

Supporting Information

Antitumor Agents 284. A New Desmosdumotin B Analogue with bicyclic B-ring as Cytotoxic and Antitubulin Agent

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Table S1. Analyses of Newly Synthesized Compounds

Comp.	Formula	C%		H%		O%	
		Calcd.	Found	Calcd.	Found	Calcd.	Found
5	C ₂₈ H ₃₀ O ₄	78.11	78.10	7.02	7.01	14.86	14.77
6	C ₂₆ H ₂₆ O ₄ ·1/4H ₂ O	76.73	76.76	6.56	6.34	-	-
7	C ₂₆ H ₂₆ O ₄ ·1/4H ₂ O	76.73	75.07	6.56	6.23		
8	C ₂₆ H ₂₆ O ₅	74.62	74.36	6.26	6.23	19.12	18.95
9	C ₂₇ H ₂₈ O ₆ ·1/4H ₂ O	71.59	71.16	6.34	6.18	-	-
10	C ₂₇ H ₂₈ O ₆ ·H ₂ O	68.51	68.60	6.48	6.20		
11	C ₂₅ H ₂₄ O ₄	77.30	76.99	6.23	6.29	16.47	16.13
12	C ₂₆ H ₂₆ O ₅	74.62	74.41	6.26	6.22	19.12	18.97
13	C ₂₄ H ₂₃ O ₄ N·1/8H ₂ O	73.59	73.58	5.98	5.96	16.85	16.82
14	C ₂₂ H ₂₂ O ₆ ·1/4H ₂ O	68.29	68.09	5.86	5.78	-	-
15	C ₂₃ H ₂₄ O ₆ ·1/4H ₂ O	68.90	68.93	6.16	6.10	-	-
16	C ₂₃ H ₂₂ O ₅	73.00	72.87	5.86	5.84	21.14	21.35
17	C ₂₃ H ₂₂ O ₄ S	70.03	69.89	5.62	5.65	-	-
18	C ₂₄ H ₂₄ O ₄ S	70.56	70.56	5.92	5.83	15.67	15.48
20	C ₂₄ H ₂₅ O ₄ N	73.64	73.50	6.44	6.40	-	-
21	C ₂₃ H ₂₂ O ₄ S·1/8H ₂ O	69.63	69.90	5.65	5.70	16.64	16.07
23	C ₂₄ H ₂₄ O ₄ S	70.56	70.38	5.92	5.92	15.67	15.82
25	C ₂₄ H ₂₄ O ₅ S	67.90	67.68	5.70	5.71	18.84	18.58
26	C ₂₃ H ₂₂ O ₅ S	67.30	67.24	5.40	5.28	19.49	19.28
29	C ₂₇ H ₂₆ O ₄	78.24	78.38	6.32	6.48	15.44	15.43
31	C ₂₇ H ₂₄ O ₅ ·1/2H ₂ O	74.13	74.39	5.76	5.57	-	-
32	C ₂₉ H ₂₆ O ₄ ·1/2H ₂ O	77.83	78.07	6.08	5.96	-	-
33	C ₂₉ H ₂₆ O ₄ ·1/2H ₂ O	77.83	78.03	6.08	5.91	-	-
34	C ₂₇ H ₂₆ O ₄	78.24	77.95	6.32	6.36	15.44	15.20
35	C ₂₃ H ₂₀ O ₄	76.65	76.72	5.59	5.52	-	-
36	C ₂₀ H ₁₈ O ₆ ·1/2H ₂ O	66.11	66.12	5.27	5.01	-	-
37	C ₂₀ H ₁₆ O ₄ S·1/4H ₂ O	67.30	67.08	4.66	4.26	-	-
40a	C ₂₆ H ₂₆ O ₄	77.59	77.68	6.51	6.47	15.90	16.04
41	C ₂₅ H ₂₄ O ₃ S	74.23	74.19	5.98	5.96	11.87	12.11
42	C ₂₅ H ₂₄ O ₂ S ₂ ·H ₂ O	68.46	68.94	5.97	5.82	-	-
43	C ₂₆ H ₂₅ BrO ₄	64.87	64.56	5.23	5.09	13.29	12.93
44	C ₂₅ H ₂₃ BrO ₄	64.25	64.00	4.96	4.94	-	-
48	C ₂₅ H ₂₆ O ₄	76.90	76.68	6.71	6.66	-	-

Table S2. HPLC Analysis of Compounds, 22, 24, 27 and 28

HPLC: Shimadzu Prominence UFLC system

(Pump: LC-20AT, UV detector: SPD-M20A)

Column: Alltima C18 (5 µm, 2.1 mm × 150 mm)

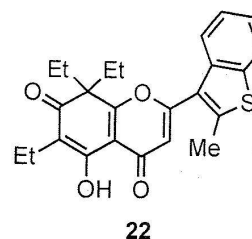
Compd	flow rate (mL/min)	CH ₃ CN %	purity	retention time (min)
22	0.15	70	99.87	9.70
24	0.15	70	98.18	10.31
27	0.15	70	98.26	11.29
28	0.15	70	99.56	7.34

Detected at 254 nm

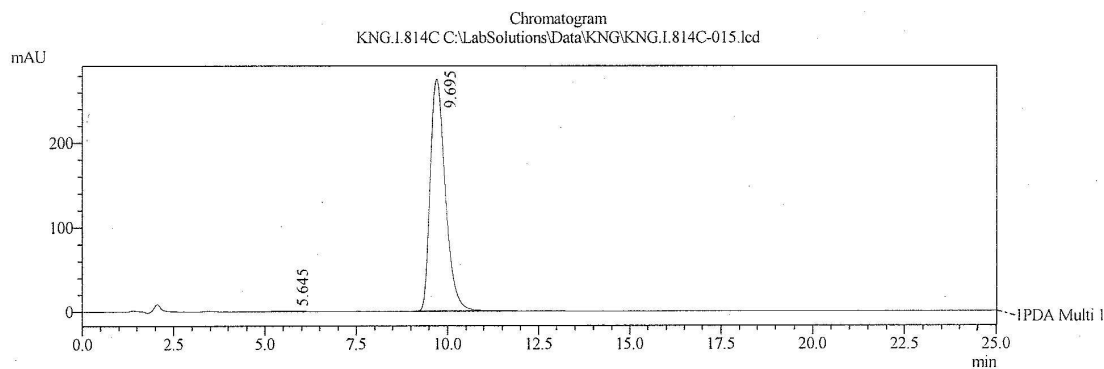
==== Shimadzu LCMSSolution Analysis Report =====

Date Acquired : 6/10/2010 5:25:48 PM Sample Type :
Sample Name : KNG.I.814C
Sample Amount : 1
Tray# : 1
Injection Volume : 5
Data File : KNG.I.814C-015.lcd
Method File : xincheng-hmt1.lcm
Original Method : C:\LabSolutions\Data\xincheng\xincheng-hmt1.lcm
Report Format : Default.lcr
Tuning File :
Processed by : Admin
Modified Date : 6/23/2010 3:30:53 PM

Sample Information
: Unknown
Sample ID : KNG.I.814C
Dilution Factor : 1
Vial# : 32



<<Comment>>
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SCL Type : CBM-20A
Power On : ON
Event1 : OFF
Event2 : OFF
Event3 : OFF
Event4 : OFF
<<Pump>>
Start B Conc.: 70.0
Pump Flow: 0.150 mL/min
<<LC Program>>
Time Unit Command Value Comment
25.00 Controller Stop



1 PDA Multi 1 / 254nm 4nm

PeakTable

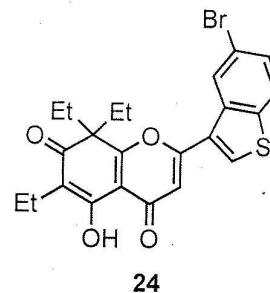
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %	Name
1	5.645	10336	884	0.131	0.319	
2	9.695	7898109	276099	99.869	99.681	
Total		7908444	276983	100.000	100.000	

==== Shimadzu LCMSsolution Analysis Report =====

Date Acquired : 6/10/2010 4:08:47 PM Sample Type
 Sample Name : KNG.I.813C
 Sample Amount : 1
 Tray# : 1
 Injection Volume : 5
 Data File : KNG.I.813C-011.lcd
 Method File : xinchon-hmt1.lcm
 Original Method : C:\LabSolutions\Data\xinchon\xinchon-hmt1.lcm
 Report Format : Default.lcr
 Tuning File :
 Processed by : Admin
 Modified Date : 6/23/2010 2:53:06 PM

Sample Information
 : Unknown
 Sample ID : KNG.I.813C
 Dilution Factor : 1
 Vial# : 31



Method

<<Comment>>

<<System Controller>>

SCL Type : CBM-20A
 Power On : ON
 Event1 : OFF
 Event2 : OFF
 Event3 : OFF
 Event4 : OFF

<<Pump>>

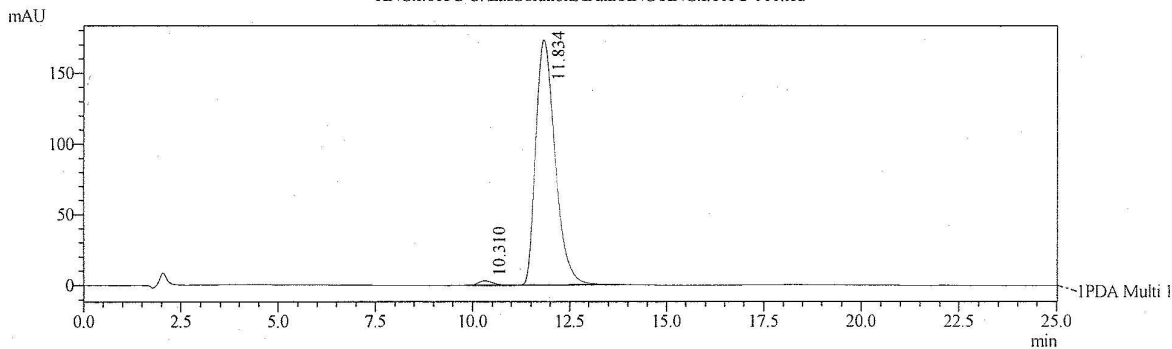
Start B Conc.: 70.0
 Pump Flow: 0.150 mL/min

<<LC Program>>

Time	Unit	Command	Value	Comment
25.00	Controller	Stop		

Chromatogram

KNG.I.813C C:\LabSolutions\Data\KNG\KNG.I.813C-011.lcd



PeakTable

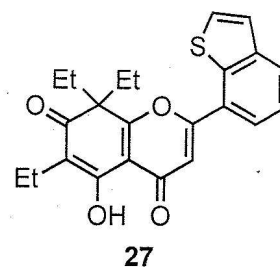
PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %	Name
1	10.310	86027	3204	1.409	1.813	
2	11.834	6020545	173508	98.591	98.187	
Total		6106573	176712	100.000	100.000	

==== Shimadzu LCMSSolution Analysis Report =====

Date Acquired : 6/10/2010 2:01:31 PM Sample Type
 Sample Name : KNG.I.815C
 Sample Amount : 1
 Tray# : 1
 Injection Volume : 10
 Data File : KNG.I.815C-007.lcd
 Method File : xinchen-hmt1.lcm
 Original Method : C:\LabSolutions\Data\xinchen\xinchen-hmt1.lcm
 Report Format : Default.lcr
 Tuning File :
 Processed by : Admin
 Modified Date : 6/23/2010 3:16:39 PM

Sample Information
 : Unknown
 Sample ID : KNG.I.815C
 Dilution Factor : 1
 Vial# : 33



Method

<<Comment>>

<<System Controller>>

SCL Type : CBM-20A
 Power On : ON
 Event1 : OFF
 Event2 : OFF
 Event3 : OFF
 Event4 : OFF

<<Pump>>

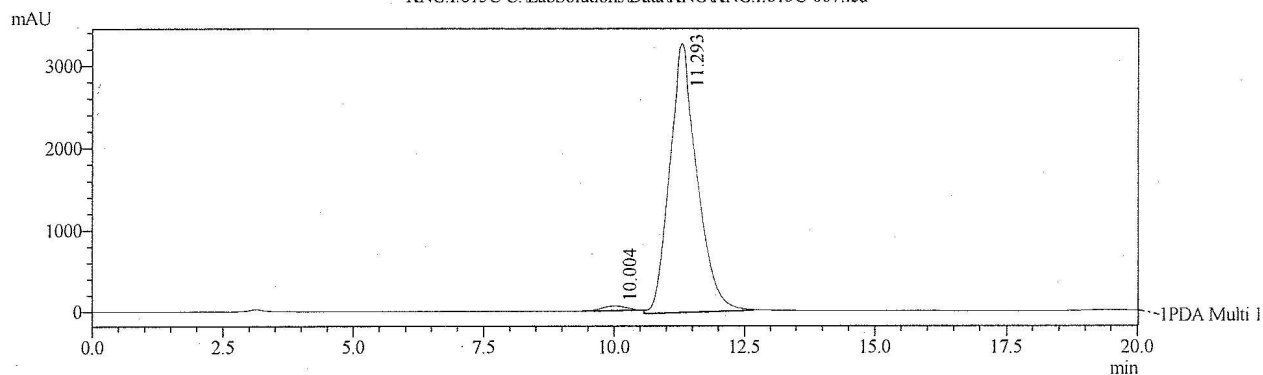
Start B Conc.: 70.0
 Pump Flow: 0.100 mL/min

<<LC Program>>

Time	Unit	Command	Value	Comment
20.00	Controller	Stop		

Chromatogram

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PeakTable

PDA Ch1 254nm 4nm

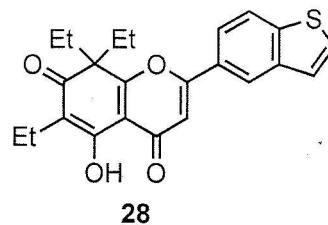
Peak#	Ret. Time	Area	Height	Area %	Height %	Name
1	10.004	1984523	58155	1.613	1.738	
2	11.293	121061658	3288359	98.387	98.262	
Total		123046181	3346514	100.000	100.000	

==== Shimadzu LCMSsolution Analysis Report =====

Date Acquired : 6/10/2010 6:34:30 PM Sample Type :
Sample Name : KNG.I.868C :
Sample Amount : 1 :
Tray# : 1 :
Injection Volume : 5 :
Data File : KNG.I.868C-002.lcd :
Method File : xinch-hmt1.lcm :
Original Method : C:\LabSolutions\Data\xinchen\xinchen-hmt1.lcm :
Report Format : Default.lcr :
Tuning File : :
Processed by : Admin :
Modified Date : 6/23/2010 3:28:09 PM :

Sample Information

: Unknown
Sample ID : KNG.I.868C
Dilution Factor : 1
Vial# : 34



Method

<<Comment>>

<<System Controller>>

SCL Type : CBM-20A
Power On : ON
Event1 : OFF
Event2 : OFF
Event3 : OFF
Event4 : OFF

<<Pump>>

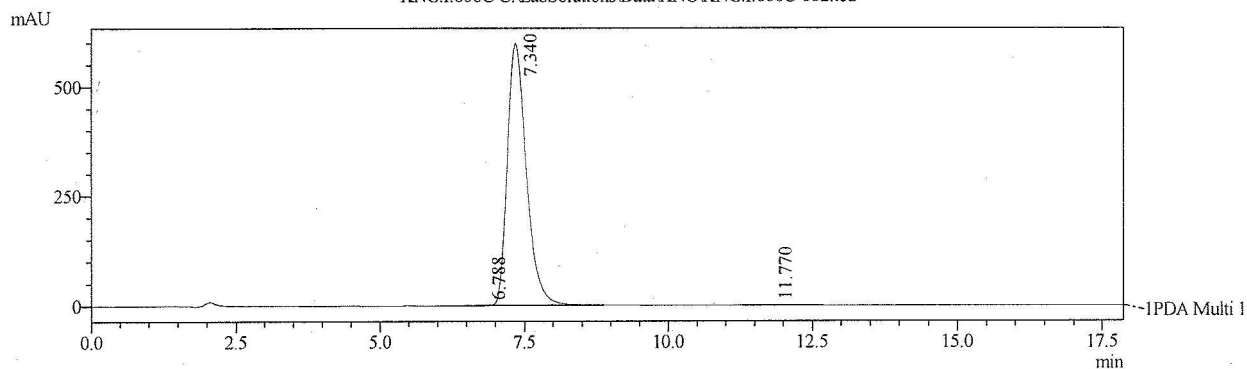
Start B Conc.: 70.0
Pump Flow: 0.150 mL/min

<<LC Program>>

Time	Unit	Command	Value	Comment
25.00	Controller	Stop		

Chromatogram

KNG.I.868C C:\LabSolutions\Data\KNG\KNG.I.868C-002.lcd



PeakTable

PDA Ch1 254nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %	Name
1	6.788	26009	1751	0.187	0.291	
2	7.340	13847574	598873	99.612	99.562	
3	11.770	27917	885	0.201	0.147	
Total		13901500	601508	100.000	100.000	

Table S3. Calculated Standard Deviation (SD)* of Antiproliferative Activities for Newly Synthesized Compounds

Cmpd	HCT-8	PC-3	A549	MCF	HepG	KB	KBV
5	1.16	0.46	0.70	-	-	0.23	0.46
6	0.02	0.10	0.02	0.05	0.05	0.02	0.02
7	0.50	0.75	0.75	1.24	0.25	0.75	1.00
8	0.22	0.07	0.05	0.14	0.05	0.07	0.10
11	0.05	0.39	0.10	0.05	0.03	0.08	0.05
12	0.48	0.48	0.96	0.24	0.72	0.24	0.72
14	0.52	0.26	1.57	0.26	0.26	0.79	0.52
15	0.05	0.10	0.03	0.05	0.05	0.05	0.08
16	0.26	0.26	0.53	-	1.06	0.79	0.79
17	1.27	0.25	1.02	0.51	0.51	0.76	0.51
19	0.84	1.15	0.47	-	0.78	0.51	0.11
20	0.26	0.51	0.51	1.02	1.28	0.51	0.77
21	0.01	0.01	-	0.01	0.01	0.01	0.01
22	0.10	6.11	0.05	-	0.10	0.05	0.02
23	4.17	-	-	-	-	3.68	5.64
24	2.33	1.48	3.38	-	1.48	1.27	0.42
25	0.94	1.18	2.59	-	0.94	0.71	0.47
26	0.56	0.95	0.37	-	0.05	0.02	0.05
27	0.61	0.43	0.20	-	0.08	0.10	0.05
28	-	-	-	-	-	0.45	-
29	0.48	0.72	0.48	0.24	0.72	0.24	0.24
34	-	0.24	0.97	0.72	0.72	1.21	0.72
35	0.11	0.40	0.05	-	0.09	0.04	0.06
36	0.05	0.06	0.04	-	1.90	0.06	0.05
37	0.07	0.05	0.01	-	0.17	0.00	0.00
40a	0.47	0.52	1.02	0.97	0.77	0.67	0.37
41	0.57	1.01	0.05	0.22	0.32	0.07	0.17
42	0.74	1.40	0.19	0.52	0.69	0.29	0.21
43	0.31	0.65	0.23	0.56	0.40	0.40	0.50
44	0.54	0.00	1.55	1.78	-	0.39	0.45
48	0.43	0.84	0.49	-	0.20	0.31	0.15

*Calculated from three or more determinations