#### **ELECTRONIC SUPPORTING INFORMATION (ESI)**

# Chrysomycins A-C, antileukemic naphthocoumarins from *Streptomyces* sporoverrucosus

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#### S1 $^{1}$ H -NMR Spectrum of chrysomycin A (1) in CD<sub>3</sub>OD

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## **S2.** HRMS Spectrum of chrysomycin A (1)

Data File Sample Type	SS.d Sample		Sa	mple Name osition	Vial 71			
Instrument Name	vishal 1	2-01-13.m	Ac	quired Time	16-07-2013 PM 8:53:39			
TRM Calibration Status	Success		D	A Method	daily_report.m			
Comment								
			Info.					
Acquisition SW 620 Version Q-T	) series TOF/6 OF B.05.01 (B	500 series 5125)						
Compound Table					1	MFG Diff		
	PT	Mass	F	ormula	MFG Formula	(ppm)	DB Formula	
Cod 72: C28 H28 OS	0.201	508.1737	C2	8 H28 O9	C28 H28 O9	-0.74	C28 H28 O9	-
cpu / Li dici ili								
		ler.	Alecalat	-	Mass			
Compound Label	m/z	RT	Algorithr	n olecular Feature	508.1737			
Cpd 72: C28 H28 O9	509.181	0.201	Find by M	olecular reactive	5 500.17.57			
MEE MS Spectrum								
Cod 72: C28 H2	3 09: +ESI M	IFE Spectru	um (0.140-0	.374 min) Frag=	175.0V SS.d			
3			509.1 228 H2			6		
3 2.5 2 1.5 1 0.5			509.1 C28 H2		00 750 800 850 900	950		
3- 2- 1.5- 1- 0- 150 200 2	50 300 35	50 400 41 Cour	1609 500 500 55 505 vs. Mass	50 600 650 7 -to-Charge (m/z)	760 750 800 850 900	950		
3 2 5 2 1.5 1 5 0 150 200 2 MS Spectrum Peak Li	50 300 35 st	50 400 45 Cour	C 50 500 50 50 500 50 50 50 50 50 50 50 50 50 50 50 50 50 50 50 50 50 50 5	50 600 650 7 -to-Charge (m/z) <b>Ion</b>	'óo 750 800 850 900 )	950		
3 2.5 1.5 1 0.5 150 200 2 <b>MS Spectrum Peak Li</b> <b>m/z z Aburd</b> 599.181 1 3	st 9252.06 C28 F	50 400 4 Cour nula 129 09	C 500 50 500 500 55 505 vs. Mass	50 600 650 7 -to-Charge (m/z) <b>Ion</b> (M+H)+	700 750 800 850 900 )	950		
3. 2.5. 2. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 2. 1.5. 1.	st 50 300 35 st 5252.06 C28 H 5827.81 C28 H	50 400 45 Cour 101a 129 09 129 09	200 500 55 100 500 55 100 500 55 100 500 55	50 800 650 7 to-Charge (m/z) Ion (M+H)+ (M+H)+	00 750 800 850 900	950		
3 2.5 2 1.5 1 0.5 0 150 200 2 MS Spectrum Peak Li <u>m/z z Aburd</u> <u>509.181 1 33</u> <u>510.1844 1 13</u> <u>Predicted Isotope Ma</u>	50 300 35 st j252.06 C28 F st27.81 C28 tch Table	50 400 41 Cour 11112 129 09 129 09	50 500 55 tts vs. Mass	50 600 650 7 100 (M+H)+ (M+H)+ 100 (M+H)+	100 750 800 850 900	950	Calc Abund Sum %	
3- 2- 1-5- 1- 0- 5- 1- 1- 1- 1- 1- 1- 1- 1- 1- 1	st Form 2252.06 C28 H 8227.81 C28 tch Table Calc m/2 Calc m/2	50 400 41 Cour 129 09 129 09 Diff (p	002 50 500 55 tts vs. Mass pm)	50 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ Abund % 100	00 750 800 850 900	950	Calc Abund Sum %	76.3
3 2.5 2 1.5 1 0.5 1 0.5 1 150 200 2 MS Spectrum Peak Li m/z z Abund 509.181 1 38 510.1844 1 1 1 Predicted Isotope Ma Isotope m/z 1 509.100 1 509.100 Ma 1 509.1000 Ma 1 509.1000 Ma 1 509.1000 Ma 1 509.1000 M	st Form 2252.06 C28 F 327.81 C28 F 12827.81 C28 F 12827.81 C28 F 1281 C28 F 1281 C38 F 1281 C381 C385 F 1281 C381 C385 F 1281 C385 C 1281 C385 C 1281	50 400 41 Cour 129 09 129 09 <b>Diff (p</b> 1806	50 500 55 its vs. Mass -0.73 -0.77	0 600 650 7 to-Charge (m/z) Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ C 100 35.23	00 750 800 850 900	950 ind Sum % 1 73.95 26.05	Calc Abund Sum %	76.3 23.6
3 2.5 2 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5	St         Form           2525.06         C28 +           3827.81         C28 +           100         C28 -           100         C28 -           100         C28 -           100         C28 -           100         C30 -           144         510	50 400 44 Cour 129 09 129 09 Diff (p 1806 1.184	50 500 55 50 70 70 70 70 70 70 70 70 70 70 70 70 70	0 800 650 7 to-Charge (m/z) Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ 100 35.23	00 750 800 850 900 ) alc Abund % Abu 30.96	950 and Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3. 2.5. 1.	50         300         35           Form         Form           252.06         C21         827.81         C28           tch Table         Calc m/z         81         509.31         10           44         510         510         510         510	50 400 48 Cour 129 09 129 09 129 09 129 09 129 09 129 09	pm) -0.77	i0 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ (M+H)+ Cl 35.23	róo 750 800 850 900 ) alc Abund % Abu 100 30.96	950 ind Sum % 1 73,95 26.05	Calc Abund Sum %	76.3 23.6
3 2.5 2 1.5 1 0.5 0 150 200 2 MS Spectrum Peak Li <u>m/z state</u> Abund <u>500.1844</u> 1 12 Predicted Isotope Ma <u>Isotope m/z</u> 2 510.18 End Of Report	st st 252.06 C28 H 252.06 C28 H 252.06 C28 H 252.06 C28 H 252.06 C28 H 252.06 C28 H 252.06 C28 H 253.06 C	50 400 41 Cour 129 09 129 09 129 09 129 09 129 09 129 09 129 09 129 09 129 09	50 500 55 ts vs. Mass pm) -0.77	50 600 650 7 to-Charge (m/z) Ion (M+H)+ (M+H)+ Abund % C 100 35.23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950	Calc Abund Sum %	76.3
3 2.5 2 1.5 1.5 1.5 1.5 1.5 1.5 1.5 2 1.5 2 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5	st st 2252.06 C28 Form 2252.06 C28 Form	50 400 41 Cour 129 09 129 09 129 09 129 09 129 09 129 09 129 09	50 500 550 50 500 550 pm) -0.73 -0.77	0 600 650 7 -to-Charge (m/z) Ion (M+H)+ (M+H)+ (M+H)+ Abund % Ct 35.23	00 750 800 850 900 ) alc Abund % Abu 30.96	950 and Sum % 73.95 26.05	Calc Abund Sum %	76.3 23.6
3- 2-5 2- 1.5 1.5 1.5 2- 1.5 1.5 2- 1.5 2- 1.5 2- 1.5 2- 1.5 2- 1.5 2- 1.5 2- 1.5 2- 1.5 2- 2- 1.5 2- 2- 1.5 2- 2- 2- 2- 2- 2- 2- 2- 2- 2-	50 300 35 st 2252.06 C28 H 327.81 C28 tch Table Cate m/z 15 500.1 16	50 400 44 Cour 129 09 129 09 129 09 129 09 129 09 129 09	50 500 550 50 500 550 tis vs. Mass pm) -0.77	50 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ 100 35.23	100 750 800 850 900 ) alc Abund % Abu 30.96	950 and Sum % 1 73.95 26.05	Calc Abund Sum %	76.3 23.6
3- 2-5 2- 1.5 1.5 0.5 0 <b>MS Spectrum Peak Li</b> <b>m/z Abude</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>MS Spectrum Peak Li</b> <b>M/z</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>Solution</b> <b>So</b>	50 300 36 st Form 252.06 (28 H 3827.81 (28 H tch Table Calc m/z 81 509.1 44 510	50 400 41 Cour 129 09 129 09 <b>Diff (p</b> .184	001 500 550 550 550 550 550 550 550 550	i0 600 650 7 to-Charge (m/z) <b>Ion</b> (M+H)+ (M+H)+ (M+H)+ <b>Abund %</b> <b>C</b> 35,23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950 ind Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3 2.5 2 1.5 1 0.5 0 <b>MS Spectrum Peak Li</b> <b>m/z x</b> Abund 509.181 1 33 510.1844 1 1.1 <b>Predicted Isotope Ma</b> <b>Iso</b> 200 2 <b>MS Spectrum Peak Li</b> <b>m/z x</b> Abund 509.181 1 33 510.1844 1 1.1 <b>Predicted Isotope Ma</b> <b>Iso</b> 201 2 <b>Iso</b> 200 2 <b>MS Spectrum Peak Li</b> <b>m</b> /z <b>x</b> Abund <b>So</b> 201 2 <b>MS Spectrum Peak Li</b> <b>m</b> /z <b>x</b> Abund <b>So</b> 201 2 <b>MS Spectrum Peak Li</b> <b>m</b> /z <b>x</b> Abund <b>So</b> 201 2 <b>MS Spectrum Peak Li</b> <b>MS Spectrum Peak Li</b> <b>MS</b>	50 300 36 st Form 1252.06 C28 F 1252.06 C28 F	50 400 41 Cour 129 09 129 09 129 09 129 09 129 09 129 09	00000000000000000000000000000000000000	50 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ Abund % C 35.23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950	Calc Abund Sum %	76.3 23.6
3. 2.5 2. 1.5 1.5 1.5 2. 1.5 1.5 1.5 2. 1.5 2. 1.5 1.5 1.5 1.5 2. 1.5 2. 1.5 2. 1.5 2. 1.5 2. 1.5 2. 1.5 2. 2. 1.5 2. 2. 2. 1.5 2. 2. 2. 2. 2. 2. 2. 2. 2. 2.	st st Form 252.06 (28 H 252.06 (28 H 26 H	50 400 41 Cour 129 09 129 09 129 09 129 09 129 109 129 109 100 100 100 100 100 100 100 100 100	-0.73 -0.77	50 800 650 7 to-Charge (m/z) Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ 25,23	00 750 800 850 900 ) alc Abund % Abu 30.96	950 and Sum % 1 73.95 26.05	Calc Abund Sum %	76.3 23.6
3- 2- 1- 2- 1- 1- 1- 1- 1- 1- 1- 1- 1- 1	50 300 35 <b>st</b> 1252.06 (28 H 225.06 (28 H 225.01 (28 H <b>tch Table</b> <b>Cate m/z</b> <b>Star 10</b> <b>Star 10</b> <b>St</b>	50 400 41 Cour 129 09 129 00 129 00 100 100 100 100 100 100 100 100 100	50 500 550 50 500 550 tts vs. Mass	50 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ 100 35.23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950 and Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3- 2- 1-5- 1-5- 0- 1-50-200-2 MS Spectrum Peak Li <u>m/z z Abund</u> <u>509.181 1 33</u> <u>510.1844 1 11</u> <b>Predicted Isotope Ma</b> <u>1500 200-2</u> <u>150-200-2</u> <u>150-200-2</u> 	50 300 36 Form 252.06 C28 Form 252.06 C28 I 827.81 C28 H Calc m/z 81 509.1 44 510	50 400 41 Cour 129 09 129 09 129 09 129 09 129 09 129 09	pm) -0.77	i0 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ Abund % C 35.23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950 ind Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3. 2.5. 2.5. 1.	50 300 36 st Form 1252.06 C28 F 1252.06 C28 F	50 400 41 Cour 129 09 129 09 129 09 129 09 129 09 129 09 129 09	00000000000000000000000000000000000000	50 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ Abund % C 35.23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950 and Sum % 73.95 26.05	Calc Abund Sum %	76.3 23.6
3.5 2.5 2.5 1.5 0.5 0.5 0.5 0.5 150 200 2 MS Spectrum Peak Li m/z z Abund 509.181 1 33 510.1844 1 12 Predicted Isotope Ma Isotope m/z 1500.200 2 Store 1	st Form 2525.06 C28 H tch Table Calc m/z Calc m/z 15 050 44 510	50 400 41 Cour 129 09 129 09 129 09 129 09 129 09 129 09	50 500 550 50 500 550 tis vs. Mass pm) -0.73 -0.77	0 800 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ 100 35.23	00 750 800 850 900 ) alc Abund % Abu 30.96	950 ind Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3. 2. 3. 2. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 1.5. 2. 1.5. 1.5. 1.5. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2	50 300 35 <b>st</b> 1252.06 C28 H 2252.05 C28 H 2252.05 C28 H <b>cate m/z</b> 1357.01 C28 H 144 510	50 400 41 Cour 129 09 129 00 129 00 100 100 100 100 100 100 100 100 100	50 500 550 50 500 550 tts vs. Mass	50 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ 100 35.23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950 and Sum % 73.95 26.05	Calc Abund Sum %	76.3
3. 2.5. 2.5. 1.5. 2.5. 1.5. 1.5. 2.5. 1.5. 1.5. 2.5. 1.5. 1.5. 2.5. 1.5. 1.5. 2.5. 1.	50 300 38 <b>Form</b> 2252.06 C28 F 827.81 C28 F <b>Calc</b> m/z 81 509.1 44 510	50 400 41 Cour 129 09 129 09 Diff (p .184	000 500 550 50	i0 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)- Cl 35,23	00 750 800 850 900 ) alc Abund % Abu 100 30.96	950 ind Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3. 2.5. 2. 1.5.	st st <u>Form</u> 252.06 C28 H 252.06 C28 H 252.06 C28 H <b>Calc m/z</b> 81 509.1 44 510	50 400 41 Cour 129 09 129 09 129 09 1806 184	-0.73 -0.77	50 800 850 7 to-Charge (m/z) Ion (M+H)+ (M+H)+ (M+H)+ 100 35.23	00 750 800 850 900 alc Abund % Abu 30.96	950 and Sum % 73.95 26.05	Calc Abund Sum %	76.3
3. 2.5. 1.	50 300 35 st 2252.06 C28 H tch Table Cate m/z 15 509.1 44 510	50 400 41 Cour 129 09 129 09 129 09 1806 184	50 500 550 50 500 550 tis vs. Mass	0 800 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ 100 35.23	00 750 800 850 900	950 ind Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3. 2.5. 1.	50 300 35 <b>st</b> 1252.06 (28 H 282.781 (28 H <b>Cale m/z</b> 15 (50 - 10 H) 14 510	50 400 41 Cour 129 09 129 09	000 500 550 500 550 500 550 500 550 50	50 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ (M+H)+ 100 % 35.23	00 750 800 850 900 alc Abund % Abu 100 30.96	950 and Sum % 1 73.95 26.05	Calc Abund Sum %	76.3
3.5 2.5 1.5 1.5 1.5 1.5 1.5 1.5 1.5 1	50 300 36 <b>st</b> 1252.06 C28 Form 1252.06 C28 IS 1252.06 C28	50 400 41 Cour 129 09 129 09 129 09 129 09 129 09 129 09 129 09 129 09 129 09 129 09	0.77	i0 600 650 7 to-Charge (m/z) (M+H)+ (M+H)+ Abund % C 35.23	00 750 800 850 900 ) alc Abund % Abu 30.96	950 and Sum % 73.95 26.05	Calc Abund Sum %	76.3



## **S3** <sup>1</sup>H -NMR Spectrum of chrysomycin B (2) in $CD_3OD$

# **S4.** HRMS Spectrum of chrysomycin B (2)

Instrument Acq Method IRM Calibra Comment	be t Name d ation State	us	SS.d Sample Instrum vishal_1 Success	nent 1 12-01-13.m	Sample Nar Position User Name Acquired Th DA Method	me SS Vial 71 me 16-07-2013 P daily_report.r	M 8:53:39 n				
Sample Gro Acquisition Version	sw	6200 se Q-TOF	eries TOF/6 B.05.01 (B	Info 500 series 5125)	•						
Compound	d Table	-									
Compo	64: C27 H	128 09	<b>RT</b> 0.2	Mass 496.1728	Formula C27 H28 O9	MFG C27	Formula H28 O9	MFG Di (ppm)	1.07	DB Formula C27 H28 O9	
Compound Cpd 64: C27	<b>1 Label</b> 7 H28 O9	<b>m</b> 49	/z 7.1801	<b>RT</b> 0.2	Algorithm Find by Molecula	Mass r Feature 496.172	28				
2	150 200	250 3	00 350	400 450 500 Counts vs. M	550 600 650 ass-to-Charge (n	700 750 800	850 900	950			
MS Spectru m/z 497.1801 498.1832 499.186 500.1914 993.3522 994.3552 995.3567	z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1	List 79574.78 24610.64 6021.46 1421.38 12668.3 7721.12 3132.06	Formula C27 H29 C27 H29 C27 H29 C27 H29 C27 H29	09 09 09 09	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+						
MS Spectru m/z 497.1801 498.1832 499.186 500.1914 993.3522 994.3552 995.3567 996.3617	z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1	List nd 79574.78 24610.64 6021.46 1421.38 12668.3 7721.12 3137.06 1285.23	Formula (C27 H29) (C27 H29) (C27 H29) (C27 H29) (C27 H29)	09 09 09 09	Ion (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+						
MS Spectru m/z 497.1801 498.1832 499.186 500.1914 993.3522 994.3552 995.3567 996.3617 Predicted I: (sotope	z         Abu           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1           1         1	List 79574.78 24610.64 6021.46 1421.38 12668.3 7721.12 3137.06 1285.23 4atch Ta	Formula C27 H29 0 C27 H29 0 C27 H29 0 C27 H29 0 C27 H29 0 D D D D D D D D D D D D D	09 09 09 09 09	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+ (2M+H)+	Calc Abund %	Ahurre	Sum 94			
MS Spectru m/z 497.1801 498.1832 499.186 500.1914 993.3522 994.3552 995.3567 995.3567 995.3567 Predicted I: (sotope 1 2 2 2 2 2 2 2 2 2 2 2 2 2	Peak           z         Abu           1         1 <t< td=""><td>List 79574.78 24610.64 6021.46 1421.38 12668.33 7721.12 3137.06 1285.23 4atch Ta [801]</td><td>Formula (27 H29) (27 H29</td><td>09 09 09 09 09 Diff (ppm) 0.</td><td>Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (2M+H)+           (2M+H)+           (2M+H)+           (2M+H)+           (2M+H)+           (2M+H)+           (2M+H)+           (2M+H)+           (2M+H)+           (2M+H)+</td><td>Calc Abund %</td><td>Abund 100</td><td>I Sum %</td><td>Calc 29</td><td>Abund Sum %</td><td>7</td></t<>	List 79574.78 24610.64 6021.46 1421.38 12668.33 7721.12 3137.06 1285.23 4atch Ta [801]	Formula (27 H29) (27 H29	09 09 09 09 09 Diff (ppm) 0.	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (2M+H)+	Calc Abund %	Abund 100	I Sum %	Calc 29	Abund Sum %	7
MS Spectru m/z 499.1801 498.1832 499.186 500.1914 993.3522 994.3552 995.3567 Predicted Is isotope 1 2 3 3 4 1 2 3 3 4 9 1 1 2 3 3 4 1 2 3 3 4 1 1 2 3 3 4 3 4 3 4 3 4 4 4 4 4 4 4 4 4 4 4 4 4	m         Peak           z         Abu           1         1           1         1           1         1           1         1           1         1           1         497.1           498.1         499.1           499.5         505.5	List nd 79574.78 24610.64 6021.46 1421.38 12668.3 7721.12 3137.06 1285.23 4atc-Ta Calc 1801 1832	Formula C27 H29 0 C27 H29 0 C2	09 09 09 09 09 09 01 0. 1. 1. 1.	Ion           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (M+H)+           (ZM+H)+           (ZM+H)+<	Calc Abund %	Abund 100 9.88 5.16	<b>Sum %</b> 71. 22.0 5.	29 05 39	Abund Sum %	7



# **S5** <sup>1</sup>H -NMR Spectrum of chrysomycin C(3) in $CD_3OD$



# **S6.** $^{13}$ C NMR Spectrum of chrysomycin C (3) in CD<sub>3</sub>OD





## **S8.** COSY Spectrum of chrysomycin C (**3**) in CD<sub>3</sub>OD



## **S9.** HSQC Spectrum of chrysomycin C (**3**) in CD<sub>3</sub>OD



## **S10.** HMBC spectrum of chrysomycin C (3) in CD<sub>3</sub>OD



# **S11**. HRMS of chrysomycin C (3)

Sample Type Instrument Na Acq Method IRM Calibratic Comment	ame on Status	SS.d Sample Instrumen vishal_12-I Success	t 1 01-13.m	Sample Name Position User Name Acquired Time DA Method	SS Vial 71 16-07-2013 PM 8:53:39 daily_report.m		
Sample Group Acquisition SV Version	₩ 6200 Q-TC	series TOF/650 0F B.05.01 (B512	Info. 0 series 25)				
Compound <sup>-</sup>	Table					- MEC 5:8	
Compour	nd Label	RT	Mass	Formula	MFG Formula	(ppm)	DB Formula
Cpd 3	1: C28 H30 O9	0.197	510.1881	C28 H30 O9	C28 H30 O9	1.68	C28 H30 O9
Compound Cpd 31: C28	<b>Label</b> H30 O9	<i>m/z</i> 511.1958	<b>RT Alg</b> 0.197 Find	<b>Jorithm</b> d by Molecular Fe	Mass eature 510.1881		
MFE MS Spectro	um						
x10 5 Cpd 2 - 1.75 - 1.5 -	31: C28 H30	O9: +ESI MFE	Spectrum (0.124 8961-113 8961-113 8961-113 8961-113 80 129 80 129 80 129 80 129 80 129 80 80 80 80 80 80 80 80 80 80 80 80 80	-0.624 min) Frag	=175.0V SS.d		
1 25			<u> </u>				
1.25 1 0.75 0.5 0.25							
1.25 1 0.75 0.5 0.25 0 MS Spectru	150 200 25 m Peak List	0 300 350	400 450 500 5 Counts vs. Mas	550 600 650 7 ss-to-Charge (m/z	700 750 800 850 900 )	950	
1.25 1 0.75 0.5 0.25 0 MS Spectru <i>m/z</i>	150 200 25 m Peak List z Abund	0 300 350	400 450 500 8 Counts vs. Mas	550 600 650 7 ss-to-Charge (m/z	700 750 800 850 900 )	950	
1.25 1 0.75 0.5 0.25 0 <b>MS Spectru</b> <i>m/z</i> 511.1958	150 200 25 m Peak List z Abund 1 1934;	<b>Formula</b> 71.98 C28 H31 ( 19 72 C28 H31 (	400 450 500 5 Counts vs. Mas	550         600         650         5           ss-to-Charge         (m/z)           Ion         (M+H)+           (M+H)+         (M+H)+	700 750 800 850 900 )	950	
1.25 1 0.75 0.25 0 <b>MS Spectru</b> <i>m/z</i> 511.1958 512.199 513.1973	150 200 25 <b>m Peak List</b> <b>z Abund</b> 1 1934; 1 579; 1 145;	Formula           1.98         C28         H31           39.72         C28         H31           63.15         C28         H31	400 450 500 5 Counts vs. Mas	550         600         650         5           s-to-Charge (m/z)         (M/H)+         (M/H)+         (M/H)+           (M+H)+         (M/H)+         (M/H)+         (M/H)+	700 750 800 850 900 )	950	
1.25 1 0.75 0.5 0.25 0 <b>MS Spectru</b> <i>m/z</i> 511.1958 512.199 513.1973 514.1945	150 200 25 m Peak List 1 1934; 1 579; 1 145; 1 31; 1	Formula 71.98 (28 H31 ( 19.72 (28 H31 ( 13.15 (28 H31 ( 15.54	400 450 500 5 Counts vs. Mas 09 09 09	550         600         650         5           s-to-Charge (m/z)         (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+         (M+H)+	700 750 800 850 900 )	950	
1.25 1 0.75 0.5 0.25 0 MS Spectru <i>m/z</i> 511.1958 512.199 513.1973 514.1945 Predicted I Isotope	150 200 25 <b>m Peak List</b> <b>z Abund</b> 1 1934; 1 579; 1 145; 1 31; sotope Mate m/z	Formula 71.98 C28 H31 73.72 C28 H31 75.54 C28 H31 75.55 C28 H3	400 450 500 5 Counts vs. Mas 09 09 09 09 09 09 09 09	550         600         650         7           s-to-Charge (m/z)         (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+         (M+H)+	700 750 800 850 900 ) alc Abund % Abun	950 d Sum % Ci	alc Abund Sum %
1.25 0.75 0.5 0.25 0.25 0.25 0.25 0.25 0.25 0.25	150         200         25           m Peak List         z         Abund           1         1934,         1         579           1         145;         1         31;           sotope Matc         m/z         511,1958         511,1958	Formula           1:98         C28 H31 (           92.72         C28 H31 (           33.15         C28 H31 (           55.54         C28 H31 (           h Table         Calc m/z           511.1963         512 (2011)	400 450 500 5 Counts vs. Mas 09 09 09 09 09 09 09 09 09 09 09 09 09	S50         600         650         7           Ion         (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+           (M+H)         (M+H)+         (M+H)+           (M+H)         (M+H)+         (M+H)+           (M+H)         (M+H)+         (M+H)+	700 750 800 850 900	950 d Sum % Cri 71.88 71.83	alc Abund Sum % 72.21 23 37
1.25 1.0.75 0.75 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.	150 200 25 <b>m Peak List</b> <b>z Abund</b> 1 1934; 1 519; 1 31; 50 <b>tope Mate</b> <b>m/z</b> 511.1958 513.1959; 513.1957; 513.1	Formula           '1.98         C28 H31 (           '9.72         C28 H31 (           :5.54         C28 H31 ( <b>table</b> C28 H31 (           Calc m/z         511.1963           512.1997         513.2023	400 450 500 5 Counts vs. Mas 09 09 09 09 09 09 09 09 09 09 09 09 09	S50         600         650         7           Ion         (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+           (M+H)         (M+H)+         (M+H)+           (M+H)         (M+H)+         (M+H)+           (M+H)         (M+H)+         (M+H)+           (M+H)         (M+H)         (M+H)+           (M+H)         (M+H)         (M+H)+           (M+H)         (M+H)         (M+H)+           (M+H)         (M+H)         (M+H)           (M+H)         (M+H)	200 750 800 850 900 alc Abund % Abun 100 30.98 6.49	950 d Sum % Ct 71.88 21.53 5.41	alc Abund Sum % 72.21 22.37 4.68
1.25 1.25 1.25 1.25 1.25 1.25 0.75 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.	150 200 25 <b>m Peak List</b> <b>z Abund</b> 1 1934 1 579 1 1455 1 31 <b>sotope Mate</b> <b>m/z</b> 511.1958 512.199 513.1973 514.1945	Formula           71.98         C28 H31 (1997)           71.98         C28 H31 (1997)           71.195         C28 H31 (1997)           71.196         S11.1963           511.1963         S12.1997           513.2023         S14.205	400 450 500 5 Counts vs. Mas 09 09 09 09 09 09 09 09 09 09 09 09 09	S50         600         650         7           Ion         (M+H)+         (M+H)+         (M+H)+           (M+H)+         (M+H)+         (M+H)+	200 750 800 850 900 alc Abund % Abun 100 30.98 6.49 1.02	950 d Sum % Ci 71.88 21.53 5.41 1.19	alc Abund Sum % 72.21 22.37 4.688 0.74

Agilent Technologies

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#### HRMS of chrysomycin D (4) **S12.**

Data File Sample Typ Instrument Acq Methor IRM Calibra Comment	e Name i ation S	e Status	SS-529 Sample Instrur vishal_ Succes	.d nent 1 12-01-13.m s	Sample Position User Na Acquire DA Met	Name SS-52 Vial 1 me d Time 22-07 hod daily_	9 7 -2013 PM 12:09:50 report.m		
Sample Gro Acquisition Version	sw	620 Q-T	0 series TOF/0 OF B.05.01 (E	5500 series 15125)	Info.				
Compoun	d Tab	ole							N. Samerak
Comp	ound L	abel	RT	Mass	Formula		MFG Formula	(ppm)	DB Formula
Cpd	49: C2	8 H30 O10	0.196	526.1835	C28 H30 O	10	C28 H30 O10	0.81	C28 H30 O10
Compoun Cpd 49: C2	<b>d Lab</b> 8 H30	<b>el</b> ) 010	<b>m/z</b> 549.1734	<b>RT</b> 4	Algorithm Find by Molecula	Mass r Feature 526.1	<b>8</b> 35		
			1						
MFE MS Spe	trum								
1.4 - 1.2 - 3 - 0.8 - 0.6 -		QQ	2 010		549.1734 C28.H30 Na O10	, ,			
0.4		1 Val	8 H3						
0.2			63		11				
0	150	200 25	0 300 350	400 450	500 550 600	650 700 750	800 850 900	950	
				Counts	vs. Mass-to-Char	ge (m/z)			
m/z	z	Abund	Formula		Ion	1			
264	1 2	703.24	C28 H32 O10	)	(M+2H)+2	1			
264.599	4 2	231.03	C28 H32 O10	)	(M+2H)+2				
528.190	3 1	770.16			(M+H)+ (M+H)+				
549.173	4 1	13959.3	C28 H30 Na	010	(M+Na)+	1			
550.175	2 1	4834.88	C28 H30 Na	010	(M+Na)+				
551.1/5 Predicted	J 1	1597.78	C28 H30 Na	010	(M+Na)+	]			
Isotope	m/2	z	Calc m/z	Diff (ppm)	) Abund %	Calc Abund %	Abund Sum %	Calc Abund	Sum %
	1	264.1	264.099	2 -2	.75 100	1	.00	75.27	76.32
	2	264.5994	264.600	9 5	.71 32.85	31	03	24.73	23.68



# **13. LCMS of active fraction**





#### 13.3. MS spectras of chrysomycins A-E





## **S14.** Screenshots of DNP database search during dereplication

Search My Searches My Account Help Tour Take the Survey
Dictionary of Natural Products
Search
Search View Results in New Window
Draw Query Clear Structure Structure Matching: Substructure   Troubleshoot Structure Search
Add Property Clear Properties Boolean Property Comparison Warde
AND  Biological Source Streptomyces Drowse] [clear]
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Kound 6935 matches from 251230 documents.

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ecular Formula
H <sub>32</sub> N <sub>2</sub> O <sub>7</sub>
H <sub>32</sub> N <sub>2</sub> O <sub>7</sub>
H <sub>28</sub> O <sub>9</sub>
H <sub>28</sub> O <sub>9</sub>
H <sub>36</sub> N <sub>4</sub> O <sub>8</sub>
H <sub>36</sub> N <sub>4</sub> O <sub>8</sub>
H <sub>28</sub> O <sub>9</sub>
H <sub>28</sub> O <sub>9</sub>
H <sub>28</sub> O <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub>
H <sub>28</sub> O <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub>
H <sub>28</sub> O <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub>
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H <sub>28</sub> O <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub> H <sub>36</sub> N <sub>4</sub> O <sub>2</sub> H <sub>48</sub> O <sub>4</sub> H <sub>30</sub> Cl <sub>2</sub> O <sub>6</sub>
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H <sub>28</sub> O <sub>9</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>10</sub> H <sub>28</sub> N <sub>4</sub> O <sub>4</sub> H <sub>36</sub> N <sub>4</sub> O <sub>2</sub> H <sub>48</sub> O <sub>4</sub> H <sub>30</sub> Cl <sub>2</sub> O <sub>6</sub> H <sub>30</sub> Cl <sub>2</sub> O <sub>6</sub> H <sub>44</sub> N <sub>4</sub> O <sub>6</sub> H <sub>40</sub> N <sub>4</sub> O <sub>6</sub>

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Dictionary of Natural Products	
Search	
Search View Results in New Window	
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Search Results	
Return to Search Columns	Page 1 of
Export As	
Found 2 matches from 251230 documents.	
Details Chemical Harmon	Molecular Formula
Chrysomycin B; 1'-Epimer (?)	C <sub>27</sub> H <sub>28</sub> O <sub>6</sub>
Napyradiomycin A.: 18-Hydroxy	CarHaaClaOa
	25 30 2 6
Return to Search Columns	Mill Drive and Mill
Export As	Page 1 of 1

**S15.** Screenshots of DNP substructure search using basic naphthocoumarin skeleton

Searc	h My Searches My Acco	unt Help T	our Tak	e the Survey	1	
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ANE	CAS Registry Nos.				[browse] [clear]	×
AND	All Text				[browse] [clear]	2
AND	Melting Point	= ~			[browse][clear]	×
AND	Boiling Point	= 🗸			[browse] [clear]	×
Search	View Results in New Window					
Sear	ch Results					
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Retur	t As Columns	Page 1 of 🕨	Goto F	Pane		
Fou	nd 27 matches from 251230 documents.					
Details	Chemical Name	Mole	cular Formula			
	Chrysomycin A Chrysomycin A: 1' Enimer(2)	C <sub>28</sub> H	2809			
	Chrysomycin B	C28 C27H	28 <sup>O</sup> 9 28 <sup>O</sup> 9			
	Chrysomycin B; 1'-Epimer (?)	C <sub>27</sub> H	<sub>28</sub> O <sub>9</sub>			
	Givocarcin M Givocarcin M 4'-Hydroxy	C26H	26 <sup>0</sup> 9			
	Gilvocarcin M; 1"-Oxo	C26PG	<sub>24</sub> O <sub>10</sub>			
	Gilvocarcin V	C <sub>27</sub> H	<sub>26</sub> O <sub>9</sub>			
	Givocarcin V; 1",2"-Dihydro Givocarcin V; 4'-Hydroxy	C <sub>27</sub> H	28O9 26O10			
	Gilvocarcin V; 4'-Hydroxy, 1",2"-dihydro	C <sub>27</sub> H	<sub>28</sub> O <sub>10</sub>			
	Ravidomycin Ravidomycin: O Do Ao	C <sub>31</sub> H	33NO9			
	Ravidomycin; O-De-Ac, N-oxide	C29 <sup>D3</sup> C29H3	31NO8 31NO9			
	Ravidomycin; N-De-Me, O-de-Ac, N-Ac	C <sub>30</sub> H	31NO9			
	Ravidomycin; N-De-Me, O-de-Ac Ravidomycin; N-De-Me	C <sub>28</sub> H	29NO8			
	Ravidomycin; Di-Ac	C35H	37NO11			
	Ravidomycin; N,N-Di-de-Me, N-Ac	C <sub>31</sub> H	31NO10			
	Ravidomycin; 1",2"-Dihydro	C <sub>31</sub> H	35NO9			
	Ravidomycin; 1",2"-Dhydro, di-Ac	C <sub>29</sub> H <sub>3</sub> C <sub>3c</sub> H <sub>3</sub>	33/1408 39NO <sub>11</sub>			
	Ravidomycin; 1",2"-Dihydro, 1"-hydroxy	C <sub>31</sub> H	35NO10			
	Ravidomycin; 1",2"-Epoxide	C <sub>31</sub> H	33NO10			
	Ravidomycin M	C <sub>31</sub> H <sub>2</sub> C <sub>52</sub> H	33 <sup>140</sup> 10 33NO9			
Ē	Ravidomycin M; O-De-Ac	C <sub>28</sub> H	NO <sub>8</sub>			