Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information of

New dimeric chromanone derivatives from the mutant strains of *Penicillium oxalicum* and their bioactivities

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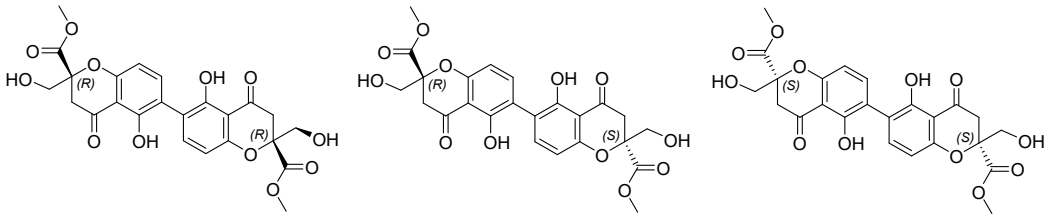


Figure S1. Structures of **1Aa**–**1Ac**

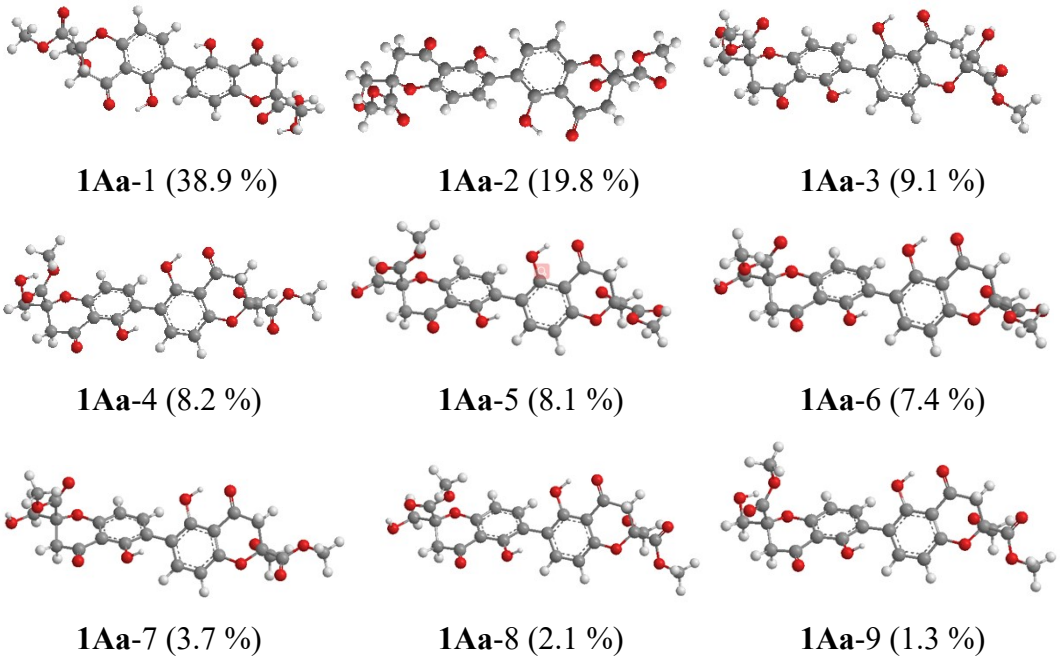


Figure S2. The optimized conformers and equilibrium populations of **1Aa**

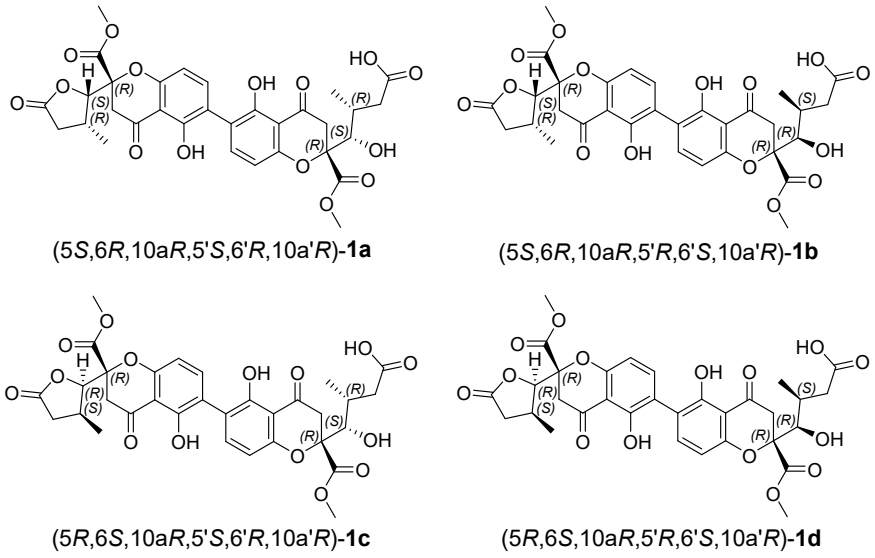


Figure S3. Structures of **1a**–**1d**

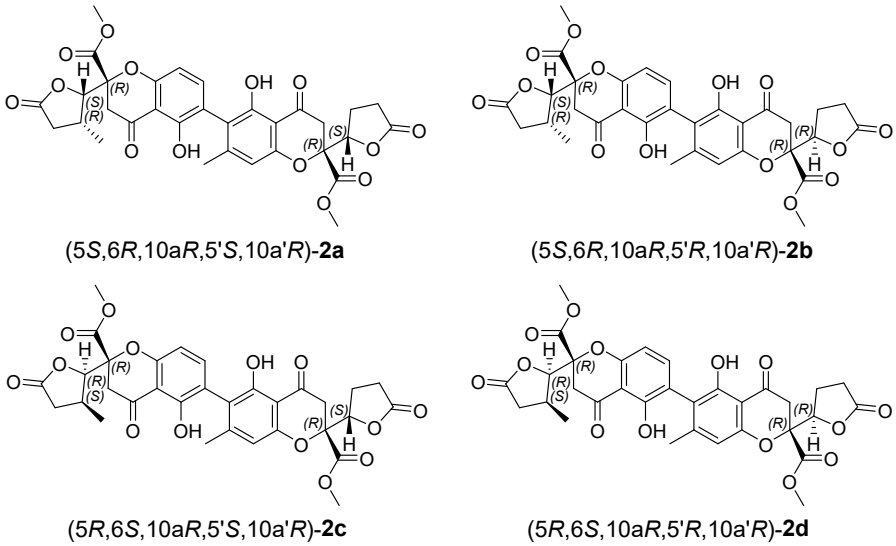


Figure S4. Structures of **2a**–**2d**

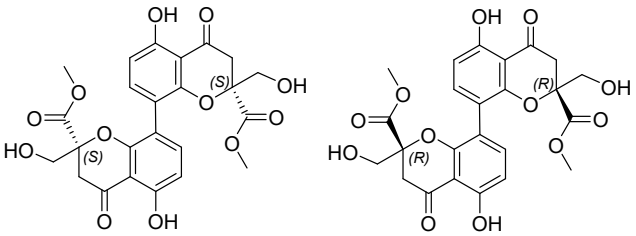


Figure S5. Structures of **3Aa** and **3Ab**

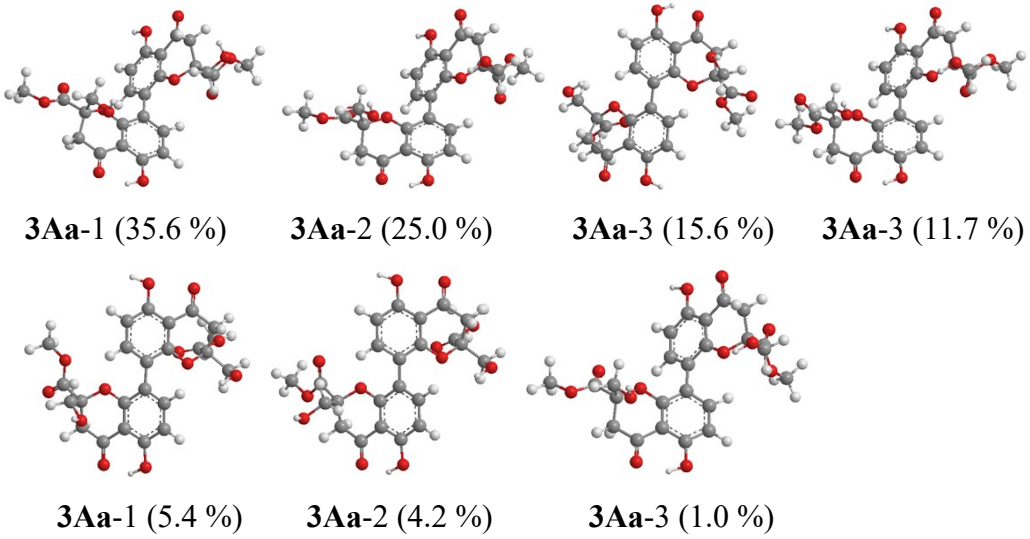
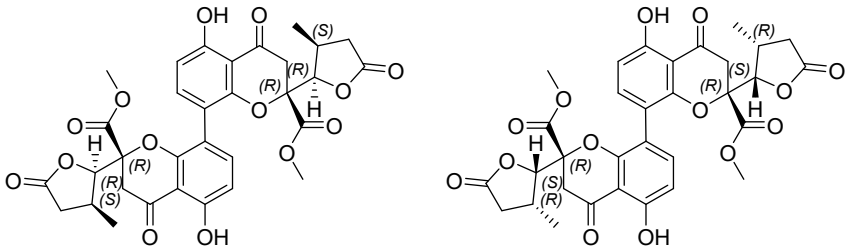


Figure S6. The optimized conformers and equilibrium populations of **3Aa**



(5*R*,6*S*,10a*R*,5'*R*,6'*S*,10a'*R*)-**3a** (5*S*,6*R*,10a*R*,5'*S*,6'*R*,10a'*R*)-**3b**

Figure S7. Structures of **3a** and **3b**

Table S1. Experimental ^{13}C NMR data of **1** and calculated ^{13}C NMR data of **1a**–**1d** in DMSO

no.	**1**	**1a**		**1b**		**1c**		**1d**	
	δ_{exp}	δ_C	$\Delta\delta_C$	δ_C	$\Delta\delta_C$	δ_C	$\Delta\delta_C$	δ_C	$\Delta\delta_C$
1	158.2	160.04	1.84	160.20	2.00	159.52	1.32	159.51	1.31
2	117.0	115.66	1.34	115.26	1.74	115.29	1.71	115.01	1.99
3	140.8	141.76	0.96	142.21	1.41	141.82	1.02	141.80	1.00
4	107.2	104.63	2.57	104.61	2.59	104.40	2.80	104.16	3.04
4a	158.3	158.02	0.28	158.96	0.66	158.59	0.29	158.60	0.30
5	81.8	82.91	1.11	82.36	0.56	81.48	0.32	82.18	0.38
6	32.6	37.57	4.97	37.47	4.87	37.32	4.72	36.50	3.90
7	36.7	36.07	0.63	36.04	0.66	36.12	0.58	35.76	0.94
8	175.5	174.89	0.61	175.18	0.32	175.46	0.04	175.61	0.11
9	195.3	193.08	2.22	192.77	2.53	193.44	1.86	193.55	1.75
9a	107.1	105.94	1.16	105.83	1.27	105.41	1.69	105.24	1.86
10	39.1	40.17	1.07	40.40	1.30	41.96	2.86	41.79	2.69
10a	83.8	88.12	4.32	87.91	4.11	86.47	2.67	86.25	2.45
11	14.7	13.58	1.12	13.47	1.23	12.94	1.76	12.29	2.41
12	169.1	172.56	3.46	170.35	1.25	170.95	1.85	172.51	3.41
13	53.6	51.99	1.61	52.09	1.51	52.50	1.10	52.22	1.38
1′	158.2	159.83	1.63	160.04	1.84	159.55	1.35	159.68	1.48
2′	115.5	114.84	0.66	115.60	0.10	114.92	0.58	115.31	0.19
3′	140.5	141.35	0.85	141.60	1.10	141.84	1.34	141.68	1.18
4′	107.2	104.31	2.89	104.88	2.32	104.31	2.89	104.64	2.56
4a′	159.2	158.90	0.30	158.78	0.42	158.75	0.45	158.54	0.66
5′	74.8	75.09	0.29	72.89	1.91	78.48	3.68	76.67	1.87
6′	30.8	31.37	0.57	33.68	2.88	31.58	0.78	33.82	3.02
7	39.8	36.88	2.92	35.80	4.00	35.66	4.14	38.01	1.79
8′	173.6	173.54	0.06	173.55	0.05	173.16	0.44	172.93	0.67
9′	197.2	194.05	3.15	195.43	1.77	193.34	3.86	194.82	2.38
9a′	106.9	105.94	0.96	105.76	1.14	105.68	1.22	105.54	1.36
10′	40.3	41.14	0.84	42.22	1.92	44.92	4.62	42.33	2.03
10a′	87.7	89.52	1.82	88.09	0.39	82.69	5.01	87.49	0.21
11′	13.9	12.36	1.54	12.49	1.41	12.53	1.37	11.36	2.54
12′	170.4	171.74	1.34	171.85	1.45	175.93	5.53	171.89	1.49
13′	53.0	51.95	1.05	52.03	0.97	52.79	0.21	52.11	0.89

Table S2. Experimental ^{1}H NMR data of **1** and calculated ^{1}H NMR data of **1a**–**1d** in DMSO

no.	**1**	**1a**		**1b**		**1c**		**1d**	
	δ_{exp}	δ_H	$\Delta\delta_H$	δ_H	$\Delta\delta_H$	δ_H	$\Delta\delta_H$	δ_H	$\Delta\delta_H$
3	7.49	7.75	-0.26	7.68	-0.19	7.66	-0.17	7.72	-0.23
4	6.68	6.51	0.17	6.46	0.22	6.43	0.25	6.46	0.22
5	4.94	4.52	0.42	4.67	0.27	4.68	0.26	4.75	0.19
6	2.98	2.99	-0.01	3.02	-0.04	2.96	0.02	2.96	0.02
7a	2.83	2.66	0.17	2.68	0.15	2.34	0.49	2.58	0.25
7b	2.33	2.30	0.03	2.30	0.03	2.57	-0.24	2.35	-0.02
10a	3.61	3.13	0.48	2.91	0.70	3.65	-0.04	3.58	0.03
10b	3.06	3.26	-0.20	3.39	-0.33	2.76	0.30	2.80	0.26
11	1.18	1.35	-0.17	1.39	-0.21	1.24	-0.06	1.27	-0.09
13	3.70	3.48	0.22	3.58	0.12	3.58	0.12	3.51	0.19
3'	7.47	7.72	-0.25	7.67	-0.20	7.64	-0.17	7.72	-0.25
4'	6.61	6.52	0.09	6.49	0.12	6.41	0.20	6.49	0.12
5'	3.89	3.96	-0.07	3.77	0.12	4.27	-0.38	3.70	0.19
6'	2.22	2.44	-0.22	2.04	0.18	2.58	-0.36	2.17	0.05
7'a	2.41	2.69	-0.28	2.89	-0.48	2.78	-0.37	2.63	-0.22
7'b	2.19	2.35	-0.16	2.24	-0.05	2.39	-0.20	2.55	-0.36
10'a	3.50	3.03	0.47	2.99	0.51	3.22	0.28	3.71	-0.21
10'b	3.01	3.35	-0.34	3.68	-0.67	3.14	-0.13	2.99	0.02
11'	0.93	1.12	-0.19	1.19	-0.26	0.85	0.08	1.14	-0.21
13'	3.64	3.55	0.09	3.61	0.03	3.50	0.14	3.58	0.06

Table S3. Statistical parameters of calculated ^{1}H and ^{13}C NMR data of **1a**–**1d** against experimental data of **1**

compound	type	CMAD	CLAD	R^2	RMSD
1a	^{13}C	1.57	4.97	0.9988	2.0223
	^{1}H	0.21	0.48	0.9824	0.2648
1b	^{13}C	1.62	4.87	0.9988	2.0348
	^{1}H	0.24	0.70	0.9729	0.3286
1c	^{13}C	2.00	5.53	0.9980	2.6157
	^{1}H	0.21	0.59	0.9811	0.2748
1d	^{13}C	1.66	3.90	0.9988	1.9940
	^{1}H	0.16	0.44	0.9897	0.2025

Table S4. Experimental ^{13}C NMR data of **2** and calculated ^{13}C NMR data of **2a**–**2d** in Chloroform

no.	**2**	**2a**		**2b**		**2c**		**2d**	
	δ_{exp}	δ_C	$\Delta\delta_C$	δ_C	$\Delta\delta_C$	δ_C	$\Delta\delta_C$	δ_C	$\Delta\delta_C$
1	159.3	160.73	1.43	160.81	1.51	160.60	1.30	160.51	1.21
2	116.6	116.30	0.30	116.38	0.22	115.94	0.66	115.96	0.64
3	141.7	143.05	1.35	143.09	1.39	143.08	1.38	142.84	1.14
4	107.9	105.26	2.64	105.02	2.88	104.81	3.09	104.47	3.43
4a	159.3	158.79	0.51	158.66	0.64	159.56	0.26	159.32	0.02
5	82.7	84.22	1.52	83.59	0.89	81.33	1.37	81.75	0.95
6	33.7	37.45	3.75	37.13	3.43	37.32	3.62	37.02	3.32
7	36.8	34.46	2.34	34.60	2.20	36.06	0.74	35.98	0.82
8	175.0	173.95	1.05	174.03	0.97	174.37	0.63	174.25	0.75
9	194.2	192.85	1.35	192.71	1.49	193.19	1.01	193.10	1.10
9a	107.7	106.25	1.45	106.11	1.59	105.57	2.13	105.44	2.26
10	40.0	44.24	4.24	43.90	3.90	41.83	1.83	41.91	1.91
10a	84.7	83.91	0.79	83.71	0.99	86.56	1.86	86.51	1.81
11	15.0	12.54	2.46	12.53	2.47	13.07	1.93	12.84	2.16
12	169.1	171.83	2.73	171.92	2.82	170.78	1.68	171.76	2.66
13	53.7	52.86	0.84	52.71	0.99	52.32	1.38	52.29	1.41
1′	159.6	160.71	1.11	160.60	1.00	160.85	1.25	160.59	0.99
2′	117.6	117.58	0.02	117.14	0.46	117.67	0.07	117.25	0.35
3′	151.5	152.97	1.47	152.96	1.46	152.97	1.47	152.71	1.21
4′	109.1	106.69	2.41	106.67	2.43	106.58	2.52	106.37	2.73
4a′	158.9	157.51	1.39	158.45	0.45	157.69	1.21	158.24	0.66
5′	81.1	81.79	0.69	78.99	2.11	82.03	0.93	79.43	1.67
6′	22.2	22.21	0.01	23.64	1.44	22.77	0.57	23.92	1.72
7	27.8	27.32	0.48	28.69	0.89	27.39	0.41	28.82	1.02
8′	175.7	175.13	0.57	175.24	0.46	174.83	0.87	175.16	0.54
9′	193.2	192.03	1.17	192.34	0.86	191.94	1.26	192.21	0.99
9a′	105.8	104.23	1.57	103.89	1.91	104.33	1.47	103.83	1.97
10′	39.6	42.72	3.12	40.67	1.07	42.87	3.27	40.73	1.13
10a′	84.2	82.71	1.49	87.01	2.81	83.16	1.04	87.15	2.95
11′	21.5	21.48	0.02	21.48	0.02	21.58	0.08	21.58	0.08
12′	169.1	171.62	2.52	171.08	1.98	172.33	3.23	171.77	2.67
13′	53.9	52.81	1.09	52.44	1.46	52.83	1.07	52.49	1.41

Table S5. Experimental ^{1}H NMR data of **2** and calculated ^{1}H NMR data of **2a**–**2d** in Chloroform

no.	**2**	**2a**		**2b**		**2c**		**2d**	
	δ_{exp}	δ_H	$\Delta\delta_H$	δ_H	$\Delta\delta_H$	δ_H	$\Delta\delta_H$	δ_H	$\Delta\delta_H$
3	7.37	7.42	-0.05	7.43	-0.06	7.43	-0.06	7.47	-0.10
4	6.67	6.63	0.04	6.62	0.05	6.60	0.07	6.61	0.06
5	4.80	4.77	0.03	4.77	0.03	4.80	0.00	4.84	-0.04
6	3.00	3.06	-0.06	3.04	-0.04	3.03	-0.03	2.99	0.01
7a	2.69	2.38	0.31	2.39	0.30	2.73	-0.04	2.58	0.11
7b	2.50	2.08	0.42	2.06	0.44	2.40	0.10	2.46	0.04
10a	3.27	3.36	-0.09	3.46	-0.19	3.44	-0.17	3.32	-0.05
10b	3.20	3.31	-0.11	3.16	0.04	3.22	-0.02	3.26	-0.06
11	1.36	1.66	-0.30	1.59	-0.23	1.35	0.01	1.30	0.06
13	3.77	3.68	0.09	3.68	0.09	3.73	0.04	3.66	0.11
4'	6.57	6.50	0.07	6.52	0.05	6.51	0.06	6.53	0.04
5'	4.88	4.80	0.08	4.69	0.19	4.78	0.10	4.68	0.20
6'	2.45	2.79	-0.34	2.46	-0.01	2.69	-0.24	2.41	0.04
7'a	2.72	2.41	0.31	2.86	-0.14	2.32	0.40	2.62	0.10
7'b	2.60	2.40	0.20	2.43	0.17	2.33	0.27	2.58	0.02
10'a	3.11	3.37	-0.26	3.60	-0.49	3.33	-0.22	3.37	-0.26
10'b	2.97	3.24	-0.27	3.06	-0.09	3.21	-0.24	3.21	-0.24
11'	2.12	2.32	-0.20	2.32	-0.20	2.31	-0.19	2.29	-0.17
13'	3.79	3.67	0.12	3.70	0.09	3.63	0.16	3.65	0.14

Table S6. Statistical parameters of calculated ^{1}H and ^{13}C NMR data of **2a**–**2d** against experimental data of **2**

compound	type	CMAD	CLAD	R^2	RMSD
2a	^{13}C	1.50	4.24	0.9990	1.8831
	^{1}H	0.18	0.42	0.9825	0.2249
2b	^{13}C	1.54	3.90	0.9990	1.8587
	^{1}H	0.15	0.49	0.9843	0.2127
2c	^{13}C	1.42	3.62	0.9991	1.7427
	^{1}H	0.13	0.40	0.9893	0.1756
2d	^{13}C	1.49	3.43	0.9991	1.7931
	^{1}H	0.10	0.26	0.9942	0.1289

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d,p)	Unscaled Shifts

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	0.15%	1.91%	97.93%	-	-
sDP4+ (C data)	7.74%	4.35%	72.56%	15.35%	-	-
sDP4+ (all data)	0.00%	0.04%	8.45%	91.51%	-	-
uDP4+ (H data)	0.01%	0.53%	0.95%	98.51%	-	-
uDP4+ (C data)	8.32%	22.56%	44.87%	24.25%	-	-
uDP4+ (all data)	0.00%	0.49%	1.74%	97.76%	-	-
DP4+ (H data)	0.00%	0.00%	0.02%	99.98%	-	-
DP4+ (C data)	1.70%	2.59%	85.89%	9.82%	-	-
DP4+ (all data)	0.00%	0.00%	0.16%	99.84%	-	-

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311G(d,p)	Unscaled Shifts

		DP4+	0.00%	0.00%	0.16%	99.84%	-
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C	x	159.3	168.134483	168.201346	167.944218	167.945856	
C	x	116.6	121.85752	121.946989	121.422941	121.513504	
C	x	141.7	149.721077	149.751762	149.695779	149.525196	
C	x	107.9	110.36324	110.124516	109.830627	109.543781	
C	x	159.3	166.111782	165.962627	166.863597	166.703866	
C		82.7	88.4489688	87.8114782	85.3770515	85.8649864	
C		33.7	39.7403222	39.4470204	39.5320246	39.2427195	
C		36.8	36.623134	36.814117	38.2221212	38.162219	
C		175	181.899454	181.967065	182.283425	182.27004	
C	x	194.2	201.580729	201.410173	201.893302	201.915454	
C	x	107.7	111.392556	111.259537	110.627093	110.553059	
C		40	46.8070425	46.4923084	44.2329797	44.334952	
C		84.7	88.1215101	87.9356251	90.8168853	90.8232218	
C		15	13.7978538	13.8366773	14.2765372	14.0400883	
C	x	169.1	179.697764	179.771036	178.544879	179.669414	
C		53.7	55.7832201	55.6668671	55.1581784	55.1559551	
C	x	159.6	168.111336	167.981439	168.199929	168.026466	
C	x	117.6	123.196072	122.737399	123.231001	122.85693	
C	x	151.5	160.048683	160.029278	160.000436	159.820309	
C	x	109.1	111.846863	111.839664	111.675012	111.522326	
C	x	158.9	164.782673	165.750711	164.911864	165.576262	
C		81.1	85.9133698	83.0259565	86.1033172	83.4423663	
C		22.2	23.8697875	25.4015453	24.3787783	25.5864798	
C		27.8	29.1880727	30.6597902	29.1896896	30.6908994	
C	x	175.7	183.134828	183.225899	182.76287	183.211965	
C	x	193.2	200.728317	201.03329	200.586833	200.989444	
C	x	105.8	109.290106	108.94805	109.332685	108.875282	
C		39.6	45.2280874	43.1263875	45.3089061	43.1110254	
C		84.2	86.8746141	91.368581	87.2752306	91.4864682	
C		21.5	23.1035054	23.156237	23.1326239	23.1523536	
C	x	169.1	179.470753	178.895356	180.162376	179.681732	
C		53.9	55.7378825	55.3829434	55.6826553	55.3646858	
H	x	7.37	7.66559338	7.673938	7.67012904	7.67161066	
H	x	6.67	6.82758094	6.80985815	6.79175568	6.77182264	
H		4.8	4.83031529	4.83334748	4.87043226	4.9139434	
H		3	2.99115475	2.99430985	2.99519644	2.98108887	
H		2.69	2.25905093	2.29177772	2.67641378	2.5511557	
H		2.5	1.94251503	1.94566288	2.32296762	2.42296383	
H		3.27	3.31245677	3.44241887	3.42462998	3.32950501	
H		3.2	3.26364159	3.11439695	3.19282272	3.25836584	
H		1.36	1.48620948	1.43772799	1.20502659	1.21363429	
H		3.77	3.65728256	3.67556192	3.73226445	3.67846951	
H	x	6.57	6.68384985	6.69709089	6.686255	6.6831775	
H		4.88	4.85979556	4.75336863	4.8525023	4.74606301	
H		2.45	2.70222147	2.36681201	2.6299884	2.36966076	
H		2.72	2.29626099	2.7997859	2.23597372	2.58861839	
H		2.6	2.27988156	2.34404338	2.24938774	2.55588536	
H		3.11	3.32152236	3.58192477	3.311886	3.38138817	
H		2.97	3.19061447	3.01191027	3.18243914	3.2115873	
H		2.12	2.20375049	2.22187009	2.22753686	2.24581217	
H		3.79	3.64194819	3.6945803	3.62864256	3.67100418	

Figure S8. Detailed DP4+ probability analysis for **2**. Isomer 1 is (5*S*,6*R*,10a*R*,5′*S*,10a′*R*)-**2a**, isomer 2 is (5*S*,6*R*,10a*R*,5′*R*,10a′*R*)-**2b**, isomer 3 is (5*R*,6*S*,10a*R*,5′*S*,10a′*R*)-**2c**, isomer 4 is (5*R*,6*S*,10a*R*,5′*R*,10a′*R*)-**2d**

Table S7. Experimental ^{13}C NMR data of **3** and calculated ^{13}C NMR data of **3a** and **3b** in DMSO

no.	**3**	**3a**		**3b**	
	δ_{exp}	δ_C	$\Delta\delta_C$	δ_C	$\Delta\delta_C$
1	160.2	160.79	0.59	161.30	1.10
2	109.5	106.79	2.71	107.21	2.29
3	141.0	140.46	0.54	143.74	2.74
4	114.0	113.46	0.54	113.56	0.44
4a	155.4	157.13	1.73	156.45	1.05
5	81.6	81.28	0.32	81.51	0.09
6	32.8	36.35	3.55	36.60	3.80
7	35.8	35.39	0.41	34.78	1.02
8	174.9	175.51	0.61	174.31	0.59
9	194.6	193.28	1.32	191.99	2.61
9a	107.3	105.58	1.72	105.14	2.16
10	39.2	41.95	2.75	40.21	1.01
10a	85.3	85.12	0.18	87.61	2.31
11	14.3	12.59	1.71	12.31	1.99
12	169.1	170.07	0.97	170.05	0.95
13	53.6	51.95	1.65	51.63	1.97
1′	160.2	160.88	0.68	161.19	0.99
2′	109.5	106.96	2.54	108.14	1.36
3′	141.0	140.72	0.28	143.23	2.23
4′	114.0	113.47	0.53	113.34	0.66
4a′	155.4	157.12	1.72	155.91	0.51
5′	81.6	82.04	0.44	84.05	2.45
6′	32.8	35.95	3.15	35.76	2.96
7	35.8	35.34	0.46	33.87	1.93
8′	174.9	175.42	0.52	174.18	0.72
9′	194.6	193.28	1.32	191.94	2.66
9a′	107.3	105.62	1.68	105.23	2.07
10′	39.2	41.98	2.78	43.02	3.82
10a′	85.3	85.11	0.19	82.87	2.43
11′	14.3	12.52	1.78	12.63	1.67
12′	169.1	171.13	2.03	171.67	2.57
13′	53.6	51.93	1.67	51.79	1.81

Table S8. Experimental ^{1}H NMR data of **3** and calculated ^{1}H NMR data of **3a** and **3b** in DMSO

no.	**3**	**3a**		**3b**	
	δ_{exp}	δ_H	$\Delta\delta_H$	δ_H	$\Delta\delta_H$
2	6.49	6.60	0.11	6.48	0.01
3	7.75	7.45	0.30	7.95	0.20
5	4.85	4.83	0.02	4.67	0.18
6	2.88	3.00	0.12	2.98	0.10
7a	2.45	2.13	0.32	2.04	0.41
7b	1.72	1.47	0.25	1.96	0.24
10a	3.56	4.18	0.62	3.43	0.13
10b	3.17	2.90	0.27	3.06	0.11
11	1.00	1.25	0.25	1.37	0.37
13	3.75	3.78	0.03	3.72	0.03
2'	6.49	6.61	0.12	6.43	0.06
3'	7.75	7.46	0.29	7.94	0.19
5'	4.85	4.86	0.01	4.65	0.20
6'	2.88	2.98	0.10	2.88	0.00
7'a	2.45	2.15	0.30	2.32	0.13
7'b	1.72	1.52	0.20	2.01	0.29
10'a	3.56	4.15	0.59	3.33	0.23
10'b	3.17	2.89	0.28	3.20	0.03
11'	1.00	1.27	0.27	1.13	0.13
13'	3.75	3.73	0.02	3.69	0.06

Table S9. Statistical parameters of calculated ^{1}H and ^{13}C NMR data of **3a** and **3b** against experimental data of **3**

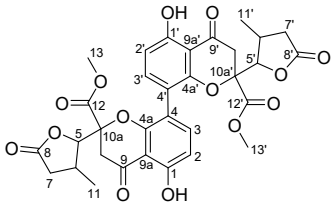
compound	type	CMAD	CLAD	R^2	RMSD
3a	^{13}C	1.35	3.55	0.9991	1.7002
	^{1}H	0.22	0.62	0.9803	0.2927
3b	^{13}C	1.78	3.82	0.9987	2.0795
	^{1}H	0.16	0.41	0.9907	0.2011

Table S10. ^{13}C NMR data of **5** and **6**

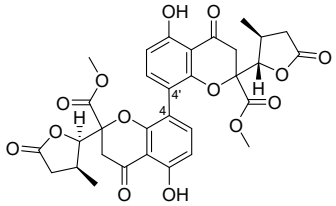
no.	**5** (**$CDCl_3$**)	**5** (DMSO-d_6)	**6** (**$CDCl_3$**)	**6** (DMSO-d_6)
1	159.3	158.4	156.2	156.1
2	117.7	116.9	110.4	109.2
3	141.4	140.7	141.4	140.9
4	107.5	107.1	115.4	114.8
4a	158.6	158.2	161.9	160.4
5	82.8	81.8	82.4	81.7
6	33.7	32.6	34.0	32.9
7	36.8	36.8	37.1	35.2
8	175.0	175.5	174.6	174.9
9	194.2	195.2	194.2	194.9
9a	107.7	107.2	107.9	107.5
10	39.9	40.0	35.3	32.9
10a	84.6	83.8	85.9	85.4
11	15.0	14.7	14.7	14.1
12	169.2	169.1	169.0	168.9
13	53.9	53.6	53.8	53.5
1′	159.3	158.4	158.5	158.0
2′	117.7	116.9	117.8	116.6
3′	141.4	140.7	141.2	140.6
4′	107.5	107.1	107.9	107.4
4a′	158.6	158.2	159.1	158.2
5′	82.8	81.8	83.0	81.9
6′	33.7	32.6	33.4	32.5
7′	36.8	36.8	39.7	36.9
8′	175.0	175.5	174.9	175.5
9′	194.2	195.2	194.7	195.3
9a′	107.7	107.2	107.5	107.0
10′	39.9	40.0	40.1	39.2
10a′	84.6	83.8	84.5	83.9
11′	15.0	14.7	15.0	14.6
12′	169.2	169.1	168.8	169.3
13′	53.9	53.6	53.8	53.5

Table S11. ^{1}H NMR data of **5** and **6**

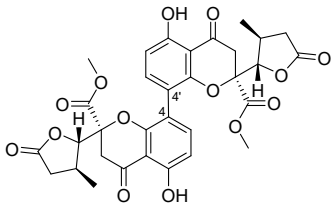
no.	**5** (CDCl$_3$)	**5** (DMSO-d_6)	**6** (CDCl$_3$)	**6** (DMSO-d_6)
2			6.63, d (3.6)	6.61, d (3.0)
3	7.53, d (8.4)	7.50, d (8.4)	7.46, d (8.4)	7.49, d (9.0)
4	6.63, d (8.4)	6.69, d (8.4)		
5	4.81, d (6.6)	4.94, d (6.6)	4.65, d (7.2)	4.84, d (7.2)
6	2.99, m	2.98, m	2.87, m	2.86, m
7	2.49, dd (17.4, 8.4)	2.33, dd (16.8, 6.0)	1.94, dd (17.4, 11.4)	1.75, dd (17.4, 10.2)
	2.71, dd (17.4, 8.4)	2.83, dd (17.4, 8.4)	2.43, dd (17.4, 7.2)	2.40, dd (17.4, 8.4)
10	3.24, m	3.06, d (17.4)	3.34, d (17.4)	3.58, d (18.0)
			3.16, d (17.4)	3.04, d (17.4)
11	1.34, d (7.2)	1.18, d (7.2)	1.23, d (7.2)	1.05, d (7.2)
13	3.77, s	3.70, s	3.80, s	3.69, s
3′	7.53, d (8.4)	7.50, d (8.4)	7.58, d (8.4)	7.60, d (9.0)
4′	6.63, d (8.4)	6.69, d (8.4)	6.62, d (3.6)	6.59, d (3)
5′	4.81, d (6.6)	4.94, d (6.6)	4.86, d (6.6)	4.95, d (6.6)
6′	2.99, m	2.98, m	2.95, m	2.97, m
7′	2.49, dd (17.4, 8.4)	2.33, dd (16.8, 6.0)	2.28, dd (17.4, 8.4)	2.32, dd (16.8, 5.4)
	2.71, dd (17.4, 8.4)	2.83, dd (17.4, 8.4)	2.73, dd (17.4, 8.4)	2.86, dd (17.4, 8.4)
10′	3.24, m	3.06, d (17.4)	3.27, d (17.4)	3.57, d (17.4)
			3.20, d (17.4)	3.08, d (17.4)
11′	1.34, d (7.2)	1.18, d (7.2)	1.30, d (7.2)	1.16, d (7.2)
13′	3.77, s	3.70, s	3.74, s	3.68, s
1-OH	11.92, s	11.83, s	11.58, s	11.55, s
1′-OH	11.92, s	11.83, s	11.83, s	11.82, s



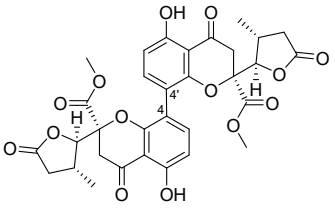
paecilin A (**4**)



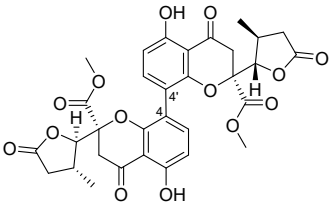
paecilin C (**3A**)



dimethyl (2S,2'S)-5,5'-dihydroxy-2,2'-bis[(2S,3S)-3-methyl-5-oxotetrahydrofuran-2-yl]4,4'-dioxo-[8,8'-bichroman]-2,2'-dicarboxylate (**3B**)



dimethyl (2S,2'S)-5,5'-dihydroxy-2,2'-bis([2R,3R]-3-methyl-5-oxotetrahydrofuran-2-yl)-4,4'-dioxo-[8,8'-bichromane]-2,2'-dicarboxylate (**3C**)



dimethyl (2S,2'S)-5,5'-dihydroxy-2-([2S,3S]-3-methyl-5-oxotetrahydrofuran-2-yl)-2'-([2R,3R]-3-methyl-5-oxotetrahydrofuran-2-yl)-4,4'-dioxo-[8,8'-bichromane]-2,2'-dicarboxylate (**3D**)

Figure S9. Structures of chromanone dimers with 4–4′ linkage

Table S12. ^{1}H NMR data of chromanone dimers with 4–4′ linkage

no.	**4**	**3A**	**3B**	**3C**	**3D**
2	6.63, d (8.5)	6.64, d (8.0)	6.60, d (8.7)	6.65, d (8.8)	6.60, d (8.7)
3	7.46, d (9.0)	7.52, d (8.5)	7.47-7.82, m	7.93, d (8.8)	7.77, d (8.7)
5	4.86, d (6.5)	4.82, d (6.5)	4.26, d (3.0)	4.34, d (3.6)	4.32, d (3.1)
6	2.95, m	3.00, m	2.39-2.57, m	2.68-2.75, m	2.77, m
7	2.74, dd (17.0, 7.0)	2.73, dd (17.0, 8.0)	2.06, dd (18.0, 9.0)	2.45, dd (18.0, 9.3)	2.33, dd (17.9, 9.3)
	2.43, dd (17.0, 7.0)	2.52, dd (17.5, 8.5)	1.82, dd (18.0, 3.6)	2.03, dd (18.0, 4.3)	1.94, dd (17.9, 3.7)
10	3.34, d (17.5)	3.29, d (17.5)	3.59, d (17.4)	3.20, d (17.0)	3.19, d (17.1)
	3.21, d (17.0)		3.03, d (17.4)	3.01, d (17.0)	3.13, d (17.1)
11	1.30, d (7.0)	1.36, d (7.0)	1.05, d (6.9)	1.15, d (7.1)	1.11, d (7.1)
13	3.78, s	3.79, s	3.76, s	3.80, s	3.76, s
2′	6.62, d (8.5)	6.63, d (8.0)	6.60, d (8.7)	6.65, d (8.8)	6.63, d (8.7)
3′	7.57, d (8.5)	7.54, d (8.5)	7.47-7.82, m	7.93, d (8.8)	7.73, d (8.7)
5′	4.65, d (7.5)	4.10, s	4.26, d (3.0)	4.34, d (3.6)	4.27, d (2.7)
6′	2.87, m	2.39, m	2.39-2.57, m	2.68-2.75, m	2.49, m
7′	2.30, dd (17.0, 8.5)	2.67, dd (17.0, 8.0)	2.06, dd (18.0, 9.0)	2.45, dd (18.0, 9.3)	2.08, dd (18.1, 9.3)
	1.96, dd (17.0, 11.0)	2.46, m	1.82, dd (18.0, 3.6)	2.03, dd (18.0, 4.3)	1.85, dd (18.1, 3.4)
10′	3.27, d (17.0)	3.22, d, (17.5)	3.59, d (17.4)	3.20, d (17.0)	3.43, d (17.3)
	3.16, d (17.0)		3.03, d (17.4)	3.01, d (17.0)	3.06, d (17.3)
11′	1.23, d (7.0)	1.11, d (6.5)	1.05, d (6.9)	1.15, d (7.1)	1.09, d (7.2)
13′	3.74, s	3.77, s	3.76, s	3.80, s	3.79, s
1-OH	11.57, s	11.92, s	11.61, s		11.56, s
1′-OH	11.82, s	12.03, s	11.61		11.64, s

Table S13. ^{13}C NMR data of chromanone dimers with 4–4′ linkage

no.	**4**	**3A**	**3B**	**3C**	**3D**
1	161.8	159.2	161.6	161.7	161.9
2	110.3	107.4	109.9	111.1	111.3
3	141.3	140.9	140.8	142.0	141.3
4	115.3	117.4	115.0	114.0	114.5
4a	156.1	158.8	156.4	155.3	156.4
5	82.8	82.6	85.9	87.3	87.5
6	33.3	33.5	29.7	29.8	29.8
7	36.9	36.7	35.4	35.9	35.9
8	174.8	174.9	175.3	174.7	175.0
9	194.5	195.9	195.3	194.1	194.5
9a	107.8	107.5	107.5	107.5	107.9
10	40.0	39.8	40.5	39.7	40.4
10a	84.3	84.5	84.9	84.9	85.3
11	14.7	14.9	20.7	20.7	20.9
12	168.9	169.1	168.9	168.6	168.7
13	53.6	53.5	53.5	53.8	53.9
1′	158.9	159.2	161.6	161.7	161.8
2′	107.8	107.3	109.9	111.1	110.1
3′	141.1	141.2	140.8	142.0	141.6
4′	117.7	117.8	115.0	114.0	115.2
4a′	158.3	158.4	156.4	155.3	155.7
5′	82.3	76.2	85.9	87.3	86.5
6′	33.9	30.7	29.7	29.8	30.0
7′	35.2	40.2	35.4	35.9	35.7
8′	174.4	174.9	175.3	174.7	176.3
9′	194.0	194.1	195.3	194.1	194.8
9a′	107.0	107.5	107.5	107.5	107.3
10′	39.6	39.8	40.5	39.7	40.7
10a′	85.7	86.8	84.9	84.9	85.0
11′	14.4	13.7	20.7	20.7	21.0
12′	168.7	169.1	168.9	168.6	169.1
13′	53.6	53.7	53.5	53.8	54.0

Table S14. Cytotoxic activities against MIA-PaCa-2 cell line of **1**–**13**

Compounds	Inhibition rate (%) in 10 μM	IC_{50} (μM)
1	0.68	
2	0.05	
3	5.21	
4	0.92	
5	5.23	
6	11.21	
7	58.41	
8	71.96	2.6
9	76.82	2.1
10	6.94	
11	5.25	
12	0.45	
13	1.99	

Table S15. Antibacterial activities (MIC, μg/mL) of **1**–**13**

Microorganism	strain no.	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	levofloxacin
Escherichia coli	ATCC 25922	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	≤0.03
Pseudomoas syringae	CPCC 101099	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	
Bacillus cereus	CPCC 101254	>64	>64	>64	>64	>64	>64	>64	32	>64	4	>32	>32	>32	
Enterococcus faecalis	ATCC 29212	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	1
Enterococcus faecium	ATCC 700221	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	128
Klebsiella pneumoniae	ATCC BAA-2146	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	>128
Staphylococcus aureus	ATCC 33591	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	0.25
Pseudomonas aeruginosa	13-17	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	
Acinetobacter baumannii	12-8	>64	>64	>64	>64	>64	>64	>64	>64	>64	>64	>32	>32	>32	

Figure S10. ^{1}H NMR spectrum of **1** in DMSO-d_6

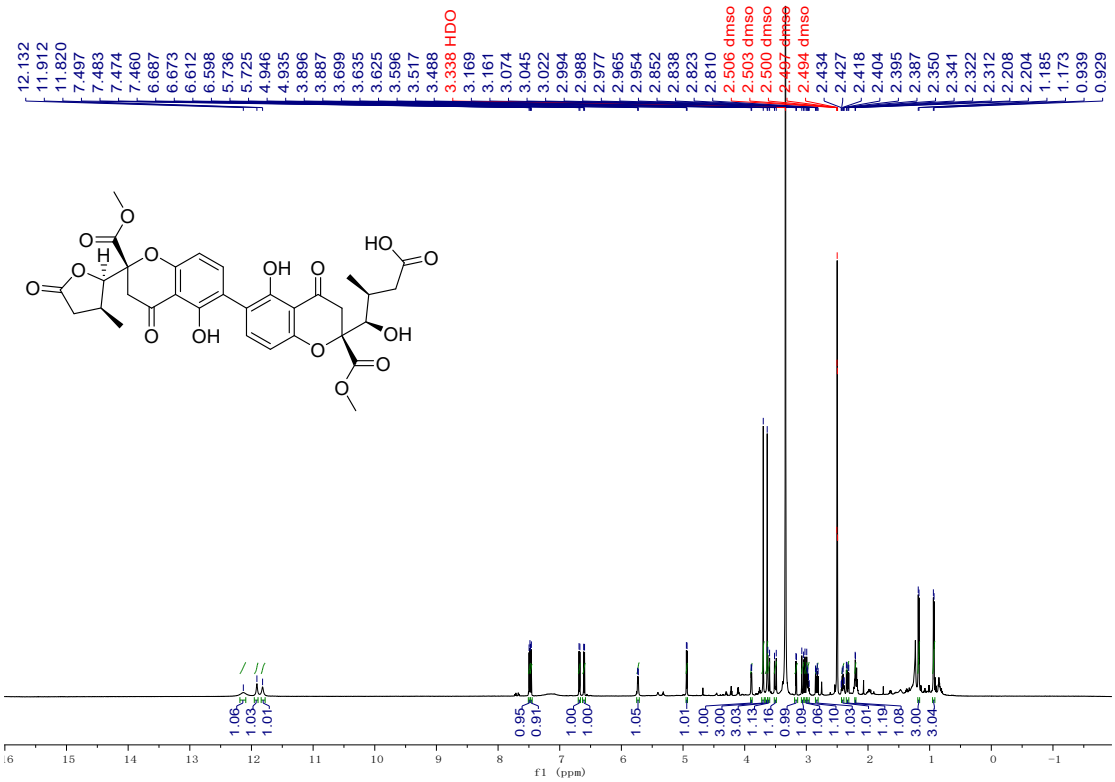


Figure S11. ^{13}C NMR spectrum of **1** in DMSO-d_6

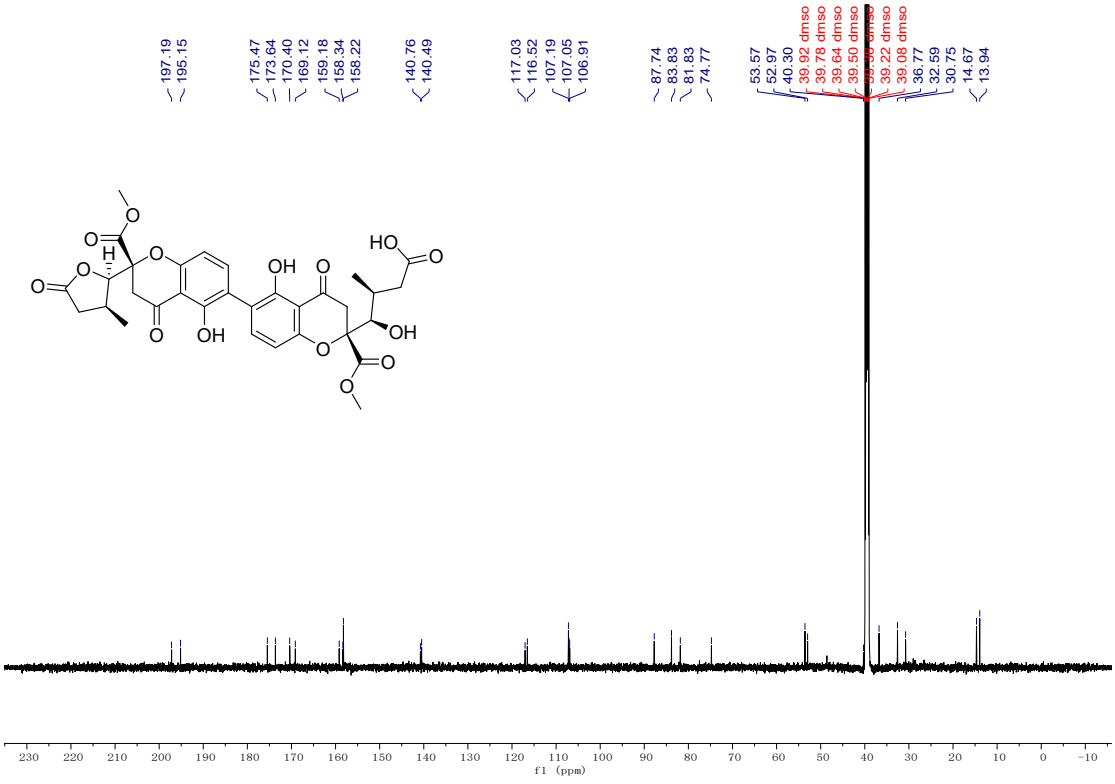


Figure S12. DEPT spectra of **1** in DMSO-d_6

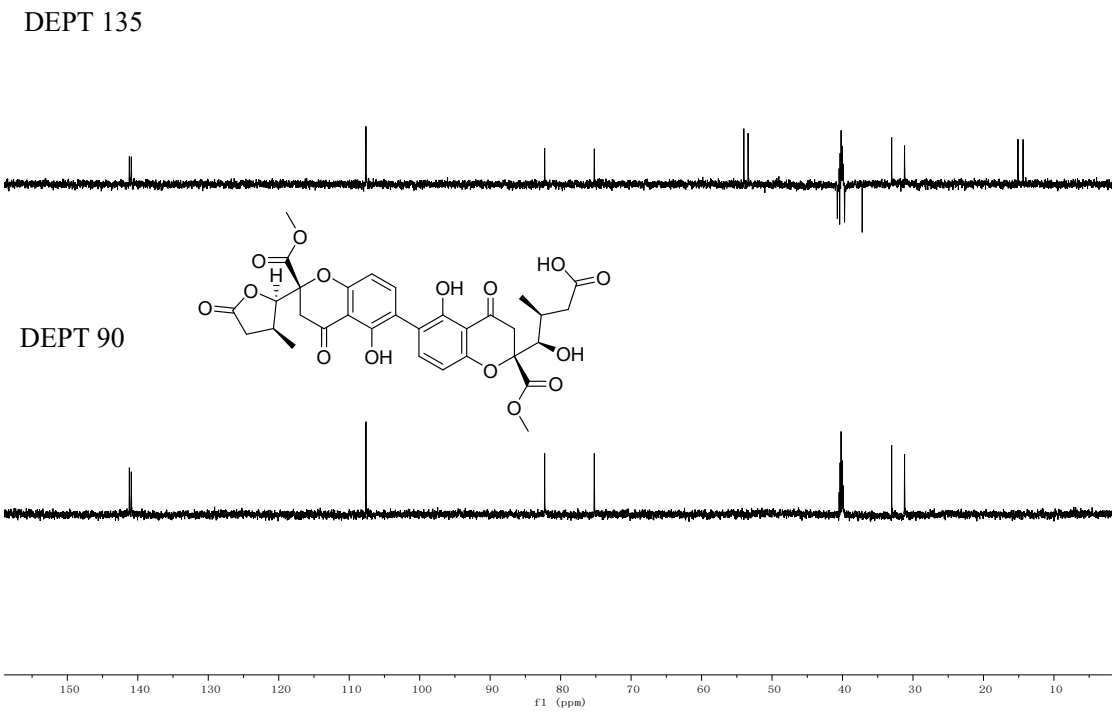


Figure S13. ^{1}H–^{1}H COSY spectrum of **1** in DMSO-d_6

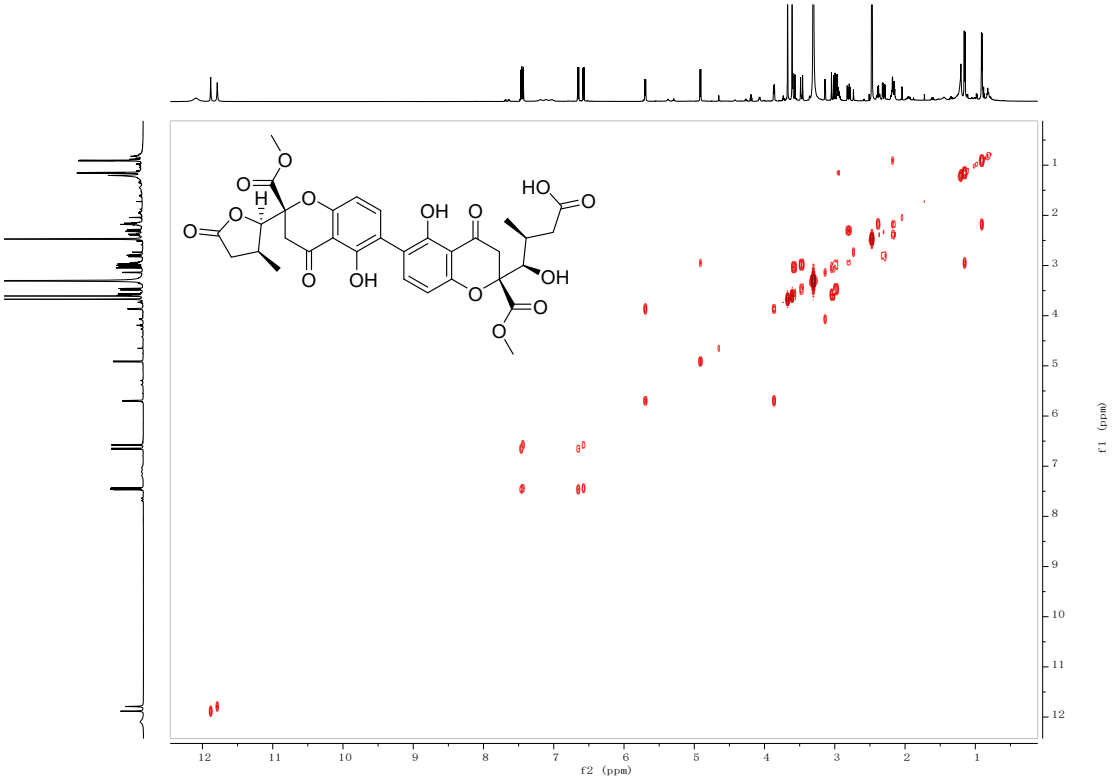


Figure S14. HSQC spectrum of **1** in DMSO-d_6

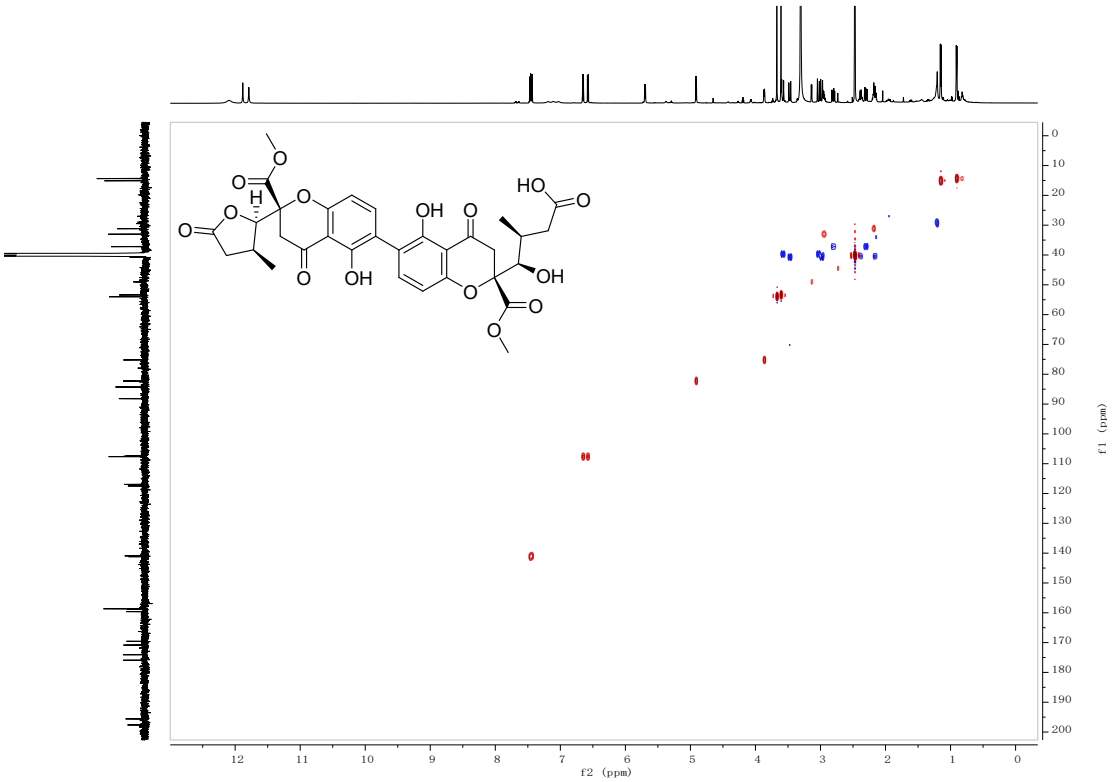


Figure S15. HMBC spectrum of **1** in DMSO-d_6

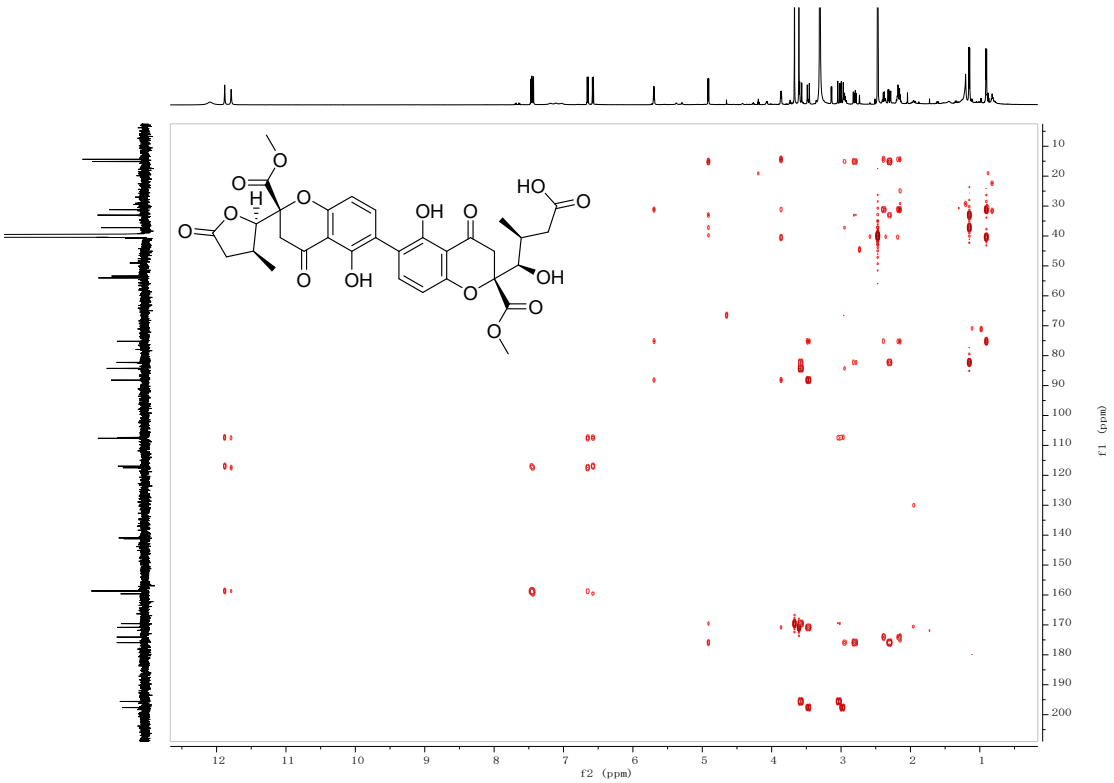


Figure S16. NOESY spectrum of **1** in DMSO-d_6

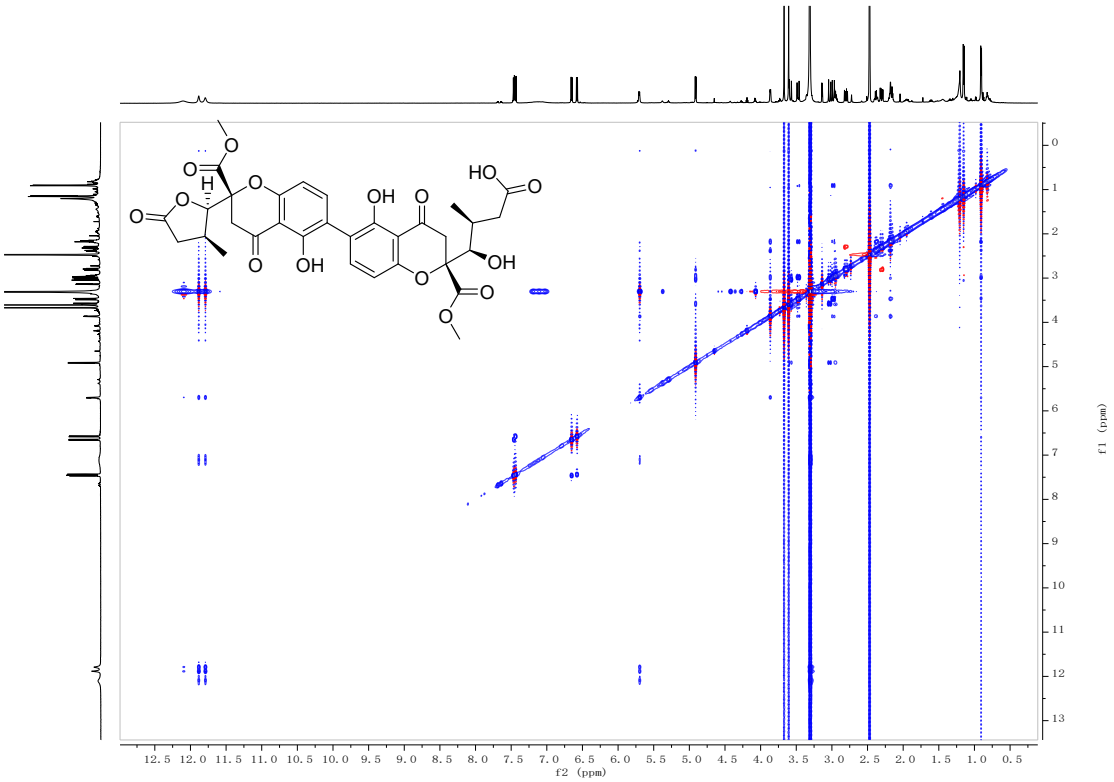


Figure S17. HRESIMS spectrum of **1**

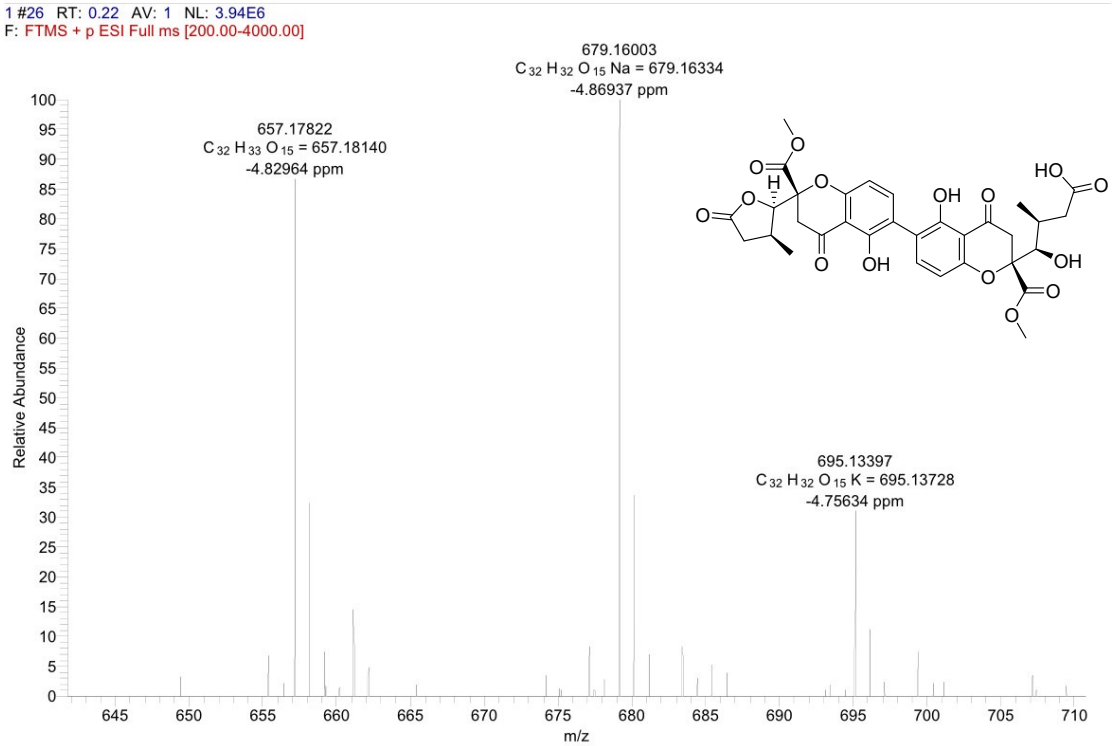
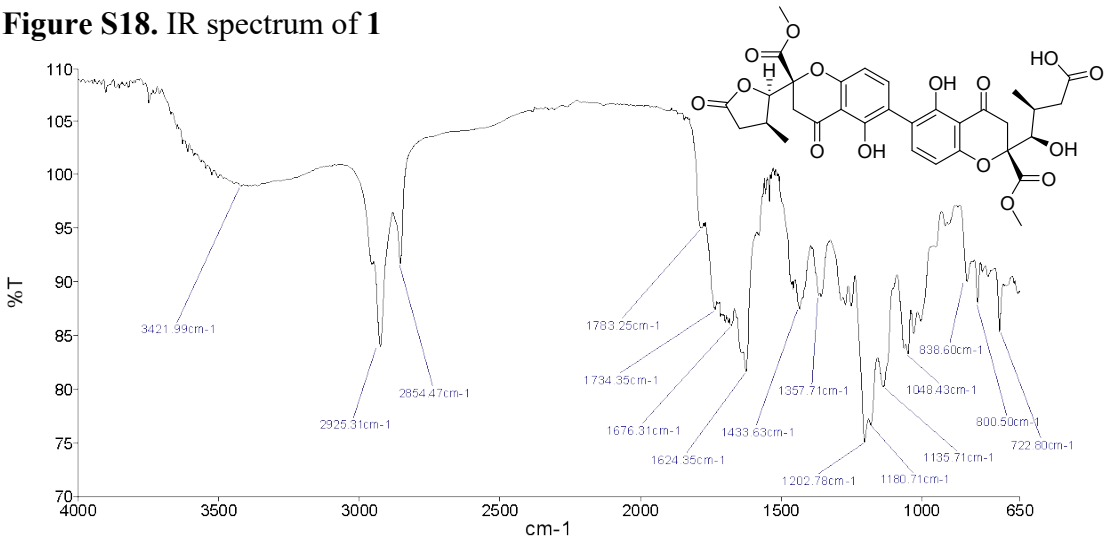


Figure S18. IR spectrum of **1**



傅立叶变换显微镜红外 (FT-IR Microscope)

Figure S19. UV spectrum of **1**

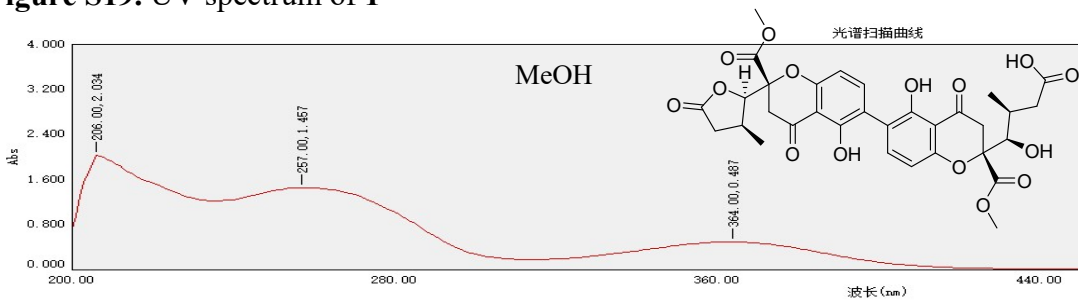
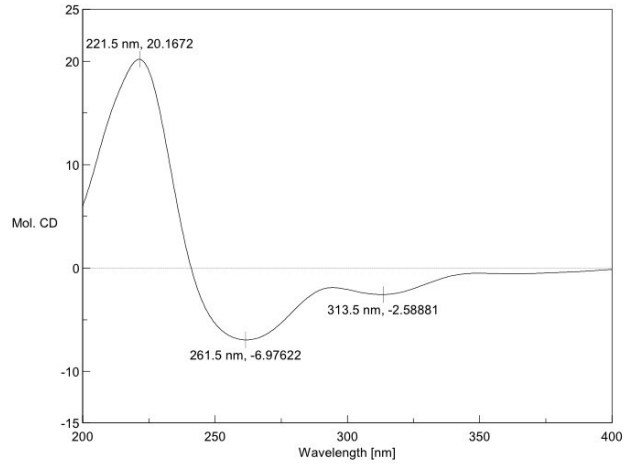


Figure S20. ECD spectrum of **1**



[Comments]

Sample name	114h-16-1-1
Comment	

[Measurement Information]

Instrument Name	IMM-CD
Instrument Type	JM-815
Serial No.	A024461168
Accessory	Standard
Accessory S/N	A005461185
Cell Length	1 mm
Measurement date	2021/7/5 10:37
Photometric Mode	CD, HT, Abs
Measure Range	400 - 200 nm
Data pitch	0.5 nm
Sensitivity	Standard
D.I.T.	1 sec
Bandwidth	1.00 nm
Start Mode	Immediately
Scanning Speed	100 nm/min
Baseline Correction	Baseline
Shutter Control	Auto
CD Detector	PMT
PMT Voltage	Auto
Accumulations	2
Solvent	MEOH
Concentration	0.5 (w/v)%

[Detailed Information]

Creation date	2021/7/5 14:23
Data array type	Linear data array * 3
Horizontal axis	Wavelength [nm]
Vertical axis(1)	Mol. CD
Vertical axis(2)	HT [V]
Vertical axis(3)	Abs
Start	400 nm
End	200 nm
Data interval	0.5 nm
Data points	401

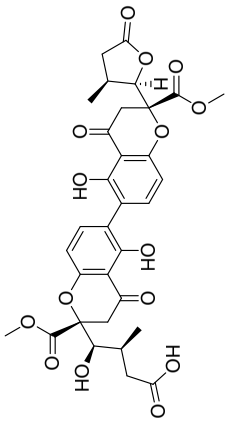


Figure S21. ^{1}H NMR spectrum of **2** in $CDCl_3$

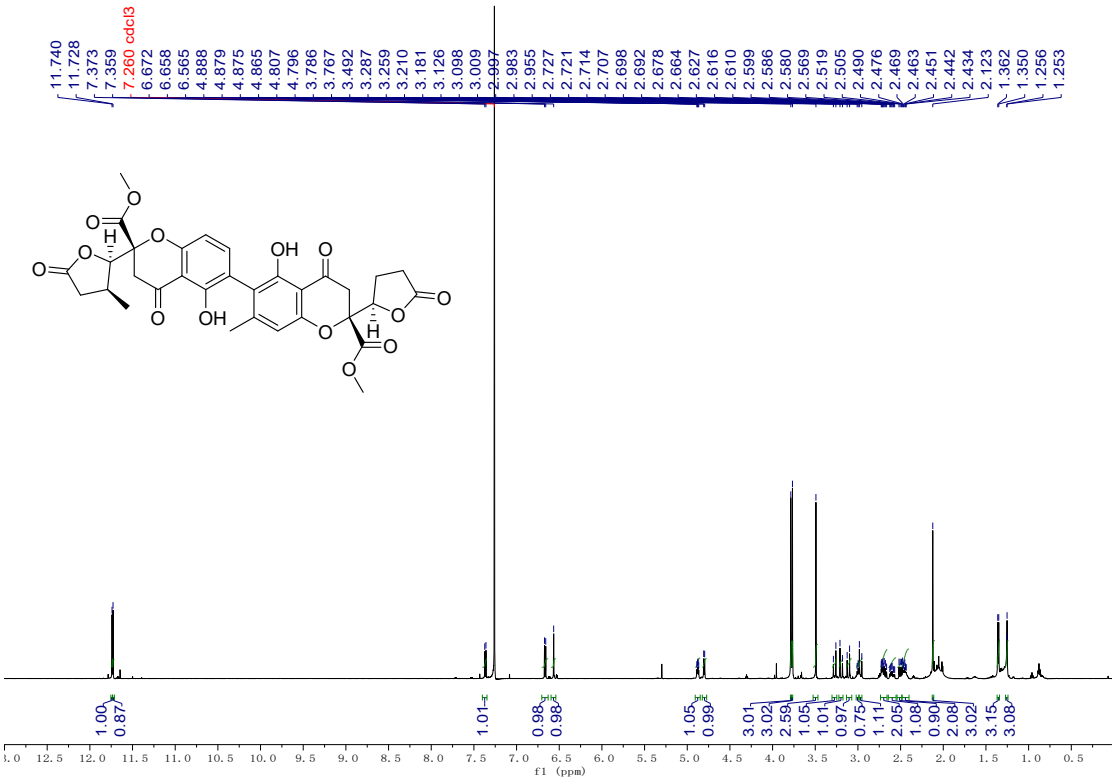


Figure S22. ^{13}C NMR spectrum of **2** in $CDCl_3$

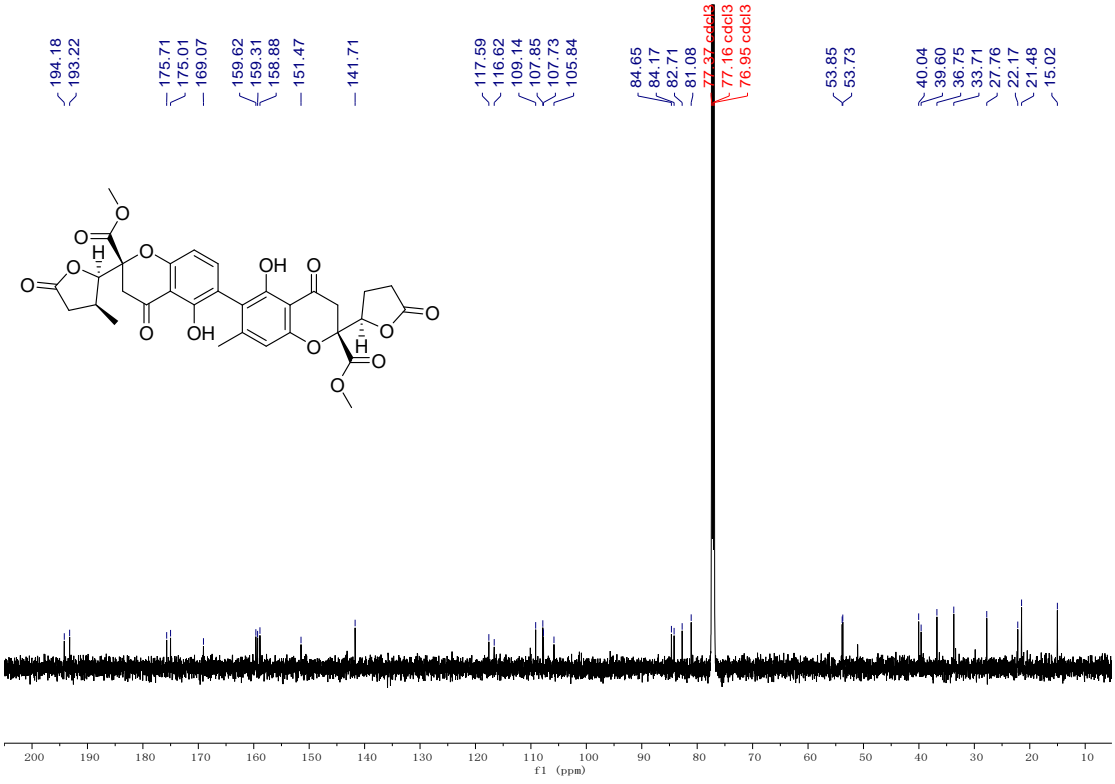


Figure S23. DEPT spectra of **2** in $CDCl_3$

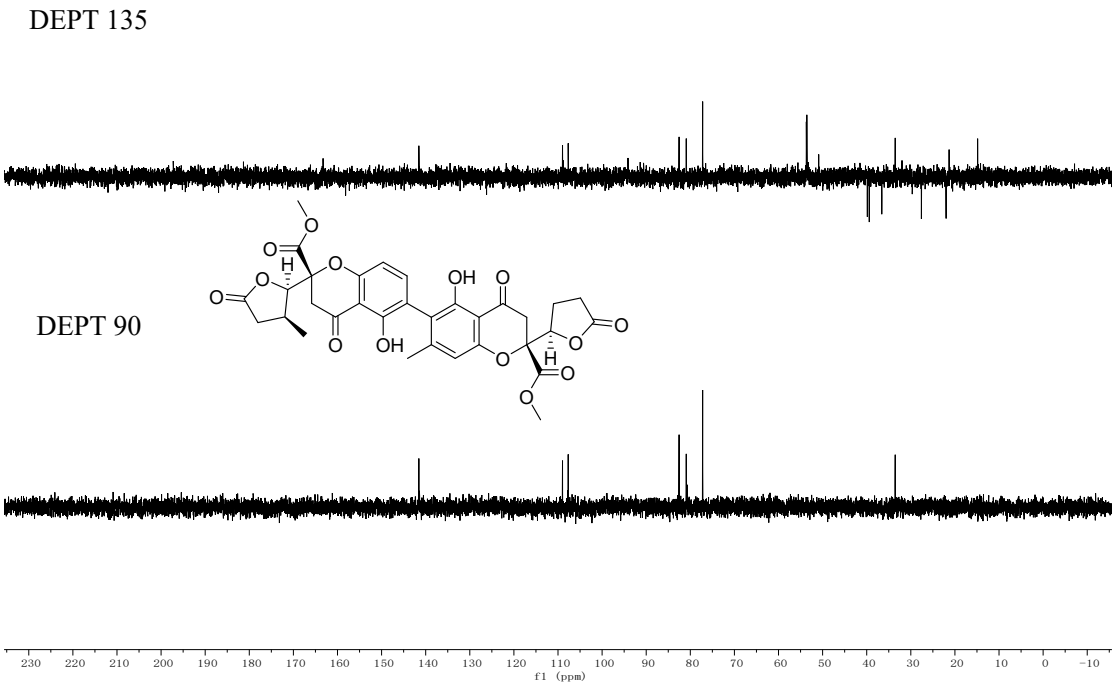


Figure S24. ^{1}H–^{1}H COSY spectrum of **2** in $CDCl_3$

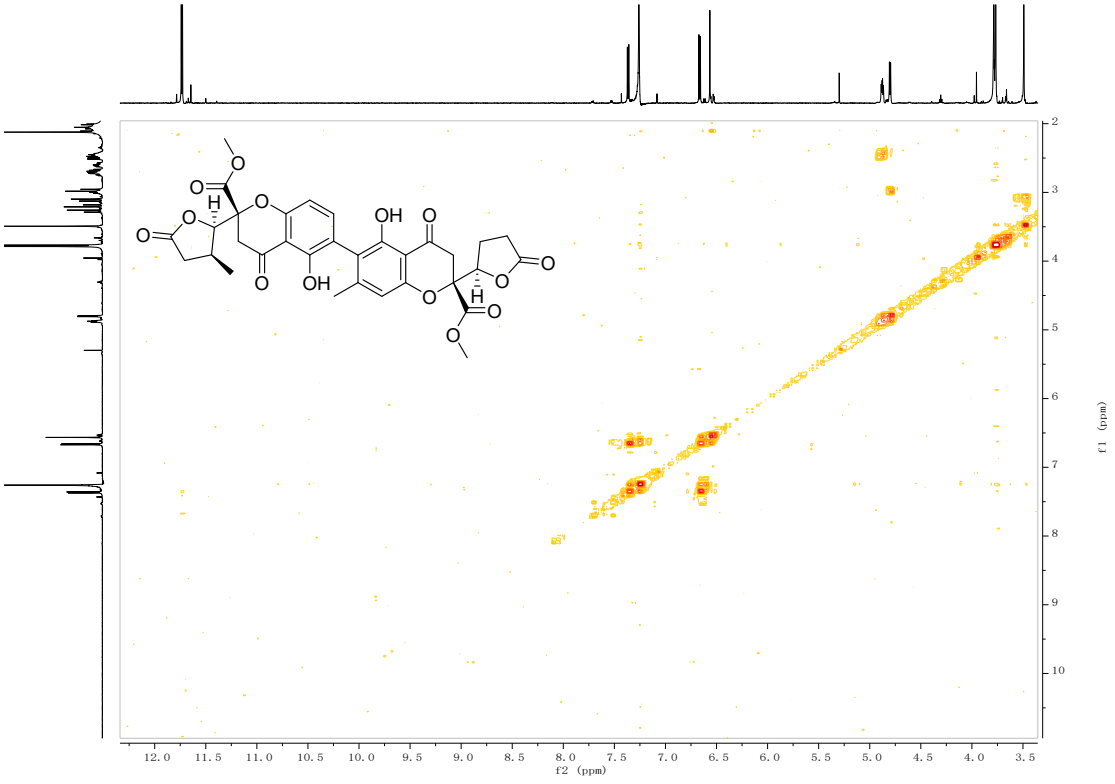


Figure S25. HSQC spectrum of **2** in $CDCl_3$

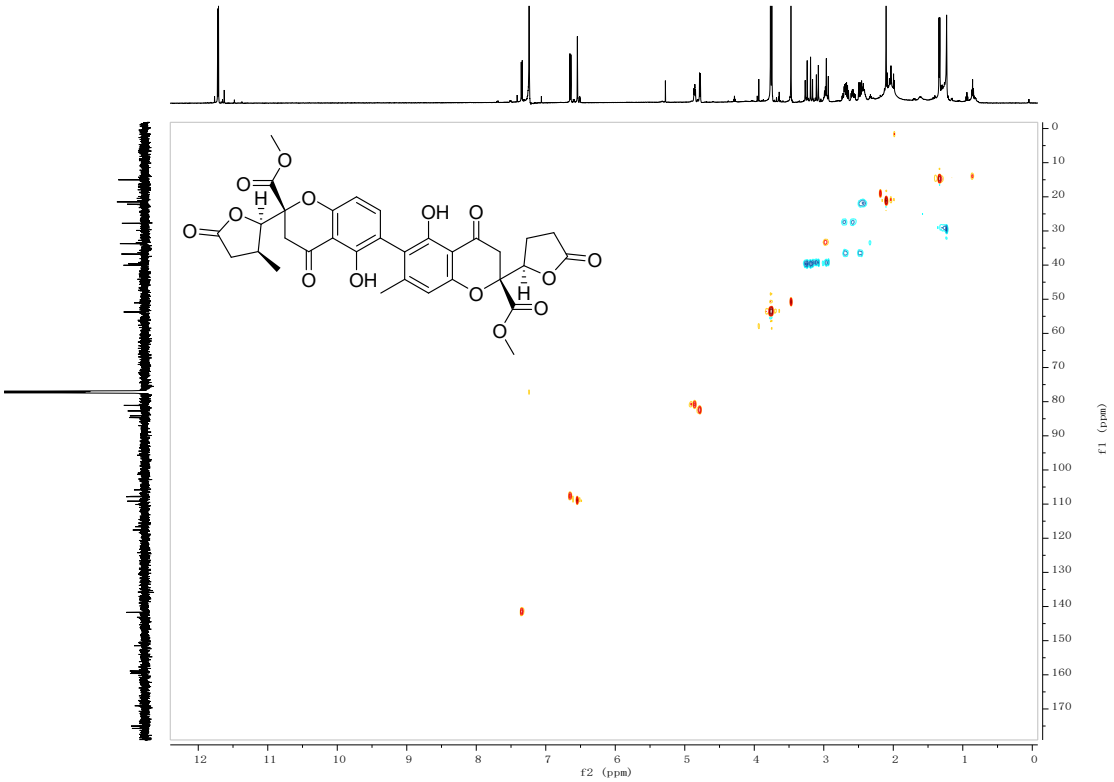


Figure S26. HMBC spectrum of **2** in $CDCl_3$

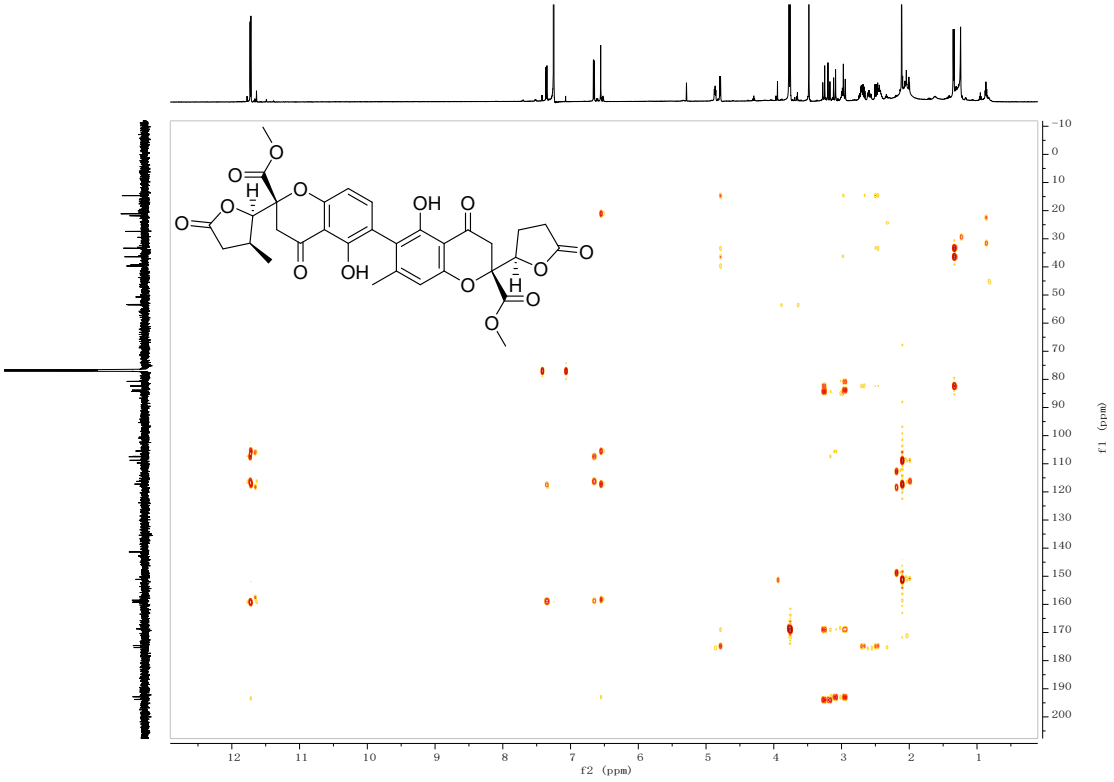


Figure S27. NOESY spectrum of **2** in $CDCl_3$

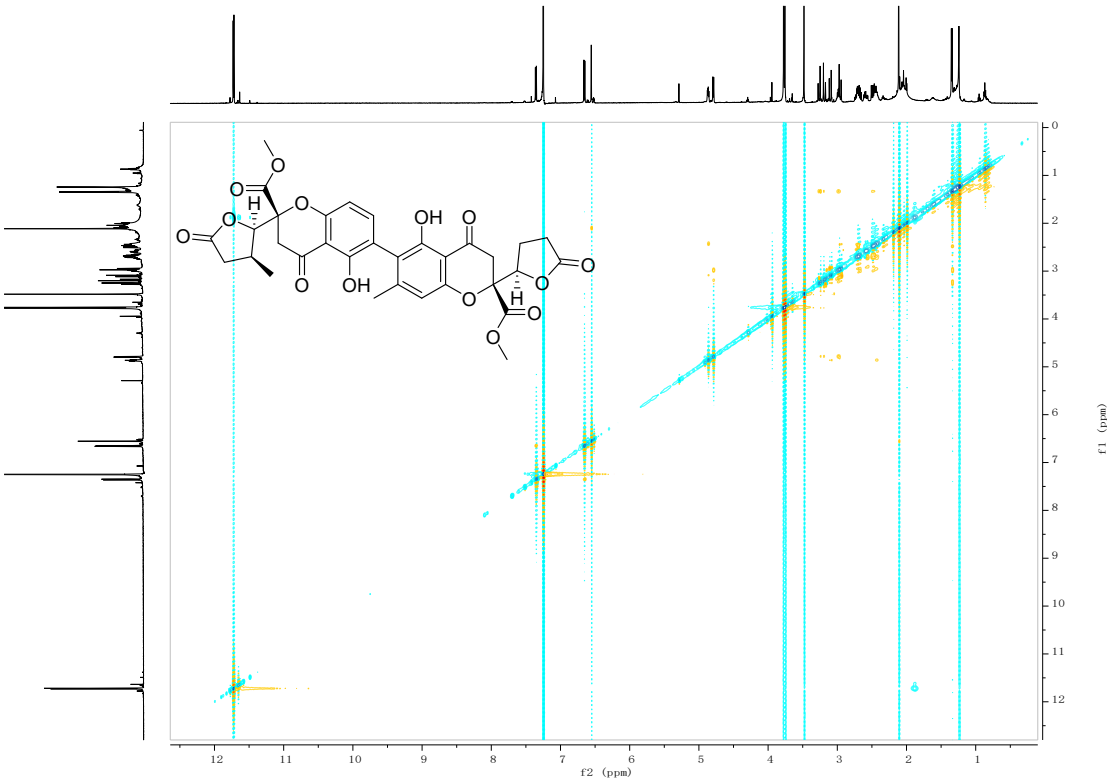


Figure S28. HRESIMS spectrum of **2**

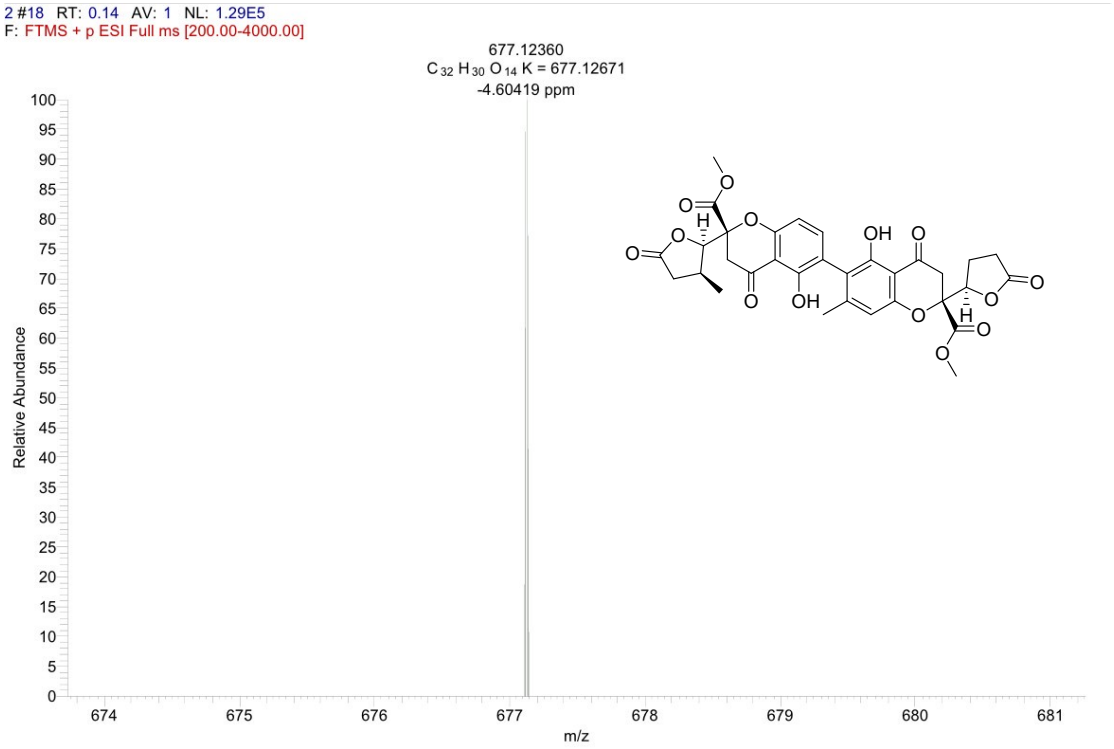
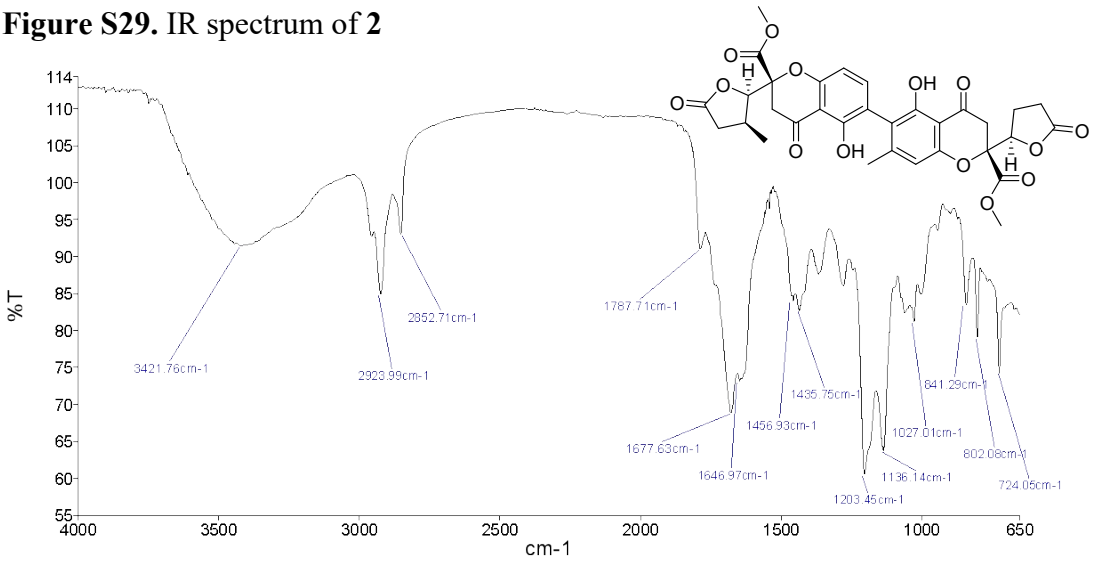


Figure S29. IR spectrum of **2**



傅立叶变换显微镜红外 (FT-IR Microscope)

Figure S30. UV spectrum of **2**

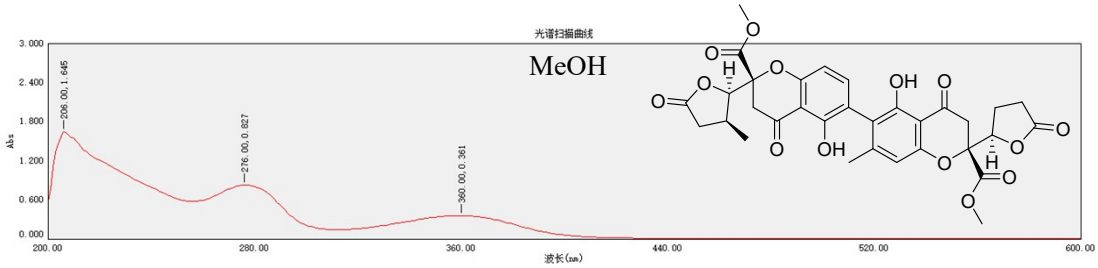
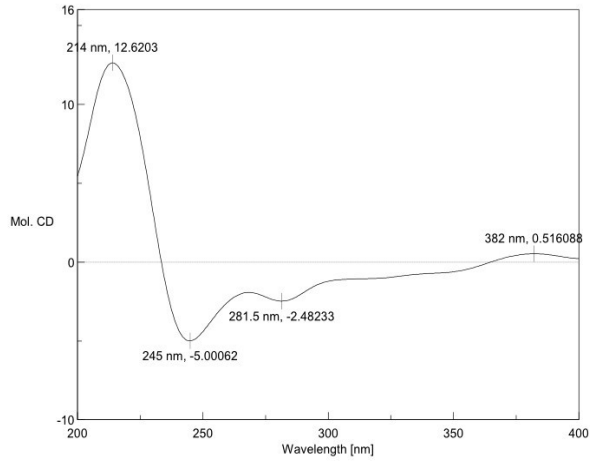


Figure S31. ECD spectrum of **2**



[Comments]
Sample name 114h-21-2-2
Comment

[Measurement Information]
Instrument Name IMM-CD
Serial No. A024461168

Accessory Standard
Accessory S/N A005461185
Cell Length 1 mm

Measurement date 2021/7/5 10:53

Photometric Mode CD, HT, Abs
Measure Range 400 - 200 nm
Data pitch 0.5 nm
Sensitivity Standard
D.I.T. 1 sec
Bandwidth 1.00 nm
Start Mode Immediately
Scanning Speed 100 nm/min
Baseline Correction Baseline
Shutter Control Auto
CD Detector PMT
PMT Voltage Auto
Accumulations 2
Solvent MEOH
Concentration 0.5 (w/v)%

[Detailed Information]
Creation date 2021/7/5 14:25

Data array type Linear data array * 3
Horizontal axis Wavelength [nm]
Vertical axis(1) Mol. CD
Vertical axis(2) HT [V]
Vertical axis(3) Abs
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End 200 nm
Data interval 0.5 nm
Data points 401

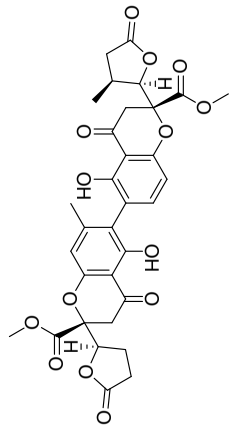


Figure S32. ^{1}H NMR spectrum of **3** in DMSO-d_6

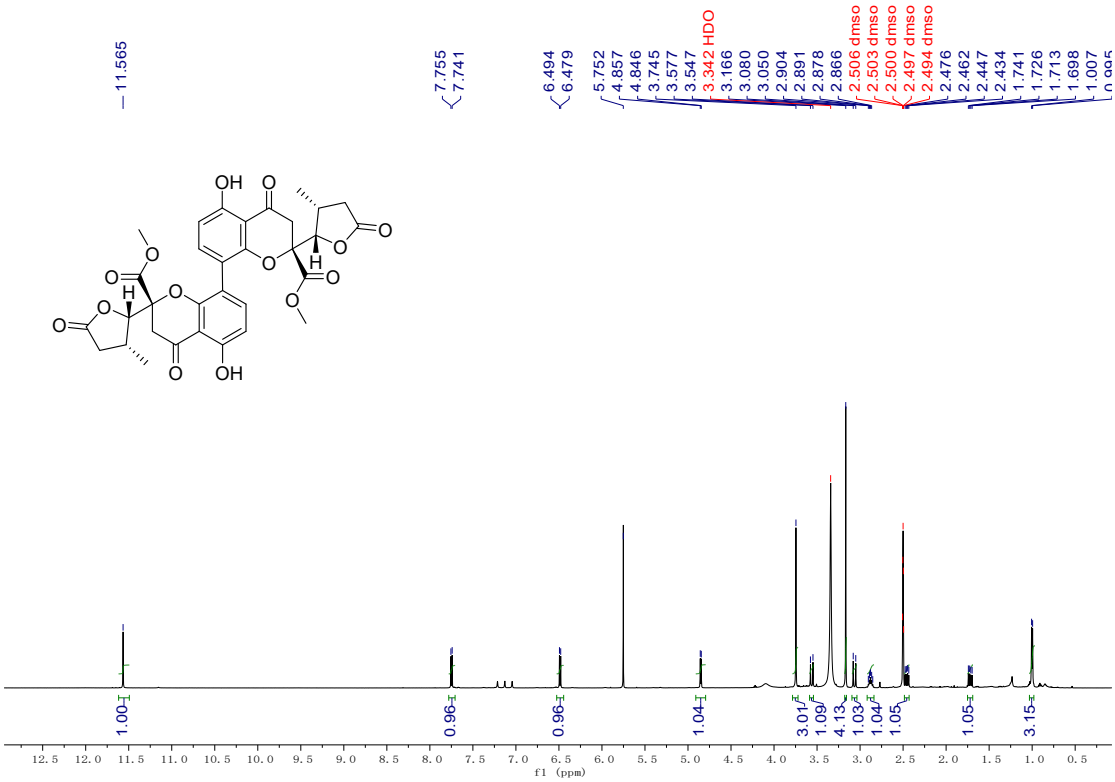


Figure S33. ^{13}C NMR spectrum of **3** in DMSO-d_6

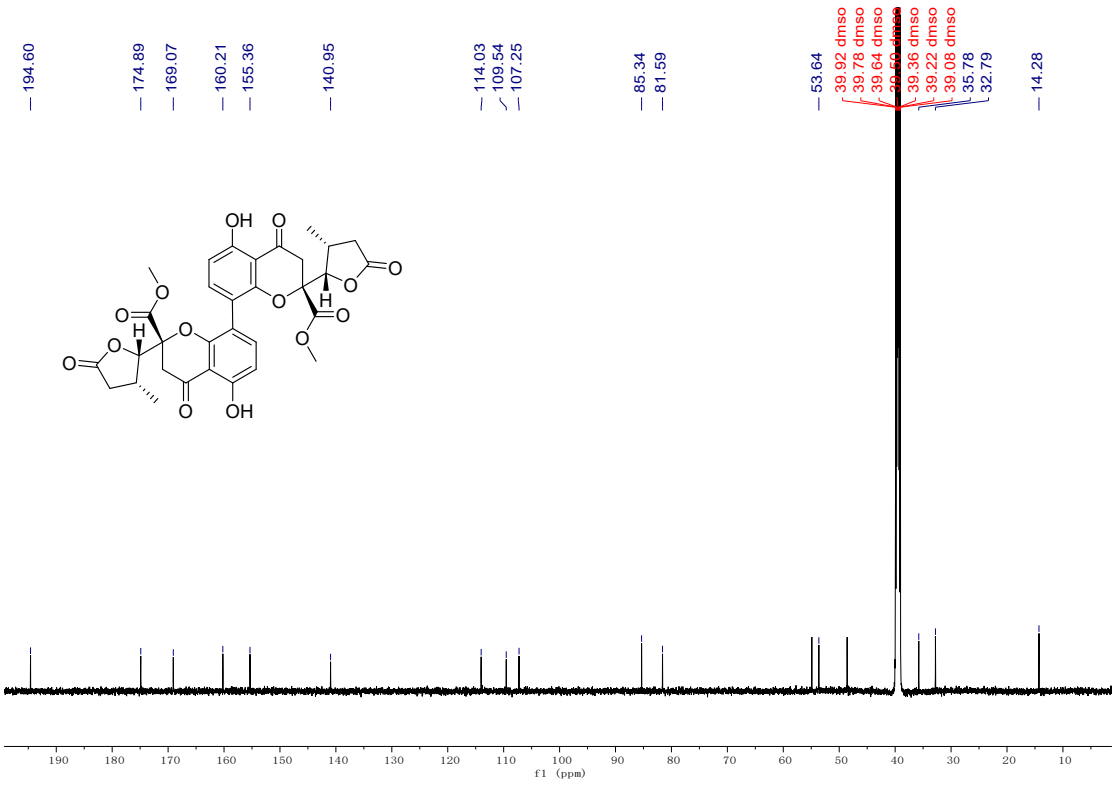


Figure S34. DEPT spectra of **3** in DMSO-d_6

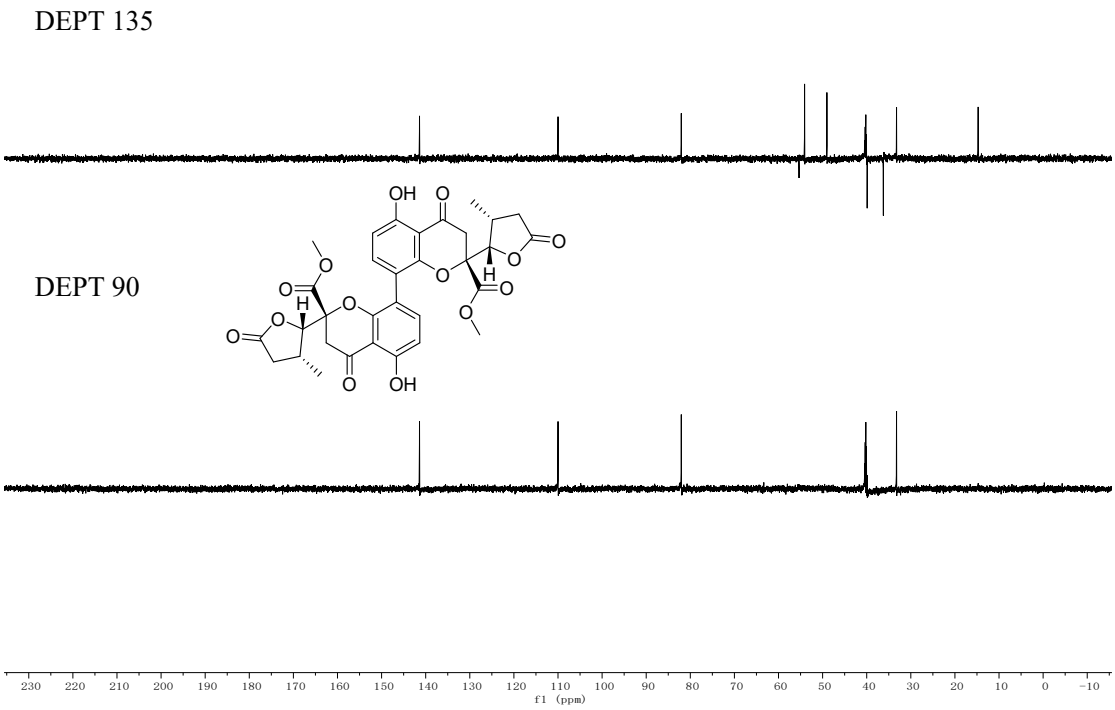


Figure S35. ^{1}H–^{1}H COSY spectrum of **3** in DMSO-d_6

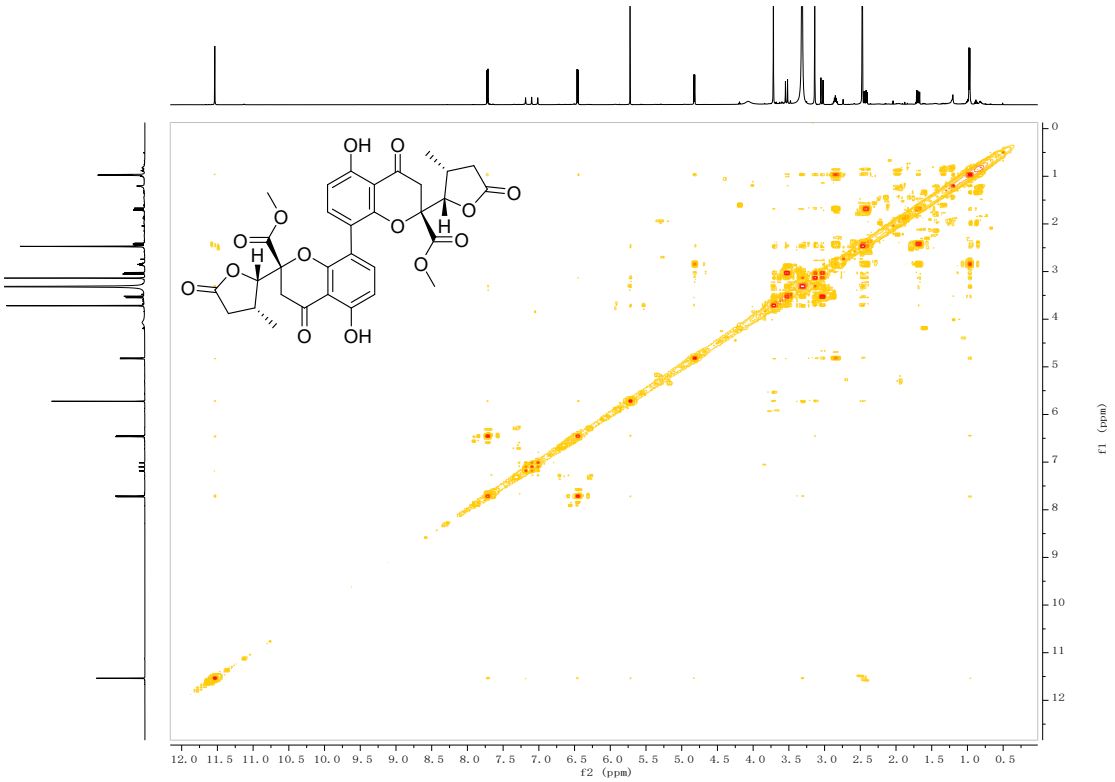


Figure S36. HSQC spectrum of **3** in DMSO-d_6

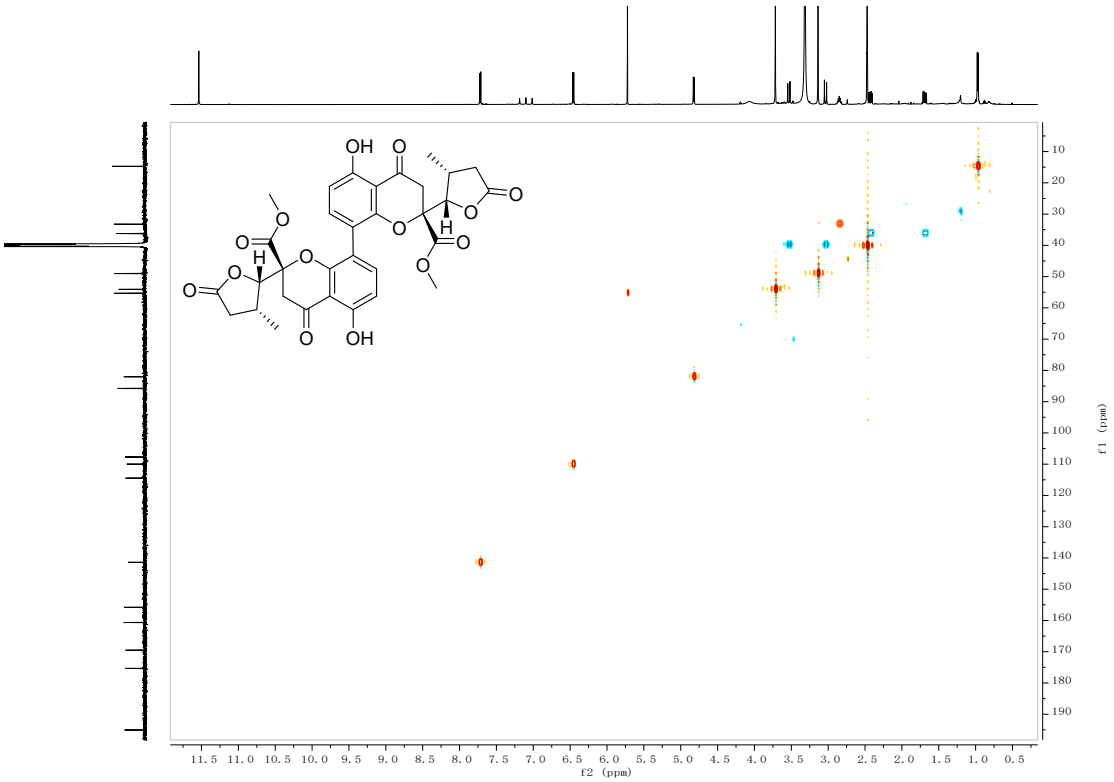


Figure S37. HMBC spectrum of **3** in DMSO-d_6

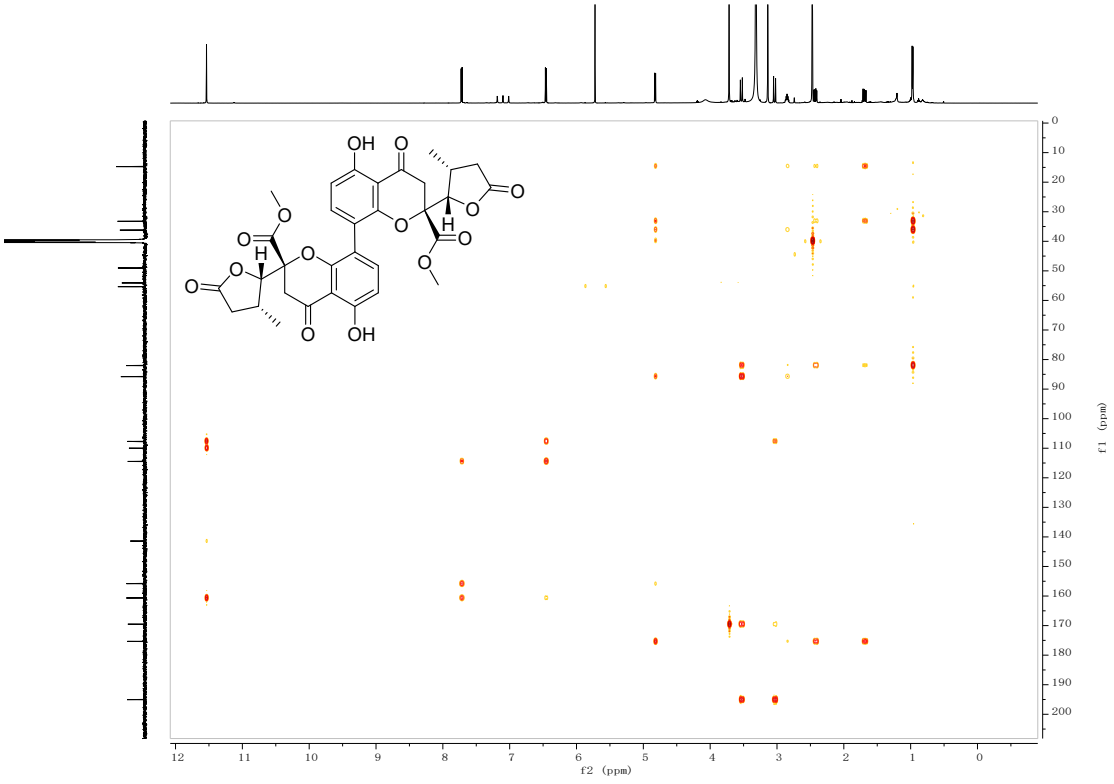


Figure S38. NOESY spectrum of **3** in DMSO-d_6

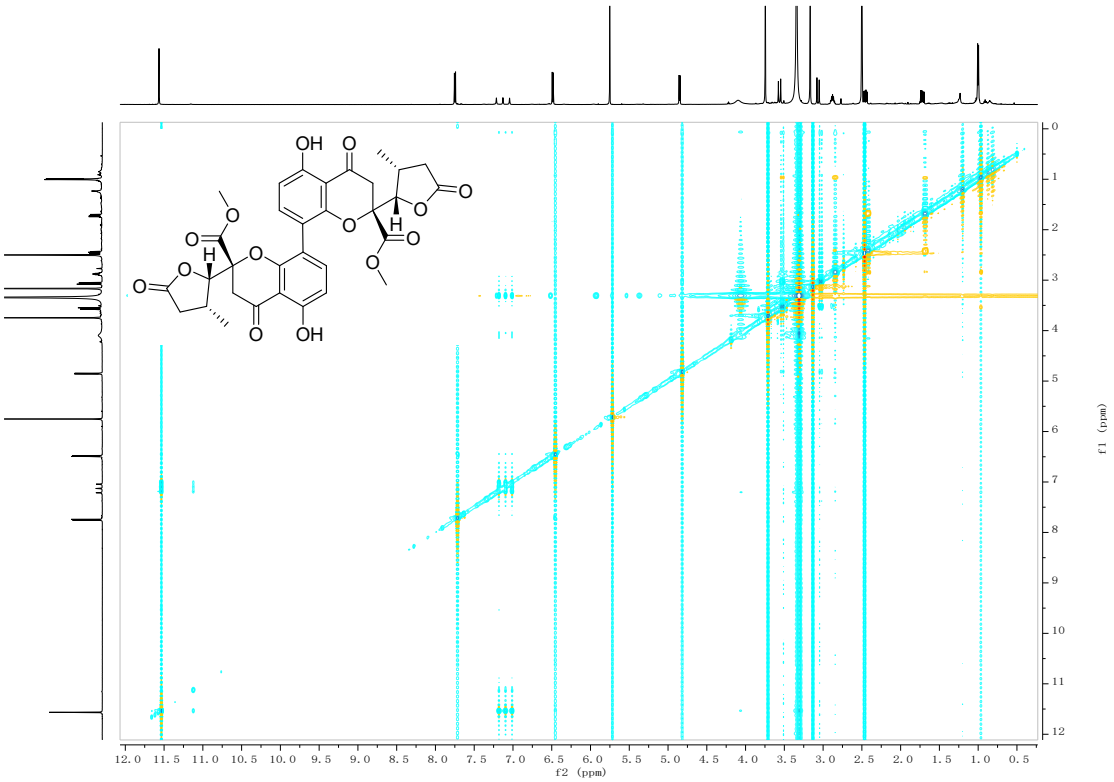


Figure S39. HRESIMS spectrum of **3**

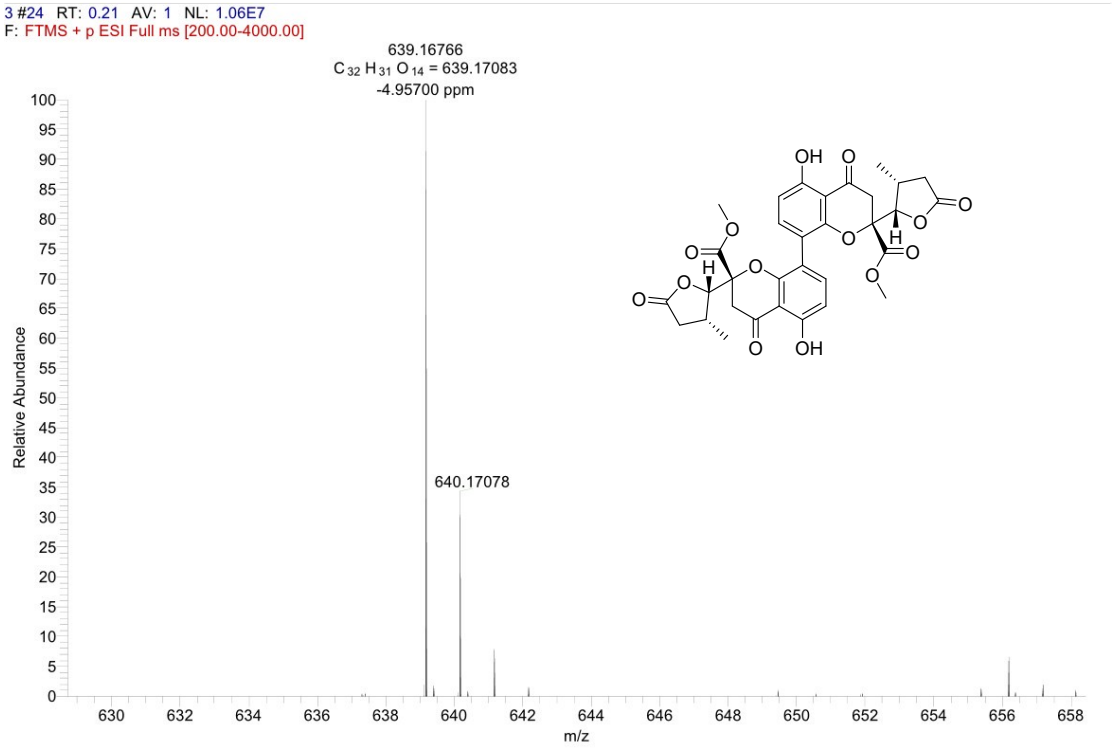
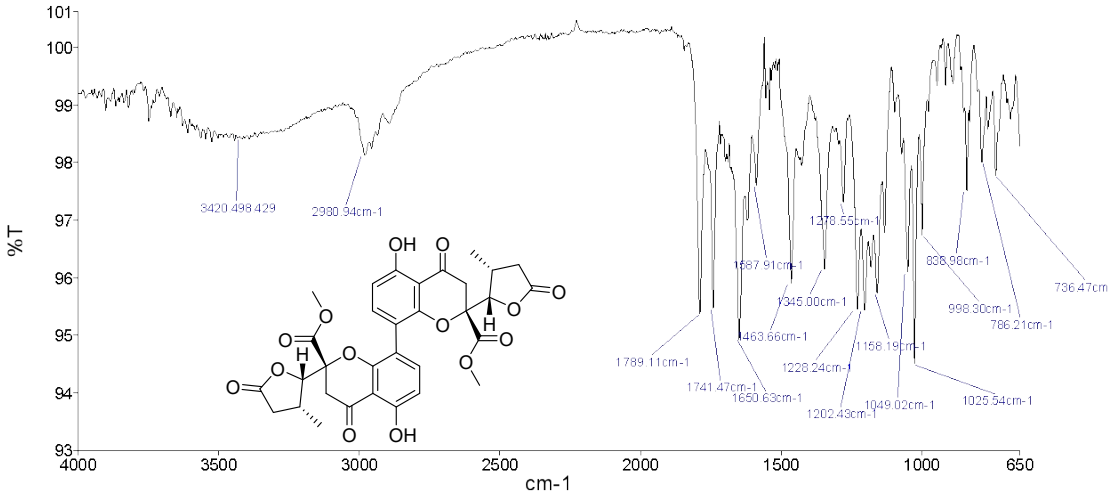


Figure S40. IR spectrum of 3



傅立叶变换显微镜红外 (FT-IR Microscope)

Figure S41. UV spectrum of **3**

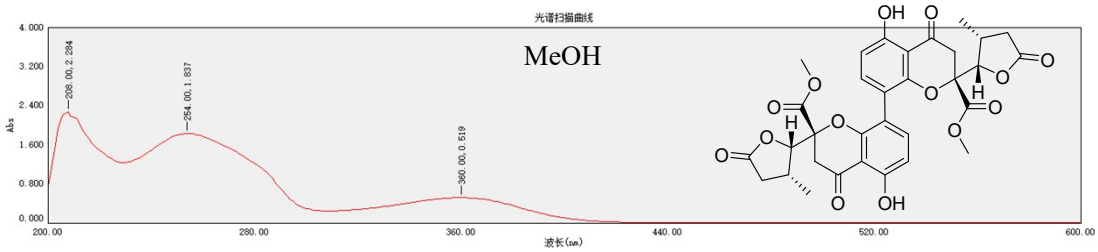
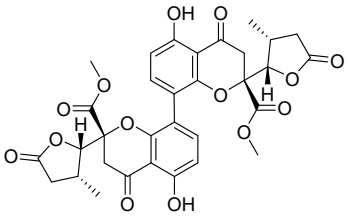
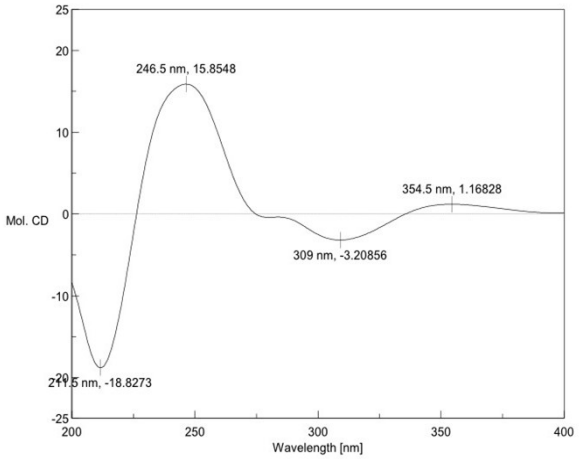


Figure S42. ECD spectrum of **3**





[Comments]
Sample name 114h-21-3-1
Comment

[Measurement Information]
Instrument Name IMM-CD
Model Name IM-45
Serial No. A024461168

Accessory Standard
Accessory S/N A005461185
Cell Length 1 mm

Measurement date 2021/7/5 11:06

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Measure Range 400 - 200 nm
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Sensitivity Standard
D.I.T. 1 sec
Bandwidth 1.00 nm
Start Mode Immediately
Scanning Speed 100 nm/min
Baseline Correction Baseline
Shutter Control Auto
CD Detector PMT
PMT Voltage Auto
Accumulations 2
Solvent MEOH
Concentration 0.5 (w/v)%

[Detailed Information]
Creation date 2021/7/5 14:27

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Vertical axis(1) Mol. CD
Vertical axis(2) HT [V]
Vertical axis(3) Abs
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End 200 nm
Data interval 0.5 nm
Data points 401