

Supplementary Information

Preparation of Derivatives of Betulinic Acid, Steviol and Isosteviol and Evaluation of Antitrypanosomal and Antimalarial Activities

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New compounds spectra

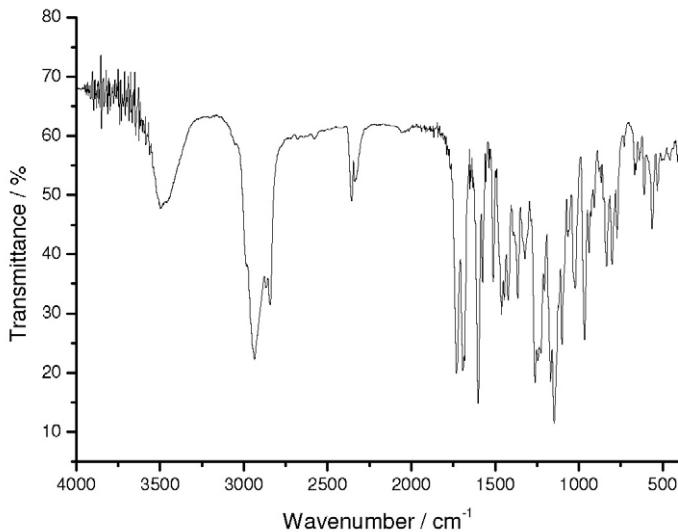


Figure S1. IR spectrum (KBr) of steviol *p*-methoxyphenacyl ester (**3e**).

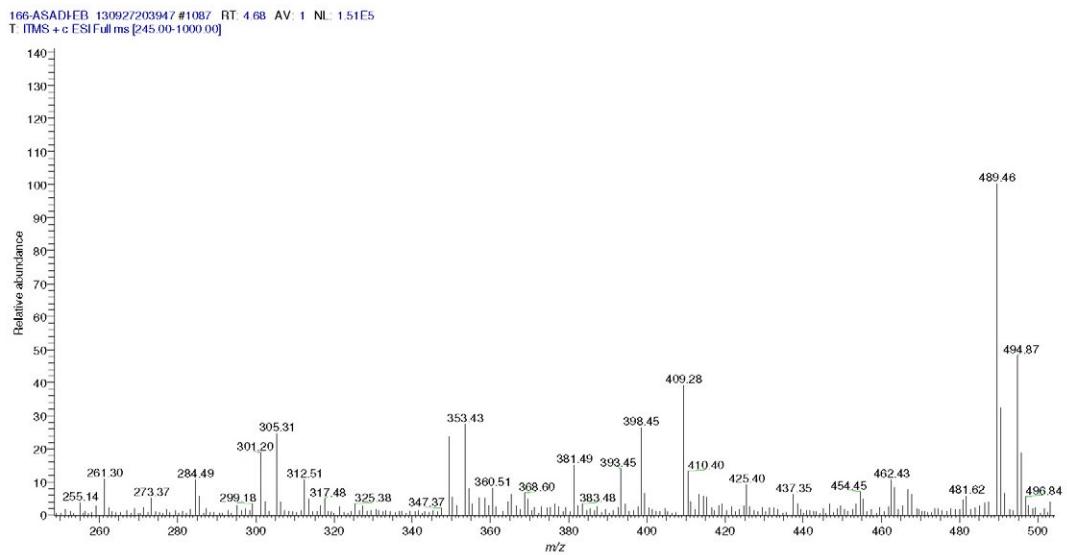


Figure S2. MS-ESI spectrum of steviol *p*-methoxyphenacyl ester (**3e**).

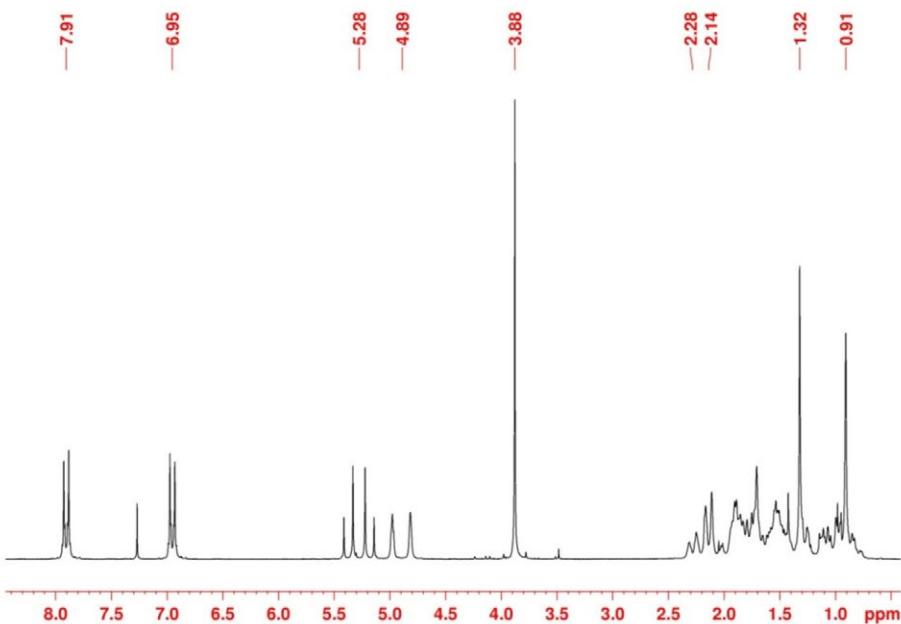


Figure S3. ^1H NMR spectrum (50 MHz, CDCl_3) of steviol *p*-methoxyphenacyl ester (**3e**).

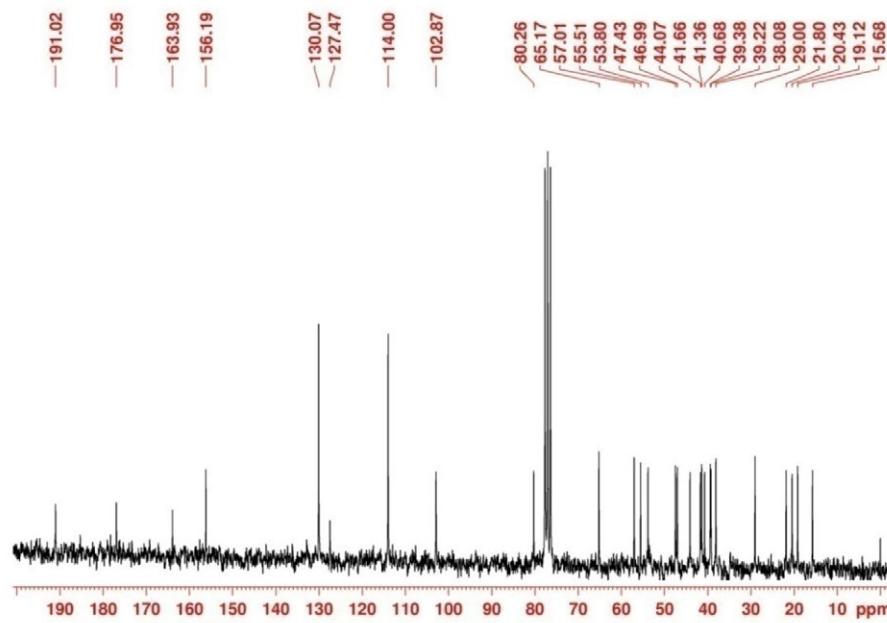


Figure S4. ¹³C NMR spectrum (50 MHz, CDCl₃) of steviol *p*-methoxyphenyl ester (**3e**).

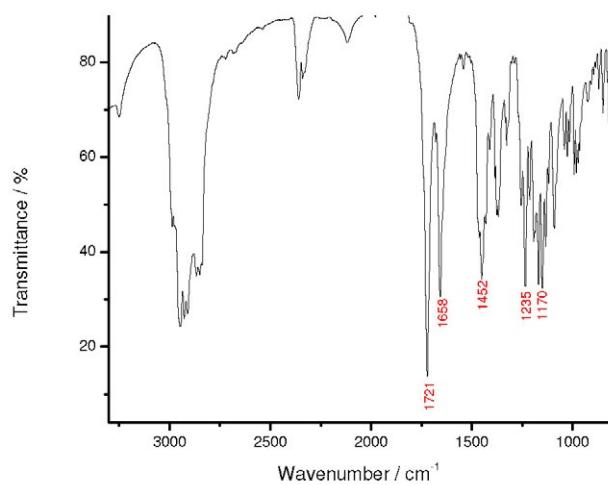


Figure S5. IR spectrum (KBr) of isosteviol isopropylhydrazone (**4d**).

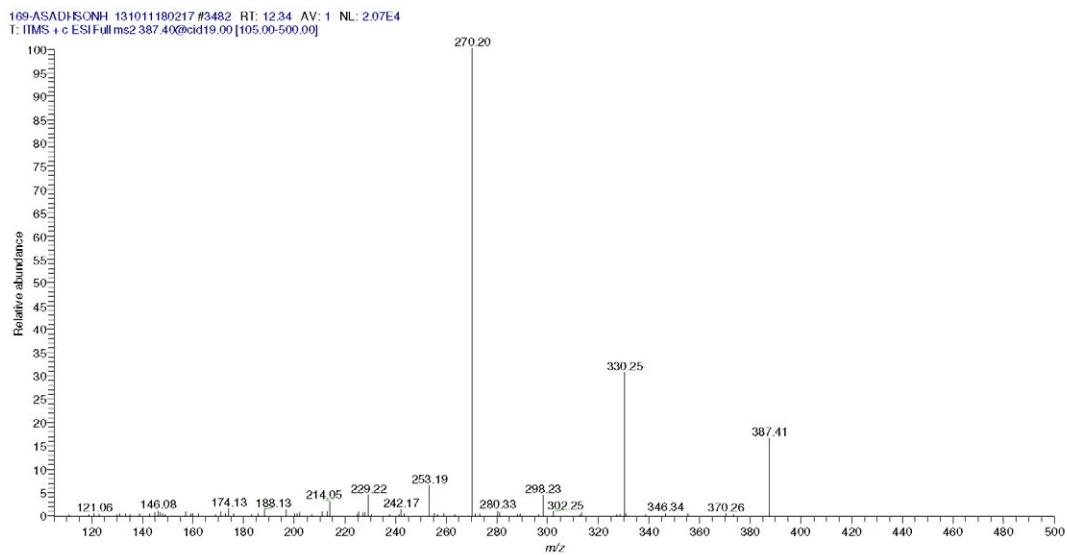


Figure S6. MS-ESI spectrum of isosteviol isopropylhydrazone (**4d**).

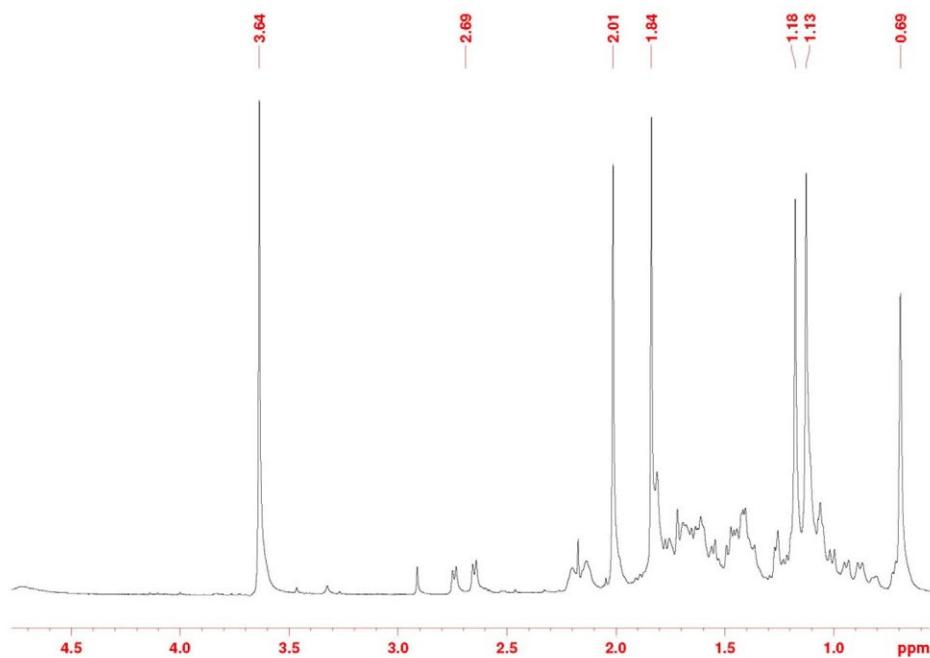


Figure S7. ^1H NMR spectrum (50 MHz, CDCl_3) of isosteviol isopropylhydrazone (**4d**).

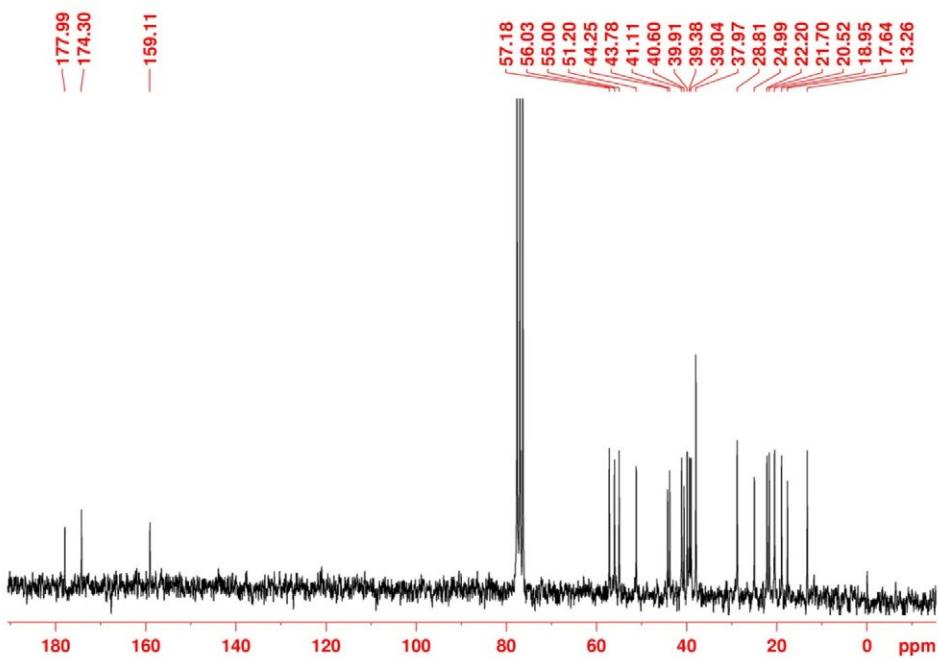


Figure S8. ¹³C NMR spectrum (50 MHz, CDCl₃) of isosteviol isopropylhydrazone (**4d**).

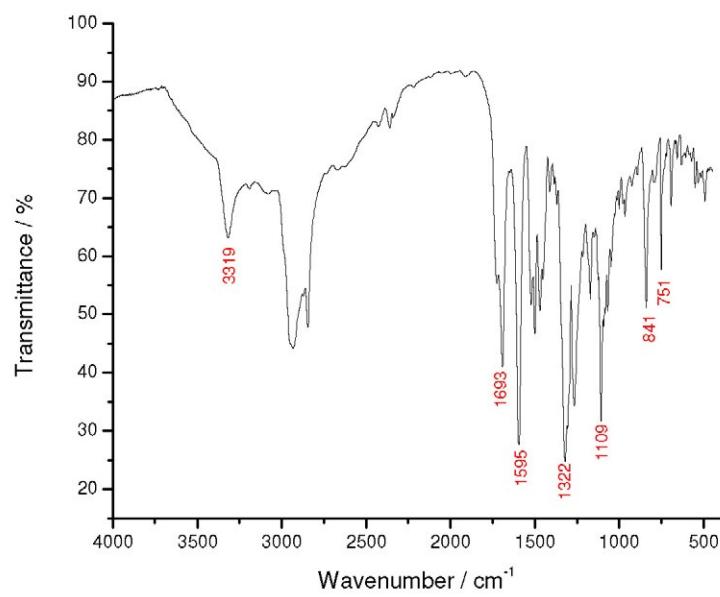


Figure S9. IR spectrum (KBr) of isosteviol 4-nitrophenylhydrazone (**4e**).

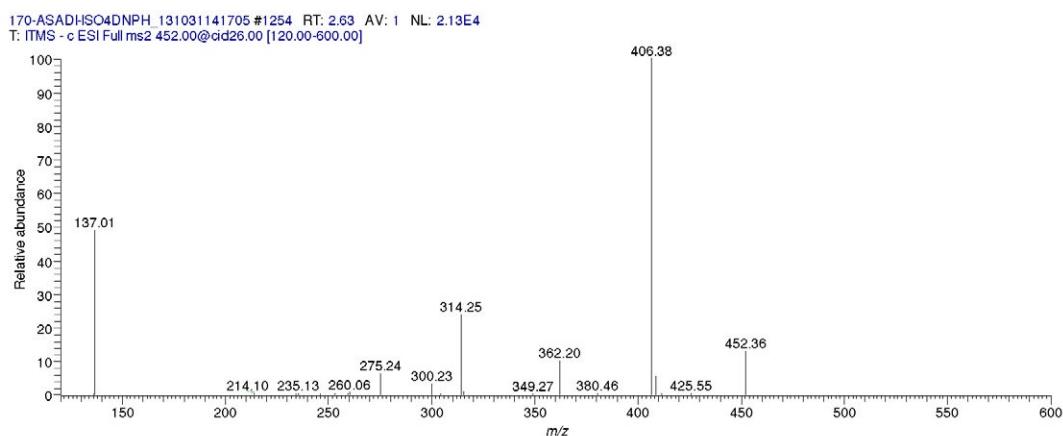


Figure S10. MS-ESI spectrum of isosteviol 4-nitrophenylhydrazone (**4e**).

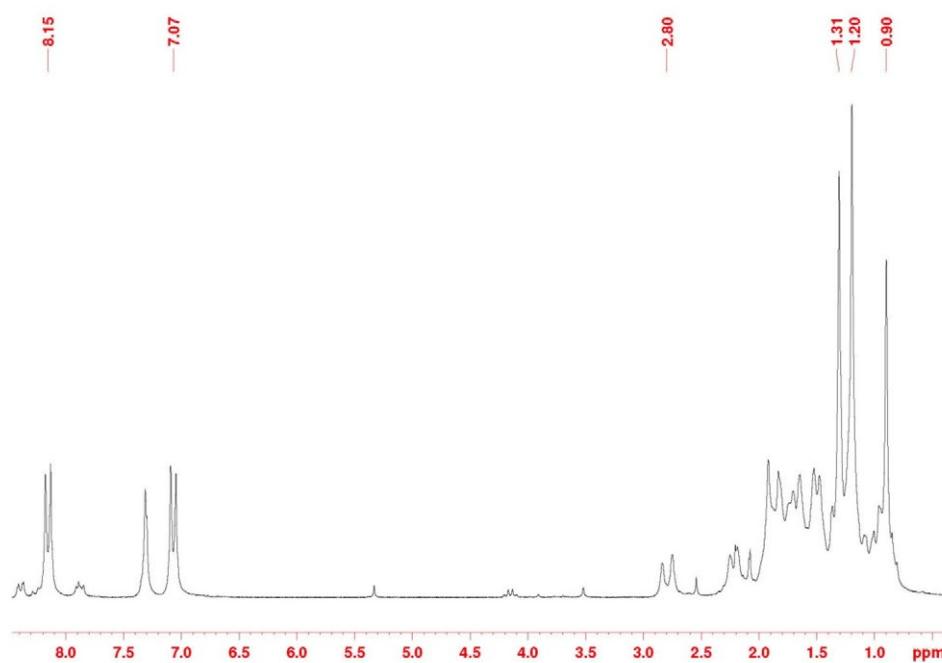


Figure S11. ^1H NMR spectrum (50 MHz, CDCl_3) of isosteviol 4-nitrophenylhydrazone (**4e**).

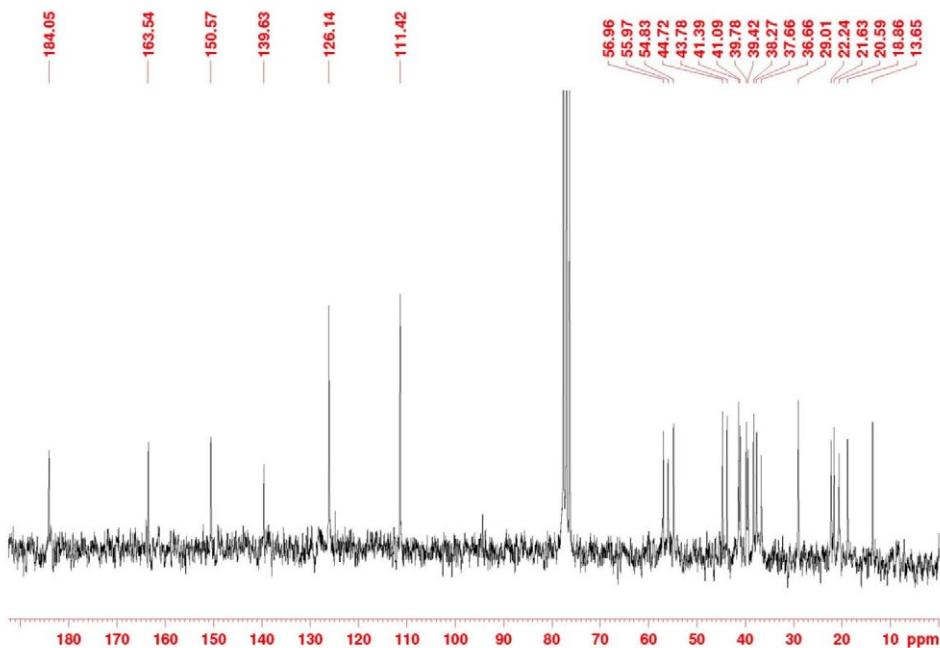


Figure S12. ¹³C NMR spectrum (50 MHz, CDCl₃) of isosteviol 4-nitrophenylhydrazone (**4e**).

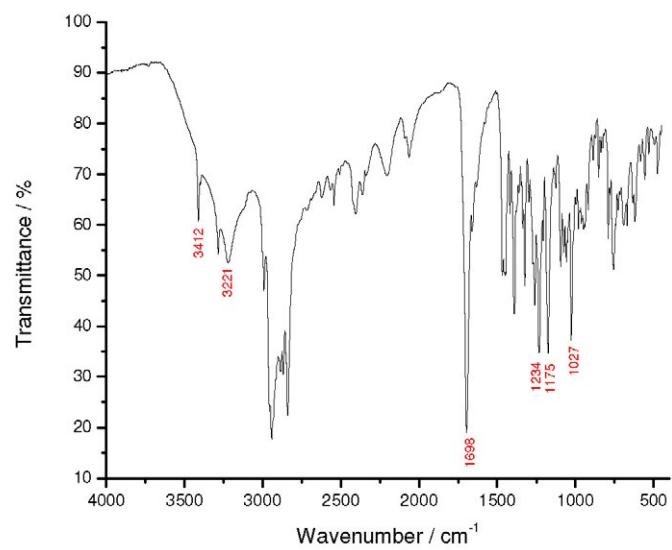


Figure S13. IR spectrum (KBr) of 17-hydroxyisosteviol hydrazone (**4k**).

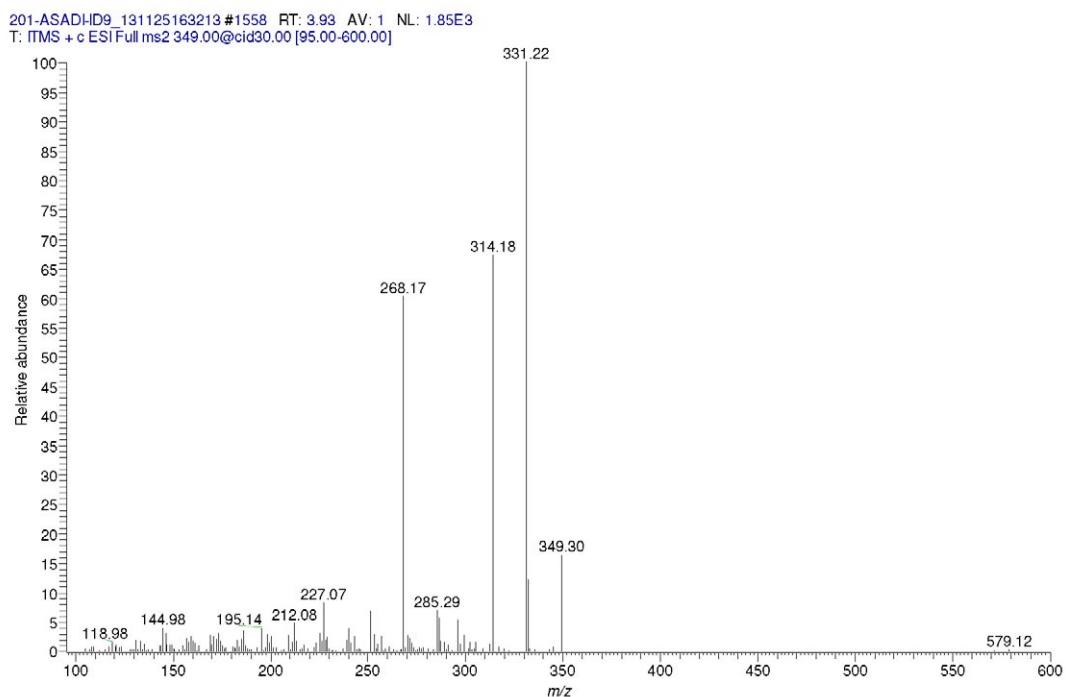


Figure S14. MS-ESI spectrum of 17-hydroxyisosteviol hydrazone (**4k**).

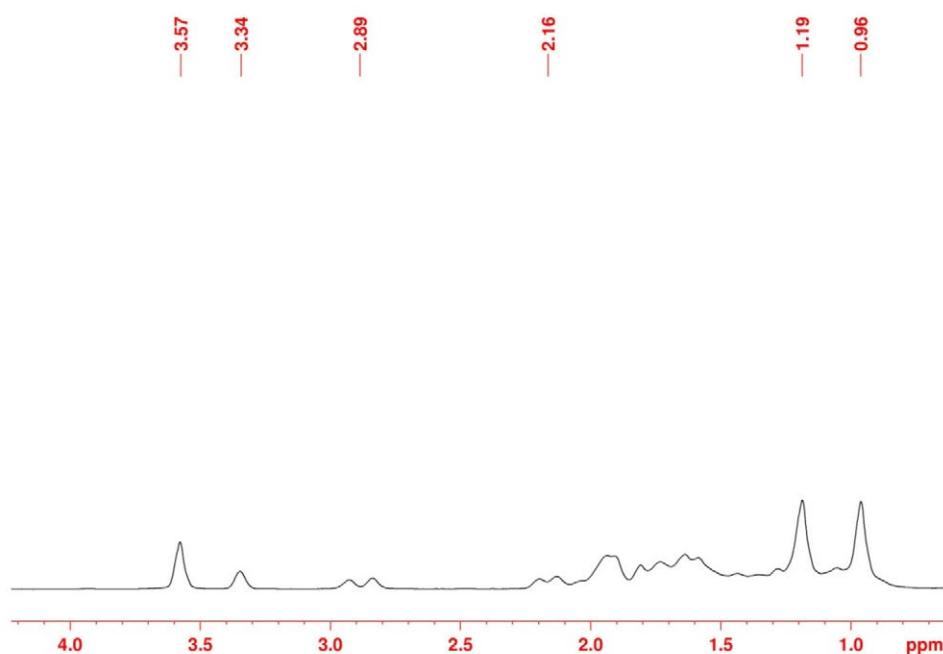


Figure S15. ^1H NMR spectrum (200 MHz, CD_3OD) of 17-hydroxyisosteviol hydrazone (**4k**).

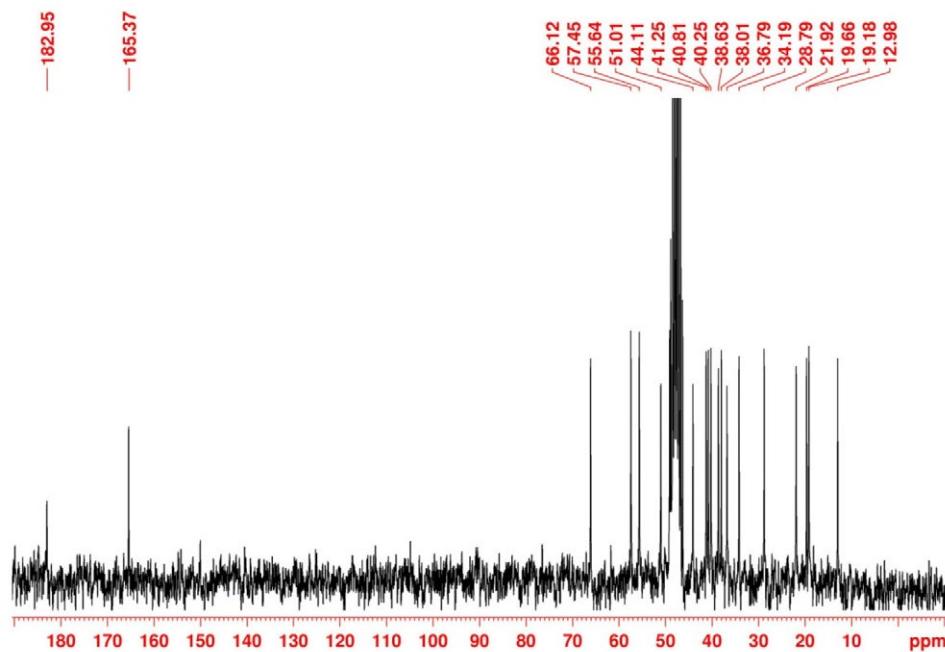


Figure S16. ¹³C NMR spectrum (50 MHz, CD₃OD) of 17-hydroxyisosteviol hydrazone (**4k**).

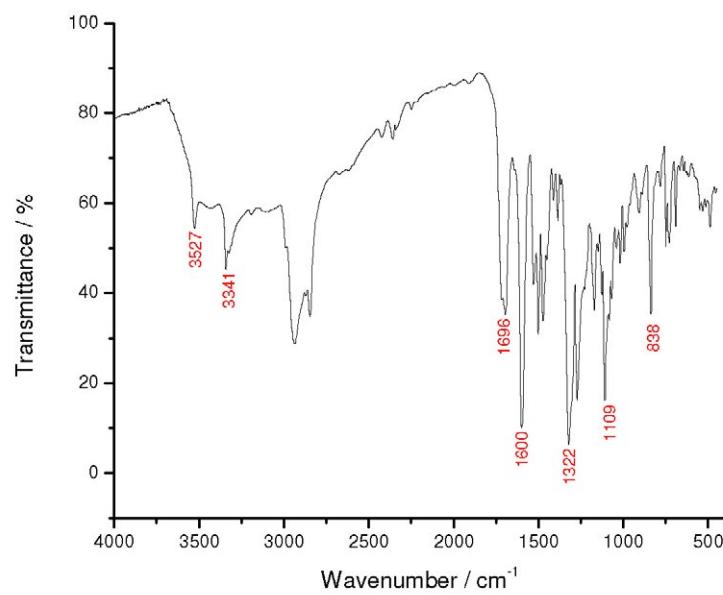


Figure S17. IR spectrum (KBr) of 17-hydroxyisosteviol, 4-nitrophenylhydrazone (**4l**).

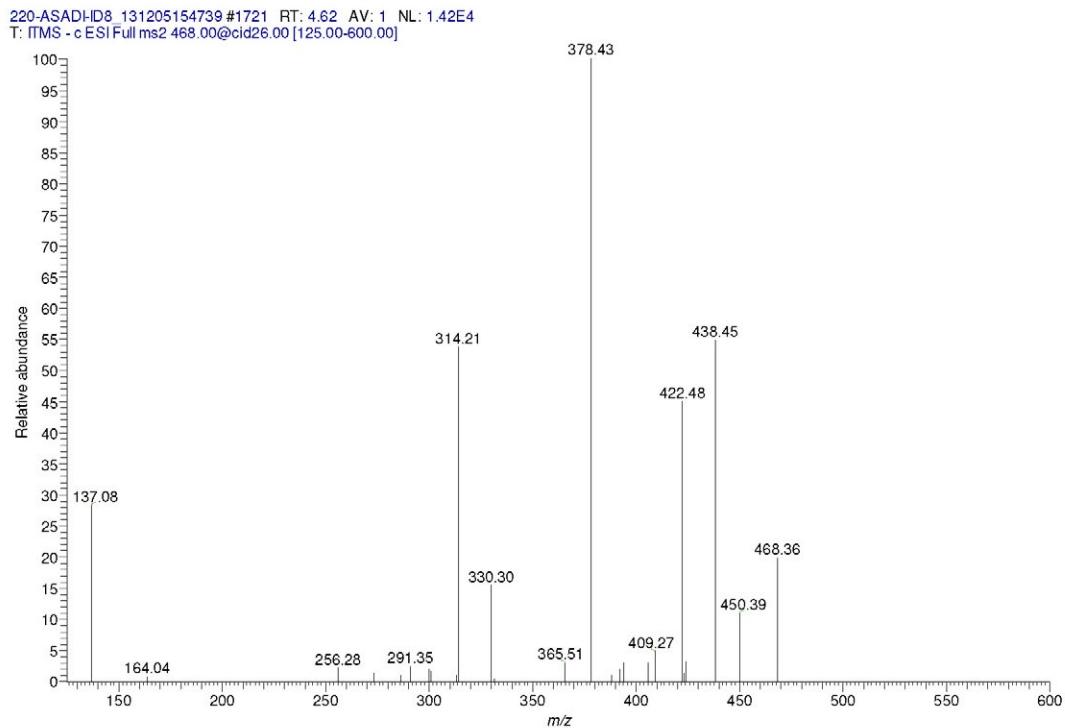


Figure S18. MS-ESI spectrum of 17-hydroxyisosteviol, 4-nitrophenylhydrazone (**4l**).

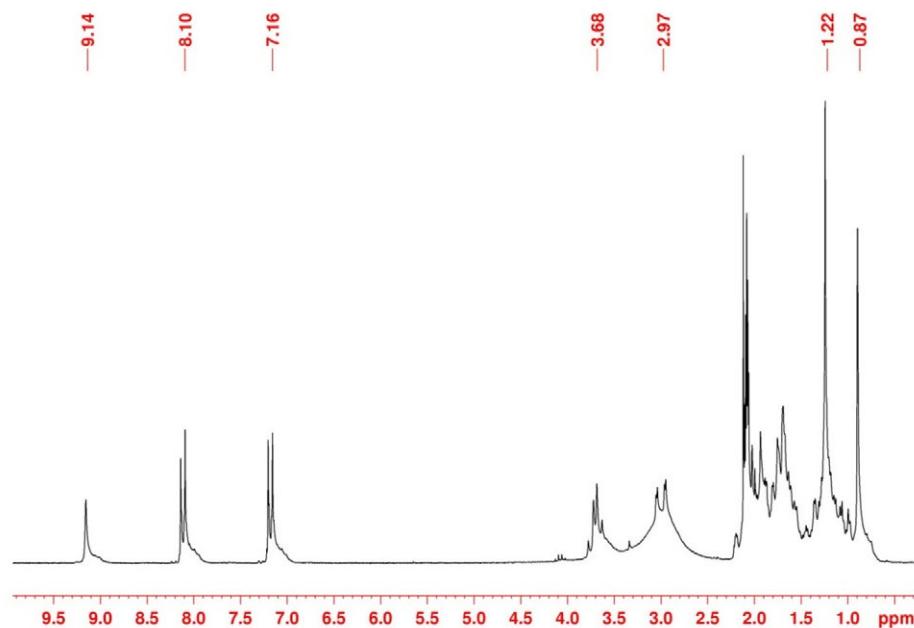


Figure S19. ^1H NMR spectrum (200 MHz, acetone- d_6) of 17-hydroxyisosteviol, 4-nitrophenylhydrazone (**4l**).

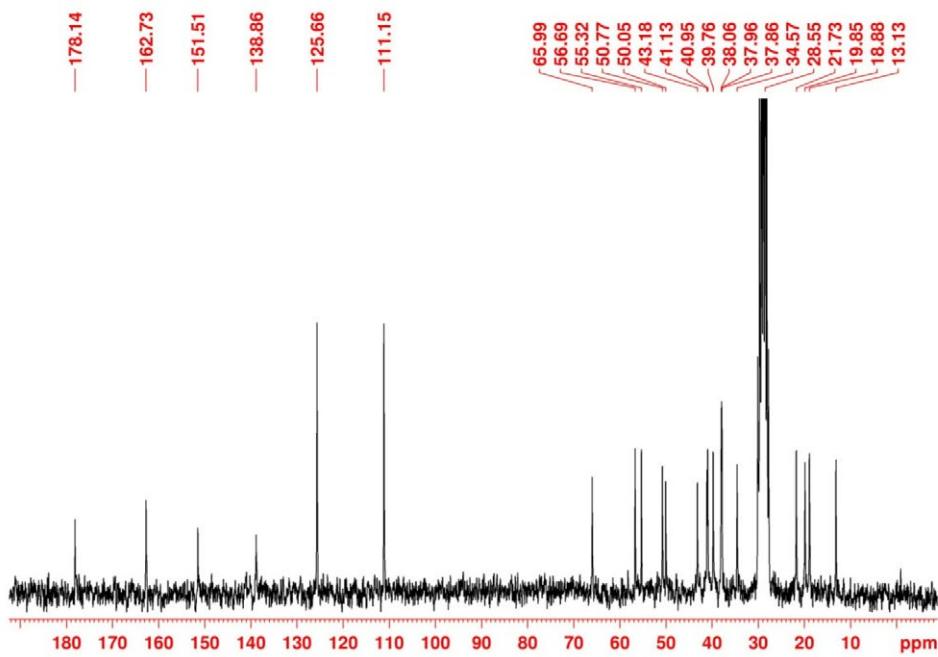


Figure S20. ¹³C NMR spectrum (50 MHz, acetone-*d*₆) of 17-hydroxyisosteviol, 4-nitrophenylhydrazone (**4l**).

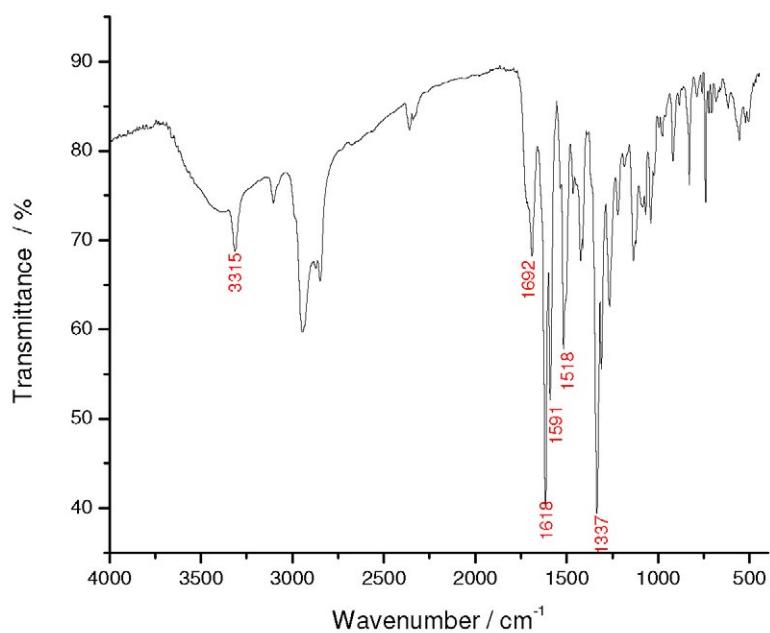


Figure S21. IR spectrum (KBr) of 17-hydroxyisosteviol-2,4-dinitrophenylhydrazone (**4m**).

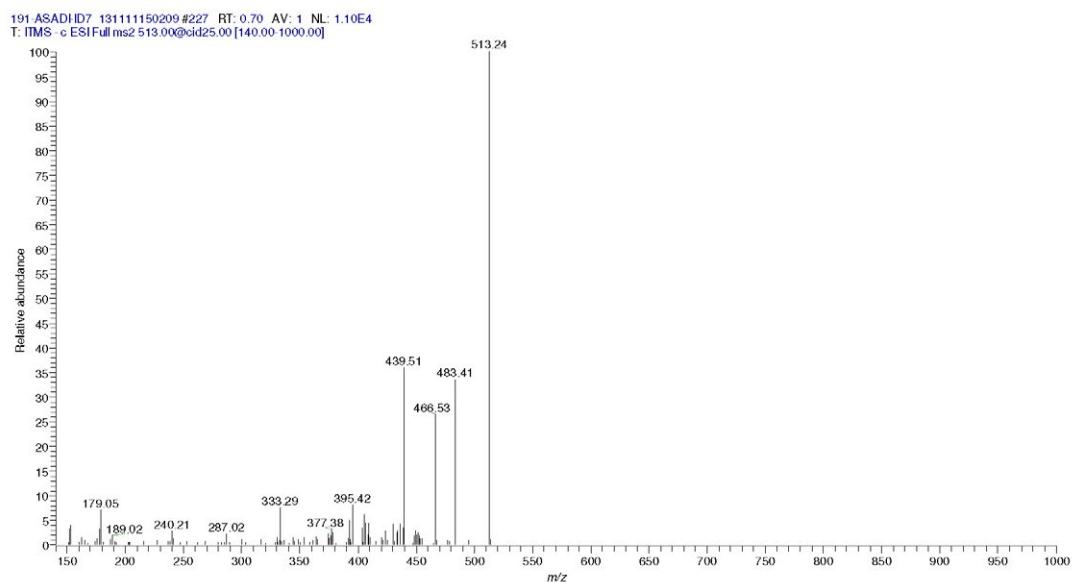


Figure S22. MS-ESI spectrum of 17-hydroxyisosteviol-2,4-dinitrophenylhydrazone (**4m**).

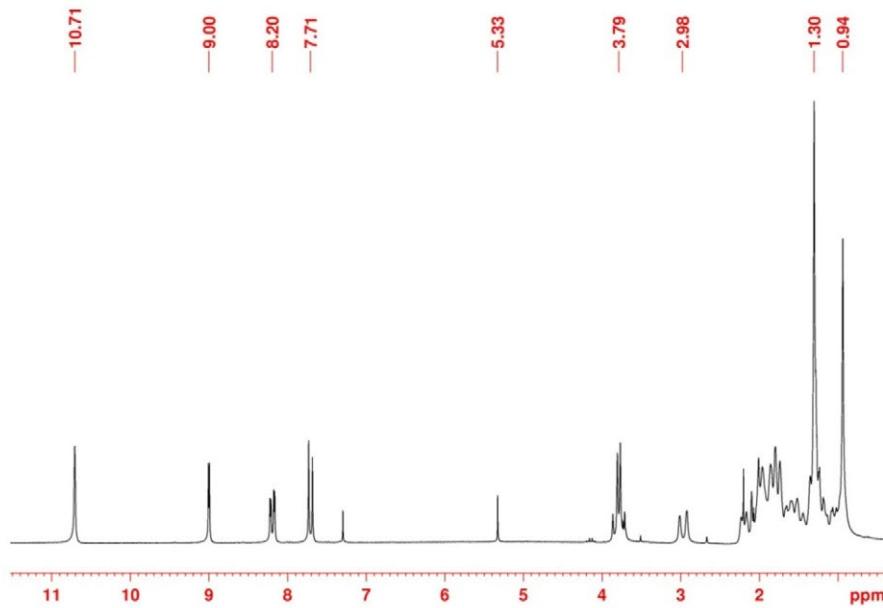


Figure S23. ^1H NMR spectrum (200 MHz, acetone- d_6) of 17-hydroxyisosteviol-2,4-dinitrophenylhydrazone (**4m**).

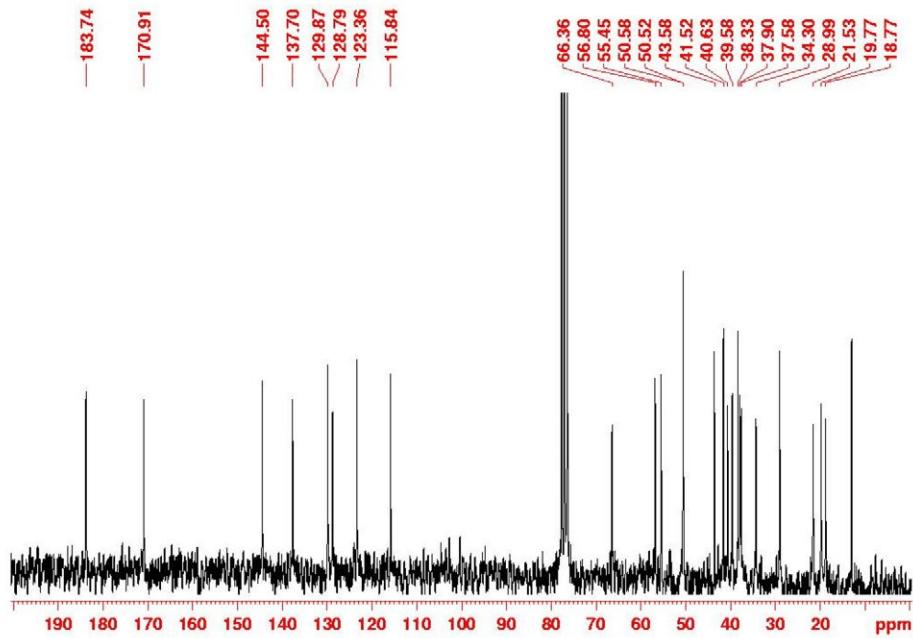


Figure S24. ¹³C NMR spectrum (50 MHz, acetone-*d*₆) of 17-hydroxyisosteviol-2,4-dinitrophenylhydrazone (**4m**).

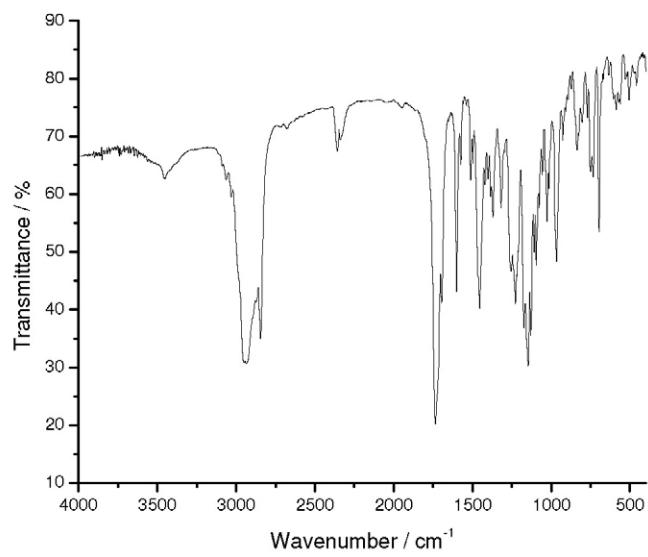


Figure S25. IR spectrum (KBr) of isosteviol *p*-methoxyphenacyl ester (**4n**).

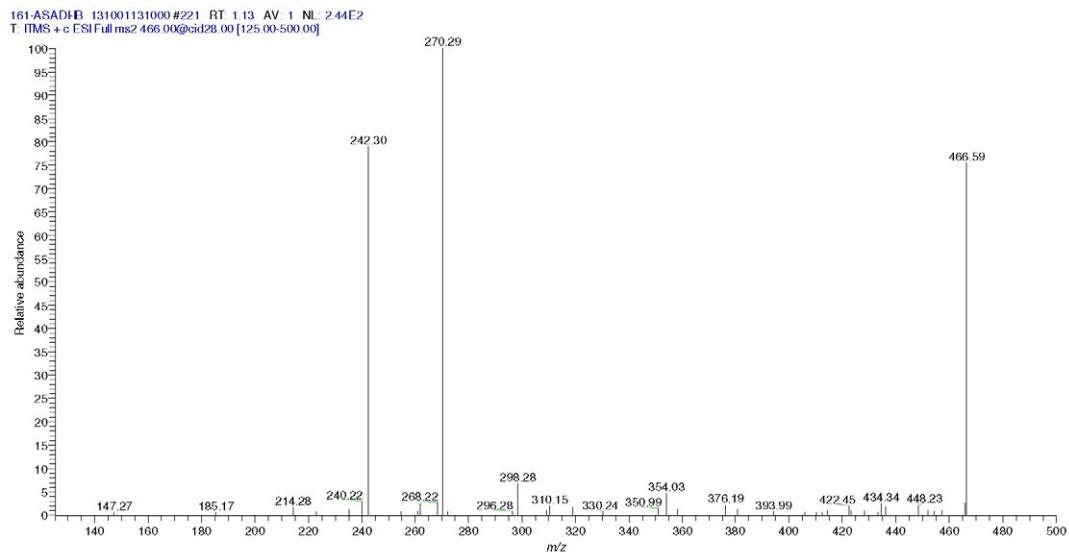


Figure S26. MS-ESI spectrum of isosteviol *p*-methoxyphenacyl ester (**4n**).

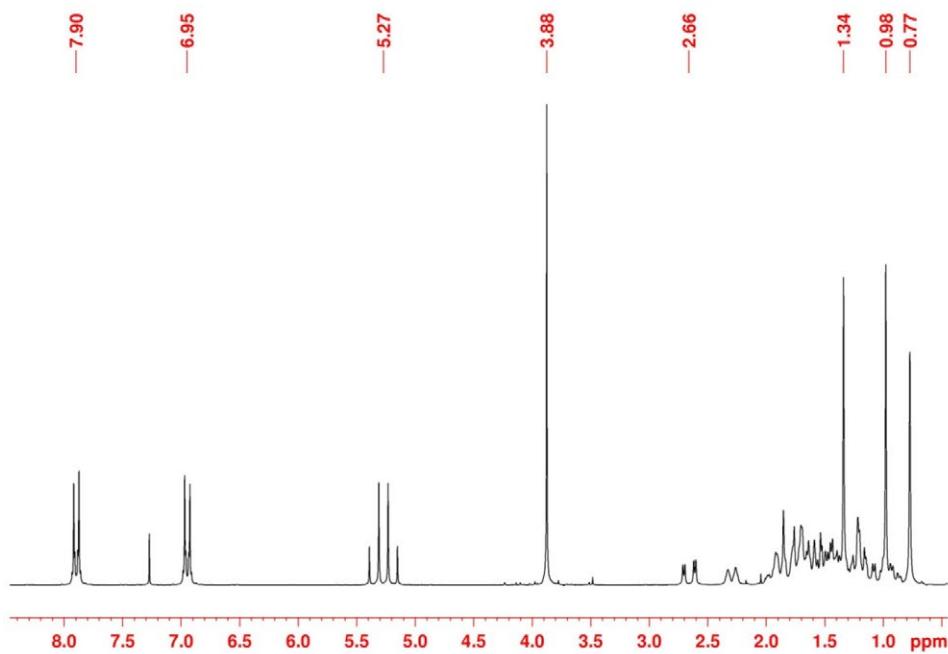


Figure S27. ^1H NMR spectrum (200 MHz, CDCl_3) of isosteviol *p*-methoxyphenacyl ester (**4n**).

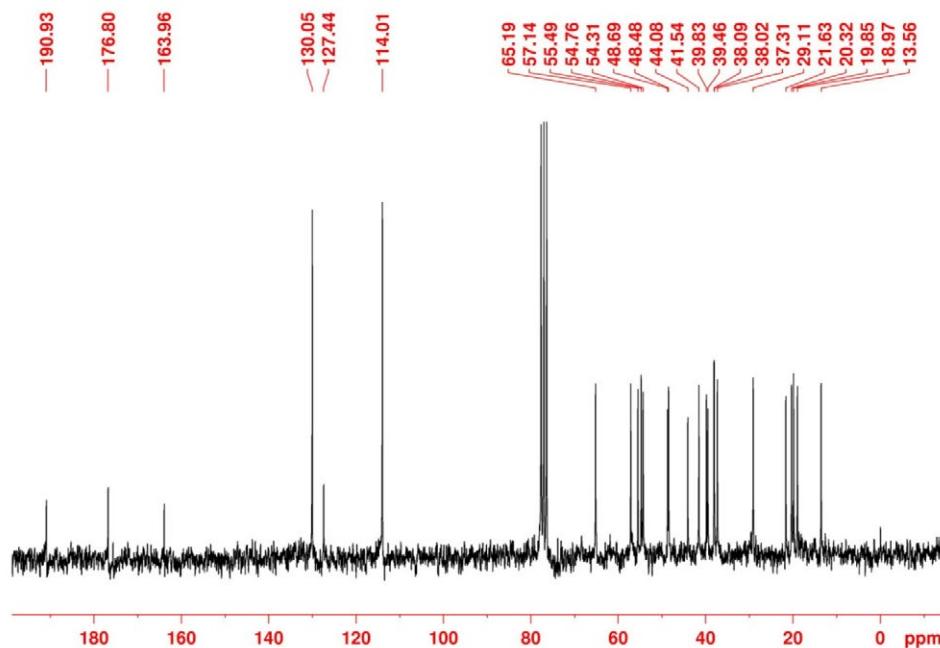


Figure S28. ¹³C NMR spectrum (50 MHz, CDCl₃) of isosteviol *p*-methoxyphenacyl ester (**4n**).

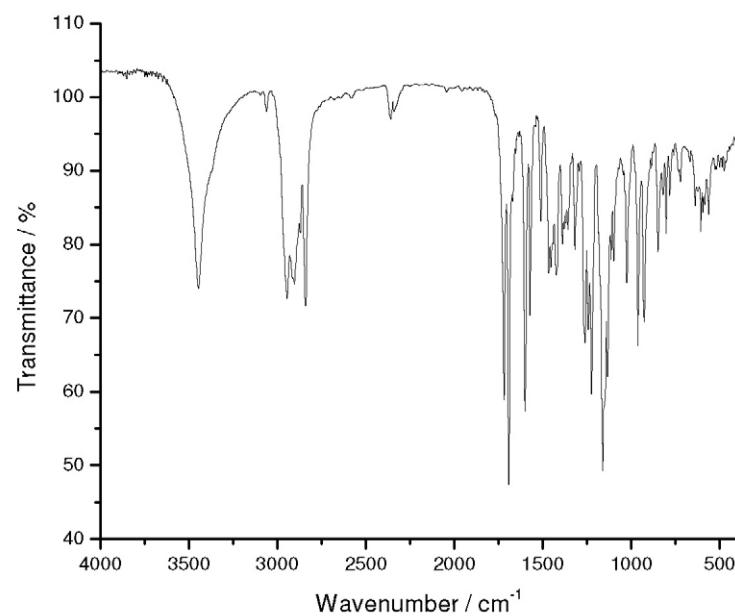


Figure S29. IR spectrum (KBr) of isosteviol oxime *p*-methoxyphenacyl ester (**4o**).

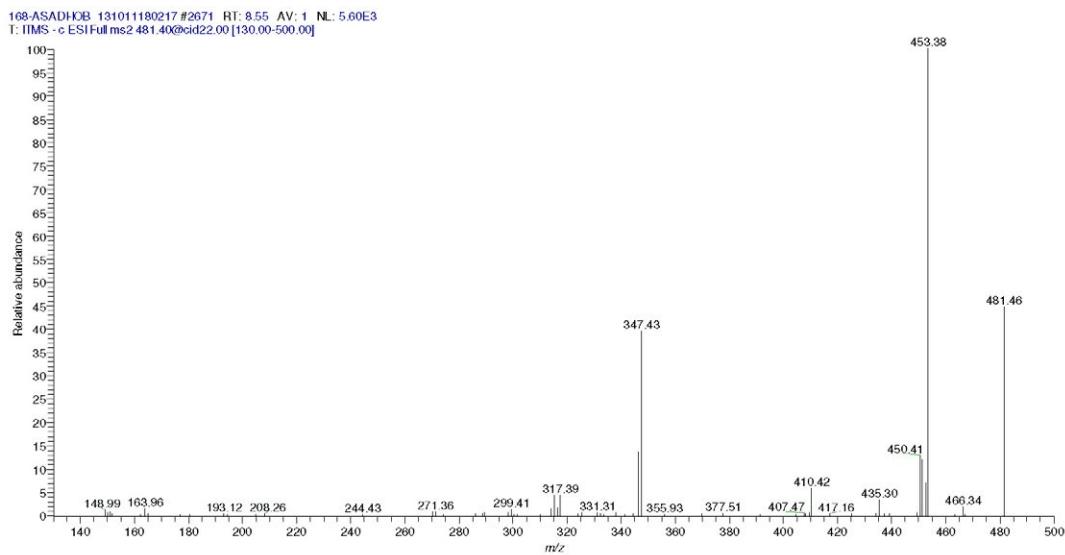


Figure S30. MS-ESI spectrum of isosteviol oxime *p*-methoxyphenacyl ester (**4o**).

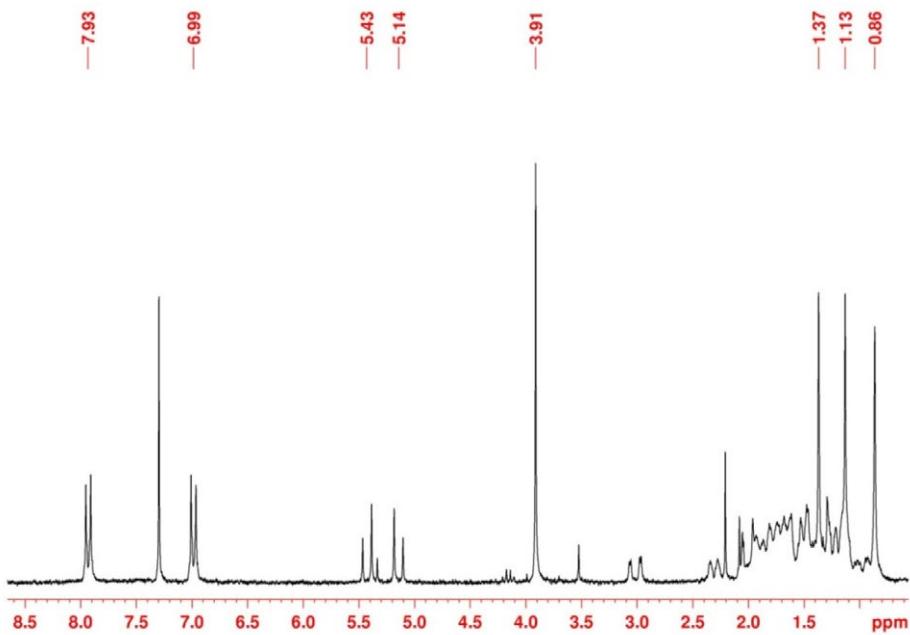


Figure S31. ^1H NMR spectrum (200 MHz, CDCl_3) of isosteviol oxime *p*-methoxyphenacyl ester (**4o**).

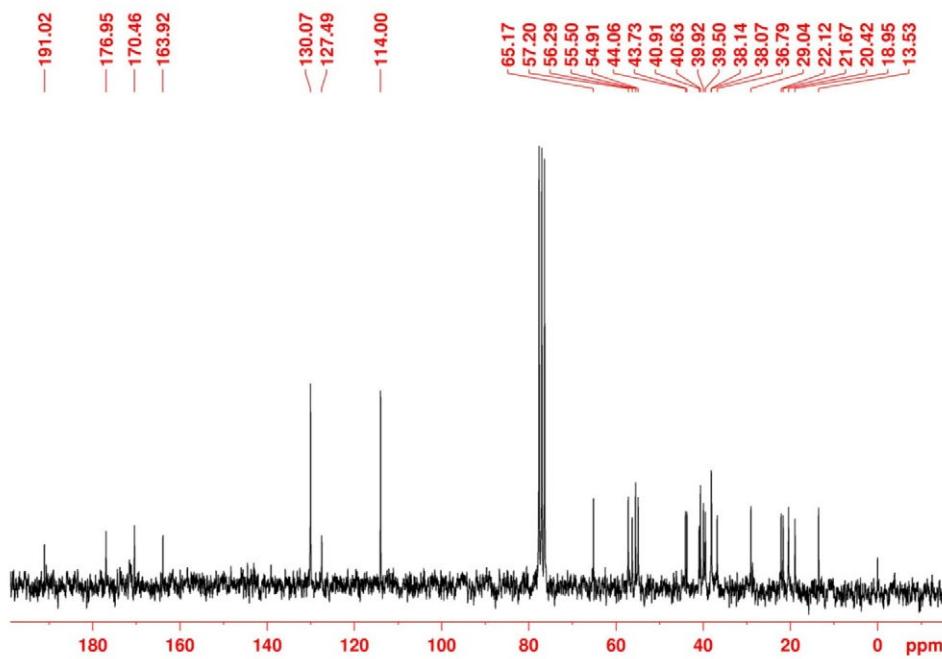


Figure S32. ¹³C NMR spectrum (50 MHz, CDCl₃) of isosteviol oxime *p*-methoxyphenacyl ester (**4o**).

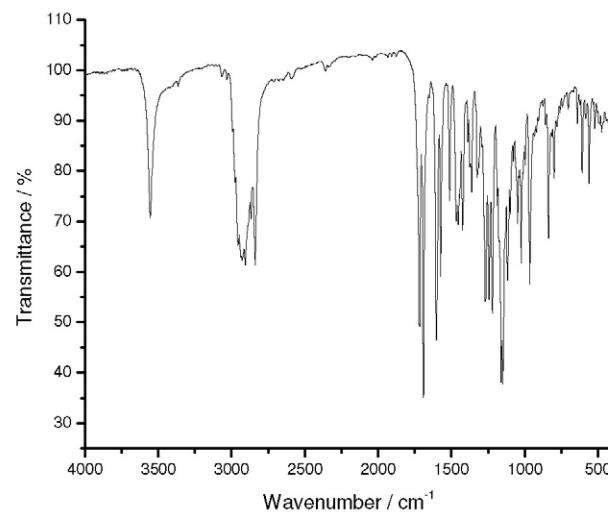


Figure S33. IR spectrum (KBr) of 16-hydroxyisosteviol *p*-methoxyphenacyl ester (**4p**).

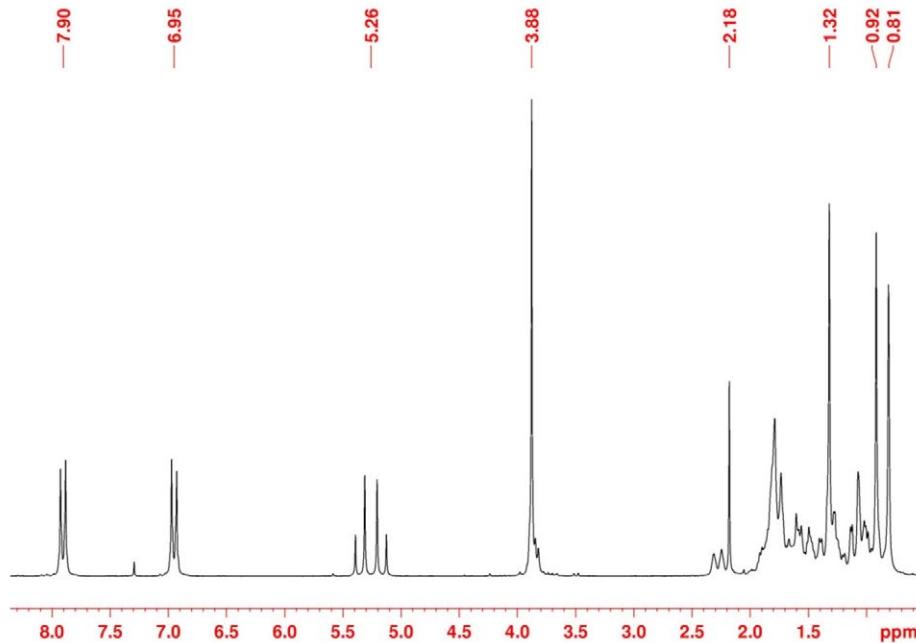


Figure S34. ¹H NMR spectrum (200 MHz, CDCl₃) of 16-hydroxyisosteviol *p*-methoxyphenacyl ester (**4p**).

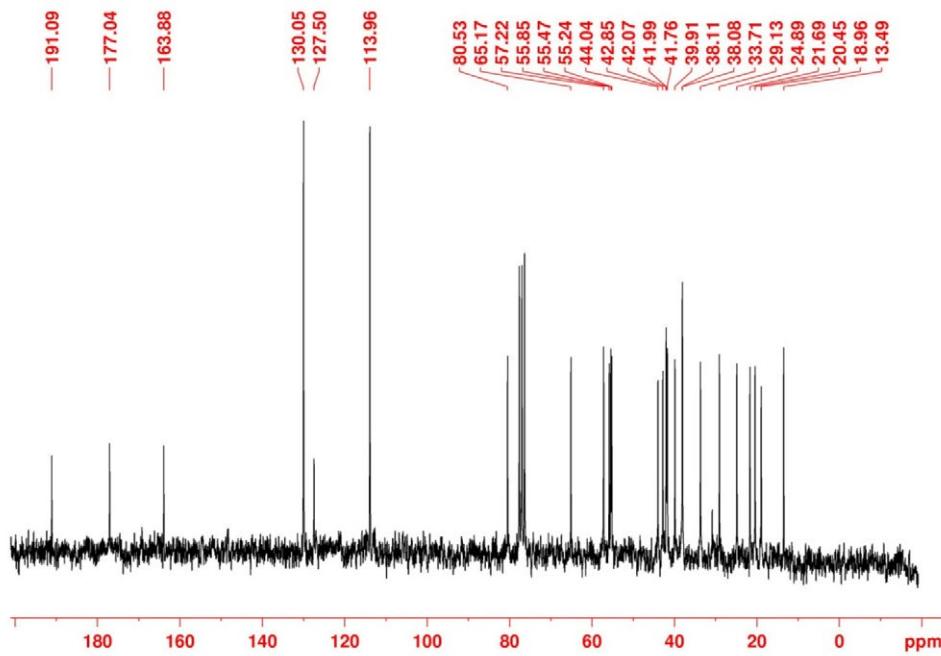


Figure S35. ¹³C NMR spectrum (50 MHz, CDCl₃) of 16-hydroxyisosteviol *p*-methoxyphenacyl ester (**4p**).

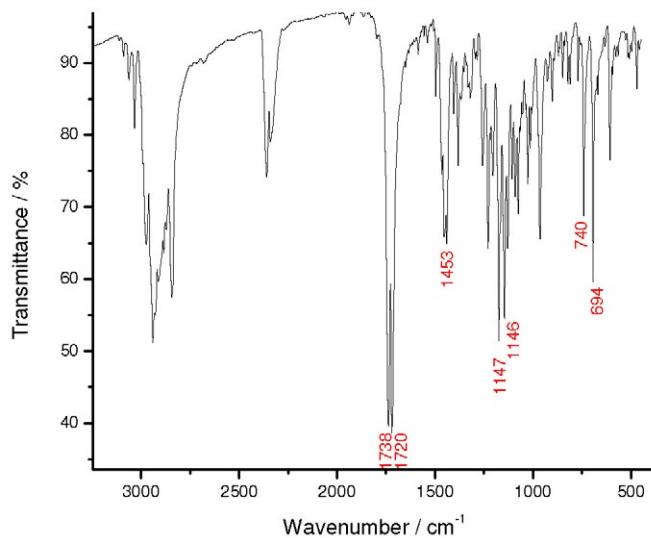


Figure S36. IR spectrum (KBr) of isosteviol benzyl ester (**4q**).

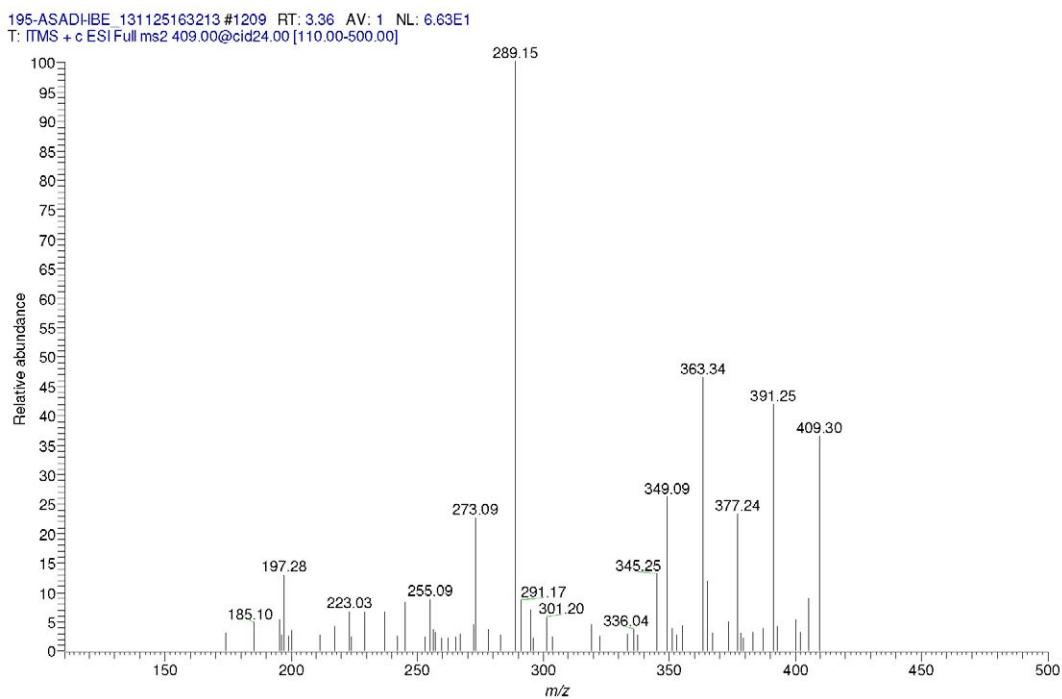


Figure S37. MS-ESI spectrum of isosteviol benzyl ester (**4q**).

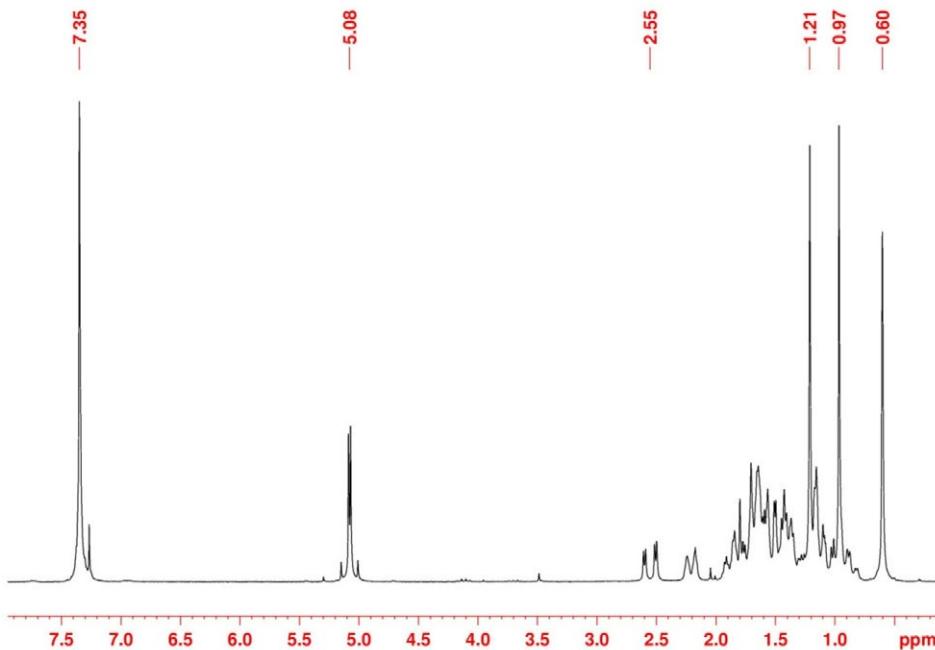


Figure S38. ¹H NMR spectrum (200 MHz, CDCl₃) of isosteviol benzyl ester (**4q**).

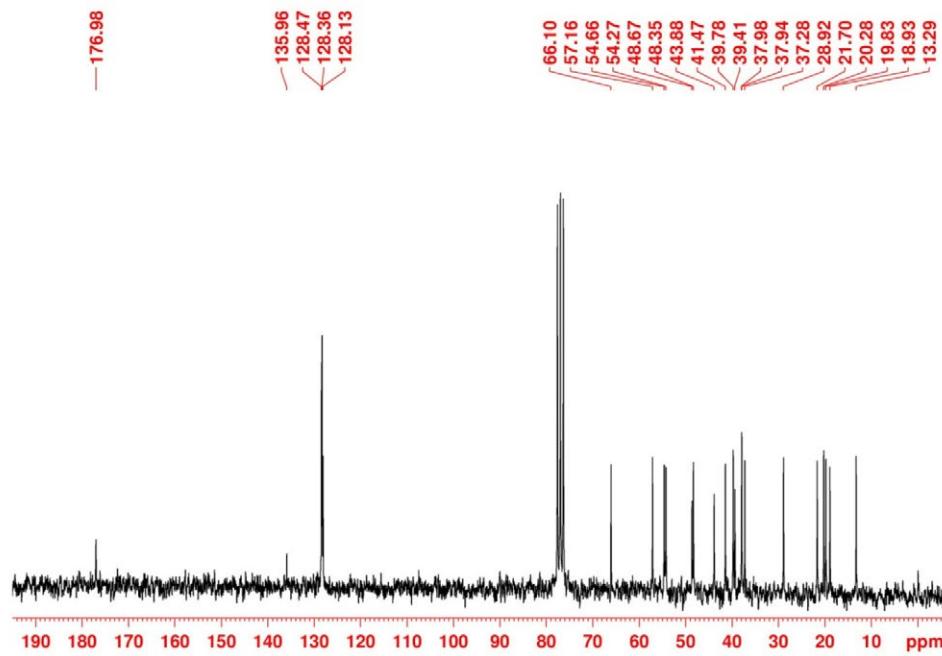


Figure S39. ¹³C NMR spectrum (50 MHz, CDCl₃) of isosteviol benzyl ester (**4q**).

Table S1. ^{13}C NMR (50 MHz, CDCl_3) data for phenacyl ester derivatives

C	3e	4n	4o	4p	4q
1	40.6	39.8	39.9	39.9	39.7
2	19.1	18.9	18.9	18.9	18.9
3	38.0	37.3	38.1	38.1	37.3
4	44.1	44.1	43.7	44.1	43.8
5	56.9	57.1	57.1	57.2	57.2
6	21.9	21.6	21.7	21.7	21.7
7	41.3	41.5	39.5	41.7	41.5
8	41.6	39.5	40.6	41.9	39.4
9	53.7	54.7	54.9	55.8	54.6
10	39.4	38.1	38.1	38.1	37.9
11	20.4	20.3	20.4	20.4	20.3
12	39.2	38.0	36.7	33.7	37.9
13	80.2	48.7	44.0	42.1	48.6
14	47.4	54.3	56.3	55.3	54.2
15	46.9	48.5	40.9	42.8	48.3
16	156.2	176.8	170.4	80.5	177.0
17	102.8	19.8	22.1	24.9	19.8
18	28.9	29.1	29.0	29.1	28.9
19	176.9	176.8	177.0	177.0	176.9
20	15.7	13.5	13.5	13.5	13.3
1'	127.4	127.4	127.0	127.5	135.9
2'	130.1	130.0	130.1	130.0	128.3
3'	113.9	114.0	113.9	113.9	128.4
4'	163.9	163.9	163.9	163.9	128.1
5'	113.9	114.0	113.9	113.9	128.4
6'	130.1	130.0	130.1	130.0	128.3
C=O ketone	191.0	190.9	190.9	191.1	—
CH_3O	65.2	65.2	65.2	65.2	
αC	55.5	55.5	55.5	55.5	65.1

Table S2. ^{13}C NMR data for hydrazone derivatives

C	4d (50 MHz, CDCl_3)	4e (50 MHz, CDCl_3)	4k (50 MHz, CD_3OD)	4l (50 MHz, acetone- d_6)	4m (50 MHz, acetone- d_6)
1	39.9	39.8	40.2	39.7	39.6
2	18.9	18.8	19.2	18.9	18.7
3	37.9	37.6	38.6	37.9	37.9
4	43.8	43.7	44.1	43.2	43.6
5	57.2	56.9	57.4	56.7	56.8
6	21.7	21.6	21.9	21.7	21.5
7	39.4	39.4	36.8	37.8	37.6
8	40.6	41.4	40.8	41.1	41.5
9	55.0	54.8	55.6	55.3	55.4
10	37.9	38.3	38.0	38.0	38.3
11	20.5	20.6	19.6	19.8	19.7
12	39.0	36.6	34.2	34.5	34.3
13	44.2	44.7	49.1	50.0	50.6
14	56.0	55.9	51.0	50.8	50.5
15	41.1	41.1	41.2	40.9	40.6
16	174.3	163.5	165.4	162.7	170.9
17	24.9	22.2	66.1	65.0	66.4
18	28.8	29.0	28.8	28.4	28.0
19	177.9	184.0	182.9	178.1	183.7
20	13.2	13.6	12.9	13.1	12.9
1'	22.2	139.6	—	138.8	128.8
2'	159.1	111.4	—	111.1	137.7
3'	17.6	126.1	—	125.6	129.9
4'	—	150.6	—	151.5	144.5
5'	—	126.1	—	125.6	123.4
CH_3O	51.2	—	—	111.1	115.8