

1 Supplementary Materials

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

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27 **Table S1.** *in silico* evaluation of Log K<sub>ow</sub>

28 **Figure S1.** Proposed fragmentation pathway based on MS/MS of [M-H]<sup>-</sup> ion at m/z 719 corresponding  
29 to compound 2

30 **Figure S2.** <sup>1</sup>H NMR spectrum of 3-O-palmitoylsilybin 2 (600 MHz, DMSO-d<sub>6</sub>, 300K)

31 **Figure S3.** Partial <sup>1</sup>H NMR spectrum of silybin (a) and 3-O-palmitoylsilybin (b) (600 MHz, DMSO-d<sub>6</sub>,  
32 300K)

33 **Figure S4.** Partial HSQC spectrum of 3-O-palmitoylsilybin (2) (600 MHz, DMSO-d<sub>6</sub>, 300K)

34 **Figure S5.** Partial HMBC spectrum of 3-O-palmitoylsilybin (2) with H3/C1' long range correlation  
35 highlighted by the red box (600 MHz, DMSO-d<sub>6</sub>, 300K)

36 **Figure S6.** <sup>13</sup>C NMR (DEPTQ) spectrum of 3-O-palmitoylsilybin 2 (150 MHz, DMSO-d<sub>6</sub>, 300K)

37 **Figure S7.** Pearson correlation analysis linking Log K<sub>ow</sub> to CUPRAC assay, FRAP assay and CD  
38 production inhibition in bulk oil and o/w emulsion

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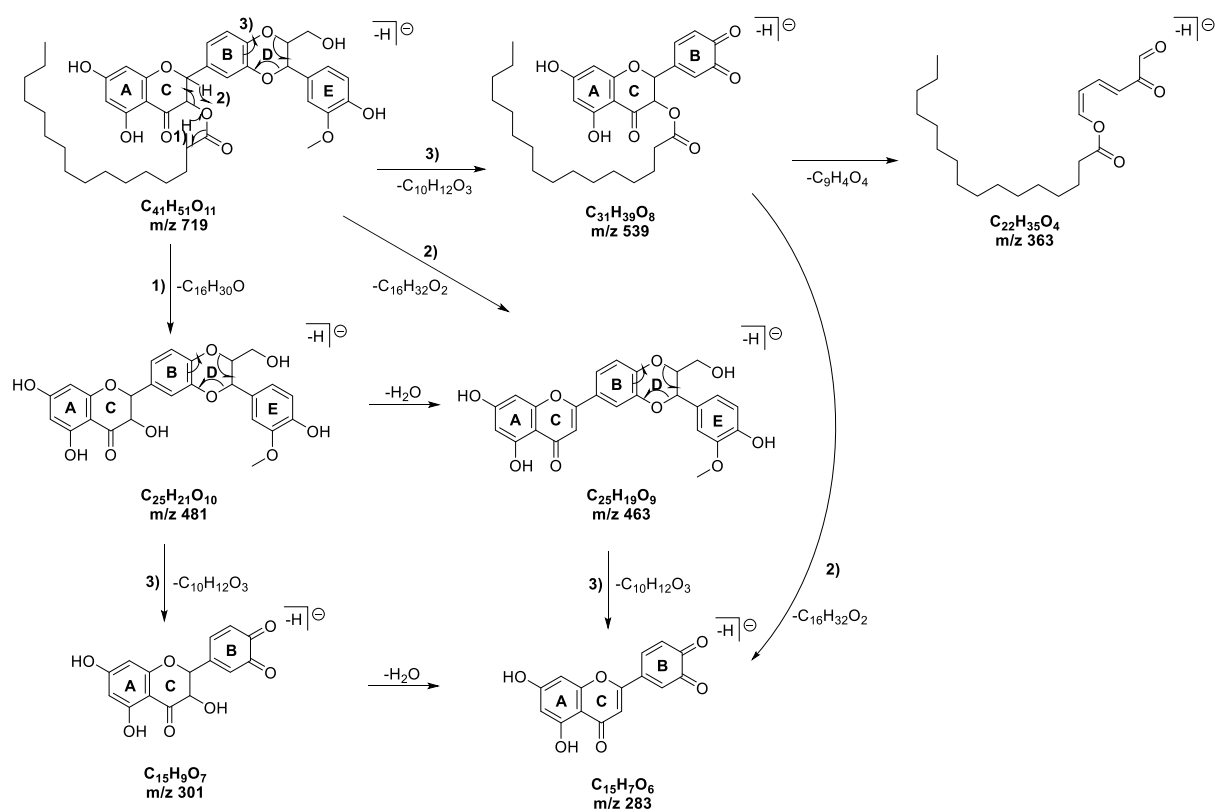
**Table S1.** *in silico* evaluation of Log K<sub>ow</sub>

	Log K <sub>ow</sub> *
Silybin	2.58 ± 0.59
Silybinyl palmitate	10.72 ± 0.60
Ascorbic acid	-2.41 ± 0.45
Ascorbyl palmitate	6.06 ± 0.59

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\* evaluated *in silico* using ACD/LogP DB; Note that according to PubChem, Log K<sub>ow</sub> for BHA is equal to 3.06

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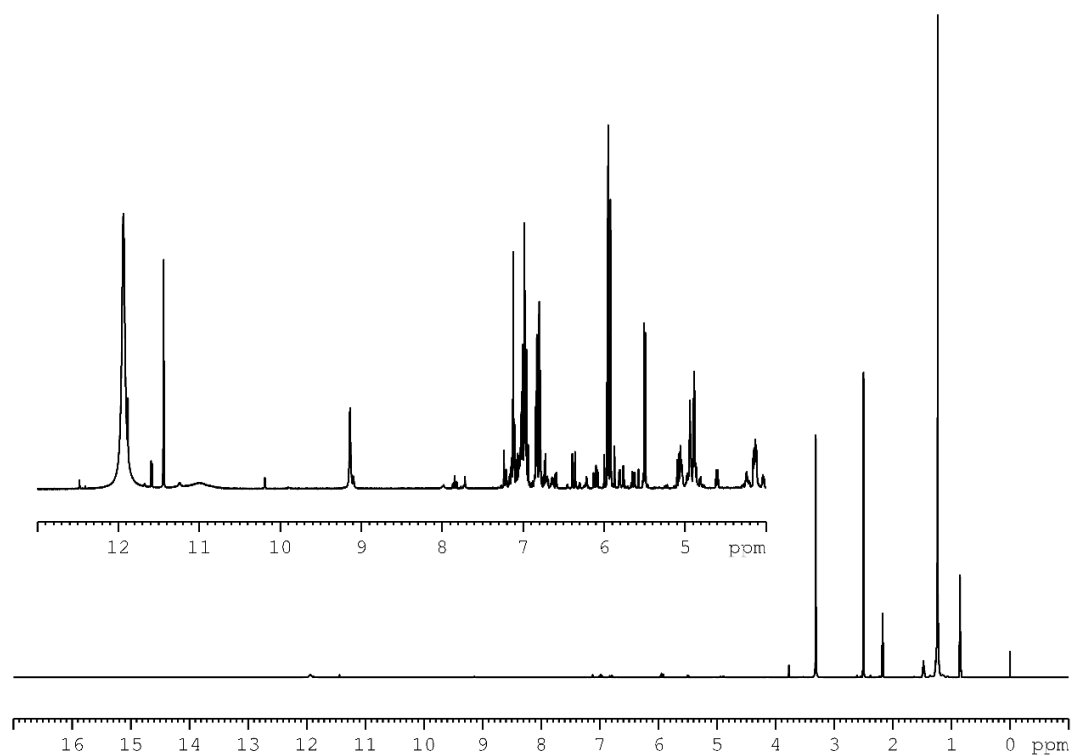
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**Figure S1.** Proposed fragmentation pathway based on MS/MS of  $[M-H]^-$  ion at  $m/z$  719 corresponding to compound 2

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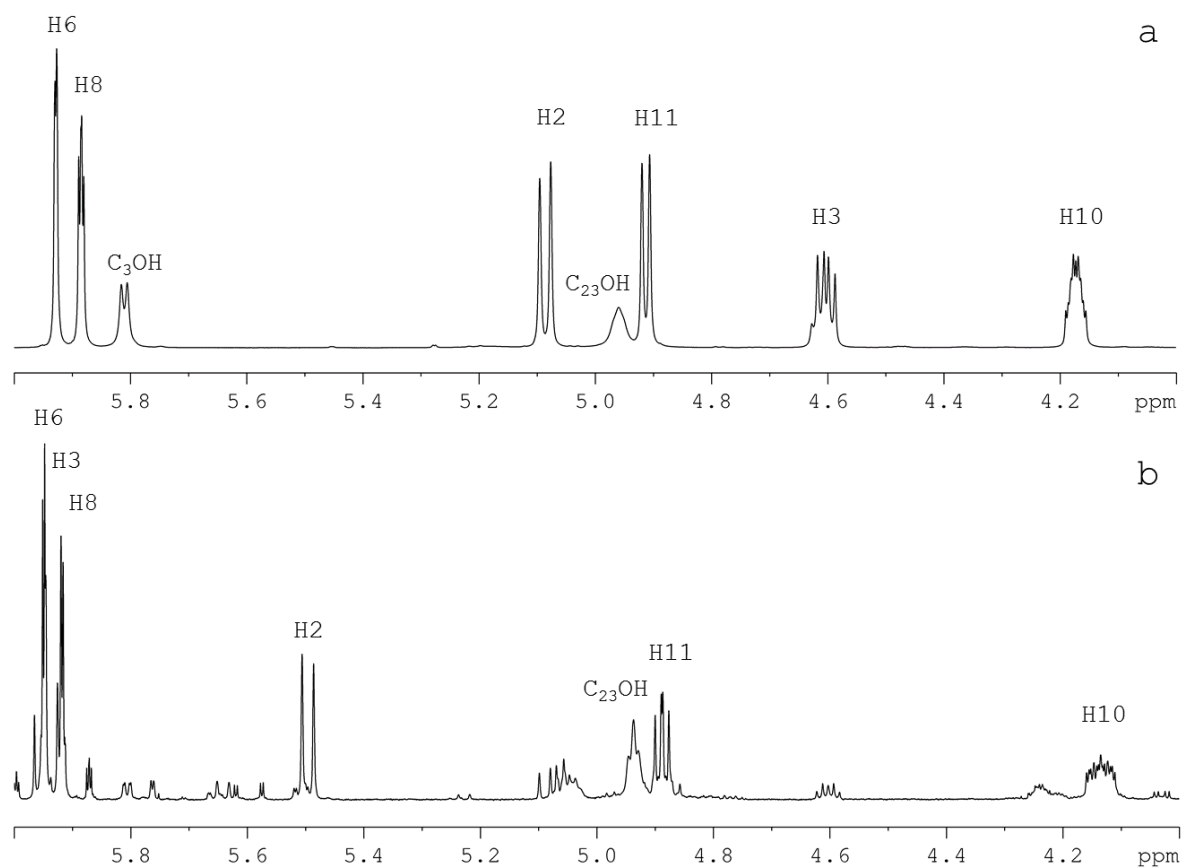


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**Figure S2.**  $^1\text{H}$  NMR spectrum of 3-O-palmitoylsilybin 2 (600 MHz,  $\text{DMSO-d}_6$ , 300K)

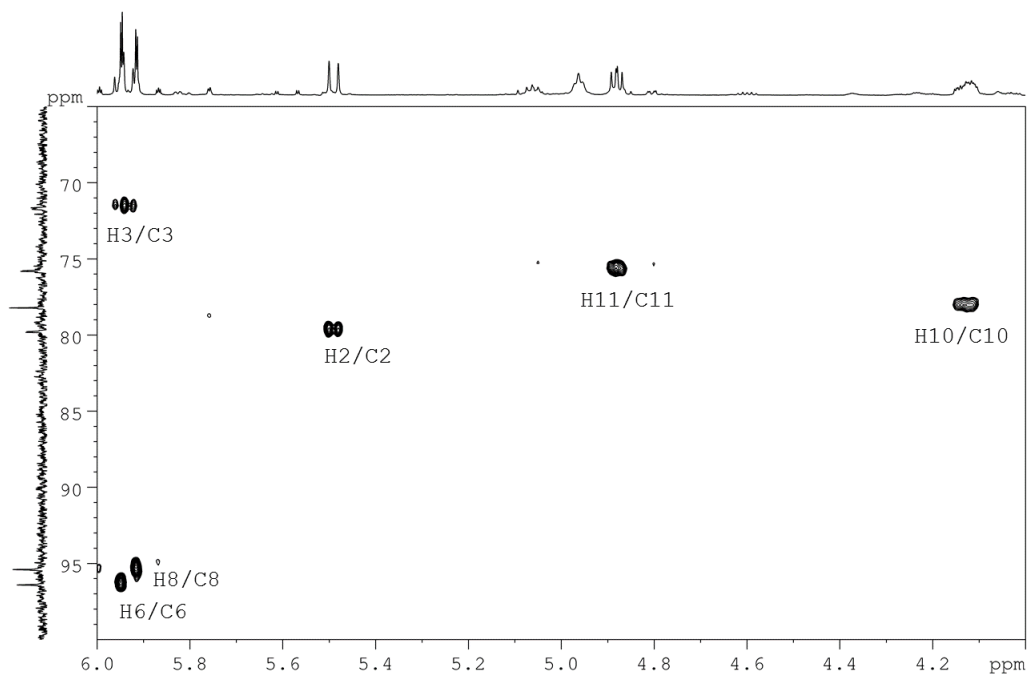


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53 **Figure S3.** Partial  $^1\text{H}$  NMR spectrum of silybin (a) and 3-O-palmitoysilybin (b) (600 MHz,  $\text{DMSO-d}_6$ , 300K)

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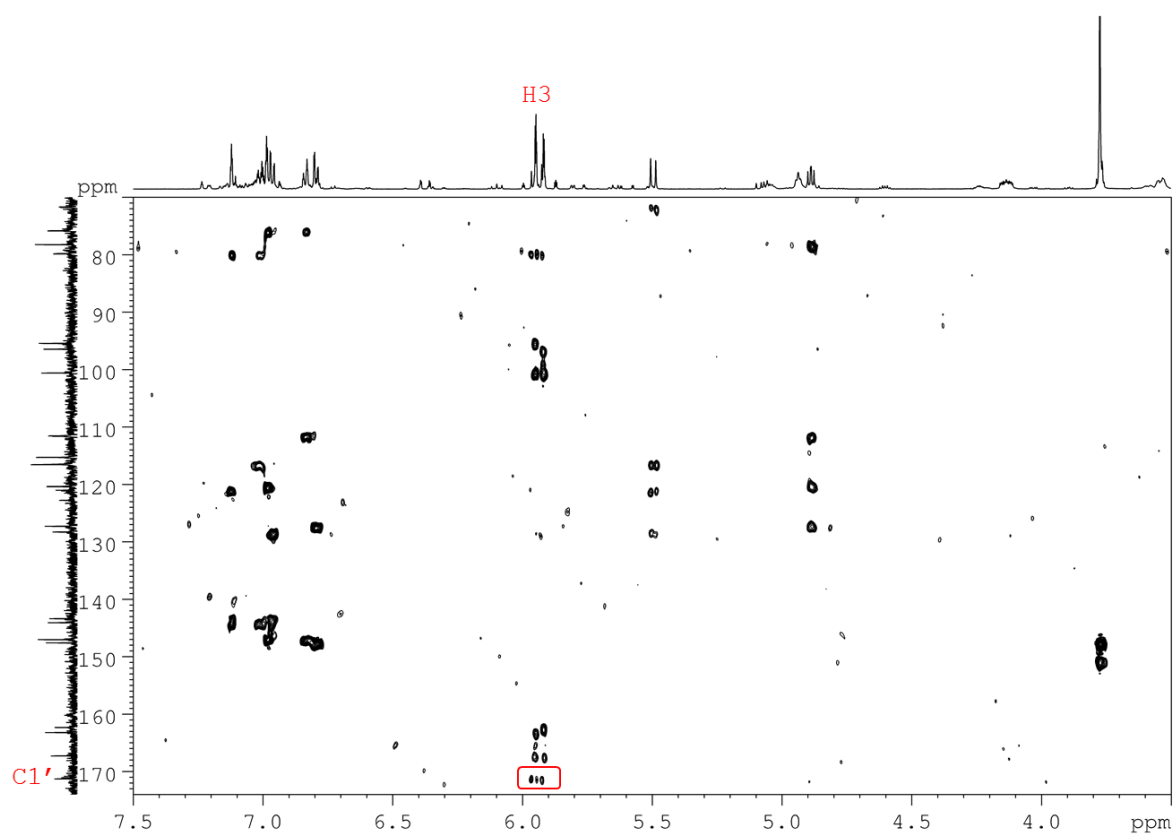
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**Figure S4.** Partial HSQC spectrum of 3-O-palmitoylsilybin (2) (600 MHz, DMSO-d<sub>6</sub>, 300K)

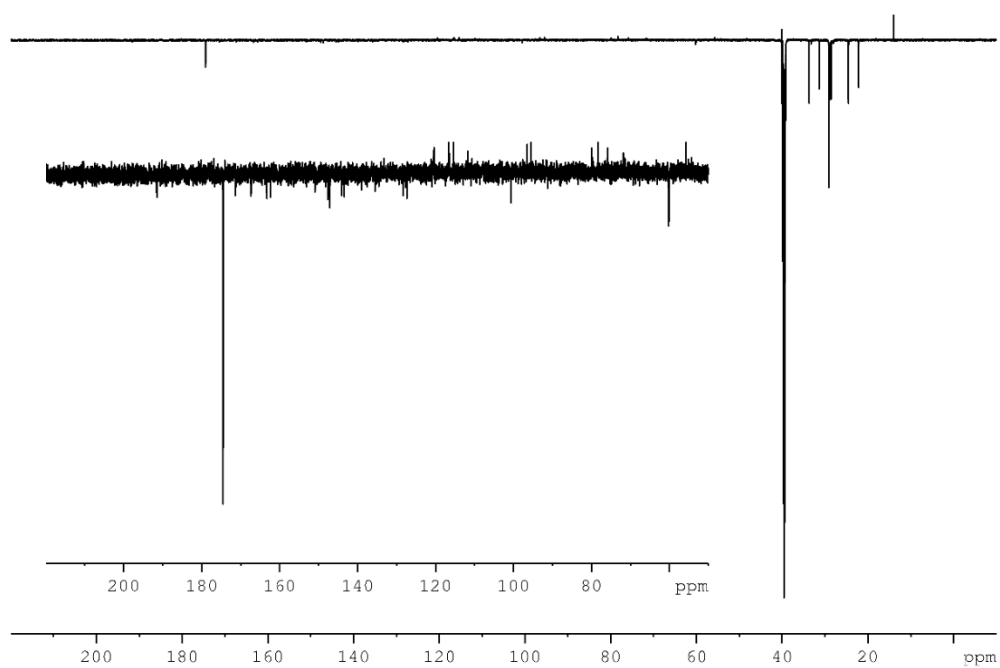
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**Figure S5.** Partial HMBC spectrum of 3-O-palmitoylsilybin (**2**) with H3/C1' long range correlation highlighted by the red box (600 MHz, DMSO-d<sub>6</sub>, 300K)

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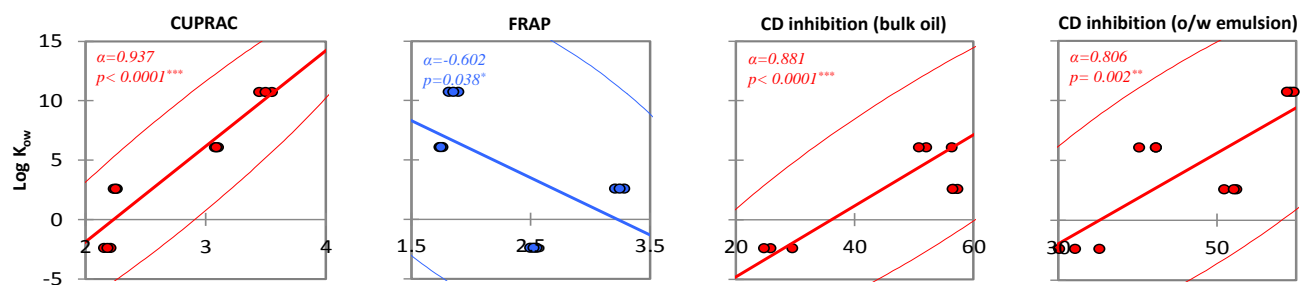


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**Figure S6.**  $^{13}\text{C}$  NMR (DEPTQ) spectrum of 3-O-palmitoylsilybin 2 (150 MHz,  $\text{DMSO-d}_6$ , 300K)





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**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



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