

Supplementary material

Identification of Novel and Potent Indole-based Benzenesulfonamides as Selective Human Carbonic Anhydrase II Inhibitors: Design, Synthesis, In Vitro, and In Silico Studies

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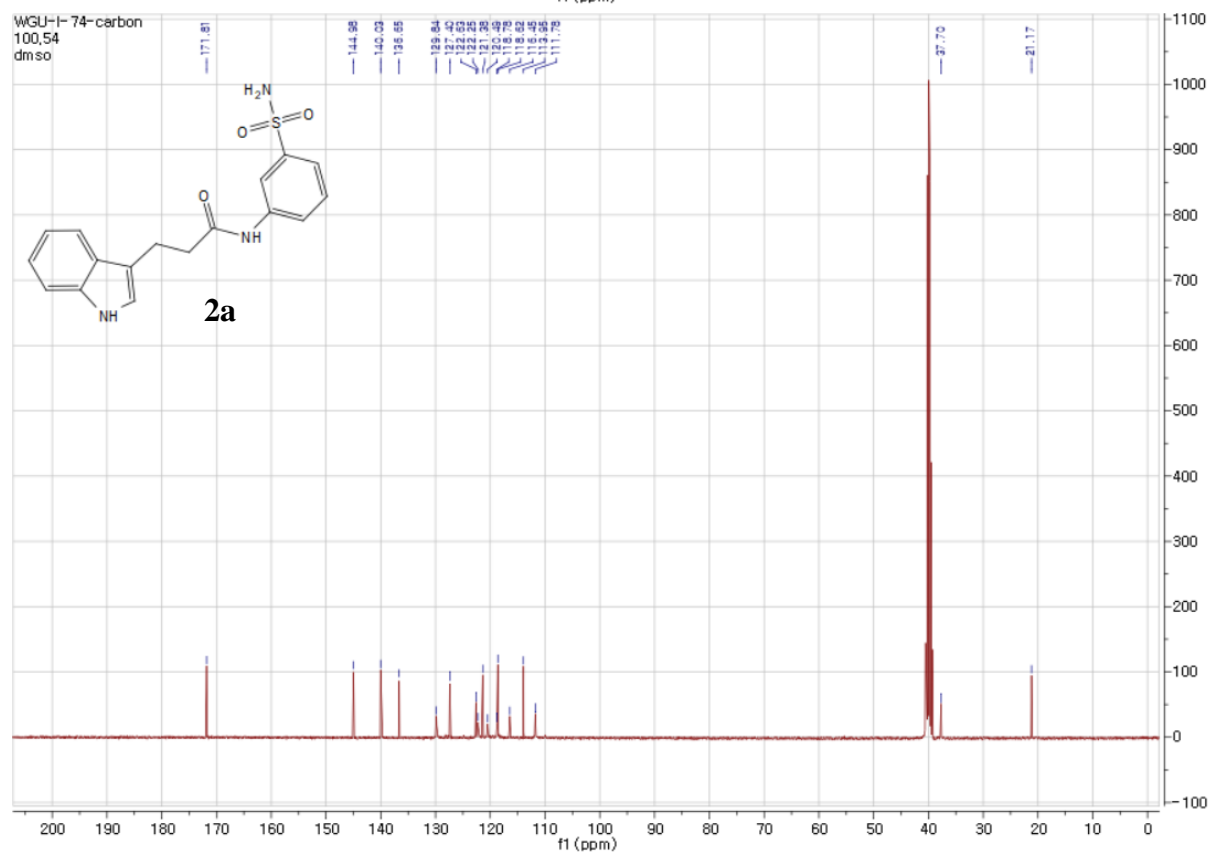
WGU-I-74
399,81
dmsol

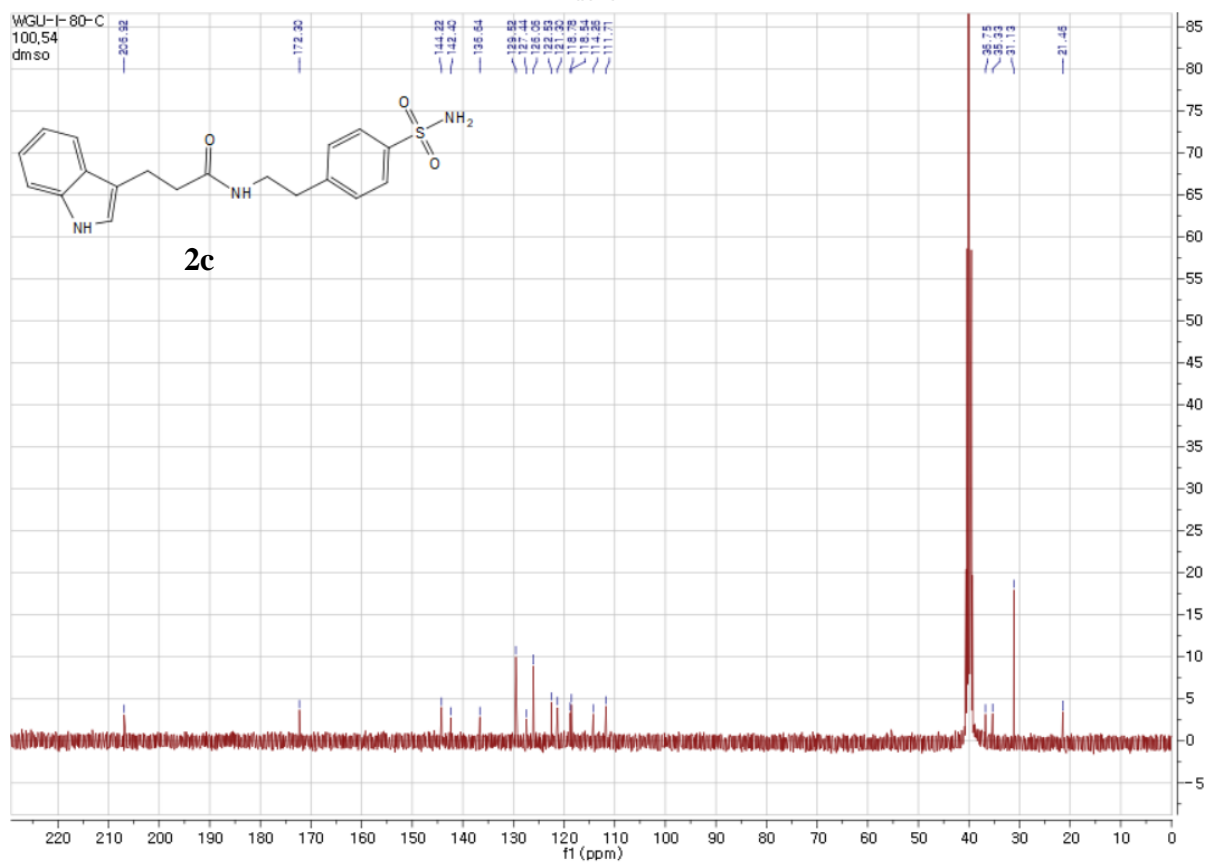
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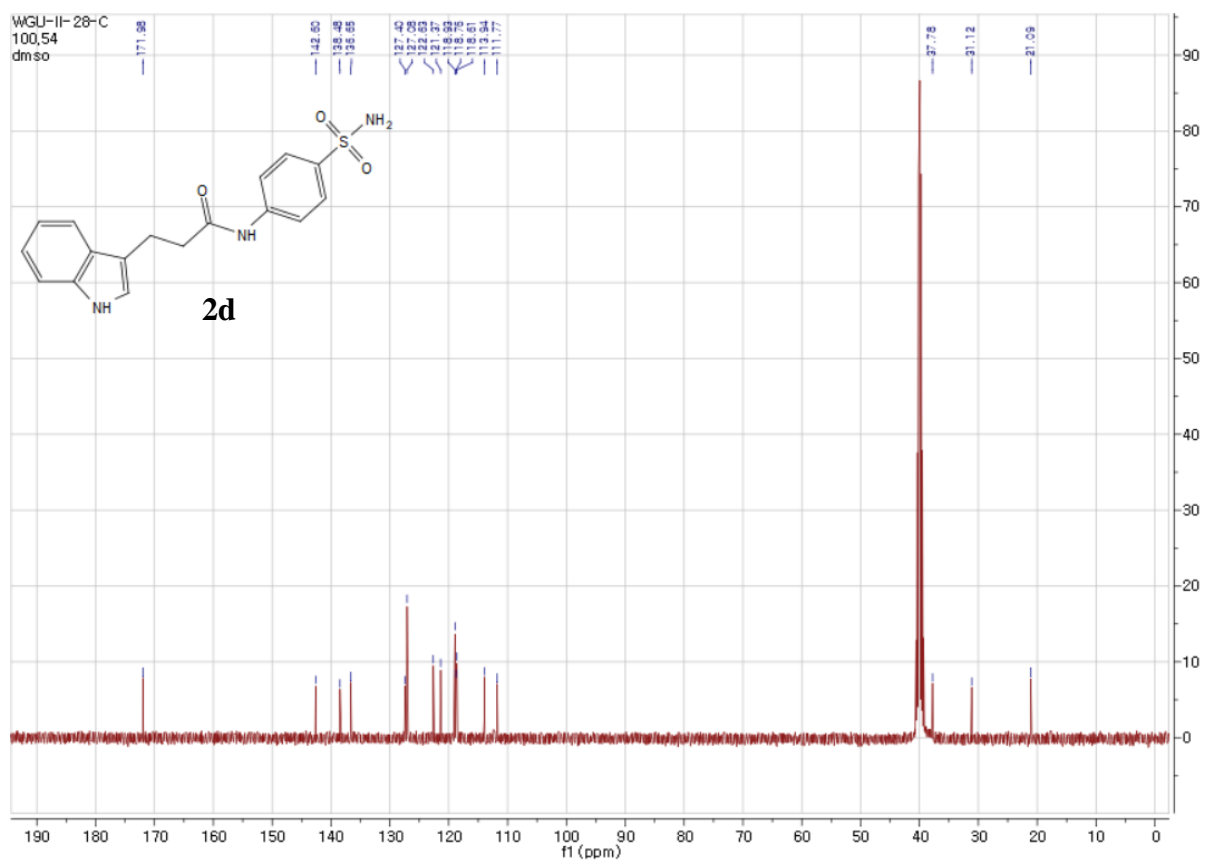
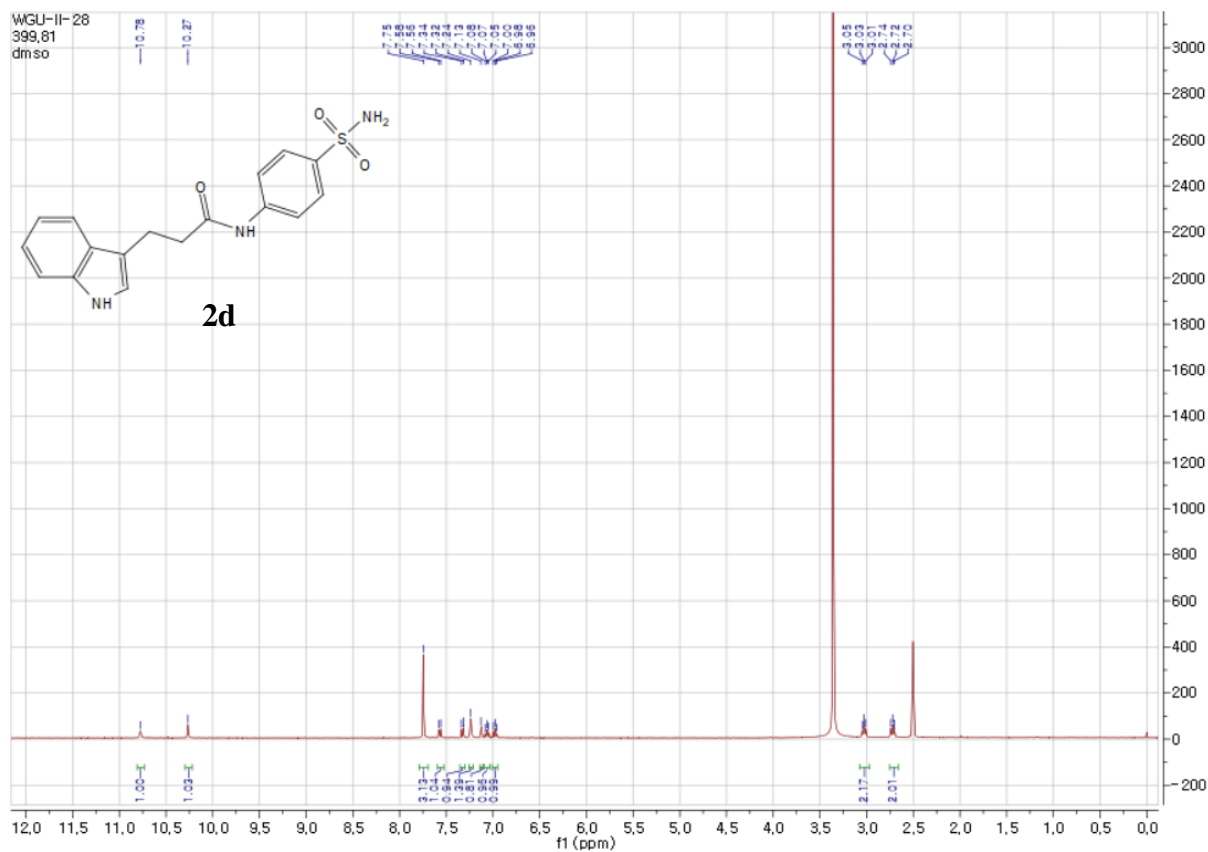
2a

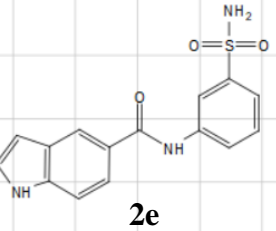
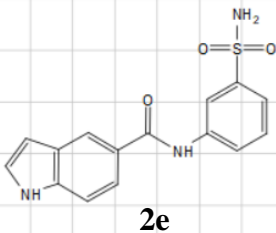
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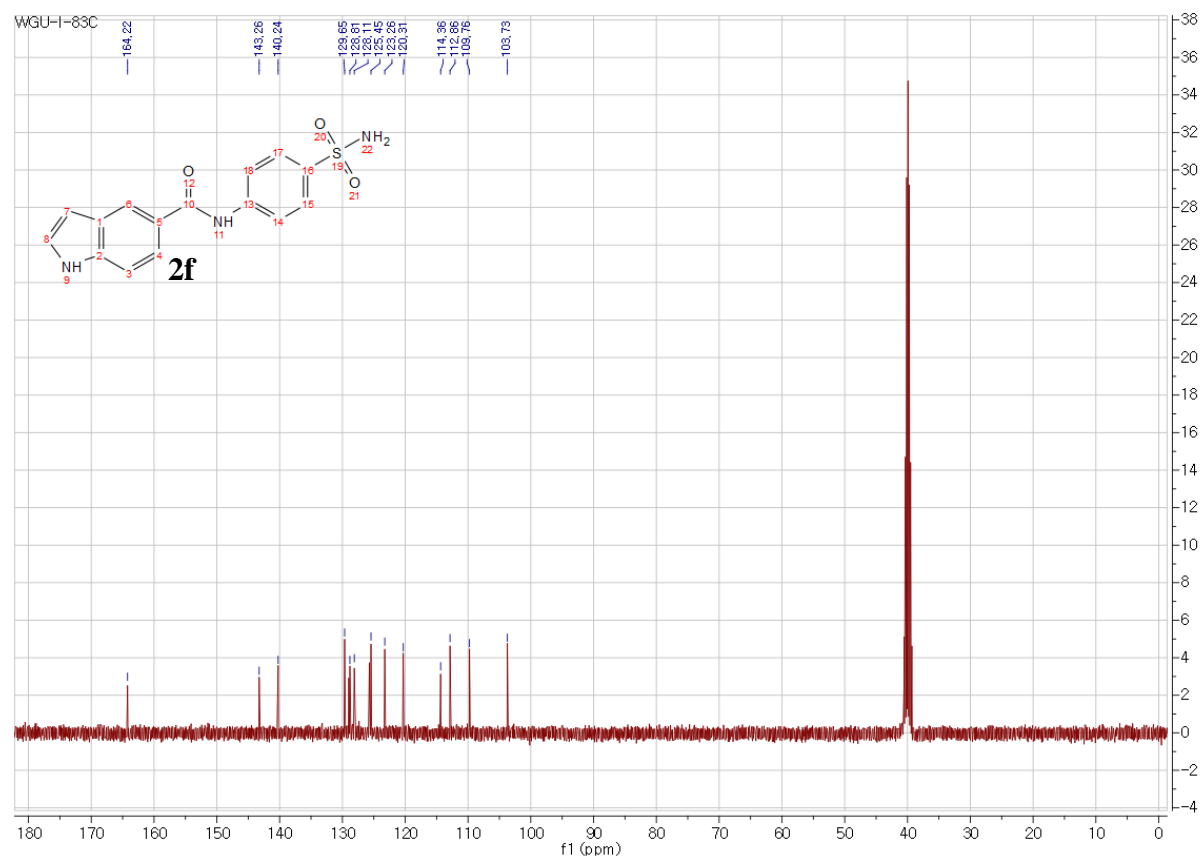
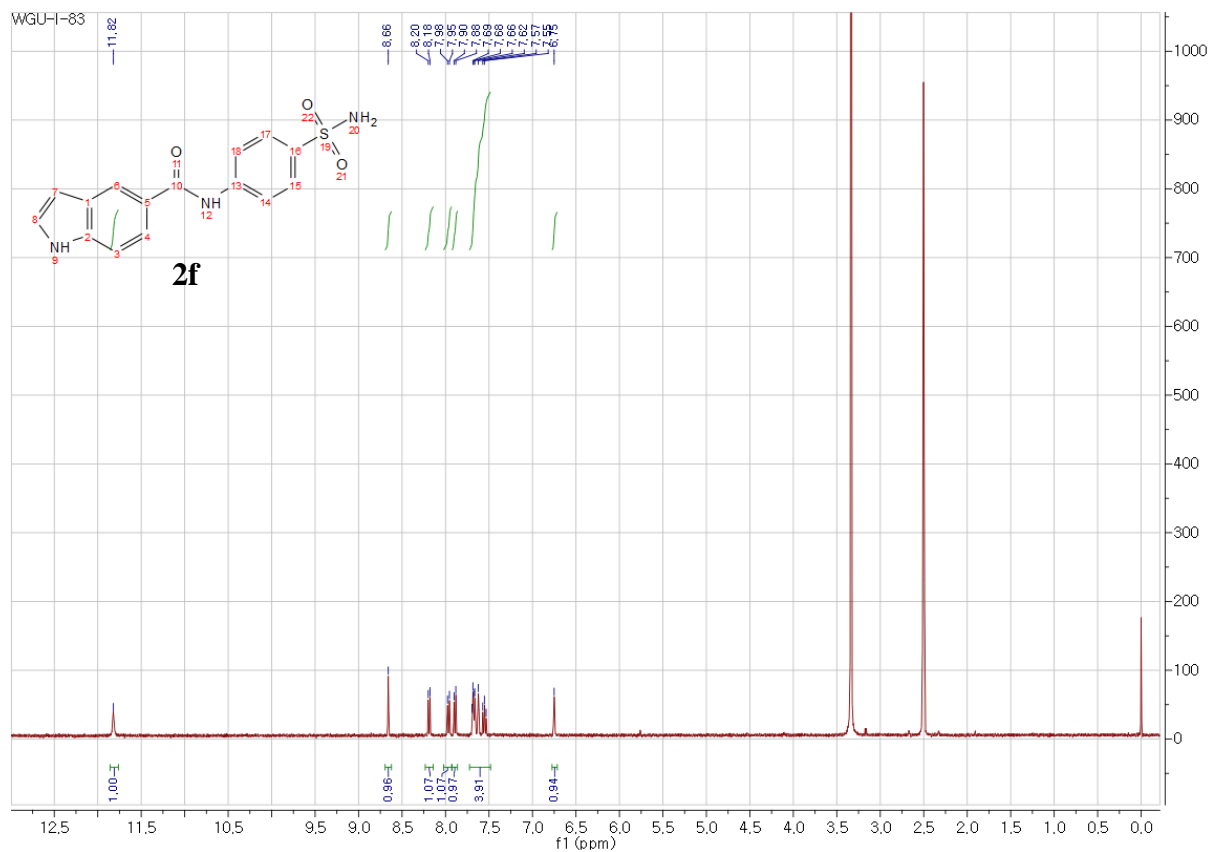
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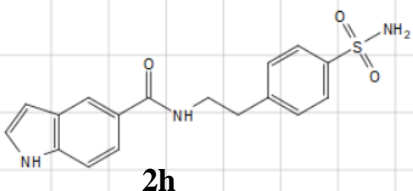
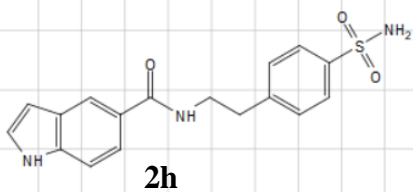


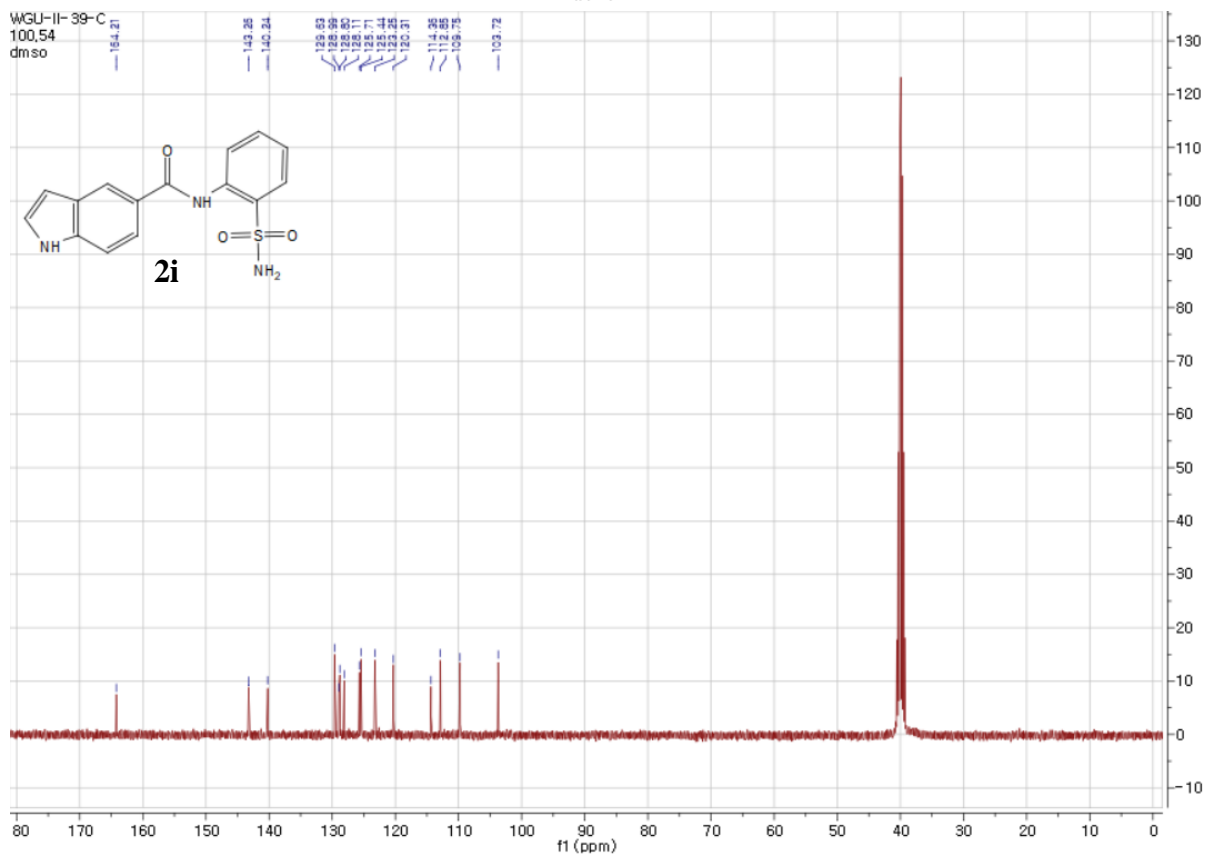
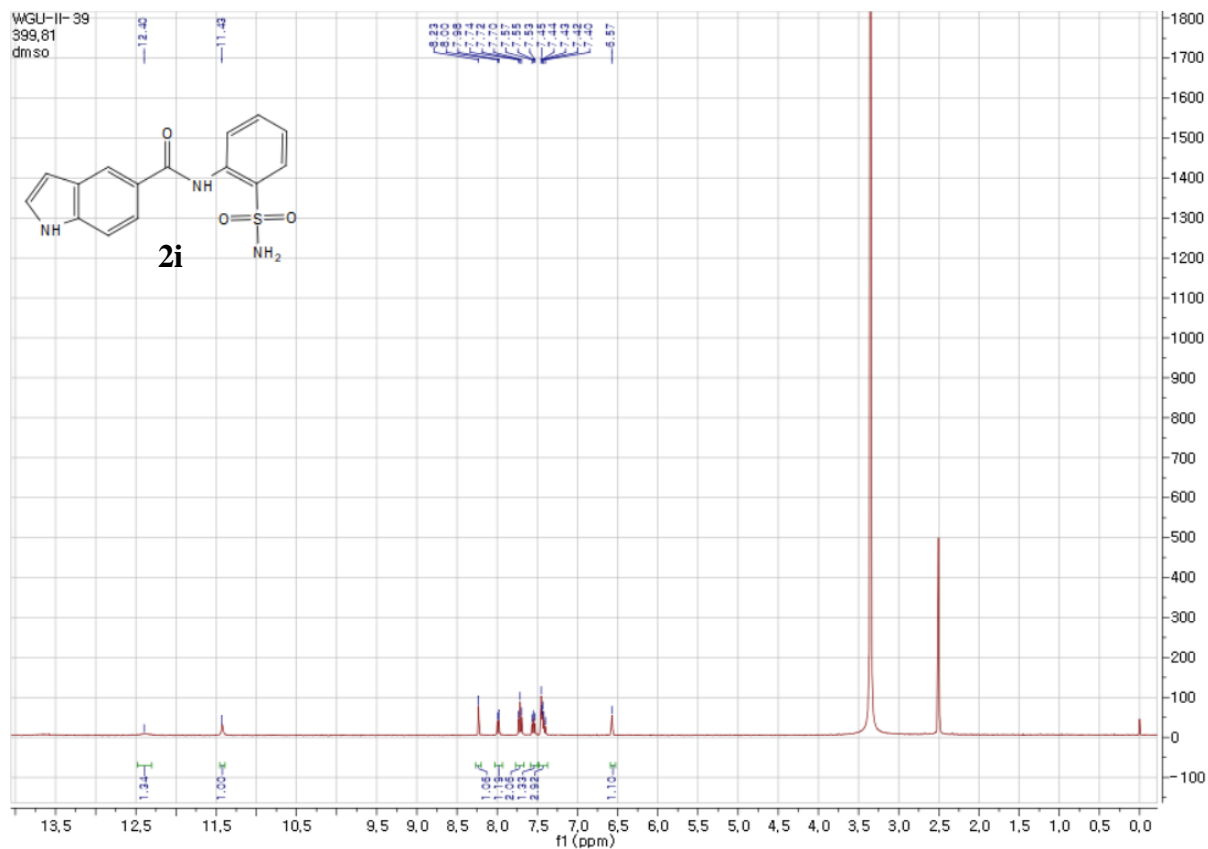


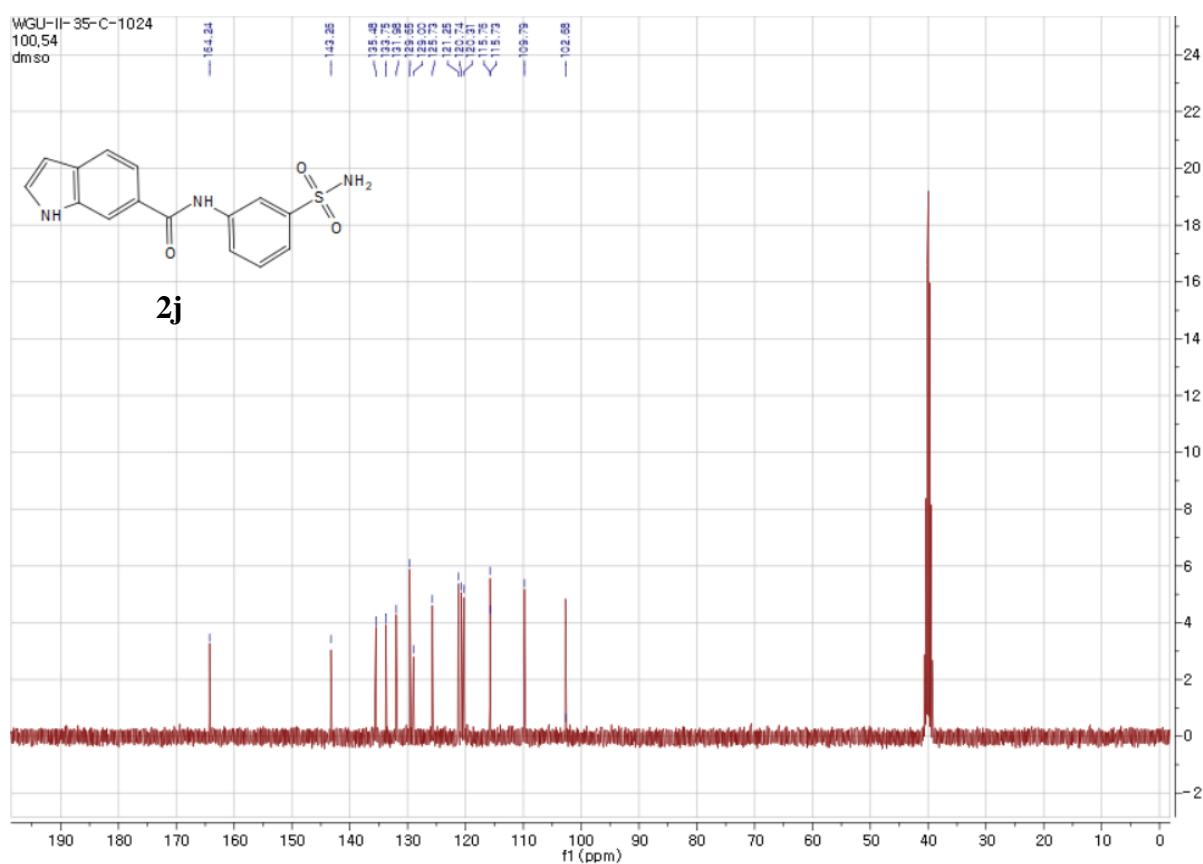
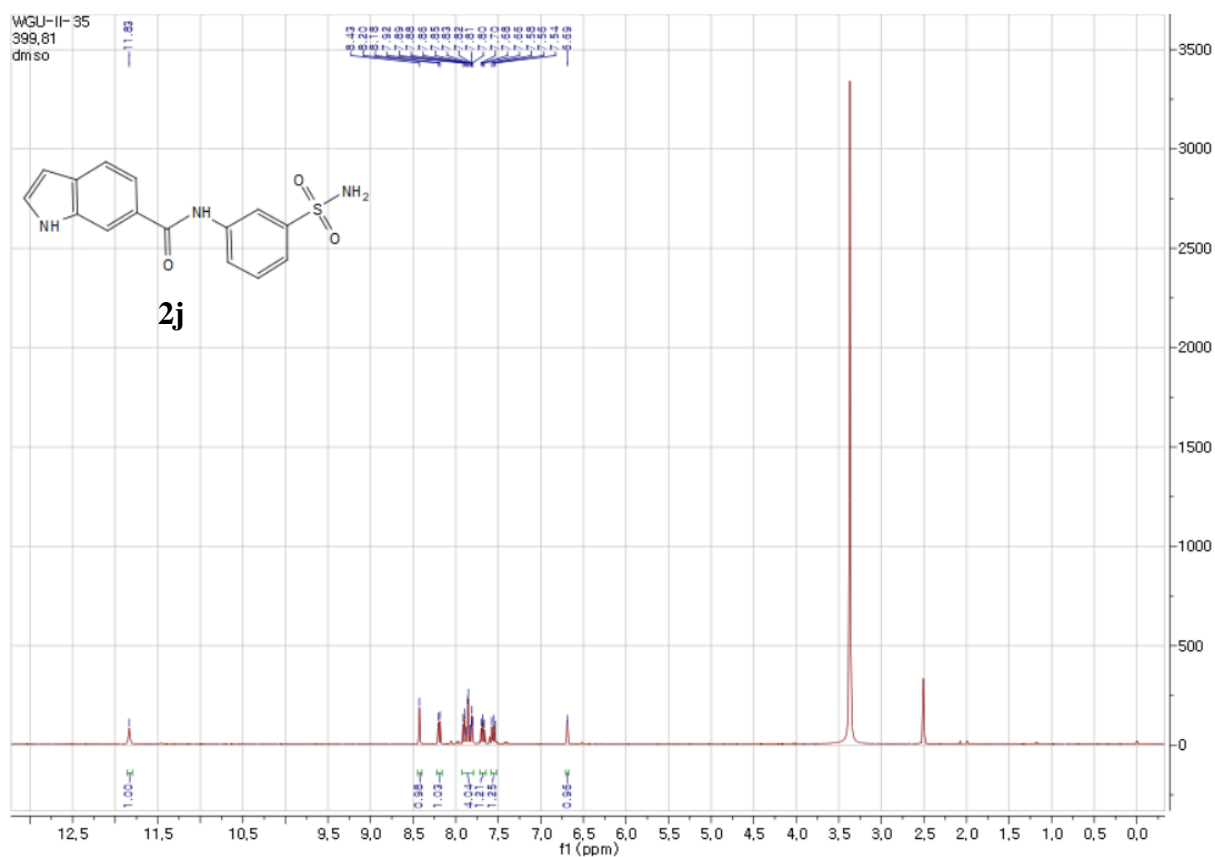


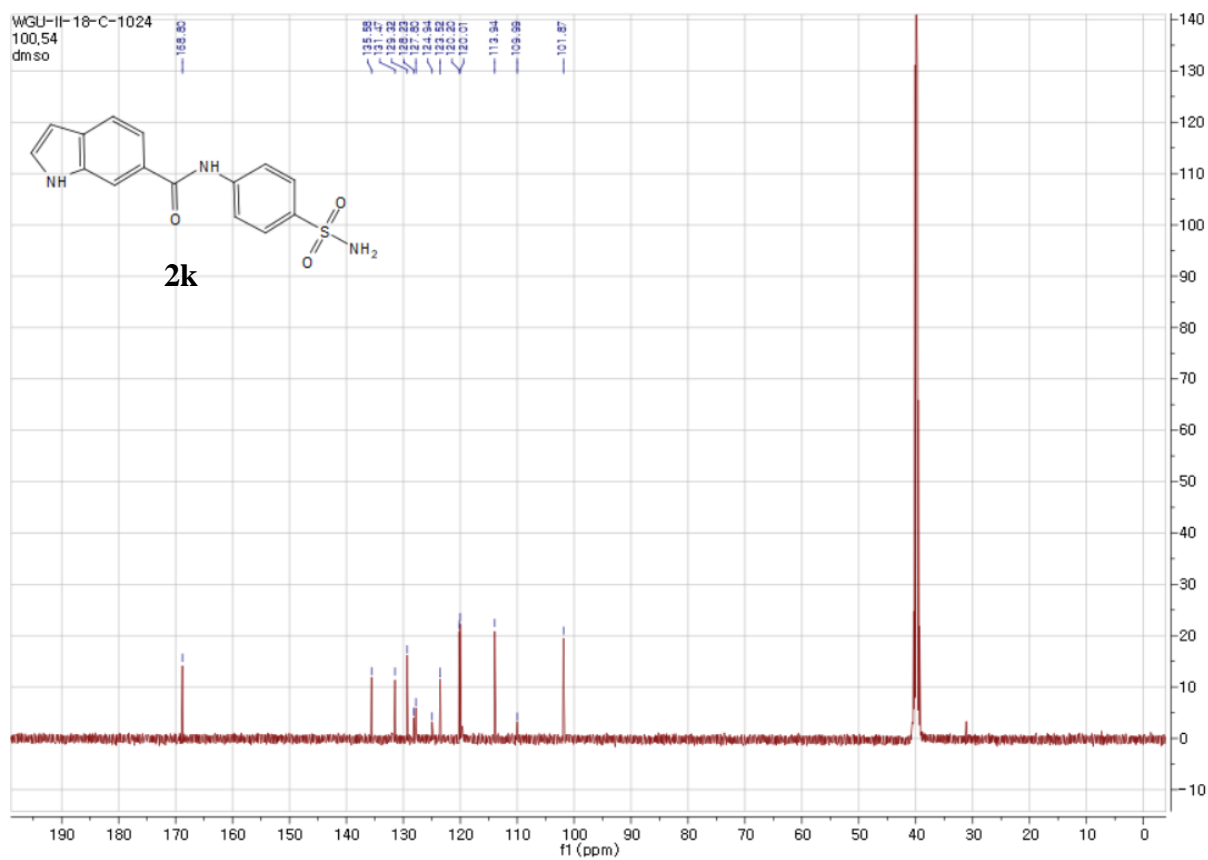
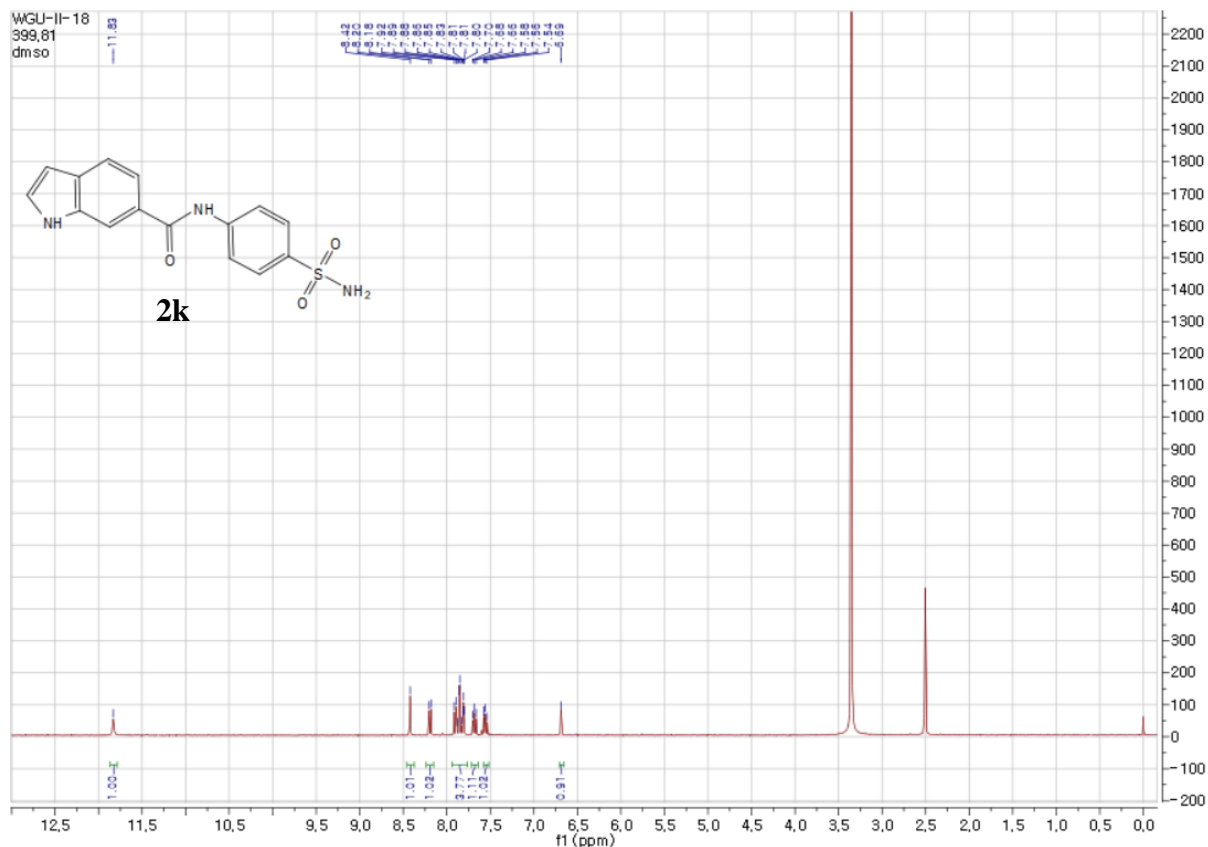


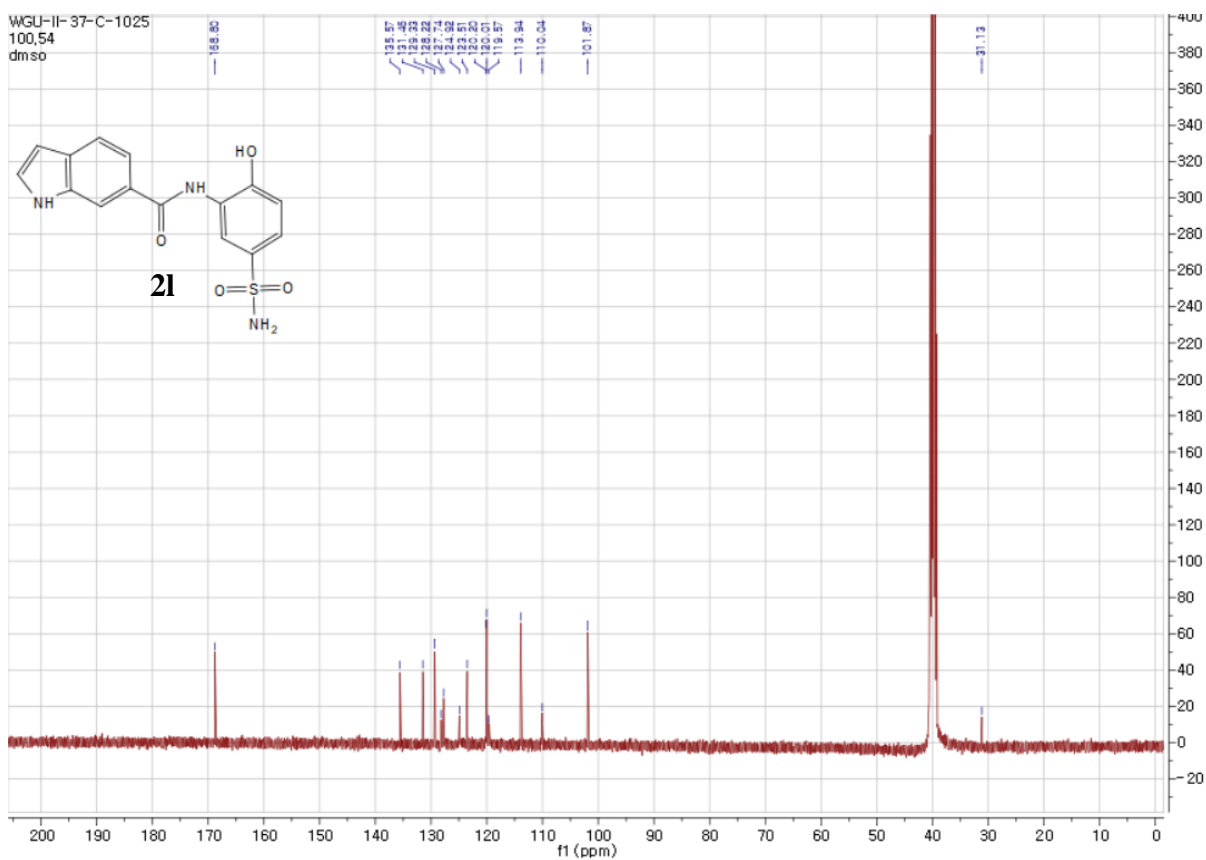
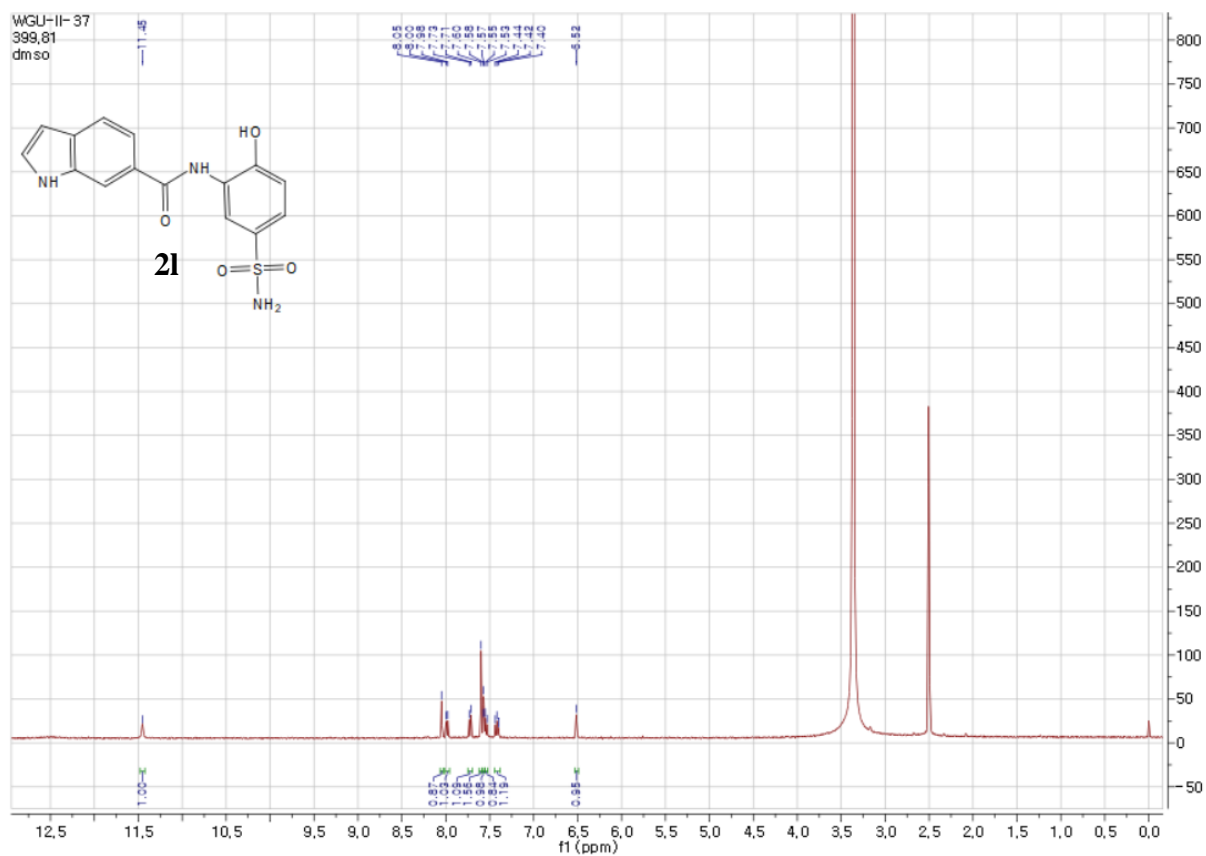


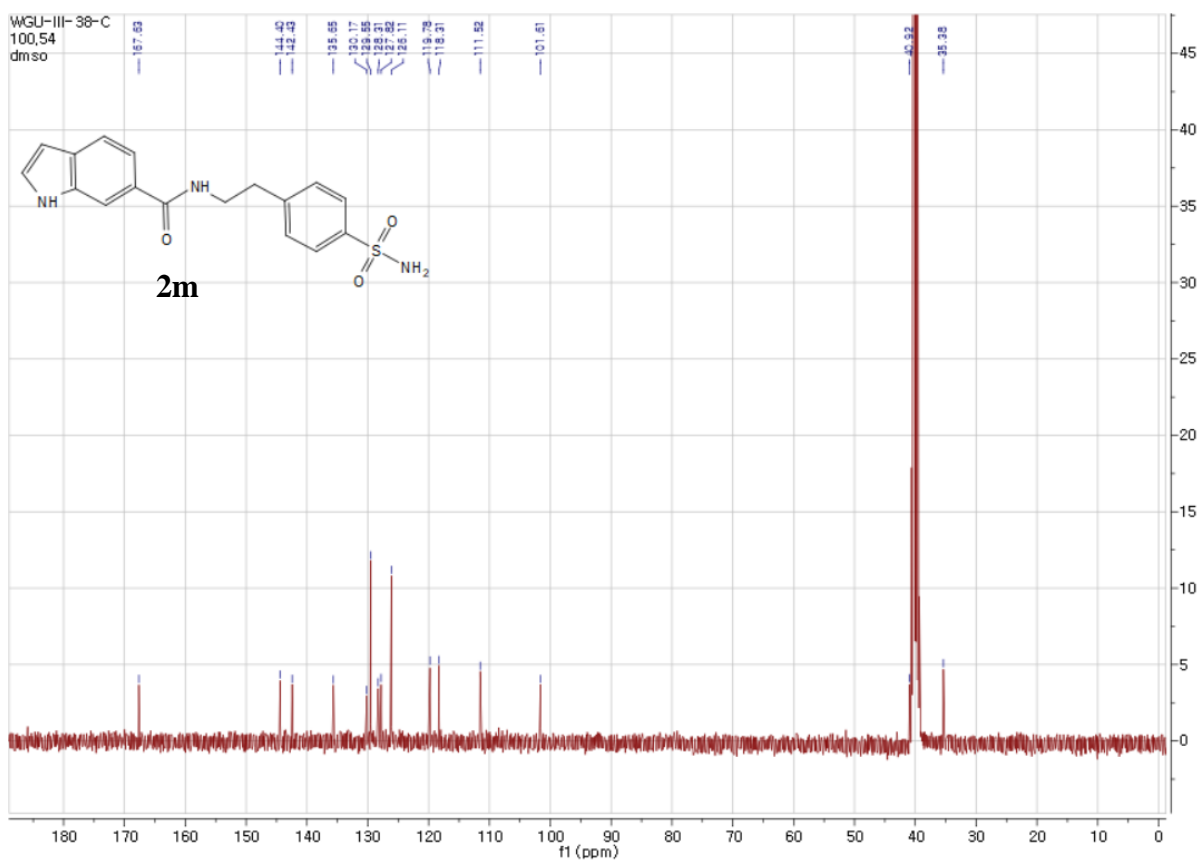
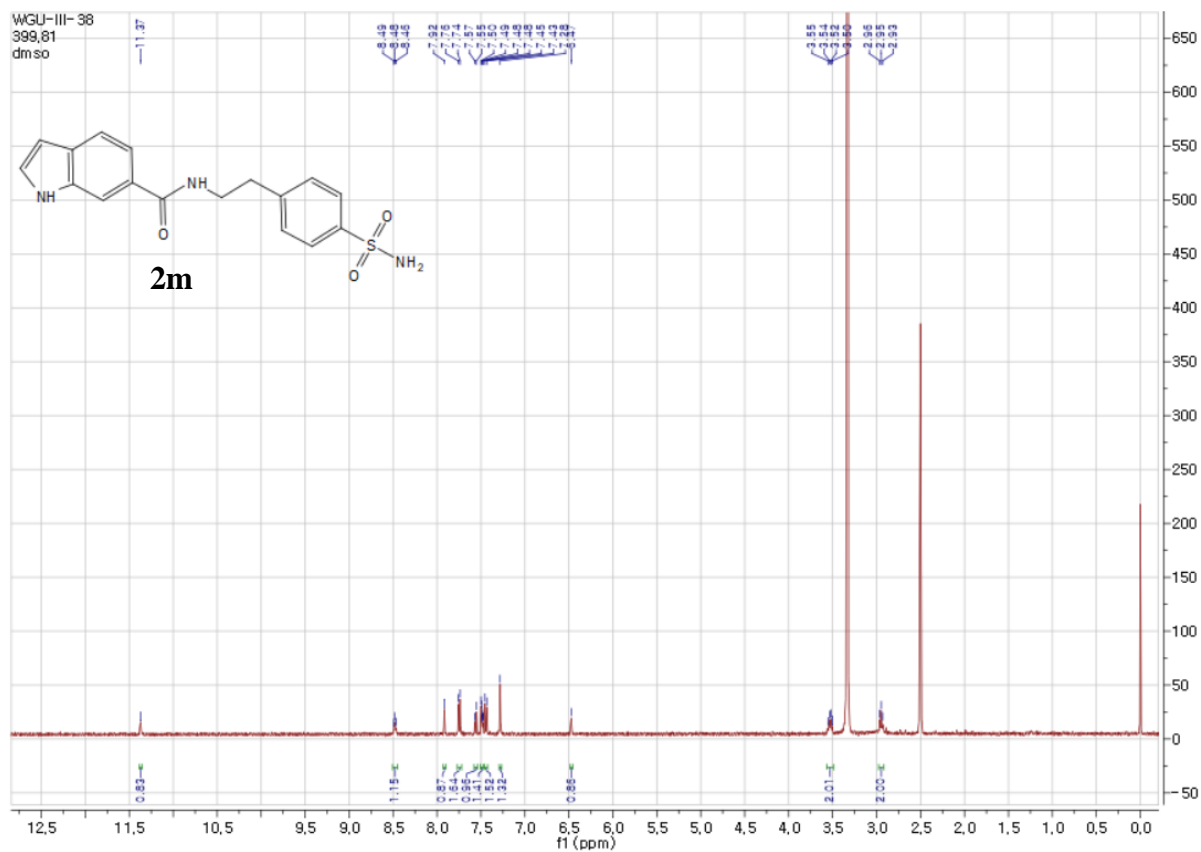


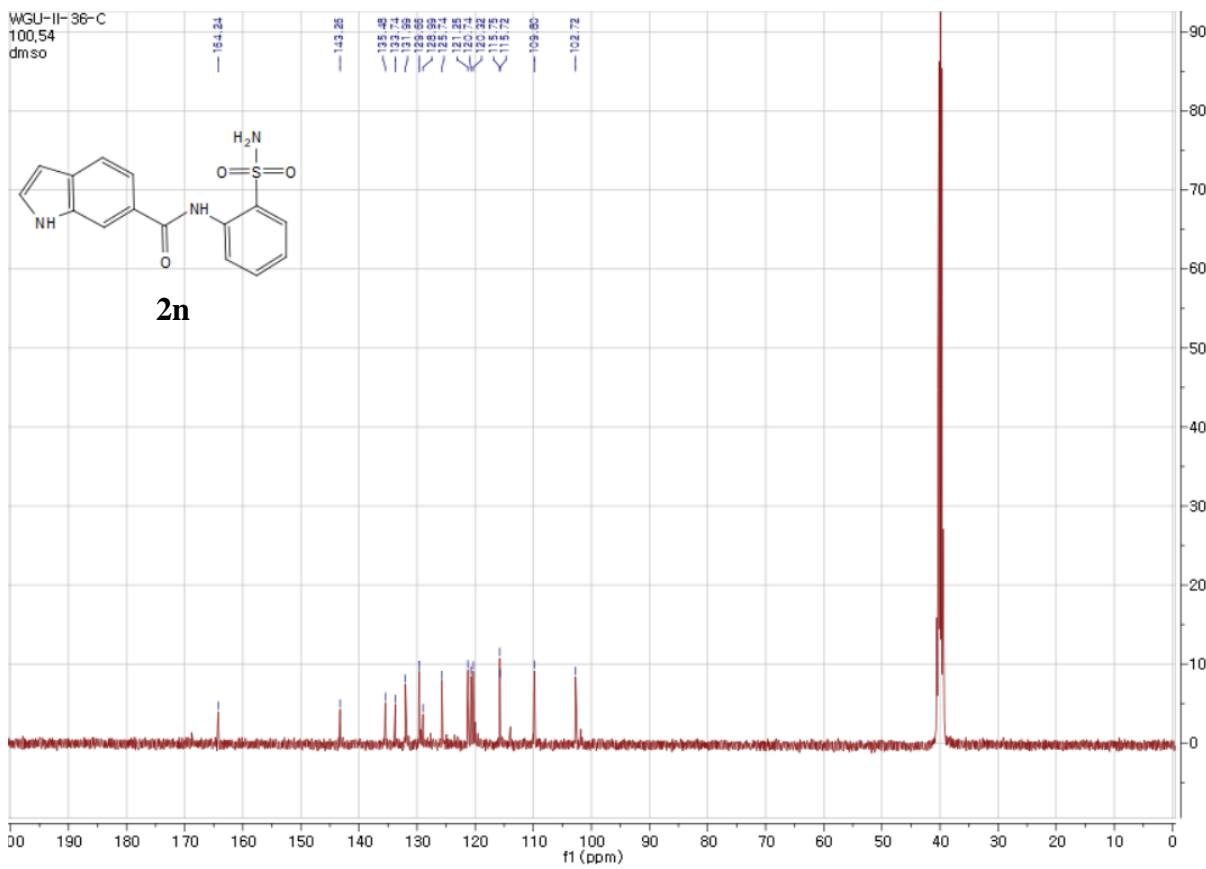
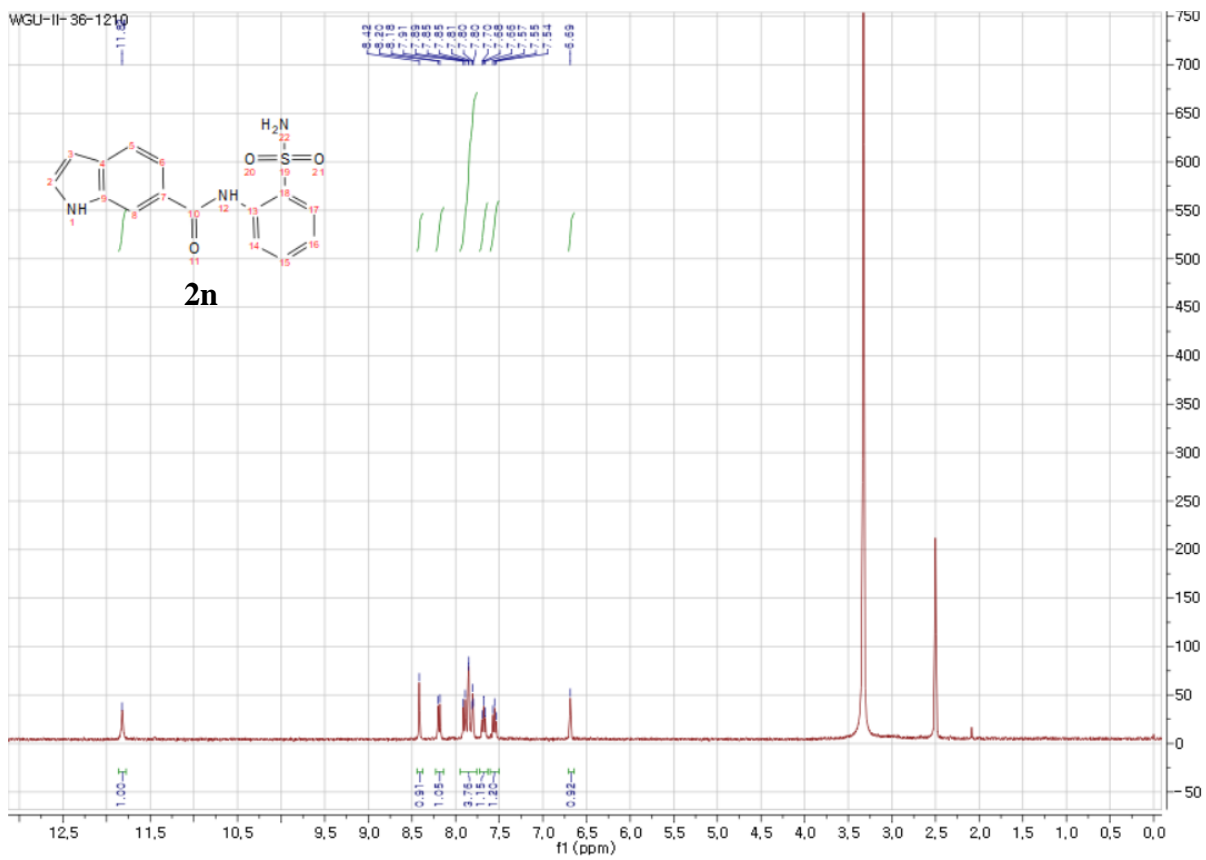






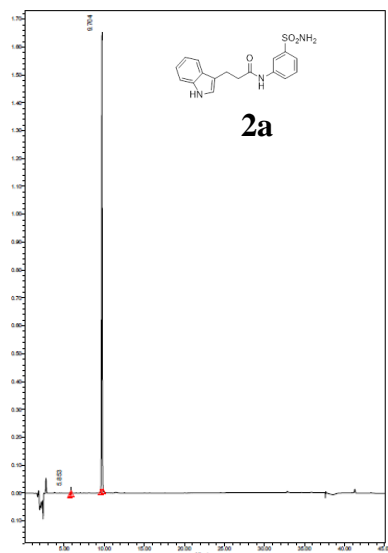




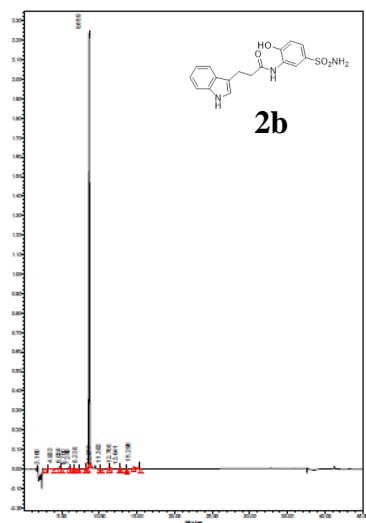


2. HPLC purity

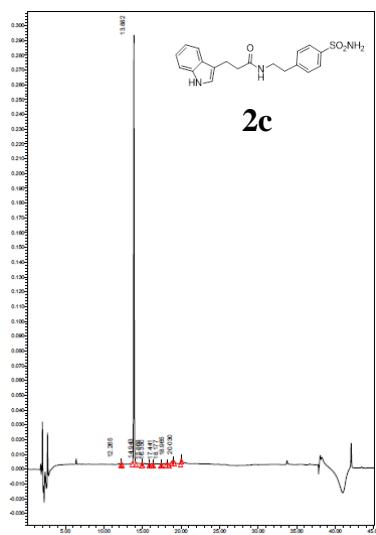
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1		5.853							21570	0.21	4841	bb	
2		9.704							10154012	99.79	1640978	bb	



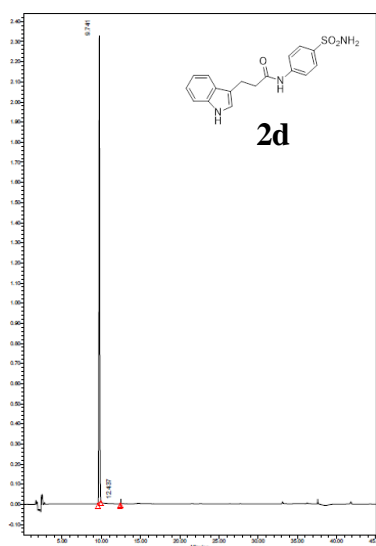
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2		4.933							48324	0.30	4938	bb	
3		6.038							18831	0.12	2398	bb	
4		6.700							1569	0.01	423	bb	
5		7.249							7081	0.04	1689	bb	
6		8.238							44044	0.28	8594	bb	
7		8.659							15369532	97.00	2242742	bb	
8		10.077							2482	0.02	311	bb	
9		11.383							40538	0.26	5556	bb	
10		12.766							17021	0.11	4020	bb	
11		13.641							1431	0.01	382	bb	
12		15.298							257785	1.63	15769	bb	



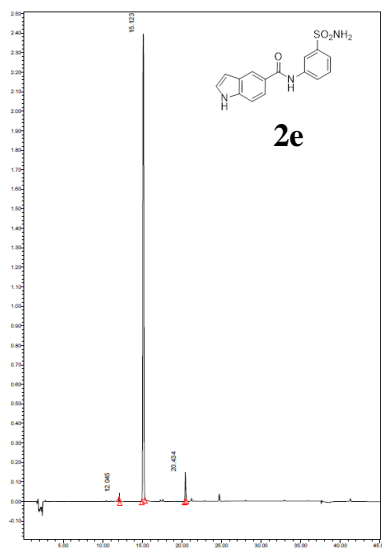
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1	12.265							909	0.06	253	bb		
2	13.882							1591817	99.00	286374	bb		
3	14.943							525	0.03	199	bb		
4	15.868							0	0.00	-0	bb		
5	16.350							376	0.02	87	bb		
6	17.441							628	0.04	145	bb		
7	18.177							880	0.05	-125	bb		
8	18.965							6813	0.42	563	bb		
9	20.030							5964	0.37	1217	bb		



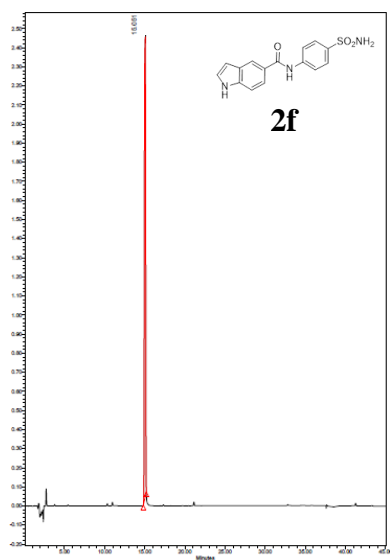
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1	9.741							16354019	99.98	2322914	bb	
2	12.437							2751	0.02	812	bb	



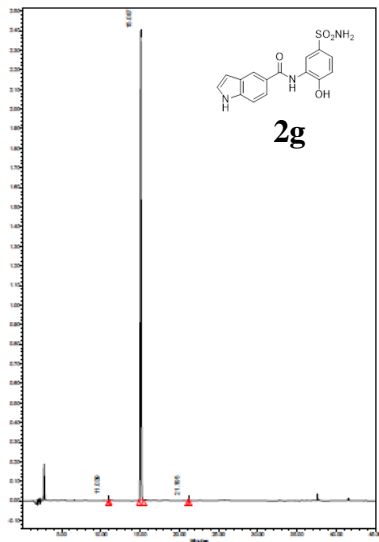
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1		12.045							13607	0.06	2636	bb	
2		15.123							23033597	96.78	2409116	bb	
3		20.434							752736	3.16	120461	bb	



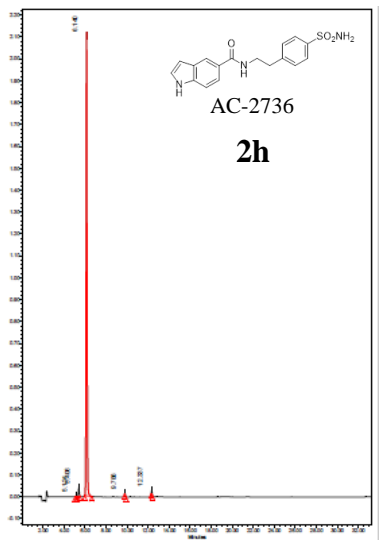
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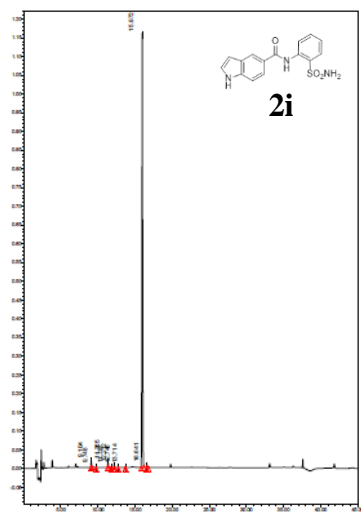
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1	11.039							40642	0.21	7378	bb	
2	15.087							19368165	99.62	2407029	bb	
3	21.195							33647	0.17	5326	bb	



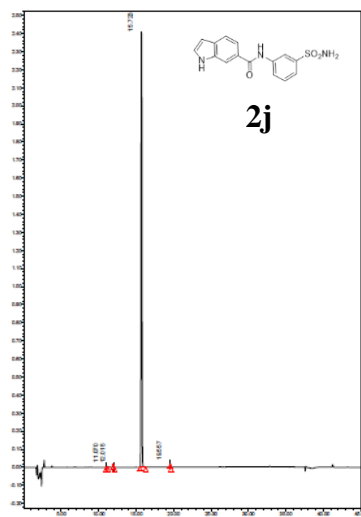
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1	5.124							14862	0.10	3240	bb	
2	5.406							224896	1.56	39342	bb	
3	6.140							14058338	97.68	2113810	bb	
4	9.788							22932	0.16	6528	bb	
5	12.337							70658	0.49	17520	bb	



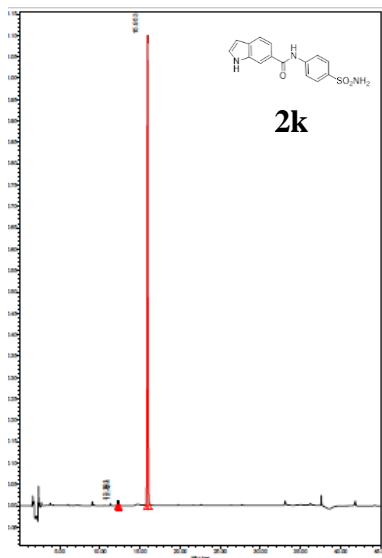
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1		9.104							54155	0.66	12032	bb	
2		9.748							764	0.01	240	bb	
3		11.355							52092	0.64	10110	bb	
4		11.797							1827	0.02	501	bb	
5		12.212							13261	0.16	2847	bb	
6		12.748							61	0.00	61	bb	
7		13.714							1949	0.02	617	bb	
8		15.972							8014764	98.02	1163330	bb	
9		16.641							37974	0.46	4672	bb	



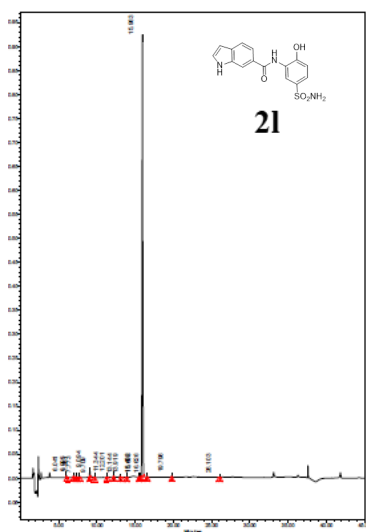
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1		11.070							29879	0.15	4607	bb	
2		12.015							25660	0.13	4915	bb	
3		15.723							20068158	99.67	2419202	bb	
4		19.557							10109	0.05	1649	bb	



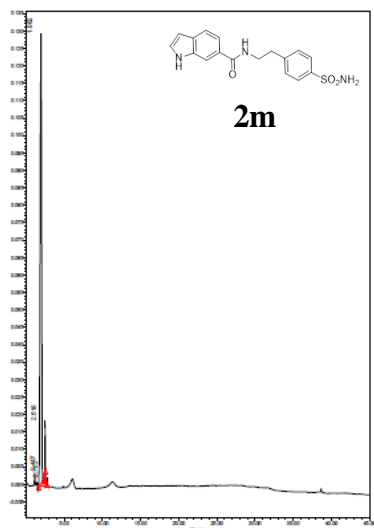
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1		12.191							1763	0.02	705	bb	
2		12.434							6031	0.08	1412	bb	
3		15.953							7503939	99.90	1092658	bb	



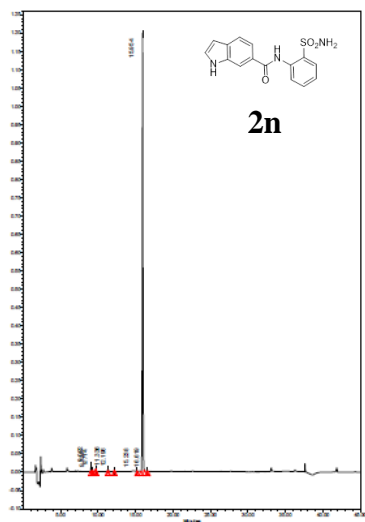
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1		6.041							11743	0.18	2638	bb	
2		6.995							3264	0.05	681	bb	
3		7.281							8370	0.13	1922	bb	
4		7.773							11908	0.19	1654	bb	
5		9.094							50125	0.78	10364	bb	
6		9.709							7152	0.11	1110	bb	
7		11.344							14838	0.23	2412	bb	
8		12.201							2902	0.05	849	bb	
9		13.144							7235	0.11	-585	bb	
10		13.919							269	0.00	-56	bb	
11		15.492							27	0.00	-14	bb	
12		15.608							0	0.00	0	bb	
13		15.963							6272192	98.03	918650	bb	



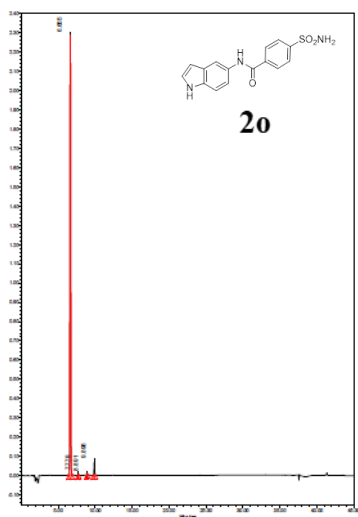
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1	1.982							1737170	96.73	129132	bb		
2	2.407							1179	0.07	597	bb		
3	2.518							55830	3.11	13988	bb		
4	2.752							1686	0.09	558	bb		



Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1	9.092							76112	0.92	13853	bb	
2	9.338							307	0.00	192	bb	
3	9.714							6898	0.08	1735	bb	
4	11.336							18297	0.22	3916	bb	
5	12.196							2351	0.03	702	bb	
6	15.238							34	0.00	34	bb	
7	15.954							8184772	98.70	1190180	bb	
8	16.619							4039	0.05	793	bb	



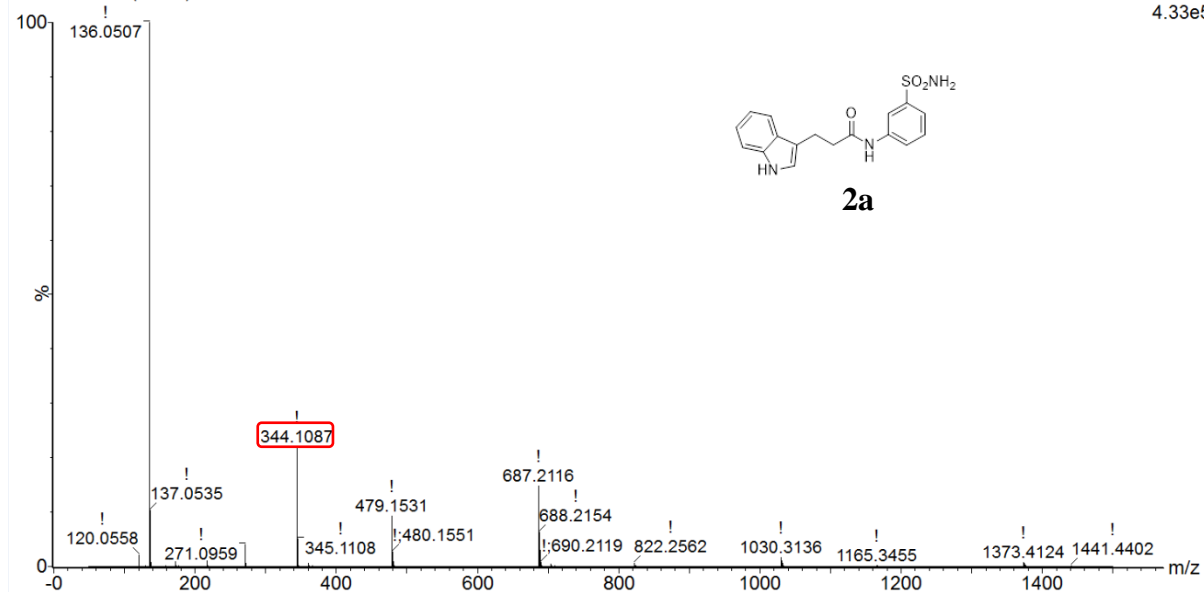
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1		6.655							16039540	97.38	2313113	bb	
2		7.778							9441	0.06	1850	bb	
3		8.891							6264	0.04	-1087	bb	
4		9.898							415866	2.52	66089	bb	



3. HRMS data

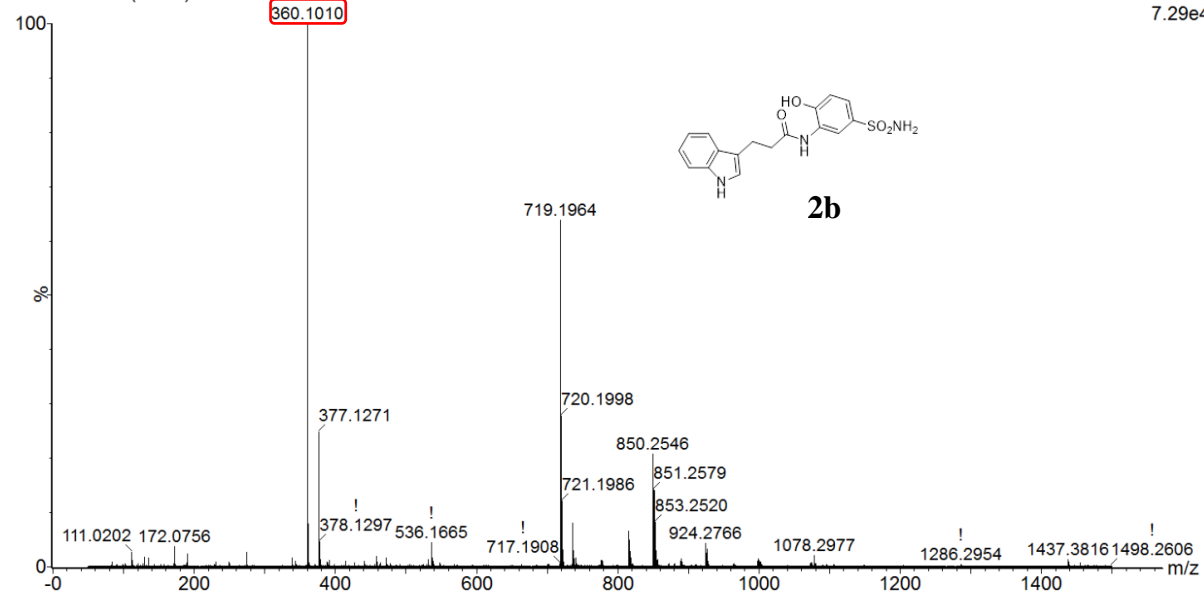
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1: TOF MS ES+
4.33e5



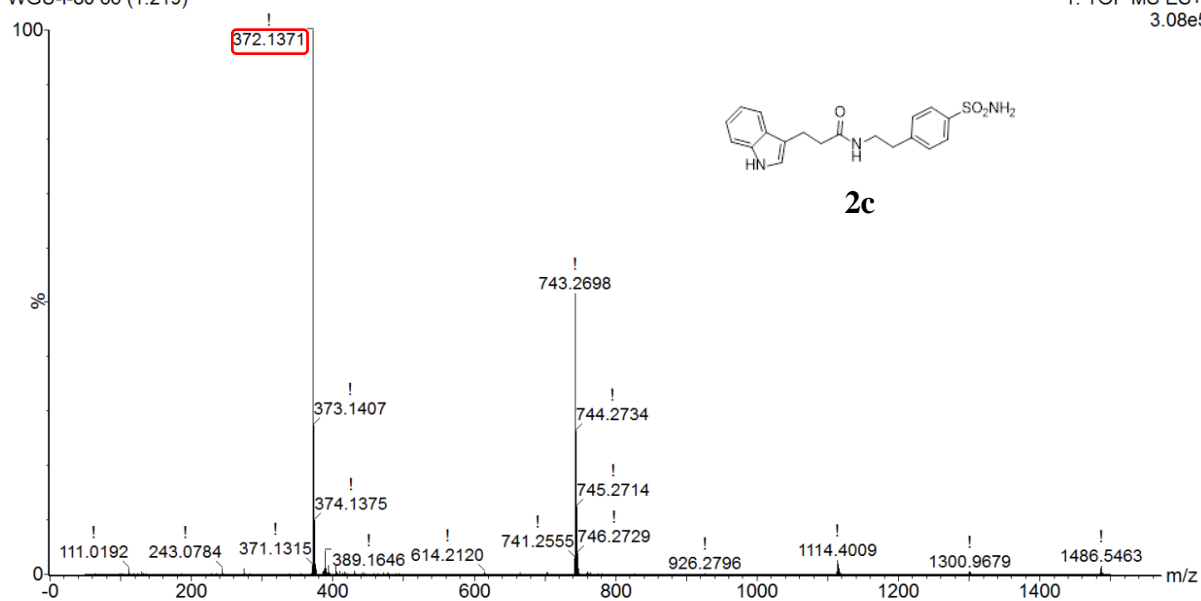
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1: TOF MS ES+
7.29e4



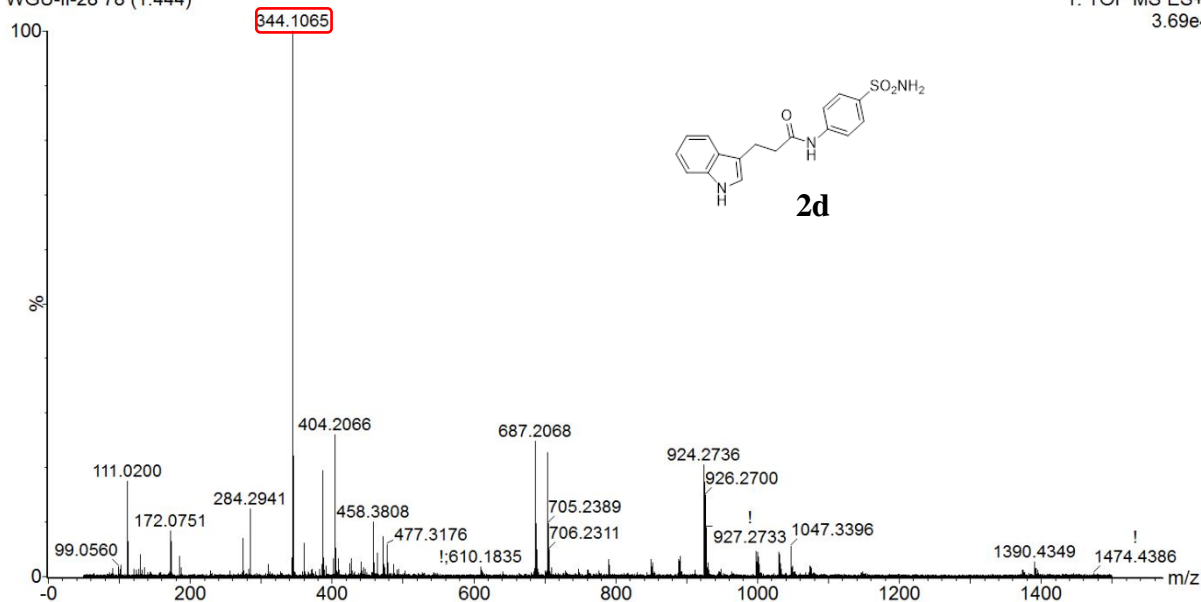
WGU-I-80 66 (1.219)

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3.08e5

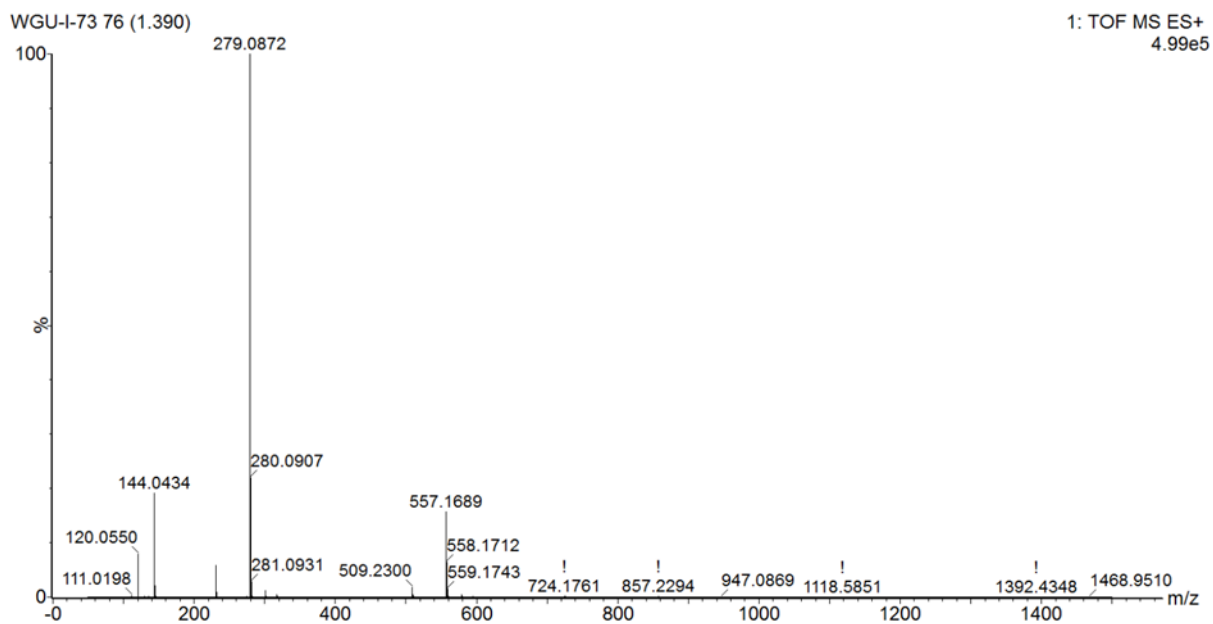


WGU-II-28 78 (1.444)

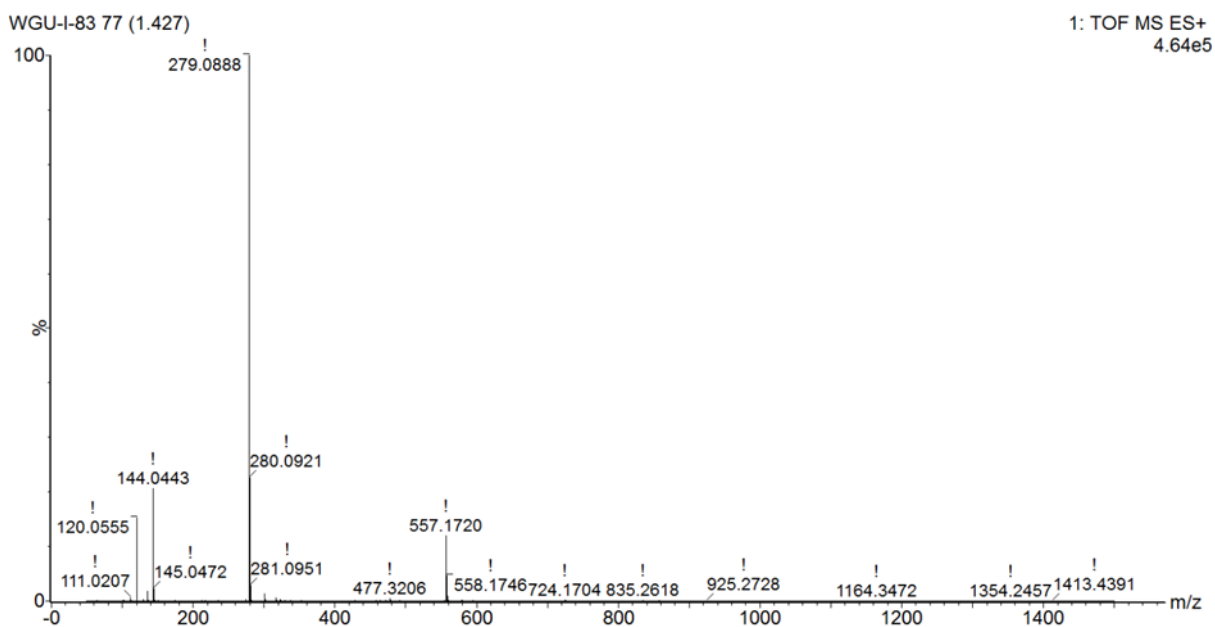
1: TOF MS ES+
3.69e4



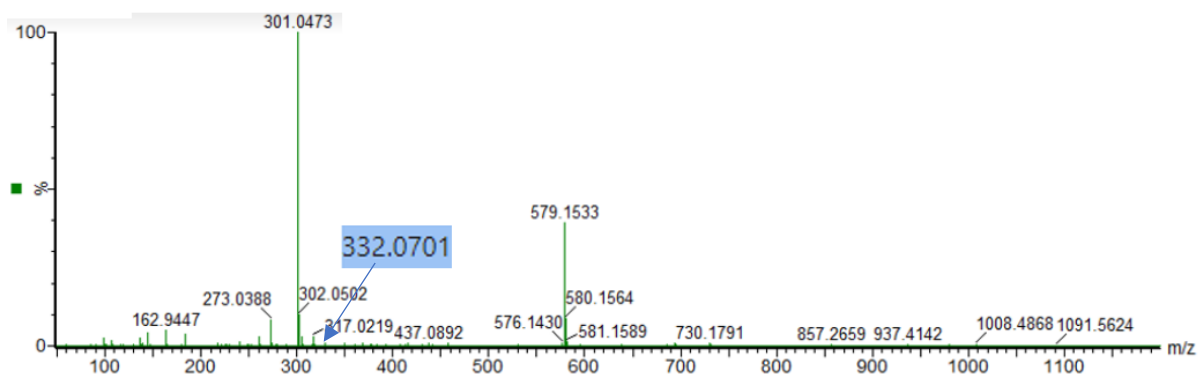
Compound 2e (Fragmentation)



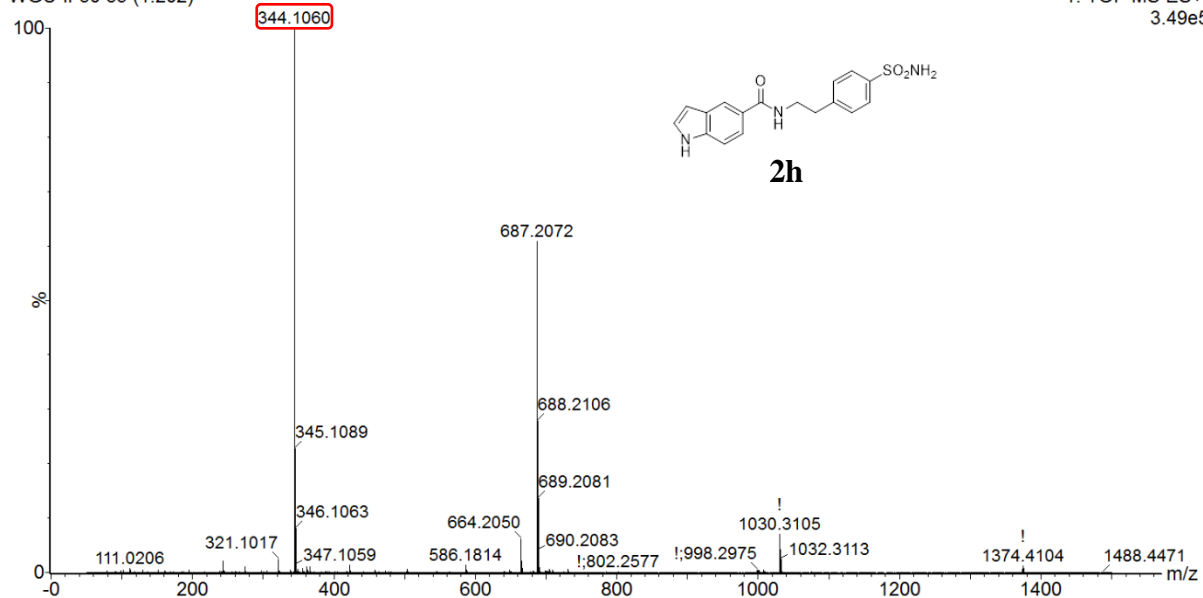
Compound 2f (Fragmentation)



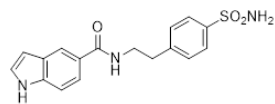
Compound 2g



WGU-II-50 65 (1.202)

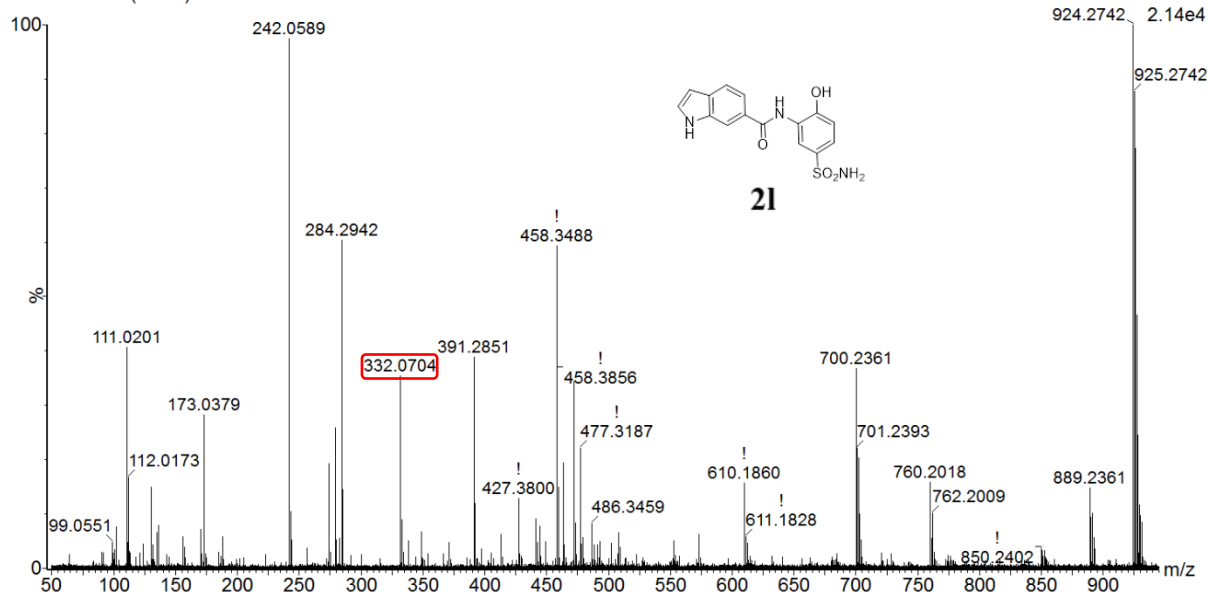


1: TOF MS ES+
3.49e5

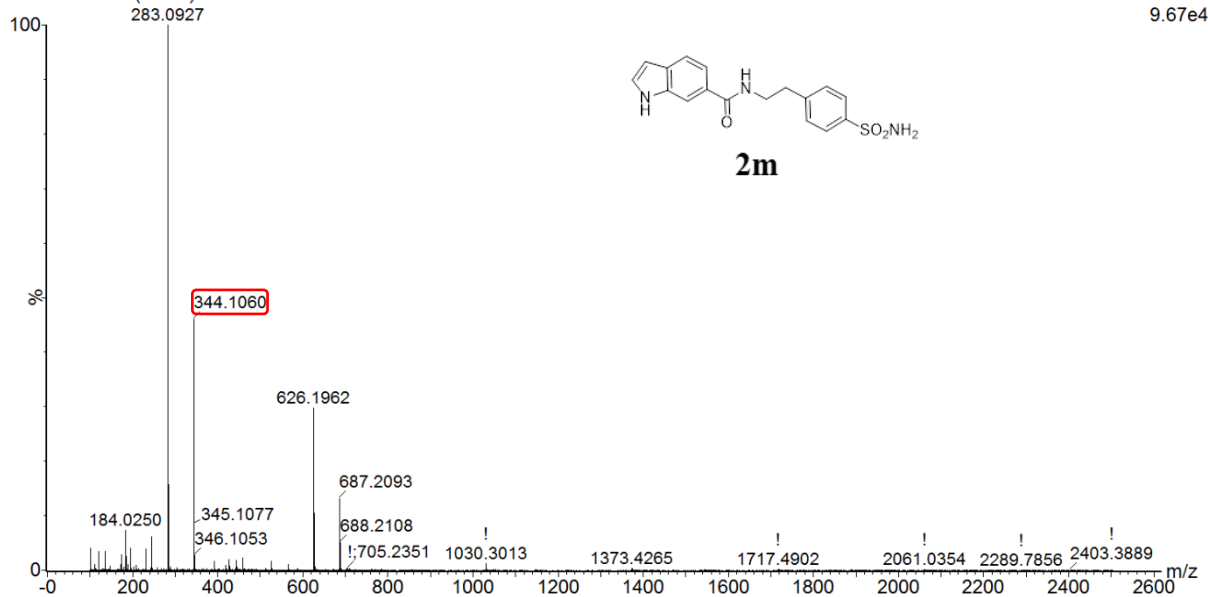


2h

WGU-II-37 68 (1.253)

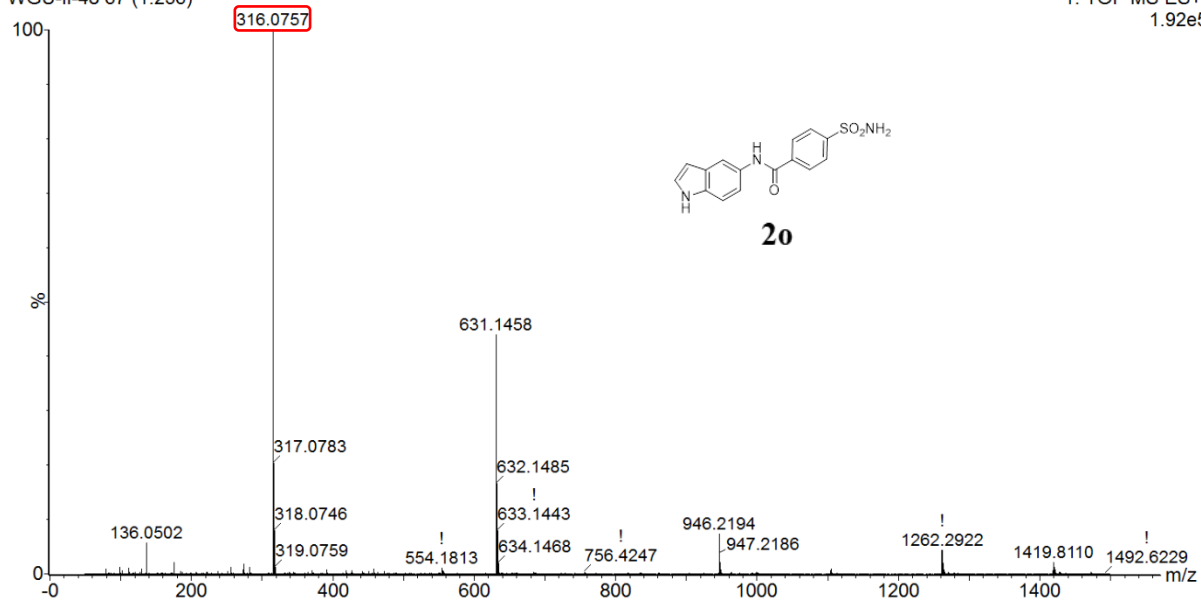


WGU-III-38 76 (1.344)



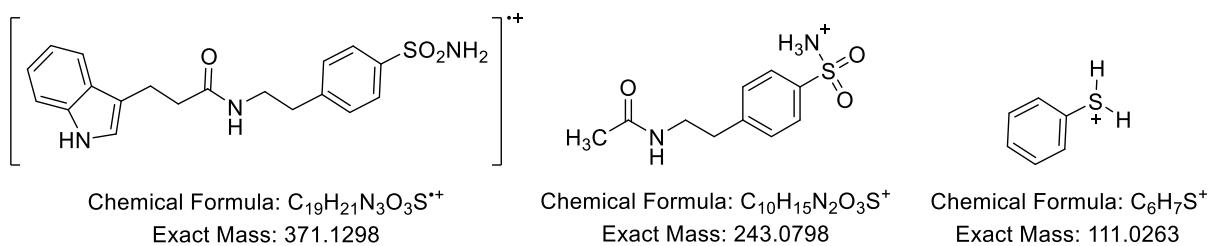
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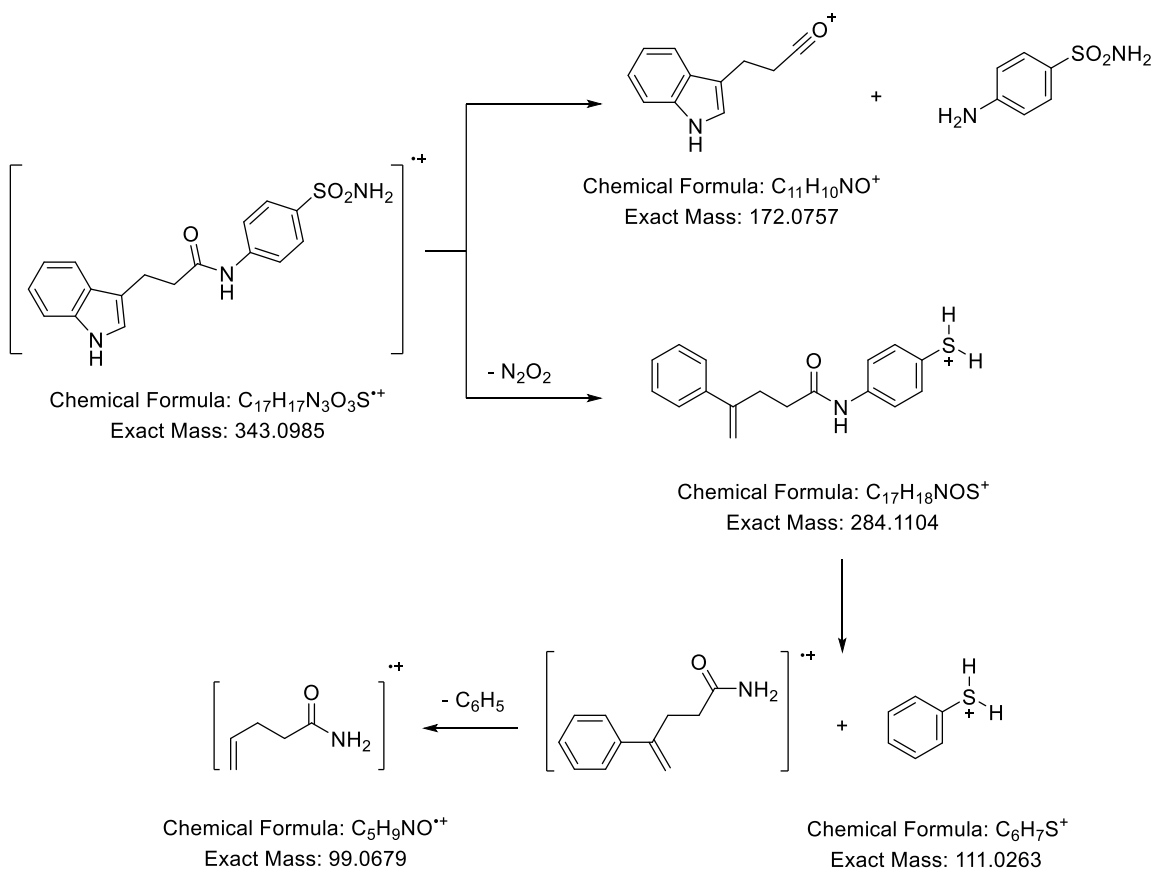


4. Interpretation of HRMS:

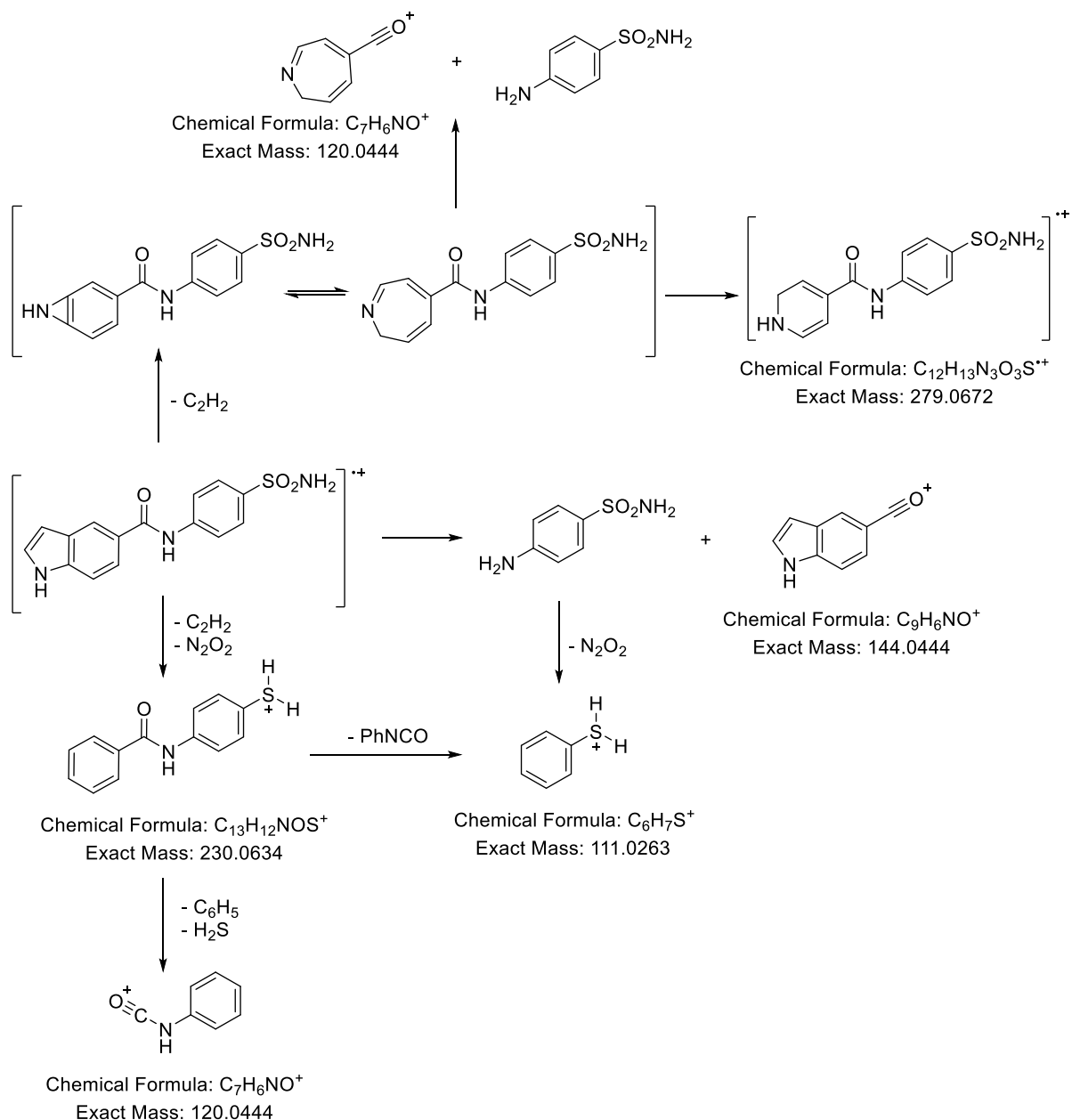
Compound 2c:



Compound 2d:



Compounds 2e and 2f:



Compound 2h:

