

# Synthesis, antifungal, and antibacterial activities of novel benzoylurea derivatives containing a pyrimidine moiety

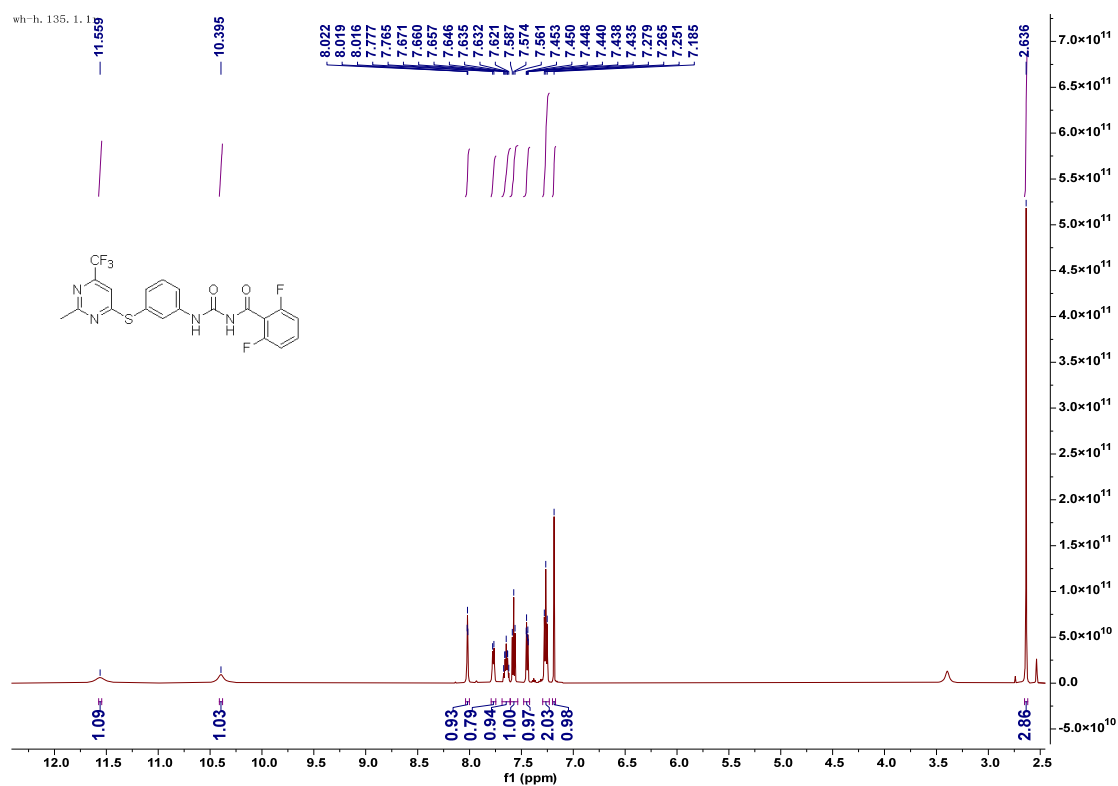


Figure S1 <sup>1</sup>H NMR spectrum of compound 4a

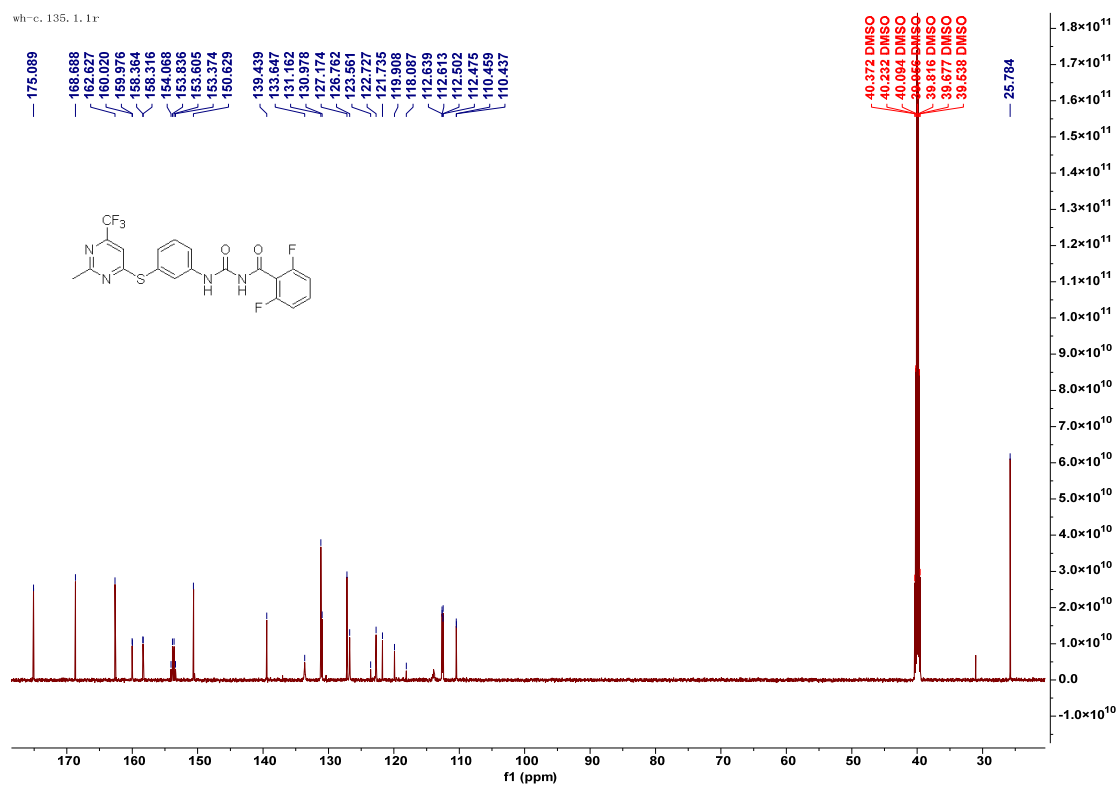
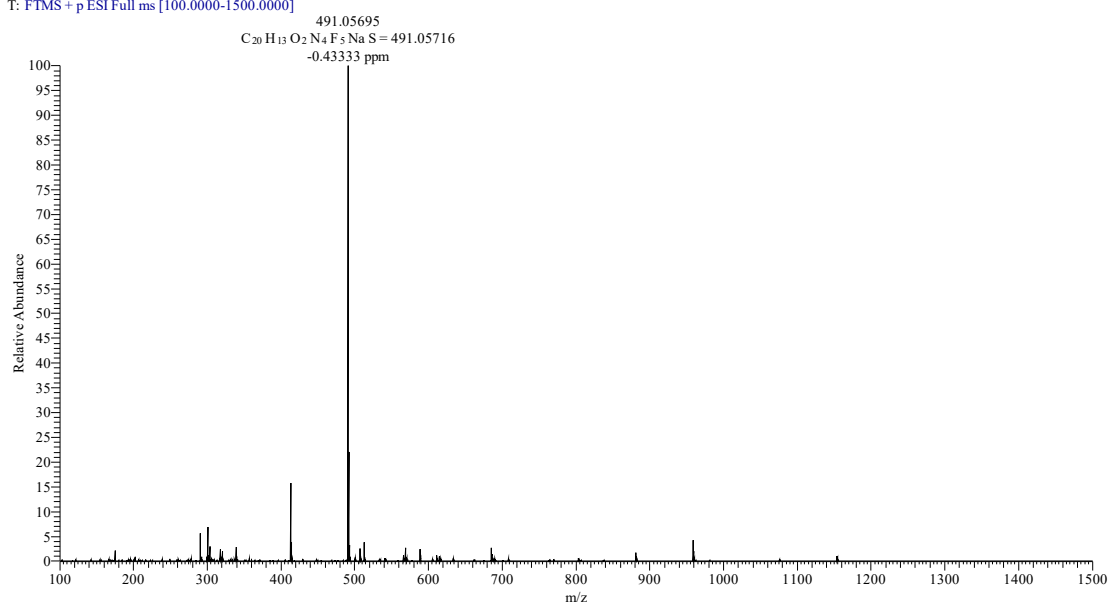
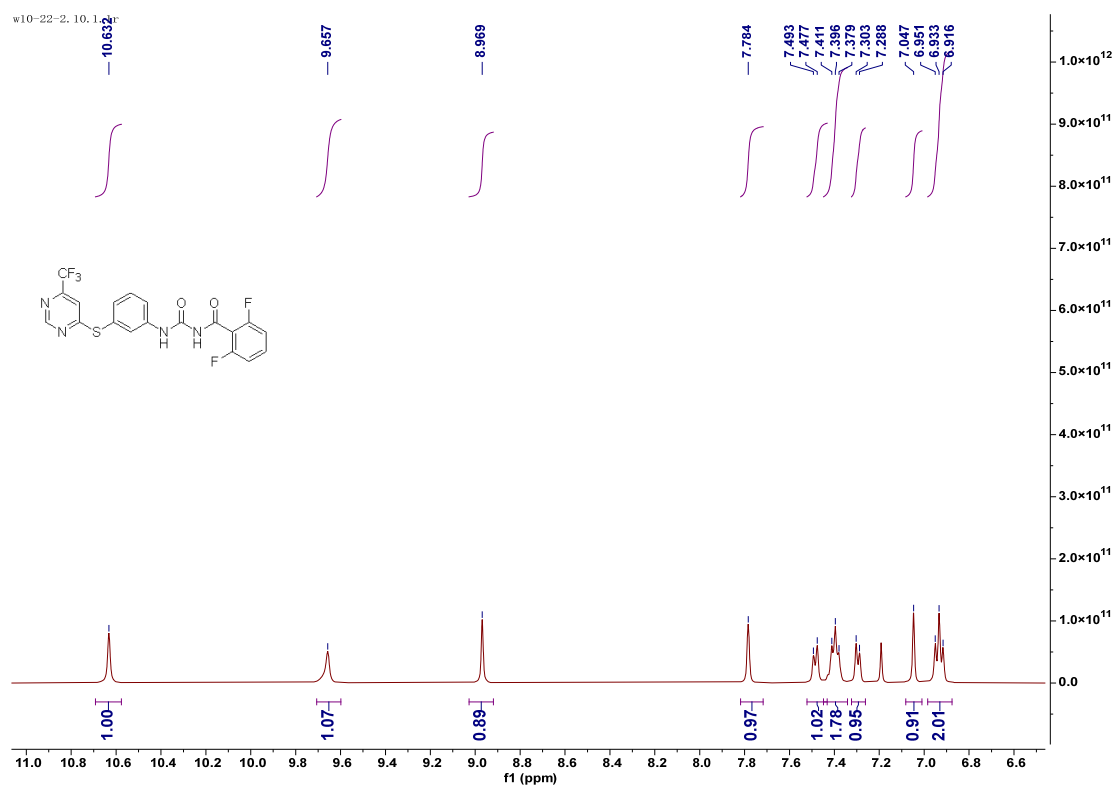


Figure S2 <sup>13</sup>C NMR spectrum of compound 4a

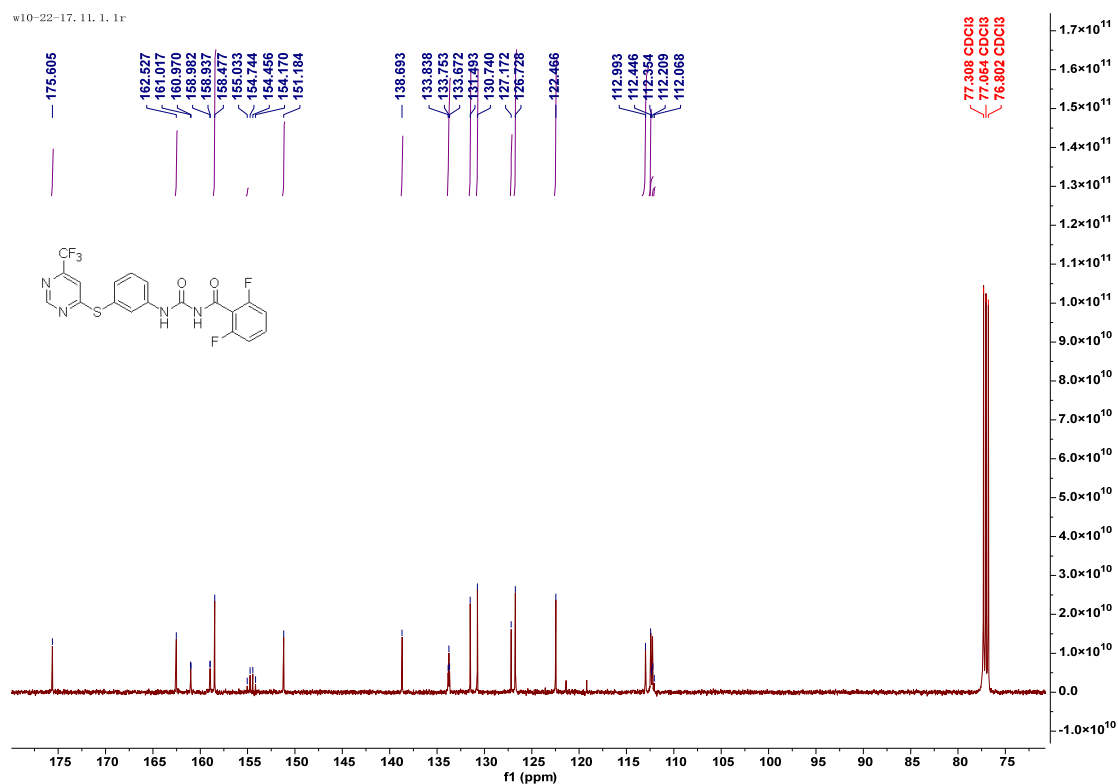
W12-05-12 #24 RT: 0.11 AV: 1 NL: 4.75E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



**Figure S3** HRMS spectrum of compound **4a**

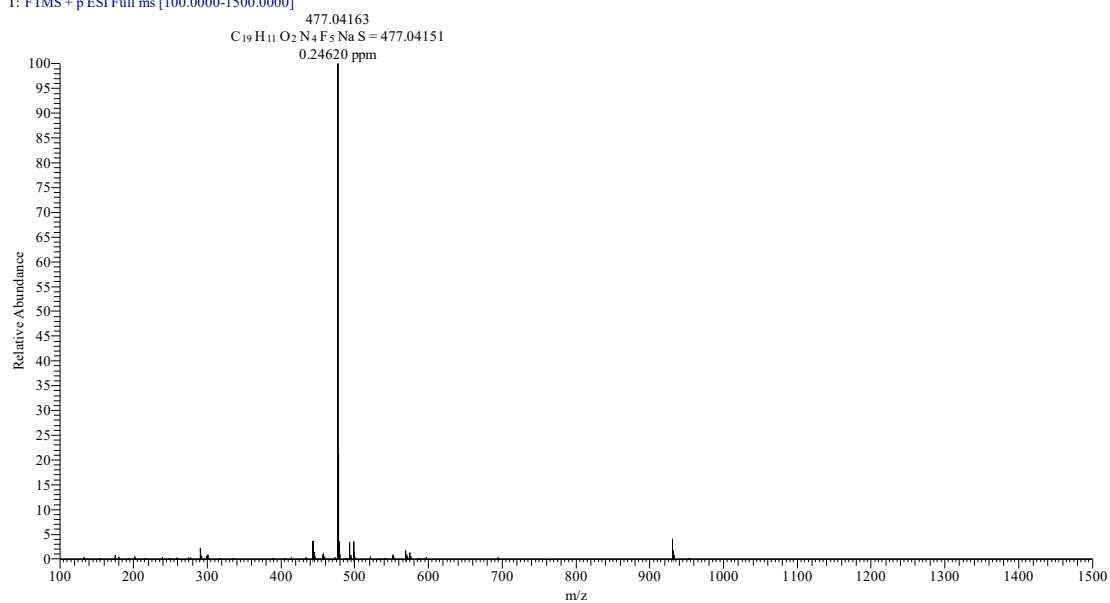


**Figure S4** <sup>1</sup>H NMR spectrum of compound **4b**



**Figure S5** <sup>13</sup>C NMR spectrum of compound **4b**

W12-05-13 #26 RT: 0.12 AV: 1 NL: 5.78E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



**Figure S6** HRMS spectrum of compound **4b**

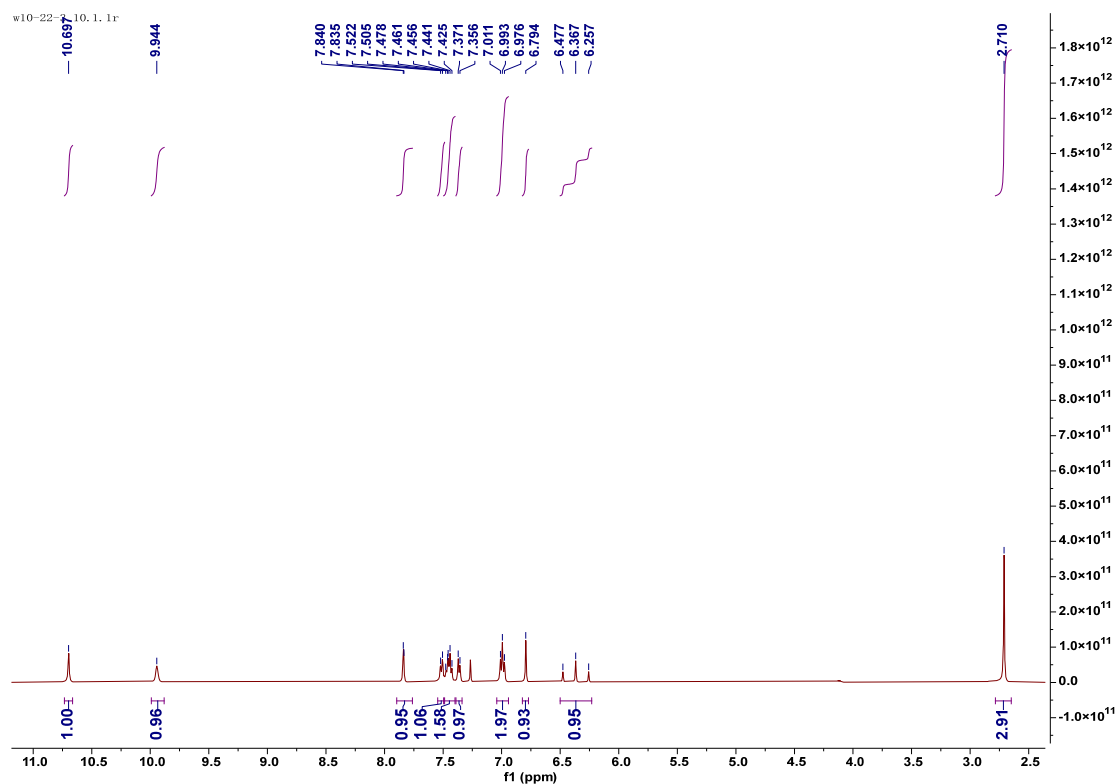


Figure S7  $^1\text{H}$  NMR spectrum of compound **4c**

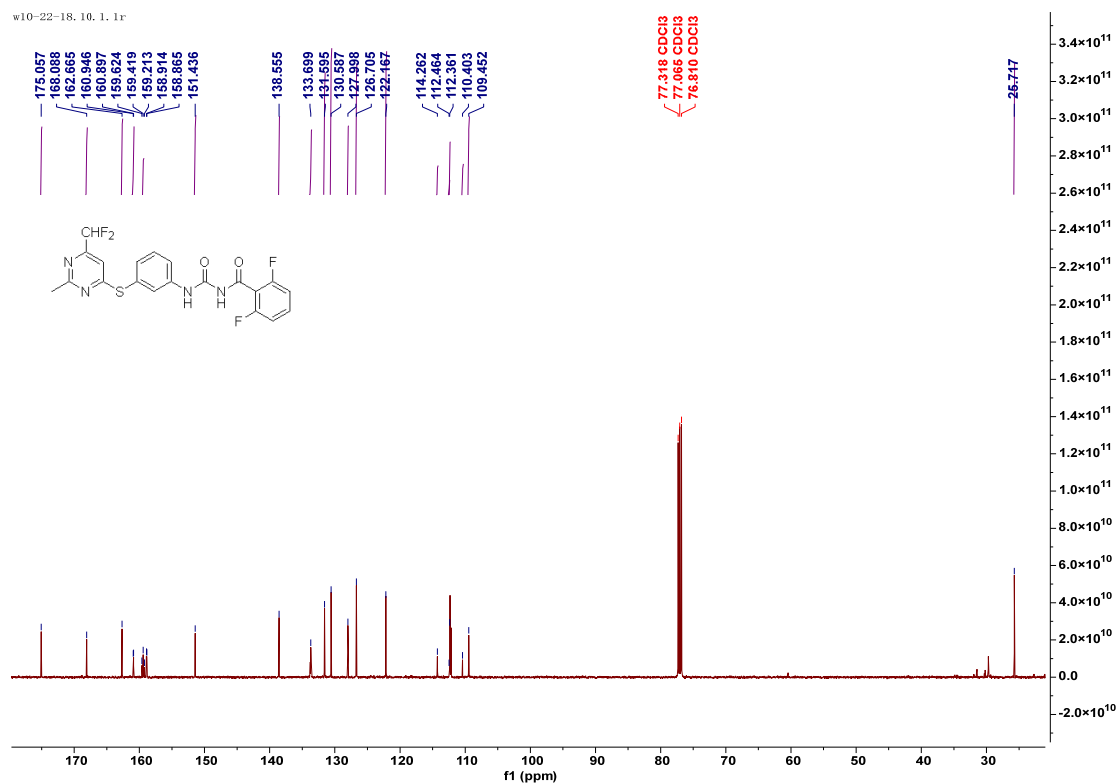


Figure S8  $^{13}\text{C}$  NMR spectrum of compound **4c**

W12-05-14 #25 RT: 0.11 AV: 1 NL: 5.92E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

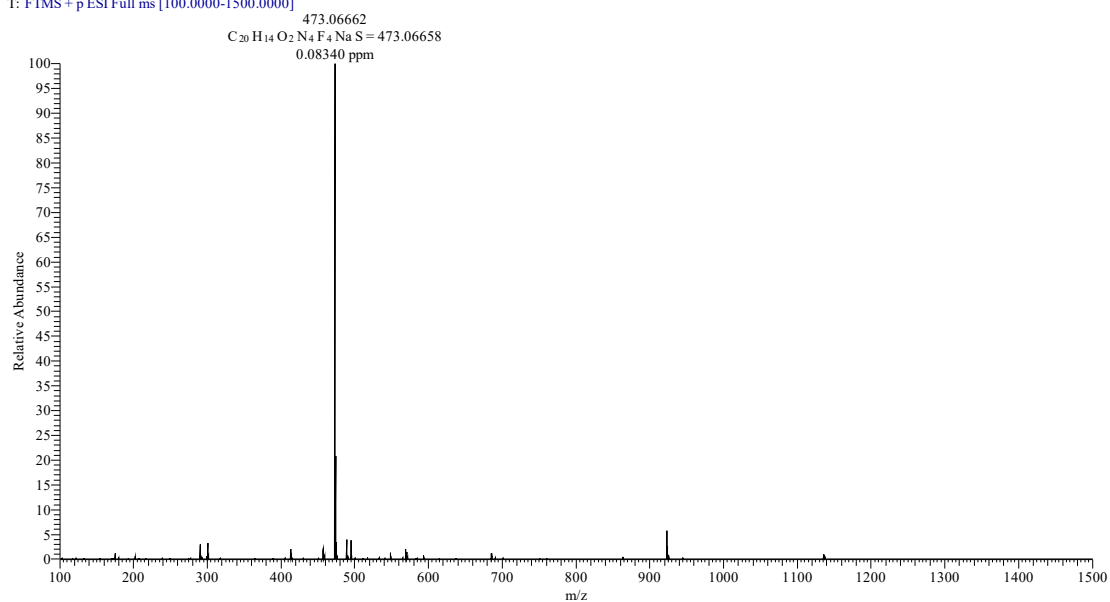


Figure S9 HRMS spectrum of compound 4c

w10-22-21. 10. 1. 1r

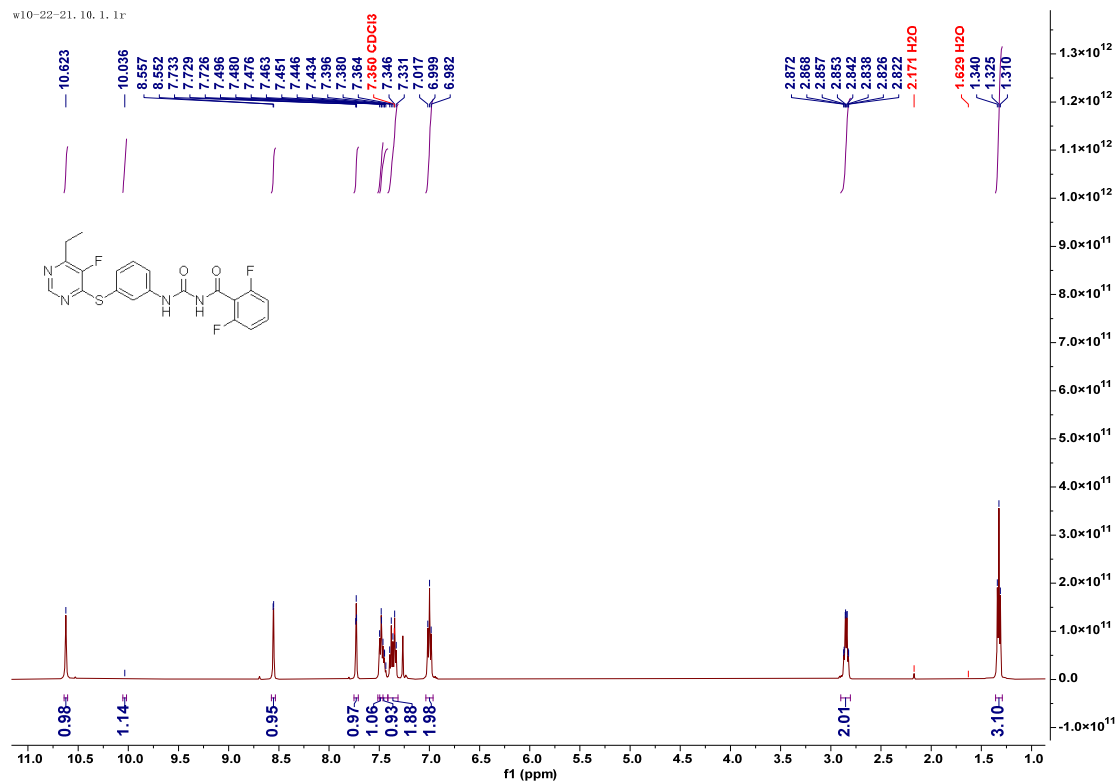


Figure S10 <sup>1</sup>H NMR spectrum of compound 4d

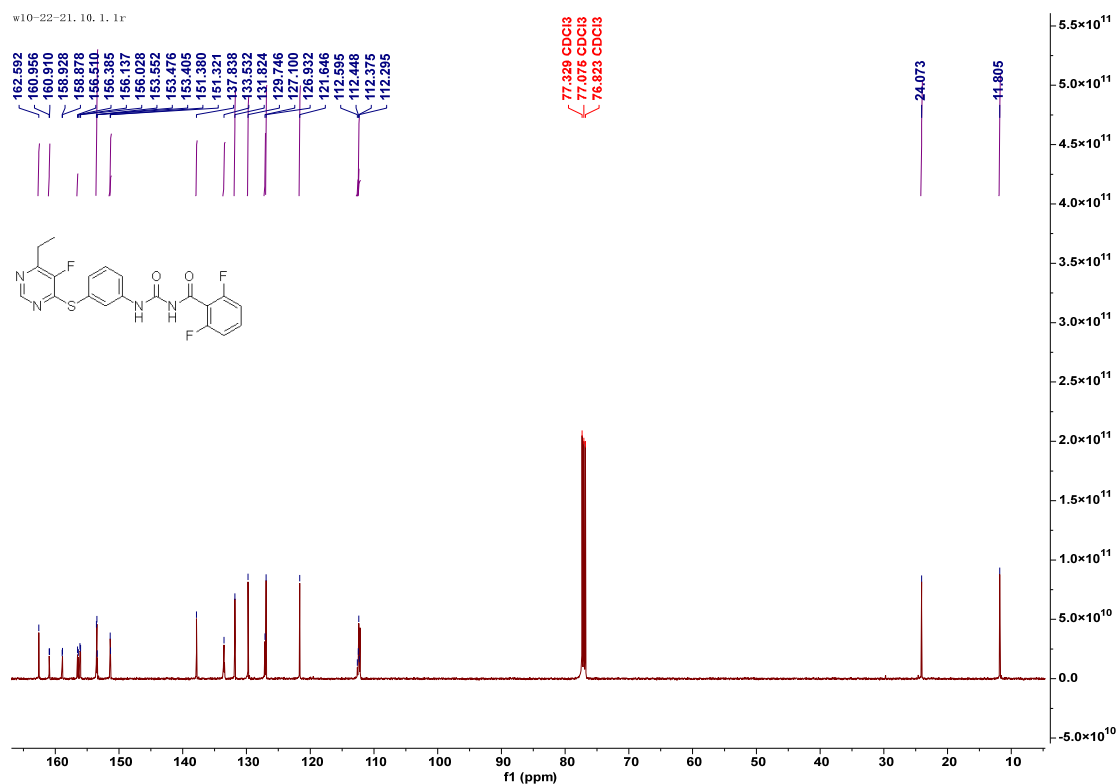


Figure S11  $^{13}\text{C}$  NMR spectrum of compound 4d

W12-05-15 #24 RT: 0.11 AV: 1 NL: 5.66E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

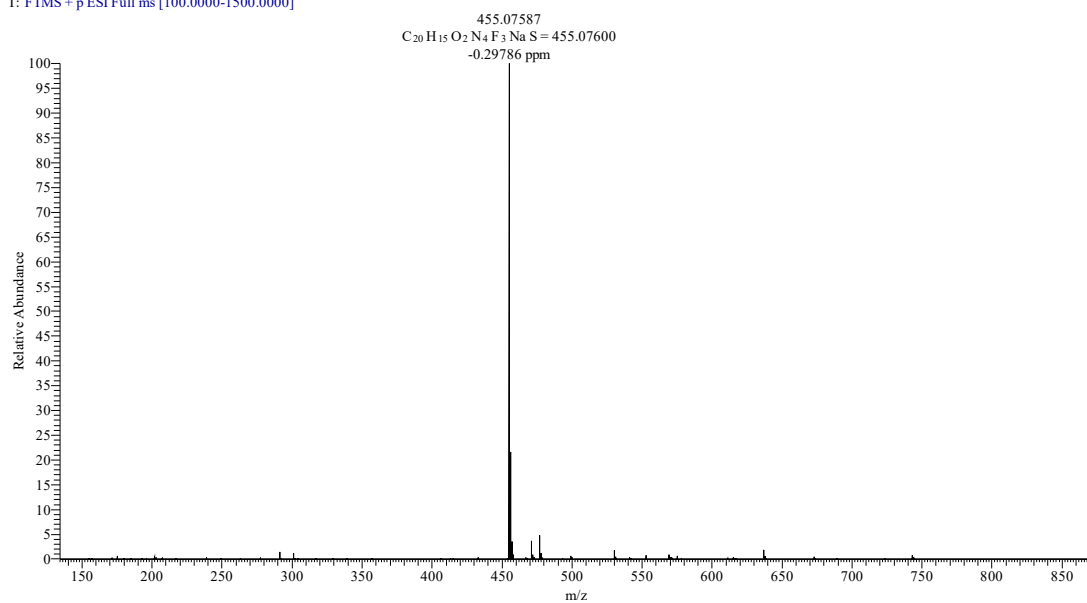


Figure S12 HRMS spectrum of compound 4d

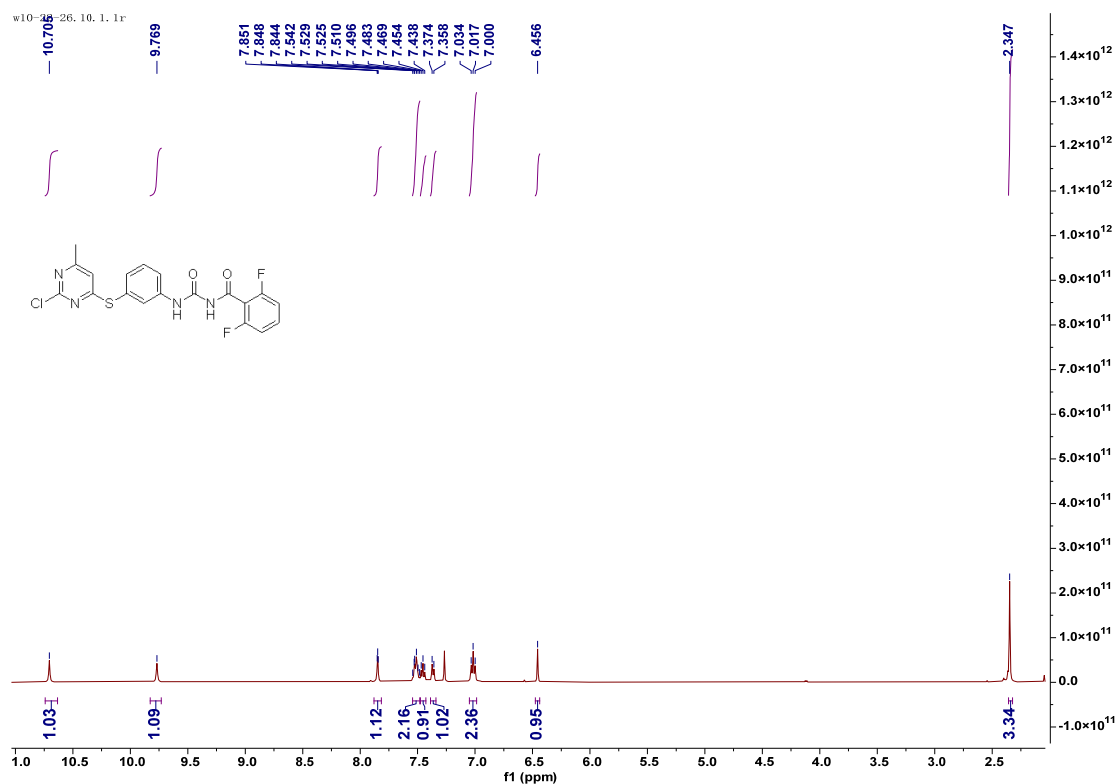


Figure S13 <sup>1</sup>H NMR spectrum of compound 4e

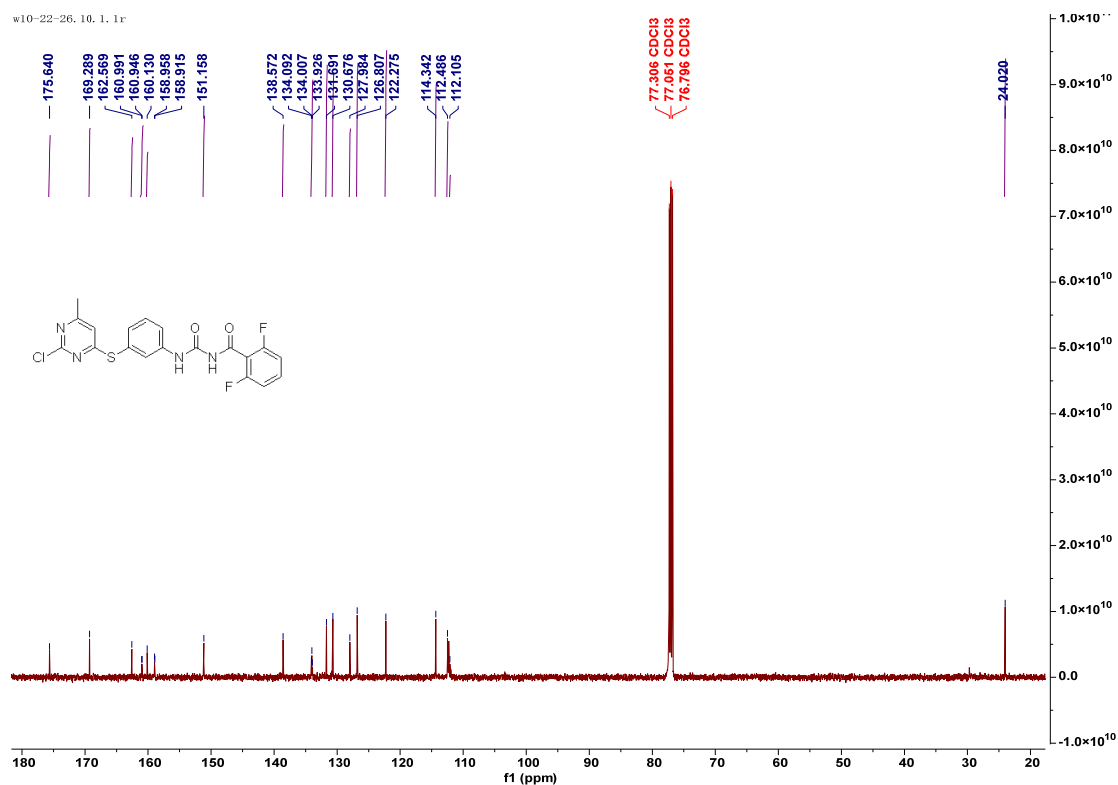


Figure S14 <sup>13</sup>C NMR spectrum of compound 4e

W12-05-16 #24 RT: 0.11 AV: 1 NL: 4.27E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

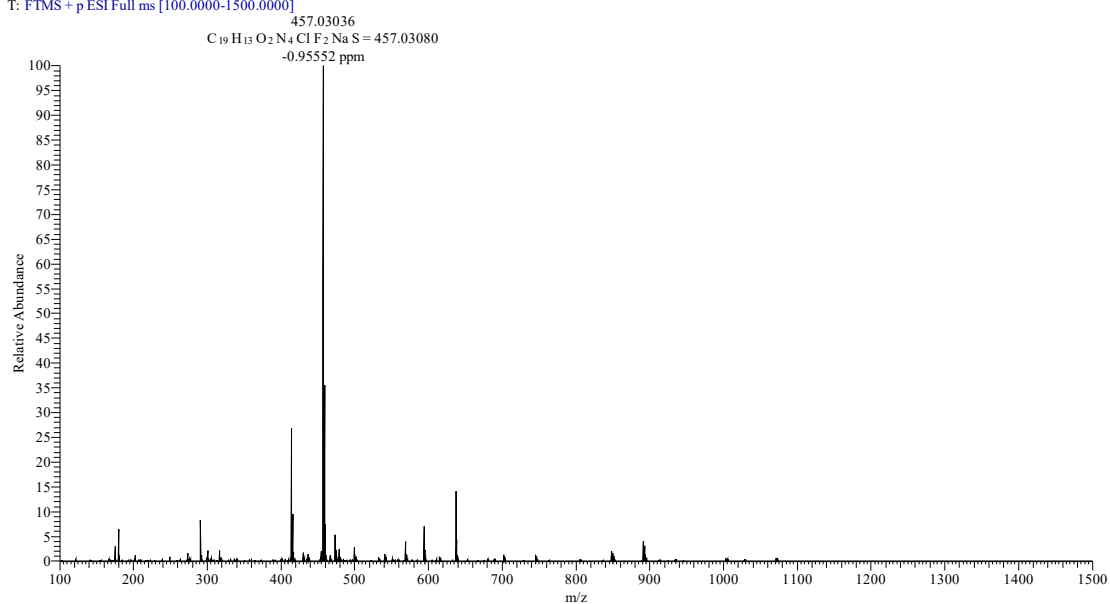


Figure S15 HRMS spectrum of compound 4e

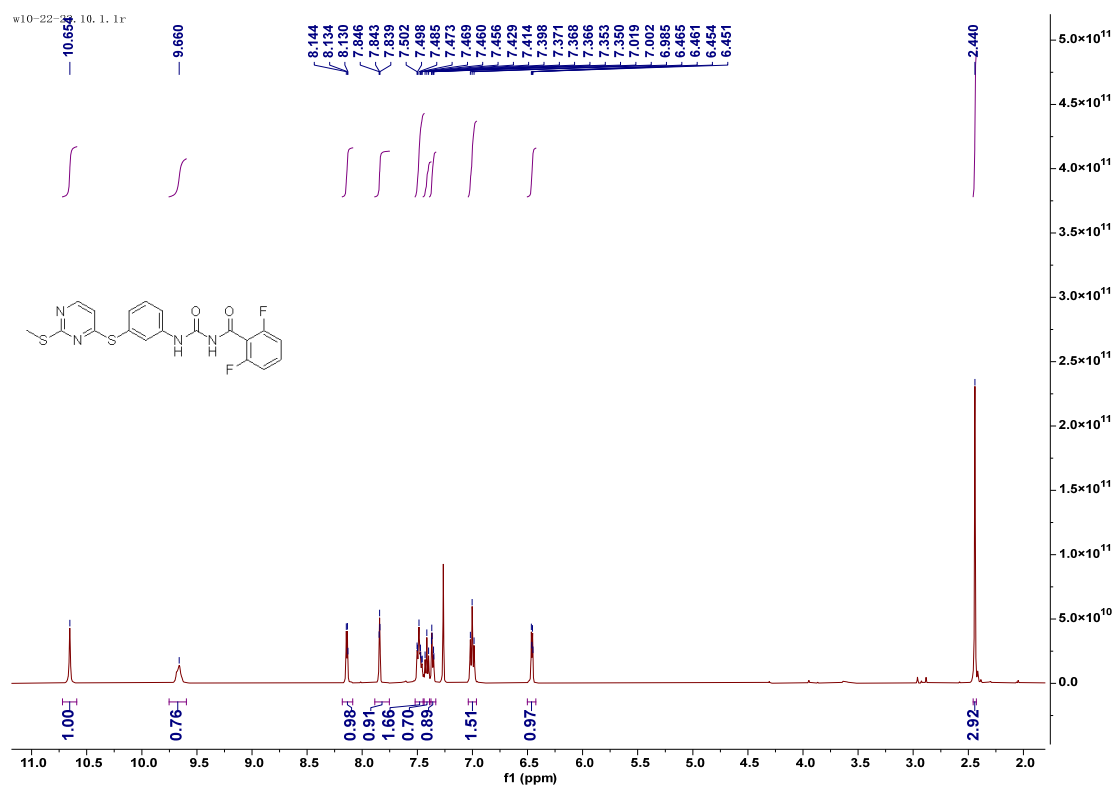


Figure S16 <sup>1</sup>H NMR spectrum of compound 4f



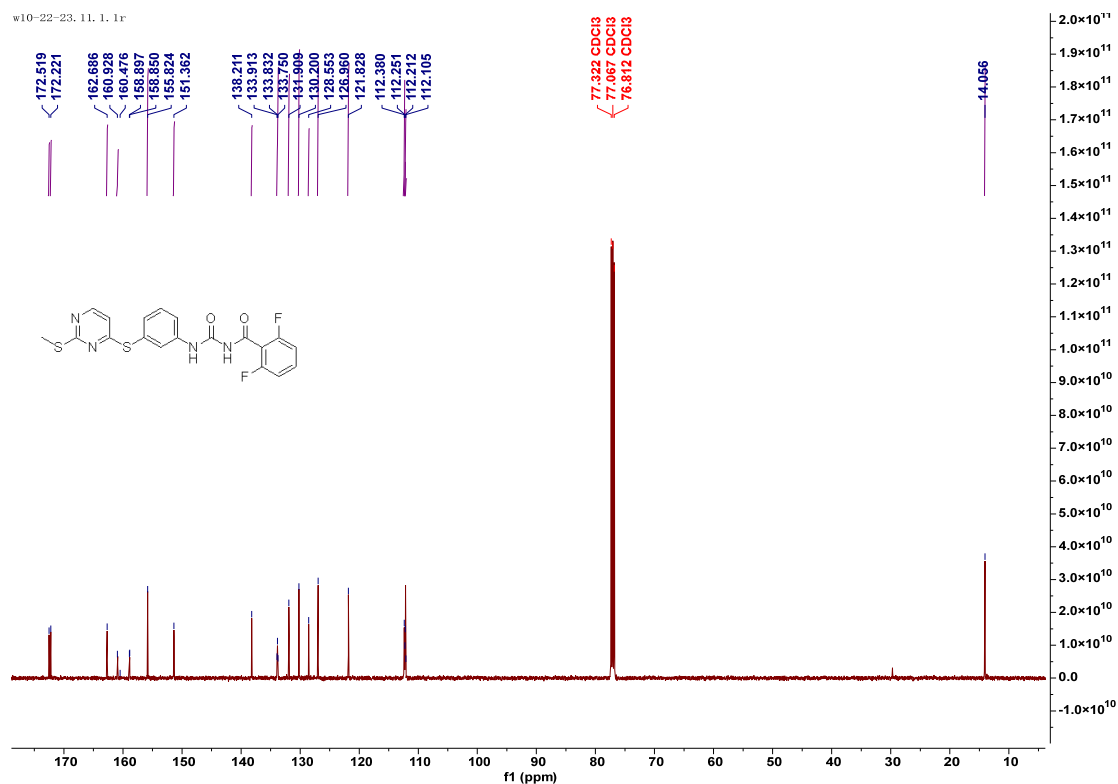


Figure S17 <sup>13</sup>C NMR spectrum of compound 4f

W12-05-17#23 RT: 0.11 AV: 1 NL: 1.54E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

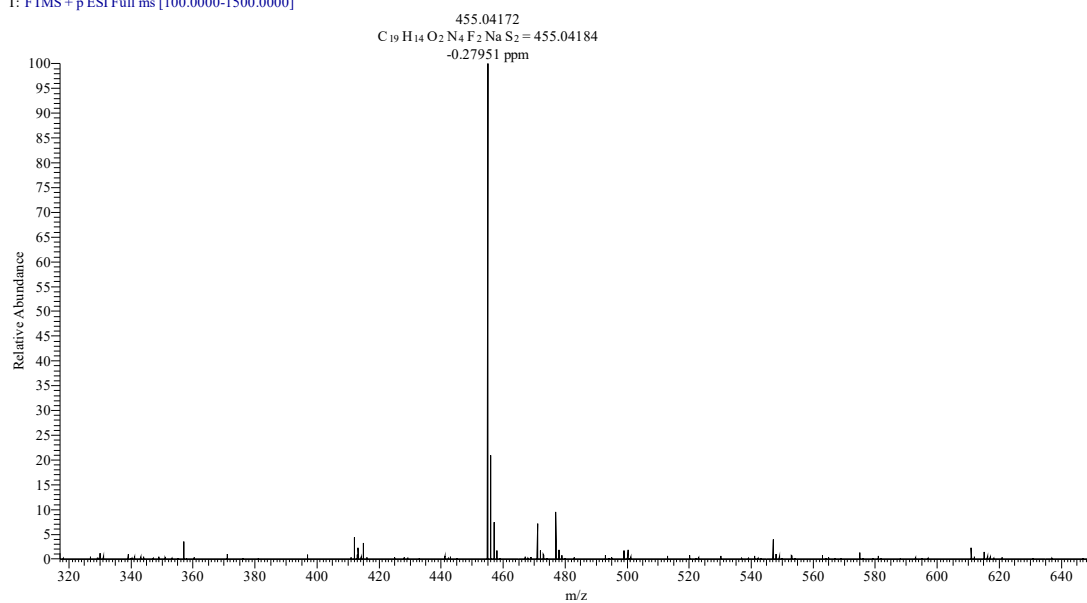


Figure S18 HRMS spectrum of compound 4f



W12-05-18 #23 RT: 0.10 AV: 1 NL: 1.19E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

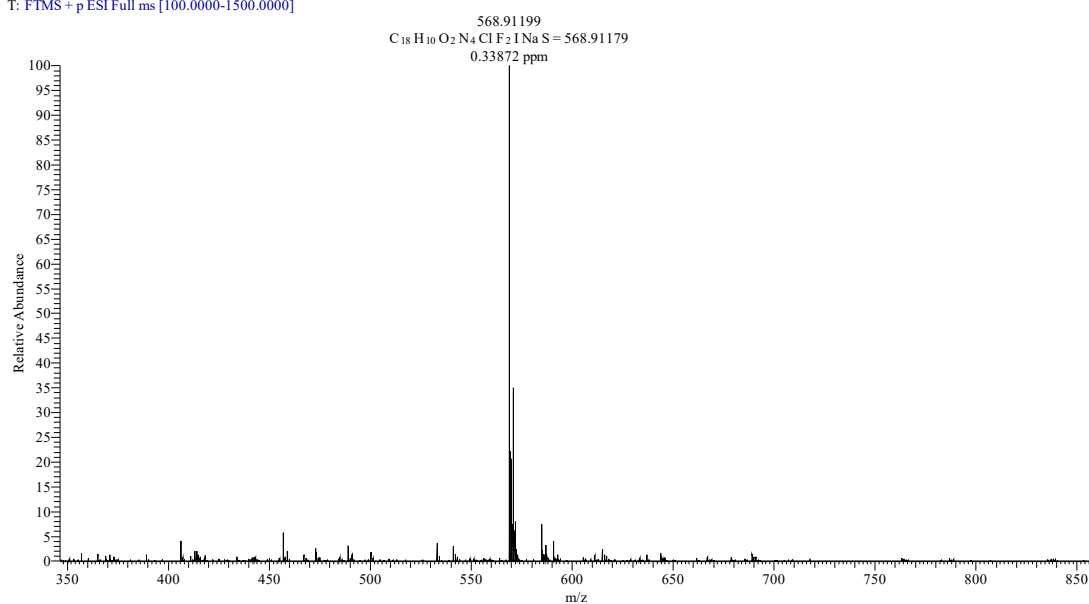


Figure S21 HRMS spectrum of compound 4g

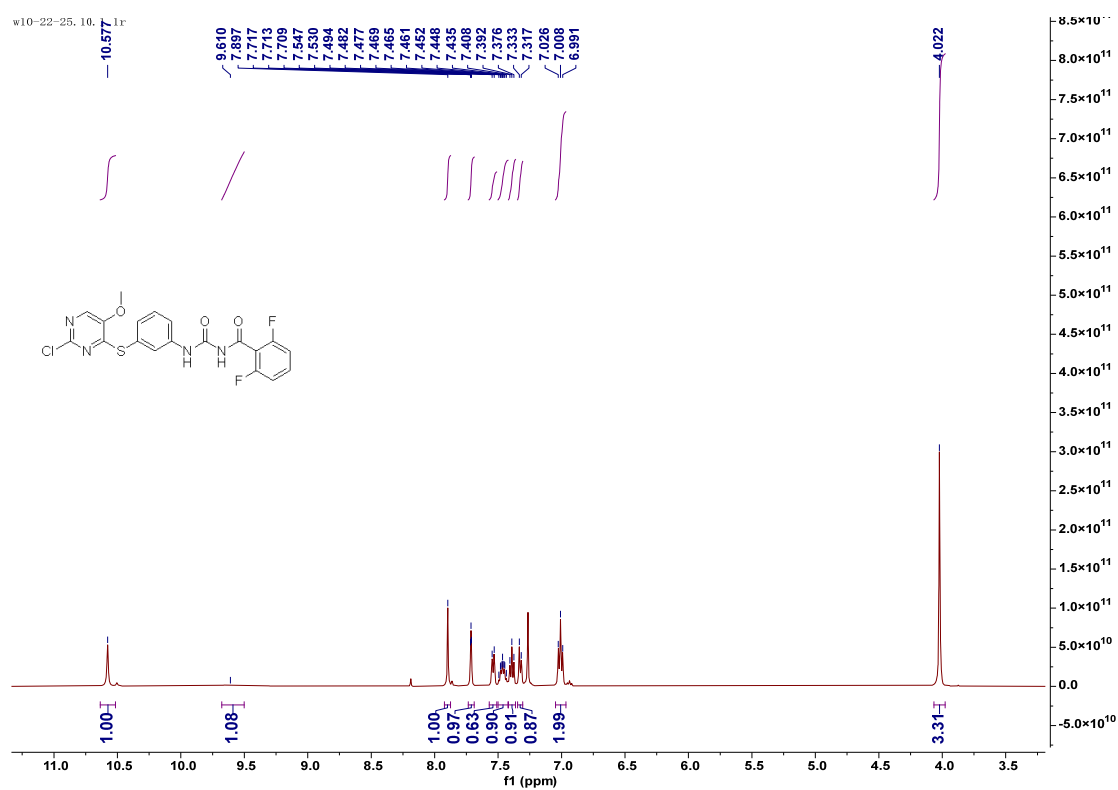
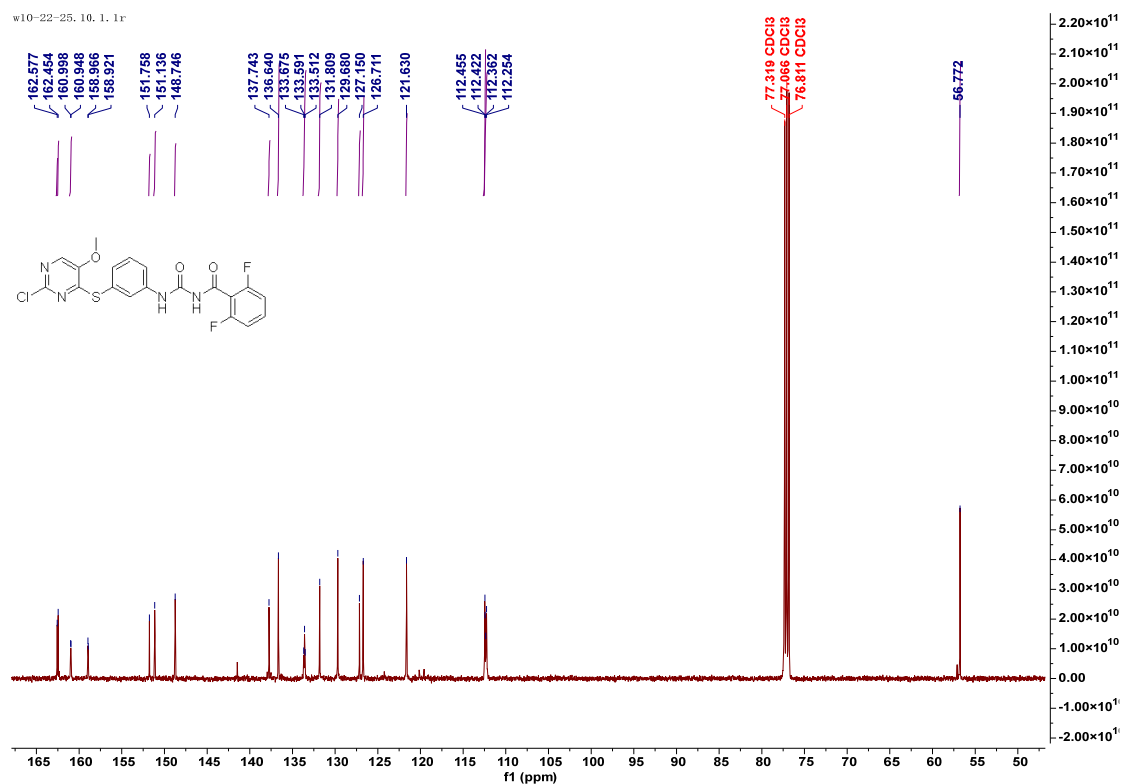
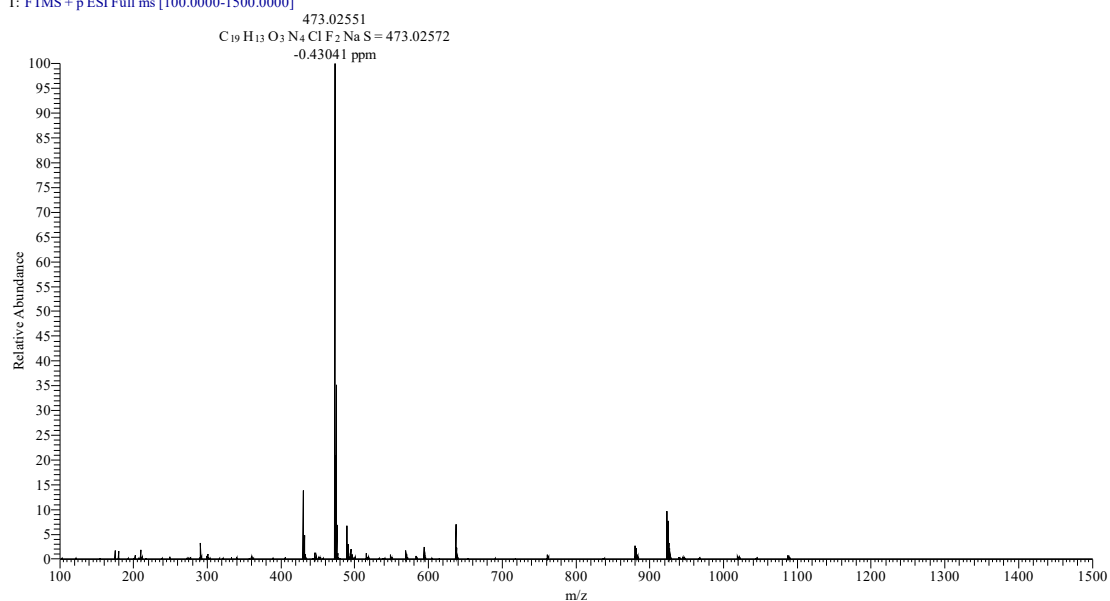


Figure S22 <sup>1</sup>H NMR spectrum of compound 4h



**Figure S23** <sup>13</sup>C NMR spectrum of compound **4h**

W12-05-19 #24 RT: 0.11 AV: 1 NL: 5.48E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



**Figure S24** HRMS spectrum of compound **4h**

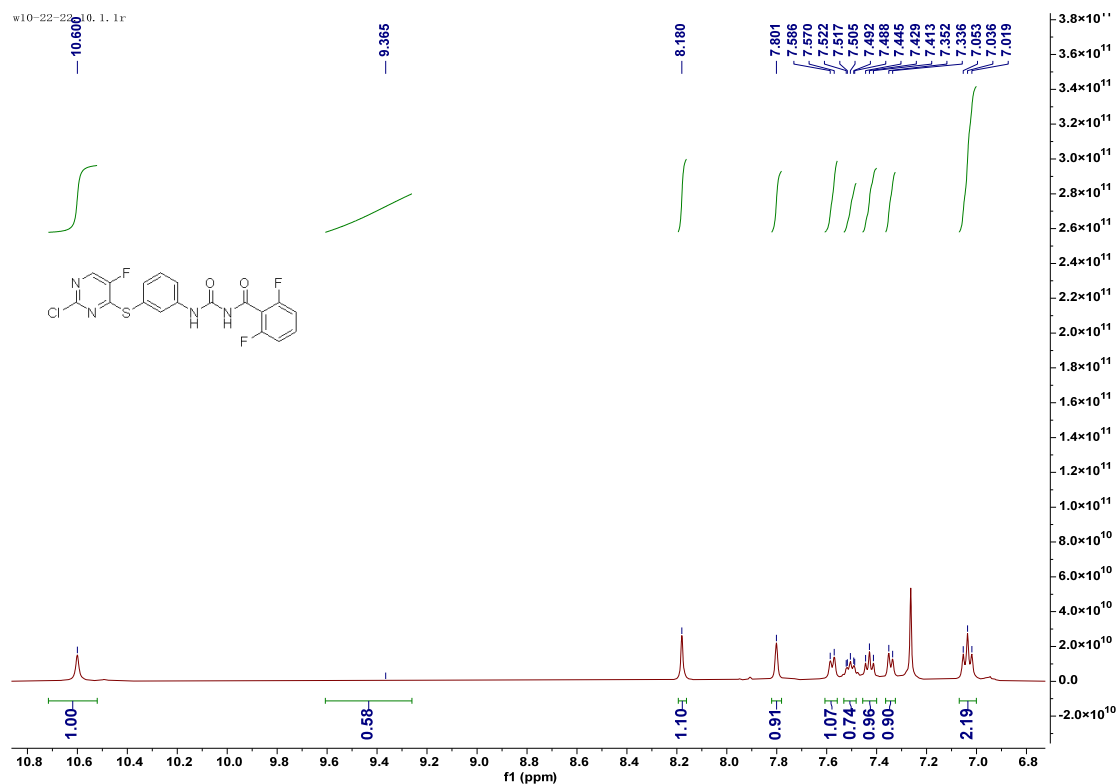


Figure S25  $^1\text{H}$  NMR spectrum of compound 4i

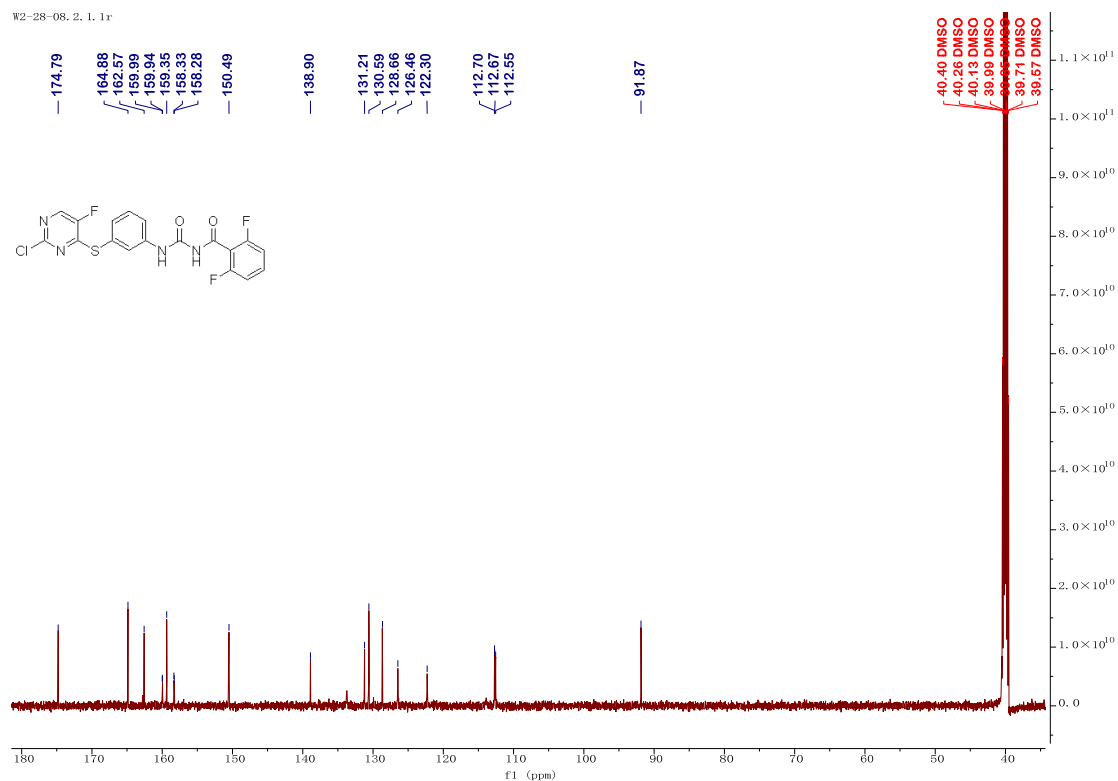


Figure S26  $^{13}\text{C}$  NMR spectrum of compound 4i

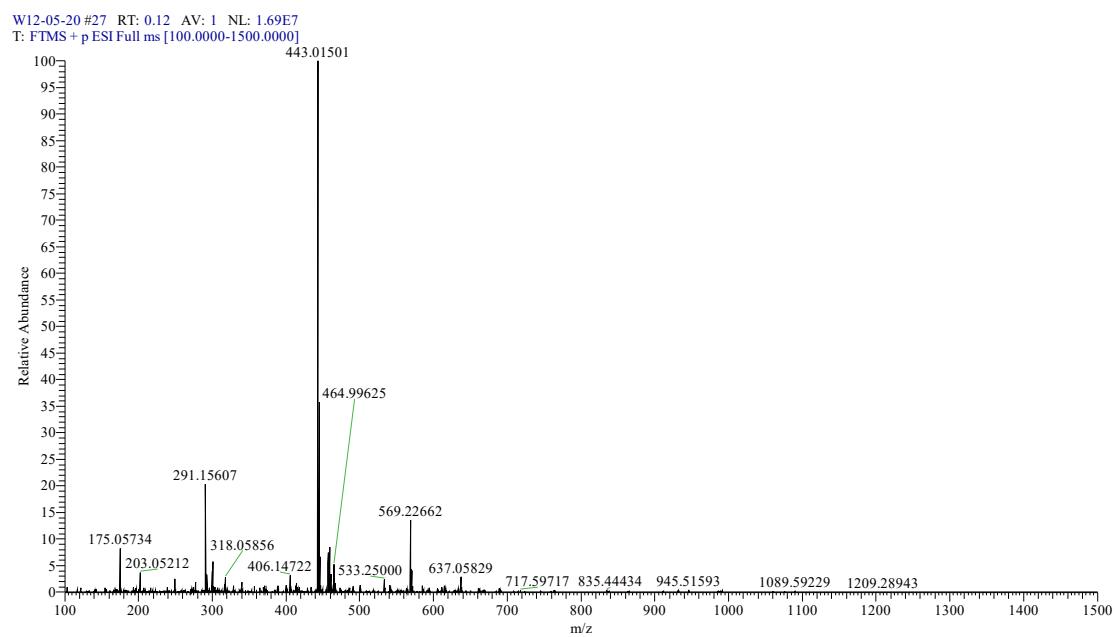


Figure S27 HRMS spectrum of compound 4i

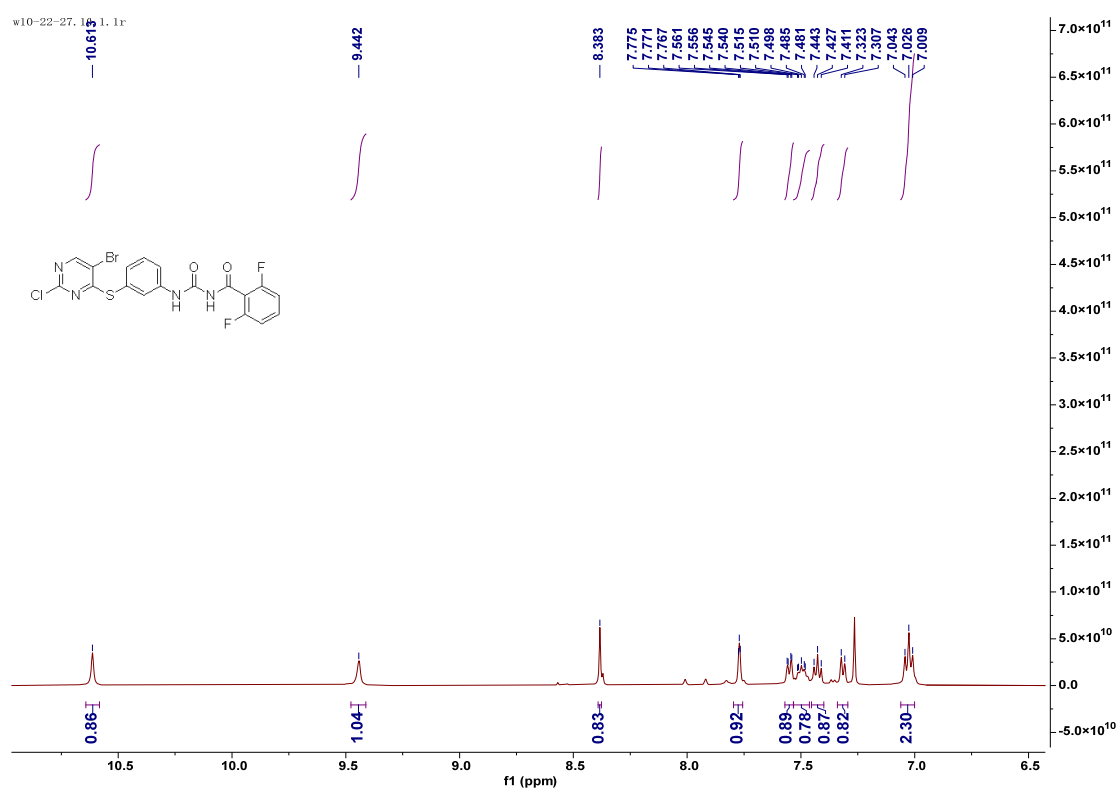
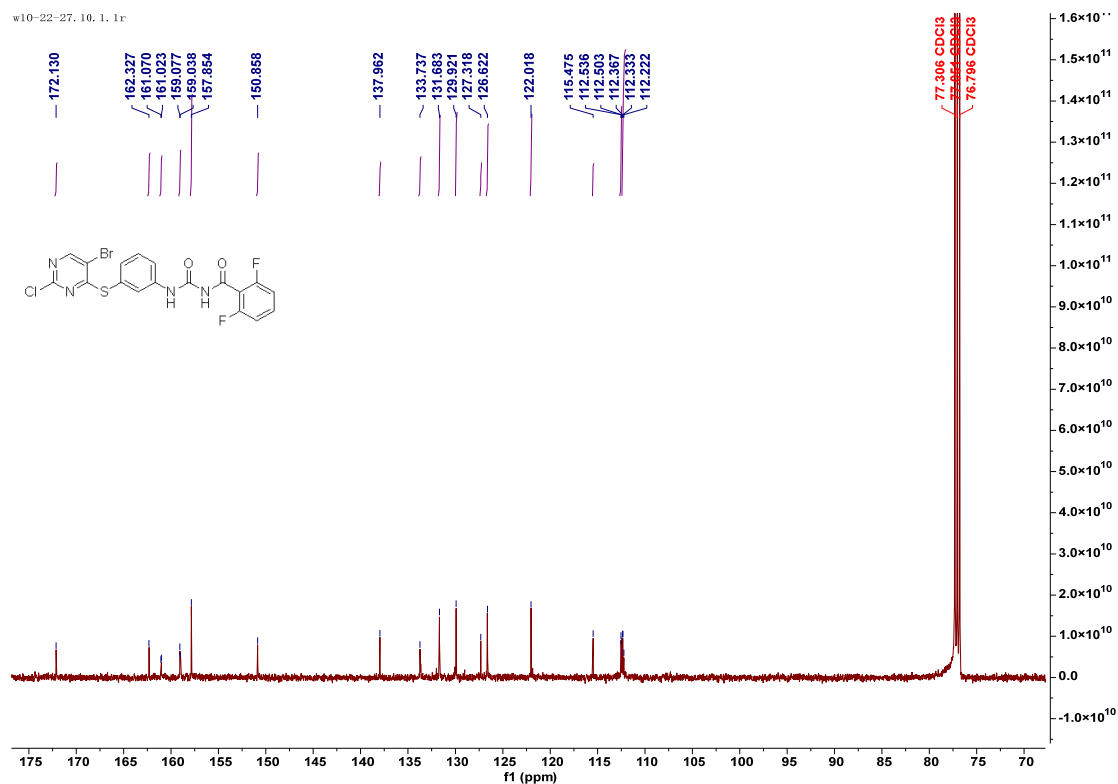
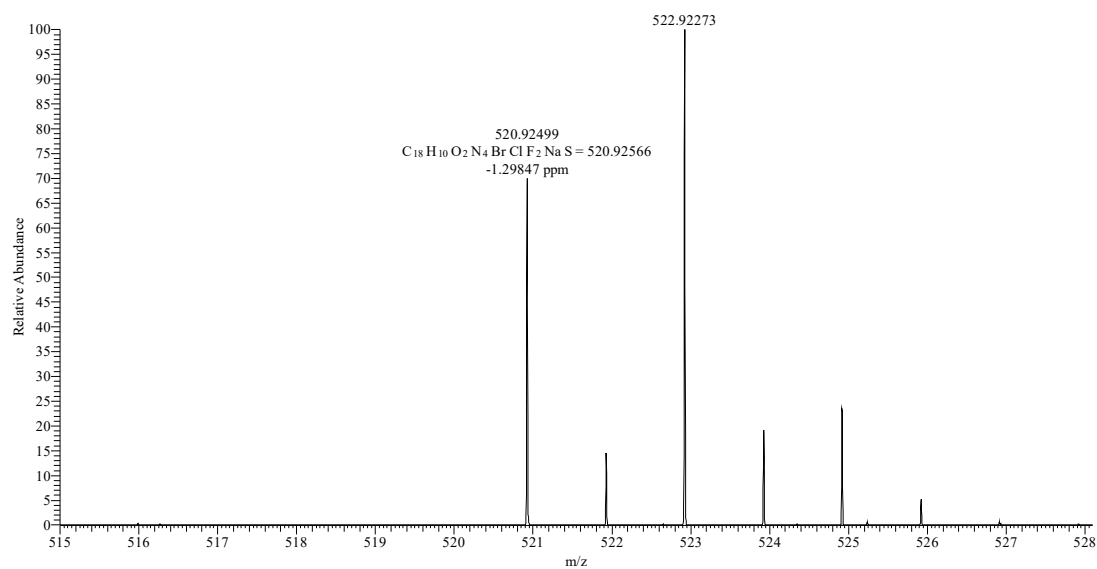


Figure S28  $^1\text{H}$  NMR spectrum of compound 4j



**Figure S29**  $^{13}\text{C}$  NMR spectrum of compound **4j**

W12-05-21 #23 RT: 0.11 AV: 1 NL: 3.30E6  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



**Figure S30** HRMS spectrum of compound **4j**

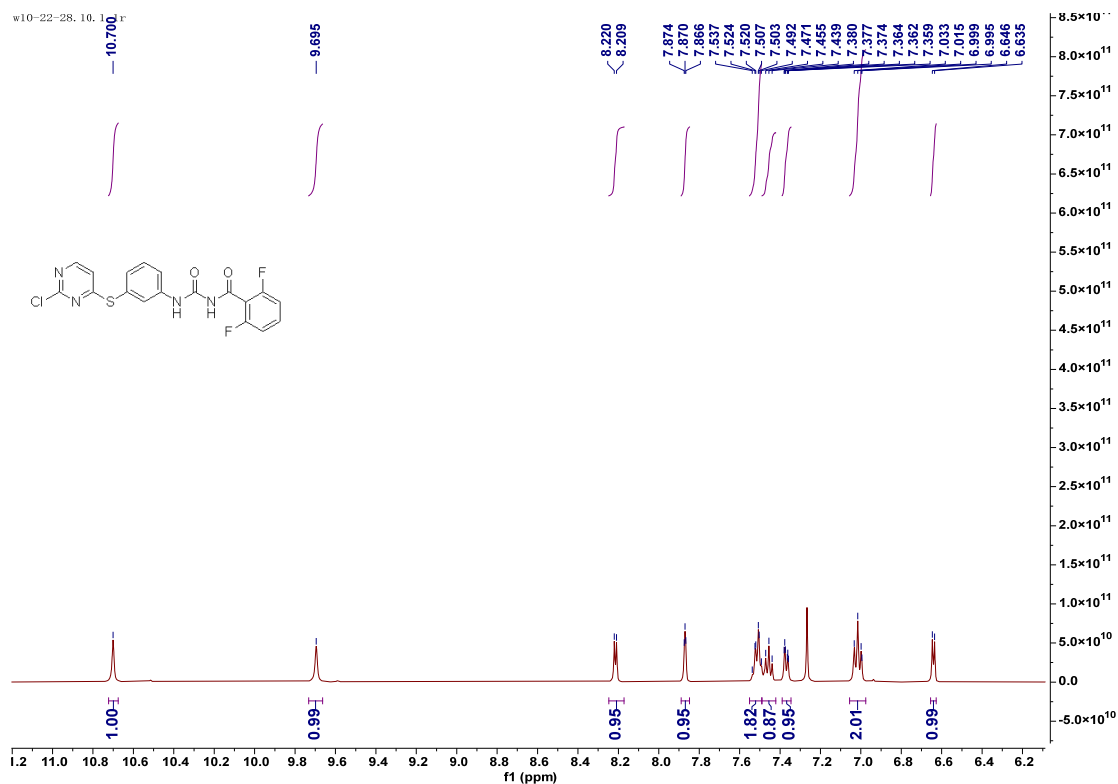


Figure S31  $^1\text{H}$  NMR spectrum of compound 4k

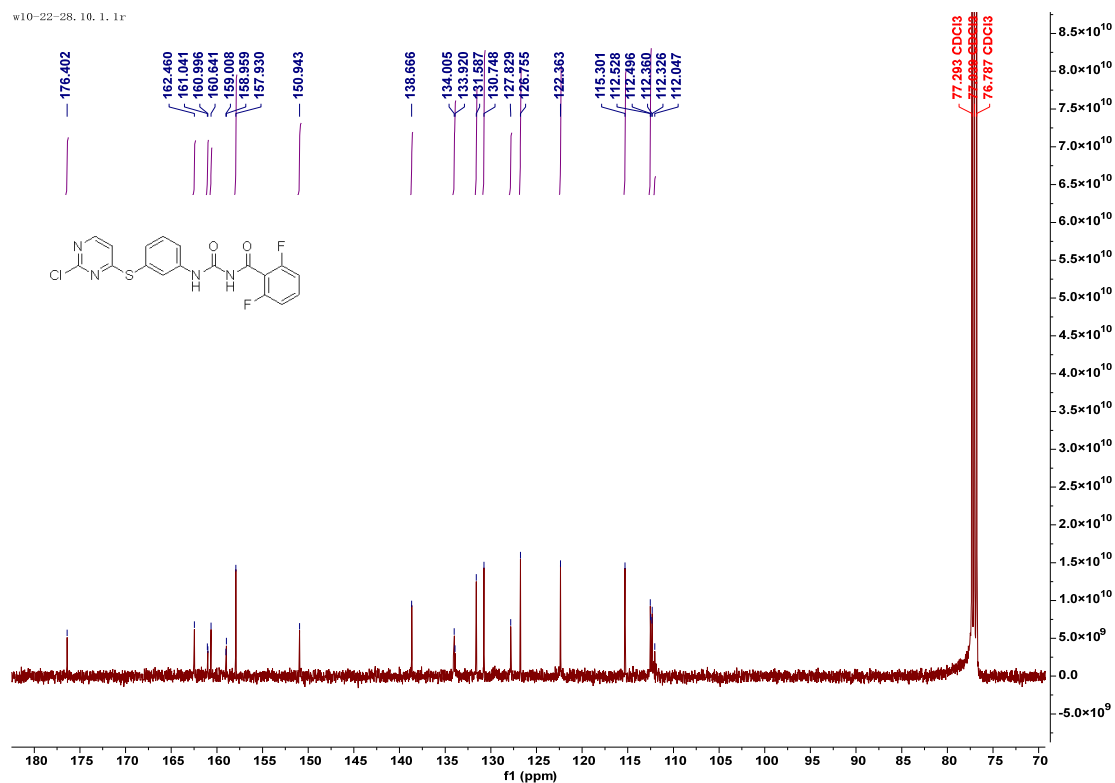
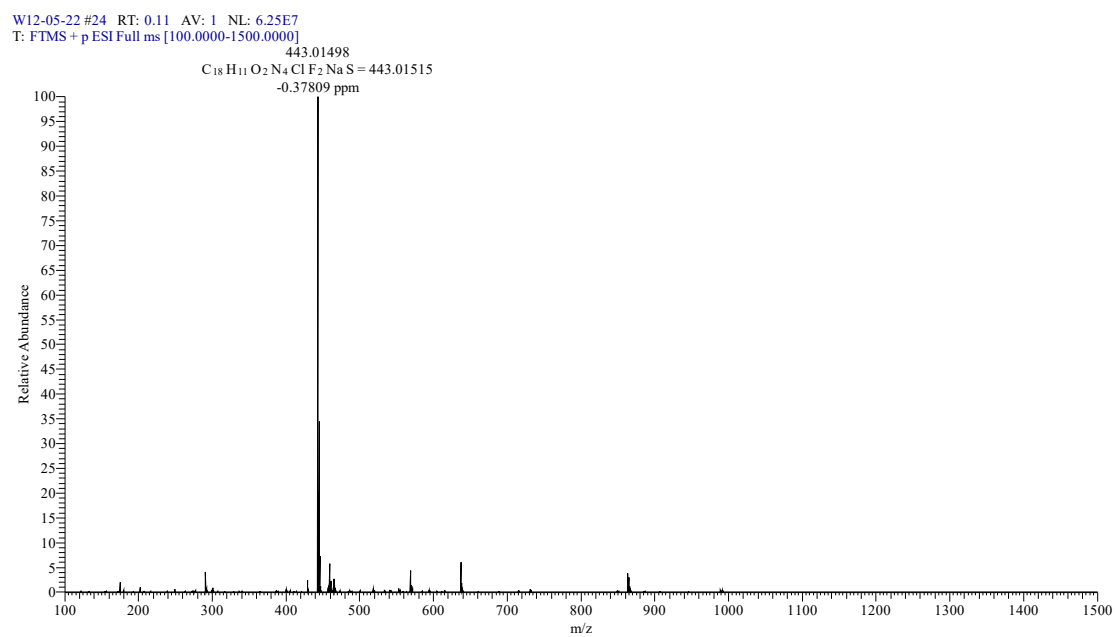
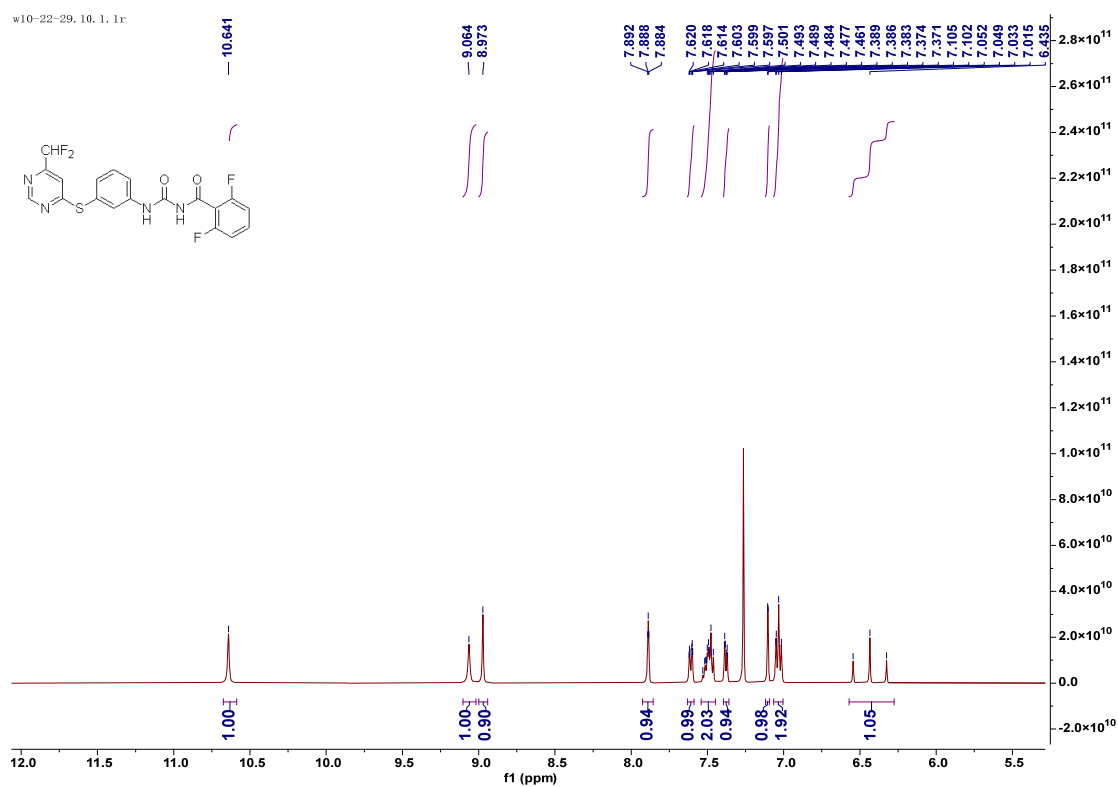


Figure S32  $^{13}\text{C}$  NMR spectrum of compound 4k

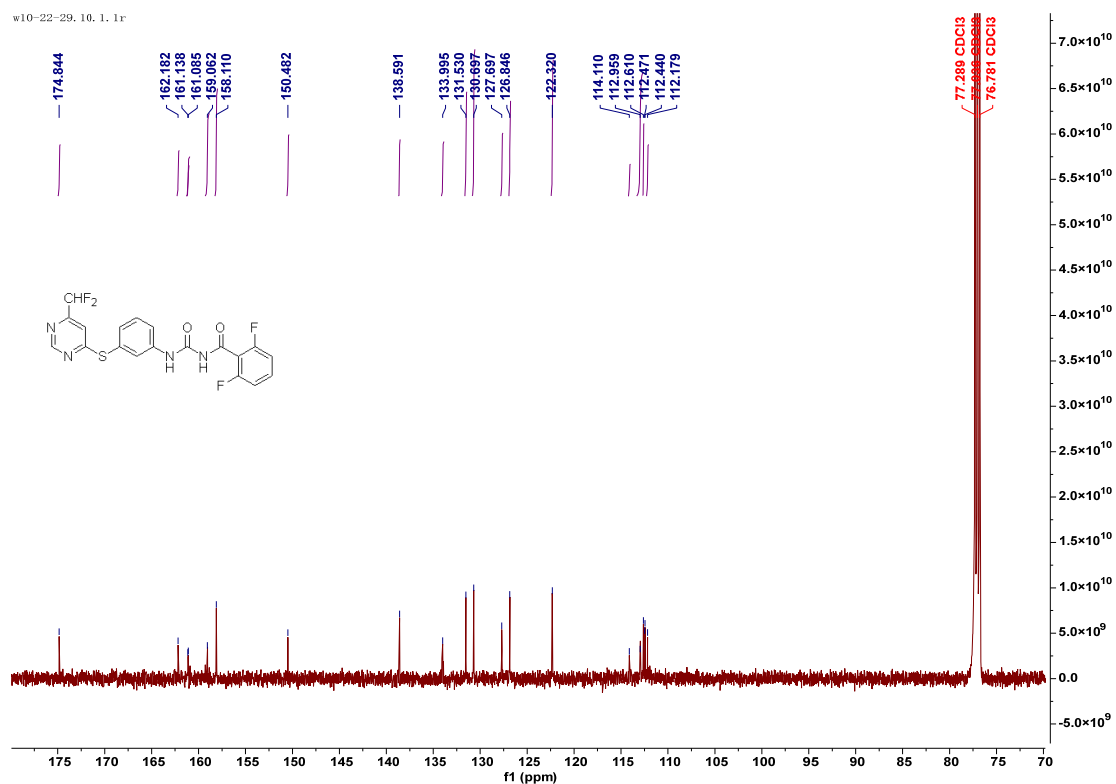




**Figure S33** HRMS spectrum of compound **4k**

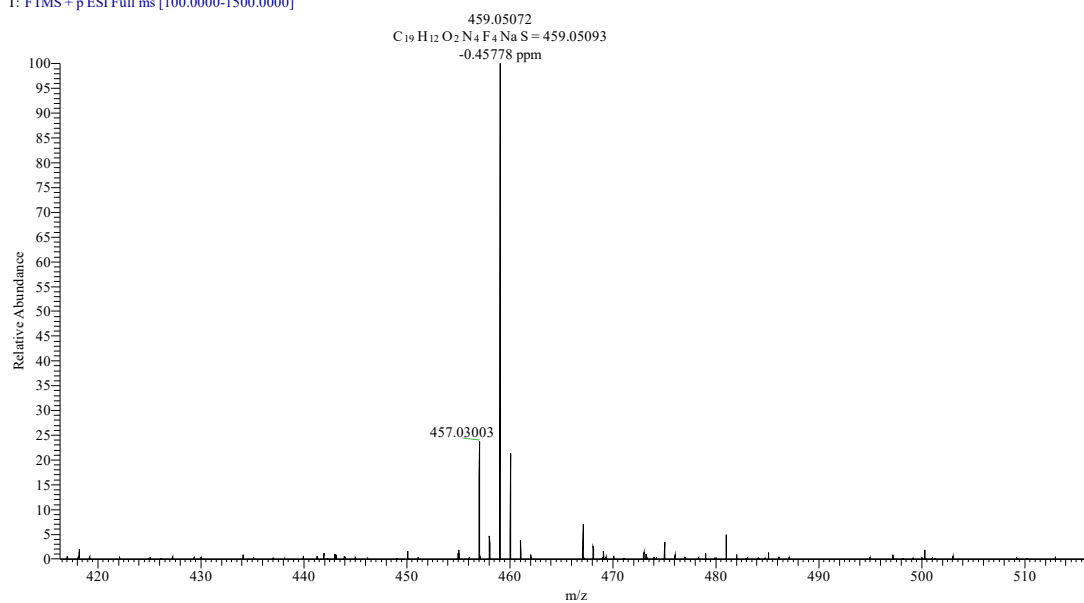


**Figure S34** <sup>1</sup>H NMR spectrum of compound **4l**



**Figure S35**  $^{13}\text{C}$  NMR spectrum of compound **4l**

W12-05-23 #21 RT: 0.09 AV: 1 NL: 9.86E6  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



**Figure S36** HRMS spectrum of compound **4l**

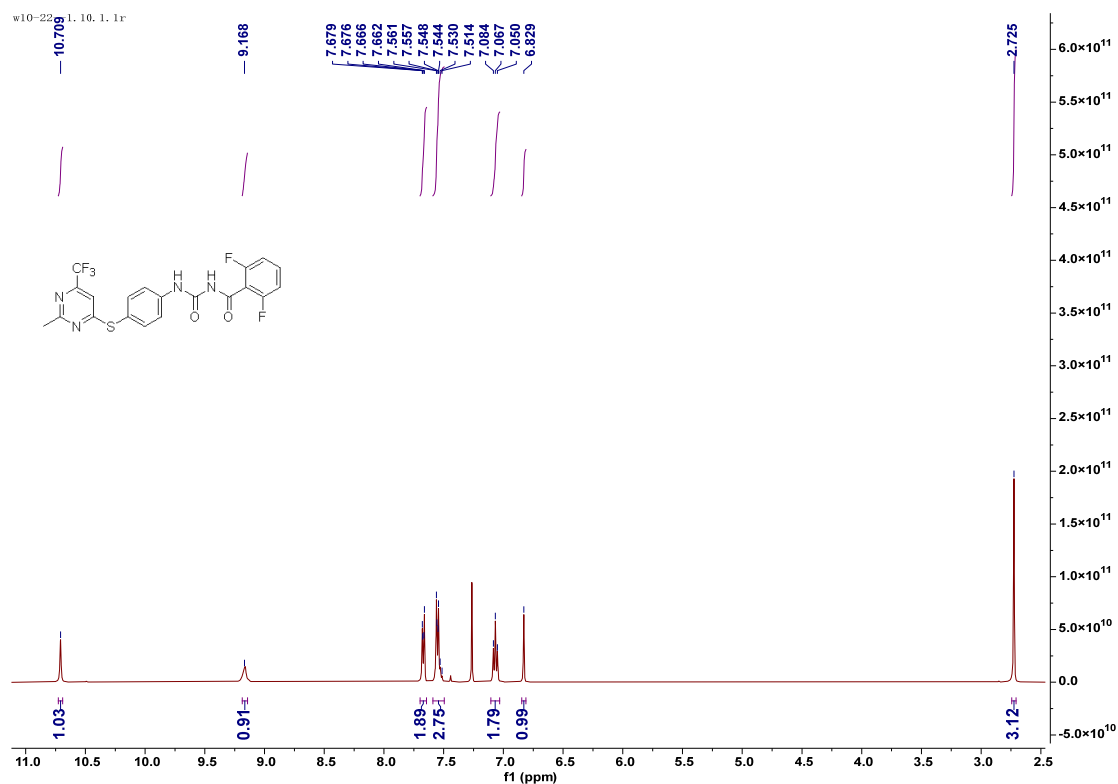


Figure S37 <sup>1</sup>H NMR spectrum of compound 4m

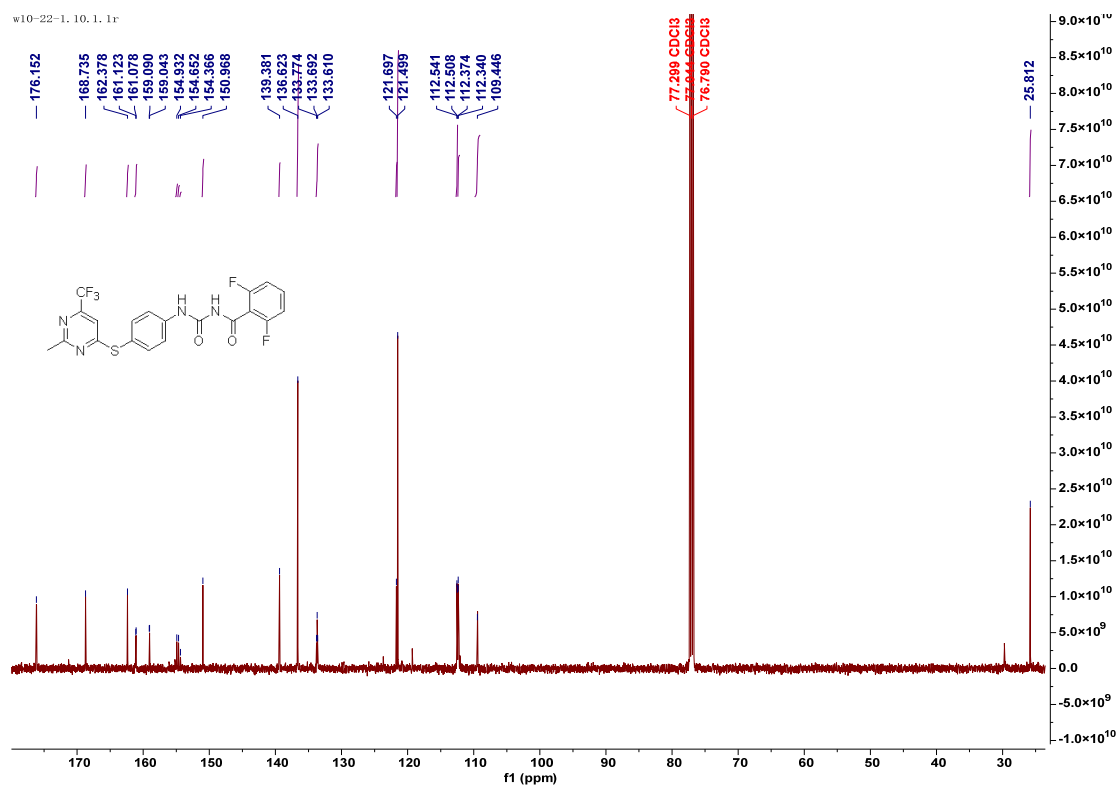


Figure S38 <sup>13</sup>C NMR spectrum of compound 4m

W12-05-1 #25 RT: 0.11 AV: 1 NL: 3.67E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

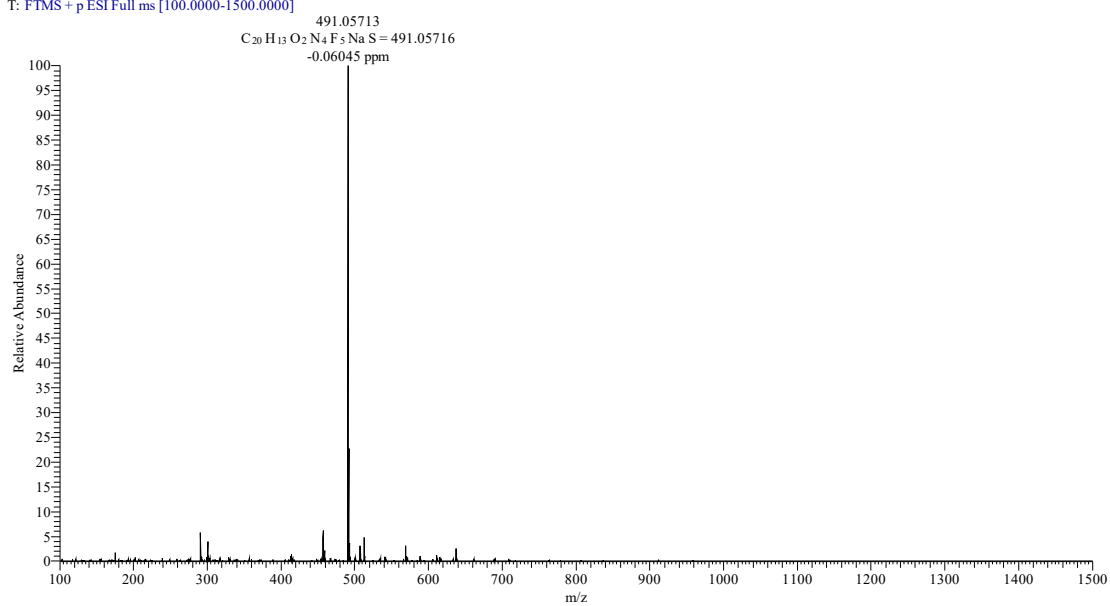


Figure S39 HRMS spectrum of compound **4m**

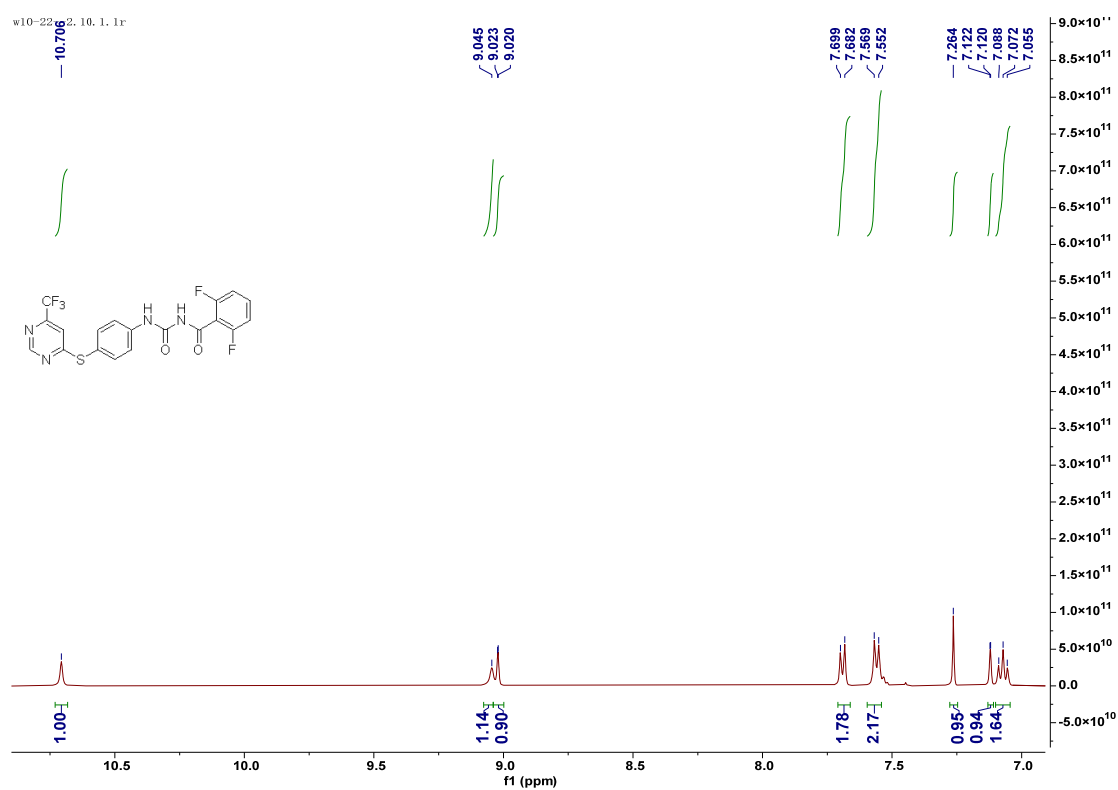


Figure S40 <sup>1</sup>H NMR spectrum of compound **4n**

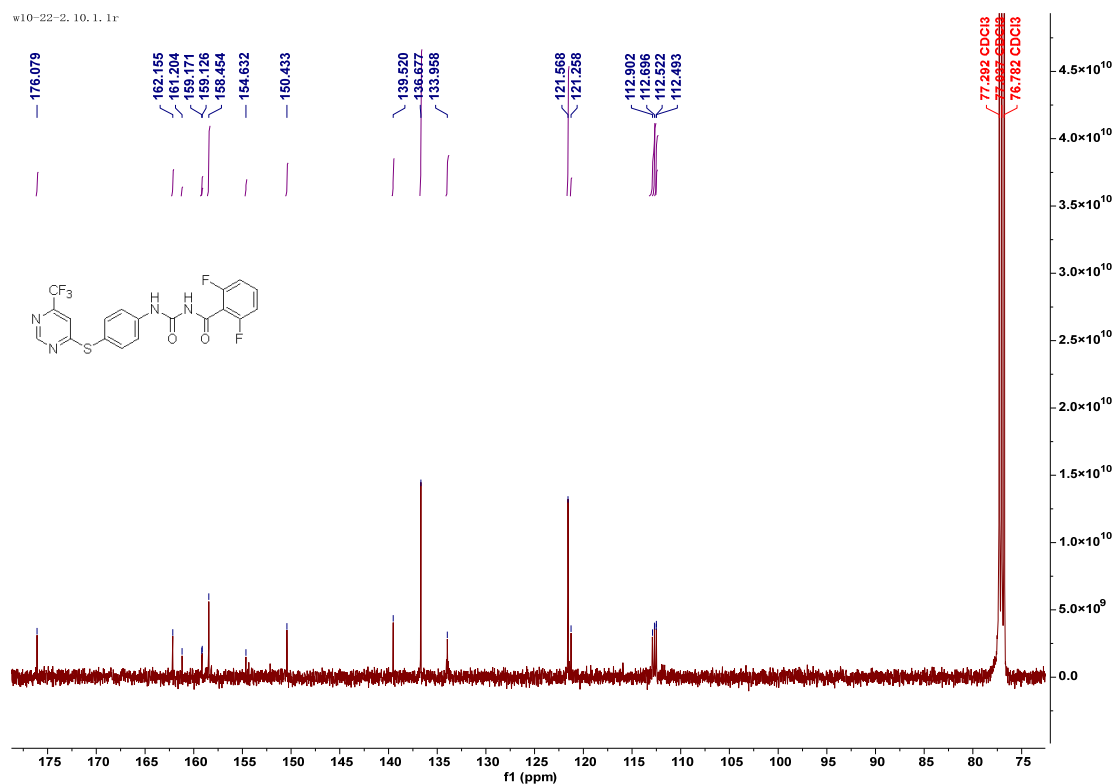


Figure S41 <sup>13</sup>C NMR spectrum of compound 4n

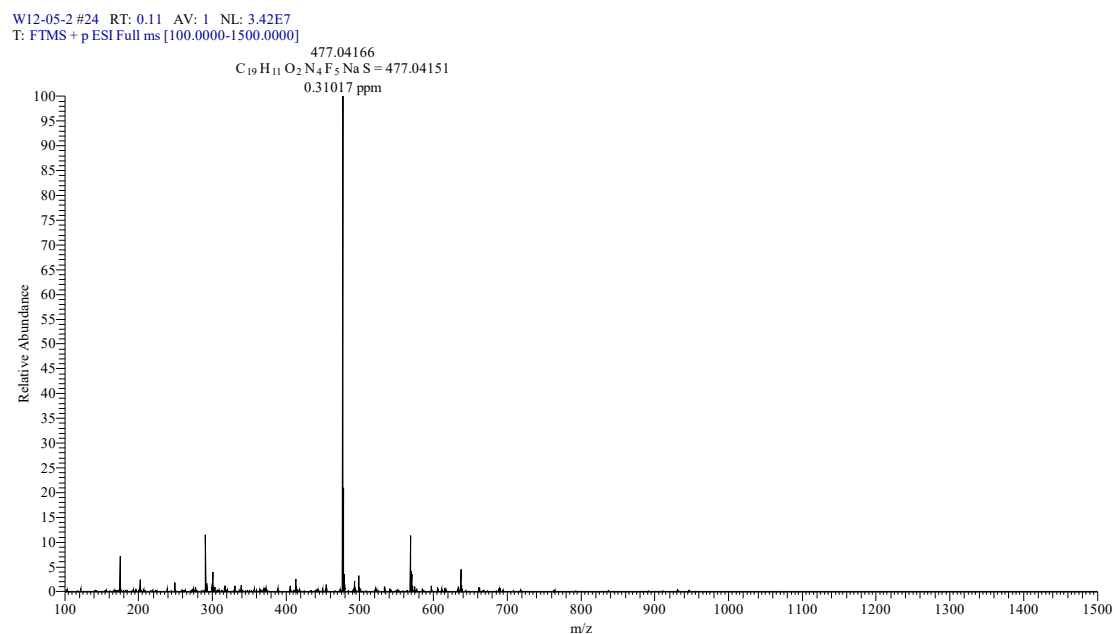


Figure S42 HRMS spectrum of compound 4n

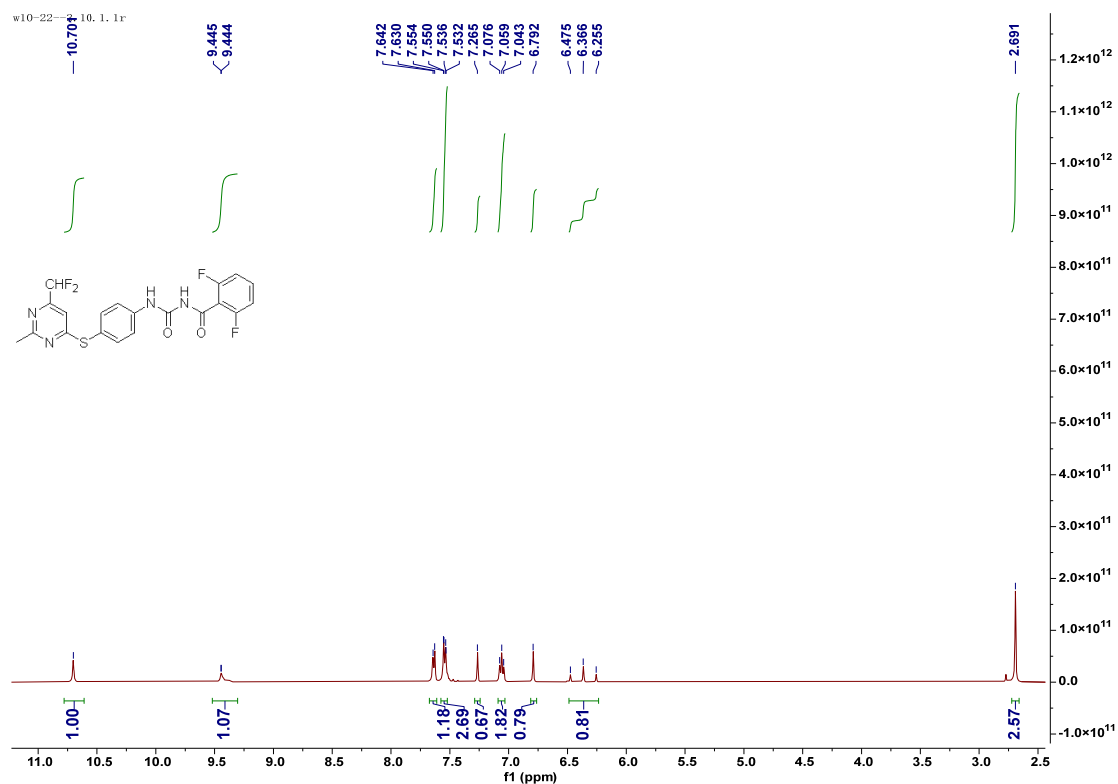


Figure S43  $^1\text{H}$  NMR spectrum of compound 40

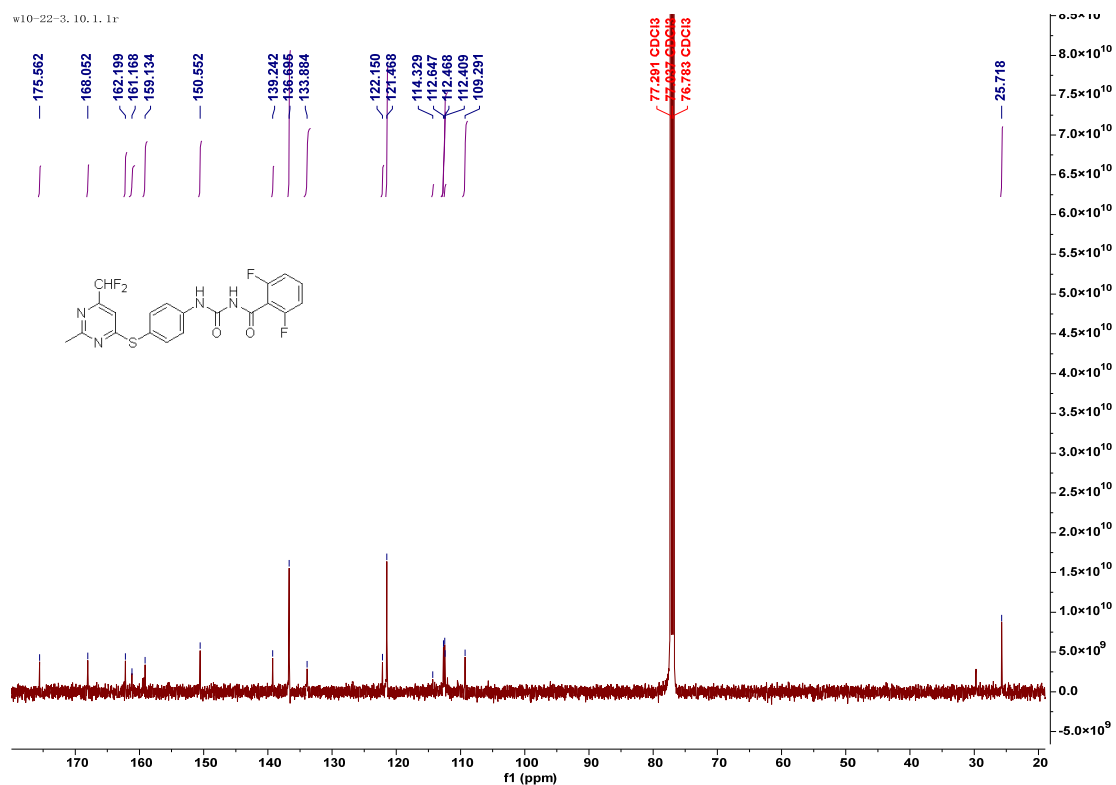


Figure S44  $^{13}\text{C}$  NMR spectrum of compound 40

W12-05-3 #20 RT: 0.09 AV: 1 NL: 3.75E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

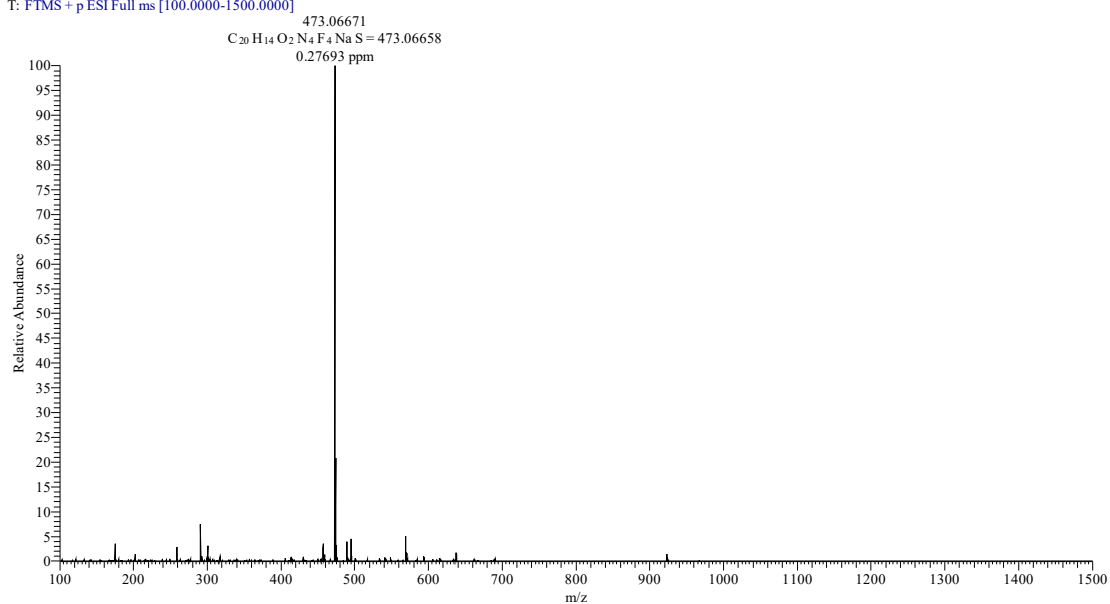


Figure S45 HRMS spectrum of compound 4o

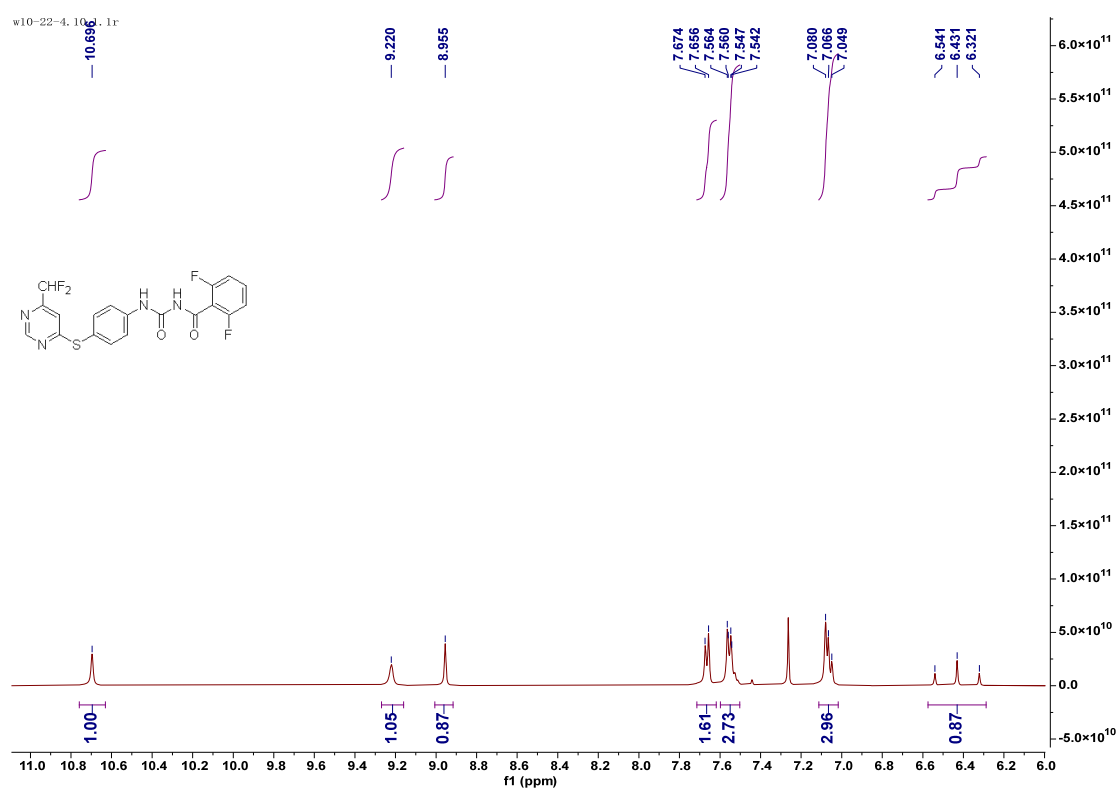


Figure S46 <sup>1</sup>H NMR spectrum of compound 4p

w10-22-4, 10, 1, 1r

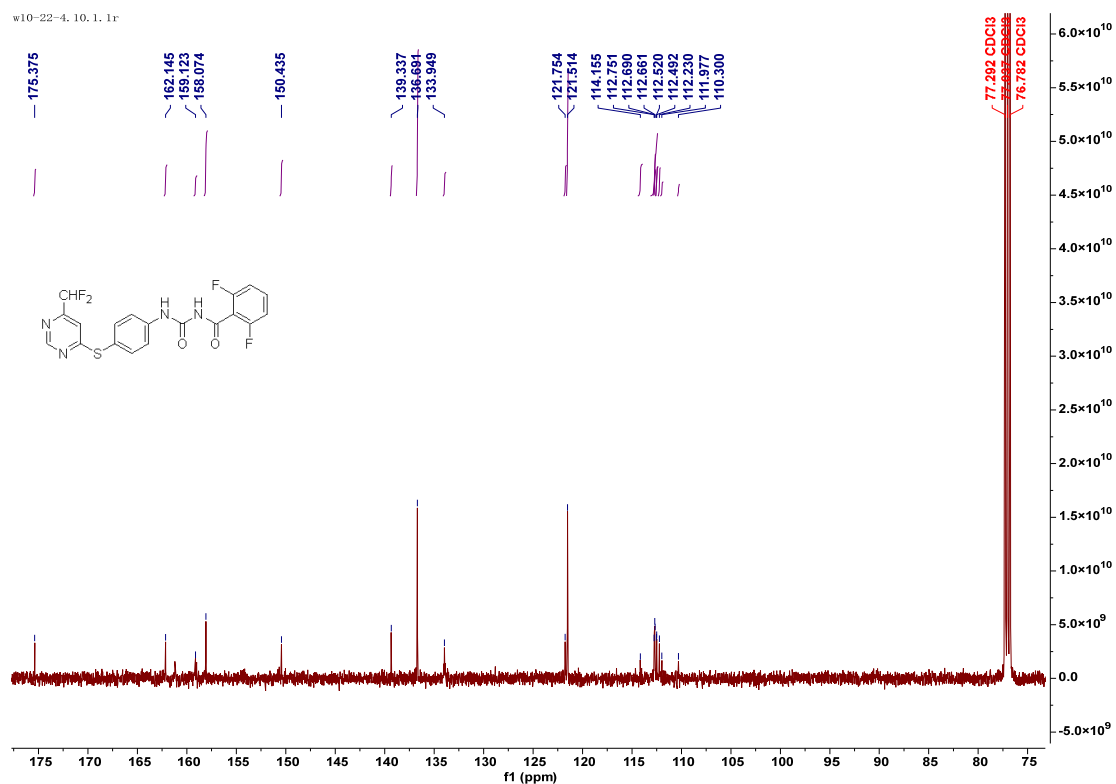


Figure S47 <sup>13</sup>C NMR spectrum of compound 4p

W12-05-4 #23 RT: 0.10 AV: 1 NL: 3.16E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

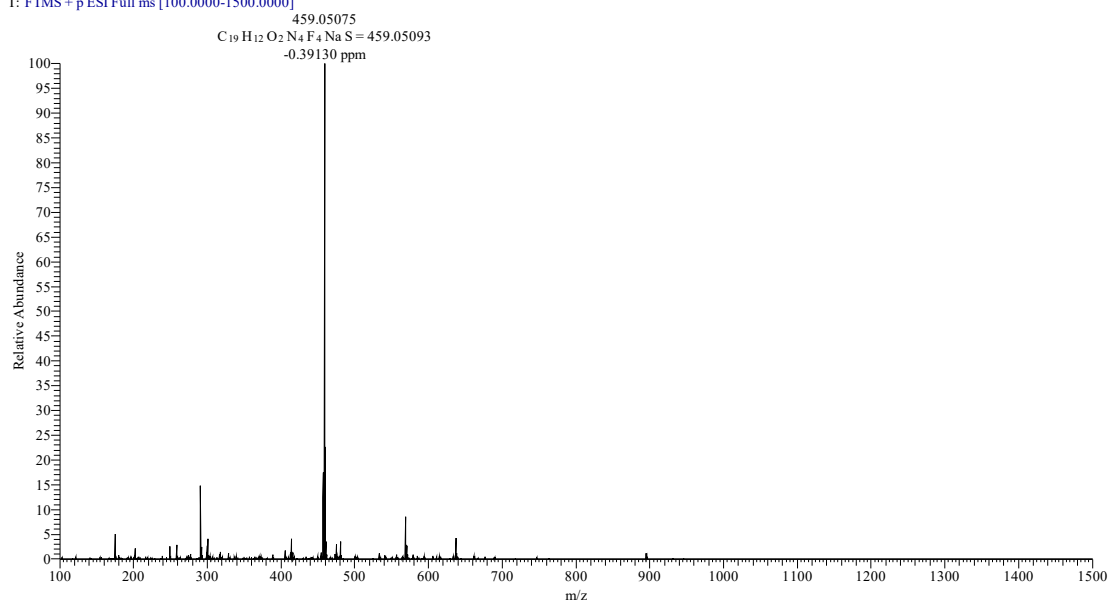


Figure S48 HRMS spectrum of compound 4p



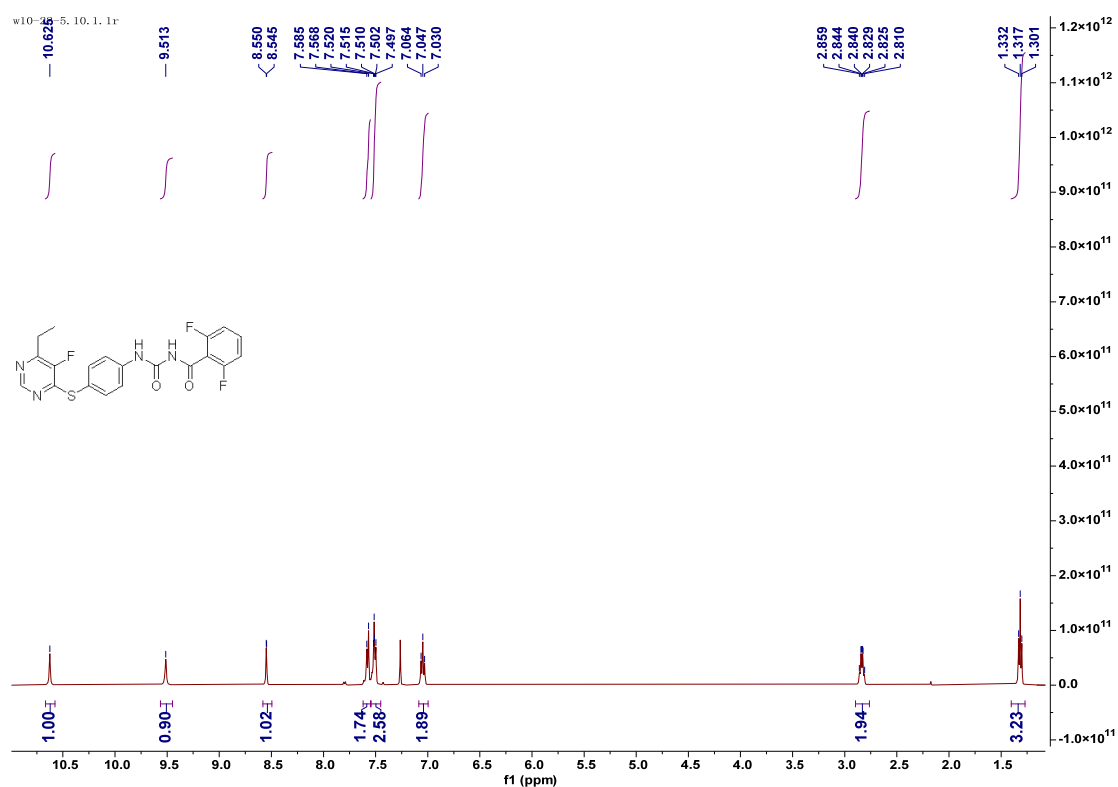


Figure S49 <sup>1</sup>H NMR spectrum of compound 4q

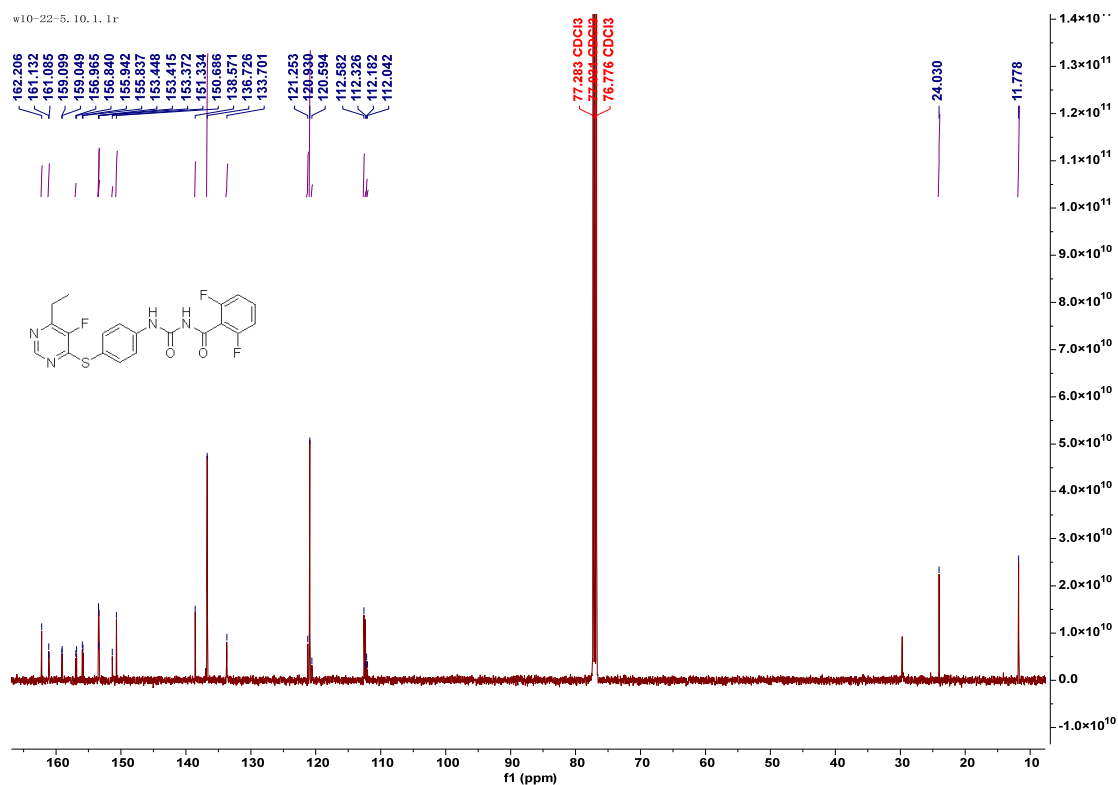


Figure S50 <sup>13</sup>C NMR spectrum of compound 4q

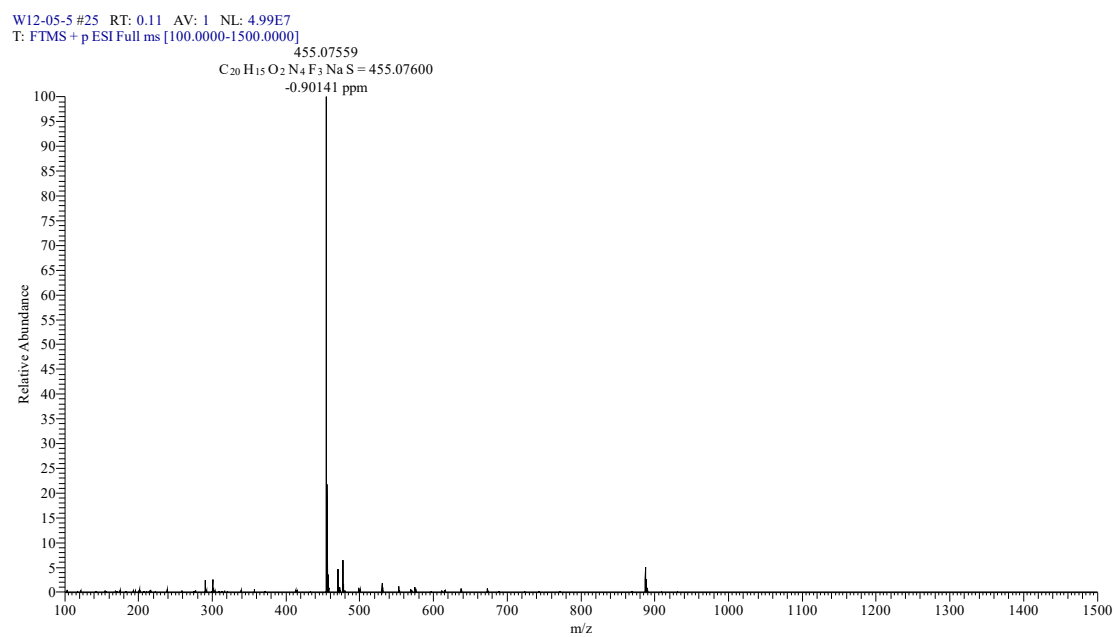


Figure S51 HRMS spectrum of compound 4q

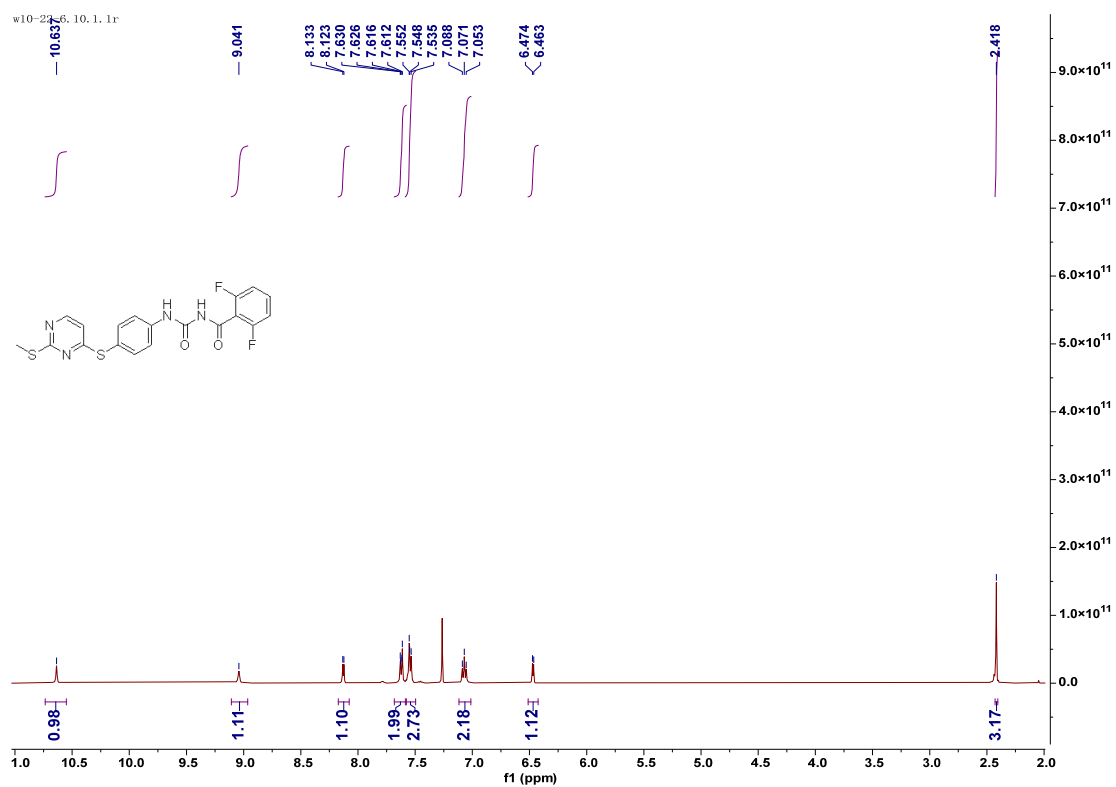


Figure S52 <sup>1</sup>H NMR spectrum of compound 4r

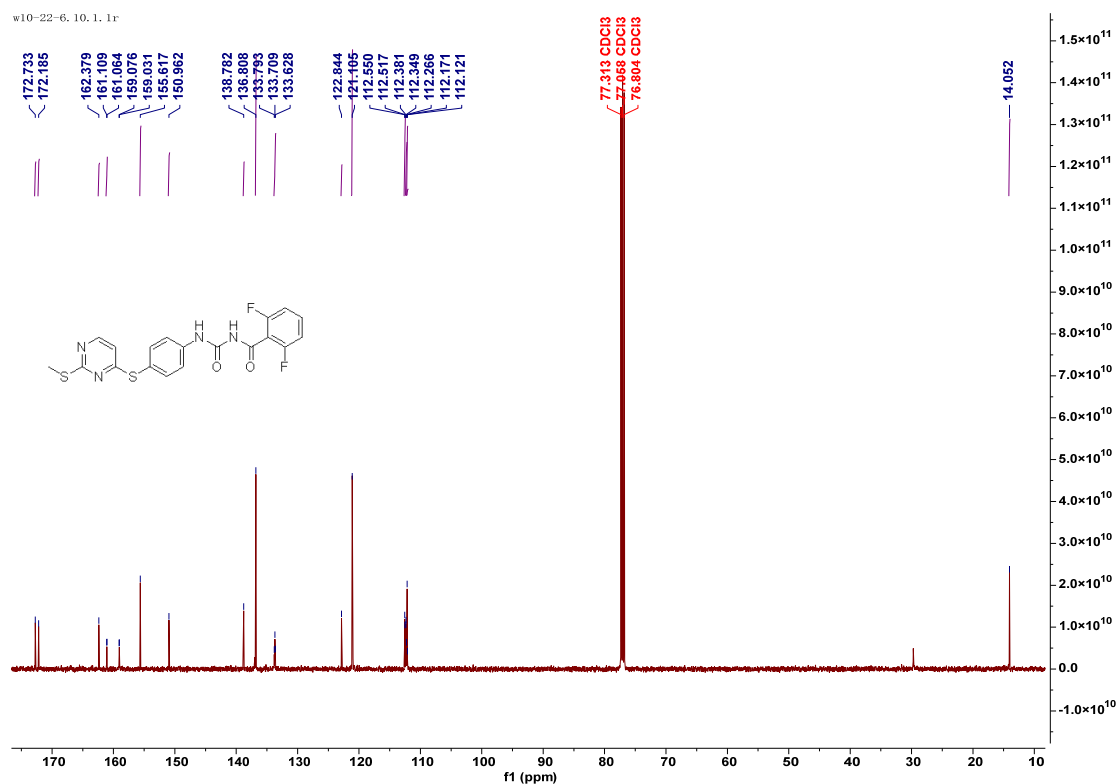


Figure S53 <sup>13</sup>C NMR spectrum of compound 4r

W12-05-06 #32 RT: 0.14 AV: 1 NL: 2.48E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

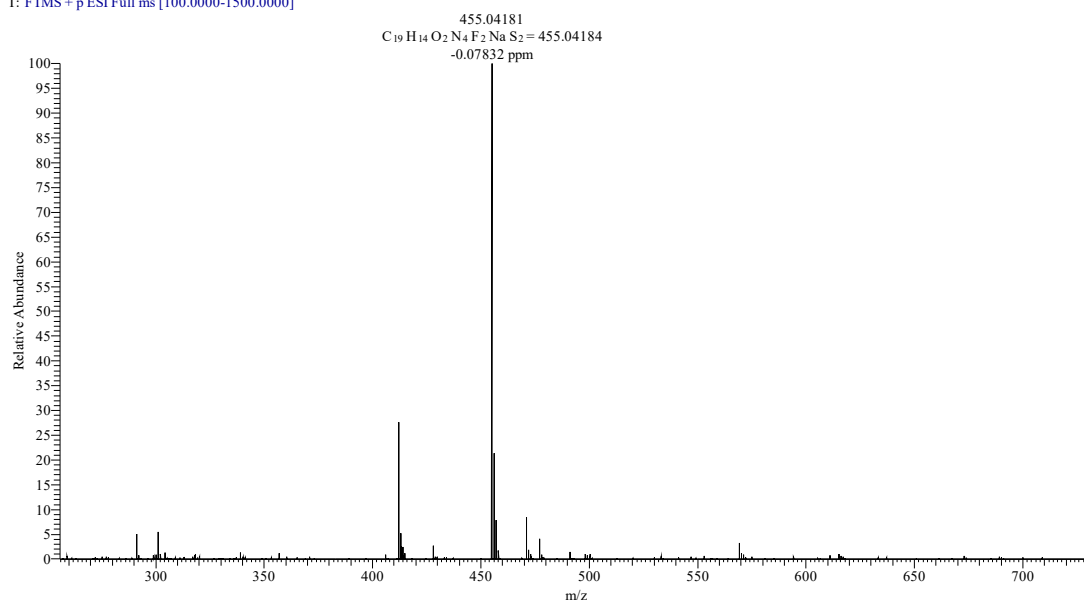


Figure S54 HRMS spectrum of compound 4r

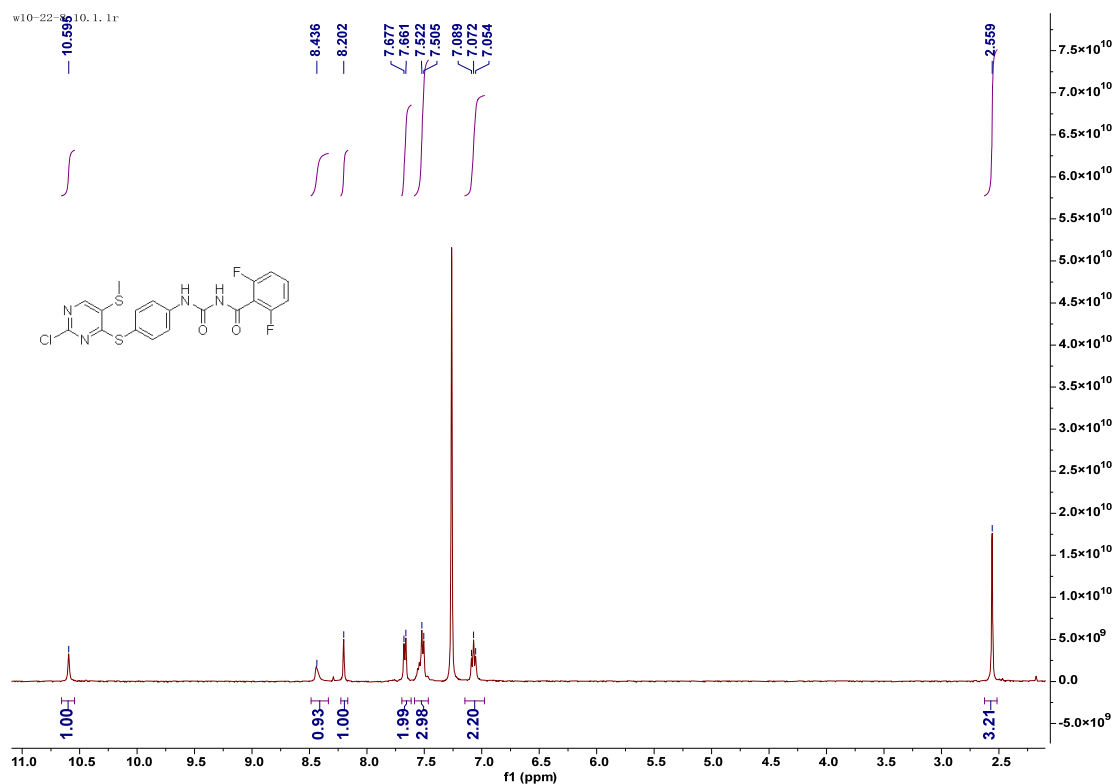


Figure S55  $^1\text{H}$  NMR spectrum of compound 4s

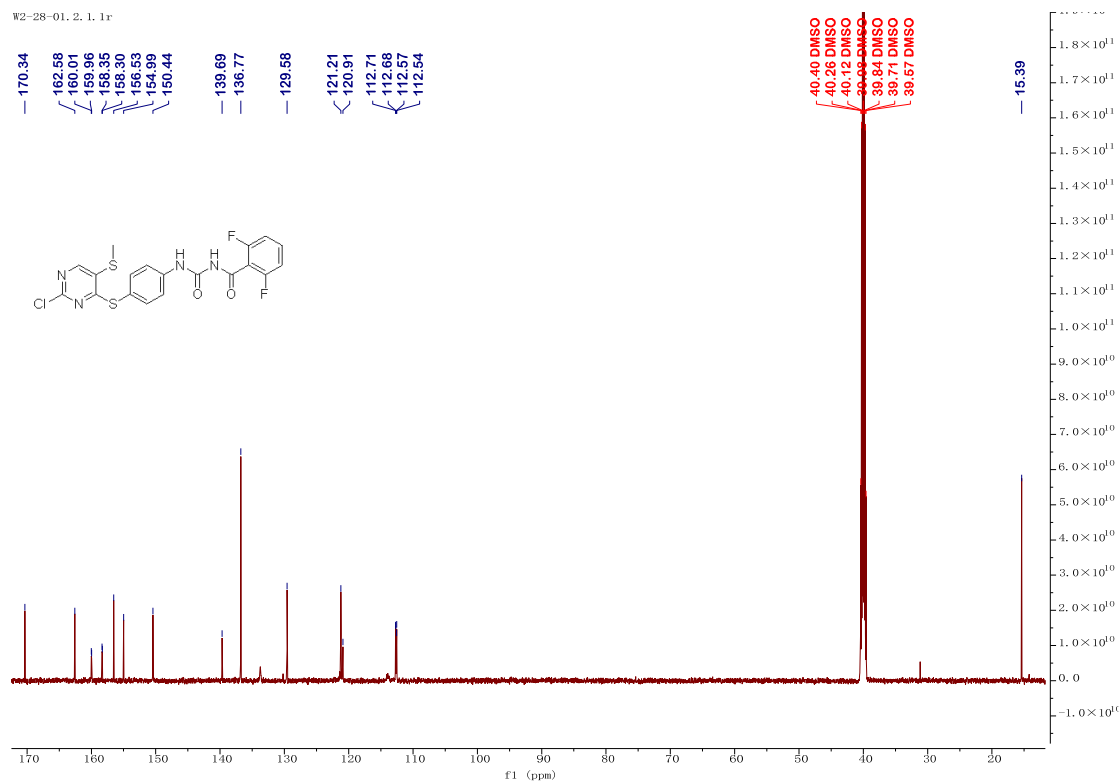


Figure S56  $^{13}\text{C}$  NMR spectrum of compound 4s

W12-05-07 #25 RT: 0.11 AV: 1 NL: 1.58E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

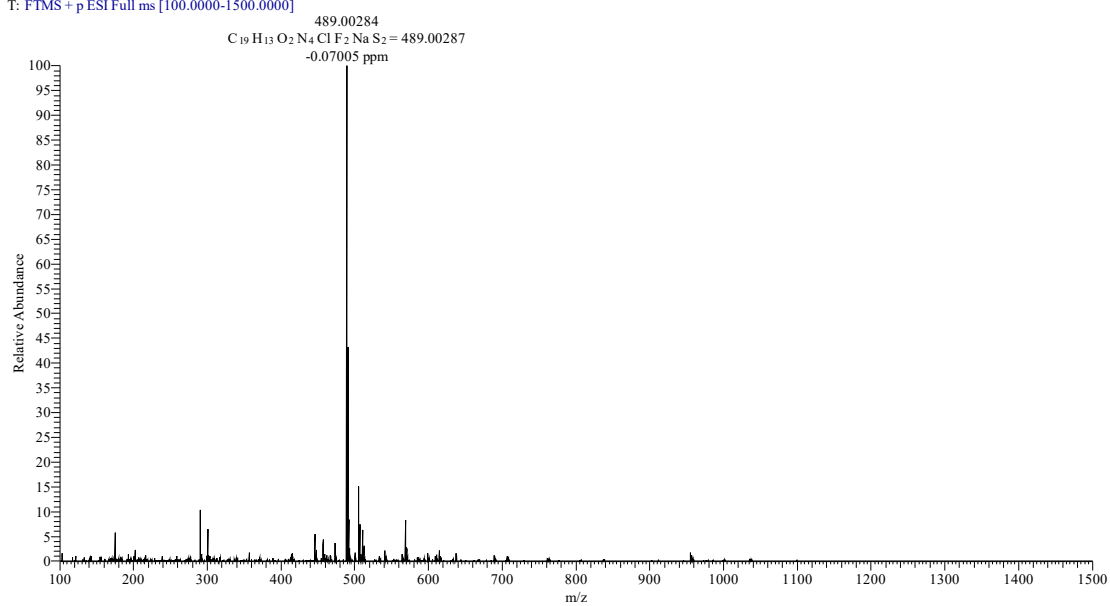


Figure S57 HRMS spectrum of compound 4s

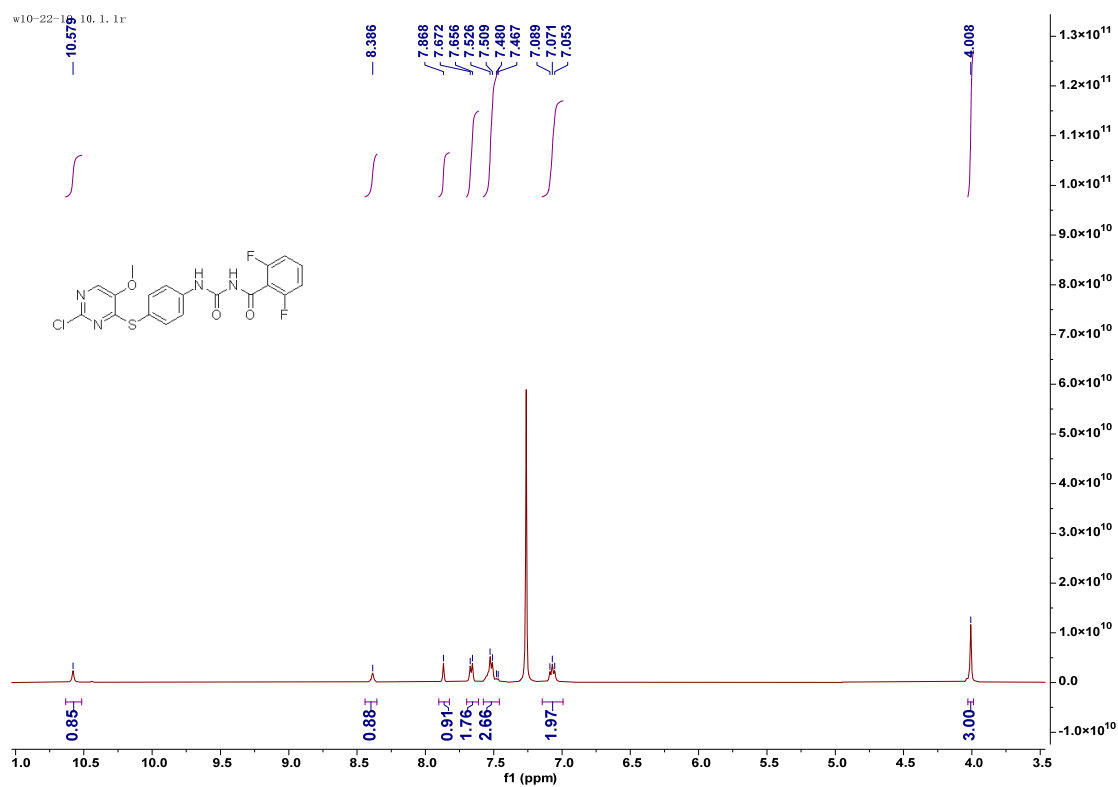


Figure S58 <sup>1</sup>H NMR spectrum of compound 4t

Chemical structure of compound 10 is shown above the spectrum. The spectrum displays peaks corresponding to the chemical shifts listed above the plot area.

**Figure S59**  $^{13}\text{C}$  NMR spectrum of compound **4t**

473.02567  
C<sub>19</sub>H<sub>13</sub>O<sub>3</sub>N<sub>4</sub>ClF<sub>2</sub>NaS = 473.02572  
-0.10783 ppm

Mass spectrum plot showing relative abundance versus m/z. The x-axis ranges from 100 to 1500 m/z. The y-axis ranges from 0 to 100 relative abundance. The base peak is at m/z 473.02567. Other significant peaks are at m/z 423.02567 and 473.02572.

**Figure S60** HRMS spectrum of compound **4t**

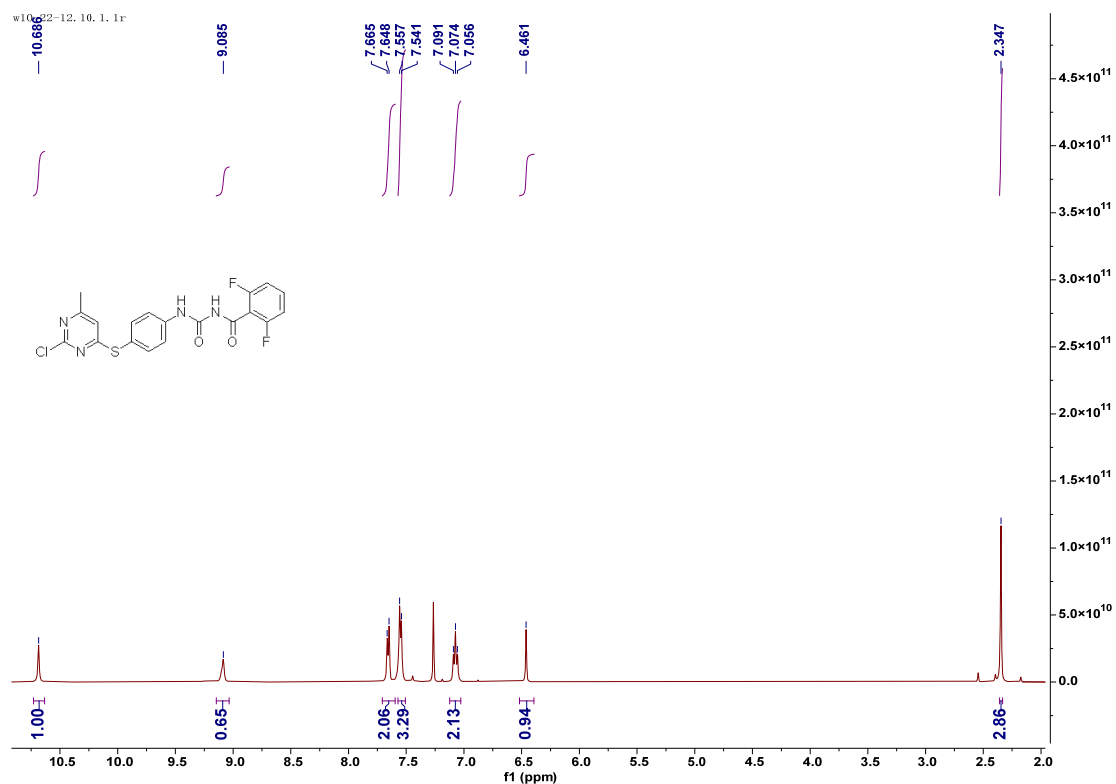


Figure S61 <sup>1</sup>H NMR spectrum of compound 4u

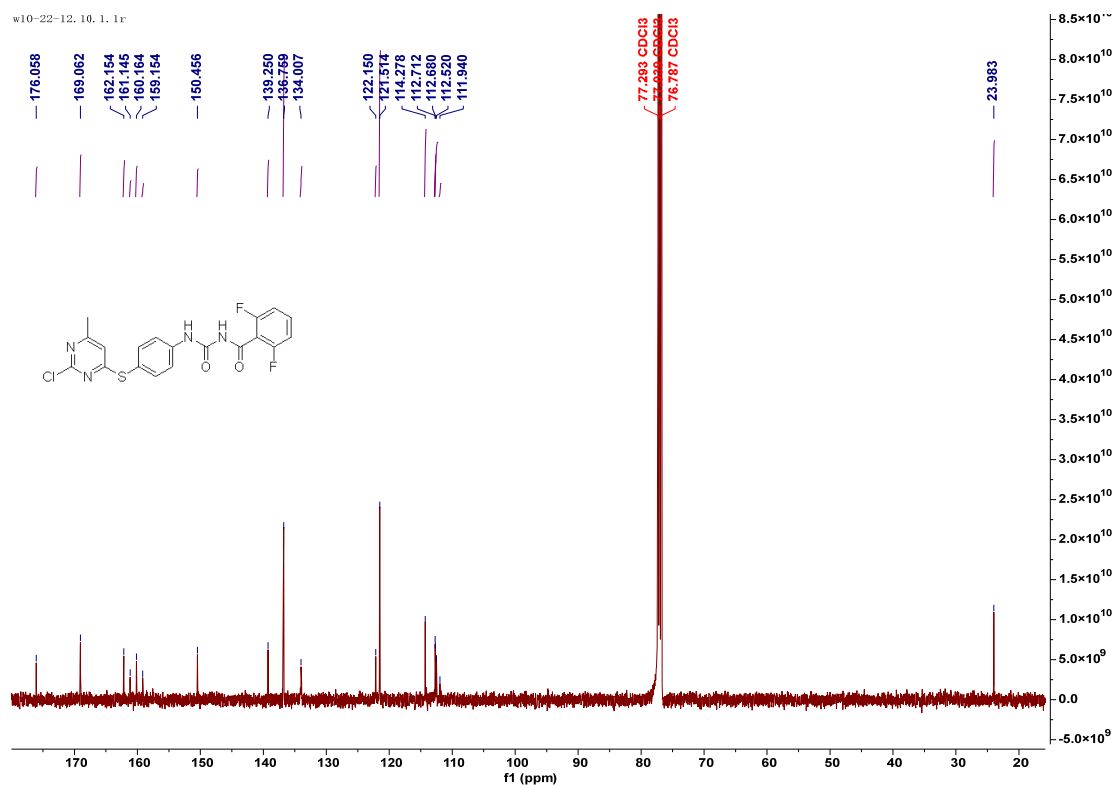
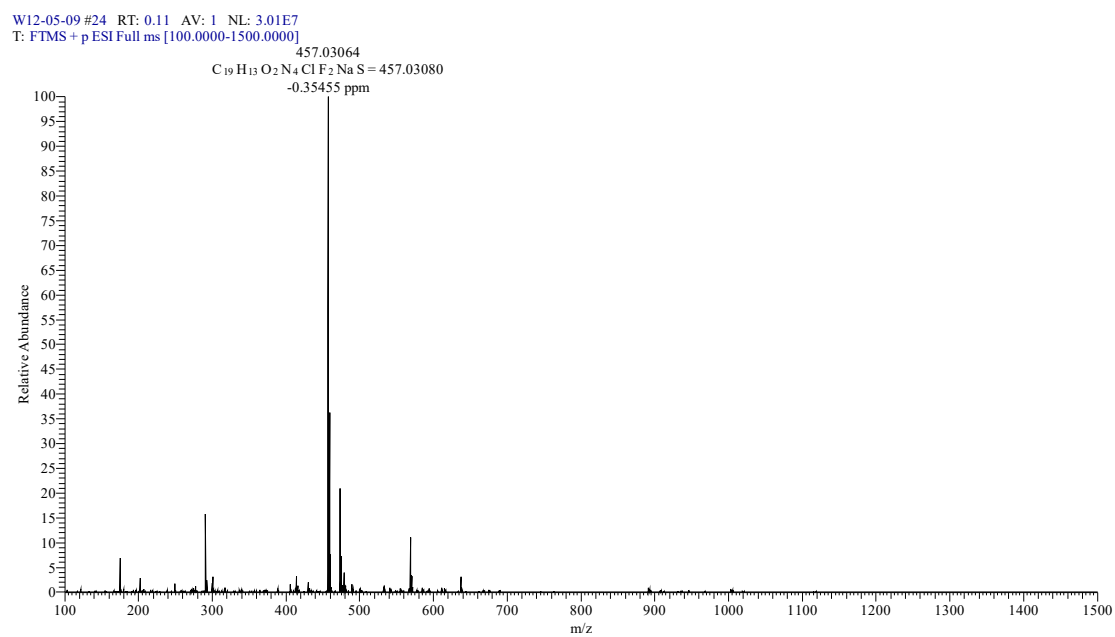
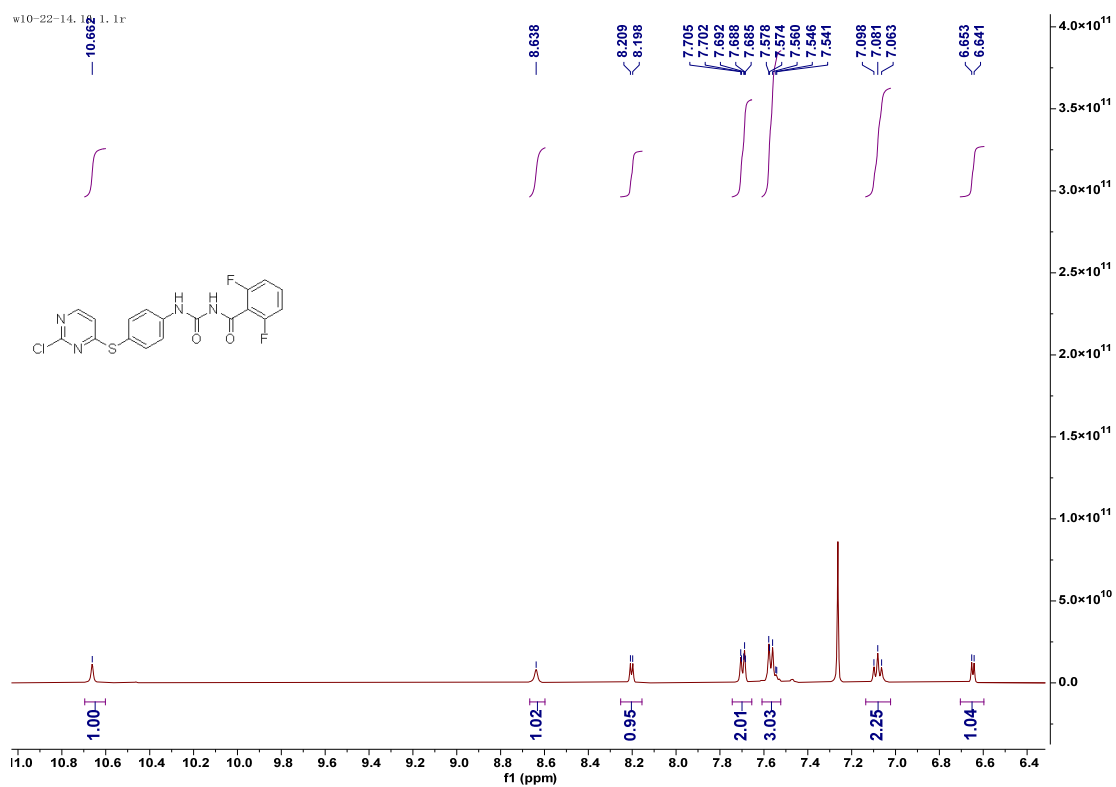


Figure S62 <sup>13</sup>C NMR spectrum of compound 4u



**Figure S63** HRMS spectrum of compound **4u**



**Figure S64** <sup>1</sup>H NMR spectrum of compound **4v**



w10-22-14, 10. 1. 1r

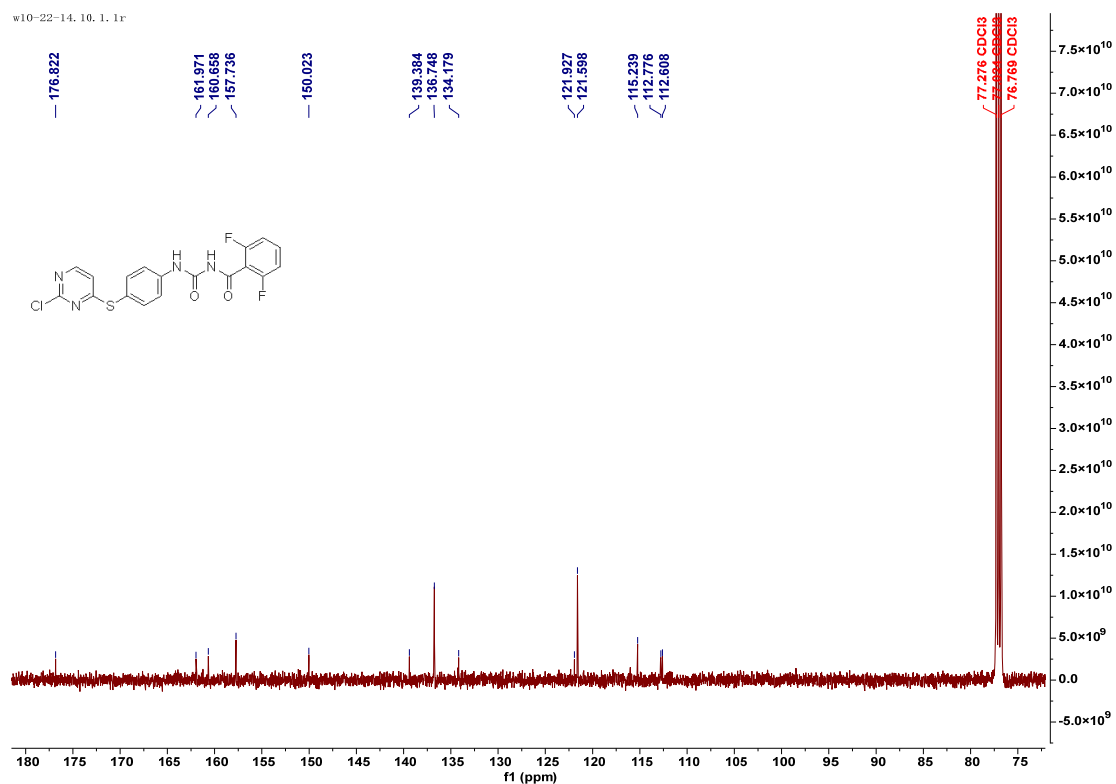


Figure S65  $^{13}\text{C}$  NMR spectrum of compound 4v

W12-05-10 #26 RT: 0.12 AV: 1 NL: 1.71E7  
T: FTMS + p ESI Full ms [100.0000-1500.0000]

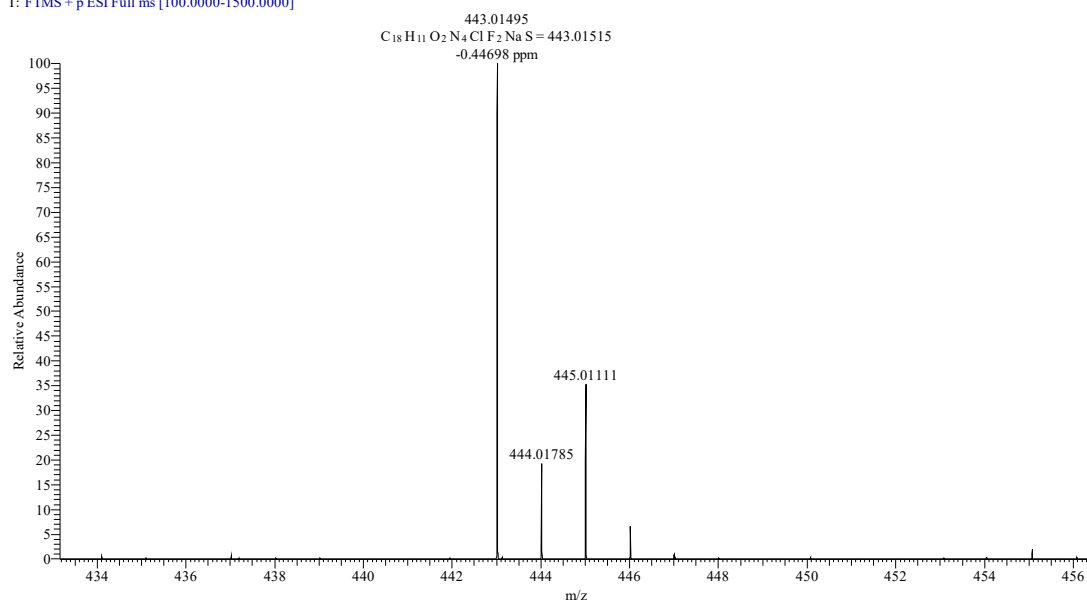


Figure S66 HRMS spectrum of compound 4v

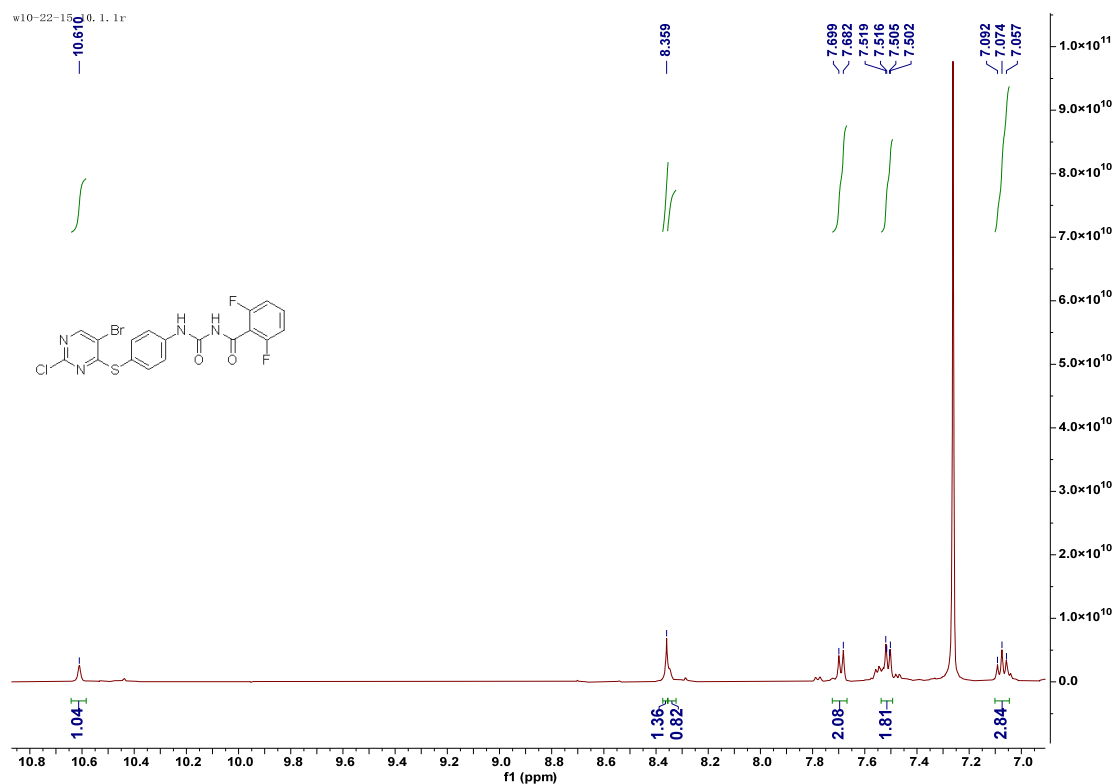


Figure S67  $^1\text{H}$  NMR spectrum of compound 4w

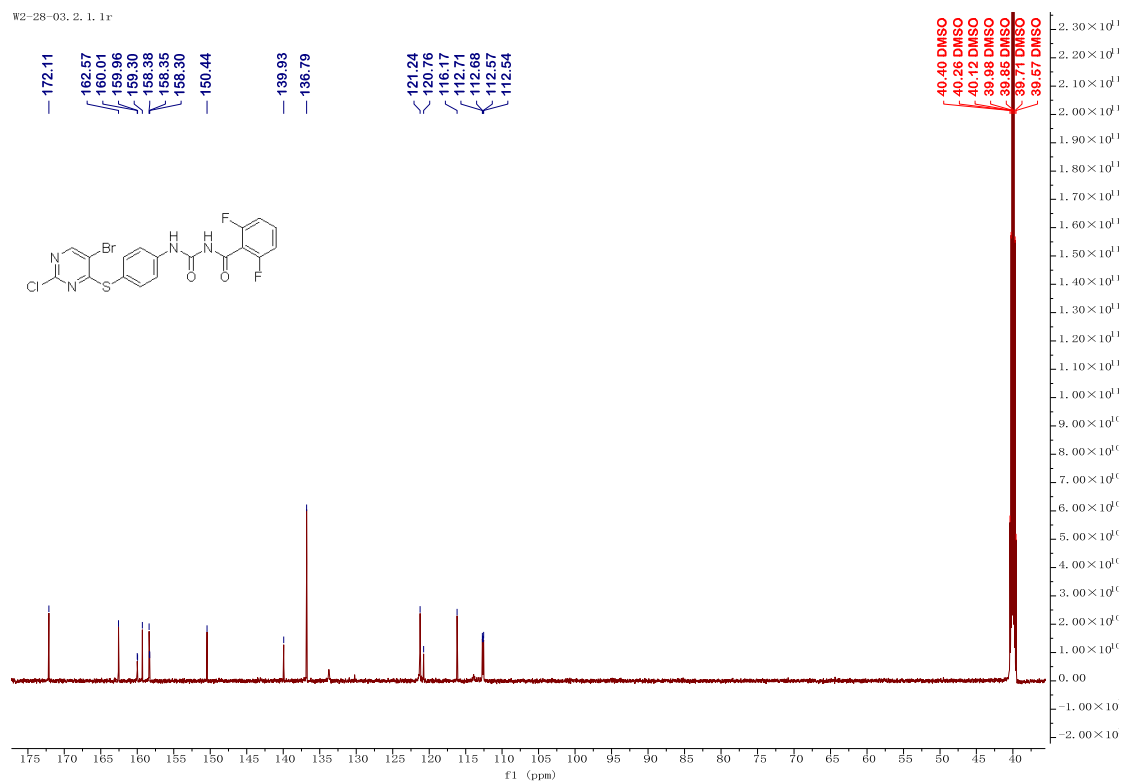
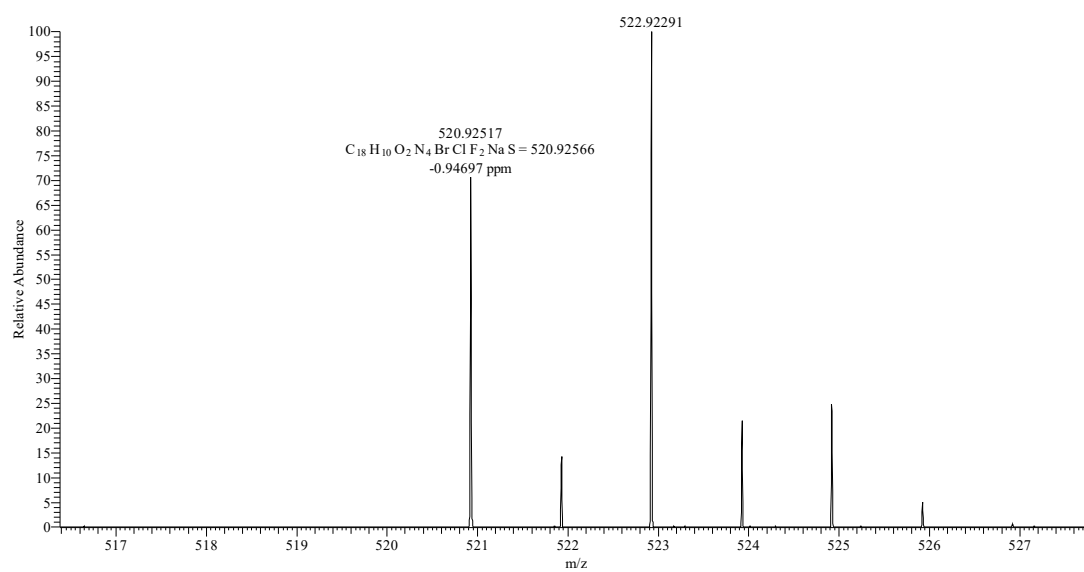


Figure S68  $^{13}\text{C}$  NMR spectrum of compound 4w

W12-05-11 #25 RT: 0.11 AV: 1 NL: 3.96E6  
T: FTMS + p ESI Full ms [100.0000-1500.0000]



**Figure S69** HRMS spectrum of compound **4w**