Supplementary Material

An enantiopure building block for naturally occurring hydroporphyrins and vitamin B_{12} from Hagemann´s ester

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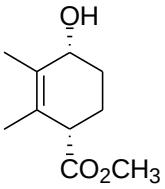
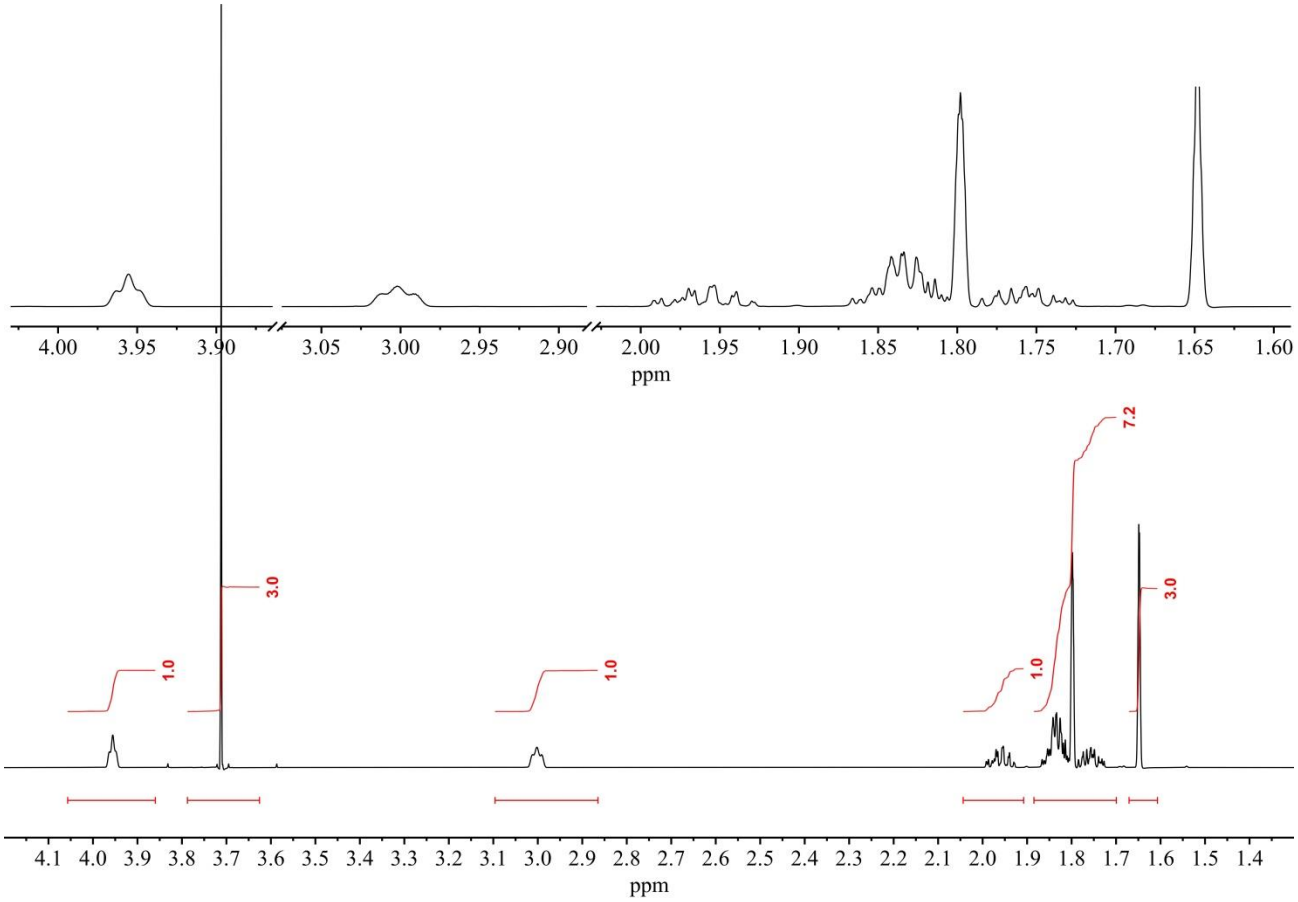
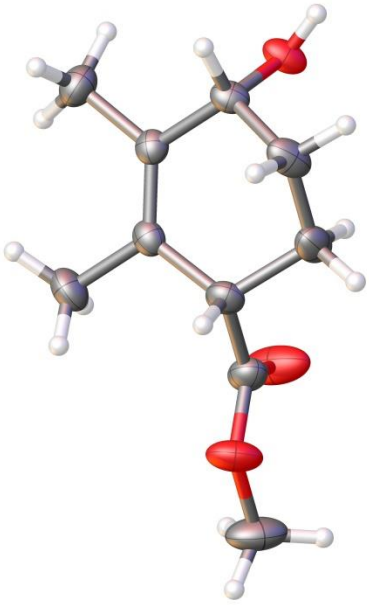
Compound 5/*rac*-5



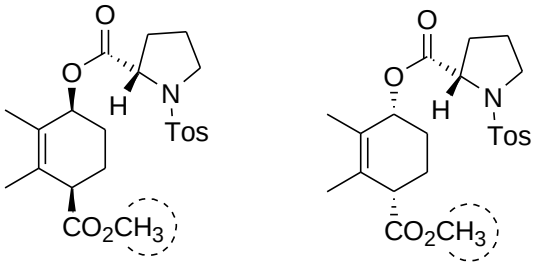
^{1}H NMR (600 MHz, $CDCl_3$)



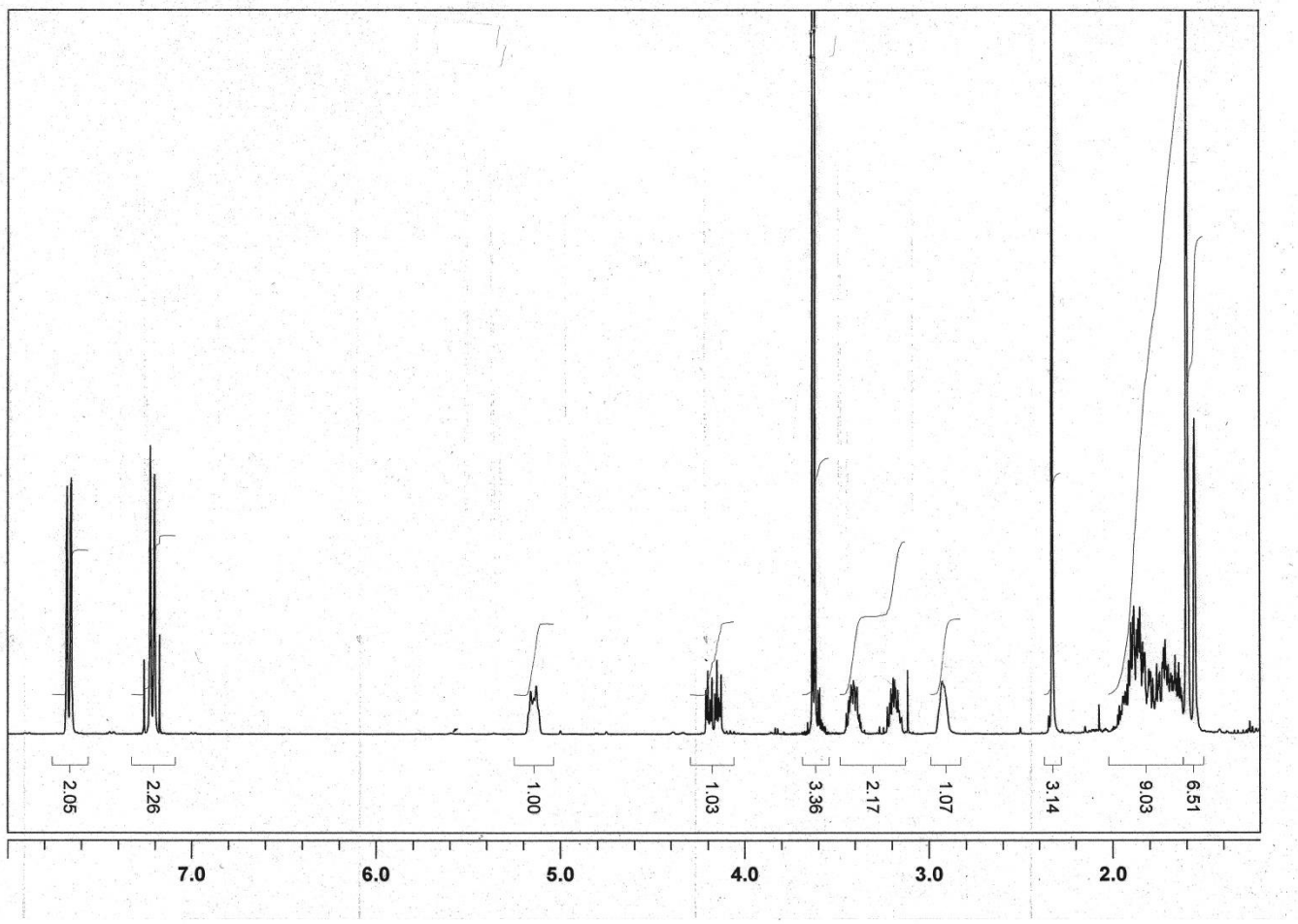
X-Ray crystal-structure analysis of *rac*-**5**: $C_{10}H_{16}O_3$ M 184.23, thermal ellipsoids are shown at 50% level. Monoclinic, space group $P2_1/n$, D_c = 1.1212 [Mg/m^3], Z = 8, unit cell a = 1289.2(2), b = 776.60(10), c = 2114.1(3) [pm], α = 90°, β = 107.420(10)°, γ = 90°, V = 2.0196(5) [nm^3], μ(MoK_α) = 0.088[mm^{-1}], wR_2 = 0.1388. Deposition Number: CCDC 2040266.



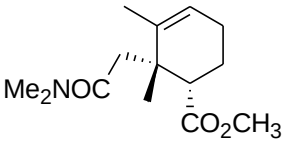
Compounds 14/15



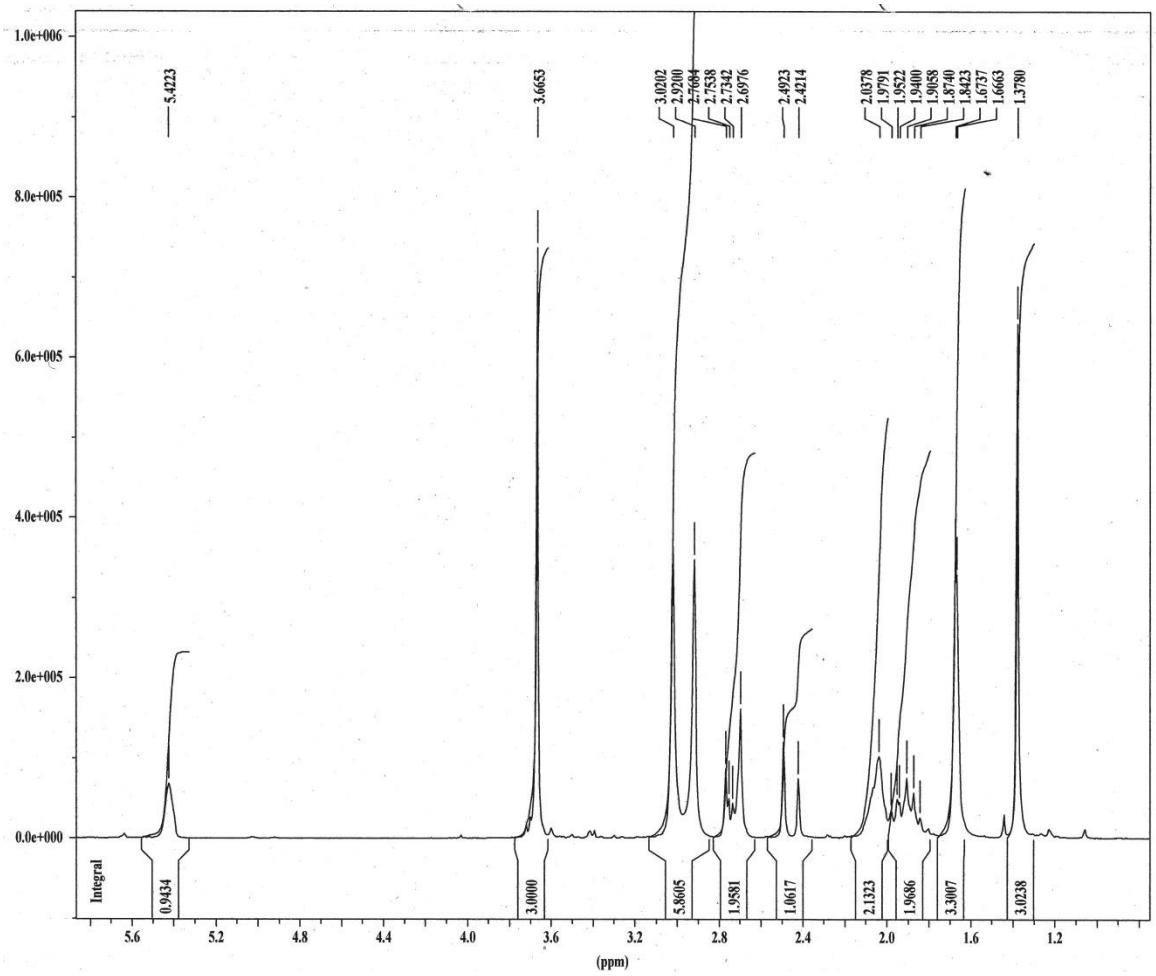
^{1}H NMR (360 MHz, $CDCl_3$)

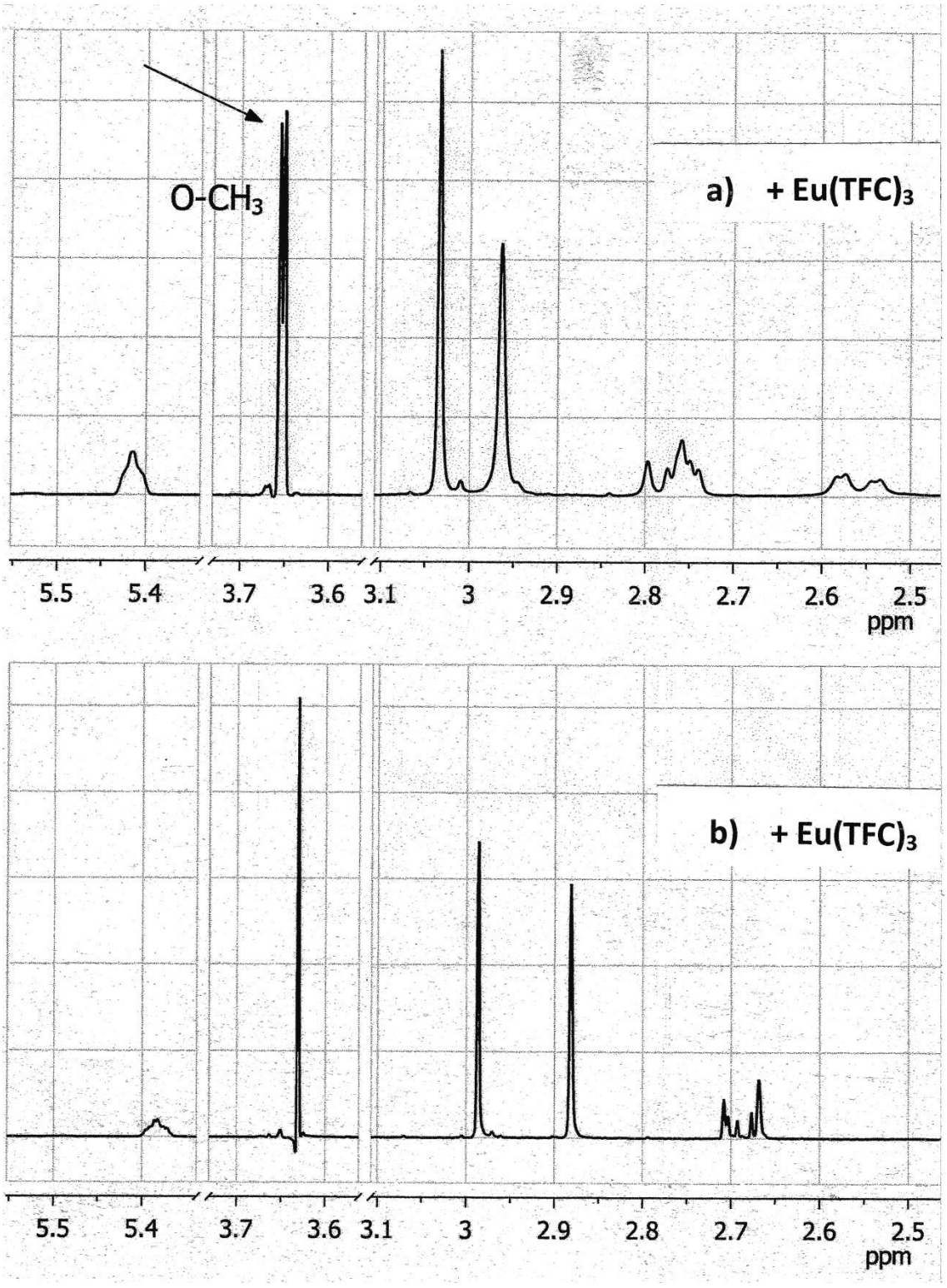


Compound 2

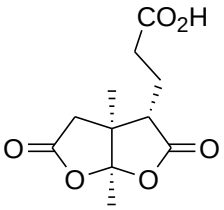


^{1}H NMR (360 MHz, $CDCl_3$)

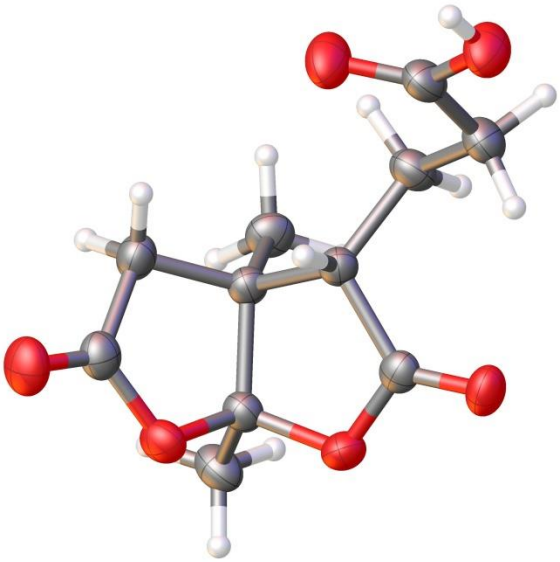



O-CH3
a) + Eu(TFC)3
5.5
5.4
3.7
3.6
3.1
3
2.9
2.8
2.7
2.6
2.5
ppm
b) + Eu(TFC)3
5.5
5.4
3.7
3.6
3.1
3
2.9
2.8
2.7
2.6
2.5
ppm

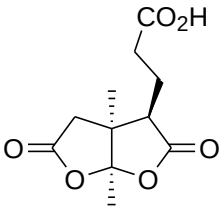
Compound *rac*-8



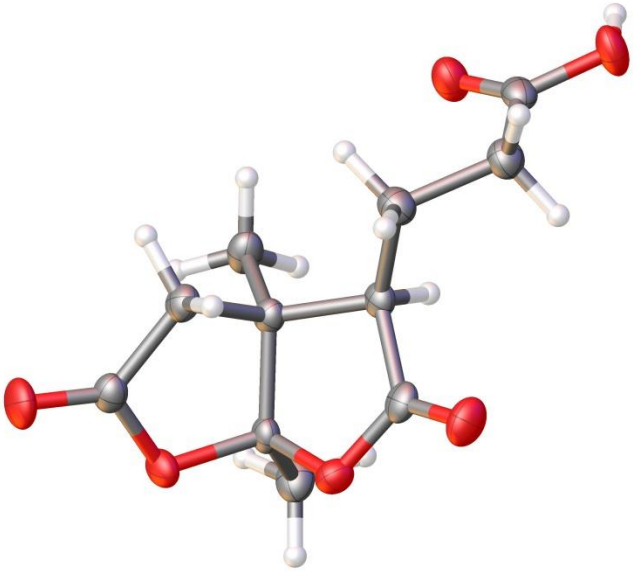
X-Ray crystal-structure analysis of *rac*-8: $C_{11}H_{14}O_6$ M 242.22, thermal ellipsoids are shown at 50 % level. Monoclinic, space group $P2_1/c$, D_c = 1.422 [Mg/m^3], Z = 4, unit cell a = 675.30(10), b = 1701.1(2), c = 1037.70(10) [pm], α = 90°, β = 108.340(10)°, γ = 90°, V = 1.1315(2) [nm^3], μ(MoK_α) = 0.117 [mm^{-1}], wR_2 = 0.1129. Deposition Number: CCDC 2040263.



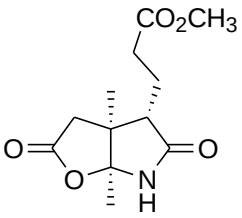
Compound *epi-rac*-8



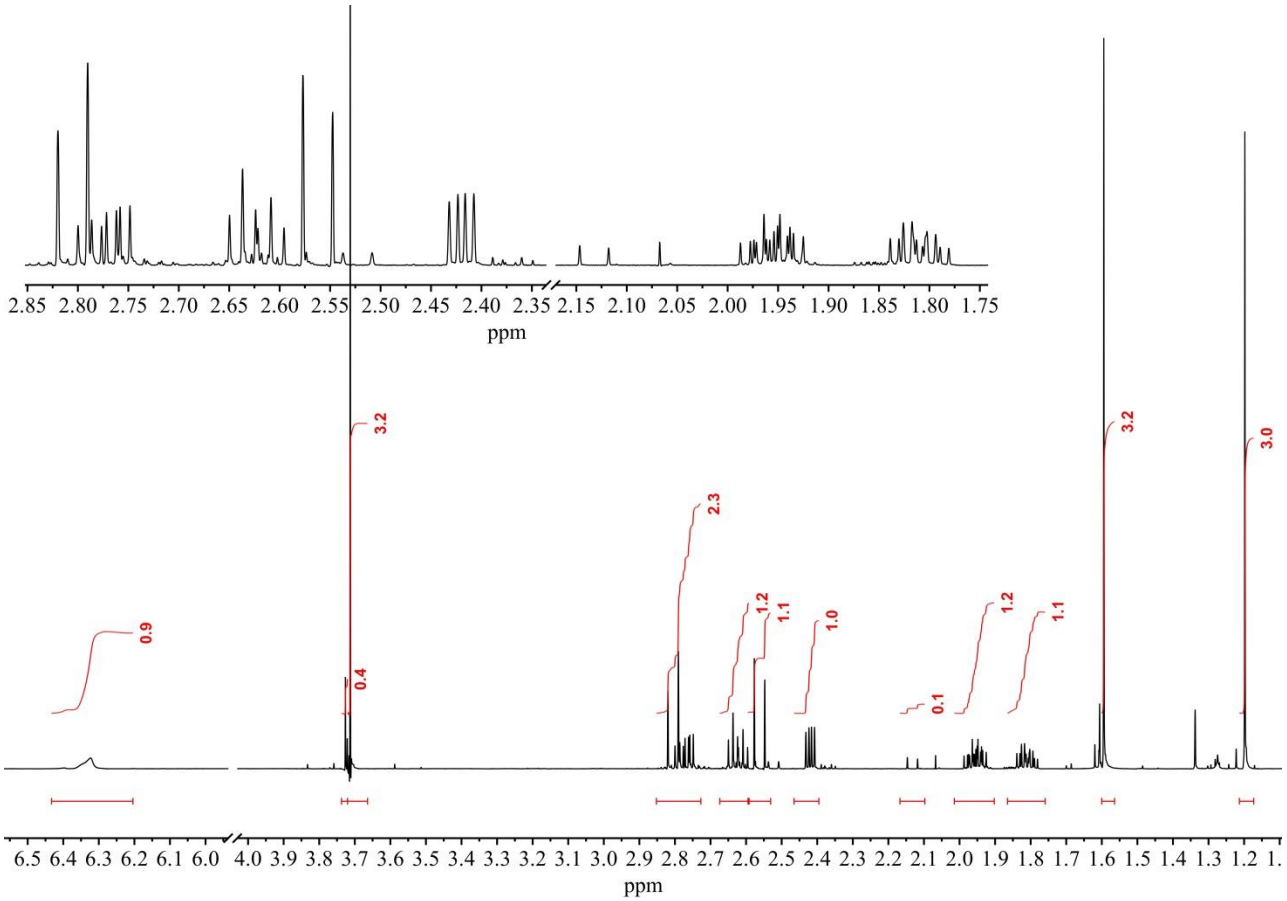
X-Ray crystal-structure analysis of *epi-rac*-8: $C_{11}H_{14}O_6$ M 242.22, thermal ellipsoids are shown at 50 % level. Monoclinic, space group $P2_1/c$, D_C = 1.433 [Mg/m^3], Z = 4, unit cell a = 811.00(10), b = 2001.5(3), c = 714.8(3) [pm], α = 90°, β = 104.62(2)°, γ = 90°, V = 1.1224(5) [nm^3], μ(MoK_α) = 0.118 [mm^{-1}], wR_2 = 0.1762. Deposition Number: CCDC 2040267.



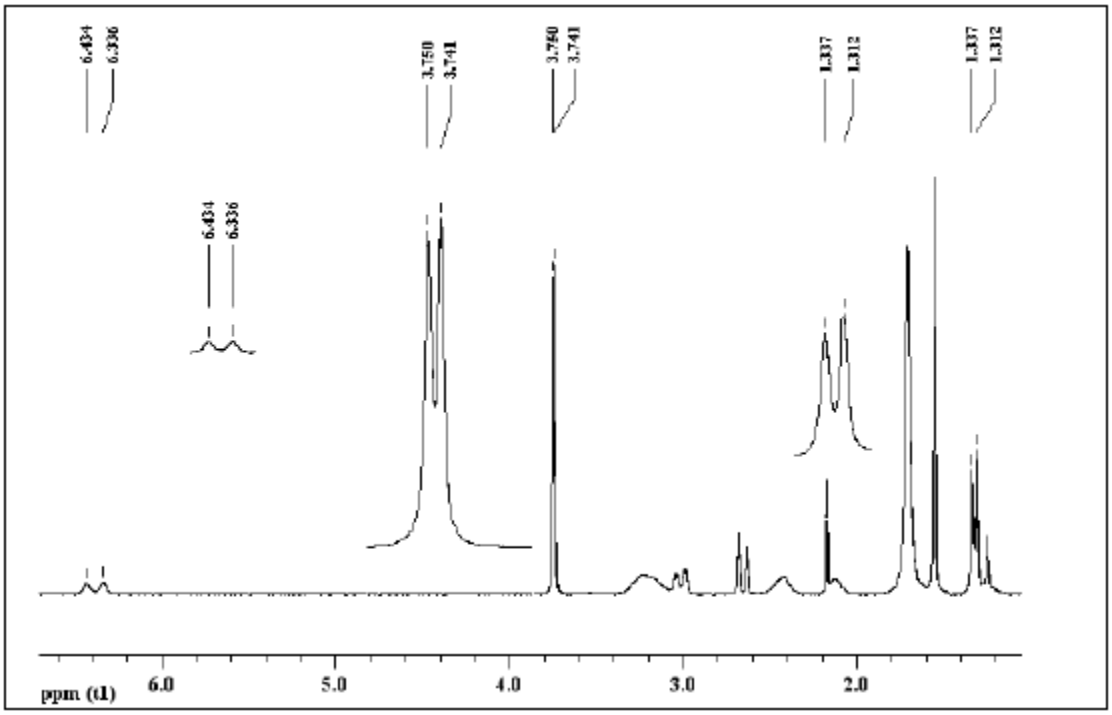
Compound 3/*rac*-3



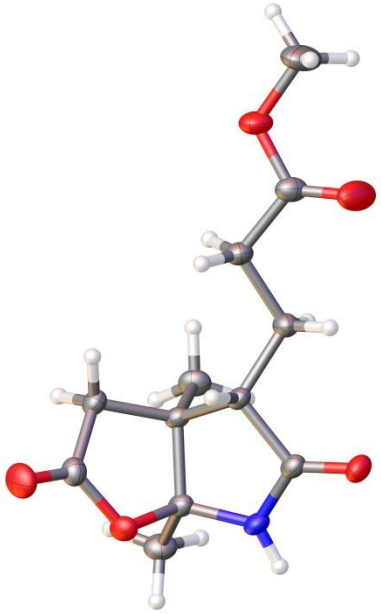
^{1}H NMR (600 MHz, $CDCl_3$): 3 + trace of 2-*epi*-**3**



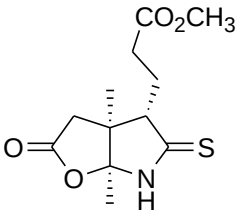
^{1}H NMR (360 MHz, $CDCl_3$) shift experiment on *rac*-3 with Eu(TFC)$_3$. Split off of -NH, -CO_2CH_3 and 1-CH_3 signals.



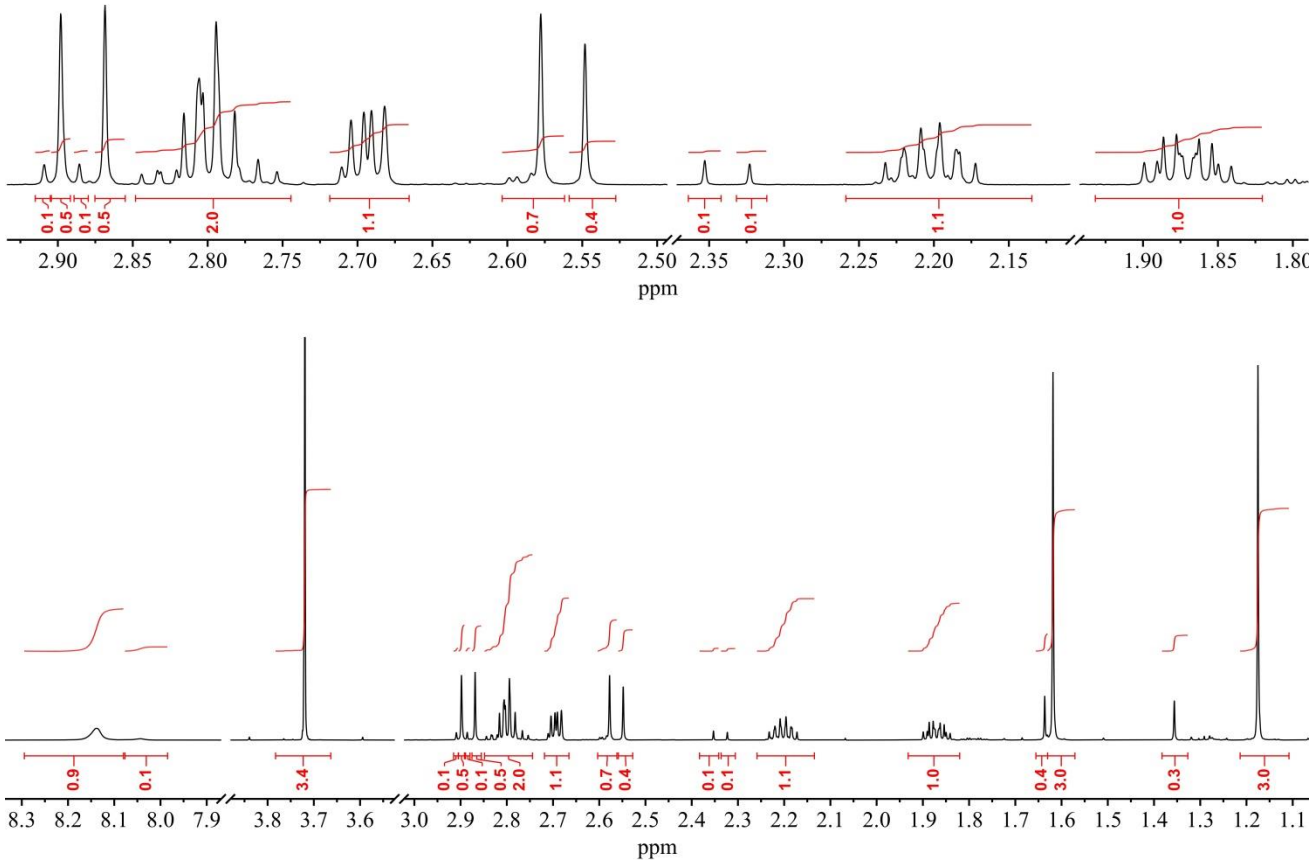
X-Ray crystal-structure analysis of *rac*-3: $C_{12}H_{17}NO_3$ M 255.27, thermal ellipsoids are shown at 50 % level. Triclinic, space group P-1, D_c = 1.340 [Mg/m^3], Z = 2, unit cell a = 669.80(10), b = 859.80(10), c = 1189.1(2) [pm], α = 98.470(10)°, β = 104.930(10)°, γ = 101.950(10)°, V = 0.63259(16) [nm^3], μ(Mo$K_α$) = 0.105 [mm^{-1}], wR_2 = 0.1297. Deposition Number : CCDC 2040265.



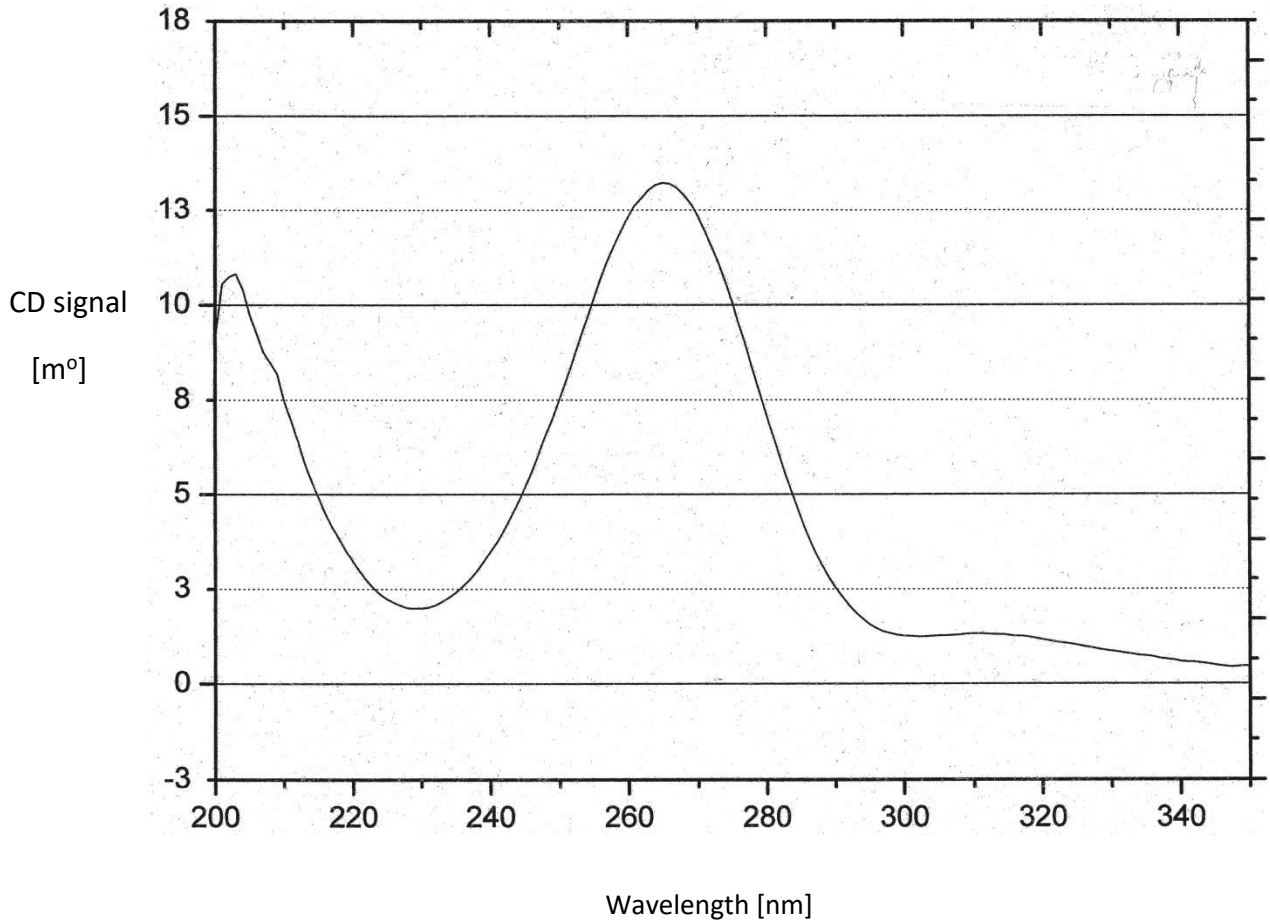
Compound 10



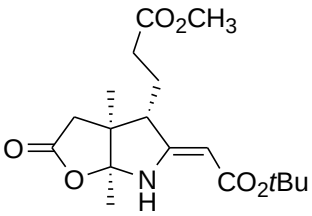
^{1}H NMR (600 MHz, $CDCl_3$): 10 + ca. 10 % of 2-*epi*-**10**



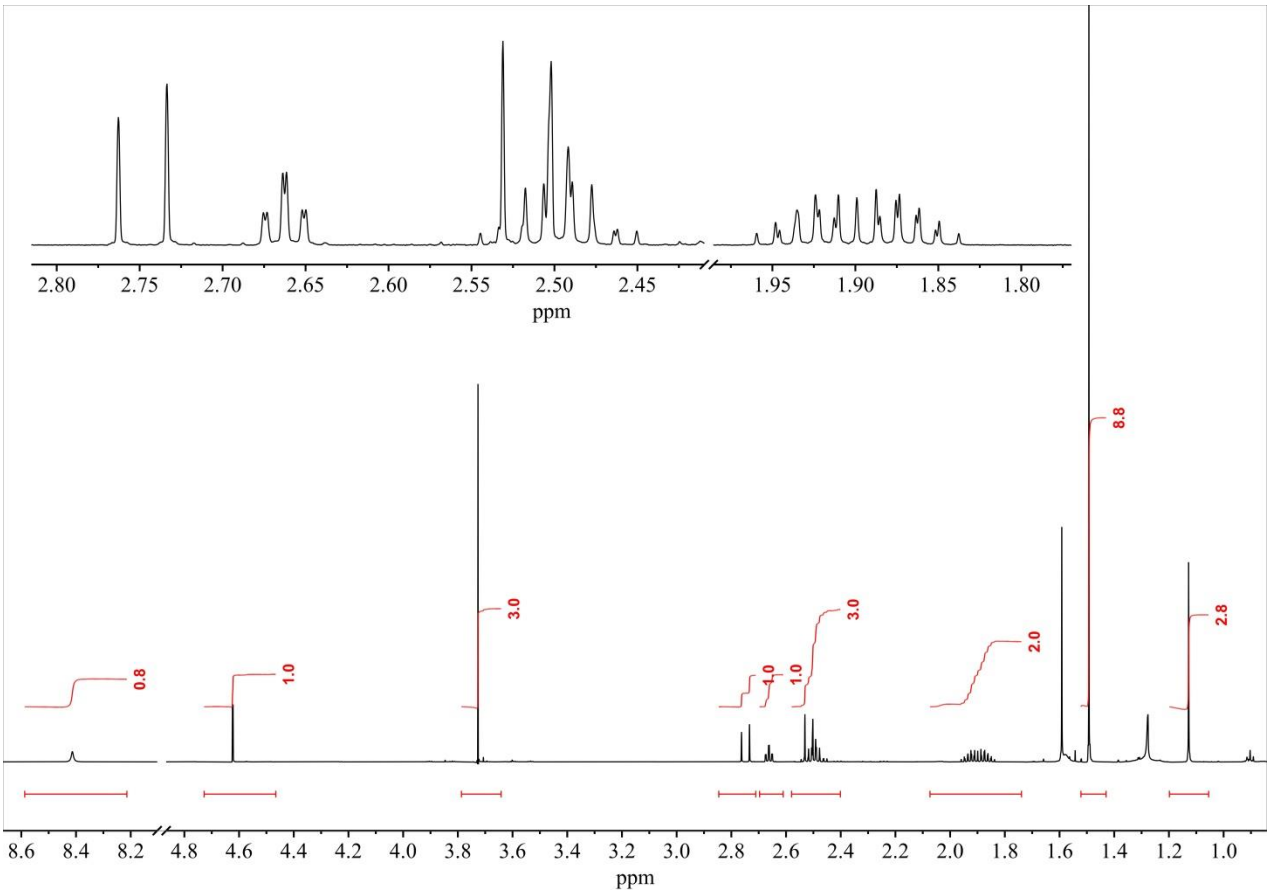
CD spectrum in CH_3OH [c = 9.40 x 10^{-5} M, Θ(λ) = 1415 (267 nm)]



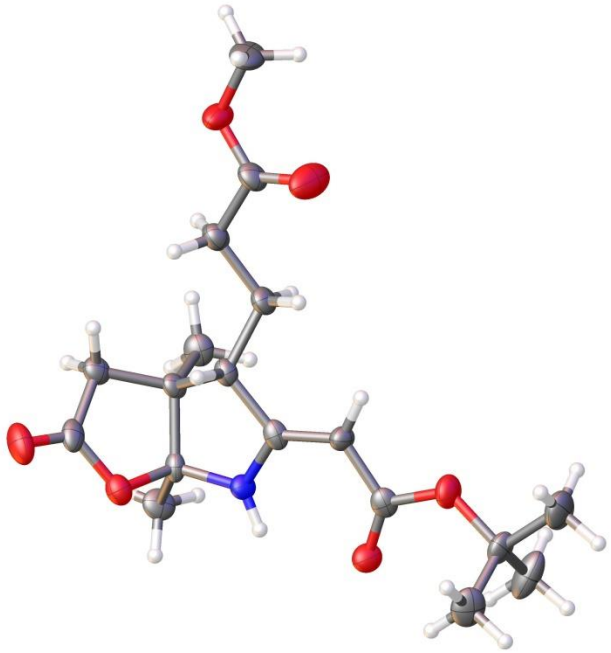
Compound 12/*rac*-12



^{1}H NMR (600 MHz, $CDCl_3$)



X-Ray crystal-structure analysis of *rac*-**12**: $C_{18}H_{27}NO_6$ M 353.41, thermal ellipsoids are shown at 50 % level. Monoclinic, space group $P2_1/n$, D_c = 1.247 [Mg/m^3], Z = 4, unit cell a = 669.1(2), b = 3324.9(6), c = 852.5(2) [pm], α = 90°, β = 96.91(2)°, γ = 90°, V = 1.8828(8) [nm^3], μ(MoK$_\alpha$) = 0.093 [mm^{-1}], wR_2 = 0.2179. Deposition Number: CCDC 2040264.



CD spectrum of 12 in CH_3OH [c = 2.86 x 10^{-5} M, Θ(λ) = 7944 (265)]