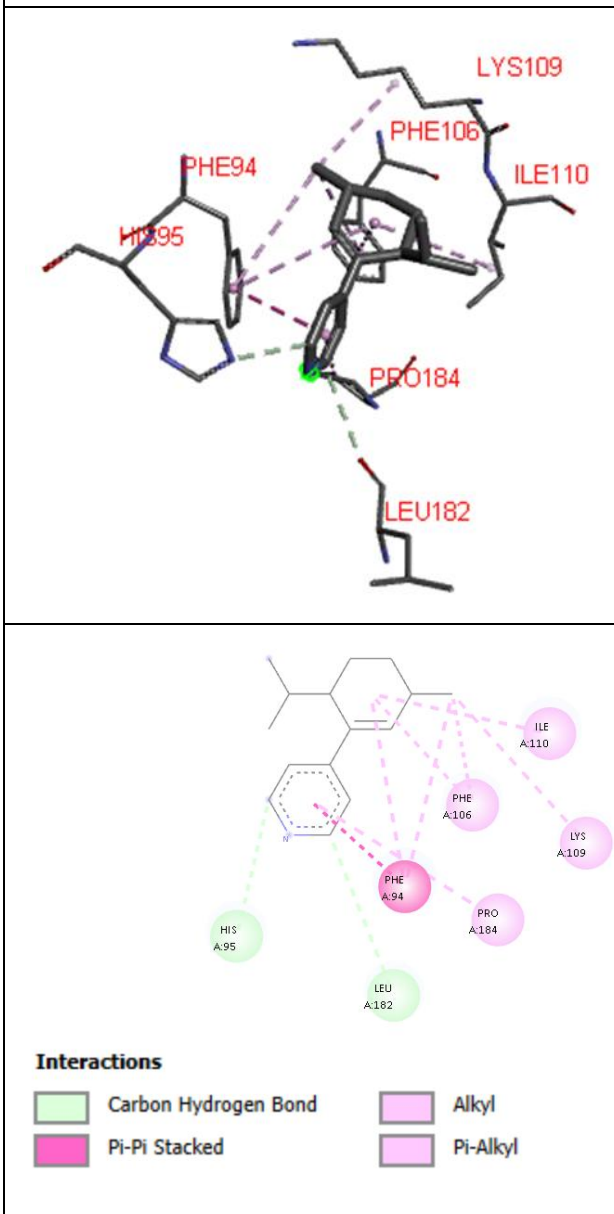
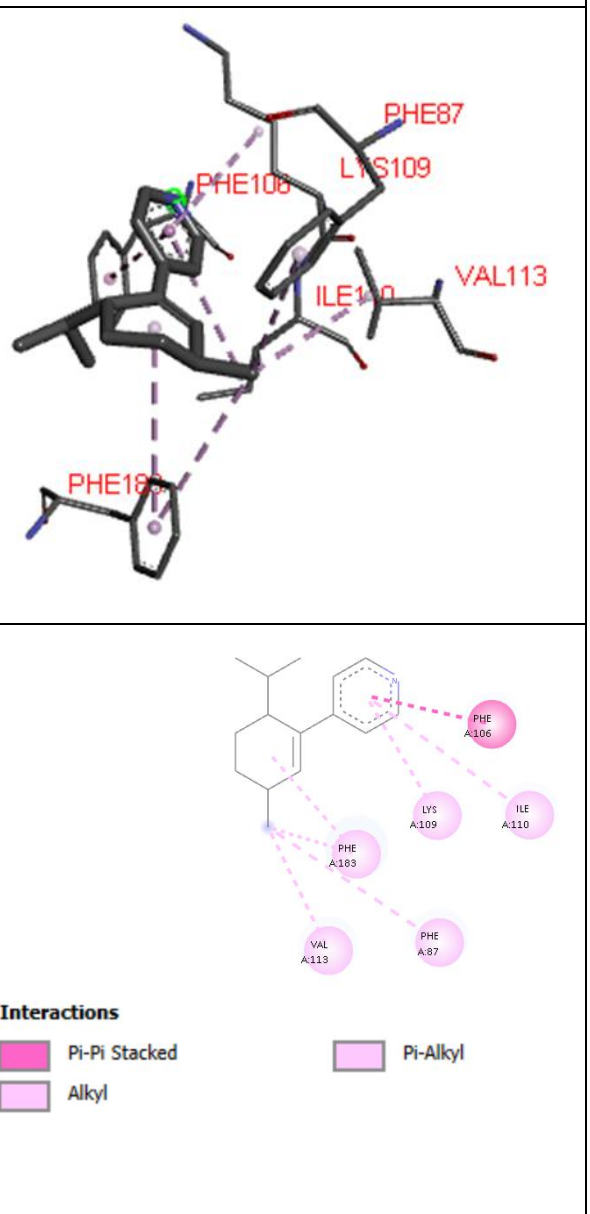
• *Synthesized Ligands of Series **6**/ent-**6** with CB2 Receptor*

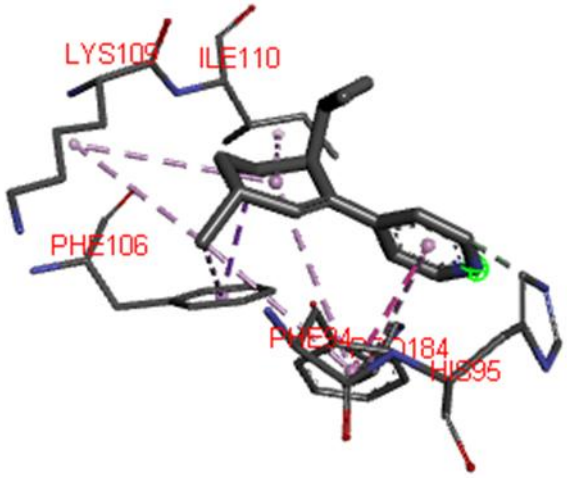
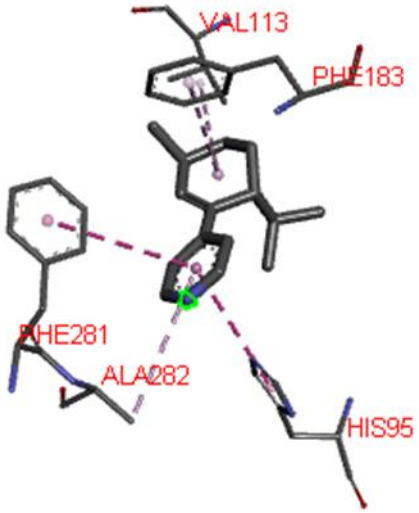
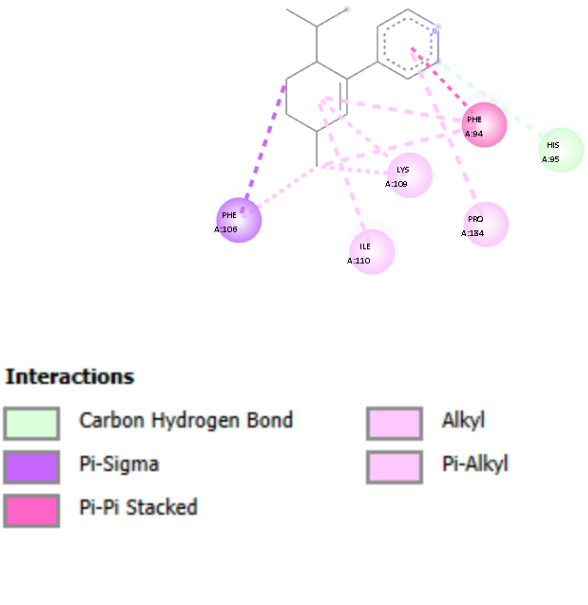
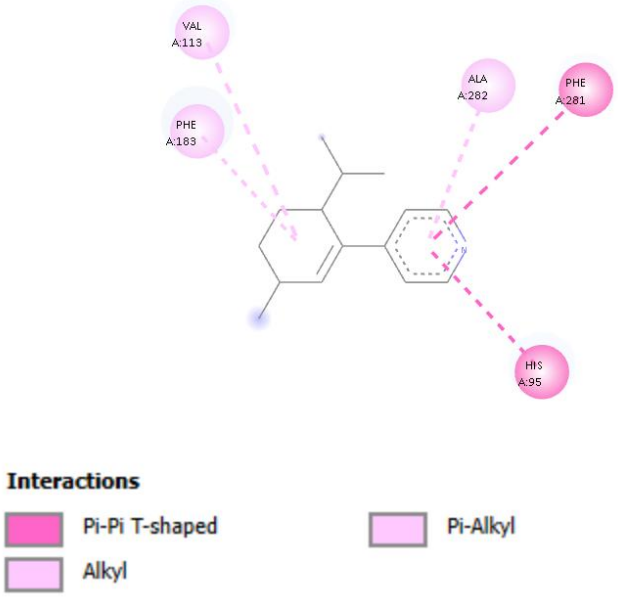
6a (II)	**ent-6a (II)**
	
	
Binding energy: -9.4	**Binding energy: -8.6**

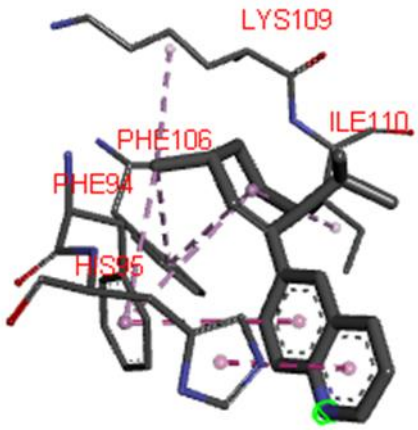
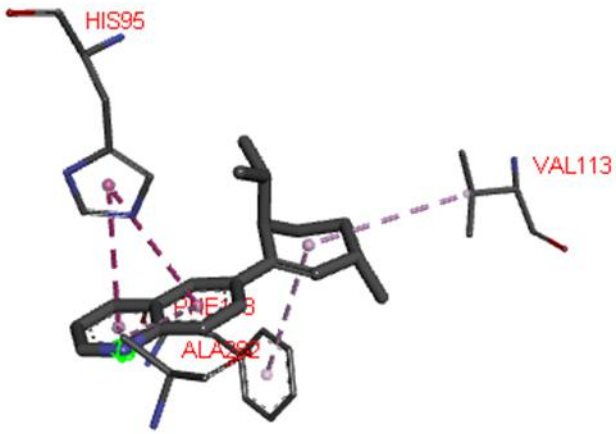
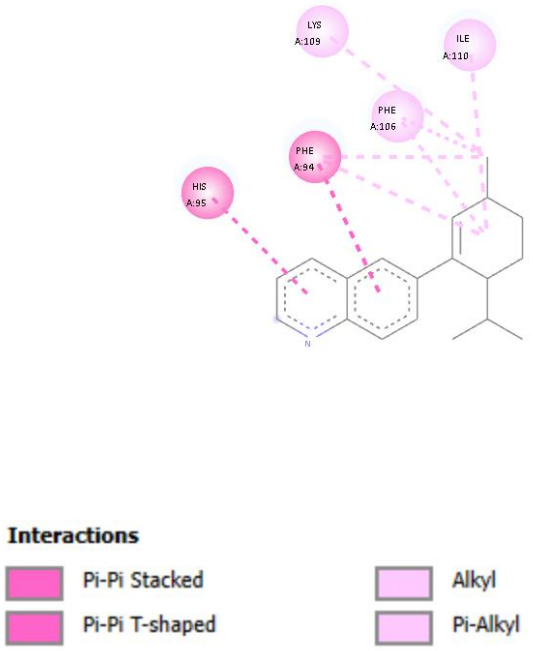
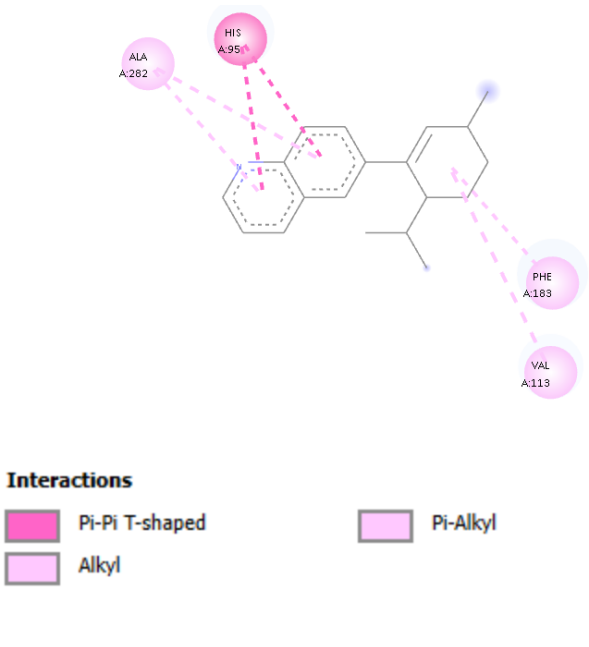
6b (l)	ent-6b (l)
	
	
Binding energy: -9.3	**Binding energy: -8.3**

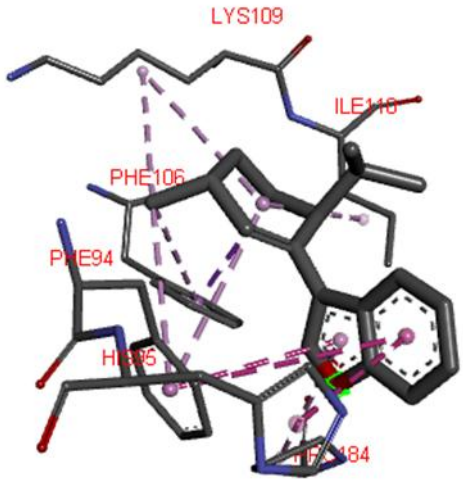
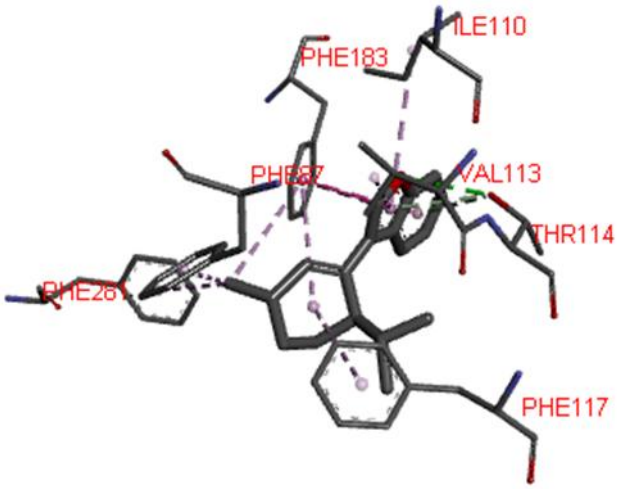
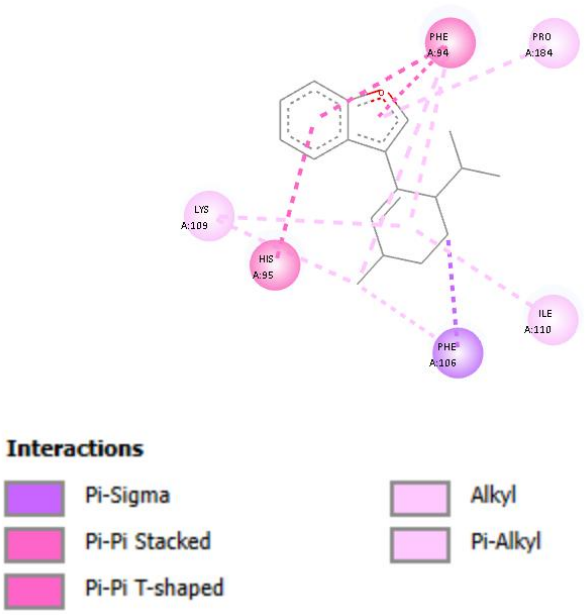
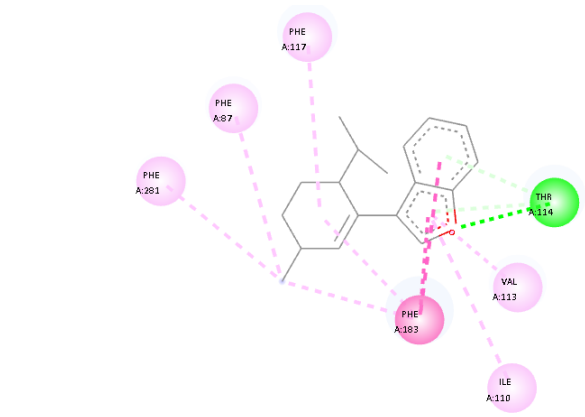
6b (II)	ent-6b (II)
	
	
Binding energy: -8.5	**Binding energy: -8.3**

6c (l)	ent-6c (l)
	
	
Binding energy: -7.6	**Binding energy: -7.7**

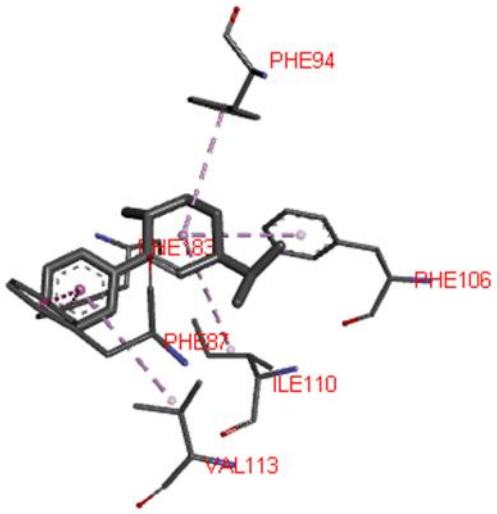
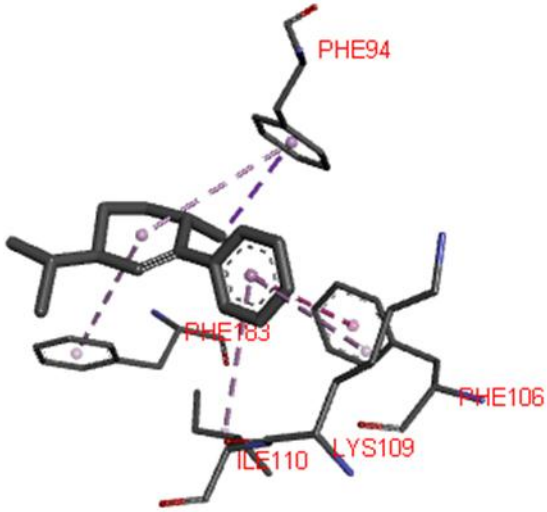
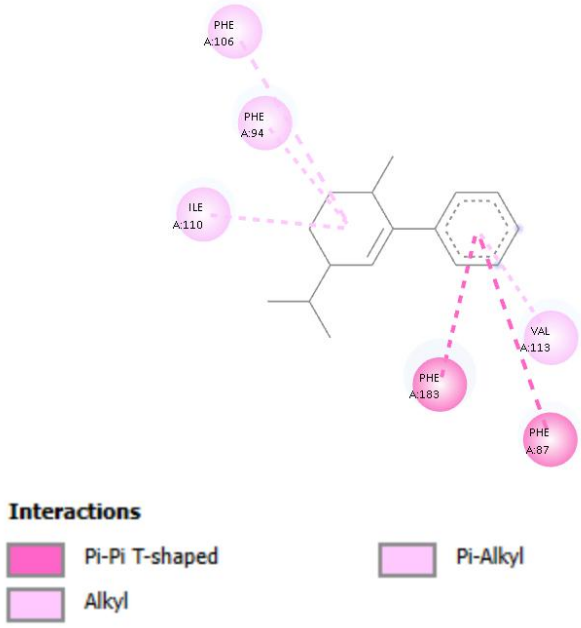
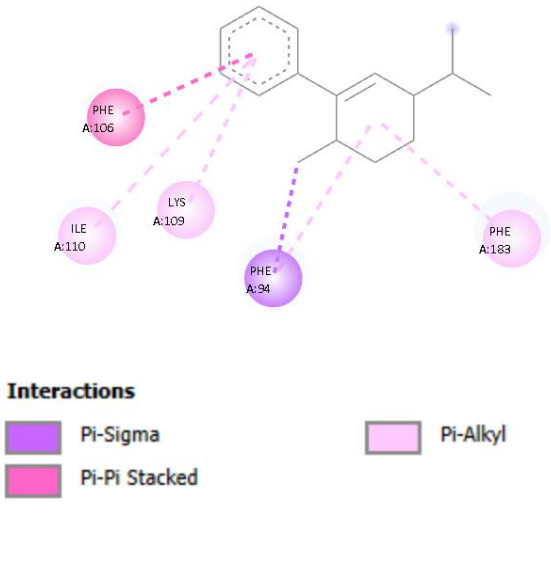
6d (l)	ent-6d (l)
	
Binding energy: -9.0	**Binding energy: -8.2**

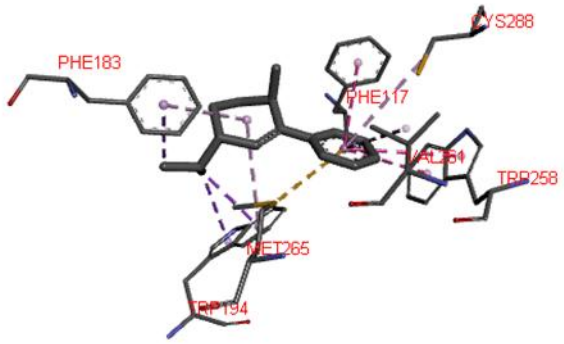
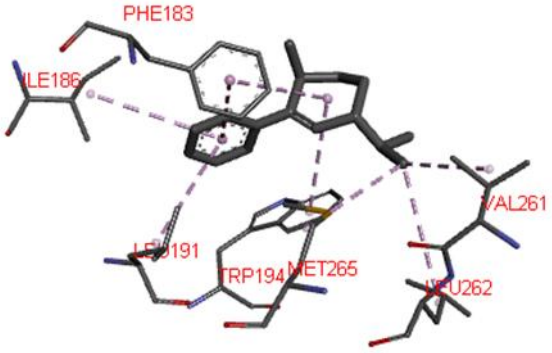
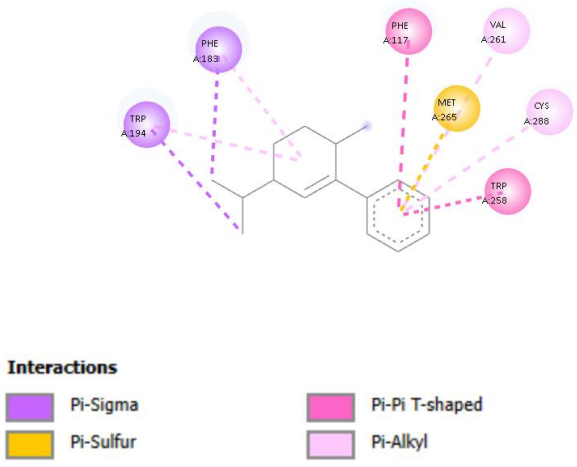
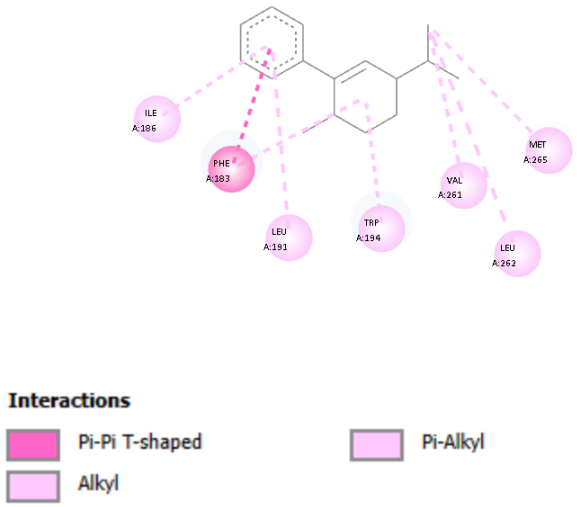
6d (II)	ent-6d (II)
	
	
Binding energy: -9.2	**Binding energy: -8.0**

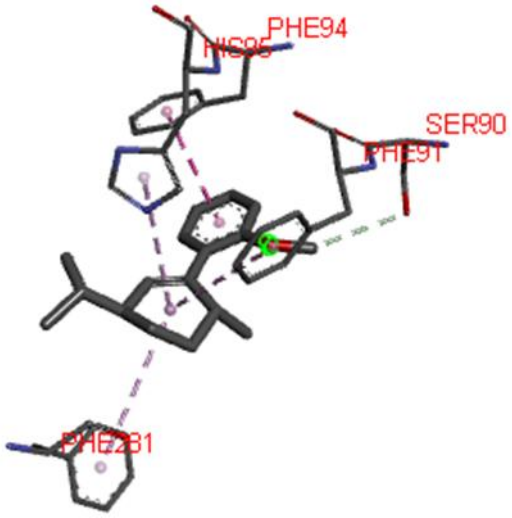
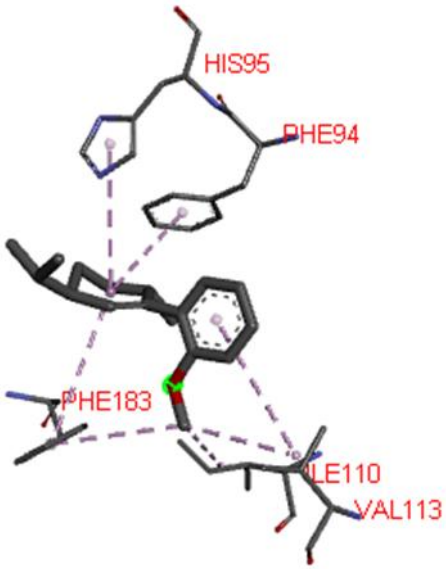
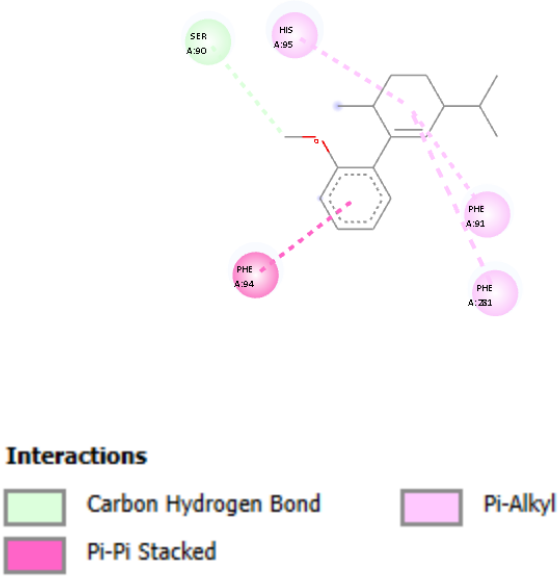
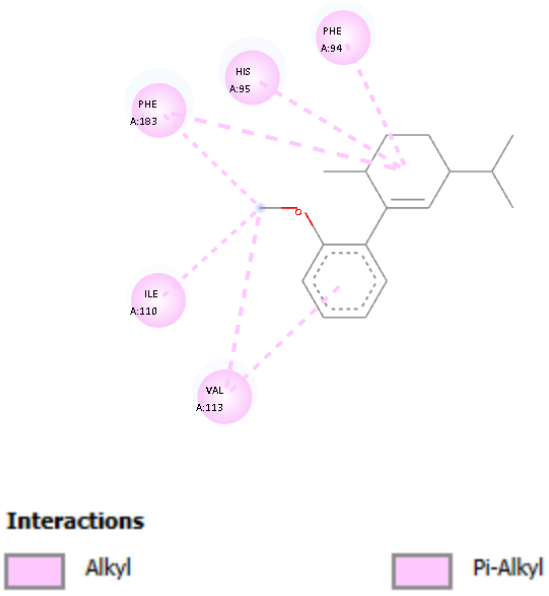
6e (II)	ent-6e (II)
	
	
Binding energy: -10.7	**Binding energy: -9.8**

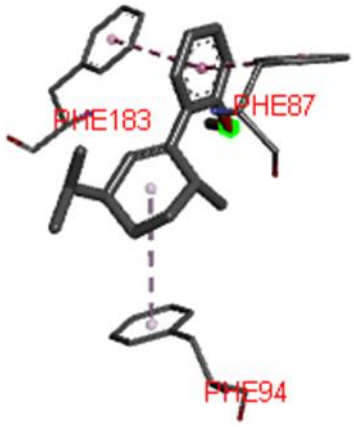
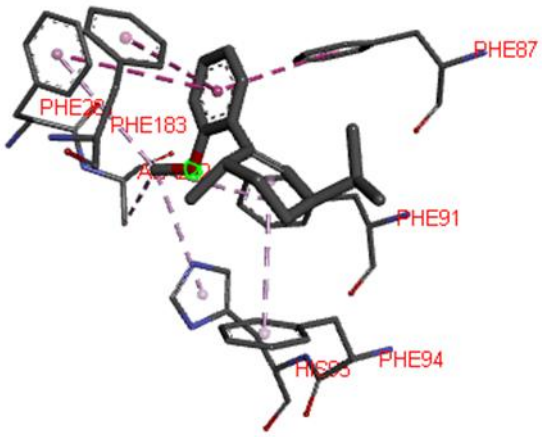
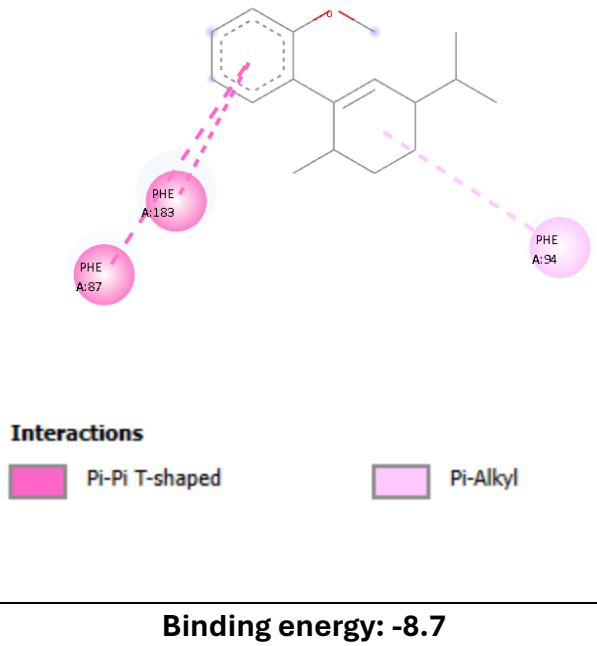
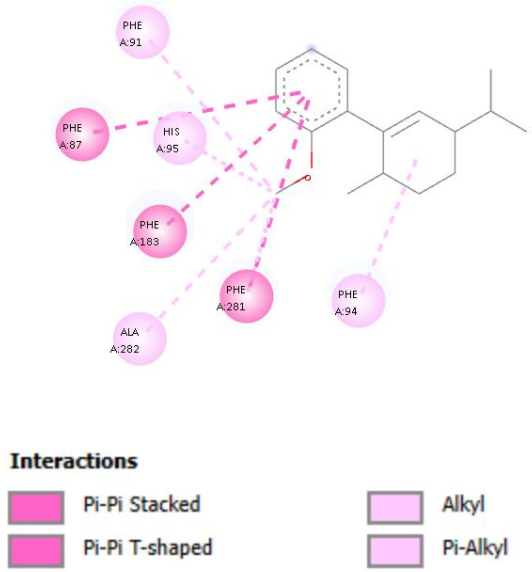
6f (II)	ent-6f (II)
	
	
Binding energy: -10.2	**Binding energy: -9.5**

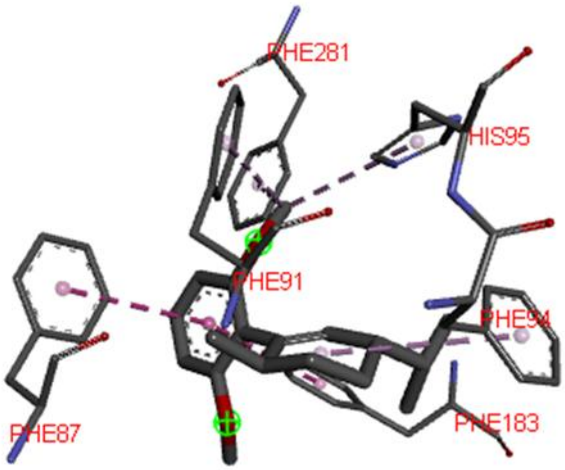
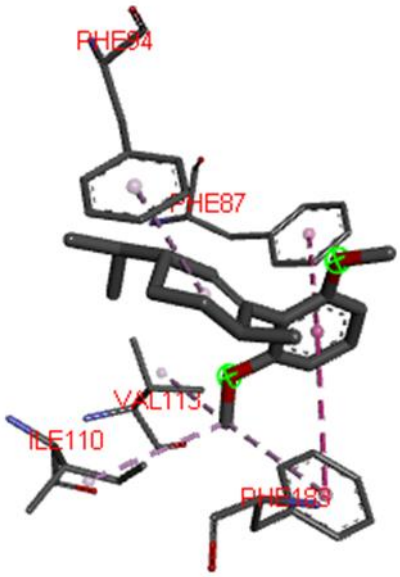
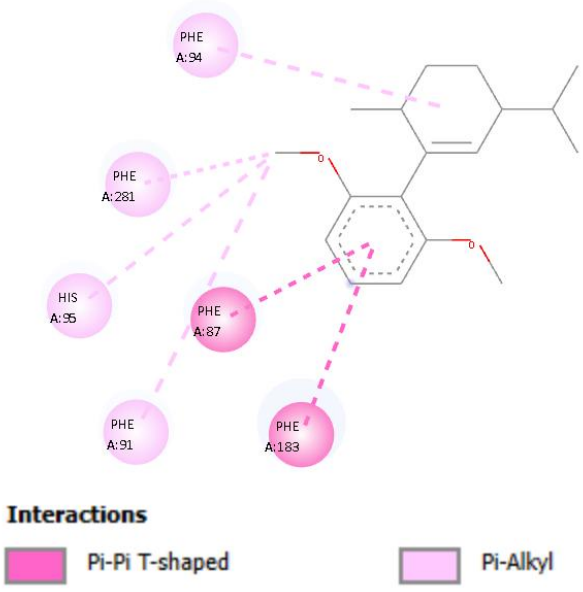
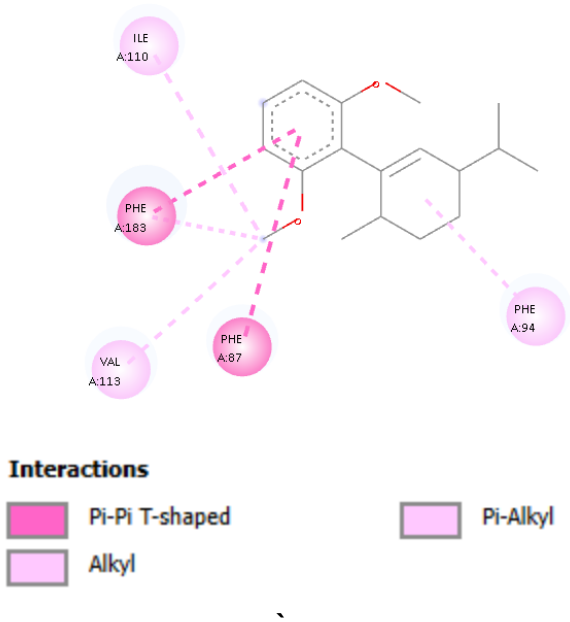
• *Synthesized Ligands of Series **7**/ent-**7** with CB2 Receptor*

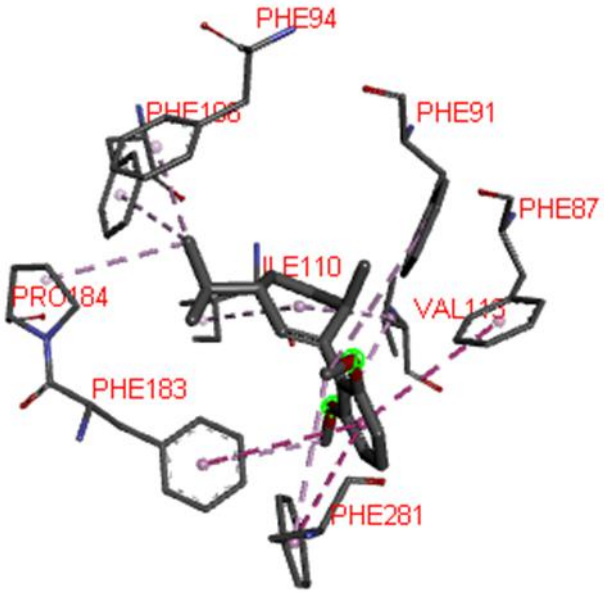
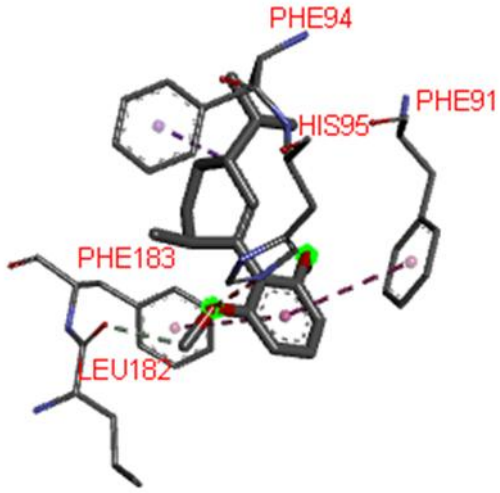
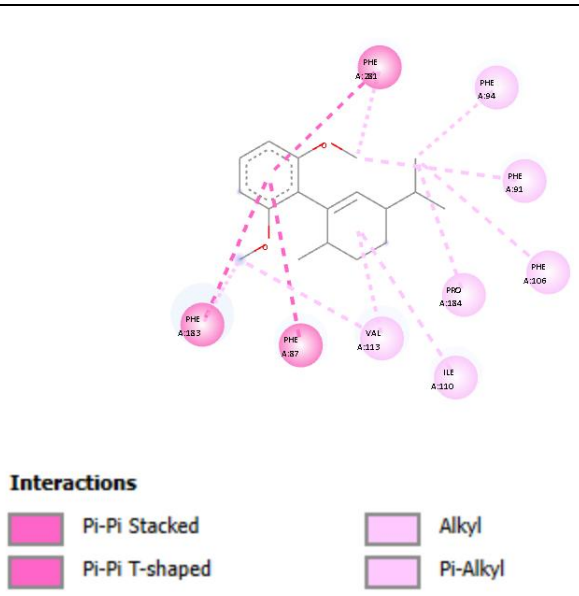
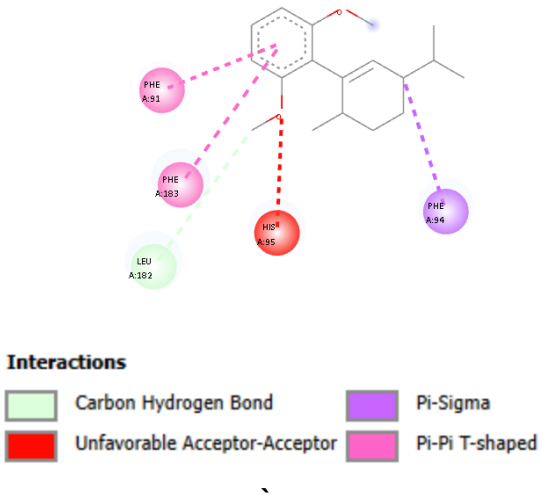
7a (I)	**ent-7a (I)**
	
	
Binding energy: -9.5	**Binding energy: -8.9**

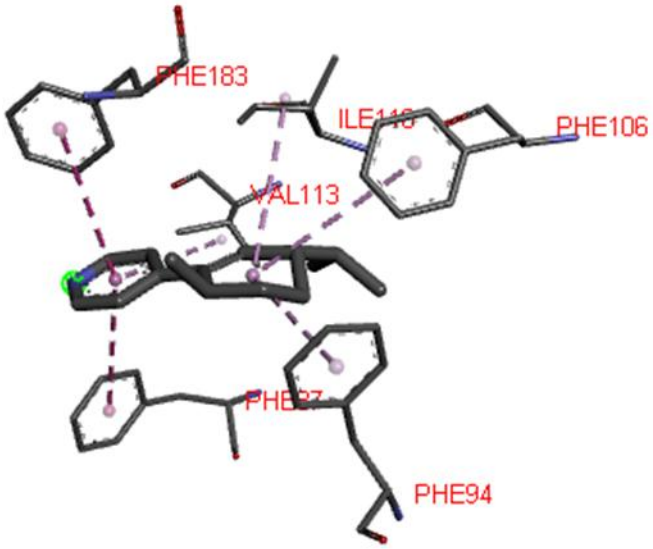
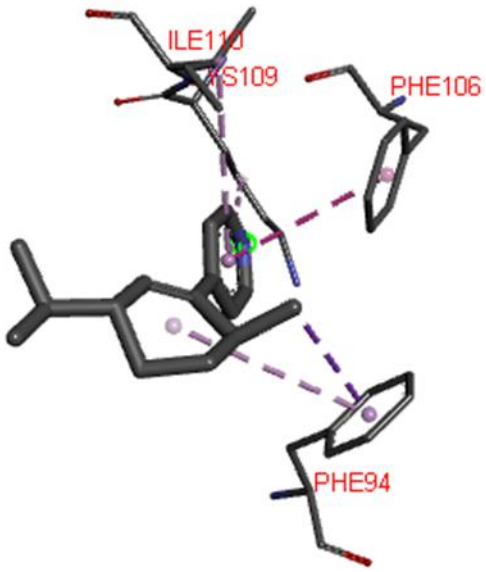
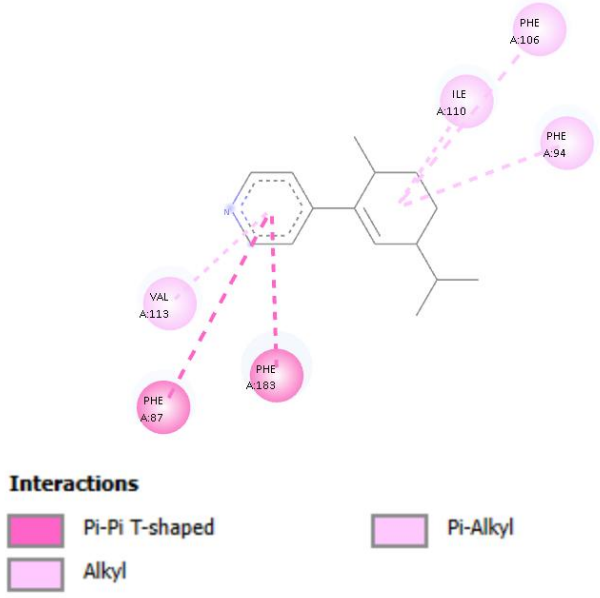
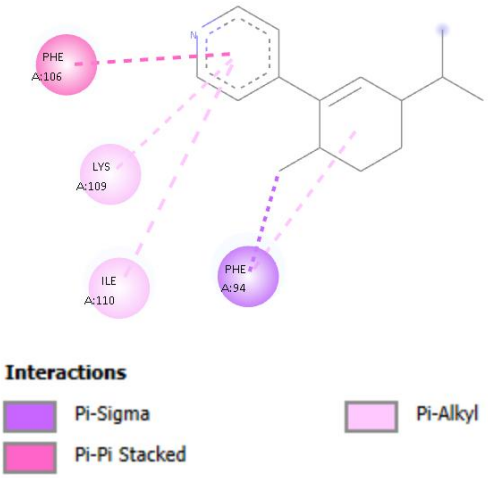
7a (II)	ent-7a (II)
	
	
Binding energy: -9.2	**Binding energy: -9.2**

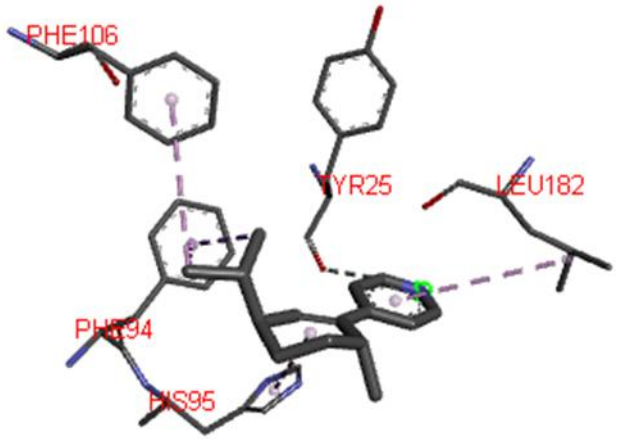
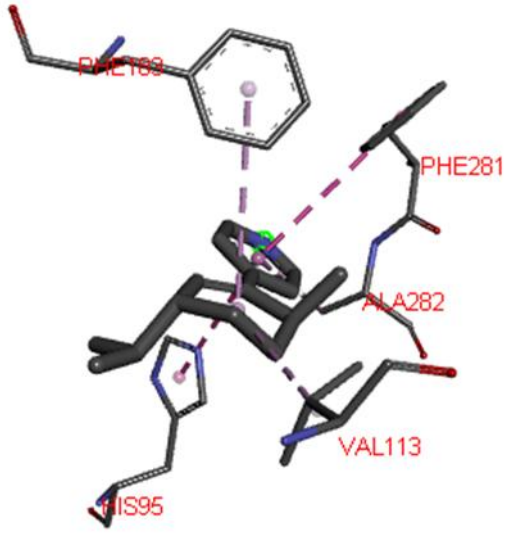
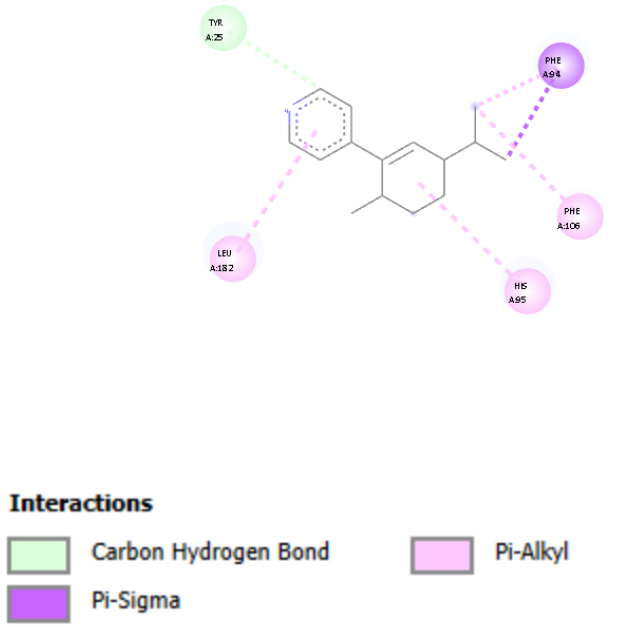
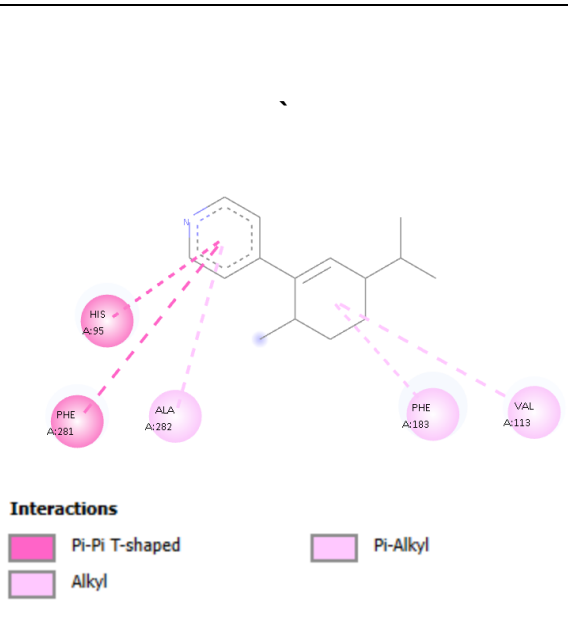
7b (l)	ent-7b (l)
	
	
Binding energy: -9.4	**Binding energy: -8.2**

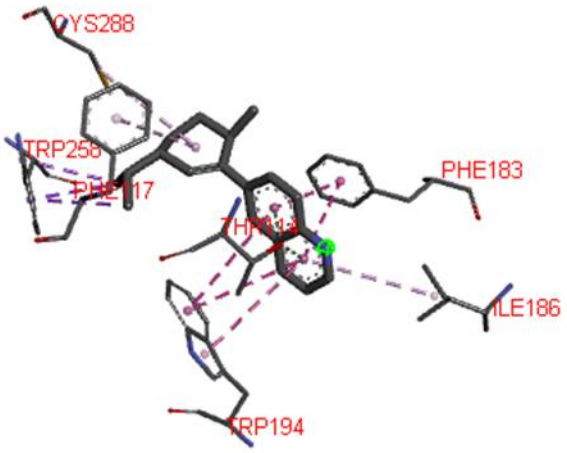
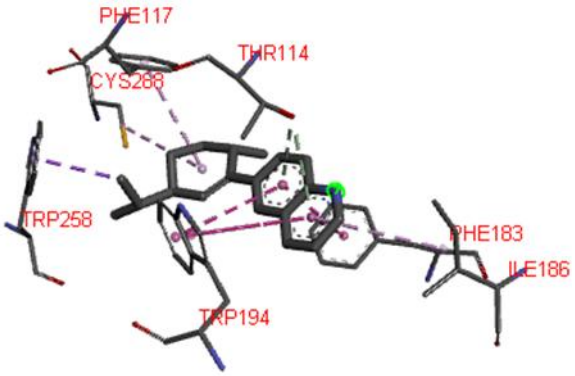
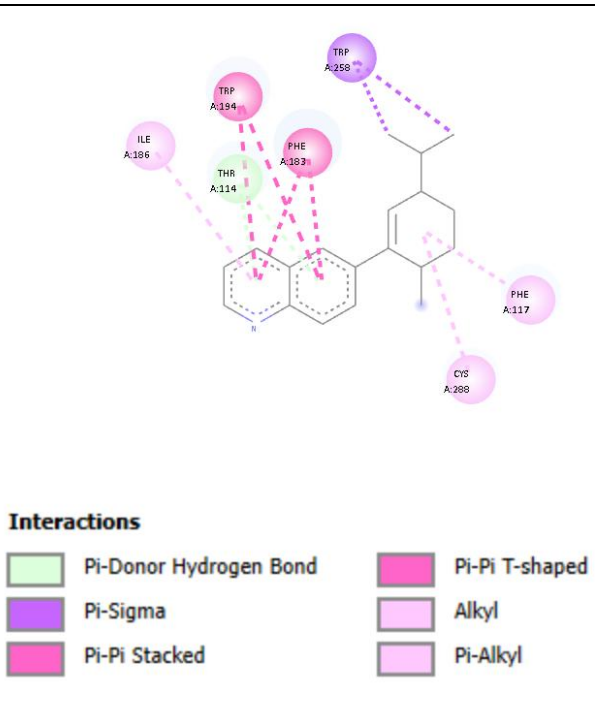
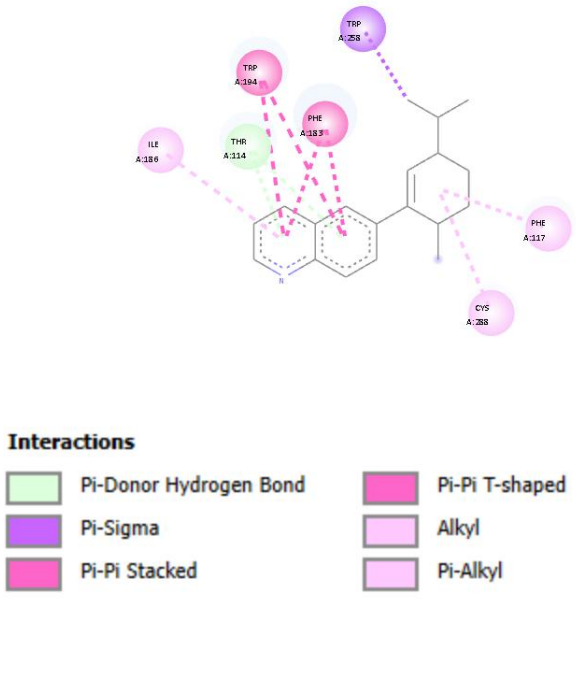
7b (II)	ent-7b (II)
	
	
Binding energy: -8.7	**Binding energy: -8.7**

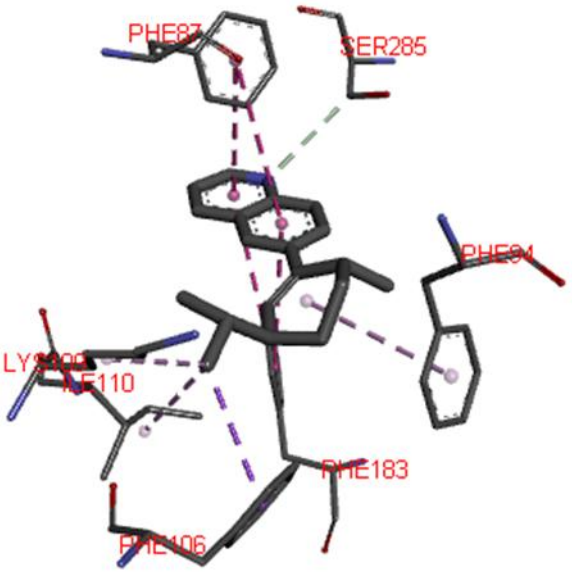
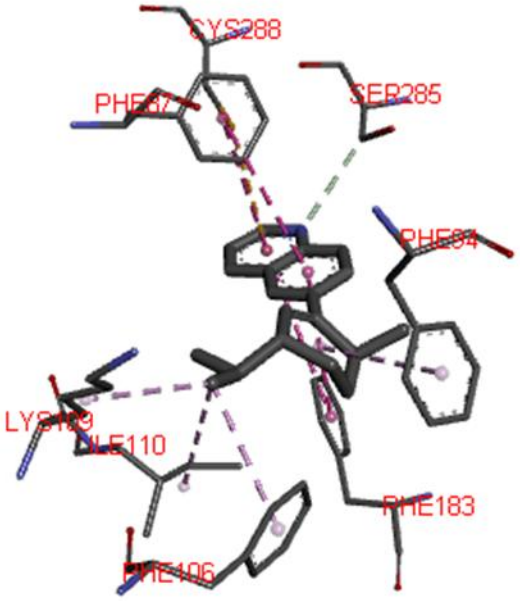
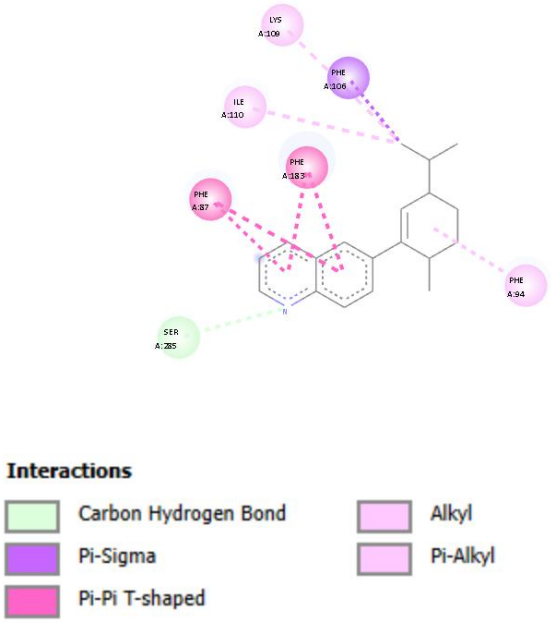
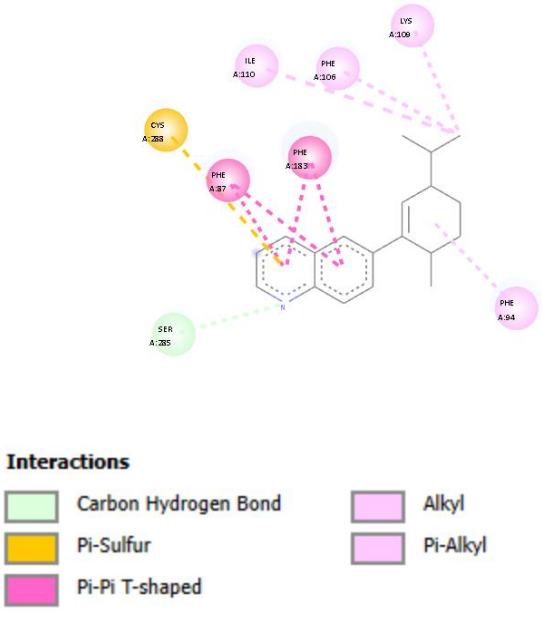
7c (I)	ent-7c (I)
	
	
Binding energy: -7.8	**Binding energy: -8.2**

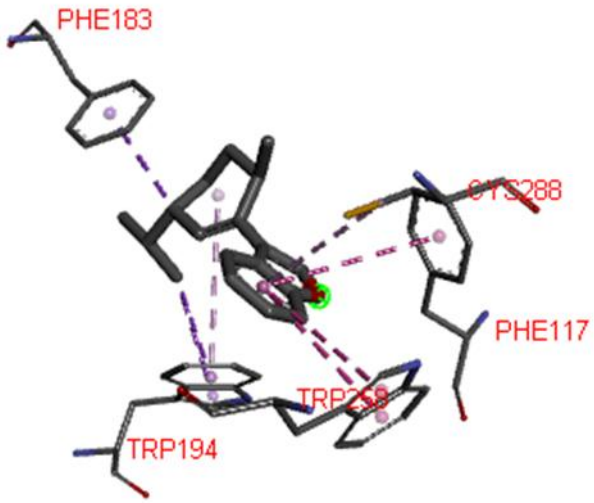
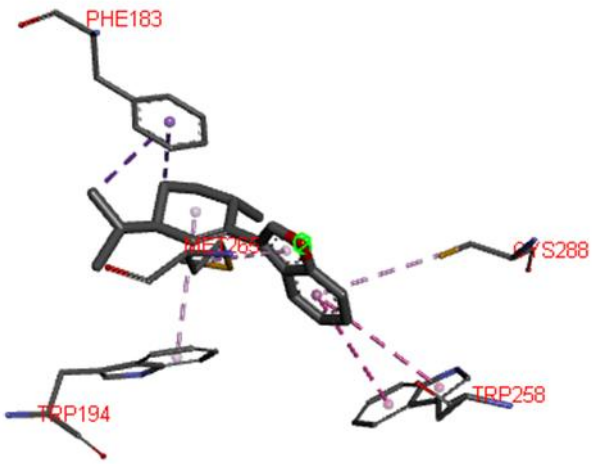
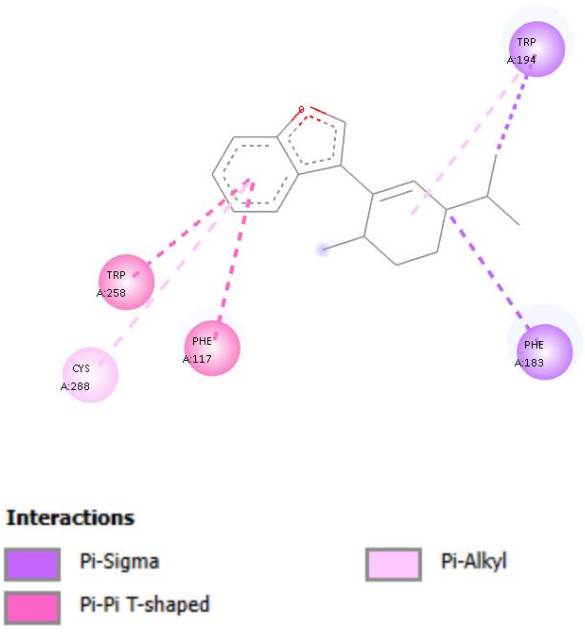
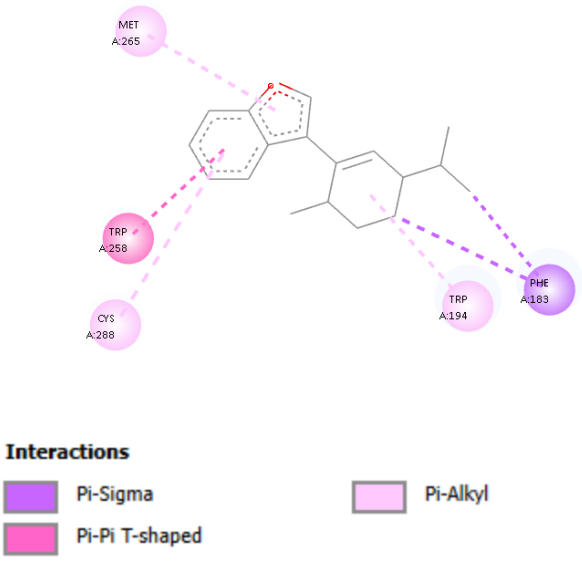
7c (II)	ent-7c (II)
	
	
Binding energy: -8.0	**Binding energy: -8.3**

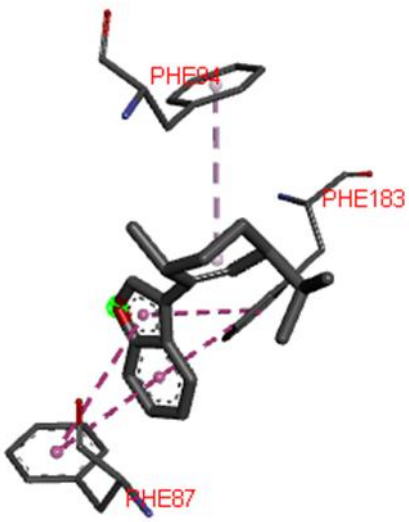
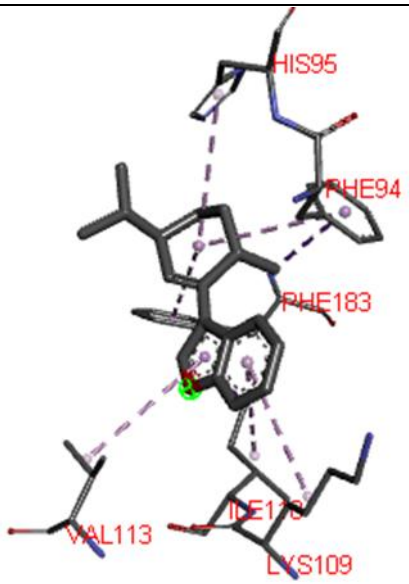
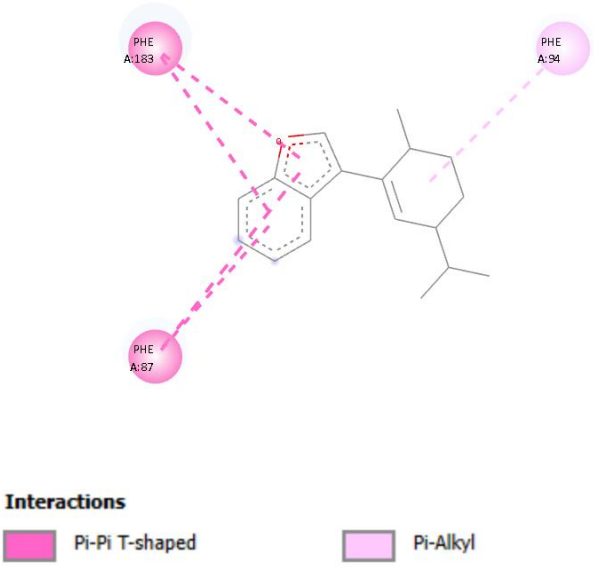
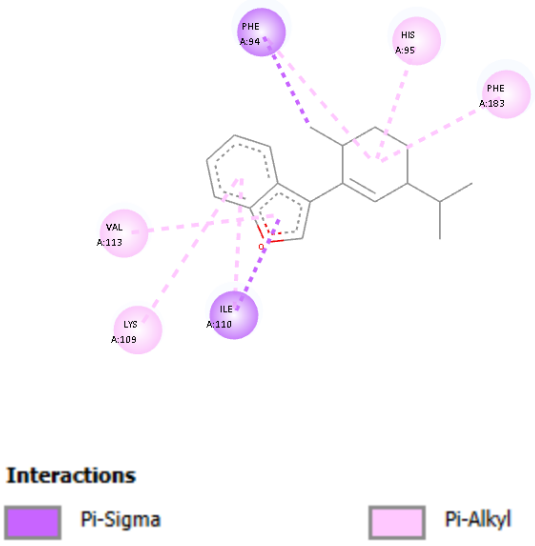
7d (I)	ent-7d (I)
	
	
Binding energy: -8.9	**Binding energy: -8.3**

7d (II)	ent-7d (II)
	
	
Binding energy: -8.2	**Binding energy: -8.3**

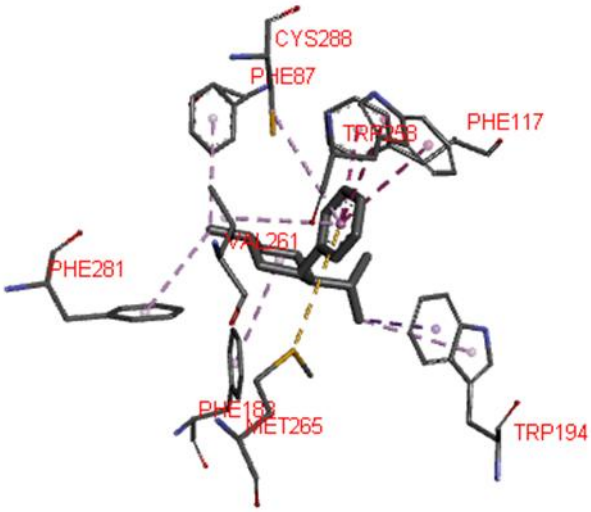
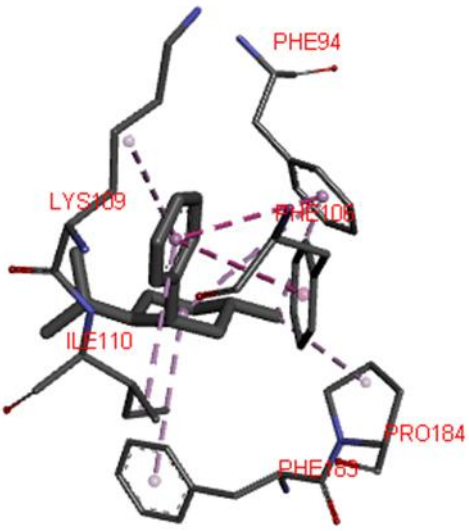
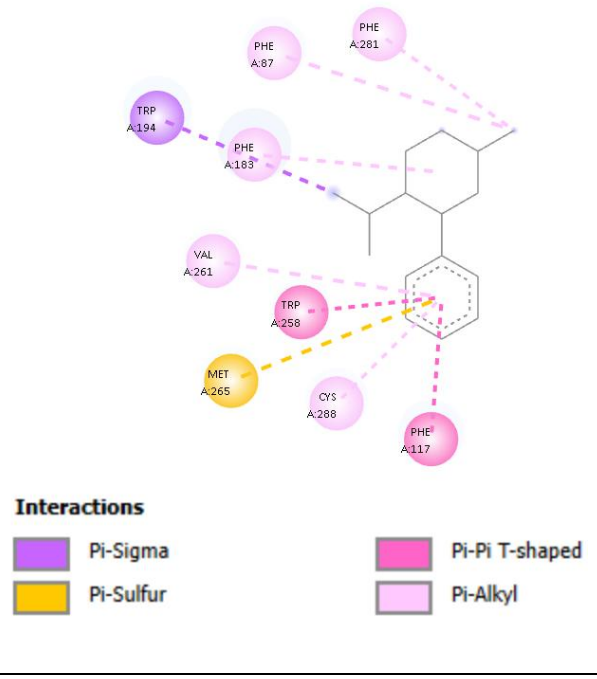
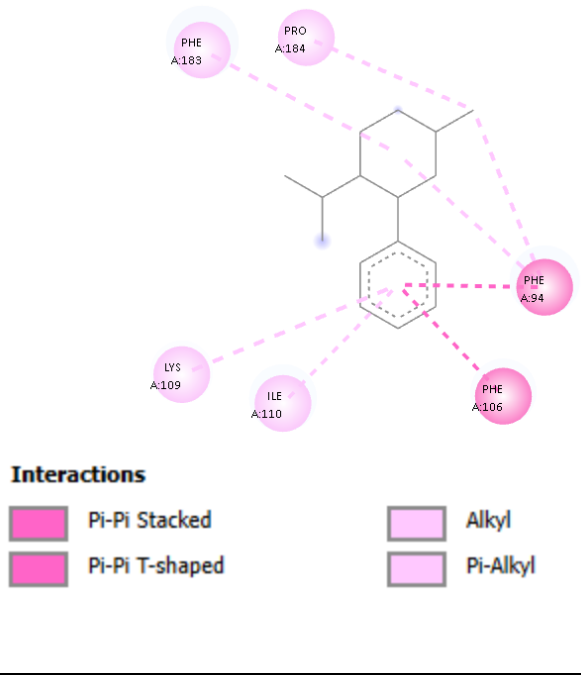
7e (I)	ent-7e (I)
	
	
Binding energy: -10.6	**Binding energy: -10.4**

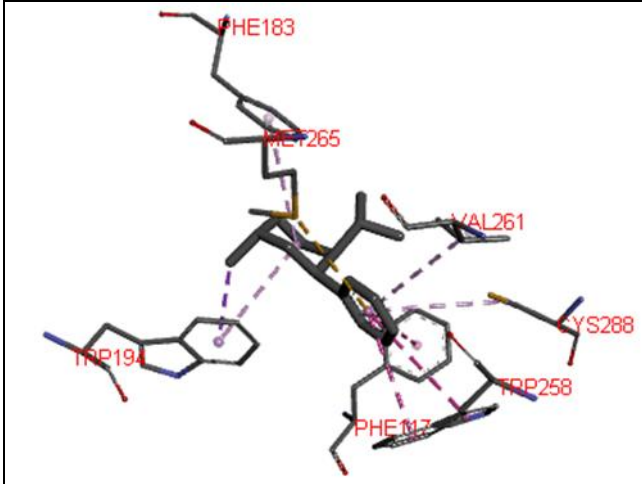
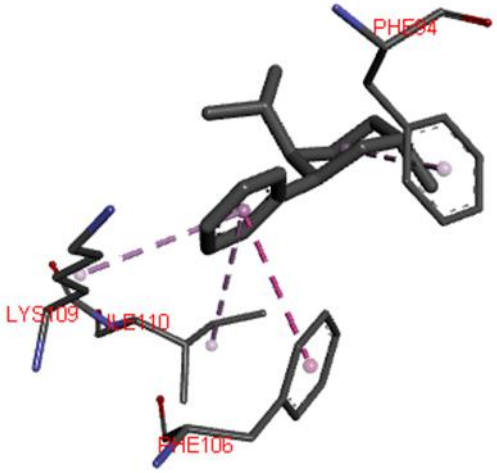
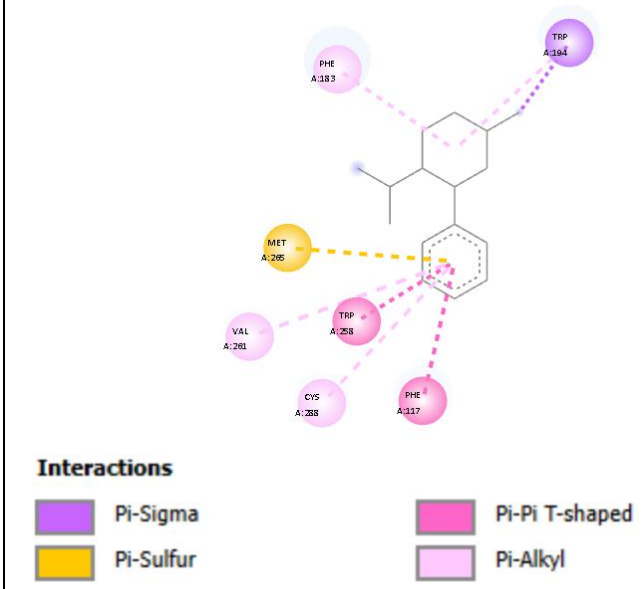
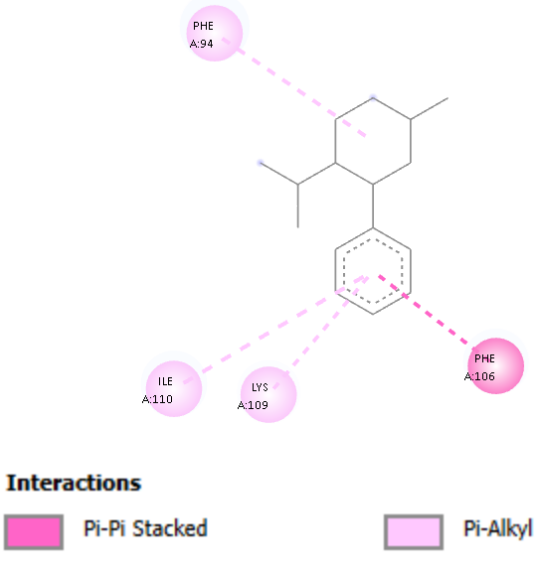
7e (II)	ent-7e (II)
	
	
Binding energy: -10.2	**Binding energy: -10.1**

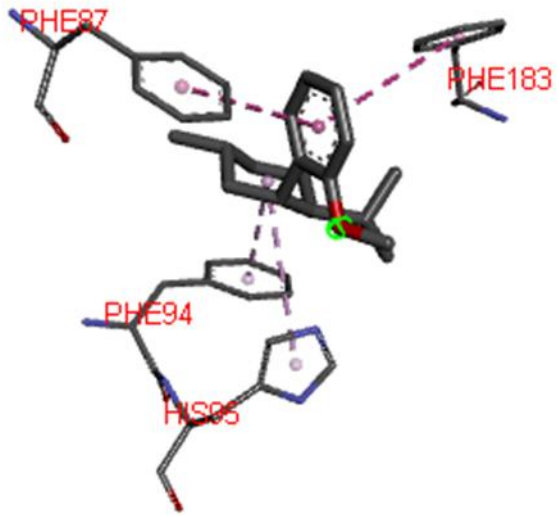
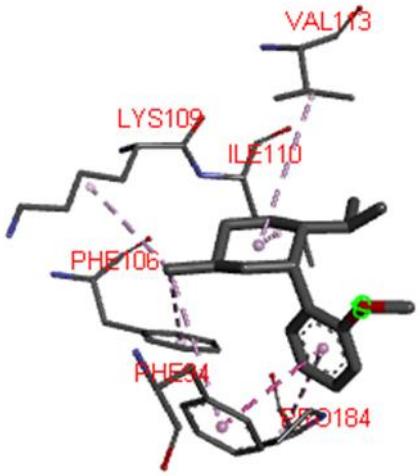
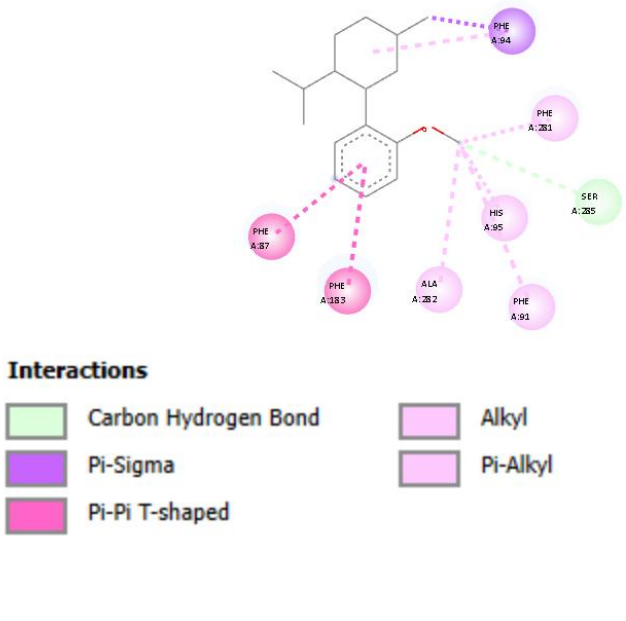
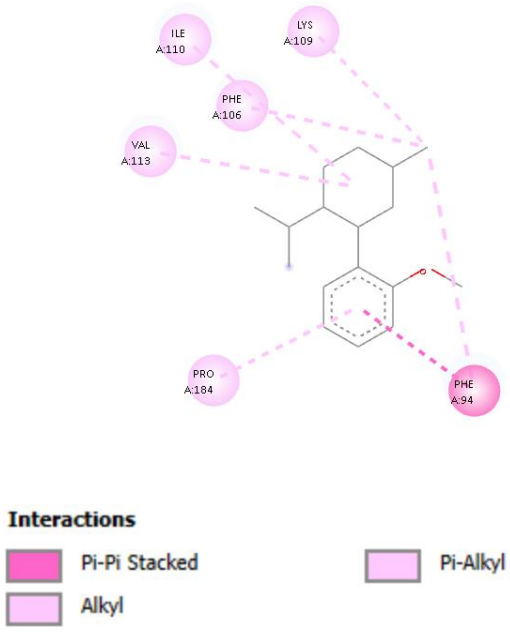
7f (l)	ent-7f (l)
	
	
Binding energy: -9.5	**Binding energy: -9.7**

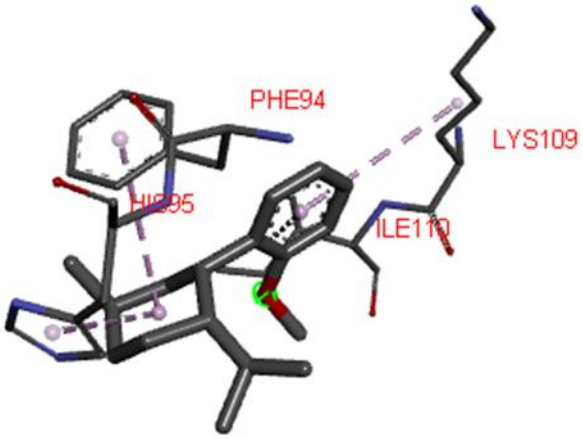
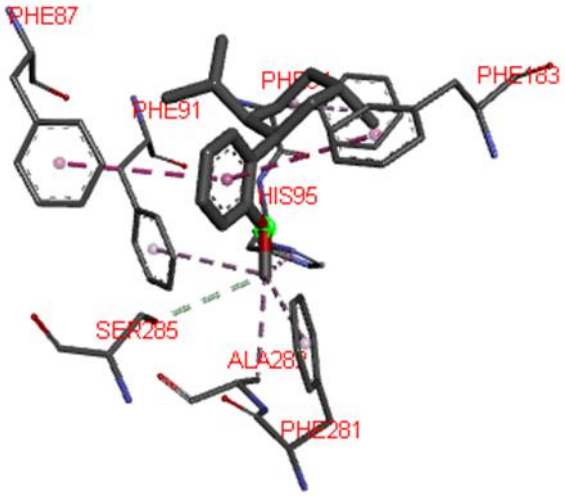
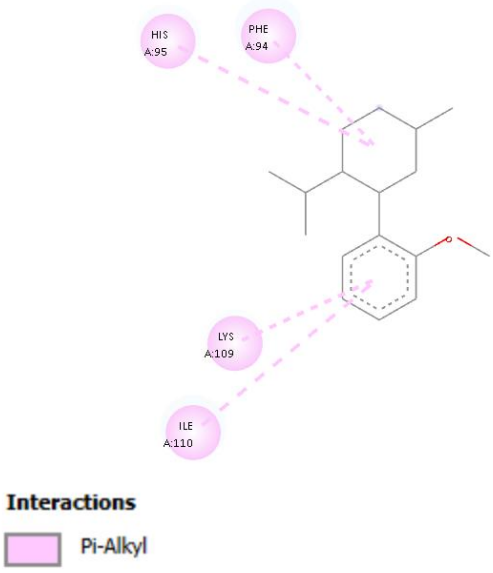
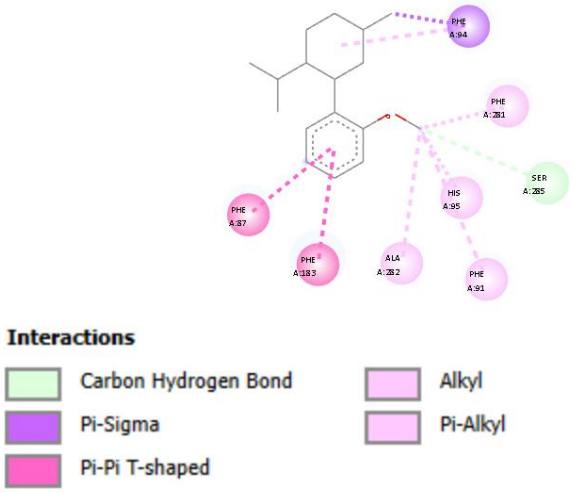
7f (II)	ent-7f (II)
	
	
Binding energy: -9.8	**Binding energy: -9.8**

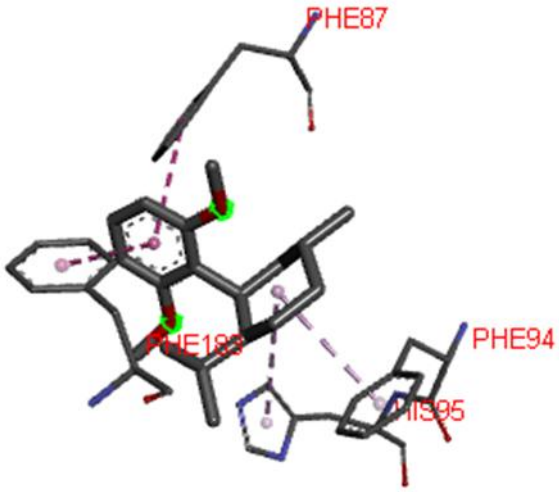
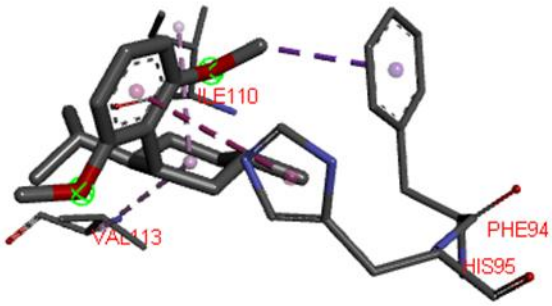
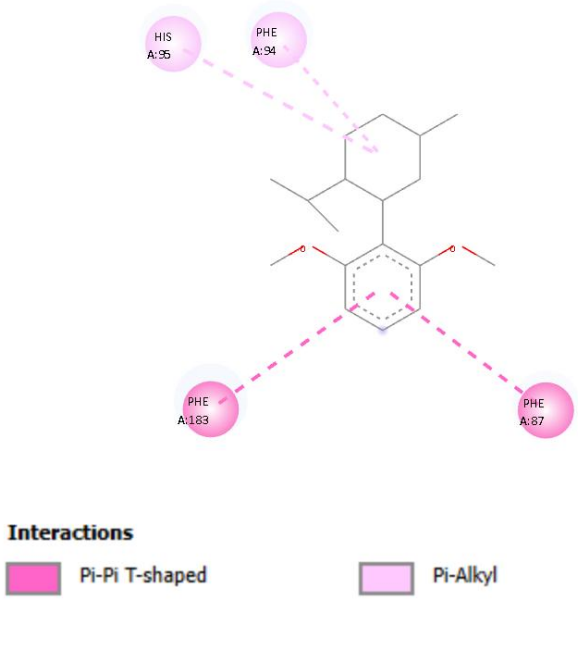
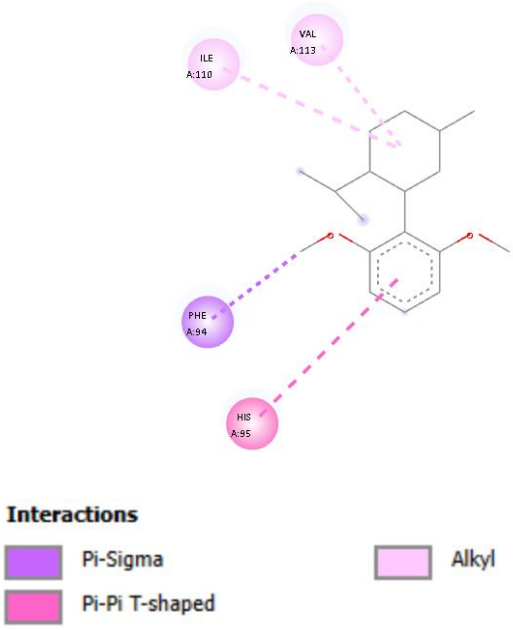
• *Synthesized Ligands of Series **8**/ent-**8** with CB2 Receptor*

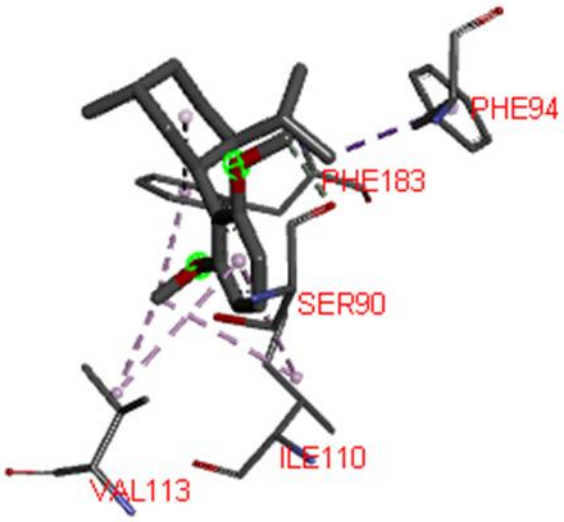
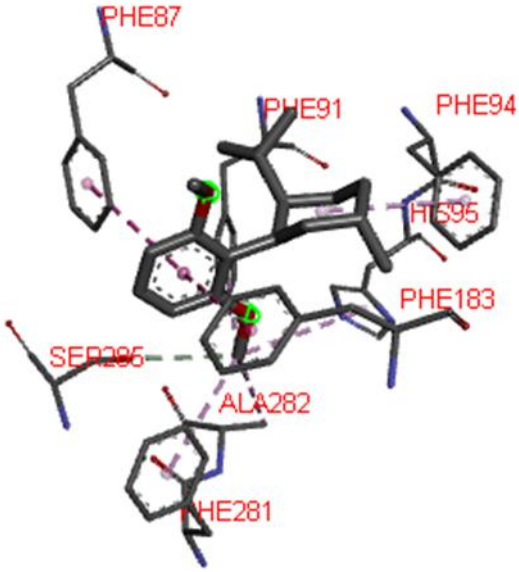
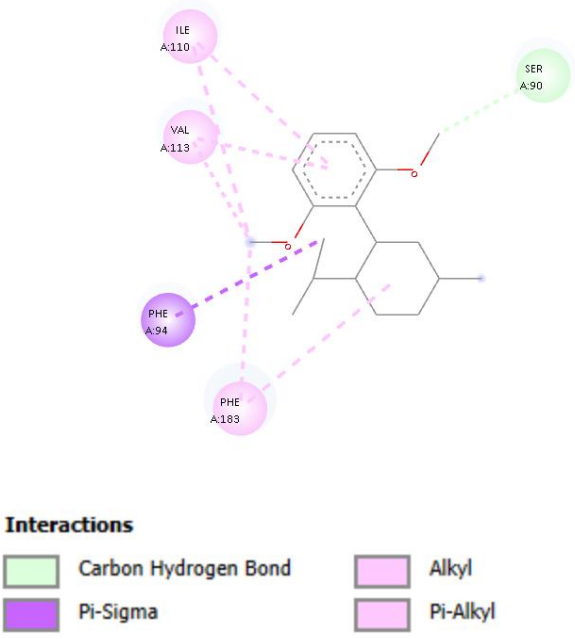
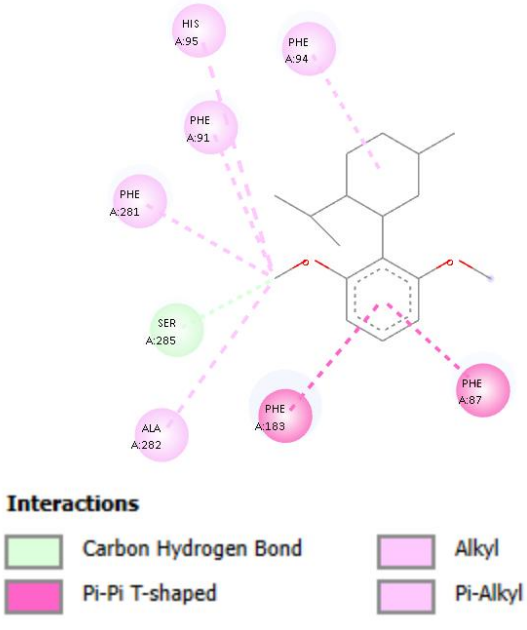
8a (I)	**ent-8a (I)**
	
	
Binding energy: -8.8	**Binding energy: -8.7**

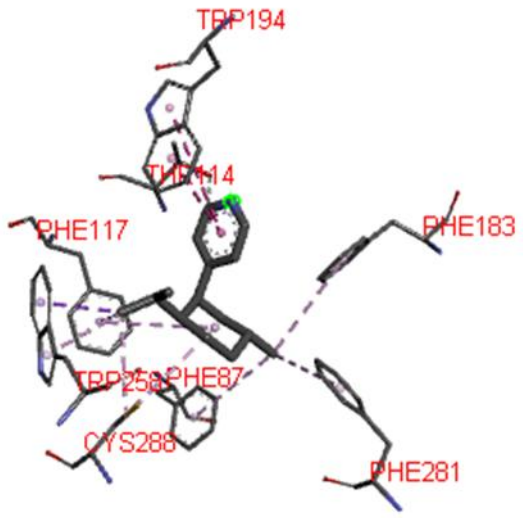
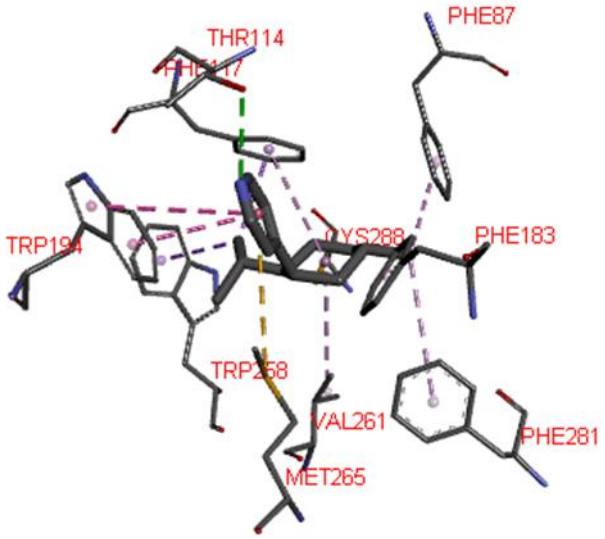
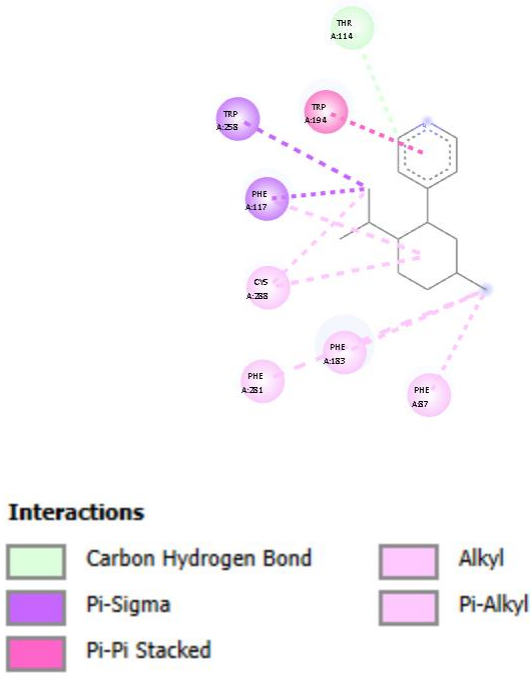
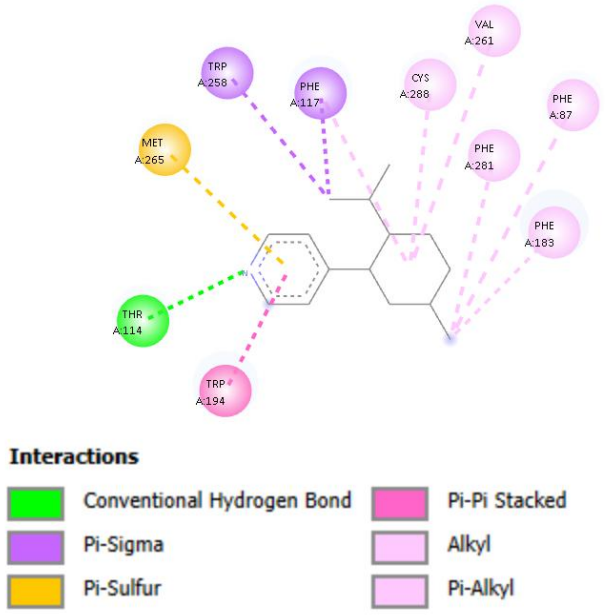
8a (II)	ent-8a (II)
	
	
Binding energy: -9.0	**Binding energy: -8.3**

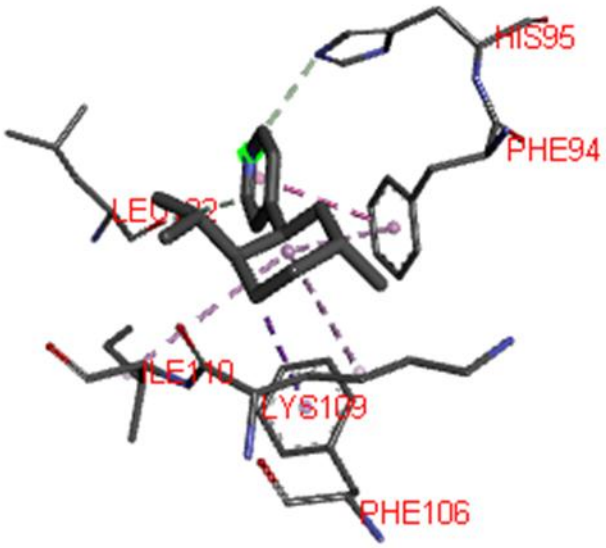
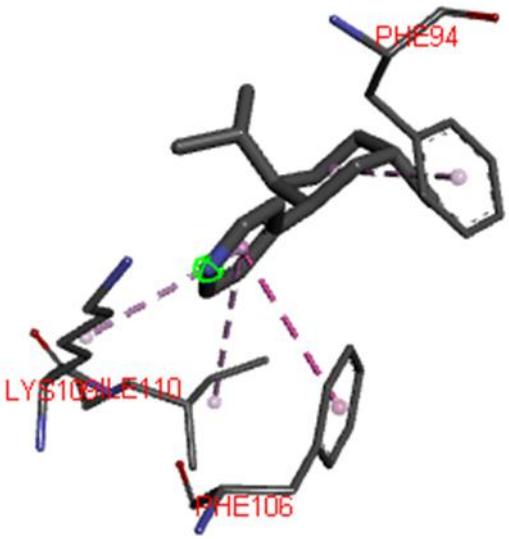
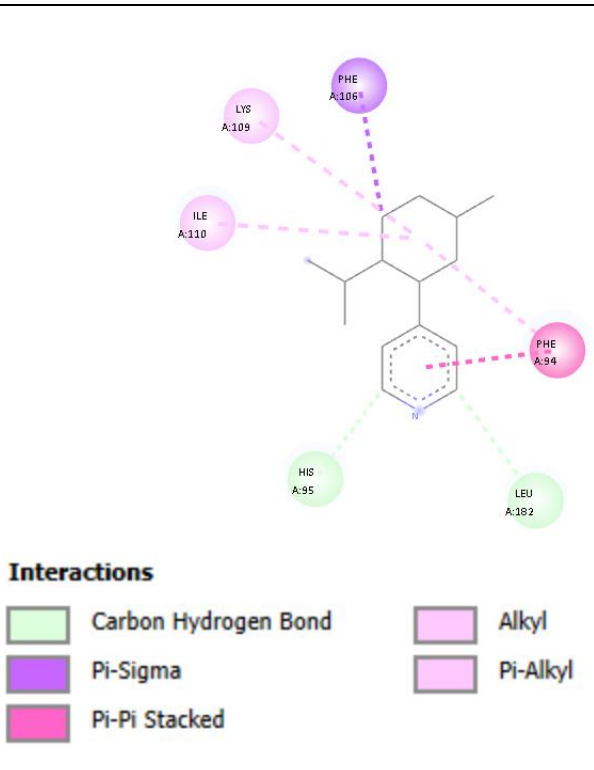
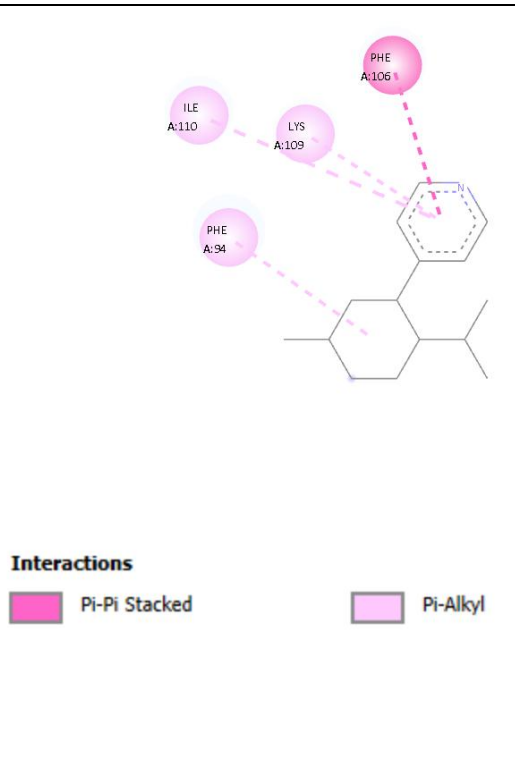
8b (l)	ent-8b (l)
	
	
Binding energy: -8.2	**Binding energy: -8.7**

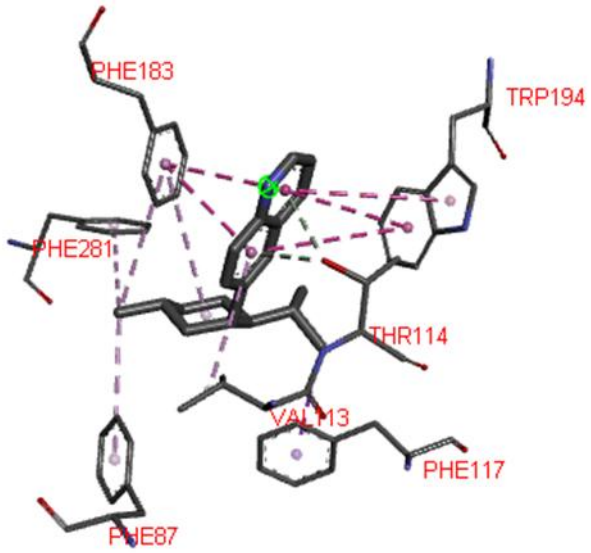
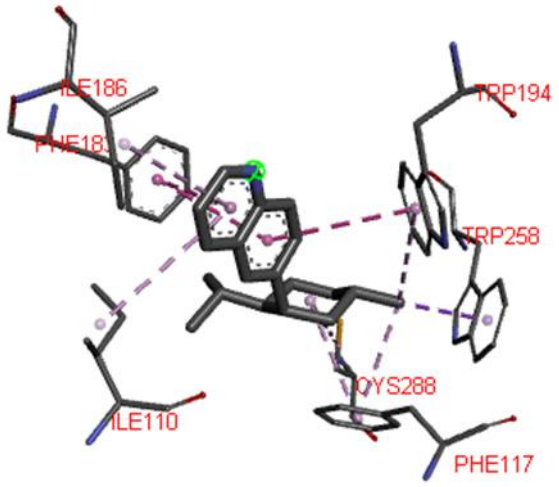
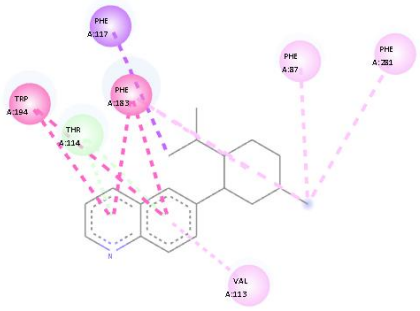
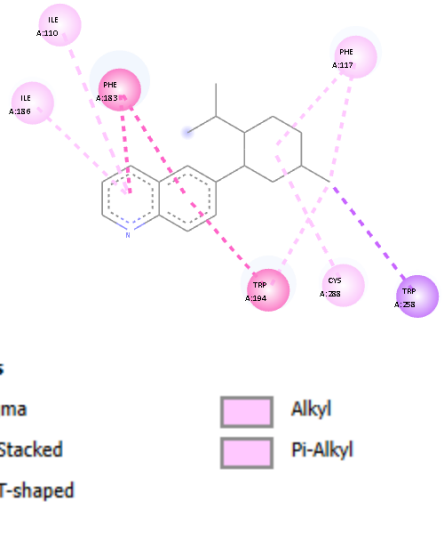
8b (II)	ent-8b (II)
	
	
Binding energy: -8.5	**Binding energy: -8.1**

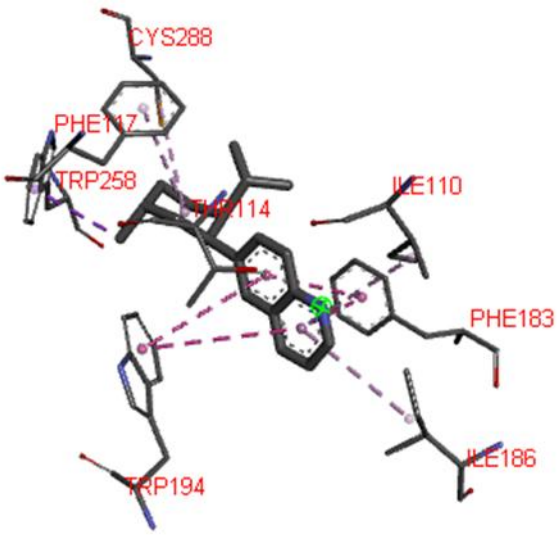
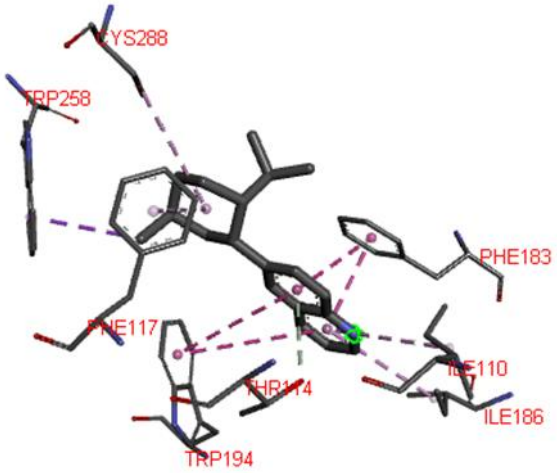
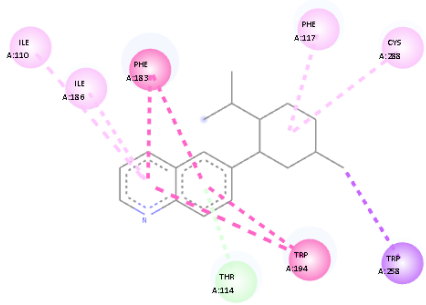
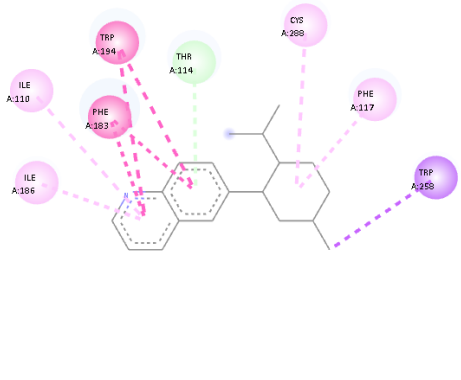
8c (l)	ent-8c (l)
	
	
Binding energy: -8.0	**Binding energy: -7.3**

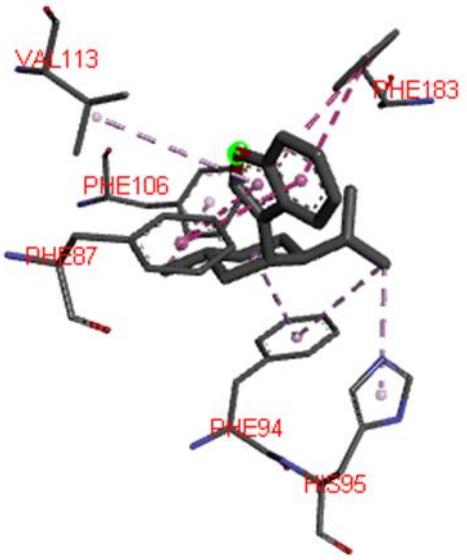
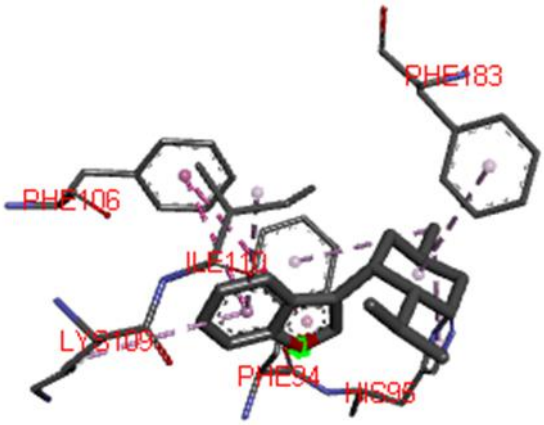
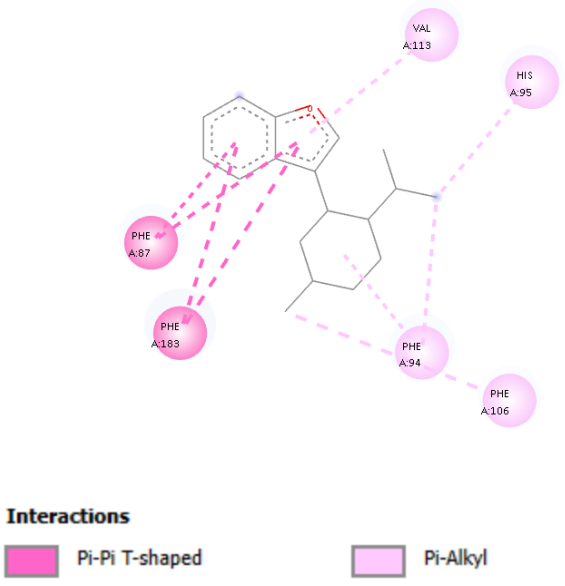
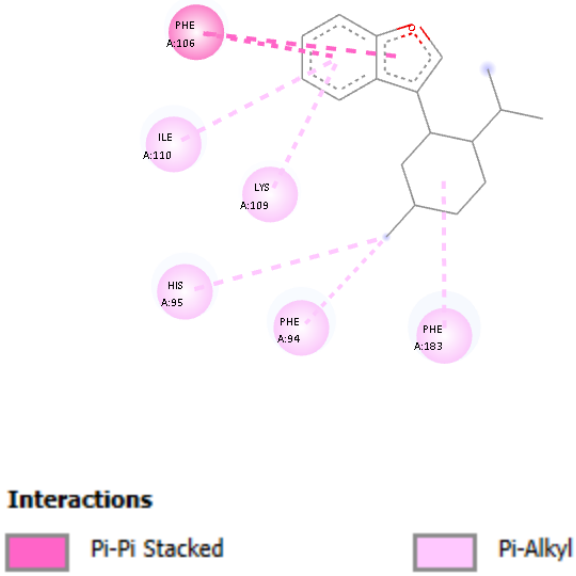
8c (II)	ent-8c (II)
	
	
Binding energy: -7.6	**Binding energy: -7.8**

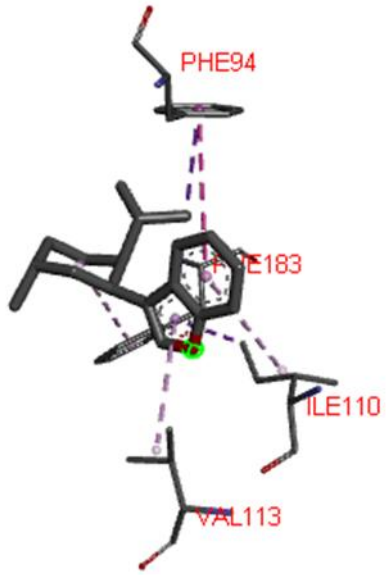
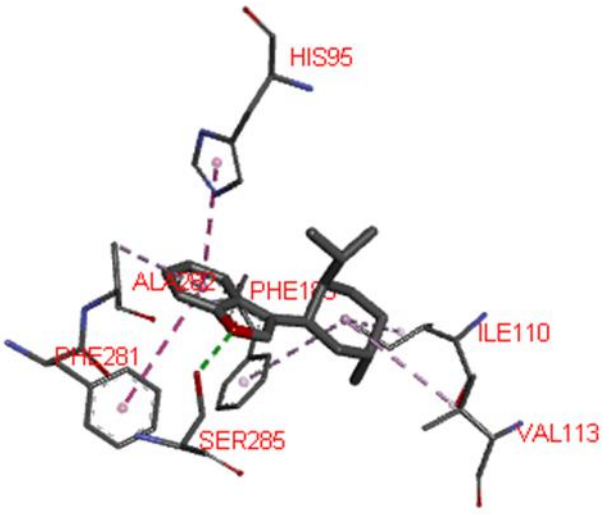
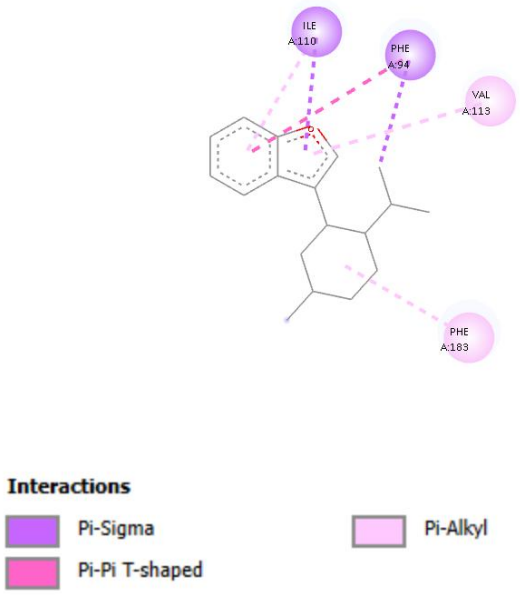
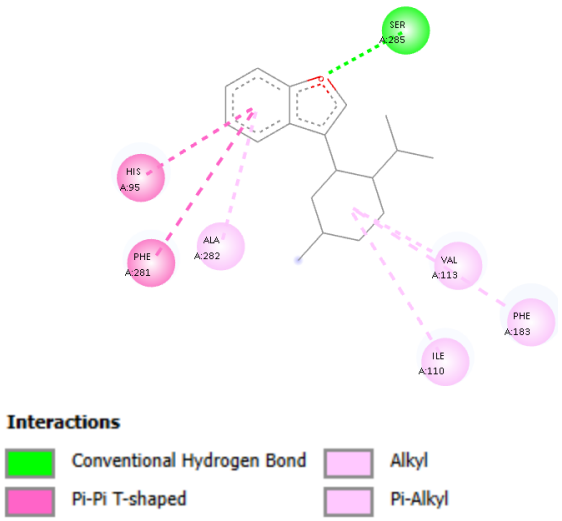
8d (I)	ent-8d (I)
	
	
Binding energy: -7.9	**Binding energy: -8.3**

8d (II)	ent-8d (II)
	
	
Binding energy: -8.3	**Binding energy: -7.6**

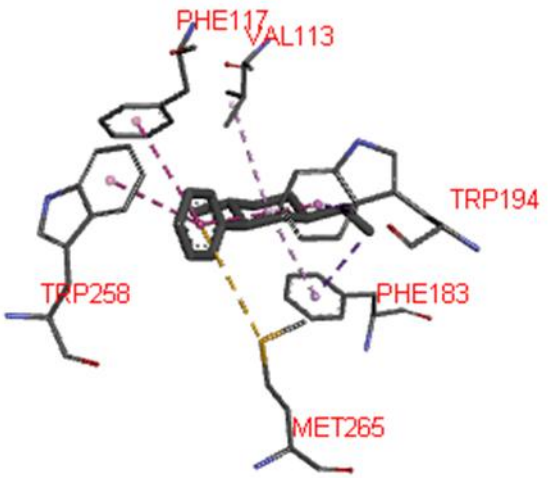
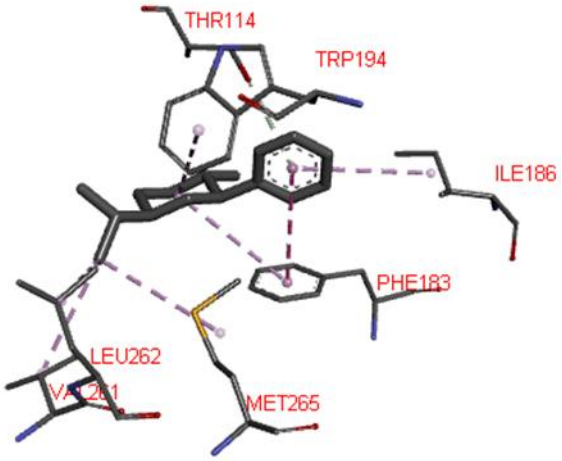
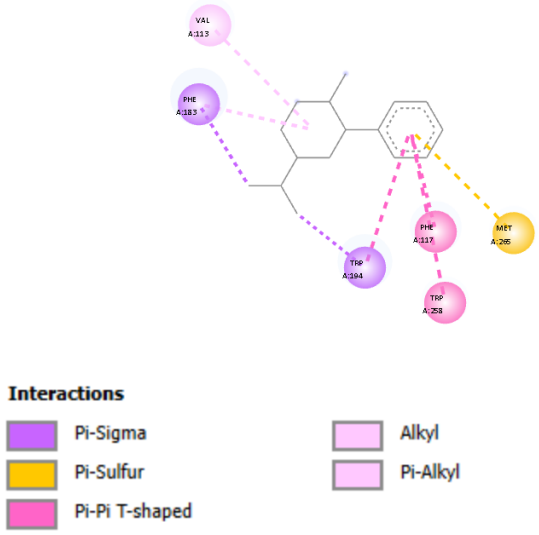
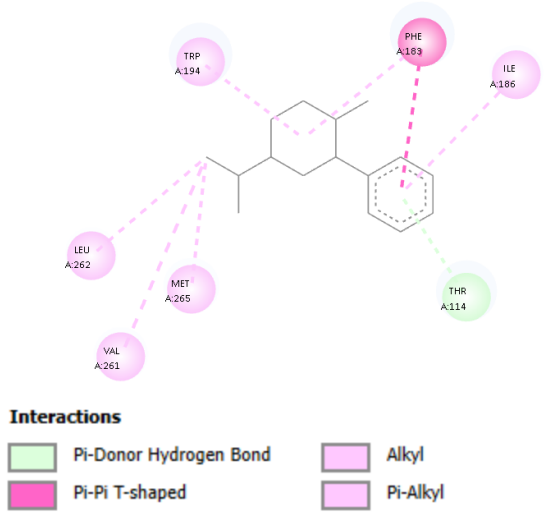
8e (l)	ent-8e (l)
	
	
Binding energy: -10.0	**Binding energy: -9.6**

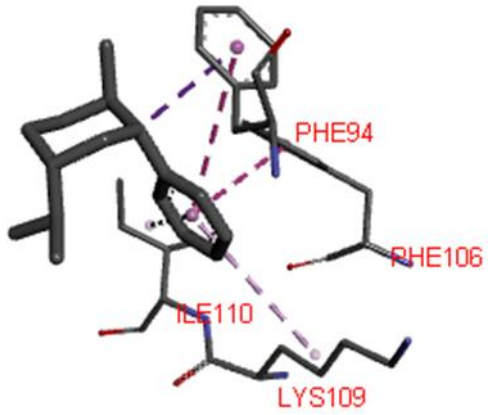
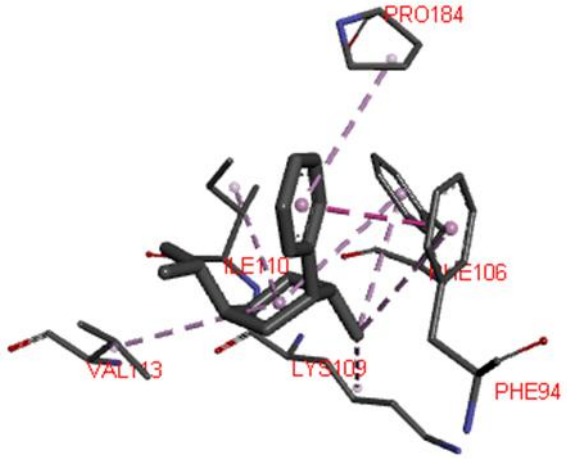
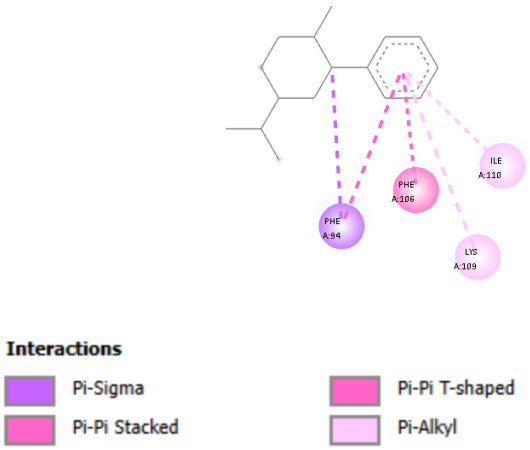
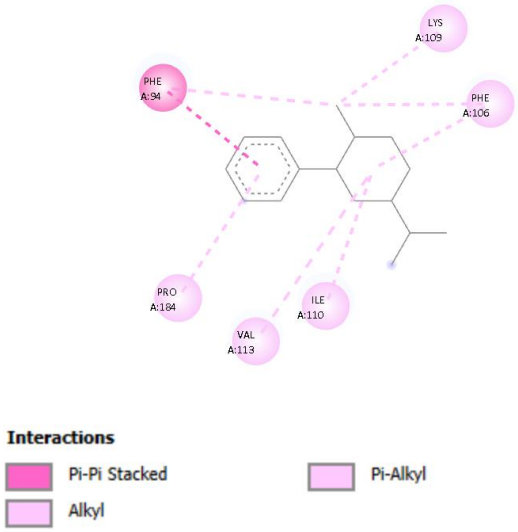
8e (II)	ent-8e (II)
	
	
Binding energy: -10.0	**Binding energy: -9.7**

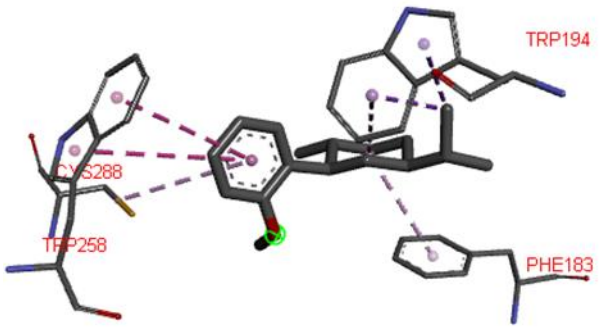
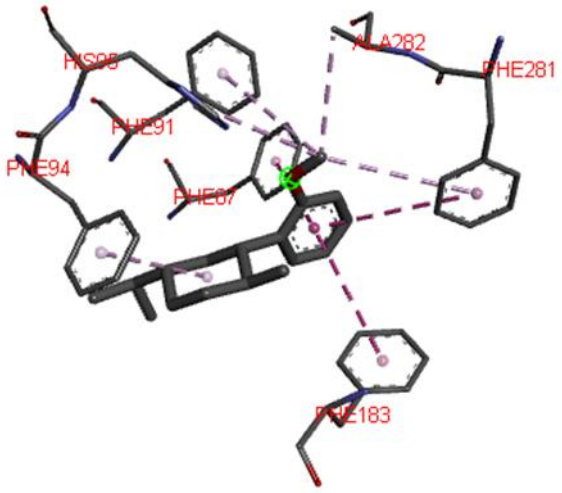
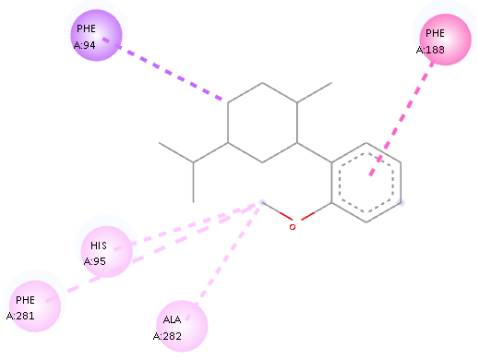
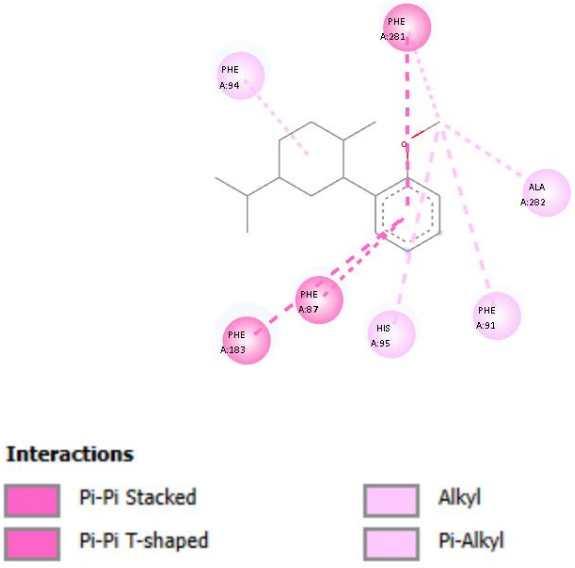
8f (l)	ent-8f (l)
	
	
Binding energy: -8.9	**Binding energy: -9.2**

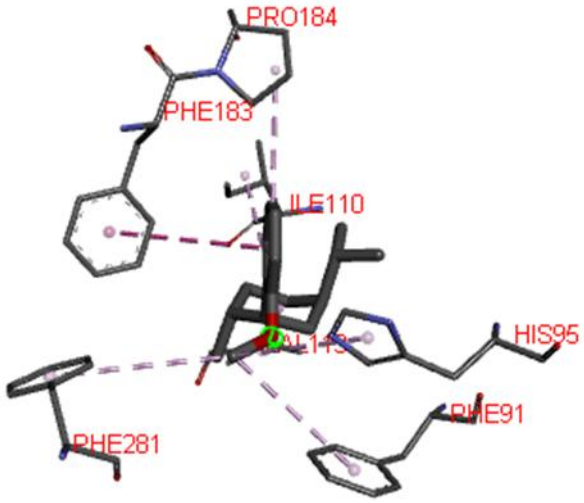
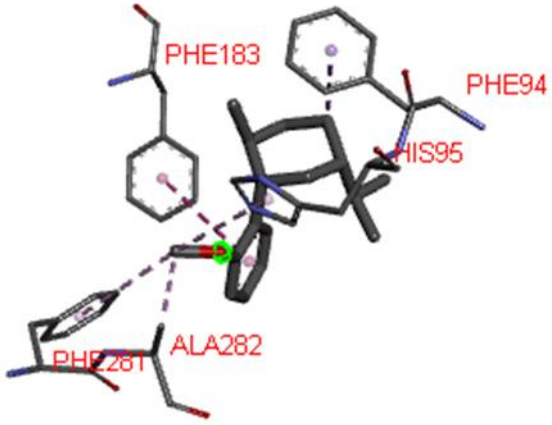
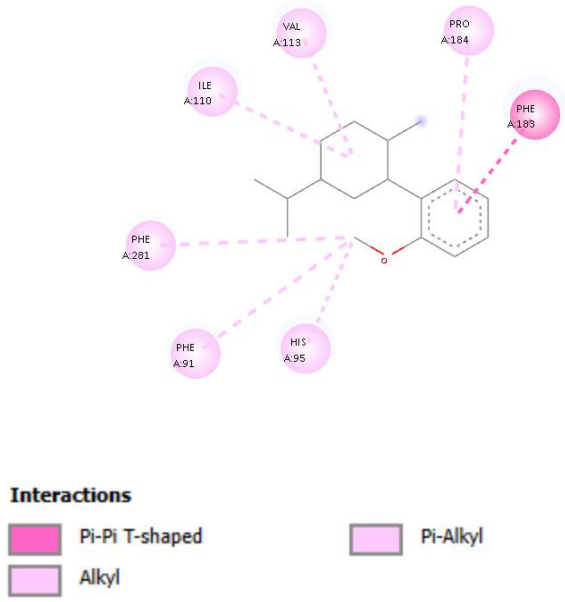
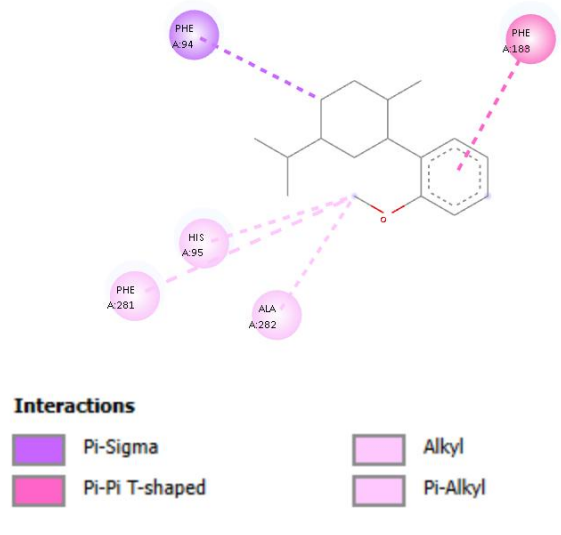
8f (II)	ent-8f (II)
	
	
Binding energy: -9.6	**Binding energy: -8.9**

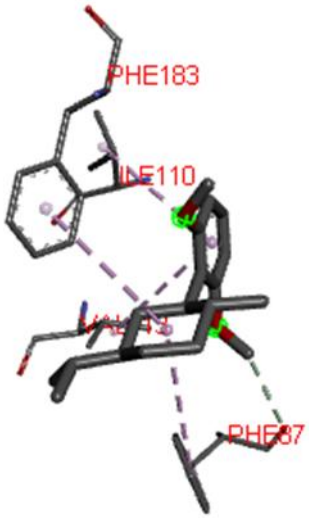
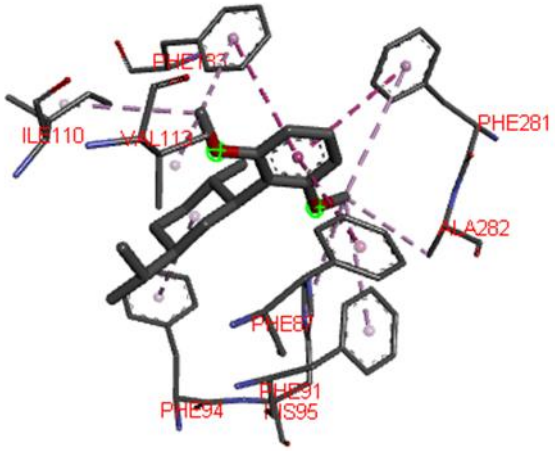
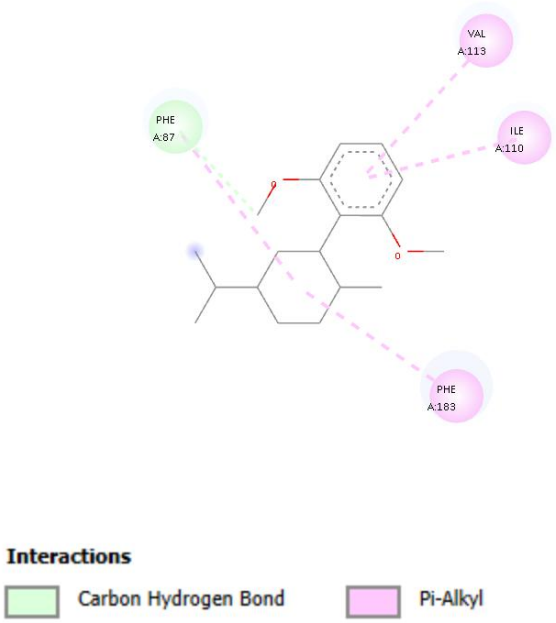
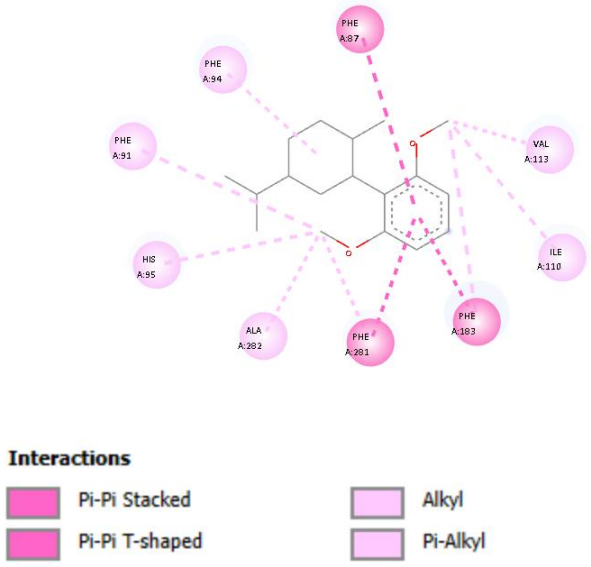
• *Synthesized Ligands of Series* ***9****/ent-****9*** *with CB2 Receptor*

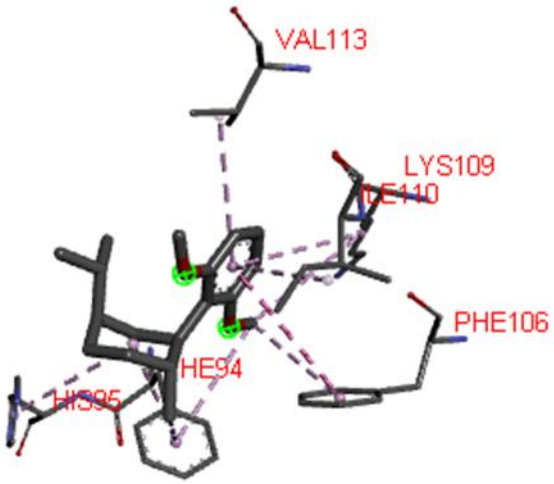
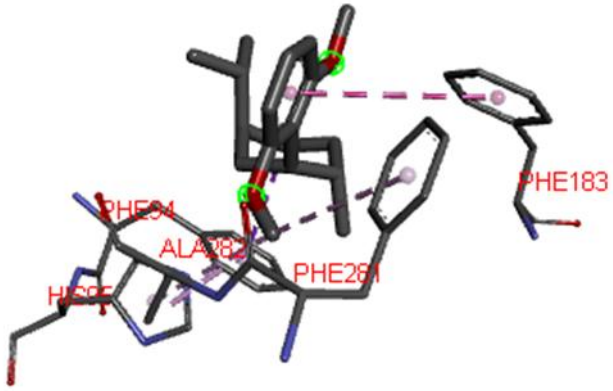
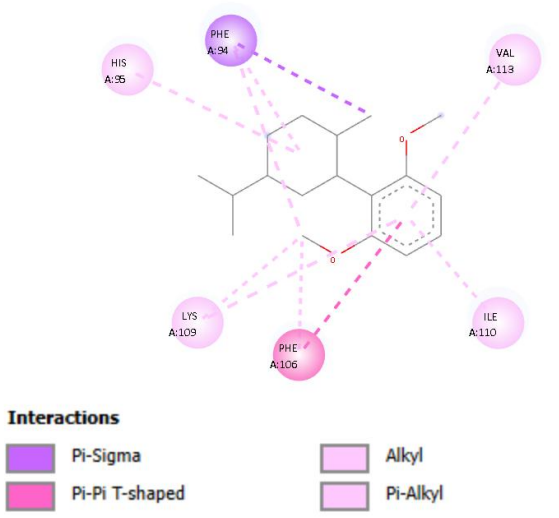
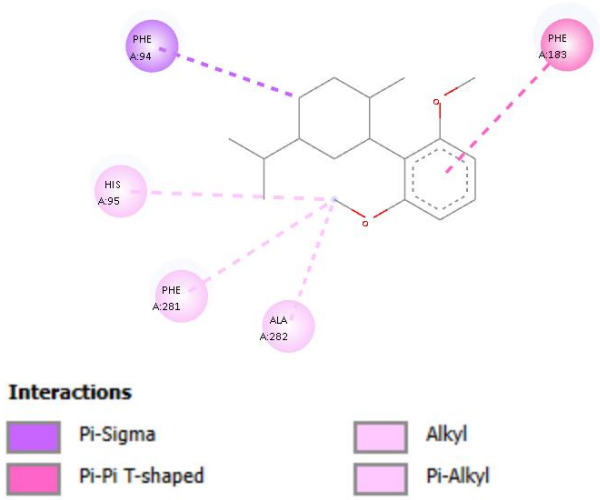
9a (I)	**ent-9a (I)**
	
	
Binding energy: -9.0	**Binding energy: -8.9**

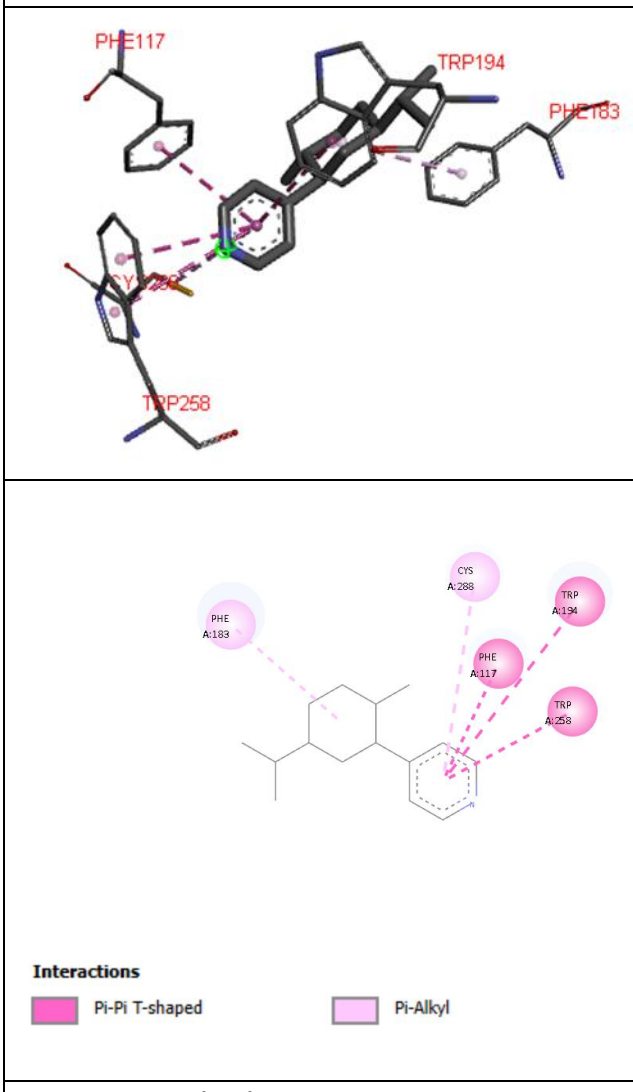
9a (II)	ent-9a (II)
	
	
Binding energy: -9.2	**Binding energy: -9.4**

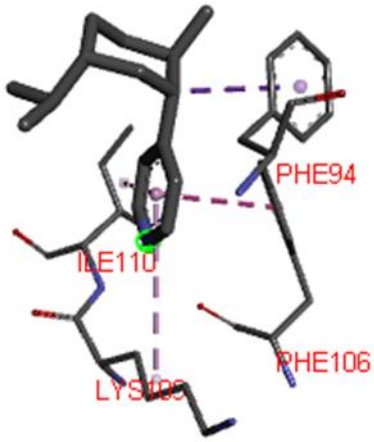
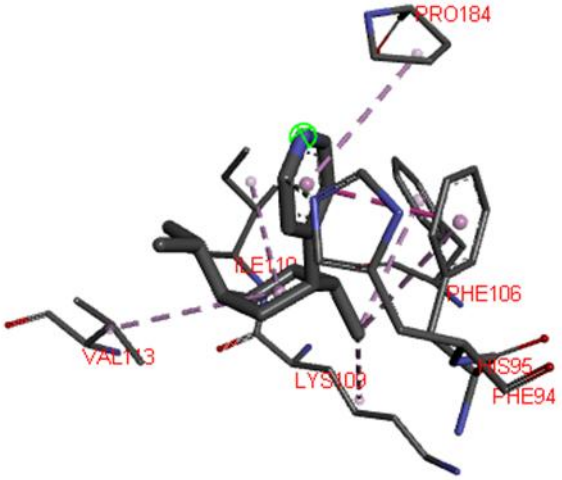
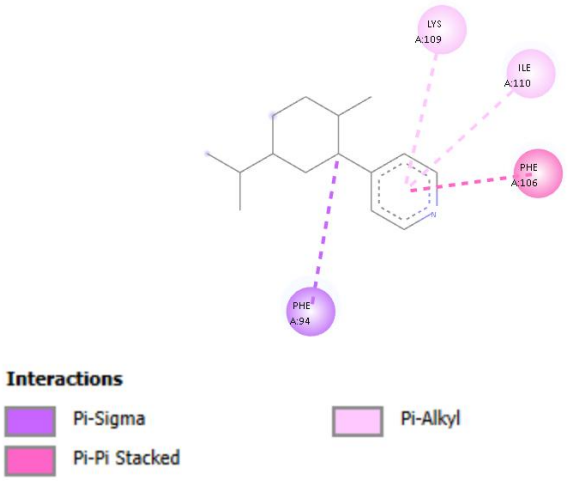
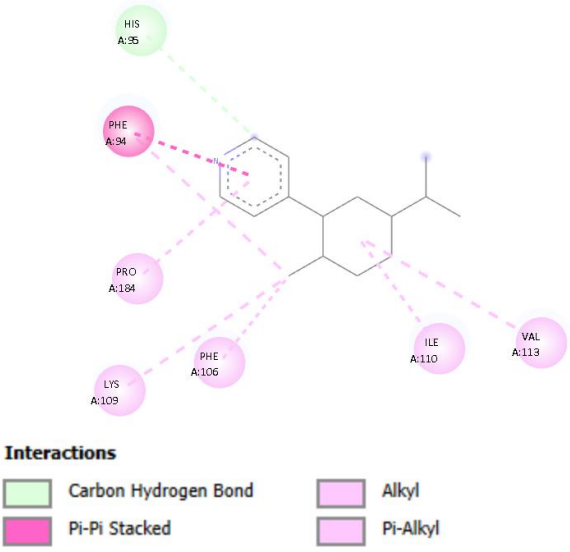
9b (I)	ent-9b (I)
	
	
Binding energy: -8.6	**Binding energy: -8.6**

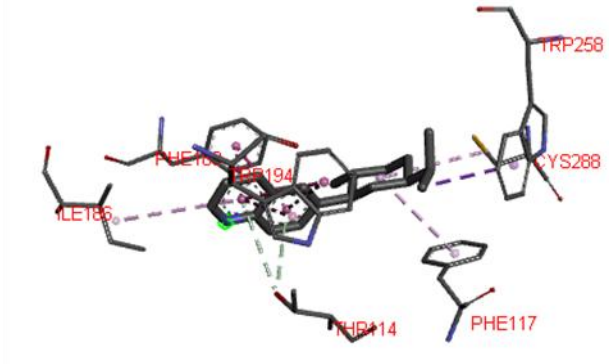
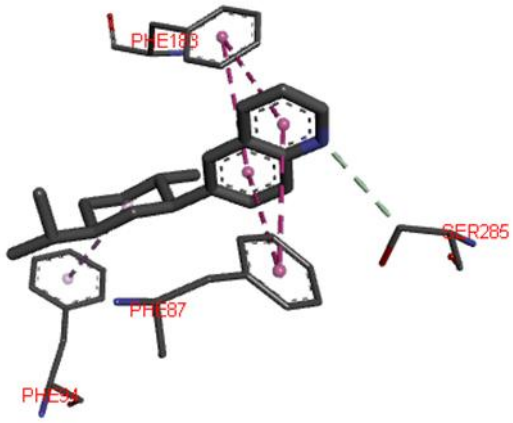
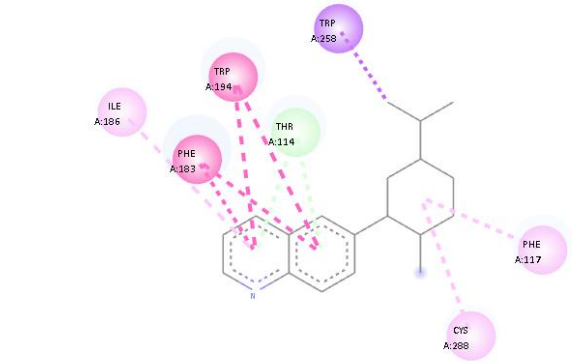
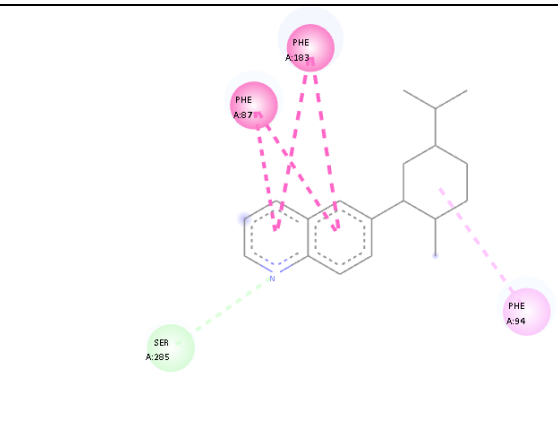
9b (II)	ent-9b (II)
	
	
Binding energy: -8.2	**Binding energy: -8.6**

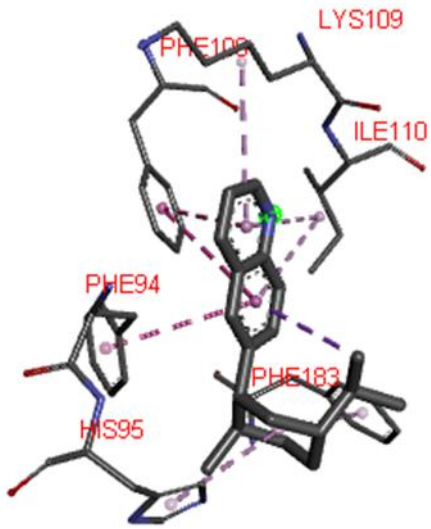
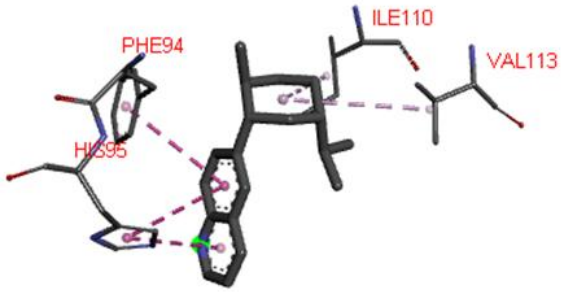
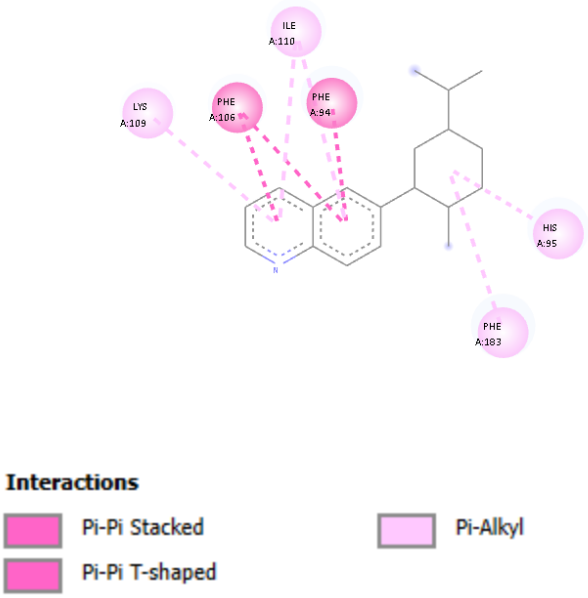
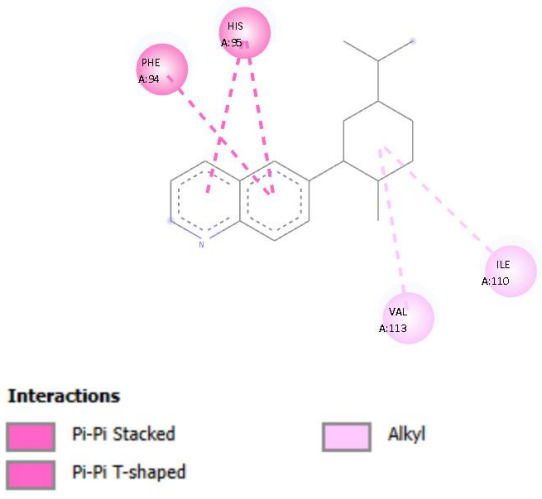
9c (l)	ent-9c (l)
	
	
Binding energy: -7.9	**Binding energy: -8.3**

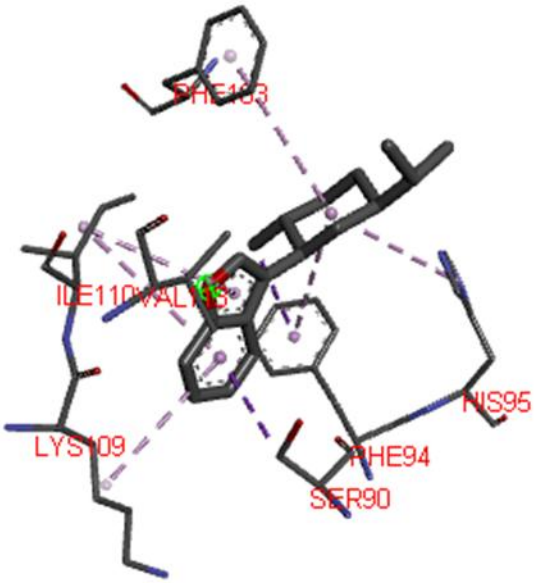
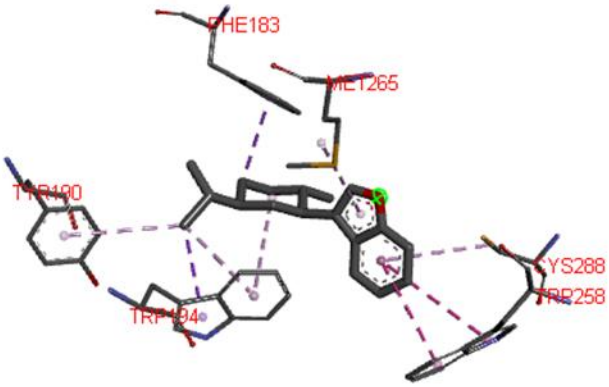
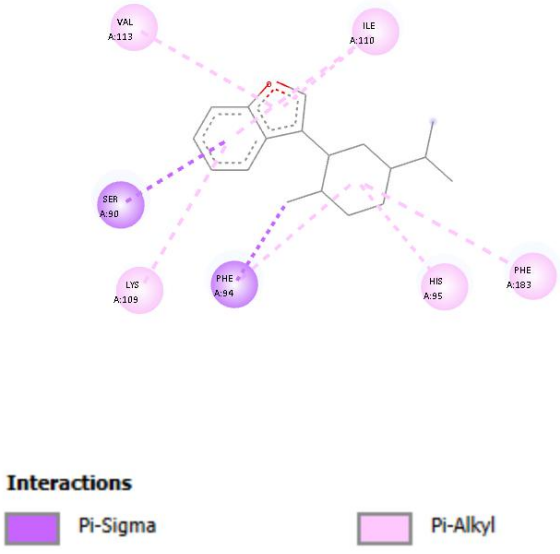
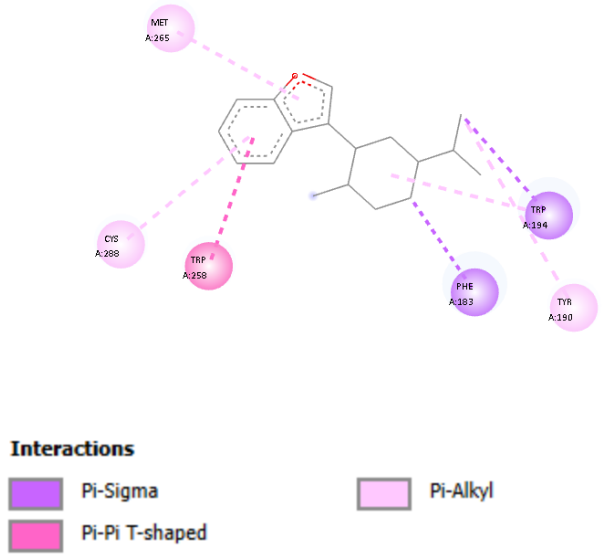
9c (II)	ent-9c (II)
	
	
Binding energy: -8.0	**Binding energy: -8.8**

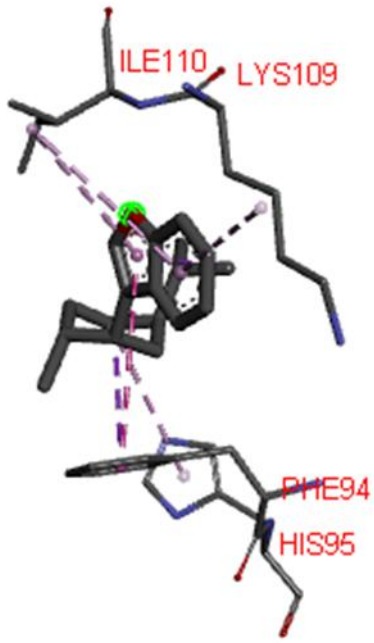
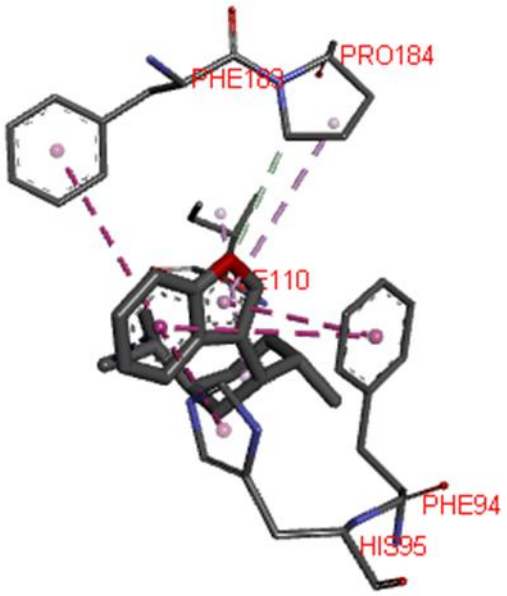
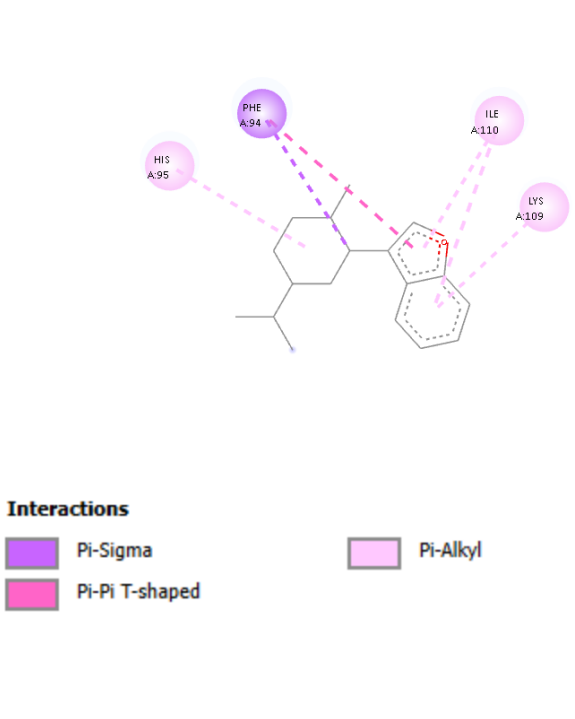
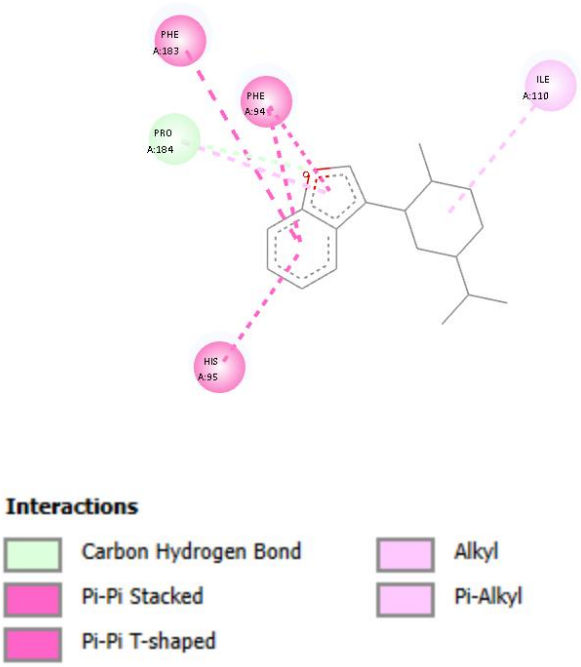
9d (I)	ent-9d (I)
	
Binding energy: -8.0	**Binding energy: -8.1**

9d (II)	ent-9d (II)
	
	
Binding energy: -8.5	**Binding energy: -9.0**

9e (I)	ent-9e (I)
	
	
Binding energy: -10.1	**Binding energy: -10.0**

9e (II)	ent-9e (II)
	
	
Binding energy: -9.4	**Binding energy: -10.3**

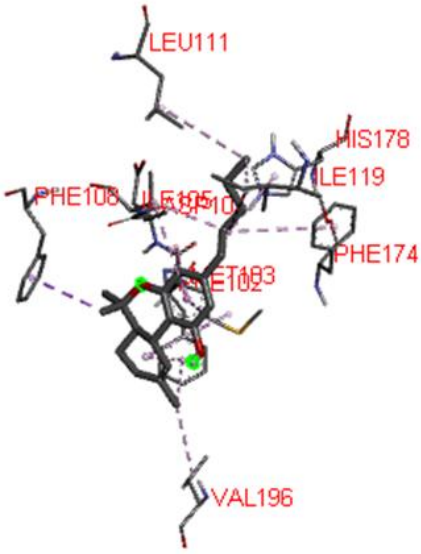
9f (I)	ent-9f (I)
	
	
Binding energy: -9.5	**Binding energy: -9.9**

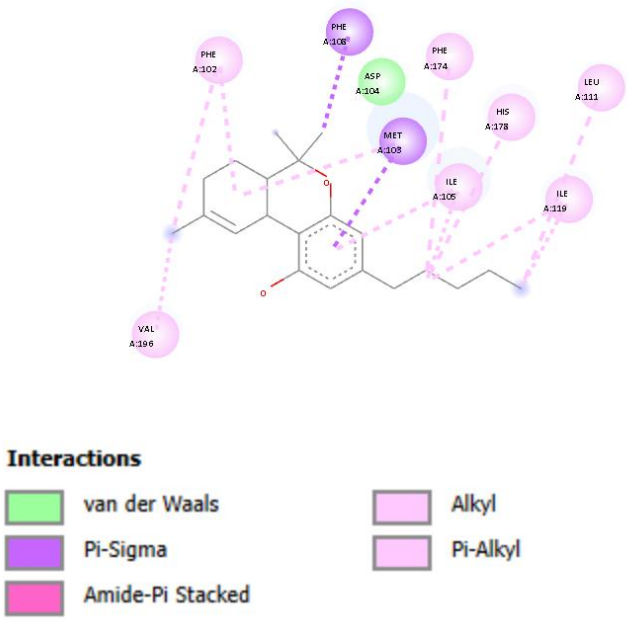
9f (II)	ent-9f (II)
	
	
Binding energy: -9.1	**Binding energy: -9.7**

VII. Molecular Docking of Known Modulators of Cannabinoid Receptors CB1 and CB2

• *CB1 Receptor Ligands*

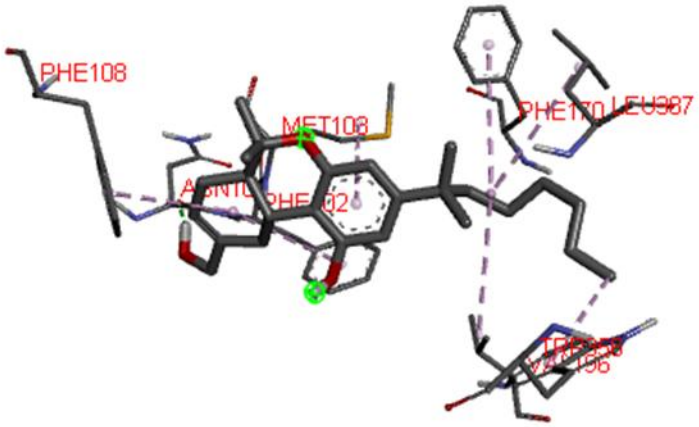
Partial agonist: Tetrahydrocannabinol (THC)

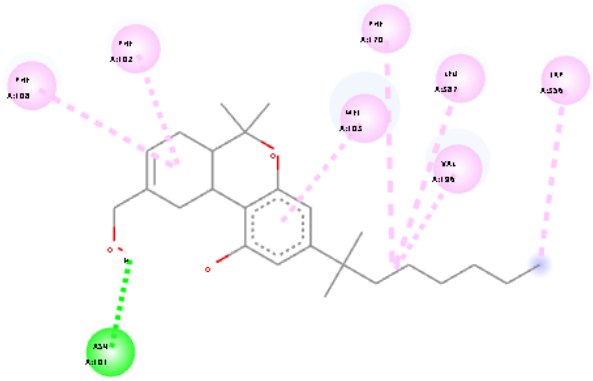




Binding energy: -9.6

Agonist: HU-210





Interactions

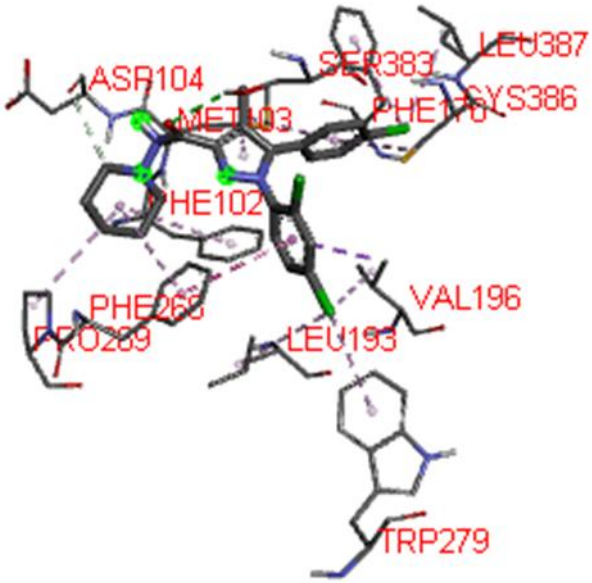
Conventional Hydrogen Bond

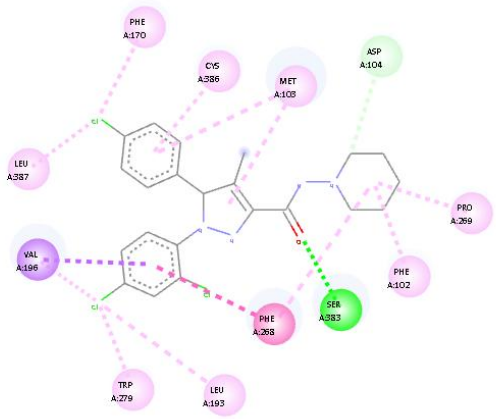
Pi-Alkyl

Alkyl

Binding energy: -9.7

Antagonist: SR141716A (Rimonabant)



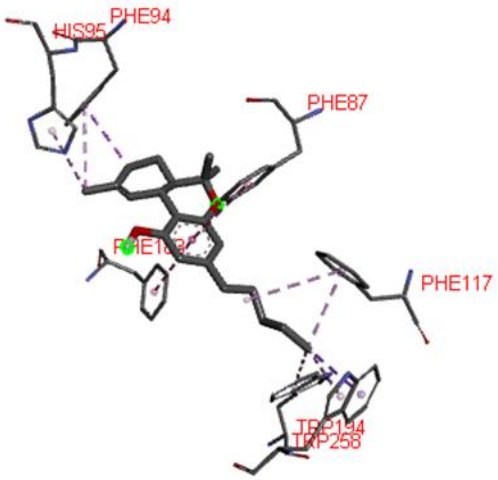
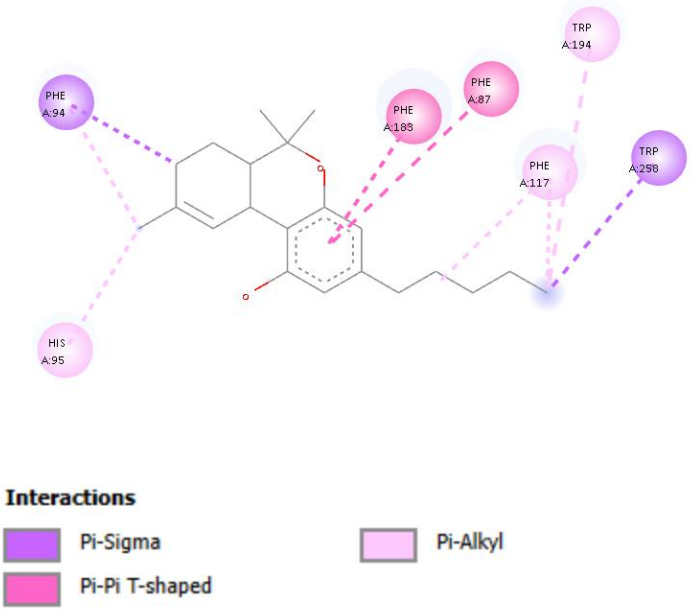


Interactions

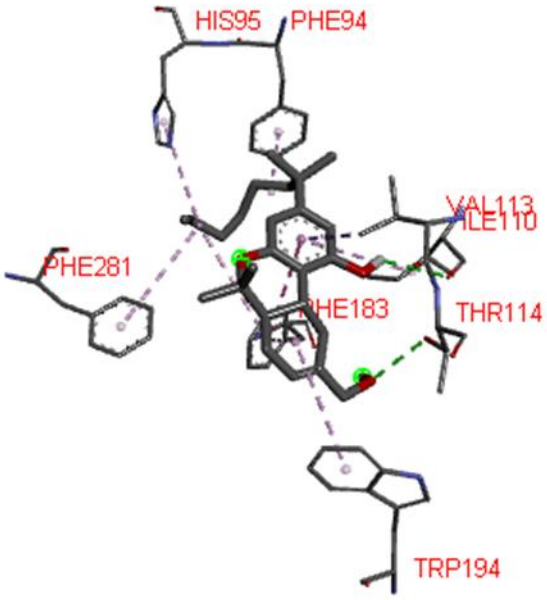
Conventional Hydrogen Bond	Pi-Pi T-shaped
Carbon Hydrogen Bond	Alkyl
Pi-Sigma	Pi-Alkyl

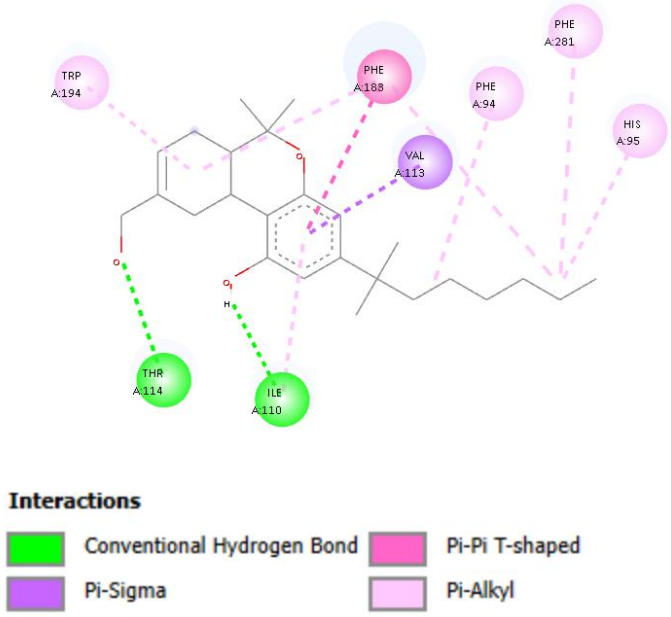
Binding energy: -11.1

• *CB2 Receptor Ligands*

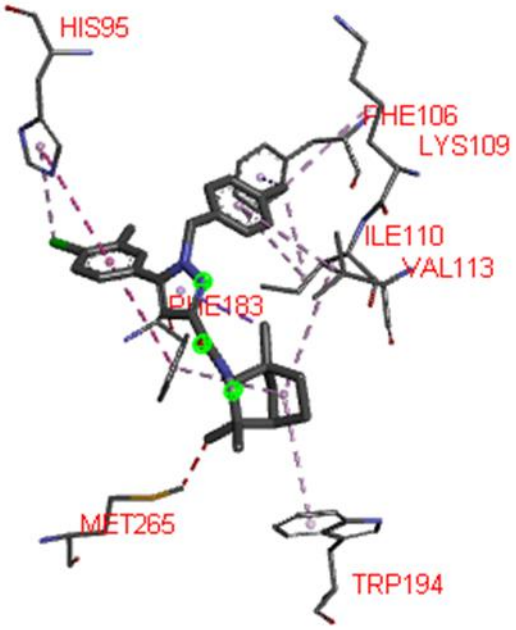
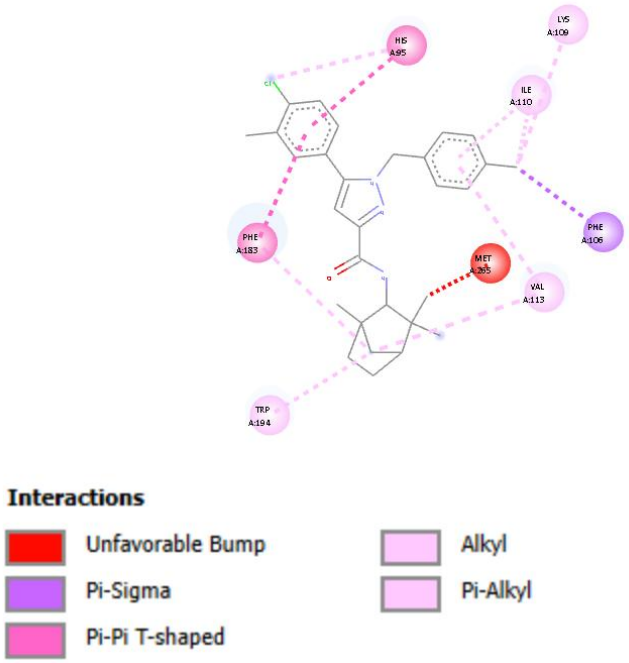
Partial agonist: Tetrahydrocannabinol (THC)


Binding energy: -10.2

Agonist: HU-210





Binding energy: -10.7

Antagonist: HY13439


Binding energy: -11.2