

# 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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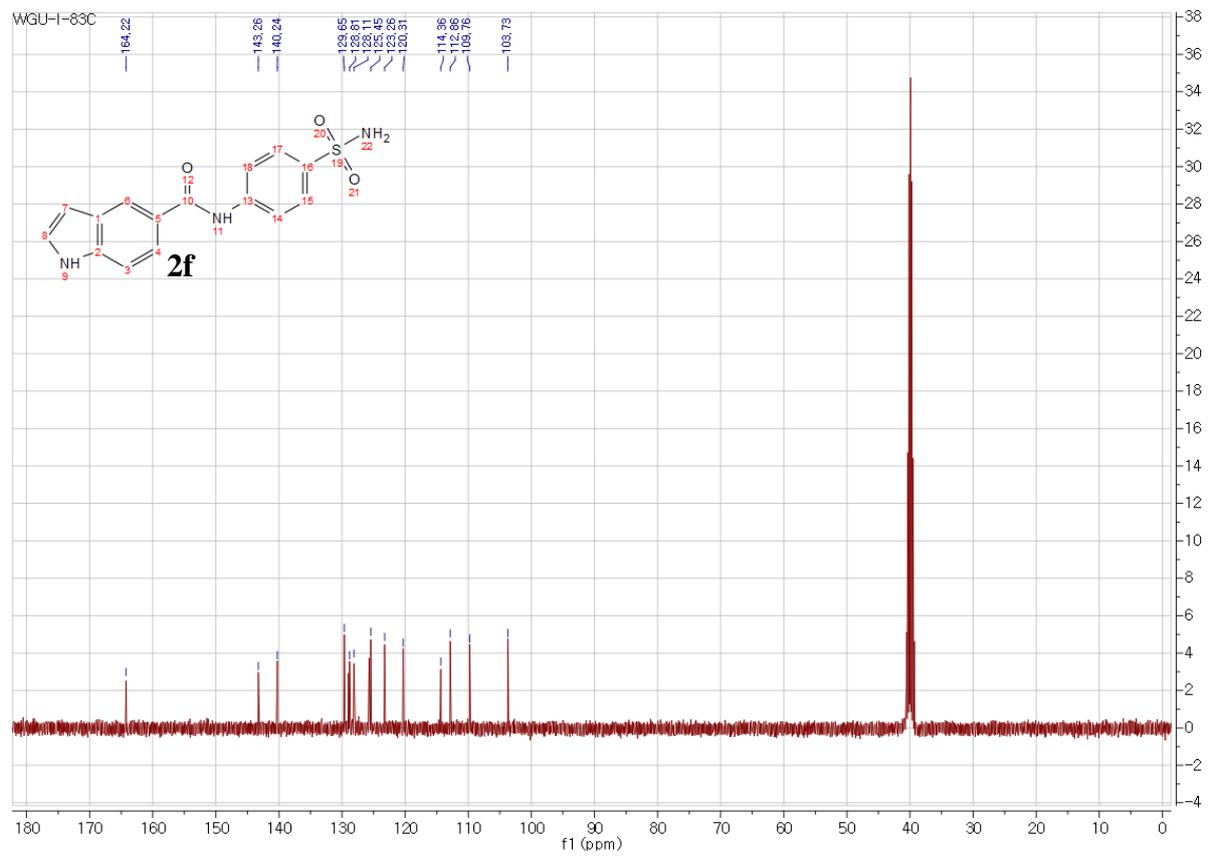
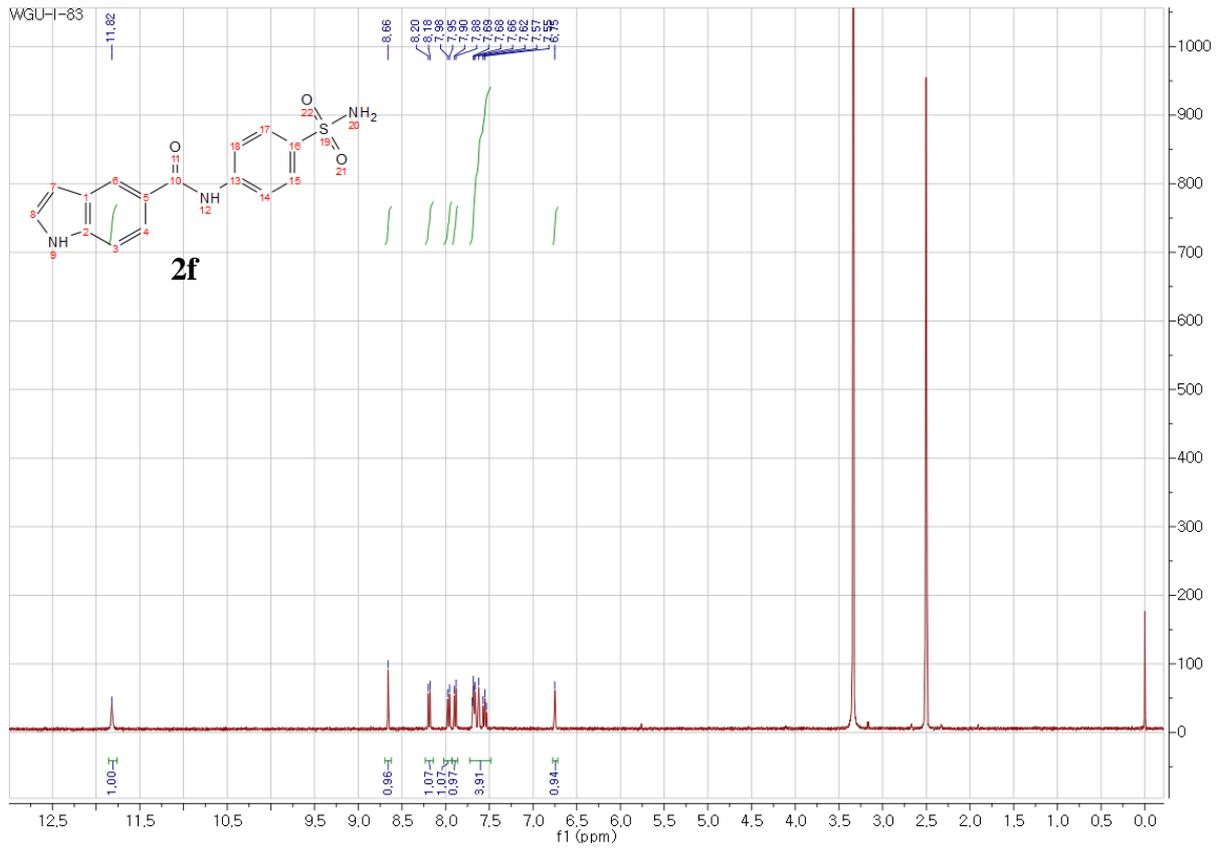




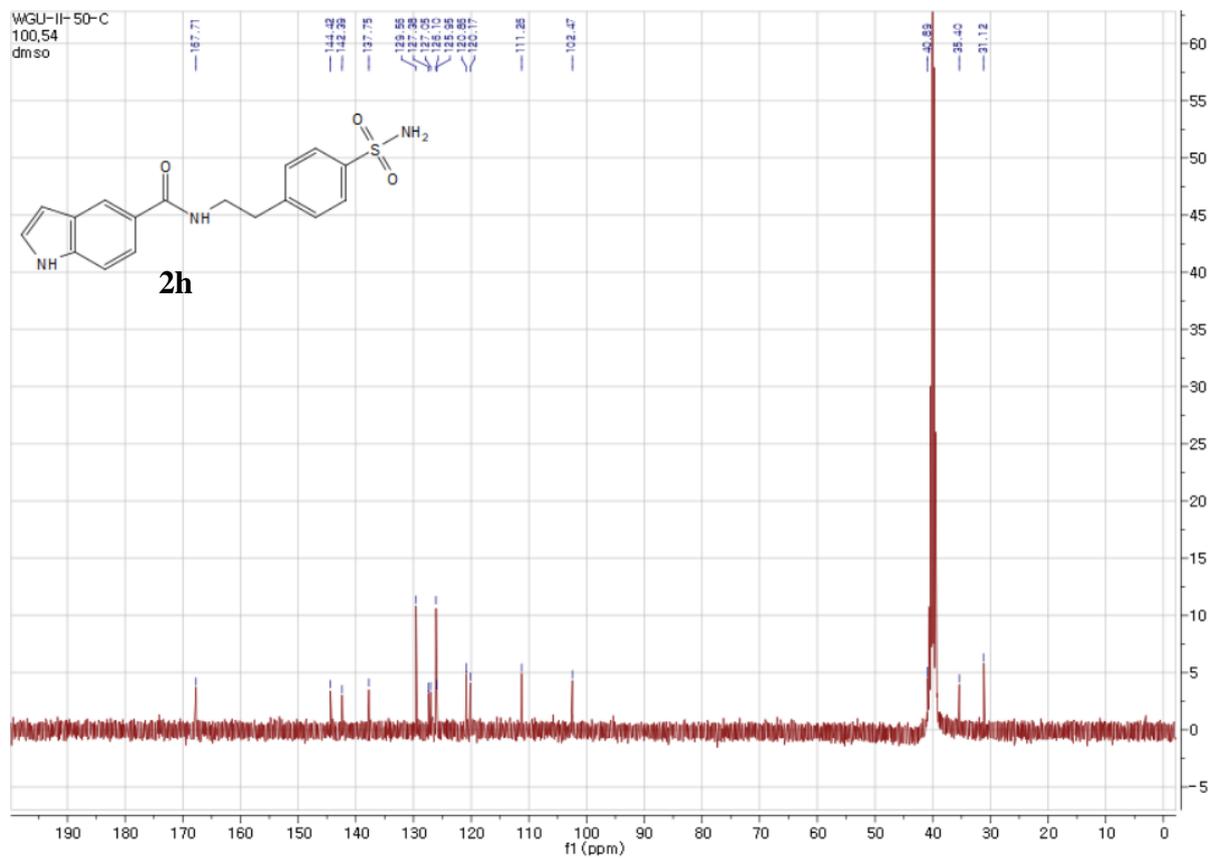
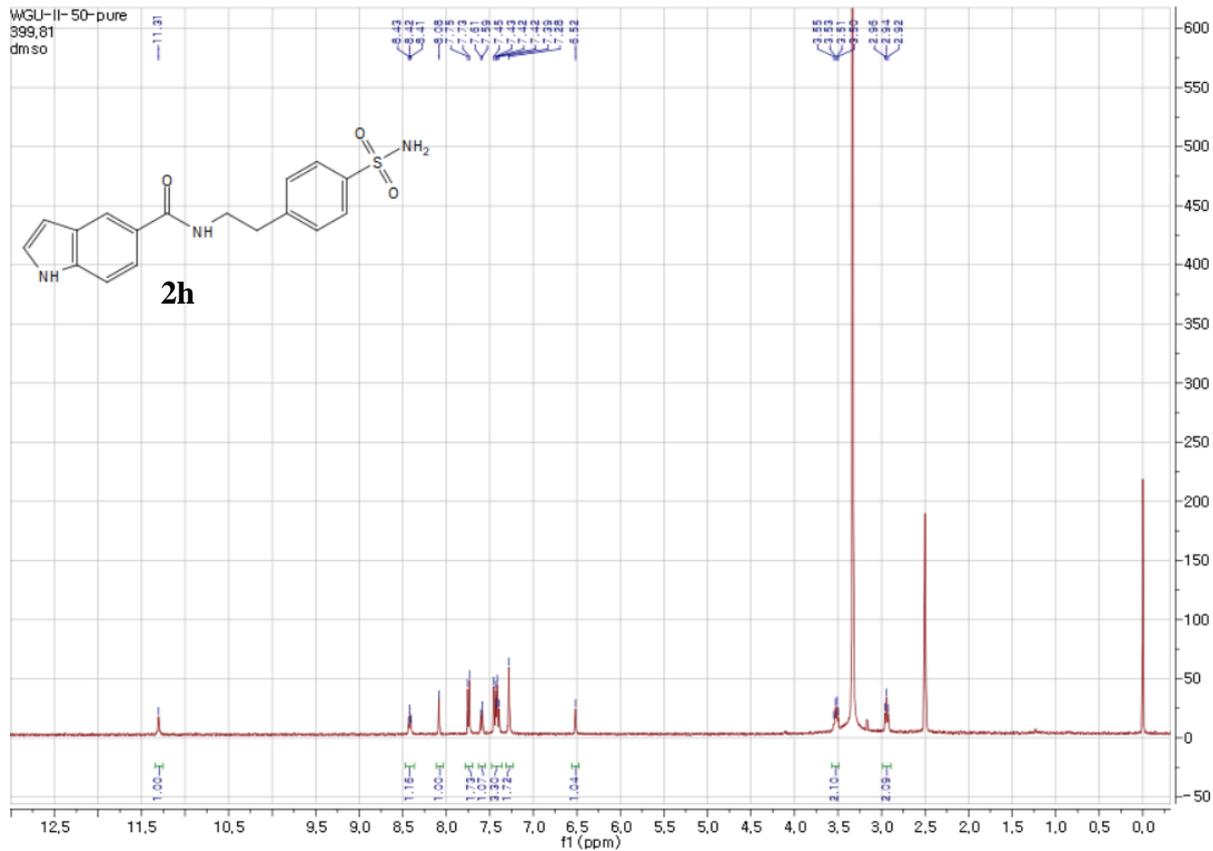




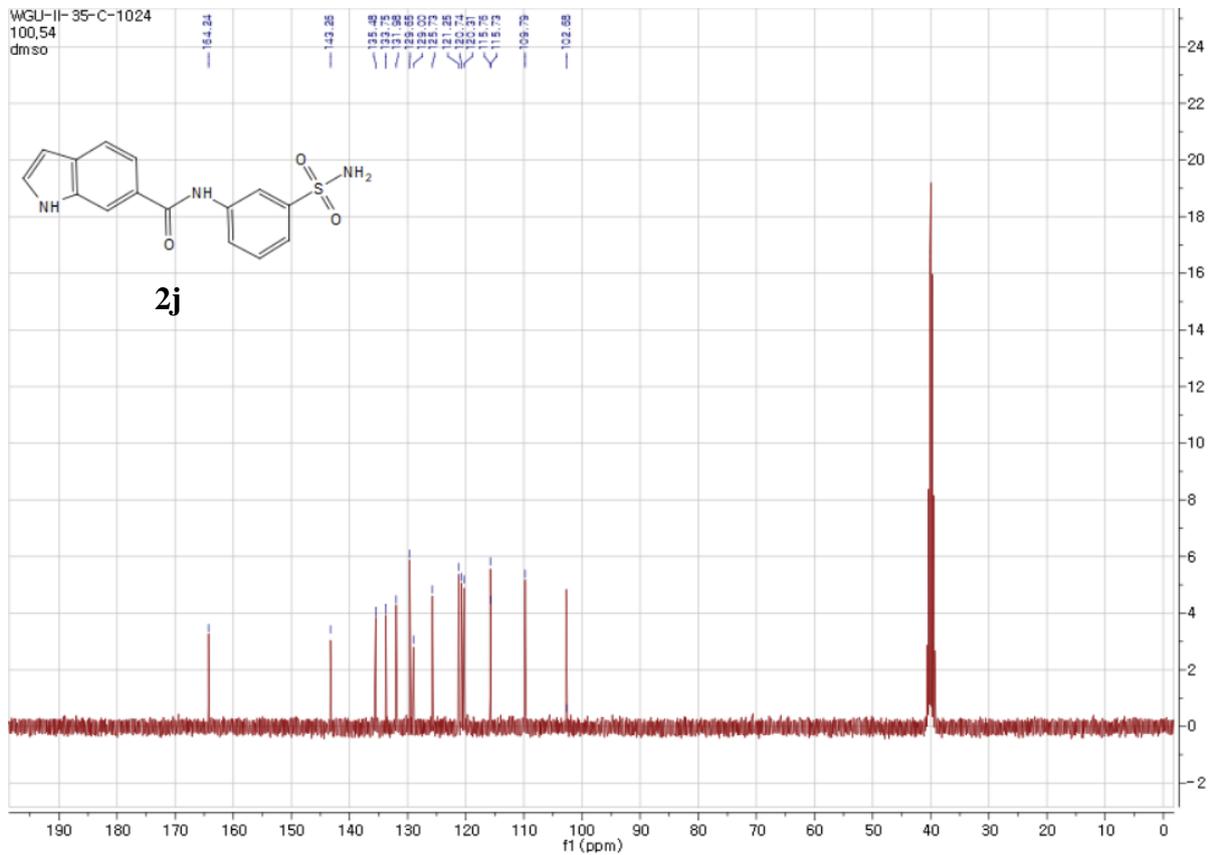
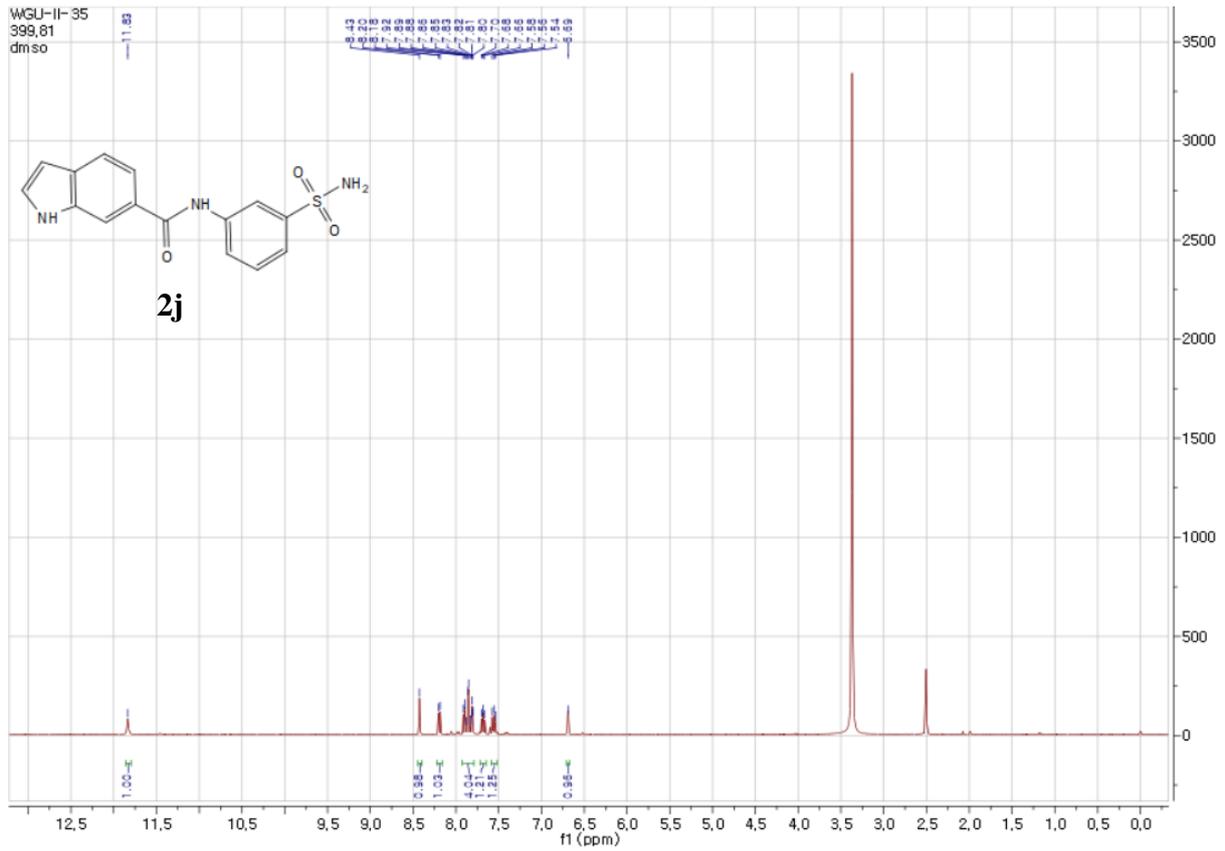


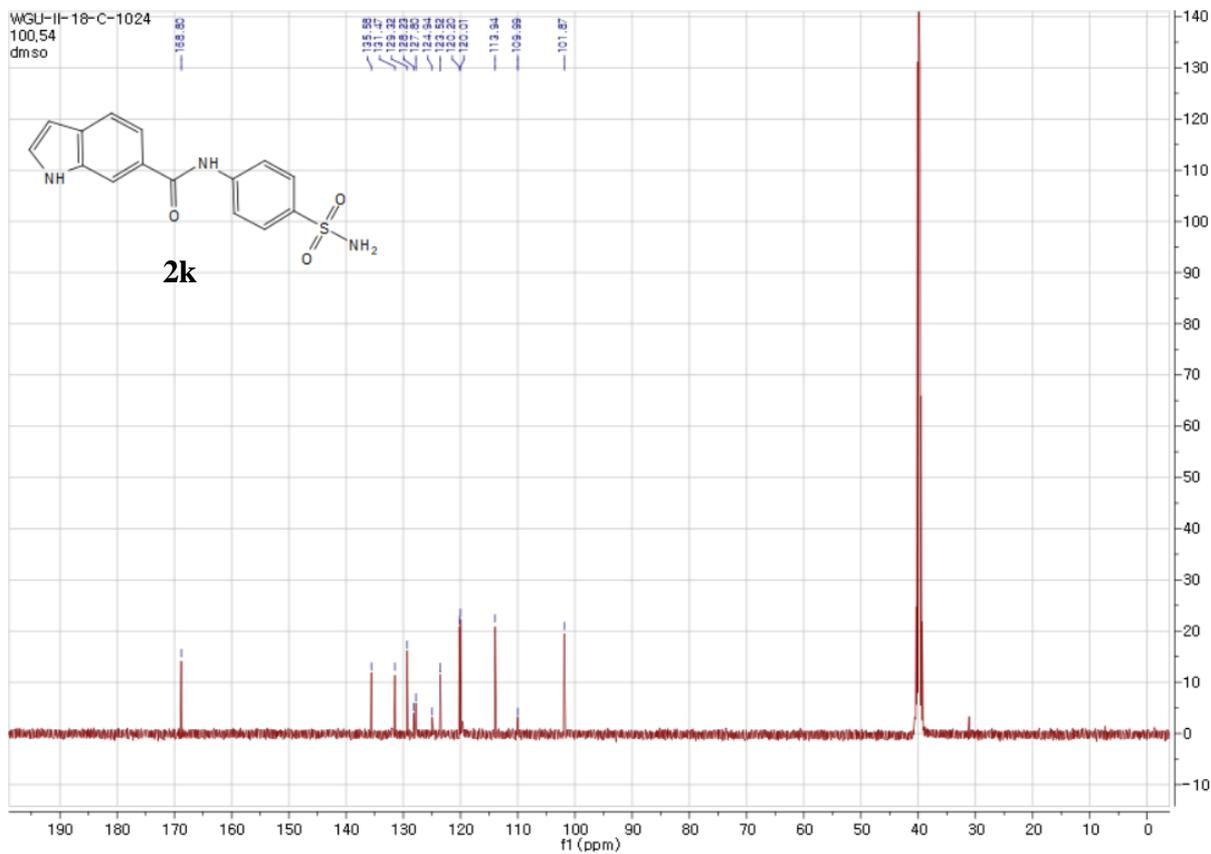
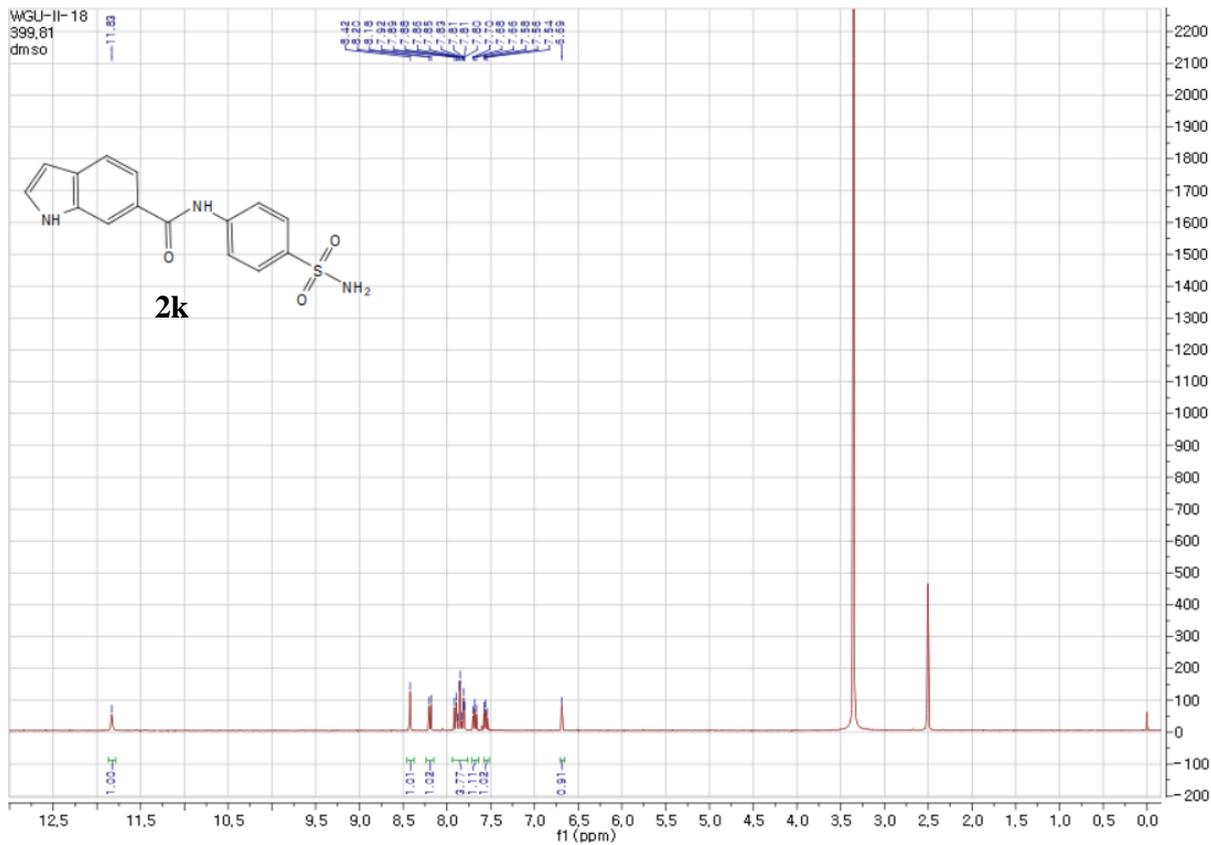


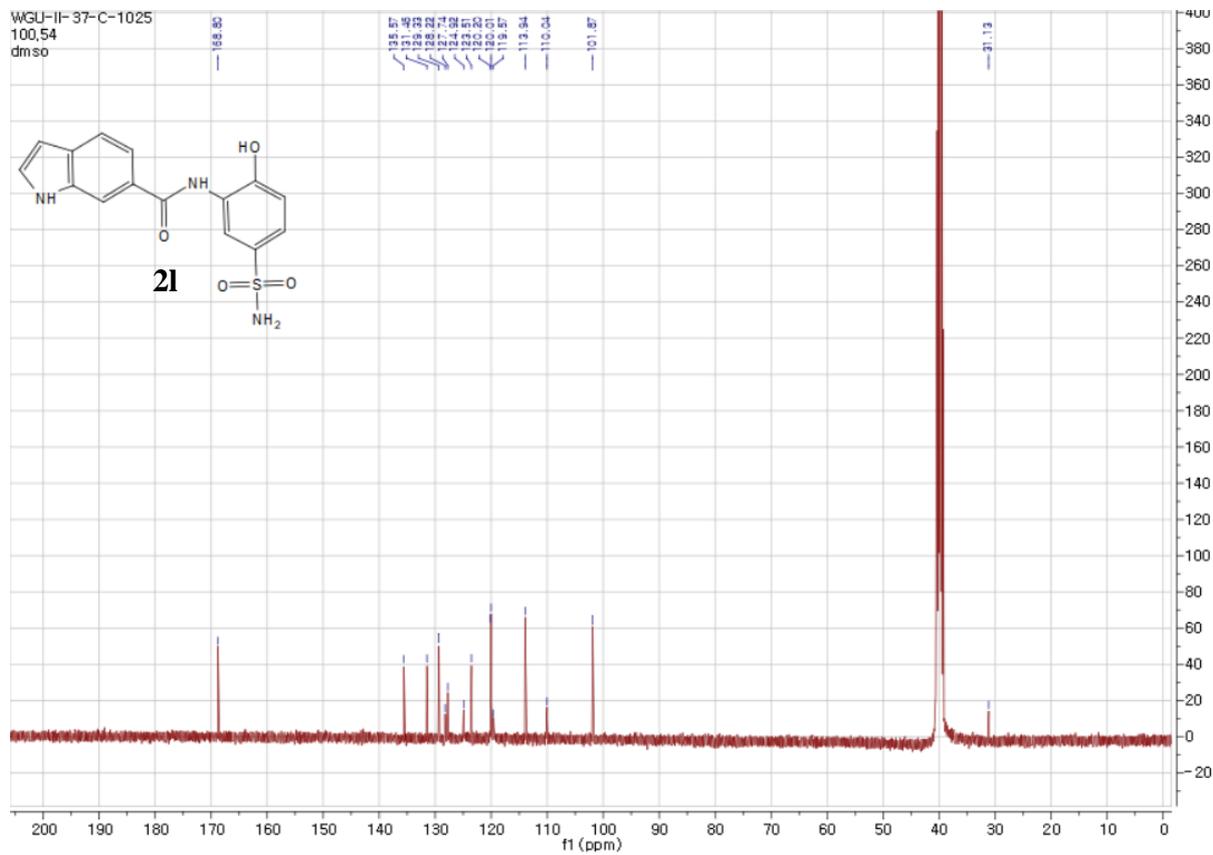
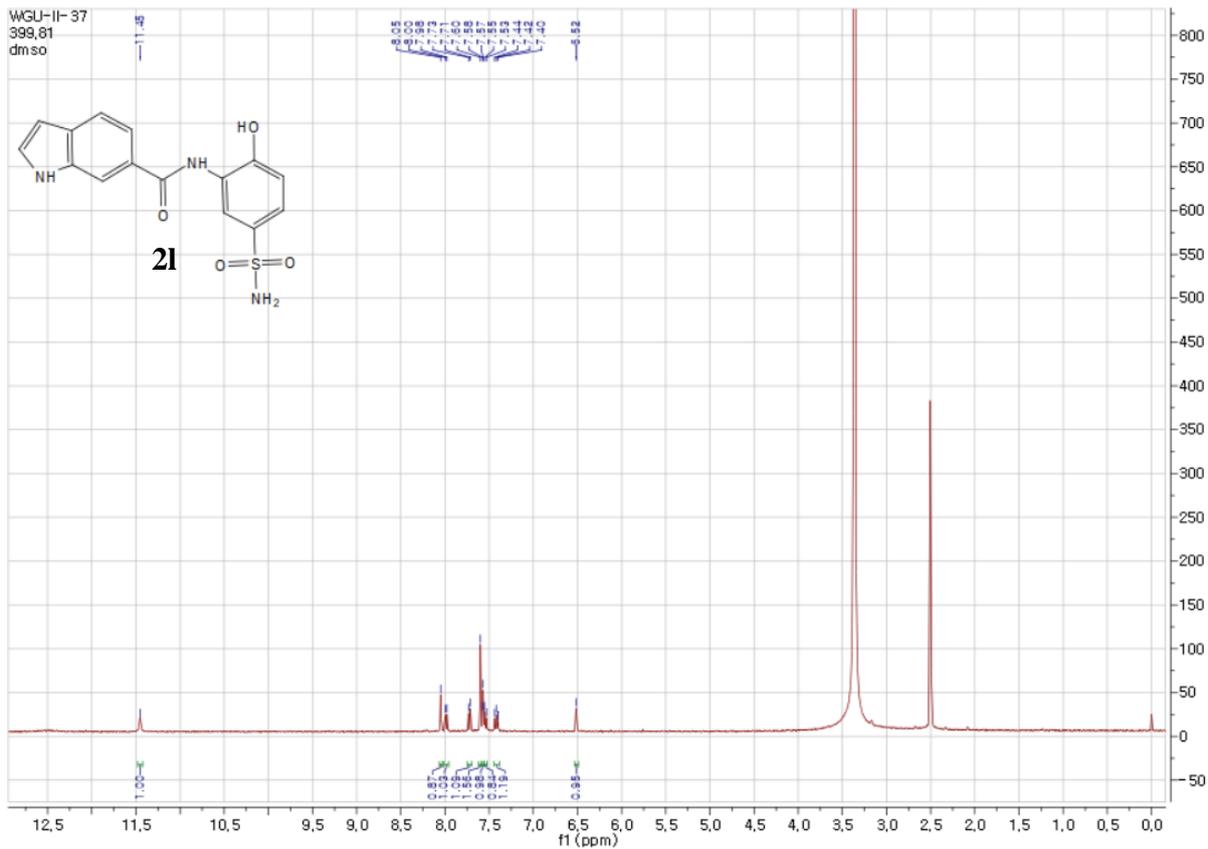


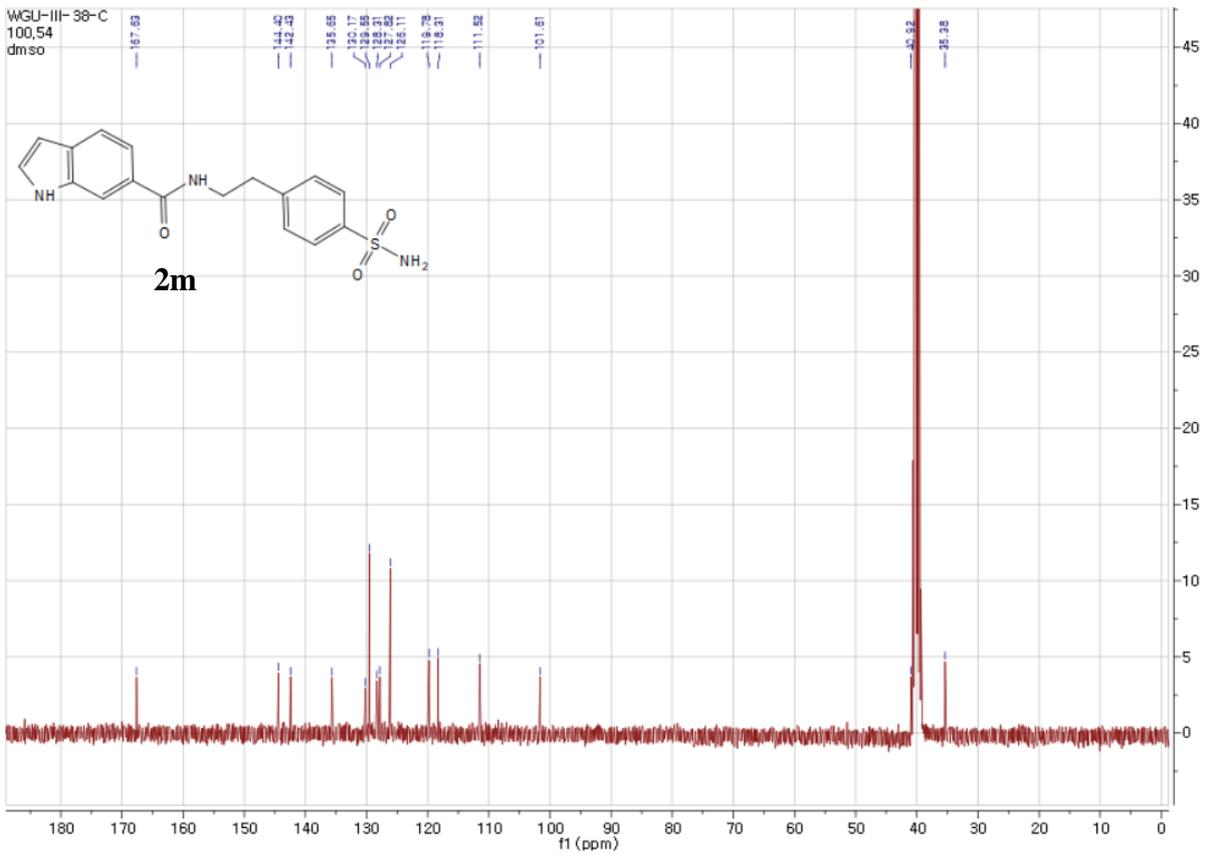
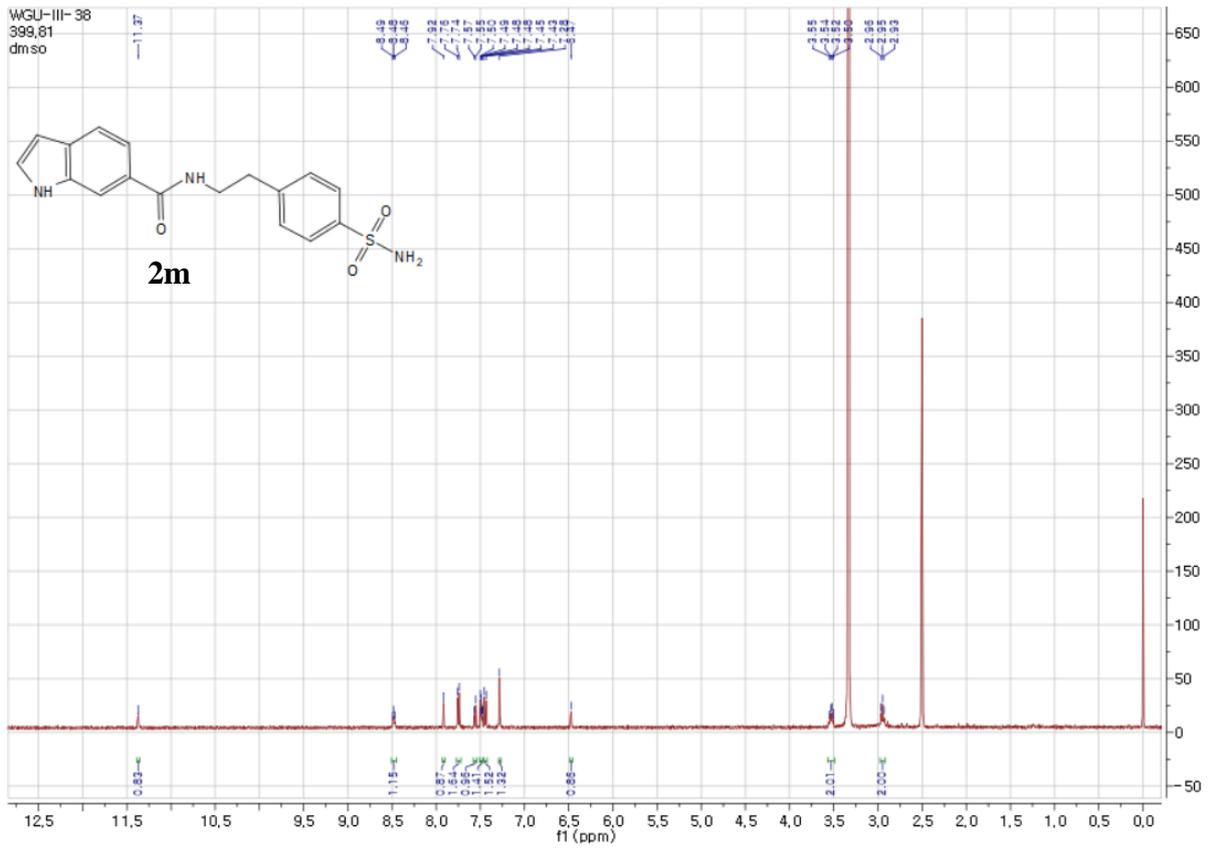


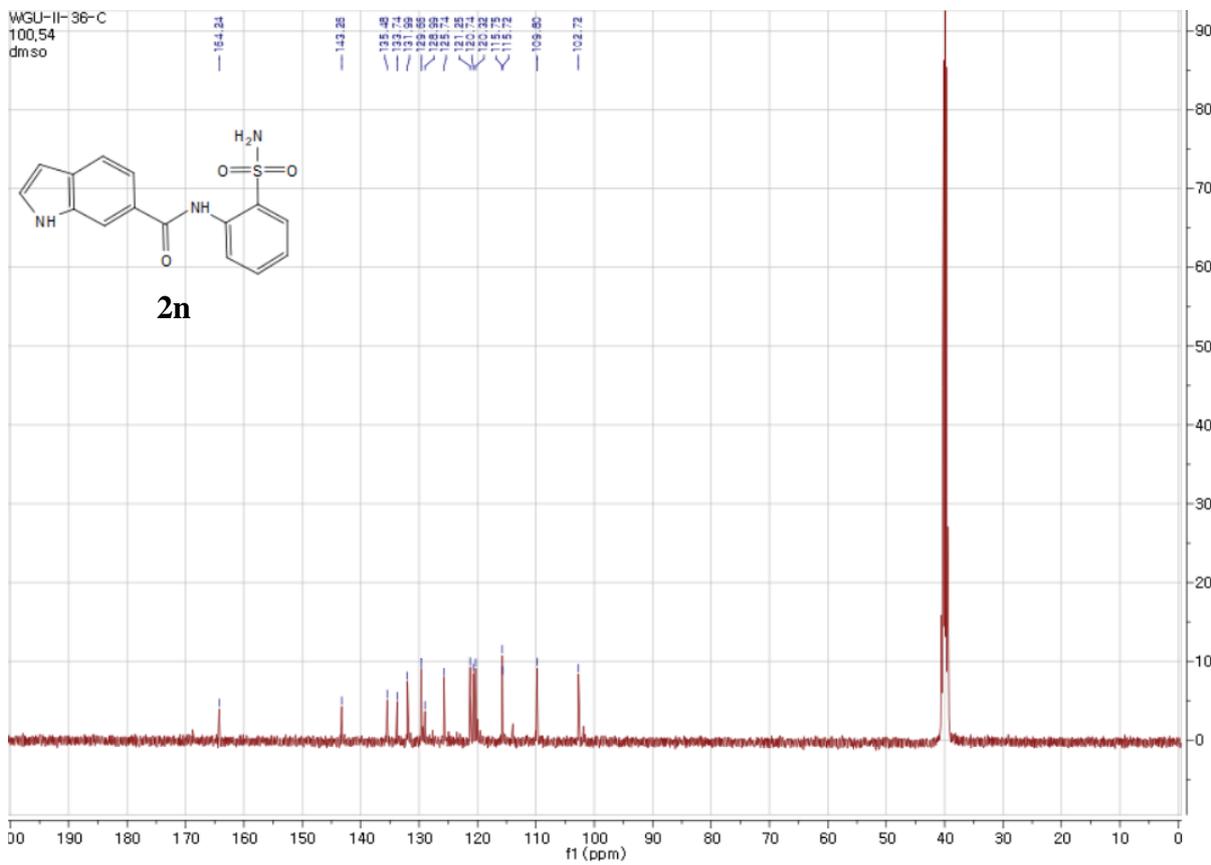
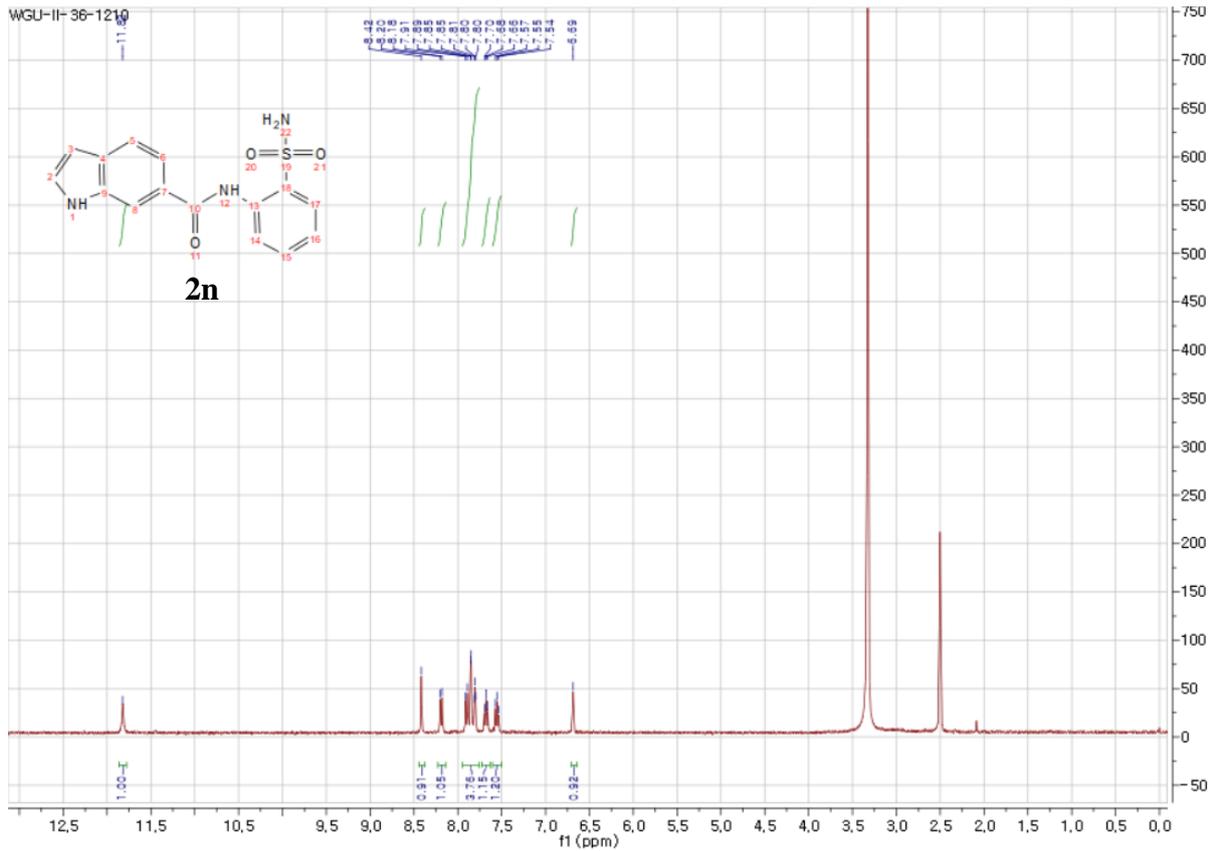


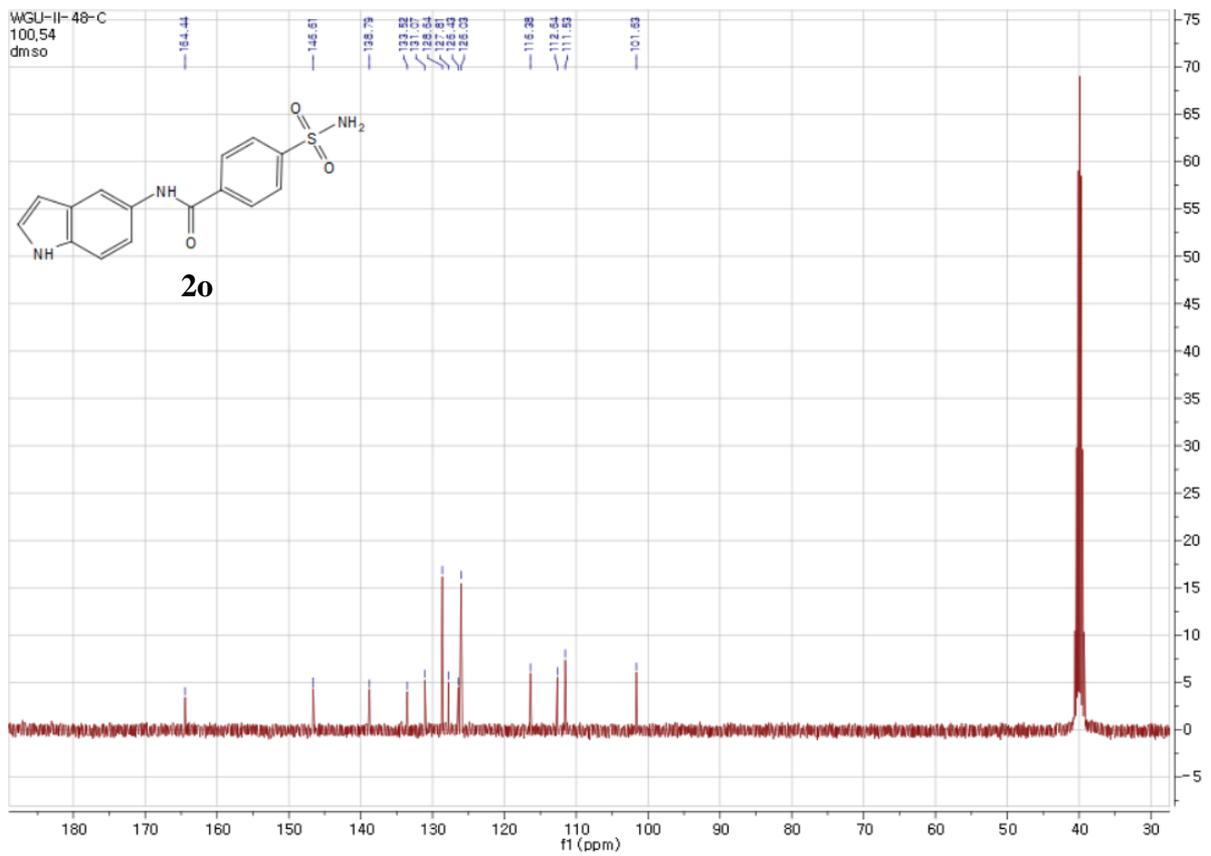
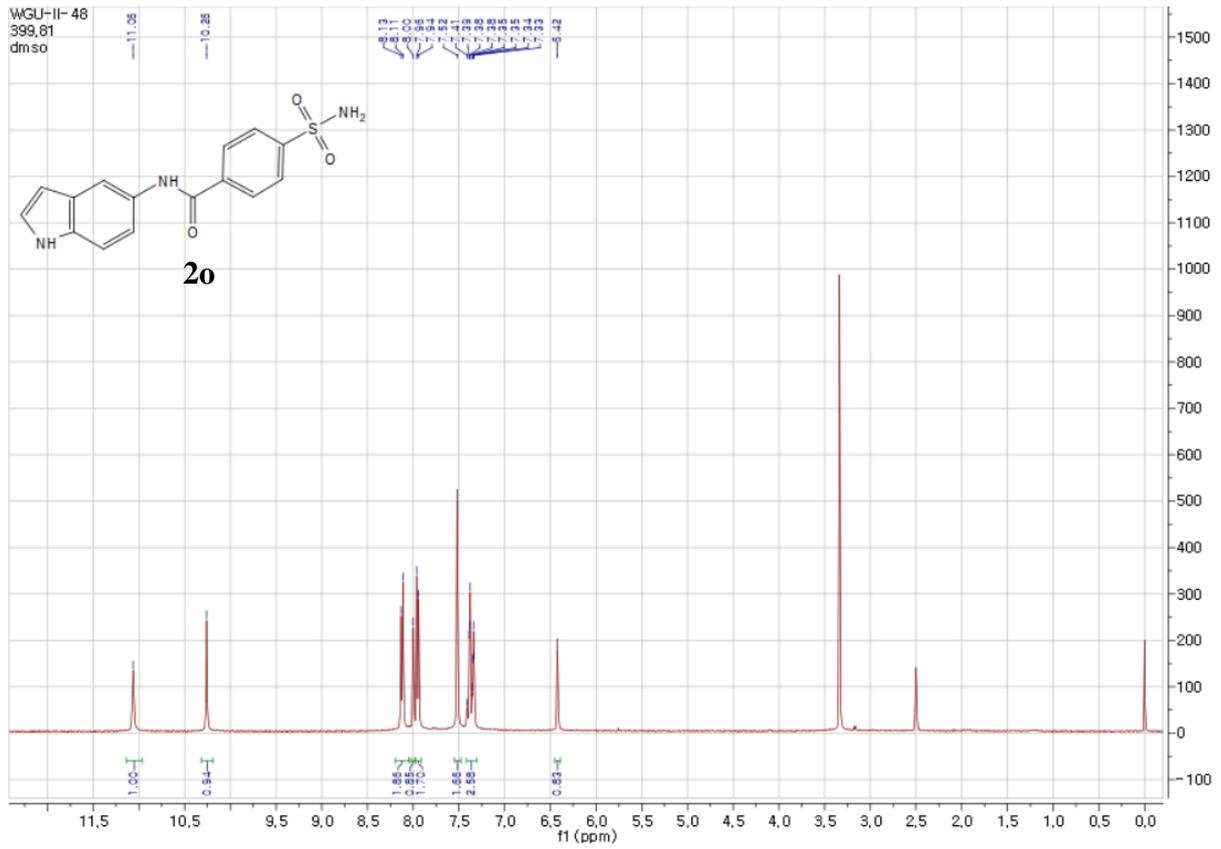






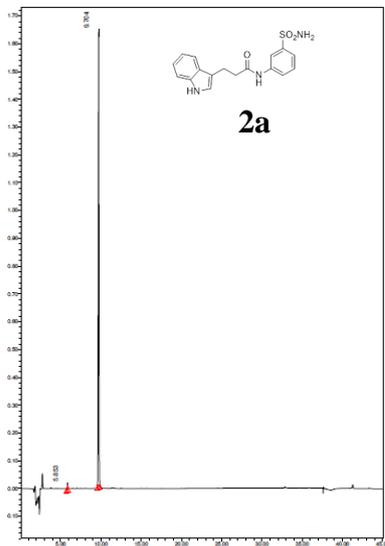




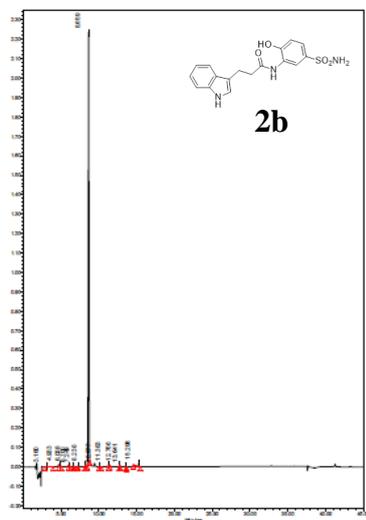


## 2. HPLC purity

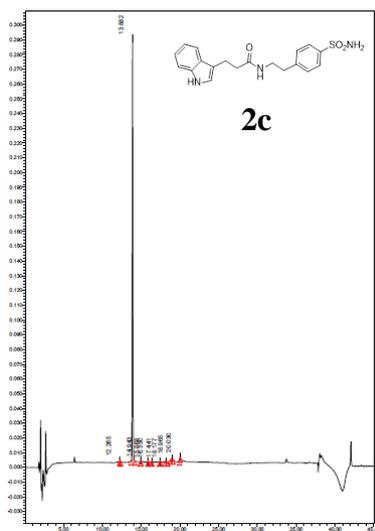
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2	9.704							10154012	99.79	1640978	bb	



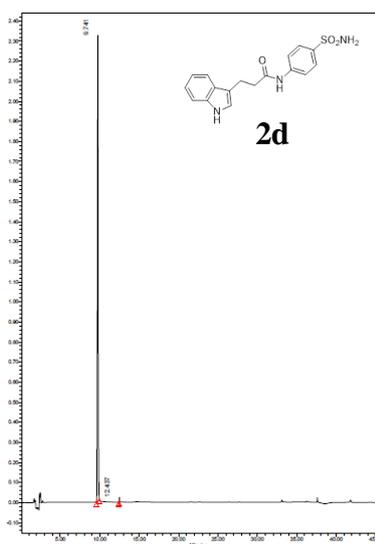
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1	3.160							35909	0.23	2232	bb	
2	4.933							48324	0.30	4938	bb	
3	6.038							18831	0.12	2398	bb	
4	6.700							1569	0.01	423	bb	
5	7.249							7081	0.04	1689	bb	
6	8.238							44044	0.28	8594	bb	
7	8.659							15369532	97.00	2242742	bb	
8	10.077							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	



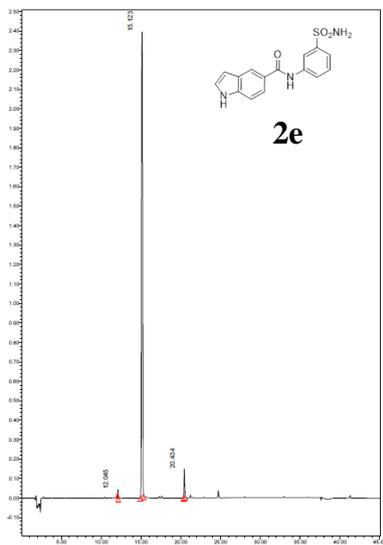
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1	12.265							909	0.06	253	bb		
2	13.882							1591817	99.00	286374	bb		
3	14.943							525	0.03	199	bb		
4	15.868							0	0.00	-0	bb		
5	16.350							376	0.02	87	bb		
6	17.441							628	0.04	145	bb		
7	18.177							880	0.05	-125	bb		
8	18.965			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



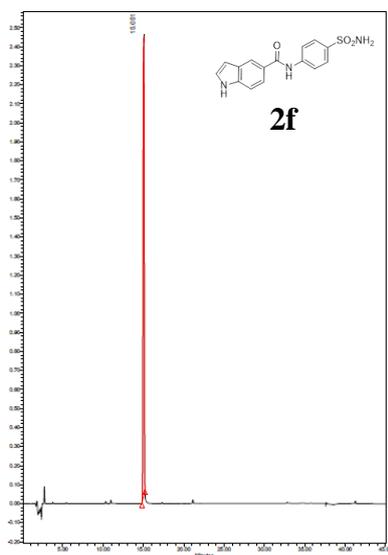
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1	9.741							16354019	99.98	2322914	bb	
2	12.437							2751	0.02	812	bb	



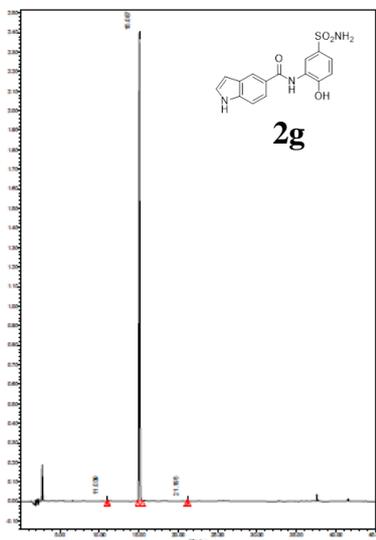
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1	12.045							13607	0.06	2636	bb	
2	15.123							23033597	96.78	2409116	bb	
3	20.434							752736	3.16	120461	bb	



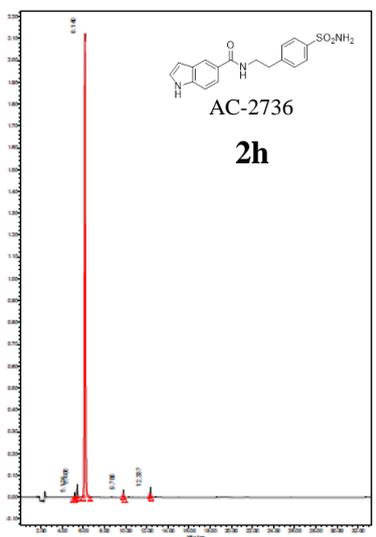
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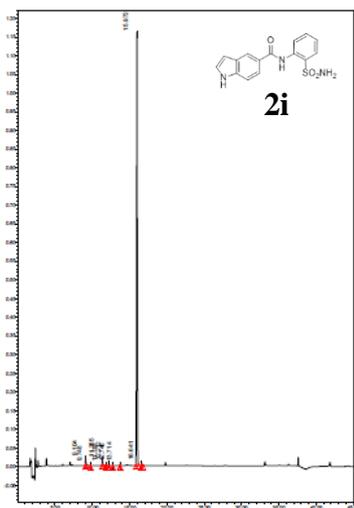
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1	11.039							40642	0.21	7378	bb	
2	15.087							19368165	99.62	2407029	bb	
3	21.195							33647	0.17	5326	bb	



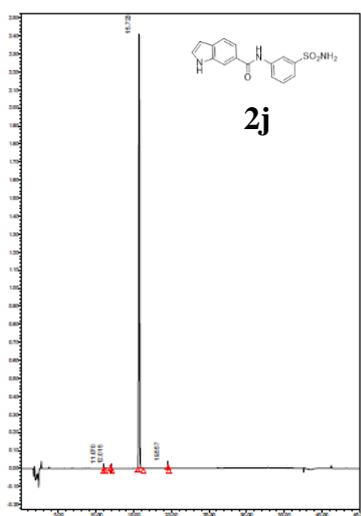
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1	5.124							14862	0.10	3240	bb	
2	5.406							224896	1.56	39342	bb	
3	6.140							14058338	97.68	2113810	bb	
4	9.788							22932	0.16	6528	bb	
5	12.337							70658	0.49	17520	bb	



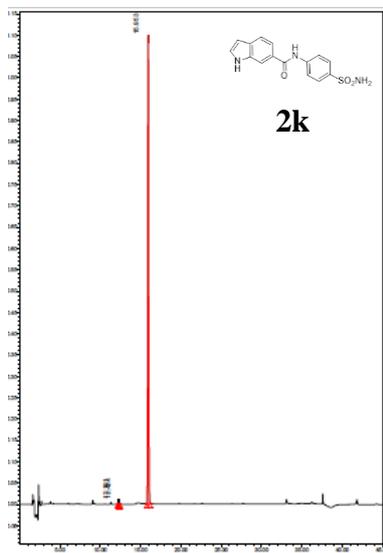
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1	9.104							54155	0.66	12032	bb	
2	9.748							764	0.01	240	bb	
3	11.355							52092	0.64	10110	bb	
4	11.797							1827	0.02	501	bb	
5	12.212							13261	0.16	2847	bb	
6	12.748							61	0.00	61	bb	
7	13.714							1949	0.02	617	bb	
8	15.972						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



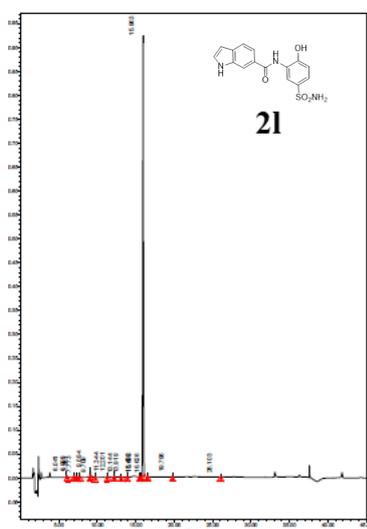
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1	11.070							29879	0.15	4607	bb	
2	12.015							25660	0.13	-4915	bb	
3	15.723							20068158	99.67	2419202	bb	
4	19.557							10109	0.05	1649	bb	



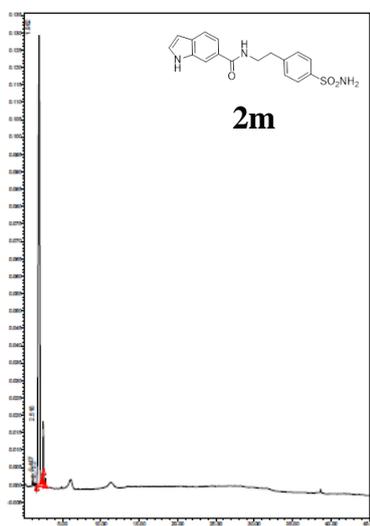
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1	12.191							1763	0.02	705	bb	
2	12.434							6031	0.08	1412	bb	
3	15.953							7503939	99.90	1092658	bb	



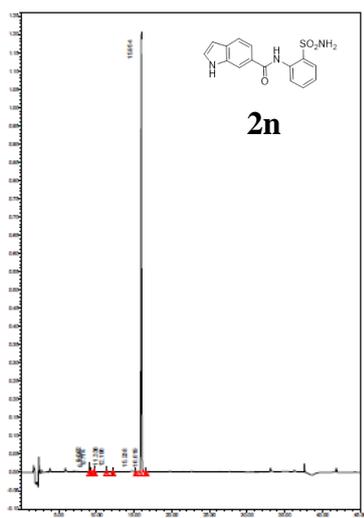
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1	6.041							11743	0.18	2638	bb	
2	6.995							3264	0.05	681	bb	
3	7.281							8370	0.13	1922	bb	
4	7.773							11908	0.19	1654	bb	
5	9.094							50125	0.78	10364	bb	
6	9.709							7152	0.11	1110	bb	
7	11.344							14838	0.23	2412	bb	
8	12.201							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	



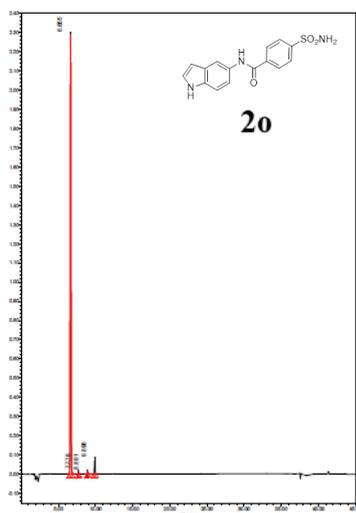
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1	1.982							1737170	96.73	129132	bb		
2	2.407							1179	0.07	597	bb		
3	2.518							55830	3.11	13988	bb		
4	2.752							1686	0.09	558	bb		



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	Units
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		



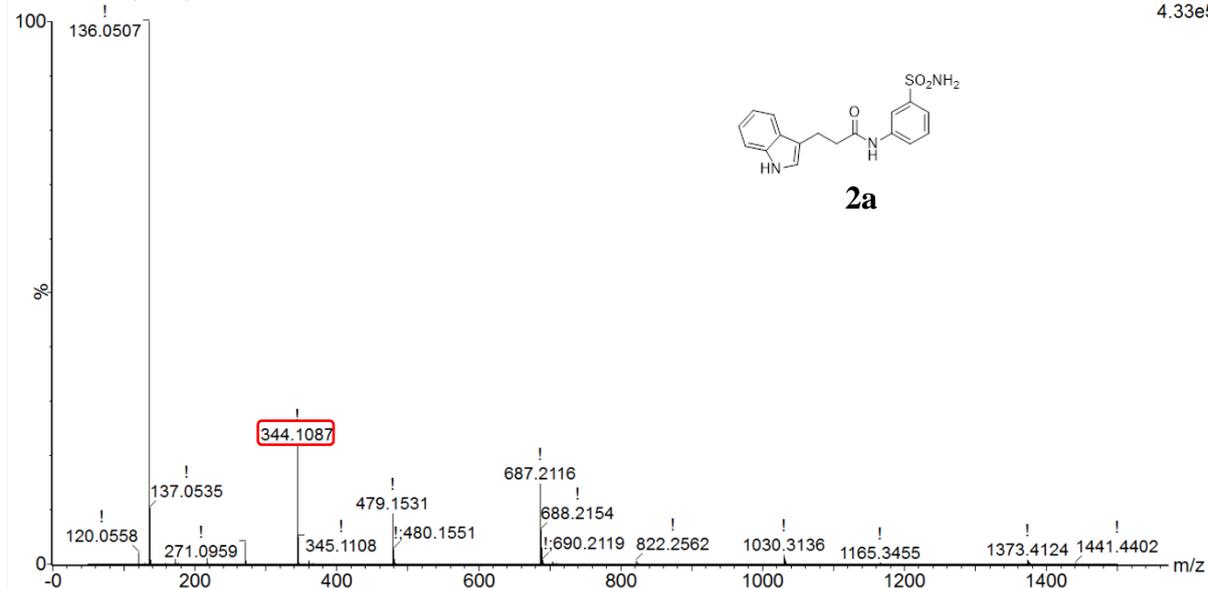
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1	6.655							16039540	97.38	2313113	bb	
2	7.778							9441	0.06	1850	bb	
3	8.891							6264	0.04	-1087	bb	
4	9.898							415866	2.52	66089	bb	



### 3. HRMS data

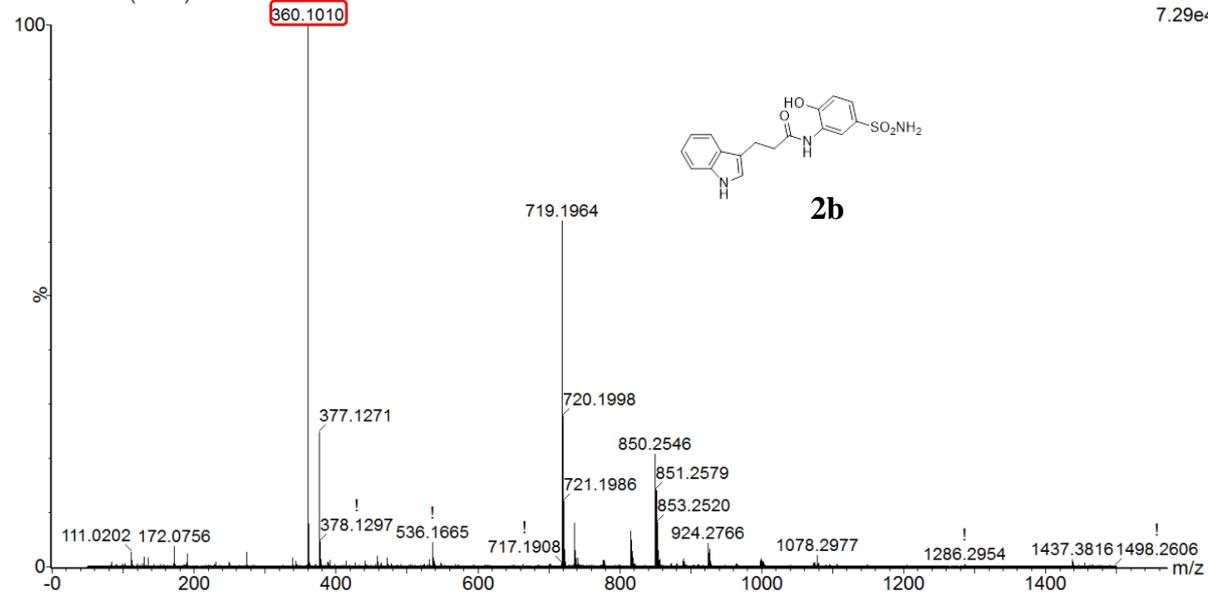
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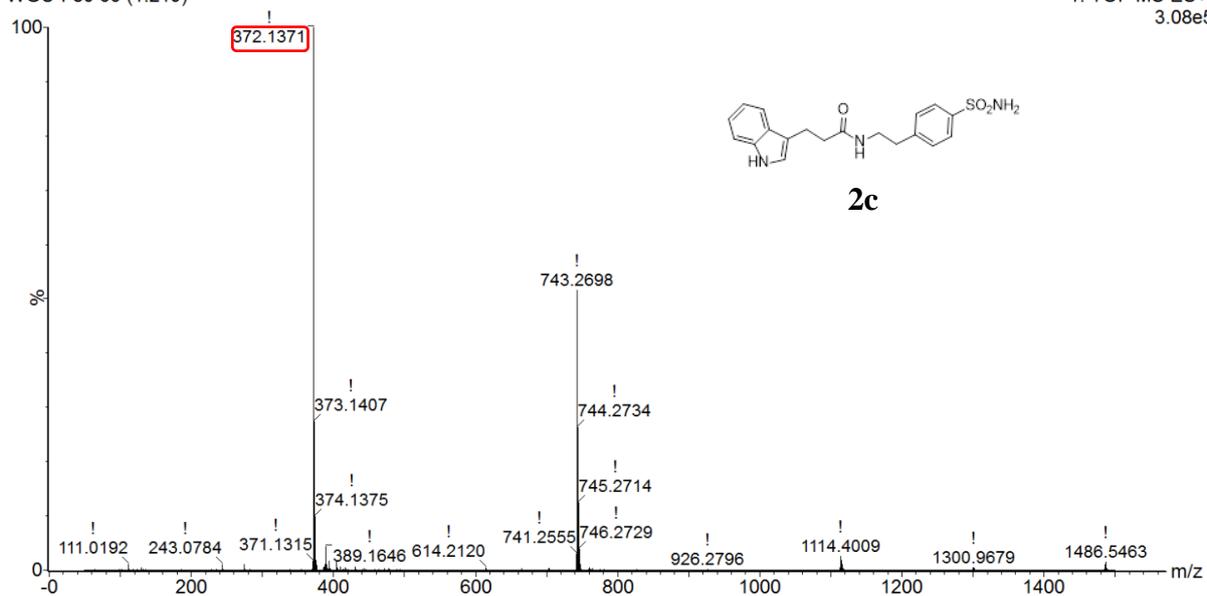
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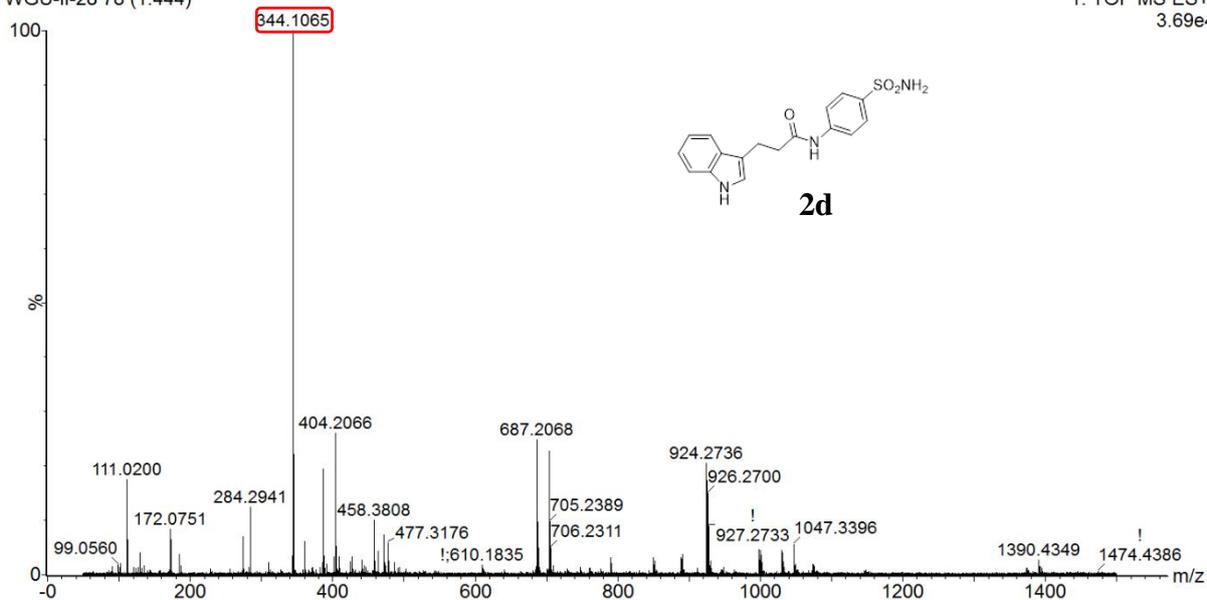
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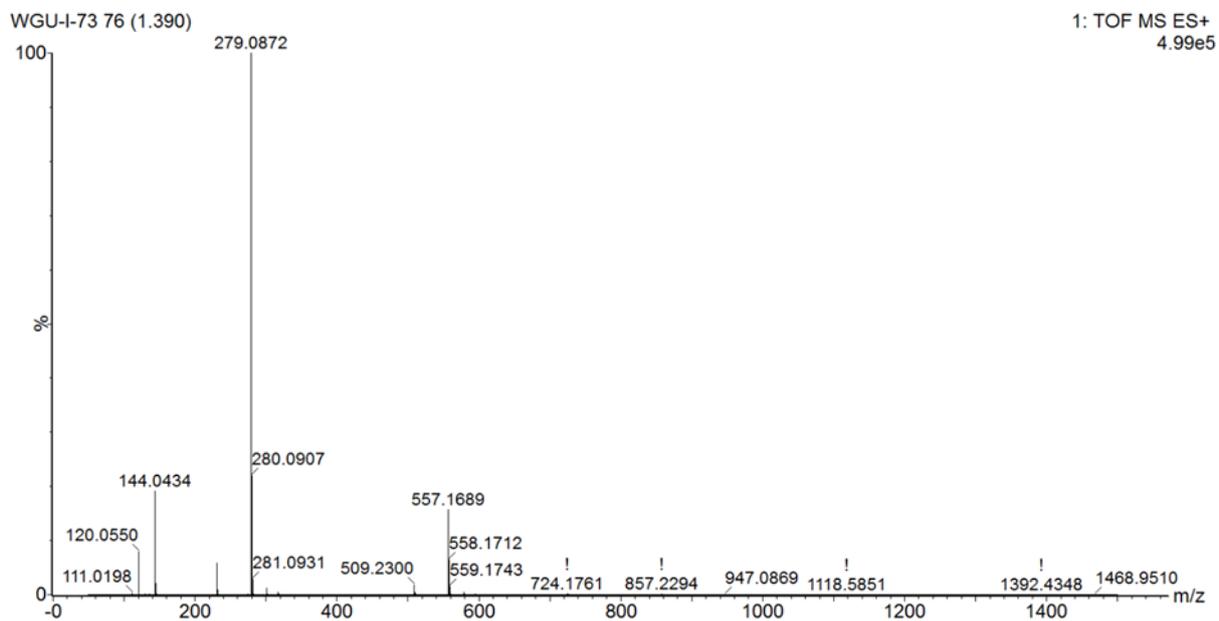


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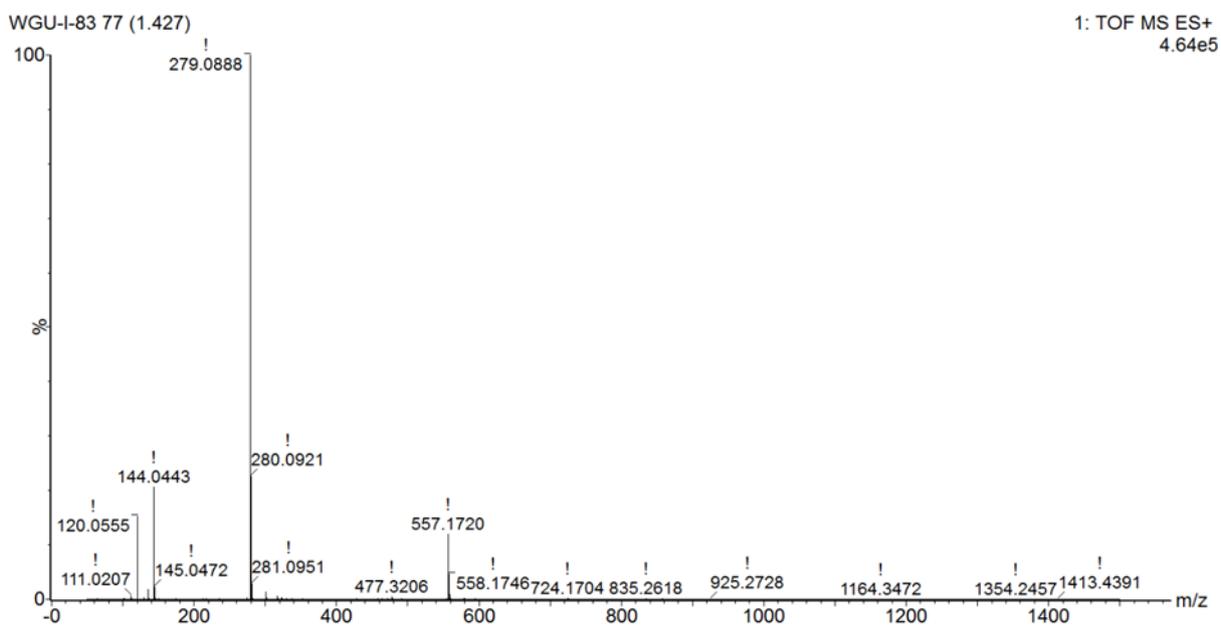
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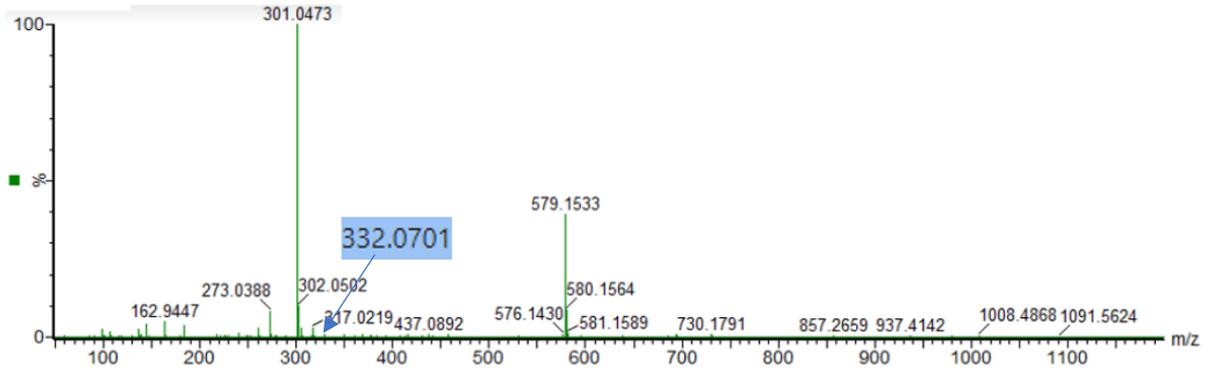
### Compound 2e (Fragmentation)



### Compound 2f (Fragmentation)

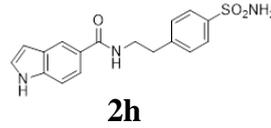
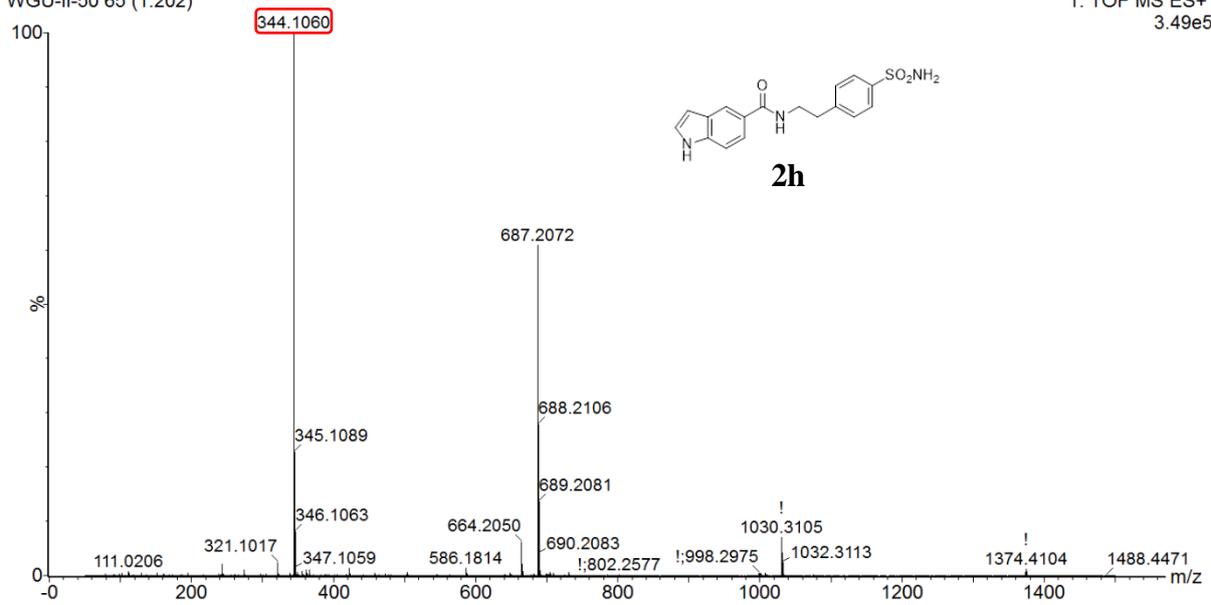


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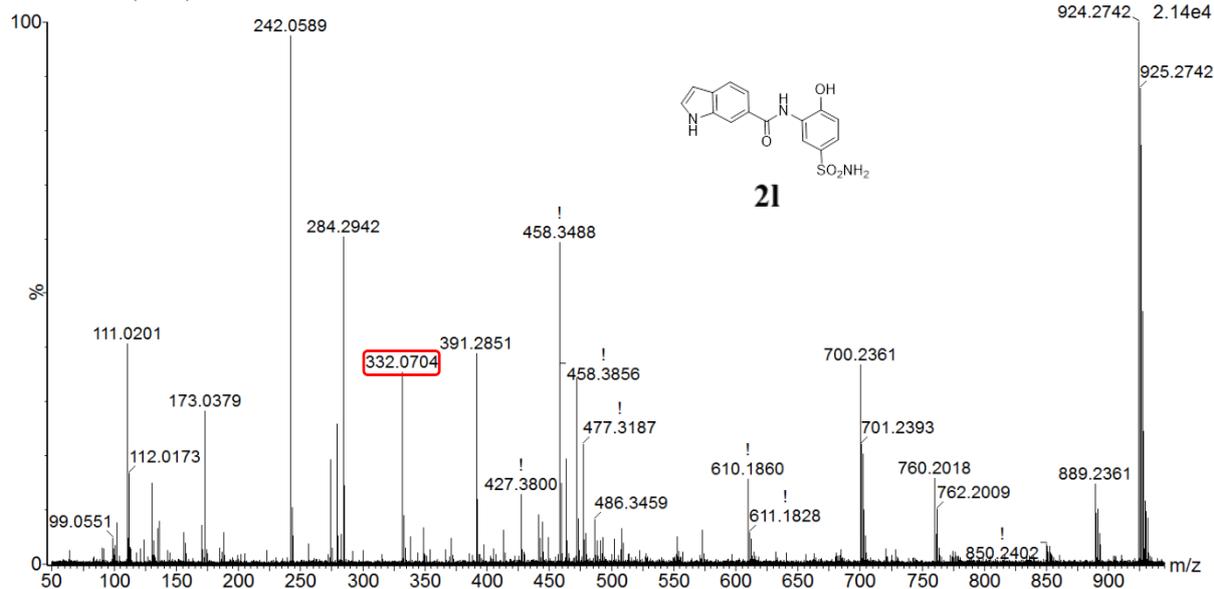


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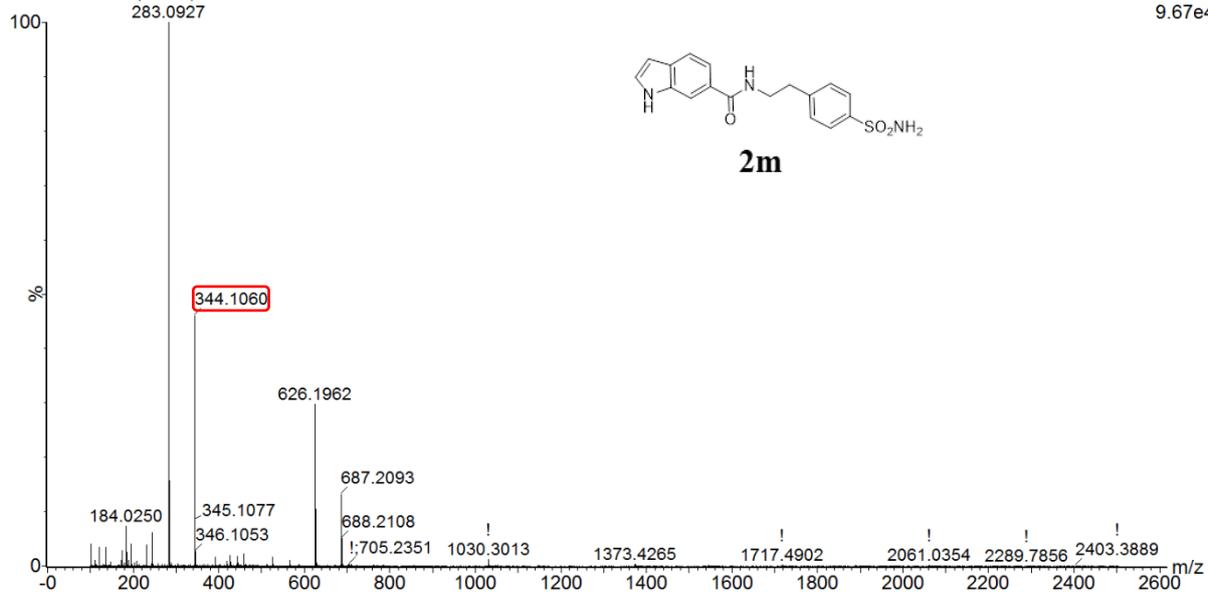
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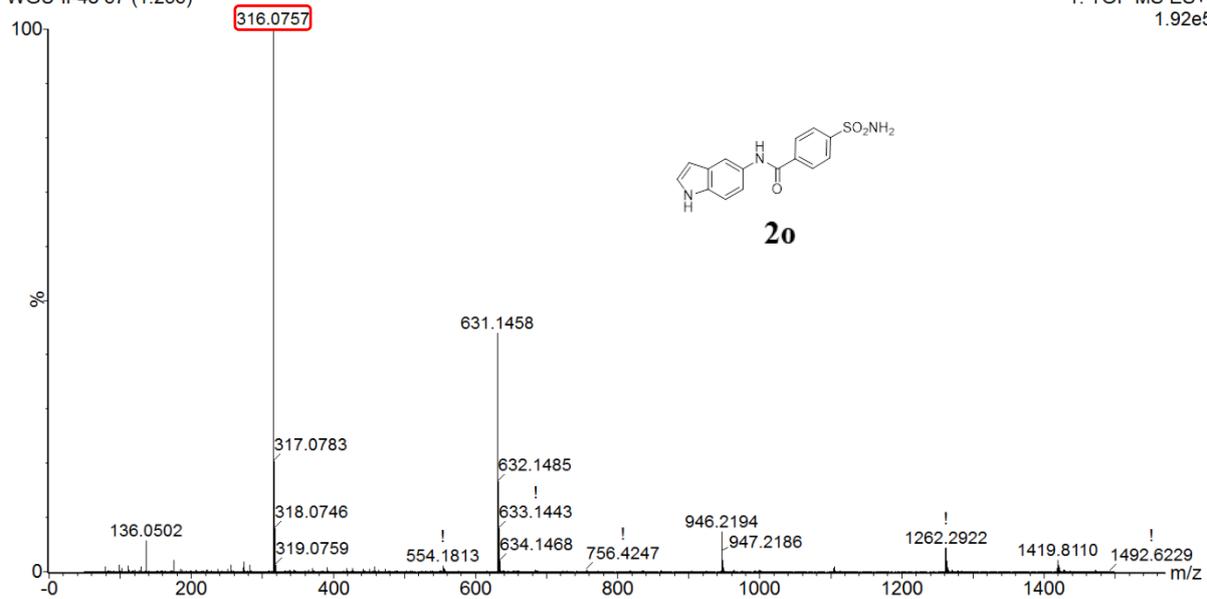


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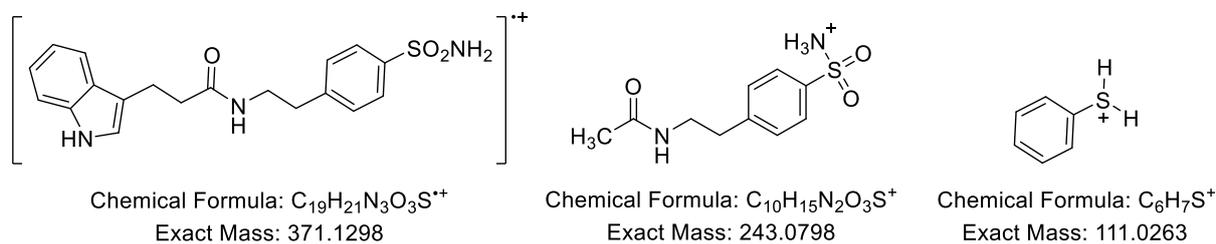
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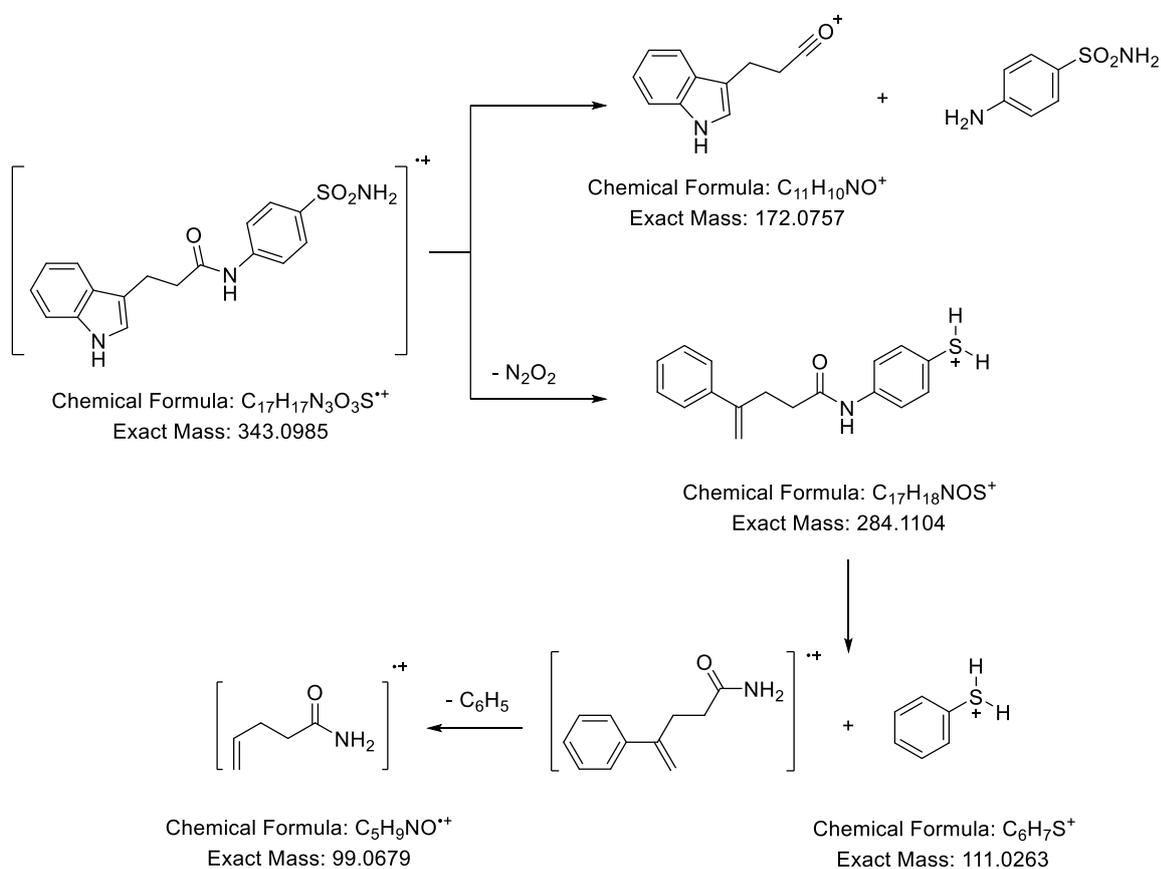


#### 4. Interpretation of HRMS:

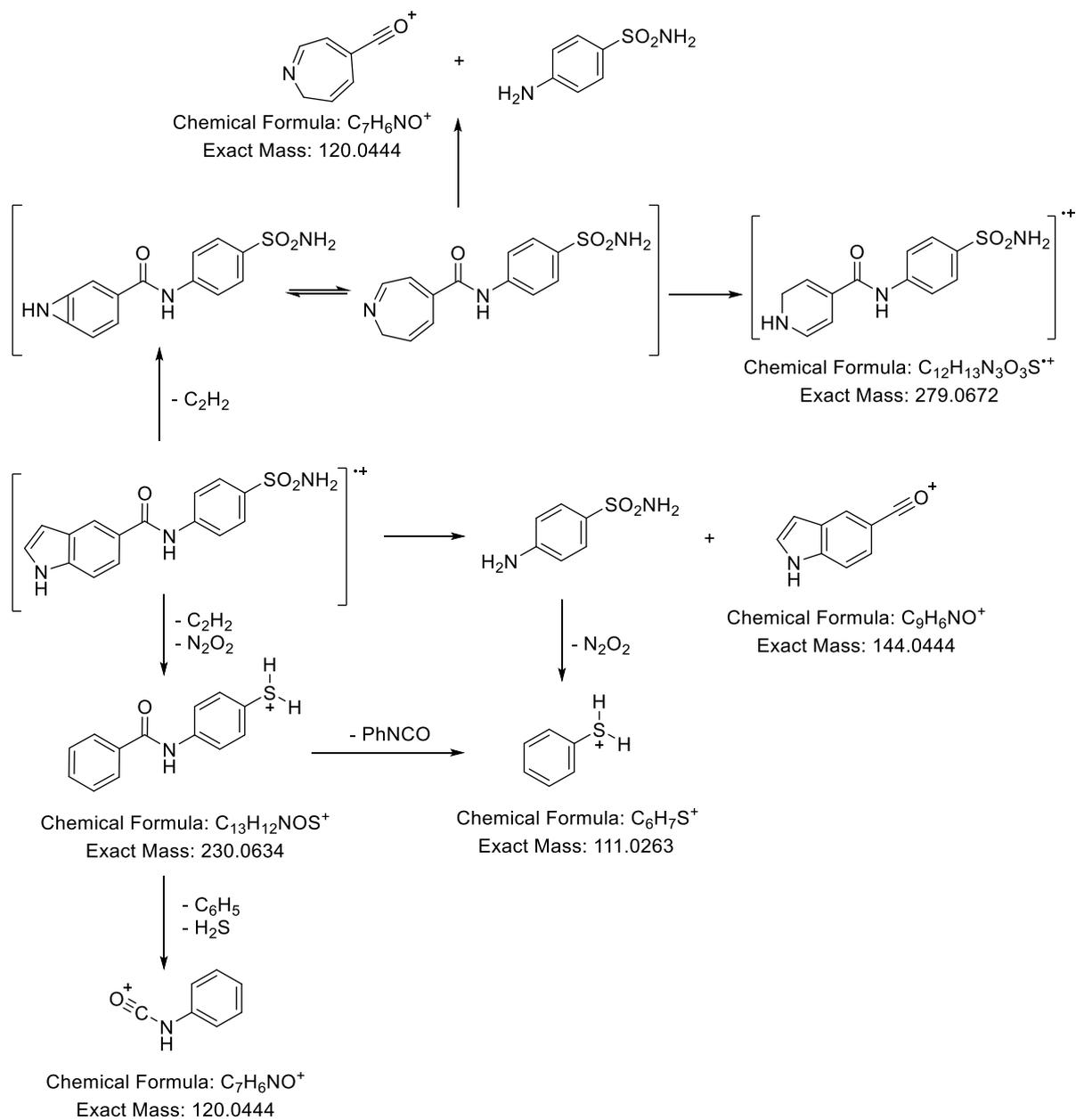
##### Compound 2c:



##### Compound 2d:



##### Compounds 2e and 2f:



### Compound 2h:

