## **Supplementary Material**

## Bioguided discovery and pharmacophore modeling of the mycotoxic indole diterpene alkaloids penitrems as breast cancer proliferation, migration, and invasion inhibitors

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**Fig. SI1.** RP-HPLC Separation of Compounds 1-5. Column: Cosmosil 5C18-AR-II (20 x 250 mm) Mobile Phase: isocratic elution (CH<sub>3</sub>CN-H<sub>2</sub>O; 80:20) UV detection shown: at 296 nm Injection volume: 2 mL Flow rate: 5 mL min<sup>-1</sup>



**Fig. SI2.** RP-HPLC Purification of Compounds **6** and **7**. Column: Cosmosil 5C18-AR-II (20 x 250 mm) Mobile Phase: isocratic elution (CH<sub>3</sub>CN-H<sub>2</sub>O; 80:20) UV detection shown: at 296 nm Injection volume: 2 mL Flow rate: 5 mL min<sup>-1</sup> Total amount injected: 25 mg

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Figure SI3. <sup>1</sup>H NMR Spectrum of Compound 8 (Acetone-d<sub>6</sub>).

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Figure SI4. PENDANT Spectrum of Compound 8 (Acetone-d<sub>6</sub>).

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**Figure SI5.** <sup>1</sup>H NMR Spectrum of Compound **9** (Acetone-d<sub>6</sub>).



Figure SI6. PENDANT Spectrum of Compound 9 (Acetone-d<sub>6</sub>).



Fig. SI7. Mean graph of the effect of  $10 \,\mu\text{M}$  dose of 1 on the percent growth of the NCI's 60 cell lines.

One Dose Mean Graph     Experiment ID: 10070590     Report Date: Feb D5, 2011       Panel/Cell Line     Growth Percent     Mean Growth Percent - Growth Percent       Lewieming CCRF-CEM H-600(T6)     23.94 23.95 20.95 2	One Dose Mean Graph       Panel/Cell Line     Growth Percent       Leukemia     2000       CCRF-CEM     21.34       HL-60(TB)     28.96       K-562     19.90       MOLT-4     36.42       RPMI-8226     20.37       SR     45.92       Non-Small Cell Lung Cancer     43.13       EKVX     63.02       HOP-62     93.85       NCI-H226     82.26       NCI-H226     82.26       NCI-H226     78.48       Colon Cancer     78.48       Colon Cancer     60.655       HCT-15     74.35       HC1-15     74.35       HC1-15     74.35       HT29     38.36       WG12     40.91       SW-620     64.13       CNS Cancer     977       SNB-19     71.77       SNB-75     68.15       U251     66.28
Panel/Cell Line     Crowth Percent     Mean Growth Percent - Growth Percent       Lawkerning GCRF-CEM H-GO(TR)     2:34 19:00 19:0	Panel/Cell Line     Growth Percent       Leukemia     21.34       CCRF-CEM     21.34       HL:60(TB)     28.96       K-562     19.90       MOLT-4     36.42       RPMI-8226     20.37       SR     45.92       Non-Small Cell Lung Cancer     45.92       A549/ATCC     43.13       EKVX     63.02       HOP-62     93.95       NCI-H26     82.26       NCI-H27     73.16       NCI-H27     78.48       Colon Cancer     70.49       COLO 205     76.49       HCT-116     25.33       HCT-15     74.35       HCT-15     74.35       HCT-15     74.35       HCT-15     74.35       HCT-15     74.35       HCT-15     74.35       HCT-2988     49.18       SF-268     49.18       SF-268     49.18       SF-268     49.18       SF-268     49.18       SF-268     49.18 <t< th=""></t<>
Levieme CCRF-CEM CCRF-CEM H-0.60(T6) 20.95 RF RFMI-9226 RFMI-9226 RC-1226 HC-126 HC-1226 HC-126	Leukemia     21.34       CCRF-CEM     21.34       HL-60(TB)     28.96       K-562     19.90       MOLT-4     36.42       RPMI-8226     20.37       SR     45.92       Non-Small Cell Lung Cancer     A5.49/ATCC       A5.49/ATCC     43.13       EKVX     63.02       HOP-62     93.95       NCI-H226     82.26       NCI-H226     82.26       NCI-H226     82.26       NCI-H227     78.48       Colon Cancer     70.65       COL 0205     76.49       HCC-2998     106.55       HCT-116     25.33       HCT-15     74.35       HT29     38.36       KM12     40.91       SW-620     64.13       CNS Cancer     95.738       SF-268     49.18       SF-268     49.18       SF-268     49.18       SF-268     49.18       SF-268     49.18       SF-268     49.18
	Metantorna     39.45       LOX.IMVI     39.45       MALME-3M     67.41       M14     34.50       MDA-MB-435     33.87       SK-MEL-2     87.84       SK-MEL-2     87.84       SK-MEL-2     94.12       SK-MEL-5     61.11       UACC-257     44.72       UACC-62     76.79       Ovarian Cancer     66.33       OVCAR-3     48.84       OVCAR-4     66.33       OVCAR-5     101.78       OVCAR-6     101.78       OVCAR-73     90.33       Real Cancer     70.34       786-0     70.34       ACHN     59.28       SIN12C     38.62       TK-10     83.97       UO-31     11.52       Prostate Cancer     77.77       PC-3     27.77       DU-145     64.39       Breast Cancer     77.75       HS 578T     42.40       BT-549     63.73       T-47D     64.48
	Range 95.03

**Fig. SI8**. Mean graph of the effect of 10  $\mu$ M dose of **2** on the percent growth of the NCI's 60 cell lines.

Developmental Ther	apeutics Program	NSC: D-752822/1	Conc: 1.00E-5 Molar	Test Date: Jul 26, 2010	
One Dose Mean Graph		Experiment ID: 10070S90		Report Date: Feb 05, 2011	
Panel/Cell Line	Growth Percent	Mean Growth	Percent - Growth Per	cent	
Leukemia CCRF-CEM H-60(TB) K-562 MOLT-4 RPMI-8226 SR Non-Small Cell Lung Cancer A 549/ATCC EK/X HOF-62 NGI-H226 NGI-H226 NGI-H227 NGI-H220 NGI-H222 Colon Cancer COLO 205 HCC-2998 HCT-116 HCT-998 HCT-116 HCT-998 HCT-116 HCT-998 SNB-75 U251 Melanoma LOX IMVI MALME-33 SNB-75 U251 Melanoma LOX IMVI MALME-33 SNB-75 U251 Melanoma LOX IMVI MALME-33 SK-MEL-2 SK-MEL-2 SK-MEL-2 SK-MEL-5 UACC-257 UA	67.99 100.62 76.91 76.91 77.48 91.94 92.64 104.16 99.24 99.24 99.24 99.24 99.24 99.41 100.50 86.01 105.66 103.80 92.44 98.87 90.56 109.93 106.14 88.93 90.70 100.59 84.36 98.98 104.83 98.98 104.83 98.98 104.83 98.98 105.52 103.52 104.83 98.98 106.43 106.43 106.43 106.43 106.44 106.79 102.81 96.88 108.79 102.81 96.21 101.41 102.83 99.19 102.81 99.19 102.81 99.19 100.65 100.41 101.18 92.23 100.65 100.41 101.18 92.23 100.65 100.41 101.18 92.23 100.65 94.75 96.61 97.45 29.46 49.09		الليعيدية مديه مدينية باللية عديا ومعنا		
100	450	100 50		100 155	
	150	100 50	0 -50	-100 -150	

Fig. SI9. Mean graph of the effect of 10  $\mu$ M dose of 4 on the percent growth of the NCI's 60 cell lines.