

Supplementary Materials:

Insights into the phytochemistry of the Cuban endemic medicinal plant *Phyllanthus orbicularis*: Fideloside, a novel bioactive 8-C-glycosyl 2,3-dihydroflavonol

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Content:	Page:
Figure S1: Chemical structure of natural products extracted from <i>Phyllanthus</i> species	2
Figure S2. ¹ H NMR spectrum of compound 3 (DMSOd6, 400 MHz)	3
Figure S3. ¹³ C NMR spectrum of compound 3 (DMSOd6, 400 MHz)	3
Figure S4. COSY spectrum of compound 3 (DMSOd6, 400 MHz)	4
Figure S5. HSQC spectrum of compound 3 (DMSOd6, 400 MHz)	5
Figure S6. HMBC spectrum of compound 3 (DMSOd6, 400 MHz)	6
Figure S7. NOESY spectrum of compound 3 (DMSOd6, 400 MHz)	7
Figure S8: ATR infrared spectrum of compound 3	8
Figure S9: Moststable conformation of the 2 <i>S</i> ,3 <i>S</i> enantiomer for compound 3	9
Table S1: DFT calculations for the 2 <i>S</i> ,3 <i>S</i> enantiomer (compound 3)	9

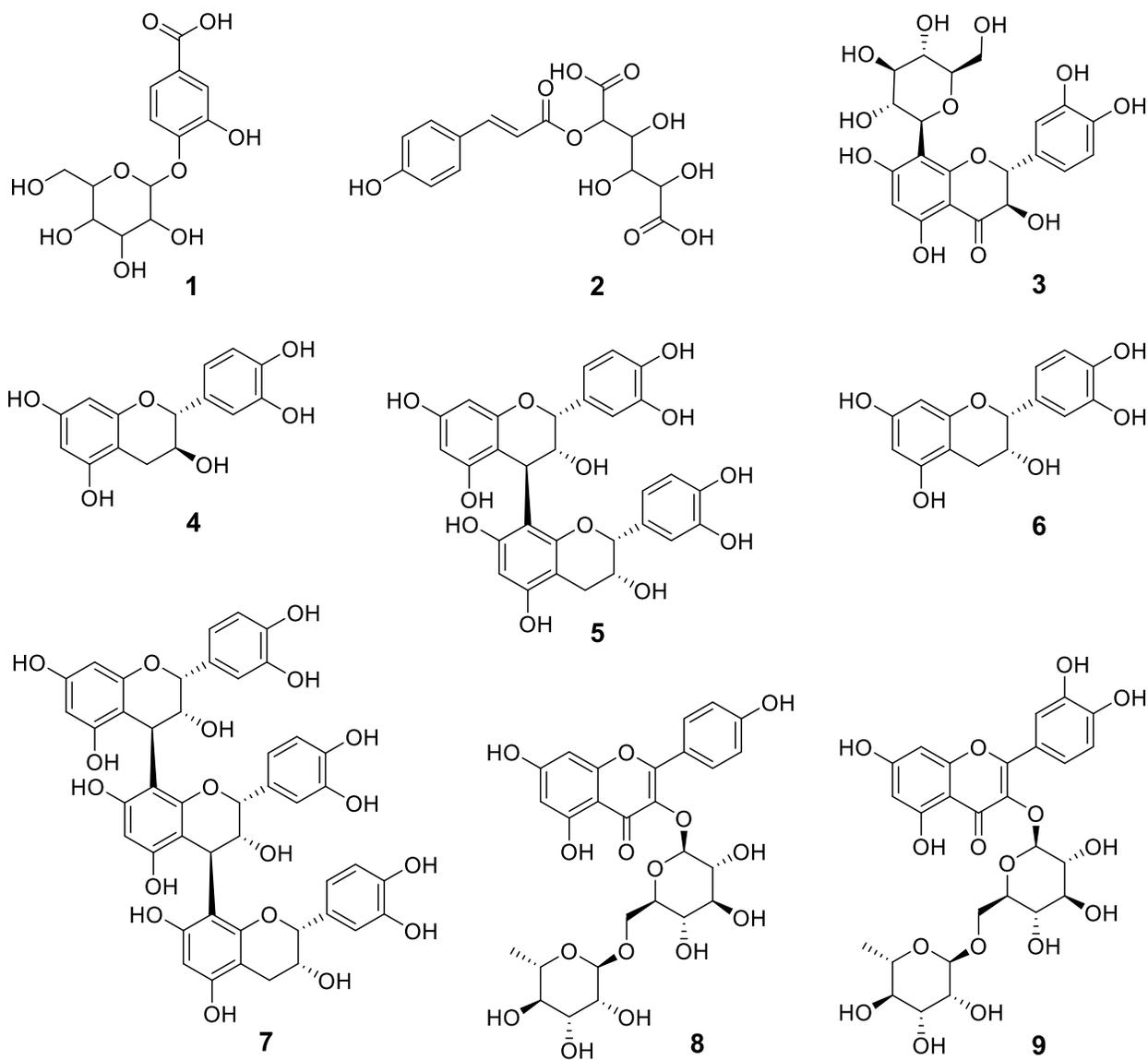


Figure S1:Chemical structure of natural products extracted from *Phyllanthus* species

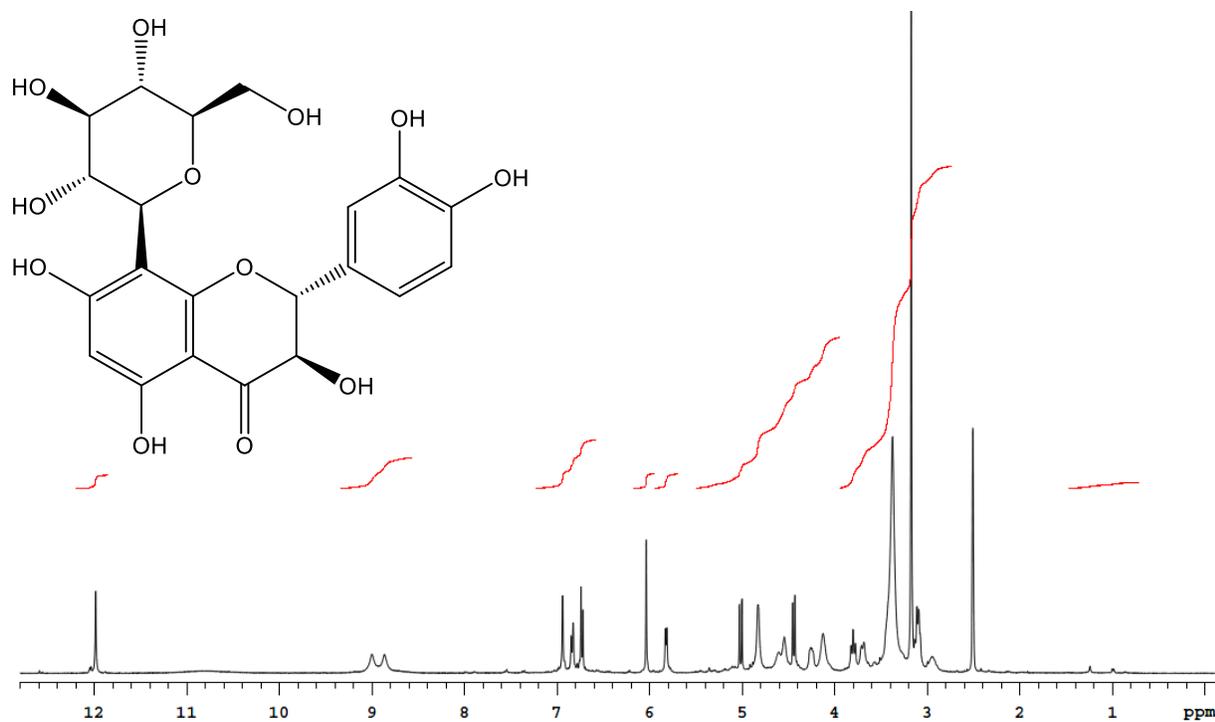


Figure S2. ¹H NMR spectrum of compound 3 (DMSO-d₆, 400 MHz)

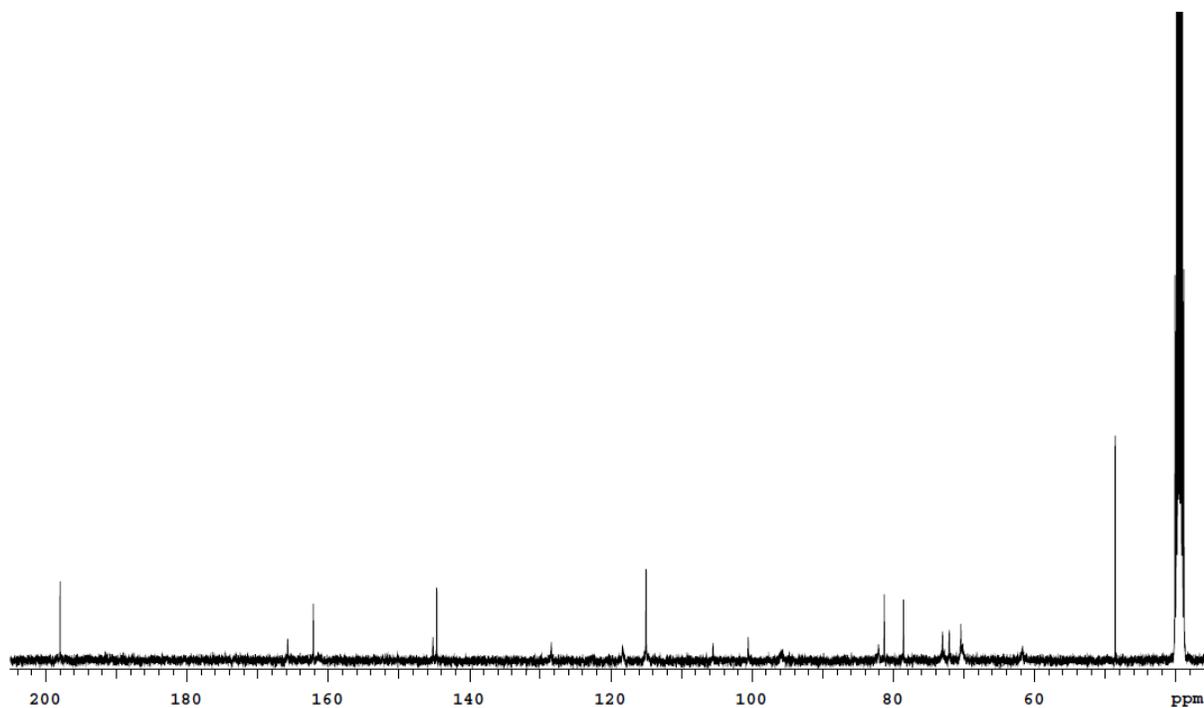


Figure S3. ¹³C NMR spectrum of compound 3 (DMSO-d₆, 400 MHz)

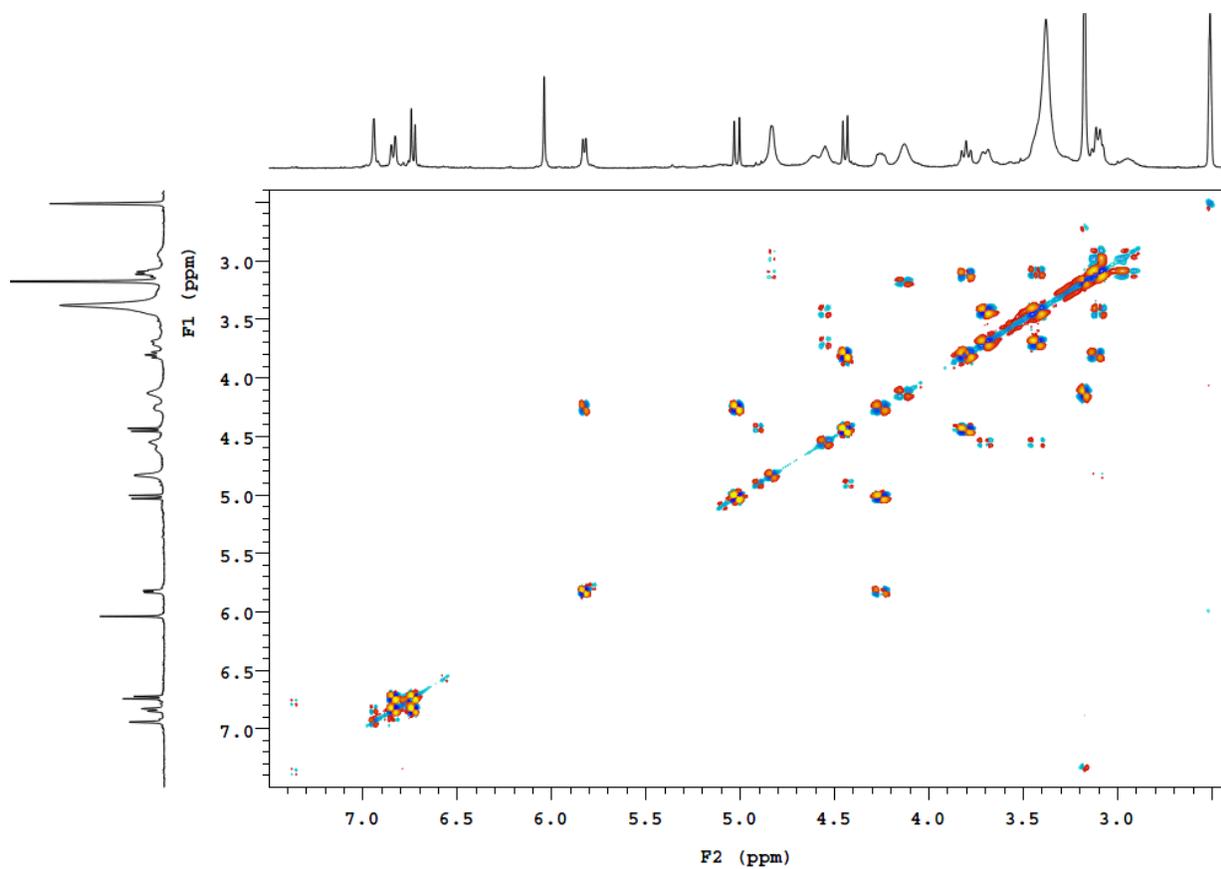


Figure S4. COSY spectrum of compound **3**(DMSO_d6, 400 MHz)

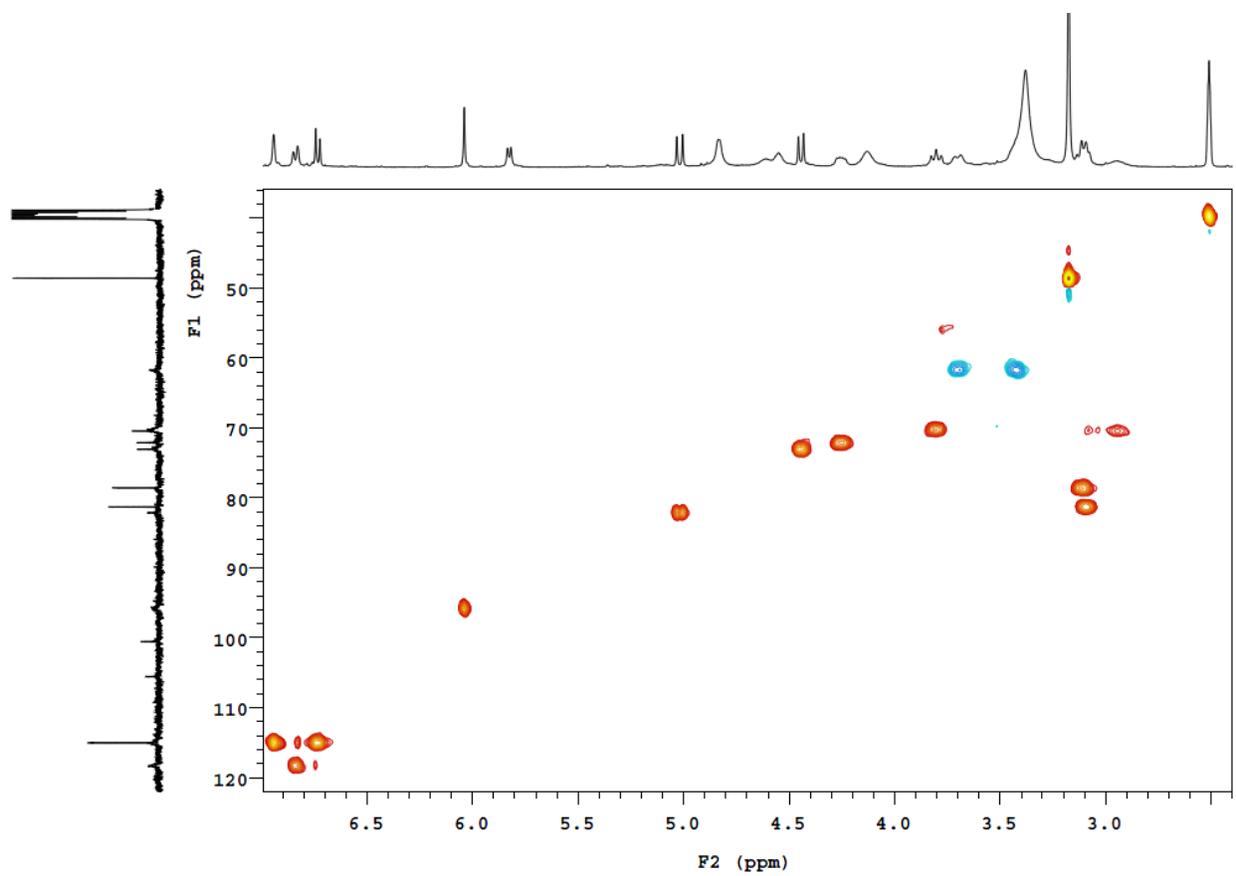


Figure S5. HSQC spectrum of compound 3(DMSOd₆, 400 MHz)

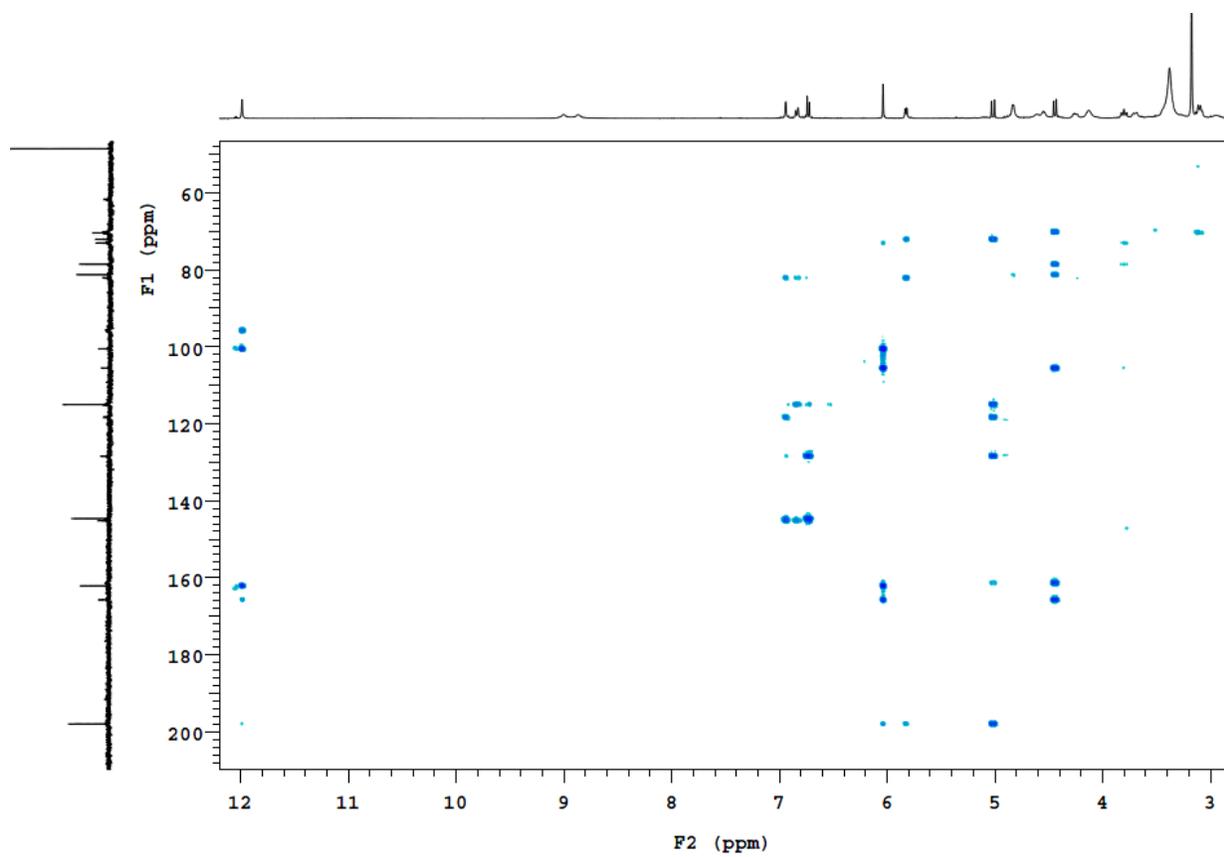


Figure S6. HMBC spectrum of compound **3** (DMSO d_6 , 400 MHz)

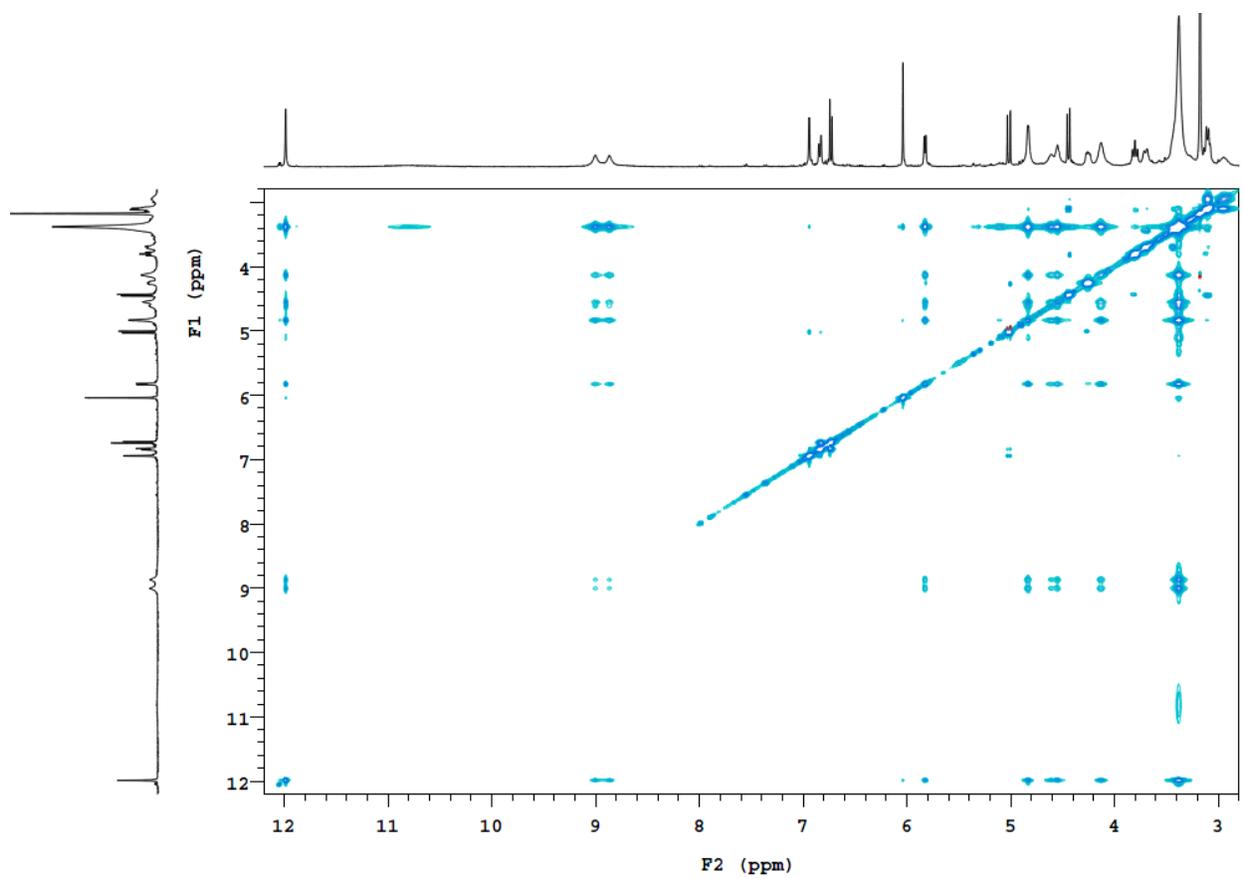


Figure S7. NOESY spectrum of compound **3** (DMSO-d₆, 400 MHz)

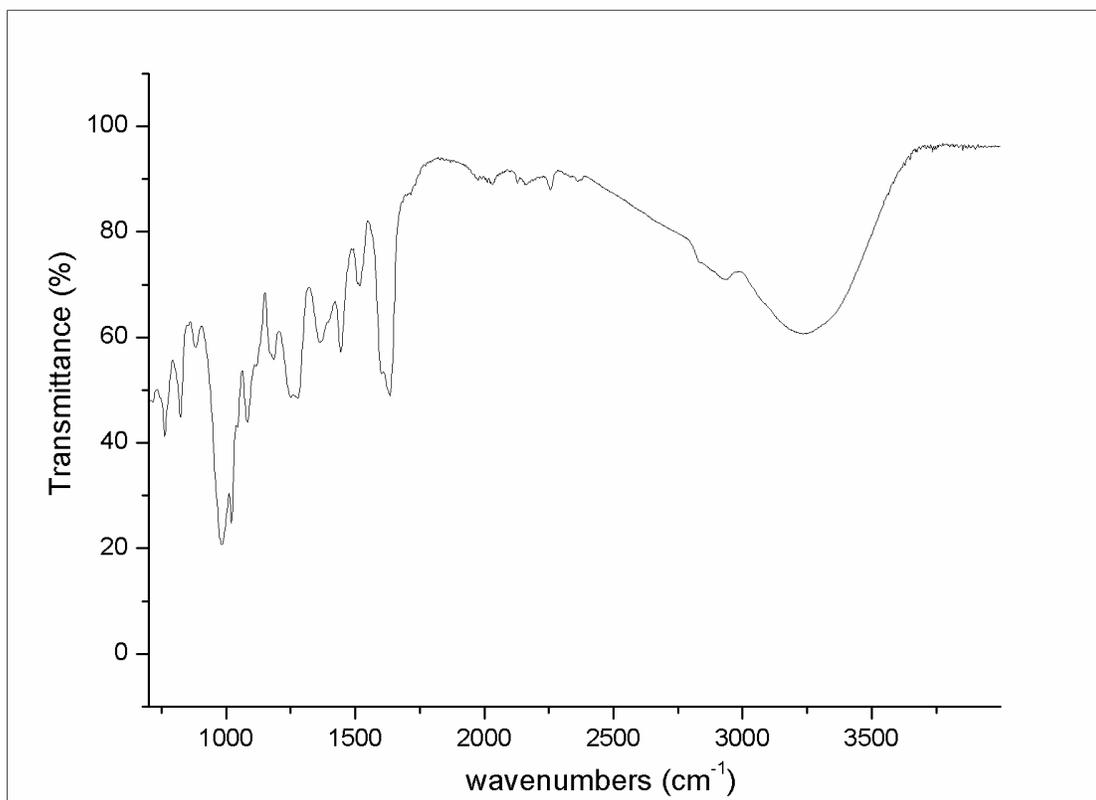


Figure S8:ATR infrared spectrum of compound **3**

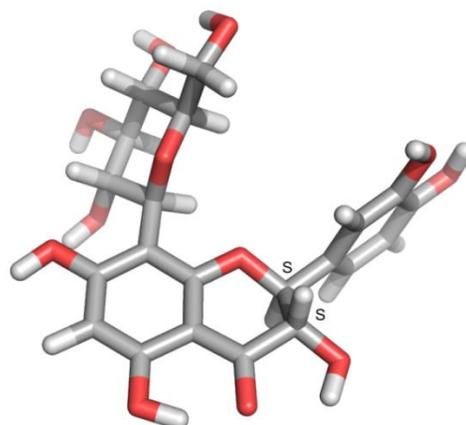
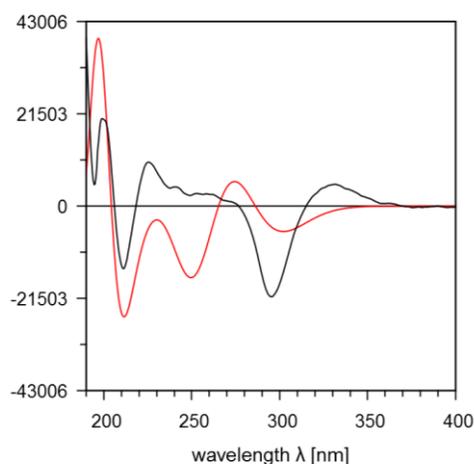


Figure S9. Comparison of experimental CD spectrum (black line) with Boltzmann weighted calculated CD spectrum (see Table S1) for the $2S,3S$ enantiomer with a similarityfactor $S = 0.5276$ for $\sigma = 0.3$ eV and -2 nm shift. right: Calculated moststable conformation of the $2S,3S$ enantiomer.

Table S1: Results of DFT calculations for the $2S, 3S$ enantiomer

Conformation	O-C2-C1'-C2' (in °)	C2'-C3'-O-H (in°)	Energy (kcal/mol)	Boltzmann weight	CD-fit
1	67.1	2.9	0.00	31.0	0.6105
2	64.7	-179.5	0.04	29.0	0.5841
3	-113.7	179.5	0.14	24.5	0.4789
4	-113.1	0.3	0.41	15.5	0.5555
Boltzmann					0.5276