SUPPLEMENTARY MATERIAL

Cytotoxic activity of steroidal glycosides from the aerial parts of *Solanum torvum* collected in Thua Thien Hue, Vietnam

Le Canh Viet Cuong[a,b], Le Thi Lien[a], Nguyen Thi Minh Phuong[c], Vo Thi Kim Thu[d], Tran Phuong Ha[a], Ton That Huu Dat[a], Pham Thi Hai Ha[e], Tran Thi Phuong Anh[b], Hoang Le Tuan Anh[a,b,*]

[a] *Mientrung Institute for Scientific Research, Vietnam Academy of Science and Technology (VAST), 321 Huynh Thuc Khang road, Hue city, Vietnam*

[b] *Graduate University of Science and Technology, VAST, 18 Hoang Quoc Viet, Hanoi, Vietnam*

[c] *Faculty of Environment and Chemical Engineering, Duy Tan University (DTU), 254 Nguyen Van Linh road, Da Nang, Vietnam*

[d] *Faculty of Food Science and Technology, Thu Dau Mot University, 06 Tran Van On road, Thu Dau Mot, Vietnam*

[e] *Faculty of Biotechnology, Nguyen Tat Thanh University, 300A Nguyen Tat Thanh road, Ho Chi Minh City, Vietnam*

* To whom correspondence should be addressed:

Hoang Le Tuan Anh, Ph.D/Assoc. Prof.

Email: hltanh@misr.vast.vn

Abstract

A phytochemical investigation of *Solanum torvum* led to the isolation of eleven steroidal glycosides, including neochlorogenin 6-*O*-*β*-D-quinovopyranoside (**1**), (22*R*,23*S*,25*R*)-3*β*-6*α*,23-trihydroxy-5*α*-spirostane 6-*O*-*β*-D-xylopyranosyl-(1→3)-*β*-D-quinovopyranoside (**2**), neochlorogenin 6-*O*-*α*-L-rhamnopyranosyl-(1→3)-*β*-D-quinovopyranoside (**3**), solagenin 6-*O*-*α*-L-rhamnopyranosyl-(1→3)-*β*-D-quinovopyranoside (**4**), paniculonin A (**5**), paniculonin B (**6**), 6α-*O*-[*β*-D-xylopyranosyl-(1→3)*β*-D-quinovopyranosyl]-(25*S*)-5α-spirostan-3*β*-ol (**7**), torvoside J (**8**), torvoside K (**9**), torvoside L (**10**), and solagenin 6-*O*-*β*-D-quinovopyranoside (**11**). Their chemical structures were elucidated by 1D-NMR and 2D-NMR data as well as comparison with the data reported in the literature. Moreover, all isolated compounds were evaluated for their cytotoxic activities against SK-LU-1, HepG2, MCF-7, and T24 cancer cell lines. Among them, compounds **1**, **3**, **7**, and **11** exhibited cytotoxicity against all four tested cell lines with IC_{50} values ranging from 7.89 ± 0.87 to 46.76 ± 3.88 μM.

Keywords: *Solanum torvum, steroid, steroidal glycoside, cytotoxic activity.*

CONTENTS

General experimental procedures

The NMR spectra were measured on Bruker AM500 MHz spectrometers with TMS as an internal standard. Column chromatography (CC) was performed on silica gel (Kiesel gel 60, 70-230 mesh and 230-400 mesh, Merck, Darmstadt, Germany), YMC*GEL (ODS-A, 12 nm S-150 μm, YMC Co., Ltd.) and Sephadex LH-20 (Sigma-Aldrich, USA) resins. TLC used pre-coated silica gel 60 F_{254} (1.05554.0001, Merck) and RP-18 F_{254S} plated (1.15685.0001, Merck), and compounds were visualized by spraying aqueous 10% H_2SO_4 and heating for 3-5 min.

Cell lines and cell culture

The SK-LU-1 **(**human lung carcinoma), HepG2 (human hepatocellular carcinoma), MCF7 (human breast carcinoma), and T24 (human urine bladder carcinoma) cell lines were a generous gift from Prof. J. M. Pezzuto, University of Long Island, USA and Prof. Jeanette Maier, Università degli Studi di Milano, Italy.

The cells were cultured as a monolayer in Dulbeco's Modified Eagle Medium (DMEM) containing 2 mM L-glutamine, 1.5 g/L sodium bicarbonate, 4.5 g/L glucose, 10 mM HEPES, 1.0 mM sodium pyruvate, and 10% Fetal Bovine Serum (FBS). The medium was further added with 0.01 mg/mL bovine insulin while LNCaP medium was supplemented with 10 nM of testosterone. The cells were subcultured after 3-5 days with the ratio of 1:3 and incubated at 37^oC, 5% CO_2 and 100% humidified.

Cytotoxicity assay

Cytotoxic assays were performed according to a method developed by Monks et al, which is being used at the National Institute of Health (USA) as a standard method for the evaluation of the cytotoxic potential of compounds or extracts using a panel of human cancer cell lines (Monks et al. 1991). Cell lines were grown in 96-well microtiter plates with each well containing 190 μl medium. After 24 hrs, 10 μl of the test samples dissolved in 10% DMSO were added to the wells. The cells were then cultured for additional 48 hrs, fixed with trichloroacetic acid, and stained with sulforhodamine B, followed by the determination of the optical densities at 515 nm using an EL× 800 Microplate Reader (Bio-Tek Instruments) (Shoemaker et al. 2002). The inhibitory rate of cell growth (IR) of cells was calculated by the following equation $IR = 100\%-[(OD_t - OD_0) / (OD_c - OD_0)] \times 100$, where: OD_t: average OD value at day 3; OD_0: average OD value at time-zero; OD_c: average OD value of the blank DMSO control sample.

The cytotoxicities were calculated and expressed as Inhibition concentration at 50 % (IC_{50} values). The IC_{50} values of promising agents will be determined by testing a series of sample final concentrations at 100, 20, 4, and 0.8 μM. Experiments were carried out in triplicate for accuracy of

data. The TableCurve 2Dv4 software was used for data analysis and for IC_{50} calculation. The IC_{50} values should be in small deviation throughout the experiments.

Table S1. Sources and biological activities of isolated compounds

Compounds	Sources	Biological activities	References
1	*S. torvum*, *S. hispidum*	Anti-mycotic activity	(González et al. 2004; Lu Y-Y et al. 2011)
2	*S. torvum*, *S. surattense*	Anti-inflammatory and cytotoxic activities	(Lu Y et al. 2011; Lee et al. 2013)
3	*S. torvum*	-	(Arthan et al. 2002; Lu Y-Y et al. 2011)
4	*S. torvum*	Anti-viral activity	(Arthan et al. 2002; Lu Y-Y et al. 2011)
5	*S. torvum*, *S. paniculatum*	-	(Ripperger and Schreiber 1968; Challal et al. 2014)
6	*S. torvum*, *S. paniculatum, S. procumbens*	Anti-inflammatory activity	(Ripperger and Schreiber 1968; Lee et al. 2013; Challal et al. 2014; Hien et al. 2018)
7	*S. hispidum*	Anti-mycotic activity	(González et al. 2004)
8	*S. torvum*, *S. surattense*, *S. cumingii*	-	(Iida et al. 2005; Lu Y et al. 2011; Li et al. 2015)
9	*S. torvum*, *S. surattense*, *S. cumingii*	-	(Iida et al. 2005; Lu Y et al. 2011; Li et al. 2015)
10	*S. torvum*, *S. surattense*, *S. cumingii*	-	(Iida et al. 2005; Lu Y et al. 2011; Li et al. 2015)
11	*S. torvum*	-	(Lu et al. 2008; Lu Y-Y et al. 2011)

Table S2. ^{1}H- and ^{13}C-NMR data of compounds **1-3**

Pos.	1		2		3	
	$\delta_C{}^{a,c}$	$\delta_H{}^{b,c}$ *(mult., J in Hz)*	$\delta_C{}^{a,d}$	$\delta_H{}^{b,d}$ *(mult., J in Hz)*	$\delta_C{}^{a,d}$	$\delta_H{}^{b,d}$ *(mult., J in Hz)*
1	38.5	1.05 (m) 1.72 (m)	37.4	0.86 (m) 1.53 (m)	37.4	0.84 (m) 1.53 (m)
2	32.7	1.29 (m) 1.99 (m)	31.5	1.57 (m) 1.98 (m)	31.5	1.35 (m) 1.55 (m)
3	71.9	3.48 (m)	70.4	3.72 (m)	70.4	3.67 (m)
4	32.8	1.18 (m) 2.42 (m)	32.5	1.61 (br d, 12.0) 3.09 (br d, 12.0)	32.4	1.54 (m) 3.02 (br d, 12.5)
5	51.8	1.18 (m)	50.9	1.29 (m)	50.9	1.22 (m)
6	80.2	3.41 (td, 4.5, 10.5)	79.2	3.59 (dd, 4.5, 11.0)	79.3	3.52 (m)
7	41.7	0.97 (overlapped) 2.20 (dt, 4.0, 8.5)	40.9	1.02 (m) 2.42 (dt-like, 4.0, 12.5)	40.9	1.09 (m) 2.39 (m)

8	35.2	1.67 (m)	34.0	1.54 (m)	33.8	1.51 (m)
9	55.1	0.71 (m)	53.6	0.52 (m)	53.5	0.51 (m)
10	37.6	-	36.4	-	36.4	-
11	22.1	1.34 (m) 1.57 (m)	20.9	1.09 (m) 1.33 (m)	20.9	1.13 (m) 1.37 (m)
12	41.6	1.17 (m) 1.75 (m)	39.6	0.98 (m) 1.60 (m)	39.7	0.99 (m) 1.60 (m)
13	41.0	-	40.9	-	40.5	-
14	57.4	1.21 (m)	56.1	1.01 (m)	56.1	1.01 (m)
15	31.9	1.44 (m) 1.78 (m)	32.0	1.39 (m) 2.01 (m)	31.7	1.96 (m)
16	82.2	4.42 (m)	81.3	4.57 (q, 6.5)	80.9	4.42 (q, 7.5)
17	63.6	1.76 (m)	65.2	3.49 (m) 4.12 (m)	62.4	1.73 (m)
18	16.9	0.81 (s)	16.2	0.77 (s)	16.3	0.74 (s)
19	13.8	0.89 (s)	13.3	0.77 (s)	13.3	0.77 (s)
20	43.5	1.88 (m)	40.4	2.62 (t-like, 6.0)	42.2	1.83 (m)
21	14.7	1.01 (d, 7.0)	16.9	1.47 (d, 7.0)	14.5	1.07 (d, 7.0)
22	111.1	-	110.4	-	109.6	-
23	27.0	1.37 (m) 1.74 (m)	69.8	4.01 (m)	26.1	1.39 (m) 1.83 (m)
24	26.8	1.44 (m) 2.04 (m)	33.9	1.78 (m) 2.27 (dt-like, 4.5, 14.0)	25.8	1.30 (m) 2.07 (m)
25	28.5	1.69 (m)	26.9	1.65 (m)	27.2	1.52 (m)
26	66.1	3.28 (m) 3.95 (dd, 2.5, 11.0)	64.2	1.73 (m)	64.9	3.31 (d, 11.0) 3.89 (dd, 2.0, 11.0)
27	16.4	1.10 (d, 7.0)	20.1	1.43 (d, 7.5)	16.0	1.00 (d, 7.0)
1′	105.3	4.29 (d, 8.0)	104.6	4.76 (d, 7.5)	105.0	4.66 (d, 8.0)
2′	76.0	3.19 (dd, 8.0, 9.0)	74.5	3.97 (dd, 8.0, 9.0)	75.7	3.90 (t, 8.5)
3′	78.0	3.30 (m)	87.1	3.99 (m)	83.1	4.15 (t, 9.0)
4′	77.1	3.01 (t, 9.0)	74.4	3.50 (m)	74.8	3.49 (m)
5′	73.0	3.31 (m)	71.9	3.65 (m)	72.0	4.70 (br d, 1.5)
6′	18.2	1.29 (d, 6.0)	18.3	1.50 (d, 6.5)	18.4	1.52 (d, 6.5)
1″			105.8	5.15 (d, 8.0)	102.5	6.10 (s)
2″			74.8	3.95 (m)	72.3	3.64 (m)
3″			77.5	4.08 (m)	72.1	4.52 (dd, 3.5, 9.5)
4″			70.4	4.10 (m)	73.6	4.25 (t, 9.5)
5″			66.8	3.63 (dd, 4.5, 11.0) 4.23 (dd, 4.5, 11.0)	69.6	4.85 (m)
6″					18.2	1.61 (d, 6.0)

Measured in [a]125 MHz, [b]500 MHz, [c]Methanol-d_4, [d]Pyridine-d_5. All the NMR data assignments were done by HSQC and HMBC spectra.

Table S3. ^{1}H- and ^{13}C-NMR data of compounds **4**-**6**

Pos.	4		5		6	
	$\delta_C^{a,d}$	$\delta_H^{b,d}$ *(mult., J in Hz)*	$\delta_C^{a,c}$	$\delta_H^{b,c}$ *(mult., J in Hz)*	$\delta_C^{a,c}$	$\delta_H^{b,c}$ *(mult., J in Hz)*
1	38.4	1.12 (m) 1.75 (m)	38.5	1.05 (m) 1.73 (m)	38.5	1.07 (dd, 3.5, 13.5) 1.72 (m)
2	37.8	2.25 (m) 2.37 (m)	31.9	1.43 (m) 1.77 (m)	31.8	1.44 (m) 1.77 (m)
3	211.6	-	71.9	3.48 (m)	71.8	3.48 (m)
4	39.6	1.63 (m) 2.34(m)	32.7	1.19 (m) 2.42 (m)	32.7	1.19 (m) 2.40 (m)
5	52.0	1.54 (m)	51.8	1.18 (m)	51.7	1.19 (m)
6	79.9	3.68 (td, 4.5, 10.5)	80.4	3.42 (m)	80.5	3.40 (m)
7	40.5	1.09 (m) 2.40 (m)	41.6	0.98 (m) 2.20 (m)	41.7	1.00 (m) 2.20 (m)
8	33.7	1.58 (m)	35.1	1.70 (m)	35.0	1.57 (m)
9	53.0	0.56 (m)	55.1	0.72 (m)	55.1	0.71 (dt, 3.5, 11.0)
10	36.5	-	37.6	-	37.6	-
11	21.1	1.21 (m) 1.36 (m)	22.1	1.35 (m) 1.57 (m)	22.1	1.35 (m) 1.78 (m)
12	39.6	1.00 (m) 2.38 (m)	41.3	1.19 (m) 1.76 (m)	41.3	1.20 (m) 1.78 (m)
13	40.6	-	42.2	-	42.0	-
14	55.9	1.01 (m)	57.4	1.20 (m)	57.4	1.21 (m)
15	31.8	1.38 (m) 1.97 (m)	32.6	1.41 (m) 1.98 (m)	32.5	1.44 (m) 1.98 (m)
16	80.9	4.42 (q, 7.5)	82.6	4.45 (m)	82.6	4.46 (m)
17	62.5	1.73 (m)	63.2	1.78 (m)	63.1	1.80 (m)
18	16.4	0.78 (s)	17.0	0.88 (s)	17.0	0.88 (s)
19	12.4	0.93 (s)	13.8	0.90 (s)	13.9	0.90 (s)
20	42.3	1.85 (m)	37.1	2.56 (m)	37.0	2.56 (m)
21	14.6	1.08 (d, 6.5)	14.3	0.98 (d, 7.0)	14.4	0.98 (d, 7.0)
22	109.6	-	112.7	-	112.6	-
23	26.1	1.40 (m) 1.83 (m)	64.0	3.70 (dd, 5.0, 11.5)	63.9	3.70 (m)
24	25.9	1.32 (m) 2.08 (m)	36.0	1.69 (m) 1.91 (m)	35.9	1.70 (m) 1.82 (m)
25	27.2	1.55 (m)	31.3	1.91 (m)	31.2	1.92 (m)
26	65.0	3.32 (br d, 11.0) 3.98 (dd, 2.5, 11.0)	65.0	3.21 (br d, 11.5) 3.87 (dd, 4.0, 11.0)	65.0	3.22 (br d, 11.0) 3.87 (dd, 2.0, 11.0)
27	16.1	1.02 (d, 7.5)	17.6	1.12 (d, 7.0)	17.6	1.13 (d, 7.0)
1′	105.2	4.61 (d, 7.5)	104.8	4.34 (d, 8.0)	105.1	4.29 (d, 8.0)
2′	75.5	3.87 (dd, 7.5, 9.0)	75.0	3.37 (m)	76.3	3.29 (dd, 8.0, 9.0)
3′	83.5	4.14 (t, 9.0)	87.8	3.45 (m)	84.4	3.44 (m)
4′	74.9	3.50 (t, 9.0)	75.2	3.08 (t, 9.0)	75.7	3.04 (t, 9.0)
5′	72.3	4.52 (m)	72.7	3.34 (m)	72.9	3.35 (m)
6′	18.5	1.54 (d, 6.0)	18.2	1.29 (d, 6.0)	18.4	1.30 (d, 6.0)
1″	102.8	6.09 (s)	106.0	4.50 (d, 7.5)	102.8	5.16 (d, 1.5)
2″	72.1	4.72 (m)	75.2	3.28 (m)	72.2	3.73 (m)

3″	72.4	3.68 (m)	77.7	3.36 (m)	72.3	3.99 (m)
4″	73.9	4.25 (t, 9.5)	71.0	3.53 (m)	73.9	3.40 (m)
5″	69.7	4.84 (dd, 6.0, 9.0)	67.1	3.25 (m) 3.92 (dd, 5.0, 11.0)	70.0	4.02 (m)
6″	18.3	1.61 (d, 6.0)			17.9	1.27 (d, 6.5)

Measured in [a]125 MHz, [b]500 MHz, [c]Methanol-d_4, [d]Pyridine-d_5. All the NMR data assignments were done by HSQC and HMBC spectra.

Table S4. ^{1}H- and ^{13}C-NMR data of compounds **7**-**9**

Pos.	**7**		**8**		**9**	
	$\delta_C{}^{a,c}$	$\delta_H{}^{b,c}$ *(mult., J in Hz)*	$\delta_C{}^{a,c}$	$\delta_H{}^{b,c}$ *(mult., J in Hz)*	$\delta_C{}^{a,c}$	$\delta_H{}^{b,c}$ *(mult., J in Hz)*
1	38.5	1.17 (m) 1.75 (m)	38.5	1.05 (m) 1.72 (m)	38.5	1.05 (m) 1.73 (m)
2	32.7	1.29 (m) 1.98 (m)	31.8	1.43 (m) 1.77 (m)	31.9	1.43 (m) 1.78 (m)
3	71.8	3.48 (m)	71.8	3.49 (m)	71.9	3.48 (m)
4	32.7	1.18 (m) 2.42 (m)	32.6	1.18 (m) 2.40 (m)	32.7	1.17 (m) 2.39 (m)
5	51.8	1.18 (m)	51.7	1.20 (m)	51.8	1.20 (m)
6	80.3	3.42 (m)	80.4	3.40 (m)	80.4	3.40 (m)
7	41.7	0.97 (m) 2.19 (m)	41.6	0.99 (m) 2.20 (m)	41.6	1.00 (m) 2.20 (m)
8	35.2	1.68 (m)	35.3	1.66 (m)	35.3	1.68 (m)
9	55.1	0.72 (m)	55.0	0.71 (m)	55.1	0.72 (m)
10	37.6	-	37.6	-	37.6	-
11	22.1	1.34 (m) 1.57 (m)	22.0	1.33 (m) 1.57 (m)	22.0	1.35 (m) 1.55 (m)
12	41.6	1.18 (m) 1.75 (m)	40.7	1.15 (m) 1.77 (m)	40.8	1.16 (m) 1.77 (m)
13	41.0	-	42.0	-	42.1	-
14	57.4	1.21 (m)	57.5	1.18 (m)	57.5	1.18 (m)
15	31.9	1.44 (m) 1.77 (m)	32.9	1.19 (m) 2.00 (m)	32.9	1.19 (m) 1.99 (m)
16	82.2	4.42 (m)	82.4	4.48 (m)	82.6	4.50 (m)
17	63.6	1.76 (m)	65.6	1.72 (m)	65.4	1.73 (m)
18	16.9	0.81 (s)	16.8	0.84 (s)	16.8	0.85 (s)
19	13.8	0.90 (s)	13.9	0.90 (s)	13.9	0.89 (s)
20	43.5	1.87 (m)	41.7	2.28 (m)	41.0	2.22 (m)
21	14.7	1.01 (d, 7.5)	17.1	1.12 (d, 7.0)	16.9	1.14 (d, 7.0)
22	111.0	-	110.0	-	111.4	-
23	27.0	1.37 (m) 1.94 (m)	71.0	3.55 (br s)	71.2	3.60 (t,3.5)
24	26.8	1.44 (m) 2.05 (m)	37.5	1.64 (m) 1.68 (m)	34.7	1.67 (m) 1.73 (m)
25	28.5	1.69 (m)	24.9	2.06 (m)	28.0	1.77 (m)
26	66.1	3.30 (m) 3.95 (dd, 2.5, 11.5)	67.5	3.38 (m) 3.49 (m)	66.3	3.41 (m) 3.48 (m)
27	16.4	1.11 (d, 7.0)	17.4	0.79 (d, 6.5)	20.2	1.23 (d, 7.0)
1′	104.9	4.34 (d, 7.5)	105.1	4.29 (d, 8.0)	105.1	4.29 (d, 8.0)

2′	75.1	3.38 (m)	76.3	3.31 (m)	76.4	3.32 (m)
3′	87.8	3.44 (m)	84.4	3.44 (m)	84.4	3.43 (m)
4′	75.3	3.08 (t, 9.0)	75.7	3.04 (dd, 9.0, 9.5)	75.8	3.04 (dd, 9.0, 9.0)
5′	72.7	3.34 (m)	72.3	3.96 (m)	73.0	3.35 (m)
6′	18.3	1.30 (d, 6.5)	18.4	1.30 (d, 6.0)	18.4	1.30 (d, 6.5)
1″	106.0	4.50 (d, 7.5)	102.7	5.16 (d, 1.5)	102.8	5.16 (d, 1.5)
2″	75.2	3.28 (m)	72.2	3.72 (dd, 3.0, 9.5)	72.3	3.96 (m)
3″	77.7	3.37 (m)	72.9	3.34 (m)	72.4	3.72 (dd, 3.5, 9.5)
4″	71.0	3.53 (m)	73.9	3.42 (m)	74.0	3.46 (m)
5″	67.1	3.25 (m) 3.92 (dd, 4.5, 11.5)	70.0	4.01 (m)	70.0	4.02 (m)
6″			17.9	1.27 (d, 6.0)	17.9	1.27 (d, 6.5)

Measured in [a]125 MHz, [b]500 MHz, [c]Methanol-d_4. All the NMR data assignments were done by HSQC and HMBC spectra.

Table S5. ^{1}H- and ^{13}C-NMR data of compounds **10**-**11**

Pos.	**10**		**11**	
	$\delta_C{}^{a,c}$	$\delta_H{}^{b,c}$ *(mult., J in Hz)*	$\delta_C{}^{a,c}$	$\delta_H{}^{b,c}$ *(mult., J in Hz)*
1	38.5	1.04 (m) 1.80 (m)	39.7	1.40 (m) 2.03 (m)
2	31.9	1.43 (m) 1.79 (m)	38.6	2.23 (m) 2.51 (m)
3	71.9	3.47 (m)	214.8	-
4	32.7	1.18 (m) 2.39 (m)	40.3	2.29 (m) 2.91 (m)
5	51.8	1.18 (m)	53.1	1.59 (m)
6	80.5	3.40 (m)	80.8	3.50 (td, 4.5, 11.0)
7	41.7	0.96 (br d, 11.5) 2.19 (m)	41.4	1.02 (m) 2.24 (m)
8	35.1	1.68 (m)	35.1	1.74 (m)
9	55.2	0.71 (td, 4.0, 12.0)	54.5	0.81 (m)
10	37.6	-	37.8	-
11	22.1	1.37 (m) 1.67 (m)	22.2	1.44 (m) 1.60 (m)
12	41.3	1.17 (m) 1.76 (m)	40.9	1.20 (m) 1.77 (m)
13	42.3	-	41.7	-
14	56.7	1.14 (m)	57.2	1.22 (m)
15	34.7	1.30 (m) 1.98 (m)	32.7	1.31 (m) 2.00 (m)
16	85.4	4.74 (m)	82.2	4.43 (m)
17	64.3	1.86 (dd, 6.0, 9.0)	63.6	1.77 (m)
18	17.1	0.89 (s)	16.9	0.84 (s)
19	13.8	0.90 (s)	13.0	1.11 (s)
20	43.8	2.22 (m)	43.5	1.49 (m)
21	16.5	1.18 (d, 7.5)	14.7	1.02 (d, 7.0)
22	113.5	-	111.1	-
23	70.8	3.65 (dd, 5.0, 12.0)	27.0	1.37 (m) 1.94 (m)

24	38.5	1.49 (m) 1.72 (m)	26.8	1.44 (m) 2.05 (m)
25	31.9	1.72 (m)	28.5	1.69 (m)
26	69.5	3.32 (m) 3.45 (m)	66.1	3.29 (m) 3.95 (dd, 2.5, 11.0)
27	16.8	0.84 (d, 6.5)	16.4	1.10 (d, 6.5)
1′	105.1	4.29 (d, 8.0)	105.4	4.27 (d, 8.0)
2′	76.4	3.29 (dd, 8.0, 9.0)	75.8	3.17 (dd, 7.5, 8.0)
3′	84.5	3.43 (m)	77.9	3.29 (m)
4′	75.8	3.04 (t, 9.0)	77.0	3.00 (t, 9.0)
5′	72.4	3.96 (m)	73.0	3.31 (m)
6′	18.4	1.30 (d, 6.0)	18.2	1.29 (d, 6.5)
1″	102.8	5.16 (d, 1.5)		
2″	72.3	3.72 (dd, 3.5, 9.5)		
3″	73.0	3.33 (m)		
4″	74.0	3.41 (m)		
5″	70.1	4.01 (m)		
6″	17.9	1.27 (d, 6.5)		

Measured in [a)]125 MHz, [b)]500 MHz, [c)]Methanol-d_4. All the NMR data assignments were done by HSQC and HMBC spectra.

Table S6. Cytotoxic activity of compounds **1-11** on four human cell lines

Compound	**IC_{50} (μM)**			
	SK-LU-1	**HepG2**	**MCF-7**	**T24**
1	8.71±1.07	12.02±1.09	7.89±0.87	11.11±1.03
2	>100	>100	>100	>100
3	13.86±1.52	15.53±1.63	25.65±2.52	26.41±3.04
4	>100	>100	>100	>100
5	>100	>100	>100	>100
6	>100	>100	>100	>100
7	46.76±3.88	31.36±3.29	17.60±1.98	12.37±1.19
8	>100	>100	>100	>100
9	>100	>100	>100	>100
10	>100	>100	>100	>100
11	12.21±1.17	10.51±1.02	10.26±0.33	19.26±1.72
Ellipticine*	1.50±0.20	1.87±0.20	1.42±0.16	2.11±0.20

*) Ellipticine was used as positive control.

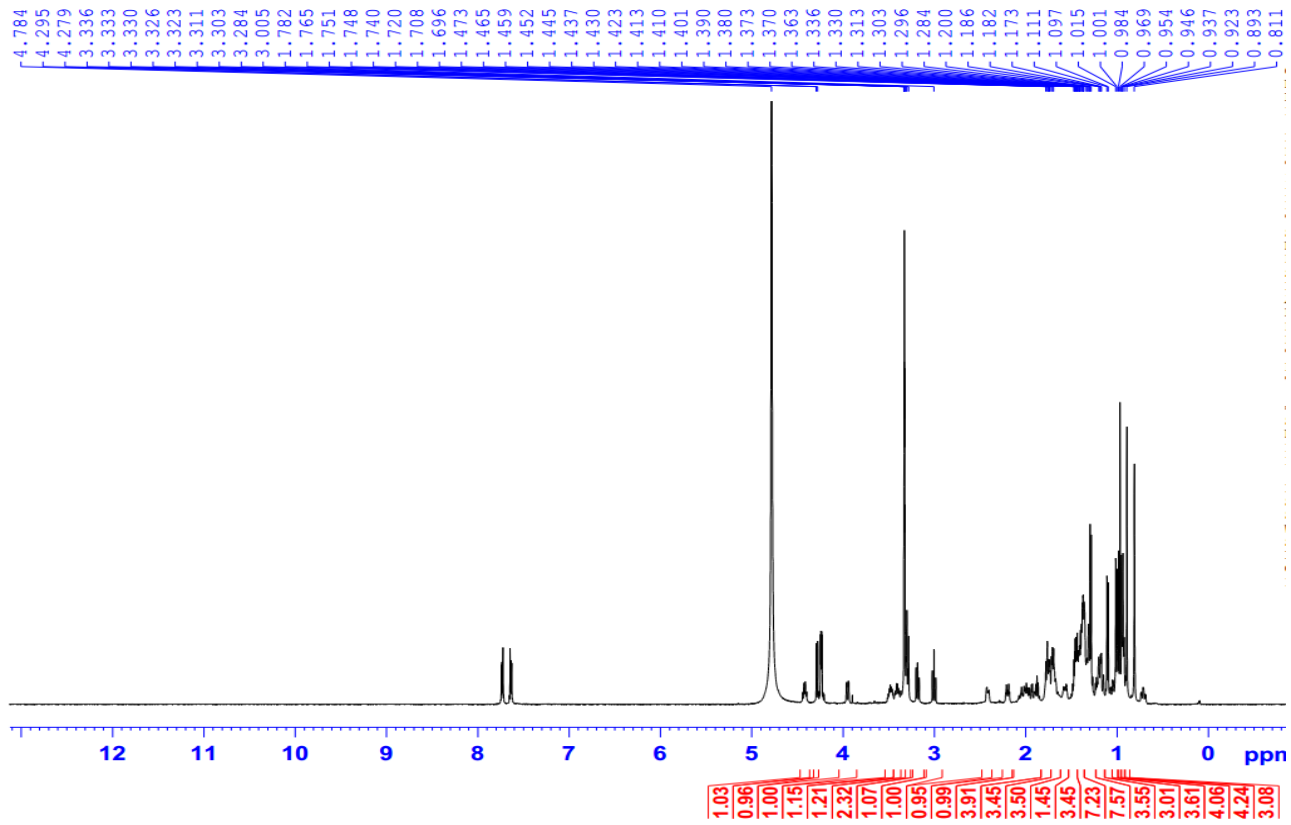

Figure S1. [1]H-NMR spectrum of compound **1** (in MeOD, 500 MHz)

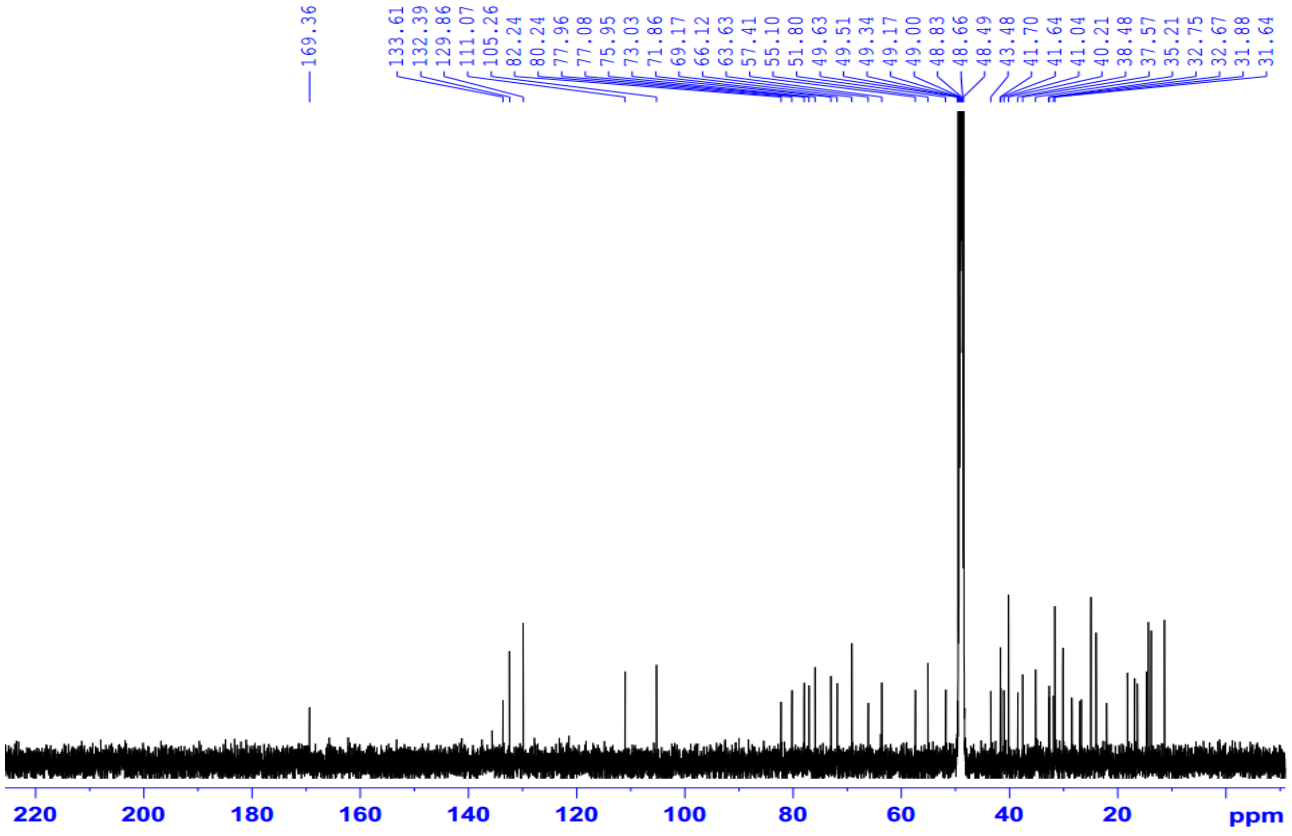

Figure S2. [13]C-NMR spectrum of compound **1** (in MeOD, 125 MHz)

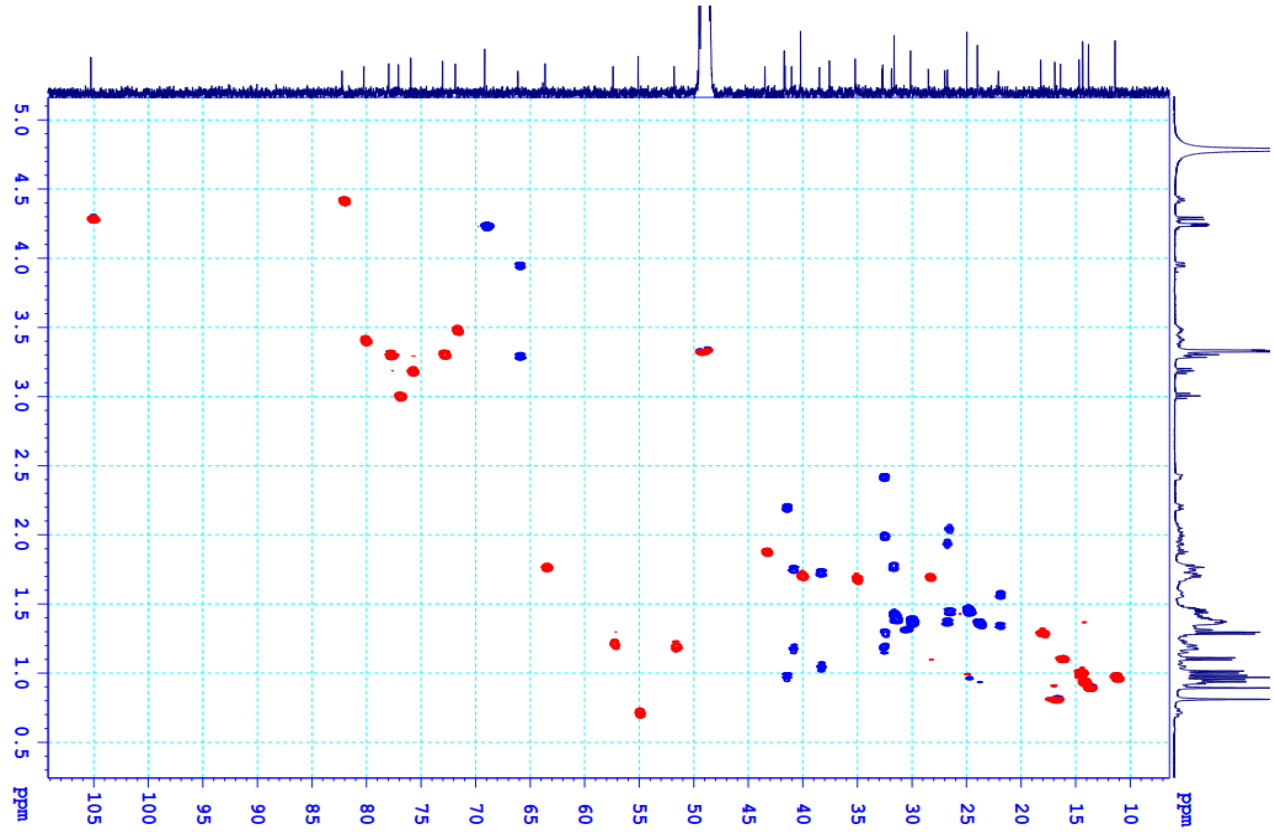

Figure S3. HSQC spectrum of compound **1**

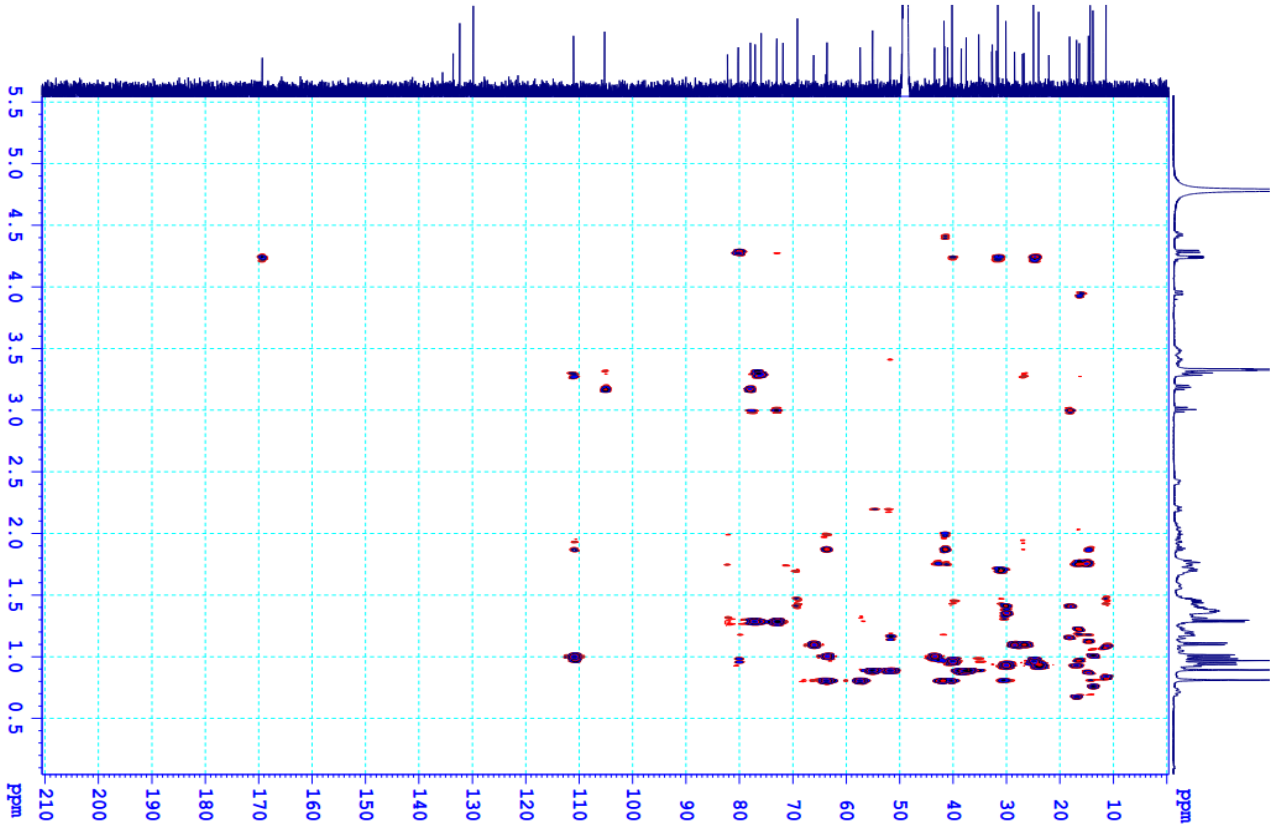

Figure S4. HMBC spectrum of compound **1**

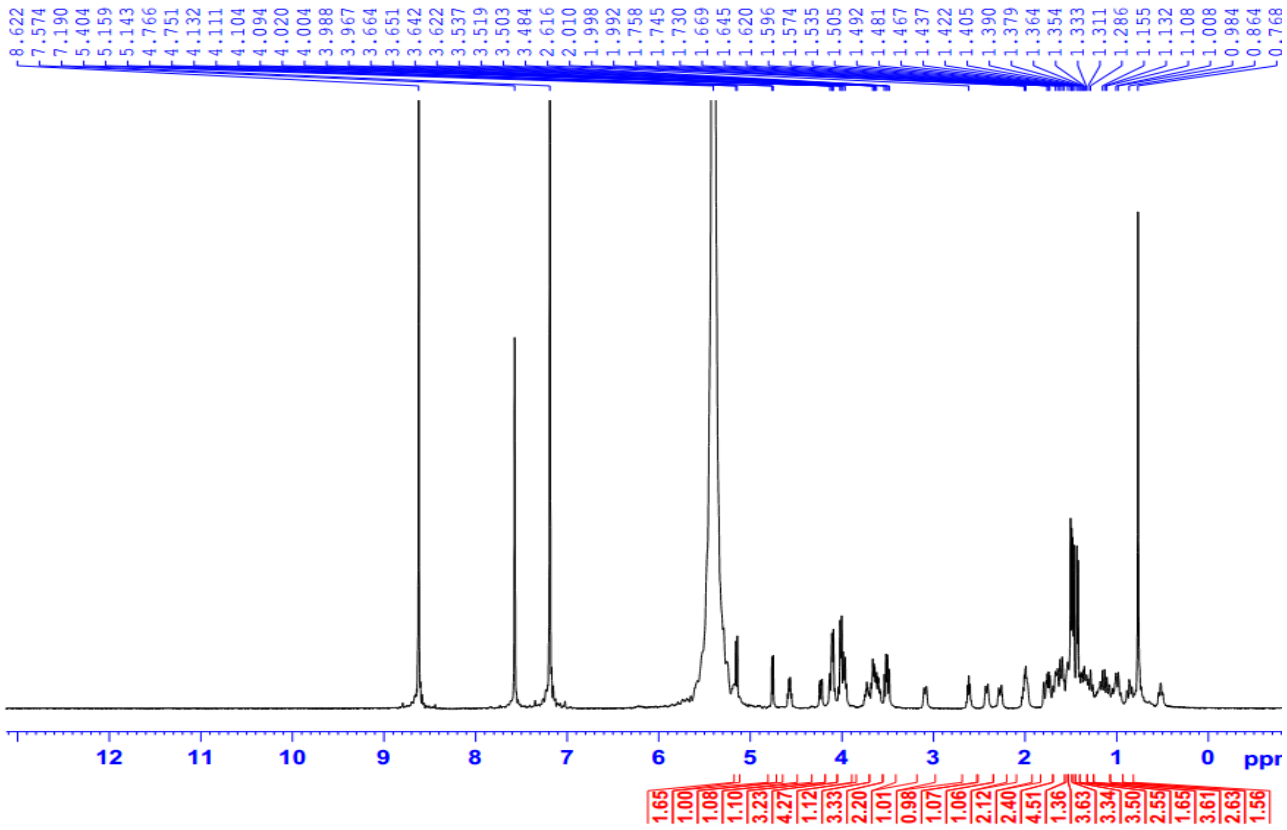

Figure S5. ^{1}H-NMR spectrum of compound **2** (in Pyridine-d_5, 500 MHz)

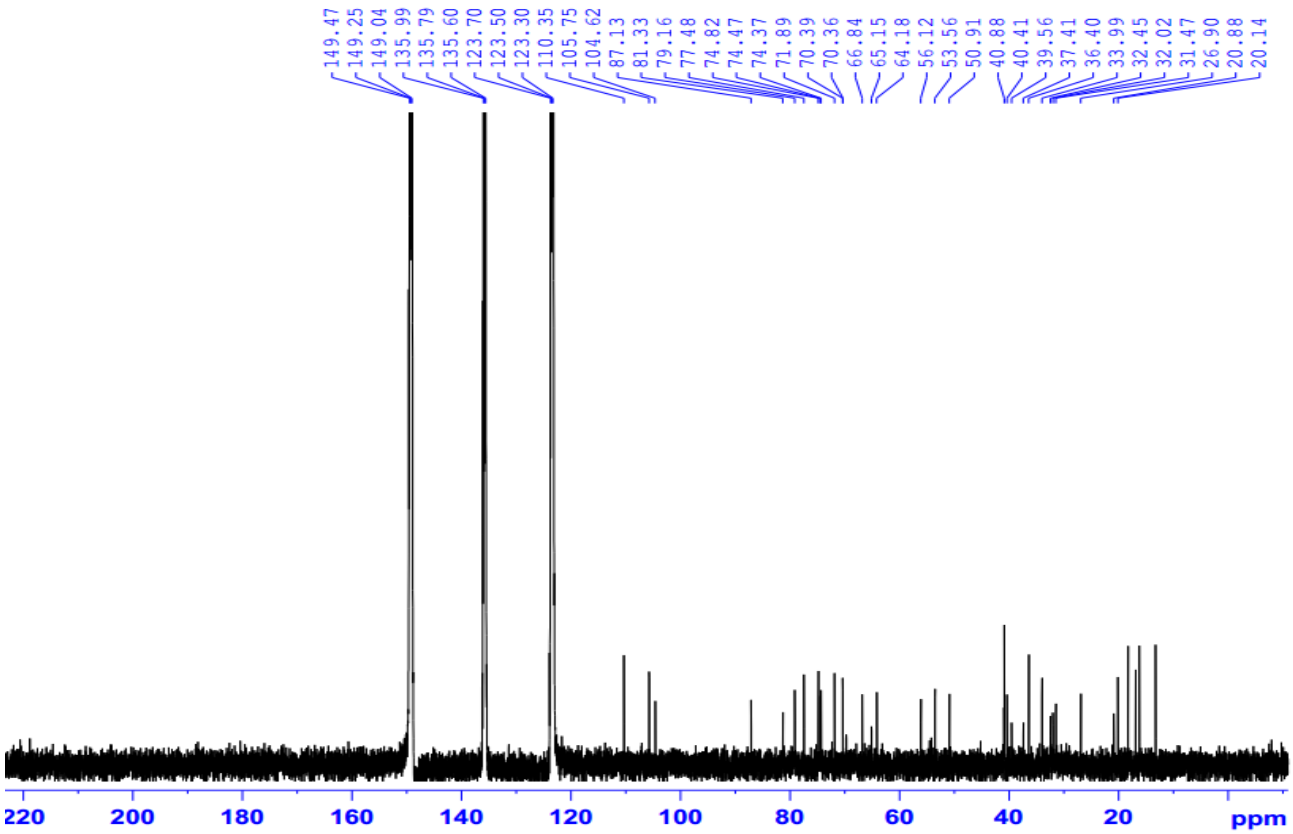

Figure S6. ^{13}C-NMR spectrum of compound **2** (in Pyridine-d_5, 125 MHz)

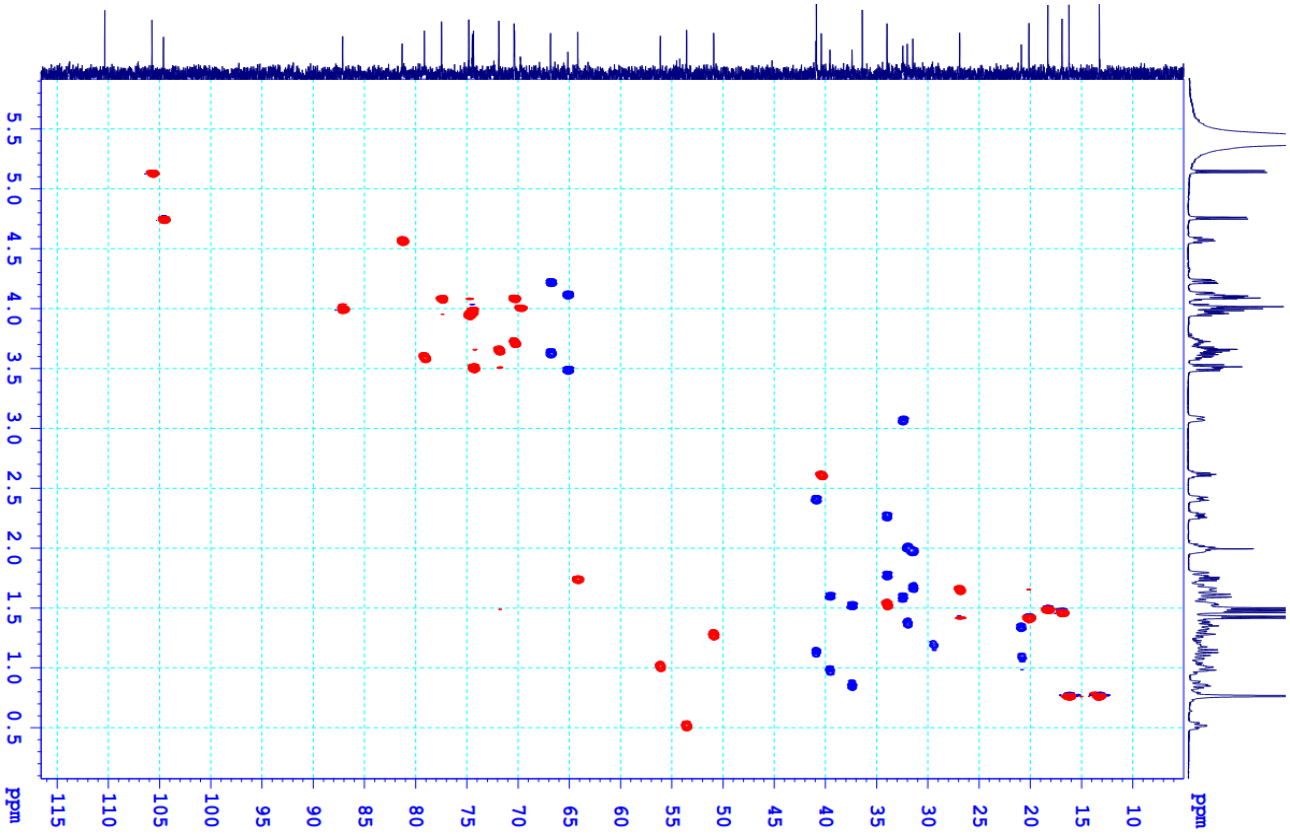

Figure S7. HSQC spectrum of compound **2**

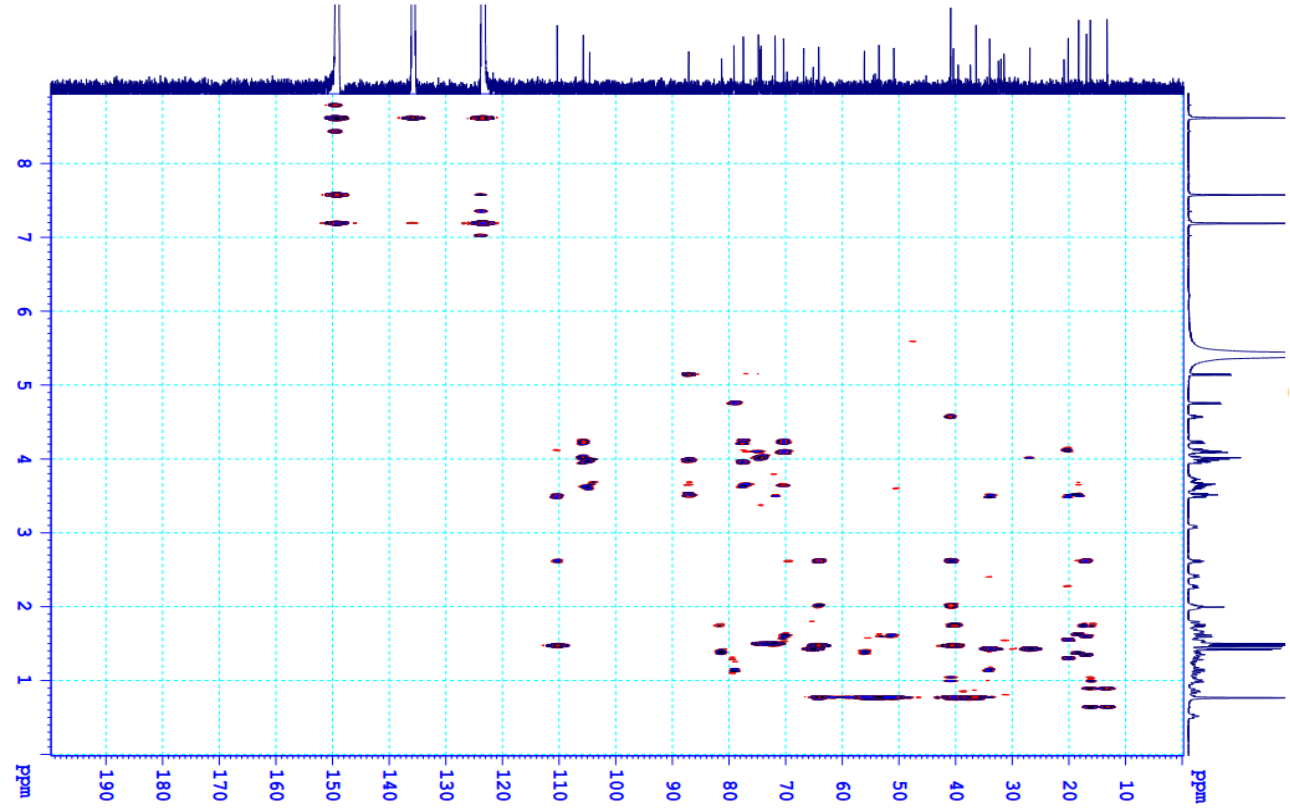

Figure S8. HMBC spectrum of compound **2**

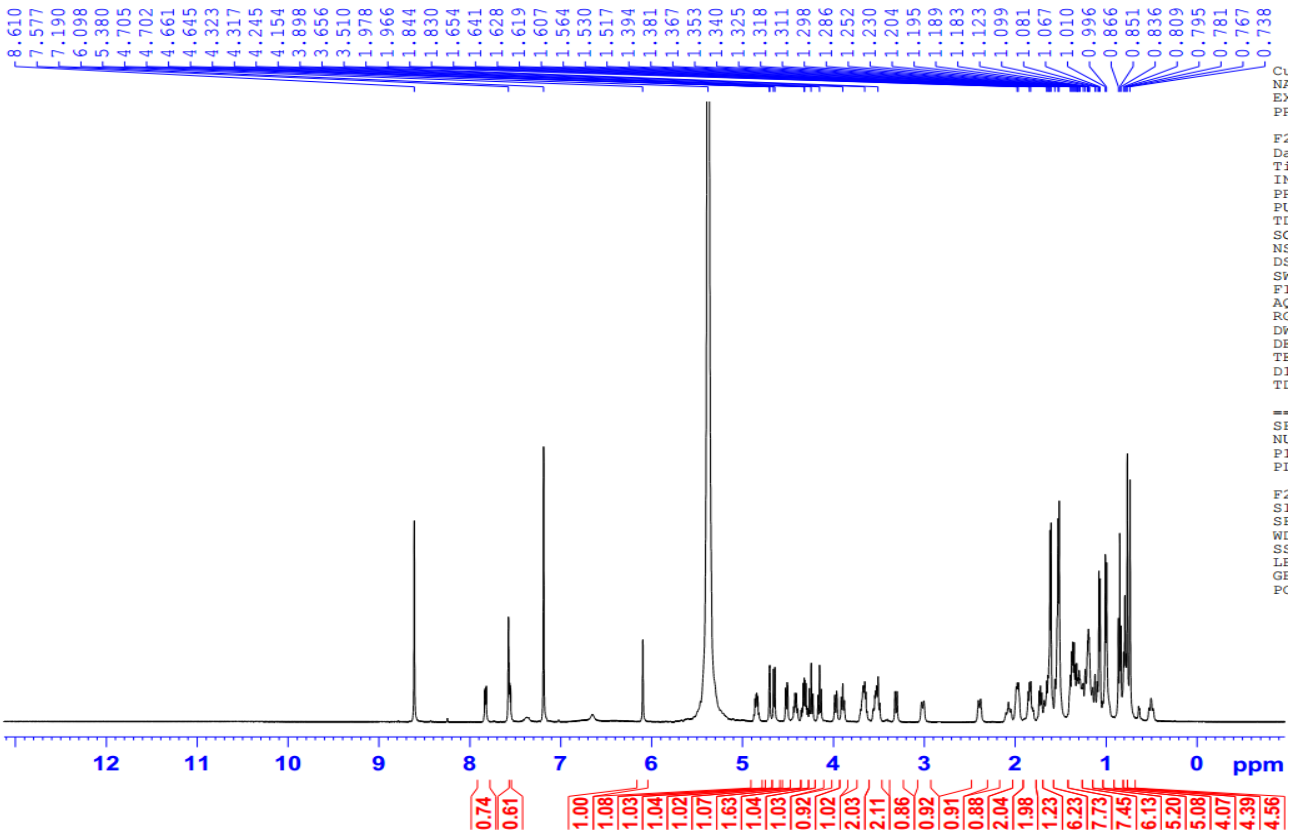

Figure S9. ^{1}H-NMR spectrum of compound **3** (in Pyridine-d_5, 500 MHz)

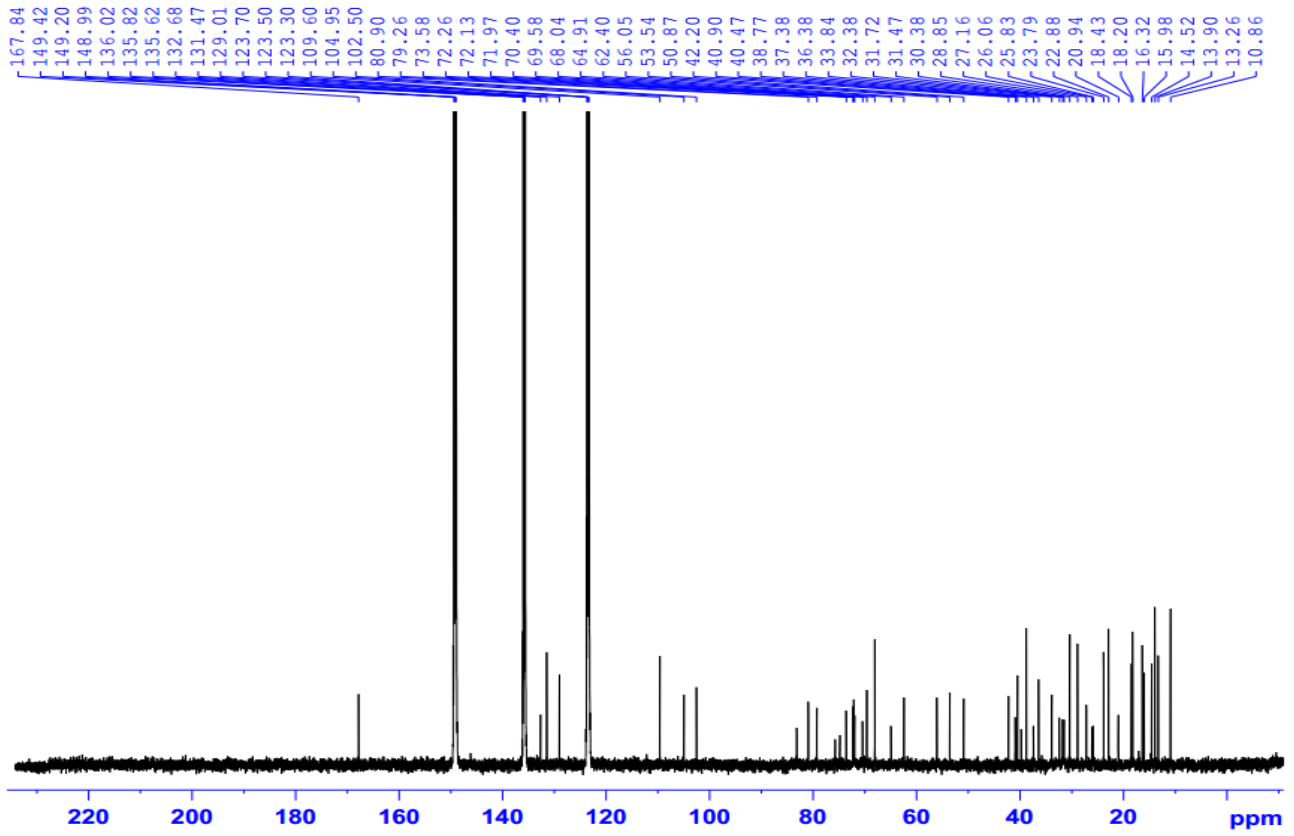

Figure S10. ^{13}C-NMR spectrum of compound **3** (in Pyridine-d_5, 125 MHz)

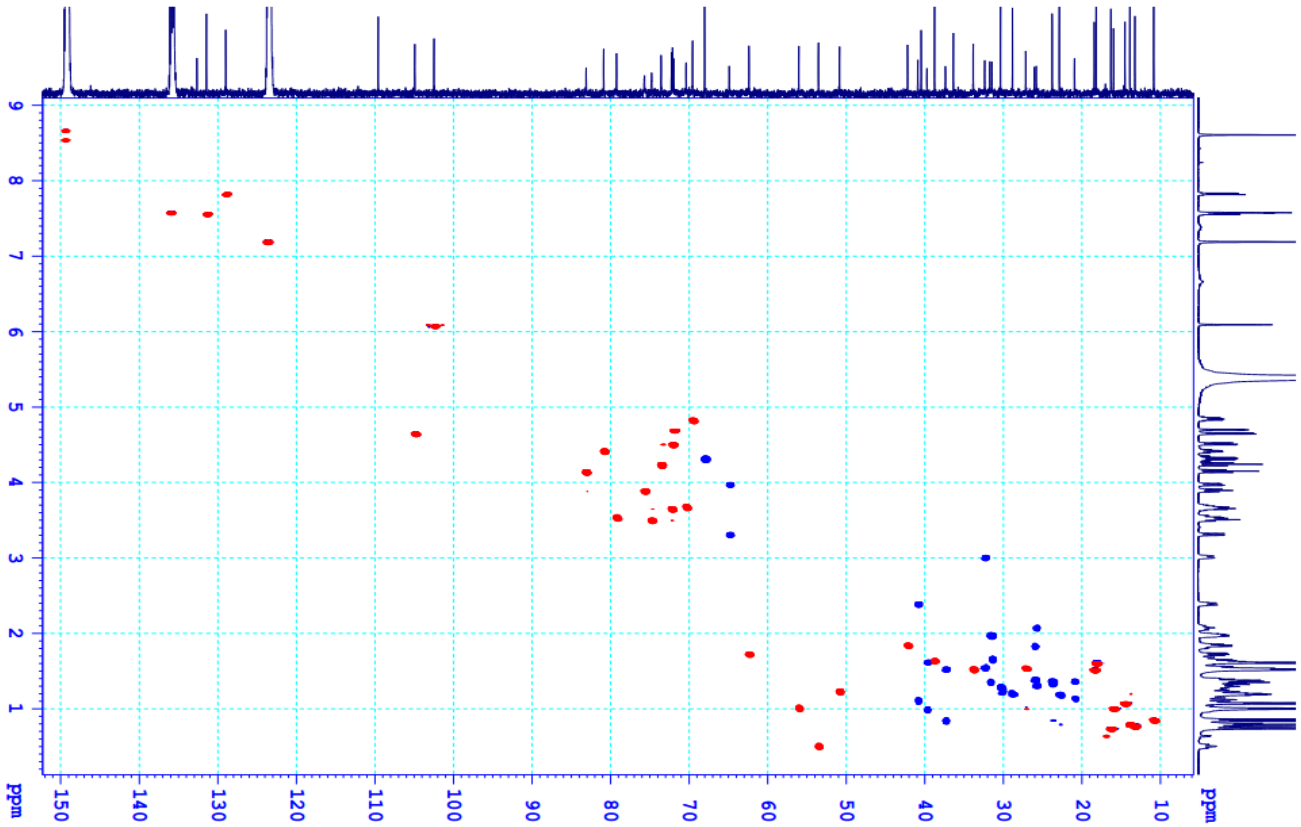

Figure S11. HSQC spectrum of compound **3**

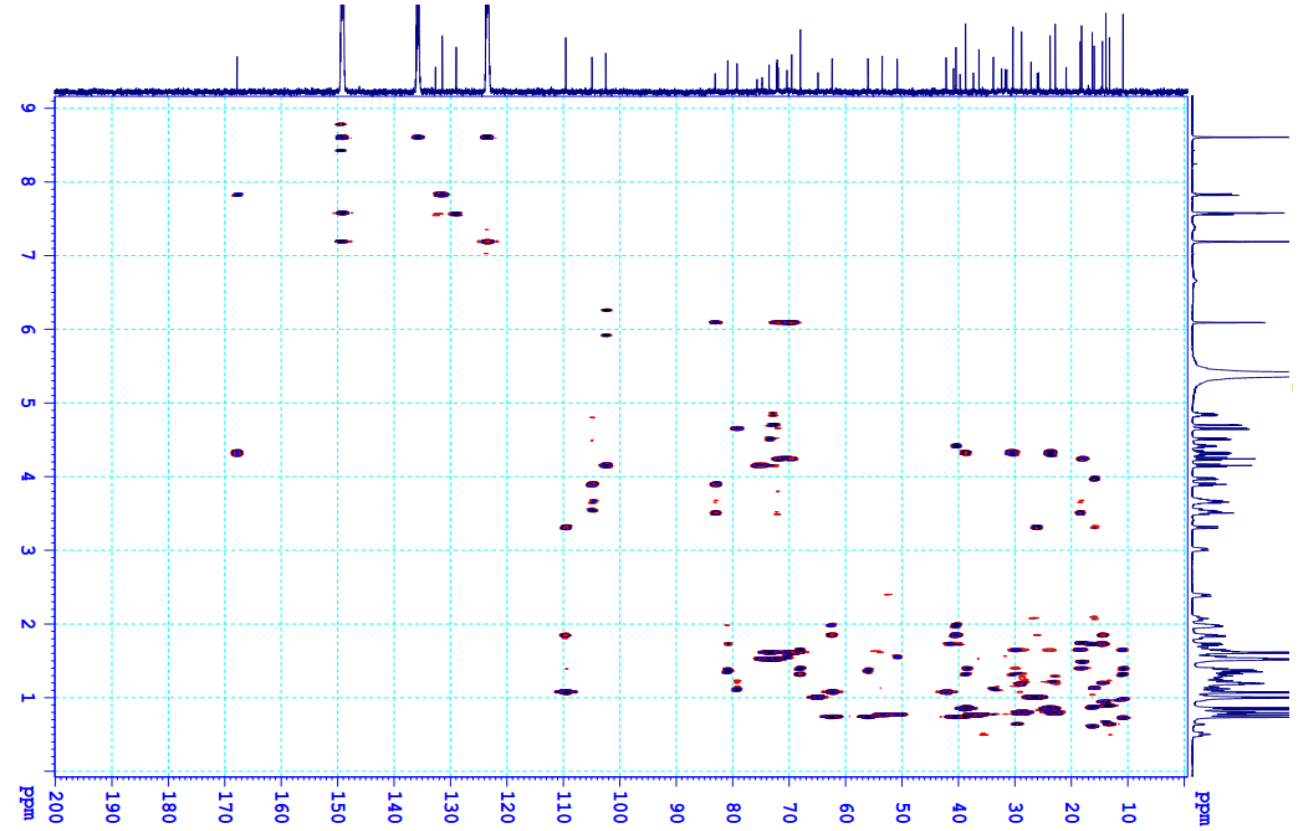

Figure S12. HMBC spectrum of compound **3**

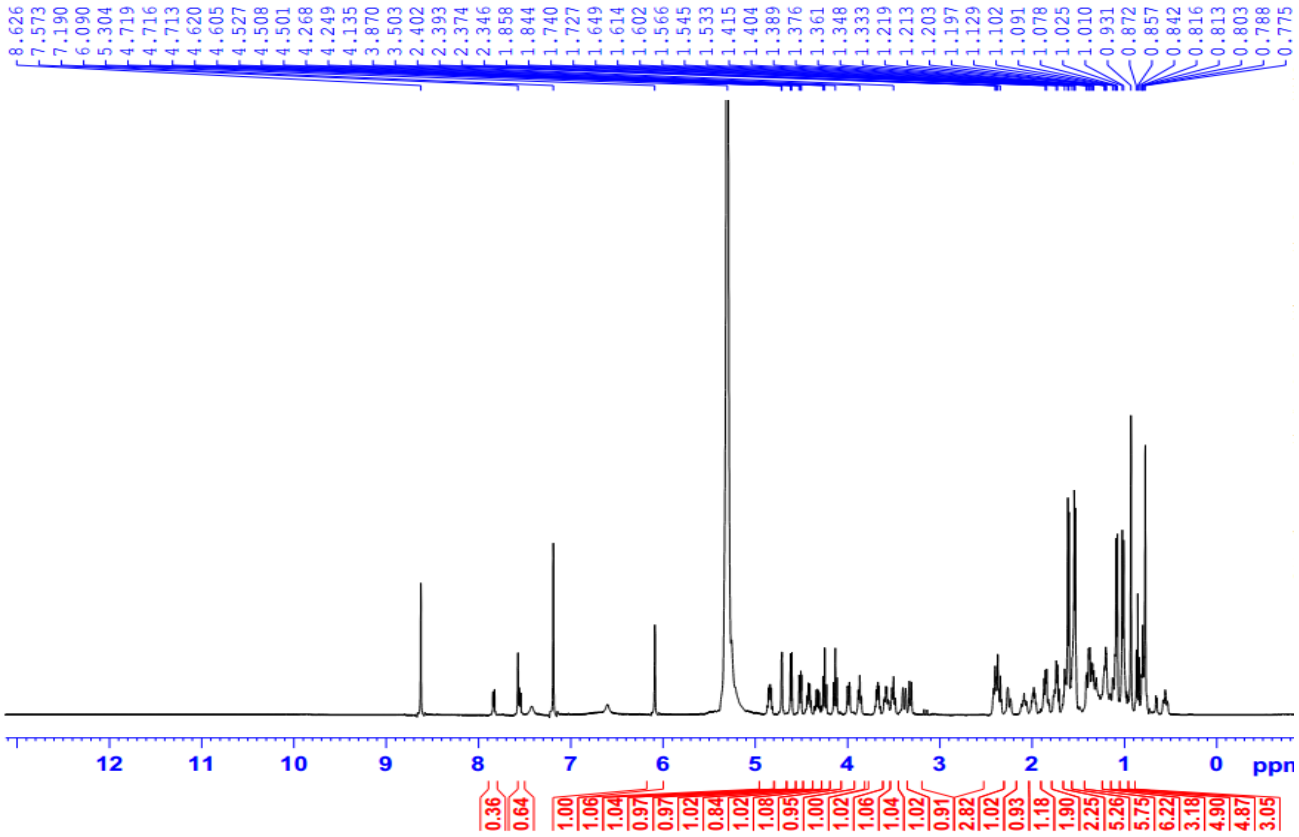

Figure S13. ^{1}H-NMR spectrum of compound **4** (in Pyridine-d_5, 500 MHz)

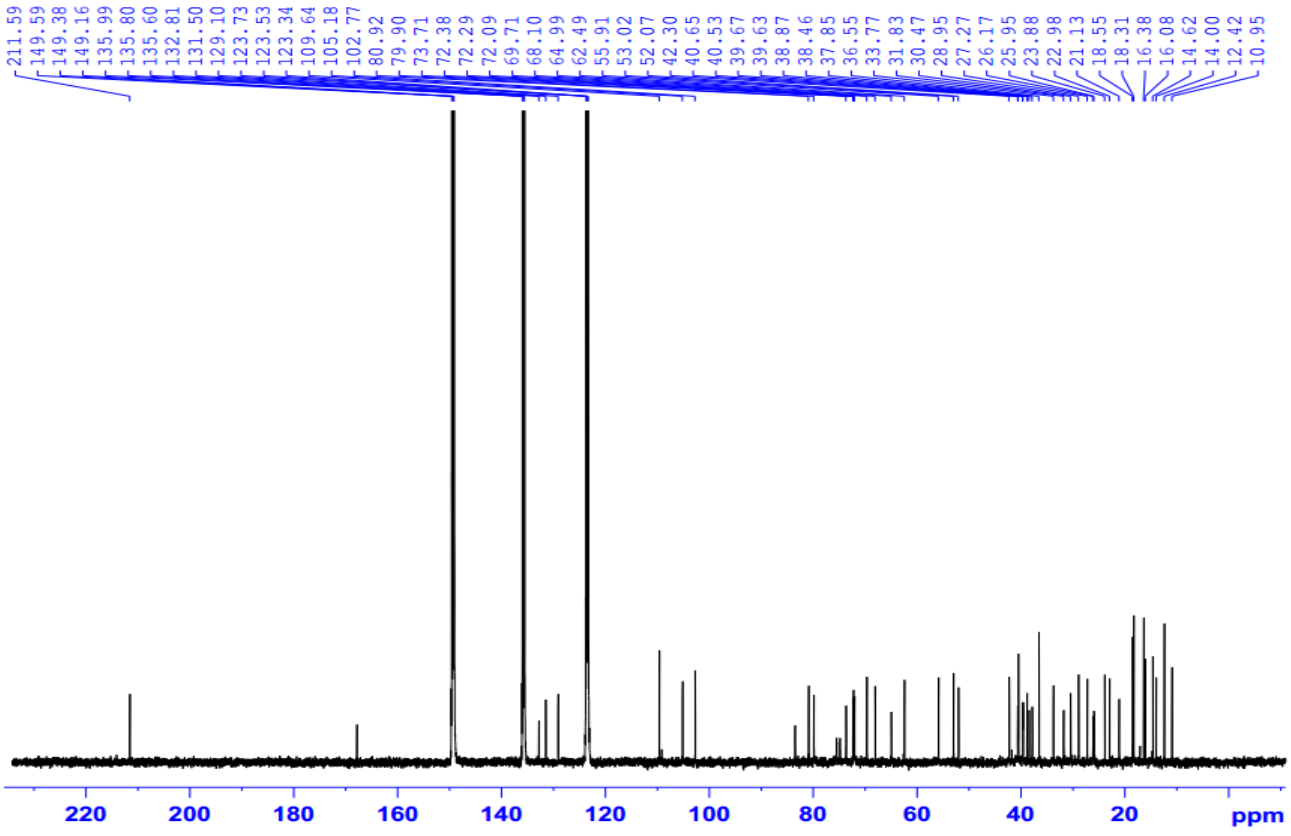

Figure S14. ^{13}C-NMR spectrum of compound **4** (in Pyridine-d_5, 125 MHz)

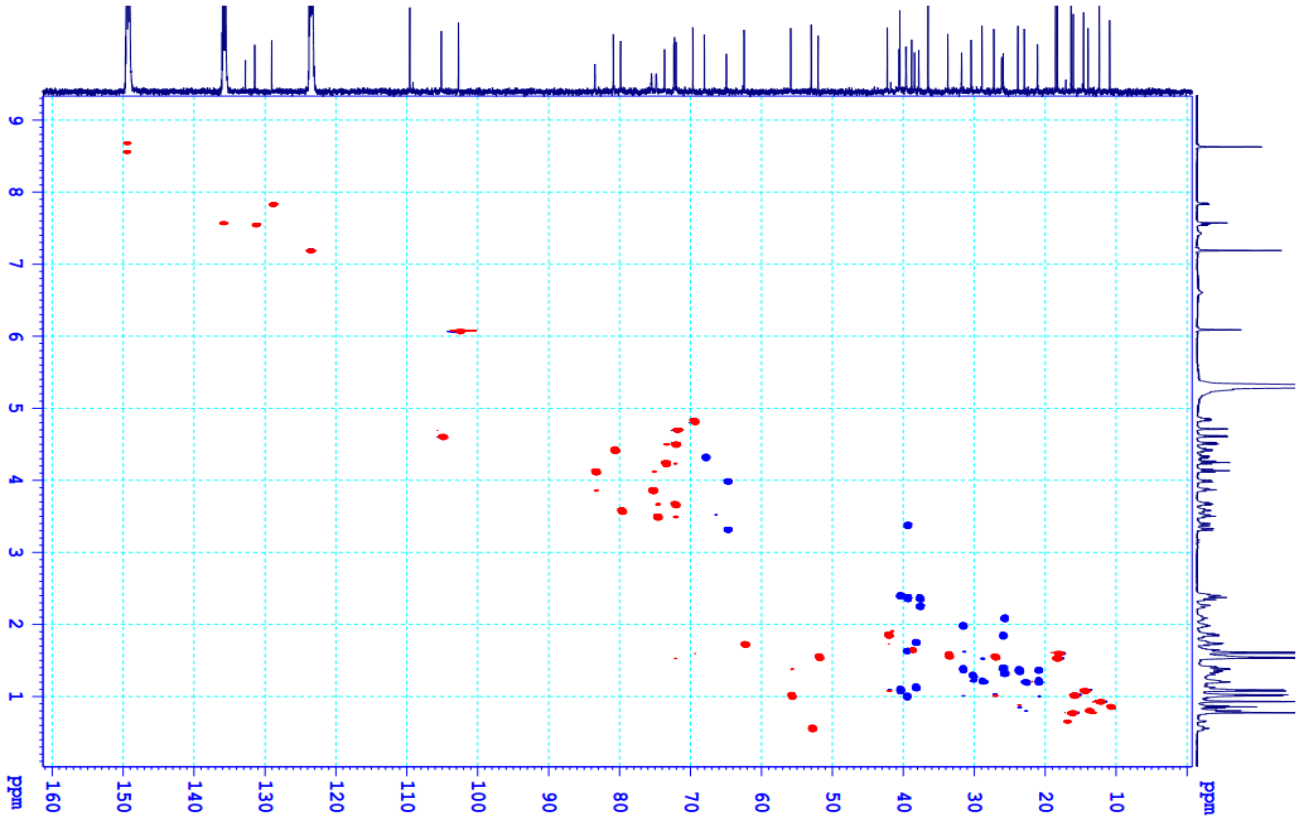

Figure S15. HSQC spectrum of compound **4**

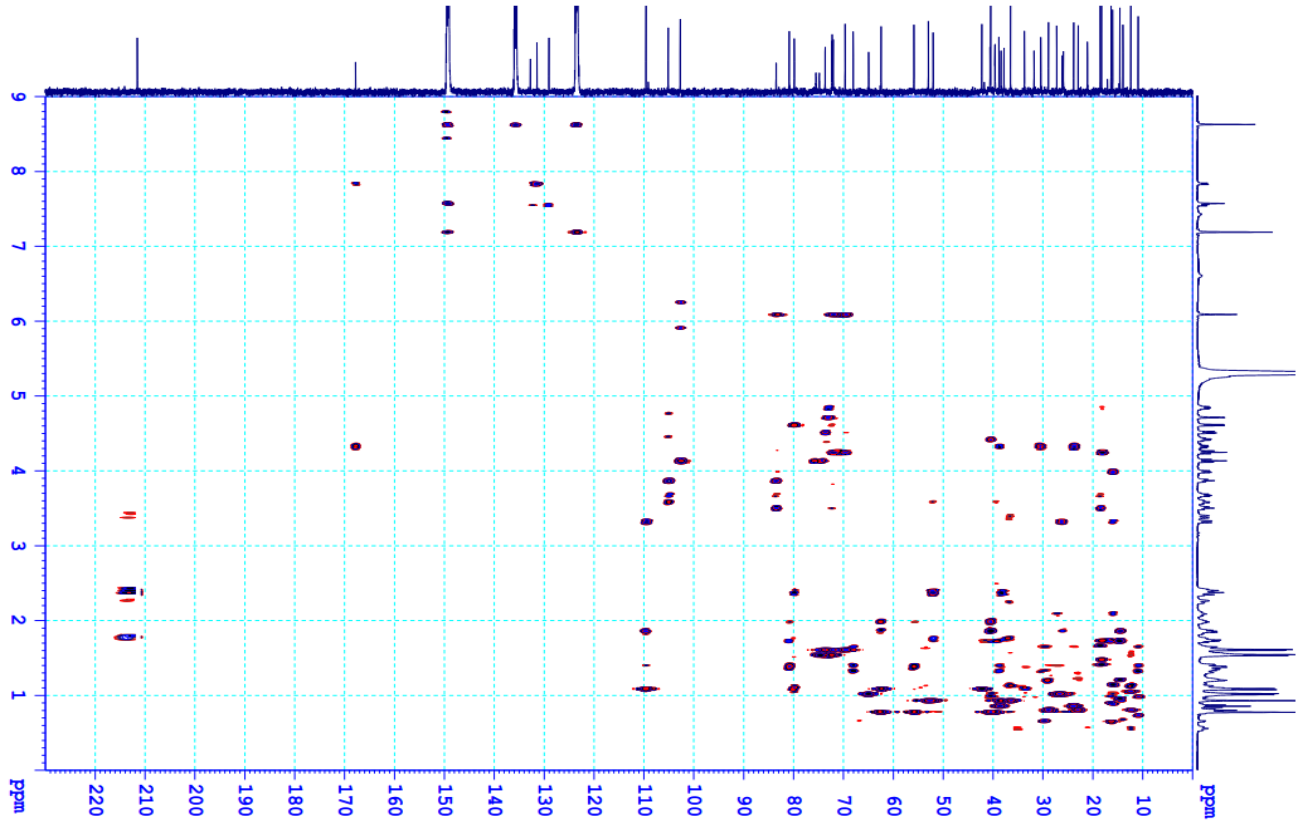

Figure S16. HMBC spectrum of compound **4**

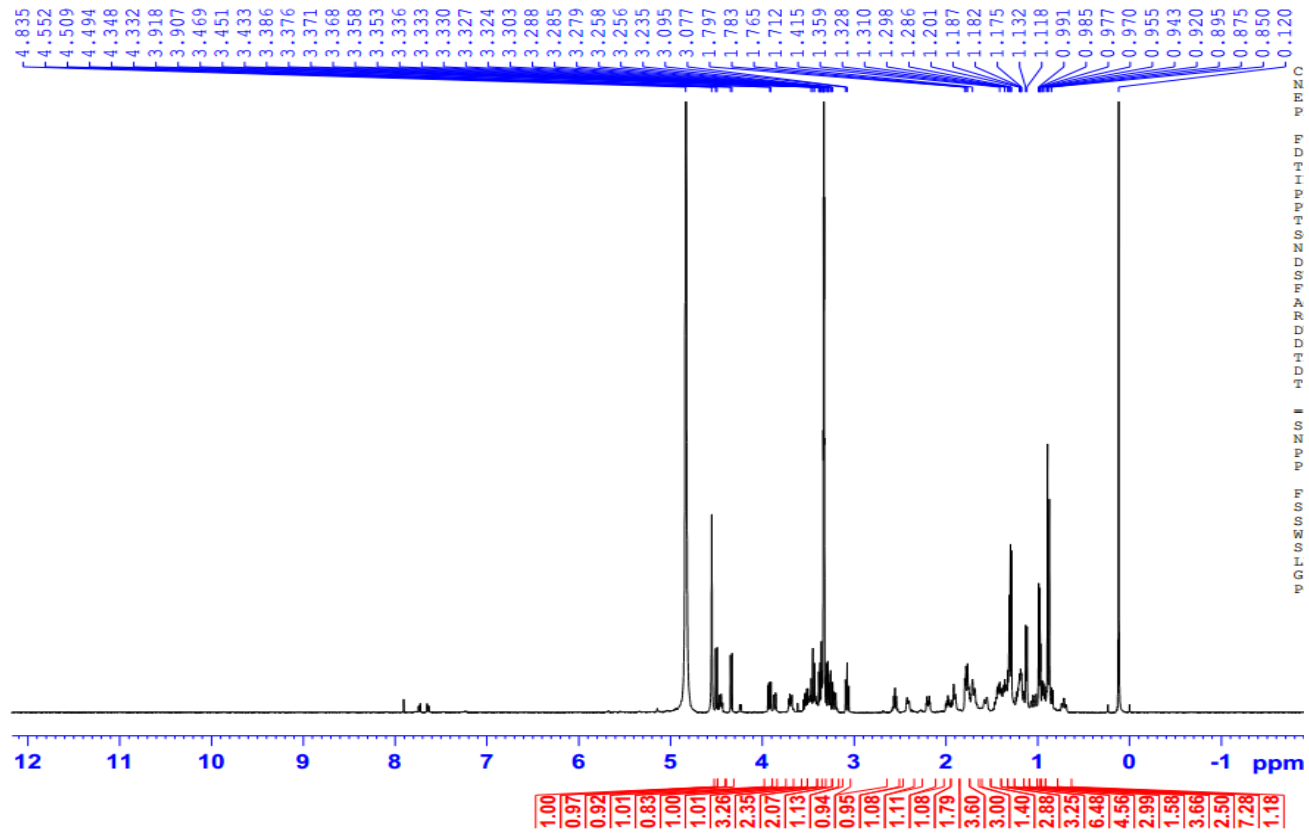

Figure S17. [1]H-NMR spectrum of compound **5** (in MeOD, 500 MHz)

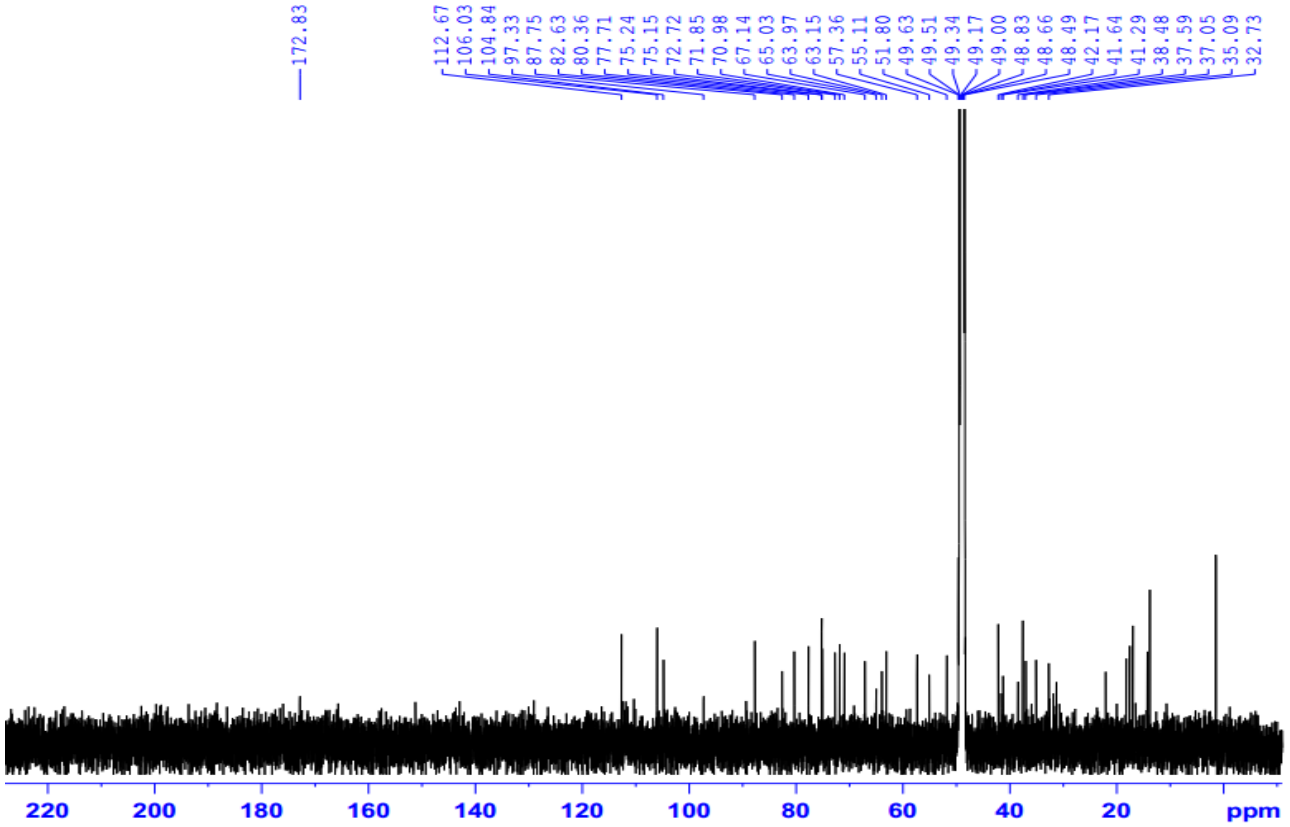

Figure S18. [13]C-NMR spectrum of compound **5** (in MeOD, 125 MHz)

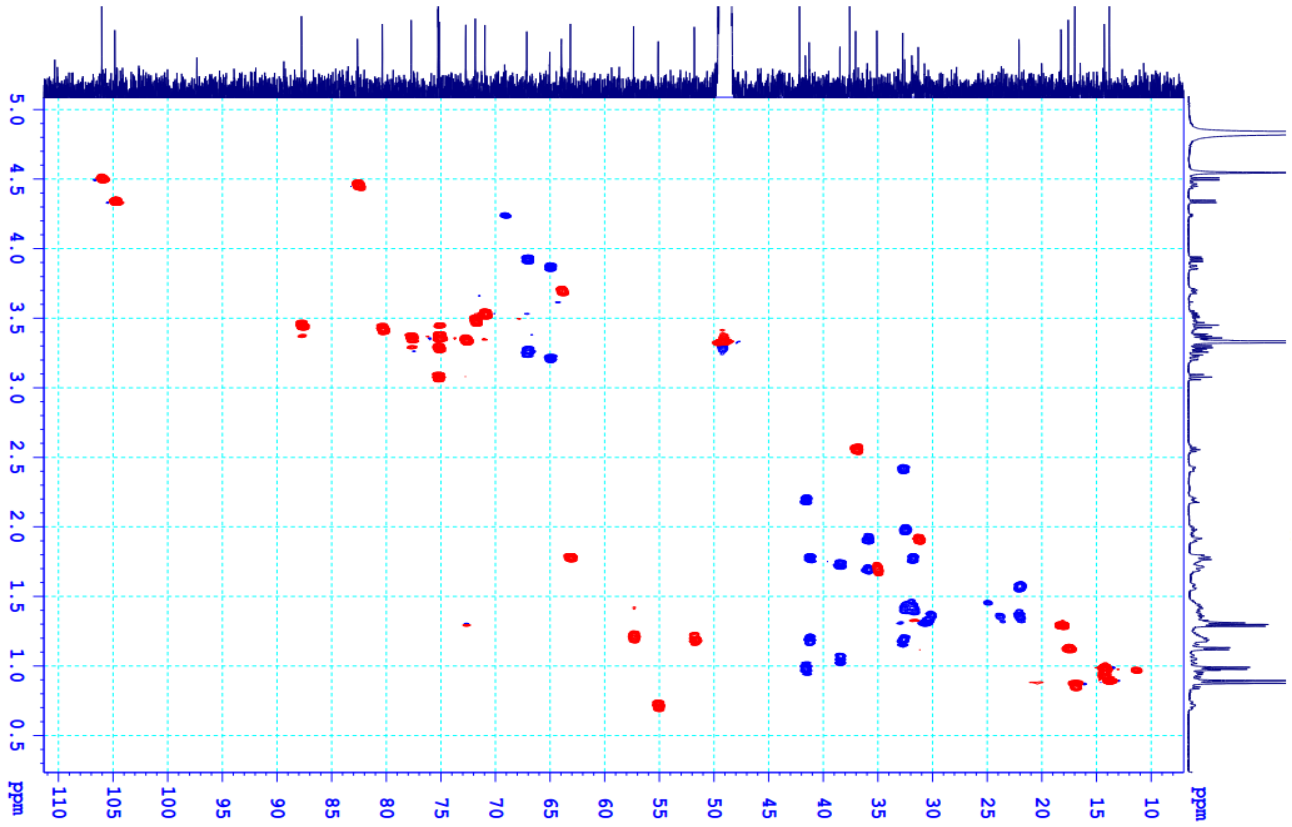

Figure S19. HSQC spectrum of compound **5**

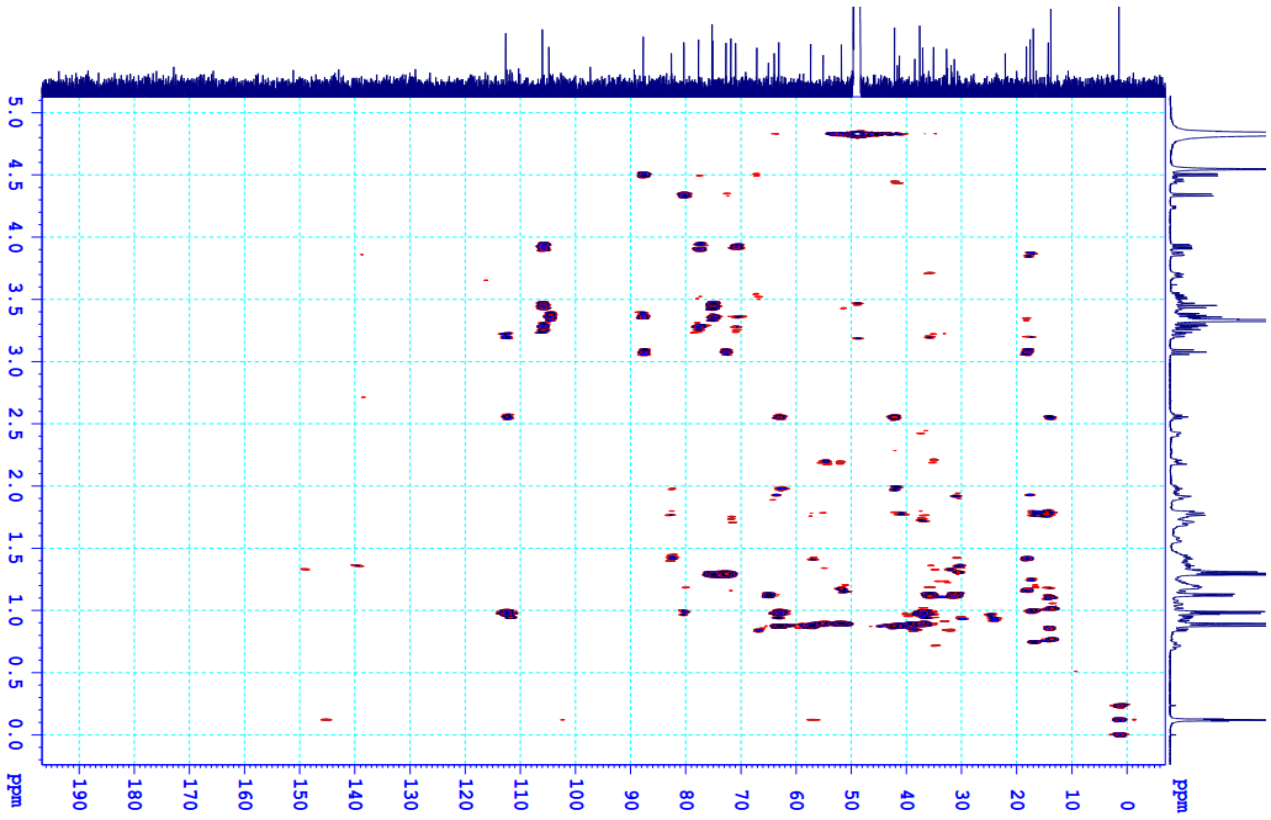

Figure S20. HMBC spectrum of compound **5**

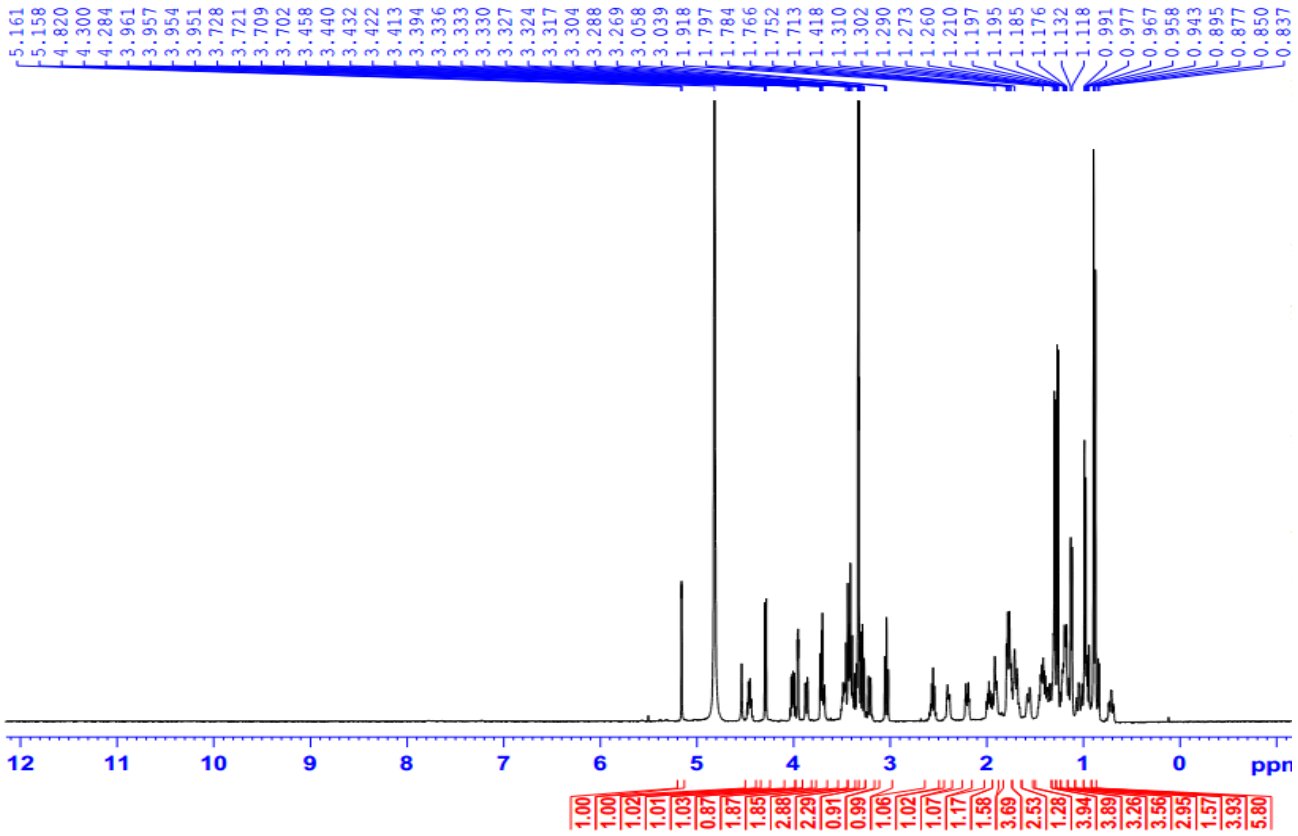

Figure S21. [1]H-NMR spectrum of compound **6** (in MeOD, 500 MHz)

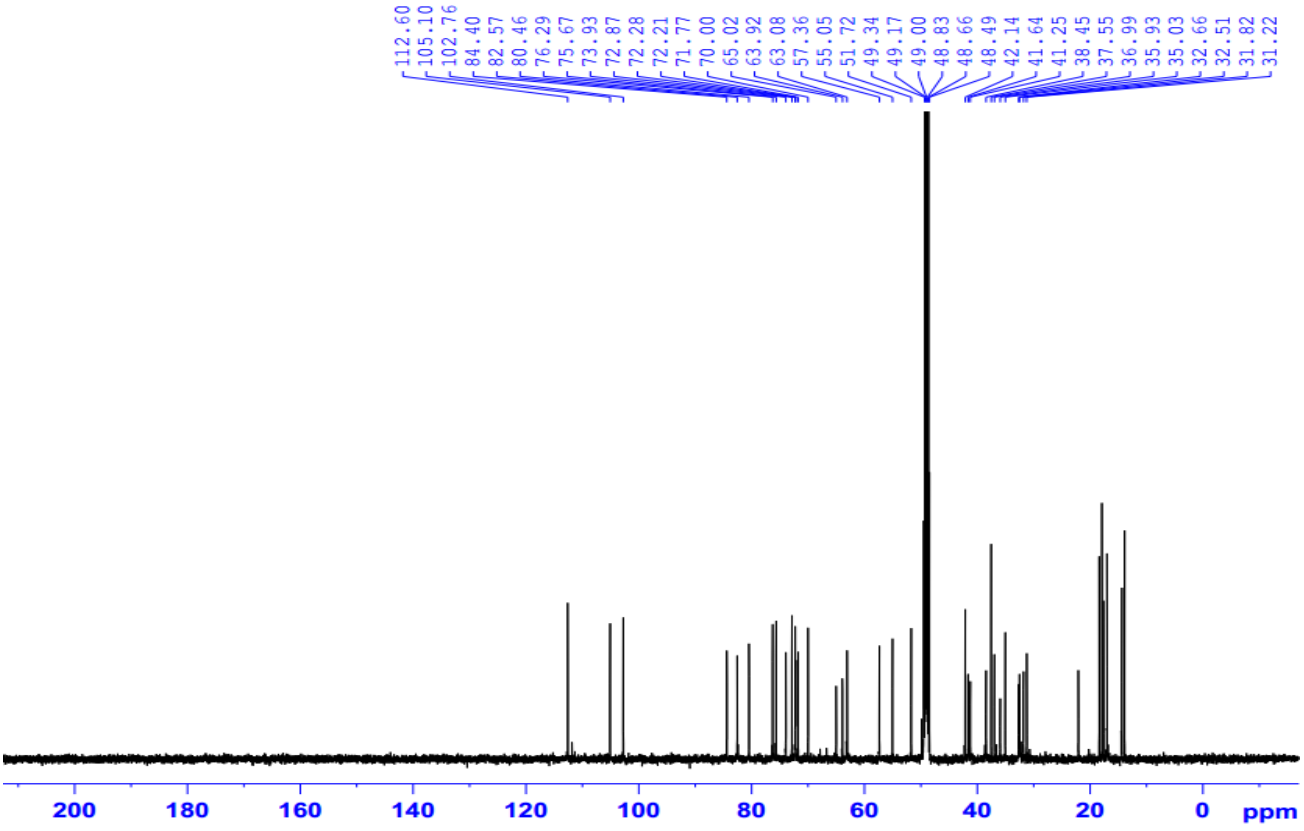

Figure S22. [13]C-NMR spectrum of compound **6** (in MeOD, 125 MHz)

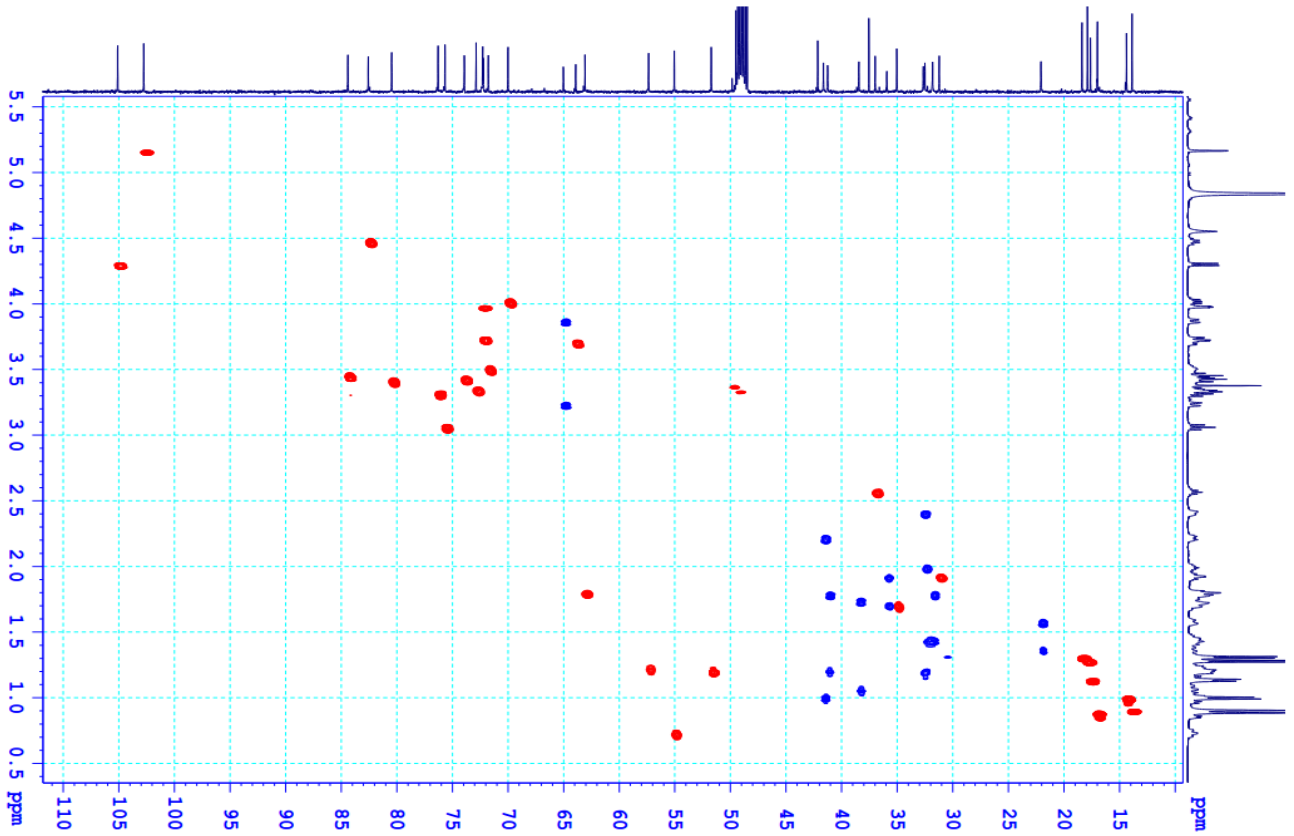

Figure S23. HSQC spectrum of compound **6**

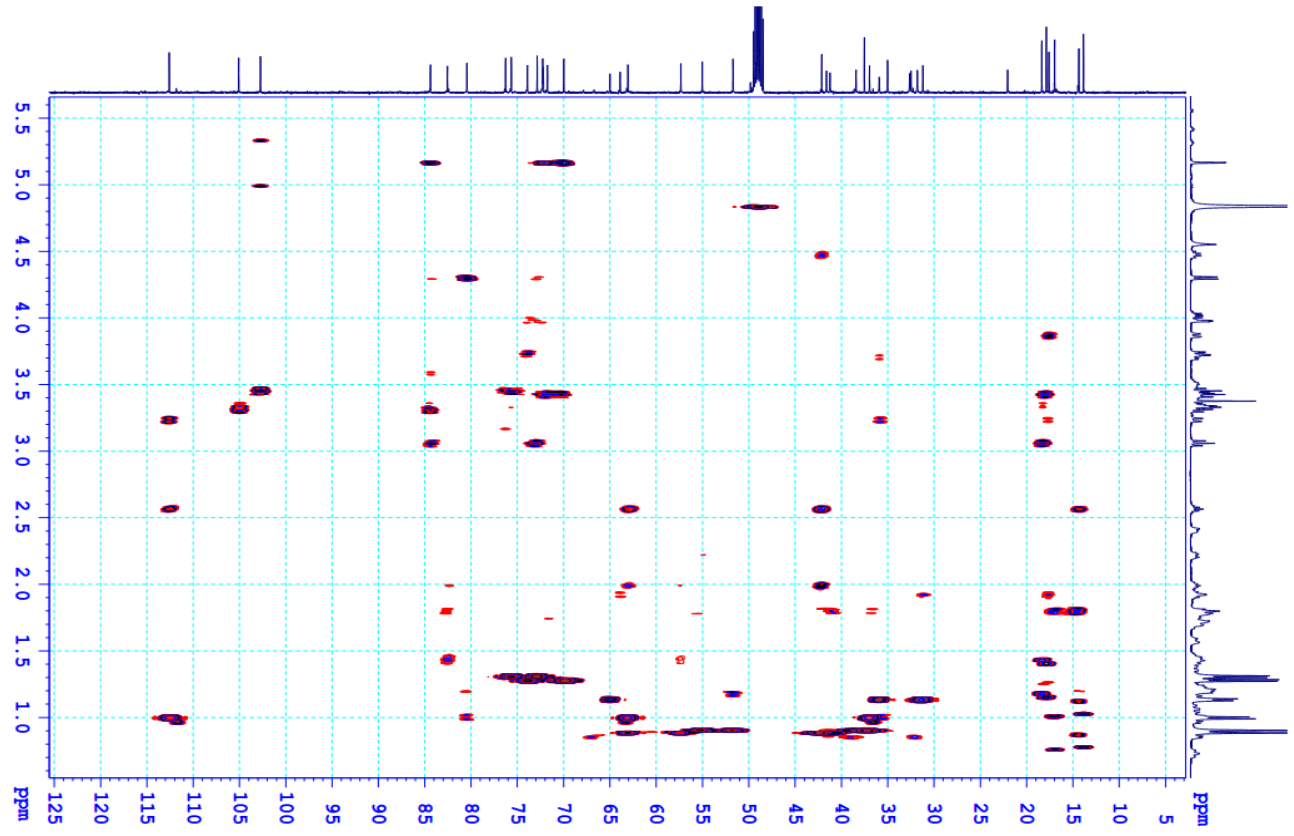

Figure S24. HMBC spectrum of compound **6**

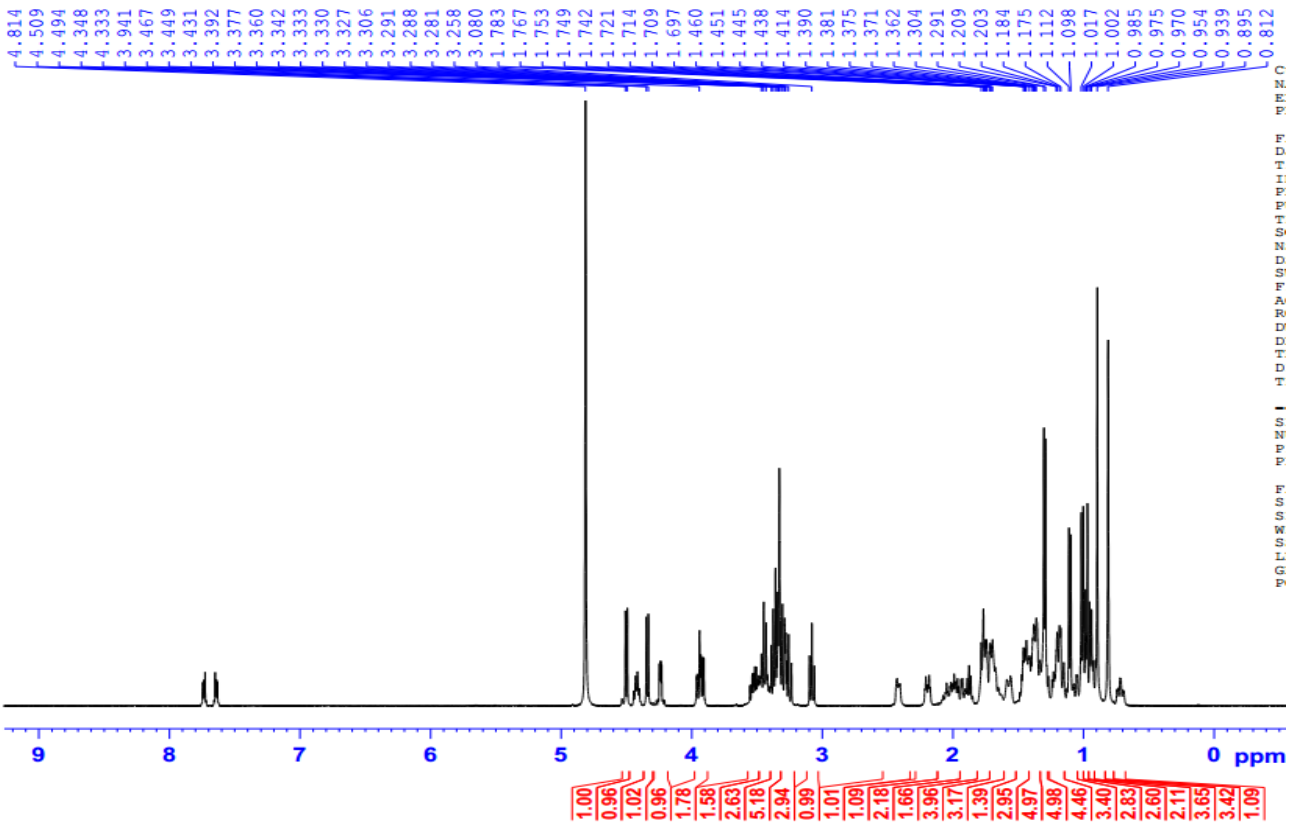

Figure S25. [1]H-NMR spectrum of compound **7** (in MeOD, 500 MHz)

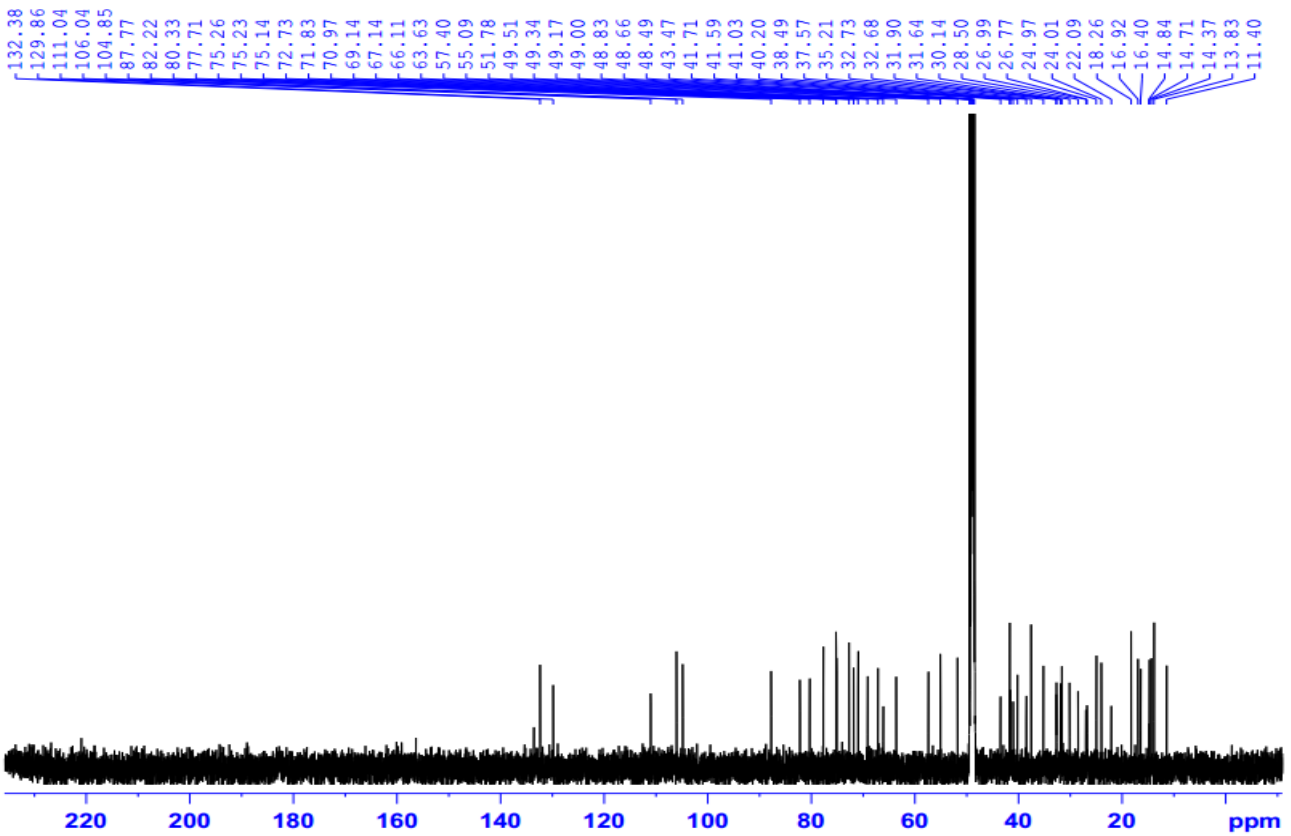

Figure S26. [13]C-NMR spectrum of compound **7** (in MeOD, 125 MHz)

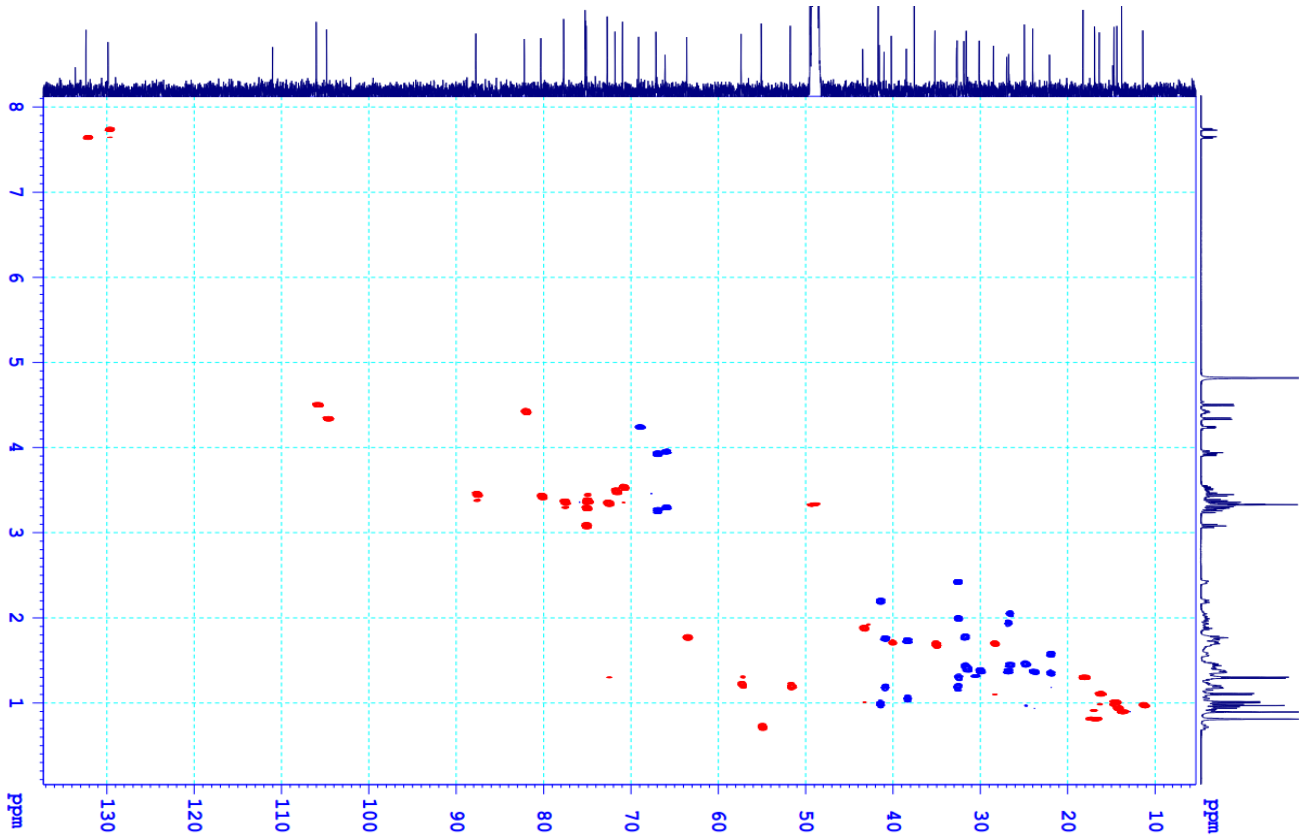

Figure S27. HSQC spectrum of compound **7**

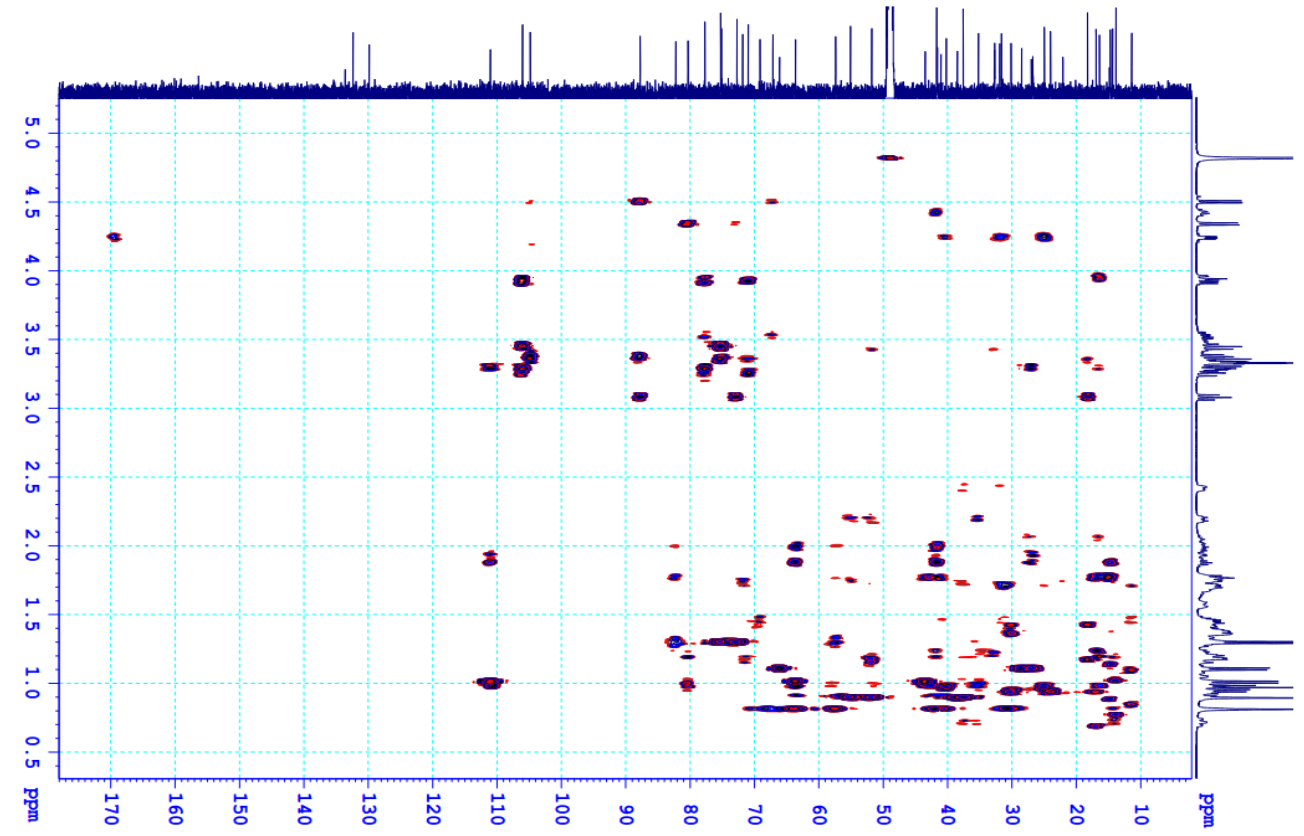

Figure S28. HMBC spectrum of compound **7**

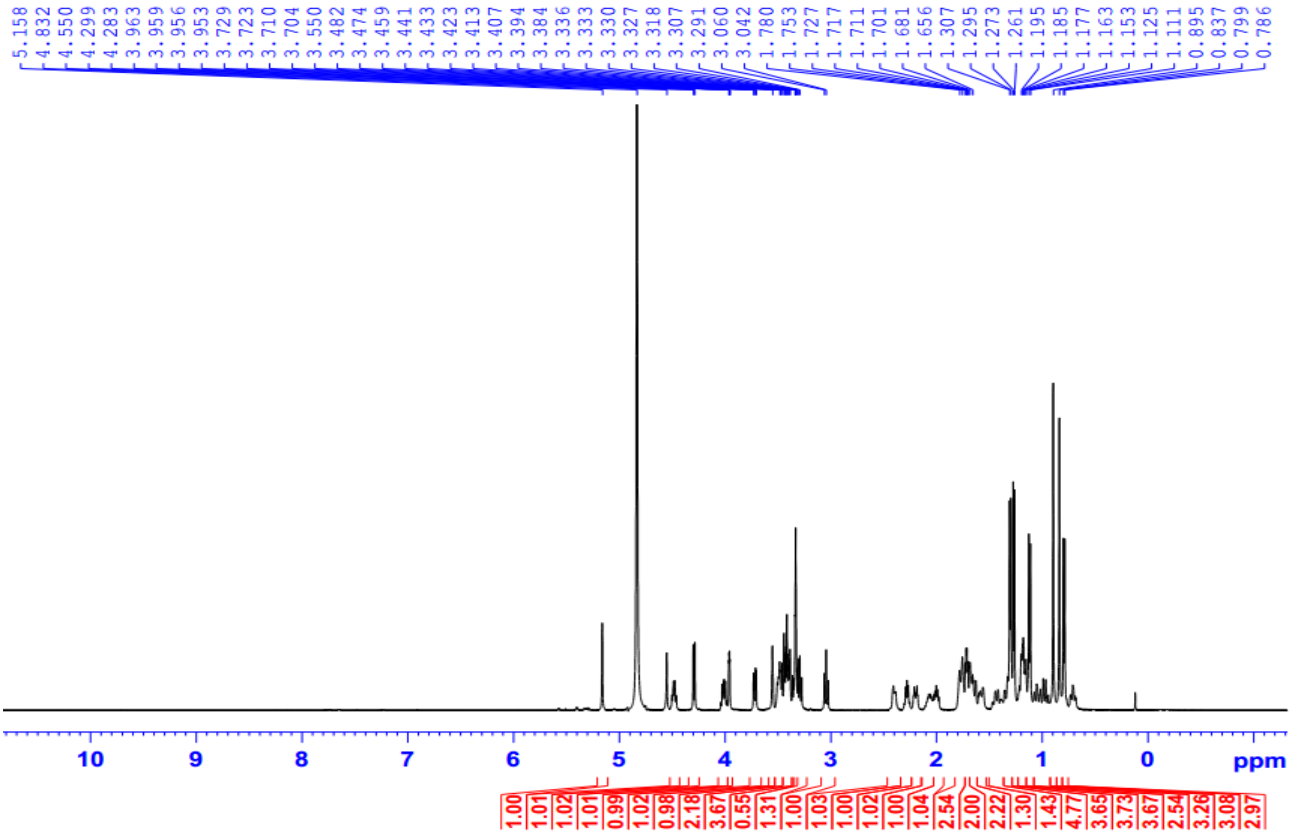

Figure S29. ^{1}H-NMR spectrum of compound **8** (in MeOD, 500 MHz)

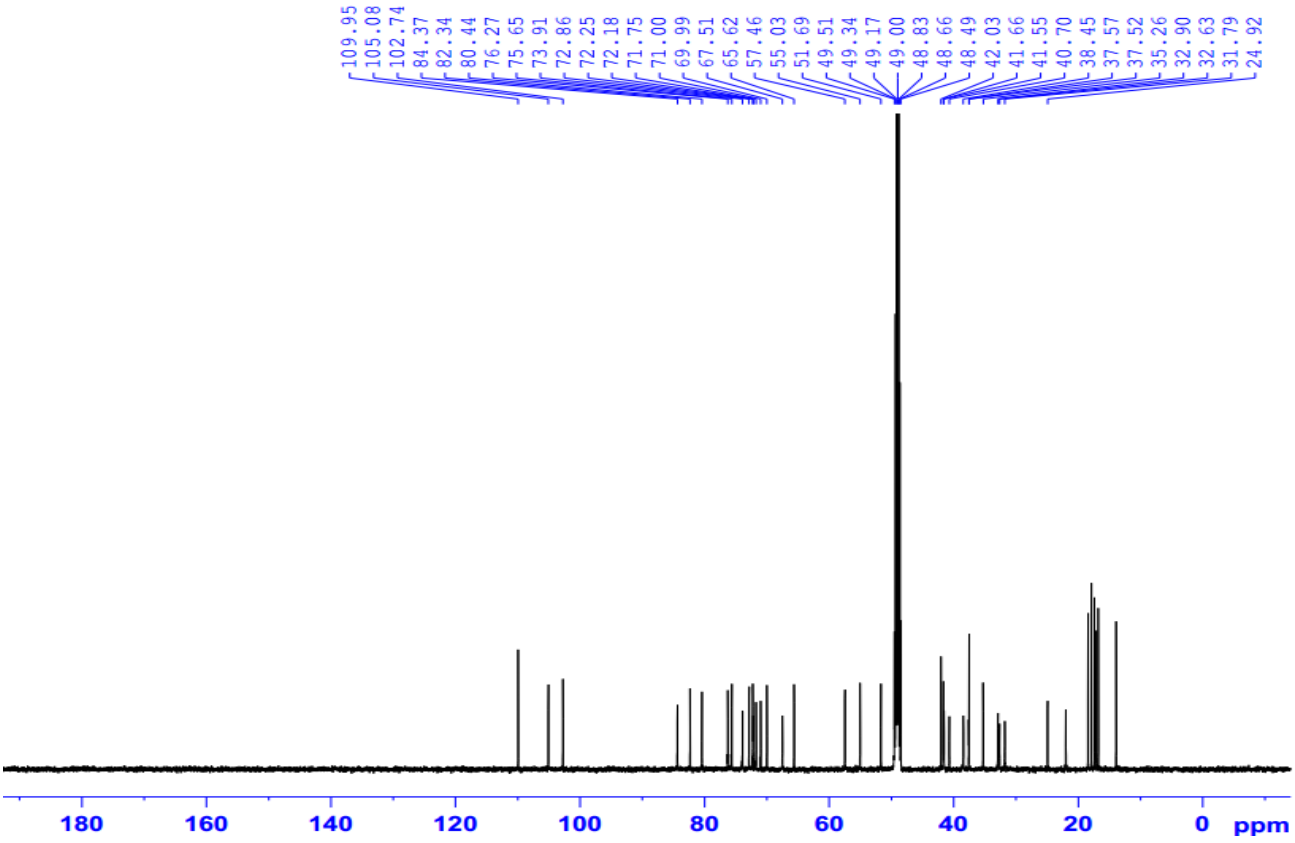

Figure S30. ^{13}C-NMR spectrum of compound **8** (in MeOD, 125 MHz)

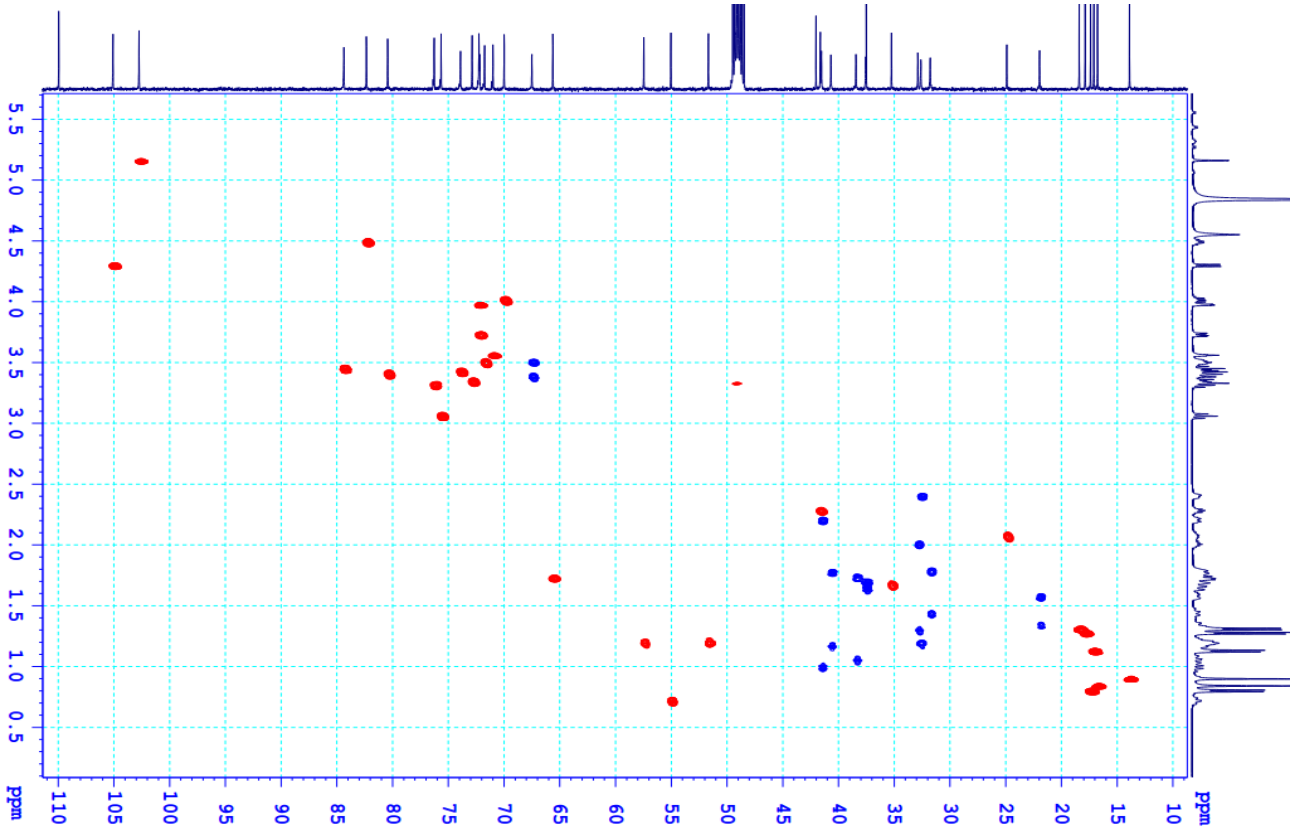

Figure S31. HSQC spectrum of compound **8**

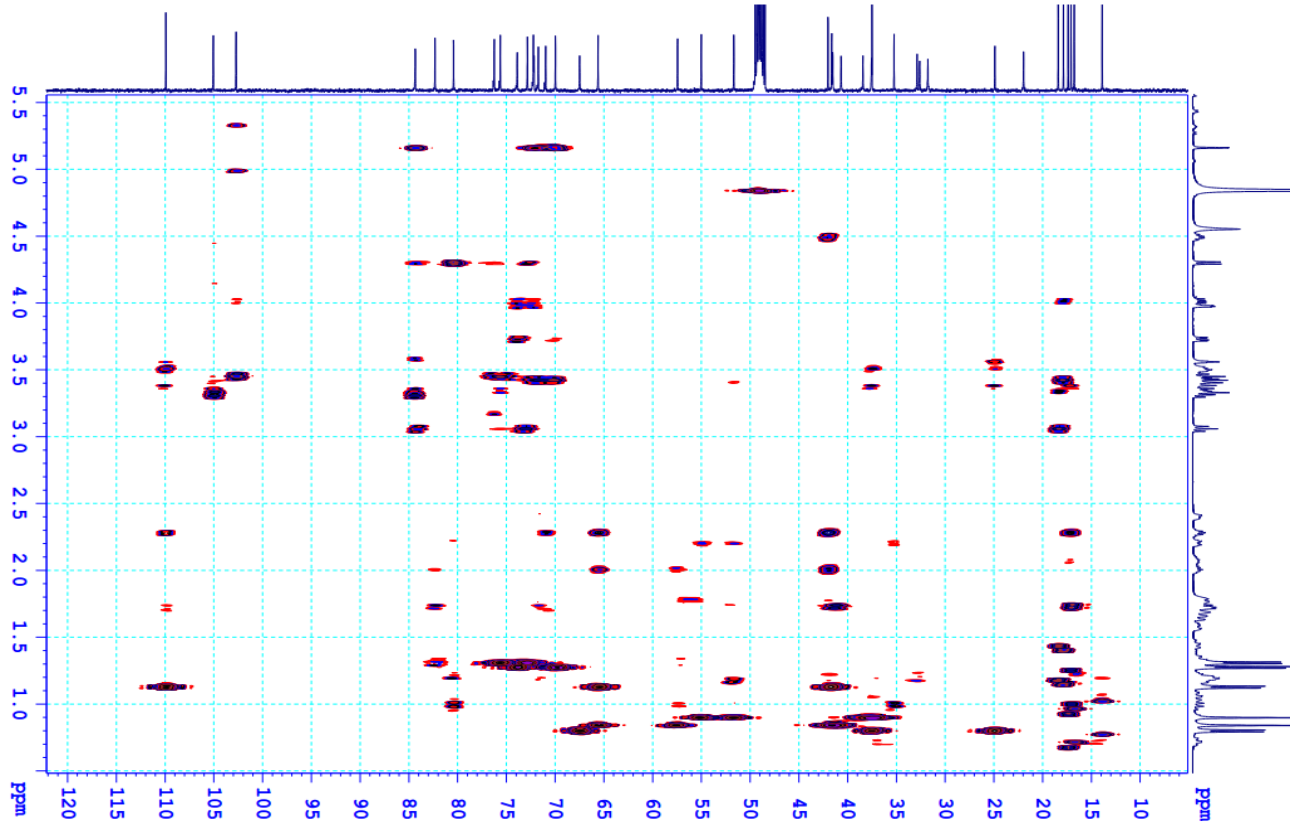

Figure S32. HMBC spectrum of compound **8**

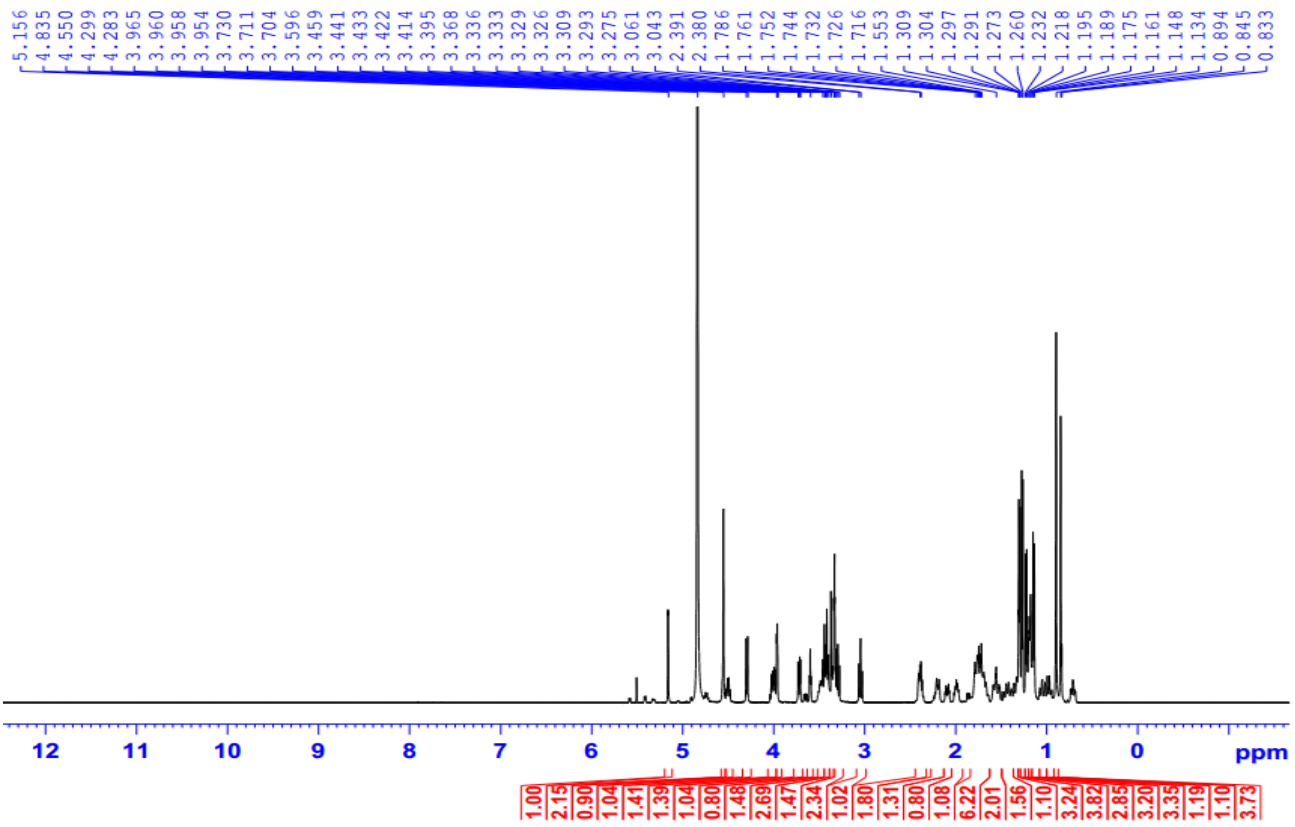

Figure S33. [1]H-NMR spectrum of compound **9** (in MeOD, 500 MHz)

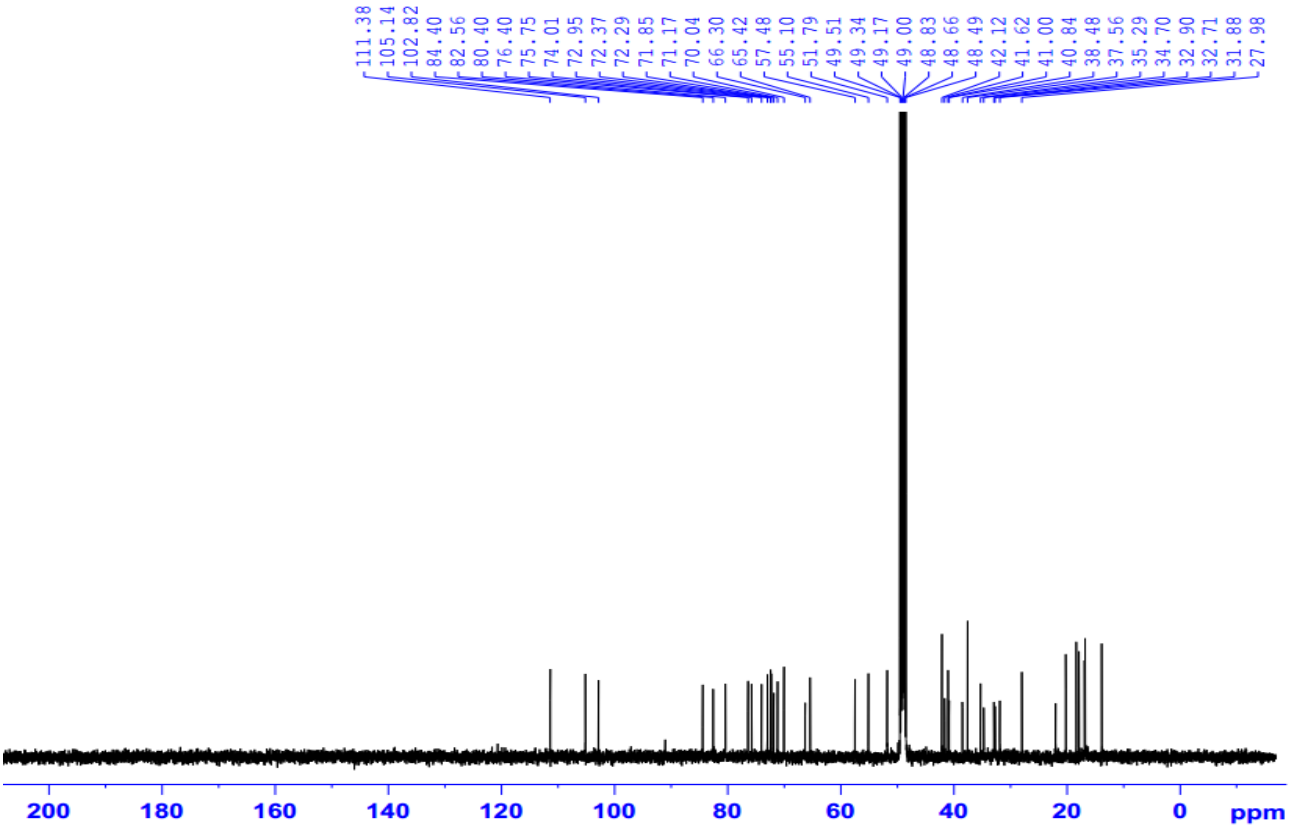

Figure S34. [13]C-NMR spectrum of compound **9** (in MeOD, 125 MHz)

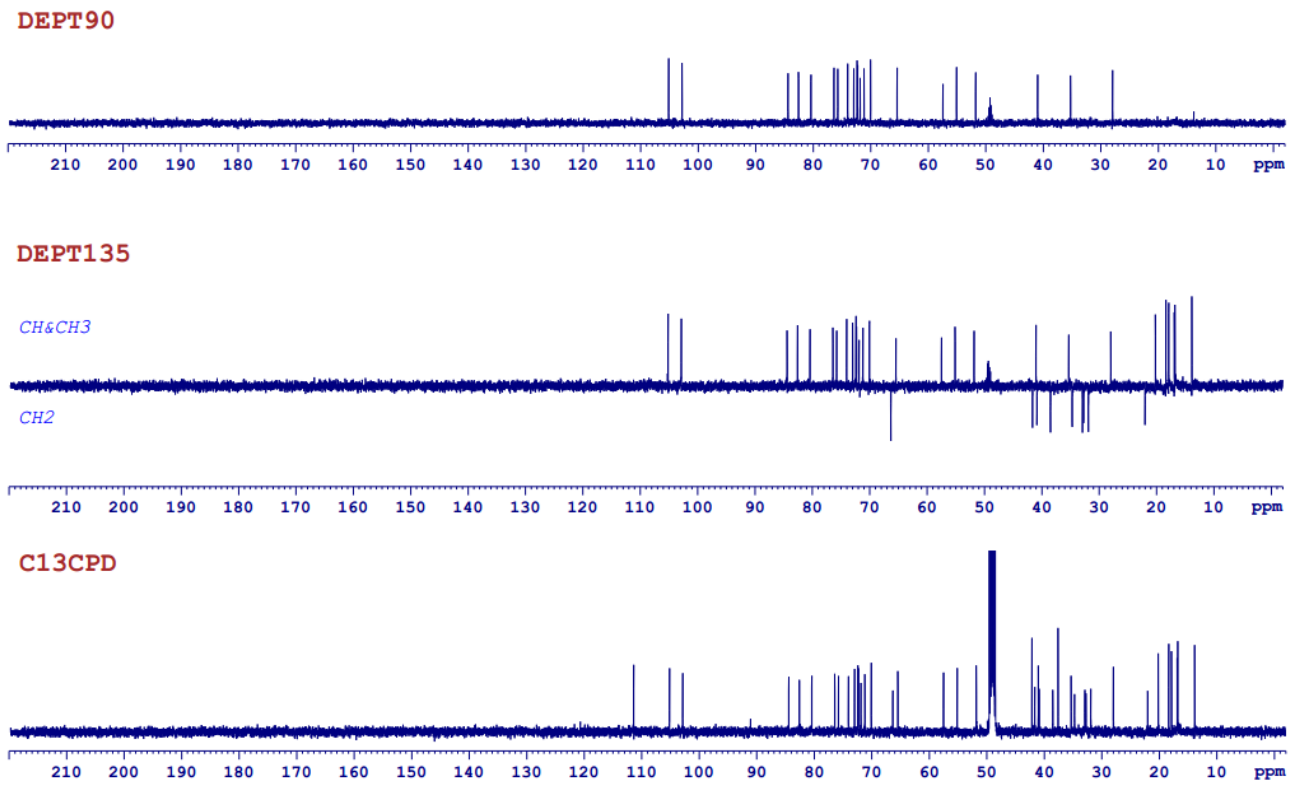

Figure S35. DEPT spectrum of compound **9**

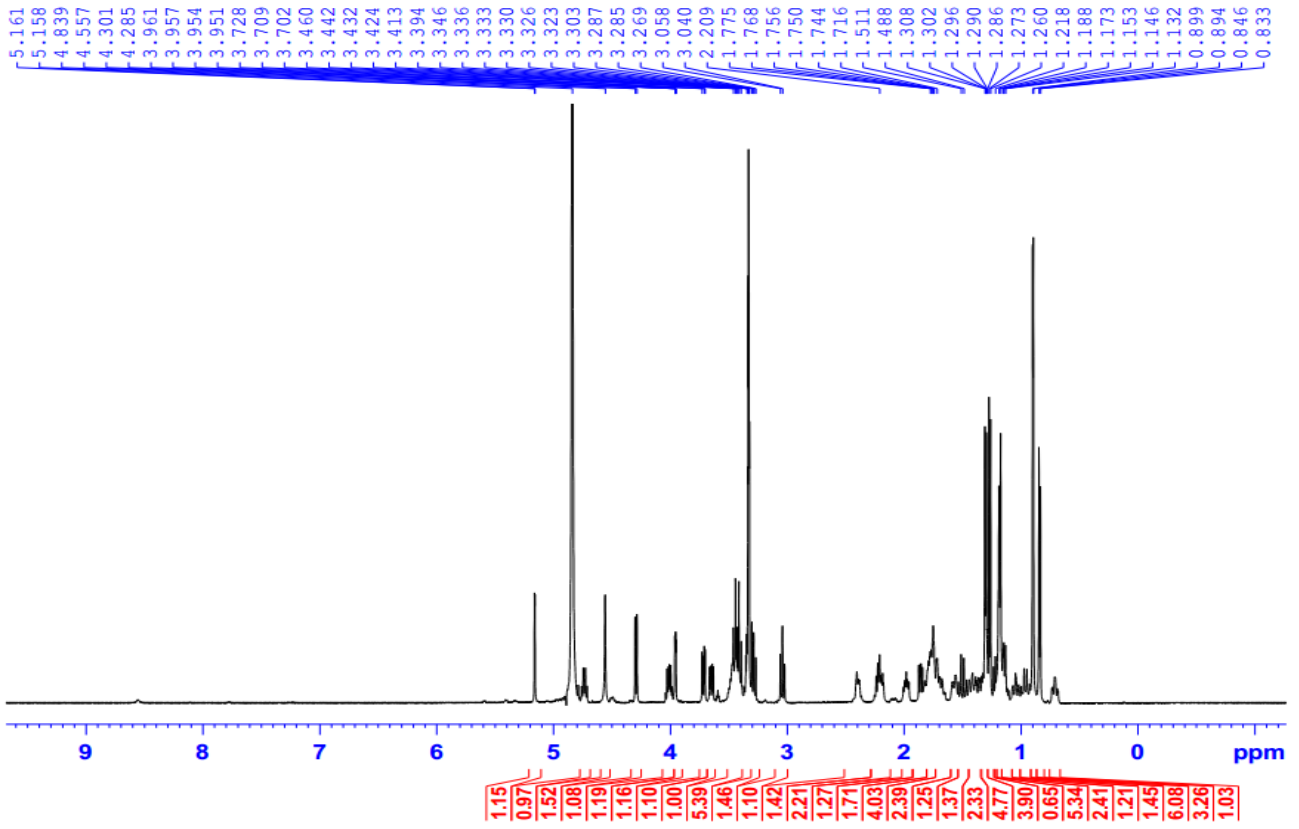

Figure S36. ^{1}H-NMR spectrum of compound **10** (in MeOD, 500 MHz)

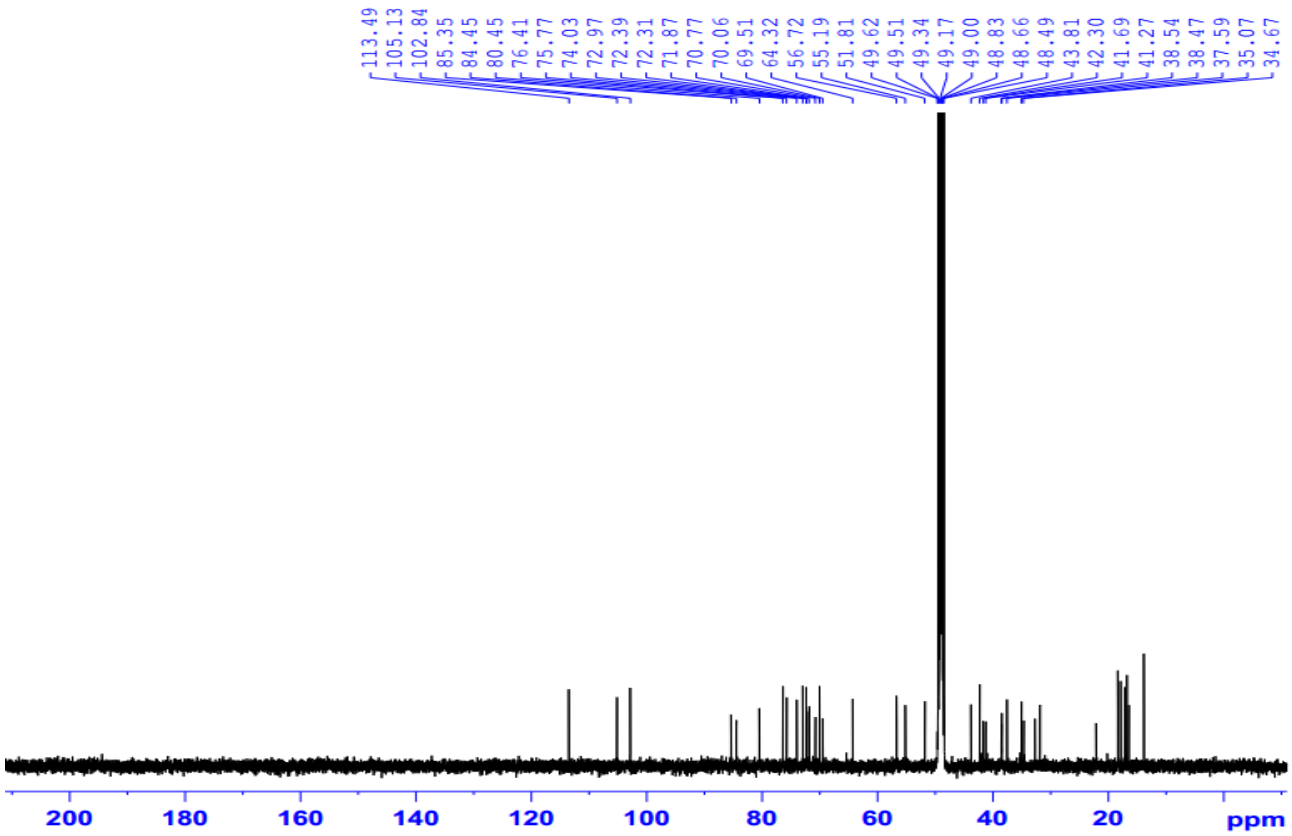

Figure S37. ^{13}C-NMR spectrum of compound **10** (in MeOD, 125 MHz)

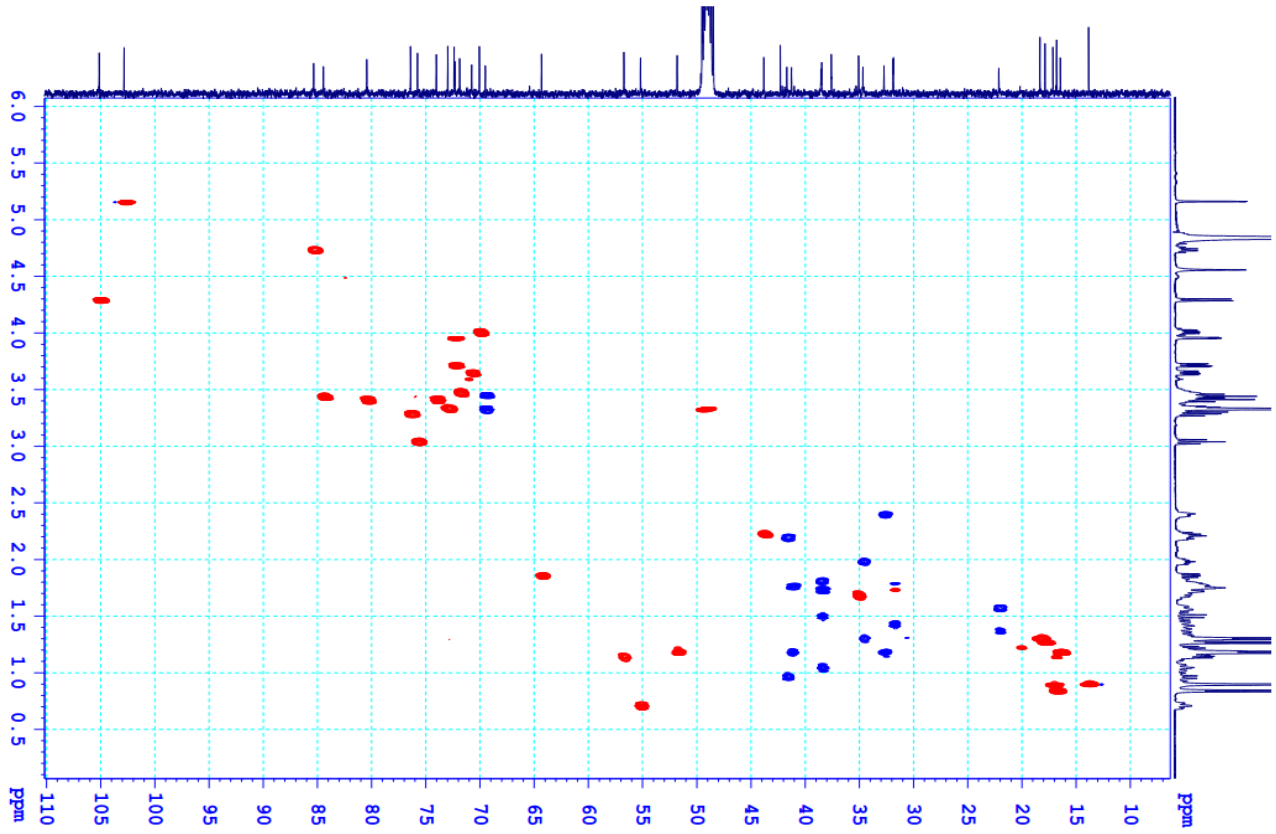

Figure S38. HSQC spectrum of compound **10**

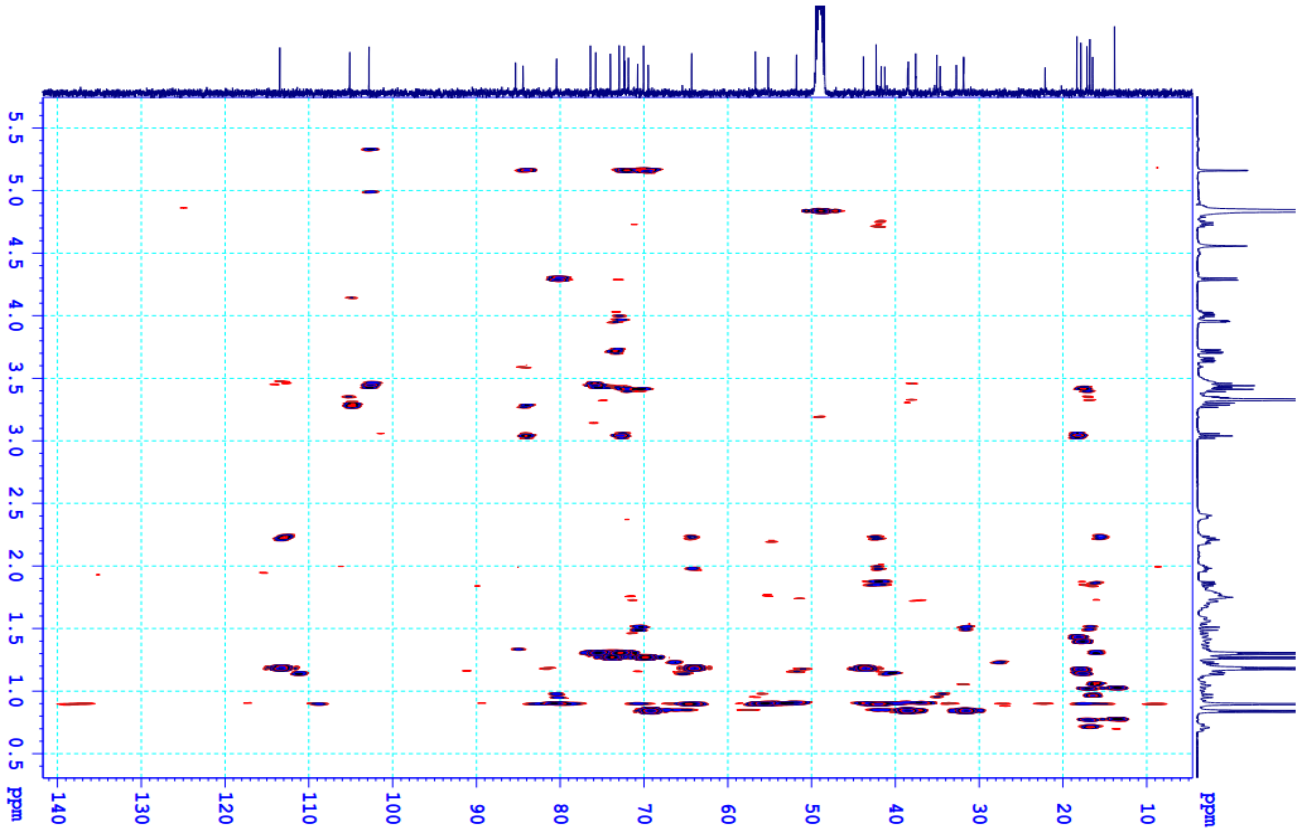

Figure S39. HMBC spectrum of compound **10**

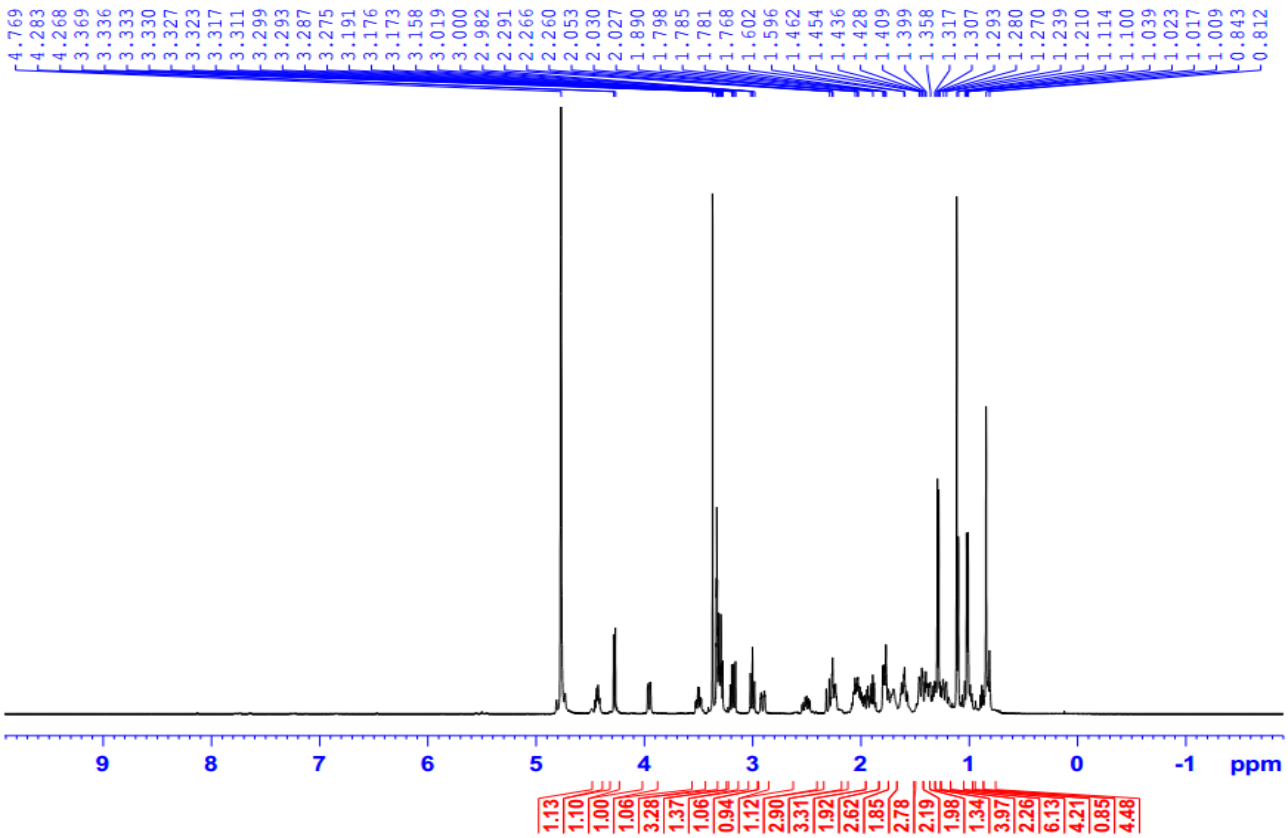

Figure S40. ^{1}H-NMR spectrum of compound **11** (in MeOD, 500 MHz)

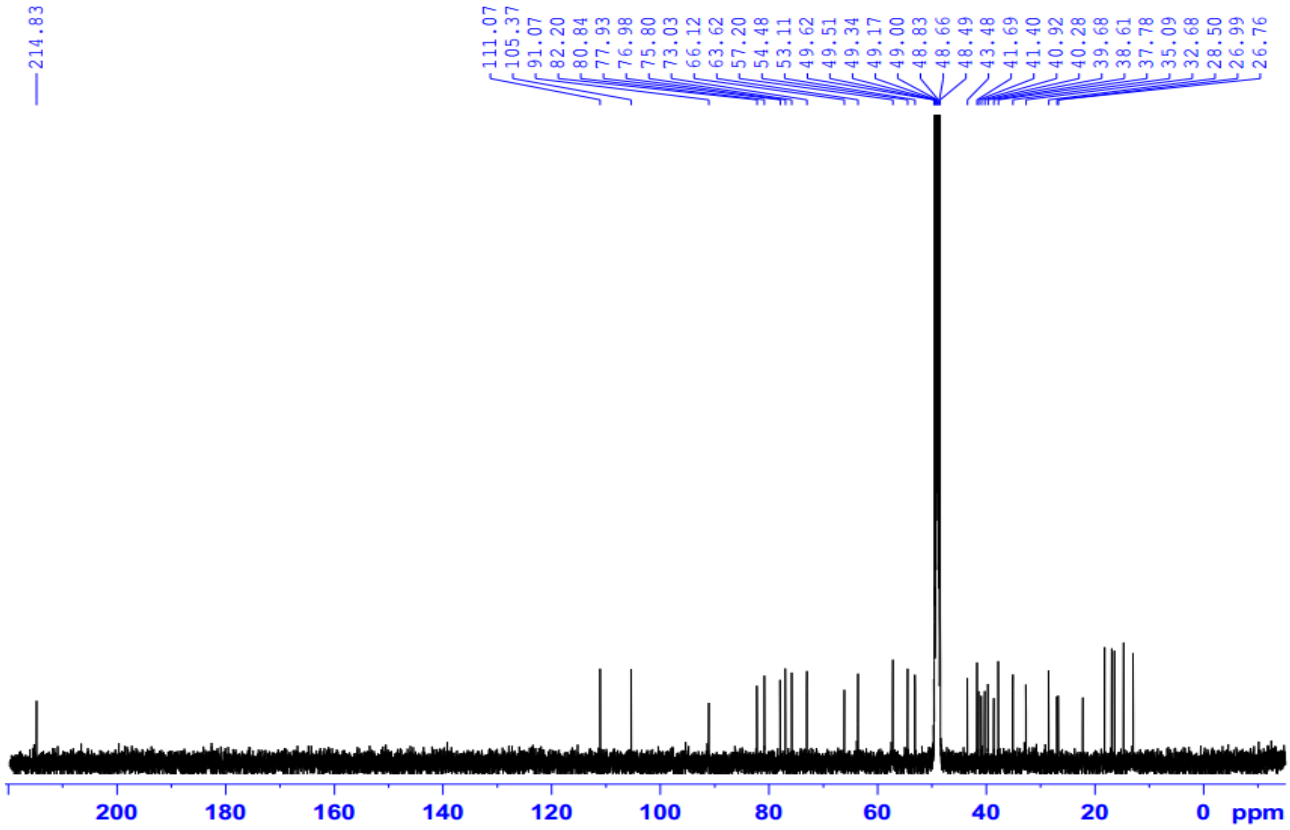

Figure S41. ^{13}C-NMR spectrum of compound **11** (in MeOD, 125 MHz)

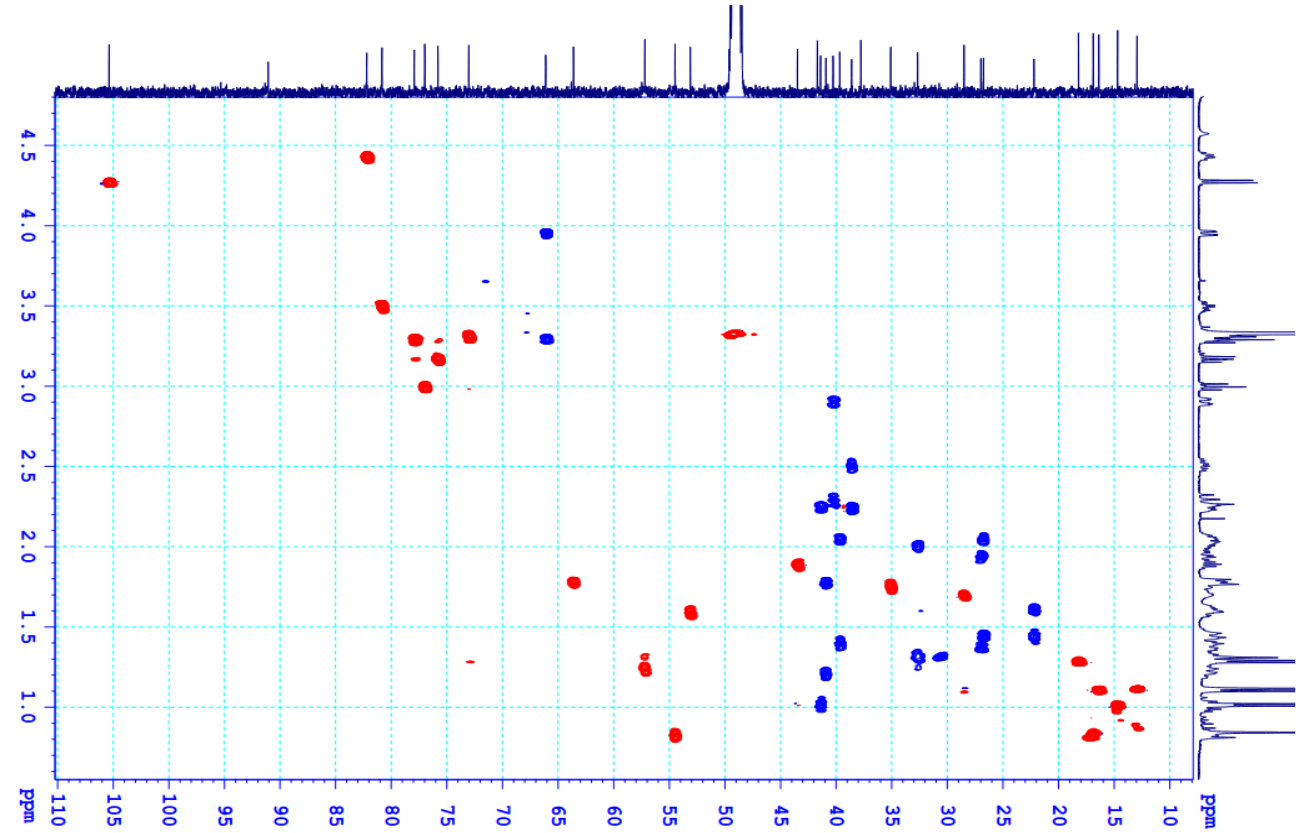

Figure S42. HSQC spectrum of compound **11**

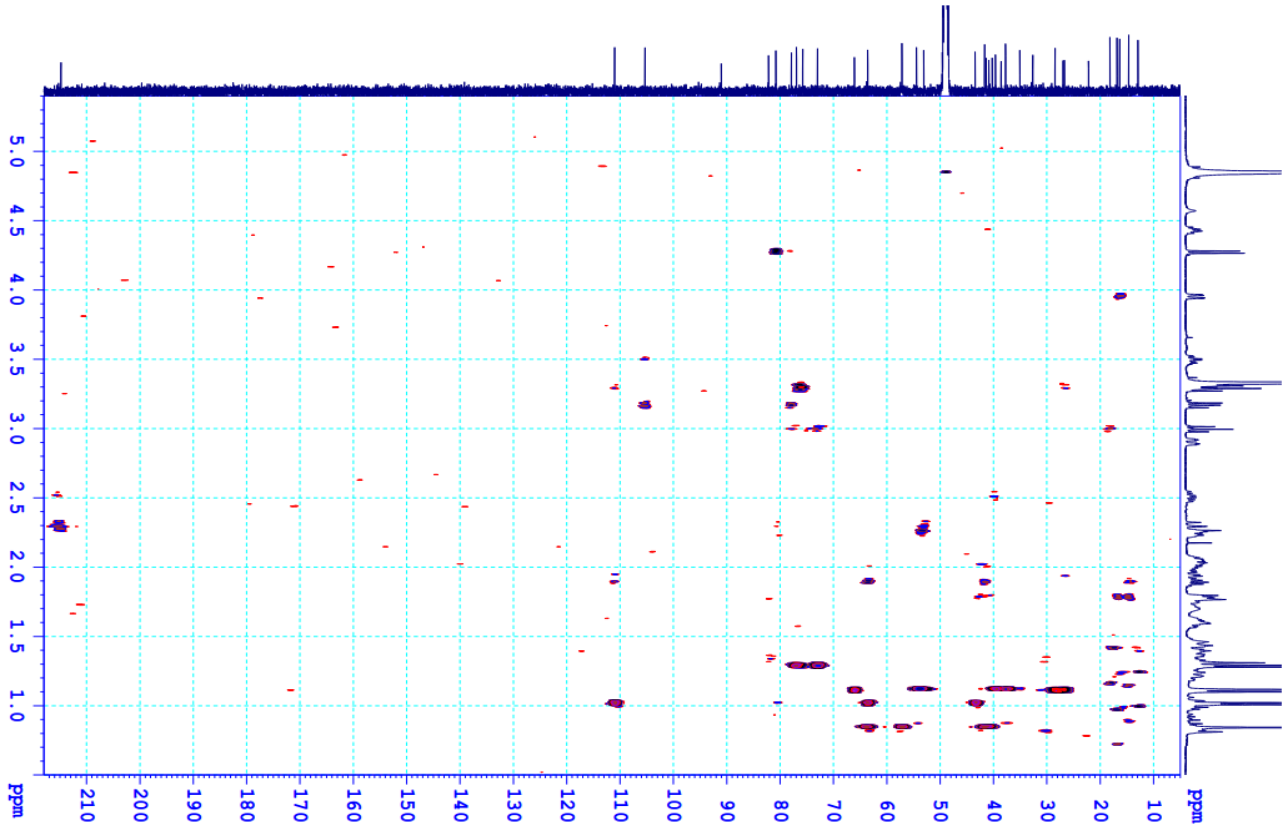

Figure S43. HMBC spectrum of compound **11**

References

Arthan D, Svasti J, Kittakoop P, Pittayakhachonwut D, Tanticharoen M, Thebtaranonth Y. 2002. Antiviral isoflavonoid sulfate and steroidal glycosides from the fruits of *Solanum torvum*. Phytochemistry. 59(4):459-463.

Challal S, Buenafe OEM, Queiroz EF, Maljevic S, Marcourt L, Bock M, Kloeti W, Dayrit FM, Harvey AL, Lerche H et al. 2014. Zebrafish bioassay-guided microfractionation identifies anticonvulsant steroid glycosides from the philippine medicinal plant *Solanum torvum*. ACS Chemical Neuroscience. 5(10):993-1004.

González M, Zamilpa A, Marquina S, Navarro V, Alvarez L. 2004. Antimycotic spirostanol saponins from *Solanum hispidum* leaves and their structure−activity relationships. Journal of Natural Products. 67(6):938-941.

Hien TTT, Tuan HA, Huong DP, Van Luong H, Mai NTT, Tai BH, Van Kiem P. 2018. Two new steroidal saponins from *Solanum procumbens*. Natural Product Communications. 13(10):1934578X1801301009.

Iida Y, Yanai Y, Ono M, Ikeda T, Nohara T. 2005. Three unusual 22-beta-*O*-23-hydroxy-(5alpha)-spirostanol glycosides from the fruits of *Solanum torvum*. Chemical and Pharmaceutical Bulletin. 53(9):1122-1125.

Lee C-L, Hwang T-L, He W-J, Tsai Y-H, Yen C-T, Yen H-F, Chen C-J, Chang W-Y, Wu Y-C. 2013. Anti-neutrophilic inflammatory steroidal glycosides from Solanum torvum. Phytochemistry. 95:315-321.

Li Q-d, Jiang H-f, Chen L, Zhang F-l, Shi B-j. 2015. Steroidal glycoside constituents from *Solanum cumingii* [10.13863/j.issn1001-4454.2015.06.024]. Zhongyaocai. 38(6):1206-1208.

Lu Y-Y, Luo J-G, Kong L-Y. 2011. Chemical Constituents from *Solanum torvum*. Chinese Journal of Natural Medicines. 9(1):30-32.

Lu Y-Y, Wang X-B, Kong L-Y. 2008. Altering hydrophilic and hydrophobic region via O–H···O and C–H···O hydrogen bonds and van der waals forces in Solagenin 6-*O*-(*β*-D-quinovopyranoside) methanol solvate monohydrate. Journal of Chemical Crystallography. 38(7):533-539.

Lu Y, Luo J, Kong L. 2011. Steroidal alkaloid saponins and steroidal saponins from *Solanum surattense*. Phytochemistry. 72(7):668-673.

Monks A, Scudiero D, Skehan P, Shoemaker R, Paull K, Vistica D, Hose C, Langley J, Cronise P, Vaigro-Wolff A et al. 1991. Feasibility of a high-flux anticancer drug screen using a diverse panel of cultured human tumor cell lines. Journal of the National Cancer Institute. 83(11):757-766. eng.

Ripperger H, Schreiber K. 1968. Structure of paniculonine A and B, two new spirostan glycosides from *Solanum paniculatum*. Chem Ber. 101(7):2450-2458.

Shoemaker RH, Scudiero DA, Melillo G, Currens MJ, Monks AP, Rabow AA, Covell DG, Sausville EA. 2002. Application of high-throughput, molecular-targeted screening to anticancer drug discovery. Current topics in medicinal chemistry. 2(3):229-246. eng.