Supplementary Information

Terpenoids from *Penicillium chrysogenum* MT-40, an Endophytic Fungus Isolated from *Huperzia serrata*

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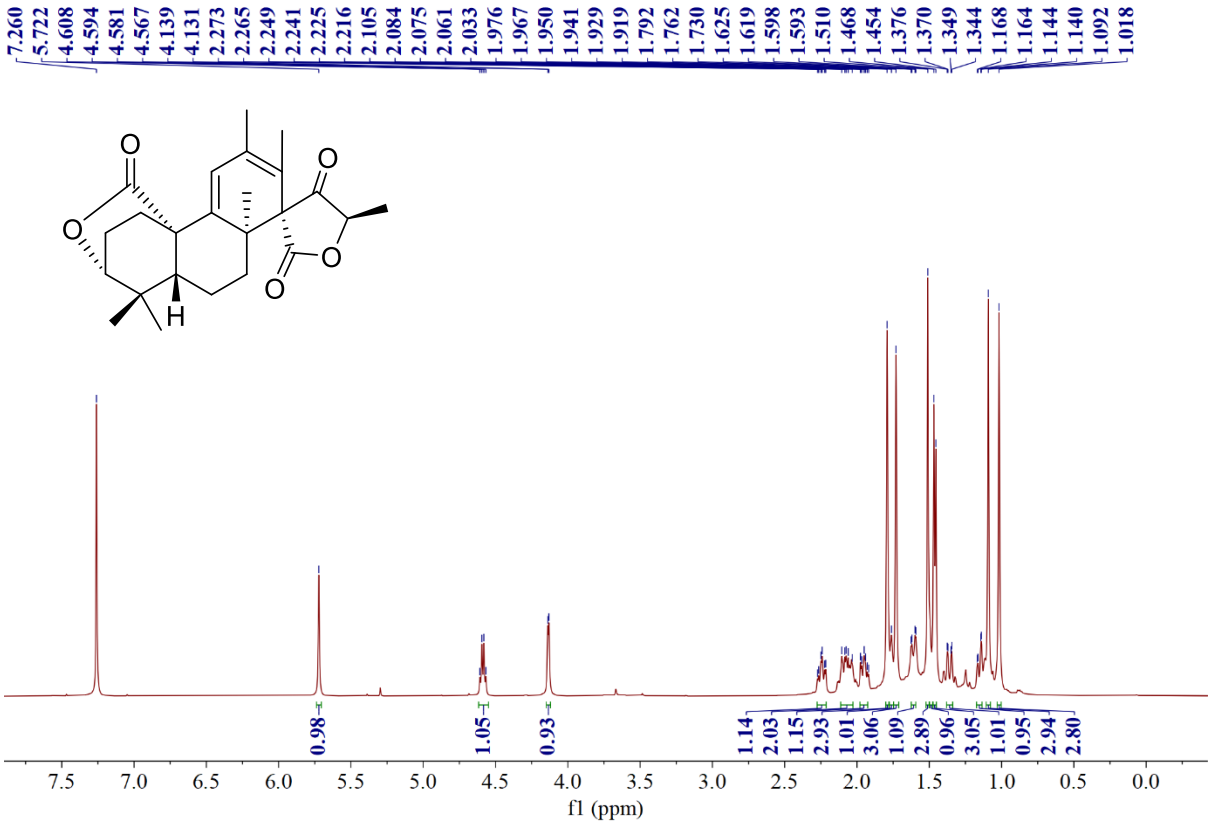


Fig. S1 ^{1}H NMR spectrum of compound **1** (in $CDCl_3$, 500 MHz)

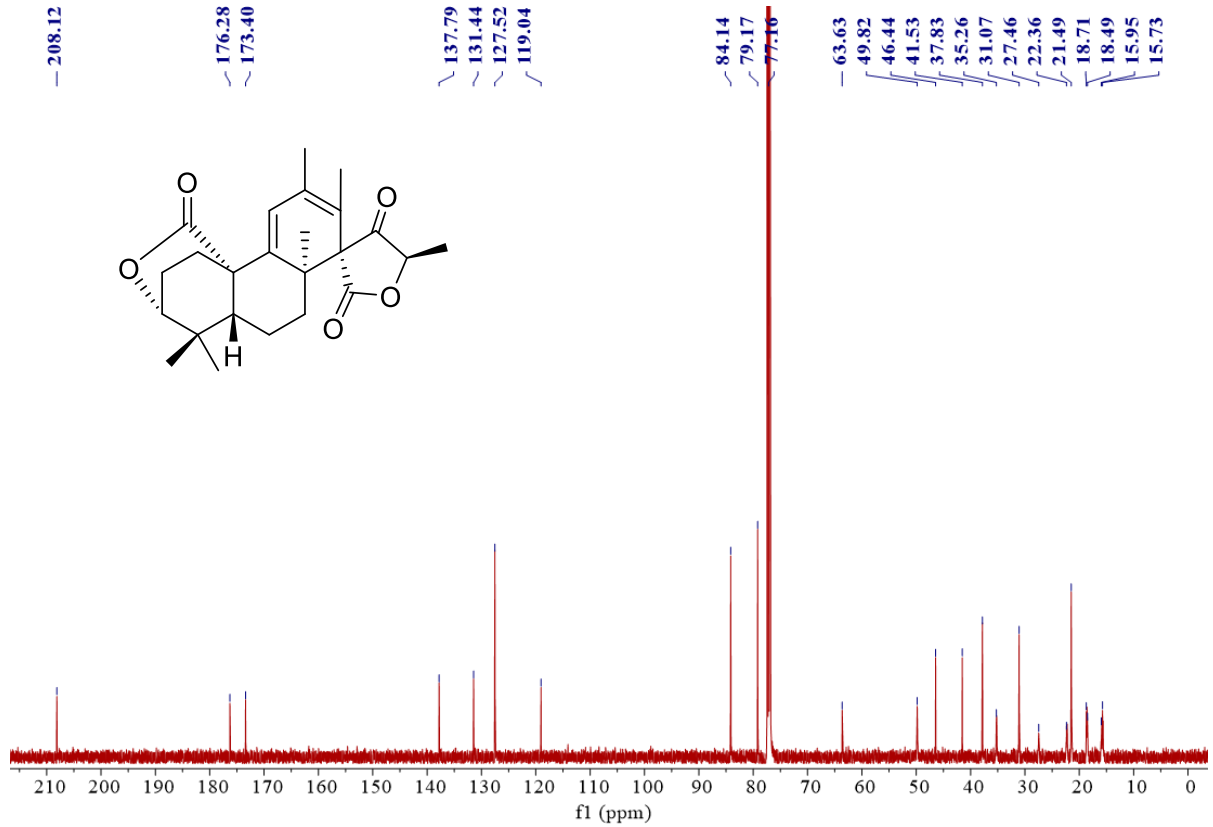


Fig. S2 ^{13}C NMR spectrum of compound **1** (in $CDCl_3$, 125 MHz)

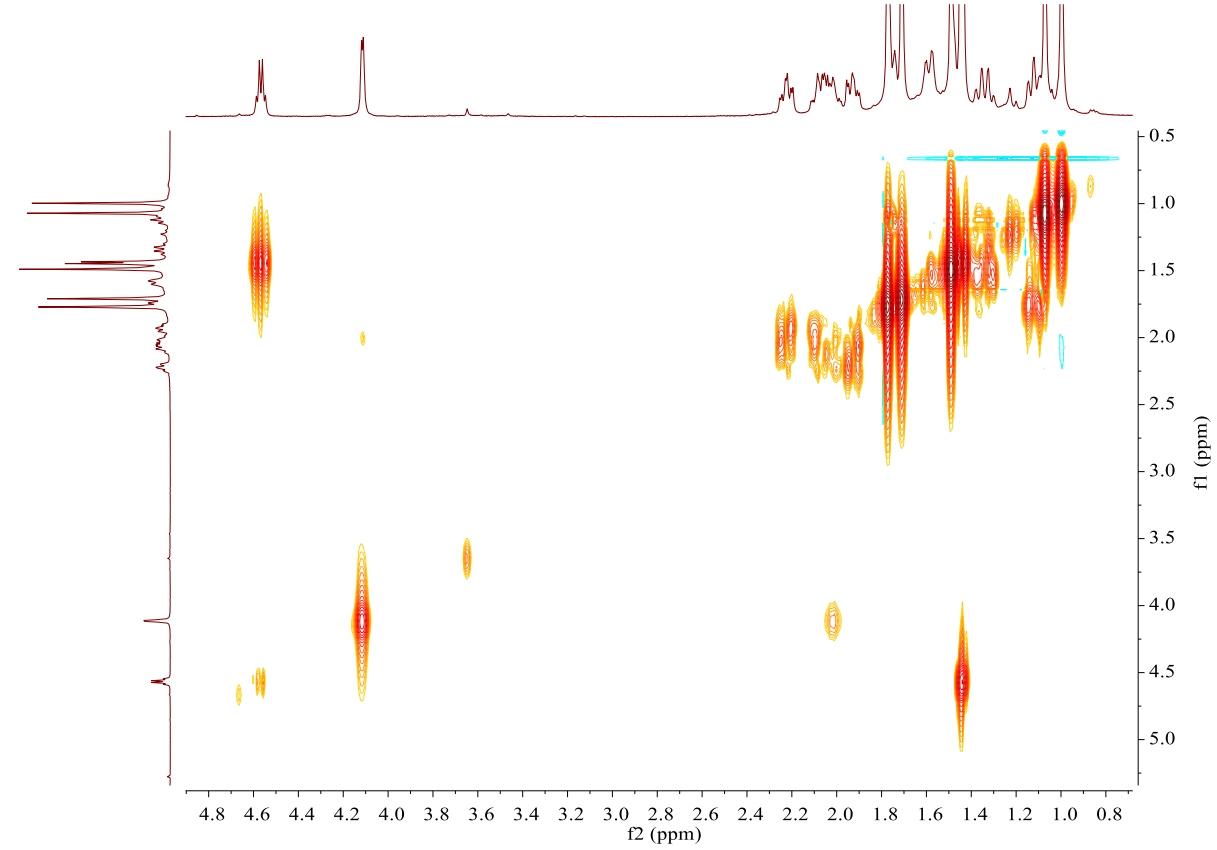


Fig. S3 ^{1}H-^{1}H COSY spectrum of compound **1**

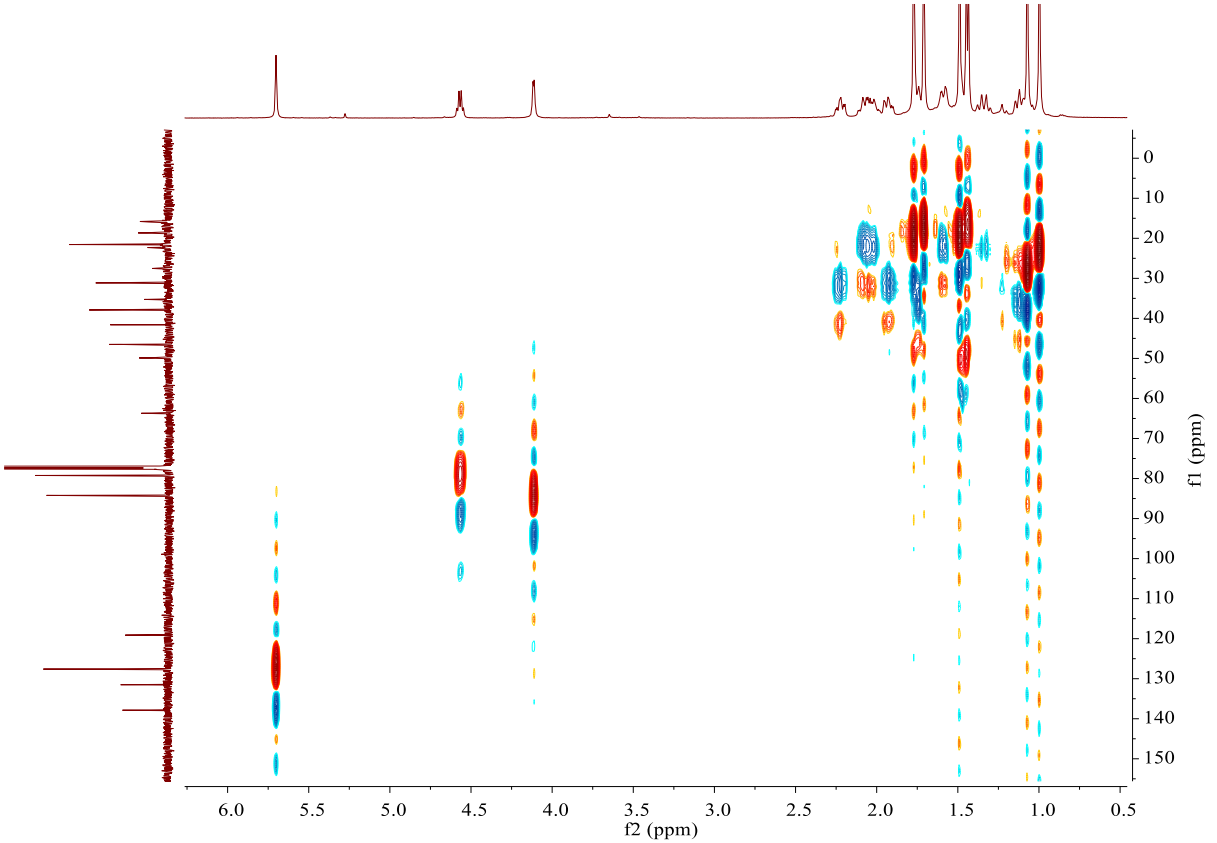


Fig. S4 gHSQC spectrum of compound **1**

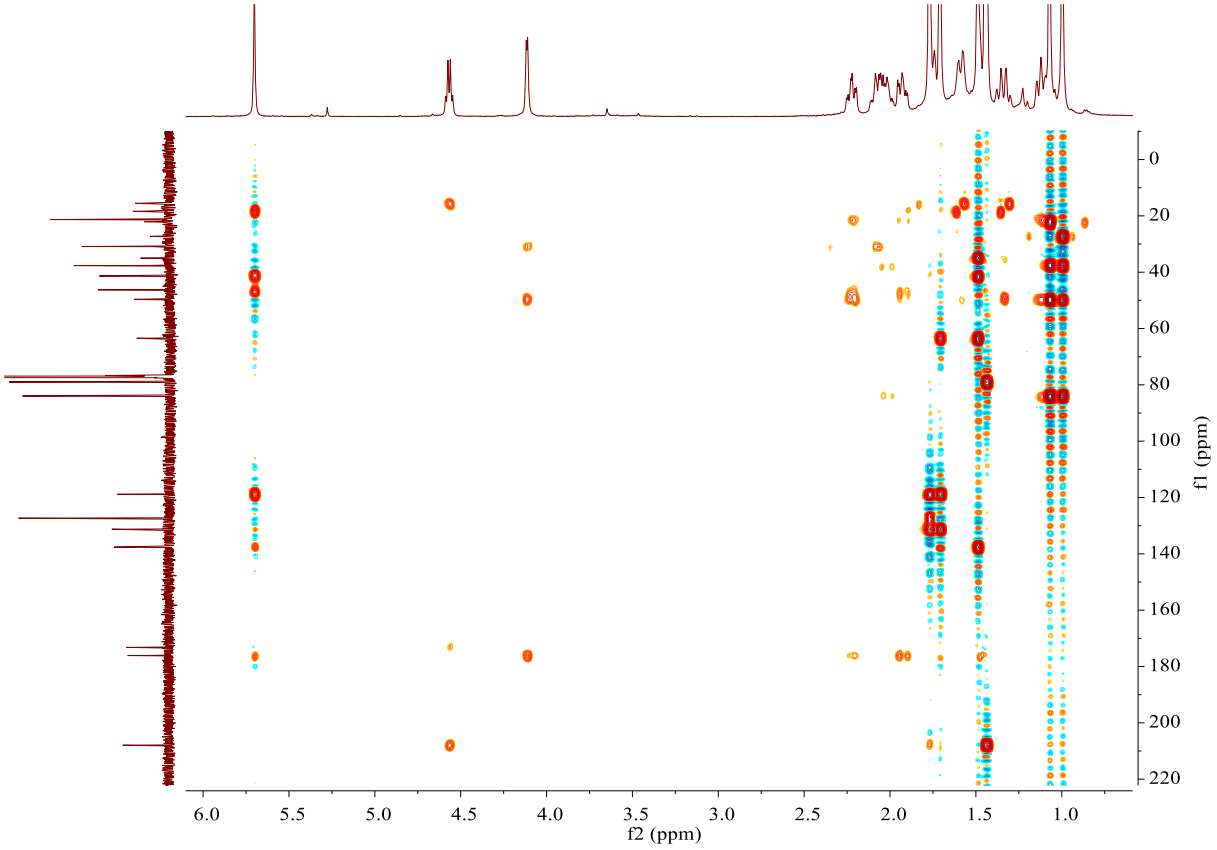


Fig. S5 gHMBC spectrum of compound **1**

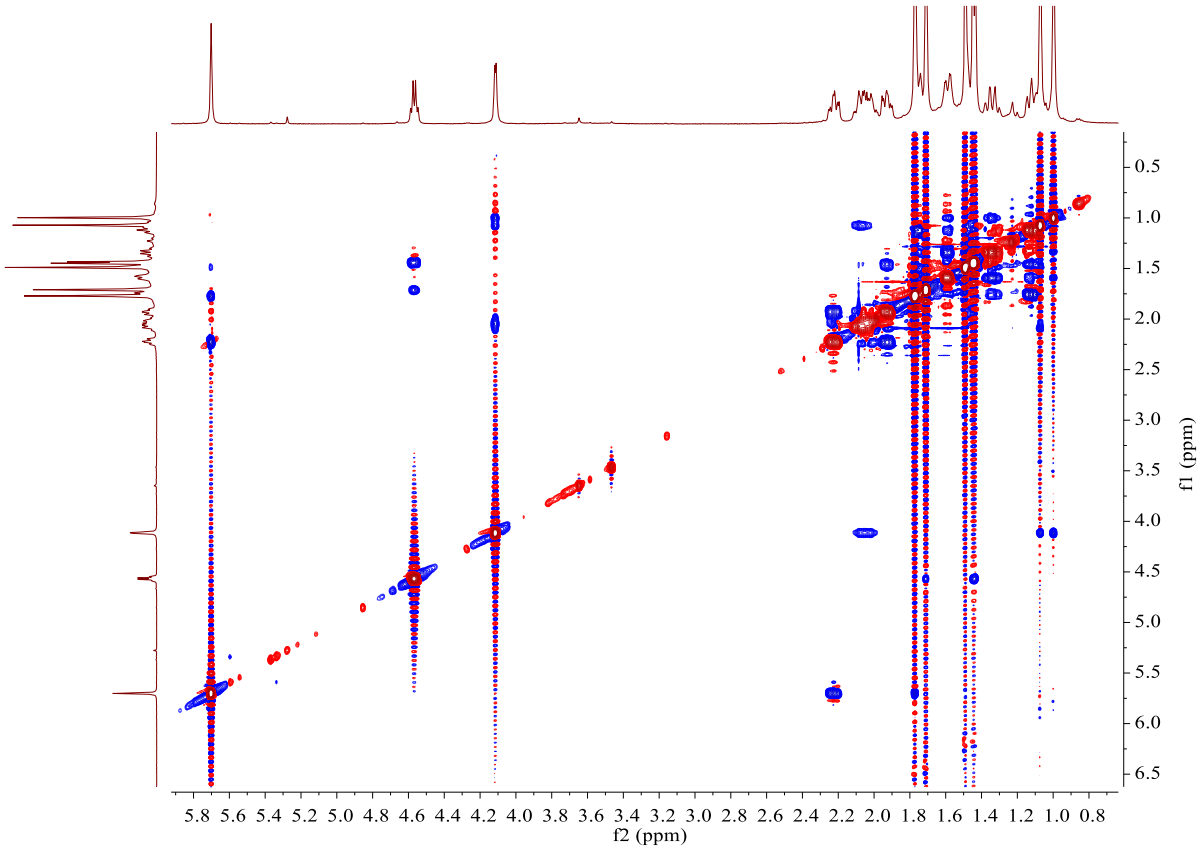
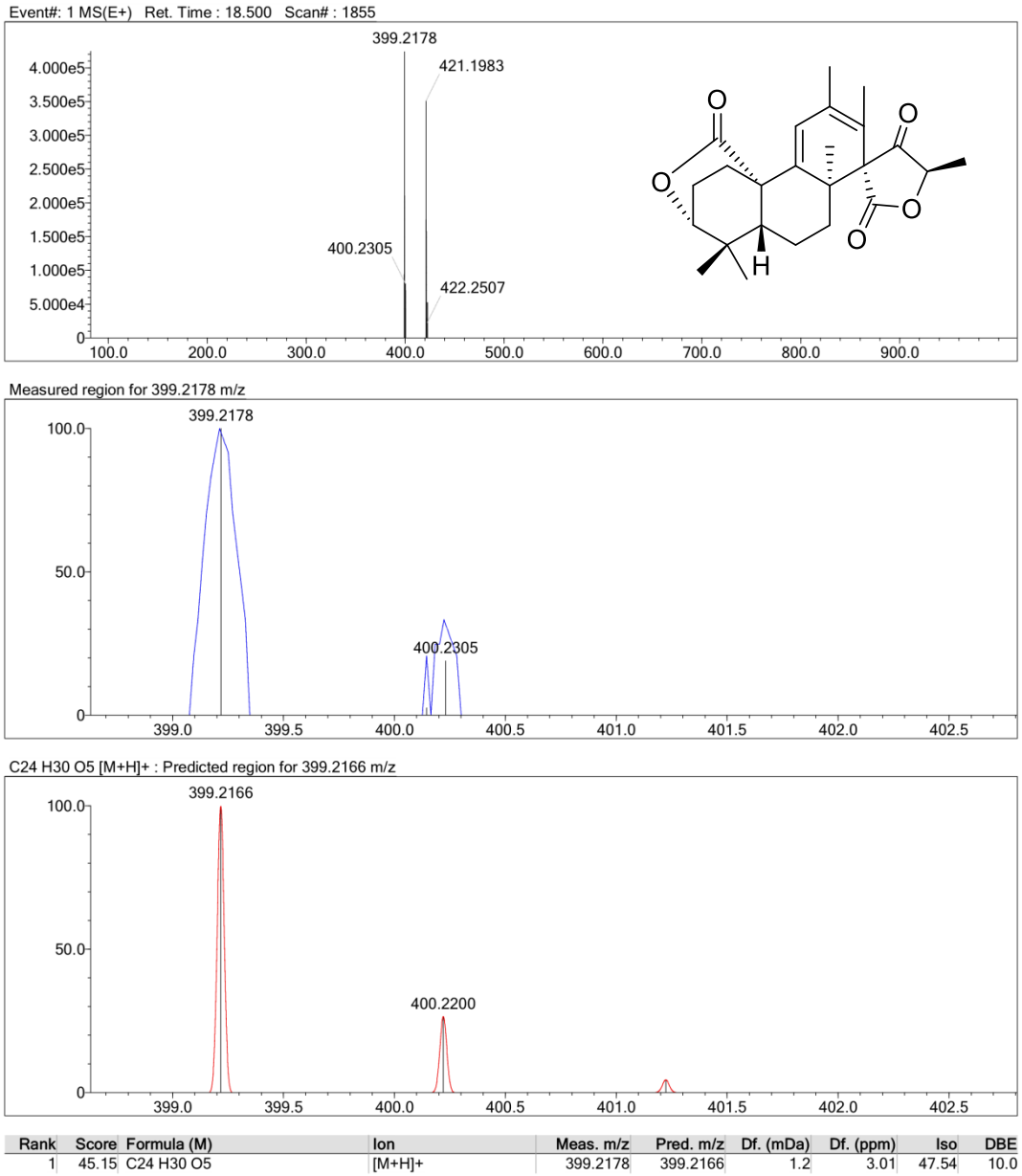


Fig. S6 NOESY spectrum of compound **1**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	45.15	C24 H30 O5	[M+H]+	399.2178	399.2166	1.2	3.01	47.54	10.0

Fig. S7 HRESIMS spectrum of compound **1**

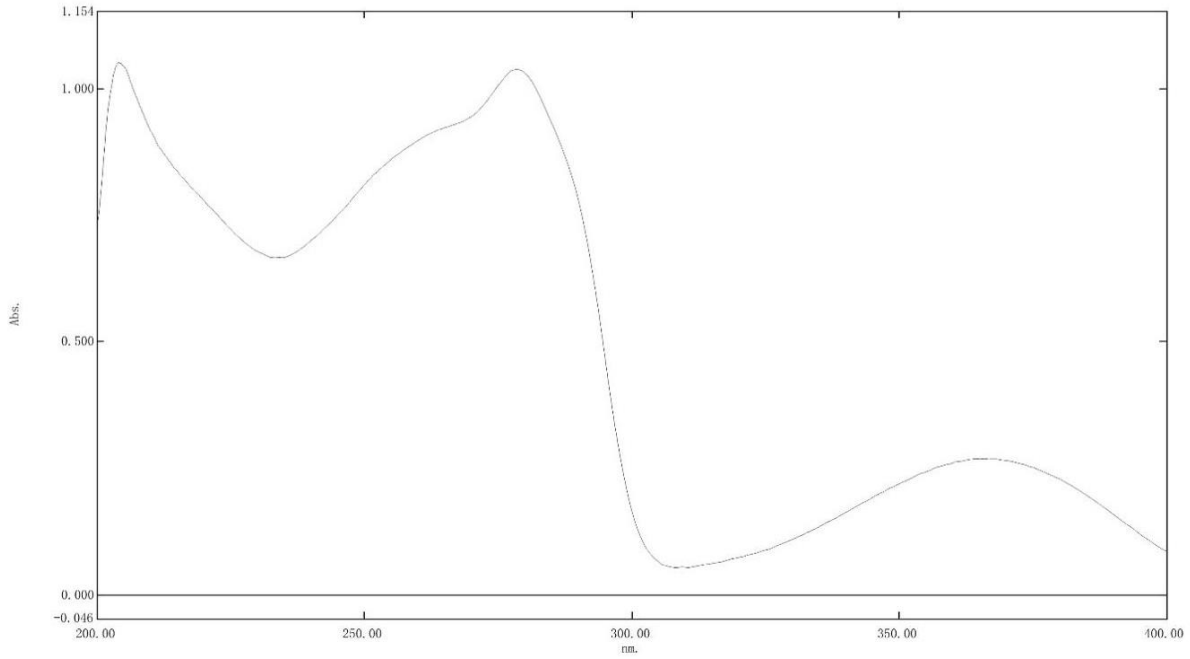


Fig. S8 UV spectrum of compound **1**

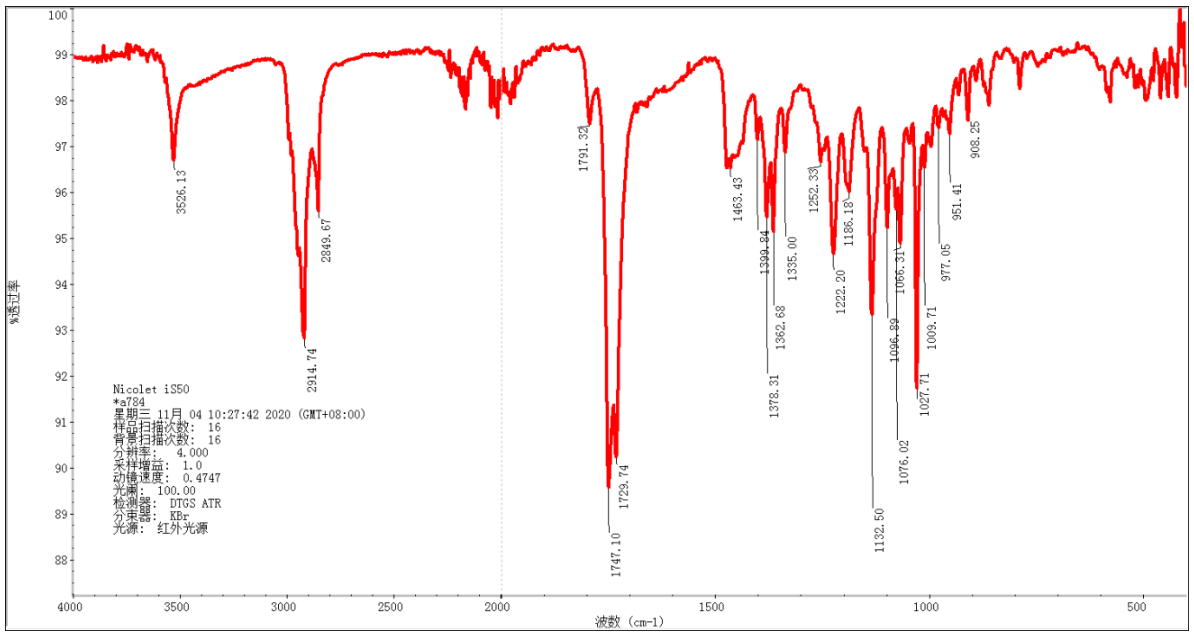


Fig. S9 IR spectrum of compound **1**

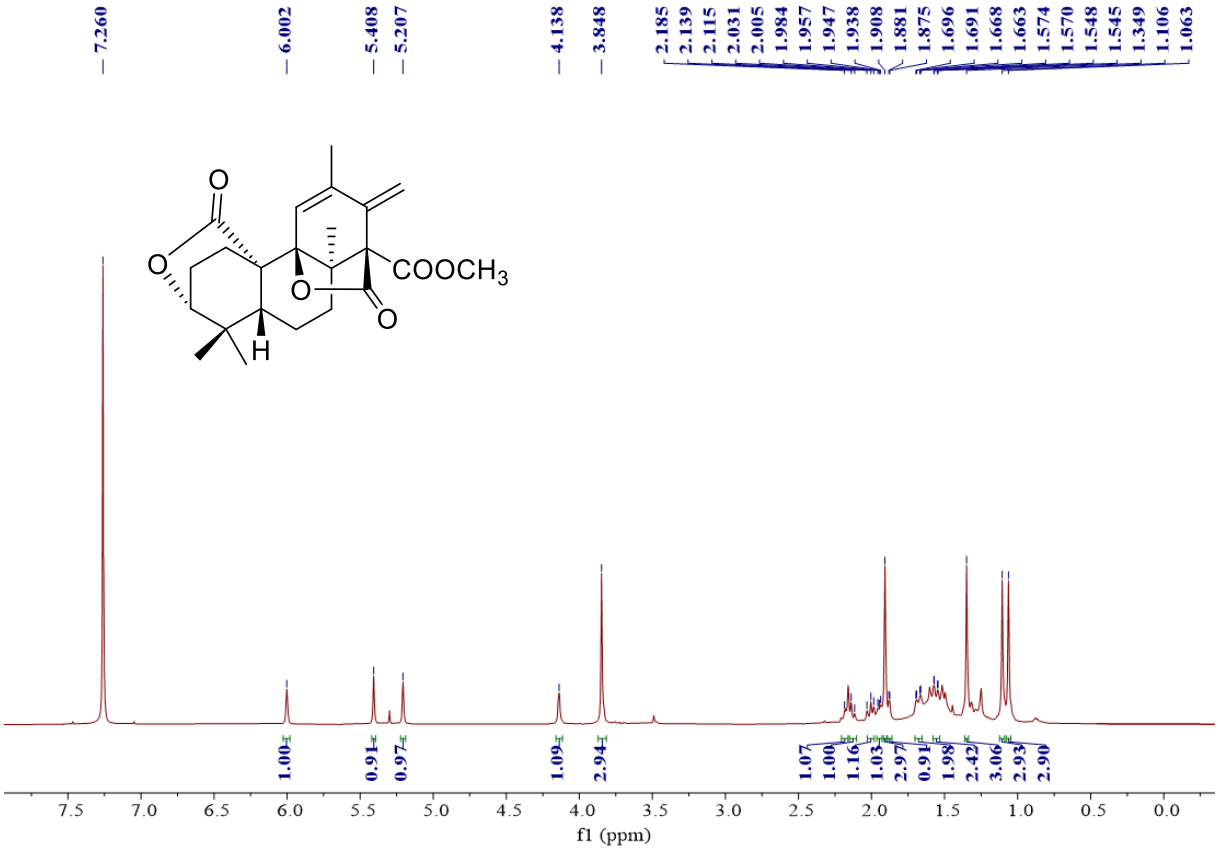


Fig. S10 ^{1}H NMR spectrum of compound **2** (in $CDCl_3$, 500 MHz)

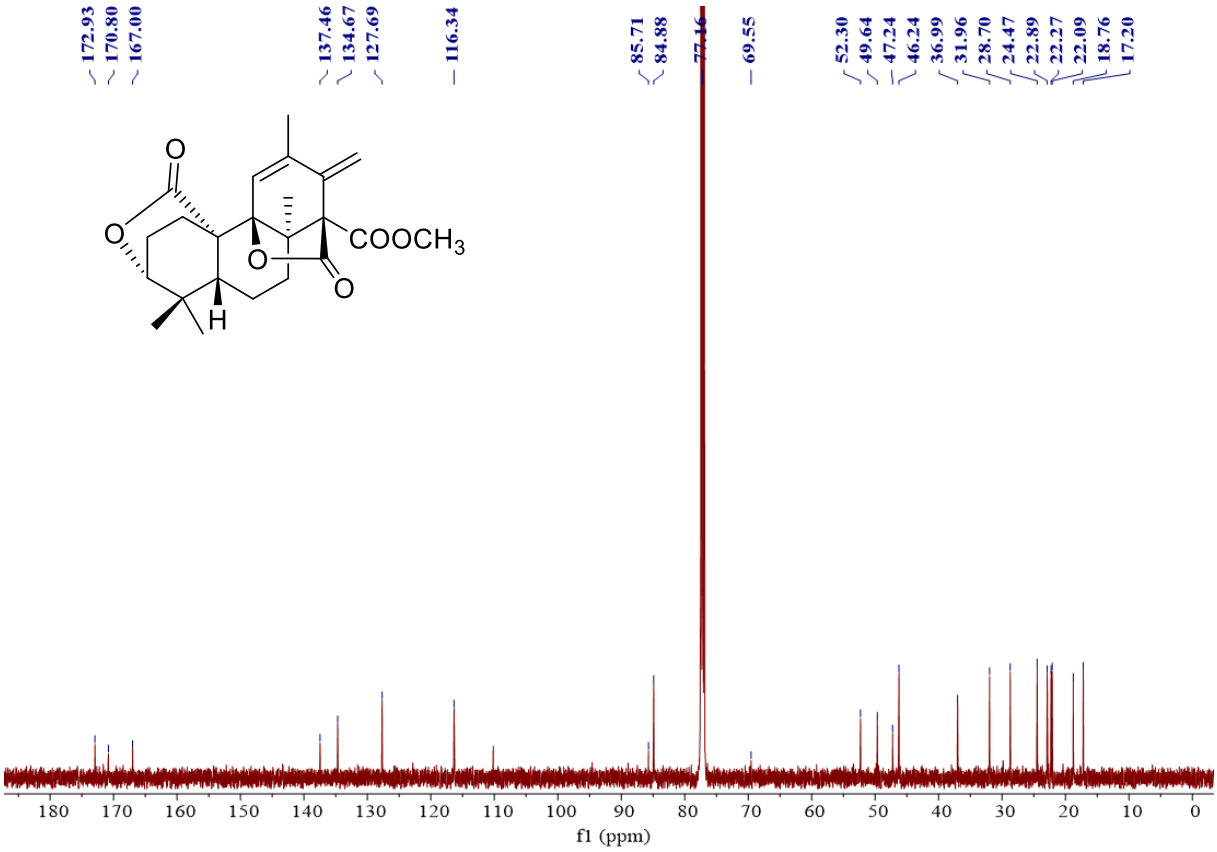


Fig. S11 ^{13}C NMR spectrum of compound **2** (in $CDCl_3$, 125 MHz)

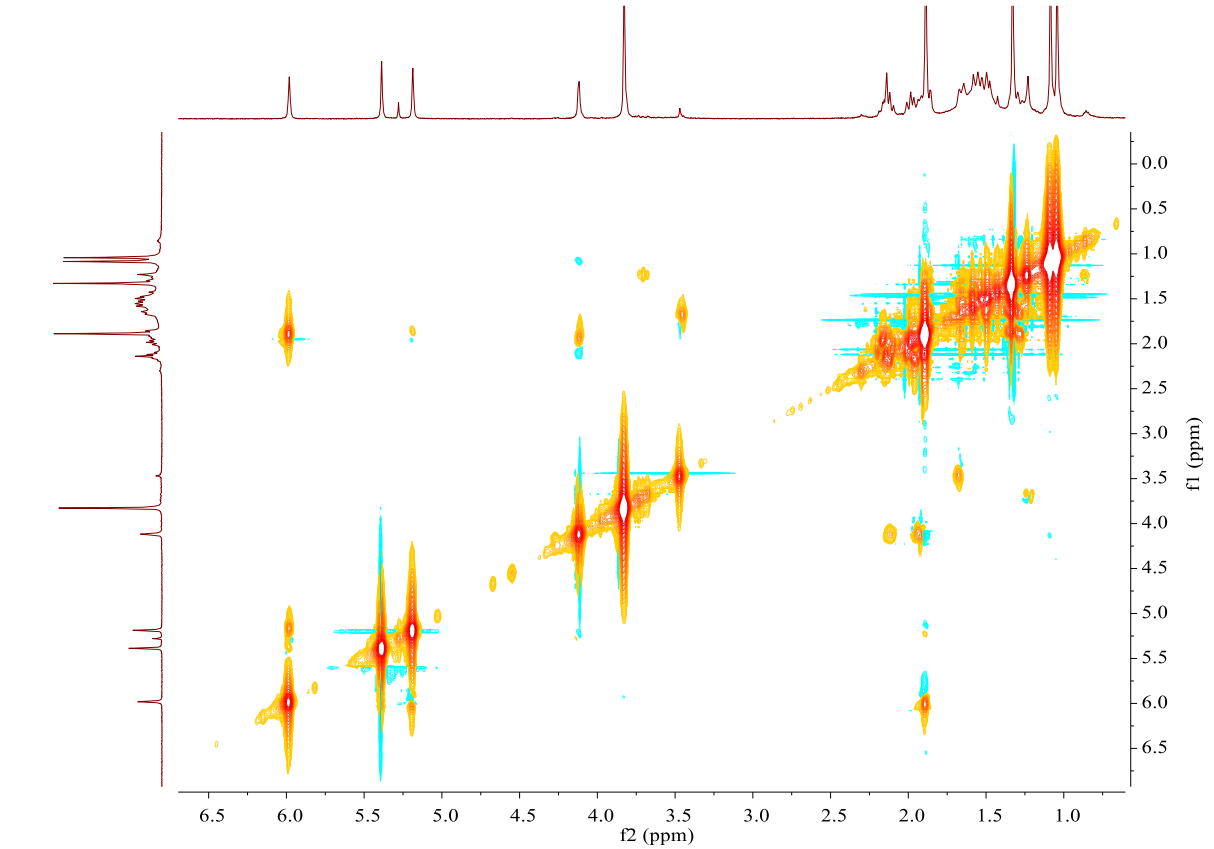


Fig.S12 ^{1}H-^{1}H COSY spectrum of compound **2**

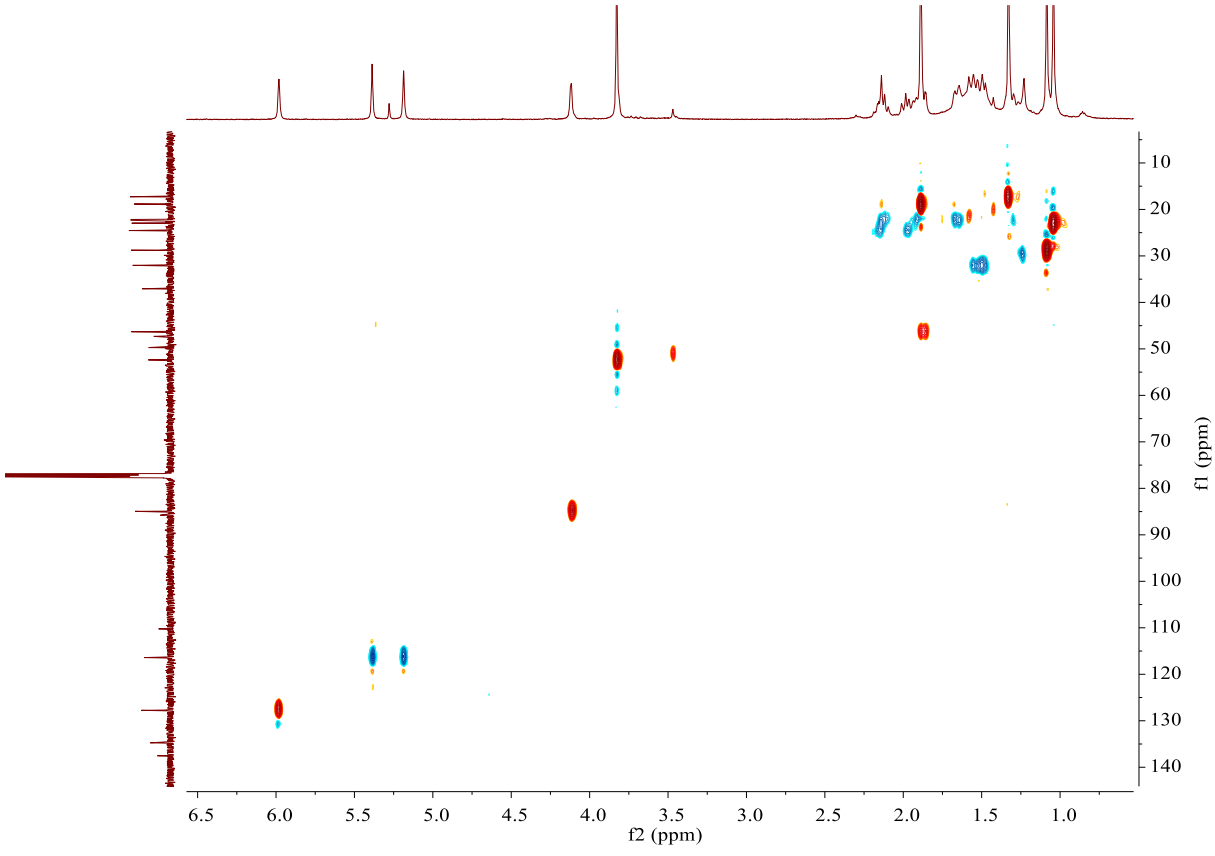


Fig. S13 gHSQC spectrum of compound **2**

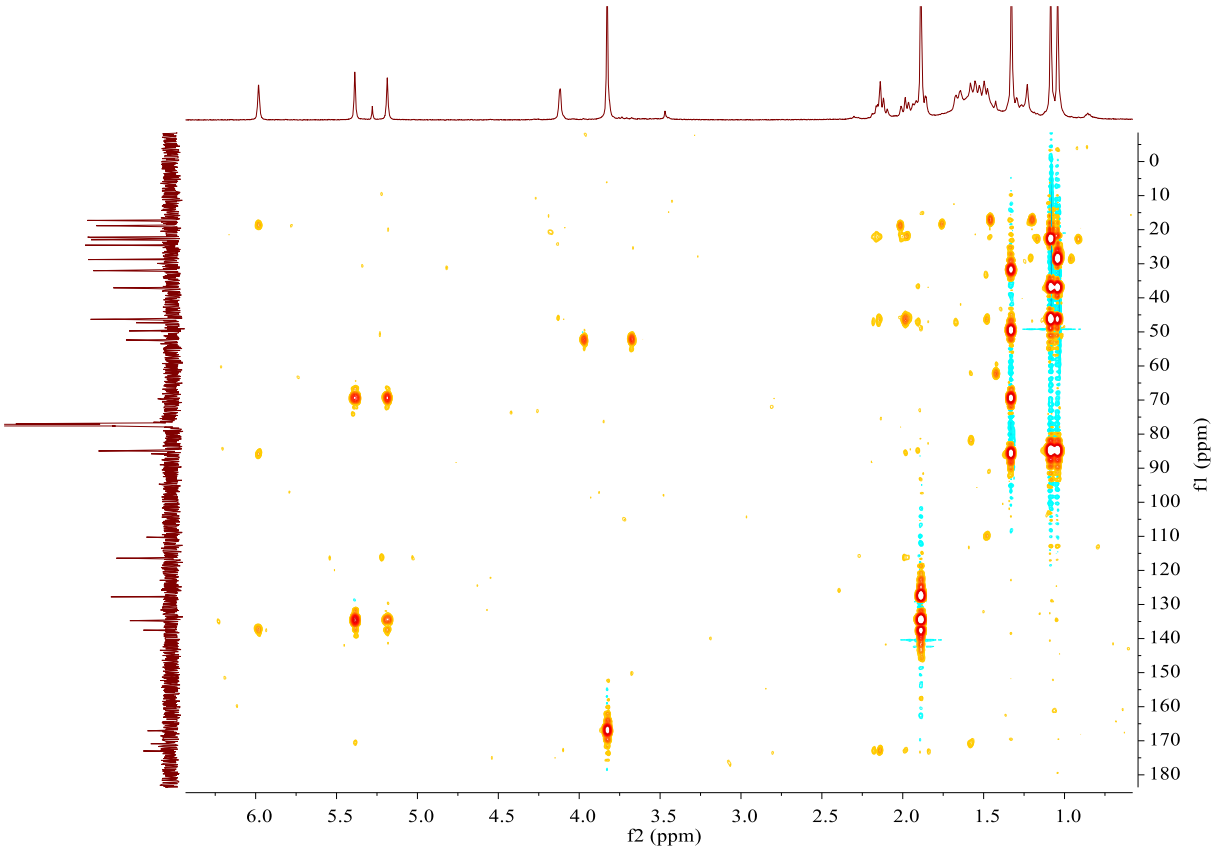


Fig. S14 gHMBC spectrum of compound **2**

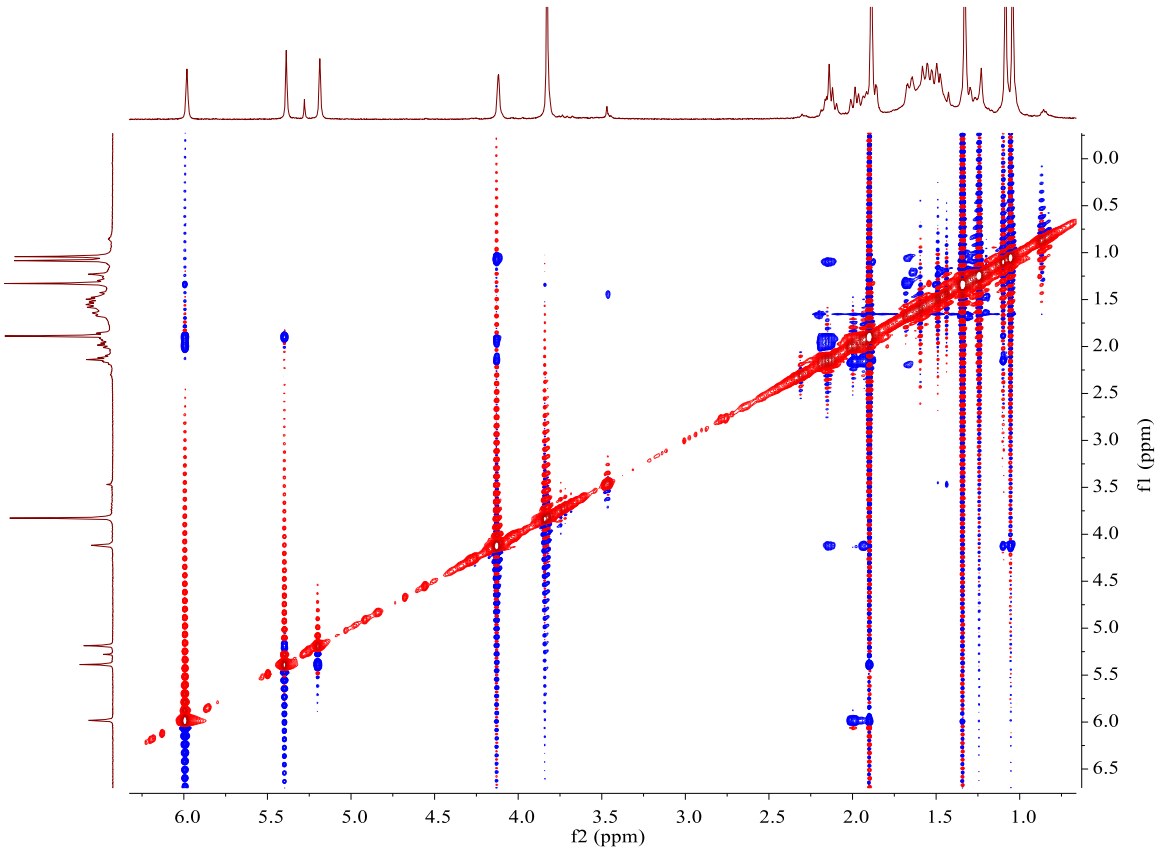
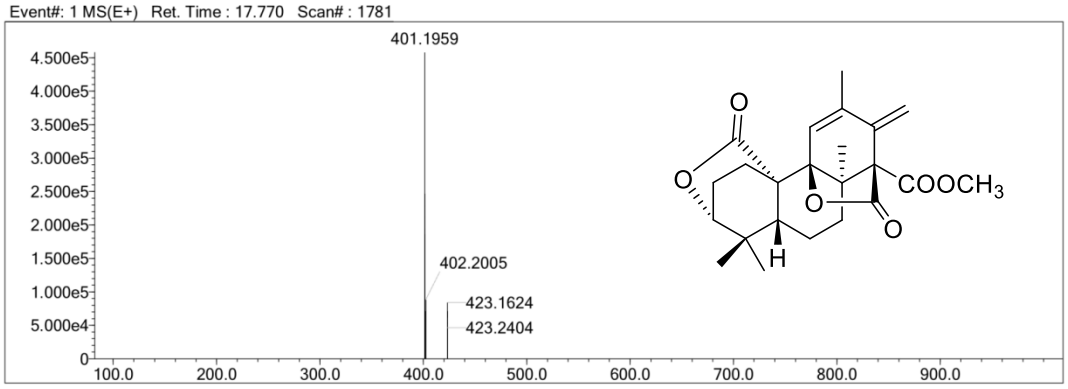
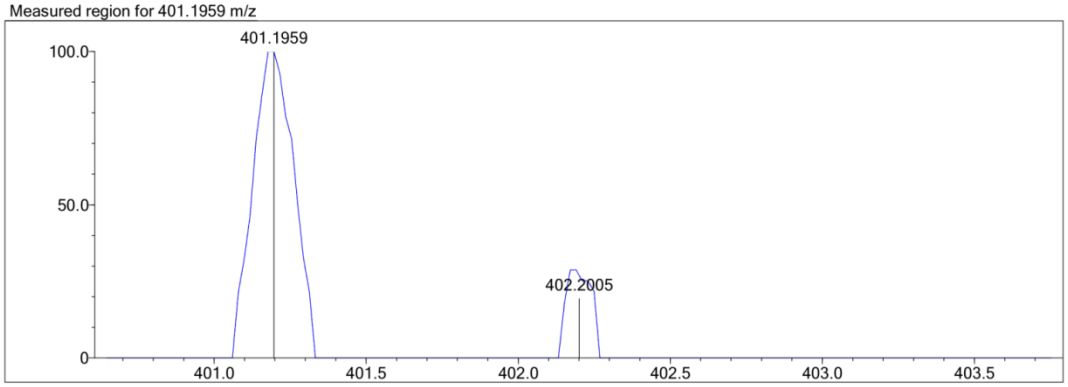
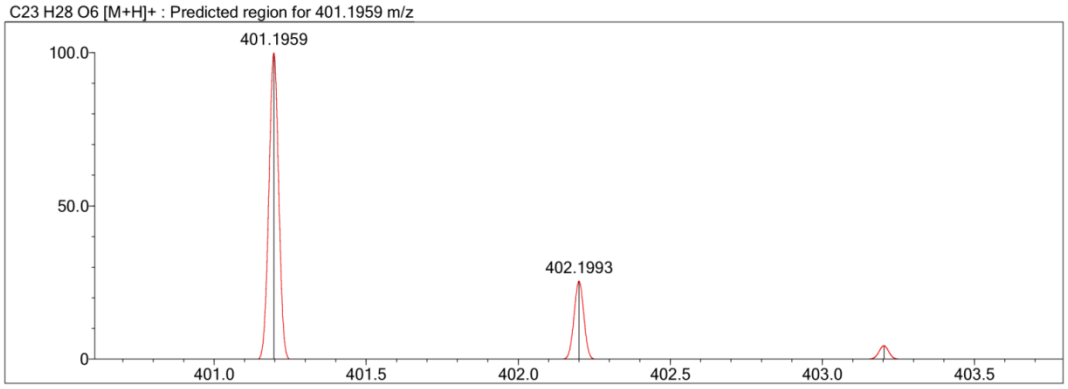


Fig. S15 NOESY spectrum of compound **2**







Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	70.02	C23 H28 O6	[M+H]+	401.1959	401.1959	0.0	0.00	70.02	10.0

Fig. S16 HRESIMS spectrum of compound **2**

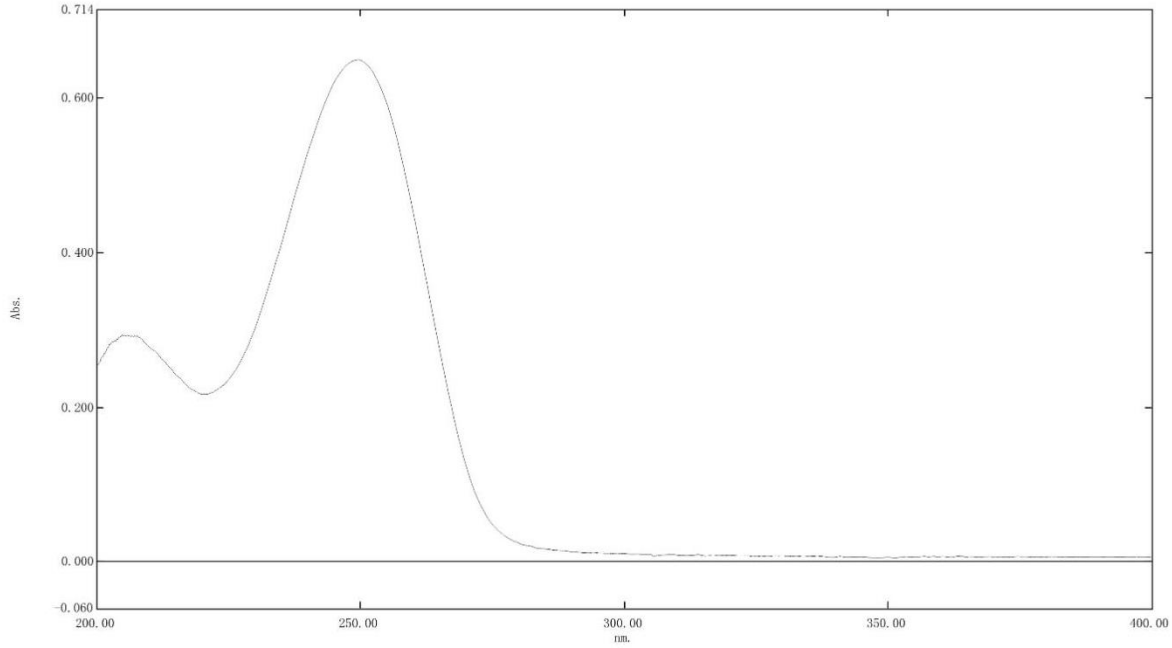


Fig. S17 UV spectrum of compound **2**

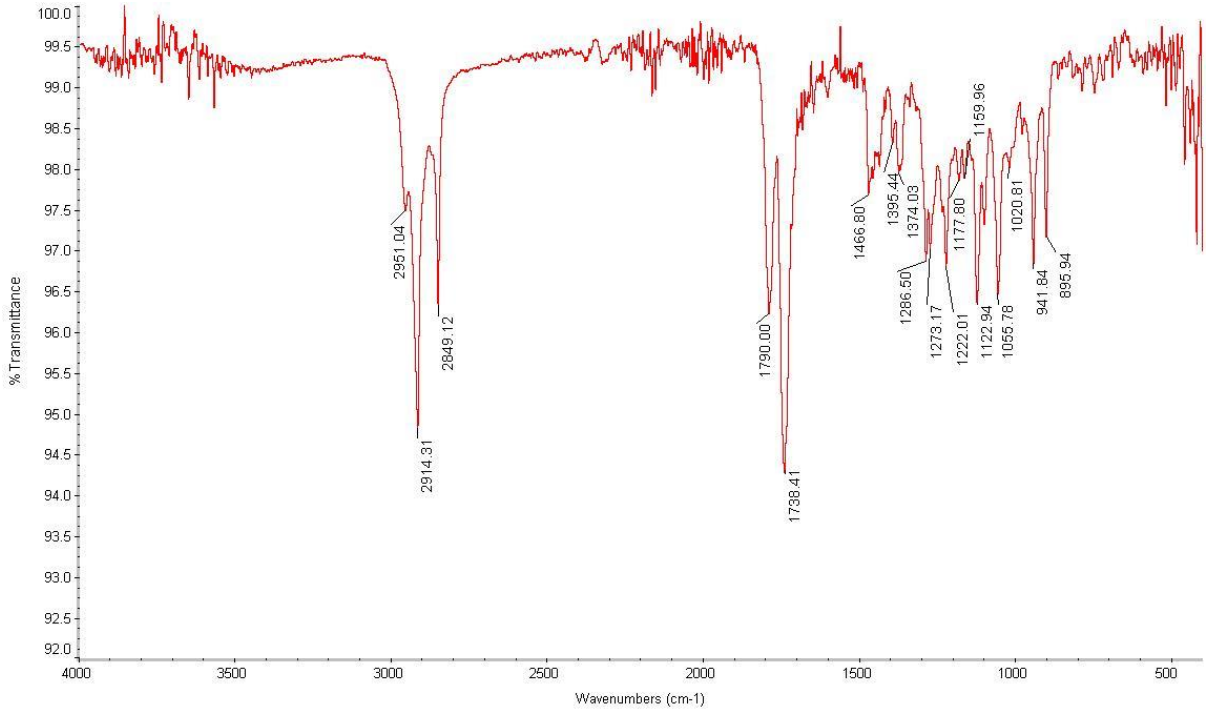


Fig. S18 IR spectrum of compound **2**

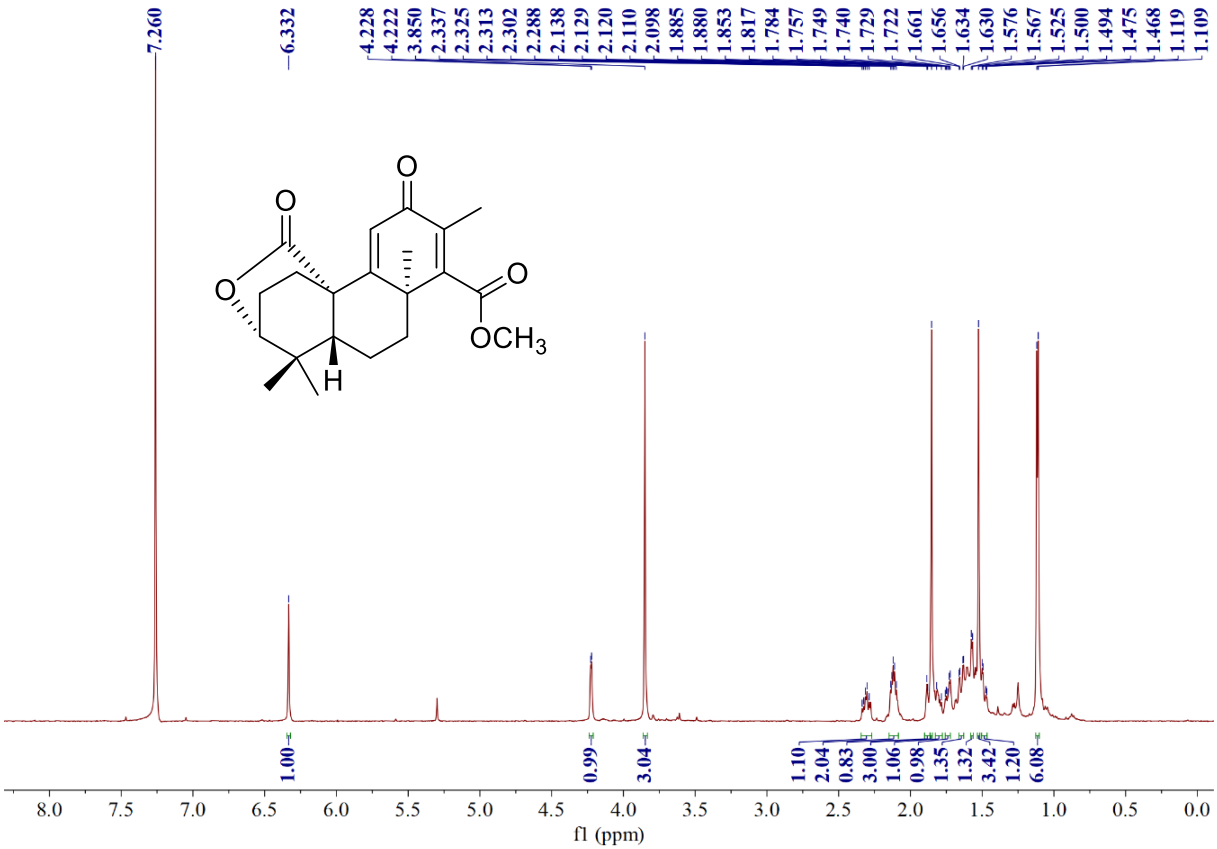


Fig. S19 ^{1}H NMR spectrum of compound **3** (in $CDCl_3$, 500 MHz)

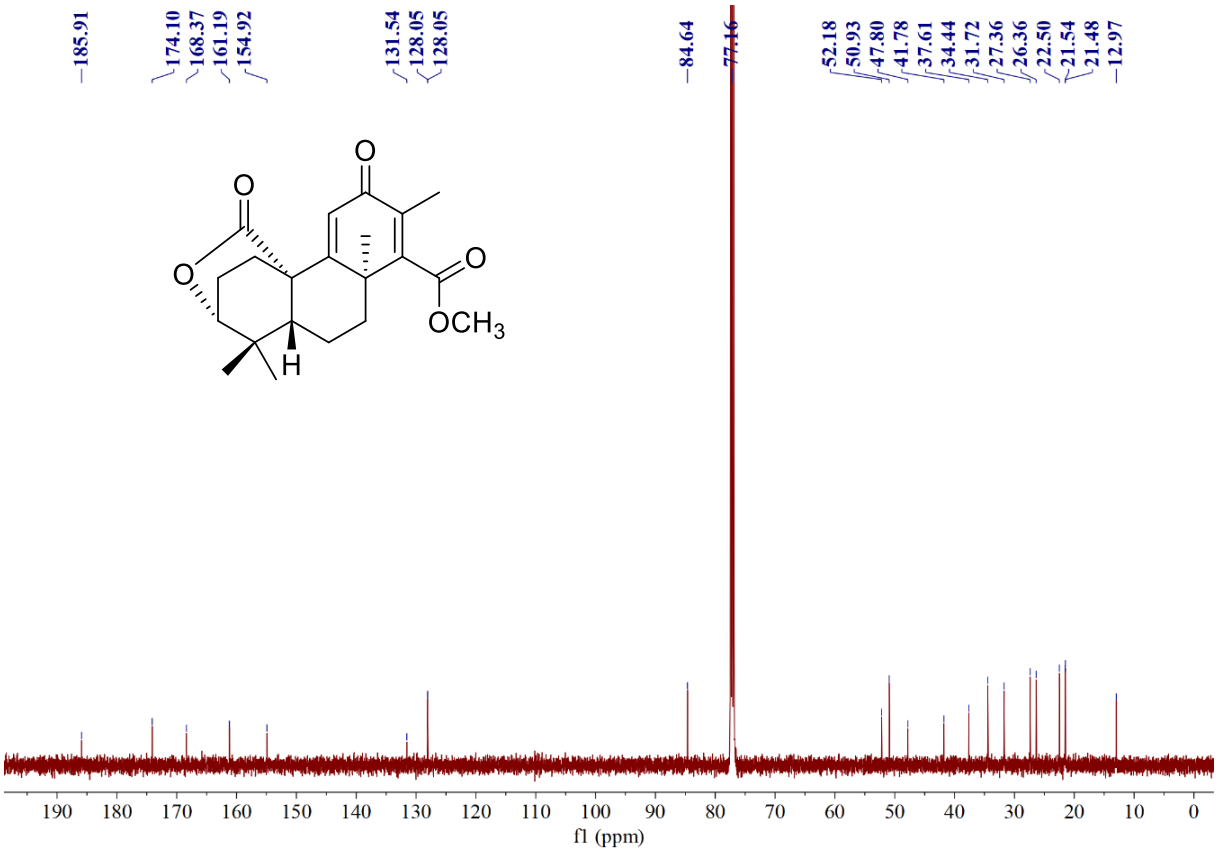


Fig. S20 ^{13}C NMR spectrum of compound **3** (in $CDCl_3$, 125 MHz)

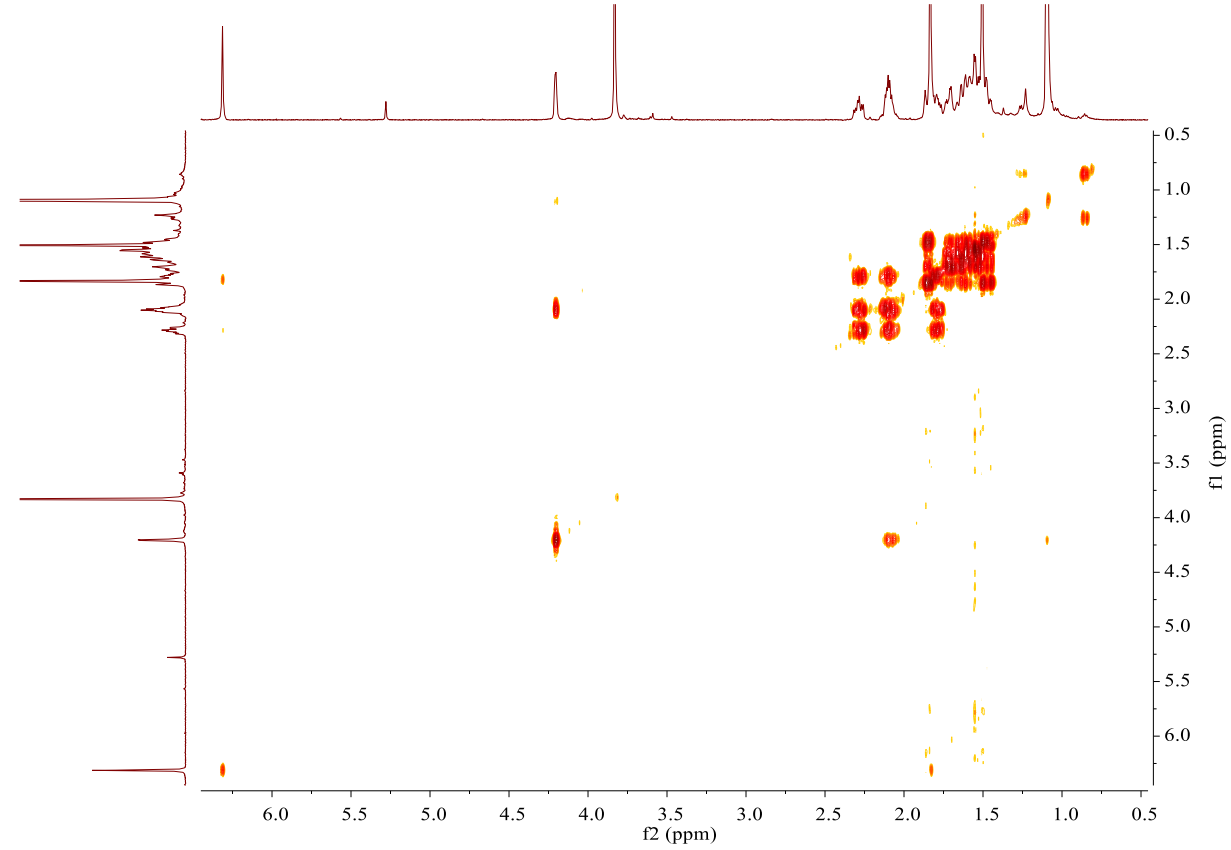


Fig. S21 ^{1}H-^{1}H COSY spectrum of compound **3**

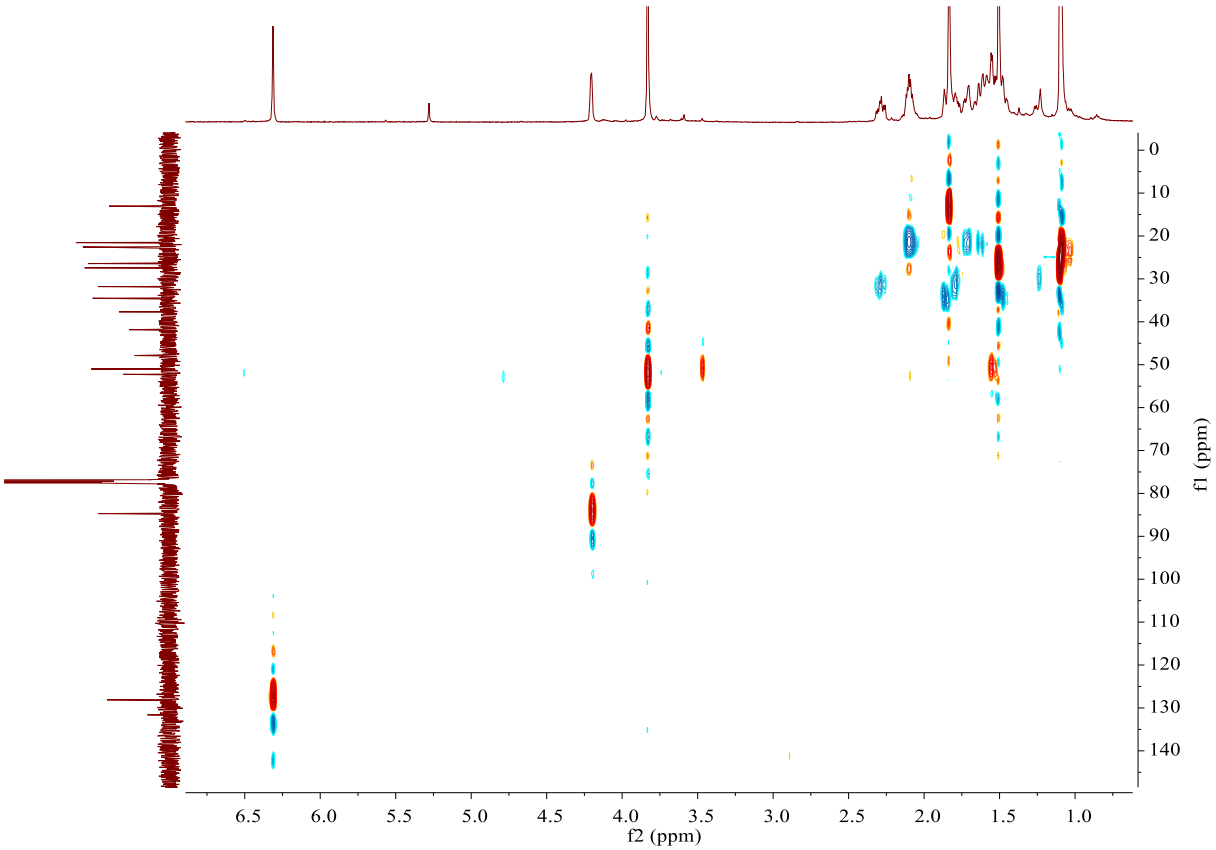


Fig. S22 gHSQC spectrum of compound **3**

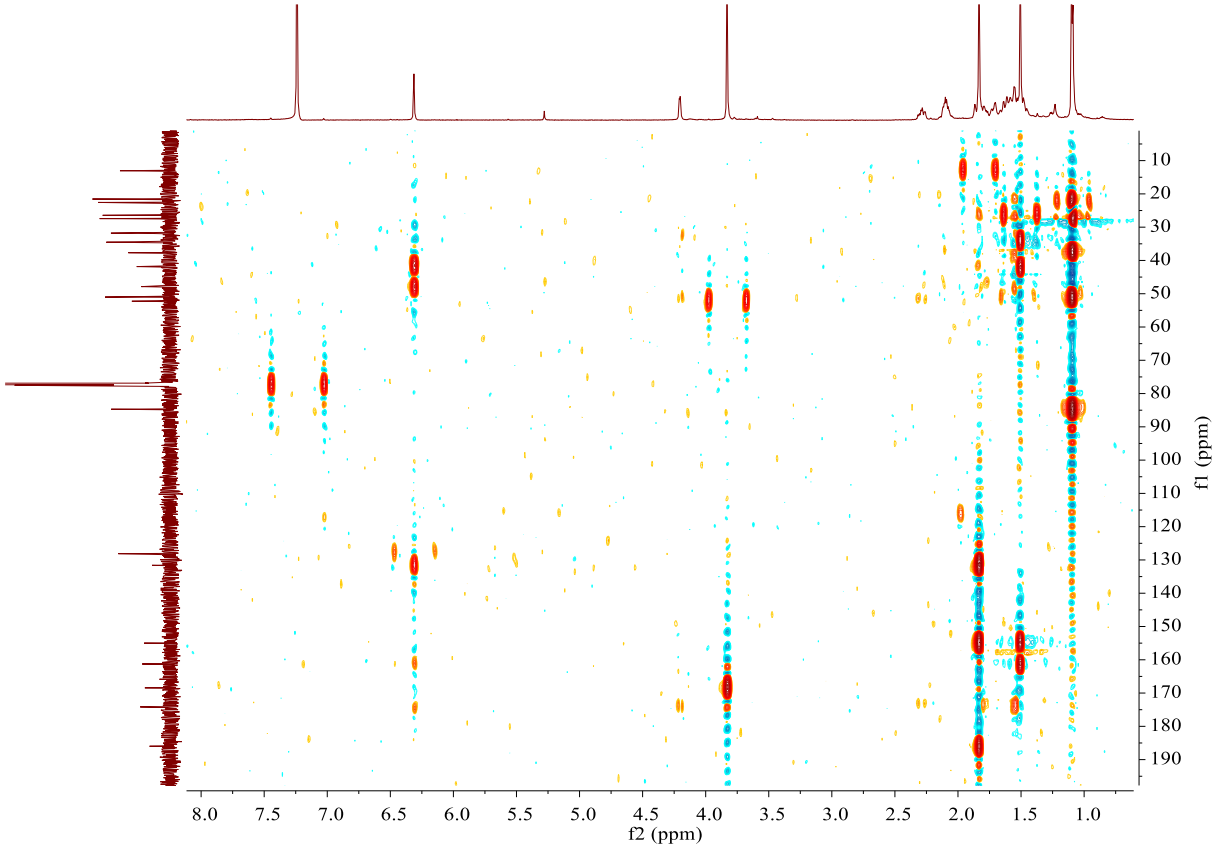


Fig. S23 gHMBC spectrum of compound **3**

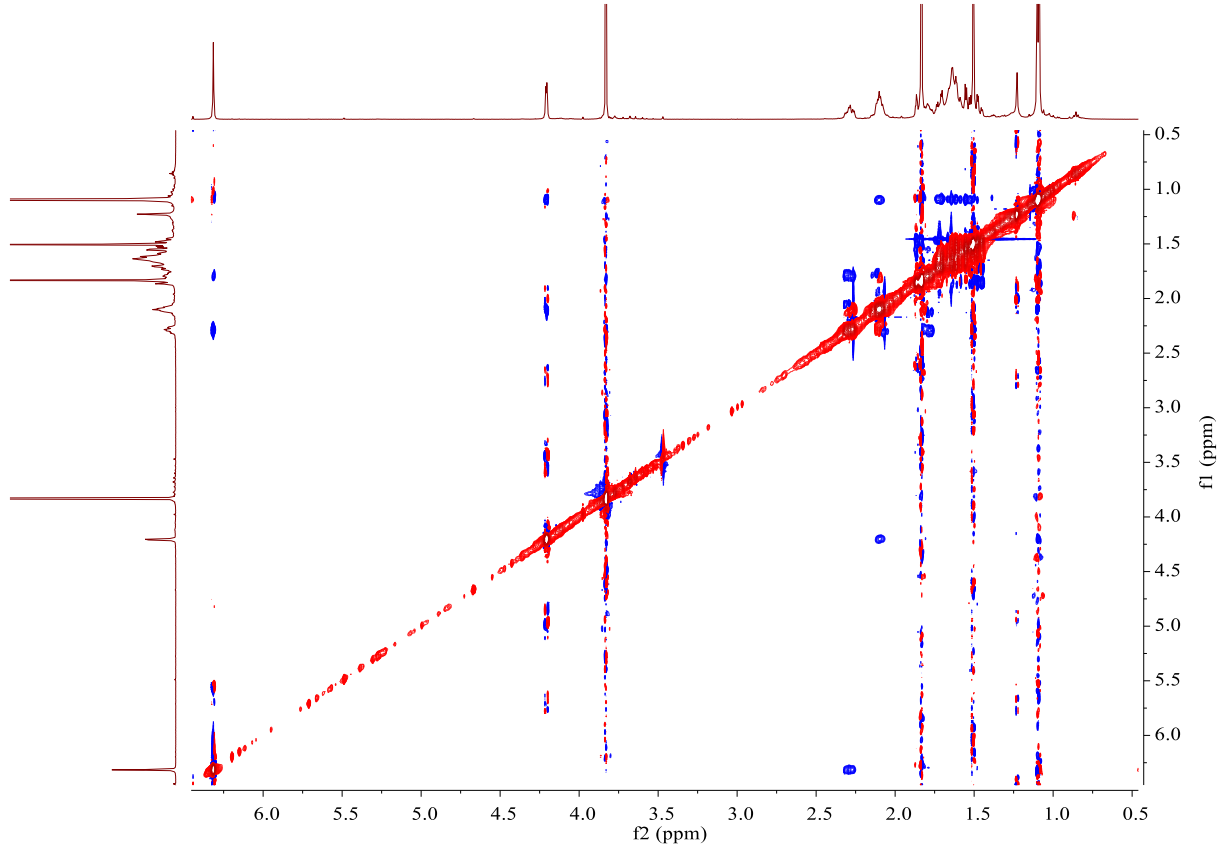
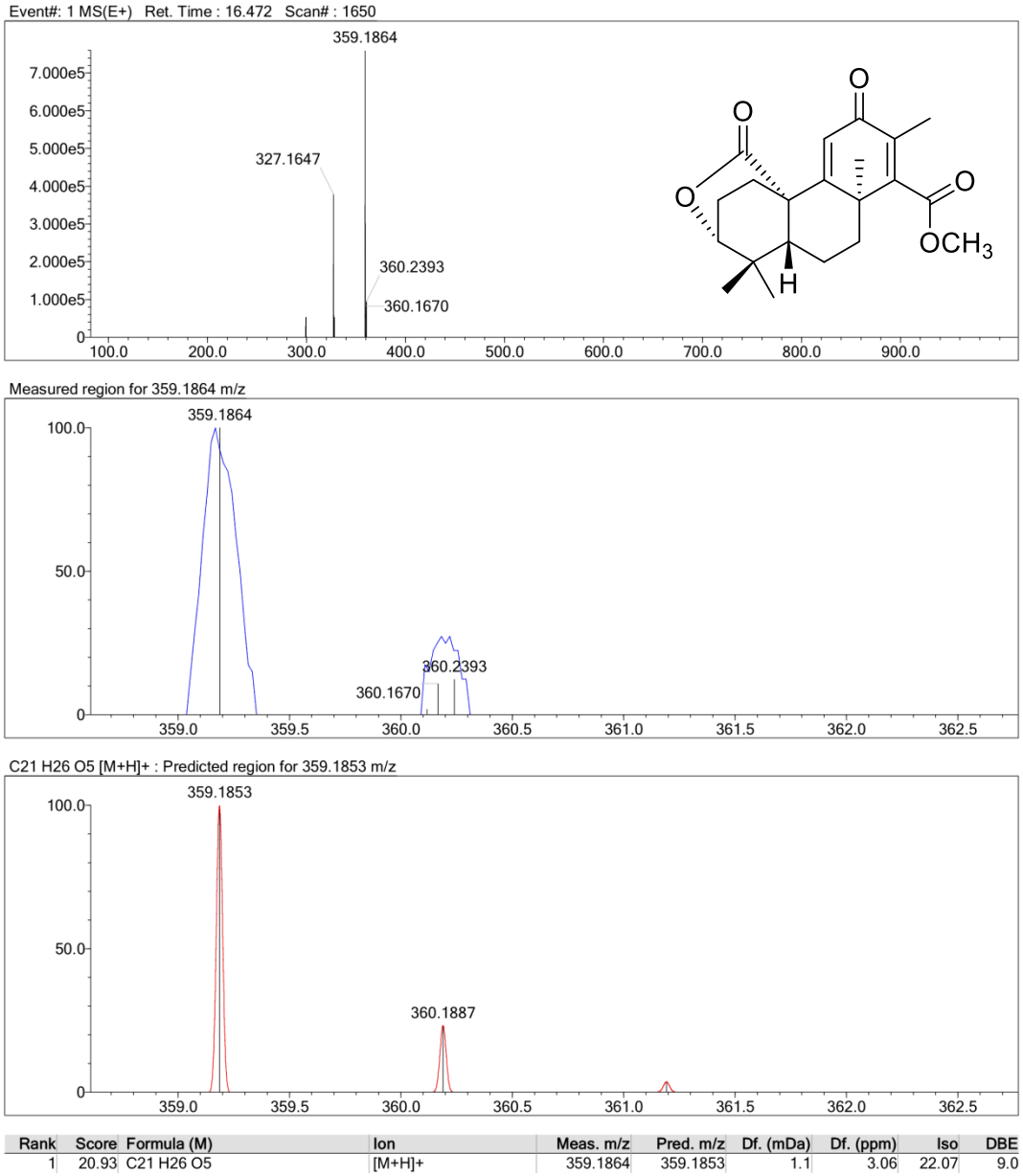


Fig. S24 NOESY spectrum of compound **3**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	20.93	C21 H26 O5	[M+H]+	359.1864	359.1853	1.1	3.06	22.07	9.0

Fig. S25 HRESIMS spectrum of compound **3**

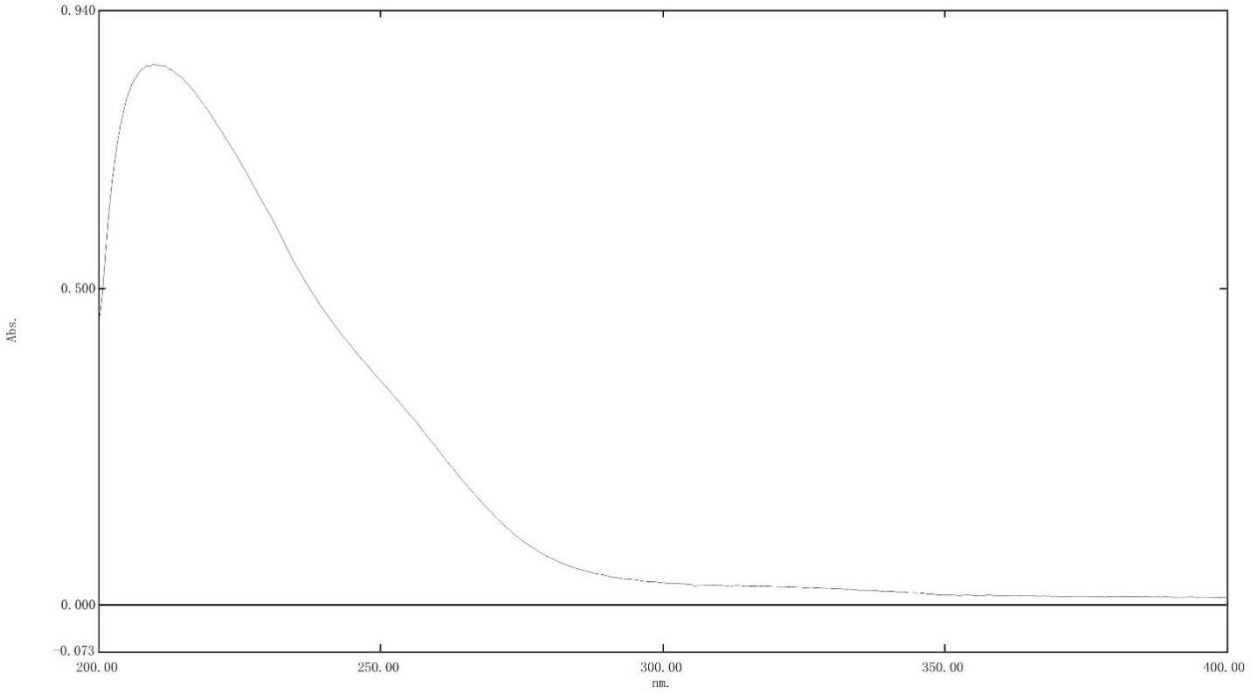


Fig. S26 UV spectrum of compound **3**

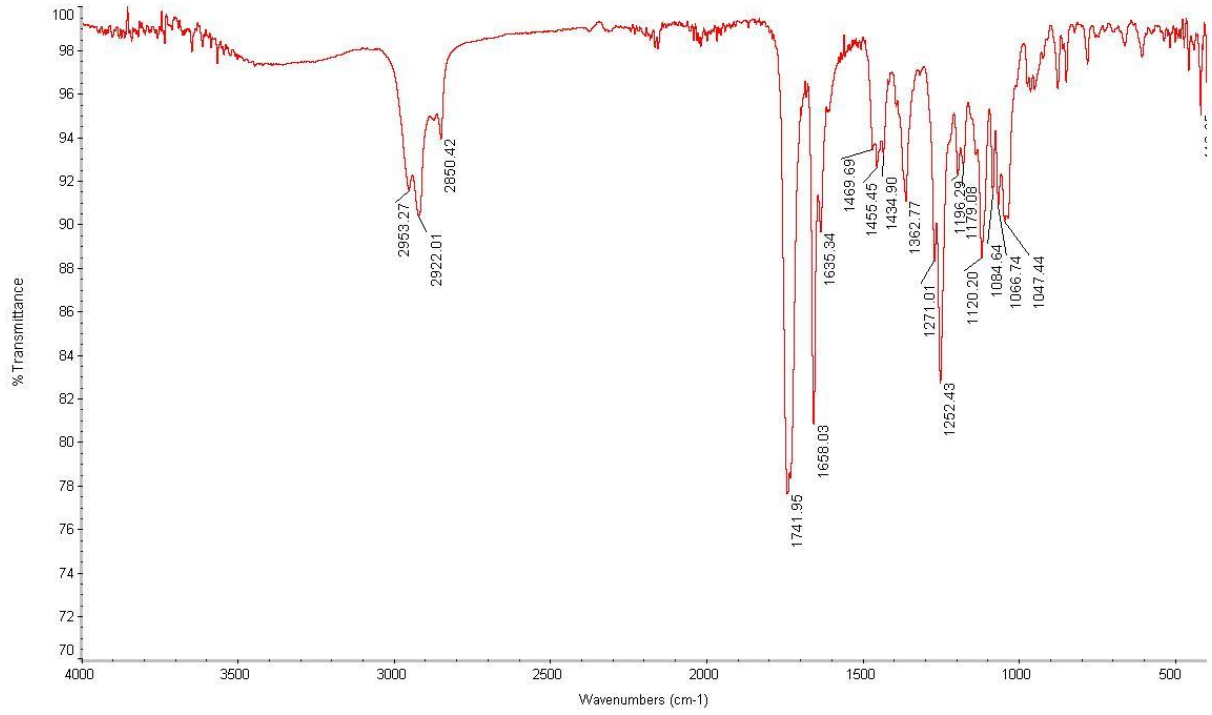


Fig. S27 IR spectrum of compound **3**

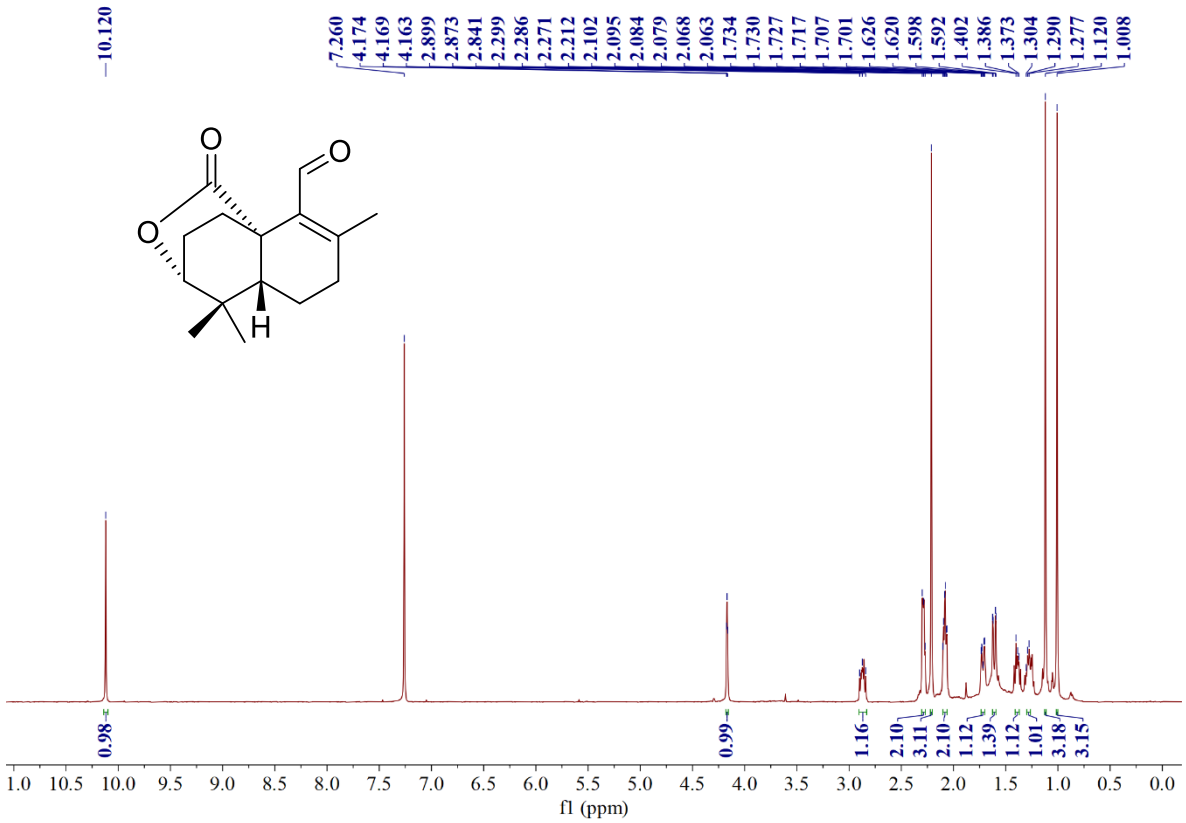


Fig. S28 ^{1}H NMR spectrum of compound **4** (in $CDCl_3$, 500 MHz)

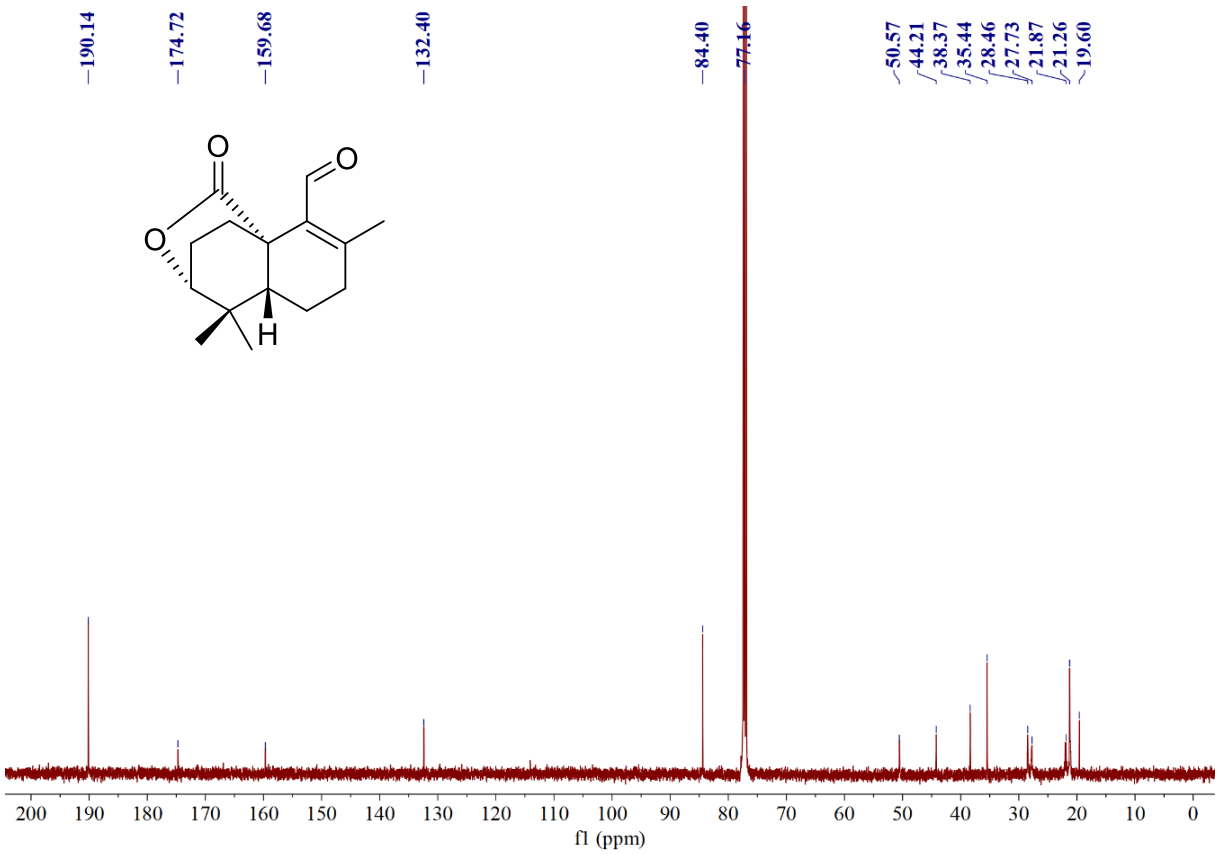


Fig. S29 ^{13}C NMR spectrum of compound **4** (in $CDCl_3$, 125 MHz)

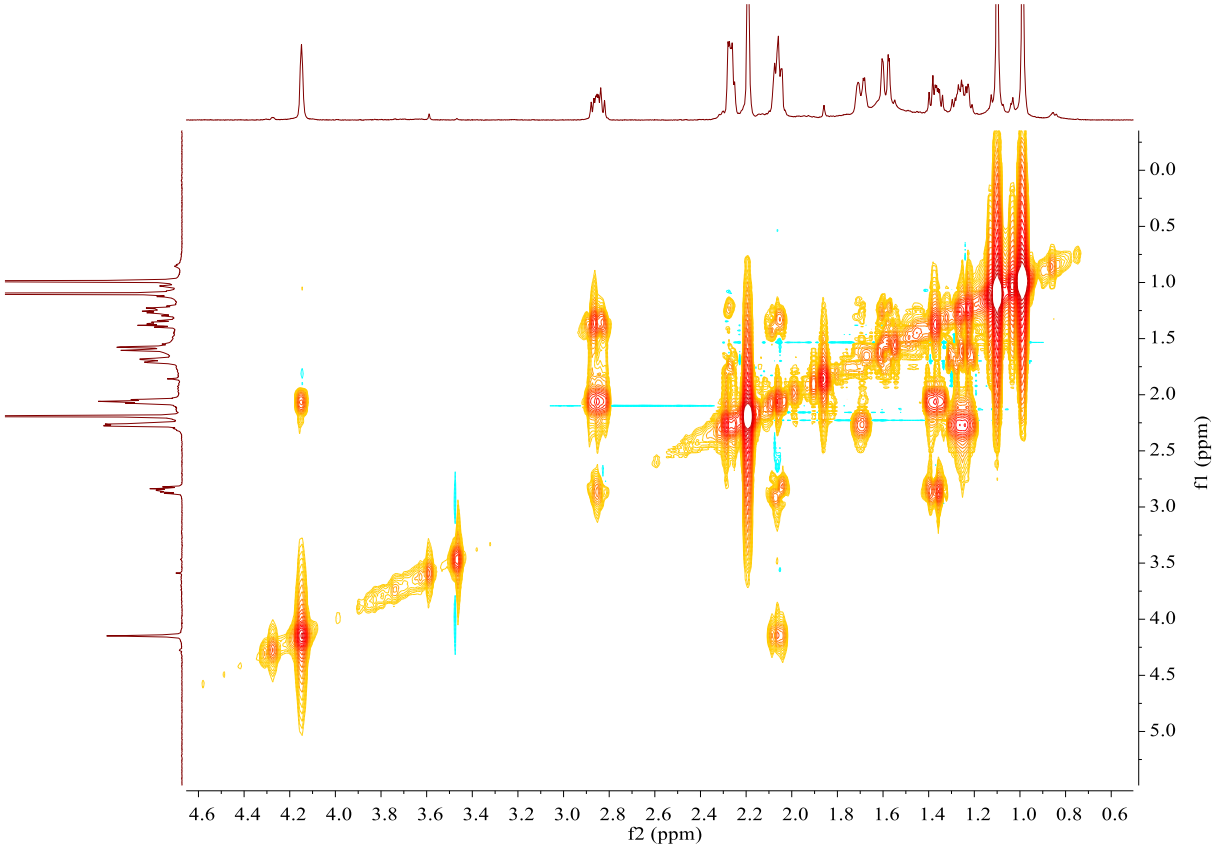


Fig. S30 ^{1}H-^{1}H COSY spectrum of compound **4**

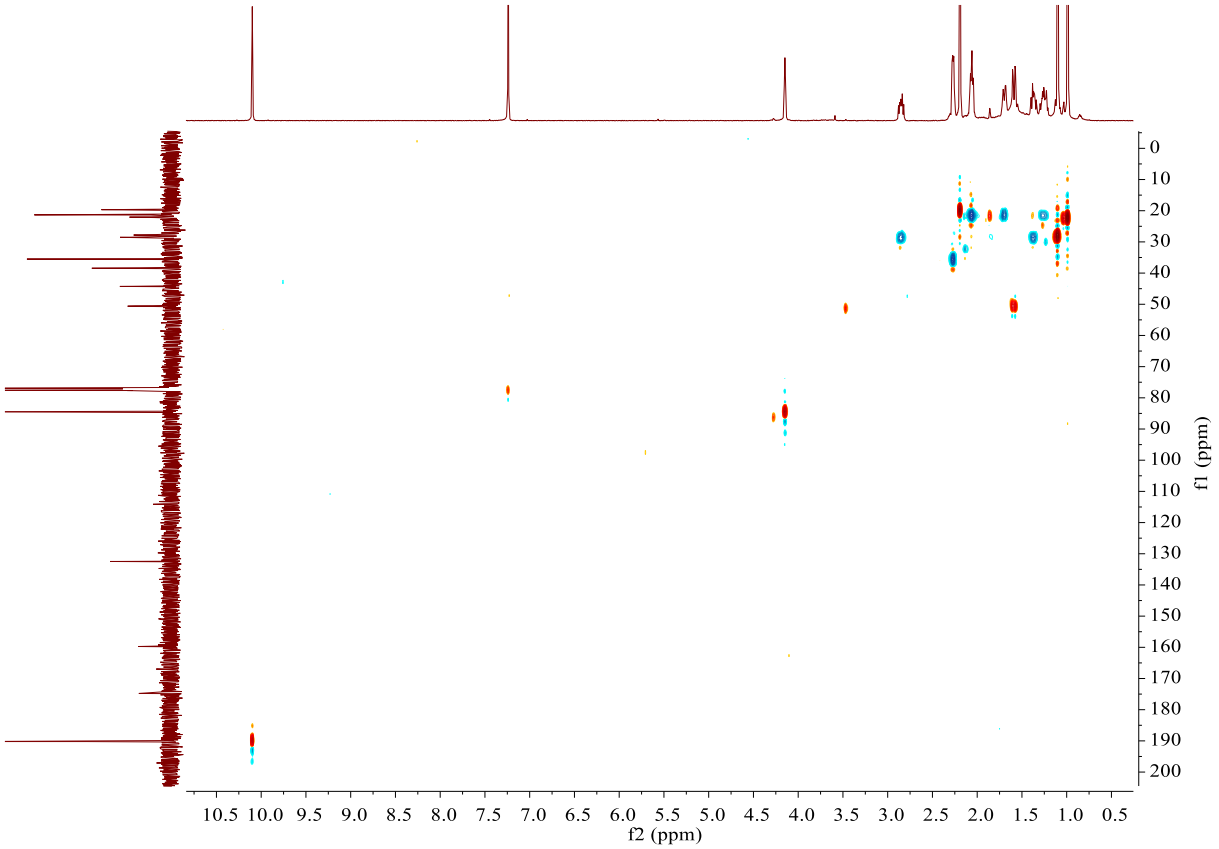


Fig. S31 gHSQC spectrum of compound **4**

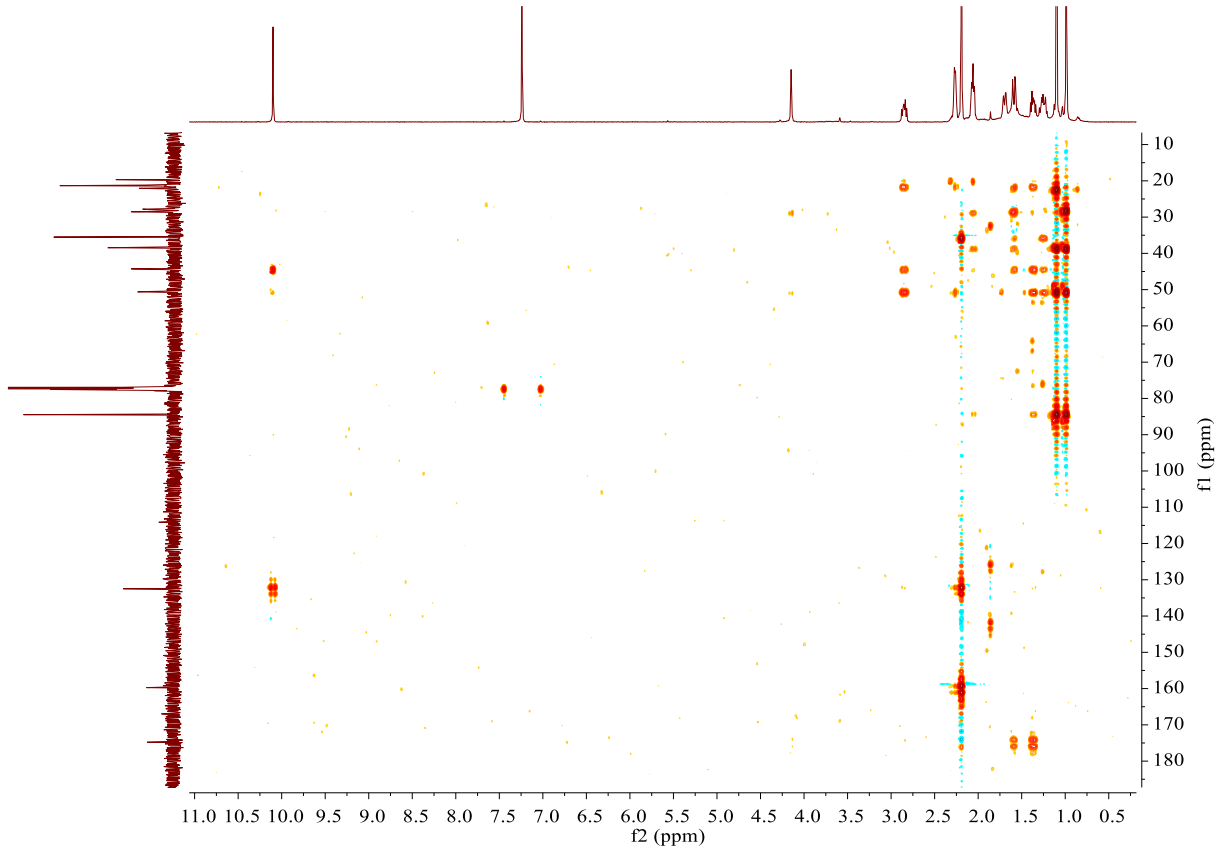


Fig. S32 gHMBC spectrum of compound **4**

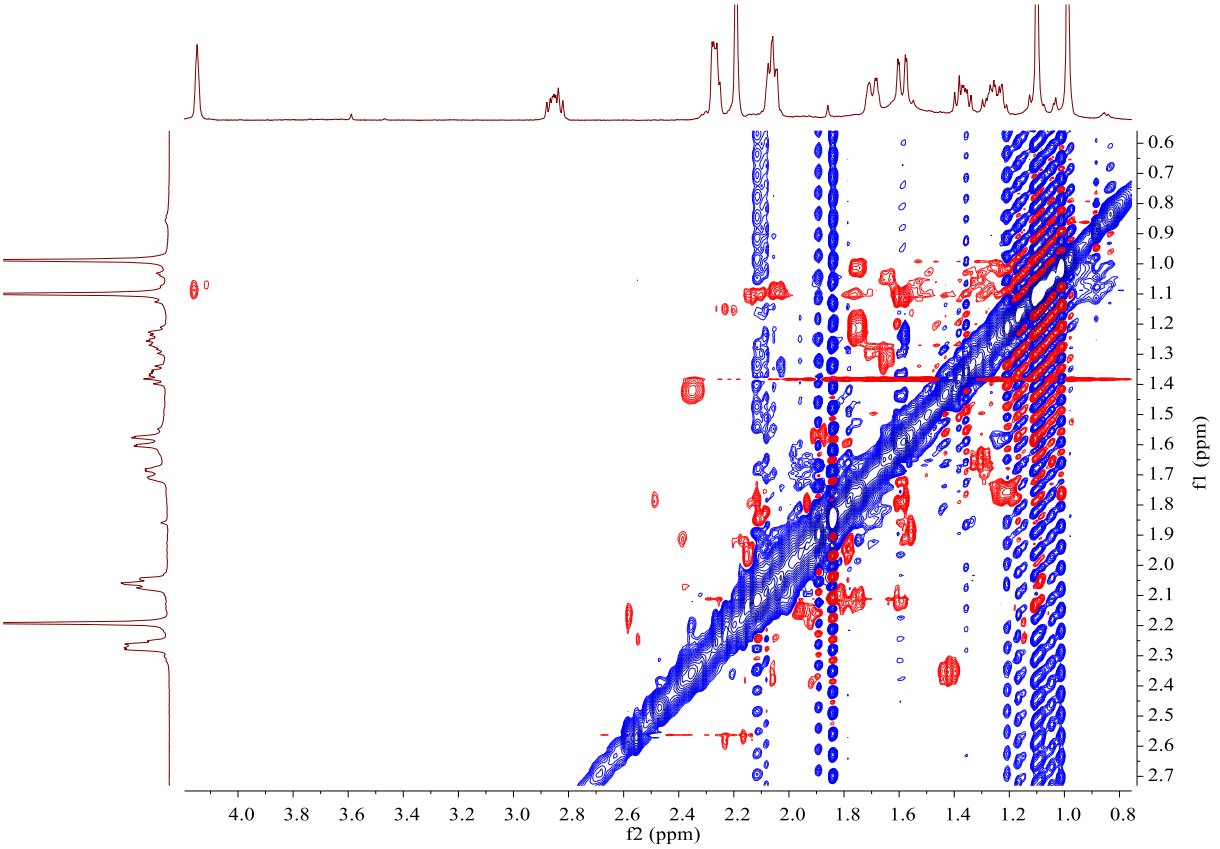
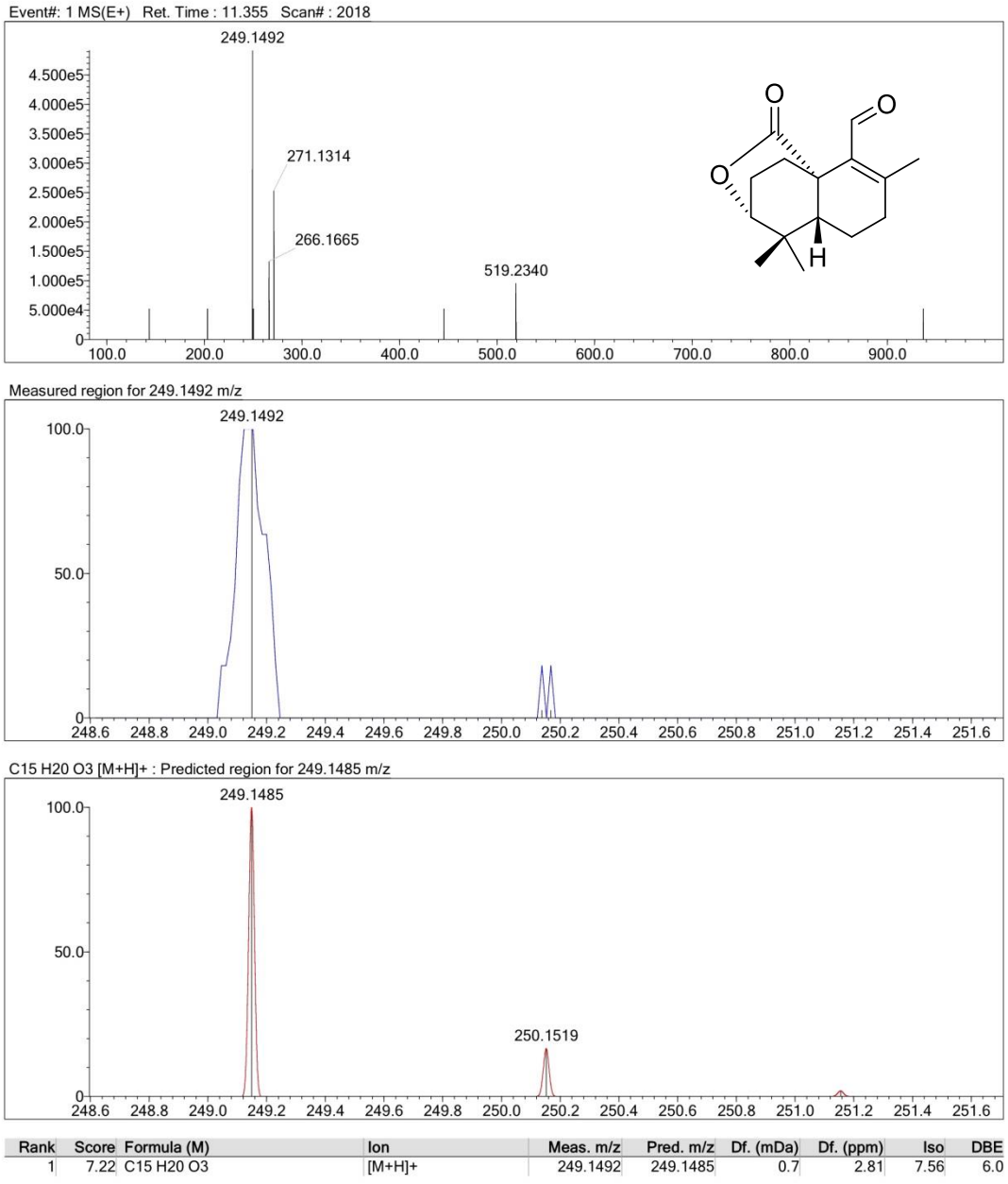


Fig. S33NOESY spectrum of compound **4**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	7.22	C15 H20 O3	[M+H]+	249.1492	249.1485	0.7	2.81	7.56	6.0

Fig. S34 HRESIMS spectrum of compound **4**

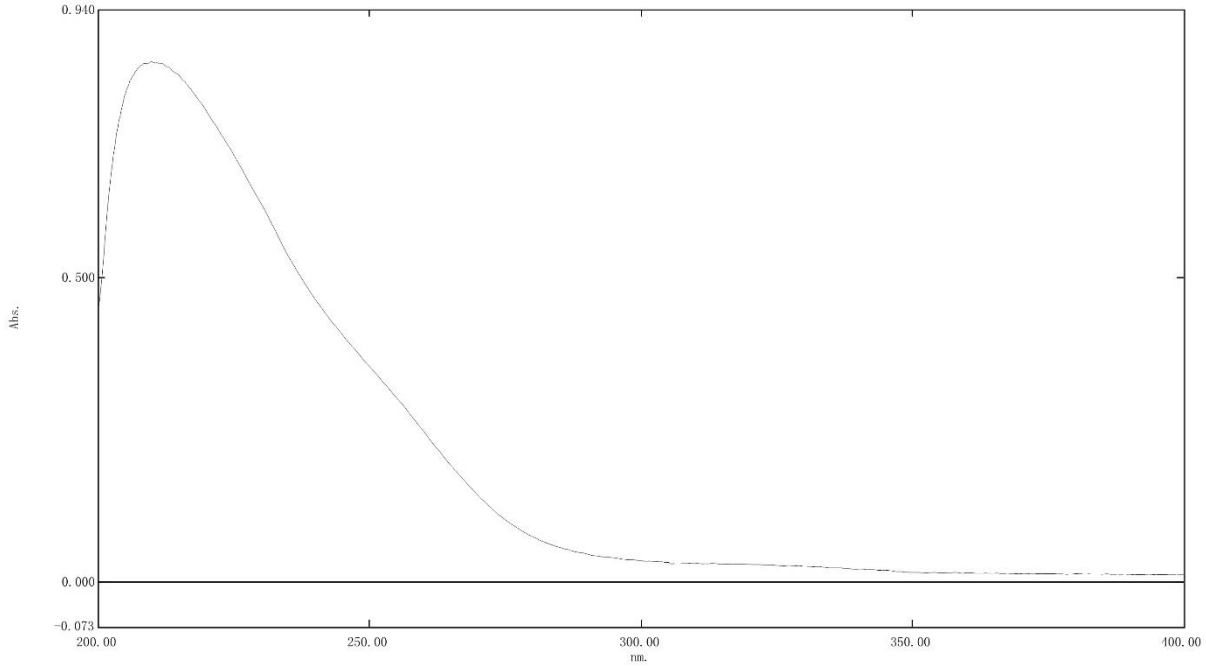


Fig. S35 UV spectrum of compound **4**

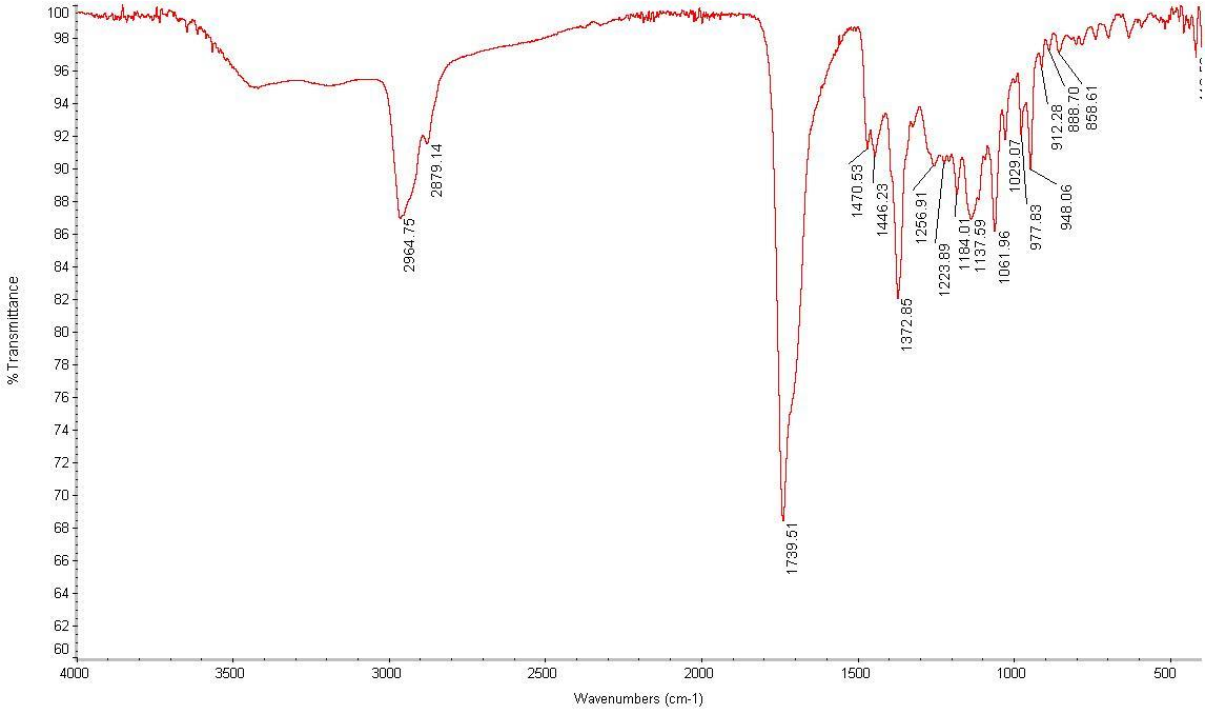


Fig. S36 IR spectrum of compound **4**

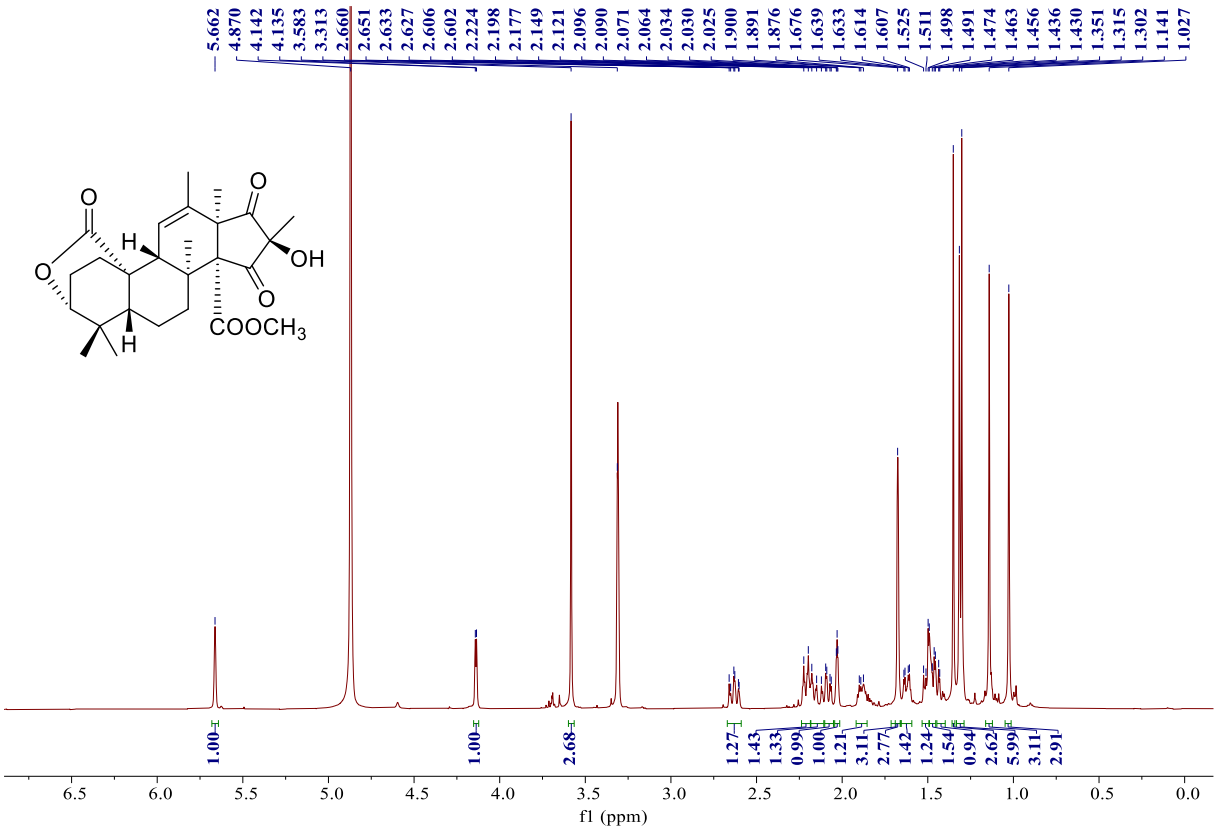


Fig. S37 ^{1}H NMR spectrum of compound **5** (in Methanol-d_4, 500 MHz)

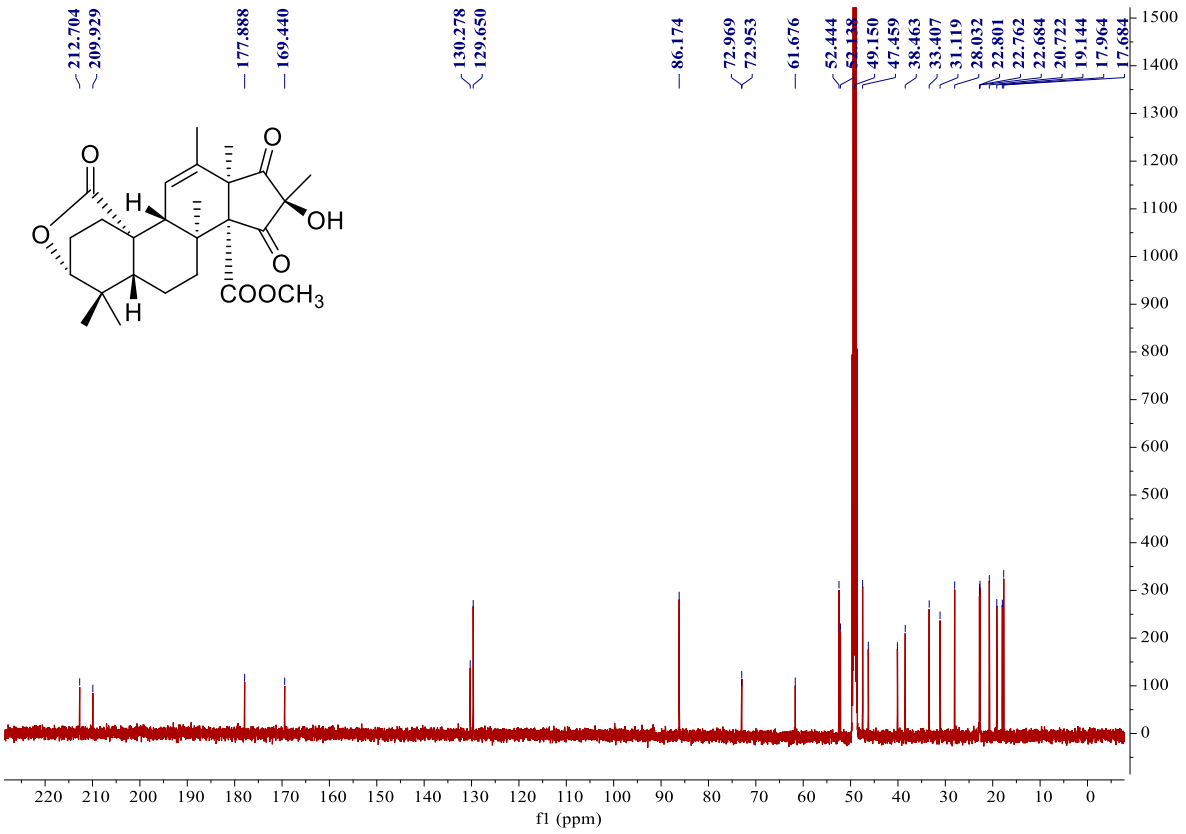


Fig. S38 ^{13}C NMR spectrum of compound **5** (in Methanol-d_4, 125 MHz)

Table S1 Optimized geometries of predominant conformers for (3*R*, 5*R*, 8*R*, 9*S*, 10*S*, 14*S*)-**2** at the B3LYP/6-31G(d) level, and Boltzmann distribution of conformers of (3*R*, 5*R*, 8*R*, 9*S*, 10*S*, 14*S*)-**2**
Cartesian Coordinates and Energies of Computed Structures.

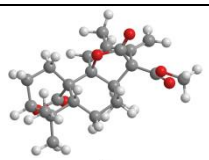
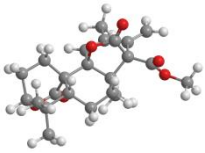
Conformer	Structure	G (Hartree)	H (Hartree)	ΔG (cal/mol)	Proportion (%)
2-1		-1344.543043	-843713.533	0	89.21
2-2		-1344.541050	-843712.282	2.112206615	10.79

Table S2 Cartesian Coordinates and Energies of (3*R*, 5*R*, 8*R*, 9*S*, 10*S*, 14*S*)-**2**
Sum of electronic and thermal Free Energies=-1344.543043

C	-1.161557	-1.78162	-0.903643	H	-1.441249	-2.840265	-0.881766
C	0.347106	-1.675936	-0.654603	H	-1.408115	-1.419461	-1.908427
C	0.857761	-0.212911	-0.699228	H	0.886501	-2.260449	-1.409111
C	-0.008325	0.682367	0.249305	H	0.571563	-2.140065	0.311825
C	2.770396	1.370615	-0.016985	H	-0.296513	2.907573	0.244543
C	1.752148	2.442731	0.078307	H	2.876813	4.109593	0.879715
C	0.448499	2.122739	0.183744	H	2.731395	4.118603	-0.878245
C	2.2187	-0.064345	0.096672	H	1.33539	4.553326	0.124148
C	2.196243	3.883549	0.049869	H	4.445175	2.660278	-0.150115
C	4.082131	1.639009	-0.117535	H	4.831784	0.860836	-0.186446
C	0.977268	0.239737	-2.161305	H	0.046096	0.066009	-2.703069
O	0.414063	0.173763	1.588884	H	1.217592	1.298795	-2.254204
C	1.718173	-0.181086	1.552559	H	1.769668	-0.339114	-2.645343
O	2.331734	-0.471307	2.550607	H	-4.205609	0.607041	2.260354
C	-3.740324	1.06471	1.383504	H	-4.155544	2.073173	1.291394
C	-4.101787	0.287429	0.12139	H	-5.178057	0.289765	-0.06346
C	-3.533266	-1.149284	0.064264	H	-1.658214	-1.434503	1.13654
C	-1.959363	-1.020782	0.16665	H	-1.853824	2.131353	1.664982
C	-1.547702	0.494343	0.224457	H	-1.856288	0.521444	2.365107
C	-2.200749	1.106251	1.509912	H	-3.667378	-2.833145	-1.33613
C	-4.029228	-1.805144	-1.243364	H	-5.12487	-1.842839	-1.23763
O	-3.539299	1.040083	-1.003301	H	-3.722862	-1.25164	-2.13482
C	-2.197366	1.190985	-0.969142	H	-5.167562	-2.012174	1.240823
O	-1.644474	1.834592	-1.838643	H	-3.712248	-3.016361	1.161744
C	-4.071294	-1.984174	1.243497	H	-3.742232	-1.597207	2.213087
C	3.211267	-1.143757	-0.334196	H	5.100052	-2.979601	0.023897
O	3.869012	-1.08366	-1.355358	H	3.938444	-4.05528	0.868134
O	3.215215	-2.202853	0.484279	H	3.73851	-3.698997	-0.879358
C	4.059866	-3.305695	0.087556				

Table S3 Optimized geometries of predominant conformers for (3*R*, 5*R*, 8*S*, 10*S*)-**3** at the B3LYP/6-31G(d) level, and Boltzmann distribution of conformers of (3*R*, 5*R*, 8*S*, 10*S*)-**3**.

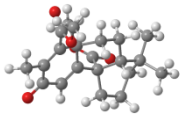
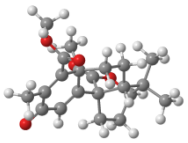
Conformer	Structure	G (Hartree)	H (Hartree)	ΔG (cal/mol)	Proportion (%)
3-1		-1191.940593	-747954.0455	0	91.31
3-2		-1191.938374	-747952.6531	2.351724274	8.69

Table S4 Cartesian Coordinates and Energies of (3*R*, 5*R*, 8*S*, 10*S*)-**3**

Sum of electronic and thermal Free Energies= -1191.940593

C	-0.03275	0.884848	-0.0106	C	-4.81126	-2.57811	-0.87623
C	-0.97085	-0.22493	0.461722	H	-1.19085	-2.37448	0.217738
C	-0.56795	-1.57458	-0.19762	H	-0.78244	-1.52449	-1.273
C	0.904353	-1.91345	0.017152	H	1.104739	-2.05163	1.084197
C	-0.53718	2.091485	-0.33587	H	1.119364	-2.87577	-0.46232
C	-1.96897	2.405057	-0.36024	H	0.092528	2.923464	-0.62774
C	-2.92231	1.281094	-0.19815	H	4.020779	0.98113	-2.1738
O	-2.36553	3.555485	-0.57239	H	4.268963	2.202465	-0.93554
C	-2.43529	0.06754	0.135757	H	5.106601	0.106543	-0.00786
C	3.700225	1.300212	-1.1789	H	2.017852	2.624621	-0.84394
C	4.029939	0.22242	-0.14991	H	1.708087	1.43829	-2.1065
C	3.358048	-1.13715	-0.4317	H	3.442646	-2.73031	-1.90872
C	1.817879	-0.84344	-0.58737	H	4.994343	-1.91899	-1.65736
C	1.480439	0.622348	-0.10451	H	3.719151	-1.13227	-2.60796
C	2.179714	1.58387	-1.13019	H	-1.18501	0.600532	2.48378
C	3.912393	-1.75651	-1.73001	H	-1.55514	-1.13323	2.36374
O	3.543585	0.709986	1.142442	H	0.130502	-0.56483	2.350491
C	2.209001	0.918743	1.213136	H	-4.65579	2.470345	0.196503
O	1.724183	1.356493	2.23587	H	-4.53663	1.921613	-1.4673
H	1.597302	-0.82719	-1.6631	H	-5.03958	0.782319	-0.20441
C	-0.88417	-0.34302	2.021323	H	4.791711	-2.19857	0.805753
C	-3.38428	-1.09455	0.288783	H	3.33649	-1.74659	1.697259
C	-4.37214	1.616196	-0.4272	H	3.292611	-3.0958	0.550388
C	3.702708	-2.09766	0.729107	H	-5.10283	-2.73177	-1.91423
O	-3.65556	-1.64789	1.337965	H	-4.31854	-3.46788	-0.47811
O	-3.88918	-1.46459	-0.89959	H	-5.68213	-2.33585	-0.26322

Table S5 Optimized geometries of predominant conformers for (3*R*, 5*R*, 10*S*)-**4** at the B3LYP/6-31G(d) level, and Boltzmann distribution of conformers of (3*R*, 5*R*, 10*S*)-**4**.

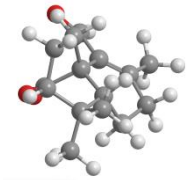
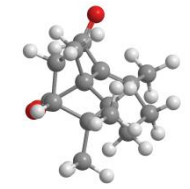
Conformer	Structure	G (Hartree)	H (Hartree)	ΔG (cal/mol)	Proportion (%)
4-1		-809.215542	-507790.4402	0	61.38
4-2		-809.215105	-507790.1659	0.463138129	38.62

Table S6 Cartesian Coordinates and Energies of (3*R*, 5*R*, 10*S*)-**4**
Sum of electronic and thermal Free Energies=-809.215542

C	1.751874	-0.13936	-0.20259	H	1.406431	2.848276	-1.00337
C	2.300934	1.106536	-0.17106	H	1.966392	3.04628	0.640314
C	1.447217	2.343567	-0.02505	H	0.075624	1.789868	1.545607
C	0.034592	2.065967	0.484841	H	-0.56435	2.98022	0.414637
C	3.774192	1.42888	-0.25646	H	4.405461	0.624917	-0.63306
C	-1.70928	-1.57094	-1.33546	H	3.91072	2.296396	-0.91356
C	-2.2691	-0.89247	-0.08643	H	4.14898	1.727719	0.731533
C	-2.11811	0.648284	-0.07892	H	-2.24498	-1.22507	-2.22384
C	-0.5934	0.943274	-0.343	H	-1.89337	-2.64683	-1.25321
C	0.243455	-0.37934	-0.21661	H	-3.30432	-1.18335	0.106891
C	-0.19167	-1.27802	-1.42245	H	0.382339	-2.2028	-1.41403
C	-2.98057	1.278839	-1.18927	H	0.059155	-0.73886	-2.34205
O	-1.52276	-1.41643	1.058399	H	-2.68784	0.940169	-2.18817
C	-0.21006	-1.07867	1.067023	H	-2.8776	2.369842	-1.16823
O	0.464514	-1.31605	2.047634	H	-4.04184	1.042866	-1.04586
H	-0.49829	1.240343	-1.39611	H	3.710436	-1.12026	-0.16038
C	2.626198	-1.32448	-0.184	H	-2.60251	2.278979	1.299672
C	-2.6294	1.185396	1.27679	H	-3.67173	0.878878	1.424376
O	2.247375	-2.49081	-0.16268	H	-2.05299	0.813843	2.127807