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

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### **Supporting Information**

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### Figure S1. Analytical HPLC of MeOH-CH<sub>3</sub>CN Partition. 35-40% MeCN in H<sub>2</sub>O over 20 minutes. Gemini NX C18, 250 x 4.6 mm, 5

µm, 1 mL/min, 235 nm.



## Figure S2. <sup>1</sup>H NMR of 15-*O*-Desmethyl-5*Z*-7-oxozeaenol (1) in DMSO- $d_6$

#### Acquisition Time (sec) 2.2719 Comment Sloan Sample 01003-58-1 Date 23 Jul 2010 15:02:24 Date Stamp 23 Jul 2010 15:02:24 File Name C:\Documents and Settings\dsayers.UNCG\Desktop\Sloan\Kannapolis Data\01003-58-1\1H\fid Frequency (MHz) 700.13 Origin Original Points Count 32768 Nucleus 1H Number of Transients 16 spect Owner nmrsu **Points Count** 32768 **Pulse Sequence** zg30 **Receiver Gain** 4.00 SW(cyclical) (Hz) 14423.08 Solvent DMSO-d6 Spectrum Offset (Hz) 4323.5869 Spectrum Type STANDARD Sweep Width (Hz) 14422.64 Temperature (degree C) 25.160 01003-58-1\_1H\_700MHz/efficalScaleFactor = 1 0.25 0.20 19 OH $\cap$ HO Normalized Intensity HO $H_2O$ 12 0.10 19 DMSO 16 14 17-OH 0.05 12 8 9-OH 9 6 15-OH 10a+10b 3 8-OH 4a 5 11 4b 3.5 11.5 11.0 10.5 9.5 9.0 7.5 7.0 5.0 3.0 2.5 2.0 1.5 1.0 0.5 0 10.0 8.5 8.0 6.5 6.0 5.5 4.5 4.0 Chemical Shift (ppm)

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## **Figure S3.** <sup>13</sup>C NMR of 15-*O*-Desmethyl-5*Z*-7-oxozeaenol (1) in DMSO- $d_6$

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# **Figure S4.** <sup>1</sup>H NMR of 7-*epi*-Zeaenol (3) in DMSO- $d_6$

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1 20.51 30	10.2 0	.0173	6	72.81	12817.6	0.0008	11	110.54	19460.2	0.0004	16	139.48	24555.4	0.0024	
2 36.78 64	75.0 0	.0029	7	74.66	13143.1	0.0005	12	127.12	22378.5	0.0063	17	158.77	27951.7	0.0008	
3 38.63 68	00.5 0	.0080	8	77.61	13663.2	0.0003	13	128.47	22617.5	0.0011	18	161.63	28455.3	0.0044	
4 55.26 97	27.7 0	.0256	9	99.86	17579.6	0.0076	14	132.53	23332.1	0.0021	19	168.96	29745.9	0.0063	
5 71.78 12	637.0 0	.0117	10	102.52	18048.8	0.0013	15	133.13	23437.7	0.0031					

## Figure S5. <sup>13</sup>C NMR of 7-*epi*-Zeaenol (3) in DMSO-*d*<sub>6</sub>

**Table S1.** NMR Data for Known Compounds **4** and **5** (500 MHz, chemical shifts in  $\delta$ , coupling constants in Hz, DMSO-*d*<sub>6</sub> for **4**, CDCl<sub>3</sub> for **5**)

Position		5E-7-Oxozeaenol (4)	5Z-7-Oxozeaenol ( <b>5</b> )				
	$\delta_{ m C}$	$\delta_{\rm H}$ (mult.; J in Hz)	$\delta_{ m C}$	$\delta_{\rm H}$ (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. <sup>1</sup>H NMR of Known Compounds 2 and 4-6 (2 and 4 in DMSO-*d*<sub>6</sub>, 5 and 6 in CDCl<sub>3</sub>,

500 MHz)