Supplementary Information

Dual SARS-CoV-2 and MERS-CoV Inhibitors from *Artemisia monosperma*: Isolation, Structure Elucidation, Molecular Modelling Studies, and *In vitro* Activities

Ahmed M. Badawy,[a,†] Marwa Samir M. Donia, [b,†] Nehal G. Hamdy, [a,†] Mayada M. El-Ayouty , [a]

Osama G. Mohamed,[c,d] Khaled M. Darwish,[e] Ashootosh Tripathi,[d,f] and Safwat A. Ahmed, [*b]

[a] *Department of Pharmacognosy, Faculty of Pharmacy, Sinai University, El-Arish 45511, Egypt;* ahmed.badawy@su.edu.eg (A.M.B.); nehal.aly@su.edu.eg (N.G.H.); miada.mohamed@su.edu.eg (M.M.E.)

[b] *Department of Pharmacognosy, Faculty of Pharmacy, Suez Canal University, Ismailia 41522, Egypt;* mdonia00@gmail.com (M.S.M.D.).

[c] *Pharmacognosy Department, Faculty of Pharmacy, Cairo University, Kasr el Aini St., Cairo 11562, Egypt;* osama.mohamed@pharma.cu.edu.eg (O.G.M.)

[d] *Natural Products Discovery Core, Life Sciences Institute, University of Michigan, Ann Arbor, MI 48109, USA,*

[e] *Department of Medicinal Chemistry, Faculty of Pharmacy, Suez Canal University, Ismailia 41522, Egypt;* Khaled_darwish@pharm.suez.edu.eg (K.M.D.)

[f] *Department of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor, MI 48109, USA;* ashtri@umich.edu (A.T.)

Correspondence: safwat_aa@yahoo.com *or* safwat_ahmed@pharm.suez.edu.eg (S.A.A.); *Tel.: +20-010-92638387; Fax: +20-064-32307*

List of figures: -

Fiqure S. 1:1H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*) 8
Fiqure S. 2: Partial expansion of ^{1}H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*). 8
Fiqure S. 3: ^{13}C-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*) 9
Fiqure S. 4: ^{1}H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*) 9
Fiqure S. 5: LC-MS/MS of compound 1 10
Fiqure S. 6: ^{1}H-NMR spectrum of compound 2 (300 MHz, DMSO-*d6*) 10
Fiqure S. 7: ^{13}C-NMR spectrum of compound 2 (300 MHz, DMSO-*d6*). 11
Fiqure S. 8:^{1}H-NMR spectrum of compound 2 (300 MHz, DMSO-*d6*) 11
Fiqure S. 9: LC-MS/MS of compound 2 12
Fiqure S. 10: ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*) 12
Fiqure S. 11: Partial expansion of ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*). 13
Fiqure S. 12: Partial expansion of ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*). 13
Fiqure S. 13: Partial expansion of ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*). 14
Fiqure S. 14: ^{13}C-NMR spectrum of 3 (400 MHz, DMSO-*d6*) 14
Fiqure S. 15: ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*) 15
Fiqure S. 16: LC-MS/MS of compound 3 15
Fiqure S. 17:^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD). 16
Fiqure S. 18: Partial expansion of ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD). 16
Fiqure S. 19: Partial expansion of ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD). 17
Fiqure S. 20: Partial expansion of ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD). 17
Fiqure S. 21: ^{13}C-NMR spectrum of compound 4 (600 MHz, CD_3OD) 18
Fiqure S. 22: ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD). 18
Fiqure S. 23: LC-MS/MS of compound 4 19
Fiqure S. 24: ^{1}H-NMR spectrum of compound 5 (600 MHz, CD_3OD). 19
Fiqure S. 25: Partial expansion of ^{1}H-NMR spectrum of compound 5 (600 MHz, CD_3OD). 20
Fiqure S. 26: Partial expansion of ^{1}H-NMR spectrum of compound 5 (600 MHz, CD_3OD). 20
Fiqure S. 27: ^{13}C-NMR spectrum of compound 5 (150 MHz, CD_3OD) 21
Fiqure S. 28: ^{1}H-NMR spectrum of compound 5 (600 MHz, CD_3OD). 21
Fiqure S. 29: LC-MS/MS of compound 5 22
Fiqure S. 30:^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD). 22
Fiqure S. 31: Partial expansion of ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD). 23
Fiqure S. 32: Partial expansion of ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD). 23
Fiqure S. 33: Partial expansion of ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD). 24
Fiqure S. 34: ^{13}C-NMR spectrum of compound 6 (150 MHz, CD_3OD) 24
Fiqure S. 35: ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD). 25
Fiqure S. 36: LC-MS/MS of compound 6 25
Fiqure S. 37: ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-*d6*) 26
Fiqure S. 38: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-*d6*). 26
Fiqure S. 39: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-d6). 27
Fiqure S. 40: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-d6). 27

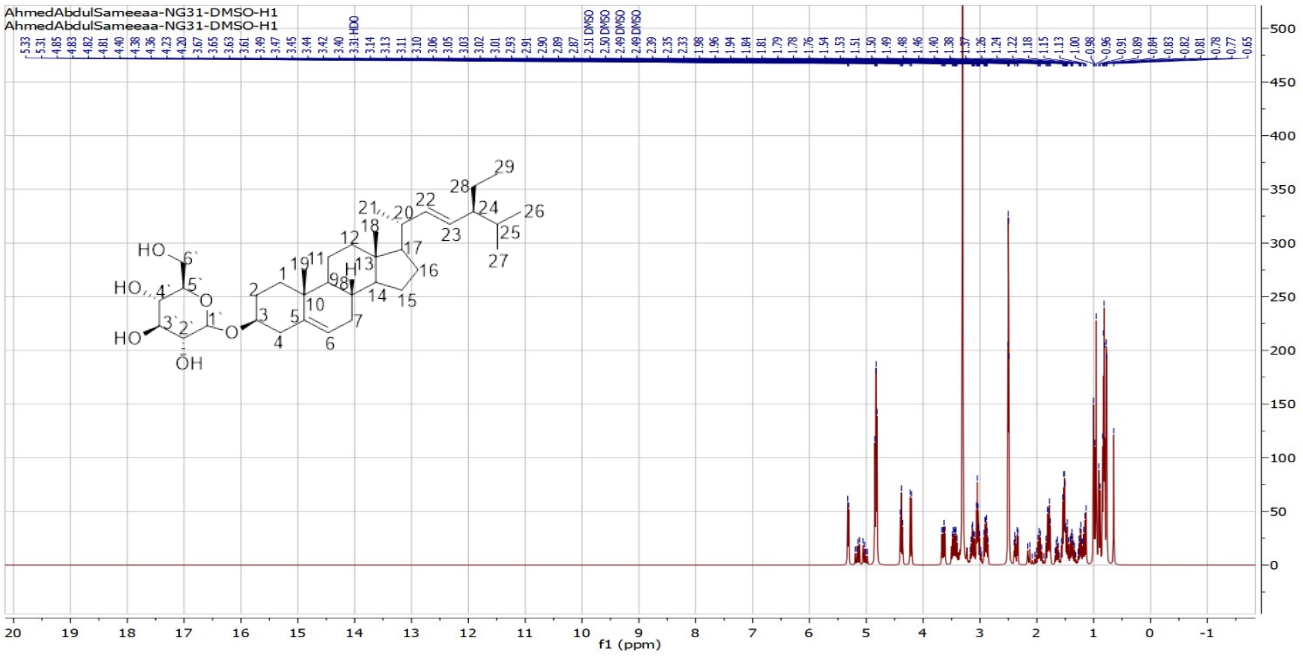
Fiqure S. 41: ^{13}C-NMR spectrum of compound 7 (75 MHz, DMSO-*d6*). 28
Fiqure S. 42: ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-*d6*) 28
Fiqure S. 43: LC-MS/MS of compound 7 29
Fiqure S. 44: ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*). 29
Fiqure S. 45: Partial expansion of ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*). 30
Fiqure S. 46: Partial expansion of ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*). 30
Fiqure S. 47: ^{13}C-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*). 31
Fiqure S. 48: ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*). 31
Fiqure S. 49: LC-MS/MS of compound 8 32

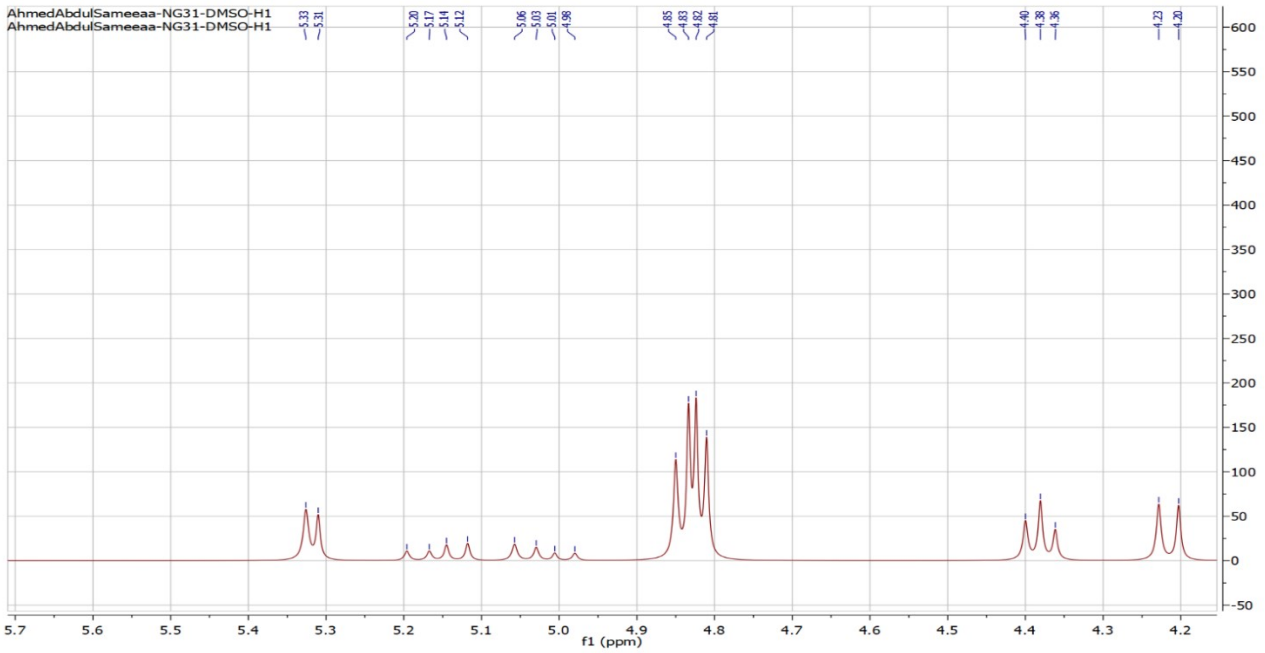
List of tables: -

Table S. 1: ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 1 (DMSO-*d6* δ in ppm, *J* in Hz). 29
Table S. 2 ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 2 (DMSO-*d6* δ in ppm, *J* in Hz). 30
Table S. 3 ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectroscopic data of compound 3 (DMSO-*d6* δ in ppm, *J* in Hz). 31
Table S. 4 ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR spectroscopic data of compound 4 (CD_3OD, δ in ppm, *J* in Hz). 32
Table S. 5 ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR spectroscopic data of compound 5 (CD_3OD, δ in ppm, *J* in Hz). 32
Table S. 6 ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR spectroscopic data of compound 6 (CD_3OD, δ in ppm, *J* in Hz). 33
Table S. 7. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 7 (DMSO-*d6* δ in ppm, *J* in Hz). 34
Table S. 8 ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 8 (DMSO-*d6* δ in ppm, *J* in Hz). 34

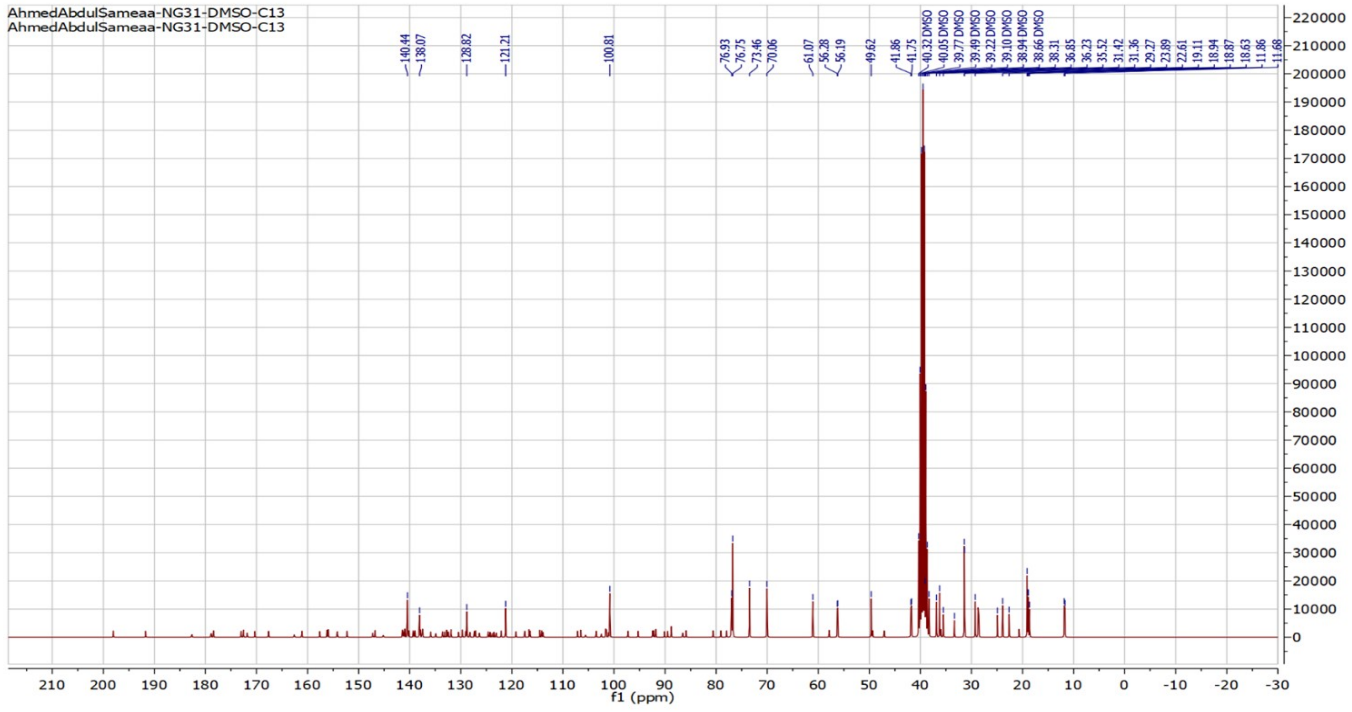
Spectroscopic data of compound 1

Fiqure S. 1:1H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*)

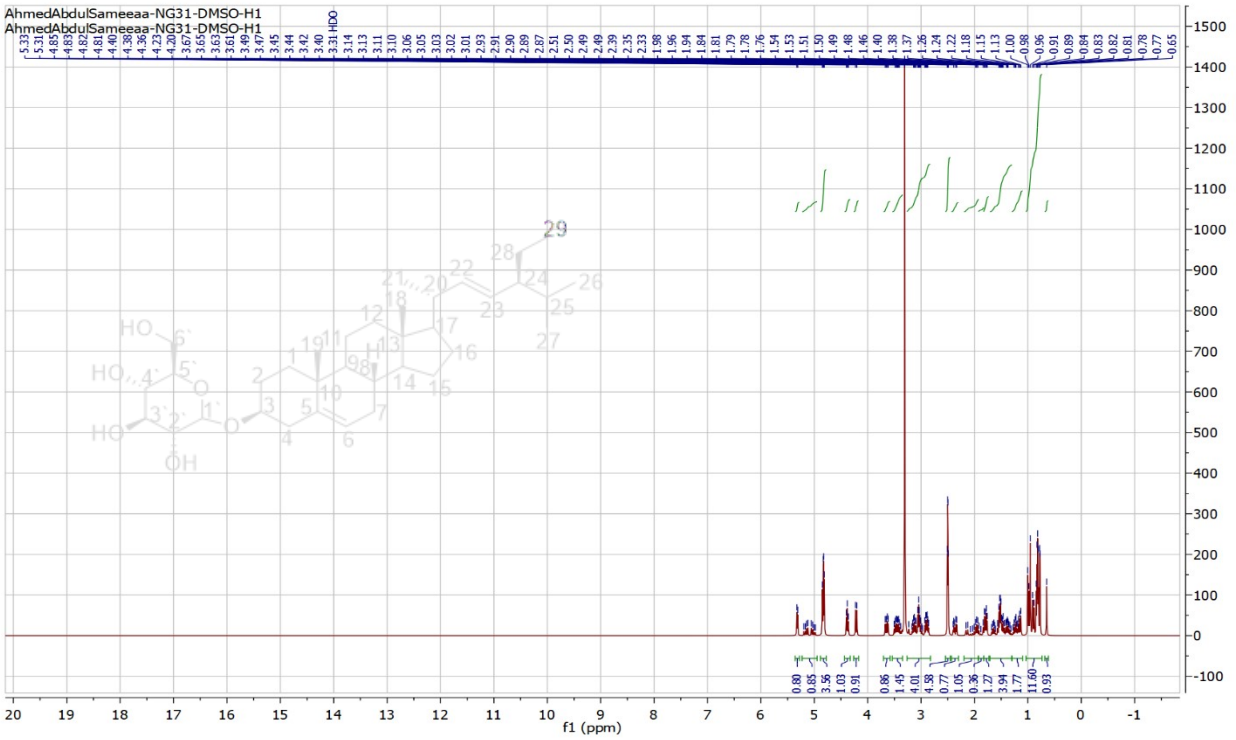




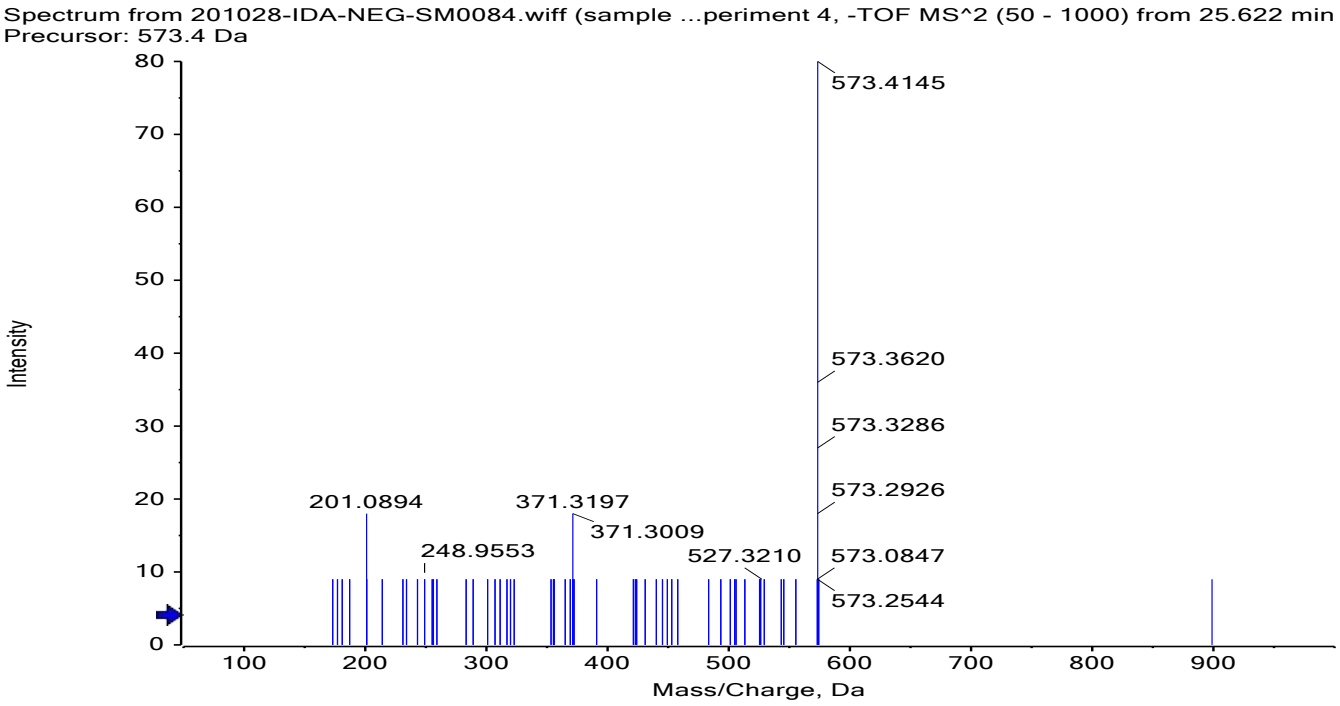
Fiqure S. 2: Partial expansion of ^{1}H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*).



Fiqure S. 3: ^{13}C-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*)



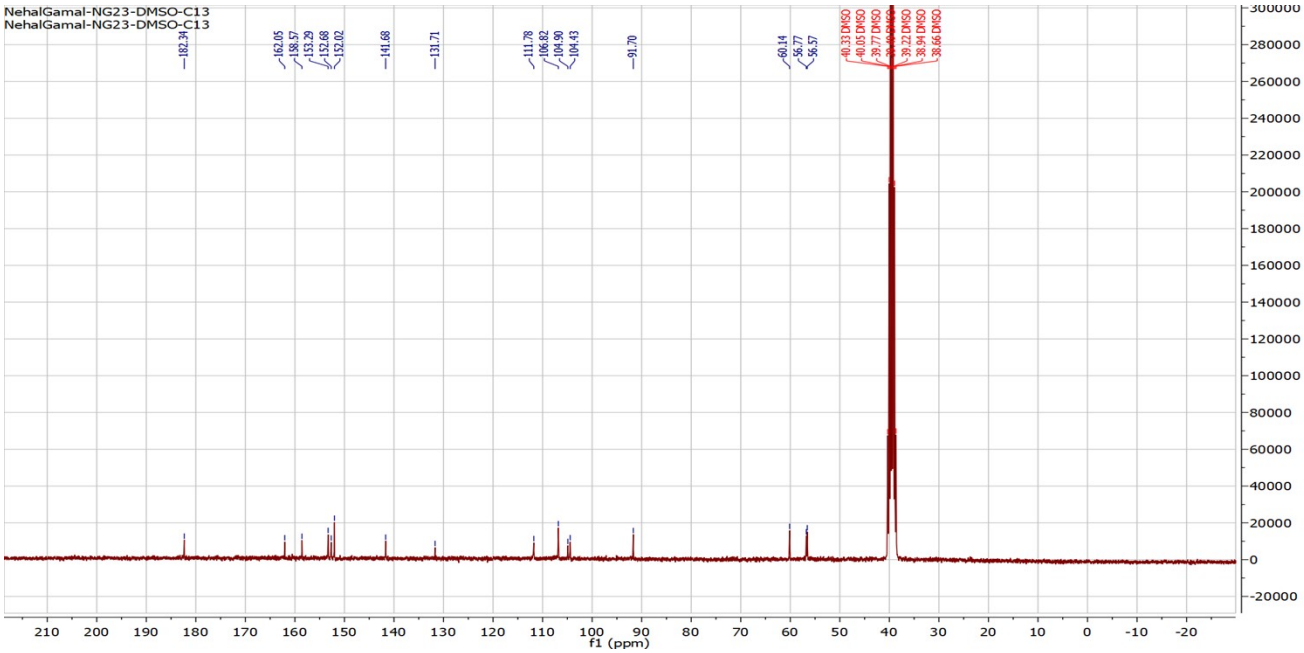
Fiqure S. 4: ^{1}H-NMR spectrum of compound 1 (300 MHz, DMSO-*d6*)

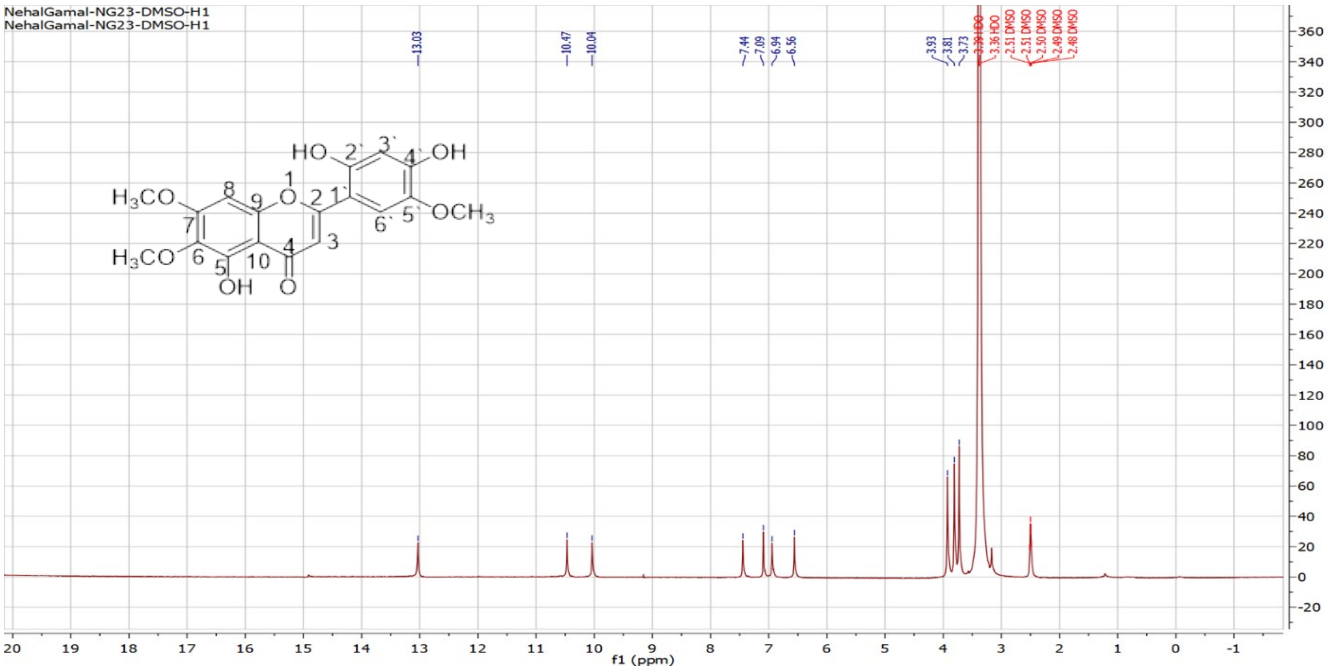


Fiqure S. 5: LC-MS/MS of compound 1

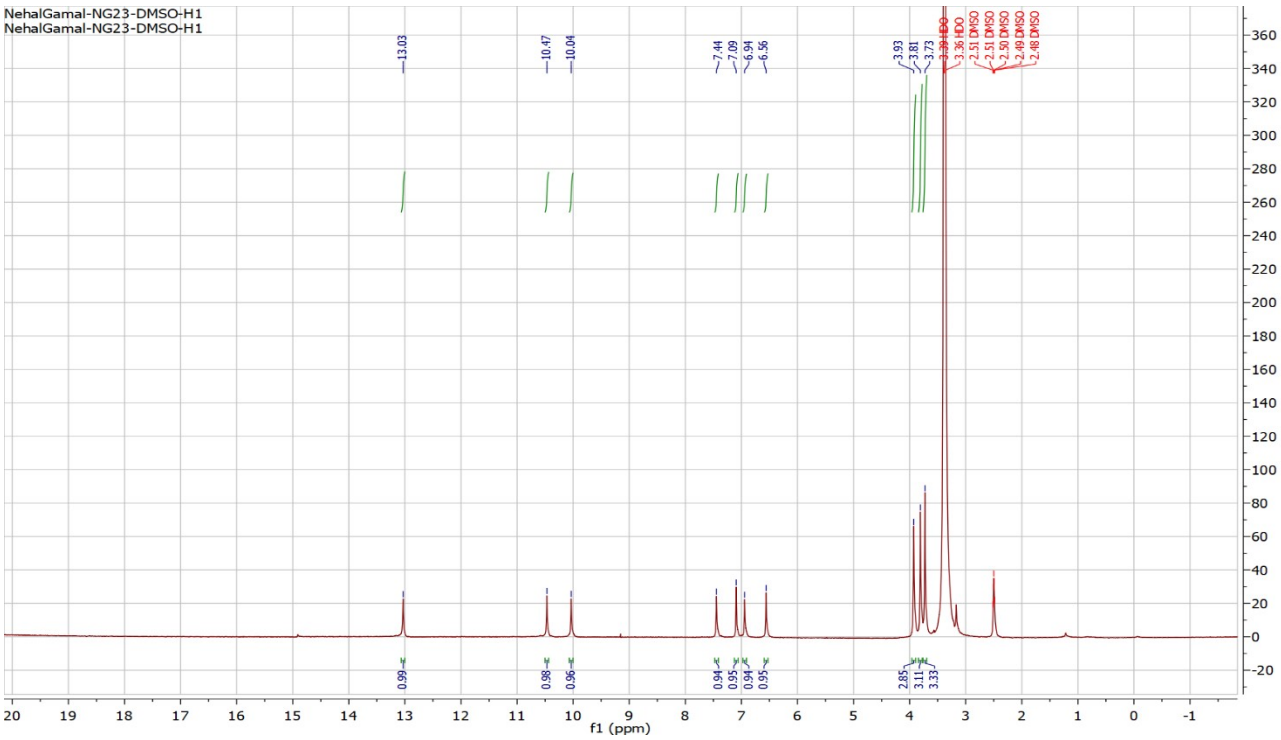
Spectroscopic data of compound 2

Fiqure S. 6: ^{1}H-NMR spectrum of compound 2 (300 MHz, DMSO-*d6*)

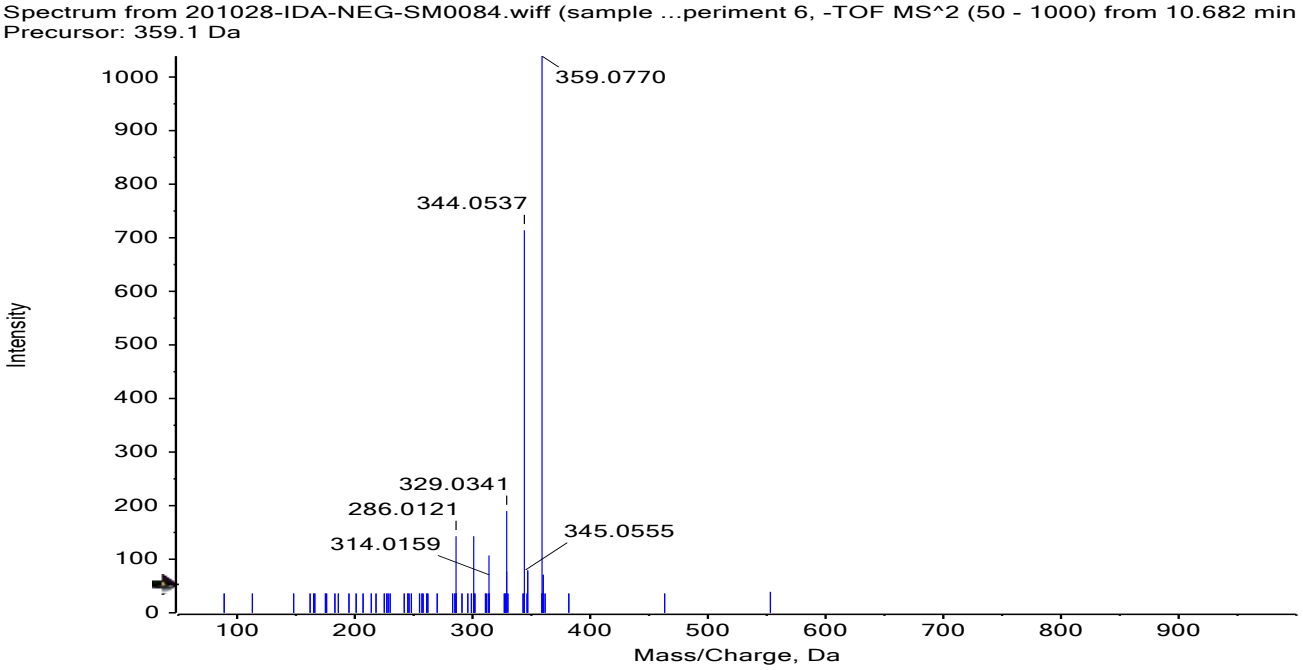




Fiqure S. 7: ^{13}C-NMR spectrum of compound 2 (300 MHz, DMSO-*d6*).

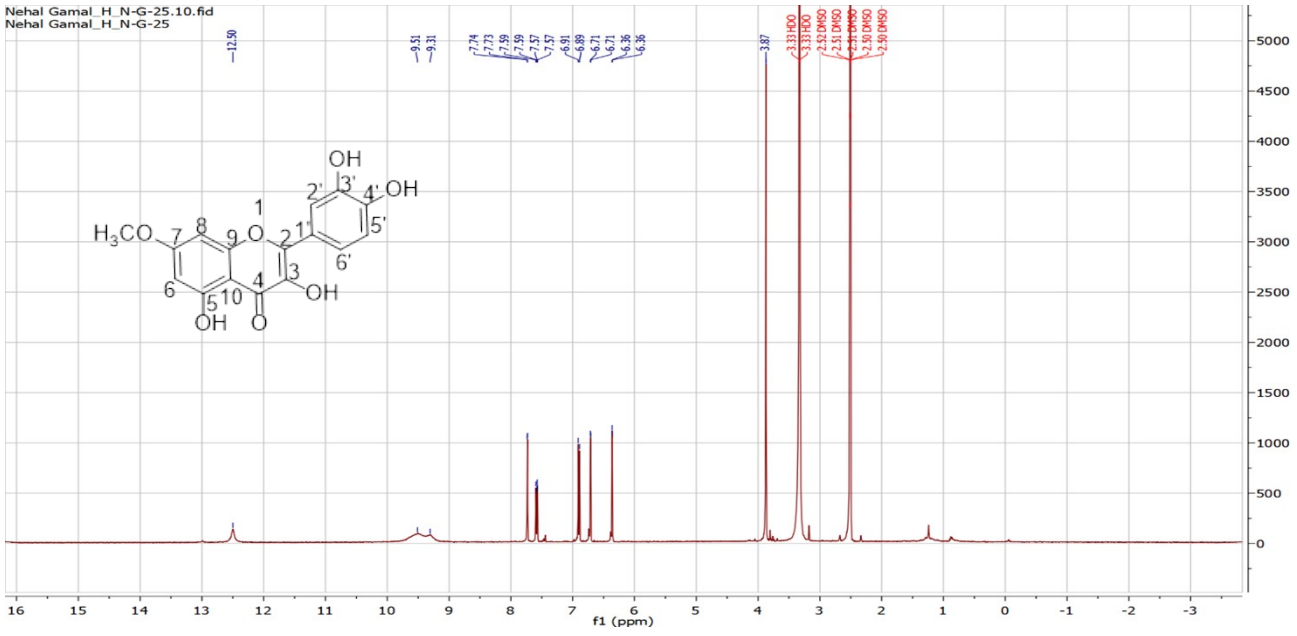


Fiqure S. 8:^{1}H-NMR spectrum of compound 2 (300 MHz, DMSO-*d6*)



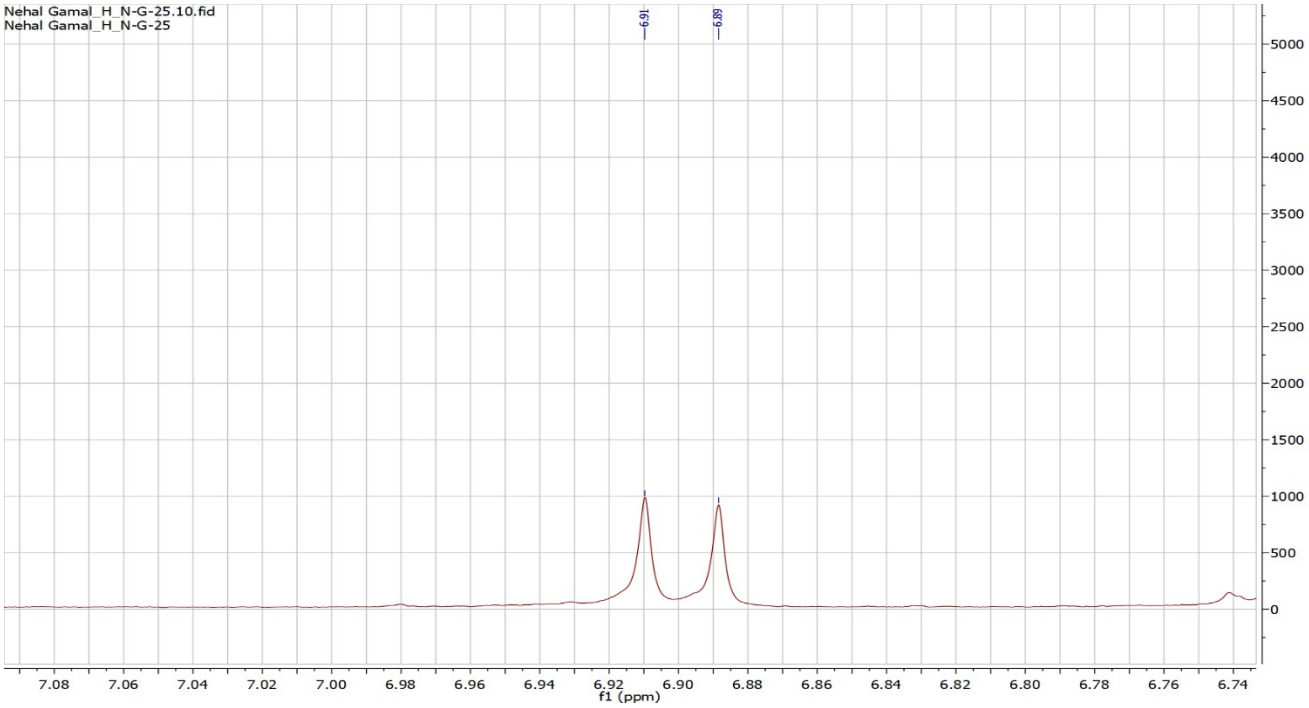
Fiqure S. 9: LC-MS/MS of compound 2

Spectroscopic data of compound 3

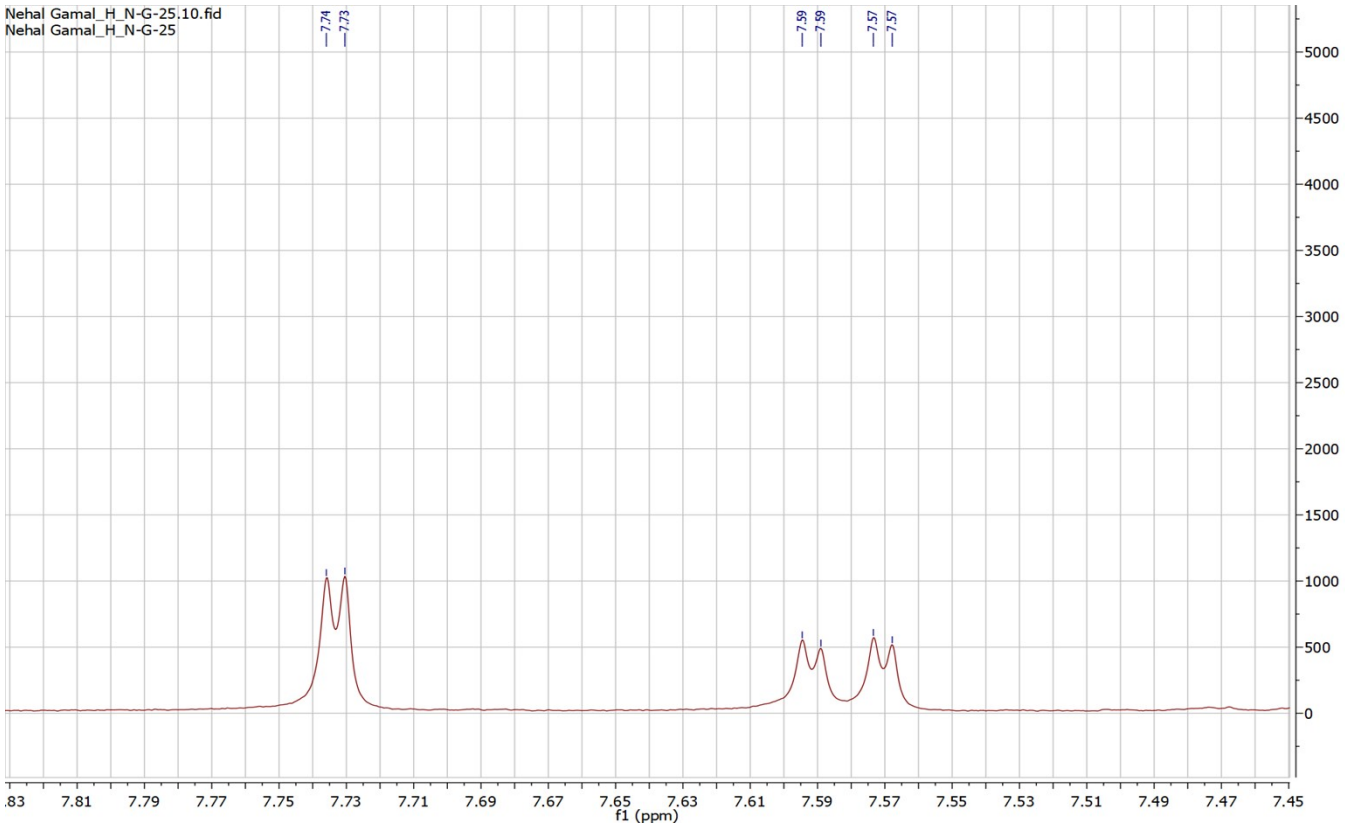


Fiqure S. 10: ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*)

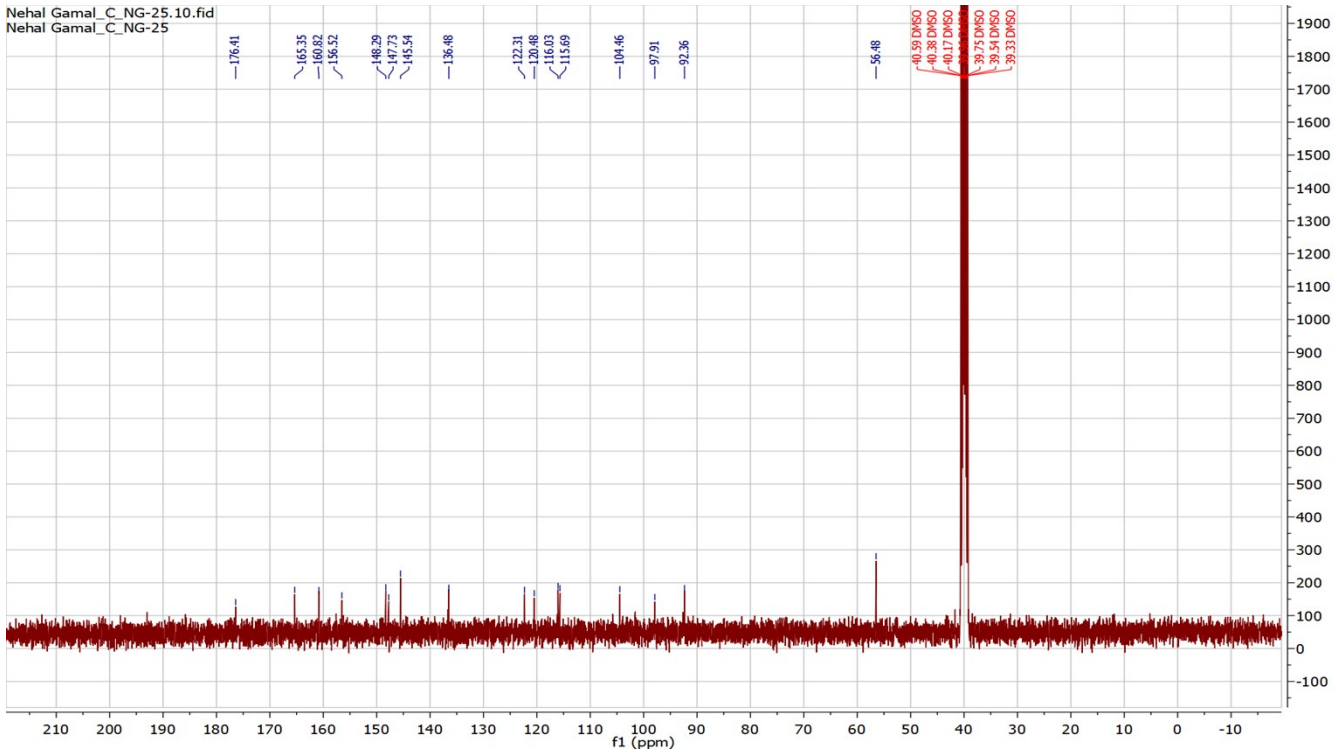
Fiqure S. 11: Partial expansion of ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*).



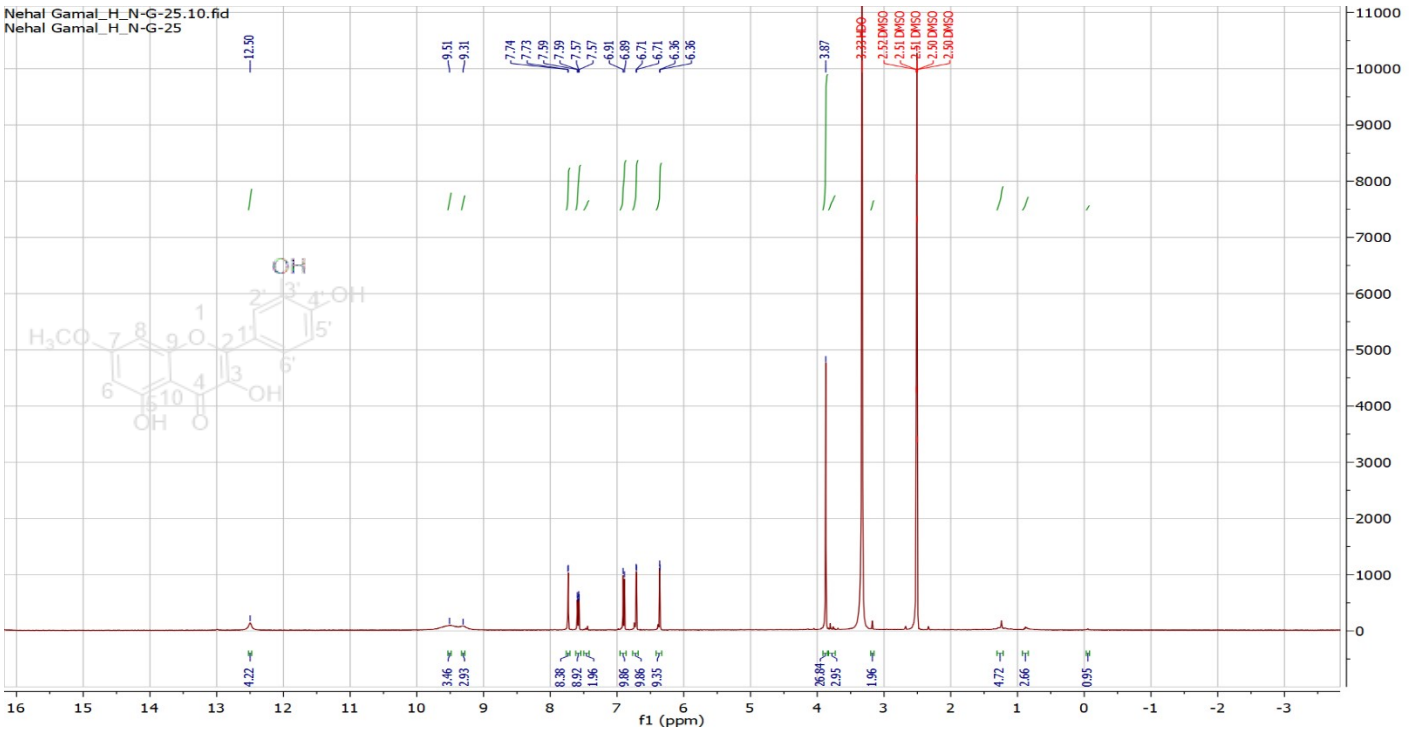
Fiqure S. 12: Partial expansion of ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*).



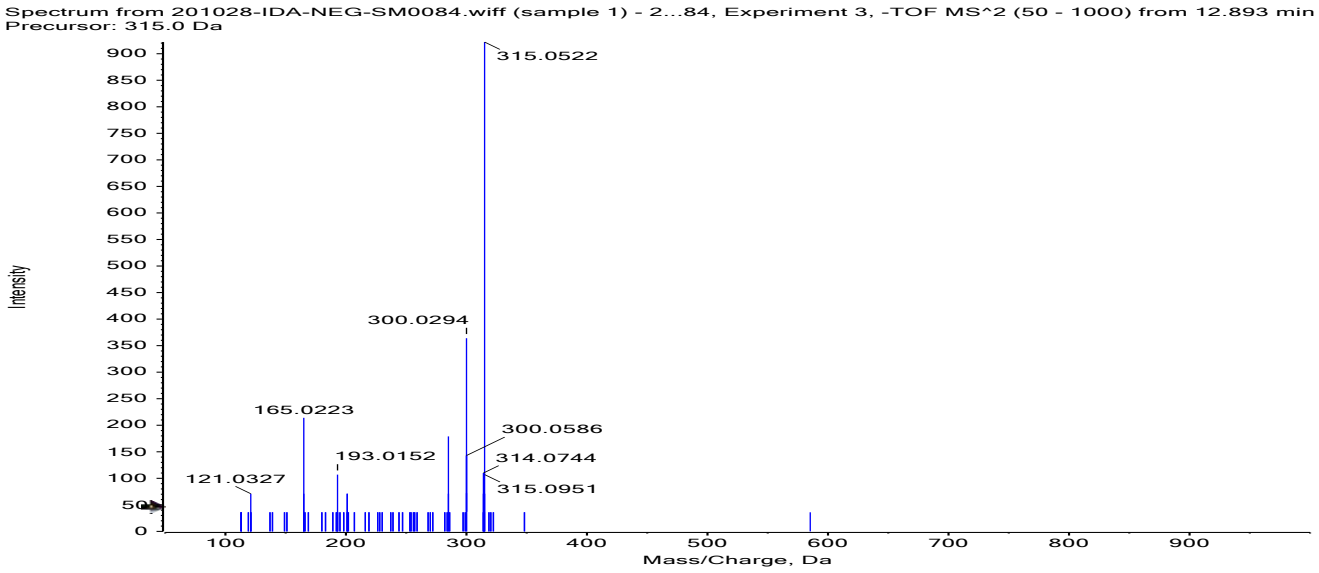
Fiqure S. 13: Partial expansion of ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*).



Fiqure S. 14: ^{13}C-NMR spectrum of 3 (400 MHz, DMSO-*d6*)

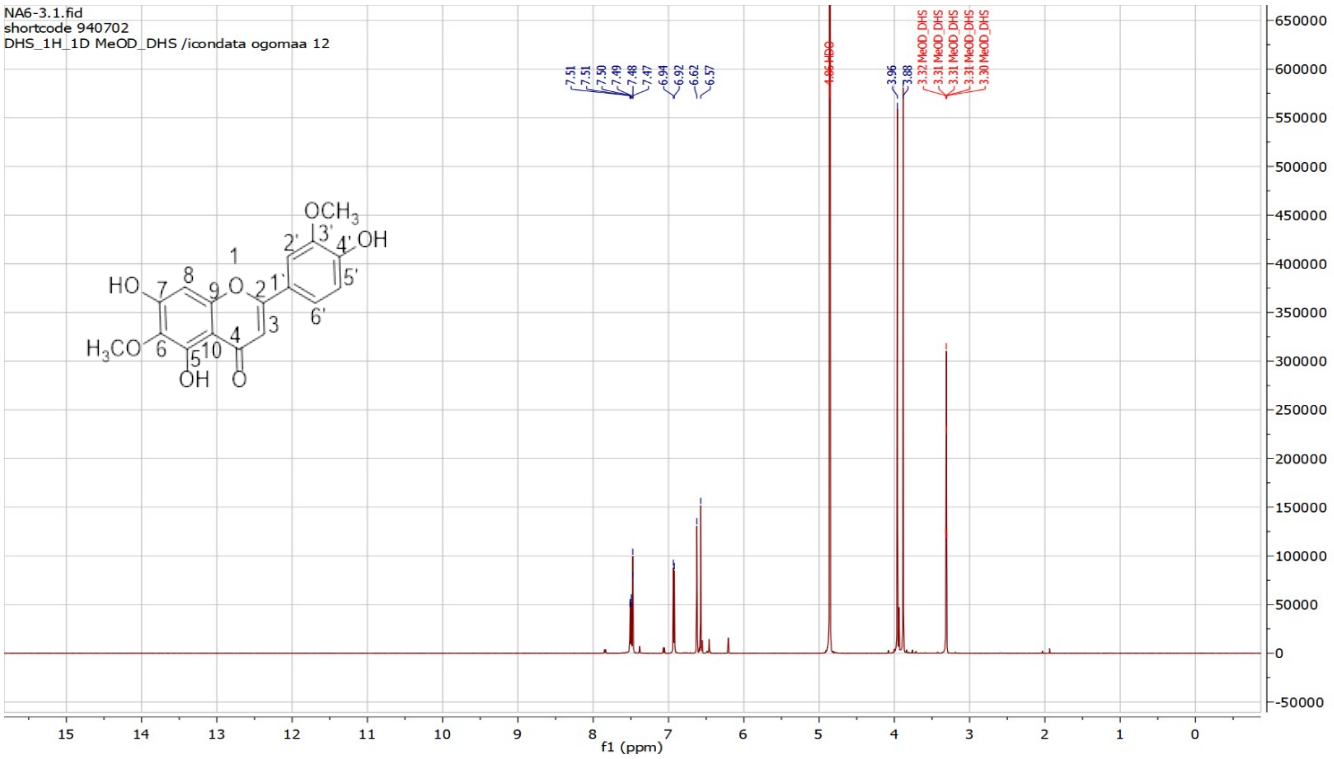


Fiqure S. 15: ^{1}H-NMR spectrum of compound 3 (400 MHz, DMSO-*d6*)

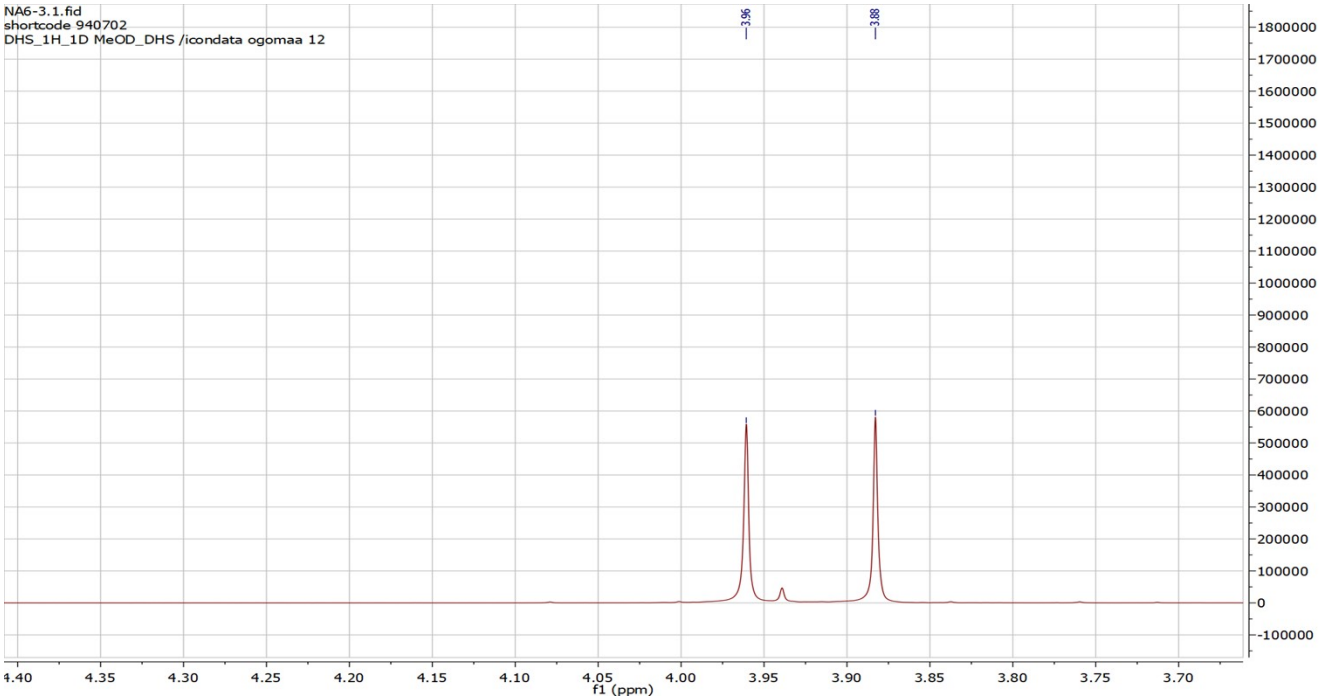


Fiqure S. 16: LC-MS/MS of compound 3

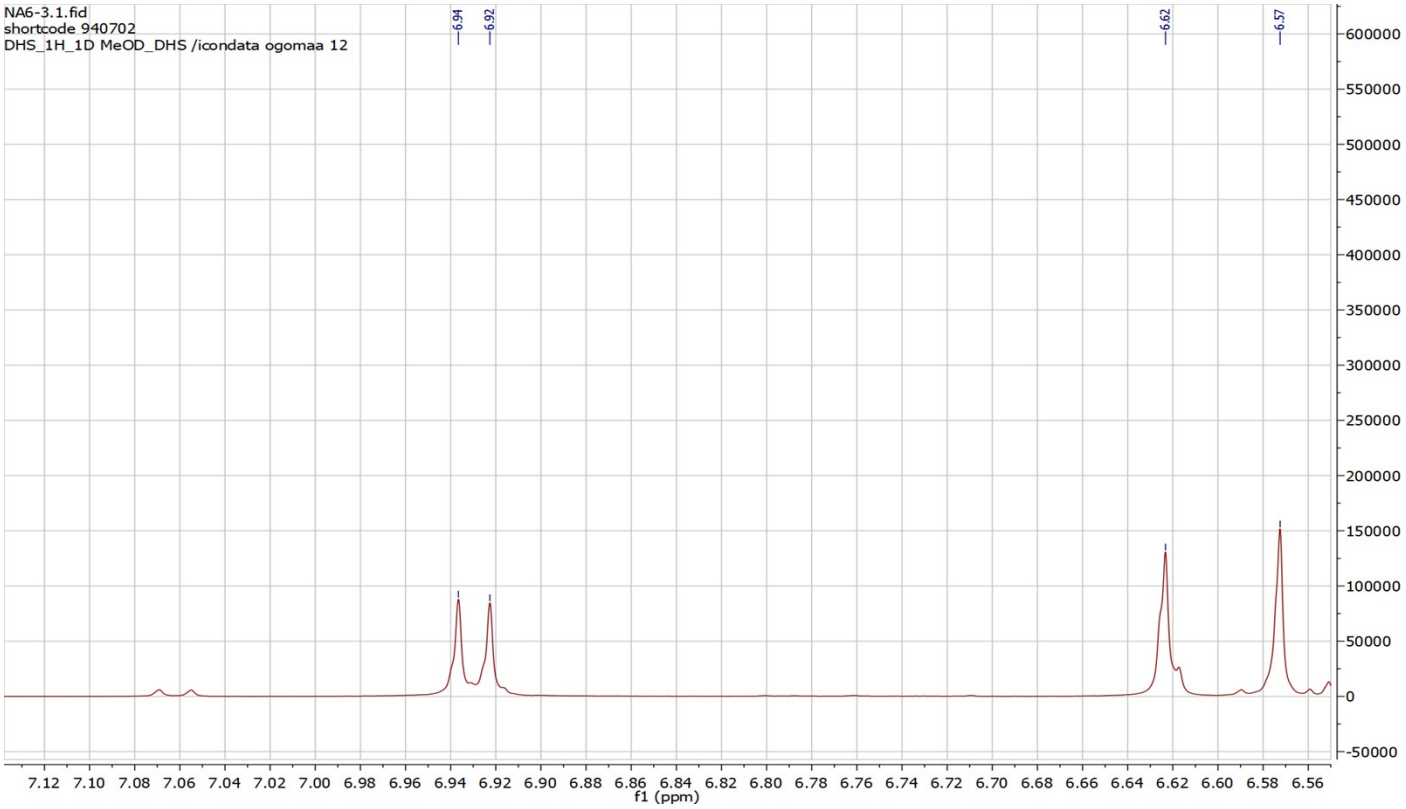
Spectroscopic data of compound 4



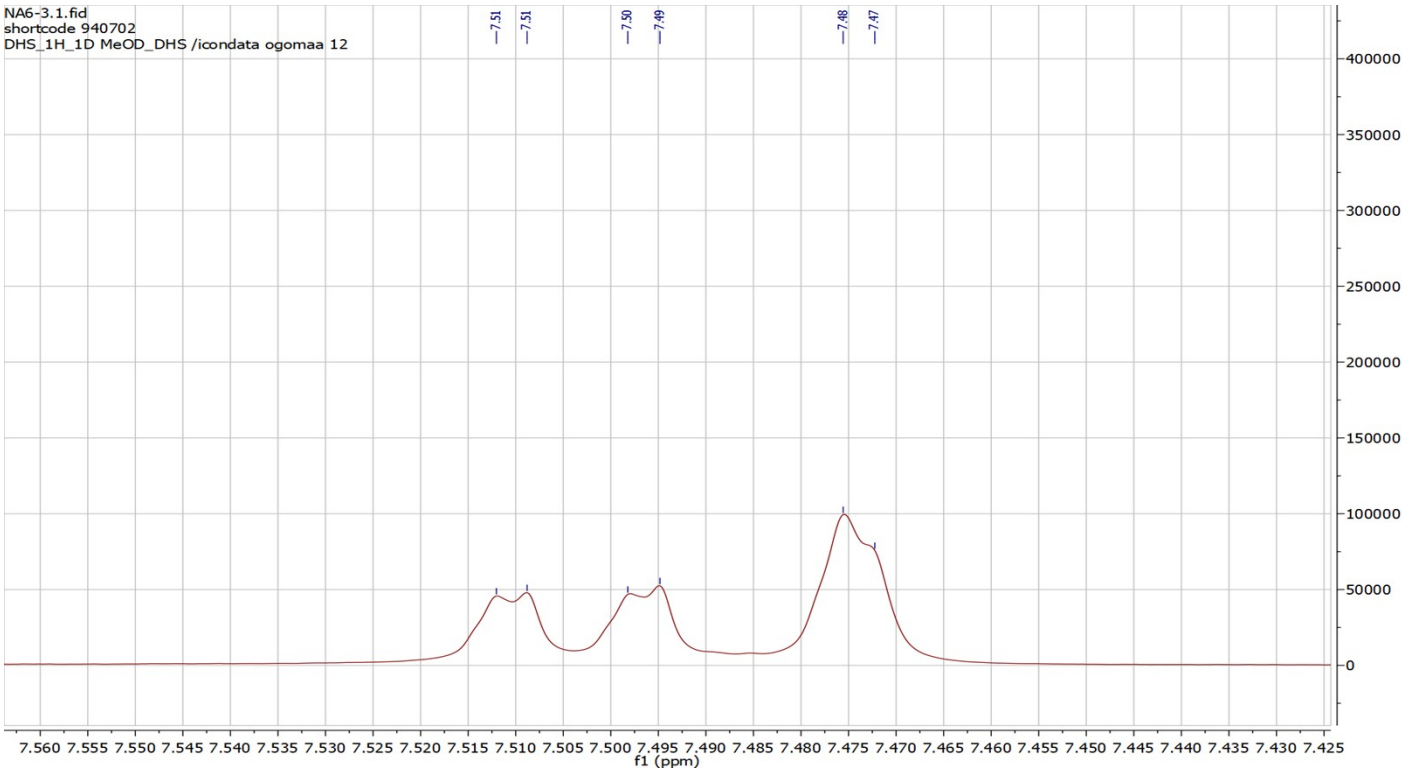
Fiqure S. 17:^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD).



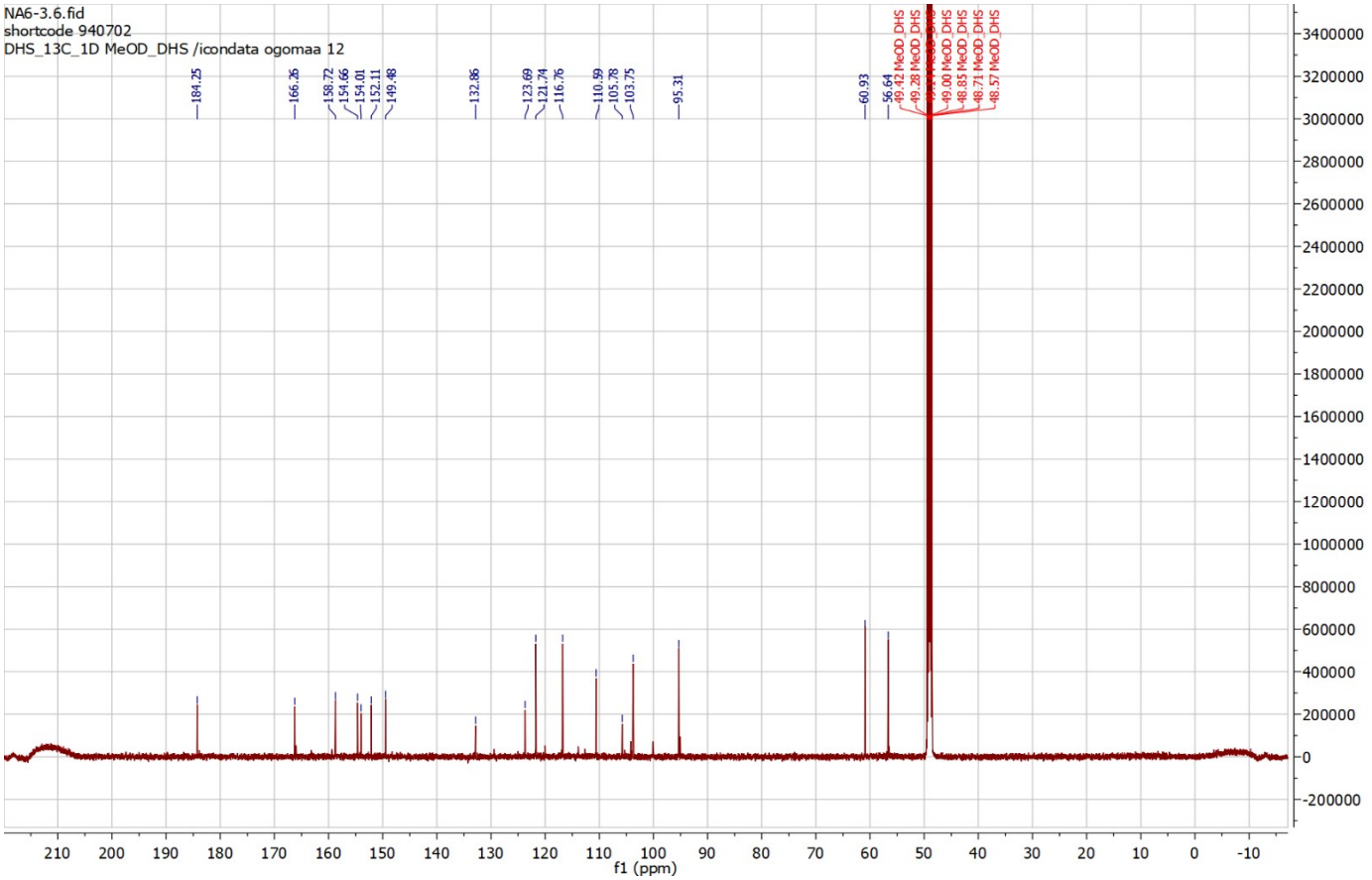
Fiqure S. 18: Partial expansion of ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD).



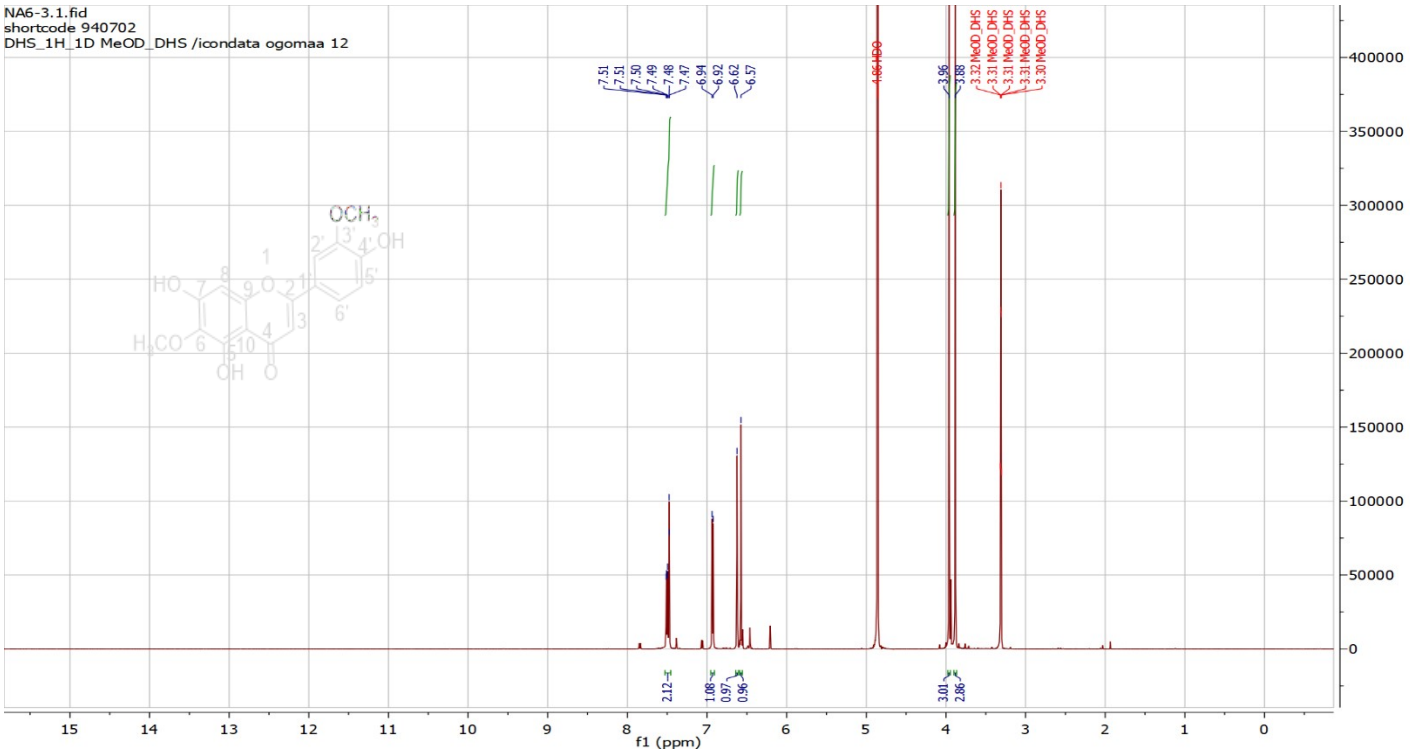
Fiqure S. 19: Partial expansion of ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD).



Fiqure S. 20: Partial expansion of ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD).

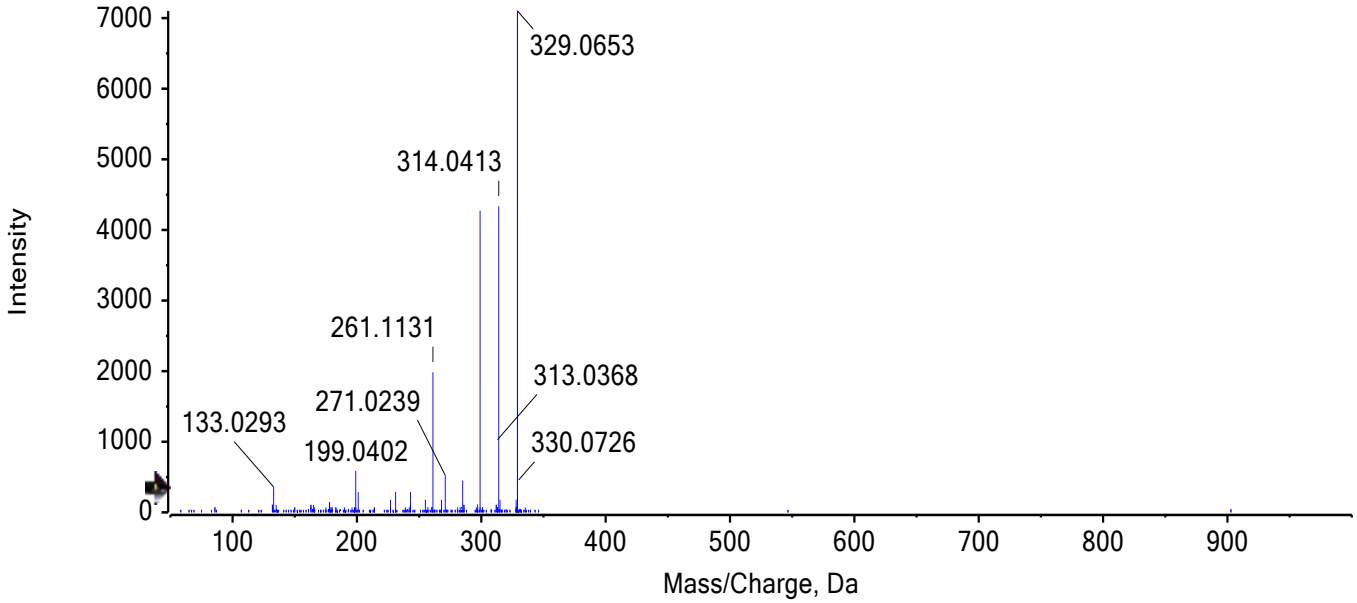


Fiqure S. 21: ^{13}C-NMR spectrum of compound 4 (600 MHz, CD_3OD).



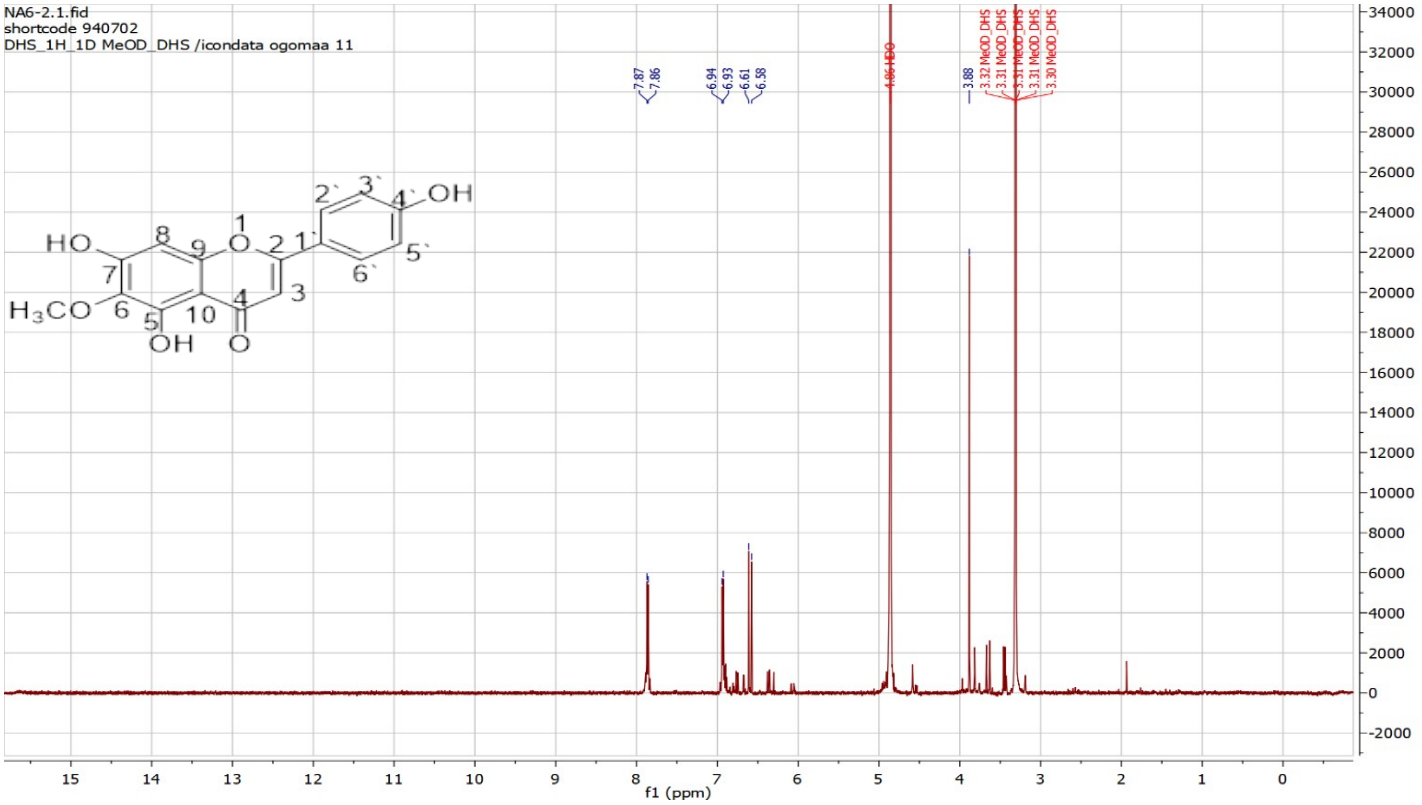
Fiqure S. 22: ^{1}H-NMR spectrum of compound 4 (600 MHz, CD_3OD).

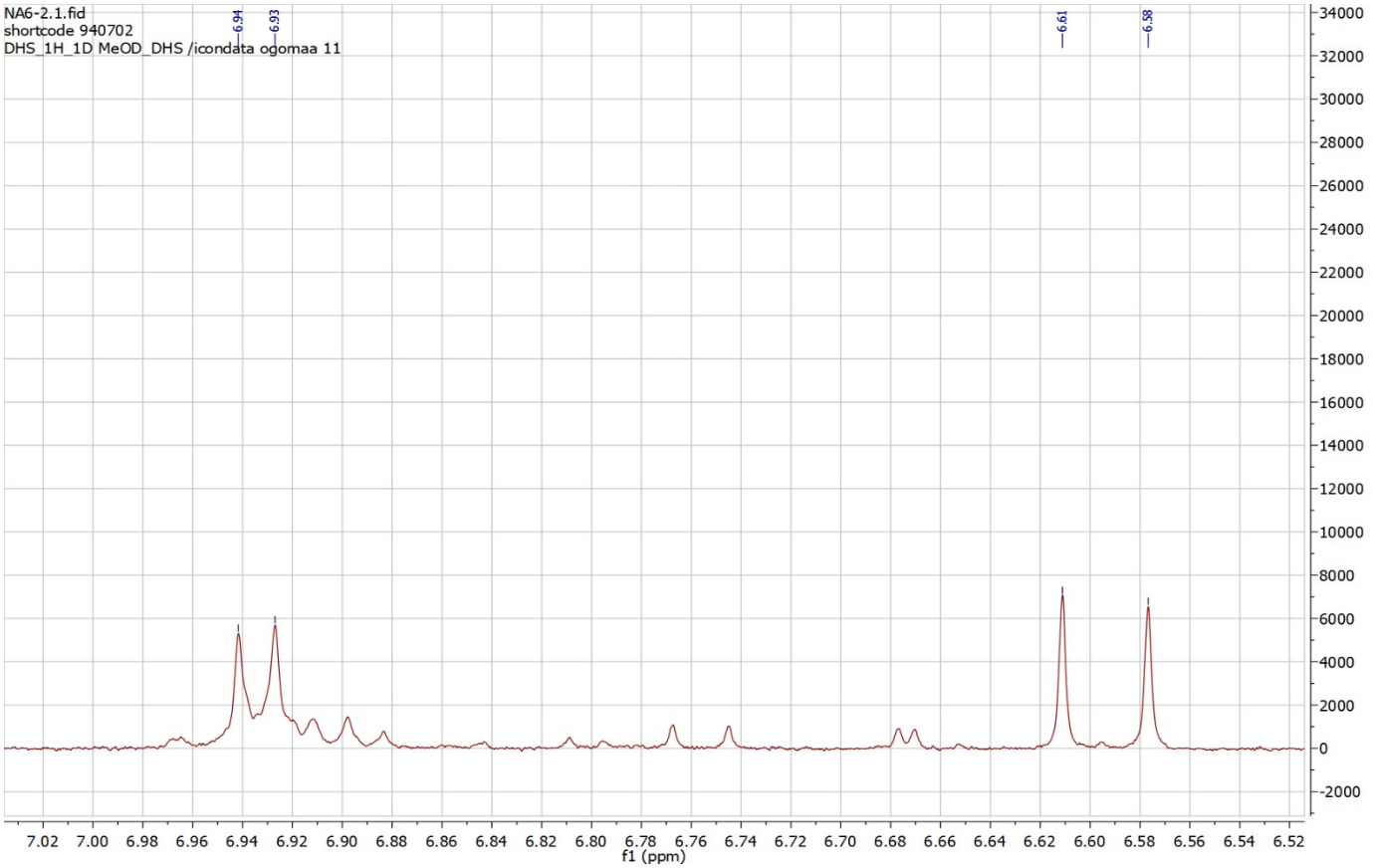
Spectrum from 201028-IDA-NEG-SM0084.wiff (sample 1) - 2...84, Experiment 3, -TOF MS^2 (50 - 1000) from 11.708 min
Precursor: 329.1 Da



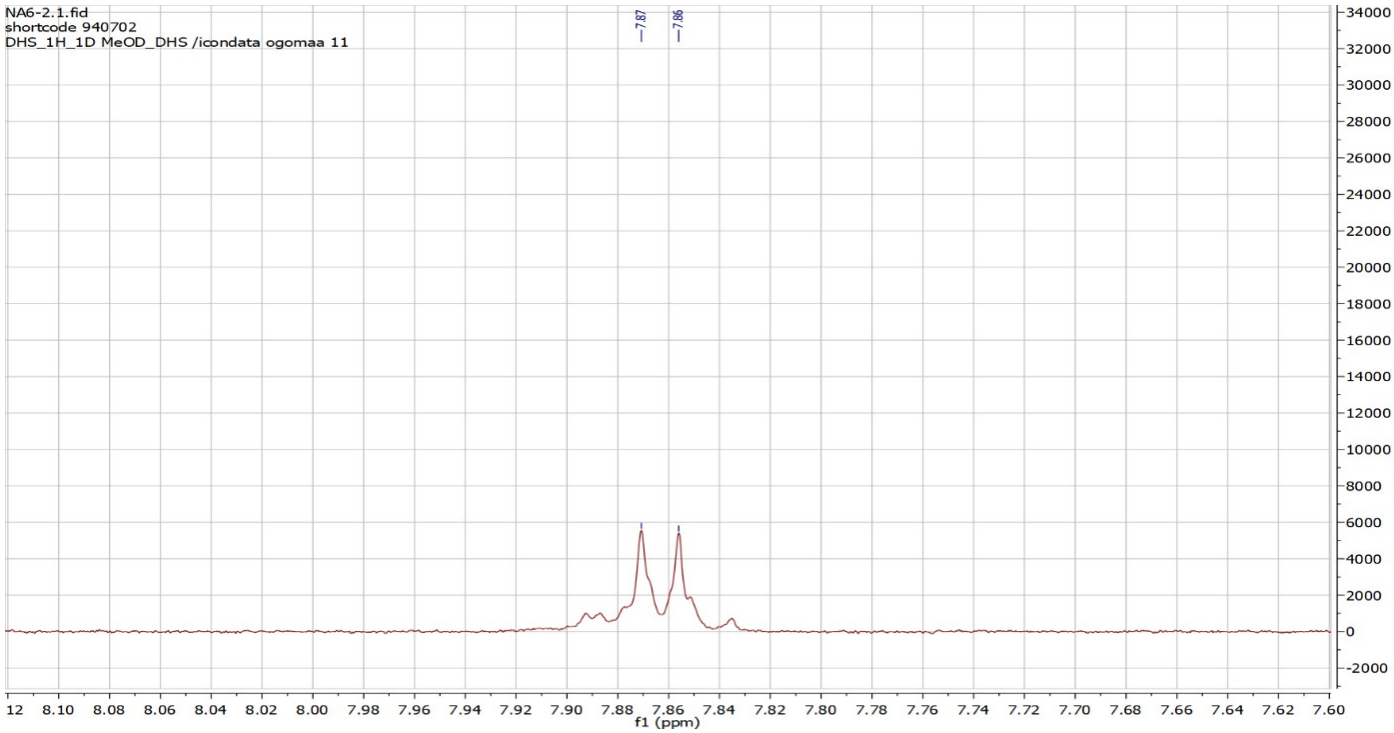
Fiqure S. 23: LC-MS/MS of compound 4

Spectroscopic data of compound 5

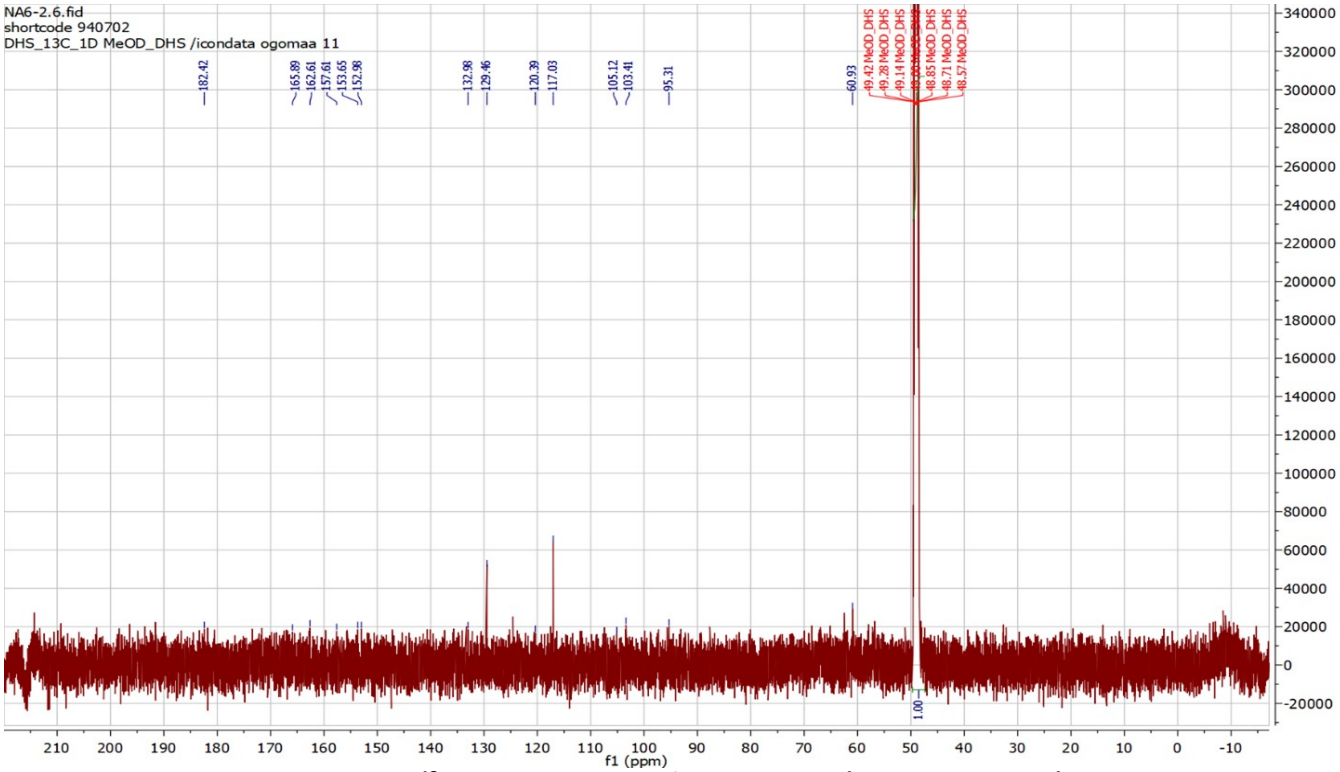

NA6-2.1.fid
shortcode 940702
DHS_1H_1D MeOD_DHS /icondata ogomaa 11
7.87
7.86
6.94
6.93
6.61
6.58
4.86 HDO
3.88
3.32 MeOD_DHS
3.31 MeOD_DHS
3.31 MeOD_DHS
3.31 MeOD_DHS
3.30 MeOD_DHS
HO
OH
H_3CO
OH
O
f1 (ppm)



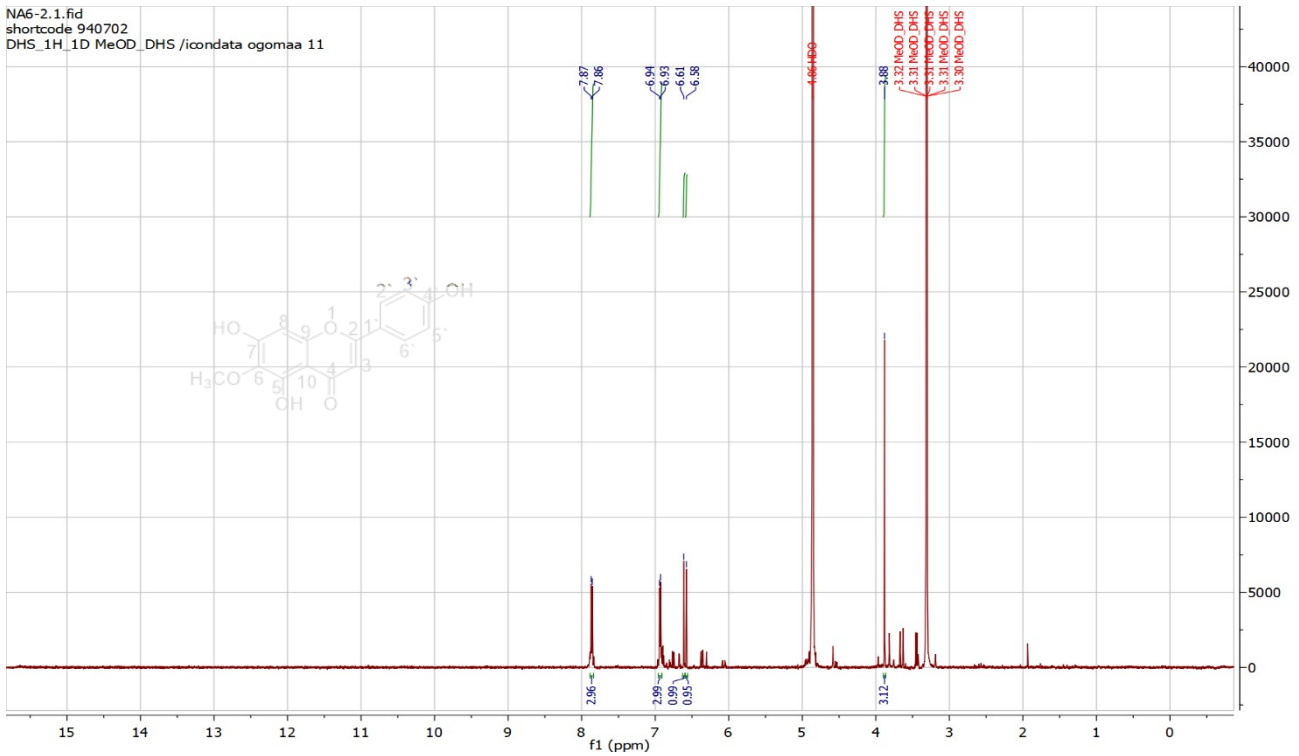
Fiqure S. 25: Partial expansion of ^{1}H-NMR spectrum of compound 5 (600 MHz, CD_3OD).



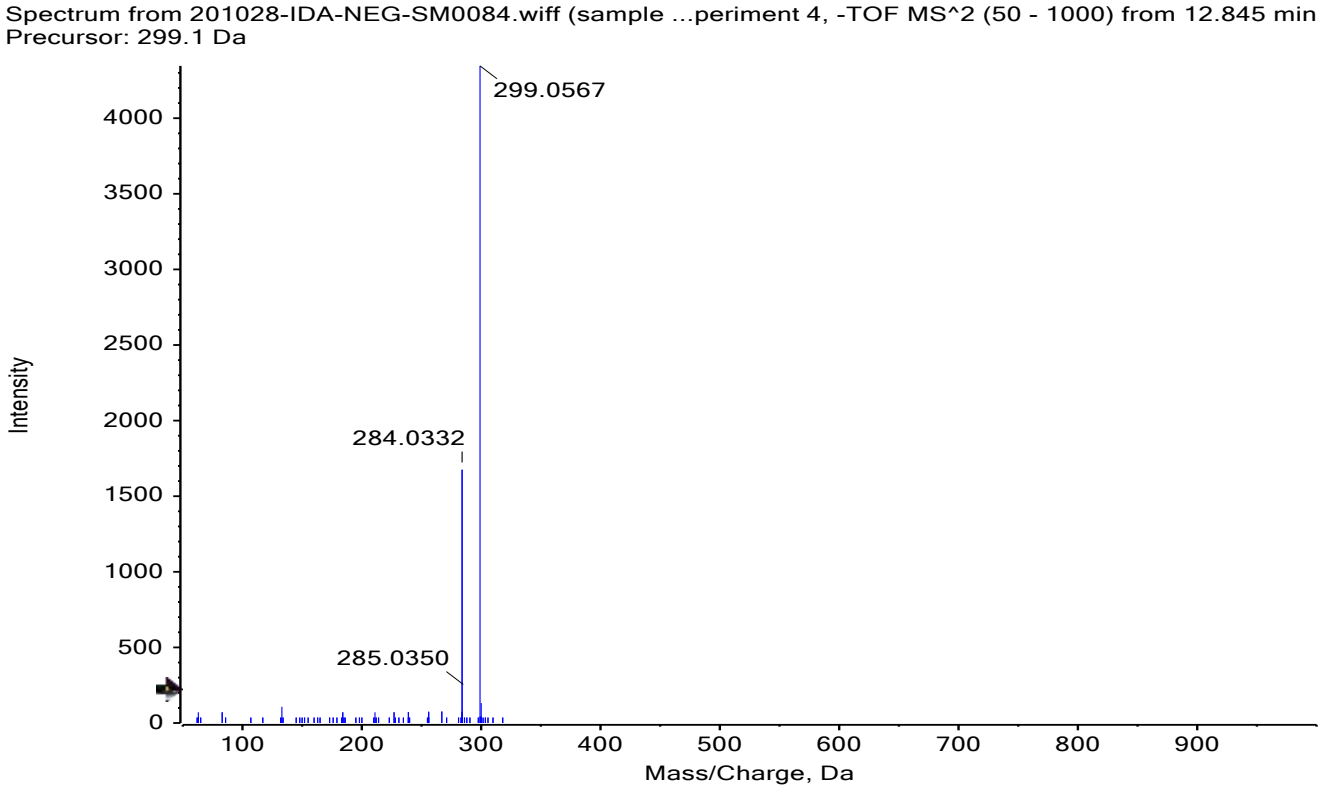
Fiqure S. 26: Partial expansion of ^{1}H-NMR spectrum of compound 5 (600 MHz, CD_3OD).



Fiqure S. 27: ^{13}C-NMR spectrum of compound 5 (150 MHz, CD_3OD)

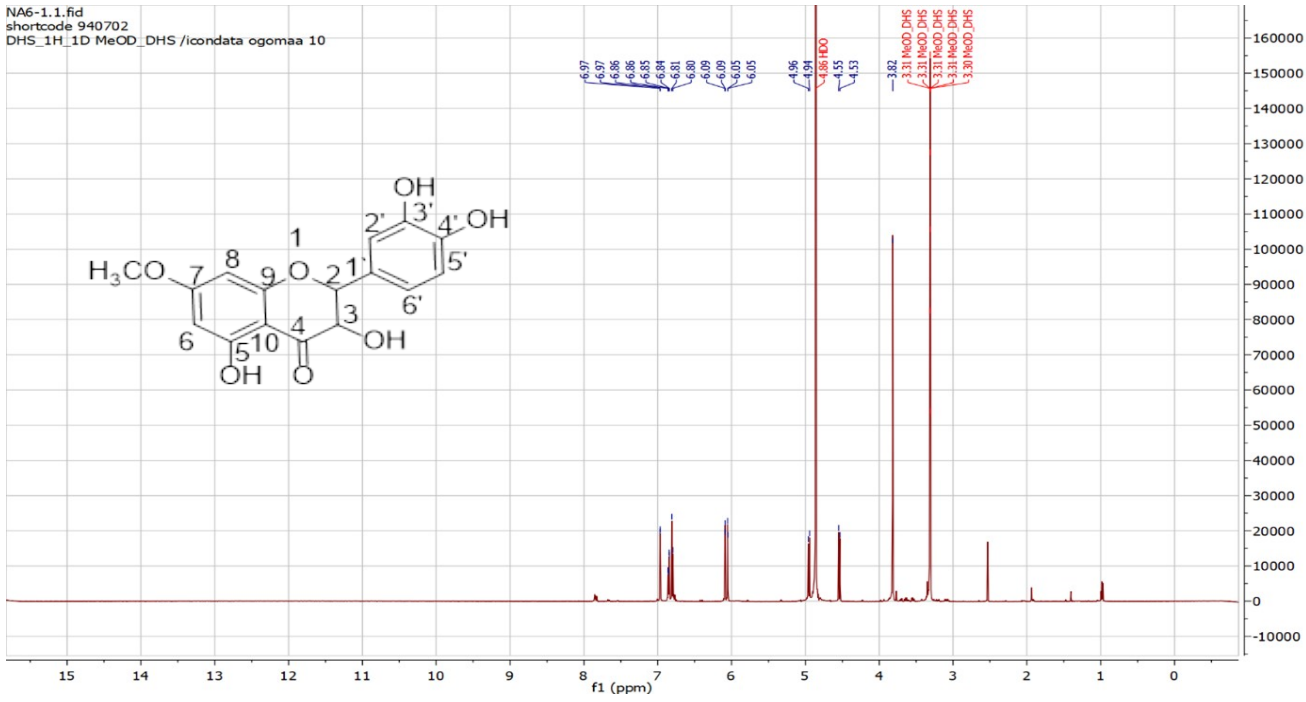


Fiqure S. 28: ^{1}H-NMR spectrum of compound 5 (600 MHz, CD_3OD).

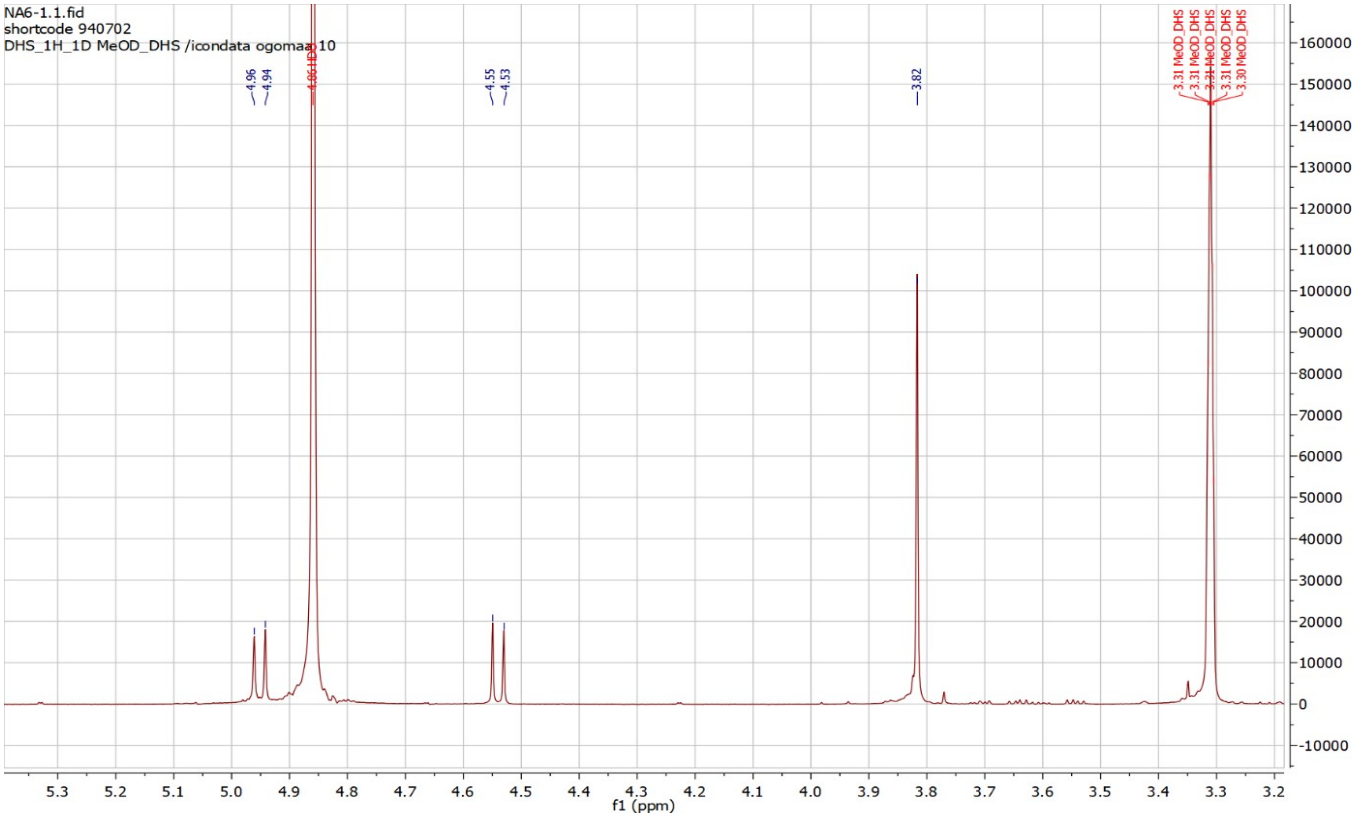


Fiqure S. 29: LC-MS/MS of compound 5

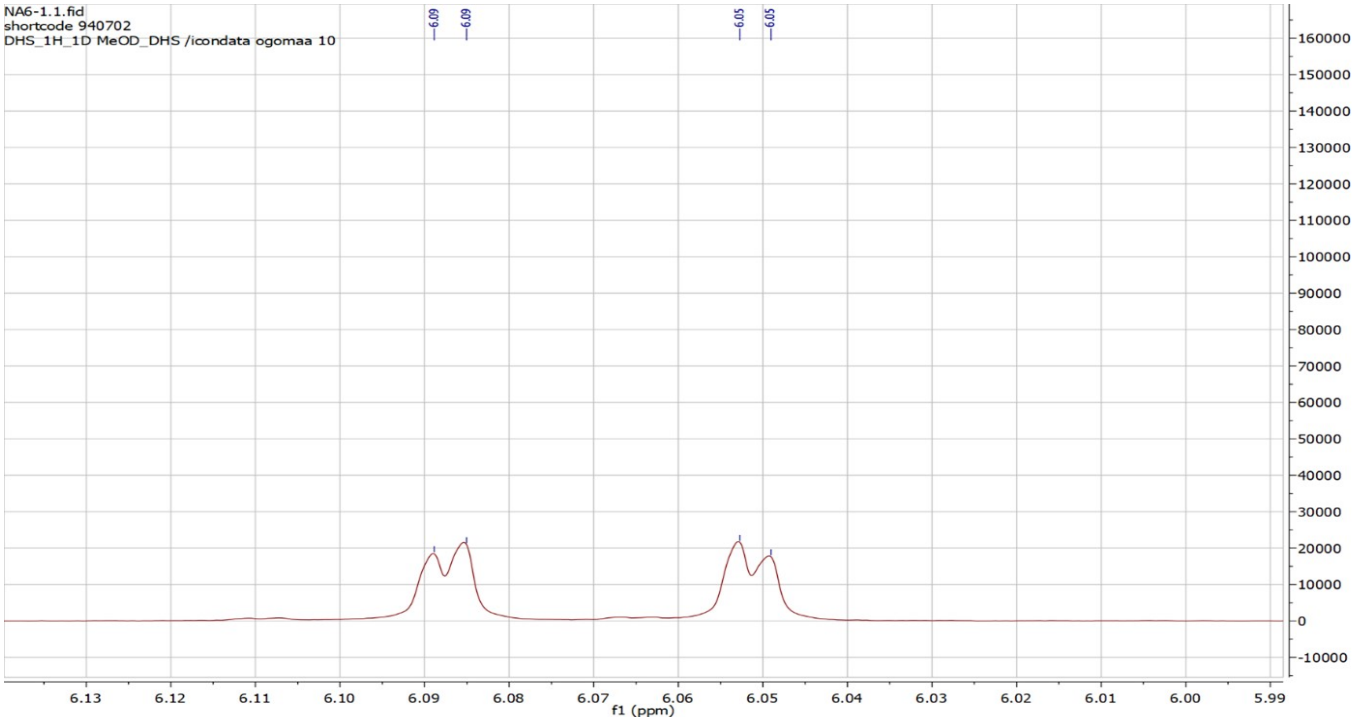
Spectroscopic data of compound 6



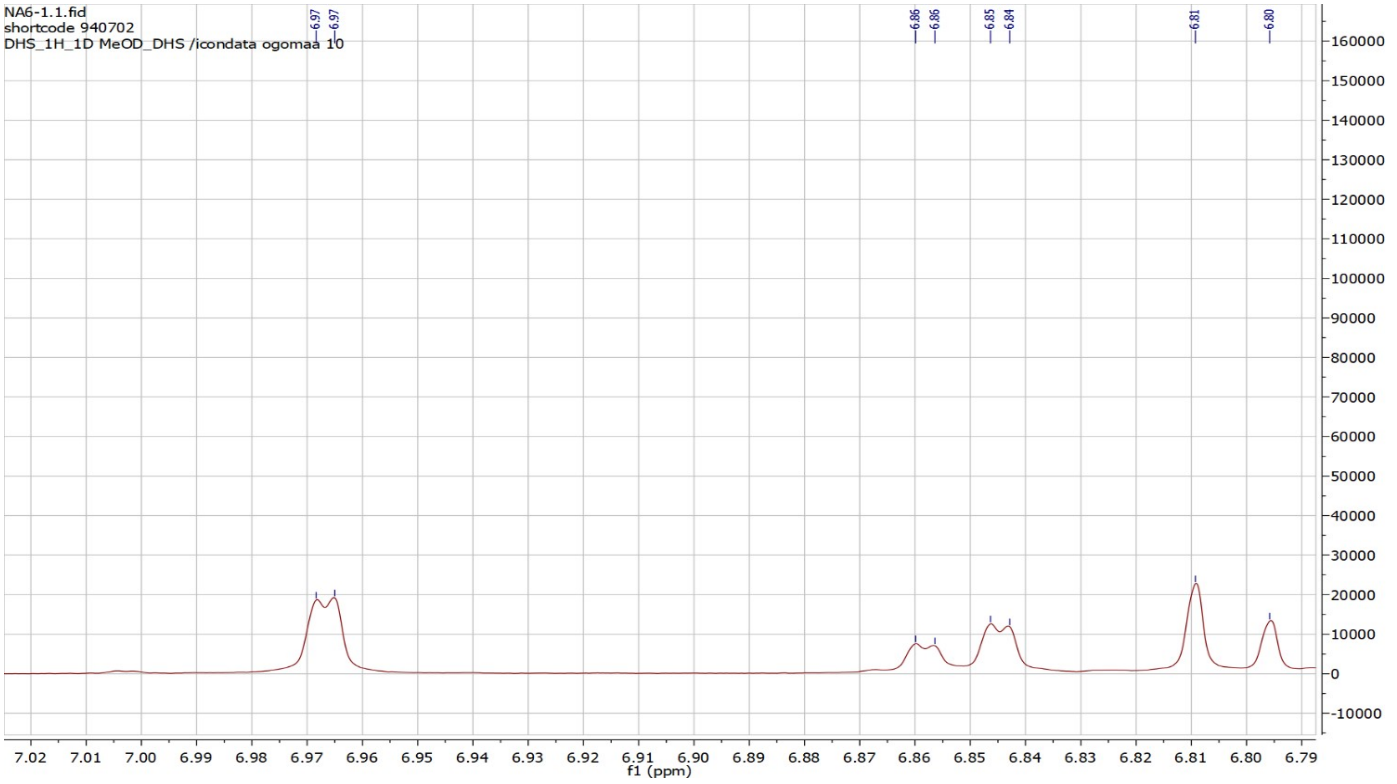
Fiqure S. 30:^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD).



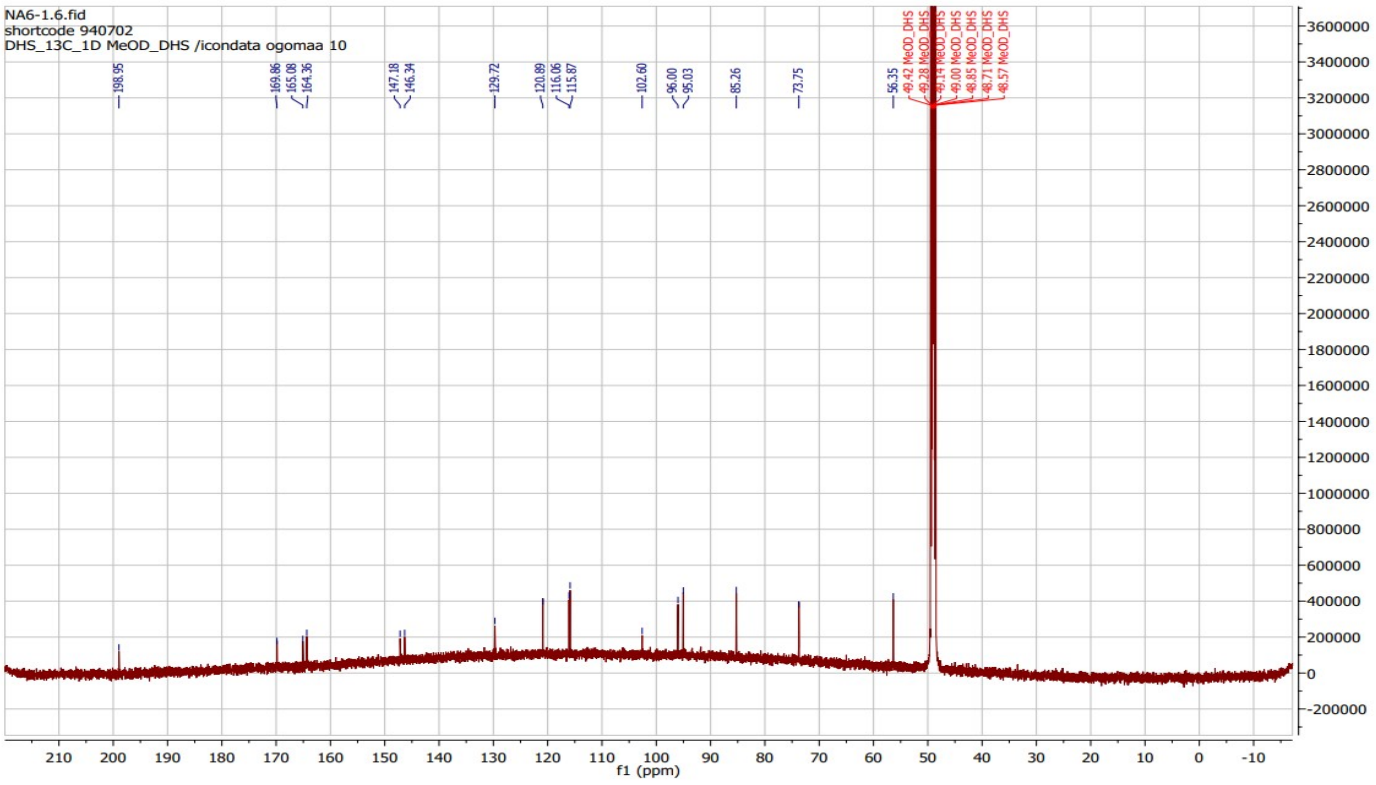
Fiqure S. 31: Partial expansion of ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD).



Fiqure S. 32: Partial expansion of ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD).



Fiqure S. 33: Partial expansion of ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD).



Fiqure S. 34: ^{13}C-NMR spectrum of compound 6 (150 MHz, CD_3OD).

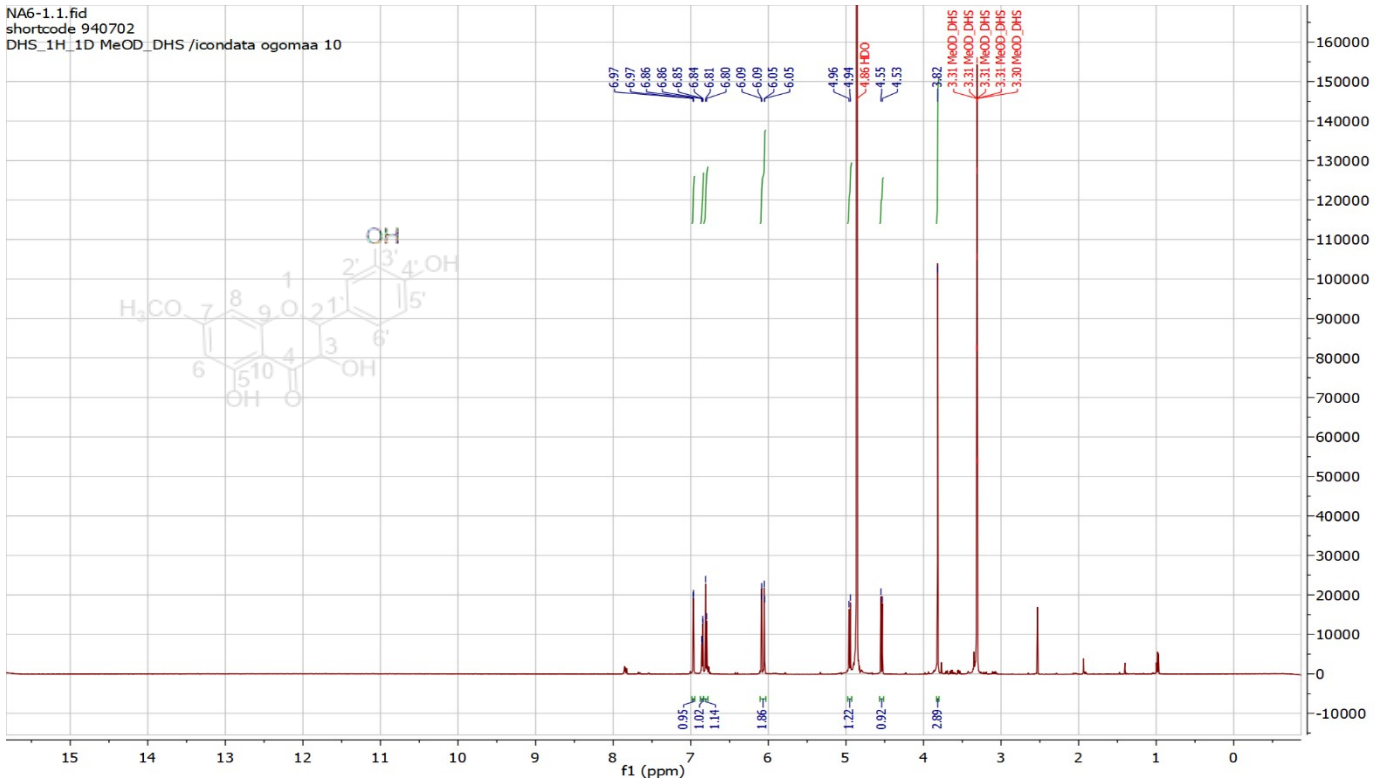


Figure S. 35: ^{1}H-NMR spectrum of compound 6 (600 MHz, CD_3OD).

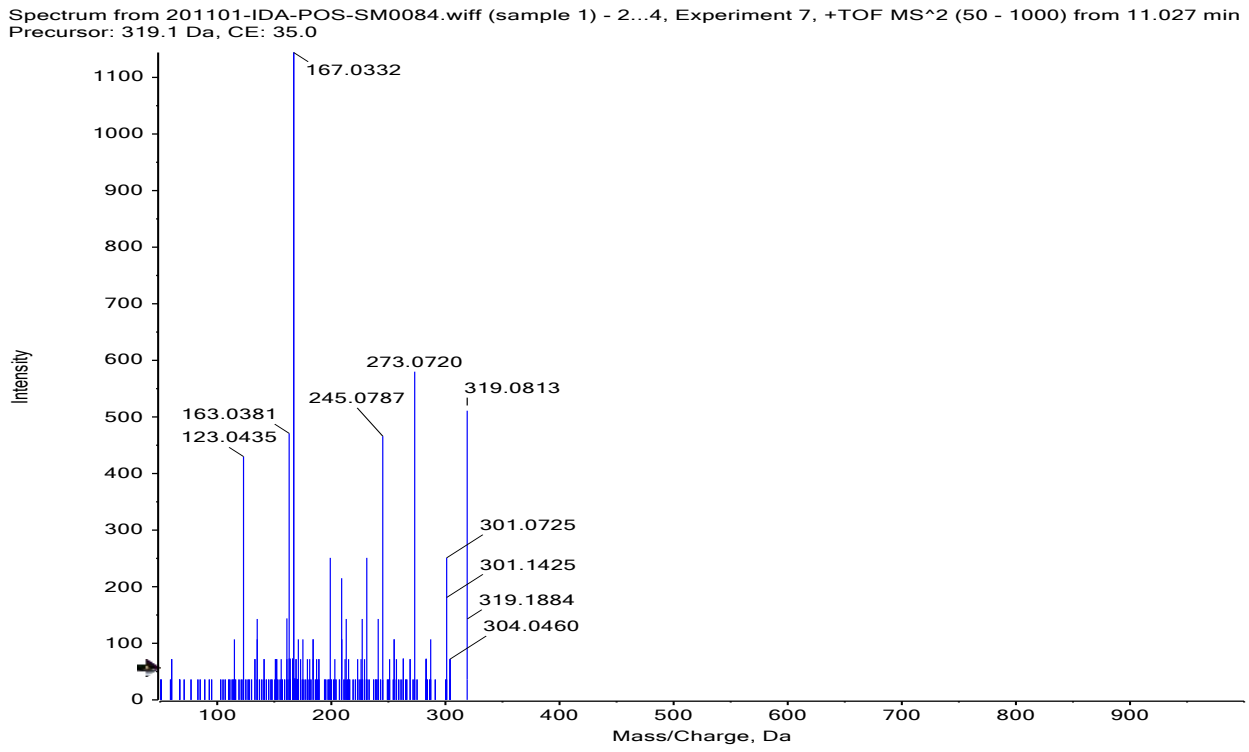
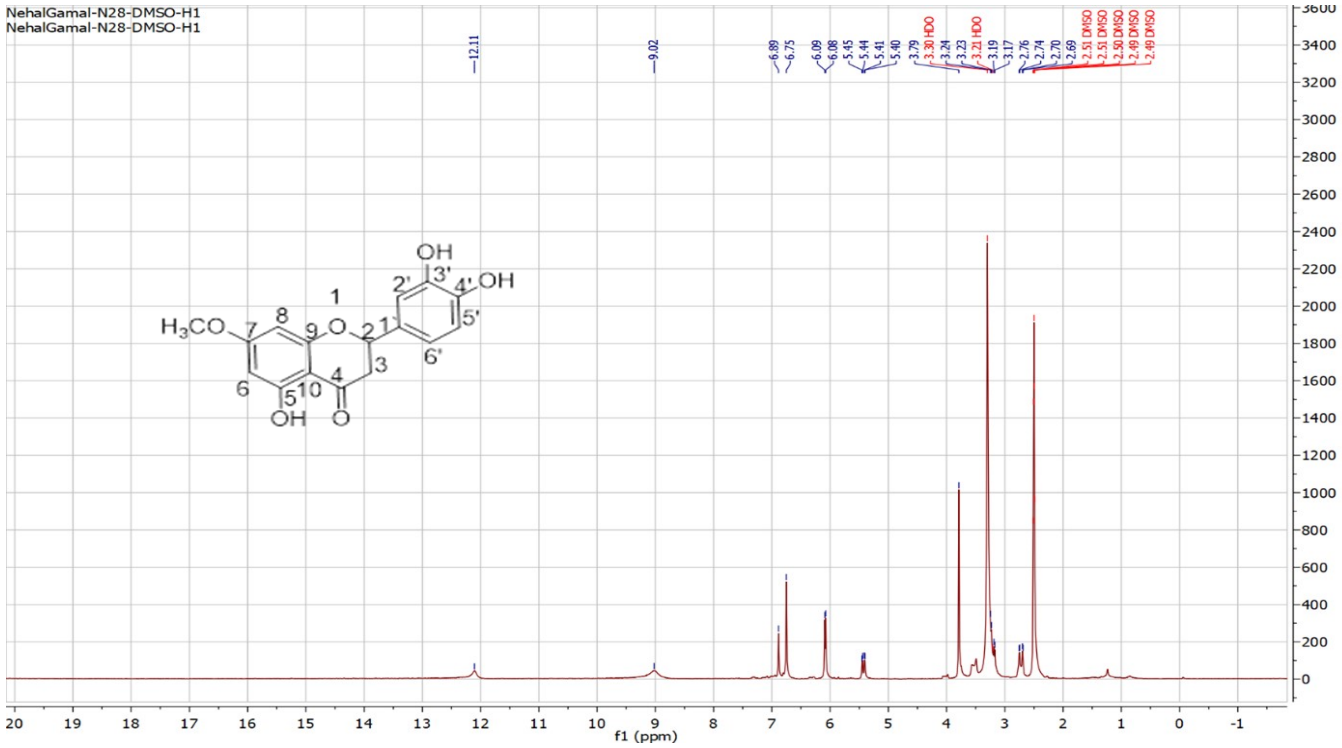
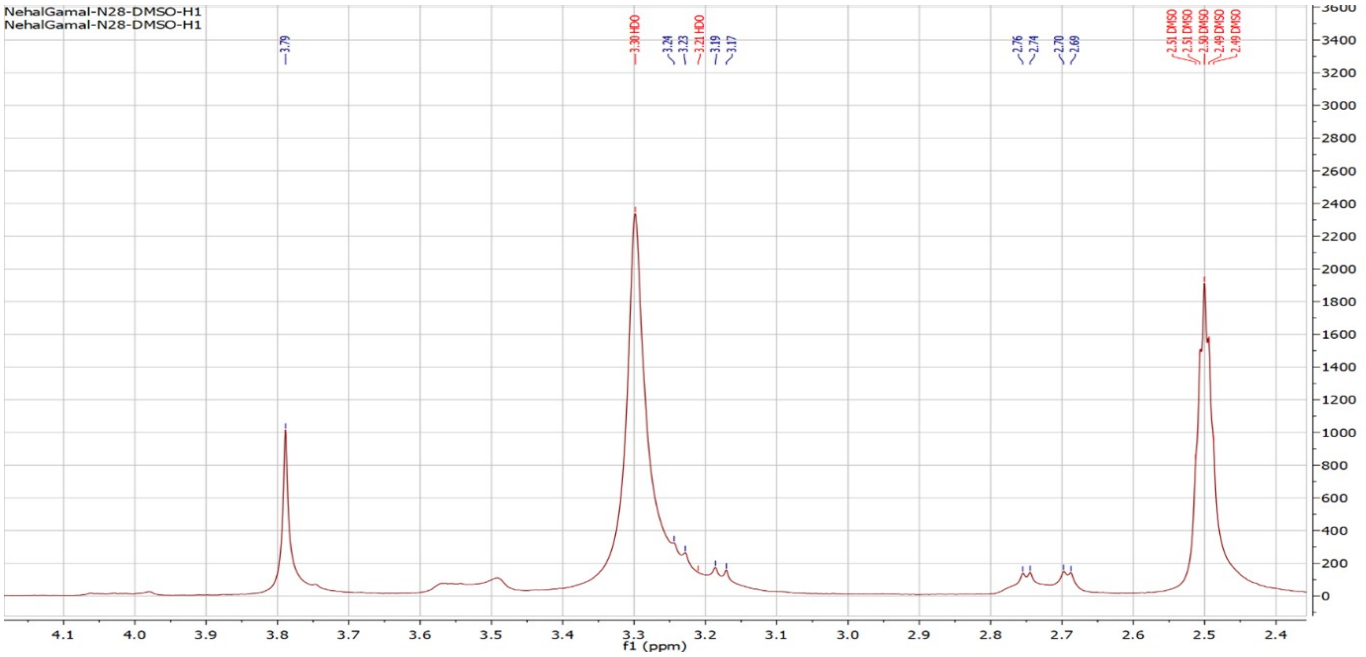


Figure S. 36: LC-MS/MS of compound 6

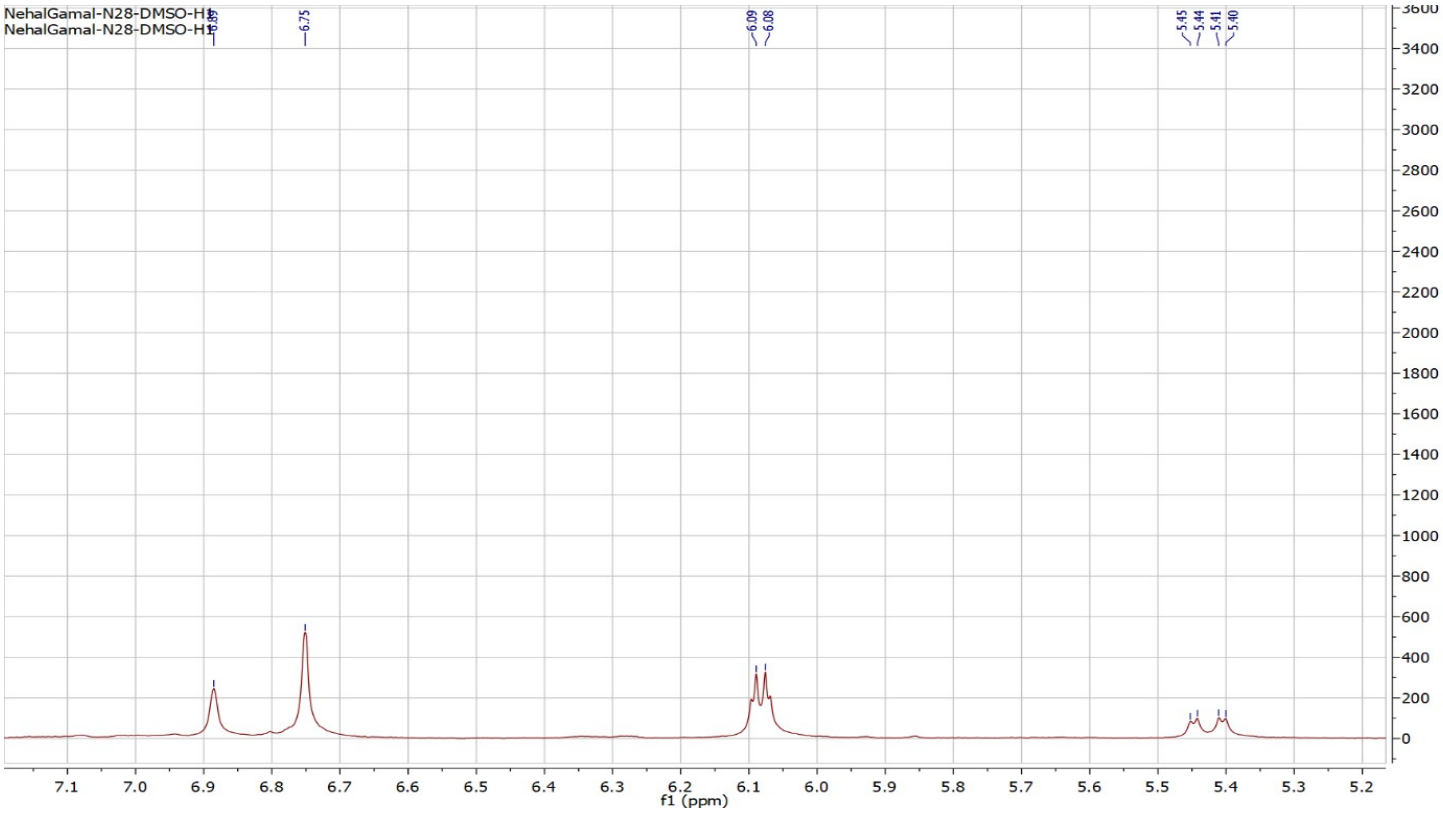
Spectroscopic data of compound 7



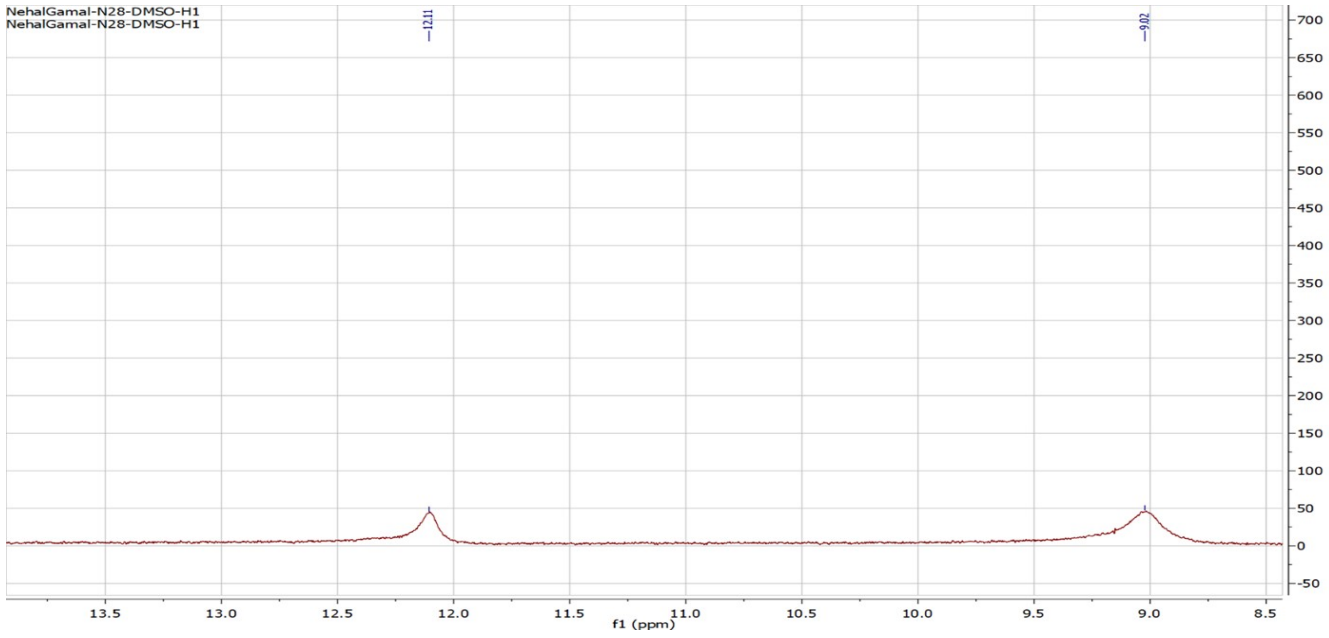
Fiqure S. 37: ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-*d6*)



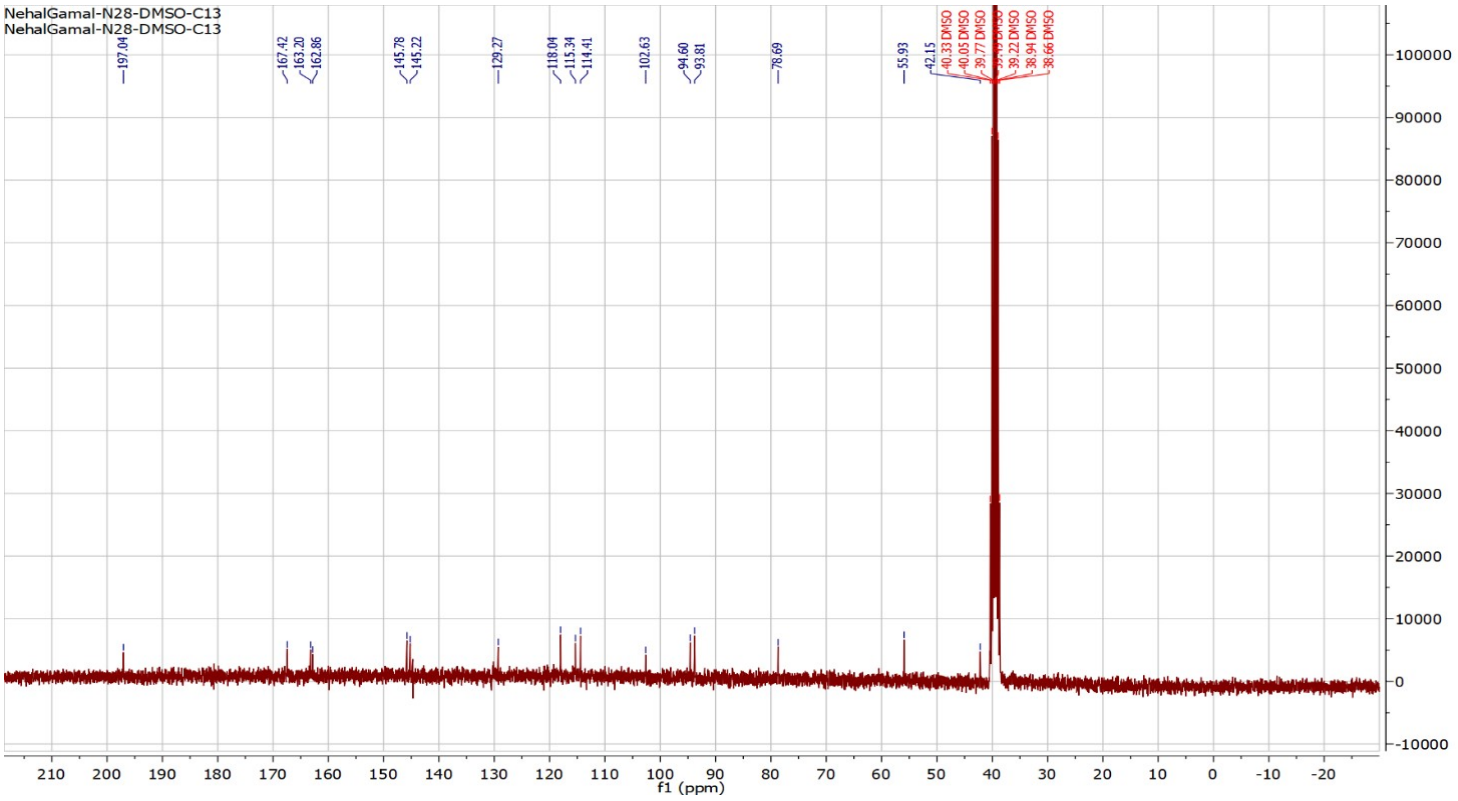
Fiqure S. 38: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-*d6*).



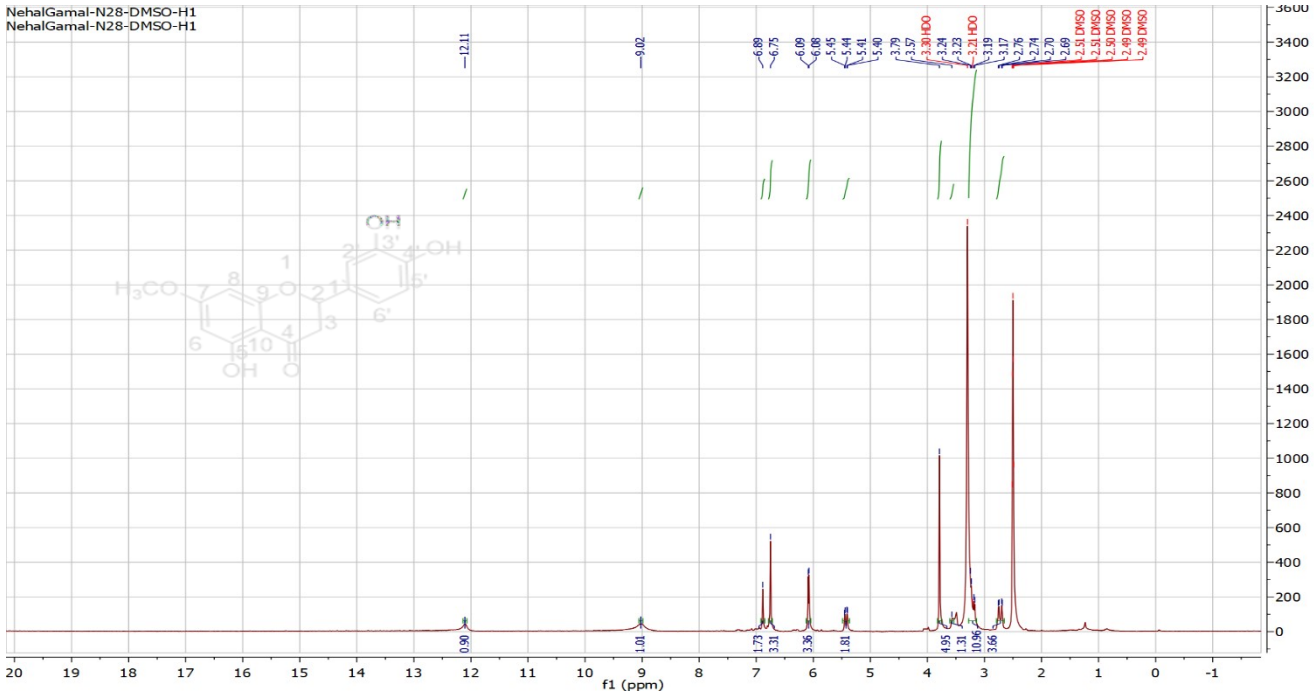
Fiqure S. 39: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-d6).



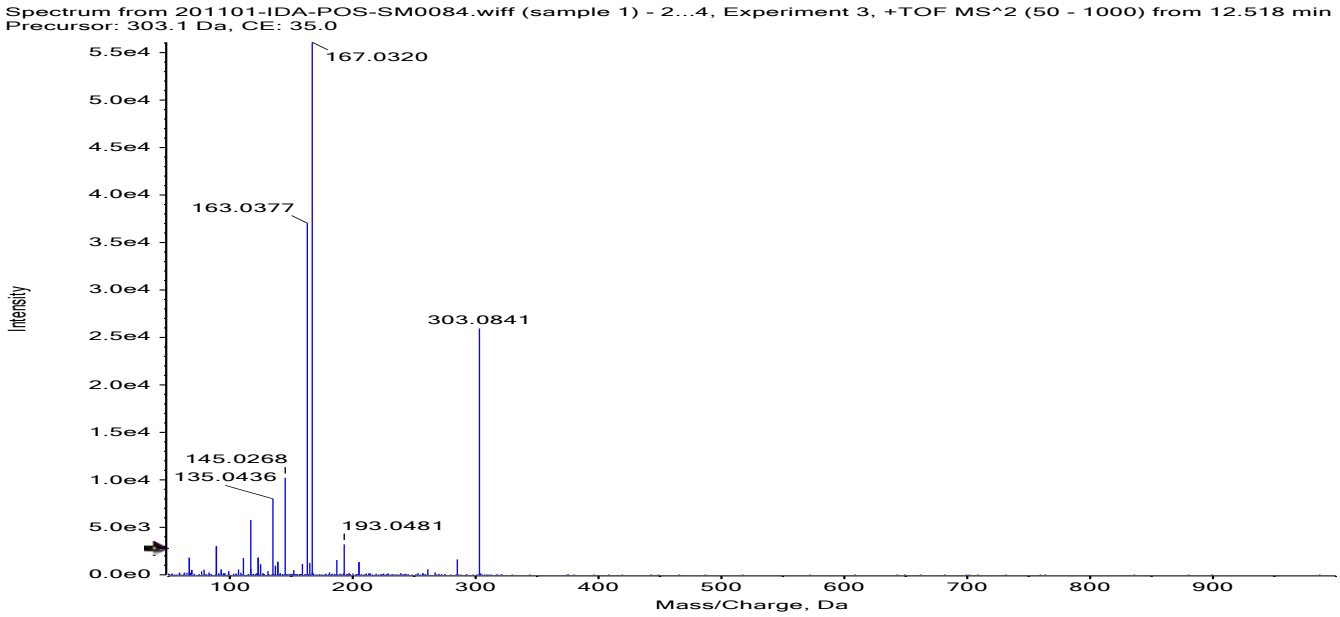
Fiqure S. 40: Partial expansion of ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-d6).



Fiqure S. 41: ^{13}C-NMR spectrum of compound 7 (75 MHz, DMSO-*d6*).

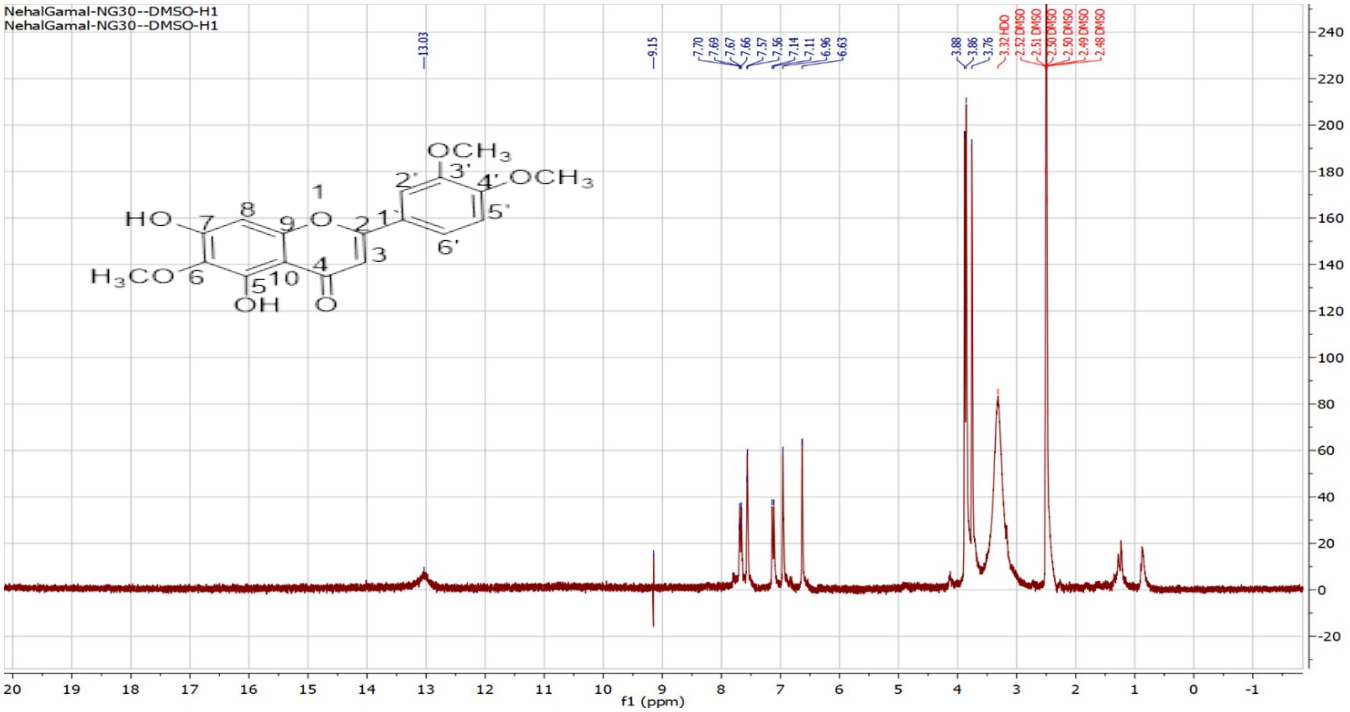


Fiqure S. 42: ^{1}H-NMR spectrum of compound 7 (300 MHz, DMSO-*d6*)

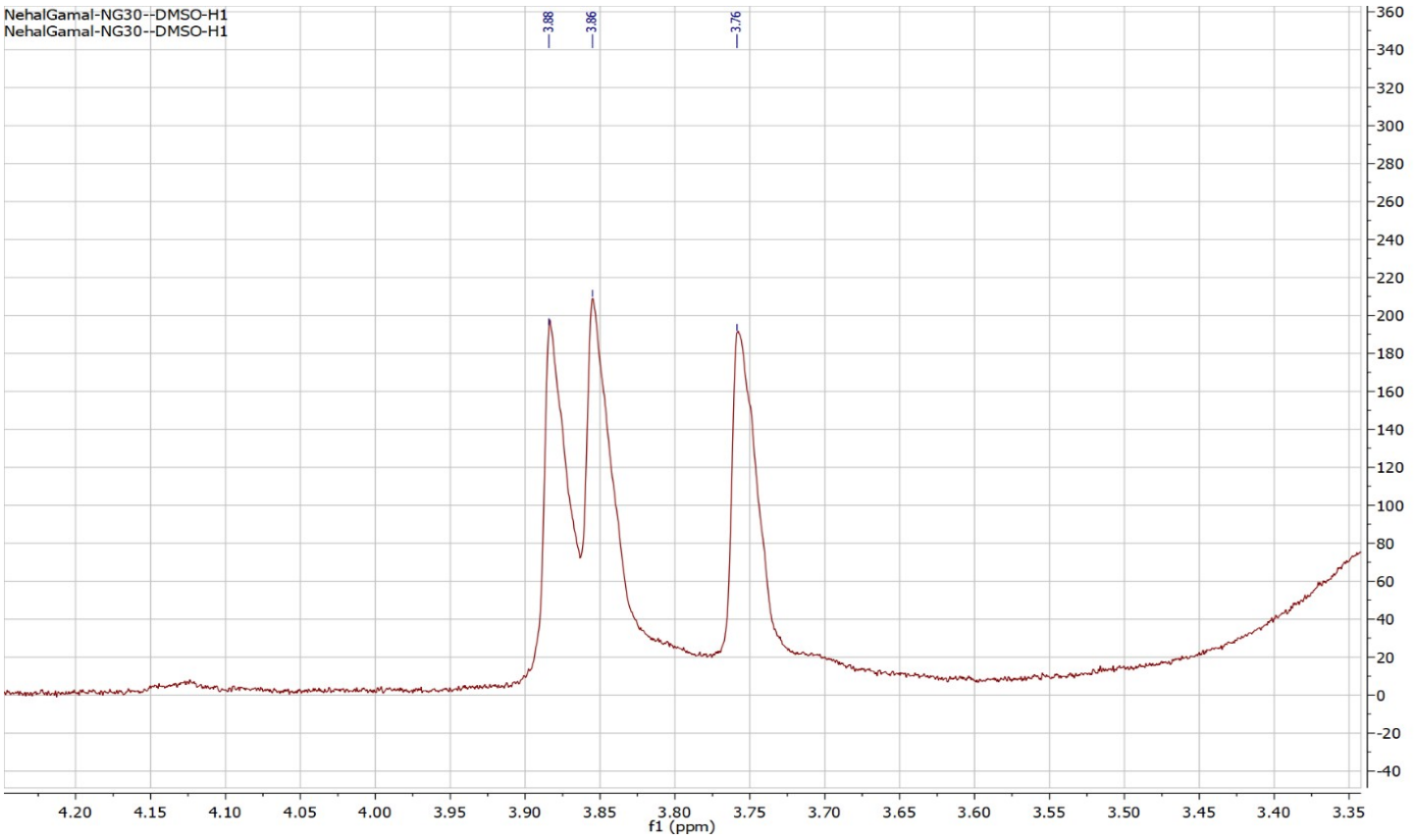


Fiqure S. 43: LC-MS/MS of compound 7

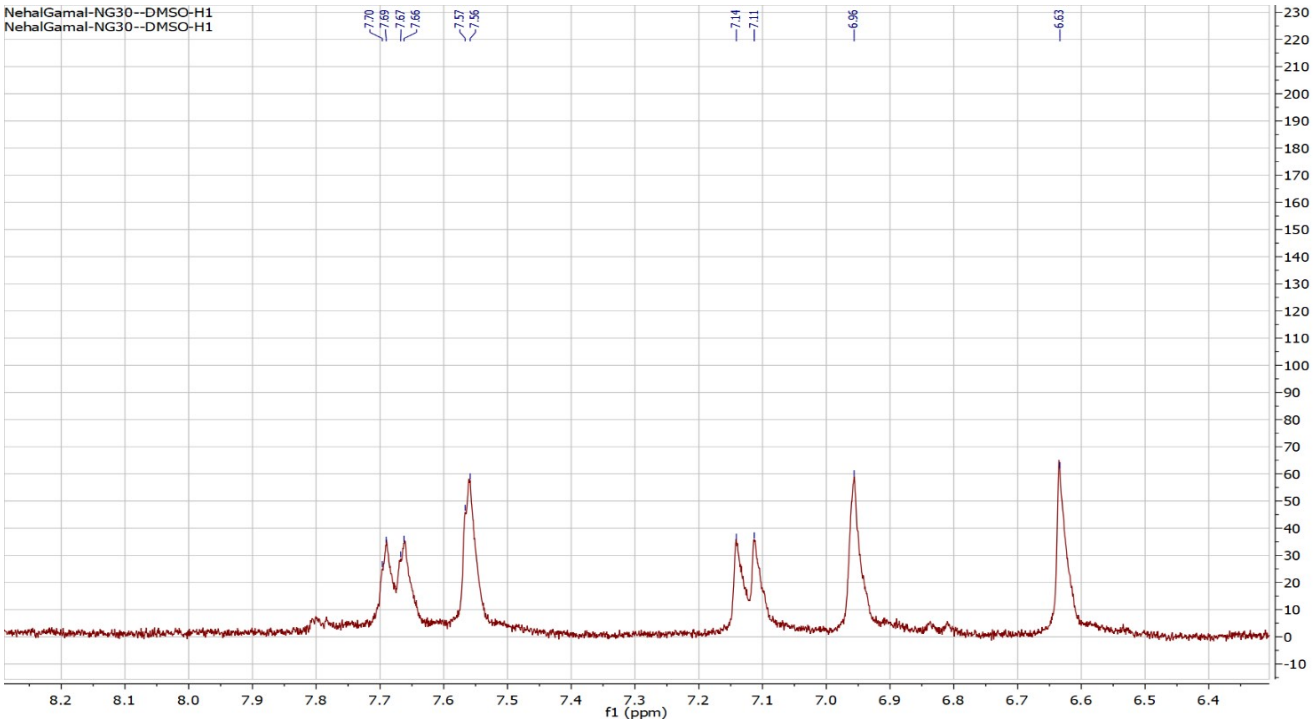
Spectroscopic data of compound 8



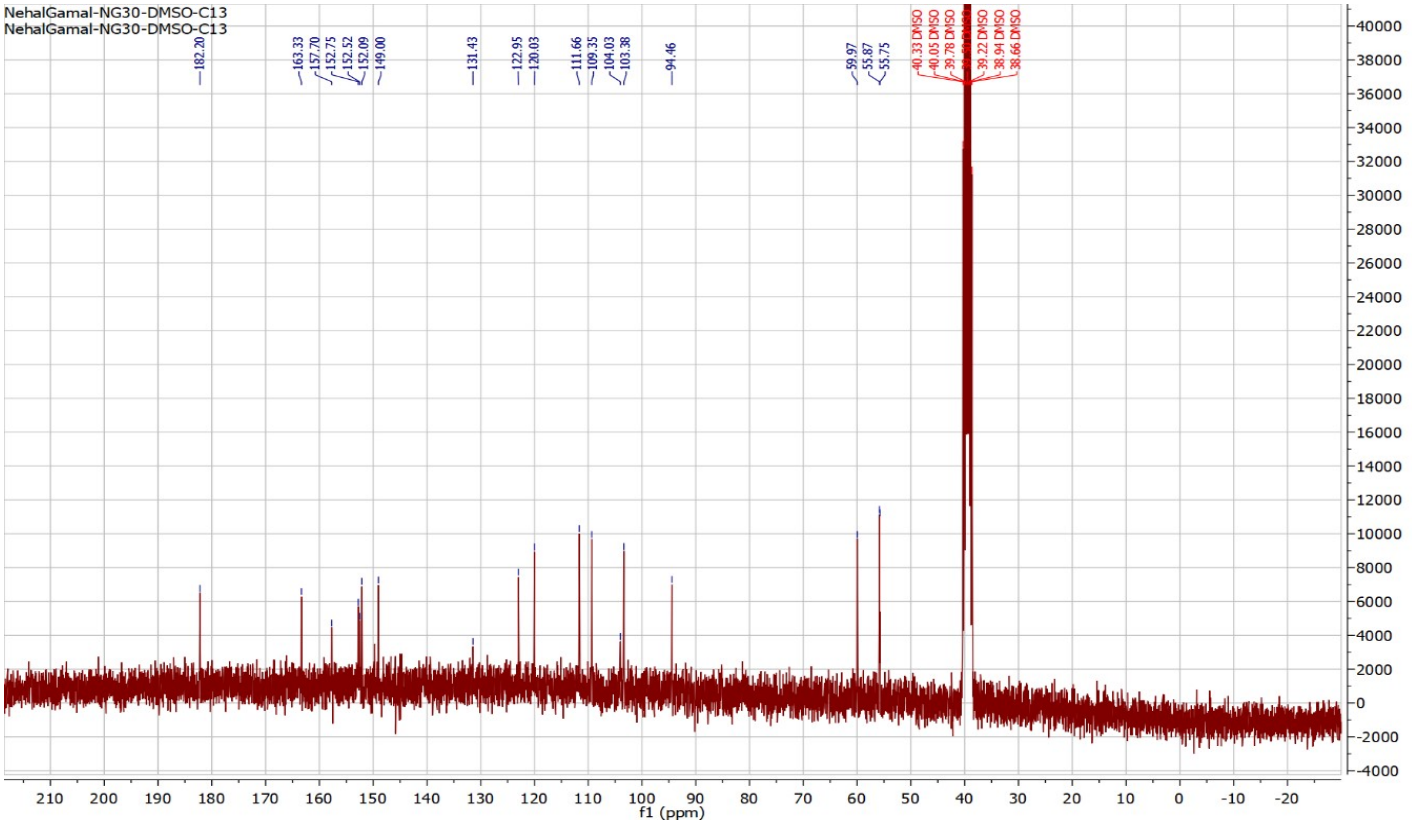
Fiqure S. 44: ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*).



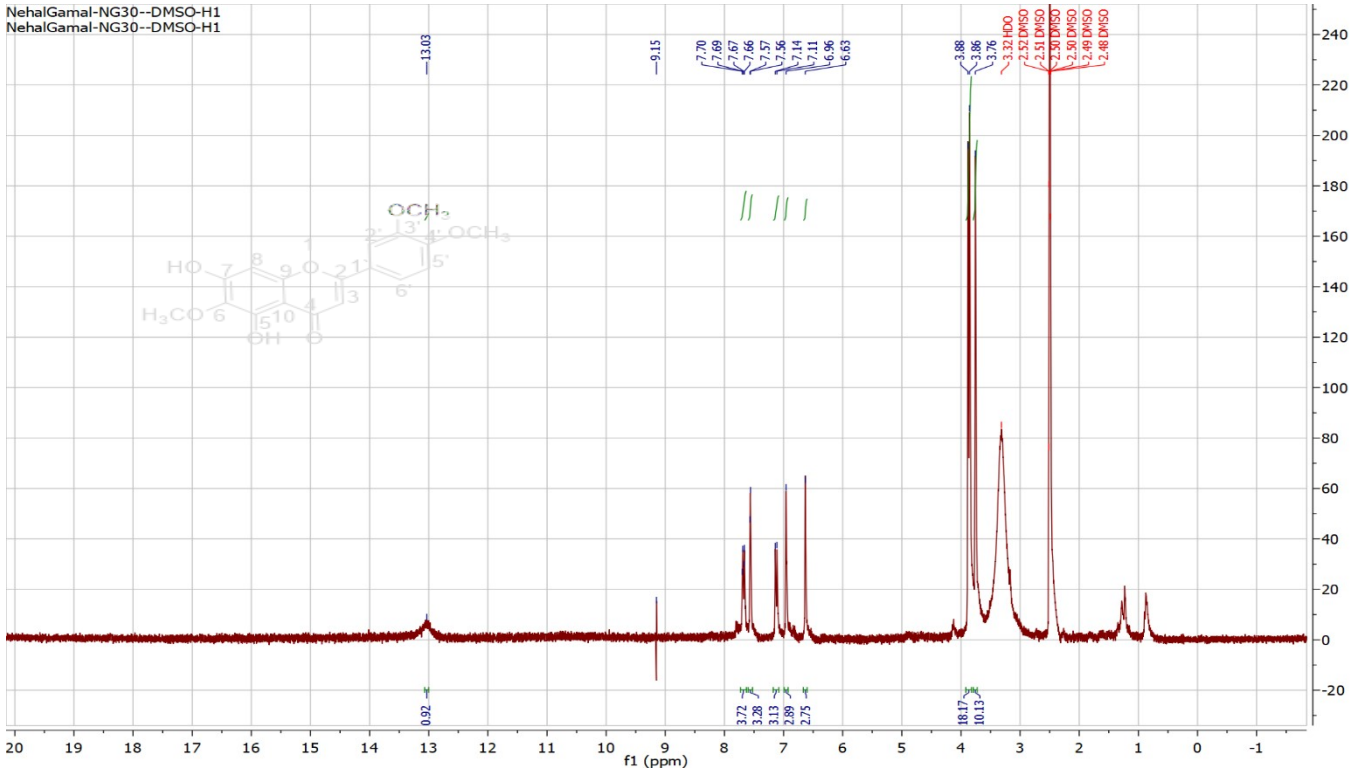
Fiqure S. 45: Partial expansion of ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*).



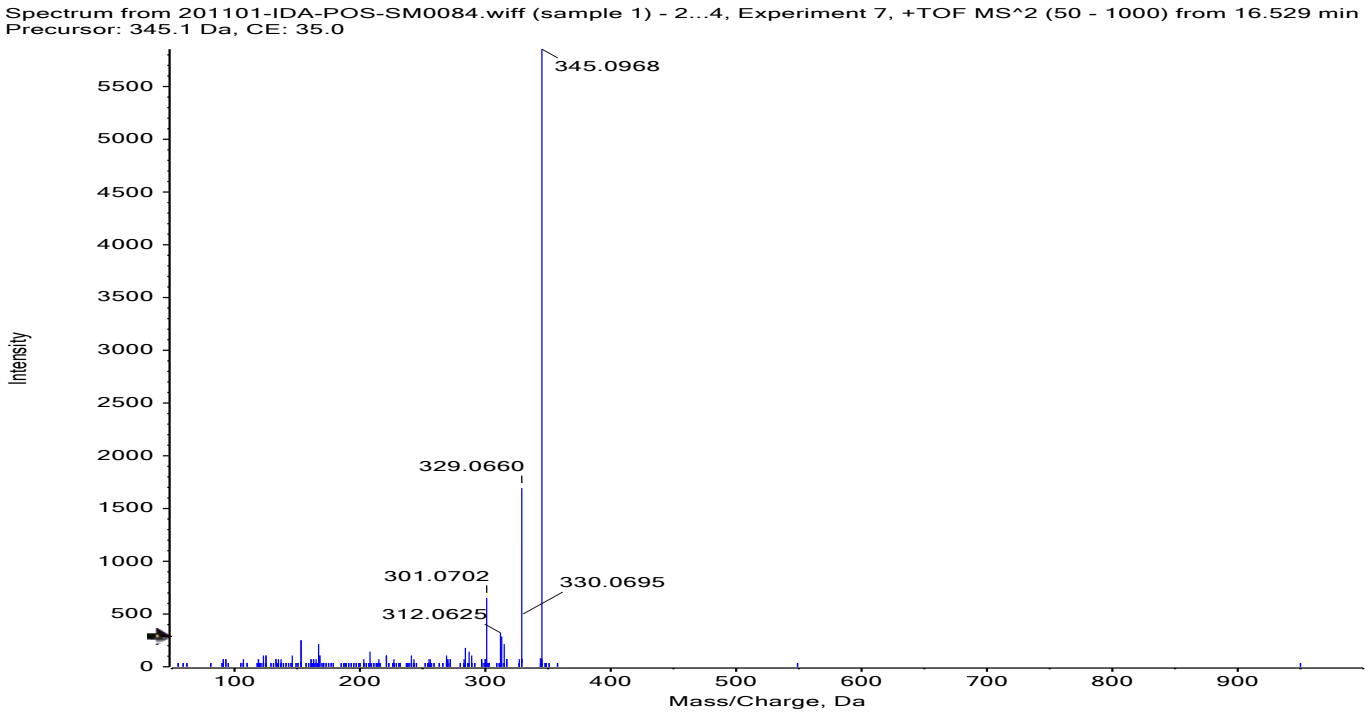
Fiqure S. 46: Partial expansion of ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*).



Fiqure S. 47: ^{13}C-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*).



Fiqure S. 48: ^{1}H-NMR spectrum of compound 8 (300 MHz, DMSO-*d6*).



Fiqure S. 49: LC-MS/MS of compound 8

Table S. 1: ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 1 (DMSO-*d6* δ in ppm, *J* in Hz).

Position	δ_c (ppm)	δ_H ppm (No. of H, *m*, *J* Hz)	Position	δ_c (ppm)	δ_H ppm (No. of H, *m*, *J* Hz)
1	38.3	2.37 (1H, *m*) & 2.12 (1H, *m*)	21	18.6	0.90 (3H, *d*, *J* = 6.2 Hz)
2	33.3	1.33 (2H, *m*)	22	138.1	5.16 (1H, *dd*, *J* = 15.1, 8.4 Hz)
3	76.9	3.44 (1H, *m*)	23	128.8	5.02 (1H, *dd*, *J* = 15.2, 8.1 Hz
4	36.8	1.80 (1H, *br d*, *J* = 10.7 Hz) & 1.17 (1H, *d*, *J* = 6.7 Hz)	24	31.3	0.98 (1H, *br s*)
5	140.4	__	25	31.3	1.64 (1H, *m*)
6	121.2	5.32 (1H, *br d*, *J* = 4.7 Hz)	26	19.1	0.82 (3H, *d*, *J* = 6.2 Hz)
7	31.4	1.42 (2H, *m*)	27	18.9	0.81 (3H, d, *J* = 6.2

					Hz)
8	31.4	1.51 (1H, *br s*)	28	23.9	0.96 (2H, *br s*)
9	49.6	1.00 (1H, *br s*)	29	11.7	0.78 (3H, *d, J* = 6.5 Hz)
10	36.2	___	1`	100.8	4.21 (1H, *d, J* = 7.5 Hz)
11	22.6	1.20 (2H, *m*)	2`	70.1	2.89 (1H, *m*)
12	41.7	2.04 (1H, *m*) & 1.15 (1H, *m*)	3`	76.8	3.14 (1H, *m*)
13	41.9	___	4`	73.5	3.08 (1H, *m*)
14	56.3	1.00 (1H, *m*)	5`	76.8	3.04 (1H, *m*)
15	24.9	1.13 (2H, *m*)	6`	61.1	3.64 (2H, *m*)
16	29.3	1.94 (1H, *br s*) & 1.78 (1H, *br s*)	2`-OH		4.82 (*br s*)
17	56.2	1.00 (1H, *m*)	3`-OH		4.85 (*br s*)
18	11.9	0.65 (3H, *s*)	4`-OH		4.81 (*br s*)
19	18.9	0.96 (3H, *br s*)	6`-OH		4.38 (*t*, *J* = 5.6 Hz)
20	35.5	1.36 (1H, *m*)			

Table S. 2 ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 2 (DMSO-*d6* δ in ppm, *J* in Hz).

Position	δ_c (ppm)	δ_H ppm (No. of H, *m, J* Hz)
2	162.1	
3	106.8	7.09 (1H, *s*)
4	182.3	
5	152.7	
6	131.7	
7	158.6	
8	91.7	6.94 (1H, *s*)
9	153.3	
10	104.4	
1`	106.8	
2`	152.0	

3`	104.9	6.56 (1H, *s*)
4`	152.0	
5`	141.7	
6`	111.8	7.44 (1H, *s*)
6-OCH3	60.1	3.93 (3H, *s*)
7-OCH3	56.8	3.81 (3H, *s*)
OCH3-5`	56.6	3.73 (3H, *s*)
5-OH		13.03 (1H, *s*)
2`-OH		10.47 (1H, *s*)
4`-OH		10.04 (1H, *s*)

Table S. 3 ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectroscopic data of compound 3 (DMSO-*d6* δ in ppm, *J* in Hz).

Position	**δ_c (ppm)**	**δ_H ppm (No. of H, *m, J* Hz)**
2	147.7	
3	136.5	
4	176.1	
5	160.8	
6	97.9	6.36 (1H, *d*, *J* = 2.2 Hz)
7	165.4	
8	92.4	6.71 (1H, *d*, *J* = 2.2 Hz)
9	156.5	
10	104.5	
1`	122.3	
2`	115.7	7.73 (1H, *d*, *J* = 2.2 Hz)
3`	145.5	
4`	148.3	
5`	116.0	6.90 (1H, *d*, *J* = 8.5 Hz,)
6`	120.5	7.58 (1H, *dd*, *J* = 8.5, 2.2 Hz,)
7-OCH3	56.5	3.87 (3H, *s*)
3-OH		9.51 (1H, *s*)

5-OH		12.50 (1H, *s*)
3`-OH		9.31 (1H, *s*)
4`-OH		9.51 (1H, *s*)

Table S. 4 ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR spectroscopic data of compound 4 (CD_3OD, δ in ppm, *J* in Hz).

Position	δ_c (ppm)	δ_H ppm (No. of H, *m, J* Hz)
2	166.3	
3	103.8	6.62 (1H, *s*)
4	184.3	
5	154.7	
6	132.9	
7	158.7	
8	95.3	6.57 (1H, *s*)
9	154.0	
10	105.8	
1`	123.7	
2`	110.6	6.93 (1H, *d*, *J* = 8.8 Hz)
3`	152.1	
4`	149.5	
5`	116.8	7.47 (1H, *d*, *J* = 2 Hz)
6`	121.7	7.50 (1H, *dd*, *J* = 8.3, 2 Hz)
6-OCH3	60.9	3.88 (3H, *s*)
3`-OCH3	56.6	3.96 (3H, *s*)

Table S. 5 ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR spectroscopic data of compound 5 (CD_3OD, δ in ppm, *J* in Hz).

Position	δ_c (ppm)	δ_H ppm (No. of H, *m, J* Hz)
2	165.9	
3	103.4	6.61 (1H, *s*)

4	182.4	
5	153.7	
6	133.0	
7	157.6	
8	95.3	6.58 (1H, *s*)
9	153.0	
10	105.1	
1`	120.4	
2`, 6`	129.5	7.86 (2H, *d*, *J* = 8.4 Hz)
3`, 5`	117.0	6.94 (2H, *d*, *J* = 8.4 Hz)
4`	162.6	
6-OCH3	60.9	3.88 (3H, *s*)

Table S. 6 ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR spectroscopic data of compound 6 (CD_3OD, δ in ppm, *J* in Hz).

Position	δ_c (ppm)	δ_H ppm (No. of H, *m, J* Hz)
2	85.3	4.95 (1H, *d*, *J* = 11.5 Hz)
3	73.8	4.54 (1H, *d*, *J* = 11.5 Hz)
4	199.0	
5	165.1	
6	96.0	6.05 (1H, *d*, *J* = 2.1 Hz)
7	169.9	
8	95.0	6.09 (1H, *d*, *J* = 2.3 Hz)
9	164.4	
10	102.6	
1`	129.7	
2`	115.9	6.97 (1H, *d*, *J* = 1.9 Hz)
3`	146.3	
4`	147.2	
5`	116.1	6.80 (1H, *d*, *J* = 8.0 Hz)

6`	120.9	6.85 (1H, *dd*, *J* = 8.1, 2.1 Hz)
7-OCH3	56.4	3.82 (3H, *s*)

Table S. 7. ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 7 (DMSO-*d6* δ in ppm, *J* in Hz).

Position	δ_c (ppm)	δ_H ppm (No. of H, *m, J* Hz)	
2	78.7	5.45 (1H, *dd, J*= 12.3, 3.1 Hz)	
3	42.2	3a	3.21 (1H, *dd, J*= 12.6, 17.1 Hz)
		3b	2.75 (1H, *dd, J*= 16.8, 3.1 Hz)
4	197.0		
5	163.2		
6	94.6	6.07(1H*, d, J*= 2.4)	
7	167.4		
8	93.8	6.09 (1H*, d, J*= 2.4)	
9	162.9		
10	102.6		
1`	129.3		
2`	114.4	6.89 (1H, *s*)	
3`	145.2		
4`	145.8		
5`	115.3	6.75 (2H, *s*)	
6`	118.0	6.75 (2H, *s*)	
7-OCH3	55.9	3.79 (3H, *s*)	
5-OH		12.10 (1H, *s*)	
3`-OH		9.02 (1H, *s*)	
4`-OH		9.02 (1H, *s*)	

Table S. 8 ^{1}H (300 MHz) and ^{13}C (75 MHz) NMR spectroscopic data of compound 8 (DMSO-*d6* δ in ppm, *J* in Hz).

Position	δ_c (ppm)	δ_H ppm (No. of H, *m, J* Hz)
2	163.3	
3	103.4	6.95 (1H, *s*)

4	182.2	
5	152.5	
6	131.4	
7	157.7	
8	94.5	6.63 (1H, *s*)
9	152.8	
10	104.0	
1`	123.0	
2`	109.4	7.56 (1H*, d, J*= 2.1)
3`	149.0	
4`	152.1	
5`	111.7	7.13 (1H*, d, J*= 8.4)
6`	120.0	7.68 (1H*, dd*, *J* = 8.3, 2 Hz)
6-OCH3	60.0	3.76 (3H, *s*)
7-OCH3	55.8	3.88 (3H, *s*)
4`-OCH3	55.9	3.86 (3H, *s*)
5-OH		13.03 (1H, *s*)