

SUPPLEMENTARY MATERIAL

MICROWAVE SYNTHESIS OF NOVEL CHENODEOXYCHOLIC ACID ESTERS AND COMPARATIVE STUDY OF CHROMATOGRAPHIC BEHAVIOR AND LIPOPHILICITY

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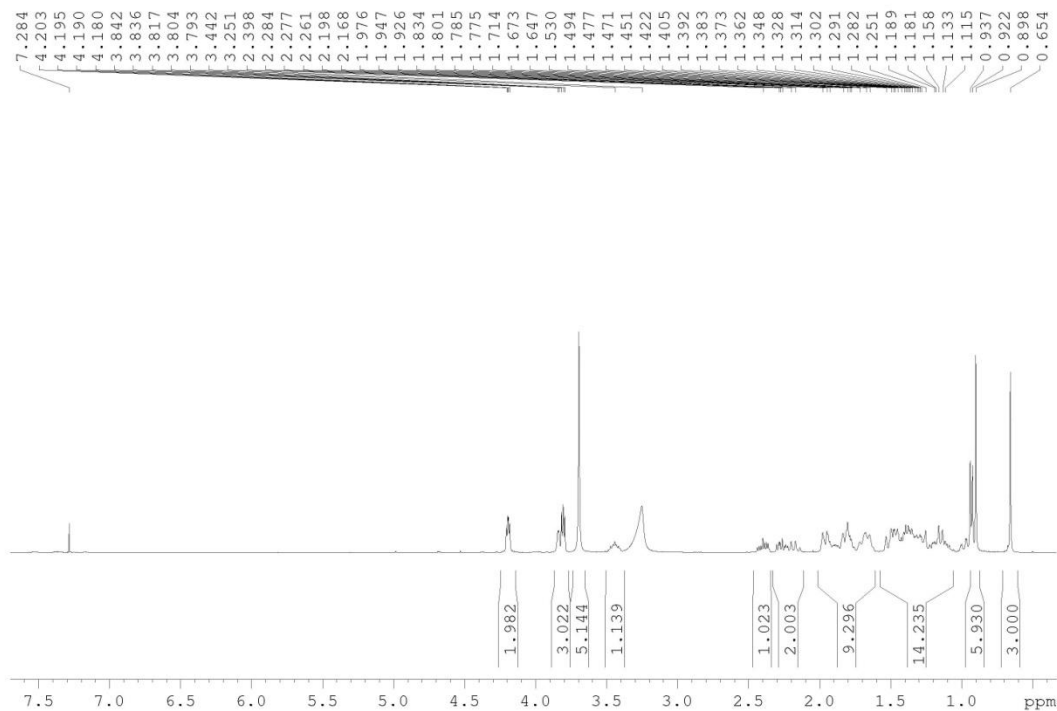
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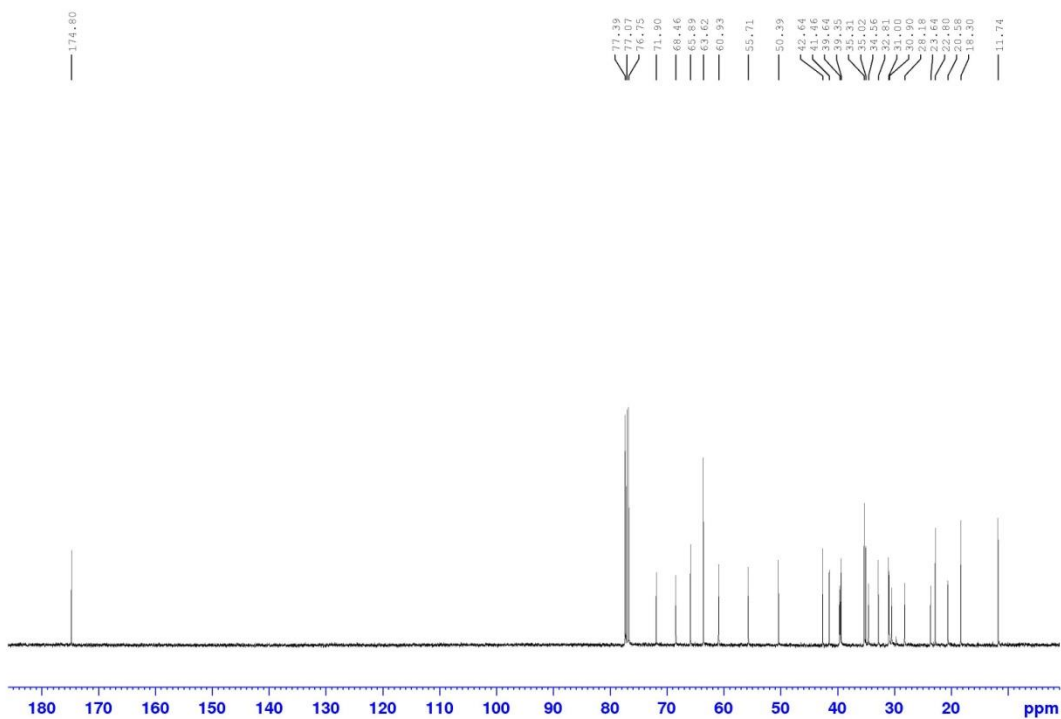
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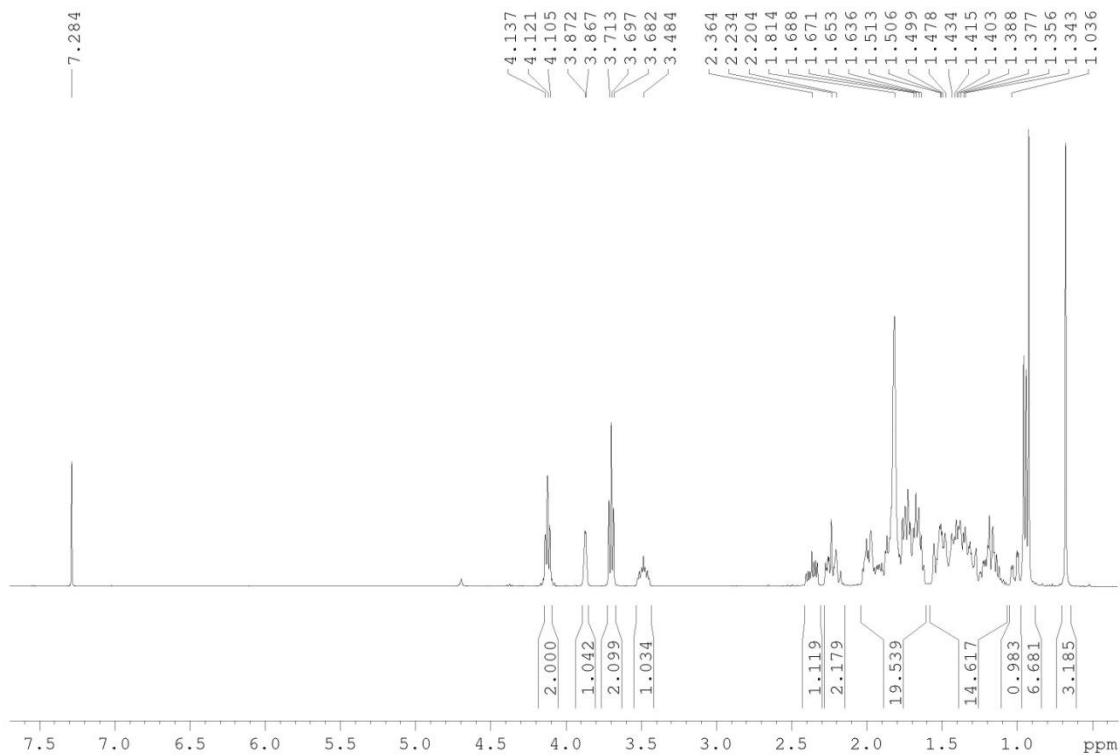
¹H NMR and ¹³C NMR spectra



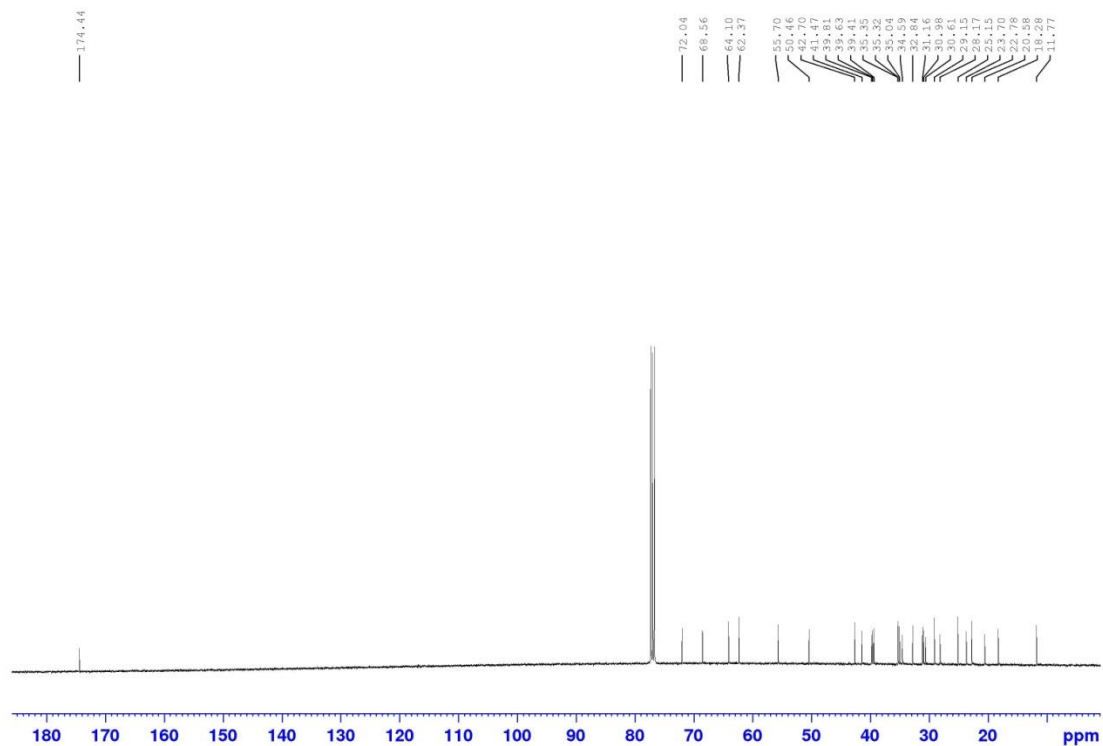
¹H NMR (250 MHz, CDCl₃) of 2'-hydroxyethyl 3α,7α-dihydroxy-5β-cholan-24-oate (1)



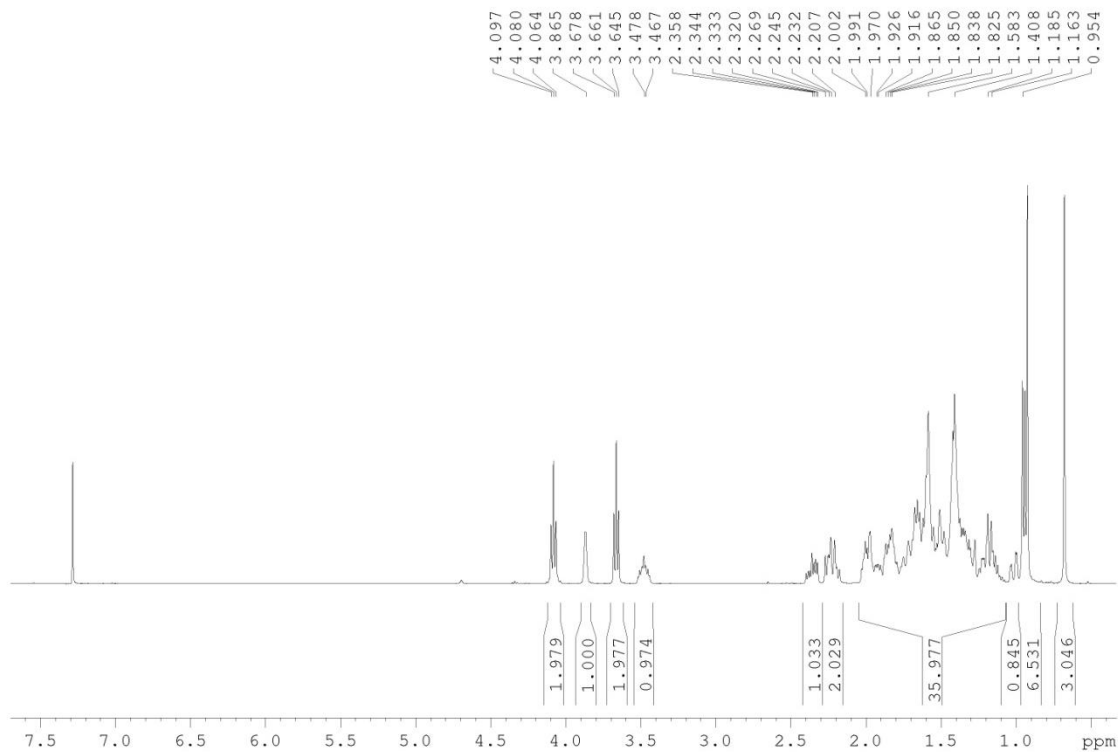
^{13}C NMR (62.9 MHz, CDCl_3) of 2'-hydroxyethyl 3 α ,7 α -dihydroxy-5 β -cholan-24-oate (**1**)



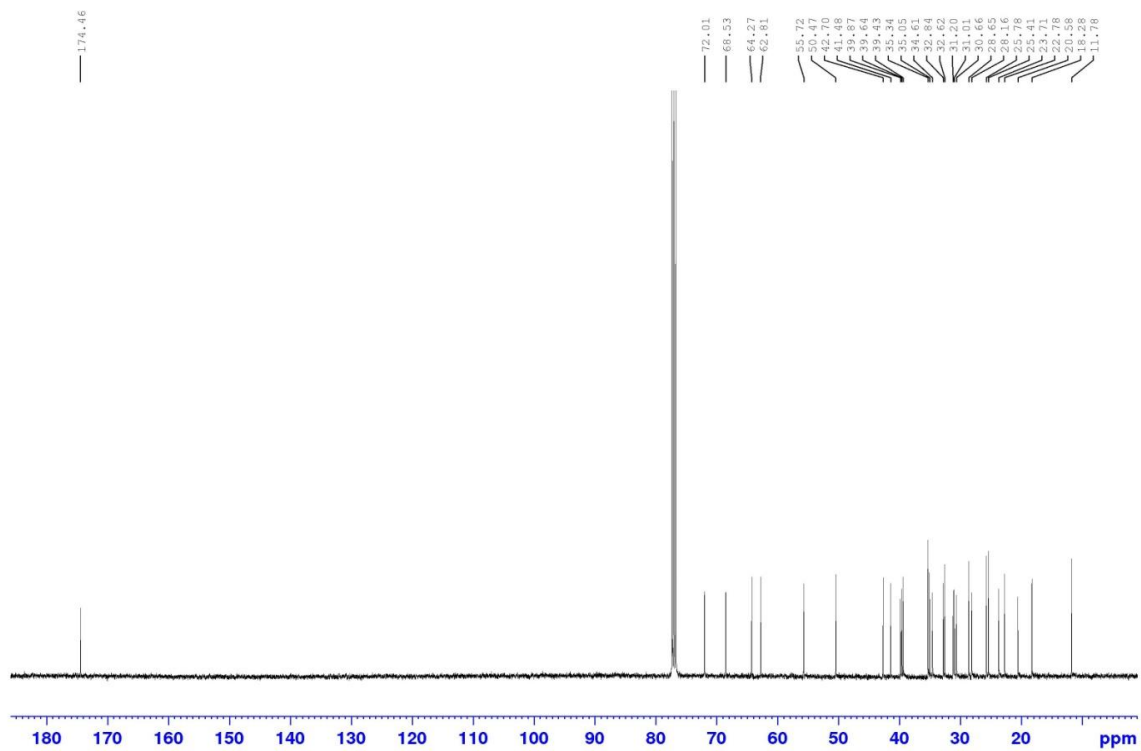
^1H NMR (250 MHz, CDCl_3) of 4'-hydroxybutyl 3 α ,7 α -dihydroxy-5 β -cholan-24-oate (**2**)



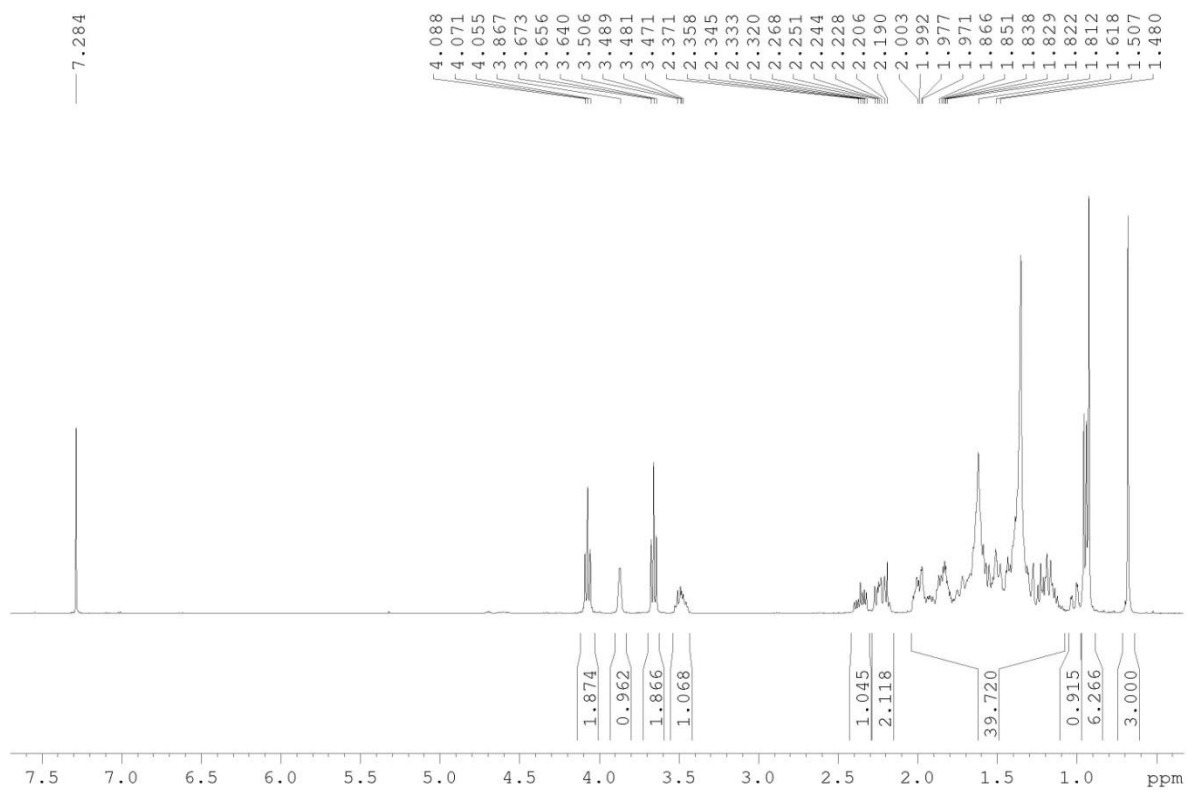
^{13}C NMR (62.9 MHz, CDCl_3) of 4'-hydroxybutyl 3 α ,7 α -dihydroxy-5 β -cholan-24-oate (2)



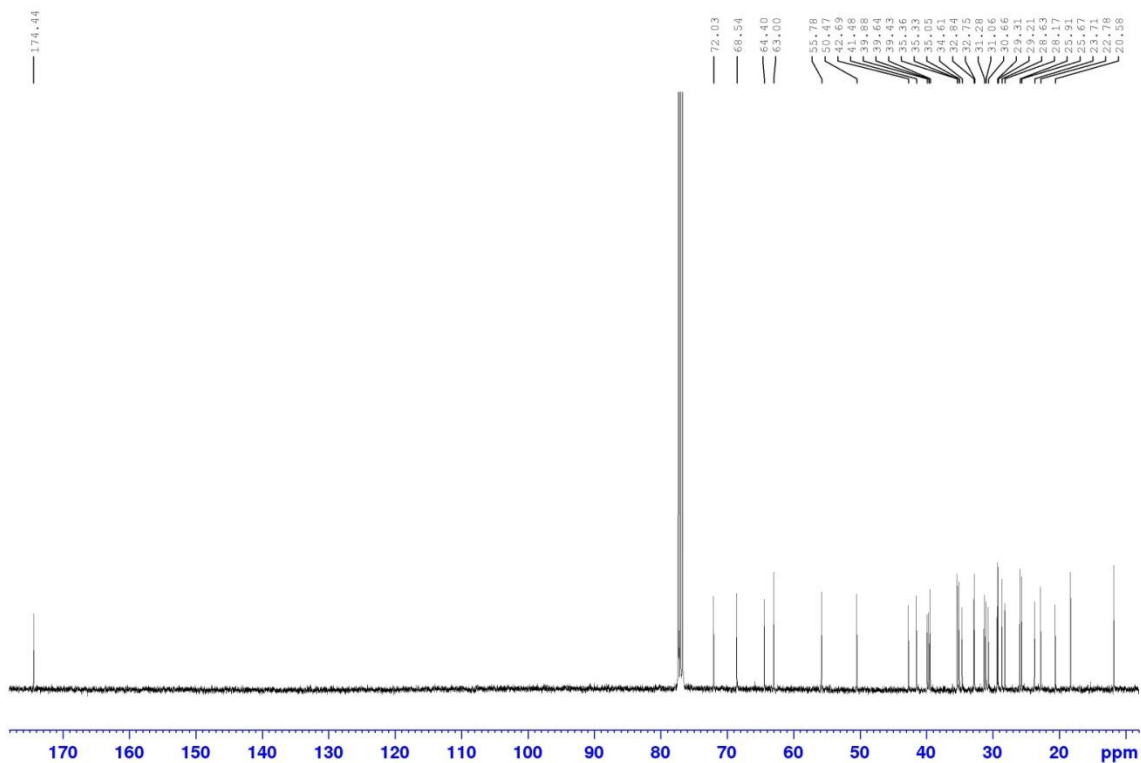
^1H NMR (250 MHz, CDCl_3) of 6'-hydroxyhexyl $3\alpha,7\alpha$ -dihydroxy- 5β -cholan-24-oate (**3**)



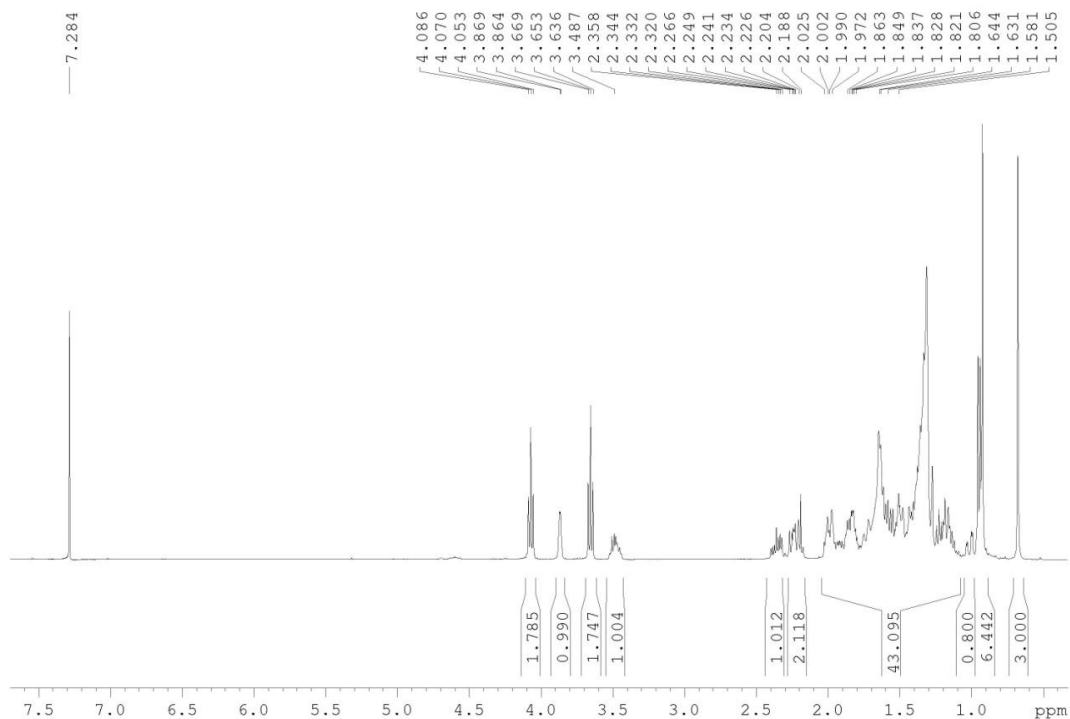
^{13}C NMR (62.9 MHz, CDCl_3) of 6'-hydroxyhexyl $3\alpha,7\alpha$ -dihydroxy- 5β -cholan-24-oate (**3**)



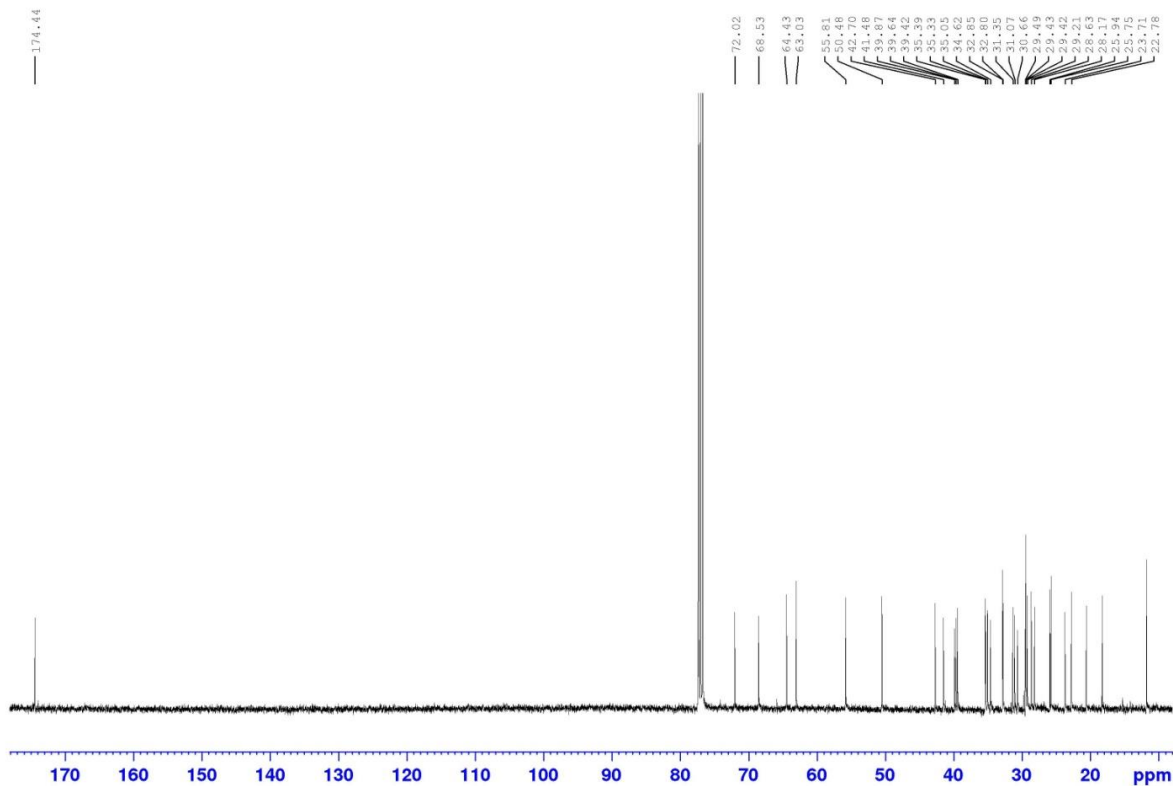
^1H NMR (250 MHz, CDCl_3) of 8'-hydroxyoctyl 3 α ,7 α -dihydroxy-5 β -cholan-24-oate (**4**)



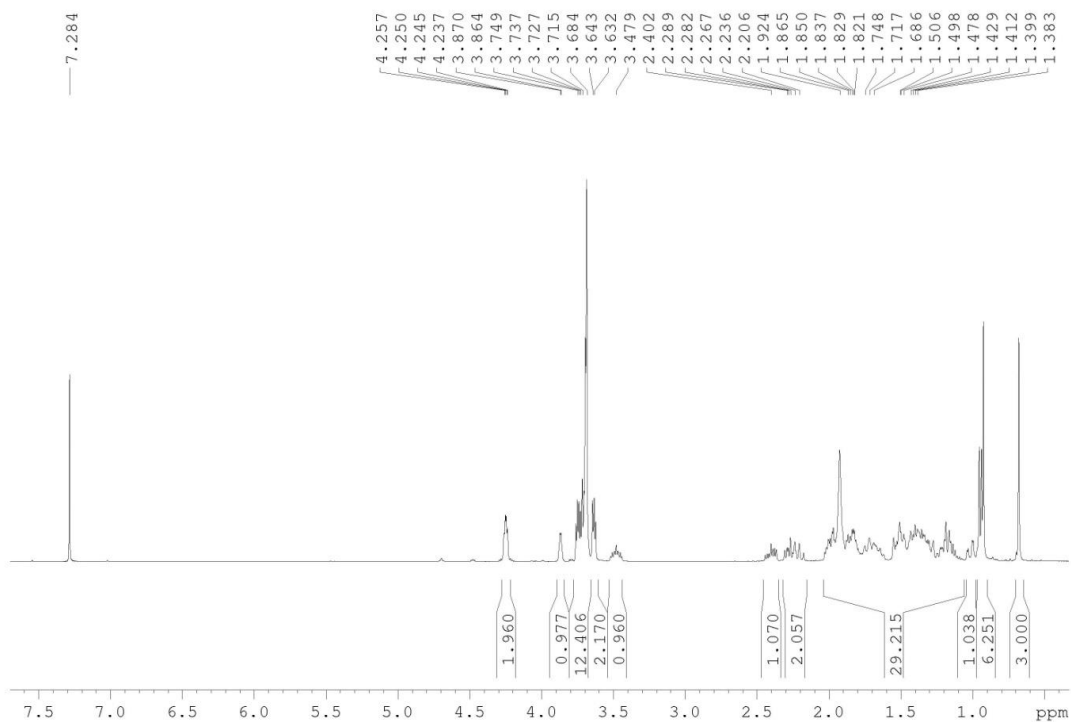
^{13}C NMR (62.9 MHz, CDCl_3) of 8^l-hydroxyoctyl 3 α ,7 α -dihydroxy-5 β -cholan-24-oate (4)



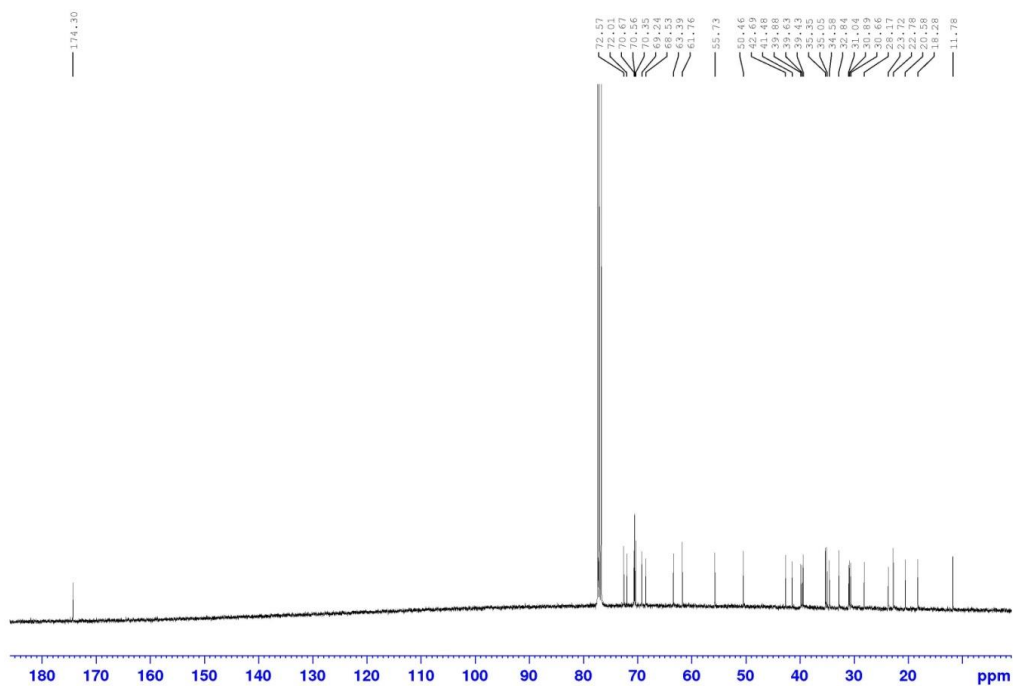
^1H NMR (250 MHz, CDCl_3) of 10^l-hydroxydecyl 3 α ,7 α -dihydroxy-5 β -cholan-24-oate (5)



^{13}C NMR (62.9 MHz, CDCl_3) of 10'-hydroxydecyl $3\alpha,7\alpha$ -dihydroxy- 5β -cholan-24-oate (5)



^1H NMR (250 MHz, CDCl_3) of 12'-hydroxy-1,4,7,10-tetraoxadodecyl $3\alpha,7\alpha$ -dihydroxy- 5β -cholan-24-oate (6)



^{13}C NMR (62.9 MHz, CDCl_3) of 12'-hydroxy-1,4,7,10-tetraoxadodecyl 3 α ,7 α -dihydroxy-5 β -cholan-24-oate (6)

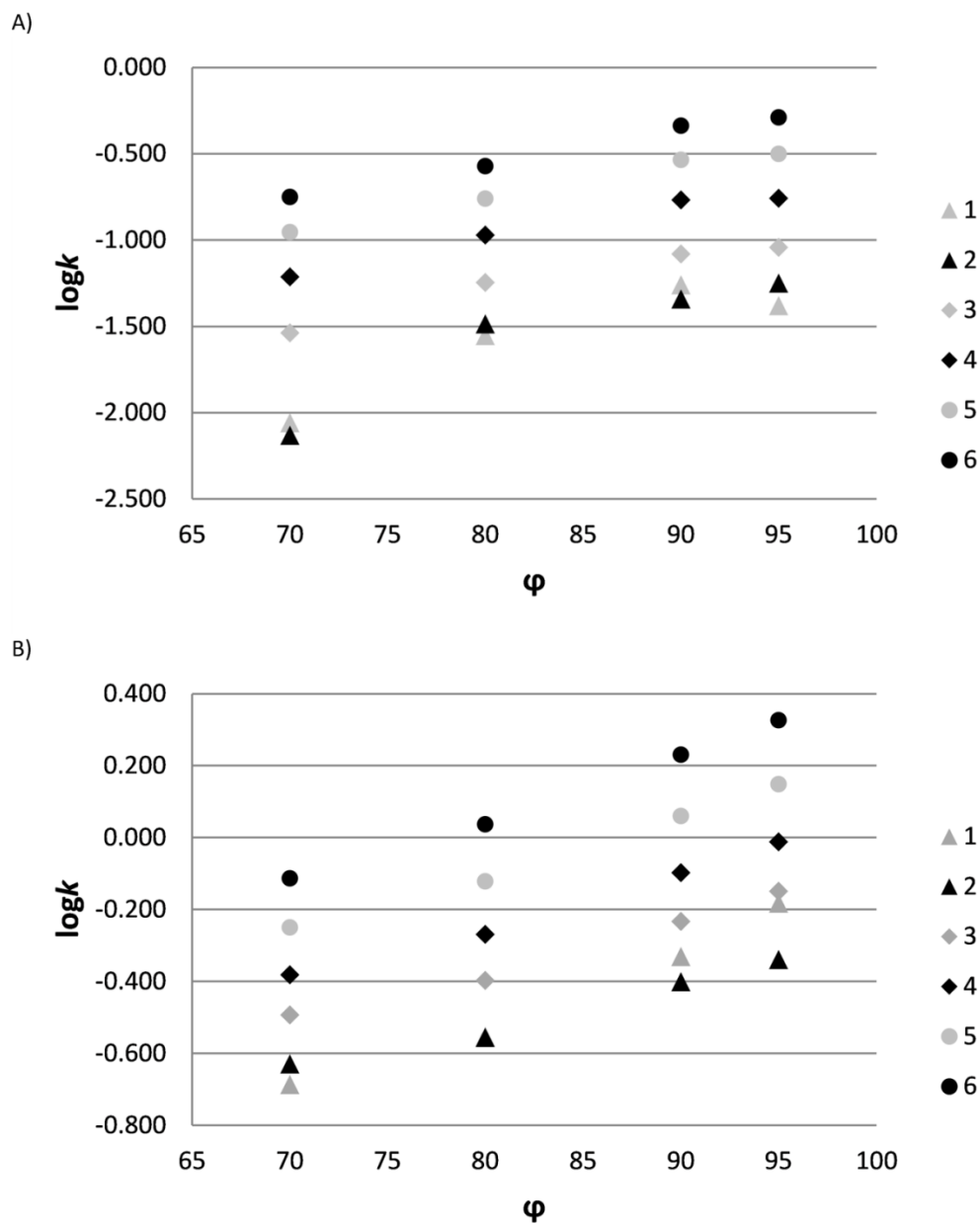


Figure S1 Logarithm of the retention factor ($\log k$) for different methanol-2-propanol (A) and acetonitrile-2-propanol (B) volume fractions.

Table S1A. (¹MarvinSketch 17.2.3; ²ChemBioDraw Ultra 12.0; ³ChemBio3D Ultra 12.0; ⁴ALOGPS 2.1).

Compound	logP ¹	logP ²	ClogP ³	ALOGPs ⁴	AC logP ⁴	ALOGP ⁴	MLOGP ⁴	Average logP ⁴
1	2.46	3.41	4.03	3.55	3.63	3.31	2.58	3.52
2	2.96	3.88	4.23	3.35	3.82	3.70	3.69	3.94
3	3.46	4.44	4.49	3.89	4.75	4.34	4.09	4.60
4	4.25	5.27	5.55	4.56	5.68	5.26	4.48	5.32
5	5.05	6.11	6.61	5.23	6.61	6.17	4.86	6.14
6	5.84	6.94	7.66	5.85	7.53	7.08	5.23	6.94