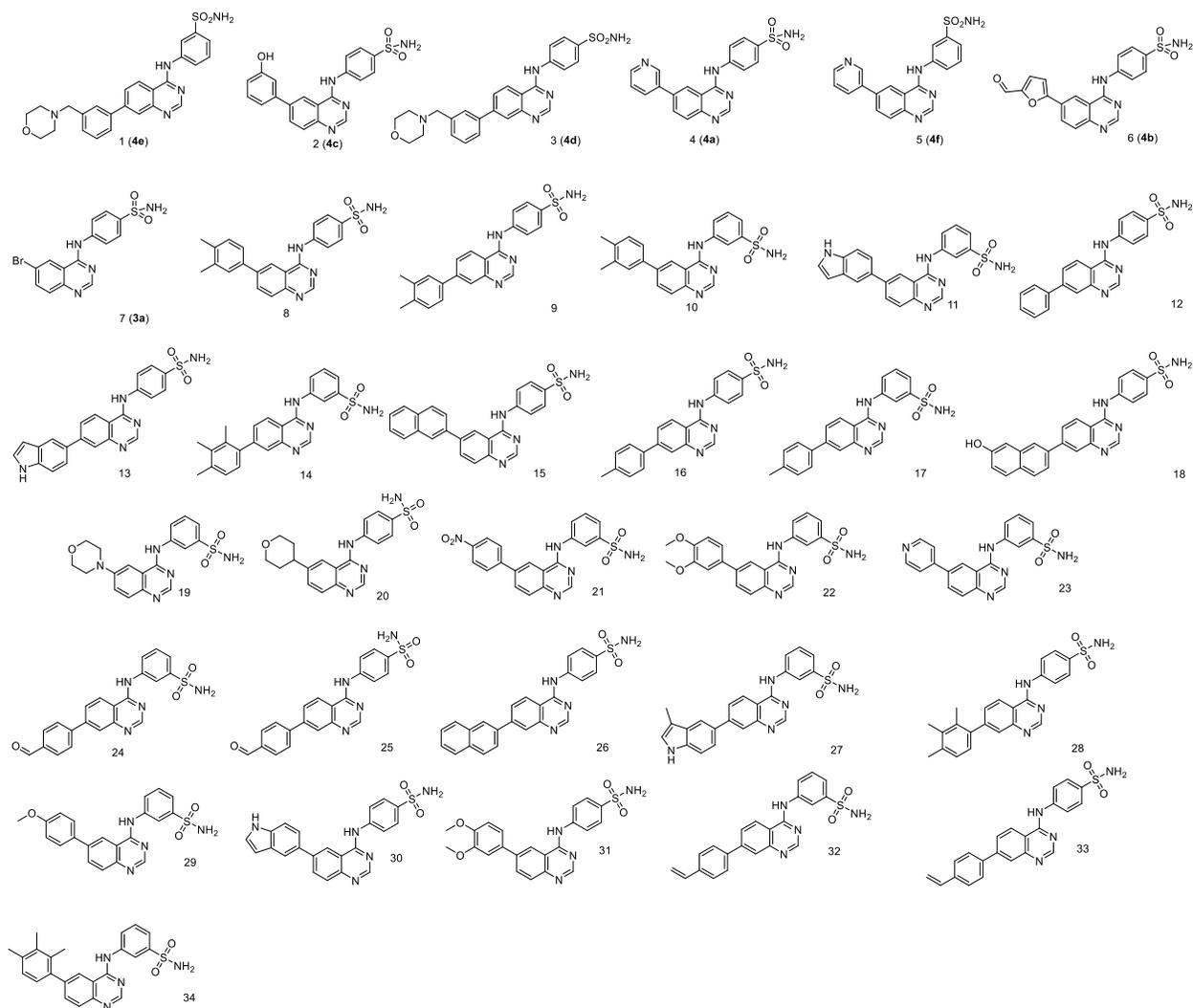


## Supplementary material

**Hit Identification of a Novel Quinazoline Sulfonamide as a promising EphB3 inhibitor: Design, Virtual Combinatorial Library, Synthesis, Biological Evaluation, and Docking Simulation Studies**

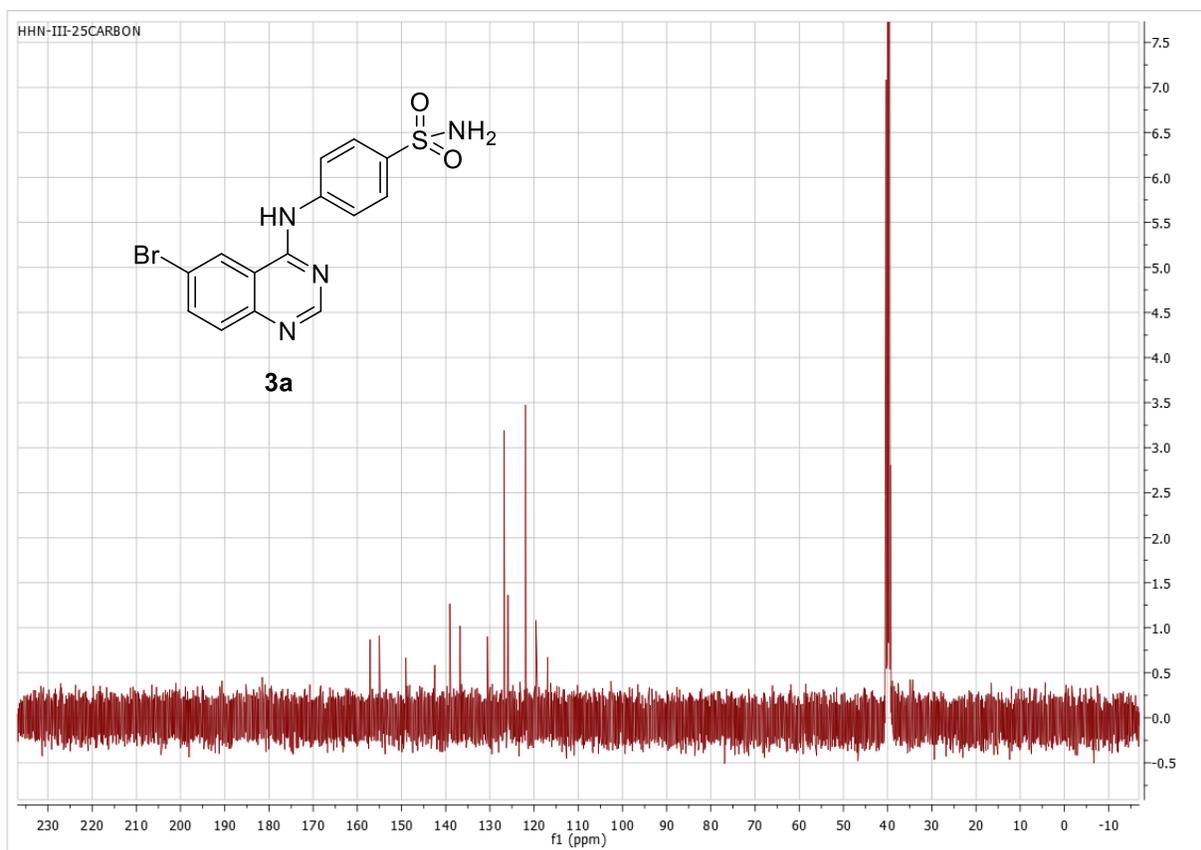
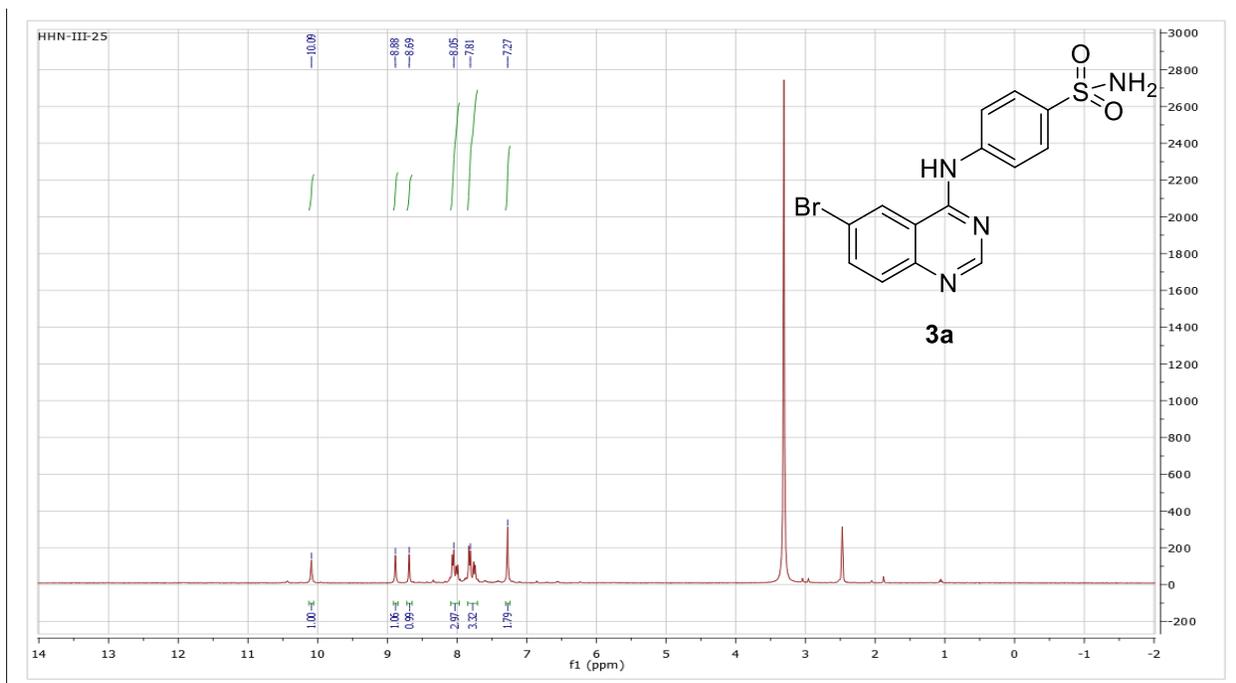
### Contents

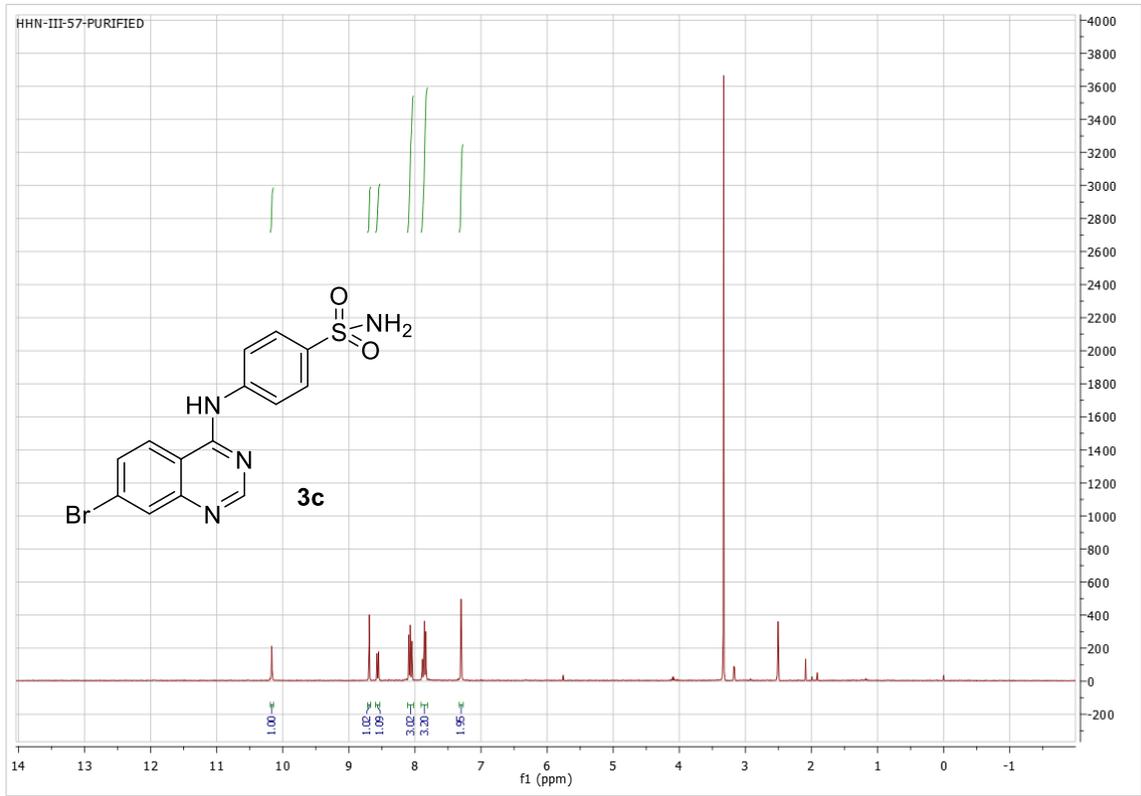
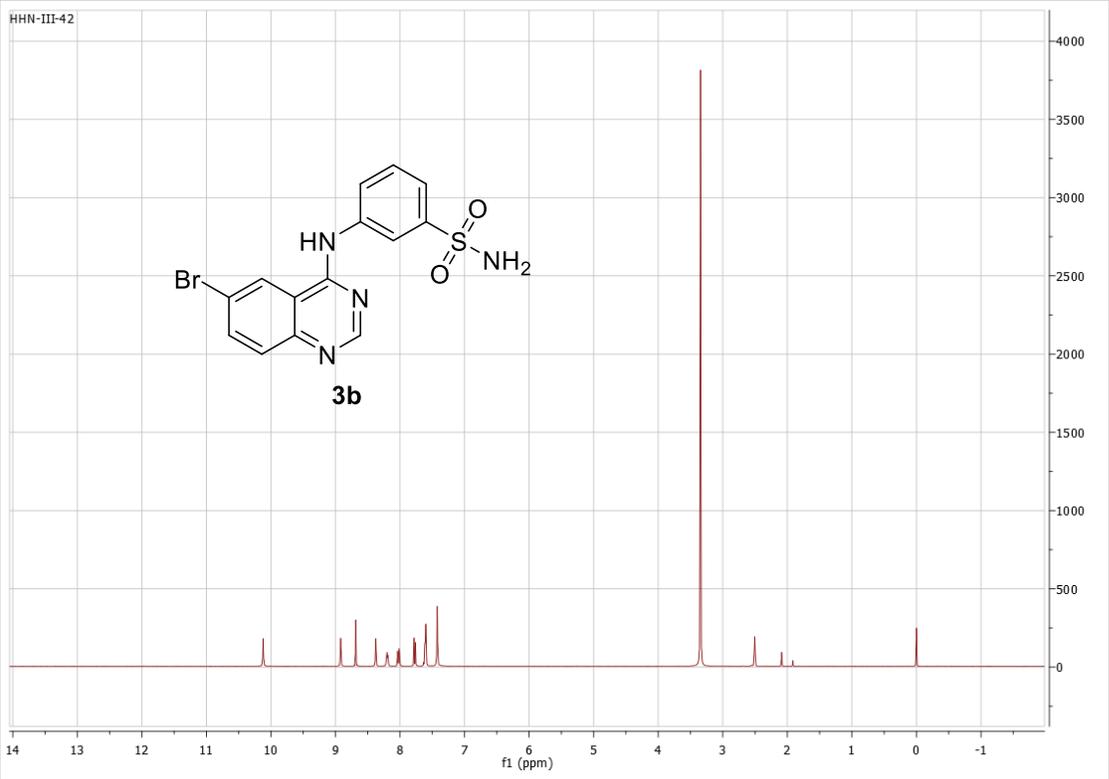
1. Figure S1. The chemical structures of the generated virtual library
2. <sup>1</sup>HNMR and <sup>13</sup>CNMR data of compounds **3a-d** and **4a-f**
3. Representative HPLC purity data of the compounds **3a-d** and **4a-f**
4. Representative HRMS data of the compounds **3a-d** and **4a-f**

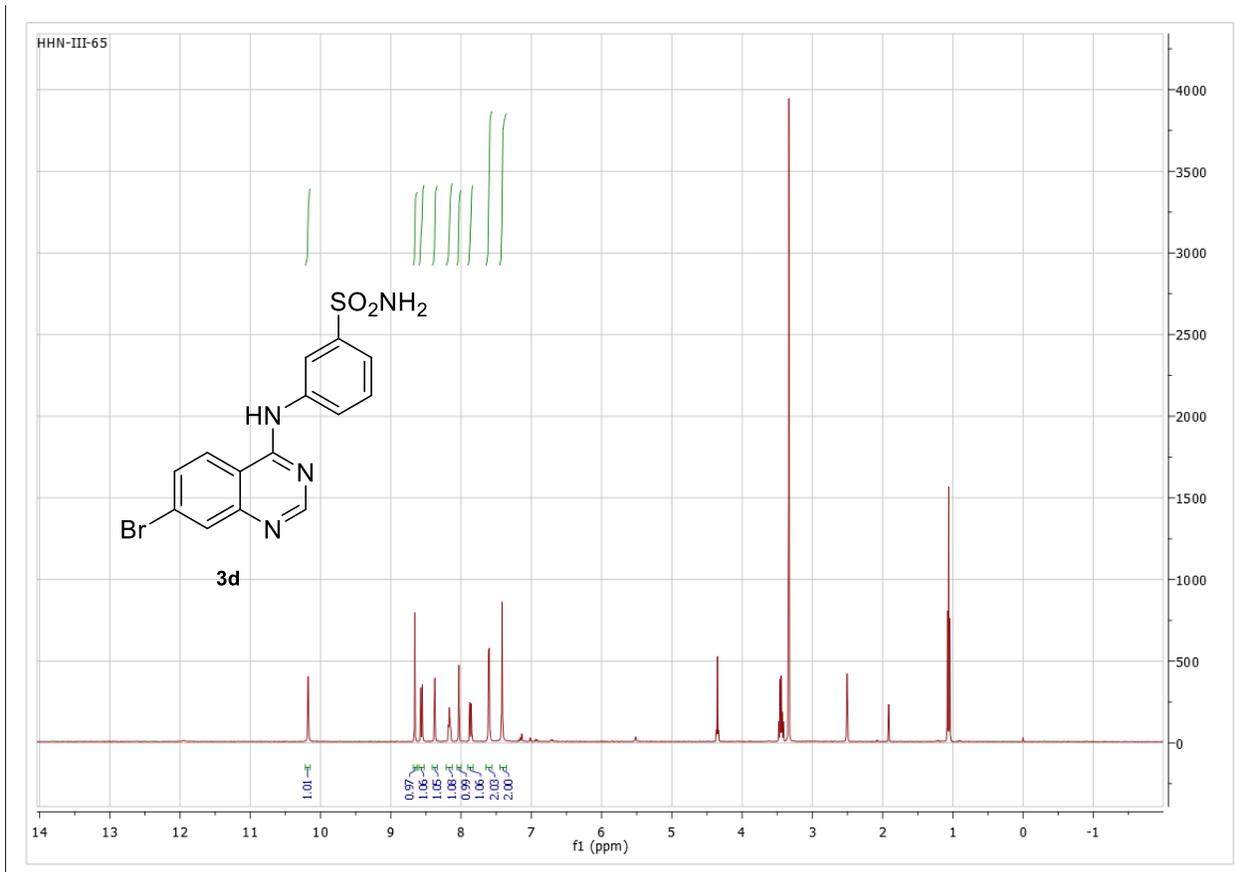
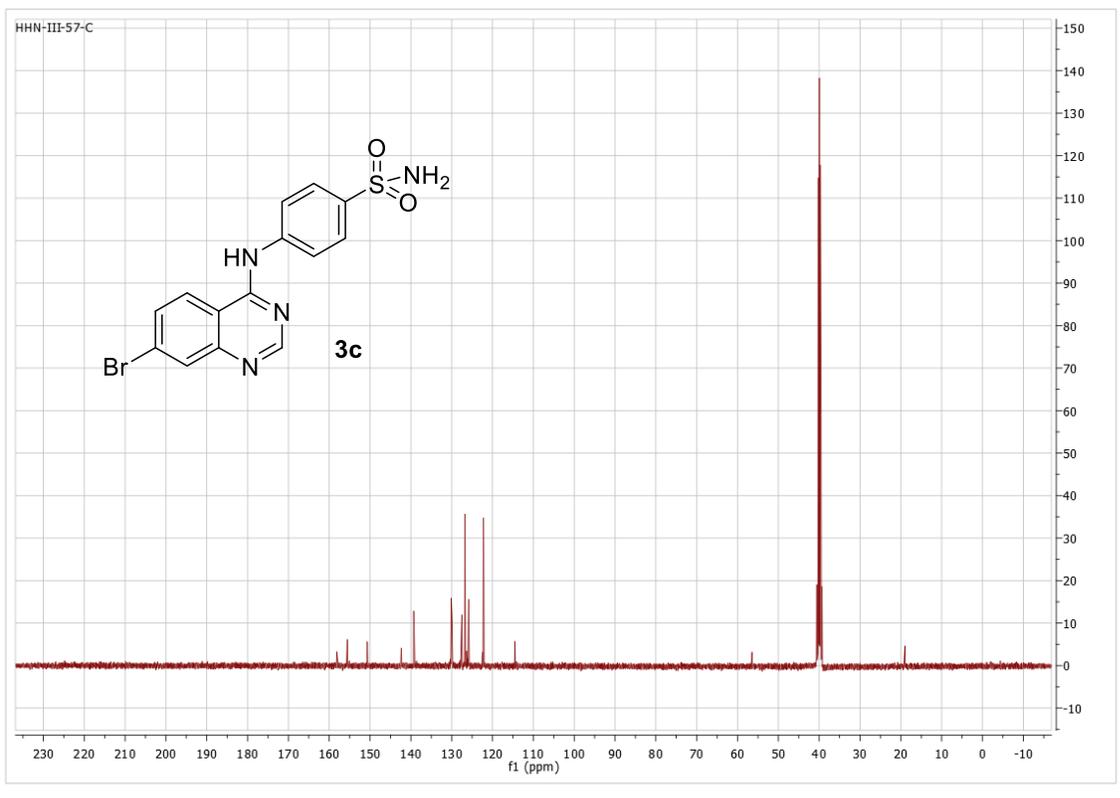


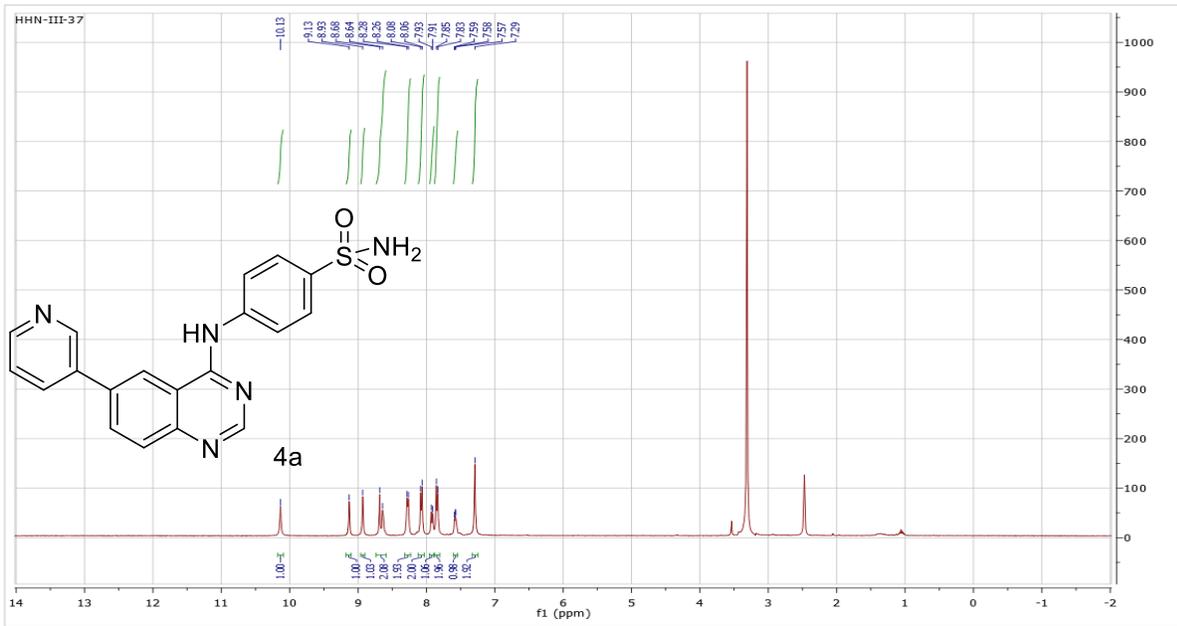
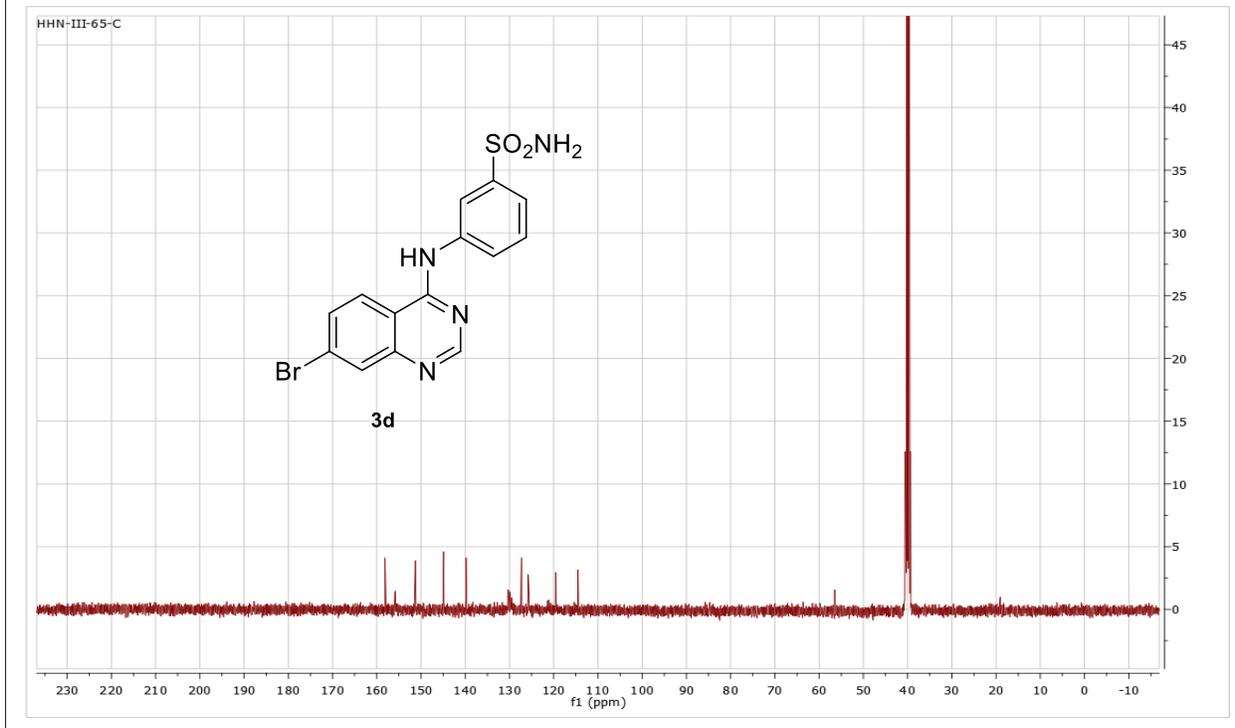
1. Figure S1. The chemical structures of the generated virtual library compounds

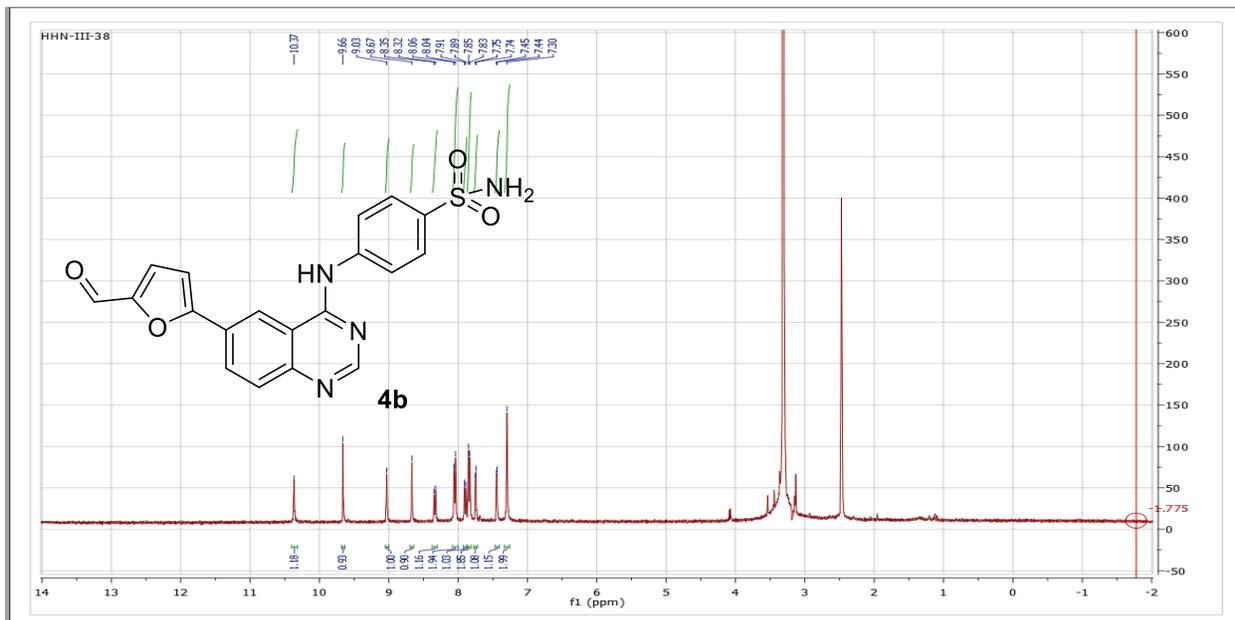
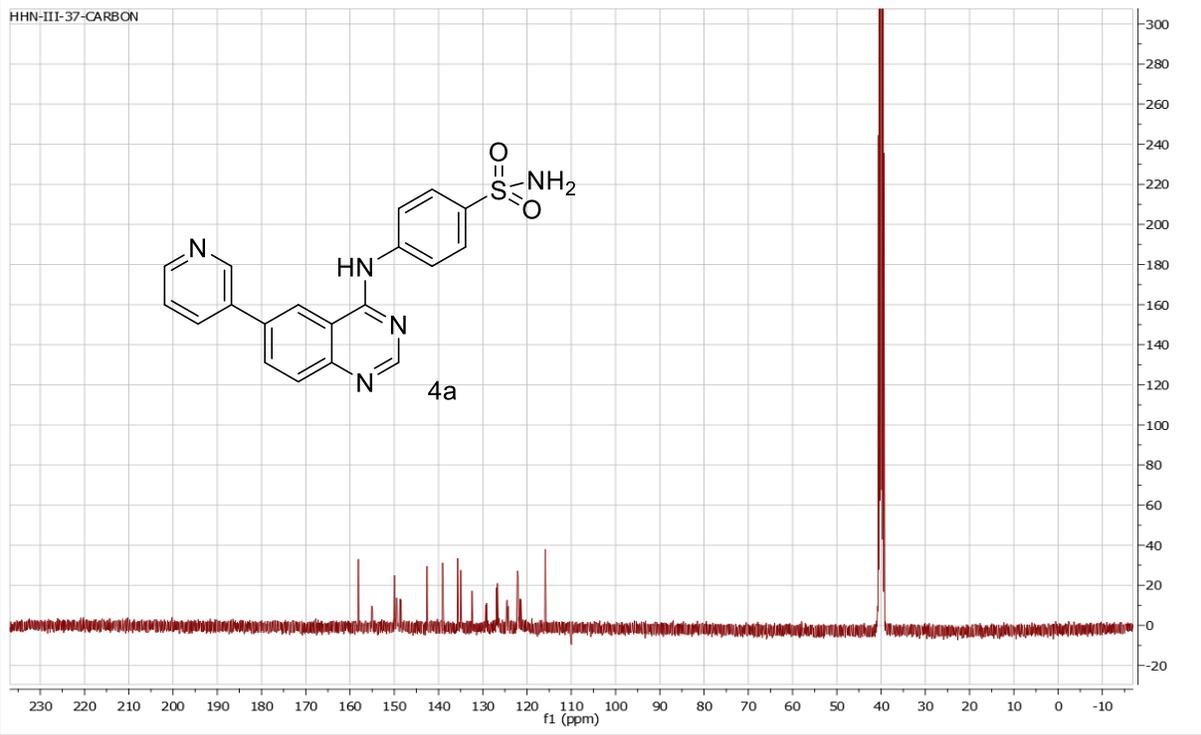
## 2. $^1\text{H}$ NMR and $^{13}\text{C}$ NMR data of compounds 3a–d and 4a–f

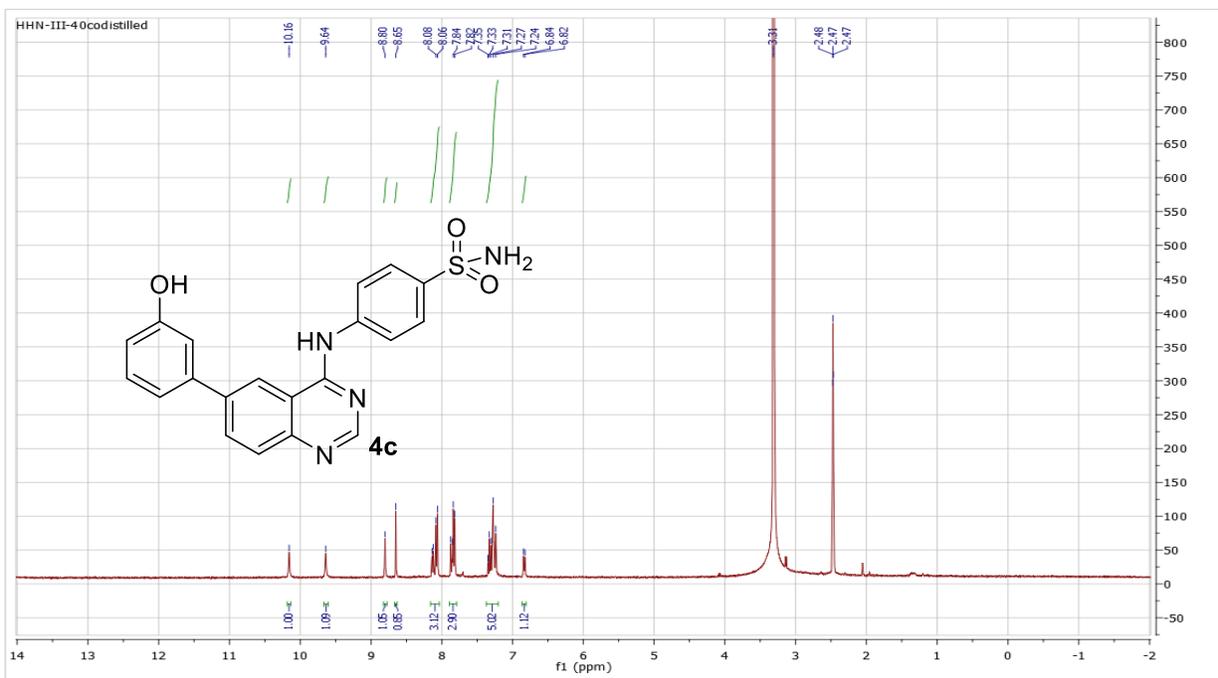
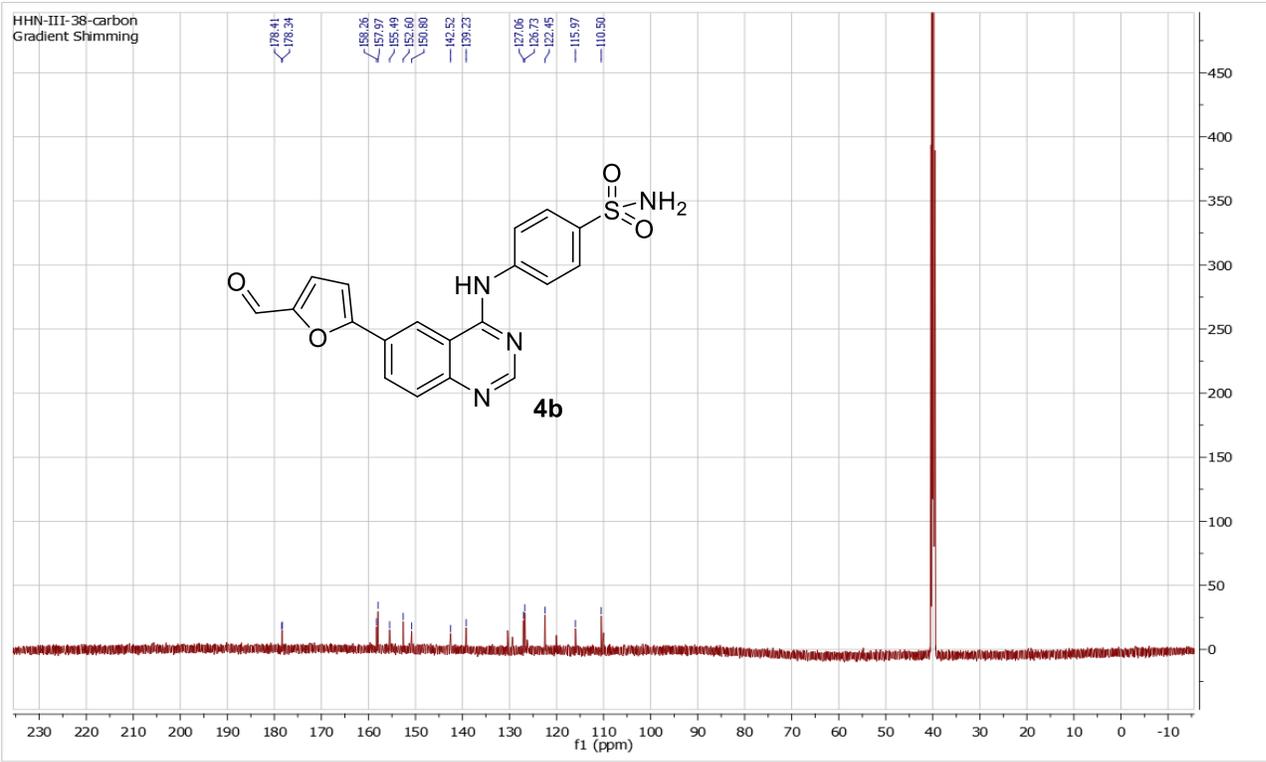


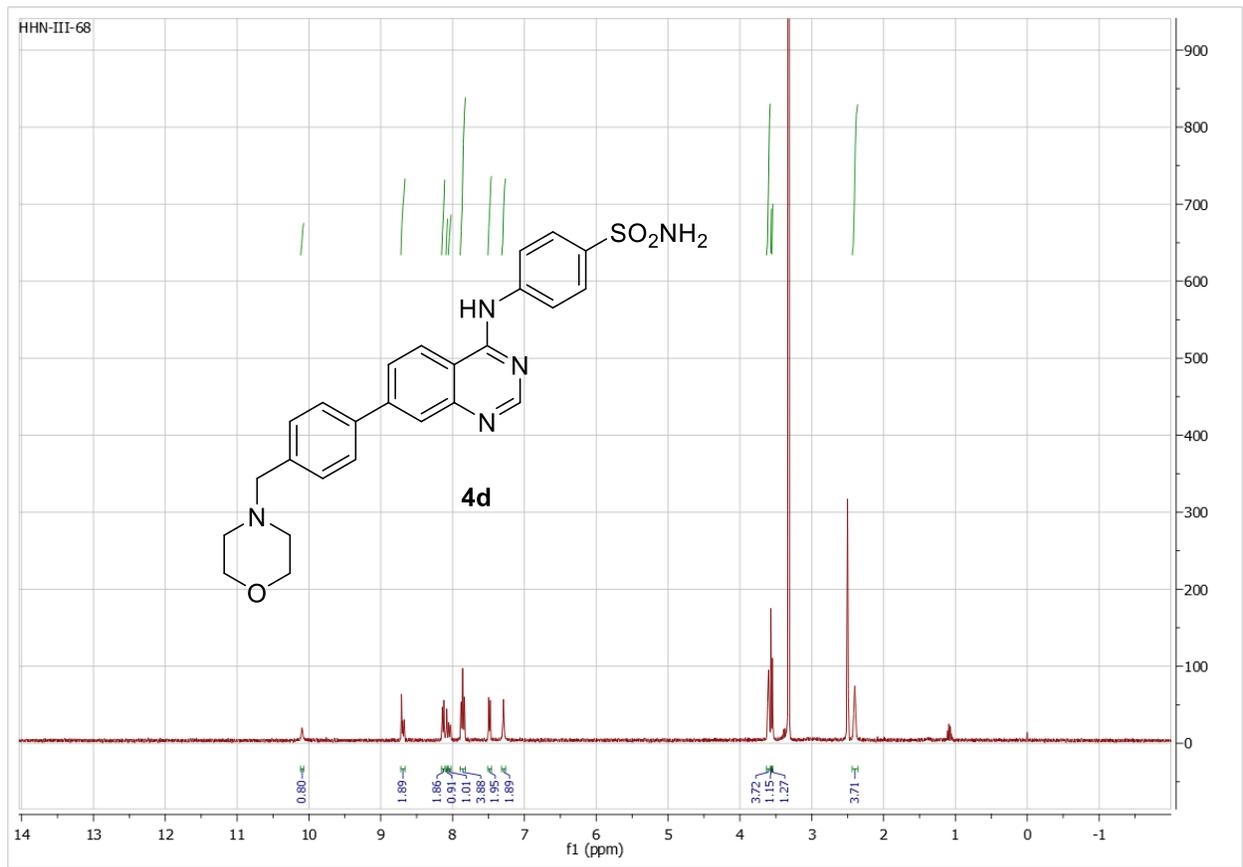
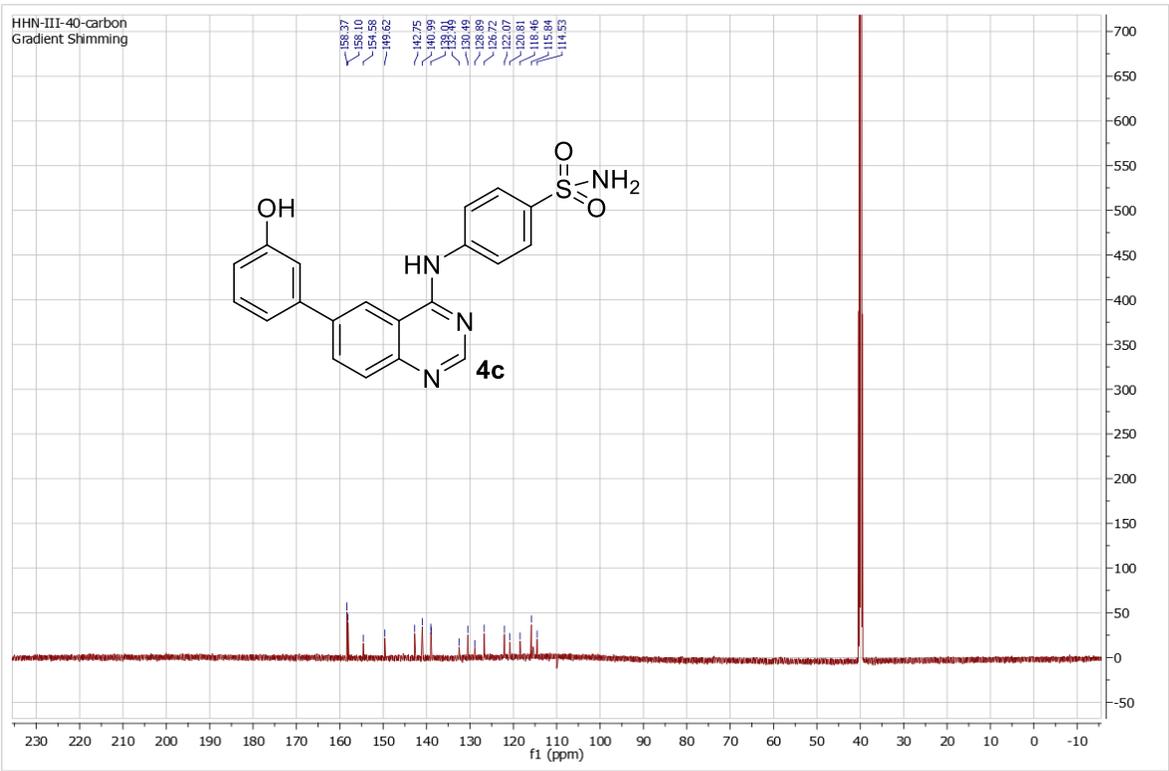


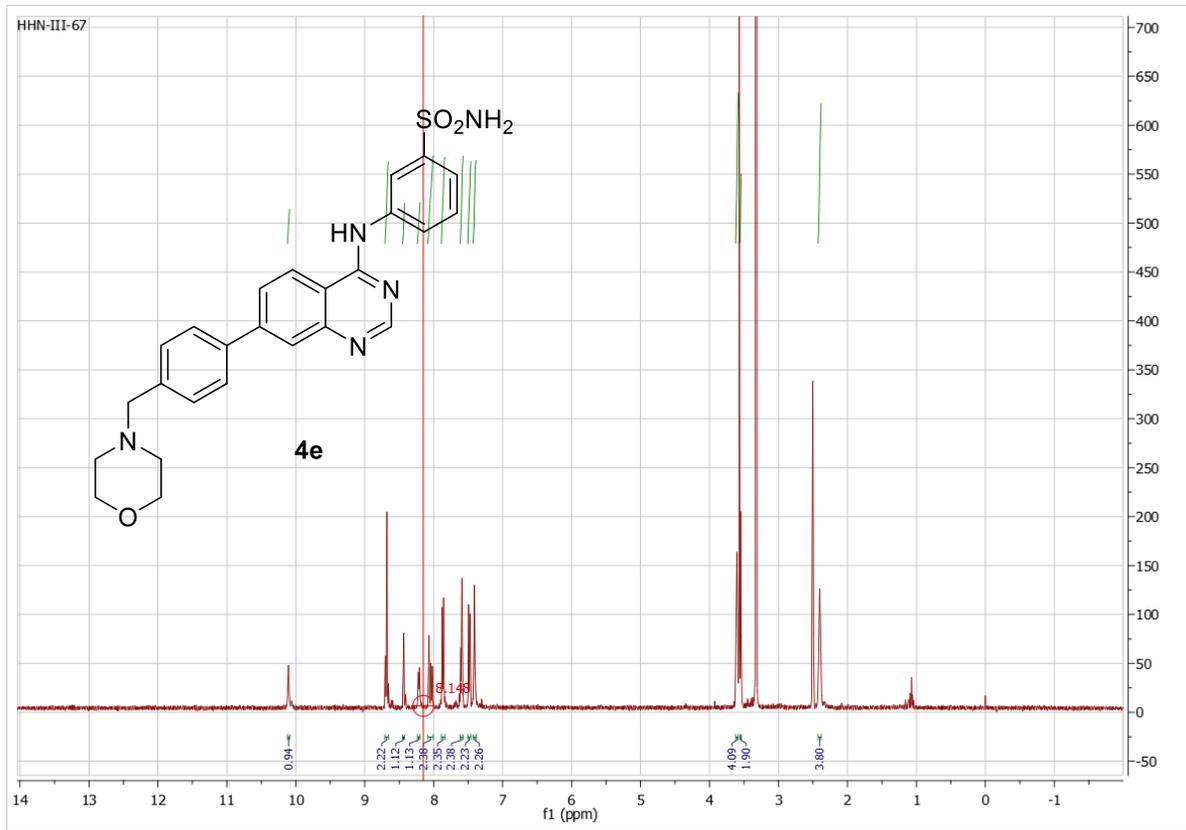
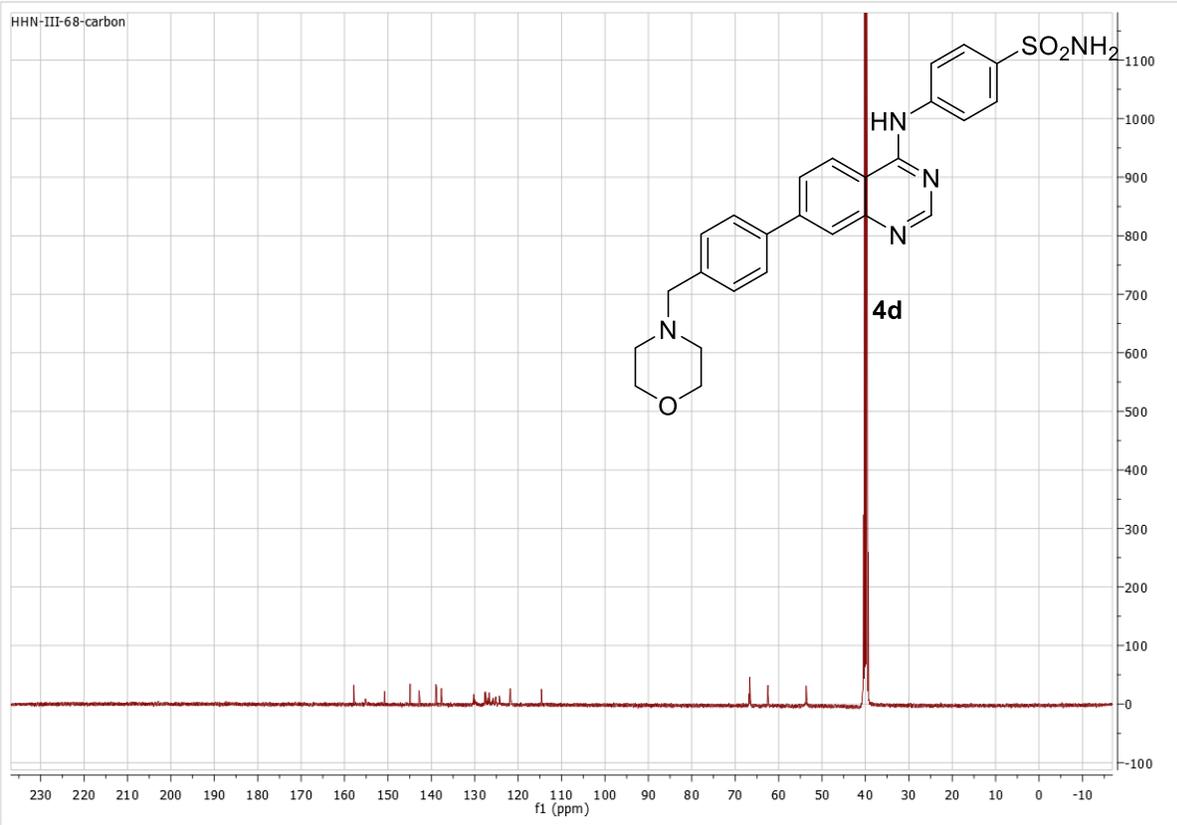




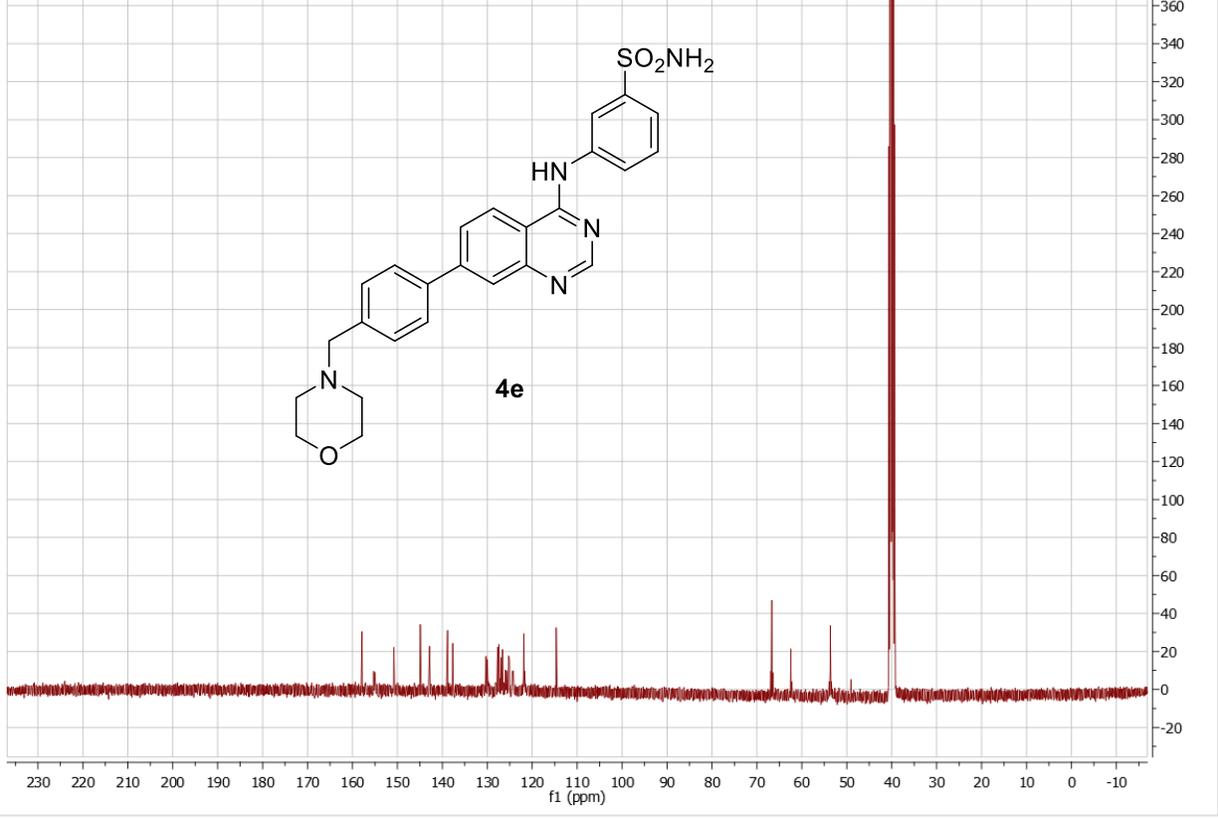




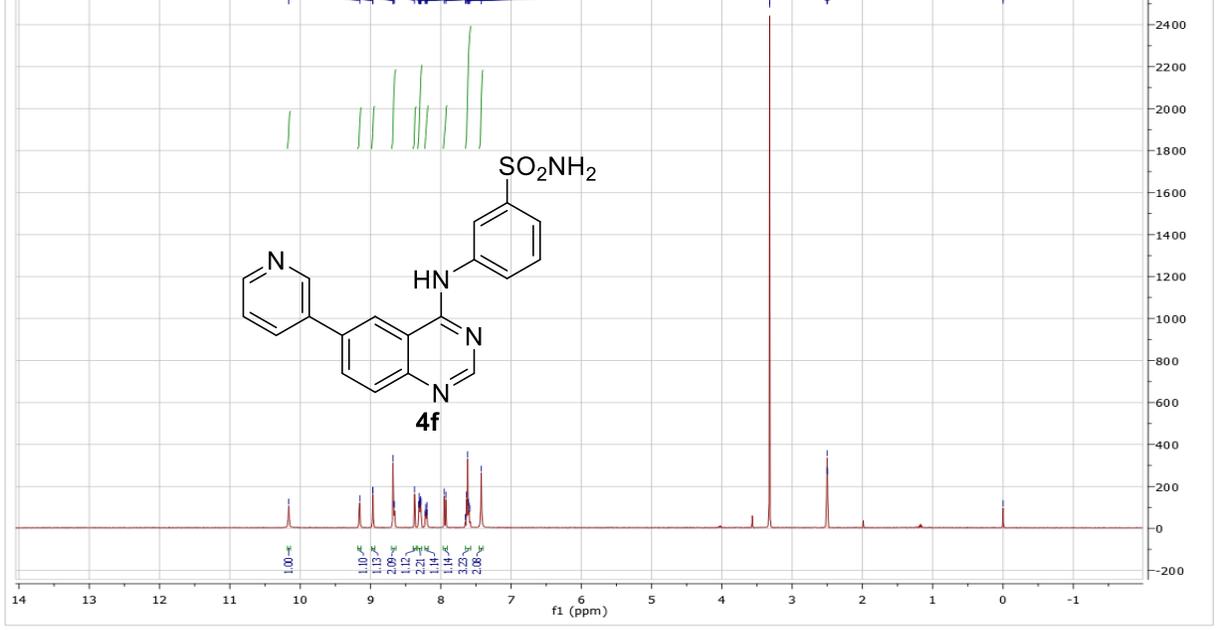




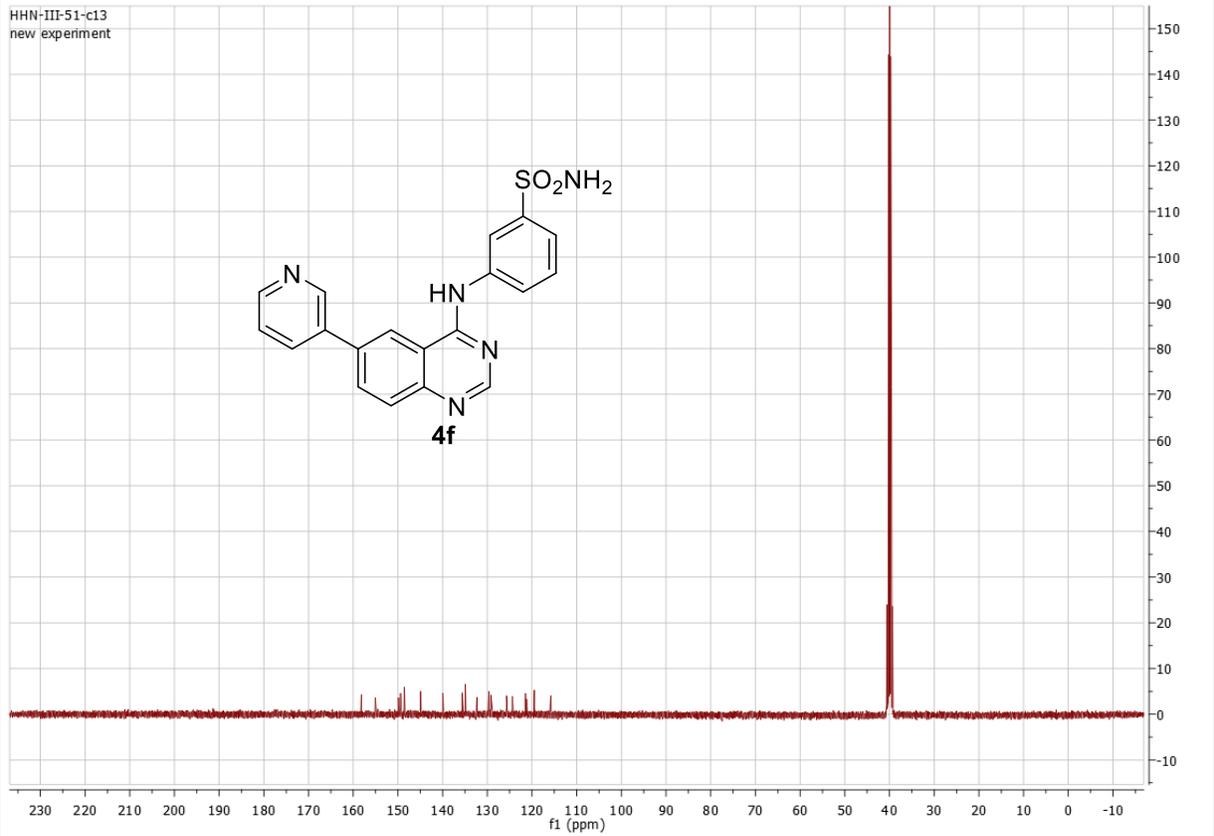
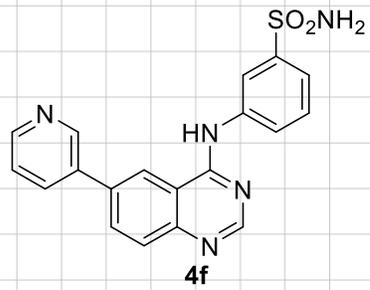
HHN-III-67carbon



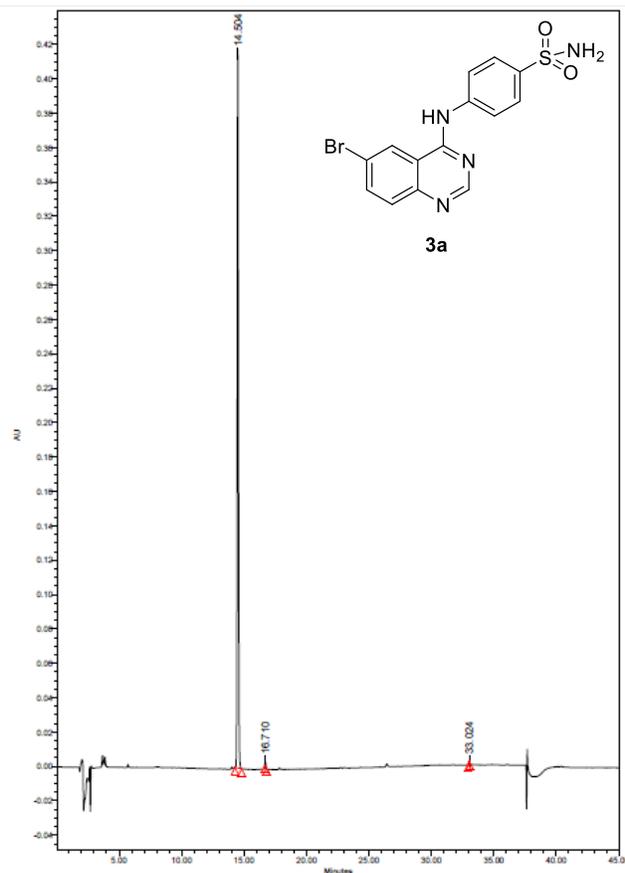
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new experiment



HHN-III-51-c13  
new experiment

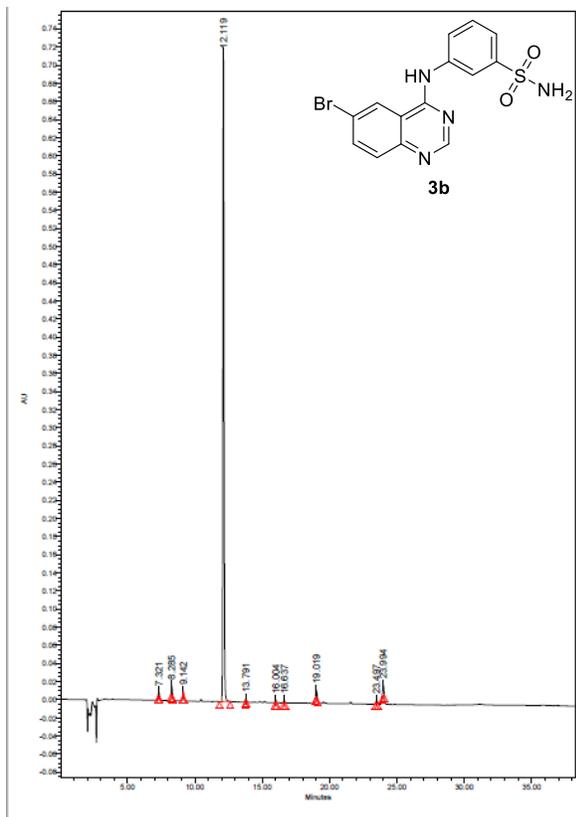


### 3. Representative HPLC purity data of the compounds 3a–d and 4a–f



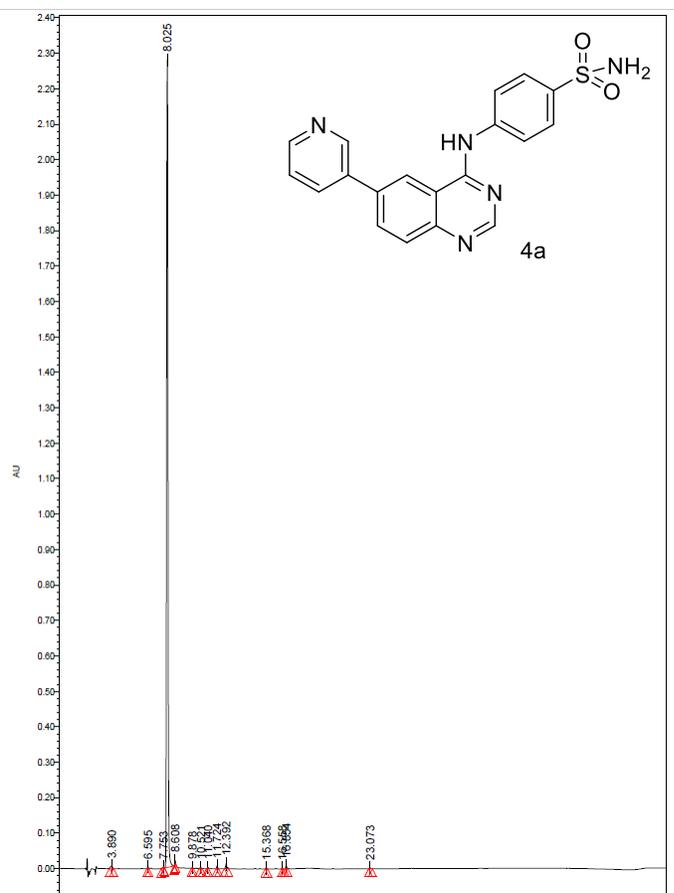
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1	14.504							2814904	99.46	418996	bb		
2	16.710							11749	0.42	2587	bb		
3	33.024							3664	0.13	851	bb		

Peak Type	Peak Codes
1 Unknown	
2 Unknown	
3 Unknown	



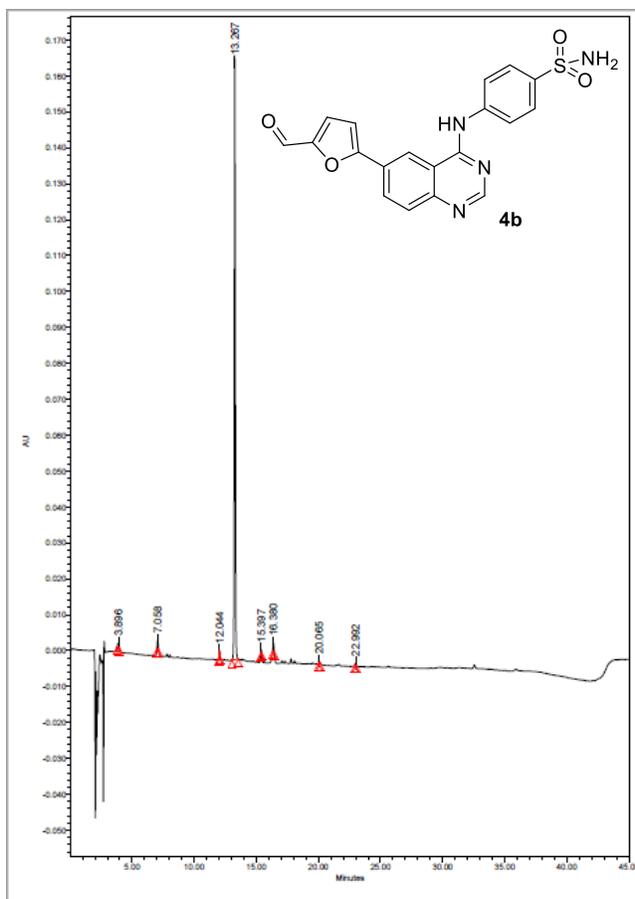
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1		7.321							19355	0.44	4478	bb		
2		8.285							40947	0.93	9778	bb		
3		9.142							12329	0.28	3927	bb		
4		12.119							4200300	95.11	719106	bb		
5		13.791							4753	0.11	1532	bb		
6		16.004							7963	0.18	1941	bb		
7		16.637							9446	0.21	1950	bb		
8		19.019							46554	1.05	8646	bb		
9		23.497							13240	0.30	2192	bb		
10		23.994							61570	1.39	11239	bb		

	Peak Type	Peak Codes
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2	Unknown	
3	Unknown	
4	Unknown	
5	Unknown	
6	Unknown	
7	Unknown	



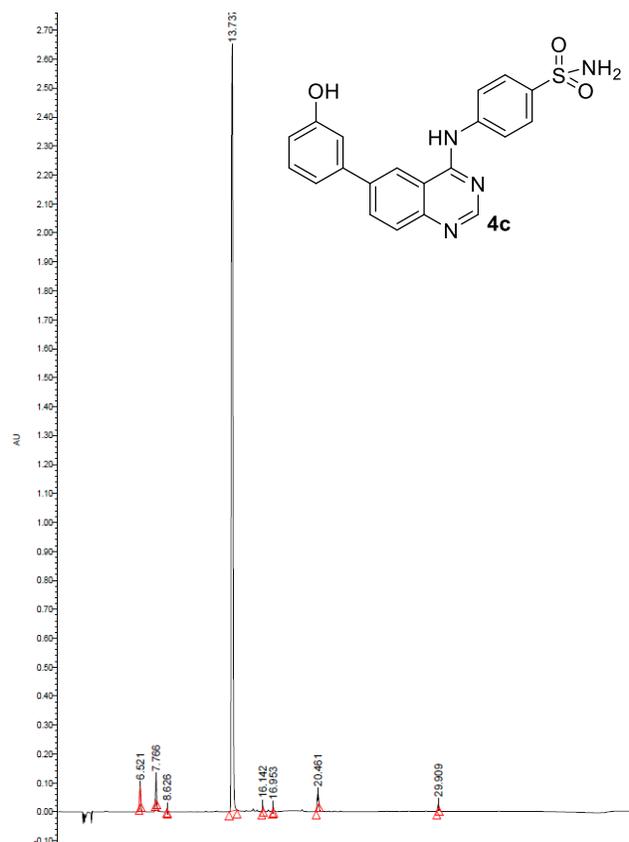
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1	3.890							63553	0.37	6105	bb		
2	6.595							22251	0.13	4998	bb		
3	7.753							21317	0.12	2894	bb		
4	8.025							16982488	97.84	2329599	bb		
5	8.608							40468	0.23	11424	bb		
6	9.878							4961	0.03	1133	bb		
7	10.521							8423	0.05	1935	bb		
8	11.040							4678	0.03	1354	bb		
9	11.724							34580	0.20	7203	bb		
10	12.392							91000	0.52	13377	bb		
11	15.368							12031	0.07	2334	bb		
12	16.558							8614	0.05	2011	bb		
13	16.854							47861	0.28	9054	bb		
14	23.073							14914	0.09	2018	bb		

Peak Type	Peak Codes
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2 Unknown	
3 Unknown	



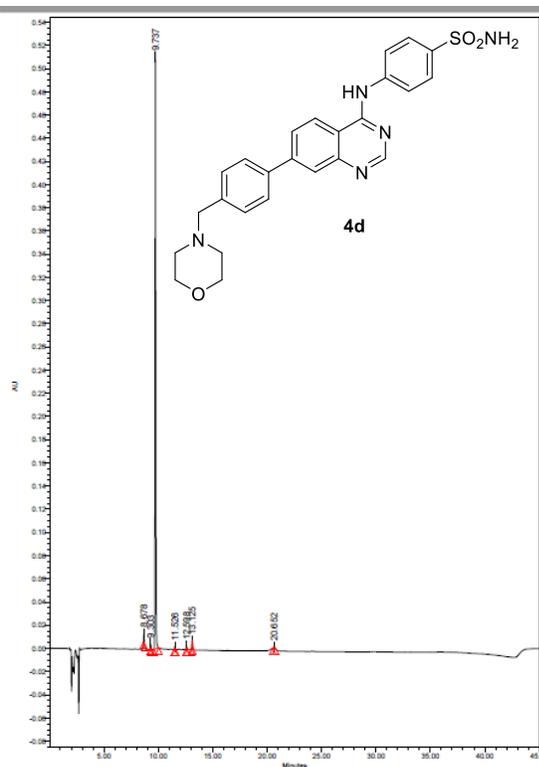
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1	3.896							9414	0.92	1205	bb		
2	7.058							11571	1.13	2388	bb		
3	12.044							5960	0.58	1692	bb		
4	13.267							977556	95.54	167740	bb		
5	15.397							2373	0.23	950	bb		
6	16.380							11354	1.11	2287	bb		
7	20.065							2506	0.24	490	bb		
8	22.992							2450	0.24	495	bb		

Peak Type	Peak Codes
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2 Unknown	
3 Unknown	
4 Unknown	
5 Unknown	
6 Unknown	
7 Unknown	
8 Unknown	



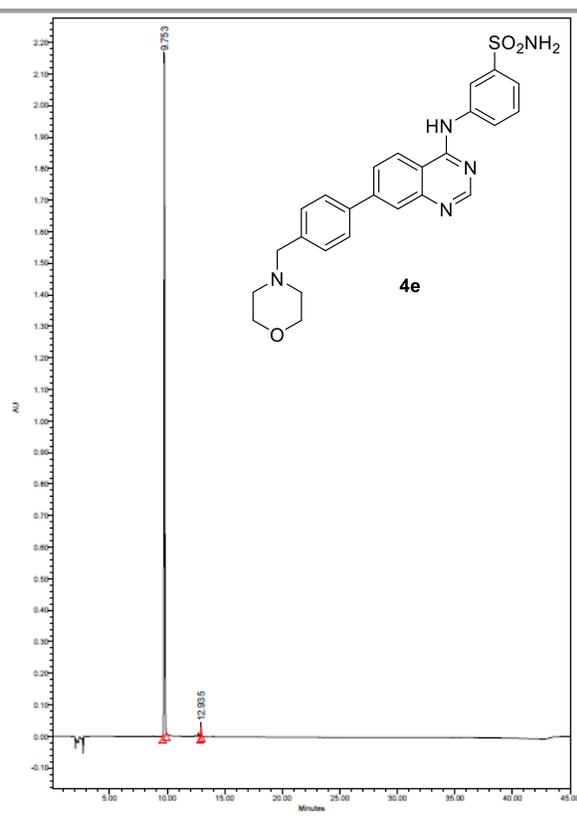
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1		6.521							356940	1.44	61650	bb		
2		7.766							366231	1.47	78682	bb		
3		8.626							9721	0.04	3802	bb		
4		13.737							23613610	95.10	2674274	bb		
5		16.142							42853	0.17	11096	bb		
6		16.953							30956	0.12	8644	bb		
7		20.461							333272	1.34	43255	bb		
8		29.909							76127	0.31	13868	bb		

	Peak Type	Peak Codes
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2	Unknown	
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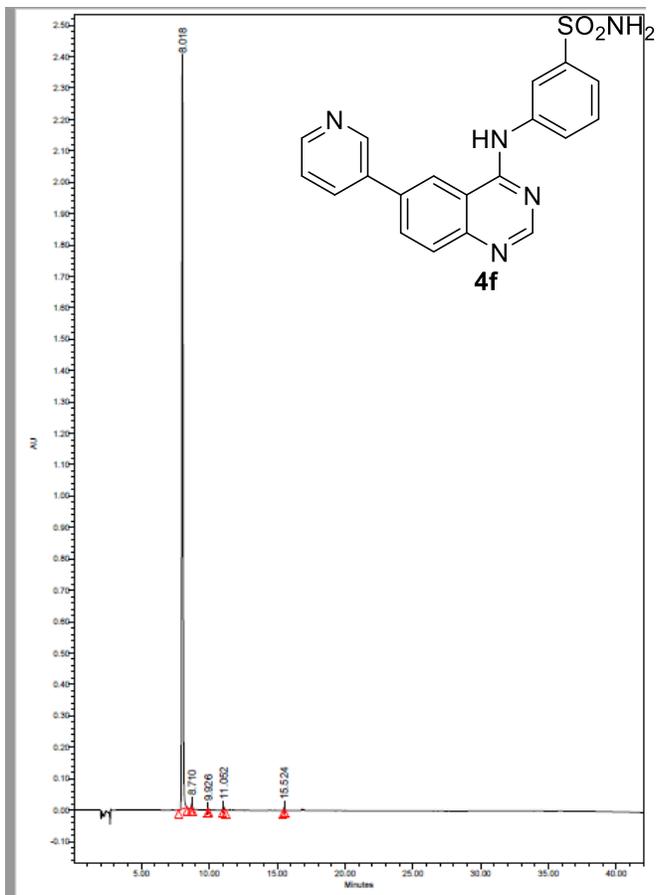
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1	8.678							28190	1.13	7920	bb		
2	9.303							14303	0.57	3748	bb		
3	9.737							2415863	96.63	506364	bb		
4	11.526							4588	0.18	1490	bb		
5	12.598							7205	0.29	2042	bb		
6	13.125							25605	1.02	6520	bb		
7	20.652							4487	0.18	505	bb		

Peak Type	Peak Codes
1 Unknown	
2 Unknown	
3 Unknown	
4 Unknown	
5 Unknown	
6 Unknown	
7 Unknown	



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	9.753							11379618	99.15	2167466	bb		
2	12.935							98094	0.85	23466	bb		

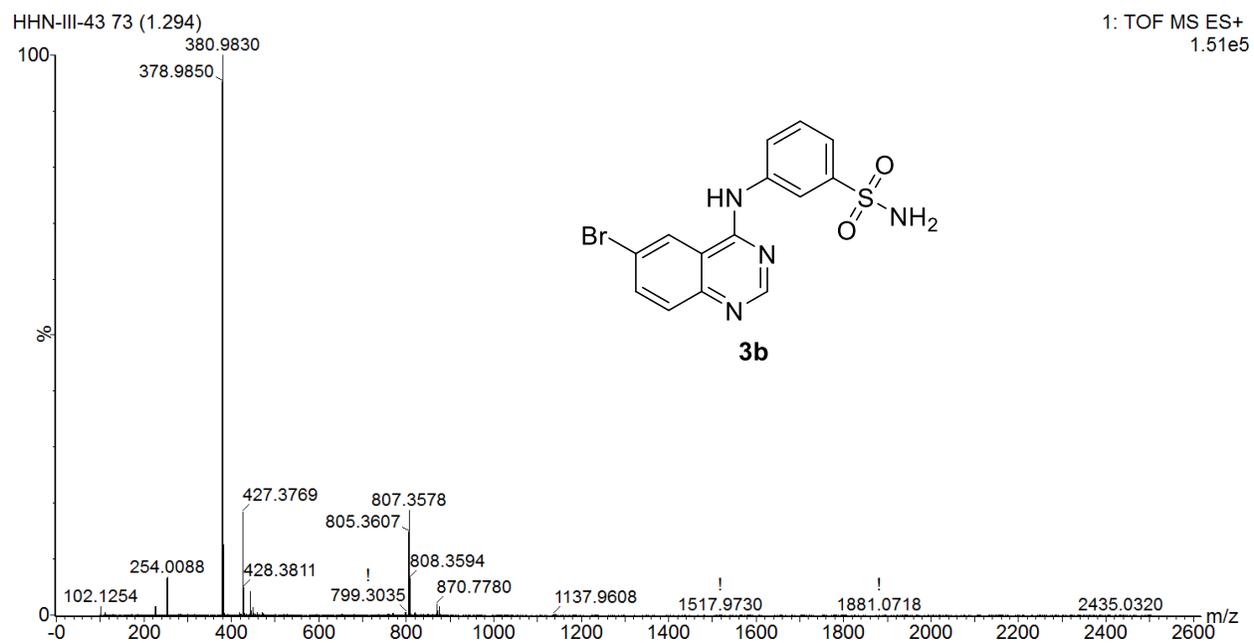
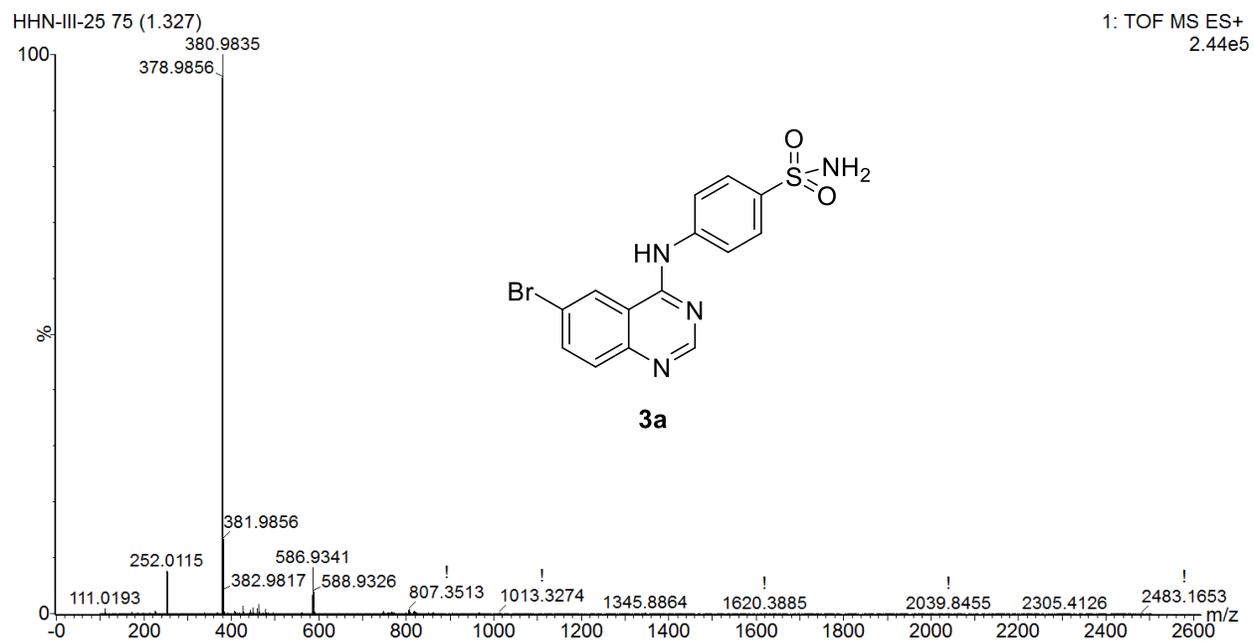
Peak Type	Peak Codes
1 Unknown	
2 Unknown	



Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	Height ( $\mu\text{V}$ )	Int Type	Amount	Units
1	8.018							14986262	98.93	2414157	bb		
2	8.710							54838	0.36	13790	bb		
3	9.926							6003	0.04	2000	bb		
4	11.052							63323	0.42	9654	bb		
5	15.524							38428	0.25	8270	bb		

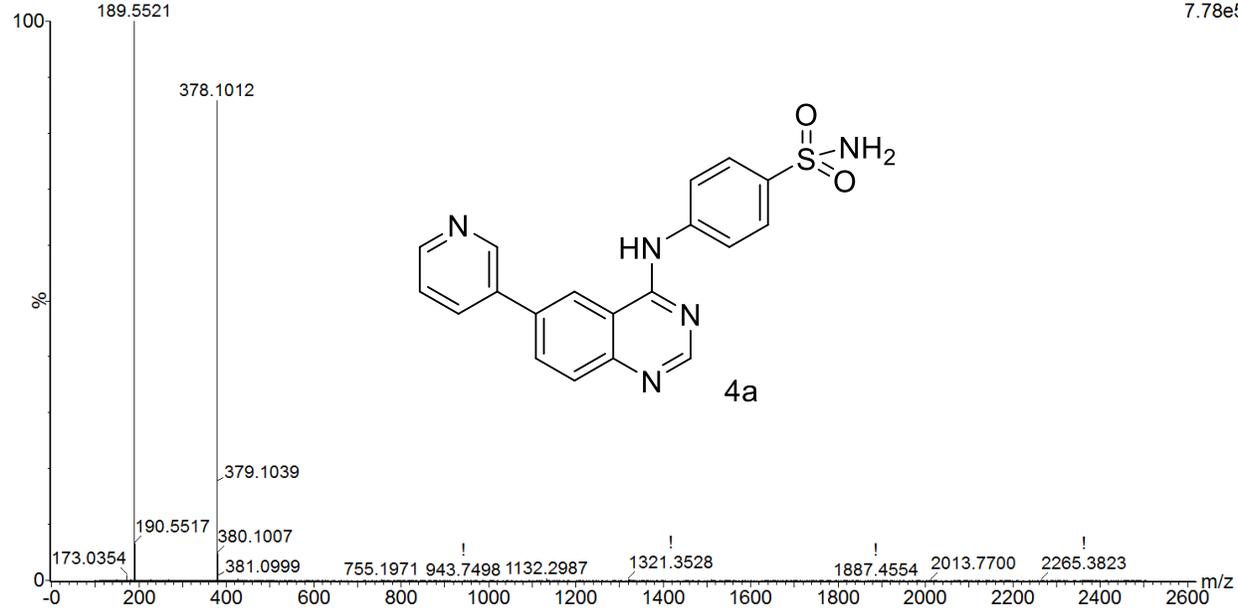
Peak Type	Peak Codes
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3	Unknown
4	Unknown
5	Unknown

#### 4. Representative HRMS data of the compounds 3a-d and 4a-f



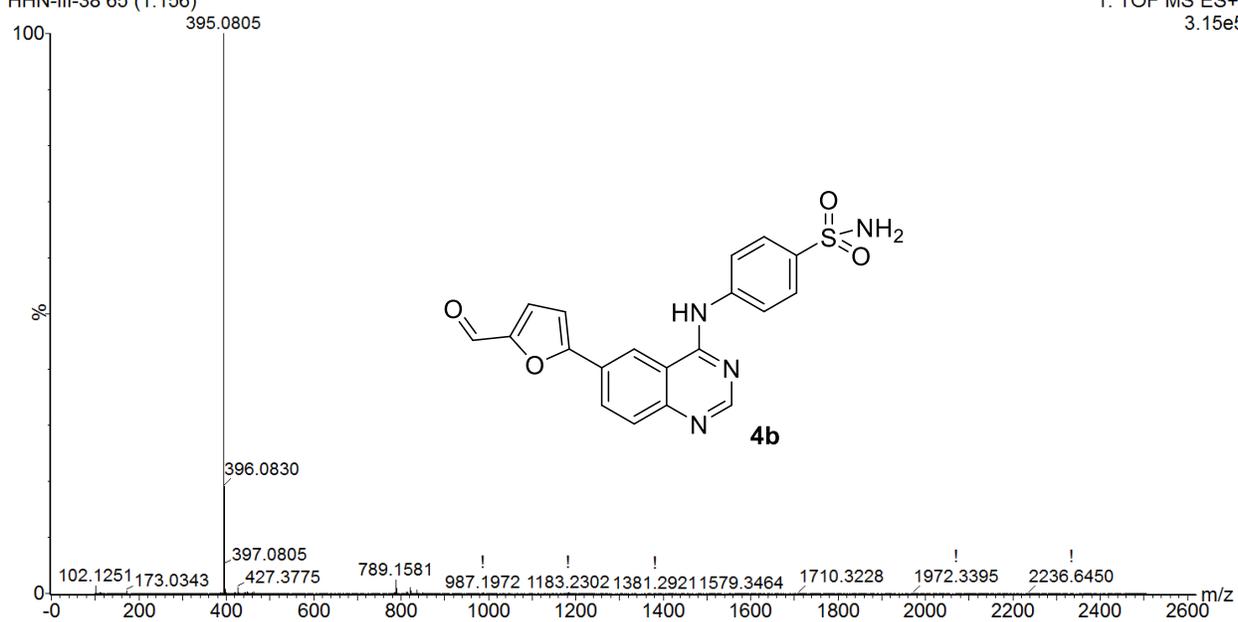
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1: TOF MS ES+  
7.78e5



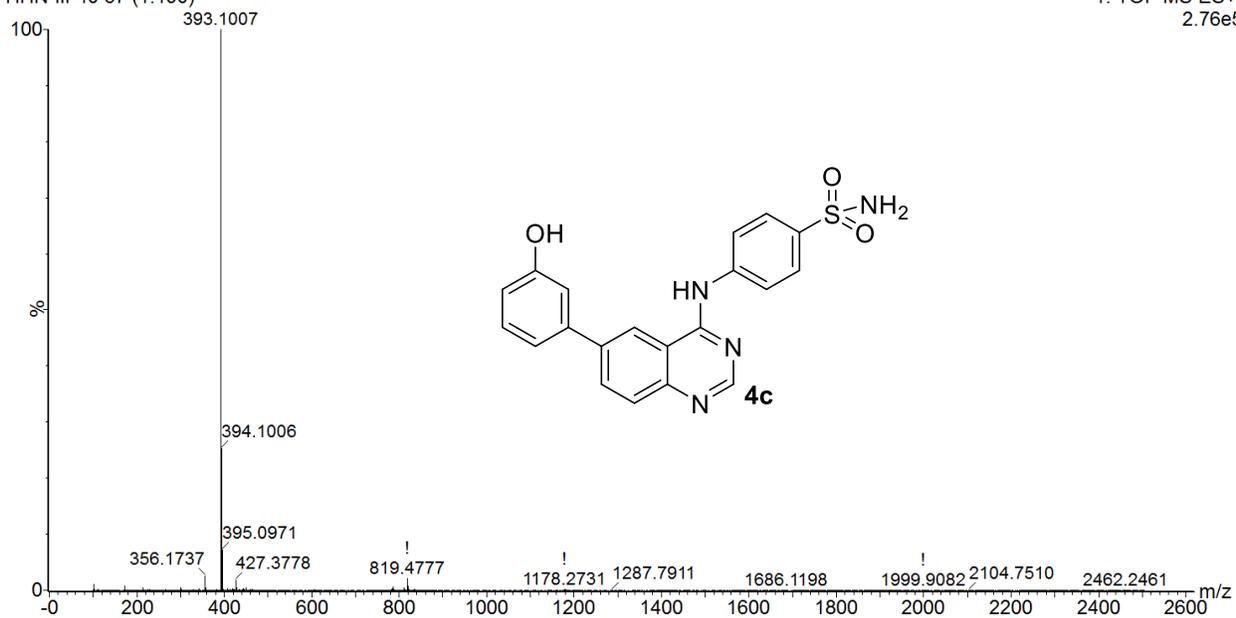
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3.15e5



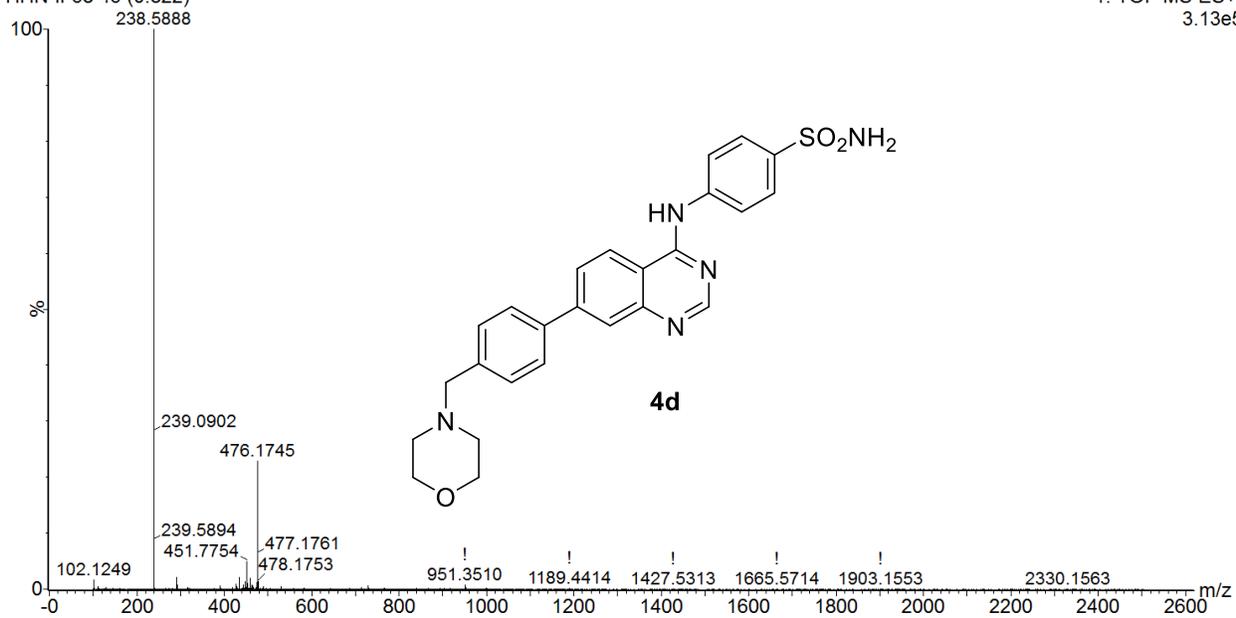
HHN-III-40 67 (1.190)

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2.76e5



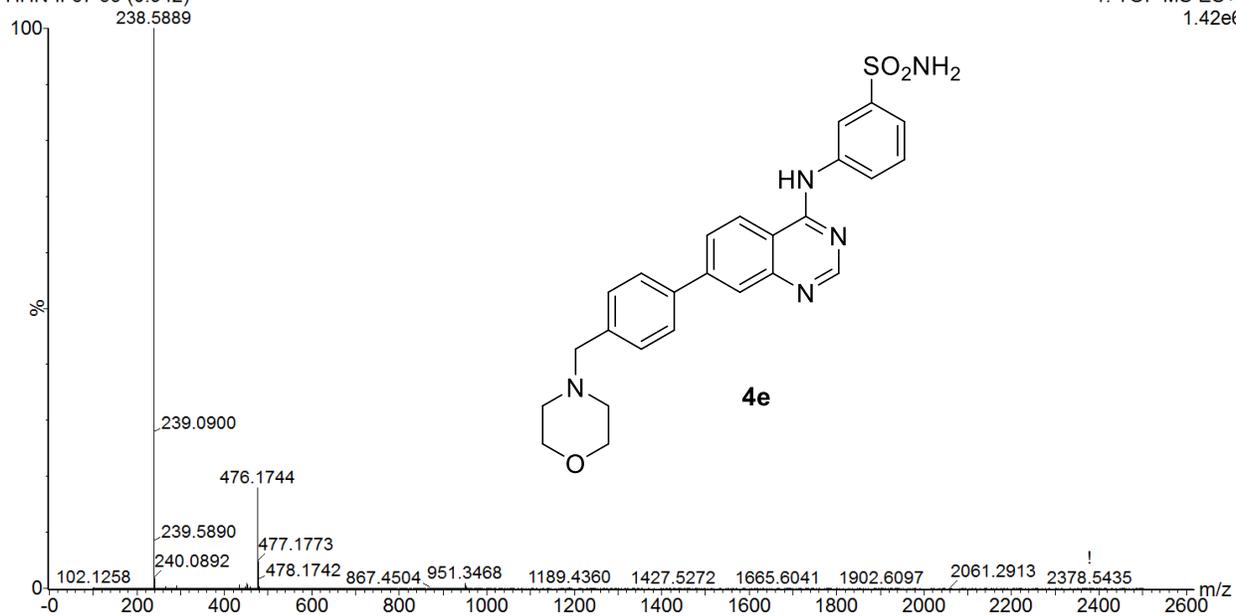
HHN-II-68 46 (0.822)

1: TOF MS ES+  
3.13e5



HHN-II-67 53 (0.942)

1: TOF MS ES+  
1.42e6



HHN-III-51 87 (1.541)

1: TOF MS ES+  
1.02e5

