Spectroscopic, molecular docking and semi-empirical studies of the albumin binding activities of 5-hydroxymethylfurfural and its synthesized derivative, di (5-furfural) ether

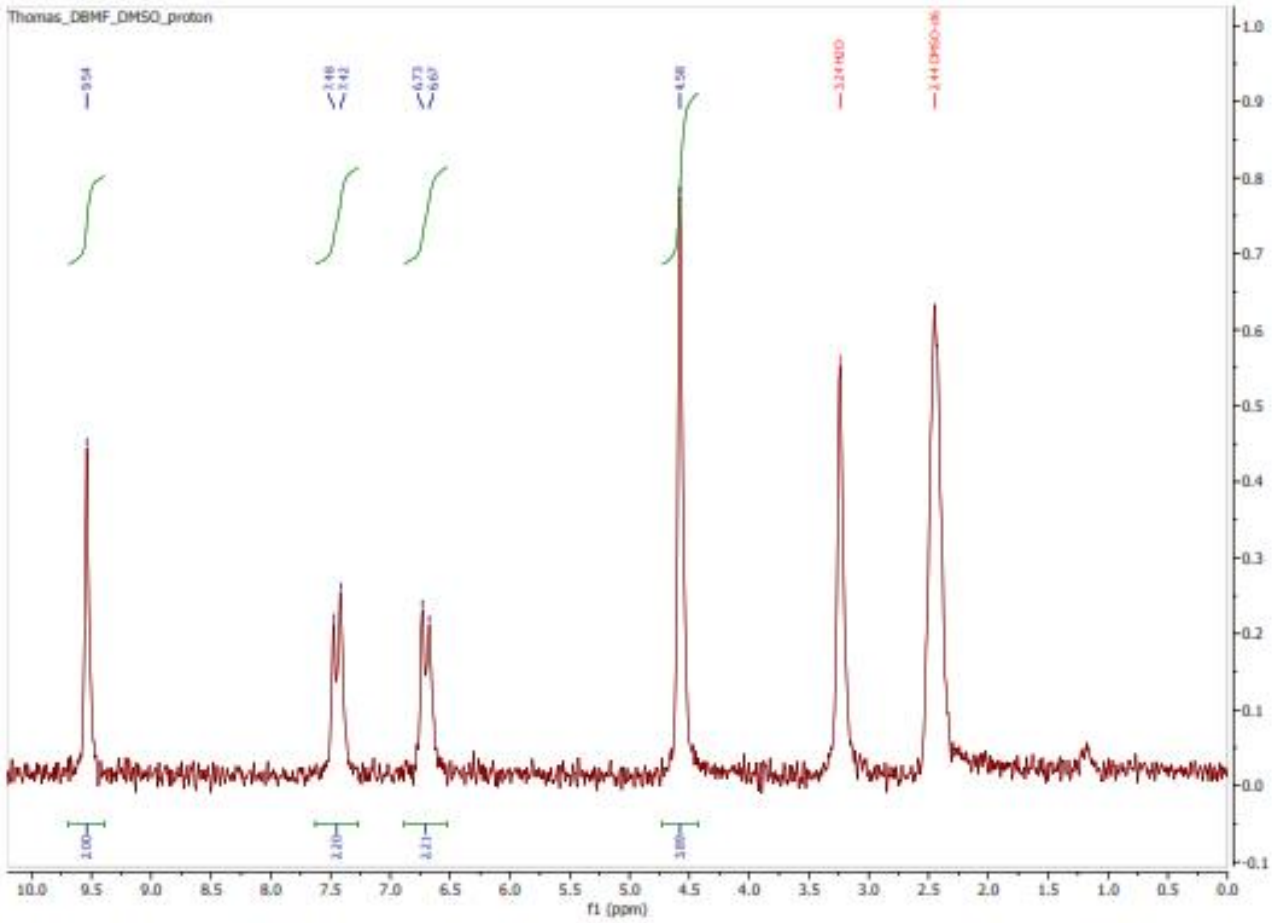


Figure 1 ^{1}H NMR of 5, 5'- oxydimethylenebis (2-furfural)

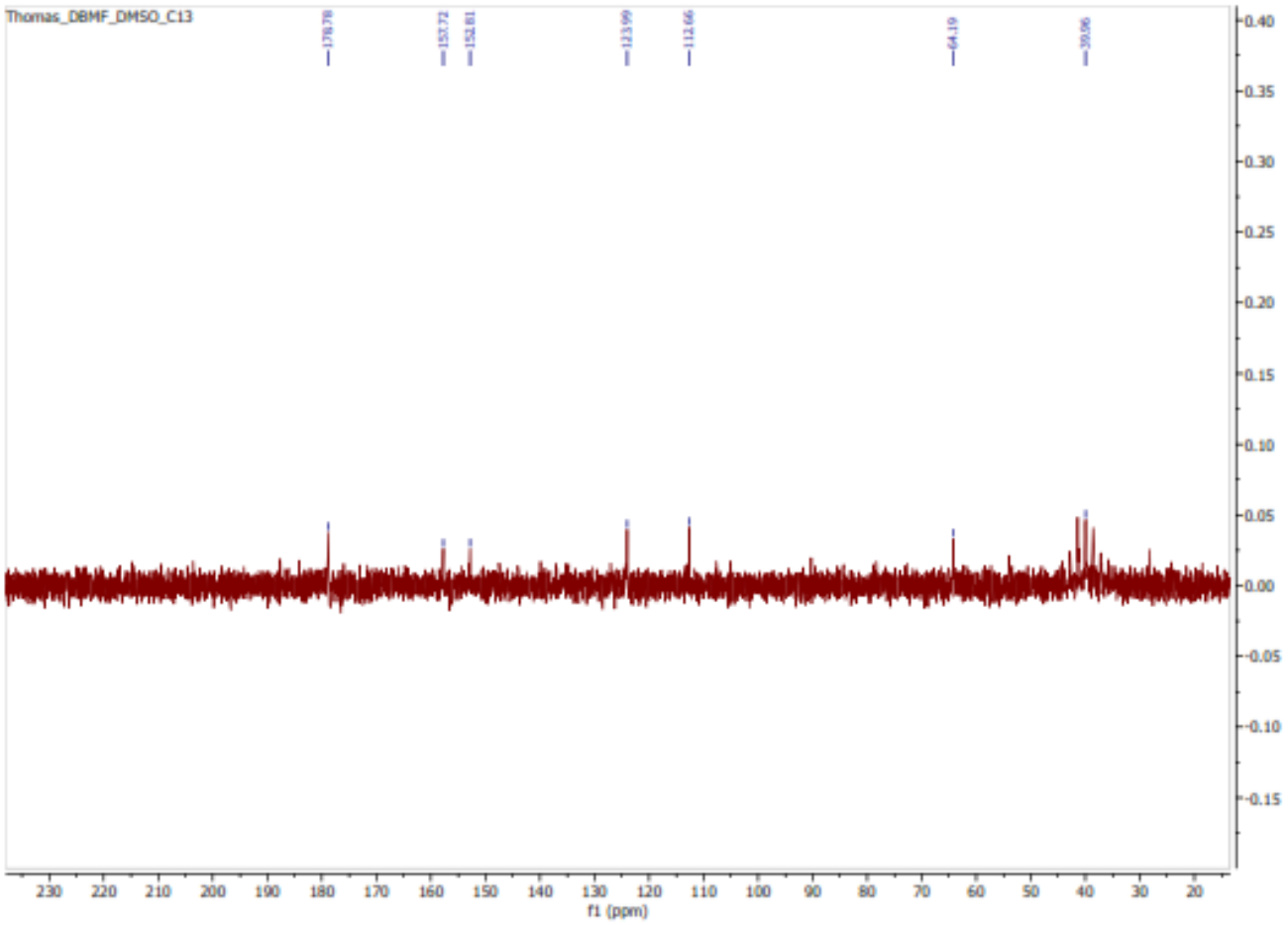


Figure 2 ^{13}CNMR of 5, 5'- oxydimethylenebis (2-furfural)

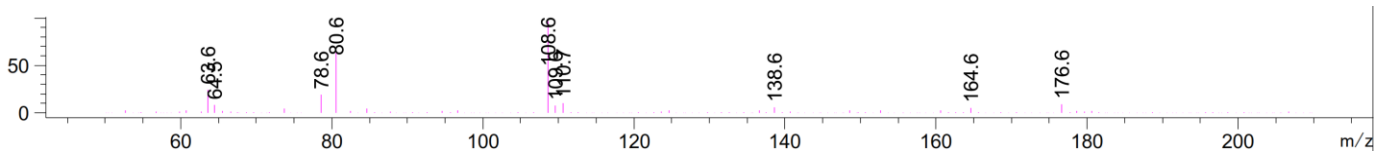
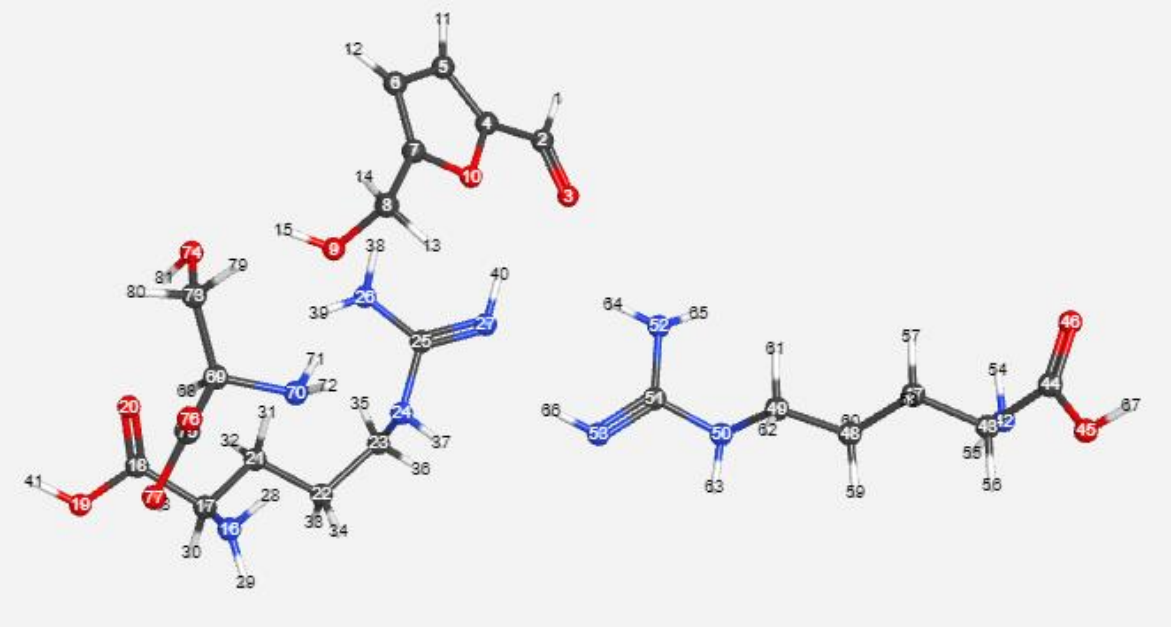


Figure 3 Mass spectrum of 5, 5'- oxydimethylenebis (2-furfural)

Figure 4 The optimised geometry and coordinates of HMF complex using the PM6-D3H+ method



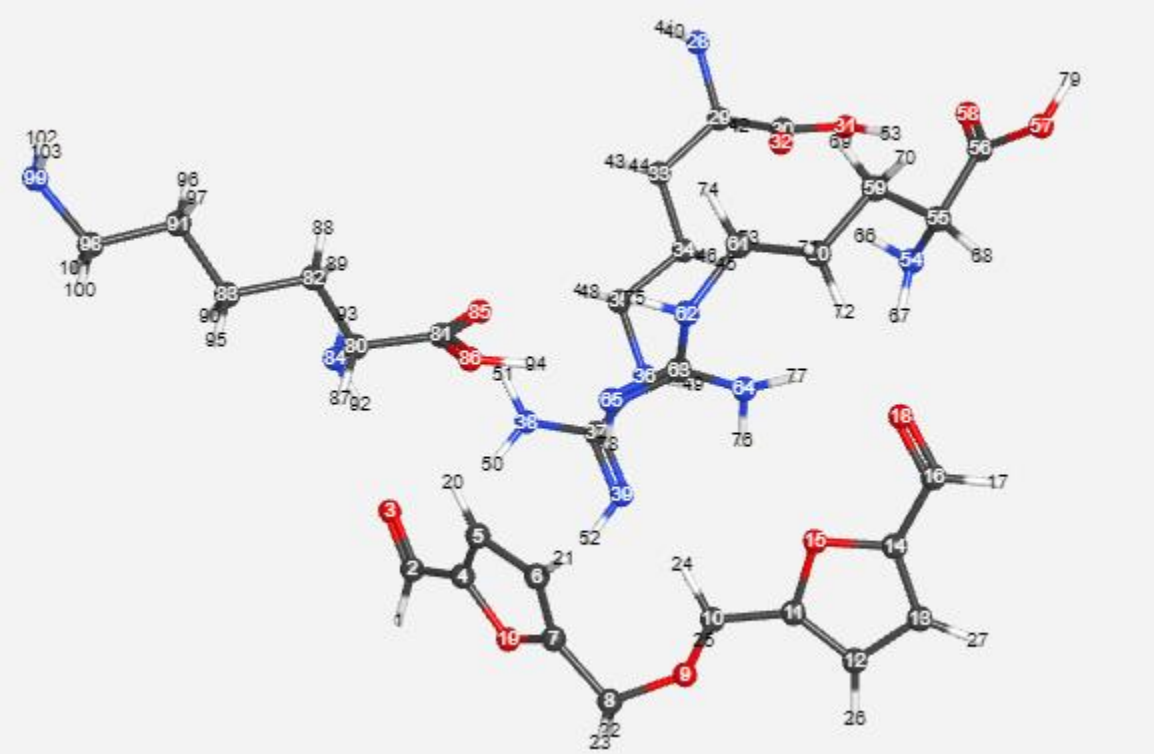
NO.	ATOM	X	Y	Z
1	H	-6.0470	0.1834	4.0341
2	C	-5.3354	-0.4160	3.4398
3	O	-5.6359	-1.5704	3.1265
4	C	-4.1158	0.2708	3.0873
5	C	-3.7342	1.5701	3.3596
6	C	-2.4427	1.8411	2.8444
7	C	-1.9381	0.7250	2.2140
8	C	-0.6575	0.4416	1.3055
9	O	0.4665	-0.5292	1.6030
10	O	-3.0804	-0.4538	2.4253
11	H	-4.3536	2.2881	3.8837
12	H	-1.9308	2.7947	2.8907
13	H	-1.1262	-0.4409	0.8939
14	H	-0.4061	1.1802	0.5452
15	H	0.5029	-0.9305	0.7206

16	N	2.1236	-6.0230	-1.5003
17	C	2.5882	-6.0700	-0.1020
18	C	4.0875	-5.7550	-0.0723
19	O	4.8129	-6.6884	0.5746
20	O	4.6242	-4.7563	-0.5324
21	C	1.8833	-5.0535	0.8098
22	C	0.3557	-5.1123	0.7675
23	C	-0.2626	-4.0734	1.7072
24	N	-1.5941	-3.7380	1.2373
25	C	-2.4112	-2.9133	1.9377
26	N	-1.7928	-1.8077	2.4664
27	N	-3.6465	-3.2870	2.0263
28	H	2.1468	-5.0545	-1.8338
29	H	1.1481	-6.3113	-1.5524
30	H	2.4297	-7.0865	0.2752
31	H	2.2058	-4.0379	0.5445
32	H	2.2213	-5.2132	1.8424
33	H	0.0058	-6.1140	1.0447
34	H	0.0053	-4.9307	-0.2545
35	H	0.3573	-3.1729	1.7272
36	H	-0.3038	-4.4747	2.7265
37	H	-2.1473	-4.5593	1.0020
38	H	-2.6455	-0.9235	2.6881
39	H	-1.2866	-1.1058	1.7830
40	H	-4.3203	-2.7240	2.5870
41	H	5.7377	-6.3782	0.4815
42	N	-13.8928	-4.0697	-0.4354
43	C	-13.1862	-3.3899	-1.5378
44	C	-14.1407	-2.4029	-2.2184

45	O	-13.9195	-2.2888	-3.5440
46	O	-14.9922	-1.7173	-1.6719
47	C	-11.9471	-2.6203	-1.0586
48	C	-10.8200	-3.5318	-0.5667
49	C	-9.5876	-2.7227	-0.1585
50	N	-8.5541	-3.6306	0.3054
51	C	-7.3757	-3.2020	0.8130
52	N	-7.4717	-2.2049	1.7132
53	N	-6.2969	-3.7775	0.4294
54	H	-14.3095	-3.3634	0.1747
55	H	-13.2416	-4.6050	0.1335
56	H	-12.9051	-4.1532	-2.2723
57	H	-12.2285	-1.9185	-0.2619
58	H	-11.5674	-2.0026	-1.8833
59	H	-10.5499	-4.2422	-1.3581
60	H	-11.1548	-4.1266	0.2911
61	H	-9.8657	-2.0166	0.6321
62	H	-9.2138	-2.1455	-1.0120
63	H	-8.3373	-4.3524	-0.3785
64	H	-6.6116	-2.0216	2.2774
65	H	-8.2475	-2.3607	2.3430
66	H	-5.4773	-3.3885	0.9200
67	H	-14.5991	-1.6469	-3.8385
68	H	3.1609	-2.5110	-1.5530
69	C	2.3603	-2.0297	-2.1240
70	N	1.2773	-3.0493	-2.3166
71	H	0.8596	-3.1892	-1.3865
72	H	0.5036	-2.5928	-2.8178
73	C	1.8330	-0.8053	-1.3709

74	O	1.3136	-1.2016	-0.0840
75	C	2.9253	-1.6259	-3.4860
76	O	3.5168	-0.5845	-3.7214
77	O	2.6949	-2.5830	-4.4216
78	H	2.2045	-3.3170	-3.9771
79	H	1.0203	-0.3180	-1.9206
80	H	2.6188	-0.0603	-1.2065
81	H	2.1142	-1.4333	0.4478

Figure 5 The optimised geometry and coordinates of OMBF complex using the PM6-D3H+ method



NO.	ATOM	X	Y	Z
1	H	-1.2582	4.3261	0.1307
2	C	-0.2435	4.4774	-0.2745
3	O	0.1911	5.6161	-0.4295
4	C	0.4837	3.2861	-0.7920
5	C	1.5775	3.0139	-1.5696
6	C	1.7789	1.6220	-1.4833
7	C	0.8199	1.1185	-0.6258
8	C	0.7382	-0.2094	0.0265
9	O	-0.5791	-0.7308	-0.0706
10	C	-0.6116	-1.9871	0.5923
11	C	-2.0005	-2.4774	0.7132
12	C	-2.5022	-3.7598	0.6218

13	C	-3.8276	-3.7023	1.0892
14	C	-4.0691	-2.3841	1.4178
15	O	-2.9832	-1.5998	1.1020
16	C	-5.2279	-1.7854	2.0107
17	H	-5.9784	-2.5025	2.3847
18	O	-5.4513	-0.5806	2.0928
19	O	-0.0839	2.0635	-0.2597
20	H	2.1948	3.7230	-2.0967
21	H	2.5904	1.0553	-1.9205
22	H	1.0207	-0.0938	1.0803
23	H	1.4439	-0.9010	-0.4499
24	H	-0.1936	-1.8980	1.6030
25	H	-0.0074	-2.7077	0.0282
26	H	-1.9482	-4.6384	0.3214
27	H	-4.5187	-4.5259	1.2026
28	N	-8.6911	6.8681	-1.2467
29	C	-8.3961	5.7972	-2.2149
30	C	-9.0884	6.0881	-3.5508
31	O	-9.5879	4.9678	-4.1161
32	O	-9.1042	7.1612	-4.1349
33	C	-6.8905	5.6576	-2.4862
34	C	-6.1356	4.9553	-1.3566
35	C	-4.6719	4.7274	-1.7398
36	N	-4.0213	3.9537	-0.7074
37	C	-2.6823	3.9188	-0.5318
38	N	-1.9382	5.3834	-0.7350
39	N	-2.0377	2.8366	0.0584
40	H	-8.4866	7.7696	-1.6848
41	H	-8.0773	6.7927	-0.4385

42	H	-8.8044	4.8613	-1.8162
43	H	-6.4474	6.6464	-2.6672
44	H	-6.7385	5.0937	-3.4150
45	H	-6.6157	3.9955	-1.1324
46	H	-6.1831	5.5509	-0.4371
47	H	-4.1894	5.7007	-1.8792
48	H	-4.6030	4.1864	-2.6901
49	H	-4.4092	3.0163	-0.5709
50	H	-0.5592	5.2032	-0.1303
51	H	-2.4410	6.0898	-0.1963
52	H	-0.6489	2.7889	0.3392
53	H	-9.7890	5.2181	-5.0545
54	N	-9.6731	1.9537	-5.6702
55	C	-8.3114	2.3059	-6.1161
56	C	-8.3545	3.6545	-6.8522
57	O	-7.3793	3.7747	-7.7761
58	O	-9.1179	4.5866	-6.6314
59	C	-7.3316	2.4139	-4.9397
60	C	-7.0452	1.0848	-4.2356
61	C	-6.1333	1.3014	-3.0268
62	N	-5.8687	0.0277	-2.3735
63	C	-5.0769	-0.0140	-1.2714
64	N	-5.5576	0.6942	-0.2258
65	N	-4.0136	-0.7251	-1.3486
66	H	-10.0078	2.6762	-5.0268
67	H	-9.6597	1.0849	-5.1407
68	H	-7.9824	1.5414	-6.8289
69	H	-7.7214	3.1273	-4.2053
70	H	-6.3826	2.8376	-5.2945

71	H	-6.5765	0.3877	-4.9410
72	H	-7.9756	0.6160	-3.8962
73	H	-6.6223	1.9868	-2.3274
74	H	-5.1877	1.7562	-3.3444
75	H	-5.4247	-0.6072	-3.0361
76	H	-5.3088	0.3580	0.7217
77	H	-6.5657	0.7678	-0.2619
78	H	-3.4335	-0.6777	-0.4898
79	H	-7.5186	4.6642	-8.1644
80	C	1.8638	6.8293	-2.5978
81	C	1.2212	6.8758	-3.9878
82	C	3.0587	7.7875	-2.5105
83	C	3.8269	7.6452	-1.1904
84	N	0.8718	7.1667	-1.5625
85	O	0.0805	7.2215	-4.2575
86	O	2.0417	6.4348	-4.9644
87	H	2.2012	5.8052	-2.4353
88	H	2.7205	8.8249	-2.6345
89	H	3.7465	7.5913	-3.3429
90	H	3.1755	7.8997	-0.3460
91	C	5.0636	8.5455	-1.1581
92	H	0.5143	6.1839	-0.9658
93	H	-0.0144	7.4058	-2.0238
94	H	1.4920	6.5103	-5.7728
95	H	4.1335	6.6002	-1.0587
96	H	4.7583	9.5916	-1.2855
97	H	5.7205	8.2948	-2.0004
98	C	5.8248	8.3827	0.1579
99	N	7.0104	9.2328	0.1890

100	H	6.1340	7.3401	0.2900
101	H	5.1799	8.6411	1.0048
102	H	6.7301	10.2070	0.0784
103	H	7.6030	9.0211	-0.6128