SUPPLEMENTARY MATERIAL

Resorcylic acid lactones from the Beibu Gulf coral-derived fungus *Curvularia lunata* GXIMD 02512 with antiproliferative effects on prostate cancer cells

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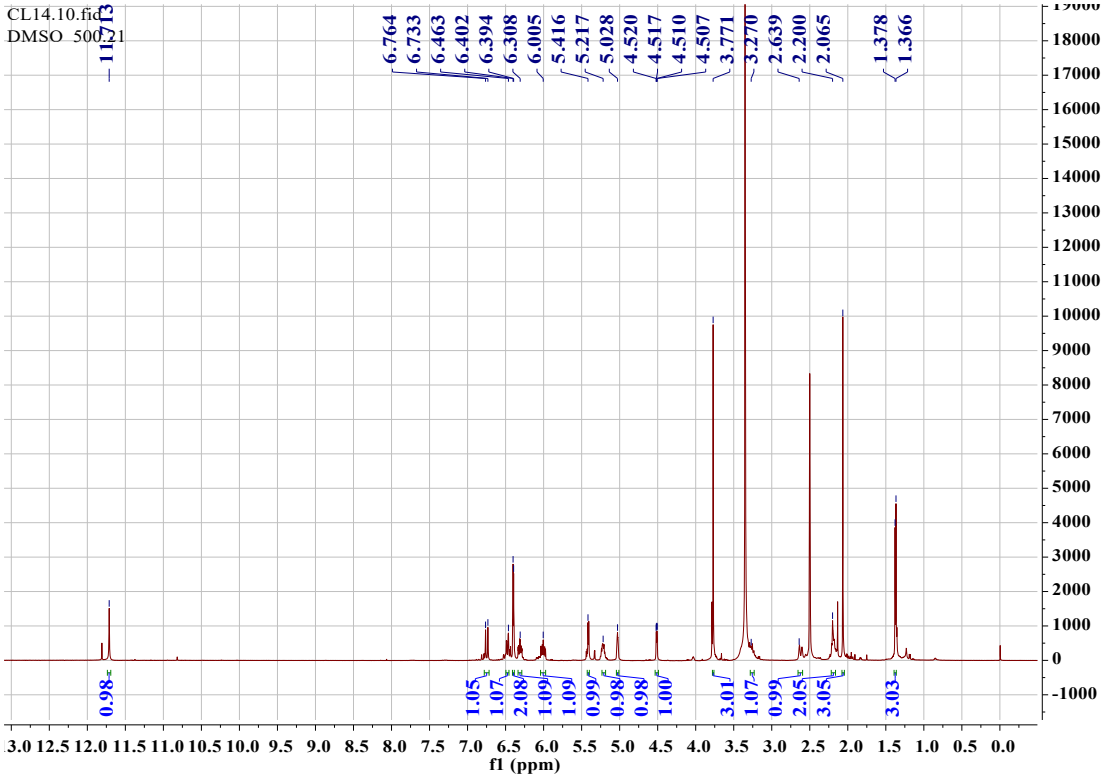
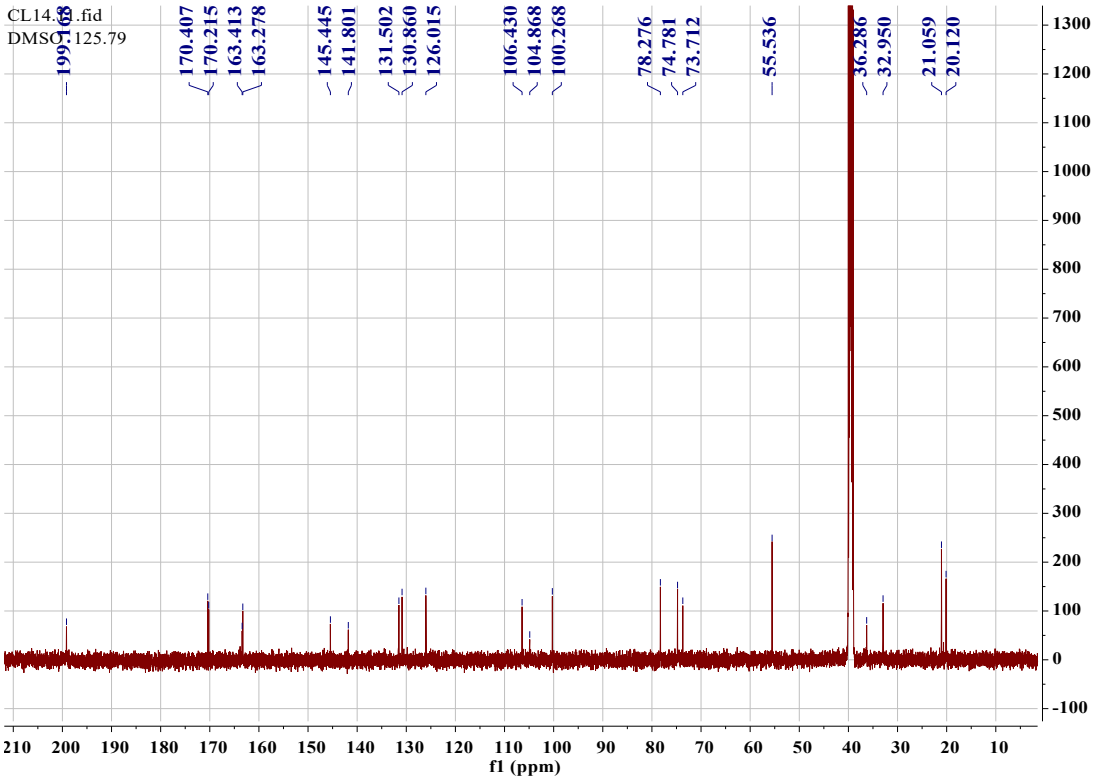


Figure S1. [1]H NMR spectrum of curvulomycin A (**1**) (500 MHz, DMSO-d_6)



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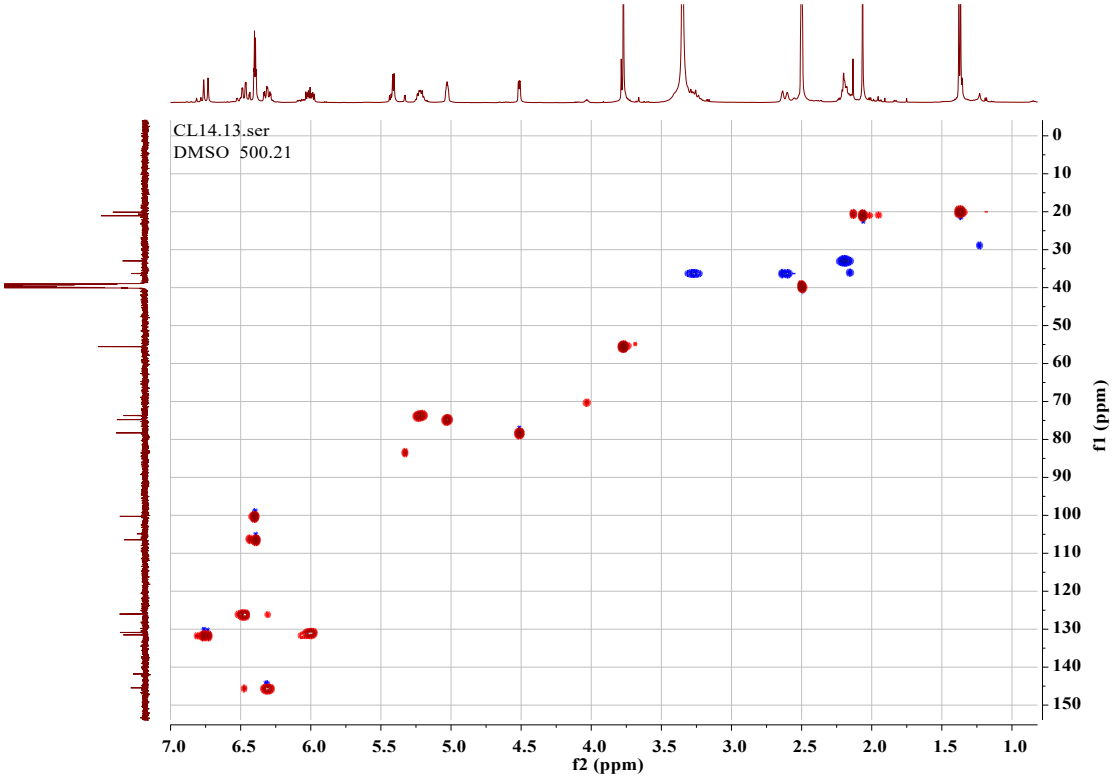

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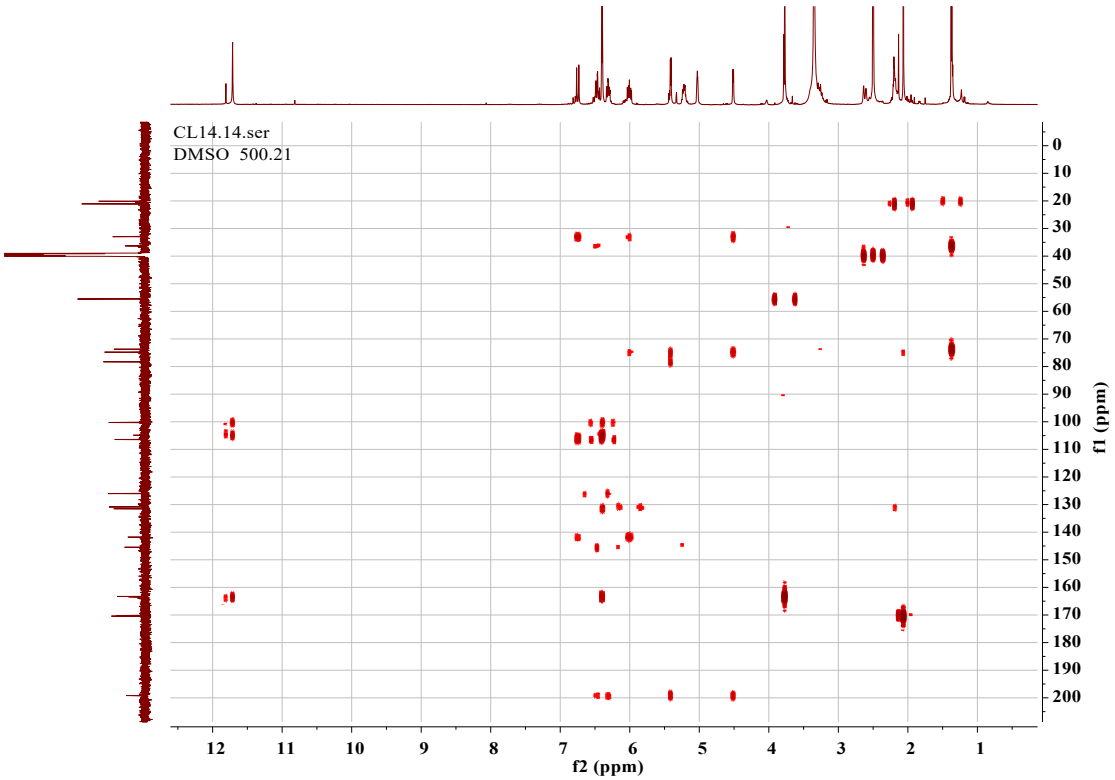
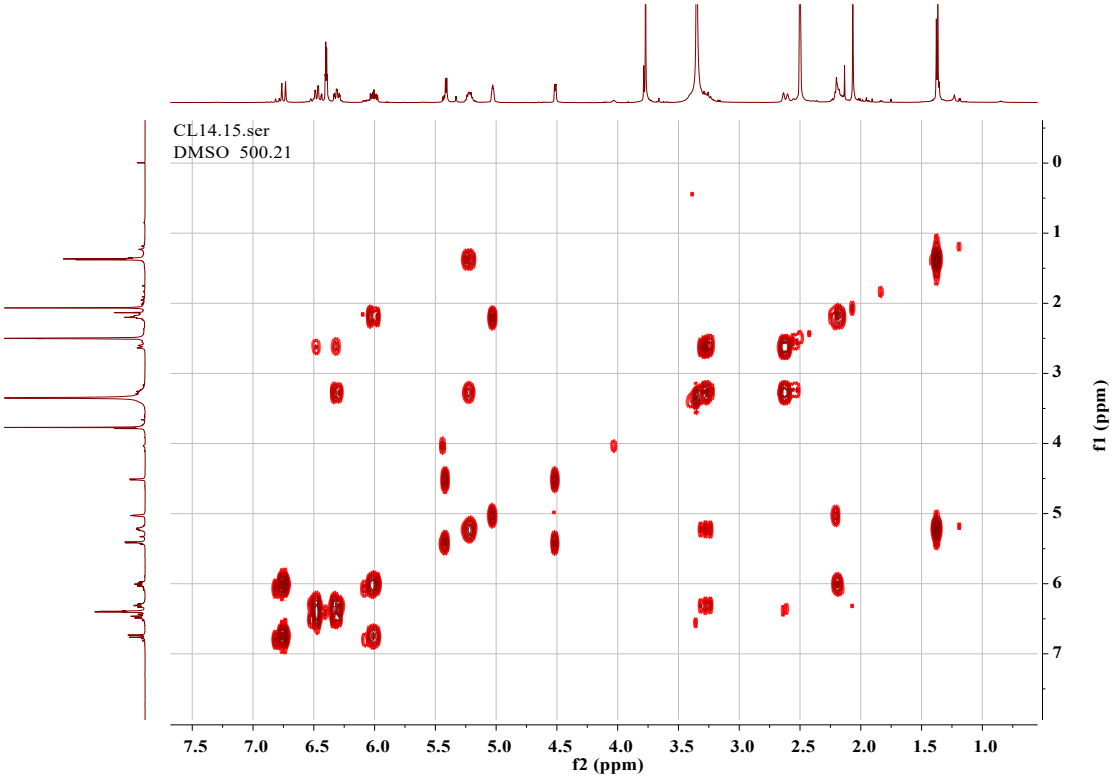


Figure S4. HMBC spectrum of curvulomycin A (**1**) (DMSO-d_6)



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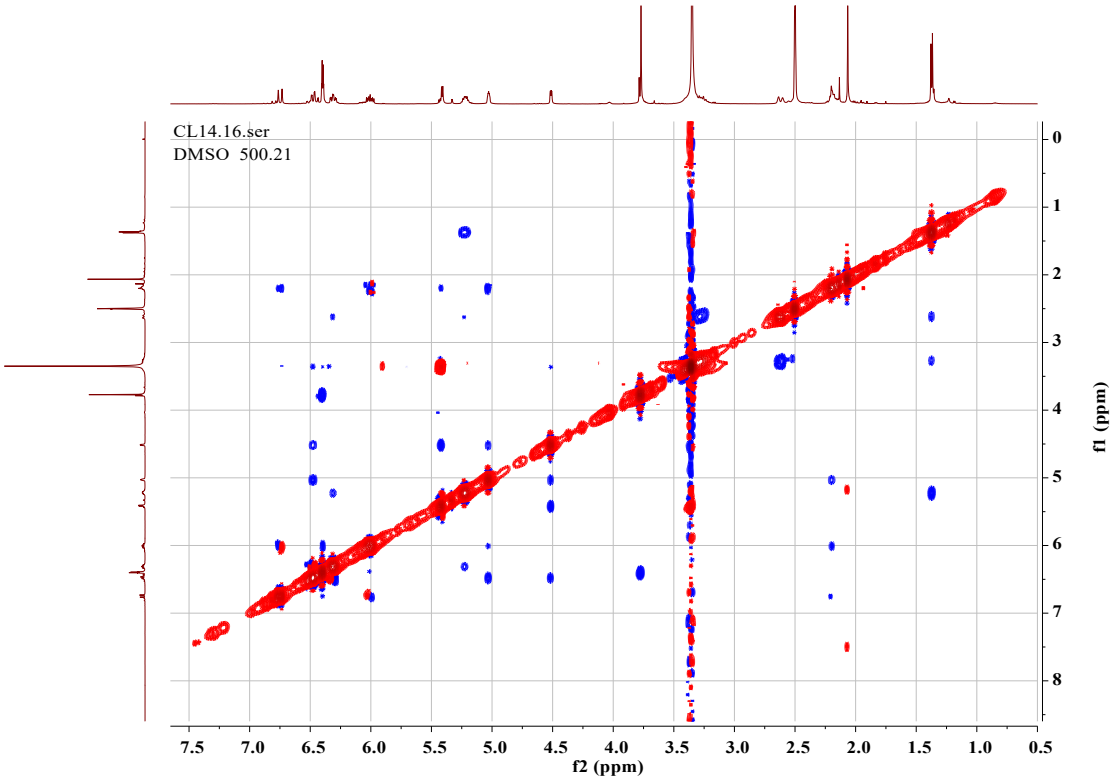


Figure S6. NOESY spectrum of curvulomycin A (**1**) (DMSO-d_6)

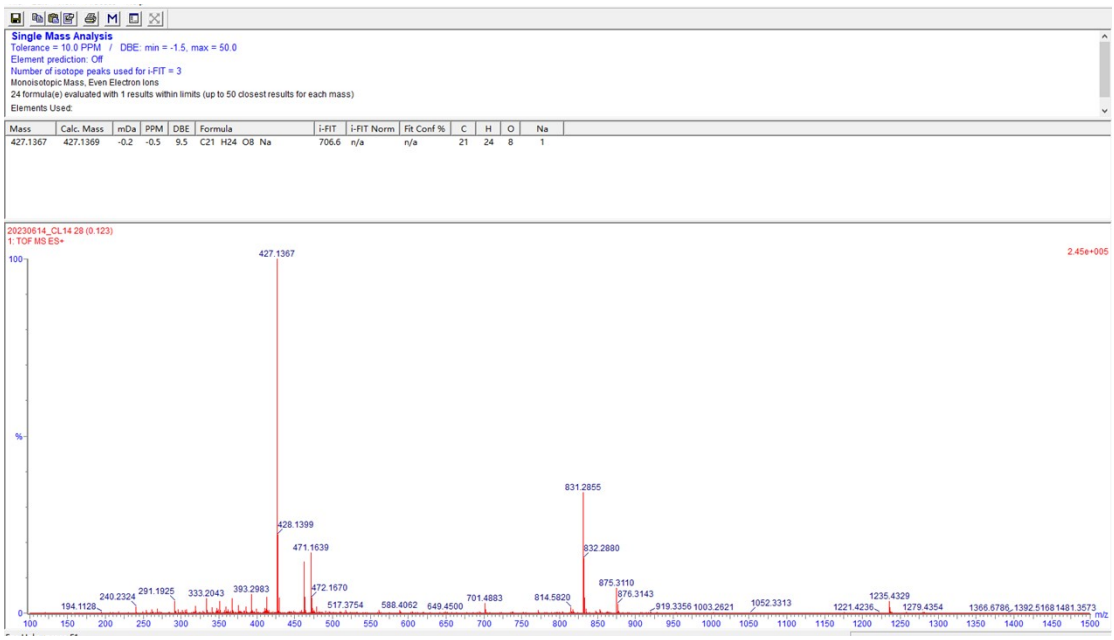


Figure S7. HR-ESI-MS spectrum of curvulomycin A (**1**)

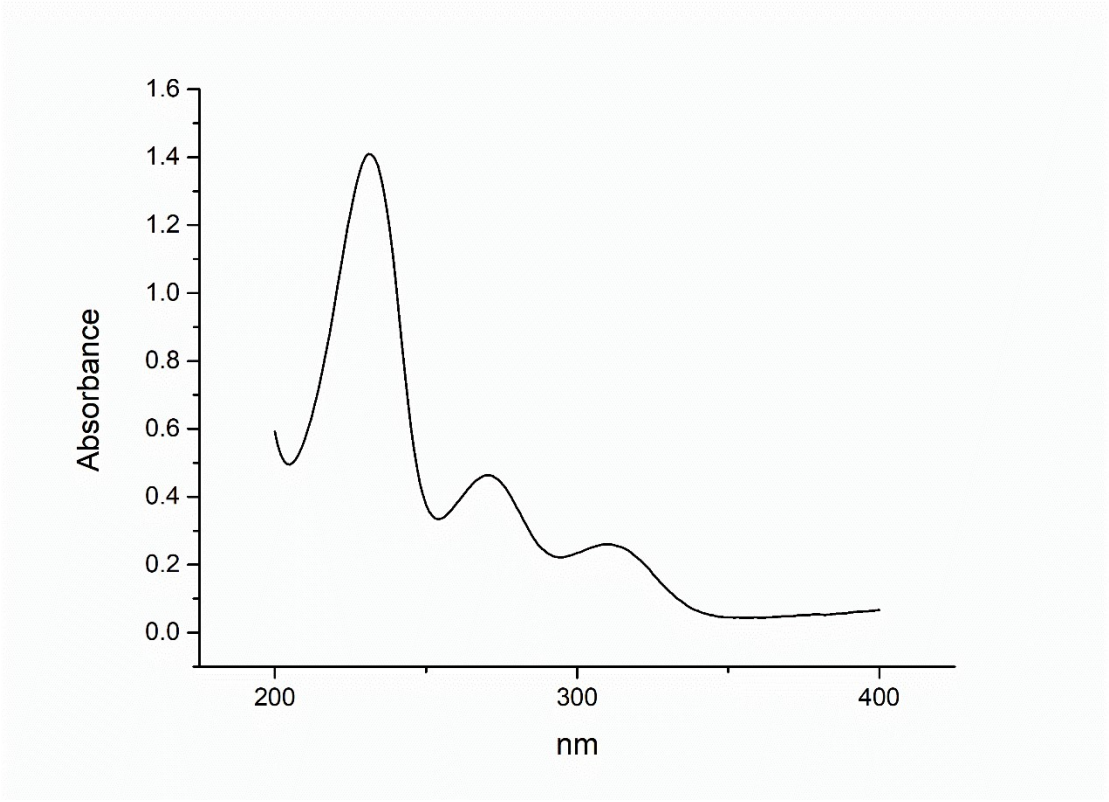


Figure S8. UV spectrum of curvulomycin A (**1**)

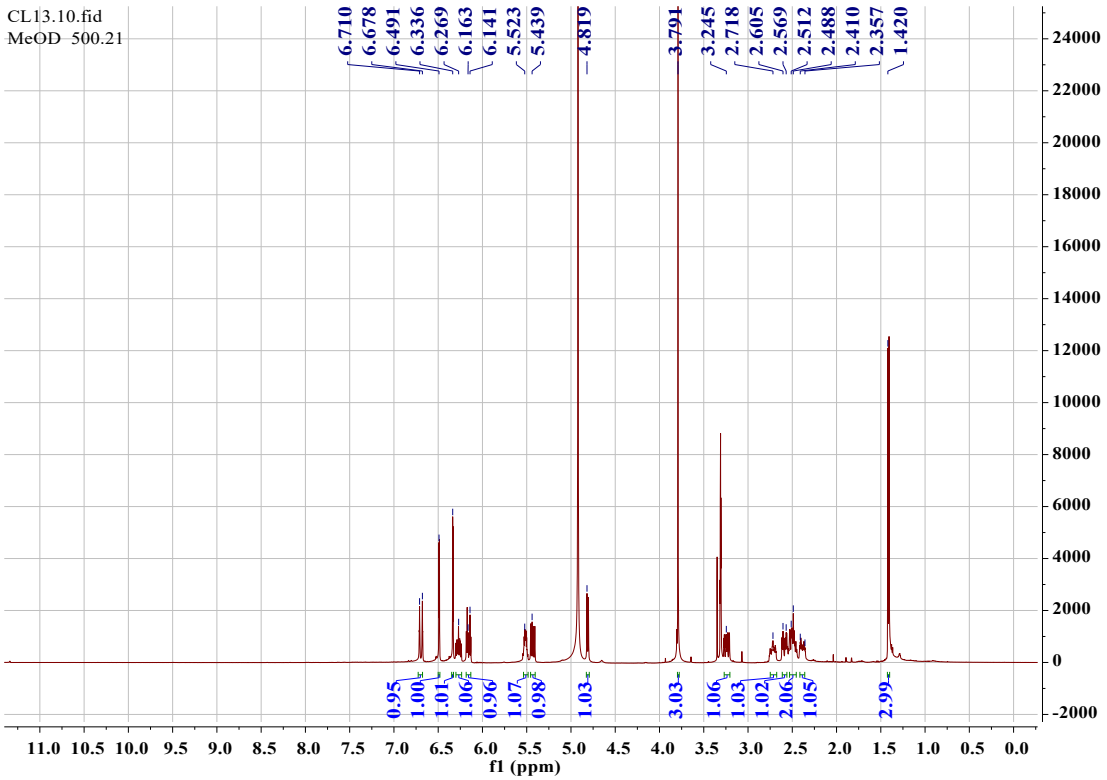


Figure S9. ^{1}H NMR spectrum of curvulomycin B (**2**) (500 MHz, CD_3OD)

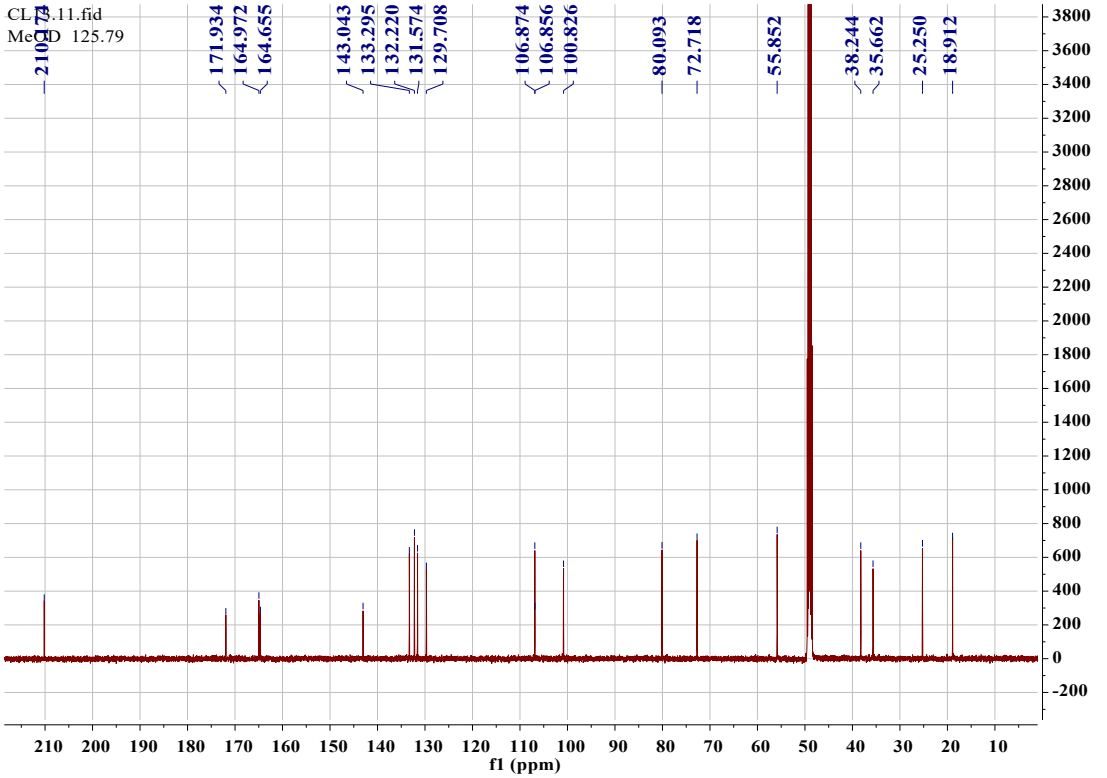


Figure S10. ^{13}C NMR spectrum of curvulomycin B (**2**) (125 MHz, CD_3OD)

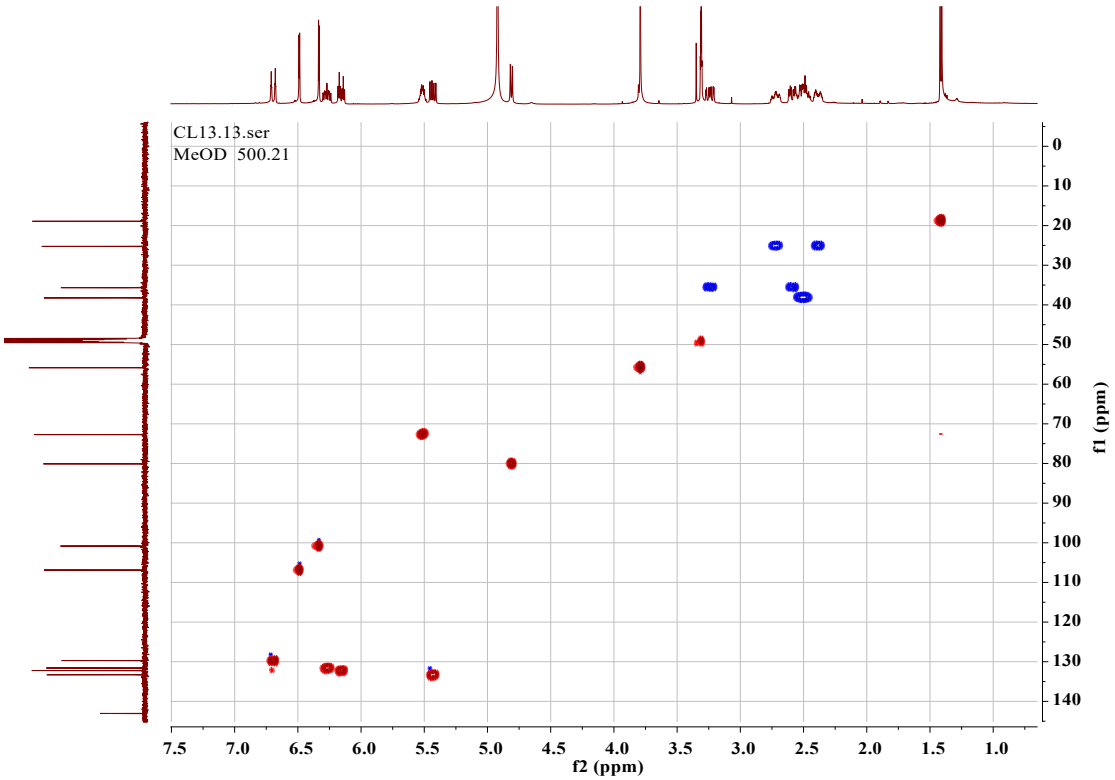


Figure S11. HSQC spectrum of curvulomycin B (**2**) (CD_3OD)

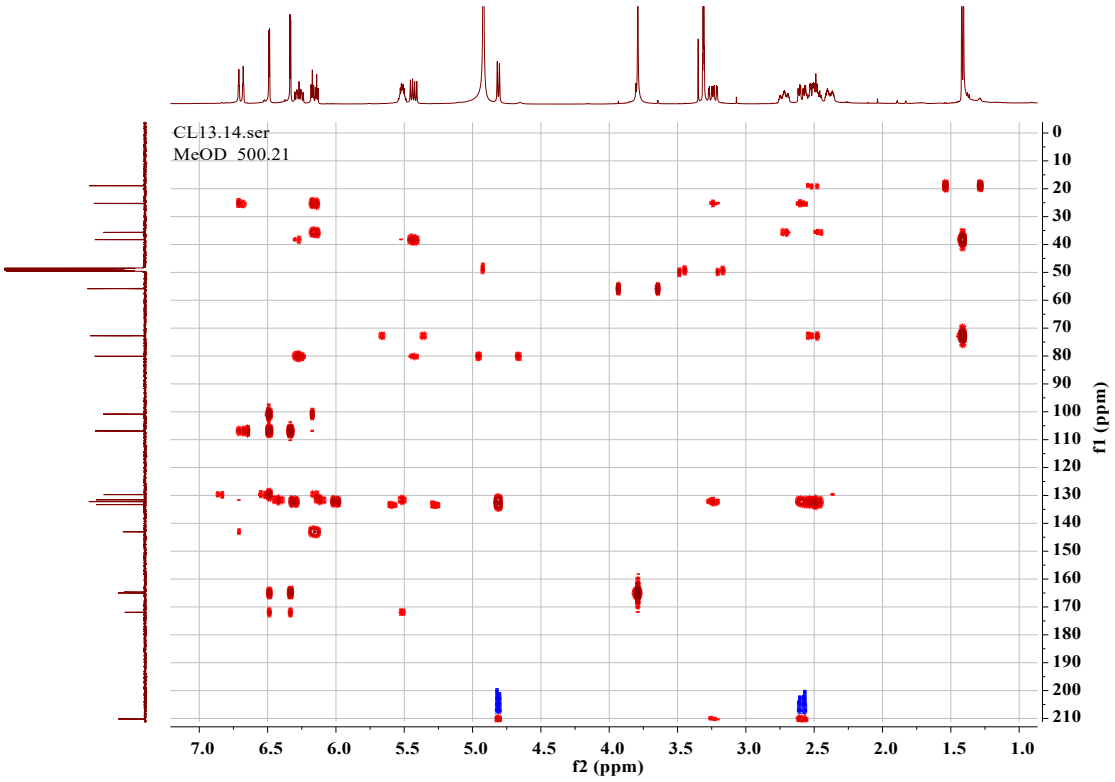


Figure S12. HMBC spectrum of curvulomycin B (**2**) (CD_3OD)

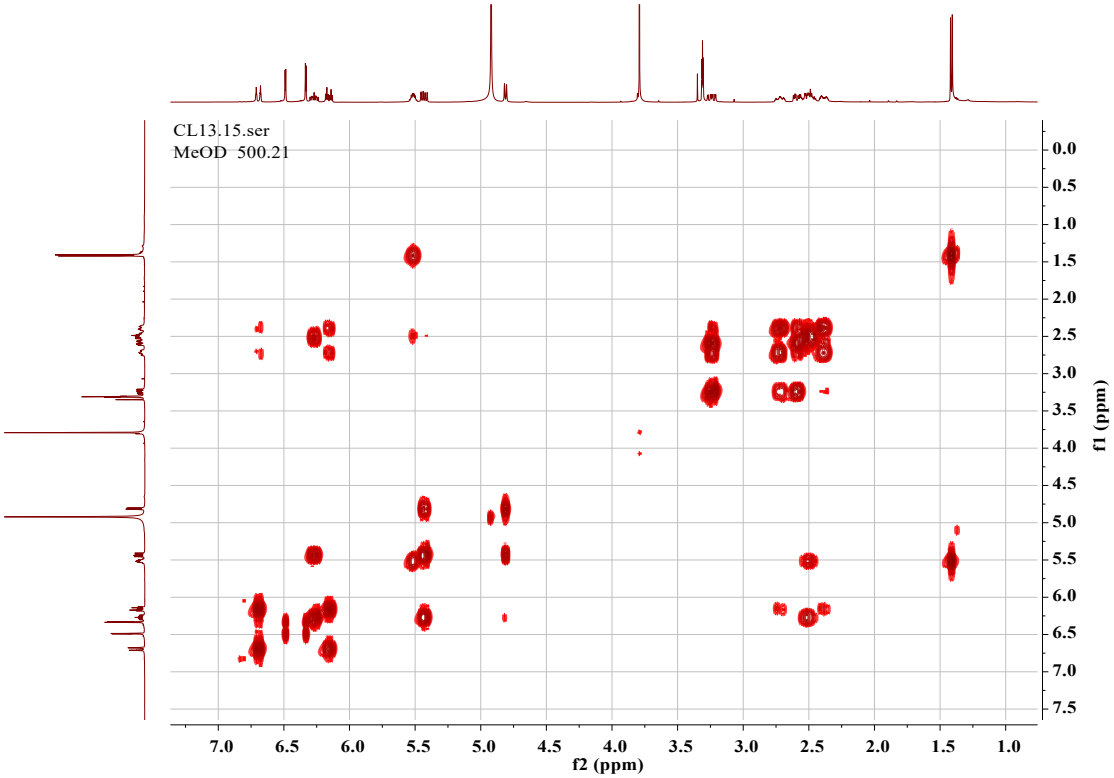


Figure S13. ^{1}H-^{1}H COSY spectrum of curvulomycin B (**2**) (CD_3OD)

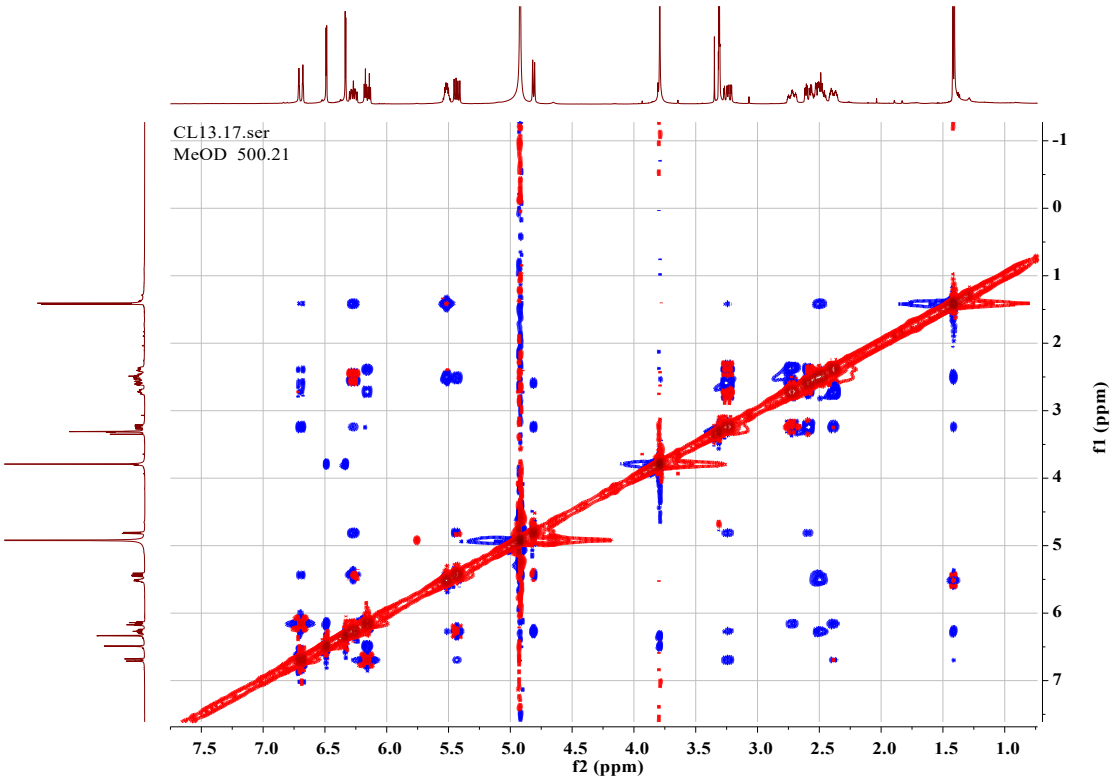


Figure S14. NOESY spectrum of curvulomycin B (**2**) (CD_3OD)

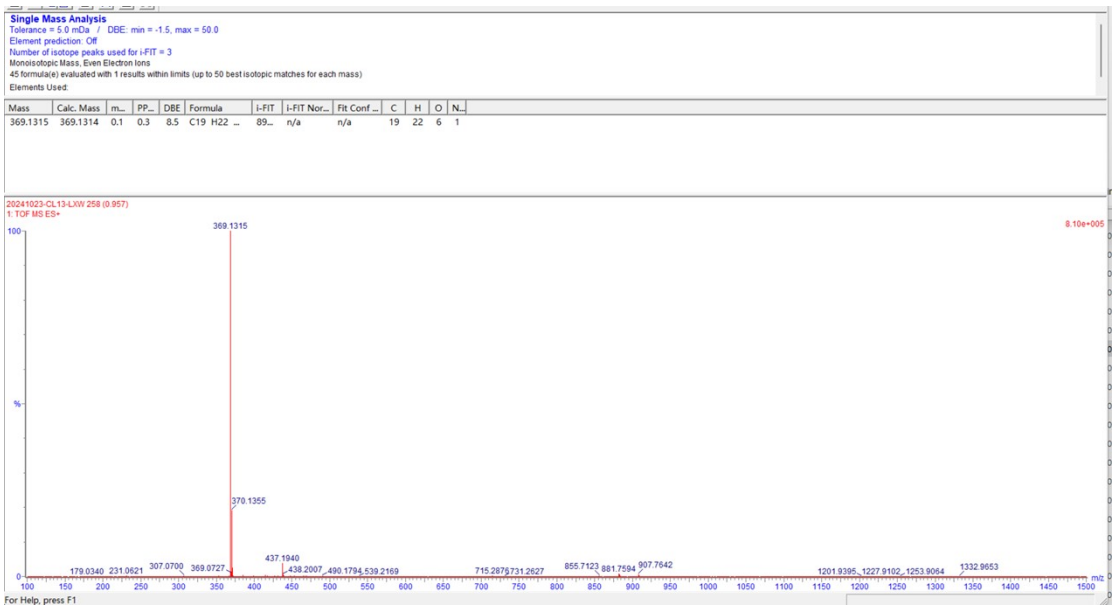


Figure S15. HR-ESIMS spectrum of curvulomycin B (**2**)

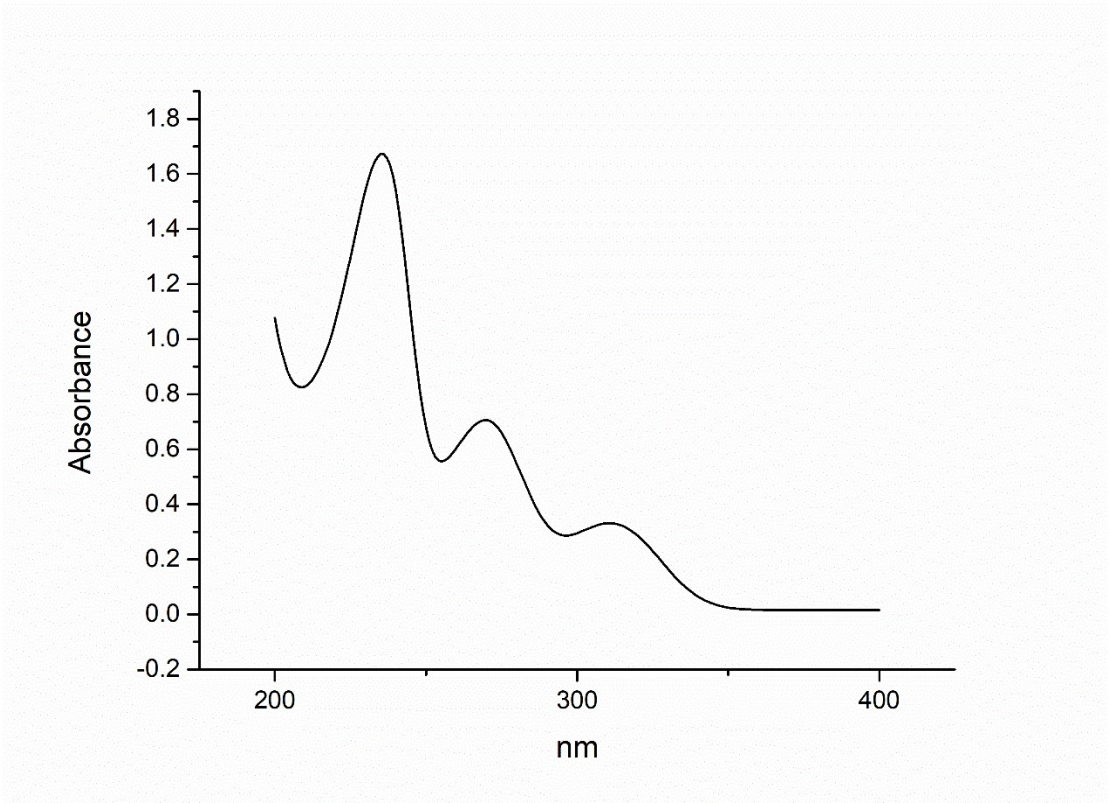


Figure S16. UV spectrum of curvulomycin B (**2**)

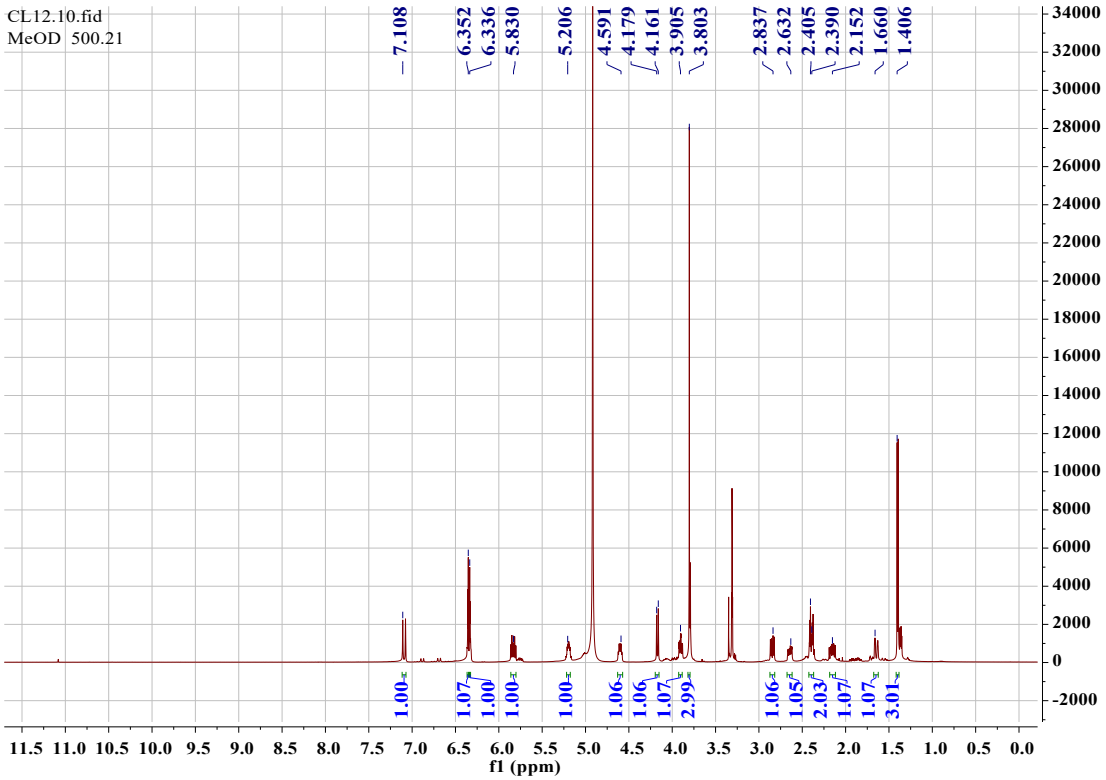


Figure S17. ^{1}H NMR spectrum of curvulomycin C (**3**) (500 MHz, CD_3OD)

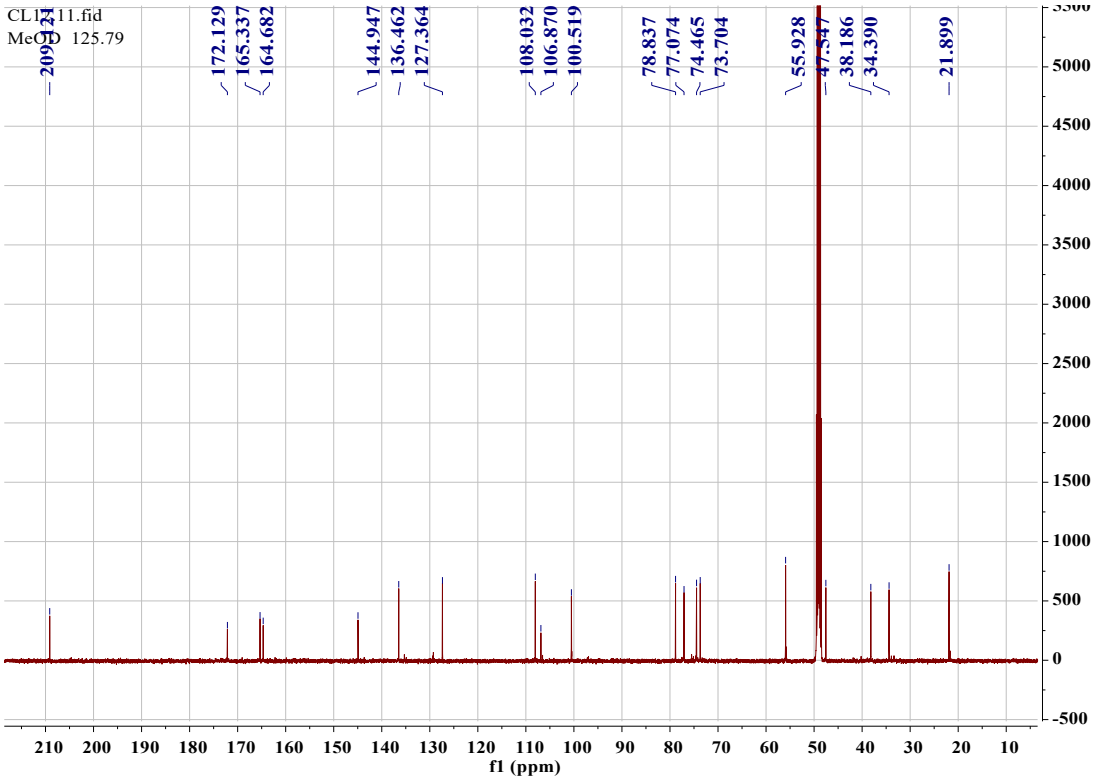


Figure S18. ^{13}C NMR spectrum of curvulomycin C (**3**) (125 MHz, CD_3OD)

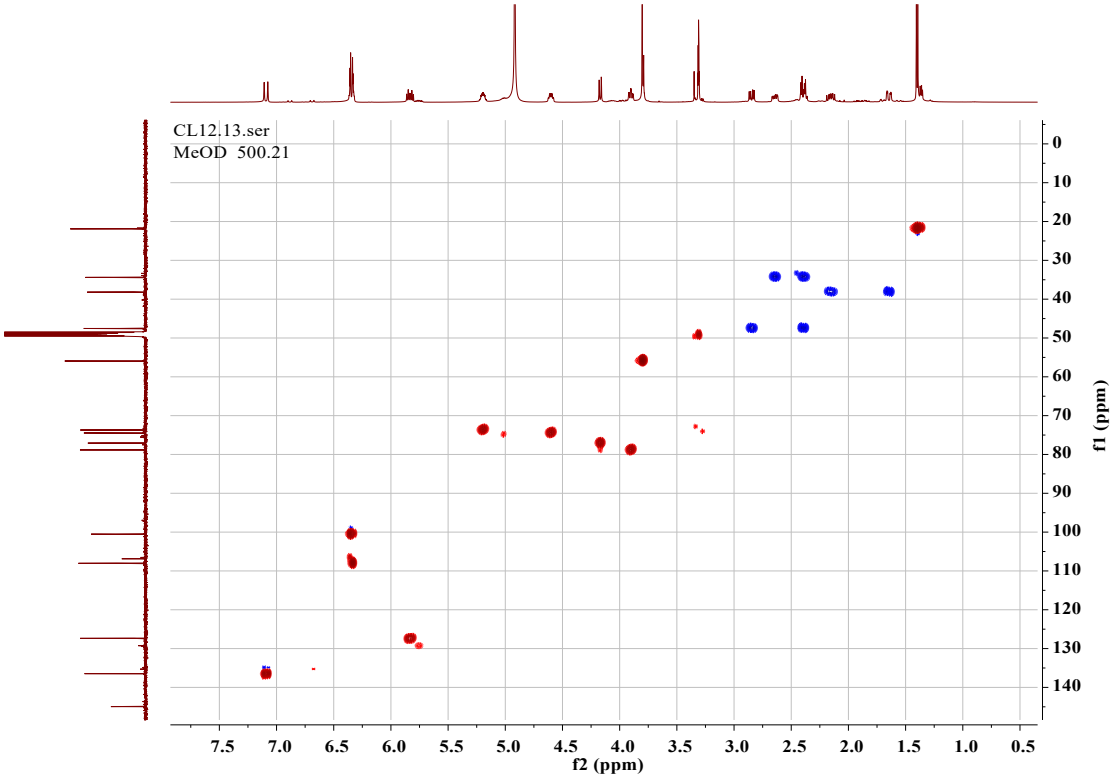


Figure S19. HSQC spectrum of curvulomycin C (**3**) (CD_3OD)

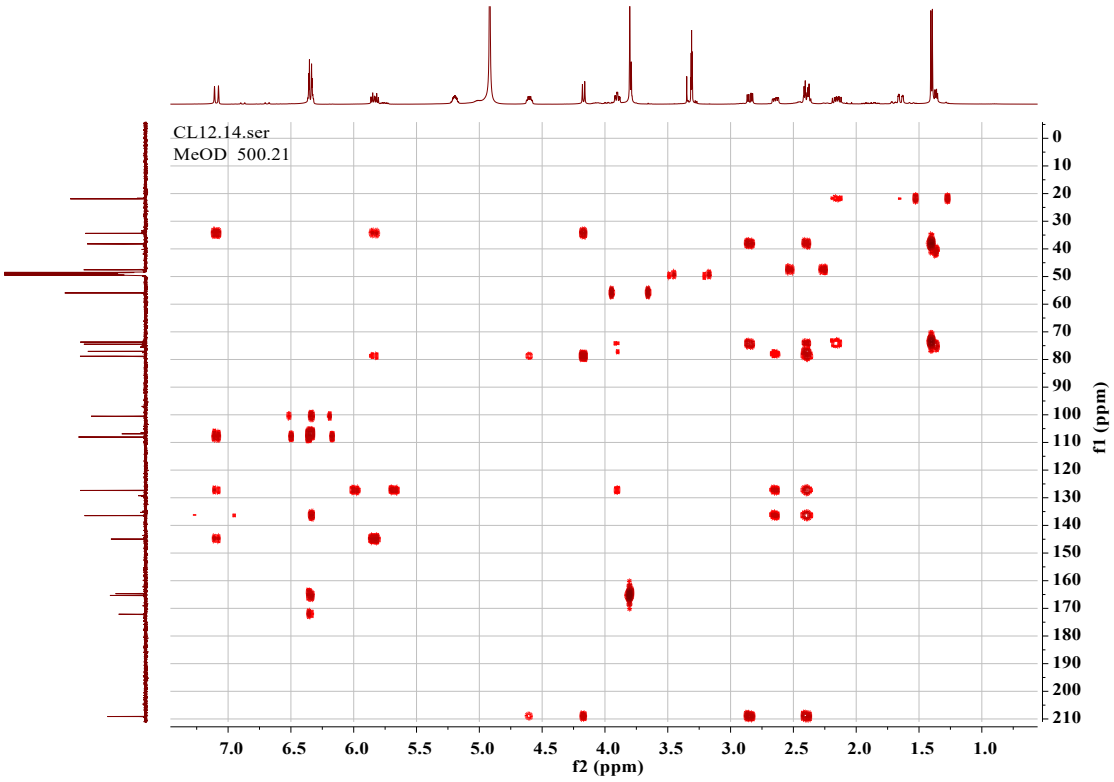


Figure S20. HMBC spectrum of curvulomycin C (**3**) (CD_3OD)

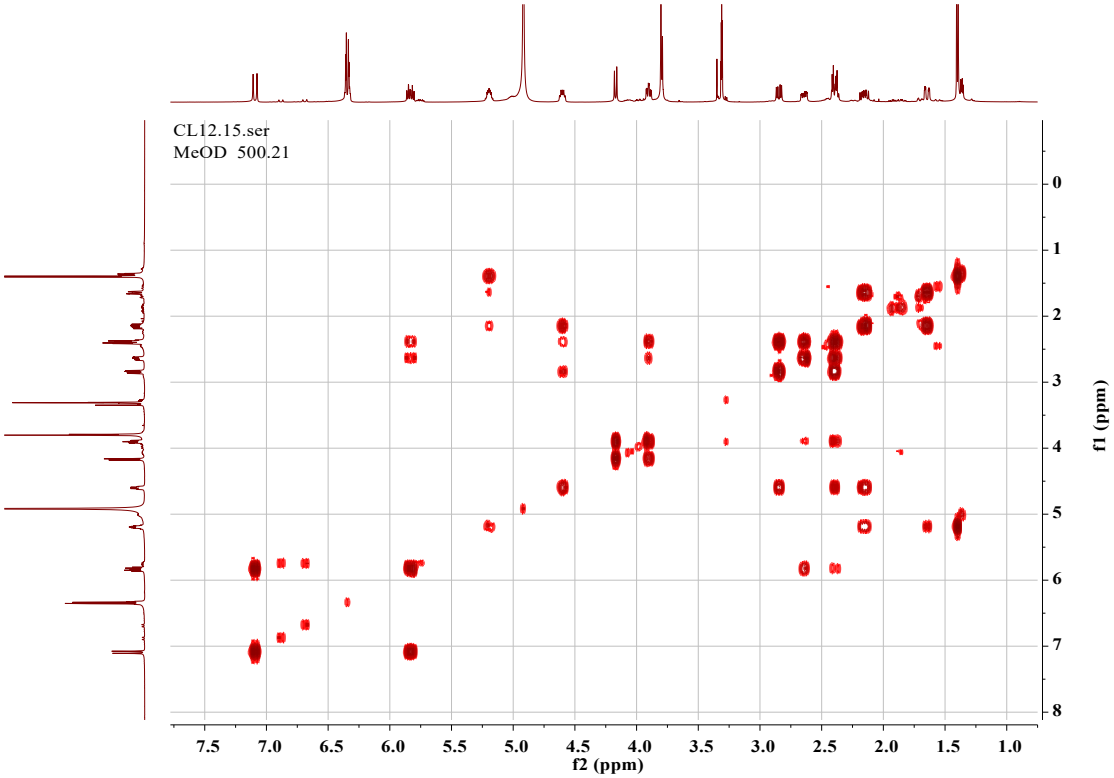


Figure S21. ^{1}H-^{1}H COSY spectrum of curvulomycin C (**3**) (CD_3OD)

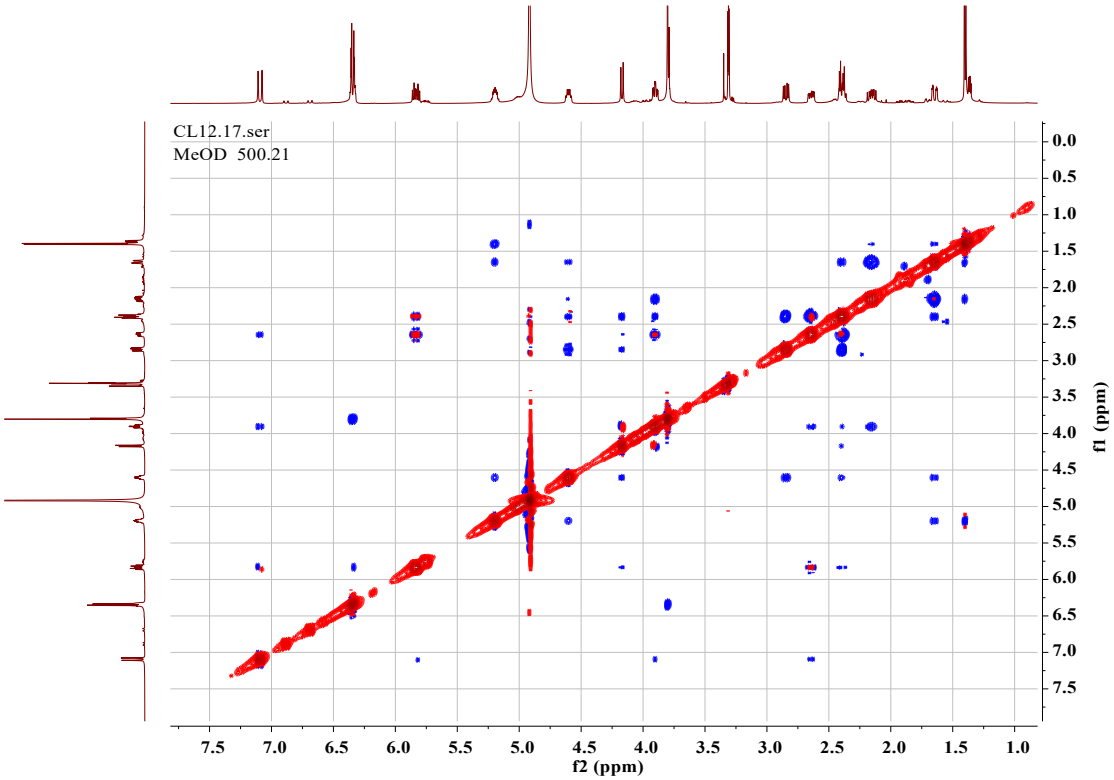


Figure S22. NOESY spectrum of curvulomycin C (**3**) (CD_3OD)

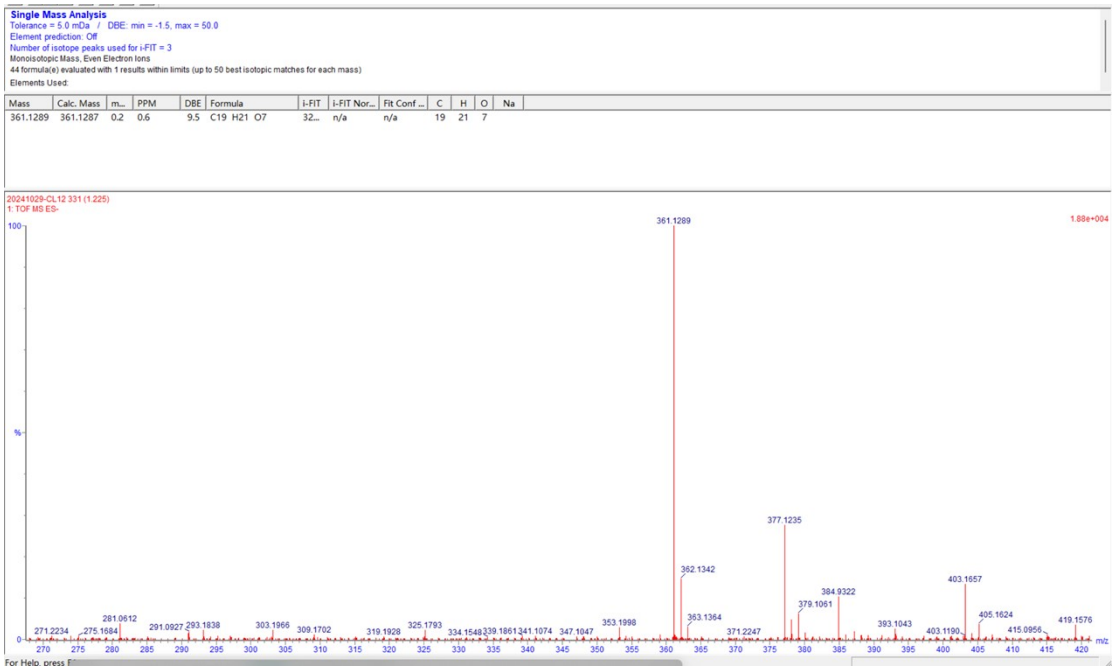


Figure S23. HR-ESIMS spectrum of curvulomycin C (**3**)

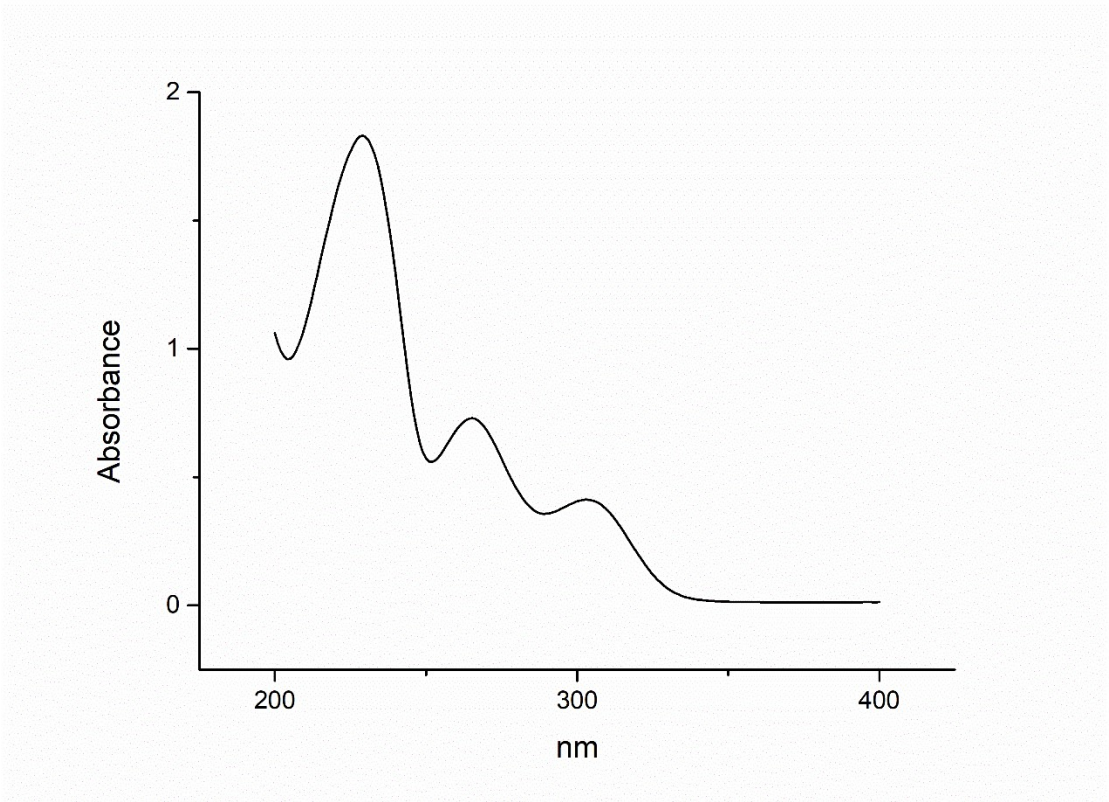


Figure S24. UV spectrum of curvulomycin C (**3**)

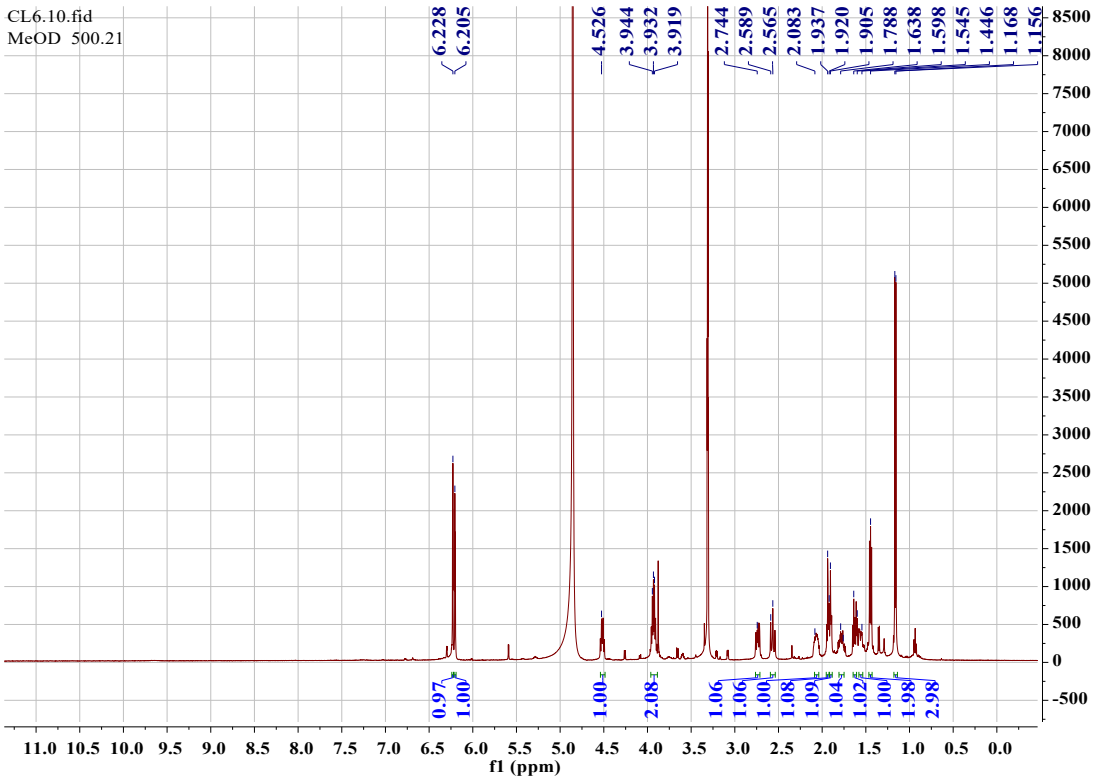


Figure S25. ^{1}H NMR spectrum of curvulomycin D (**4**) (500 MHz, CD_3OD)

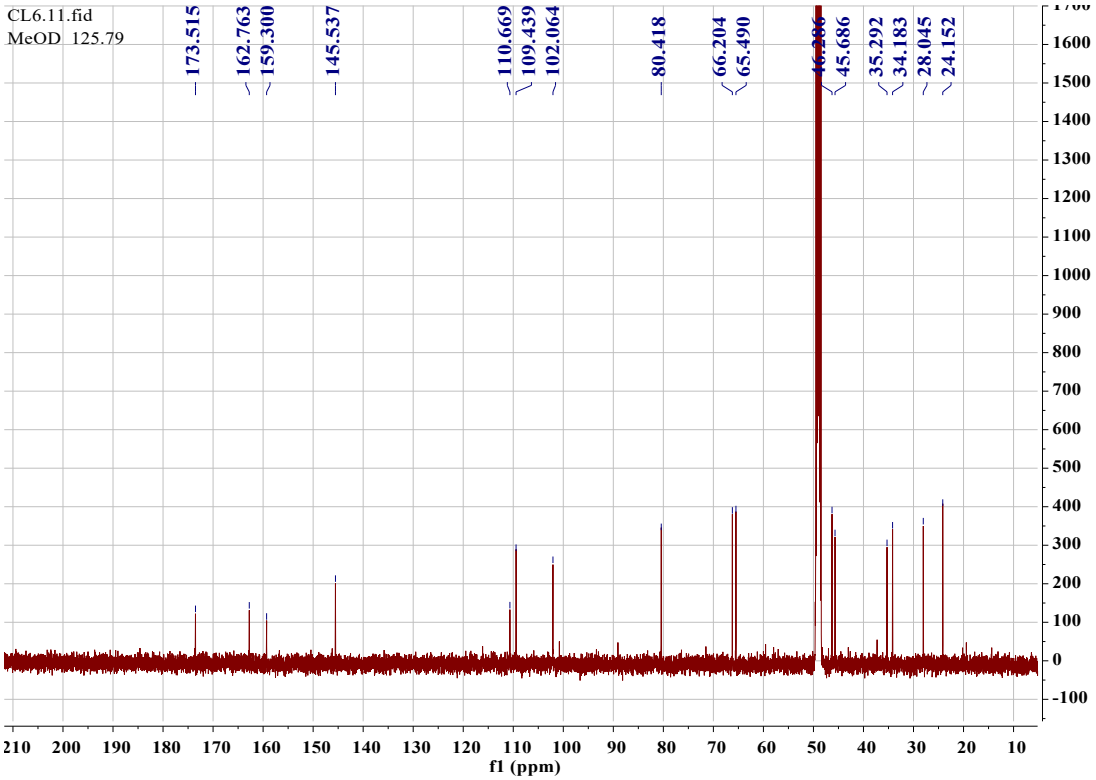


Figure S26. ^{13}C NMR spectrum of curvulomycin D (**4**) (125 MHz, CD_3OD)

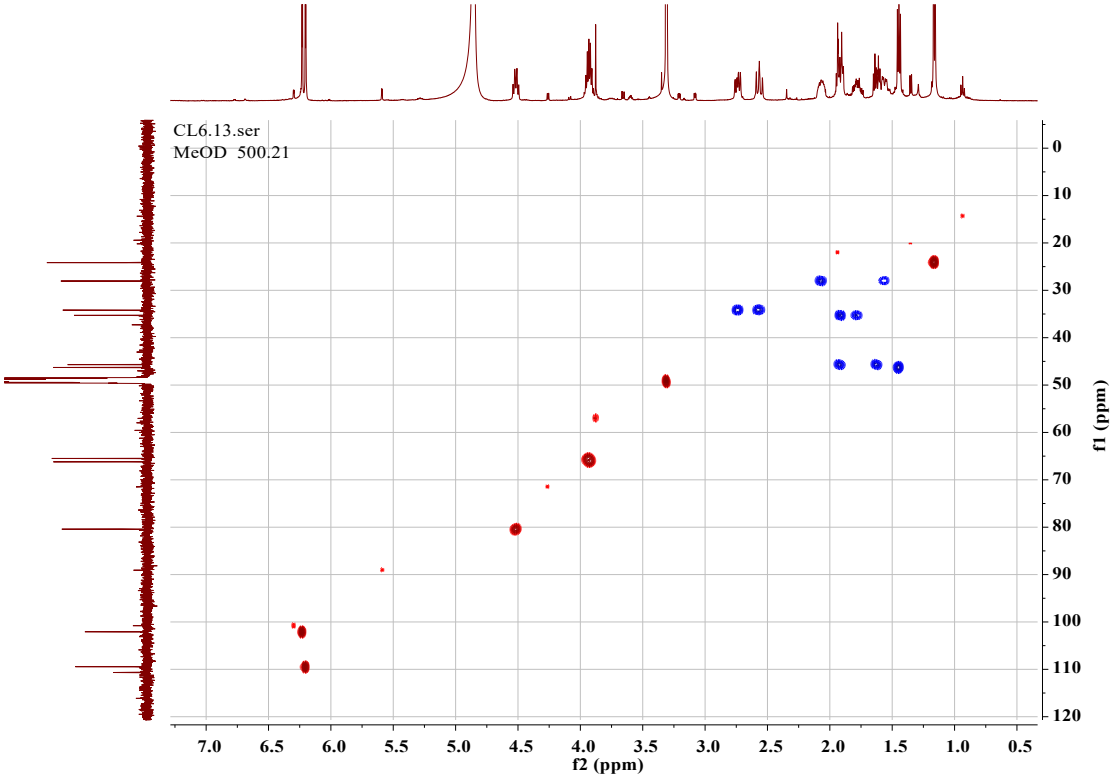


Figure S27. HSQC spectrum of curvulomycin D (**4**) (CD_3OD)

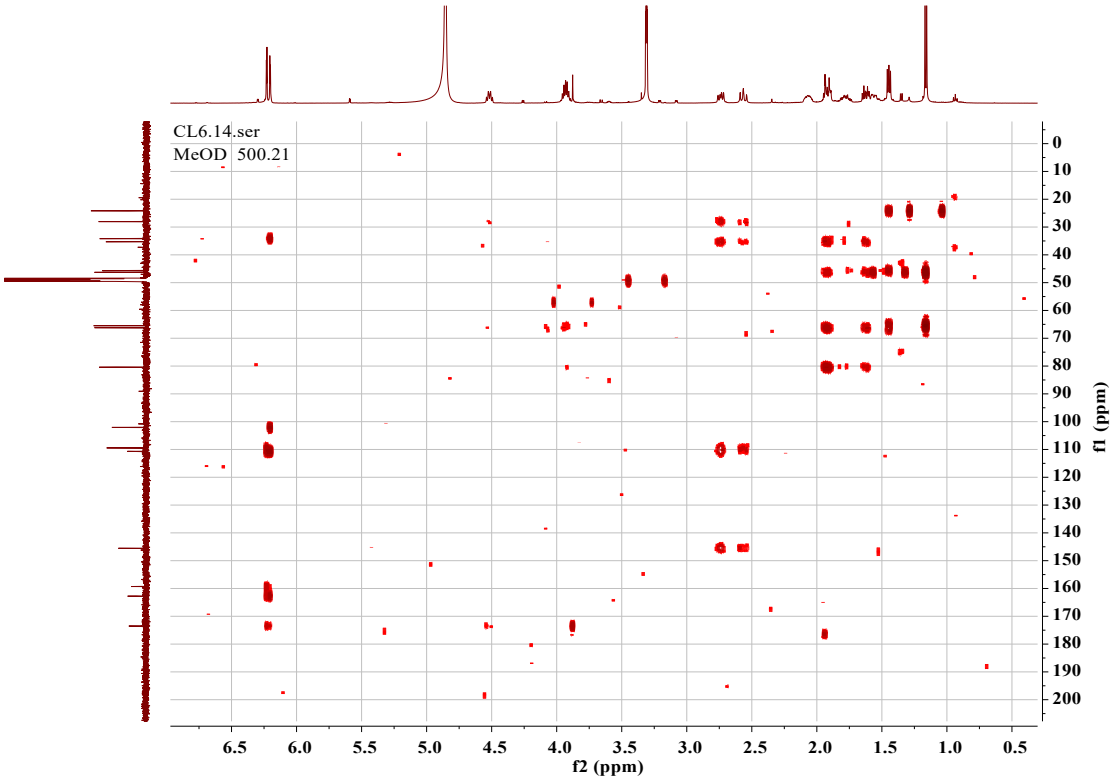


Figure S28. HMBC spectrum of curvulomycin D (**4**) (CD_3OD)

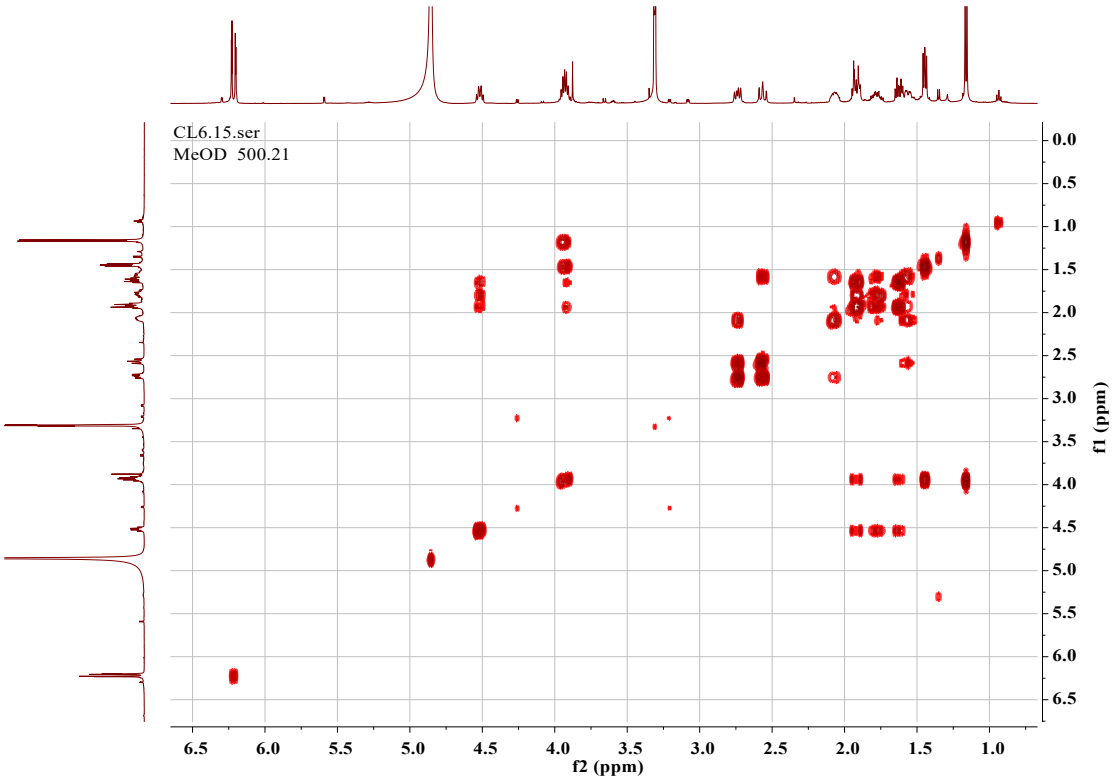


Figure S29. ^{1}H-^{1}H COSY spectrum of curvulomycin D (**4**) (CD_3OD)

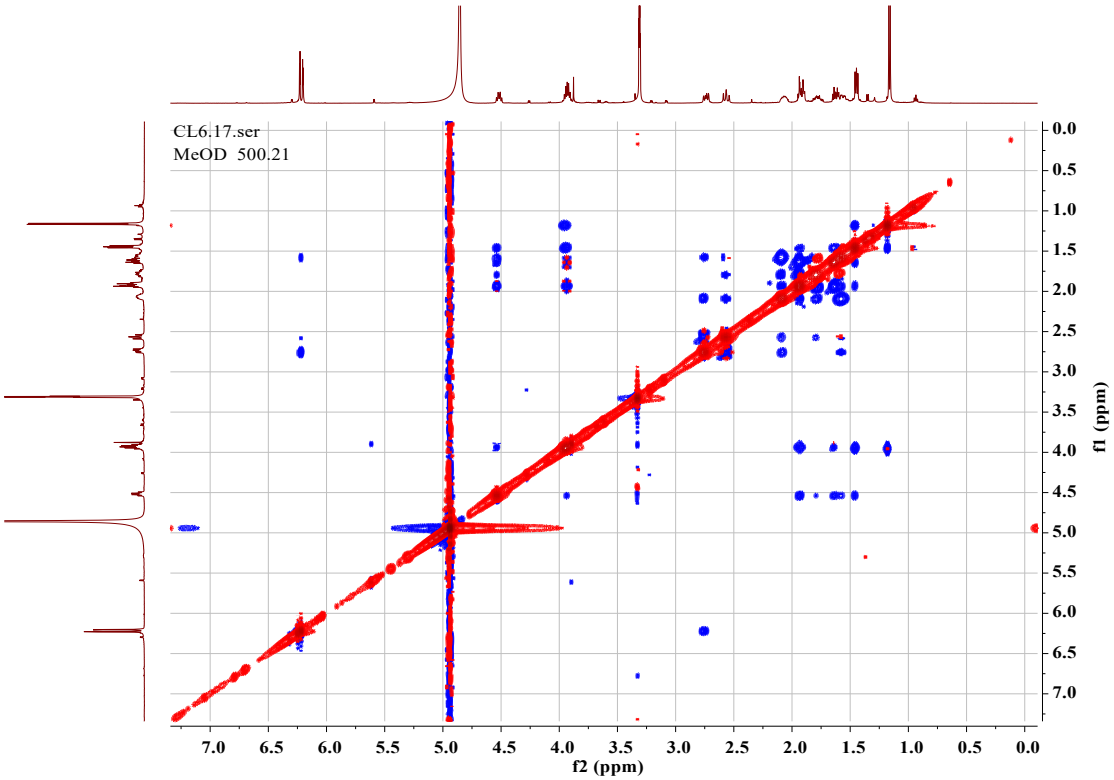


Figure S30. NOESY spectrum of curvulomycin D (**4**) (CD_3OD)

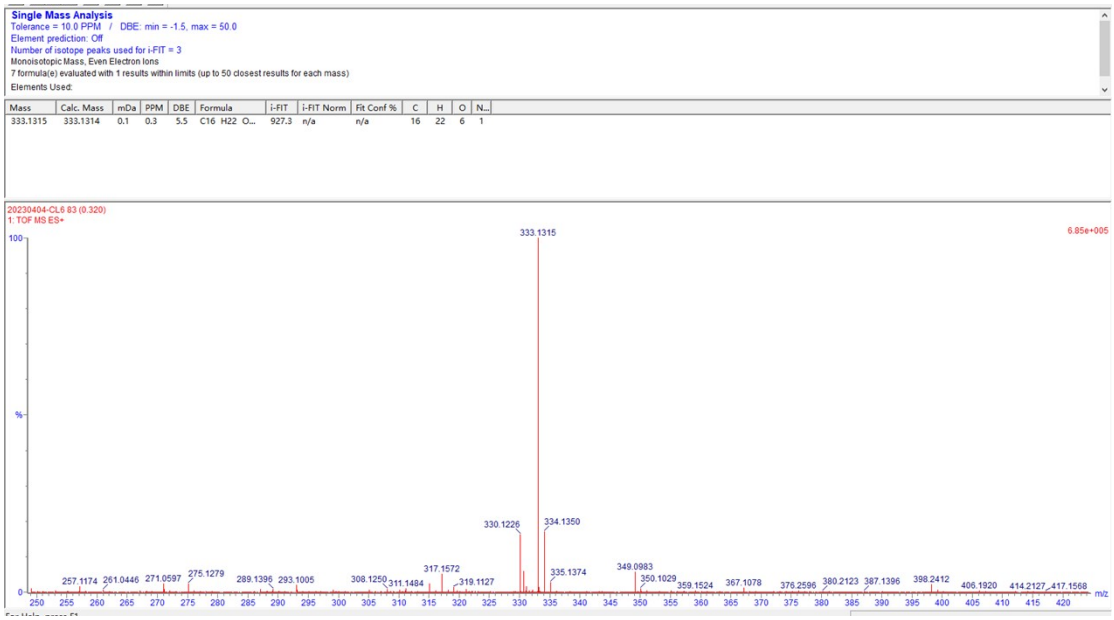


Figure S31. HR-ESIMS spectrum of curvulomycin D (**4**)

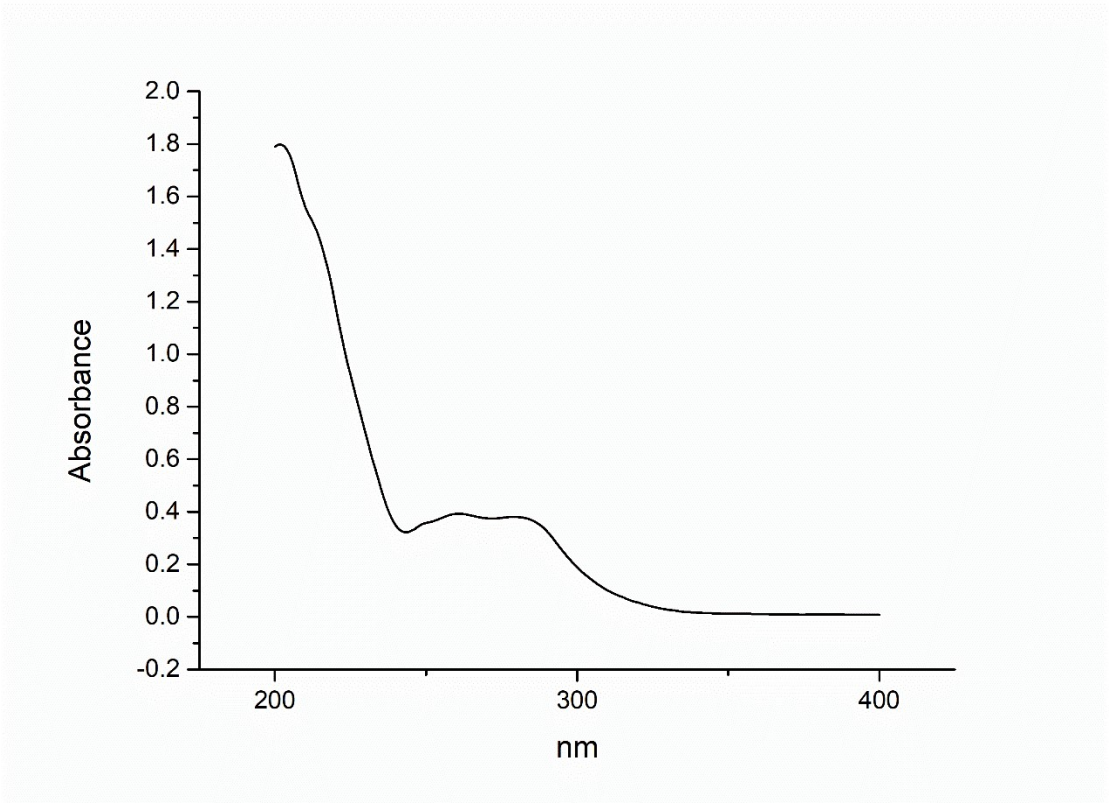


Figure S32. UV spectrum of curvulomycin D (**4**)

Table S1. Energies of **1** at MMFF94 force field.

Conformer	Energy (kJ/mol)	Population (%)
1	402.05	74.1
2	405.42	19.0
3	410.69	2.3
4	411.40	1.7
5	412.72	1.0
6	413.65	0.7
7	414.86	0.4
8	415.08	0.4
9	416.63	0.2
10	417.37	0.2

Table S2. Energies of **1** at B3LYP/6–31+g(d) level in methanol.

Conformer	E (Hartree)	E (kcal/mol)	Population (%)
1	–1416.9590411	–889155.967880661	57.74
2	–1416.9583689	–889155.546068439	28.31
3	–1416.9542291	–889152.948302541	0.35
4	–1416.9572385	–889154.836731135	8.54
5	–1416.9520956	–889151.609509956	0.04
6	–1416.9535322	–889152.510990822	0.17
7	–1416.9566886	–889154.491663386	4.77
8	–1416.9500591	–889150.331585841	0.00
9	–1416.9514036	–889151.175273036	0.02
10	–1416.9525845	–889151.916299595	0.06

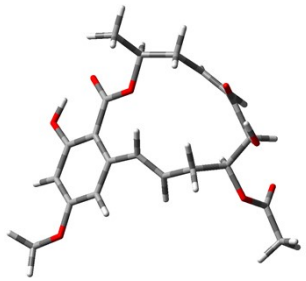
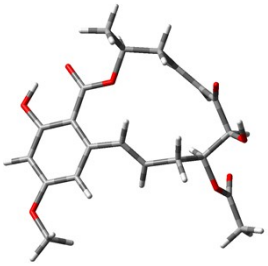
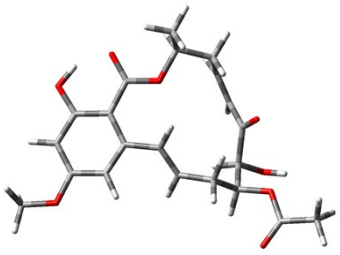
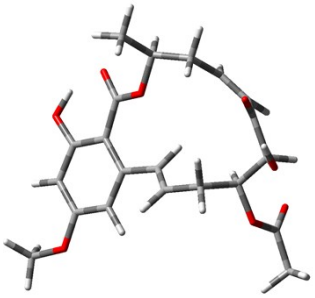
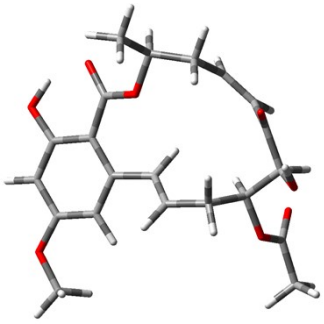
		
Conf.1 (57.74%)	Conf.2 (28.31%)	Conf.3 (0.35%)
		
Conf.4 (8.54%)	Conf.7 (4.77%)	

Figure S33. The optimized conformers and equilibrium populations of **1**.

Table S3. Energies of **2** at MMFF94 force field.

Configuration	Conformer	Energy (kJ/mol)	Population (%)
(2*S*,6*S*)-**2**	1	346.18	46.3
(2*S*,6*S*)-**2**	2	348.67	17.0
(2*S*,6*S*)-**2**	3	349.29	13.2
(2*S*,6*S*)-**2**	4	351.14	6.3
(2*S*,6*S*)-**2**	5	351.91	4.6
(2*S*,6*S*)-**2**	6	352.20	4.1
(2*S*,6*S*)-**2**	7	352.61	3.5
(2*S*,6*S*)-**2**	8	355.11	1.3
(2*S*,6*S*)-**2**	9	355.59	1.0
(2*S*,6*S*)-**2**	10	355.66	1.0
(2*S*,6*R*)-**2**	1	345.69	60.7
(2*S*,6*R*)-**2**	2	348.91	16.6
(2*S*,6*R*)-**2**	3	350.98	7.2

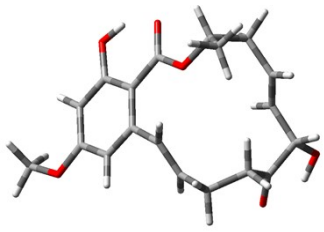
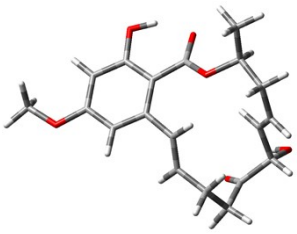
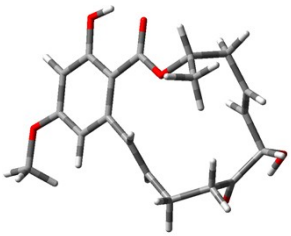
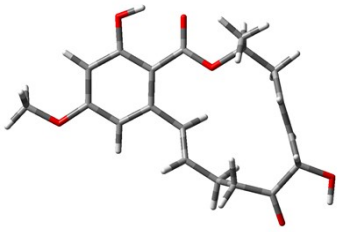
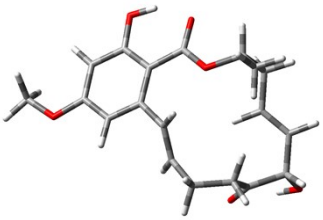
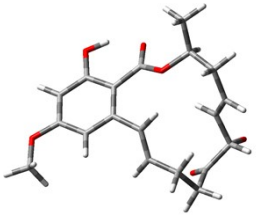
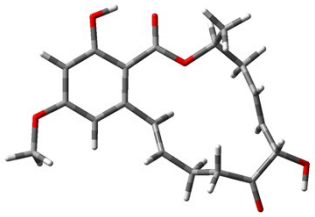
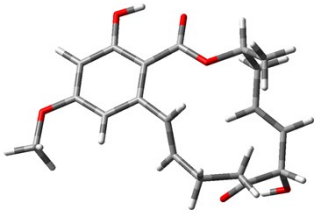
(2*S*,6*R*)-**2**	4	352.45	4.0
(2*S*,6*R*)-**2**	5	353.00	3.2
(2*S*,6*R*)-**2**	6	354.21	2.0
(2*S*,6*R*)-**2**	7	354.26	1.9
(2*S*,6*R*)-**2**	8	356.92	0.7
(2*S*,6*R*)-**2**	9	357.68	0.5
(2*S*,6*R*)-**2**	10	357.75	0.5

Table S4. Energies of **2** at B3LYP/6–31+g(d) level in methanol.

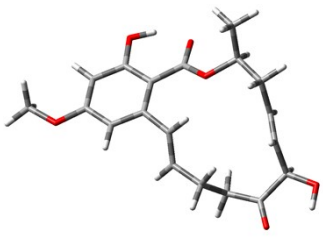
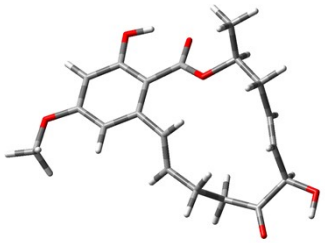
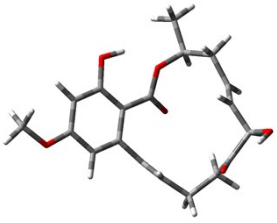
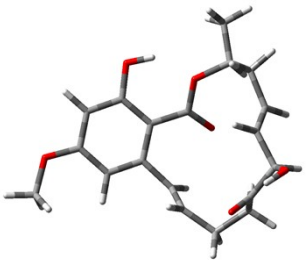
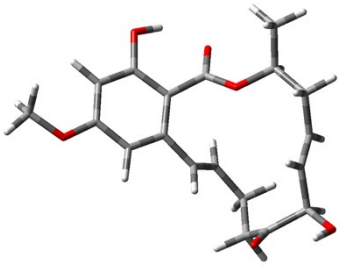
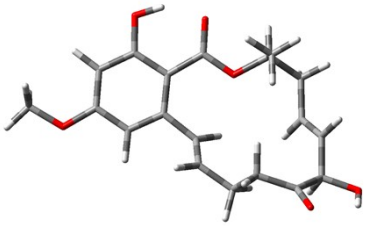
Configuration	Conformer	E (Hartree)	E (kcal/mol)	Population (%)
(2*S*,6*S*)-**2**	1	–1188.9984326	–746108.406440826	52.20
(2*S*,6*S*)-**2**	2	–1188.9953884	–746106.496174884	2.07
(2*S*,6*S*)-**2**	3	–1188.99778	–746107.9969278	26.13
(2*S*,6*S*)-**2**	4	–1188.9969369	–746107.467874119	10.69
(2*S*,6*S*)-**2**	5	–1188.9876645	–746101.649350395	0.00
(2*S*,6*S*)-**2**	6	–1188.9950427	–746106.279244677	1.44
(2*S*,6*S*)-**2**	7	–1188.9948419	–746106.153240669	1.16
(2*S*,6*S*)-**2**	8	–1188.996322	–746107.08201822	5.57
(2*S*,6*S*)-**2**	9	–1188.9873343	–746101.442146593	0.00
(2*S*,6*S*)-**2**	10	–1188.9944116	–746105.883223116	0.74
(2*S*,6*R*)-**2**	1	–1188.9960827	–746106.931855077	52.97
(2*S*,6*R*)-**2**	2	–1188.9954523	–746106.536272773	27.15
(2*S*,6*R*)-**2**	3	–1188.9917733	–746104.227663483	0.55
(2*S*,6*R*)-**2**	4	–1188.9913124	–746103.938444124	0.34
(2*S*,6*R*)-**2**	5	–1188.9901694	–746103.221200194	0.10
(2*S*,6*R*)-**2**	6	–1188.9942583	–746105.787025833	7.66
(2*S*,6*R*)-**2**	7	–1188.993209	–746105.12857959	2.52
(2*S*,6*R*)-**2**	8	–1188.9936112	–746105.380964112	3.86
(2*S*,6*R*)-**2**	9	–1188.9925838	–746104.736260338	1.30

(2*S*,6*R*)-**2**	10	–1188.9935378	–746105.334904878	3.57

(2*S*,6*S*)-**2**

		
Conf.1 (52.20%)	Conf.2 (2.07%)	Conf.3 (26.13%)
		
Conf.4 (10.69%)	Conf.6 (1.44%)	Conf.7 (1.16%)
		
Conf.8 (5.57%)	Conf.10 (0.74%)	

(2*S*,6*R*)-**2**

		
Conf.1 (52.97%)	Conf.2 (27.15%)	Conf.3 (0.55%)
		

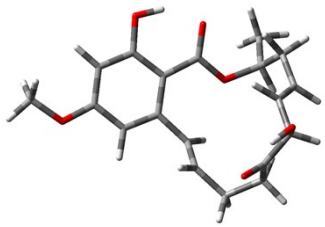
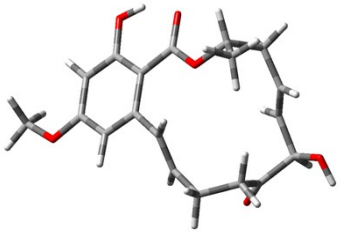
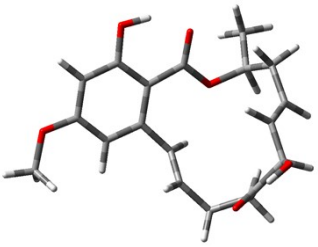
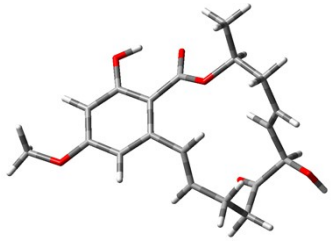
Conf.4 (0.34%)	Conf.5 (0.10%)	Conf.6 (7.66%)
		
Conf.7 (2.52%)	Conf.8 (3.86%)	Conf.9 (1.30%)
		
Conf.10 (3.57%)		

Figure S34. The optimized conformers and equilibrium populations of **2**.

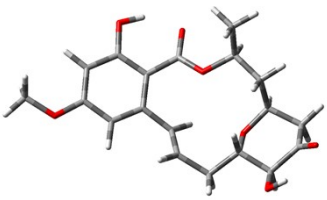
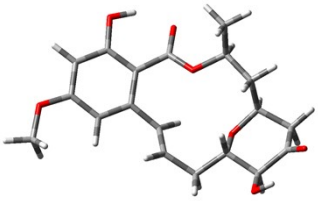
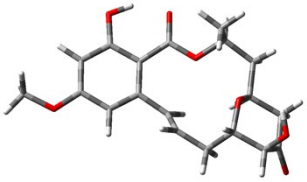
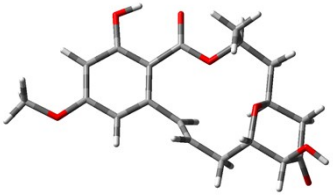
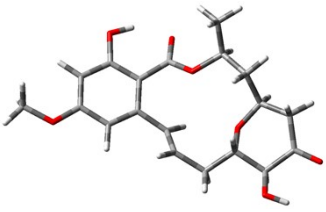
Table S5. Energies of **3** at MMFF94 force field.

Configuration	Conformer	Energy (kJ/mol)	Population (%)
(2*S*,4*S*,7*S*,8*S*)-**3**	1	384.20	73.5
(2*S*,4*S*,7*S*,8*S*)-**3**	2	386.75	26.3
(2*S*,4*S*,7*S*,8*S*)-**3**	3	401.03	0.1
(2*S*,4*S*,7*S*,8*S*)-**3**	4	403.46	0.0
(2*S*,4*S*,7*S*,8*S*)-**3**	5	404.07	0.0
(2*S*,4*R*,7*R*,8*R*)-**3**	1	391.59	49.1
(2*S*,4*R*,7*R*,8*R*)-**3**	2	393.47	22.9
(2*S*,4*R*,7*R*,8*R*)-**3**	3	394.40	15.8
(2*S*,4*R*,7*R*,8*R*)-**3**	4	396.21	7.6
(2*S*,4*R*,7*R*,8*R*)-**3**	5	398.86	2.6
(2*S*,4*R*,7*R*,8*R*)-**3**	6	401.71	0.8
(2*S*,4*R*,7*R*,8*R*)-**3**	7	404.57	0.3

Table S6. Energies of **3** at B3LYP/6–31+g(d) level in methanol.

Configuration	Conformer	E (Hartree)	E (kcal/mol)	Population (%)
(2*S*,4*S*,7*S*,8*S*)-**3**	1	–1264.2557302	–793333.113257802	60.31
(2*S*,4*S*,7*S*,8*S*)-**3**	2	–1264.2552559	–793332.815629809	36.48
(2*S*,4*S*,7*S*,8*S*)-**3**	3	–1264.2528249	–793331.290152999	2.77
(2*S*,4*S*,7*S*,8*S*)-**3**	4	–1264.2510894	–793330.201109394	0.44
(2*S*,4*S*,7*S*,8*S*)-**3**	5	–1264.2469321	–793327.592362071	0.01
(2*S*,4*R*,7*R*,8*R*)-**3**	1	–1264.2559161	–793333.229911911	61.37
(2*S*,4*R*,7*R*,8*R*)-**3**	2	–1264.2529505	–793331.368968255	2.65
(2*S*,4*R*,7*R*,8*R*)-**3**	3	–1264.2553502	–793332.874804002	33.68
(2*S*,4*R*,7*R*,8*R*)-**3**	4	–1264.2522876	–793330.952991876	1.31
(2*S*,4*R*,7*R*,8*R*)-**3**	5	–1264.2491383	–793328.976774633	0.05
(2*S*,4*R*,7*R*,8*R*)-**3**	6	–1264.2488024	–793328.765994024	0.03
(2*S*,4*R*,7*R*,8*R*)-**3**	7	–1264.2519429	–793330.736689179	0.91

(2*S*,4*S*,7*S*,8*S*)-**3**

		
Conf.1 (60.31%)	Conf.2 (36.48%)	Conf.3 (2.77%)
		
Conf.4 (0.44%)	Conf.5 (0.01%)	

(2*S*,4*R*,7*R*,8*R*)-**3**

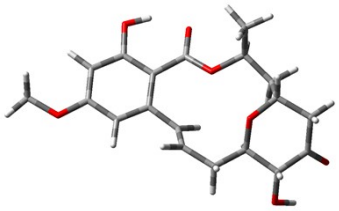
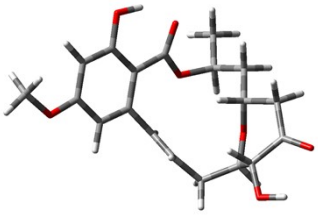
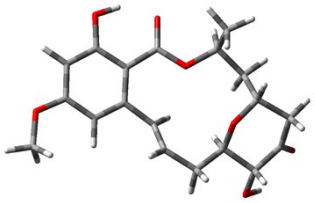
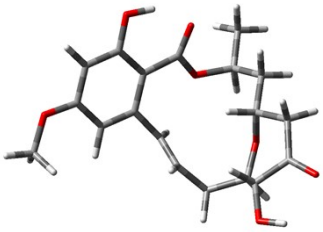
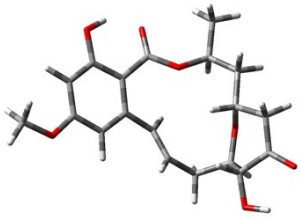
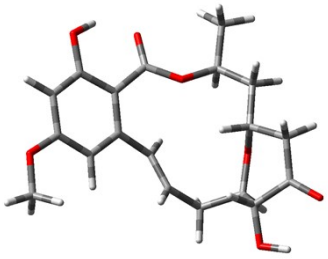
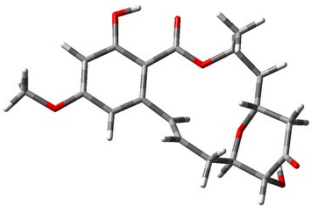
		
Conf.1 (61.37%)	Conf.2 (2.65%)	Conf.3 (33.68%)
		
Conf.4 (1.31%)	Conf.5 (0.05%)	Conf.6 (0.03%)
		
Conf.7 (0.91%)		

Figure S35. The optimized conformers and equilibrium populations of **3**.

Table S7. Energies of **4** at MMFF94 force field.

Configuration	Conformer	Energy (kJ/mol)	Population (%)
(4*R*, 6*S*, 8*S*)-**4**	1	180.45	47.3
(4*R*, 6*S*, 8*S*)-**4**	2	183.06	16.5
(4*R*, 6*S*, 8*S*)-**4**	3	183.28	15.1
(4*R*, 6*S*, 8*S*)-**4**	4	183.95	11.5
(4*R*, 6*S*, 8*S*)-**4**	5	187.62	2.6
(4*R*, 6*S*, 8*S*)-**4**	6	189.15	1.4
(4*R*, 6*S*, 8*S*)-**4**	7	189.19	1.4
(4*R*, 6*S*, 8*S*)-**4**	8	189.47	1.2
(4*R*, 6*S*, 8*S*)-**4**	9	189.88	1.1
(4*R*, 6*S*, 8*S*)-**4**	10	192.54	0.4

(4*S*, 6*R*, 8*R*)-**4**	1	183.06	32.8
(4*S*, 6*R*, 8*R*)-**4**	2	183.28	30.0
(4*S*, 6*R*, 8*R*)-**4**	3	183.95	22.9
(4*S*, 6*R*, 8*R*)-**4**	4	189.15	2.8
(4*S*, 6*R*, 8*R*)-**4**	5	189.19	2.8
(4*S*, 6*R*, 8*R*)-**4**	6	189.47	2.5
(4*S*, 6*R*, 8*R*)-**4**	7	189.88	2.1
(4*S*, 6*R*, 8*R*)-**4**	8	189.90	2.1
(4*S*, 6*R*, 8*R*)-**4**	9	193.31	0.5
(4*S*, 6*R*, 8*R*)-**4**	10	193.54	0.5
(4*S*, 6*R*, 8*S*)-**4**	1	186.46	50.7
(4*S*, 6*R*, 8*S*)-**4**	2	190.33	10.6
(4*S*, 6*R*, 8*S*)-**4**	3	190.36	10.5
(4*S*, 6*R*, 8*S*)-**4**	4	190.69	9.2
(4*S*, 6*R*, 8*S*)-**4**	5	191.57	6.5
(4*S*, 6*R*, 8*S*)-**4**	6	193.19	3.4
(4*S*, 6*R*, 8*S*)-**4**	7	194.79	1.8
(4*S*, 6*R*, 8*S*)-**4**	8	195.78	1.2
(4*S*, 6*R*, 8*S*)-**4**	9	196.25	1.0
(4*S*, 6*R*, 8*S*)-**4**	10	196.51	0.9
(4*R*, 6*S*, 8*R*)-**4**	1	186.46	37.6
(4*R*, 6*S*, 8*R*)-**4**	2	187.36	26.2
(4*R*, 6*S*, 8*R*)-**4**	3	190.33	7.9
(4*R*, 6*S*, 8*R*)-**4**	4	190.36	7.8
(4*R*, 6*S*, 8*R*)-**4**	5	190.69	6.8
(4*R*, 6*S*, 8*R*)-**4**	6	191.57	4.8
(4*R*, 6*S*, 8*R*)-**4**	7	193.19	2.5
(4*R*, 6*S*, 8*R*)-**4**	8	194.79	1.3
(4*R*, 6*S*, 8*R*)-**4**	9	195.78	0.9

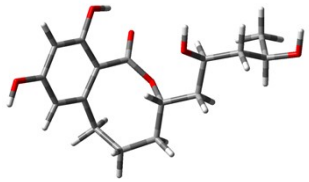
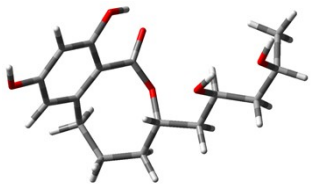
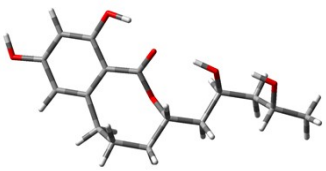
(4*R*, 6*S*, 8*R*)-**4**	10	196.25	0.7

Table S8. Energies of **4** at B3LYP/6–31+g(d) level in methanol.

Configuration	Conformer	E (Hartree)	E (kcal/mol)	Population (%)
(4*R*, 6*S*, 8*S*)-**4**	1	–1074.6438965	–674349.791492715	0.03
(4*R*, 6*S*, 8*S*)-**4**	2	–1074.6482776	–674352.540676776	2.99
(4*R*, 6*S*, 8*S*)-**4**	3	–1074.6500363	–674353.644278613	19.32
(4*R*, 6*S*, 8*S*)-**4**	4	–1074.6502969	–674353.807807719	25.47
(4*R*, 6*S*, 8*S*)-**4**	5	–1074.6486764	–674352.790927764	4.57
(4*R*, 6*S*, 8*S*)-**4**	6	–1074.6481131	–674352.437451381	2.52
(4*R*, 6*S*, 8*S*)-**4**	7	–1074.6499711	–674353.603364961	18.03
(4*R*, 6*S*, 8*S*)-**4**	8	–1074.6483035	–674352.556929285	3.08
(4*R*, 6*S*, 8*S*)-**4**	9	–1074.6502322	–674353.767207822	23.78
(4*R*, 6*S*, 8*S*)-**4**	10	–1074.6457216	–674350.936761216	0.20
(4*S*, 6*R*, 8*R*)-**4**	1	–1074.6482776	–674352.540676776	3.14
(4*S*, 6*R*, 8*R*)-**4**	2	–1074.6500356	–674353.643839356	20.25
(4*S*, 6*R*, 8*R*)-**4**	3	–1074.6502972	–674353.807995972	26.73
(4*S*, 6*R*, 8*R*)-**4**	4	–1074.6481131	–674352.437451381	2.64
(4*S*, 6*R*, 8*R*)-**4**	5	–1074.6499708	–674353.603176708	18.91
(4*S*, 6*R*, 8*R*)-**4**	6	–1074.6483034	–674352.556866534	3.23
(4*S*, 6*R*, 8*R*)-**4**	7	–1074.6502322	–674353.767207822	24.95
(4*S*, 6*R*, 8*R*)-**4**	8	–1074.64276	–674349.0783276	0.01
(4*S*, 6*R*, 8*R*)-**4**	9	–1074.6452307	–674350.628716557	0.12
(4*S*, 6*R*, 8*R*)-**4**	10	–1074.6435866	–674349.597027366	0.02
(4*S*, 6*R*, 8*S*)-**4**	1	–1074.6448259	–674350.374700509	2.11
(4*S*, 6*R*, 8*S*)-**4**	2	–1074.6468365	–674351.636372115	17.77
(4*S*, 6*R*, 8*S*)-**4**	3	–1074.645307	–674350.67659557	3.51
(4*S*, 6*R*, 8*S*)-**4**	4	–1074.6453548	–674350.706590548	3.69
(4*S*, 6*R*, 8*S*)-**4**	5	–1074.6447544	–674350.329833544	1.95

(4*S*, 6*R*, 8*S*)-**4**	6	–1074.6439081	–674349.798771831	0.80
(4*S*, 6*R*, 8*S*)-**4**	7	–1074.6477521	–674352.210920271	46.91
(4*S*, 6*R*, 8*S*)-**4**	8	–1074.6468436	–674351.640827436	17.91
(4*S*, 6*R*, 8*S*)-**4**	9	–1074.6446947	–674350.292371197	1.84
(4*S*, 6*R*, 8*S*)-**4**	10	–1074.6453061	–674350.676030811	3.51
(4*R*, 6*S*, 8*R*)-**4**	1	–1074.6448254	–674350.374386754	2.18
(4*R*, 6*S*, 8*R*)-**4**	2	–1074.6398926	–674347.279005426	0.01
(4*R*, 6*S*, 8*R*)-**4**	3	–1074.6468365	–674351.636372115	18.42
(4*R*, 6*S*, 8*R*)-**4**	4	–1074.6453069	–674350.676532819	3.64
(4*R*, 6*S*, 8*R*)-**4**	5	–1074.6453547	–674350.706527797	3.83
(4*R*, 6*S*, 8*R*)-**4**	6	–1074.6447544	–674350.329833544	2.03
(4*R*, 6*S*, 8*R*)-**4**	7	–1074.6439112	–674349.800717112	0.83
(4*R*, 6*S*, 8*R*)-**4**	8	–1074.6477518	–674352.210732018	48.60
(4*R*, 6*S*, 8*R*)-**4**	9	–1074.6468436	–674351.640827436	18.56
(4*R*, 6*S*, 8*R*)-**4**	10	–1074.6446958	–674350.293061458	1.90

(4*R*, 6*S*, 8*S*)-**4**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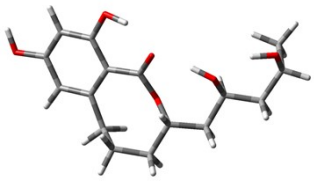
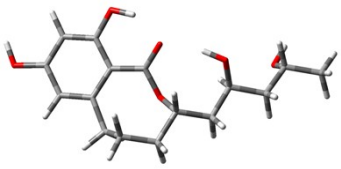
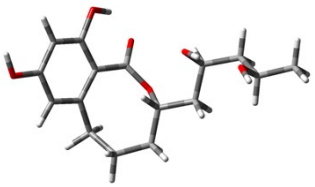
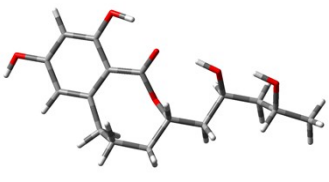
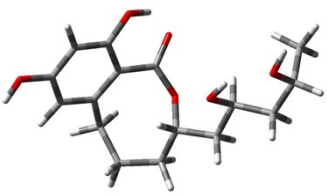
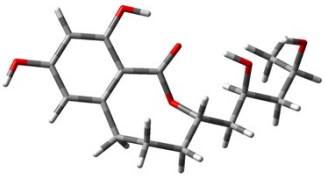
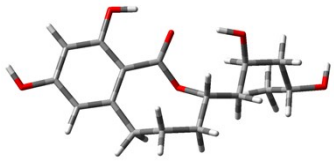
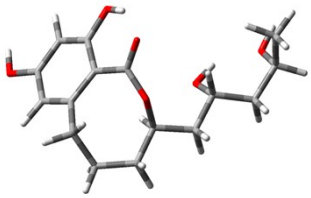
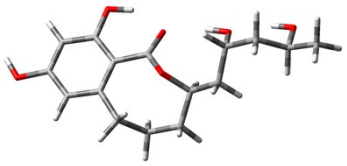
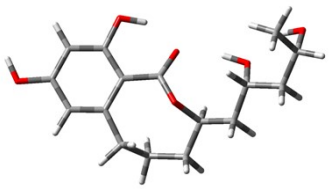
		
Conf.4 (25.47%)	Conf.5 (4.57%)	Conf.6 (2.52%)
		

Conf.7 (18.03%)	Conf.8 (3.08%)	Conf.9 (23.78%)
		
Conf.10 (0.20%)		

(4*S*, 6*R*, 8*R*)-**4**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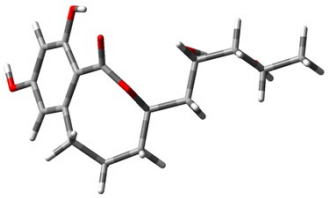
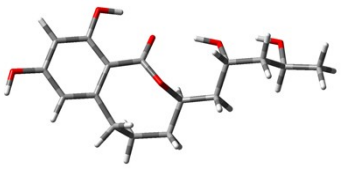
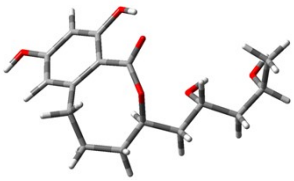
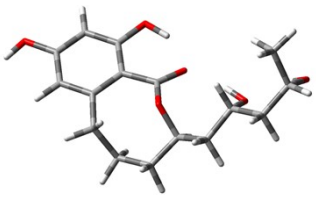
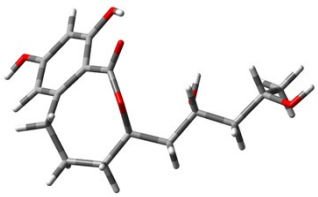
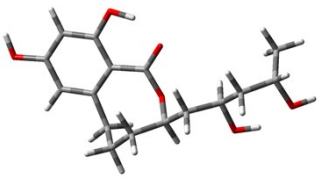
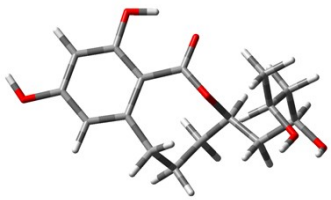
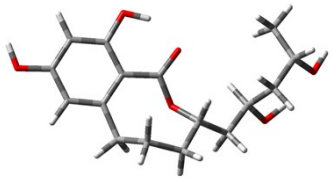
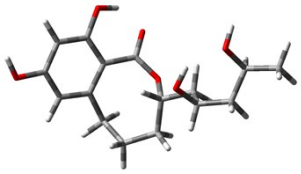
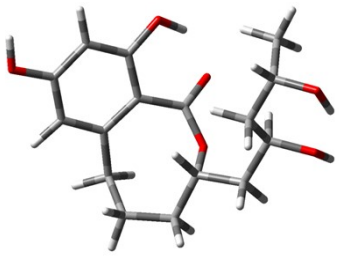
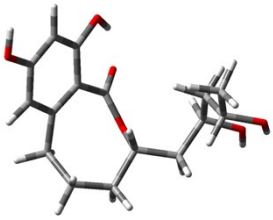
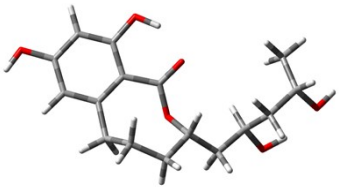
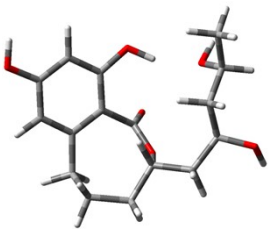
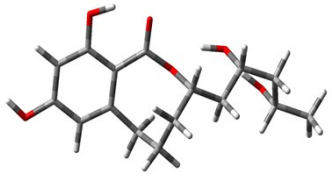
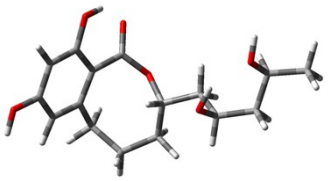
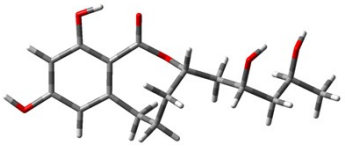
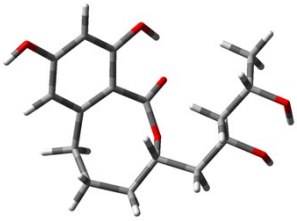
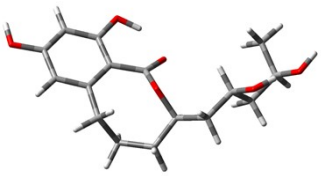
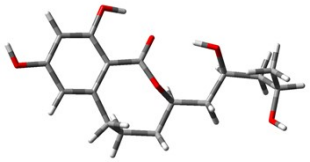
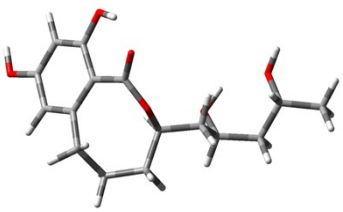
		
Conf.4 (2.64%)	Conf.5 (18.91%)	Conf.6 (3.23%)
		
Conf.7 (24.95%)	Conf.8 (0.01%)	Conf.9 (0.12%)
		
Conf.10 (0.02%)		

(4*S*, 6*R*, 8*S*)-**4**

		
Conf.1 (2.11%)	Conf.2 (17.77%)	Conf.3 (3.51%)
		
Conf.4 (3.69%)	Conf.5 (1.95%)	Conf.6 (0.80%)
		
Conf.7 (46.91%)	Conf.8 (17.91%)	Conf.9 (1.84%)
		
Conf.10 (3.51%)		

(4*R*, 6*S*, 8*R*)-**4**

		
Conf.1 (2.18%)	Conf.2 (0.01%)	Conf.3 (18.42%)

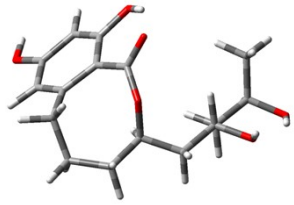
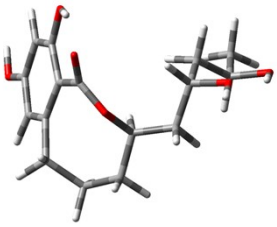
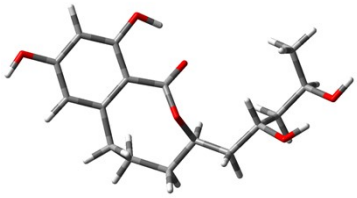
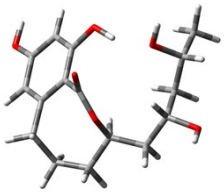
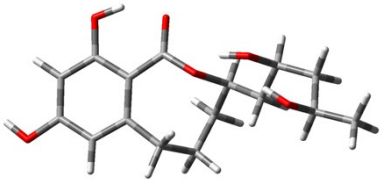
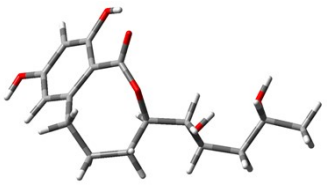
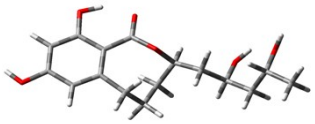
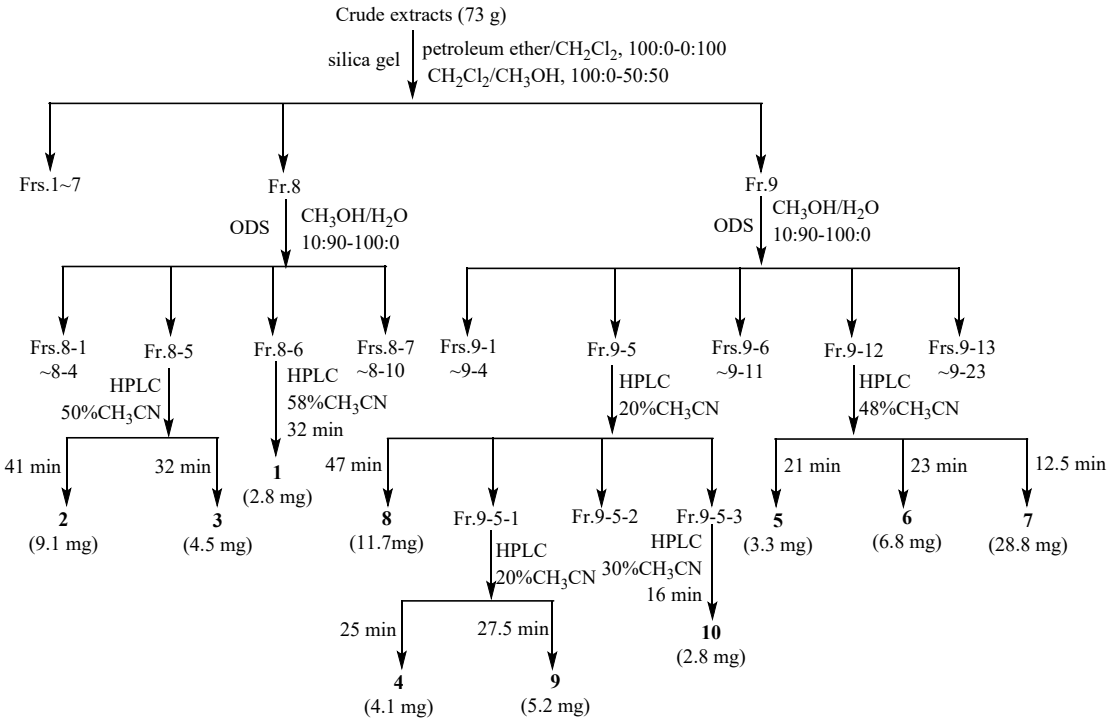
		
Conf.4 (3.64%)	Conf.5 (3.83%)	Conf.6 (2.03%)
		
Conf.7 (0.83%)	Conf.8 (48.60%)	Conf.9 (18.56%)
		
Conf.10 (1.90%)		

Figure S36. The optimized conformers and equilibrium populations of **4**.

Table S9. Specific data of the half-bandwidth and UV shifts for compounds **1**−**4**.

Compounds	Half-bandwidth (eV)	UV shift (nm)
1	0.3	–11
2	0.3	+6
3	0.23	+15
4	0.2	0



Scheme S1. The isolation process of compounds **1–10**.

Physicochemical data of known compounds 5–12.

LL-Z1640-2 (**5**): white powder, ECD (0.25 mg/mL, CH_3OH) $\lambda_{max}(\Delta\varepsilon)$ 239 (+22.1), 270 (−20.3) nm; ^{1}H NMR (500 MHz, DMSO-d_6) δ_H: 11.76 (1H, s, 16-OH), 6.74 (1H, d, J = 15.4 Hz, H-11), 6.43 (1H, d, J = 2.7 Hz, H-13), 6.39 (1H, d, J = 2.6 Hz, H-15), 6.15 – 6.24 (1H, m, H-4), 6.00 – 6.12 (1H, m, H-10), 5.21 (1H, m, H-5), 5.00 (1H, m, H-2), 4.38 (1H, s, H-7), 3.85 (1H, s, H-8), 3.78 (3H, s, H-19), 3.13 – 3.24 (1H, m, H-3a), 2.55 – 2.65 (1H, m, H-3b), 2.09 (2H, d, J = 7.0 Hz, H-9), 1.37 (3H, d, J = 6.0 Hz, H-1).^{13}C NMR (125 MHz, DMSO-d_6) δ_C: 20.0 (CH_3, C-1), 36.0(CH_2, C-9), 36.3 (CH_2, C-3), 55.5 (CH_3, C-19), 72.7 (CH, C-2), 73.7 (CH, C-8), 81.7 (CH, C-7), 100.2 (CH, C-15), 104.7 (qC, C-17), 106.0 (CH, C-13), 126.7 (CH, C-10), 130.9 (CH, C-11), 132.4 (CH, C-5), 142.3 (qC, C-12), 143.9 (CH, C-4), 163.4 (qC, C-14), 163.6 (qC, C-16), 170.4 (qC, C-18), 200.9 (qC, C-6).

Deoxy-aigialomycin C (**6**): white powder; ^{1}H NMR (500 MHz, $CDCl_3$) δ_H: 11.81 (1H, s, 16-OH), 7.11 (1H, dt, J = 15.9, 1.9 Hz, H-11), 6.53 (1H, d, J = 2.6 Hz, H-13), 6.38 (1H, d, J = 2.6 Hz, H-15), 6.13 (1H, dt, J = 16.0, 5.2 Hz, H-4), 5.94 (1H, ddd, J = 15.1, 9.2, 5.6 Hz, H-10), 5.53 – 5.60 (1H, m, H-5), 5.48 – 5.53 (1H, m, H-2), 3.88 (1H, t, J = 8.6 Hz, H-6), 3.82 (3H, s, H-19), 3.48 – 3.56 (1H, m, H-7), 2.56 (2H, m, H-8), 2.41 (1H, m, H-3a), 2.00 – 2.12 (2H, m, H-9), 1.63 (1H, ddd, J = 14.6, 7.2, 3.9 Hz, H-3b), 1.40 (3H, d, J = 6.5 Hz, H-1).^{13}C NMR (125 MHz, $CDCl_3$) δ_C: 18.7 (CH_3, C-1), 27.2 (CH_2, C-8), 31.0 (CH_2, C-9), 37.5 (CH_2, C-3), 55.5 (CH_3, C-19), 71.6 (CH, C-2), 73.2 (CH, C-6), 77.2 (CH, C-7), 100.0 (CH, C-15), 104.2 (qC, C-17), 106.9 (CH, C-13), 128.8 (CH, C-4), 130.1 (CH, C-10), 132.4 (CH, C-5), 134.3 (CH, C-11), 142.8 (qC, C-12), 164.0 (qC, C-14), 165.4 (qC, C-16), 171.3 (qC, C-18).

Zeaenol (**7**): white powder; ^{1}H NMR (500 MHz, DMSO-d_6) δ_H: 11.29 (1H, s, 16-OH), 6.85 (1H, d, J = 15.5 Hz, H-11), 6.45 (1H, d, J = 2.5 Hz, H-13), 6.37 (1H, d, J = 2.6 Hz, H-15), 6.08 (1H, m, H-4), 5.79 (1H, m, H-10), 5.56 (1H, dd, J = 15.5, 7.4 Hz, H-5), 5.15 (1H, m, H-2), 4.49 – 4.78 (1H, m, H-6), 3.88 (1H, t, J = 7.7 Hz, H-8), 3.77 (3H, s, H-19), 3.52 (1H, d, J = 7.5 Hz, H-7), 2.53 (2H, m, H-3), 2.45 (1H, dd, J = 7.3, 3.5 Hz, H-9a), 2.37 (1H, m, H-9b), 1.37 (3H, d, J = 6.3 Hz, H-1). ^{13}C NMR (125 MHz,

DMSO-d_6) δ_C: 19.3 (CH_3, C-1), 35.5 (CH_2, C-9), 36.9 (CH_2, C-3), 55.4 (CH_3, C-19), 72.2 (CH, C-2), 72.4 (CH, C-6), 73.5 (CH, C-8), 78.1 (CH, C-7), 100.0 (CH, C-15), 104.9 (qC, C-17), 106.5 (CH, C-13), 126.6 (CH, C-4), 130.5 (CH, C-10), 132.4 (CH, C-5), 132.8 (CH, C-11), 141.5 (qC, C-12) , 162.0 (qC, C-14), 162.8 (qC, C-16), 169.9 (qC, C-18).

8-Hydroxy-6-methoxy-3-methylisocoumarin (**8**): yellow oil; ^{1}H NMR (500 MHz, CD_3OD) δ_H: 6.45 (1H, d, J = 2.1 Hz, H-8), 6.31 (1H, d, J = 2.1 Hz, H-6), 6.21 (1H, s, H-4), 3.89 (3H, s, H-11), 2.19 (3H, s, H-12).^{13}C NMR (125 MHz, CD_3OD) δ_C: 19.2 (CH_3, C-12), 56.3 (CH_3, C-11), 99.5 (CH, C-8), 101.8 (CH, C-6), 103.7 (qC, C-10), 104.9 (CH, C-4), 144.0 (qC, C-5), 156.2 (qC, C-3), 162.3 (qC, C-9), 165.1 (qC, C-7), 166.3 (qC, C-1).

2-Methyl-5-carboxymethyl-7-hydroxychromone (**9**): white powder; ^{1}H NMR (500 MHz, DMSO-d_6) δ_H: 11.98 (1H, s, 12-OH), 10.64 (1H, s, 7-OH), 6.71 (1H, d, J = 2.3 Hz, H-8), 6.65 (1H, d, J = 2.3 Hz, H-6), 5.97 (1H, s, H-3), 4.00 (2H, s, H-11), 2.28 (3H, s, H-13).^{13}C NMR (125 MHz, DMSO-d_6) δ_C: 19.4 (CH_3, C-13), 40.2 (CH_2, C-11), 101.5 (CH, C-8), 110.5 (CH, C-6), 114.3 (qC, C-10), 117.9 (CH, C-3), 138.0 (qC, C-5), 158.9 (qC, C-9), 160.9 (qC, C-7), 164.2 (qC, C-2), 172.1 (qC, C-12), 177.9 (qC, C-4).

2-Methyl-5-carboxymethyl-7-hydroxychromanone (**10**): white powder; ^{1}H NMR (500 MHz, DMSO-d_6) δ_H: 11.95 (1H, s, 12-OH), 10.48 (1H, s, 7-OH), 6.29 (1H, d, J = 2.3 Hz, H-8), 6.24 (1H, d, J = 2.3 Hz, H-6), 4.51 (1H, m, H-2), 3.79 (2H, d, J = 4.4 Hz, H-11), 2.56 (2H, dd, J = 16.6, 12.0 Hz, H-3), 1.36 (3H, d, J = 6.2 Hz, H-13).^{13}C NMR (125 MHz, DMSO-d_6) δ_C: 20.5 (CH_3, C-13), 40.6 (CH_2, C-11), 44.7 (CH_2, C-3), 73.4 (CH, C-2), 101.8 (CH, C-8), 112.0 (qC, C-10), 114.2 (CH, C-6), 139.5(qC, C-5), 162.8 (qC, C-9), 164.1 (qC, C-7), 172.0 (qC, C-12), 191.3(qC, C-4).

The ITS sequence of *Curvularia lunata* GXIMD 02512

CTGTACGCGGCTGTGCTCTCGGGCCAGTTTTGCGGAGGCTGAATTATTTATTACCCTT
GTCTTTTGCGCACTTGTTGTTTCCTGGGCGGGTTCGCCCGCCACCAGGACCACATCATAAA
CCTTTTTTATGCAGTTGCAATCAGCGTCAGTATAACAAATGTAAATCATTTACAACTTTCA
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GAATTGCAGAATTCAGTGAATCATCGAATCTTTGAACGCACATTGCGCCCTTTGGTATTCC
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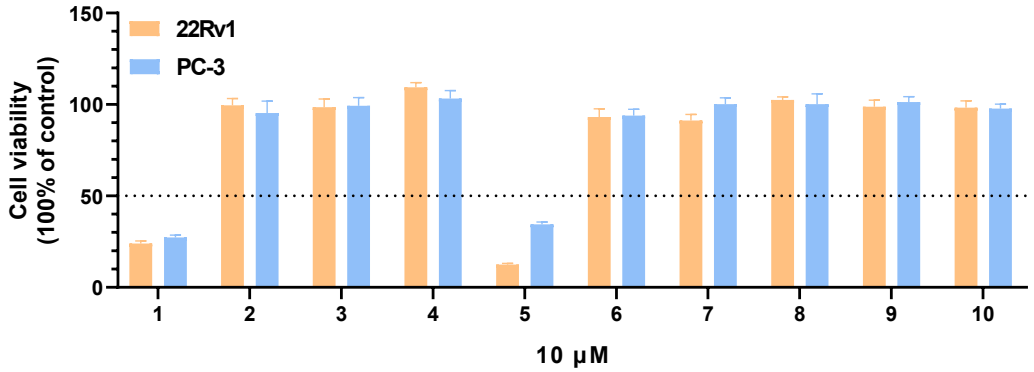

Figure S37. The cell viability of 22RV1 and PC-3 cell lines by treating with compounds **1**–**10** at 10 μM after 72 h

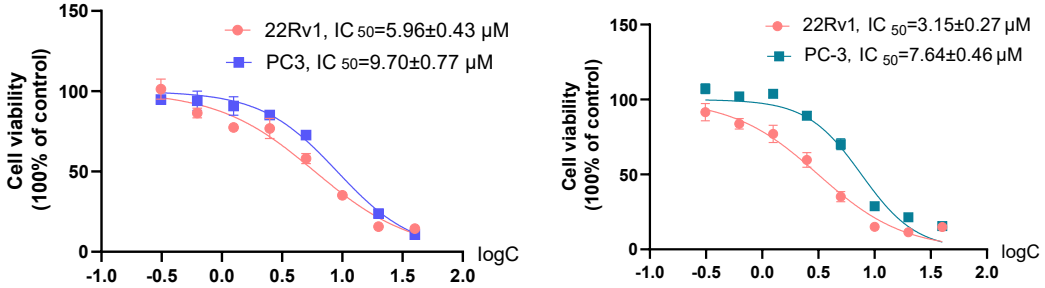

Figure S38. Cytotoxicity against 22RV1 and PC-3 cell lines of **1** (left) and **5** (right)

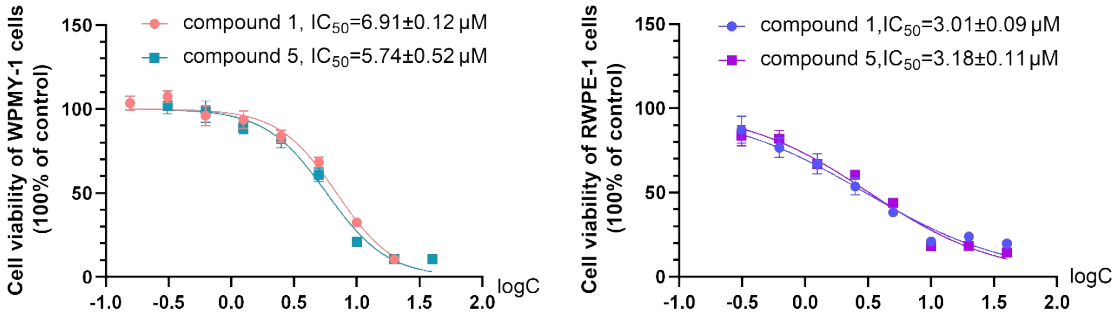

Figure S39. Cytotoxicity of compounds **1** and **5** towards two normal prostate cancer cells, WPMY-1 (left) and RWPE-1 (right).

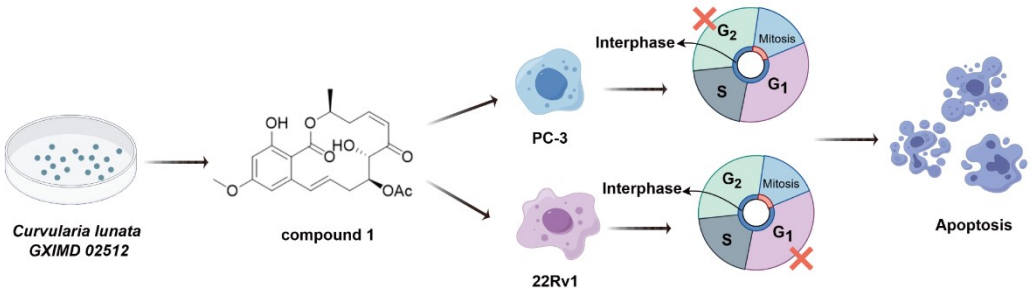

Figure S40. the primary anti-PC mechanism of compound **1**.