Antibacterial and Antioxidant Activities, *In Silico* Molecular Docking, ADMET and DFT Analysis of Compounds from roots of *Cyphostemma cyphopetalum*

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The NMR data used to establish the structures of the compounds isolated in this work are depicted as Supplementary information.

Supplementary Tables 1-7 display the tabulated spectra used to determine the structure of compounds **2-8**, respectively.

Supplementary Figures 1-6 display the spectra used to determine the structure of newly obtained spongiane diterpenoid lactone hydroxyl derivatives, 3-hydroxyisoagatholactone (**1)**.

Supplementary Table 1 ^{1}H (400 MHz, $CDCl_3$), ^{13}C and DEPT-135 NMR spectra of compound **2**

Compound 2			40
No	**^{1}H (*J*)**	**^{13}C**	**^{13}C**
1		37.2	37.2
2		31.6	31.6
3	3.50 (m, 1H)	71.9	71.8
4	2.31 (d, 2H)	42.2	42.2
5		140.8	140.7
6	5.33 (bs, 1H)	121.8	121.7
7	2.04 (m, 2H)	32.0	31.9
8		32.0	31.9
9		50.2	50.1
10		36.6	36.5
11		21.1	21.0
12		39.8	39.7
13		42.4	42.3
14		56.8	56.7
15		24.8	24.3
16		28.2	29.7
17		56.1	56.0
18	0.66 (s, 3H)	11.9 C	12.2
19	0.86 (m, 3H)	19.1	19.4
20		36.2	36.5
21	0.99(m, 3H)	18.8	18.9
22		34.0	33.9
23		26.1	26.2
24		45.9	45.8
25		29.2	29.1
26	0.83 (m, 3H)	19.9	19.8
27	0.79 (m, 3H)	19.5	19.4
28		23.1	23.0
29	0.81 (m, 3H)	12.0	12.2

Supplementary Table 2 ^{1}H (400 MHz, MeOD), ^{13}C, COSY, HSQC and HMBC spectra of compound **3**

Compound 3					[41,42]	
No	**^{1}H (*J*)**	**^{13}C**	**COSY**	**HMBC**	***^{1}H* (*J*)**	**^{13}C**
1		133.8				134.4
2, 6	7.16 (d, 8.6Hz, 2H)	128.2	H-3,5	C-4, 3/5	7.14 (d, 9.0 Hz)	128.7
3, 5	6.79 (d, 8.6Hz, 2H)	116.3	H-2,6	C-1, 4,	6.76 (d, 9.0 Hz)	116.8
4		159.4				158.9
7	5.39 (d, 6.6 Hz, 1H)	94.8		C-1, 8,	5.36 (d, 6.5 Hz)	95.3
8	4.37 (d, 6.6 Hz, 1H)	58.2	H-10/14	C-1, 7, 9, 11’	4.35 (d, 6.5 Hz)	58.8
9		147.3				147.9
10, 14	6.19 (d, 3.0 Hz, 2H)	107.6		C-8	6.16 (d, 2.0 Hz)	108.0
11, 13		159.9				160.5
12	6.18 (d, 2.0 Hz, 1H)	102.2			6.18 (t, 2.0 Hz)	102.7
1’		131.1				130.8
2’, 6’	7.06 (d, 8.7 Hz, 2H)	128.8		C-4, 3’/5’	7.03 (d, 9.0 Hz	129.3
3’, 5’	6.67 (d, 8.8 Hz, 2H)	116.3		C-4’,C2’/6’	6.65 (d, 9.0 Hz)	116.9
4’		158.3				159.0
7’	6.84 (d, 16.4 Hz, 1H)	130.3	H-8’	C-2’/6’, 8’	6.81(d, 16.0 Hz)	130.9
8’	6.59 (d, 16.5 Hz, 1H)	123.6	H-7’	C-1’, 7’, 9’, 14’	6.56(d, 16.0 Hz)	124.2
9’		136.8				137.4
10’		120.0				120.6
11’		162.7				163.2
12’	6.25 (s, 1H)	96.8		C-9’,	6.25 (d, 2.0 Hz)	97.4
13’		159.7				160.2
14’	6.63 (s, 1H)	104.3		C-7’, 9’,	6.63 (d, 2.0 Hz)	104.9

Supplementary Table 3 ^{1}H (400 MHz, MeOD), and ^{13}C spectra of compound **4.**

Compound 4			[43,44]	
No	**^{1}H (*J*)**	**^{13}C,**	**1H NMR**	**^{13}C NMR**
1	-	130.4	-	128.07
2, 6	δ 7.35 (d, 8.4 Hz, 2H)	128.7	7.35 (d)	127.75
3, 5	6.77 (d, 8.5 Hz, 2H)	116.4	6.71 (d)	115.43
4		158.2		157.16
1”	6.96 (d, 16.3 Hz, 1H)	129.3	6.87 (d)	128.02
2”	6.80 (d, 16.3 Hz, 1H)	126.9	6.76 (d)	125.60
1’	-	141.2	-	139.19
2’, 6’	6.45 (d, 2.1 Hz, 2H)	105.7	6.34 (brs)	104.23
3’, 5’		159.6		158.28
4’	6.16 (bs, 1H)	102.6	6.07 (brs)	101.67
4-OH	9.29 (OH)	OH	9.48 (OH)	
3’, 5’- OH	9.11 (OH)	OH	9.12 (OH)	

Supplementary Table 4 ^{1}H (400 MHz, MeOD), ^{13}C, COSY, and HMBC spectra of compound **5**

Compound 5					45,46	
No	**^{1}H (*J*)**	**^{13}C**	**COSY**	**HMBC**	**^{1}H (*J*)**	**^{13}C**
1		136.9				134.7
2, 6	7.15 (d, 8.6 Hz, 2H)	127.6	H-3/5	C-3/5, 7	7.18 (d, 8.5)	128.6
3, 5	6.77 (d, 8.6 Hz, 2H)	116.4			6.79 (d, 8.5)	116.9
4		158.4				159.0
7	5.37 (d, 6.6 Hz, 1H)	94.9	H-8	C-2/6, 8, 9	5.40 (d, 5.5)	95.3
8	4.35 (d, 6.6 Hz, 1H)	58.3		C-9,14/10’	4.40 (d, 5.5)	59.4
9		147.3				148.0
10, 14	6.17 (d, 2.3 Hz, 2H)	107.0	H-14	C-9,	6.14 (s)	107.8
11, 13		159.7				160.6
12	6.24 (s, 1H)	101.5	H-10/14		6.14 (s)	102.7
1’		133.8				131.1
2’, 6’	6.92 (d, 8.4 Hz, 2H)	130.5	H-3’/5’		6.69 (d, 8.5)	129.2
3’ 5’	6.72 (d, 8.6 Hz, 2H)	115.7		C-2’/3’,7’	6.51 (d, 8.5)	116.7
4’		158.4				158.8
7’	6.82 (d, 16.4 Hz, 1H)	130.4	H-8’	C-8’,9’	6.38 (s)	129.2
8’	6.58 (d, 16.9 Hz, 1H)	123.7		C-1’,14’		123.0
9’		133.9				135.0
10’		120.0				120.8
11’		160.0				163.5
12’	6.18 (s, 1H)	96.6			6.42 (s)	92.0
13’		162.8				163.5
14’		120.3				120.8
1”		137.8				134.2
2”, 6”	7.04 (d, 8.8 Hz, 2H)	128.3	H-3”/5”	C-3”/5”	7.18(dd, 2.0, 8.5)	128.6
3”, 5”	6.66 (d, 8.6 Hz, 2H).	116.2			6.78 (dd, 2.0, 8.5)	116.9
4”		157.8				159.0
7”	5.19 (d, 6.2 Hz, 1H)	94.8	H-8”	C-1”,8”,9	5.40 (d, 5.5)	95.3
8”	3.79 (d, 6.4 Hz, 1H)	57.7		C-7”,9”	4.40 (d, 5.5)	59.4
9”		147.4				148.0
10”, 14”	5.93 (d, 2.2 Hz, 2H)	106.7	H-10,14”	C-9”,8”	6.14 (s)	107.8
11”, 13”		158.5				160.6
12”	6.18(dd, 6.8, 2.3Hz, 1H)	101.8	H-10”/14”		6.14 (s)	102.7

Supplementary Table 5 ^{1}H (400 MHz, MeOD), ^{13}C, COSY, and HMBC spectra of compound **6**

Compound 6					[47,48]	
No	**^{1}H (*J*)**	**^{13}C,**	**COSY**	**HMBC**	**^{1}H**	**^{13}C**
1, 1’		133.9				131.7
2/6, 2’/6’	7.27 (d, 8.4 Hz, 4H)	128.8	H-3/5; 3’/5’	C-4/7; C-4’/7’	7.17 d (8.4)	128.1
3/5, 3’/5’	6.76 (d, 8.4 Hz, 4H)	116.1		C-1; C-1’	6.64 d (8.4)	114.2
4, 4’		158.0				155.9
7, 7’	5.40 (d, 4.4 Hz, 2H)	85.9	H-8, 8’	C-2/6; C-2’/6’	5.82 d (4.4)	83.6
8, 8’	3.58 (d, 4.4 Hz, 2H)	59.0		C-9, 10/14; C-9’, 10’/14’	3.84 dd (4.4, 6.2	59.2
9, 9’		142.1				142.6
10/14; 10’/14’	6.02 (s, 4H)	109.0		C-8, 12; C-8’, 12’	6.08 d (2.2)	108.0
11/13; 11’/ 13’		158.8				157.7
12, 12’	6.23 (bs, 2H)	101.8			6.05 t (2.2	100.5

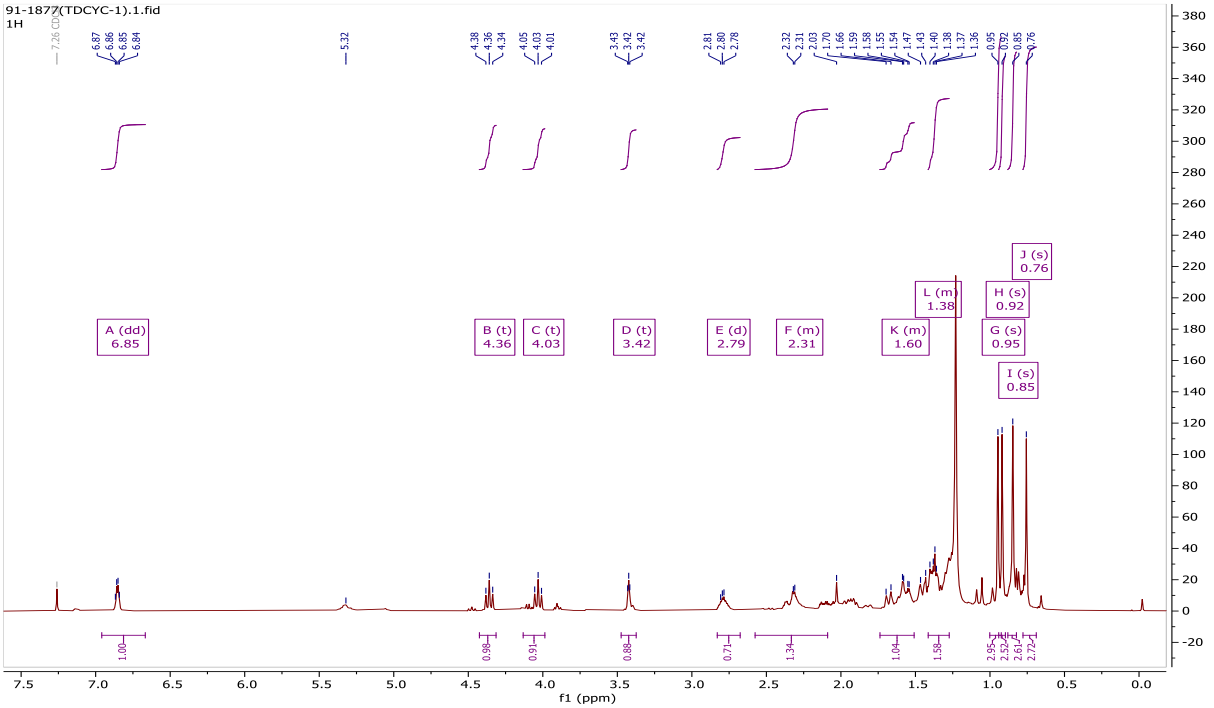
Supplementary Table 6 ^{1}H (400 MHz, MeOD), and ^{13}C spectra of compound **7**

No	**Compound 7**		[49]	
	$^{1}H(J)$	**^{13}C**	**^{1}H (*J*)**	**^{13}C**
1		137.8		134.2
2, 6	6.93 (d, 8.5 Hz, 2H)	131.1	7.15 (d, 8.4)	128.7
3, 5	6.58 (d, 8.5 Hz, 2H)	116.2	6.83 (d, 8.4)	116.5
4		158.4		159.1
7	5.18 (d, 6.2 Hz, 1H)	94.9	5.35 (d, 5.1)	93.7
8	3.78 (d, 6.2 Hz, 1H)	57.5	4.4 (d, 5.1)	56.9
9		147.4		148.0
10, 14	5.93 (d, 2.2 Hz, 2H)	107.3	6.04 (d, 2.2)	106.9
11, 13		160.1		160.0
12	6.09 (brs, 1H)	101.8	6.04 (, 2.2)	102.0
1’		131.1		131.2
2’, 6’	7.14 (d, 8.6 Hz, 2H)	128.5	6.93 (d, 8.4)	127.5
3’, 5’	6.71 (d, 8.6 Hz, 2H)	115.9	6.65 (d, 8.4)	115.4
4’		157.8		158.0
7’	4.07 (d, 6.6 Hz,1H)	72.9	4.93 (d, 8.7)	75.3
8’	4.07 (d, 6.6 Hz, 1H)	73.2	4.58 (d, 8.7)	76.5
9’		146.8		134.6
10’		126.6		119.2
11’		162.8		161.9
12’	6.23 (d, *J*2.2 Hz, 1H)	96.8	6.37 (d, 2.2)	96.7
13’		159.6		159.1
14’	6.53 (brs, 1H)	107.7	6.67 (d, 2.2)	108.2

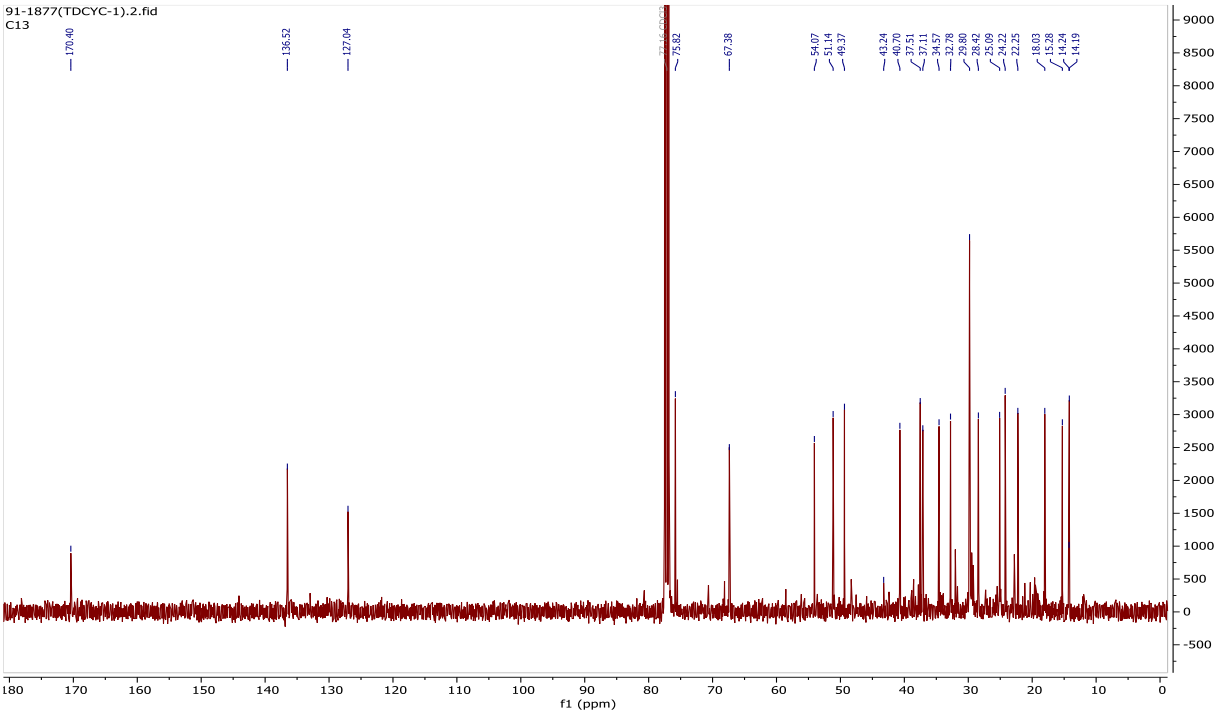
Supplementary Table 7 ^{1}H (400 MHz, MeOD), ^{13}C, COSY, HSQC and HMBC spectra of compound **8**

Compound 8					6	
No	**^{1}H (*J*)**	**^{13}C**	**COSY**	**HMBC**	**^{1}H**	**^{13}C**
1		131.2				131.3
2, 6	7.30 (d, *J* = 8.6 Hz, 2H)	128.8	H-3, 5	C-7	7.05 (d, 8.5)	129.9
3, 5	6.79 (d, *J* = 8.6 Hz, 2H)	116.1	H-2, 6		6.82 (d, 8.5)	115.2
4		157.4				157.4
7	5.43 (d, *J* = 6.6 Hz, 1H)	85.9	H-8	C-1, 2,6	4.30 (d, 8.0)	86.9
8	3.59 (dd, *J* = 6.6, 6.3 Hz, 1H)	59.1	H-7	C-14	3.42 (dd, 8.4, 3.5)	60.7
9		142.2				146.3
10		125.6				122.7
11		158.1				154.5
12	6.17 (d, *J* = 2.4 Hz, 1H)	103.6	H-10/14		6.27 (d, 2.0)	102.0
13		159.4				158.1
14	6.25 (d, *J* = 2.4 Hz, 1H)	106.9			5.74 (d, 1.8)	105.3
1’		133.9				137.4
2’, 6’	6.97 (d, *J* = 8.6 Hz, 2H)	128.8	H-3’, 5’		6.89 (d, 8.4)	128.8
3’, 5’	6.71 (d, *J* = 8.6 Hz, 2H)	116.1		C-1’, 7’	6.77 (d, 8.6)	115.1
4’		156.5				155.9
7’	4.10 (d, *J* = 6.5 Hz, 1H)	55.6		C-1’, 8’	3.93 (d, 3.0)	55.2
8’	4.20 (dd, *J* = 6.6, 6.3 Hz, 1H)	61.0		C-1’, 9’	3.46 (t, 3.5)	58.8
9’		150.3				150.5
10’, 14’	6.05 (s, 2H)	109.0		C-8’	6.09 (d, 1.8)	105.8
11’, 13’		158.9				158.9
12’	6.14 (d, *J* = 2.0 Hz, 1H)	101.8		C-10’, 14’, 8’	6.20 (d, 1.8)	100.7
OCH_3	3.58 (d, *J* = 4.8 Hz, 3H)	59.1		C-10’,14’	2.96 (3H, s)	55.8

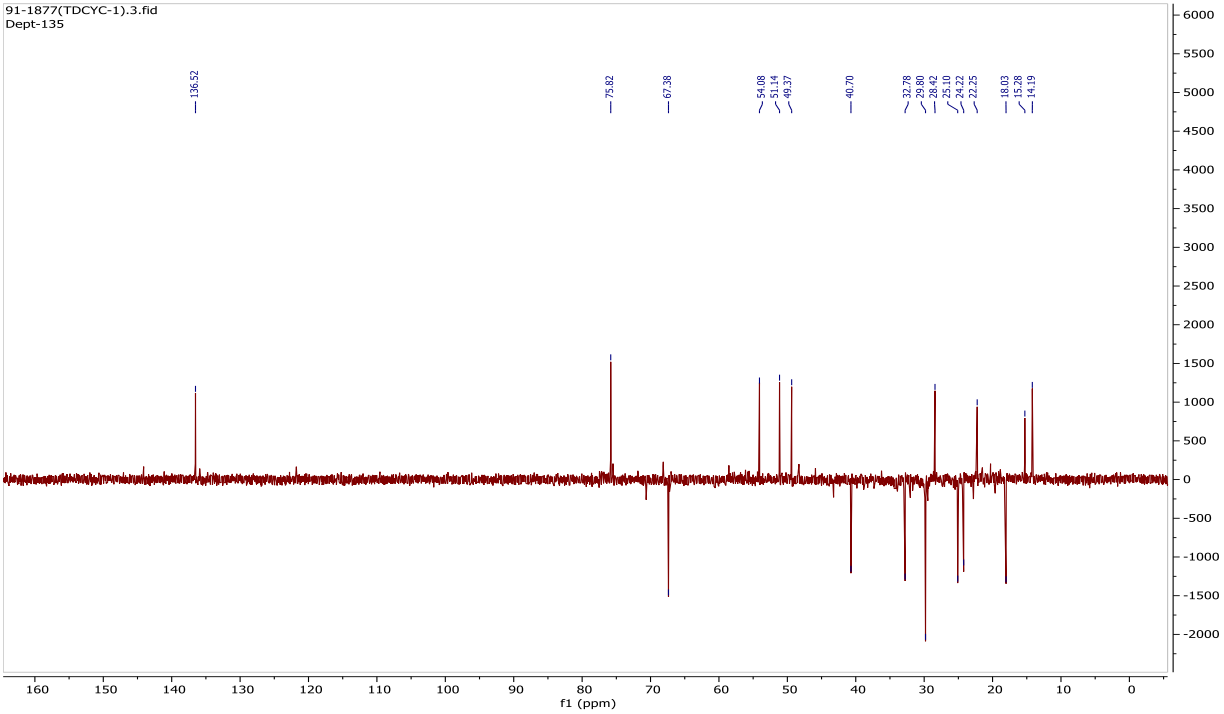
Supplementay Figure 1 ^{1}H NMR spectra of compound **1**.



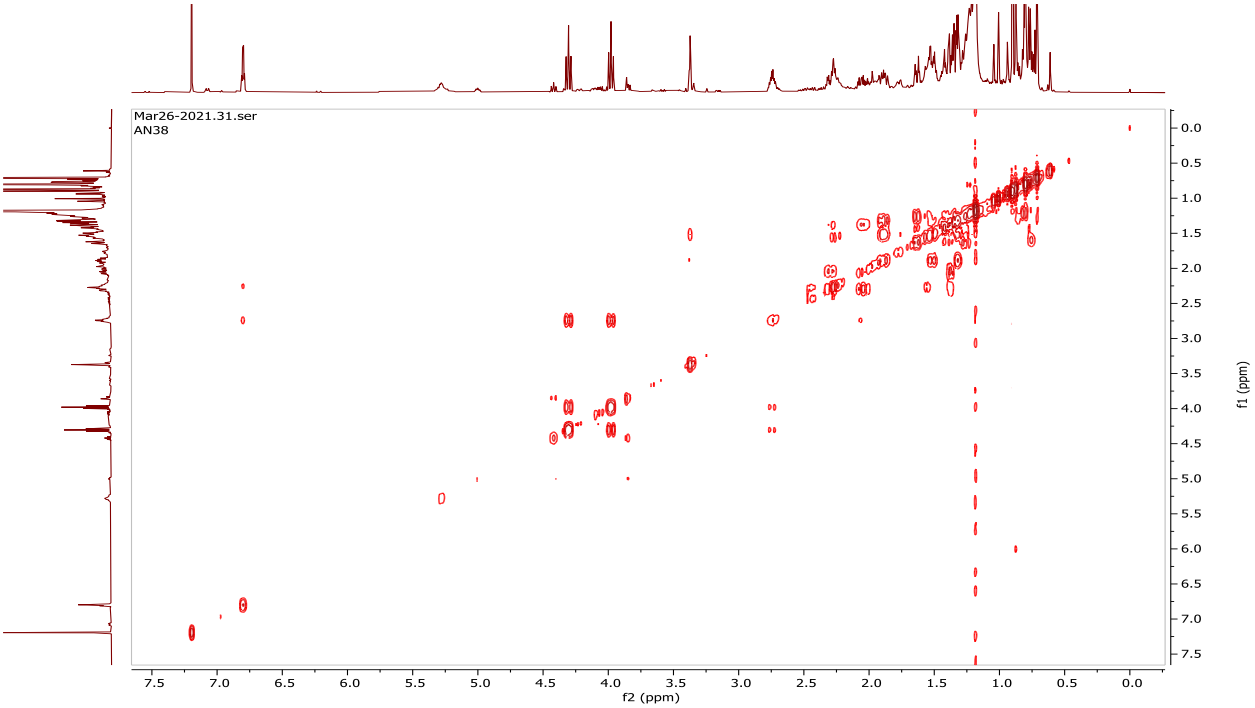
Supplementary Figure 2 13C NMR spectra of compound **1**.



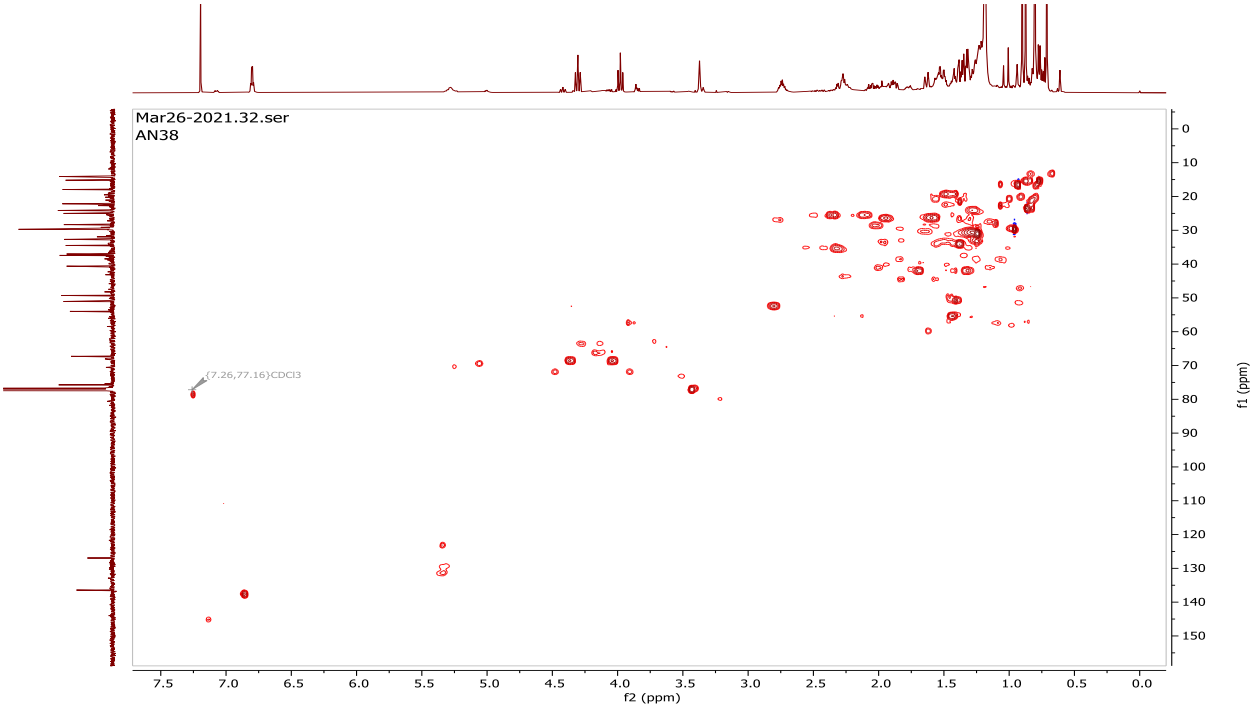
Supplementary Figure 3 DEPT-135 NMR spectra of compound 1.



Supplementary Figure 4 COSY spectrum of compound **1**.



Supplementary Figure 5 HSQC spectrum of compound **1**.



Supplementary Figure 6 HMBC spectra of compound **1**.