Supporting Information for

A Monocarbocyclic Sesterterpenoid Biosynthetic Precursor of Leucosceptroids from *Leucosceptrum canum* and Its Metabolic Isomerization by a Specialist Insect

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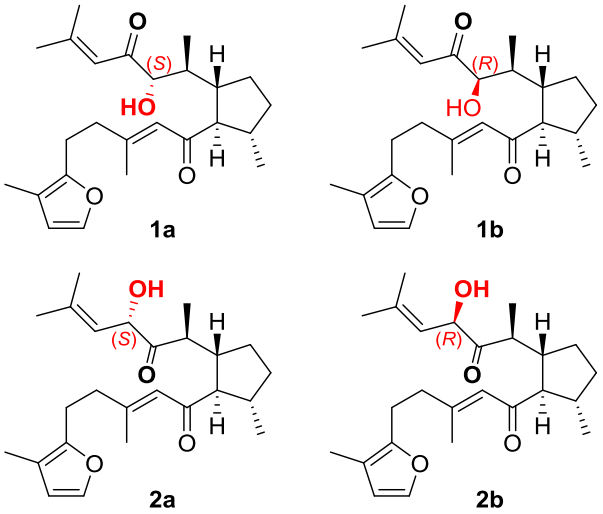
Table of Contents

Quantum chemical calculations



Conformational analyses of the structures (**1a**, **1b**, **2a**, and **2b**) were carried out via Monte Carlo searching using molecular mechanism with MMFF force field in the Spartan 18 program.[1] The force field minimum energy conformers thus obtained were subsequently optimized by applying the density functional theory (DFT) with the B3LYP/6-31G (d) level in vacuum, implemented in the Gaussian 09 software package.[2] Harmonic vibrational frequencies were also performed to confirm no imaginary frequencies of the finally optimized conformers. Gauge independent atomic orbital (GIAO) calculations of NMR chemical shifts were accomplished by DFT at the mPW1PW91/6-311+G (d,p) level in acetone or chloroform with the polarizable continuum model (PCM) in Gaussian 09 software. NMR chemical shifts of TMS were calculated in the same level and used as the references. The experimental and calculated data were analyzed by the improved probability DP4+ method for isomeric compounds. Regression analysis of calculated versus experimental NMR chemical shifts of **1** and **2** were carried out. ECD calculations further were conducted at the B3LYP/6-31G (d) level with the PCM in MeOH. The program SpecDis 1.64 was used for comparisons of the calculated curves and experimental CD spectra.

References

1. Spartan 18; Wavefunction Inc.:Irvine, CA.
2. Gaussian 09, Revision A.1, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Table S1. Optimized lowest energy 3D conformers and energy analysis for **1a**

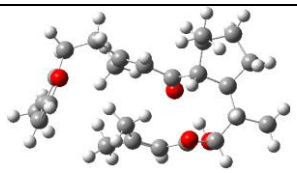
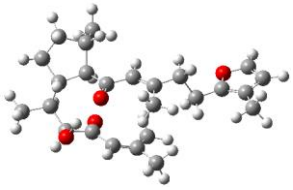
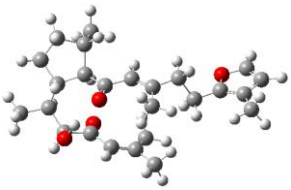
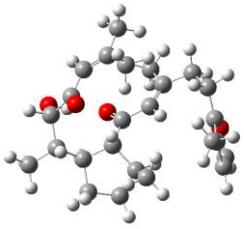
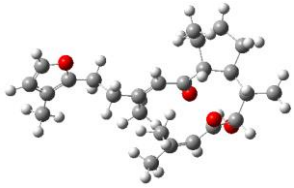
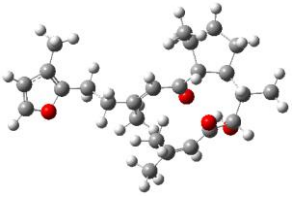
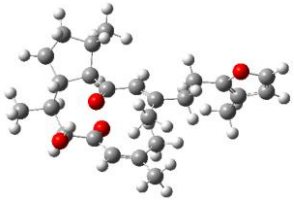
Conformers		Free energies		
No.	3D conformers	E (Hartree)	ΔE (Hartree)	Distribution
1a-1		-1274.442300	0.001091	8.54%
1a-2		-1274.442067	0.001324	6.67%
1a-3		-1274.442074	0.001317	6.72%
1a-4		-1274.443391	0	27.10%
1a-5		-1274.443158	0.000233	21.17%
1a-6		-1274.443222	0.000169	22.66%
1a-7		-1274.442131	0.00126	7.14%

Table S2. Optimized lowest energy 3D conformers and energy analysis for **1b**

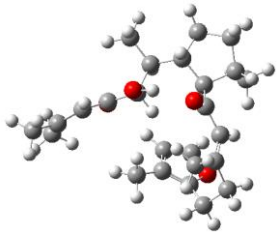
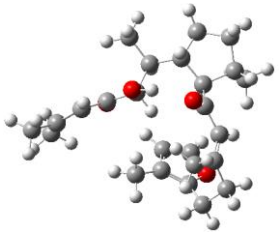
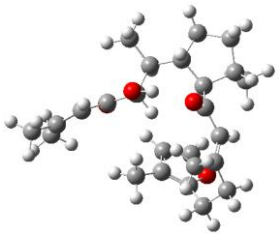
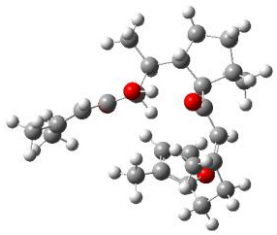
Conformers		Free energies		
No.	3D conformers	E (Hartree)	ΔE (Hartree)	Distribution
1b-1		-1274.446947	0	26.26%
1b-2		-1274.446889	0.000058	24.70%
1b-3		-1274.446926	0.000021	25.69%
1b-4		-1274.446836	0.000111	23.35%

Table S3. Optimized lowest energy 3D conformers and energy analysis for **2a**

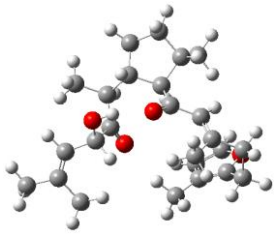
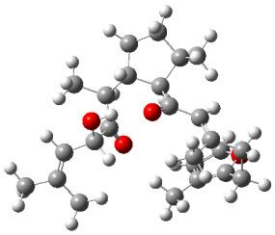
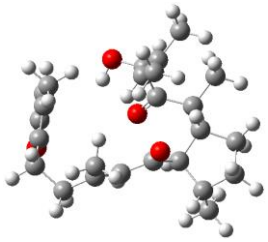
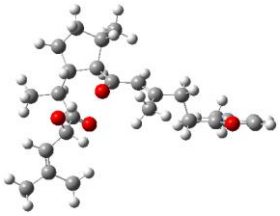
Conformers		Free energies		
No.	3D conformers	E (Hartree)	ΔE (Hartree)	Distribution
2a-1		-1274.442749	0.000447	26.76%
2a-2		-1274.442635	0.000561	23.71%
2a-3		-1274.443196	0	42.95%
2a-4		-1274.441424	0.001772	6.58%

Table S4. Optimized lowest energy 3D conformers and energy analysis for **2b**

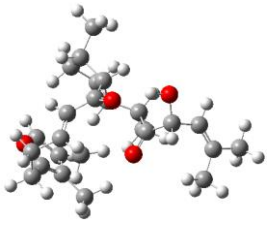
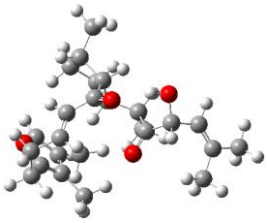
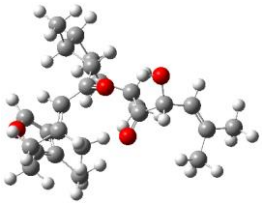
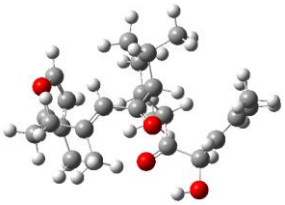
Conformers		Free energies		
No.	3D conformers	E (Hartree)	ΔE (Hartree)	Distribution
2b-1		-1274.447744	0.001043	16.49%
2b-2		-1274.447663	0.001124	15.14%
2b-3		-1274.447859	0.000928	18.63%
2b-4		-1274.448787	0	49.75%

Table S5. Calculated ^{13}C NMR results of **1a** and **1b**

No.	Experimental NMR data	**1a**			**1b**		
		Shielding tensors	Unscaled shifts	Scaled shifts	Shielding tensors	Unscaled shifts	Scaled shifts
C-1	28.0	156.2816273	32.4	27.8	156.6900849	32.0	28.1
C-2	159.7	16.32415205	172.3	161.7	14.18655403	174.5	164.2
C-3	119.1	61.73268613	126.9	118.3	62.77780852	125.9	117.8
C-4	201.2	-28.08088168	216.7	204.2	-24.23704768	212.9	200.9
C-5	78.2	100.9102812	87.7	80.8	105.1828442	83.5	77.3
C-6	36.7	143.9709574	44.7	39.6	140.9544294	47.7	43.1
C-7	46.6	145.6178087	43.0	38.1	142.5111286	46.1	41.6
C-8	30.7	153.4232475	35.2	30.6	154.4298642	34.2	30.2
C-9	33.5	153.0980953	35.5	30.9	151.9006352	36.7	32.6
C-10	39.4	144.3914754	44.3	39.2	146.0185257	42.6	38.3
C-11	60.3	120.7866662	67.9	61.8	121.7540273	66.9	61.4
C-12	205.1	-26.14561454	214.8	202.4	-25.27713834	213.9	201.9
C-13	125.4	59.15919644	129.5	120.8	57.25915889	131.4	123.0
C-14	156.6	13.61830319	175.0	164.3	15.81736161	172.8	162.6
C-15	39.6	142.8202272	45.8	40.7	144.8997731	43.7	39.3
C-16	24.2	160.6074333	28.0	23.7	160.9163251	27.7	24.0
C-17	149.4	32.23716066	156.4	146.5	32.32436029	156.3	146.9
C-18	114.4	65.89051623	122.8	114.3	63.53858359	125.1	117.0
C-19	112.7	68.9920718	119.7	111.3	68.30020865	120.3	112.5
C-20	140.0	41.41729064	147.2	137.7	41.6854432	147.0	137.9
C-21	21.4	163.0973111	25.5	21.3	162.6403655	26.0	22.4
C-22	12.5	166.8394561	21.8	17.8	174.0824077	14.6	11.4
C-23	22.5	162.5193349	26.1	21.9	162.7627815	25.9	22.3
C-24	19.0	163.0932188	25.6	21.3	165.1666274	23.5	20.0
C-25	9.7	176.1975907	12.4	8.8	176.4145666	12.2	9.2

Table S6. Calculated ^{1}H NMR results of **1a** and **1b**

No.	Experimental NMR data	**1a**			**1b**		
		Shielding tensors	Unscaled shifts	Scaled shifts	Shielding tensors	Unscaled shifts	Scaled shifts
H-1	1.95	30.02532713	1.85	1.87	29.73423314	2.14	2.20
H-3	6.12	24.68294546	7.19	6.76	24.37422371	7.50	7.03
H-5	4.22	28.17199046	3.70	3.57	28.56271717	3.31	3.26
H-6	2.23	29.4645495	2.41	2.38	29.9657403	1.90	1.99
H-7	2.26	29.56779798	2.30	2.29	29.55842549	2.31	2.36
H-8a	2.03	30.04683697	1.82	1.85	30.05872335	1.81	1.91
H-8b	1.79	30.35301084	1.52	1.57	30.41049709	1.46	1.59
H-9a	2.02	30.36755276	1.50	1.55	30.17802569	1.69	1.80
H-9b	1.28	30.61278334	1.26	1.33	30.48310291	1.39	1.53
H-10	2.12	30.08310433	1.79	1.81	29.9500247	1.92	2.01
H-11	2.59	29.62599267	2.24	2.23	29.77874264	2.09	2.16
H-13	5.99	25.52036167	6.35	6.00	25.84748517	6.02	5.70
H-15	2.41	29.27296813	2.60	2.56	29.3903498	2.48	2.51
H-16	2.73	29.02442697	2.85	2.78	28.94028929	2.93	2.92
H-19	6.12	25.30119823	6.57	6.20	24.87662626	6.99	6.58
H-20	7.19	24.29252131	7.58	7.12	24.29049709	7.58	7.11
H-21	2.2	29.82801553	2.04	2.05	29.53652425	2.33	2.38
H-22	0.51	1.14512628	1.15	1.22	31.06564552	0.80	1.00
H-23	1.05	1.136635943	1.14	1.22	30.66329053	1.21	1.37
H-24	2.11	2.314735776	2.31	2.30	29.73369655	2.14	2.20
H-25	1.92	29.77124277	2.10	2.10	30.38485997	1.49	1.62
5-OH	3.68	27.93003659	3.94	3.79	28.54311346	3.33	3.28

Table S7. Calculated ^{13}C NMR results of **2a** and **2b**

No.	Experimental NMR data	**2a**			**2b**		
		Shielding tensors	Unscaled shifts	Scaled shifts	Shielding tensors	Unscaled shifts	Scaled shifts
C-1	25.9	160.0284043	28.2	24.9	160.1099391	28.2	25.3
C-2	138.8	39.12503076	149.1	140.1	37.97926586	150.3	141.5
C-3	122.8	58.1905415	130.1	122.0	58.51370351	129.8	122.0
C-4	76.7	108.5413678	79.7	74.0	108.5111136	79.8	74.4
C-5	214.7	-41.28291441	229.6	216.7	-37.75147553	226.0	213.5
C-6	42.3	129.130983	59.1	54.4	136.9255263	51.3	47.4
C-7	48.4	138.0686393	50.2	45.9	136.2220314	52.1	48.1
C-8	31.3	152.9293104	35.3	31.7	154.6324782	33.6	30.5
C-9	34.5	152.6893126	35.6	31.9	152.0600983	36.2	33.0
C-10	39.3	144.0537074	44.2	40.2	145.1376664	43.1	39.6
C-11	60.8	122.2181298	66.1	61.0	118.9886307	69.3	64.4
C-12	204	-25.67658828	214.0	201.8	-29.24740981	217.5	205.4
C-13	126.1	57.96610023	130.3	122.2	58.60524591	129.7	121.9
C-14	157.5	12.17593463	176.1	165.8	15.36083965	172.9	163.0
C-15	40.1	142.9611266	45.3	41.2	146.1780017	42.1	38.6
C-16	24.8	161.0961189	27.2	23.9	160.9544267	27.3	24.5
C-17	150.4	32.64783651	155.6	146.3	32.33929868	155.9	146.9
C-18	115.2	62.75064096	125.5	117.6	62.75926485	125.5	117.9
C-19	113.6	69.12356913	119.2	111.5	68.14882661	120.1	112.8
C-20	141	41.06253471	147.2	138.3	41.6206935	146.7	138.0
C-21	18.9	166.9213448	21.4	18.4	167.3286511	20.9	18.5
C-22	17.6	172.1477836	16.1	13.4	167.4349106	20.8	18.4
C-23	22.3	163.6001085	24.7	21.5	164.7683747	23.5	20.9
C-24	19.1	163.7260865	24.5	21.4	166.3524244	21.9	19.4
C-25	9.8	175.8836038	12.4	9.8	176.2379502	12.0	10.0

Table S8. Calculated ^{1}H NMR results of **2a** and **2b**

No.	Experimental	**2a**			**2b**		
	NMR data	Shielding tensors	Unscaled shifts	Scaled shifts	Shielding tensors	Unscaled shifts	Scaled shifts
H-1	1.76	29.97555121	2.25	1.85	29.96554458	2.26	1.94
H-3	4.95	26.8212665	5.41	4.90	26.39887444	5.83	5.31
H-4	4.78	26.96415464	5.27	4.76	27.04675202	5.18	4.69
H-6	2.99	29.82865625	2.40	1.99	29.2084563	3.02	2.65
H-7	2.17	29.28421207	2.95	2.52	30.25104934	1.98	1.67
H-8a	1.65	29.89293374	2.34	1.93	29.99029404	2.24	1.91
H-8b	1.54	30.51088818	1.72	1.33	30.60161252	1.63	1.34
H-9a	1.94	30.18988603	2.04	1.65	30.09325574	2.14	1.82
H-9b	1.15	30.51728952	1.71	1.33	30.54749232	1.68	1.39
H-10	2.07	29.96908641	2.26	1.86	29.85561437	2.37	2.04
H-11	2.71	29.6364116	2.59	2.18	29.97086281	2.26	1.93
H-13	6.12	25.86169763	6.37	5.83	25.85630073	6.37	5.82
H-15	2.45	29.30349743	2.93	2.50	29.25747892	2.97	2.61
H-16	2.8	28.88090053	3.35	2.91	28.87897759	3.35	2.96
H-19	6.18	25.17955187	7.05	6.49	25.28053609	6.95	6.36
H-20	7.31	24.16212957	8.07	7.47	24.19536042	8.03	7.39
H-21	1.87	30.03232105	2.20	1.80	30.08875019	2.14	1.82
H-22	0.89	30.54475617	1.69	1.30	30.8352645	1.39	1.12
H-23	1.04	30.79280381	1.44	1.06	30.96025812	1.27	1.00
H-24	2.13	29.53713965	2.69	2.28	29.77271269	2.46	2.12
H-25	1.93	29.85826124	2.37	1.97	29.58138468	2.65	2.30
4-OH	4.04	27.19152935	5.04	4.54	27.48573831	4.74	4.28

Table S9. DP4+ evaluation of theoretical and experimental data of **1**

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Shielding Tensors

		DP4+	0.00%	100.00%	–	–	–
Nuclei	sp2?	xperimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		28	156.3	156.7			
C	x	159.7	16.3	14.2			
C	x	119.1	61.7	62.8			
C	x	201.2	-28.1	-24.2			
C		78.2	100.9	105.2			
C		36.7	144.0	141.0			
C		46.6	145.6	142.5			
C		30.7	153.4	154.4			
C		33.5	153.1	151.9			
C		39.4	144.4	146.0			
C		60.3	120.8	121.8			
C	x	205.1	-26.15	-25.28			
C	x	125.4	59.16	57.26			
C	x	156.6	13.62	15.82			
C		39.6	142.82	144.90			
C		24.2	160.61	160.92			
C	x	149.4	32.24	32.32			
C	x	114.4	65.89	63.54			
C	x	112.7	68.99	68.30			
C	x	140	41.42	41.69			
C		21.4	163.10	162.64			
C		12.5	166.84	174.08			
C		22.5	162.52	162.76			
C		19	163.09	165.17			
C		9.7	176.20	176.41			
H		1.95	30.03	29.73			
H	x	6.12	24.68	24.37			
H		4.22	28.17	28.56			
H		2.23	29.46	29.97			
H		2.26	29.57	29.56			
H		2.03	30.05	30.06			
H		1.79	30.35	30.41			
H		2.02	30.37	30.18			
H		1.28	30.61	30.48			
H		2.12	30.08	29.95			
H		2.59	29.63	29.78			
H	x	5.99	25.52	25.85			
H		2.41	29.27	29.39			
H		2.73	29.02	28.94			
H	x	6.12	25.30	24.88			
H	x	7.19	24.29	24.29			
H		2.2	29.83	29.54			
H		0.51	1.15	31.07			
H		1.05	1.14	30.66			
H		2.11	2.31	29.73			
H		1.92	29.77	30.38			
H		3.68	27.93	28.54			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	100.00%	–	–	–	–
sDP4+ (C data)	0.01%	99.99%	–	–	–	–
sDP4+ (all data)	0.00%	100.00%	–	–	–	–
uDP4+ (H data)	0.00%	100.00%	–	–	–	–
uDP4+ (C data)	0.00%	100.00%	–	–	–	–
uDP4+ (all data)	0.00%	100.00%	–	–	–	–
DP4+ (H data)	0.00%	100.00%	–	–	–	–
DP4+ (C data)	0.00%	100.00%	–	–	–	–
DP4+ (all data)	0.00%	100.00%	–	–	–	–

Table S10. DP4+ evaluation of theoretical and experimental data of **2**

Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-311+G(d,p)		Shielding Tensors	
		DP4+	0.00%	100.00%	–	–	–
Nuclei	sp2?	Experimenta	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
C		25.9	160.0	160.1			
C	x	138.8	39.1	38.0			
C	x	122.8	58.2	58.5			
C		76.7	108.5	108.5			
C	x	214.7	-41.3	-37.8			
C		42.3	129.1	136.9			
C		48.4	138.1	136.2			
C		31.3	152.9	154.6			
C		34.5	152.7	152.1			
C		39.3	144.1	145.1			
C		60.8	122.2	119.0			
C	x	204	-25.68	-29.25			
C	x	126.1	57.97	58.61			
C	x	157.5	12.18	15.36			
C		40.1	142.96	146.18			
C		24.8	161.10	160.95			
C	x	150.4	32.65	32.34			
C	x	115.2	62.75	62.76			
C	x	113.6	69.12	68.15			
C	x	141	41.06	41.62			
C		18.9	166.92	167.33			
C		17.6	172.15	167.43			
C		22.3	163.60	164.77			
C		19.1	163.73	166.35			
C		9.8	175.88	176.24			
H		1.76	29.98	29.97			
H	x	4.95	26.82	26.40			
H		4.78	26.96	27.05			
H		2.99	29.83	29.21			
H		2.17	29.28	30.25			
H		1.65	29.89	29.99			
H		1.54	30.51	30.60			
H		1.94	30.19	30.09			
H		1.15	30.52	30.55			
H		2.07	29.97	29.86			
H		2.71	29.64	29.97			
H	x	6.12	25.86	25.86			
H		2.45	29.30	29.26			
H		2.8	28.88	28.88			
H	x	6.18	25.18	25.28			
H	x	7.31	24.16	24.20			
H		1.87	30.03	30.09			
H		0.89	30.54	30.84			
H		1.04	30.79	30.96			
H		2.13	29.54	29.77			
H		1.93	29.86	29.58			
H		4.04	27.19	27.49			

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-311+G(d,p)	Shielding Tensors

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	30.14%	69.86%	–	–	–	–
sDP4+ (C data)	0.00%	100.00%	–	–	–	–
sDP4+ (all data)	0.00%	100.00%	–	–	–	–
uDP4+ (H data)	2.96%	97.04%	–	–	–	–
uDP4+ (C data)	0.01%	99.99%	–	–	–	–
uDP4+ (all data)	0.00%	100.00%	–	–	–	–
DP4+ (H data)	1.30%	98.70%	–	–	–	–
DP4+ (C data)	0.00%	100.00%	–	–	–	–
DP4+ (all data)	0.00%	100.00%	–	–	–	–

Figure S1. Regression analysis of experimental *vs* calculated NMR data of **1a** and **1b**

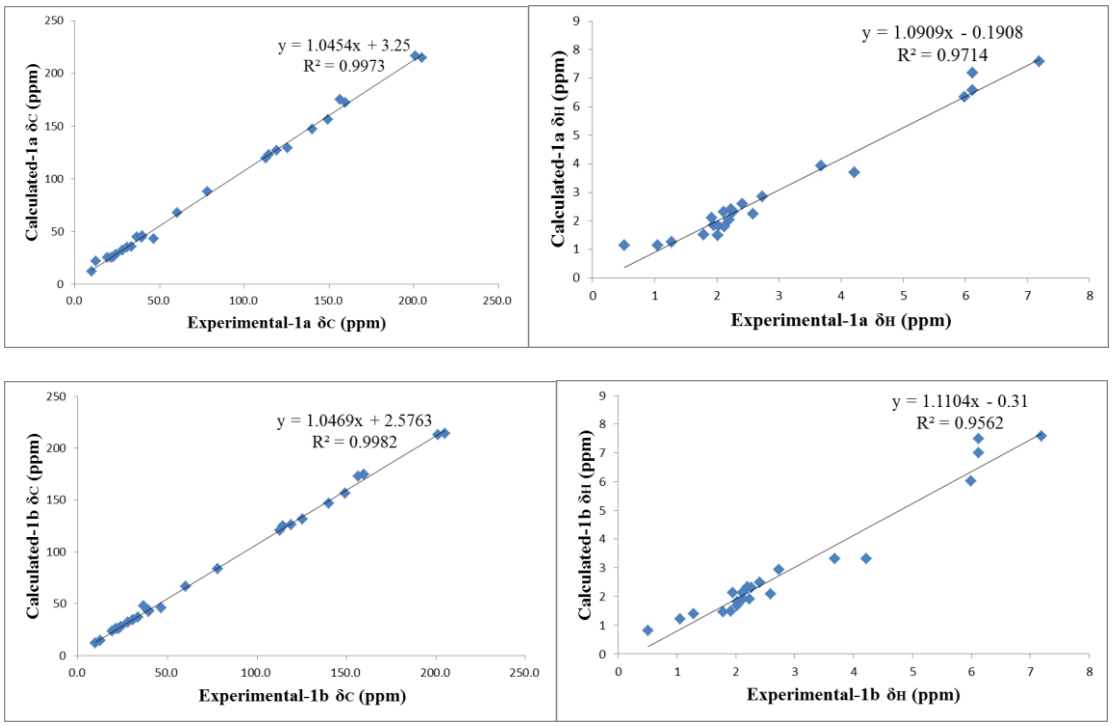


Figure S2. Regression analysis of experimental *vs* calculated NMR data of **2a** and **2b**

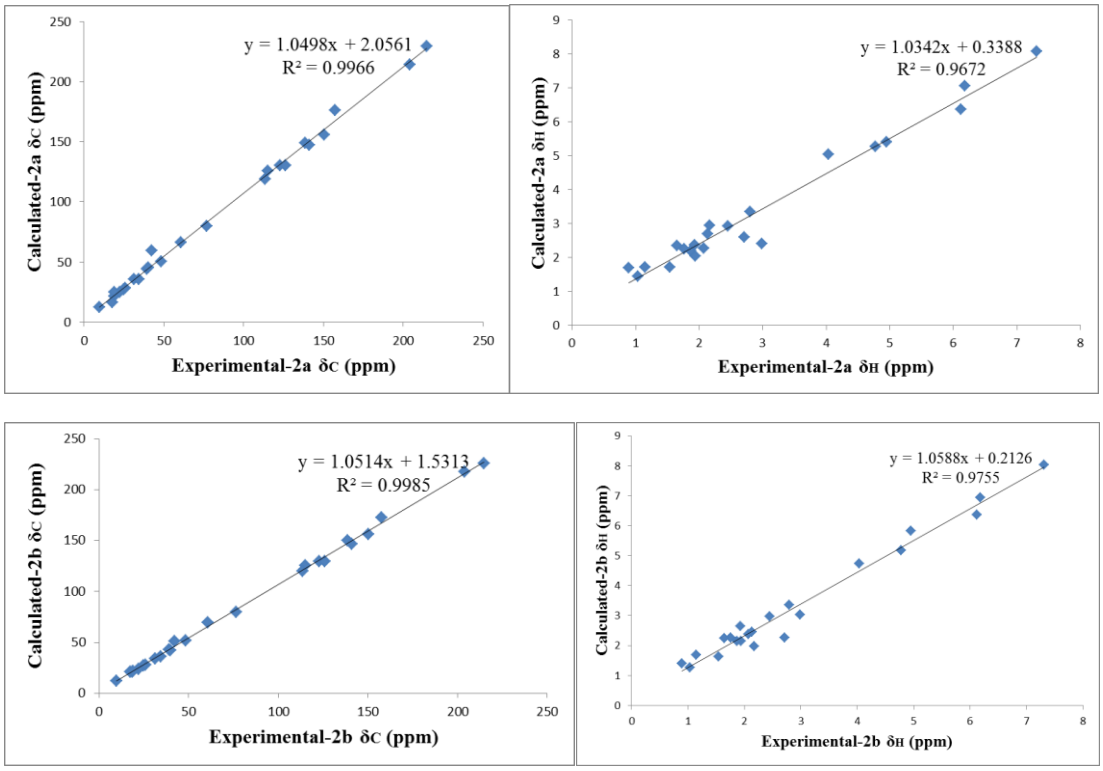


Figure S3. HRESIMS of compound **1**

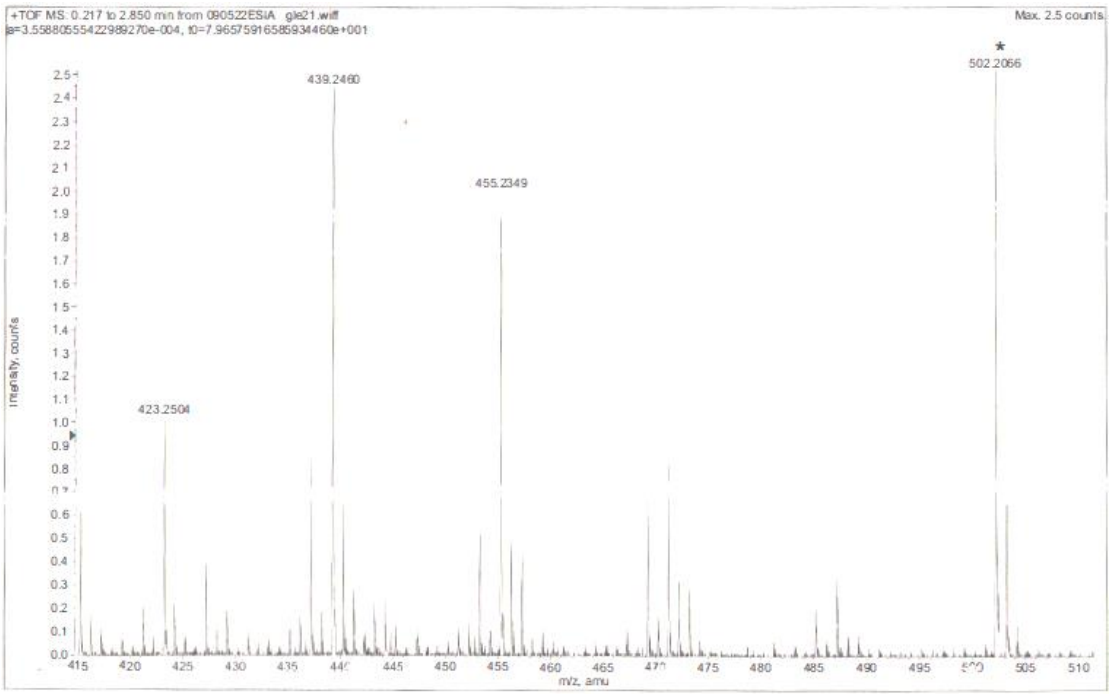


Figure S4. IR spectrum of compound **1**

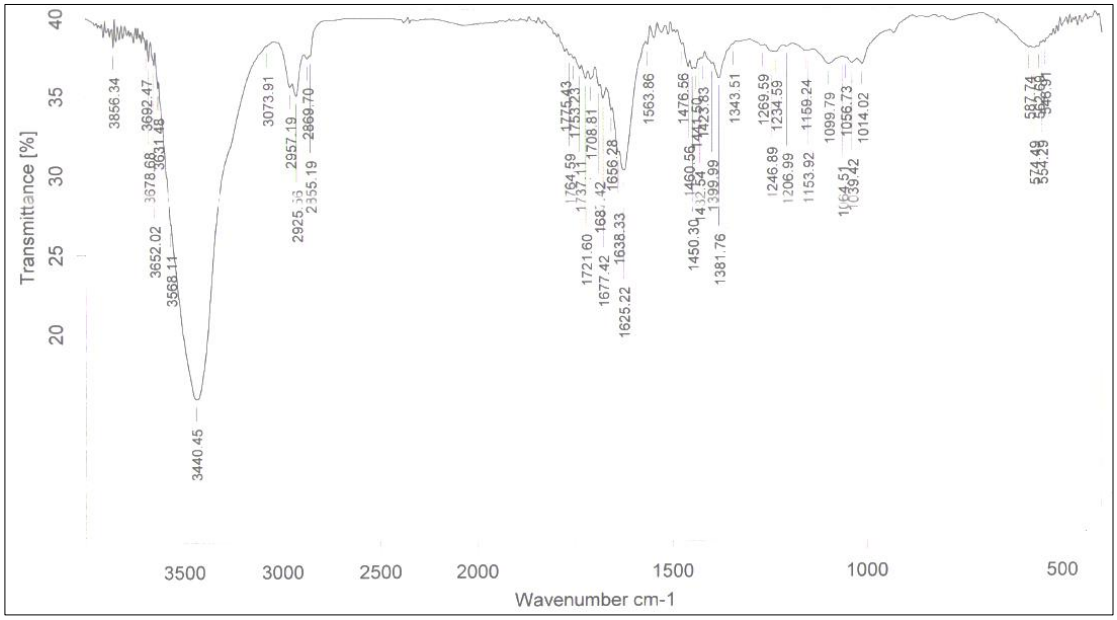


Figure S5. ^{1}H NMR spectrum of compound **1** in $CDCl_3$ (400 MHz)

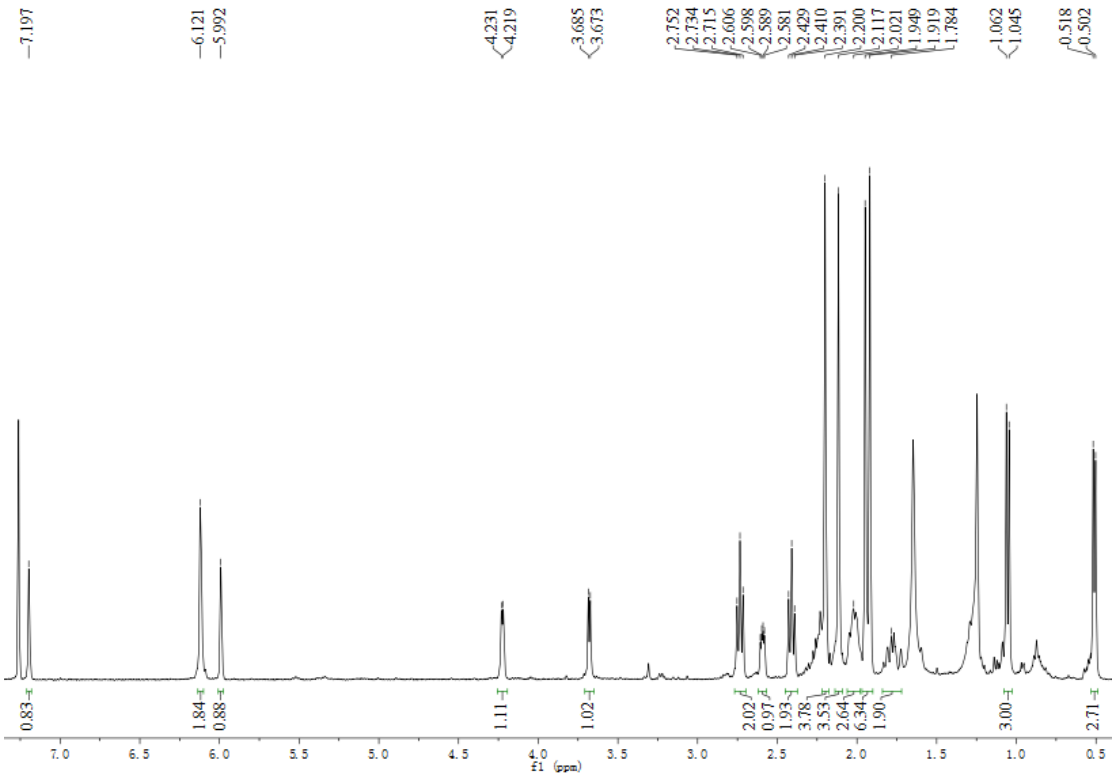


Figure S6. Expanded ^{1}H NMR spectrum of compound **1**

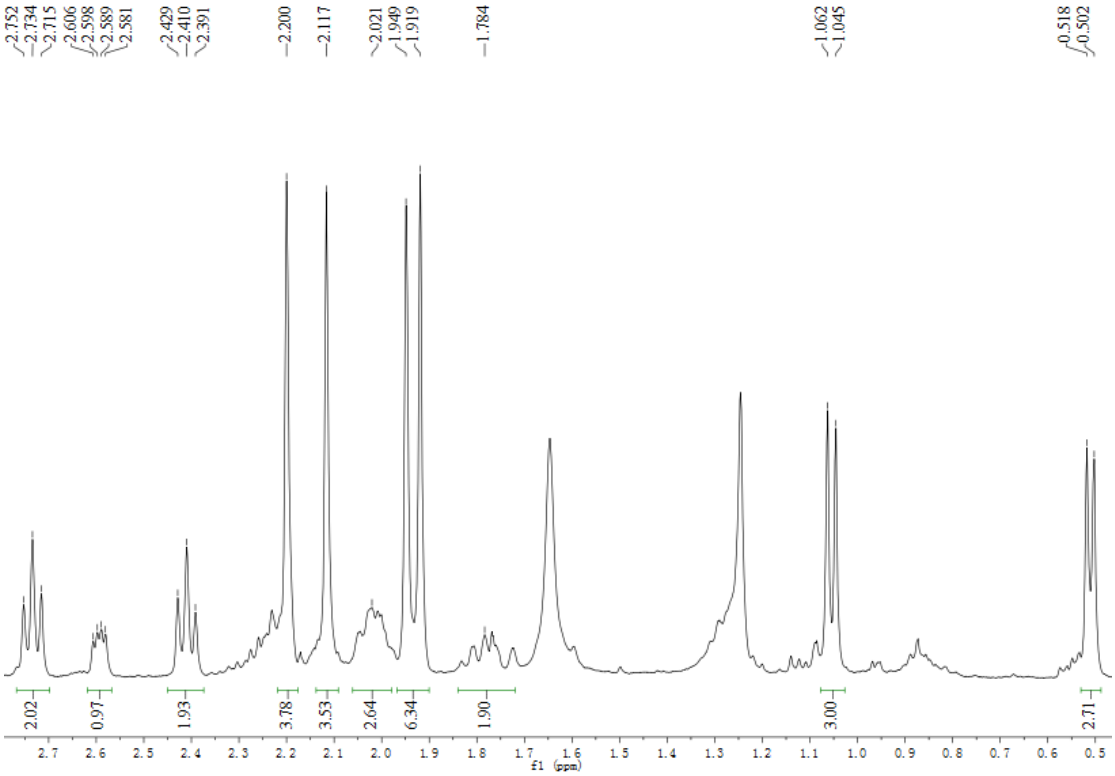


Figure S7. ^{13}C NMR (DEPT) spectrum of compound **1** in $CDCl_3$ (100 MHz)

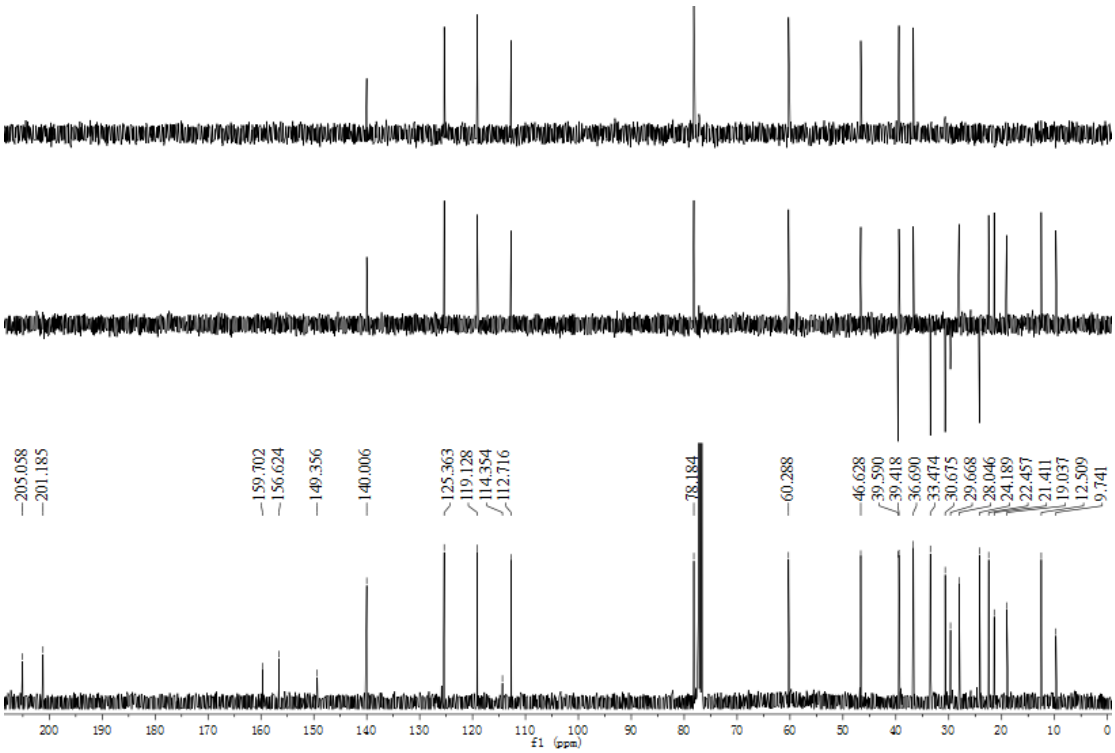


Figure S8. Expanded ^{13}C NMR (DEPT) spectrum of compound **1**

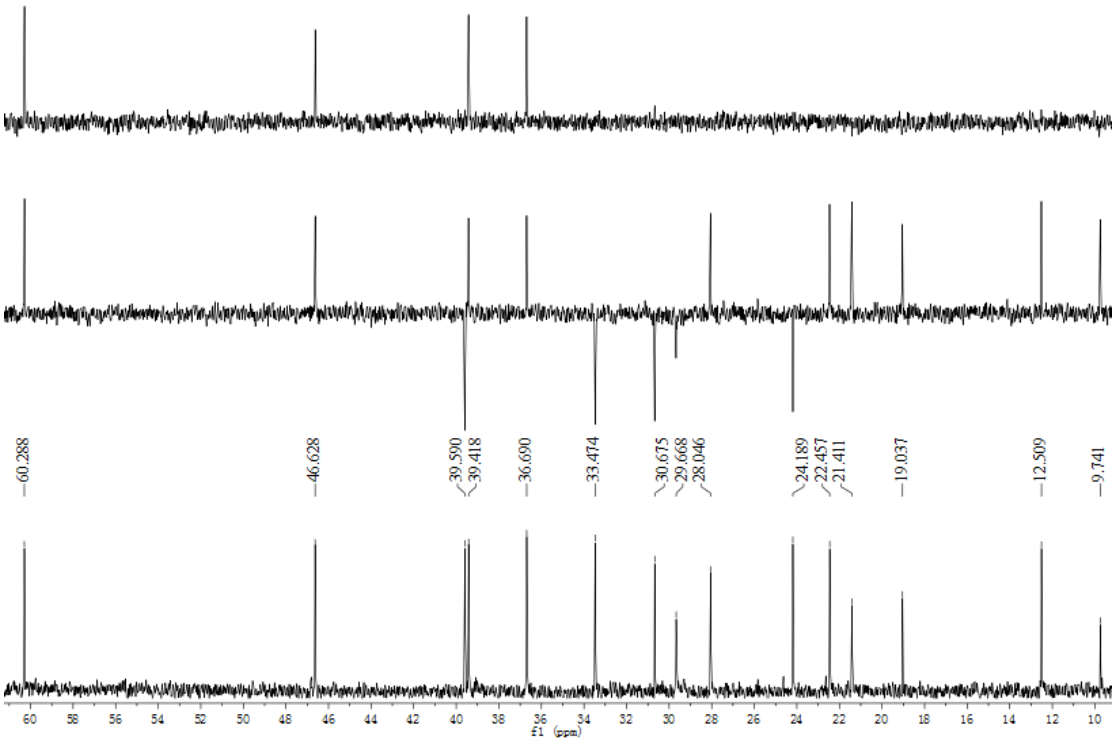


Figure S9. ^{1}H-^{1}H COSY spectrum of compound **1** in $CDCl_3$

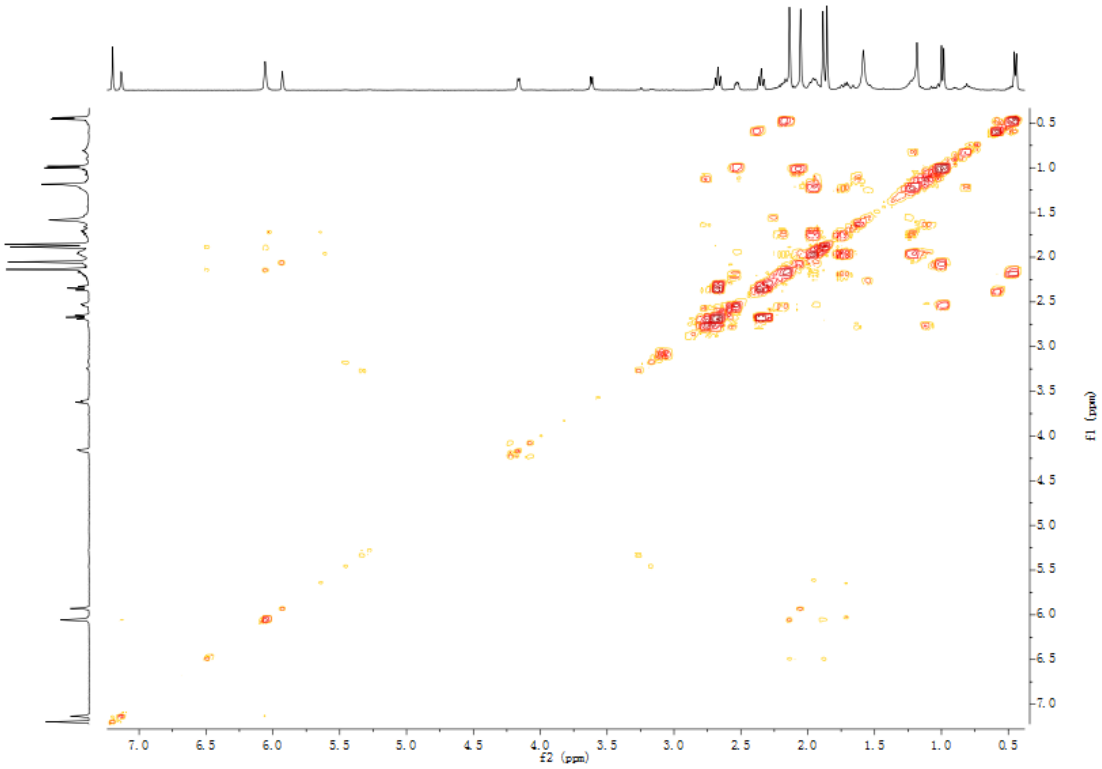


Figure S10. Expanded ^{1}H-^{1}H COSY spectrum of compound **1**

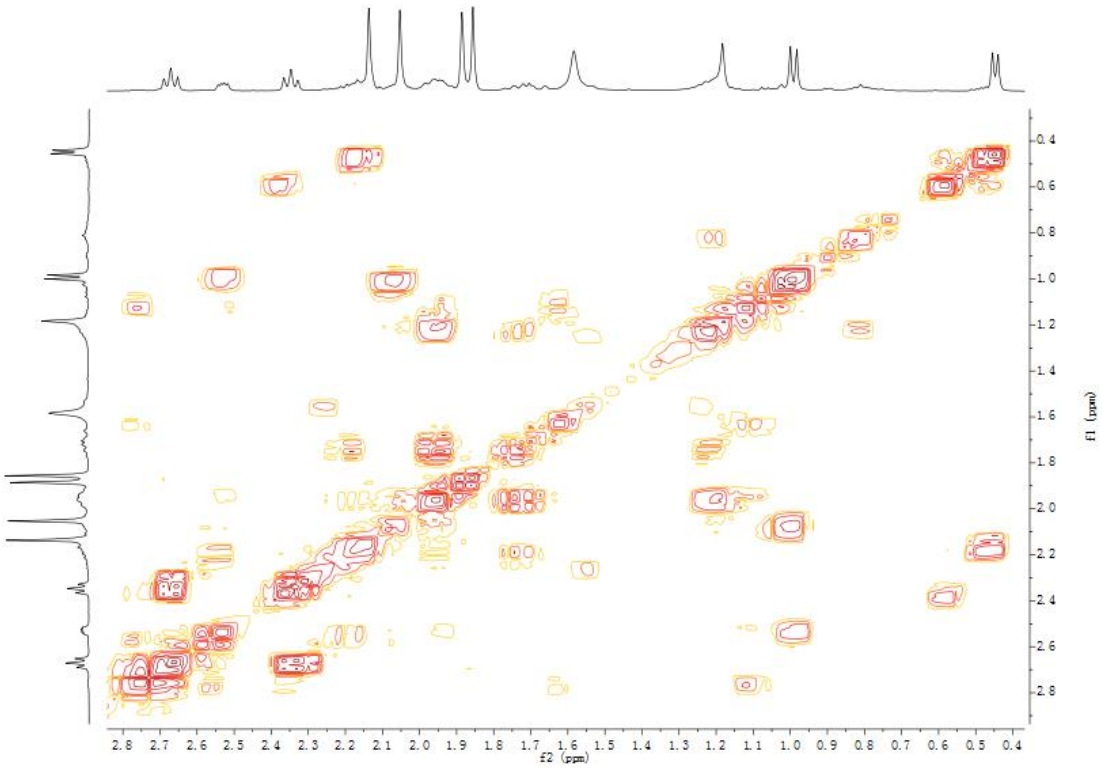


Figure S11. HSQC spectrum of compound **1** in $CDCl_3$

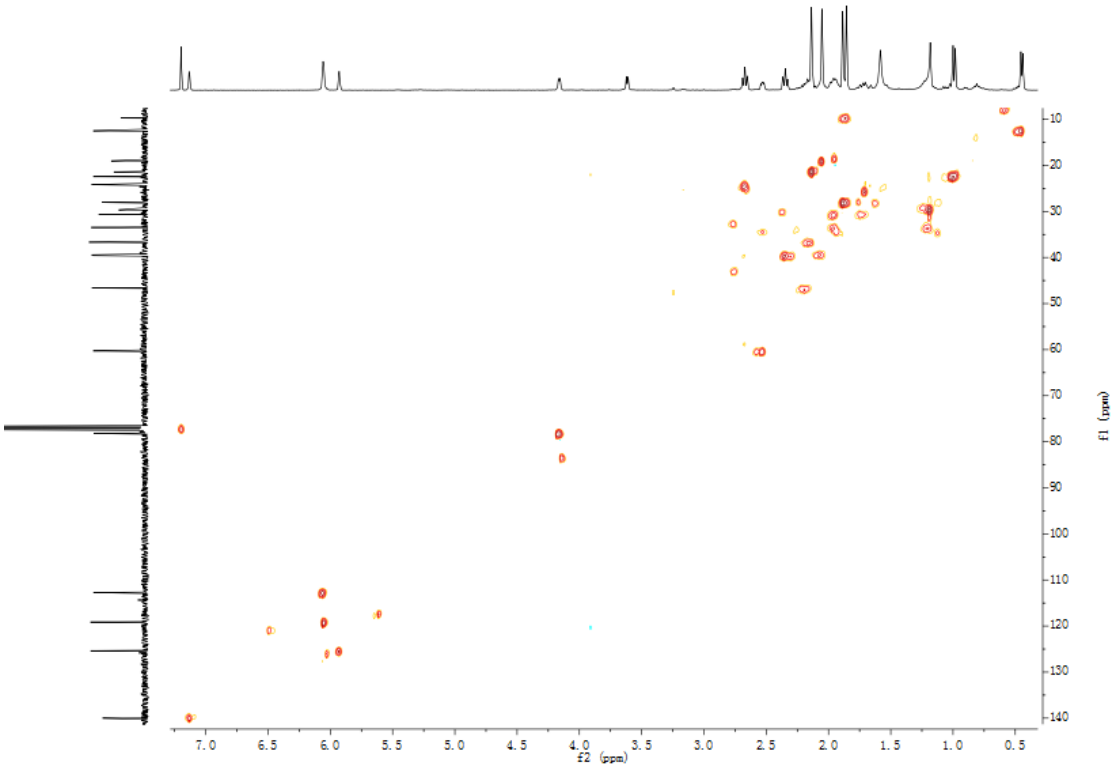


Figure S12. Expanded HSQC spectrum of compound **1**

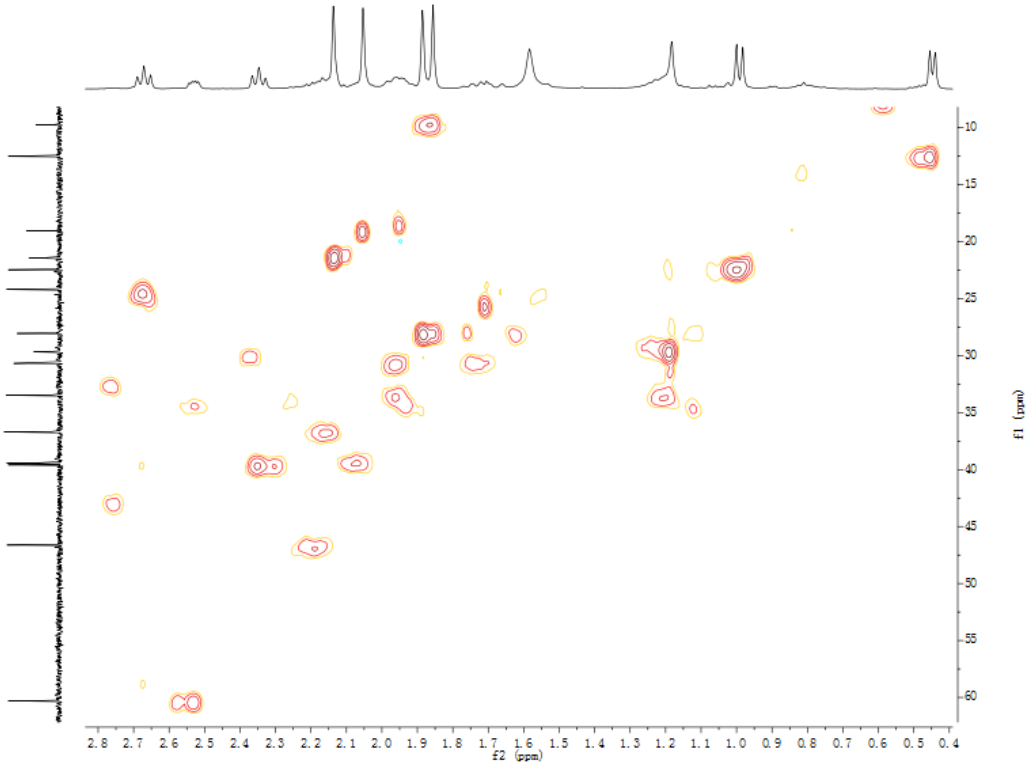


Figure S13. HMBC spectrum of compound **1** in $CDCl_3$

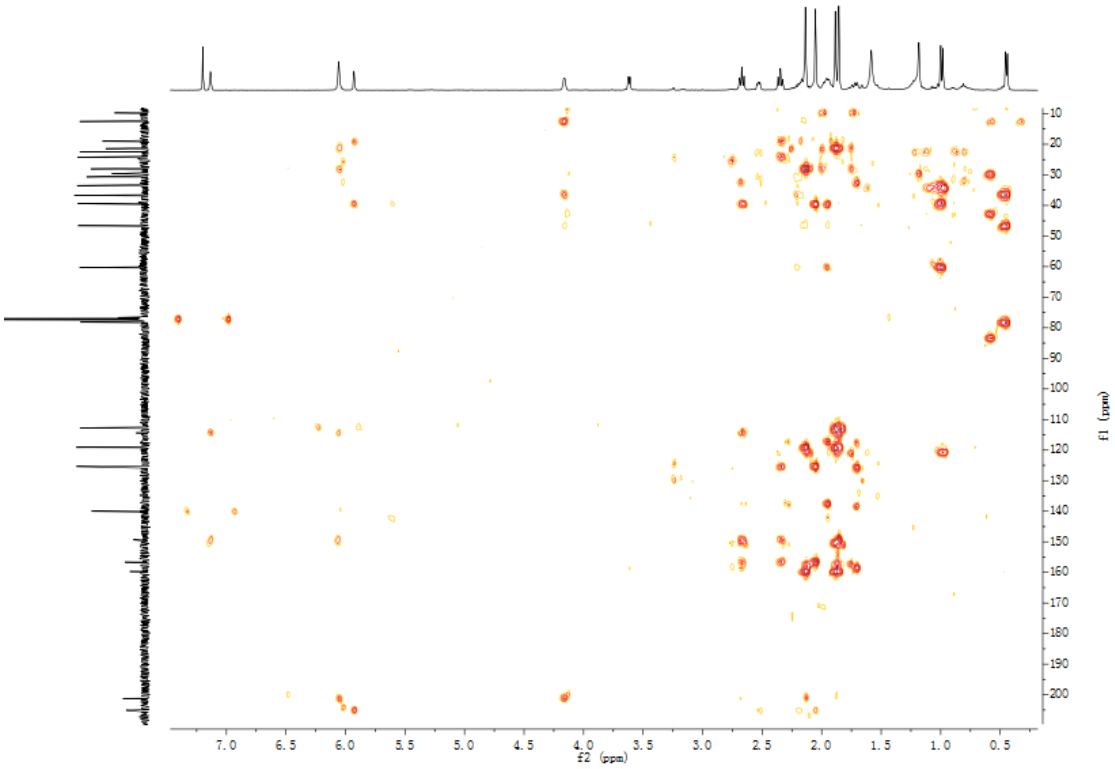


Figure S14. Expanded HMBC spectrum of compound **1**

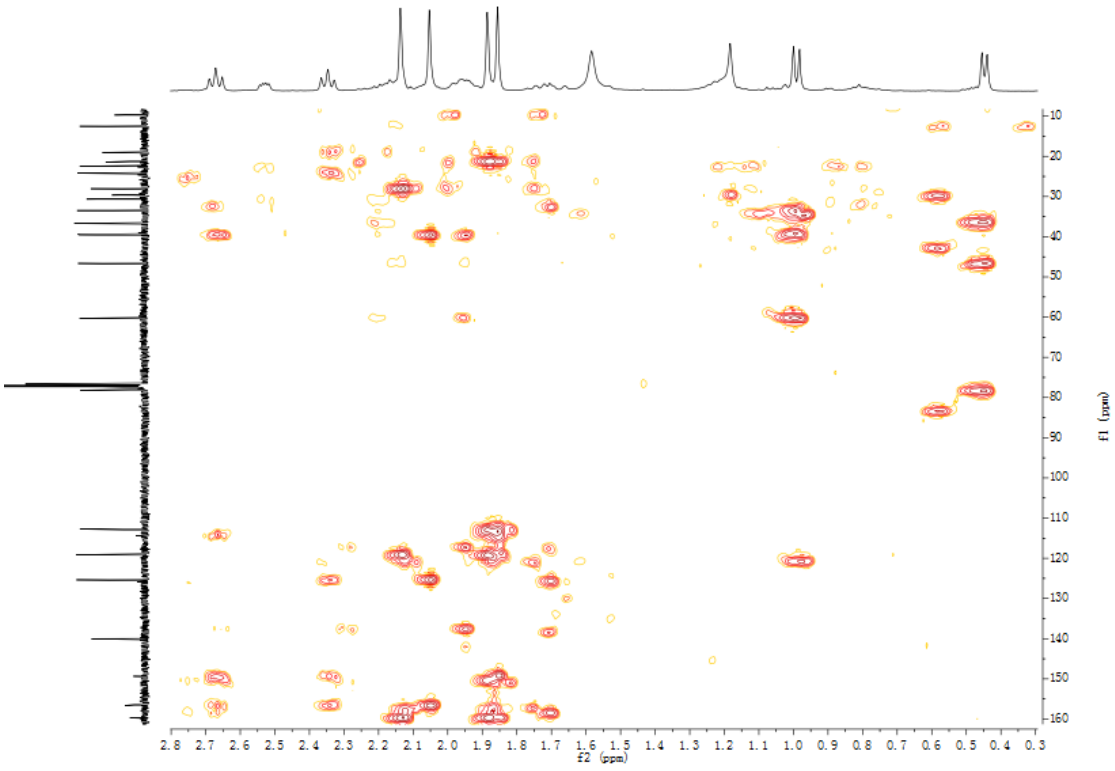


Figure S15. ROESY spectrum of compound **1** in $CDCl_3$

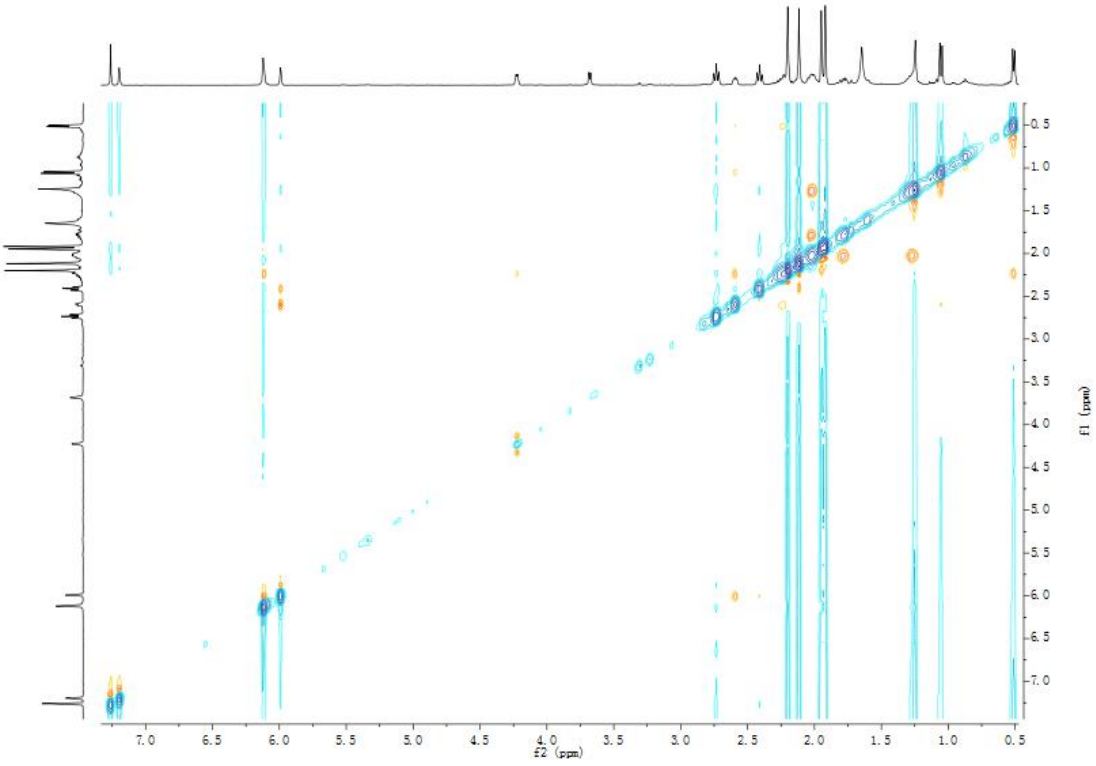


Figure S16. Expanded ROESY spectrum of compound **1**

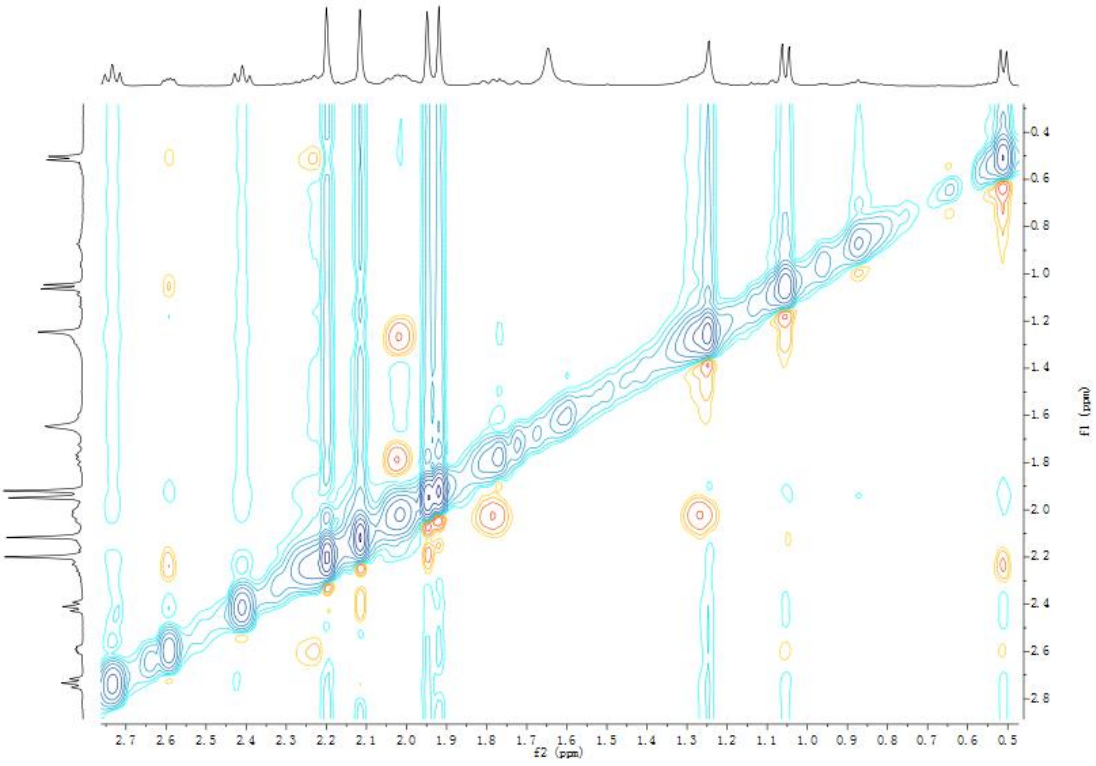


Figure S17. HRESIMS of compound **2**

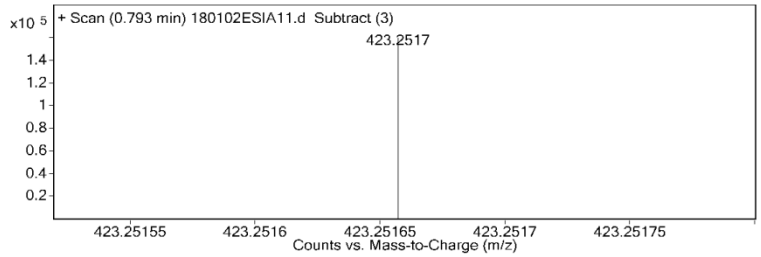
Qualitative Analysis Report

Data Filename	180102ESIA11.d	**Sample Name**	glm-3-1a
Sample Type	Sample	**Position**	
Instrument Name	Agilent G6230 TOF MS	**User Name**	KIB
Acq Method	ESI.m	**Acquired Time**	1/2/2018 11:37:11 AM
IRM Calibration Status	Success	**DA Method**	ESI.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
200	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
423.2517	1	158881.97	C25 H36 Na O4	M+
424.2542	1	34520	C25 H36 Na O4	M+
439.2338	1	14621.36		
455.2402	1	13544.43		
823.5134	1	119152.66		
824.5169	1	57281.3		
837.4919	1	41421.52		
838.4947	1	18775.66		
839.5069		79884.73		
840.5102	1	34274.27		

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff.(mDa)	Diff. (ppm)	DBE
C25 H36 Na O4	423.2511	423.2517	-0.6	1.3	7.5

--- End Of Report ---

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

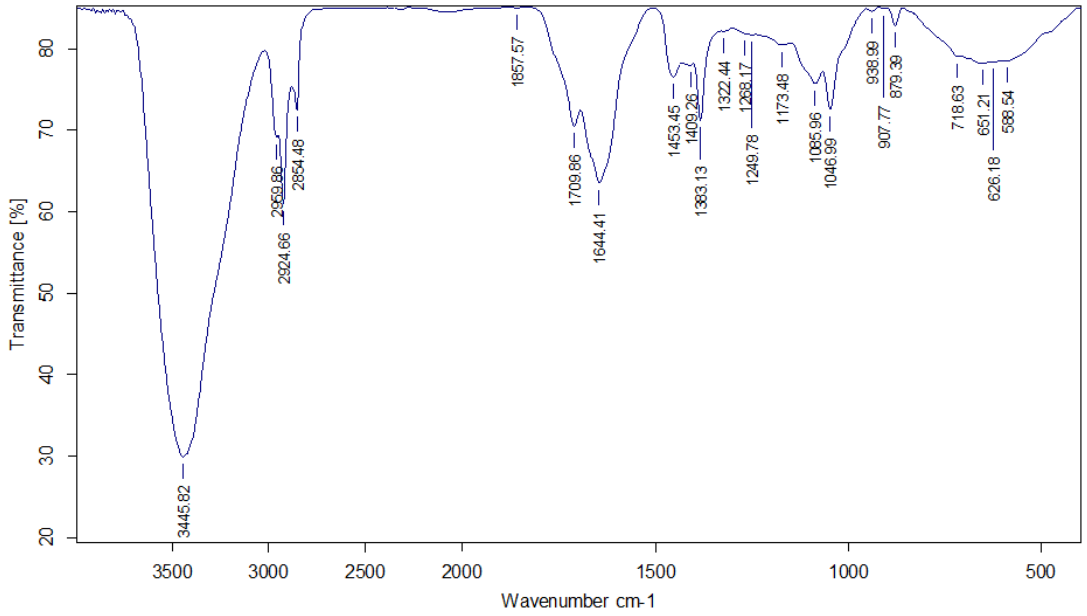


Figure S19. ^{1}H NMR spectrum of compound **2** in acetone-d_6 (800 MHz)

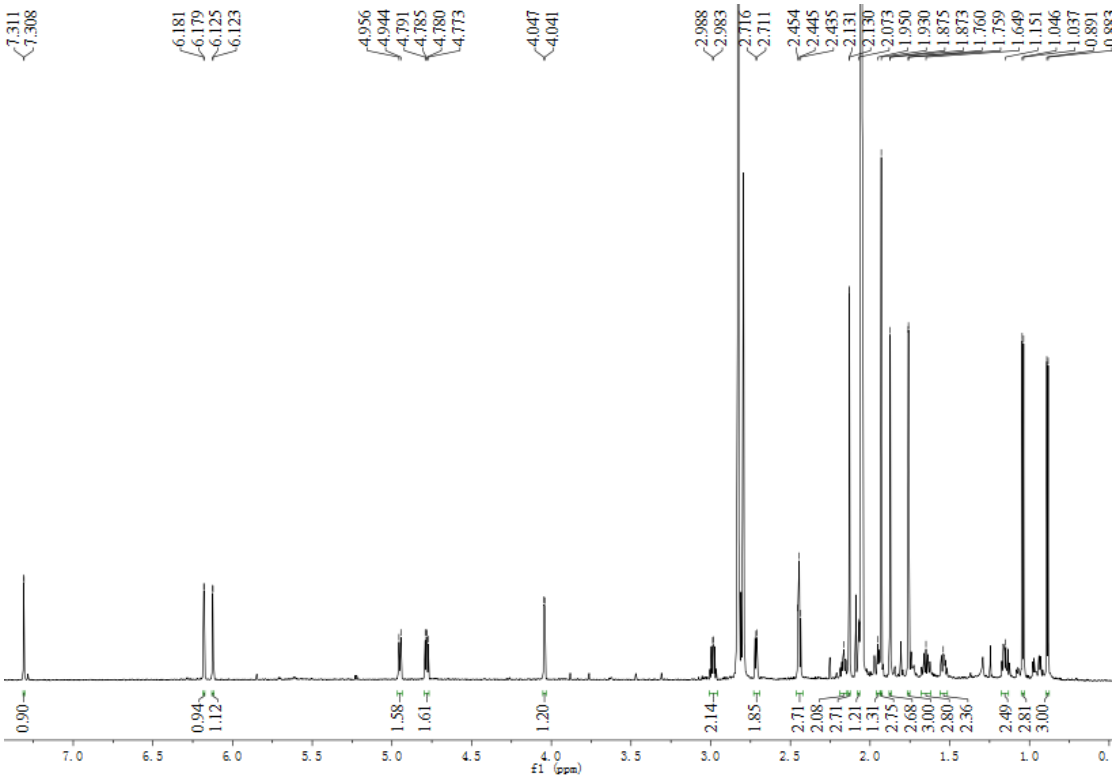


Figure S20. Expanded ^{1}H NMR spectrum of compound **2**

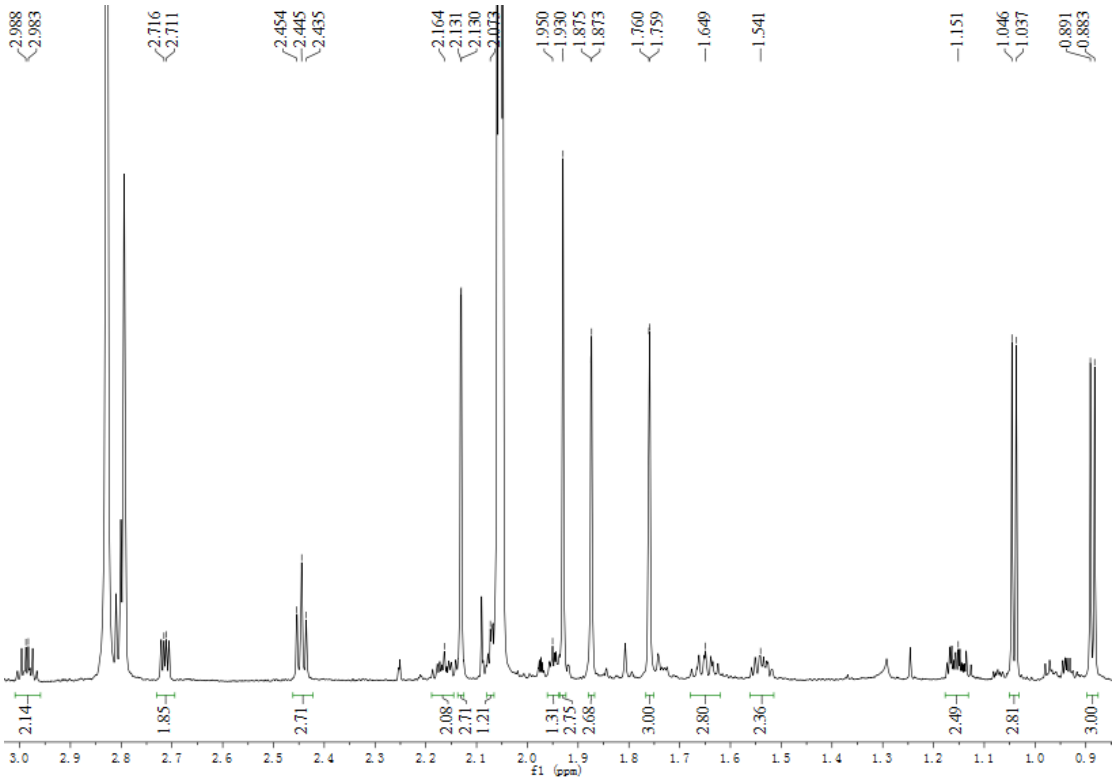


Figure S21. ^{13}C NMR (DEPT) spectrum of compound **2** in acetone-d_6 (200 MHz)

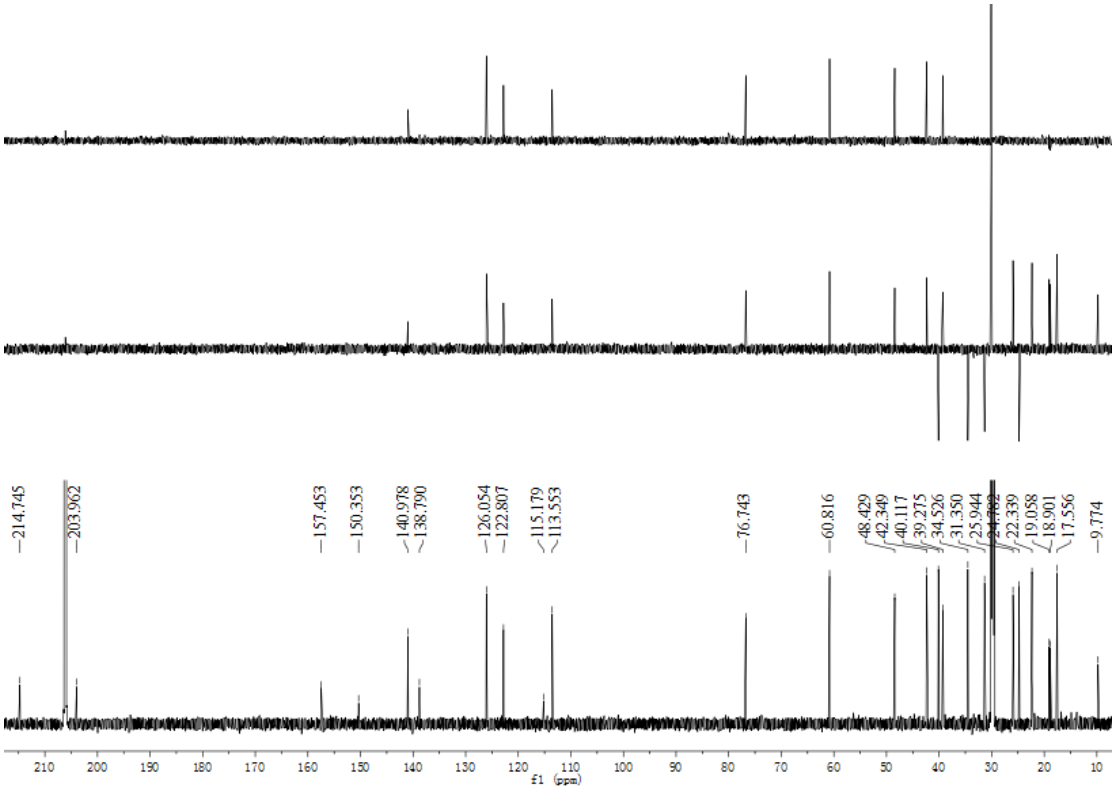


Figure S22. Expanded ^{13}C NMR (DEPT) spectrum of compound **2**

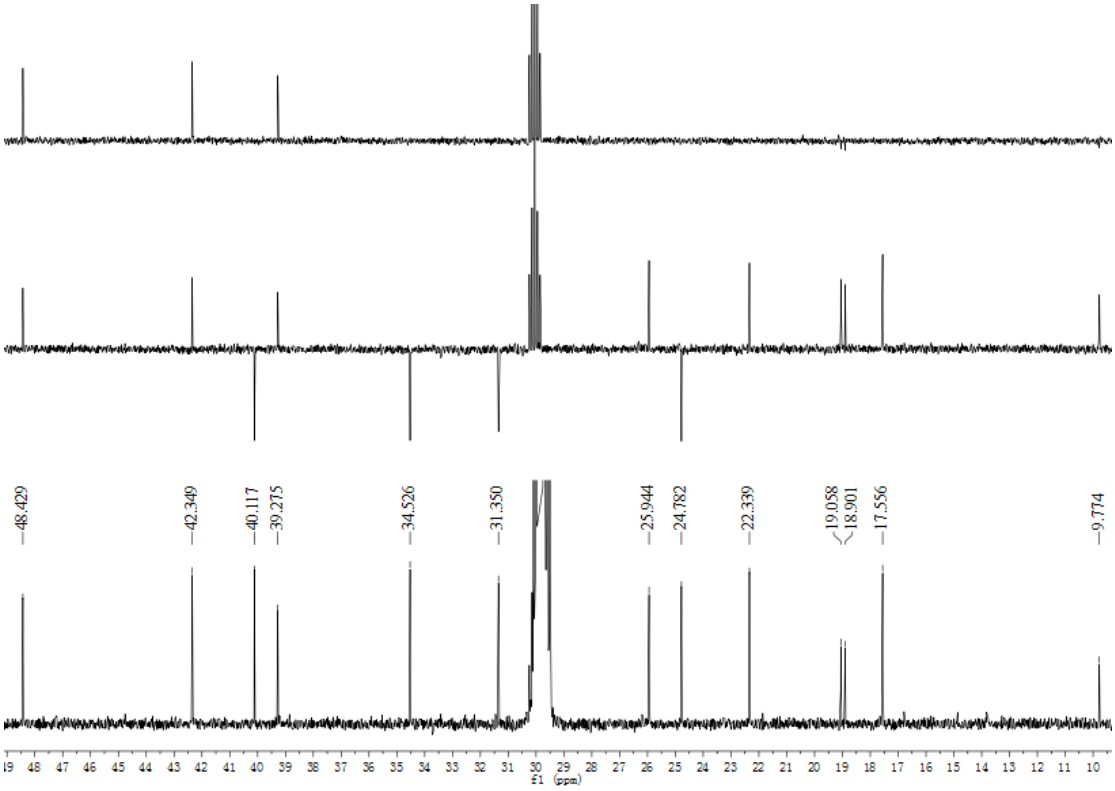


Figure S23. ^{1}H-^{1}H COSY spectrum of compound **2** in acetone-d_6

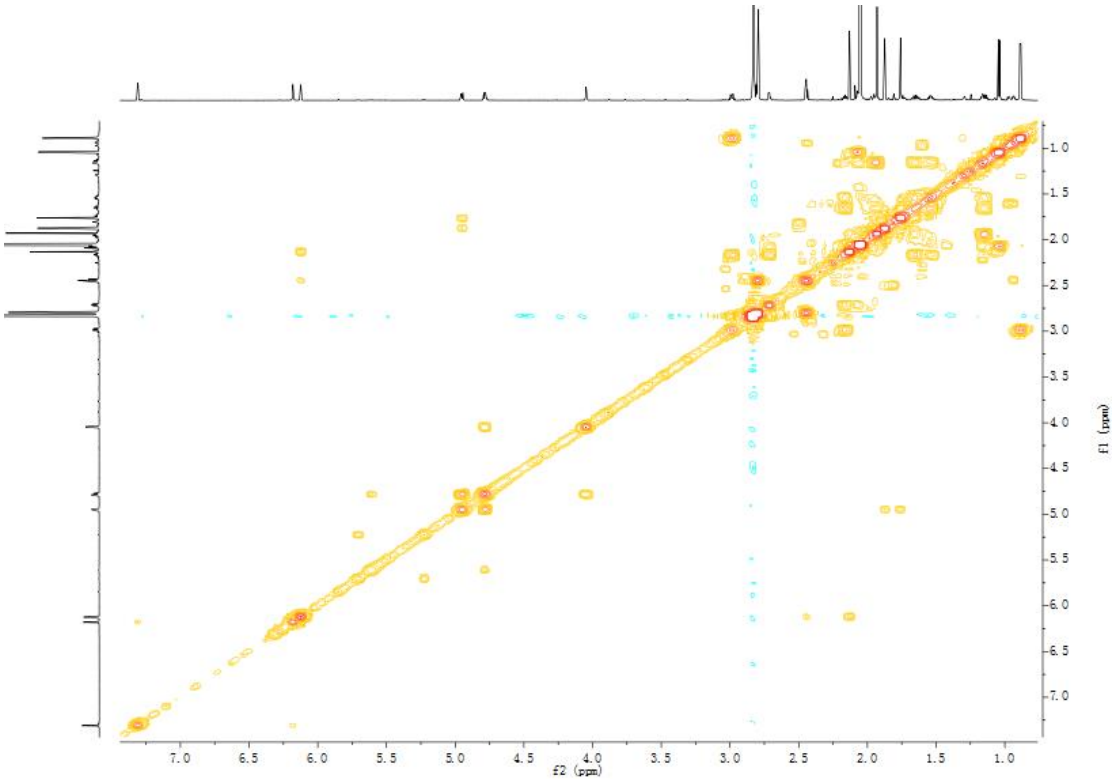


Figure S24. Expanded ^{1}H-^{1}H COSY spectrum of compound **2**

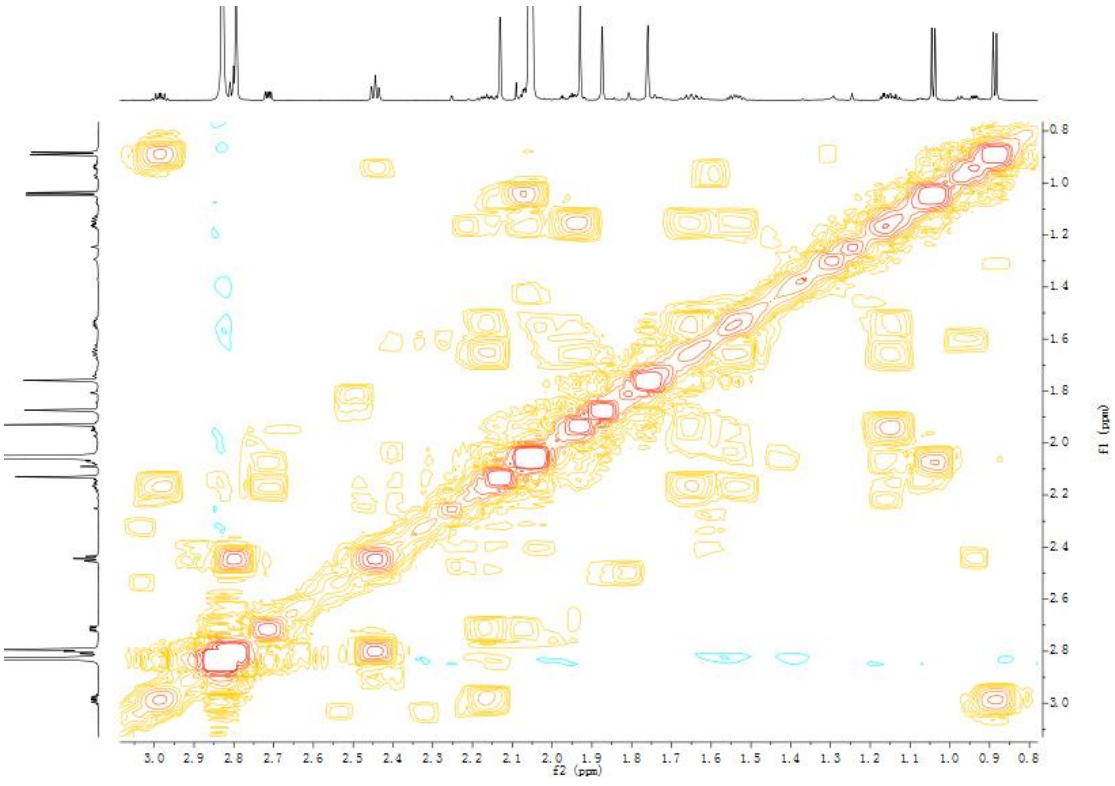


Figure S25. HSQC spectrum of compound **2** in acetone-d_6

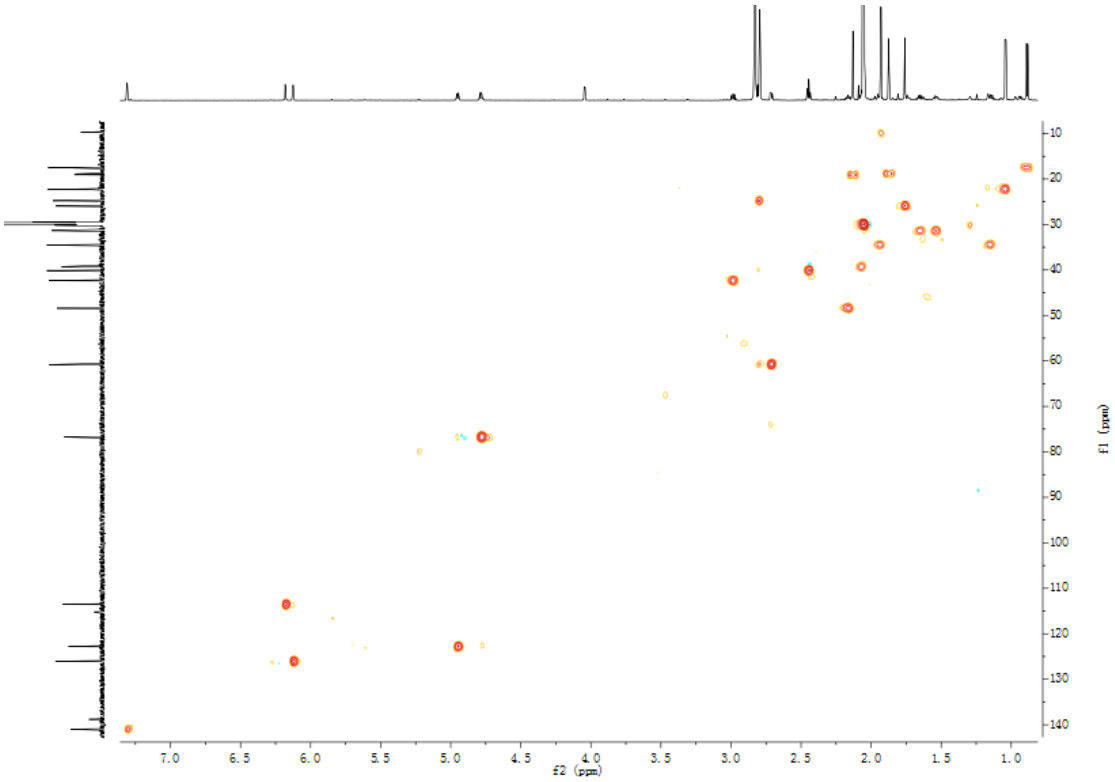


Figure S26. Expanded HSQC spectrum of compound **2**

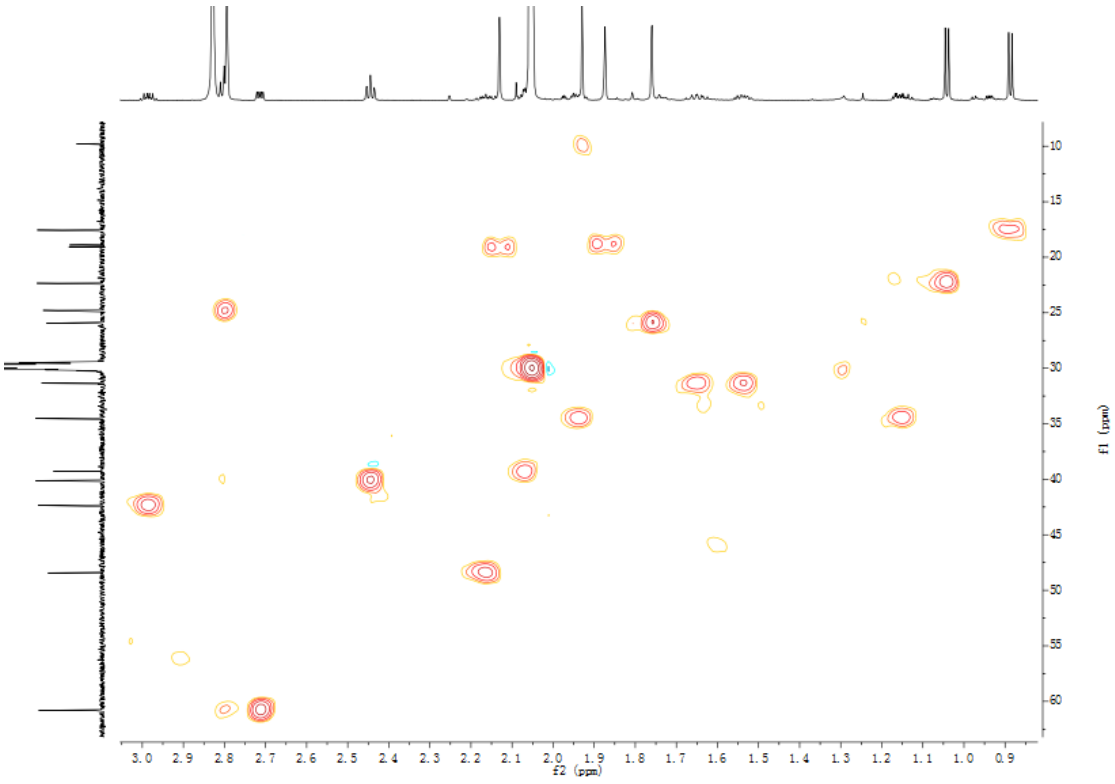


Figure S27. HMBC spectrum of compound **2** in acetone-d_6

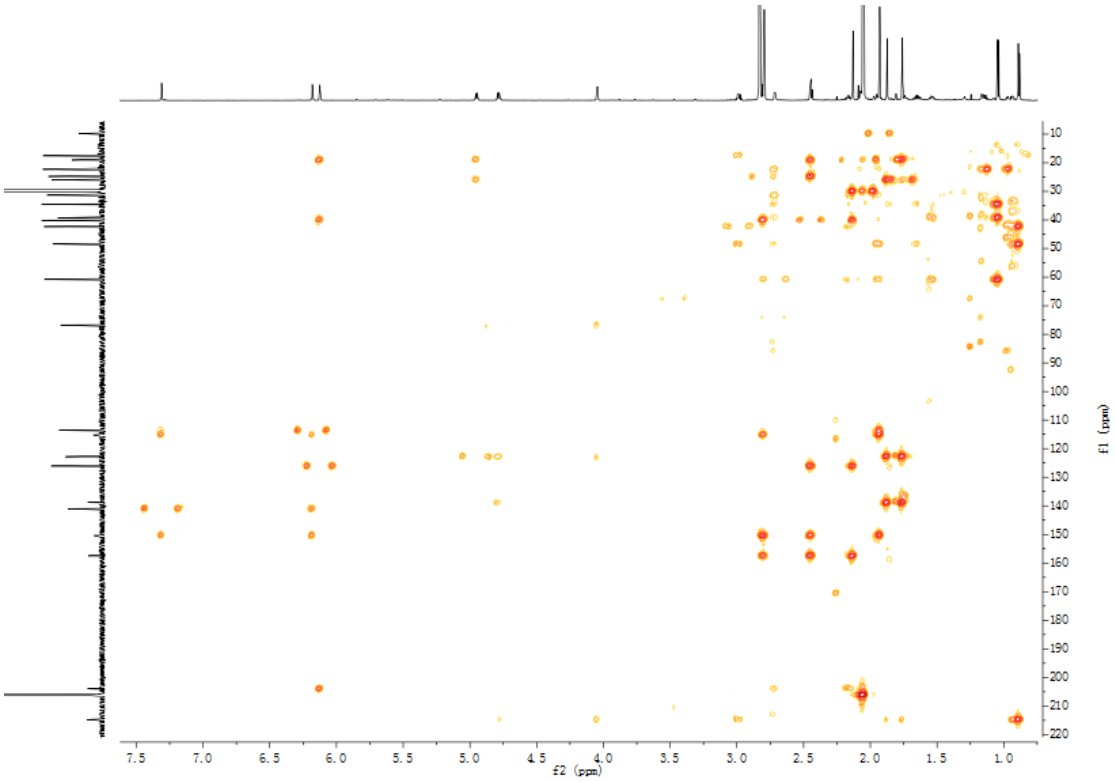


Figure S28. Expanded HMBC spectrum of compound **2**

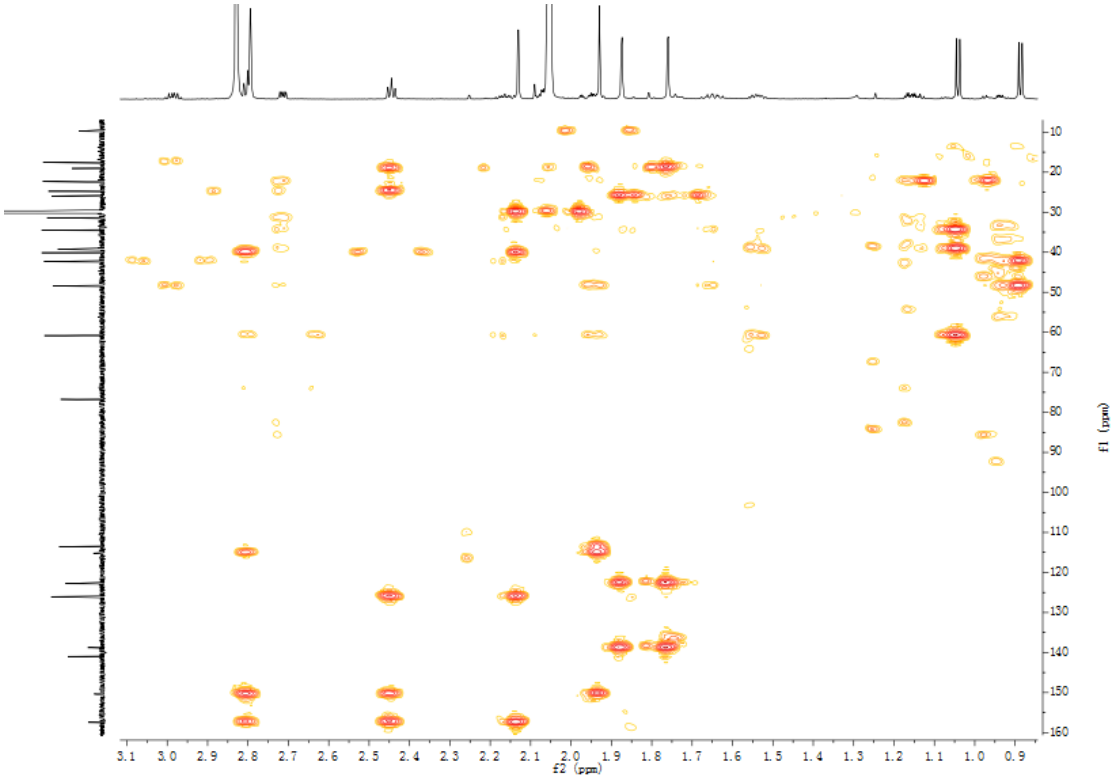


Figure S29. ROESY spectrum of compound **2** in acetone-d_6

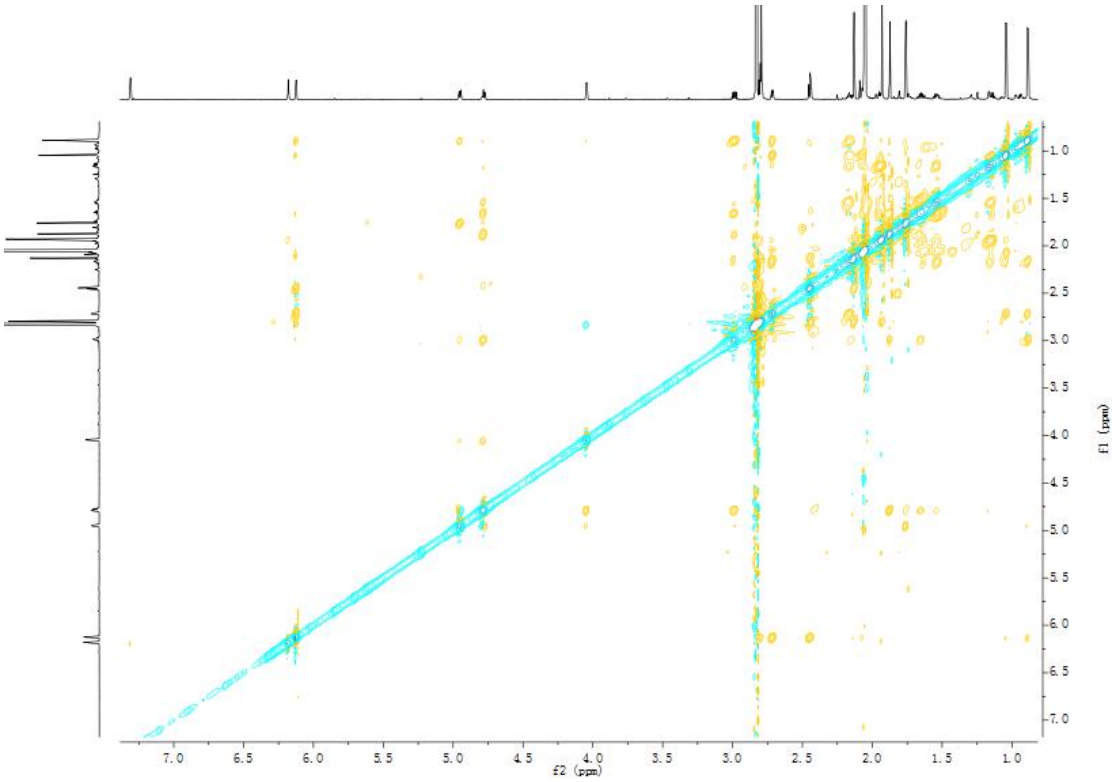


Figure S30. Expanded ROESY spectrum of compound **2**