

Supporting information

Design, synthesis and biological evaluation of novel pteridinone derivatives possessing a sulfonyl moiety as potent dual inhibitors of PLK1 and BRD4

Fei Chen, Yu Wang, Zhanfeng Gao, Shihui Wang, Jiuyu Liu, Xinhua Cui, Yuehan Wang, Zhiwei Li, Mingze Qin, Yajing Liu, Ping Gong, Yanfang Zhao, Yunlei Hou*

^a*School of Pharmaceutical Engineering, Shenyang Pharmaceutical University, 103 Wenhua Road, Shenhe District, Shenyang, 110016, China.*

Mass, ¹H NMR and ¹³C NMR spectrum of compounds

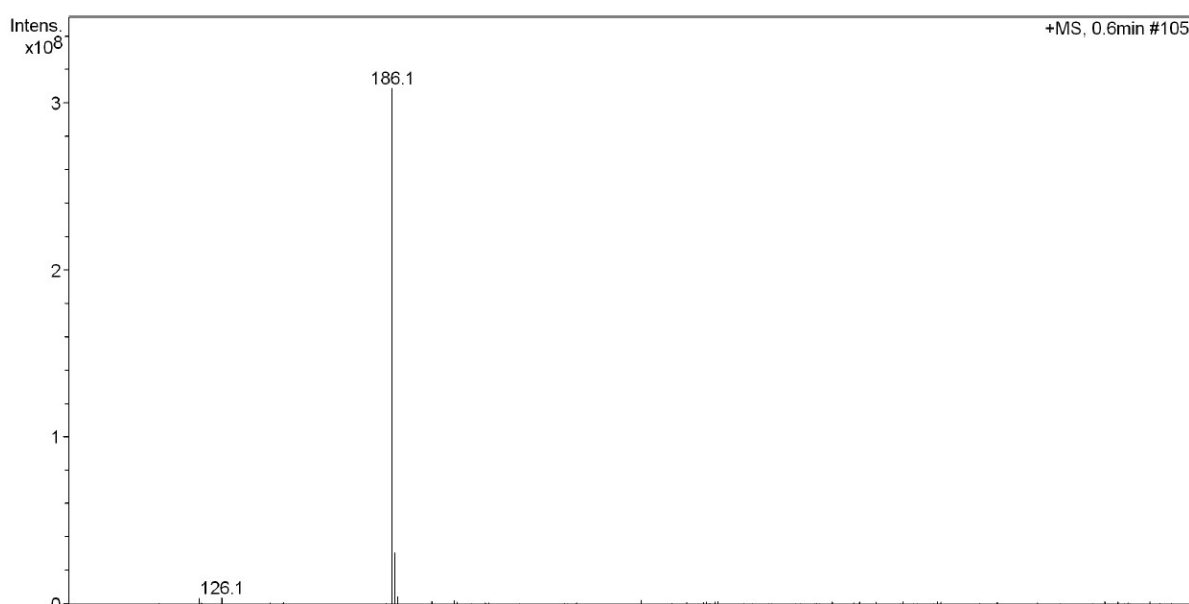


Fig. 1 Mass spectrum of compound 2

*Corresponding author. E-mail address: houyunlei901202@163.com(Y.L. Hou), yanfangzhao@126.com (Y.F. Zhao), lyjpharm@126.com (Y.J. Liu).

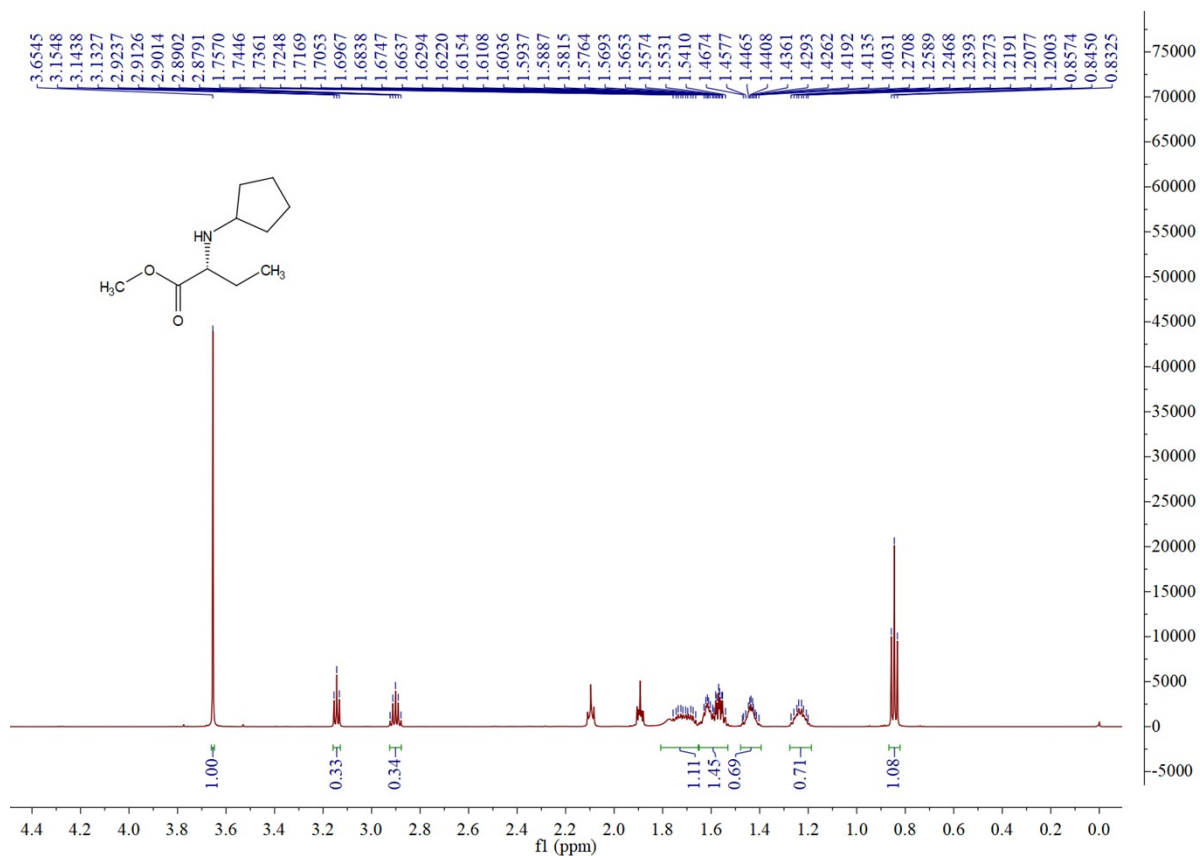


Fig. 2 ¹H NMR spectrum of compound 3

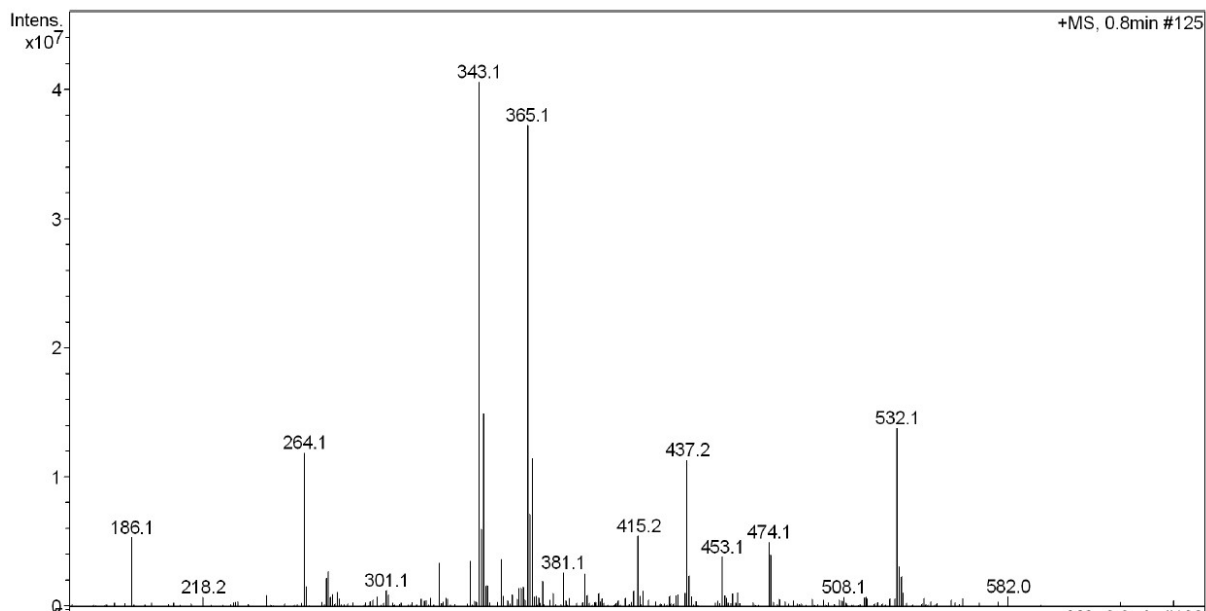


Fig. 3 Mass spectrum of compound 4

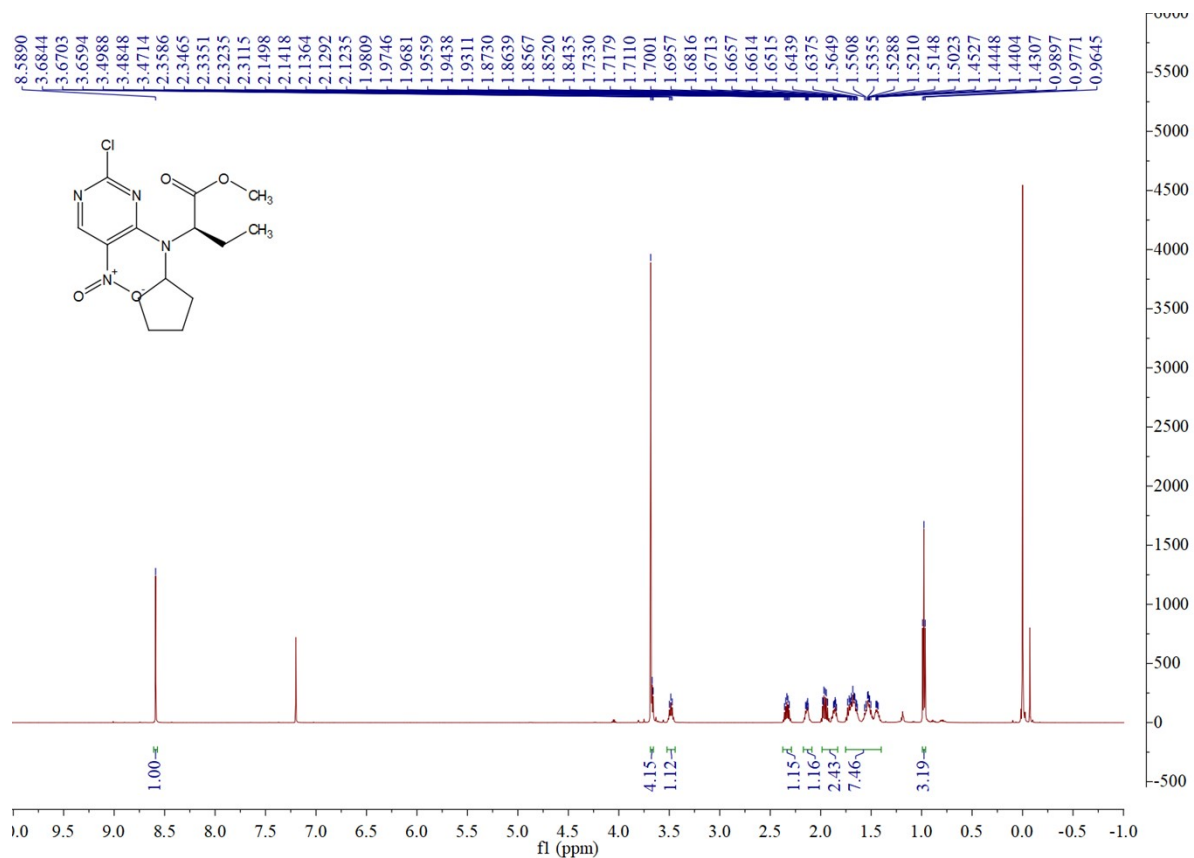


Fig. 4 ^1H NMR spectrum of compound 4

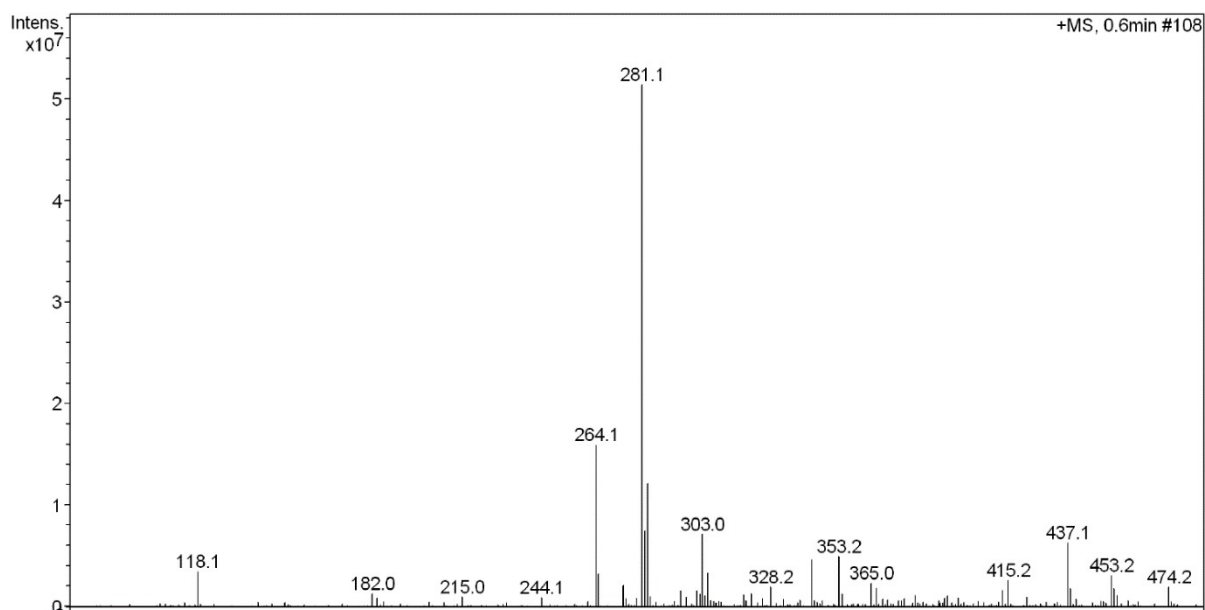


Fig. 5 Mass spectrum of compound 5

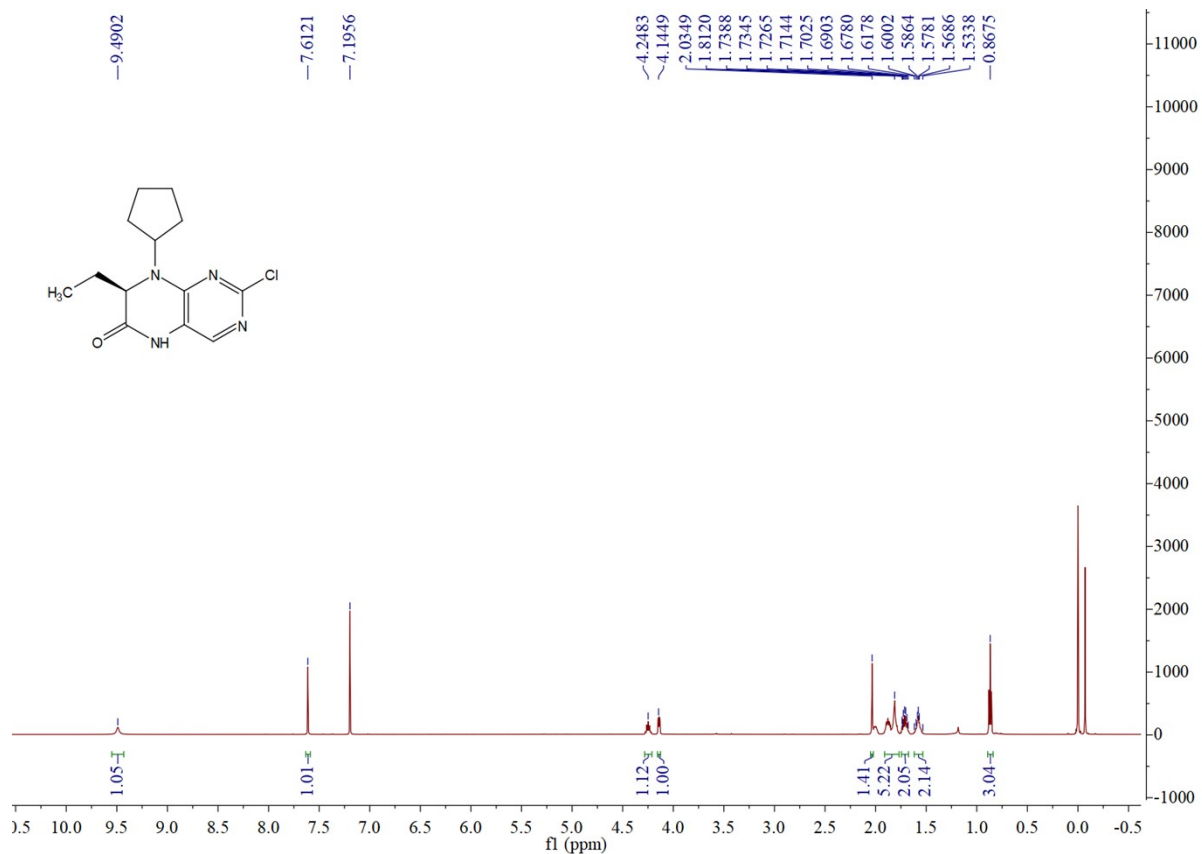


Fig. 6 ^1H NMR spectrum of compound 5

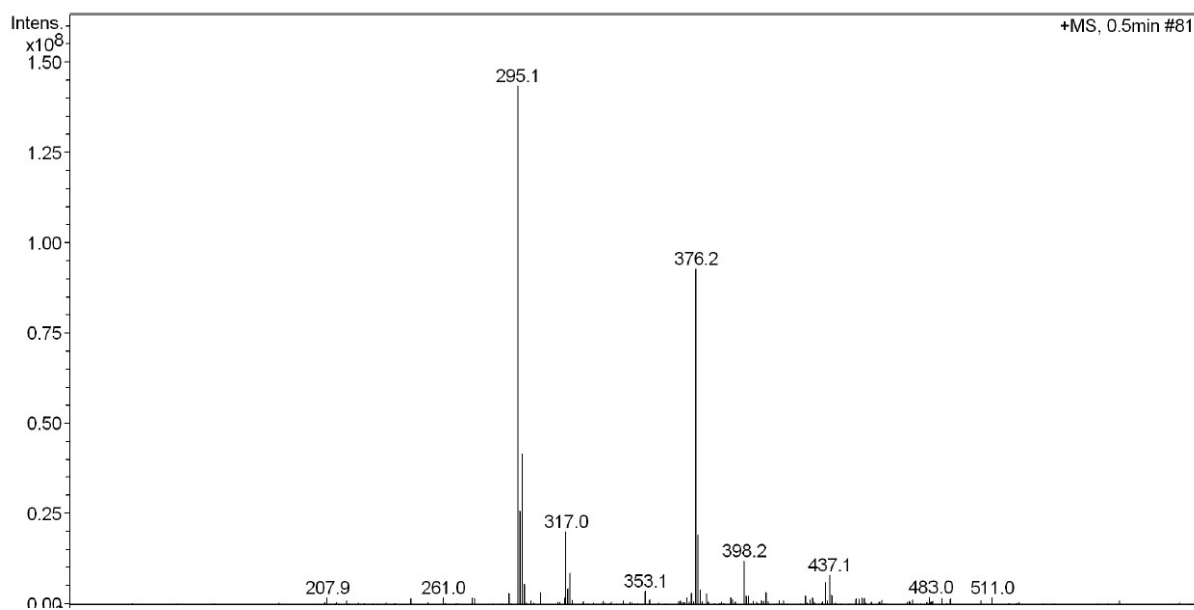


Fig. 7 Mass spectrum of compound 6

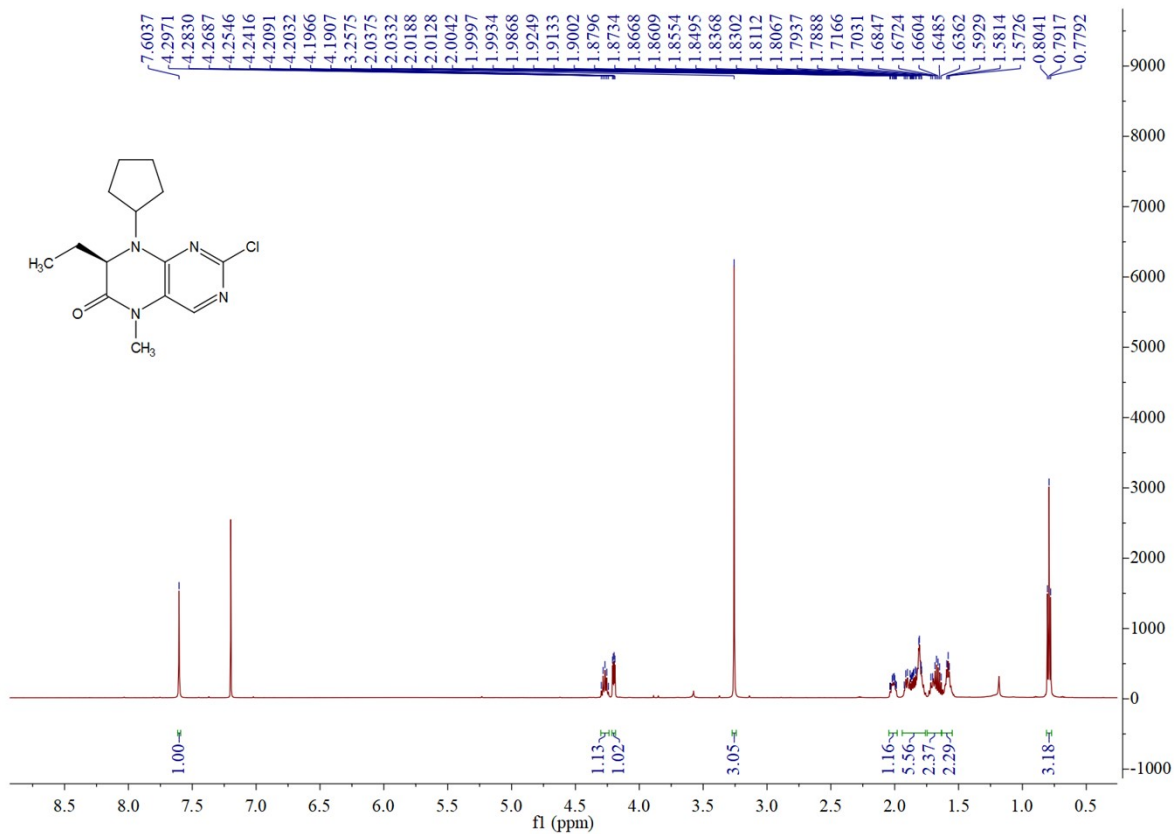
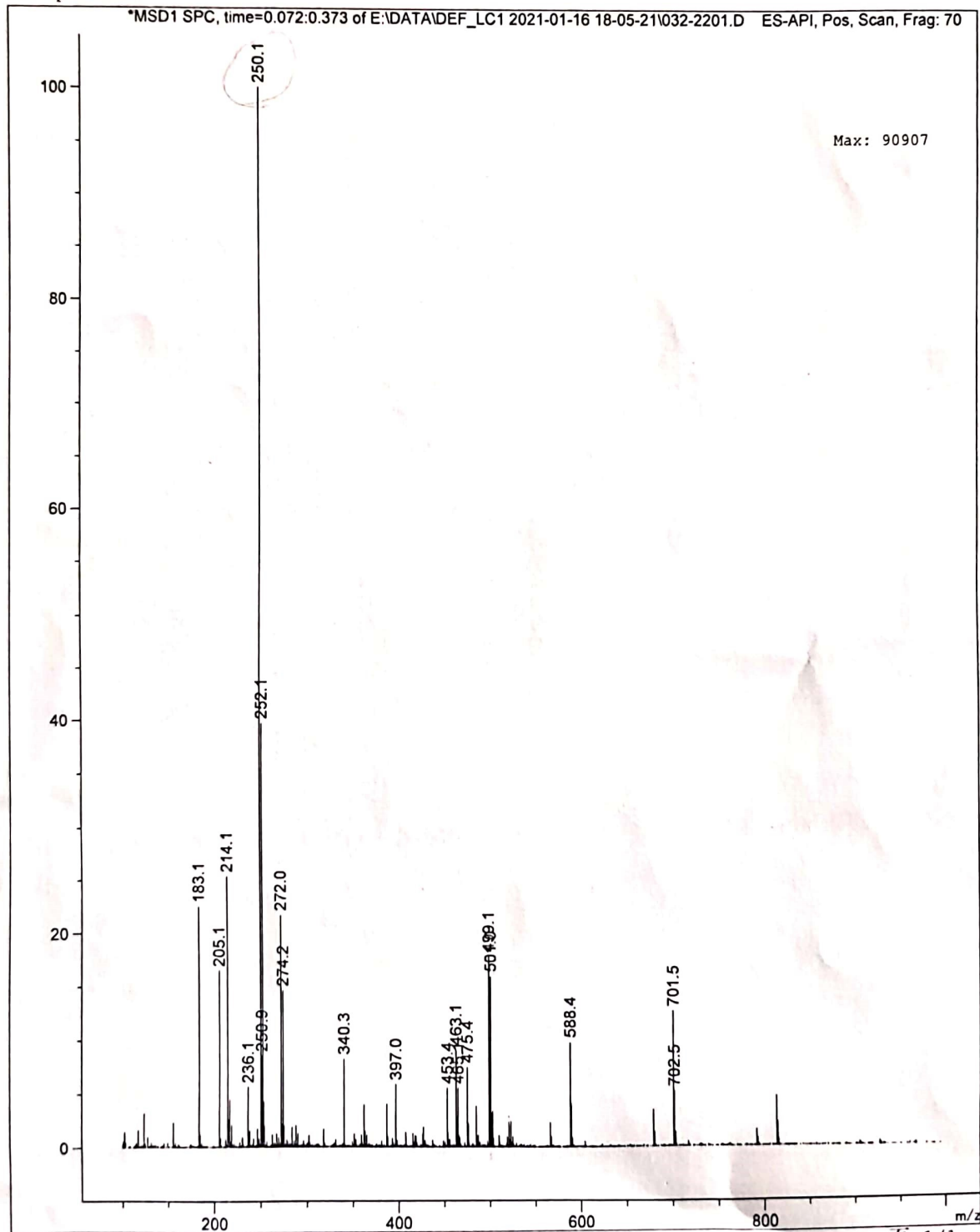


Fig. 8 ¹H NMR spectrum of compound 6

MS Spectrum



1 2021/1/16 23:00:53

页 1/1

Fig. 9 Mass spectrum of compound 11

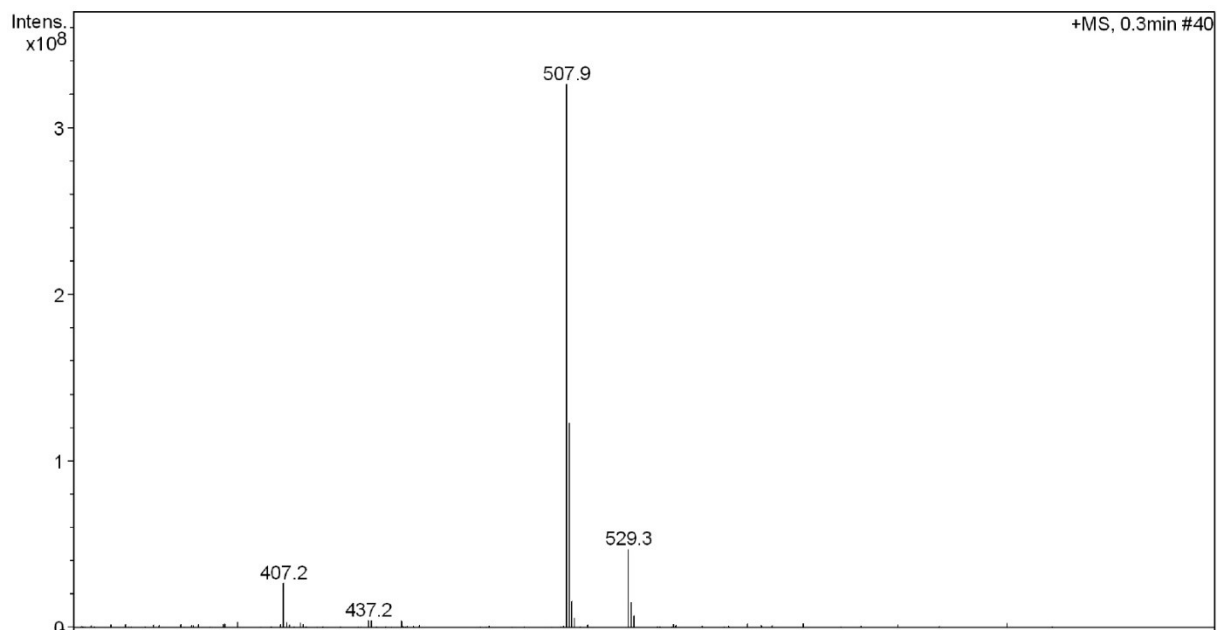


Fig. 10 Mass spectrum of compound 12

MS Spectrum

*MSD1 SPC, time=0.072:0.346 of E:\DATA\DEF_LC1 2021-01-16 18-05-21\029-1901.D ES-API, Pos, Scan, Frag: 70

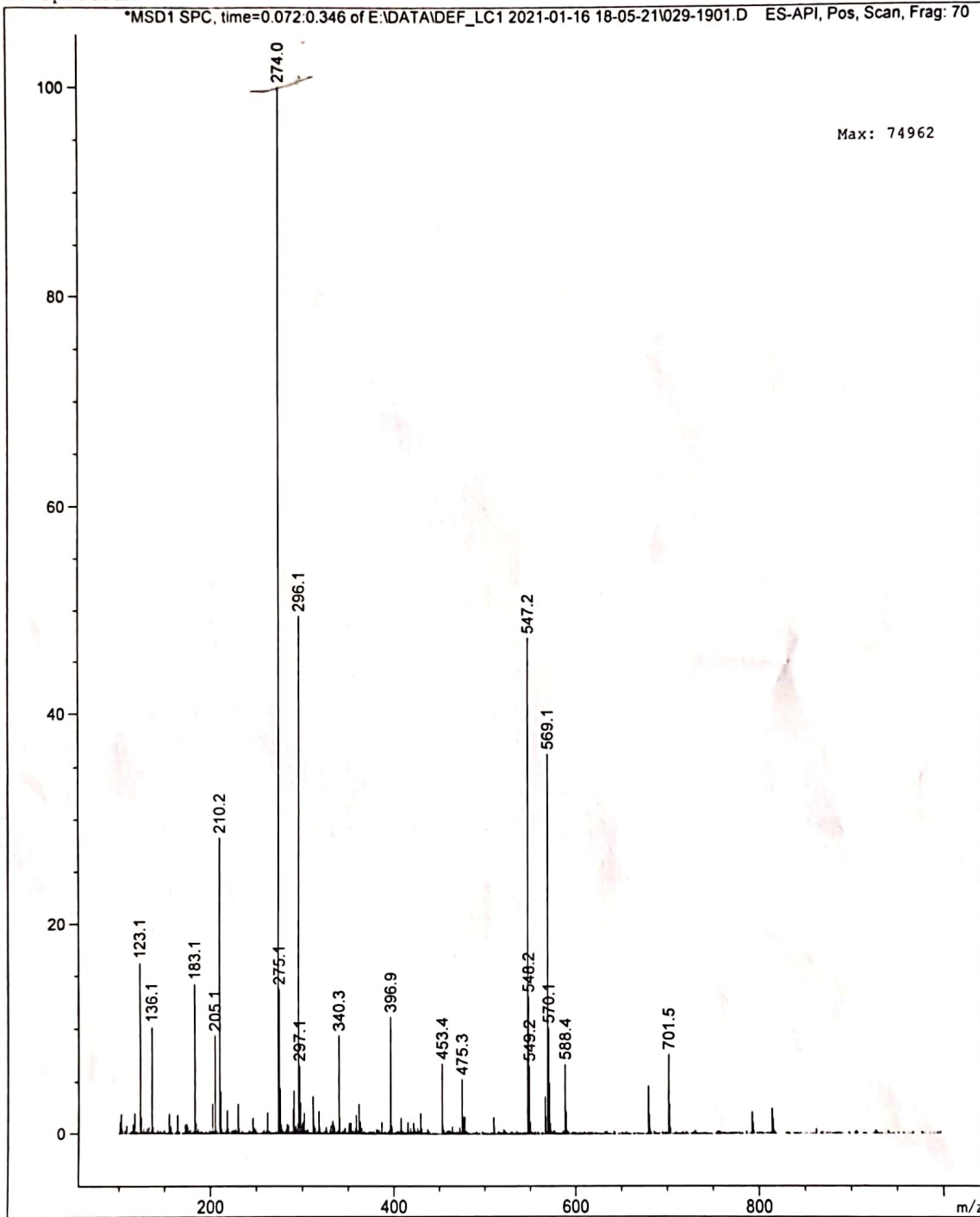


Fig. 11 Mass spectrum of compound 15

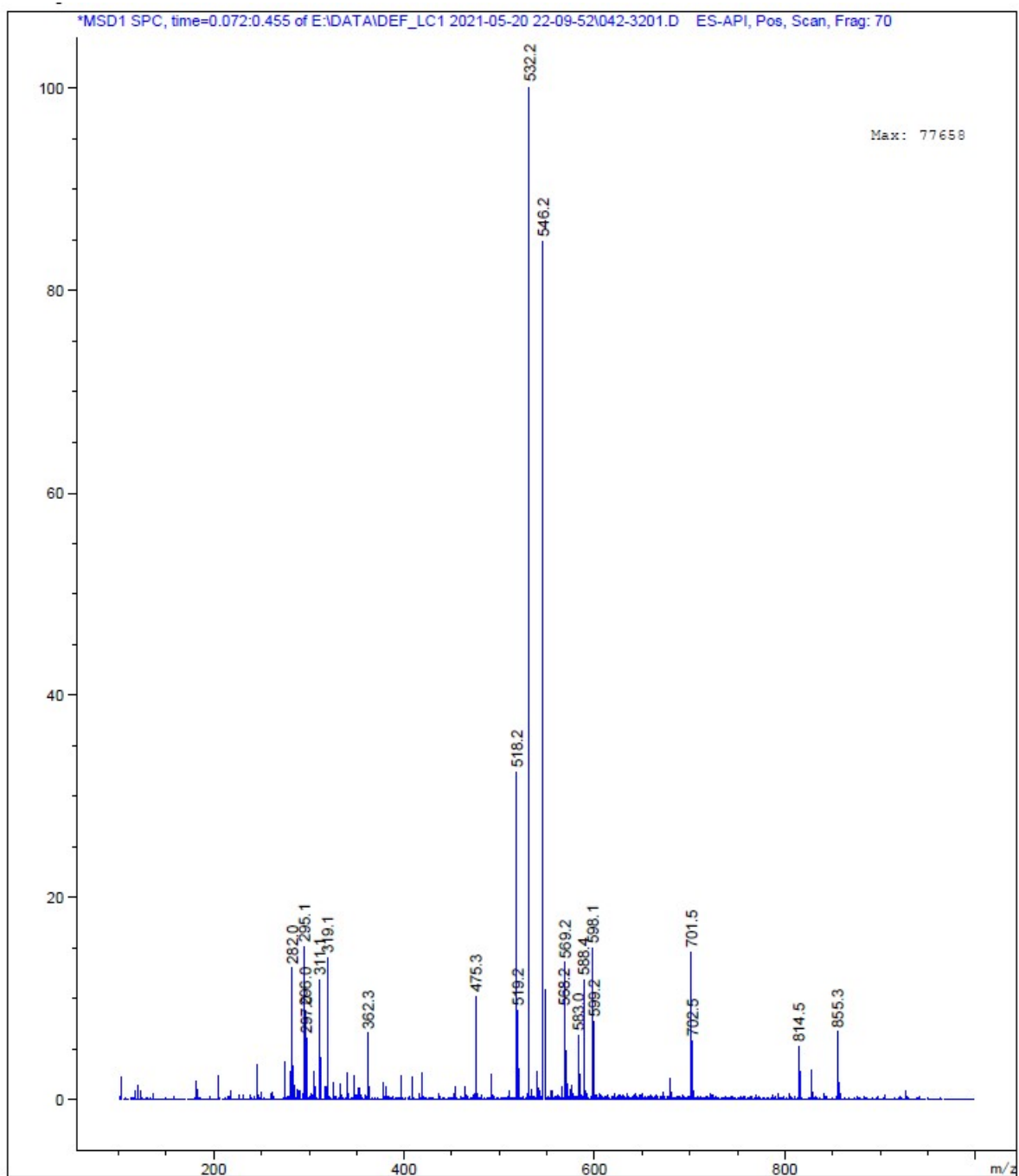


Fig. 12 Mass spectrum of compound 16

MS Spectrum

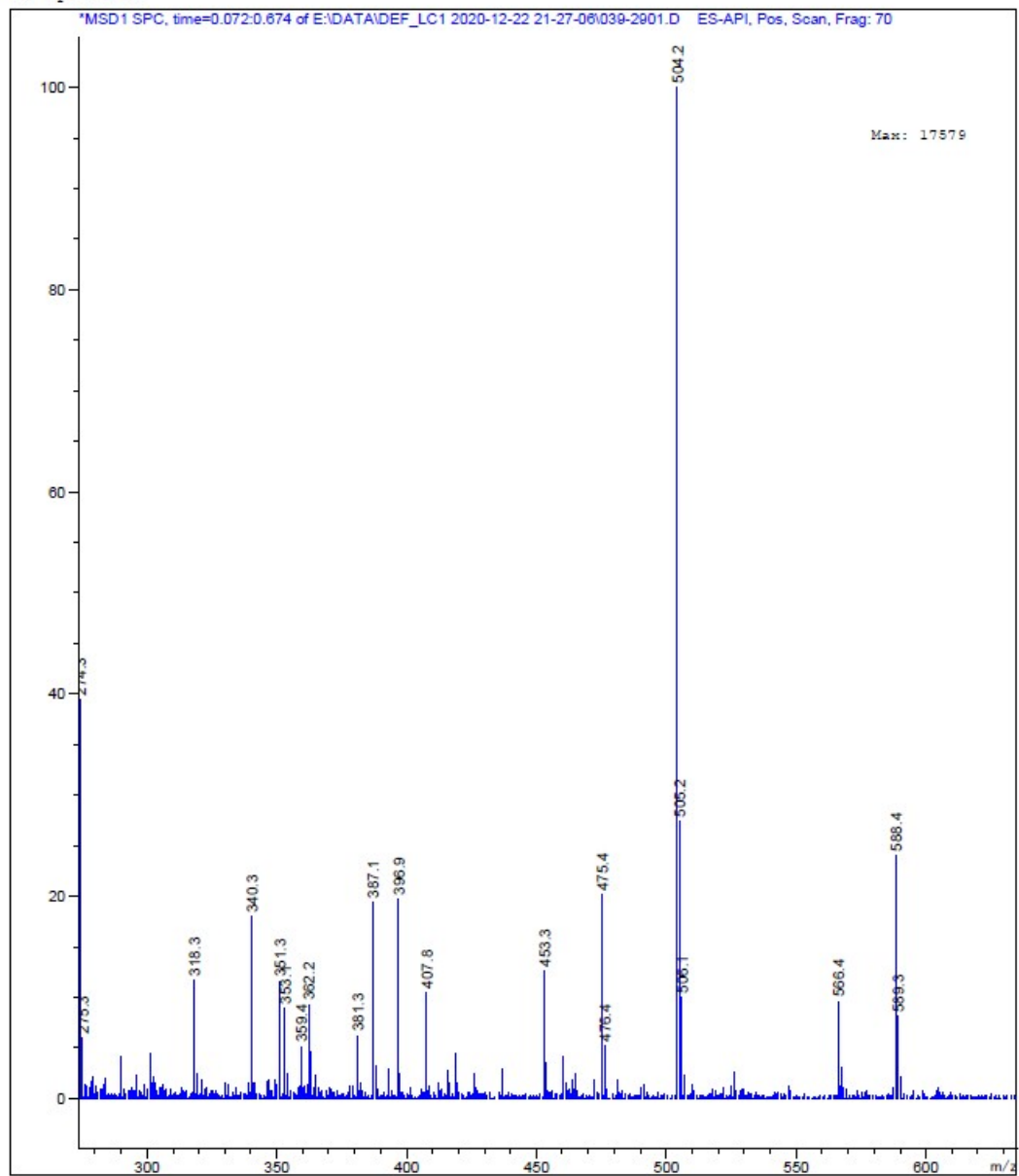


Fig. 13 Mass spectrum of compound 17

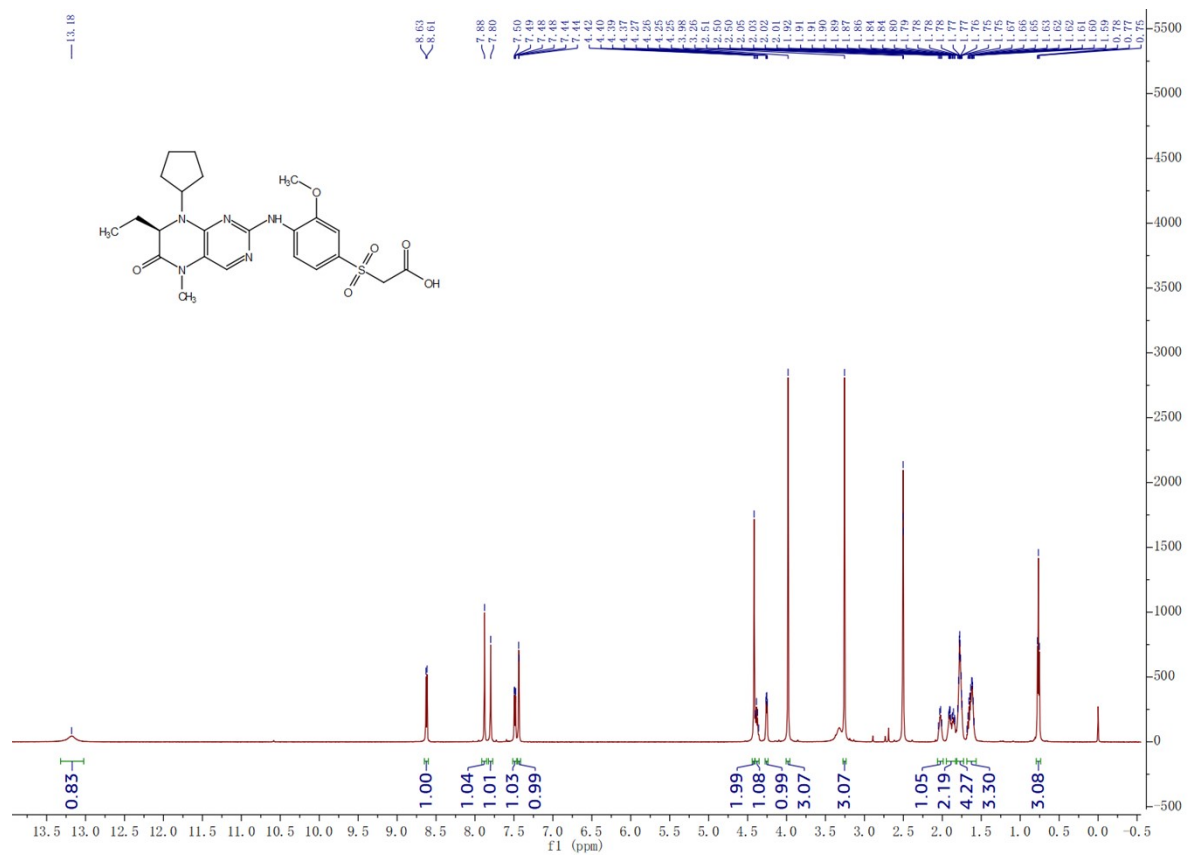


Fig. 14 ^1H NMR spectrum of compound 17

MS Spectrum

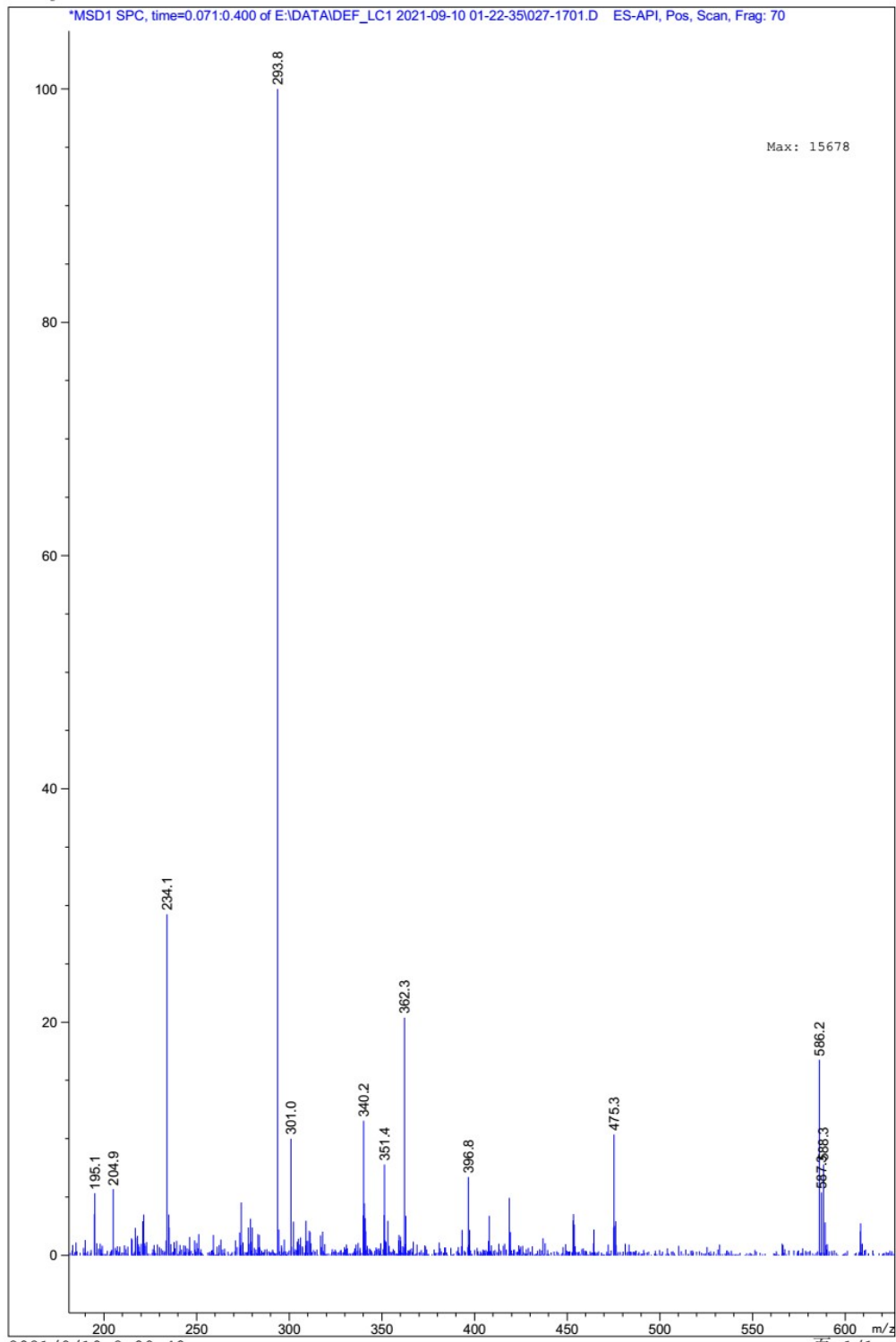


Fig. 15 Mass spectrum of compound A1

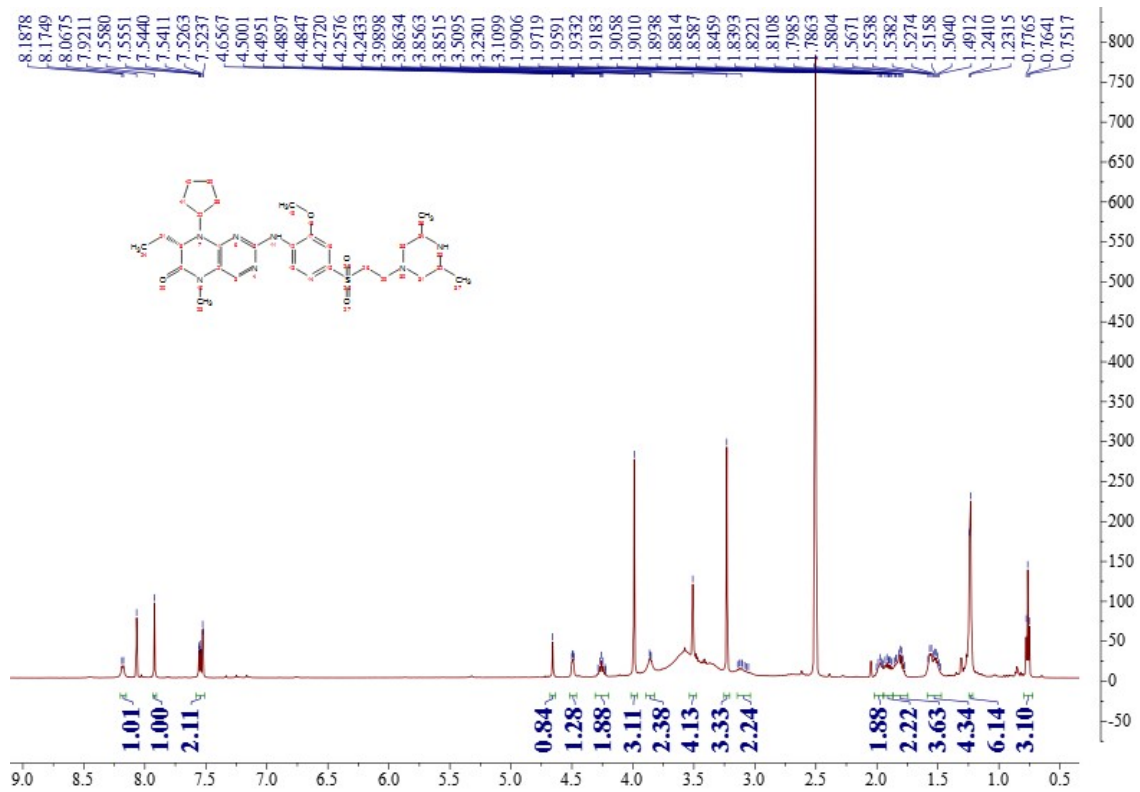


Fig. 16 ^1H NMR spectrum of compound A1

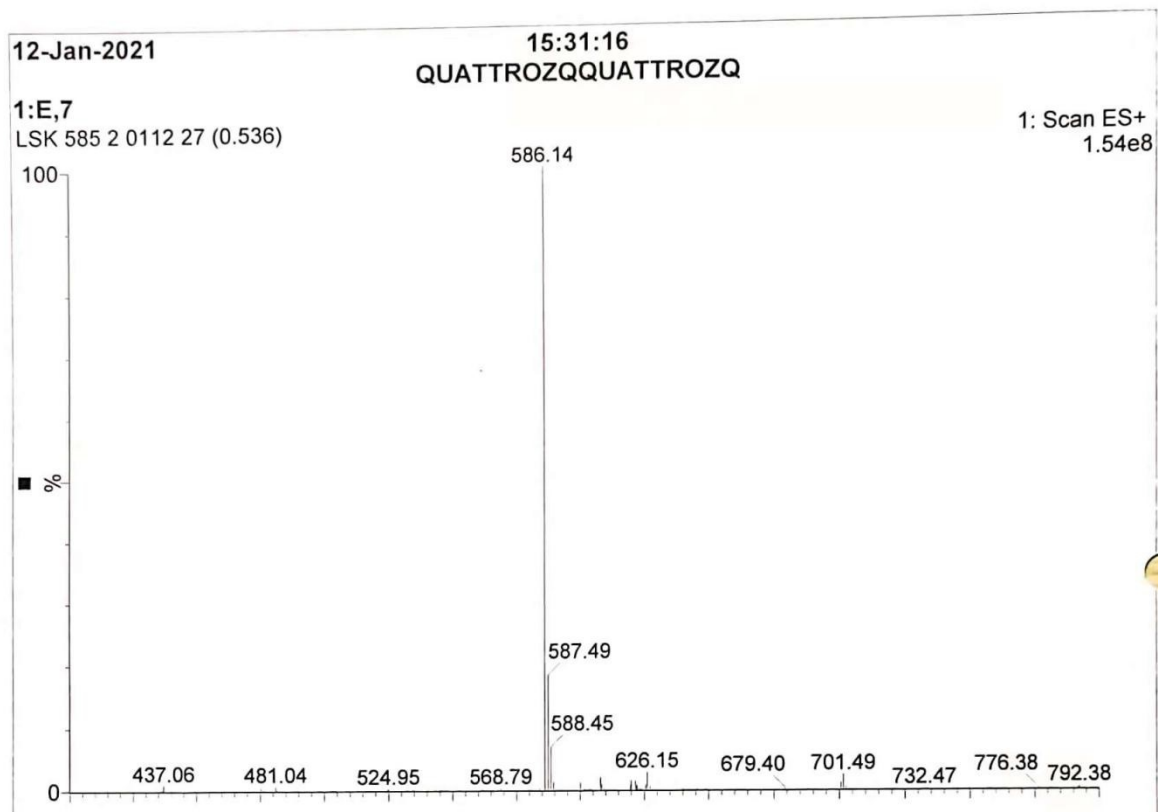


Fig. 17 Mass spectrum of compound A2

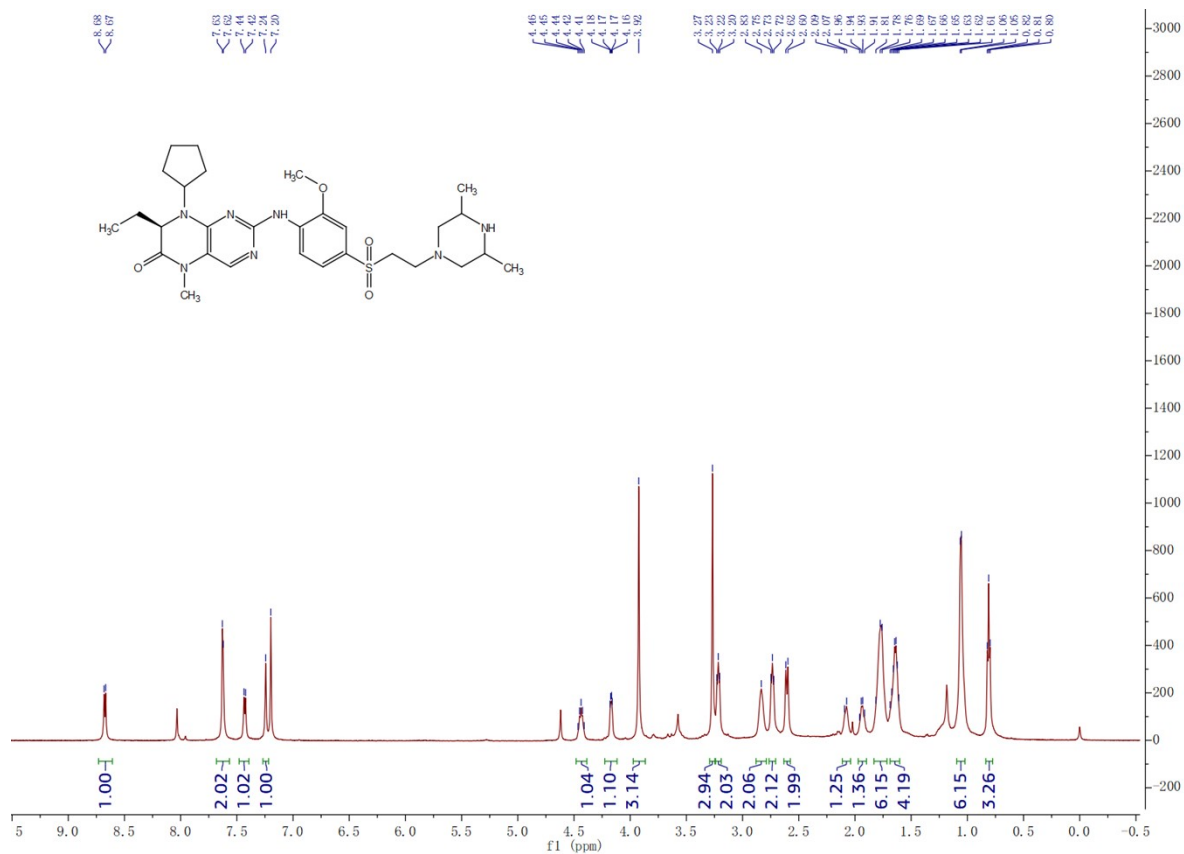


Fig. 18 ^1H NMR spectrum of compound A2

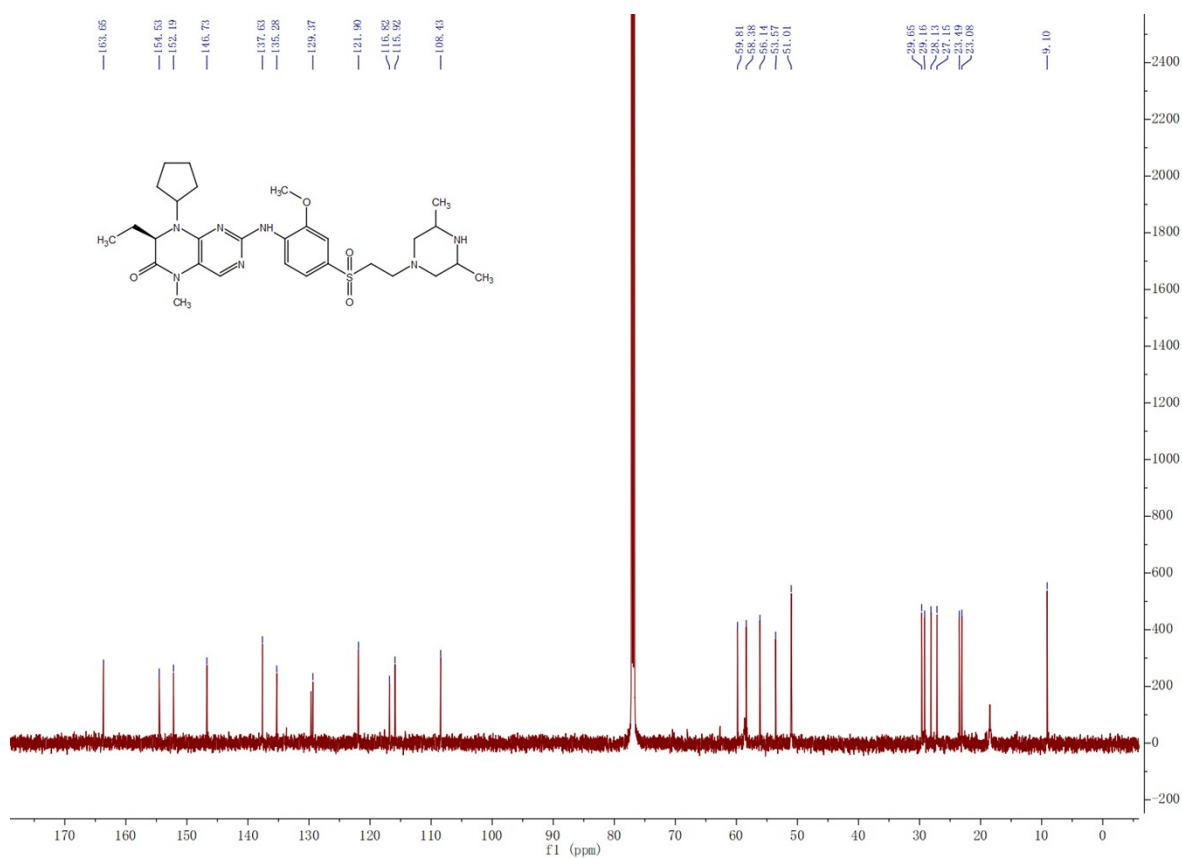


Fig. 19 ^{13}C NMR spectrum of compound A2

MS Spectrum

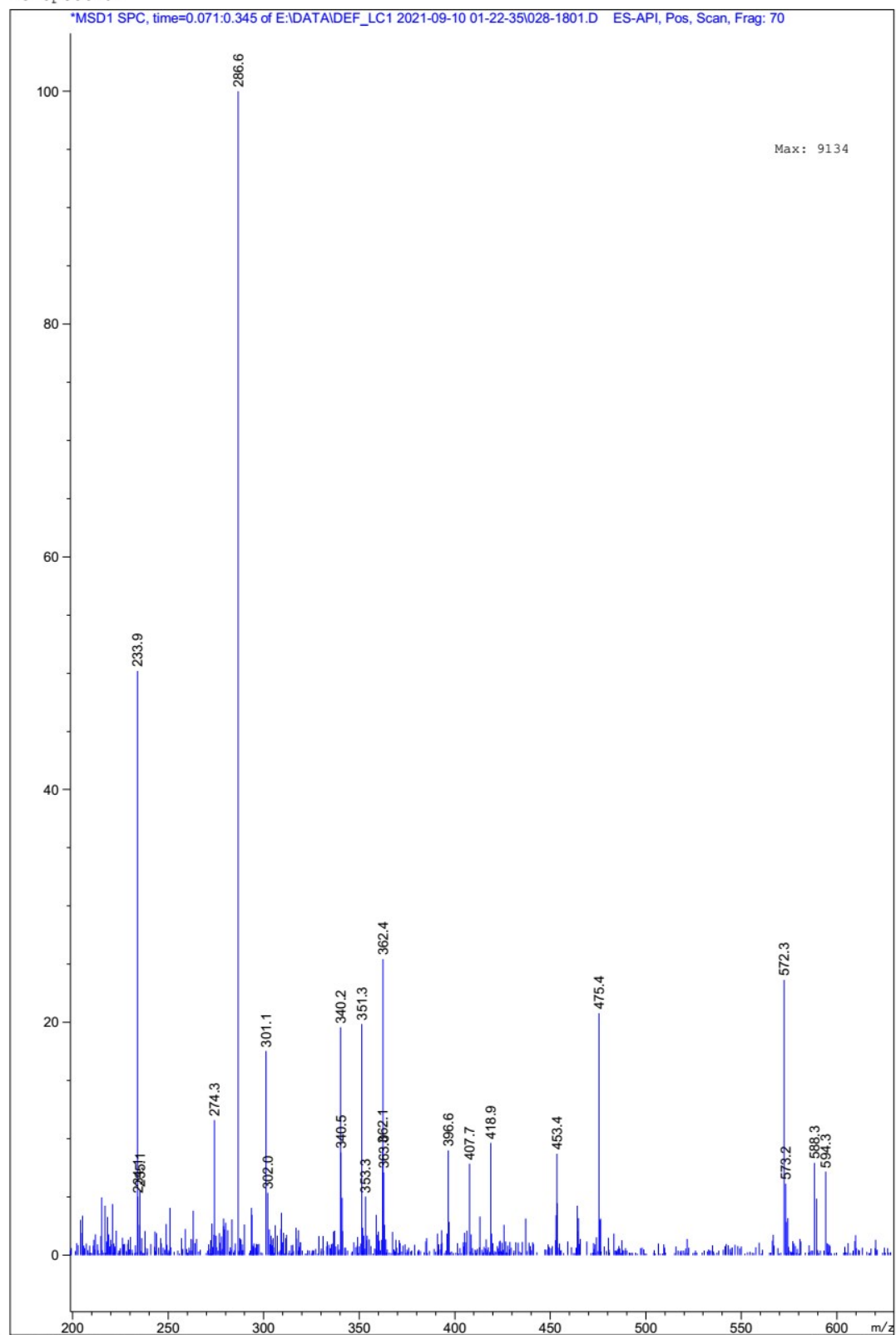


Fig. 20 Mass spectrum of compound A3

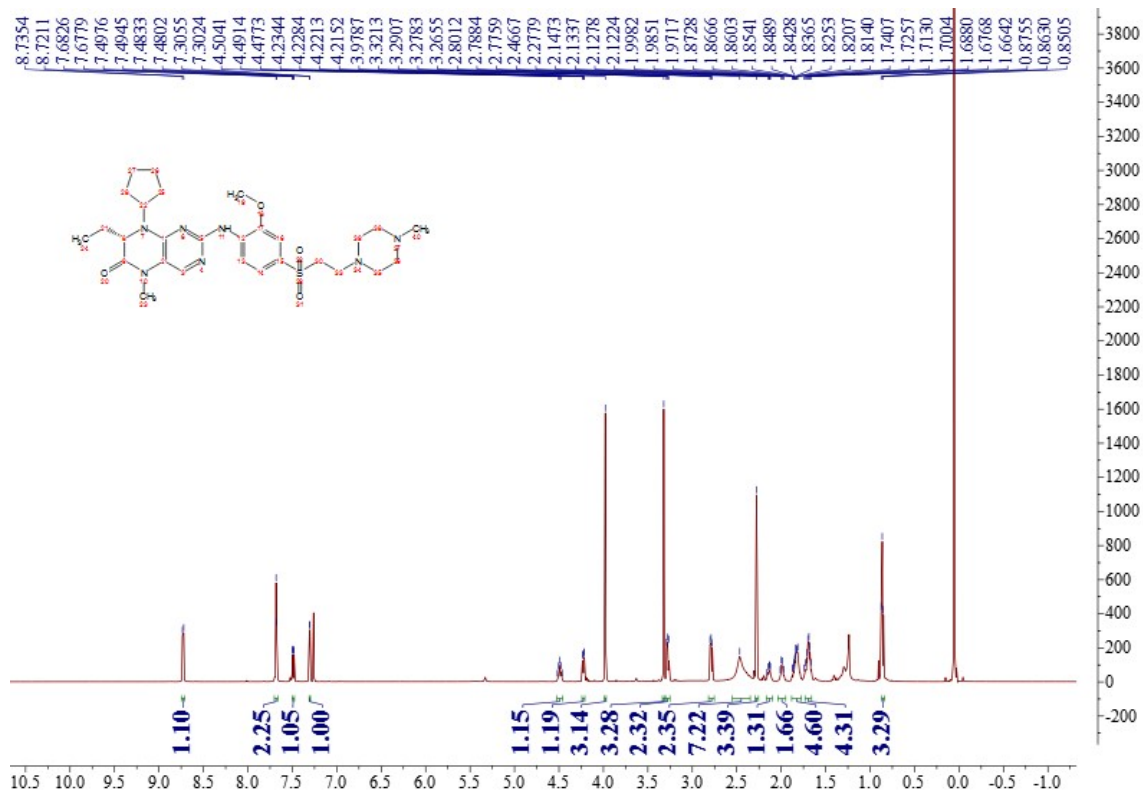


Fig. 21 ^1H NMR spectrum of compound A3

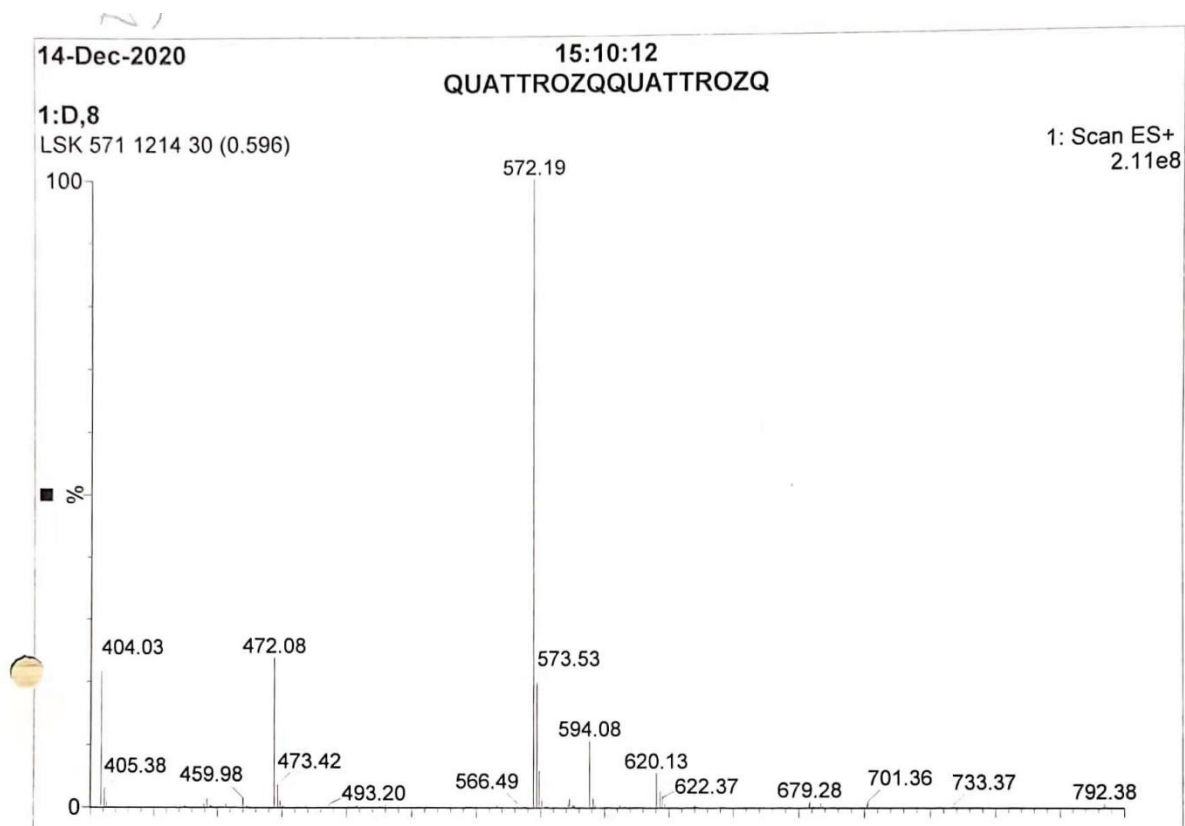


Fig. 22 Mass spectrum of compound A4

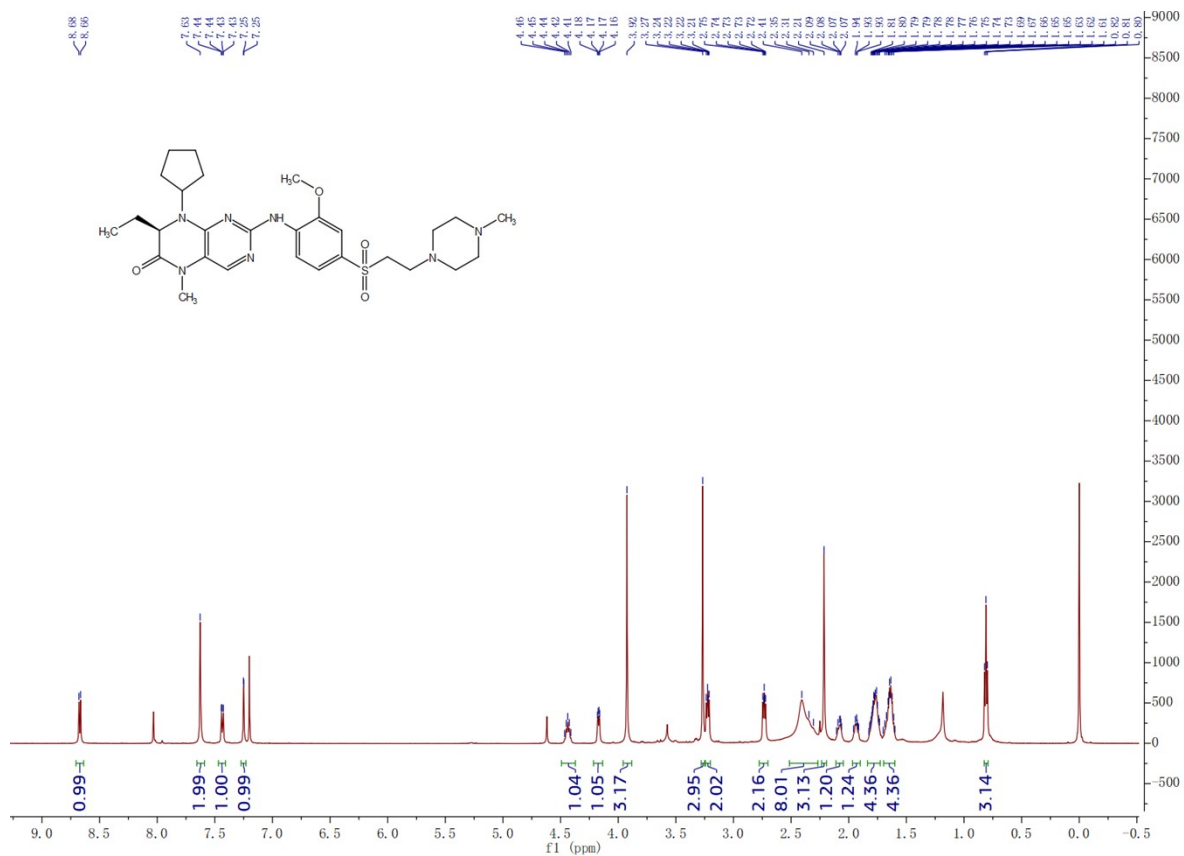


Fig. 23 ^1H NMR spectrum of compound A4

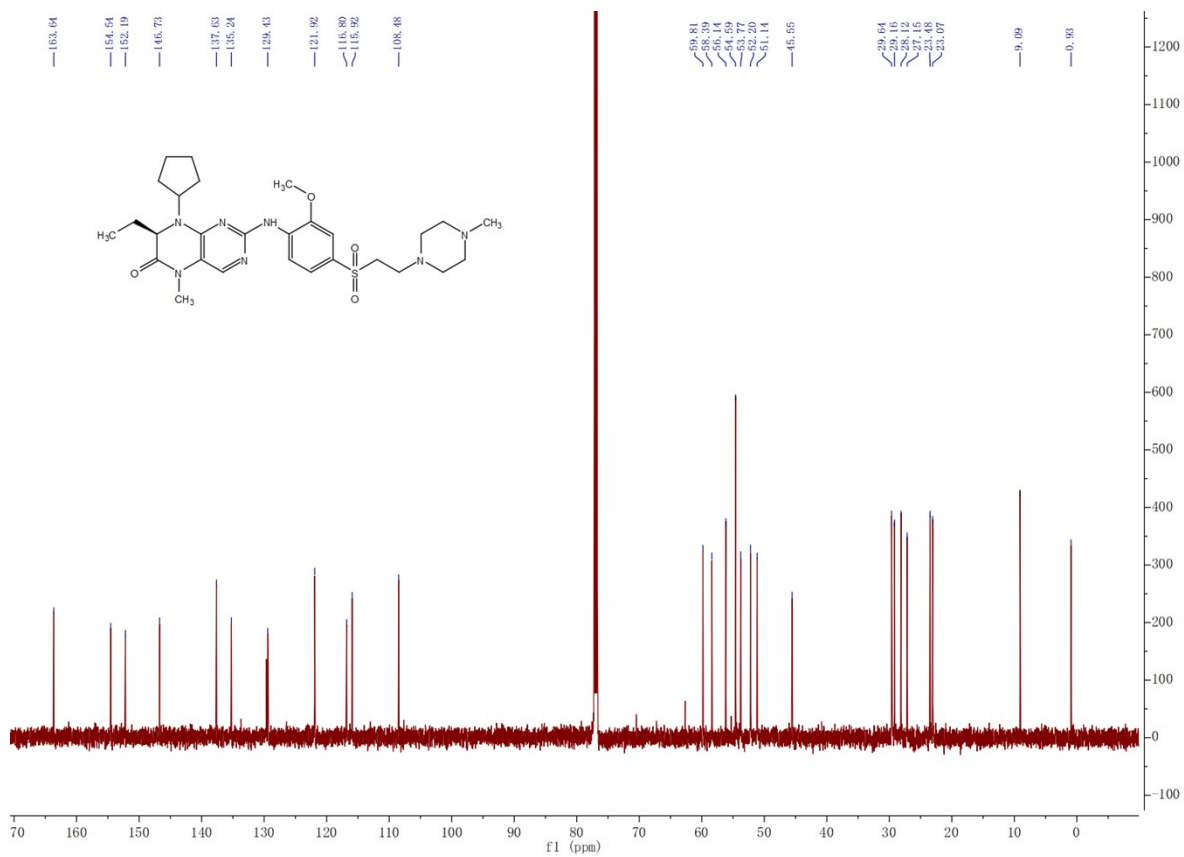


Fig. 24 ^{13}C NMR spectrum of compound A4

MS Spectrum

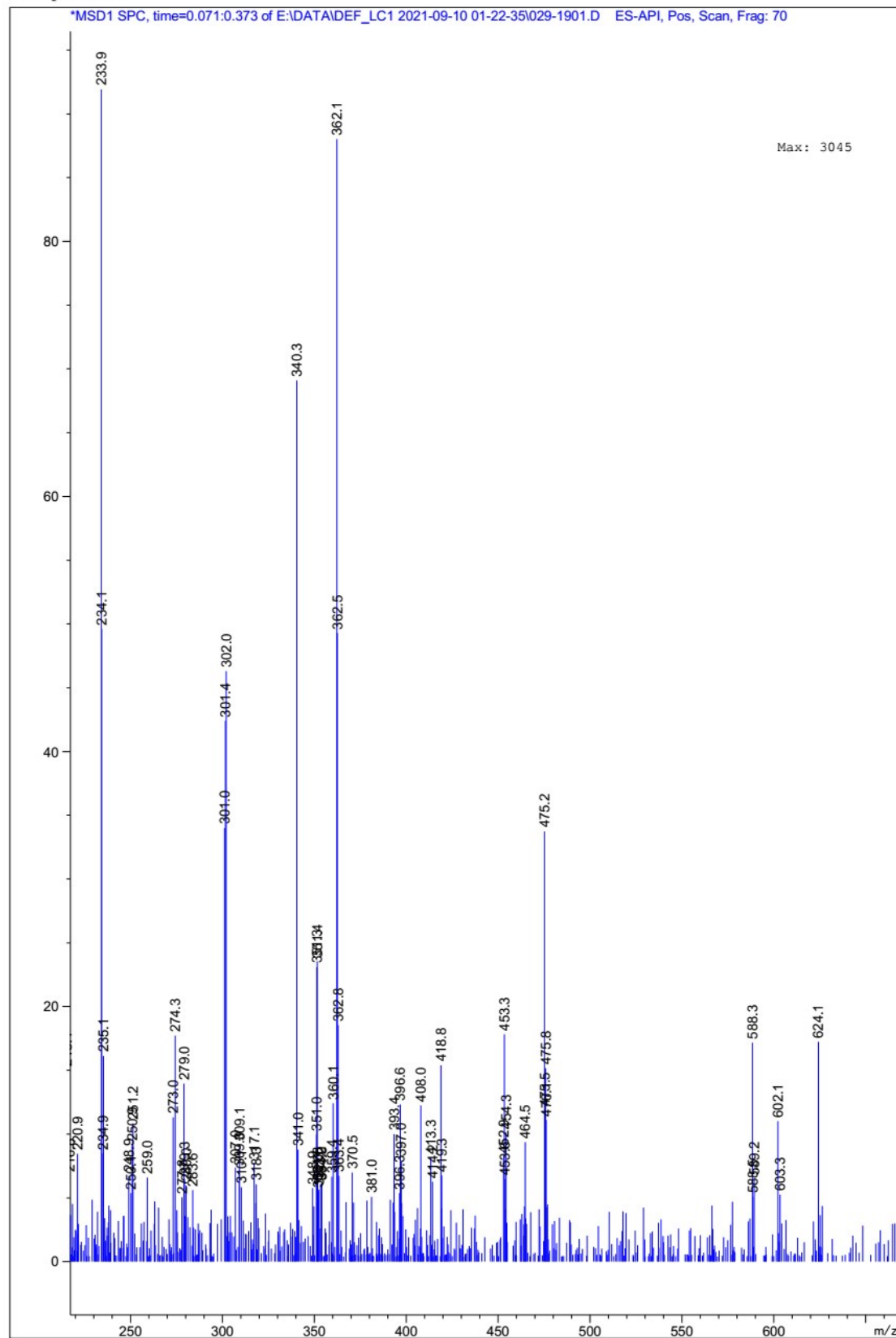


Fig. 25 Mass spectrum of compound A5

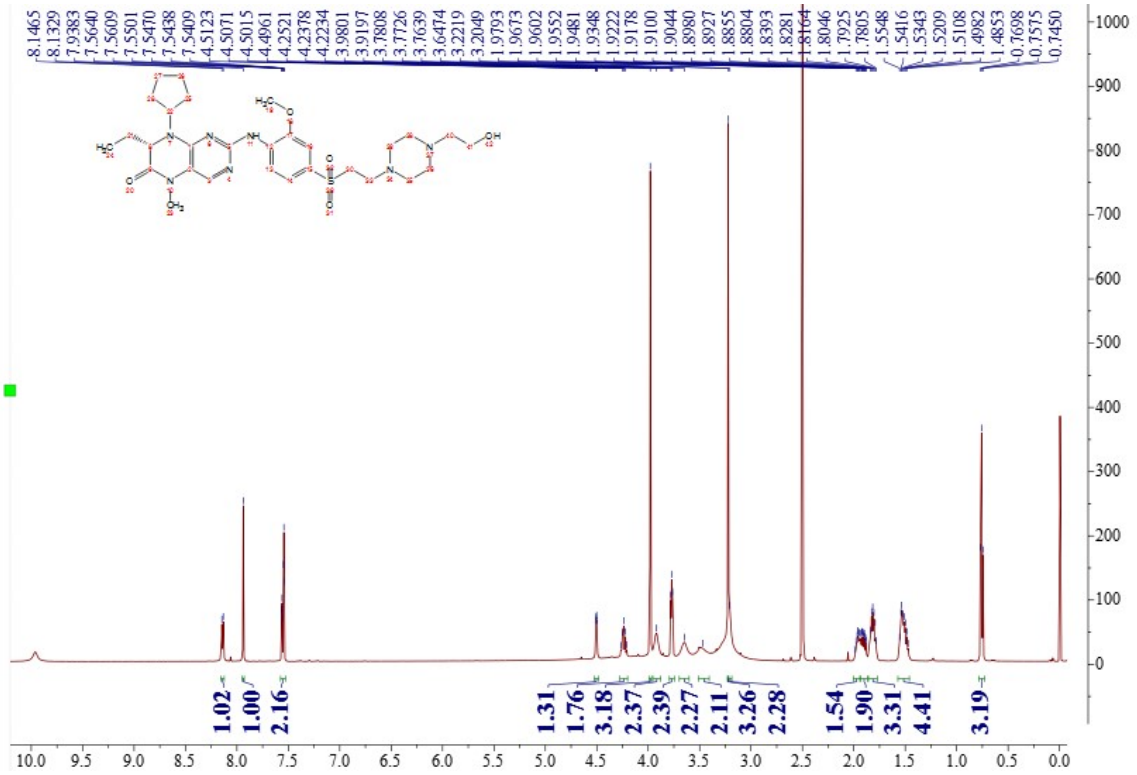


Fig. 26 ^1H NMR spectrum of compound A5

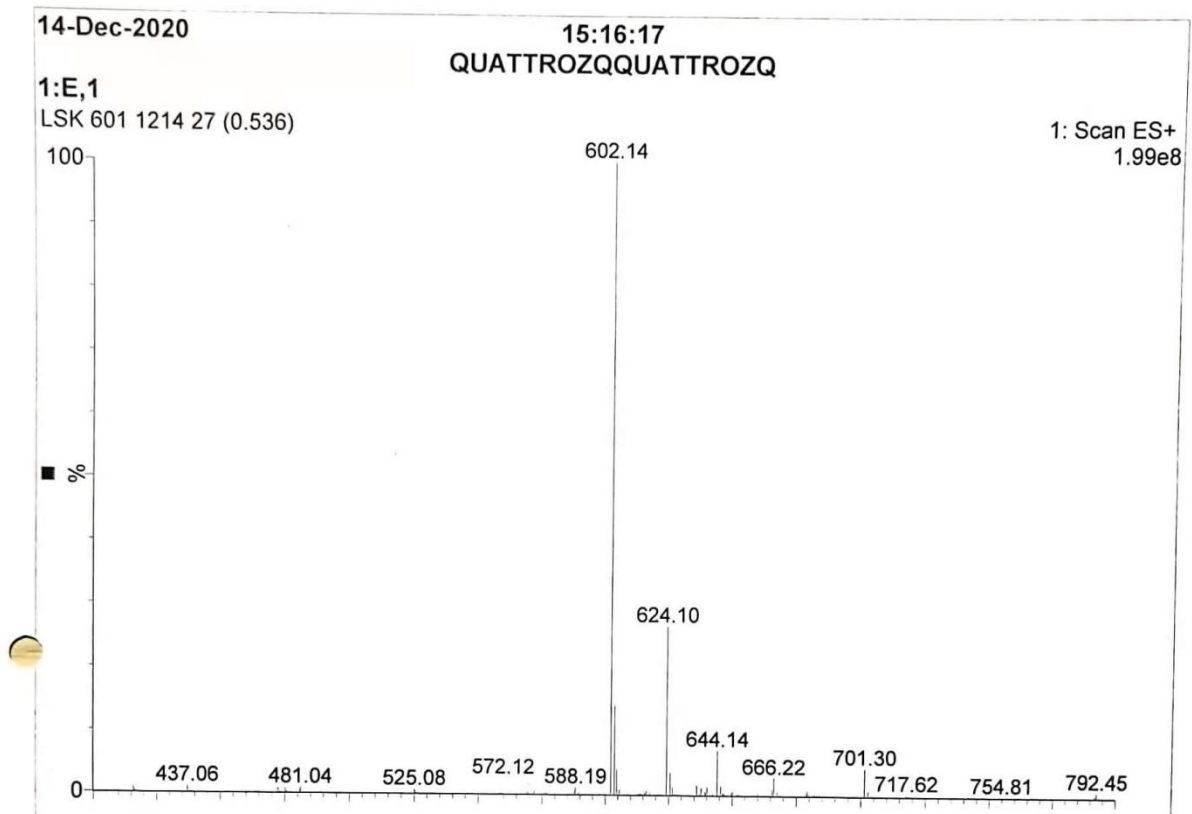
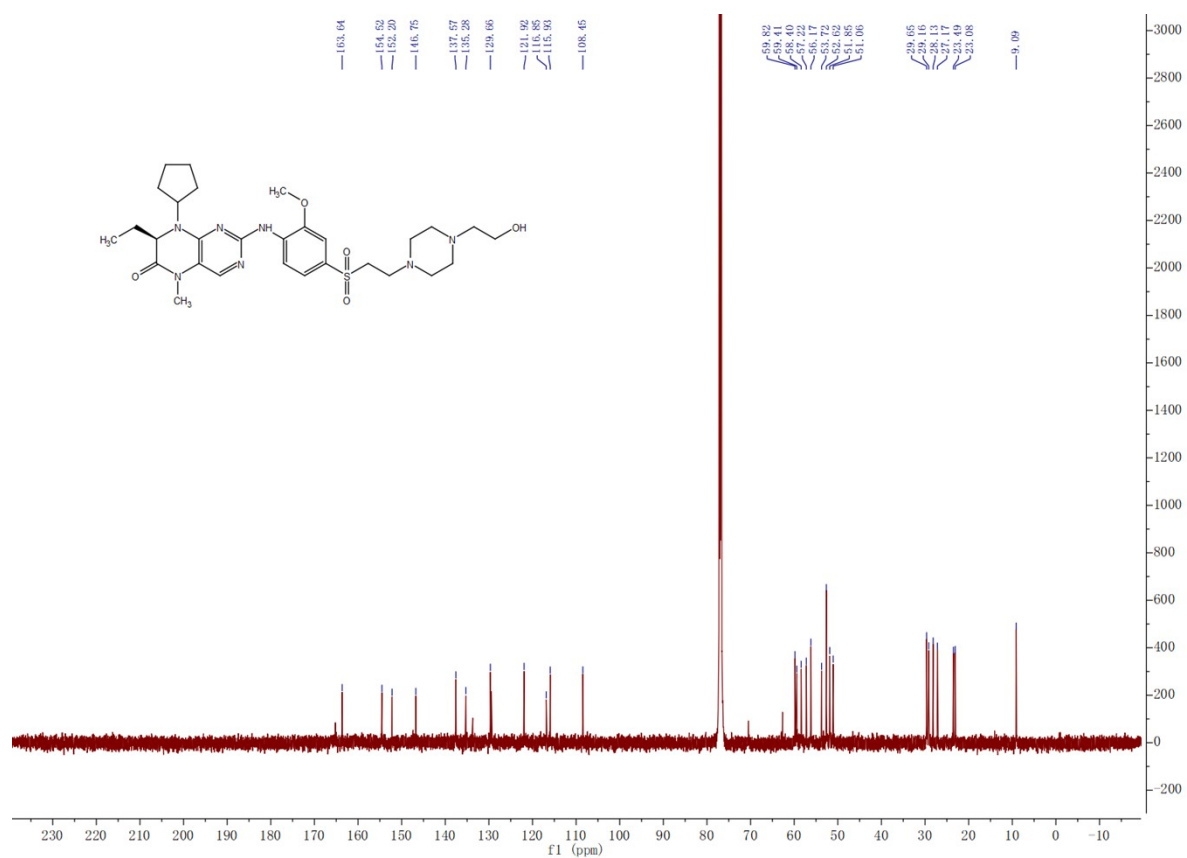
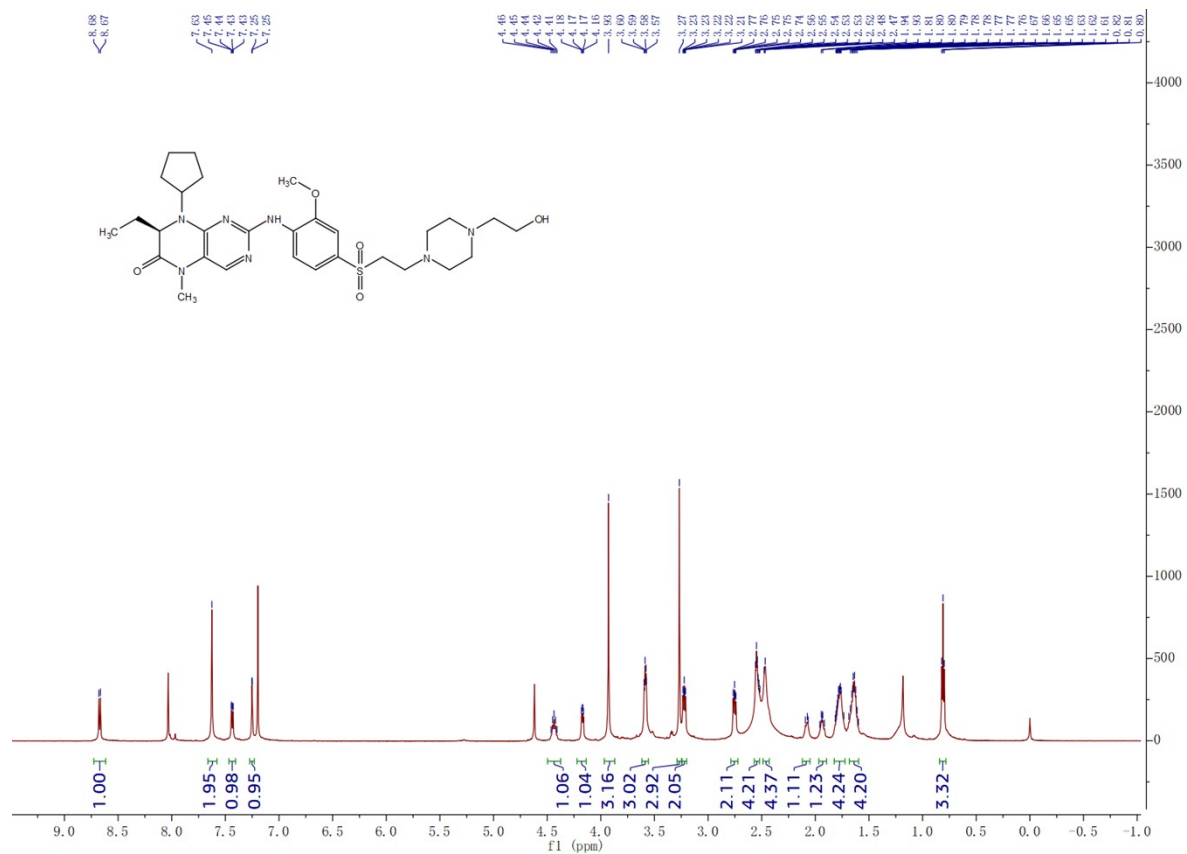


Fig. 27 Mass spectrum of compound A6



MS Spectrum

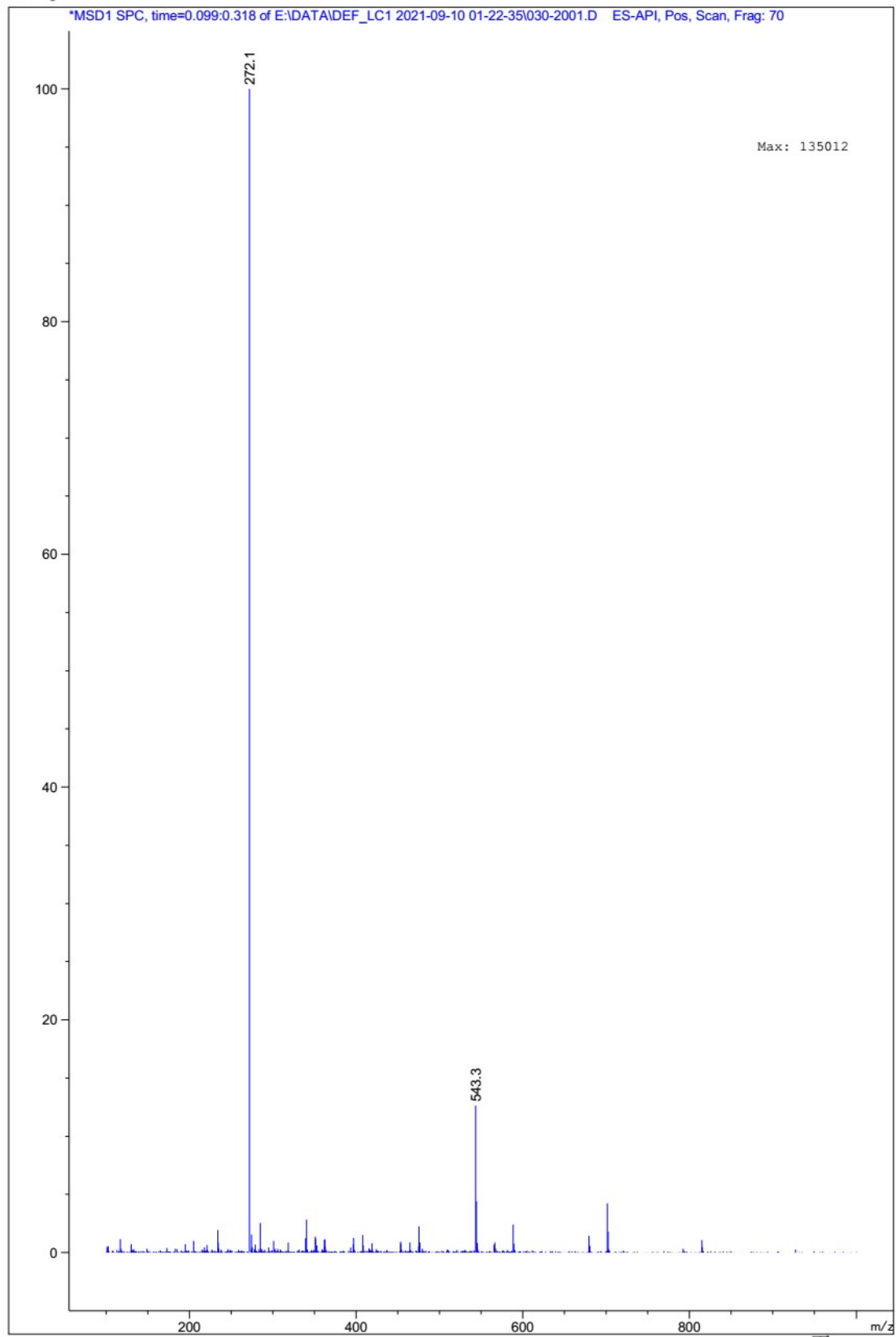


Fig. 30 Mass spectrum of compound A7

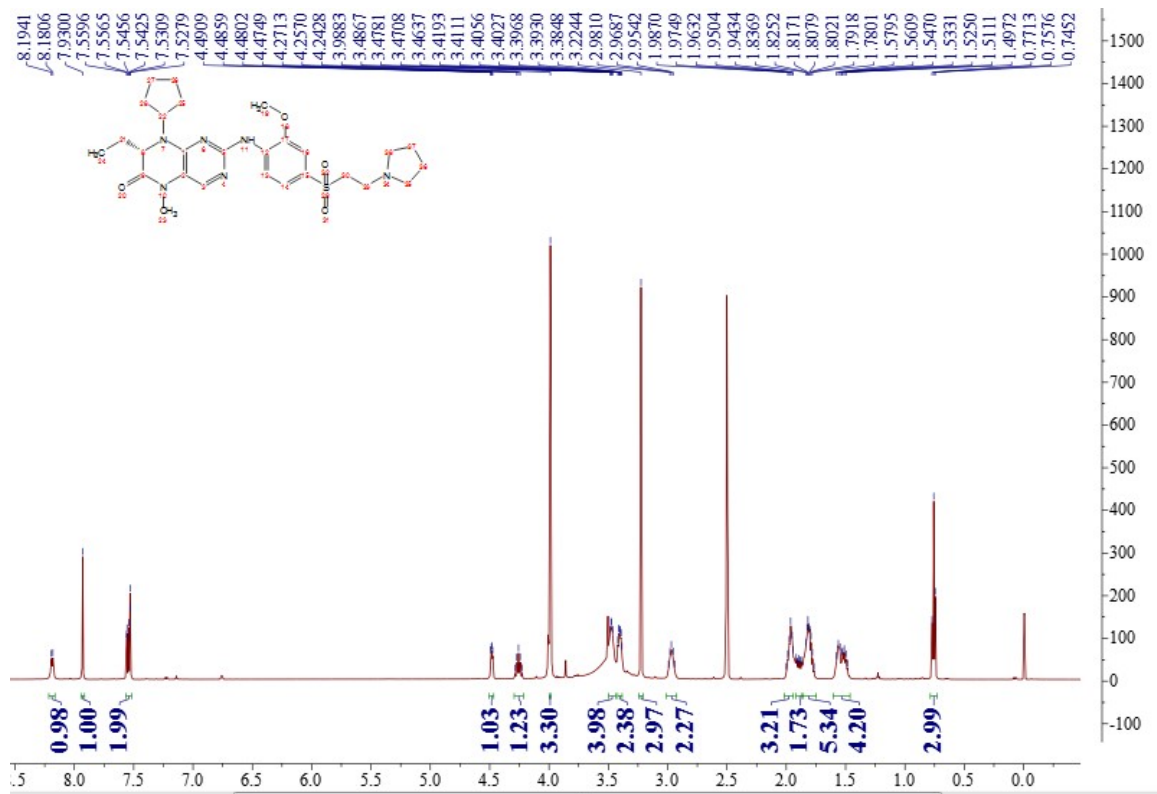


Fig. 31 ^1H NMR spectrum of compound A7

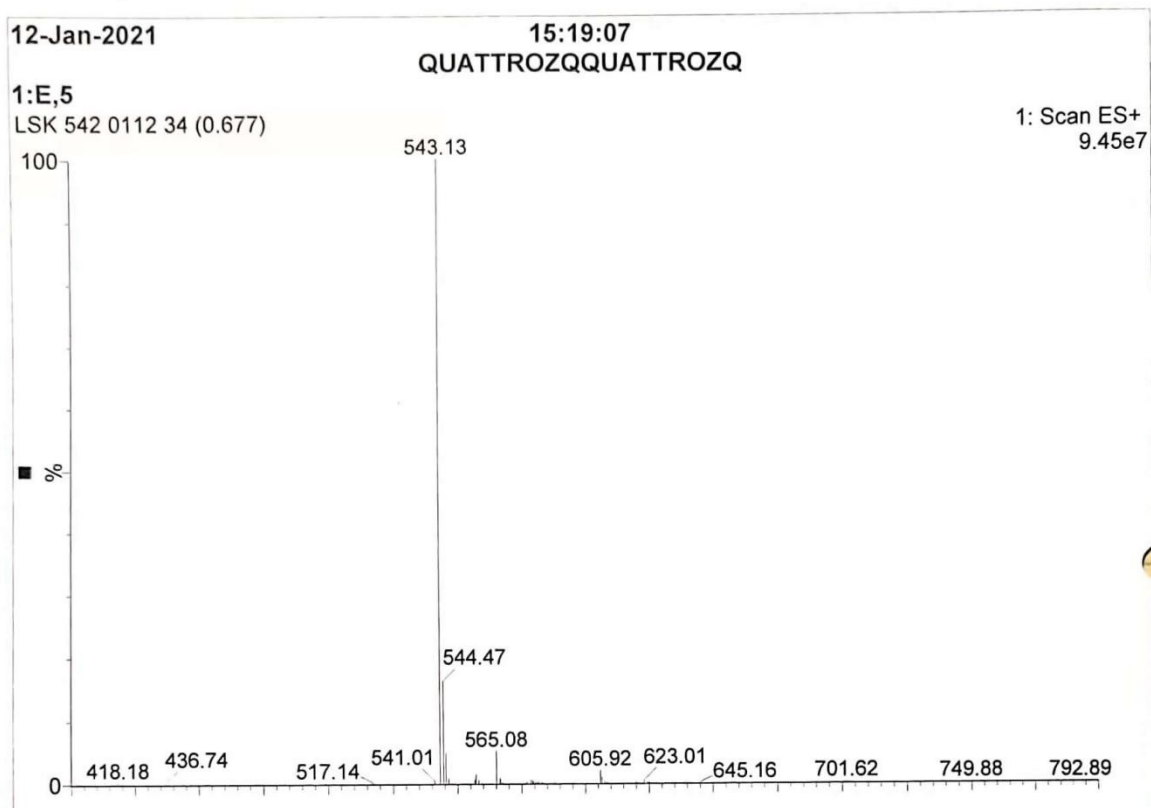
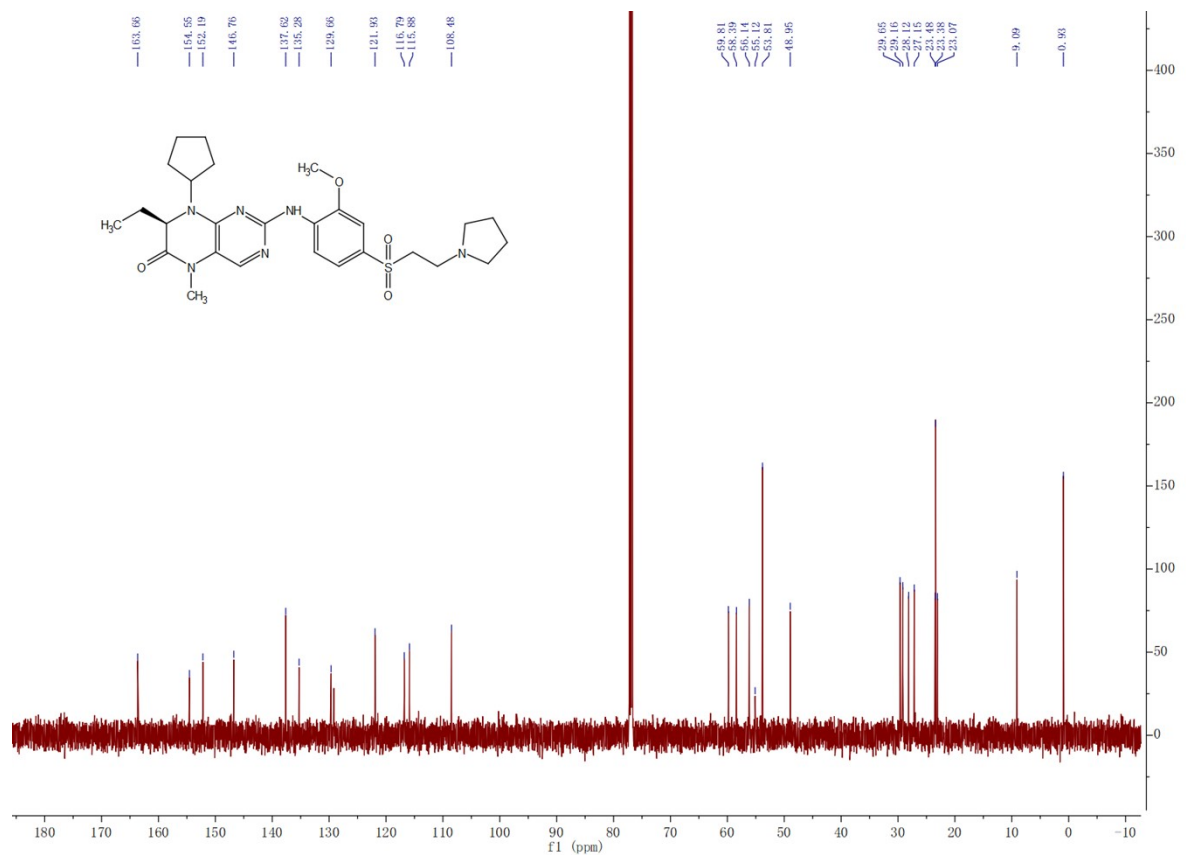
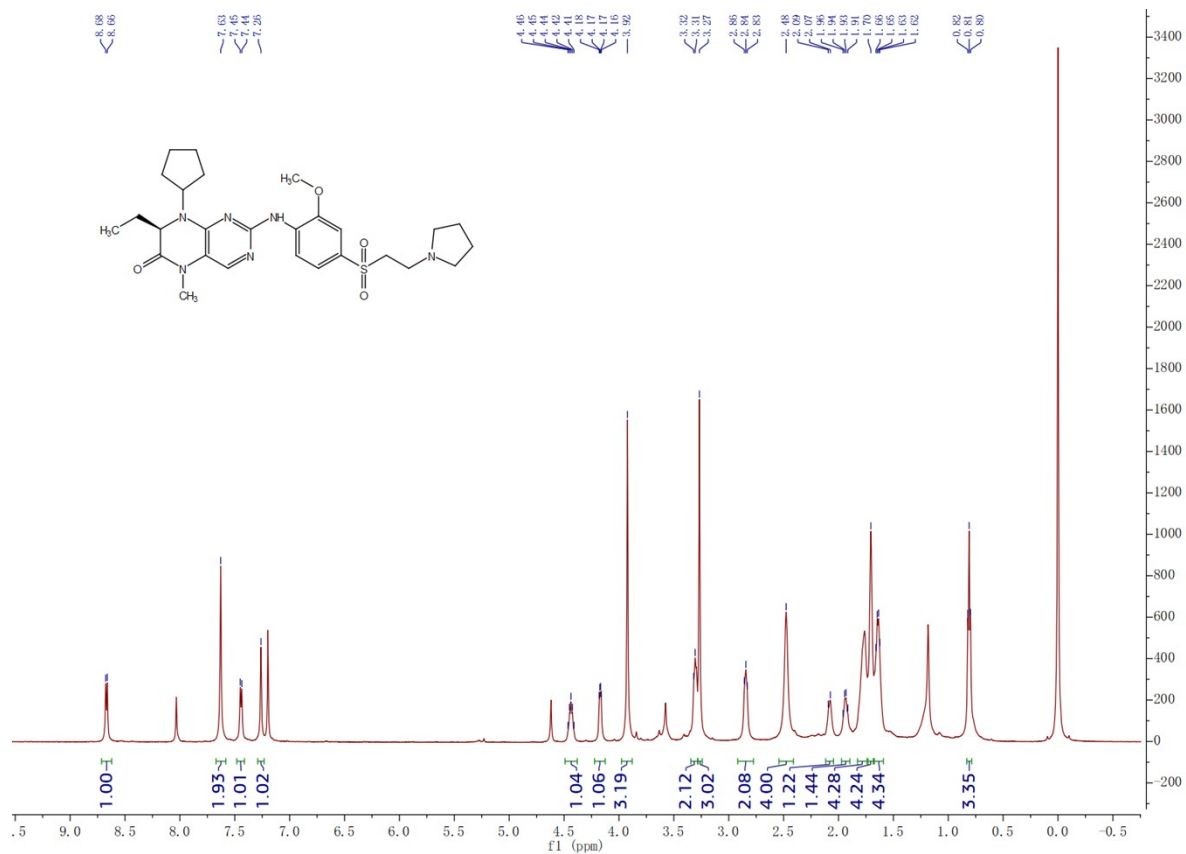


Fig. 32 Mass spectrum of compound A8



MS Spectrum

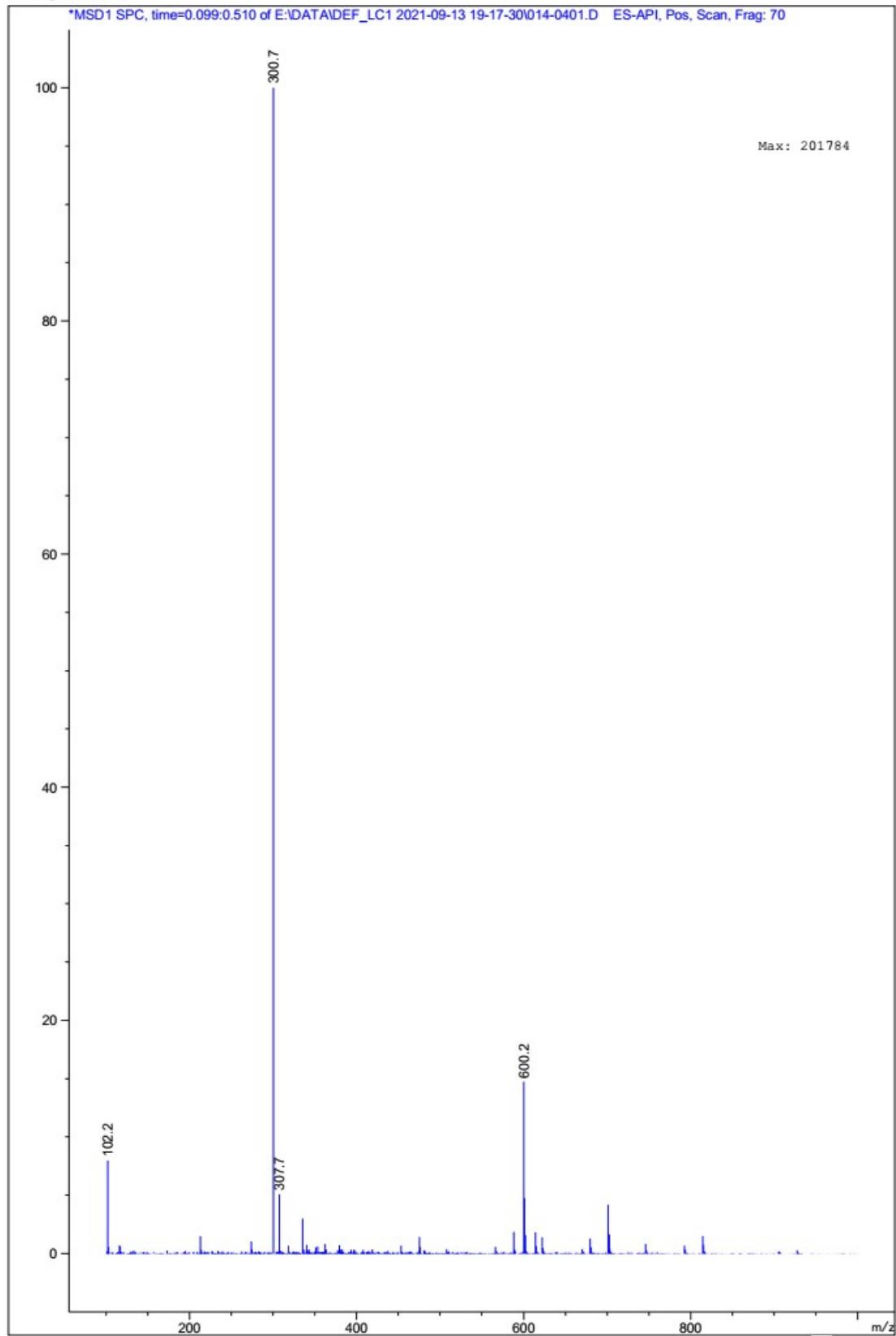


Fig. 35 Mass spectrum of compound B1

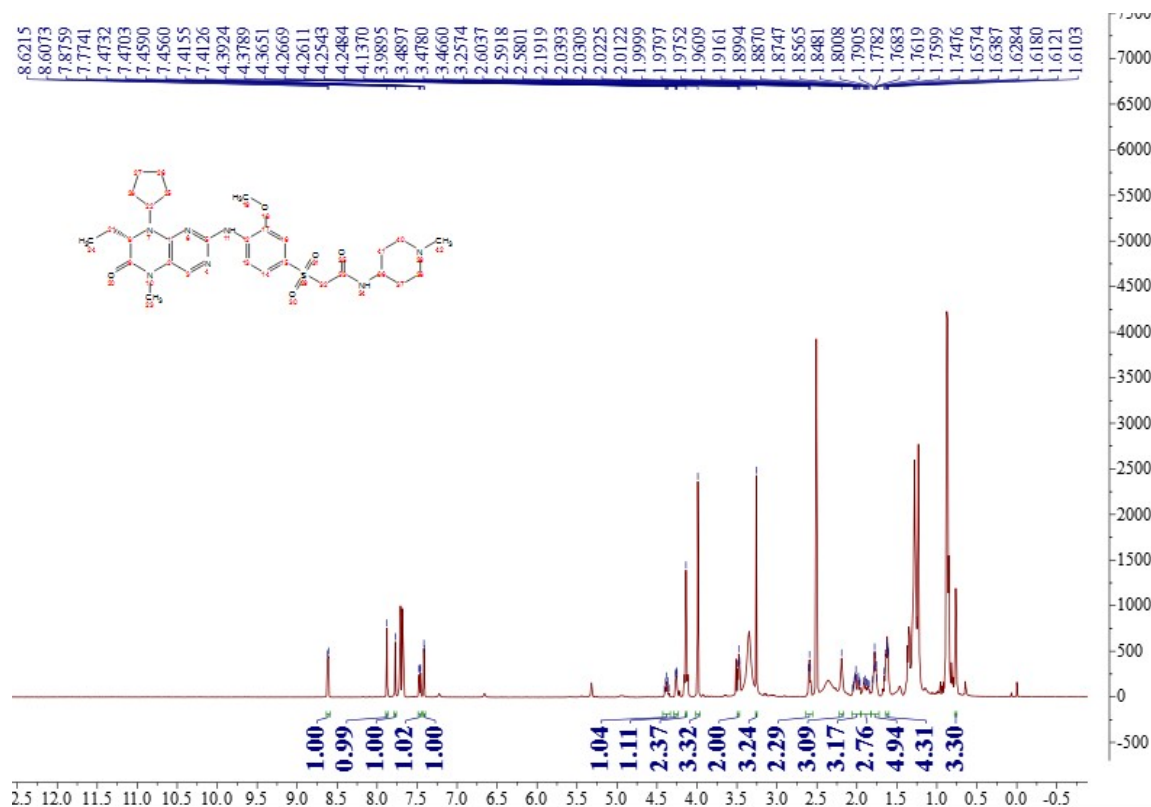


Fig. 36 ¹H NMR spectrum of compound B1

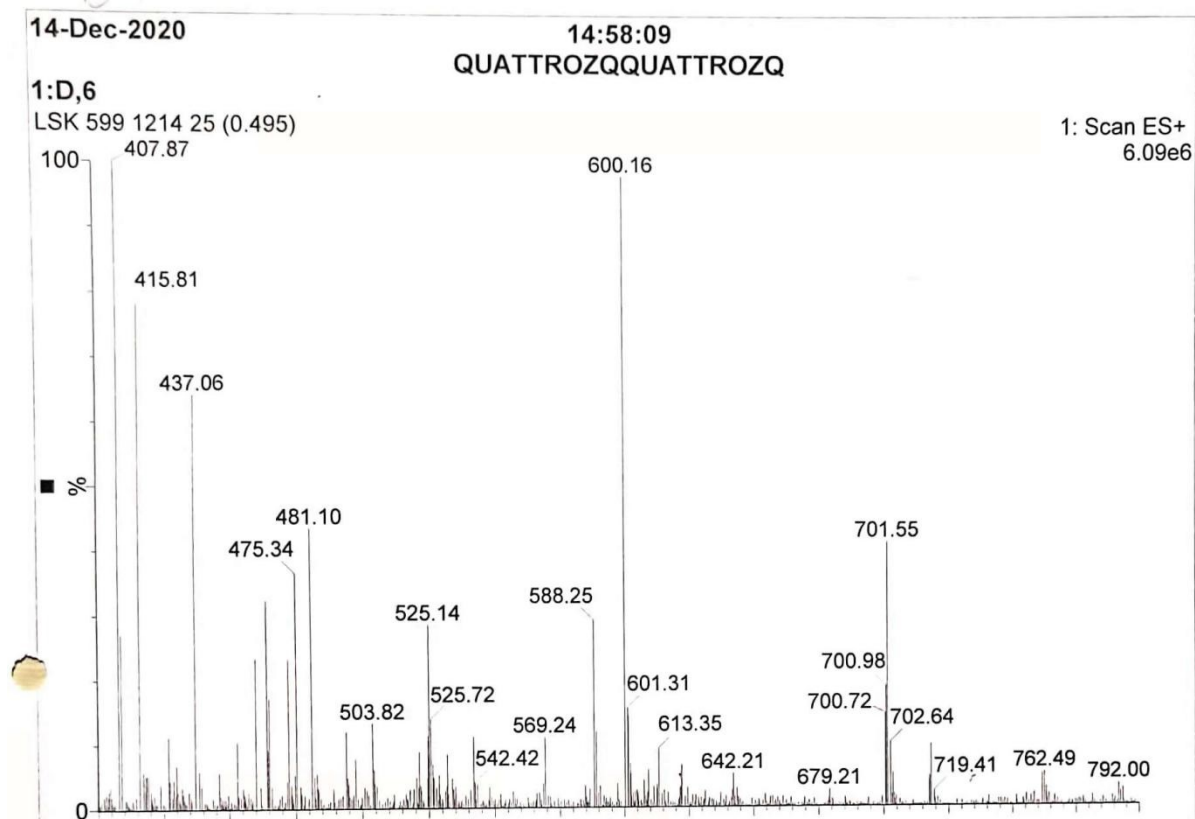


Fig. 37 Mass spectrum of compound B2

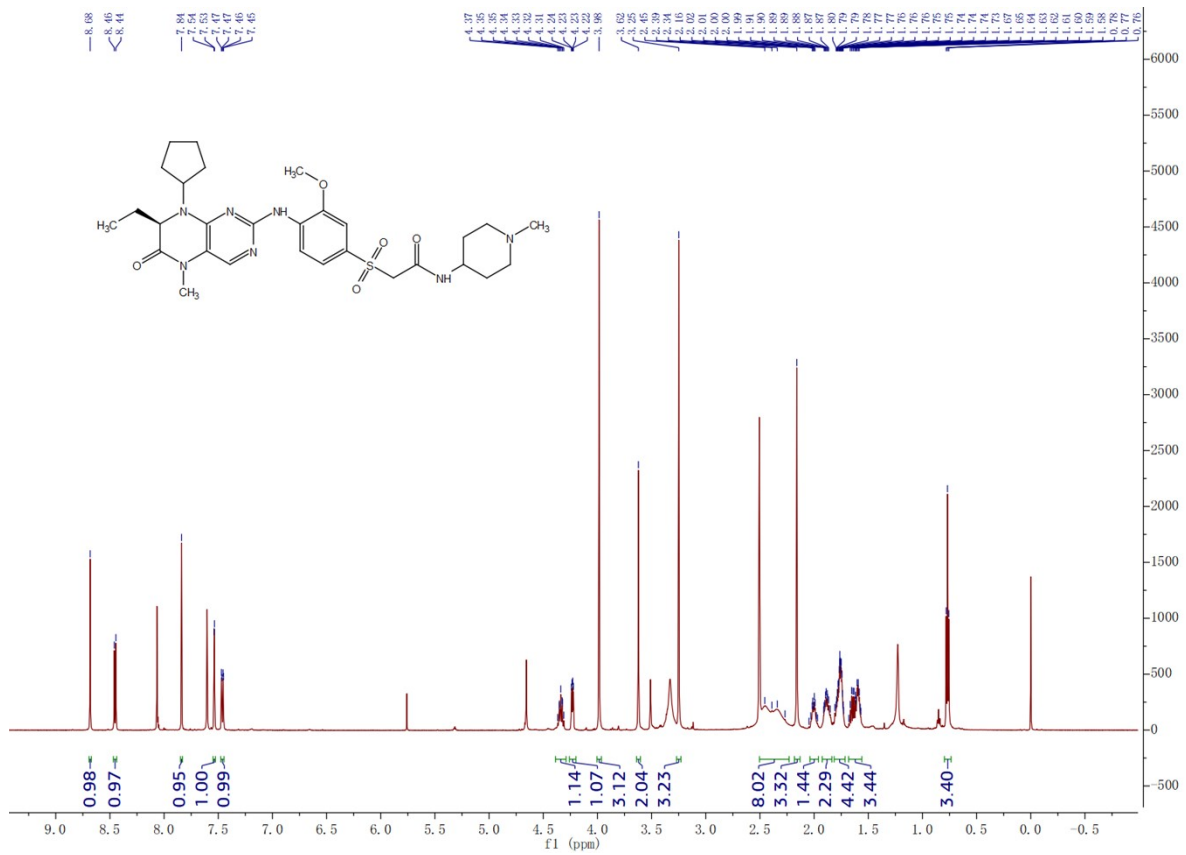


Fig. 38 ¹H NMR spectrum of compound B2

MS Spectrum

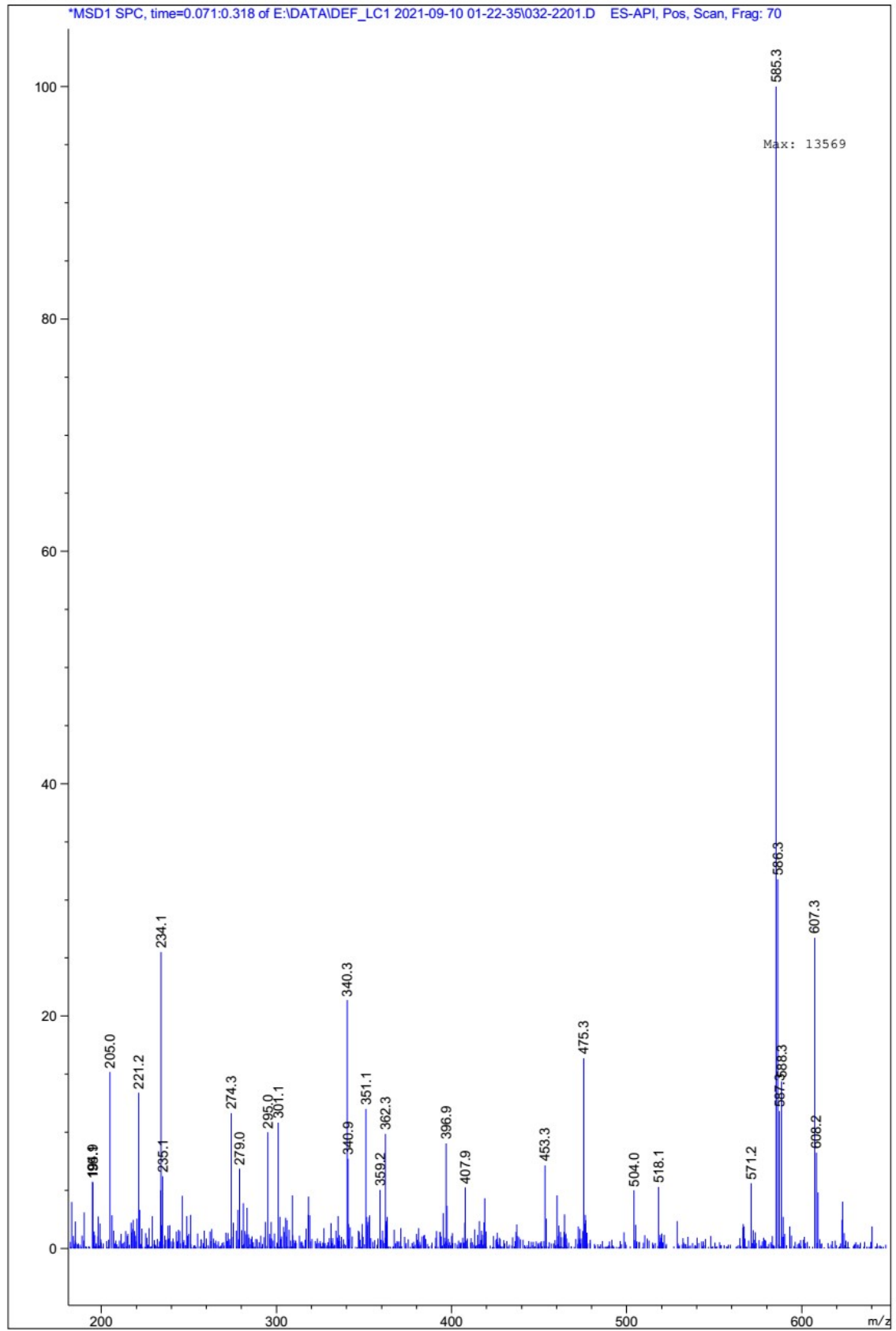


Fig. 39 Mass spectrum of compound B3

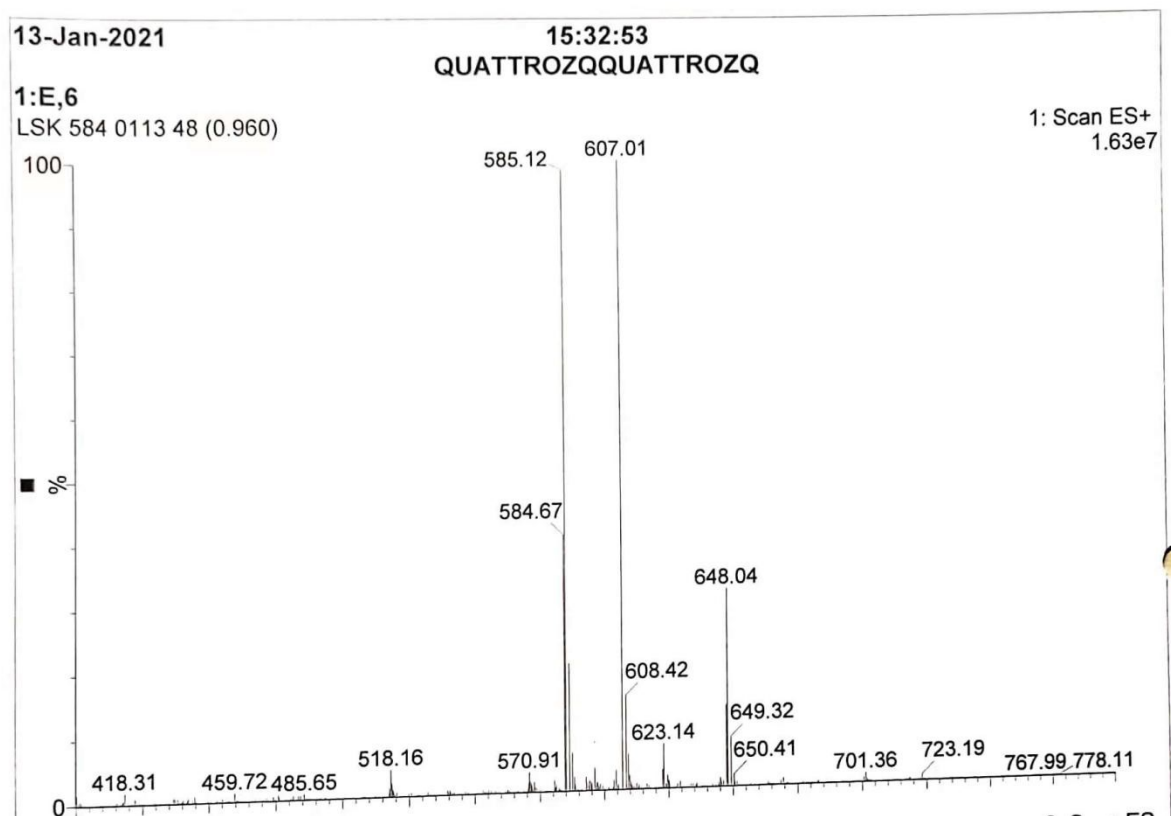


Fig. 40 Mass spectrum of compound B4

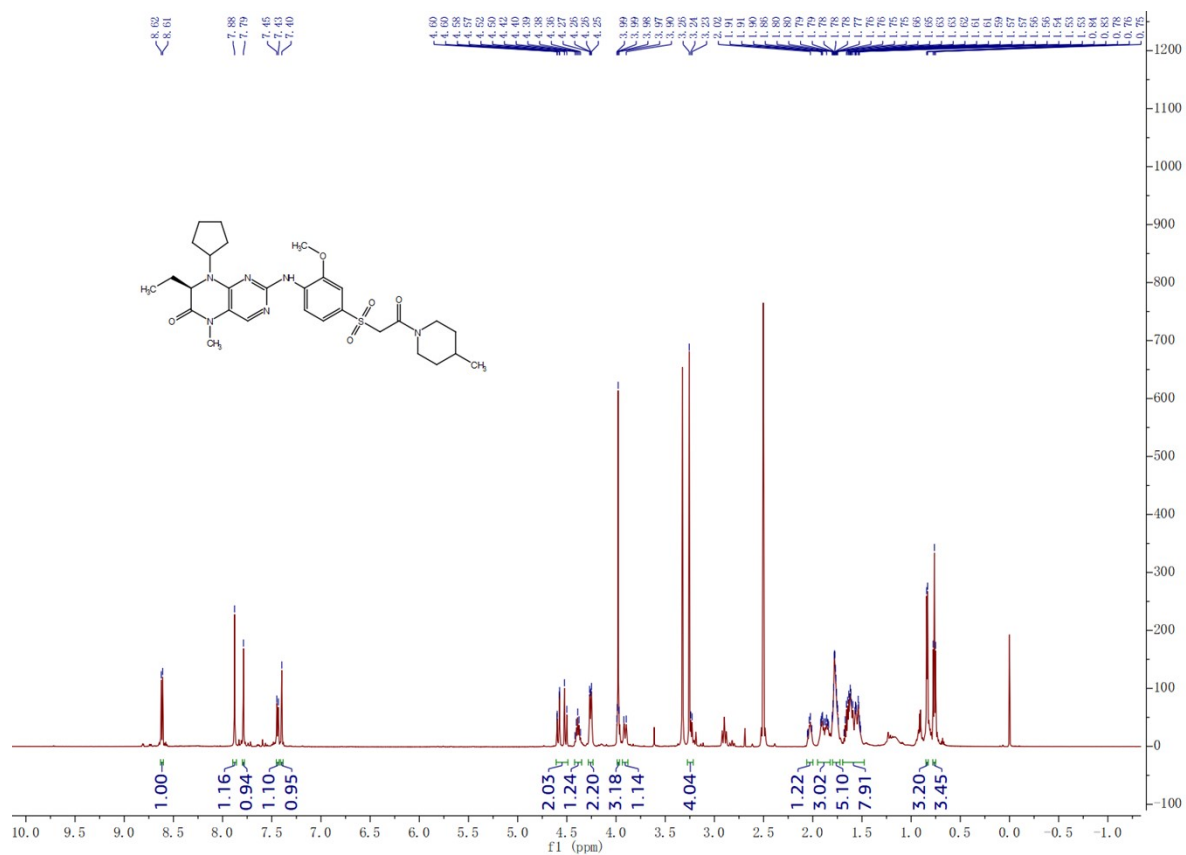


Fig. 41 ¹H NMR spectrum of compound B4

MS Spectrum

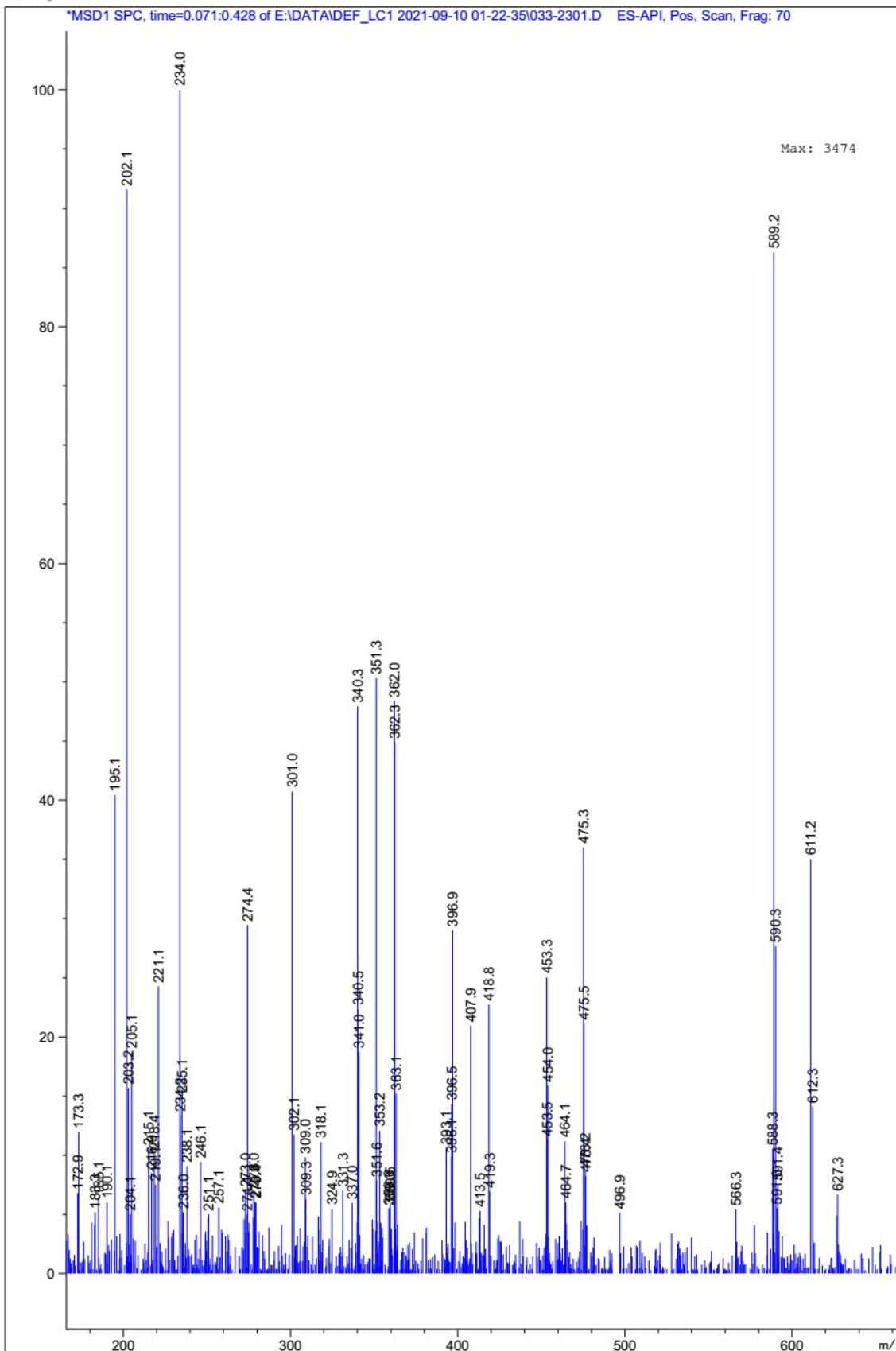


Fig. 42 Mass spectrum of compound B5

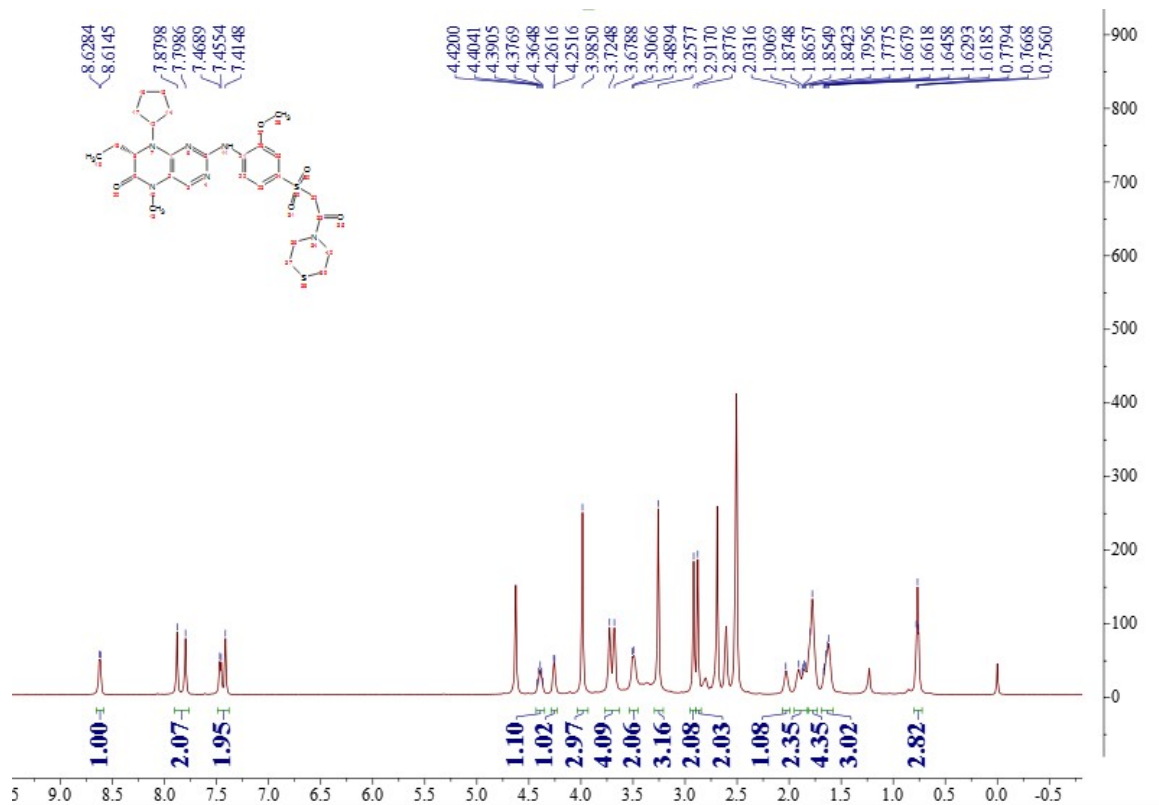


Fig. 43 ^1H NMR spectrum of compound B5

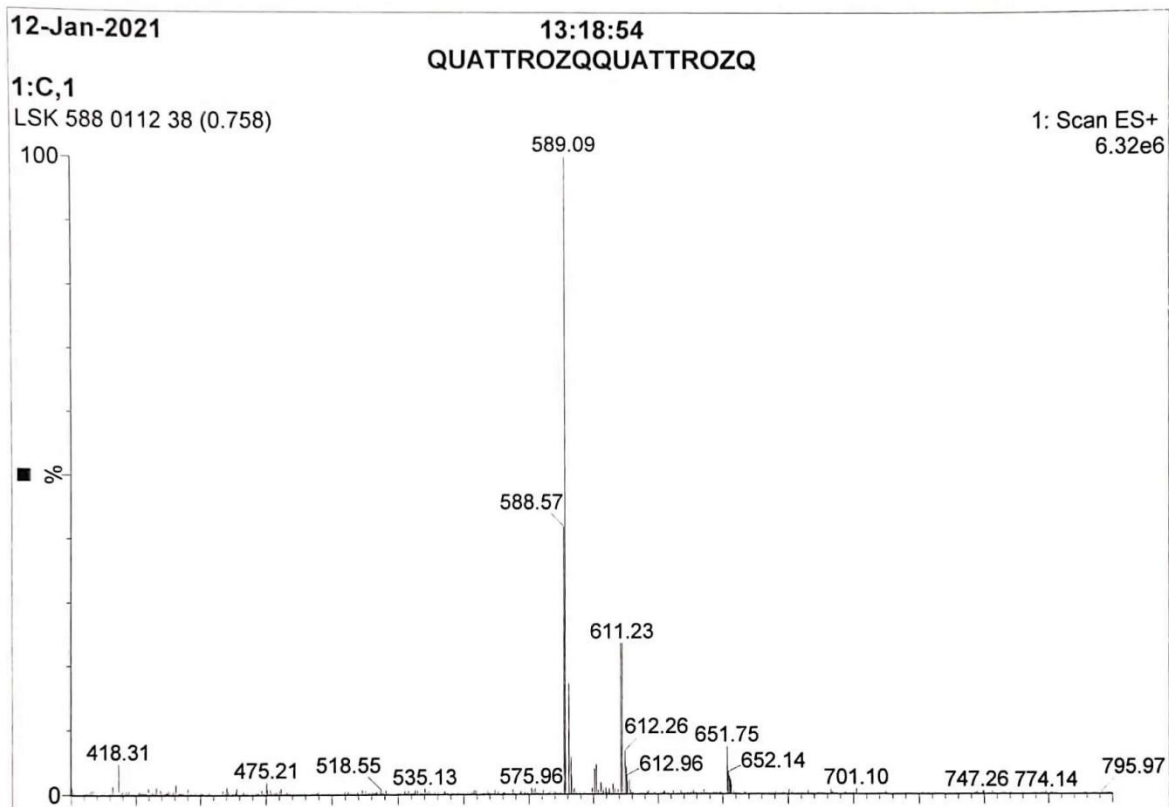


Fig. 44 Mass spectrum of compound B6

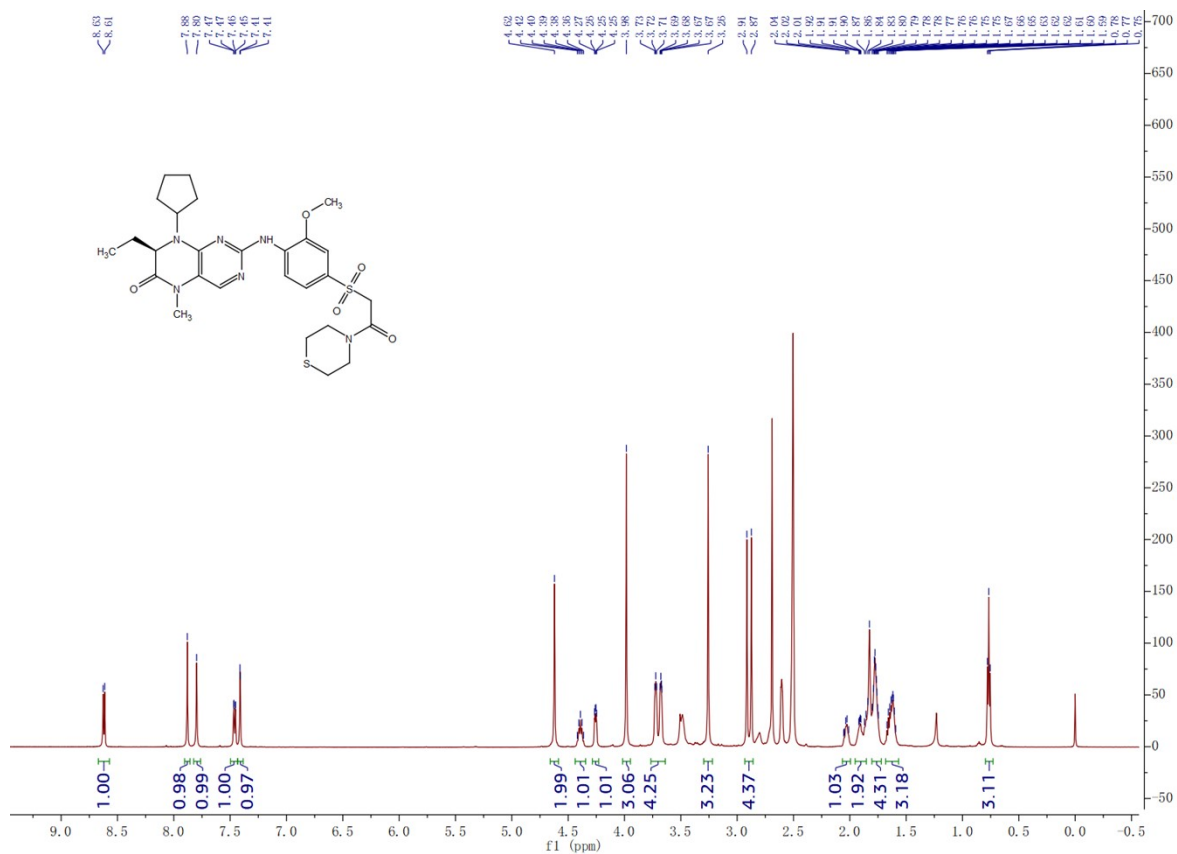


Fig. 45 ¹H NMR spectrum of compound B6

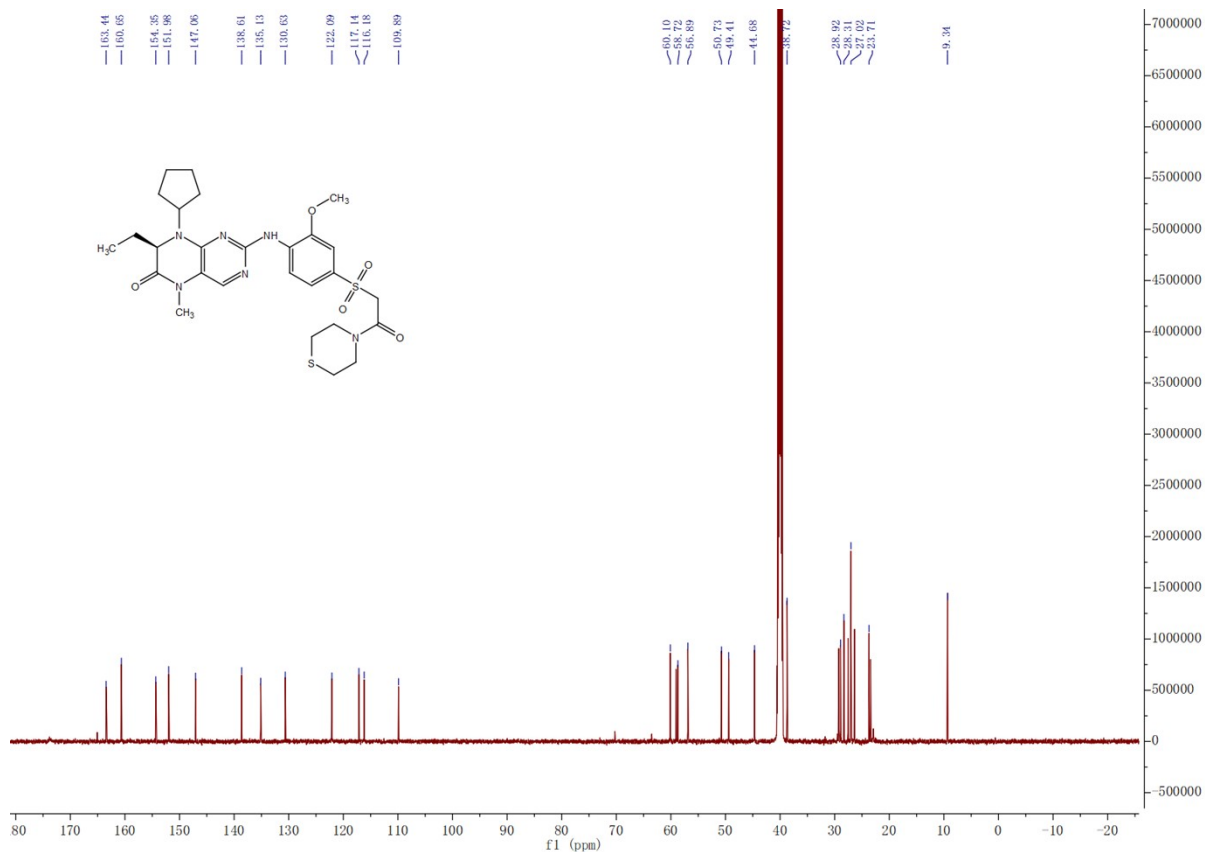


Fig. 46 ¹³C NMR spectrum of compound B6

MS Spectrum

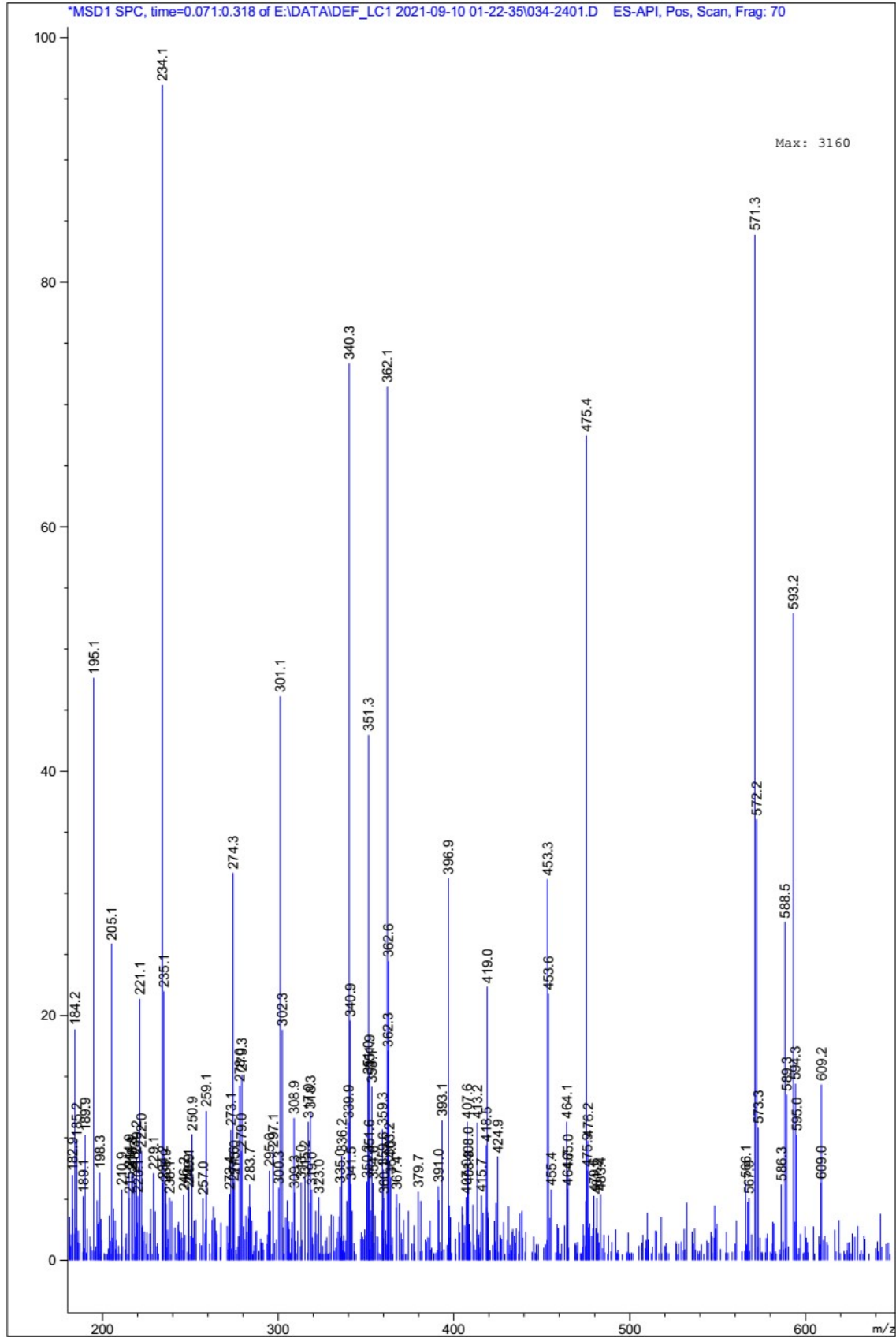


Fig. 47 Mass spectrum of compound B7

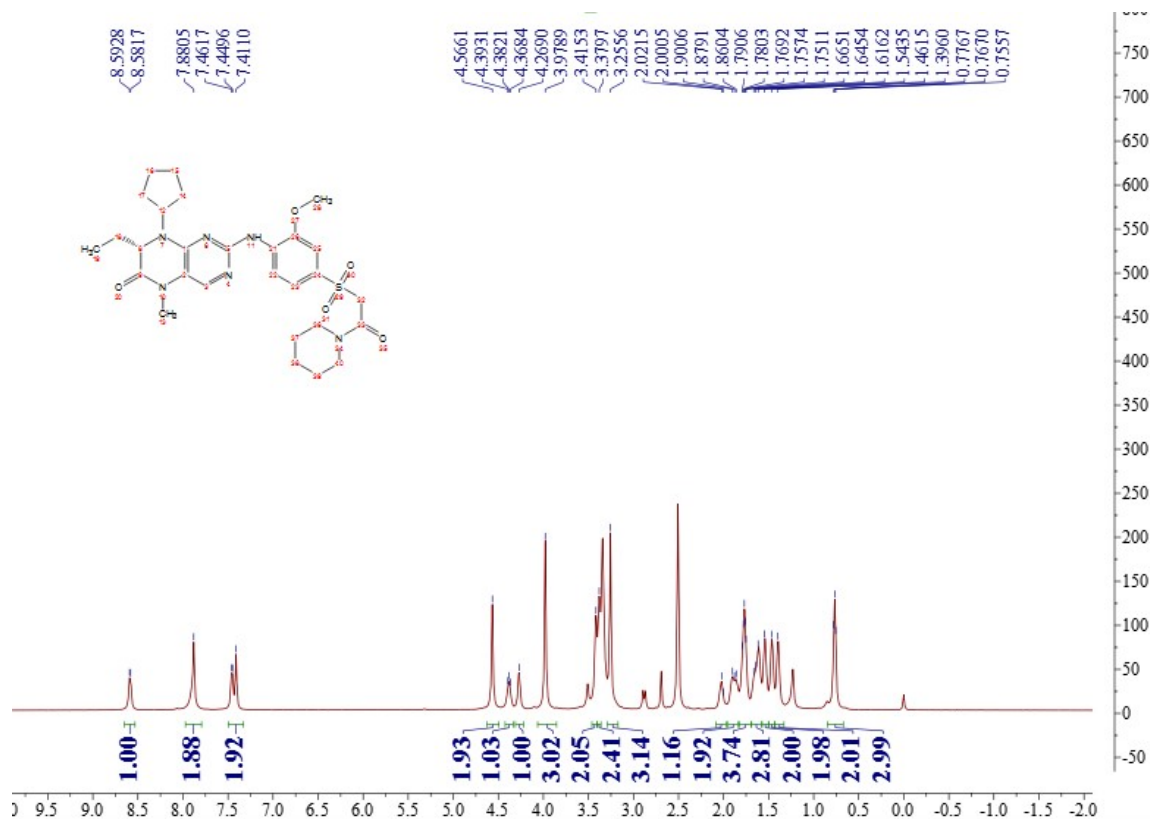


Fig. 48 ¹H NMR spectrum of compound B7

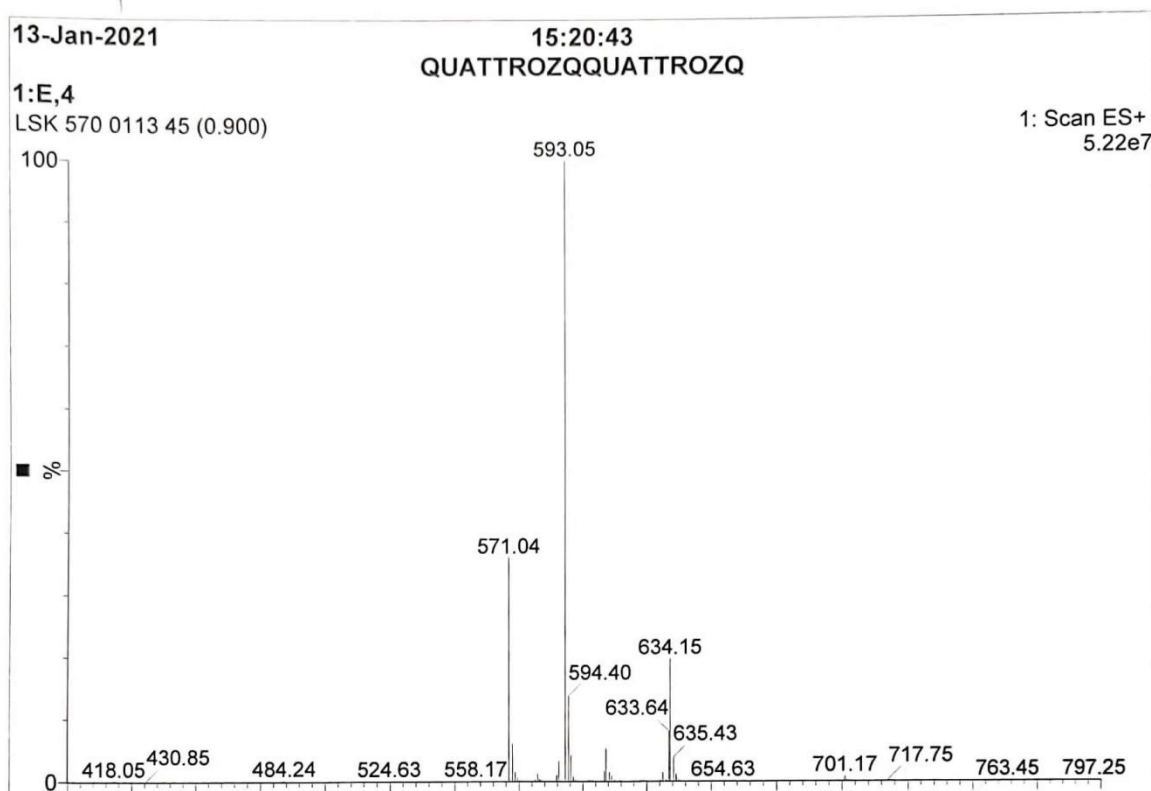


Fig. 49 Mass spectrum of compound B8

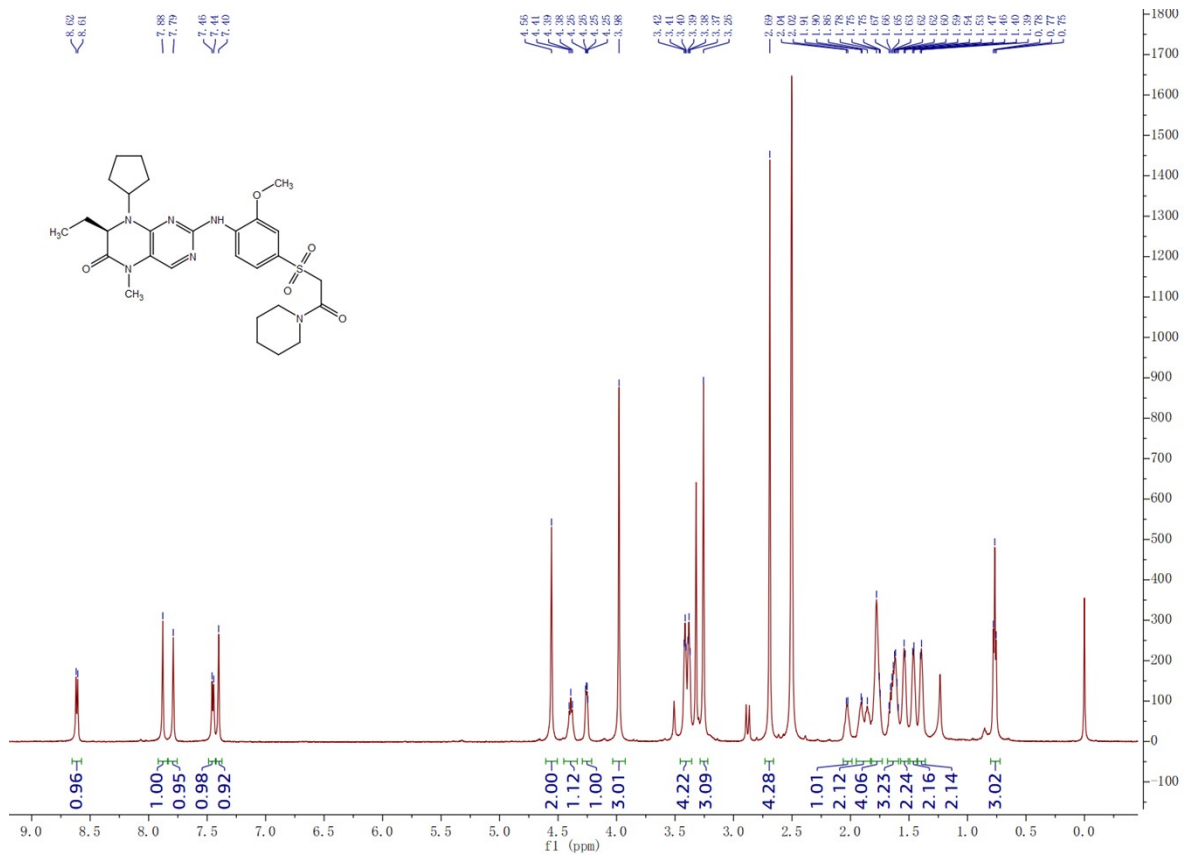


Fig. 50 ¹H NMR spectrum of compound B8

MS Spectrum

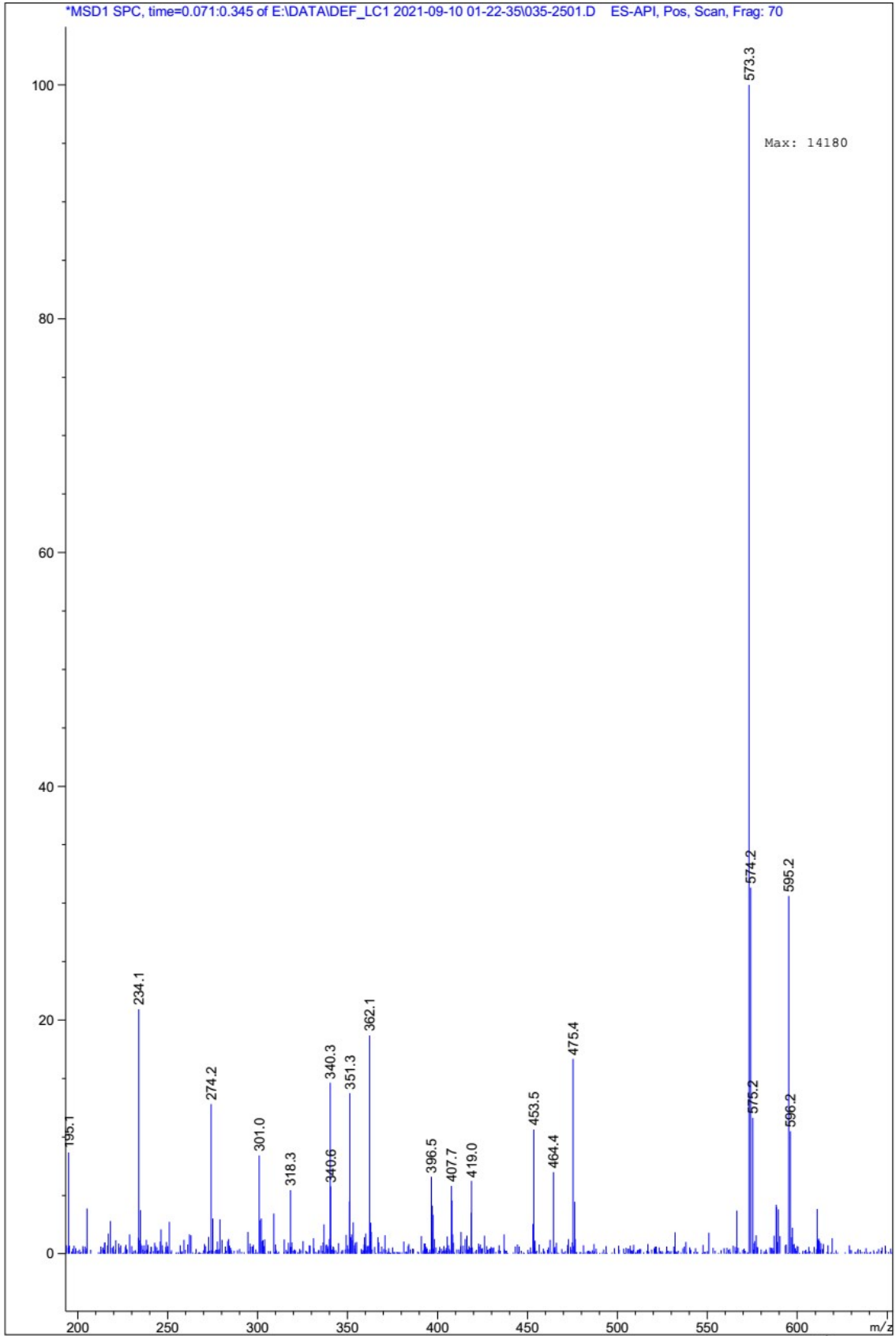


Fig.51 Mass spectrum of compound B9

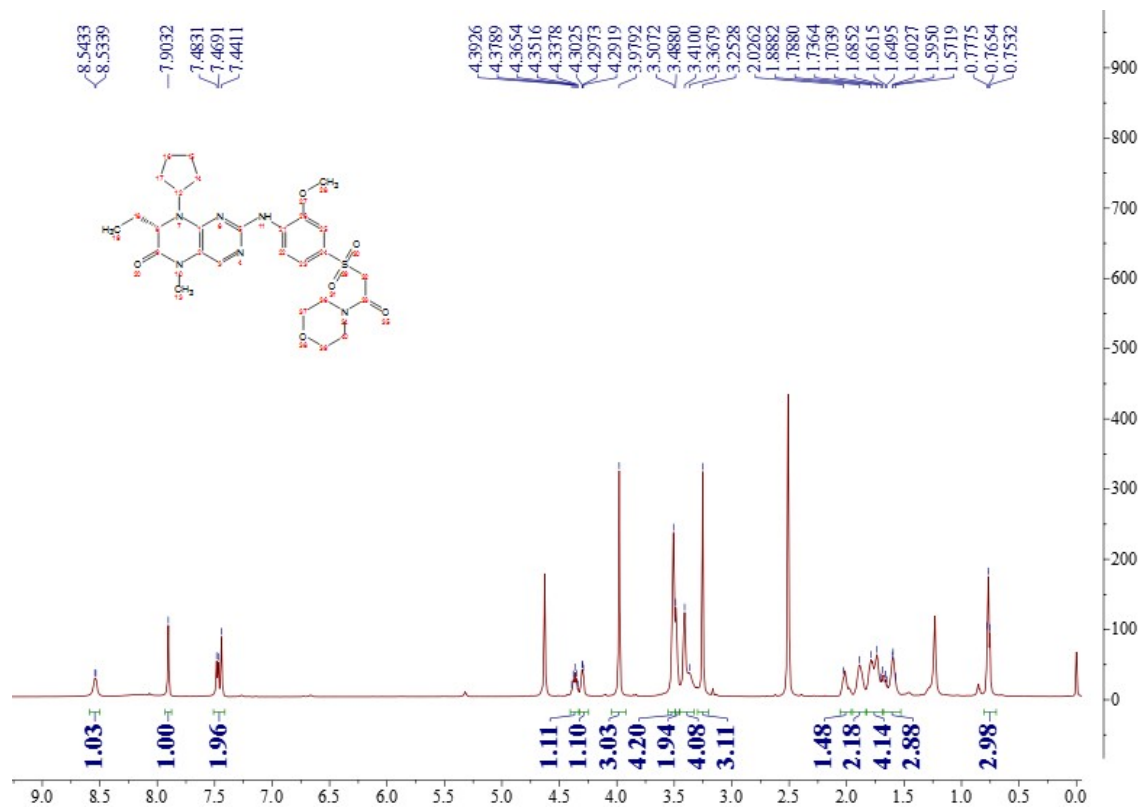


Fig. 52 ^1H NMR spectrum of compound B9

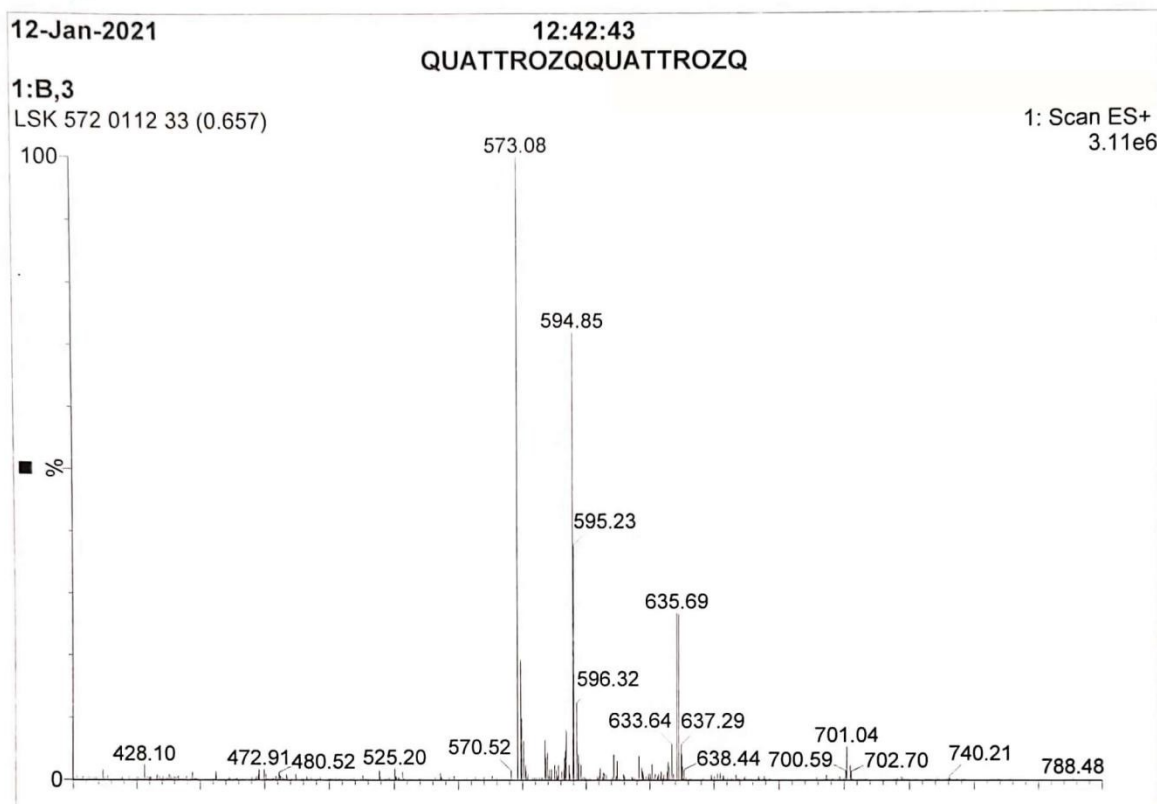


Fig. 53 Mass spectrum of compound B10

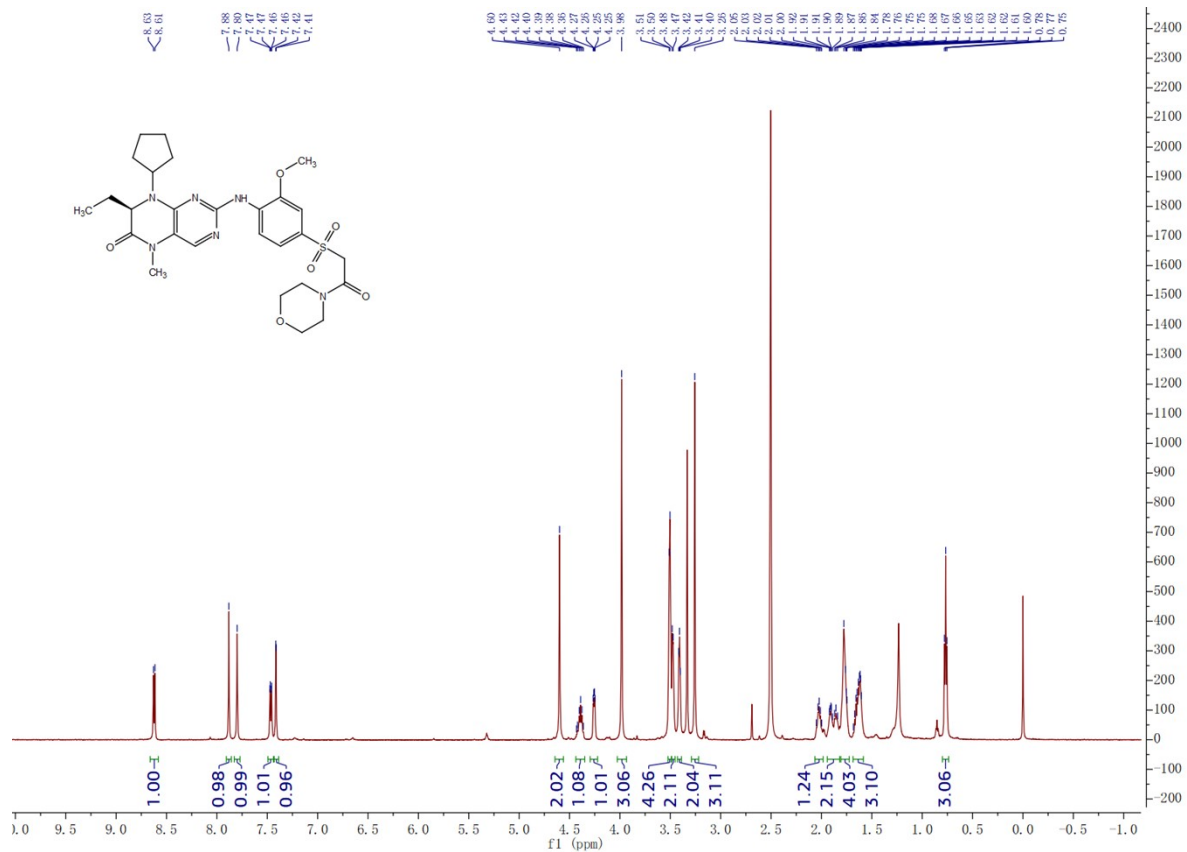


Fig. 54 ¹H NMR spectrum of compound B10

MS Spectrum

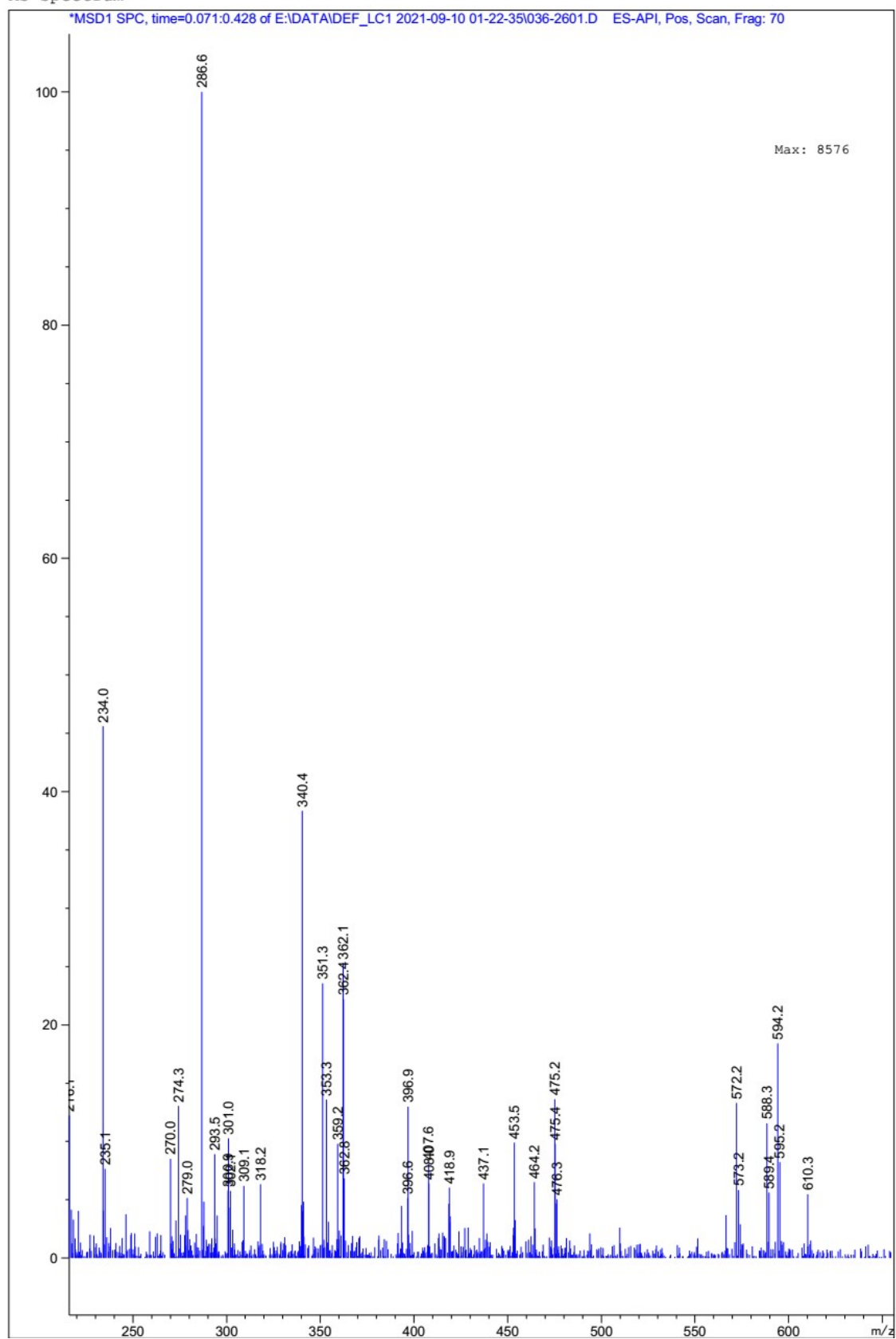


Fig. 55 Mass spectrum of compound B11

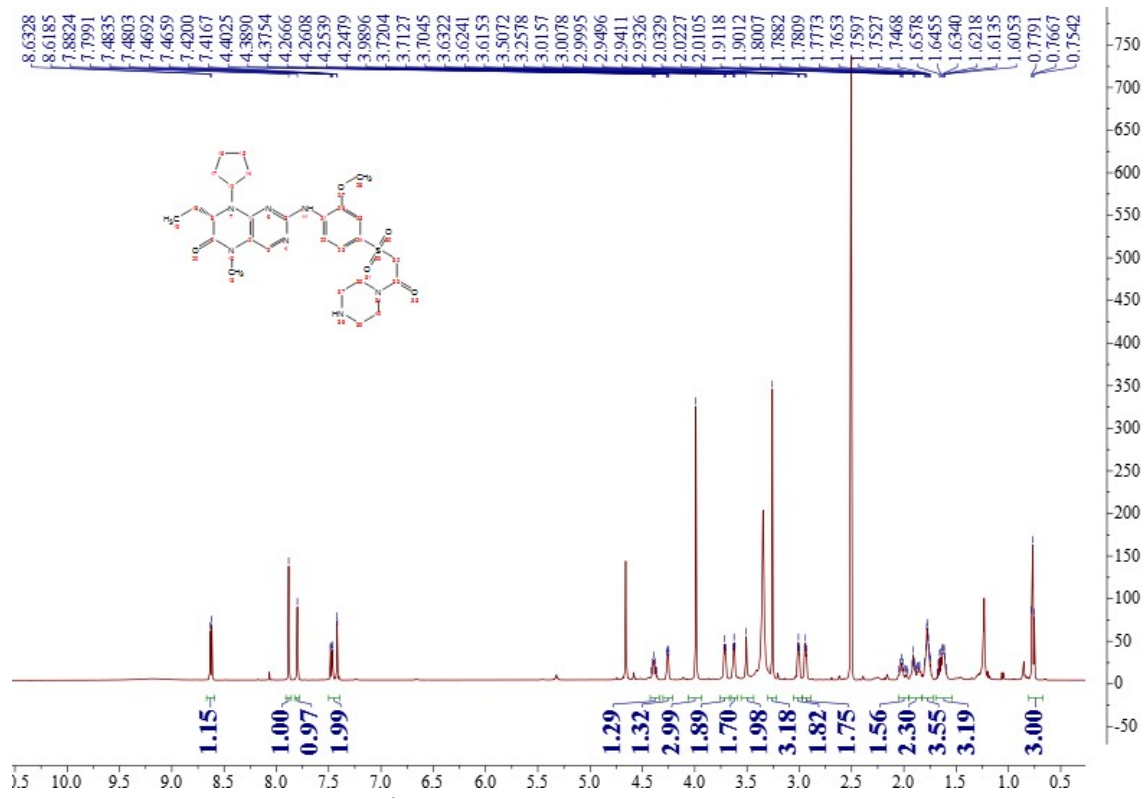


Fig. 56 ¹H NMR spectrum of compound B11

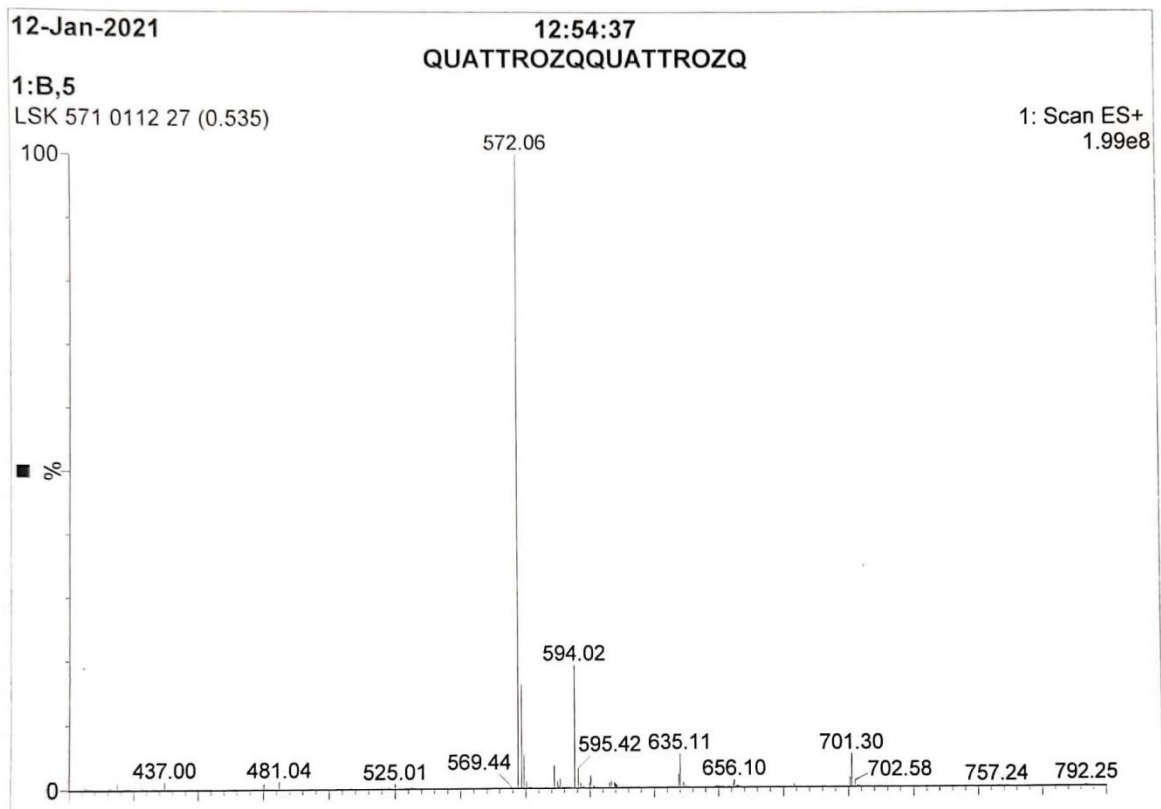


Fig. 57 Mass spectrum of compound B12

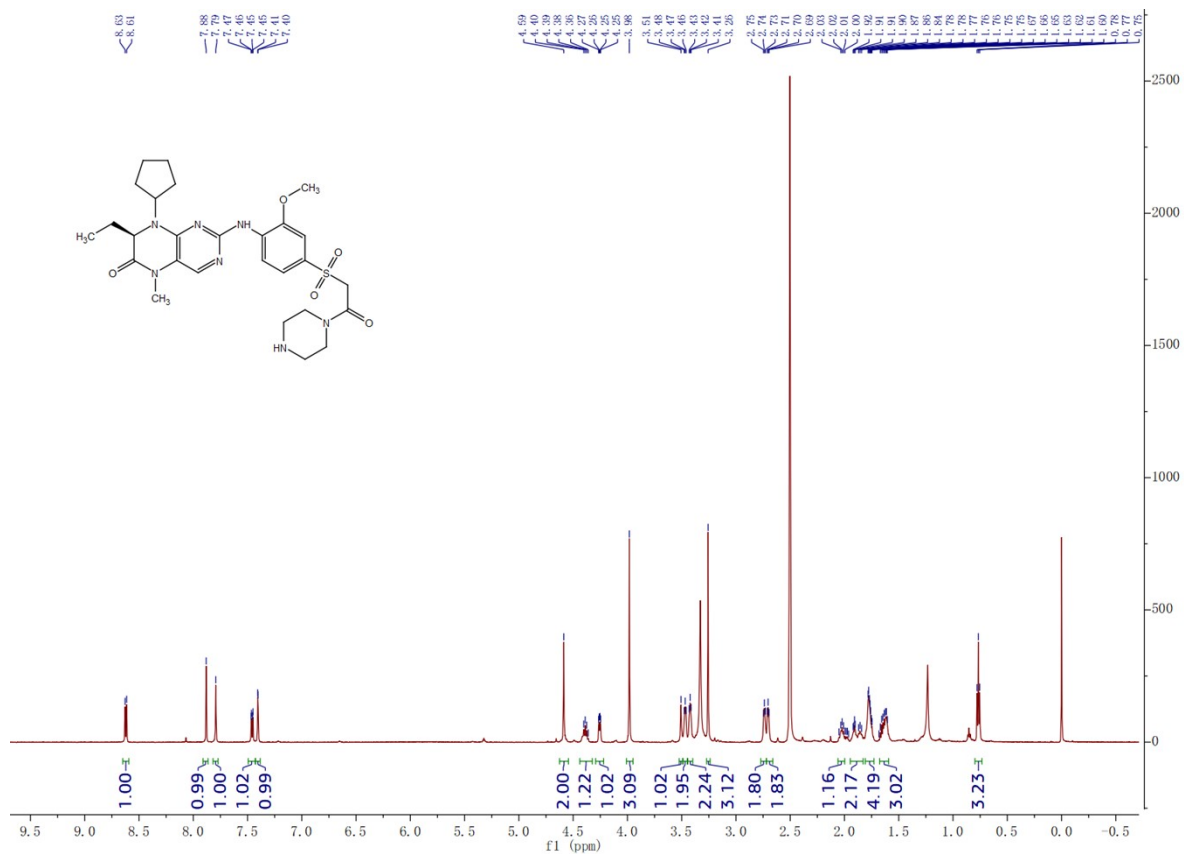


Fig. 58 ¹H NMR spectrum of compound B12

MS Spectrum

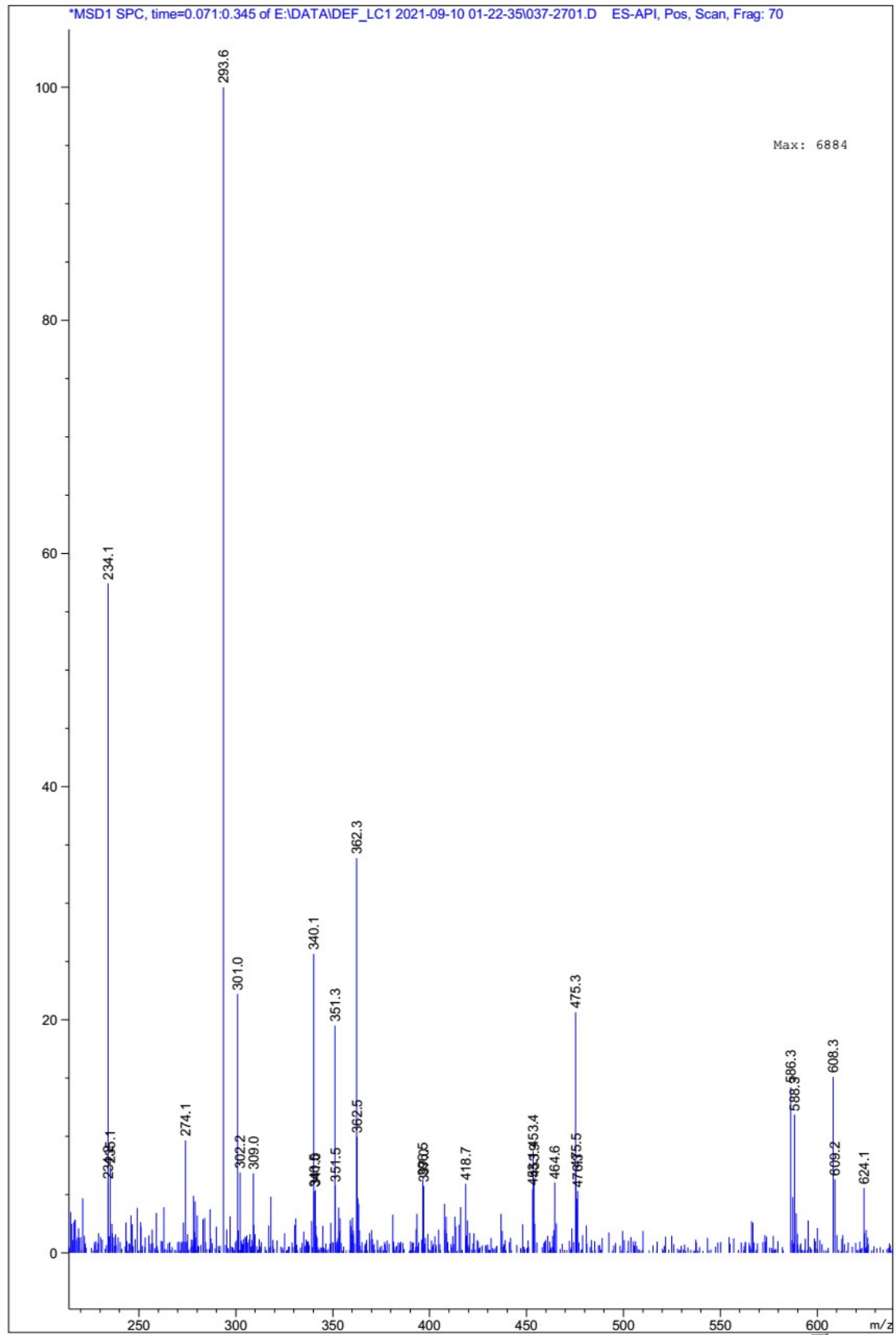


Fig. 59 Mass spectrum of compound B13

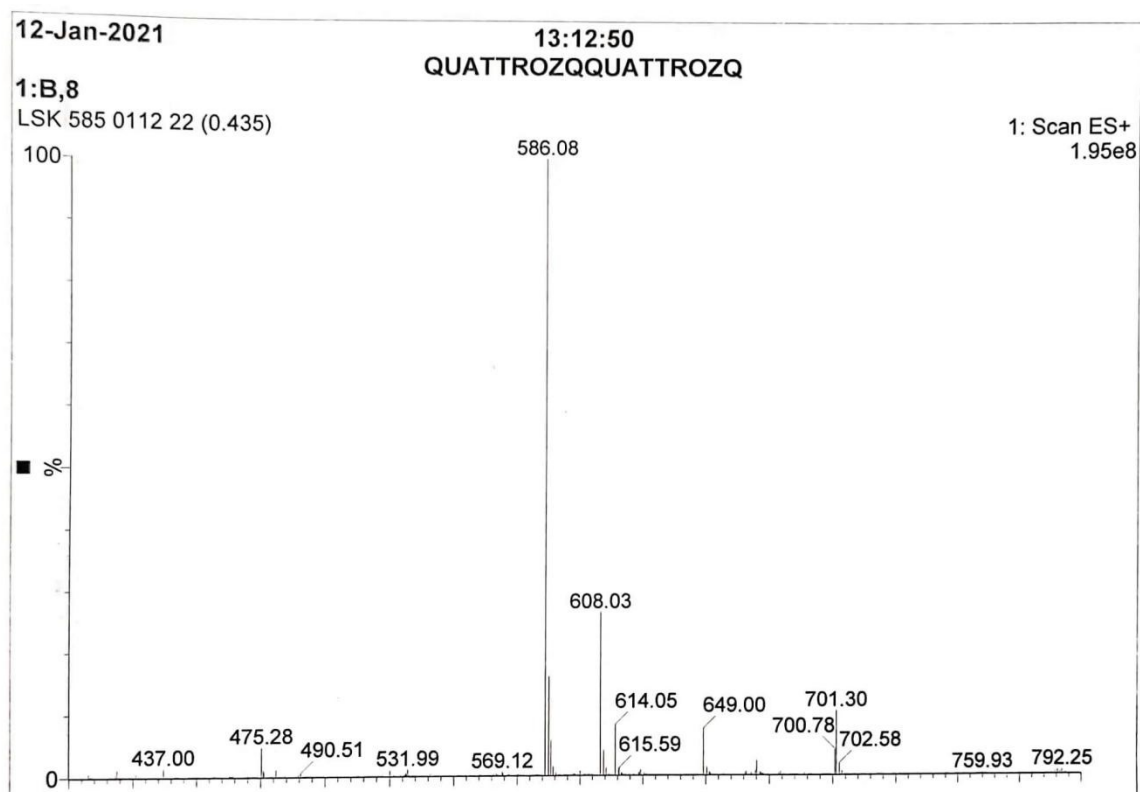


Fig. 60 Mass spectrum of compound B14

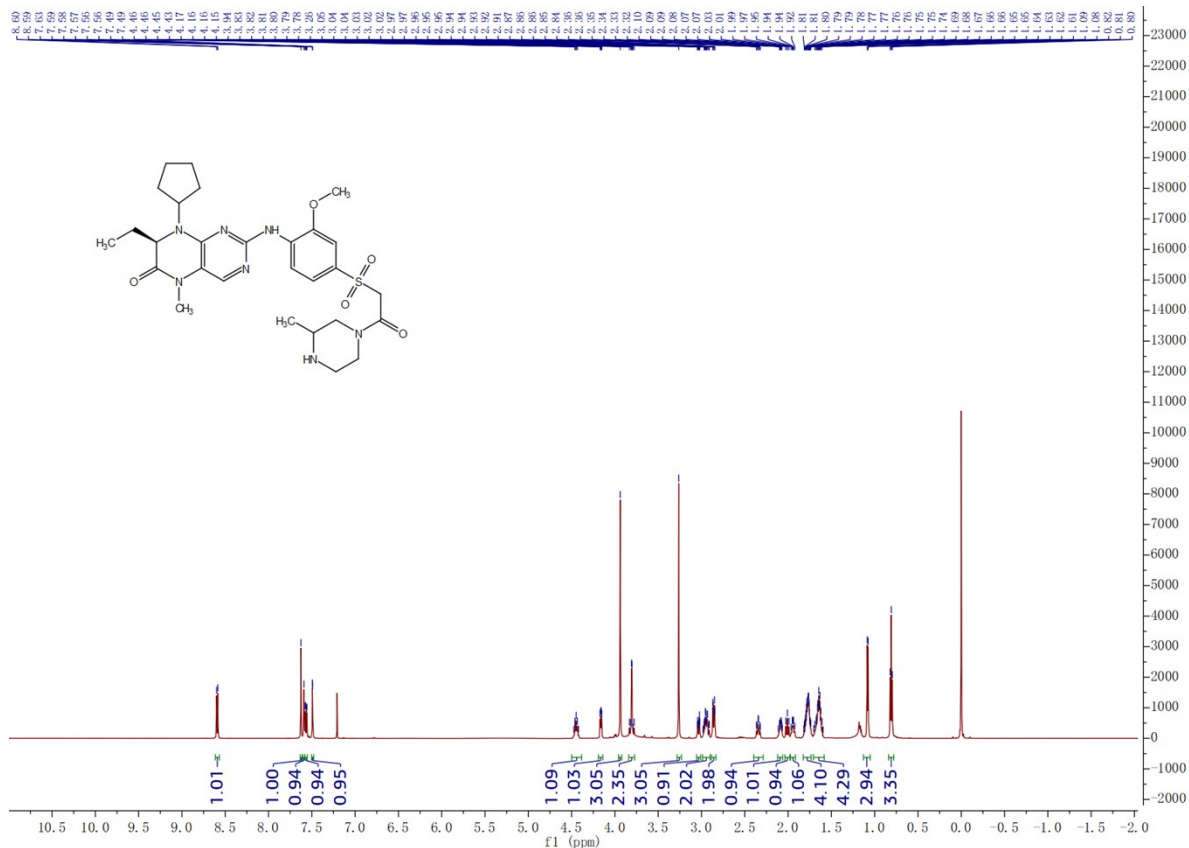


Fig. 61 ¹H NMR spectrum of compound B14

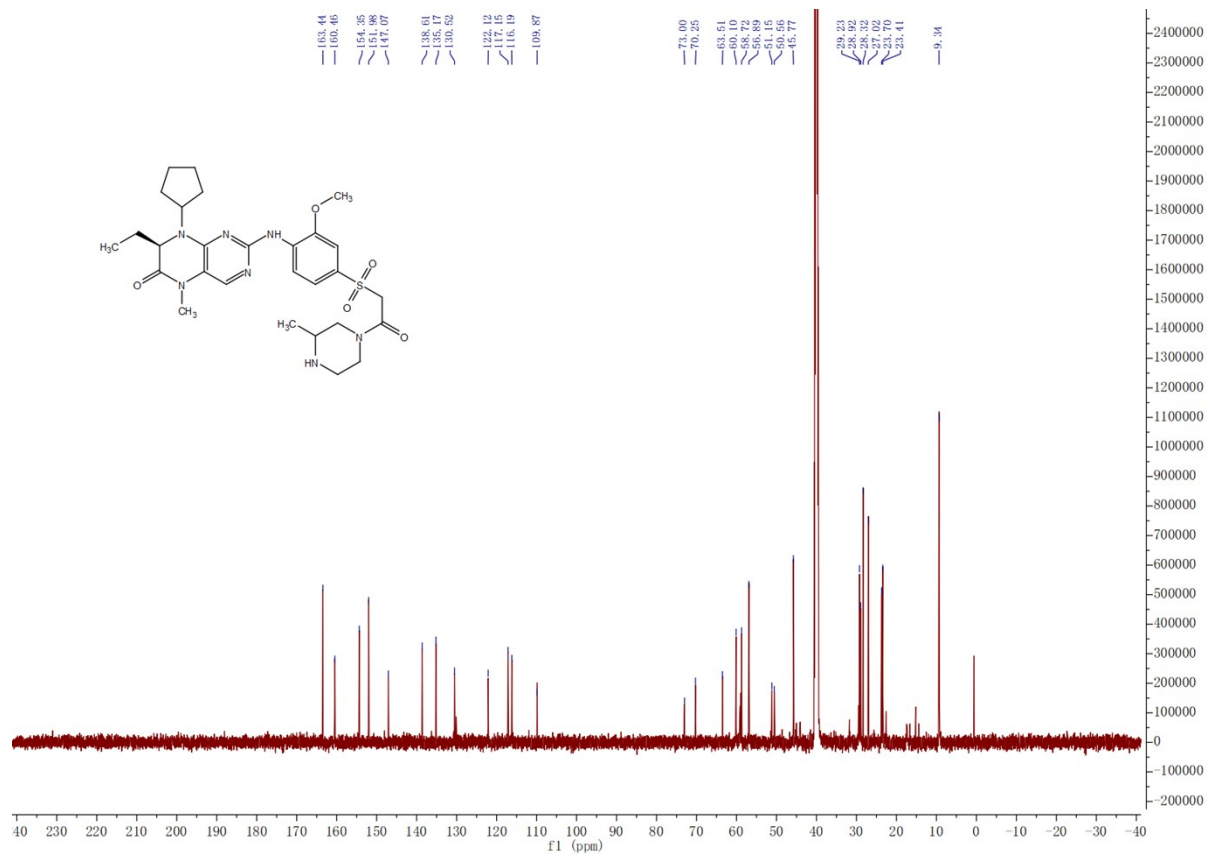


Fig. 62 ^{13}C NMR spectrum of compound B14