Resorcylic Acid Lactones with Cytotoxic and NF-κB Inhibitory Activities and Their Structure-activity Relationships

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Supporting Information

Contents:

Figure S1. Analytical HPLC of MeOH-CH_3CN Partition. 35-40% MeCN in H_2O over 20 minutes. Gemini NX C18, 250 x 4.6 mm, 5 µm, 1 mL/min, 235 nm.

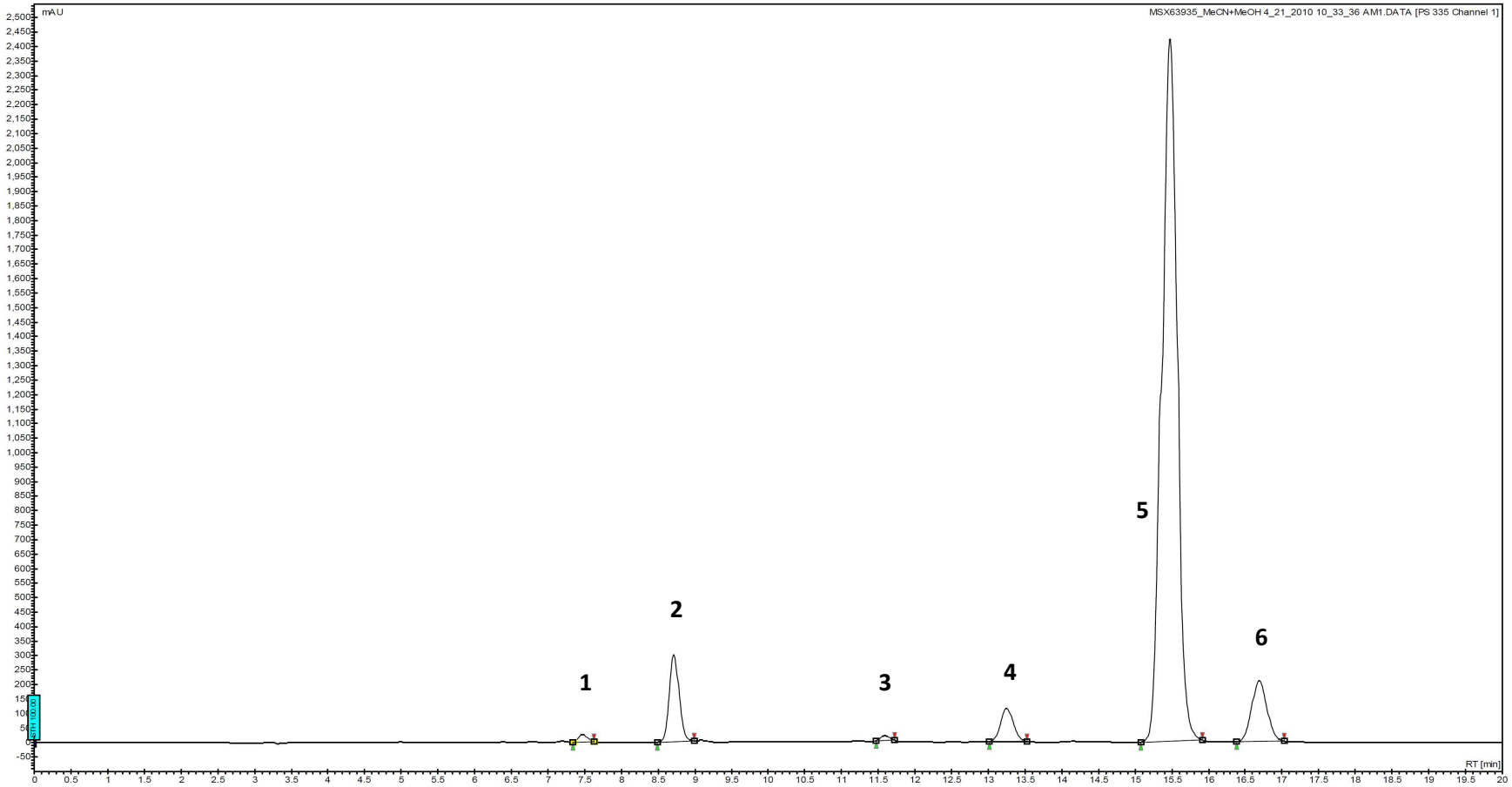

Figure S2. ^{1}H NMR of 15-*O*-Desmethyl-5*Z*-7-oxozeaenol (**1**) in DMSO-d_6

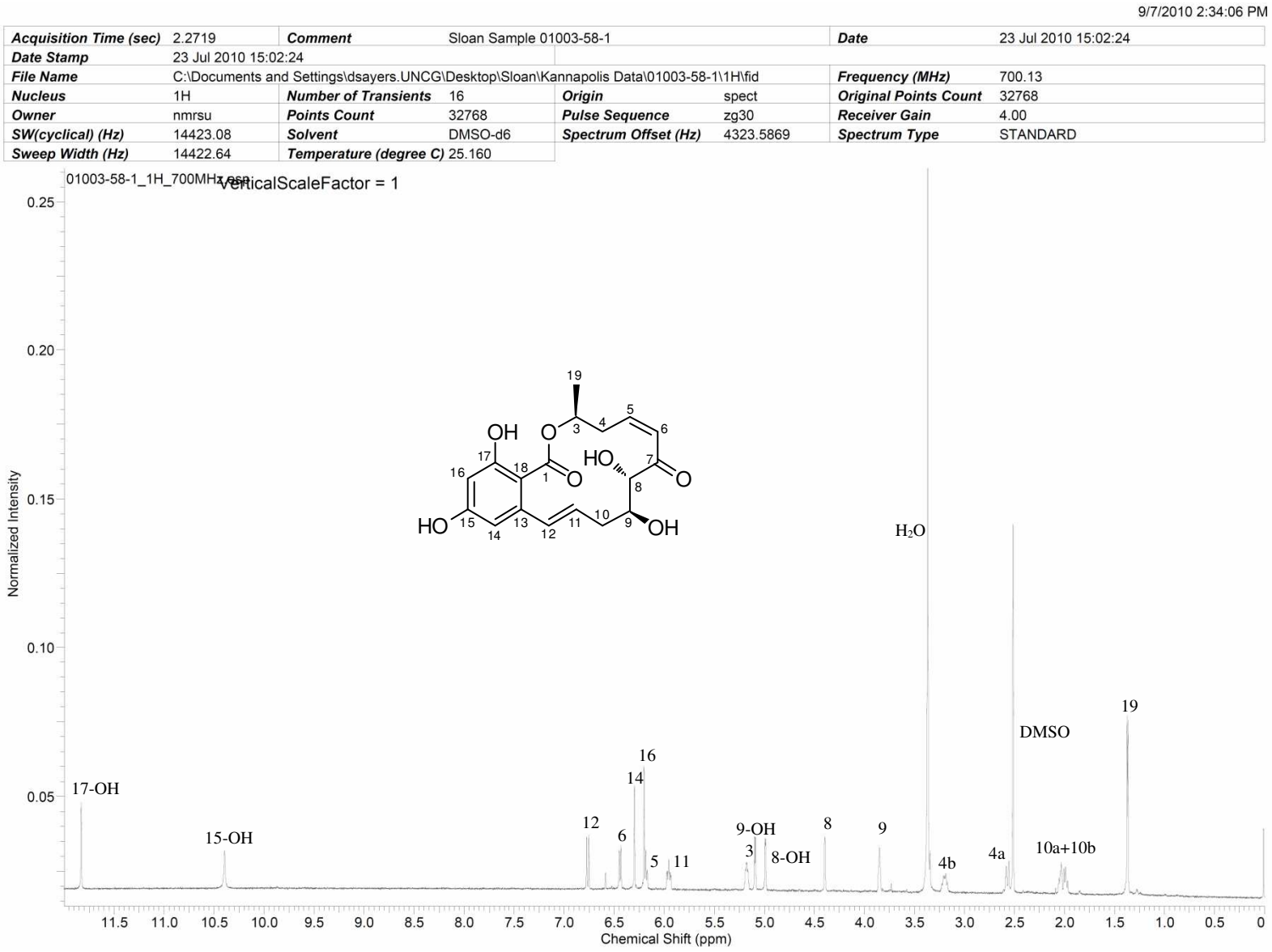

Figure S3. ^{13}C NMR of 15-*O*-Desmethyl-5*Z*-7-oxozeaenol (**1**) in DMSO-d_6

9/7/2010 2:48:38 PM

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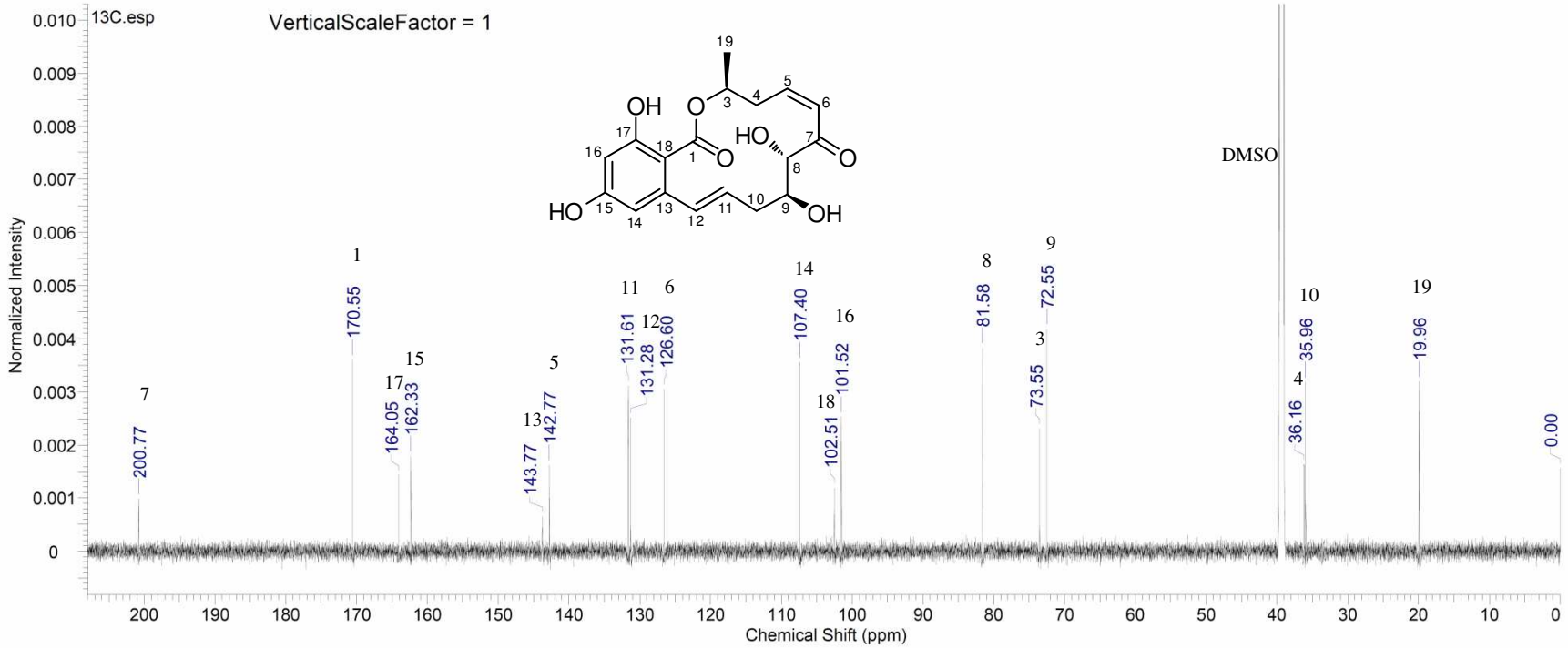
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	256.00
SW(cyclical) (Hz)	41666.67	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	17498.6523	***Spectrum Type***	STANDARD
Sweep Width (Hz)	41665.39	***Temperature (degree C)***	25.160				



No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0016
2	19.96	3513.3	0.0032
3	35.96	6329.9	0.0032
4	36.16	6365.5	0.0016
5	72.55	12771.6	0.0042

No.	(ppm)	(Hz)	Height
6	73.55	12948.4	0.0023
7	81.58	14362.3	0.0038
8	101.52	17871.9	0.0025
9	102.51	18047.3	0.0012
10	107.40	18908.2	0.0036

No.	(ppm)	(Hz)	Height
11	126.60	22288.0	0.0030
12	131.28	23110.7	0.0025
13	131.61	23170.5	0.0031
14	142.77	25135.0	0.0016
15	143.77	25310.5	0.0006

No.	(ppm)	(Hz)	Height
16	162.33	28578.4	0.0018
17	164.05	28879.8	0.0014
18	170.55	30024.2	0.0036
19	200.77	35345.7	0.0010

Figure S4. ^{1}H NMR of 7-*epi*-Zeaenol (**3**) in DMSO-d_6

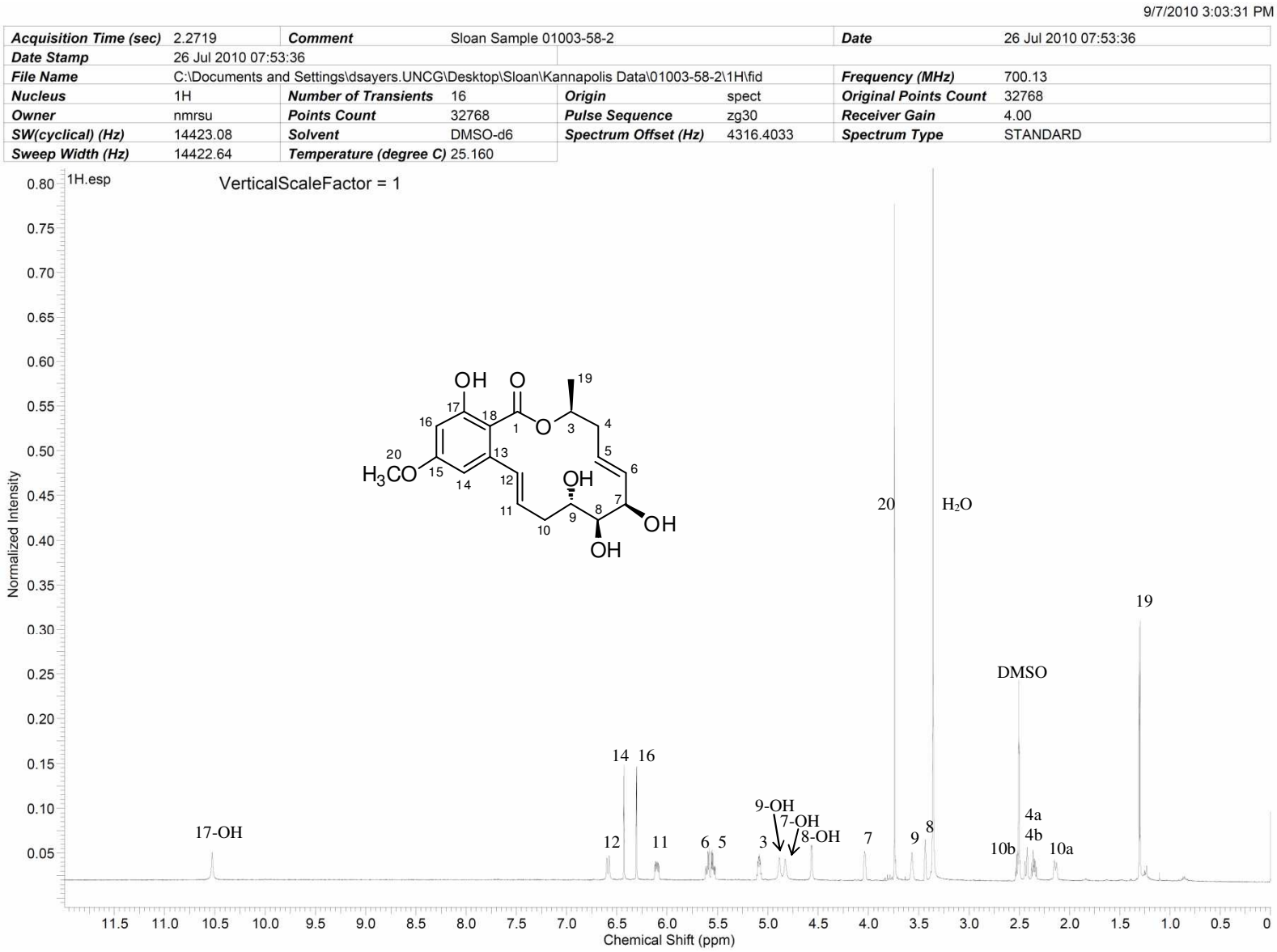


Figure S5. ^{13}C NMR of 7-*epi*-Zeaenol (**3**) in DMSO-d_6

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Acquisition Time (sec)	0.7864	***Comment***	Sloan Sample 01003-58-2			***Date***	26 Jul 2010 11:07:44
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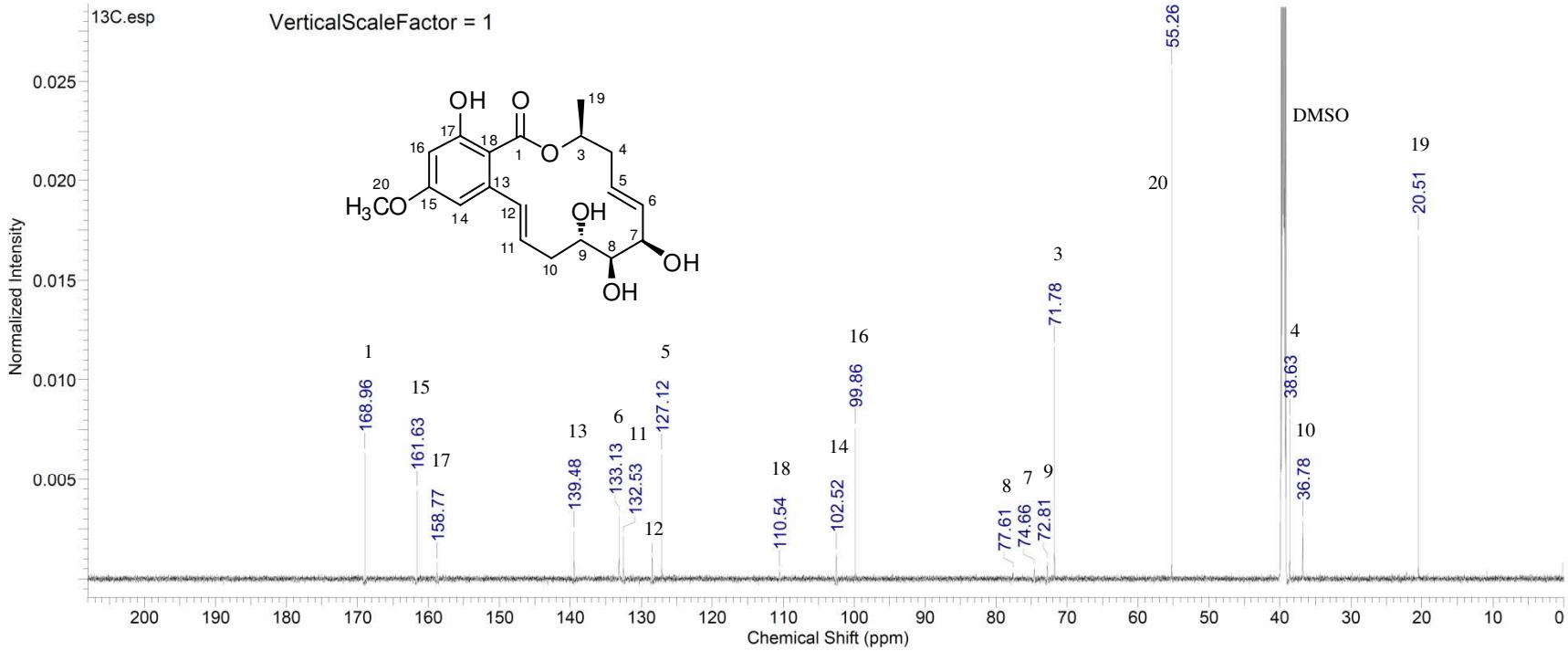
Nucleus	13C	***Number of Transients***	4096	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	256.00
SW(cyclical) (Hz)	41666.67	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	17526.8105	***Spectrum Type***	STANDARD
Sweep Width (Hz)	41665.39	***Temperature (degree C)***	25.160				



No.	(ppm)	(Hz)	Height
1	20.51	3610.2	0.0173
2	36.78	6475.0	0.0029
3	38.63	6800.5	0.0080
4	55.26	9727.7	0.0256
5	71.78	12637.0	0.0117

No.	(ppm)	(Hz)	Height
6	72.81	12817.6	0.0008
7	74.66	13143.1	0.0005
8	77.61	13663.2	0.0003
9	99.86	17579.6	0.0076
10	102.52	18048.8	0.0013

No.	(ppm)	(Hz)	Height
11	110.54	19460.2	0.0004
12	127.12	22378.5	0.0063
13	128.47	22617.5	0.0011
14	132.53	23332.1	0.0021
15	133.13	23437.7	0.0031

No.	(ppm)	(Hz)	Height
16	139.48	24555.4	0.0024
17	158.77	27951.7	0.0008
18	161.63	28455.3	0.0044
19	168.96	29745.9	0.0063

Table S1. NMR Data for Known Compounds **4** and **5** (500 MHz, chemical shifts in δ, coupling constants in Hz, DMSO-d_6 for **4**, $CDCl_3$ for **5**)

Position	5*E*-7-Oxozeaenol (**4**)		5*Z*-7-Oxozeaenol (**5**)	
	δ_C	δ_H (mult.; *J* in Hz)	δ_C	δ_H (mult.; *J* in Hz)
1	168.2	---	171.5	---
3	70.2	5.13, qdd (6.0, 8.7, 2.8)	73.9	5.24, qdd (6.2, 11.4, 2.4)
4a	37.8	2.44, ddd (14.4, 8.7, 8.7)	37.2	2.50, dd (17.2, 2.4)
4b	37.8	2.59, ddd (14.4, 6.2, 2.8)	37.2	3.57, dd (17.2, 11.4)
5	142.3	6.82, ddd (15.7, 8.7, 6.2)	147.7	6.21, ddd (11.7, 11.0, 2.7)
6	130.3	6.49, d (15.7)	125.4	6.33, dd (11.7, 2.7)
7	200.7	---	199.3	---
8	78.2	4.32, dd (5.1, 4.0)	81.0	4.51, d (2.1)
9	71.9	4.02, m	73.8	3.99, ddd (5.5, 2.7, 2.1)
10a	36.0	2.14, ddd (15.3, 6.5, 2.9)	37.7	2.12, ddd (15.8, 11.0, 2.7)
10b	36.0	2.36, ddd (15.3, 6.5, 6.5)	37.7	2.21, ddd (15.8, 5.5, 2.1)
11	130.5	6.17, ddd (15.7, 6.5, 6.5)	130.4	5.98, ddd (15.1, 11.0, 4.1)
12	128.6	6.27, d (15.7)	133.1	6.87, d (15.1)
13	138.4	---	143.3	---
14	102.6	6.45, d (2.3)	108.4	6.40, d (2.7)
15	161.3	---	164.4	---
16	100.1	6.32, d (2.3)	100.4	6.39, d (2.7)
17	157.9	---	166.1	---
18	111.5	---	103.6	---
19	20.1	1.35, d (6.0)	20.9	1.47, d (6.2)
20	55.2	3.74, s	55.6	3.80, s
7-OH	---	---	---	---
8-OH	---	5.17, d (5.1)	---	---
9-OH	---	4.99, d (5.7)	---	---
15-OH	---	---	---	---
17-OH	---	10.34, s	---	12.14, s

Figure S6. ^{1}H NMR of Known Compounds **2** and **4**-**6** (**2** and **4** in DMSO-d_6, **5** and **6** in $CDCl_3$, 500 MHz)