Supporting Information

***Rec. Nat. Prod*. 9:4 (2015) 553-560**

Characterization of one Novel Flavone and four New Source Compounds from the Bark of *Millettia ovalifolia* and In-Vitro Inhibition of Carbonic Anhydrase-II by the Novel Flavonoid

Taj Ur Rahman[*], Khanzadi Fatima Khattak[1], Wajiha Liaqat[2], Khair Zaman[1] and Syed Ghulam Musharraf[3]

1Department of Chemistry, Abdul Wali Khan University, Mardan

[2]Institute of Chemical Sciences, University of Peshwar-25120, Pakistan

[3]International Center for Chemical and Biological Sciences, H.E.J. Research Institute of Chemistry, University of Karachi, Karachi-75270, Pakistan

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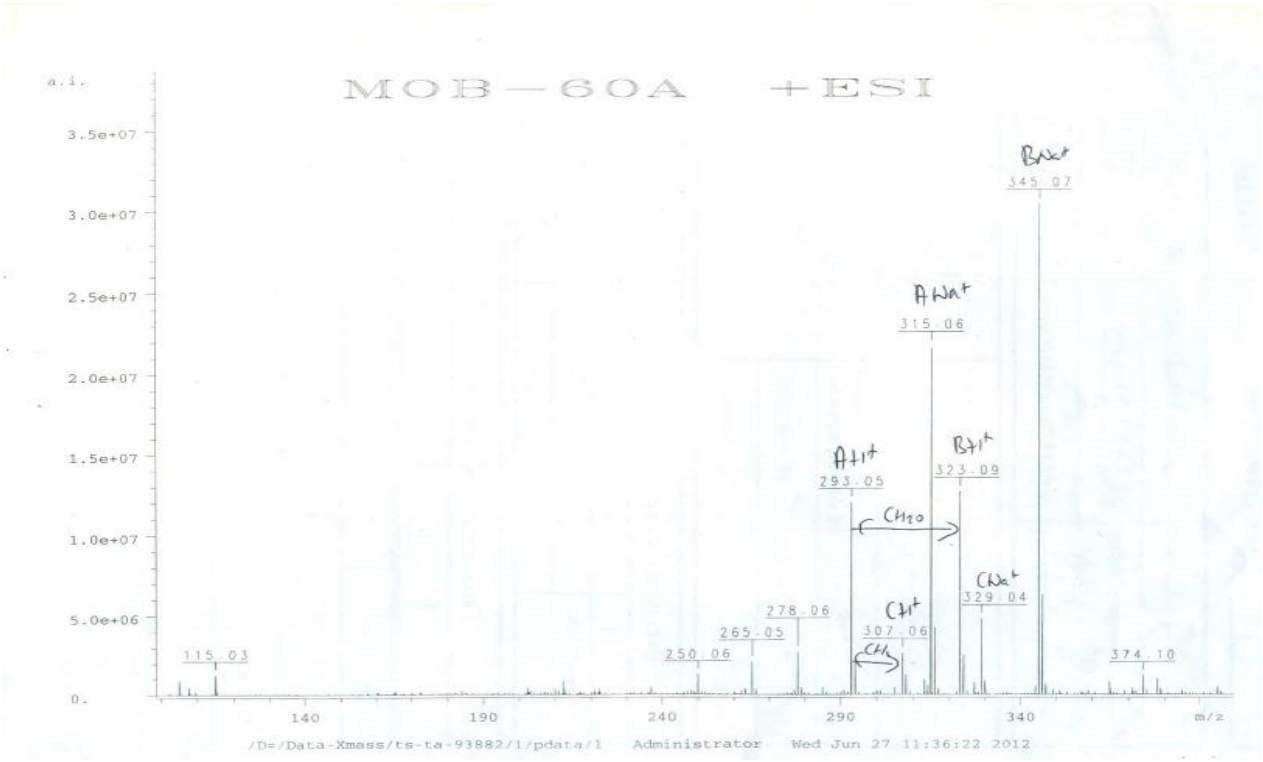
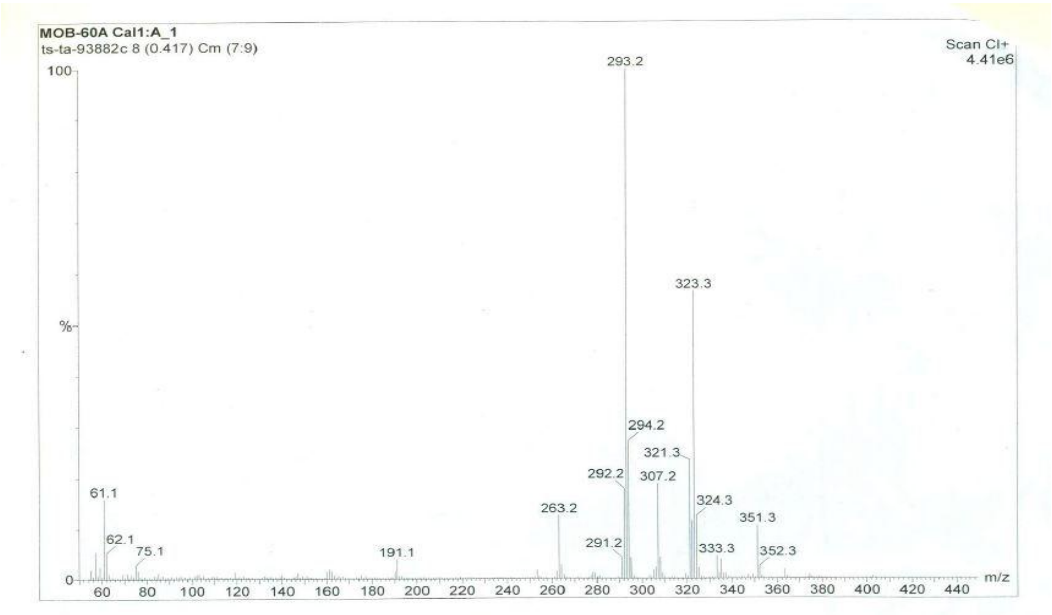


S1: ESI-MS Spectrum of Compound **1 (**7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one**)**



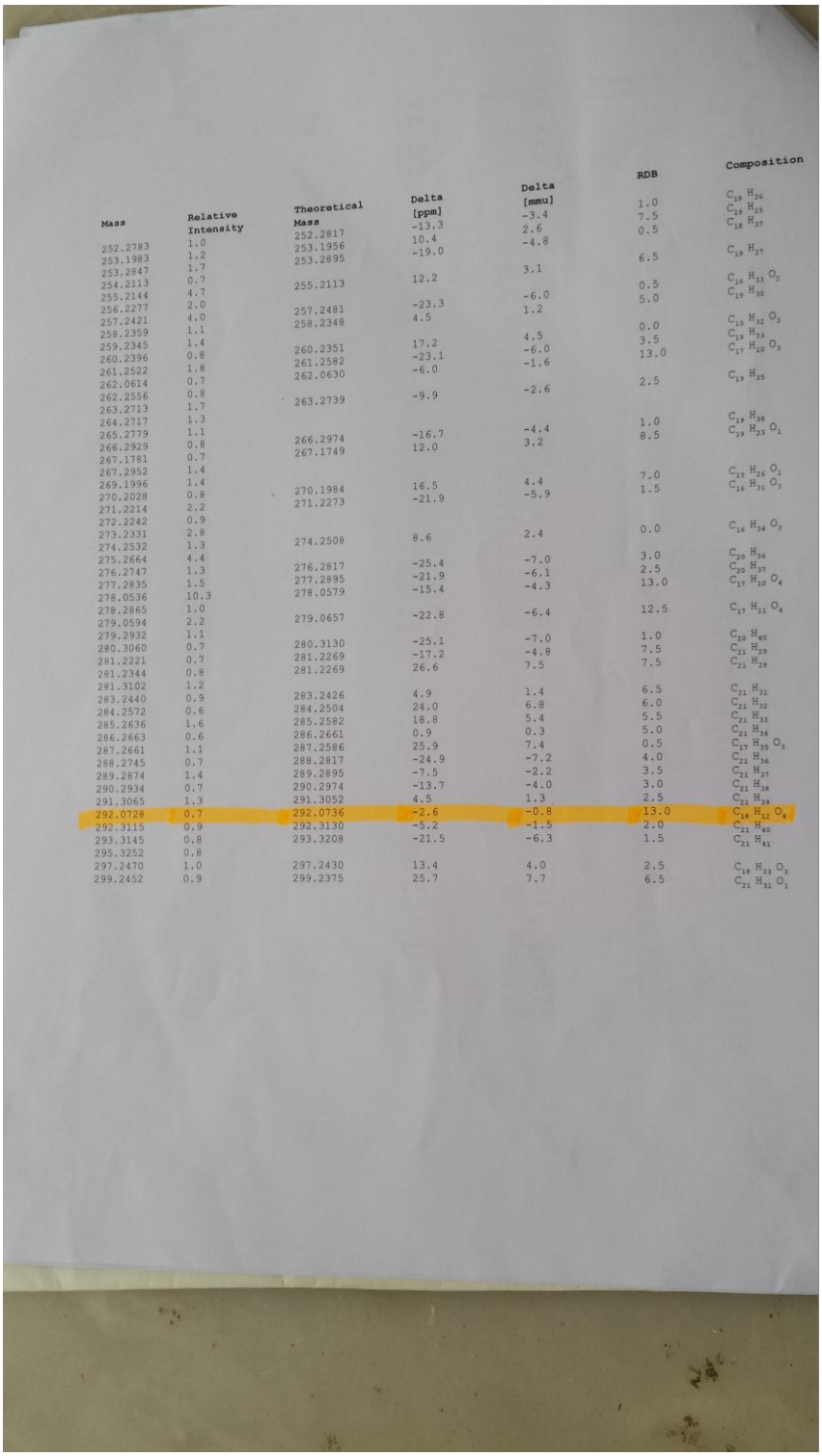
S2: CI-MS Spectrum of Compound **1** (7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one**)**

File : C:\Xcalibur\data\mob-60a-261214-c14.RAW
Full ms [39.500 - 650.500] - Range: 100.000 - 300.000
Scan No. 1 of 1

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
100.0536	0.9	100.0524	12.2	1.2	2.0	$C_5 H_8 O_2$
100.0772	0.8					
100.1203	1.6					
101.0535	2.7					
102.0363	1.4					
103.0315	1.7					
104.0267	1.5	104.0262	4.8	0.5	6.0	$C_7 H_4 O_1$
105.0225	10.7					
106.0180	3.9					
107.0123	14.0	107.0133	-9.1	-1.0	5.5	$C_6 H_3 O_2$
108.0078	6.0					
109.0037	28.8					
109.9665	2.5					
110.9993	36.0					
112.9291	1.1					
113.9412	1.4					
114.9379	4.0					
115.9513	1.6					
116.9584	4.4					
118.8968	7.3					
119.9358	0.8					
119.9662	0.7					
120.0073	5.0					
121.0250	11.8					
122.0414	4.9					
123.0591	19.6					
124.0748	7.6					
125.0951	22.5	125.0966	-12.7	-1.6	2.5	$C_8 H_{13} O_1$
126.0269	0.6					
126.1078	5.9	126.1045	26.1	3.3	2.0	$C_8 H_{14} O_1$
127.0490	2.0					
127.1265	10.3					
128.0475	2.6	128.0473	0.9	0.1	3.0	$C_6 H_8 O_3$
128.1371	0.9					
129.0781	5.9					
130.0749	1.9	130.0783	-25.6	-3.3	6.0	$C_{10} H_{10}$
131.0848	5.3	131.0861	-9.8	-1.3	5.5	$C_{10} H_{11}$
132.0858	2.0					
133.0909	9.1					
134.0898	3.9					
135.0892	11.6					
136.0858	4.3	136.0888	-22.1	-3.0	4.0	$C_9 H_{12} O_1$
137.0864	12.7					
138.0850	5.6					
139.0022	0.8	139.0031	-6.5	-0.9	5.5	$C_6 H_3 O_4$
139.0856	10.9					
140.0146	0.6	140.0110	26.2	3.7	5.0	$C_6 H_4 O_4$
140.0195	0.7					
140.0258	0.6	140.0262	-3.3	-0.5	9.0	$C_{10} H_4 O_1$
140.0831	4.0	140.0837	-4.2	-0.6	3.0	$C_8 H_{12} O_2$
141.0818	7.7					
141.9893	1.4					
142.0778	0.8	142.0783	-3.0	-0.4	7.0	$C_{11} H_{10}$
142.8947	1.2					
144.9970	7.3					
146.0015	2.5	146.0004	7.3	1.1	8.0	$C_8 H_2 O_3$
146.9021	1.1					
147.0110	7.5	147.0082	19.0	2.8	7.5	$C_8 H_3 O_3$
147.9080	2.1					
148.0160	2.8	148.0160	-0.0	-0.0	7.0	$C_8 H_4 O_3$
148.9171	8.0					
149.0266	9.1	149.0239	18.4	2.7	6.5	$C_8 H_5 O_3$
149.9244	1.5					
150.0311	3.0	150.0317	-4.1	-0.6	6.0	$C_8 H_6 O_3$
151.0435	9.9	151.0395	26.4	4.0	5.5	$C_8 H_7 O_3$
151.9636	1.0					
152.0509	4.6	152.0473	23.5	3.6	5.0	$C_8 H_8 O_3$

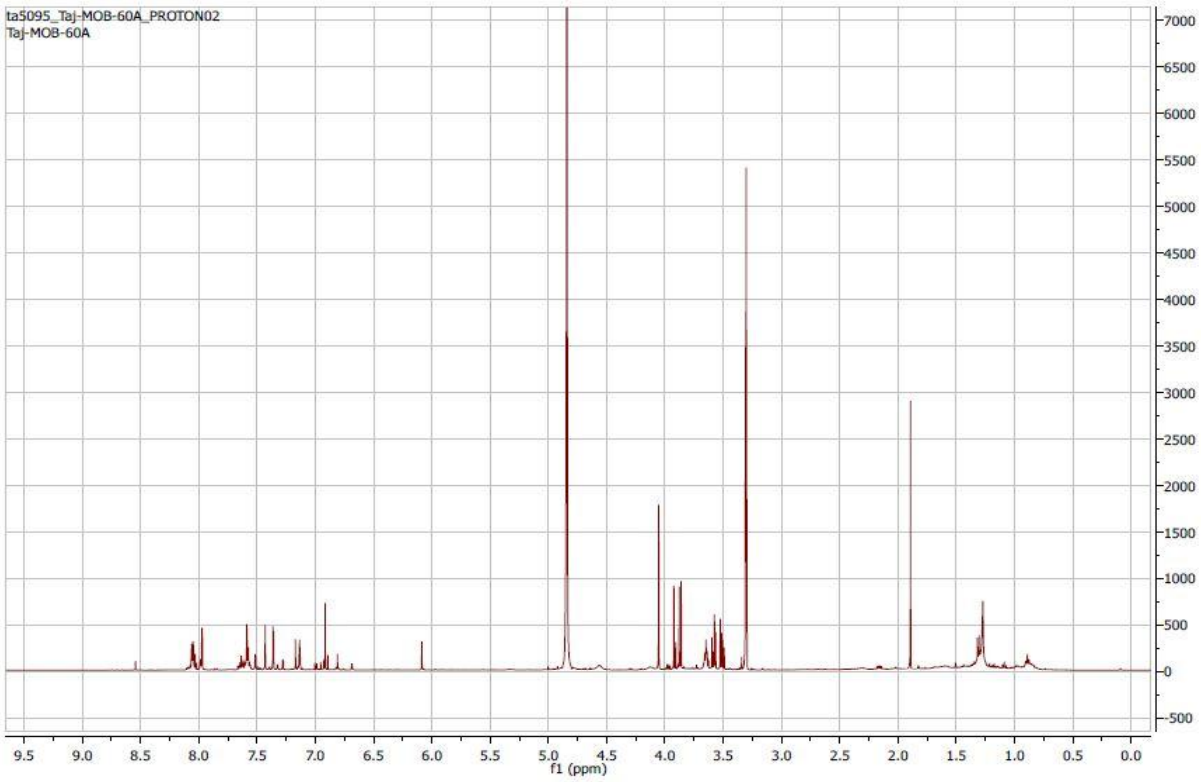
Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
152.0683	1.1					
153.0604	7.5					
153.9888	8.7					
154.0729	2.7					
154.8854	2.8					
155.0442	5.8	155.0663	-12.4	-1.9	7.5	$C_{12} H_{11}$
156.0559	1.1					
156.8981	8.7	156.9889	1.3	0.2	7.0	$C_{14} H_{..}$
157.8325	3.8					
158.0369	2.1	158.0368	0.1	0.0	6.0	$C_{10} H_8 O_2$
159.0498	5.8					
159.9545	1.2					
160.0590	3.7					
160.9858	0.8	160.9875	-10.2	-1.6	4.5	$C_8 H_9 O_4$
161.0767	0.2					
161.9441	1.3					
162.0560	2.0	162.0550	7.7	1.3	1.0	$C_{10} H_{10} O_2$
163.1089	1.7	163.1123	-14.9	-2.4	4.5	$C_{10} H_{14} O_1$
164.0487	3.7					
164.1223	3.4	164.1201	26.8	2.6	4.0	$C_{10} H_{16} O_1$
165.0467	2.3					
165.1393	7.5					
166.0997	1.8	166.0630	-59.4	-9.9	6.0	$C_9 H_{10} O_3$
166.1328	3.5					
167.8269	1.1					
167.8728	1.9	167.0708	18.8	1.8	4.5	$C_{11} H_{11} O_1$
167.1695	6.4					
168.8468	2.8	168.0786	12.7	2.1	4.0	$C_{11} H_{12} O_1$
168.1822	2.7					
169.2022	2.4	169.1017	2.5	0.4	7.5	$C_{13} H_{13}$
169.1563	4.8	169.1956	9.1	0.9	0.5	$C_{12} H_{19}$
170.3148	0.7					
170.8041	0.7	170.2035	8.7	0.6	0.0	$C_{12} H_{26}$
171.1177	3.8					
172.2317	1.2					
173.2393	3.9					
174.1429	1.8	174.1409	9.9	1.7	5.0	$C_{11} H_{18}$
175.8148	0.8	176.0184	-21.7	-3.8	12.5	$C_{10} H_6 O_4$
176.1578	1.7					
176.8286	7.7					
176.1579	1.6	176.1565	8.1	1.4	4.0	$C_{11} H_{20}$
177.8294	8.9	177.0540	-26.4	-4.7	11.5	$C_{10} H_5 O_3$
177.1726	4.8					
178.8868	1.2					
178.2196	2.1	178.1722	3.5	0.6	3.0	$C_{13} H_{22}$
179.8941	1.5					
179.1841	9.3	179.1800	22.9	4.1	2.5	$C_{14} H_{23}$
180.8884	8.8	180.0909	-24.8	-4.5	9.0	$C_{11} H_{16}$
180.1884	2.7	180.1878	8.7	1.6	2.0	$C_{11} H_{24}$
181.8976	1.1	181.1017	-22.8	-4.1	8.5	$C_{11} H_{17}$
181.1933	3.8	181.1956	-12.7	-2.7	1.5	$C_{13} H_{25}$
182.1923	9.4					
183.1913	1.8					
183.8966	1.2	183.1021	-19.1	-3.5	3.5	$C_{10} H_{15} O_1$
183.1919	4.2					
184.8969	6.7	184.0888	-18.4	-1.9	8.3	$C_{12} H_{12} O_1$
185.1858	2.7					
186.8957	1.3	186.1043	-35.8	-6.6	7.3	$C_{14} H_{14} O_1$
187.8936	8.8					
187.1814	3.6					
188.1828	1.2	188.1776	23.1	4.3	6.5	$C_{13} H_{24} O_1$
189.1193	1.2					
189.1851	3.7					
190.1123	8.6					
190.1882	1.8					
191.1032	8.9					
191.1823	4.3					
192.1919	2.6					
192.1841	2.8	192.1979	1.8	0.3	3.8	$C_{14} H_{26}$
193.8973	2.8	193.1017	-23.1	-4.5	9.5	$C_{11} H_{17}$

Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
193.1887	4.4					
194.1952	8.7	194.0943	4.9	0.9	5.0	$C_{14}H_{26}O$
194.2009	3.1	194.2035	-13.4	-3.0	2.0	$C_{14}H_{26}$
195.1927	5.9	195.1023	2.7	0.5	4.5	$C_{13}H_{25}O$
196.1987	1.0					
196.2022	3.2					
196.2093	2.1					
197.1183	1.5	197.1178	7.9	1.6	3.5	$C_{12}H_{17}O_2$
197.2239	3.0					
199.1484	1.4	199.1487	-10.4	-0.1	4.5	$C_{15}H_{19}$
200.1473	1.4					
201.1617	2.7	201.1643	-13.0	-2.6	5.5	$C_{16}H_{21}$
202.1645	3.3					
203.1678	9.9	203.1672	1.9	0.4	6.5	$C_{15}H_{23}O$
203.1732	2.4					
204.1743	1.2	204.1725	10.3	3.3	0.0	$C_{12}H_{22}O_2$
205.1840	0.7	205.1919	11.2	2.3	10.5	$C_{15}H_{25}$
205.1947	3.7	205.1956	-4.9	-0.9	3.5	$C_{16}H_{25}$
206.2021	1.6	206.2035	-6.7	-1.4	3.0	$C_{16}H_{26}$
207.1230	0.8					
207.2065	3.4	207.2113	-13.4	-2.8	2.5	$C_{15}H_{27}$
208.2040	2.5					
209.1622	0.9					
209.2045	2.7	209.2269	-11.6	-2.4	1.5	$C_{15}H_{29}$
210.2346	1.8	210.2348	-0.8	-0.2	1.5	$C_{15}H_{30}$
211.1478	1.2	211.1487	-5.9	-0.8	7.5	$C_{14}H_{19}$
211.2402	3.8	211.2426	-11.3	-2.3	3.5	$C_{15}H_{31}$
213.1692	5.7	213.1643	22.7	4.8	6.5	$C_{16}H_{21}$
214.1698	1.7	214.1722	-11.4	-2.4	6.5	$C_{16}H_{22}$
215.1828	3.5	215.1800	8.8	1.9	5.5	$C_{16}H_{23}$
216.1853	1.1	216.1878	-12.1	-2.6	5.5	$C_{16}H_{24}$
217.0687	8.8	217.0653	15.4	3.3	12.5	$C_{14}H_{9}O_2$
217.1838	2.6	217.1956	-54.5	-11.8	4.5	$C_{16}H_{25}$
218.2380	2.3	218.2035	157.5	34.3	4.5	$C_{16}H_{26}$
219.2049	5.4	219.2113	-29.8	-6.5	3.5	$C_{16}H_{27}$
220.2134	1.4	220.2191	-26.1	-5.7	3.5	$C_{16}H_{28}$
221.0916	1.0	221.0914	0.7	0.2	8.5	$C_{14}H_{13}O_2$
221.2230	2.8	221.2269	-16.0	-3.5	3.5	$C_{16}H_{29}$
222.2295	1.9	222.2348	-24.5	-5.4	3.5	$C_{16}H_{30}$
223.1244	0.8					
223.2389	2.1	223.2426	-16.3	-3.6	1.5	$C_{16}H_{31}$
224.2515	1.3	224.2504	5.0	1.1	1.0	$C_{16}H_{32}$
225.1853	0.6	225.1643	4.4	1.0	7.5	$C_{15}H_{21}$
225.2547	2.4	225.2582	-15.7	-3.5	0.5	$C_{16}H_{33}$
227.1938	2.2	227.1800	14.0	3.2	6.5	$C_{15}H_{23}$
228.1960	1.7					
228.2031	1.6					
238.2006	1.2	238.2035	-12.4	-2.9	5.0	$C_{17}H_{26}$
251.1880	1.1					
252.1915	1.2					
253.2024	2.3	253.2269	-19.8	-4.8	3.5	$C_{18}H_{29}$
254.2118	1.5					
255.2325	2.3					
256.2148	3.9	256.2140	20.5	4.6	3.5	$C_{16}H_{28}O$
257.1419	1.7					
257.2355	2.6					
258.2647	1.2					
259.2661	2.2					
261.1980	1.6	261.1956	14.3	3.6	6.5	$C_{16}H_{25}$
262.2072	0.9	262.2035	16.5	3.7	6.0	$C_{16}H_{26}$
263.2219	2.7					
264.2158	0.8					
265.2178	1.6	265.2217	25.4	6.0	3.5	$C_{16}H_{29}O$
266.2175	0.6	266.2348	-8.0	-2.0	3.0	$C_{16}H_{30}O$
267.2457	2.4	267.2426	-7.7	-1.9	3.5	$C_{16}H_{31}$
268.2445	1.2	268.2504	-28.9	-5.9	3.0	$C_{16}H_{32}$
269.2574	2.1	269.2582	-3.4	-0.9	2.5	$C_{16}H_{33}$
282.0660	0.8	282.0630	6.2	1.6	12.0	$C_{16}H_{10}O_2$
282.2581	1.4					
283.2686	1.4					



Mass	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
252.2783	1.0	252.2817	-13.3	-3.4	1.0	$C_{18}H_{36}$
253.1983	1.2	253.1956	10.4	2.6	7.5	$C_{19}H_{25}$
253.2847	1.7	253.2895	-19.0	-4.8	0.5	$C_{18}H_{37}$
254.2113	0.7			3.1	6.5	$C_{19}H_{27}$
255.2144	4.7	255.2113	12.2		0.5	$C_{16}H_{33}O_2$
256.2277	2.0			-6.0	5.0	$C_{19}H_{30}$
257.2421	4.0	257.2481	-23.3	1.2		
258.2359	1.1	258.2348	4.5		0.0	$C_{15}H_{32}O_3$
259.2345	1.4			4.5	3.5	$C_{19}H_{33}$
260.2396	0.8	260.2351	17.2	-6.0	13.0	$C_{17}H_{10}O_3$
261.2522	1.8	261.2582	-23.1	-1.6		
262.0614	0.7	262.0630	-6.0		2.5	$C_{19}H_{35}$
262.2556	0.8			-2.6		
263.2713	1.7	263.2739	-9.9			
264.2717	1.3				1.0	$C_{19}H_{38}$
265.2779	1.1			-4.4	8.5	$C_{19}H_{23}O_1$
266.2929	0.8	266.2974	-16.7	3.2		
267.1781	0.7	267.1749	12.0		7.0	$C_{19}H_{26}O_1$
267.2952	1.4				1.5	$C_{16}H_{31}O_3$
269.1996	1.4			4.4		
270.2028	0.8	270.1984	16.5	-5.9		
271.2214	2.2	271.2273	-21.9			
272.2242	0.9				0.0	$C_{16}H_{34}O_3$
273.2331	2.8			2.4		
274.2532	1.3	274.2508	8.6		3.0	$C_{20}H_{36}$
275.2664	4.4			-7.0	2.5	$C_{20}H_{37}$
276.2747	1.3	276.2817	-25.4	-6.1	13.0	$C_{17}H_{10}O_4$
277.2835	1.5	277.2895	-21.9	-4.3		
278.0536	10.3	278.0579	-15.4		12.5	$C_{17}H_{11}O_4$
278.2865	1.0			-6.4		
279.0594	2.2	279.0657	-22.8			
279.2932	1.1			-7.0	1.0	$C_{20}H_{40}$
280.3060	0.7	280.3130	-25.1	-4.8	7.5	$C_{21}H_{29}$
281.2221	0.7	281.2269	-17.2	7.5	7.5	$C_{21}H_{29}$
281.2344	0.8	281.2269	26.6			
281.3102	1.2			1.4	6.5	$C_{21}H_{31}$
283.2440	0.9	283.2426	4.9	6.8	6.0	$C_{21}H_{32}$
284.2572	0.6	284.2504	24.0	5.4	5.5	$C_{21}H_{33}$
285.2636	1.6	285.2582	18.8	0.3	5.0	$C_{21}H_{34}$
286.2663	0.6	286.2661	0.9	7.4	0.5	$C_{17}H_{35}O_3$
287.2661	1.1	287.2586	25.9	-7.2	4.0	$C_{21}H_{36}$
288.2745	0.7	288.2817	-24.9	-2.2	3.5	$C_{21}H_{37}$
289.2874	1.4	289.2895	-7.5	-4.0	3.0	$C_{21}H_{38}$
290.2934	0.7	290.2974	-13.7	1.3	2.5	$C_{21}H_{39}$
291.3065	1.3	291.3052	4.5	-0.8	13.0	$C_{18}H_{12}O_4$
292.0728	0.7	292.0736	-2.6	-1.5	2.0	$C_{21}H_{40}$
292.3115	0.9	292.3130	-5.2	-6.3	1.5	$C_{21}H_{41}$
293.3145	0.8	293.3208	-21.5			
295.3252	0.8			4.0	2.5	$C_{18}H_{33}O_3$
297.2470	1.0	297.2430	13.4	7.7	6.5	$C_{21}H_{31}O_1$
299.2452	0.9	299.2375	25.7			

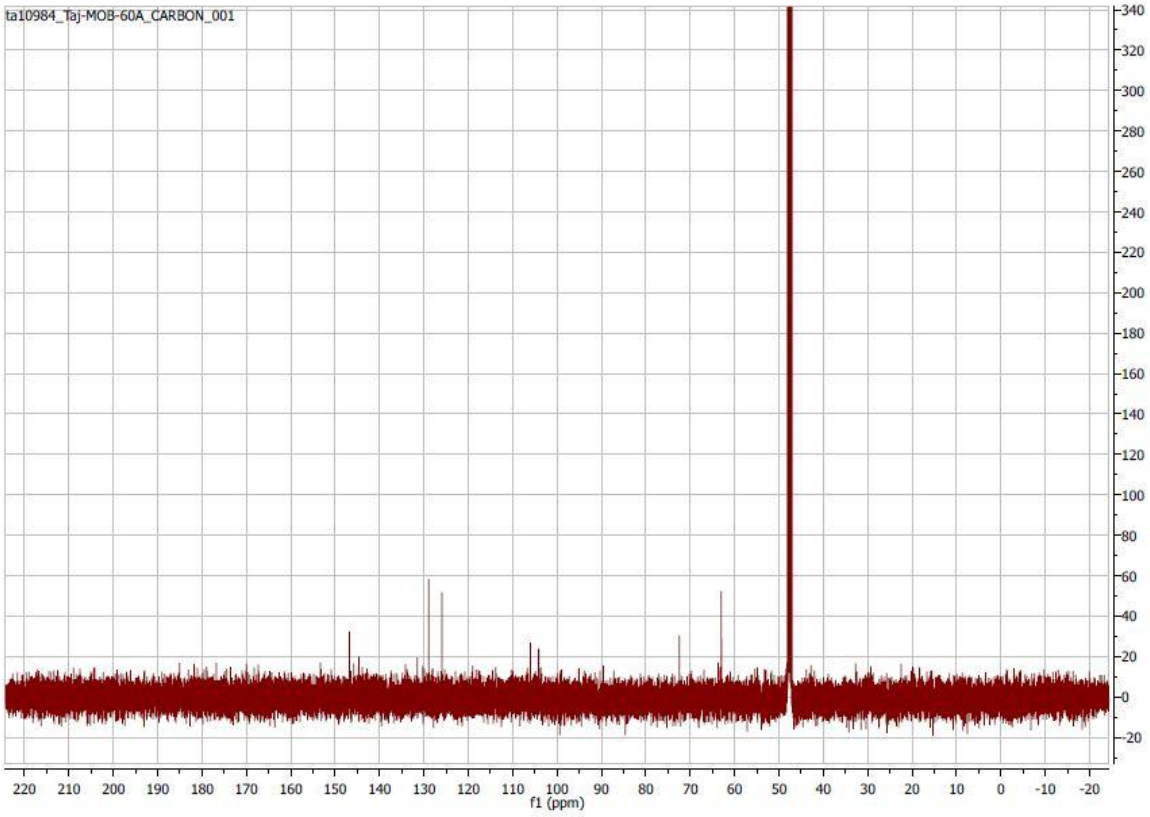
S3: HRMS Spectrum of Compound **1 (**7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one**)**



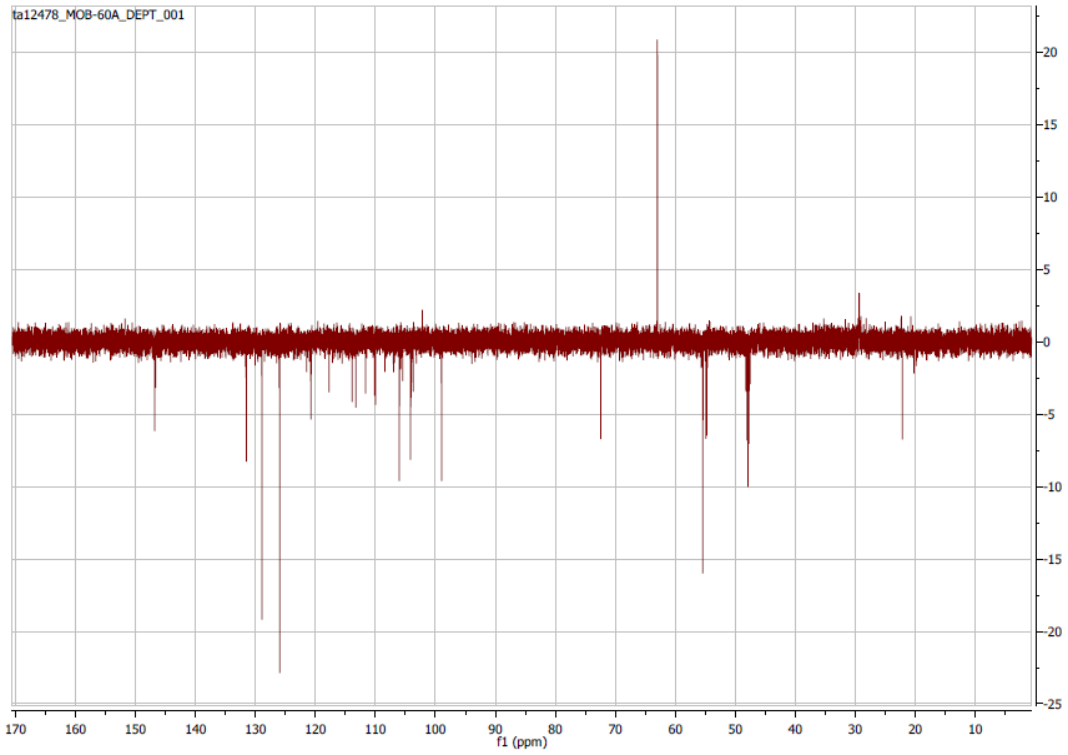
S4: ^{1}H-NMR (400 M*Hz*, MeOD) Spectrum of Compound **1 (**7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one**)**

*(7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one) (**1**):* ^{1}H-NMR (400 M*Hz*, MeOD), *δ*: 6.92 (s, H-2), 7.05 (d, *J*= 10 *Hz*, H-4a), 8.05 (d, *J*= 10 *Hz*, H-5) 8.05 (d, *J*= 10 *Hz*, H-7) 7.47 (d, *J*= 10*Hz*, H-8) 7.45 (2H, dd, J= 9,2 *Hz*, H-2′) 6.98 (2H, dd, *J*= 9, 2*Hz*, H-3′) 3.61 (s, OCH_3) 6.98 (2H, dd, *J*= 9, 2 *Hz*, H-5′) 7.45 (2H, dd, *J*= 9, 2*HZ*, H-6′).

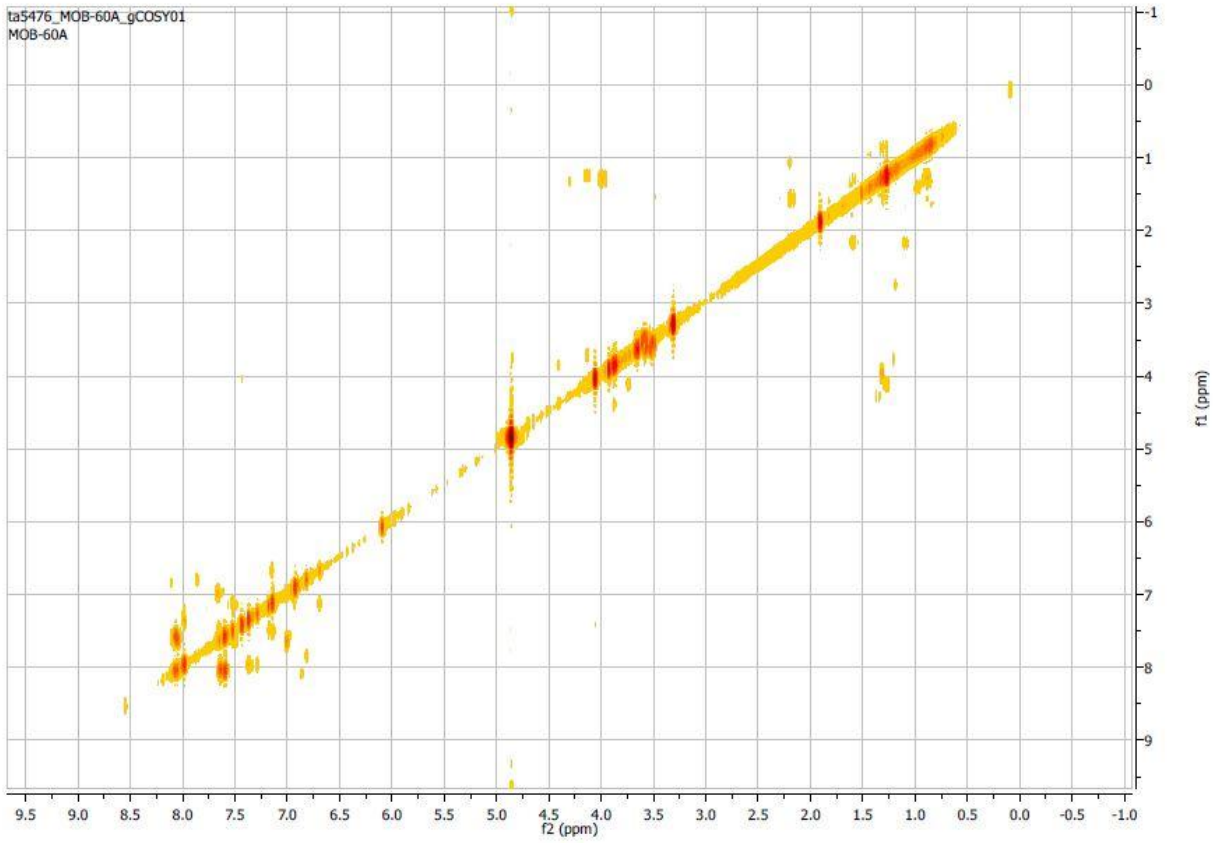
^{13}C-NMR (100 M*Hz*, MeOD), *δ*: 103.5(C-2) 160.1(C-3) 158.1(C-4) 104.1(C-4a) 125.1(C-5) 113.2(C-6) 147.3(C-7) 105.1(C-8) 164.2(C-8a) 107.1(C-9) 178.9(C-10) 126.2(C-1′) 130.2(C-2′) 116.2(C-3′) 165.1(C-4′) 116.2(C-5′) 130.2(C-6′) 55.2(OCH_3)



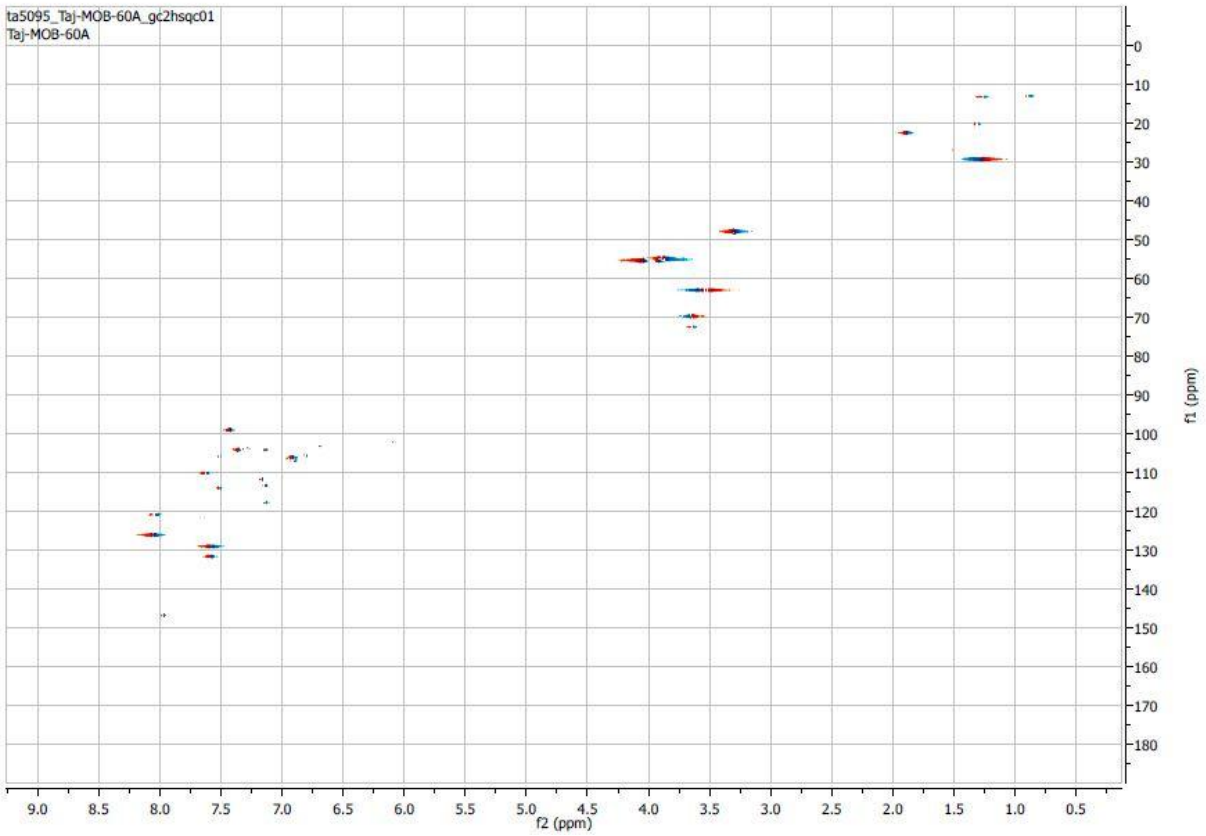
S5: ^{13}C-NMR Spectrum (100 M*Hz*, MeOD) Spectrum of Compound **1** (7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one)



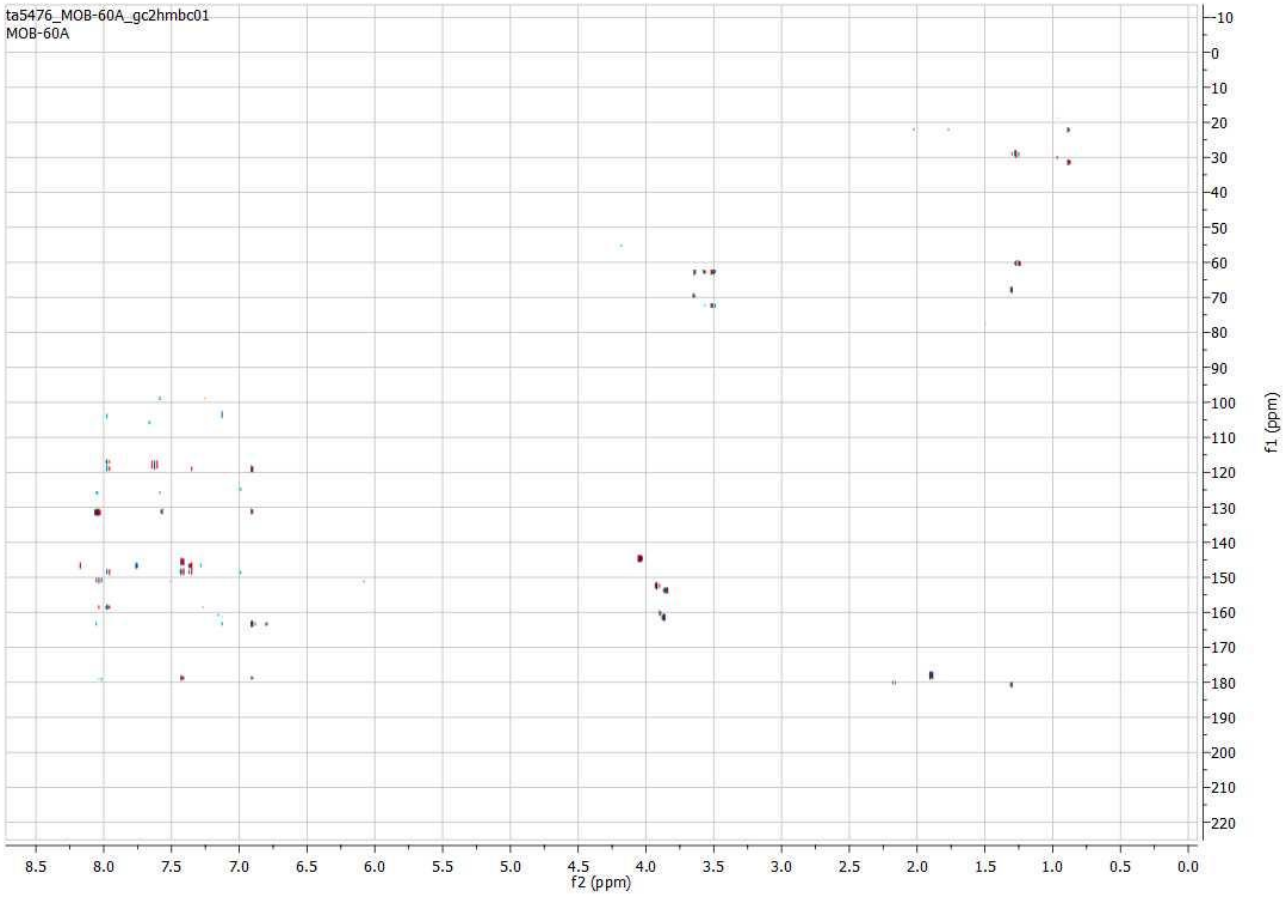
S6: ^{13}C-NMR DEPT Spectrum of Compound **1** (7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one**)**)



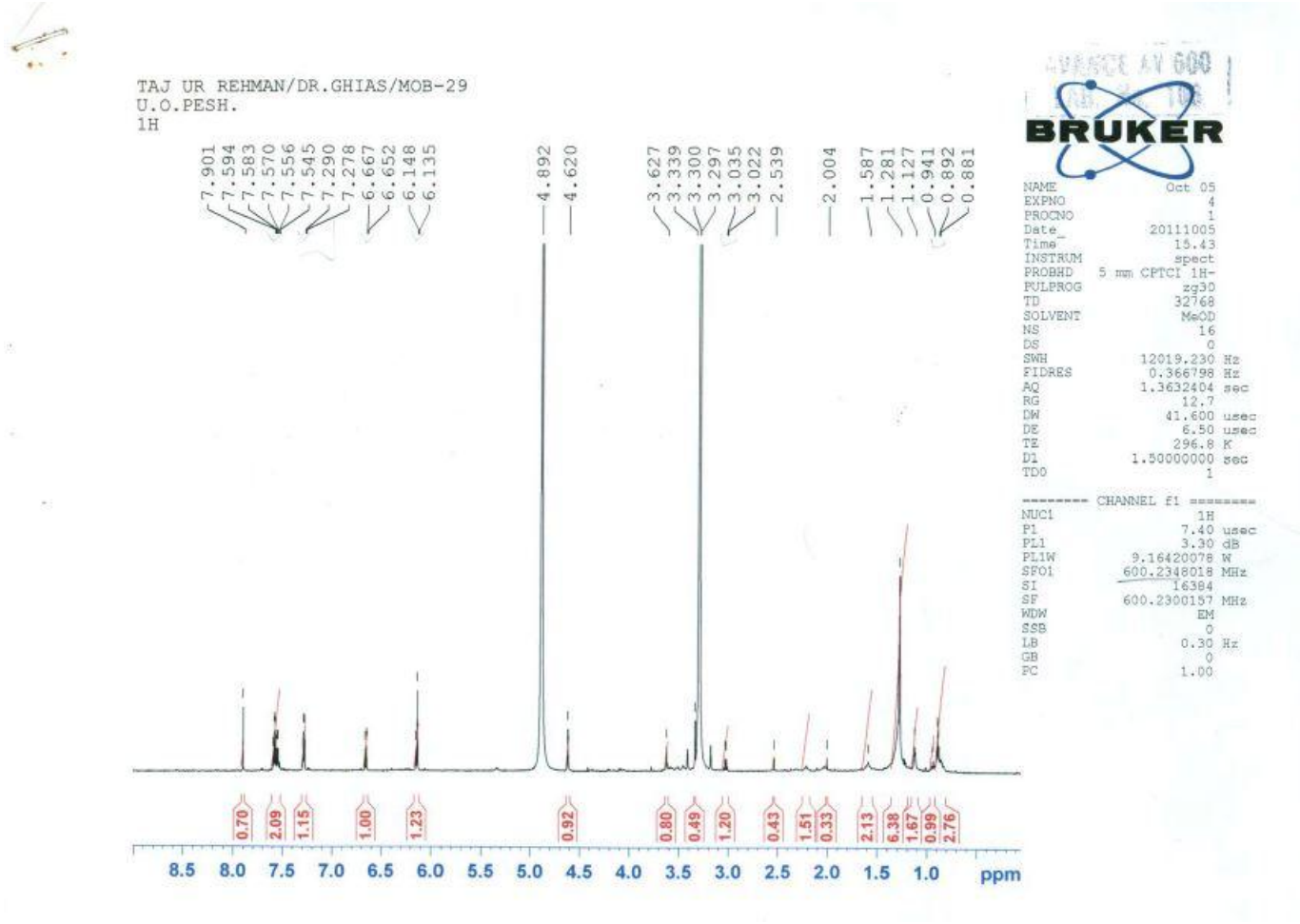
S7: COSY (400 M*Hz*) Spectrum of Compound **1** (7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one)



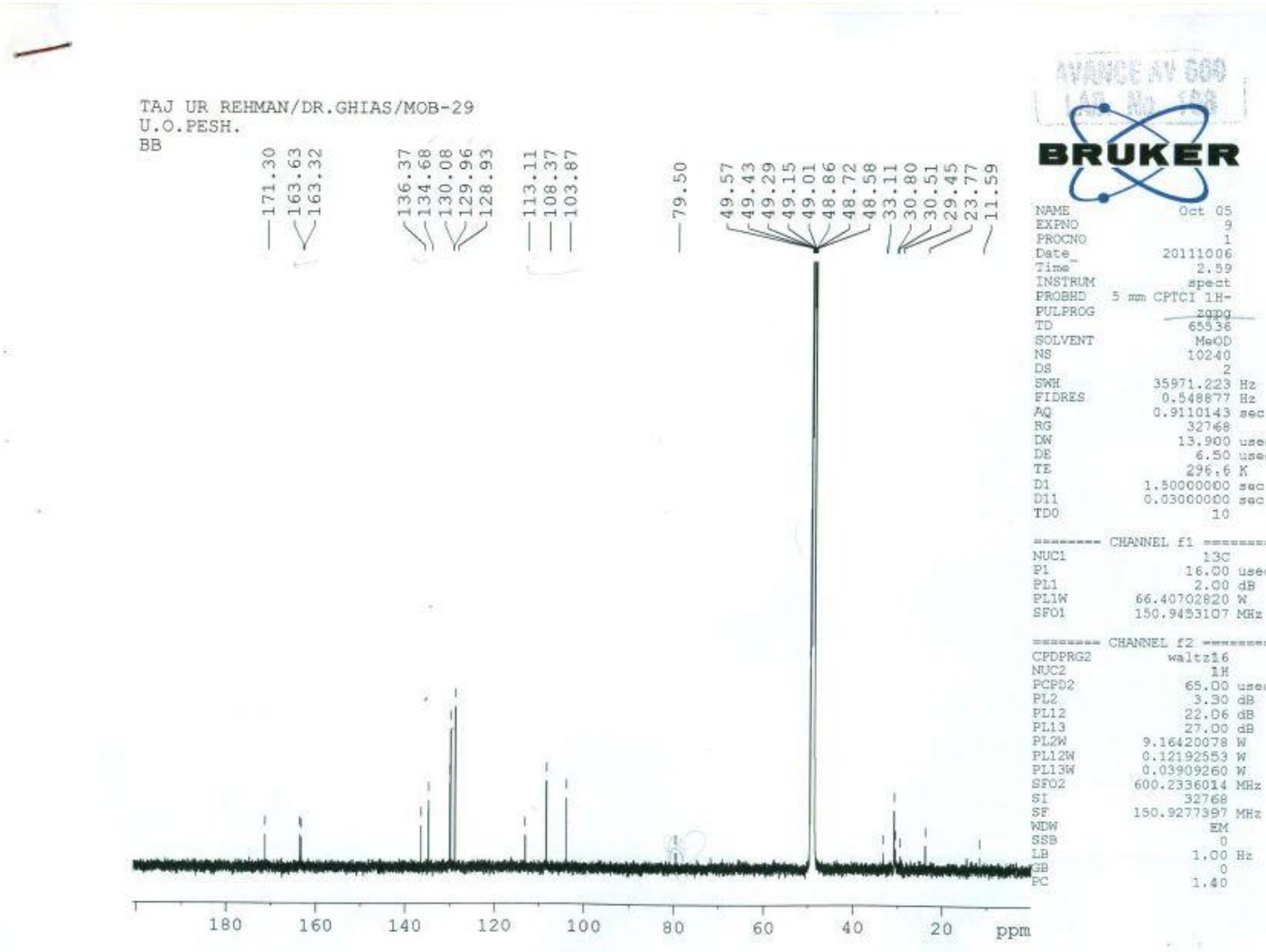
S8: HSQC (400 M*Hz*) Spectrum of Compound **1** (7-(4-methoxyphenyl)-9H-furo[2,3-f]chromen-9-one**)**)



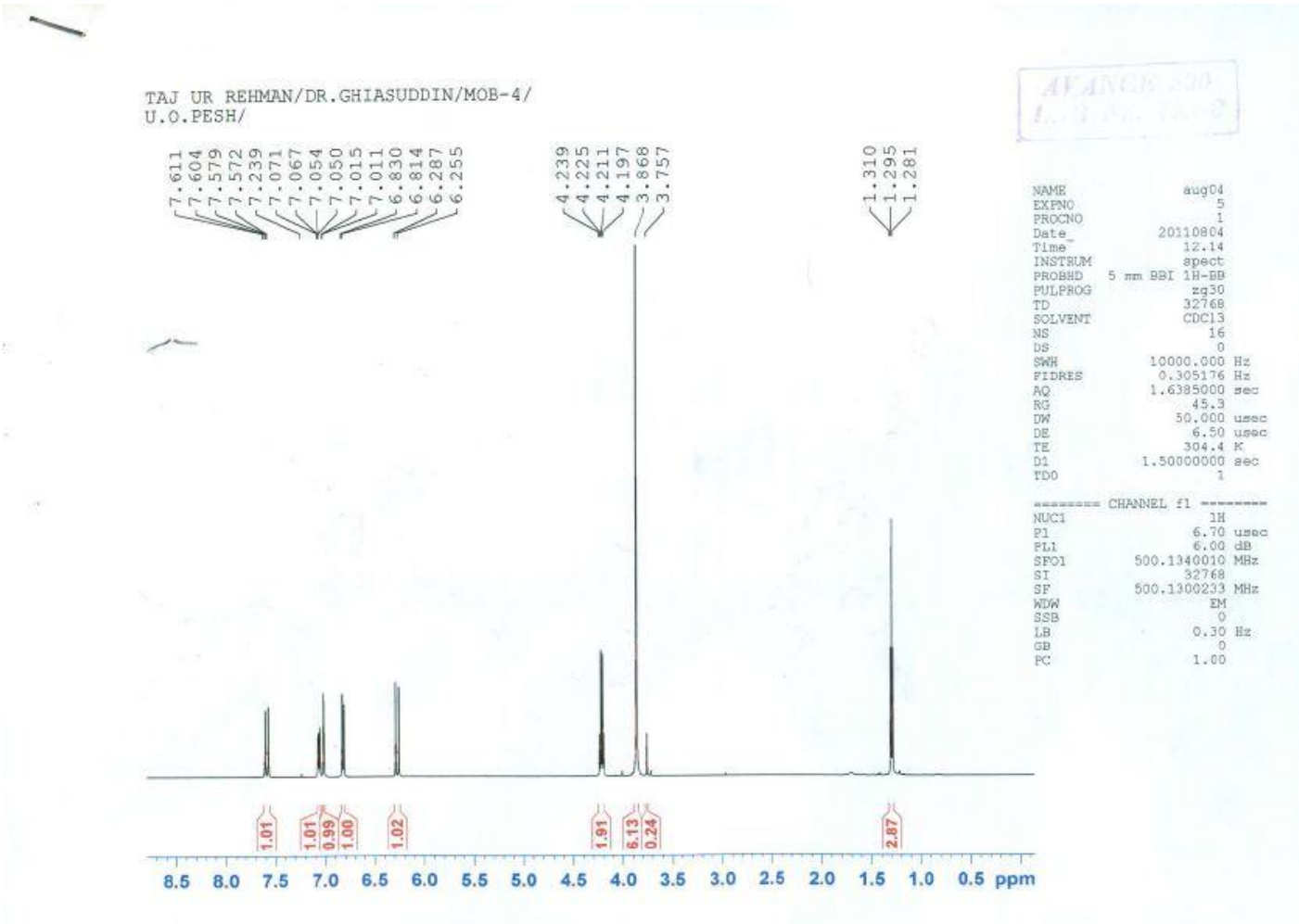
S9: HMBC (400 M*Hz*) Spectrum of Compound **1** (7-(3,4-Dihydroxyphenoxy)-5-hydroxy-2-(4-hydroxy-3-methoxyphenyl)-4H-chromen-4-one)



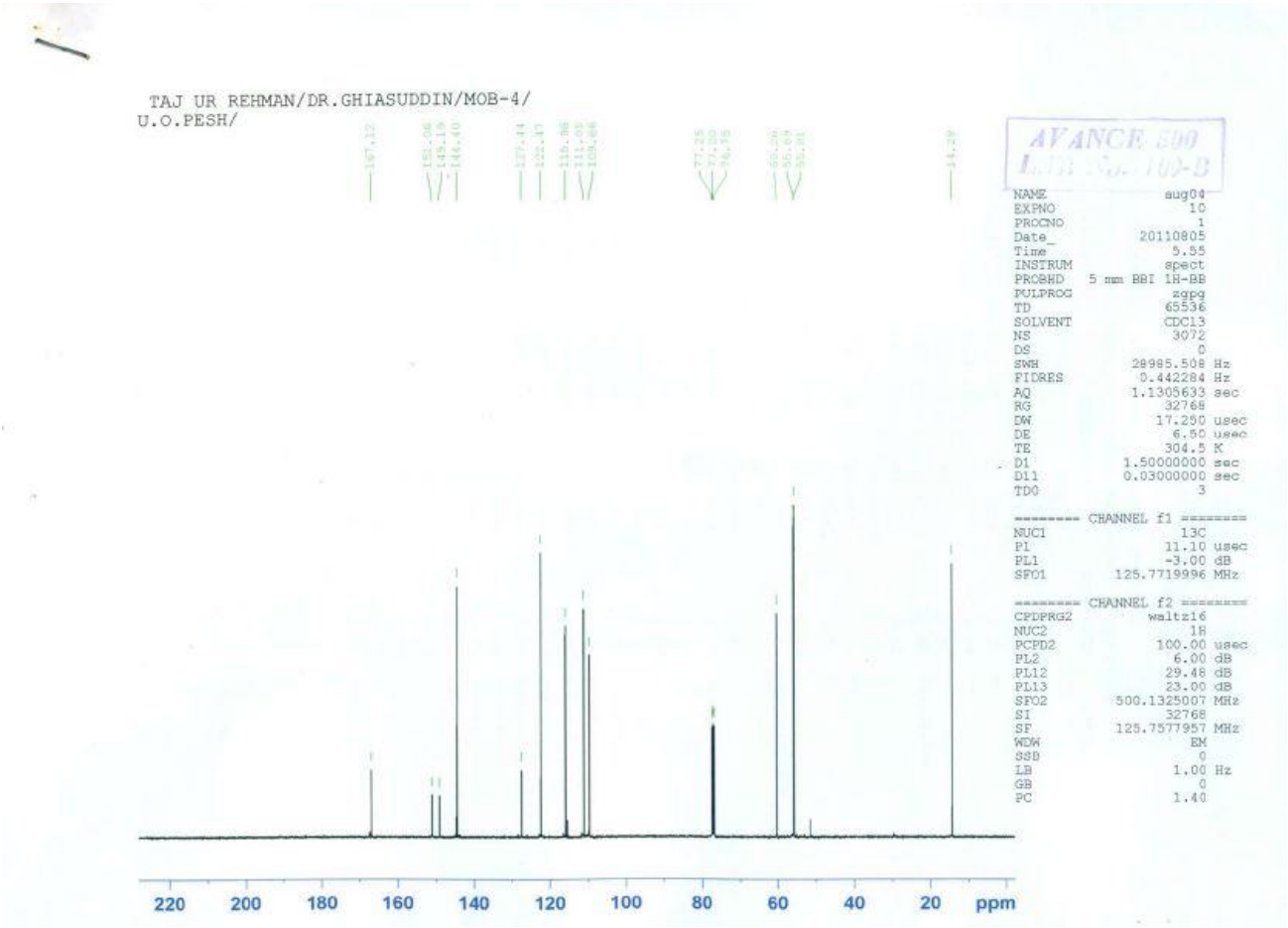
S10: [1]H-NMR (600 M*Hz*, MeOD) Spectrum of Compound **2** (3,7-dihydroxy-2-phenyl-4H-chromen-4-one)



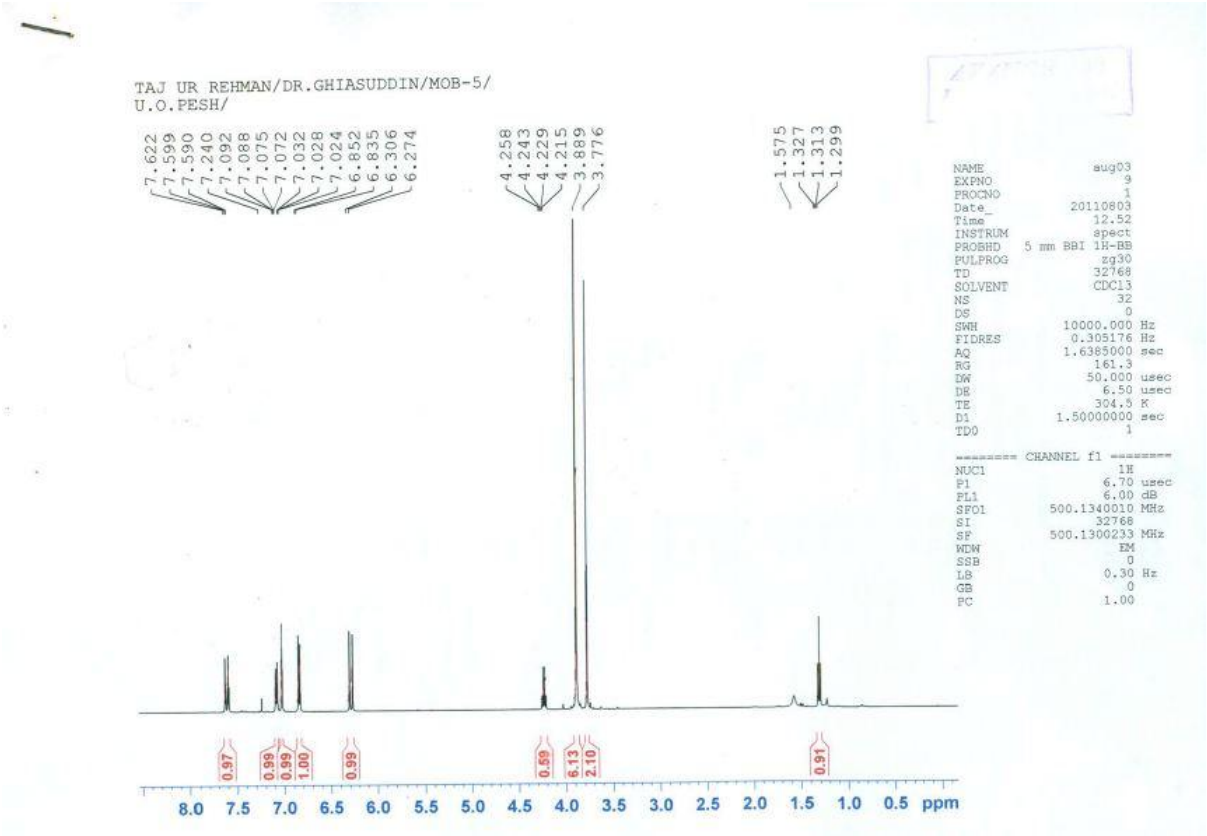
S11: ^{13}CNMR (150 M*Hz*, MeOD) Spectrum of Compound **2** (3,7-dihydroxy-2-phenyl-4H-chromen-4-one)



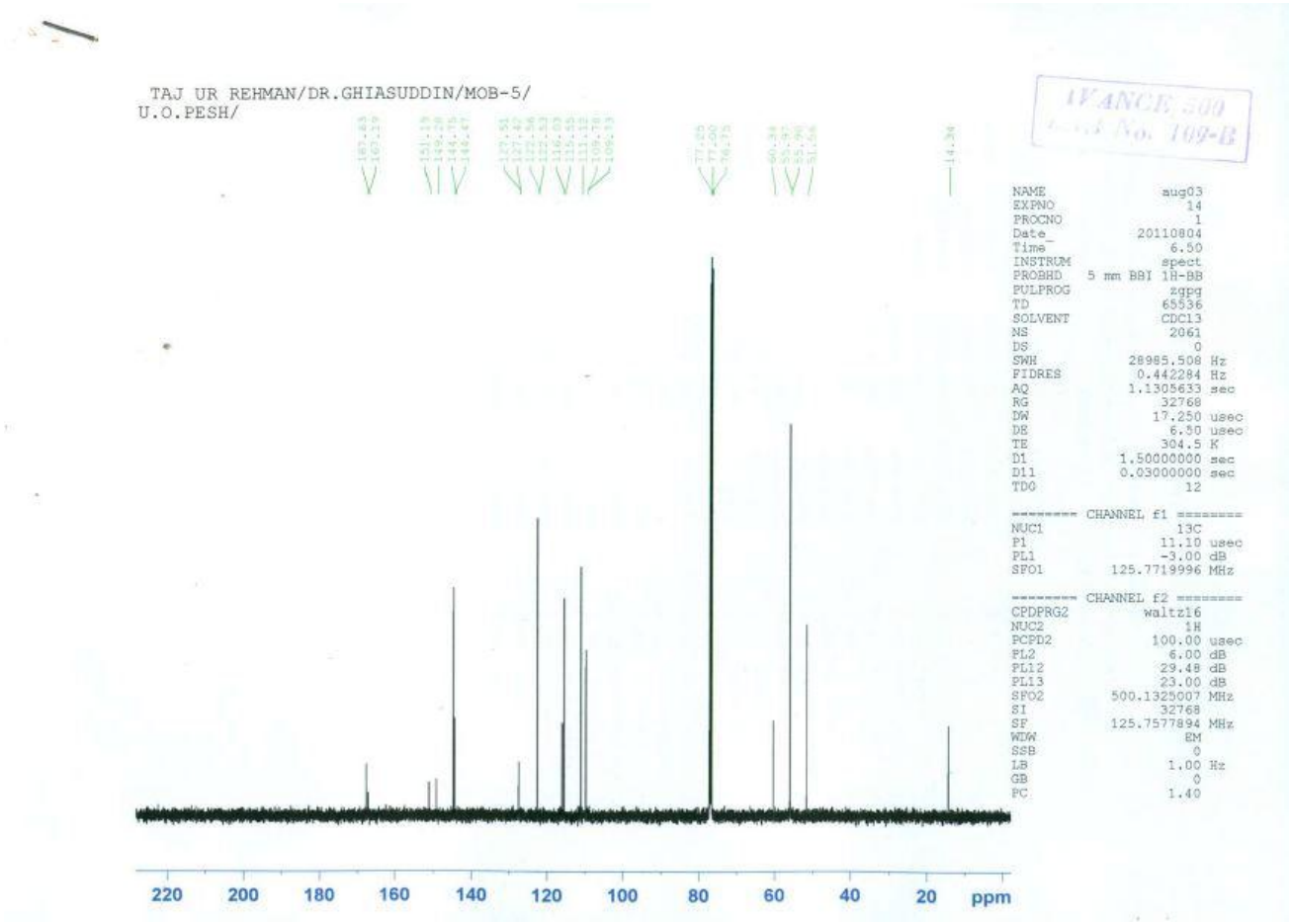
S12: ^{1}HNMR (500 M*Hz*, $CDCl_3$) Spectrum of Compound **3** ((*E*)-ethyl-3-(3,4-dimethoxyphenyl)acrylate)



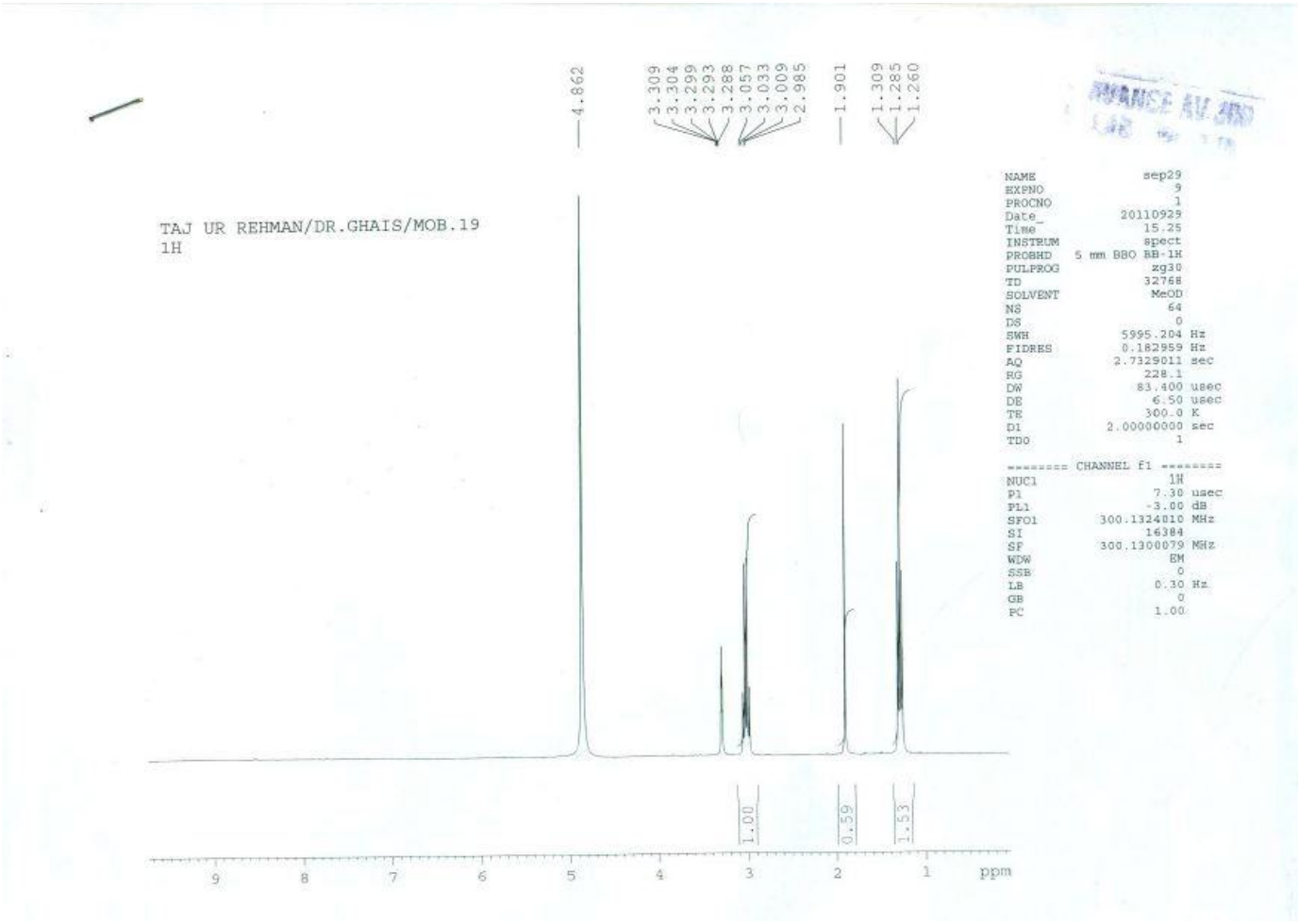
S13: ^{13}CNMR (125 M*Hz*, $CDCl_3$) Spectrum of Compound **3** ((*E*)-ethyl-3-(3,4-dimethoxyphenyl)acrylate)



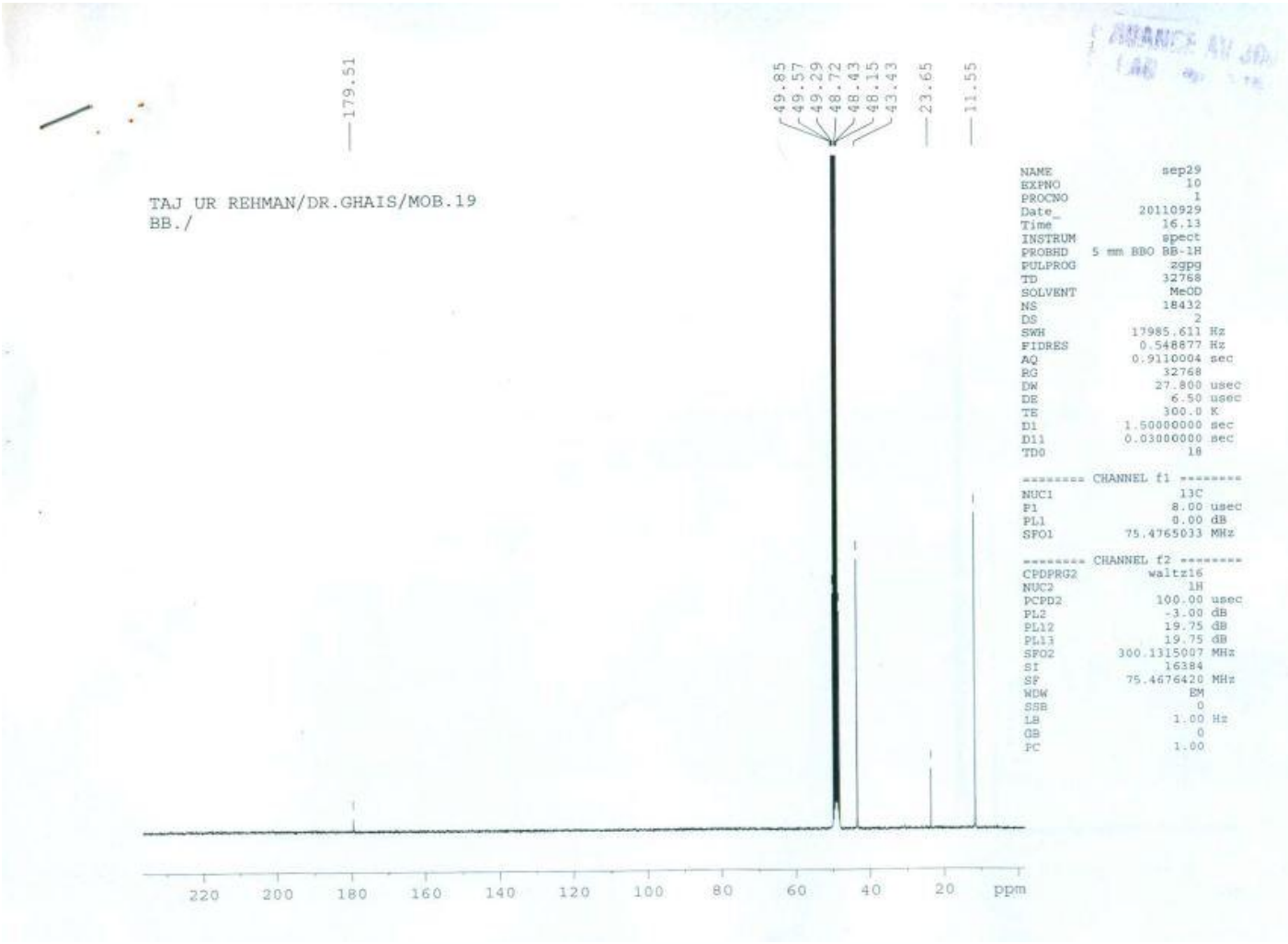
S14: ^{1}HNMR (500 M*Hz*, $CDCl_3$) Spectrum of compound **4** ((*E*)-Methyl-3-(3,4-dimethoxyphenyl)acrylate)



S15: ^{13}CNMR (125 M*Hz*, $CDCl_3$) Spectrum of compound **4** ((*E*)-Methyl-3-(3,4-dimethoxyphenyl)acrylate)



S16: [1]HNMR (300 M*Hz*, MeOD) of compound **5** (N-ethylacetamide)



S17: ^{13}CNMR (75 M*Hz*, MeOD) of compound **5** (N-ethylacetamide)