Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

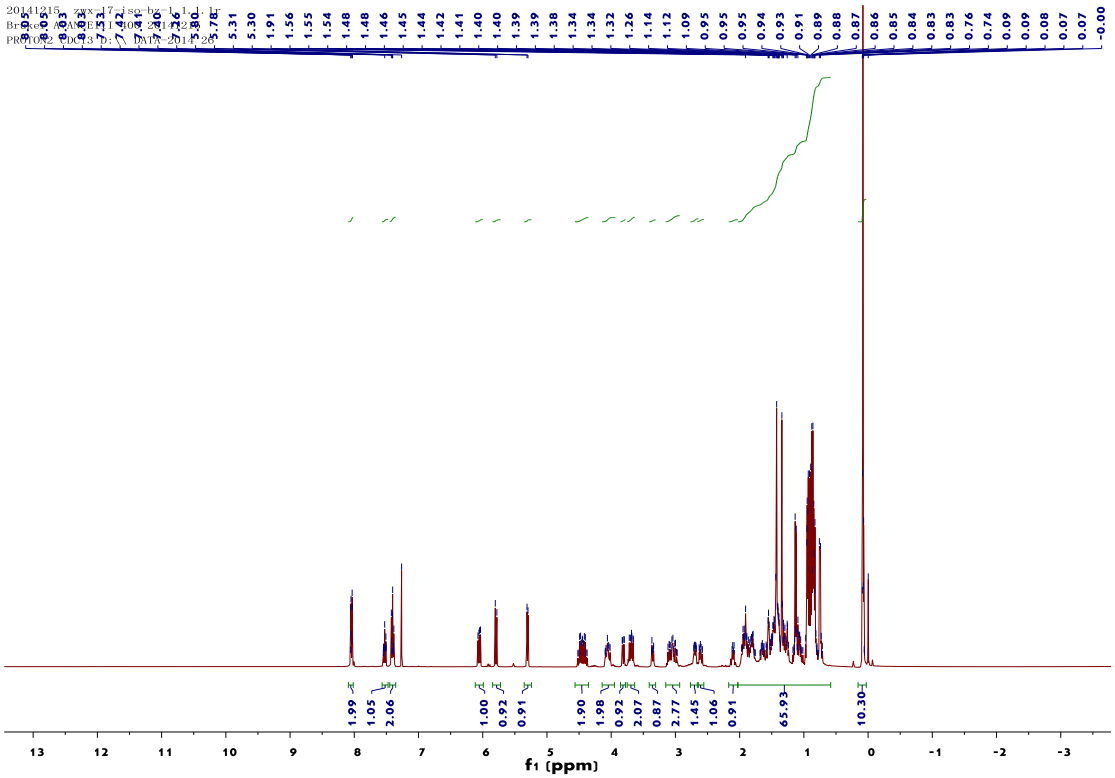
Supplementary information

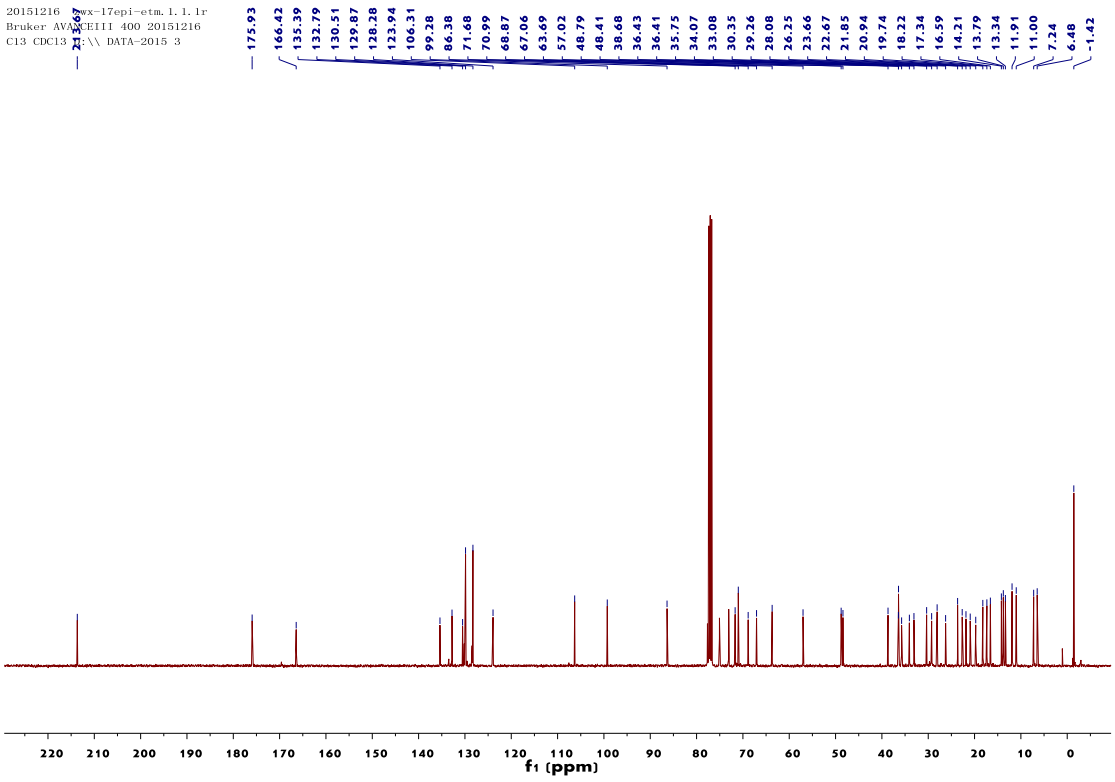
1.^{1}H NMR and ^{13}C NMR of 2,3,4,5,8,9,10

2. Crystal Data of 9

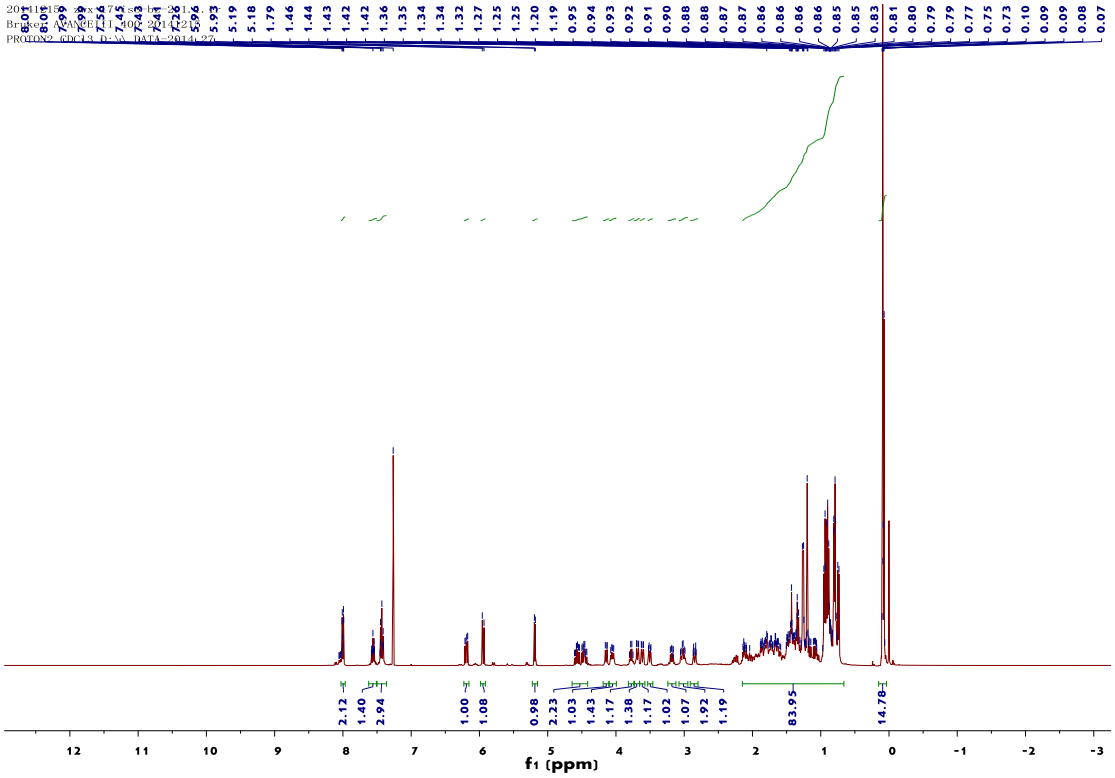
3. Dose-response curves

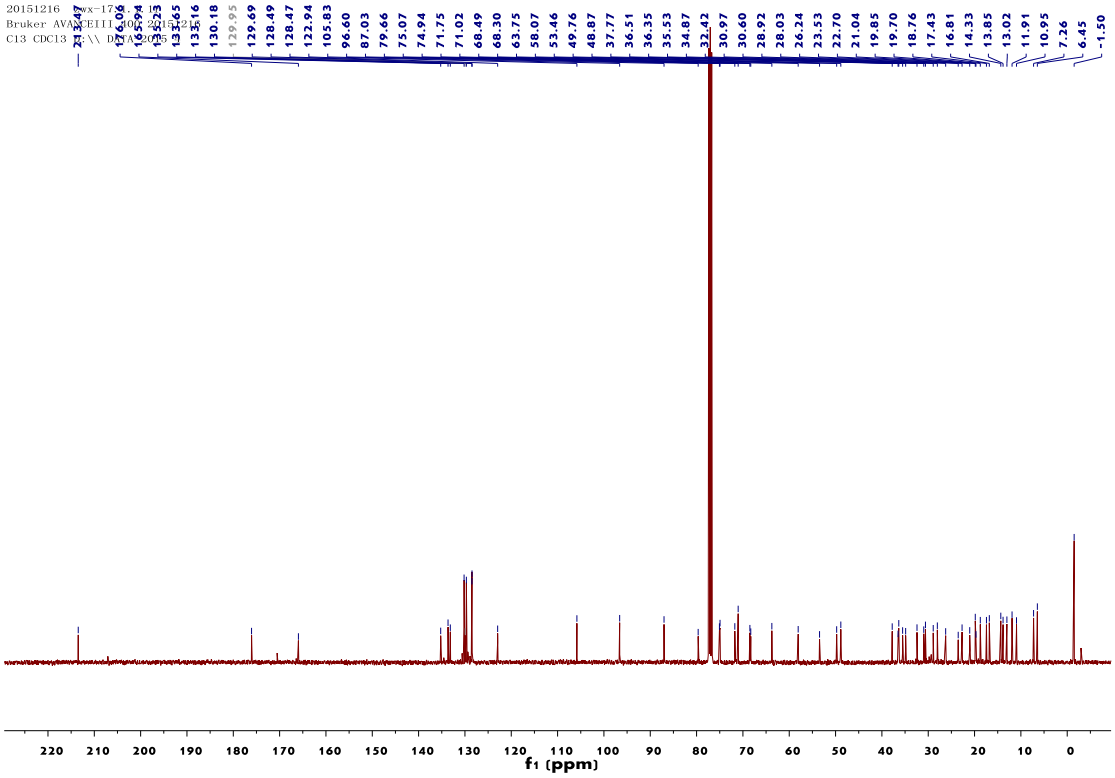
*intermediate **8***



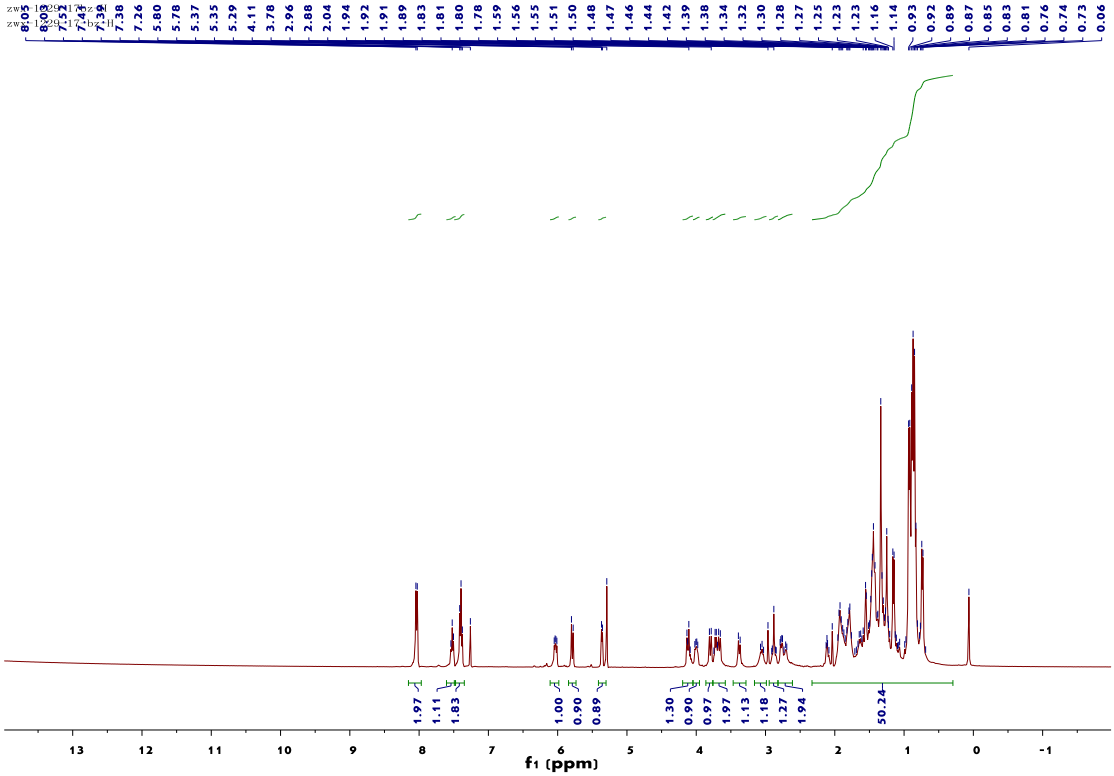


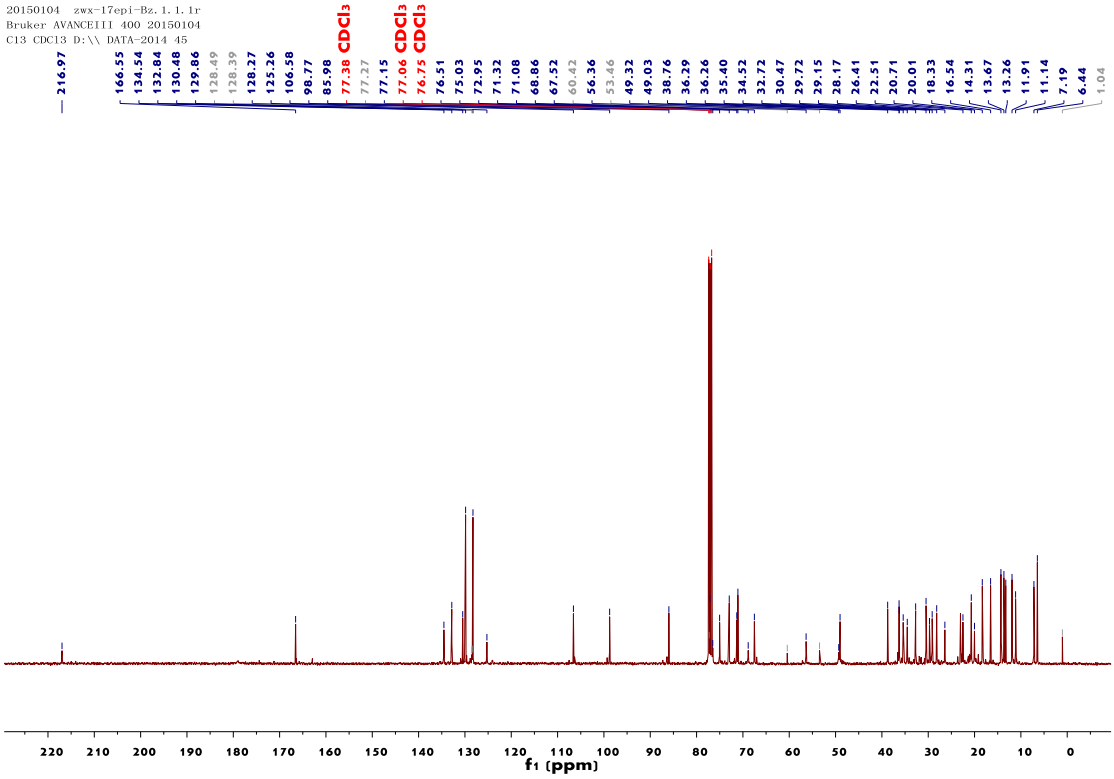
intermediate 9



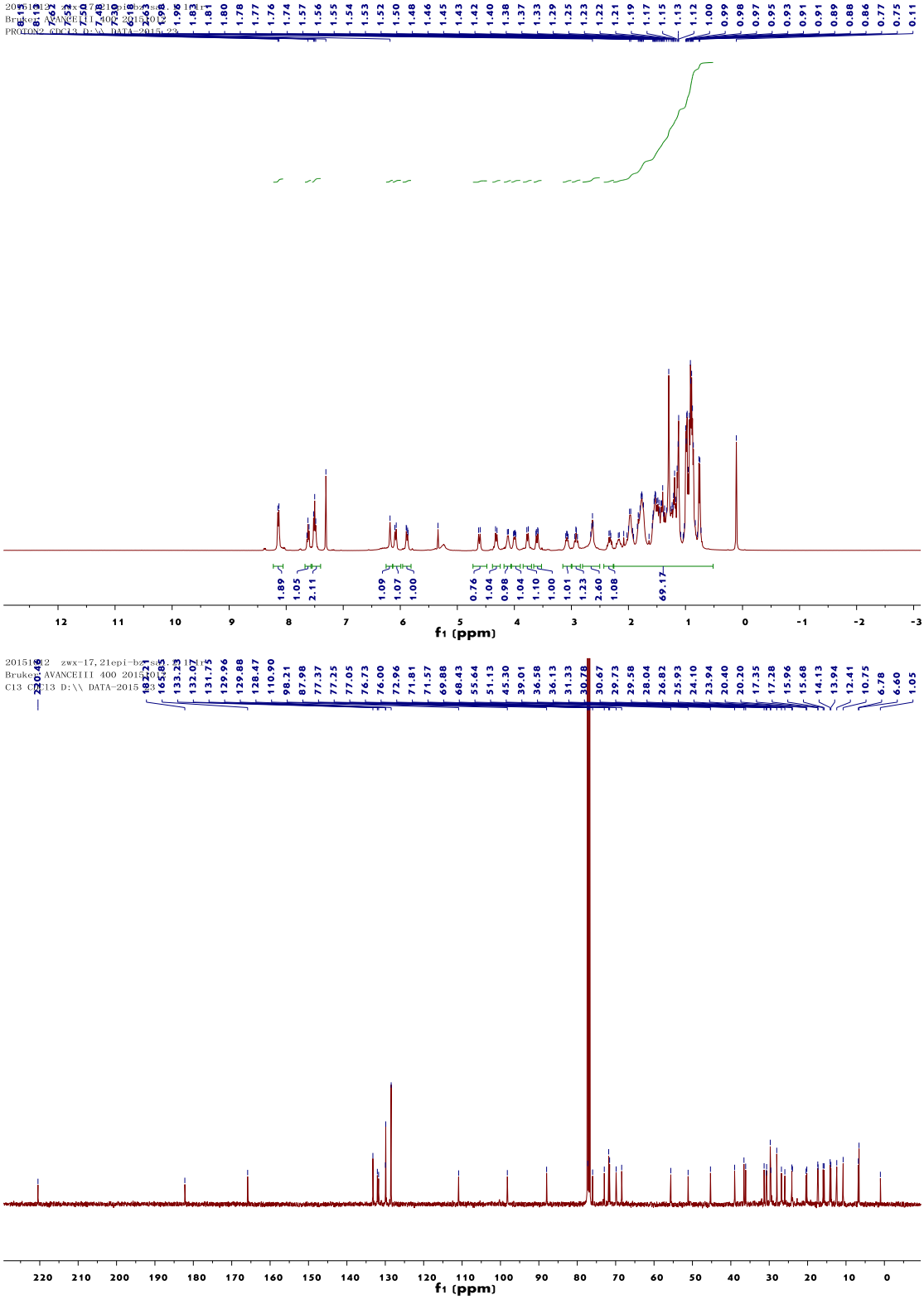


17-epi-20-O-Bz-salinomycin sodium salt ***(4)***

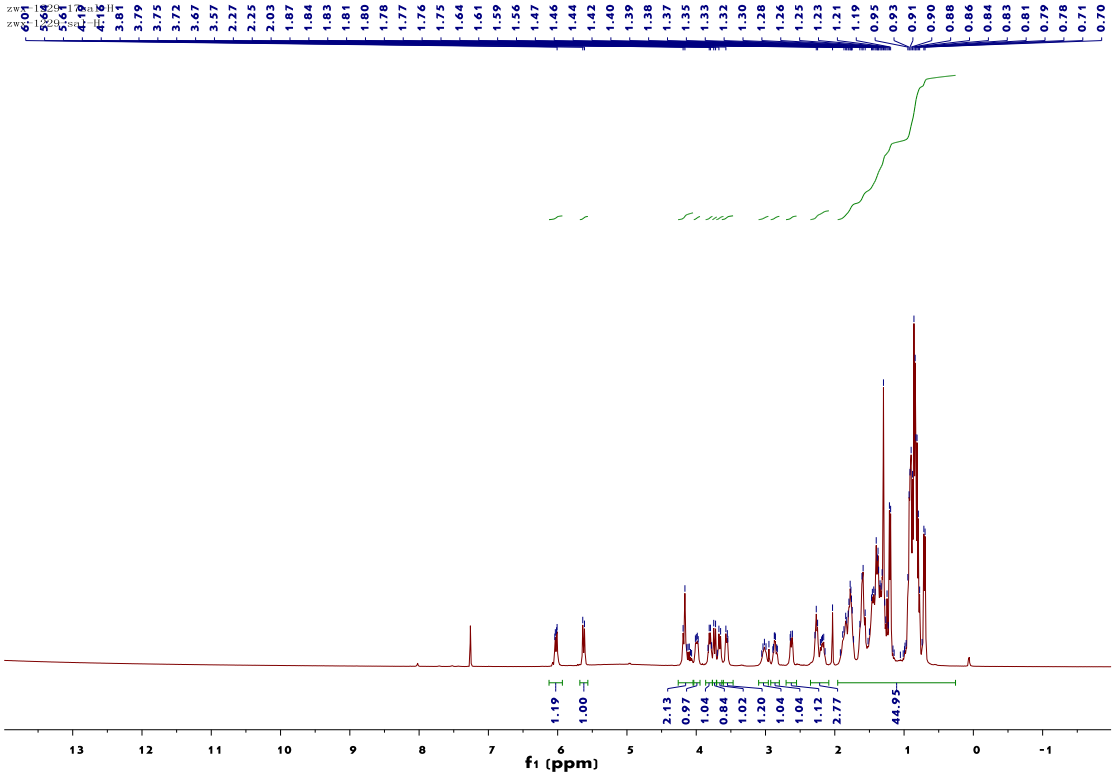


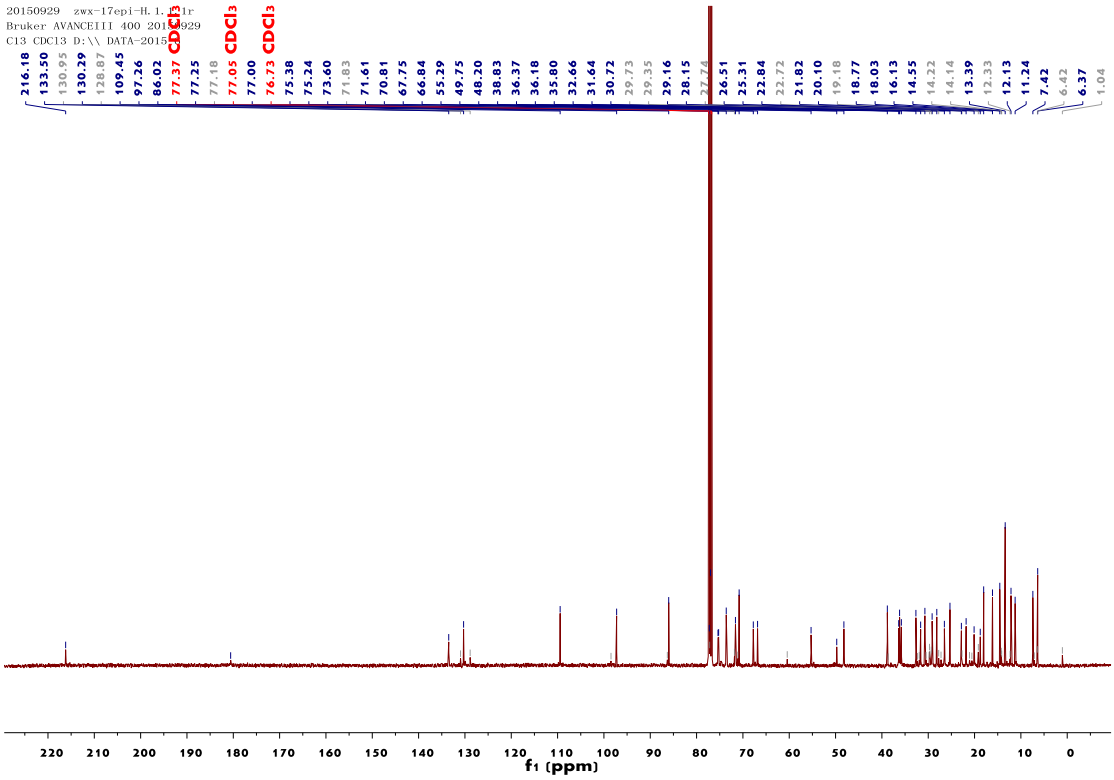


17,21-di-epi-20-O-Bz-salinomycin sodium salt (***5***)

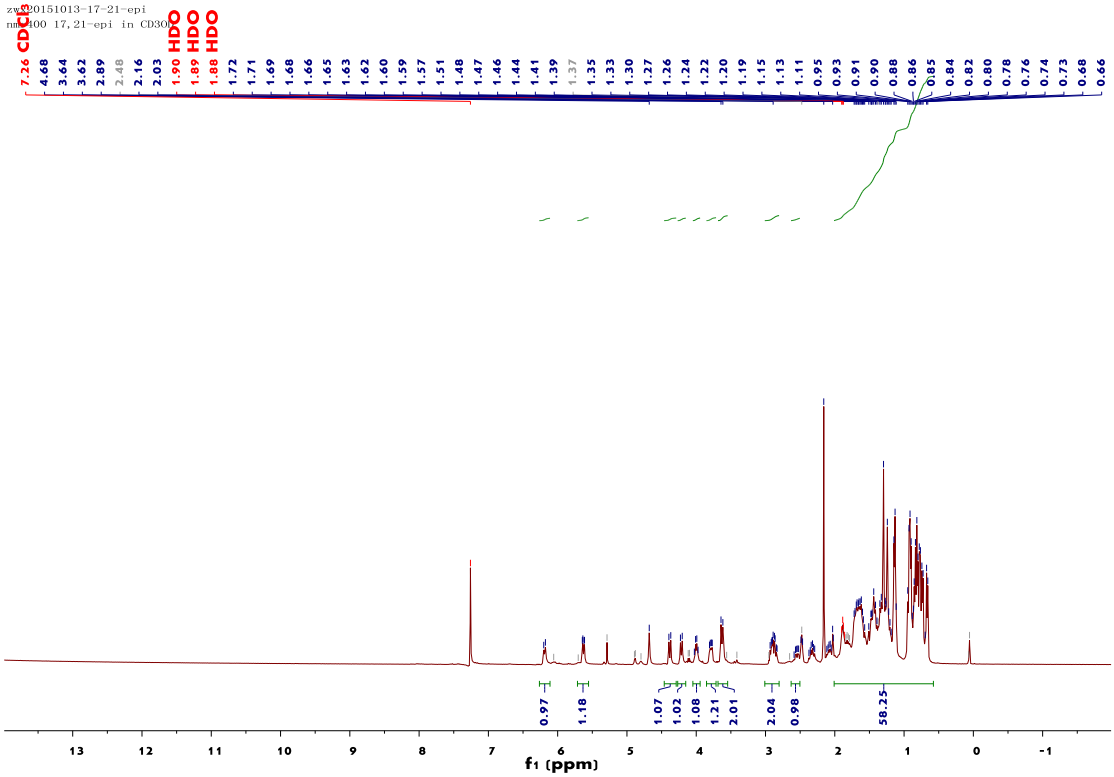


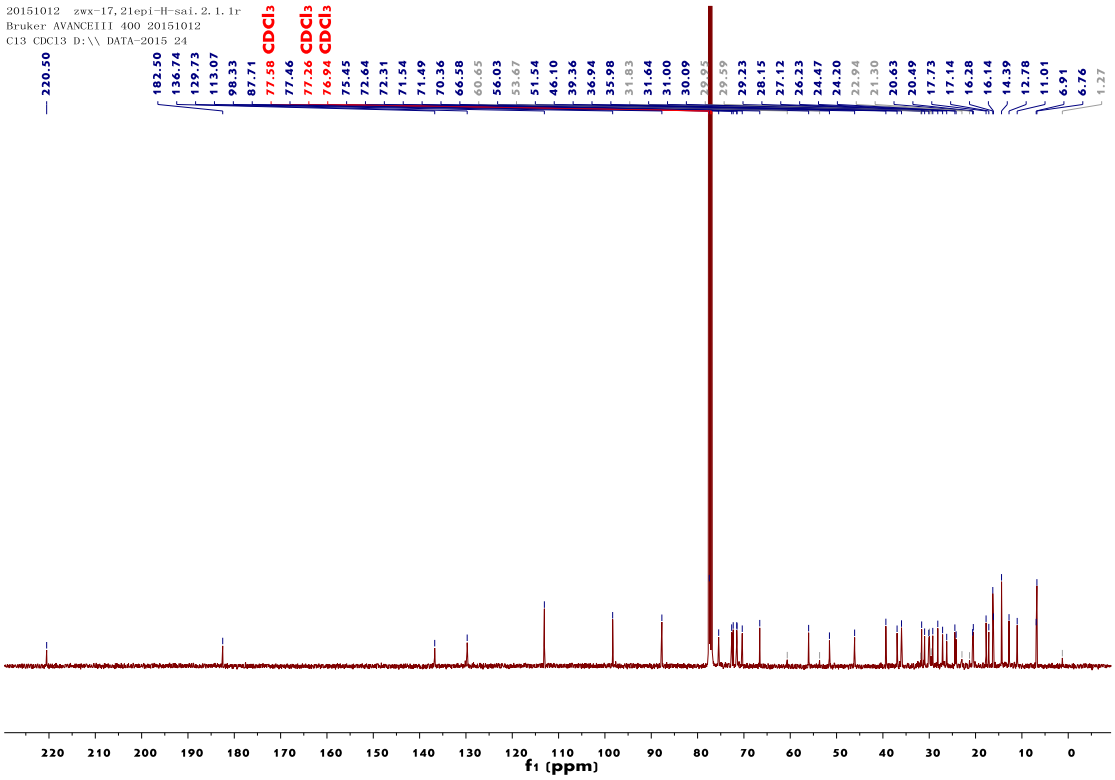
*17-epi-salinomycin sodium salt (**2**)*





*17, 21-di-epi-salinomycin sodium salt (**3**)*





Crystal data and structure refinement details of compound 9:

A suitable crystal was selected and analyzed on a Xcalibur, Atlas, Gemini ultra diffractometer. The crystal was kept at 293(2) K during data collection. Using Olex2, the structure was solved with the Superflip structure solution program using Charge Flipping and refined with the ShelXL refinement package using Least Squares minimisation.

Crystal Data for $C_{55}H_{88}O_{11}Si$ (*M* =953.34 g/mol): monoclinic, space group $P2_1$ (no. 4), a=12.1784(3) Å b=10.4550(2) Å c=22.4818(4) Å α=90.0000° β=99.8798(18)° γ=90.0000° V=2820.05(10) Å3 Z=2, μ(CuKα) = 0.803 mm^{-1}, *Dcalc* = 1.123 g/cm^3, 41478 reflections measured (7.368° ≤ 2^{Θ} ≤ 134.002°), 10003 unique (R_{int} = 0.0390, R_{sigma} = 0.0221) which were used in all calculations. The final R_1 was 0.0447 (I > 2σ(I)) and wR_2 was 0.1313 (all data).

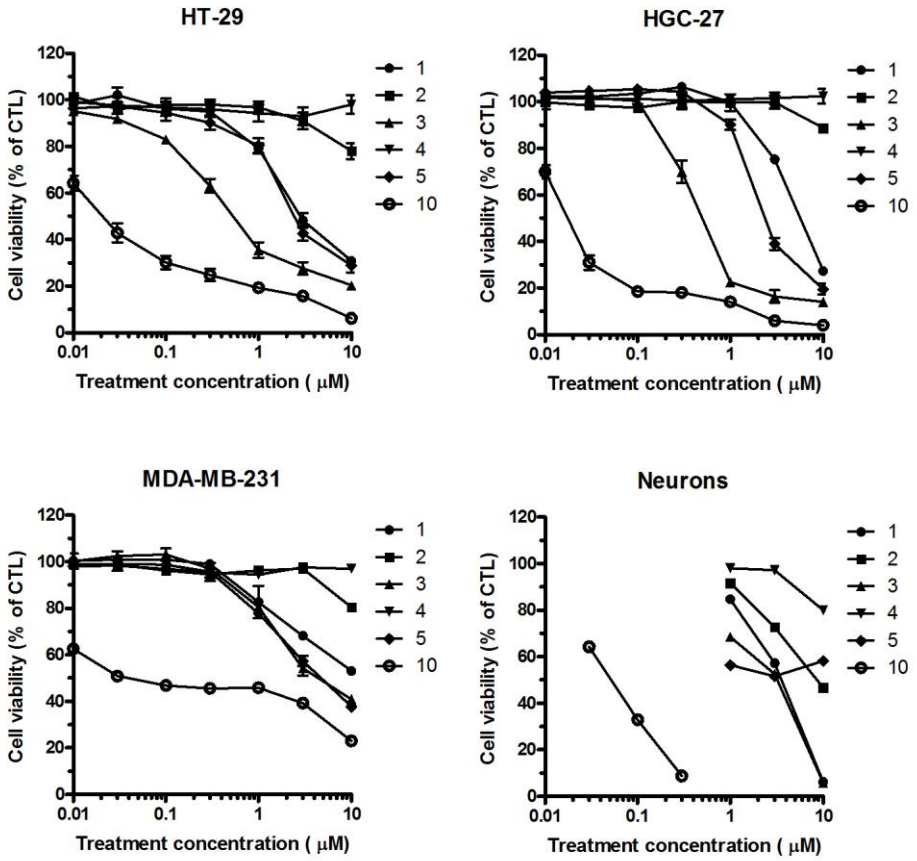
Atomic parameters:

Atom	x/a	y/b	z/c	U [Å^2]
O1	-0.7429(2)	-0.4023(2)	-0.58095(9)	
O7	-0.8458(2)	-0.5181(3)	-0.66126(9)	
O41	-0.5484(2)	-0.5023(2)	-0.97813(9)	
O38	-0.7989(2)	-0.3382(3)	-0.46195(9)	
O18	-0.6722(2)	-0.6807(2)	-0.86992(10)	
H18	-0.60440	-0.68960	-0.86480	0.1080
O28	-0.7669(2)	0.0078(2)	-0.71355(10)	
O24	-0.8571(2)	-0.2301(2)	-0.61603(10)	
O20	-0.6904(3)	-0.4000(3)	-0.79542(11)	
O49	-0.3543(3)	-0.4861(3)	-0.86019(11)	
C2	-0.8111(4)	-0.5119(4)	-0.59784(14)	
O51	-0.4361(2)	-0.6776(3)	-0.86476(12)	
O40	-0.9389(3)	-0.2849(3)	-0.41476(12)	
C6	-0.7921(3)	-0.2879(3)	-0.56473(14)	
C5	-0.8704(3)	-0.3112(4)	-0.51975(15)	
H5	-0.91470	-0.23420	-0.51620	0.0920
C11	-0.7611(3)	-0.5298(3)	-0.69843(13)	
H11	-0.71740	-0.45060	-0.69510	0.0780
C46	-0.6173(3)	-0.6130(3)	-0.99444(12)	
H46	-0.58030	-0.68710	-0.97300	0.0730
C39	-0.8452(4)	-0.3221(3)	-0.41287(15)	
C13	-0.7640(3)	-0.4780(3)	-0.80978(14)	
C12	-0.8234(3)	-0.5429(3)	-0.76432(13)	
H12	-0.82600	-0.63440	-0.77400	0.0780
C15	-0.7025(3)	-0.5641(3)	-0.90184(12)	
H15	-0.64000	-0.50420	-0.89260	0.0750
C16	-0.7248(3)	-0.5887(3)	-0.97073(13)	
H16	-0.75830	-0.51090	-0.99030	0.0760
C42	-0.4391(3)	-0.5073(4)	-0.99249(15)	
H42	-0.40670	-0.42190	-0.98470	0.0880
C32	-0.8695(3)	0.0122(3)	-0.81580(17)	

C29	-0.8191(3)	-0.1086(3)	-0.69893(15)	
H29	-0.77610	-0.18080	-0.71070	0.0830
C60	-0.7678(4)	-0.3542(3)	-0.35677(15)	
C35	-0.9293(3)	0.1234(3)	-0.80229(19)	
H35A	-0.91430	0.13890	-0.75960	0.1160
H35B	-1.00780	0.10980	-0.81510	0.1160
H35C	-0.90590	0.19590	-0.82310	0.1160
C45	-0.6303(3)	-0.6389(3)	-1.06252(13)	
H45	-0.66820	-0.72140	-1.07070	0.0840
C47	-0.3630(3)	-0.6011(4)	-0.95101(16)	
H47	-0.37950	-0.68810	-0.96620	0.0940
C48	-0.3888(3)	-0.5934(4)	-0.88814(16)	
C14	-0.8014(3)	-0.5089(4)	-0.87696(13)	
H14	-0.86090	-0.57300	-0.88100	0.0820
C33	-0.7542(3)	0.0163(4)	-0.77588(15)	
H33	-0.72330	0.10120	-0.78130	0.0900
C27	-0.8092(4)	-0.1098(4)	-0.63073(16)	
C3	-0.9172(4)	-0.5094(5)	-0.57390(17)	
H3	-0.96760	-0.57550	-0.58510	0.1210
C30	-0.9361(3)	-0.1171(4)	-0.73425(17)	
H30A	-0.98130	-0.04880	-0.72210	0.0940
H30B	-0.96940	-0.19810	-0.72600	0.0940
C4	-0.9452(4)	-0.4209(5)	-0.53812(17)	
H4	-1.01260	-0.42700	-0.52420	0.1130
C21	-0.9456(3)	-0.4951(4)	-0.77461(16)	
H21A	-0.94960	-0.41790	-0.75110	0.0970
H21B	-0.96790	-0.47290	-0.81690	0.0970
C31	-0.9329(3)	-0.1064(4)	-0.80153(16)	
H31A	-0.89740	-0.18190	-0.81460	0.0900
H31B	-1.00850	-0.10270	-0.82380	0.0900
C25	-0.6960(4)	-0.1961(4)	-0.54315(16)	
H25A	-0.71210	-0.14250	-0.51050	0.1000
H25B	-0.62720	-0.24230	-0.52970	0.1000
C17	-0.8083(3)	-0.6970(4)	-0.98692(15)	
H17A	-0.82640	-0.70490	-1.03000	0.1140
H17B	-0.87480	-0.67860	-0.97090	0.1140
H17C	-0.77630	-0.77560	-0.97000	0.1140
C10	-0.6825(4)	-0.6413(4)	-0.67906(16)	
H10	-0.72490	-0.72060	-0.68810	0.1050
C26	-0.6888(4)	-0.1174(4)	-0.59879(17)	
H26A	-0.64240	-0.15910	-0.62400	0.1050
H26B	-0.65910	-0.03290	-0.58790	0.1050

C64	-0.7314(8)	-0.3668(6)	-0.24852(19)	
H64	-0.75480	-0.35630	-0.21160	0.1560
C43	-0.4436(4)	-0.5337(5)	-1.05920(16)	
H43A	-0.36870	-0.54730	-1.06710	0.1050
H43B	-0.47470	-0.46000	-1.08240	0.1050
C65	-0.8045(5)	-0.3403(4)	-0.30196(16)	
H65	-0.87700	-0.31380	-0.30090	0.1240
C50	-0.3734(4)	-0.4725(5)	-0.79751(18)	
H50A	-0.35490	-0.55170	-0.77570	0.1170
H50B	-0.45130	-0.45350	-0.79720	0.1170
C44	-0.5146(4)	-0.6511(4)	-1.07912(15)	
H44A	-0.52150	-0.66140	-1.12250	0.1010
H44B	-0.47820	-0.72660	-1.06000	0.1010
C54	-0.3023(4)	-0.3669(5)	-0.76795(18)	
H54A	-0.32720	-0.28750	-0.78820	0.1130
H54B	-0.22640	-0.38170	-0.77410	0.1130
C8	-0.7377(6)	-0.6269(5)	-0.57594(18)	
H8	-0.78340	-0.70390	-0.58510	0.1330
C34	-0.6715(3)	-0.0790(5)	-0.79158(17)	
H34A	-0.60920	-0.08410	-0.75910	0.1300
H34B	-0.64620	-0.05240	-0.82780	0.1300
H34C	-0.70630	-0.16140	-0.79780	0.1300
C61	-0.6602(4)	-0.3964(4)	-0.35704(18)	
H61	-0.63480	-0.40600	-0.39350	0.1080
C59	-0.7002(4)	-0.5376(5)	-1.10077(15)	
H59A	-0.77550	-0.54120	-1.09350	0.1370
H59B	-0.69920	-0.55350	-1.14270	0.1370
H59C	-0.66970	-0.45440	-1.09010	0.1370
C62	-0.5907(5)	-0.4242(5)	-0.3038(2)	
H62	-0.51910	-0.45450	-0.30440	0.1290
C36	-0.8583(4)	0.0208(5)	-0.88194(18)	
H36A	-0.81190	0.09390	-0.88710	0.1070
H36B	-0.81980	-0.05510	-0.89230	0.1070
C23	-0.5855(5)	-0.6443(6)	-0.7134(2)	
H23A	-0.61280	-0.66280	-0.75520	0.1700
H23B	-0.53360	-0.70930	-0.69670	0.1700
H23C	-0.54890	-0.56270	-0.71010	0.1700
C57	-0.2656(5)	-0.4965(5)	-0.6443(2)	
H57A	-0.32460	-0.55710	-0.65610	0.1610
H57B	-0.25680	-0.48190	-0.60160	0.1610
H57C	-0.19740	-0.52960	-0.65410	0.1610
C19	-0.8465(5)	-0.3870(5)	-0.91012(17)	

H19A	-0.90250	-0.34990	-0.89020	0.1570
H19B	-0.87860	-0.40760	-0.95100	0.1570
H19C	-0.78670	-0.32710	-0.91000	0.1570
C37	-0.8735(6)	-0.0005(5)	-0.6075(2)	
H37A	-0.95190	-0.01240	-0.62110	0.1730
H37B	-0.85060	0.07940	-0.62250	0.1730
H37C	-0.85840	0.00030	-0.56410	0.1730
C9	-0.6420(5)	-0.6359(5)	-0.61069(18)	
H9A	-0.59870	-0.71200	-0.59810	0.1330
H9B	-0.59370	-0.56230	-0.60120	0.1330
C56	-0.4383(4)	-0.2849(6)	-0.6718(3)	
H56A	-0.46040	-0.21350	-0.69800	0.1650
H56B	-0.43290	-0.25840	-0.63050	0.1650
H56C	-0.49270	-0.35190	-0.68030	0.1650
C58	-0.1914(5)	-0.2257(5)	-0.6576(2)	
H58A	-0.11940	-0.26190	-0.65900	0.1620
H58B	-0.19590	-0.20190	-0.61690	0.1620
H58C	-0.20230	-0.15140	-0.68310	0.1620
C52	-0.2397(4)	-0.5729(6)	-0.9525(2)	
H52A	-0.22920	-0.56650	-0.99420	0.1240
H52B	-0.22010	-0.49100	-0.93340	0.1240
C63	-0.6261(7)	-0.4078(6)	-0.2503(2)	
H63	-0.57780	-0.42480	-0.21450	0.1560
C22	-1.0271(4)	-0.5922(6)	-0.7575(2)	
H22A	-1.02460	-0.66840	-0.78110	0.1580
H22B	-1.10100	-0.55720	-0.76530	0.1580
H22C	-1.00720	-0.61250	-0.71540	0.1580
Si55	-0.30047(9)	-0.34503(10)	-0.68460(4)	
C1	-0.9659(4)	0.0330(7)	-0.9257(2)	
H1A	-0.95020	0.04520	-0.96570	0.1930
H1B	-1.00700	0.10500	-0.91470	0.1930
H1C	-1.00920	-0.04340	-0.92460	0.1930
C1AA	-0.1630(5)	-0.6733(8)	-0.9214(3)	
H1AA	-0.17880	-0.75370	-0.94170	0.2130
H1AB	-0.17390	-0.68120	-0.88020	0.2130
H1AC	-0.08720	-0.64940	-0.92220	0.2130
C0AA	-0.6957(8)	-0.6252(6)	-0.5069(2)	
H0AA	-0.65460	-0.54790	-0.49600	0.2360
H0AB	-0.64810	-0.69760	-0.49570	0.2360
H0AC	-0.75820	-0.62900	-0.48610	0.2360


HT-29
HGC-27
MDA-MB-231
Neurons
Cell viability (% of CTL)
Treatment concentration (μM)
0
20
40
60
80
100
120
0.01
0.1
1
10
1
2
3
4
5
10