

New Biologically Active Chromanes and Chromenes from the Monotypic Plant Species *Koeberlinia spinosa*

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S1 Spectroscopic Data for **1** (3*E*,7*E*)-9-hydroxy-1-((*S*)-6-hydroxy-2,8-dimethylchroman-2-yl)-4,8-dimethylnona-3,7-dien-2-one.

Table S1. ¹H and ¹³C NMR Assignments for Compound **1**^a

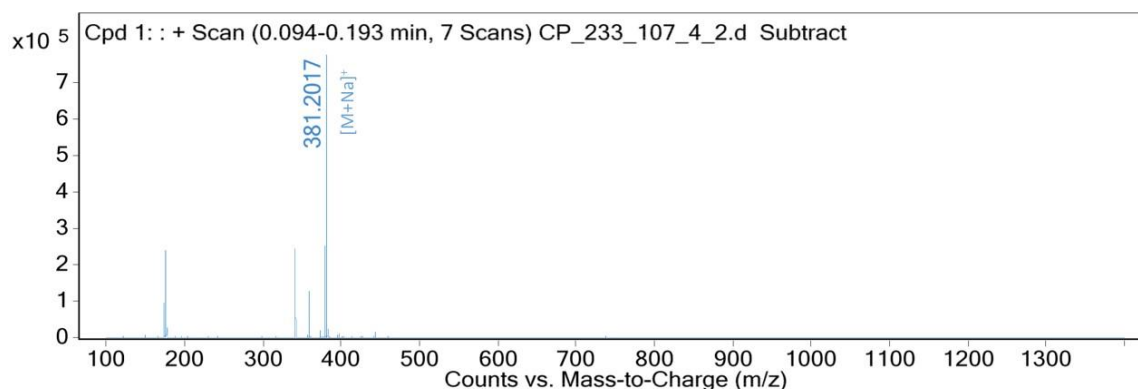
position	δ _C , type	δ _H (J in Hz)	HMBC
2	76.2, C		
3	33.1, CH ₂	1.90, dt (13.6, 6.9) 1.79, dt (13.6, 6.9)	2, 4, 4a, 1', 12' 2, 4, 4a, 1', 12'
4	23.3, CH ₂	2.71, t (6.9)	2, 3, 4a, 5, 6, 8, 8a
4a	122.0, C		
5	113.7, CH	6.35, d (2.9)	4, 6, 7, 8, 8a
6	150.8, C		
7	116.8, CH	6.43, d (2.9)	5, 6, 8a, 13'
8	127.8, C		
8a	145.7, C		
1'	53.7, CH ₂	2.82, d (13.1) 2.55, d (13.1)	2, 3, 2', 3', 12' 2, 3, 2', 3', 12'
2'	201.7, C		
3'	126.2, CH	6.19, br s	2', 4', 5', 11'
4'	159.5, C		
5'	41.9, CH ₂	2.19, m ^b	3', 4', 6', 7', 11'
6'	26.7, CH ₂	2.20, m ^b	4', 5', 7', 8'
7'	125.1, CH	5.36, br t (6.7)	5', 6', 9', 10'
8'	137.0, C		
9'	68.7, CH ₂	3.89, s	7', 8', 10'
10'	13.7, CH ₃	1.63, d (1.4)	7', 8', 9'
11'	19.6, CH ₃	2.12, d (1.2)	1', 2', 3', 4'
12'	25.3, CH ₃	1.34, s	2, 3, 1'
13'	16.5, CH ₃	2.06, s	7, 8, 8a

^aNMR data obtained in CD₃OD at 500 MHz for δ_H and 125 MHz for δ_C.

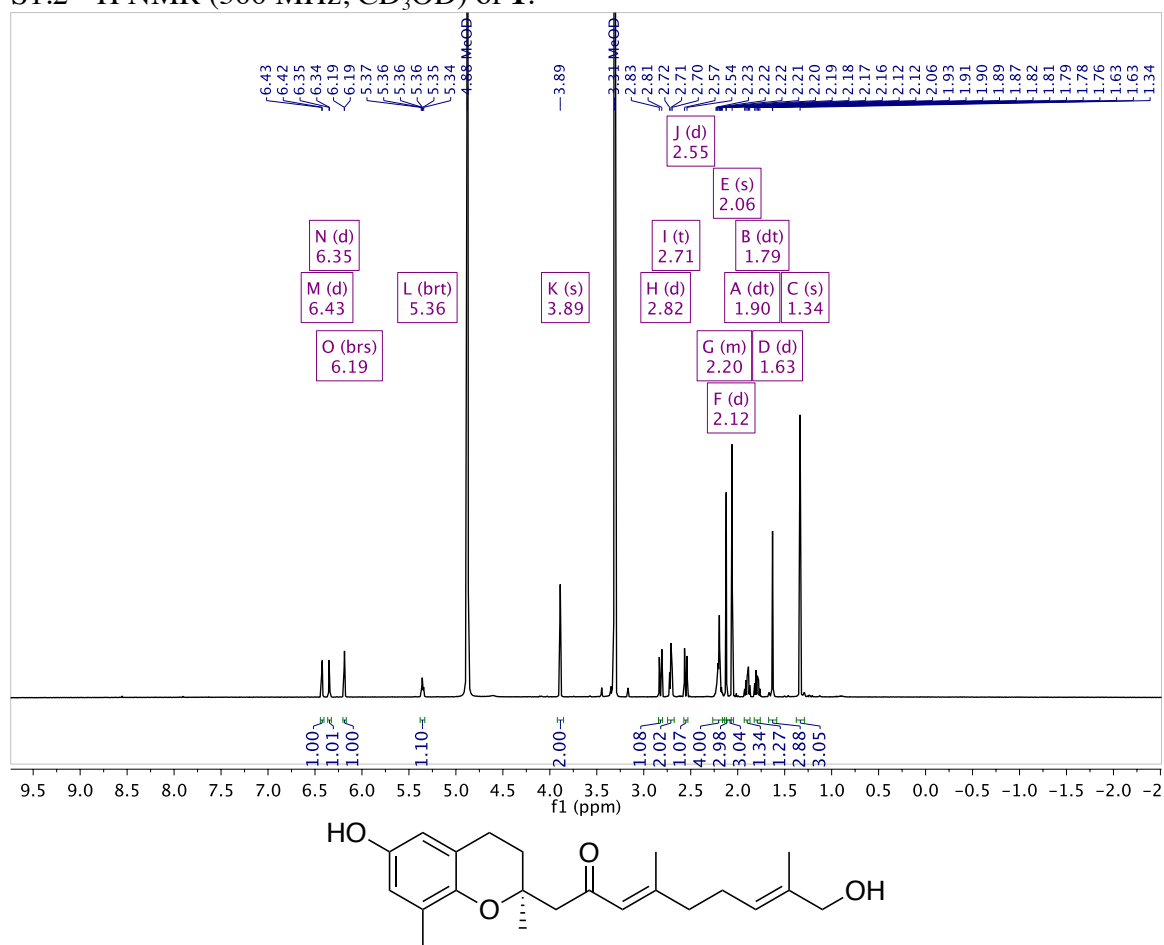
Assignments were made utilizing ¹H, ¹³C, HSQC, and HMBC experiments.

^bOverlapping signals, assignments were made via HSQC correlations.

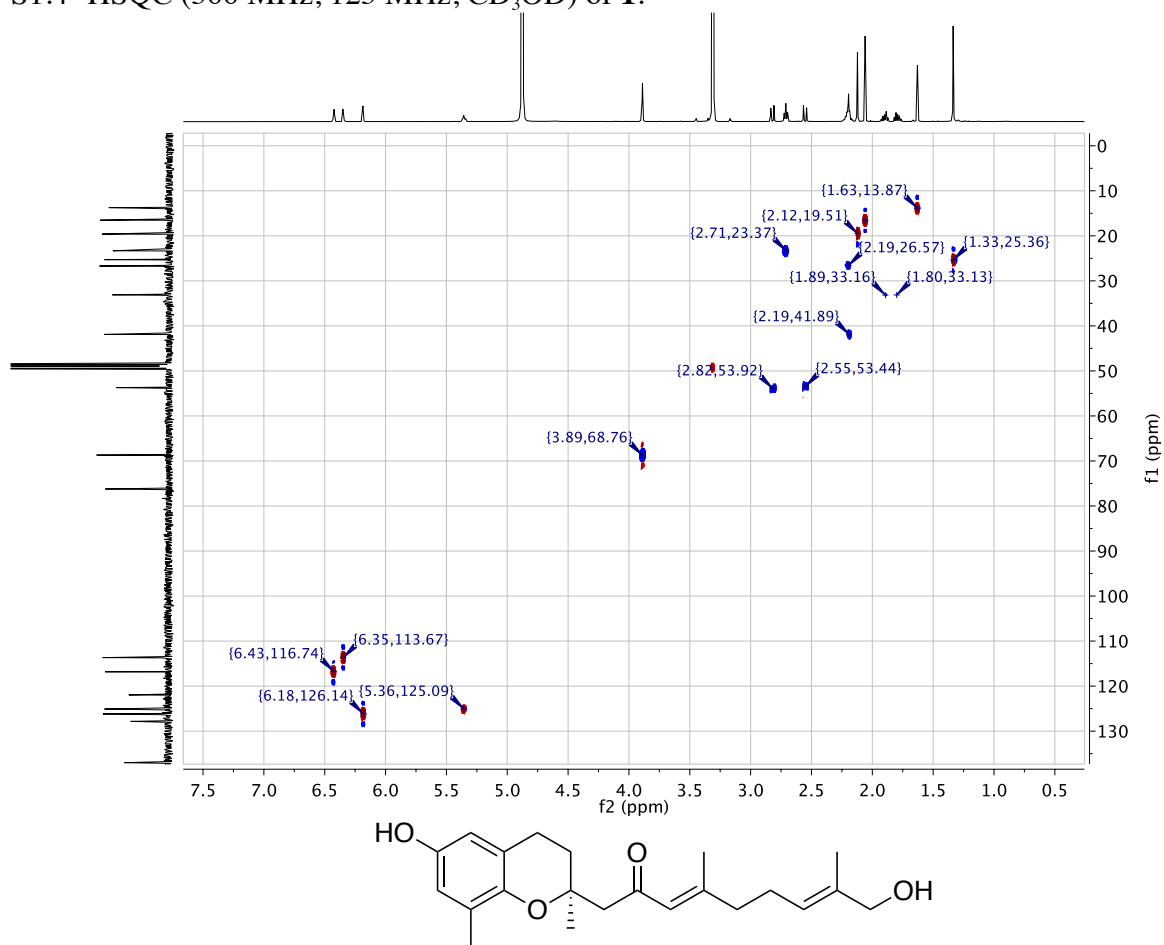
S1.1 HRESIMS Spectroscopic Data of **1**.



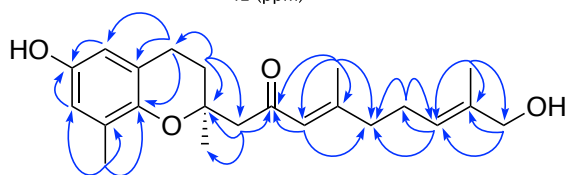
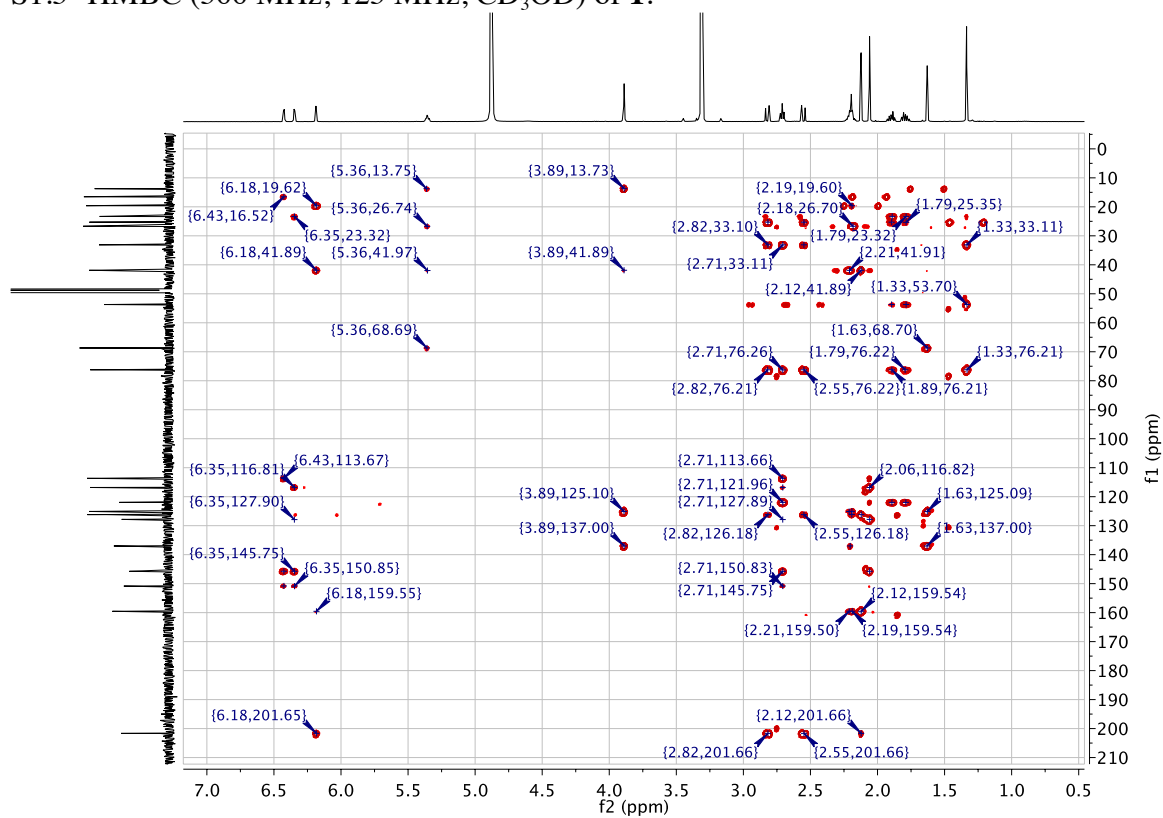
S1.2 ^1H NMR (500 MHz, CD_3OD) of **1**.



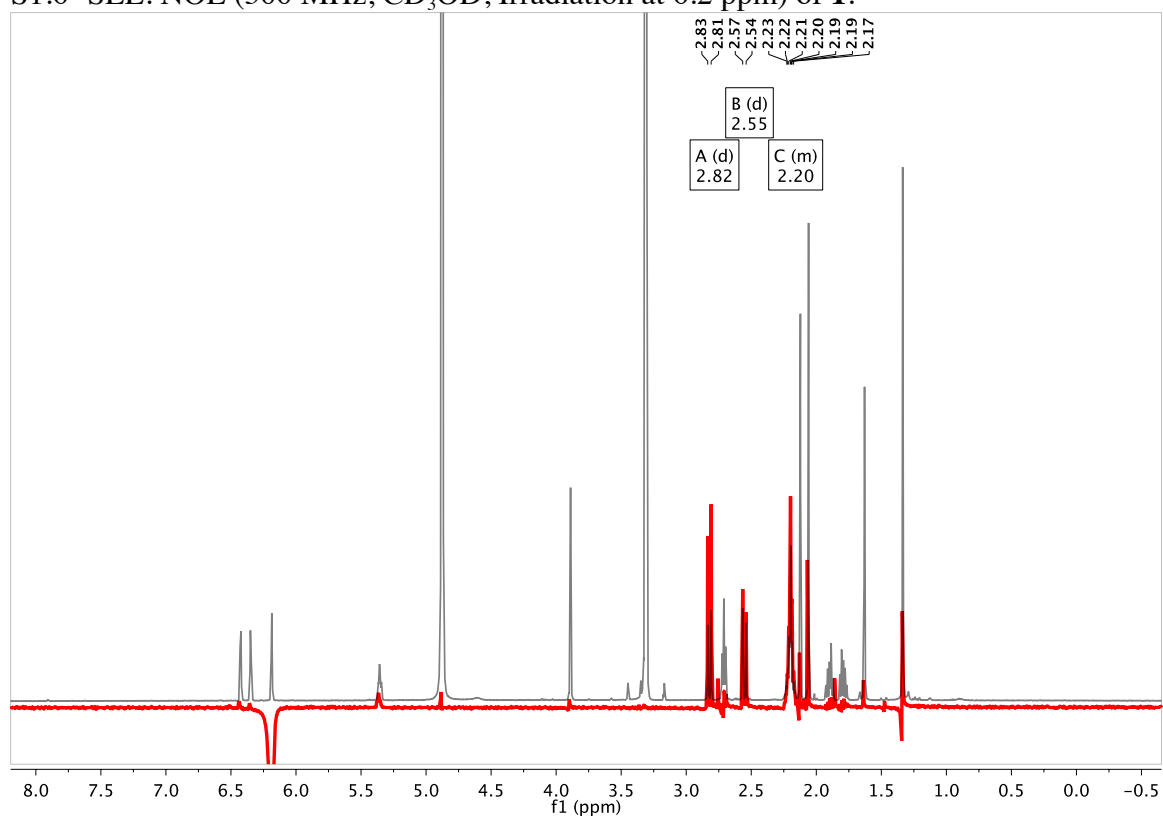
S1.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **1**.



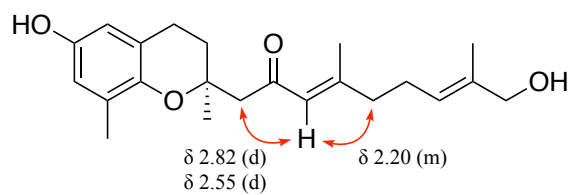
S1.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **1**.



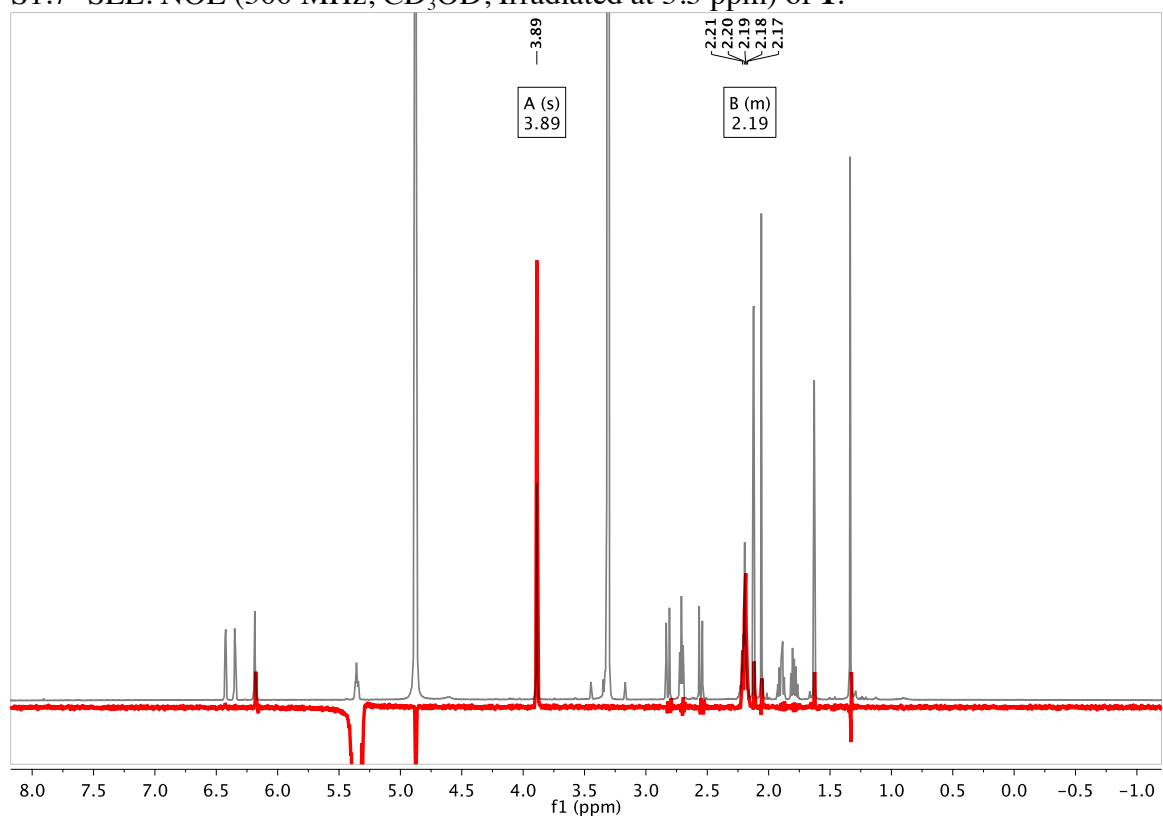
S1.6 SEL. NOE (500 MHz, CD₃OD, Irradiation at 6.2 ppm) of **1**.



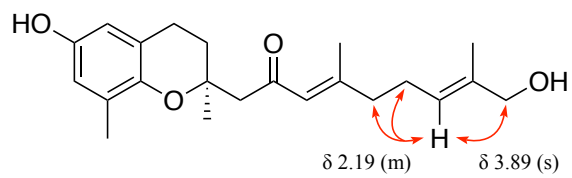
SEL. NOE in red. ¹H NMR in gray.



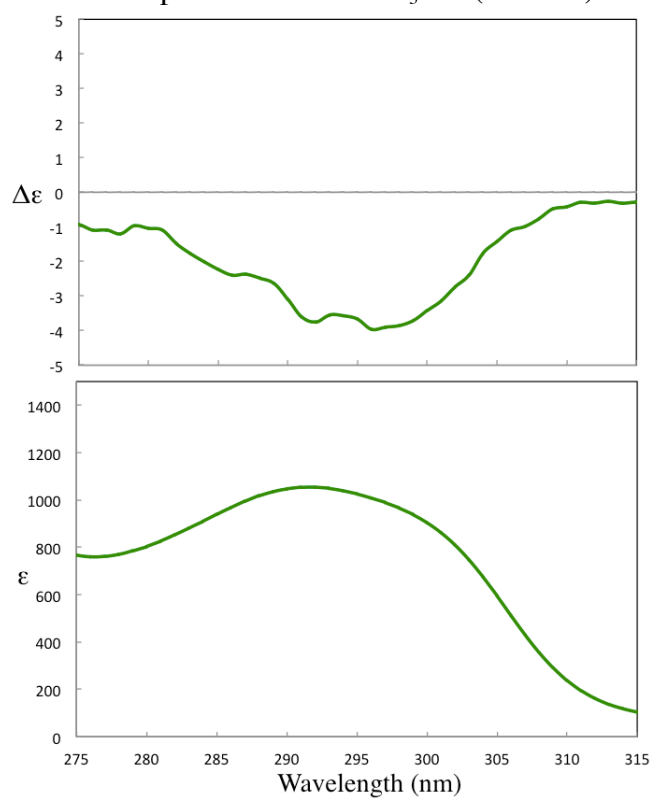
S1.7 SEL. NOE (500 MHz, CD₃OD, Irradiated at 5.3 ppm) of **1**.



SEL. NEO in red. ¹H NMR in gray.

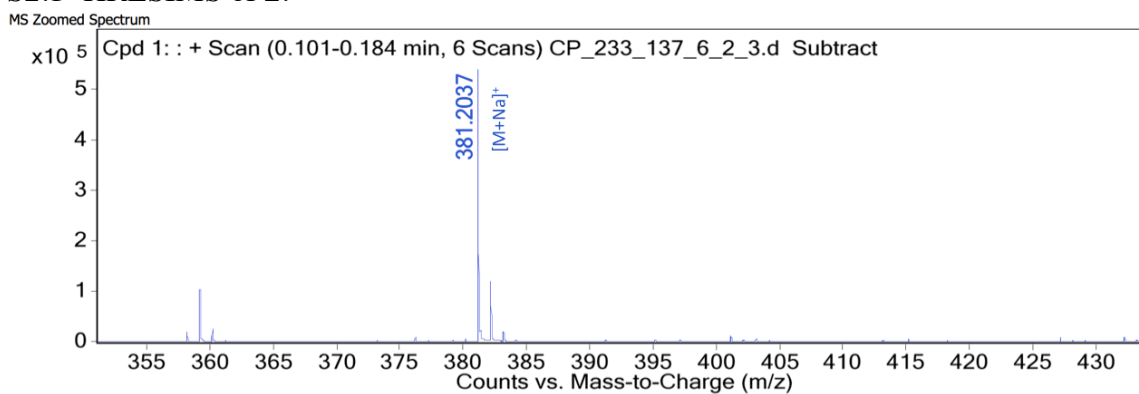


S1.8 ECD Spectrum of **1** in CH₃OH (0.5 mM)

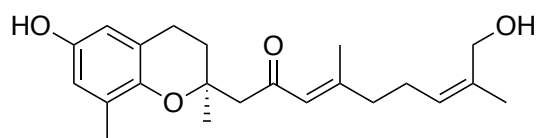
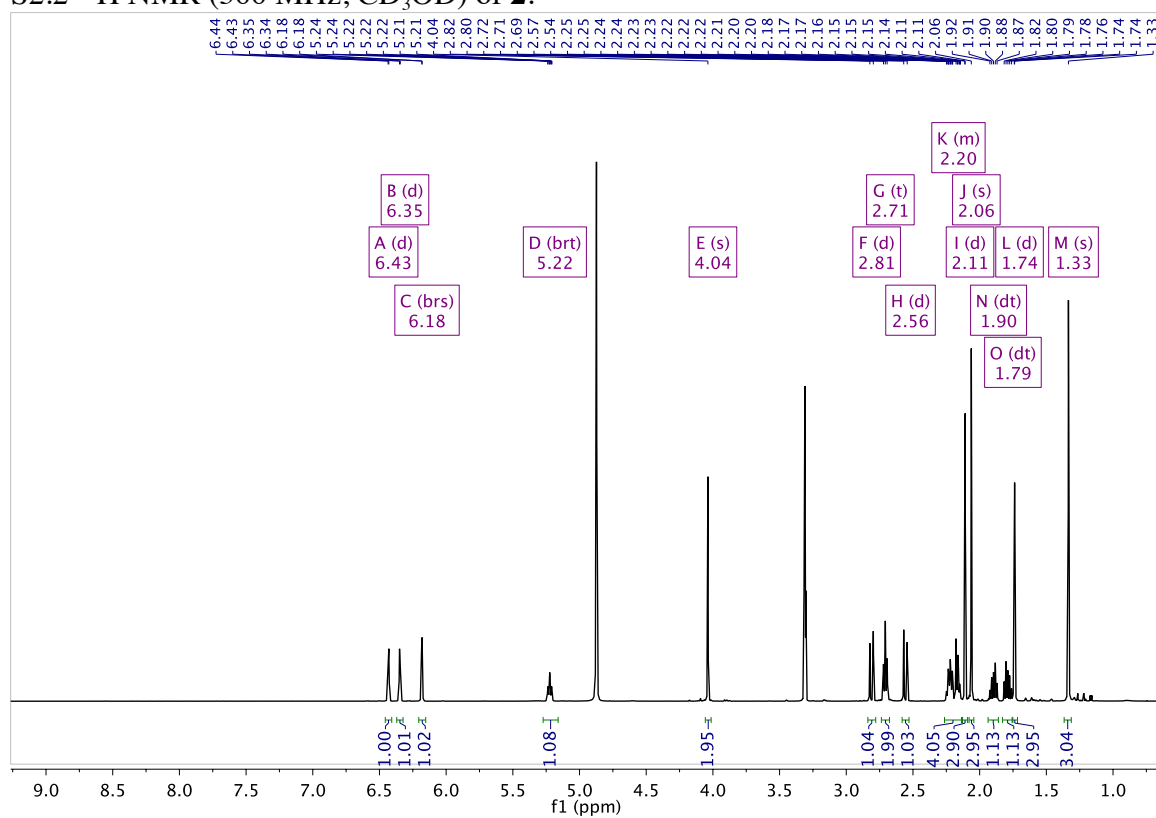


S2 Spectroscopic Data for **2** (3*E*,7*Z*)-9-hydroxy-1-((*S*)-6-hydroxy-2,8-dimethylchroman-2-yl)-4,8-dimethylnona-3,7-dien-2-one.

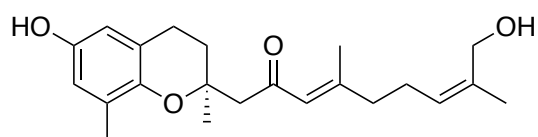
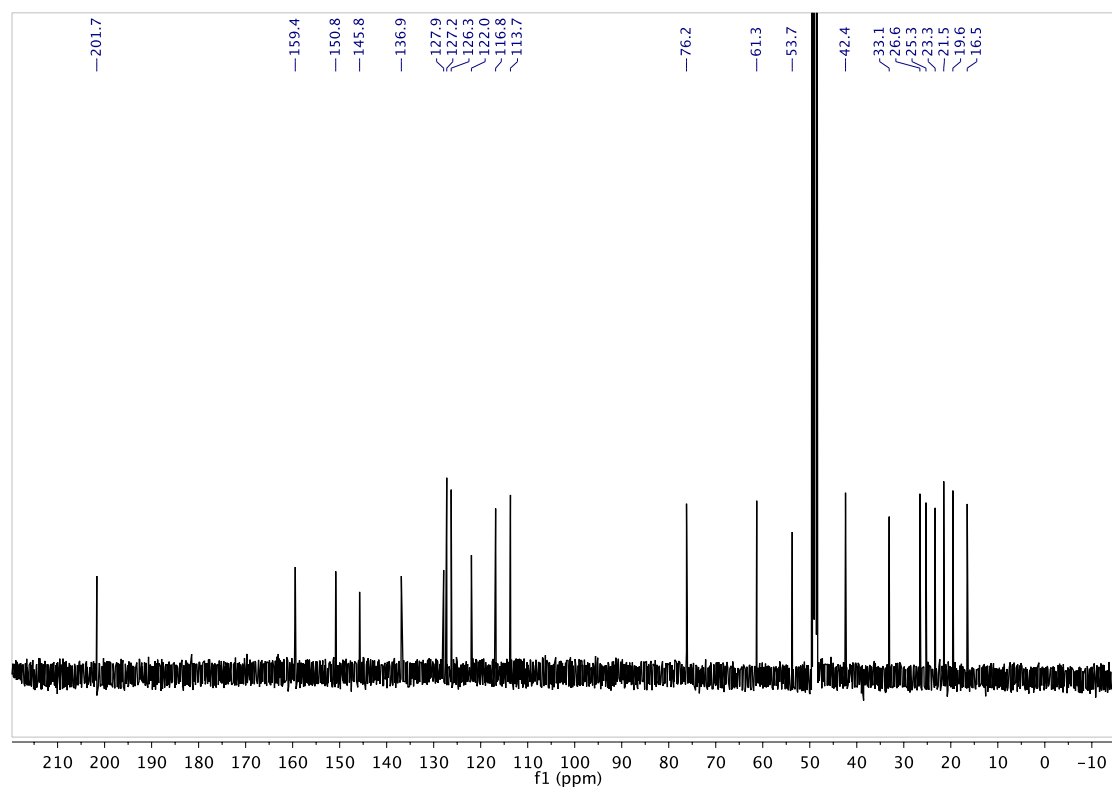
S2.1 HRESIMS of **2**.



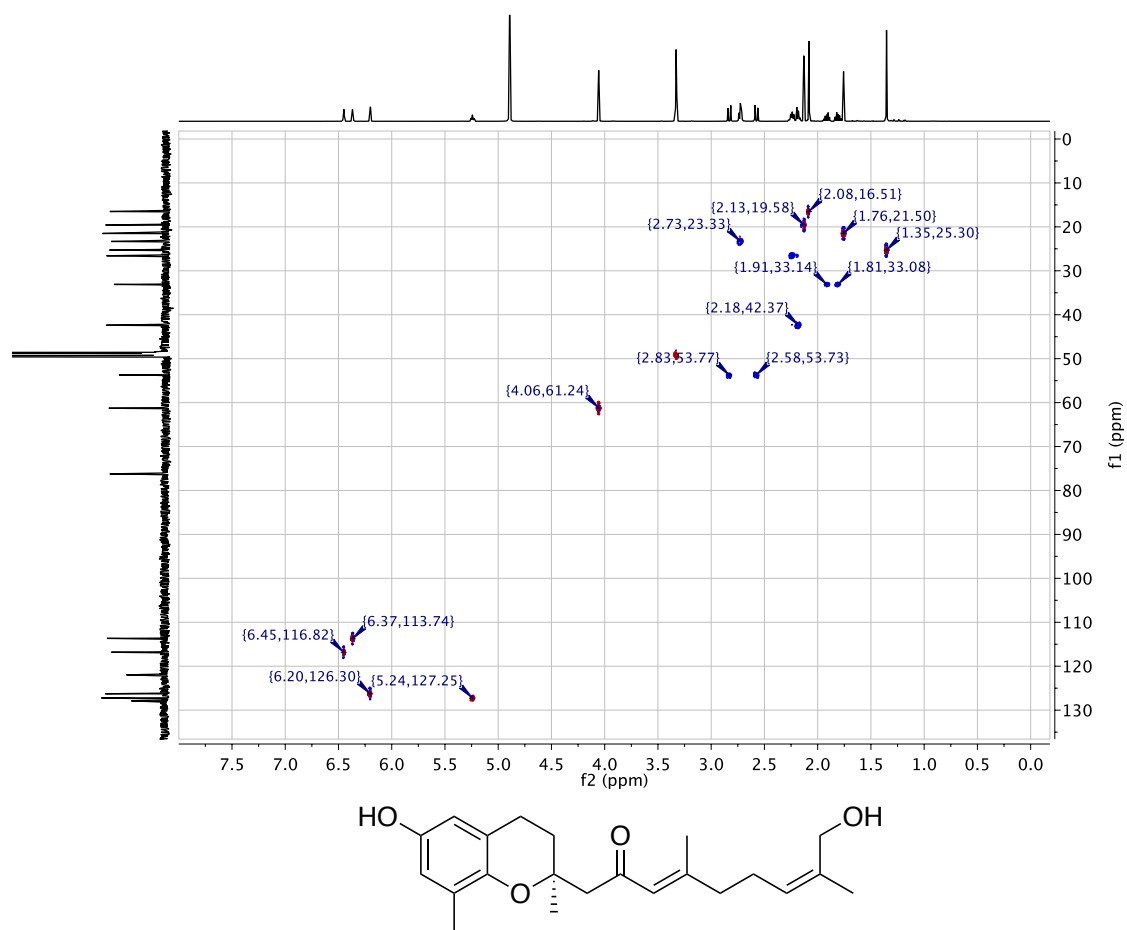
S2.2 ^1H NMR (500 MHz, CD_3OD) of **2**.



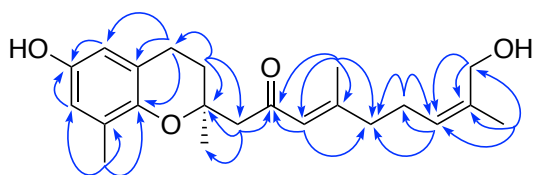
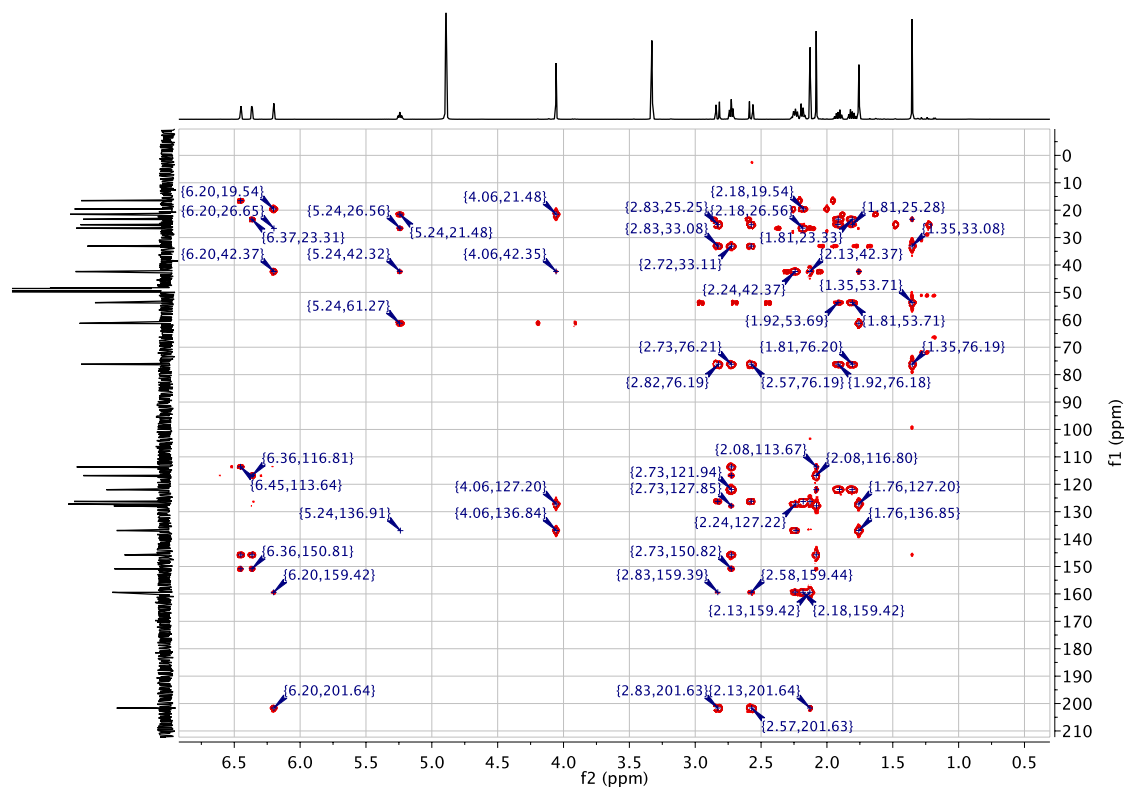
S2.3 ^{13}C NMR (125 MHz, CD_3OD) of **2**.



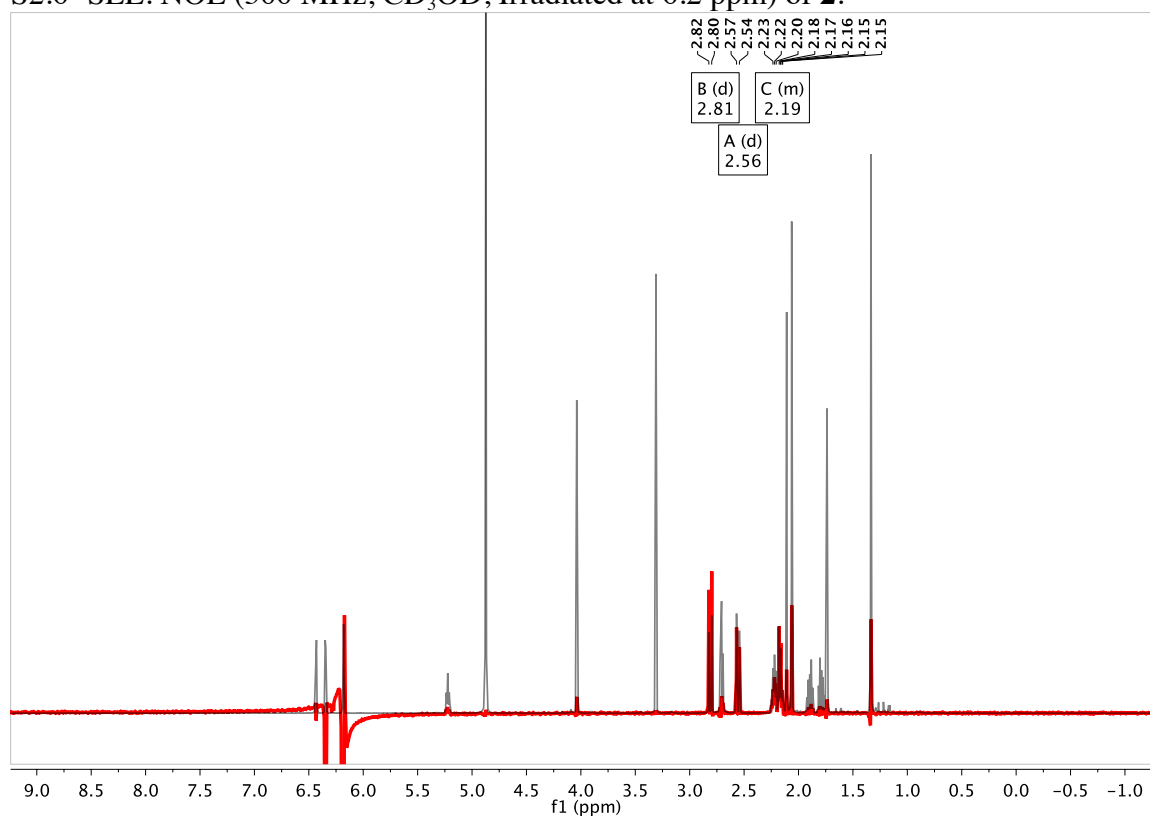
S2.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **2**.



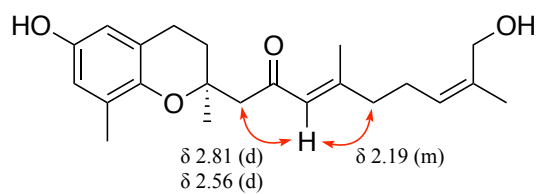
S2.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **2**.



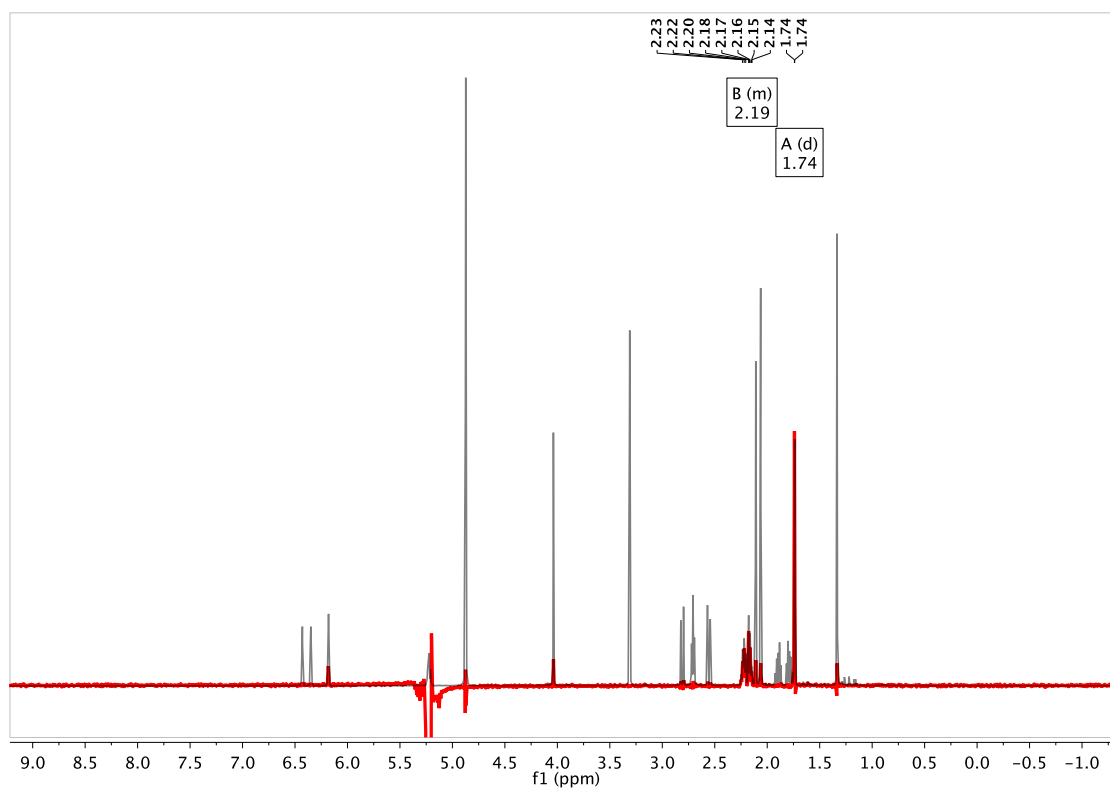
S2.6 SEL. NOE (500 MHz, CD₃OD, Irradiated at 6.2 ppm) of **2**.



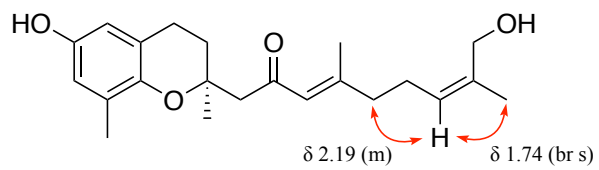
SEL. NOE in red. ¹H NMR in gray.



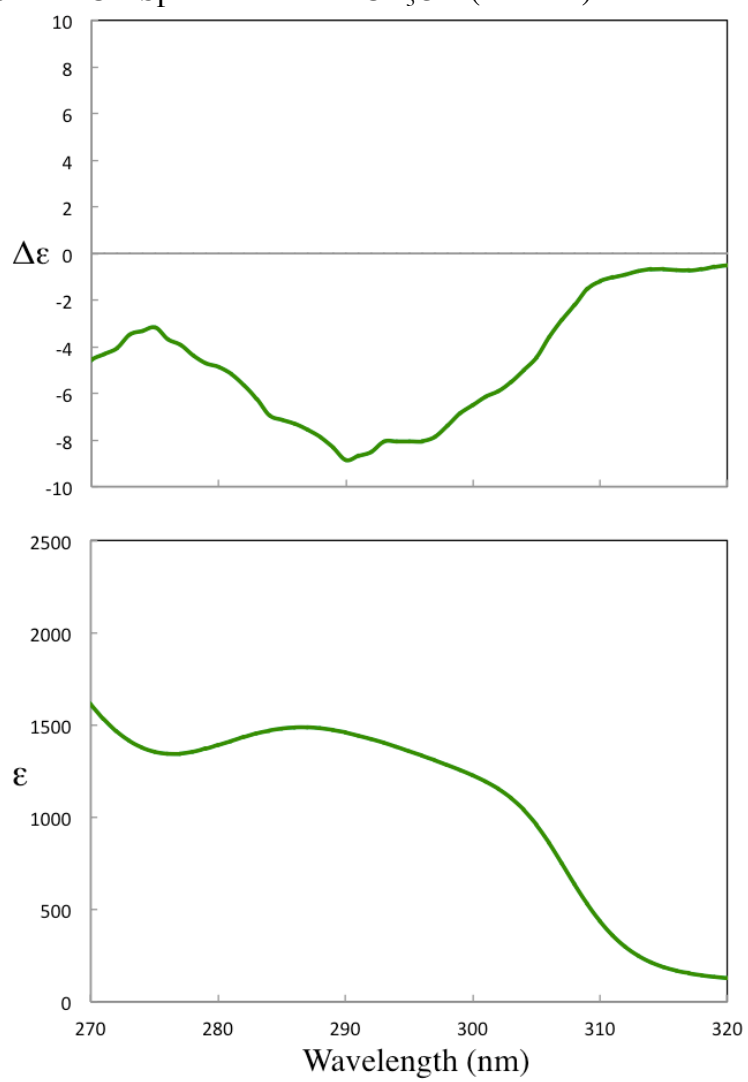
S2.7 SEL. NOE (500 MHz, CD₃OD, Irradiated at 5.3 ppm) of **2**.



SEL. NOE in red. ¹H NMR in gray.

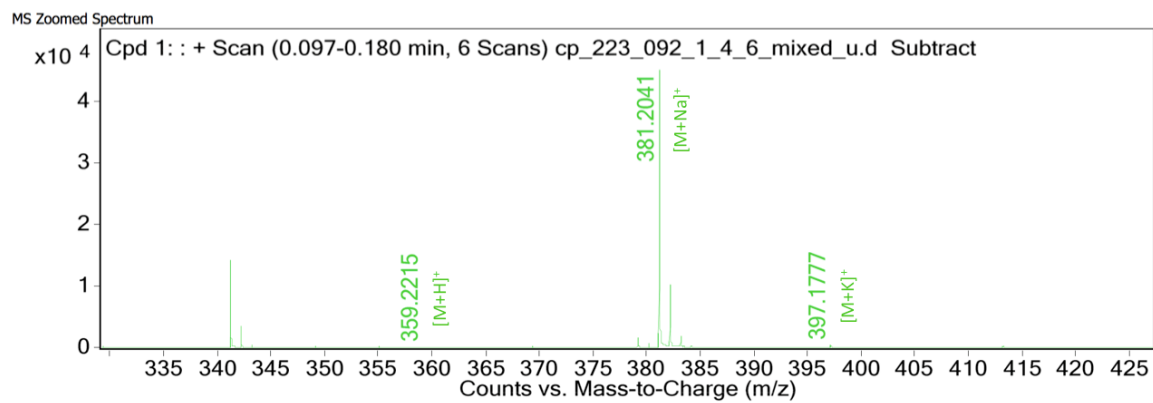


S2.8 ECD Spectrum of **2** in CH₃OH (1.0 mM).

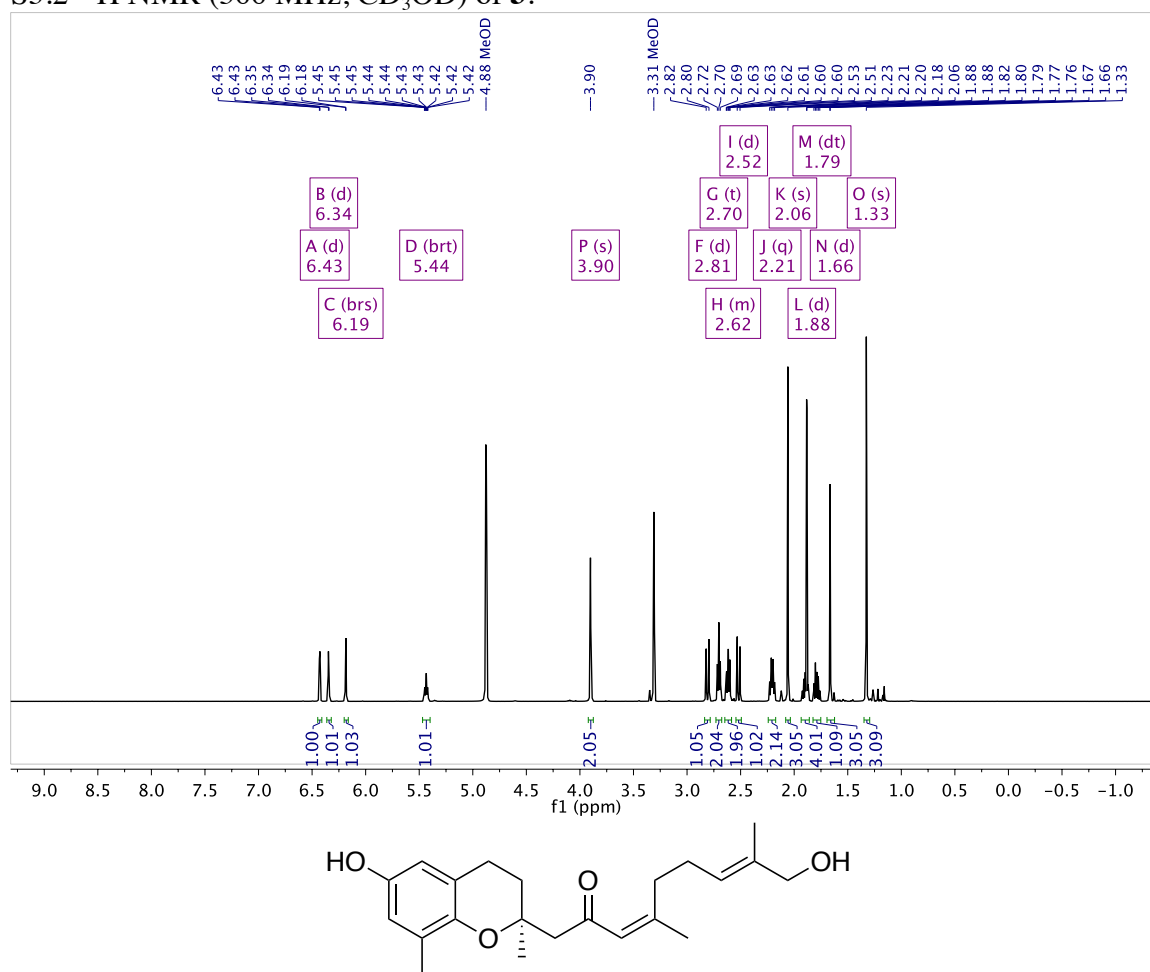


S3 Spectroscopic Data for **3** (3*Z*,7*E*)-9-hydroxy-1-((*S*)-6-hydroxy-2,8-dimethylchroman-2-yl)-4,8-dimethylnona-3,7-dien-2-one.

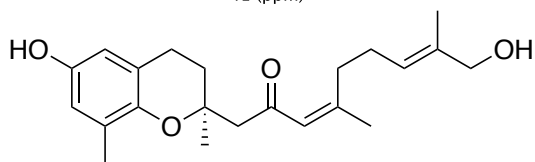
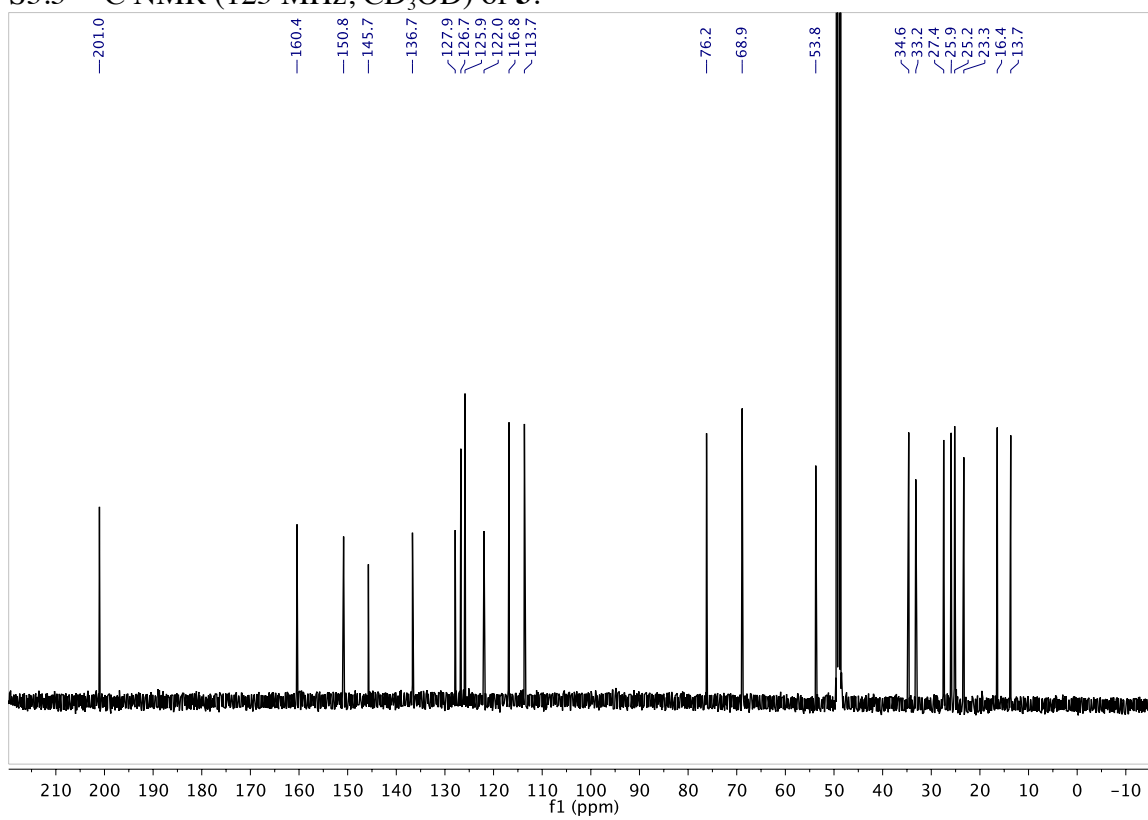
S3.1 HREIMS of **3**.



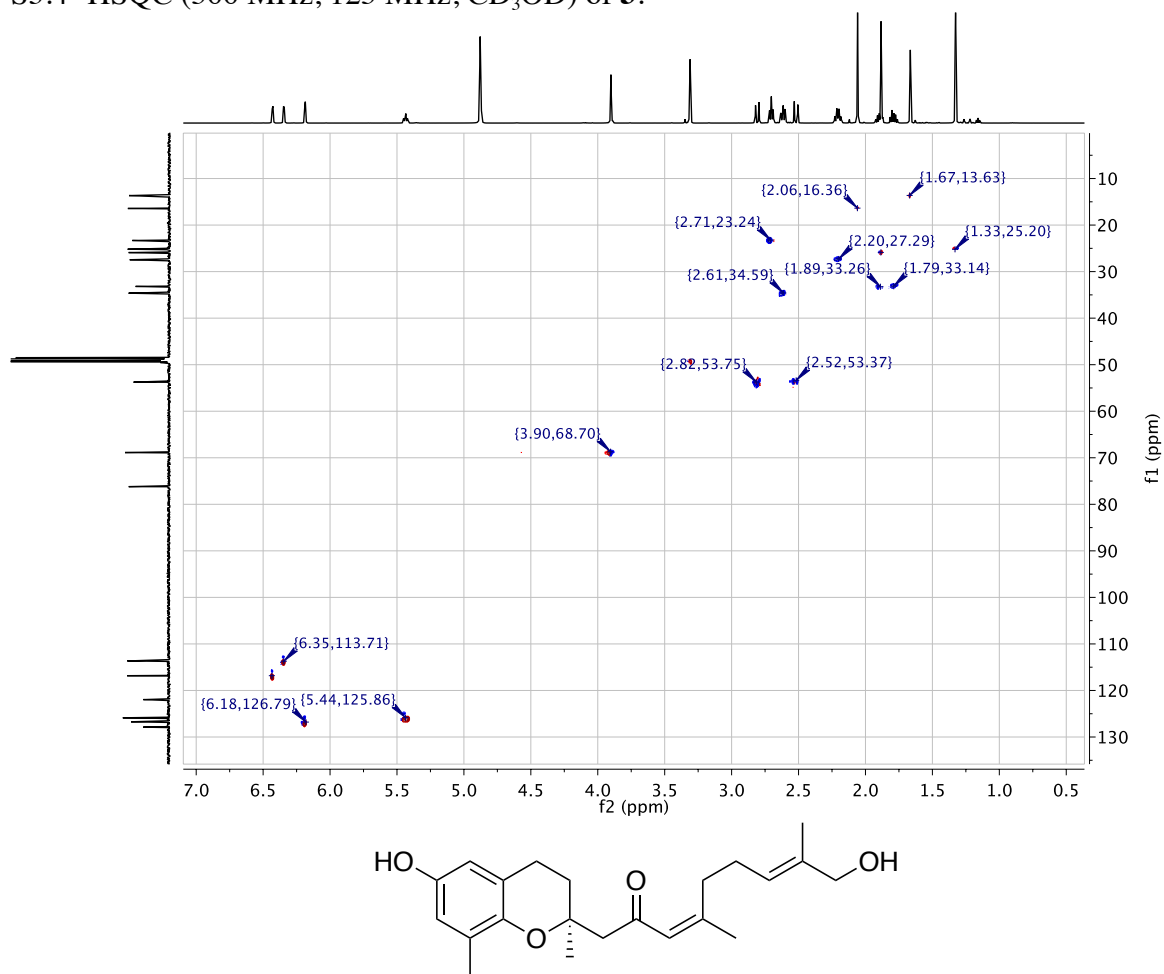
S3.2 ^1H NMR (500 MHz, CD_3OD) of **3**.



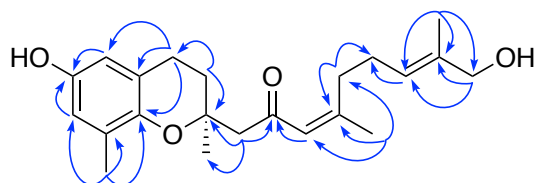
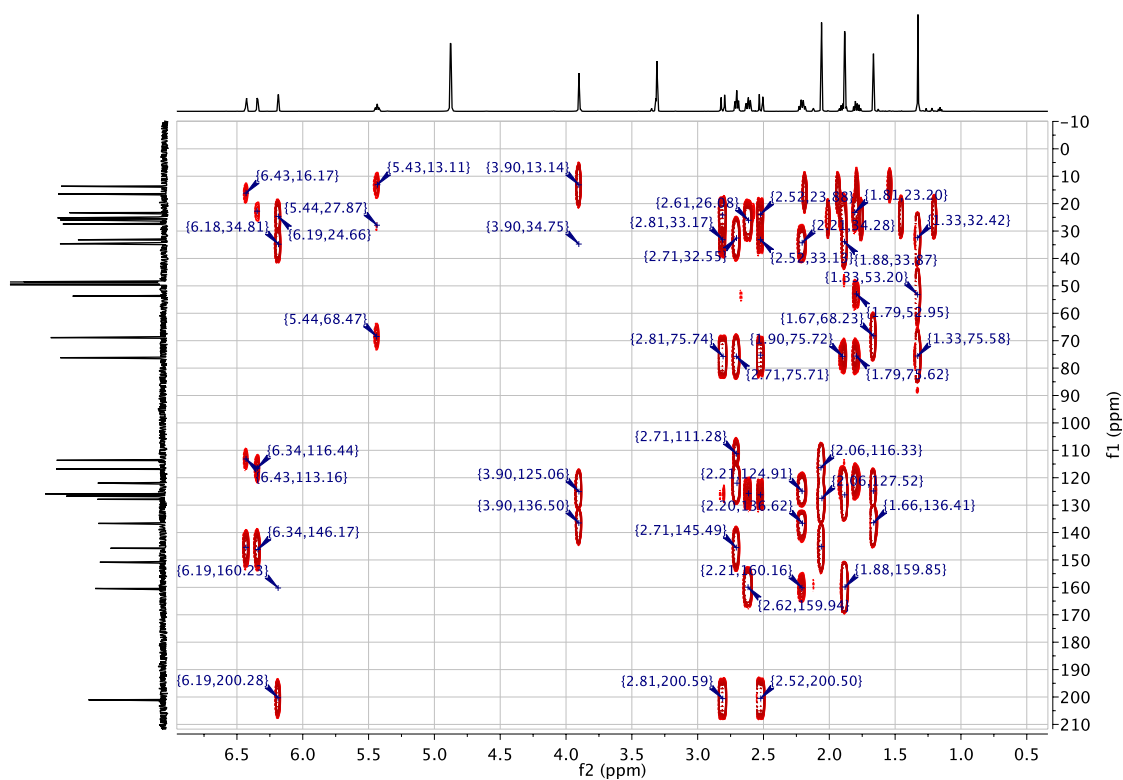
S3.3 ^{13}C NMR (125 MHz, CD_3OD) of **3**.



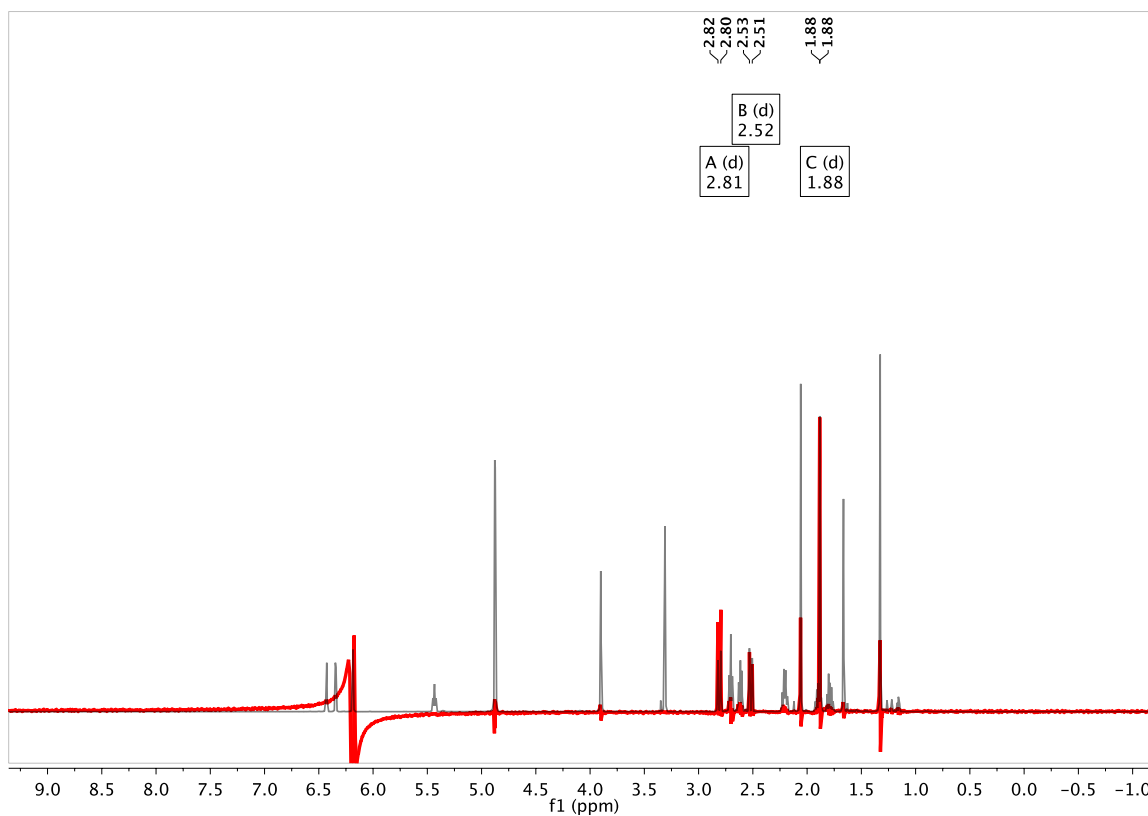
S3.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **3**.



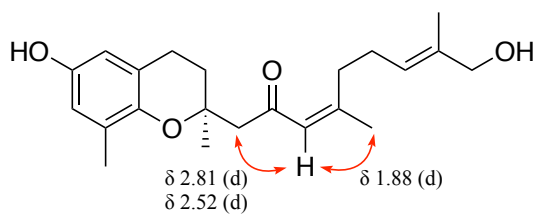
S3.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **3**.



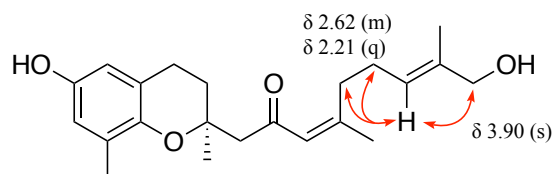
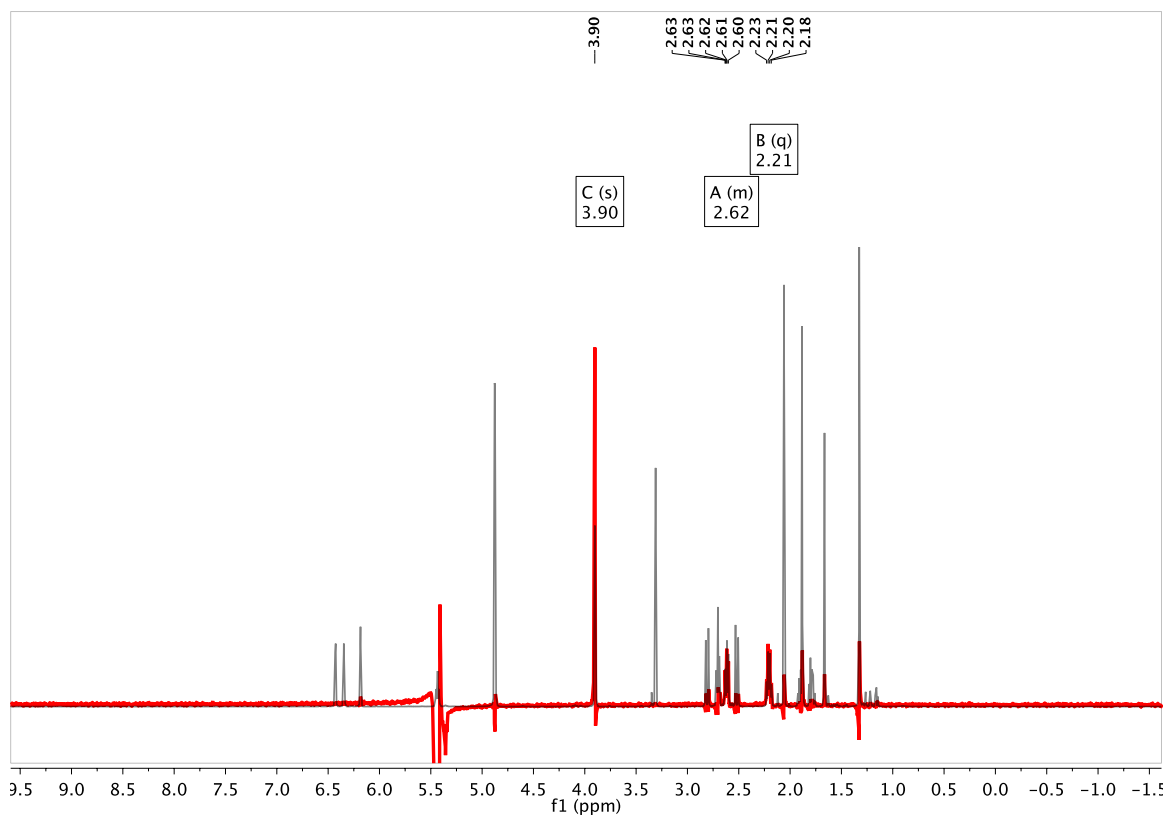
S3.6 SEL. NOE (500 MHz, CD₃OD, Irradiated at 6.2 ppm) of **3**.



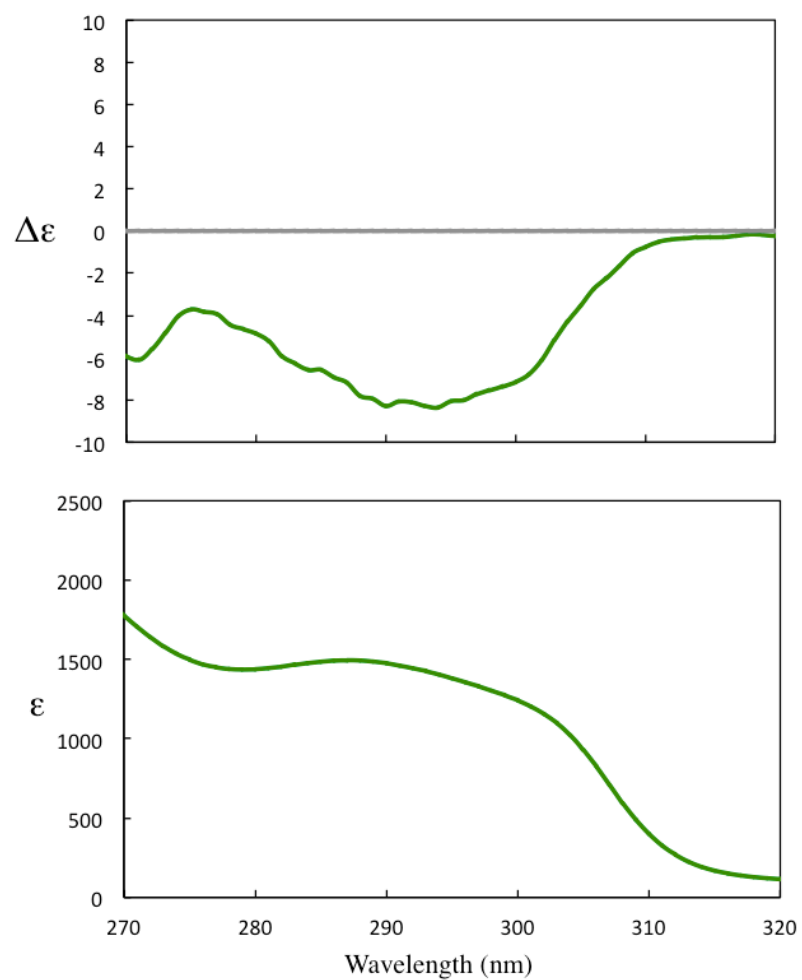
SEL. NOE in red. ¹H NMR in gray.



S3.7 SEL. NOE (500 MHz, CD₃OD, Irradiated at 5.4 ppm) of **3**.

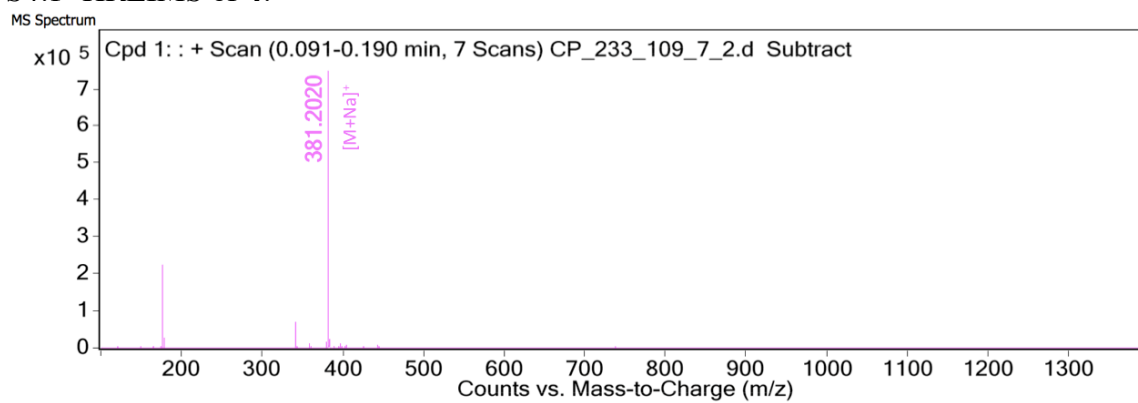


S3.8 ECD Spectrum of **3** in CH₃OH (1.0 mM).

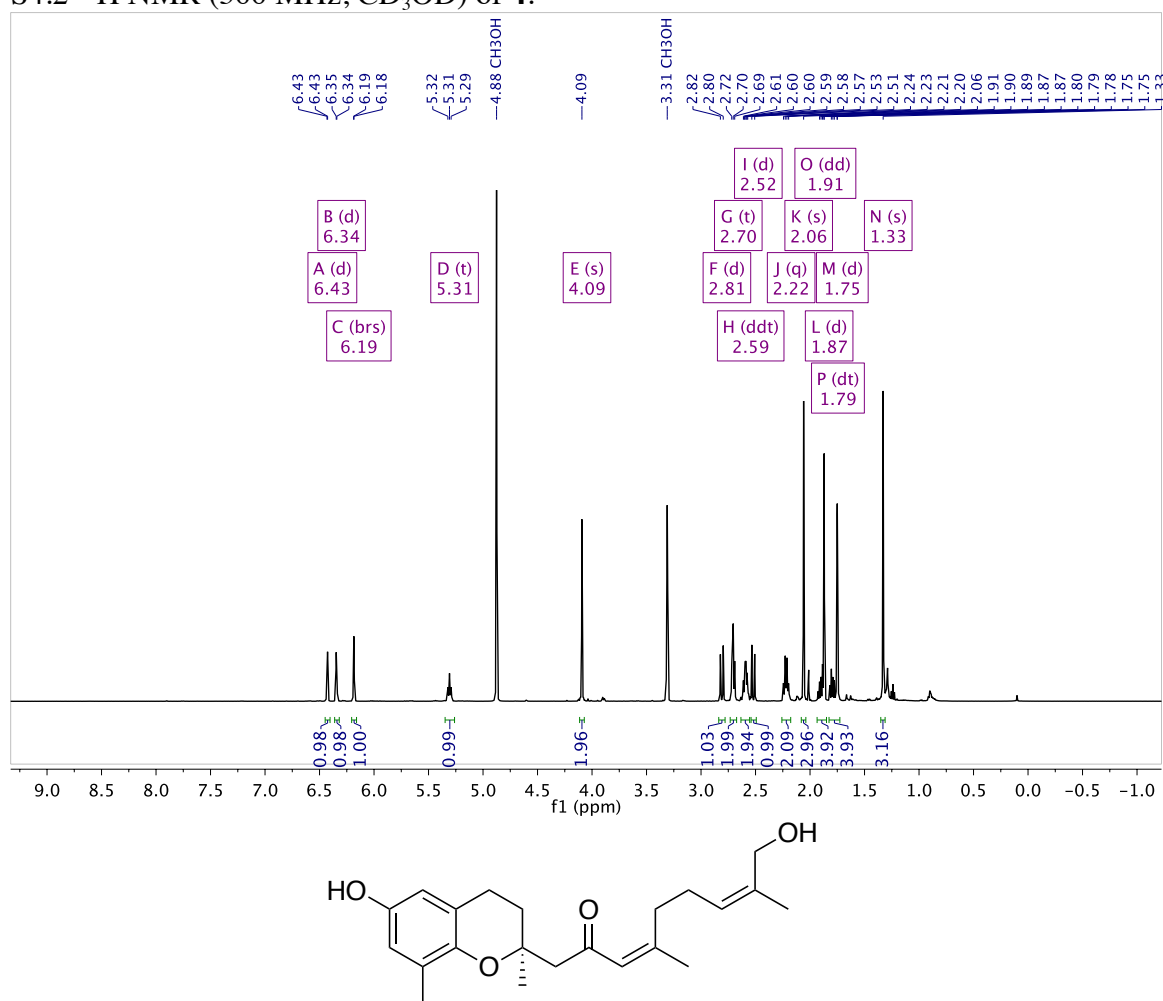


S4 Spectroscopic Data for **4** (3Z,7Z)-9-hydroxy-1-((S)-6-hydroxy-2,8-dimethylchroman-2-yl)-4,8-dimethylnona-3,7-dien-2-one.

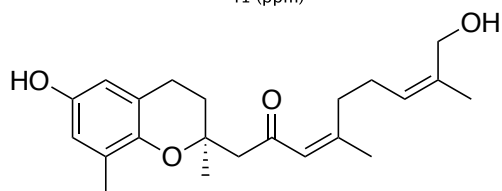
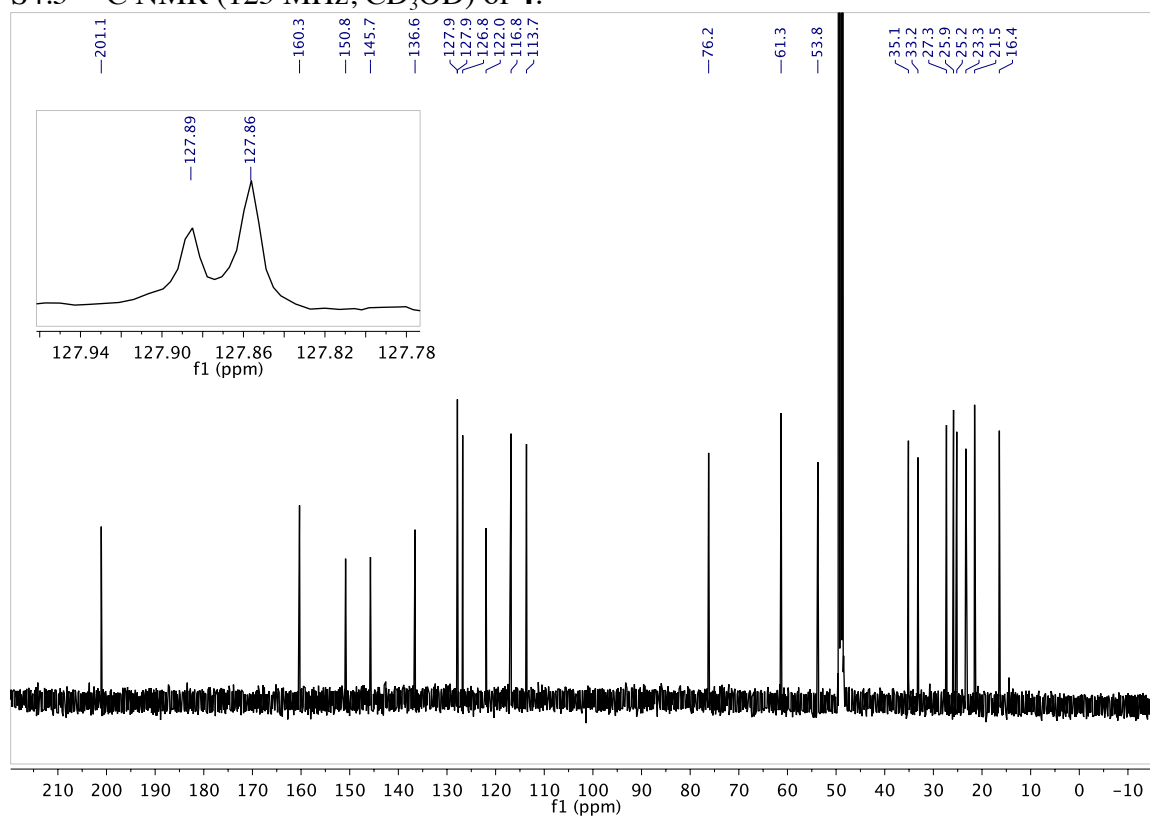
S4.1 HREIMS of **4**.



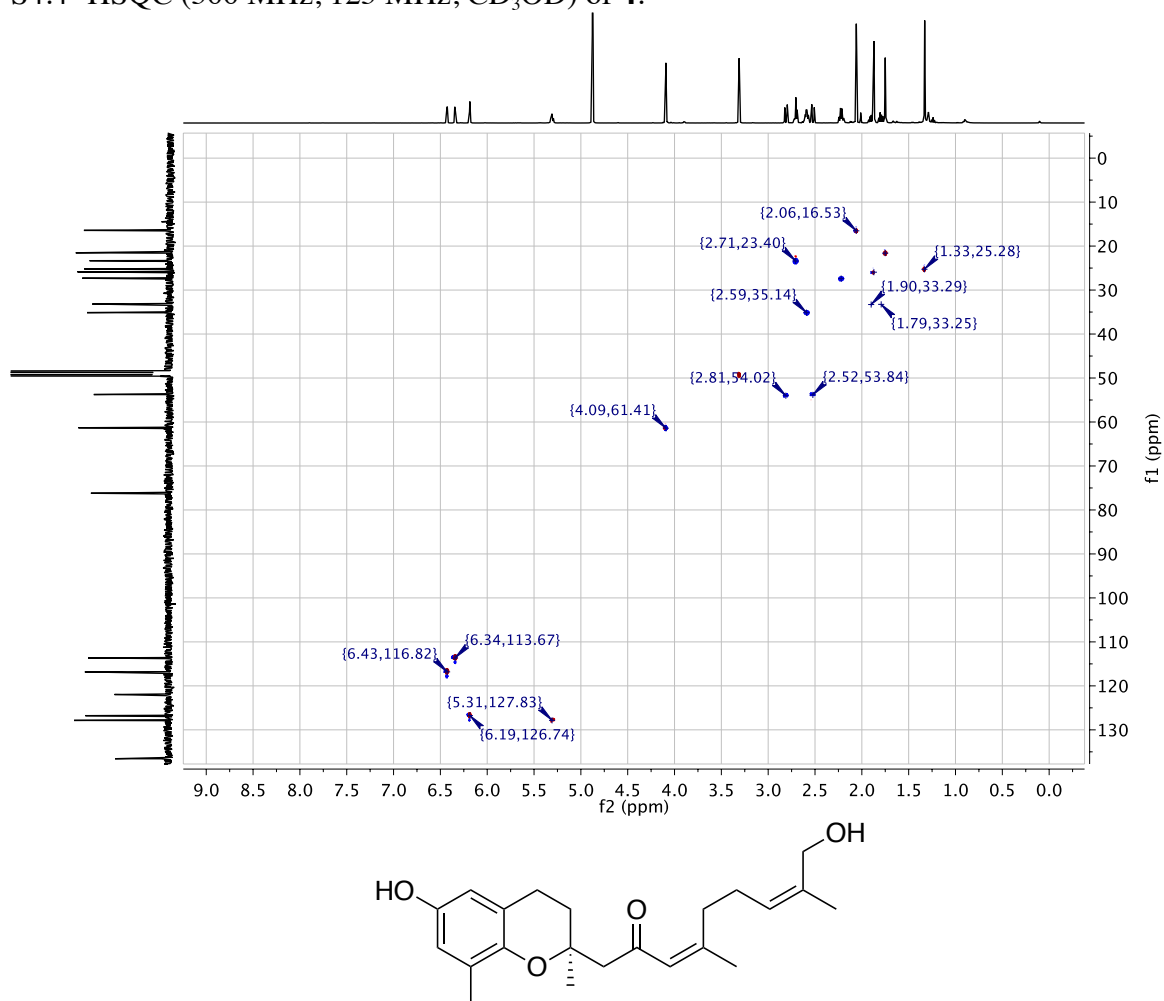
S4.2 ^1H NMR (500 MHz, CD_3OD) of **4**.



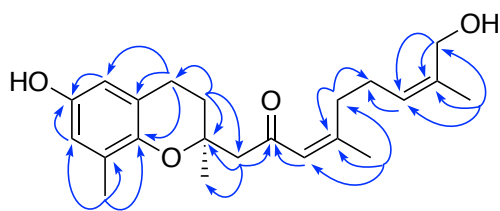
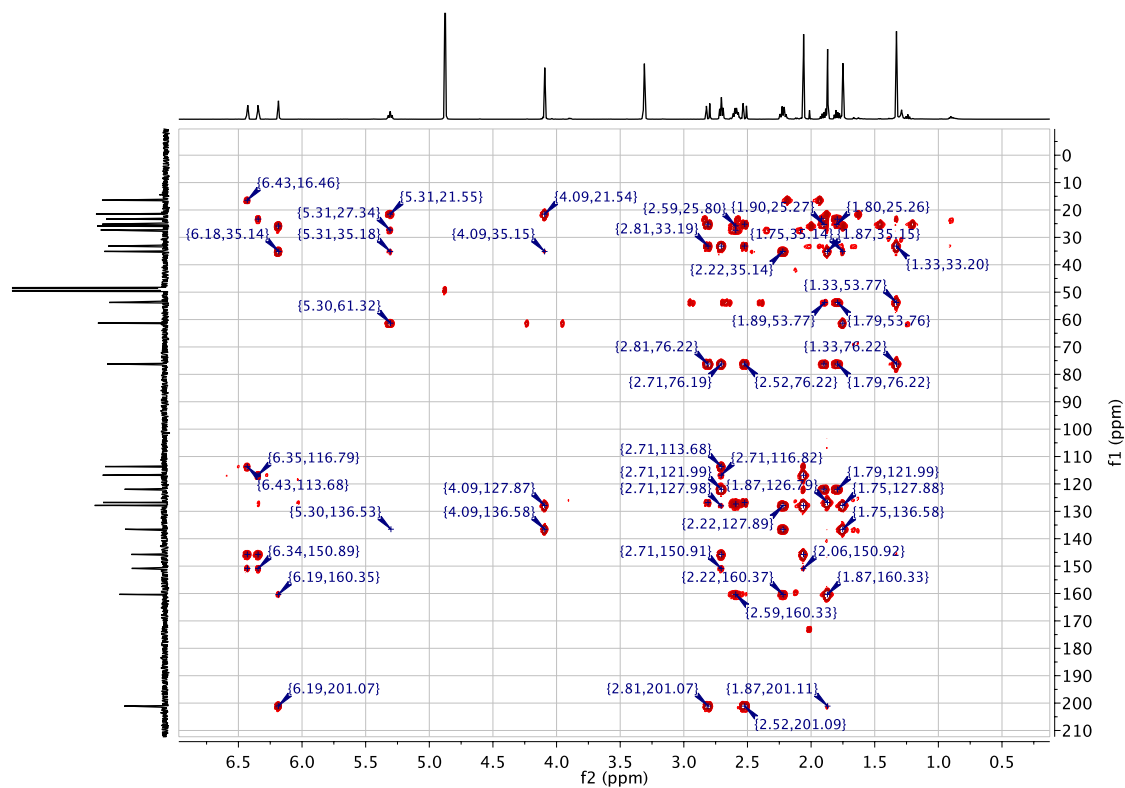
S4.3 ^{13}C NMR (125 MHz, CD_3OD) of **4**.



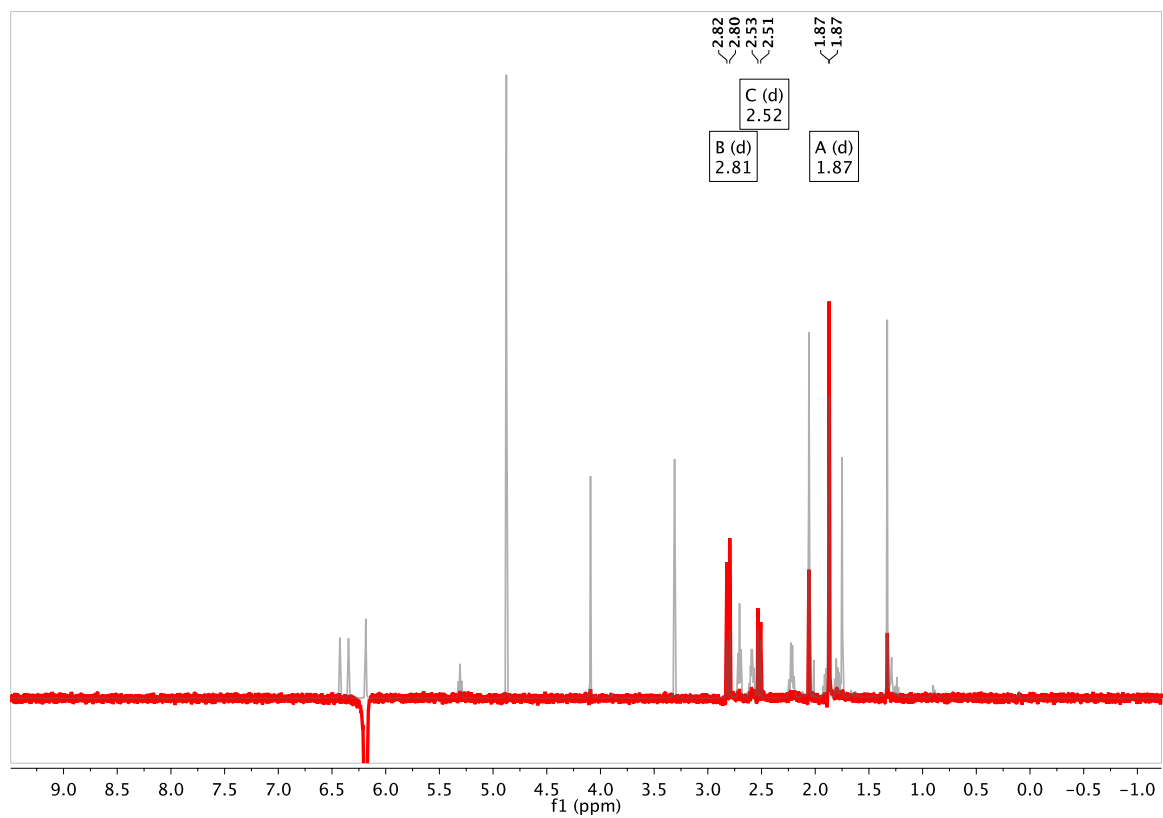
S4.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **4**.



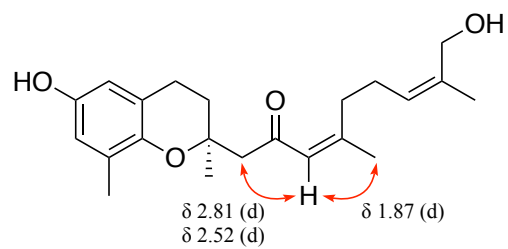
S4.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **4**.



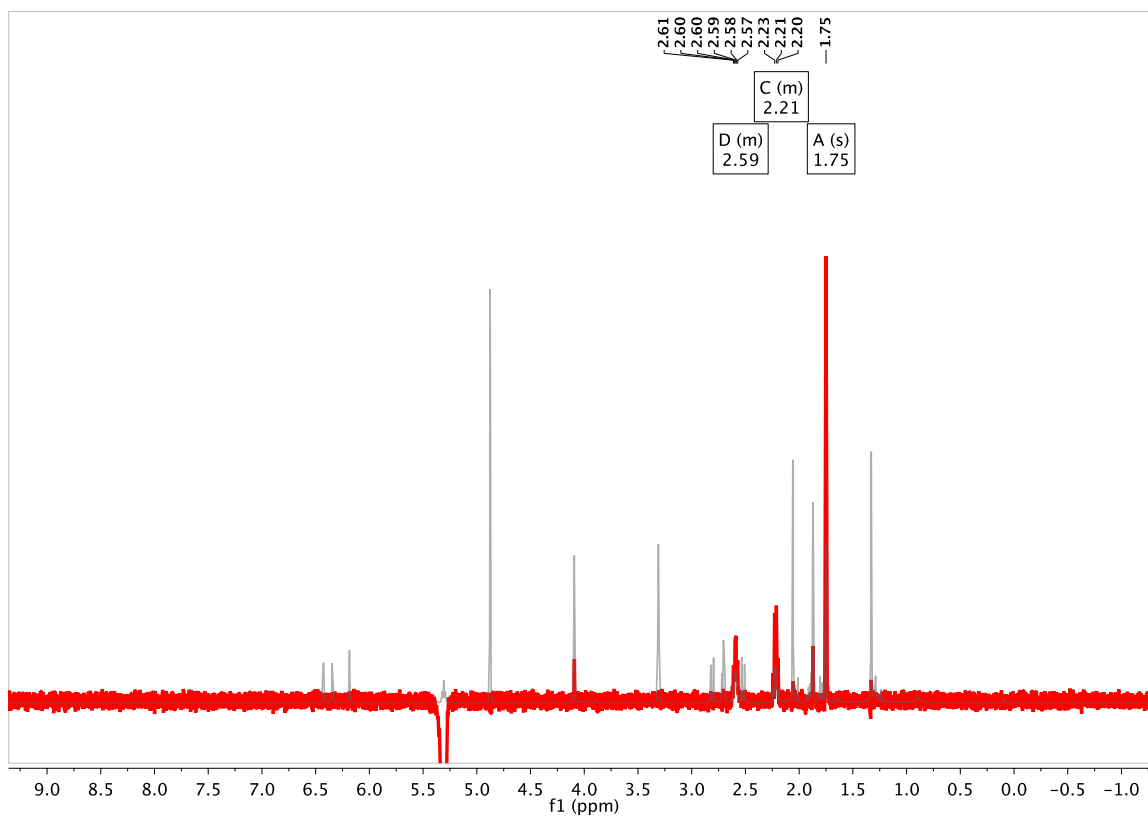
S4.6 SEL. NOE (500 MHz, CD₃OD, Irradiated at 6.2 ppm) of **4**.



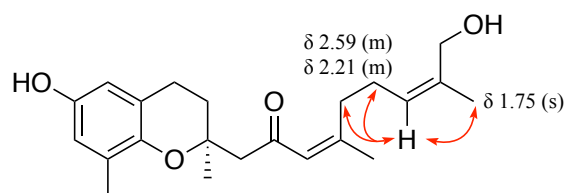
SEL. NOE in red. ¹H NMR in gray.



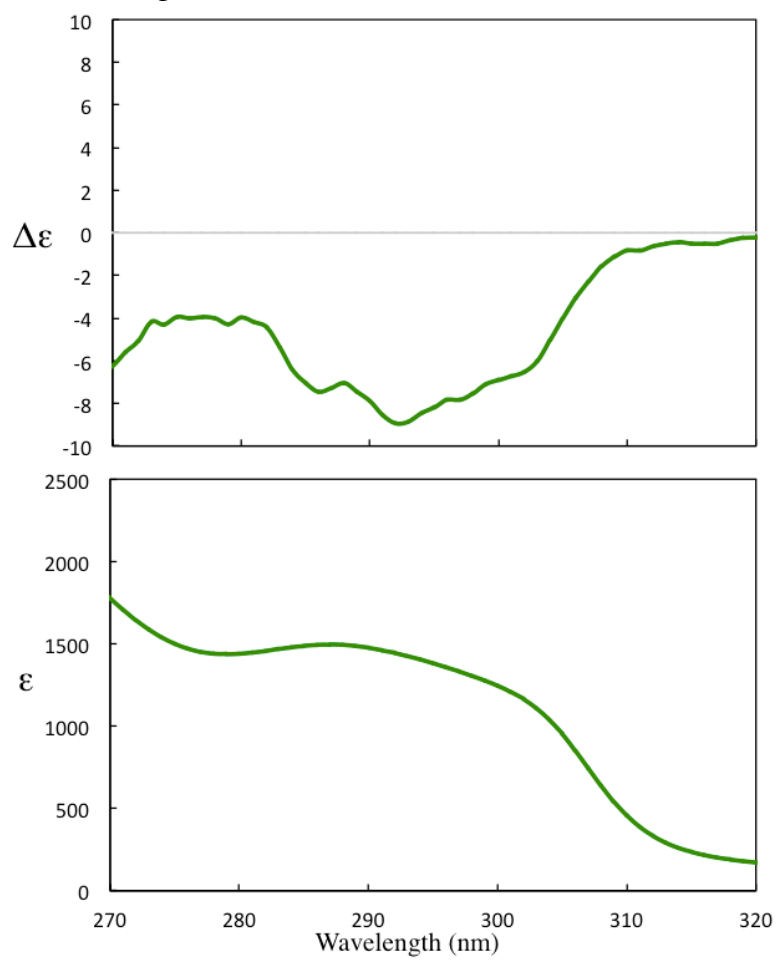
S4.7 SEL. NOE (500 MHz, CD₃OD, Irradiated at 5.5 ppm) of **4**.



SEL. NOE in red. ¹H NMR in gray.

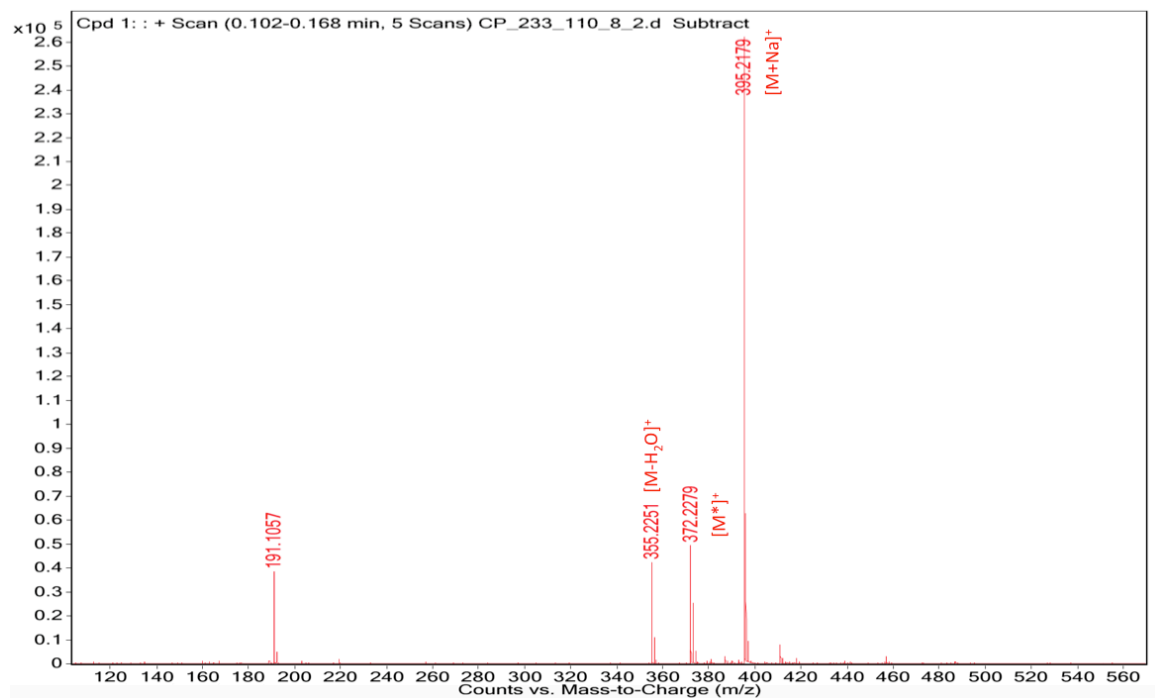


S4.8 ECD Spectrum of **4** in CH₃OH (1.0 mM).

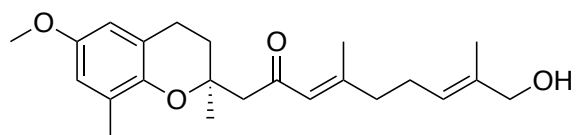
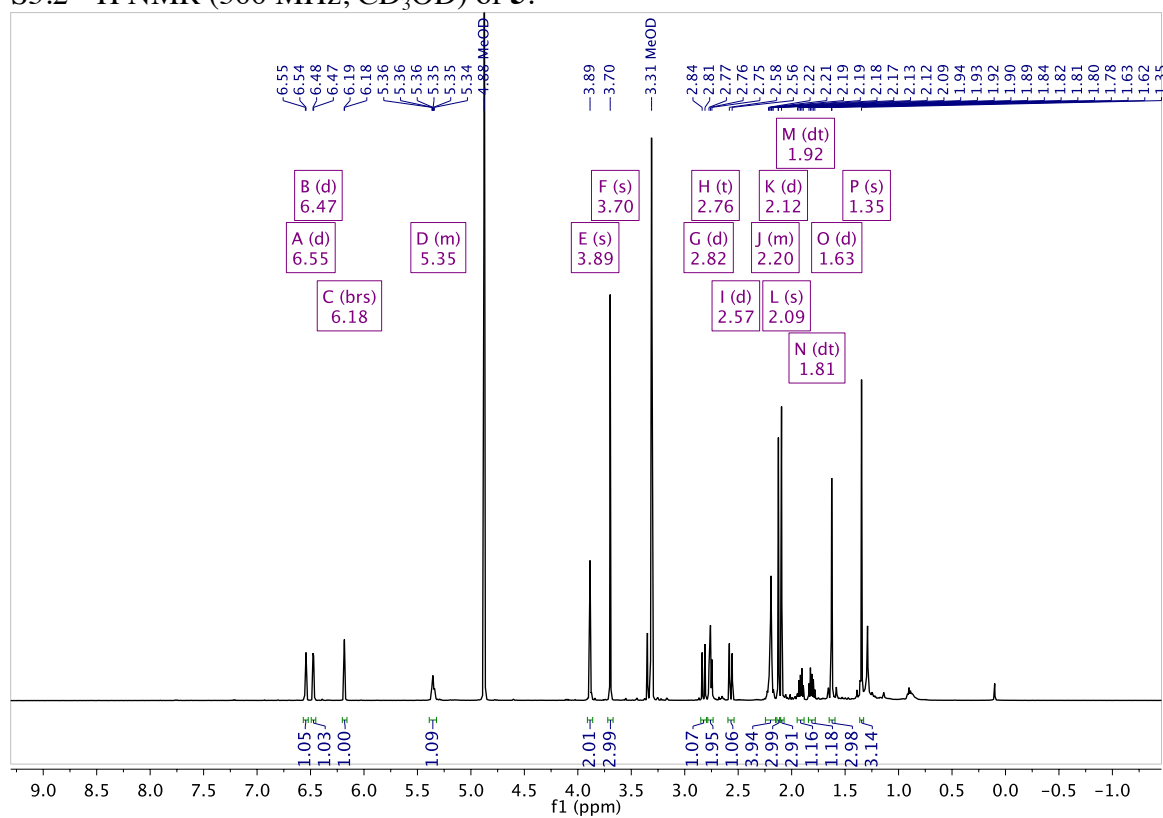


S5 Spectroscopic Data for **5** (3*E*,7*E*)-9-hydroxy-1-((*S*)-6-methoxy-2,8-dimethylchroman-2-yl)-4,8-dimethylnona-3,7-dien-2-one.

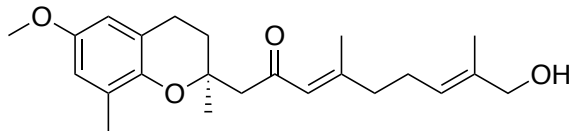
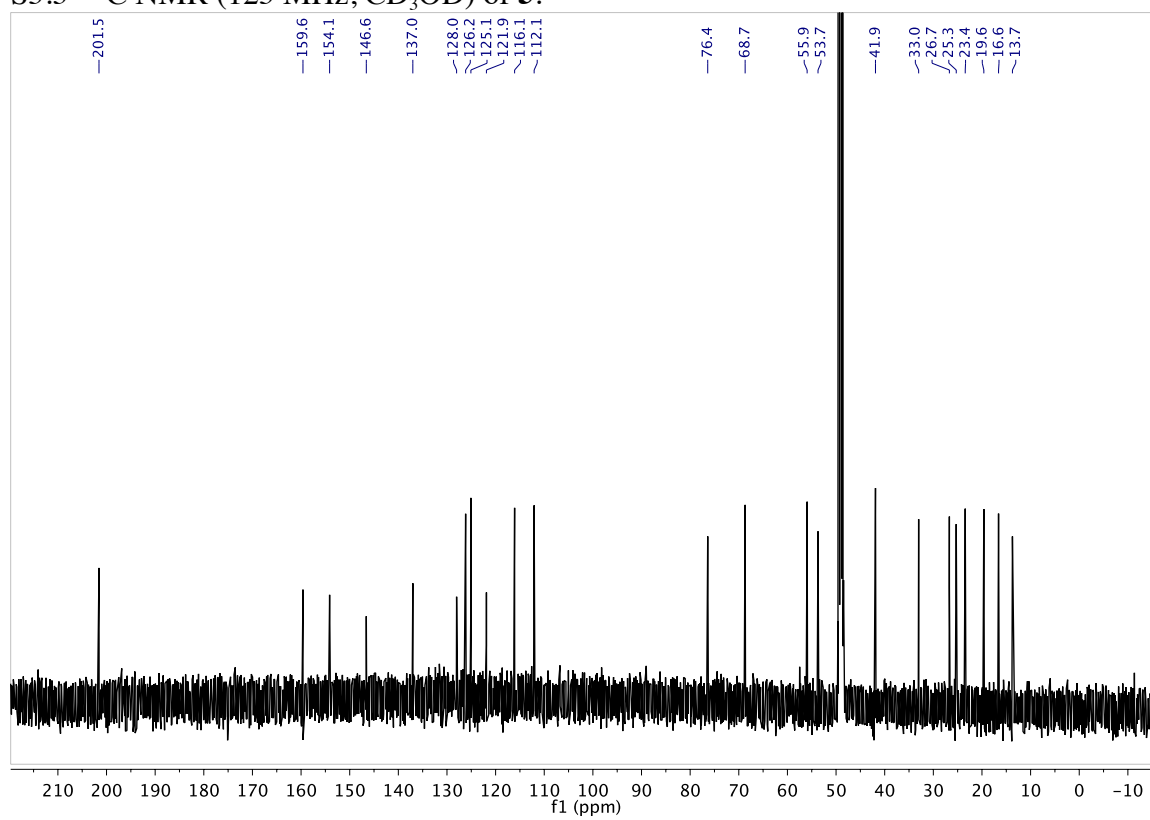
S5.1 HRESIMS of **5**.



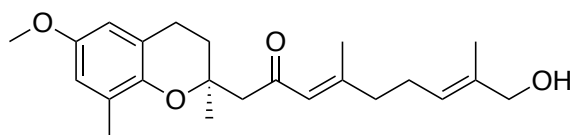
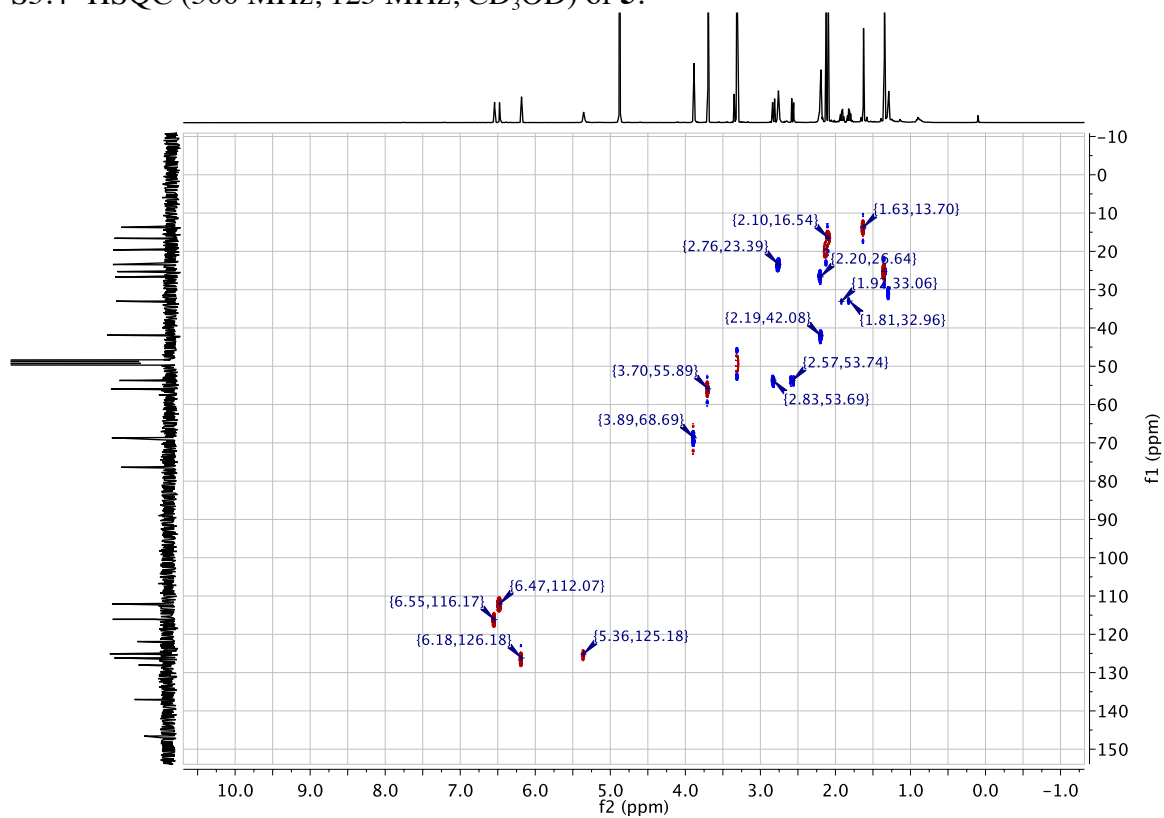
S5.2 ^1H NMR (500 MHz, CD_3OD) of **5**.



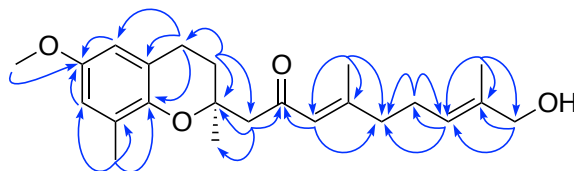
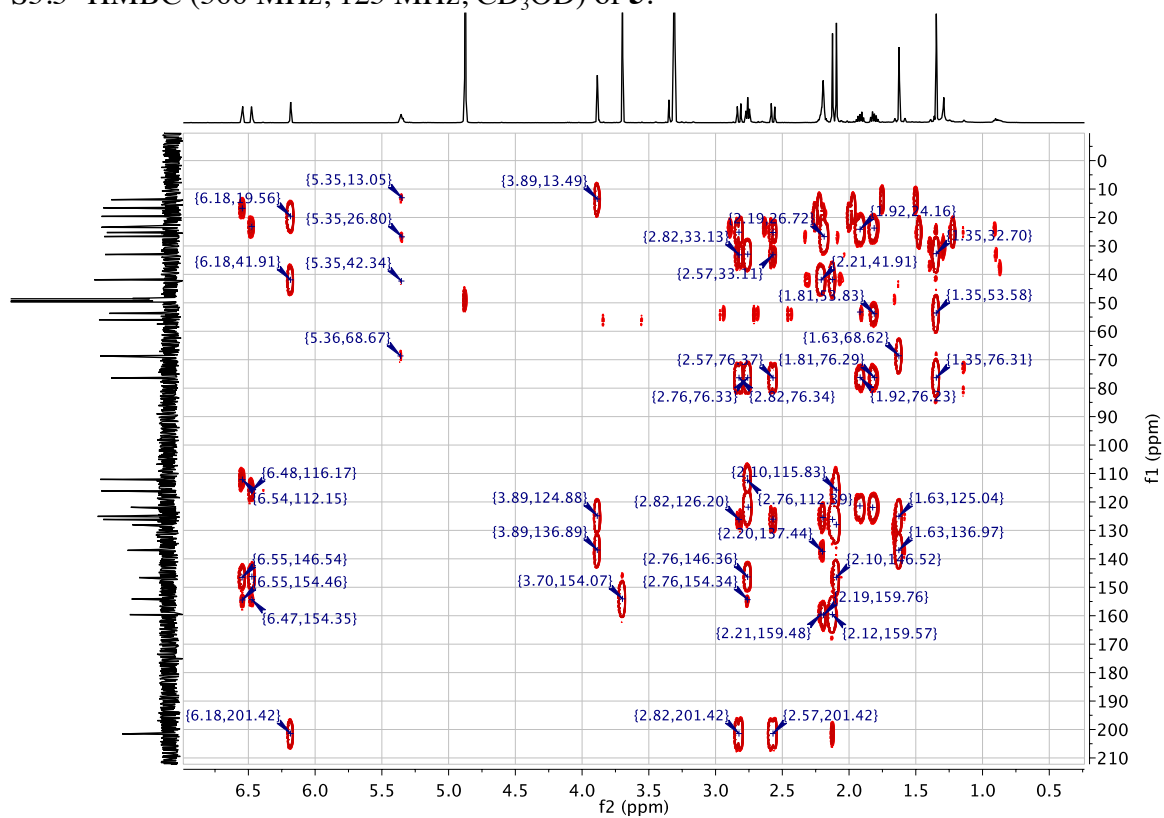
S5.3 ^{13}C NMR (125 MHz, CD_3OD) of **5**.



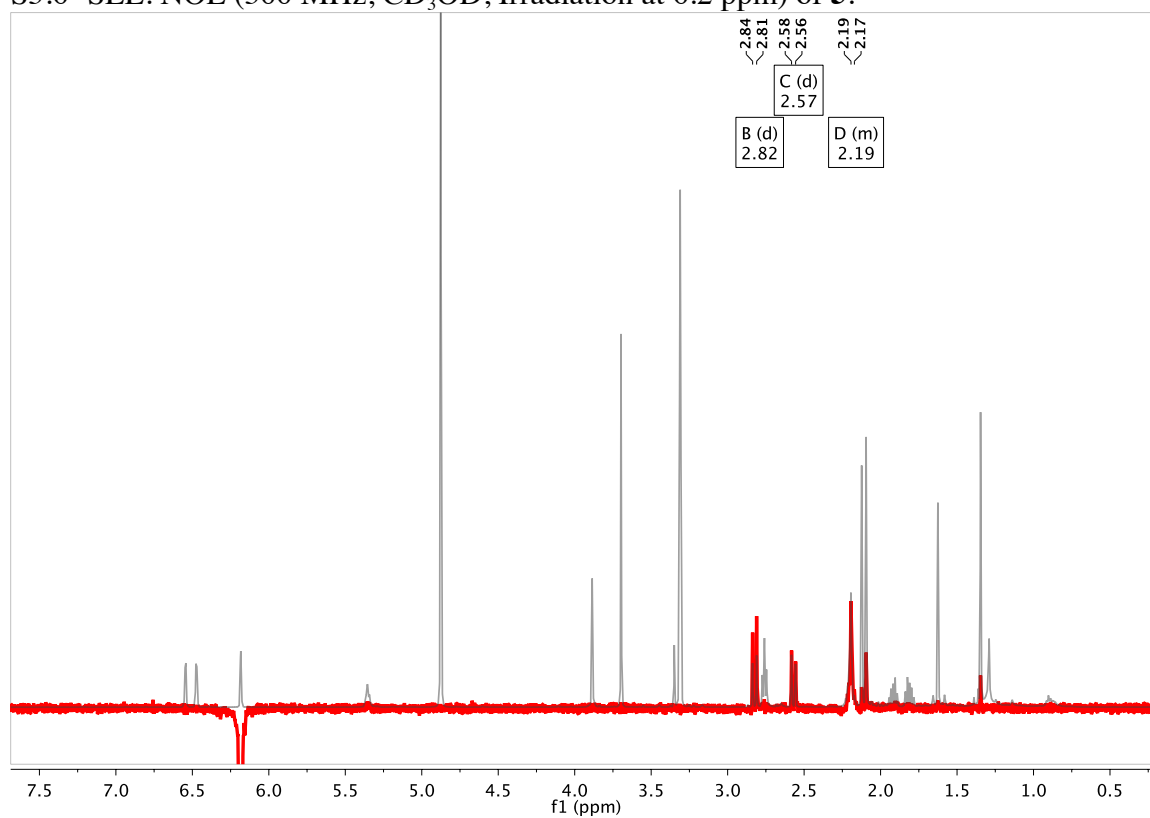
S5.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **5**.



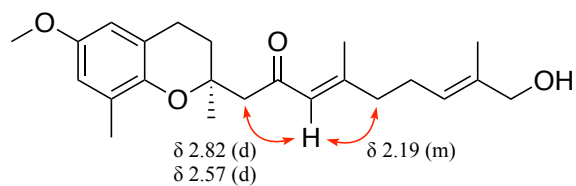
S5.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **5**.



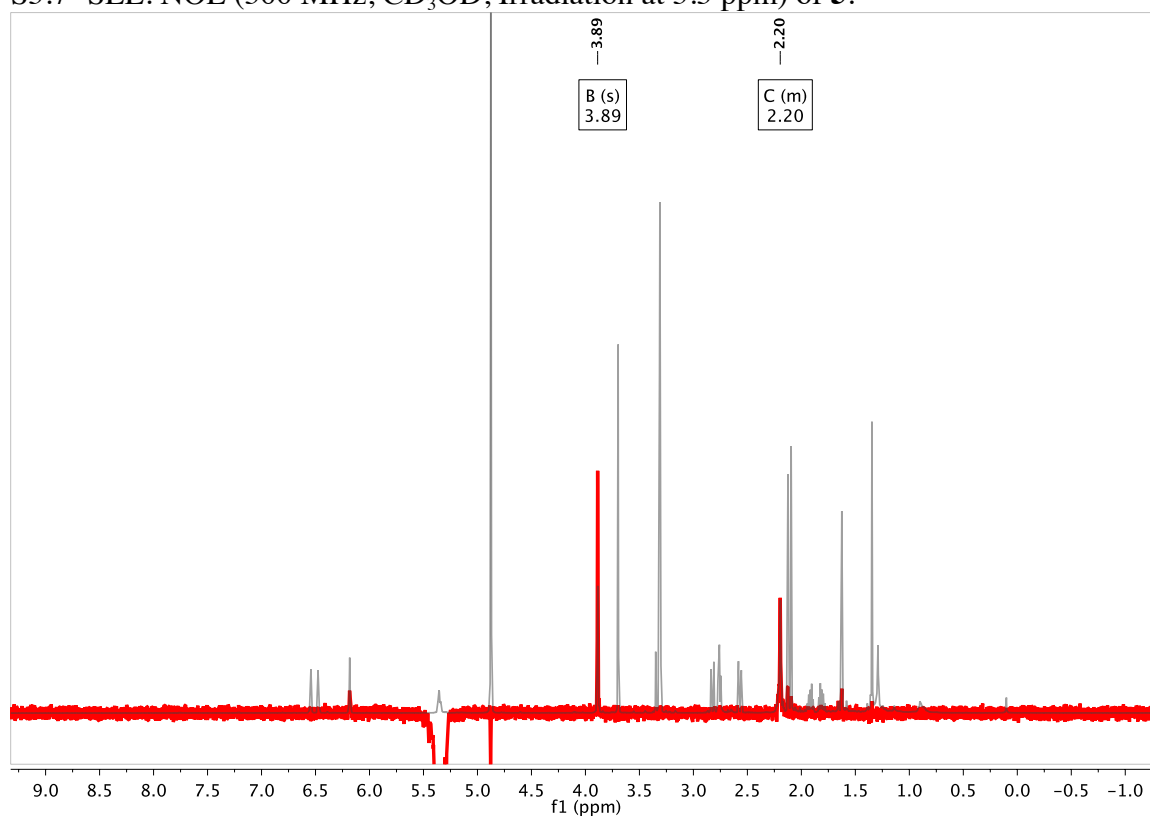
S5.6 SEL. NOE (500 MHz, CD₃OD, Irradiation at 6.2 ppm) of **5**.



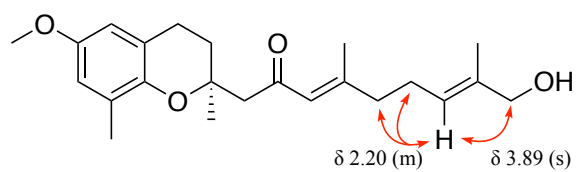
SEL. NOE in red. ¹H NMR in gray.



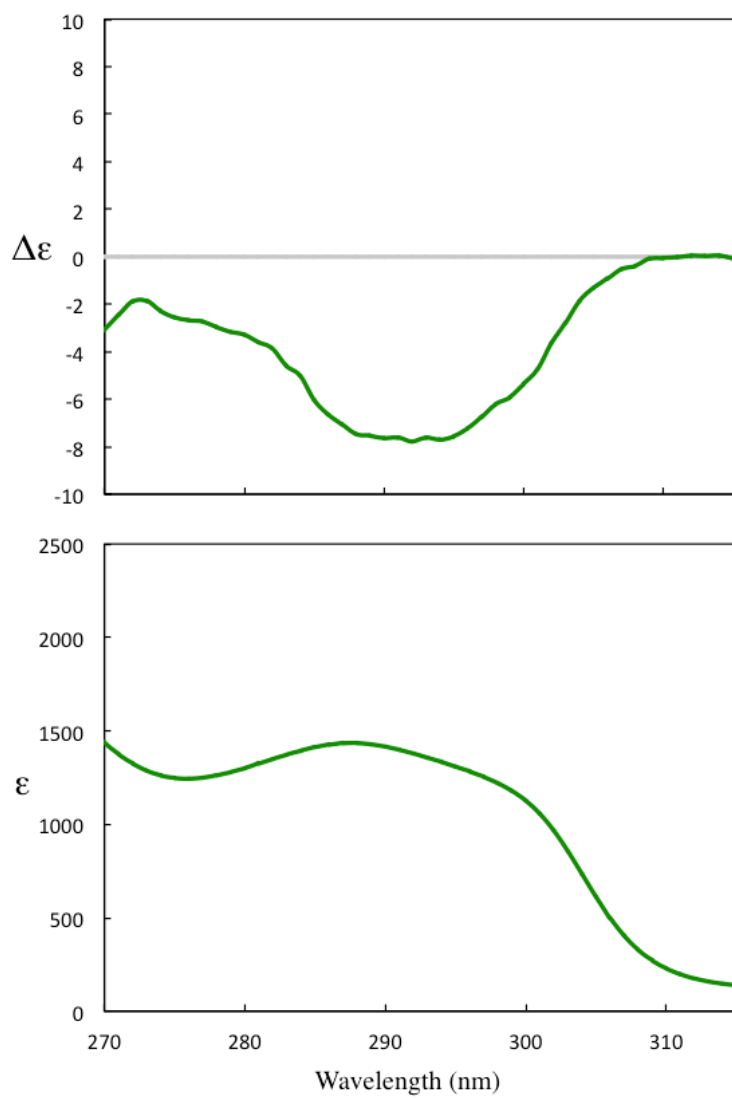
S5.7 SEL. NOE (500 MHz, CD₃OD, Irradiation at 5.5 ppm) of **5**.



SEL. NOE in red. ¹H NMR in gray.

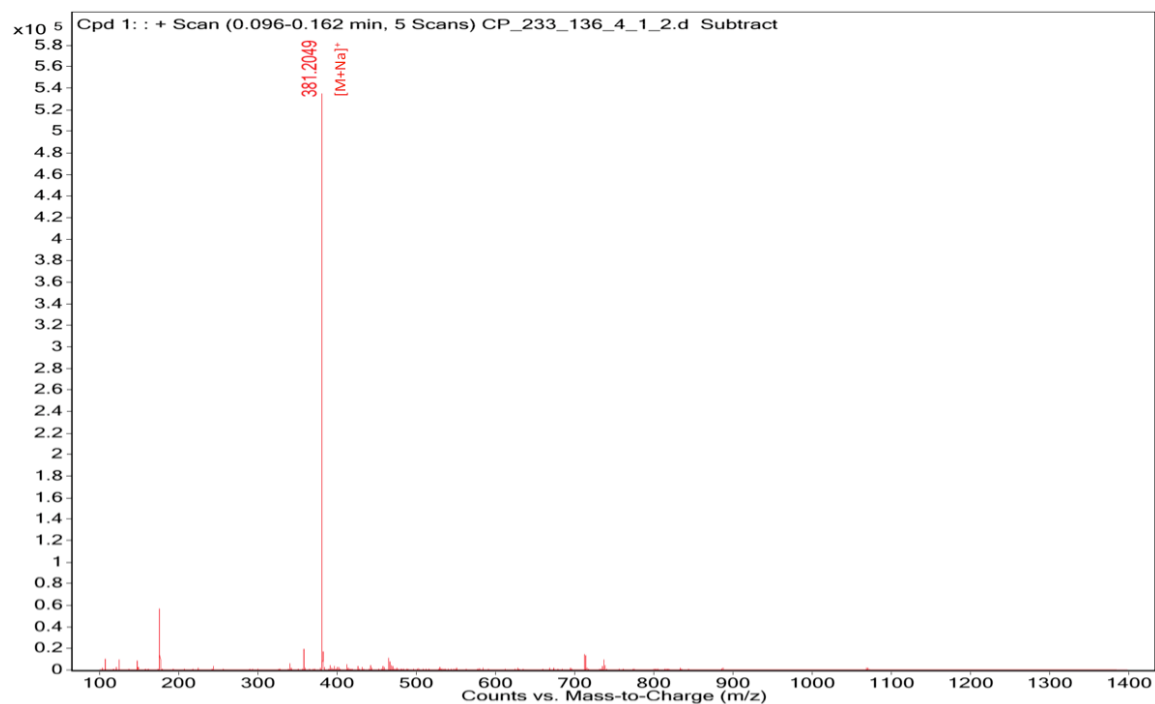


S5.8 ECD spectrum of **5** in CH₃OH (1.0 mM).



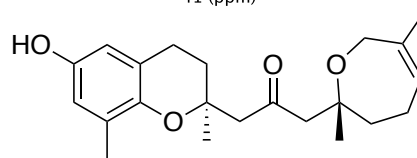
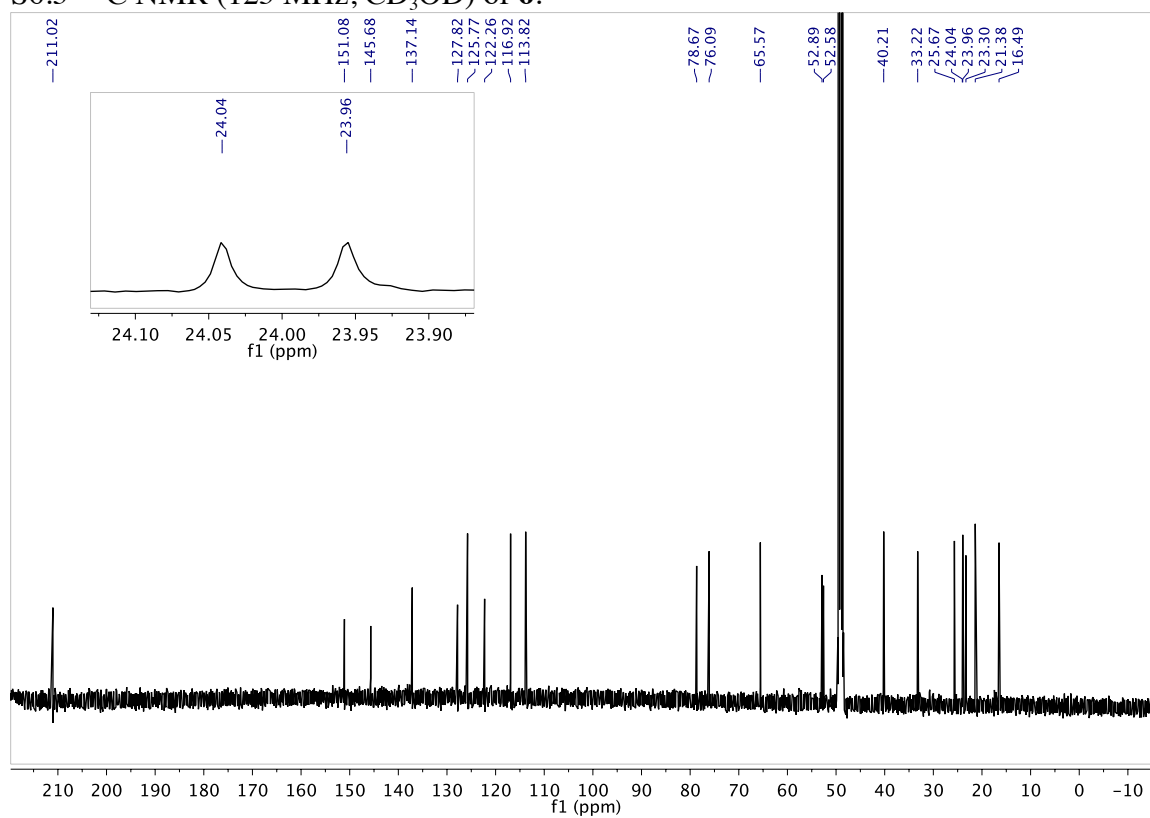
S6 Spectroscopic Data for **6** 1-((*S*)-2,6-dimethyl-2,3,4,7-tetrahydrooxepin-2-yl)-3-((*S*)-6-hydroxy-2,8-dimethylchroman-2-yl)propan-2-one.

S6.1 HRESIMS of **6**.

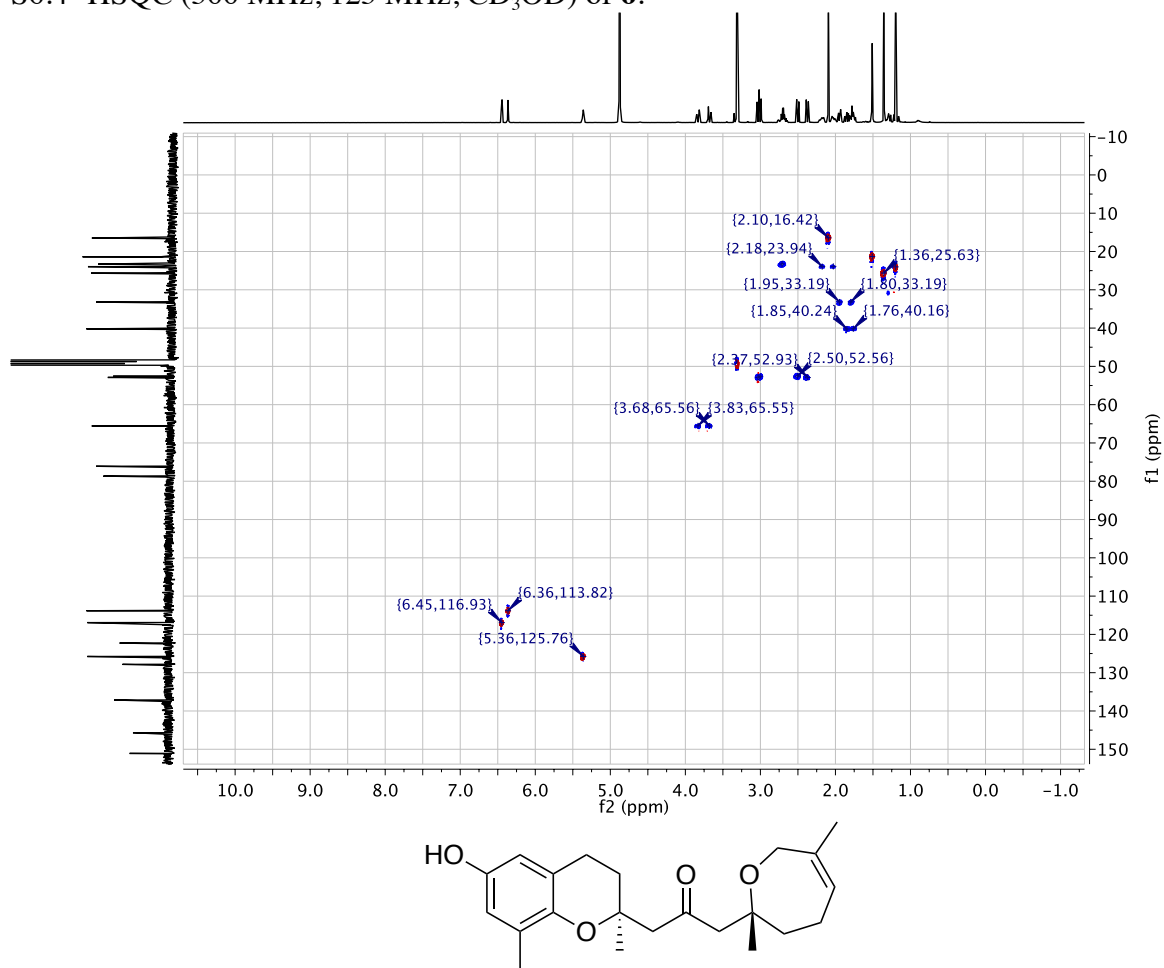


[illegible]

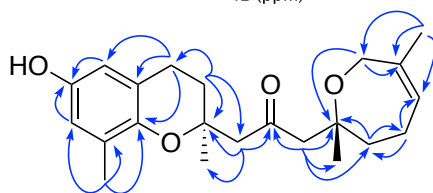
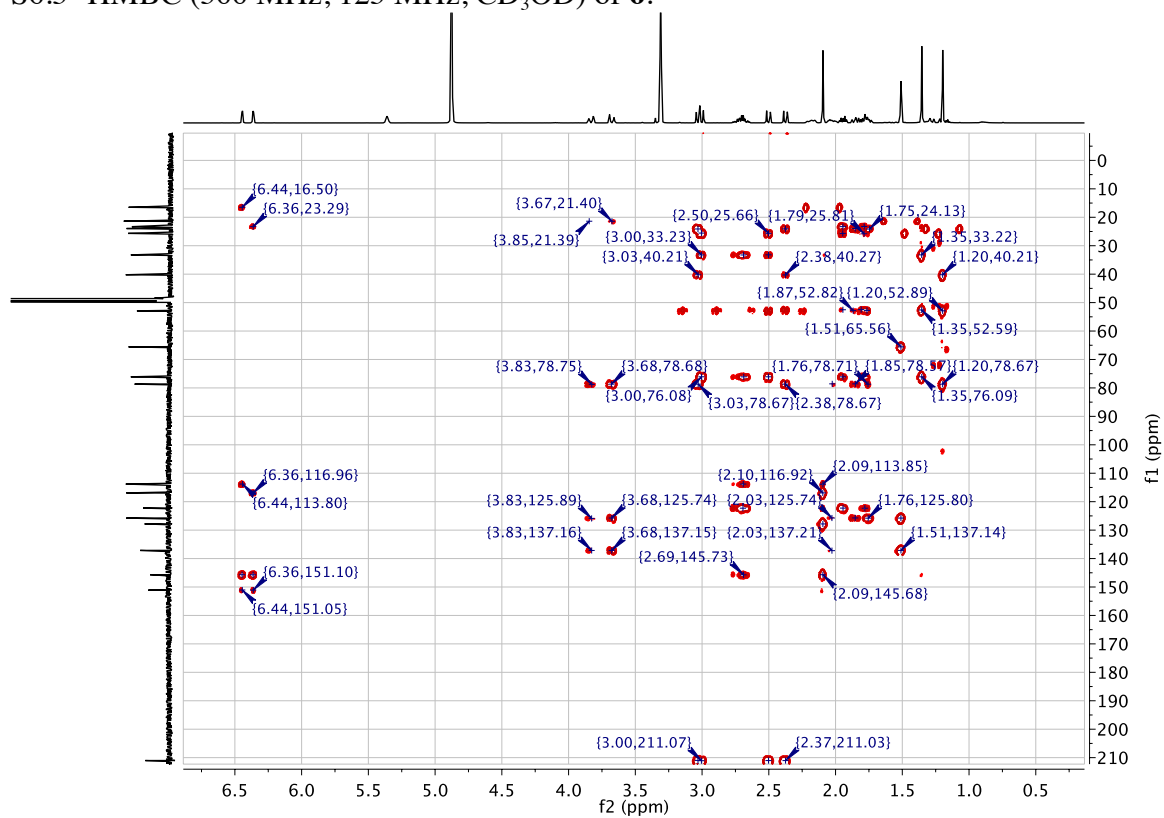
S6.3 ^{13}C NMR (125 MHz, CD_3OD) of **6**.



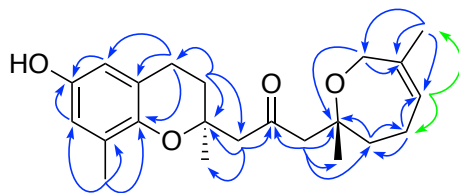
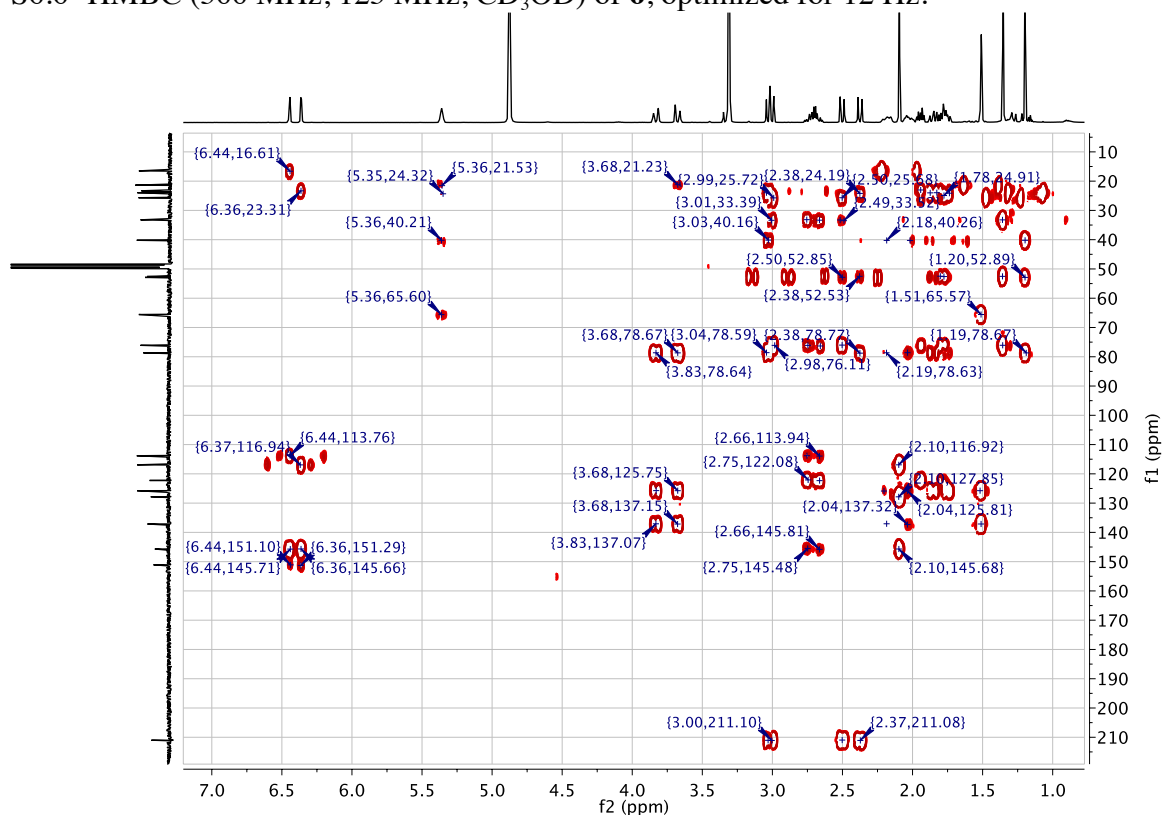
S6.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **6**.



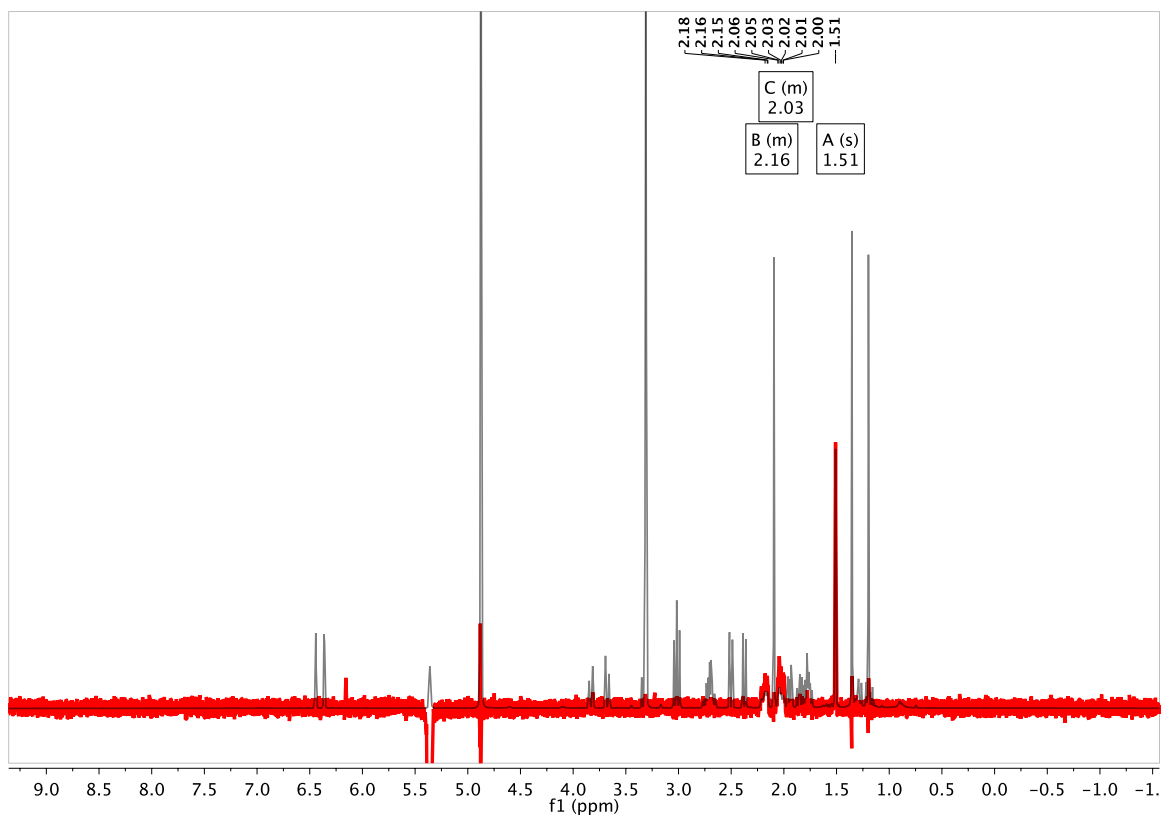
S6.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **6**.



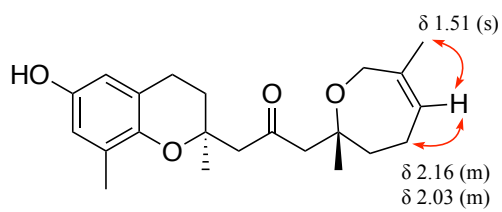
S6.6 HMBC (500 MHz, 125 MHz, CD₃OD) of **6**, optimized for 12 Hz.



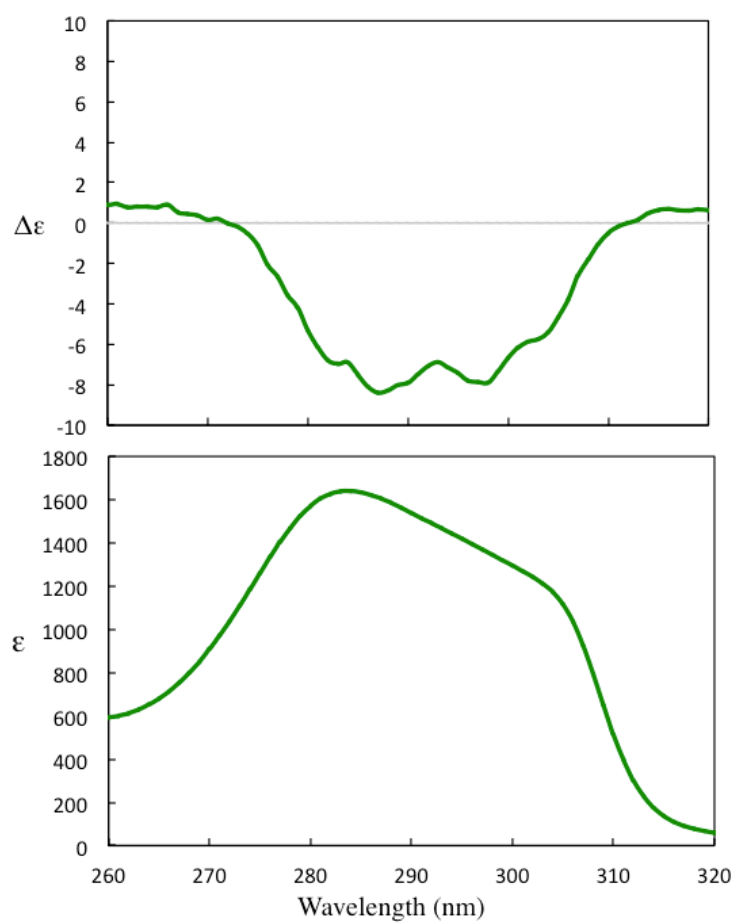
S6.7 SEL. NOE (500 MHz, CD₃OD, Irradiation at 5.4 ppm) of **6**.



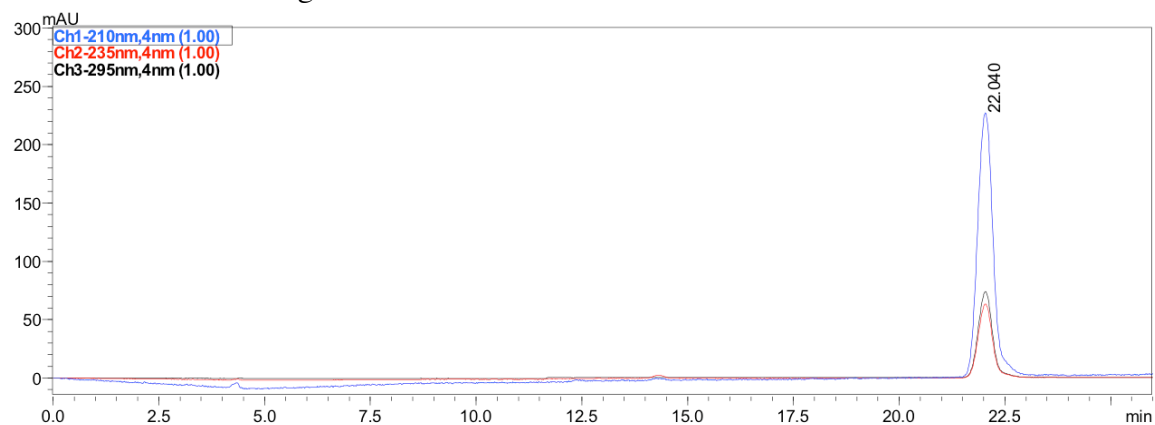
SEL. NOE in red. ¹H NMR in gray.



S6.8 ECD spectrum of **6** in CH₃OH (1.0 mM).

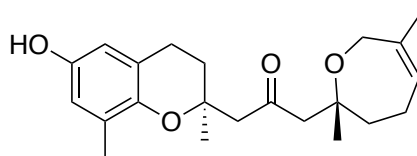


S6.9 HPLC chromatogram of **6**.



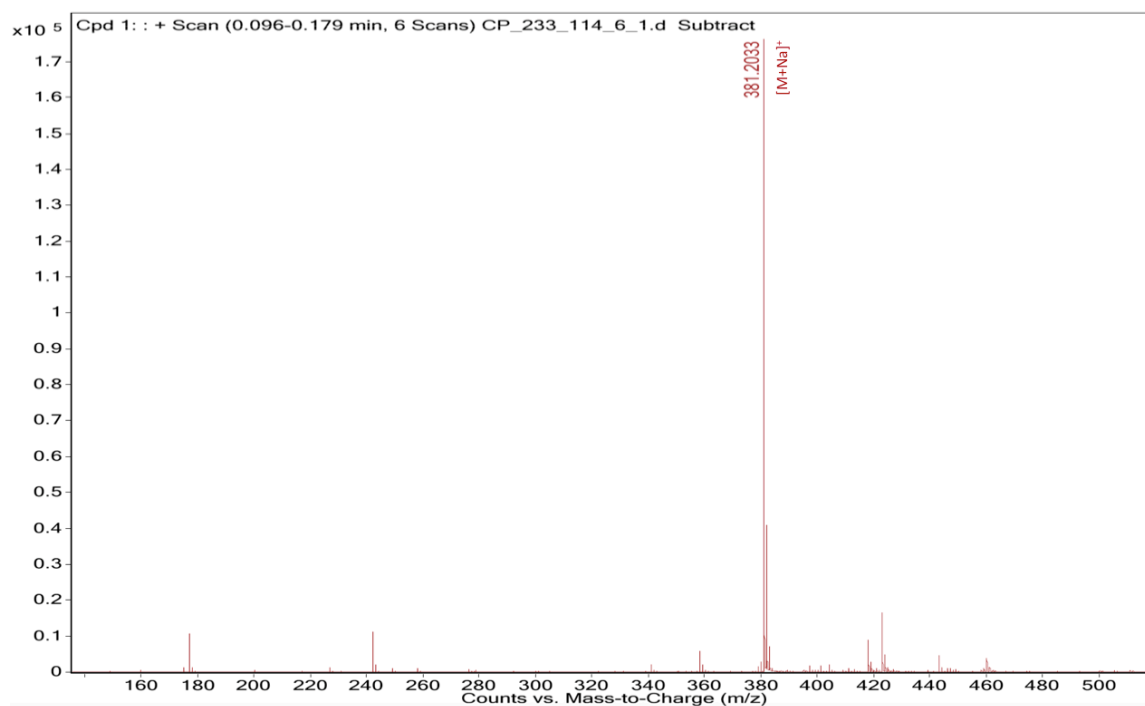
Phenomenex 5 μm , 100 Å, Luna C₁₈(2) (250 x 10 mm) column with H₂O/MeOH at 3 mL/min.

Time (min)	MeOH %
0	70
26	81.7

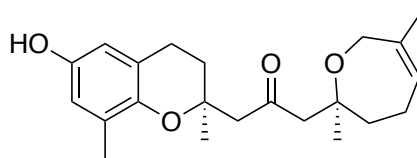
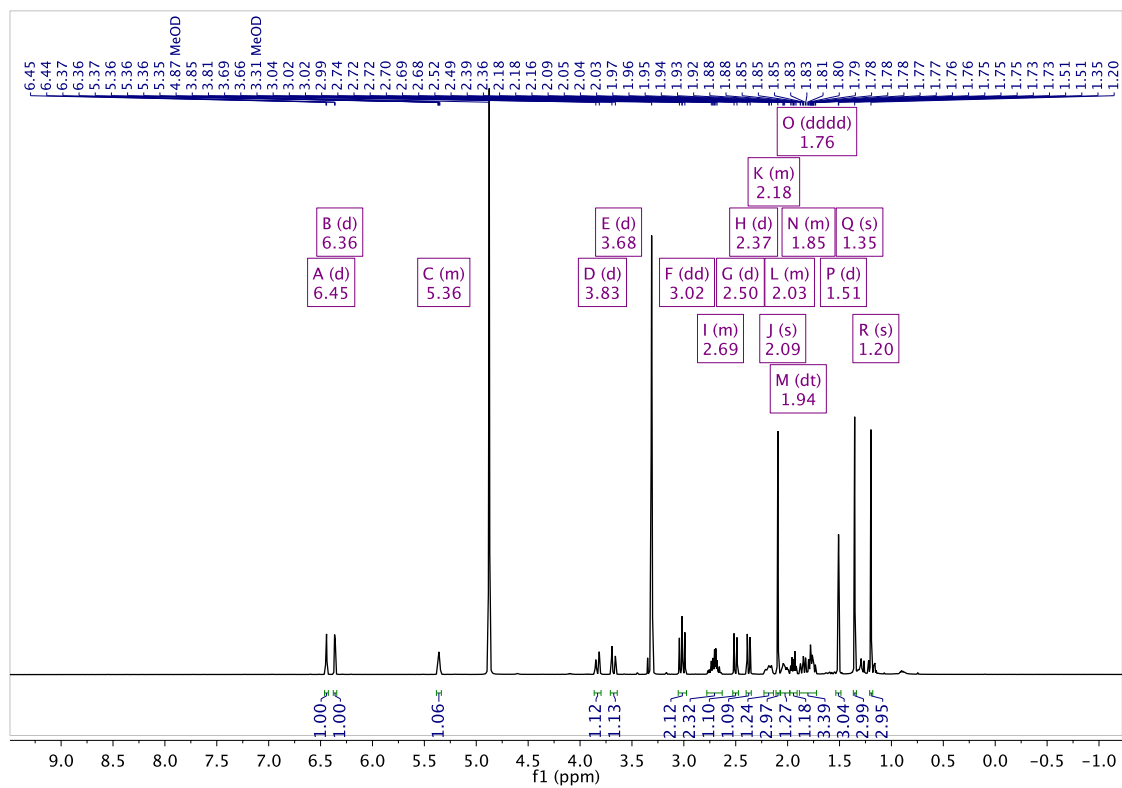


S7 Spectroscopic Data for **7** 1-((*R*)-2,6-dimethyl-2,3,4,7-tetrahydrooxepin-2-yl)-3-((*S*)-6-hydroxy-2,8-dimethylchroman-2-yl)propan-2-one.

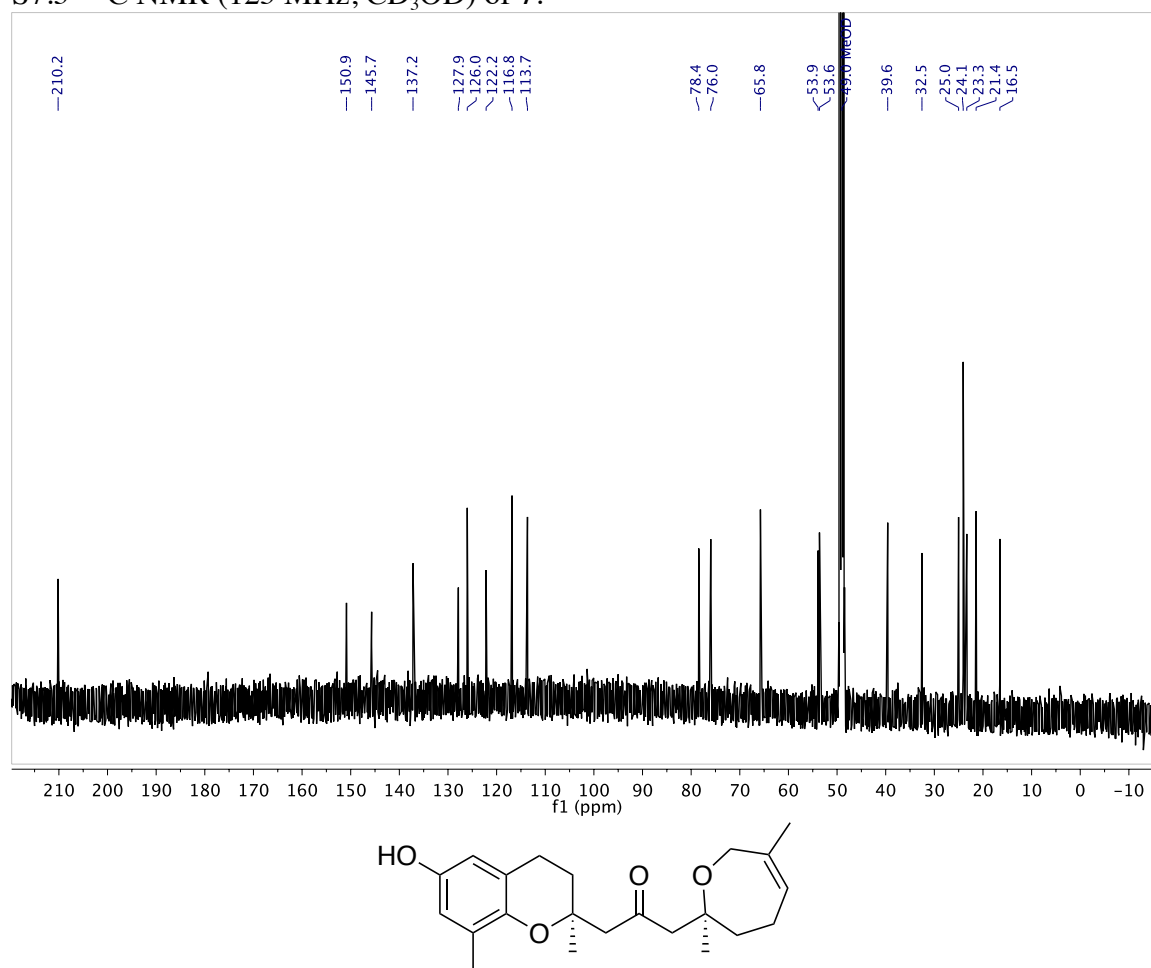
S7.1 HRESIMS of **7**.



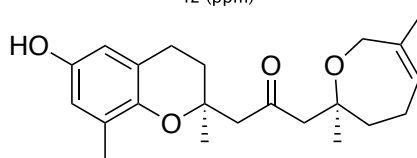
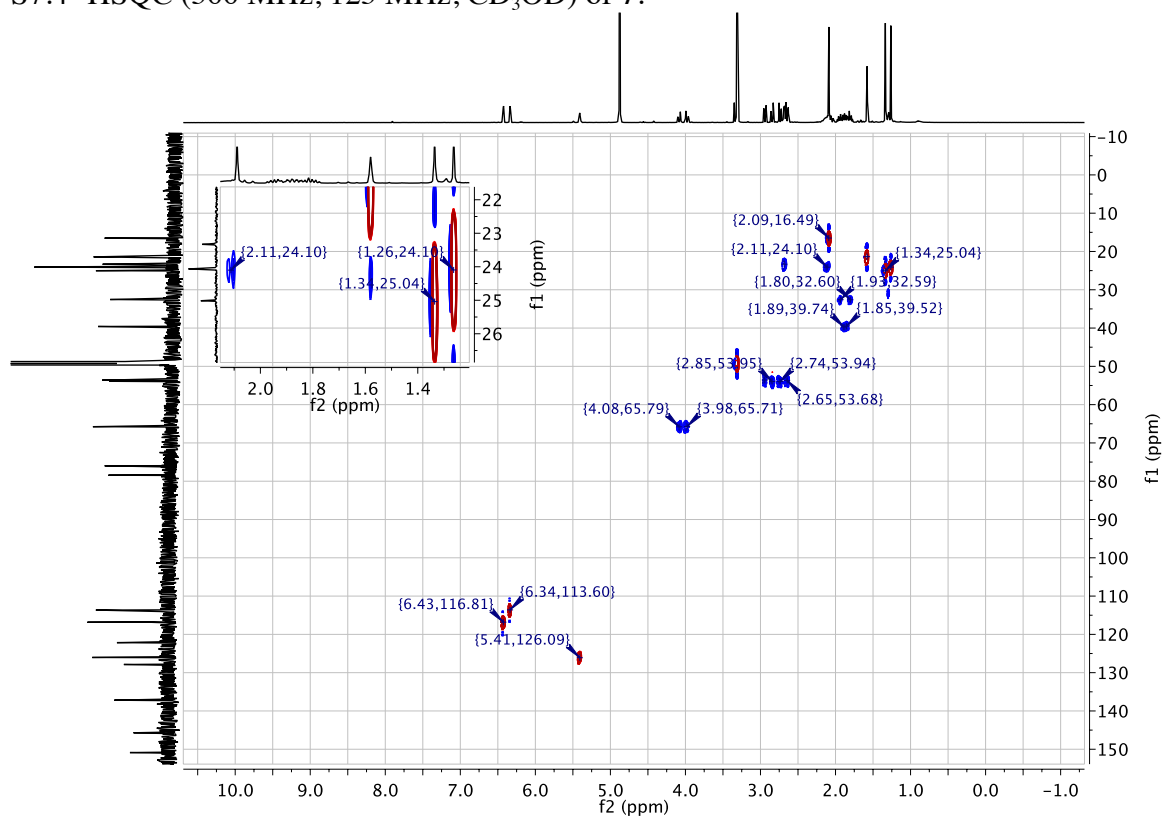
S7.2 ^1H NMR (500 MHz, CD_3OD) of **7**.



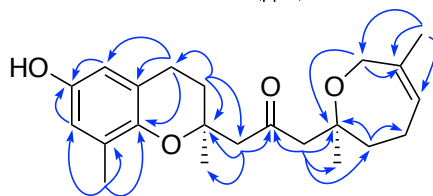
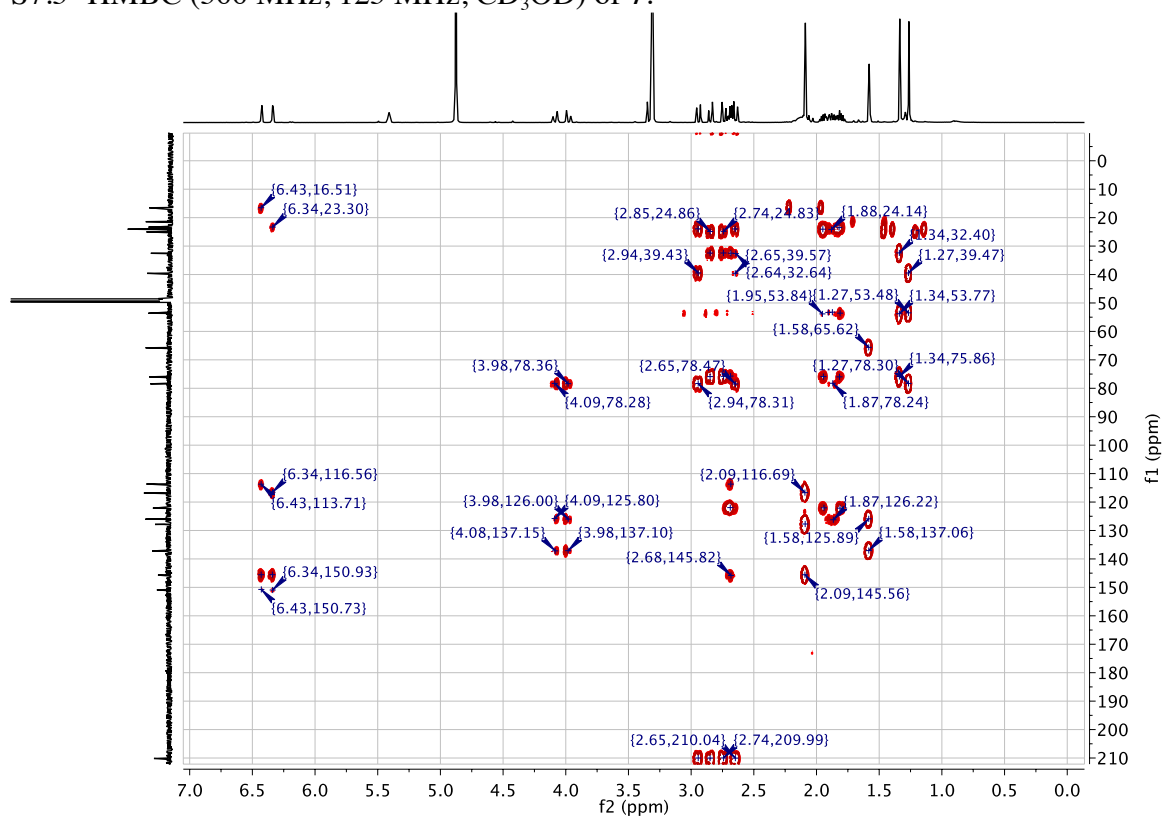
S7.3 ^{13}C NMR (125 MHz, CD_3OD) of **7**.



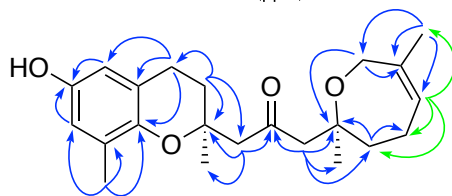
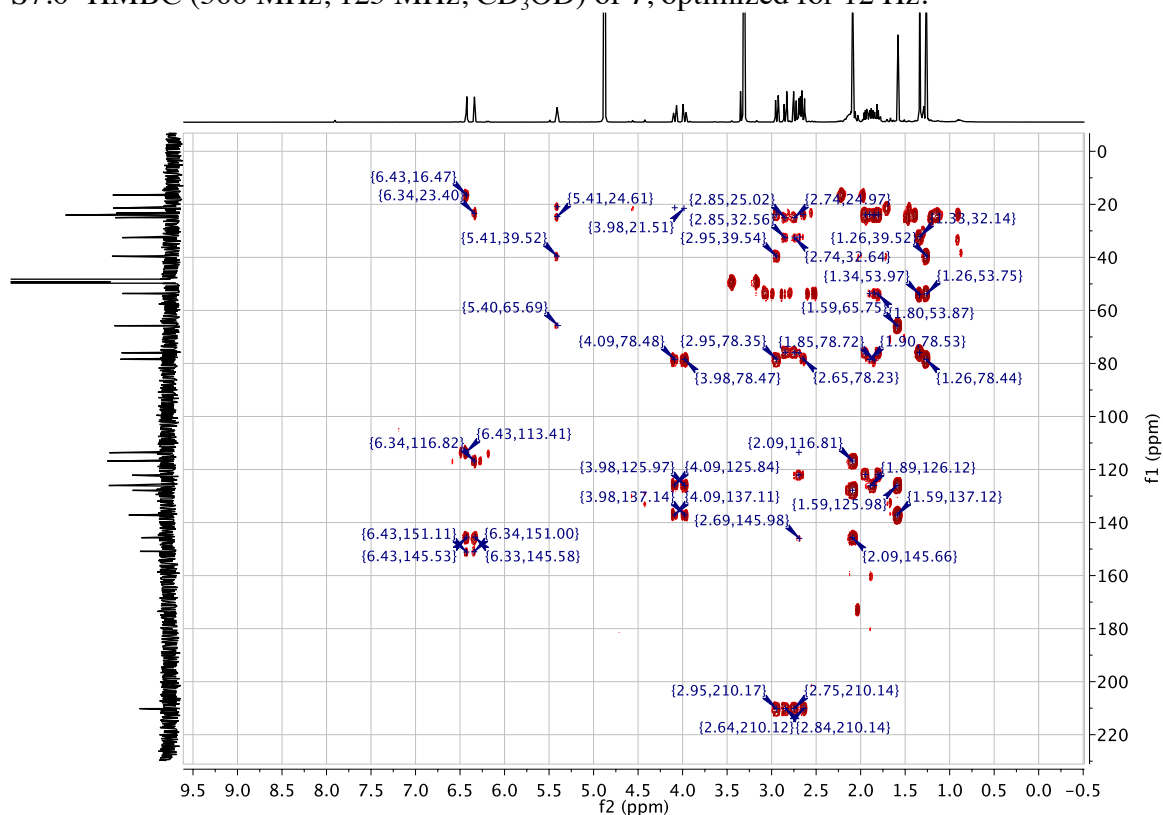
S7.4 HSQC (500 MHz, 125 MHz, CD₃OD) of 7.



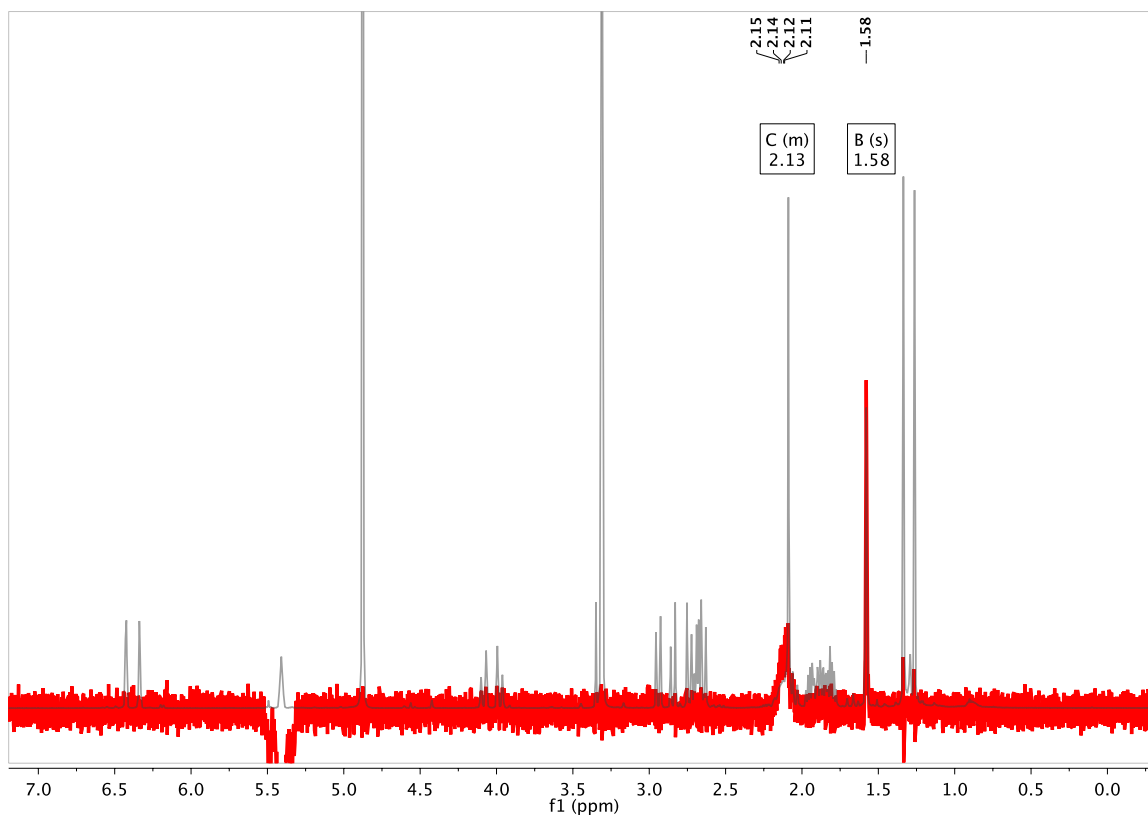
S7.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **7**.



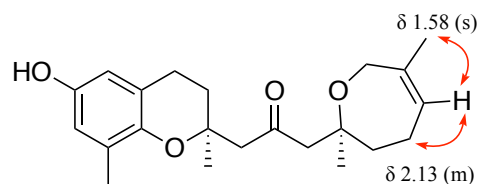
S7.6 HMBC (500 MHz, 125 MHz, CD₃OD) of **7**, optimized for 12 Hz.



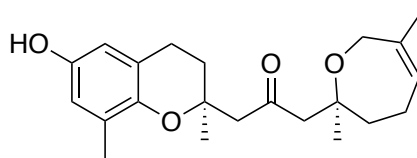
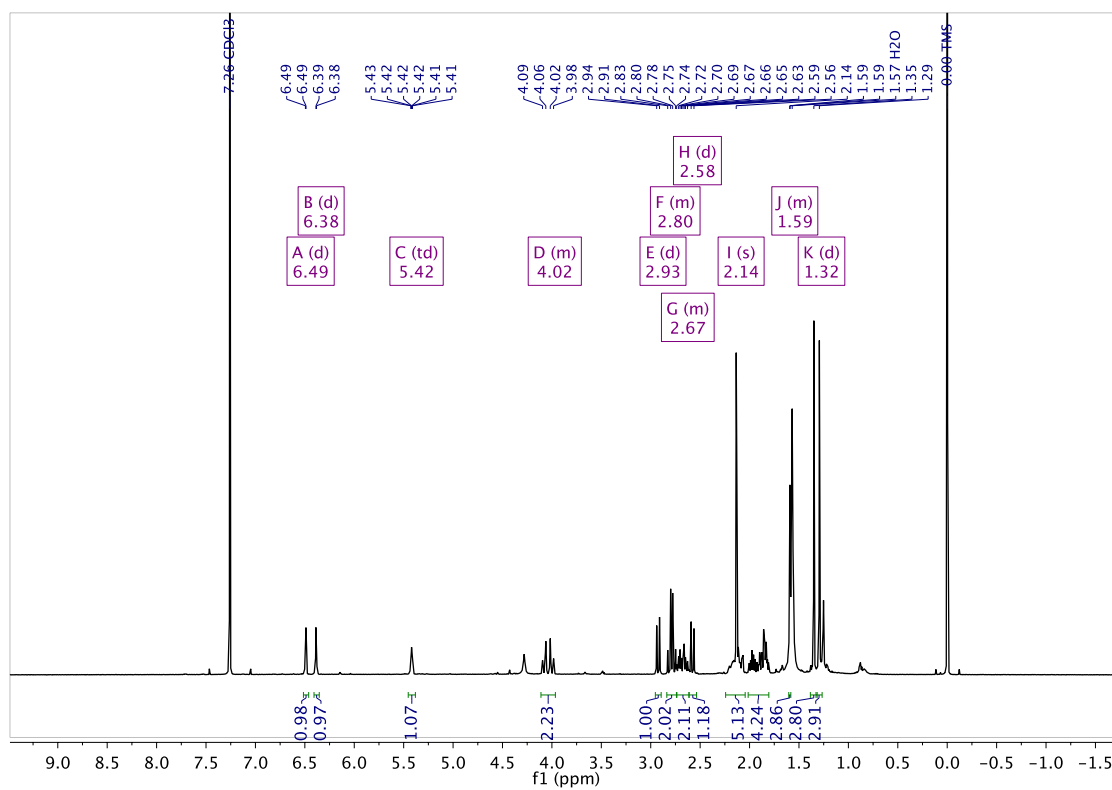
S7.7 SEL. NOE (500 MHz, CD₃OD, Irradiation at 5.4 ppm) of **7**.



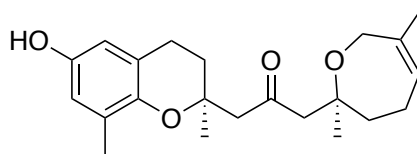
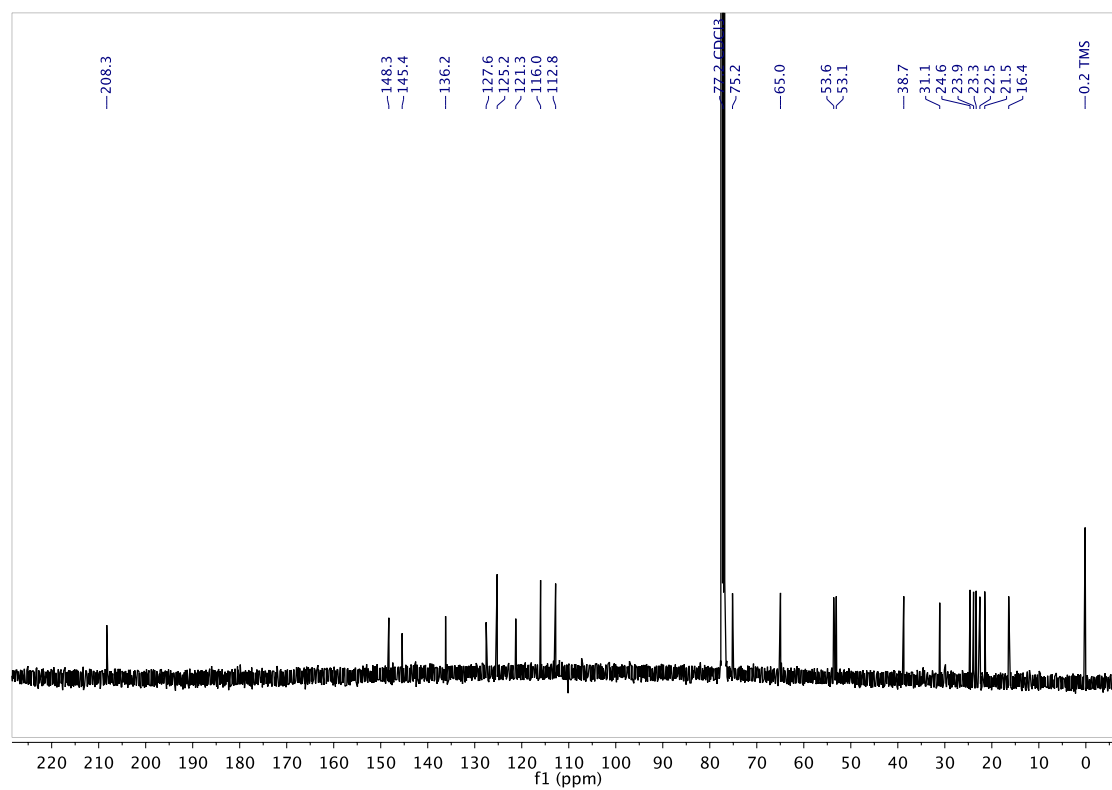
SEL. NOE in red. ¹H NMR in gray.



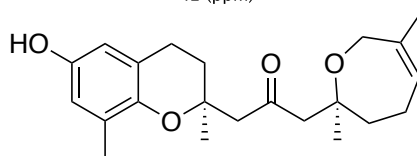
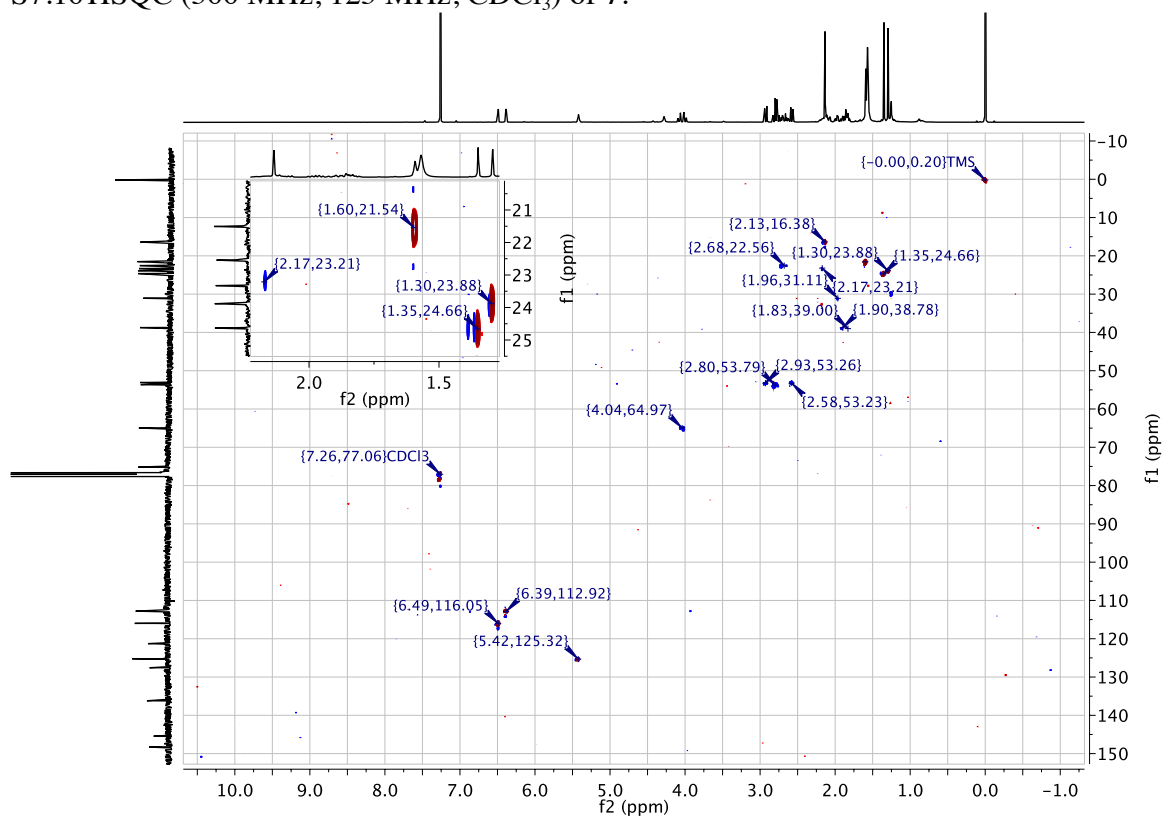
S7.8 ^1H NMR (500 MHz, CDCl_3) of **7**.



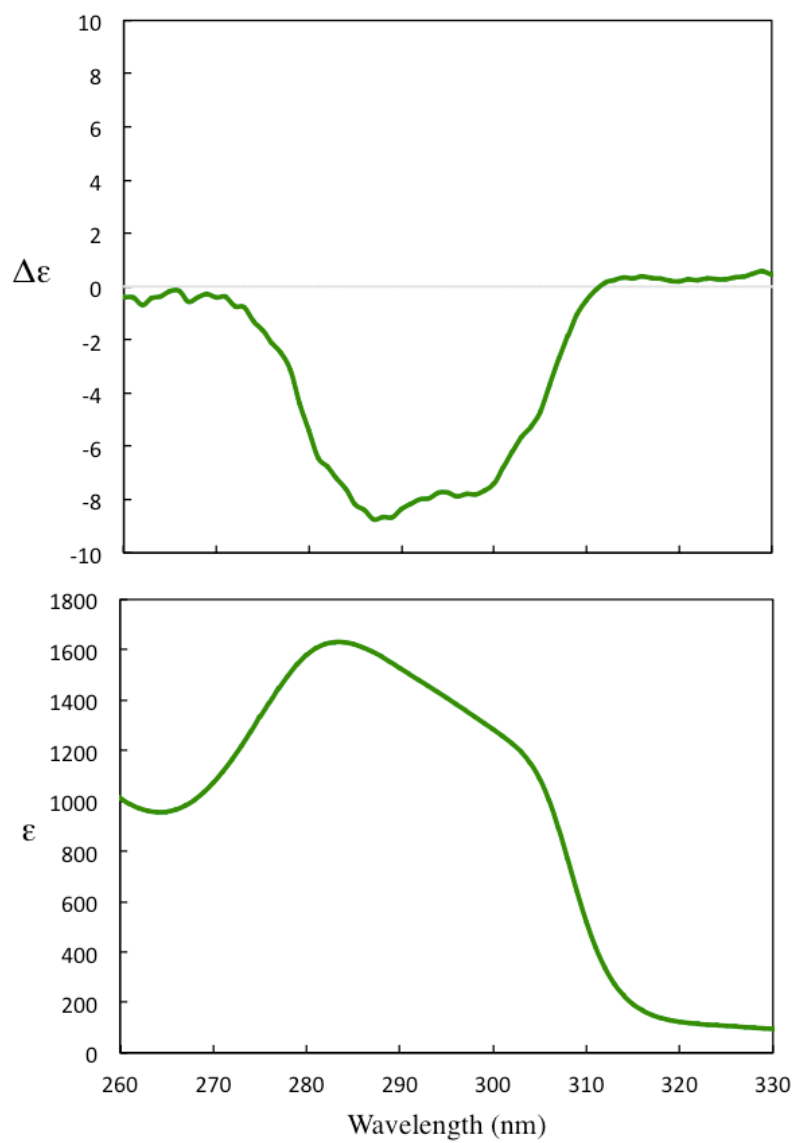
S7.9 ^{13}C NMR (125 MHz, CDCl_3) of **7**.



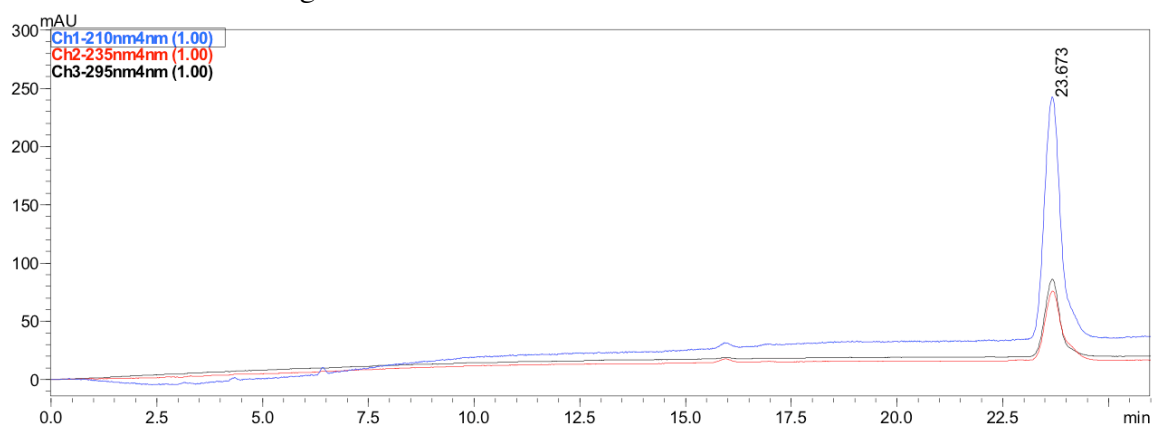
S7.10HSQC (500 MHz, 125 MHz, CDCl₃) of 7.



S7.11 ECD spectrum of **7** in CH₃OH (1.0 mM).

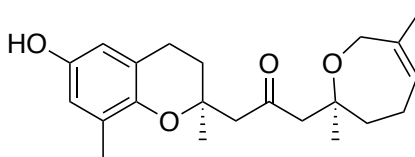


S7.12 HPLC Chromatogram of 7.



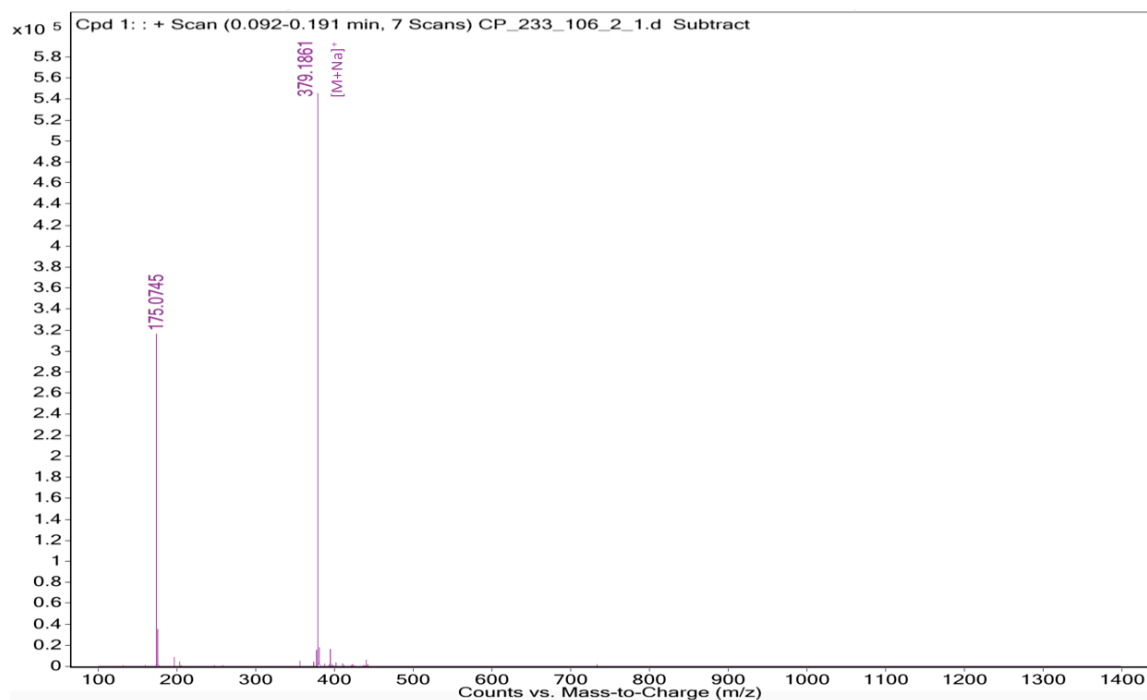
Phenomenex 5 μ m, 100 Å, Luna C₁₈(2) (250 x 10 mm) column with H₂O/MeOH at 3 mL/min.

Time (min)	MeOH %
0	70
26	81.7

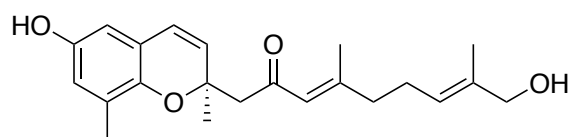
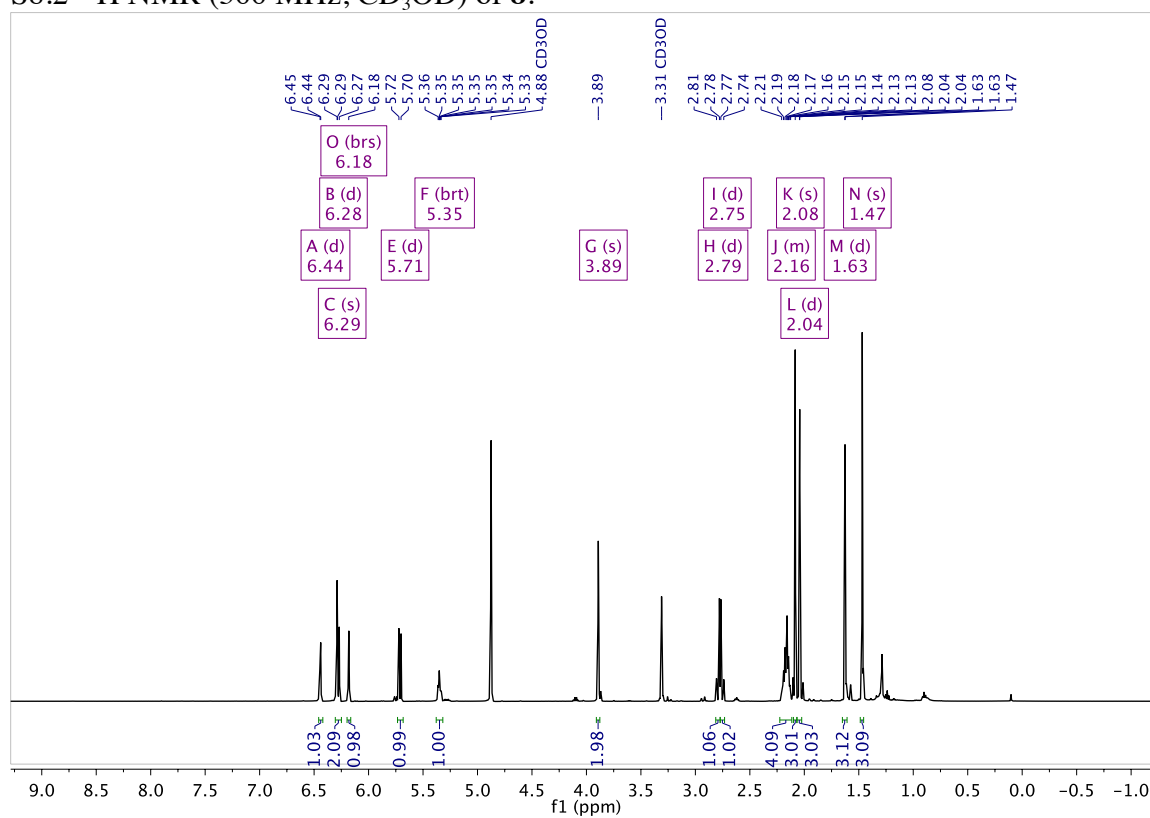


S8 Spectroscopic Data for **8** (3*E*,7*E*)-9-hydroxy-1-((*R*)-6-hydroxy-2,8-dimethyl-2*H*-chromen-2-yl)-4,8-dimethylnona-3,7-dien-2-one.

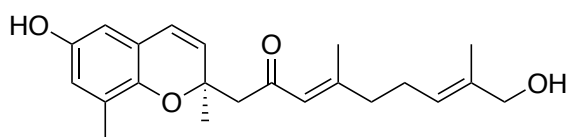
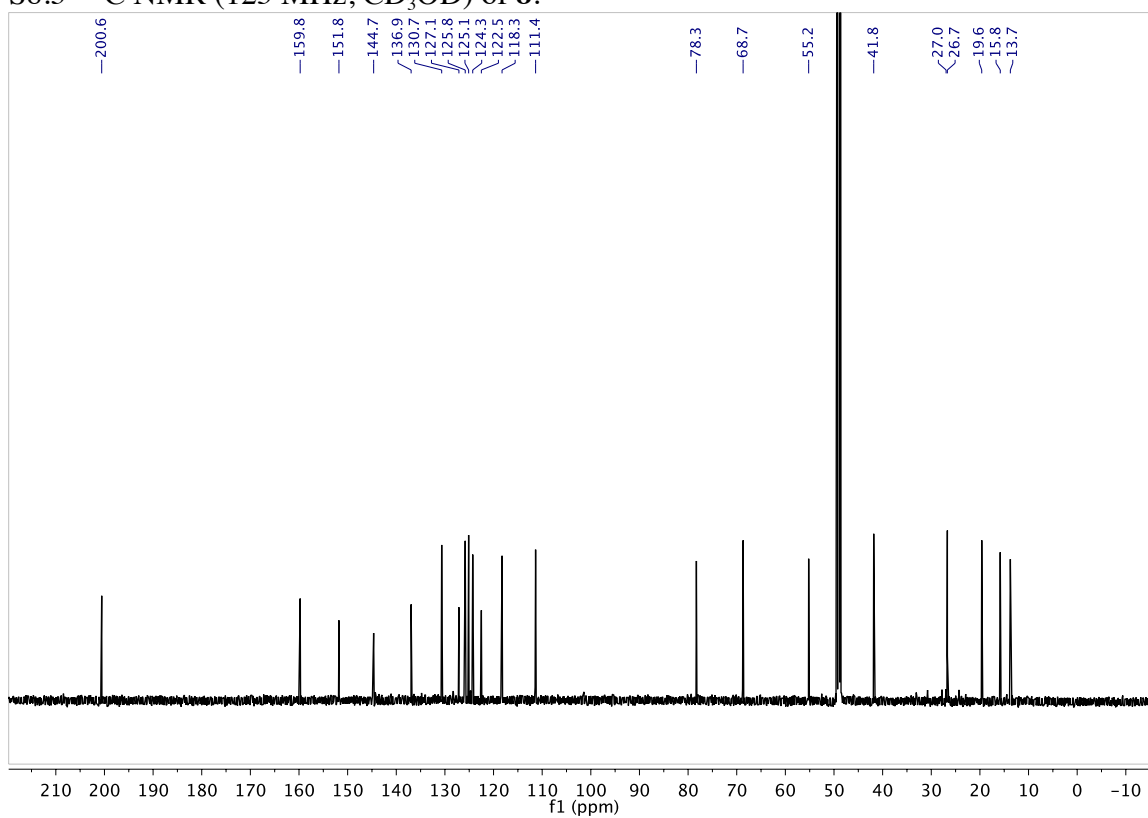
S8.1 HRESIMS of **8**.



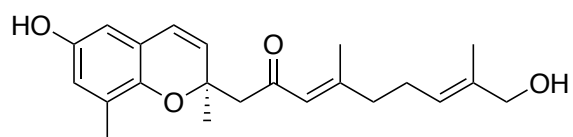
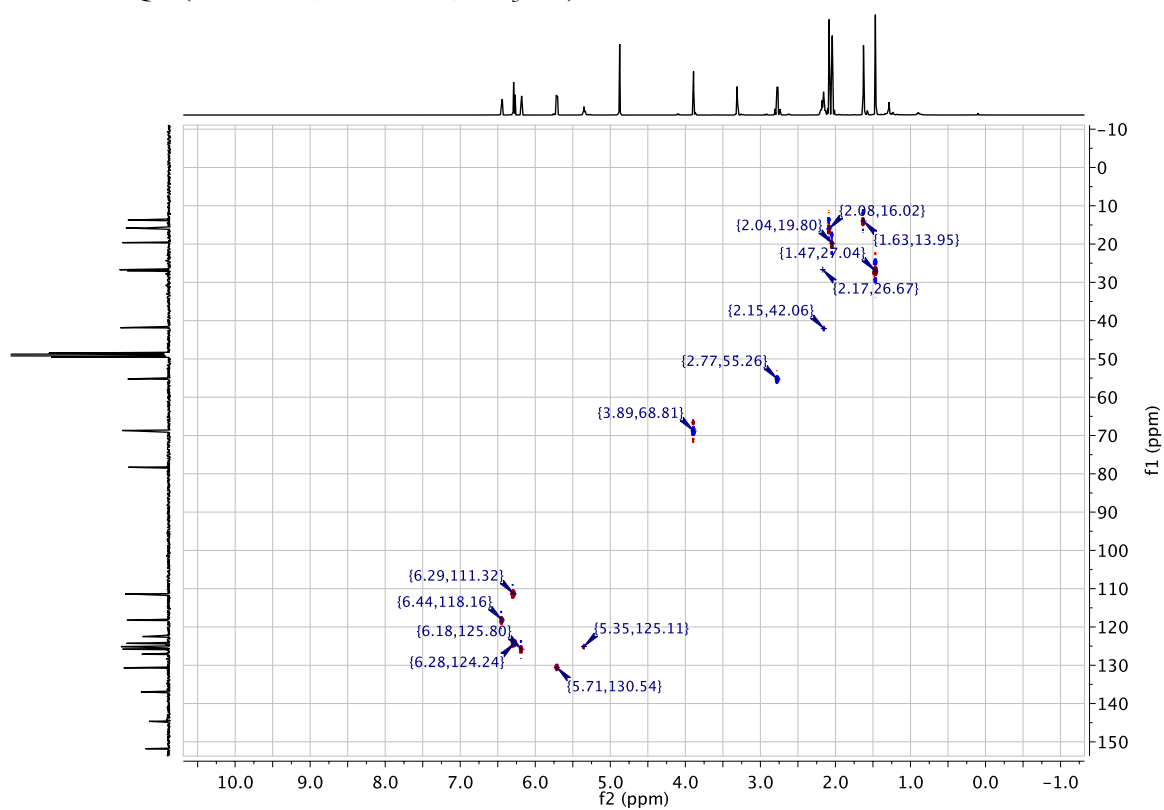
S8.2 ^1H NMR (500 MHz, CD_3OD) of **8**.



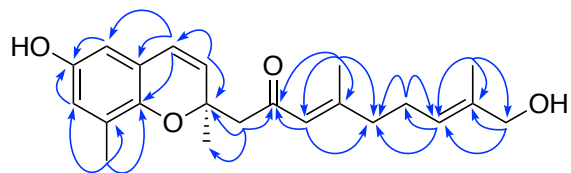
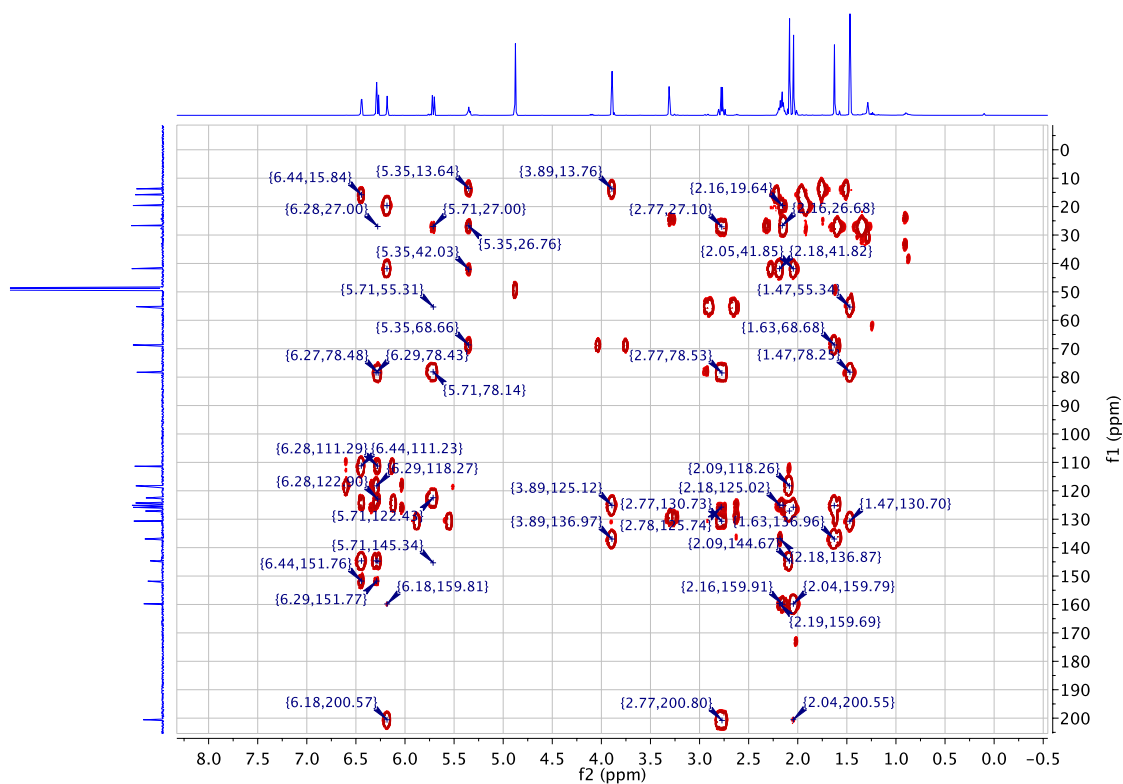
S8.3 ^{13}C NMR (125 MHz, CD_3OD) of **8**.



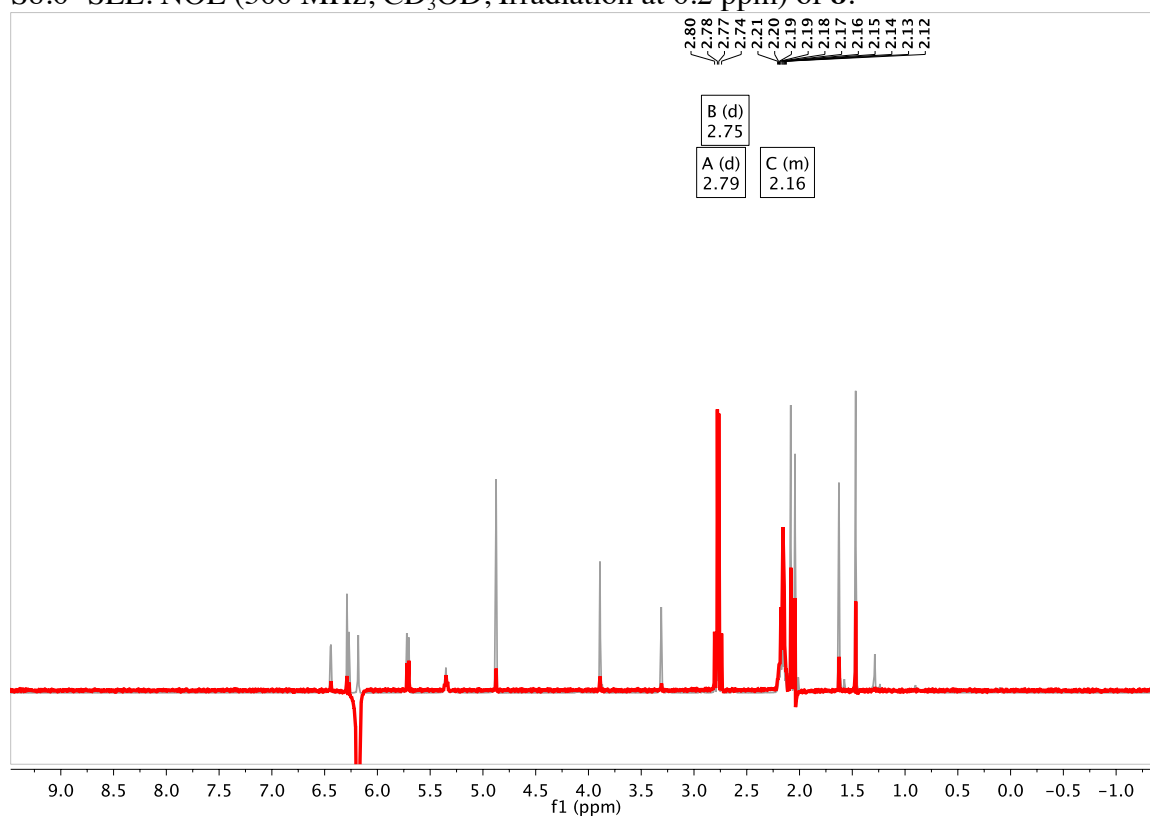
S8.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **8**.



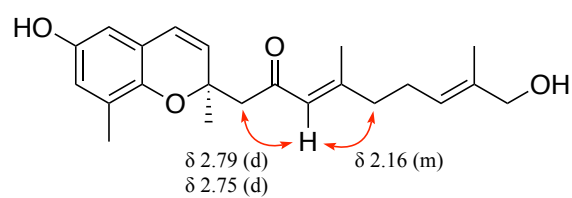
S8.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **8**.



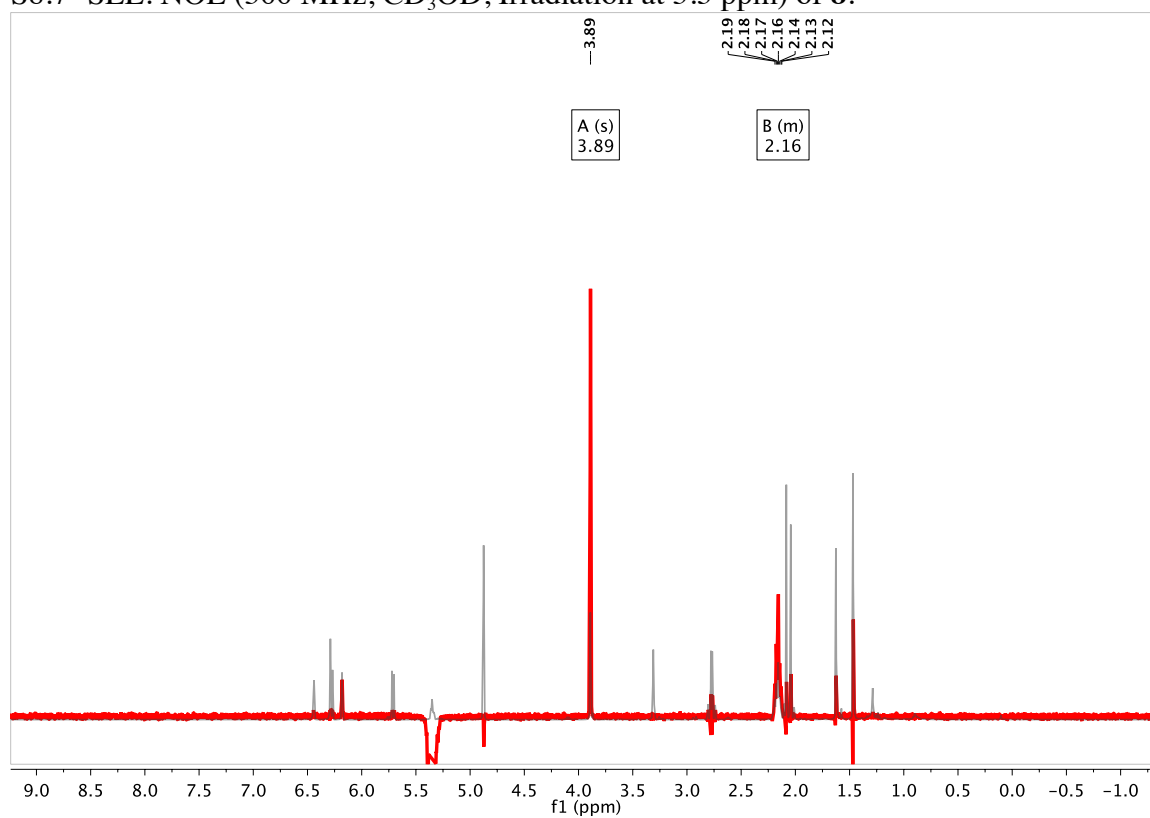
S8.6 SEL. NOE (500 MHz, CD₃OD, Irradiation at 6.2 ppm) of **8**.



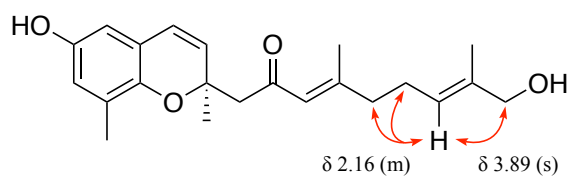
SEL. NOE in red. ¹H NMR in gray.



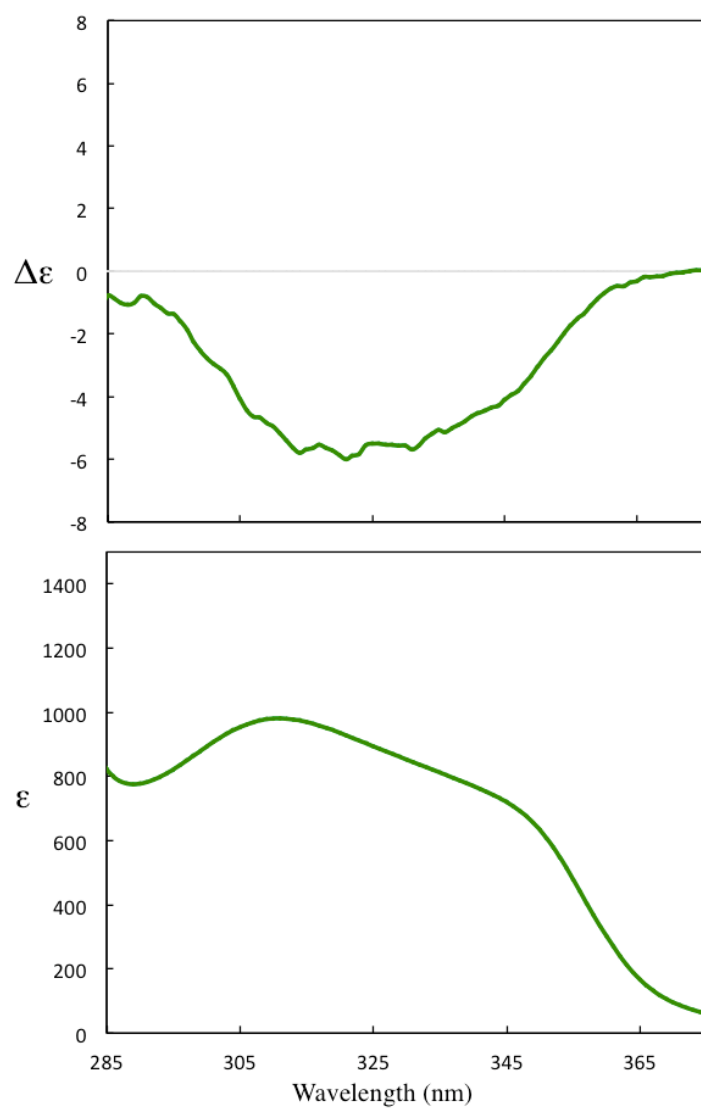
S8.7 SEL. NOE (500 MHz, CD₃OD, Irradiation at 5.3 ppm) of **8**.



SEL. NOE in red. ¹H NMR in gray.

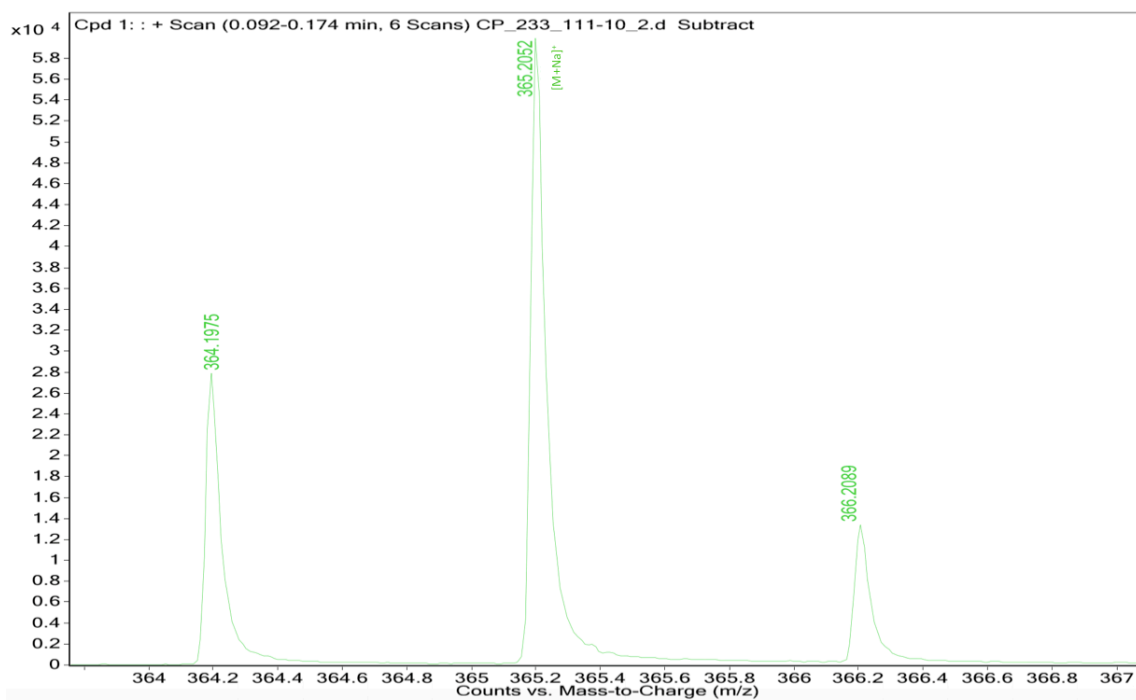


S8.8 ECD spectrum of **8** in CHCl₃ (1.0 mM).

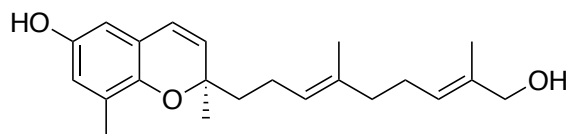
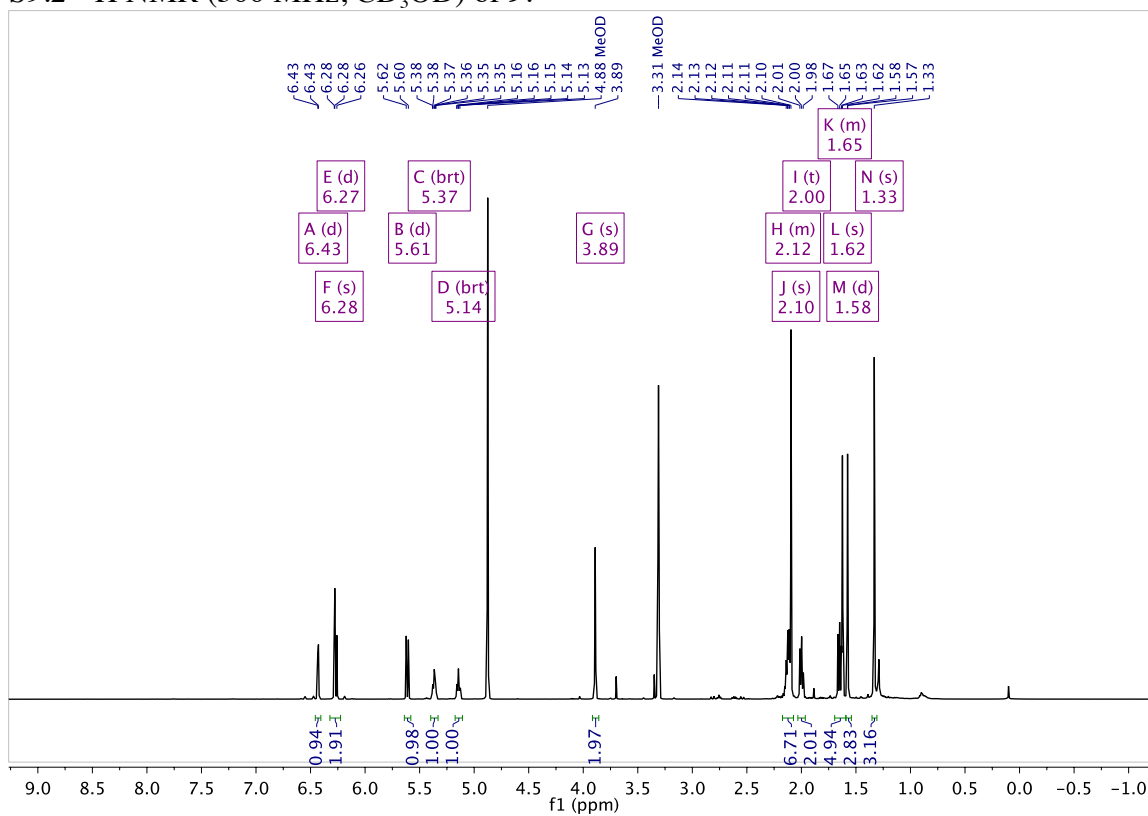


S9 Spectroscopic Data for **9** (*R*)-2-((3*E*,7*E*)-9-hydroxy-4,8-dimethylnona-3,7-dien-1-yl)-2,8-dimethyl-2*H*-chromen-6-ol.

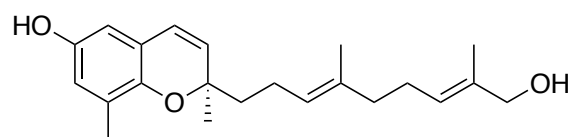
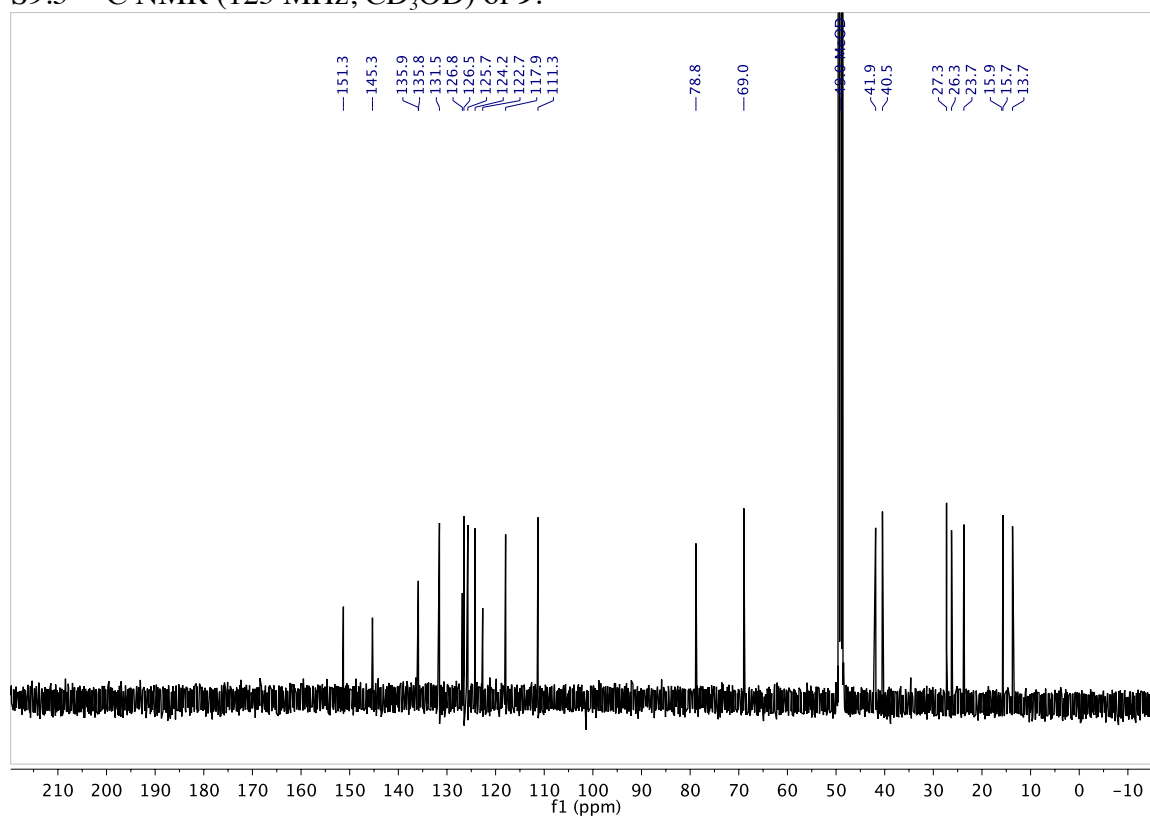
S9.1 HRESIMS of **9**.



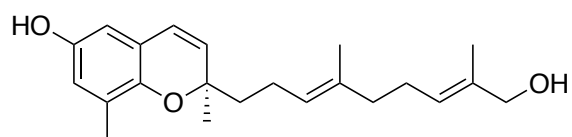
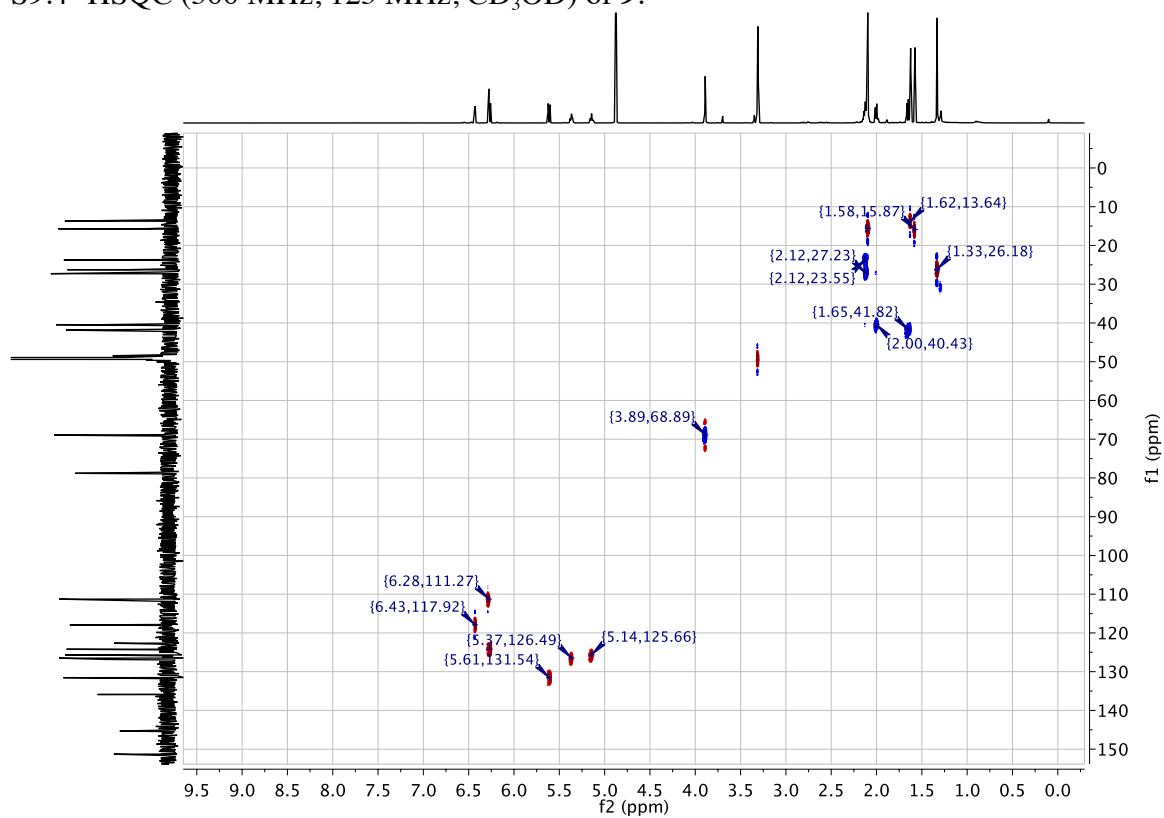
S9.2 ^1H NMR (500 MHz, CD_3OD) of **9**.



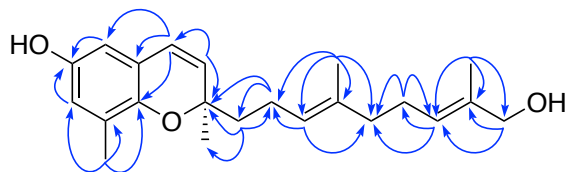
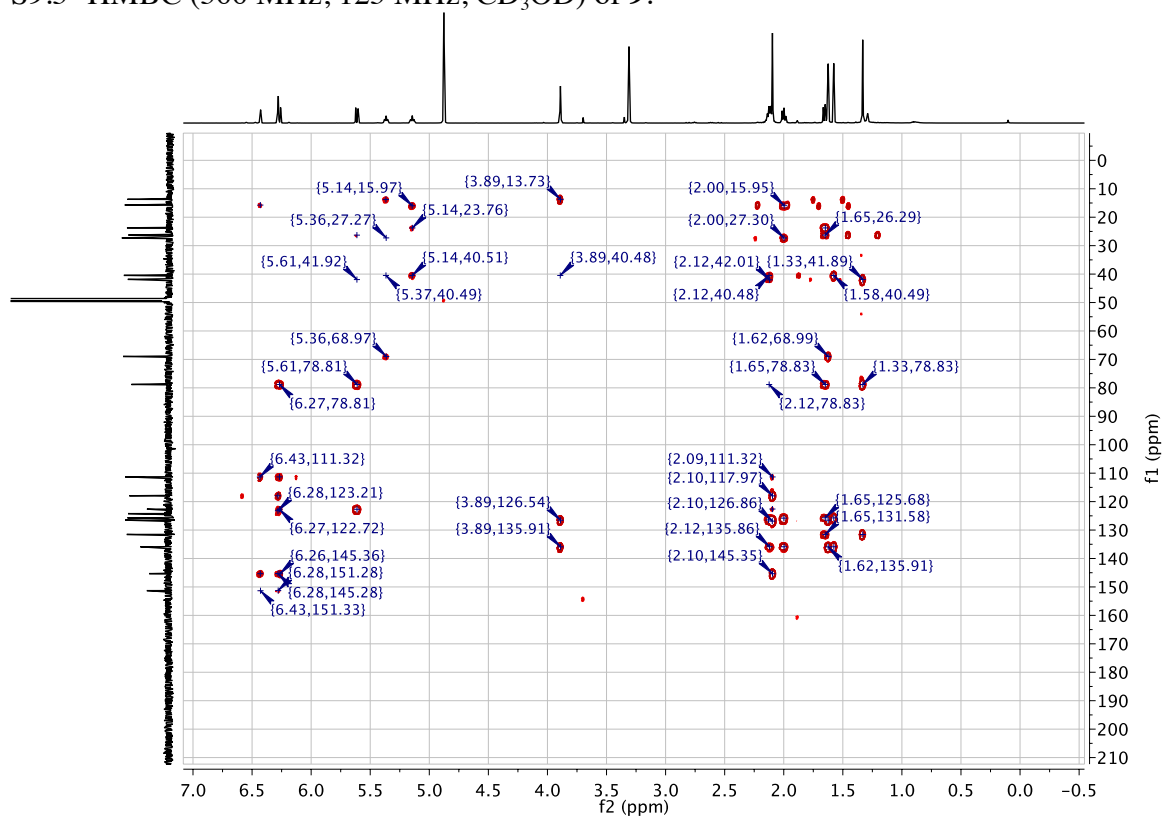
S9.3 ^{13}C NMR (125 MHz, CD_3OD) of **9**.



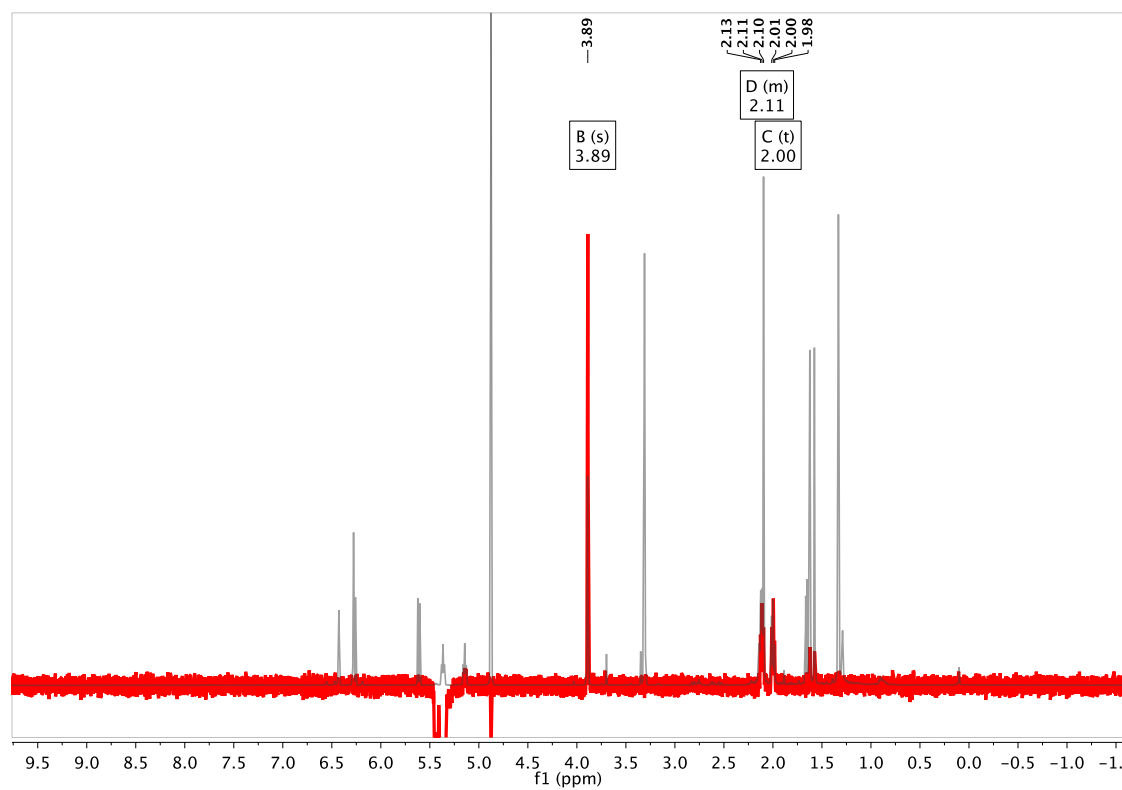
S9.4 HSQC (500 MHz, 125 MHz, CD₃OD) of **9**.



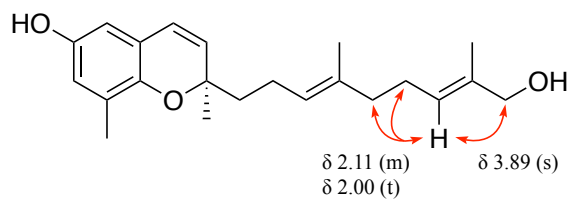
S9.5 HMBC (500 MHz, 125 MHz, CD₃OD) of **9**.



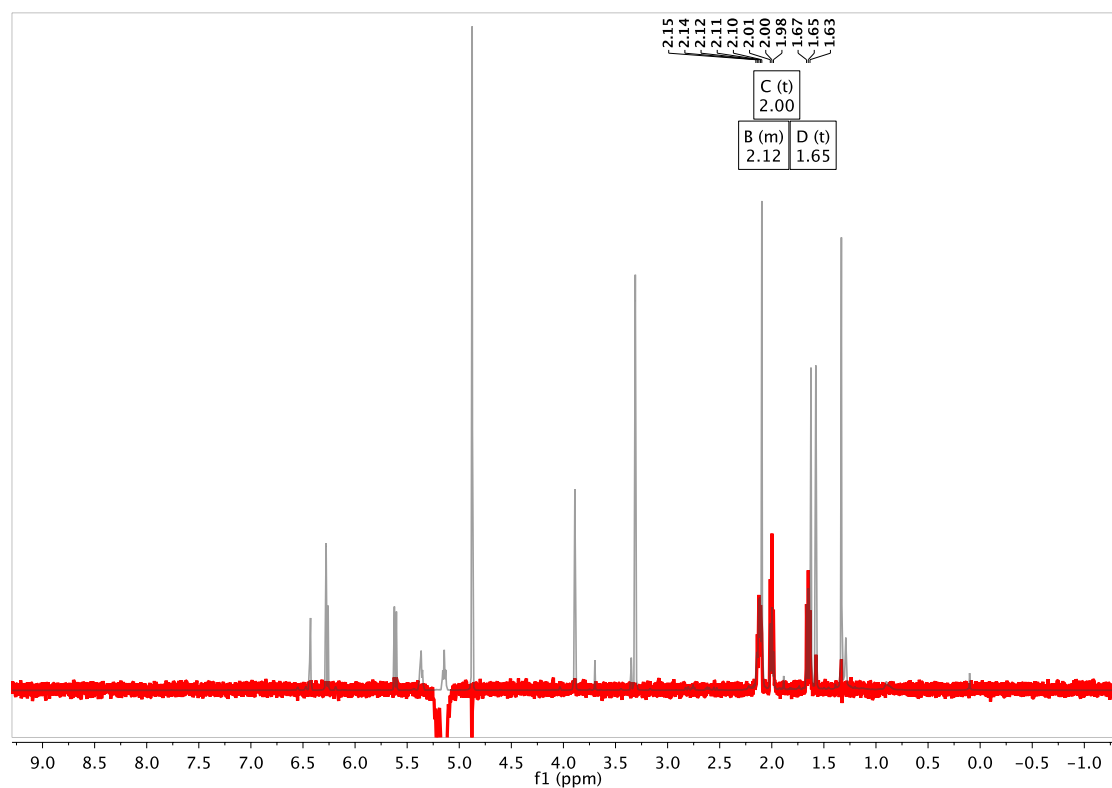
S9.6 SEL. NOE (500 MHz, CD₃OD, Irradiation at 5.4 ppm) of **9**.



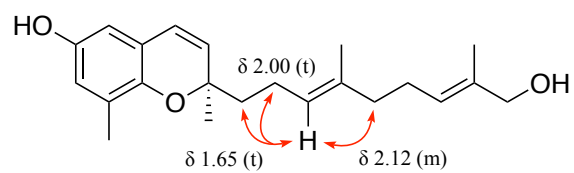
SEL. NOE in red. ¹H NMR in gray.



S9.7 SEL. NOE (500 MHz, CD₃OD, Irradiation at 5.1 ppm) of **9**.



SEL. NOE in red. ¹H NMR in gray.



S9.8 ECD spectrum of **9** in CHCl₃ (1.0 mM).

