molecules

MDPI

Supplementary Materials

Synthesis of 3-O-palmitoyl-silybin, a new-to-nature antioxidant flavonolignan with increased protective action against oxidative damages in lipophilic media

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Table S1. *in silico* evaluation of Log K_{ow}

	Log K_{ow} *
Silybin	2.58 ± 0.59
Silybinyl palmitate	10.72 ± 0.60
Ascorbic acid	-2.41 ± 0.45
Ascorbyl palmitate	6.06 ± 0.59

* evaluated *in silico* using ACD/LogP DB; Note that according to PubChem, Log K_{ow} for BHA is equal to 3.06

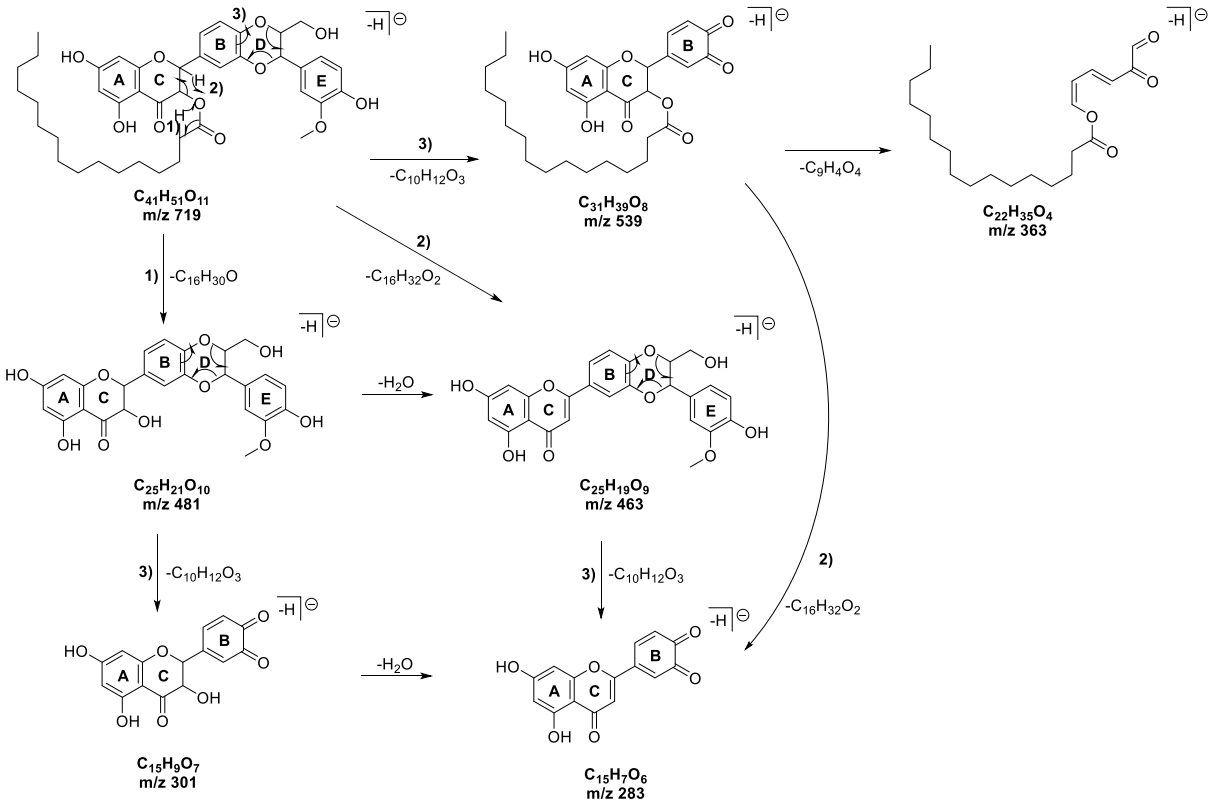


Figure S1. Proposed fragmentation pathway based on MS/MS of $[M-H]^-$ ion at m/z 719 corresponding to compound **2**

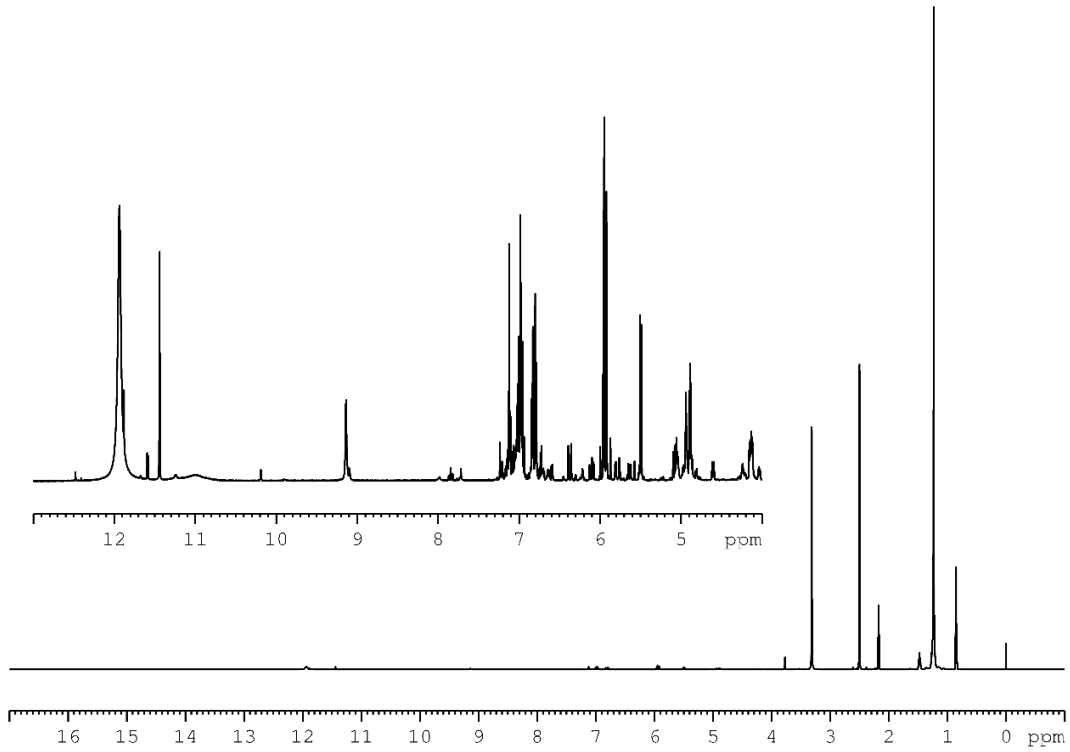


Figure S2. ^{1}H NMR spectrum of 3-O-palmitoylsilybin 2 (600 MHz, DMSO-d_6, 300K)

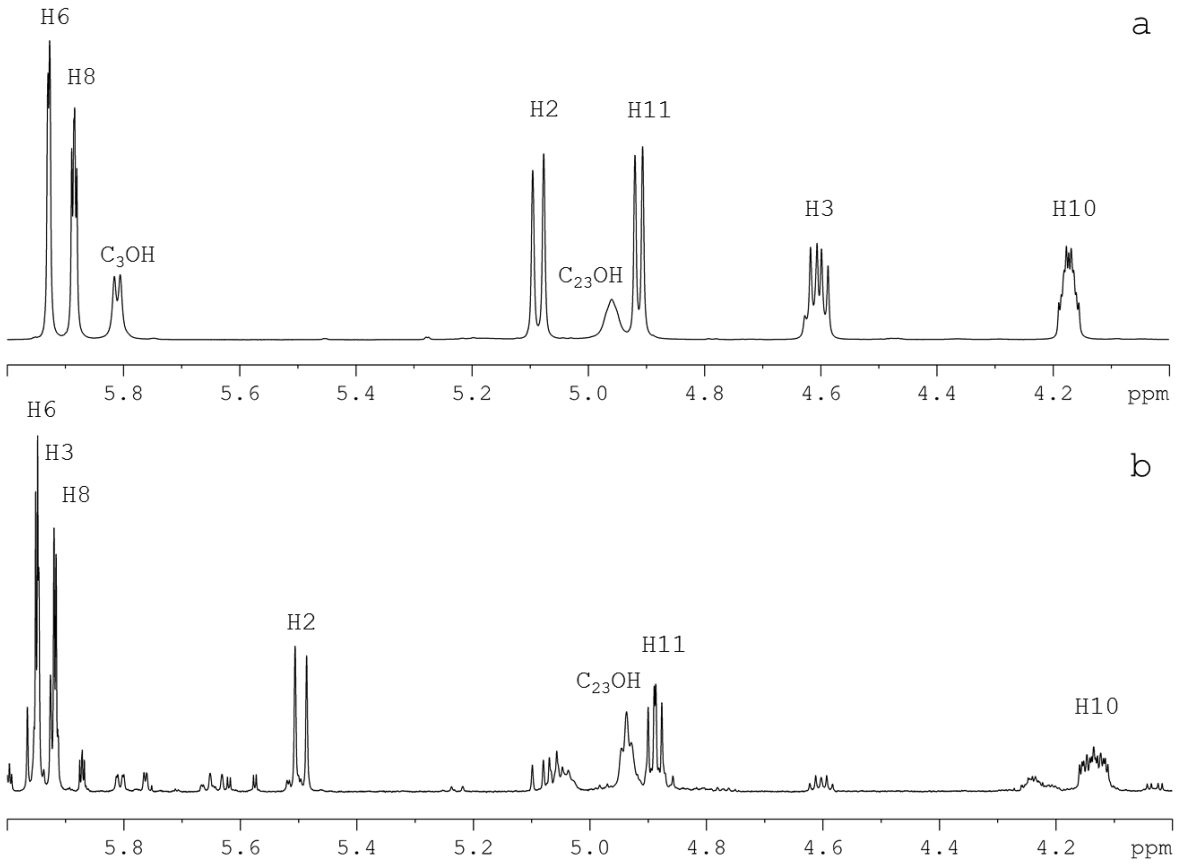


Figure S3. Partial ^{1}H NMR spectrum of silybin (a) and 3-O-palmitoylsilybin (b) (600 MHz, DMSO-d_6, 300K)

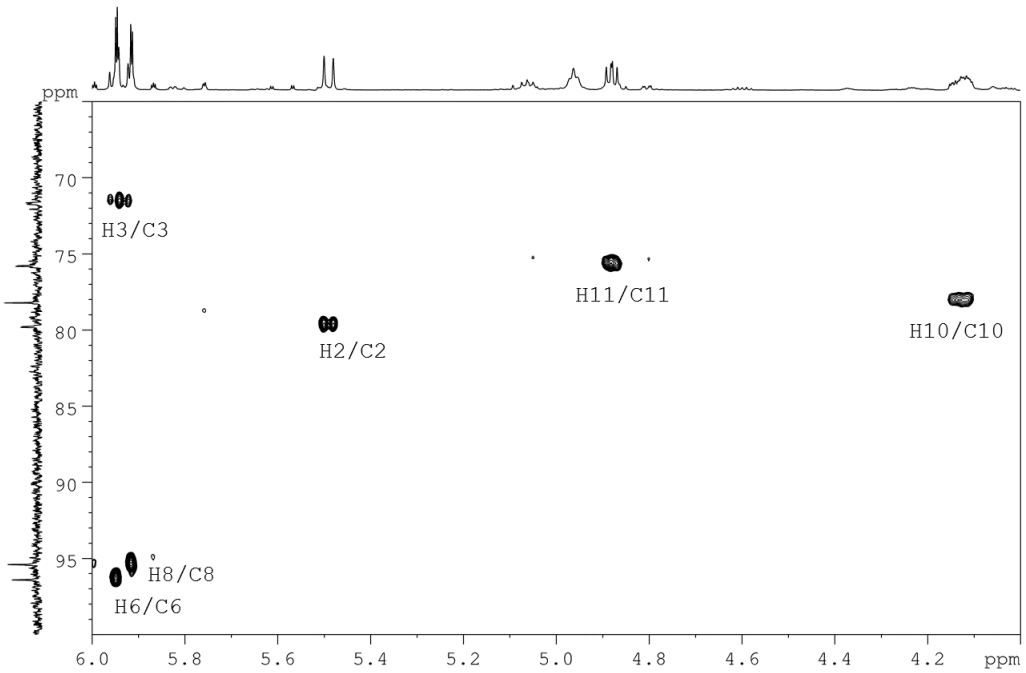


Figure S4. Partial HSQC spectrum of 3-O-palmitoylsilybin (**2**) (600 MHz, DMSO-d_6, 300K)

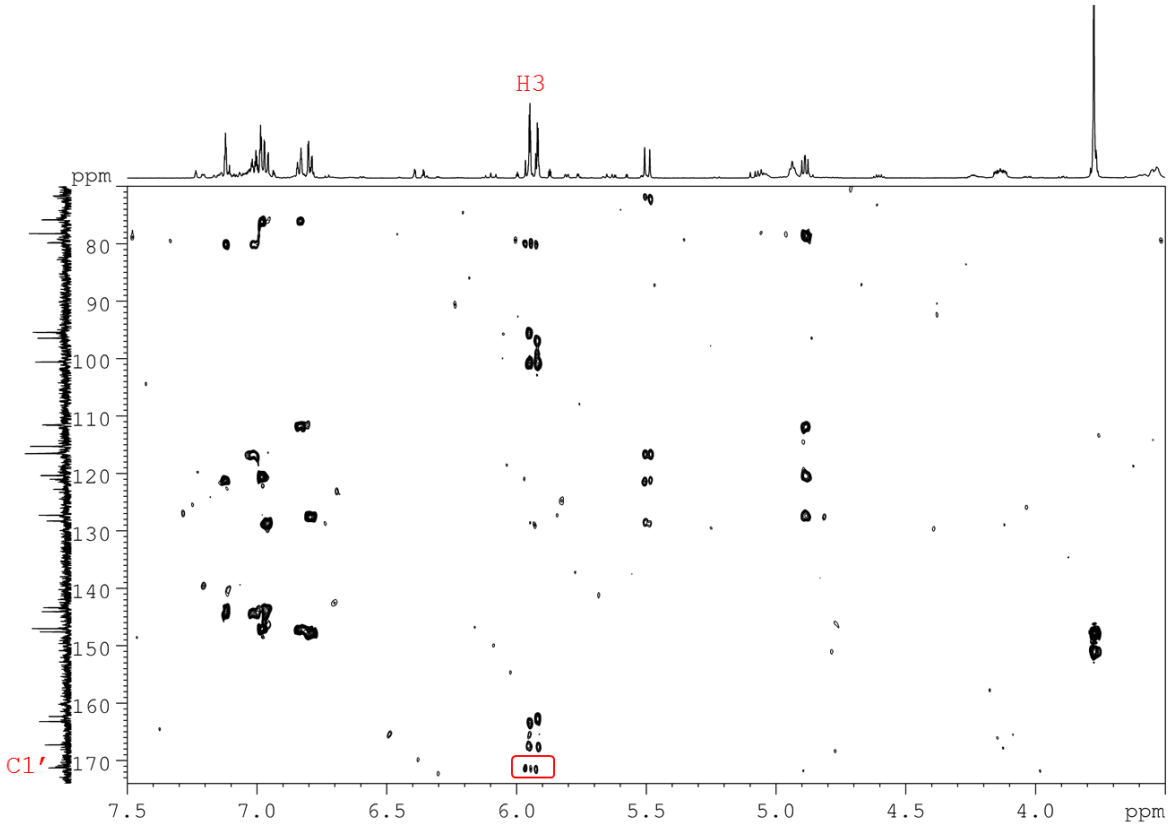
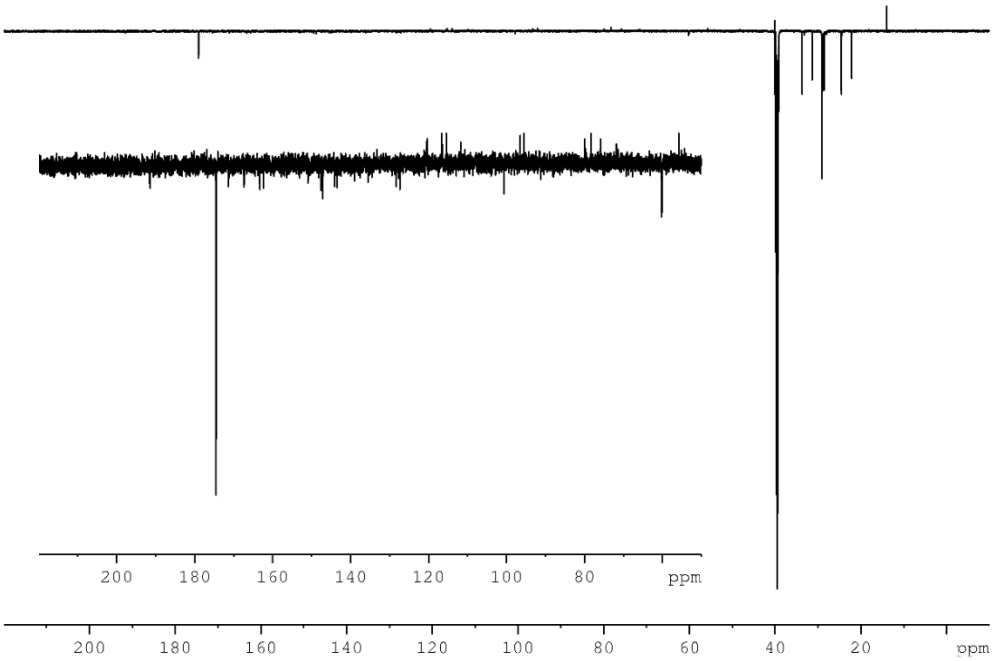


Figure S5. Partial HMBC spectrum of 3-O-palmitoylsilybin (**2**) with H3/C1' long range correlation highlighted by the red box (600 MHz, DMSO-d_6, 300K)

64



65

66 **Figure S6.** ^{13}C NMR (DEPTQ) spectrum of 3-O-palmitoylsilybin **2** (150 MHz, DMSO-d_6, 300K)

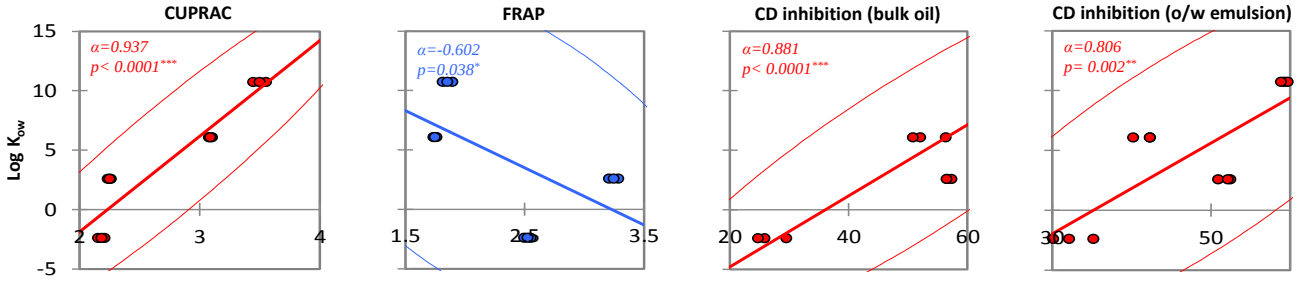


Figure S7. Pearson correlation analysis linking Log K_{ow} to CUPRAC and FRAP assays, and CD production inhibition in bulk oil and o/w emulsion