

Supplementary Information

Discovery of ureido-like Apcin analogs as Cdc20-specific inhibitors against cancer

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¹ Department of Medicinal Chemistry, Xiangya School of Pharmaceutical Sciences, Central South University, Changsha 410013, Hunan, China

² Hunan Key Laboratory of Organ Fibrosis; Changsha 410013, Hunan, China

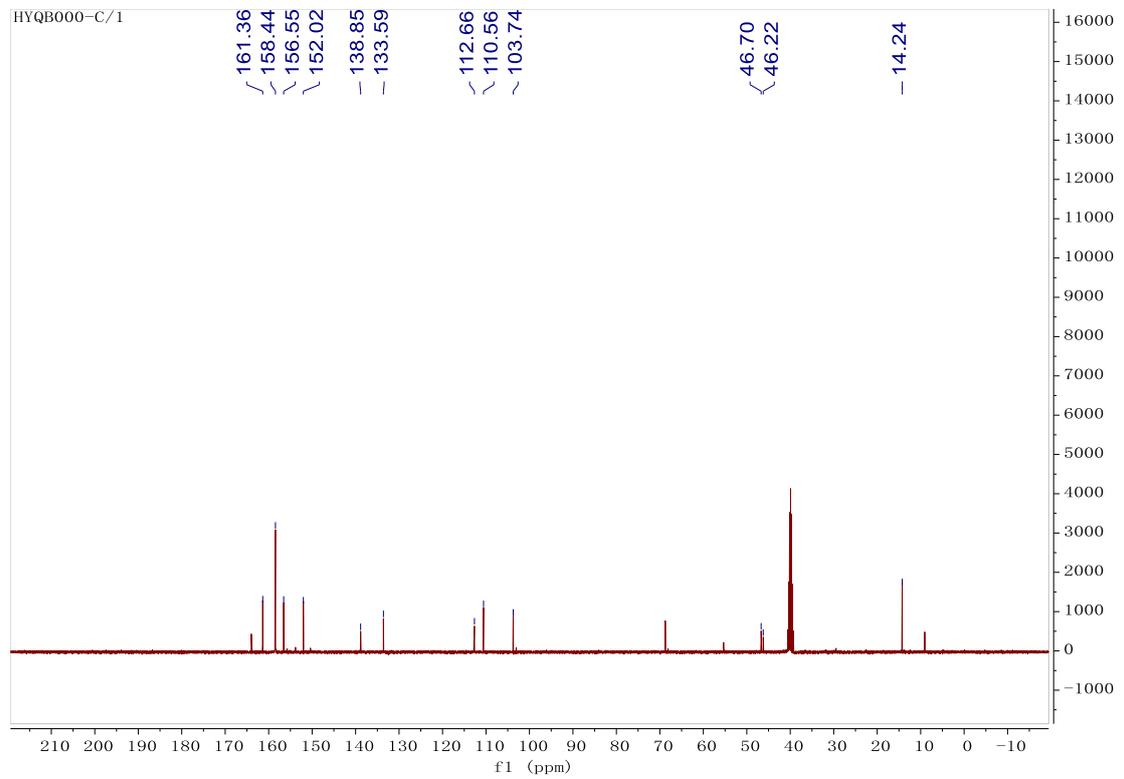
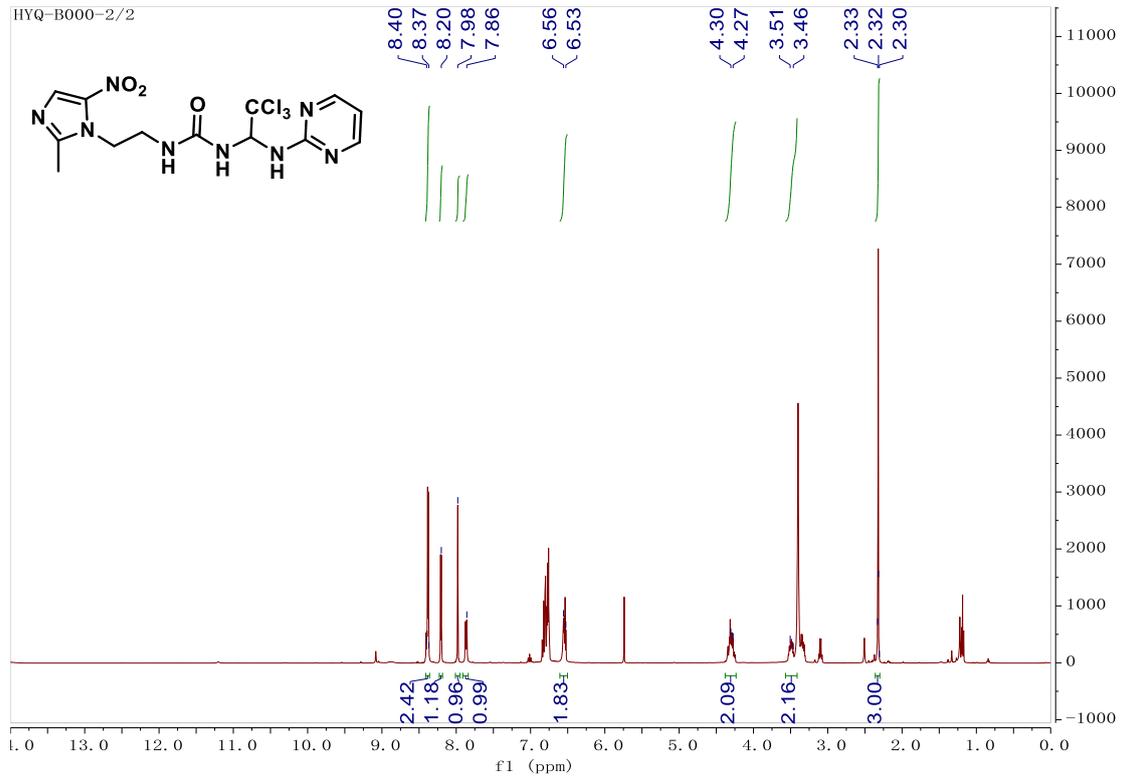
³ Hunan Key Laboratory of Diagnostic and Therapeutic Drug Research for Chronic Diseases; Changsha 410013, Hunan, China

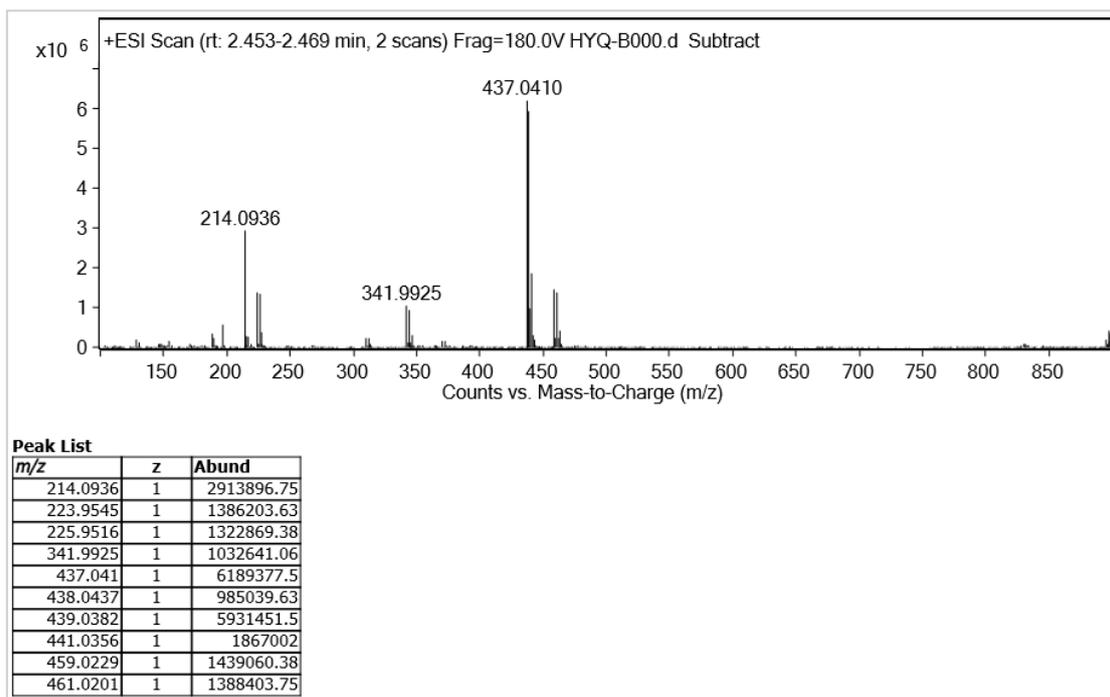
* Correspondence: (Email: cz_job@csu.edu.cn) +86-826500370.

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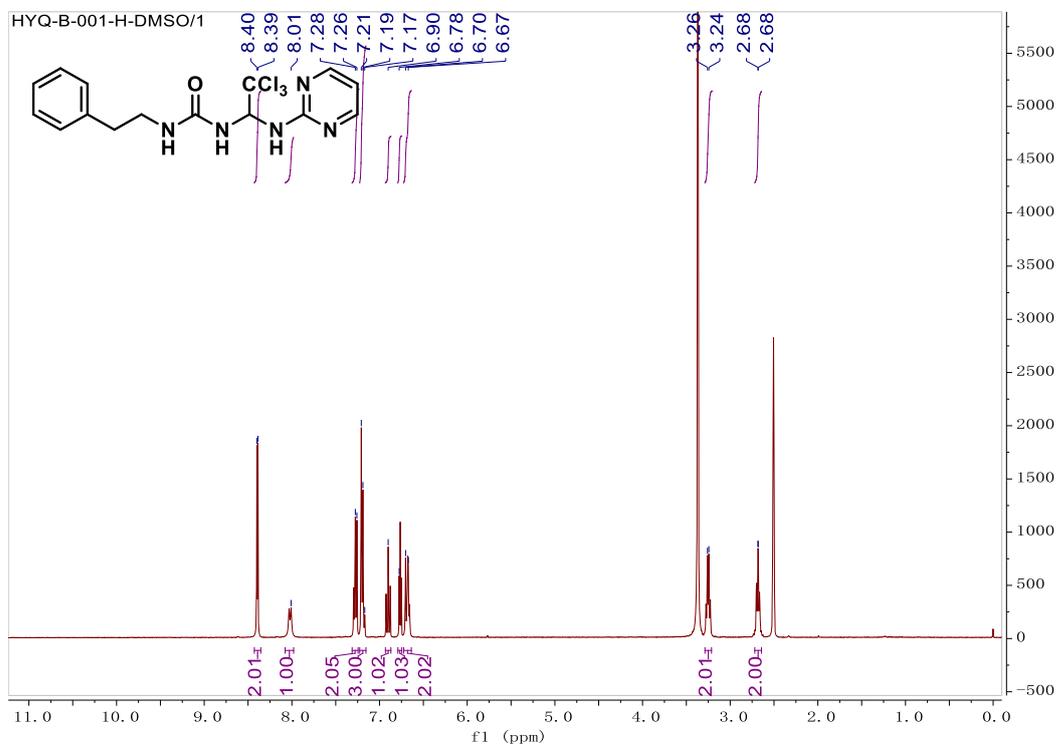
NMR, HRMS and HMBC spectra of compounds	page	2-48
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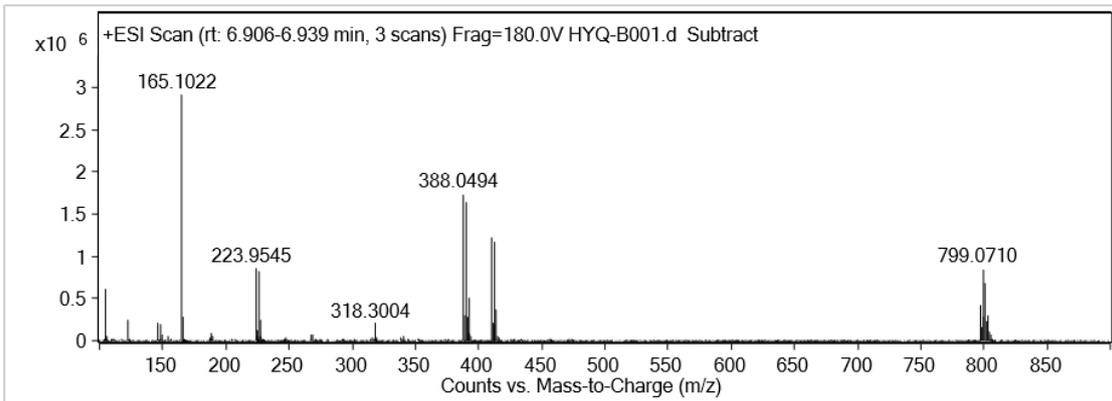
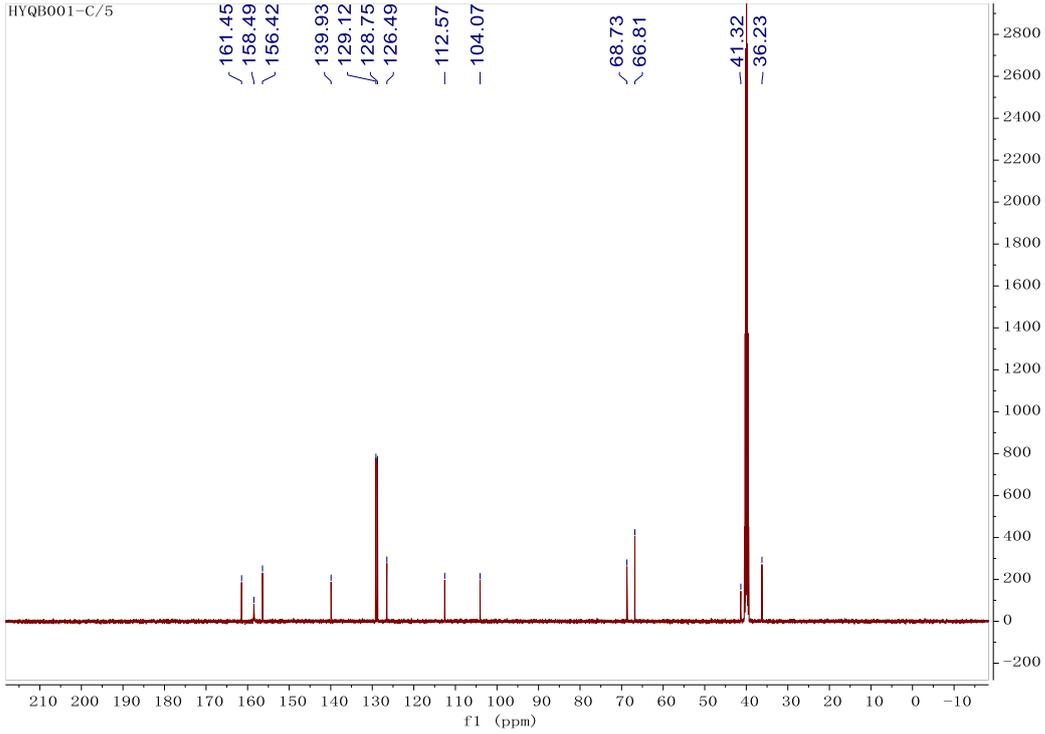
Compound 1





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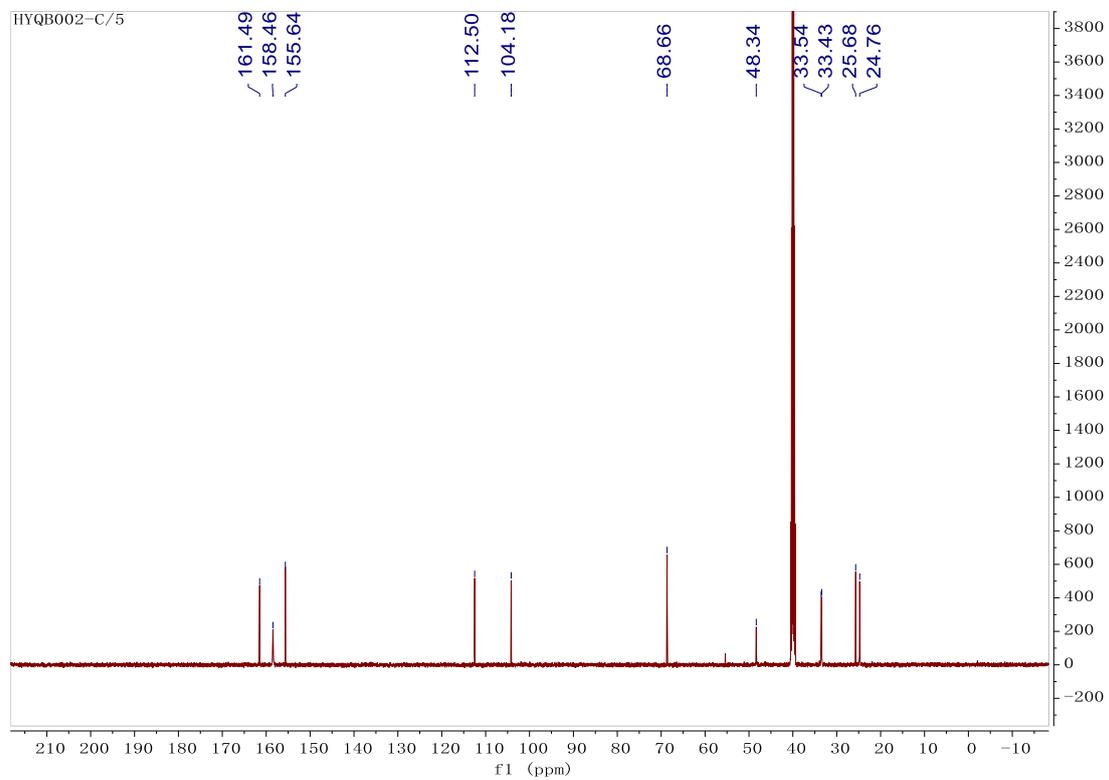
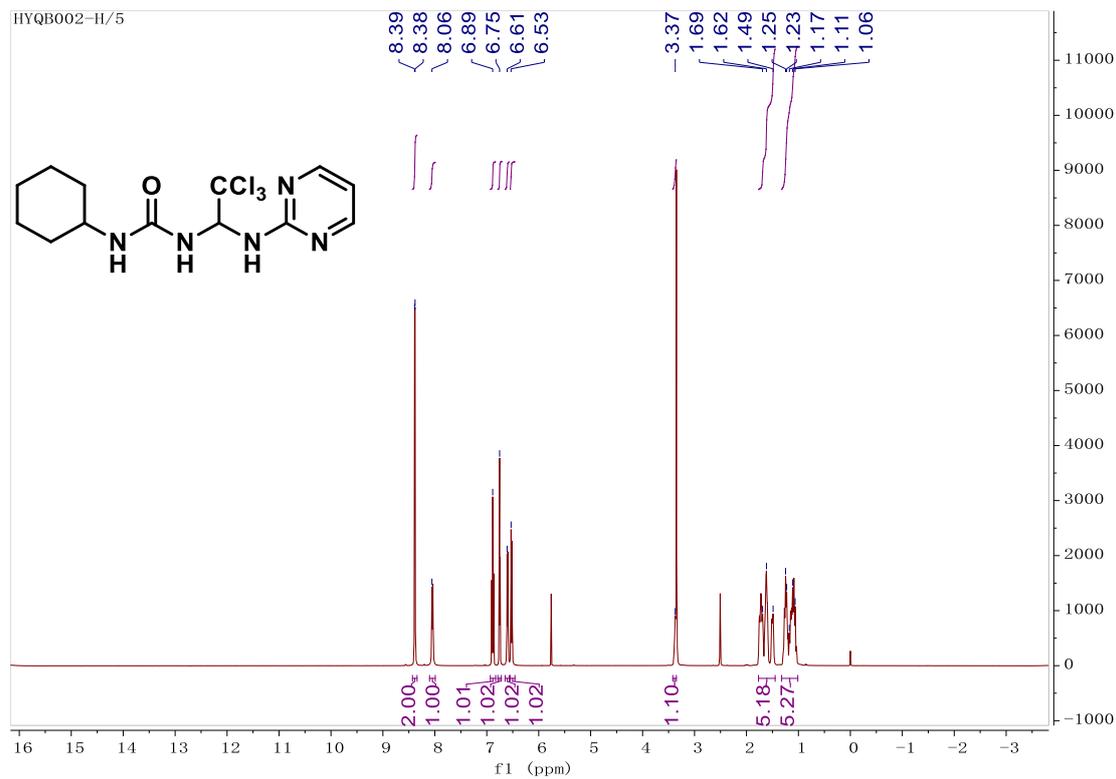


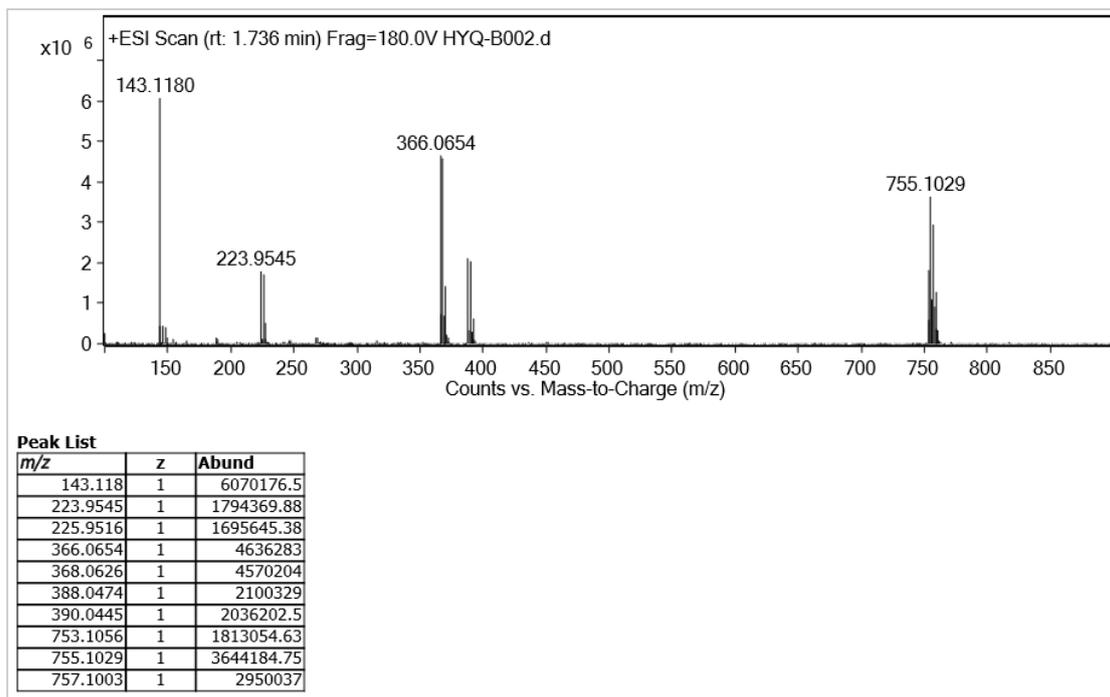


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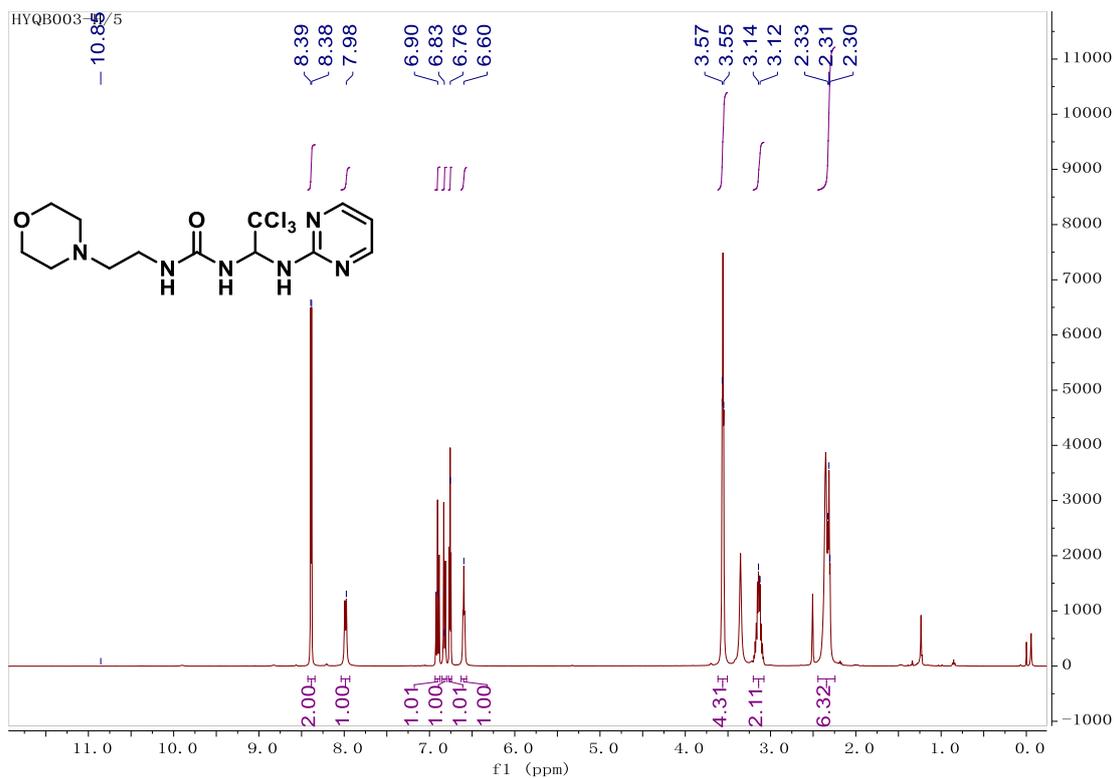
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390.0466	1	1640183.38
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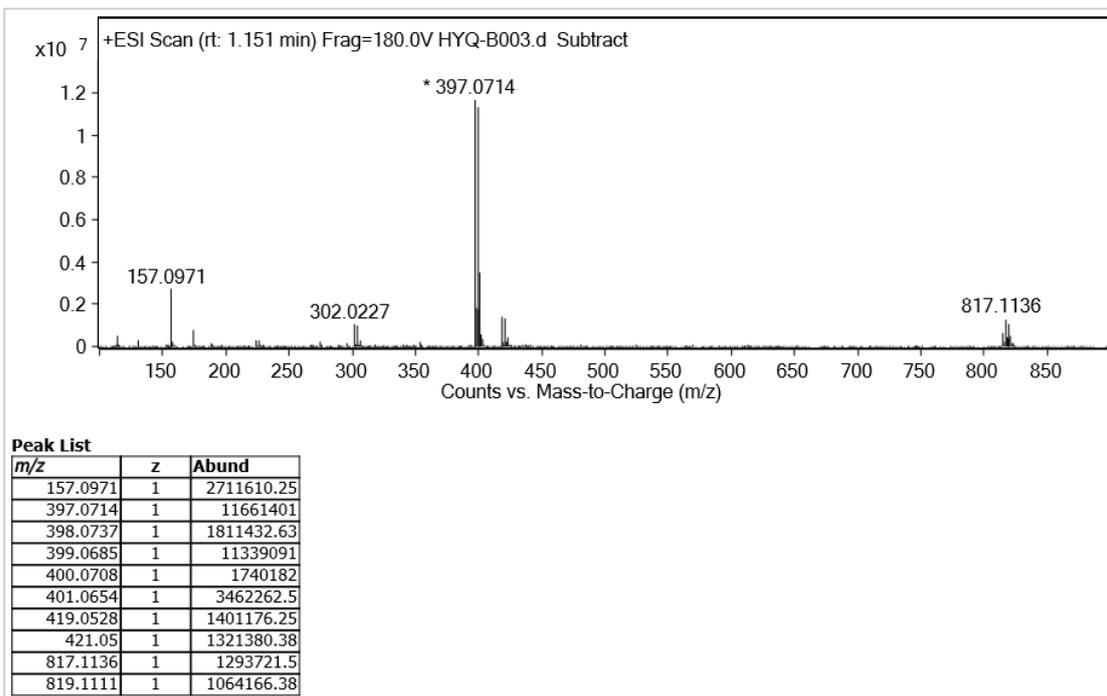
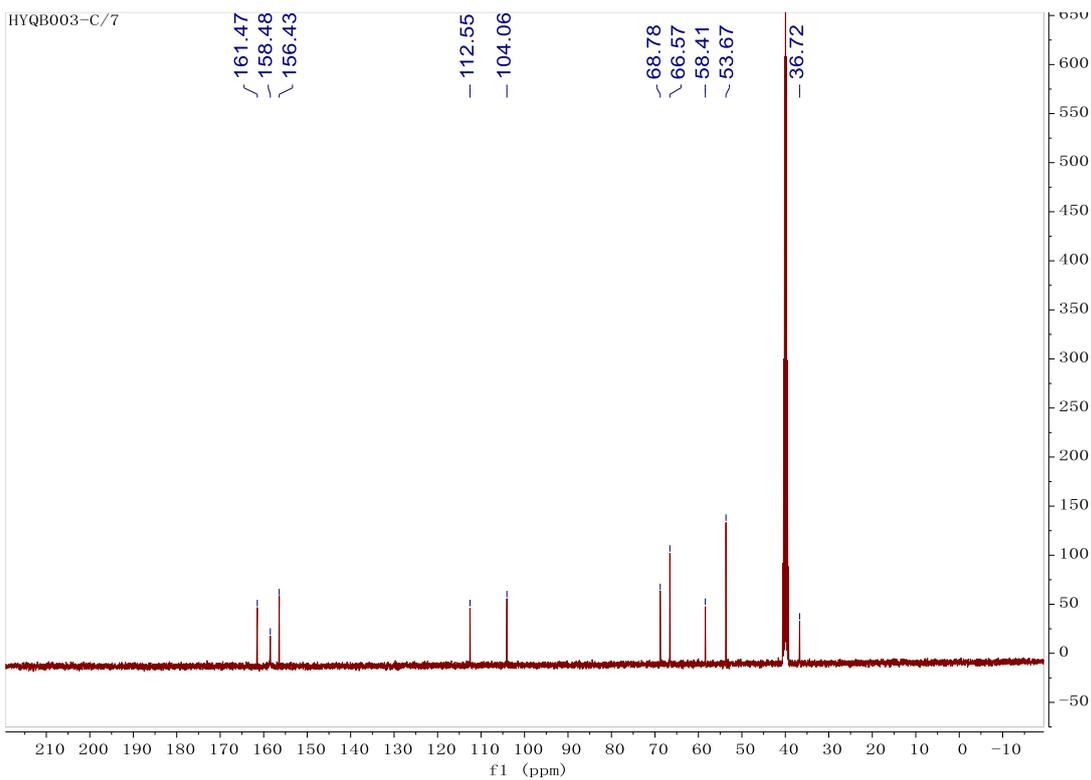
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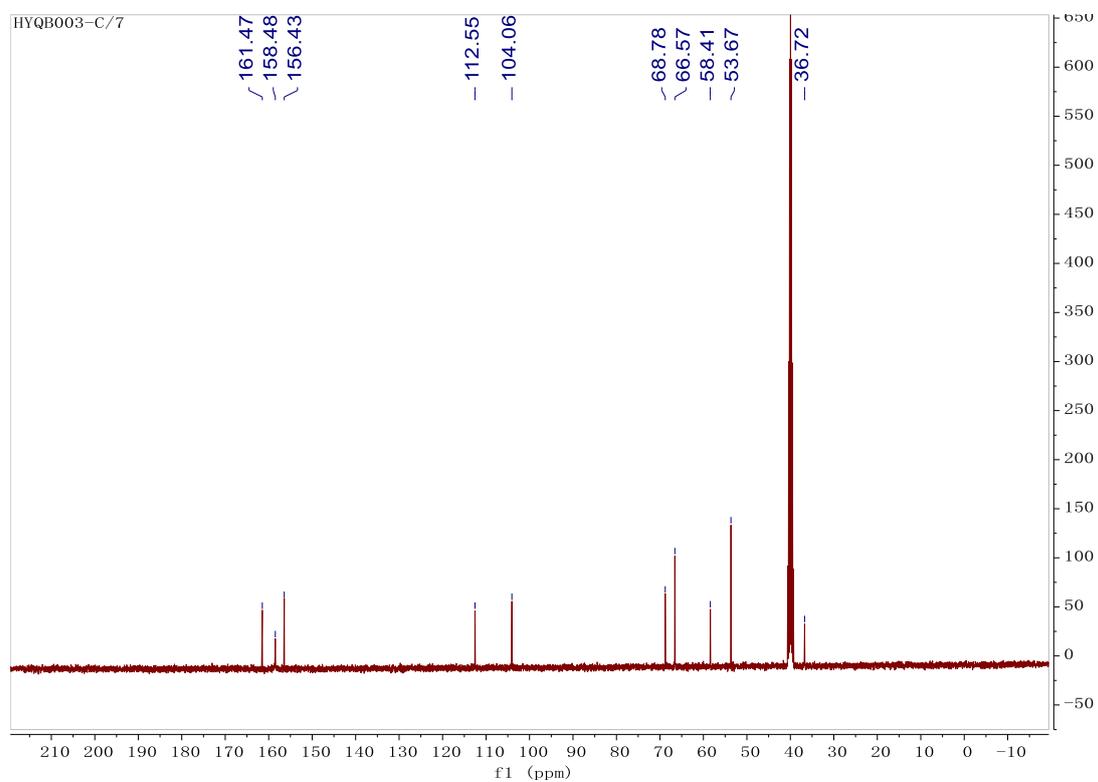
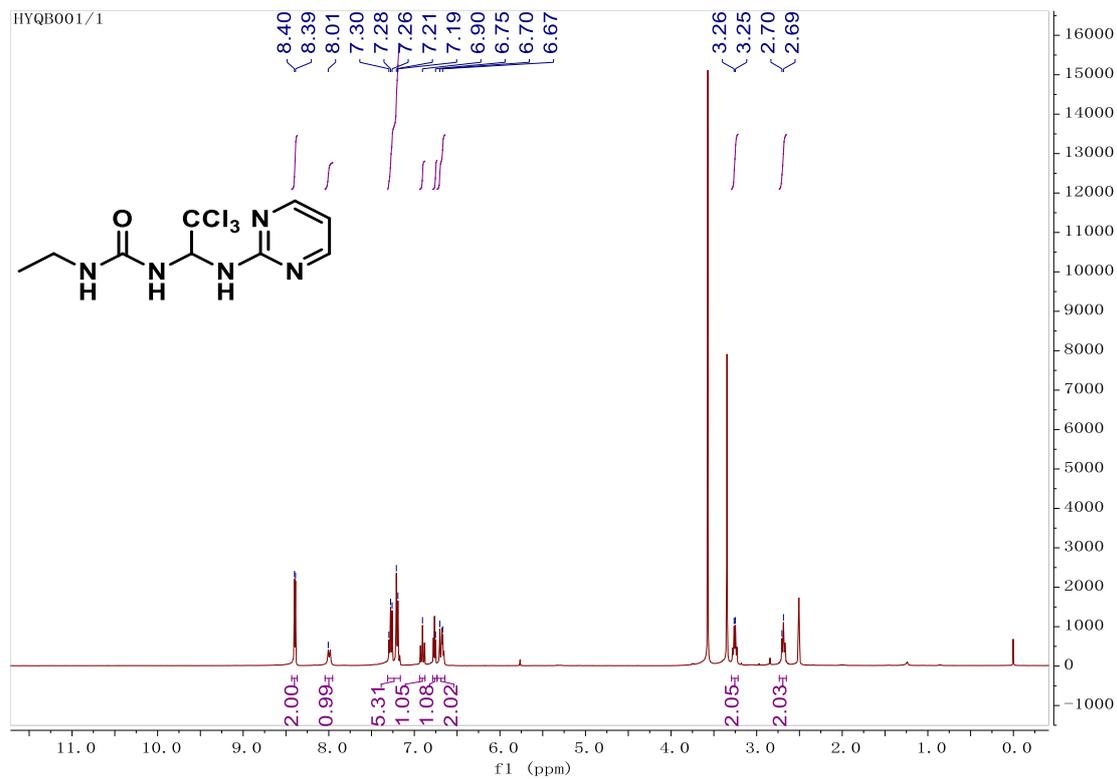


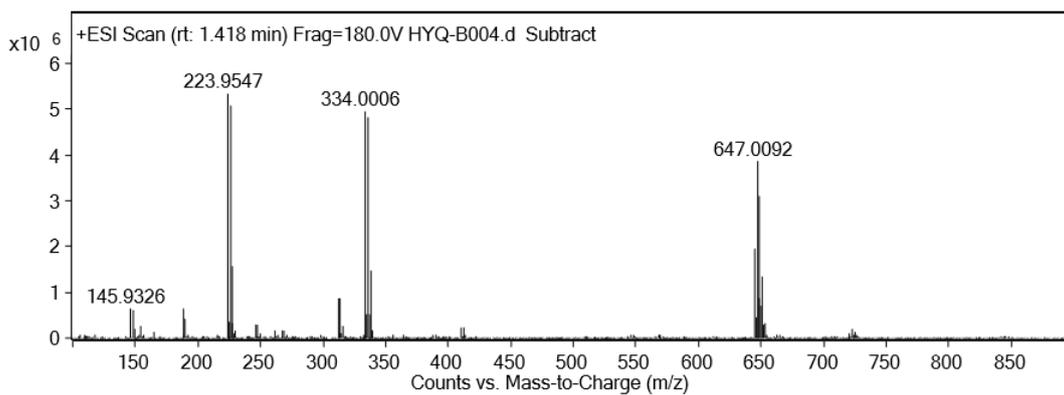
Compound 4





Compound 5

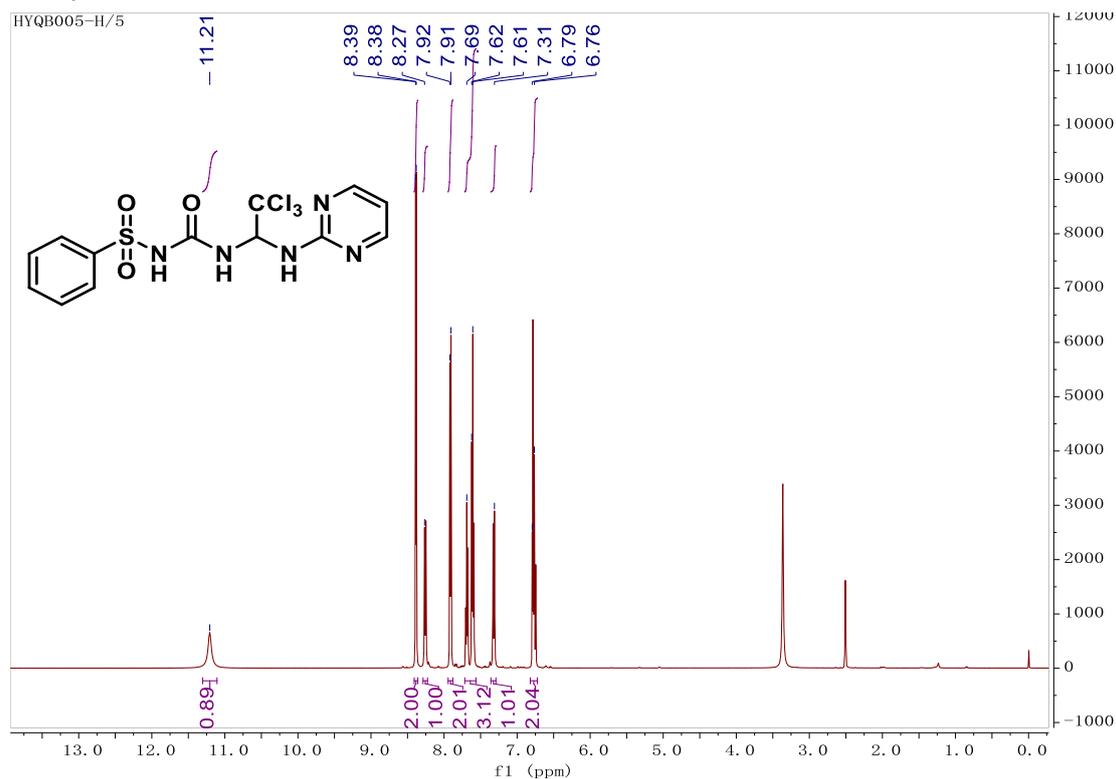


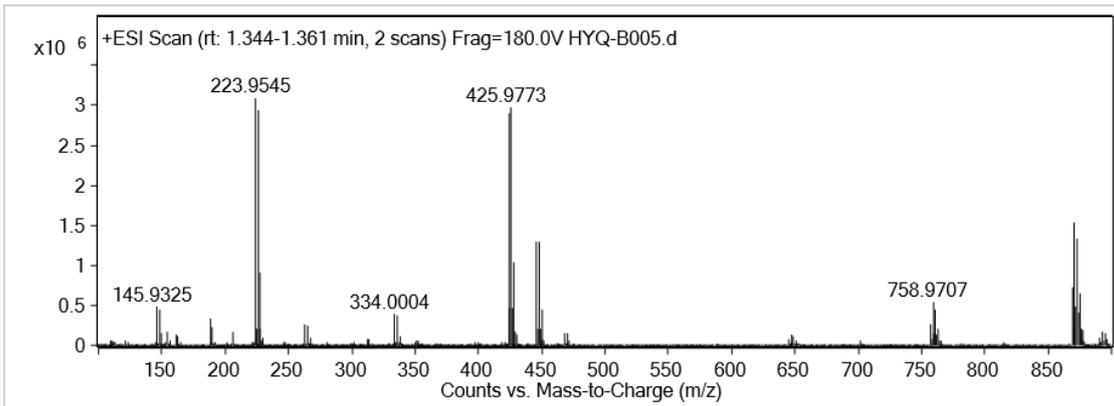
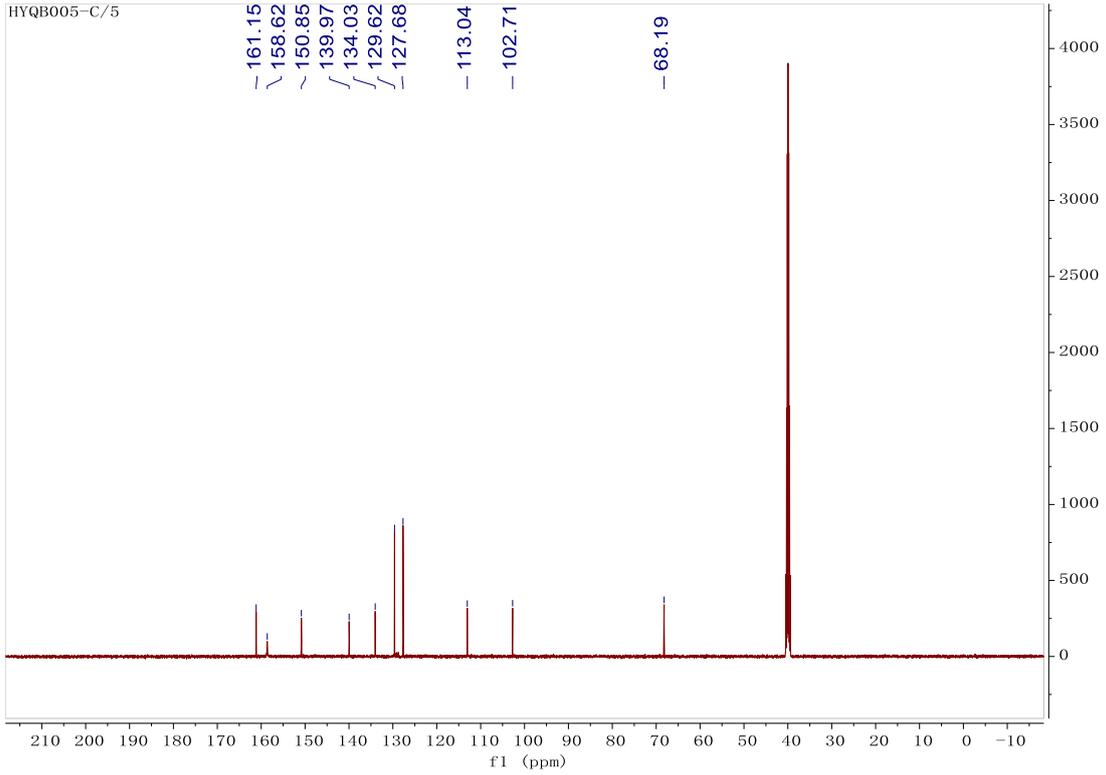


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334.0006	1	4929472
335.9977	1	4800584.5
337.9949	1	1480485.63
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651.0039	1	1337346.38

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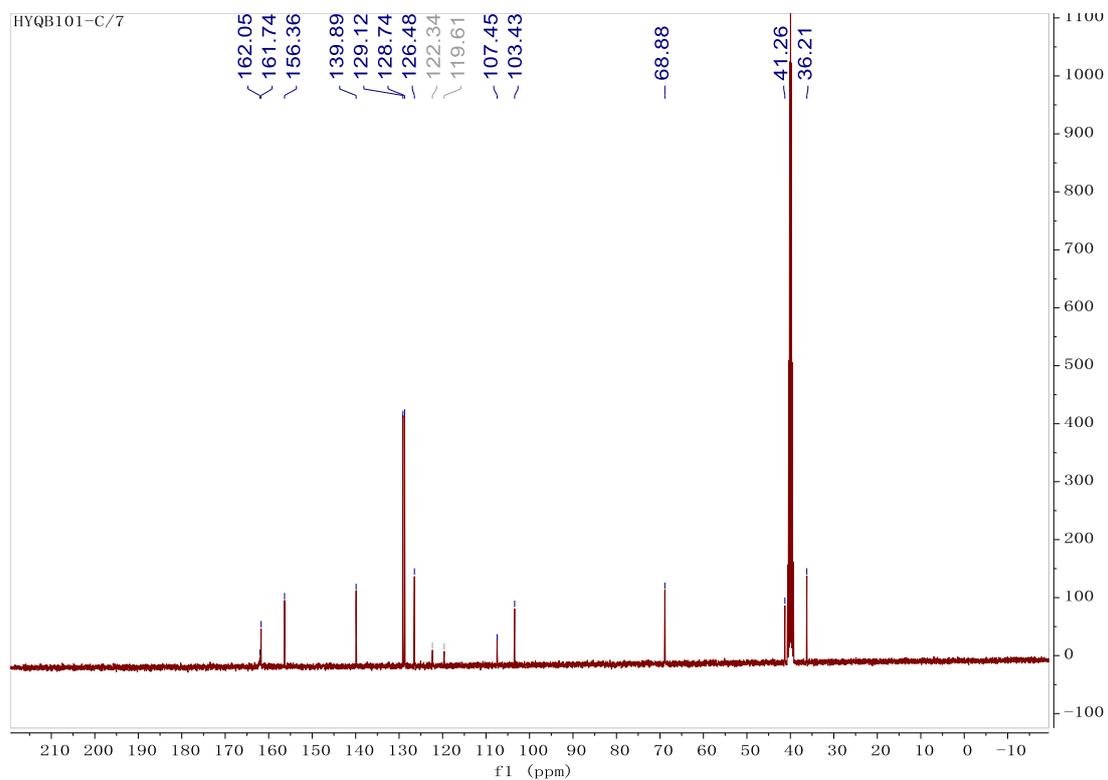
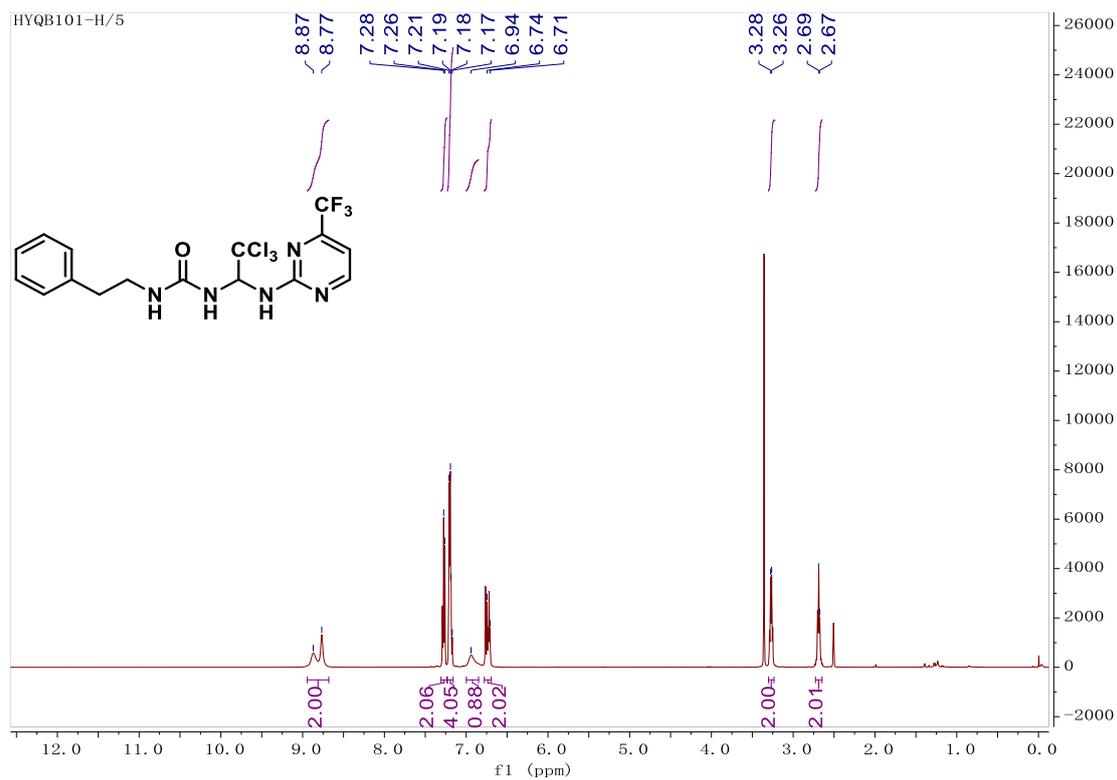


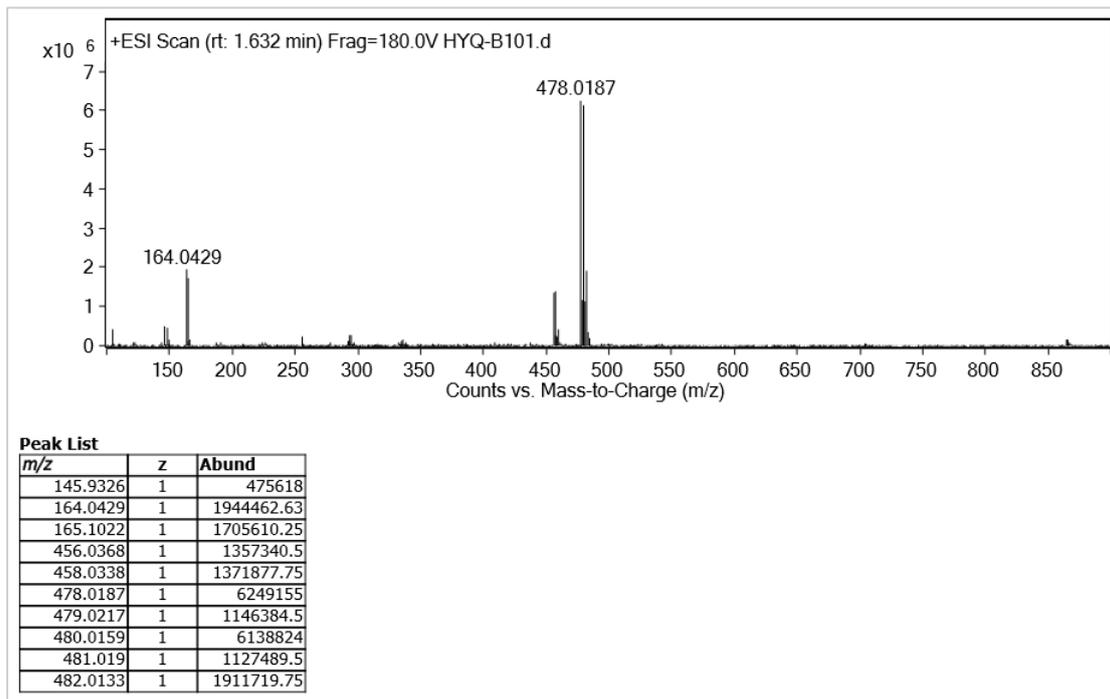


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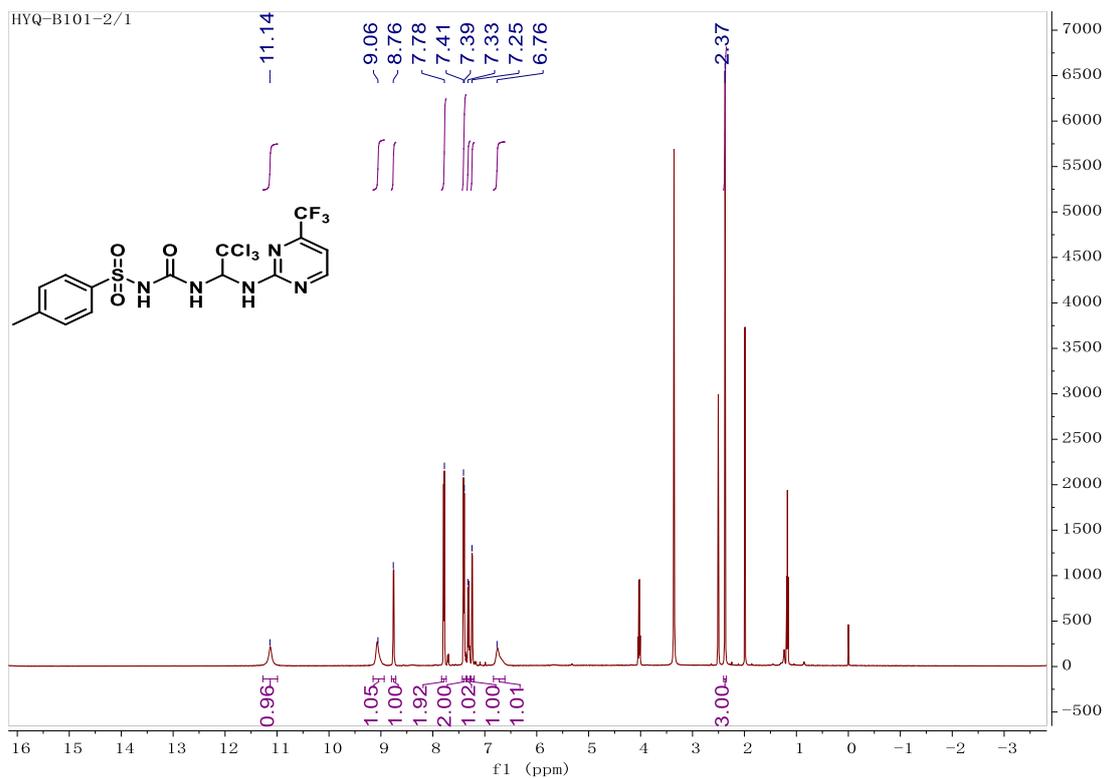
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425.9773	1	2975801.75
427.9746	1	1032621.13
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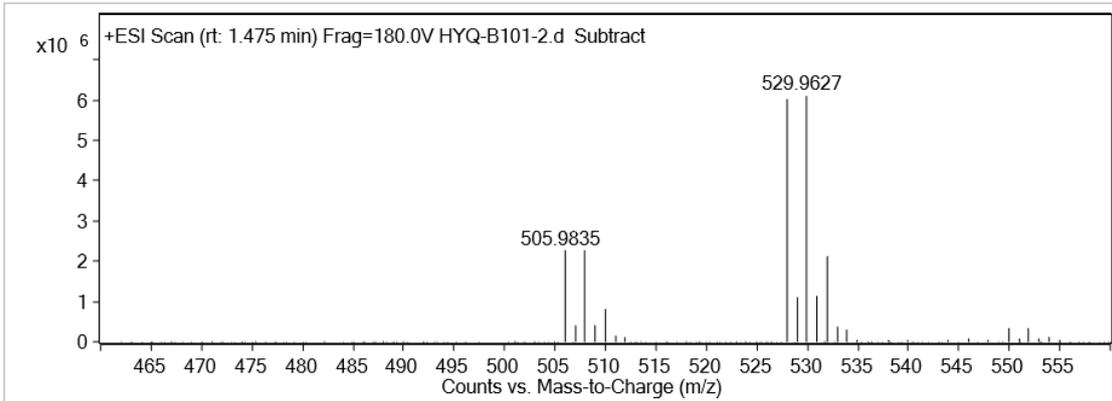
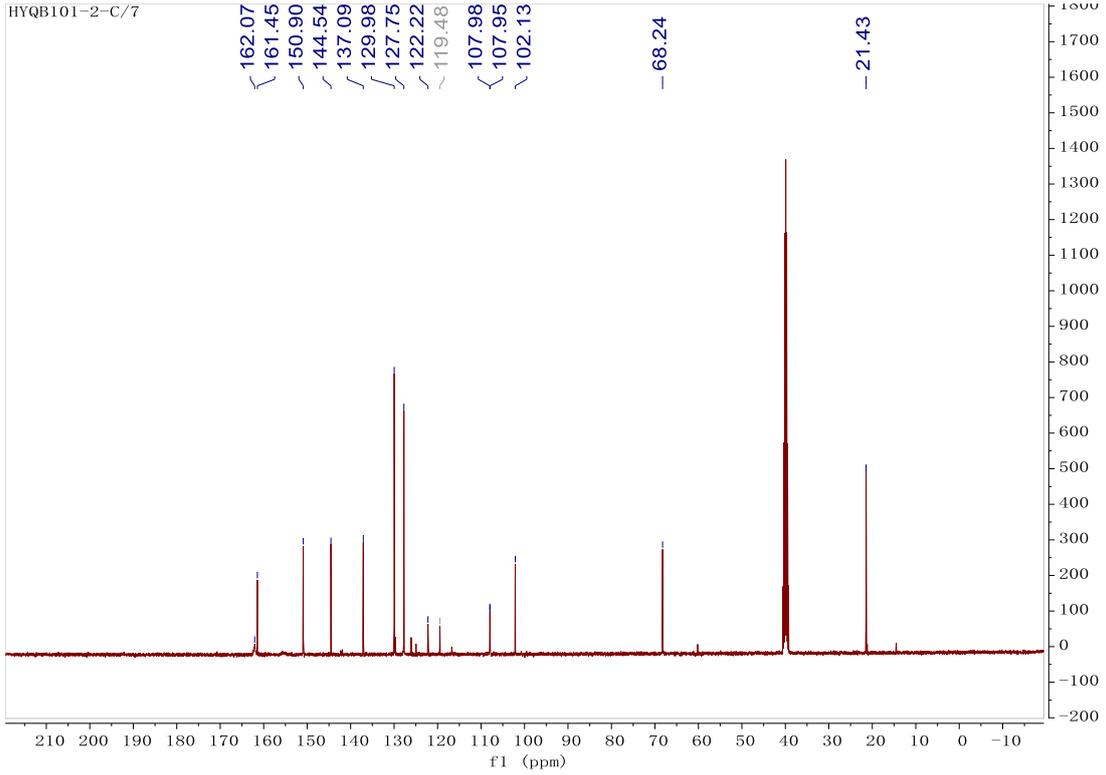
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Compound 8

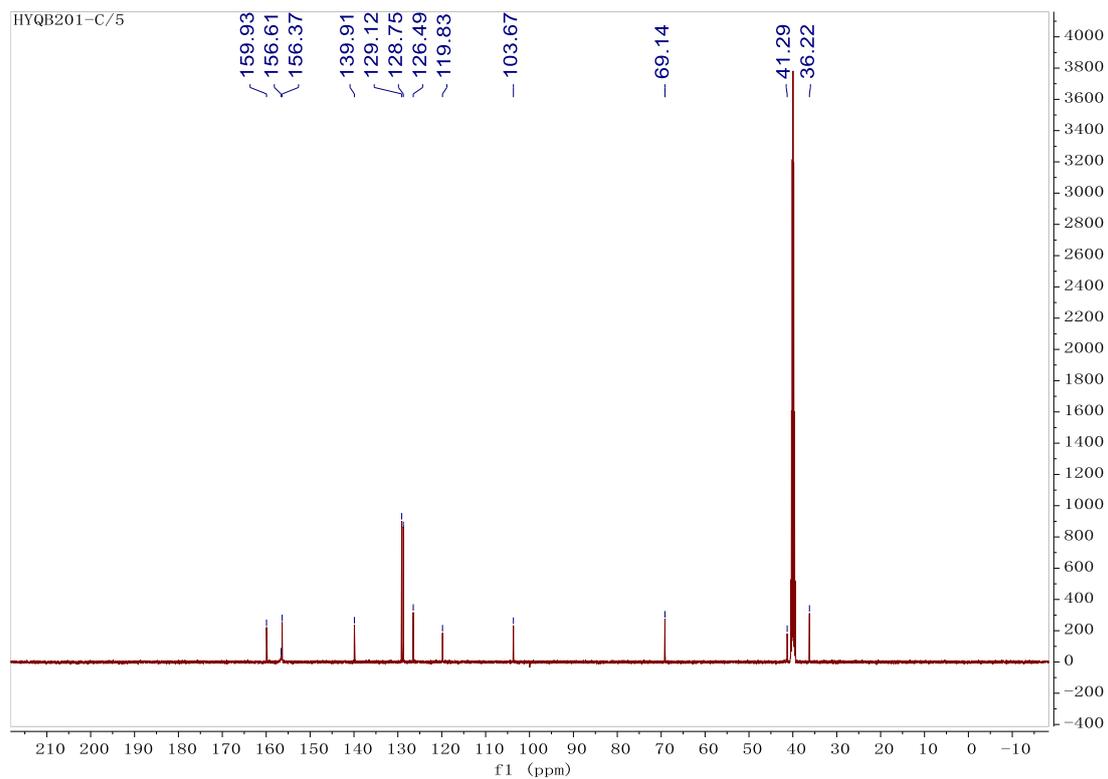
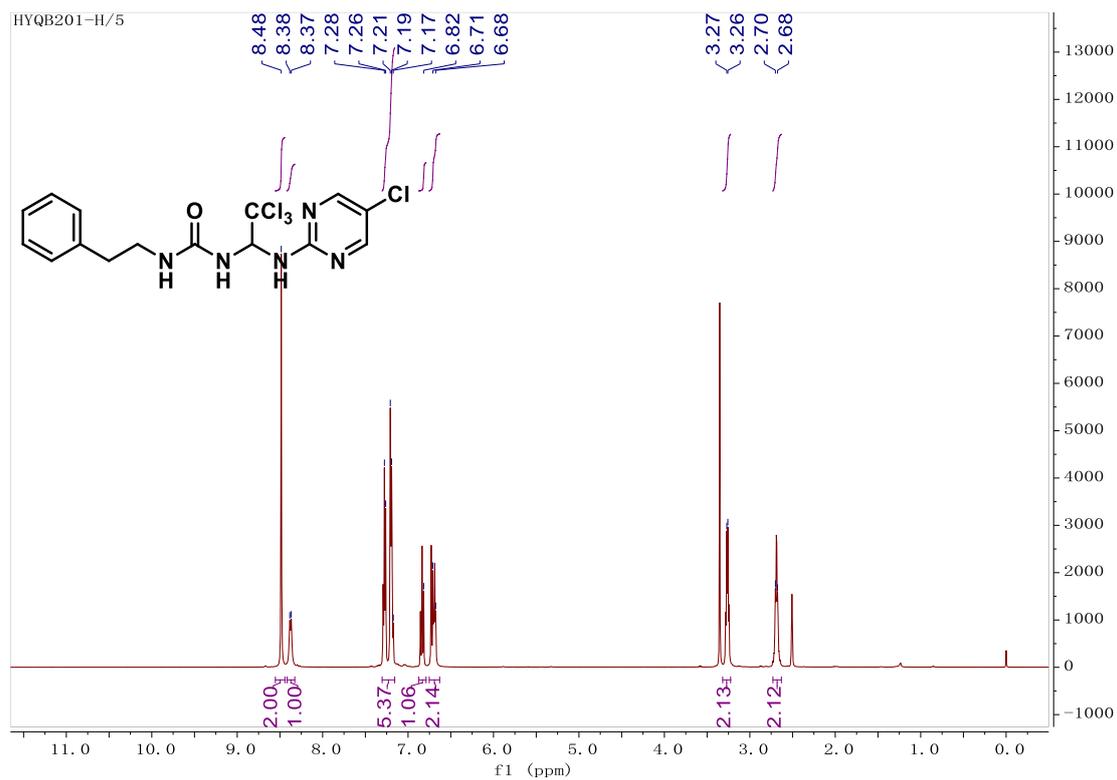


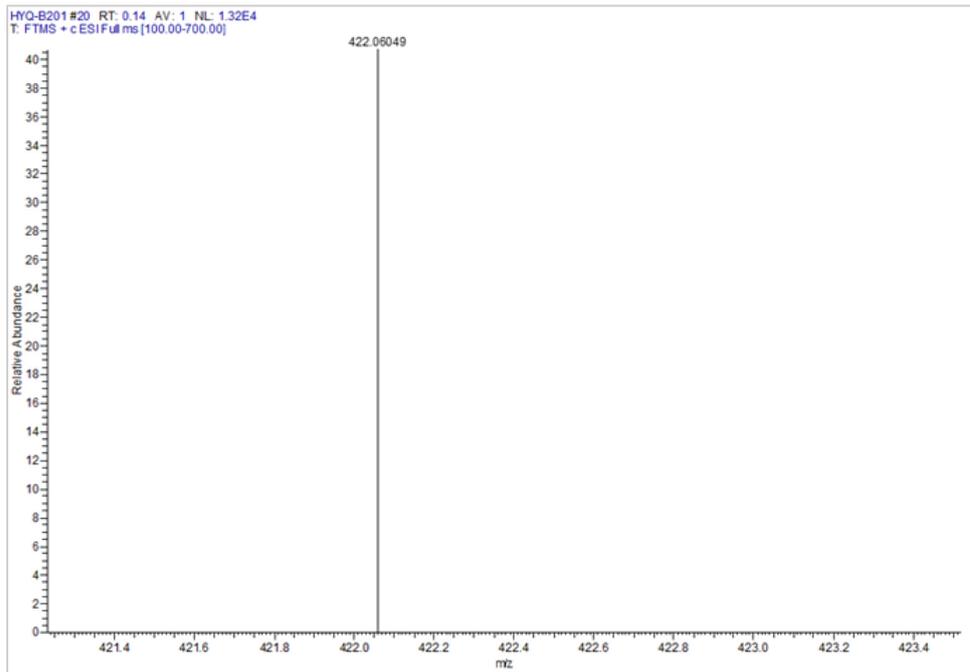


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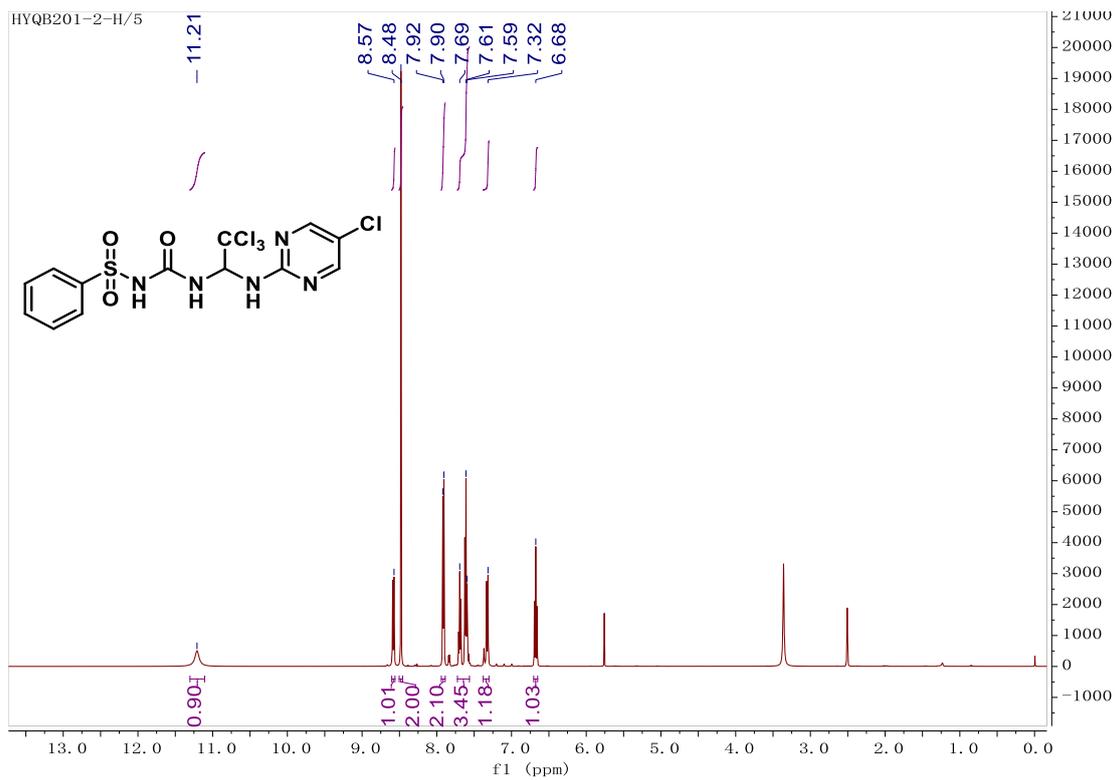
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507.9807	1	2272734.5
527.9656	1	6023426
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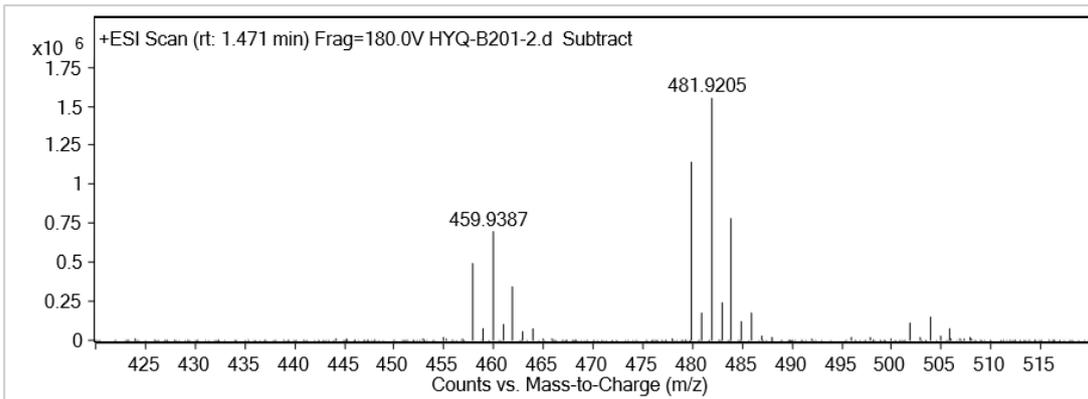
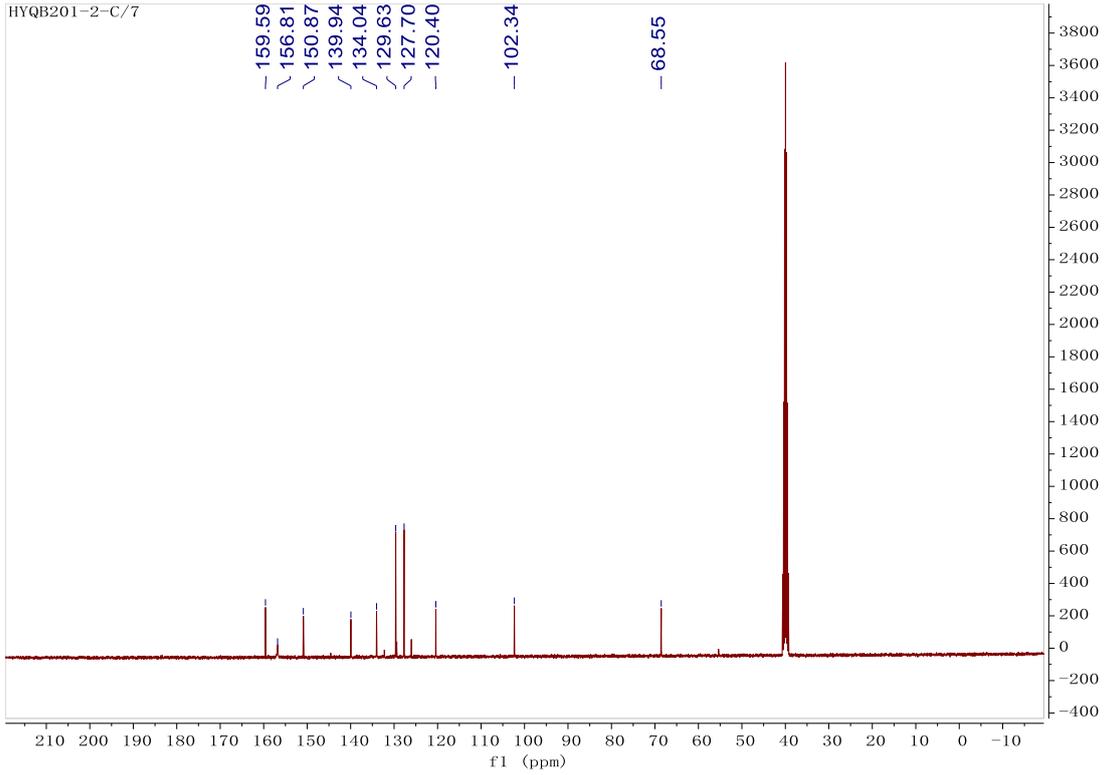
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Compound 10

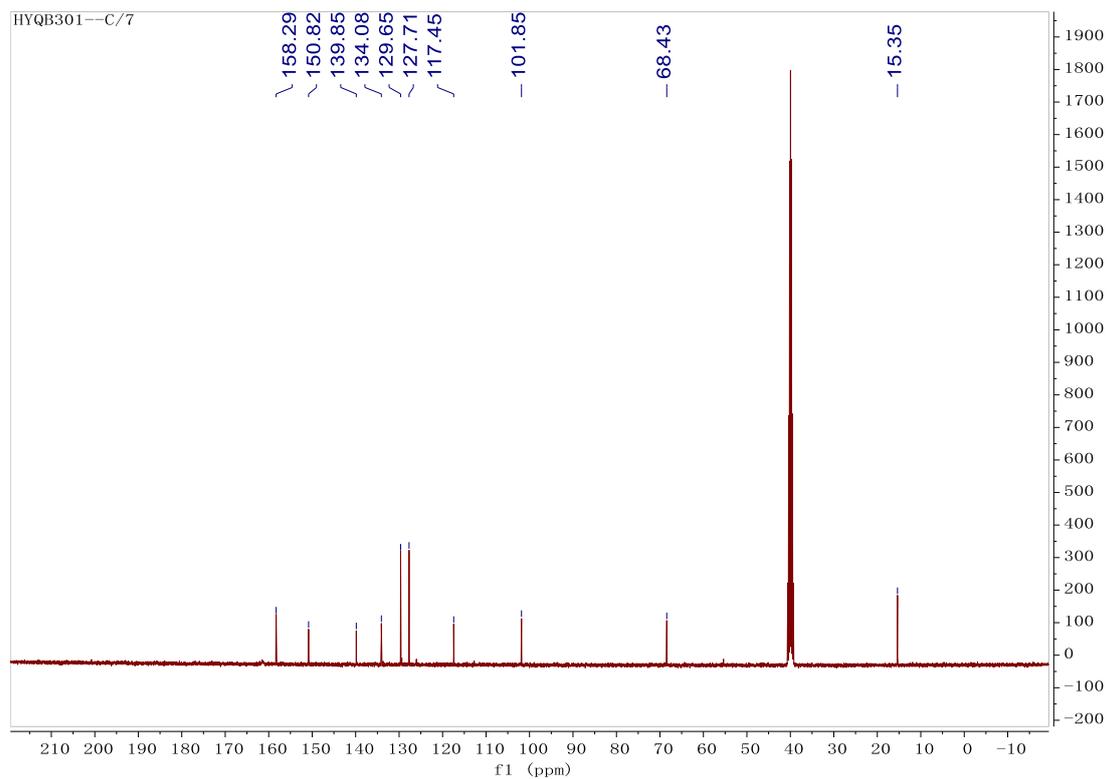
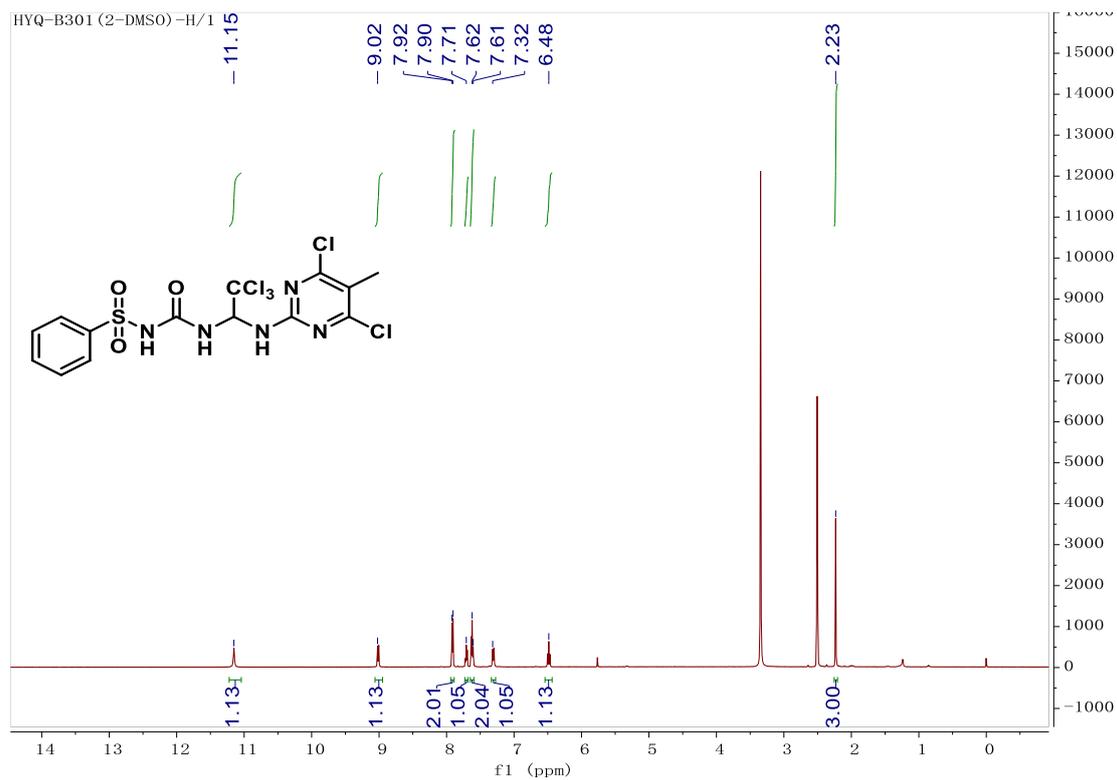


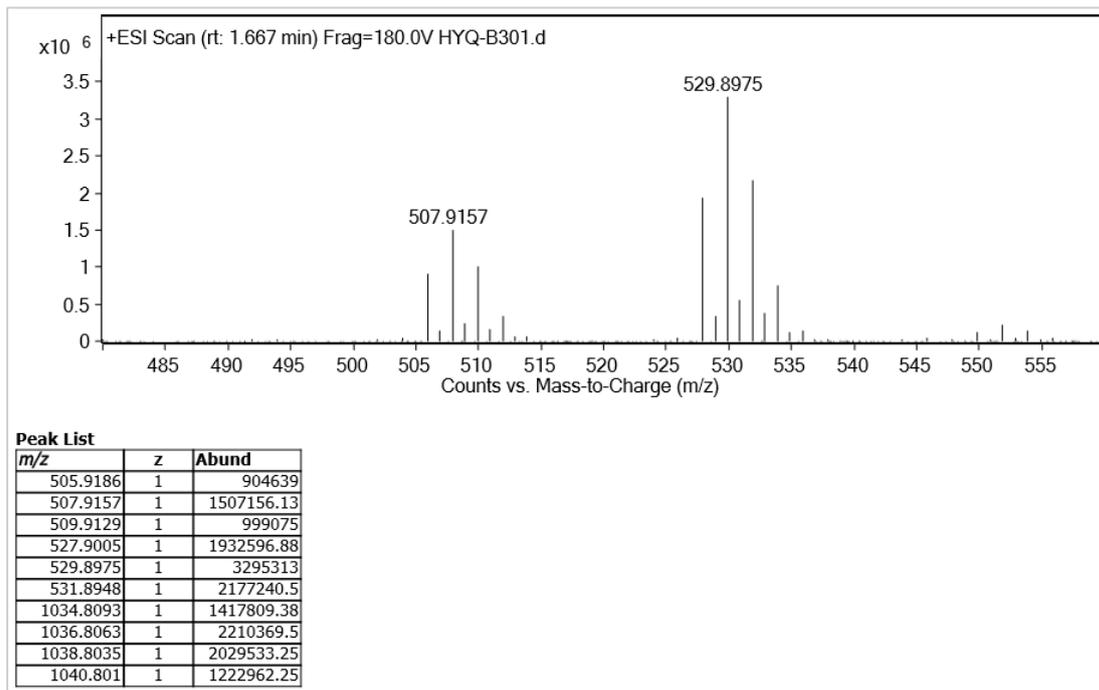


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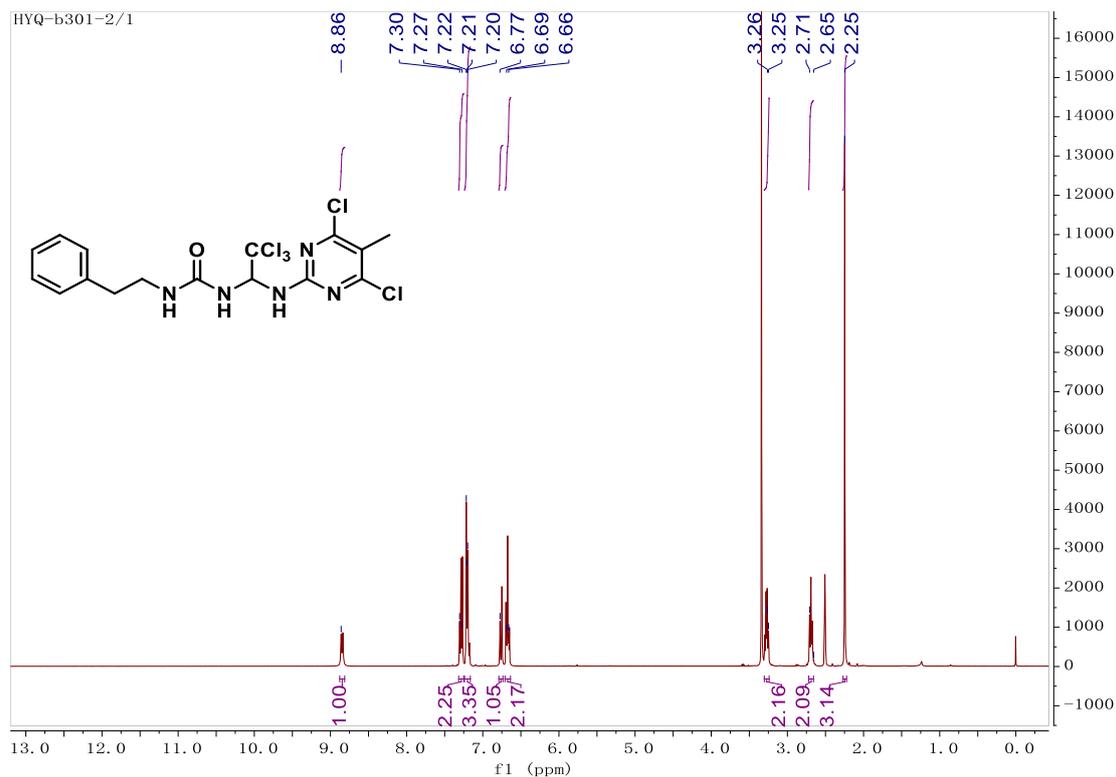
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479.9235	1	1146159.88
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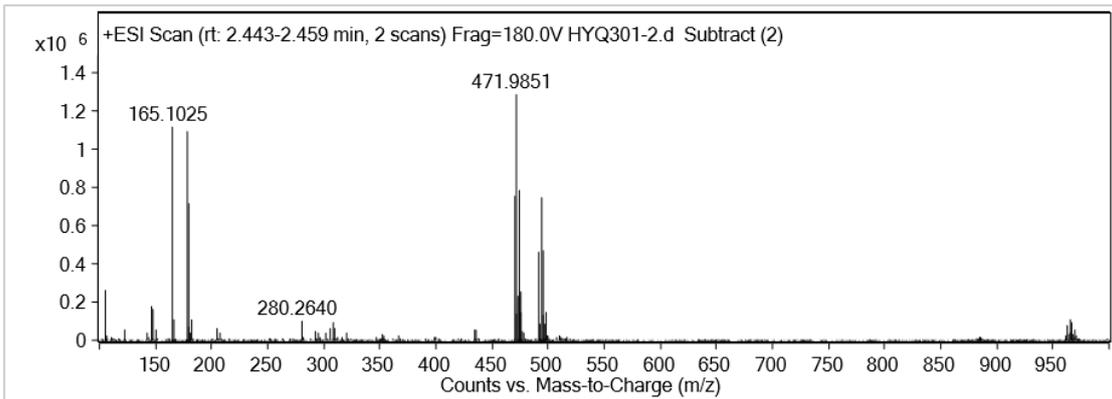
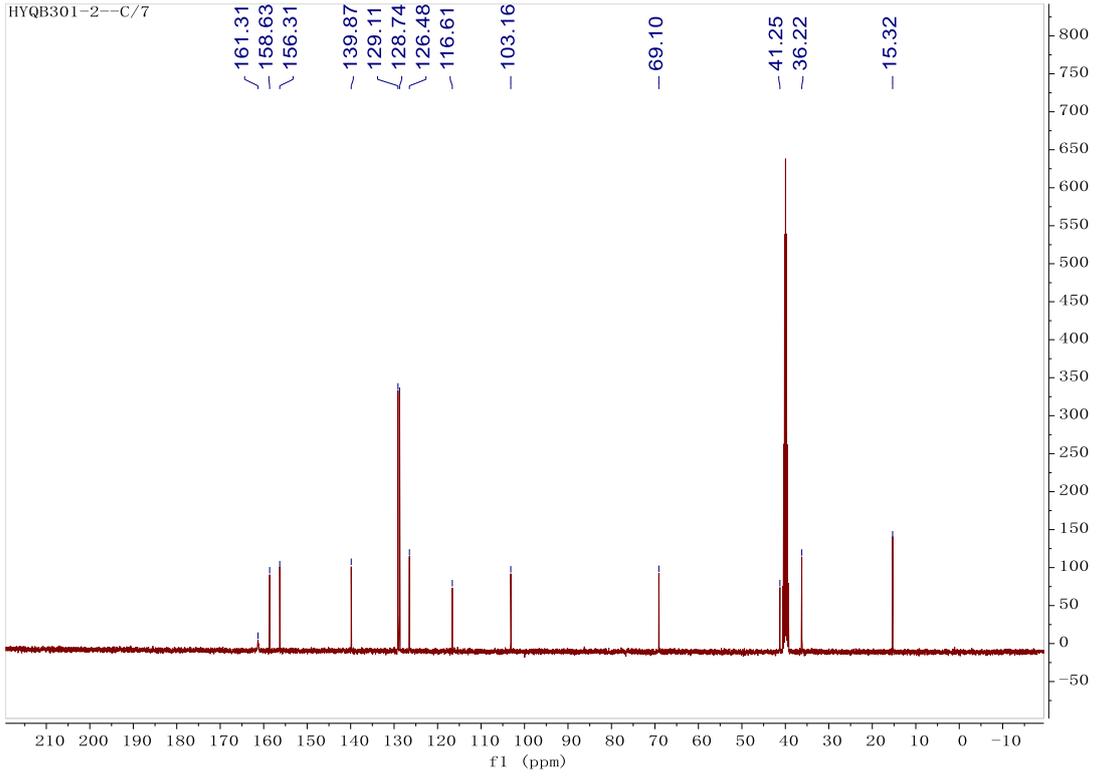
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Compound 12

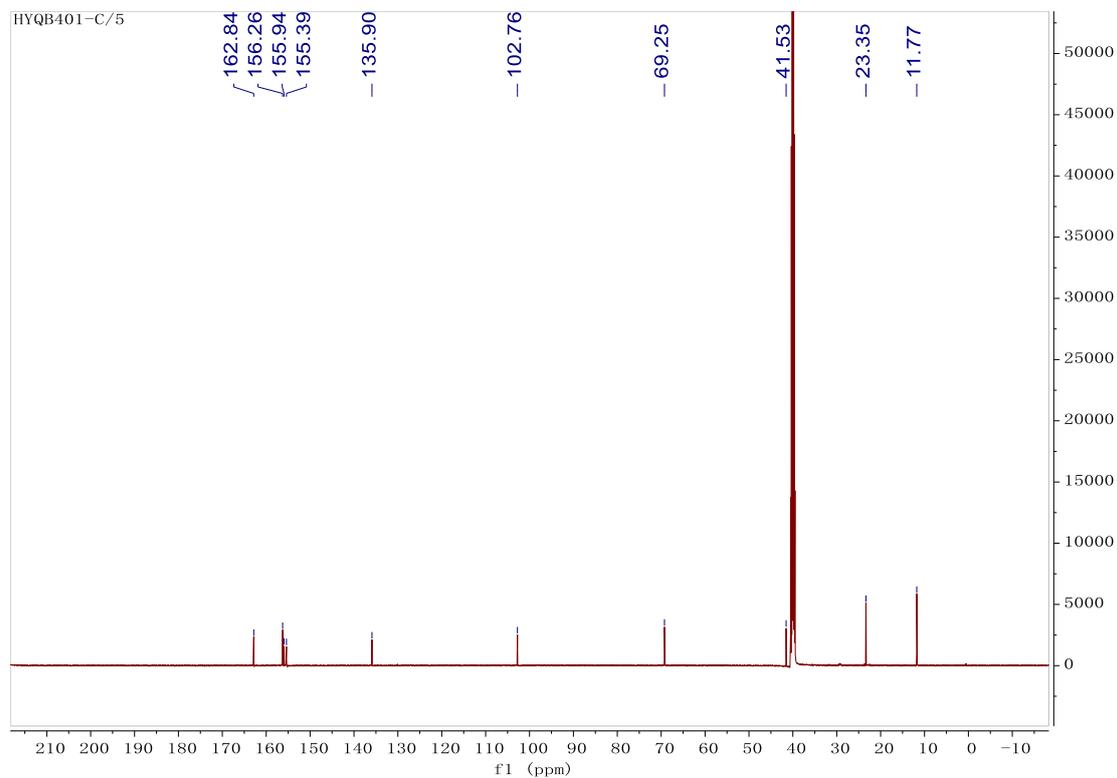
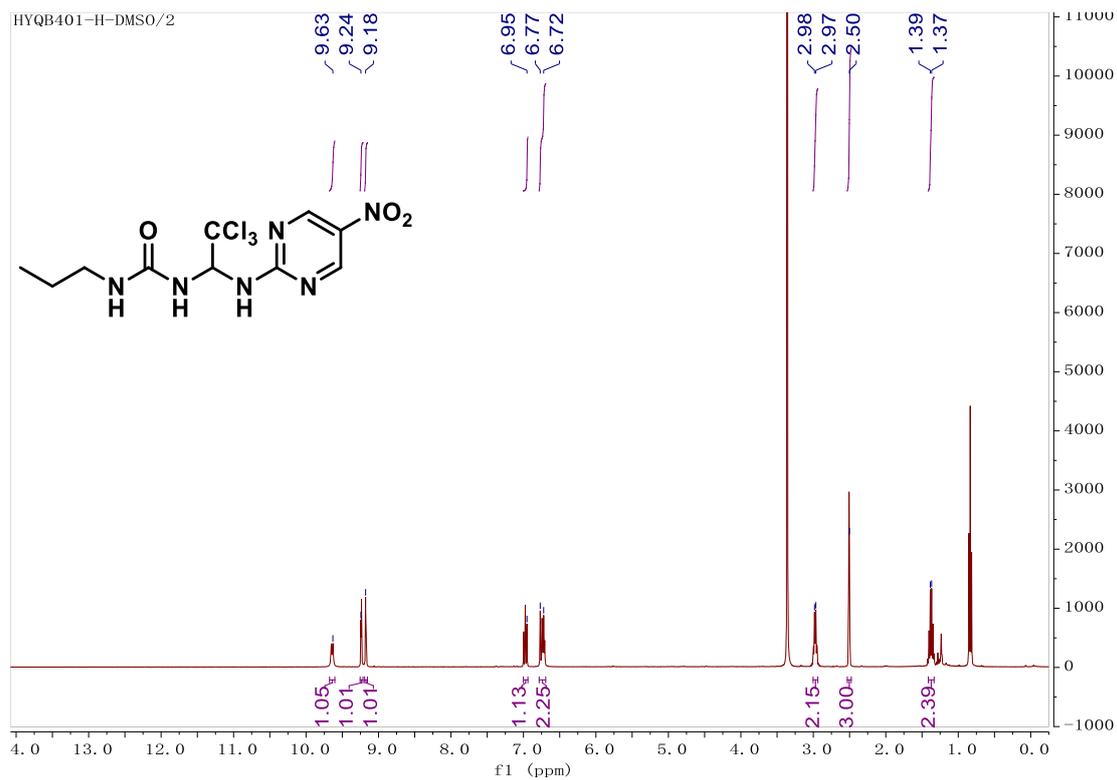


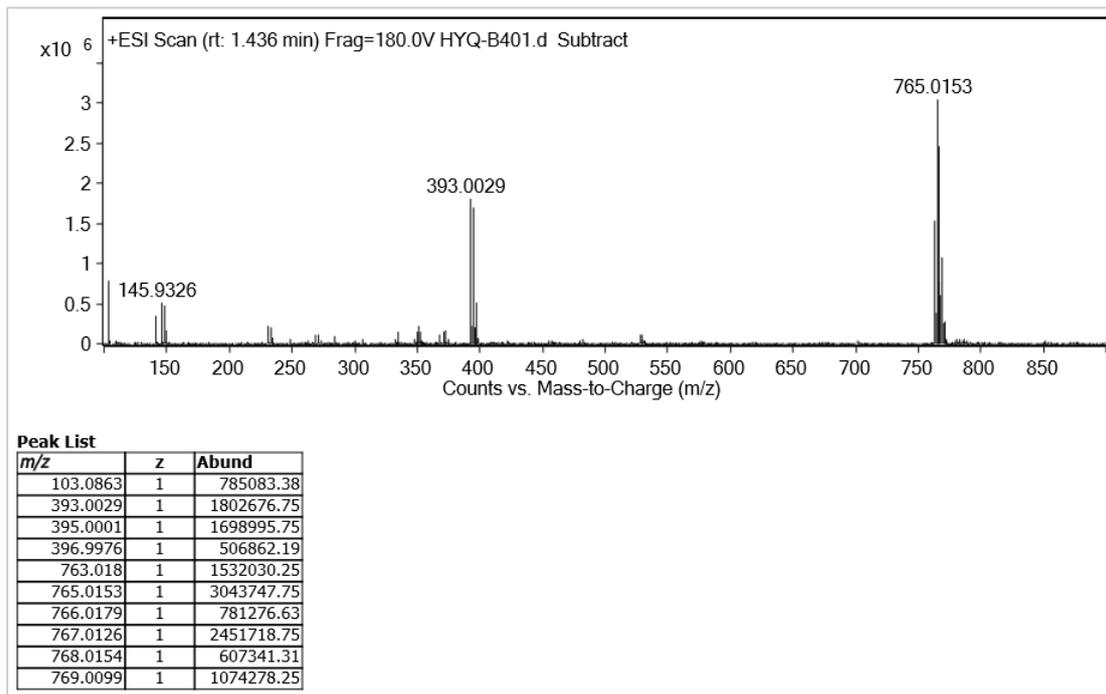


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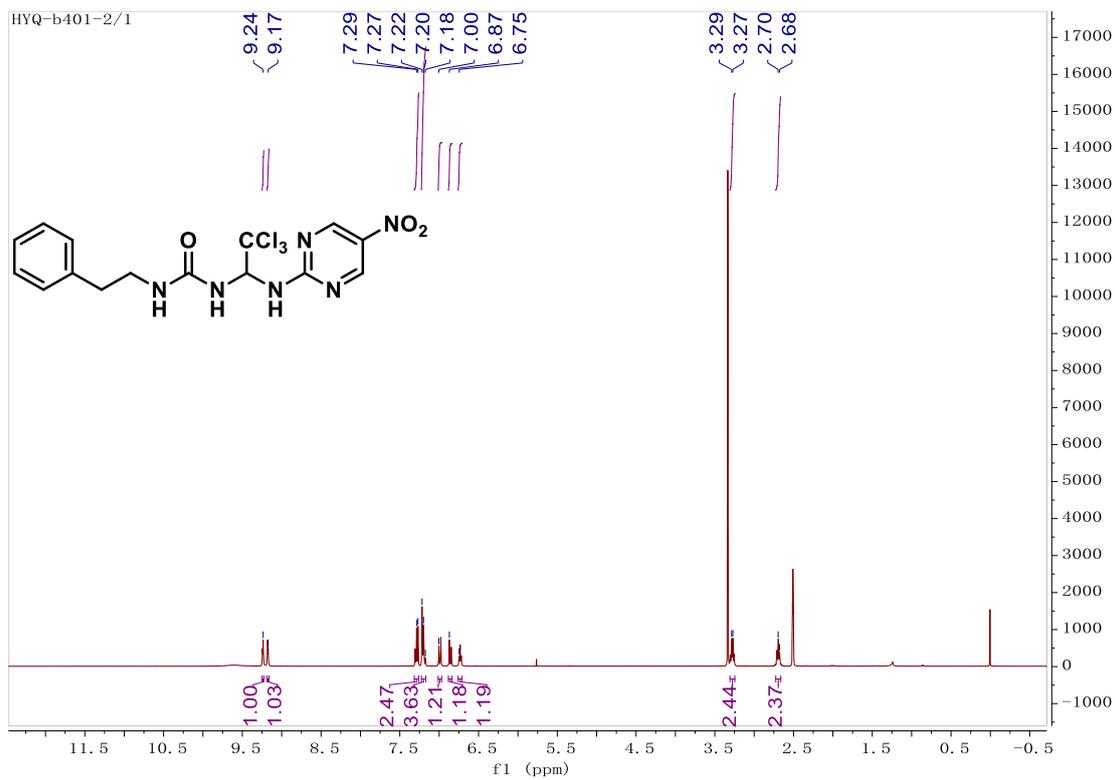
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469.988	1	751841
471.9851	1	1285317.88
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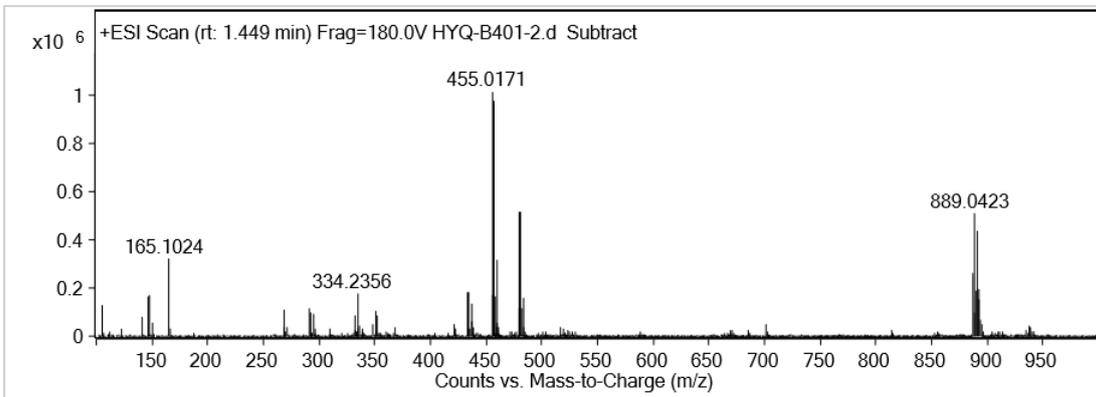
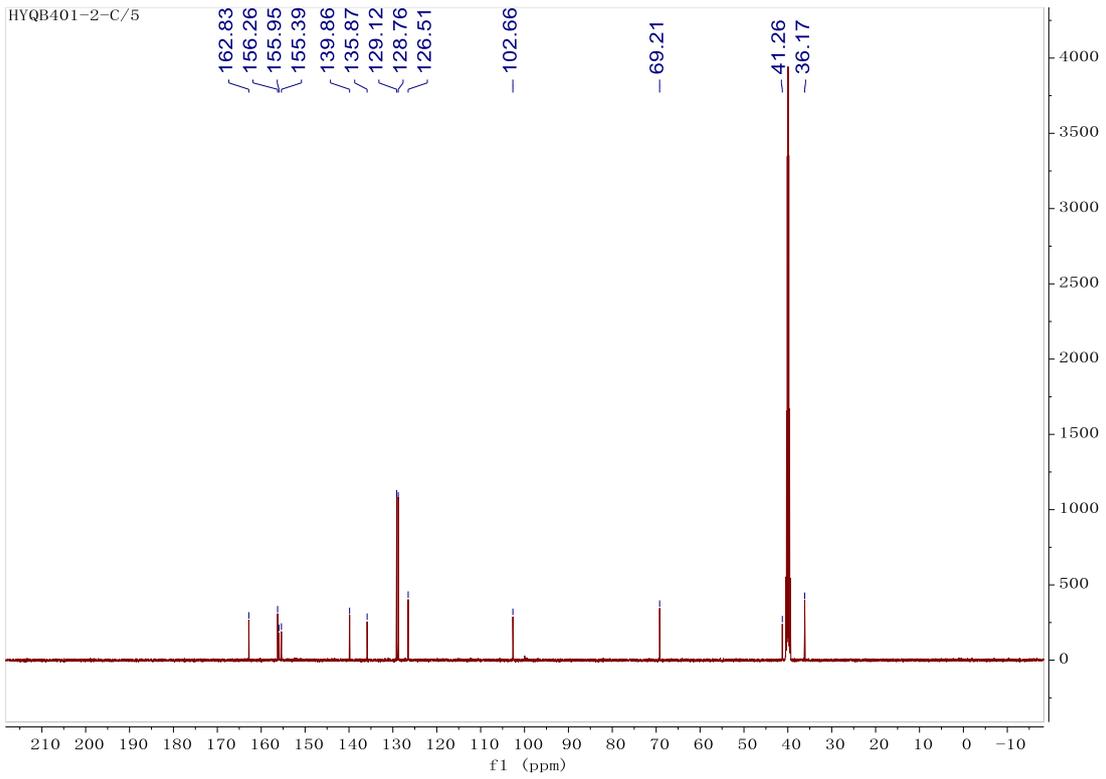
Compound 13





Compound 14

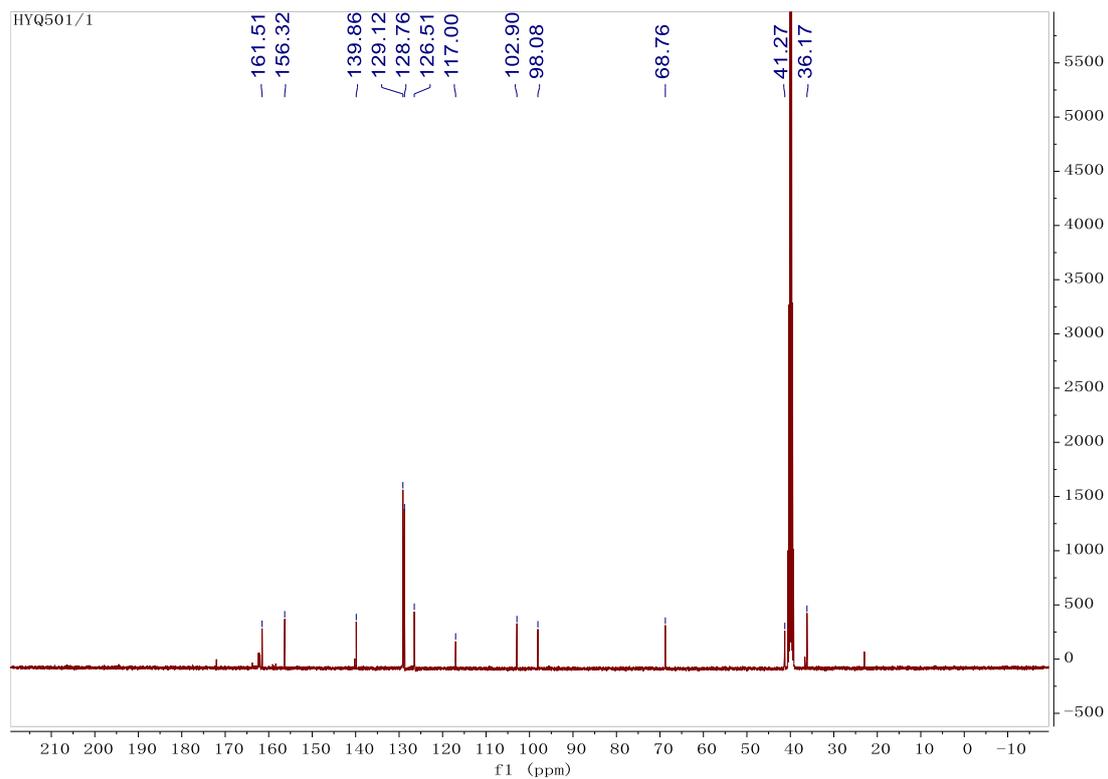
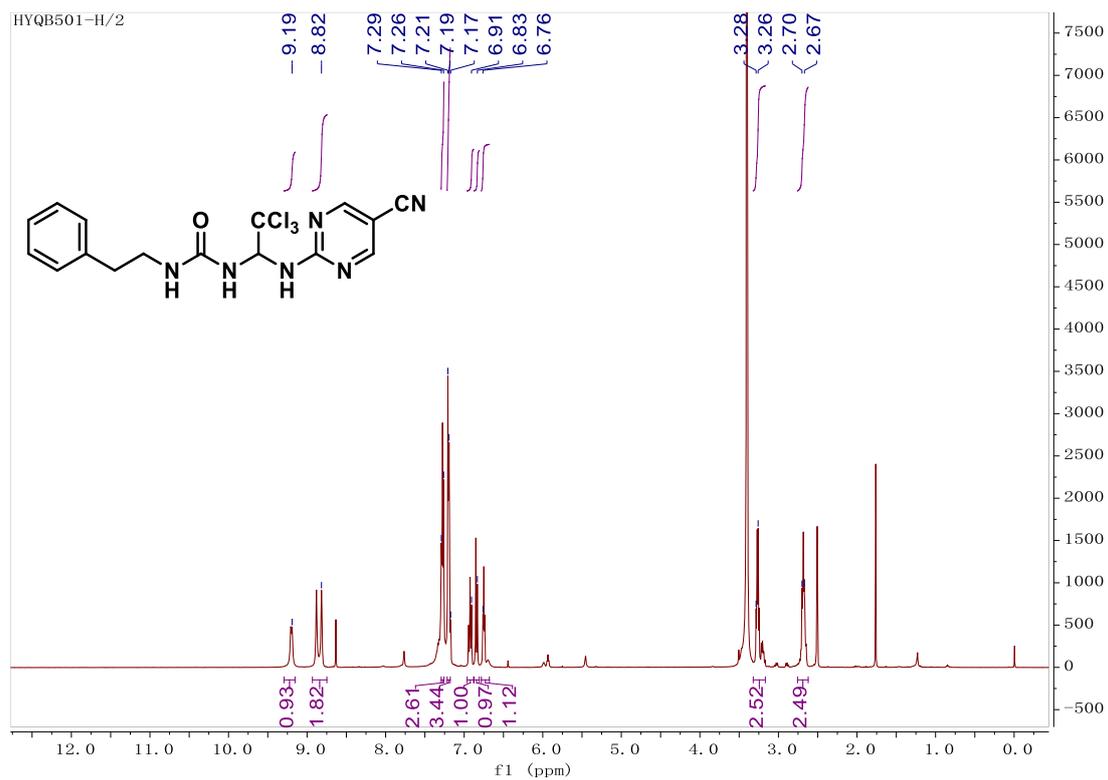


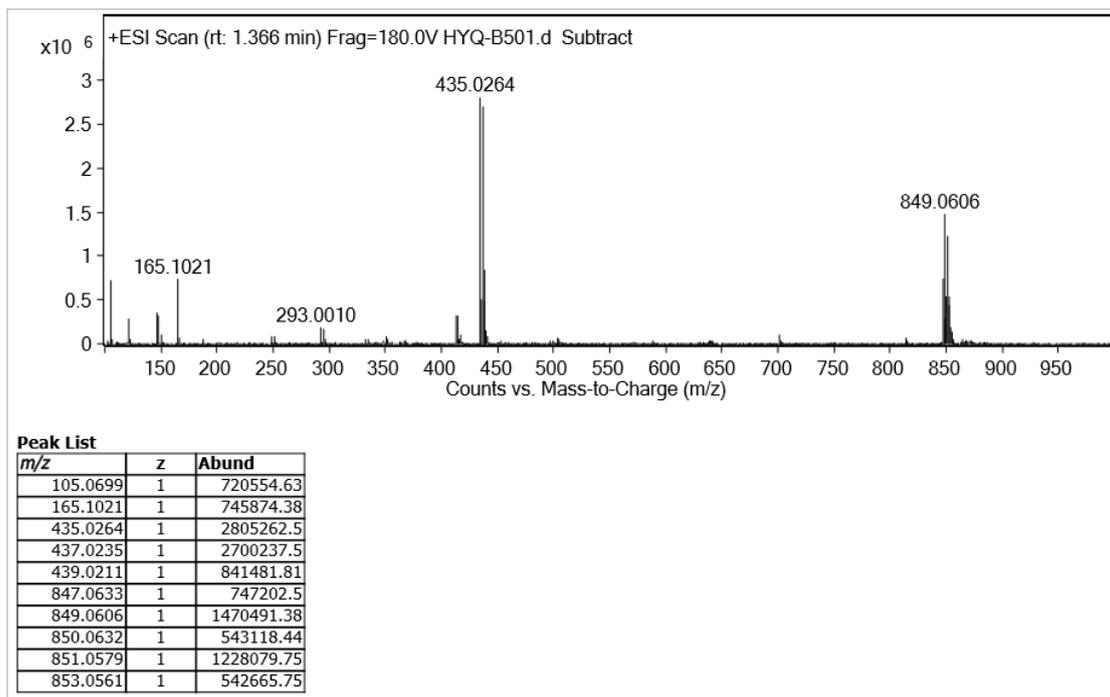


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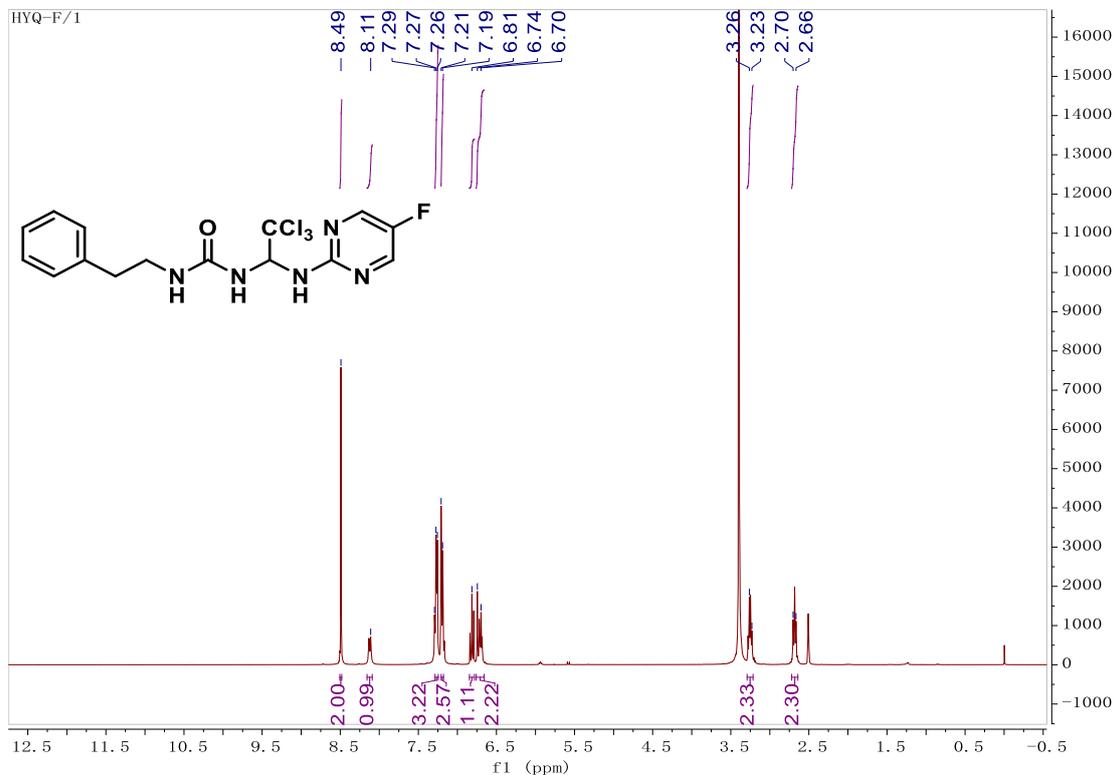
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479.0787	1	517871.5
481.076	1	517401.22
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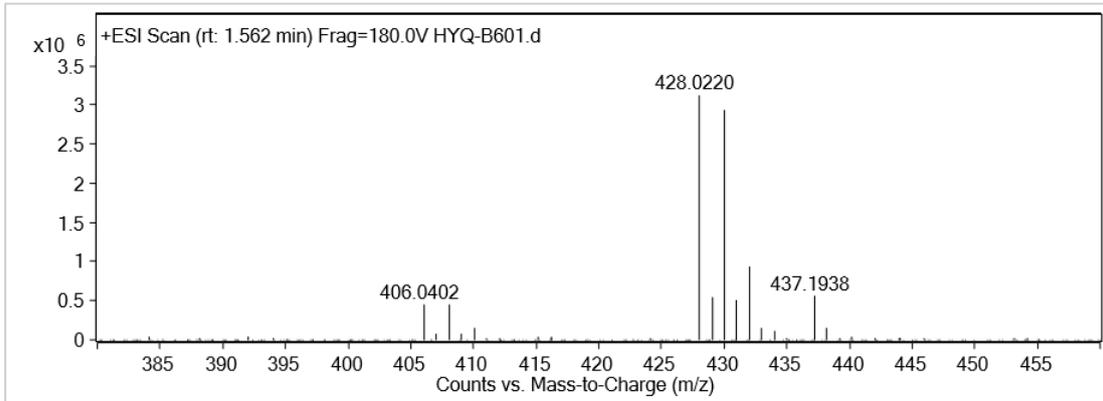
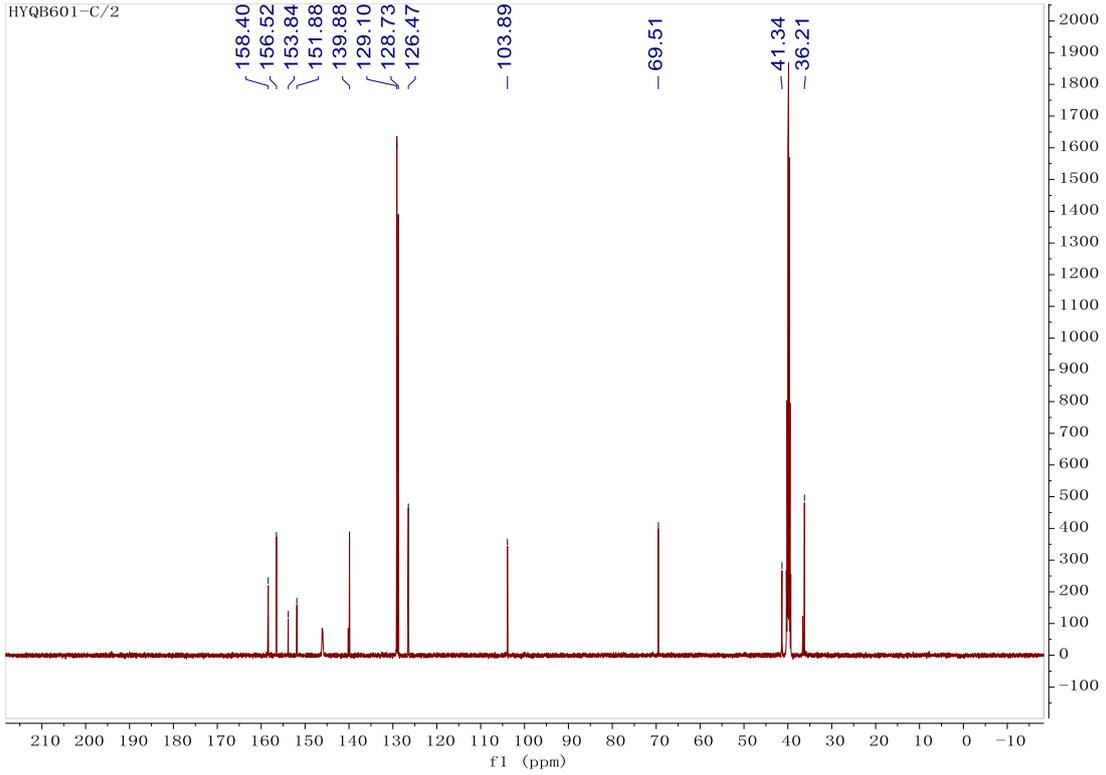
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Compound 16

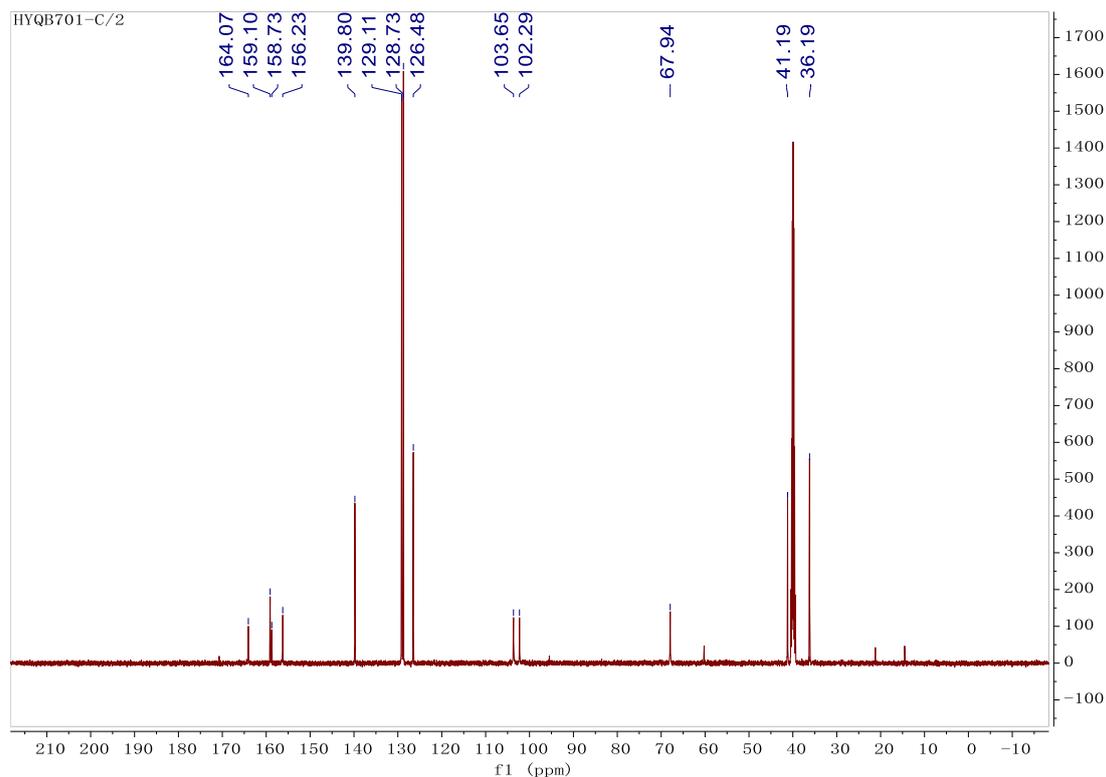
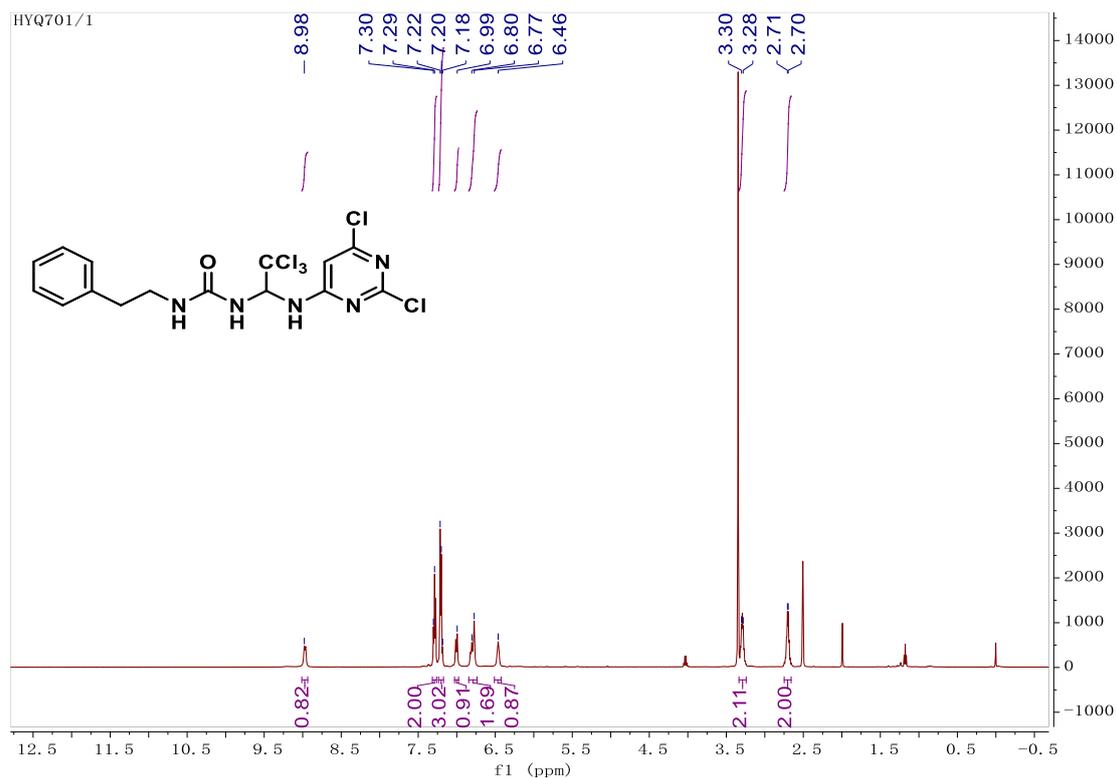


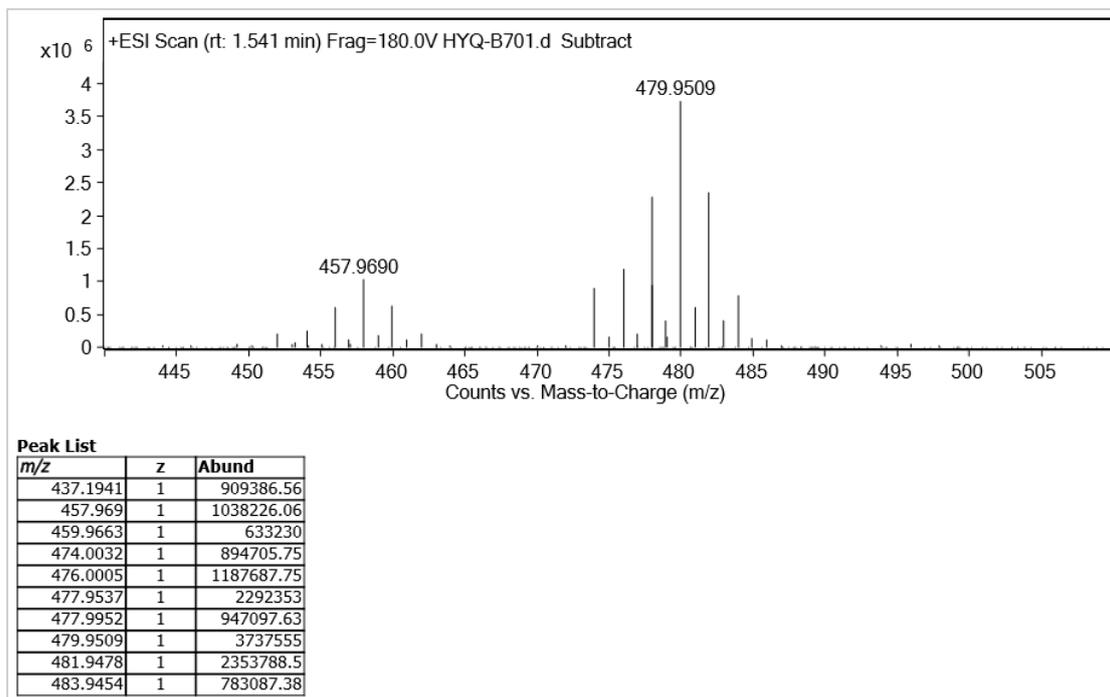


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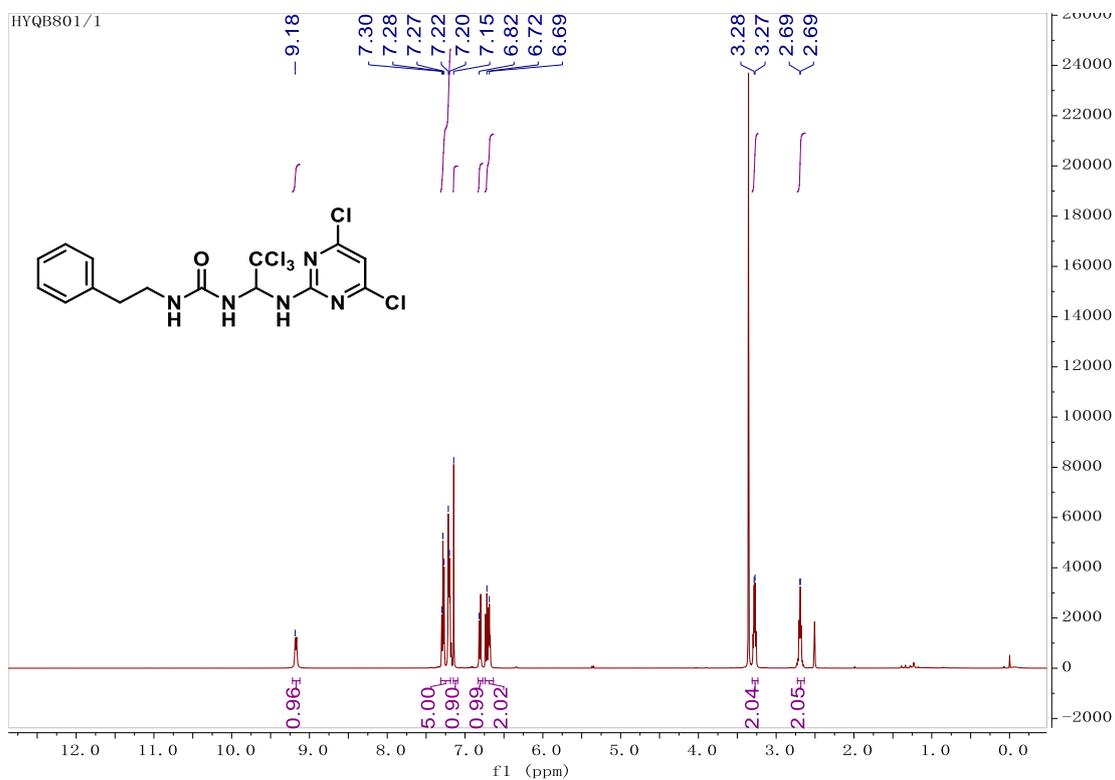
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291.1471	1	1649376.88
428.022	1	3121466.25
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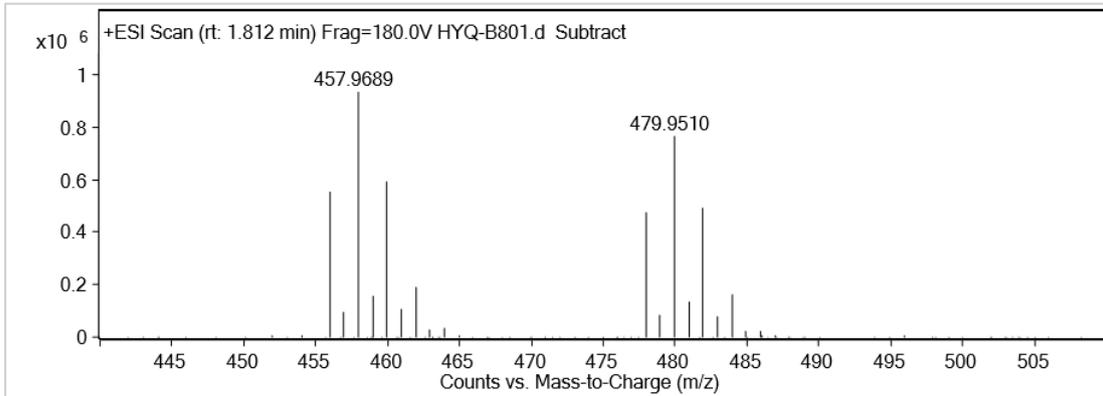
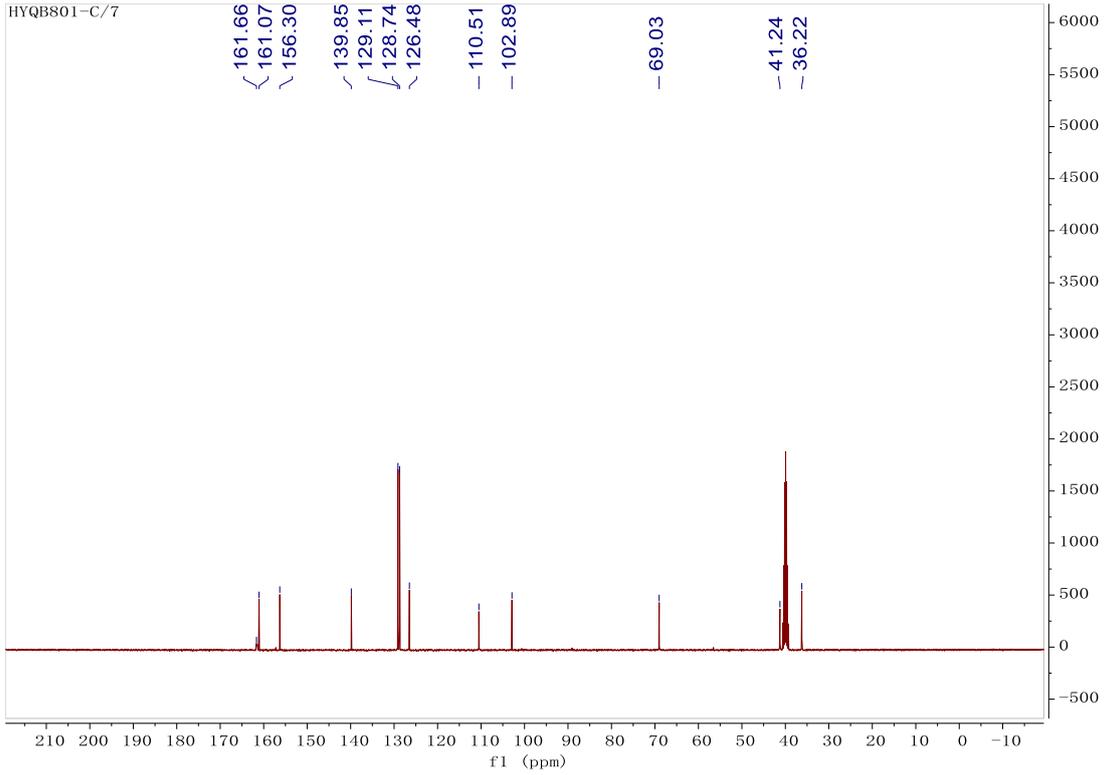
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Compound 18

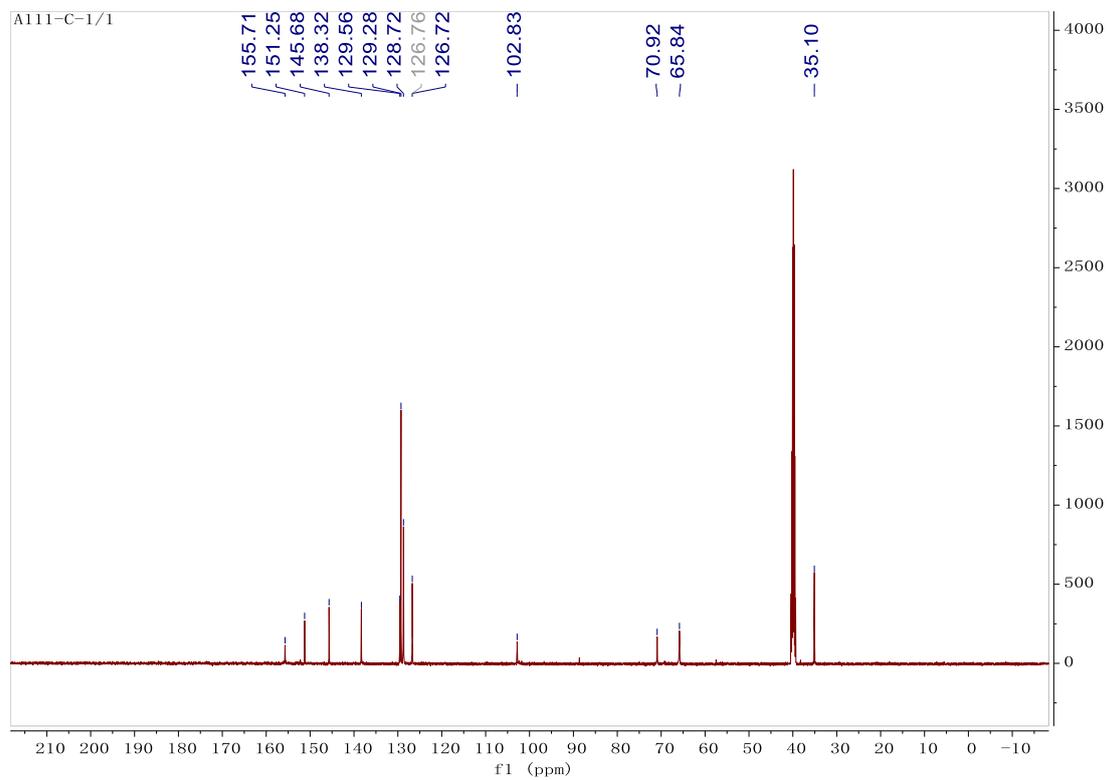
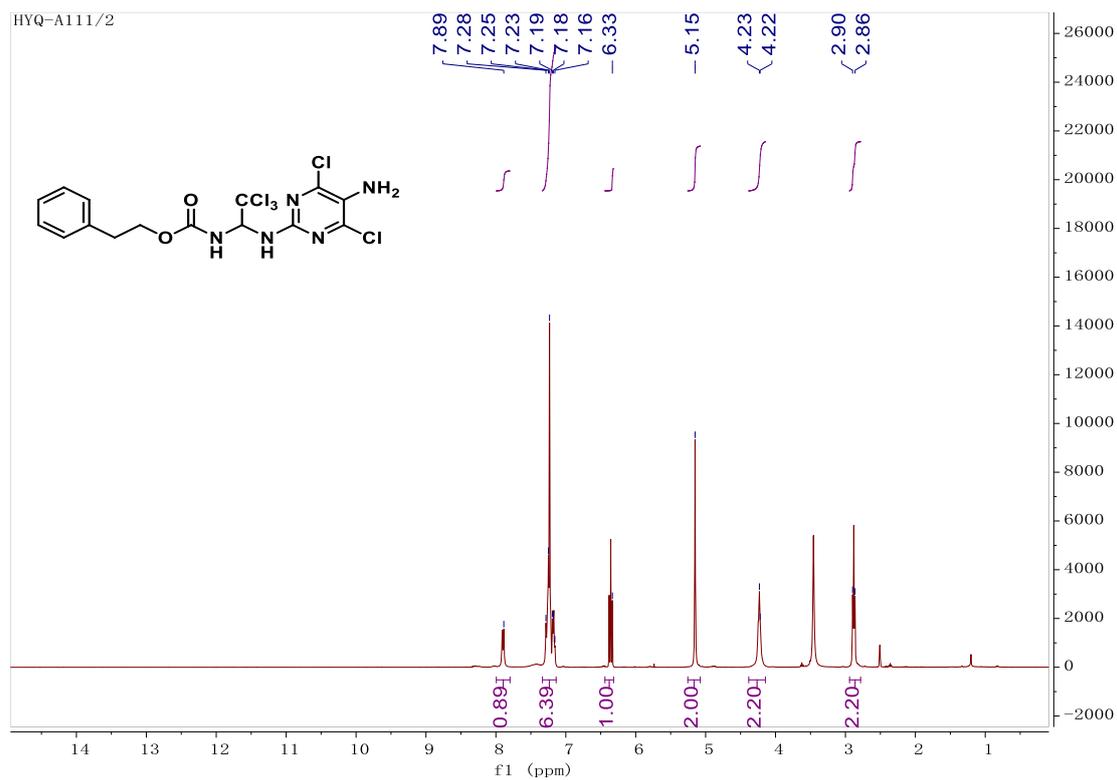


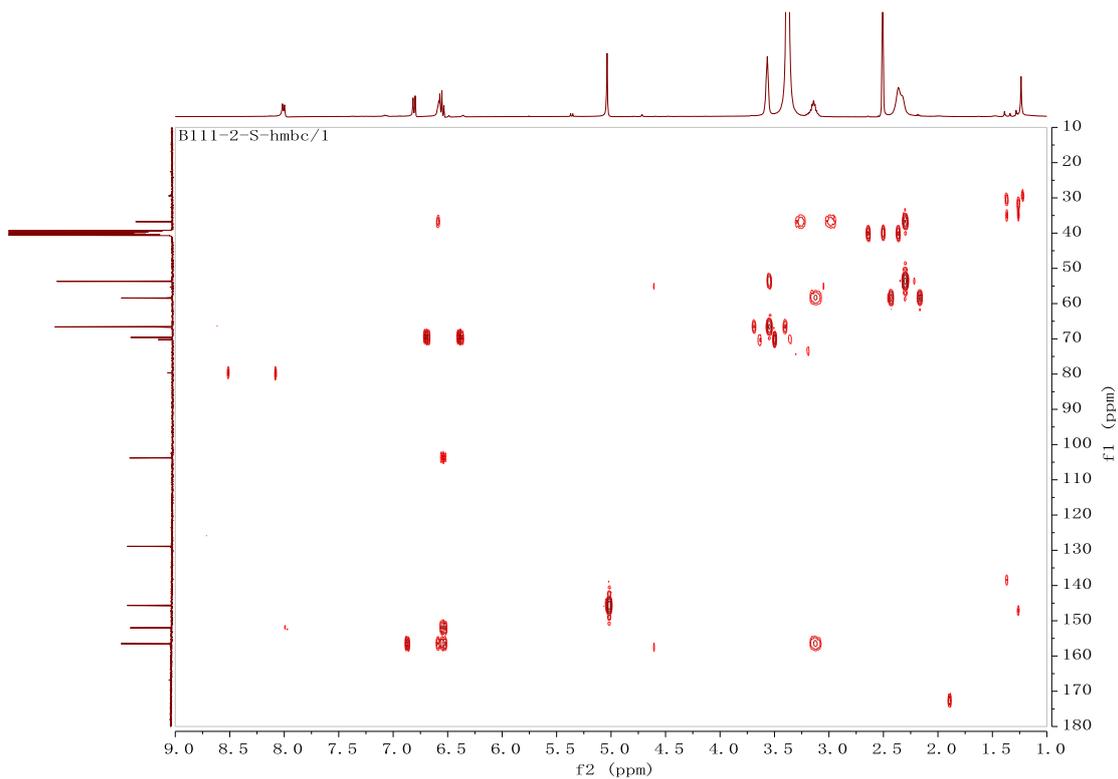
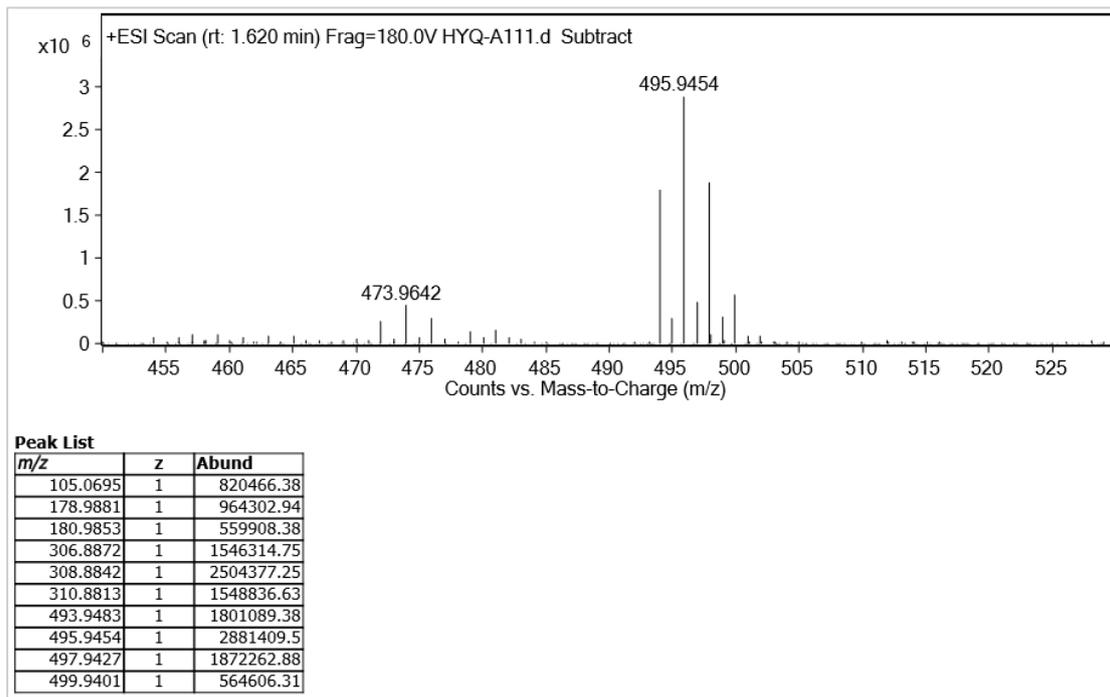


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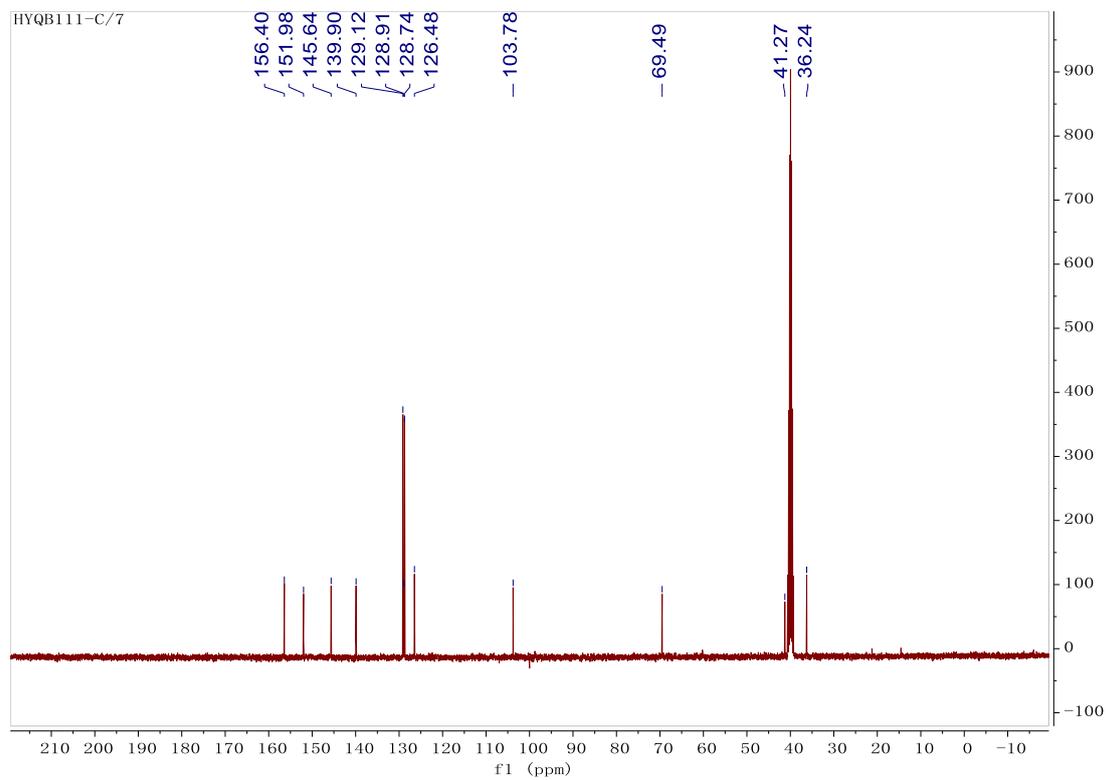
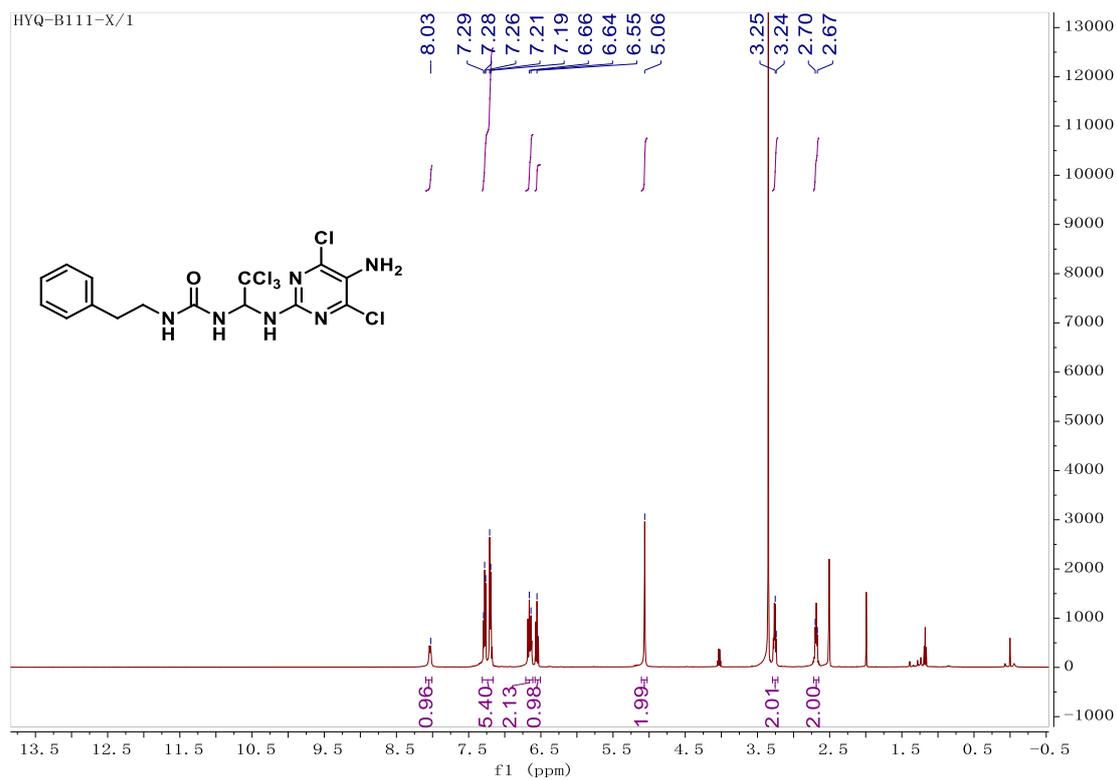
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165.9748	1	496365.72
455.972	1	555500.81
457.9689	1	933681.19
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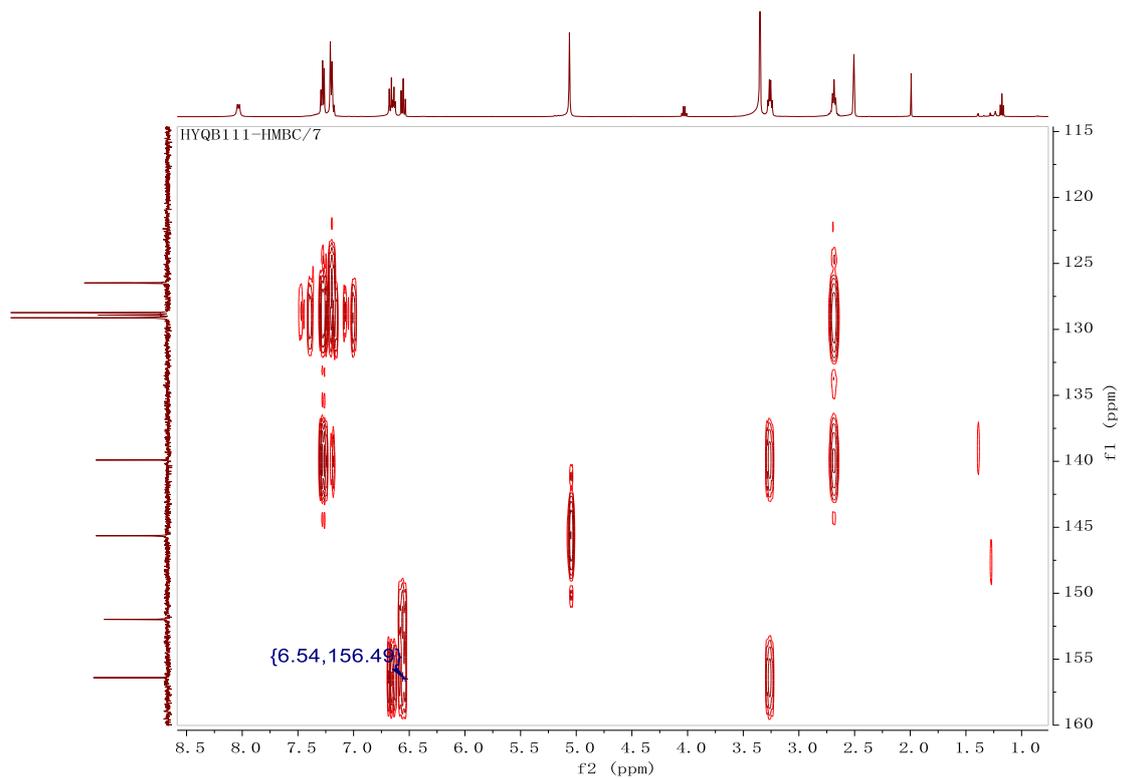
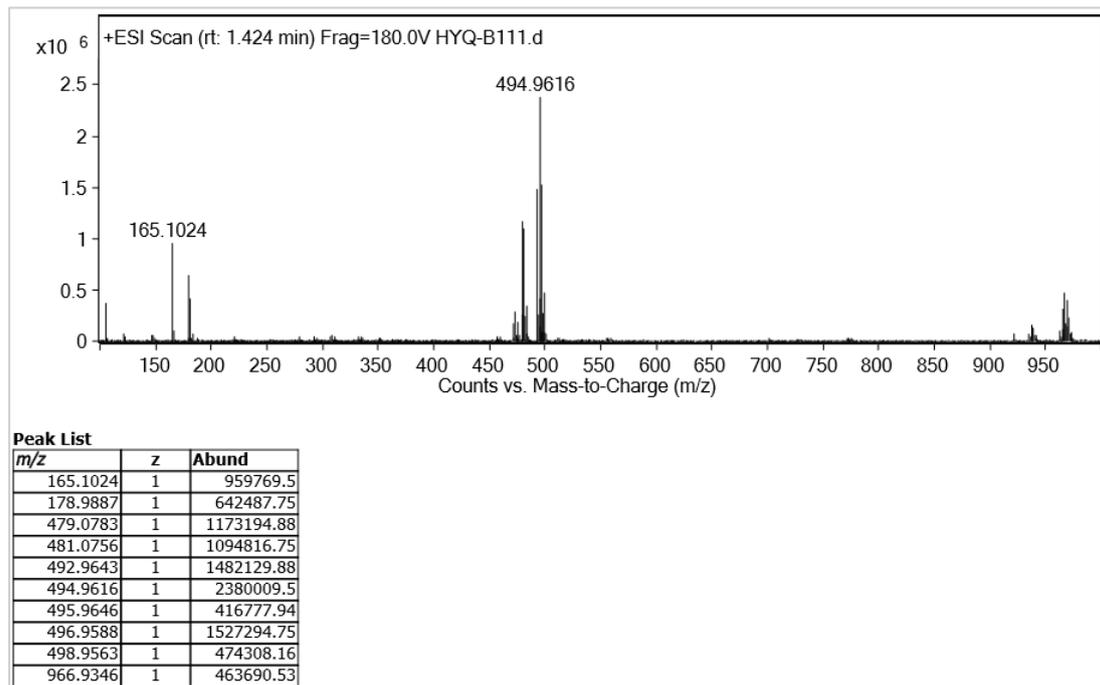
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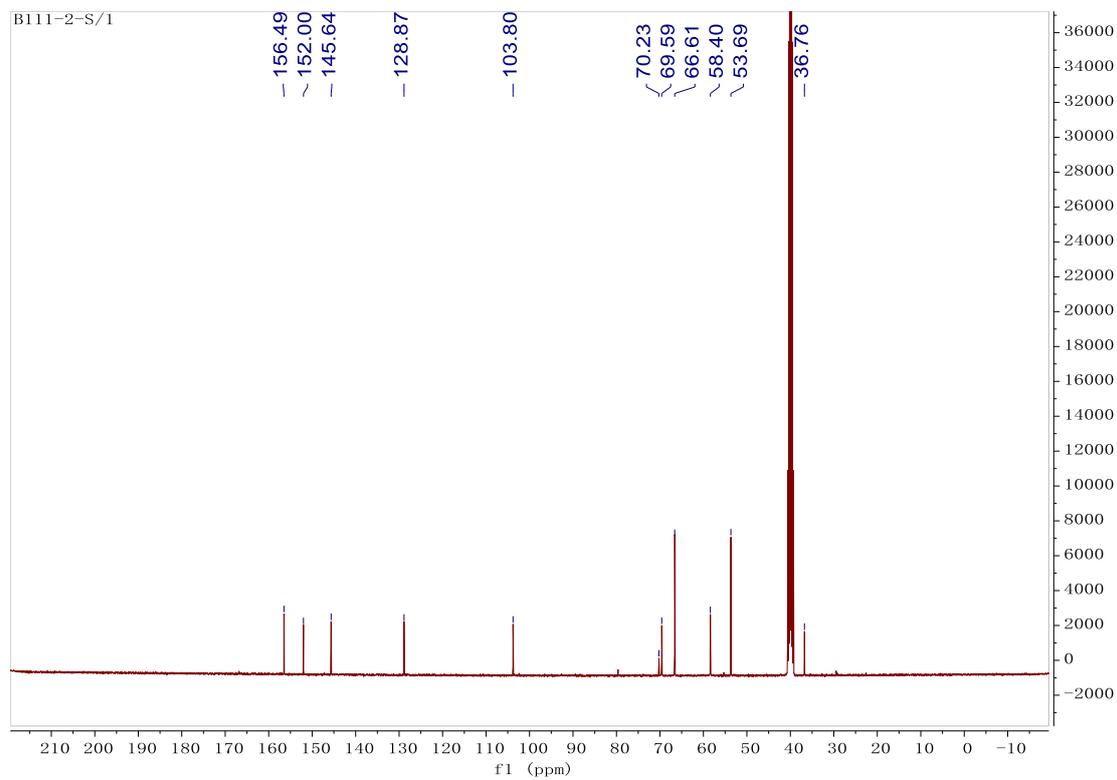
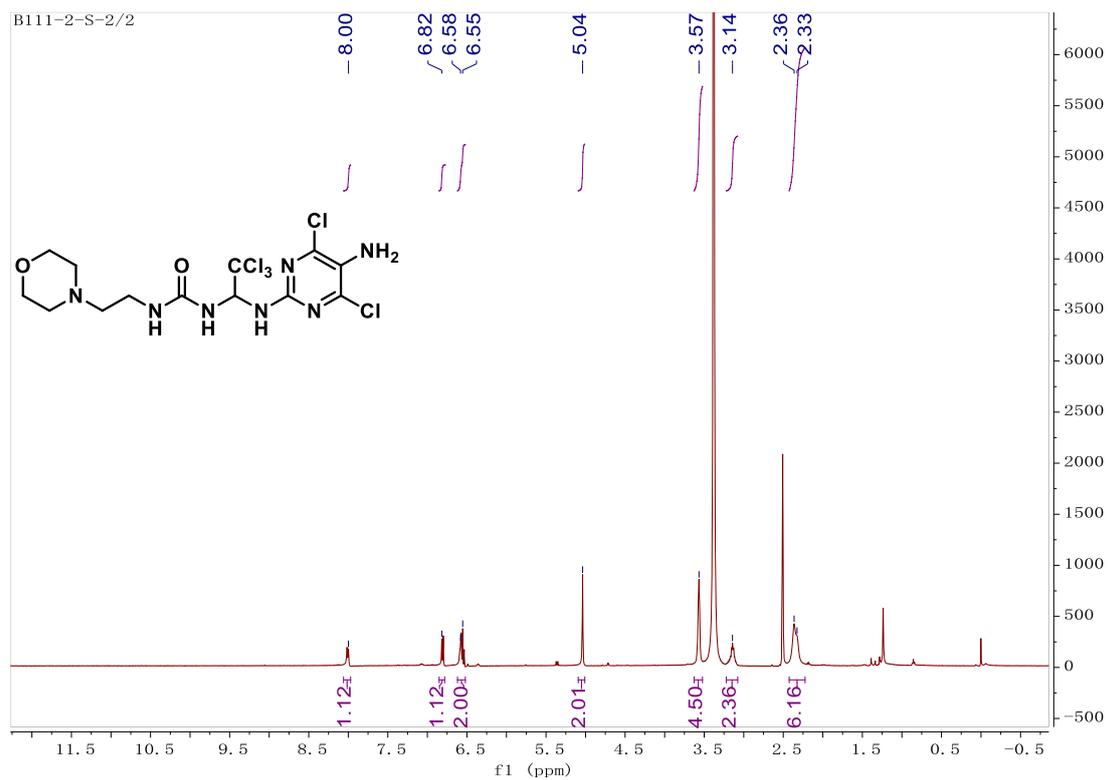


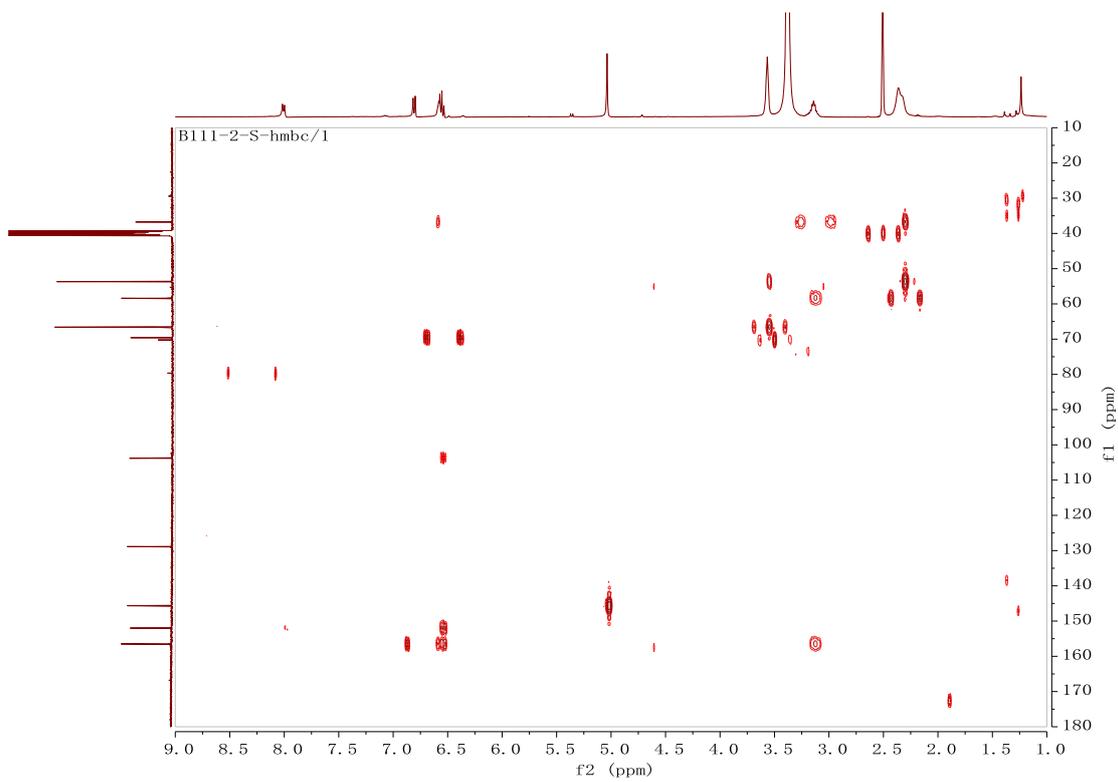
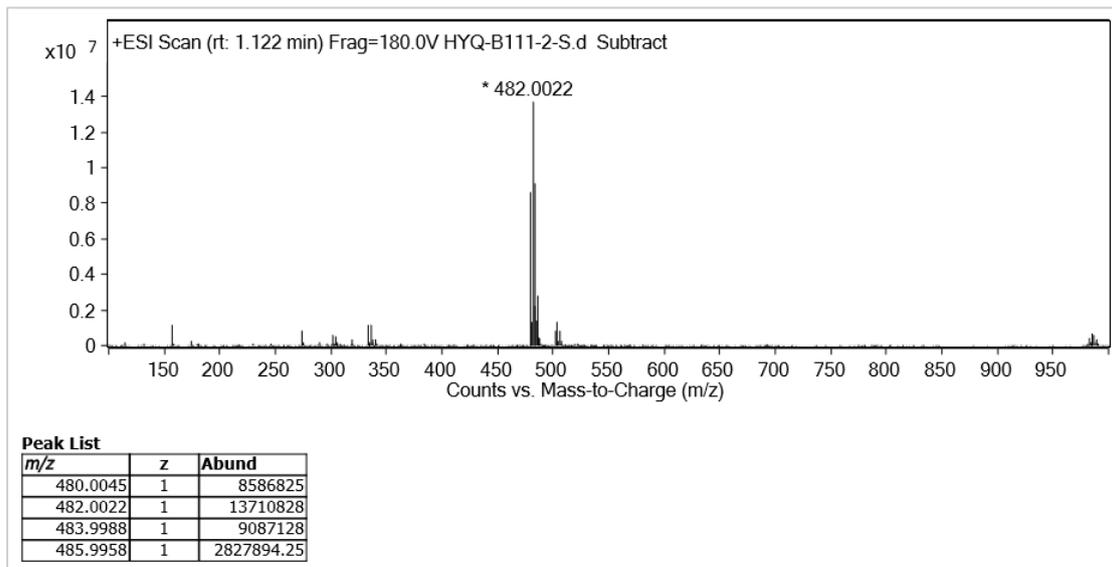
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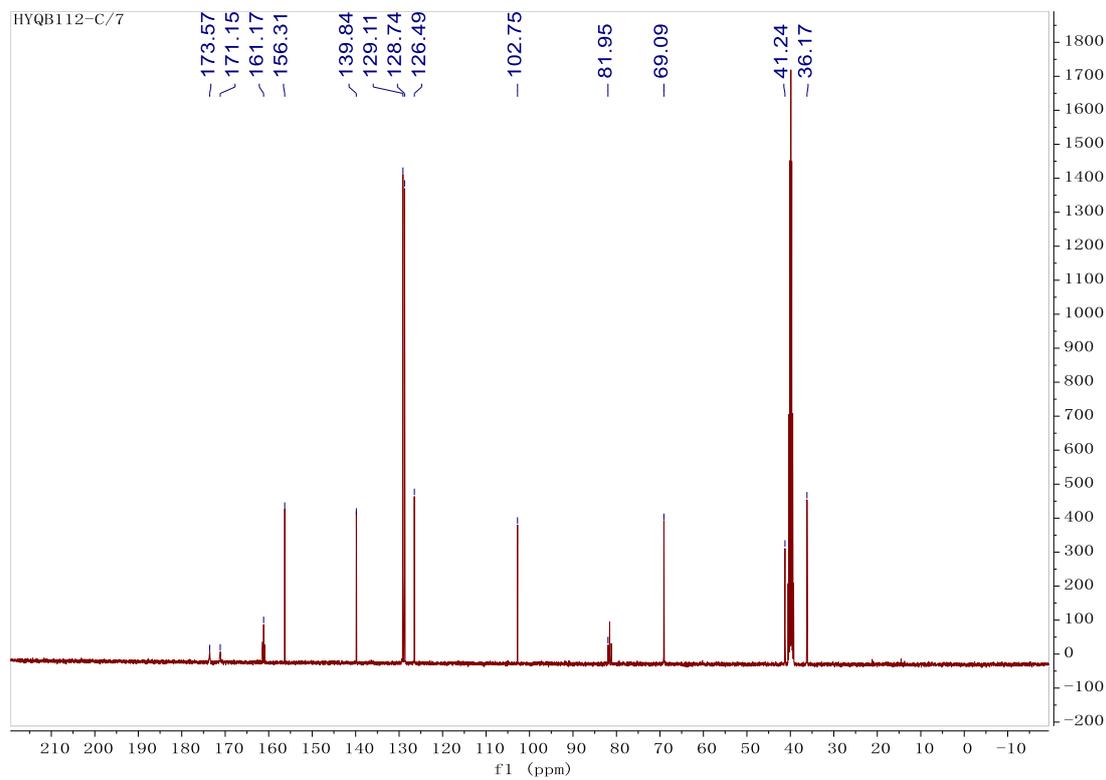
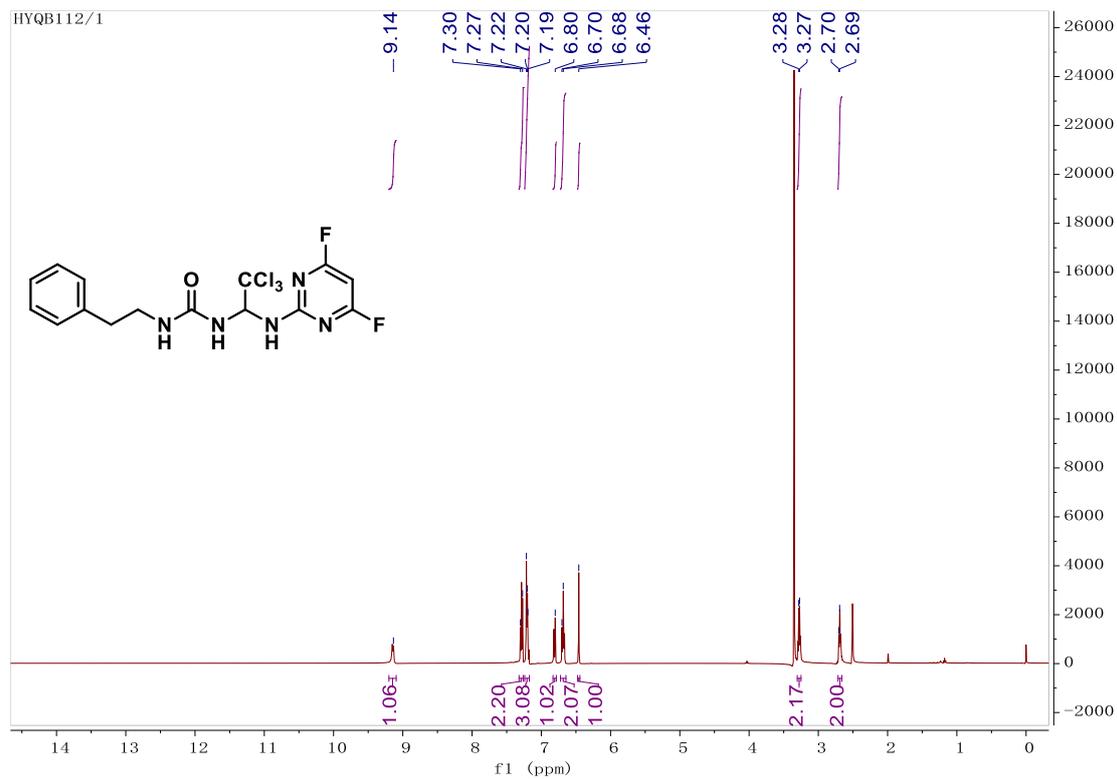


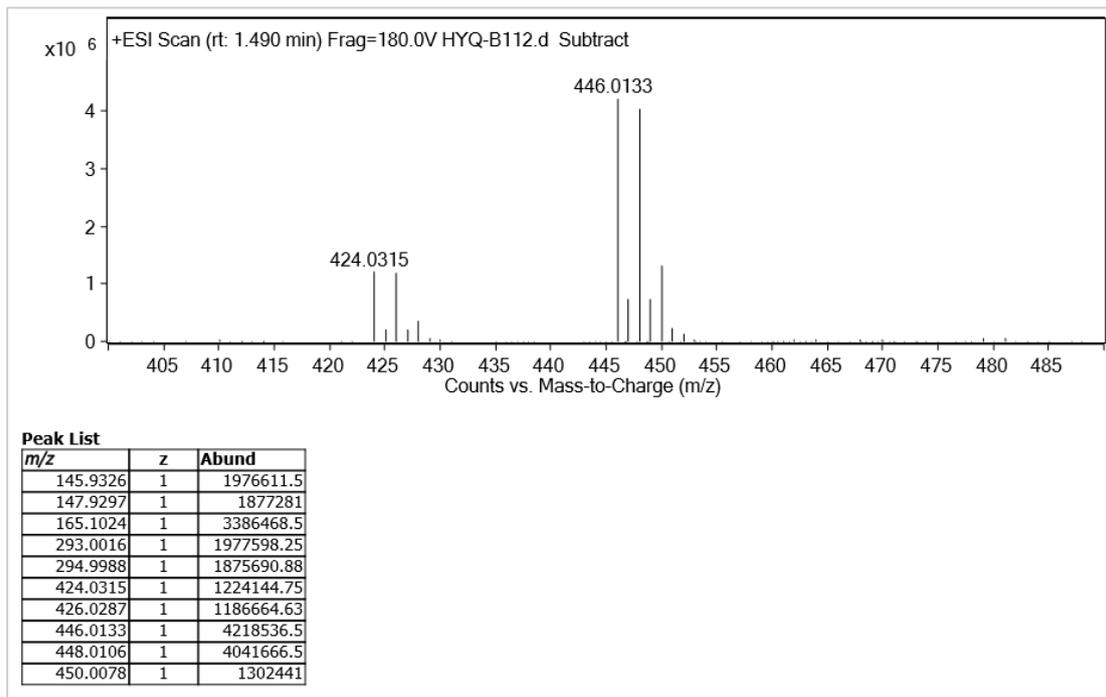
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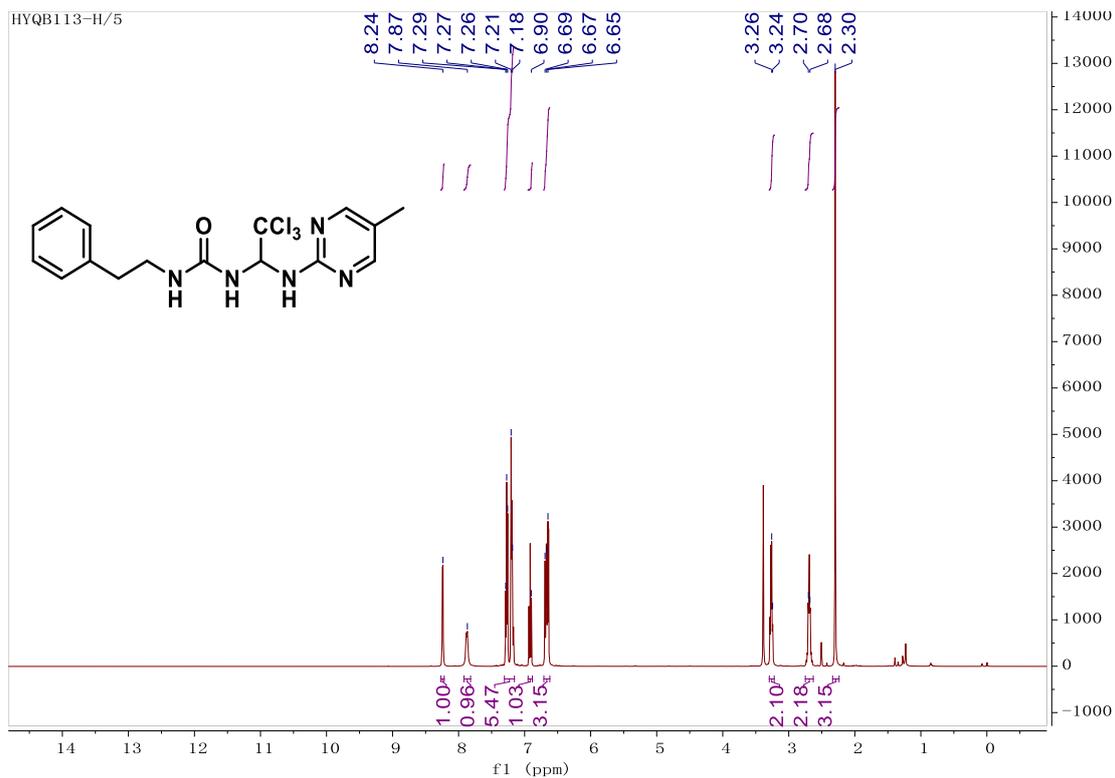


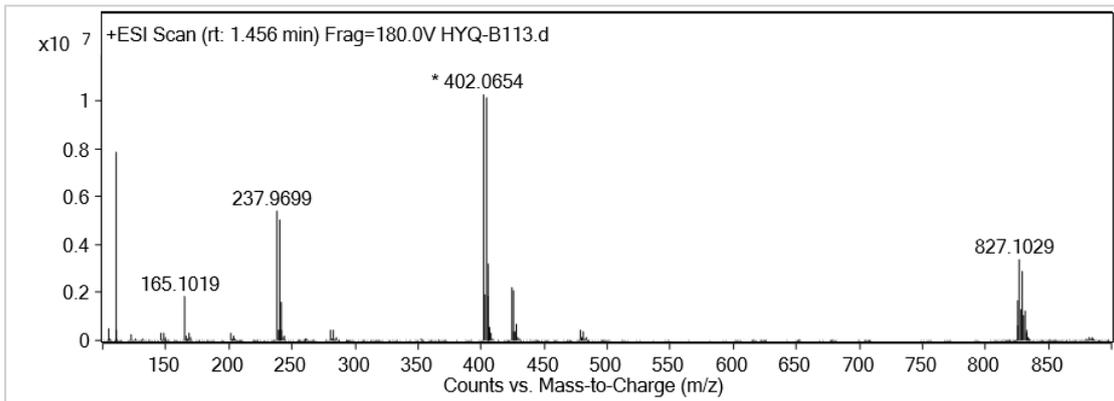
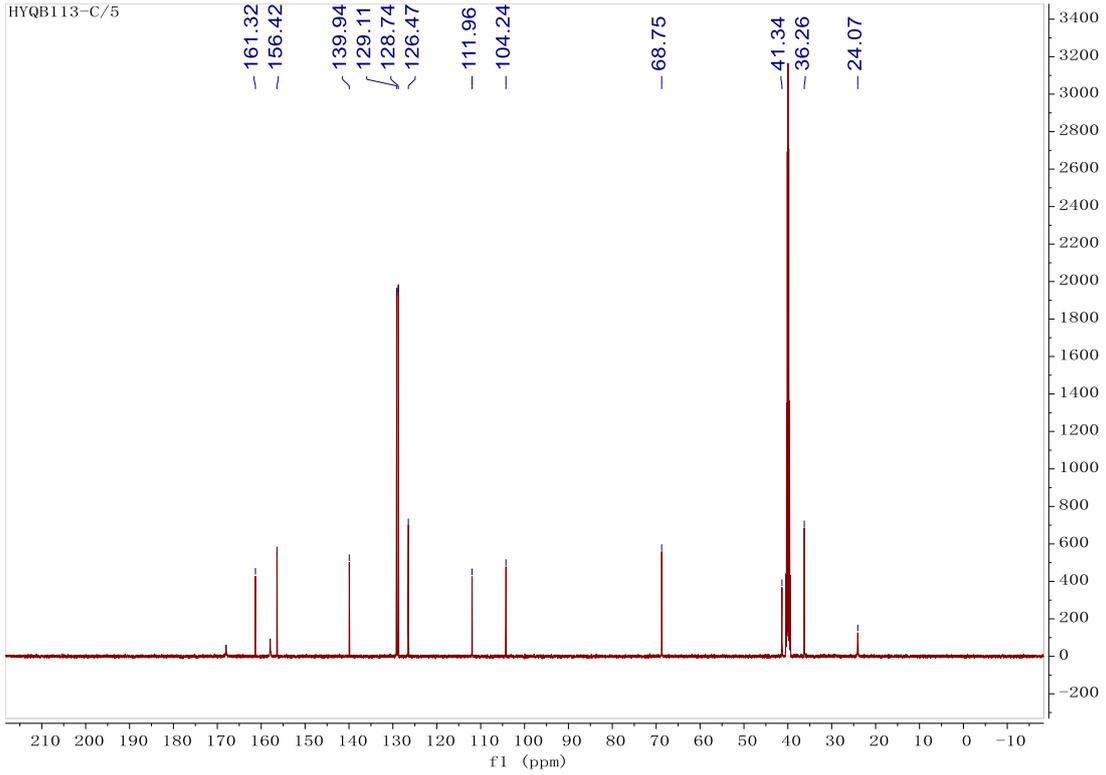
Compound 22





Compound 23

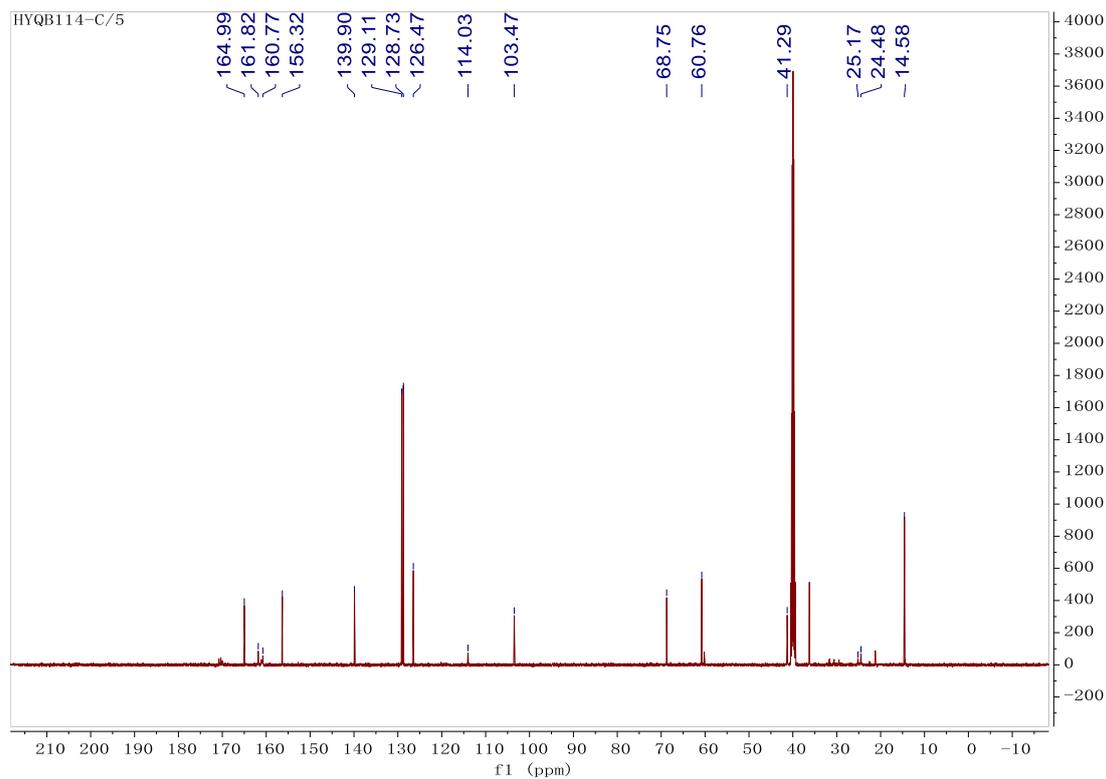
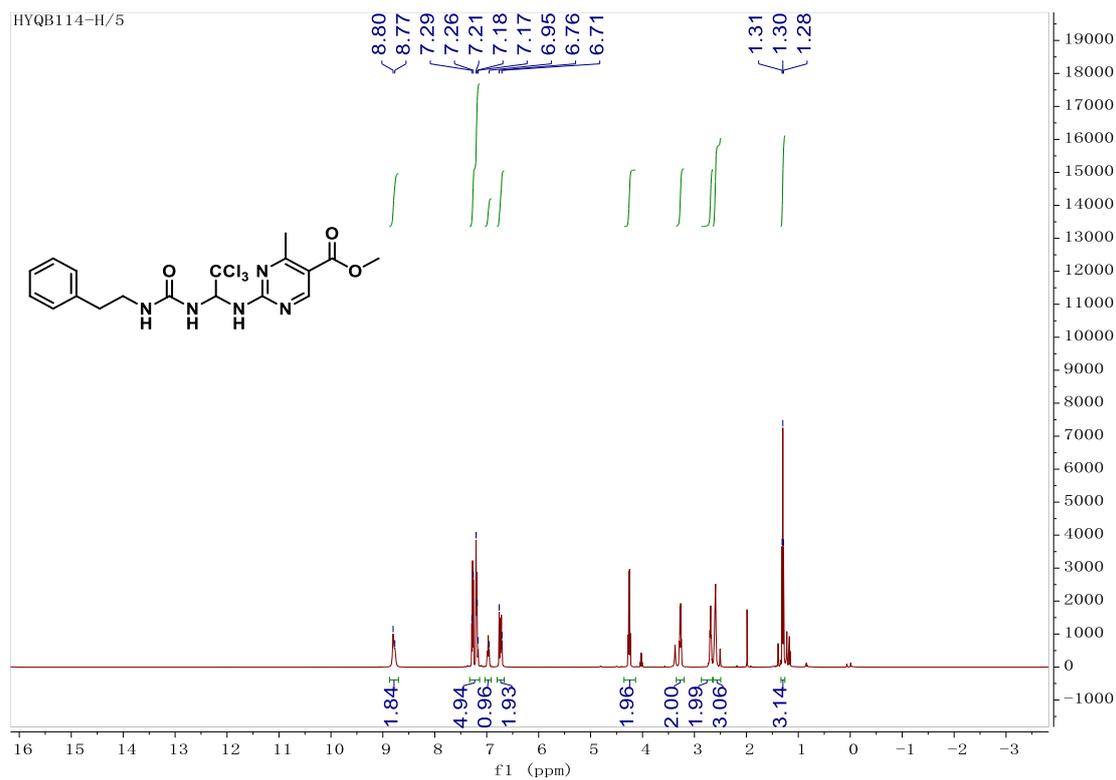


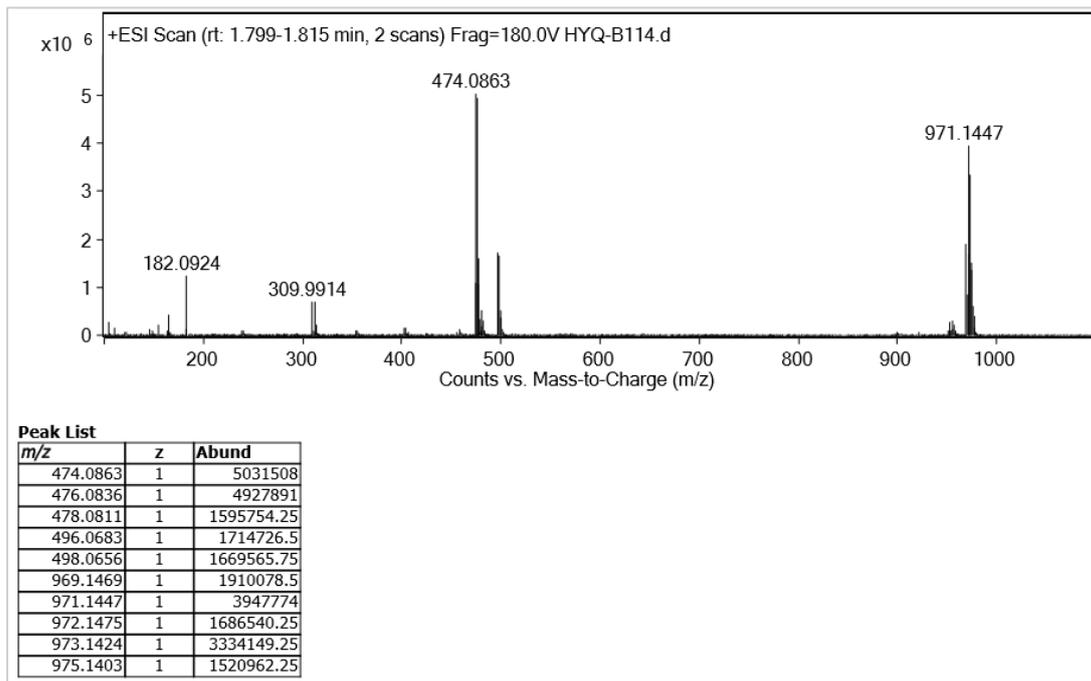


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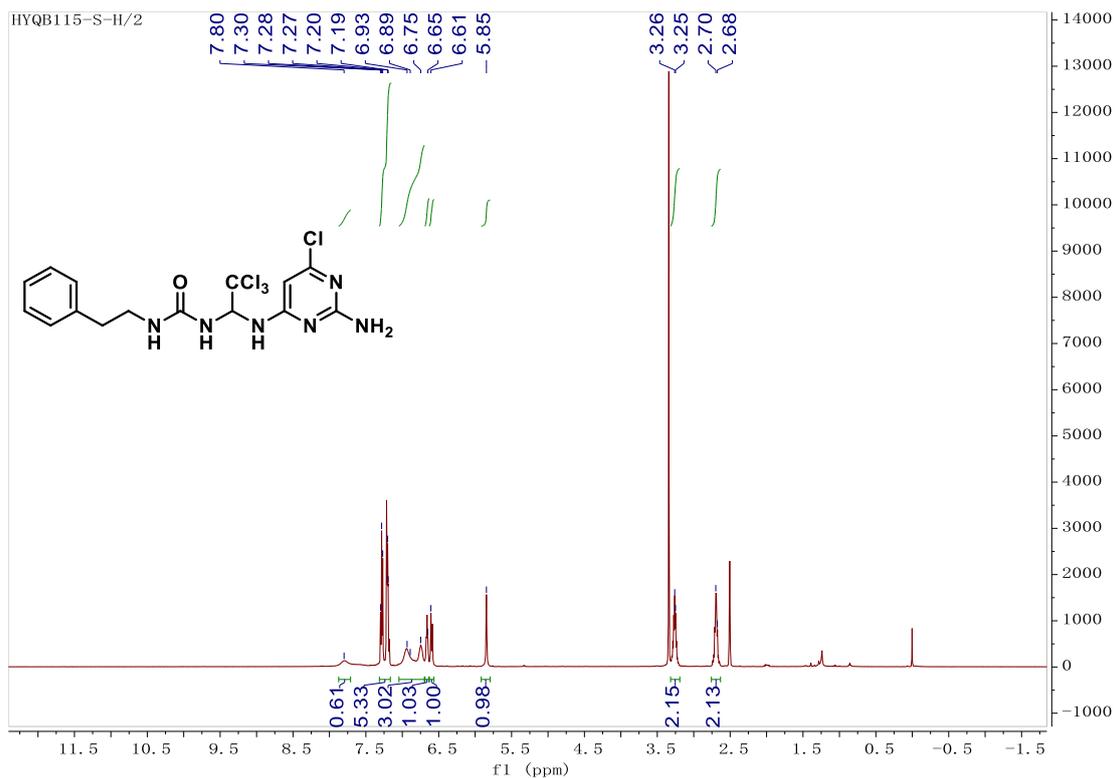
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404.0626	1	10105609
406.0596	1	3168678
424.0469	1	2190224.25
426.0441	1	2118229.25
827.1029	1	3394894
829.1002	1	2891291

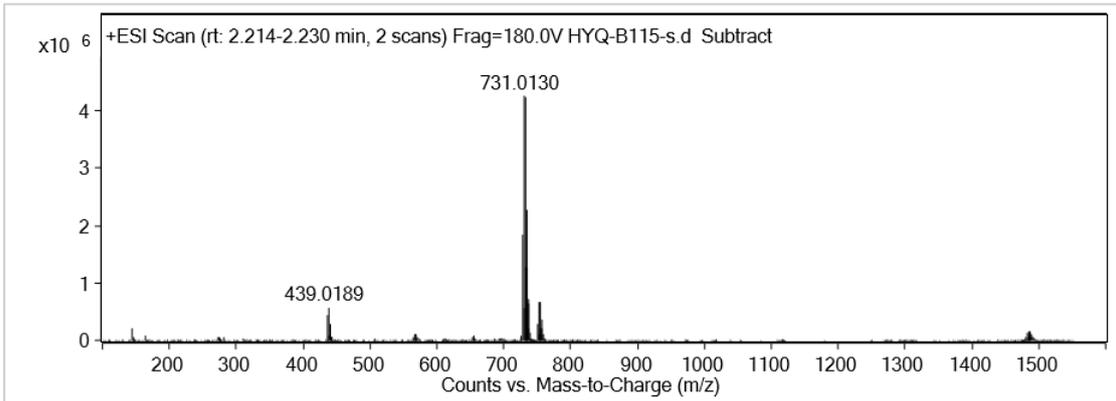
Compound24





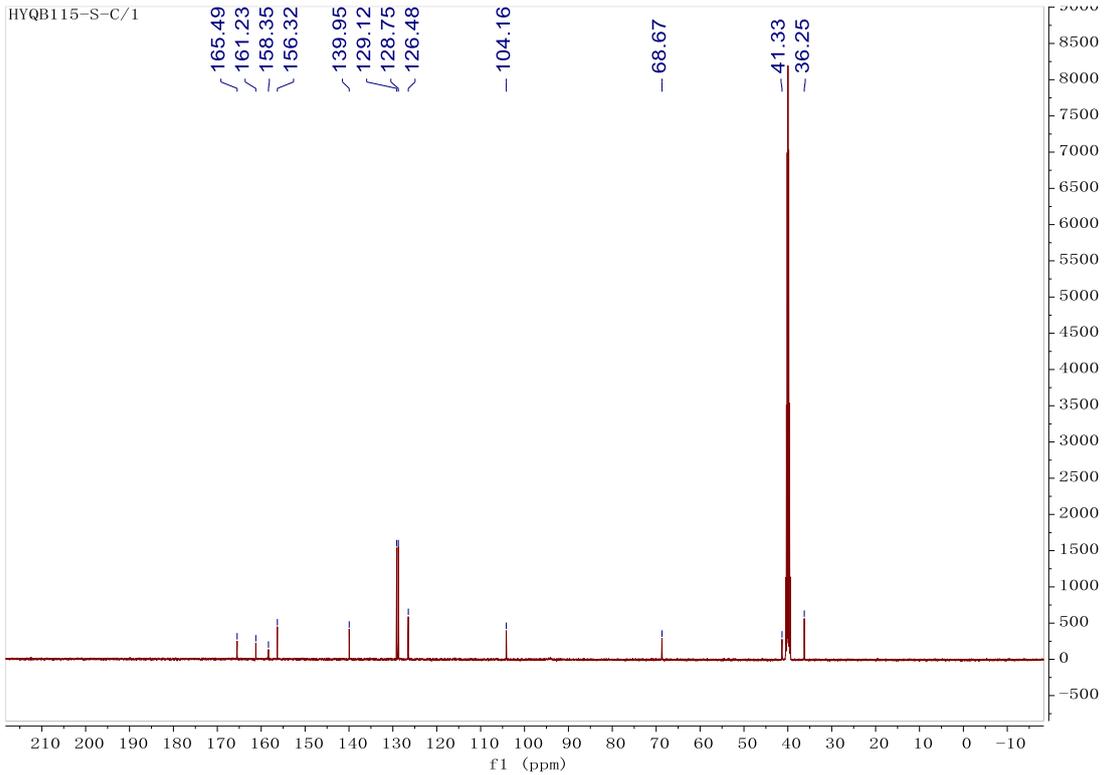
Compound 25

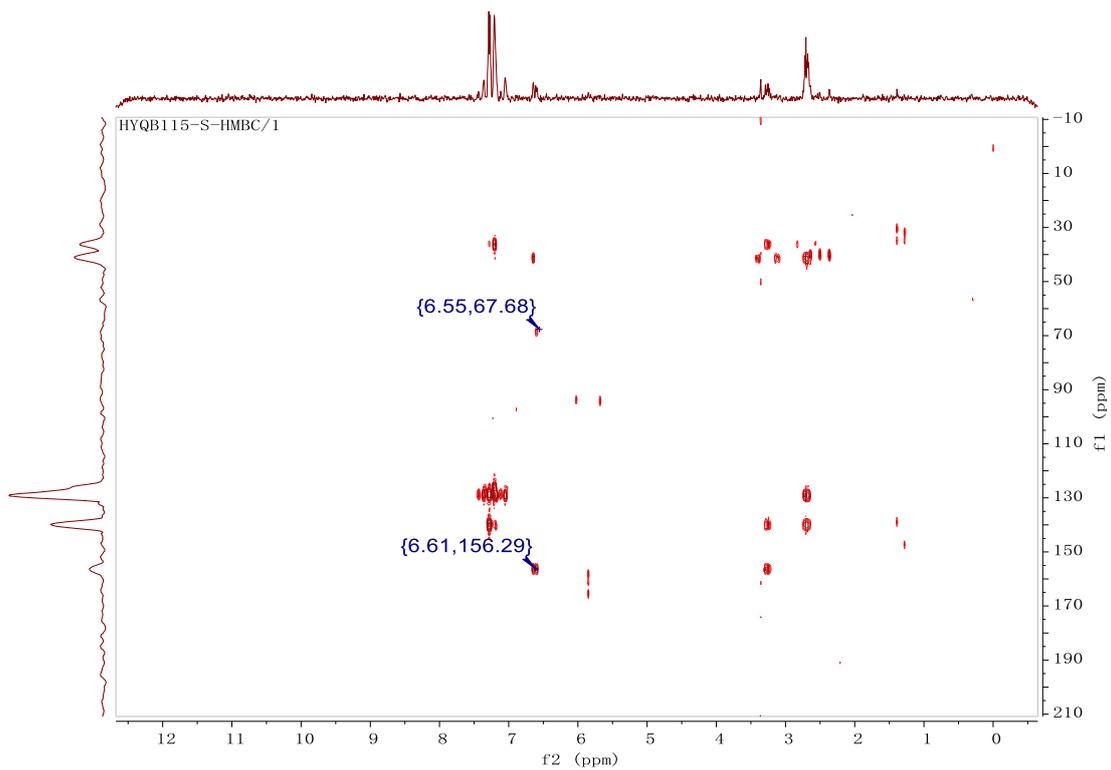




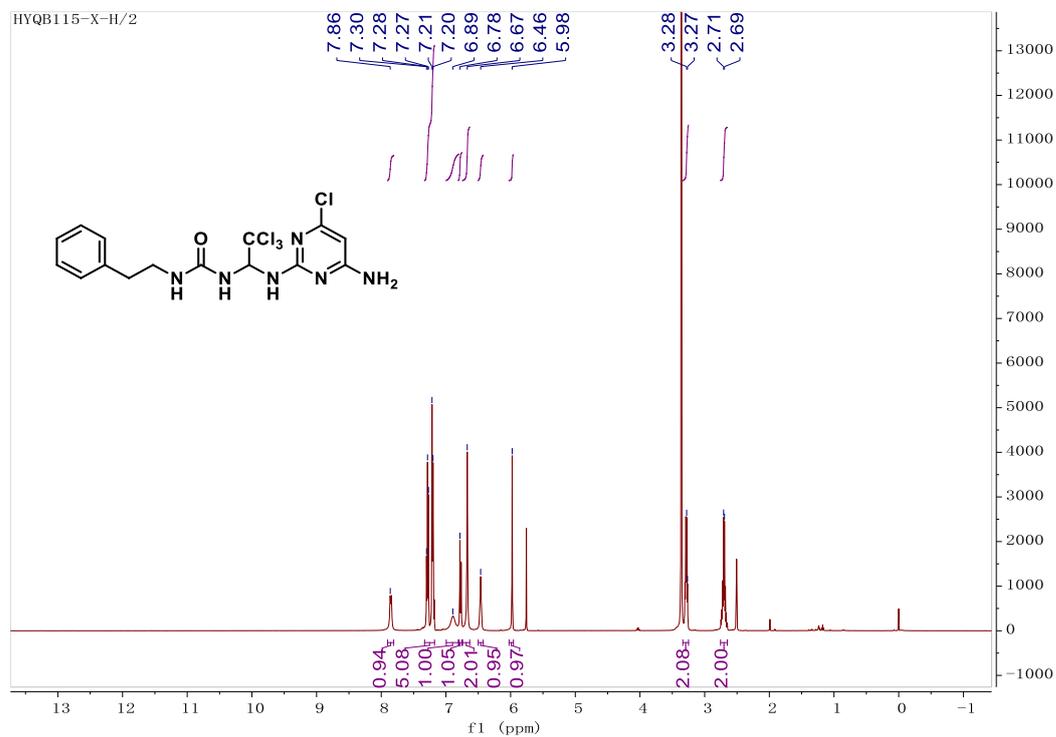
Peak List

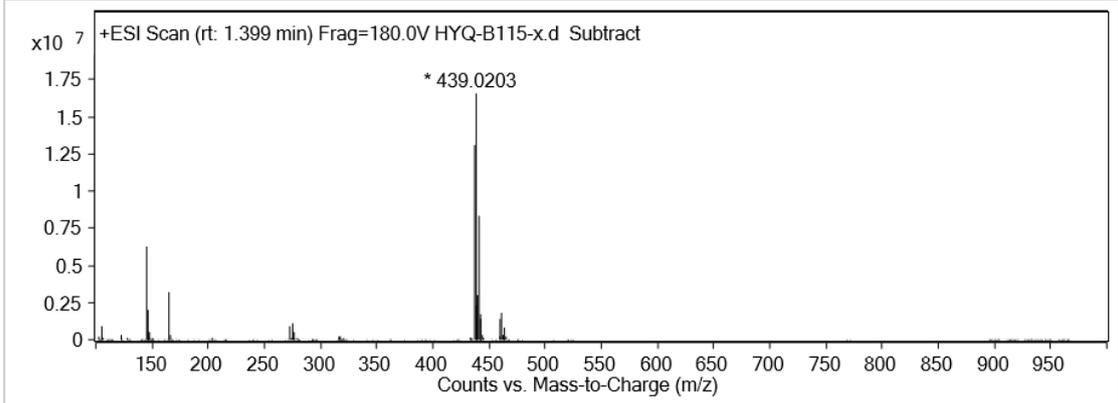
m/z	z	Abund
729.0162	1	1839294.75
731.013	1	4260150.5
732.0158	1	1281294.25
733.0103	1	4241561.5
734.013	1	1251993.5
735.0077	1	2261063.25
736.0103	1	649382.75
737.0056	1	727508.88
752.9949	1	659895.44
754.9923	1	674211.88





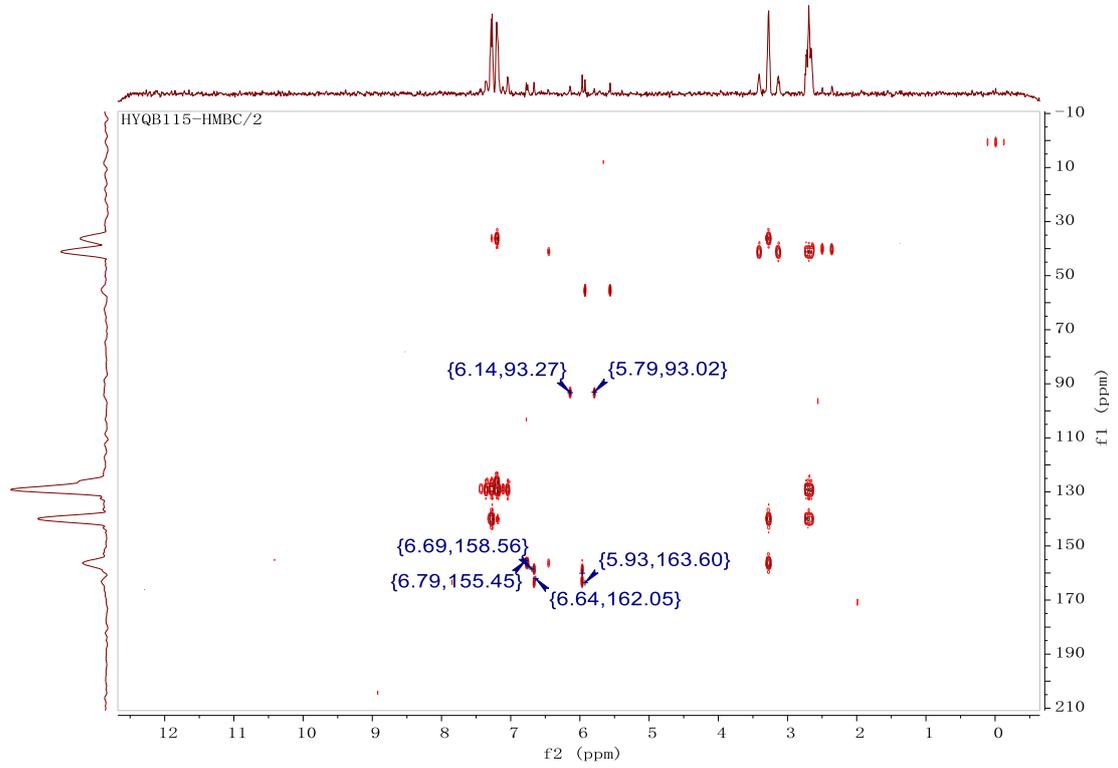
Compound 26



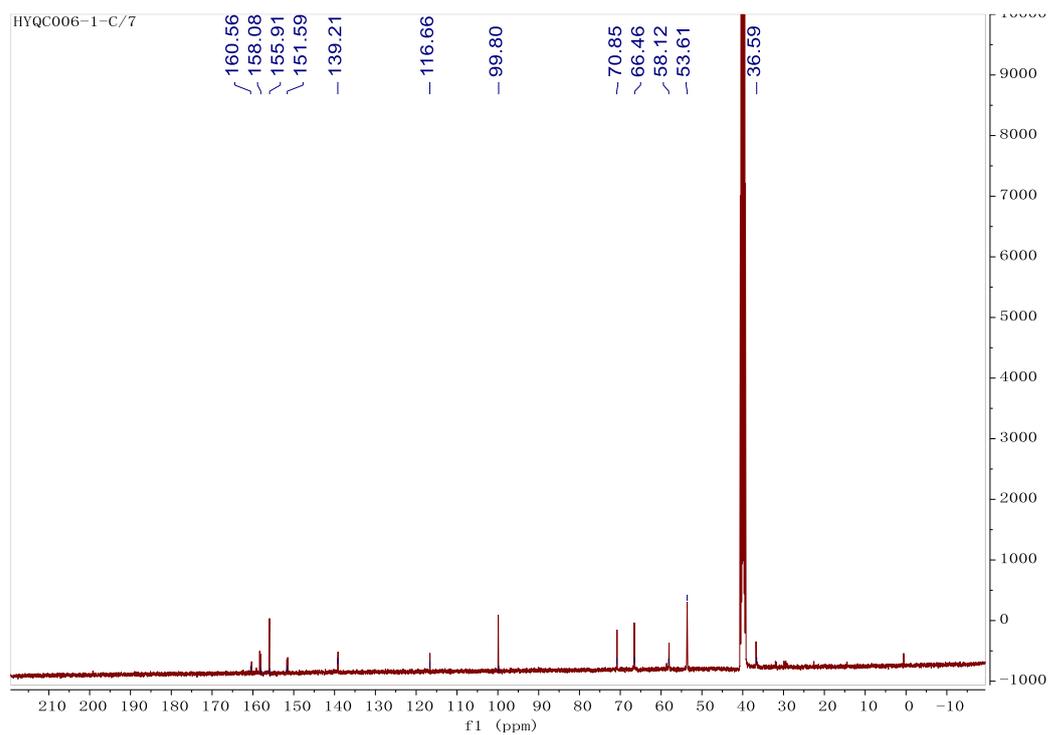
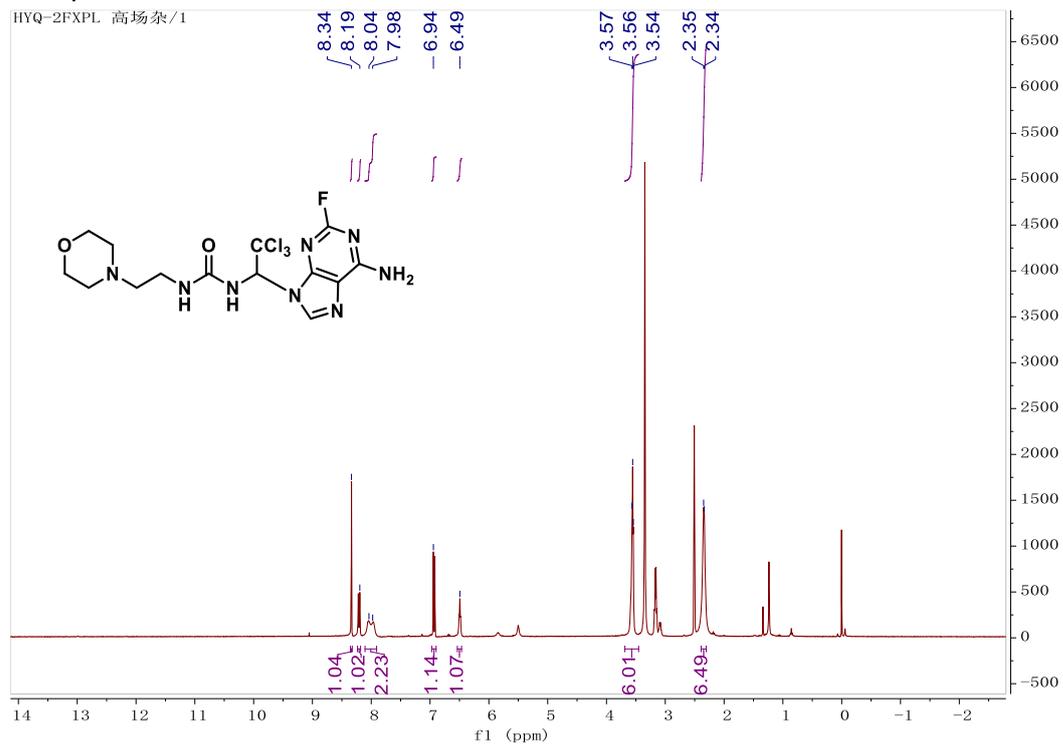


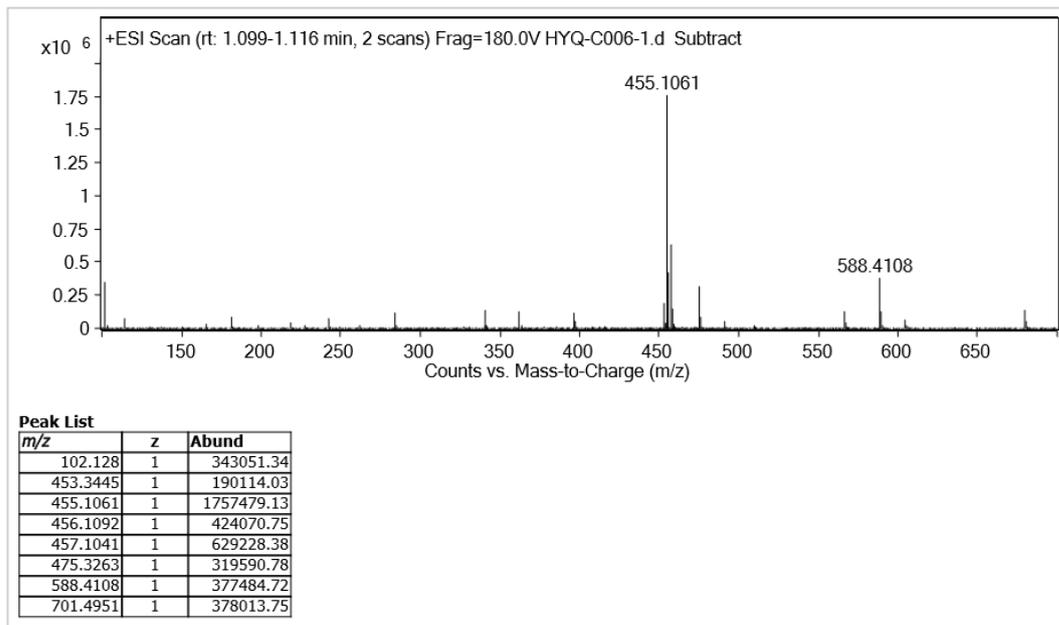
Peak List

m/z	z	Abund
145.0277	1	6224761
165.1024	1	3181428.25
437.0226	1	13036265
439.0203	1	16558550
440.0221	1	2990025.25
441.0166	1	8315304.5

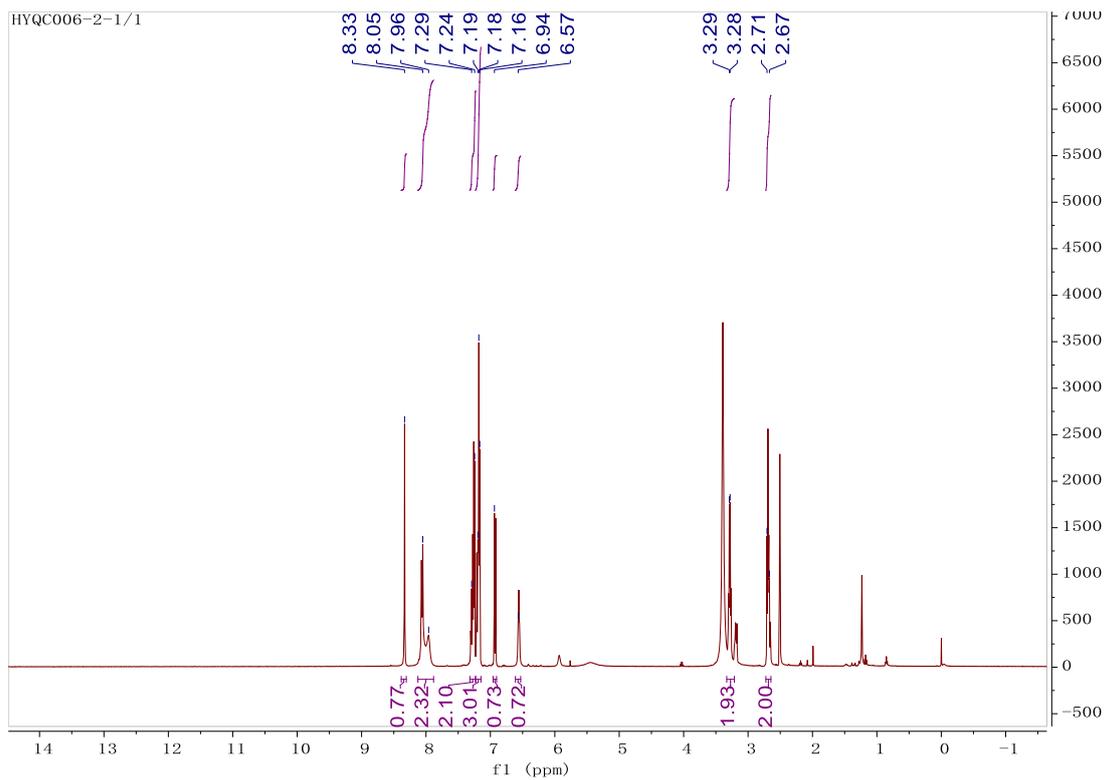


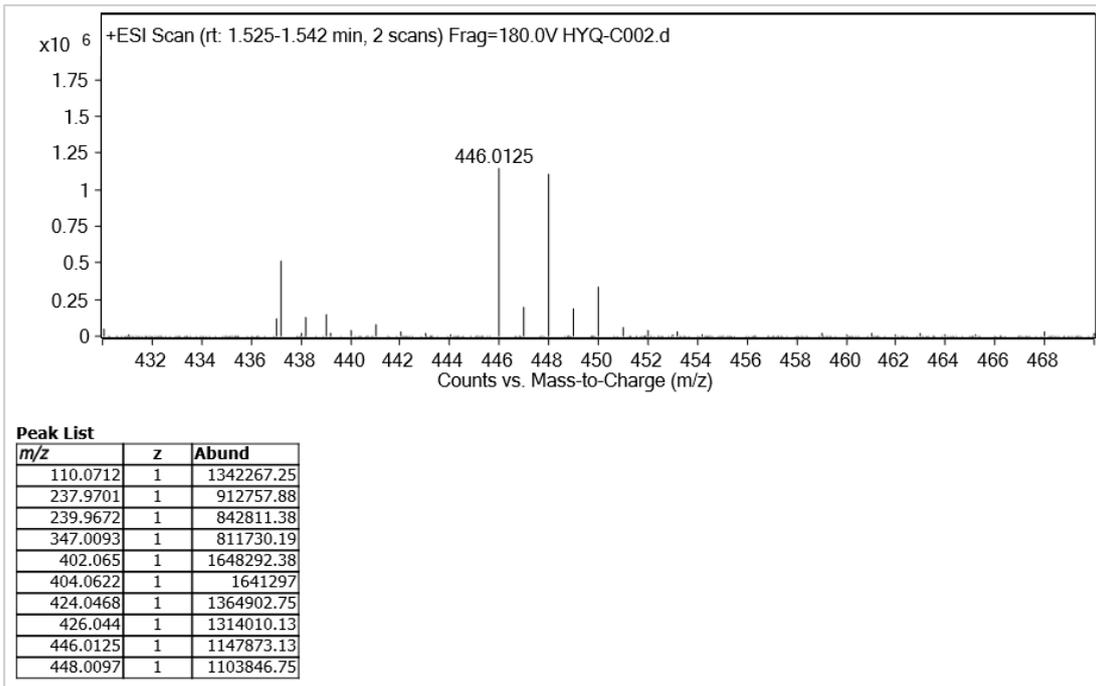
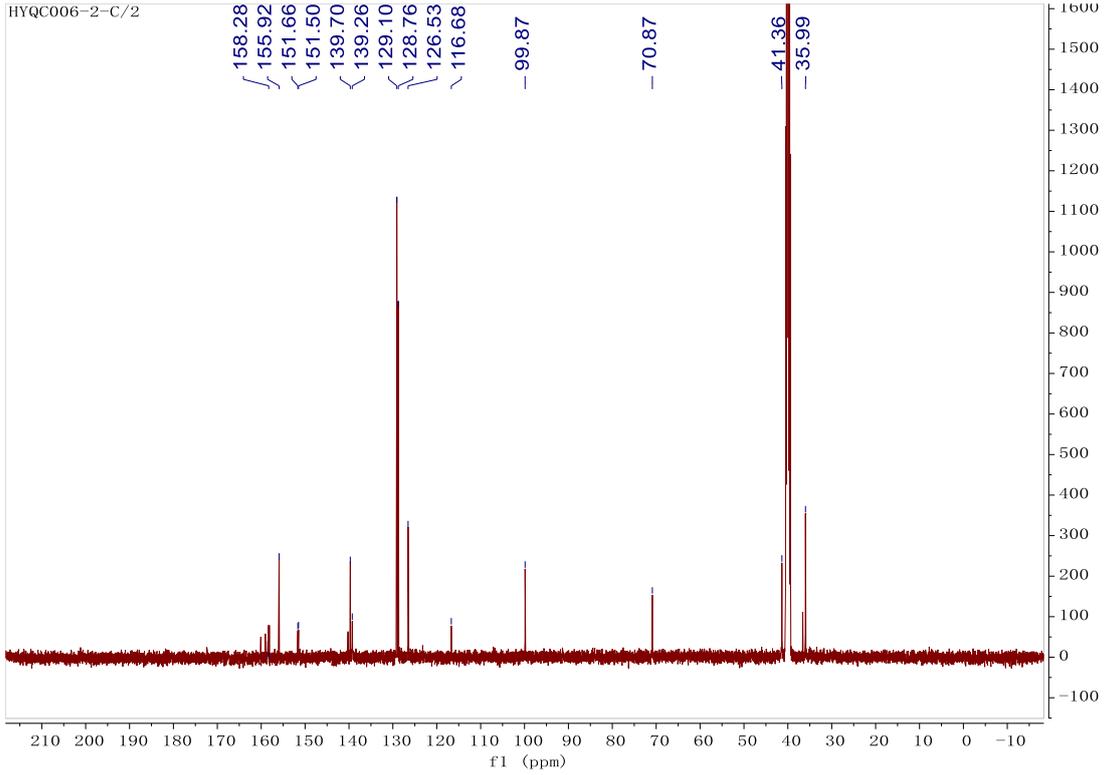
Compound 27



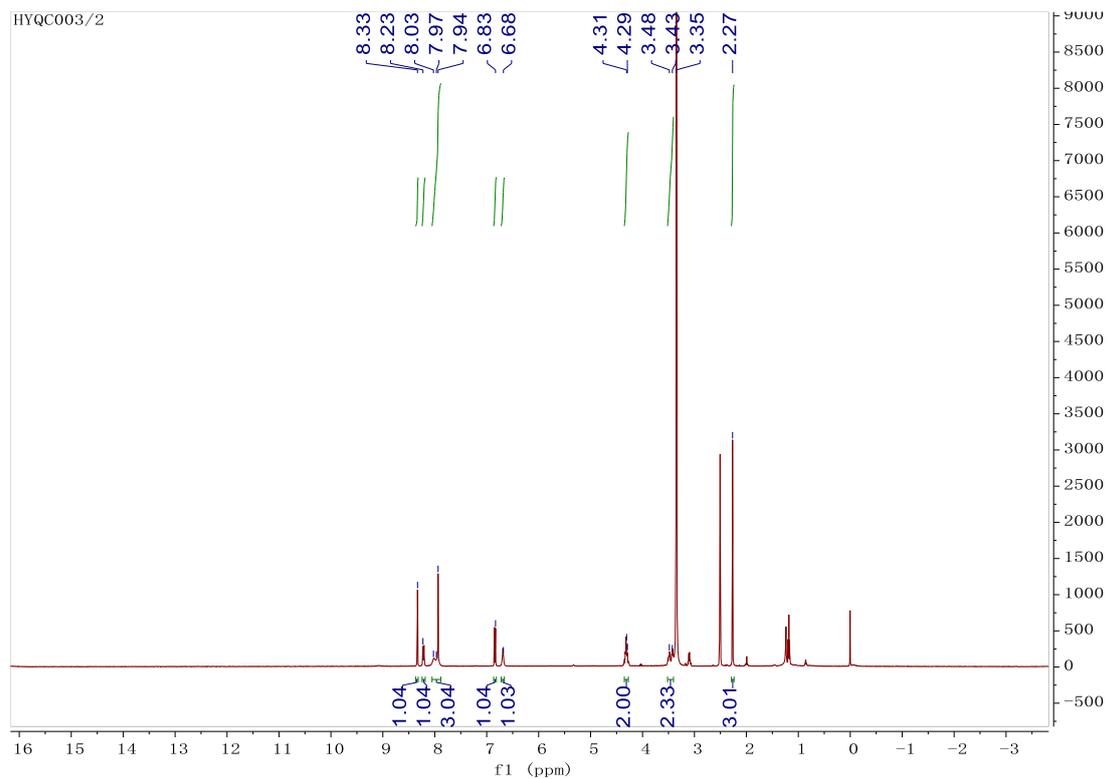
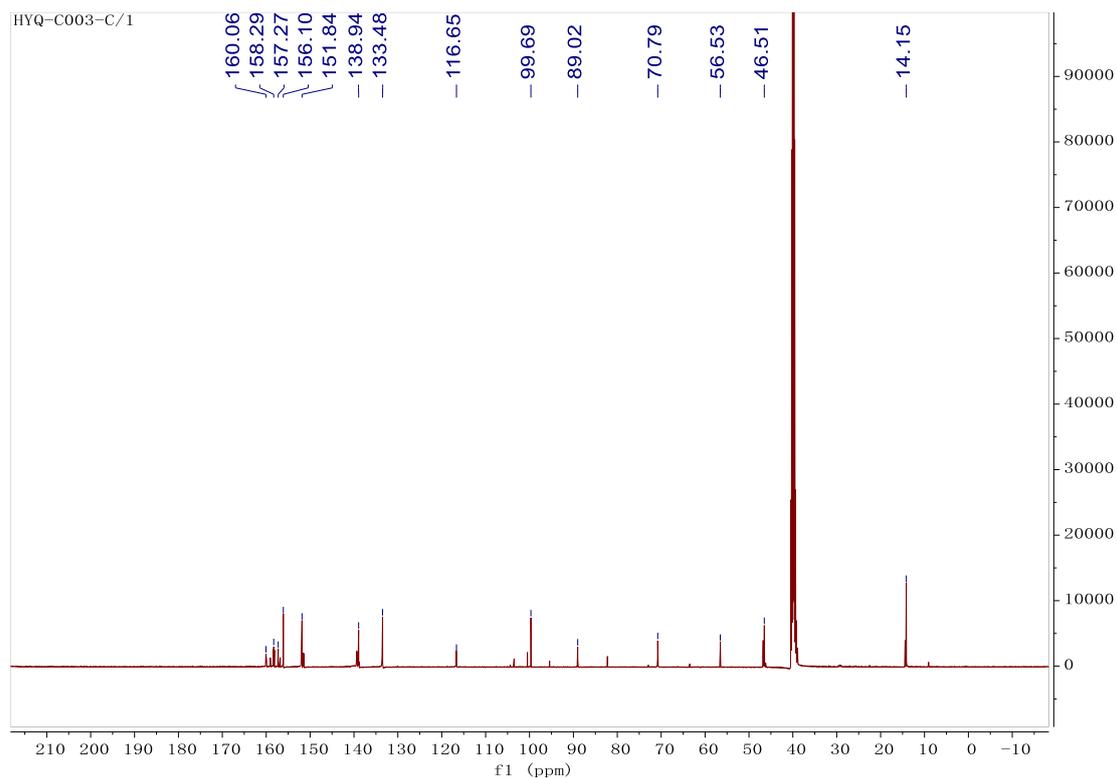


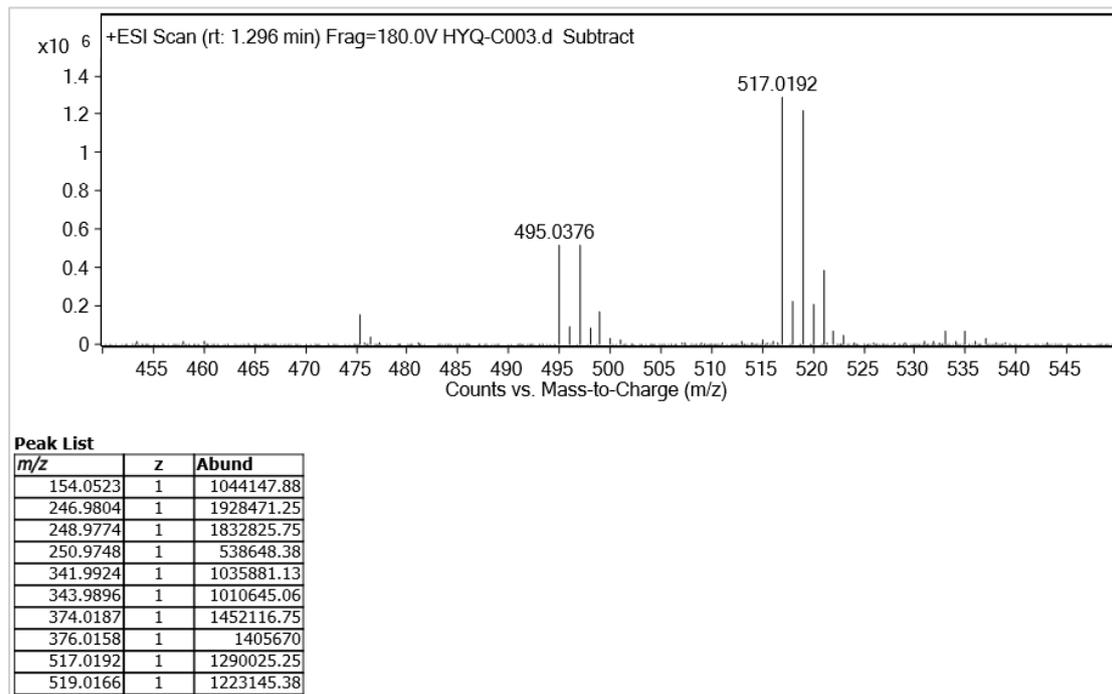
Compound 28



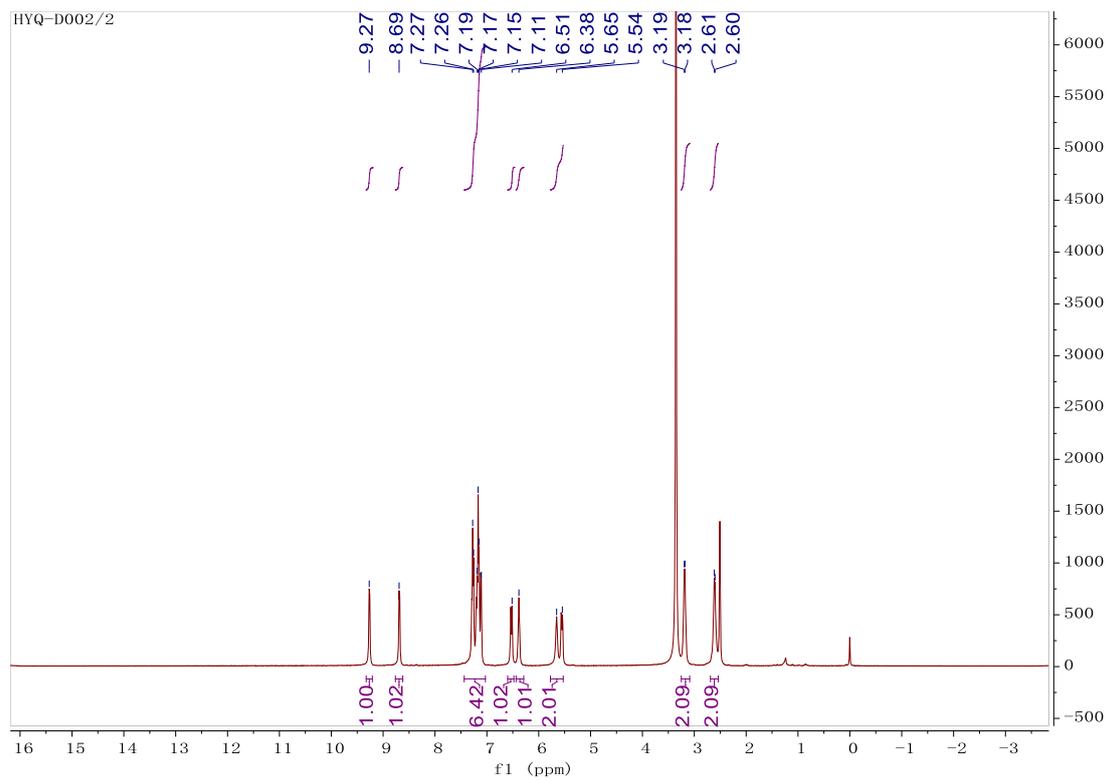


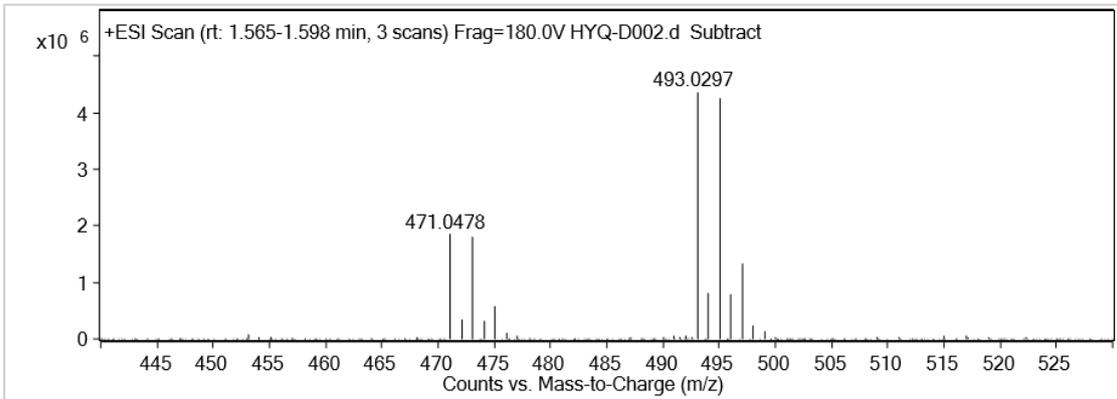
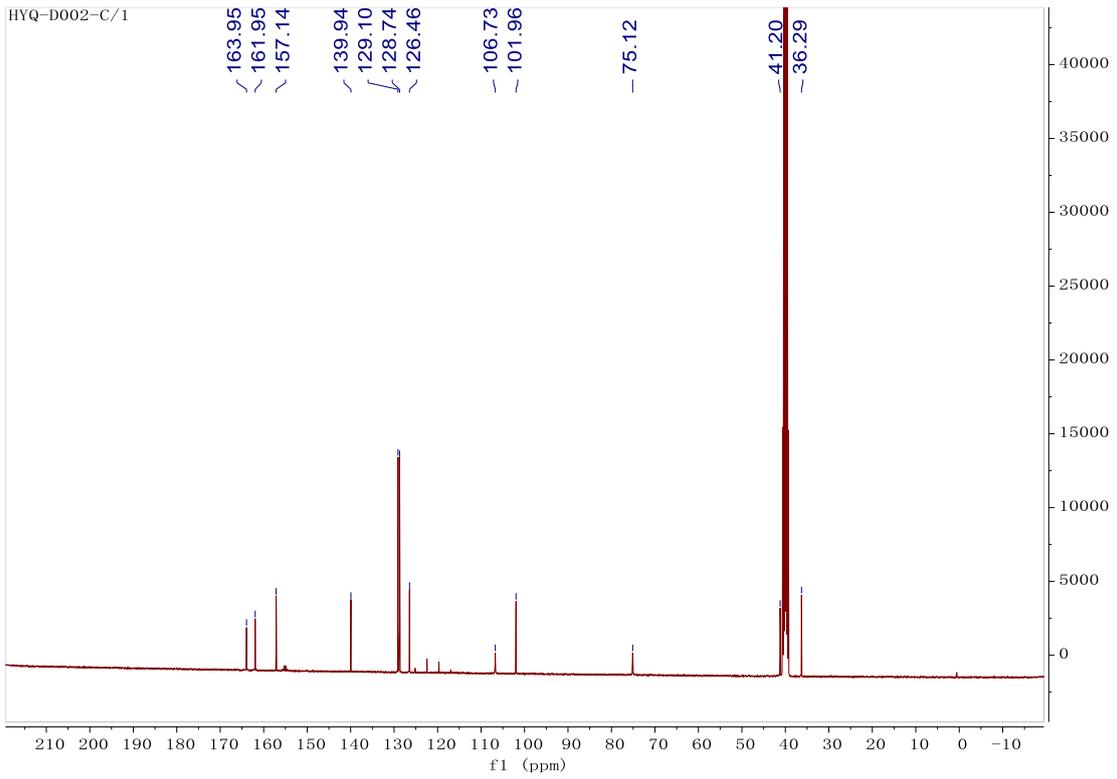
Compound 29





Compound 30





Peak List

m/z	z	Abund
165.1022	1	2057486.63
179.0539	1	2366741.75
409.0957	1	1080793.38
471.0478	1	1852333.88
473.045	1	1798070.88
493.0297	1	4356592.5
494.0325	1	820580.25
495.027	1	4253897
496.0299	1	778167.38
497.0245	1	1321068.63