

Supplementary Information

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

Yiqin He ^{1,2,3}, Xiangyang Le ^{1,2,3}, Gaoyun Hu ^{1,2,3}, Qianbin Li ^{1,2,3}, Zhuo Chen ^{1,2,3*}

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.

Contents

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

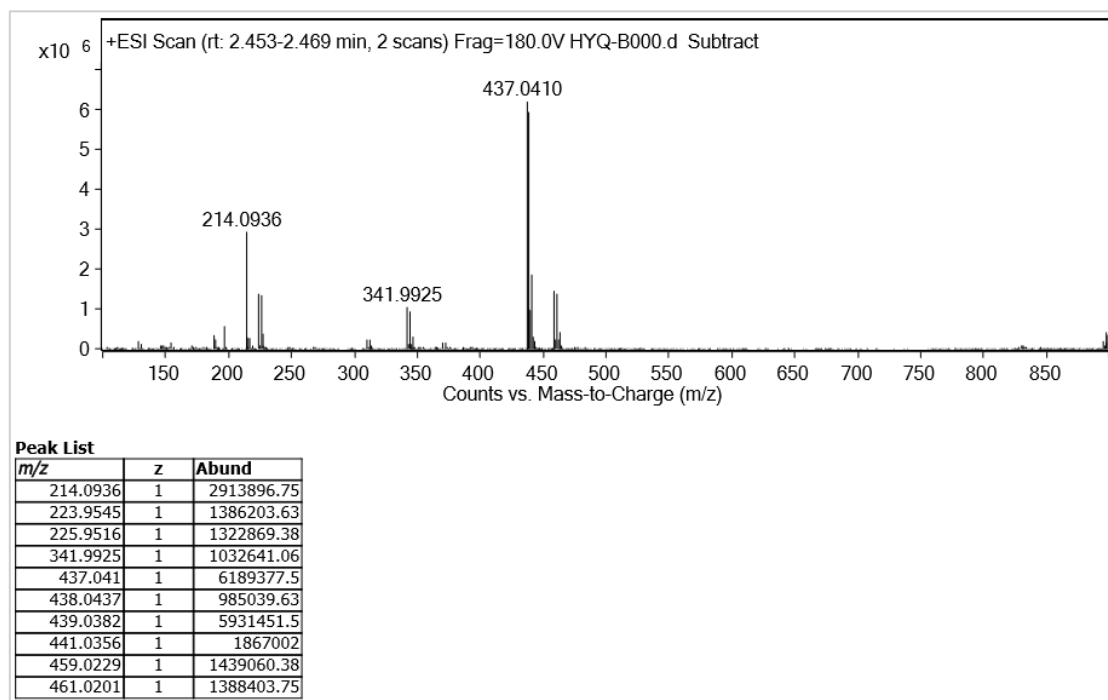
HYQ-B000-2/2

Chemical structure of compound 10: CC1=CN(C=C1[N+](=O)[O-])CCNC(=O)NC(CCl)N2=CC=CC=N2

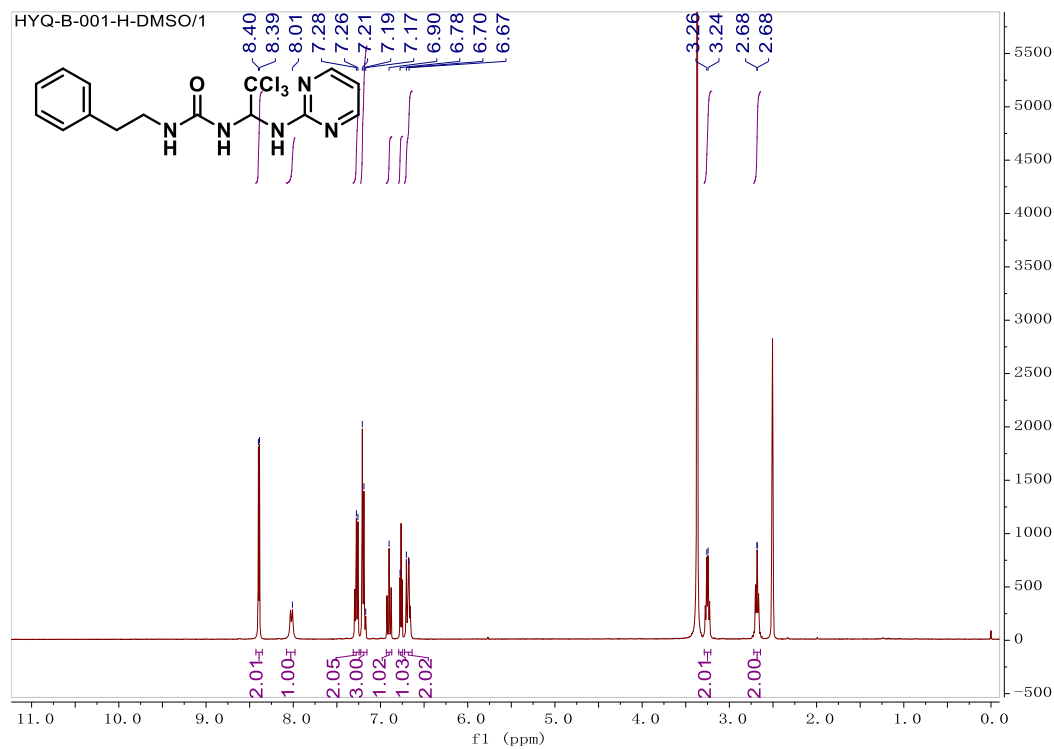
¹H NMR spectrum (CDCl₃) showing peaks and integration values:

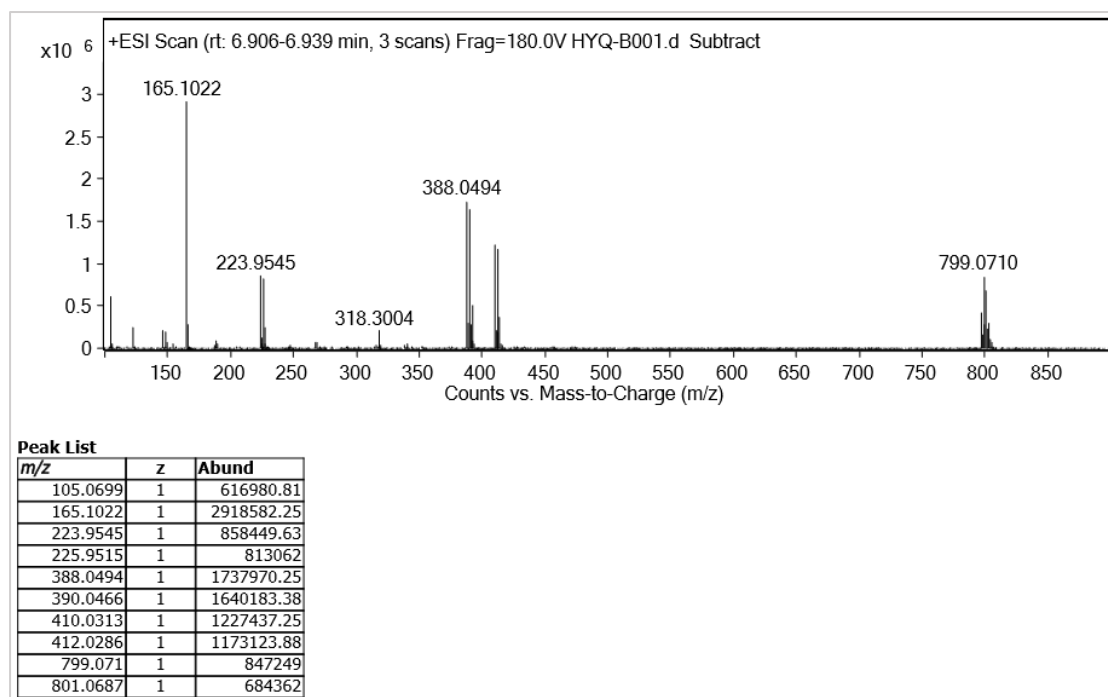
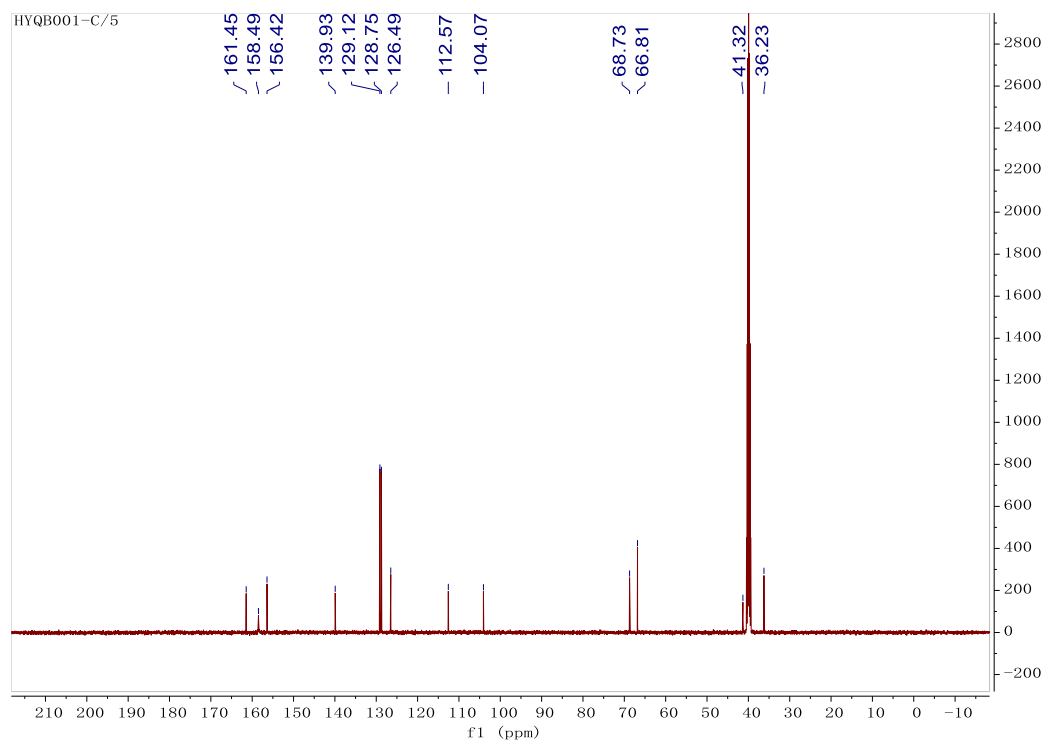
Chemical Shift (ppm)	Integration
8.40, 8.37, 8.20, 7.98, 7.86	2.42, 1.18, 0.96, 0.99
6.56, 6.53	1.83
4.30, 4.27, 3.51, 3.46	2.09, 2.16
2.33, 2.32, 2.30	3.00



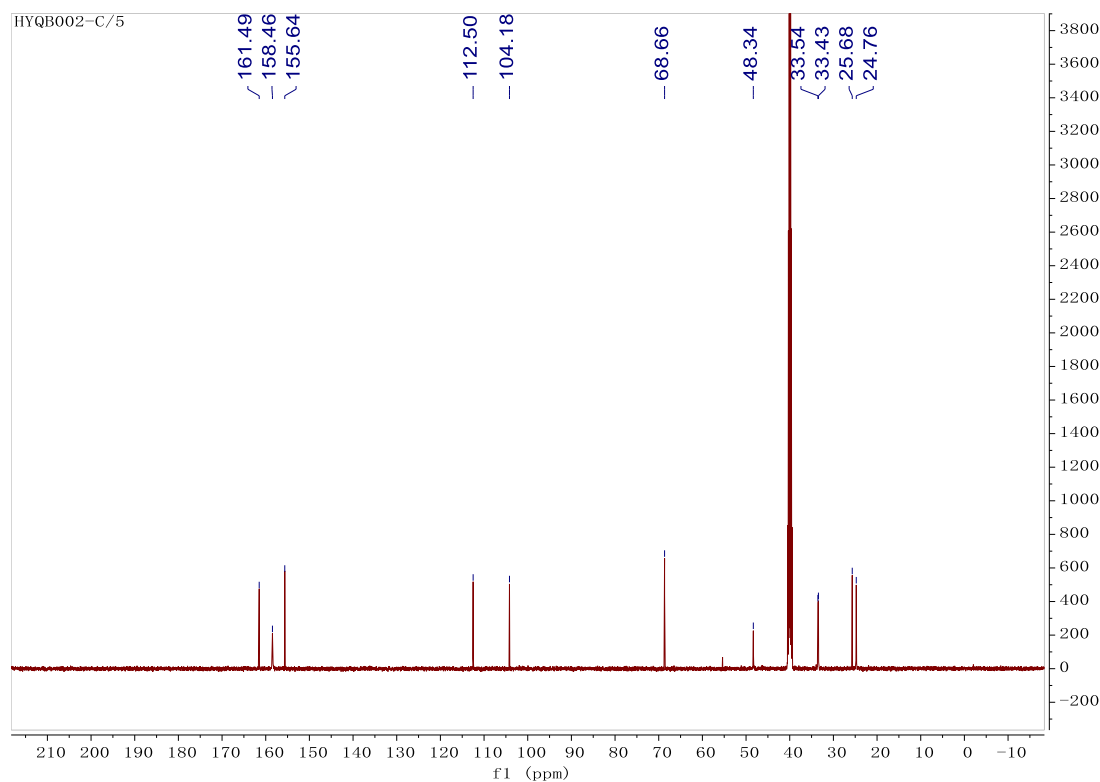
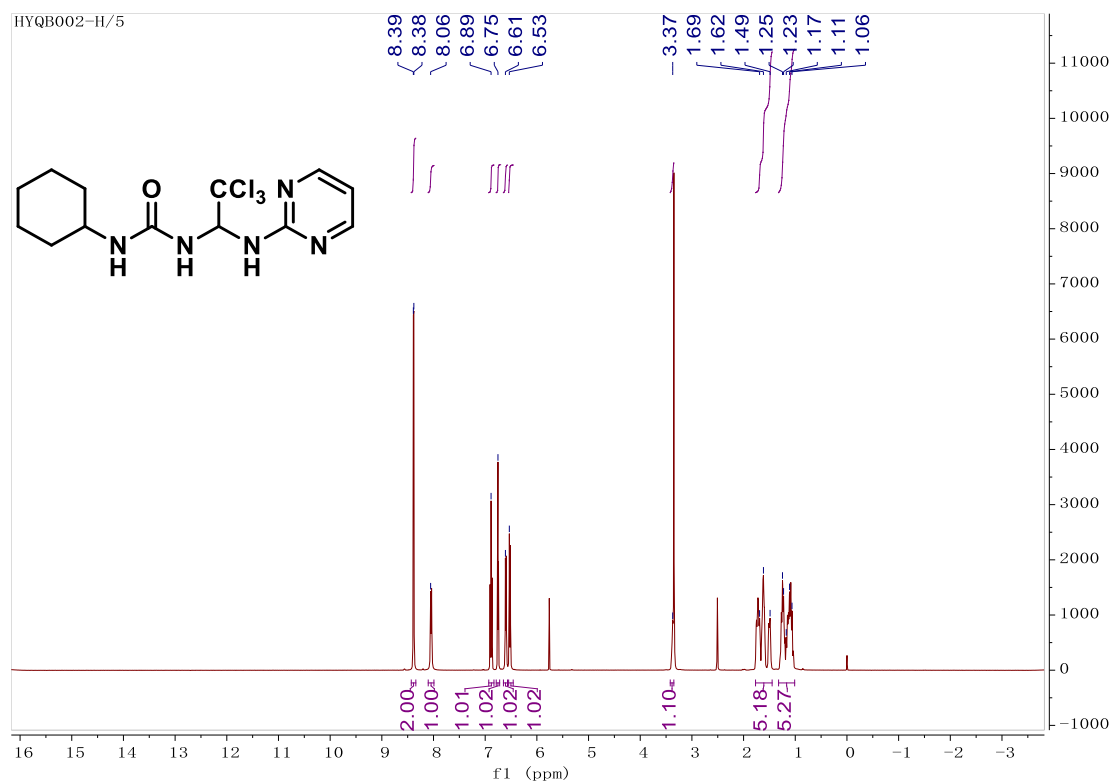


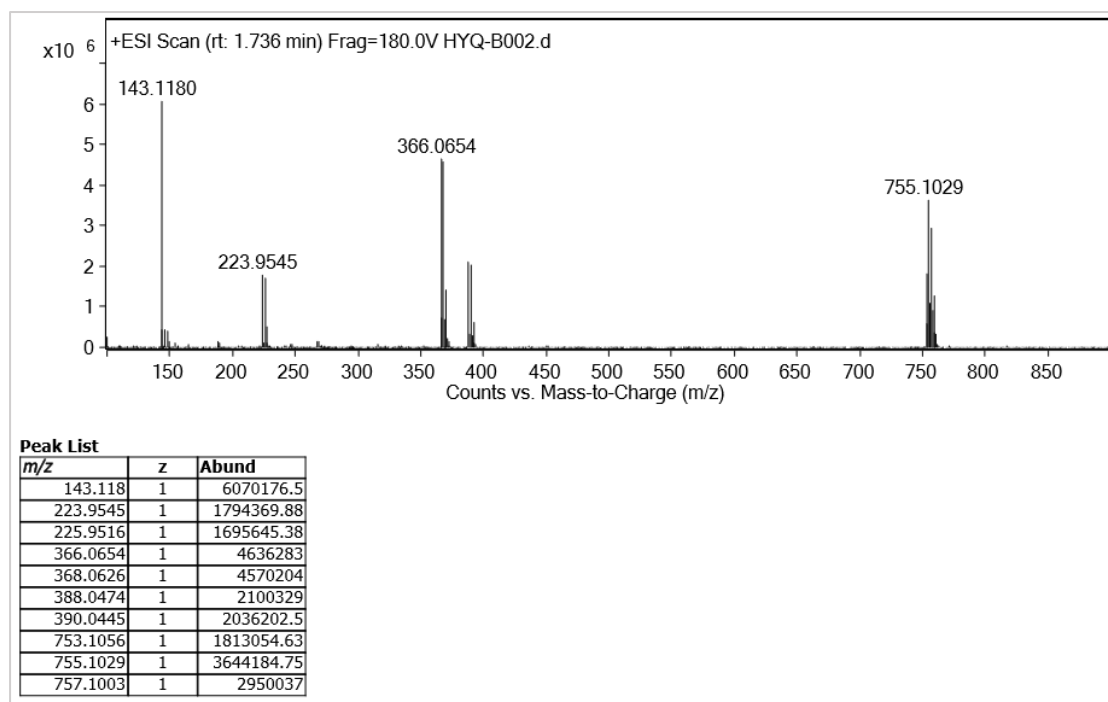
Compound 2



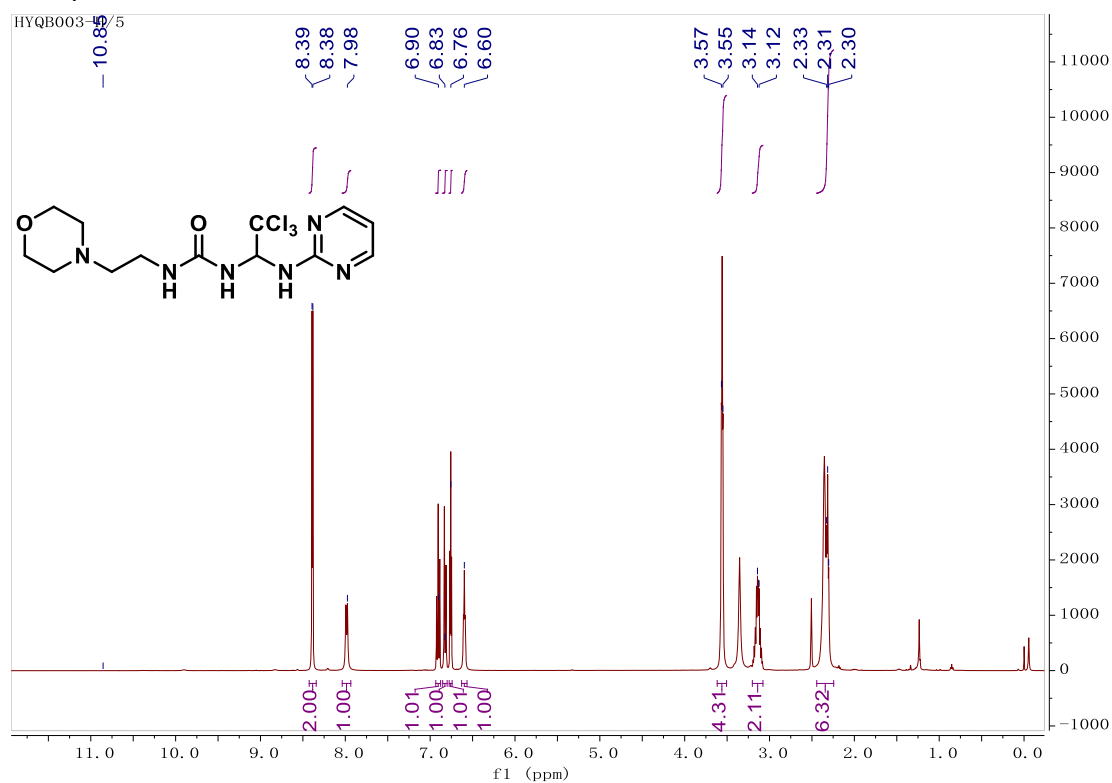


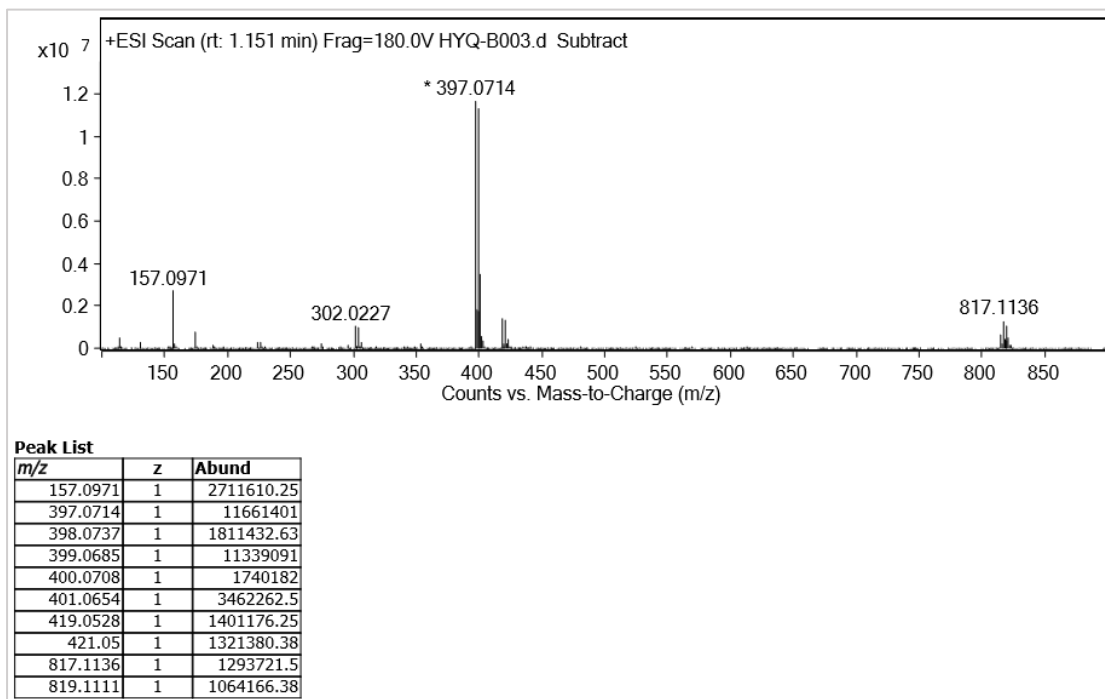
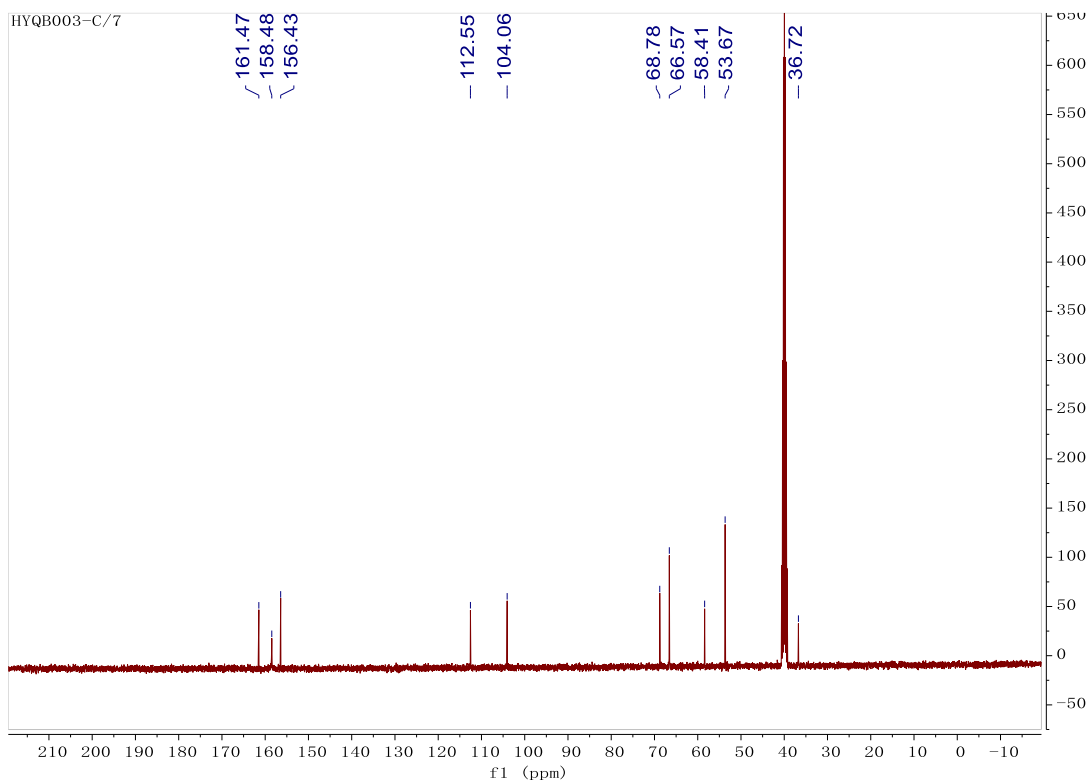
Compound 3



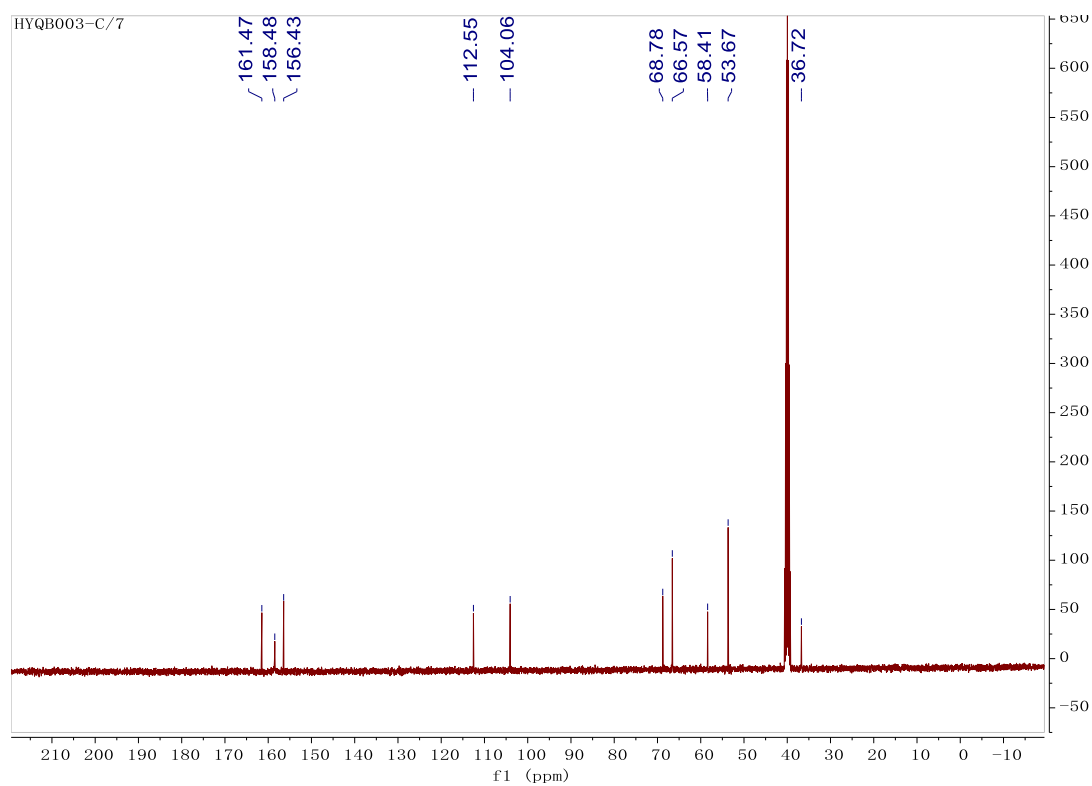
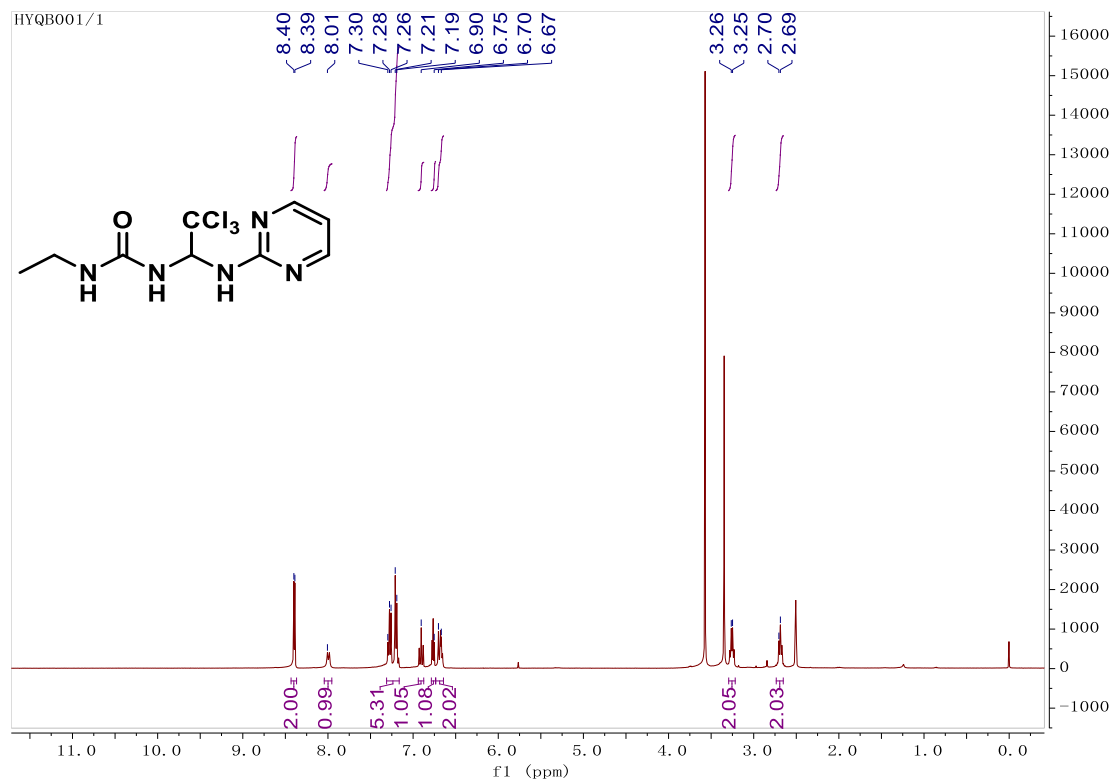


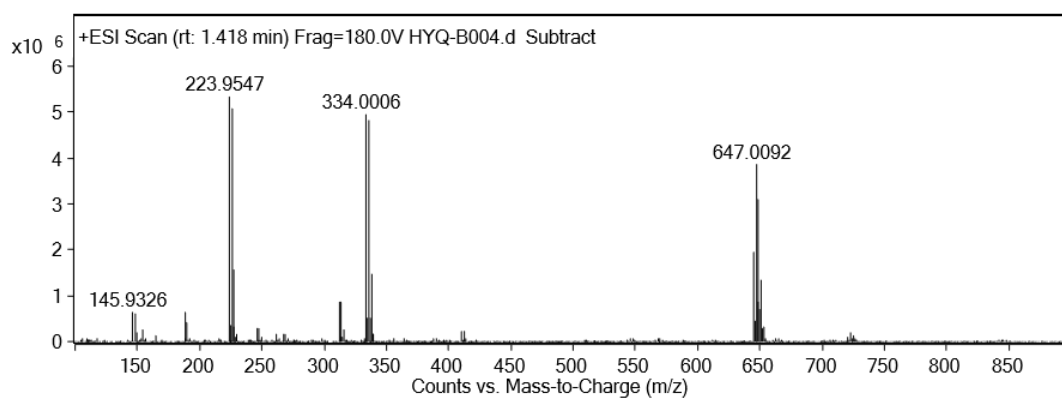
Compound 4





Compound 5

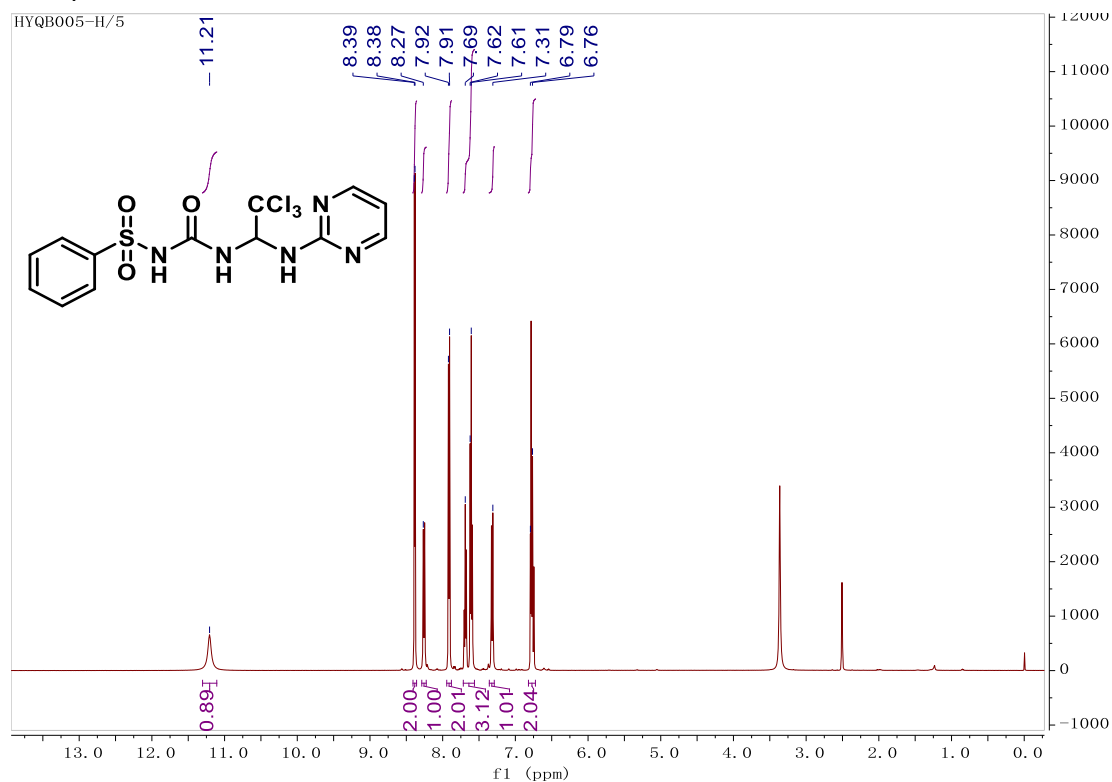


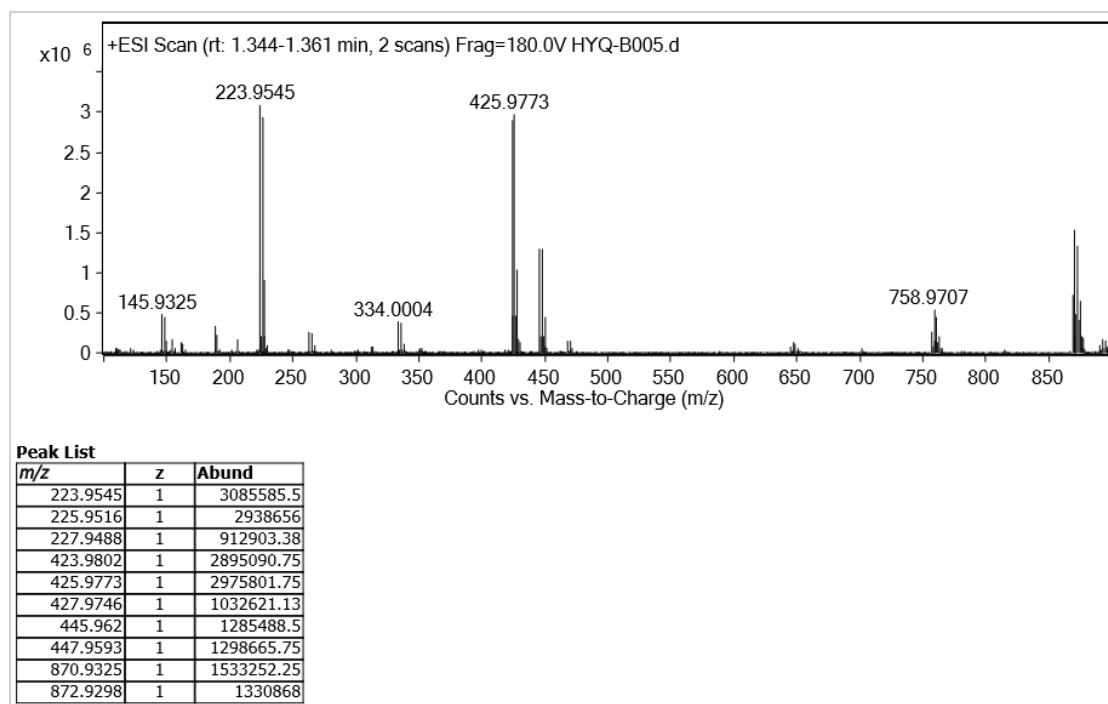
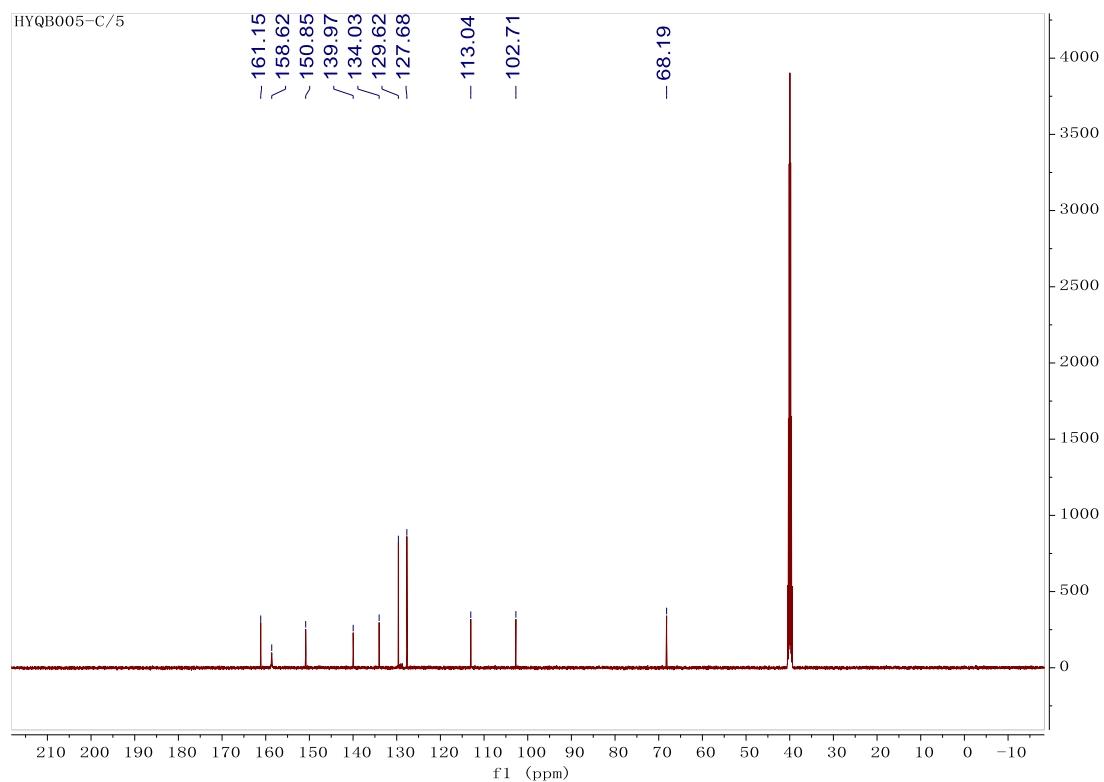


Peak List

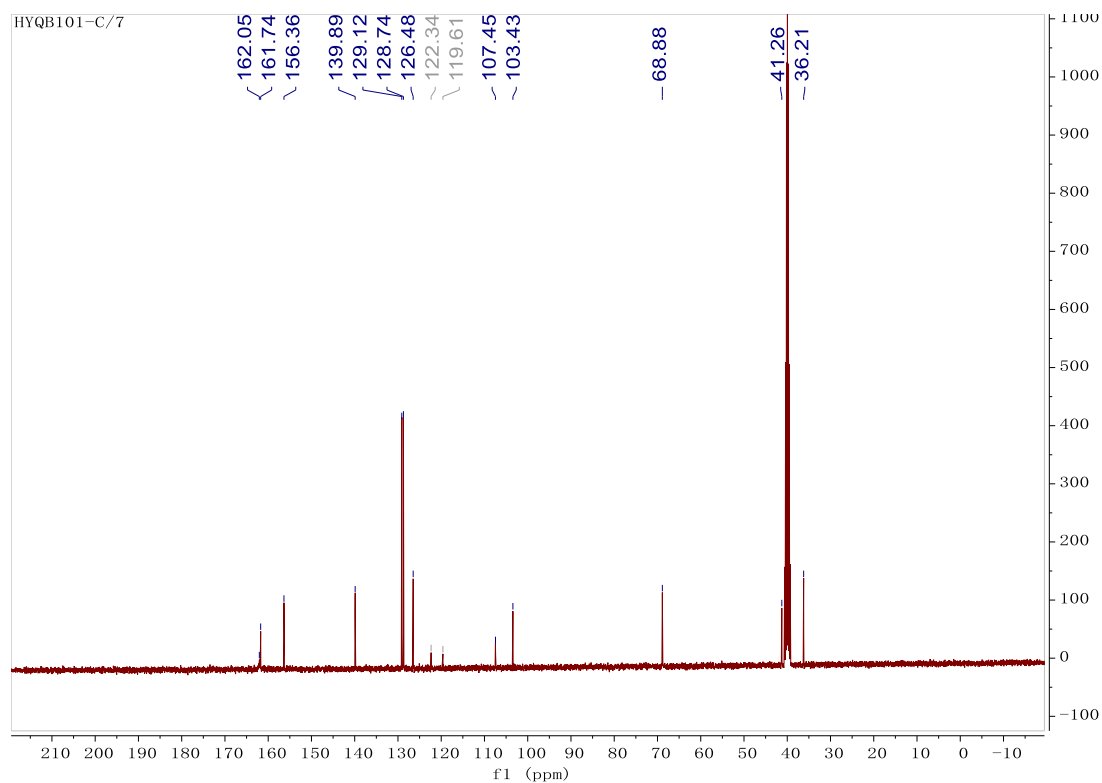
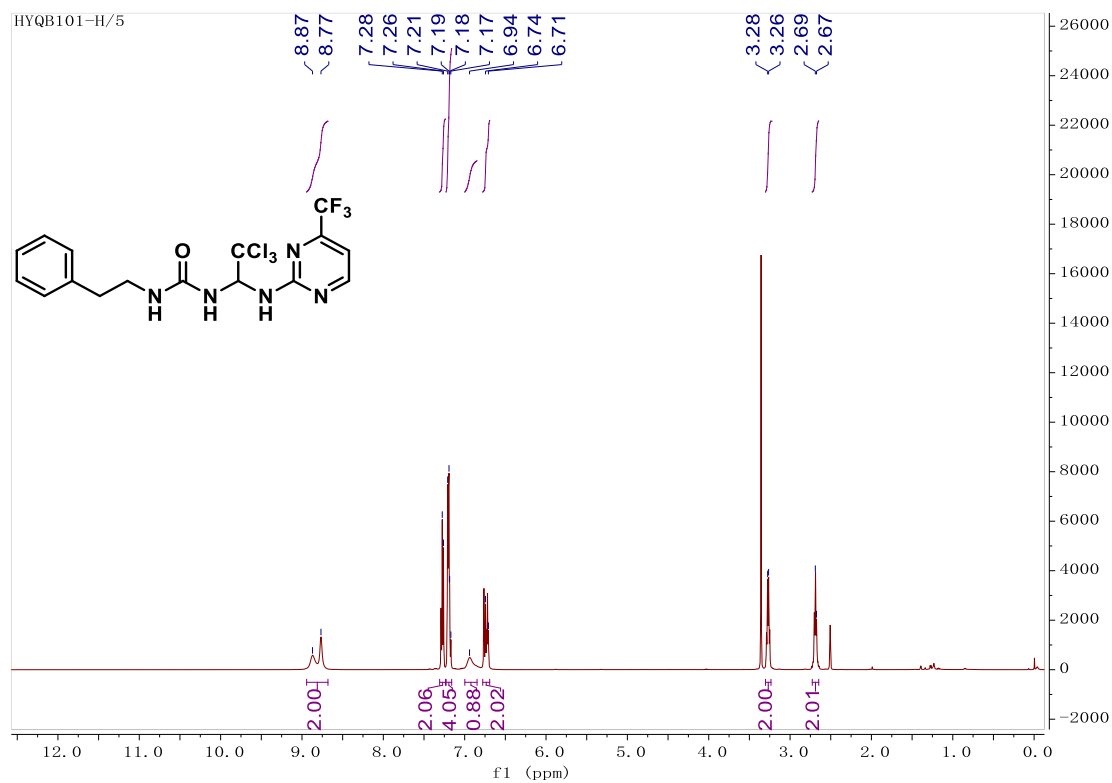
m/z	z	Abund
223.9547	1	5329879
225.9518	1	5086102.5
227.9488	1	1556247.63
334.0006	1	4929472
335.9977	1	4800584.5
337.9949	1	1480485.63
645.0121	1	1946913
647.0092	1	3872751
649.0065	1	3084400.5
651.0039	1	1337346.38

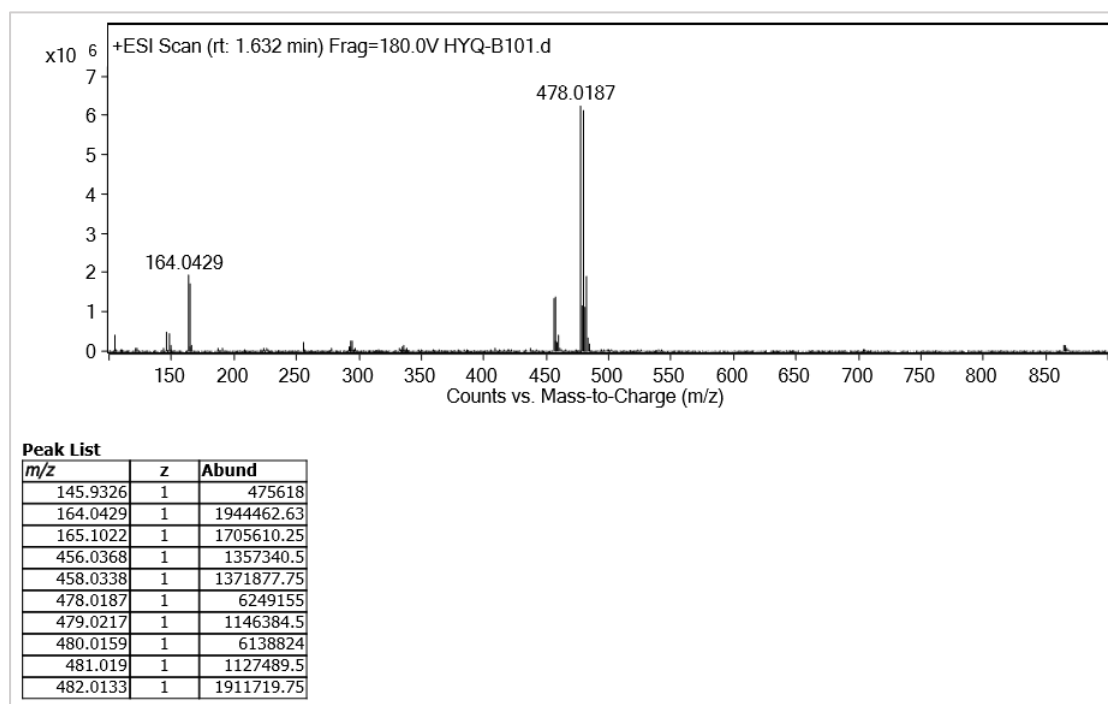
Compound 6



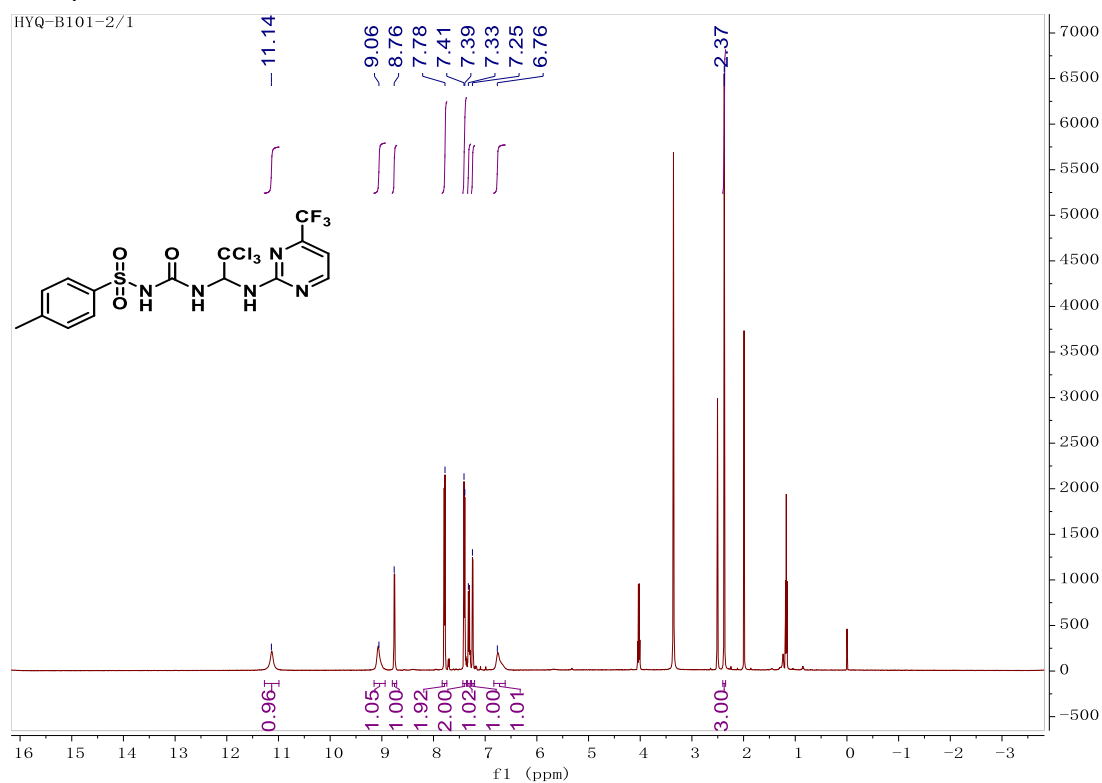


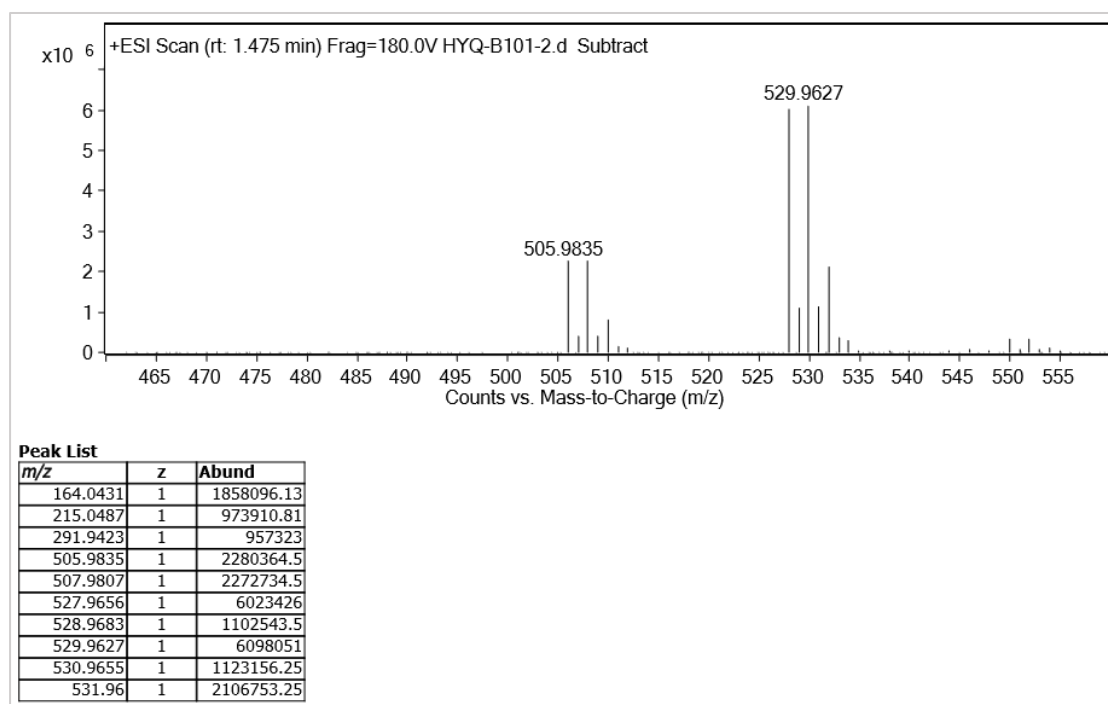
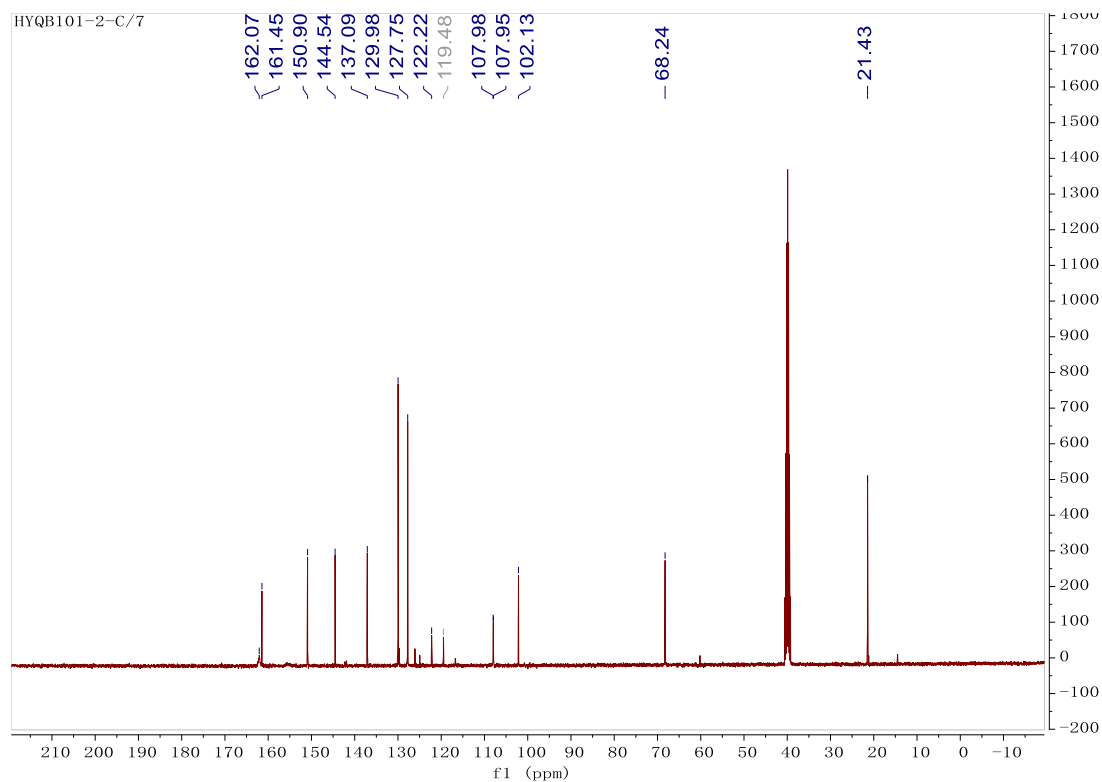
Compound 7



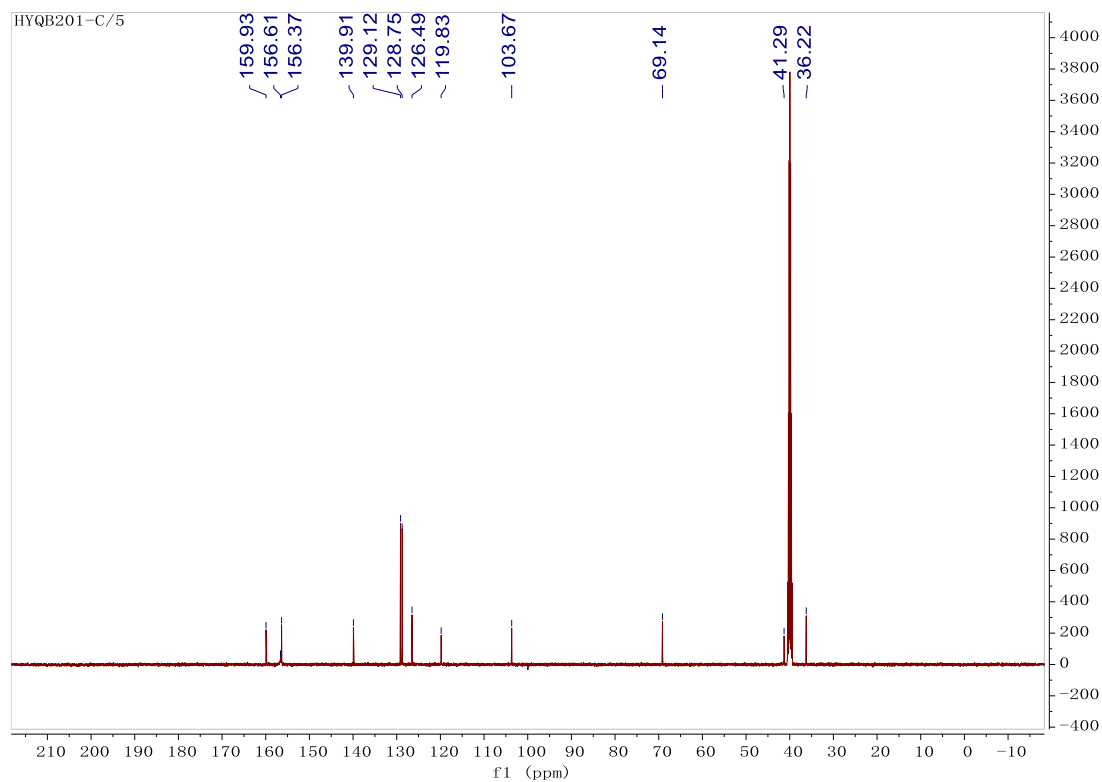
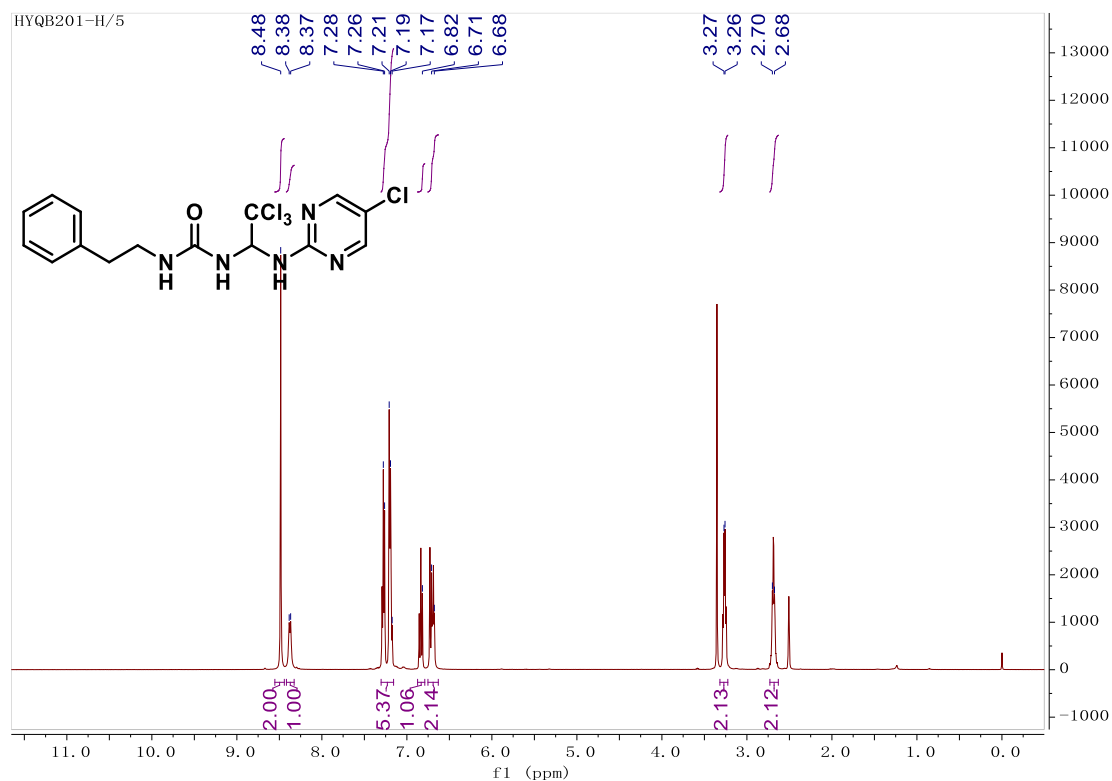


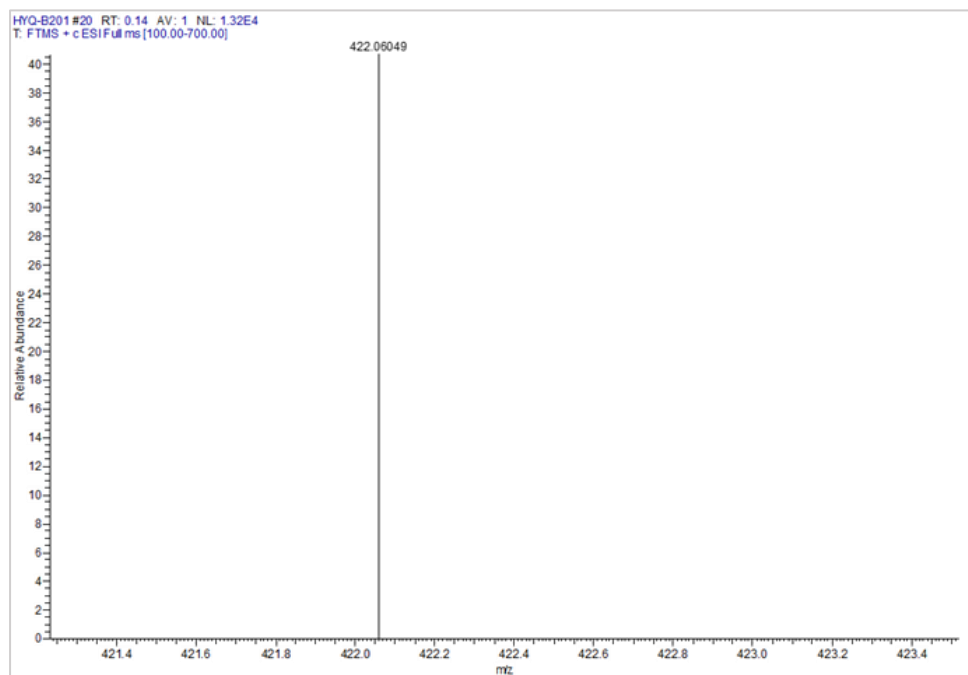
Compound 8



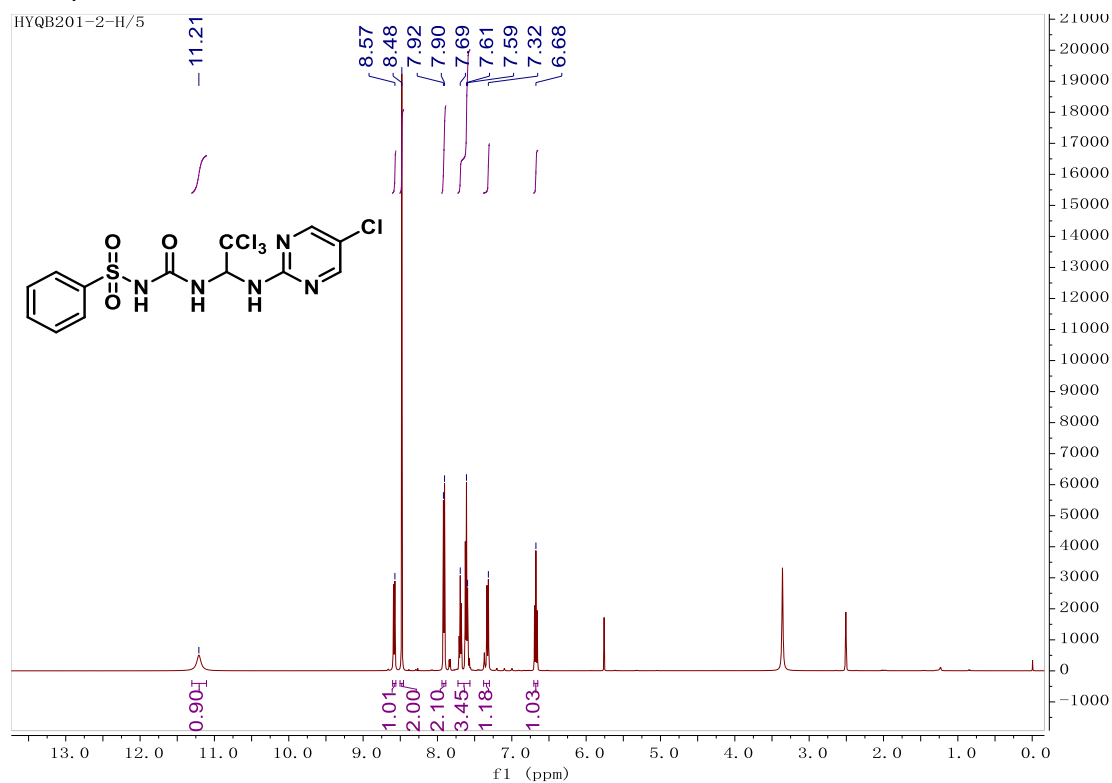


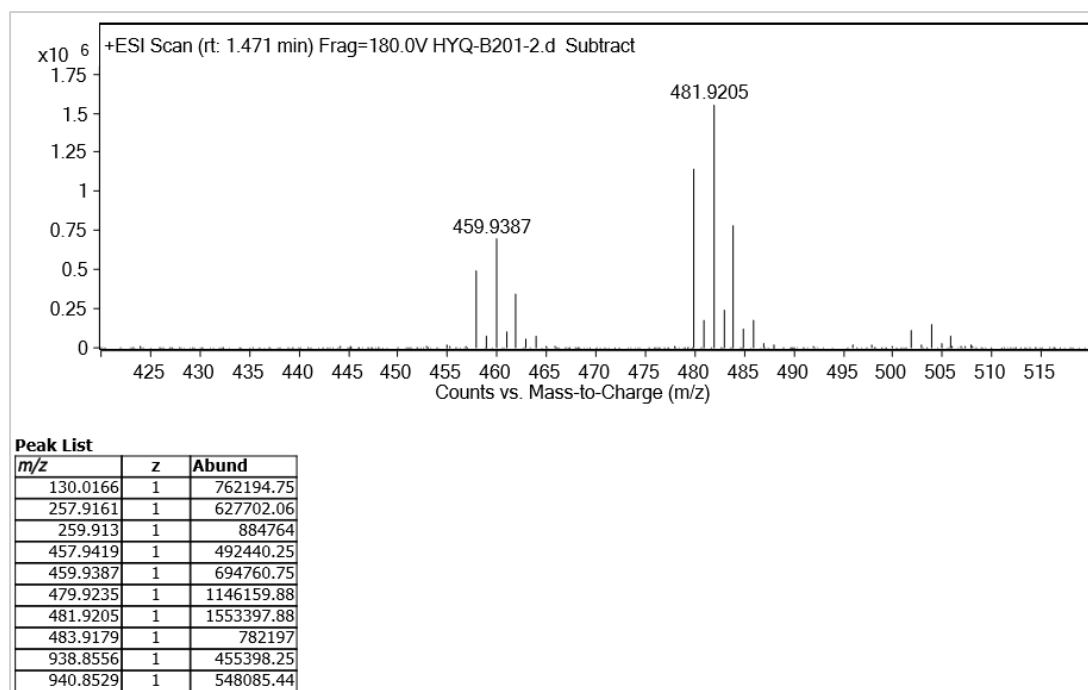
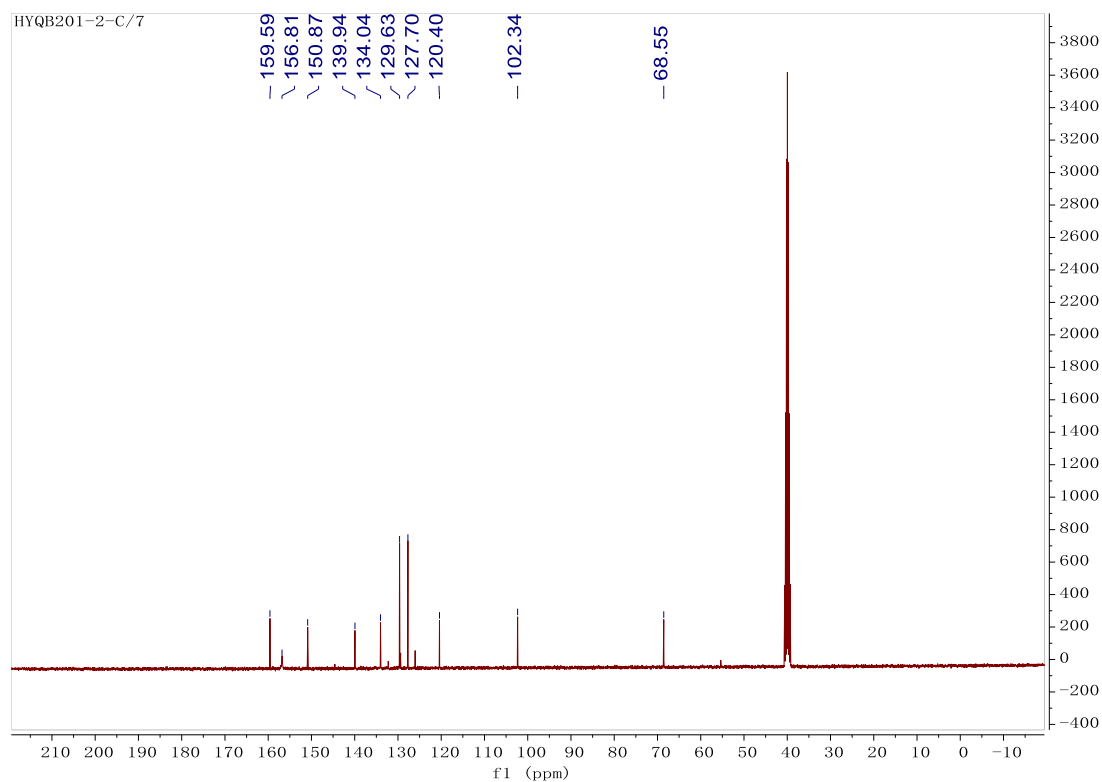
Compound 9



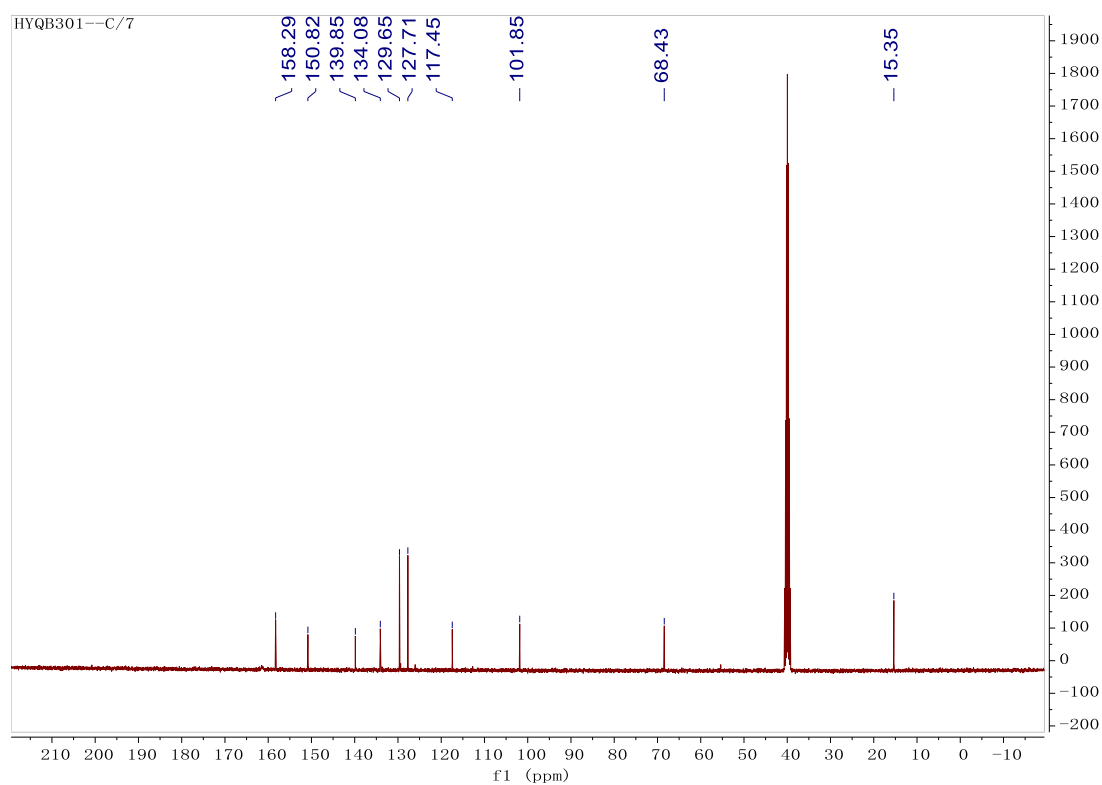
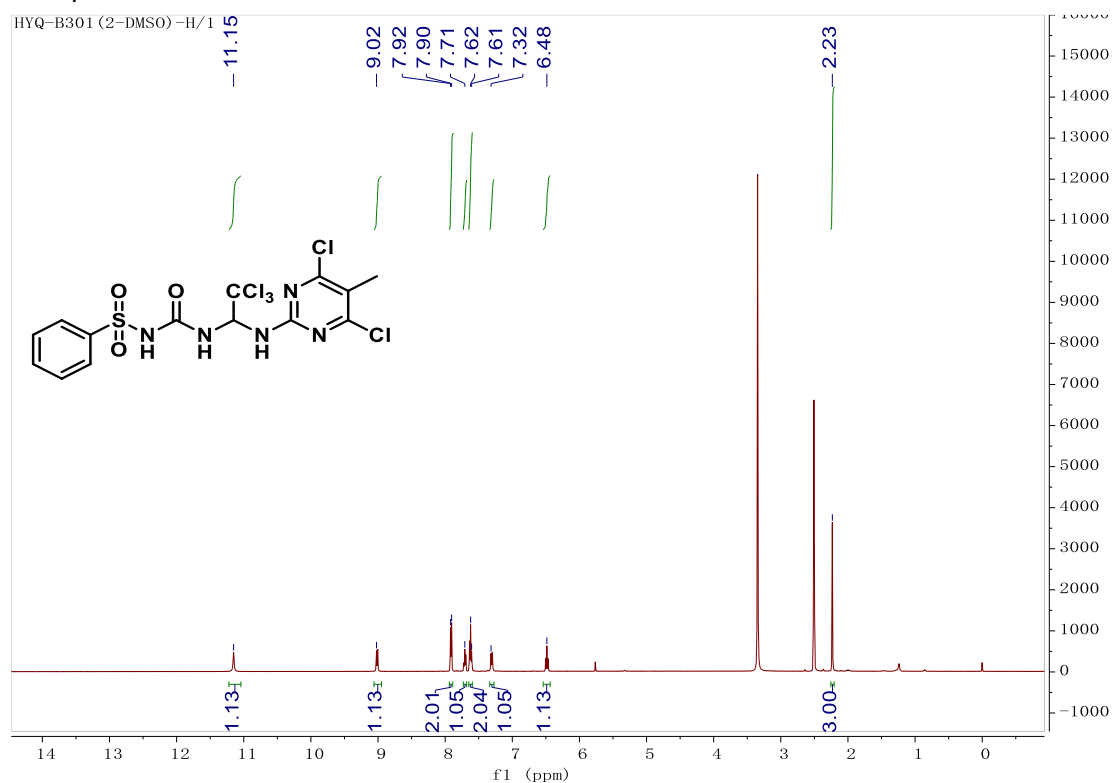


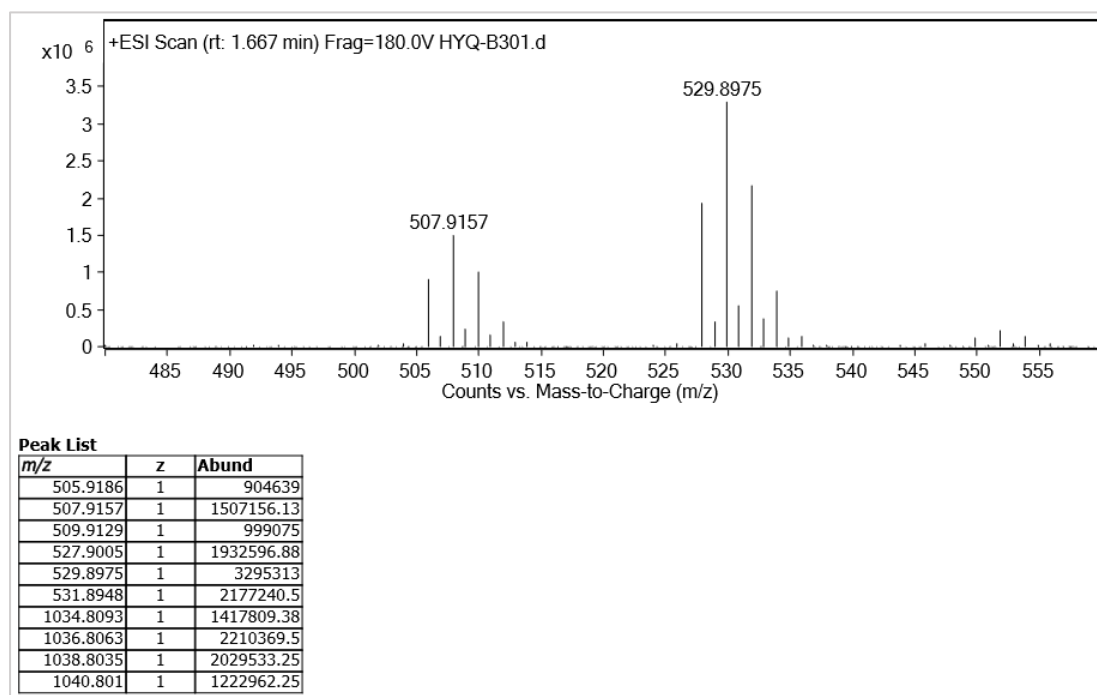
Compound 10



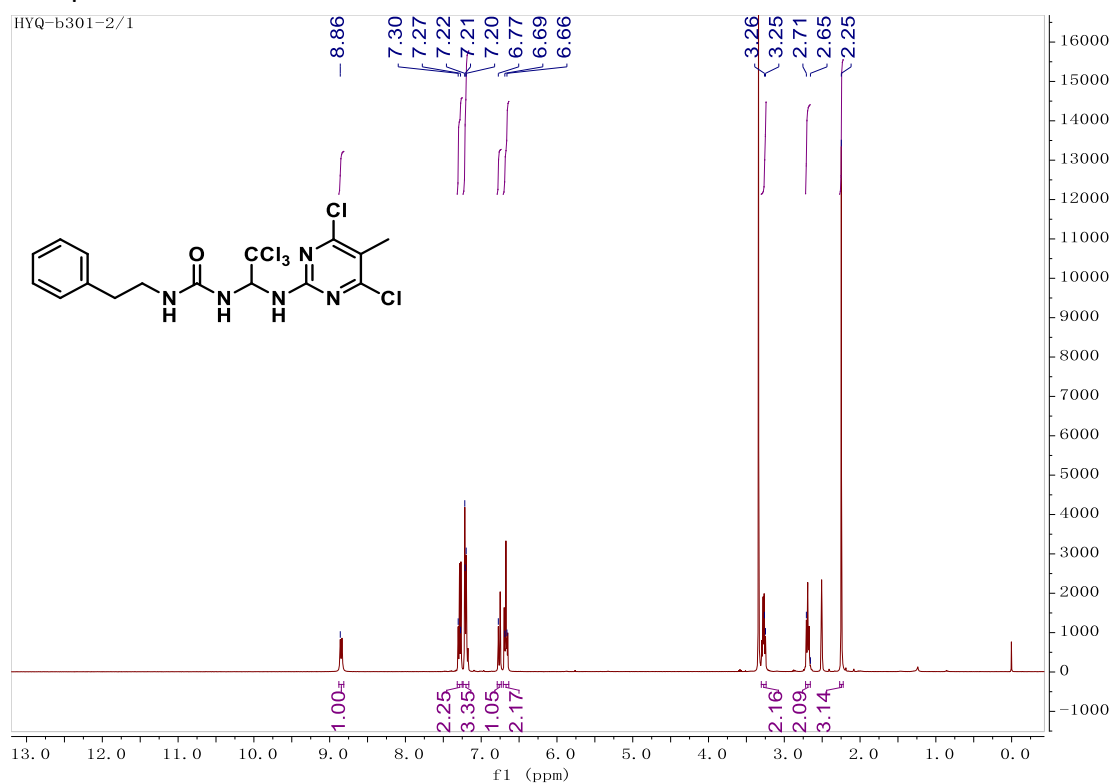


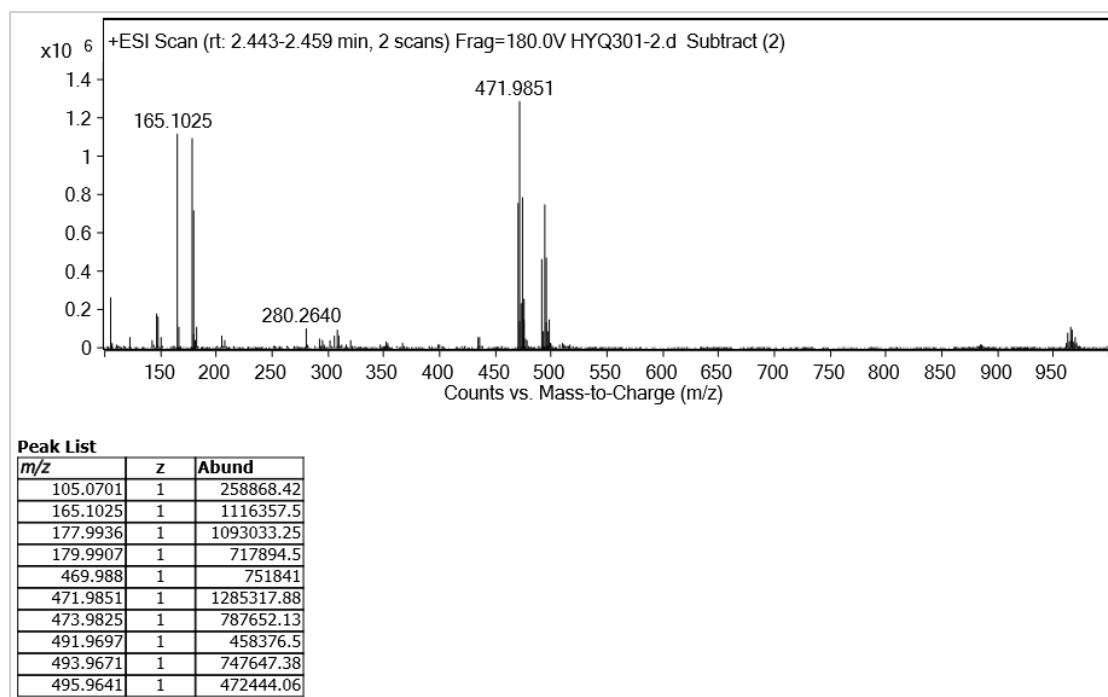
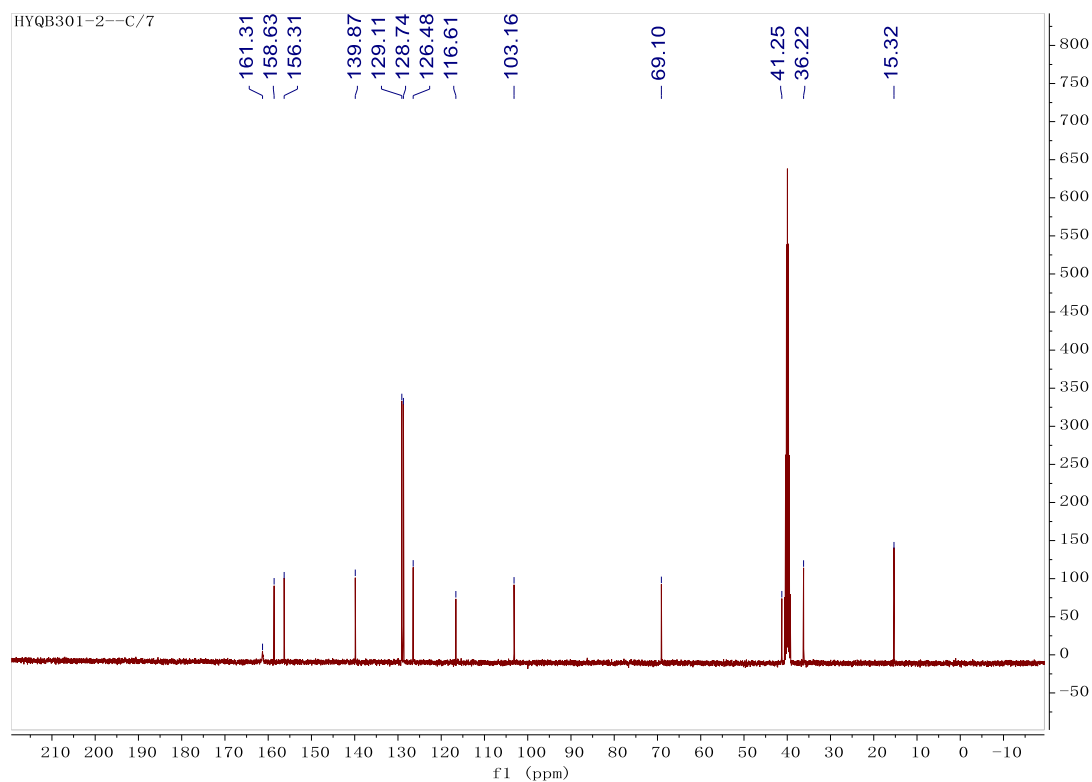
Compound 11





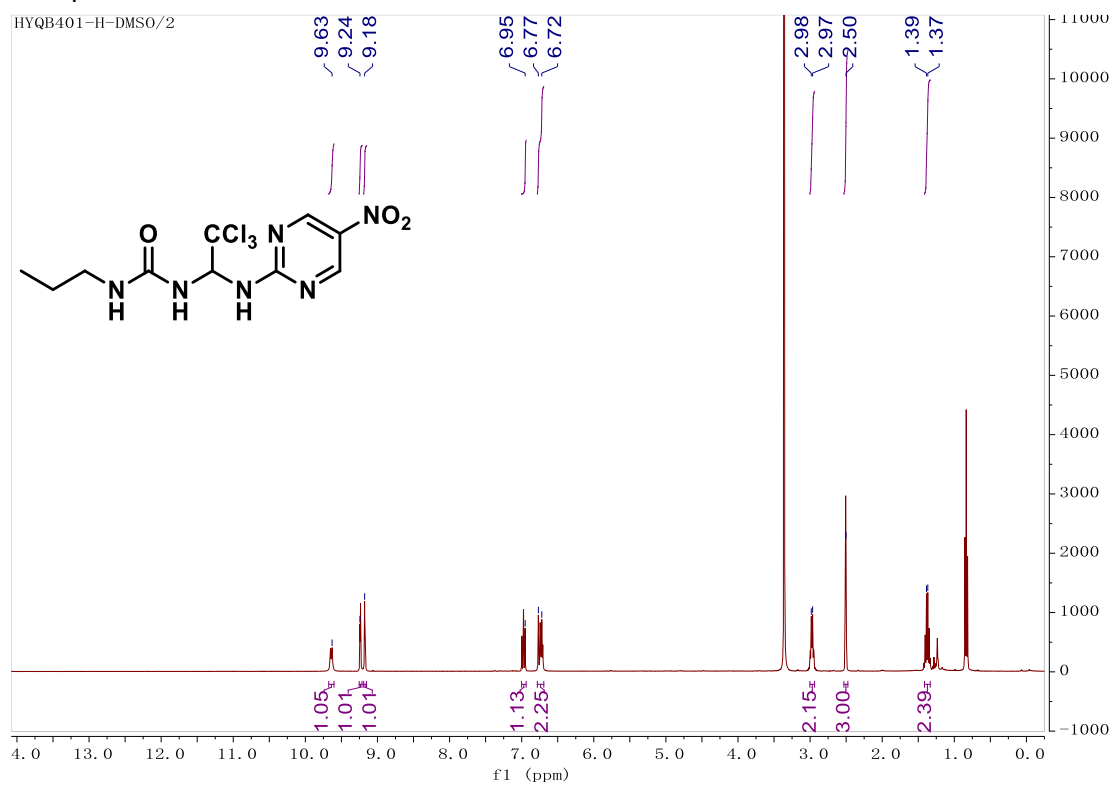
Compound 12



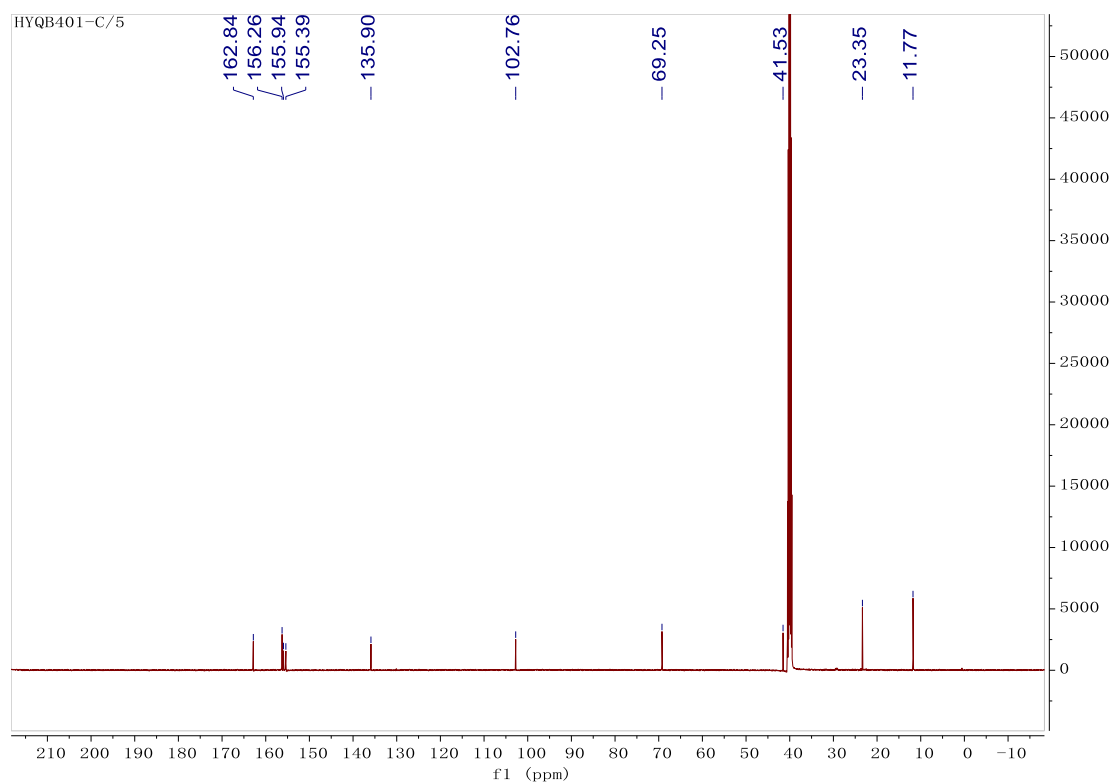


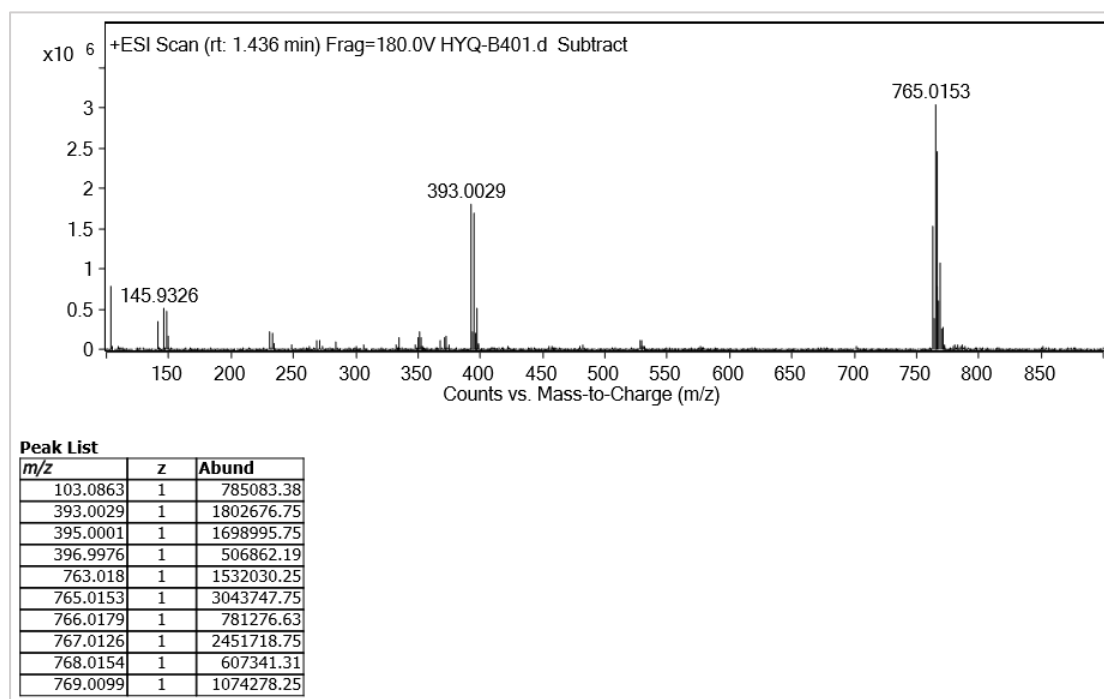
Compound 13

HYQB401-H-DMSO/2

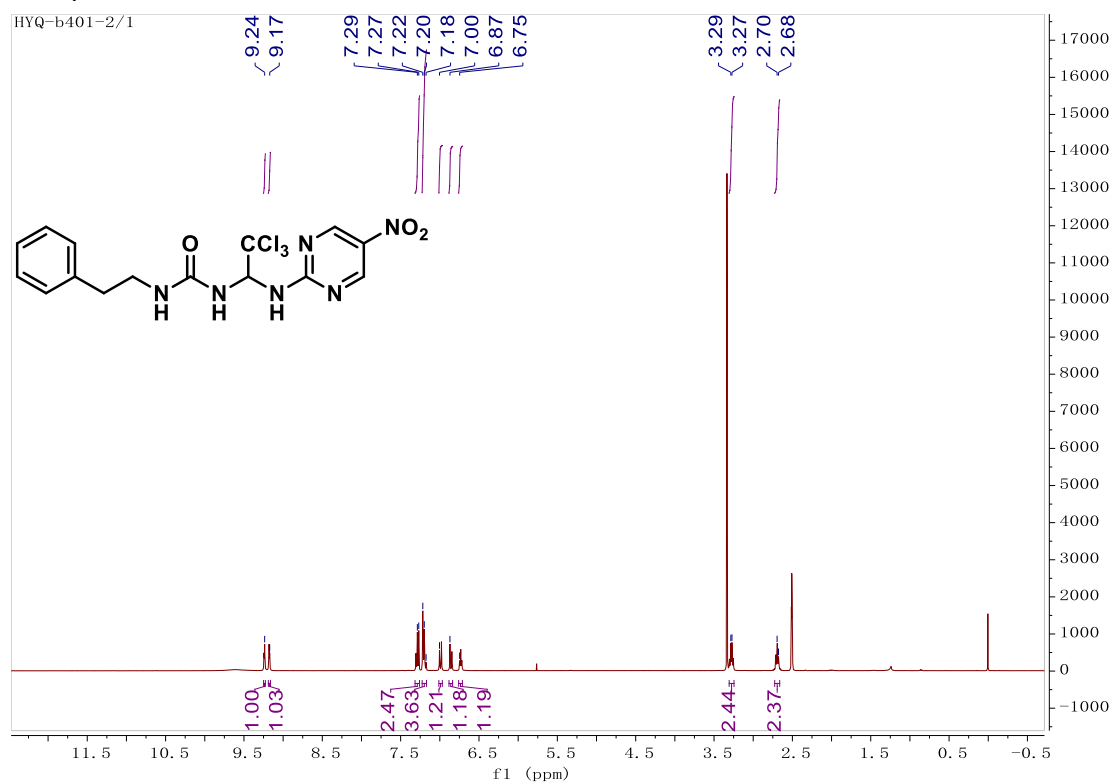


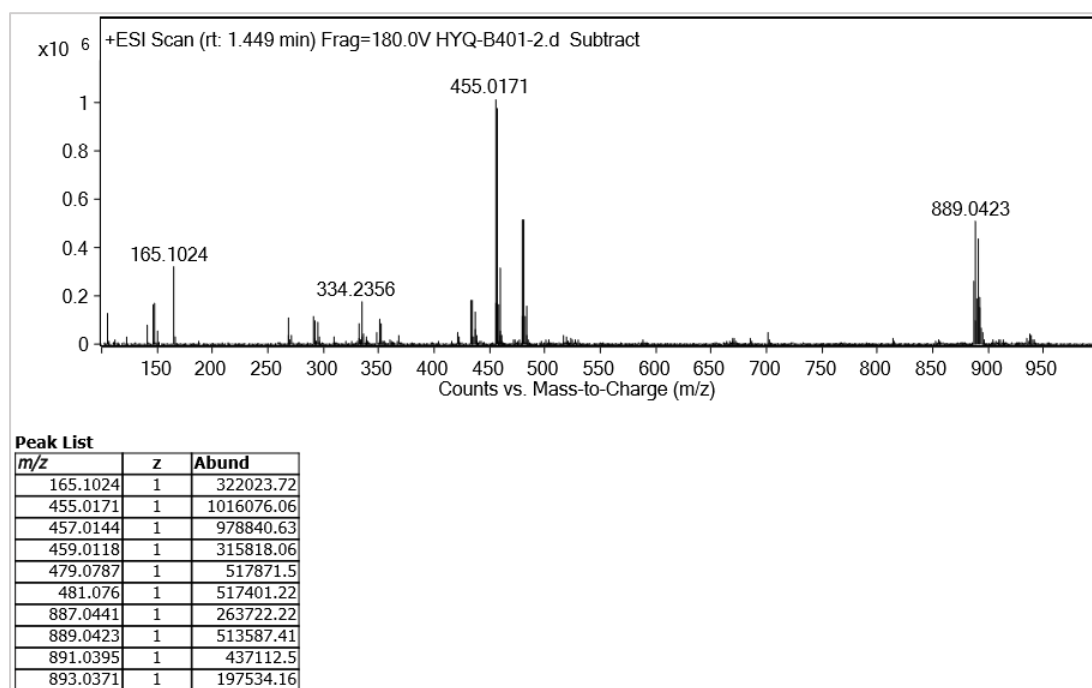
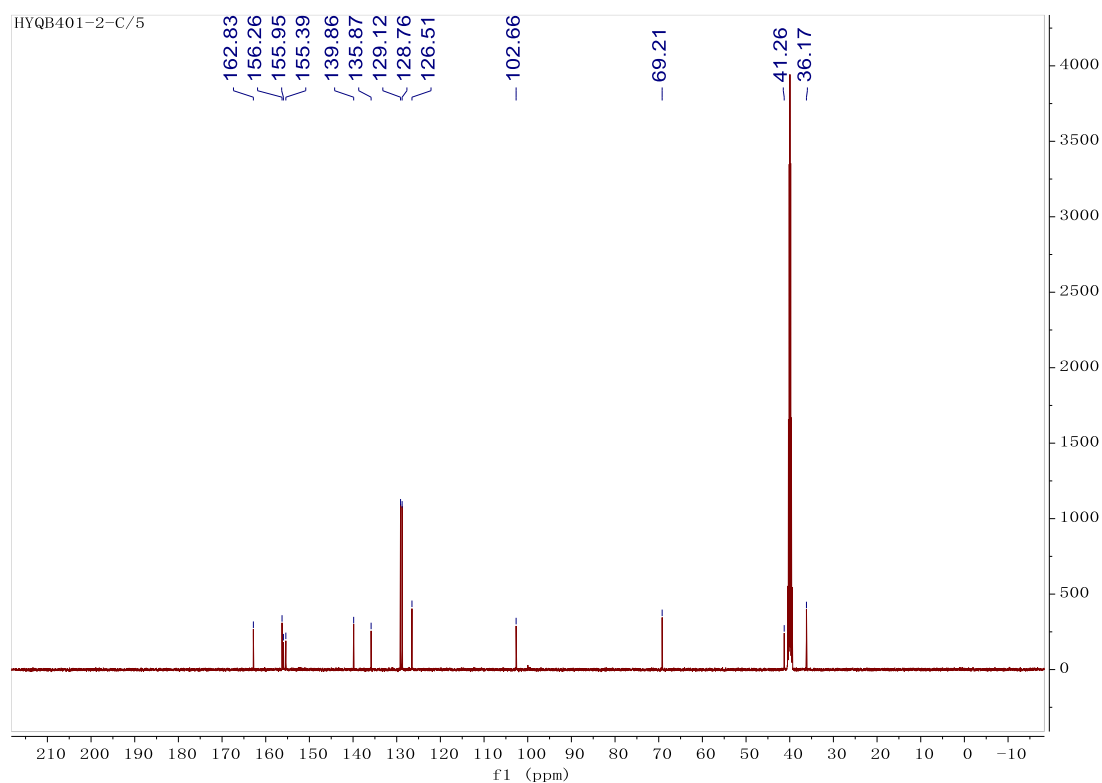
HYQB401-C/5



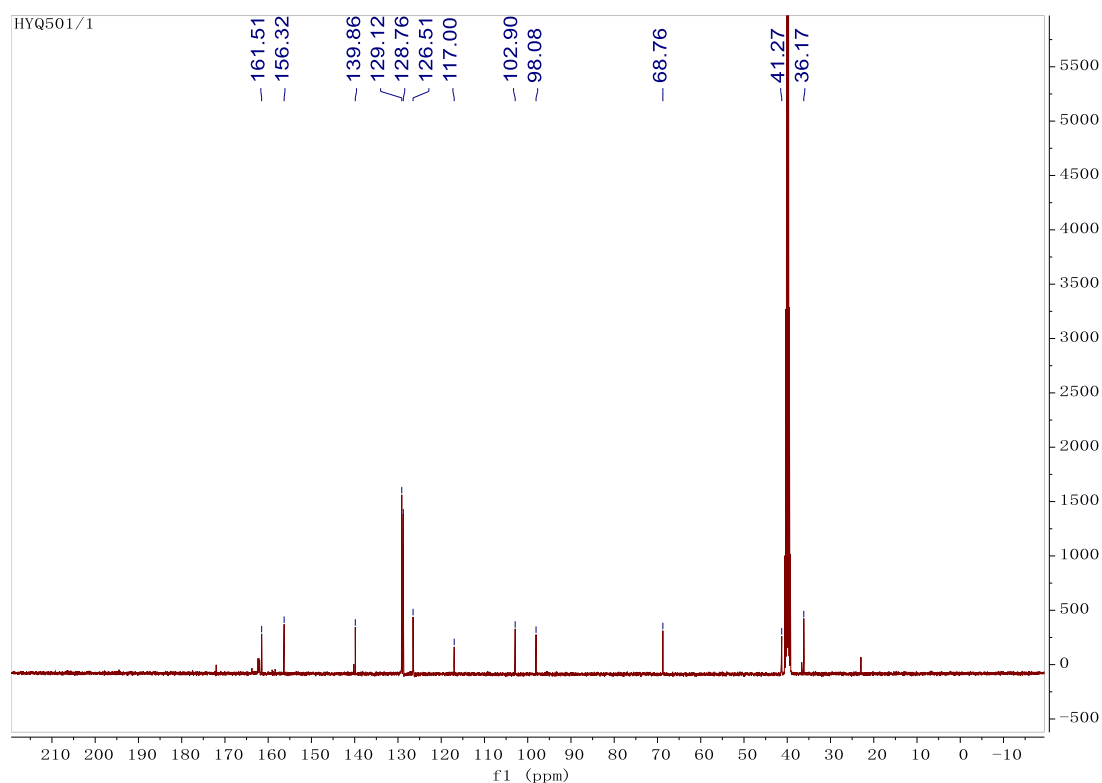
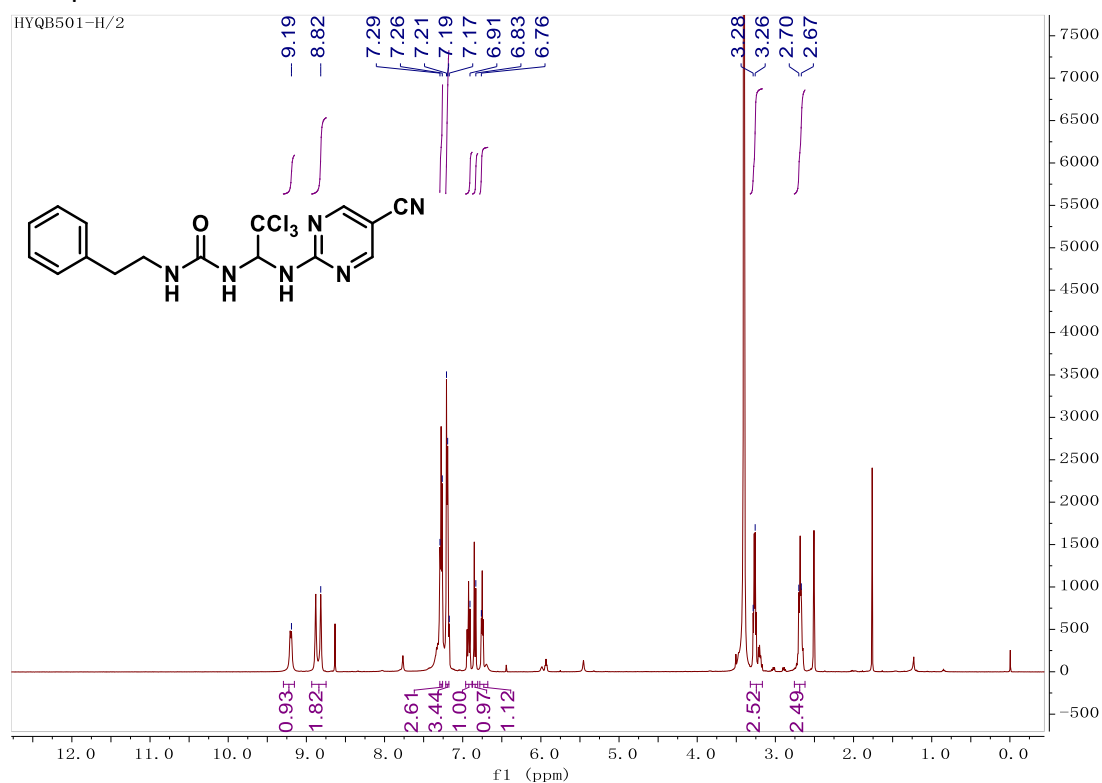


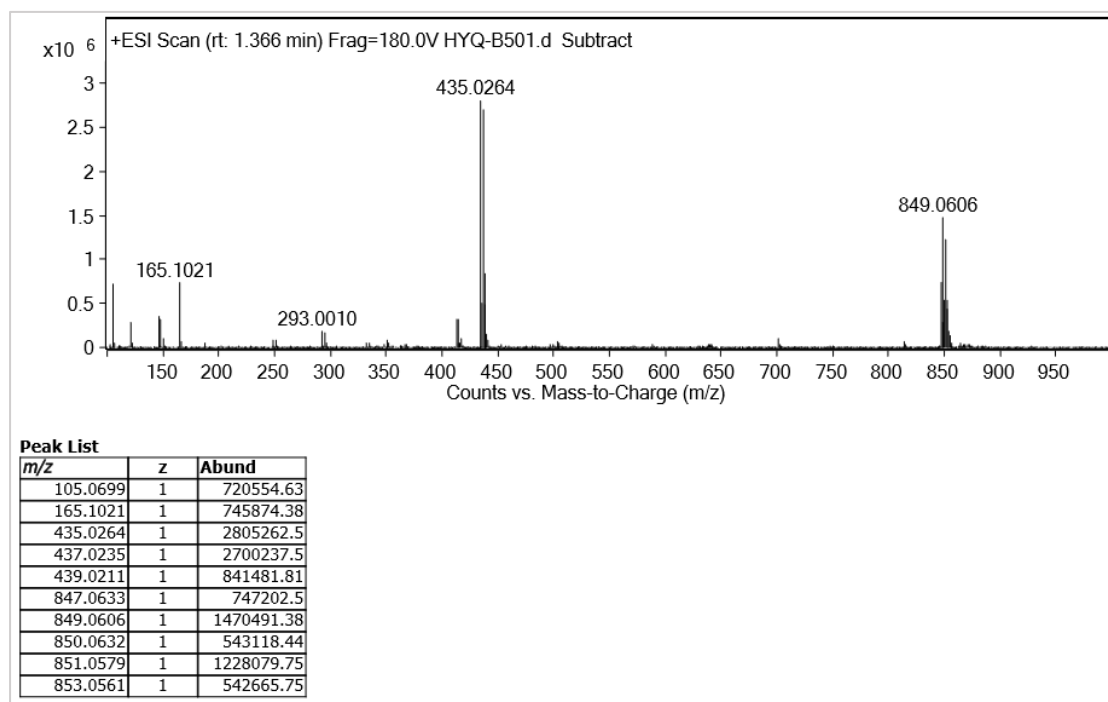
Compound 14



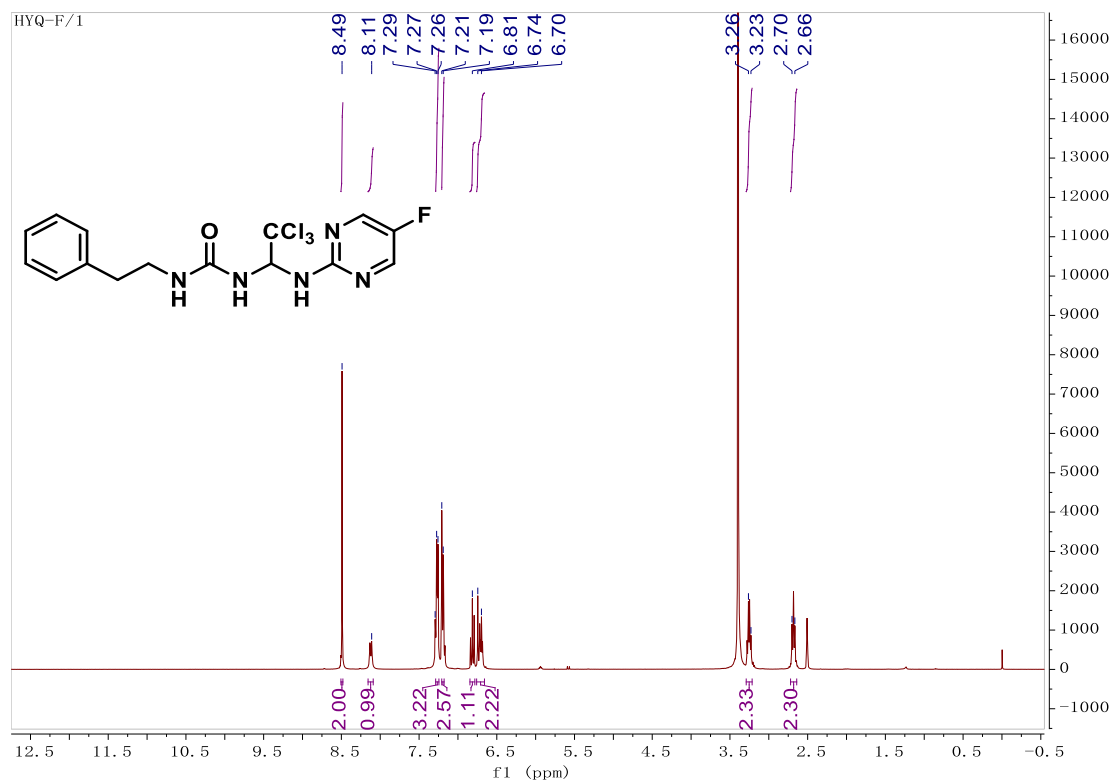


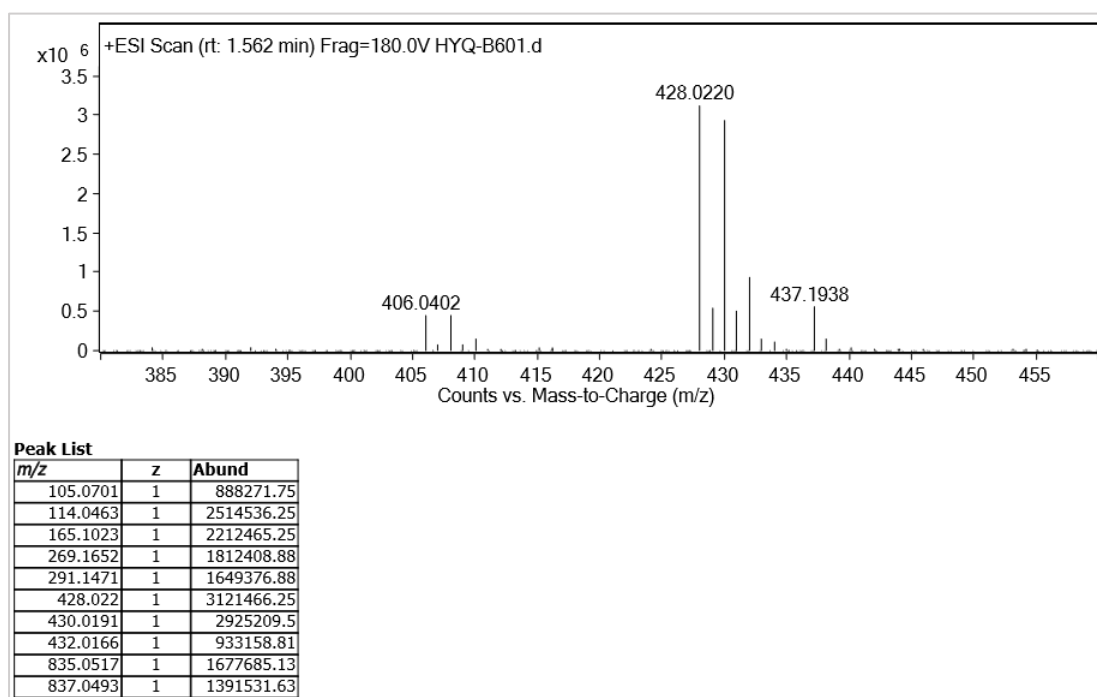
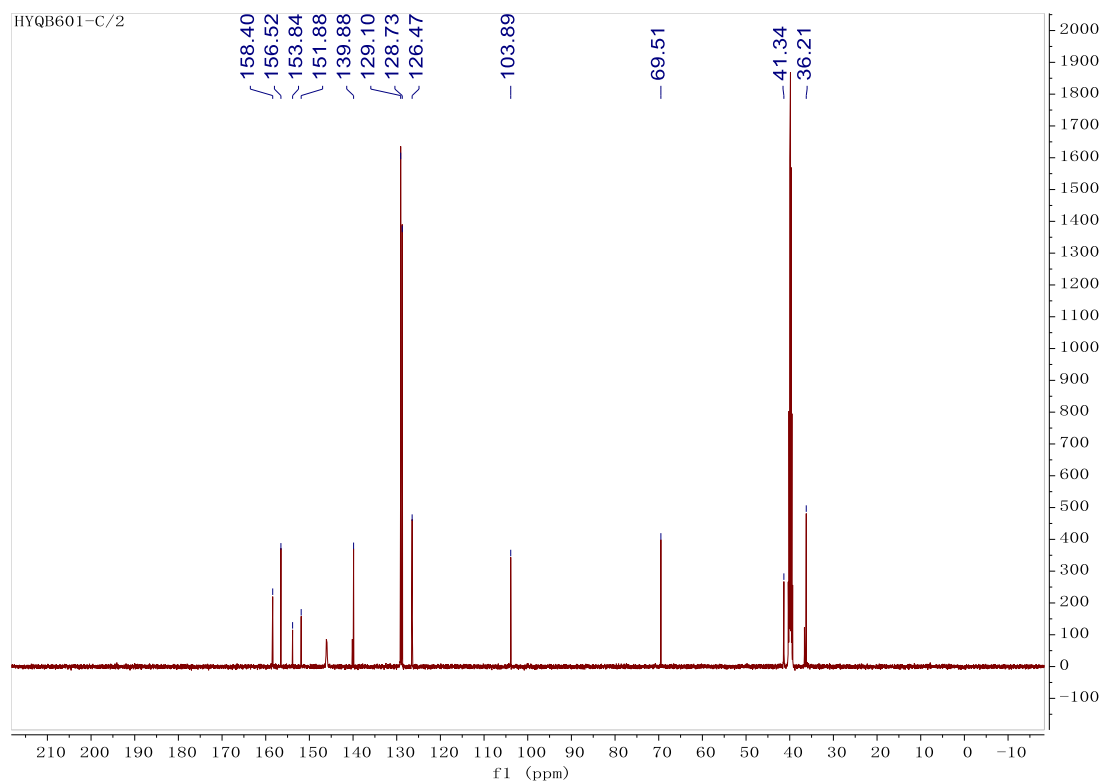
Compound 15



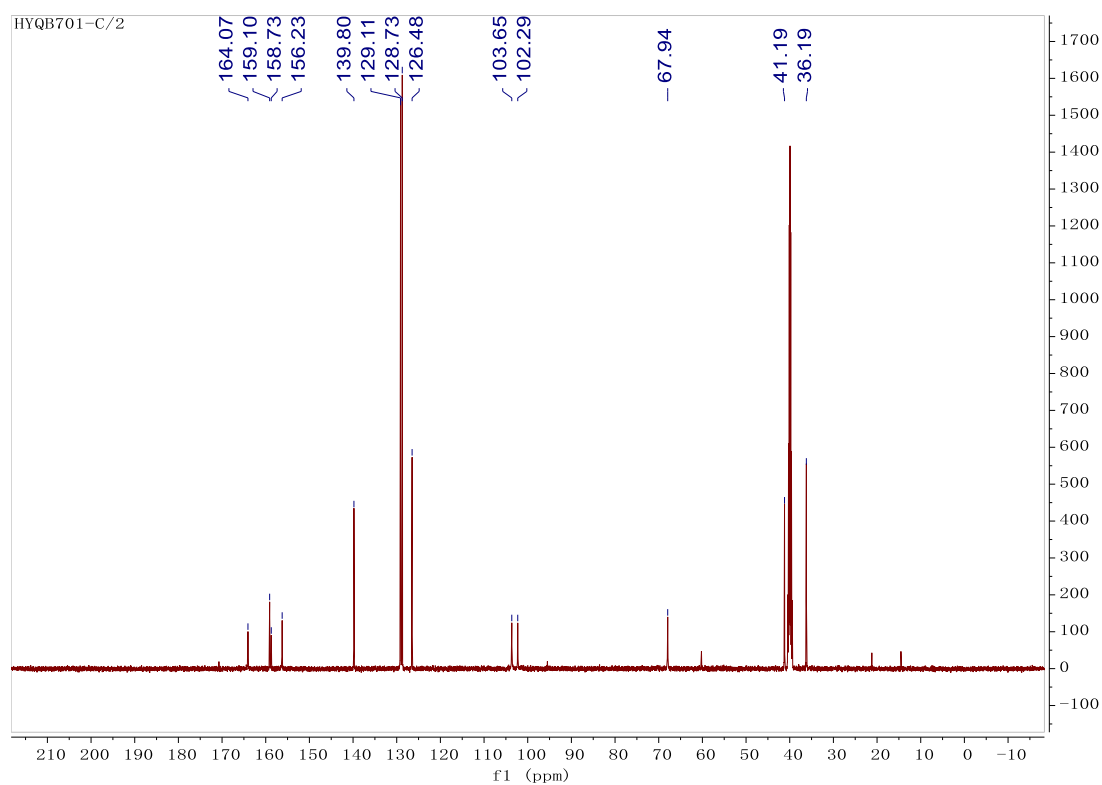
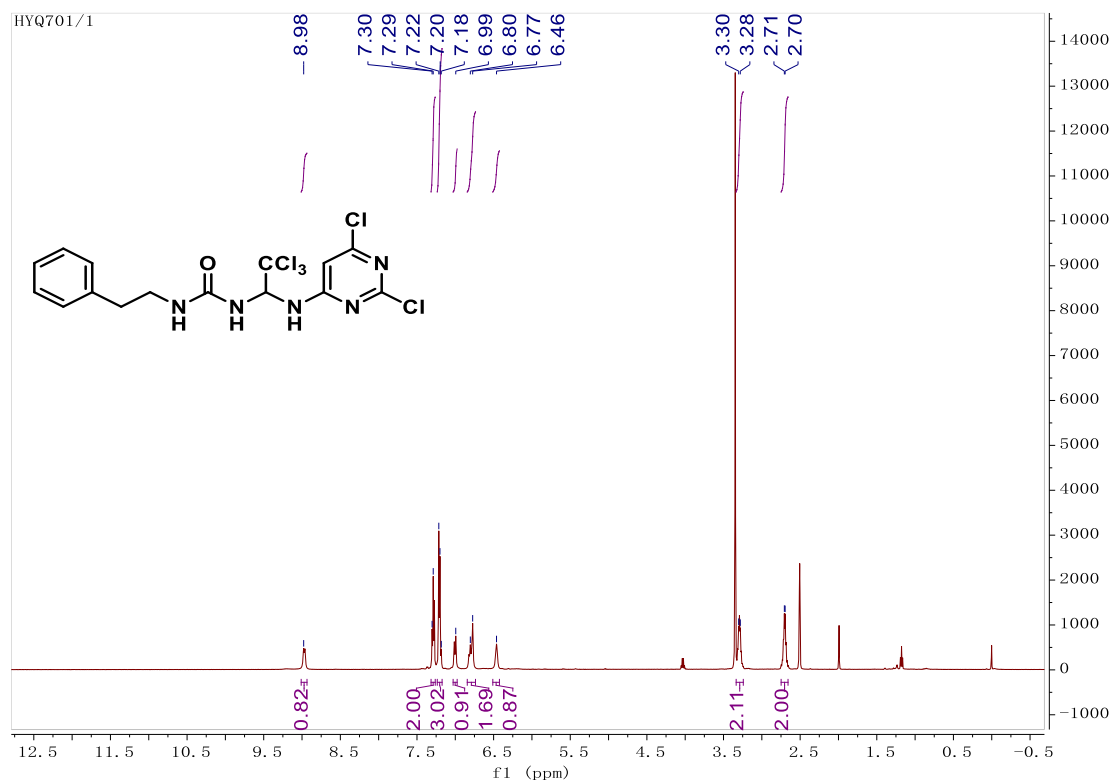


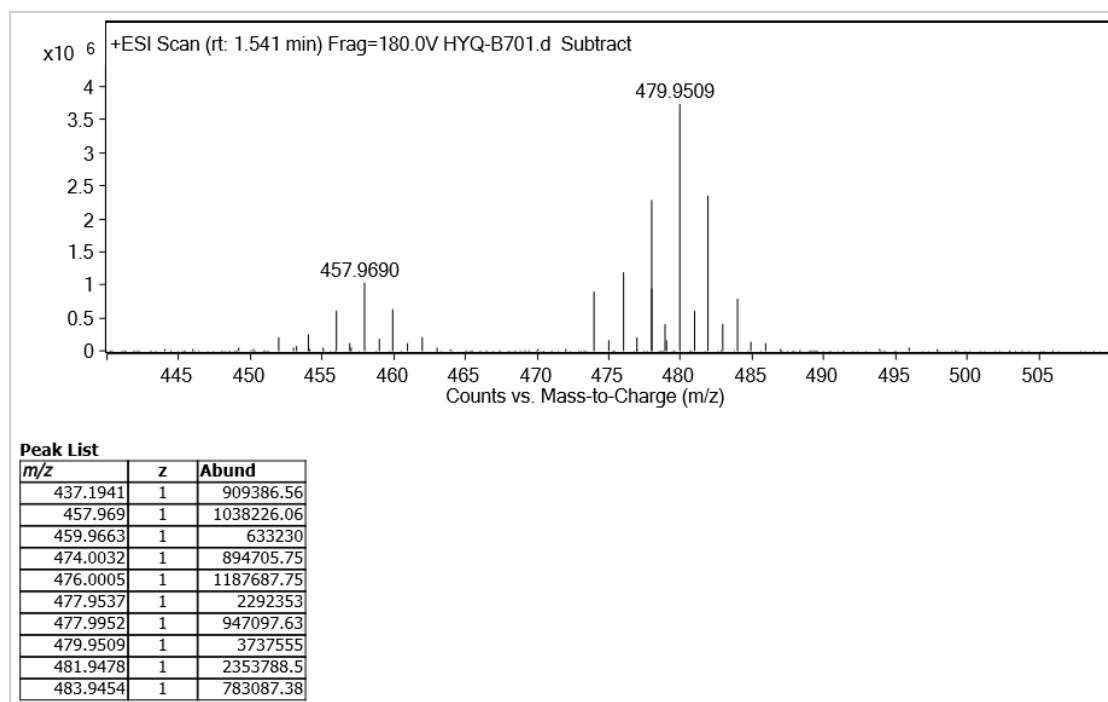
Compound 16



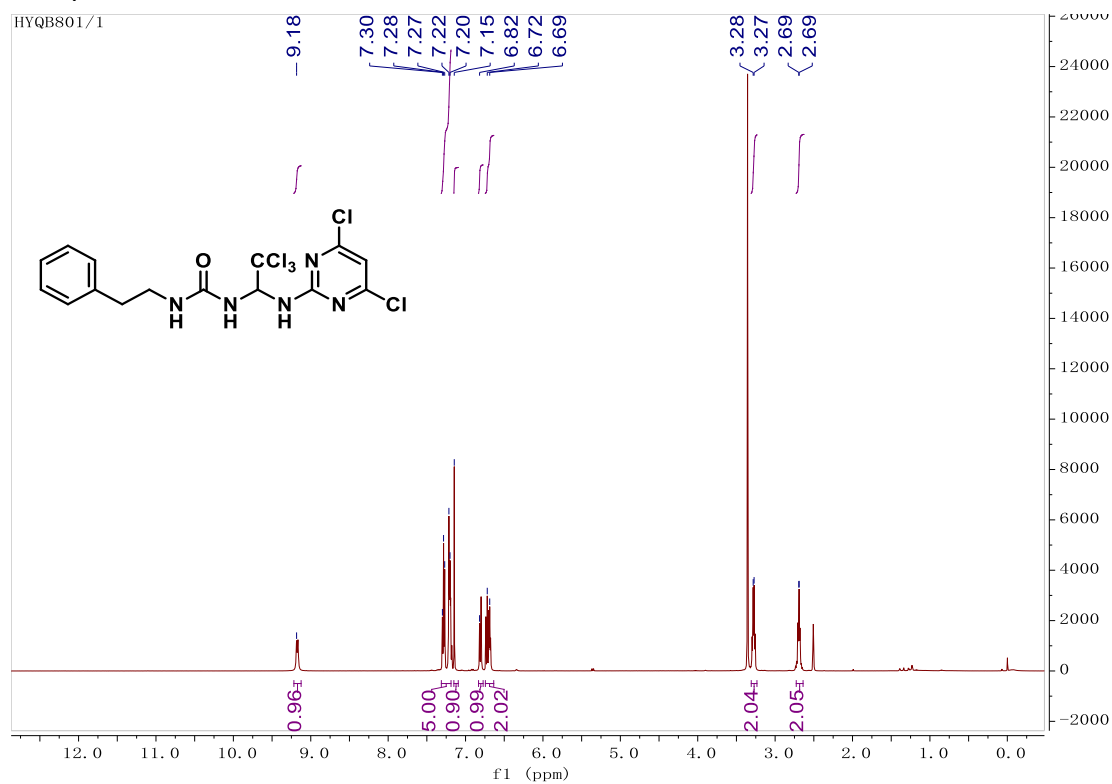


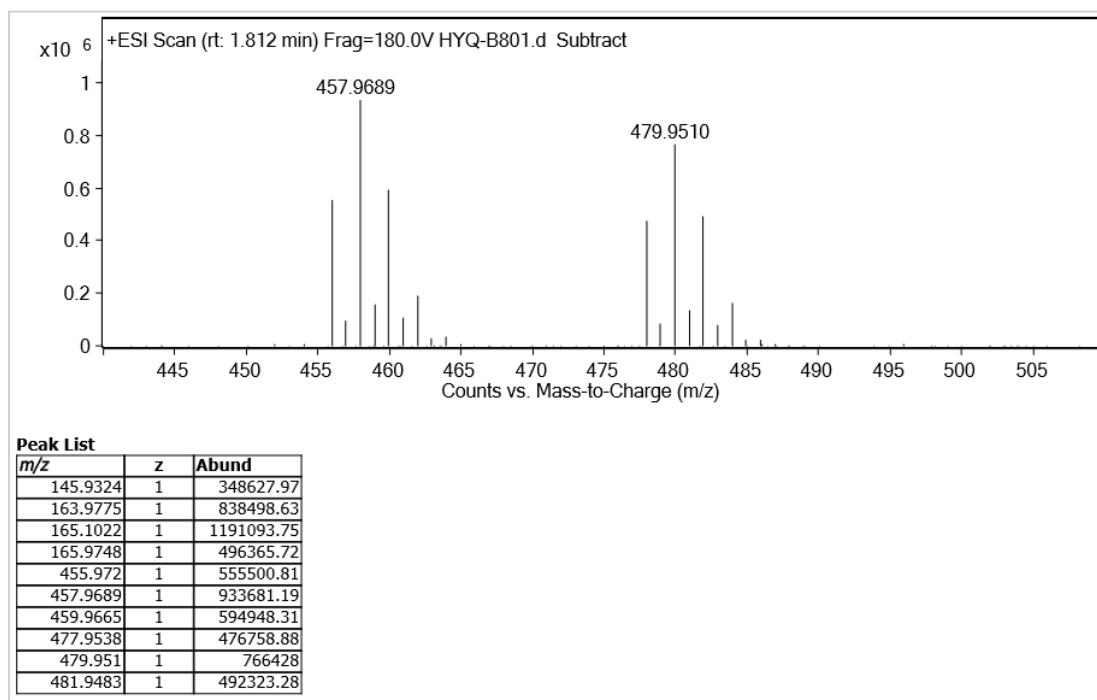
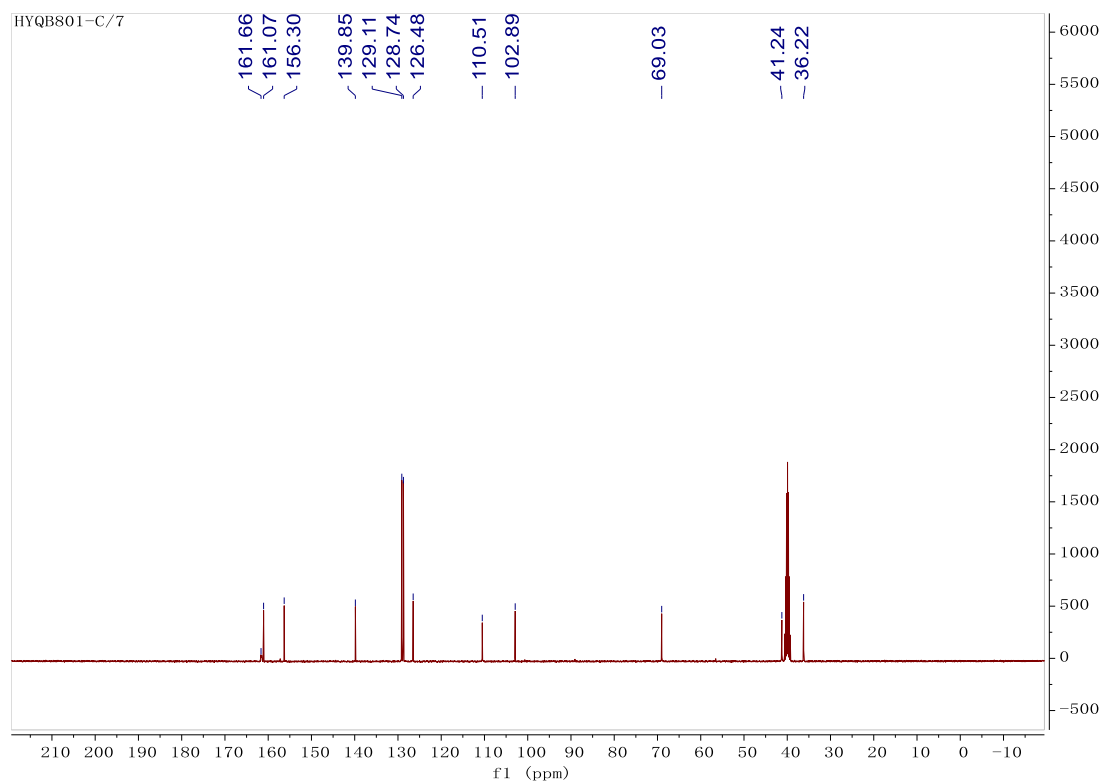
Compound 17



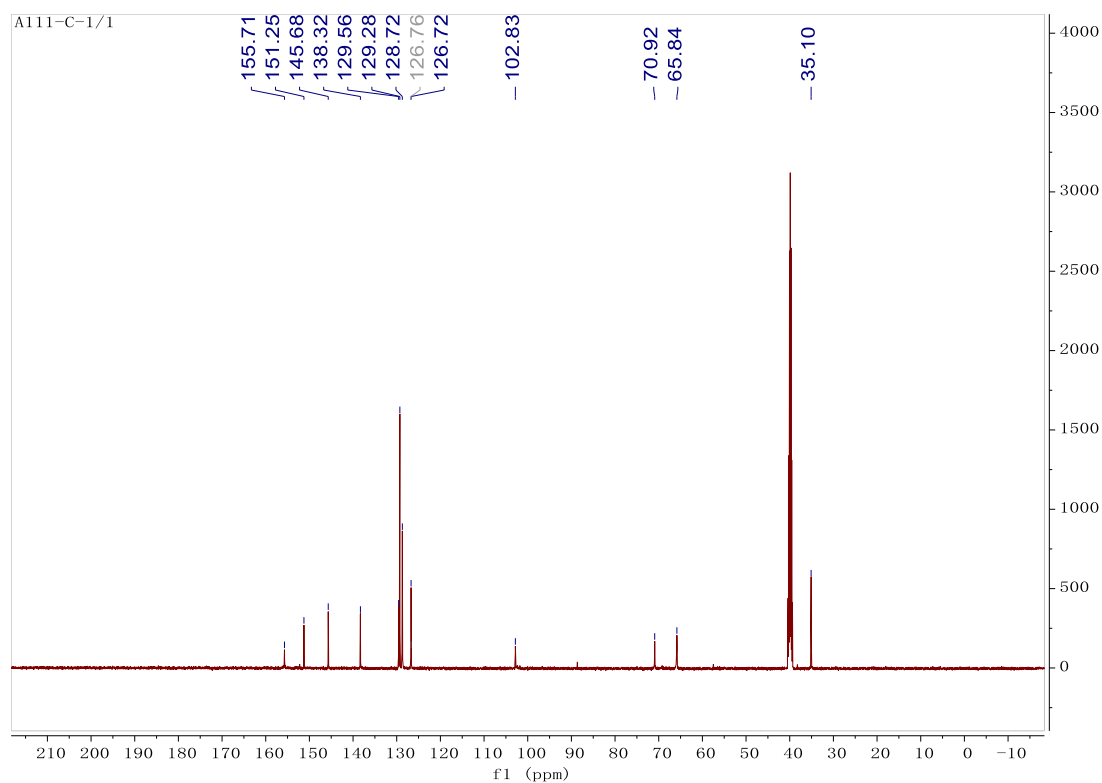
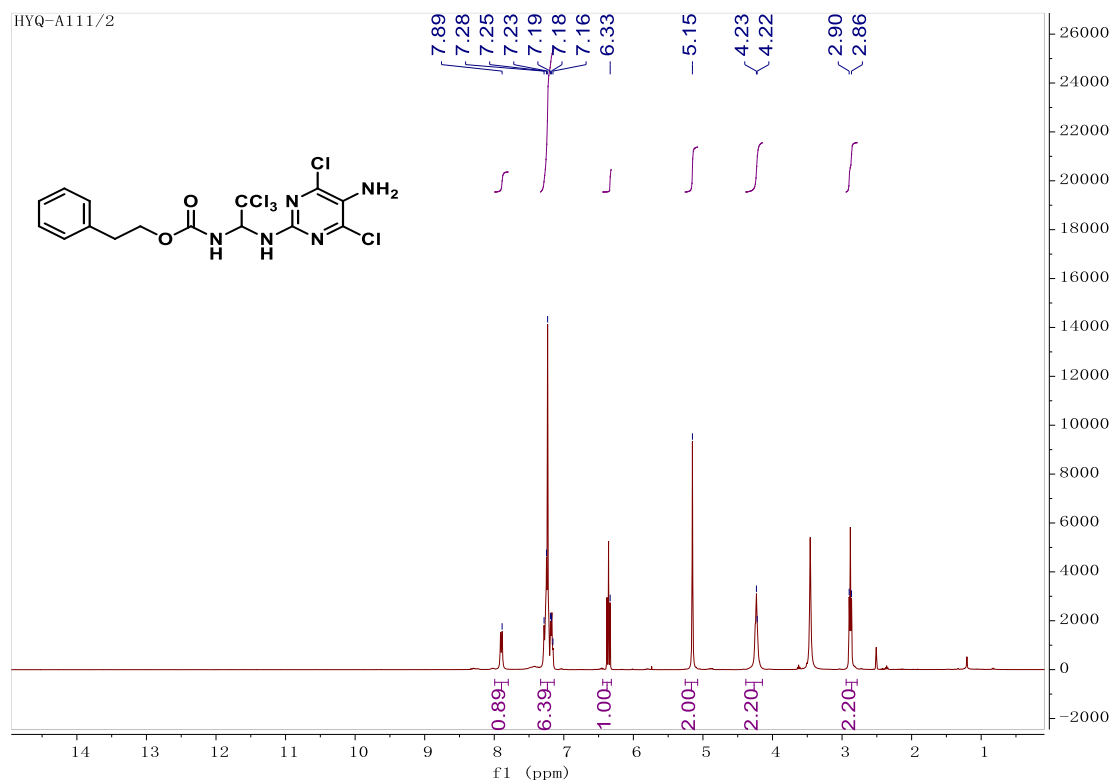


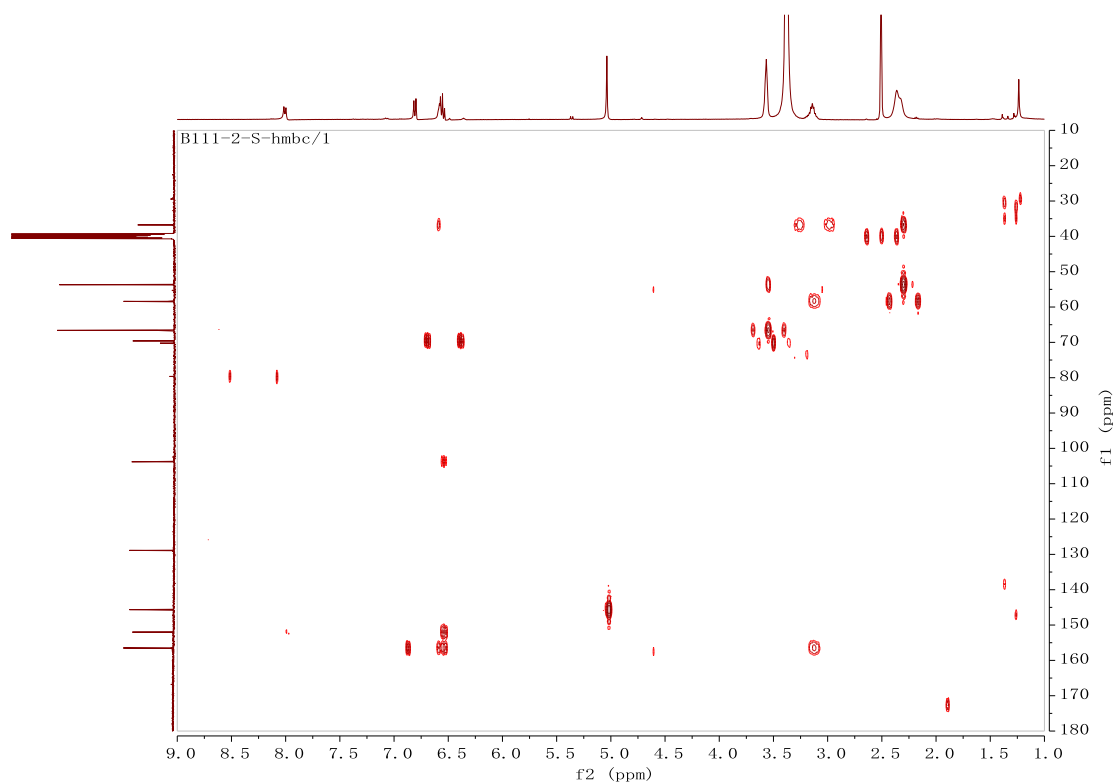
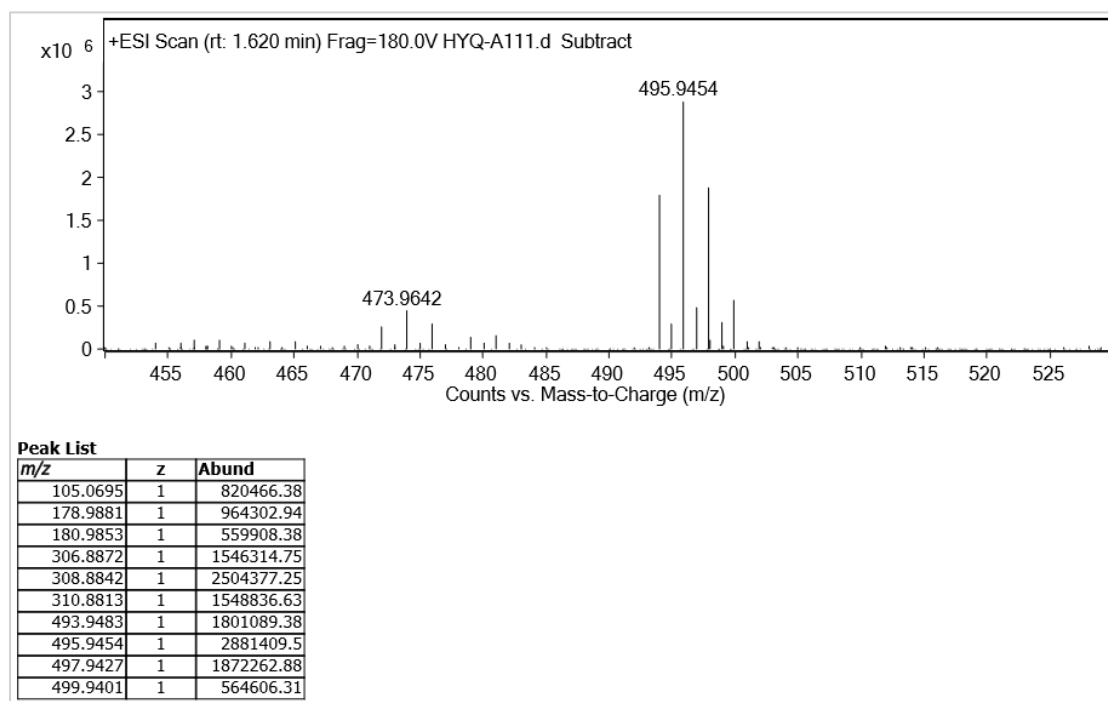
Compound 18



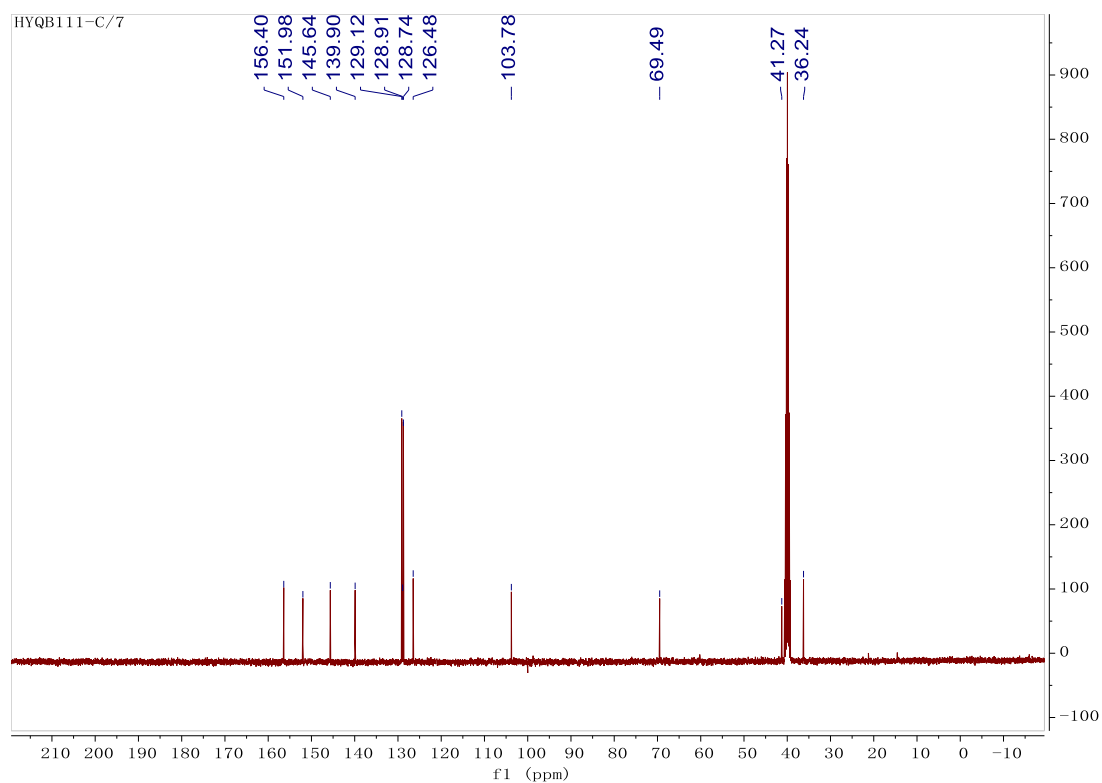
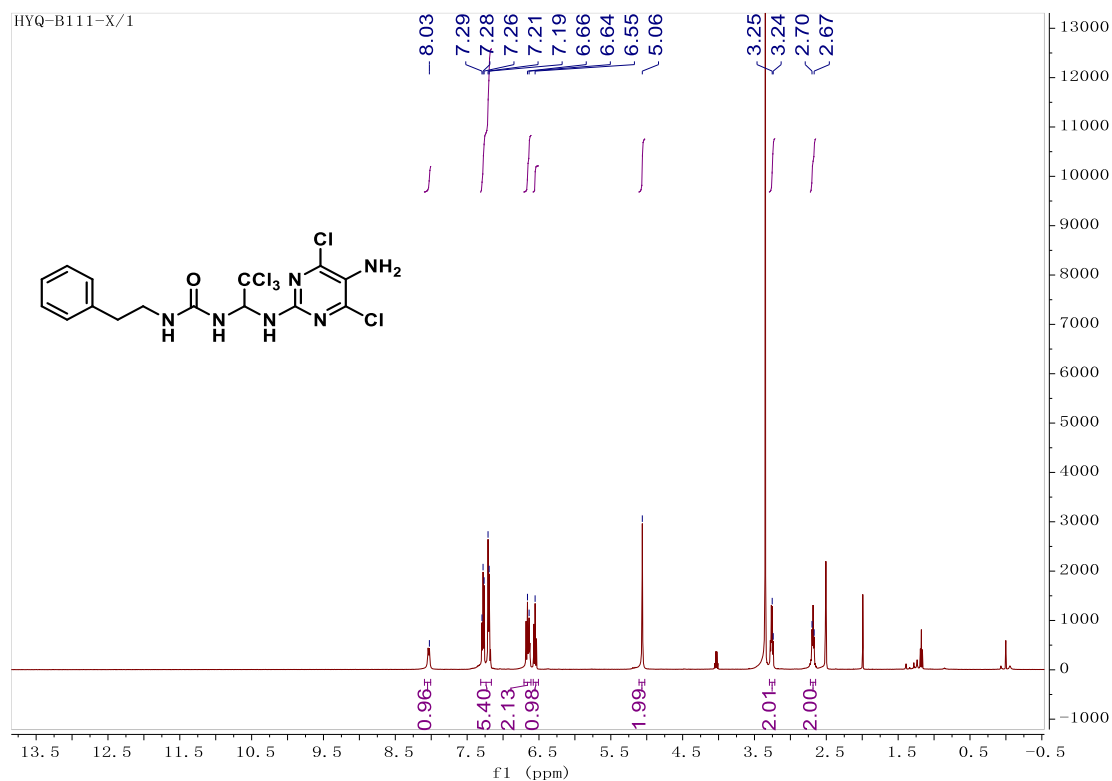


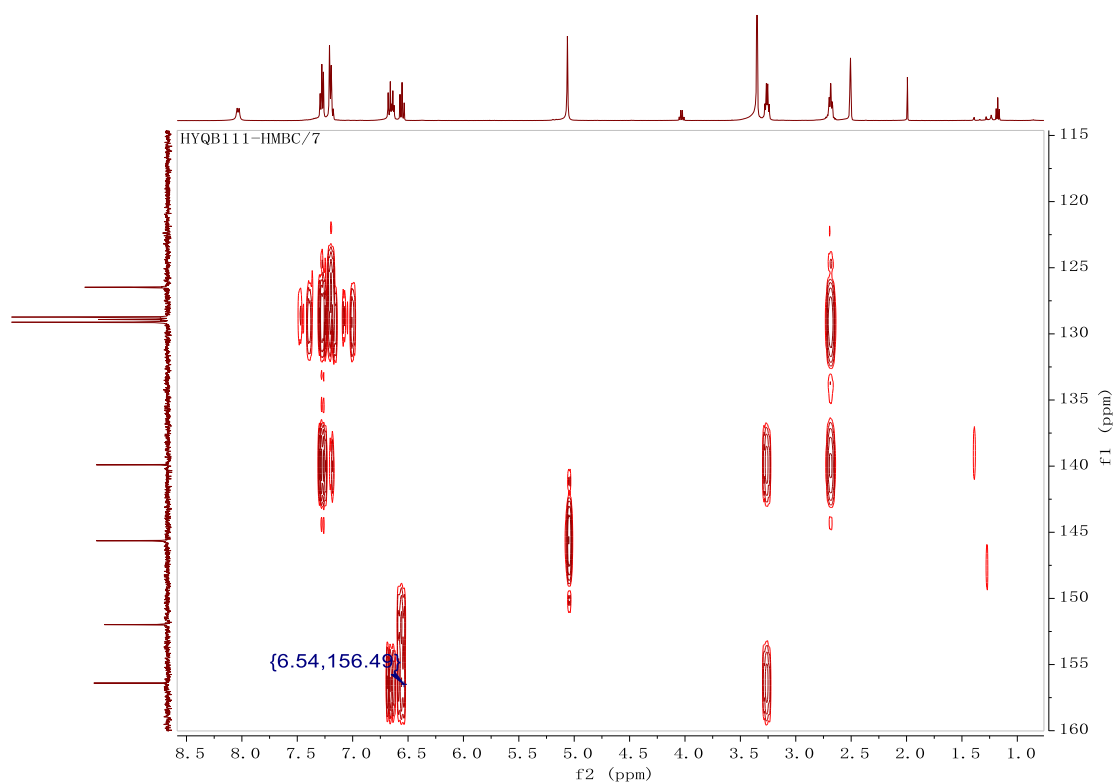
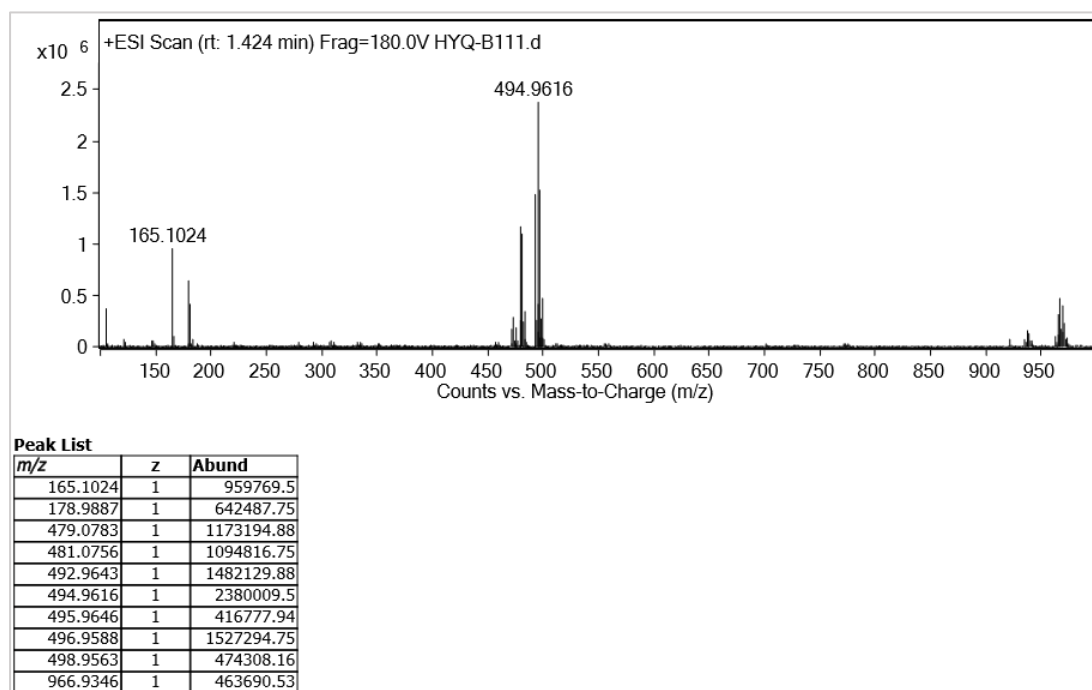
Compound 19



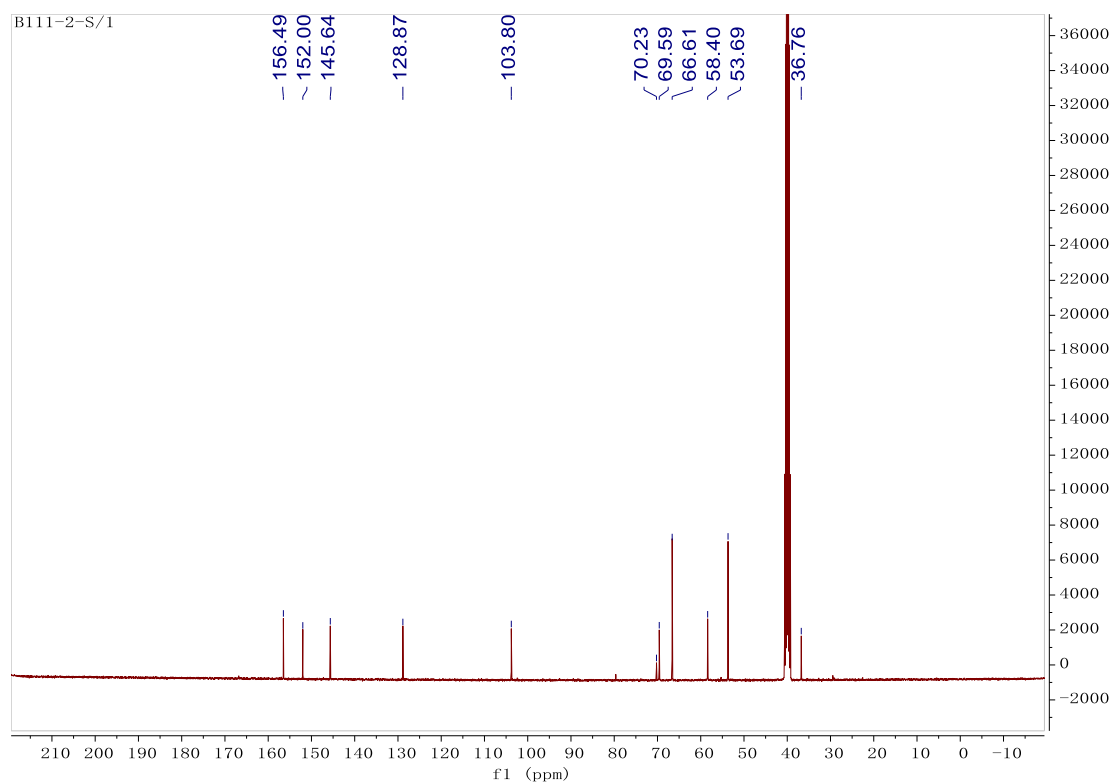
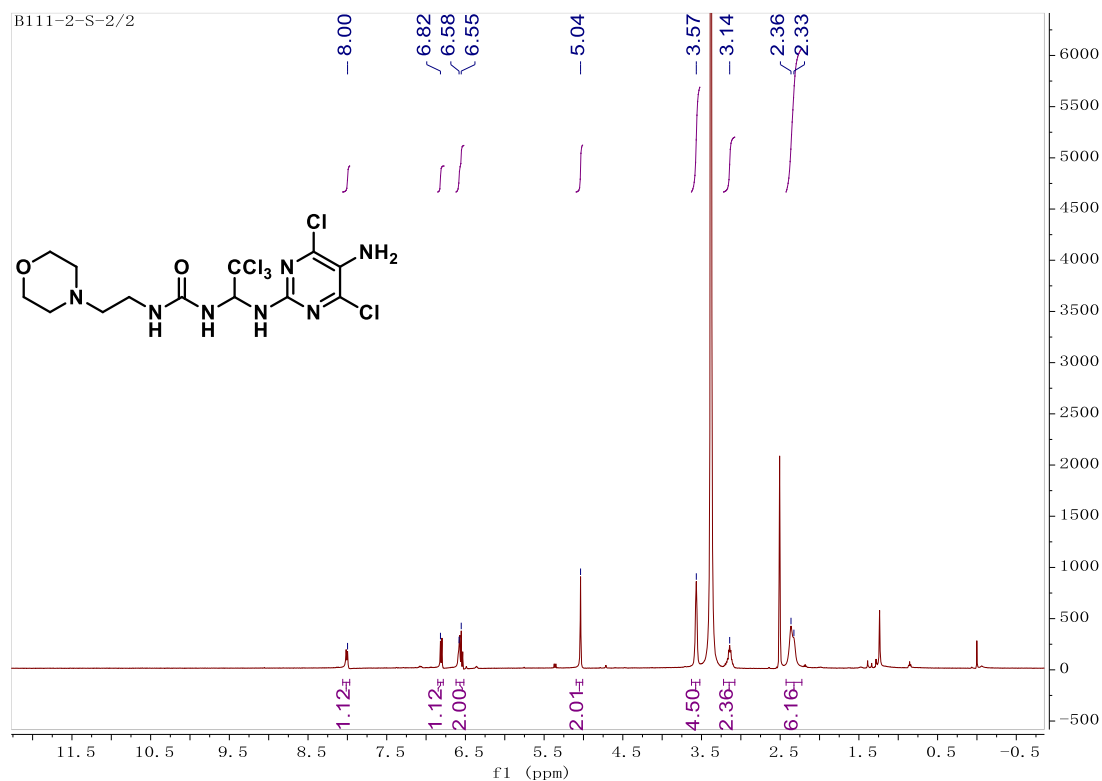


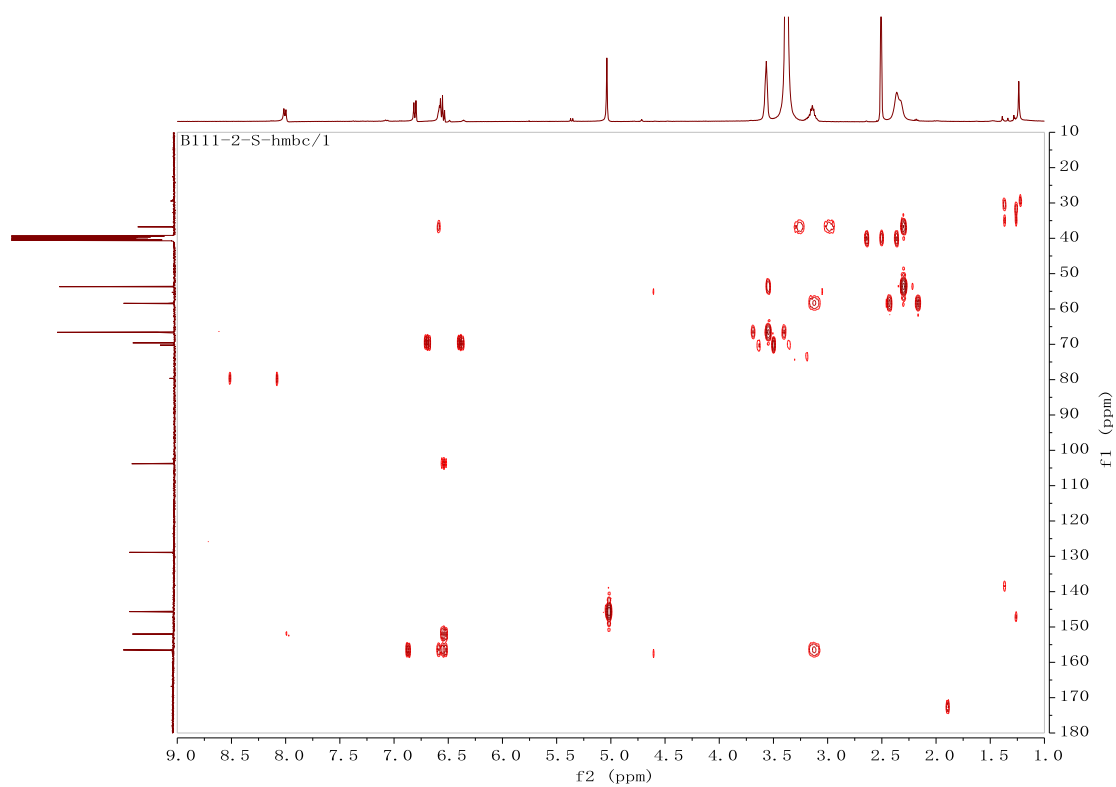
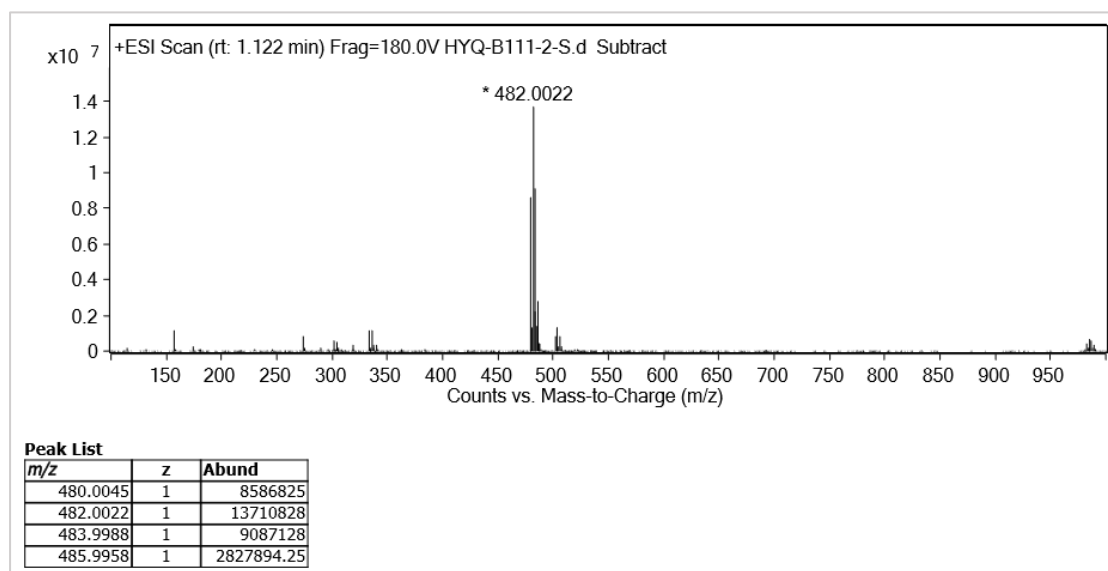
Compound 20



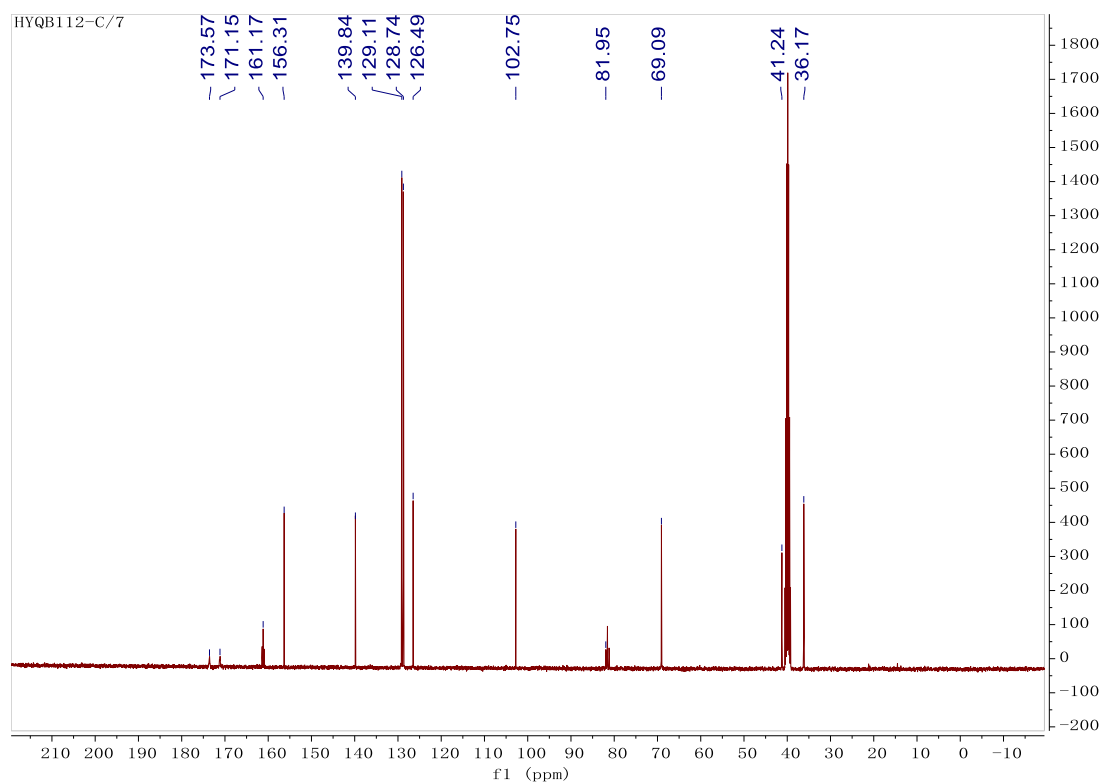
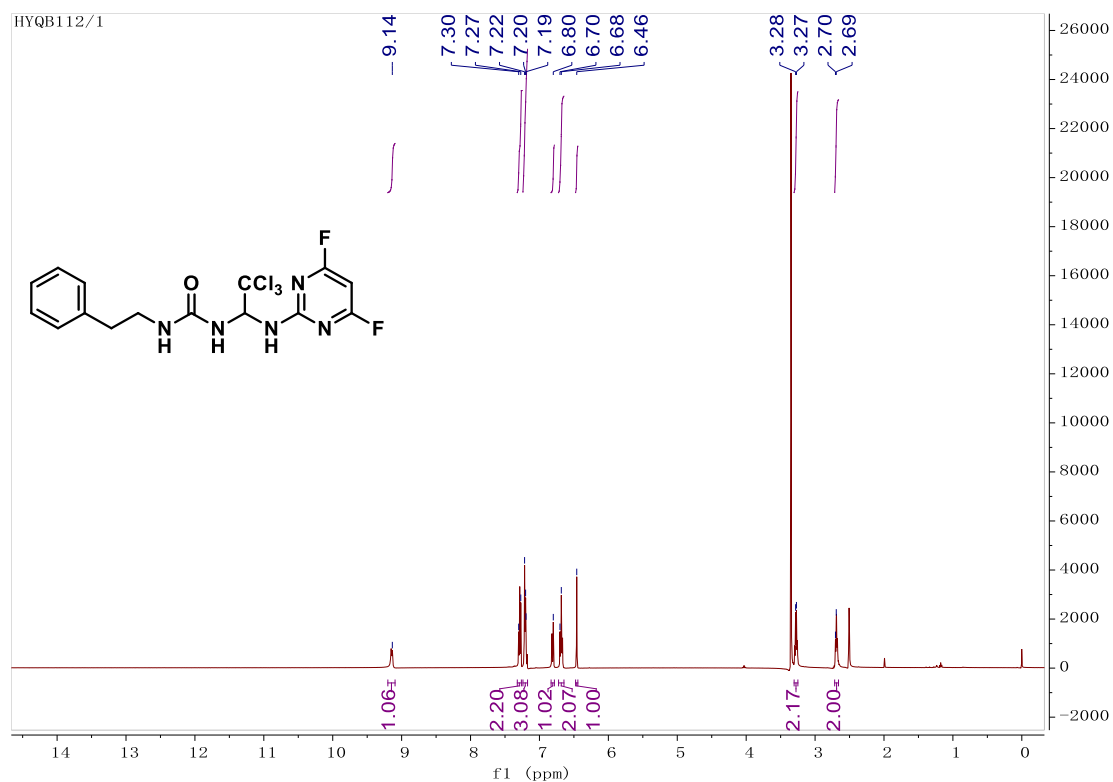


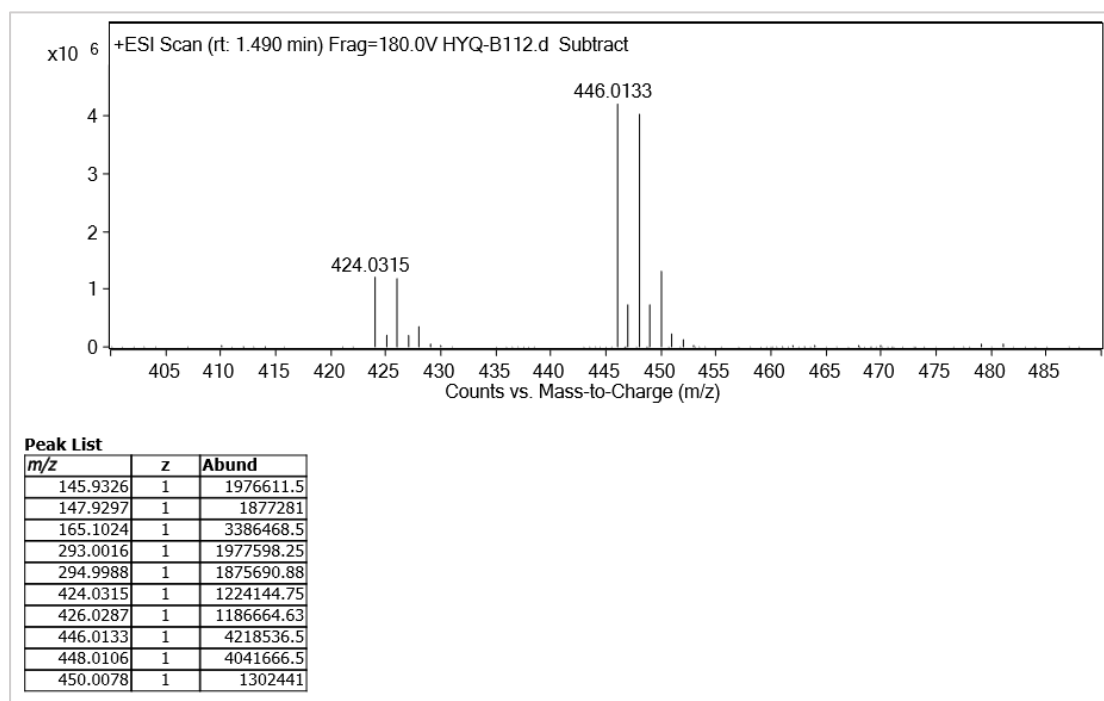
Compound 21



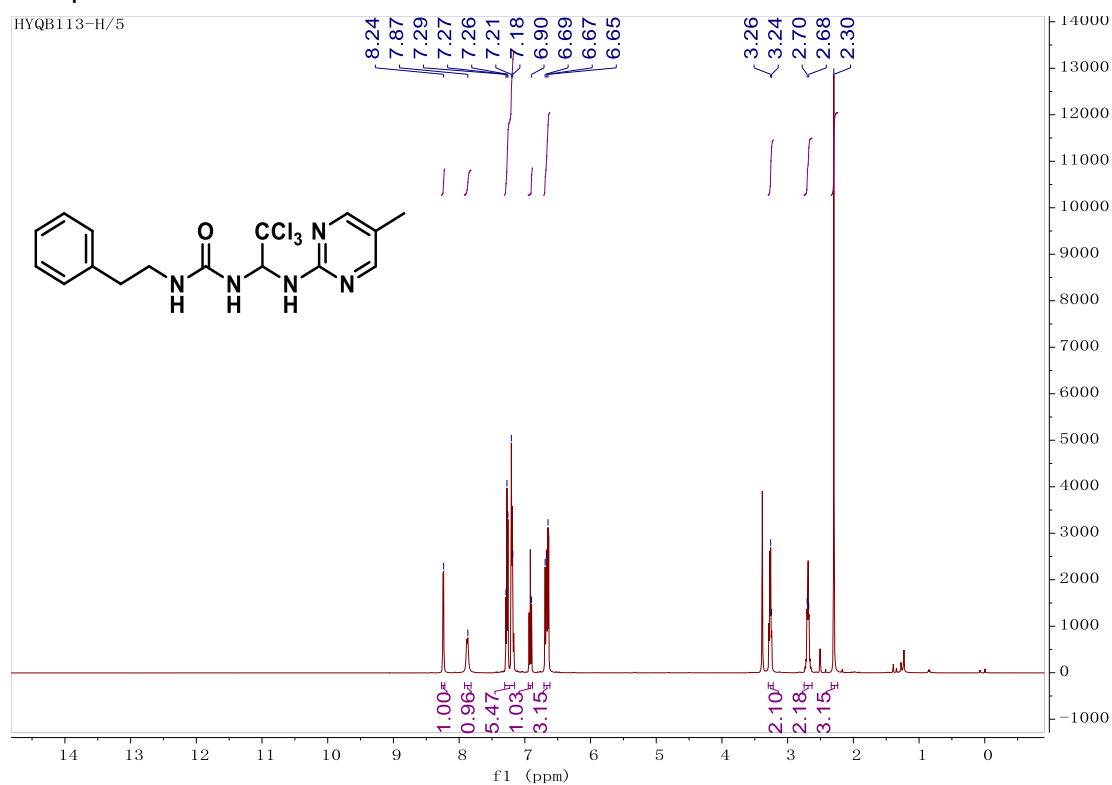


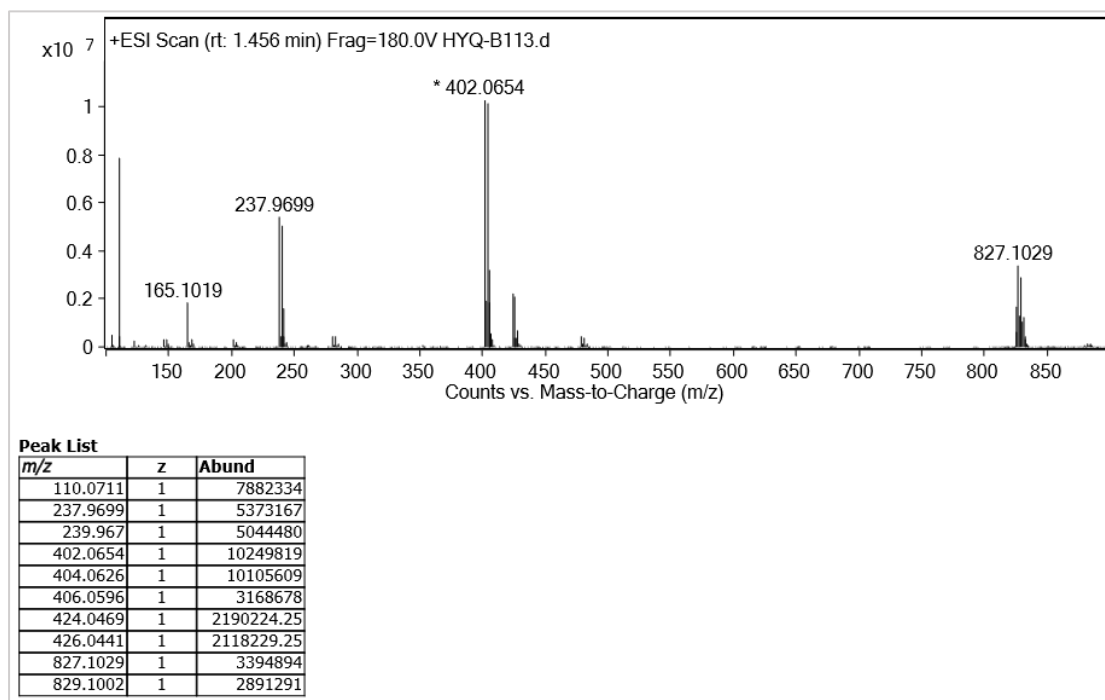
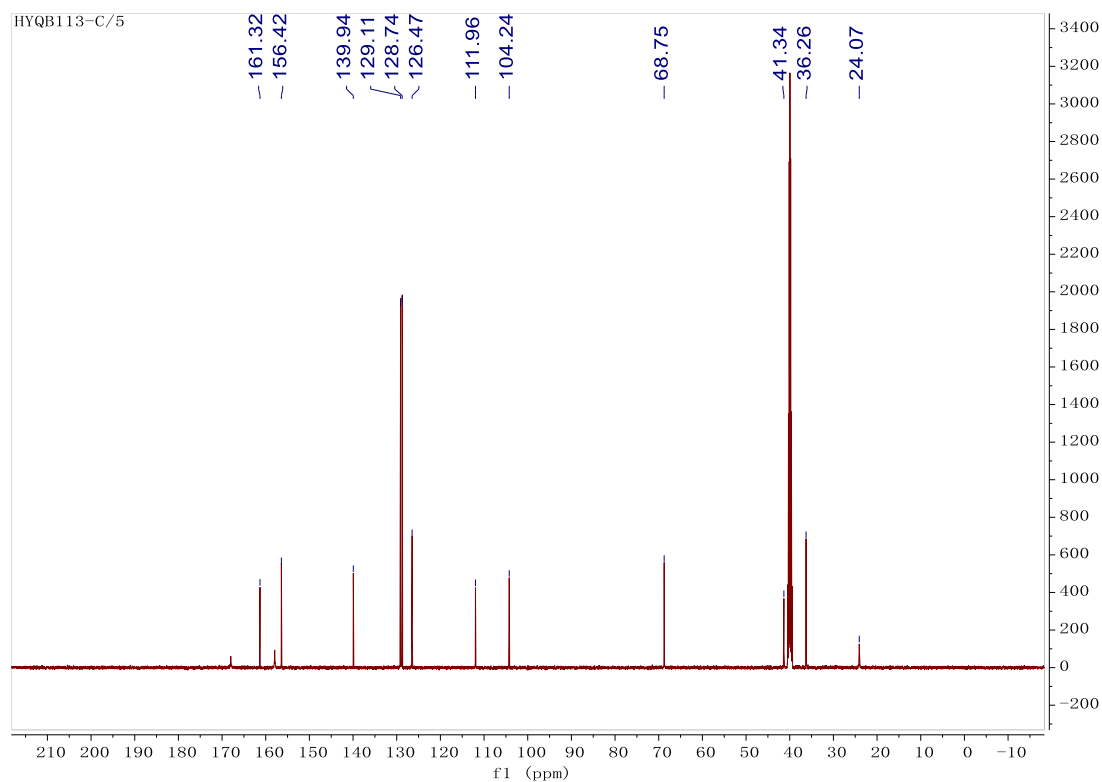
Compound 22



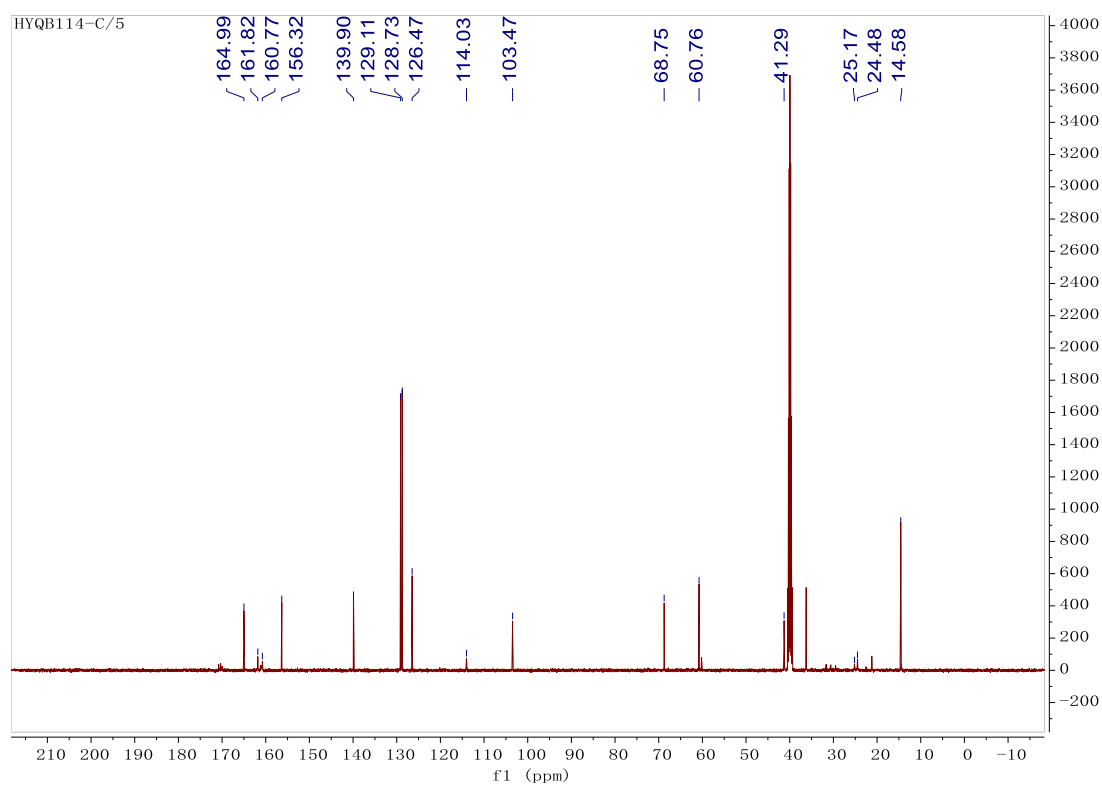
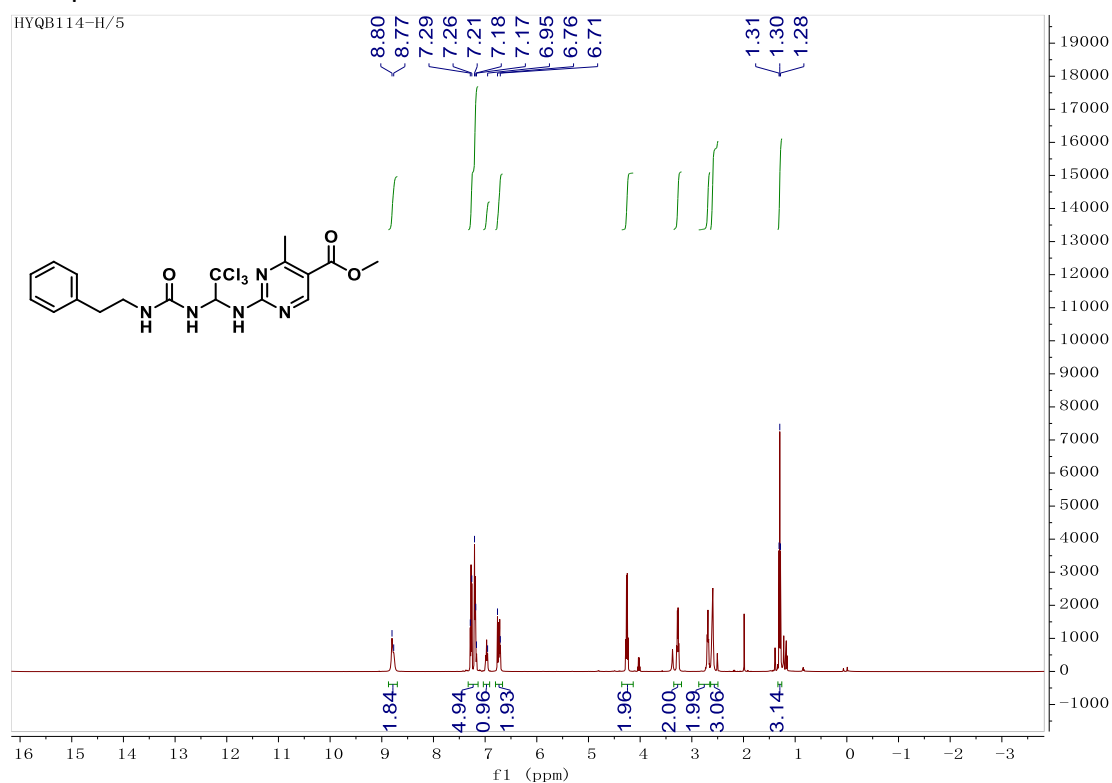


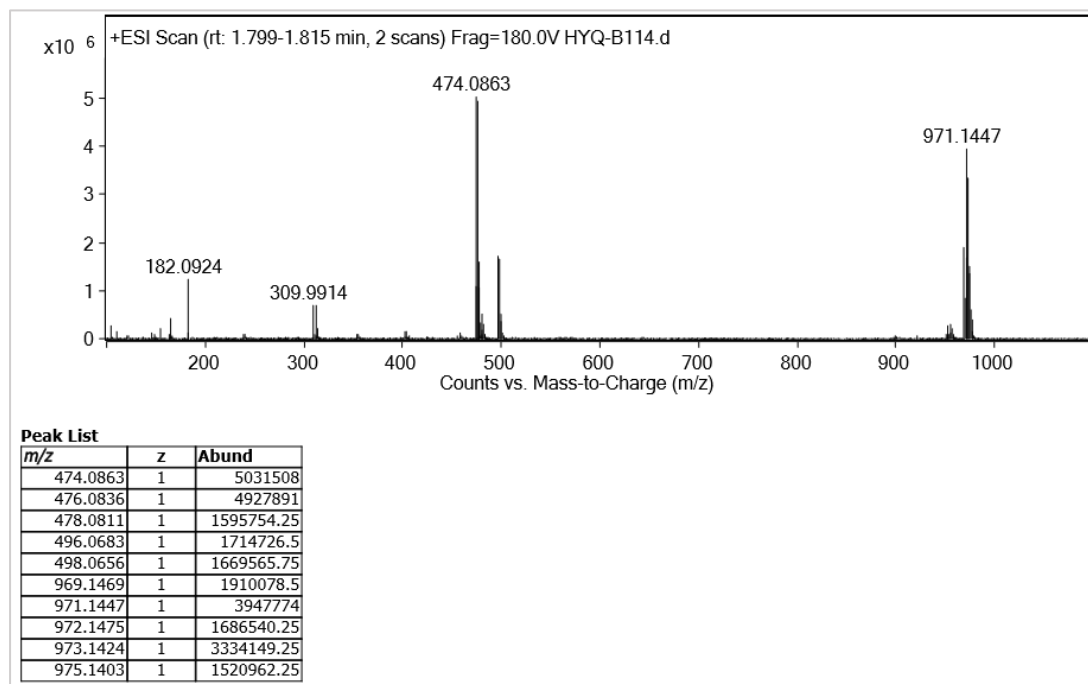
Compound 23



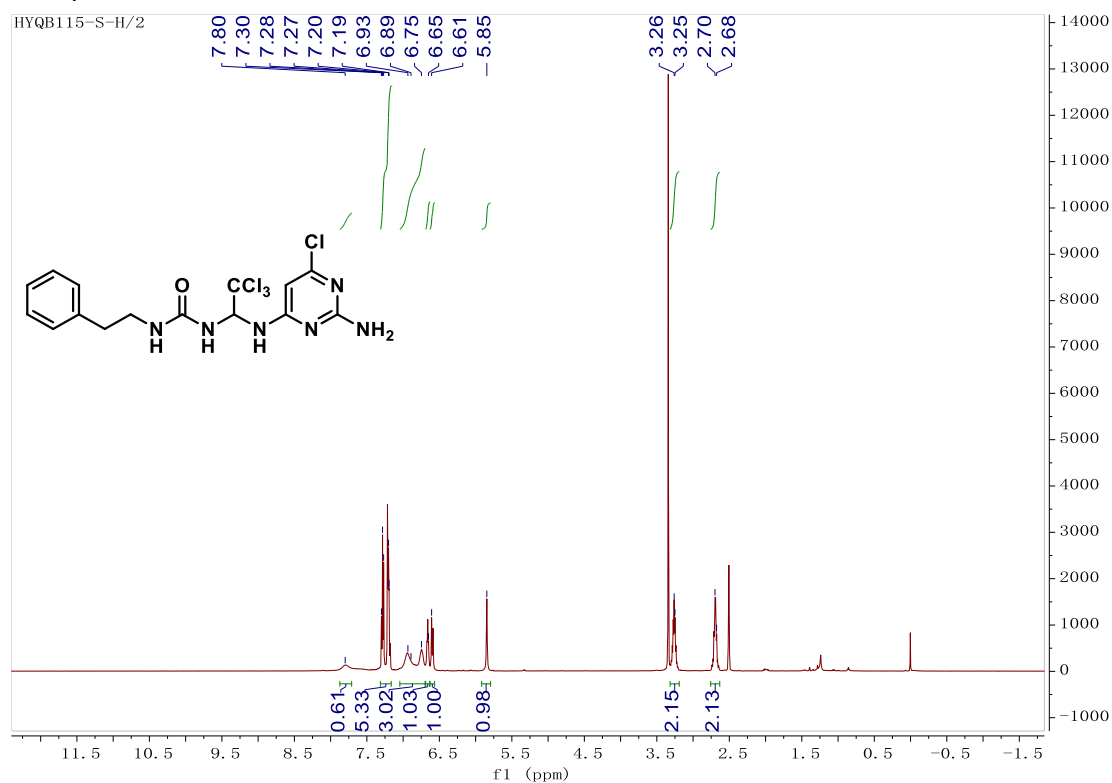


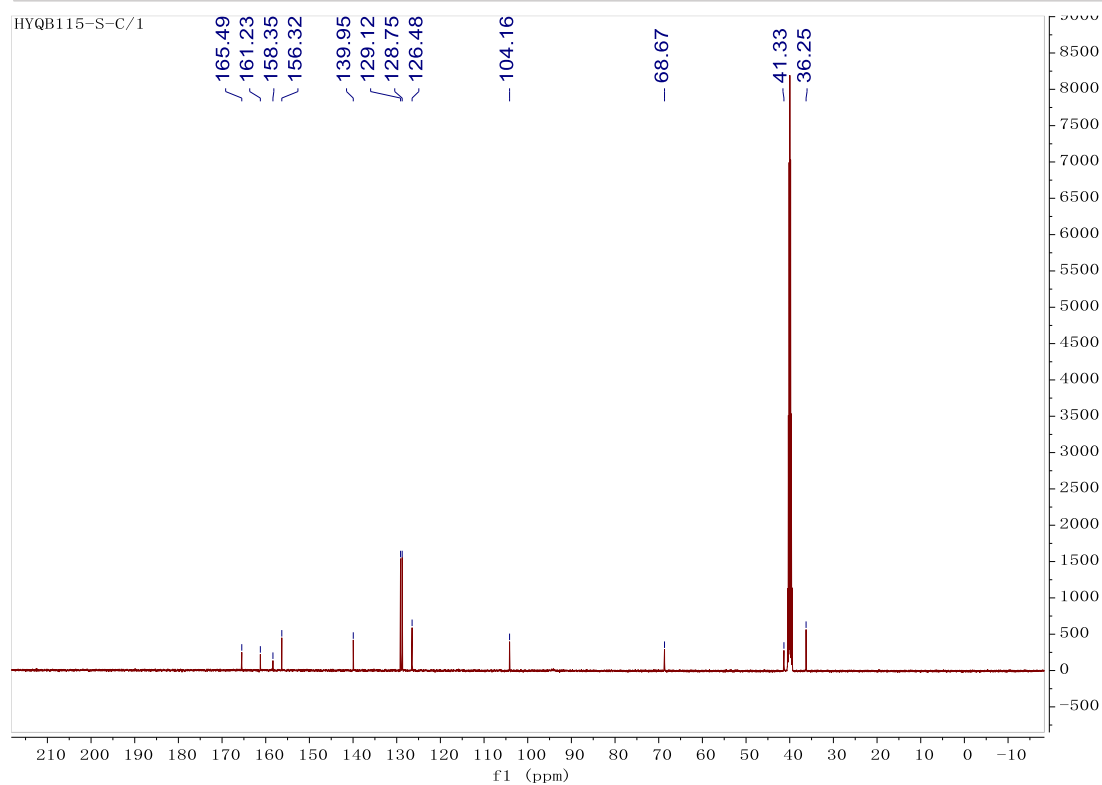
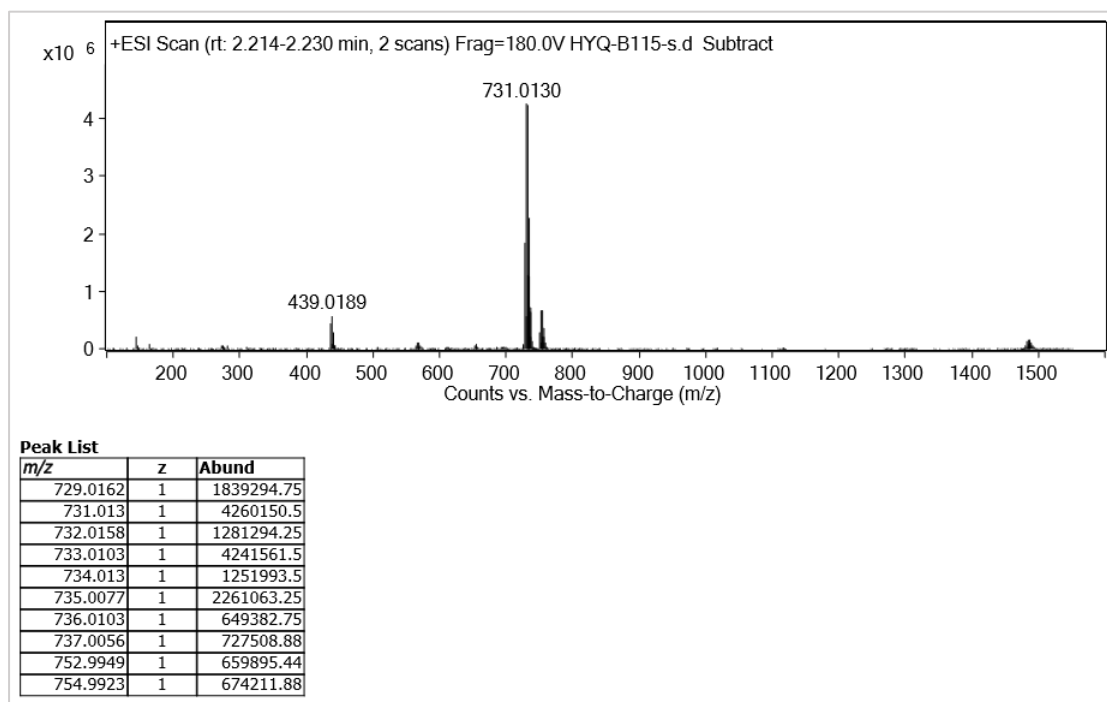
Compound24

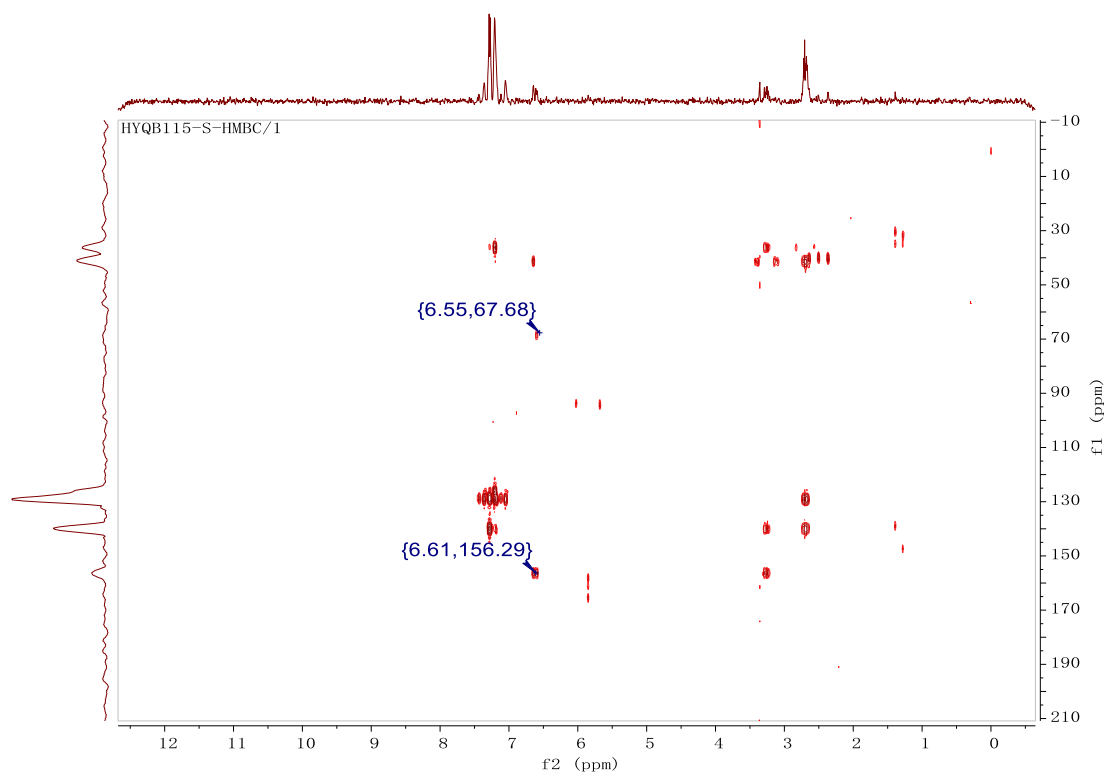




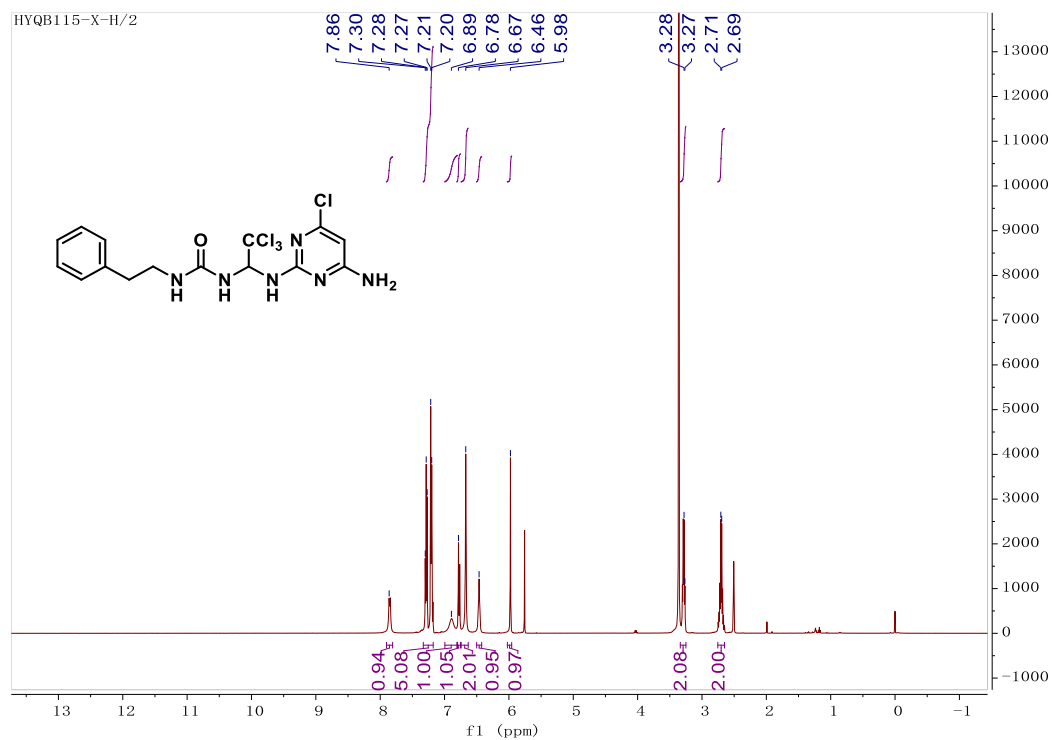
Compound 25

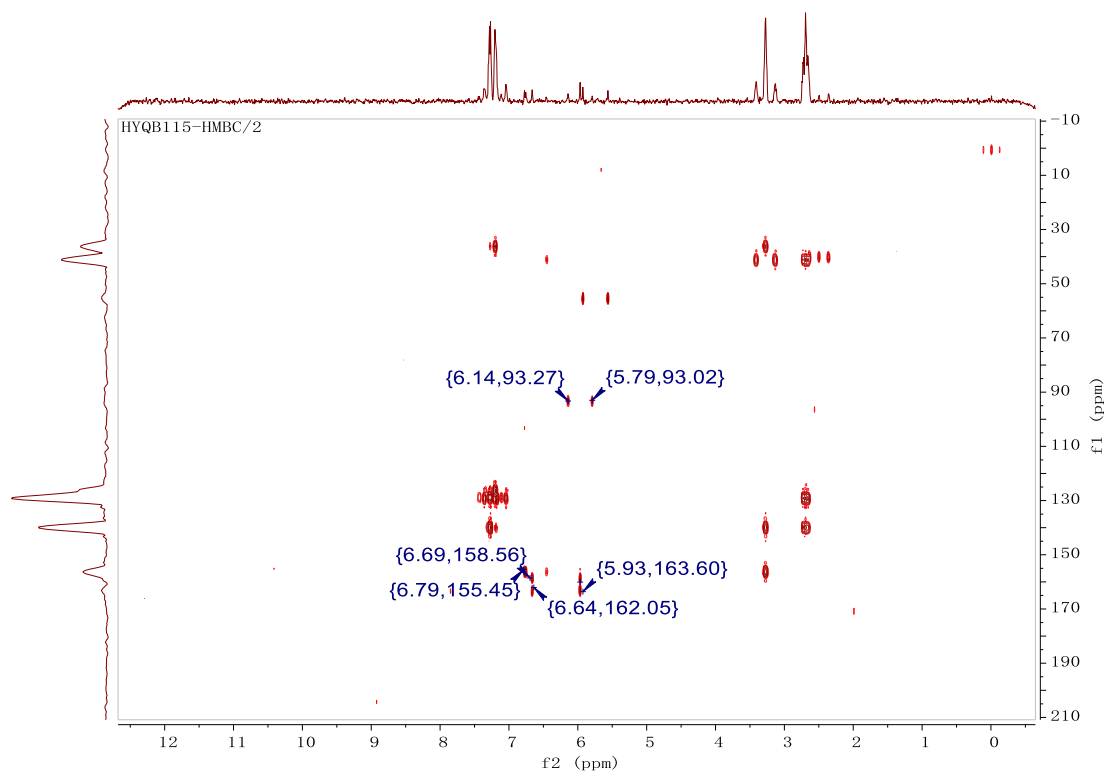
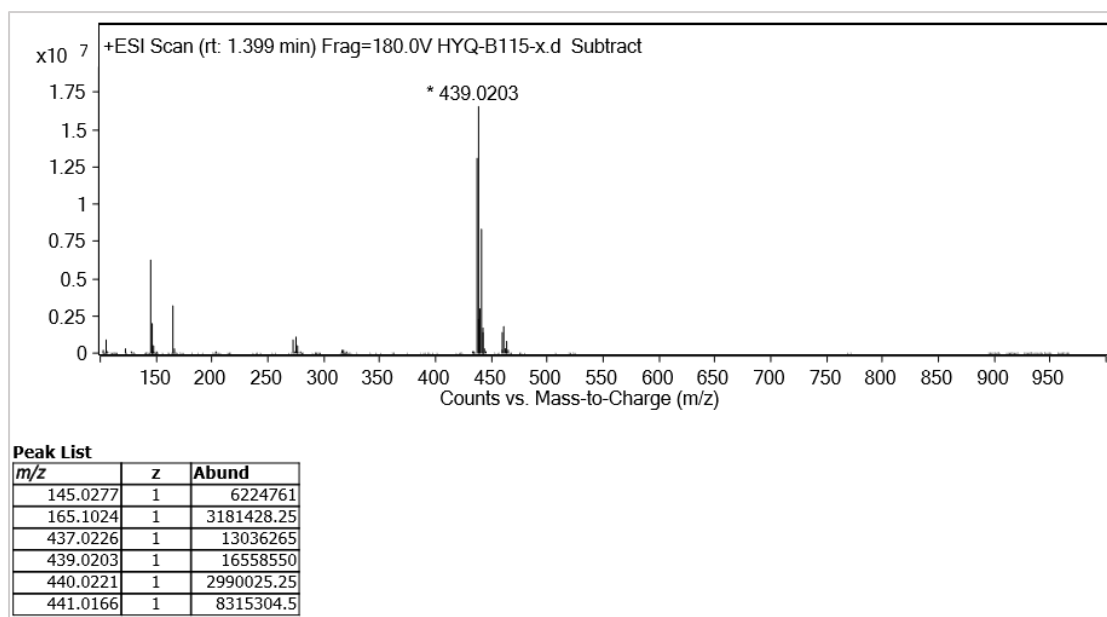




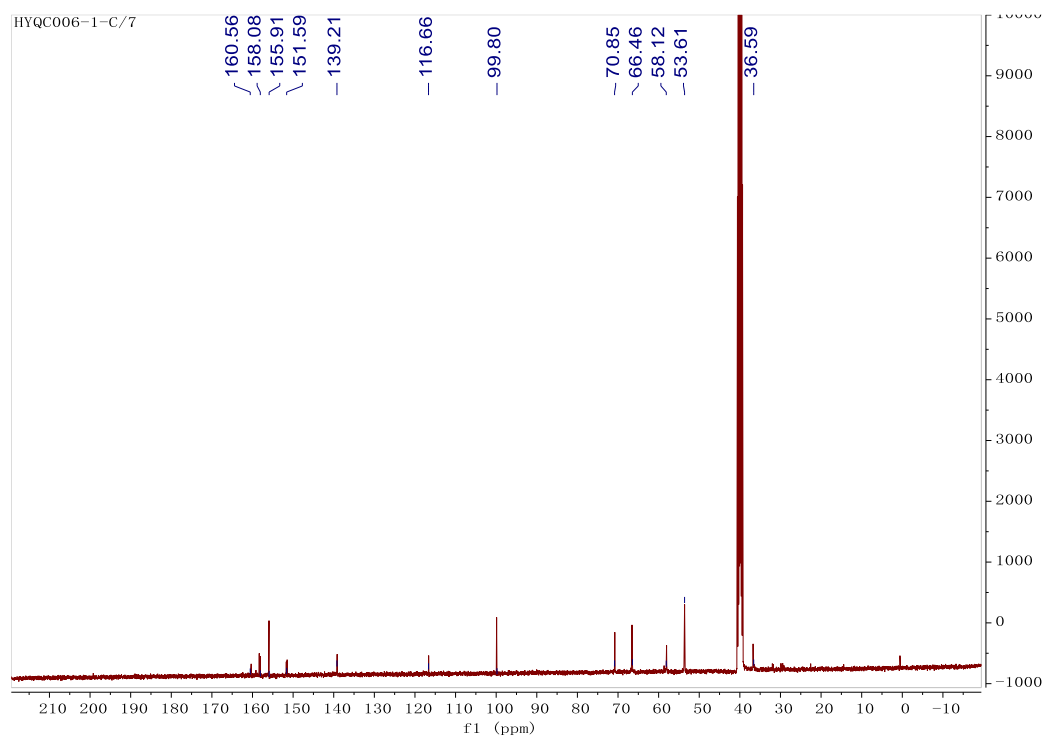
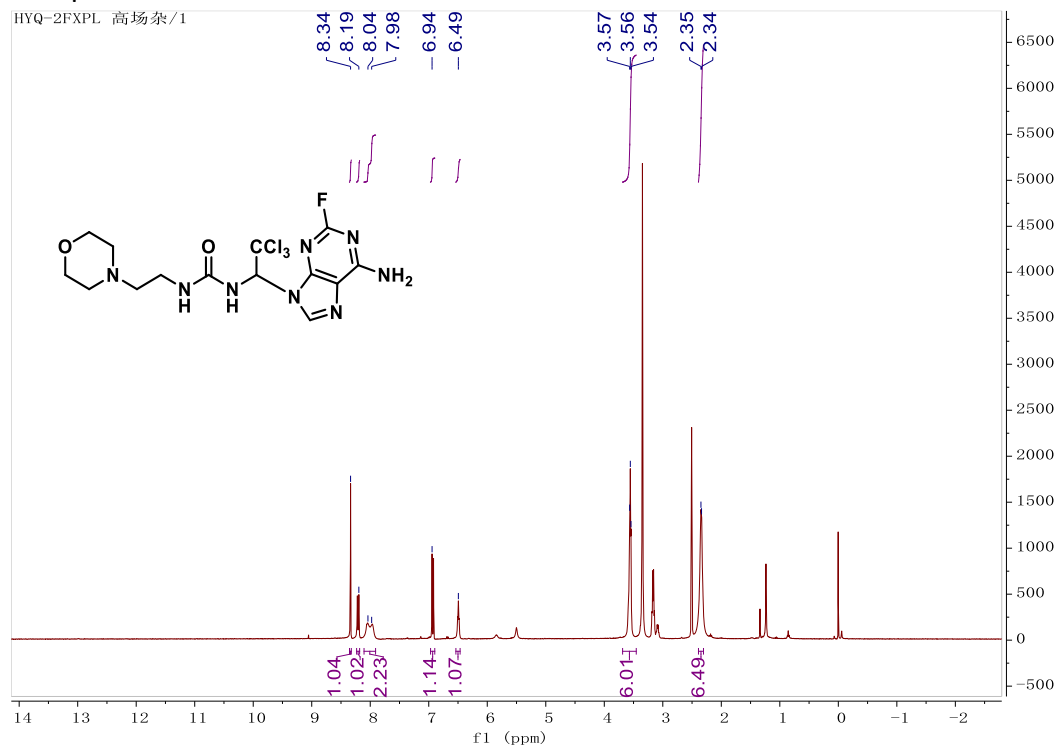


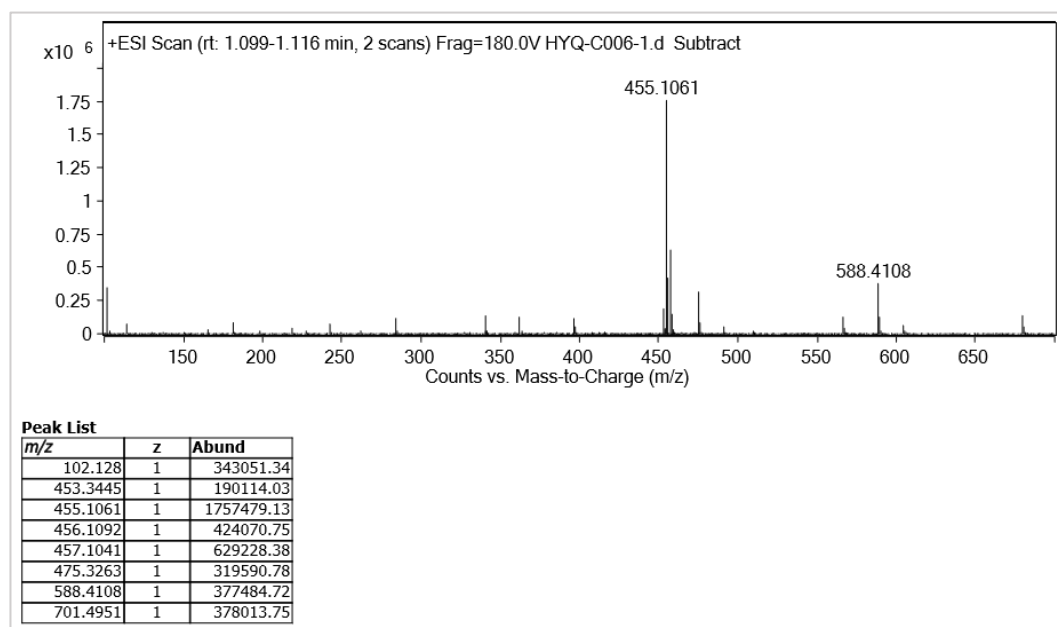
Compound 26



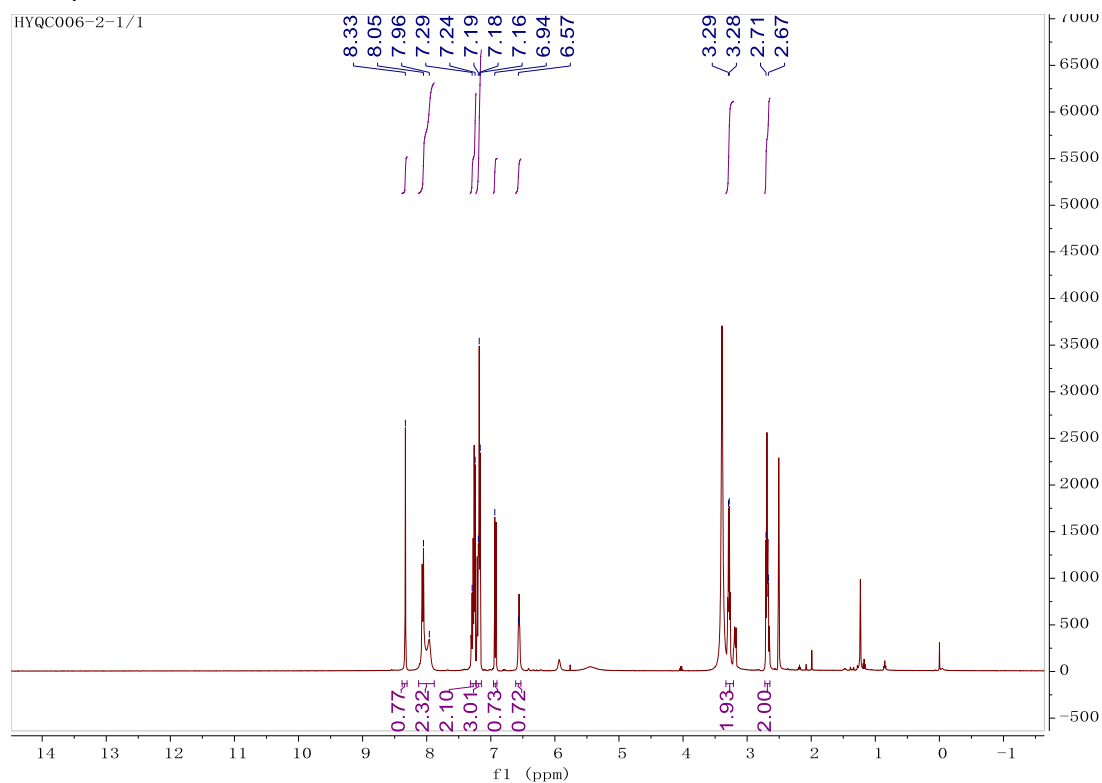


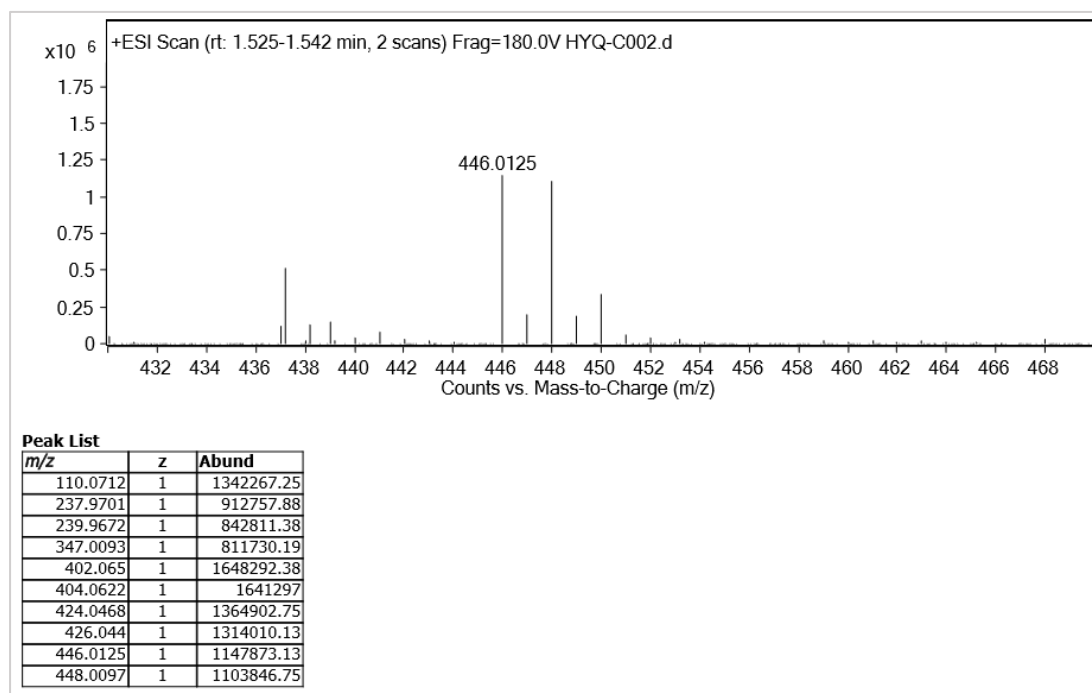
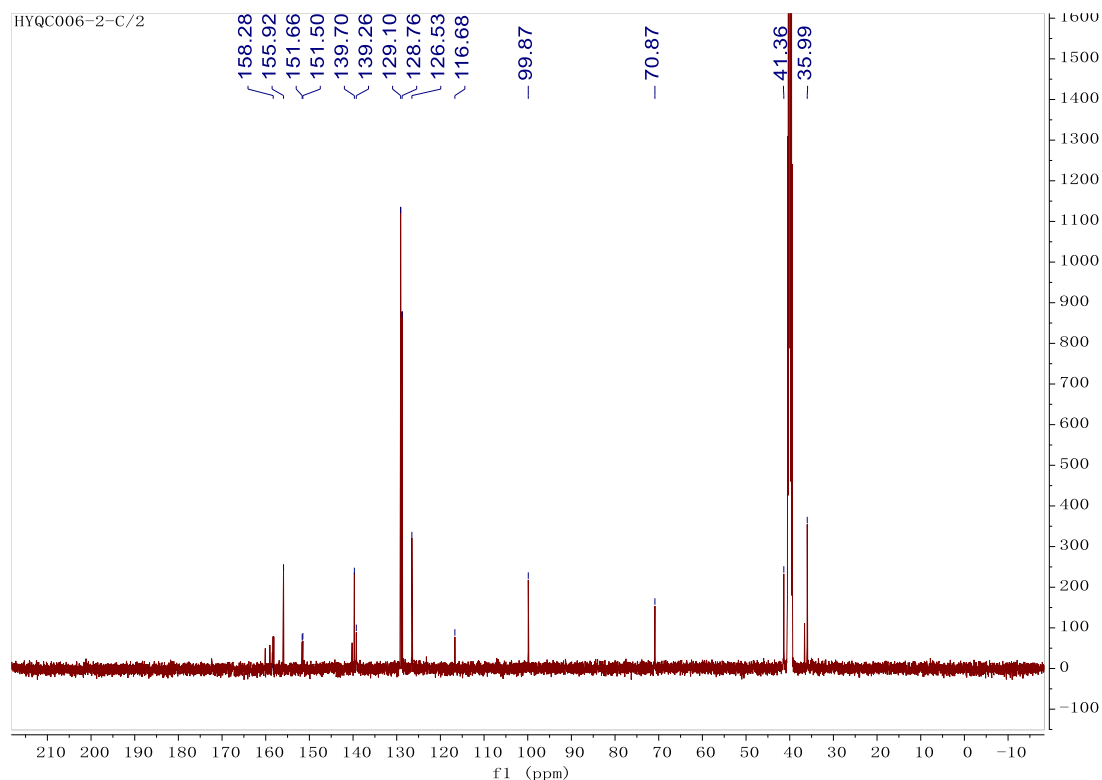
Compound 27



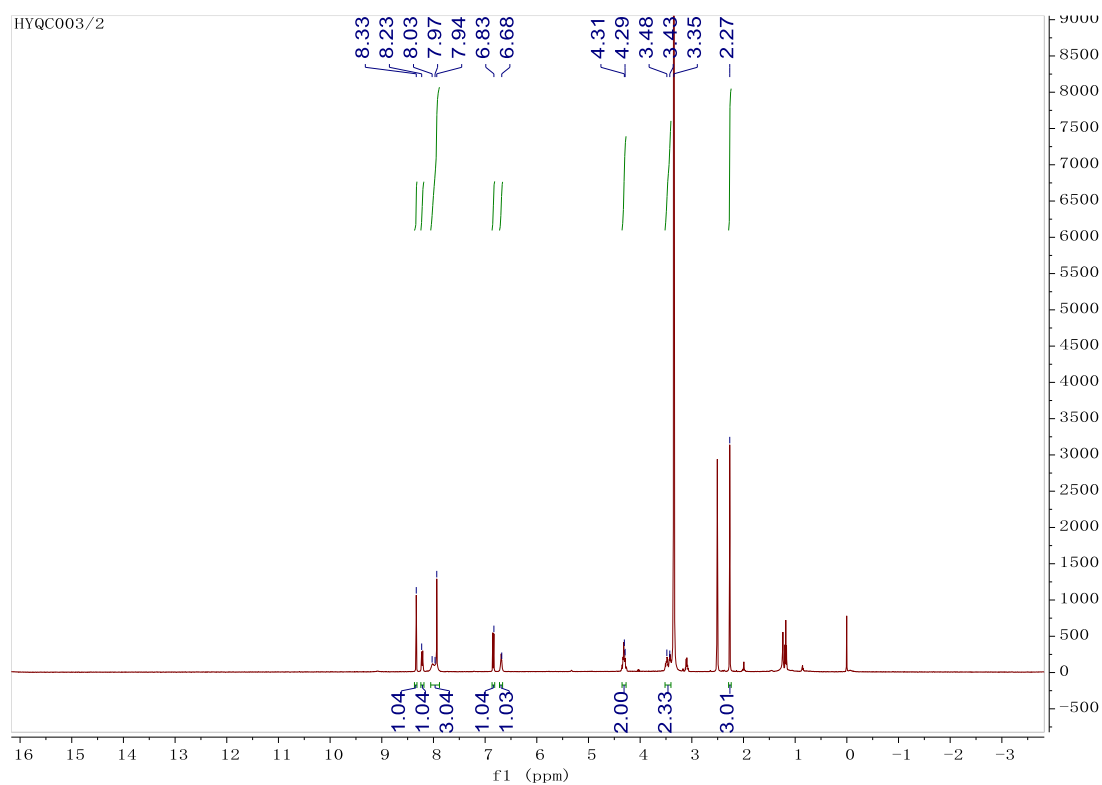
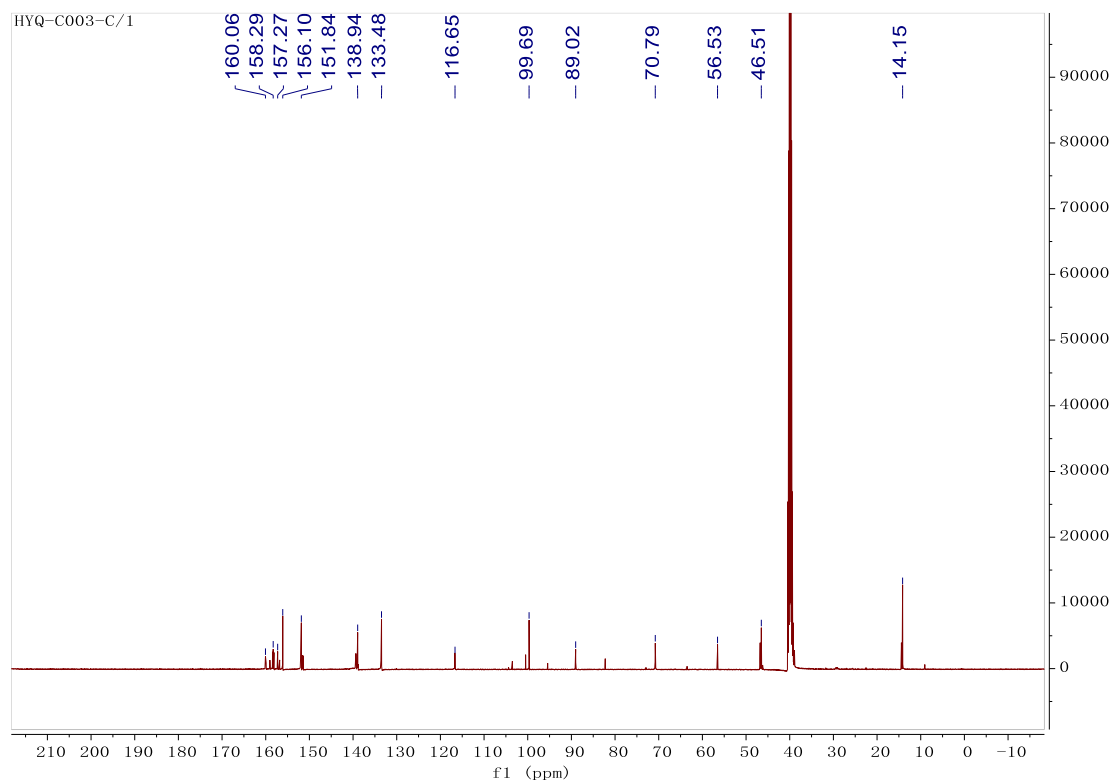


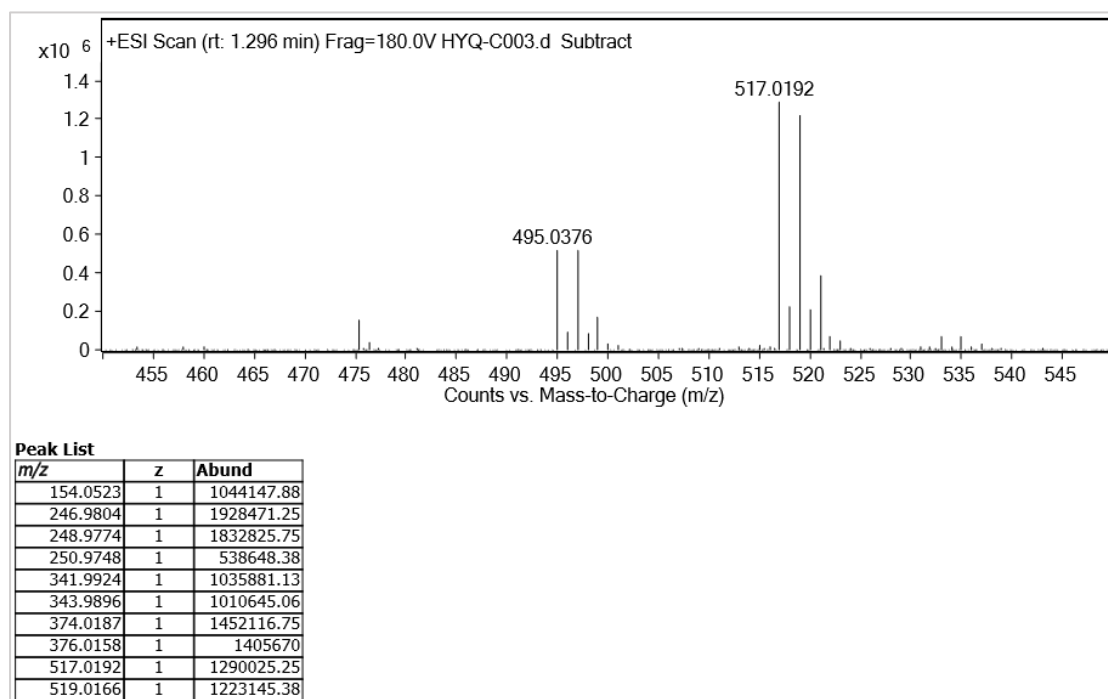
Compound 28





Compound 29





Compound 30

