Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Amichalasines F−J: Cytochalasan heterotrimers with mirror imaged core structures from *Aspergillus micronesiensis*

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Table S1. ^{1}H and ^{13}C NMR data for compound 1.

				1			
no.	δ_H (*J* in Hz)	δ_C	type	*no.*	δ_H (*J* in Hz)	δ_C	type
1		175.4	C	1′		175.8	C
3	2.95 ddd (10.8, 5.1, 2.6)	53.0	CH	3′	3.02 m	52.8	CH
4	2.65 m	51.2	CH	4′	2.62 t (4.4)	53.9	CH
5	2.30 m	36.5	CH	5′	2.54 m	37.2	CH
6		143.7	C	6′		142.6	C
7	5.24 s	126.2	CH	7′	5.24 s	126.6	CH
8	2.56 m	44.4	CH	8′	3.00 m	46.3	CH
9		68.6	C	9′		69.9	C
10a	1.27 m	49.8	CH_2	10′a	1.37 m	49.9	CH_2
10b	1.19 m			10′b	1.21 m		
11	1.20 d (7.2)	14.7	CH_3	11′	1.25 d (7.2)	14.0	CH_3
12	1.76 s	20.3	CH_3	12′	1.77 s	20.3	CH_3
13	6.43 d (9.6)	127.0	CH	13′	6.07 d (9.8)	126.6	CH
14		138.7	C	14′		138.7	C
15a	2.19 m	41.2	CH_2	15′a	2.12 m	38.2	CH_2
15b	2.02 m			15′b	2.05 m		
16a	2.25 m	21.3	CH_2	16′a	1.91 m	22.3	CH_2
16b	1.63 m			16′b	1.91 m		
17a	2.73 m	37.8	CH_2	17′a	2.51ddd (16.3, 7.2, 6.0)	44.6	CH_2
17b	2.22 m			17′b	2.36 dt (16.3, 6.0)		
18		209.9	C	18′		208.9	C
19	3.51 d (7.1)	57.2	CH	19′	3.38 d (5.8)	56.0	CH
20	5.16 dd (7.1, 4.9)	58.9	CH	20′	4.64 d (5.8)	49.8	CH
21		205.0	C	21′		216.7	C
22	1.64 m	26.3	CH	22′	1.72 m	26.2	CH
23	0.91 d (6.5)	24.4	CH_3	23′	0.95 d (6.6)	24.4	CH_3
24	0.93 d (6.5)	21.4	CH_3	24′	0.90 d (6.6)	21.2	CH_3
25	1.29 s	15.2	CH_3	25′	1.49 s	15.4	CH_3
1″	4.37 s	83.6	CH	6″		130.8	C
2″		67.6	C	7″		159.1	C
3″		198.2	C	8″	5.61 d (4.9)	82.8	CH
4″		93.0	C	9″	1.49 s	13.8	CH_3
5″		196.7	C				

600 MHz for ^{1}H and 150 MHz for ^{13}C, measured in CD_3OD.

Table S2. ^{1}H and ^{13}C NMR data for compounds 2 and 3.

	2[a]								**3**[b]						
no.	δ_H (*J* in Hz)	δ_C	type	*no.*	δ_H (*J* in Hz)	δ_C	type	*no.*	δ_H (*J* in Hz)	δ_C	type	*no.*	δ_H (*J* in Hz)	δ_C	type
1		175.0	C	1′		174.7	C	1		176.4	C	1′		176.6	C
3	3.18 m	51.6	CH	3′	3.02 m	51.7	CH	3	3.08 m	53.4	CH	3′	3.09 m	53.2	CH
4	2.36 m	55.4	CH	4′	2.12 m	55.6	CH	4	2.09 t (4.5)	57.2	CH	4′	2.16 m	56.4	CH
5	2.64 m	35.6	CH	5′	2.57 m	35.8	CH	5	2.64 m	37.7	CH	5′	2.15 m	37.0	CH
6		139.3	C	6′		140.2	C	6		140.7	C	6′		141.6	C
7	5.44 brs	126.1	CH	7′	5.39 brs	125.4	CH	7	5.44 brs	127.0	CH	7′	5.41 brs	126.3	CH
8	3.39 brd (11.2)	43.1	CH	8′	3.43 brd (11.0)	43.9	CH	8	3.39 brd (11.2)	46.0	CH	8′	3.45 brd (11.0)	45.5	CH
9		68.8	C	9′		69.4	C	9		68.0	C	9′		71.7	C
10a	1.65 m	48.4	CH_2	10′a	1.51 m	47.6	CH_2	10a	1.71 m	49.8	CH_2	10′a	1.47 m	49.4	CH_2
10b	1.16 m			10′b	1.16 m			10b	1.15 m			10′b	1.04 m		
11	1.22 d (7.2)	13.8	CH_3	11′	1.20 d (7.3)	13.9	CH_3	11	1.24 d (7.2)	14.5	CH_3	11′	1.25 d (7.2)	14.2	CH_3
12	1.76 s	20.2	CH_3	12′	1.76 s	20.4	CH_3	12	1.79 s	20.4	CH_3	12′	1.81 s	20.1	CH_3
13	5.97 d (11.2)	125.1	CH	13′	6.04 d (11.0)	127.9	CH	13	6.01 d (11.2)	125.9	CH	13′	6.10 d (11.0)	128.6	CH
14		136.1	C	14′		134.7	C	14		136.8	C	14′		136.2	C
15a	2.09 m	35.0	CH_2	15′a	2.27 m	35.6	CH_2	15a	2.72 m	34.3	CH_2	15′a	2.35 m	36.7	CH_2
15b	2.09 m			15′b	2.19 m			15b	1.87 m			15′b	2.17 m		
16a	1.83 m	32.5	CH_2	16′a	2.93 ddd (15.5, 12.0)	37.0	CH_2	16a	3.00 m	35.3	CH_2	16′a	2.95 m	38.5	CH_2
16b	1.57 m			16′b	2.63 dd (15.5. 7.3)			16b	2.05 m			16′b	2.51 m		
17	4.49 dd (5.1, 9.5)	75.1	CH	17′		210.1	C	17		211.4	C	17′		210.8	C
18		206.5	C	18′	5.37 brd (3.2)	73.5	CH	18	3.09 m	79.8	CH	18′	5.13 s	74.9	CH
19	3.49 dd (7.2, 4.5)	57.7	CH	19′	2.46 d (7.3)	48.0	CH	19	2.77 m	50.5	CH	19′	2.51 m	49.7	CH
20	4.37 d (7.2)	47.4	CH	20′	3.80 d (7.3)	52.2	CH	20	4.16 d (5.4)	47.2	CH	20′	3.88 d (6.7)	53.5	CH
21		213.7	C	21′		215.9	C	21		213.0	C	21′		218.7	C
22	1.74 m	25.5	CH	22′	1.51 m	25.5	CH	22	1.87 m	26.9	CH	22′	1.62 m	26.0	CH
23	1.02 d (6.5)	23.7	CH_3	23′	0.97 d (6.4)	23.5	CH_3	23	1.18 d (6.6)	24.6	CH_3	23′	1.00 d (6.5)	23.9	CH_3
24	0.96 d (6.5)	21.8	CH_3	24′	0.91 d (6.4)	21.3	CH_3	24	1.00 d (6.6)	21.5	CH_3	24′	0.94 d (6.5)	22.0	CH_3
25	1.53 s	16.6	CH_3	25′	1.53 s	14.6	CH_3	25	1.48 s	15.8	CH_3	25′	1.58 s	14.5	CH_3
1″	4.13 s	83.5	CH	6″		132.5	C	1″	3.93 s	84.2	CH	6″		133.5	C
2″		64.9	C	7″		155.4	C	2″		66.8	C	7″		155.5	C
3″		196.1	C	8″	5.45 d (4.5)	79.9	CH	3″		198.1	C	8″	5.56 d (5.1)	82.6	CH
4″		89.4	C	9″	1.88 s	14.1	CH_3	4″		91.3	C	9″	1.89 s	13.5	CH_3
5″		196.7	C					5″		197.4	C				

[a]600 MHz for ^{1}H and 150 MHz for ^{13}C, measured in $CDCl_3$.

[b]600 MHz for ^{1}H and 150 MHz for ^{13}C, measured in CD_3OD.

Table S3. ^{1}H and ^{13}C NMR data for compounds 4 and 5.

	4[c]								**5**[d]						
no.	δ_H (*J* in Hz)	δ_C	type	*no.*	δ_H (*J* in Hz)	δ_C	type	*no.*	δ_H (*J* in Hz)	δ_C	type	*no.*	δ_H (*J* in Hz)	δ_C	type
1		177.4	C	1′		176.5	C	1		175.8	C	1′		173.9	C
3	3.11 m	53.9	CH	3′	3.09 m	53.3	CH	3	3.06 m	51.0	CH	3′	2.72 m	50.6	CH
4	2.07 t (4.4)	57.9	CH	4′	2.16 t (4.2)	56.7	CH	4	3.38 m	50.0	CH	4′	2.35 m	51.5	CH
5	2.65 m	37.4	CH	5′	2.65 m	37.2	CH	5	2.36 m	35.5	CH	5′	2.29 m	35.7	CH
6		140.6	C	6′		141.7	C	6		139.2	C	6′		141.0	C
7	5.51 brs	127.0	CH	7′	5.42 brs	126.2	CH	7	5.35 brs	125.5	CH	7′	5.12 brs	125.5	CH
8	3.60 brd (11.2)	44.4	CH	8′	3.47 brd (11.1)	45.8	CH	8	3.24 m	42.7	CH	8′	2.41 m	45.6	CH
9		69.3	C	9′		71.4	C	9		68.0	C	9′		65.1	C
10a	1.86 m	49.7	CH_2	10′a	1.47 m	49.5	CH_2	10a	1.41 m	48.9	CH_2	10′a	1.43 m	47.6	CH_2
10b	1.14 m			10′b	1.05 m			10b	1.16 m			10′b	0.99 m		
11	1.25 d (7.0)	14.6	CH_3	11′	1.27 d (7.0)	14.2	CH_3	11	1.17 d (7.1)	13.7	CH_3	11′	1.14 d (7.0)	13.1	CH_3
12	1.82 s	20.4	CH_3	12′	1.82 s	20.1	CH_3	12	1.74 s	20.1	CH_3	12′	1.69 s	19.8	CH_3
13	5.89 d (11.2)	125.3	CH	13′	6.12 d (11.1)	128.3	CH	13	5.92 d (11.0)	123.8	CH	13′	6.04 d (9.8)	125.4	CH
14		138.0	C	14′		136.3	C	14		135.9	C	14′		137.9	C
15a	1.99 m	37.5	CH_2	15′a	2.33 m	36.6	CH_2	15a	1.92 m	35.9	CH_2	15′a	2.06 m	34.1	CH_2
15b	1.99 m			15′b	2.19 m			15b	1.81 m			15′b	1.93 m		
16a	1.29 m	29.5	CH_2	16′a	2.93 m	38.5	CH_2	16a	1.23 m	29.2	CH_2	16′a	2.16 m	32.5	CH_2
16b	1.29 m			16′b	2.51 m			16b	1.04 m			16′b	1.83 m		
17	3.92 m	71.9	CH	17′		210.9	C	17	3.61 m	67.6	CH	17′	3.93 m	74.0	CH
18	2.93 m	78.6	CH	18′	5.09 s	74.8	CH	18	3.22 m	77.5	CH	18′		211.2	C
19	2.40 t (5.8)	53.1	CH	19′	2.52 m	49.7	CH	19	1.65 m	51.1	CH	19′	3.72 d (5.1)	44.1	CH
20	3.96 d (5.8)	48.9	CH	20′	3.90 d (6.5)	53.3	CH	20	3.81 t (4.7)	52.0	CH	20′	5.26 d (5.1)	47.3	CH
21		213.7	C	21′		219.1	C	21		207.6	C	21′		209.5	C
22	1.86 m	26.7	CH	22′	1.63 m	26.0	CH	22	1.69 m	24.4	CH	22′	1.68 m	24.1	CH
23	1.16 d (6.5)	24.5	CH_3	23′	1.00 d (6.5)	24.0	CH_3	23	1.13 d (6.5)	23.6	CH_3	23′	0.83 d (6.6)	24.2	CH_3
24	1.00 d (6.5)	21.5	CH_3	24′	0.94 d (6.5)	21.9	CH_3	24	0.94 d (6.5)	21.4	CH_3	24′	0.81 d (6.6)	21.1	CH_3
25	1.50 s	16.5	CH_3	25′	1.58 s	14.7	CH_3	25	1.29 s	16.0	CH_3	25′	1.33 s	15.2	CH_3
1″	3.95 s	85.1	CH	6″		133.6	C	1″	5.01 d (5.2)	83.1	CH	6″		125.0	C
2″		67.2	C	7″		155.9	C	2″		68.5	C	7″		160.3	C
3″		198.8	C	8″	5.45 d (5.0)	82.5	CH	3″		195.4	C	8″	5.05 s	81.8	CH
4″		91.3	C	9″	1.94 s	13.8	CH_3	4″		88.3	C	9″	1.83 s	11.5	CH_3
5″		197.4	C					5″		195.6	C				

[c]400 MHz for ^{1}H and 100 MHz for ^{13}C, measured in CD_3OD.

[d]500 MHz for ^{1}H and 125 MHz for ^{13}C, measured in DMSO-d_6.

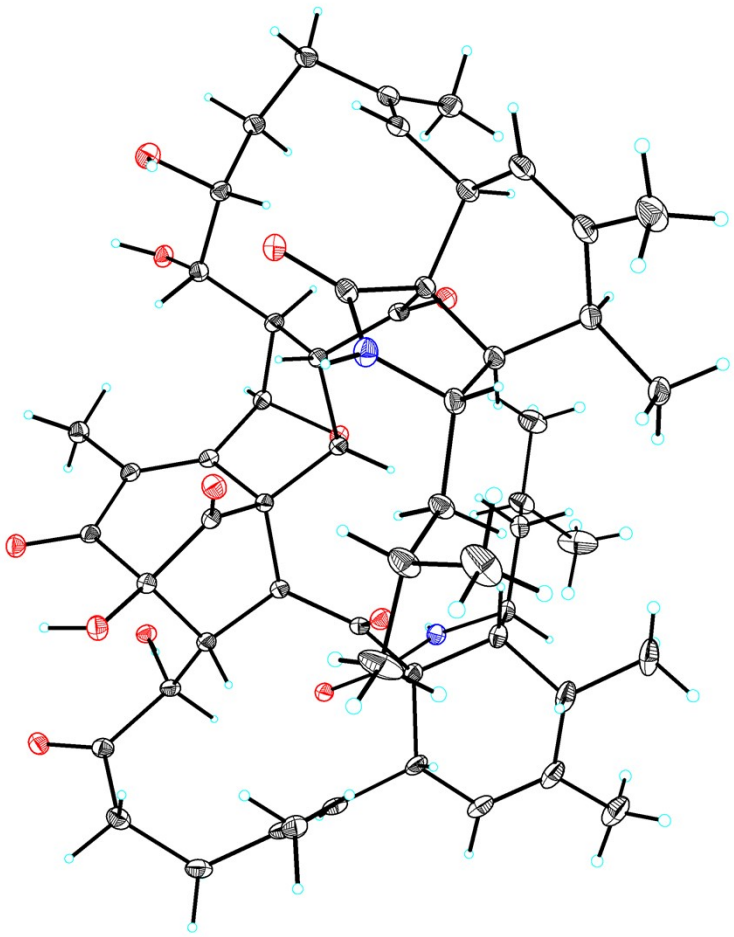


Fig. S1. X-ray drawing of compound **4**

ECD calculation

The theoretical calculation of compound **1** was performed using Gaussian 09[1] and figured using GaussView 5.0[2]. Conformation search using molecular mechanics calculations was performed in Discovery Studio 3.5 Client with MMFF force field with 20 kcal mol^{-1} upper energy limit.[3]

The optimized conformation geometries and thermodynamic parameters of all selected conformations were provided. The predominant conformers were optimized at B3LYP/6-31G(d,p) level. The theoretical calculation of ECD was performed using time dependent Density Functional Theory (TDDFT) at B3LYP/6-31G(d,p) level in MeOH with PCM model[4]. The ECD spectrum of compound **1** was obtained by weighing the Boltzmann distribution rate of each geometric conformation[5].

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E) = \frac{1}{2.297\times10^{-39}} \times \frac{1}{\sqrt{2\pi\sigma}} \sum_{i}^{A} \Delta E_i R_i e^{-[(E-E_i)/(2\sigma)]^2} \qquad (1)$$

The σ represented the width of the band at $1/e$ height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition i, respectively. R_{vel} had been used in this work.

(1) Gaussian 09, Revision C.01,M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

(2) GaussView, Version 5, Dennington, R.; Keith, T.; Millam, J. *Semichem Inc.*, Shawnee Mission, KS, **2009**.

(3) Smith, S. G.; Goodman, J. M. *J. Am. Chem. Soc.* **2010**, *132*, 12946−12959.

(4) (a) Miertus, S.; Scrocc, E.; Tomasi, J. *J. Chem. Phys.* **1981**, *55*, 117. (b) Miertus, S.; Tomasi, J. *J. Chem. Phys.* **1982**, *65*, 239. (c) Cossi, M.; Barone, V.; Cammi, R.; Tomasi, J. *Chem. Phys. Lett.* **1996**, *255*, 327.

(5) Tähtinen, P.; Bagno, A.; Klika, K. D.; Pihlaja, K. *J. Am. Chem. Soc.* **2003**, *125*, 4609−4618.

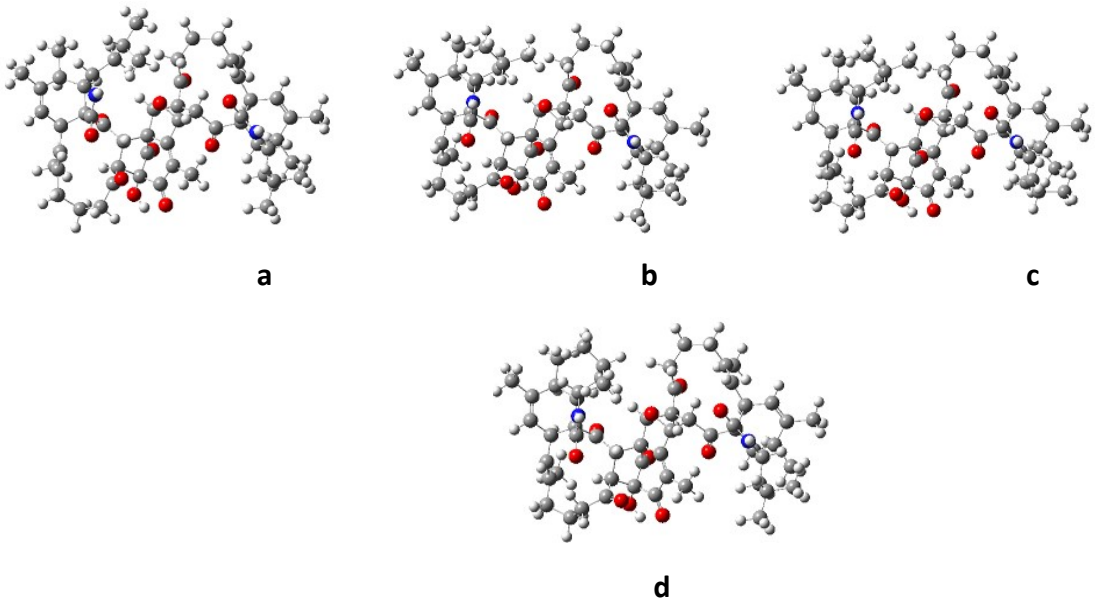


Fig. S2. Optimized geometries of predominant conformers for compound **1** at the B3LYP/6-31G(d,p) level in the gas phase.

Table S4. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized compound **1** at B3LYP/6-31G(d,p) level in the gas phase.

Conformations	E+ZPE	G	%
1a	-3076.013711	-3076.116442	70.7
1b	-3076.011805	-3076.113952	5.1
1c	-3076.013348	-3076.115161	18.2
1d	-3076.013002	-3076.114111	6

E+ZPE, G: total energy with zero point energy (ZPE) and Gibbs free energy in the gas phase at B3LYP/6-31G(d,p) level. %: Boltzmann distributions, using the relative Gibbs free energies as weighting factors.

Table S5. Optimized Z-matrixes of compound **1** in the gas phase (Å) at B3LYP/6-31G(d,p) level.

1a				**1b**			
C	0.627113	-2.34719	0.348245	C	0.706555	-2.31217	0.389827
C	0.026309	-3.35318	-0.5427	C	0.087898	-3.36482	-0.46523
C	-1.11387	-2.91485	-1.49516	C	-1.09963	-2.91557	-1.39104
C	-0.72992	-1.52188	-2.04433	C	-0.69236	-1.55407	-1.9628
C	-0.85499	-0.63598	-0.80265	C	-0.79918	-0.62459	-0.76847
C	0.245818	-1.06777	0.160715	C	0.322998	-1.04054	0.190677
C	-0.58751	0.88272	-0.82215	C	-0.52463	0.89209	-0.82553
O	-0.34466	1.122662	0.582988	O	-0.26849	1.161483	0.57201
C	0.778845	0.232559	0.721724	C	0.859251	0.273832	0.716753
O	0.410984	-4.51662	-0.61583	O	0.512392	-4.50064	-0.52098
C	6.543346	-0.37265	-1.32306	C	6.633019	-0.31872	-1.29032
C	5.406662	-0.72429	-0.32067	C	5.484135	-0.66436	-0.29978
C	4.373641	0.430472	-0.11875	C	4.442515	0.487536	-0.12632
C	4.865967	1.767337	-0.84674	C	4.931539	1.812311	-0.87809
C	6.355569	1.941681	-0.6232	C	6.415664	2.00598	-0.63595
C	7.197217	0.933441	-0.8888	C	7.269727	0.999947	-0.86859
C	2.984497	0.051482	-0.70228	C	3.060573	0.090133	-0.71563
C	1.769904	0.886479	-0.31174	C	1.835881	0.914841	-0.33584
C	0.789949	1.197626	-1.49053	C	0.845879	1.184152	-1.51617
C	4.07501	3.012885	-0.52003	C	4.123	3.056484	-0.59203
C	0.90199	2.630883	-2.01633	C	0.954011	2.597511	-2.09219
C	0.61382	3.809659	-1.0836	C	0.646046	3.804584	-1.20302
C	1.391984	5.087121	-1.43962	C	1.420289	5.075334	-1.5901
C	2.844462	5.120845	-0.90346	C	2.867509	5.13664	-1.04242
C	3.719186	3.979684	-1.38521	C	3.75858	3.992806	-1.48665
C	4.283569	0.607239	1.412367	C	4.34233	0.694802	1.399884

C	5.952036	-1.08945	1.097395	C	6.011351	-1.00926	1.130074
N	5.152138	-0.25767	1.987115	N	5.199849	-0.1655	1.998001
O	3.541815	1.367259	2.030635	O	3.60219	1.472356	1.998044
O	2.87313	-0.87973	-1.4789	O	2.966602	-0.84254	-1.4924
C	5.829349	-2.58555	1.429318	C	5.885856	-2.50085	1.479883
C	6.294343	-3.01656	2.835168	C	6.328772	-2.91241	2.898592
C	5.977732	-4.50274	3.060079	C	6.013039	-4.3967	3.136911
C	7.785857	-2.73998	3.080773	C	7.815102	-2.62773	3.165626
C	7.499897	-1.5486	-1.56156	C	7.602254	-1.49036	-1.49706
C	8.691297	1.067522	-0.76652	C	8.760531	1.148459	-0.72502
C	4.116015	4.02413	-2.84087	C	4.162326	4.000903	-2.94108
O	1.159897	2.817484	-3.19285	O	1.223362	2.745524	-3.27176
C	-6.07551	2.276514	-0.35832	C	-5.81279	2.402973	-0.48675
C	-4.67027	1.841137	0.163376	C	-4.58284	1.767076	0.228361
C	-4.51674	0.282974	0.267488	C	-4.5541	0.198533	0.117593
C	-5.84661	-0.45054	-0.21024	C	-5.85043	-0.3579	-0.62639
C	-7.02371	0.203947	0.474262	C	-7.06858	0.361597	-0.09766
C	-7.16397	1.536618	0.411341	C	-7.08556	1.700445	-0.02936
C	-3.38929	-0.20971	-0.66914	C	-3.32819	-0.22696	-0.71762
C	-2.23727	-1.09155	-0.18153	C	-2.1766	-1.04789	-0.13286
C	-2.42284	-2.55544	-0.69748	C	-2.37582	-2.55294	-0.57278
C	-5.80415	-1.9494	-0.04824	C	-5.97817	-1.85901	-0.55204
C	-2.70332	-3.57371	0.41455	C	-2.64331	-3.51991	0.592117
C	-3.31331	-4.9224	0.051273	C	-3.88742	-4.39569	0.585269
C	-4.40359	-5.03378	-1.02756	C	-4.45482	-4.89313	-0.76756
C	-5.75227	-4.34733	-0.69376	C	-5.8073	-4.24759	-1.16974
C	-5.81777	-2.86809	-1.02969	C	-5.71674	-2.76955	-1.50613
C	-4.26936	0.017986	1.761317	C	-4.50105	-0.29201	1.57023
C	-4.33211	2.411846	1.58169	C	-4.50563	2.099517	1.755249
N	-4.13961	1.216084	2.386637	N	-4.49528	0.788212	2.387081
O	-4.20293	-1.07258	2.31206	O	-4.46033	-1.45856	1.946561
O	-3.44078	0.11114	-1.84623	O	-3.28547	0.108459	-1.89115
C	-3.12442	3.366062	1.558858	C	-3.26608	2.935223	2.118139
C	-2.75902	4.066011	2.889809	C	-3.07201	3.255881	3.613936
C	-1.86128	3.206257	3.796031	C	-1.72641	3.966303	3.824019
C	-2.06853	5.410494	2.607185	C	-4.22284	4.088127	4.200202
C	-6.22527	3.801425	-0.43812	C	-5.81602	3.933847	-0.37995
C	-8.31651	2.26856	1.044017	C	-8.27917	2.475338	0.460847
C	-5.92275	-2.56702	-2.50769	C	-5.29926	-2.4638	-2.92585
O	-2.31079	-3.36749	1.548007	O	-1.85549	-3.56848	1.519806
O	-1.33196	-3.89673	-2.45086	O	-1.38445	-3.86214	-2.37471
C	1.666784	-2.83002	1.318185	C	1.754309	-2.7775	1.356658
O	-0.41034	-1.24129	-3.16786	O	-0.33938	-1.36991	-3.10401

H	2.099512	1.798559	0.175356	H	2.155565	1.843649	0.125963
H	-2.17788	-1.10998	0.905176	H	-2.13209	-0.97634	0.952164
H	4.865961	-1.58326	-0.72636	H	4.953857	-1.53103	-0.70268
H	-3.93981	2.22501	-0.55412	H	-3.69185	2.178792	-0.25562
H	-3.20631	-2.59568	-1.454	H	-3.18865	-2.60458	-1.29334
H	0.961321	0.543288	-2.34541	H	1.013929	0.498385	-2.34706
H	-1.42044	1.488801	-1.17012	H	-1.35789	1.494339	-1.17831
H	1.146899	0.23349	1.745507	H	1.236314	0.297361	1.737048
H	6.038505	-0.18615	-2.28383	H	6.140773	-0.15122	-2.26102
H	4.724529	1.540488	-1.91296	H	4.807786	1.558774	-1.94048
H	6.711165	2.914794	-0.29451	H	6.757621	2.988061	-0.3197
H	3.793768	3.126207	0.523667	H	3.834612	3.195805	0.446531
H	-0.46309	4.005297	-1.19776	H	-0.43011	3.989768	-1.34082
H	0.75026	3.525293	-0.03631	H	0.76674	3.555045	-0.14492
H	0.862295	5.952786	-1.02587	H	0.880798	5.949539	-1.20805
H	1.381862	5.201303	-2.52793	H	1.4194	5.156265	-2.68148
H	2.813199	5.114964	0.192703	H	2.826621	5.159419	0.053167
H	3.288486	6.080691	-1.20203	H	3.304512	6.092896	-1.36244
H	7.002817	-0.78448	1.178804	H	7.060772	-0.70191	1.220904
H	5.255574	-0.25532	2.992109	H	5.297087	-0.14288	3.003342
H	6.403297	-3.14669	0.68017	H	6.473374	-3.07044	0.74783
H	4.779926	-2.87623	1.296894	H	4.839623	-2.79575	1.334049
H	5.715002	-2.44633	3.577632	H	5.735189	-2.33482	3.623913
H	6.260149	-4.81904	4.069558	H	6.278816	-4.69912	4.155174
H	4.910433	-4.70935	2.929723	H	4.948969	-4.60859	2.990353
H	6.527582	-5.131	2.349101	H	6.577304	-5.03209	2.443768
H	8.084182	-3.07543	4.079394	H	8.097588	-2.94908	4.173478
H	8.033948	-1.67605	3.007484	H	8.061367	-1.56405	3.082411
H	8.406498	-3.27714	2.353257	H	8.449588	-3.17246	2.455859
H	8.230281	-1.30739	-2.33931	H	8.341917	-1.2551	-2.2679
H	6.942963	-2.42956	-1.89579	H	7.057061	-2.38076	-1.82562
H	8.059765	-1.82869	-0.66358	H	8.151258	-1.75251	-0.58702
H	8.963561	2.066426	-0.4152	H	9.17999	0.432844	-0.00731
H	9.11622	0.33598	-0.06836	H	9.276983	0.971142	-1.67674
H	9.191047	0.903104	-1.72938	H	9.019269	2.155627	-0.38725
H	3.241769	3.925293	-3.49244	H	4.88799	3.223524	-3.18726
H	4.58351	4.991034	-3.06652	H	3.292912	3.871975	-3.59386
H	4.830338	3.24489	-3.11311	H	4.618582	4.966943	-3.19223
H	-6.11108	1.912552	-1.39614	H	-5.67353	2.166264	-1.55199
H	-5.89501	-0.20728	-1.27783	H	-5.69154	-0.05567	-1.66822
H	-7.73739	-0.42295	1.003207	H	-7.92607	-0.23197	0.210826
H	-5.74349	-2.2965	0.979671	H	-6.29903	-2.23085	0.417806
H	-2.45105	-5.52088	-0.28093	H	-3.65327	-5.23308	1.248393

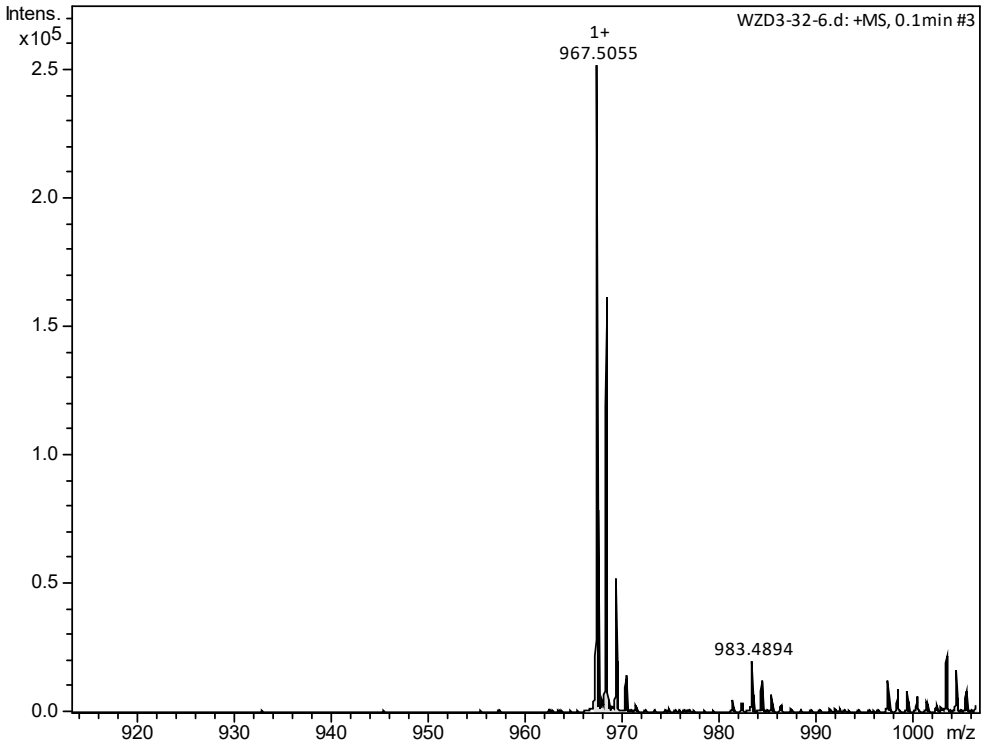
H	-3.64714	-5.36474	0.995562	H	-4.63481	-3.78978	1.113117
H	-4.59121	-6.10509	-1.16671	H	-4.61703	-5.97385	-0.69056
H	-4.01102	-4.67971	-1.98661	H	-3.71899	-4.76997	-1.56981
H	-6.5404	-4.86392	-1.25894	H	-6.20679	-4.79587	-2.03287
H	-5.97896	-4.50012	0.367771	H	-6.51562	-4.39614	-0.3459
H	-5.19535	2.964729	1.977036	H	-5.41213	2.634781	2.062676
H	-4.03716	1.233495	3.390654	H	-4.46605	0.652364	3.387632
H	-3.36529	4.138772	0.816681	H	-3.32164	3.8803	1.559271
H	-2.24905	2.823072	1.180141	H	-2.37844	2.403247	1.752062
H	-3.69396	4.282428	3.43028	H	-3.0248	2.30303	4.162778
H	-1.61279	3.743019	4.717794	H	-1.54092	4.156709	4.886233
H	-2.32324	2.258134	4.083034	H	-0.89531	3.368213	3.436837
H	-0.92329	2.962487	3.284706	H	-1.71172	4.932997	3.306097
H	-1.79531	5.919824	3.537322	H	-4.32133	5.043982	3.671231
H	-2.71619	6.081774	2.033099	H	-4.04173	4.313141	5.256375
H	-1.14828	5.259689	2.030021	H	-5.1876	3.573626	4.137876
H	-7.17075	4.07536	-0.91519	H	-6.6312	4.36528	-0.96783
H	-5.41871	4.231761	-1.04077	H	-4.87894	4.34505	-0.76941
H	-6.20248	4.28688	0.542578	H	-5.93157	4.287766	0.649164
H	-8.97909	1.572108	1.564883	H	-8.03598	3.107125	1.324173
H	-7.97909	3.018889	1.76978	H	-8.67336	3.145937	-0.31301
H	-8.91448	2.806338	0.297492	H	-9.08468	1.798139	0.757252
H	-5.16077	-3.10905	-3.07962	H	-6.07109	-2.81652	-3.62238
H	-6.8941	-2.90726	-2.89067	H	-5.12604	-1.40367	-3.11414
H	-5.81517	-1.50946	-2.75065	H	-4.37861	-2.99832	-3.19198
H	-0.70767	-4.6137	-2.22481	H	-0.84031	-3.63165	-3.14611
H	2.138781	-2.00761	1.859551	H	2.498949	-3.3876	0.836991
H	1.20926	-3.50679	2.047728	H	2.254012	-1.94785	1.861457
H	2.437038	-3.40164	0.791838	H	1.289889	-3.4194	2.113039
1c				**1d**			
C	0.681527	-2.3703	0.404955	C	0.756637	-2.33648	0.331295
C	0.06474	-3.41634	-0.43413	C	0.164906	-3.3629	-0.5492
C	-1.13484	-3.02536	-1.34315	C	-1.02969	-2.95976	-1.45915
C	-0.74375	-1.66809	-1.97506	C	-0.65247	-1.57682	-2.04125
C	-0.83725	-0.71765	-0.77874	C	-0.77283	-0.66817	-0.81517
C	0.284106	-1.10403	0.18354	C	0.344506	-1.06912	0.145887
C	-0.56577	0.798166	-0.87338	C	-0.52343	0.853329	-0.85753
O	-0.31043	1.102749	0.518106	O	-0.28567	1.11701	0.545253
C	0.818529	0.220982	0.68395	C	0.854402	0.247022	0.693848
O	0.507318	-4.55309	-0.53905	O	0.626291	-4.48867	-0.68671
C	6.586659	-0.41388	-1.2983	C	6.657829	-0.24062	-1.24773
C	5.443801	-0.73542	-0.29273	C	5.505908	-0.60466	-0.26752
C	4.401477	0.418816	-0.14941	C	4.443802	0.529634	-0.10315

C	4.890233	1.727477	-0.92817	C	4.918983	1.864033	-0.84651
C	6.374918	1.924895	-0.69299	C	6.398177	2.079807	-0.5926
C	7.226812	0.912739	-0.9067	C	7.269919	1.087828	-0.82013
C	3.022343	0.005837	-0.73518	C	3.075418	0.110709	-0.70955
C	1.795099	0.838612	-0.38183	C	1.832091	0.912948	-0.34187
C	0.805733	1.076989	-1.56917	C	0.850524	1.173366	-1.53108
C	4.08042	2.976593	-0.66809	C	4.088657	3.094275	-0.56224
C	0.915531	2.477494	-2.17597	C	0.941705	2.592563	-2.09534
C	0.599953	3.70379	-1.31559	C	0.606451	3.788268	-1.20029
C	1.376211	4.966735	-1.72407	C	1.362406	5.074016	-1.57348
C	2.819283	5.04272	-1.16696	C	2.804126	5.156115	-1.01385
C	3.716765	3.893388	-1.58302	C	3.717565	4.029033	-1.45576
C	4.293761	0.654579	1.371199	C	4.323008	0.730842	1.422288
C	5.981153	-1.04026	1.144221	C	6.025575	-0.94215	1.166932
N	5.153913	-0.18706	1.990469	N	5.1908	-0.11402	2.027779
O	3.542721	1.435939	1.951555	O	3.561534	1.491925	2.014871
O	2.931786	-0.94834	-1.48566	O	3.006424	-0.82267	-1.48794
C	5.887578	-2.53269	1.516942	C	5.922767	-2.43622	1.514225
C	6.668742	-3.02707	2.75843	C	6.360281	-2.84172	2.936394
C	8.191396	-2.93973	2.568693	C	6.061271	-4.32975	3.173277
C	6.245588	-2.36294	4.078956	C	7.840973	-2.53866	3.213925
C	7.555337	-1.58864	-1.49018	C	7.64676	-1.39723	-1.44524
C	8.718192	1.061779	-0.76919	C	8.757164	1.260298	-0.66672
C	4.127155	3.872647	-3.03549	C	4.134357	4.050711	-2.90631
O	1.194643	2.600656	-3.35592	O	1.220398	2.754492	-3.27073
C	-5.74741	2.425679	-0.53153	C	-5.71203	2.402364	-0.5056
C	-4.52099	1.786272	0.186588	C	-4.49269	1.747169	0.210629
C	-4.54409	0.213786	0.156803	C	-4.50059	0.177683	0.116684
C	-5.88443	-0.32988	-0.51436	C	-5.82655	-0.35391	-0.58989
C	-7.05915	0.457806	0.014888	C	-7.01524	0.404662	-0.04994
C	-7.02938	1.798232	0.003221	C	-6.99673	1.744871	-0.01391
C	-3.36575	-0.29829	-0.70166	C	-3.30784	-0.28777	-0.74849
C	-2.21277	-1.12126	-0.11883	C	-2.14868	-1.11426	-0.18363
C	-2.40834	-2.63151	-0.52728	C	-2.31862	-2.61173	-0.647
C	-6.05814	-1.82058	-0.3708	C	-5.98565	-1.85057	-0.50148
C	-2.66214	-3.58815	0.64974	C	-2.57407	-3.613	0.491929
C	-3.99099	-4.31323	0.75825	C	-3.89537	-4.35652	0.559003
C	-4.62121	-4.878	-0.54097	C	-4.50504	-4.8812	-0.76646
C	-5.98413	-4.23421	-0.90644	C	-5.87339	-4.24277	-1.12147
C	-5.8754	-2.77287	-1.30251	C	-5.77979	-2.76683	-1.46402
C	-4.44941	-0.20278	1.630512	C	-4.41255	-0.2943	1.57291
C	-4.39991	2.195099	1.691551	C	-4.40676	2.101493	1.734263
N	-4.38357	0.916919	2.388896	N	-4.3621	0.793893	2.375592

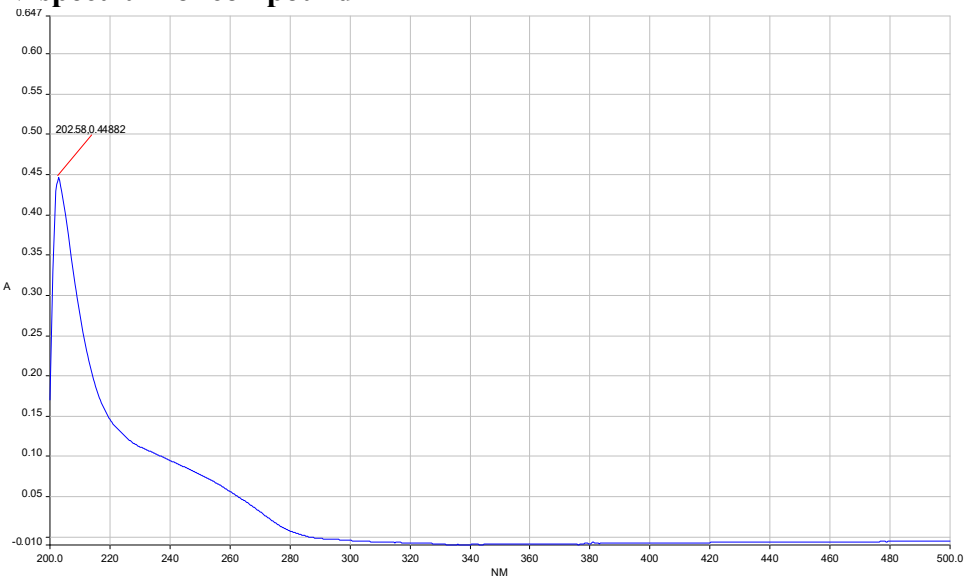
O	-4.42207	-1.3493	2.067353	O	-4.3727	-1.45682	1.96546
O	-3.36065	-0.02635	-1.89156	O	-3.29545	0.026065	-1.92799
C	-3.14562	3.037025	1.980161	C	-3.18723	2.983511	2.066516
C	-2.92604	3.453683	3.448475	C	-3.11568	3.636709	3.467916
C	-1.55894	4.137892	3.597906	C	-4.23721	4.661623	3.699418
C	-4.04631	4.357915	3.985392	C	-3.04226	2.636771	4.634217
C	-5.69387	3.959421	-0.51402	C	-5.67485	3.934915	-0.43246
C	-8.17975	2.643538	0.479349	C	-8.16242	2.562436	0.473785
C	-5.52697	-2.5308	-2.75255	C	-5.41796	-2.46954	-2.90041
O	-1.79339	-3.74311	1.491121	O	-1.71281	-3.78745	1.337174
O	-1.39382	-4.05439	-2.23856	O	-1.26293	-3.96208	-2.3912
C	1.745662	-2.81387	1.36459	C	1.814417	-2.79782	1.289435
O	-0.42065	-1.45245	-3.11226	O	-0.32124	-1.31879	-3.16724
H	2.111598	1.778665	0.058794	H	2.129222	1.843508	0.131398
H	-2.155	-1.0212	0.96292	H	-2.10308	-1.05189	0.901464
H	4.911508	-1.61364	-0.66728	H	4.99348	-1.47948	-0.67586
H	-3.62808	2.143024	-0.33624	H	-3.59253	2.13083	-0.27976
H	-3.22467	-2.69727	-1.24487	H	-3.12408	-2.66214	-1.37795
H	0.974183	0.371953	-2.38356	H	1.037046	0.496382	-2.36504
H	-1.3992	1.390911	-1.24188	H	-1.36165	1.445756	-1.21551
H	1.195395	0.26703	1.703578	H	1.220061	0.265615	1.718528
H	6.087662	-0.26509	-2.26854	H	6.171898	-0.08085	-2.22284
H	4.765654	1.452272	-1.98509	H	4.807362	1.612496	-1.9107
H	6.718885	2.91283	-0.39782	H	6.722474	3.066926	-0.27332
H	3.787597	3.135816	0.366431	H	3.787993	3.223832	0.474111
H	-0.47519	3.885209	-1.46596	H	-0.47161	3.956353	-1.34506
H	0.712288	3.477702	-0.25131	H	0.723469	3.53357	-0.14297
H	0.832708	5.848349	-1.36536	H	0.805631	5.937091	-1.19082
H	1.383512	5.023864	-2.8169	H	1.368916	5.161236	-2.66433
H	2.770388	5.086473	-0.07231	H	2.754141	5.172969	0.081492
H	3.255767	5.993987	-1.50223	H	3.228072	6.120863	-1.32585
H	7.024556	-0.70967	1.22254	H	7.068618	-0.61695	1.268502
H	5.234047	-0.15456	2.99631	H	5.276905	-0.09162	3.034122
H	6.243783	-3.1088	0.654684	H	6.526149	-2.99515	0.786876
H	4.825525	-2.78239	1.631645	H	4.883013	-2.74865	1.359126
H	6.417119	-4.09322	2.846598	H	5.754358	-2.27133	3.657222
H	8.71566	-3.38949	3.418475	H	6.324255	-4.62867	4.193297
H	8.512264	-3.46629	1.663444	H	5.000762	-4.55474	3.020191
H	8.533751	-1.90115	2.49209	H	6.637524	-4.9585	2.48395
H	6.685211	-2.88951	4.932325	H	8.11973	-2.85411	4.224673
H	5.15808	-2.37172	4.209897	H	8.075	-1.47232	3.129695
H	6.594697	-1.32433	4.143338	H	8.487116	-3.07753	2.510268
H	8.288258	-1.36652	-2.27133	H	8.389717	-1.15118	-2.20948

H	7.009005	-2.4854	-1.79909	H	7.118064	-2.29589	-1.7783
H	8.111959	-1.83351	-0.58021	H	8.191277	-1.65057	-0.53002
H	9.138064	0.360926	-0.03719	H	9.183649	0.551553	0.053691
H	9.232591	0.863357	-1.7178	H	9.282345	1.091277	-1.61517
H	8.979091	2.075477	-0.45335	H	8.997569	2.271542	-0.32757
H	4.860048	3.09581	-3.26096	H	4.873176	3.285053	-3.15003
H	3.261925	3.722695	-3.68927	H	3.27275	3.912794	-3.56745
H	4.577188	4.836457	-3.30569	H	4.578934	5.024519	-3.14821
H	-5.64863	2.123314	-1.58447	H	-5.5935	2.138924	-1.56698
H	-5.75019	-0.08127	-1.57337	H	-5.68203	-0.06669	-1.63775
H	-7.92482	-0.08734	0.383971	H	-7.88217	-0.15984	0.285668
H	-6.34368	-2.14314	0.627457	H	-6.27838	-2.21234	0.481133
H	-3.84167	-5.09756	1.50487	H	-3.74564	-5.16522	1.279072
H	-4.65679	-3.57046	1.214335	H	-4.57422	-3.63736	1.033324
H	-4.78126	-5.95346	-0.40786	H	-4.6509	-5.96304	-0.67534
H	-3.92377	-4.79174	-1.38207	H	-3.80122	-4.75374	-1.59687
H	-6.4304	-4.80822	-1.72871	H	-6.30458	-4.79256	-1.968
H	-6.65578	-4.33833	-0.04601	H	-6.55119	-4.38629	-0.27158
H	-5.29477	2.752236	1.994336	H	-5.32651	2.615565	2.039855
H	-4.32701	0.831689	3.393888	H	-4.29928	0.66697	3.374921
H	-3.19991	3.944282	1.361746	H	-3.16666	3.796993	1.329385
H	-2.27063	2.471014	1.636235	H	-2.28277	2.386936	1.89154
H	-2.90004	2.540343	4.062307	H	-2.16704	4.19157	3.470738
H	-1.35829	4.397988	4.642466	H	-4.09518	5.185678	4.650443
H	-0.74877	3.489974	3.248397	H	-4.26154	5.415276	2.904816
H	-1.52149	5.064656	3.012418	H	-5.22341	4.184344	3.739333
H	-4.11641	5.28085	3.3968	H	-4.01171	2.158687	4.82433
H	-3.85199	4.643696	5.024408	H	-2.76579	3.149014	5.561598
H	-5.02743	3.872161	3.95942	H	-2.29967	1.852656	4.45342
H	-6.50853	4.385428	-1.10664	H	-6.48732	4.373611	-1.01879
H	-4.75364	4.312937	-0.94969	H	-4.73378	4.313707	-0.84449
H	-5.77022	4.376937	0.494792	H	-5.76662	4.313992	0.589875
H	-7.88615	3.322345	1.289508	H	-7.88943	3.212445	1.314218
H	-8.57812	3.274961	-0.32479	H	-8.55298	3.220437	-0.31266
H	-8.99614	2.015608	0.846067	H	-8.97921	1.914108	0.802163
H	-6.36313	-2.84591	-3.39067	H	-6.24373	-2.77011	-3.55879
H	-5.29415	-1.49054	-2.98169	H	-5.19363	-1.41951	-3.08999
H	-4.66389	-3.134	-3.06006	H	-4.54547	-3.05301	-3.21918
H	-0.7464	-4.75174	-2.01124	H	-0.60737	-4.65688	-2.18007
H	2.509657	-3.3936	0.838107	H	2.585954	-3.35993	0.754953
H	2.220607	-1.97192	1.872791	H	2.280104	-1.96728	1.824197
H	1.304114	-3.47446	2.118377	H	1.369663	-3.48037	2.021599

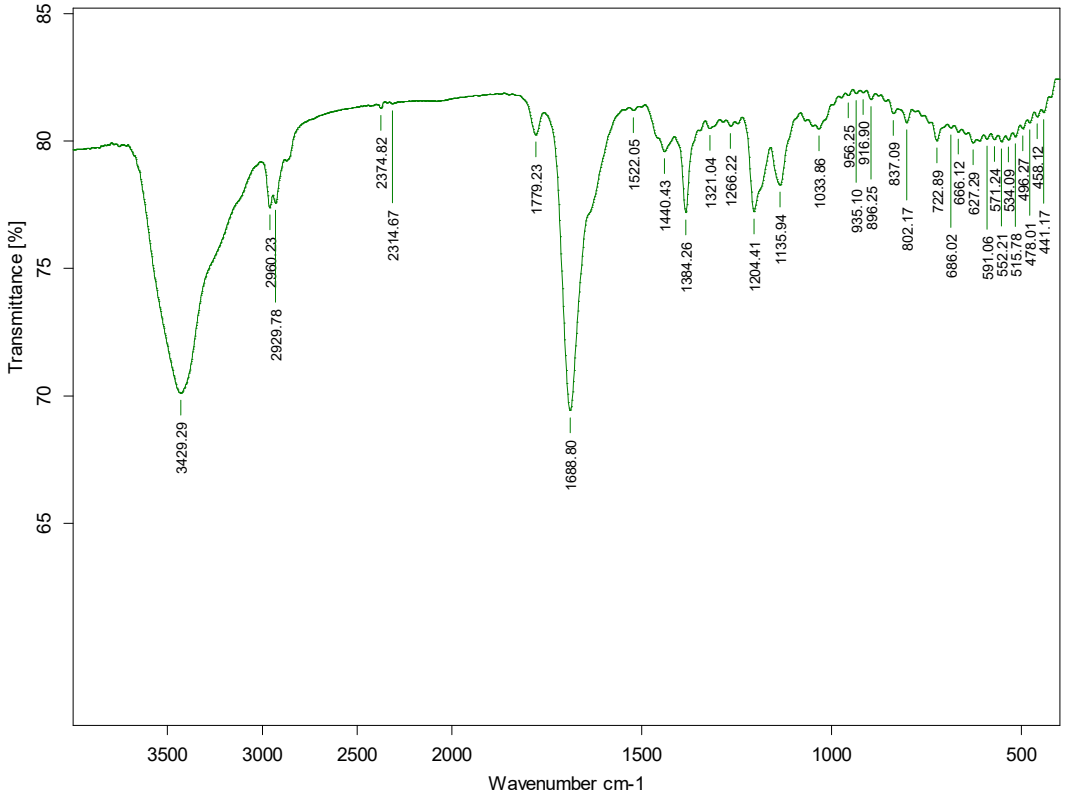
HRESIMS of compound 1



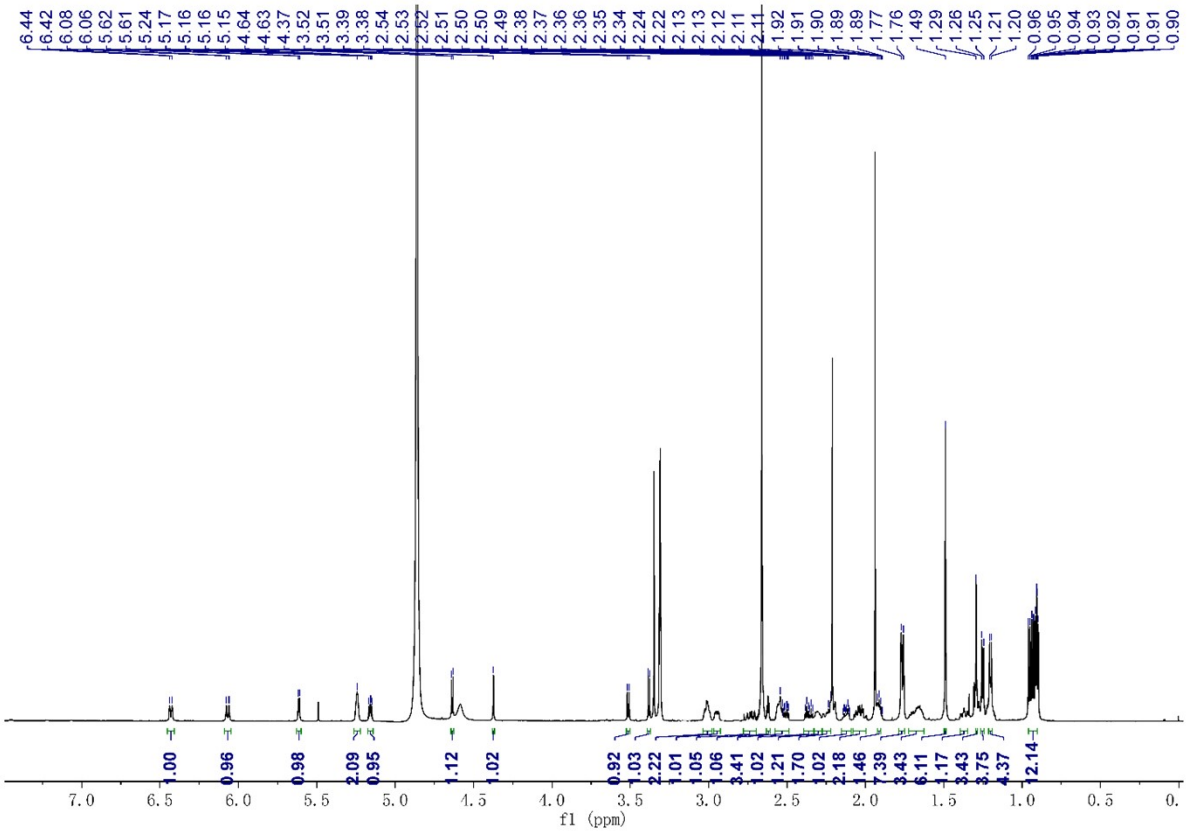
UV spectrum of compound 1



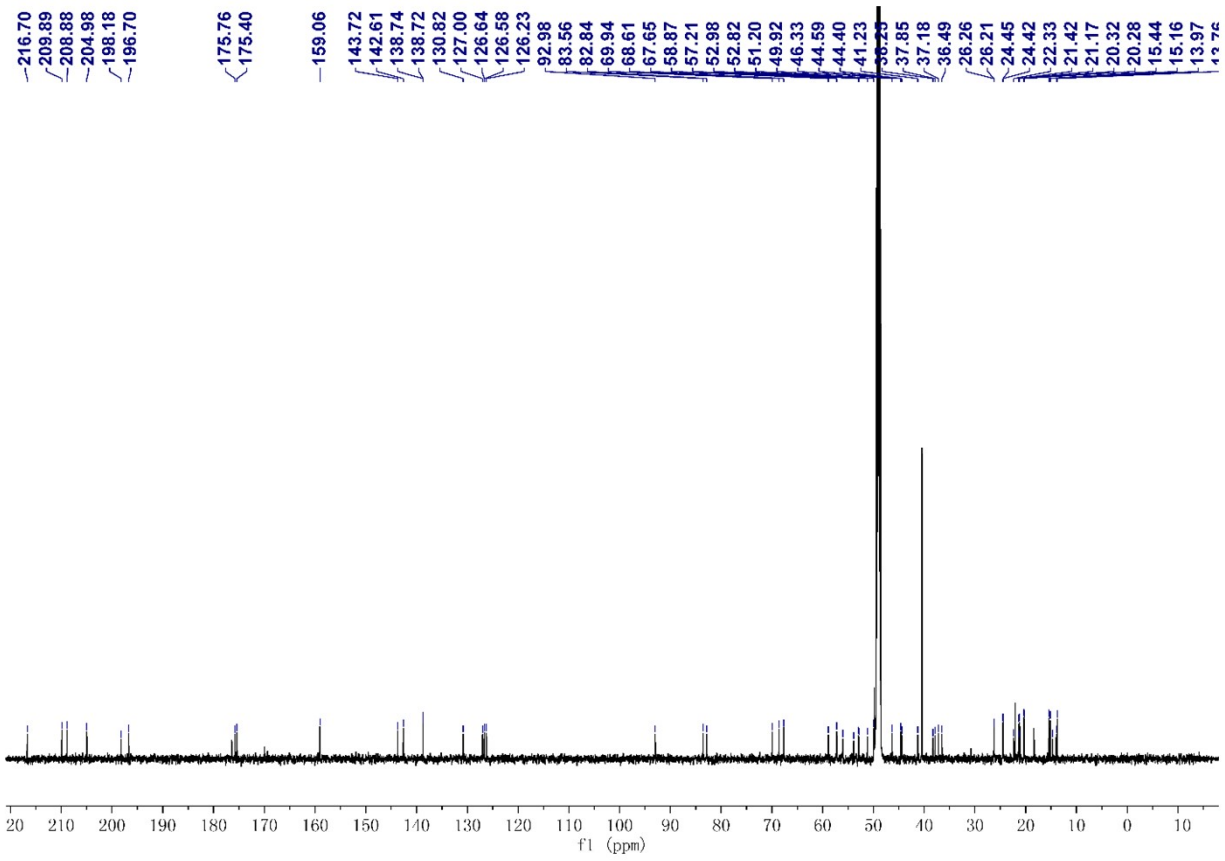
IR spectrum of compound 1



^{1}H NMR of compound 1

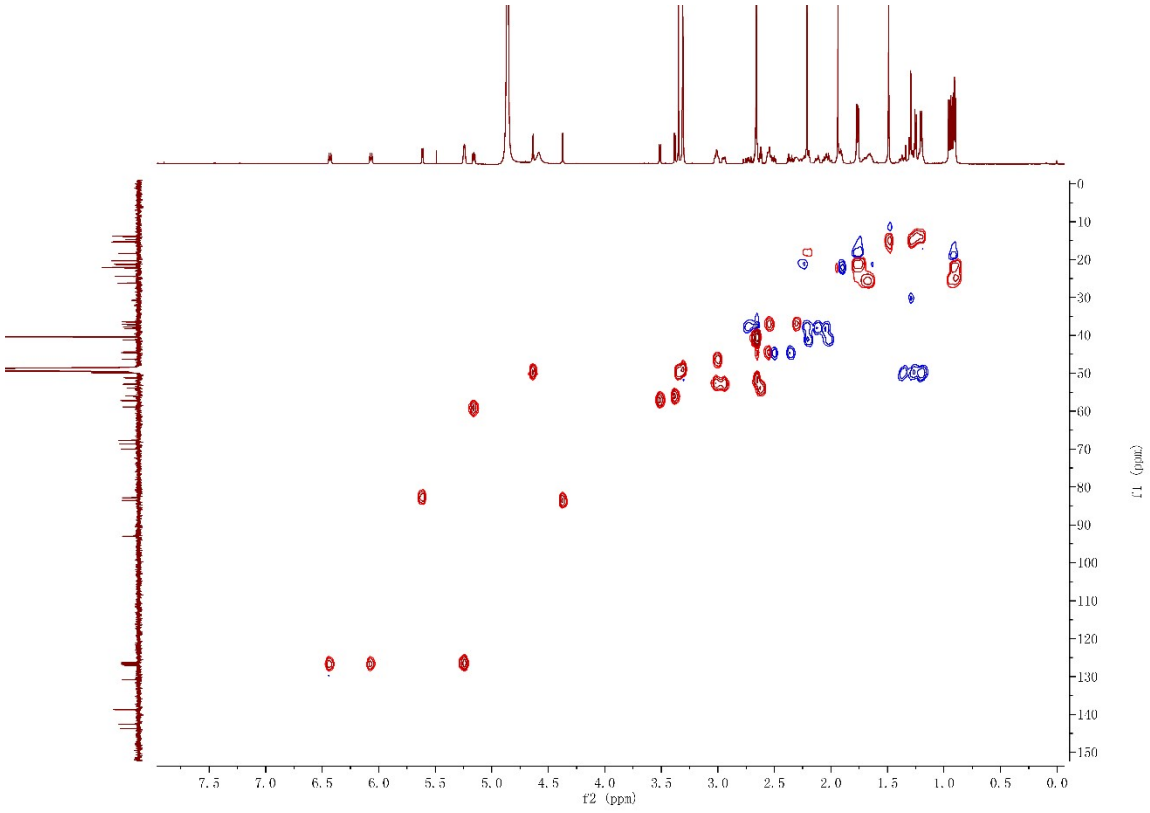


^{13}C NMR of compound 1

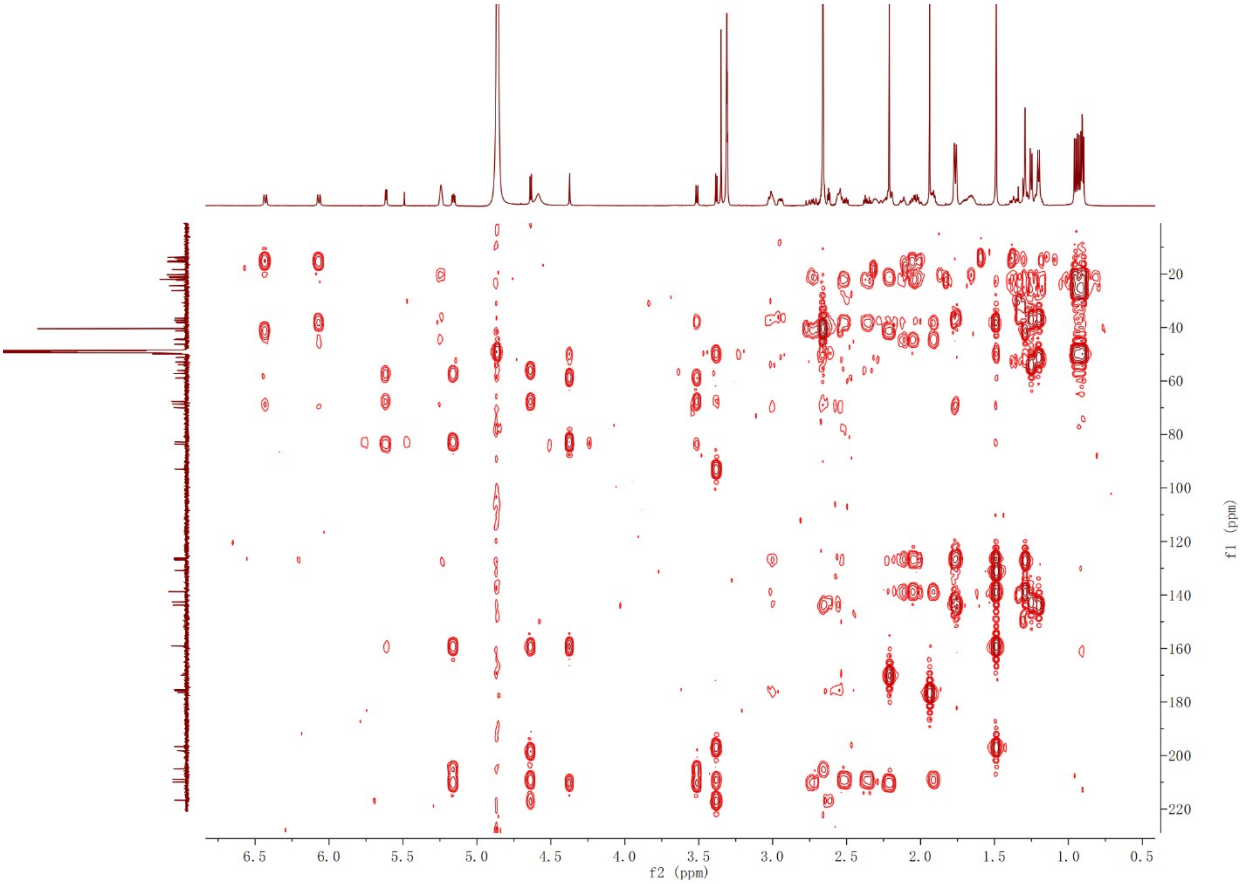


HS

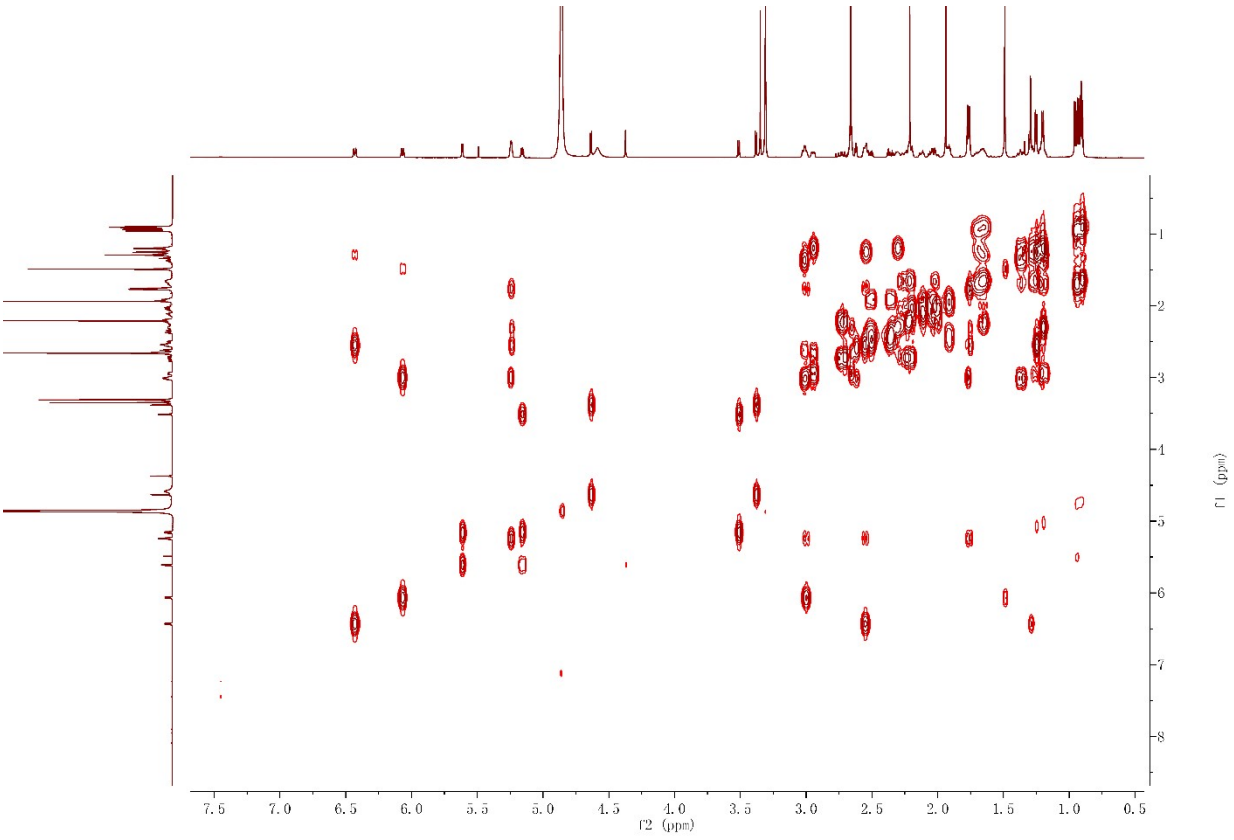
QC of compound 1



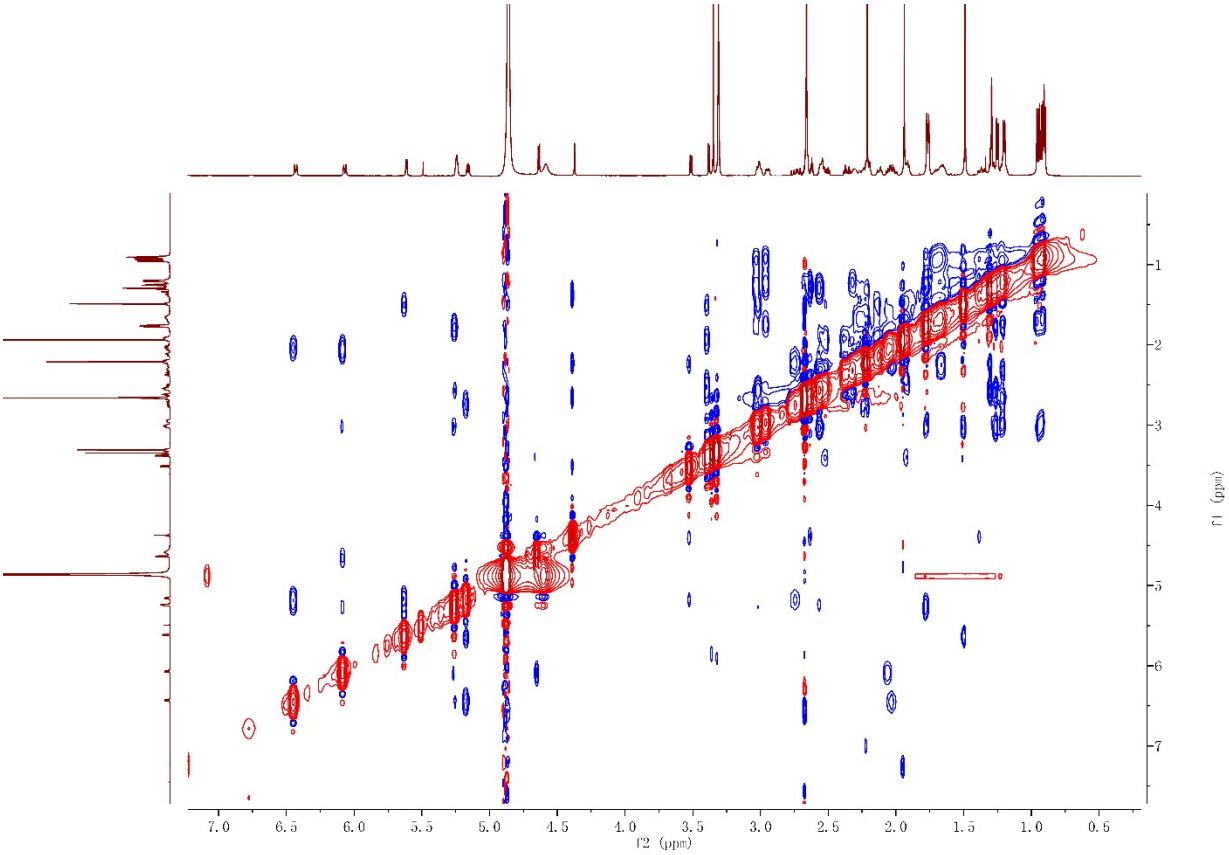
HMBC of compound 1



$^{1}H-^{1}H$ COSY of compound 1

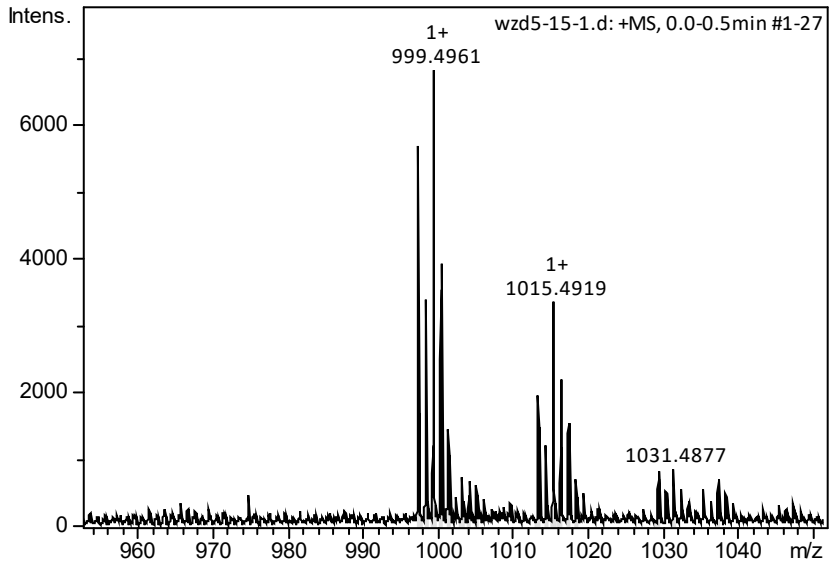


NOESY of compound 1

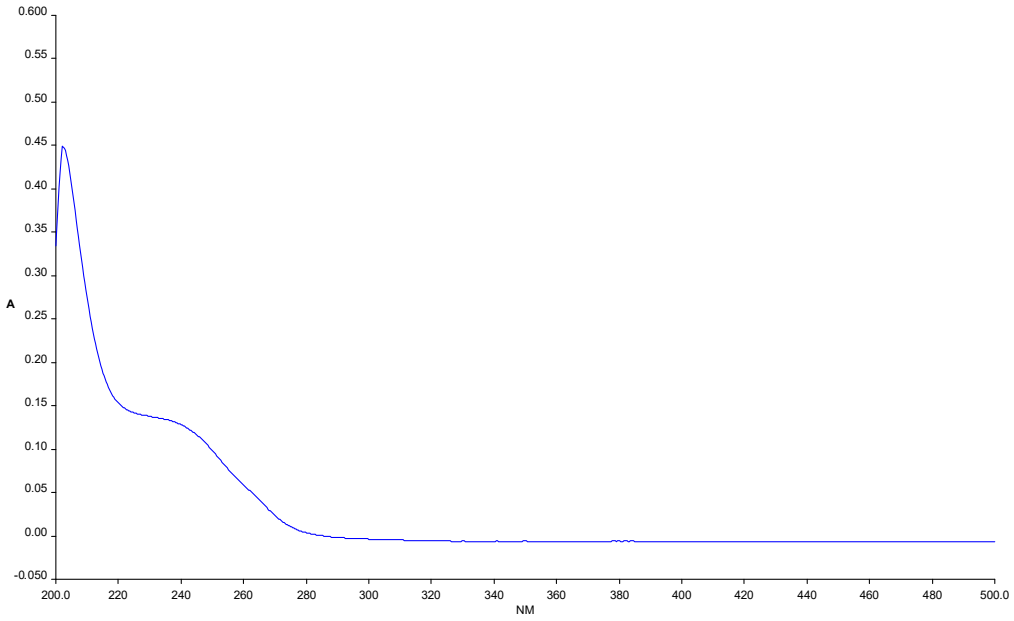


HRE

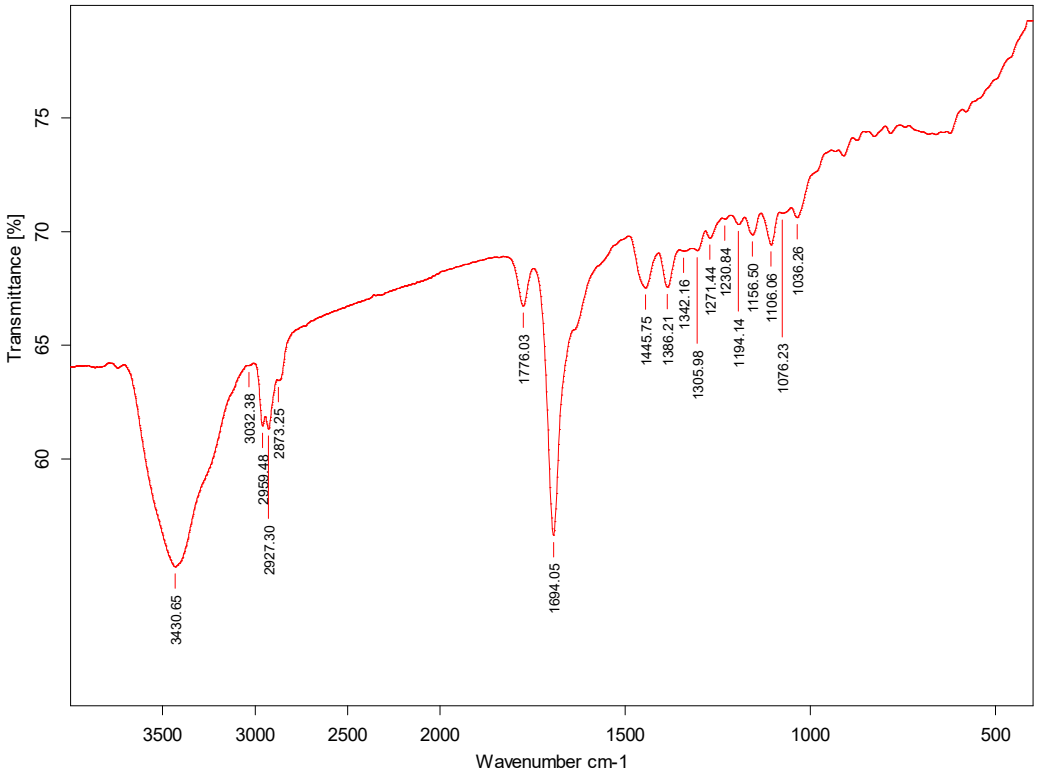
SIMS of compound 2



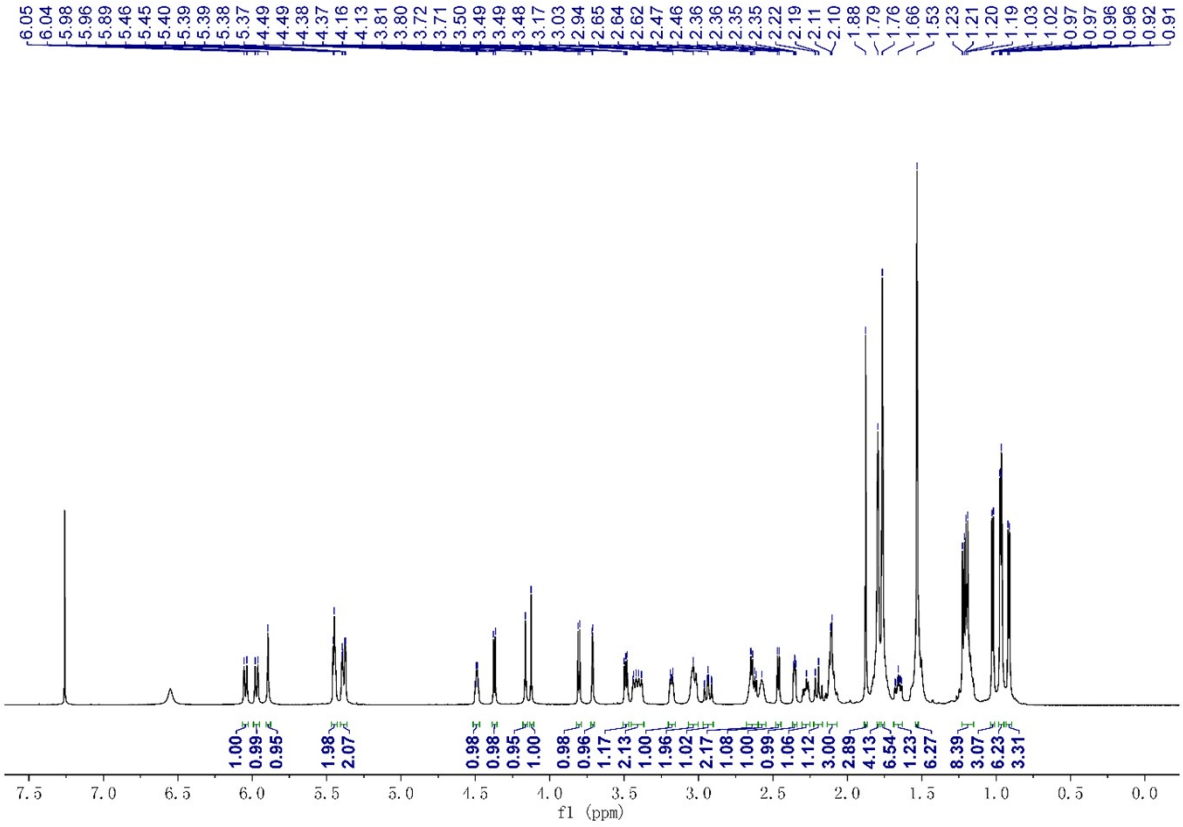
UV spectrum of compound 2



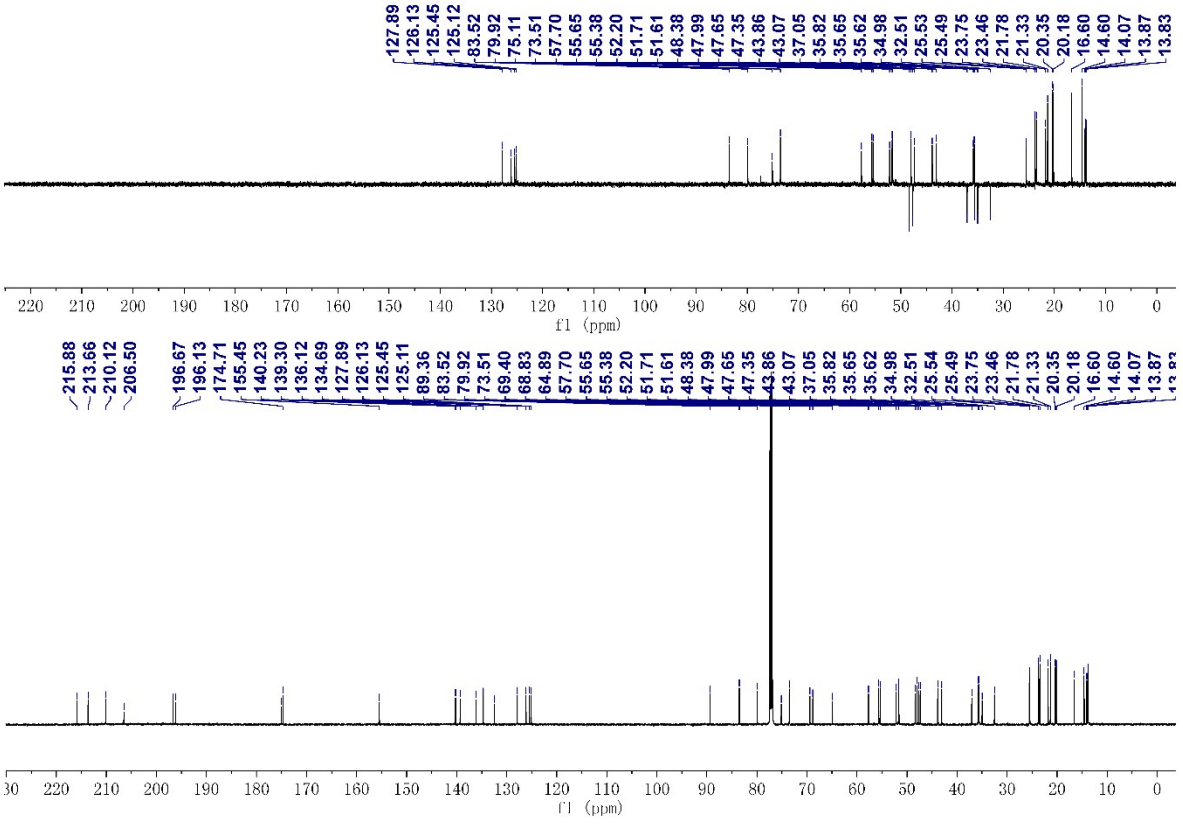
IR spectrum of compound 2



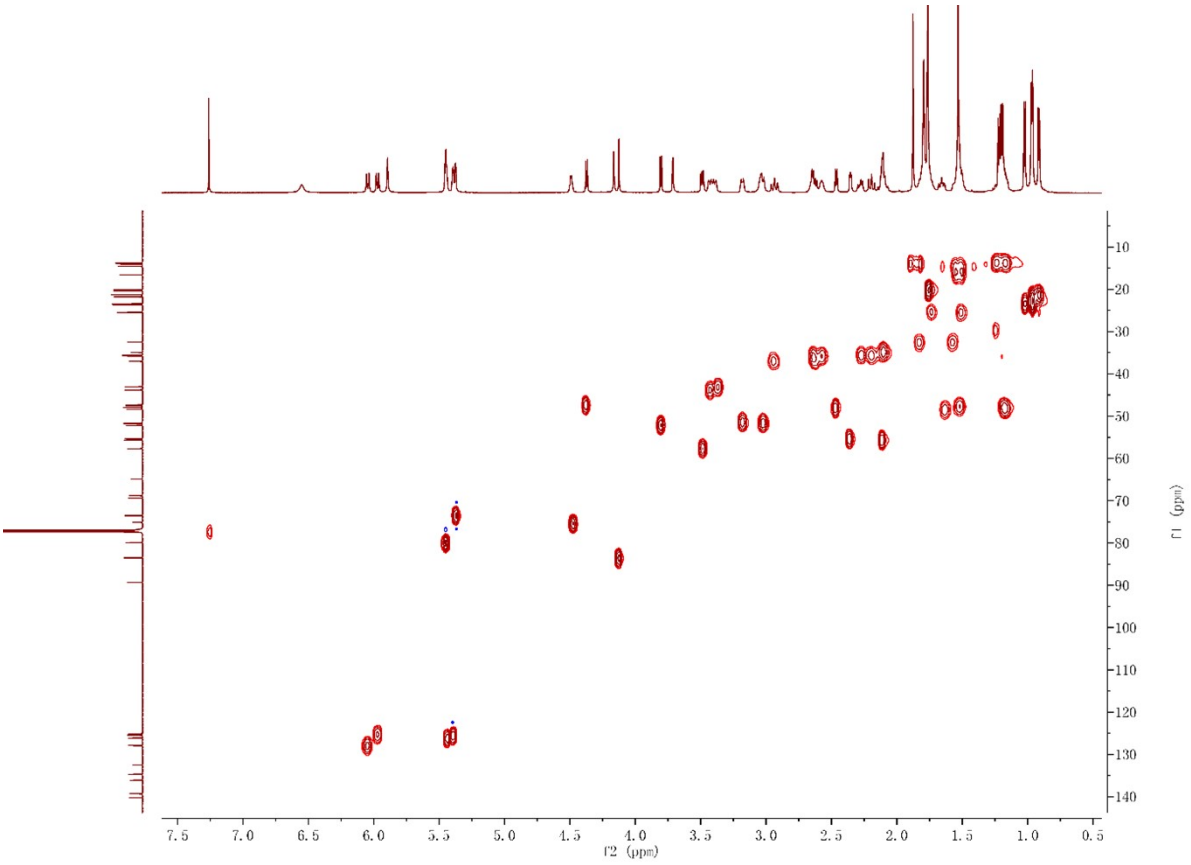
^{1}H NMR of compound 2



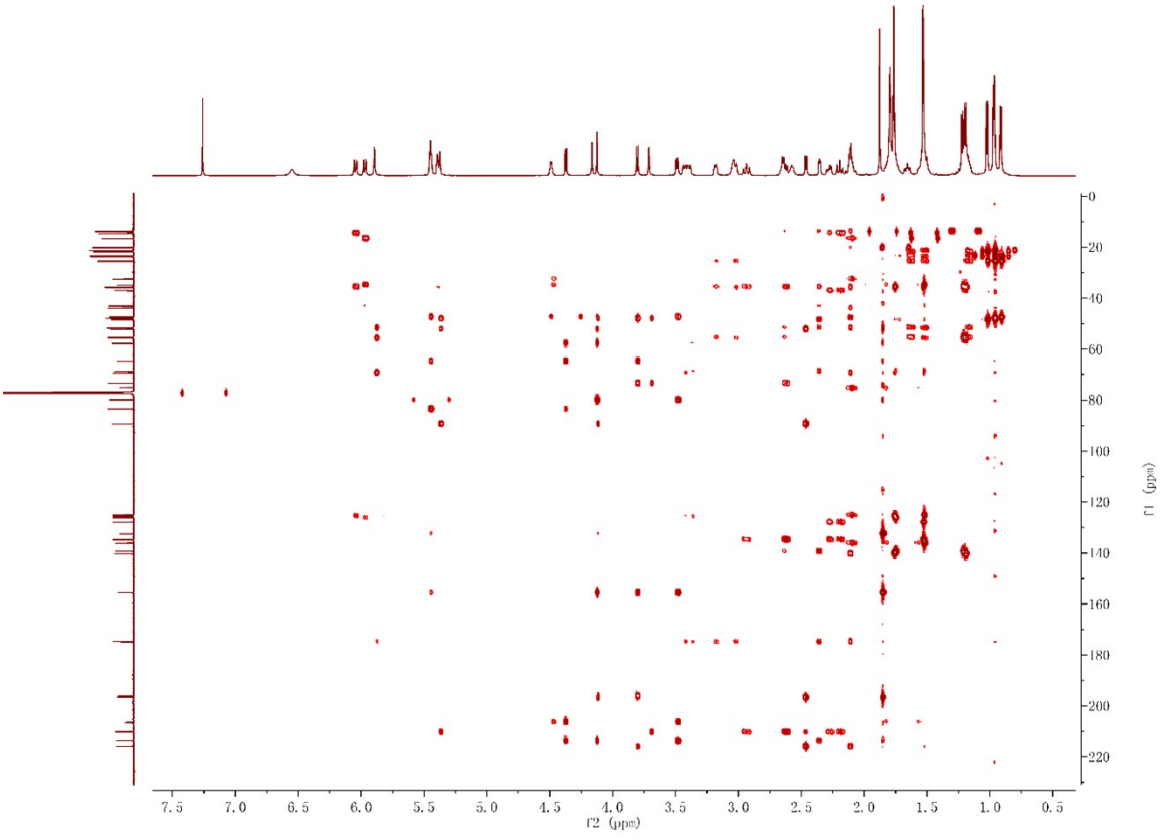
^{13}C NMR and DEPT of compound 2



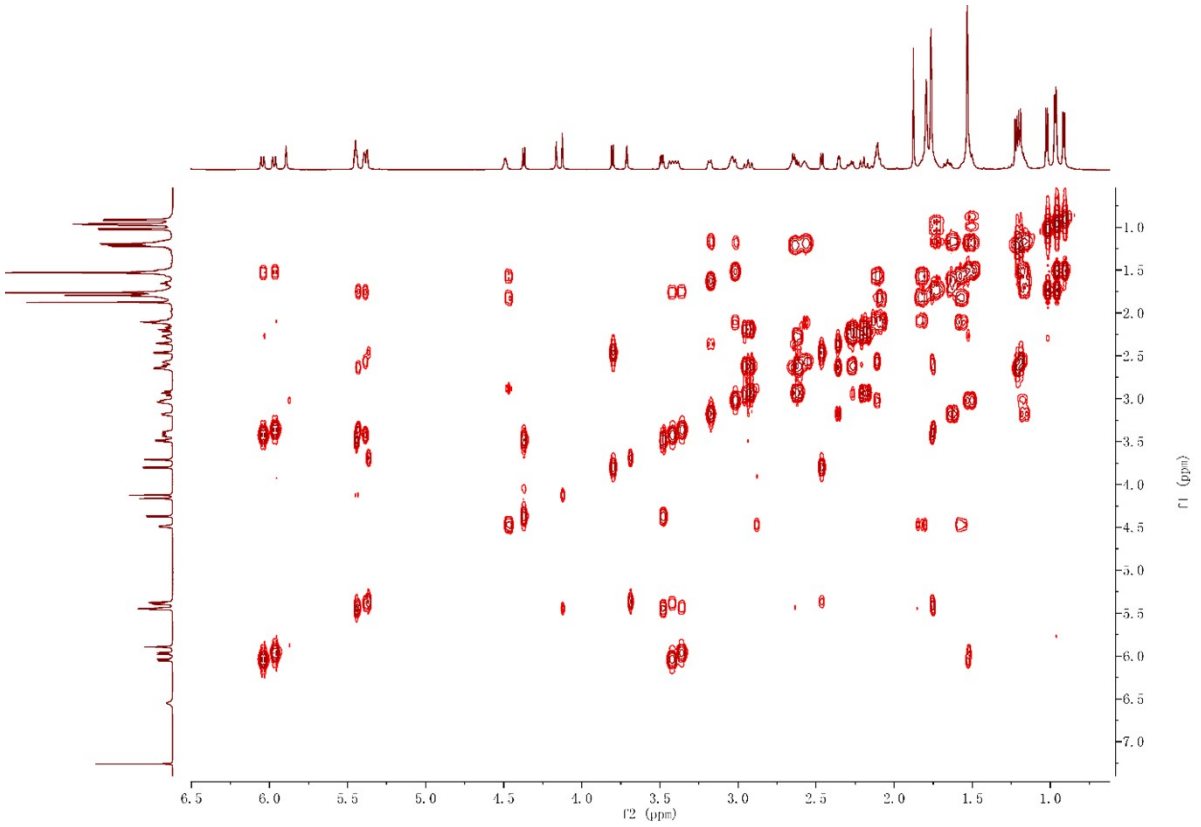
HSQC of compound 2



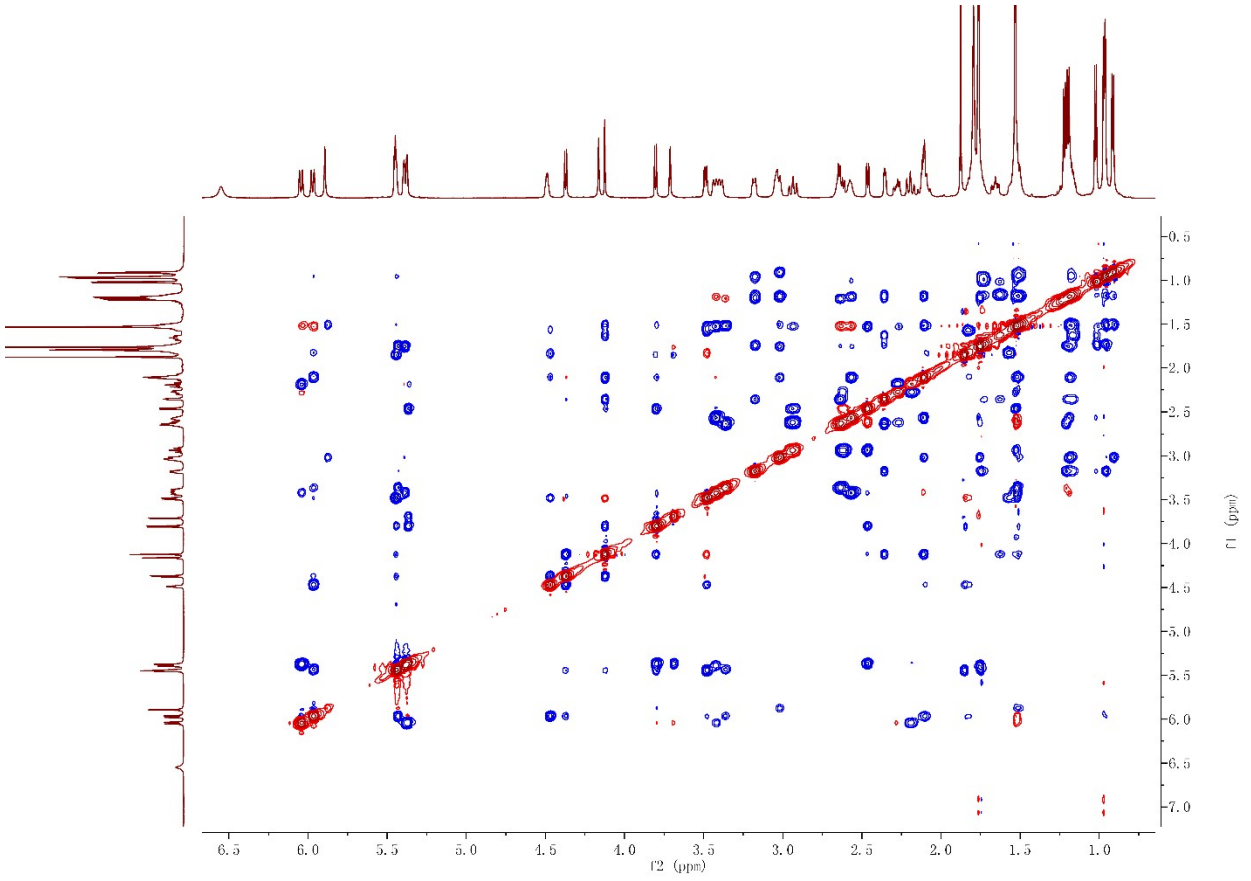
HMBC of compound 2



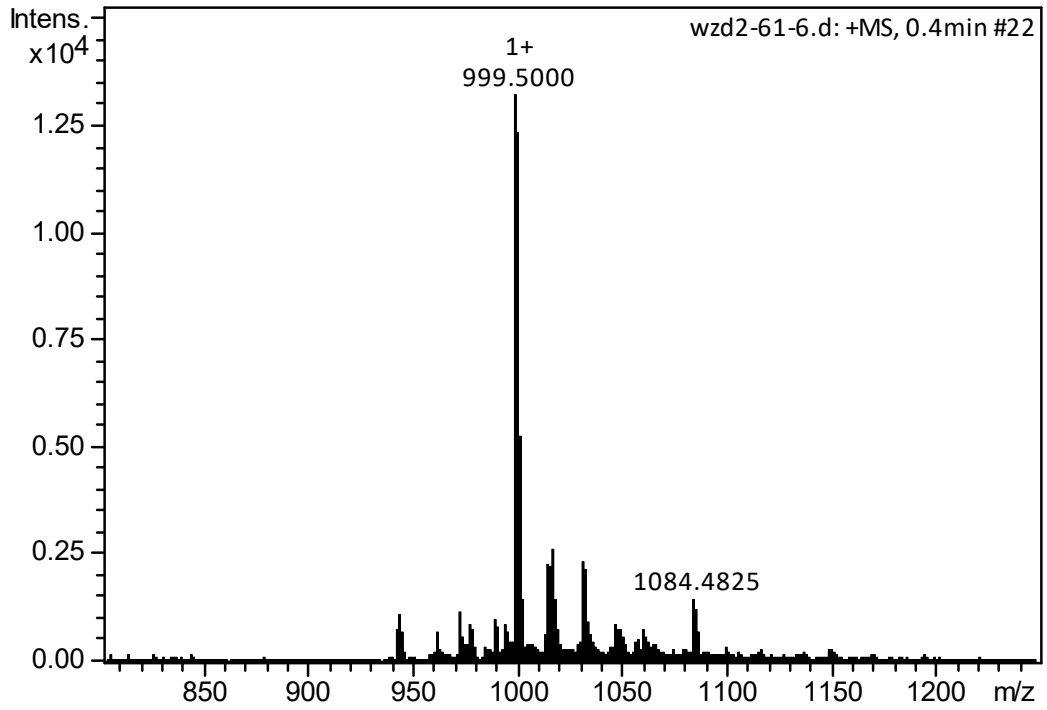
$^{1}H-^{1}H$ COSY of compound 2



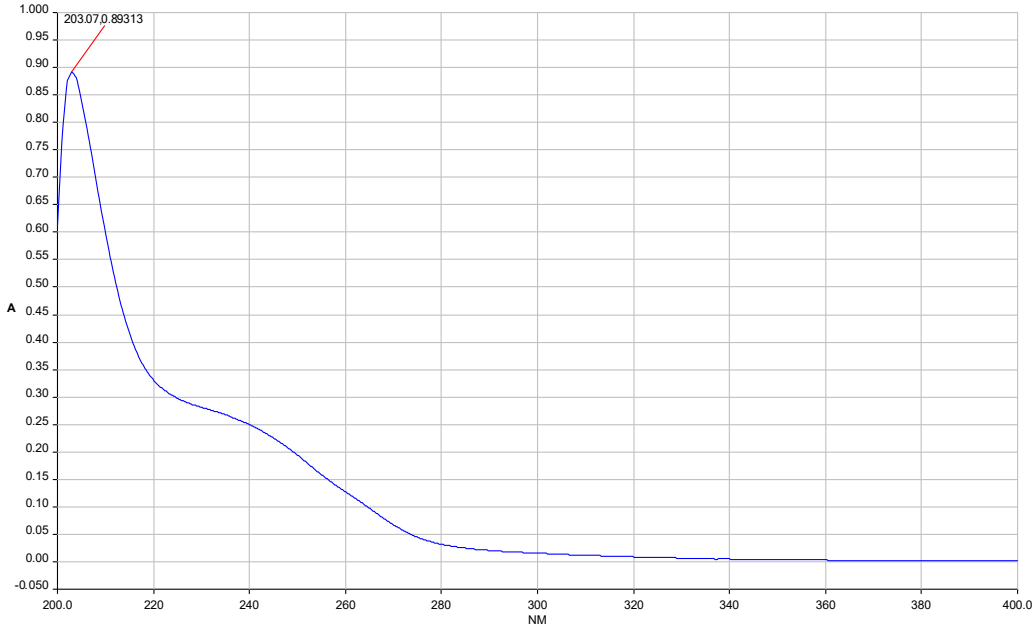
ROESY of compound 2



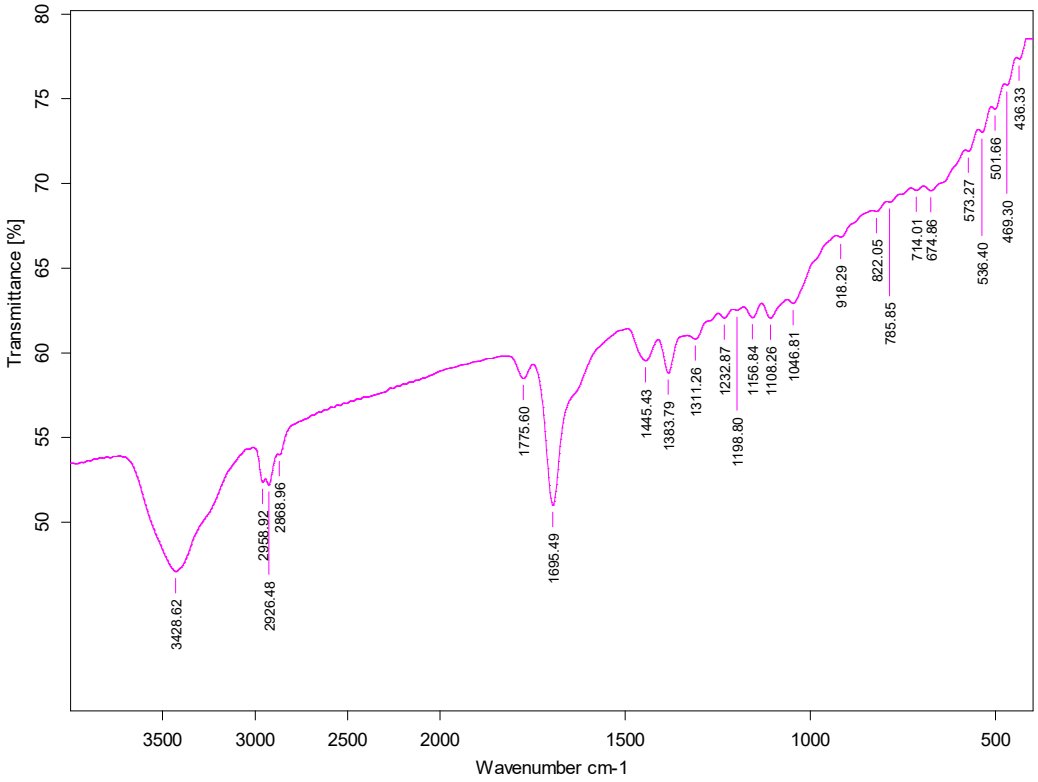
HRESIMS of compound 3



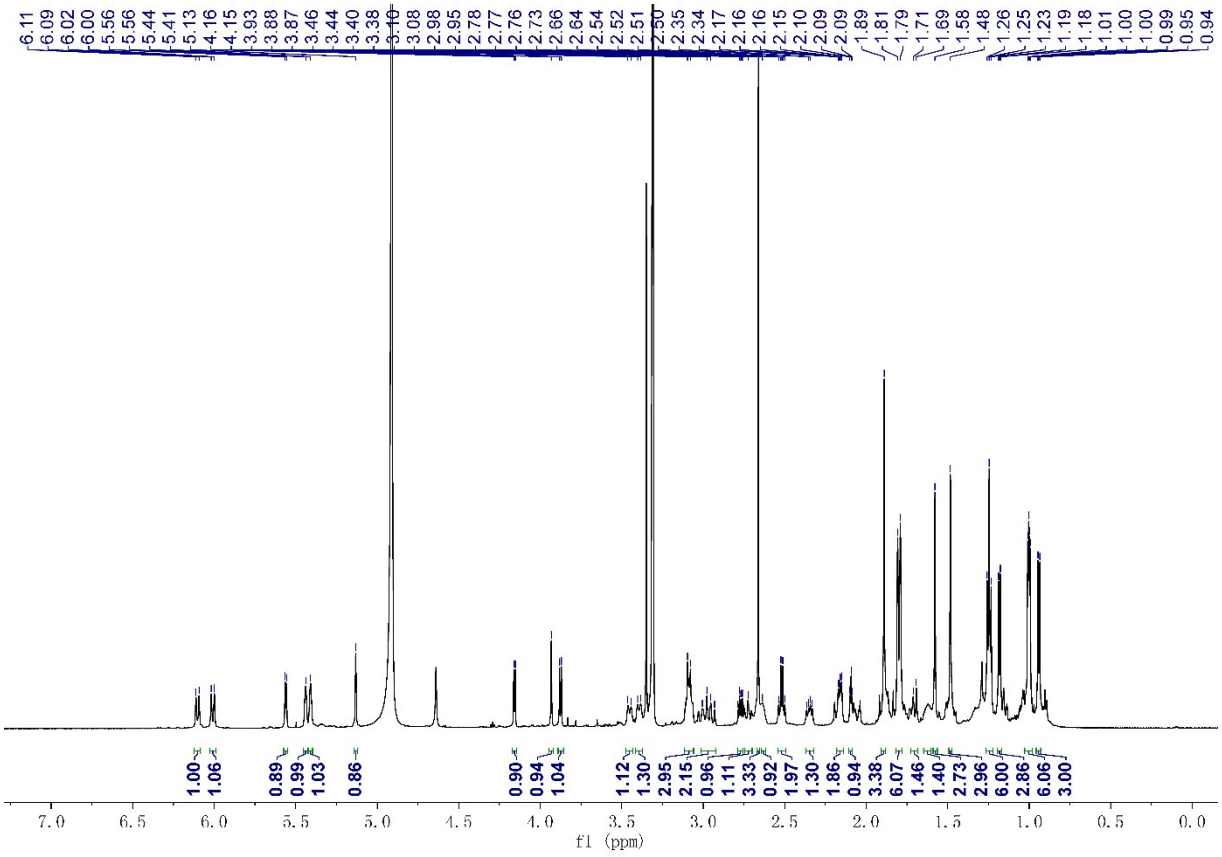
UV spectrum of compound 3



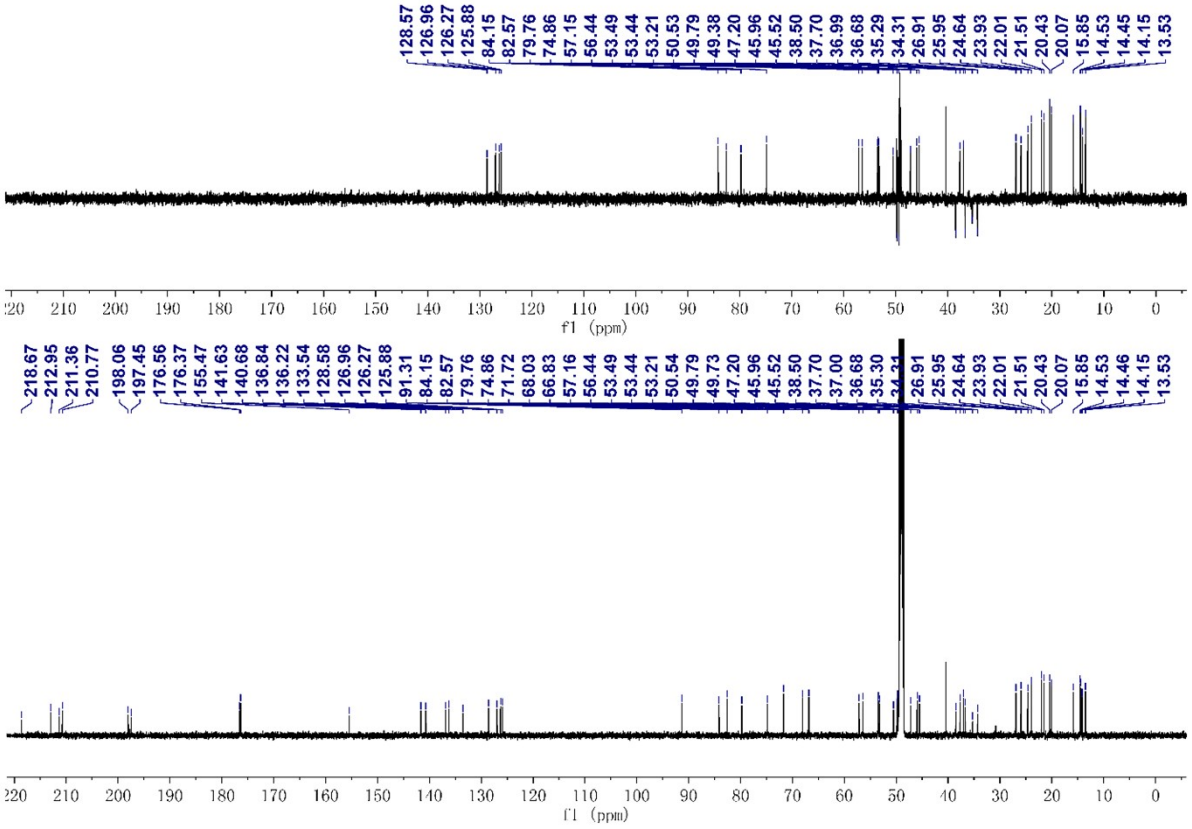
IR spectrum of compound 3



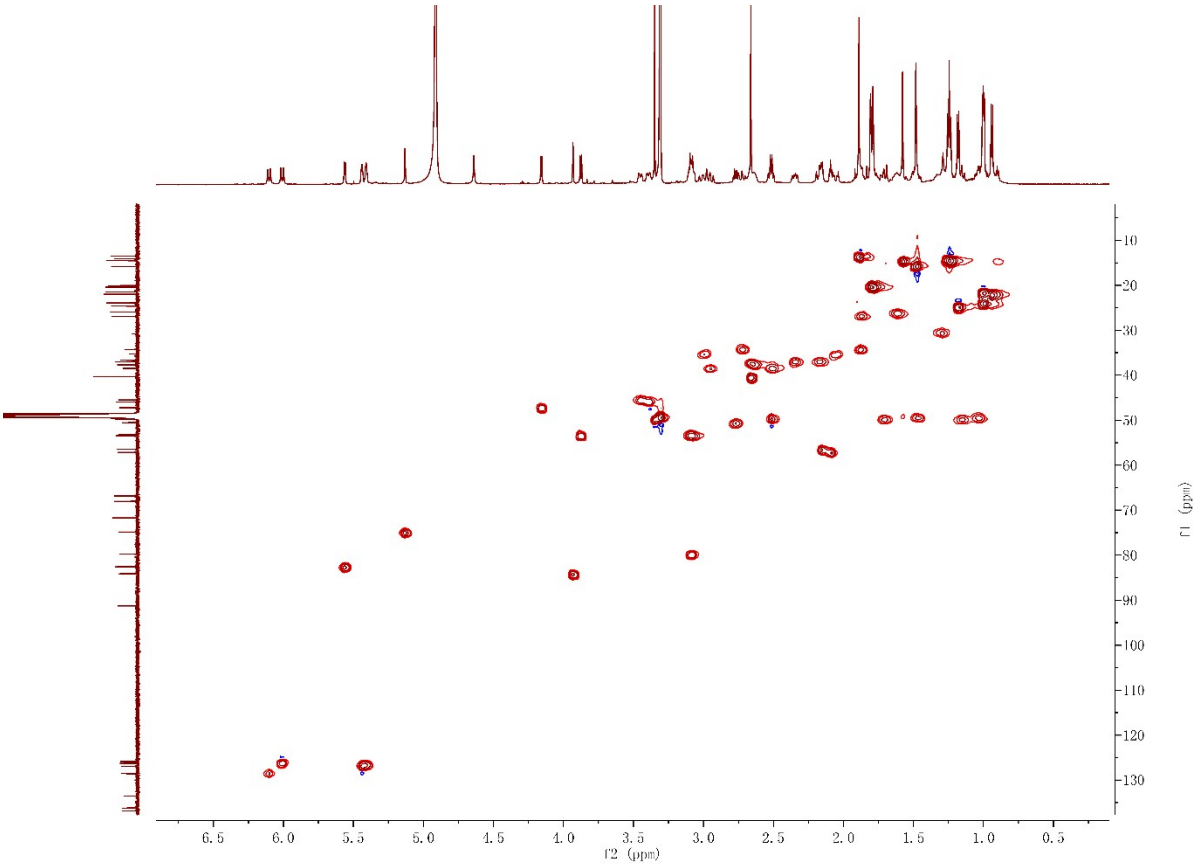
^{1}H NMR of compound 3



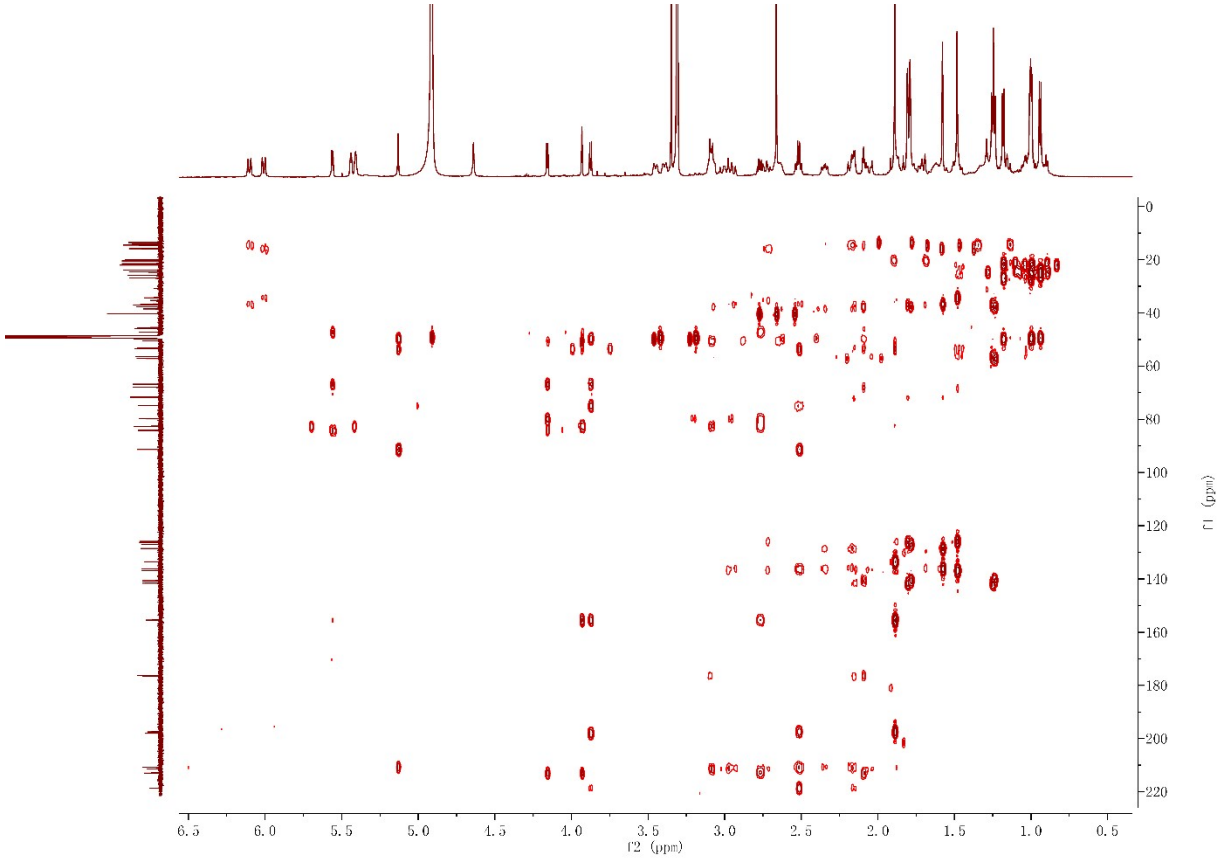
^{13}C NMR and DEPT of compound 3



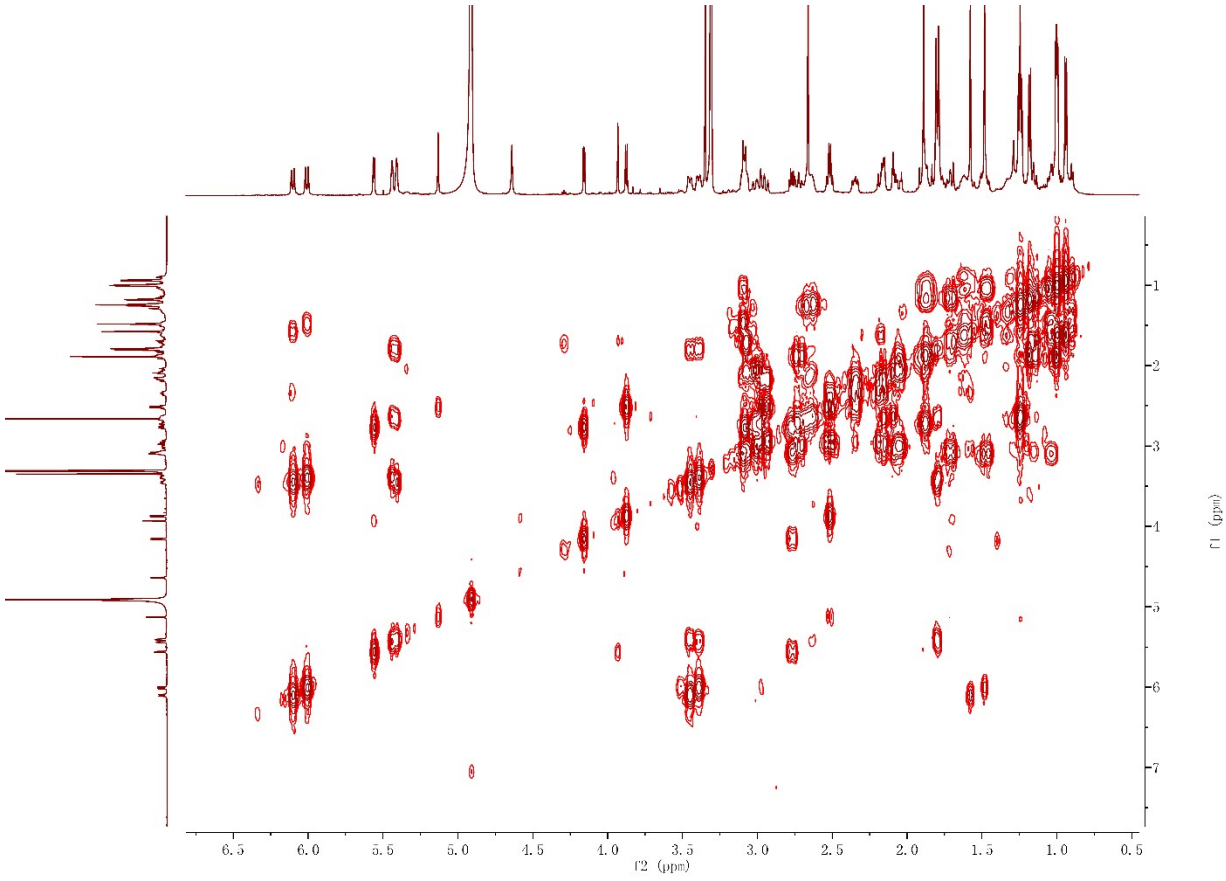
HSQC of compound 3



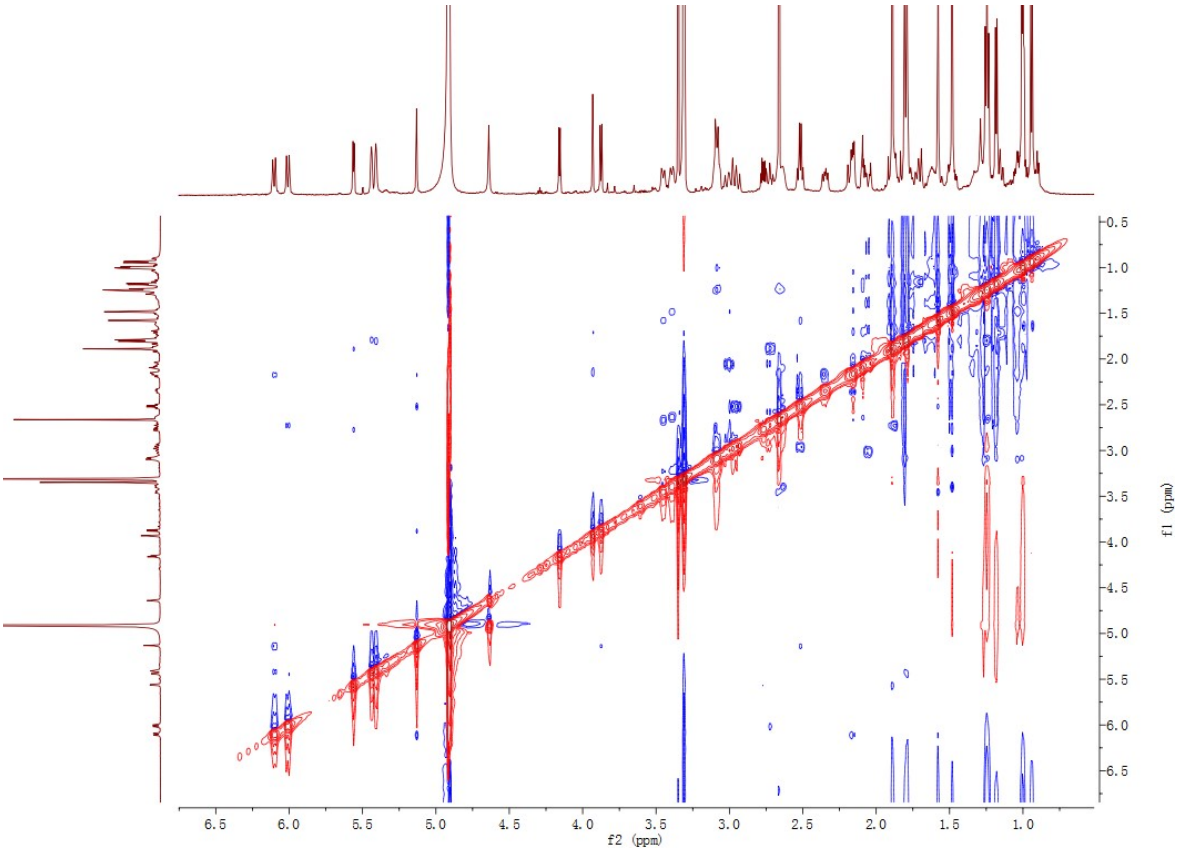
HMBC of compound 3



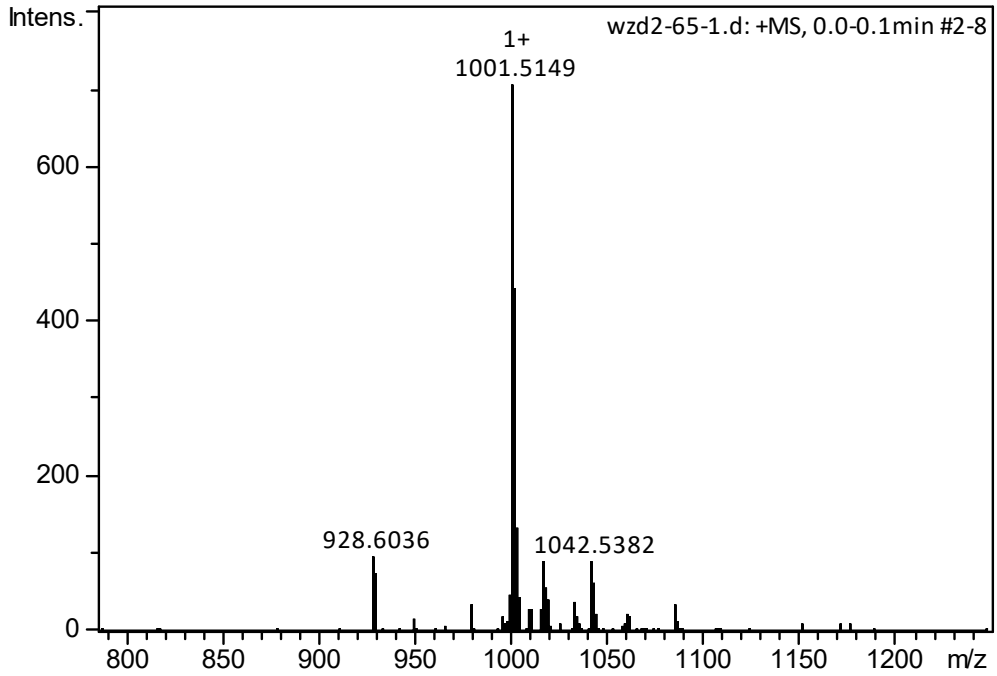
$^{1}H-^{1}H$ COSY of compound 3



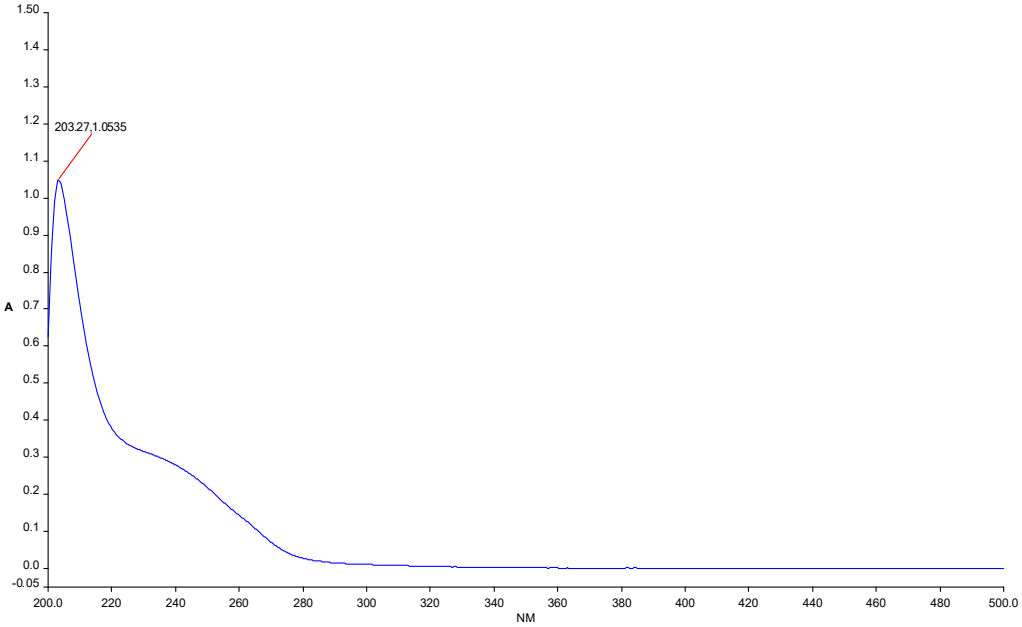
ROESY of compound 3



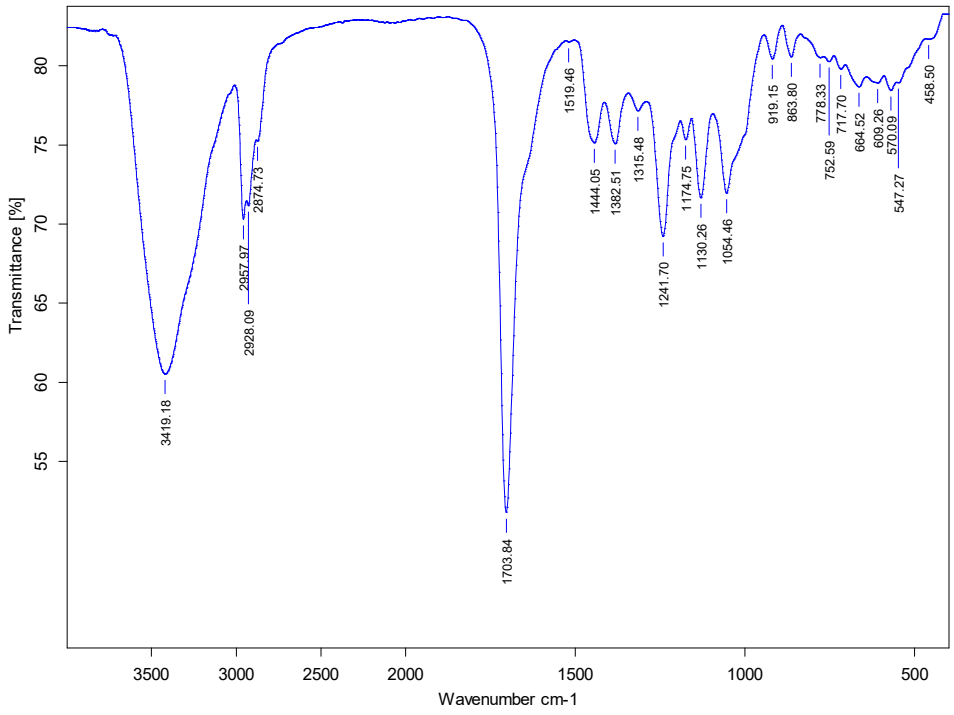
HRESIMS of compound 4



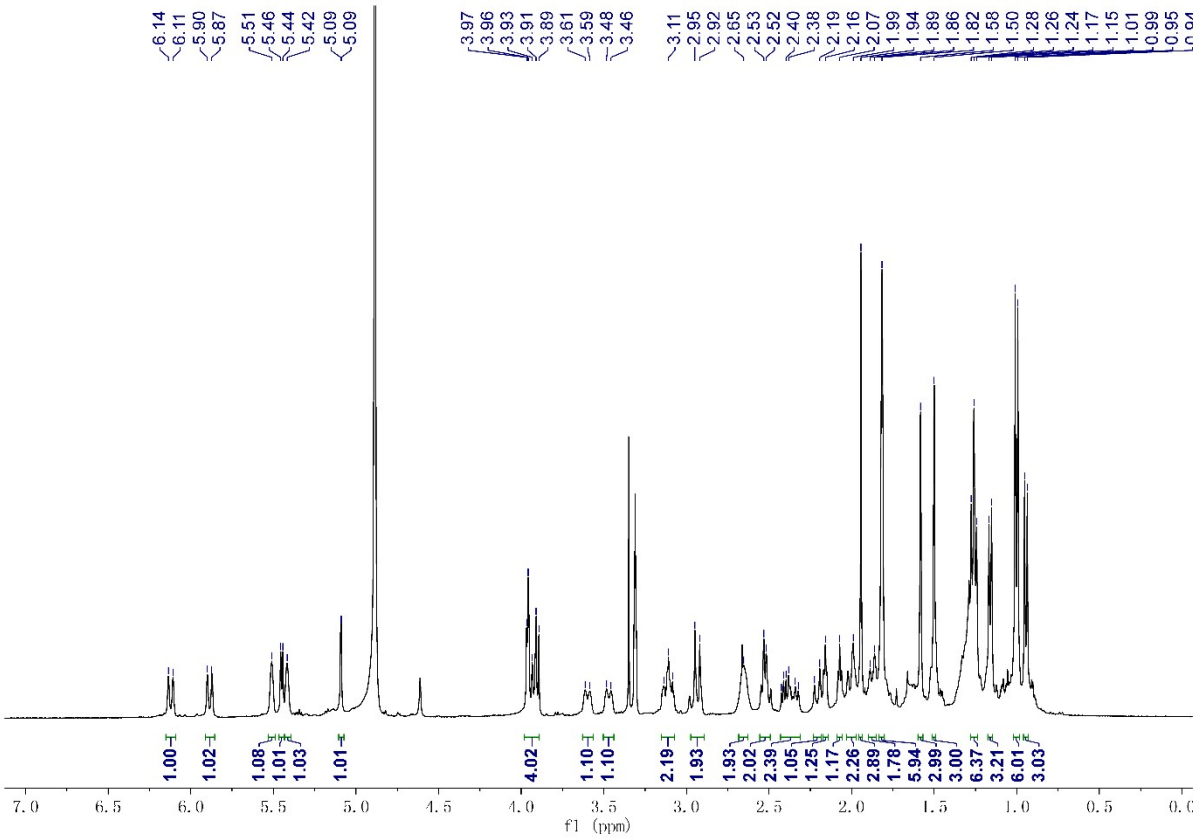
UV spectrum of compound 4



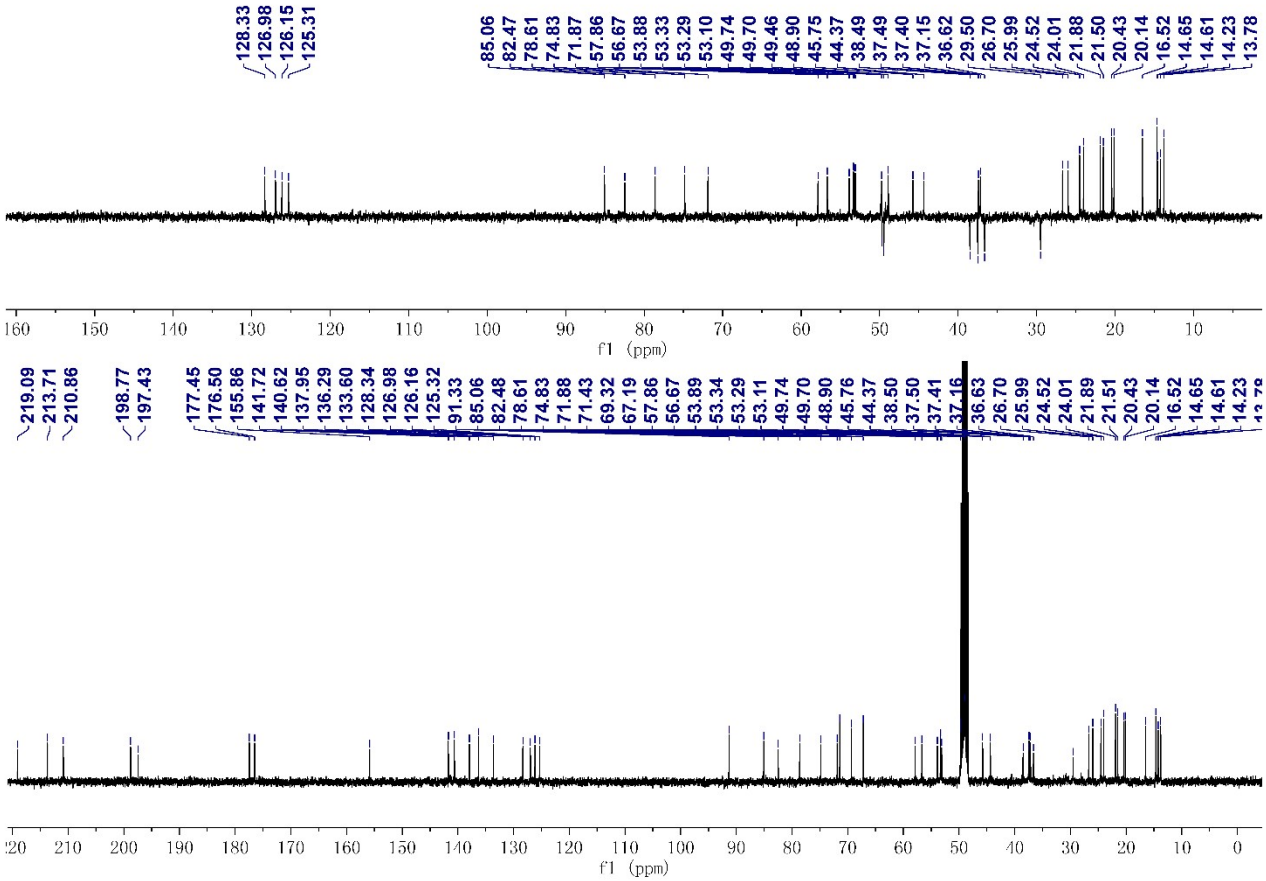
IR spectrum of compound 4



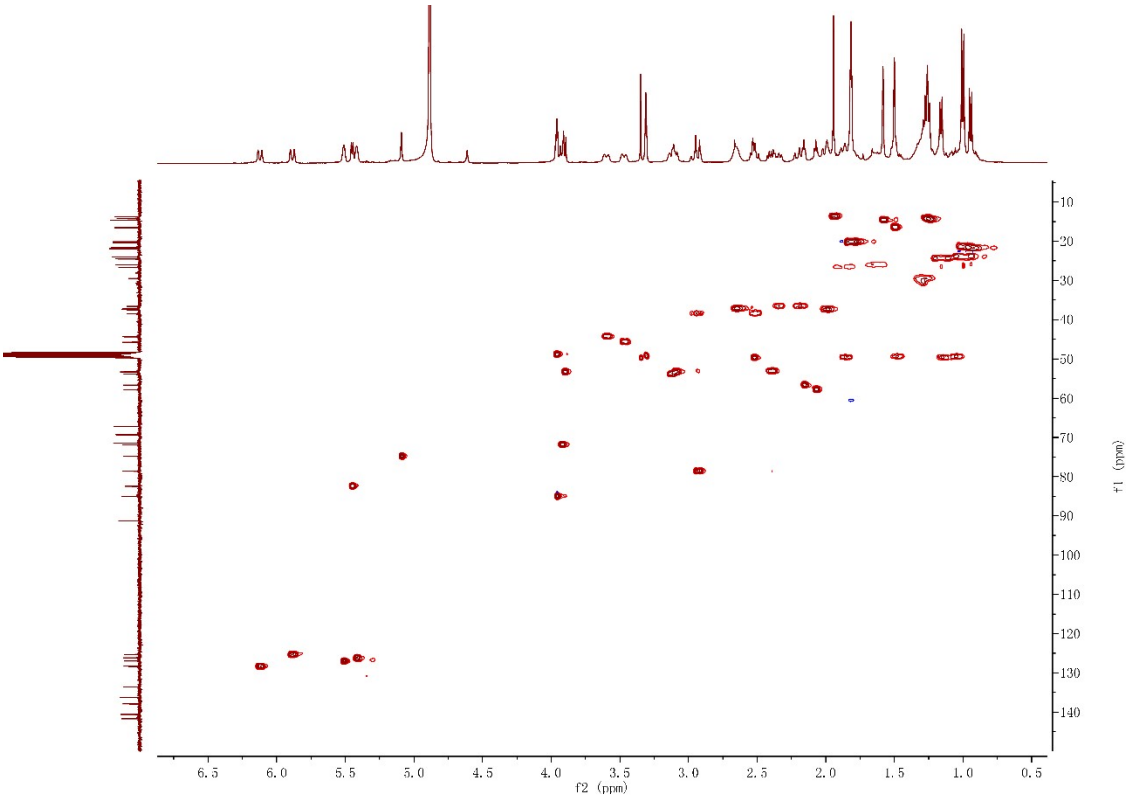
^{1}H NMR of compound 4



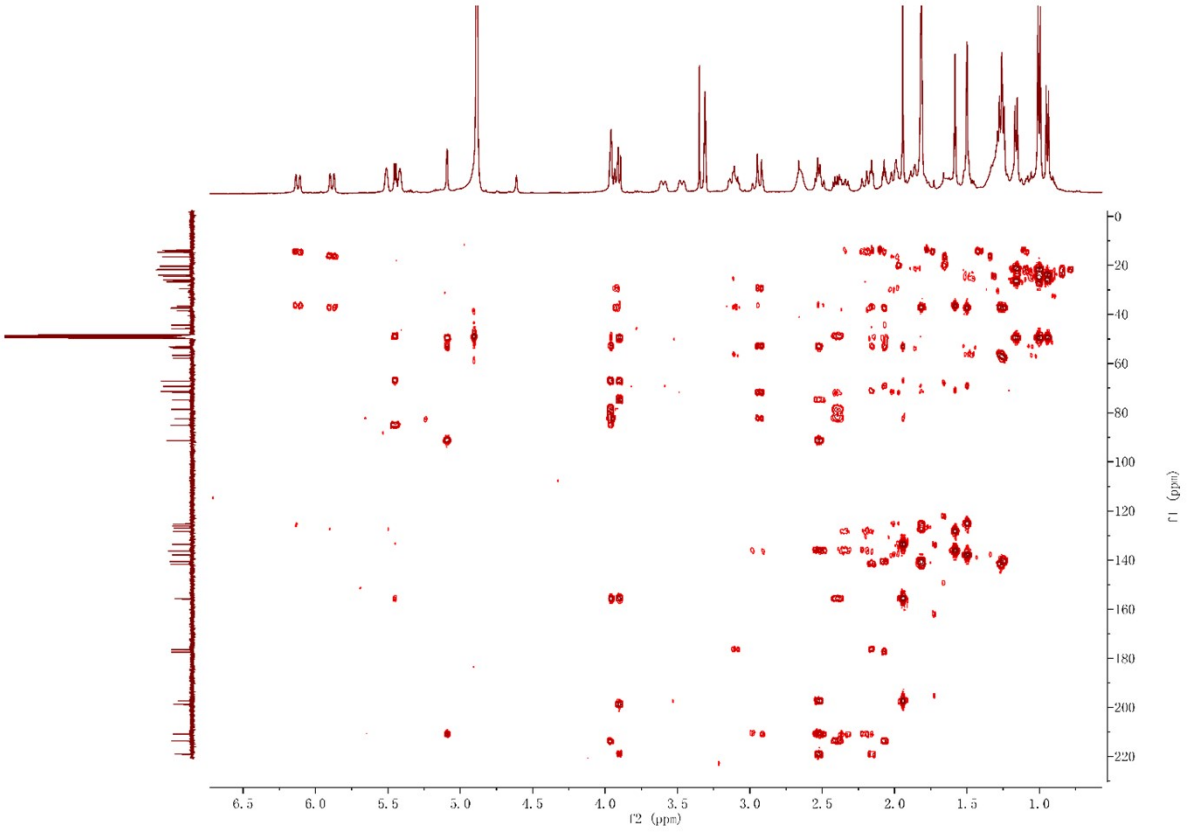
^{13}C NMR and DEPT of compound 4



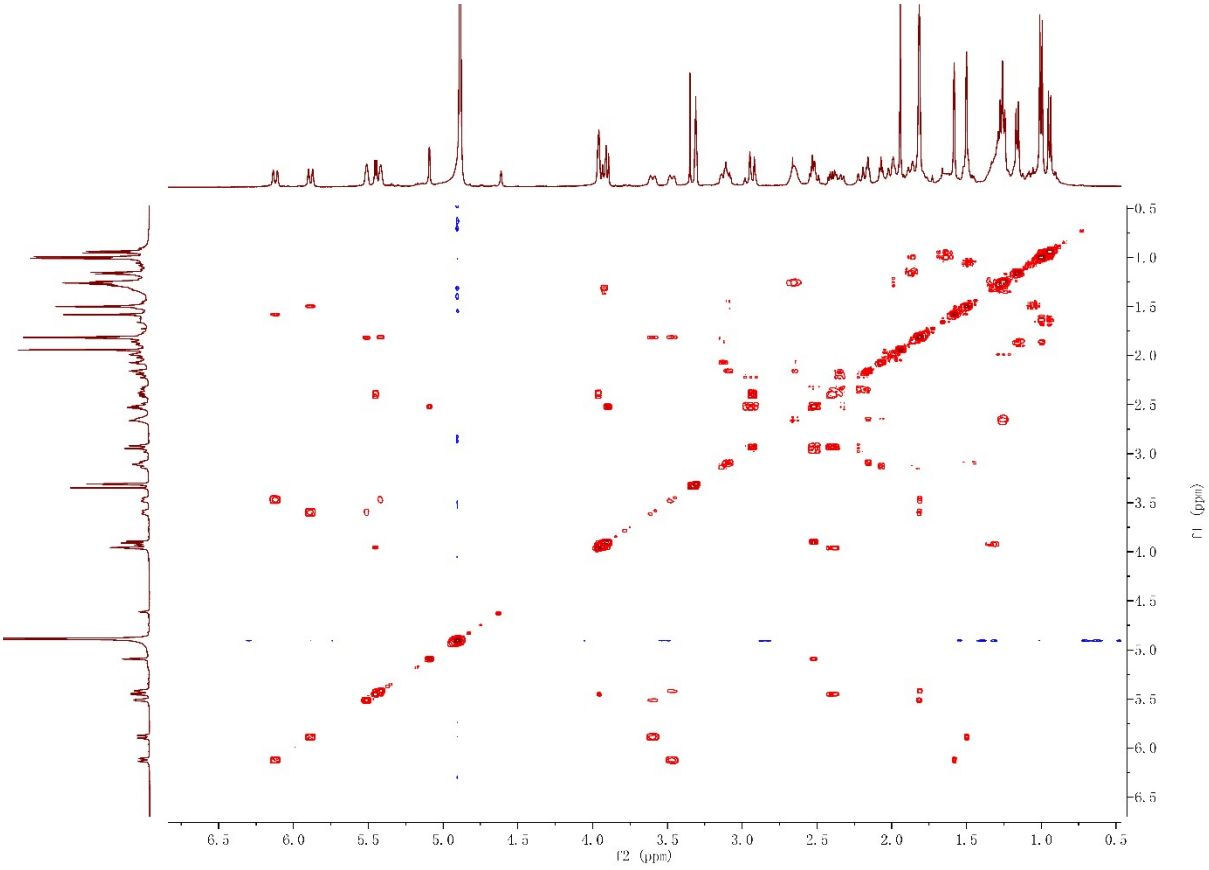
HSQC of compound 4



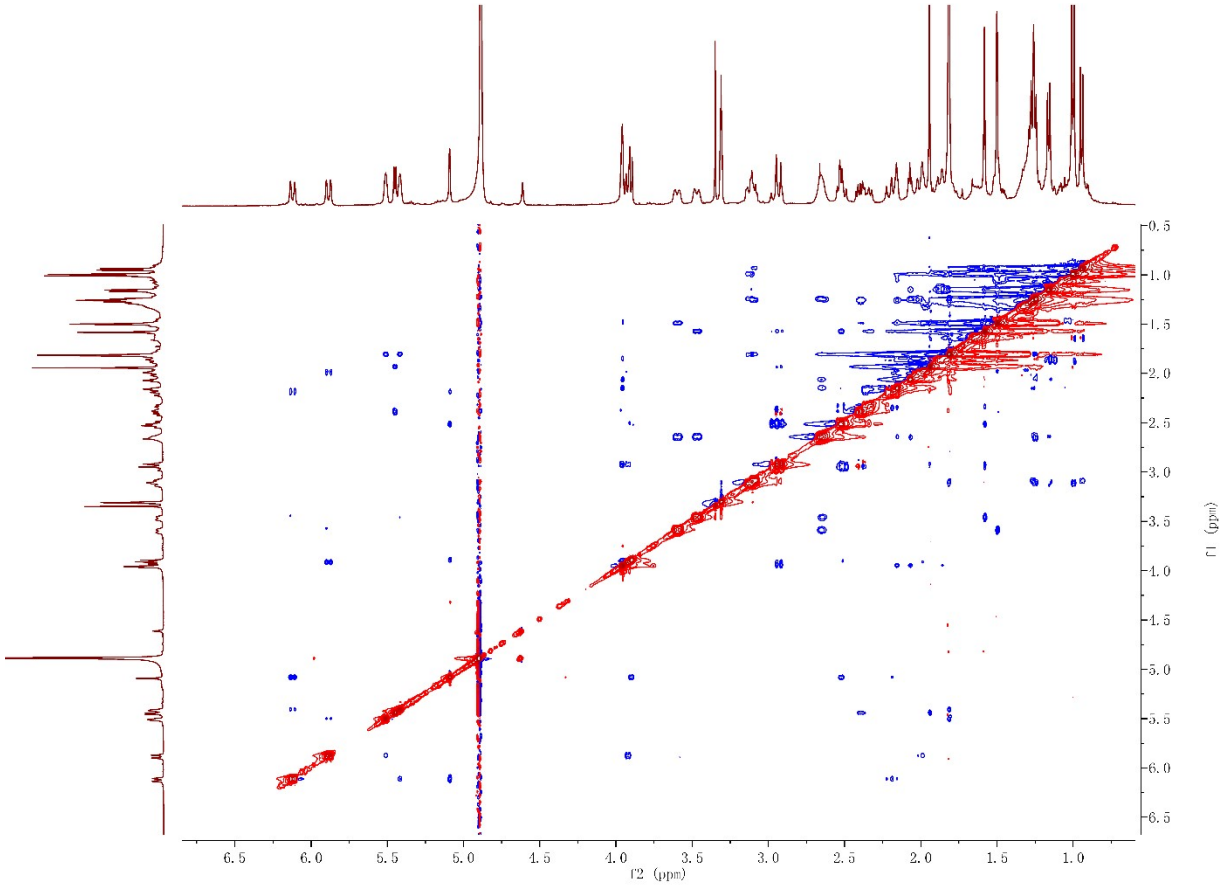
HMBC of compound 4



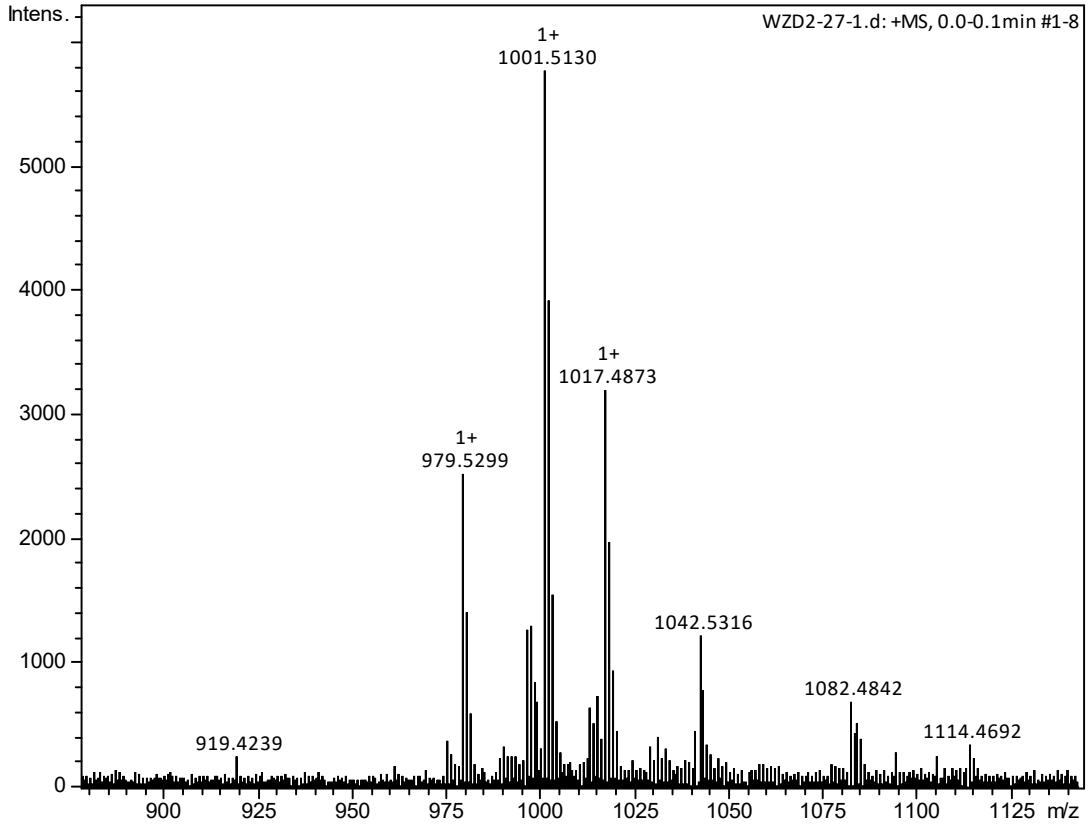
$^{1}H-^{1}H$ COSY of compound 4



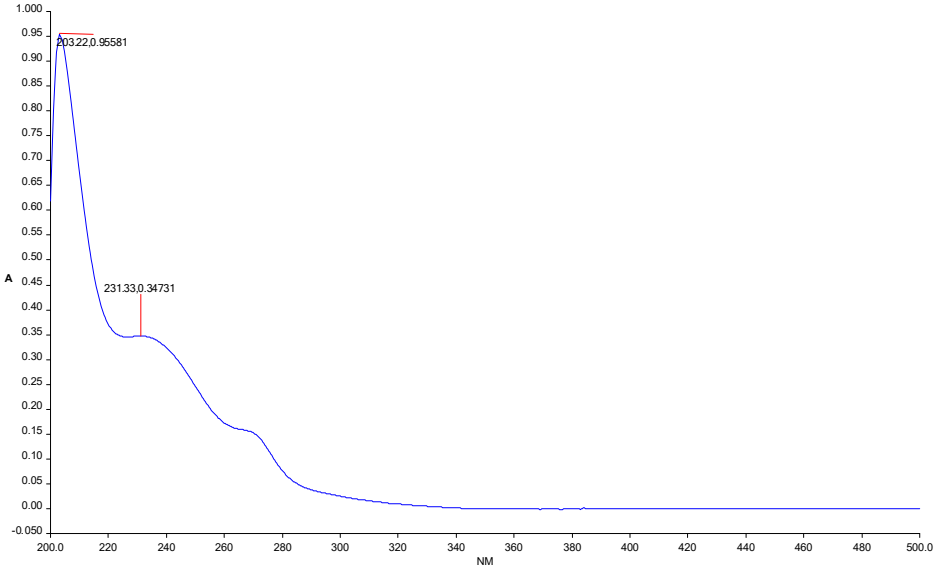
NOESY of compound 4



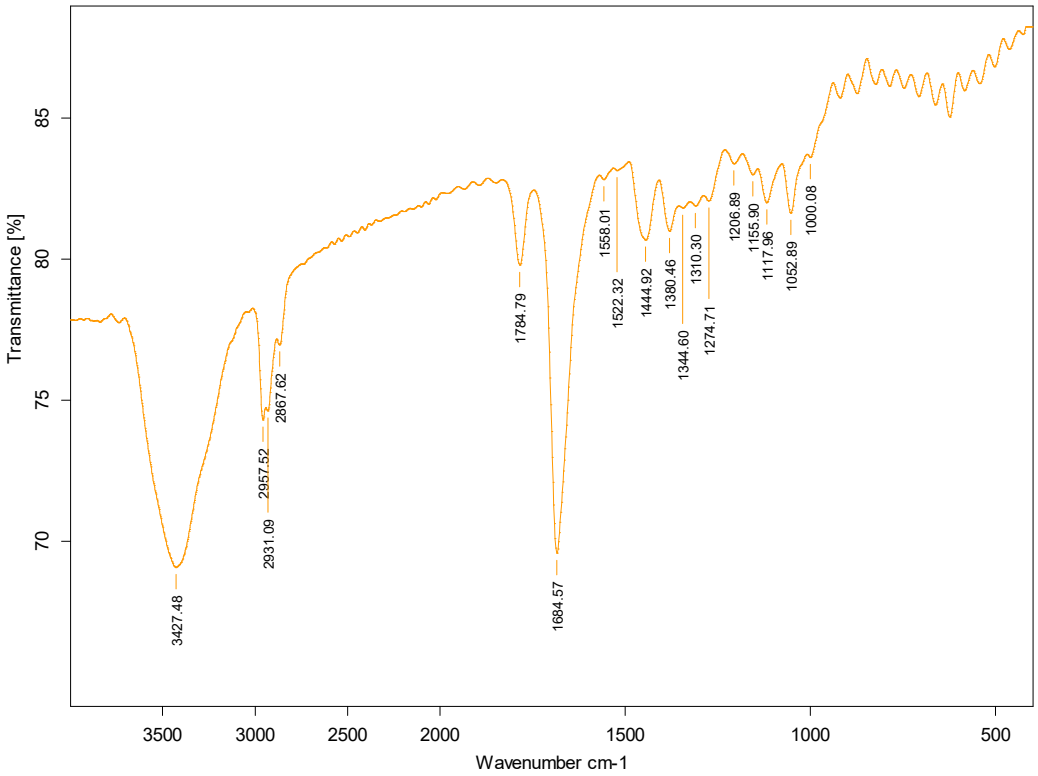
HRESIMS of compound 5



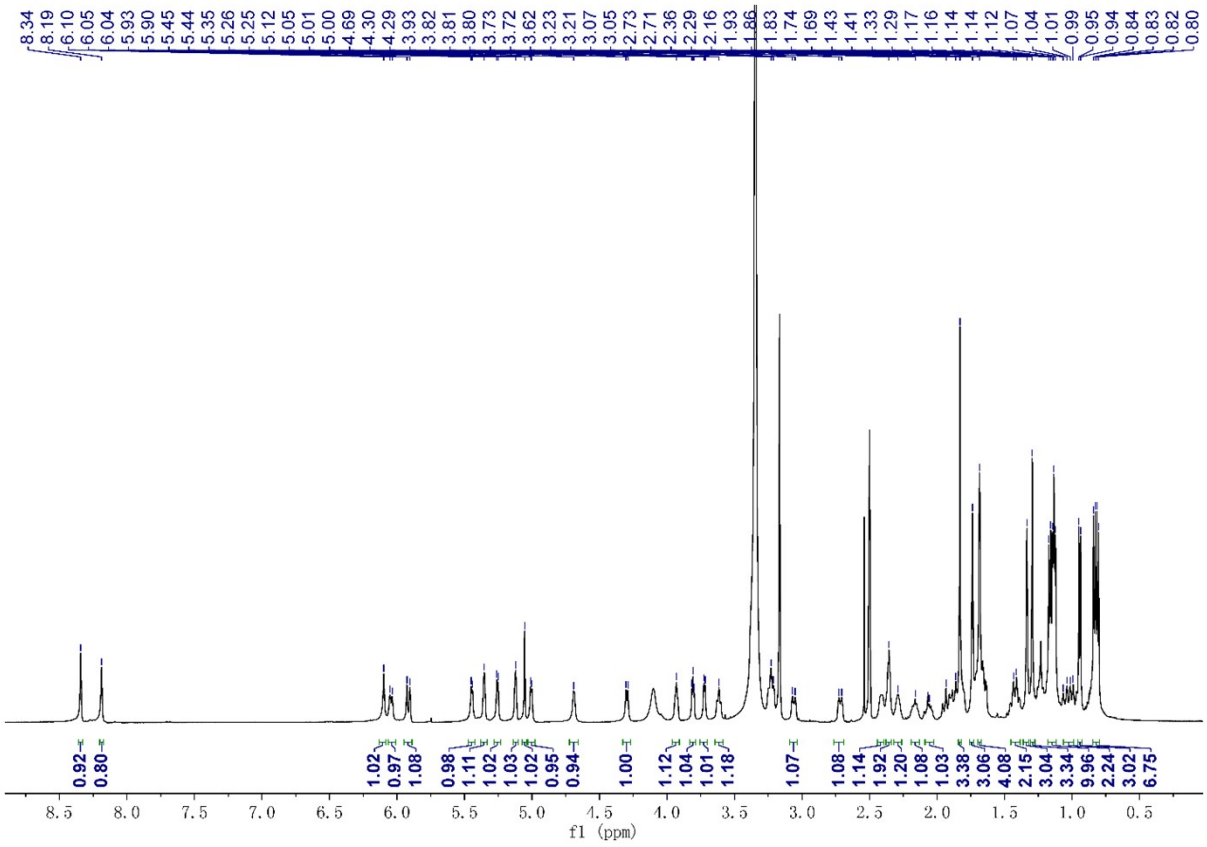
UV spectrum of compound 5



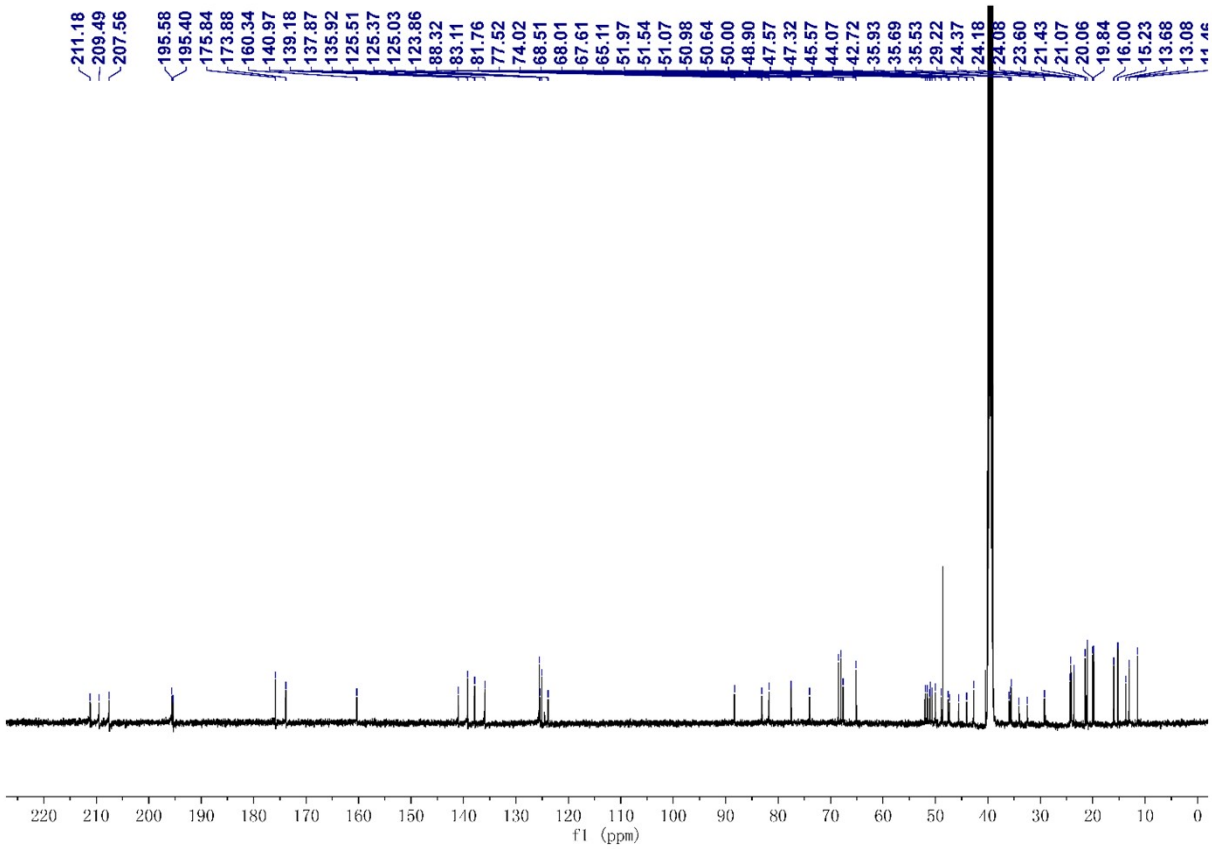
IR spectrum of compound 5



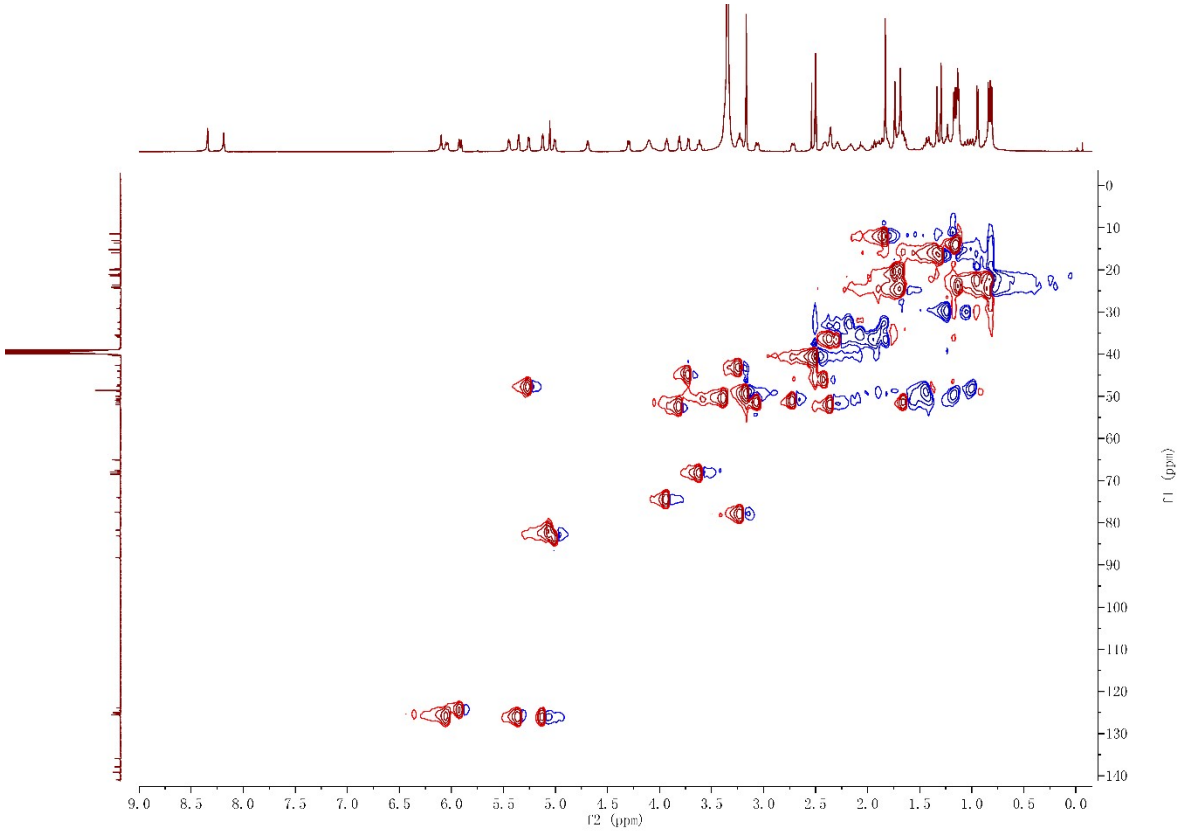
^{1}H NMR of compound 5



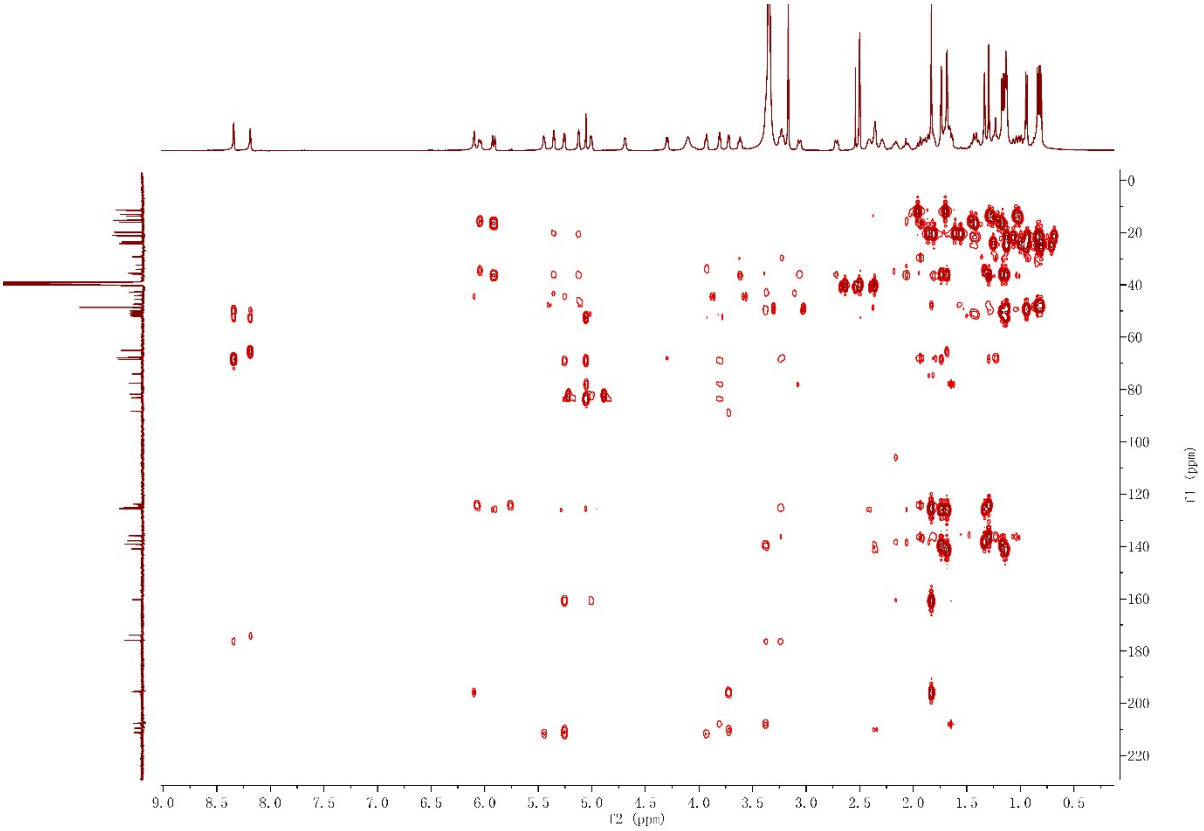
^{13}C NMR of compound 5



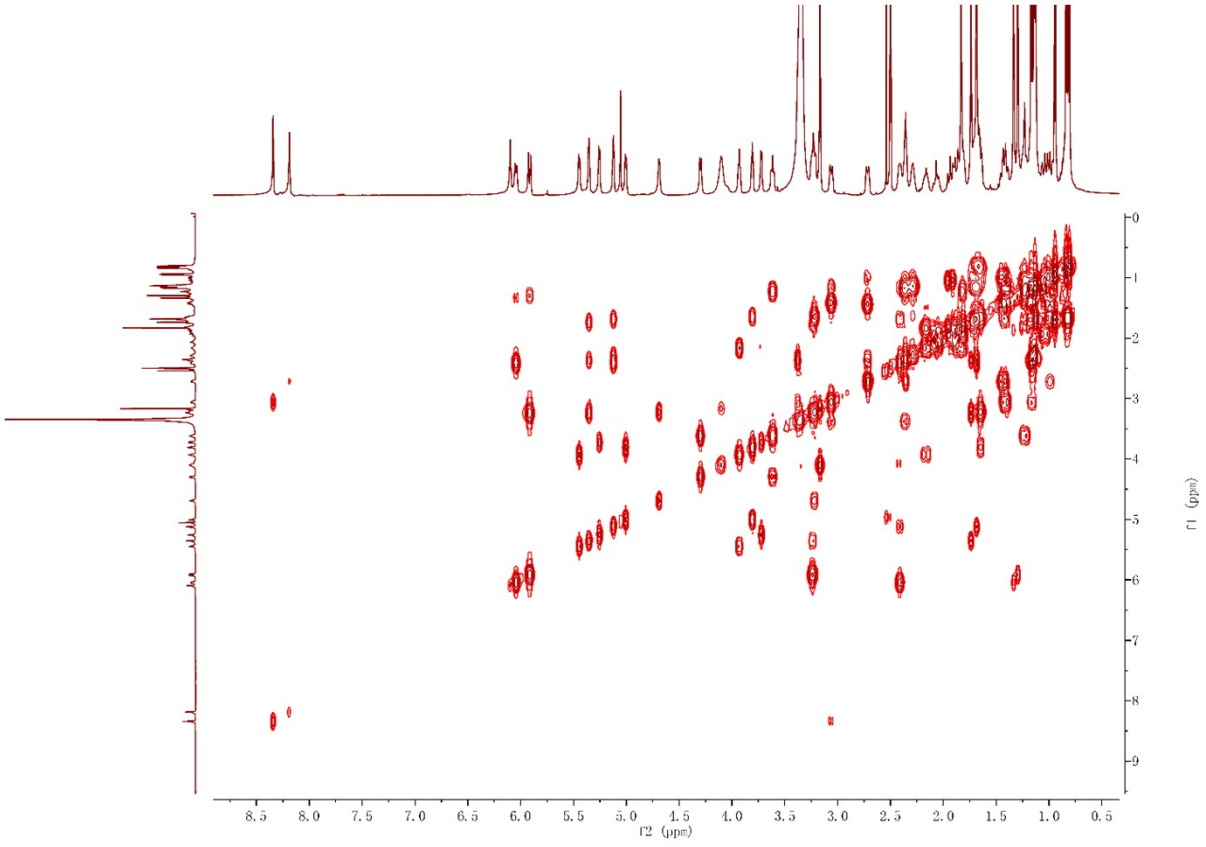
HSQC of compound 5



HMBC of compound 5



$^{1}H-^{1}H$ COSY of compound 5



NOESY of compound 5