CYP27A1 acts on the pre-vitamin D3 photoproduct, lumisterol, producing biologically active hydroxy-metabolites.

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Supplememtal section

Table S1 Chemical shift assignments (solvent: CD_3OD)

	25(S)-27(OH)L3 (2A)		25(R)-27(OH)L3 (2B)		25(OH)L3 (3)	
Atom	^{1}H	^{13}C	^{1}H	^{13}C	^{1}H	^{13}C
1	1.61 α, 1.71 β	34.6	1.61 α, 1.71 β	34.5	1.62 α, 1.72 β	34.6
2	2.46 α, 2.25 β	38.9	2.46 α, 2.24 β	39.0	2.47 α, 2.25 β	38.9
3	4.04	67.0	4.04	66.9	4.05	66.9
4	2.42 α, 2.28 β	38.9	2.42 α, 2.28 β	38.9	2.43 α, 2.29 β	38.9
5	NA	140.8	NA	140.7	NA	140.7
6	5.58	121.9	5.58	121.8	5.59	121.8
7	5.43	116.8	5.43	116.8	5.44	116.8
8	NA	ND	NA	ND	NA	ND
9	2.32	47.2	2.32	47.1	2.33	47.1
10	NA	38.0	NA	38.0	NA	37.9
11	1.54 α/β	20.0	1.54 α/β	19.9	1.55 α/β	20.0
12	1.55 α, 1.99 β	38.7	1.53 α, 2.00 β	38.7	1.55 α, 2.00 β	38.7
13	NA	42.9	NA	42.9	NA	42.9
14	2.54	50.7	2.56	50.8	2.55	50.6
15	1.44 α, 1.69 β	23.4	1.42 α, 1.72 β	23.4	1.45 α, 1.70 β	23.4
16	1.72 α/β	29.6	1.71 α/β	29.6	1.72 α/β	29.6
17	1.38	58.6	1.38	58.7	1.40	58.5
18	0.64	18.8	0.64	18.8	0.65	18.8
19	0.76	13.9	0.76	13.9	0.77	14.0
20	1.37	37.5	1.37	37.4	1.39	37.5
21	0.95	18.9	0.95	18.8	0.97	18.9
22	1.45 1.04	37.2	1.41	36.9	1.07 1.46	37.4
23	1.46 1.17	24.6	1.28 1.35	24.5	1.27 1.46	21.9
24	1.02 1.43	34.7	1.06 1.35	34.6	1.46 1.35	45.3
25	1.58	36.8	1.57	36.8	NA	71.4
26	0.91	17.2	0.91	16.9	1.19	29.1
27	3.33, 3.42	68.4	3.33, 3.40	68.6	1.19	29.1

NA – Not applicable (ternary carbons); ND – Not determined.

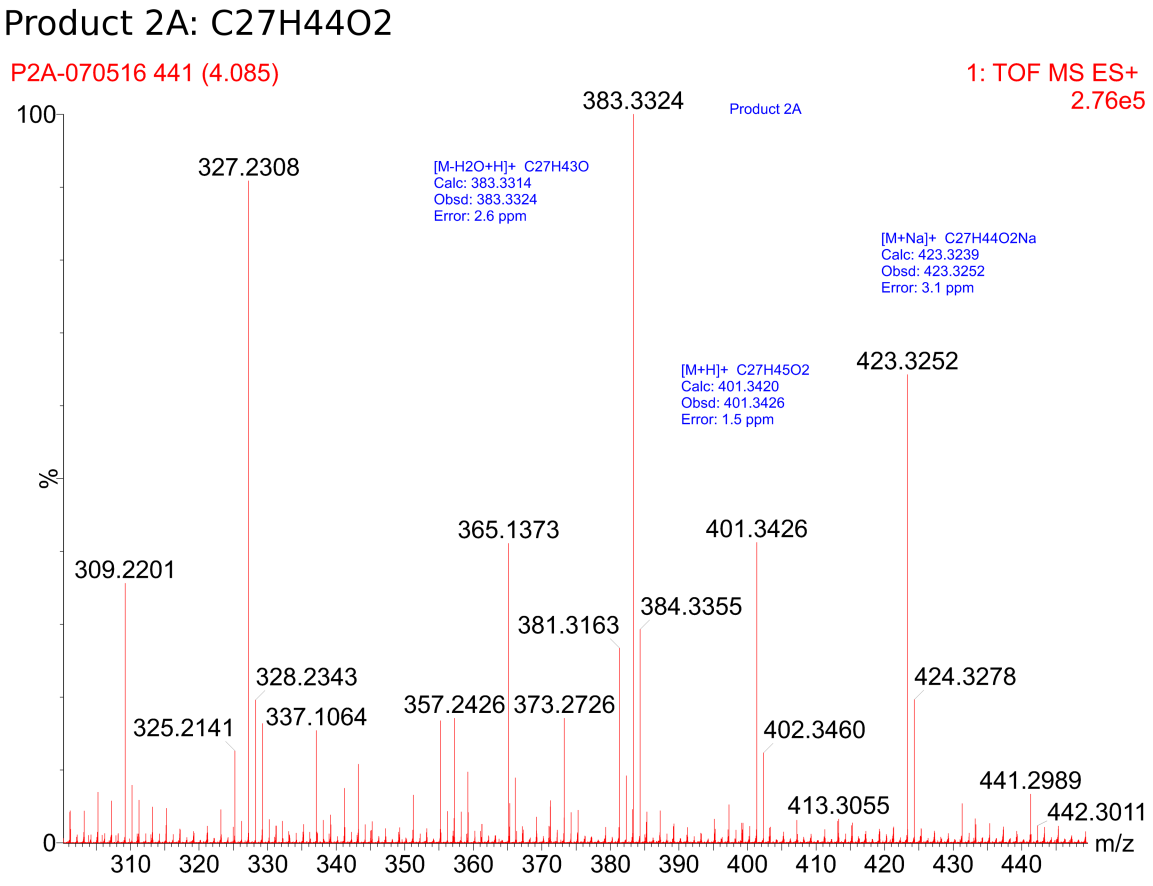

Fig. S1 (A) High resolution MS of lumisterol product 2A (25(S)-27(OH) L3) using ESI in the positive mode. Calculated mass and observed mass values as well as the errors are labeled for $[M + Na]^+$, $[M + H]^+$, and $[M - H_2O + H]^+$.

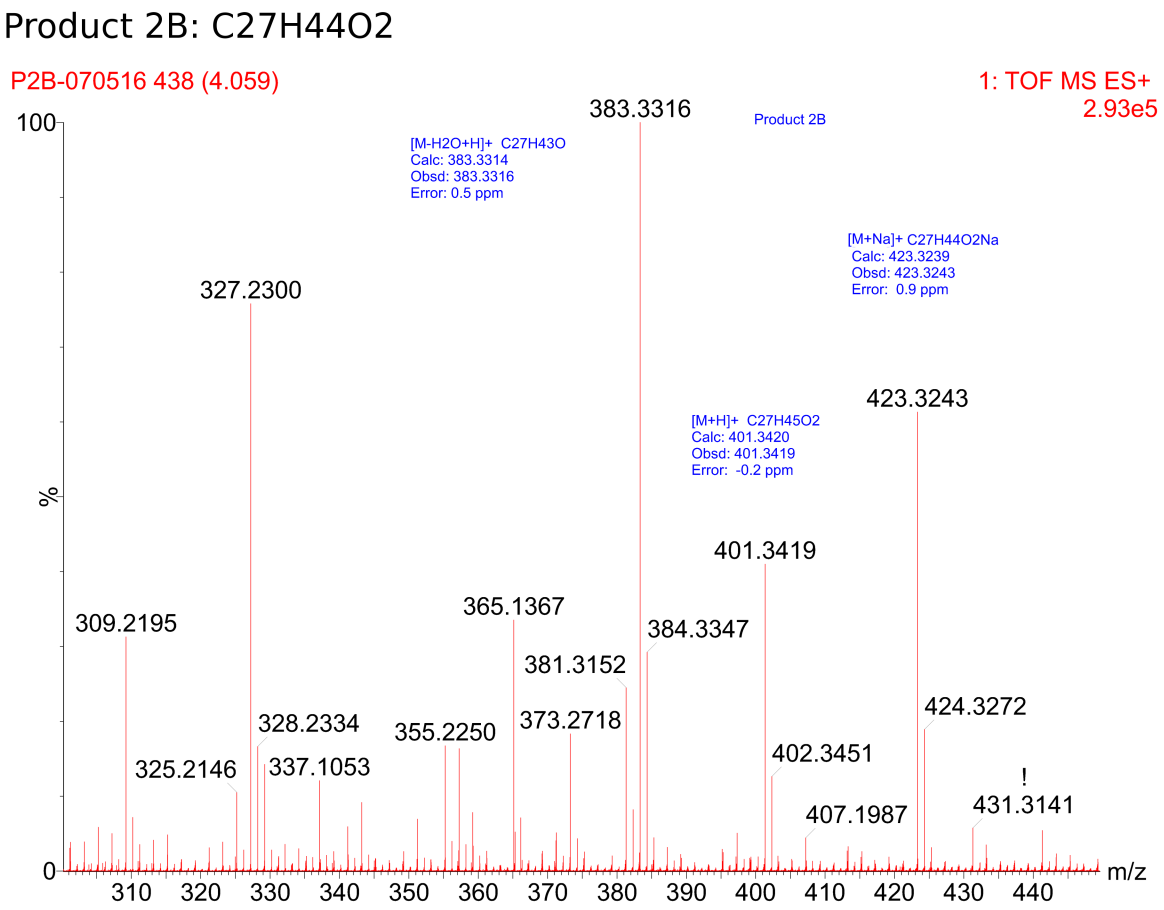

Fig. S1 (B) High resolution MS of lumisterol product 2B (25(R)-27(OH)L3) using ESI in the positive mode. Calculated mass and observed mass values as well as the errors are labeled for $[M + Na]^+$, $[M + H]^+$, and $[M - H_2O + H]^+$.

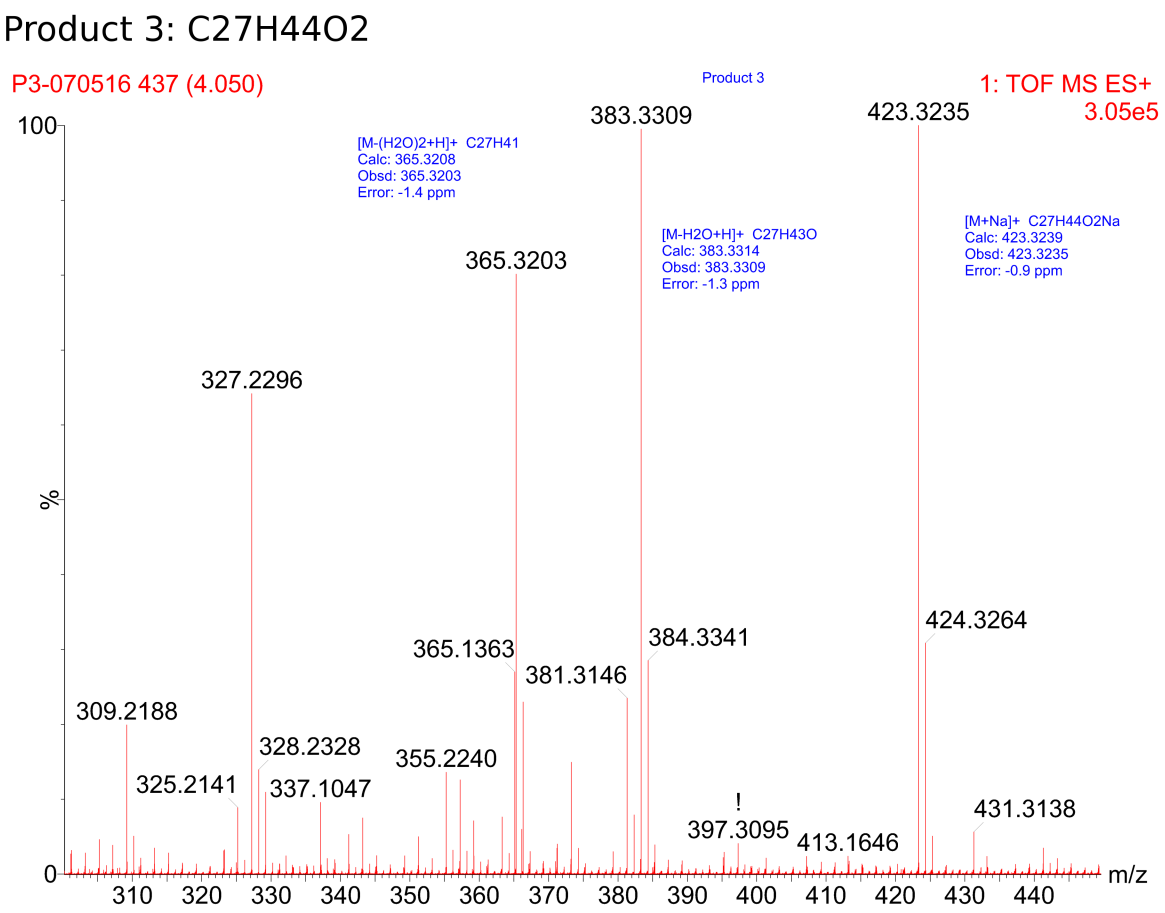

Fig. S1 (C) High resolution MS of lumisterol product 3 (25(OH)L3) using ESI in the positive mode. Calculated mass and observed mass values as well as the errors are labeled for $[M + Na]^+$, $[M - H_2O + H]^+$, and $[M - (H_2O)_2 + H]^+$.

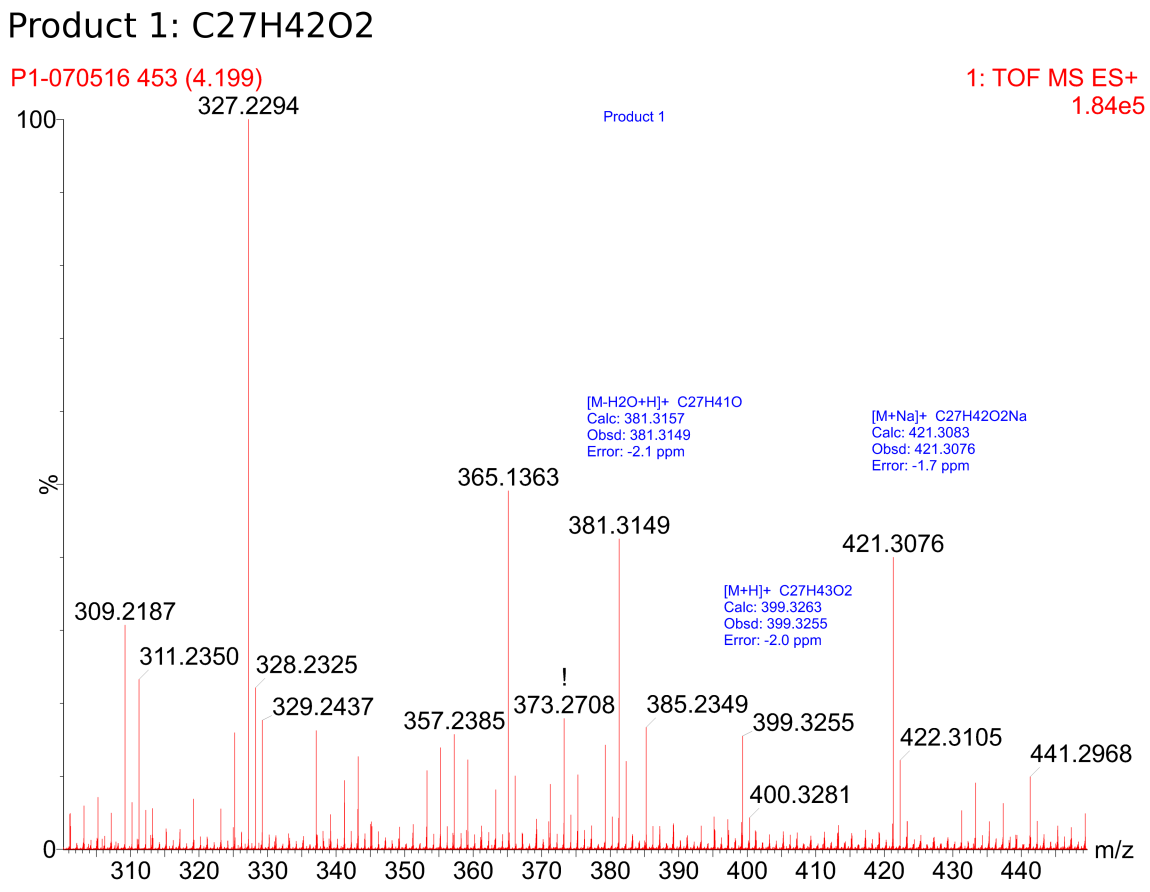

Fig. S1 (D) High resolution MS of lumisterol product 1 using ESI in the positive mode. Calculated mass and observed mass values as well as the errors are labeled for $[M + Na]^+$, $[M + H]^+$, and $[M - H_2O + H]^+$.

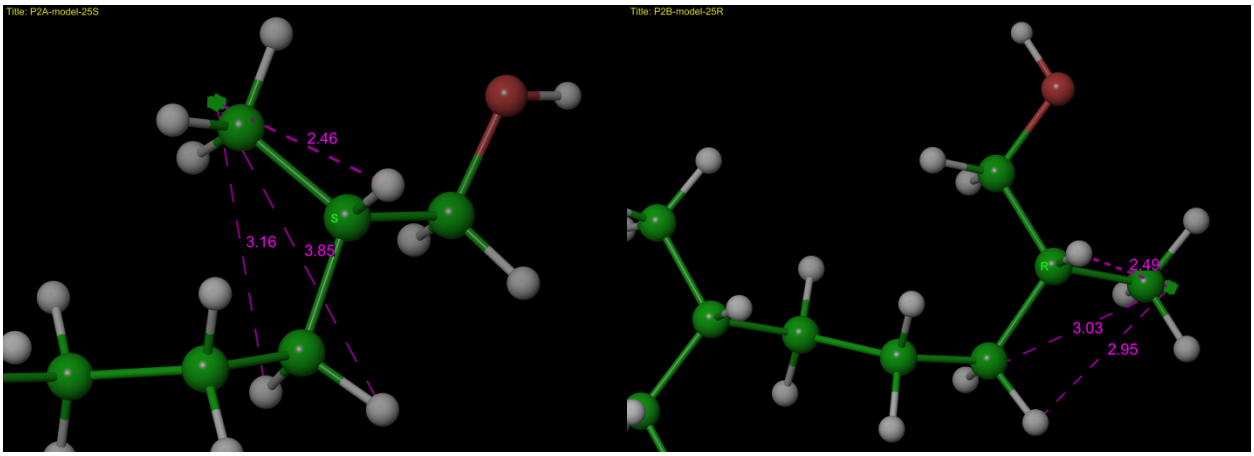

Fig. S2. Molecular models of (25*S*)-27(OH)L3 (left), and (25*R*)-27(OH)L3 (right). A centroid pseudo atom is created to represent the three protons of 26-CH_3 for the distance measurement. Carbon, hydrogen, and oxygen atoms are shown in green, white, and red, respectively. Only the side chain region is shown for clarity. The measured distances are consistent with the NMR results (Figs 2-4).

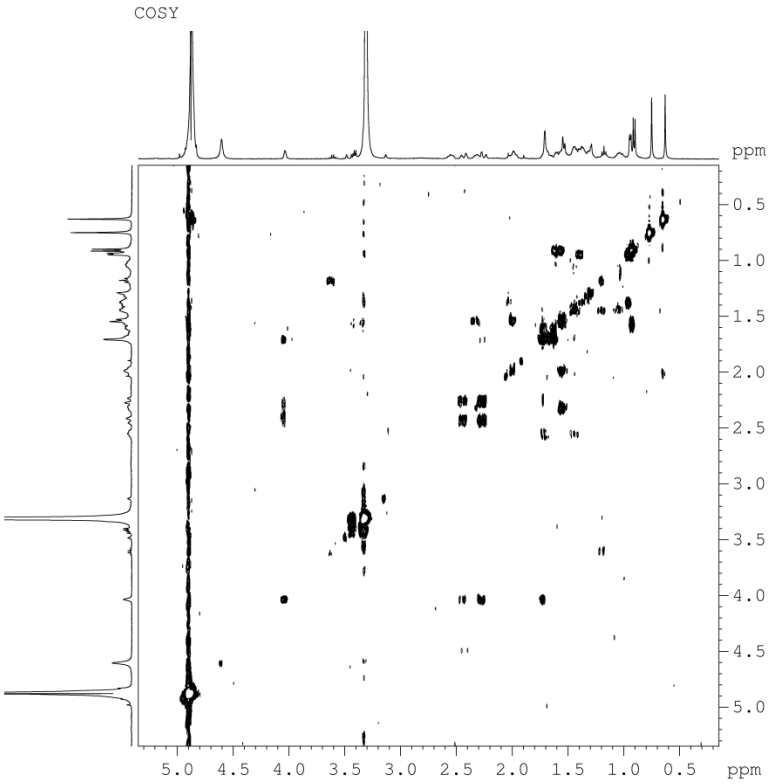

Fig. S3. COSY of (25*S*)-27(OH)L3 (product 2A)

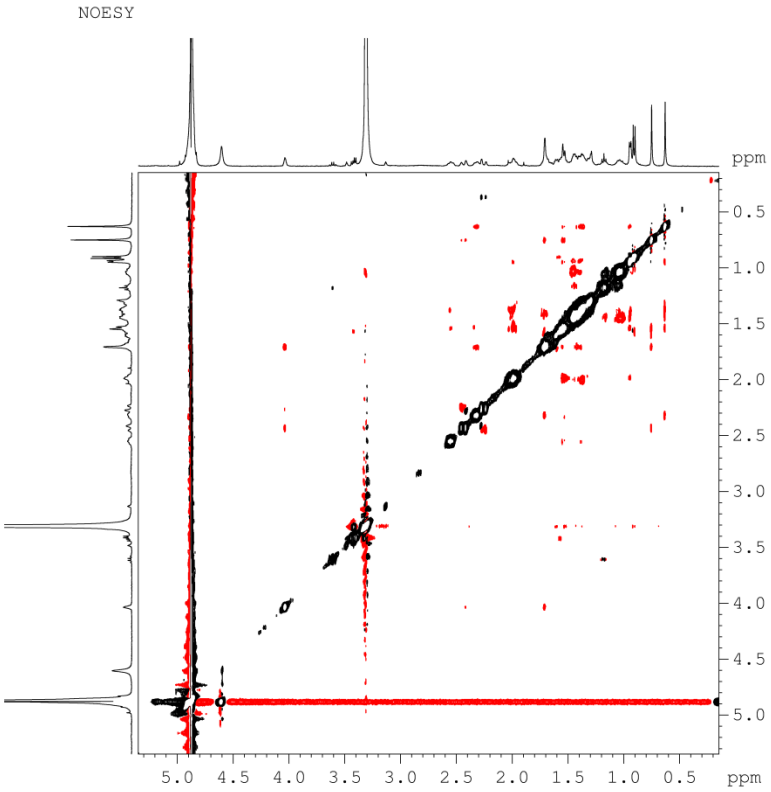

Fig. S4. NOESY of (25*S*)-27(OH)L3 (product 2A)

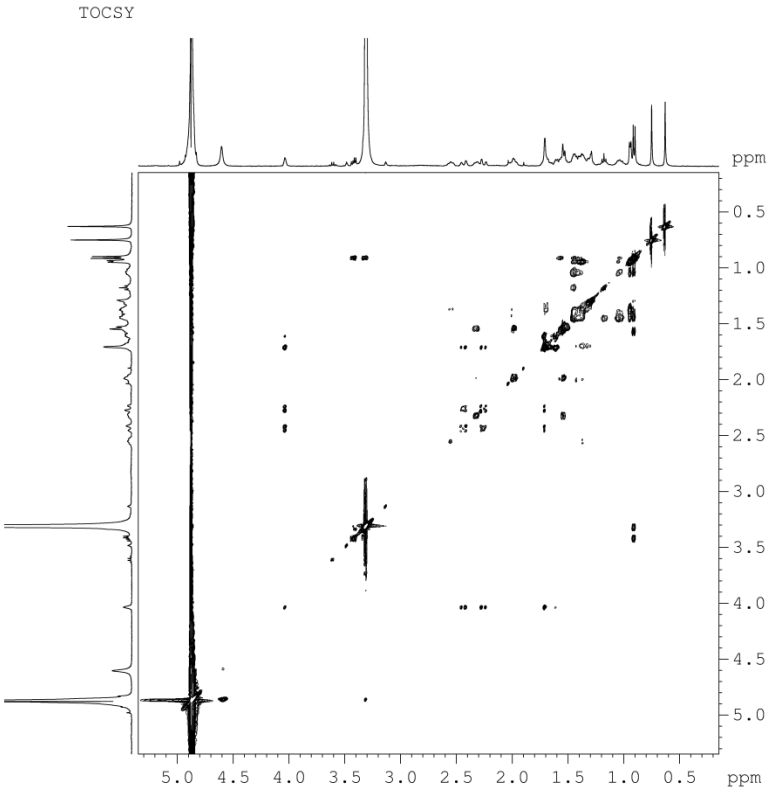

Fig. S5. TOCSY of (25*S*)-27(OH)L3 (product 2A)

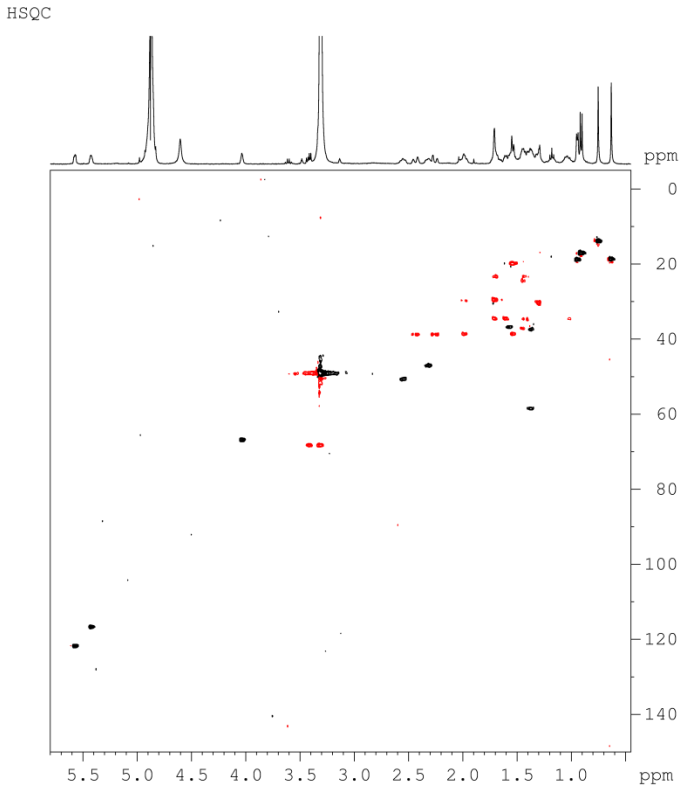

Fig. S6. HSQC of (25*S*)-27(OH)L3 (product 2A)

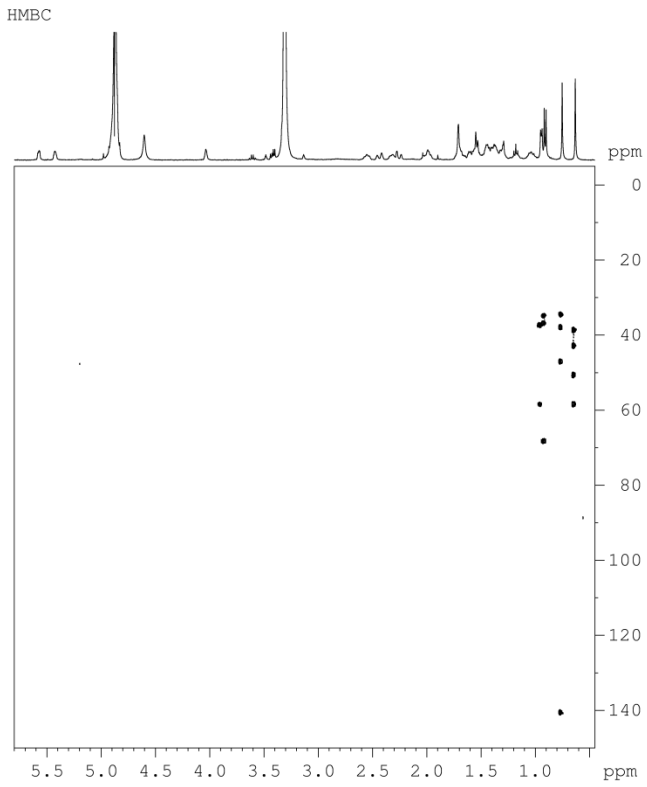

Fig. S7. HMBC of (25*S*)-27(OH)L3 (product 2A)

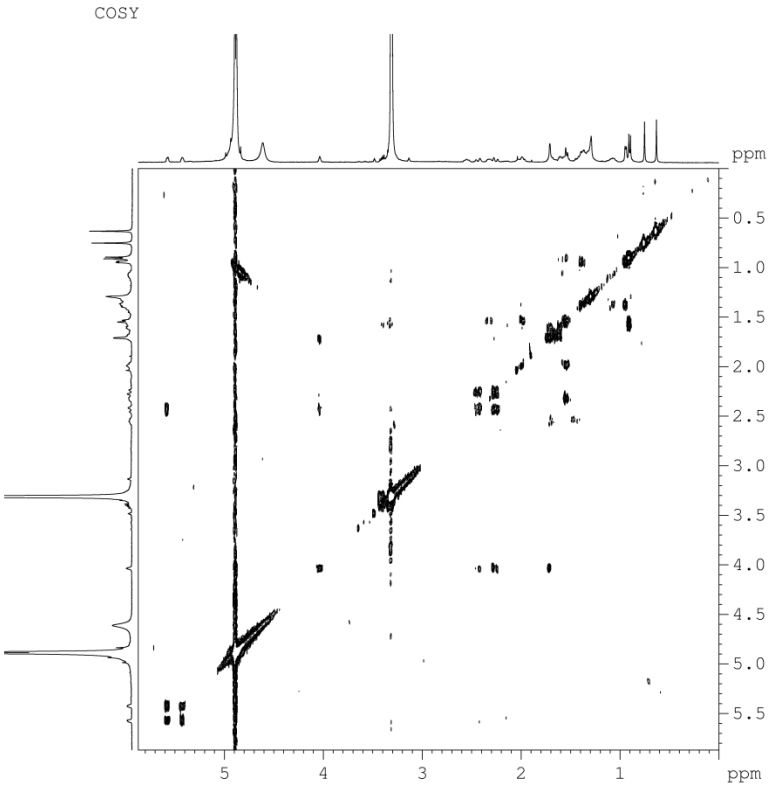

Fig. S8. COSY of (25*R*)-27(OH)L3 (product 2B)

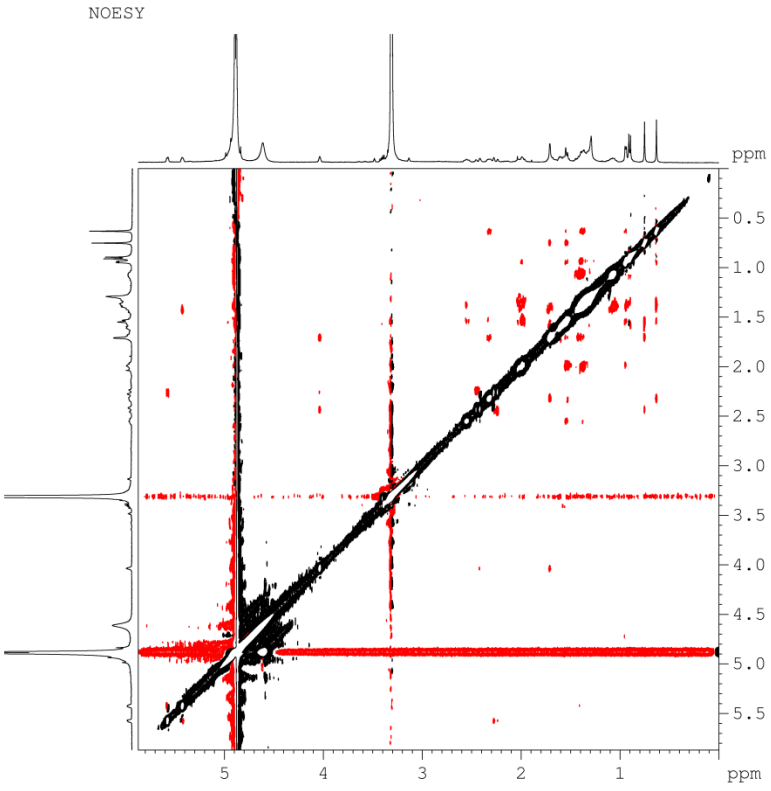

Fig. S9. NOESY of (25*R*)-27(OH)L3 (product 2B)

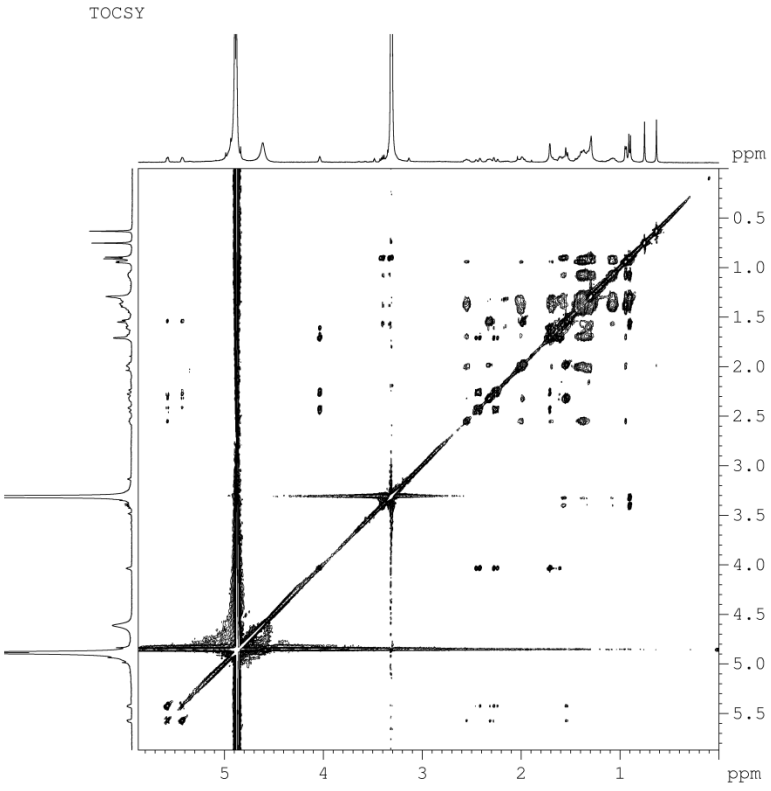

Fig. S10. TOCSY of (25*R*)-27(OH)L3 (product 2B)

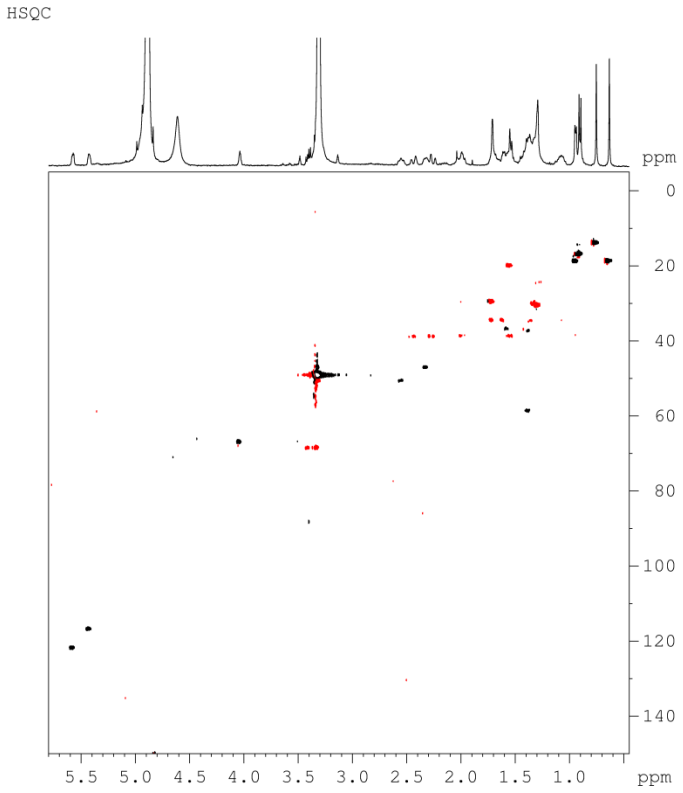

Fig. S11. HSQC of (25*R*)-27(OH)L3 (product 2B)

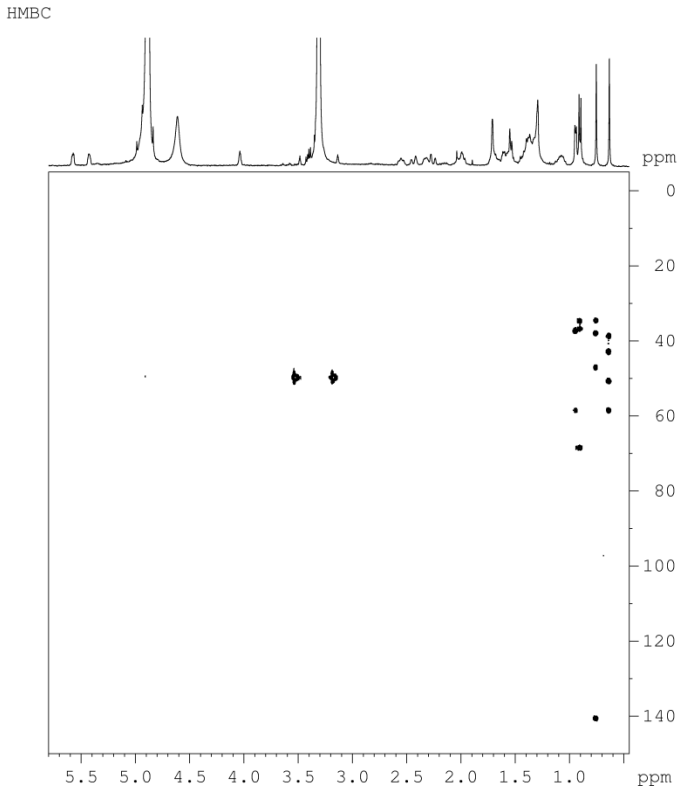

Fig. S12. HMBC of (25*R*)-27(OH)L3 (product 2B)

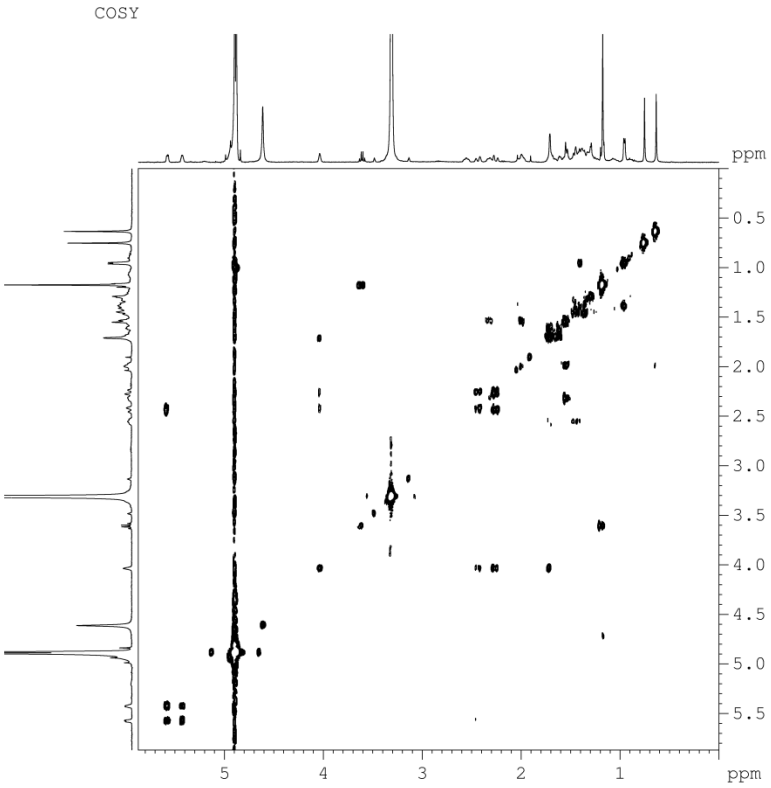

Fig. S13. COSY of 25(OH)L3 (product 3)

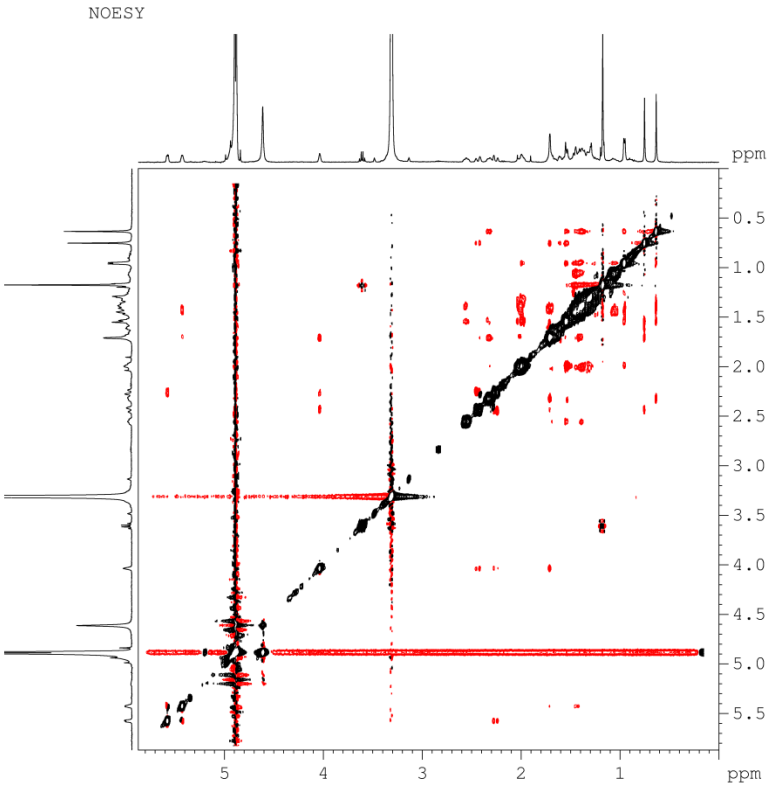

Fig. S14. NOESY of 25(OH)L3 (product 3)

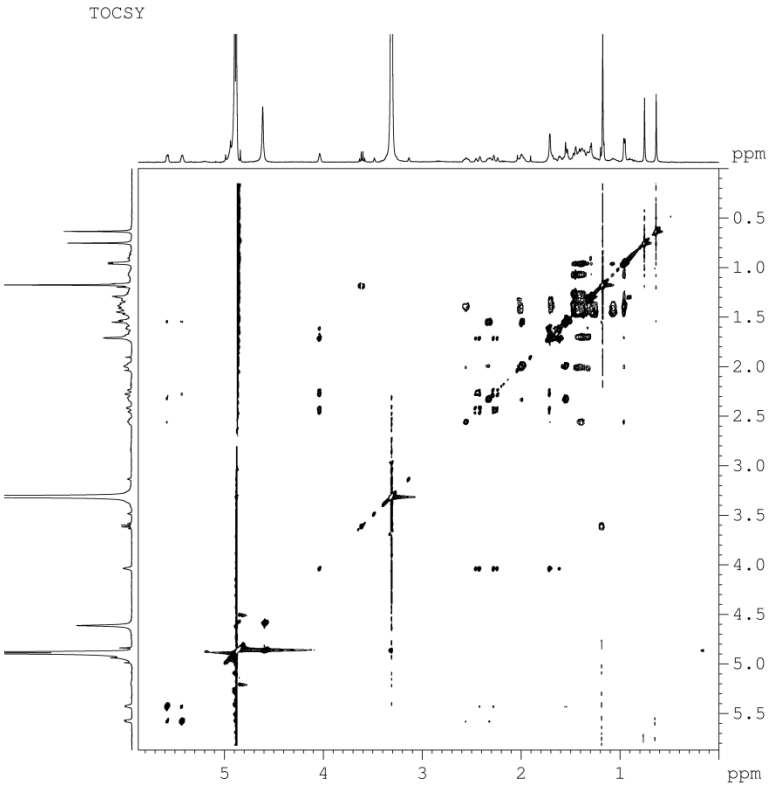

Fig. S15. TOCSY of 25(OH)L3 (product 3)

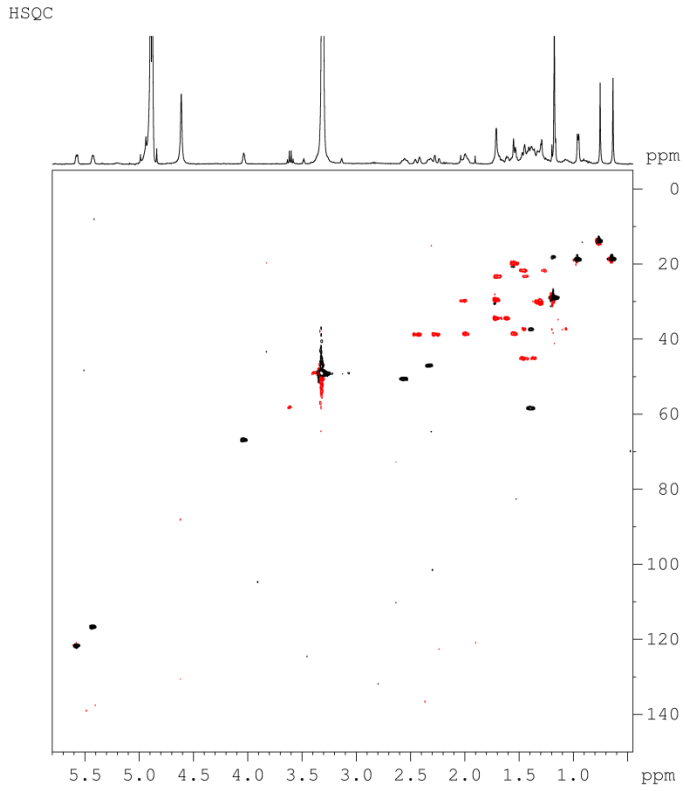

Fig. S16. HSQC of 25(OH)L3 (product 3)

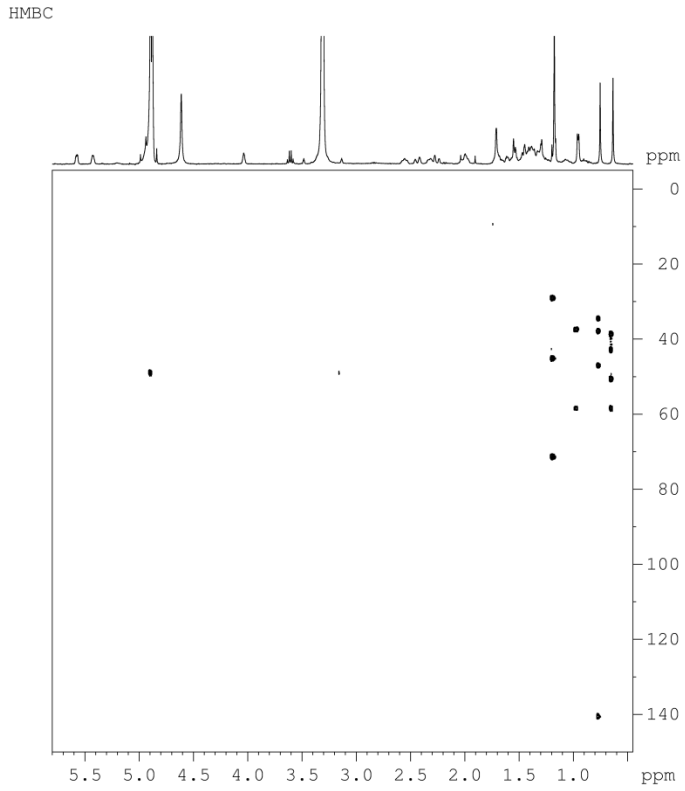

Fig. S17. HMBC of 25(OH)L3 (product 3)