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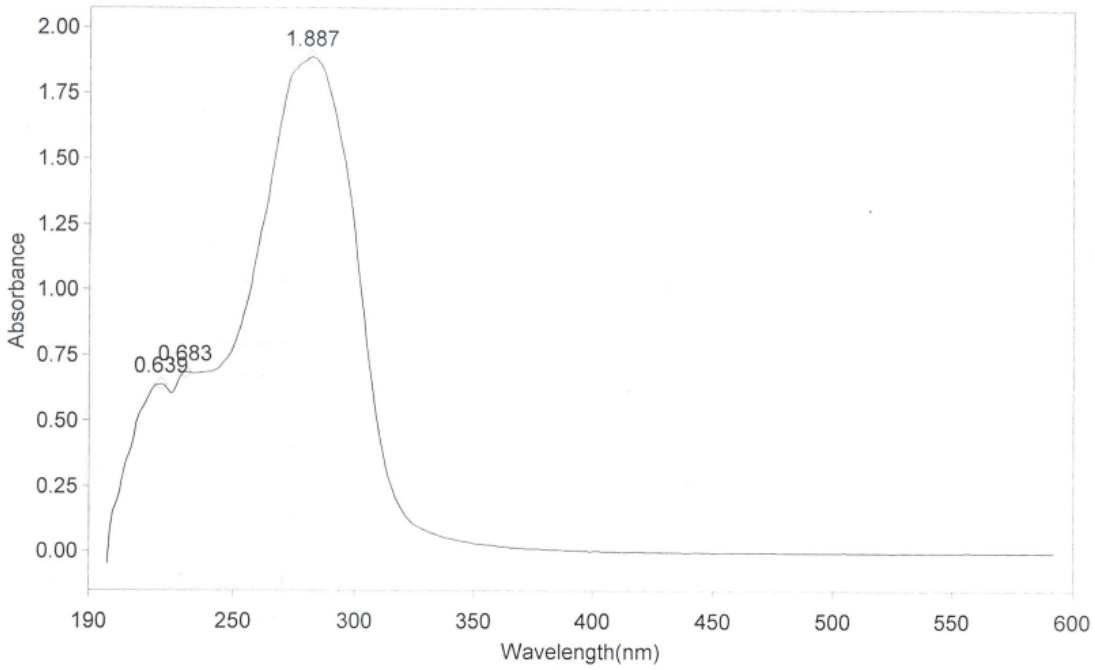
THERMO ELECTRON ~ VISIONpro SOFTWARE V4.10

Operator Name	ZAINAB RIZVI	Date of Report	2/28/2019
Department	ANALYTICAL LAB NANOTECH	Time of Report	11:08:49AM
Organization	HEJ KARACHI UNIVERSITY		
Information	SHD-MF-23B/OWOOLA/PROF.DR.M.IQBAL CHAUDHARY		

Scan Graph



Results Table - SHD-MF-23B-OWOOLA.sre,SHD-MF-23B,Cycle01

nm	A
220.00	0.639
230.00	0.683
282.00	1.887

Peak Pick Method
Find 8 Peaks Above -3.0000 A
Start Wavelength 190.00 nm
Stop Wavelength 350.00 nm
Sort By Wavelength

Sensitivity	Manual
Rising Points	3
Falling Points	3
Min. Change	0.0000

Page 1, Scan Graph

Figure S1: Ultra-Violent Spectrum 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

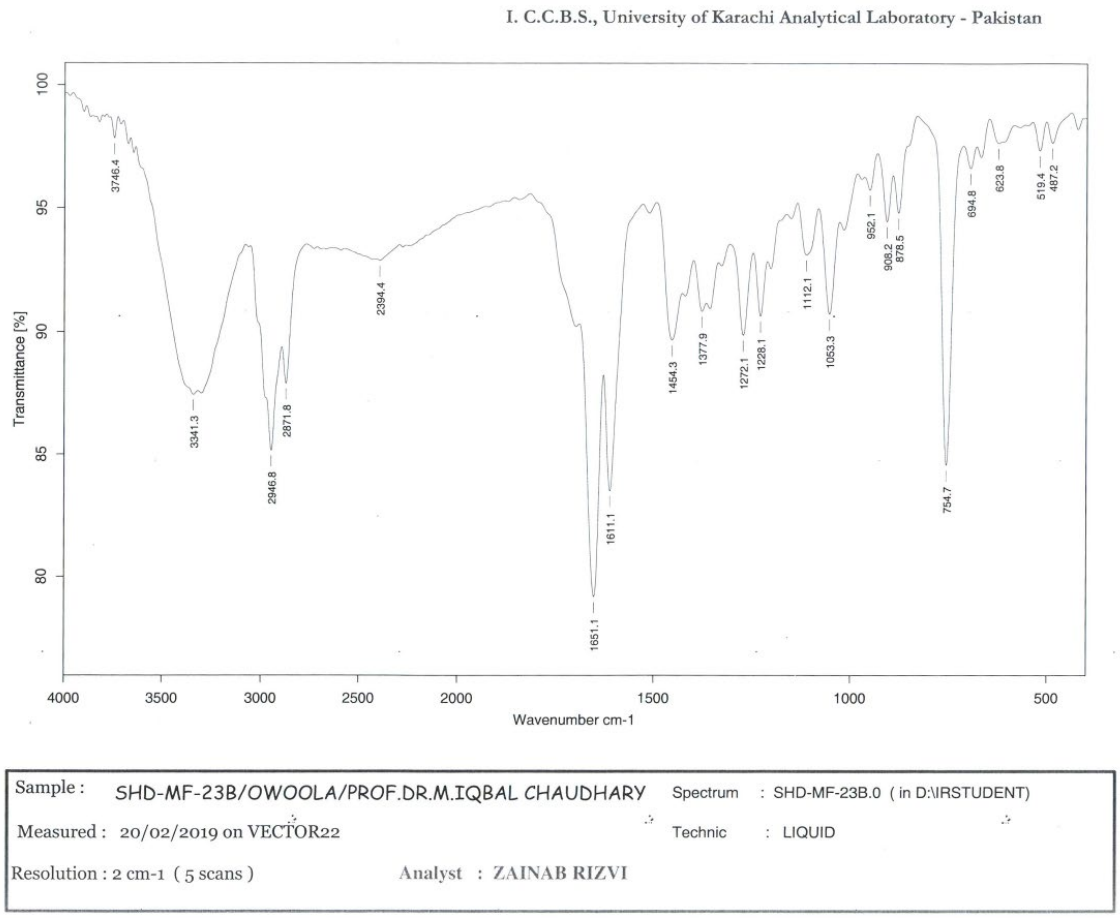


Figure S2: Fourier-Transform Infra-Red of 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

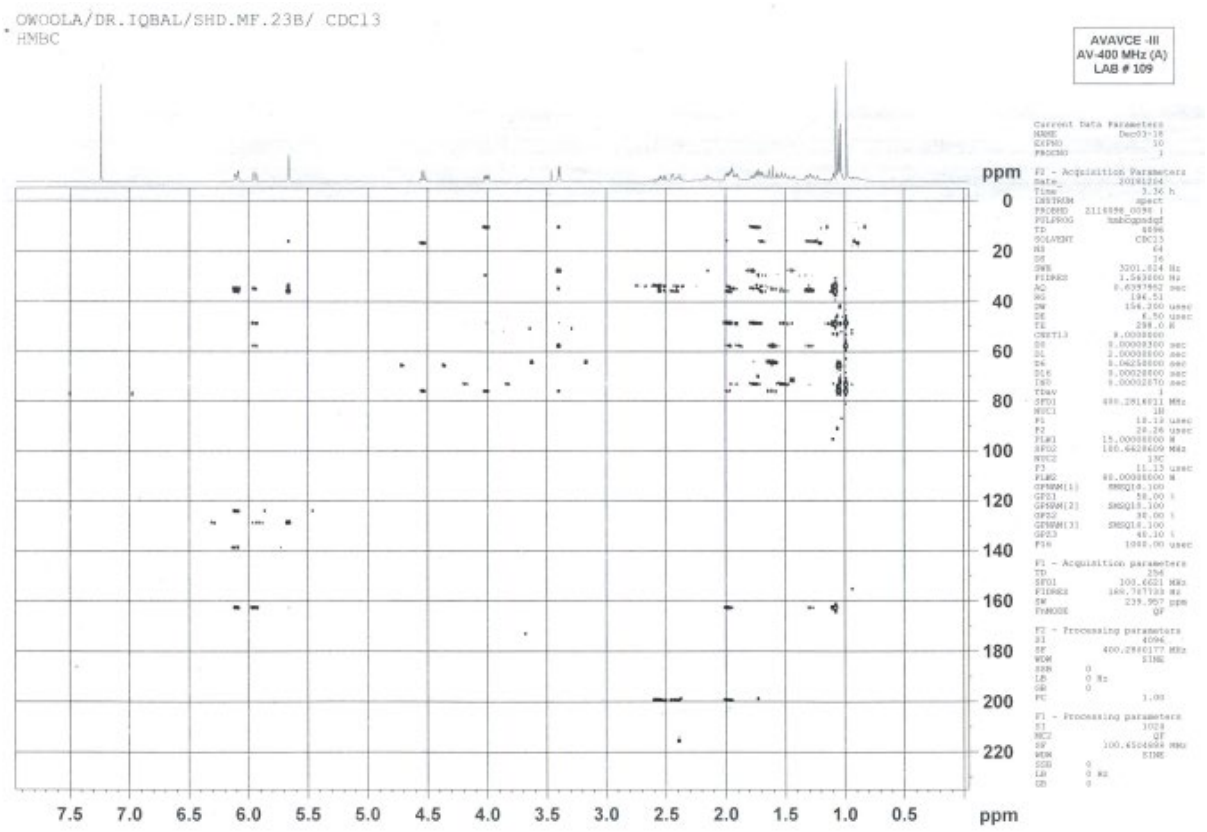


Figure S3: HMBC Spectrum of 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

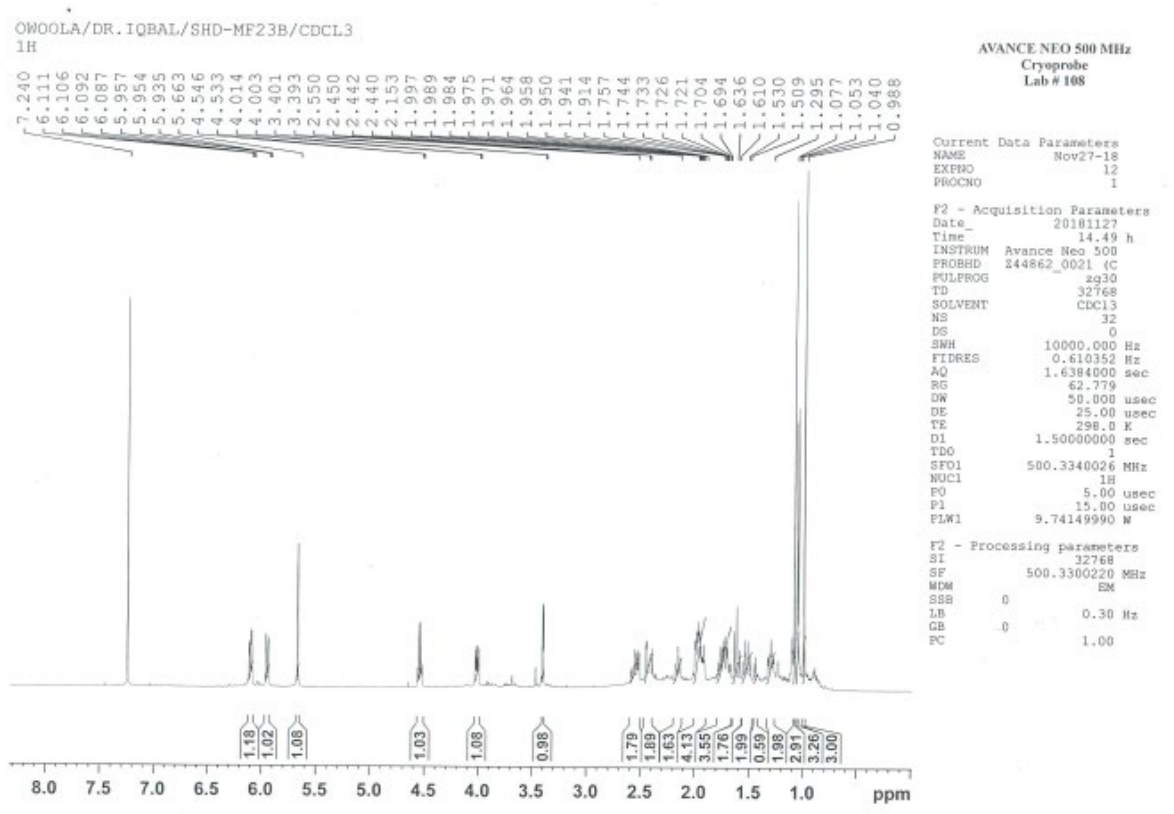


Figure S4: H-NMR Spectrum of 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

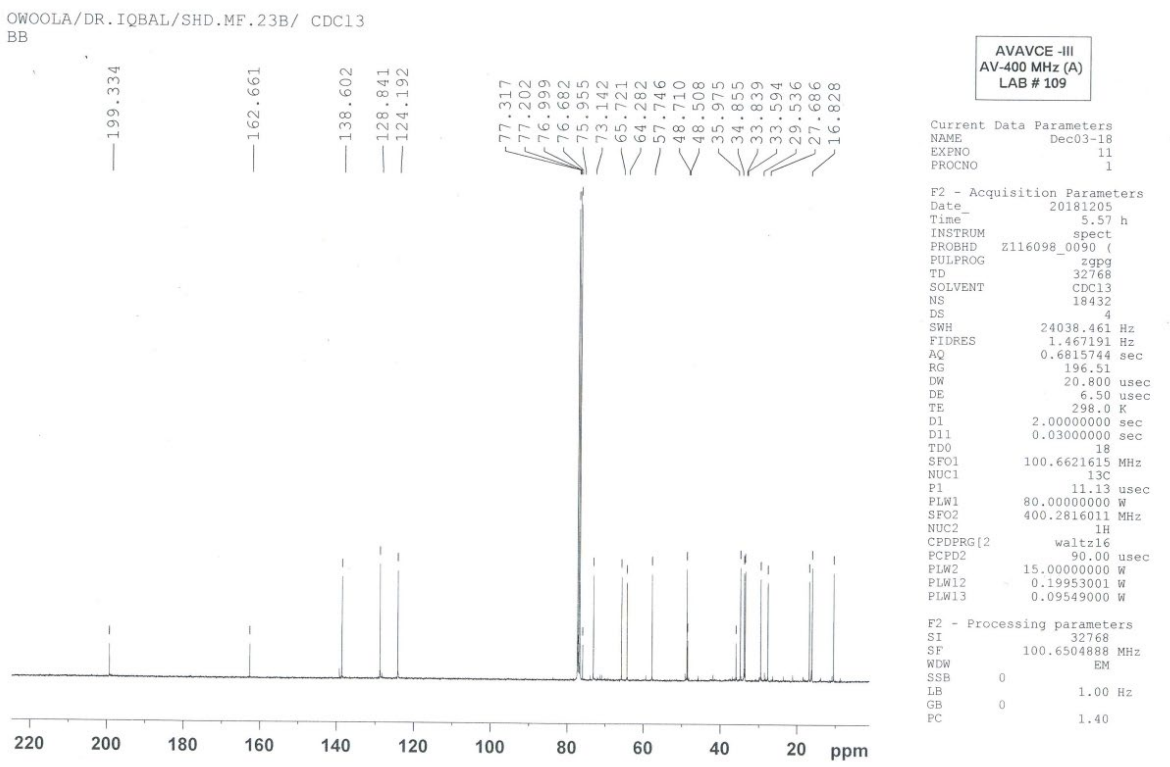


Figure S5: C-13 Spectrum of 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

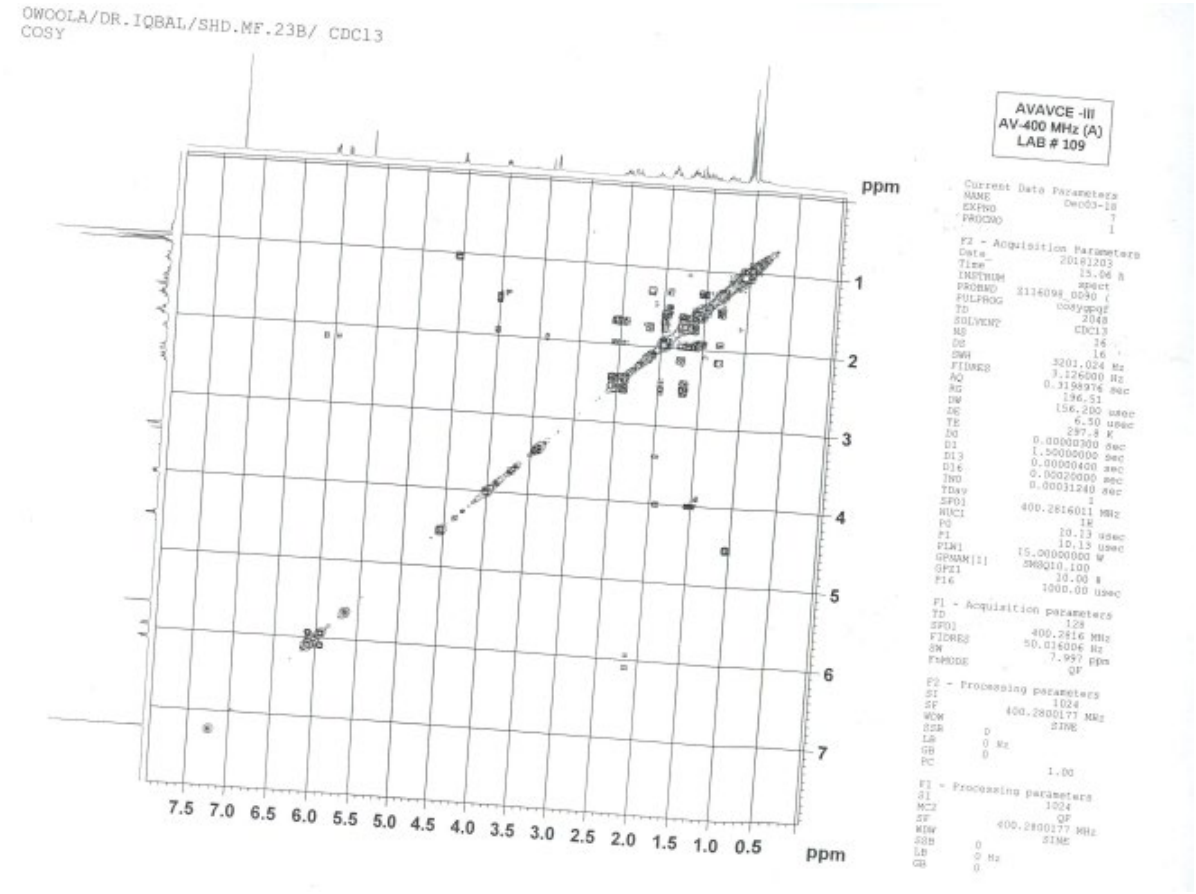


Figure S6: COSY Spectrum of 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

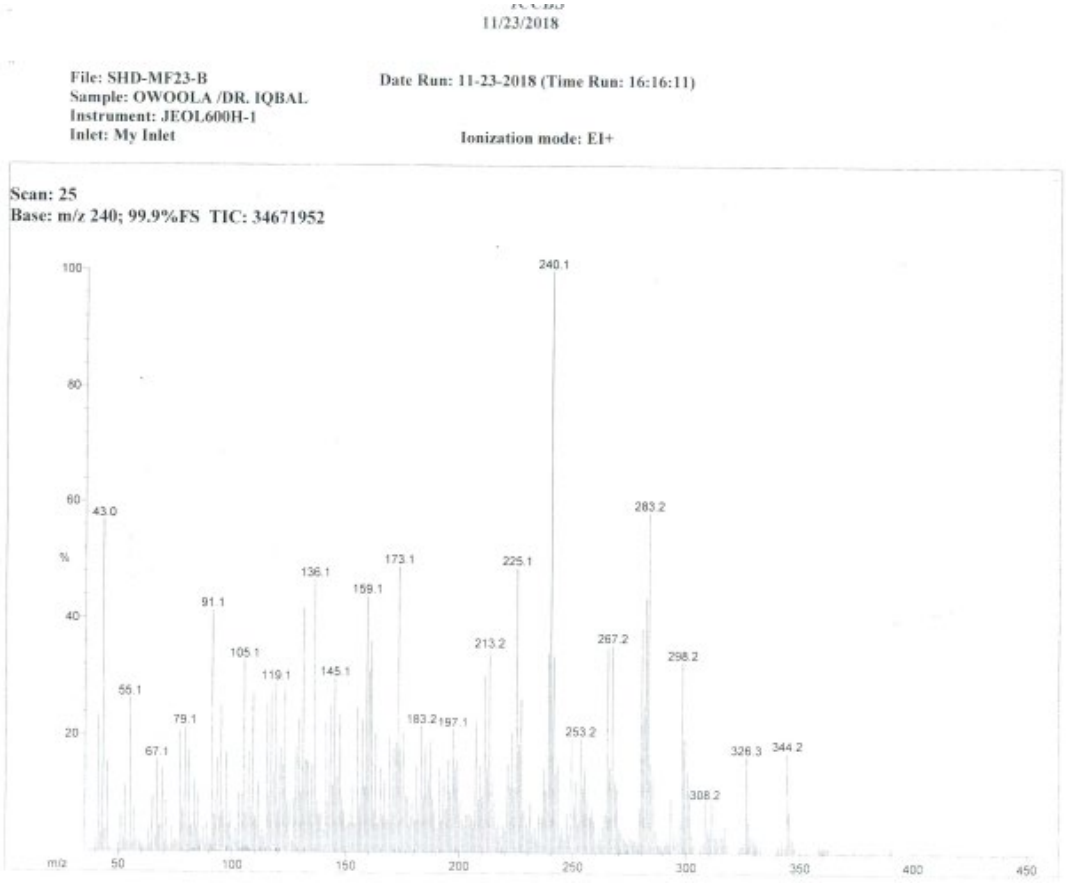


Figure S7: EI-MS of 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

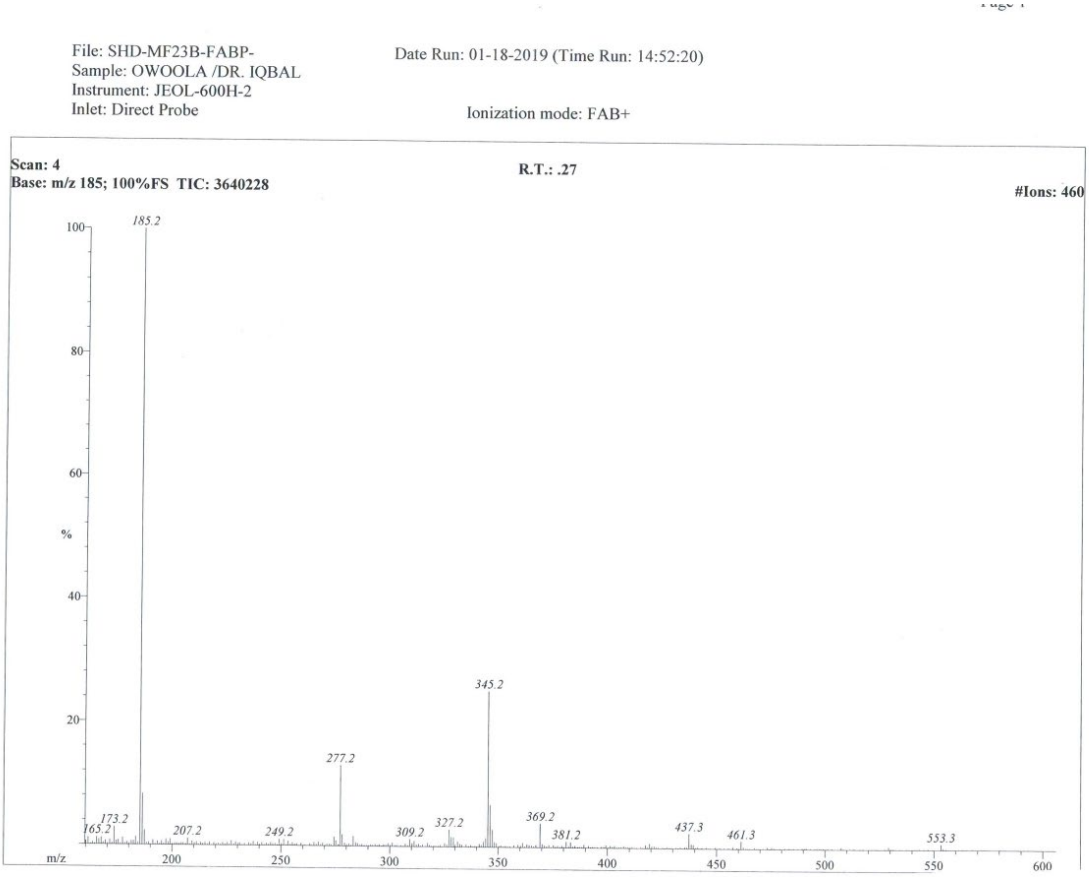


Figure S8: FAB spectrum of 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

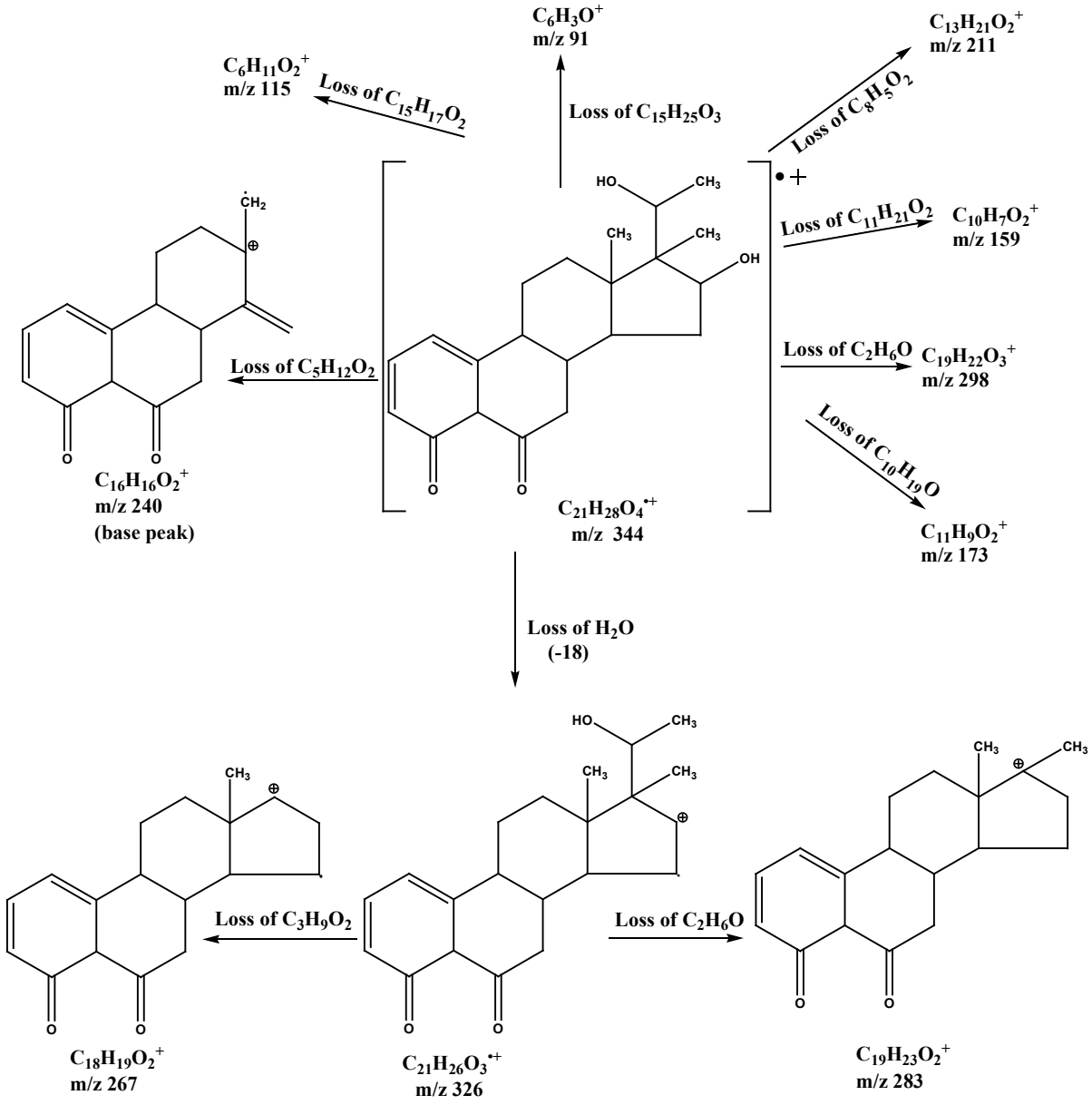


Figure S9**:** Proposed EI-MS fragmentation mechanistic pathways for 16-hydroxy-17-(1-hydroxyethyl)-13,17-dimethyl-5H-cyclopenta[a]phenanthrene-4,6-dione

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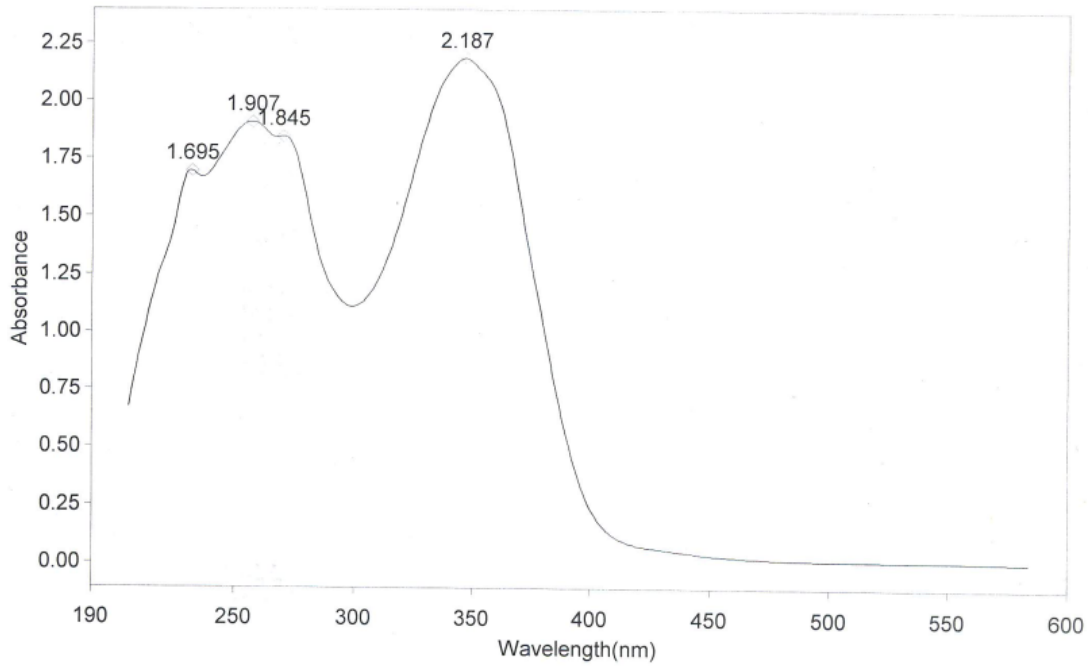
Department	ANALYTICAL LAB NANOTECH	Time of Report	10:45:08AM
Organization	HEJ KARACHI UNIVERSITY		
Information	SHH-42-4/OWOOLA/PROF.DR.M.IQBAL CHAUDHARY		

Scan Graph



Results Table - SHH-42-4-OWOOLA.sre,SHH-42-4,Cycle01

nm	A
232.00	1.695
257.00	1.907
270.00	1.845
347.00	2.187
Sensitivity	Manual
Rising Points	3
Falling Points	3
Min. Change	0.0000

Peak Pick Method
Find 8 Peaks Above -3.0000 A
Start Wavelength 190.00 nm
Stop Wavelength 400.00 nm
Sort By Wavelength

Page 1, Scan Graph

Figure S10: Ultra-Violent Spectrum of 2-(4-ethoxy-3-methoxyphenyl)-5-hydroxy-3,7,8-trimethoxy-4H-Chromen-4-one

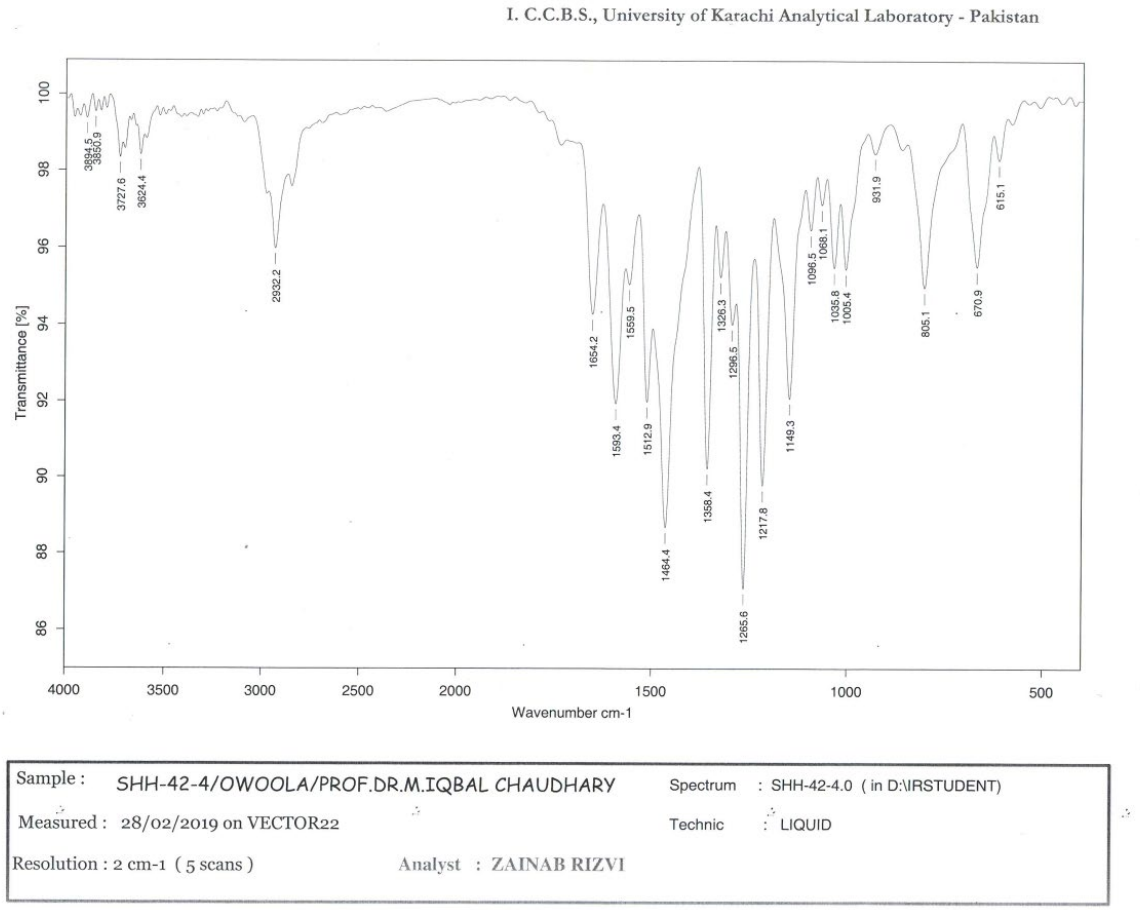


Figure S11: Fourier-Transform InfraRed Spectrum of 2-(4-ethoxy-3-methoxyphenyl)-5-hydroxy-3,7,8-trimethoxy-4H-Chromen-4-one

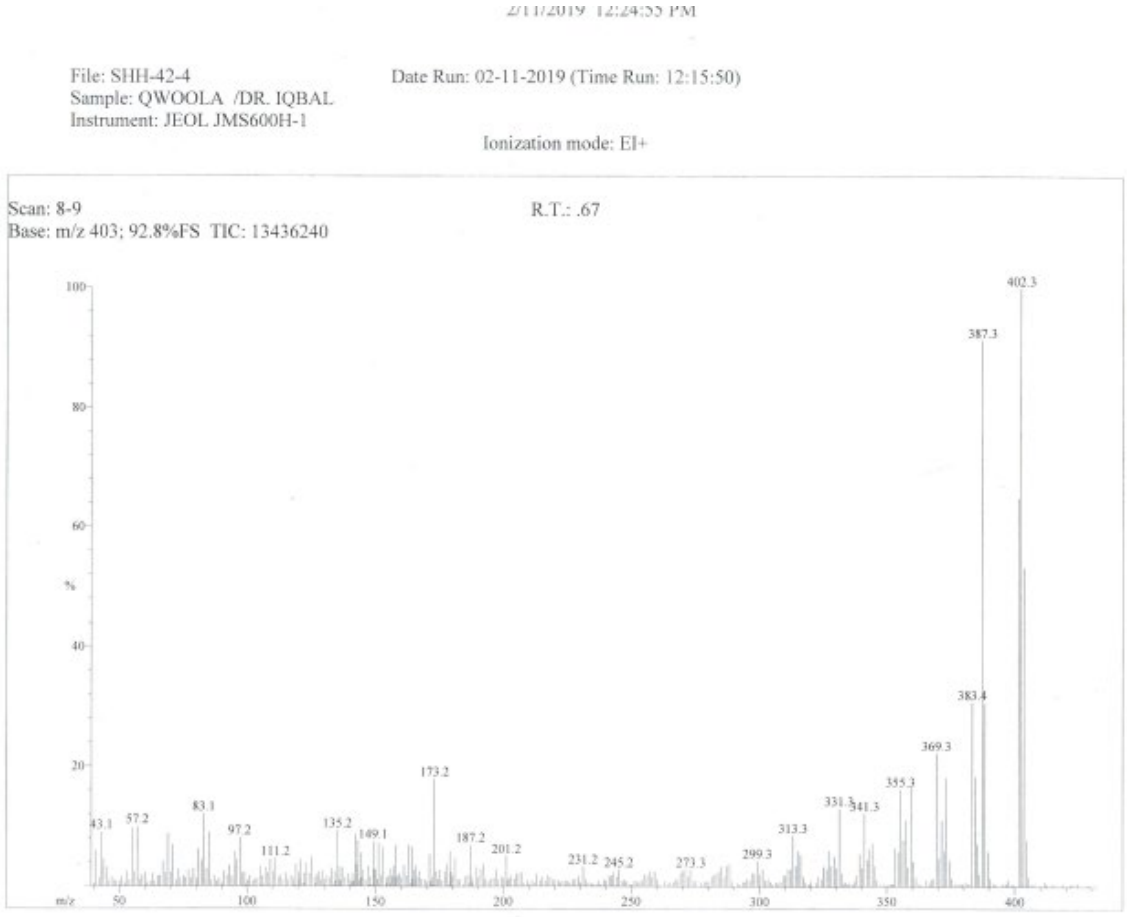


Figure S12: EI-MS Spectrum of 2-(4-ethoxy-3-methoxyphenyl)-5-hydroxy-3,7,8-trimethoxy-4H-Chromen-4-one

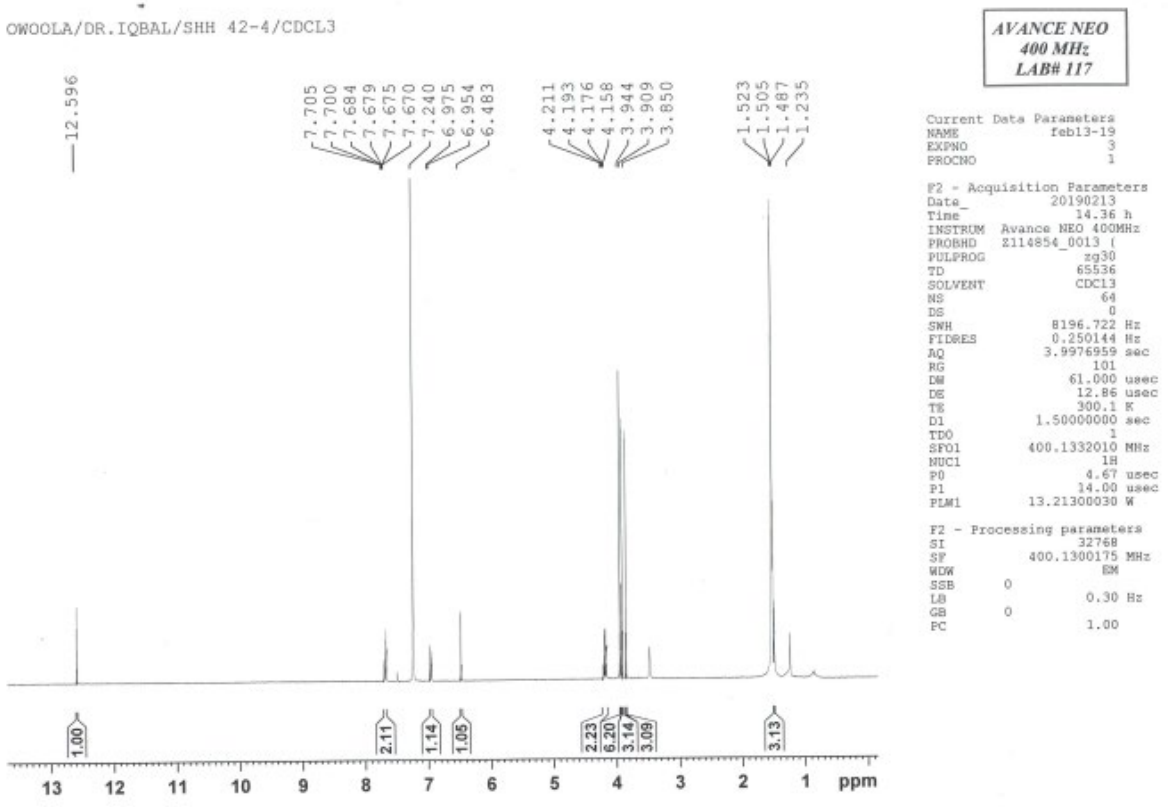


Figure S13: H-NMR Spectrum of 2-(4-ethoxy-3-methoxyphenyl)-5-hydroxy-3,7,8-trimethoxy-4H-Chromen-4-one

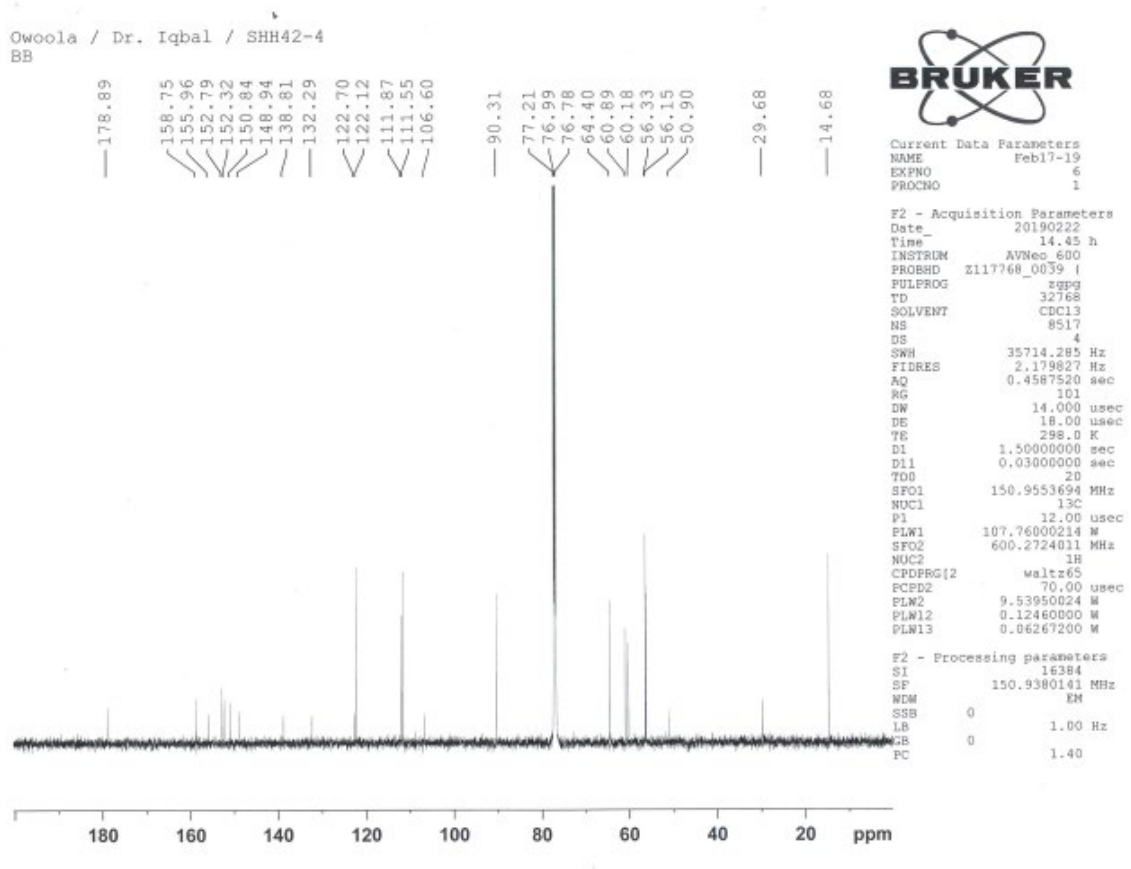


Figure S14: C-13 spectrum of 2-(4-ethoxy-3-methoxyphenyl)-5-hydroxy-3,7,8-trimethoxy-4H-Chromen-4-one

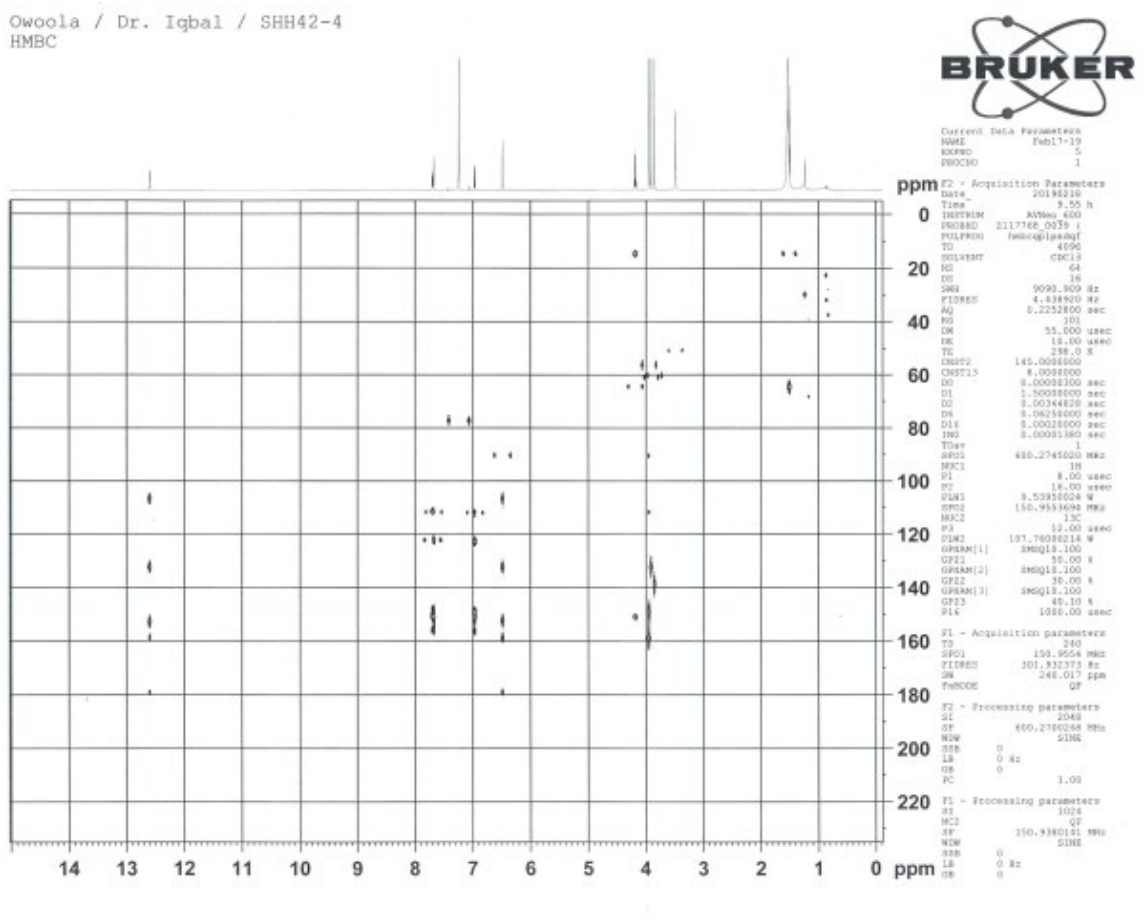


Figure S15: HMBC Spectrum of 2-(4-ethoxy-3-methoxyphenyl)-5-hydroxy-3,7,8-trimethoxy-4H-Chromen-4-one

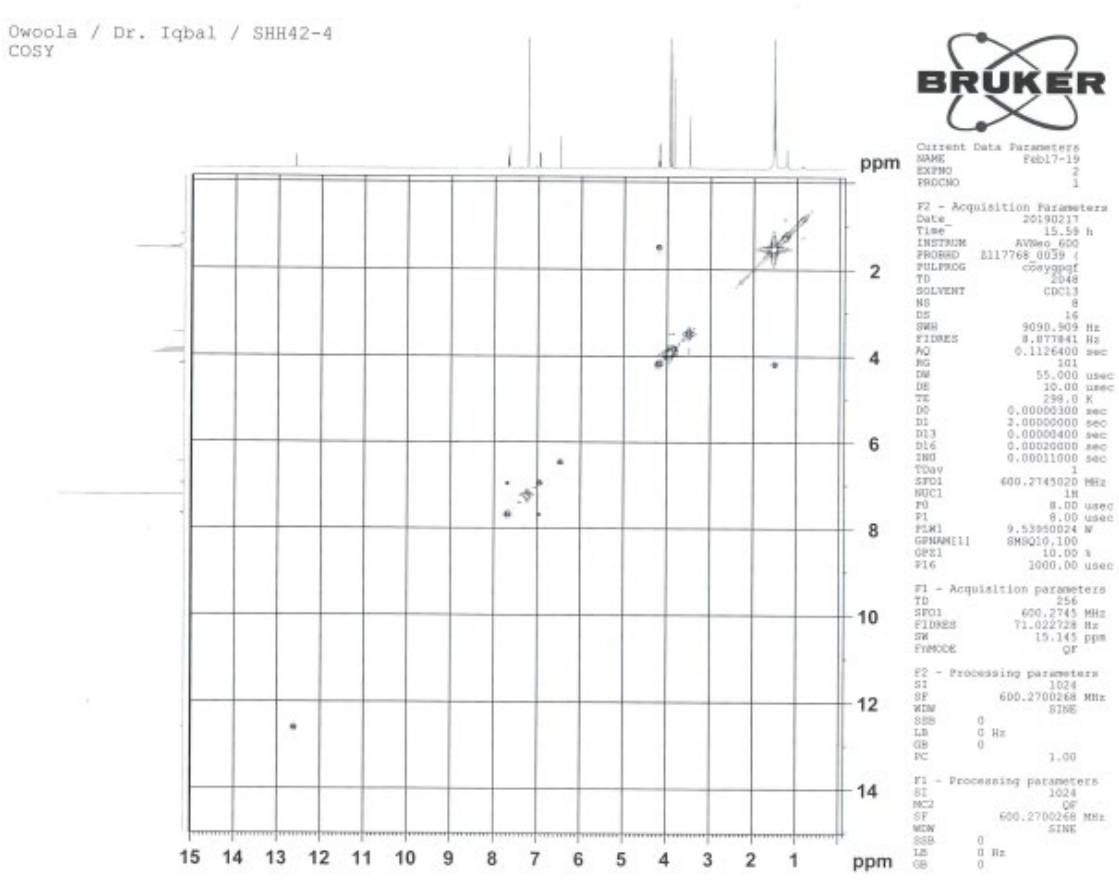


Figure S16: COSY Spectrum of 2-(4-ethoxy-3-methoxyphenyl)-5-hydroxy-3,7,8-trimethoxy-4H-Chromen-4-one

Table S1: ^{1}H and ^{13}C NMR data of compounds 3 and 4

	^{1}H NMR chemical shifts δ in ppm (coupling constant *J* in Hz)		^{13}C NMR chemical shifts δ in ppm
Position	3	4	
1	1.46 m	1.12 m 1.57 m	37.5
2	1.53 m	1.07 d (6.8)	29.3
3	3.50 t dd (5.0, 4.5, 3.6)	3.95 m	78.1
4	2.29 m	1.91 d (13.2) 1.98 d (13.2)	39.8
5	--	--	140.9
6	5.32 d (4.0)	5.34 d (3.6)	121.9
7	2.03 m	1.27 d (6.0) 1.89 m	32.2
8	1.68 m	1.57 m	32.1
9	1.53 m	1.30 m	50.4
10	--	--	36.9
11	1.52 m	1.42 m	21.3
12	1.51 m	2.74 dd (2.4, 13.2) 2.49 m	39.9
13	--	--	42.5
14	1.49 m	1.12 d (10)	56.8
15	1.58 m	1.57 m	24.5
16	1.84 s d (3.5)	1.74 m	28.5
17	1.45	1.07 d (6.8)	56.1
18	0.68 Overlapping Doublet	0.66 s	12.0
19	0.99 s	0.92 s	19.2
20	1.62 m	1.42 m	36.4
21	0.91 d (6.5)	0.98 d (6.4)	19.2
22	4.99 dd (8.5, 8.5)	1.42 m	34.2
23	5.14 dd (8.5, 8.5)	1.25 m	29.3
24	1.23 m	0.91 t (3.6)	50.4
25	1.57 m	1.74 m	29.5
26	0.84 (Overlapping d)	0.88 d (1.6)	19.0
27	0.86 d (6.5)	0.88 d (1.6)	19.9
28	1.14 m	1.25 m	23.4
29	0.83 t (4.0)	0.87 t (1.6)	12.0
1'	--	5.05 d (7.6)	102.6
2'	--	4.05 t (8.0)	75.3

3	--	3.95 m	78.6
4	--	4.31 m	71.7
5	--	4.31 m	78.5
6	--	4.42 dd (5.2), 11.6)	62.9
		4.57 dd (2.4), 12.0)	

Table S2: ^{1}H and ^{13}C NMR data of compounds 5-8

	^{1}H NMR chemical shifts δ in ppm (coupling constant *J* in Hz), (400 MHz)				^{13}C NMR chemical shifts δ in ppm (100 MHz)			
Position	5 (DMSO)	6 ($CDCl_3$)	7 (C_5D_5N)	8 (C_5D_5N)	5 (DMSO)	6 ($CDCl_3$)	7(C_5D_5N)	8(C_5D_5N)
1	--	α 0.94 s β 1.56 s	1.72 d (14.1) 2.05 m	1.84 t (12) 1.96 m	138.4	39.1	24.9	42.5
1a	--	--	--	--	135.9	--	--	--
2	--	α 1.82 s β 1.82 s	2.20 m 1.72 d (14.1)	4.29 m	--	28.1	25.6	67.2
3	8.56 d (4.80)	α 3.47 d (6.8)	4.36 br s	4.11 d (3.6)	136.9	78.1	74.9	78.7
4	8.40 d (4.80)	--	2.21 m 1.72 d (14.1)	--	117.9	39.2	36.3	48.5
4a	--	--	--	--	130.7	--	--	--
5	8.31 d (7.60)	α 0.89 s	3.58 m	2.01-2.07 m	122.8	55.8	74.1	44.7
5a	--	--	--	--	120.0	--	--	--
6	7.30 m	α 1.56 s β 1.37 s	1.79 s 2.32 m	1.46, 1.94 m	119.8	18.8	36.9	18.9

7	7.60 d (7.90)	α 1.56 s β 1.37 s	1.32 m 1.60 dd (3.6, 13.6)	2.09 m 1.75 m	128.6	33.6	21.7	33.7
8	7.83 d (7.90)	--	2.36 m	--	113.0	39.9	41.7	42.3
8a	--	--	--	--	141.6	--	--	--
9	--	α 1.65 d (9.2)	1.71 d (14.1)	1.96 m	--	48.1	39.5	49.4
10	--	--	--	--	187.3	37.3	55.4	39.1
11	--	α 1.97 d (4.0) β 1.97 d (4.0)	1.94, q 2.60 m	1.96 2.10 m	--	23.6	18.6	24.4
12	--	α 5.49 s	1.70 d (14.1) 2.30 m	5.46 br s	--	125.6	39.7	126.7
13	--	--	--	--	--	139.2	49.1	139.3
14	--	--	4.74, br s	--	--	42.5	85.3	40.2
15	--	α 1.28 s β 2.33 dd (4.6, 13.2)	1.05, q 2.07 m	1.62 m 2.34 m	--	28.7	30.8	29.2
16	--	α 2.12 dd (4.0, 13.2) β 2.00 s	1.81 m 2.07 m	1.99-2.06 m	--	24.9	30.6	25.3
17	--	--	3.37,t, (9.6,18.4)	--	--	48.0	48.6	49.4

18	--	β 2.63 d (11.6)	1.13 s	2.63 br. d	--	53.6	18.3	54.4
19	--	α 1.48 s	10.4 s	1.43 m	--	39.5	208.6	40.4
20	--	β 1.06 s	--	1.38 m	--	39.4	174.1	40.4
21	--	α 1.53 s, β 1.45 s	4.90 d (2) 4.94 s	1.36 m 1.46 m	--	31.0	74.1	31.8
22	--	α 1.97 d (4.0) β 1.97 d (4.0)	6.07 d (1.2)	1.96 m	--	37.4	116.7	38.1
23	--	α 1.24 s	--	3.77, 3.93 d (10.8)	--	28.8	172.6	71.3
24	--	0.89 s	--	0.88 s	--	16.5	--	17.9
25	--	β 1.01 s	--	1.01 s	--	15.6	--	17.4
26	--	β 1.01 s	--	1.08 s	--	17.5	--	17.7
27	--	α 1.24 s	--	1.16 s	--	23.9	--	24.2
28	--	--	--	--	--	179.8	--	181.7
29	--	β 1.02 s	--	0.98 d (6.6)	--	17.4	--	17.6
30	--	α 1.94	--	0.93 d (6.6)	--	20.8	--	21.6
1	--	--	5.40 d (16, 9.6)	--	--	--	97.8	--
2	9.24 s	--	1.90 m 2.32 m	--	137.8	--	39.5	--

3'	--	--	4.38 m	--	114.2	--	68.5	--
3a'	--	--	--	--	127.2	--		--
4'	8.55 d (6.4)	--	3.60 m	--	122.0	--	73.8	--
5'	7.30 m	--	4.25 m	--	121.6	--	70.5	--
6'	7.30 m	--	1.55 d (6)	--	121.7	--	18.9	--
7'	7.56 d (7.2)	--	--	--	112.2	--	--	--
7a'	--	--	--	--	135.0	--	--	--
9 NH	12.09 br. S	--	--	--	--	--	--	--
1' NH	11.98 br. S	--	--	--	--	--	--	--