Macedonian Journal of Chemistry and Chemical Engineering, Vol. **42**, No. 2, pp. 165–174 (2023)

SUPPLEMENTARY MATERIAL

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

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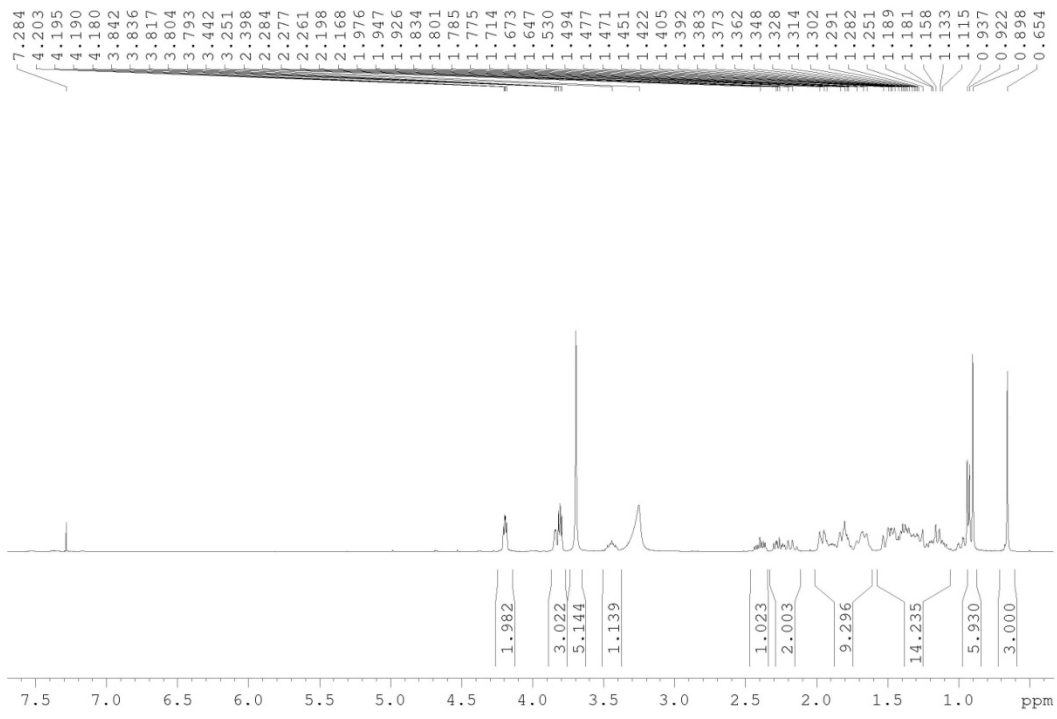
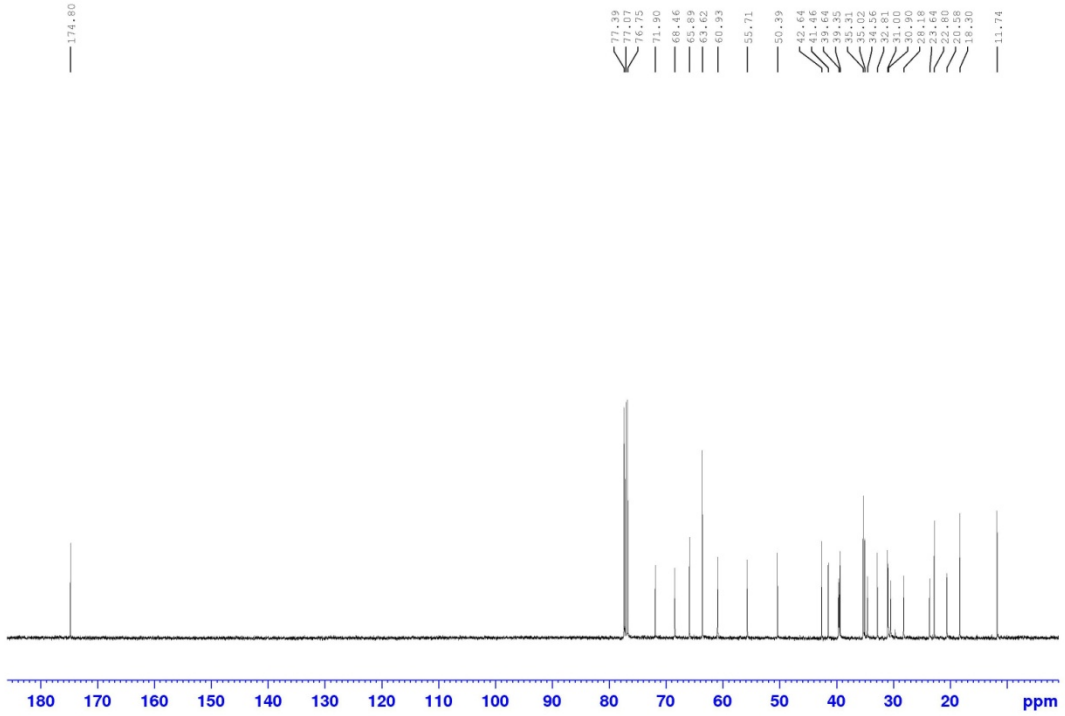
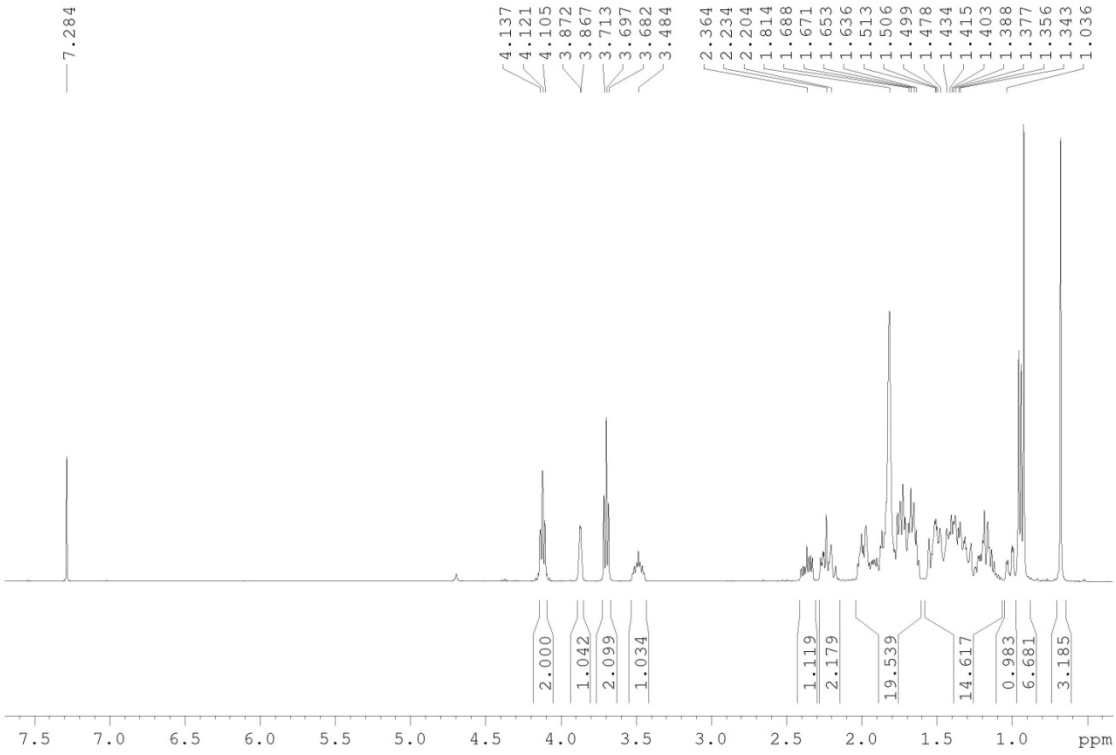
^{1}H NMR and ^{13}C NMR spectra



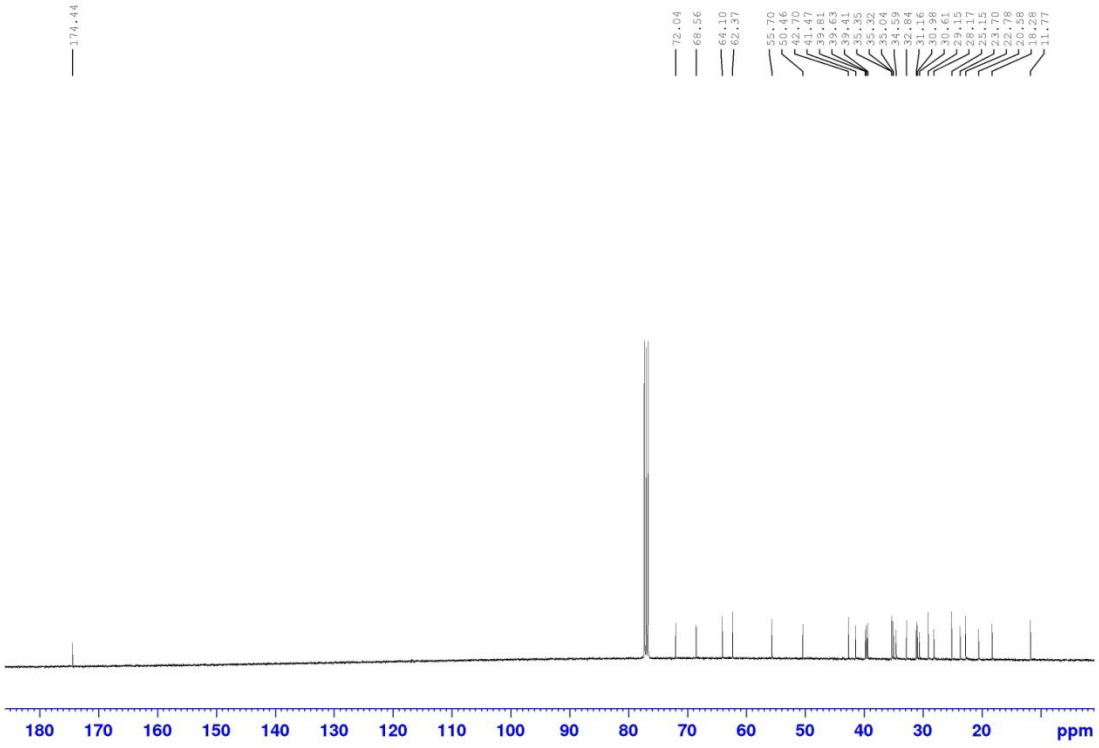
^{1}H NMR (250 MHz, $CDCl_3$) of 2'-hydroxyethyl 3α,7α-dihydroxy-5β-cholan-24-oate (**1**)



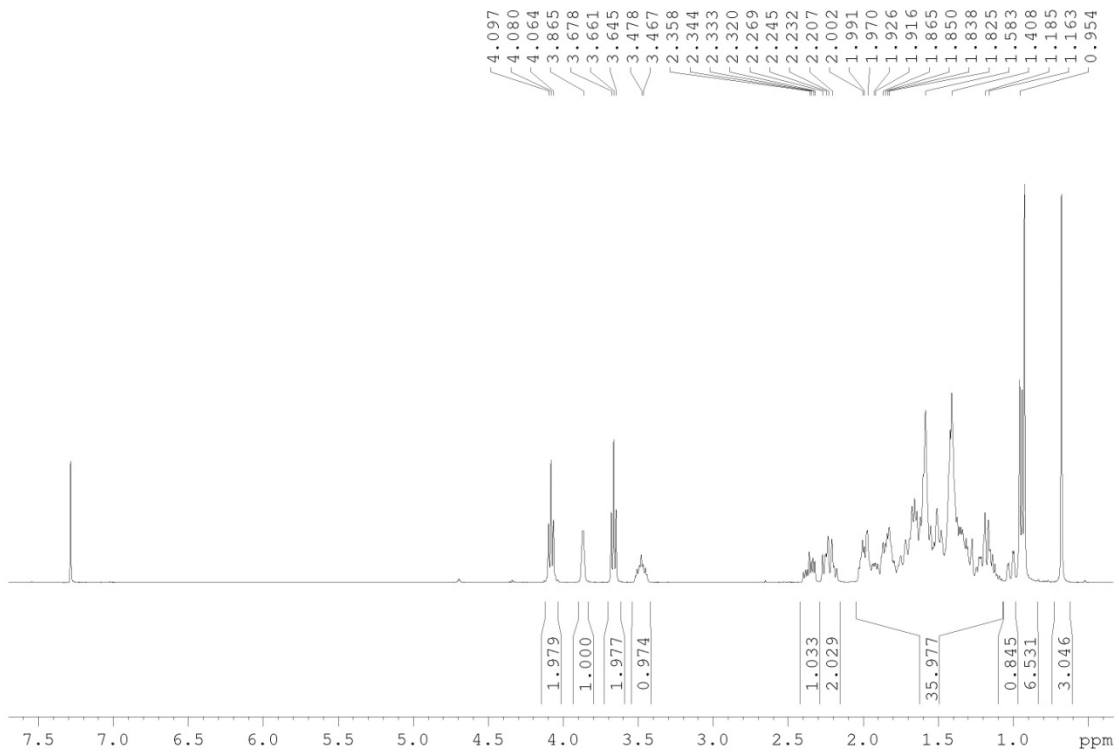
^{13}C NMR (62.9 MHz, $CDCl_3$) of 2'-hydroxyethyl 3α,7α-dihydroxy-5β-cholan-24-oate (**1**)



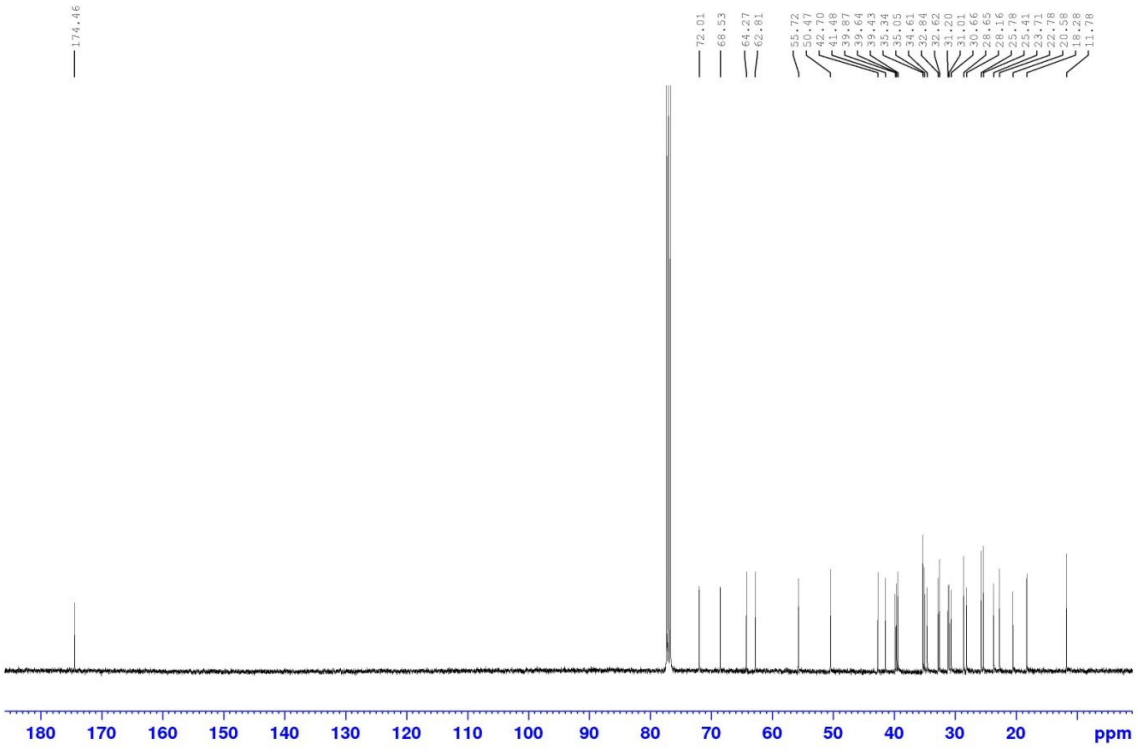
^{1}H NMR (250 MHz, $CDCl_3$) of 4'-hydroxybutyl 3α,7α-dihydroxy-5β-cholan-24-oate (**2**)



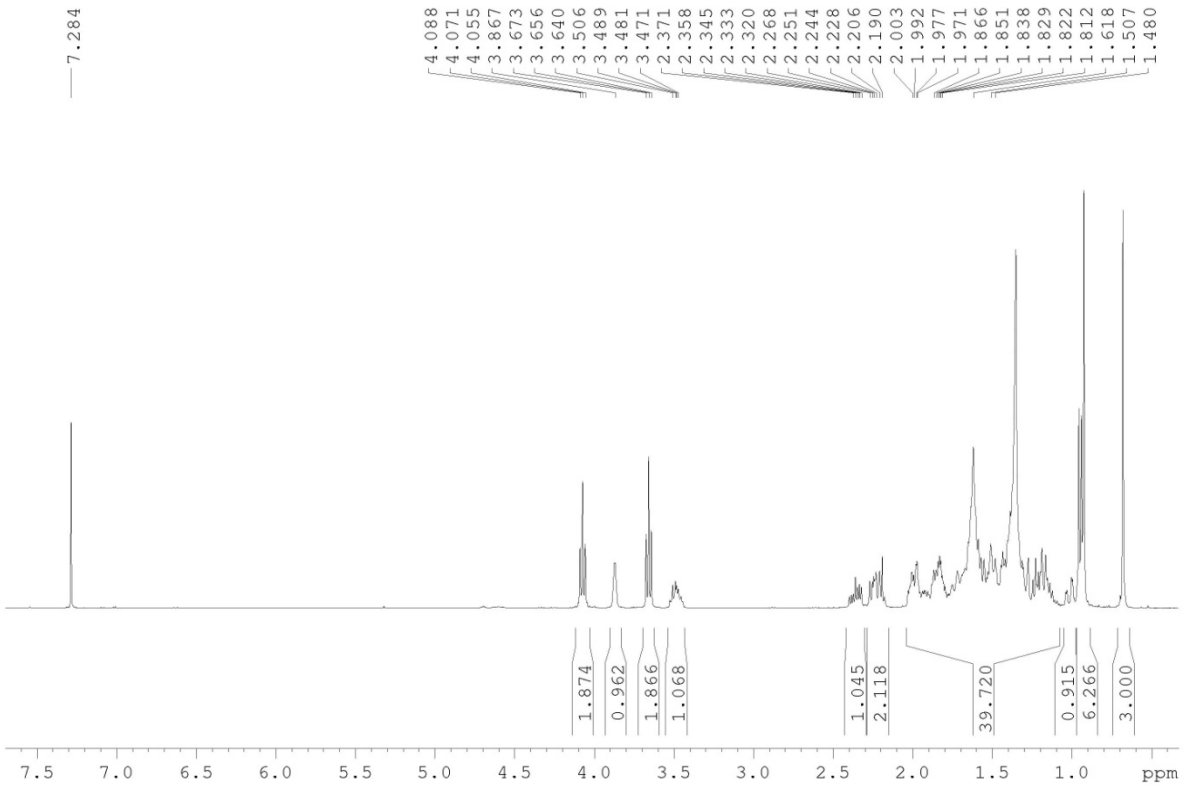
^{13}C NMR (62.9 MHz, $CDCl_3$) of 4'-hydroxybutyl 3α,7α-dihydroxy-5β-cholan-24-oate (**2**)



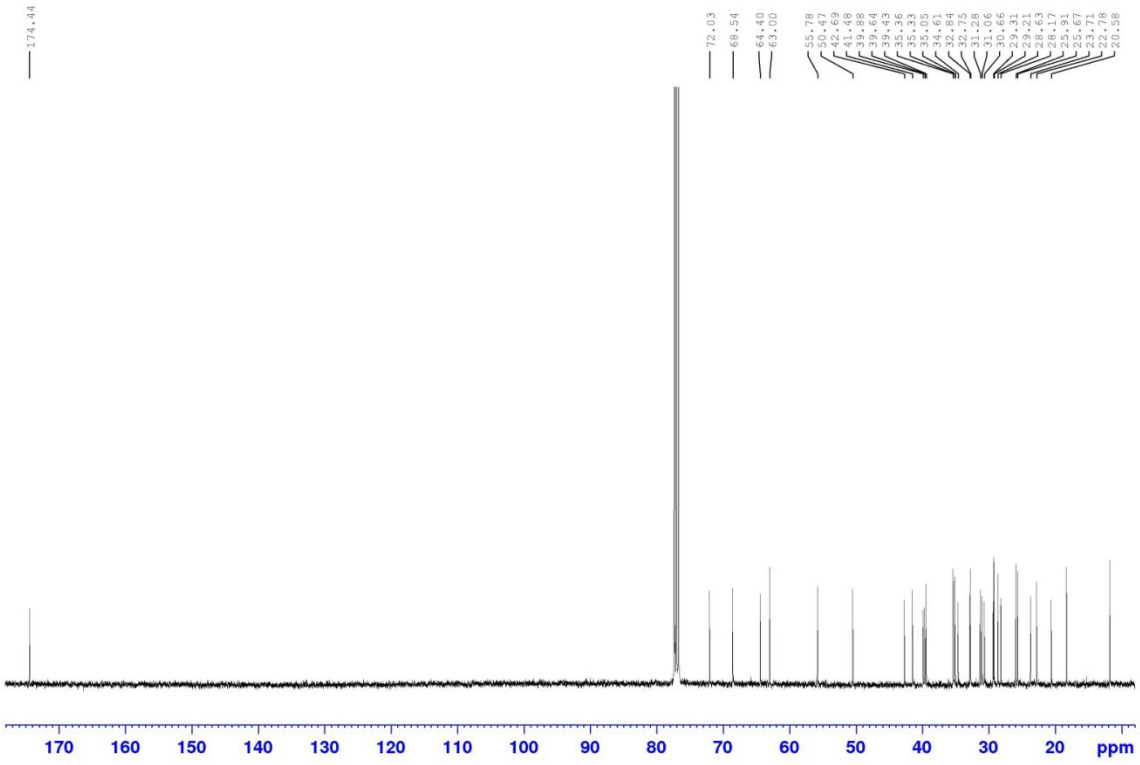
^{1}H NMR (250 MHz, $CDCl_3$) of 6'-hydroxyhexyl 3α,7α-dihydroxy-5β-cholan-24-oate (**3**)



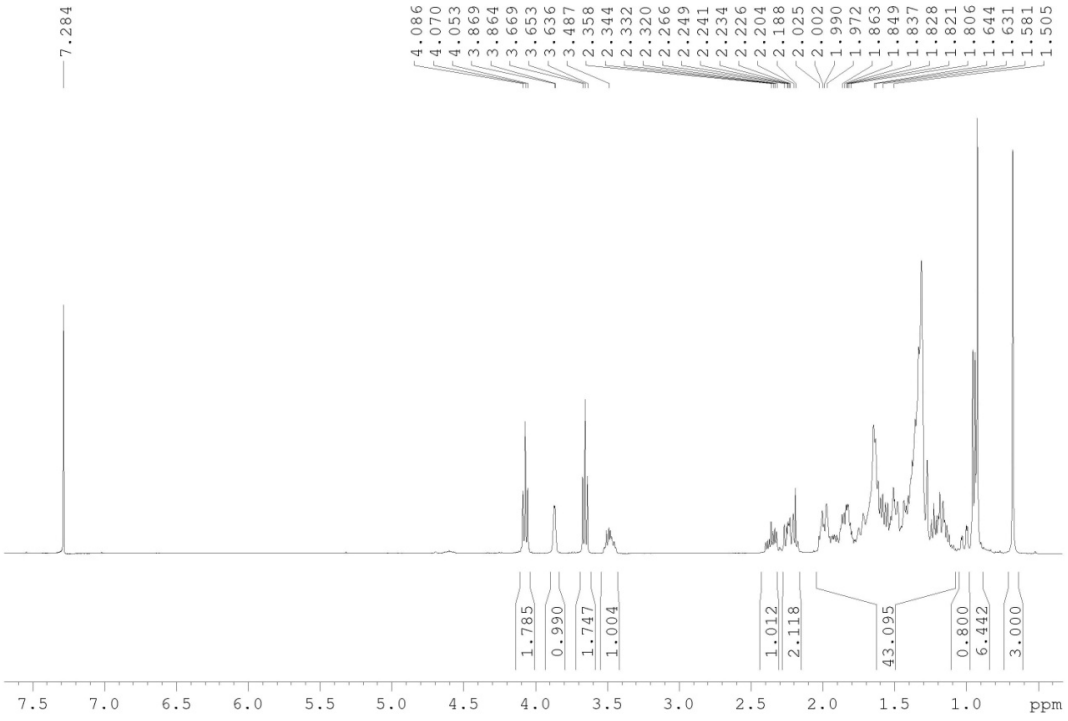
^{13}C NMR (62.9 MHz, $CDCl_3$) of 6'-hydroxyhexyl 3α,7α-dihydroxy-5β-cholan-24-oate (**3**)



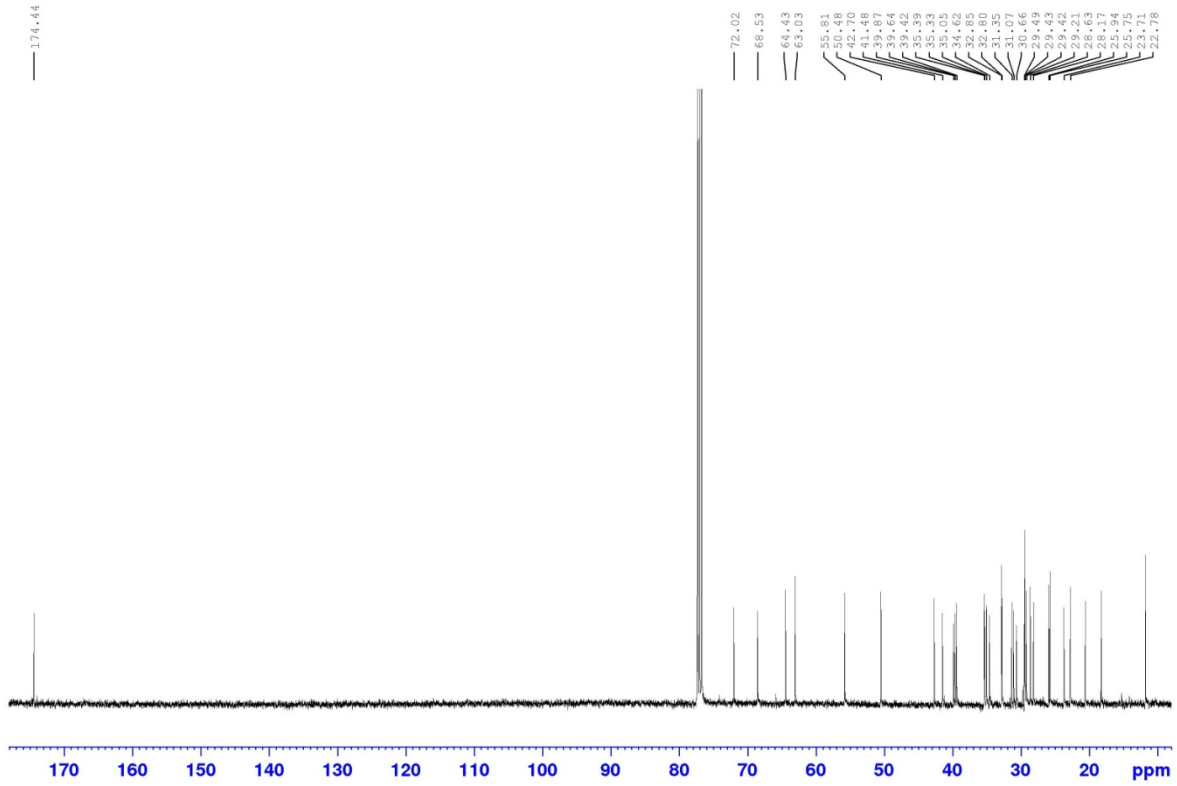
^{1}H NMR (250 MHz, $CDCl_3$) of 8'-hydroxyoctyl 3α,7α-dihydroxy-5β-cholan-24-oate (**4**)



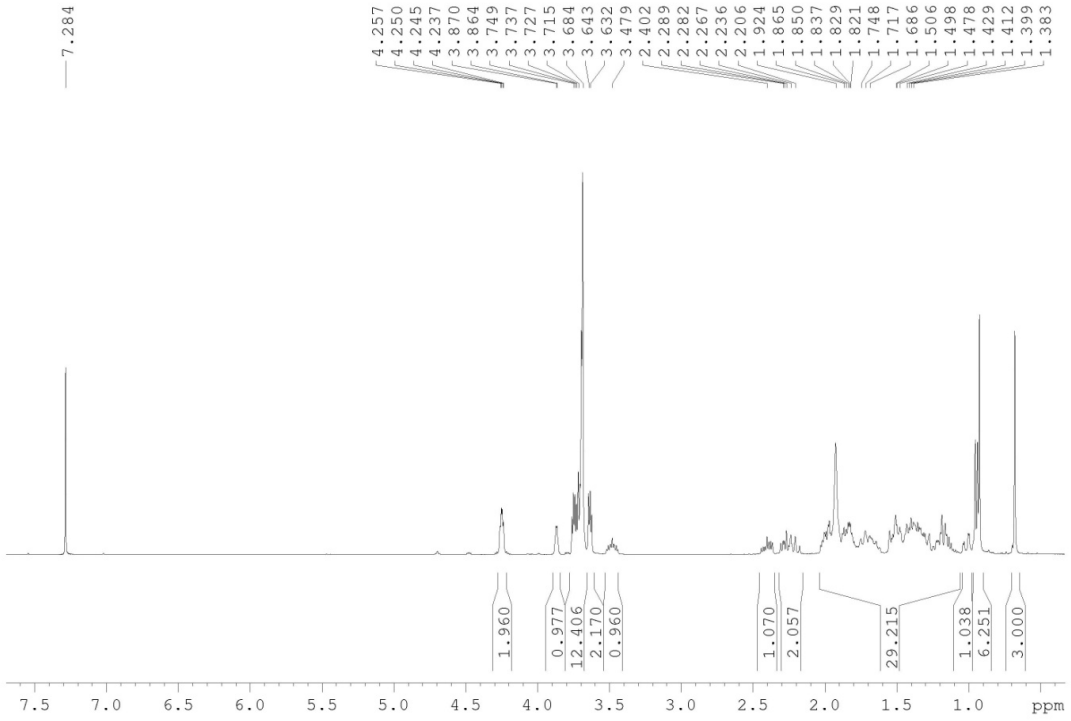
^{13}C NMR (62.9 MHz, $CDCl_3$) of 8'-hydroxyoctyl 3α,7α-dihydroxy-5β-cholan-24-oate (**4**)



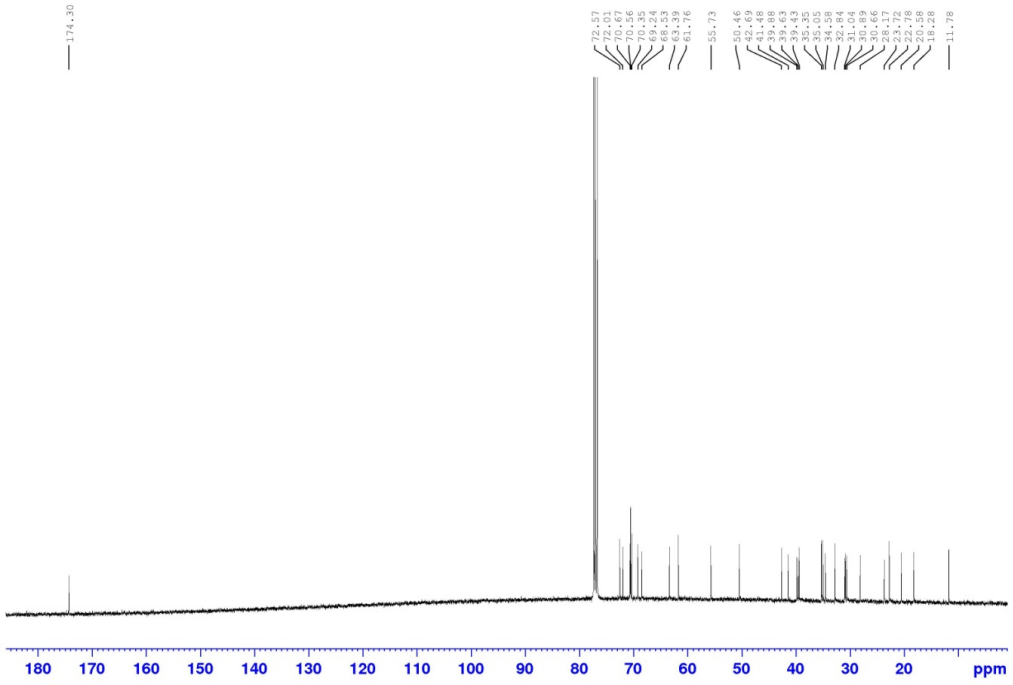
^{1}H NMR (250 MHz, $CDCl_3$) of 10'-hydroxydecyl 3α,7α-dihydroxy-5β-cholan-24-oate (**5**)



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



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



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

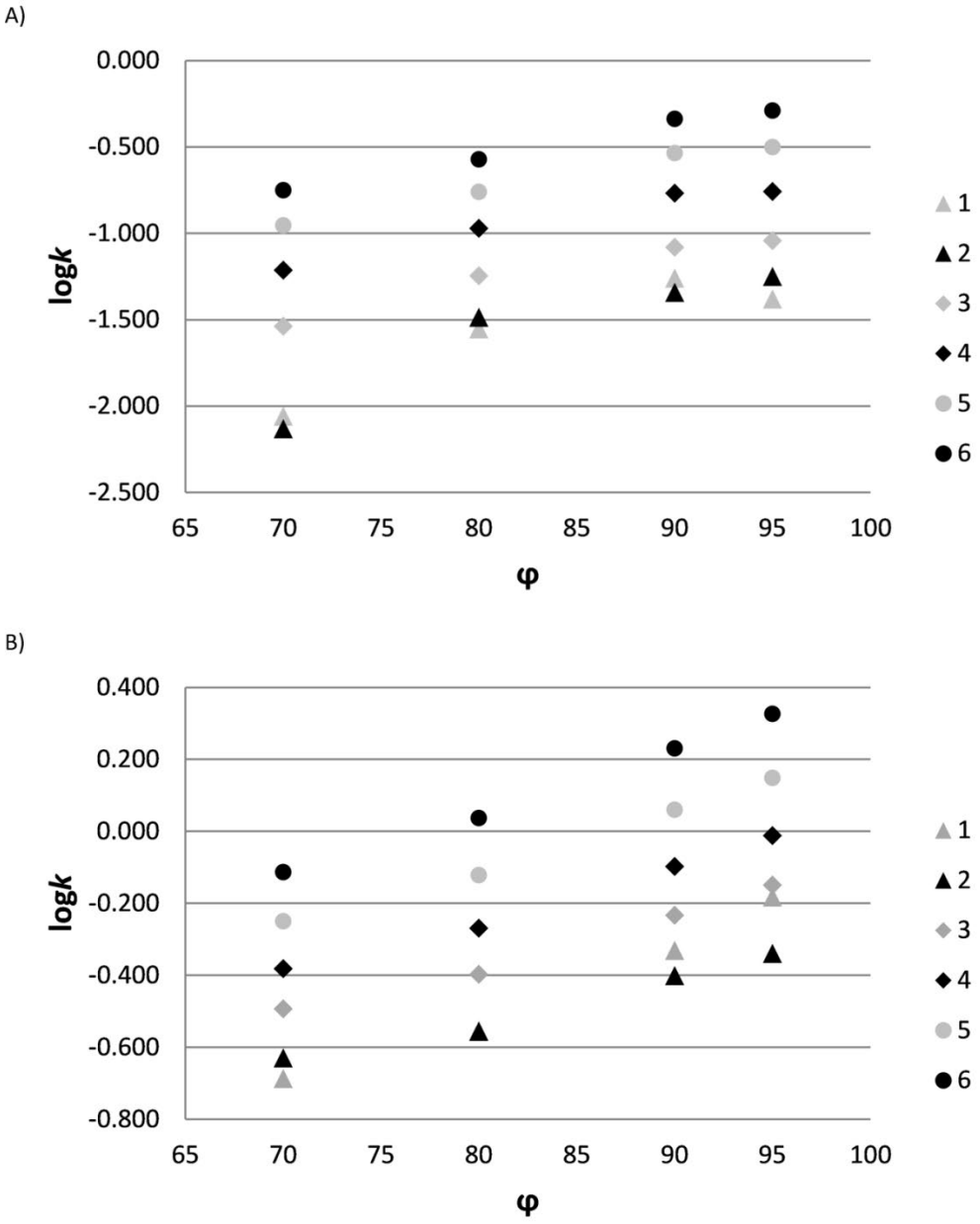


Figure S1 Logarithm of the retention factor (log*k*) for different methanol-2-propanol (A) and acetonitrile-2-propanol (B) volume fractions.

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

Compound	log*P*[1]	log*P*[2]	Clog*P*[3]	ALOG*P*s[4]	AC log*P*[4]	ALOG*P*[4]	MLOG*P*[4]	Average log*P*[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