Electronic supplementary information

Diterpenoids from the aerial parts of Isodon serra and their anti-hepatocarcinoma potential

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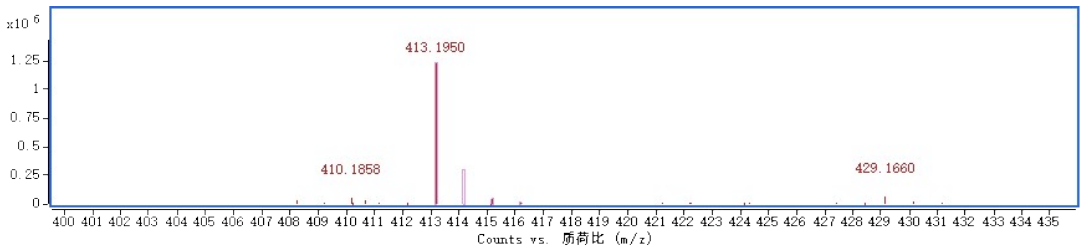
Content



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	*m/z*
$C_{22}H_{30}O_6$	100	390.2043	390.2042	413.1935	-0.1	413.1950

Fig. S1. HR-ESI-MS (+) spectrum of compound **1**

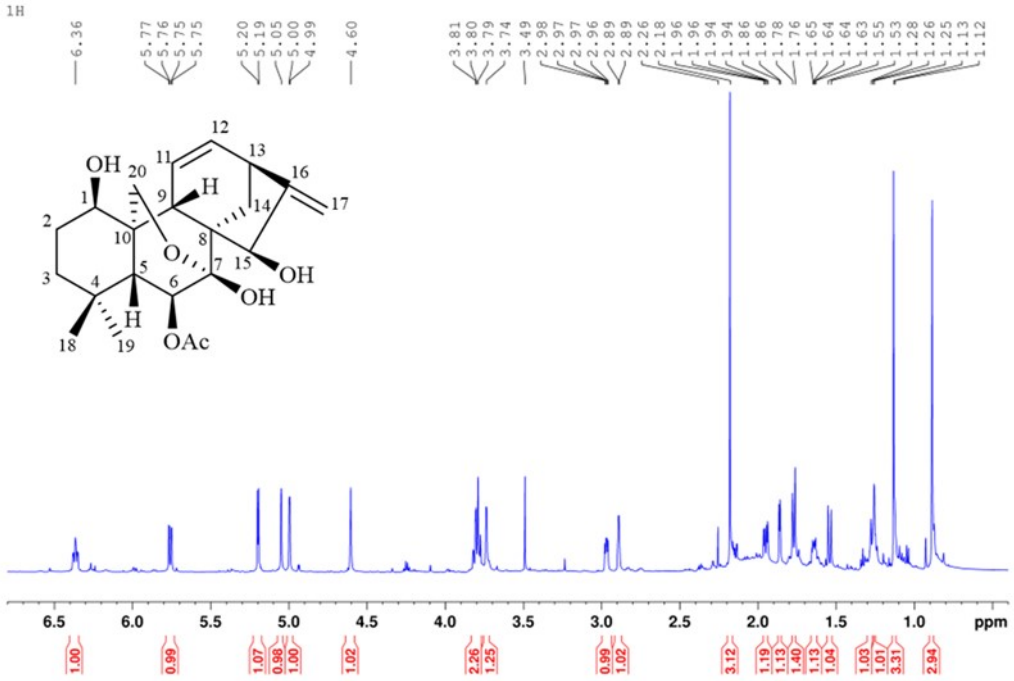


Fig. S2. ^{1}H NMR spectrum for compound **1**

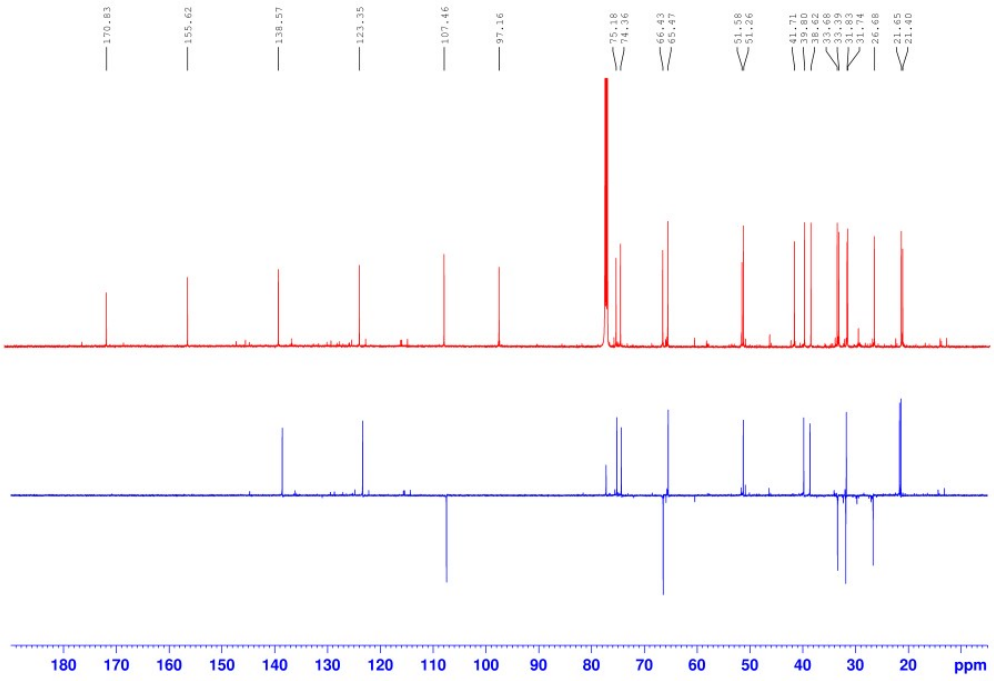


Fig. S3. ^{13}C and DEPT 135 NMR spectra for compound **1**

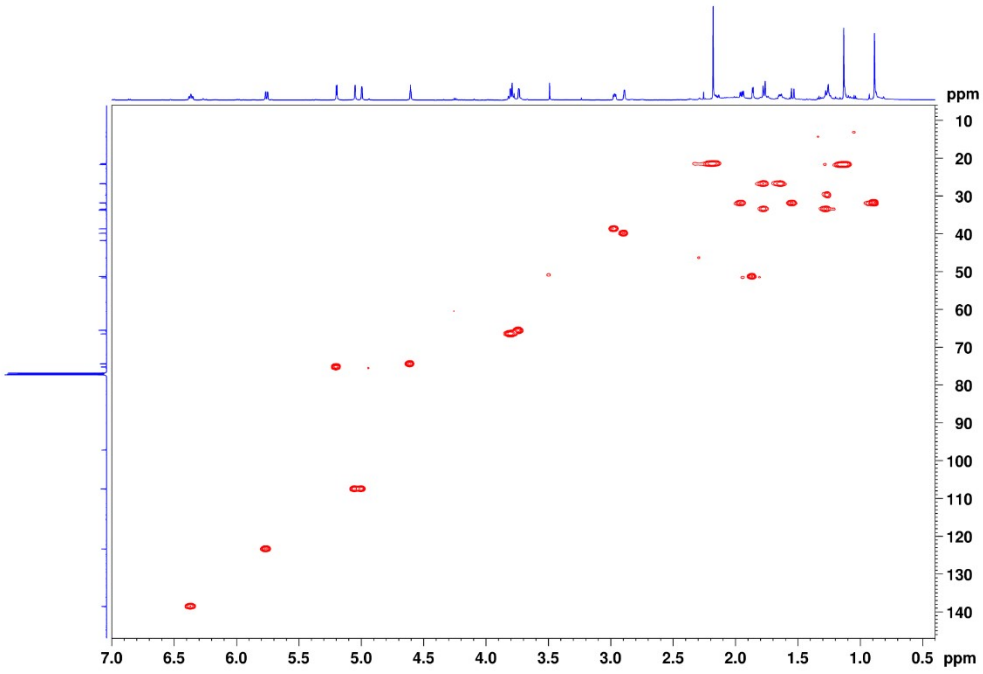


Fig. S4. HSQC NMR spectrum for compound **1**

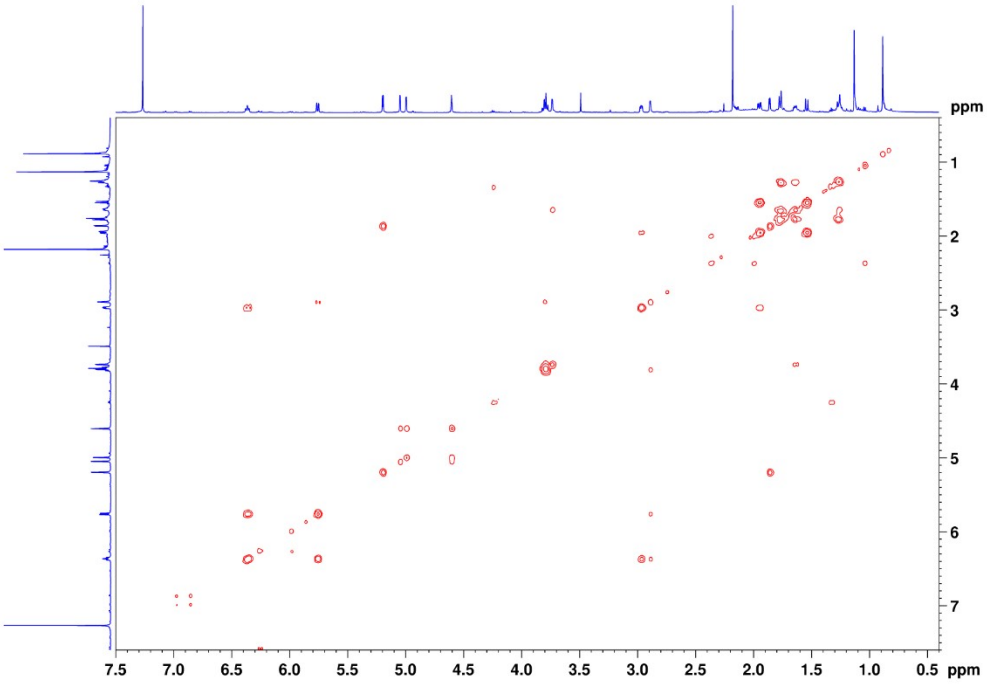


Fig. S5. ^{1}H–^{1}H COSY NMR spectrum for compound **1**

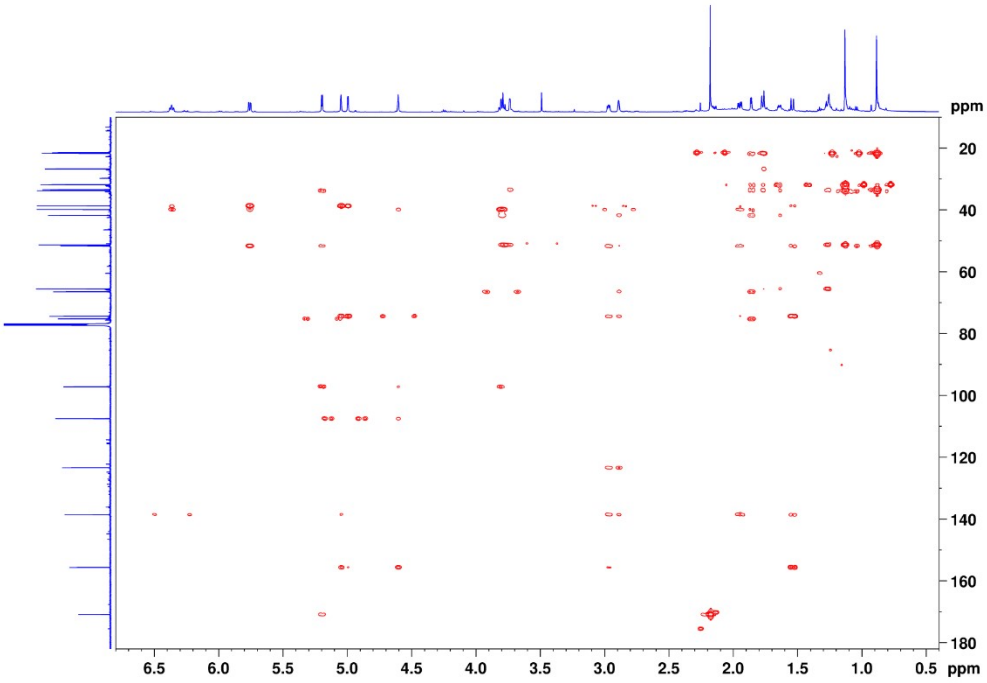


Fig. S6. HMBC NMR spectrum for compound **1**

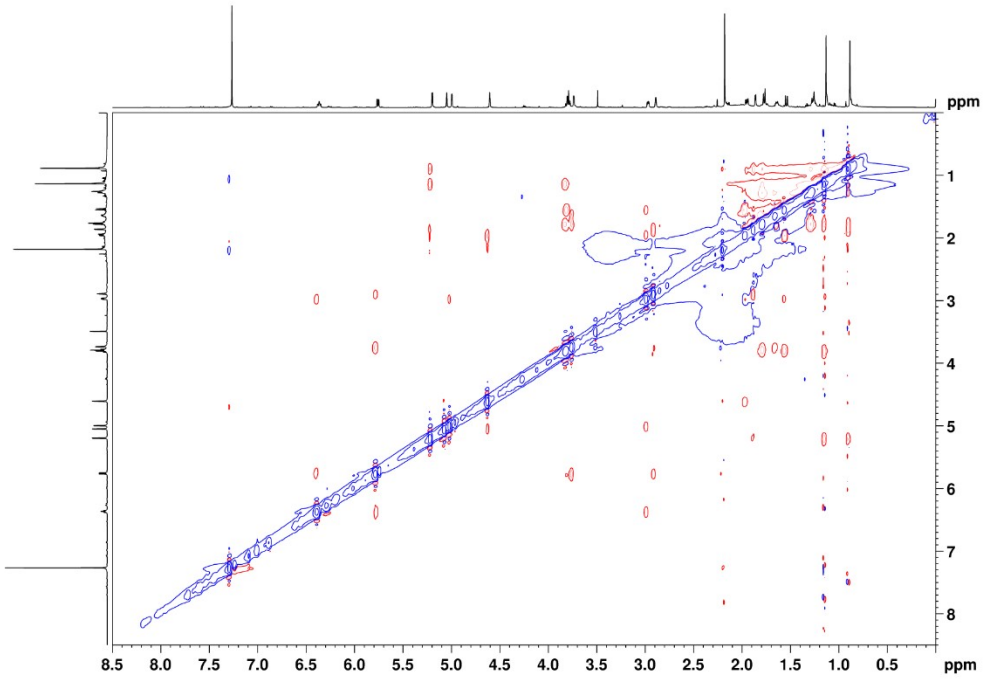


Fig. S7. NOESY NMR spectrum for compound **1**

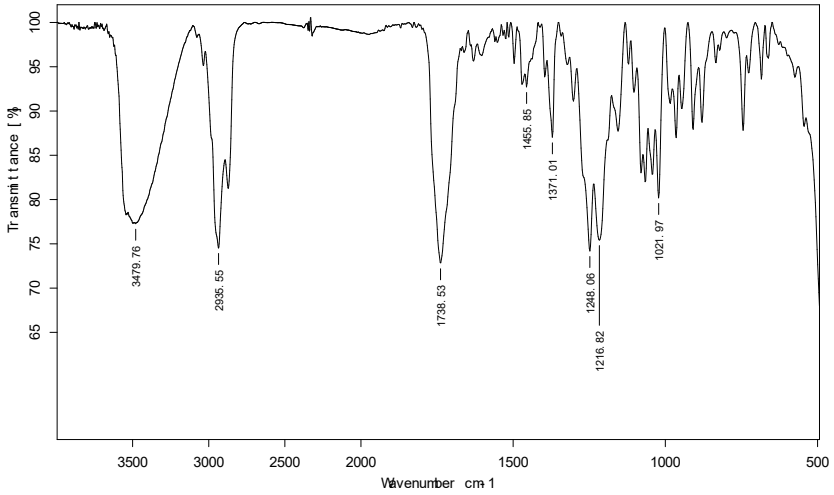


Fig. S8. IR spectrum of compound **1** (KBr)

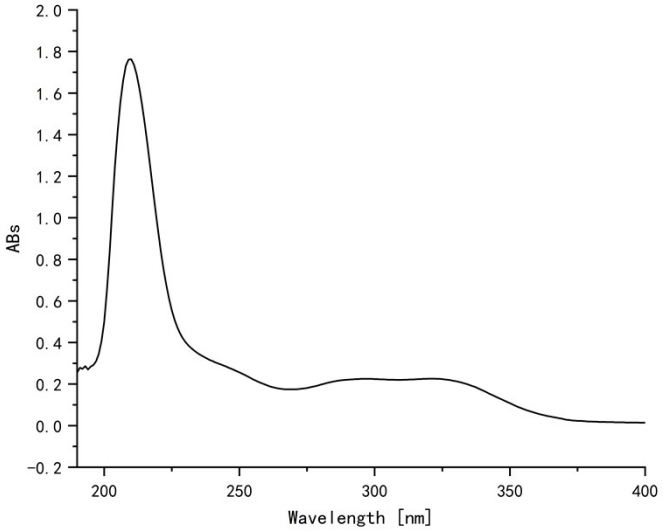


Fig. S9. UV spectrum of compound **1** in MeOH

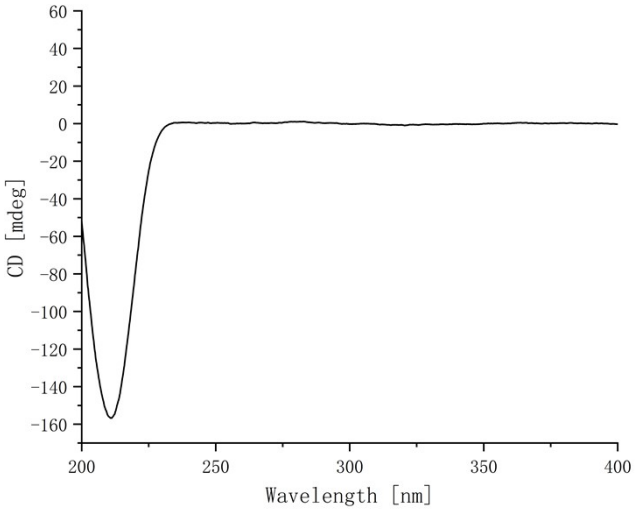
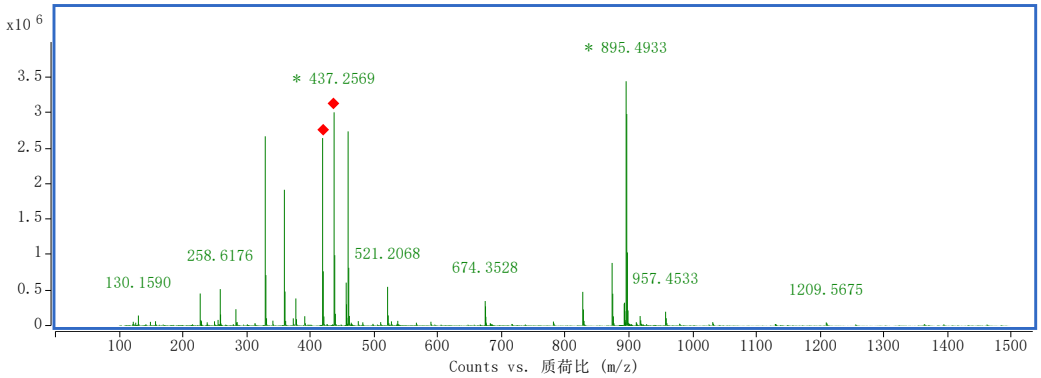


Fig. S10. CD spectrum of compound **1** in MeOH



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	*m/z*

$C_{24}H_{36}O_7$	100	436.2461	436.2461	437.2534	-0.05	437.2569

Fig. S11. HR-ESI-MS (+) spectrum of compound **2**

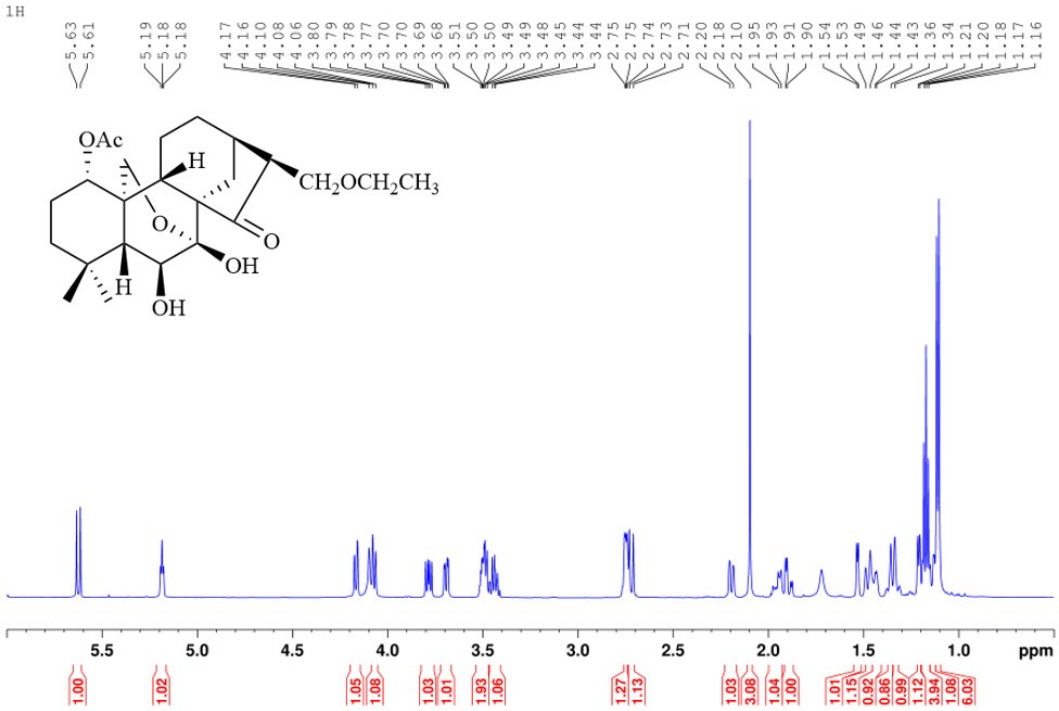


Fig. S12. ^{1}H NMR spectrum for compound **2**

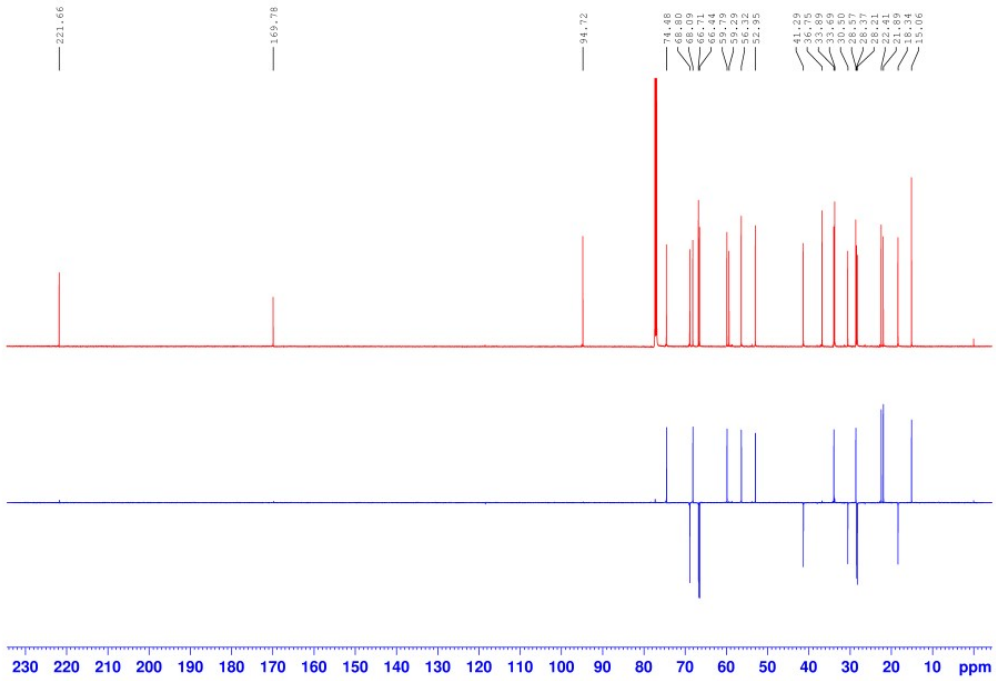


Fig. S13. ^{13}C and DEPT 135 NMR spectra for compound **2**

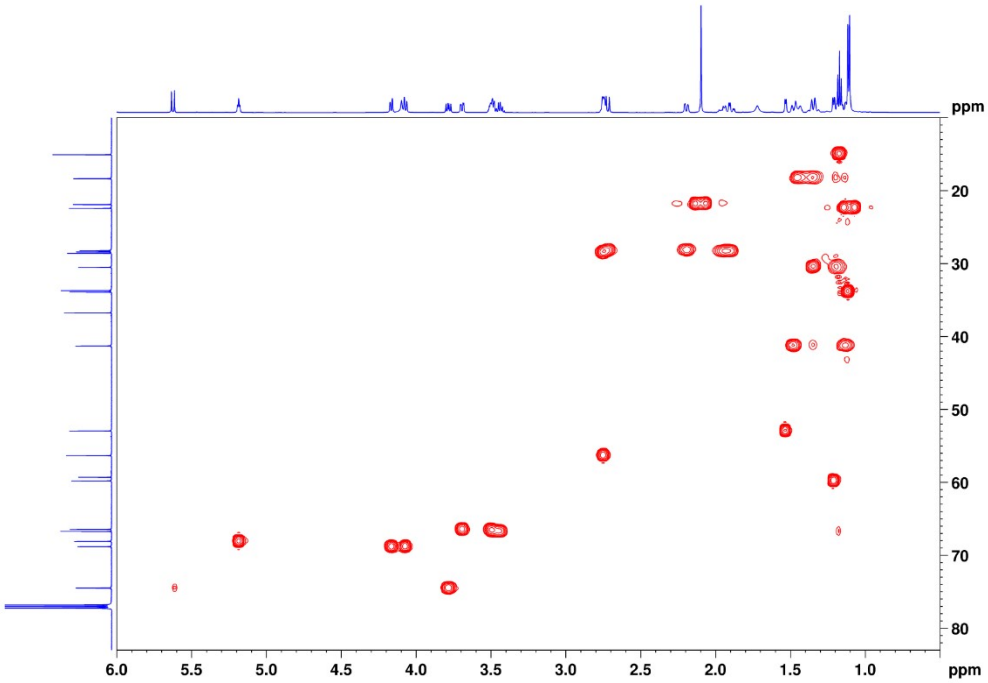


Fig. S14. HSQC NMR spectrum for compound **2**

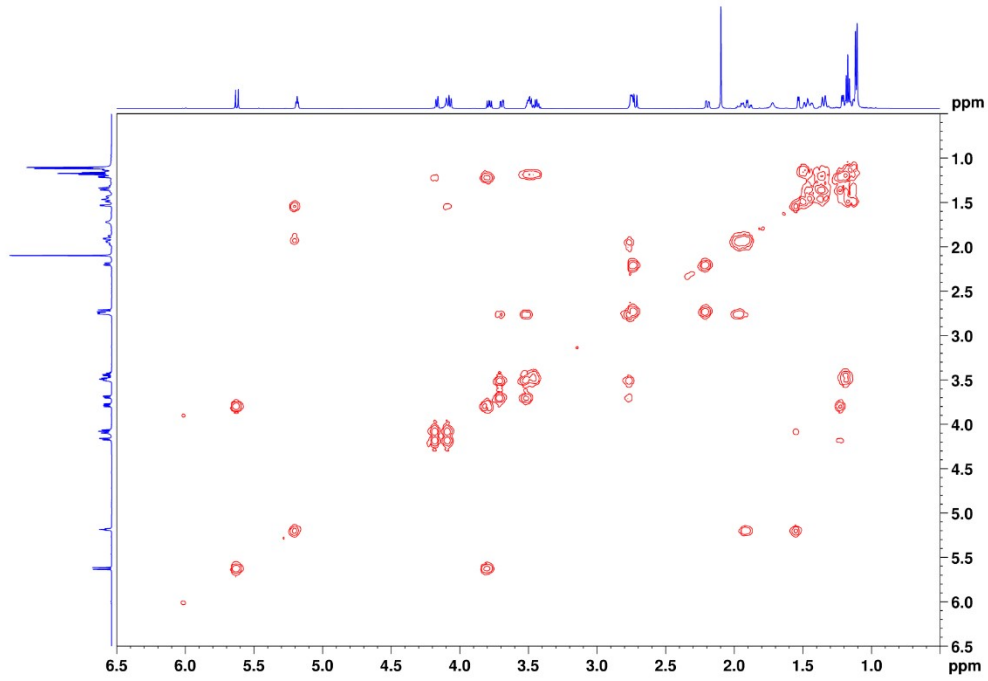


Fig. S15. ^{1}H–^{1}H COSY NMR spectrum for compound **2**

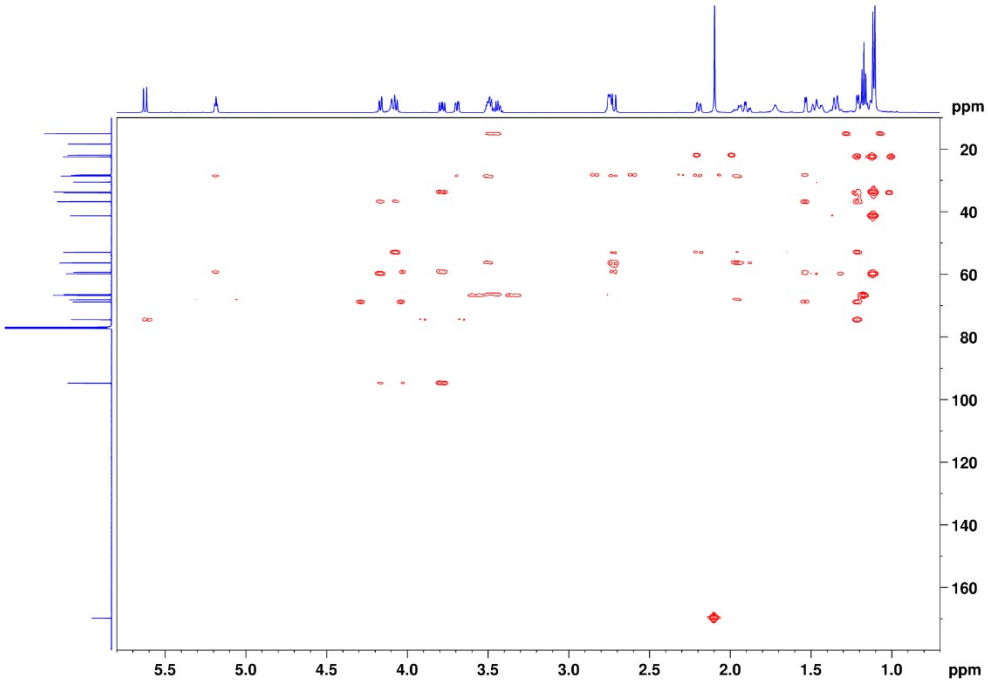


Fig. S16. HMBC NMR spectrum for compound **2**

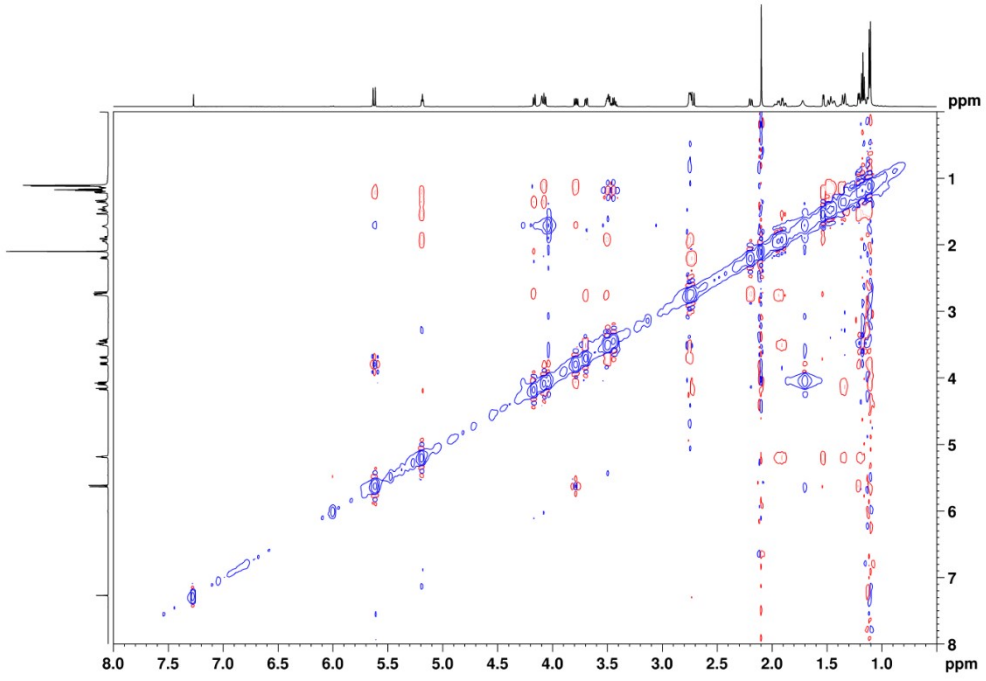


Fig. S17. NOESY NMR spectrum for compound **2**

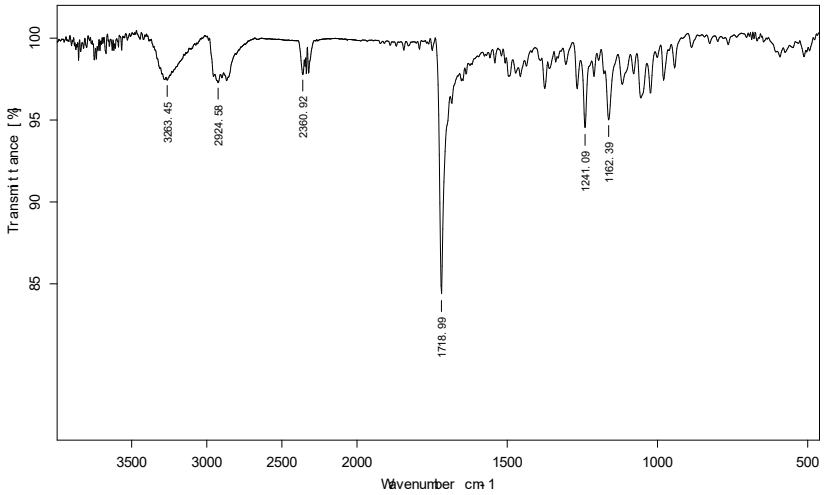


Fig. S18. IR spectrum of compound **2** (KBr)

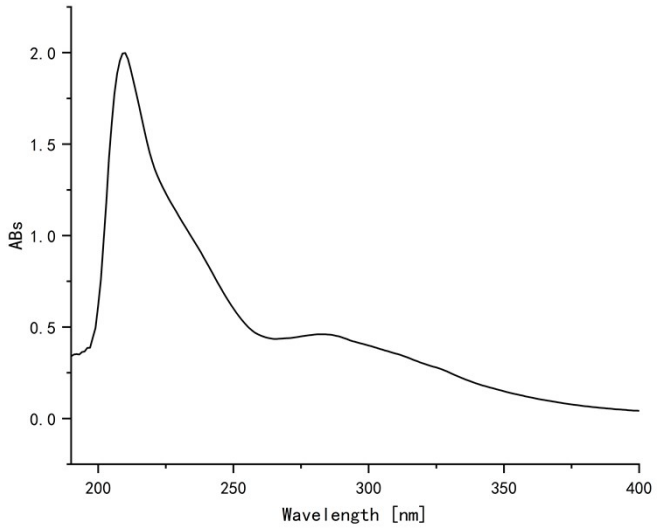


Fig. S19. UV spectrum of compound **2** in MeOH

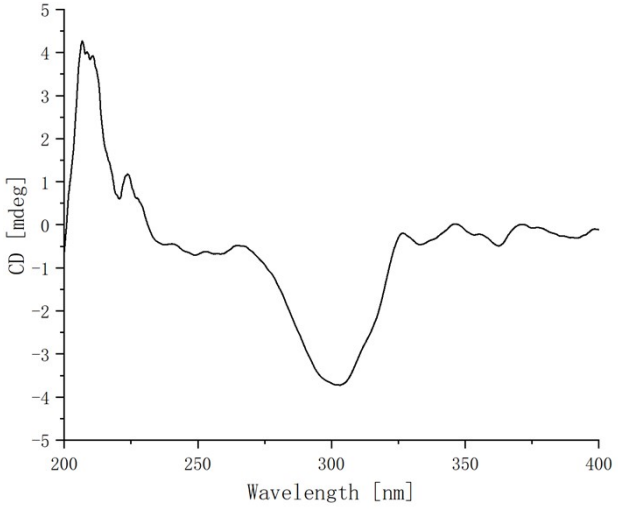
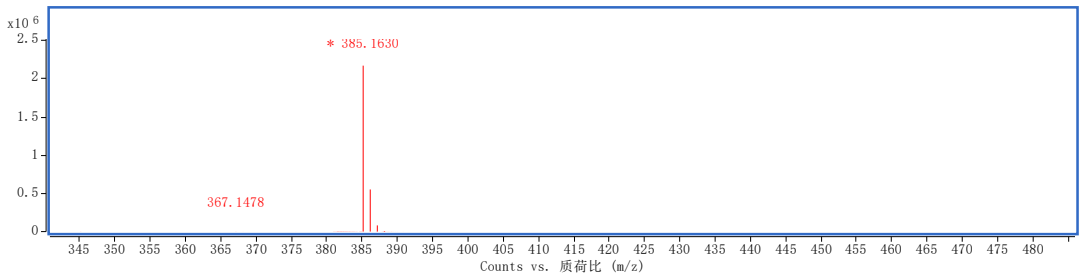


Fig. S20. CD spectrum of compound **2** in $CHCl_3$



Formula (M)	Score (MFG)	Mass	Mass (MFG)	m/z (Calc)	Diff (ppm)	*m/z*
$C_{20}H_{26}O_6$	100	362.1730	362.1729	385.1622	-0.11	385.1630

Fig. S21. HR-ESI-MS (+) spectrum of compound **3**

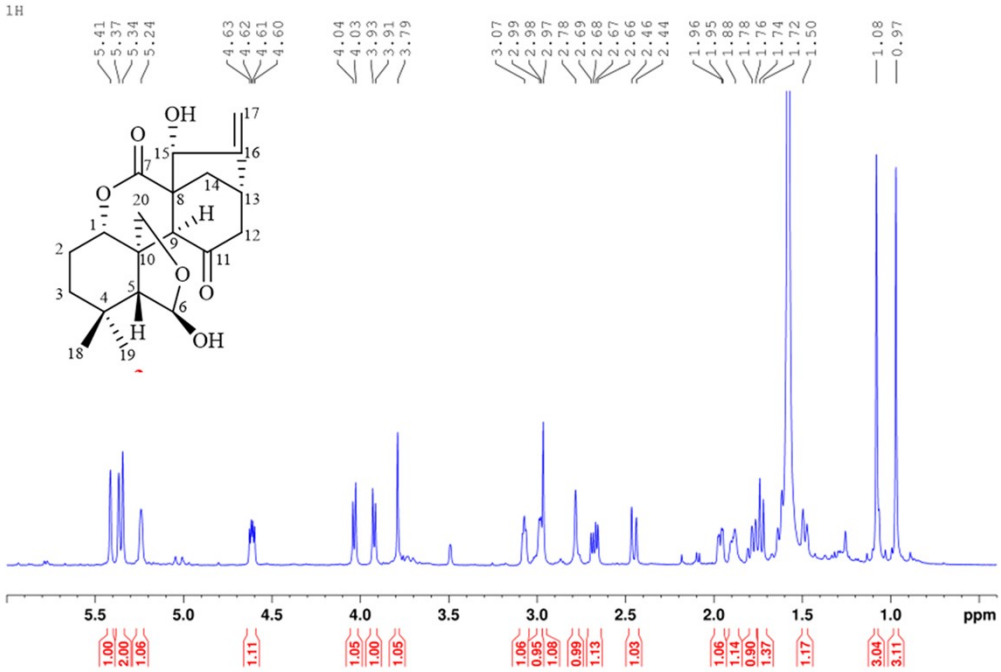


Fig. S22. ^{1}H NMR spectrum for compound **3**

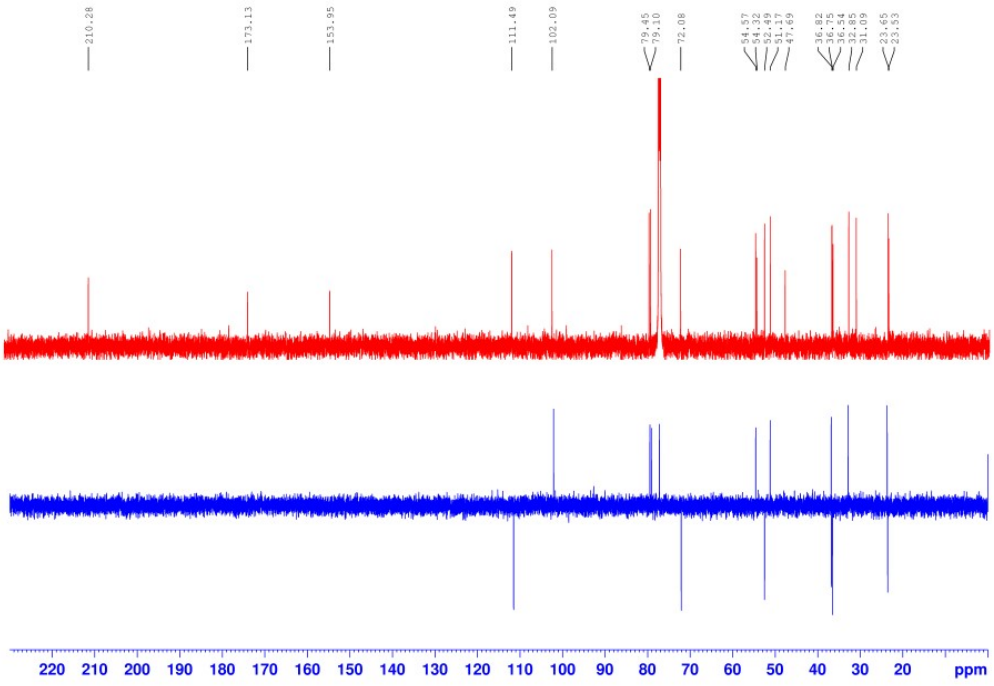


Fig. S23. ^{13}C and DEPT 135 NMR spectra for compound **3**

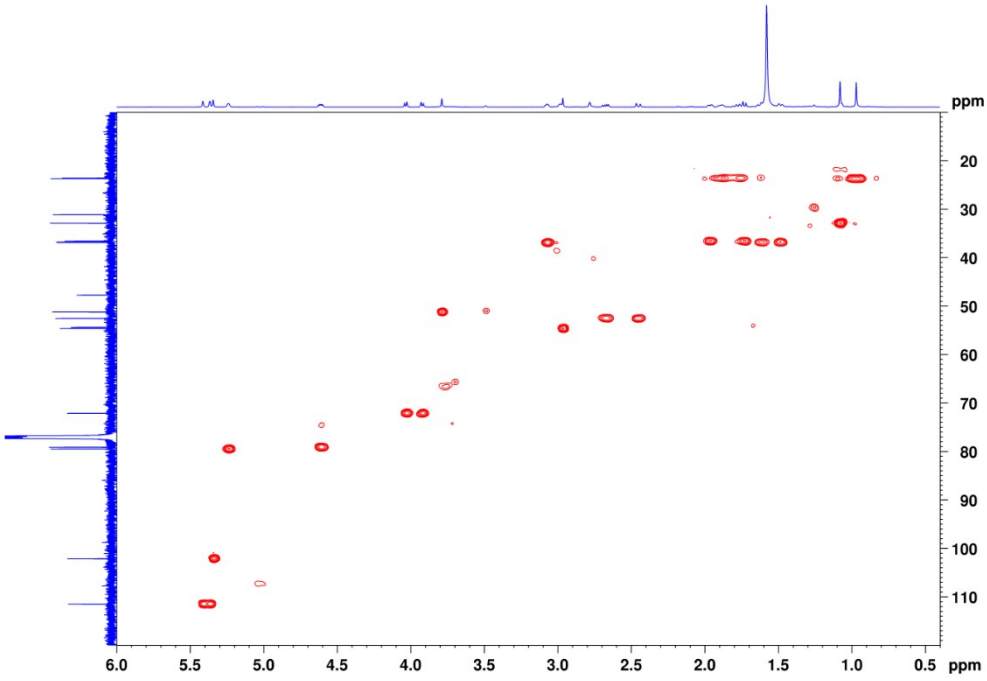


Fig. S24. HSQC NMR spectrum for compound **3**

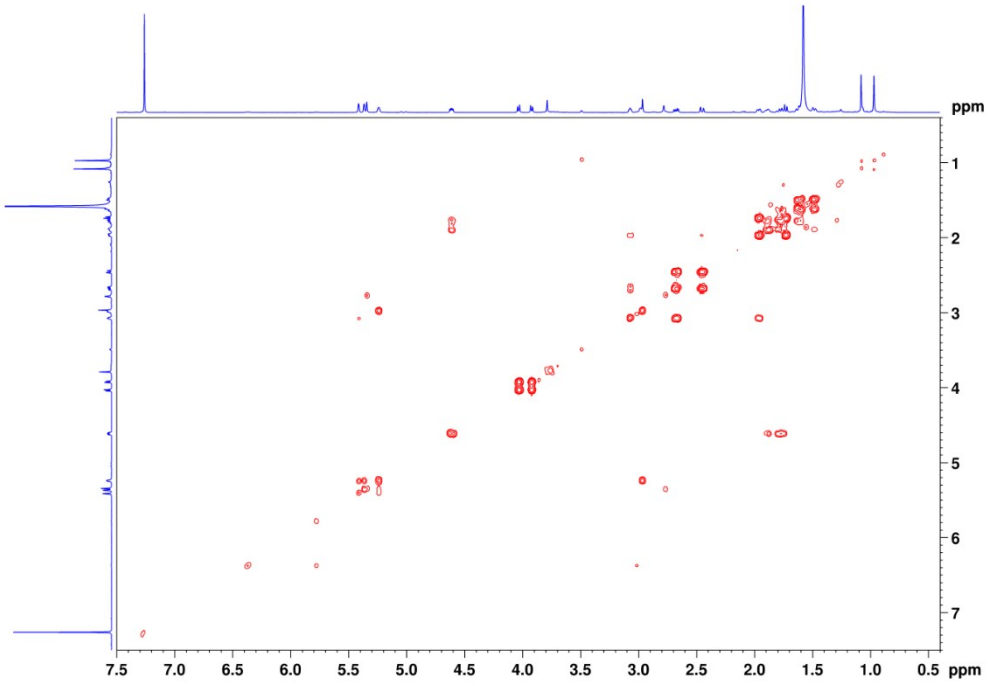


Fig. S25. ^{1}H–^{1}H COSY NMR spectrum for compound **3**

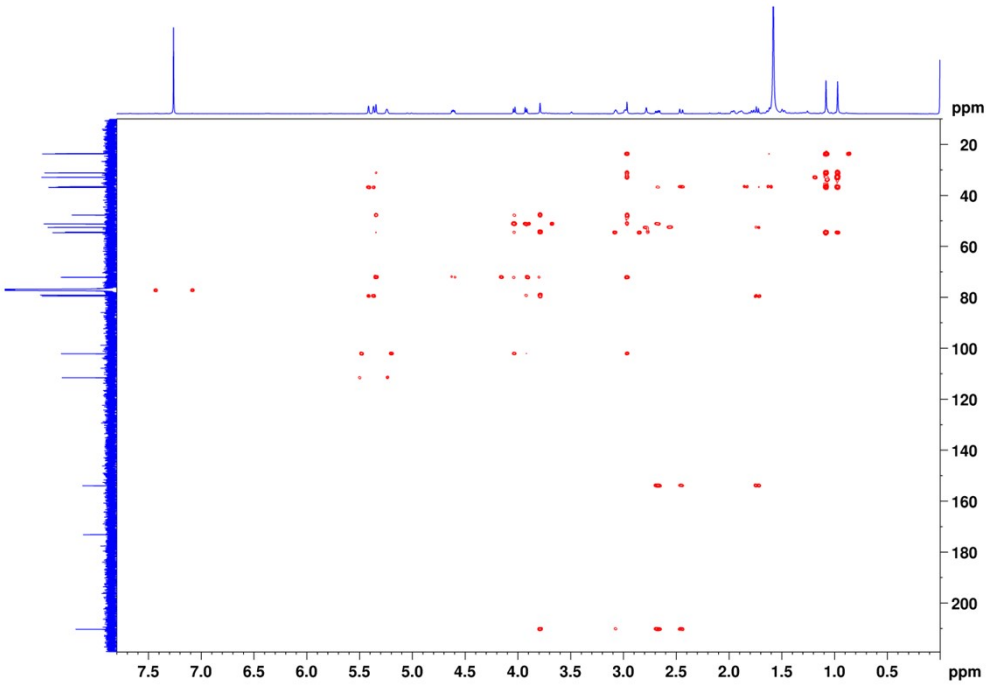


Fig. S26. HMBC NMR spectrum for compound **3**

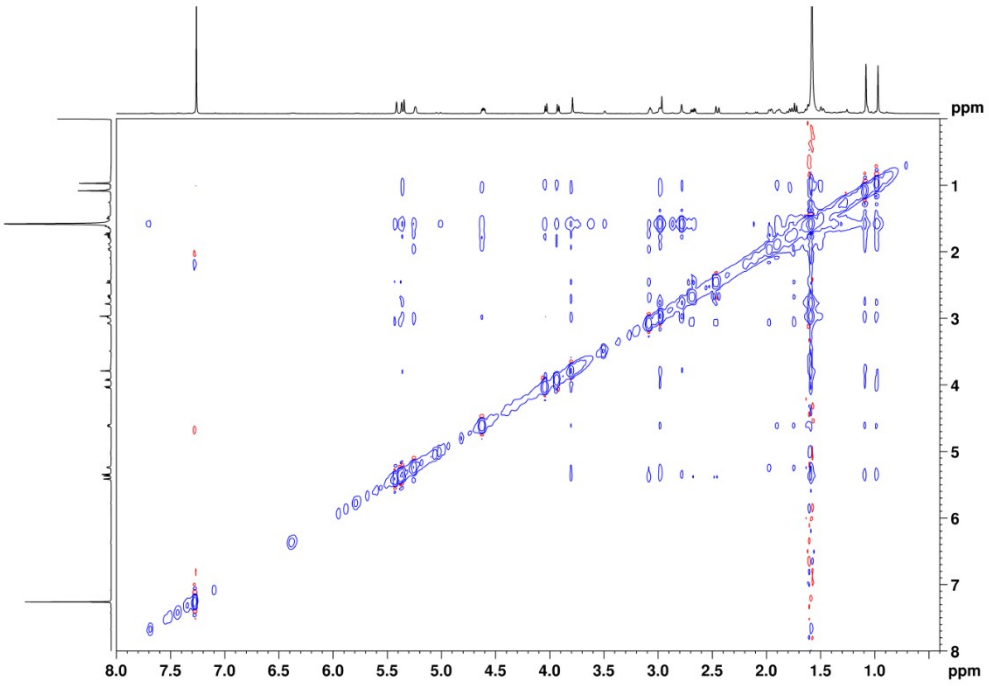


Fig. S27. NOESY NMR spectrum for compound **3**

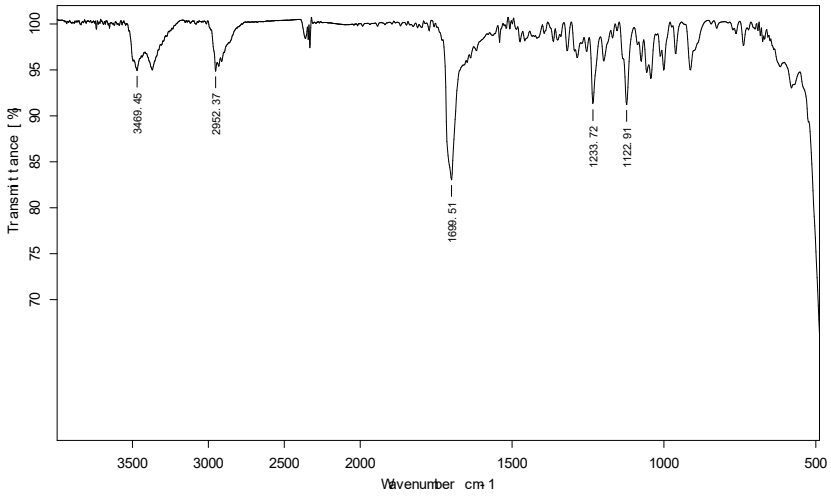


Fig. S28. IR spectrum of compound **3** (KBr)

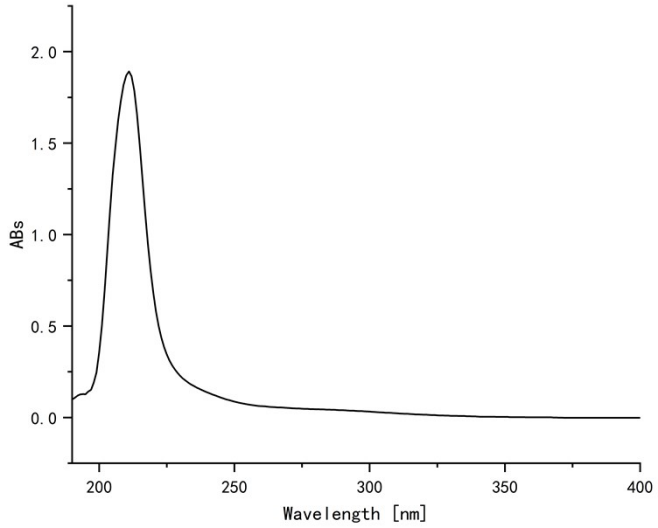


Fig. S29. UV spectrum of compound **3** in MeOH

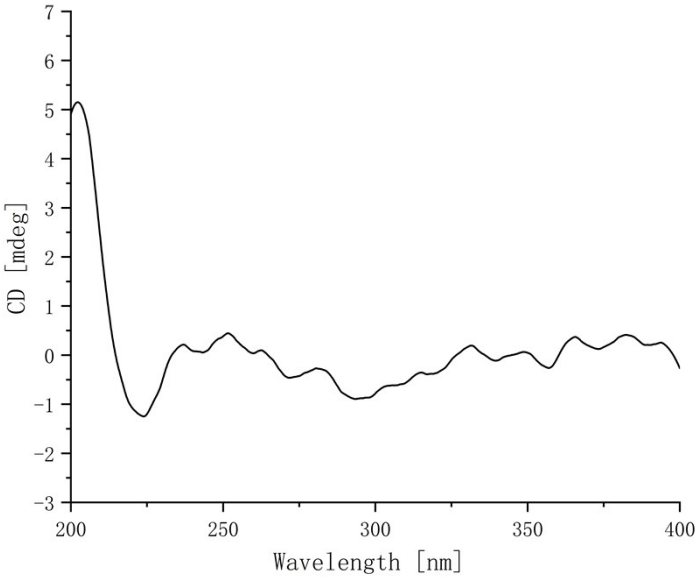


Fig. S30. CD spectrum of compound **3** in MeOH

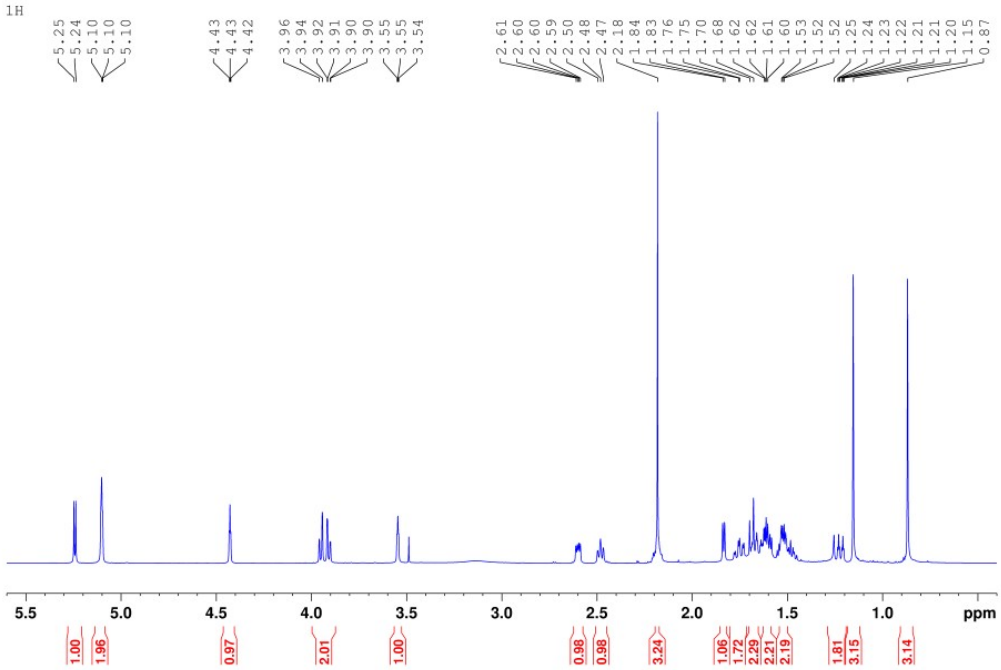


Fig. S31. [1]H NMR spectrum for compound **4**

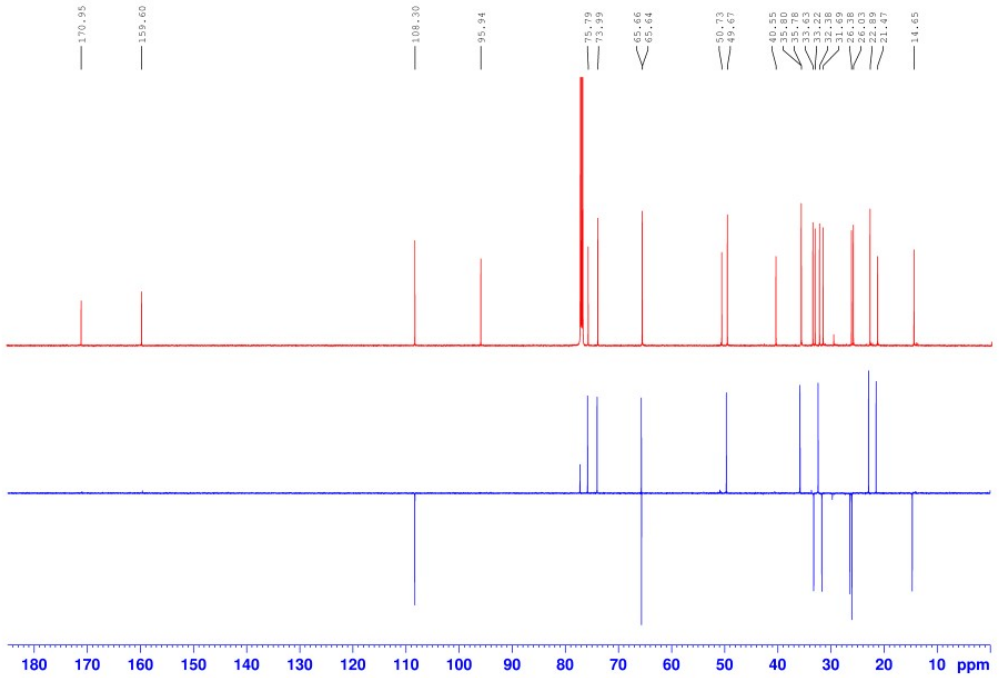


Fig. S32. [13]C and DEPT 135 NMR spectra for compound **4**

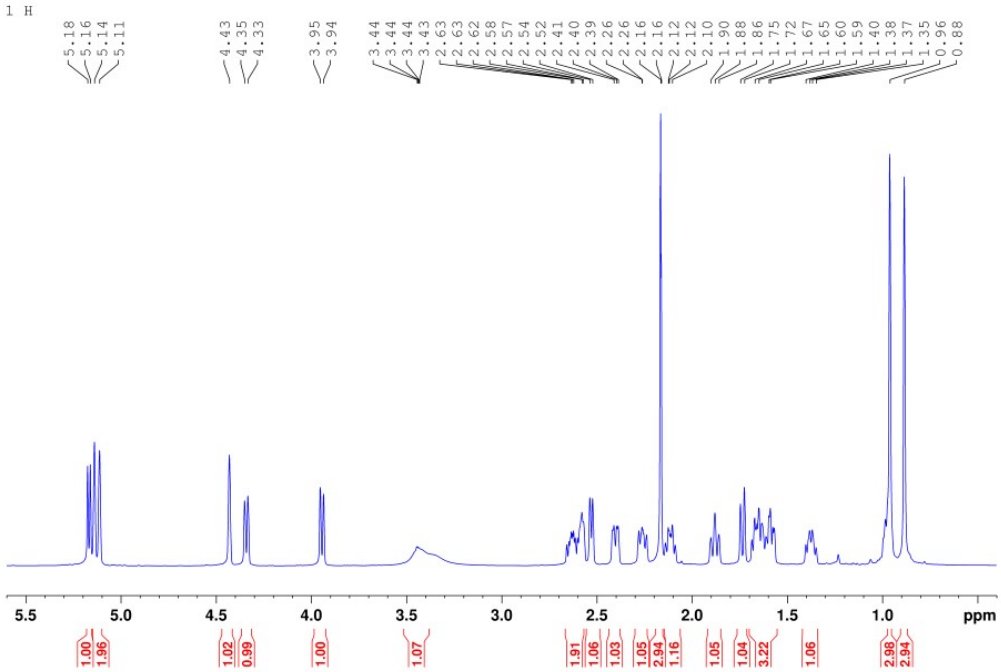


Fig. S33. [1]H NMR spectrum for compound **5**

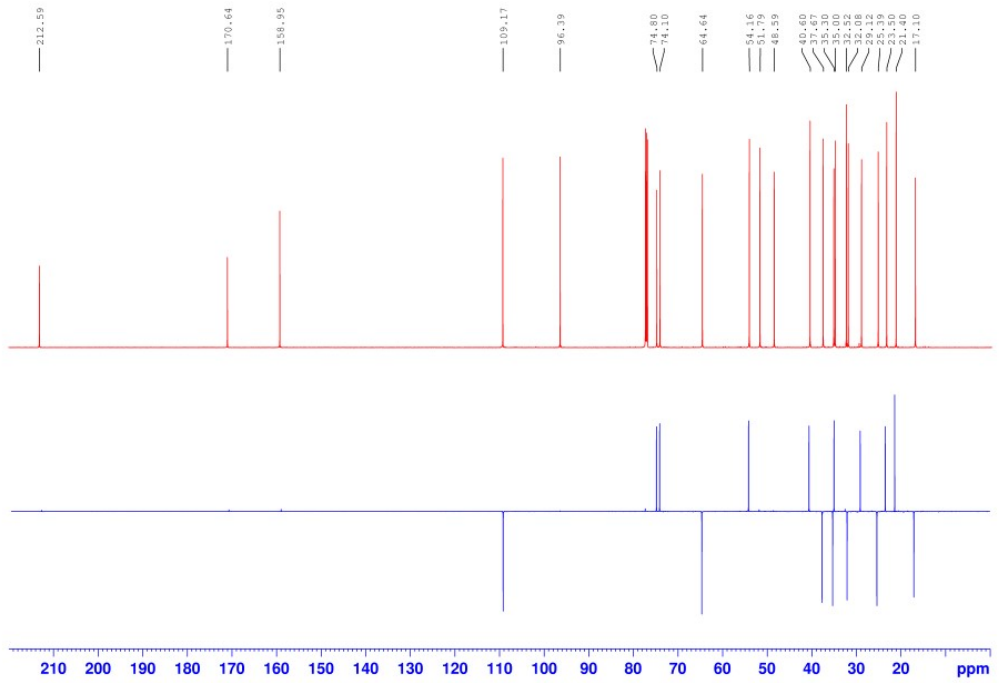


Fig. S34. [13]C and DEPT 135 NMR spectra for compound **5**

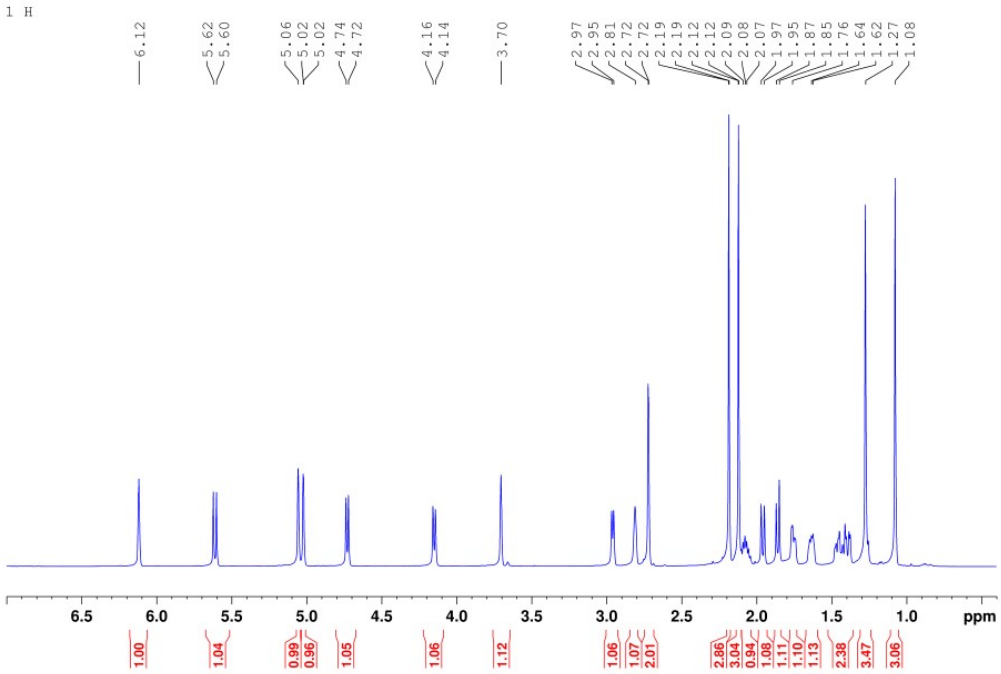


Fig. S35. ^{1}H NMR spectrum for compound **6**

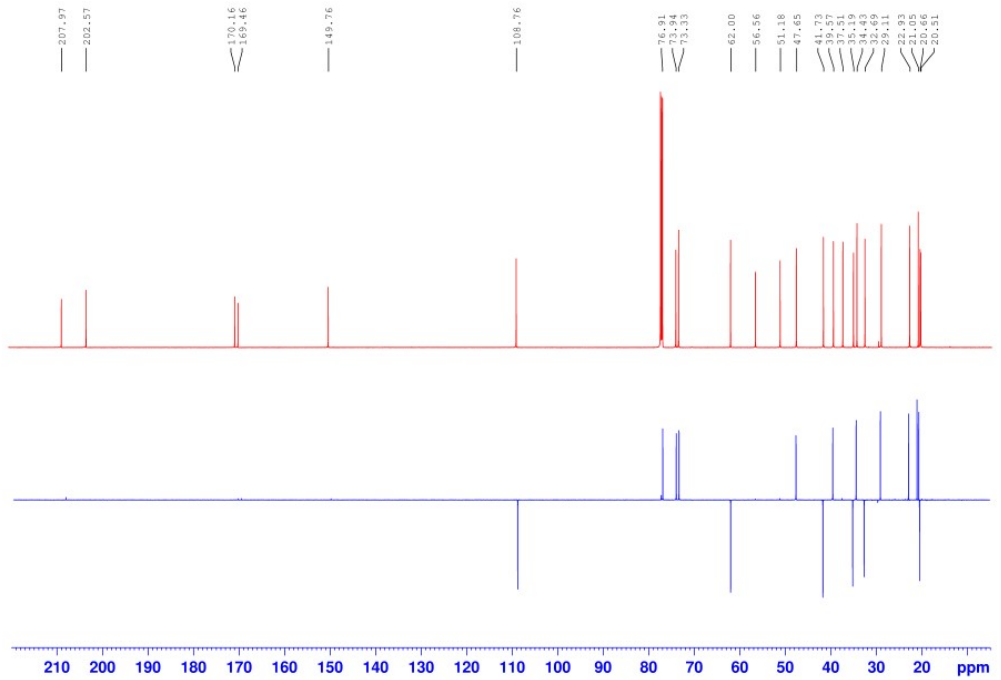


Fig. S36. ^{13}C and DEPT 135 NMR spectra for compound **6**

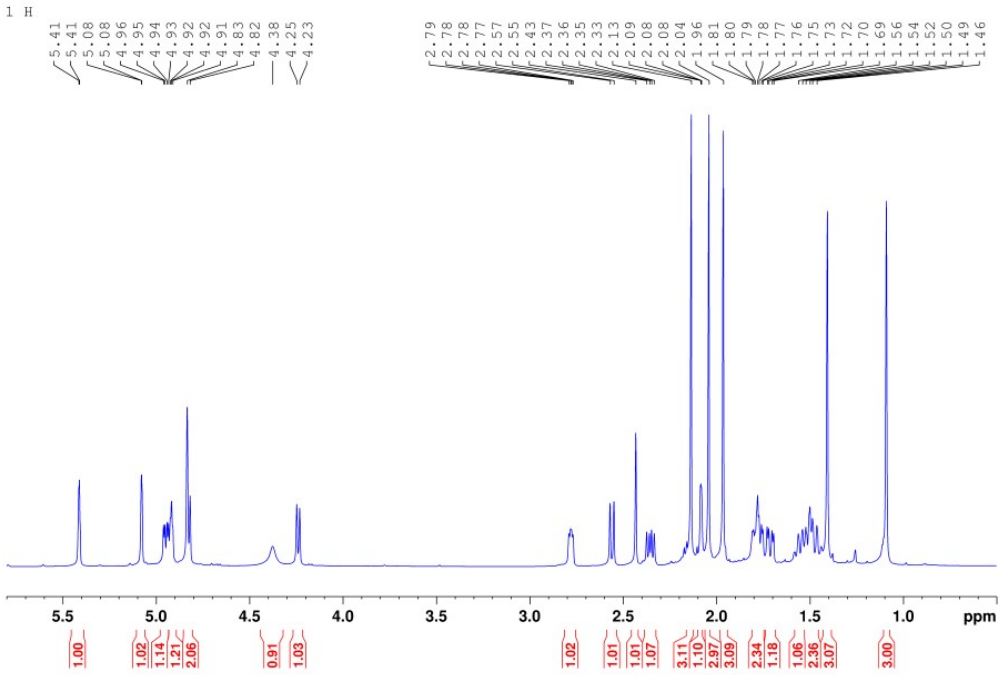


Fig. S37. ^{1}H NMR spectrum for compound **7**

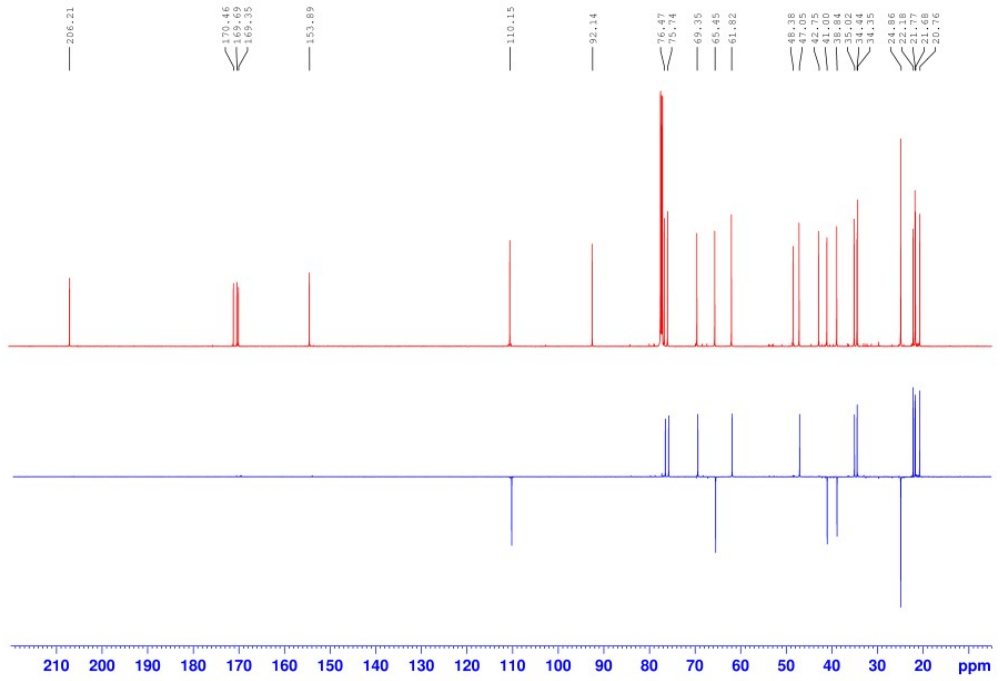


Fig. S38. ^{13}C and DEPT 135 NMR spectra for compound **7**

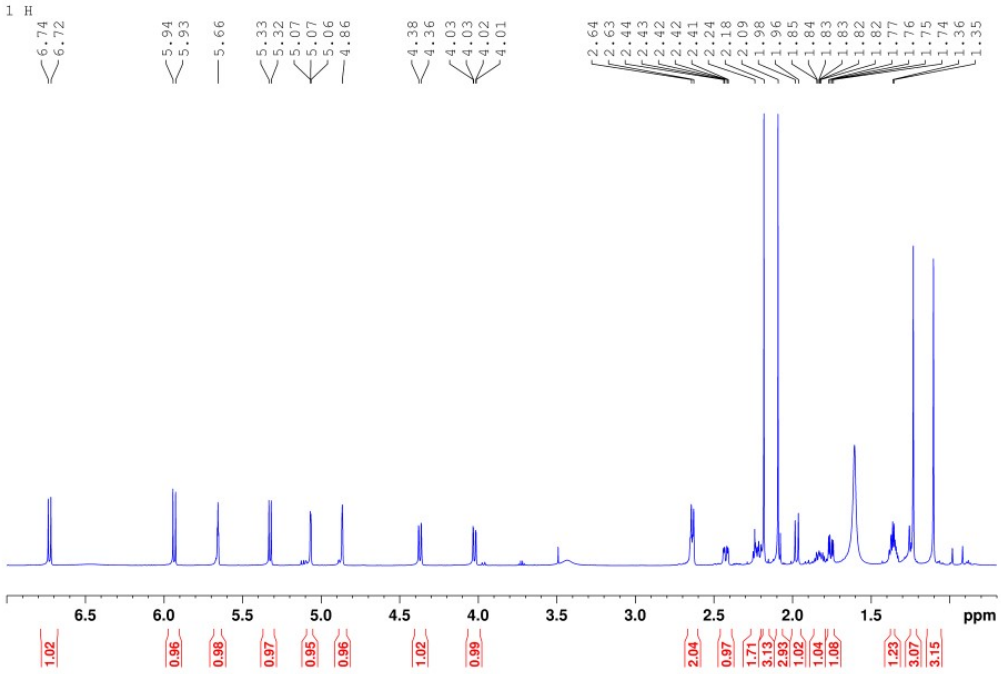


Fig. S39. [1]H NMR spectrum for compound **8**

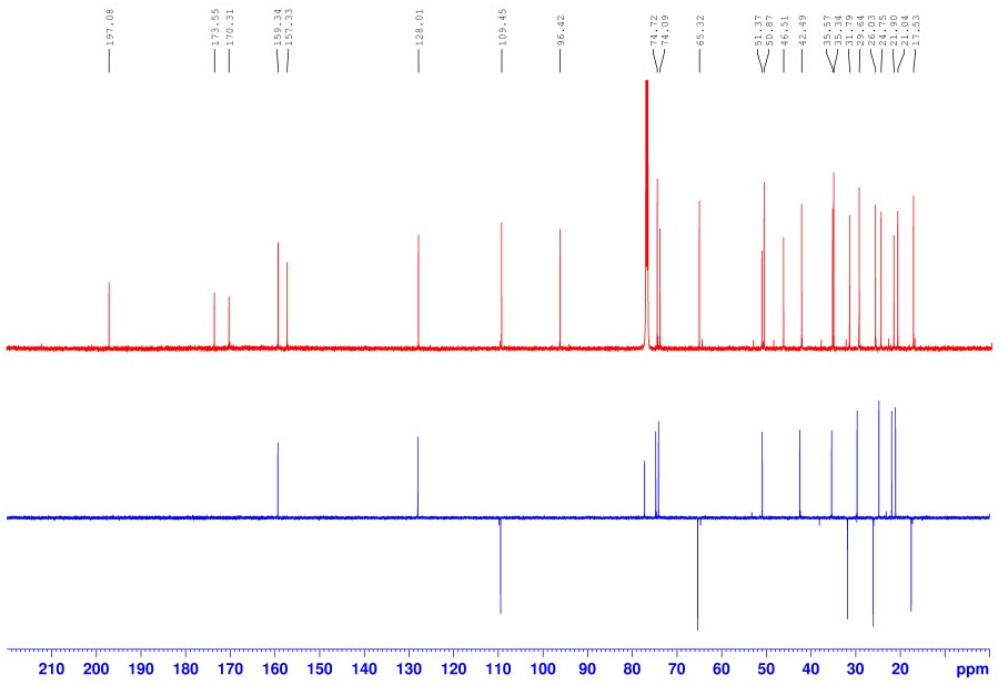


Fig. S40. [13]C and DEPT 135 NMR spectra for compound **8**

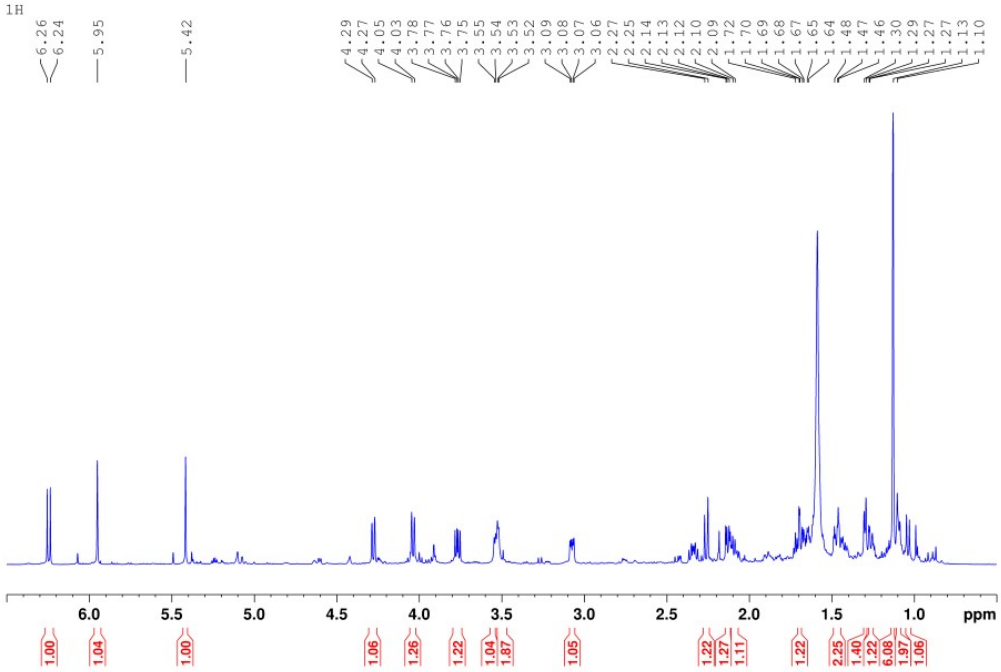


Fig. S41. [1]H NMR spectrum for compound **9**

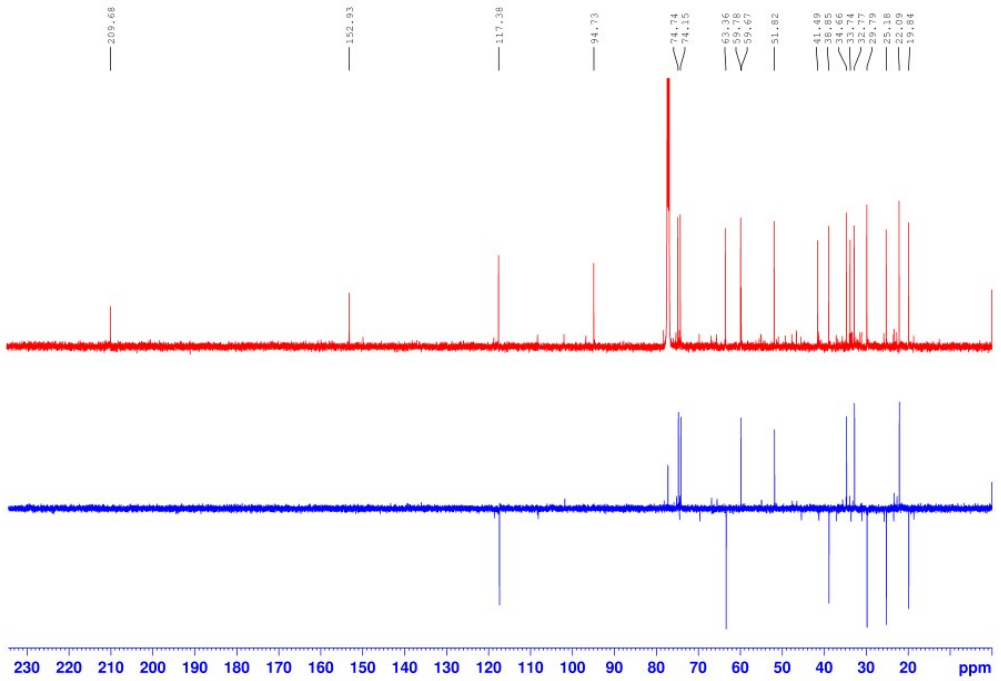


Fig. S42. [13]C and DEPT 135 NMR spectra for compound **9**

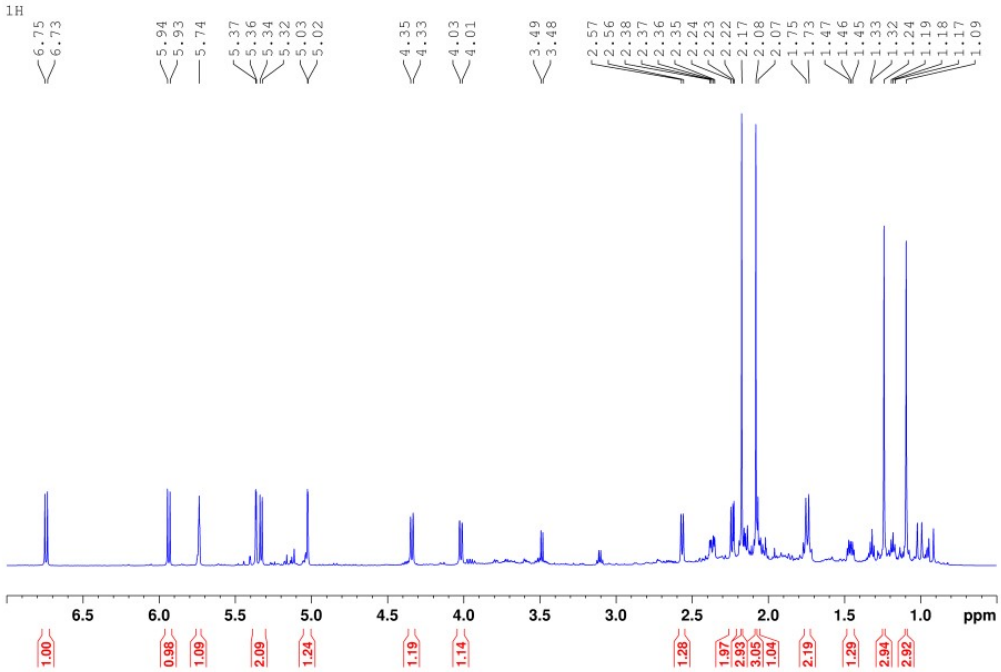


Fig. S43. [1]H NMR spectrum for compound **10**

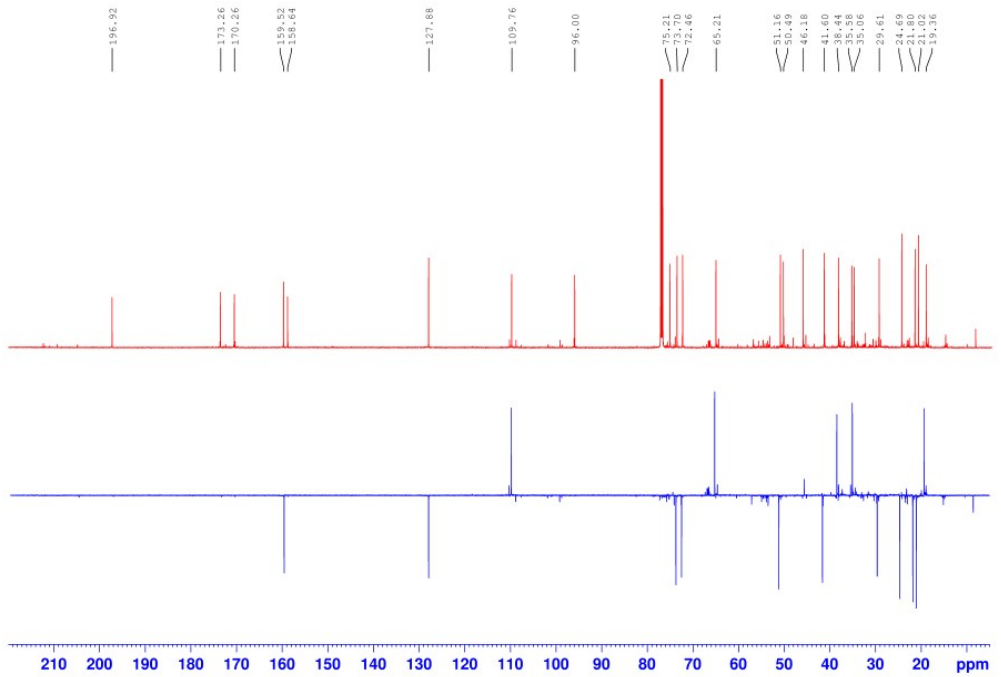


Fig. S44. [13]C and DEPT 135 NMR spectra for compound **10**

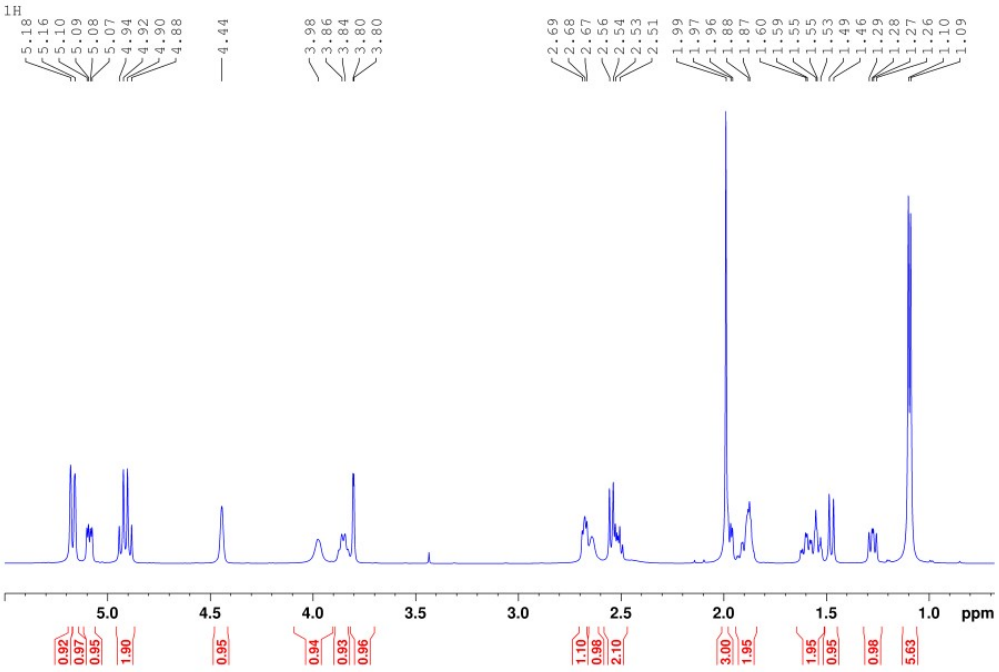


Fig. S45. [1]H NMR spectrum for compound **11**

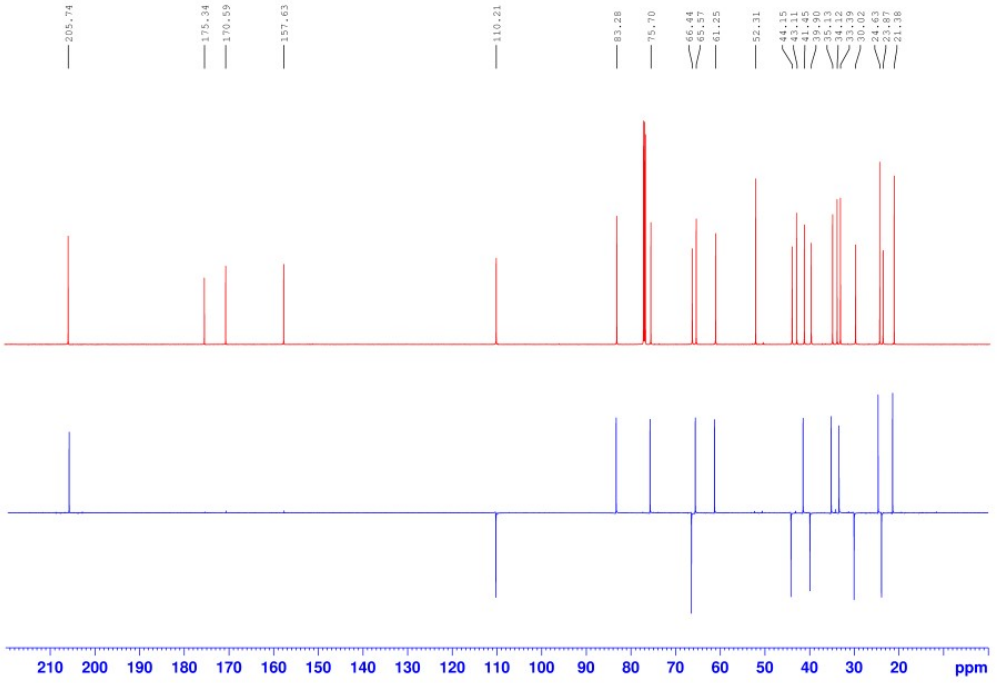


Fig. S46. [13]C and DEPT 135 NMR spectra for compound **11**

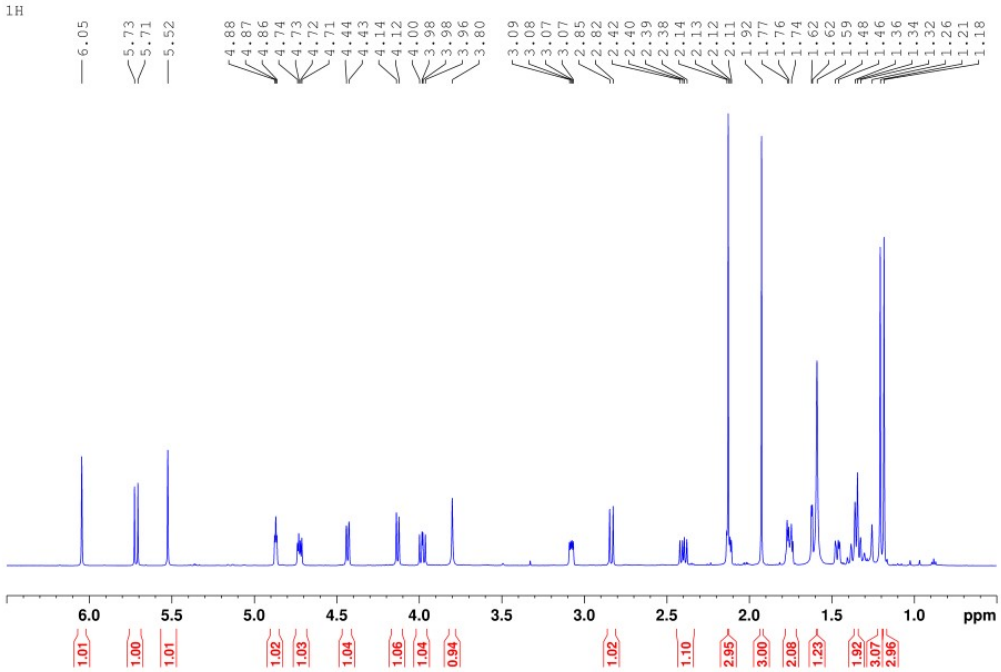


Fig. S47. [1]H NMR spectrum for compound **12**

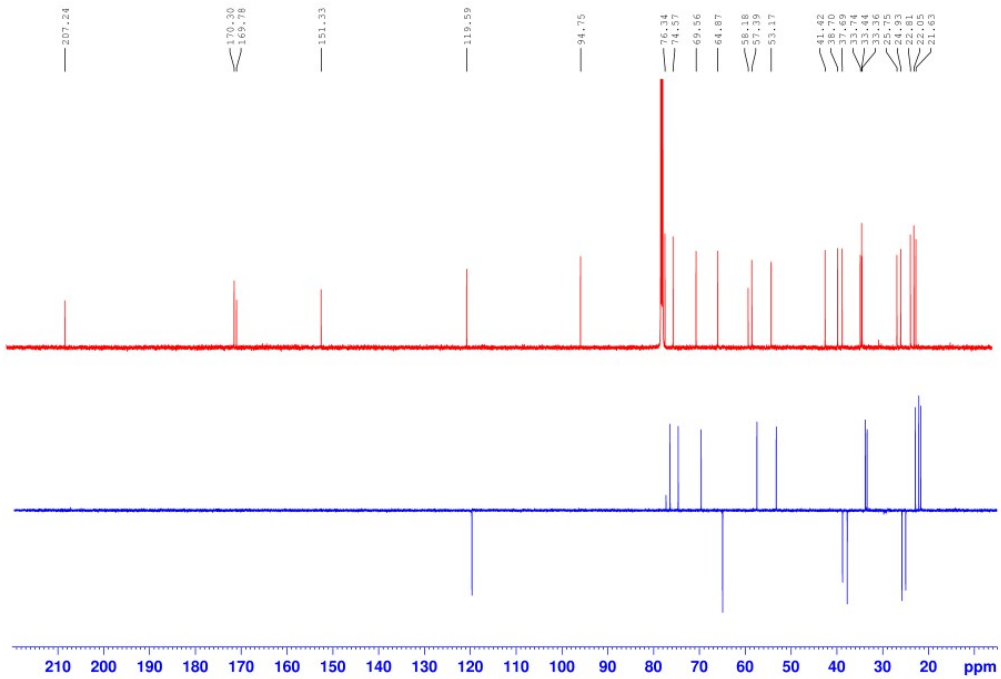


Fig. S48. [13]C and DEPT 135 NMR spectra for compound **12**

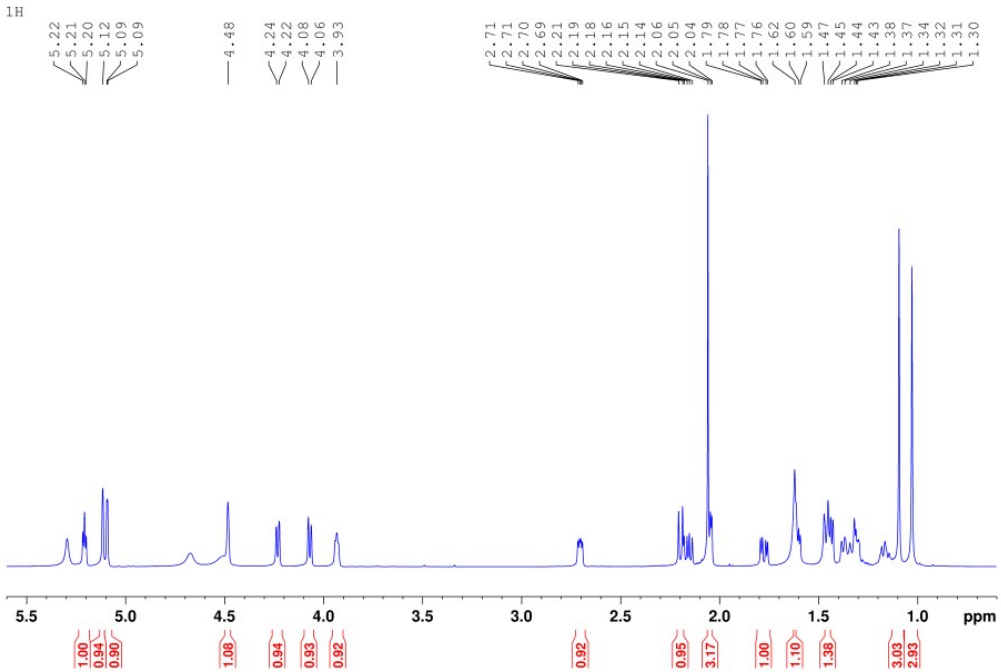


Fig. S49. [1]H NMR spectrum for compound **13**

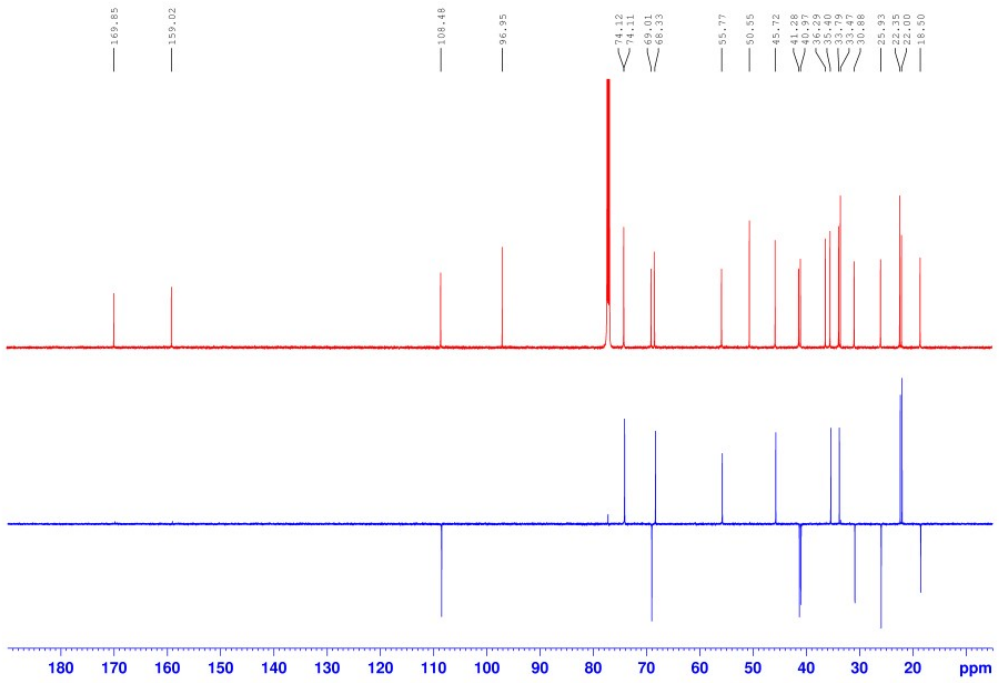


Fig. S50. [13]C and DEPT 135 NMR spectra for compound **13**

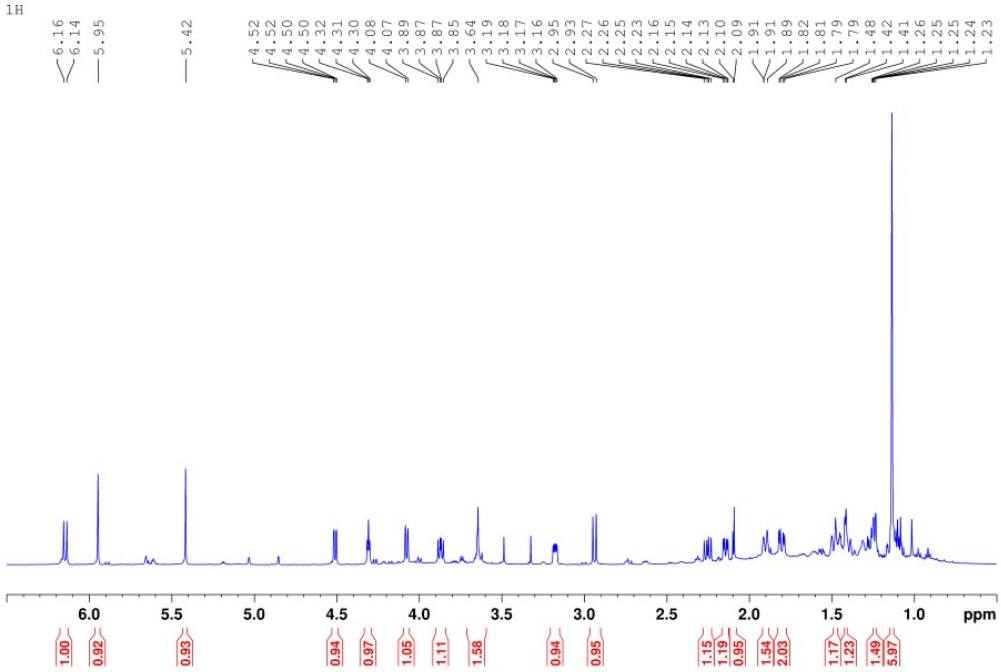


Fig. S51. [1]H NMR spectrum for compound **14**

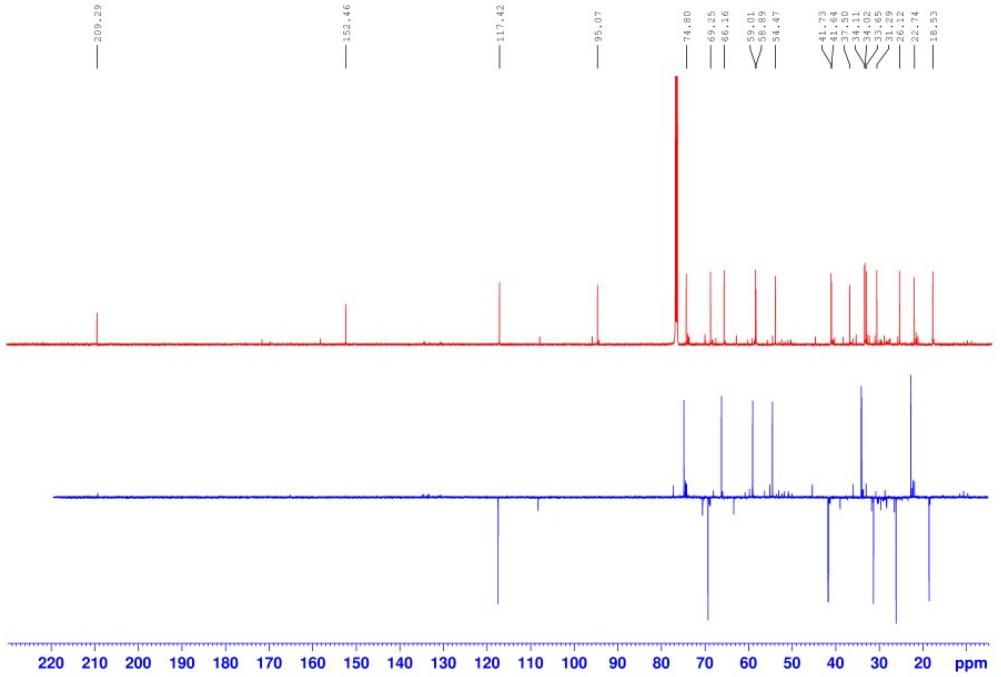


Fig. S52. [13]C and DEPT 135 NMR spectra for compound **14**

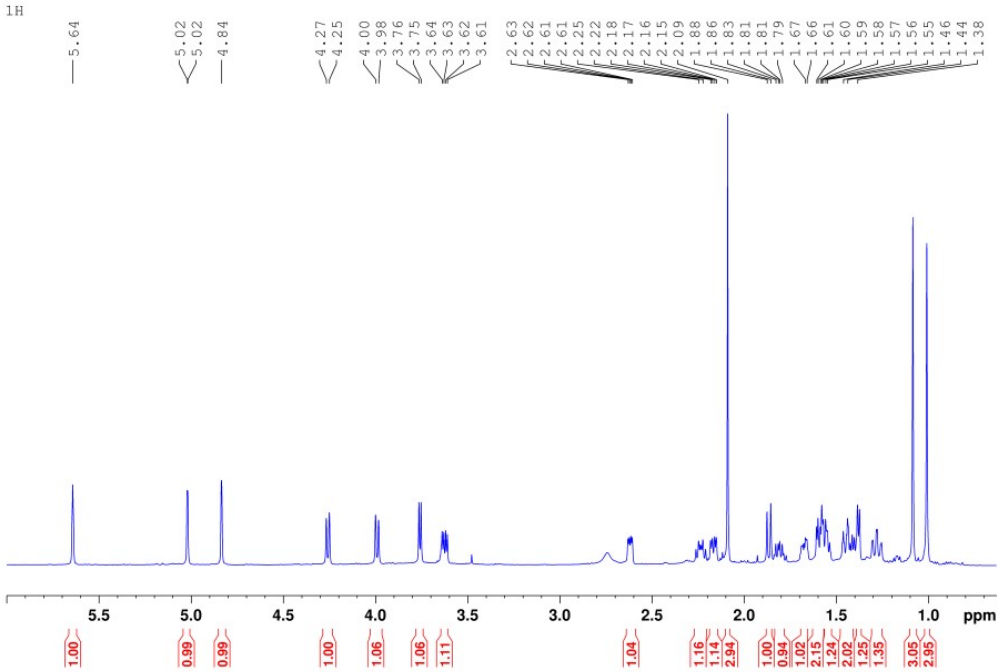


Fig. S53. [1]H NMR spectrum for compound **15**

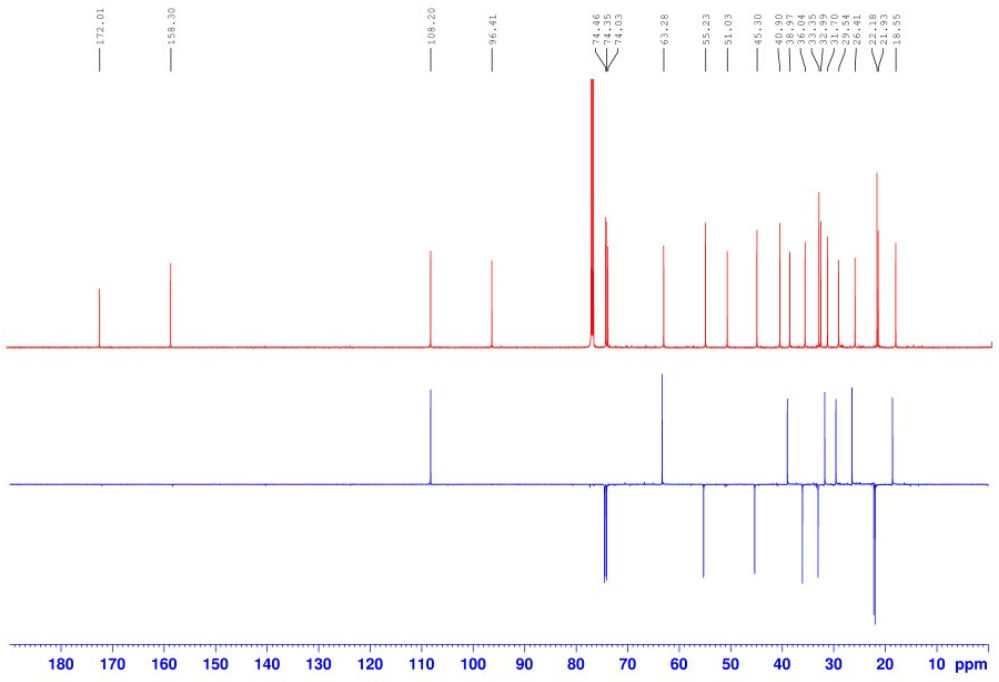


Fig. S54. [13]C and DEPT 135 NMR spectra for compound **15**

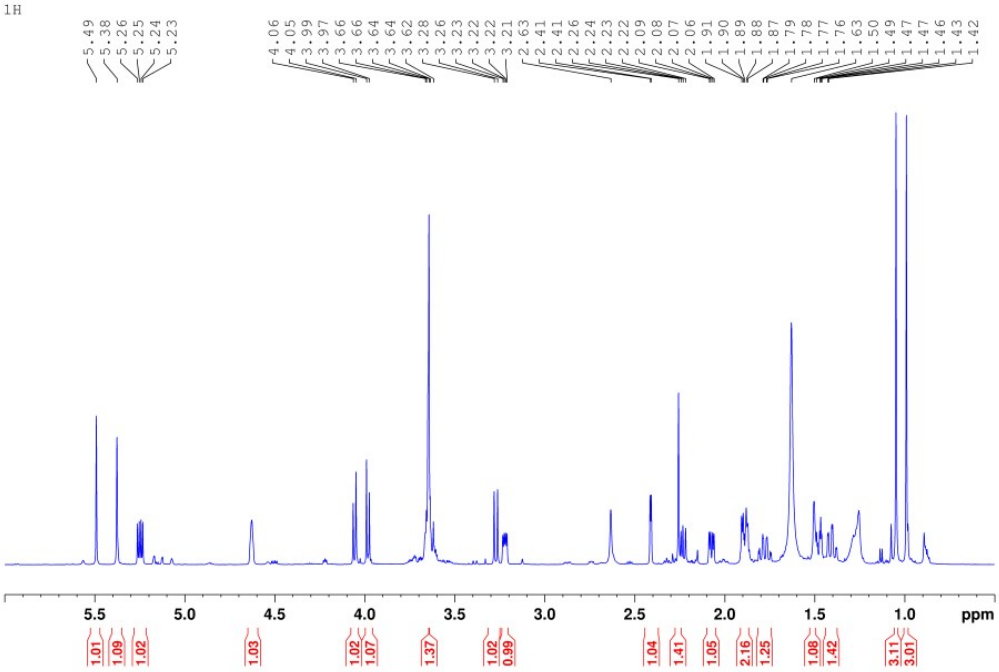


Fig. S55. [1]H NMR spectrum for compound **16**

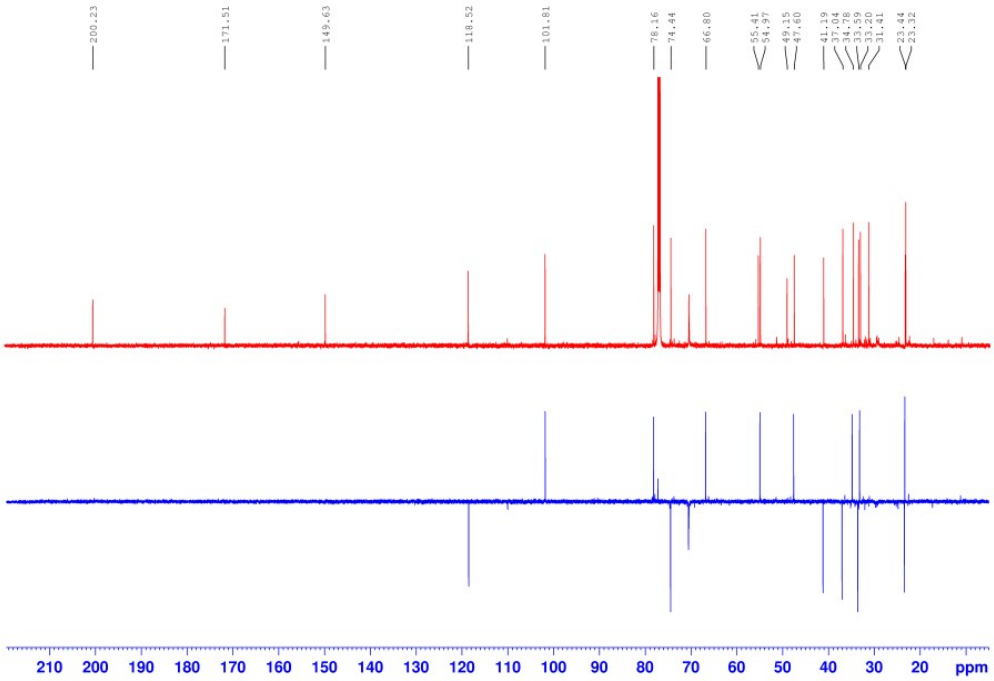


Fig. S56. [13]C and DEPT 135 NMR spectra for compound **16**

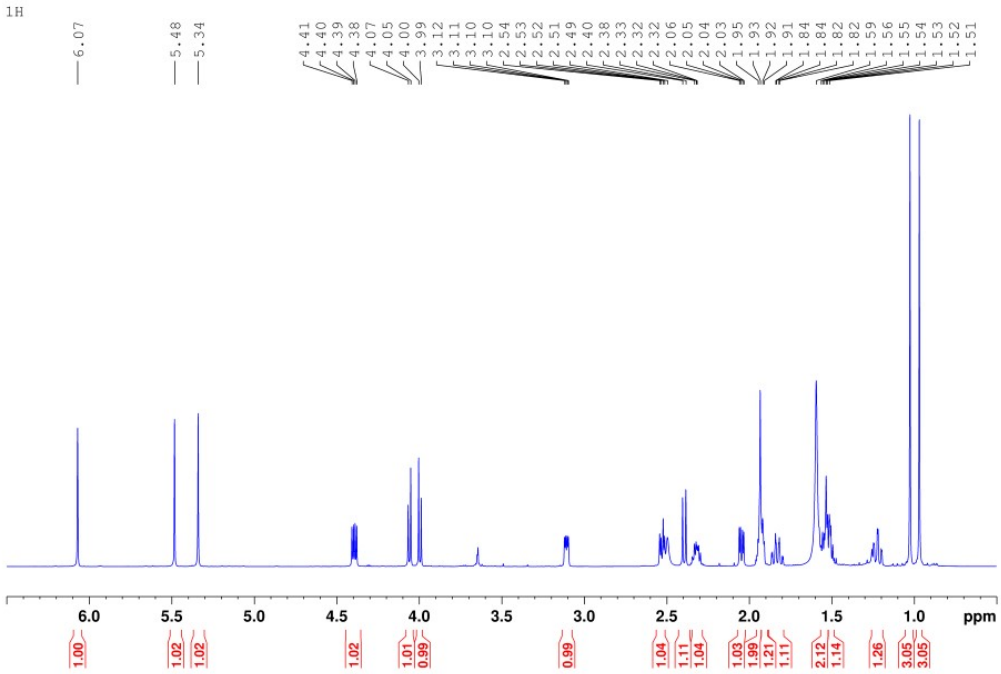


Fig. S57. [1]H NMR spectrum for compound **17**

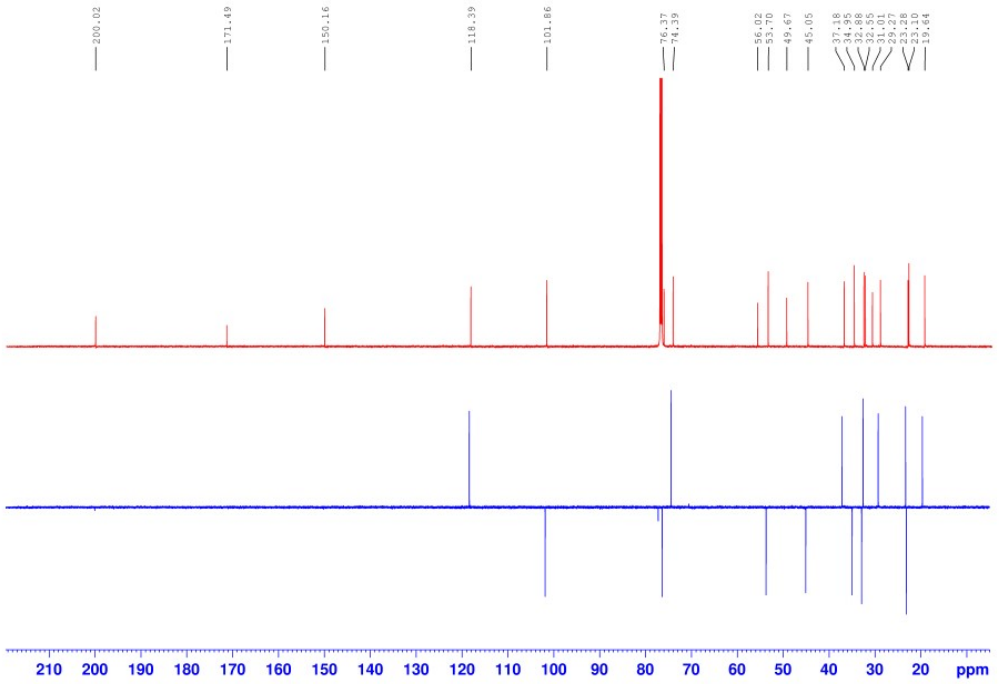


Fig. S58. [13]C and DEPT 135 NMR spectra for compound **17**

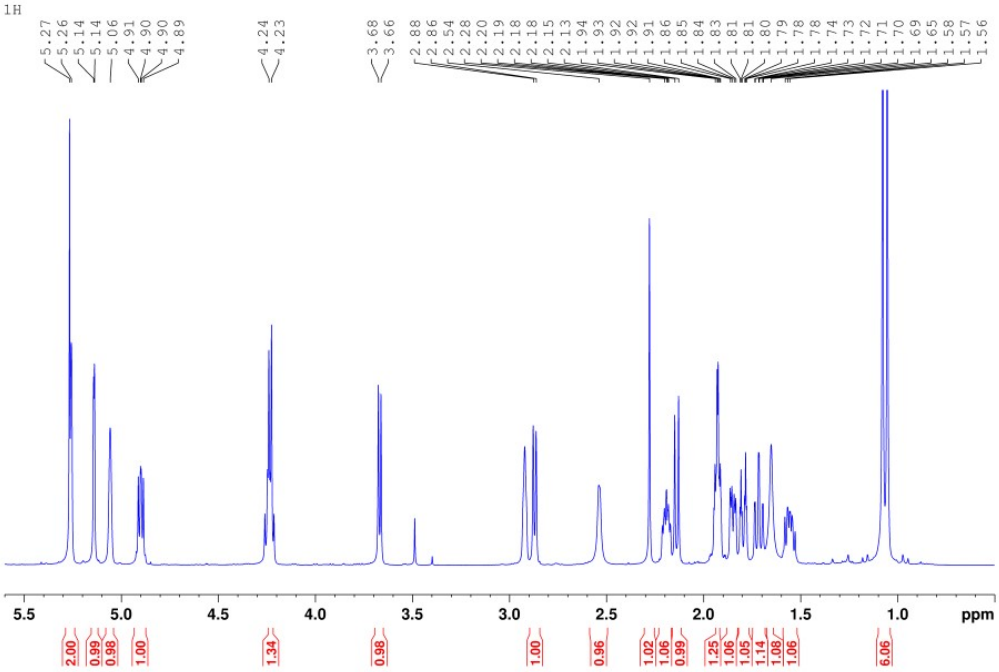


Fig. S59. ^{1}H NMR spectrum for compound **18**

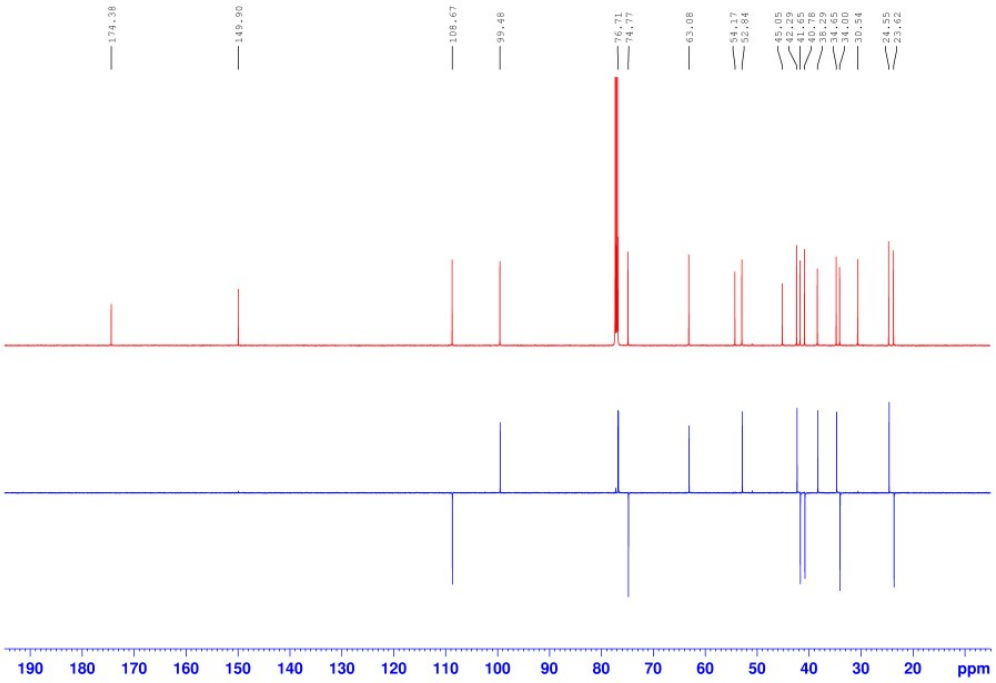


Fig. S60. ^{13}C and DEPT 135 NMR spectra for compound **18**

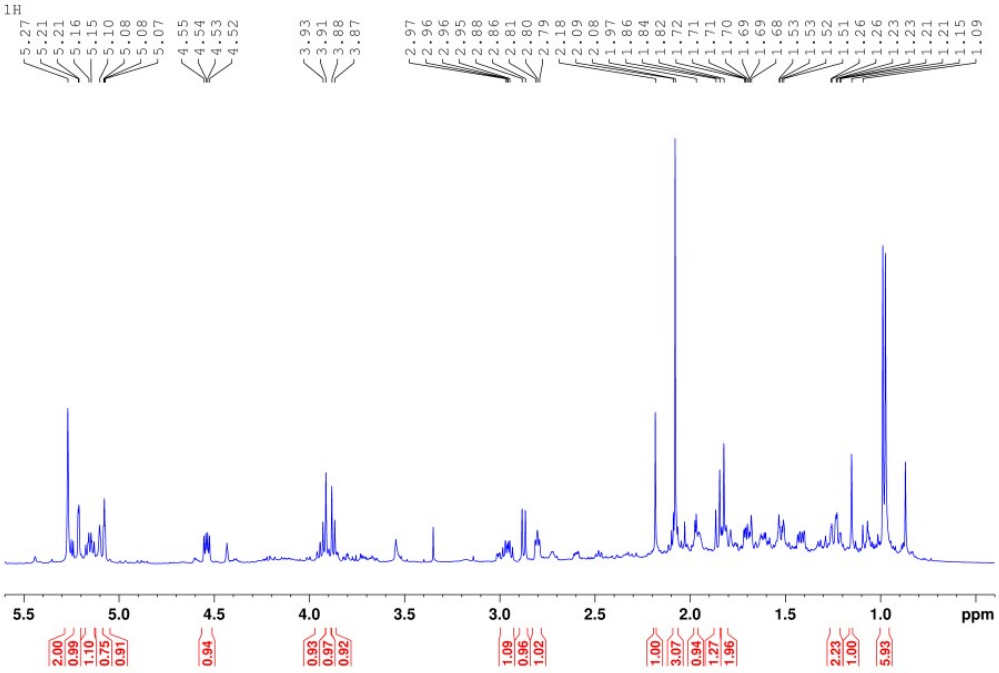


Fig. S61. [1]H NMR spectrum for compound **19**

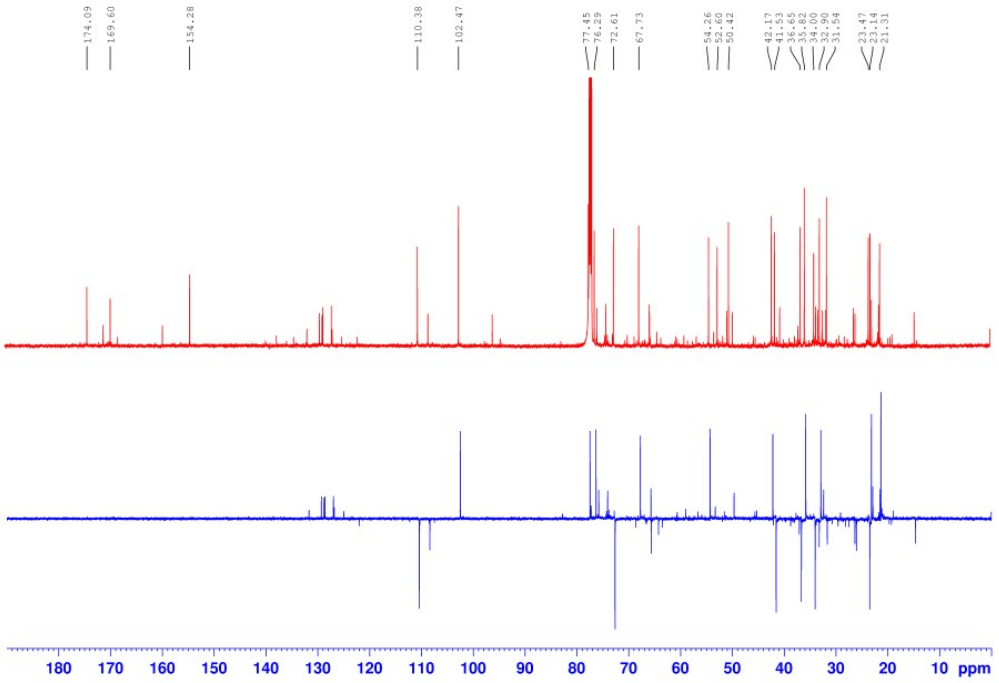


Fig. S62. [13]C and DEPT 135 NMR spectra for compound **19**

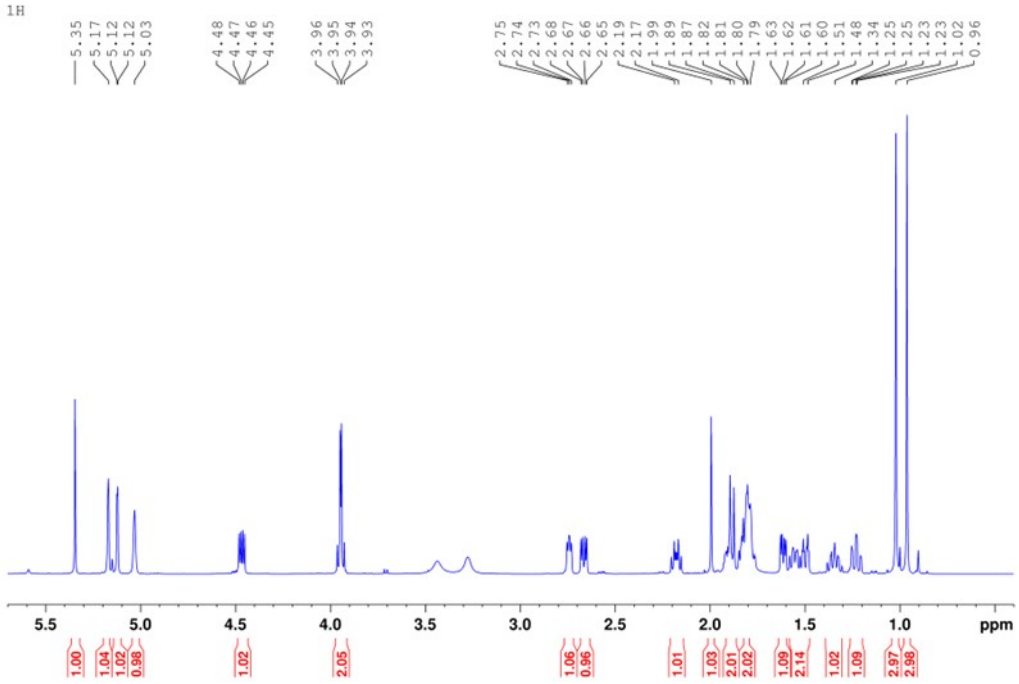


Fig. S63. [1]H NMR spectrum for compound **20**

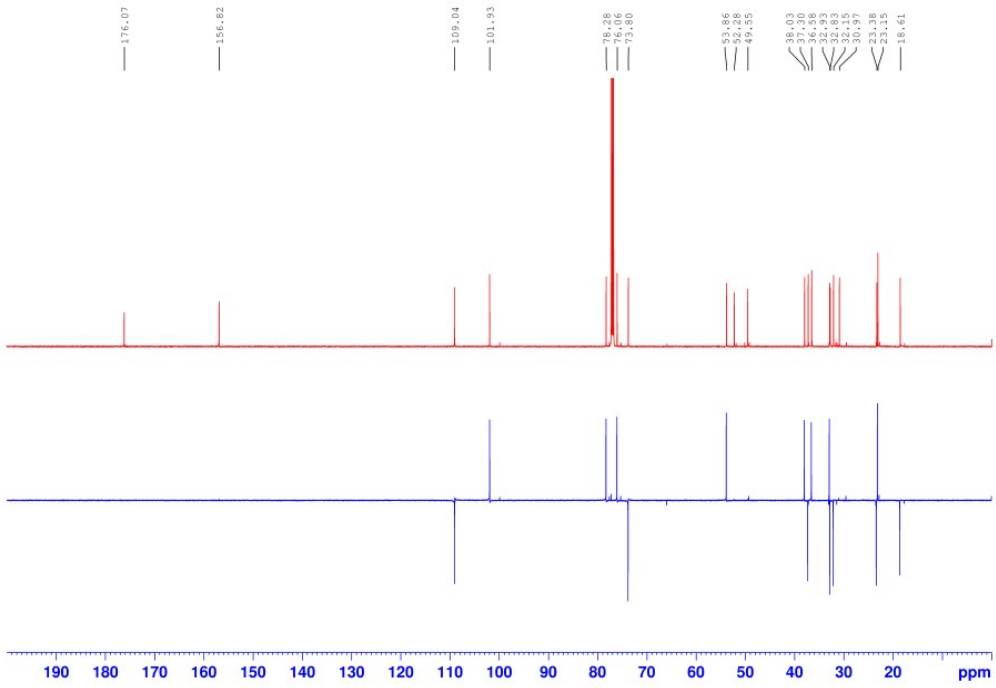


Fig. S64. [13]C and DEPT 135 NMR spectra for compound **20**

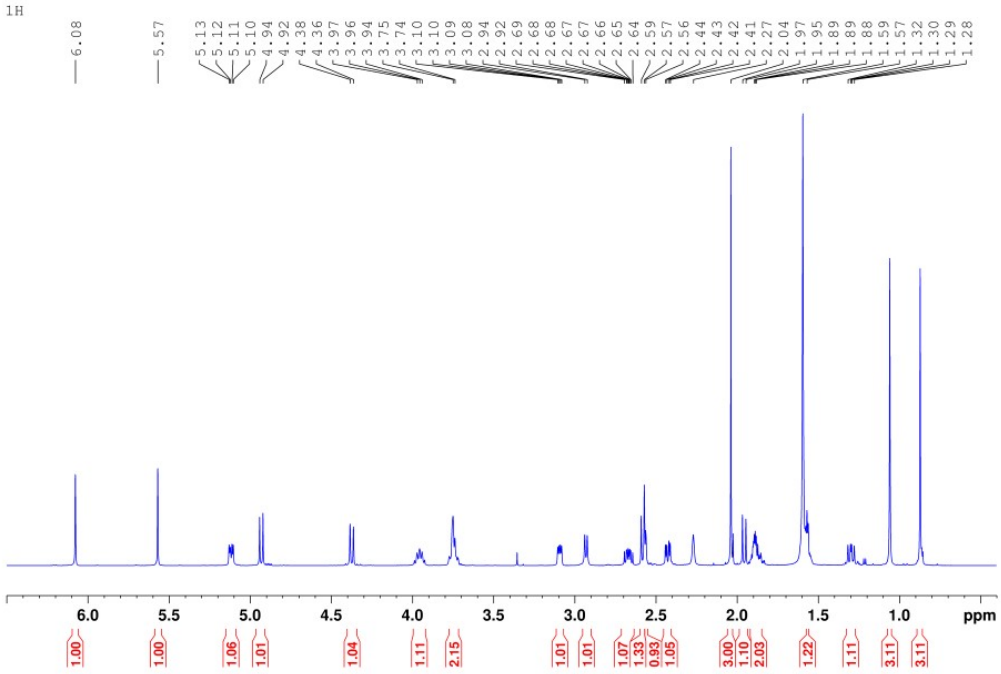


Fig. S65. [1]H NMR spectrum for compound **21**

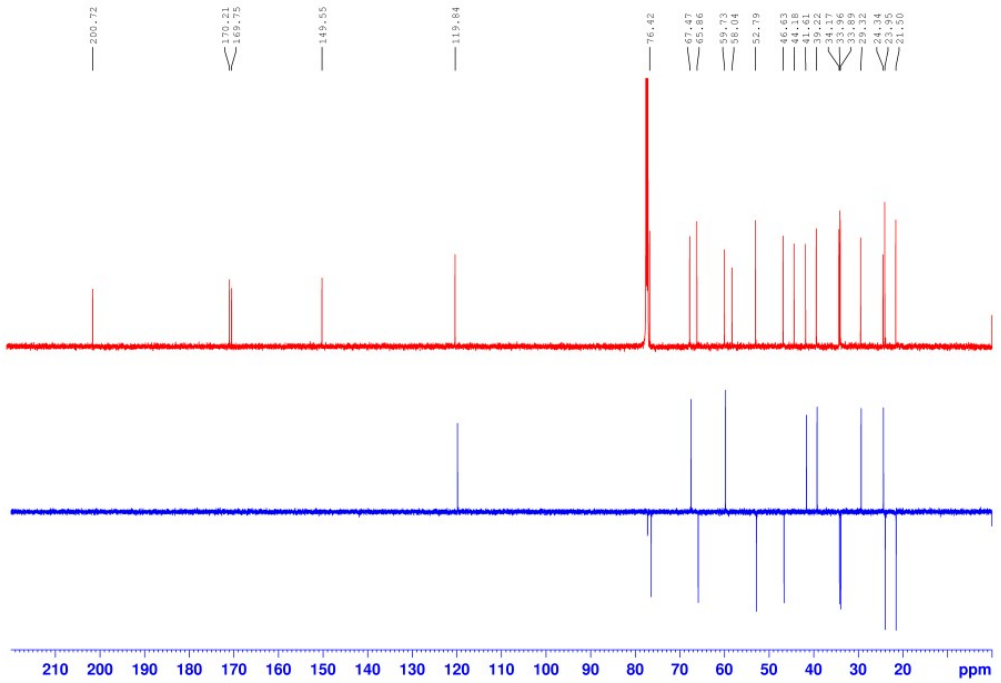


Fig. S66. [13]C and DEPT 135 NMR spectra for compound **21**

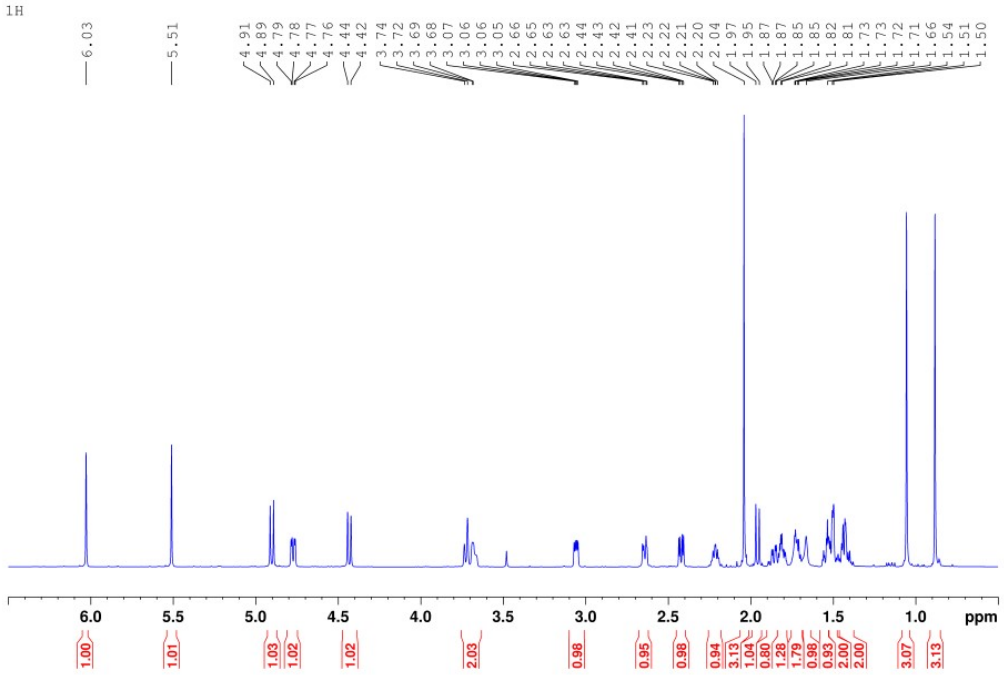


Fig. S67. [1]H NMR spectrum for compound **22**

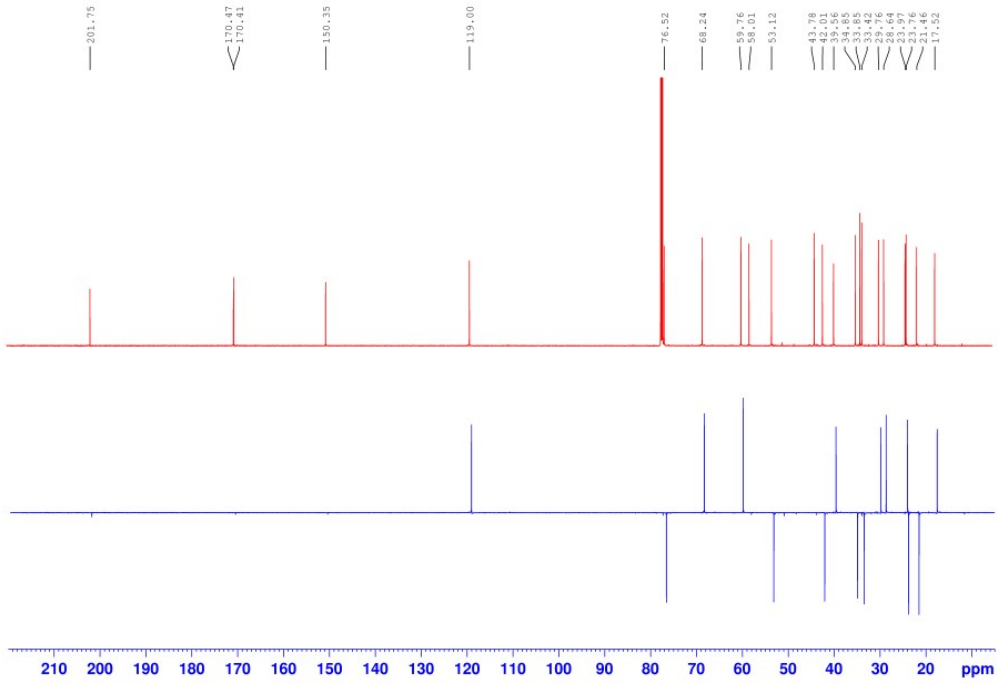


Fig. S68. [13]C and DEPT 135 NMR spectra for compound **22**

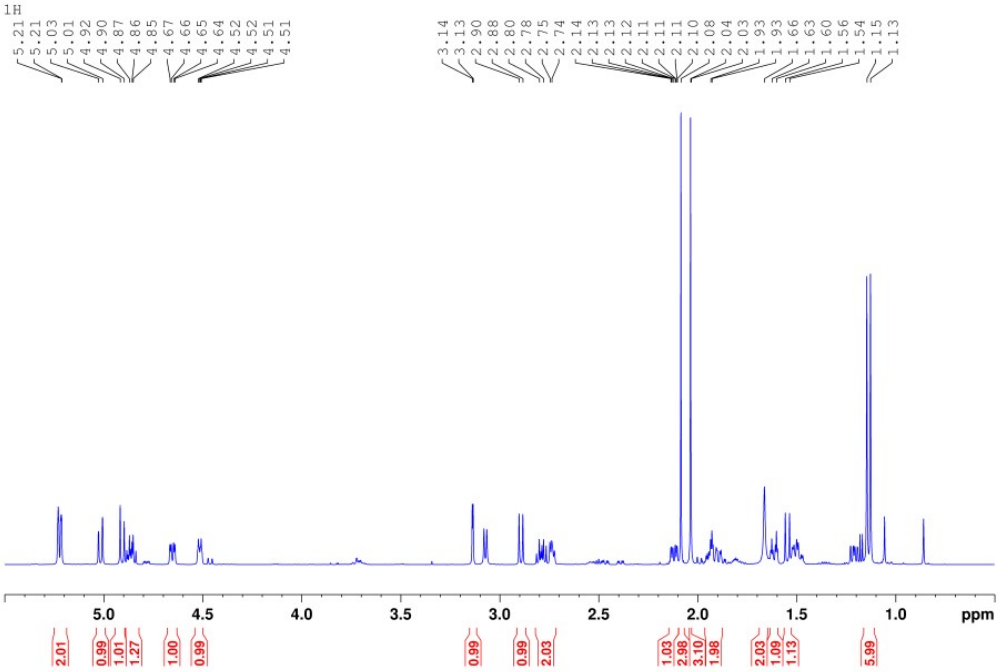


Fig. S69. [1]H NMR spectrum for compound **23**

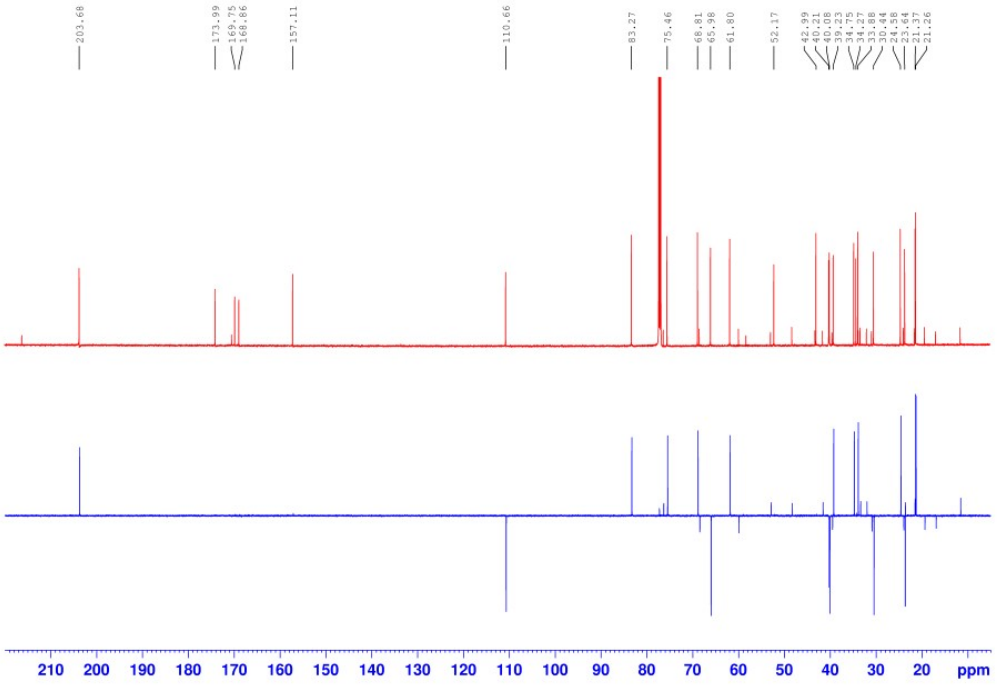


Fig. S70. [13]C and DEPT 135 NMR spectra for compound **23**

Table S1. Key conformers of compound **1**.

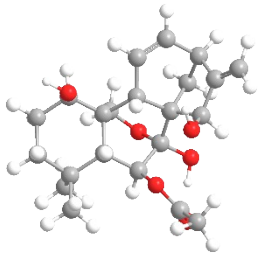
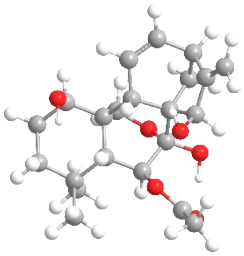
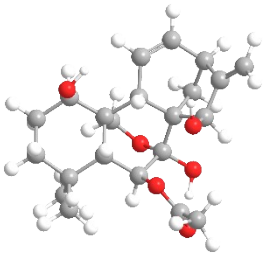
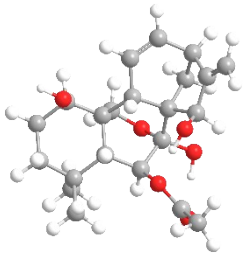
			
Conformer **1-1** 79.82%	Conformer **1-2** 13.98%	Conformer **1-3** 3.93%	Conformer **1-4** 2.27%

Table S2. Conformers and Bolzmann distributions of the optimized **1**.

species	*E'=E+ZPE*	*E*	*H*	*G*	*ΔG*	*ΔE(kcal/mol)*	*p%*
1-1	-1307.189372	-1307.164159	-1307.163215	-1307.240857	0	0	79.82%
1-2	-1307.187959	-1307.162715	-1307.161771	-1307.239213	0.001644	1.031625618	13.98%
1-3	-1307.186562	-1307.161184	-1307.16024	-1307.238016	0.002841	1.782754489	3.93%
1-4	-1307.186094	-1307.160767	-1307.159823	-1307.237498	0.003359	2.107804411	2.27%

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy

Table S3. Optimized Z-matrixes of isomer **1** in the gas phase (Å) at B3LYP/6-31G(d) level.

1-1					**1-2**			
atom	X	Y	Z		atom	X	Y	Z
C	-2.94781	-2.62934	-0.22802		C	-3.10239	-2.46472	-0.26741
C	-3.58265	-1.37063	-0.82946		C	-3.70104	-1.1553	-0.79406
C	-3.05156	-0.06029	-0.19958		C	-3.09528	0.106015	-0.13042
C	-1.48383	-0.07673	-0.30043		C	-1.53441	0.024645	-0.27987
C	-0.74235	-1.3807	0.160426		C	-0.84406	-1.32046	0.121282
C	-1.42523	-2.63396	-0.4214		C	-1.58543	-2.5224	-0.49338
C	-0.80264	1.133114	0.376678		C	-0.771	1.192083	0.38868
C	0.379803	0.675848	1.251486		C	0.387368	0.654327	1.257686
C	1.465743	-0.13309	0.51696		C	1.427441	-0.20964	0.51388
C	0.744705	-1.23926	-0.329		C	0.645734	-1.22195	-0.38376
C	2.47605	-0.72136	1.535331		C	2.353625	-0.91728	1.540463
C	3.519044	-1.33058	0.586504		C	3.392012	-1.55915	0.610069
C	2.862832	-2.53394	-0.07228		C	2.680378	-2.65907	-0.16453
C	1.57198	-2.50313	-0.421		C	1.409137	-2.51716	-0.55849
C	-0.68034	-1.44286	1.697546		C	-0.7744	-1.42751	1.654471
O	-0.2644	-0.17682	2.225785		O	-0.30723	-0.19424	2.209664
C	3.705135	-0.20919	-0.43419		C	3.718442	-0.3986	-0.32176
C	2.458695	0.675121	-0.38799		C	2.523511	0.560398	-0.3079
C	4.746117	-0.01204	-1.23968		C	4.813364	-0.22614	-1.06282
O	2.0256	0.984869	-1.70422		O	2.178677	1.0333	-1.60436
O	0.973194	1.73379	1.929089		O	1.030965	1.64568	1.982842
O	-1.11087	-2.66854	-1.82035		O	-1.29798	-2.51658	-1.90032
C	-3.57564	1.128593	-1.03437		C	-3.58656	1.345625	-0.91013

C	-3.62733	0.092289	1.227513		C	-3.62683	0.232611	1.316401
O	-0.38572	2.098935	-0.63957		O	-0.33985	2.094134	-0.66337
O	-0.71277	3.823935	0.801629		O	-0.18081	3.837363	0.776835
C	-0.38644	3.415325	-0.29289		C	-0.09623	3.378024	-0.35087
C	0.060689	4.272559	-1.44987		C	0.300605	4.159554	-1.57607
H	-3.36539	-3.52726	-0.70695		H	-3.56648	-3.32276	-0.7762
H	-3.18963	-2.7241	0.83753		H	-3.32429	-2.59991	0.798024
H	-3.37184	-1.35887	-1.90595		H	-3.52492	-1.10536	-1.87589
H	-4.67423	-1.40899	-0.72015		H	-4.78937	-1.15511	-0.65024
H	-1.27064	0.001418	-1.37259		H	-1.35307	0.125477	-1.35532
H	-0.99896	-3.52253	0.07249		H	-1.18561	-3.44624	-0.04362
H	-1.48771	1.660147	1.040161		H	-1.41193	1.761197	1.065145
H	0.690456	-0.86221	-1.35742		H	0.57621	-0.77749	-1.38519
H	2.89714	0.092554	2.134584		H	2.805786	-0.1636	2.193619
H	2.042262	-1.456	2.215557		H	1.846775	-1.64923	2.169303
H	4.456015	-1.61267	1.076371		H	4.275492	-1.9485	1.125079
H	3.471267	-3.41343	-0.27397		H	3.238341	-3.56014	-0.41262
H	1.118802	-3.35258	-0.92304		H	0.923858	-3.29892	-1.13556
H	-1.64184	-1.67475	2.161825		H	-1.74418	-1.63046	2.113957
H	0.028808	-2.22714	2.000096		H	-0.10346	-2.25284	1.935509
H	2.701939	1.602221	0.153226		H	2.771848	1.457376	0.270049
H	4.756711	0.805149	-1.95552		H	4.925335	0.643155	-1.7065
H	5.612366	-0.66943	-1.22739		H	5.633118	-0.94025	-1.05353
H	1.202408	1.494683	-1.61141		H	2.346699	0.308061	-2.2271
H	0.292358	2.398335	2.134123		H	0.502612	2.466595	1.941888
H	-1.55146	-3.44459	-2.20072		H	-1.79866	-3.24356	-2.30271
H	-4.67155	1.112561	-1.07516		H	-3.24048	1.327031	-1.95009
H	-3.20049	1.091077	-2.06378		H	-3.2355	2.279392	-0.4558
H	-3.28106	2.091984	-0.60161		H	-4.68282	1.379896	-0.91999
H	-3.41012	-0.75664	1.879567		H	-3.48864	-0.67295	1.911646
H	-3.26447	0.992429	1.733136		H	-3.15945	1.055509	1.865529
H	-4.71882	0.179436	1.164761		H	-4.70443	0.434612	1.286152
H	-0.62284	4.148588	-2.29636		H	0.536684	5.187118	-1.2981
H	0.084384	5.317723	-1.1408		H	1.167603	3.674175	-2.03577
H	1.056045	3.958972	-1.78323		H	-0.51121	4.147108	-2.31085
1-3					**1-4**			
atom	X	Y	Z		atom	X	Y	Z
C	-3.10209	-2.47488	-0.27988		C	-3.08249	-2.4945	-0.28832
C	-3.70355	-1.1597	-0.79305		C	-3.69341	-1.18347	-0.79719
C	-3.09636	0.101144	-0.1289		C	-3.09219	0.077529	-0.12954
C	-1.53481	0.020289	-0.27713		C	-1.52994	0.007947	-0.28018
C	-0.84151	-1.32631	0.119853		C	-0.83388	-1.33404	0.119927
C	-1.58362	-2.53448	-0.50252		C	-1.57054	-2.53524	-0.52169
C	-0.77224	1.190696	0.388807		C	-0.77985	1.181084	0.391424

C	0.385358	0.654041	1.258363		C	0.381533	0.652367	1.258944
C	1.426696	-0.20728	0.514197		C	1.431842	-0.19733	0.512852
C	0.648339	-1.2237	-0.38141		C	0.660296	-1.23191	-0.37114
C	2.35576	-0.90939	1.541871		C	2.377263	-0.87414	1.541087
C	3.396963	-1.54716	0.612355		C	3.420541	-1.51029	0.611043
C	2.689638	-2.64999	-0.16228		C	2.717653	-2.64191	-0.12206
C	1.417119	-2.51658	-0.55548		C	1.439242	-2.52792	-0.50204
C	-0.77372	-1.42936	1.653218		C	-0.7635	-1.44257	1.652341
O	-0.30915	-0.19412	2.209503		O	-0.29818	-0.20655	2.209799
C	3.720067	-0.3841	-0.31716		C	3.713726	-0.35964	-0.3444
C	2.517255	0.564661	-0.3129		C	2.50591	0.581603	-0.32782
C	4.819581	-0.2011	-1.04916		C	4.795923	-0.18383	-1.10352
O	2.165481	1.013699	-1.61781		O	2.136833	1.02635	-1.62851
O	1.028129	1.647795	1.981092		O	1.019571	1.64849	1.982774
O	-1.29229	-2.68185	-1.89914		O	-1.41481	-2.5536	-1.9472
C	-3.5895	1.3448	-0.90093		C	-3.59008	1.319447	-0.90144
C	-3.62552	0.219675	1.319505		C	-3.62185	0.193407	1.31917
O	-0.3417	2.09159	-0.66319		O	-0.35441	2.092991	-0.65476
O	-0.20297	3.837031	0.776388		O	-0.22333	3.830907	0.794799
C	-0.10556	3.378283	-0.34981		C	-0.13435	3.379821	-0.33579
C	0.29837	4.159434	-1.57278		C	0.240833	4.176604	-1.55809
H	-3.55372	-3.3263	-0.80178		H	-3.5275	-3.34519	-0.81688
H	-3.32886	-2.60562	0.784938		H	-3.29377	-2.64191	0.777211
H	-3.55809	-1.09535	-1.88298		H	-3.53201	-1.12762	-1.88012
H	-4.79094	-1.16198	-0.64489		H	-4.77991	-1.19179	-0.63912
H	-1.35105	0.138969	-1.35368		H	-1.35047	0.110548	-1.35617
H	-1.19047	-3.45507	-0.05667		H	-1.16707	-3.46714	-0.09368
H	-1.41616	1.758041	1.063799		H	-1.42755	1.740652	1.069156
H	0.586045	-0.77727	-1.38341		H	0.606852	-0.79043	-1.3774
H	2.804066	-0.15287	2.194372		H	2.820121	-0.10258	2.179012
H	1.851637	-1.64299	2.170996		H	1.885938	-1.60461	2.183862
H	4.281533	-1.93303	1.127963		H	4.317569	-1.873	1.121457
H	3.251606	-3.54872	-0.4095		H	3.27419	-3.55454	-0.3259
H	0.935859	-3.3018	-1.13055		H	0.967877	-3.37718	-0.99582
H	-1.74281	-1.63432	2.112726		H	-1.73222	-1.64804	2.111397
H	-0.10079	-2.25276	1.934368		H	-0.08846	-2.2642	1.935516
H	2.757335	1.470795	0.254162		H	2.745641	1.488729	0.238189
H	4.931426	0.67089	-1.68943		H	4.89112	0.68064	-1.75655
H	5.644685	-0.90883	-1.03487		H	5.62457	-0.88746	-1.09702
H	2.399229	0.301068	-2.23395		H	2.398274	0.330188	-2.25199
H	0.491058	2.463131	1.954169		H	0.480987	2.463369	1.948428
H	-1.63529	-1.90289	-2.36353		H	-0.4735	-2.63404	-2.1582
H	-4.68562	1.376224	-0.91162		H	-4.68645	1.343977	-0.91392
H	-3.24368	1.336145	-1.9416		H	-3.24215	1.310262	-1.9409

H	-3.24097	2.276312	-0.44053		H	-3.24887	2.253633	-0.43996
H	-3.49377	-0.69239	1.905546		H	-3.49312	-0.72156	1.902181
H	-3.15088	1.034048	1.874712		H	-3.14939	1.005487	1.880242
H	-4.70136	0.430209	1.291492		H	-4.69773	0.403973	1.290165
H	-0.51163	4.151415	-2.30974		H	-0.58187	4.166241	-2.28077
H	0.536694	5.185896	-1.29281		H	0.47278	5.203044	-1.27264
H	1.16489	3.671957	-2.03111		H	1.104459	3.70356	-2.03645

Table S4. Key conformers of compound **2**.

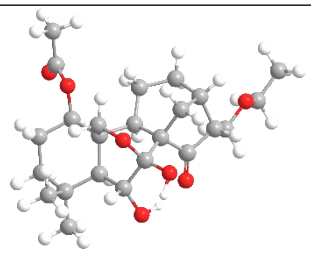
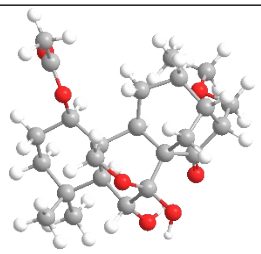
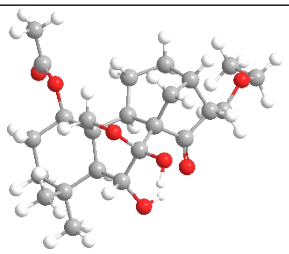
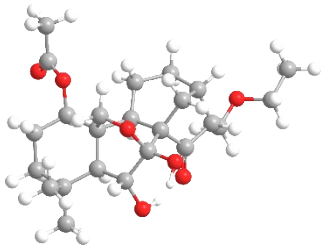
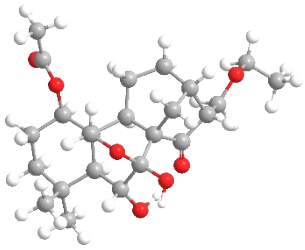
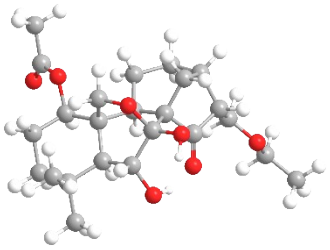
		
Conformer **2-1** 60.74%	Conformer **2-2** 15.14%	Conformer **2-3** 8.25%
		
Conformer **2-4** 7.90%	Conformer **2-5** 6.58%	Conformer **2-6** 1.39%

Table S5. Conformers and Bolzmann distributions of the optimized **2**.

species	*E'=E+ZPE*	*E*	*H*	*G*	*ΔG*	*ΔE(kcal/mol)*	*p%*
2-1	-1462.202372	-1462.172763	-1462.171819	-1462.262087	0	0	60.74%
2-2	-1462.202284	-1462.1729	-1462.171955	-1462.260776	0.001311	0.822664954	15.14%
2-3	-1462.200254	-1462.170696	-1462.169752	-1462.260203	0.001884	1.182227898	8.25%
2-4	-1462.200065	-1462.170516	-1462.169572	-1462.260163	0.001924	1.207328278	7.90%
2-5	-1462.200026	-1462.170464	-1462.16952	-1462.25999	0.002097	1.315887422	6.58%
2-6	-1462.199026	-1462.169454	-1462.16851	-1462.258525	0.003562	2.235188839	1.39%

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy

Table S6. Optimized Z-matrixes of isomer **2** in the gas phase (Å) at B3LYP/6-31G(d) level.

2-1					**2-2**			
atom	X	Y	Z		atom	X	Y	Z
C	-3.72171	1.086331	-0.91976		C	3.281379	0.877034	0.977047
C	-3.79524	-0.15051	-1.81354		C	3.06428	-0.17473	2.062364
C	-3.31027	-1.42983	-1.09738		C	2.56285	-1.51939	1.493153
C	-1.851	-1.17599	-0.57713		C	1.252089	-1.25364	0.667842
C	-1.53091	0.192069	0.158513		C	1.193456	0.001545	-0.30427
C	-2.27692	1.369924	-0.51429		C	1.959108	1.209997	0.29063

C	-1.29393	-2.32361	0.304925		C	0.773555	-2.47836	-0.14981
C	-0.34529	-1.75016	1.376649		C	-0.01448	-2.0041	-1.38928
C	0.73123	-0.76886	0.859659		C	-1.05978	-0.90004	-1.12098
C	0.023449	0.380915	0.022218		C	-0.33192	0.347319	-0.44666
C	1.588492	-0.1707	2.00132		C	-1.826	-0.47683	-2.39778
C	2.723908	0.498391	1.203964		C	-2.89826	0.46145	-1.80922
C	2.157222	1.739928	0.455147		C	-2.21999	1.799328	-1.40639
C	0.61197	1.759189	0.389284		C	-0.69553	1.655553	-1.17866
C	-1.85847	0.081407	1.666235		C	1.726616	-0.39304	-1.70168
O	-1.1747	-1.02222	2.282886		O	0.944865	-1.4462	-2.2899
C	3.139952	-0.67751	0.279076		C	-3.43719	-0.41283	-0.63991
C	1.812645	-1.34791	-0.05661		C	-2.22426	-1.23686	-0.19517
O	0.245291	-2.79109	2.095659		O	-0.60135	-3.09773	-2.0269
O	-0.7145	-3.41524	-0.39538		O	0.063928	-3.47025	0.578828
O	1.658022	-2.15925	-0.95948		O	-2.23698	-2.00396	0.756016
C	-4.33071	-1.82734	-0.00659		C	3.701672	-2.19536	0.694772
C	-3.26741	-2.57682	-2.13108		C	2.218312	-2.44613	2.680102
C	4.023333	-0.41108	-0.93276		C	-4.19444	0.203165	0.534629
O	5.228865	0.165791	-0.47004		O	-3.31263	0.967651	1.340607
C	6.152349	0.446528	-1.51107		C	-3.91251	1.42839	2.544225
C	7.400808	1.054695	-0.89368		C	-2.87756	2.215051	3.330545
O	-2.28284	2.502432	0.40262		O	2.234977	2.16231	-0.77749
O	-2.04663	3.965983	-1.31521		O	1.943486	3.912441	0.637073
C	-2.18844	3.74444	-0.13226		C	2.216722	3.479845	-0.46162
C	-2.27235	4.795506	0.949883		C	2.563595	4.320406	-1.66845
H	-4.34131	0.961358	-0.02437		H	4.010747	0.532873	0.234591
H	-4.10079	1.967184	-1.44997		H	3.677652	1.801956	1.410739
H	-3.17846	0.017772	-2.70874		H	2.330624	0.2075	2.78777
H	-4.8222	-0.29711	-2.17167		H	3.99322	-0.3387	2.623435
H	-1.23637	-1.16132	-1.48808		H	0.480616	-1.0674	1.427794
H	-1.72529	1.673356	-1.40987		H	1.314555	1.711916	1.019385
H	-2.10129	-2.76943	0.890603		H	1.631632	-3.00604	-0.57364
H	0.247688	0.221985	-1.04132		H	-0.71265	0.45866	0.57647
H	1.962629	-0.98219	2.634014		H	-2.26562	-1.36559	-2.86313
H	1.031306	0.512811	2.643942		H	-1.1842	-0.00226	-3.14191
H	3.569069	0.794329	1.829759		H	-3.70906	0.663499	-2.51719
H	2.490073	2.6508	0.965777		H	-2.37771	2.528561	-2.21048
H	2.57301	1.803629	-0.55702		H	-2.69057	2.208128	-0.50971
H	0.295718	2.505181	-0.34693		H	-0.34555	2.512201	-0.59497
H	0.217289	2.093019	1.353645		H	-0.17671	1.703595	-2.14169
H	-1.56095	0.998573	2.183927		H	1.689206	0.462382	-2.38101
H	-2.93319	-0.04835	1.834639		H	2.77284	-0.71835	-1.64937
H	3.678248	-1.40108	0.913338		H	-4.12454	-1.14907	-1.08748
H	0.107204	-3.58726	1.547267		H	-0.5581	-3.82289	-1.37363

H	0.087261	-3.07494	-0.85092		H	-0.76781	-3.04882	0.893283
H	-4.10091	-2.80337	0.431595		H	3.444462	-3.22014	0.40989
H	-5.32718	-1.90904	-0.45743		H	4.598547	-2.25605	1.32314
H	-4.40317	-1.10743	0.813314		H	3.980125	-1.65872	-0.21699
H	-2.61709	-2.32264	-2.97727		H	1.467727	-1.98553	3.334434
H	-2.88726	-3.50297	-1.69166		H	1.817281	-3.40424	2.339637
H	-4.27233	-2.76676	-2.52829		H	3.114443	-2.63623	3.283915
H	3.524384	0.259563	-1.65226		H	-4.63012	-0.61138	1.133583
H	4.210653	-1.35931	-1.46008		H	-5.02401	0.830274	0.167091
H	5.700704	1.141226	-2.23978		H	-4.27718	0.568568	3.129829
H	6.399205	-0.47975	-2.05686		H	-4.78642	2.059645	2.311127
H	8.137176	1.28768	-1.67054		H	-3.30991	2.581398	4.267981
H	7.855053	0.358187	-0.18164		H	-2.52389	3.075194	2.753012
H	7.154358	1.978461	-0.36019		H	-2.01611	1.583558	3.570573
H	-2.2193	5.786887	0.498938		H	2.619957	5.369541	-1.37632
H	-3.20763	4.687953	1.508607		H	3.517383	3.996632	-2.09647
H	-1.45067	4.667795	1.662665		H	1.798394	4.19449	-2.44218
2-3					**2-4**			
atom	X	Y	Z		atom	X	Y	Z
C	-3.70527	0.843238	-1.07558		C	3.617187	1.150724	0.965139
C	-3.63042	-0.40468	-1.95385		C	3.675459	-0.0513	1.90648
C	-3.09311	-1.63632	-1.19237		C	3.232885	-1.36228	1.221072
C	-1.69289	-1.26673	-0.58536		C	1.788644	-1.1478	0.643661
C	-1.52232	0.130434	0.145819		C	1.481137	0.18322	-0.16055
C	-2.31302	1.239916	-0.58904		C	2.185491	1.396566	0.49358
C	-1.1137	-2.35706	0.352599		C	1.274195	-2.34004	-0.20433
C	-0.26453	-1.70143	1.460247		C	0.369182	-1.82527	-1.3413
C	0.765272	-0.65426	0.979875		C	-0.73878	-0.83395	-0.91624
C	0.01794	0.43914	0.100022		C	-0.07942	0.358071	-0.09746
C	1.533678	0.007971	2.149063		C	-1.55153	-0.29281	-2.11759
C	2.643564	0.761415	1.390987		C	-2.72661	0.397435	-1.39804
C	2.011957	1.962968	0.630805		C	-2.2043	1.676081	-0.6809
C	0.474593	1.859162	0.495937		C	-0.66397	1.713885	-0.54726
C	-1.93197	0.008331	1.63216		C	1.870032	0.014121	-1.6482
O	-1.18789	-1.0182	2.309516		O	1.232467	-1.12934	-2.24118
C	3.176636	-0.37582	0.477554		C	-3.17154	-0.74195	-0.44156
C	1.920747	-1.16045	0.114146		C	-1.85413	-1.38472	-0.02417
O	0.359272	-2.68601	2.228276		O	-0.17918	-2.90301	-2.0391
O	-0.42675	-3.42159	-0.28957		O	0.673583	-3.40214	0.522433
O	1.867115	-1.99994	-0.77471		O	-1.73237	-2.15446	0.919325
C	-4.14633	-2.10133	-0.16016		C	4.296469	-1.78213	0.180692
C	-2.89875	-2.78585	-2.20531		C	3.170016	-2.47267	2.292799
C	4.052937	-0.0383	-0.72301		C	-4.09769	-0.4323	0.728322

O	5.193124	0.649321	-0.24124		O	-5.28774	0.12207	0.197478
C	6.06263	1.137697	-1.2566		C	-6.31993	0.33448	1.154043
C	6.916336	0.051883	-1.90961		C	-6.09009	1.555608	2.043456
O	-2.45846	2.380854	0.30546		O	2.213202	2.493103	-0.46573
O	-2.23234	3.833622	-1.4228		O	1.893031	4.016617	1.185028
C	-2.42399	3.618836	-0.2456		C	2.083221	3.75294	0.017569
C	-2.64067	4.676472	0.811394		C	2.195413	4.764234	-1.09928
H	-4.36703	0.681681	-0.21688		H	4.272423	1.003588	0.09905
H	-4.11637	1.687094	-1.64093		H	3.96238	2.056582	1.475994
H	-2.97564	-0.19785	-2.81343		H	3.025343	0.14019	2.772989
H	-4.61981	-0.6333	-2.37002		H	4.691134	-0.16991	2.304949
H	-1.02205	-1.22047	-1.45464		H	1.145317	-1.10123	1.533677
H	-1.73259	1.572288	-1.45567		H	1.595029	1.726007	1.354512
H	-1.92186	-2.84313	0.904388		H	2.107998	-2.80687	-0.73408
H	0.314711	0.301536	-0.94873		H	-0.34834	0.240356	0.961032
H	1.944312	-0.77312	2.797217		H	-1.89126	-1.13351	-2.7314
H	0.903486	0.6478	2.768743		H	-0.97345	0.369489	-2.76404
H	3.443086	1.115156	2.046003		H	-3.54647	0.656736	-2.07187
H	2.248037	2.890258	1.16534		H	-2.5211	2.560052	-1.24617
H	2.465704	2.073231	-0.36074		H	-2.66659	1.780564	0.307373
H	0.133694	2.580004	-0.2539		H	-0.38744	2.492537	0.170879
H	0.009334	2.154651	1.441362		H	-0.22856	2.011617	-1.5058
H	-1.75413	0.954123	2.152606		H	1.575625	0.90202	-2.21655
H	-2.99888	-0.2184	1.735513		H	2.952281	-0.101	-1.77125
H	3.764796	-1.04914	1.12251		H	-3.68197	-1.49478	-1.06434
H	0.299701	-3.50062	1.692985		H	-0.05874	-3.67319	-1.45109
H	0.371429	-3.03497	-0.71359		H	-0.15069	-3.04917	0.925193
H	-3.87039	-3.05314	0.30394		H	4.089253	-2.7704	-0.241
H	-5.10441	-2.26247	-0.66902		H	5.275225	-1.84598	0.671506
H	-4.32335	-1.38157	0.643796		H	4.397702	-1.08308	-0.65393
H	-2.21805	-2.48928	-3.01283		H	2.4821	-2.20096	3.102963
H	-2.47723	-3.67543	-1.72974		H	2.824462	-3.42153	1.873588
H	-3.85974	-3.05549	-2.66073		H	4.161937	-2.62843	2.734917
H	3.508607	0.587183	-1.45032		H	-3.61368	0.256366	1.437369
H	4.318251	-0.97141	-1.23905		H	-4.30664	-1.3626	1.278755
H	6.705881	1.867769	-0.75394		H	-6.45246	-0.57059	1.76924
H	5.479619	1.679048	-2.02025		H	-7.23259	0.46937	0.563845
H	7.622017	0.503116	-2.61697		H	-6.95804	1.717032	2.693451
H	6.308362	-0.67129	-2.46342		H	-5.94752	2.45172	1.430139
H	7.489047	-0.49093	-1.15022		H	-5.21223	1.436332	2.687543
H	-2.6462	5.661661	0.344068		H	2.119	5.770866	-0.68711
H	-3.58787	4.503006	1.331999		H	3.149636	4.645011	-1.62238
H	-1.84305	4.626412	1.560332		H	1.398944	4.60305	-1.83361

2-5					2-6			
atom	X	Y	Z		atom	X	Y	Z
C	-3.81511	0.912122	-0.80253		C	-3.82974	-0.07011	-1.13072
C	-3.87183	-0.35102	-1.65985		C	-3.42862	-1.35652	-1.85108
C	-3.28426	-1.58396	-0.93955		C	-2.59405	-2.30246	-0.96069
C	-1.81514	-1.24308	-0.50245		C	-1.34405	-1.50916	-0.43723
C	-1.527	0.159402	0.17983		C	-1.55616	-0.04393	0.129418
C	-2.36785	1.279072	-0.48111		C	-2.59207	0.726701	-0.72288
C	-1.16024	-2.3351	0.380662		C	-0.49405	-2.29721	0.593592
C	-0.17751	-1.68697	1.376267		C	0.105064	-1.3282	1.63102
C	0.818878	-0.67462	0.766368		C	0.827943	-0.09137	1.050594
C	0.006241	0.423022	-0.04753		C	-0.14552	0.642578	0.033487
C	1.724382	-0.01274	1.832561		C	1.309421	0.88416	2.149993
C	2.764104	0.696801	0.943723		C	2.237859	1.807163	1.338746
C	2.085873	1.903635	0.233207		C	1.380065	2.675561	0.366606
C	0.540728	1.836701	0.26271		C	-0.07563	2.171872	0.229163
C	-1.76676	0.073219	1.705478		C	-1.94891	-0.09663	1.624035
O	-0.9816	-0.96761	2.311579		O	-0.99954	-0.84781	2.39883
C	3.167501	-0.46711	-0.00263		C	3.123576	0.755648	0.62206
C	1.862754	-1.22782	-0.20685		C	2.127981	-0.34874	0.277111
O	0.503318	-2.67763	2.086476		O	0.944986	-2.02335	2.503562
O	-0.57279	-3.42419	-0.31692		O	0.482925	-3.17147	0.047484
O	1.694478	-2.08381	-1.06559		O	2.319628	-1.22698	-0.55013
C	-4.22496	-2.00377	0.213205		C	-3.49621	-2.89712	0.144854
C	-3.23601	-2.75554	-1.9452		C	-2.09516	-3.47614	-1.83216
C	3.895737	-0.15042	-1.31768		C	4.021008	1.202356	-0.53236
O	5.036461	0.669072	-1.13873		O	5.122998	0.321778	-0.59393
C	6.174176	0.000794	-0.61096		C	5.971536	0.558811	-1.7056
C	7.340302	0.975841	-0.61891		C	7.119844	-0.43505	-1.65007
O	-2.38664	2.435548	0.405166		O	-3.03897	1.8942	0.026659
O	-2.3182	3.857078	-1.36213		O	-3.14736	3.135636	-1.86966
C	-2.38677	3.664388	-0.16772		C	-3.30634	3.023775	-0.67345
C	-2.4713	4.74213	0.887642		C	-3.81066	4.111885	0.245582
H	-4.38082	0.78194	0.127285		H	-4.43983	-0.28727	-0.24618
H	-4.26543	1.7578	-1.33428		H	-4.4359	0.564077	-1.78745
H	-3.31326	-0.17621	-2.59134		H	-2.84577	-1.09698	-2.74737
H	-4.90746	-0.55862	-1.95797		H	-4.3229	-1.88255	-2.20876
H	-1.24724	-1.22582	-1.44316		H	-0.70951	-1.383	-1.32524
H	-1.87944	1.584953	-1.41184		H	-2.10281	1.087151	-1.63354
H	-1.91234	-2.79475	1.026329		H	-1.139	-2.94449	1.192123
H	0.177058	0.254696	-1.11954		H	0.209834	0.443576	-0.98616
H	2.18308	-0.7923	2.449946		H	1.8639	0.326848	2.911848
H	1.181086	0.656014	2.502178		H	0.492581	1.402716	2.654377
H	3.635621	1.04263	1.506065		H	2.852956	2.451621	1.974733

H	2.397308	2.831059	0.727249		H	1.352929	3.710227	0.727278
H	2.439297	1.991738	-0.79958		H	1.848703	2.719721	-0.62459
H	0.139456	2.551596	-0.46264		H	-0.54912	2.677573	-0.61846
H	0.187383	2.163925	1.245356		H	-0.63951	2.46795	1.118821
H	-1.49971	1.020709	2.183304		H	-2.0024	0.916829	2.035086
H	-2.8211	-0.11659	1.934498		H	-2.93504	-0.55139	1.764935
H	3.801119	-1.1508	0.58595		H	3.795765	0.321613	1.379017
H	0.366322	-3.49632	1.571892		H	1.149297	-2.86072	2.044587
H	0.185472	-3.06411	-0.82883		H	1.150328	-2.61313	-0.41004
H	-3.92281	-2.95585	0.659975		H	-2.98132	-3.67168	0.721307
H	-5.23805	-2.14605	-0.1818		H	-4.36867	-3.37348	-0.3185
H	-4.29069	-1.26785	1.019298		H	-3.86936	-2.15323	0.853536
H	-2.64635	-2.49237	-2.8321		H	-1.50795	-3.11378	-2.685
H	-2.78483	-3.64823	-1.50389		H	-1.45944	-4.16012	-1.26337
H	-4.24942	-3.0076	-2.28161		H	-2.94749	-4.04165	-2.22917
H	3.238279	0.402499	-1.99561		H	4.363283	2.238222	-0.35831
H	4.158421	-1.09395	-1.8186		H	3.471714	1.19479	-1.48785
H	6.403818	-0.88693	-1.2237		H	6.352102	1.594926	-1.67876
H	5.981777	-0.35284	0.41518		H	5.40351	0.44517	-2.64428
H	8.241455	0.497624	-0.21977		H	7.690911	-0.31059	-0.72435
H	7.111409	1.852656	-0.00448		H	7.796188	-0.28638	-2.49898
H	7.547355	1.316749	-1.63826		H	6.738248	-1.46038	-1.68302
H	-2.49459	5.720498	0.406756		H	-4.05036	4.999911	-0.34009
H	-3.36969	4.603364	1.497648		H	-4.69839	3.768753	0.786419
H	-1.60837	4.679257	1.559119		H	-3.04783	4.355793	0.992691

Table S7. Key conformers of compound **3**.

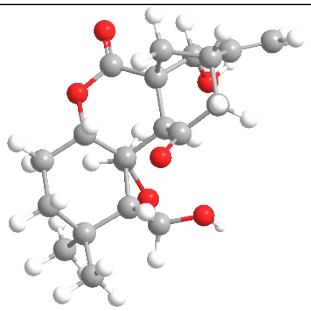
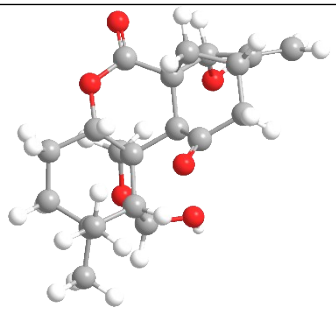
	
Conformer **3-1** 99.78%	Conformer **3-2** 0.22%

Table S8. Conformers and Bolzmann distributions of the optimized **3**.

species	*E'=E+ZPE*	*E*	*H*	*G*	*ΔG*	*ΔE(kcal/mol)*	*p%*
3-1	-1228.64088	-1228.618337	-1228.617393	-1228.689615	0	0	99.78%
3-2	-1228.635118	-1228.61262	-1228.611675	-1228.683859	0.005756	3.611944682	0.22%

E, E', H, G: total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy

Table S9. Optimized Z-matrixes of isomer **3** in the gas phase (Å) at B3LYP/6-31G(d) level.

3-1					**3-2**			
atom	X	Y	Z		atom	X	Y	Z
C	-2.28372	2.052085	0.82678		C	2.344688	2.067223	-0.6812
C	-3.22586	0.94363	1.31339		C	3.433453	1.165828	-0.06991
C	-3.35607	-0.22465	0.306744		C	3.275329	-0.32648	-0.43299
C	-1.93017	-0.82747	0.025863		C	1.916245	-0.87442	0.137315
C	-0.75982	0.204812	-0.15242		C	0.754123	0.195776	0.197128
C	-0.88504	1.474862	0.703493		C	0.953471	1.409169	-0.72487
C	0.653907	-0.36276	0.174489		C	-0.64963	-0.38928	-0.1321
C	1.762218	0.776303	0.113158		C	-1.76831	0.735408	-0.19516
C	1.237374	2.173039	-0.22378		C	-1.25917	2.157439	0.01247
O	-0.01784	2.503128	0.14544		O	0.005004	2.456958	-0.34295
C	0.790428	-1.0843	1.522638		C	-0.75159	-1.21916	-1.41872
C	2.190281	-1.60691	1.836002		C	-2.13817	-1.78931	-1.7091
C	3.26467	-0.58283	1.371466		C	-3.23363	-0.74252	-1.35909
C	2.604717	0.815775	1.425409		C	-2.58405	0.651686	-1.52354
C	-0.85087	0.490089	-1.67948		C	0.796321	0.646957	1.70229
C	-1.84791	-1.58917	-1.29696		C	1.958963	-1.32868	1.602015
O	-0.85746	-2.6006	-1.17584		O	0.91452	-2.27966	1.775379
O	1.928347	2.99979	-0.78217		O	-1.97342	3.034884	0.453584
C	2.905452	0.365304	-0.86653		C	-2.93269	0.407784	0.790301
C	3.606942	-0.74283	-0.1062		C	-3.60567	-0.77387	0.120132
C	4.3437	-1.70187	-0.66302		C	-4.34418	-1.68806	0.745801
O	2.50443	-0.04306	-2.16086		O	-2.56658	0.129709	2.128901
O	-1.50538	-0.63667	-2.2819		O	1.752656	-0.17629	2.380508
O	-0.10742	-1.18807	2.340622		O	0.161763	-1.37799	-2.2093
C	-4.21112	-1.33326	0.956232		C	3.299725	-0.51526	-1.96692
C	-4.11181	0.271785	-0.94957		C	4.487558	-1.09727	0.131111
H	-2.2628	2.88753	1.536035		H	2.622831	2.359712	-1.69931
H	-2.61405	2.464202	-0.13275		H	2.265139	2.9958	-0.10739
H	-4.22137	1.359768	1.513359		H	3.427941	1.258115	1.022318
H	-2.85153	0.551622	2.269444		H	4.417195	1.520282	-0.4033
H	-1.70384	-1.49986	0.849584		H	1.622525	-1.72743	-0.47147
H	-0.52878	1.248231	1.714318		H	0.708794	1.118017	-1.74983
H	0.912205	-1.10314	-0.59019		H	-0.92239	-1.06854	0.684403
H	2.336623	-2.57545	1.341458		H	-2.28235	-2.7115	-1.13211
H	2.23496	-1.7701	2.917334		H	-2.15932	-2.04899	-2.77205
H	4.150813	-0.66615	2.008467		H	-4.10482	-0.89221	-2.00445
H	3.339533	1.624909	1.360206		H	-3.32501	1.457265	-1.54271
H	2.009808	0.974752	2.331211		H	-1.97058	0.7376	-2.42688
H	0.132941	0.600517	-2.14231		H	-0.18456	0.528508	2.173475
H	-1.43603	1.390086	-1.89789		H	1.117616	1.684544	1.824087
H	-2.79138	-2.0446	-1.61927		H	2.906271	-1.75753	1.935978

H	-0.671	-2.91264	-2.07686		H	0.82281	-2.42112	2.732147
H	3.567848	1.237453	-0.94736		H	-3.60339	1.277339	0.769386
H	4.48146	-1.74559	-1.73914		H	-4.50558	-1.63649	1.818254
H	4.822186	-2.47679	-0.06854		H	-4.80129	-2.5191	0.213578
H	2.428442	0.759015	-2.70196		H	-2.4899	0.983595	2.584108
H	-4.31098	-2.20279	0.29539		H	3.307682	-1.58104	-2.22216
H	-5.22189	-0.96649	1.172884		H	4.204967	-0.06118	-2.3892
H	-3.76718	-1.67709	1.897559		H	2.431399	-0.08309	-2.46781
H	-5.07157	0.704435	-0.64168		H	5.392183	-0.81522	-0.42052
H	-3.57223	1.036001	-1.51348		H	4.670765	-0.87408	1.187674
H	-4.33335	-0.5438	-1.64438		H	4.36279	-2.18193	0.024946