

Supplementary Data

Lead Optimization of TOPK Inhibitors using Complementary Computational and Synthetic Approaches

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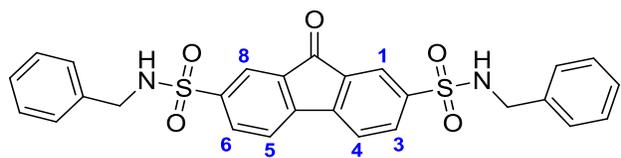
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E-mail: nashari@just.edu.jo (Nizar A. Al-Shar'i)

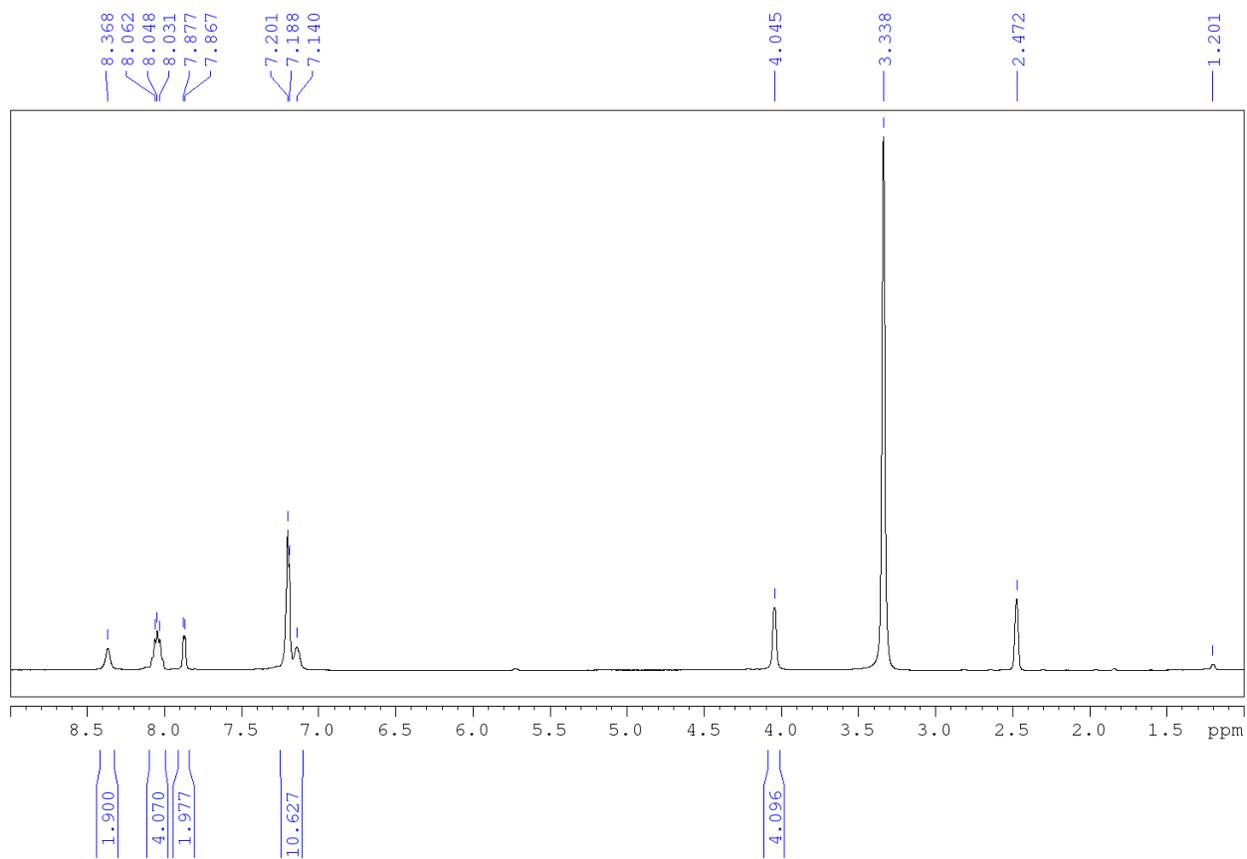
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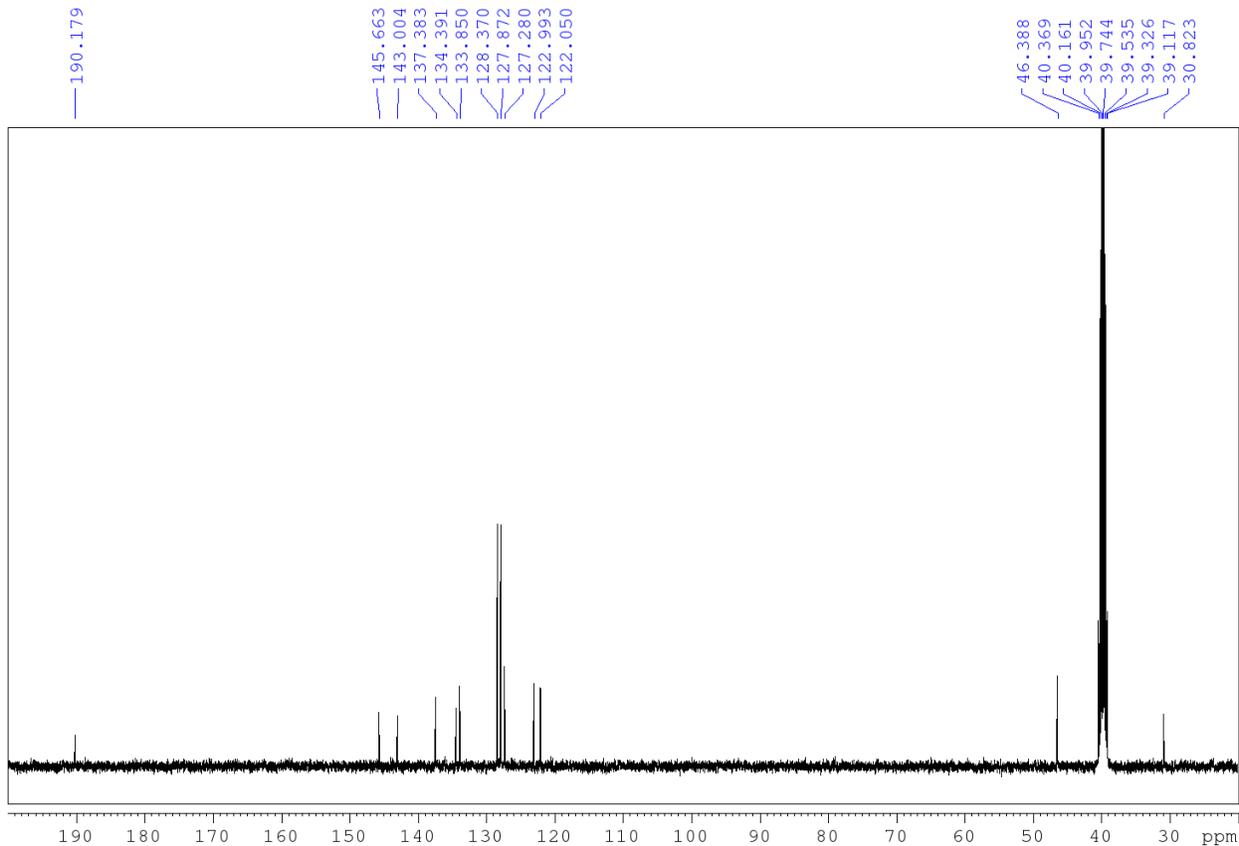
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¹³ C NMR spectrum of compound 1	S-4
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Compound 1

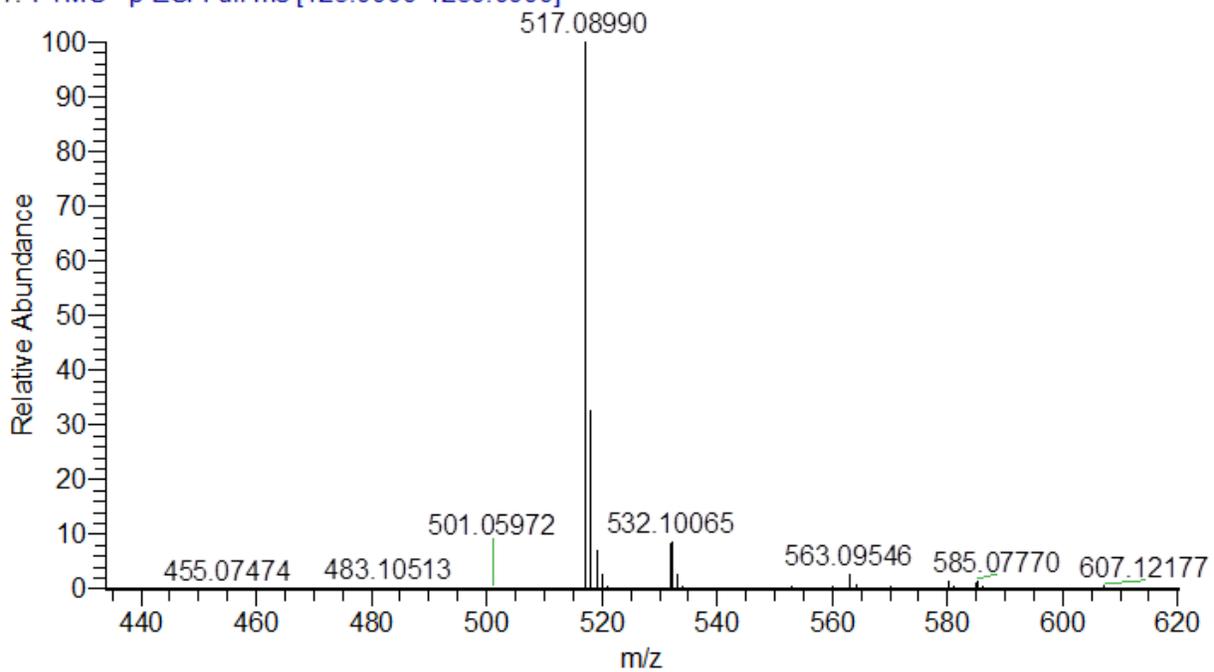


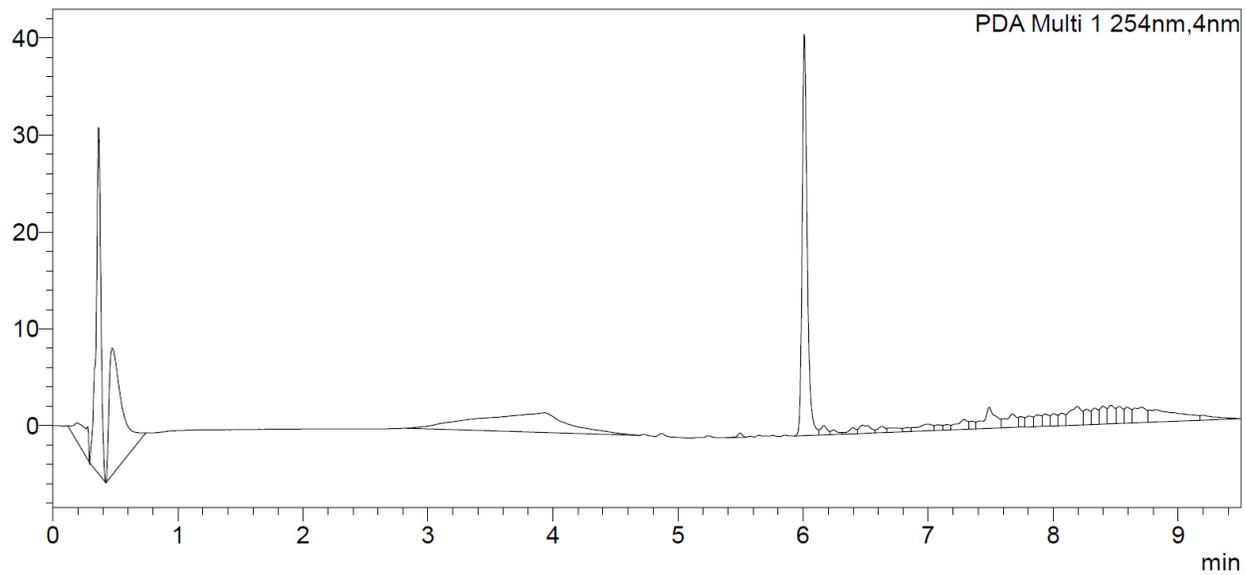
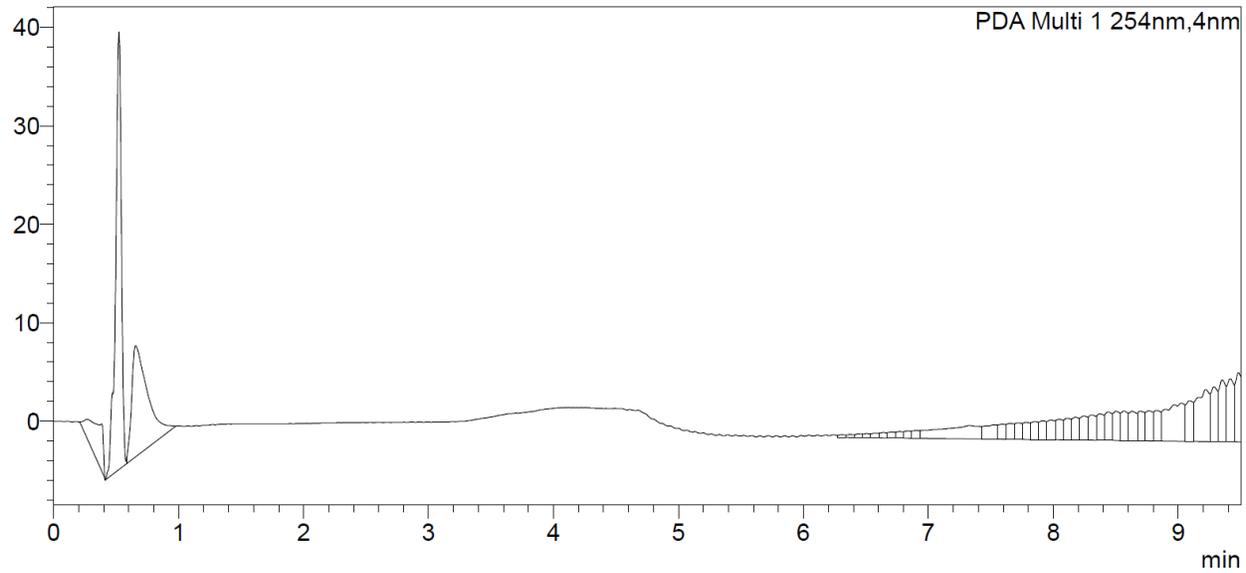
*N*²,*N*⁷-dibenzyl-9-oxo-9*H*-fluorene-2,7-disulfonamide



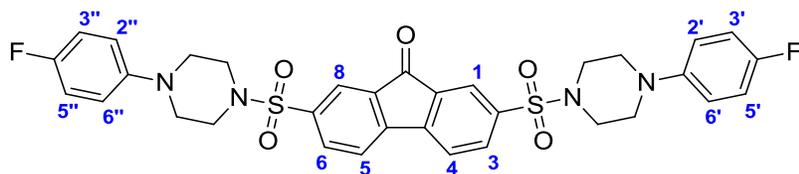


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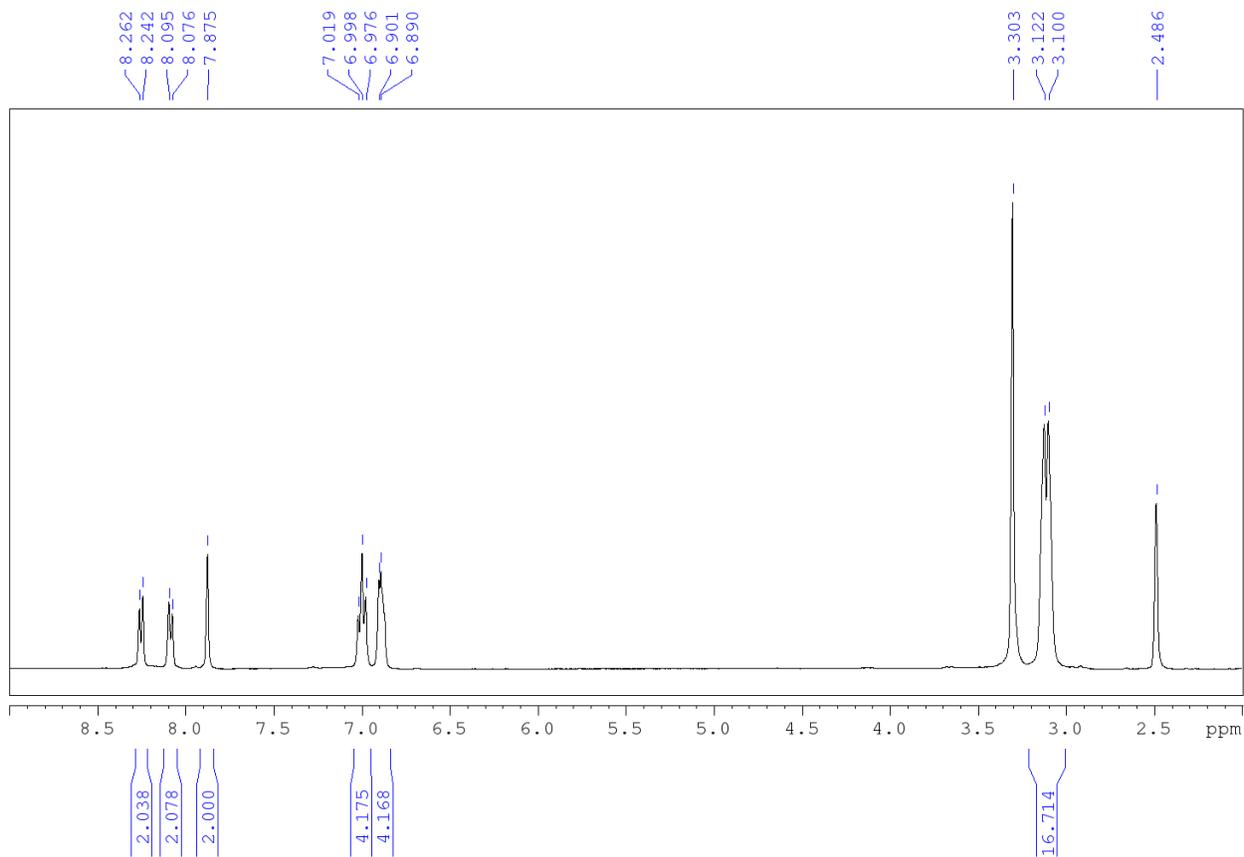


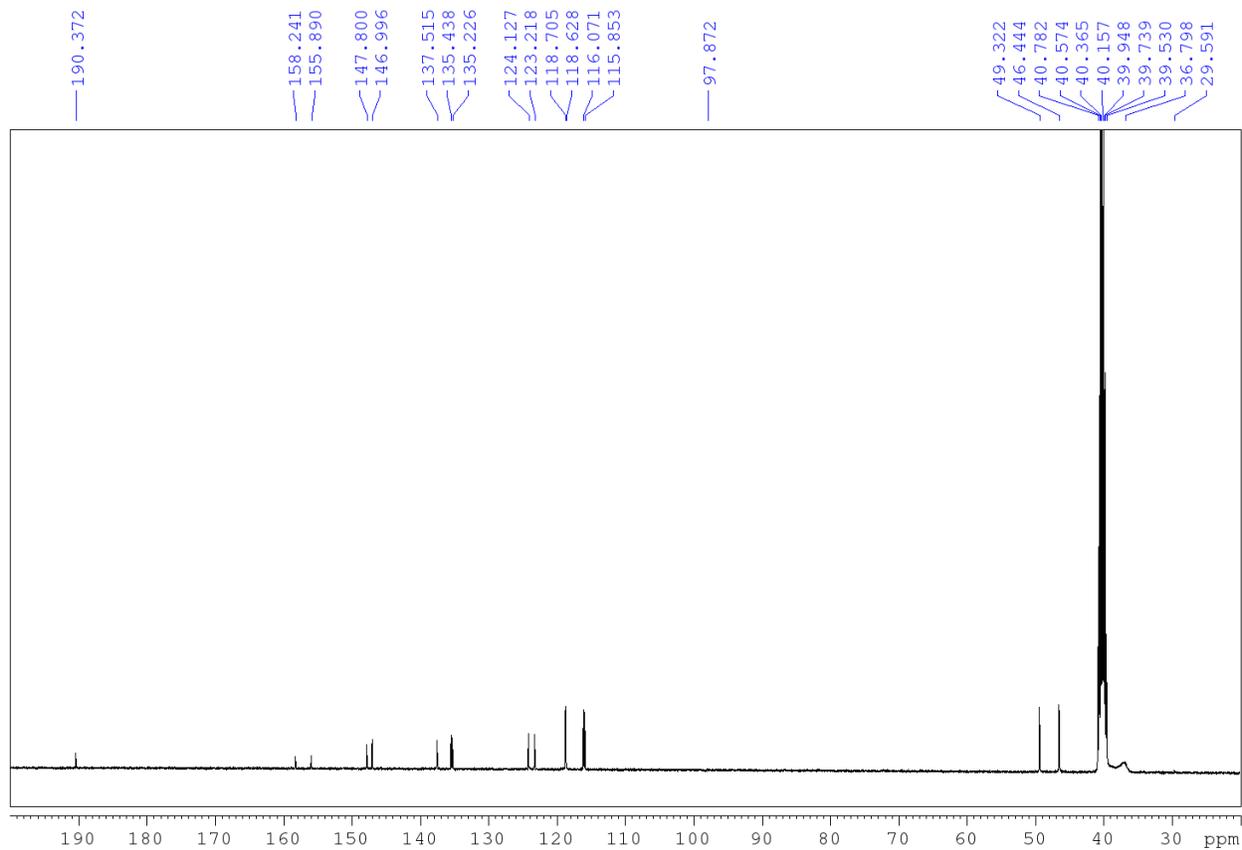


Compound 6

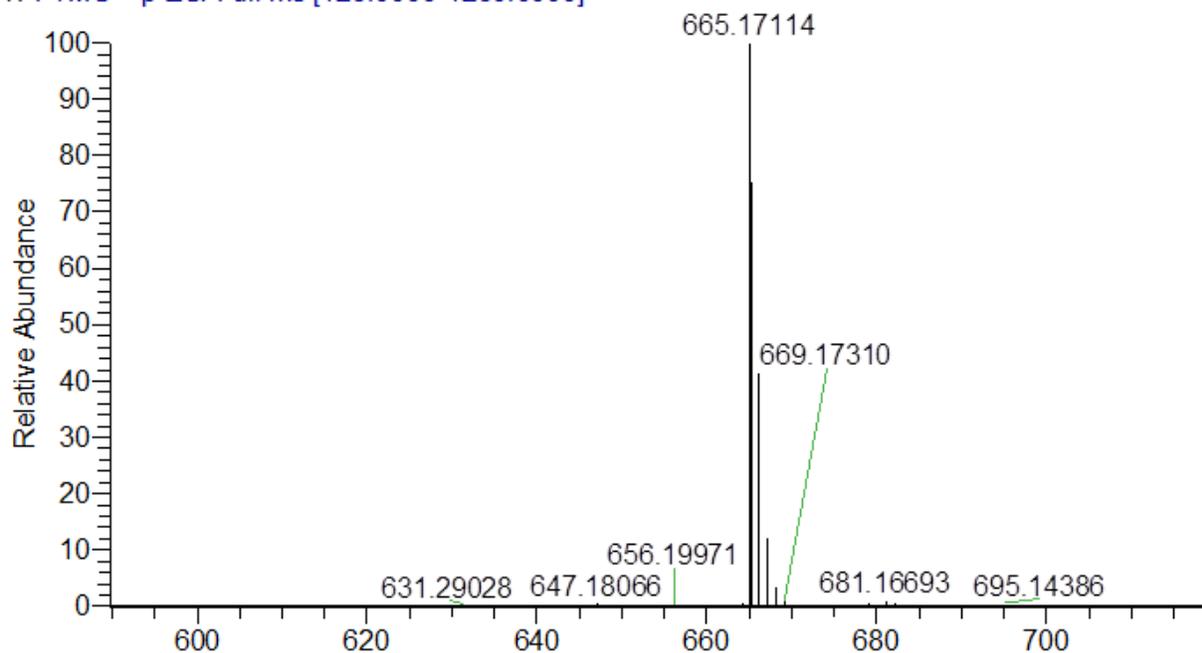


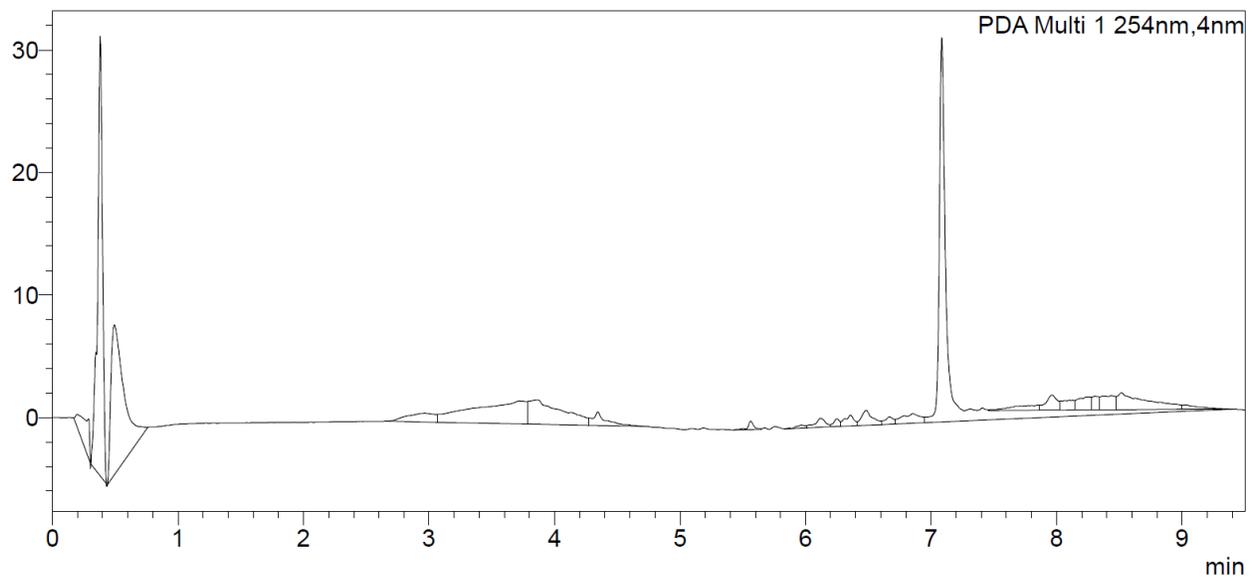
2,7-bis((4-fluorophenyl)piperazin-1-yl)sulfonyl-9H-fluoren-9-one



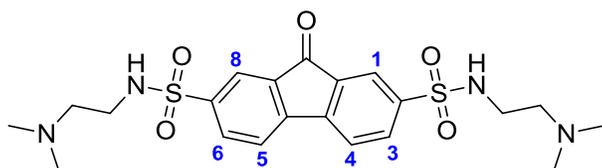


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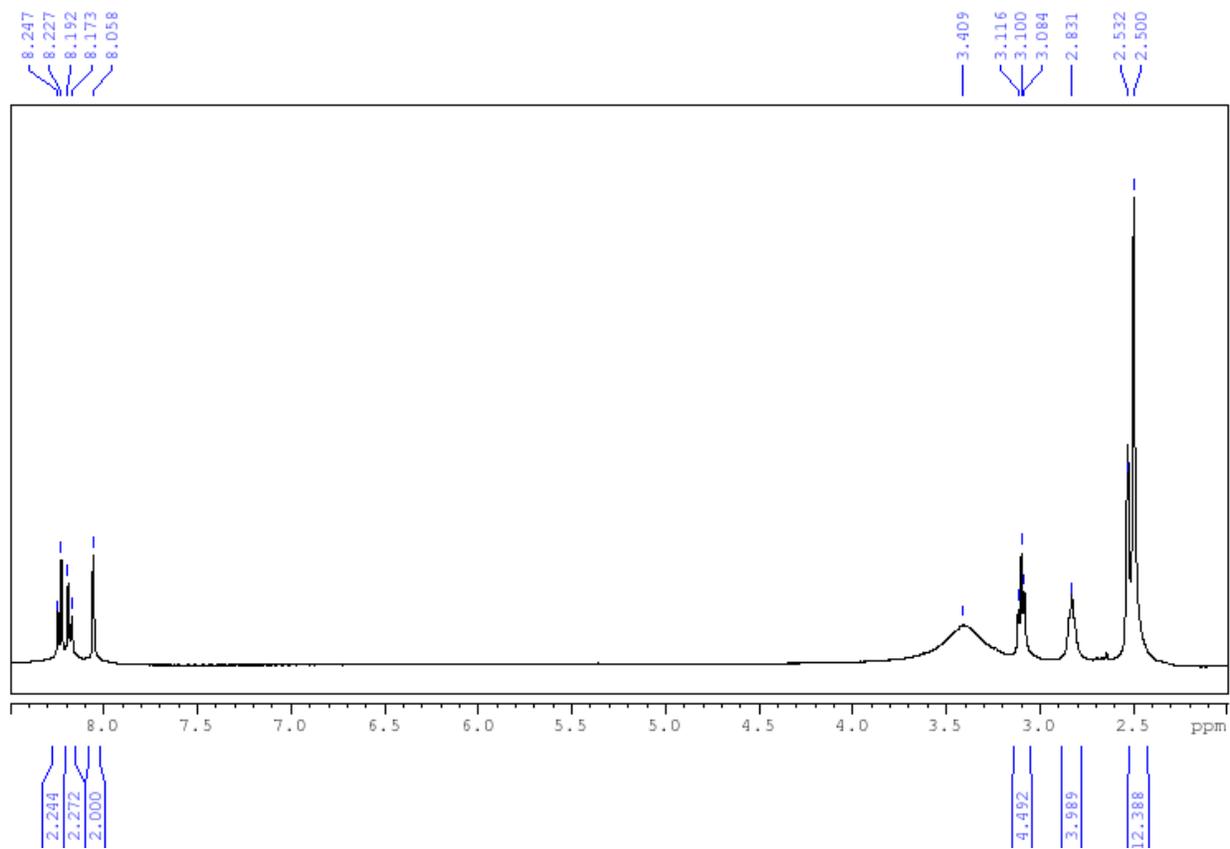


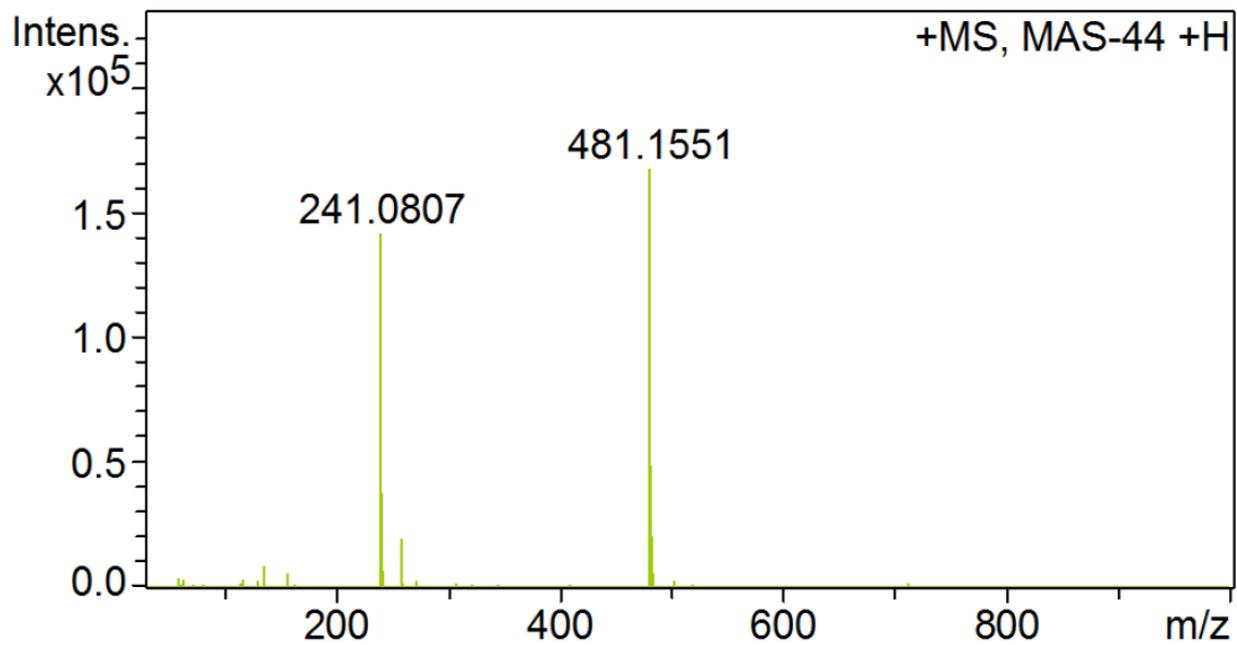
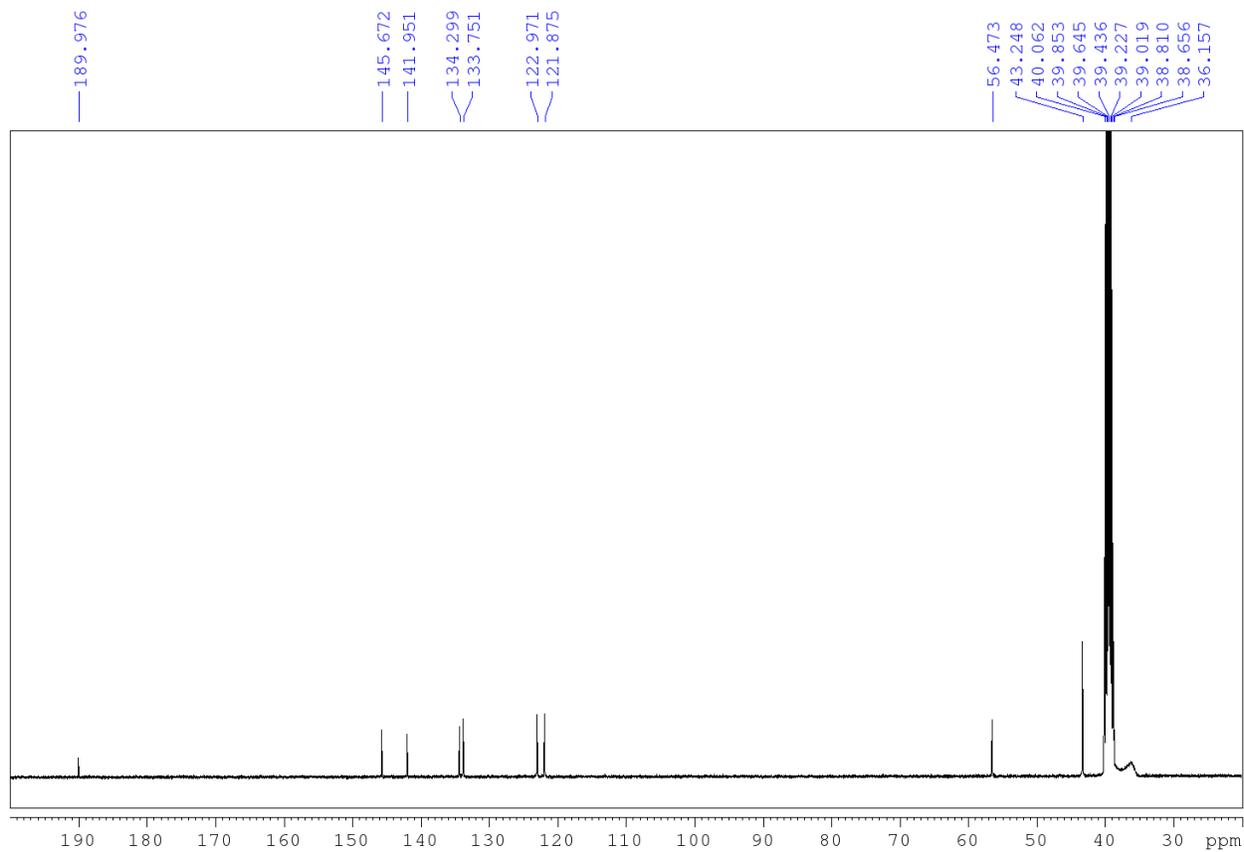


Compound 7

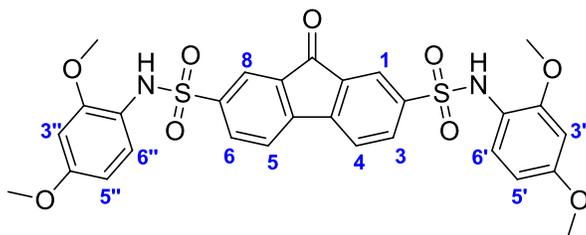


*N*²,*N*⁷-bis(2-(dimethylamino)ethyl)-9-oxo-9*H*-fluorene-2,7-disulfonamide

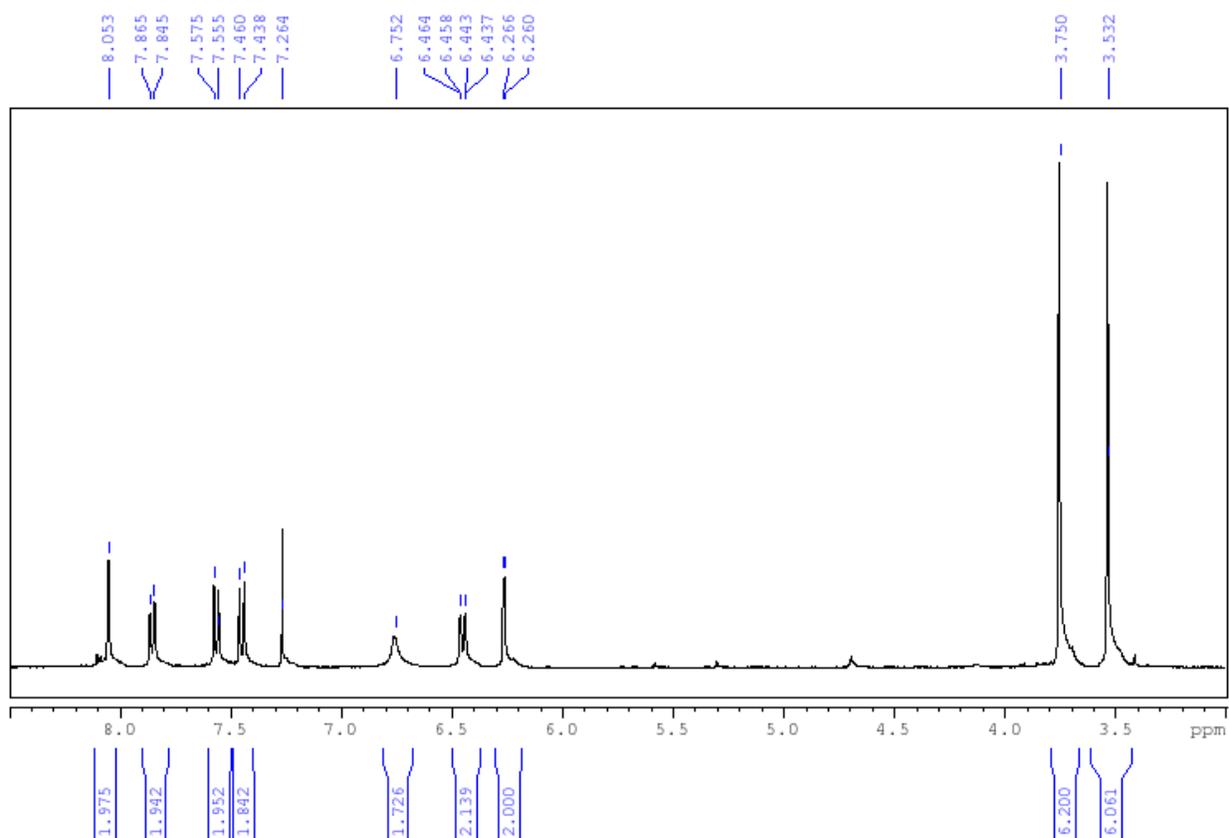


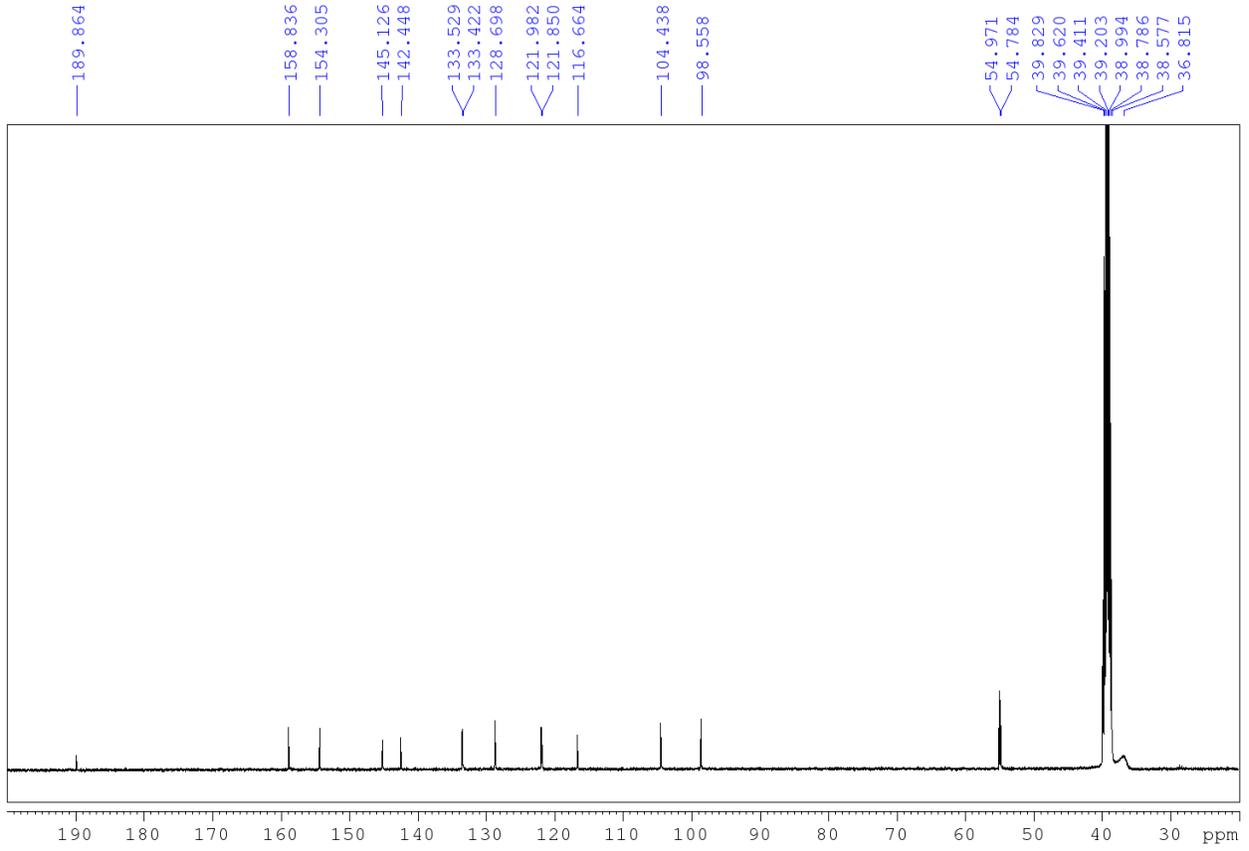


Compound 8

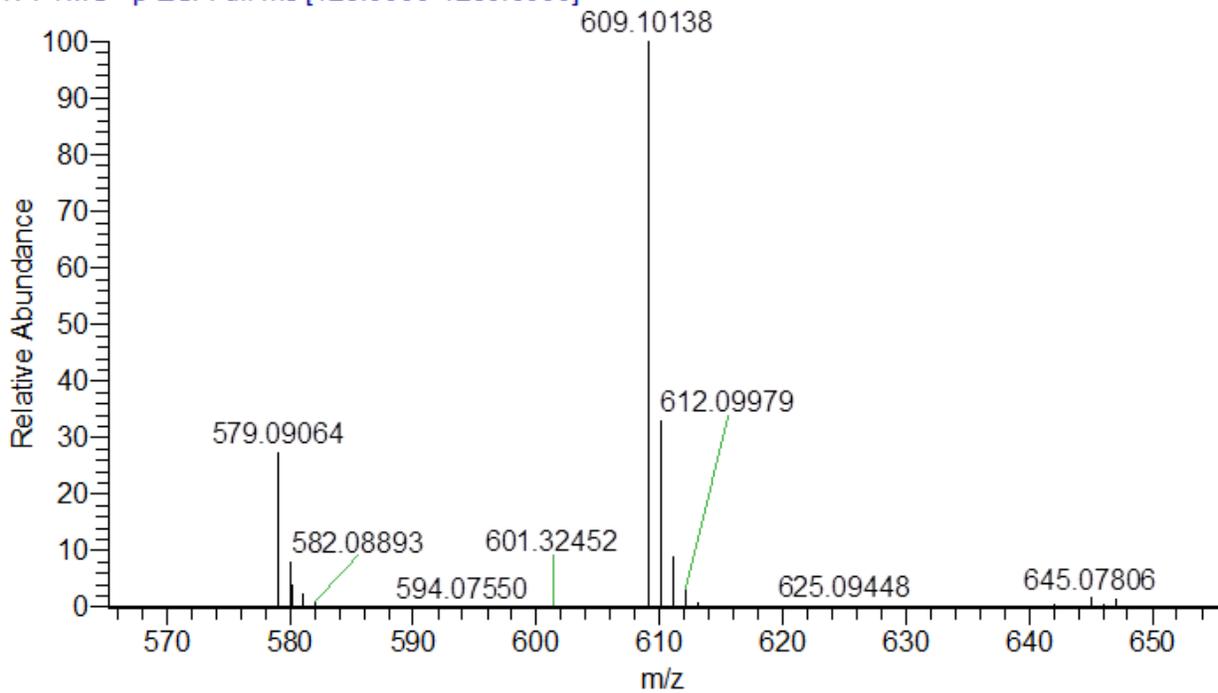


*N*²,*N*⁷-bis(2,4-dimethoxyphenyl)-9-oxo-9*H*-fluorene-2,7-disulfonamide

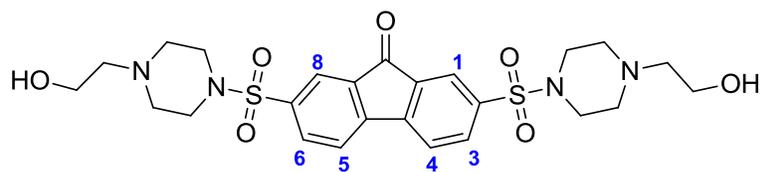




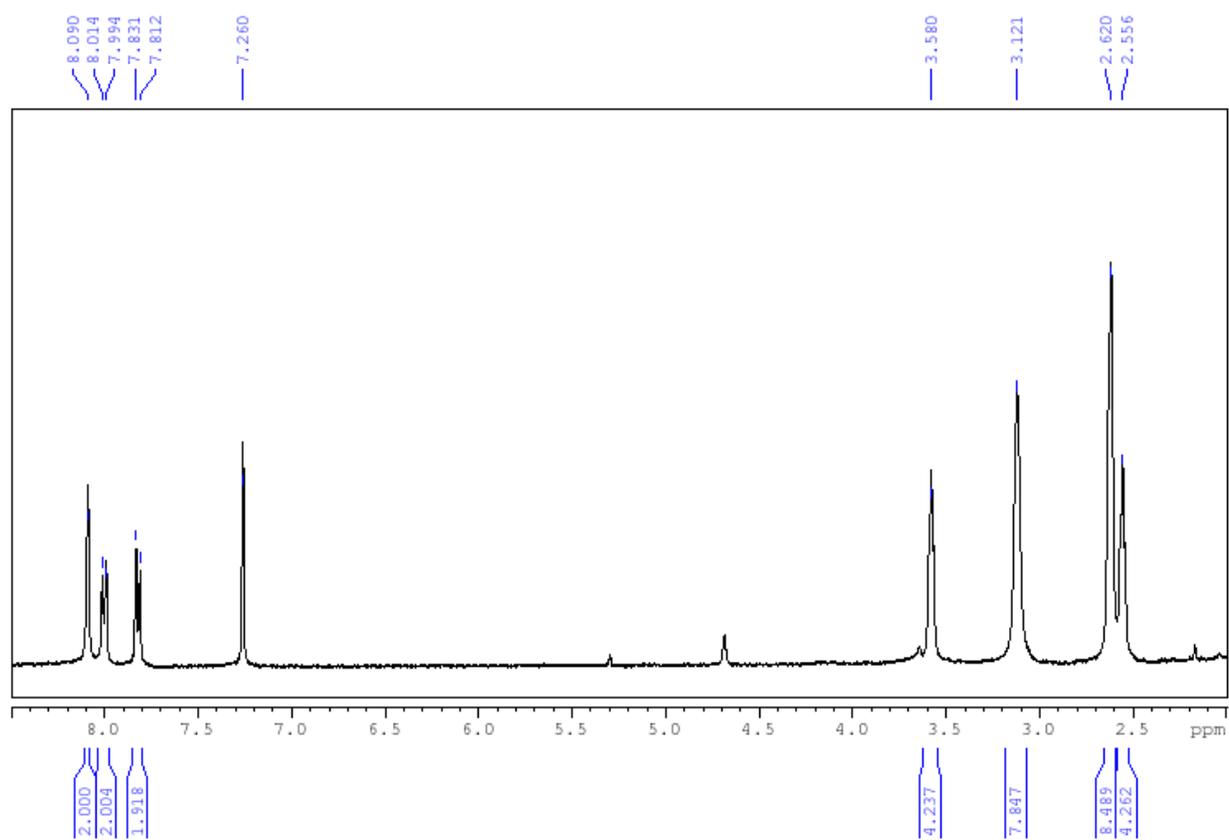
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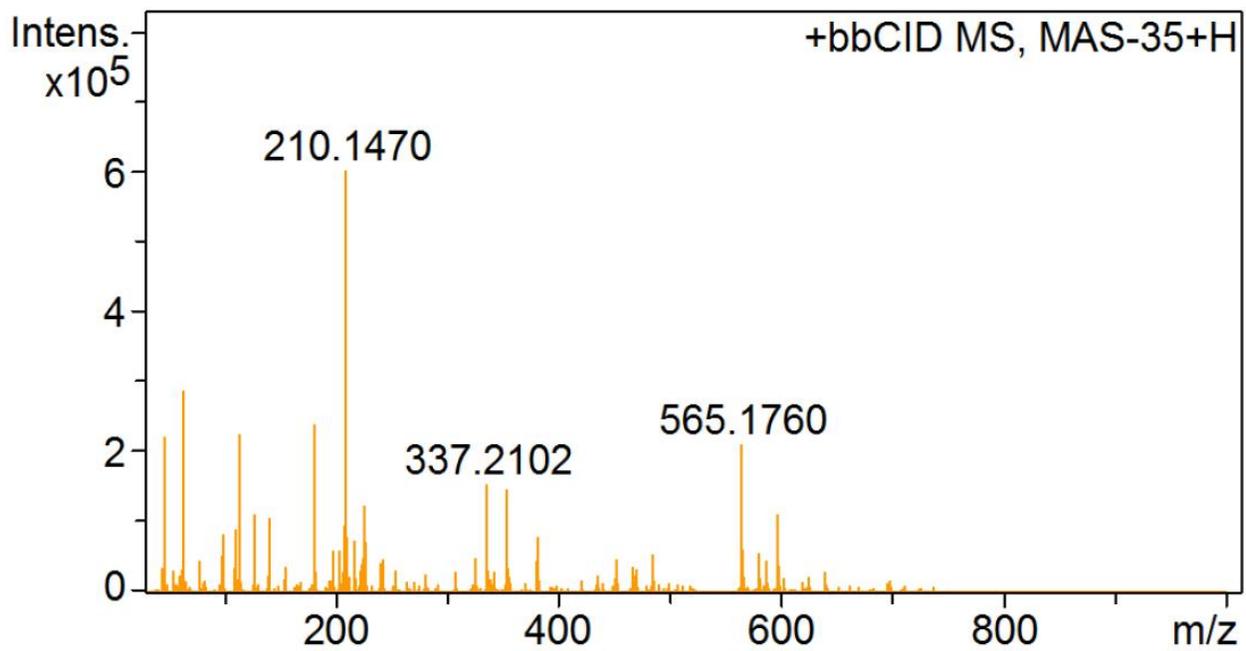
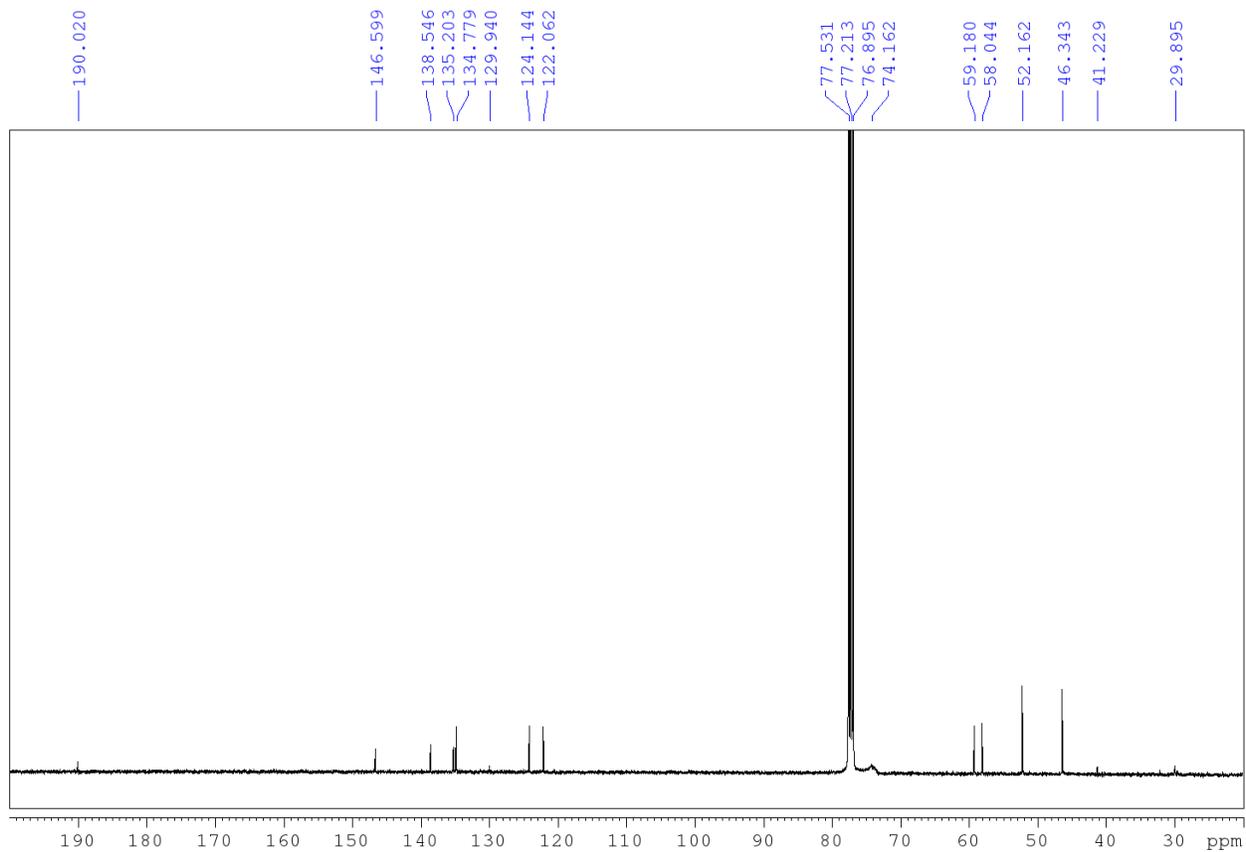


Compound 9

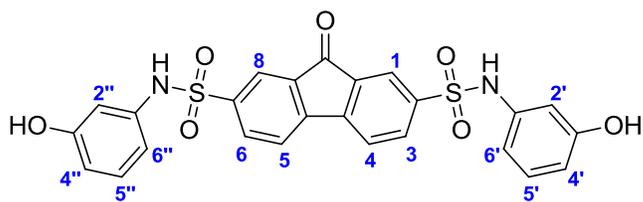


2,7-bis((4-(2-hydroxyethyl)piperazin-1-yl)sulfonyl)-9H-fluoren-9-one

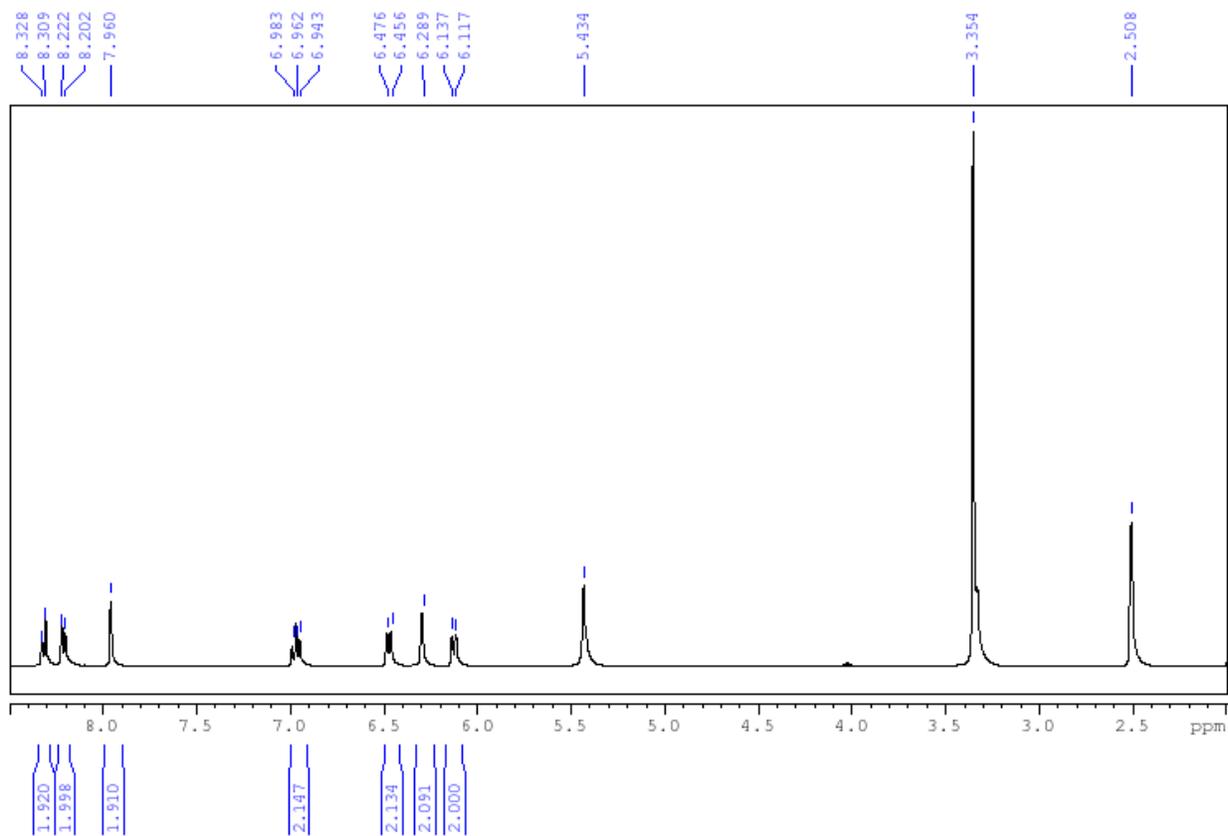


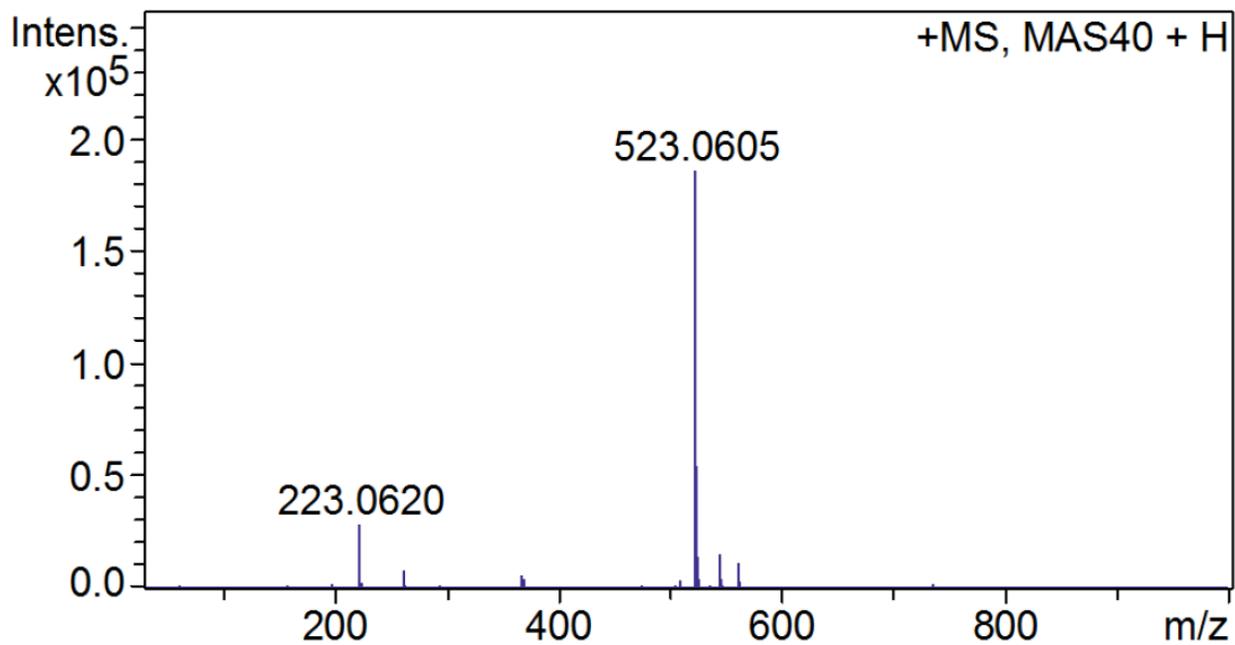
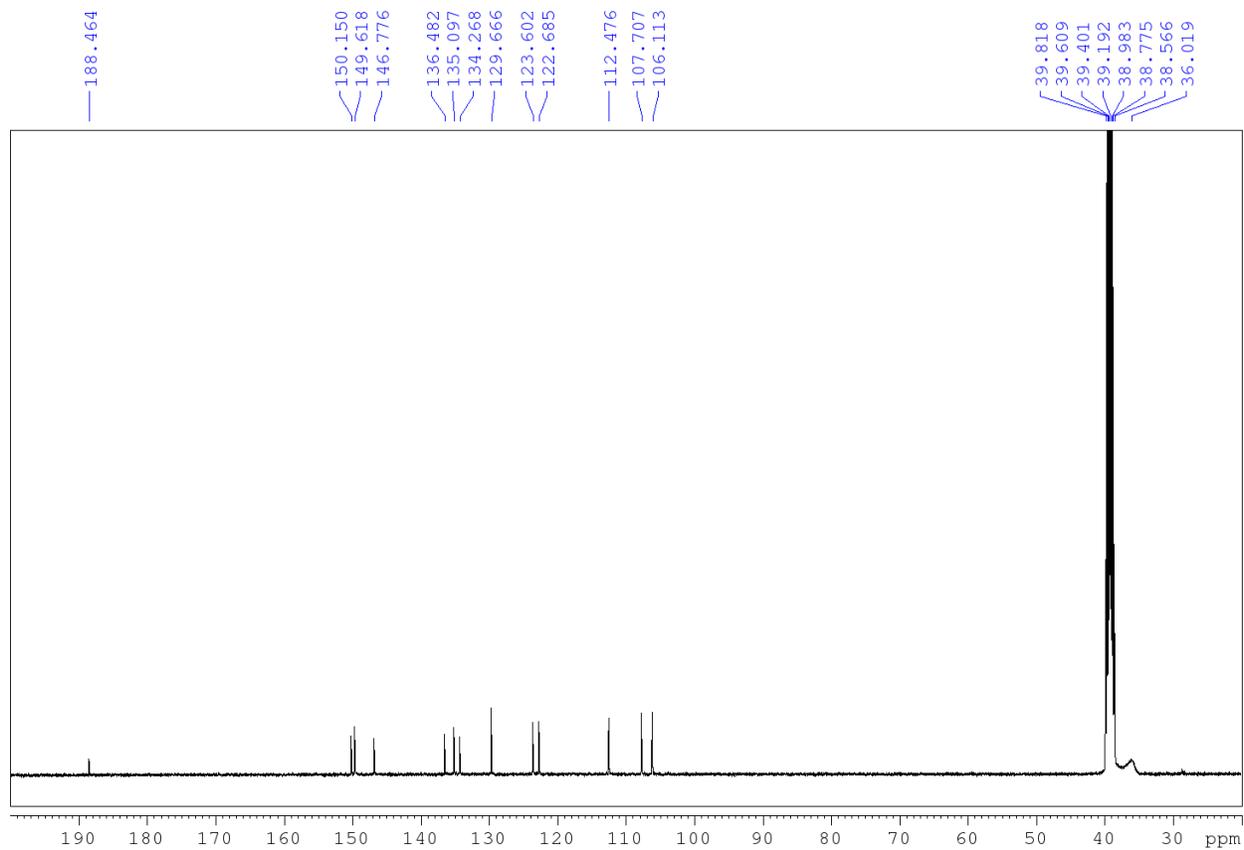


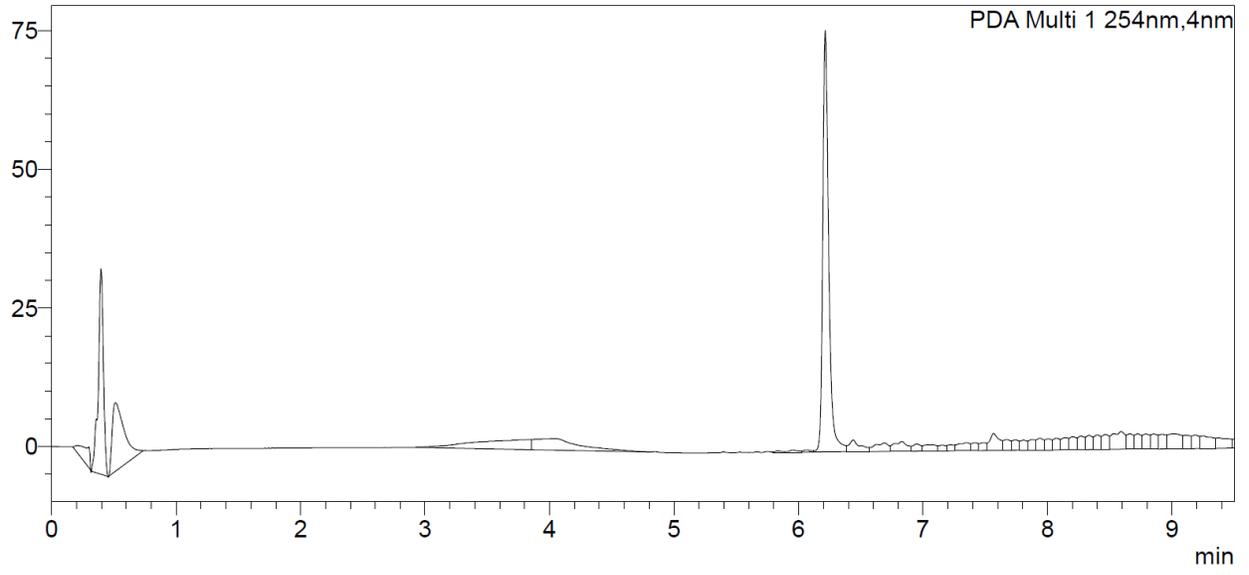
Compound 10



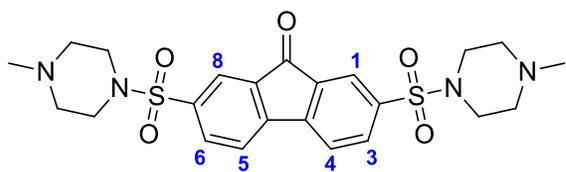
*N*²,*N*⁷-bis(3-hydroxyphenyl)-9-oxo-9*H*-fluorene-2,7-disulfonamide



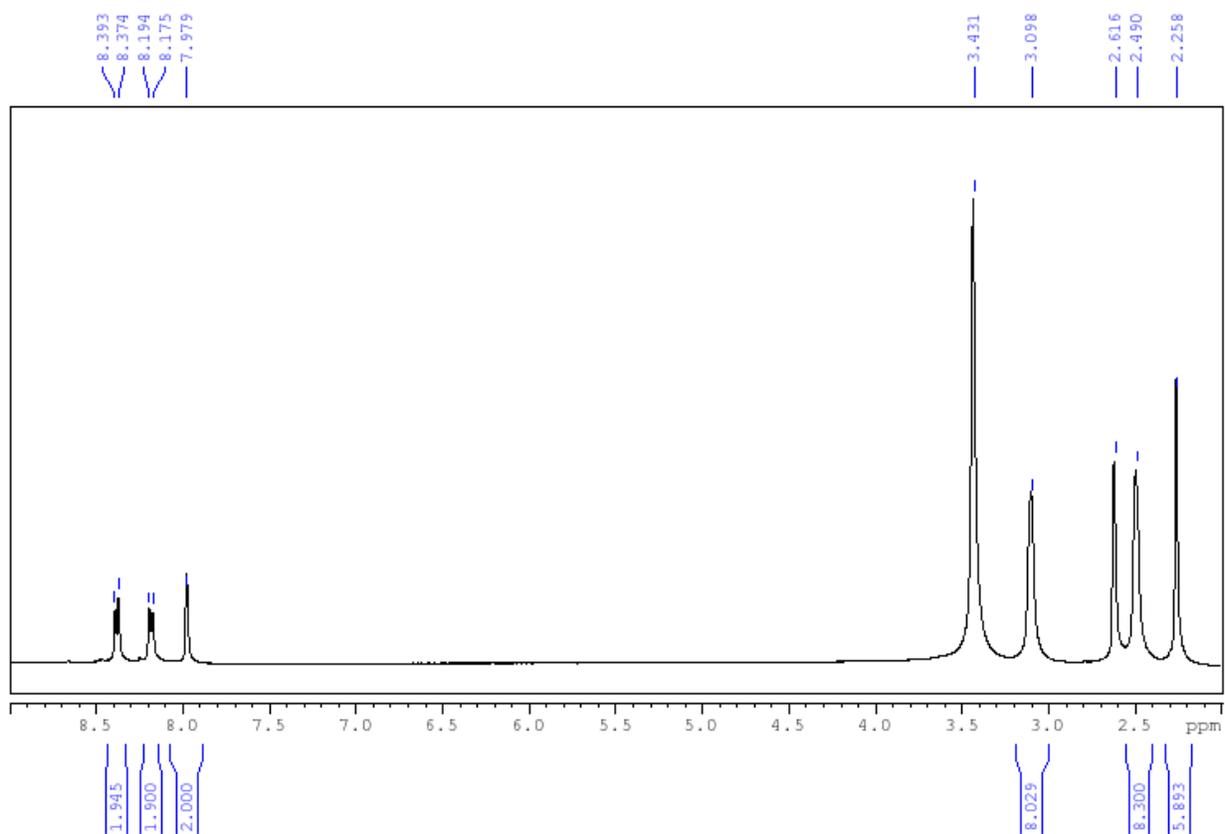


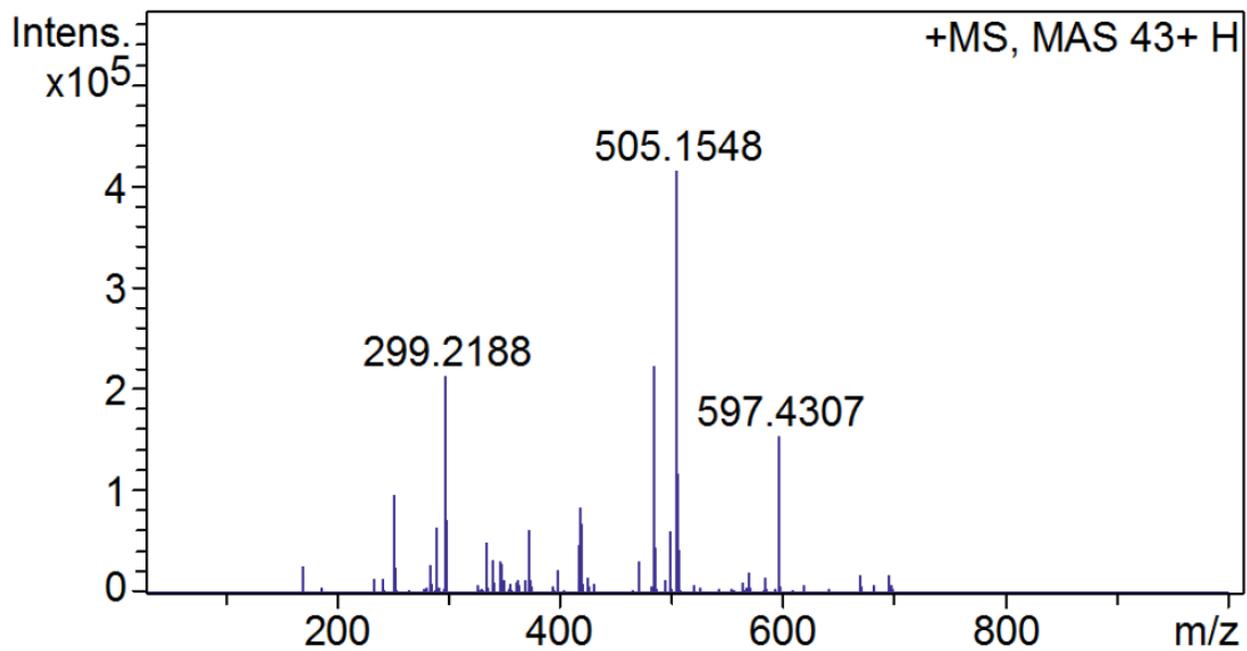
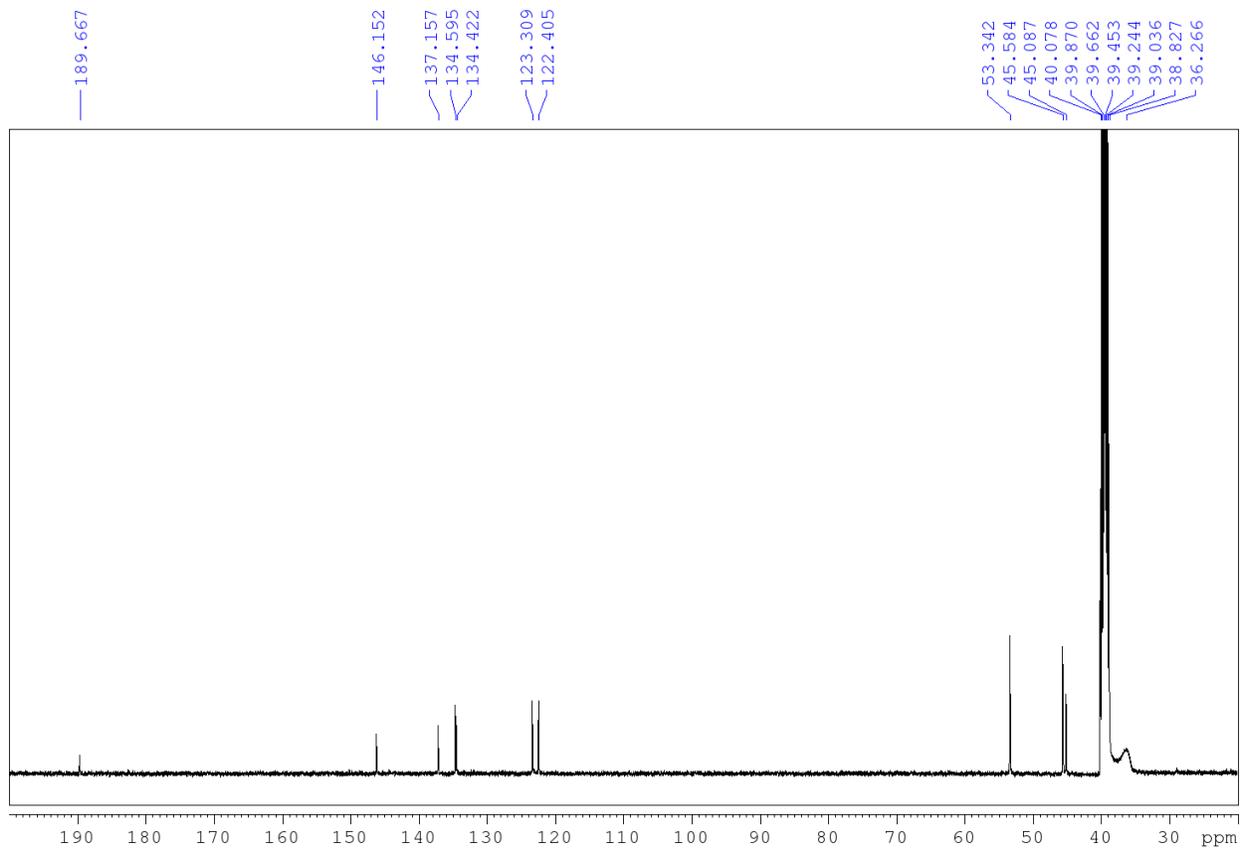


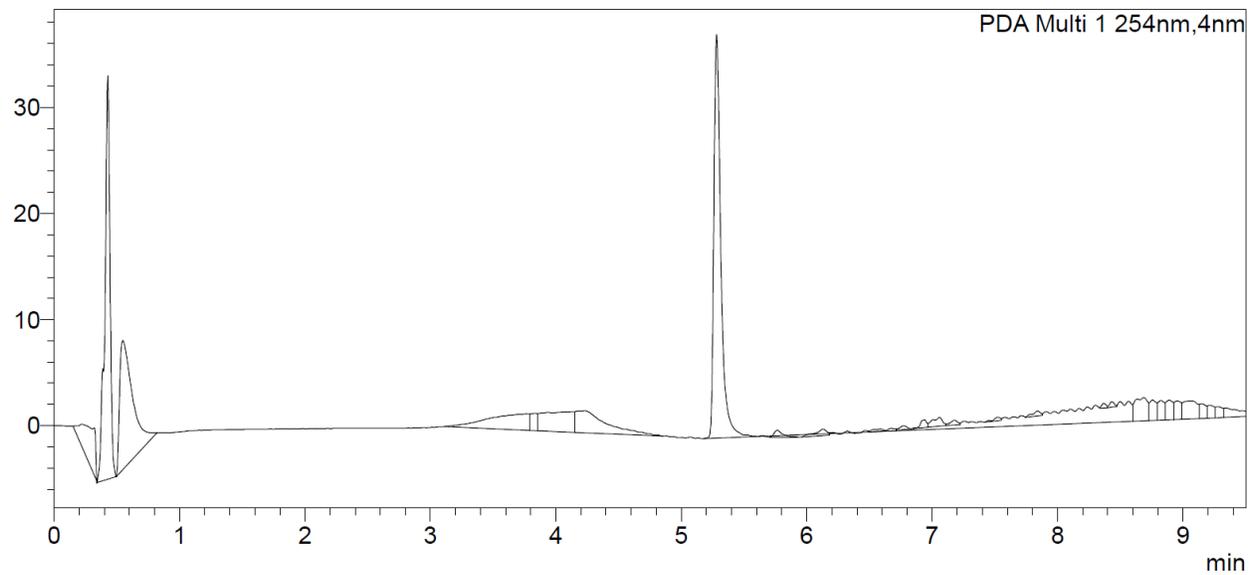
Compound 11



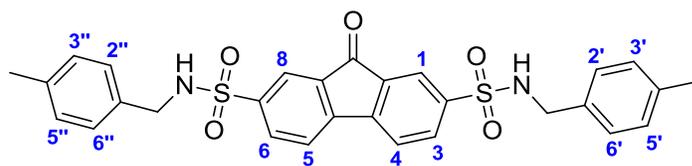
2,7-bis((4-methylpiperazin-1-yl)sulfonyl)-9H-fluoren-9-one



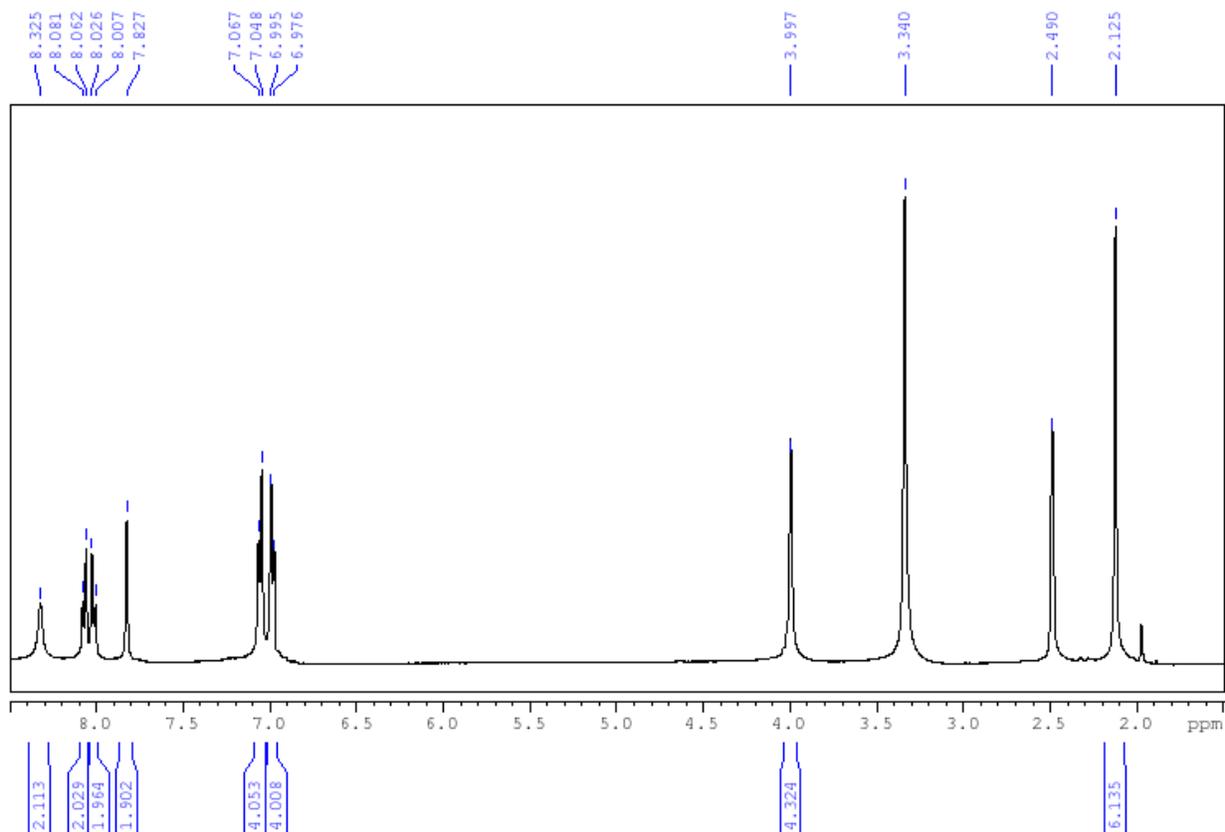


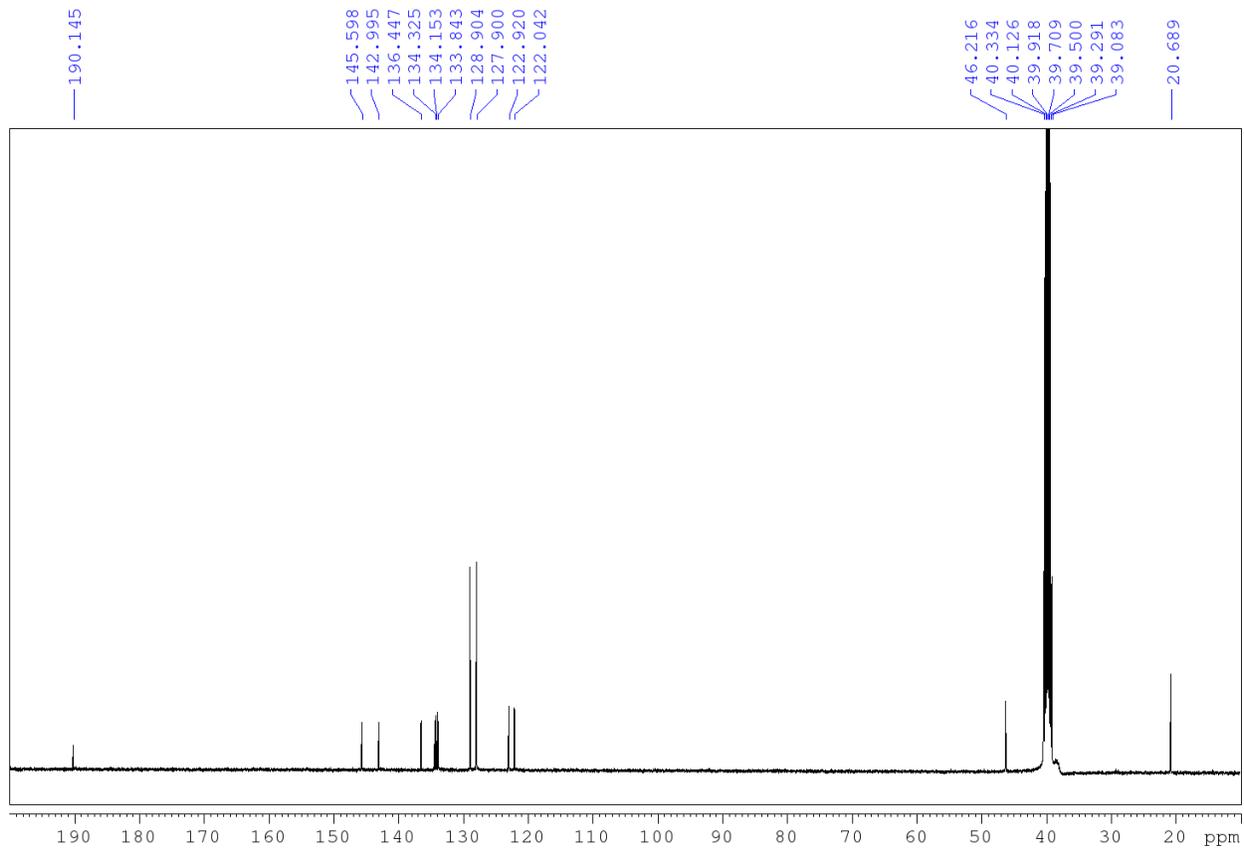


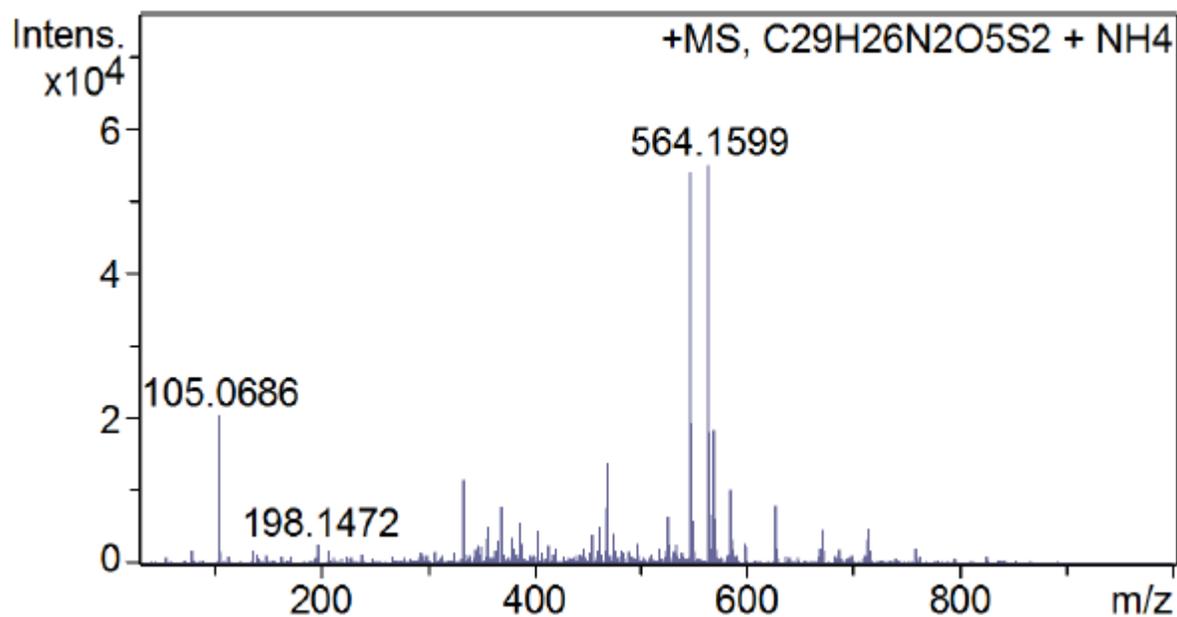
Compound 12



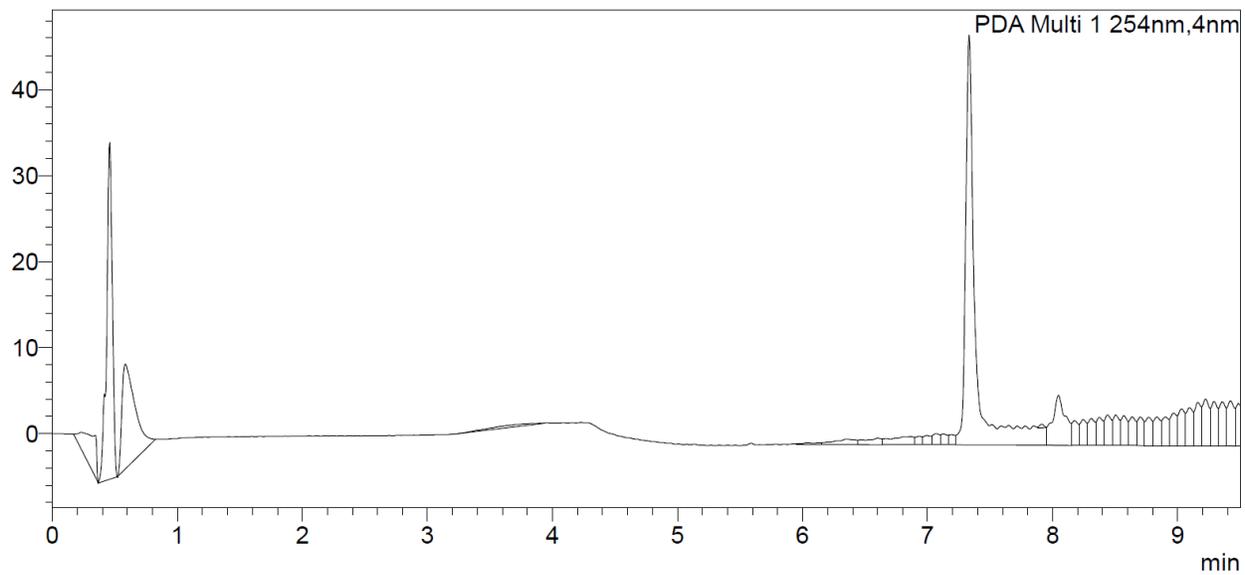
*N*²,*N*⁷-bis(4-methylbenzyl)-9-oxo-9*H*-fluorene-2,7-disulfonamide



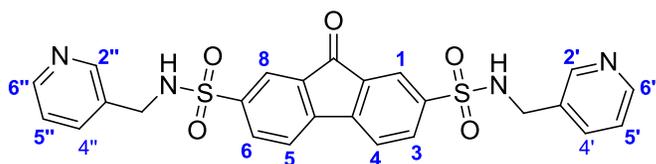




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2	334.2583	37746	474287.3	11682	21.2	0.0089
3	469.8352	22697	568542.1	14004	25.5	0.0207
4	547.1334	41411	2190926.0	53964	98.1	0.0132
5	548.1367	39481	790968.6	19482	35.4	0.0139
6	564.1599	41266	2232347.0	54984	100.0	0.0137
7	565.1631	39112	741694.9	18268	33.2	0.0145
8	569.1155	41655	751928.2	18520	33.7	0.0137
9	585.0894	39628	417076.3	10273	18.7	0.0148
10	626.4220	34746	332932.2	8200	14.9	0.0180



Compound 13



9-oxo- N^2,N^7 -bis(pyridin-3-ylmethyl)-9H-fluorene-2,7-disulfonamide

