Supplementary Information

Structure-based design of 2,4-diaminopyrimidine derivatives bearing pyrrolyl group as ALK & ROS1 inhibitors

Jie Wang[a], Shangfei Wei[a], Tong Li[a], Lingyun Xing [a], Meng Cao[a], Nan Jiang[a], Ming Guo[a], Daiying Zuo[b, *], Xin Zhai[a,*]

[a] Key Laboratory of Structure-Based Drug Design and Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, PR China

[b] Department of Pharmacology, Shenyang Pharmaceutical University, Shenyang 110016, China.

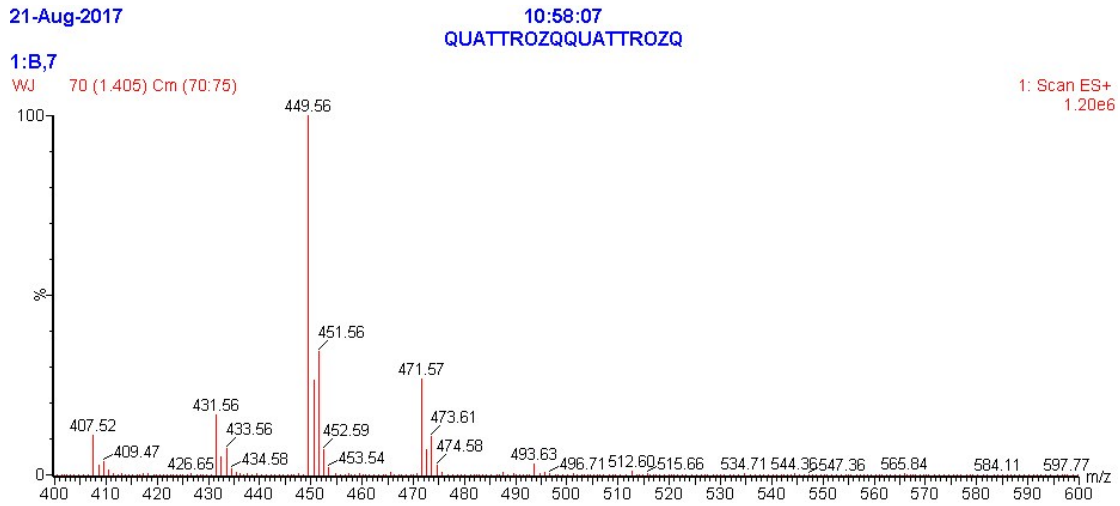

Fig. 1-1 MS spectrum of **9a**

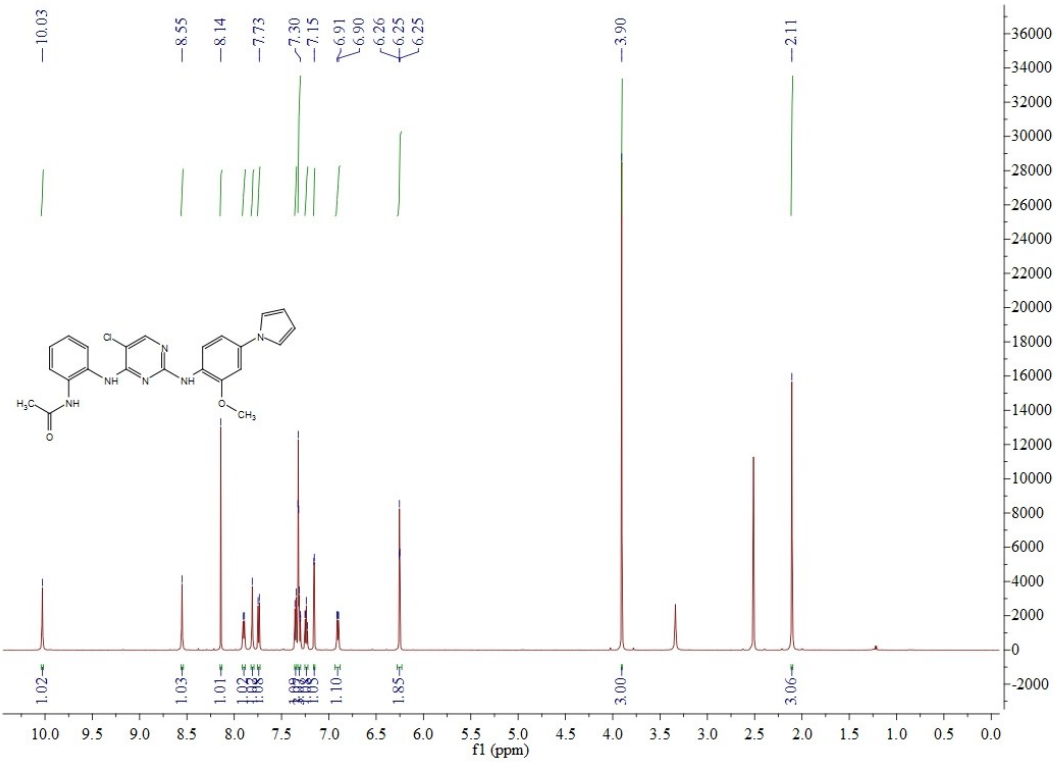

Fig. 1-2 ^{1}H-NMR spectrum of **9a**

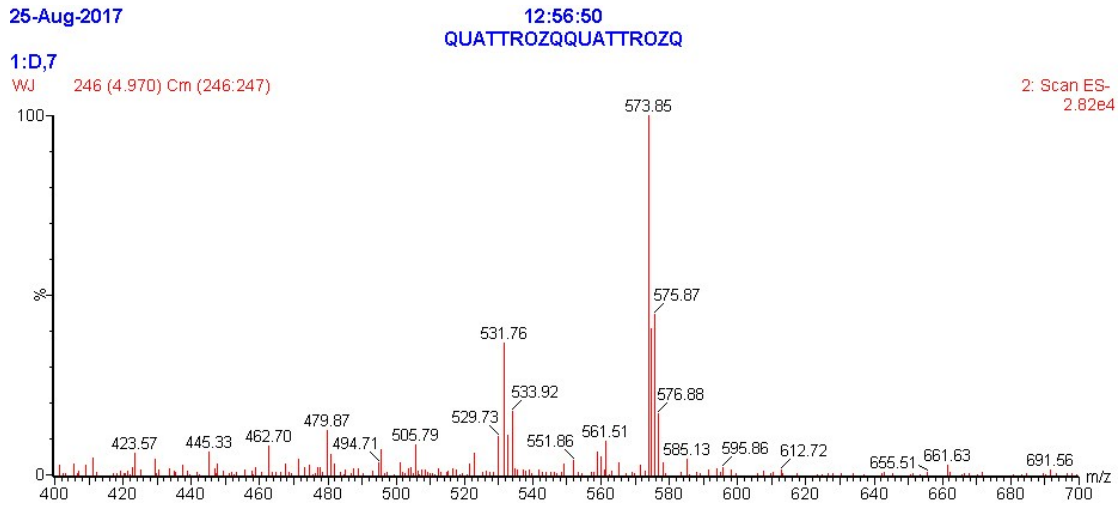

Fig. 2-1 MS spectrum of **9b**

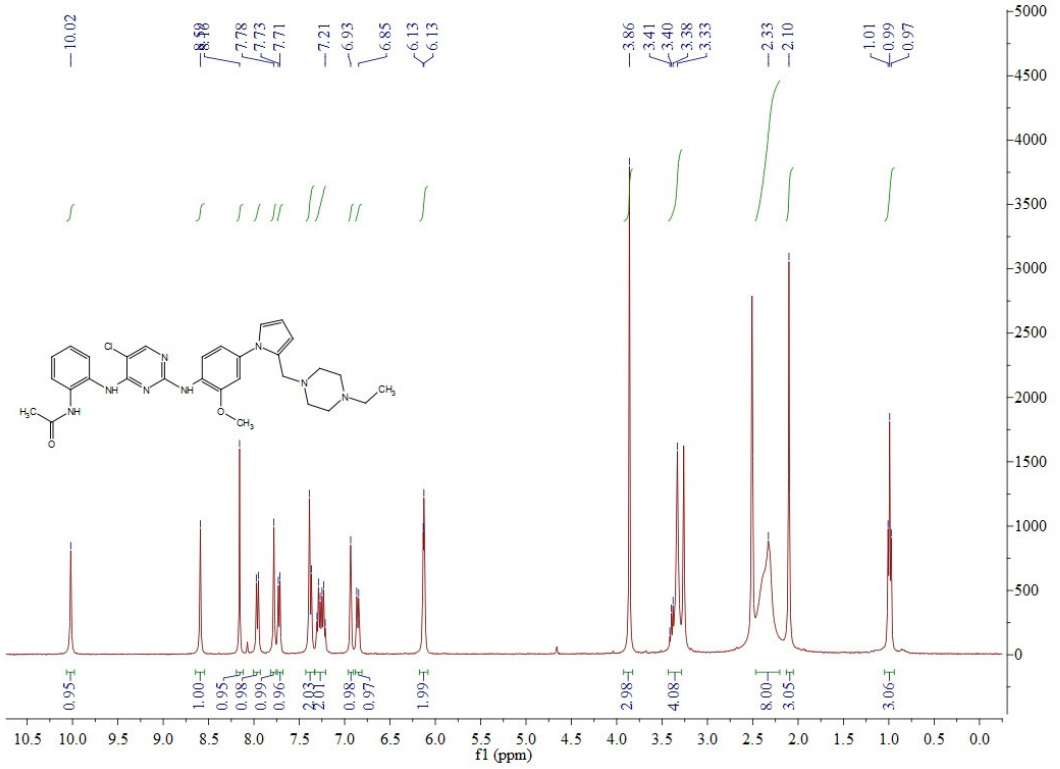

Fig. 2-2 ^{1}H-NMR spectrum of **9b**

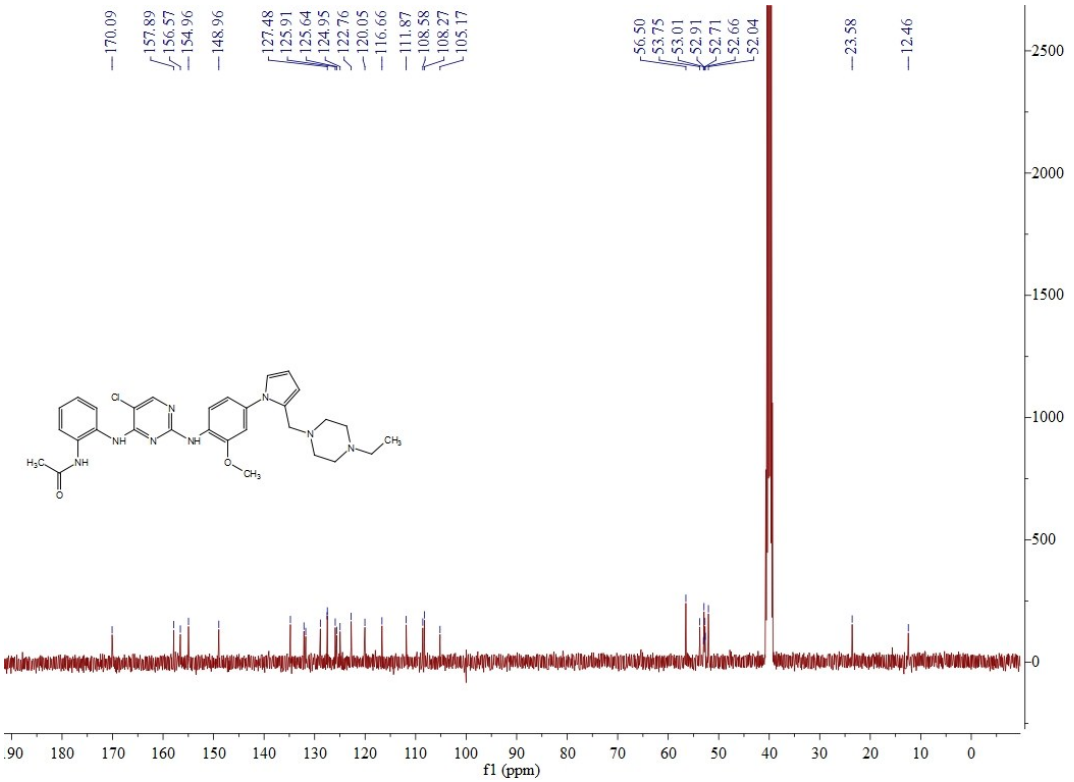

Fig. 2-3 ^{13}C-NMR spectrum of **9b**

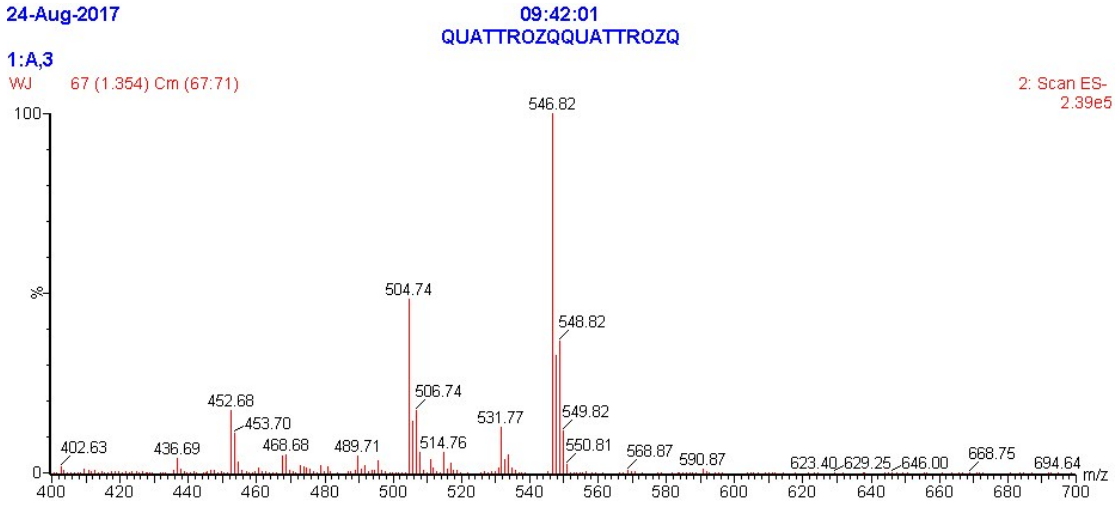

Fig. 3-1 MS spectrum of **9c**

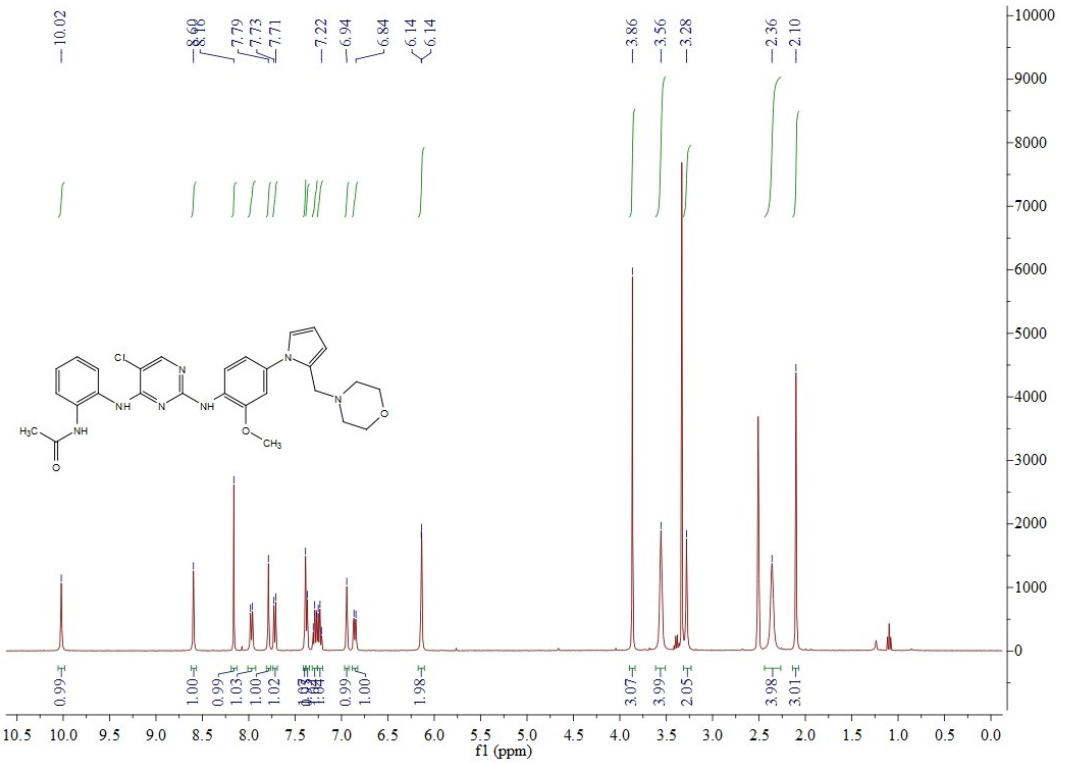

Fig. 3-2 ^{1}H-NMR spectrum of **9c**

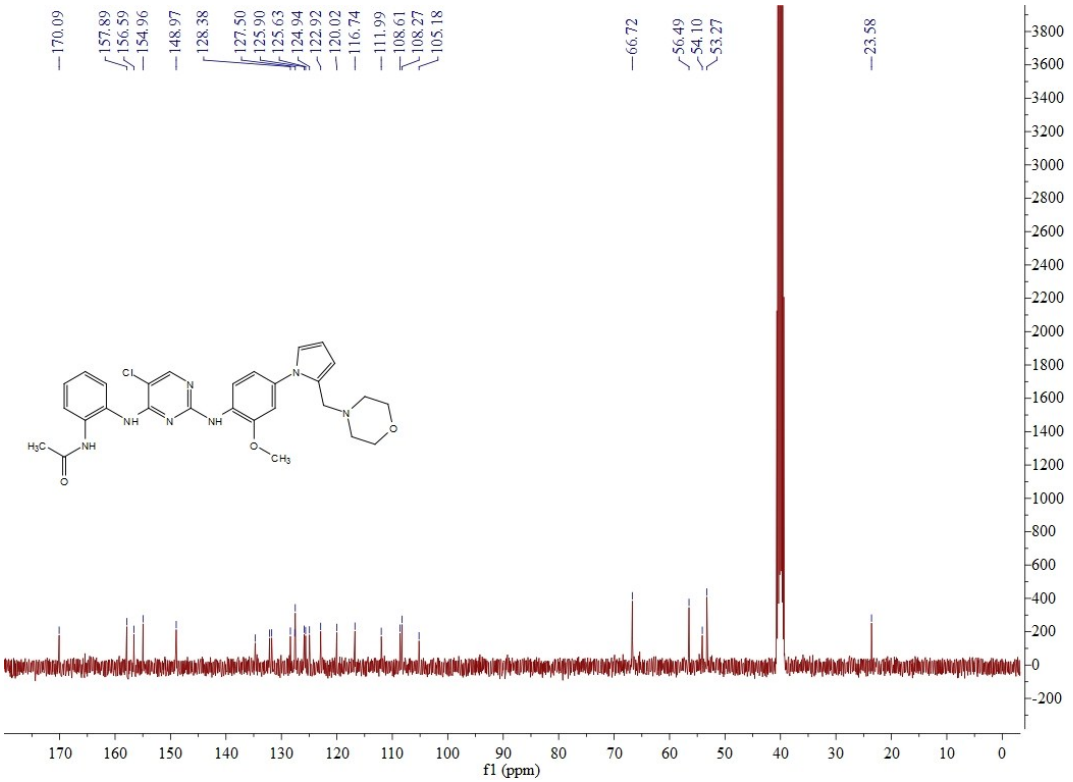

Fig. 3-3 ^{13}C-NMR spectrum of **9c**

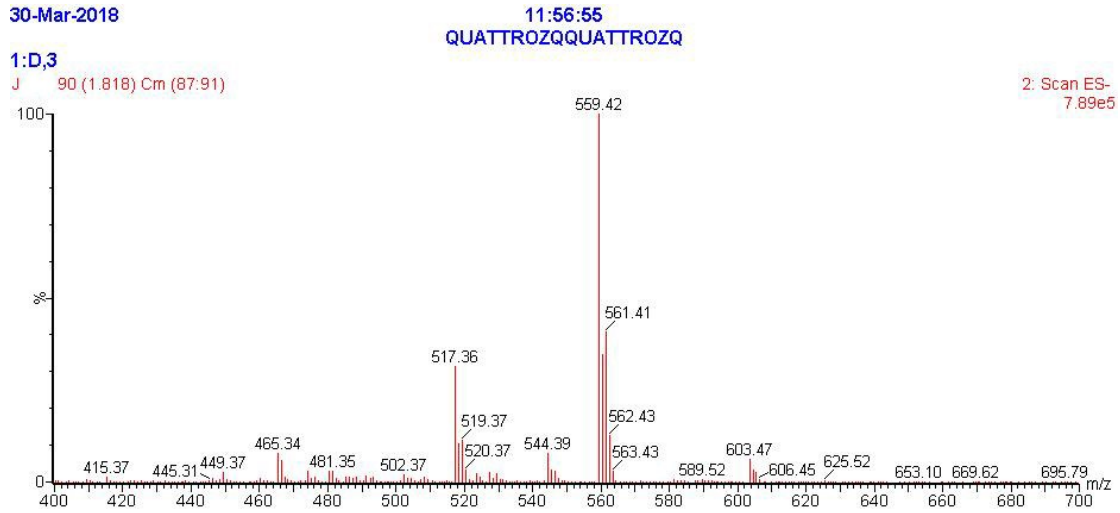

Fig. 4-1 MS spectrum of **9d**

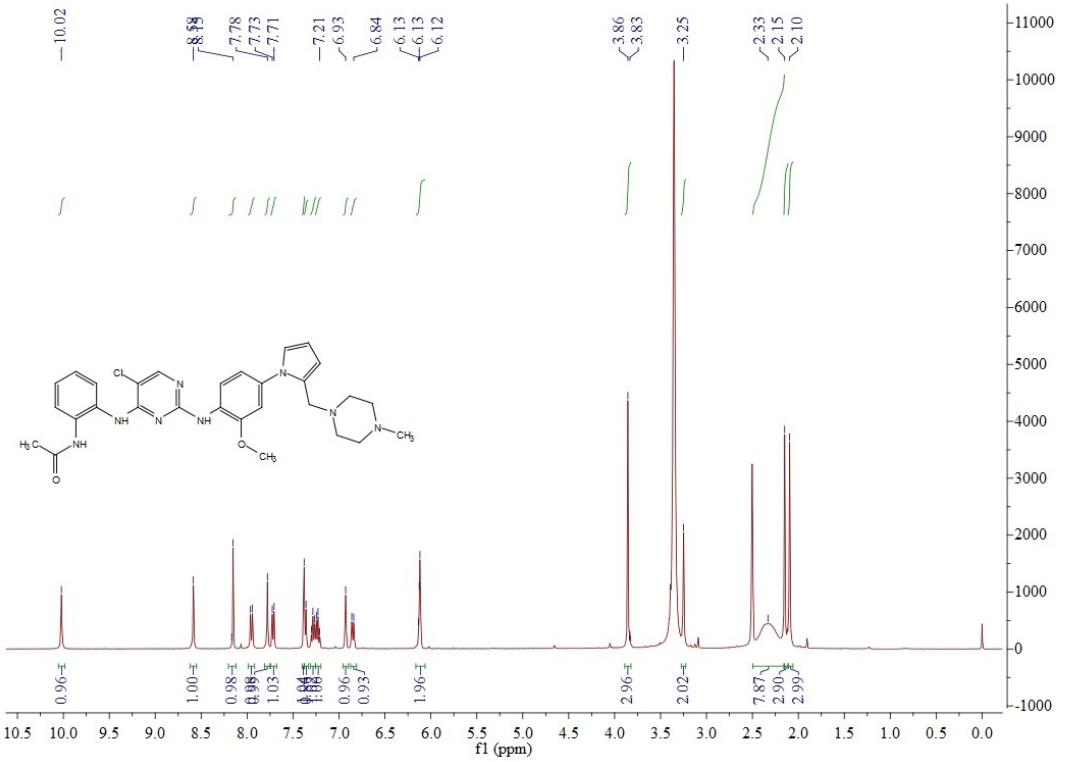

Fig. 4-2 ^{1}H-NMR spectrum of **9d**

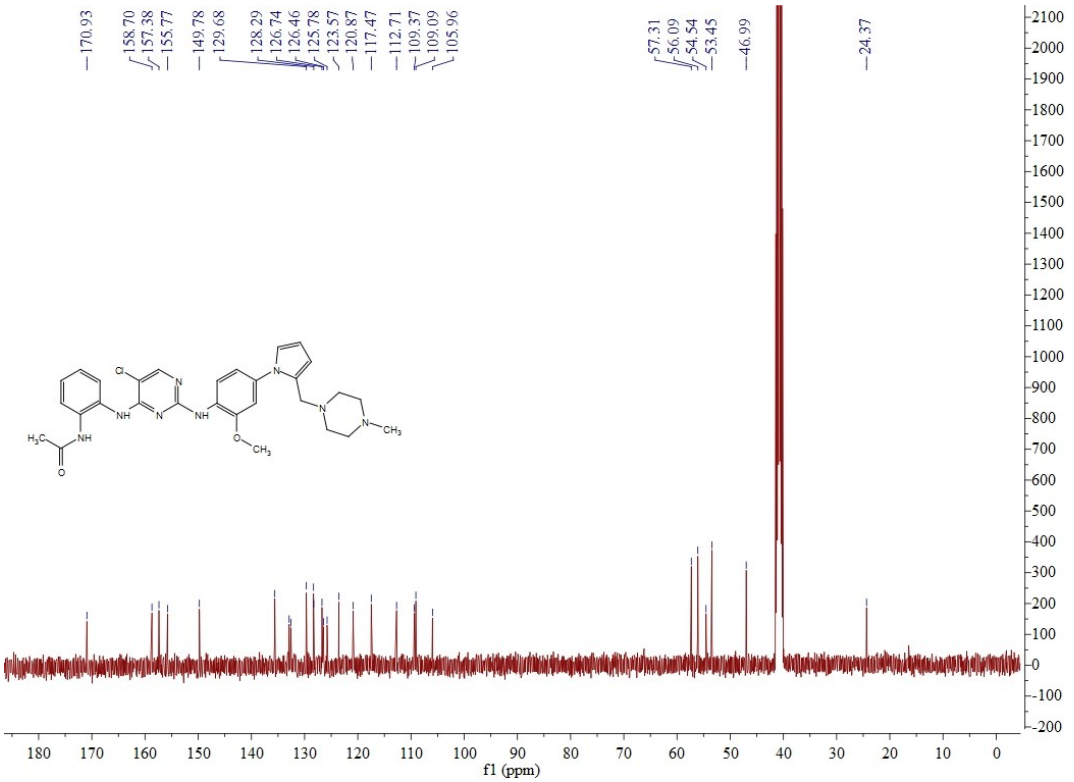

Fig. 4-3 ^{13}C-NMR spectrum of **9d**

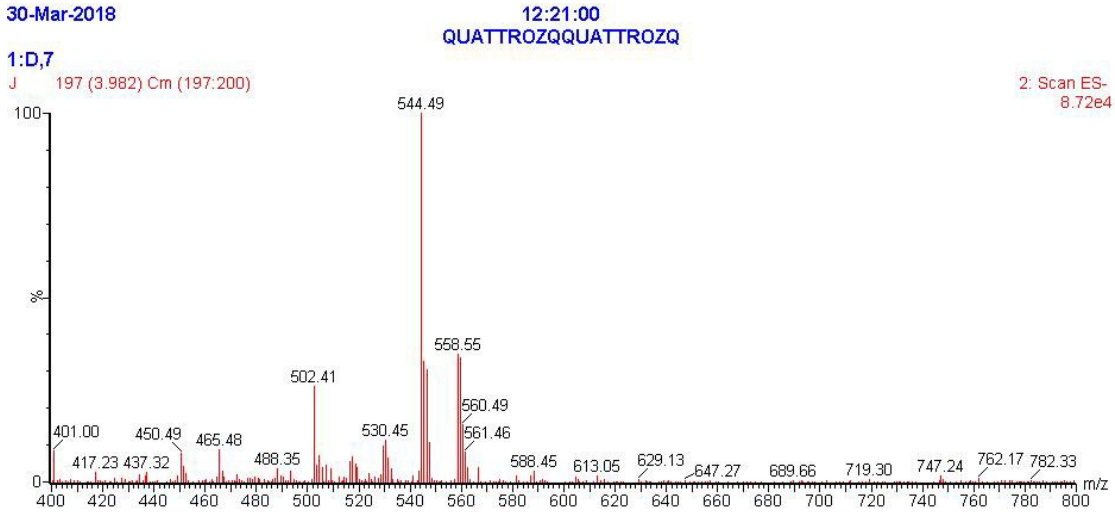

Fig. 5-1 MS spectrum of **9e**

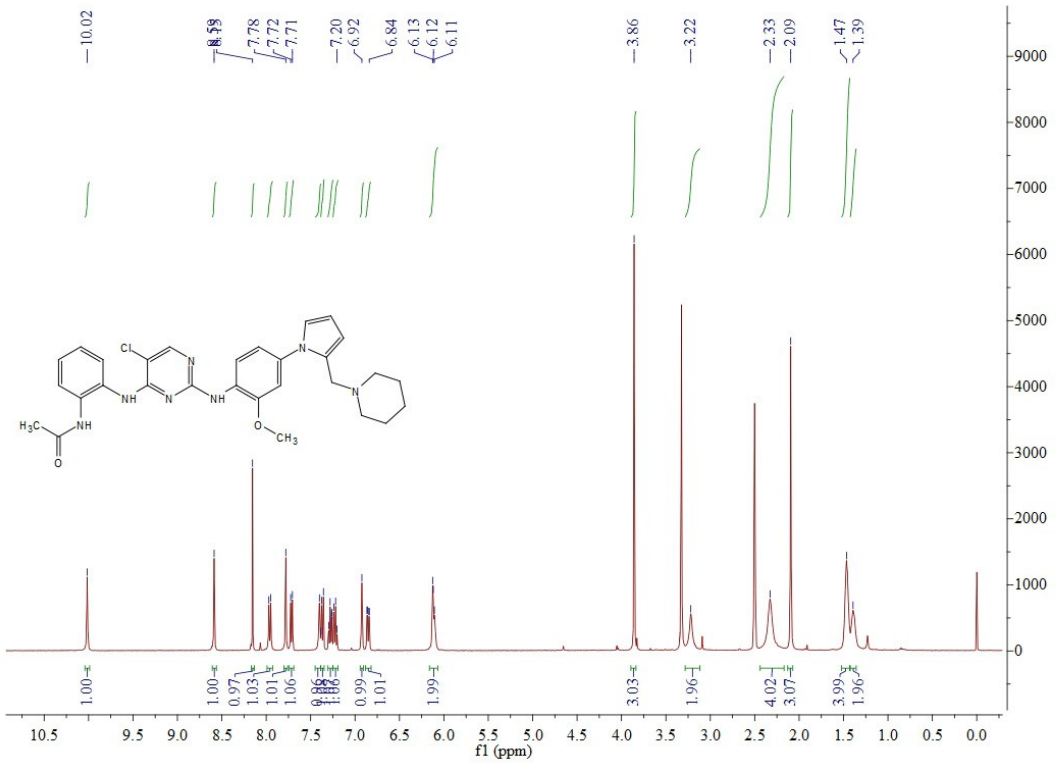

Fig. 5-2 ^{1}H-NMR spectrum of **9e**

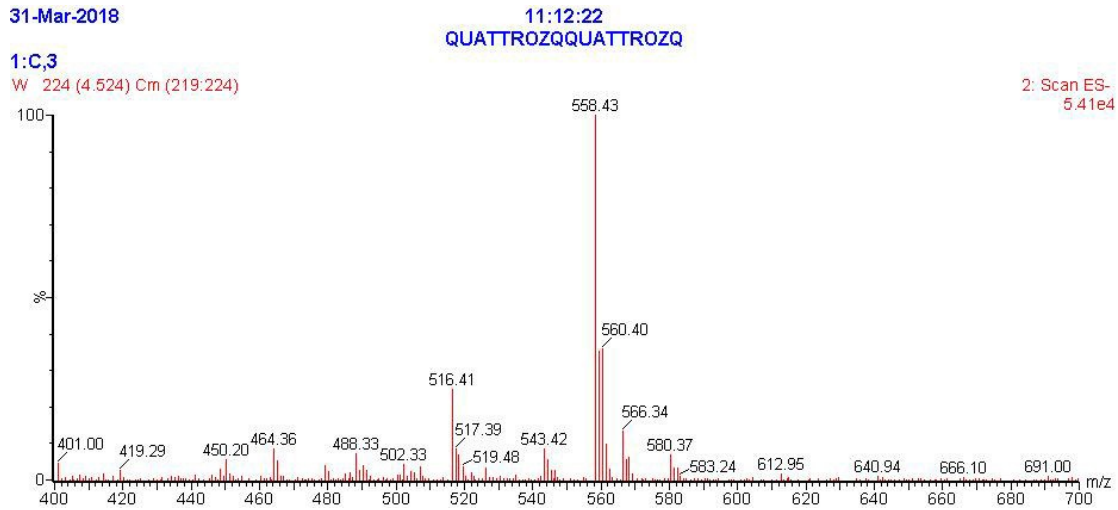

Fig. 6-1 MS spectrum of **9f**

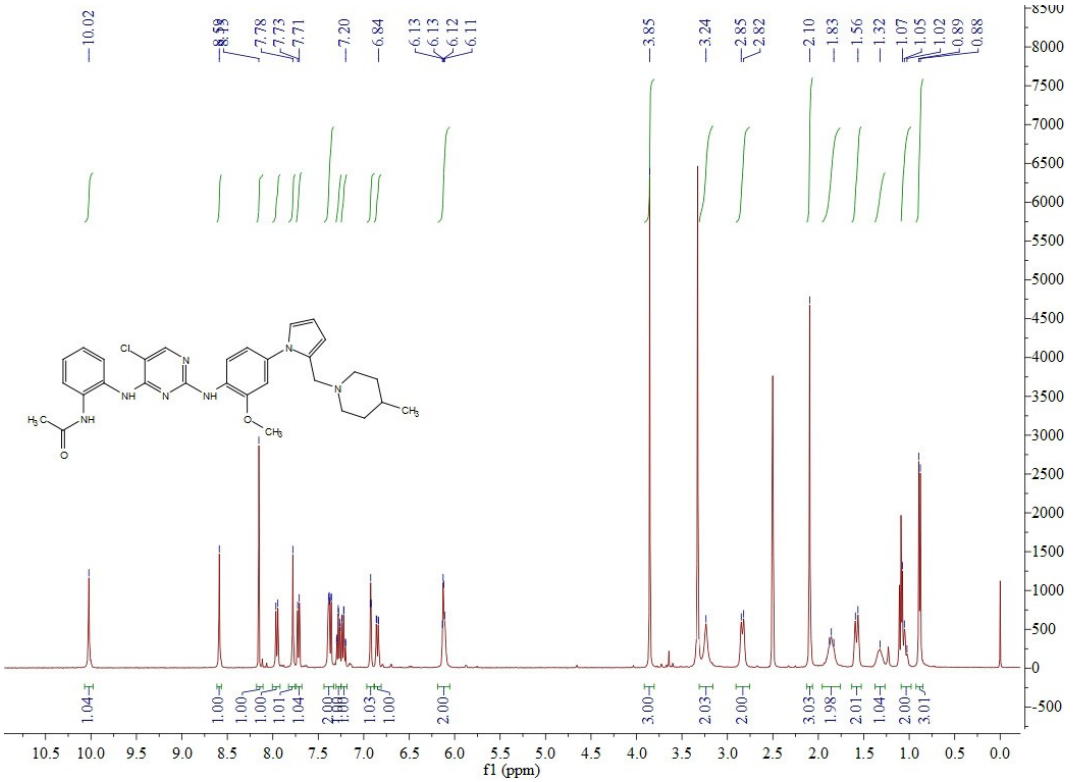

Fig. 6-2 ^{1}H-NMR spectrum of **9f**

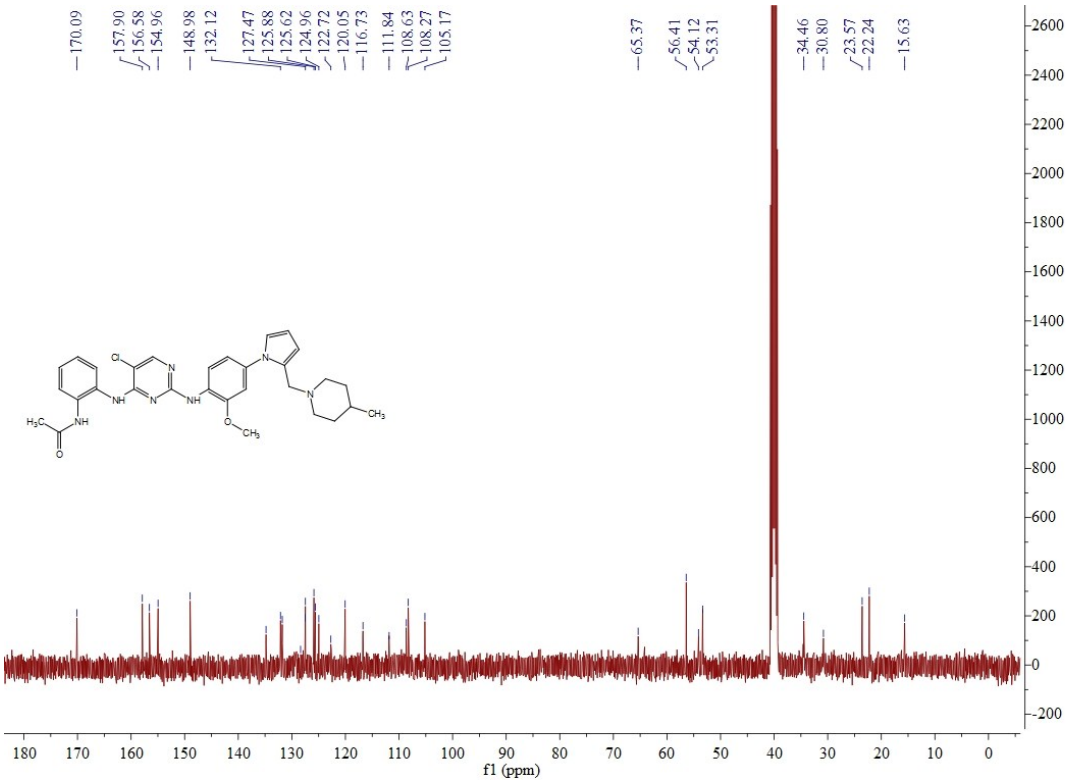

Fig. 6-3 ^{13}C-NMR spectrum of **9f**

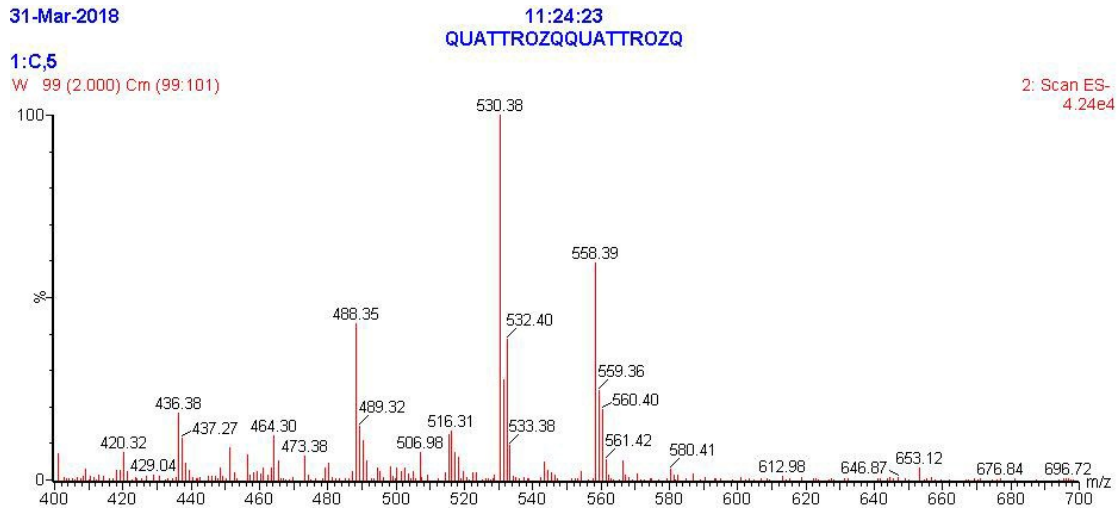

Fig. 7-1 MS spectrum of **9g**

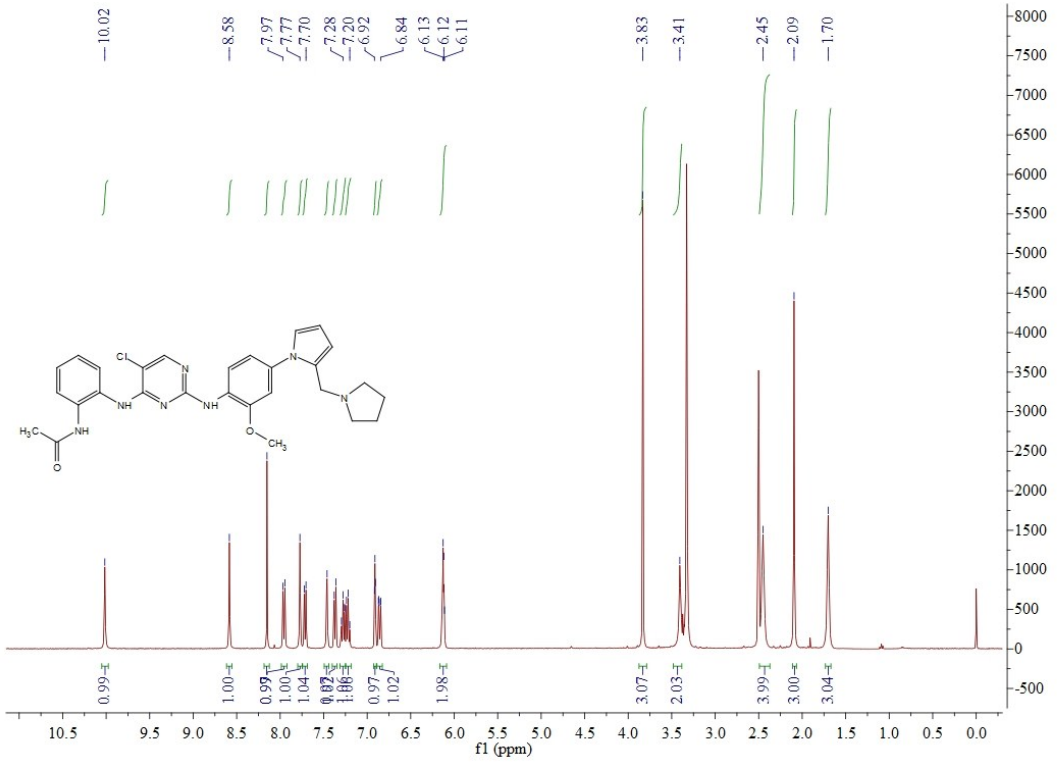

Fig. 7-2 ^{1}H-NMR spectrum of **9g**

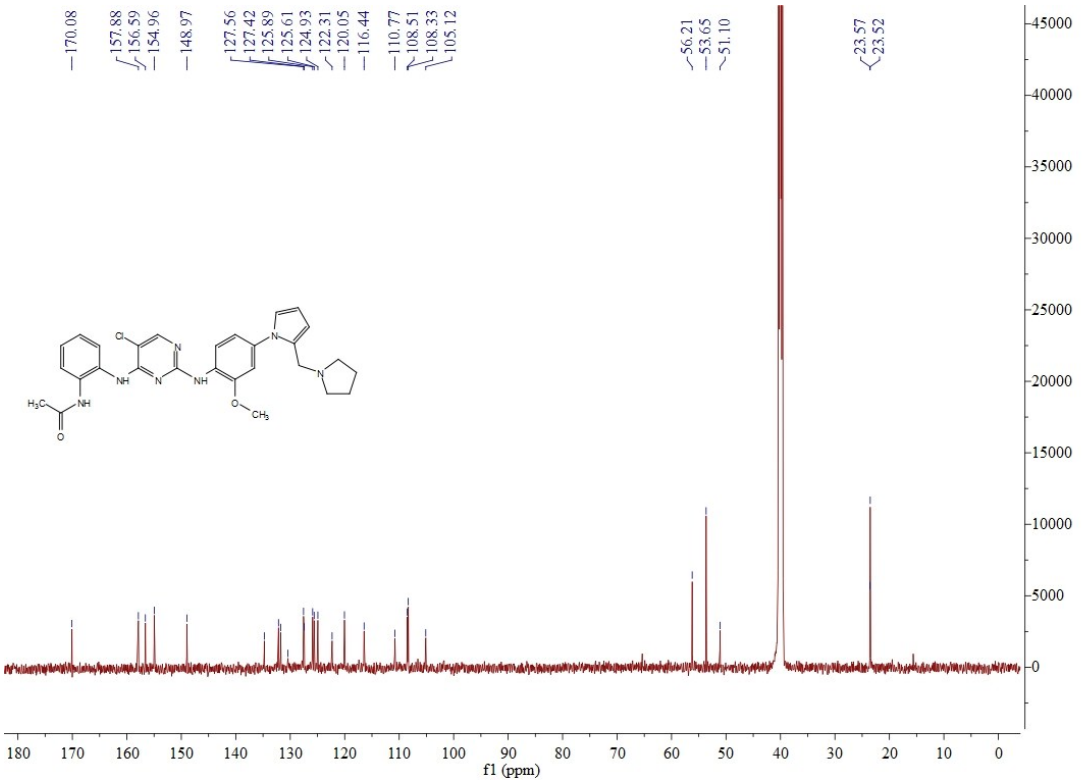

Fig. 7-3 ^{13}C-NMR spectrum of **9g**

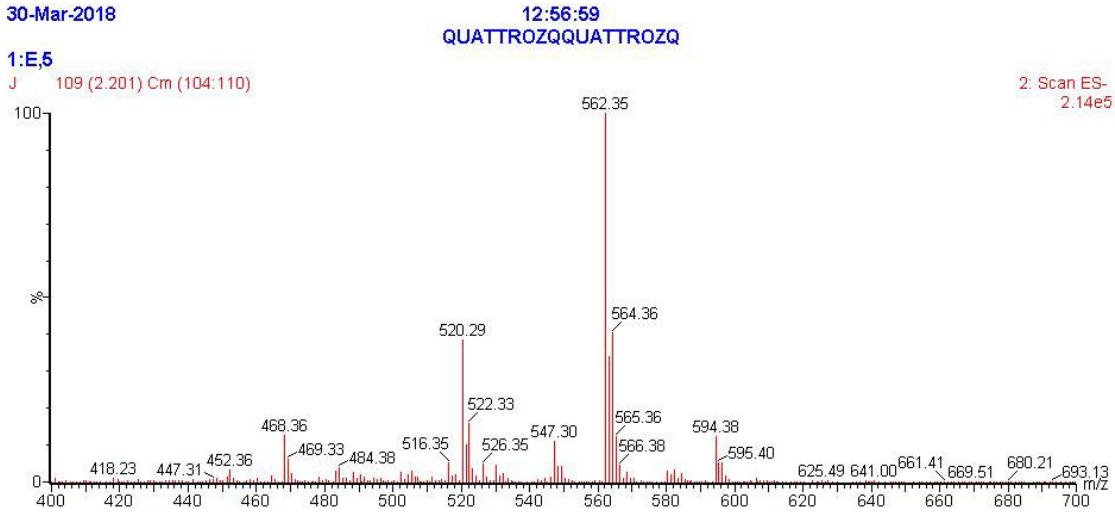

Fig. 8-1 MS spectrum of **9h**

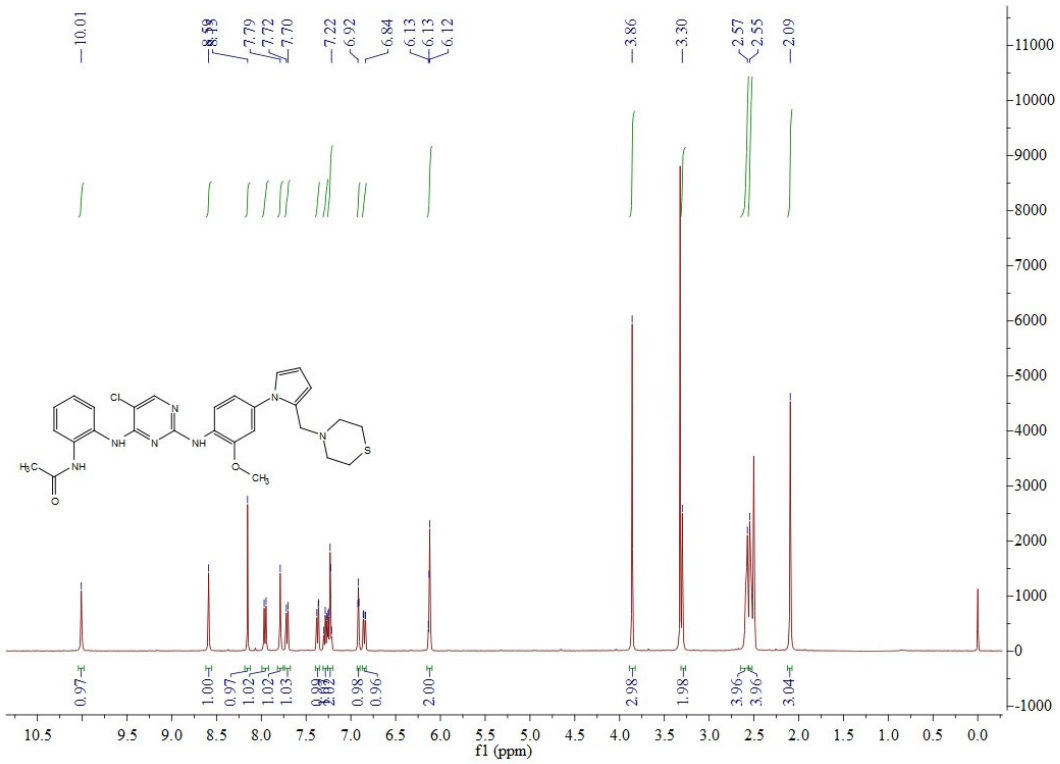

Fig. 8-2 ^{1}H-NMR spectrum of **9h**

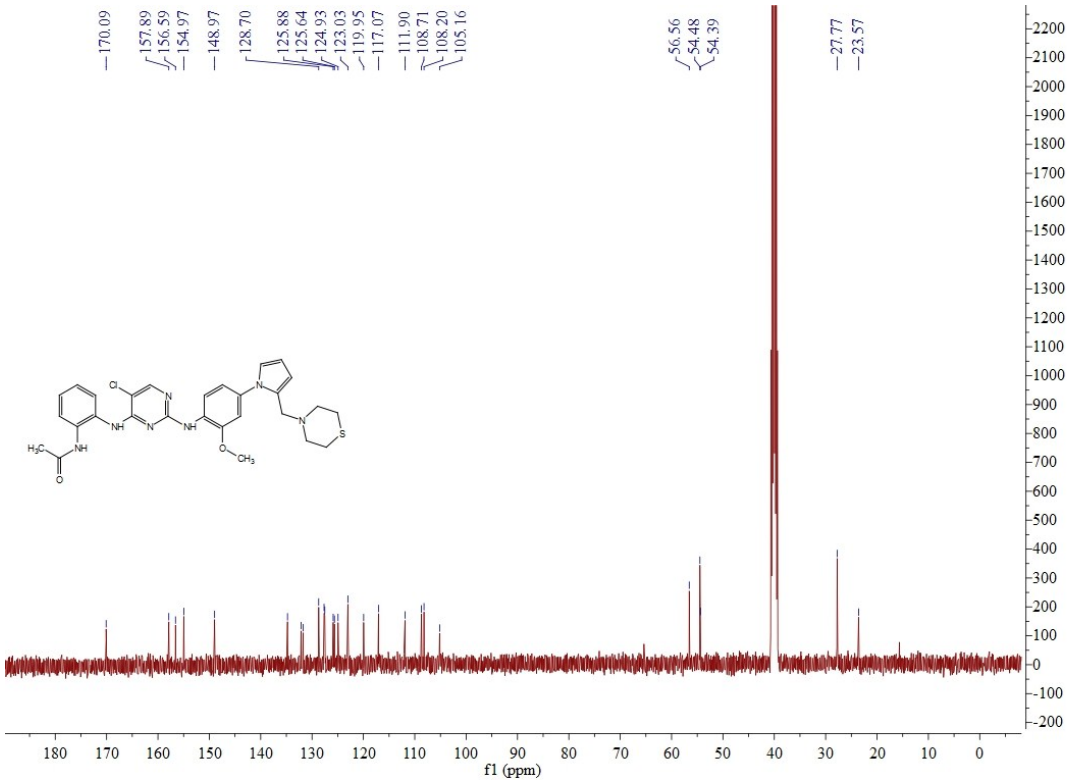

Fig. 8-3 ^{13}C-NMR spectrum of **9h**

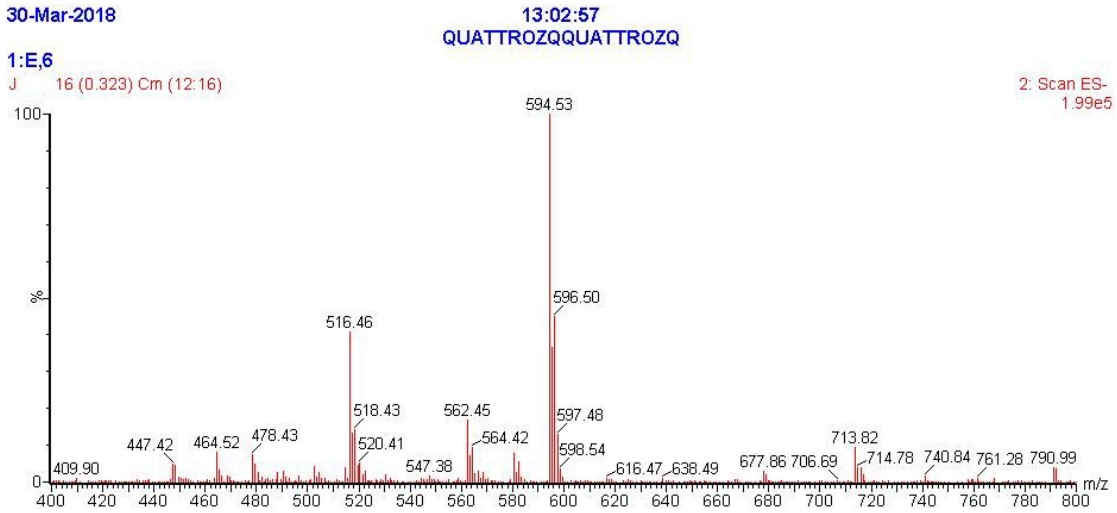

Fig. 9-1 MS spectrum of **9i**

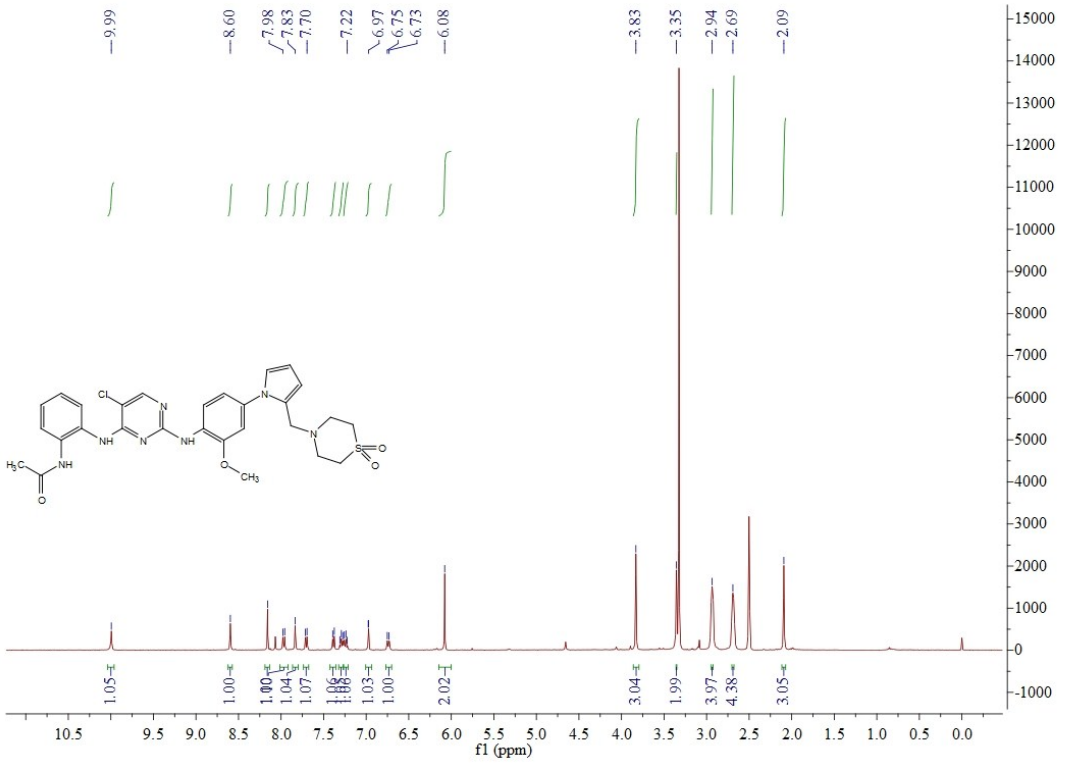

Fig. 9-2 ^{1}H-NMR spectrum of **9i**

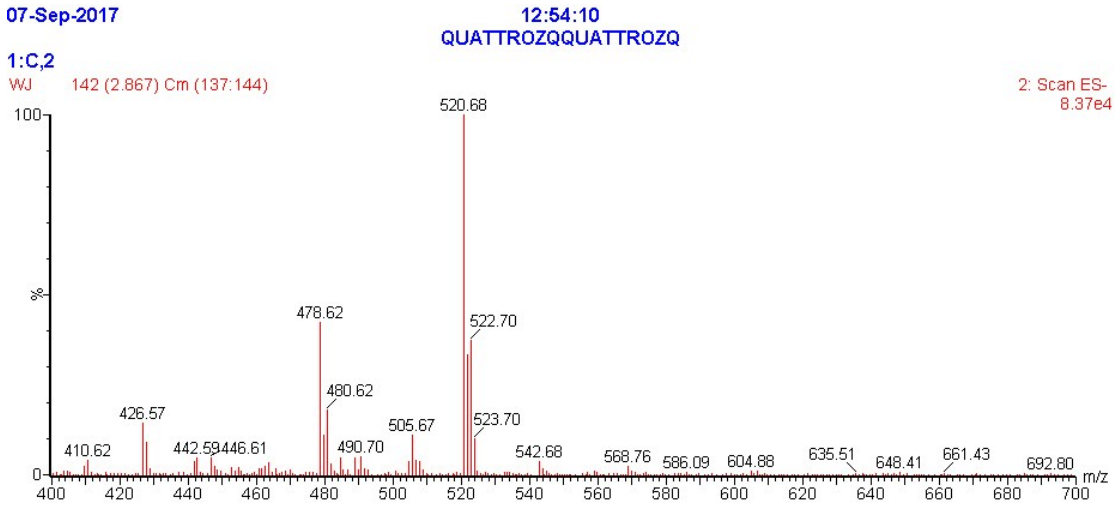

Fig. 10-1 MS spectrum of **9j**

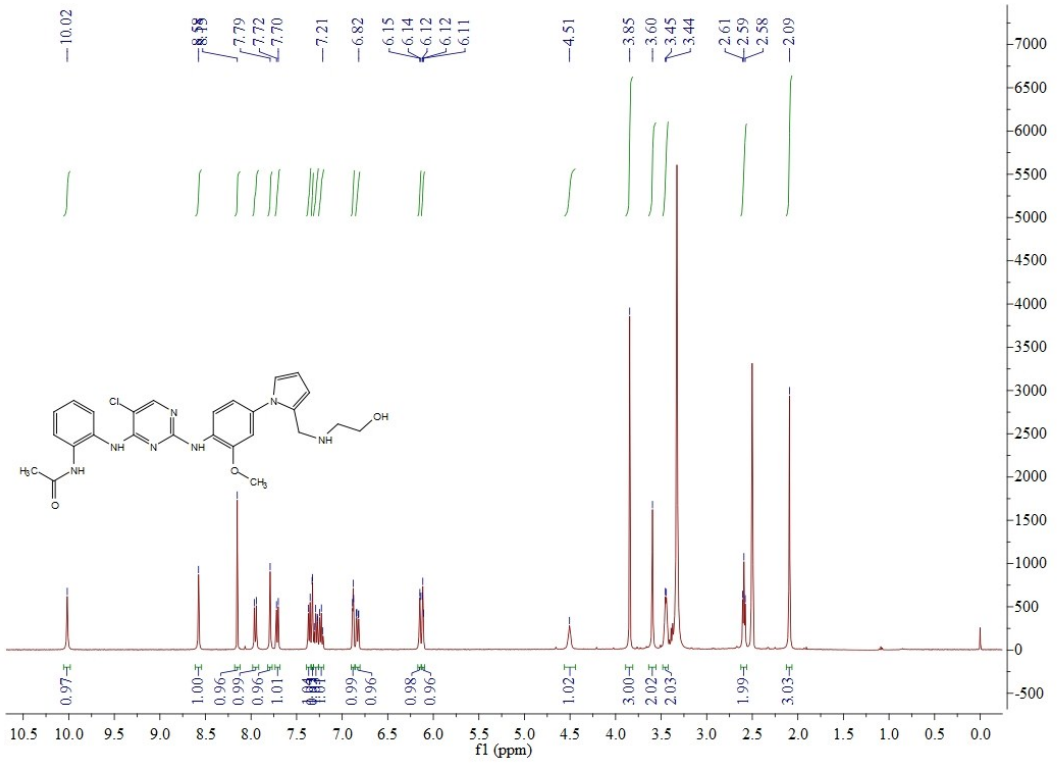

Fig. 10-2 ^{1}H-NMR spectrum of **9j**

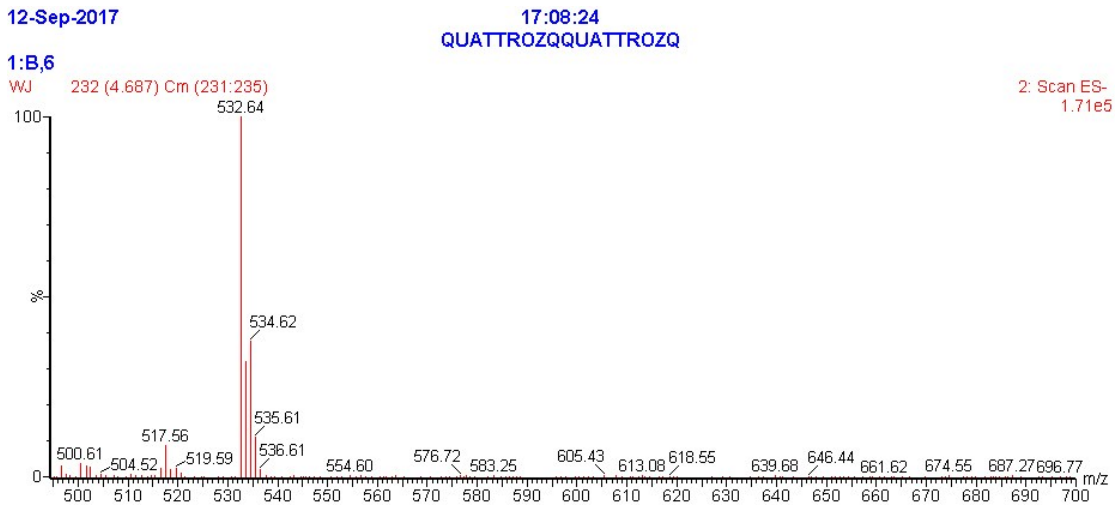

Fig. 11-1 MS spectrum of **9k**

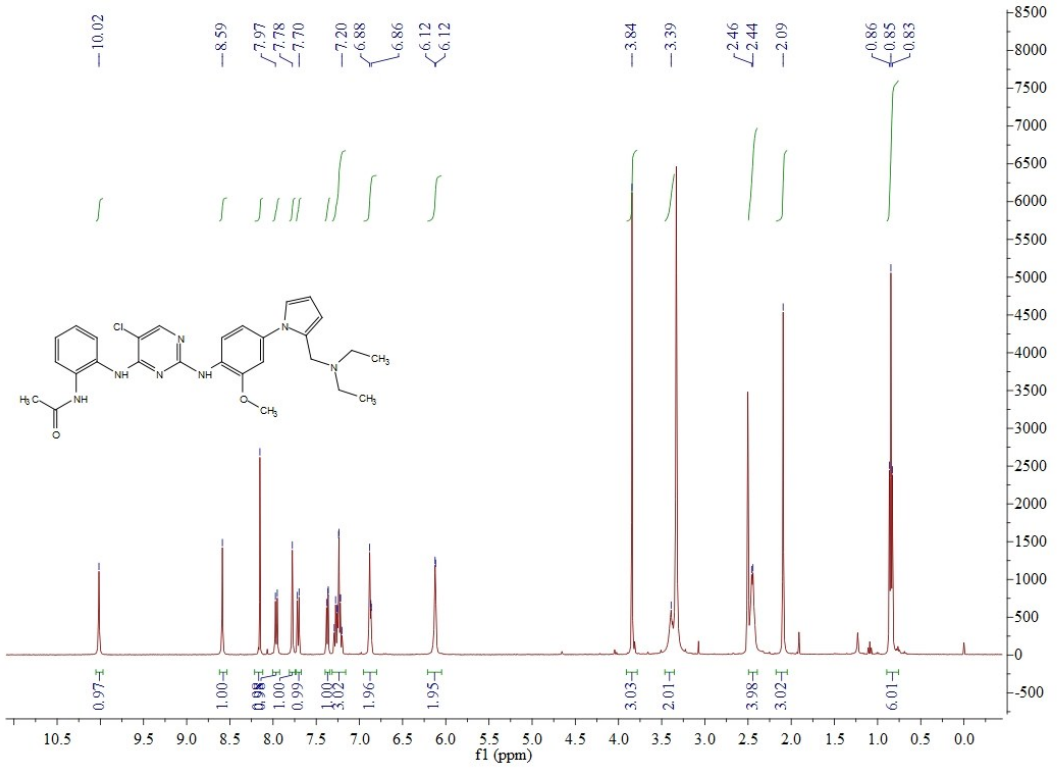

Fig. 11-2 ^{1}H-NMR spectrum of **9k**

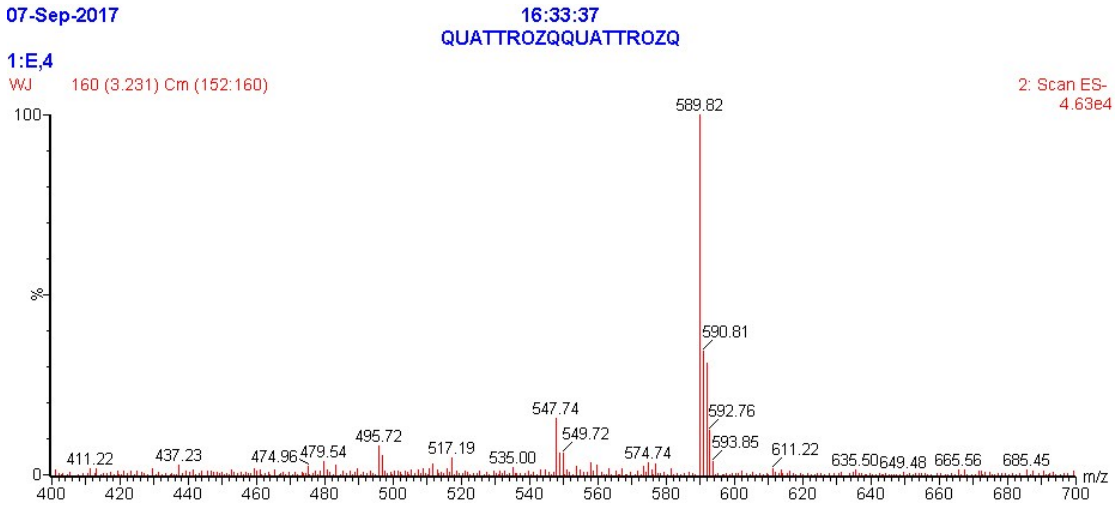

Fig. 12-1 MS spectrum of **9l**

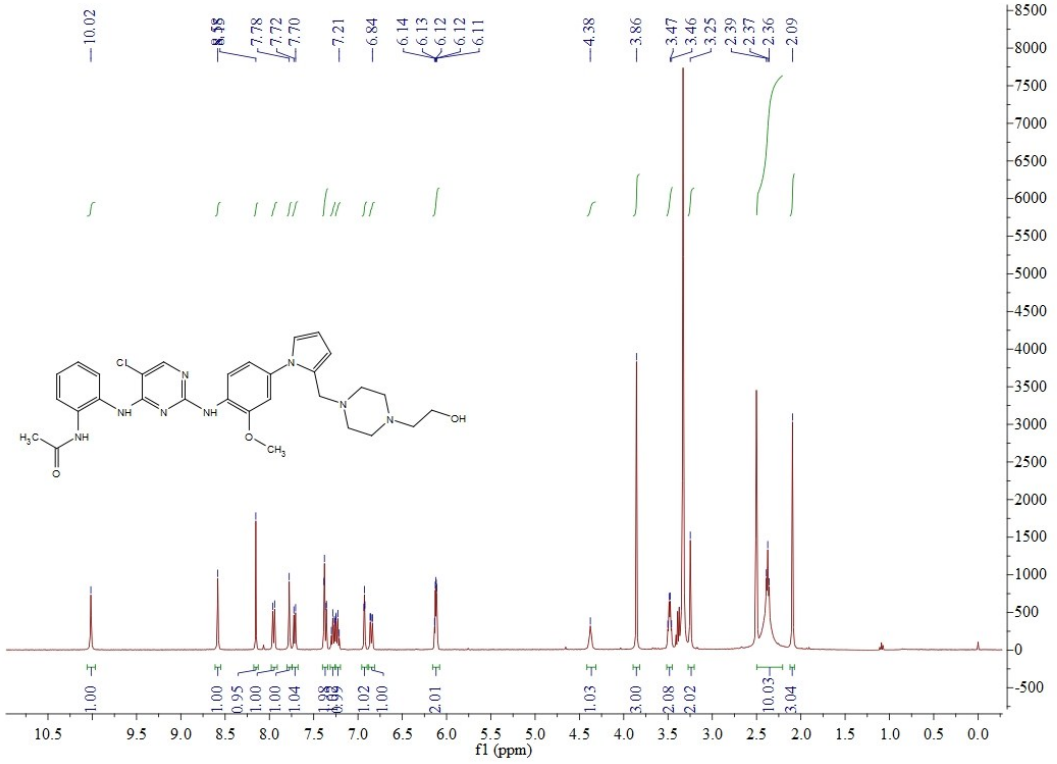

Fig. 12-2 ^{1}H-NMR spectrum of **9l**

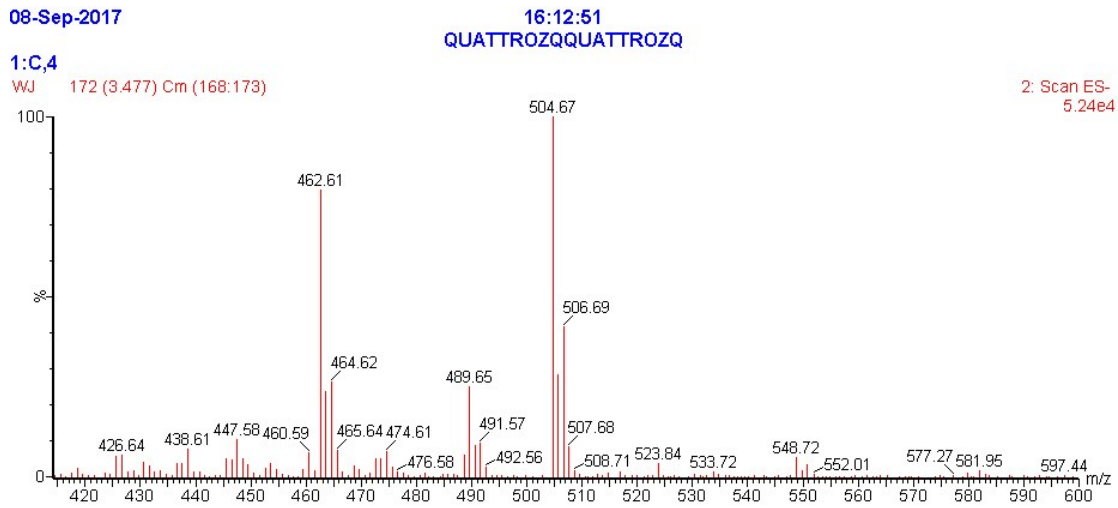

Fig. 13-1 MS spectrum of **9m**

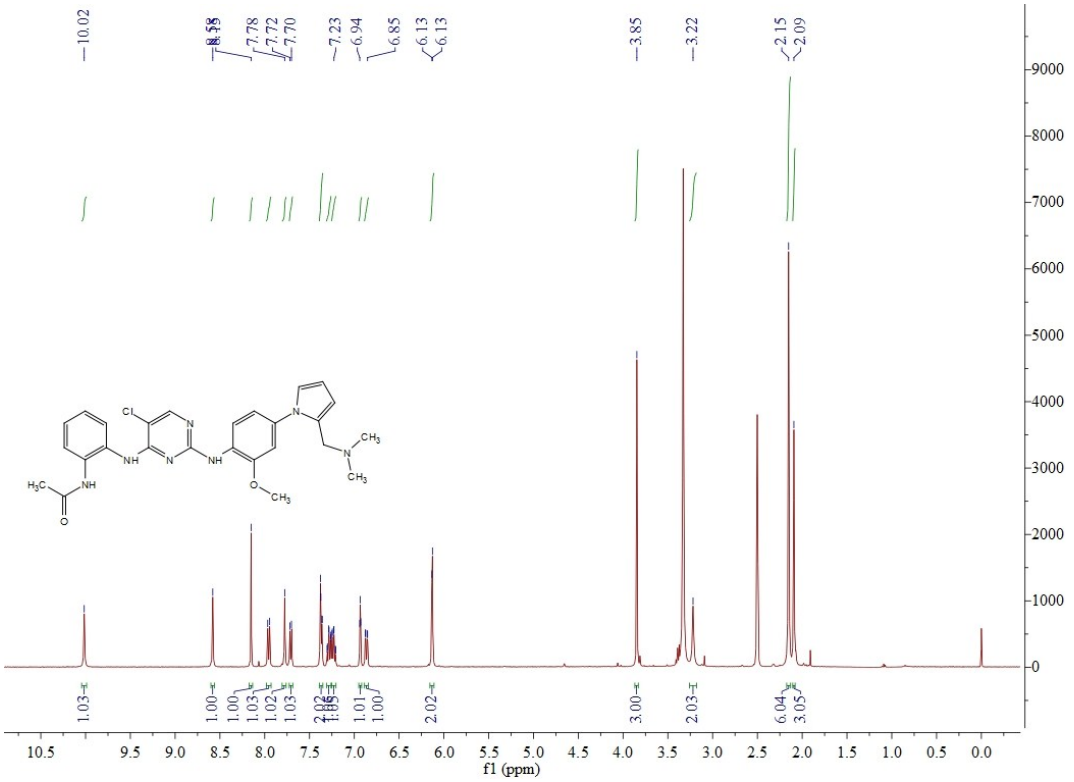

Fig. 13-2 ^{1}H-NMR spectrum of **9m**

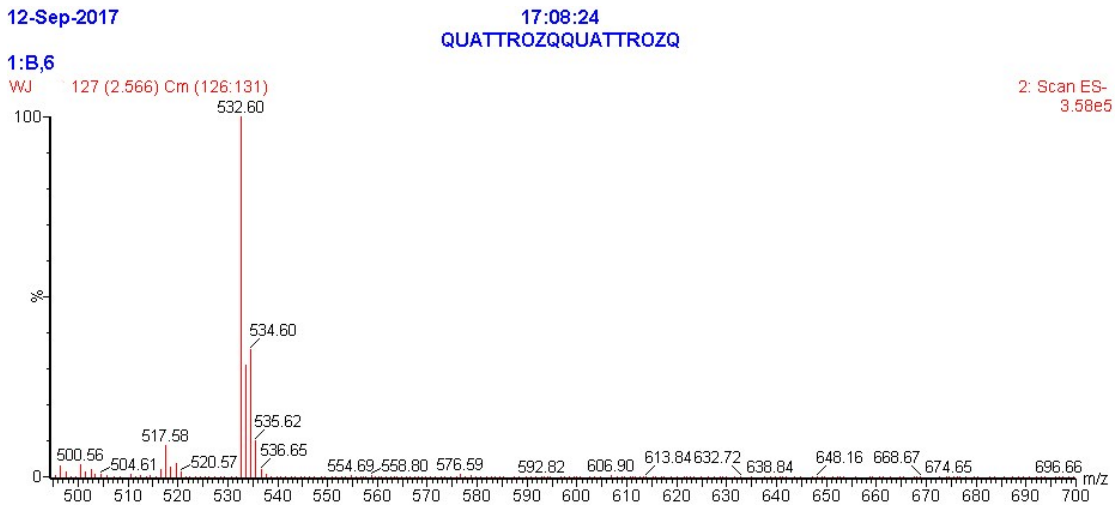

Fig. 14-1 MS spectrum of **9n**

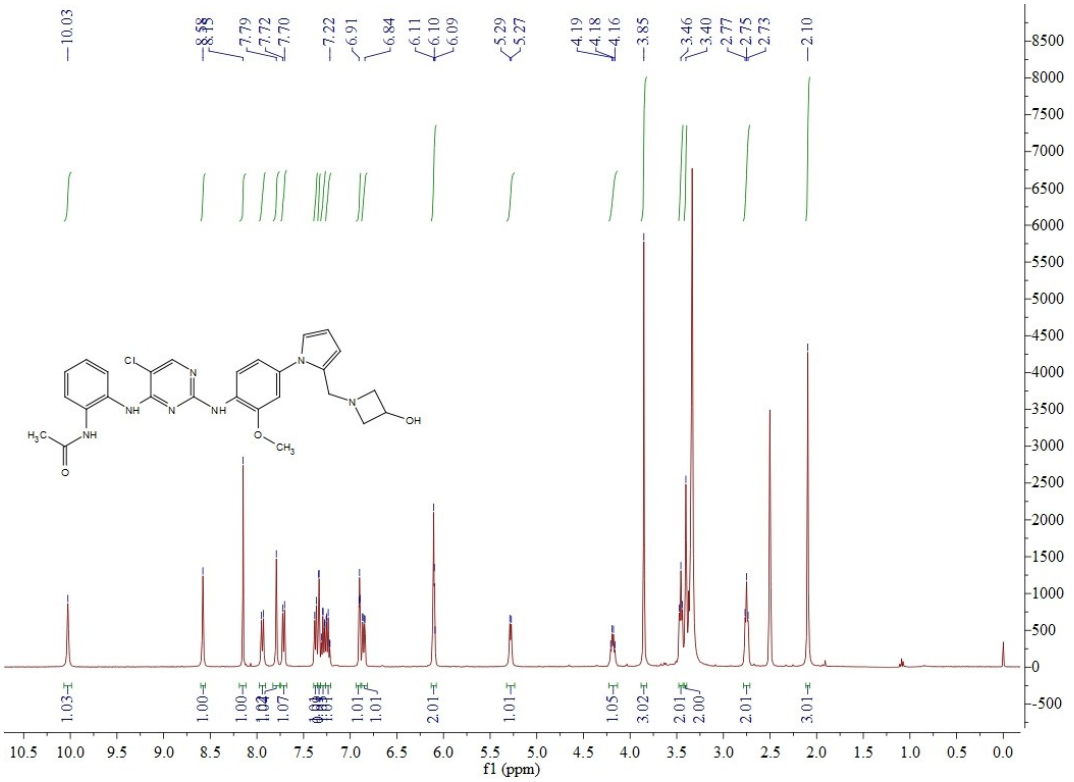

Fig. 14-2 ^{1}H-NMR spectrum of **9n**

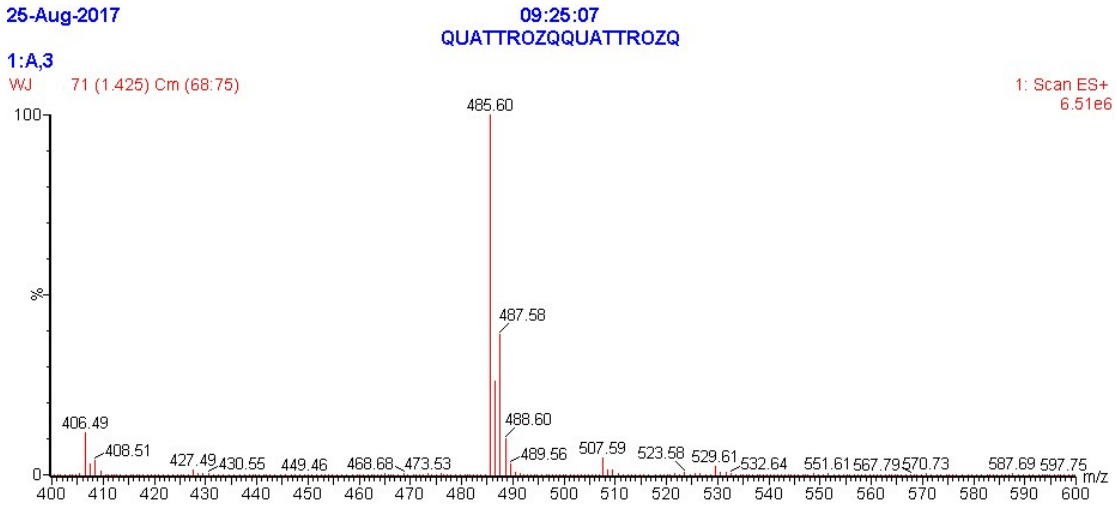

Fig. 15-1 MS spectrum of **10a**

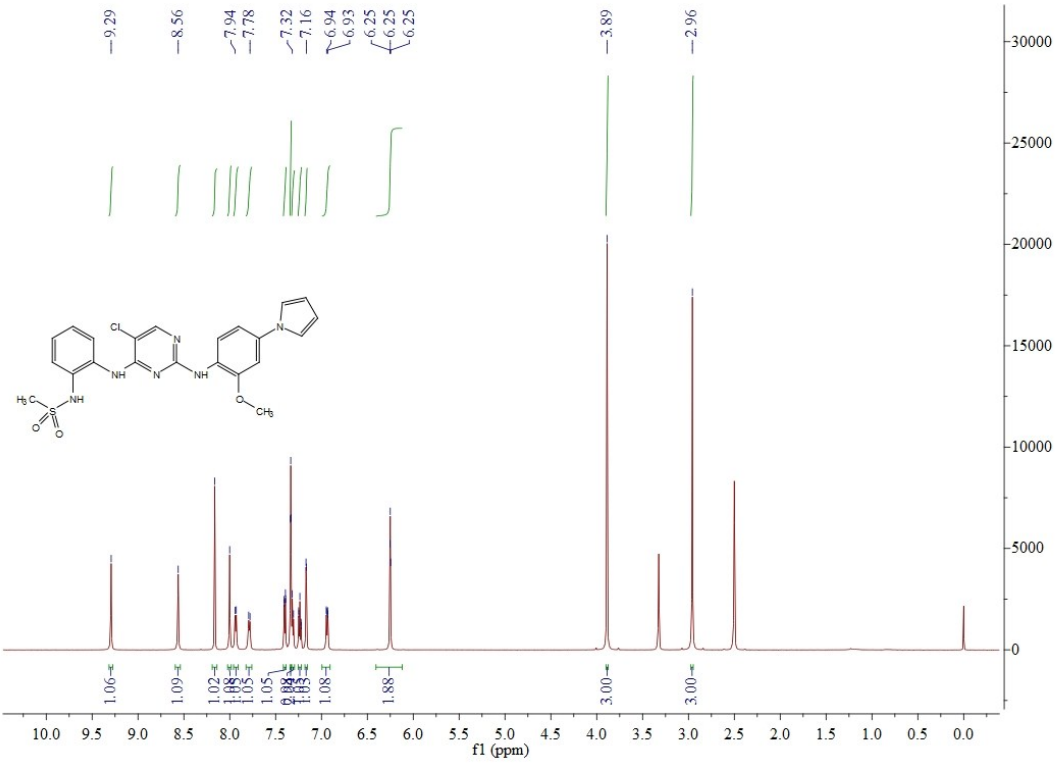

Fig. 15-2 ^{1}H-NMR spectrum of **10a**

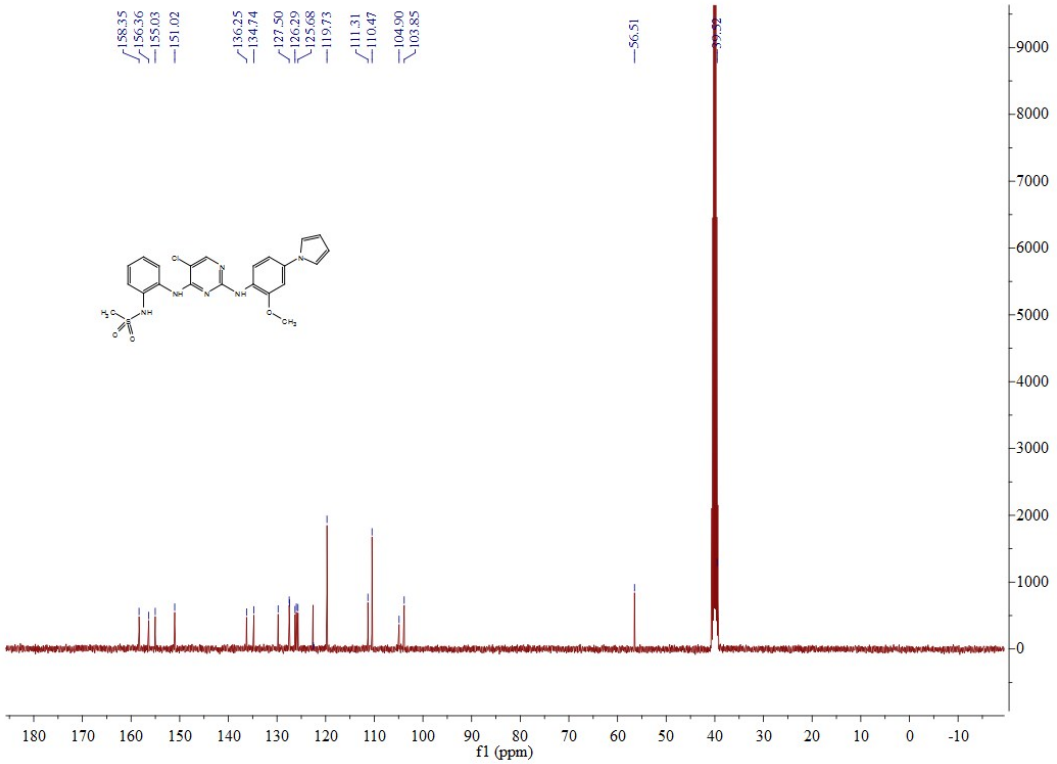

Fig. 15-3 ^{13}C-NMR spectrum of **10a**

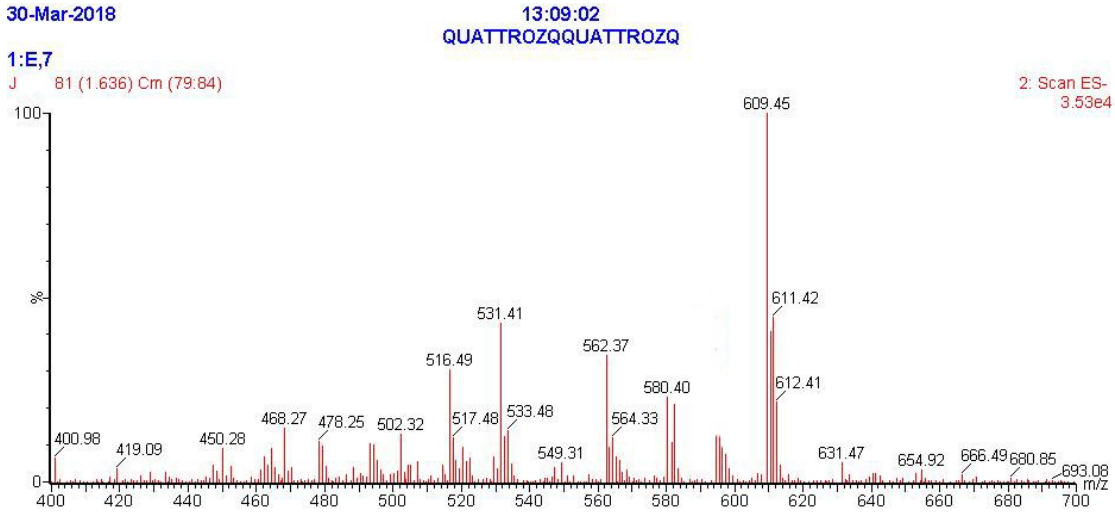

Fig. 16-1 MS spectrum of **10b**

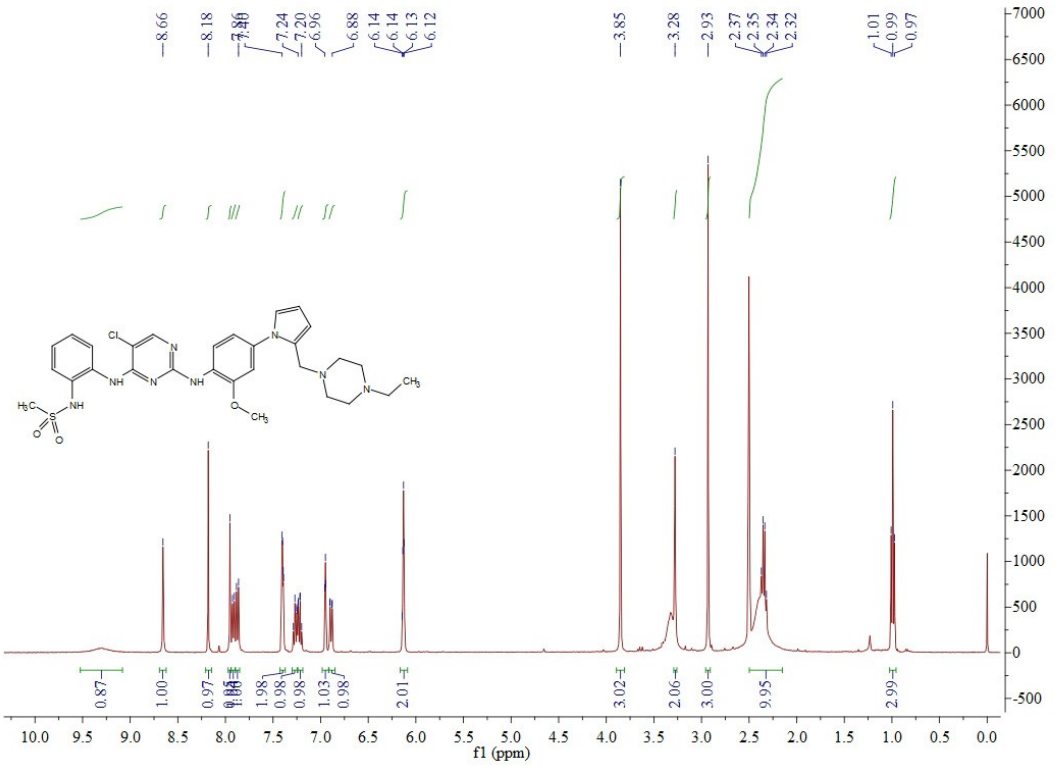

Fig. 16-2 ^{1}H-NMR spectrum of **10b**

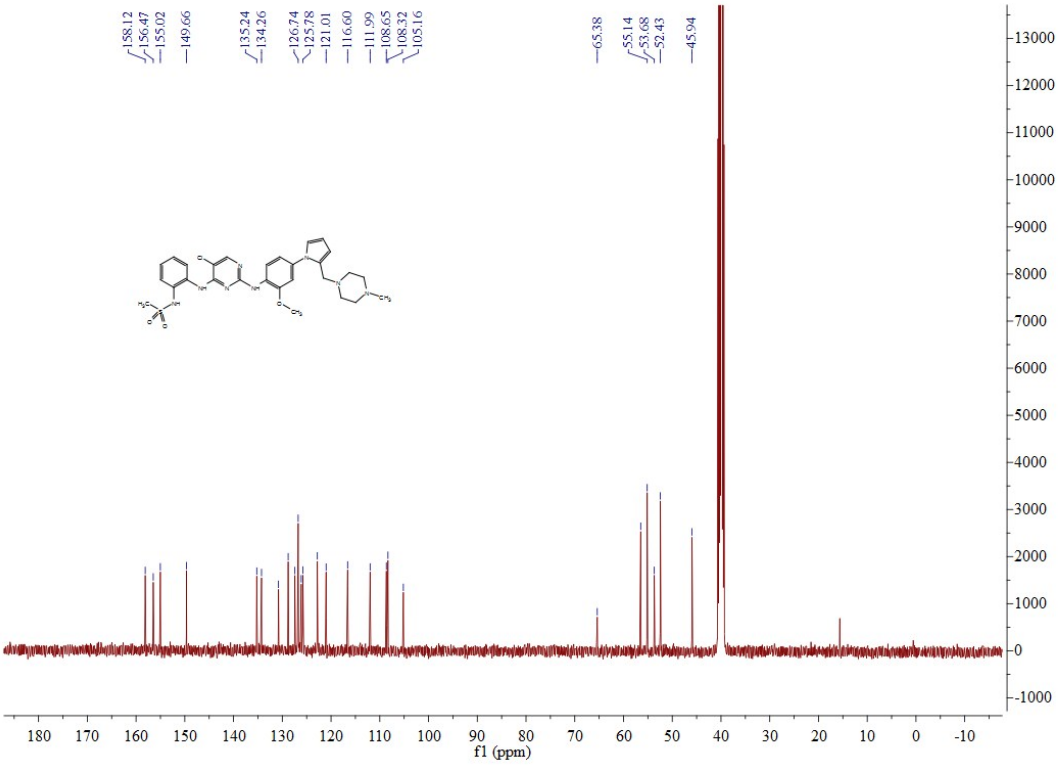

Fig. 16-3 ^{13}C-NMR spectrum of **10b**

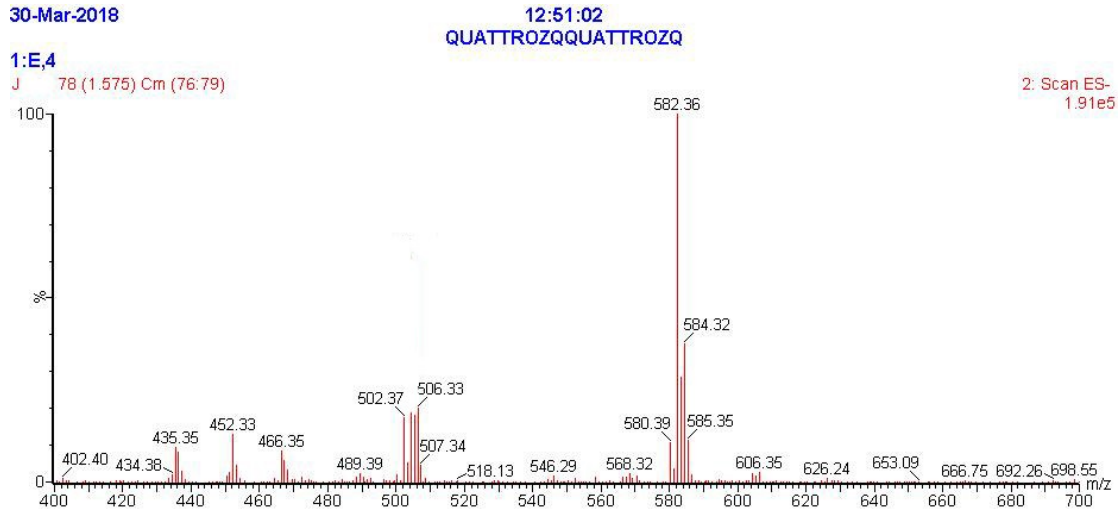

Fig. 17-1 MS spectrum of **10c**

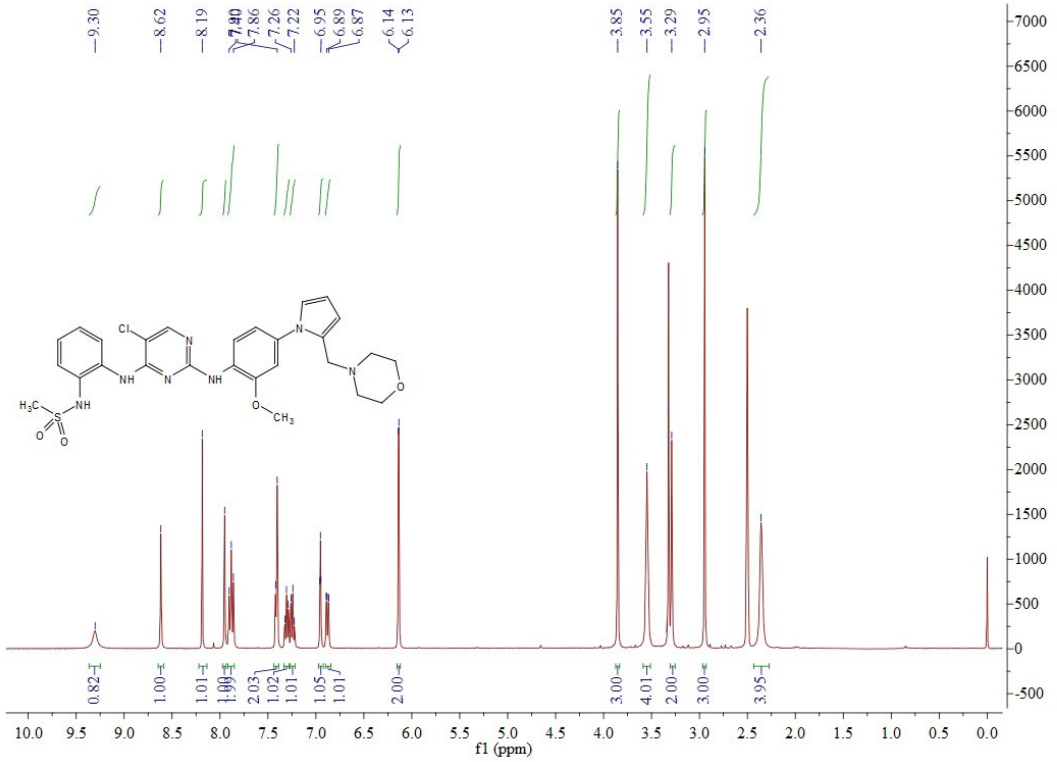

Fig. 17-2 ^{1}H-NMR spectrum of **10c**

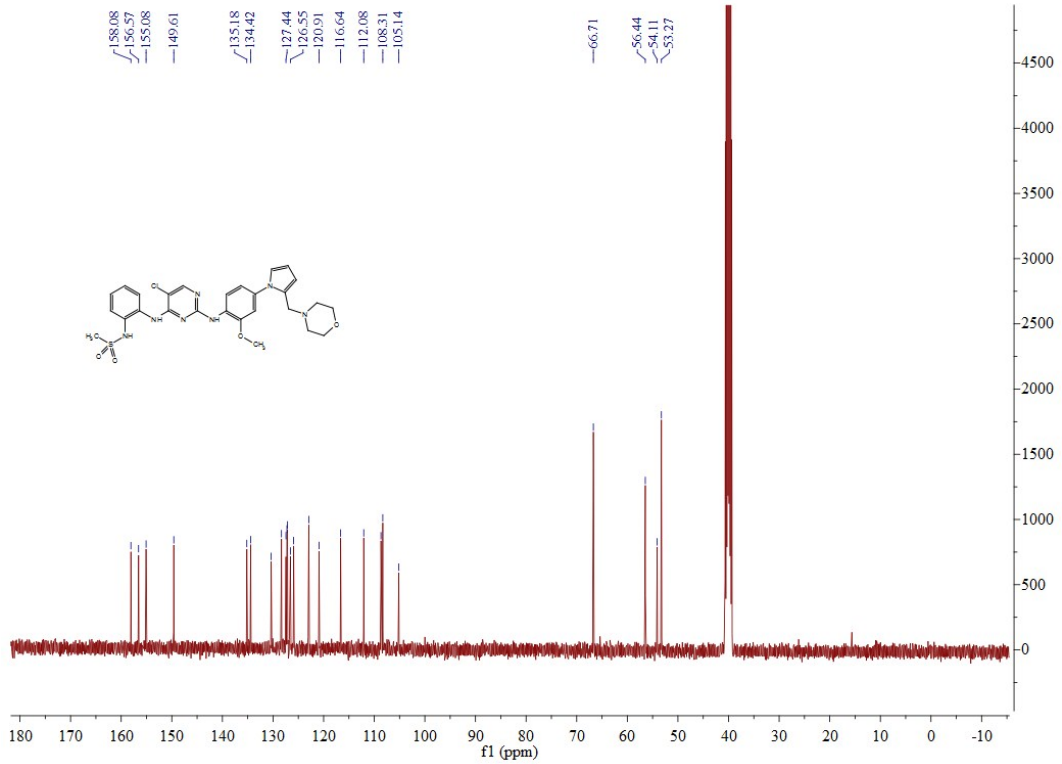

Fig. 17-3 ^{13}C-NMR spectrum of **10c**

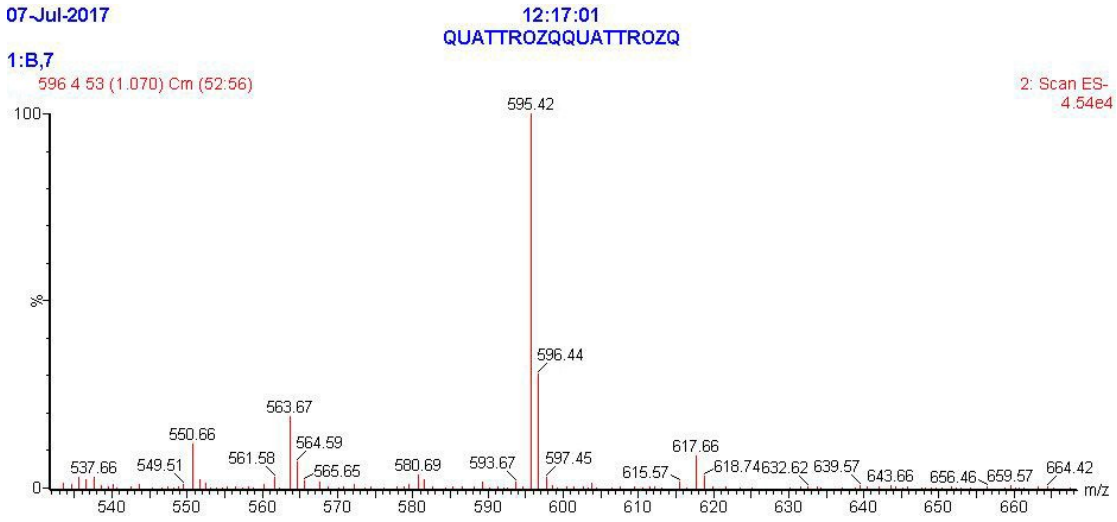

Fig. 18-1 MS spectrum of **10d**

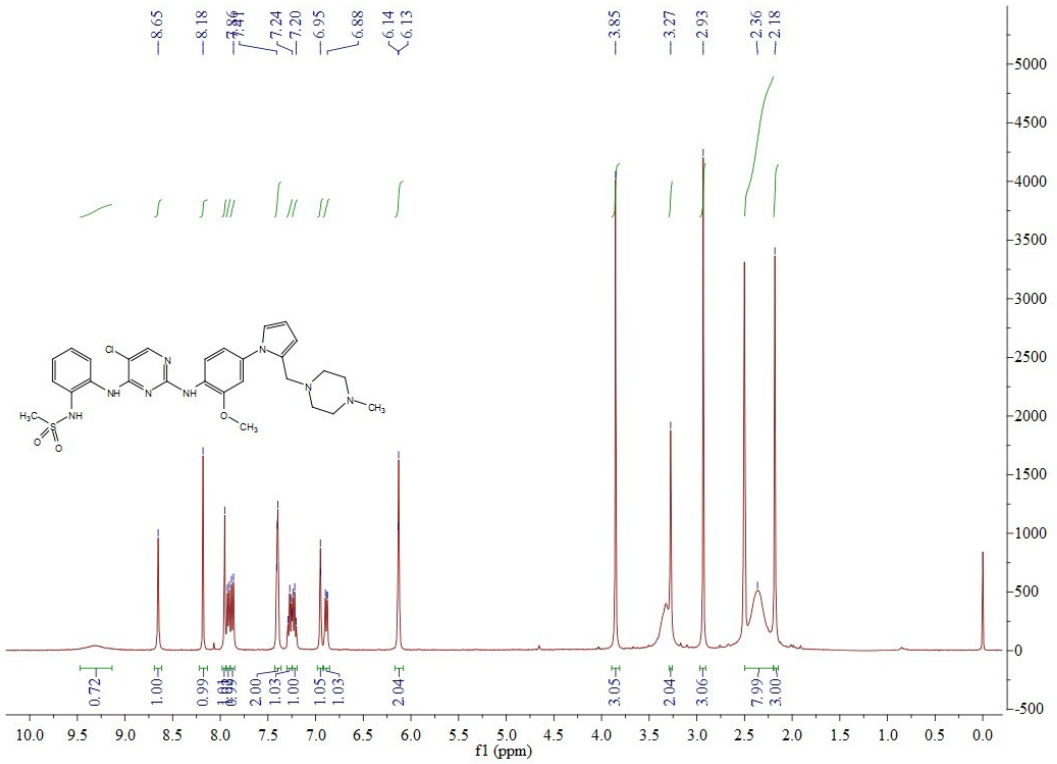

Fig. 18-2 ^{1}H-NMR spectrum of **10d**

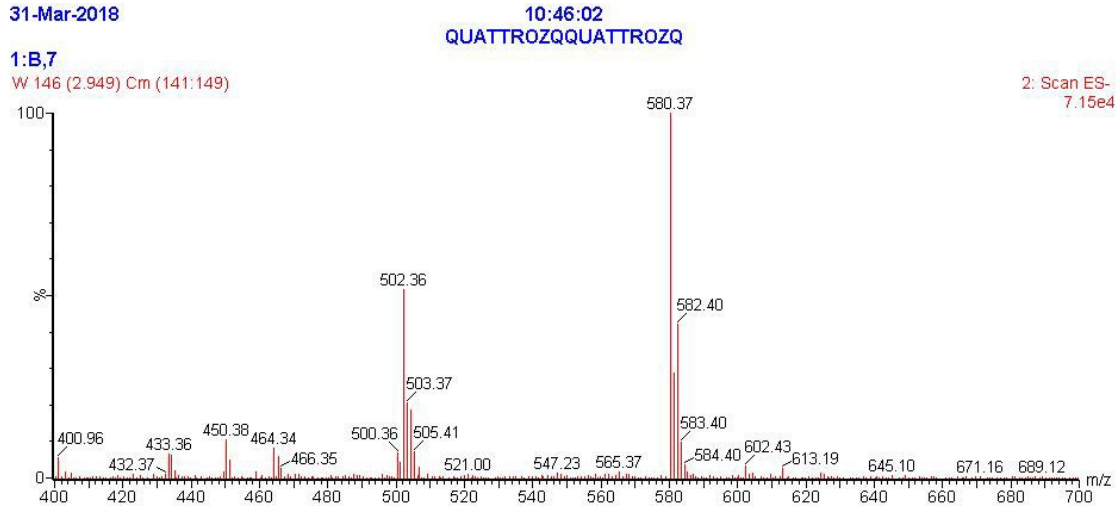

Fig. 19-1 MS spectrum of **10e**

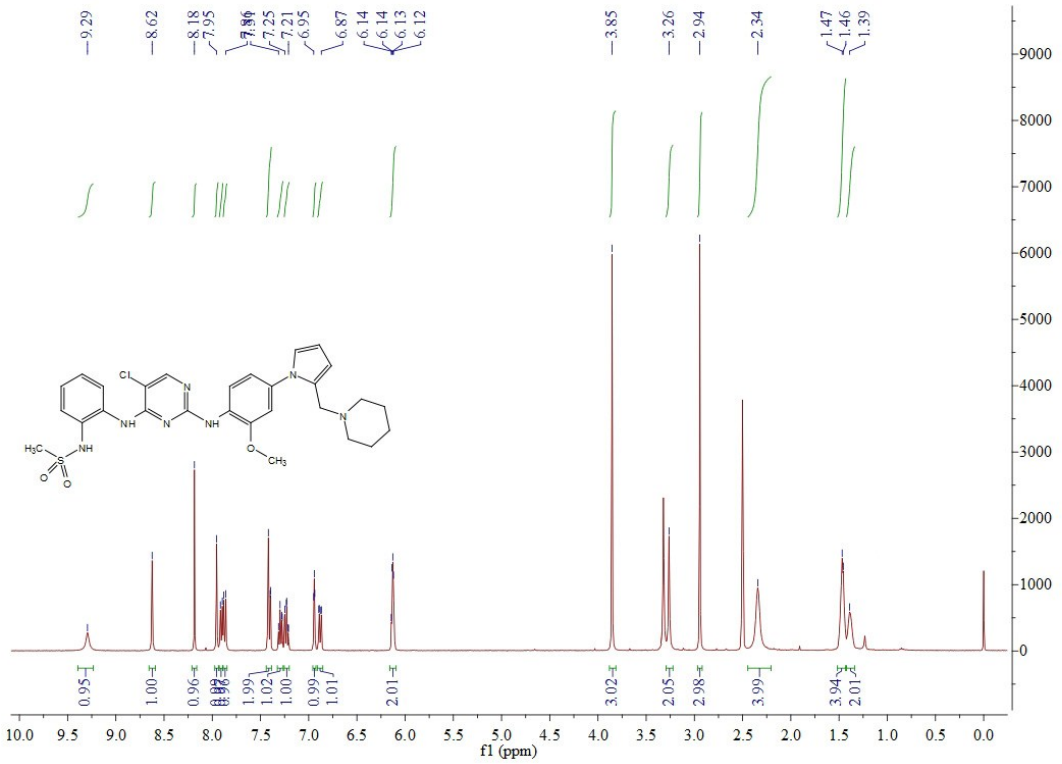

Fig. 19-2 ^{1}H-NMR spectrum of **10e**

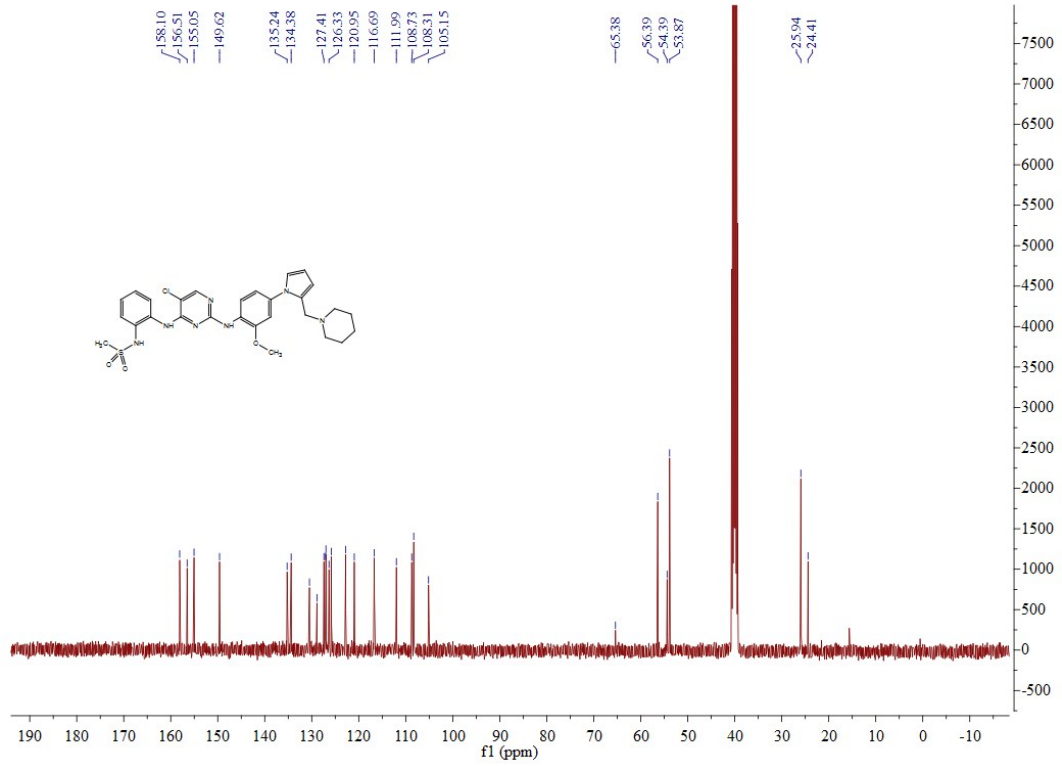

Fig. 19-3 ^{13}C-NMR spectrum of **10e**

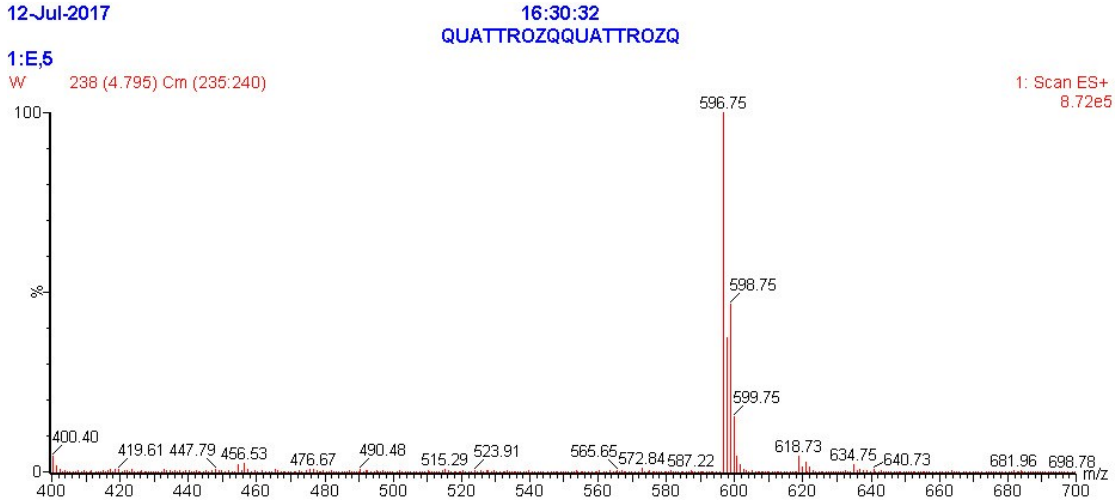

Fig. 20-1 MS spectrum of **10f**

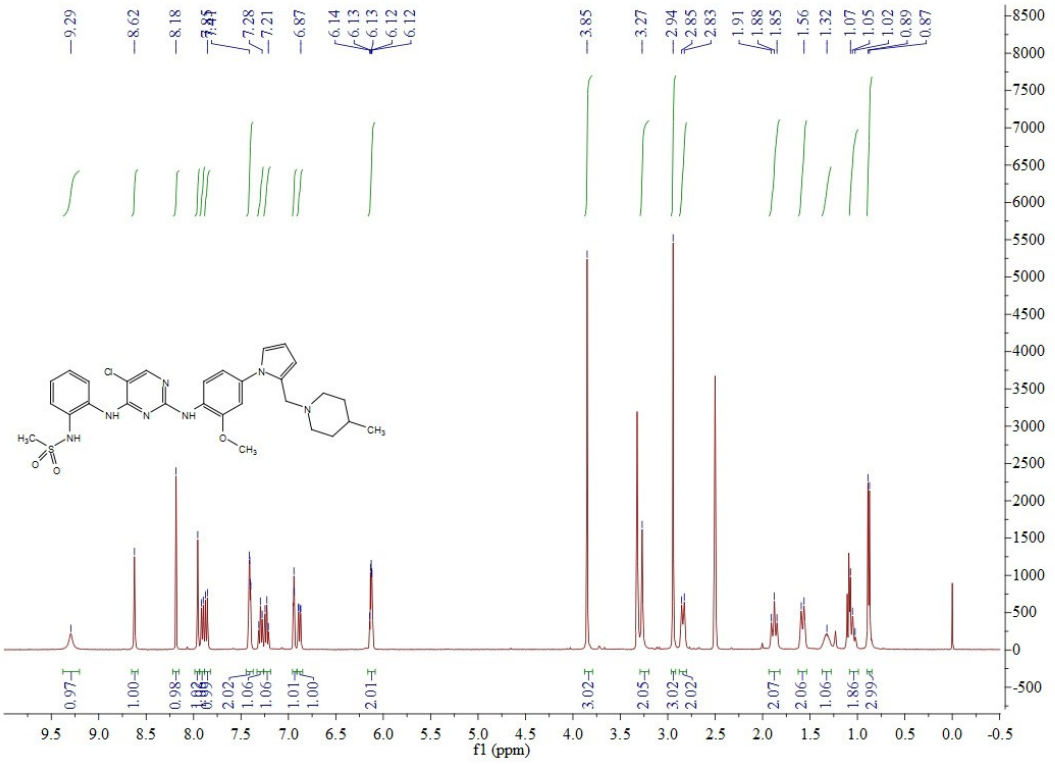

Fig. 20-2 ^{1}H-NMR spectrum of **10f**

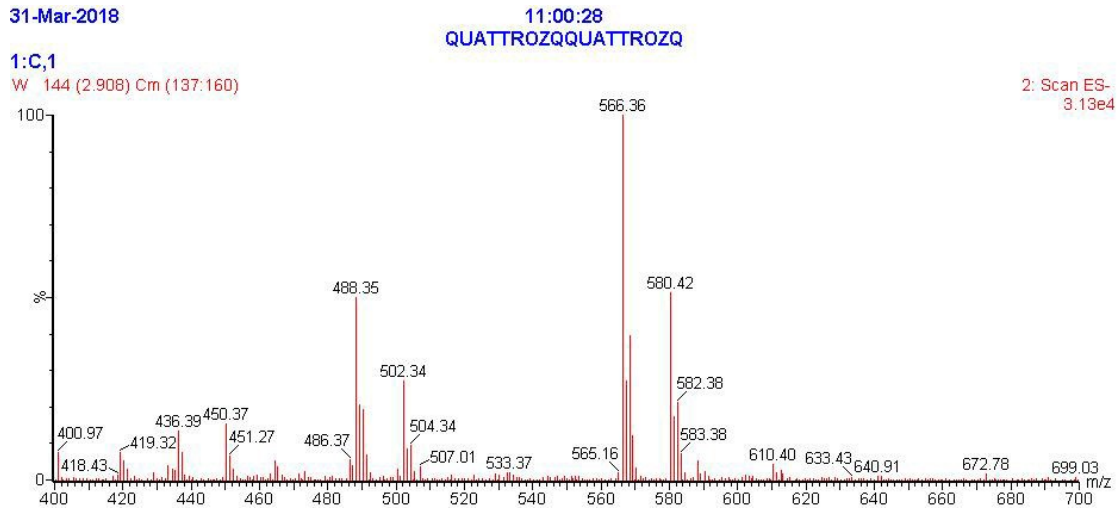

Fig. 21-1 MS spectrum of **10g**

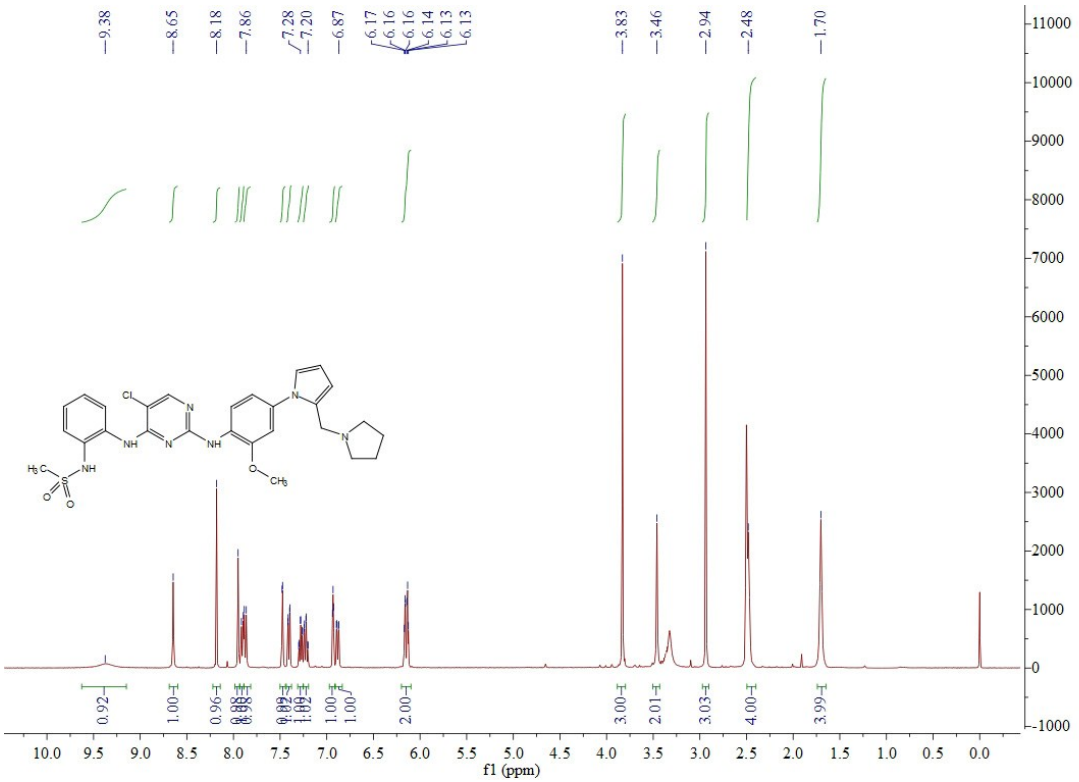

Fig. 21-2 ^{1}H-NMR spectrum of **10g**

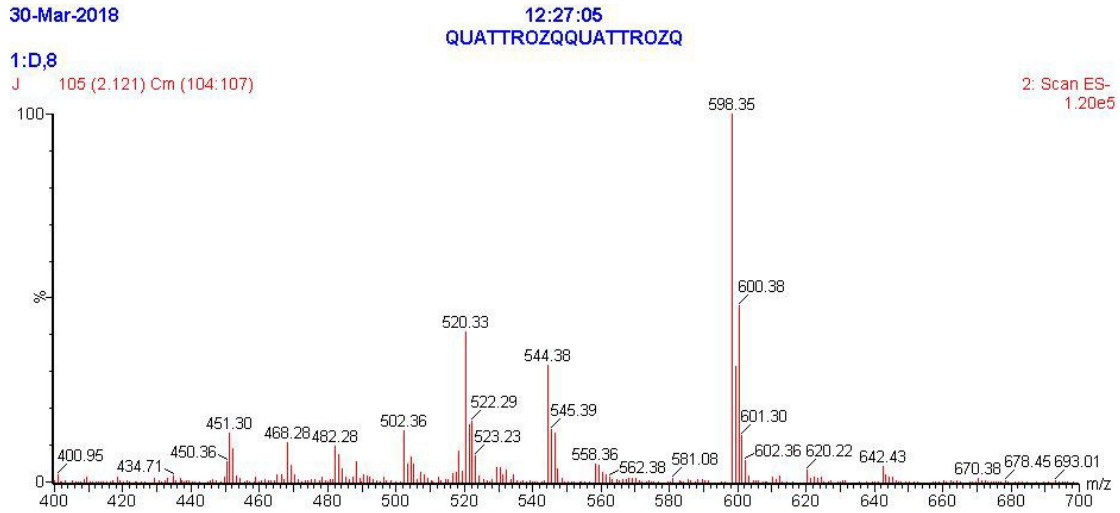

Fig. 22-1 MS spectrum of **10h**

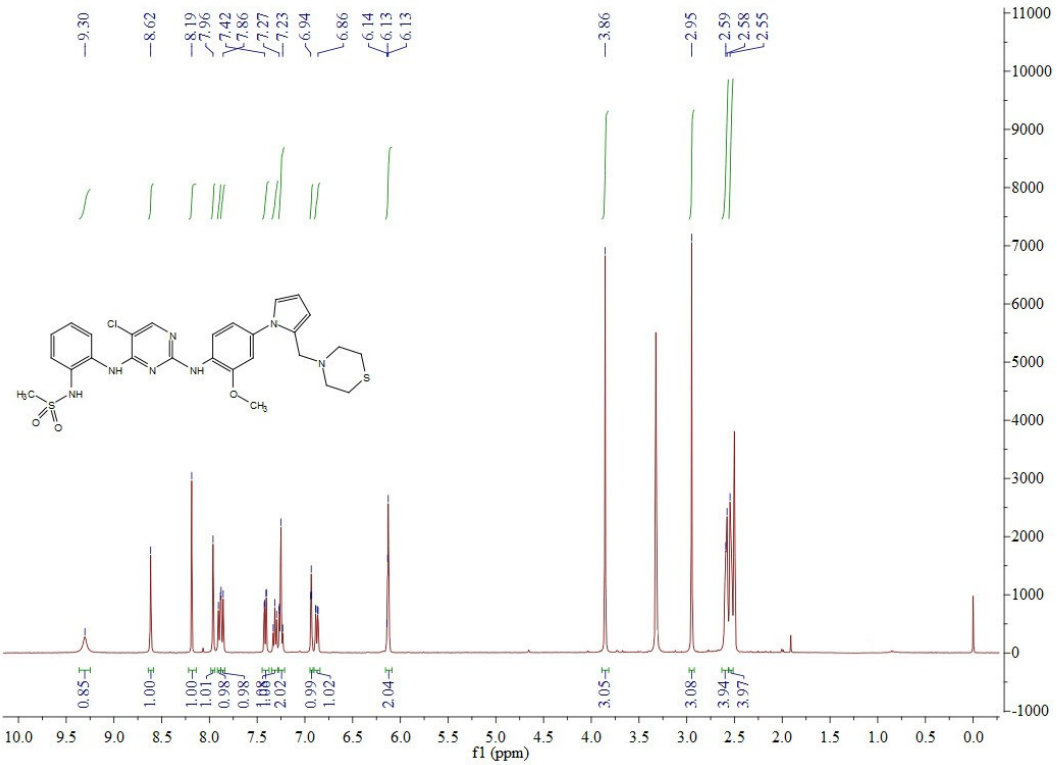

Fig. 22-2 ^{1}H-NMR spectrum of **10h**

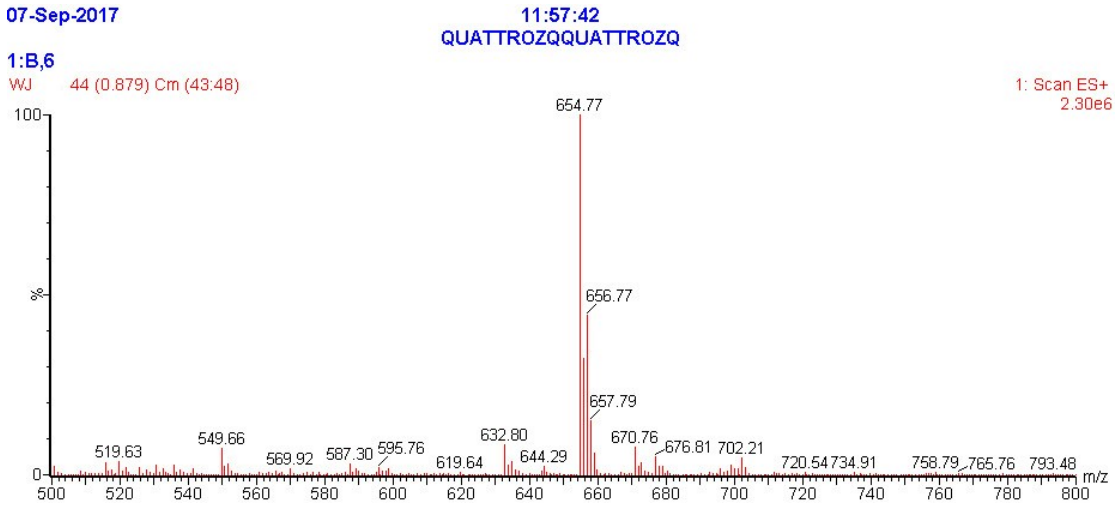

Fig. 23-1 MS spectrum of **10i**

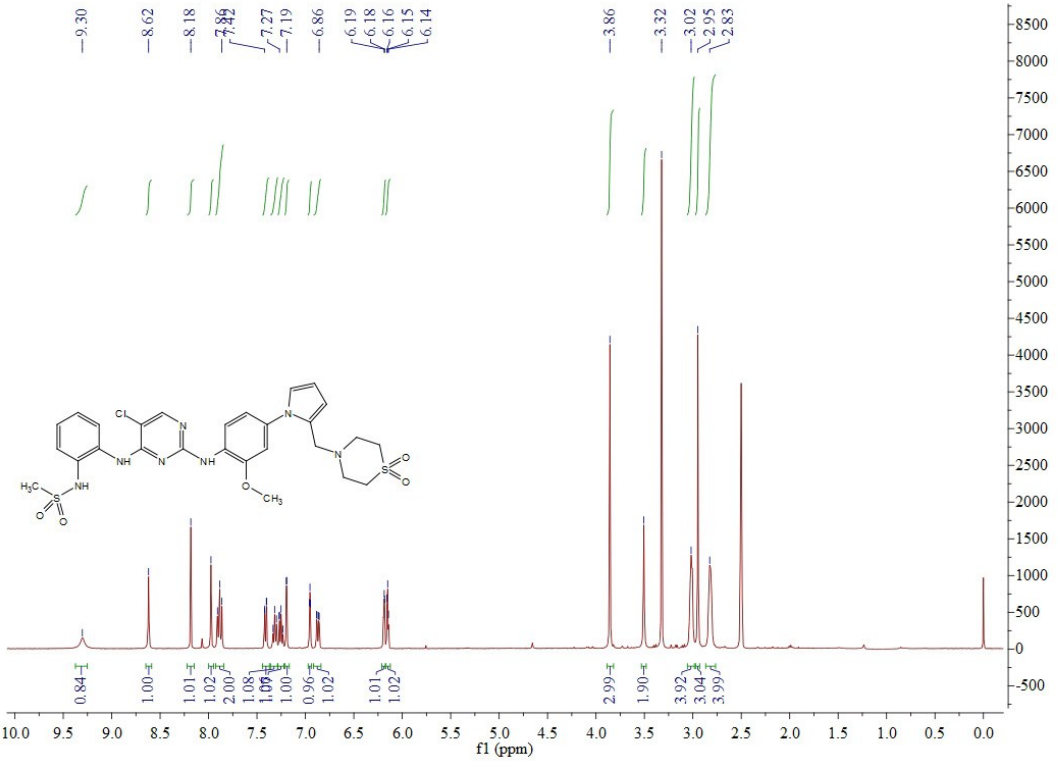

Fig. 23-2 ^{1}H-NMR spectrum of **10i**

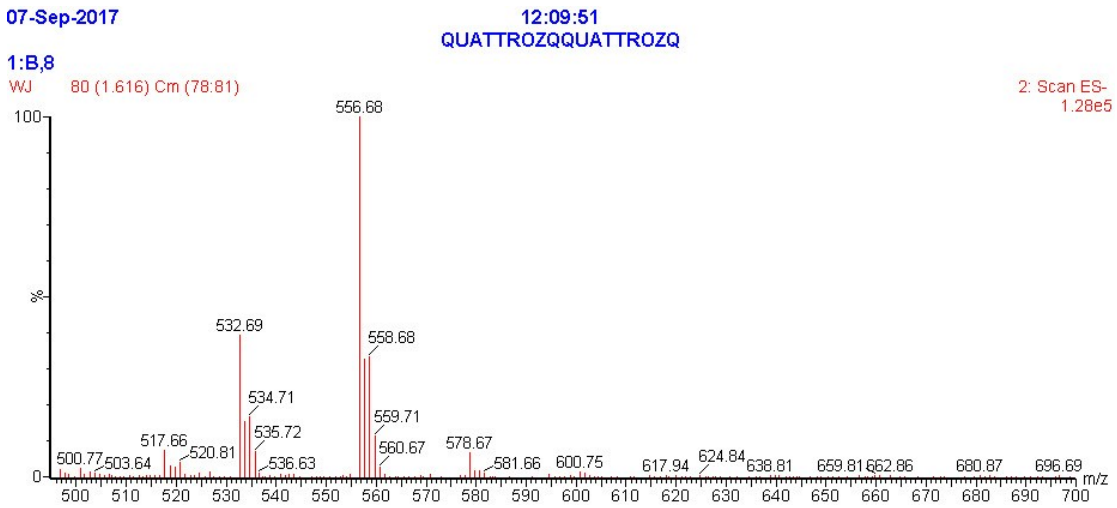

Fig. 24-1 MS spectrum of **10j**

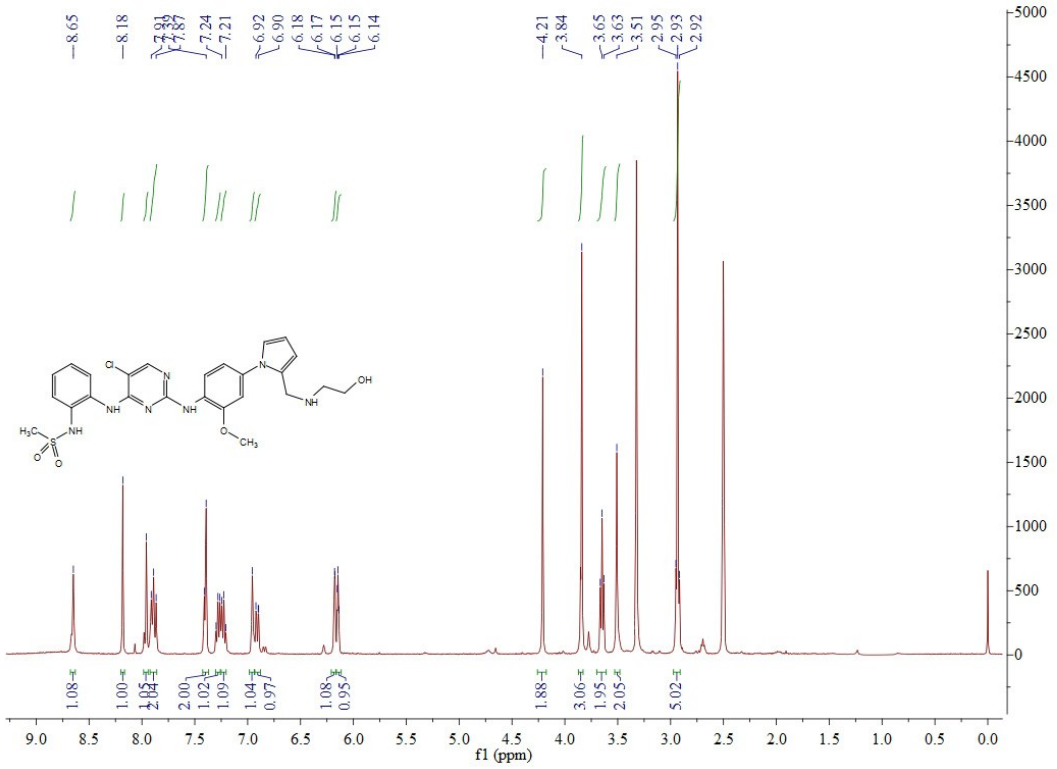

Fig. 24-2 ^{1}H-NMR spectrum of **10j**

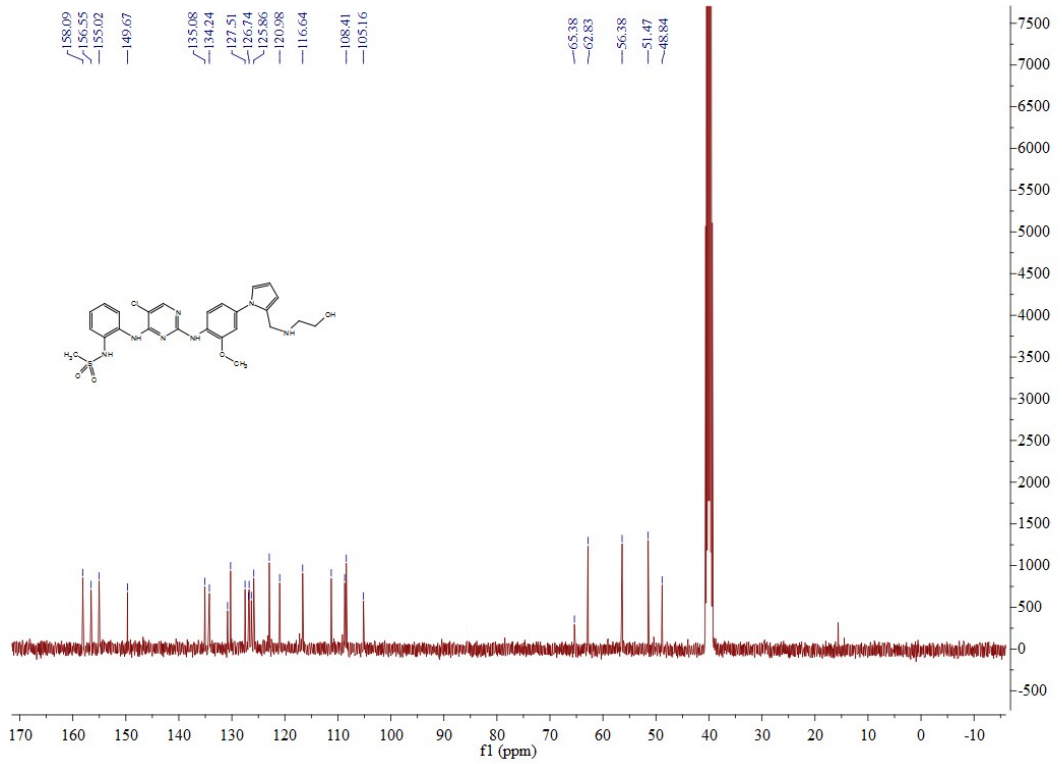

Fig. 24-3 ^{13}C-NMR spectrum of **10j**

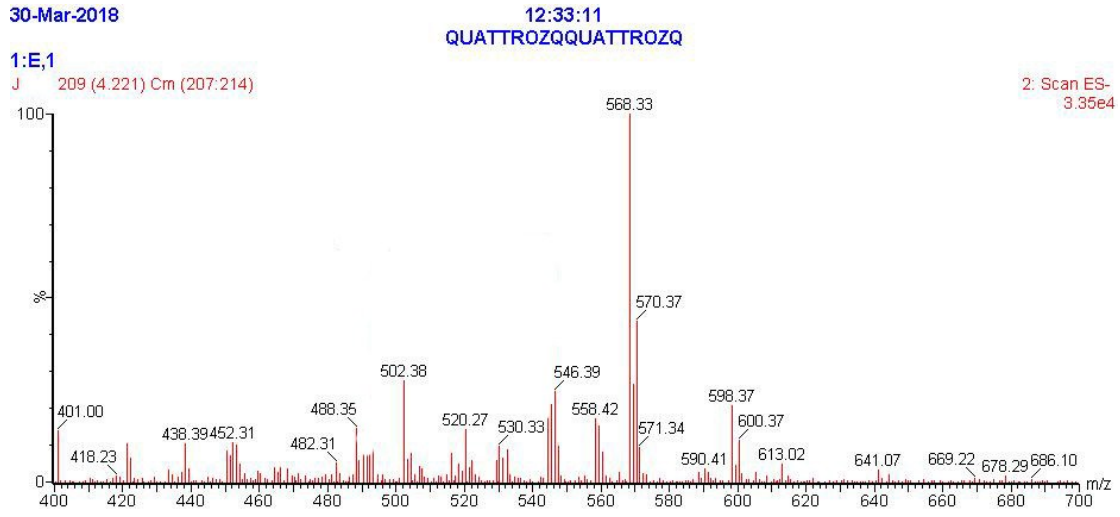

Fig. 25-1 MS spectrum of **10k**

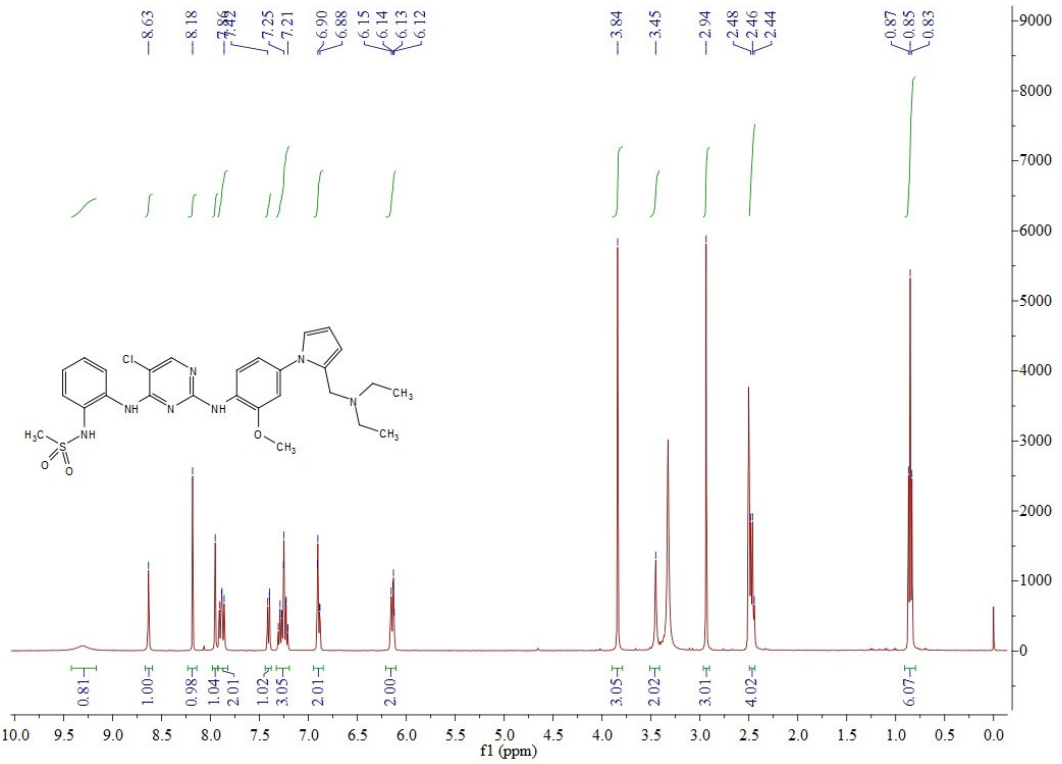

Fig. 25-2 ^{1}H-NMR spectrum of **10k**

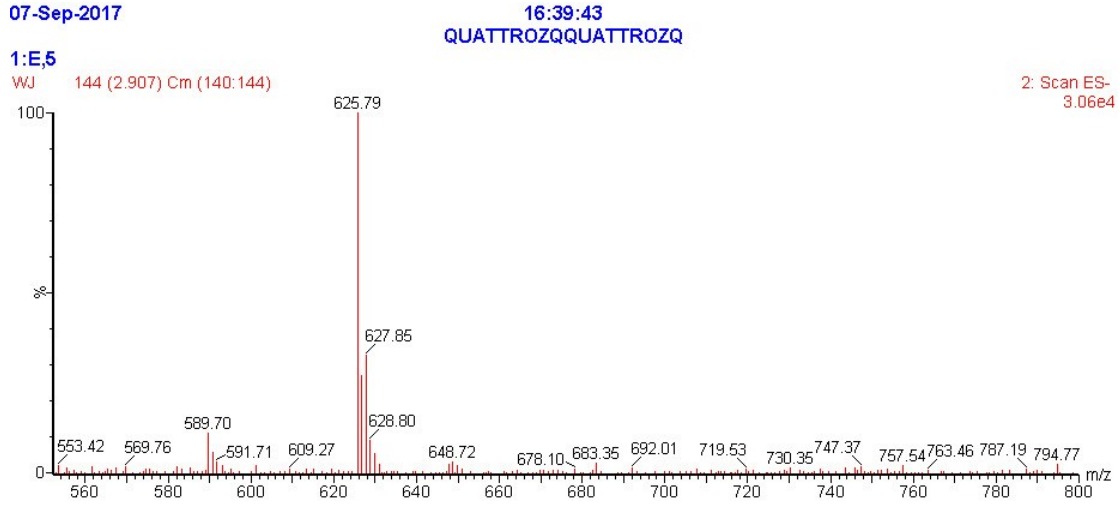

Fig. 26-1 MS spectrum of **10l**

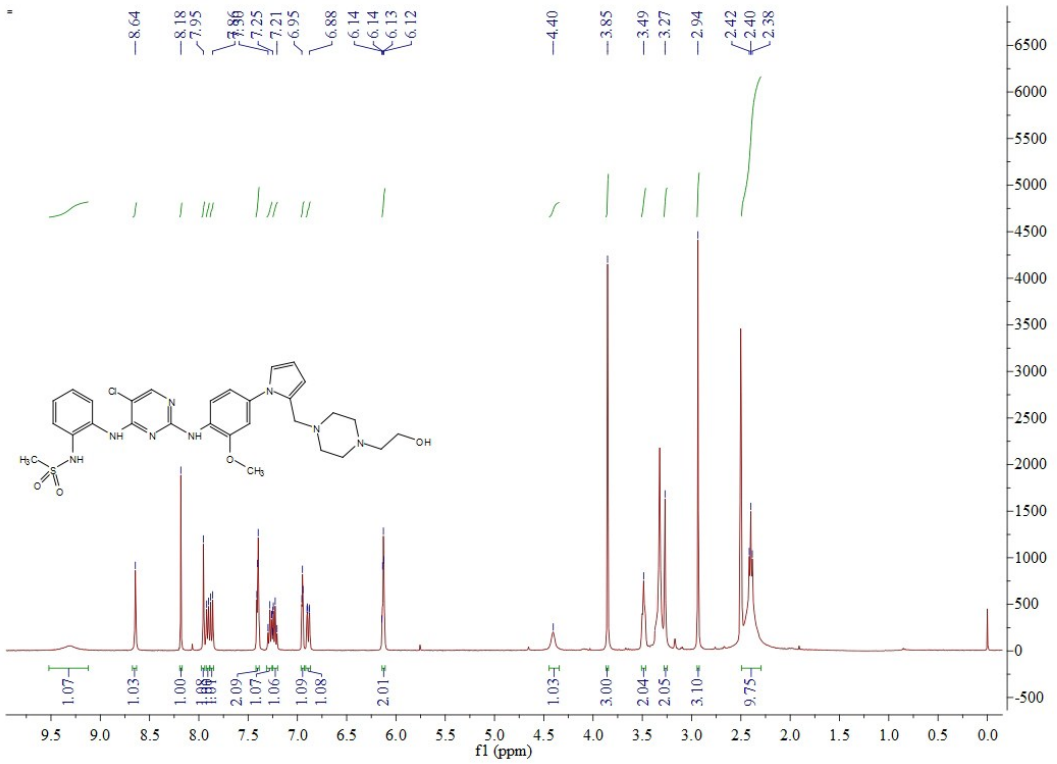

Fig. 26-2 ^{1}H-NMR spectrum of **10l**

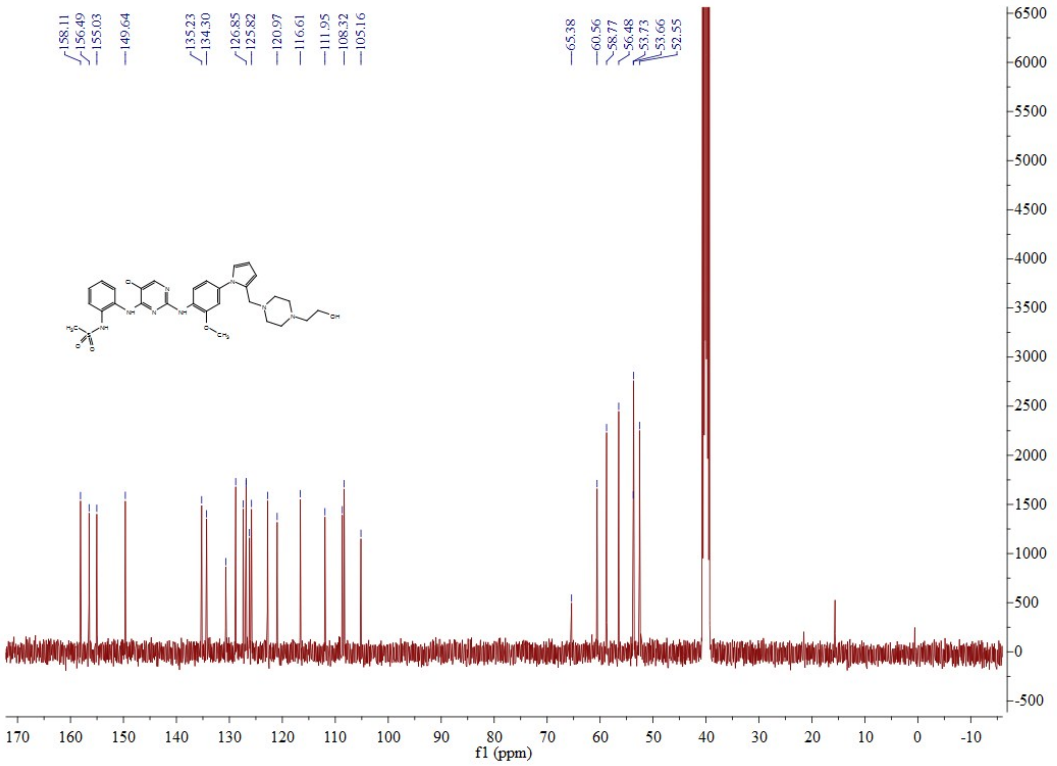

Fig. 26-3 ^{13}C-NMR spectrum of **10l**

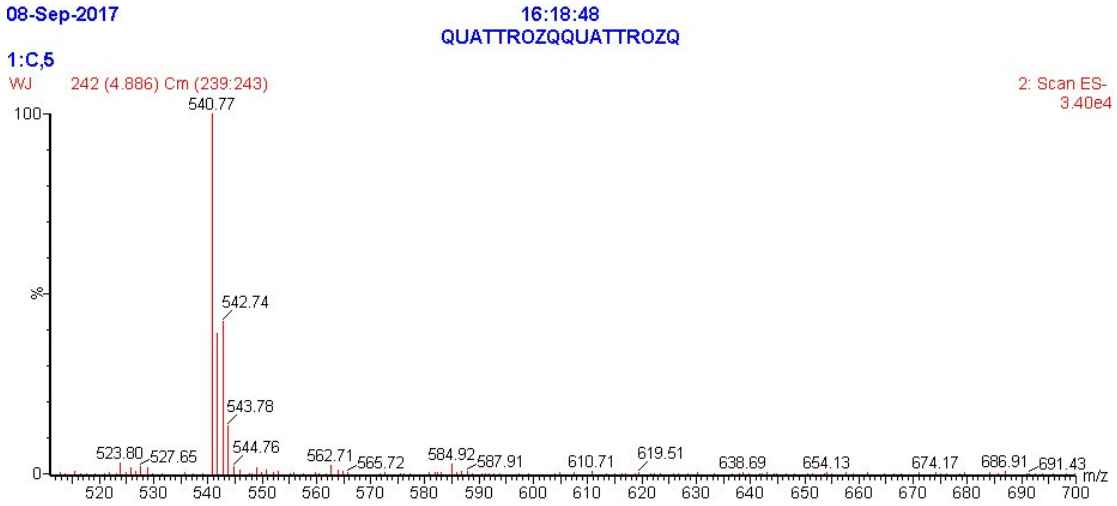

Fig. 27-1 MS spectrum of **10m**

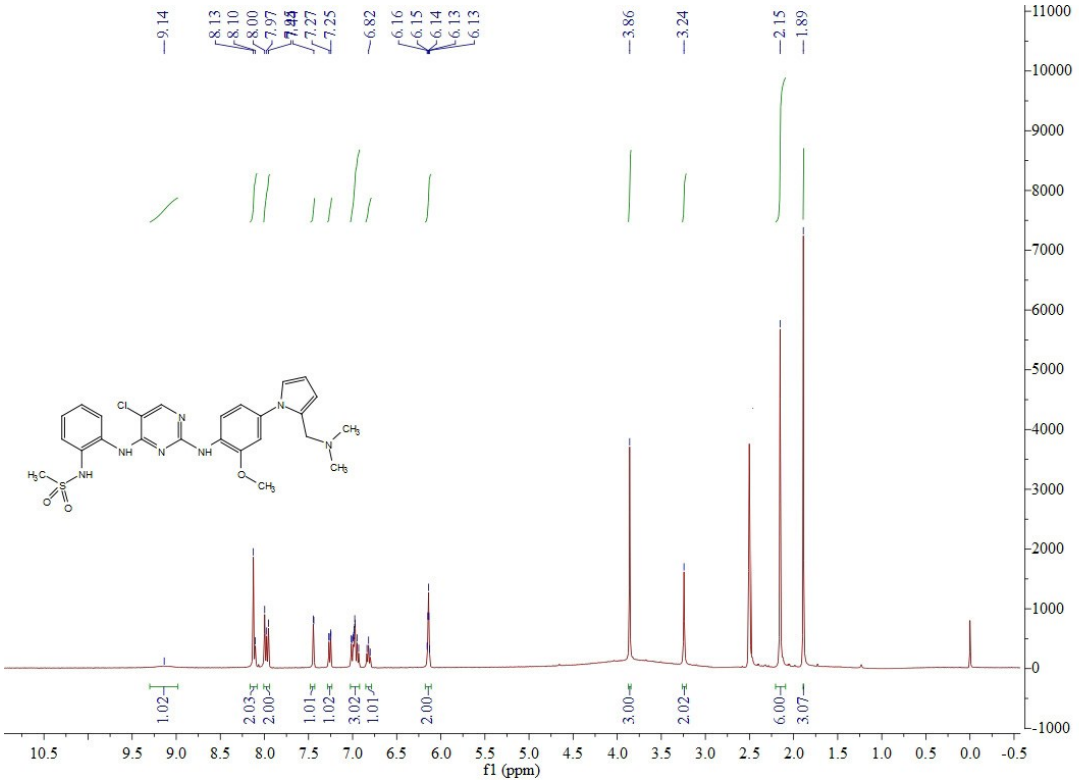

Fig. 27-2 ^{1}H-NMR spectrum of **10m**

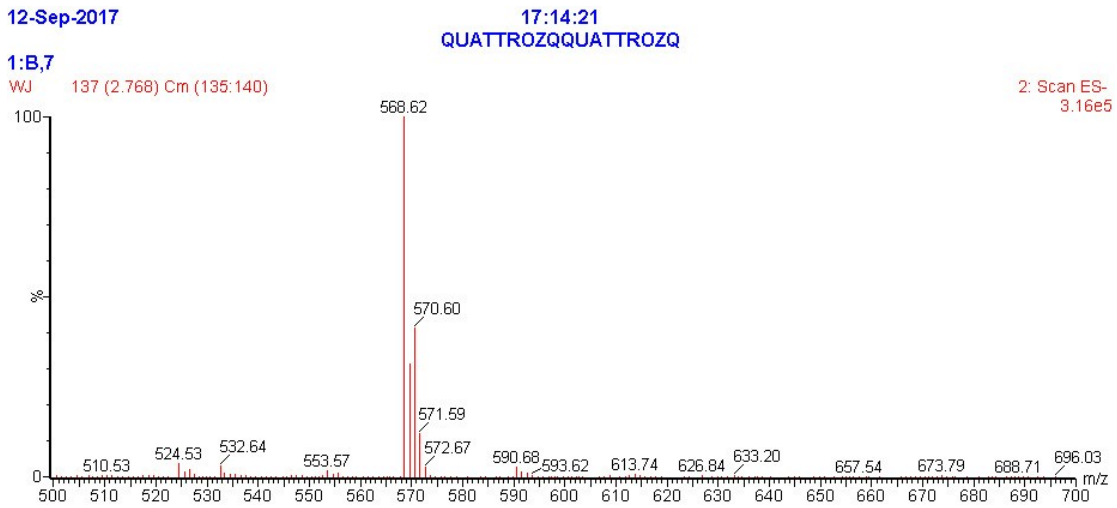

Fig. 28-1 MS spectrum of **10n**

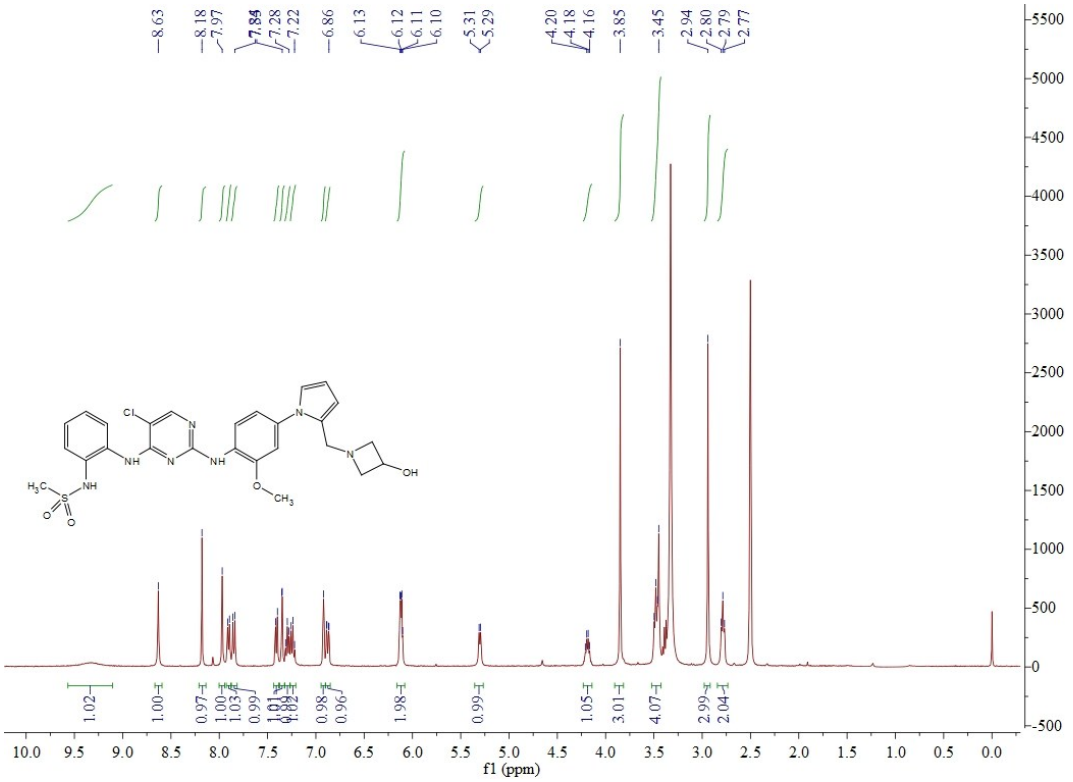

Fig. 28-2 ^{1}H-NMR spectrum of **10n**