

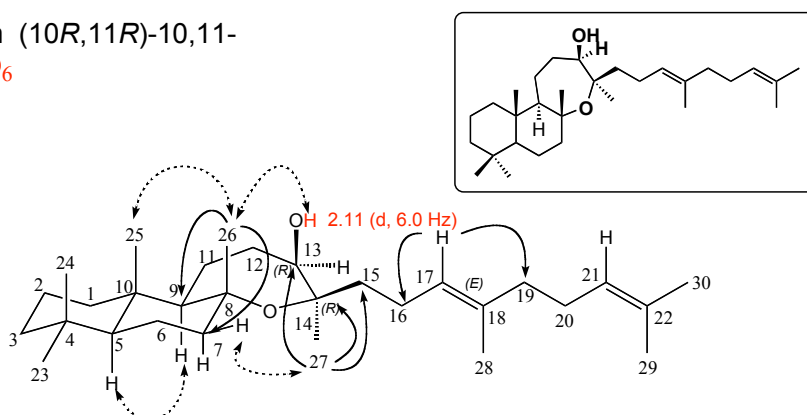
Product **26** (oil) from (10*R*,11*R*)-10,11-DihydroxySQ in C_6D_6

$[\alpha]_D^{25} = -22.9$
($c = 0.142$, in $CHCl_3$)

→ Major HMBC
← Major NOE

COSY: H13-H12, H-12-H11

HRFABMS (glycerol)
M+H, Found: 445.4113
Calcd: 445.4046

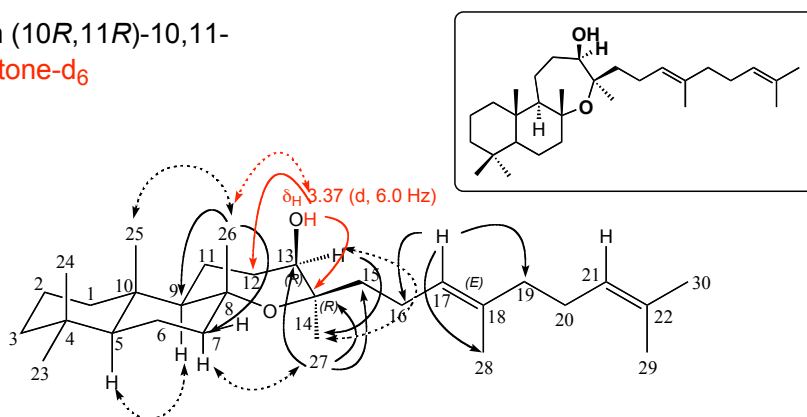


NMR data in C_6D_6 , solvent peak : 1H ; 7.28 ppm, ^{13}C ; 128.0 ppm

NO.	1H	^{13}C	NO.	1H	^{13}C	NO.	1H	^{13}C	NO.	1H	^{13}C
1	0.84(m) ; 1.79(m)	40.43	9	1.61(m)	59.88	17	5.51 (t, 7.0Hz)	125.69	25	0.791 (3H,s)	16.14
2	1.47(m); 1.64(m)	19.11	10	—	39.39	18	—	134.62	26	1.357 (3H,s)	24.69
3	1.21(m); 1.44(m)	42.25	11	1.51(m) ; 1.74(m)	17.39	19	2.26 (2H,t, 6.8Hz)	40.24	27	1.357 (3H,s)	24.20
4	—	33.50	12	1.65(m) ; 2.00(m)	32.97	20	2.33 (2H,t, 6.8Hz)	27.26	28	1.845 (3H, s)	16.16
5	0.87(m)	56.64	13	3.62 (t, 6.0Hz)	74.73	21	5.39 (t, 6.8Hz)	125.01	29	1.704 (3H, s)	17.75
6	1.23(m) ; 1.68(m)	21.48	14	—	80.73	22	—	131.11	30	1.813 (3H, s)	25.85
7	1.72(m) ; 1.98(m)	44.00	15	1.59(m) ; 2.16(dd,13.2, 13.2, 4.8 Hz)	41.71	23	0.958 (3H,s)	33.55	OH	2.109 (1H, d, 6.0 Hz)	
8	—	80.44	16	2.31(m) ; 2.41(m)	23.21	24	0.866 (3H, s)	21.50			

Product **26** (oil) from (10*R*,11*R*)-10,11-DihydroxySQ in $acetone-d_6$

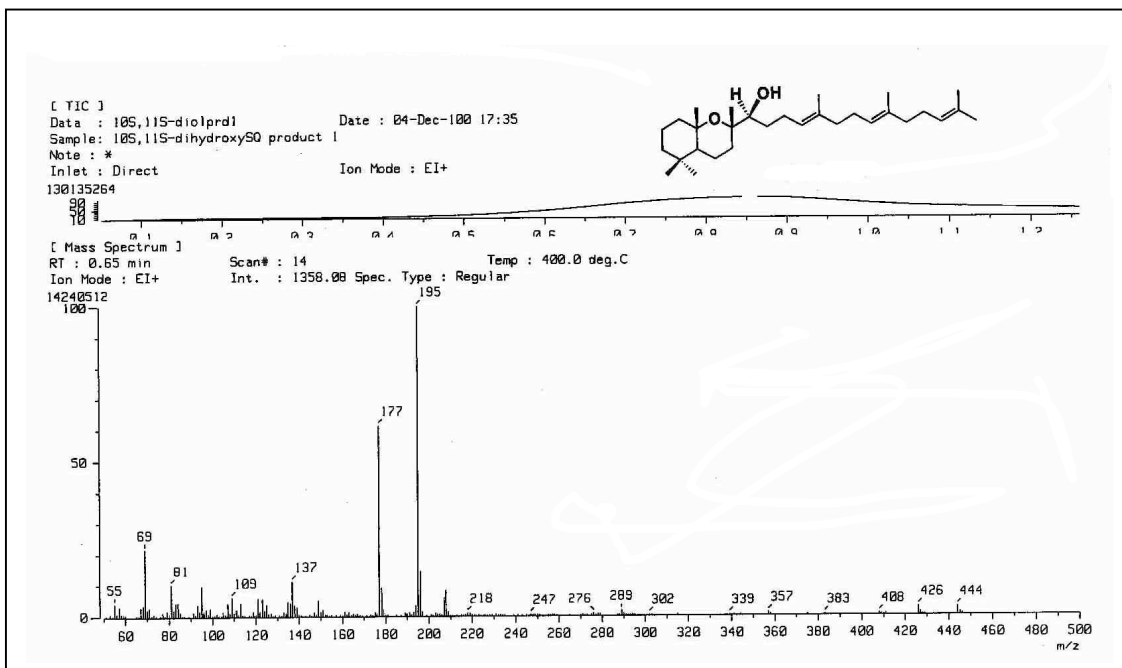
→ Major HMBC
← Major NOE
COSY: H13/H12, H12/H11



NMR data in $acetone-d_6$, solvent peak : 1H ; 2.04 ppm, ^{13}C ; 29.80 ppm

NO.	1H	^{13}C	NO.	1H	^{13}C	NO.	1H	^{13}C	NO.	1H	^{13}C
1	0.92(m) ; 1.83(m)	40.95	9	1.38 (m)	62.17	17	5.16 (t, 6.8 Hz)	125.20	25	0.807 (3H,s)	16.26
2	1.42(m) ; 1.65(m)	19.50	10	—	39.49	18	—	134.59	26	1.336 (3H,s)	23.53
3	1.16(m); 1.35(m)	42.68	11	1.47(m); 1.72(m)	19.11	19	1.96 (2H,t, 6.8Hz)	40.48	27	1.202 (3H,s)	26.99
4	—	33.97	12	1.69(m) ; 1.85(m)	32.68	20	2.33 (2H,t, 7.2 Hz)	27.45	28	1.616 (3H, s)	16.06
5	0.91(m)	57.08	13	3.67 (t, 6.0 Hz)	75.59	21	5.10 (bt, 6.8Hz)	126.34	29	1.582 (3H, s)	17.71
6	1.27(ddd,12.4,12.4,3.2 Hz) ; 1.62(m)	21.47	14	—	81.33	22	—	131.56	30	1.645 (3H, s)	25.82
7	1.57(m) ; 1.77(m)	45.30	15	1.35(m) ; 1.83(m)	40.20	23	0.880 (3H,s)	33.79	OH	3.37 (d, 6.0 Hz)	
8	—	80.28	16	2.02 (m) ; 2.08(m)	23.31	24	0.794 (3H, s)	21.79			

Product 27



Product 27 (oil) from (10S,11S)-10,11-DihydroxySQ

$[\alpha]_D^{25} = -9.01$
 (c 0.233, CHCl₃)

HRFABMS(glycerol)
 M+H, Found: 445.4120
 Calcd: 445.4046

→ Major HMBC
 ← Major NOE

Selected COSY 45; H10-H11, H11-H12, H12-H13

NMR data in C₆D₆, solvent peak : ¹H; 7.28 ppm, ¹³C; 128.0 ppm

NO.	¹ H	¹³ C	NO.	¹ H	¹³ C	NO.	¹ H	¹³ C	NO.	¹ H	¹³ C
1	1.34(m) ; 1.71(m)	41.92	9	—	75.11	17	5.42 (t, 6.8Hz)	124.91	25	1.274 (3H, s)	23.54
2	1.48 (2H,m)	20.26	10	3.43(ddd, 10.4, 5.0, 2.0Hz)	79.63	18	—	134.86	26	1.255 (3H, s)	22.39
3	1.198(m) ; 1.33(m)	41.62	11	1.59(m) ; 1.71(m)	31.28	19	2.21 (2H,m)	40.26*	27	1.826 (3H, s)	16.19
4	—	33.39	12	2.49(m) ; 2.69(m)	25.62	20	2.30 (2H,m)	27.23**	28	1.725 (3H, s)	16.11
5	1.16 (dd, 12.0, 2.0Hz)	54.37	13	5.53 (t, 6.8Hz)	125.34	21	5.37 (t, 7.0Hz)	124.97	29	1.690 (3H, s)	17.73
6	1.40 (m) ; 1.50(m)	16.34	14	—	135.27	22	—	131.05	30	1.806 (3H, s)	25.84
7	1.46(m) ; 1.74(m)	34.83	15	2.25 (2H,m)	40.21*	23	0.910 (3H, s)	32.20			
8	—	75.73	16	2.33 (2H,m)	27.11**	24	0.768 (3H, s)	20.87			

The signals of C15 and C19 and those of C16 and C19 are interchangeable due to the close values

