

## Design, synthesis, antifungal activity and 3D-QSAR study of novel pyrazole carboxamide and niacinamide derivatives containing benzimidazole moiety

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Table 1. Crystallographic data of compound **T1**.....S1

Spectrograms of title compounds **T1-T20**.....S2

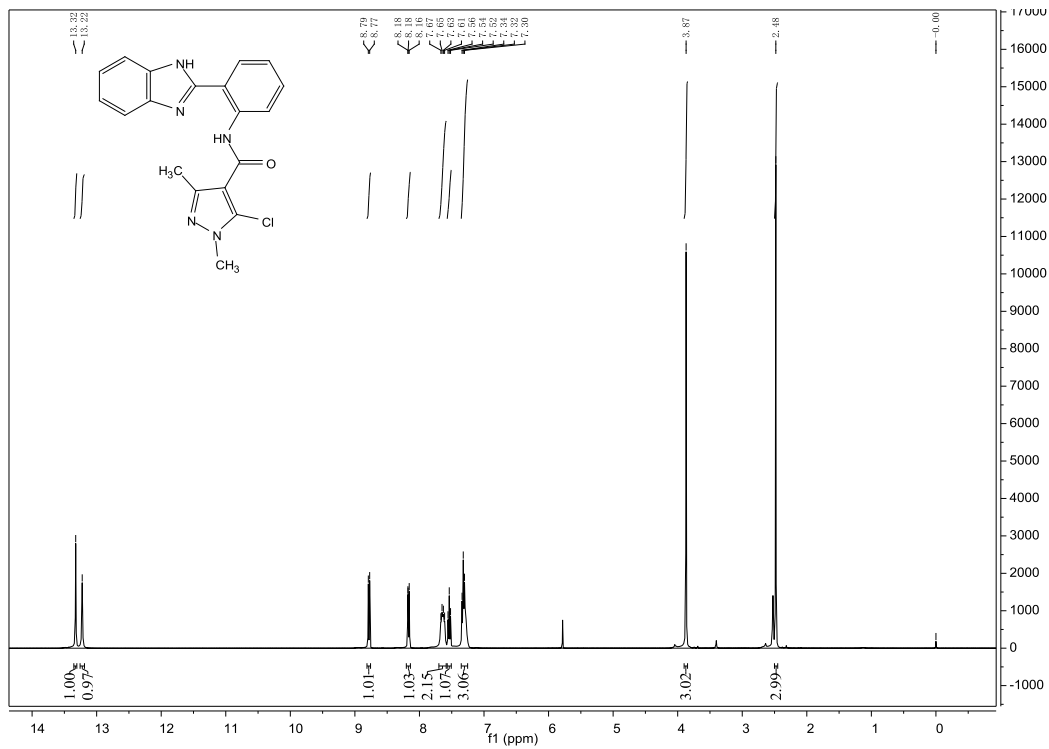
FTIR spectrograms of title compounds **T1-T20**.....S32

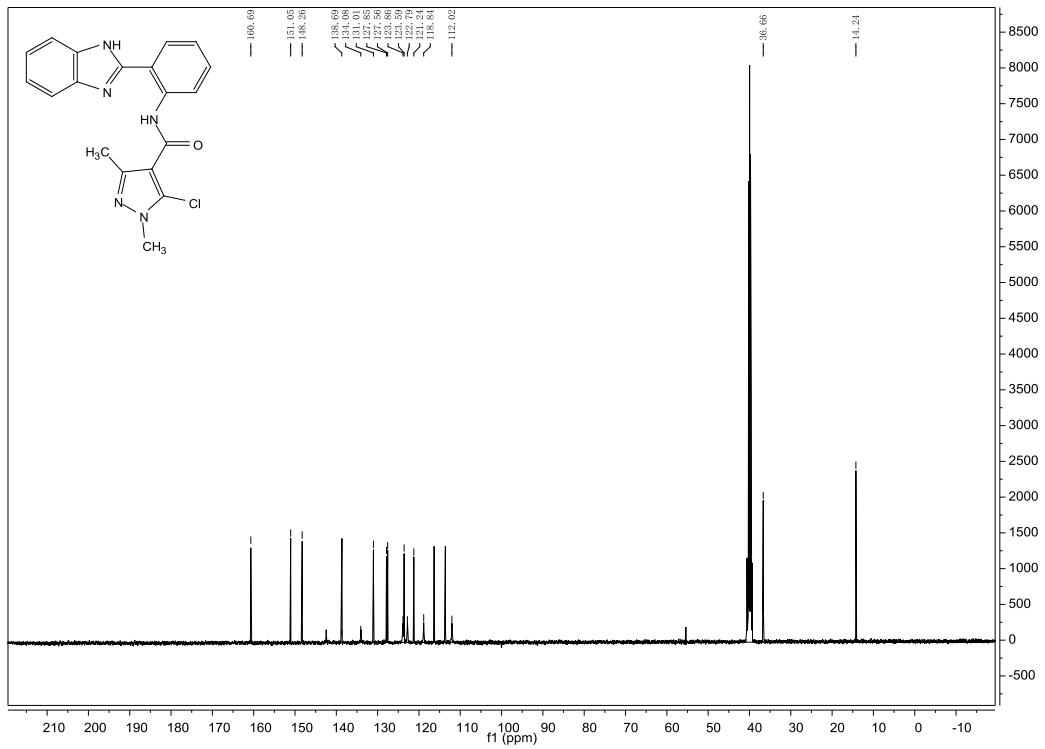
Table 1. Crystallographic data of compound **T1**

Chemical formula	C <sub>19</sub> H <sub>16</sub> ClN <sub>5</sub> O
Formula weight	365.82
Temperature[K]	100.00(10)
Crystal system	Monoclinic
Space group	P21/c
<i>a</i> [Å]	9.2973(4)
<i>b</i> [Å]	16.7097(7)
<i>c</i> [Å]	11.0503(5)
$\alpha$ [°]	90
$\beta$ [°]	94.760(4)
$\gamma$ [°]	90
<i>V</i> [Å <sup>3</sup> ]	1710.80(13)
<i>Z</i>	4
$\rho$ (calculated)[g/cm <sup>3</sup> ]	1.420
$\mu$ [mm <sup>-1</sup> ]	0.242
<i>F</i> (000)	760

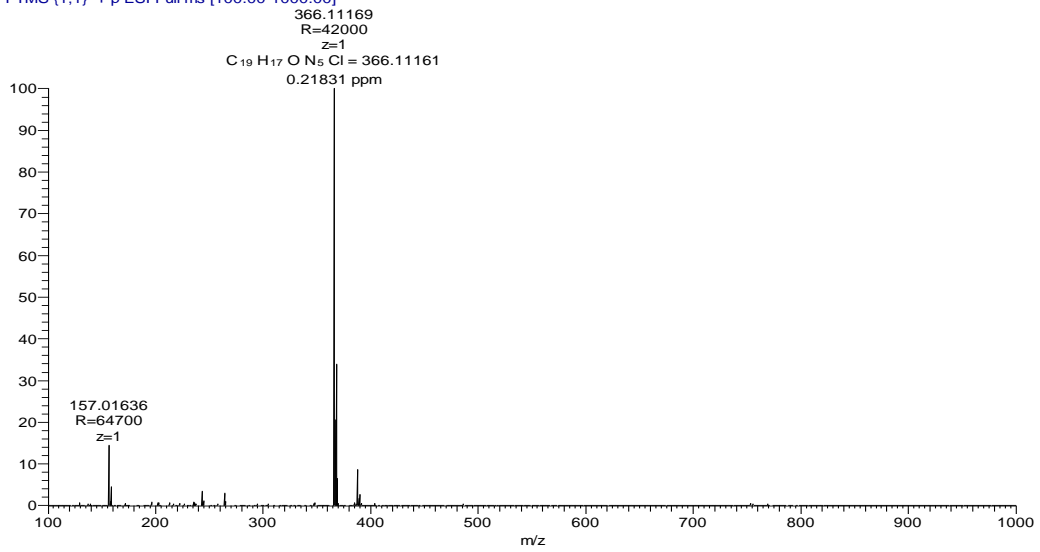
Crystal size [mm <sup>3</sup> ]	0.11 × 0.12 × 0.13
Colour, shape	Yellow, block
Radiation [Å]	MoKα (λ = 0.71073)
Theta Min-Max [°]	2.2, 26.4
<i>h, k, l</i>	-8 ≤ <i>h</i> ≤ 11, -20 ≤ <i>k</i> ≤ 17, -13 ≤ <i>l</i> ≤ 12
Reflections collected	11996
Independent reflections	3489
Data/restraints/parameters	2886/0/237
Goodness-of-fit	1.041
Final R indexes [ <i>I</i> ≥ 2σ ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0428, <i>wR</i> <sub>2</sub> = 0.1021
Final R indexes [all data]	<i>R</i> <sub>1</sub> = 0.0538, <i>wR</i> <sub>2</sub> = 0.0949
Min. and Max. Resd. Dens [e Å <sup>-3</sup> ]	-0.28, 0.28

<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound **T1**

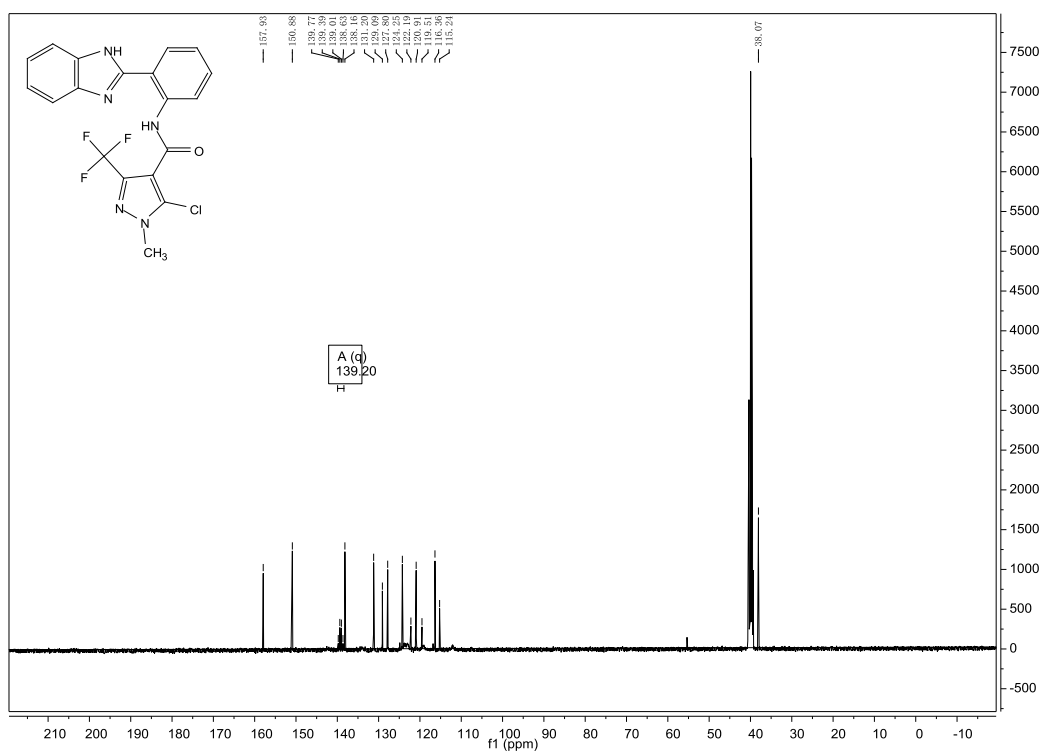
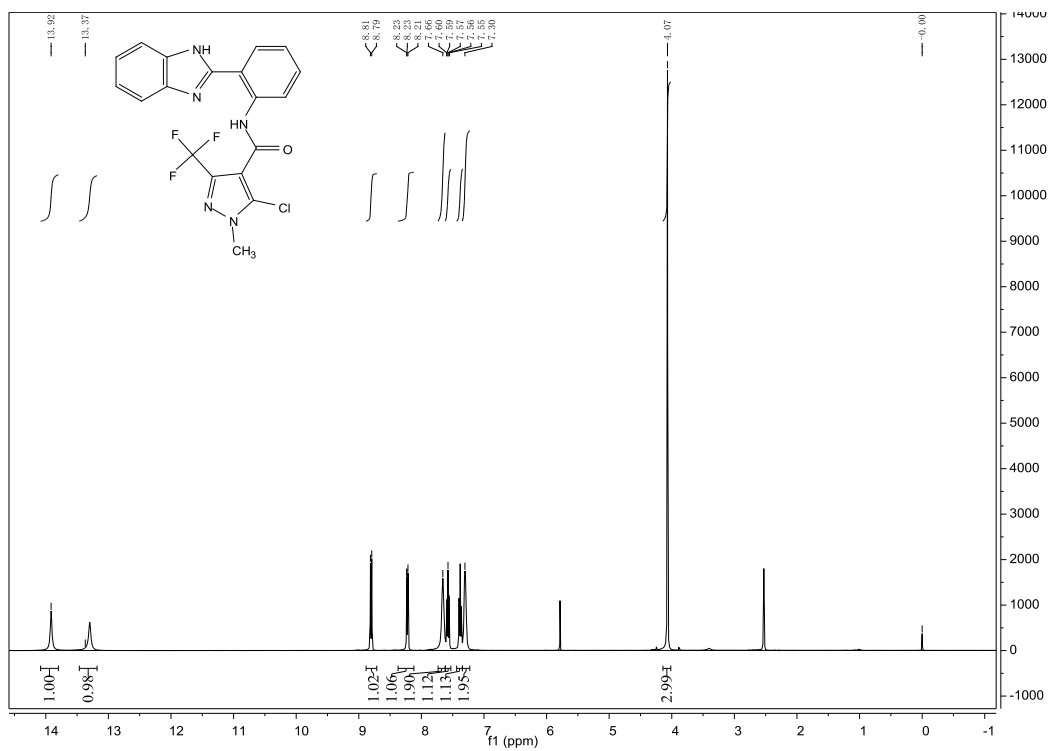




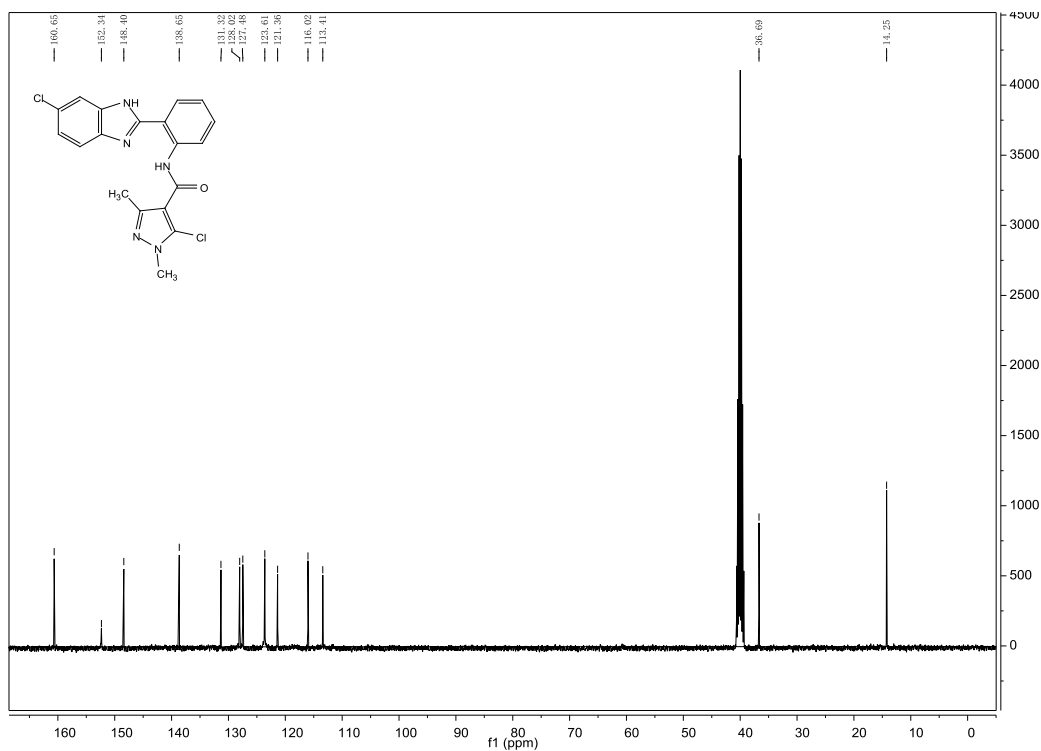
B35 #27 RT: 0.39 AV: 1 NL: 2.89E6  
 T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]



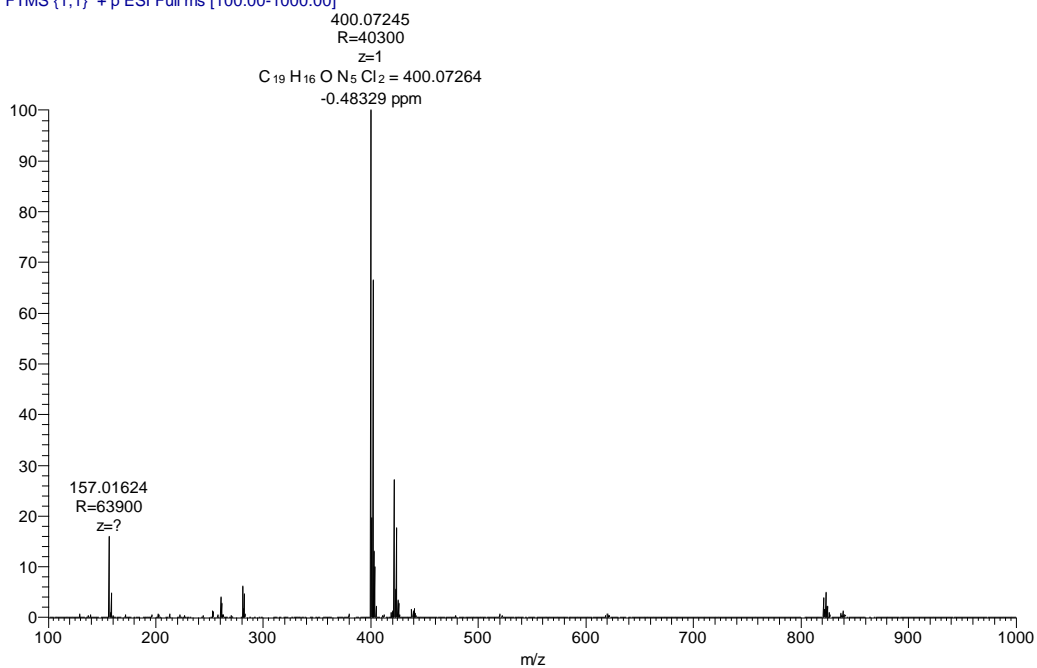
<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound **T2**



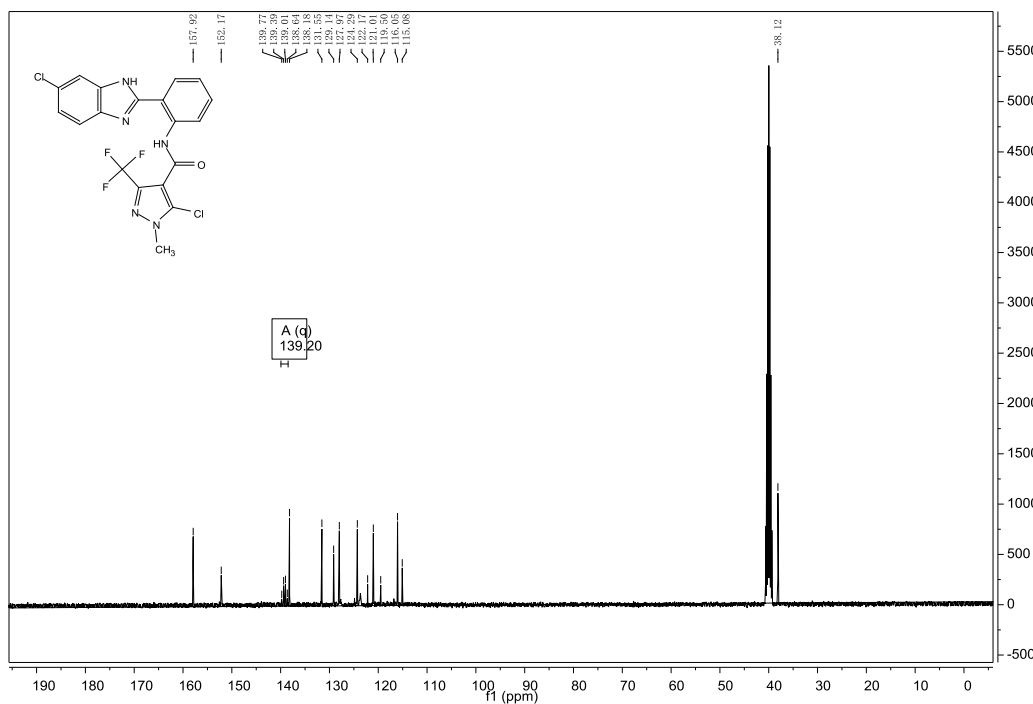
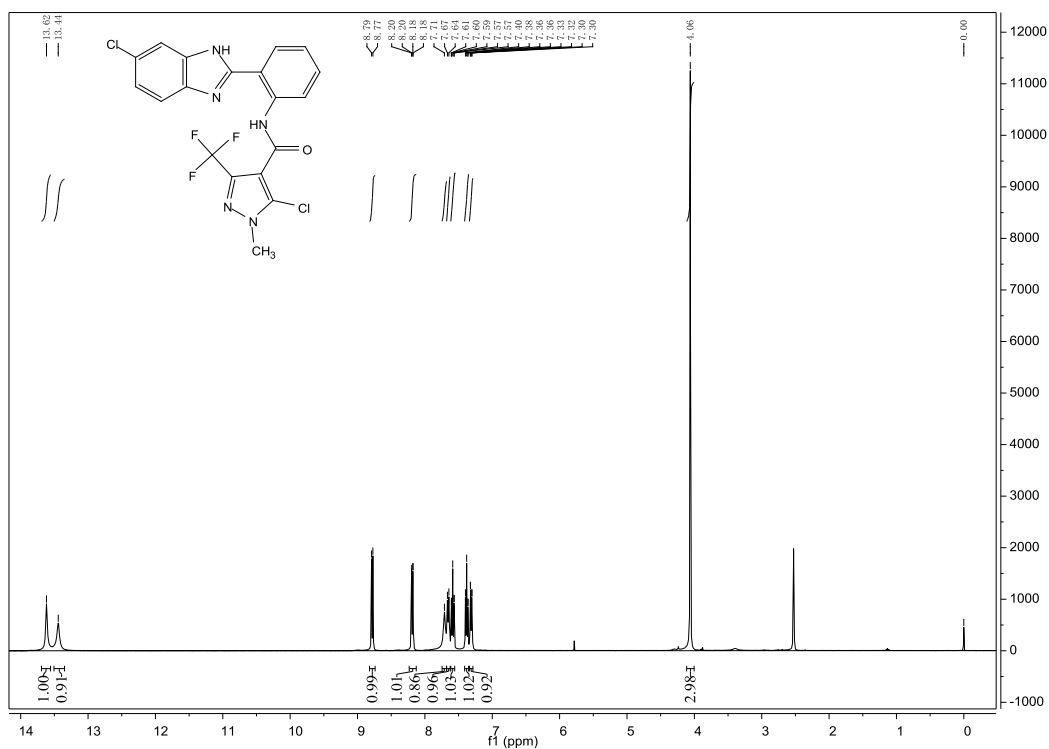




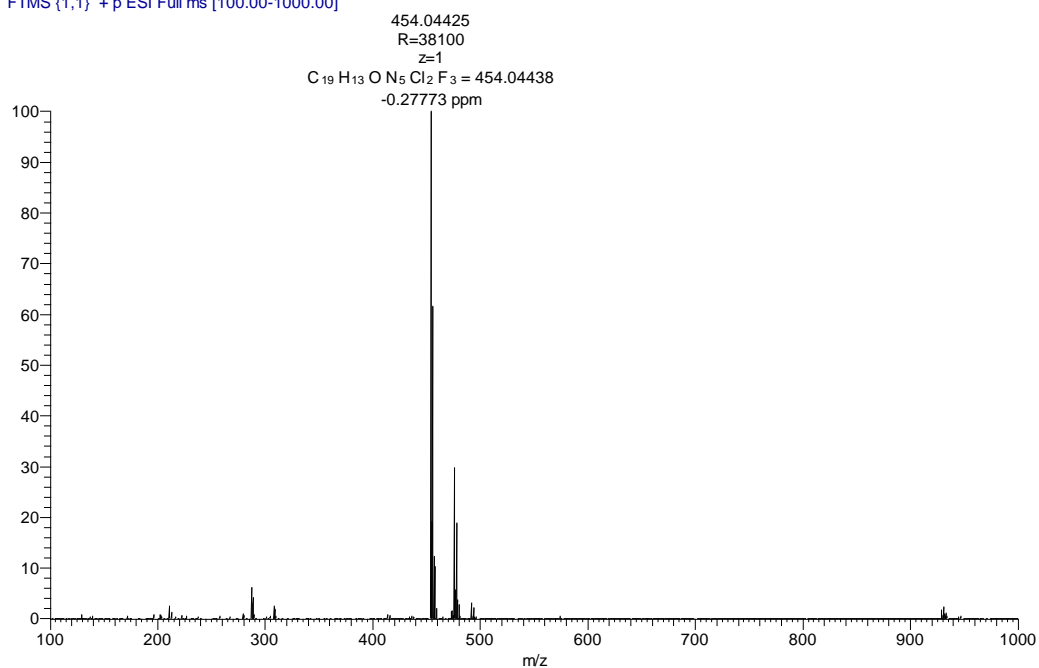
B42 #31 RT: 0.43 AV: 1 NL: 2.57E6  
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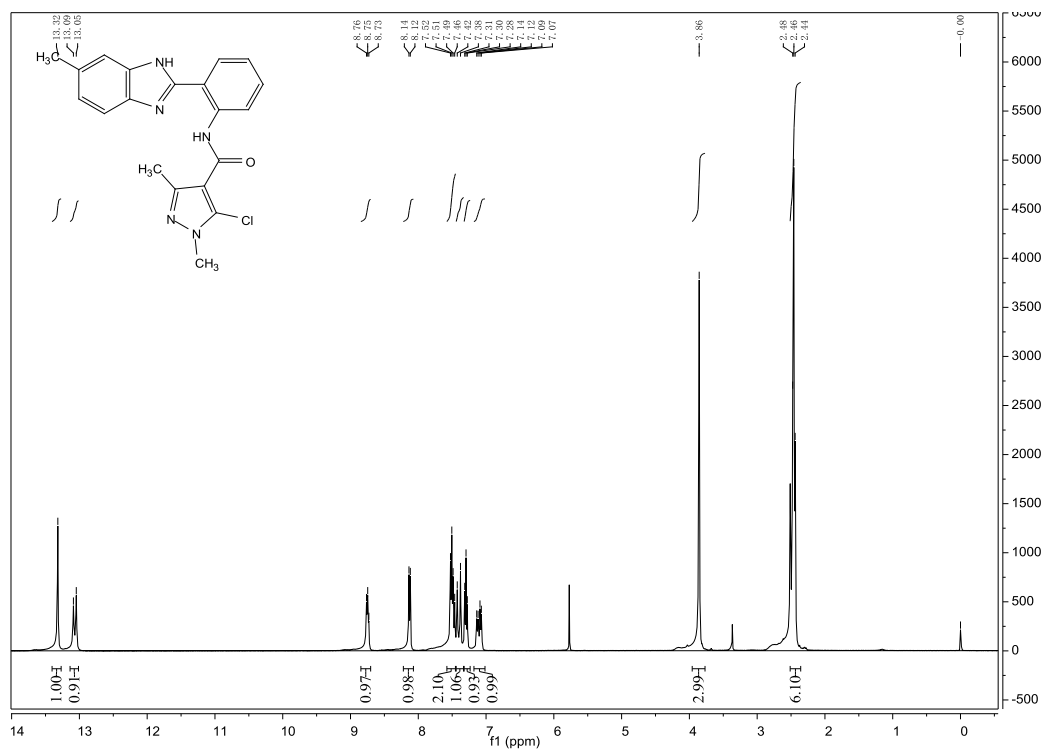
$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T4**



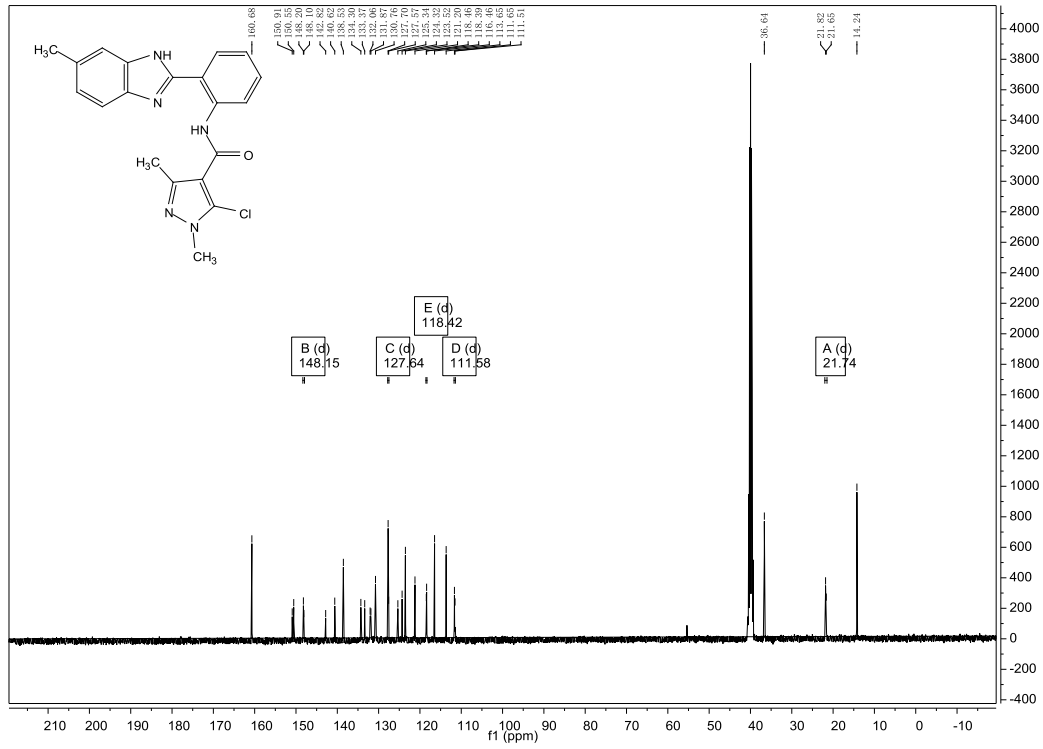
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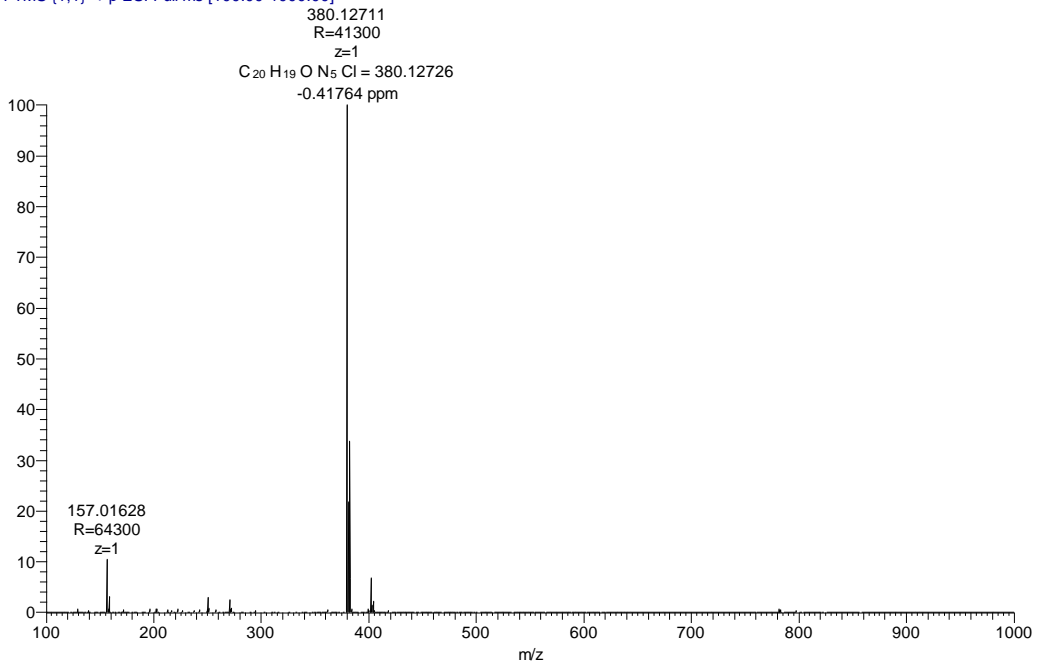
<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound T5



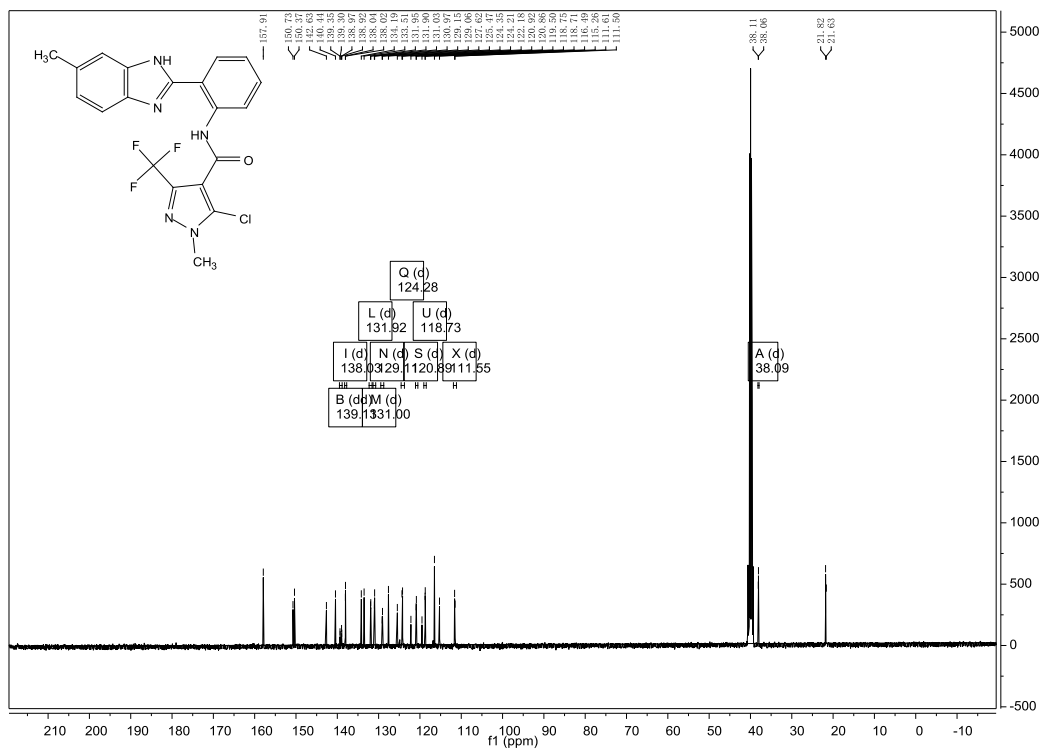
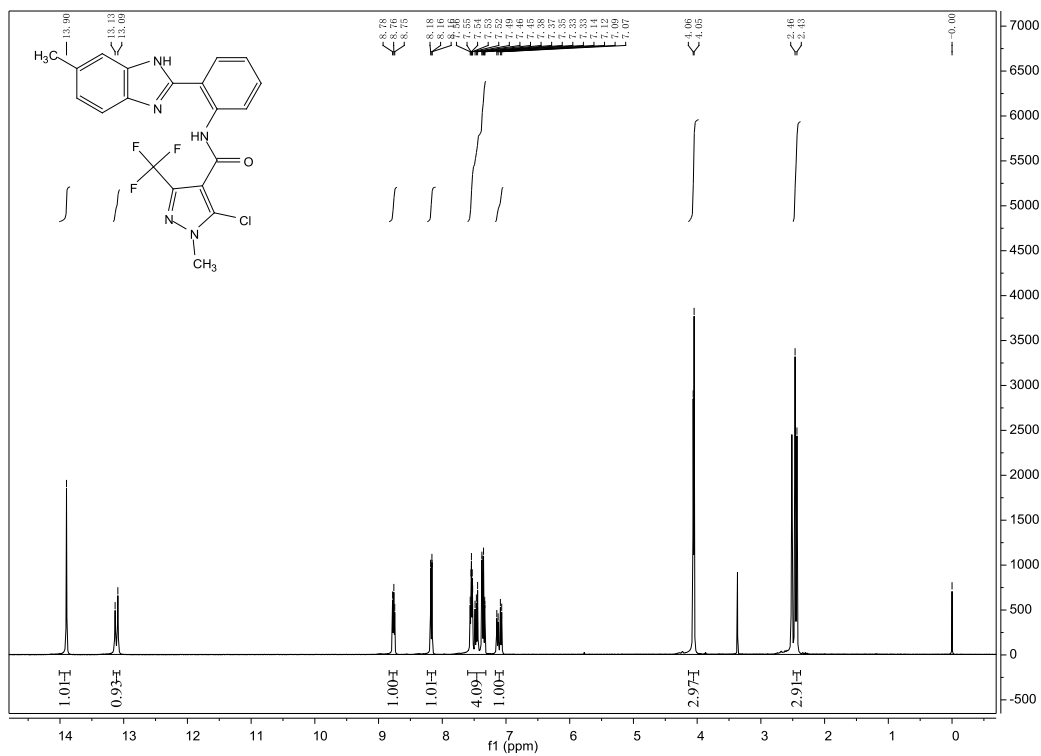




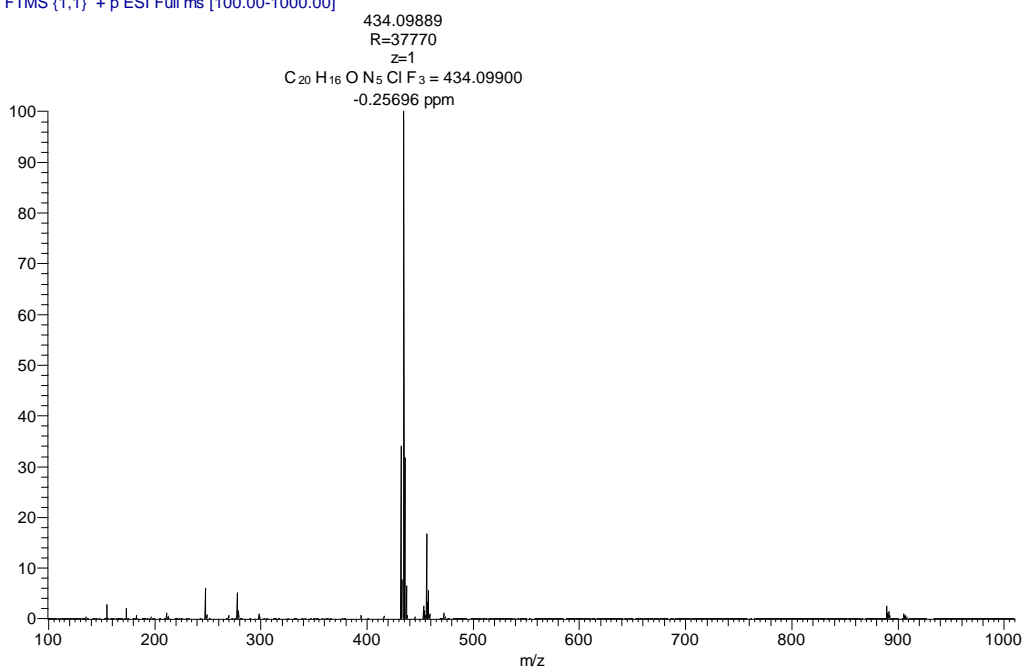
B48 #29 RT: 0.42 AV: 1 NL: 3.11E6  
 T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]



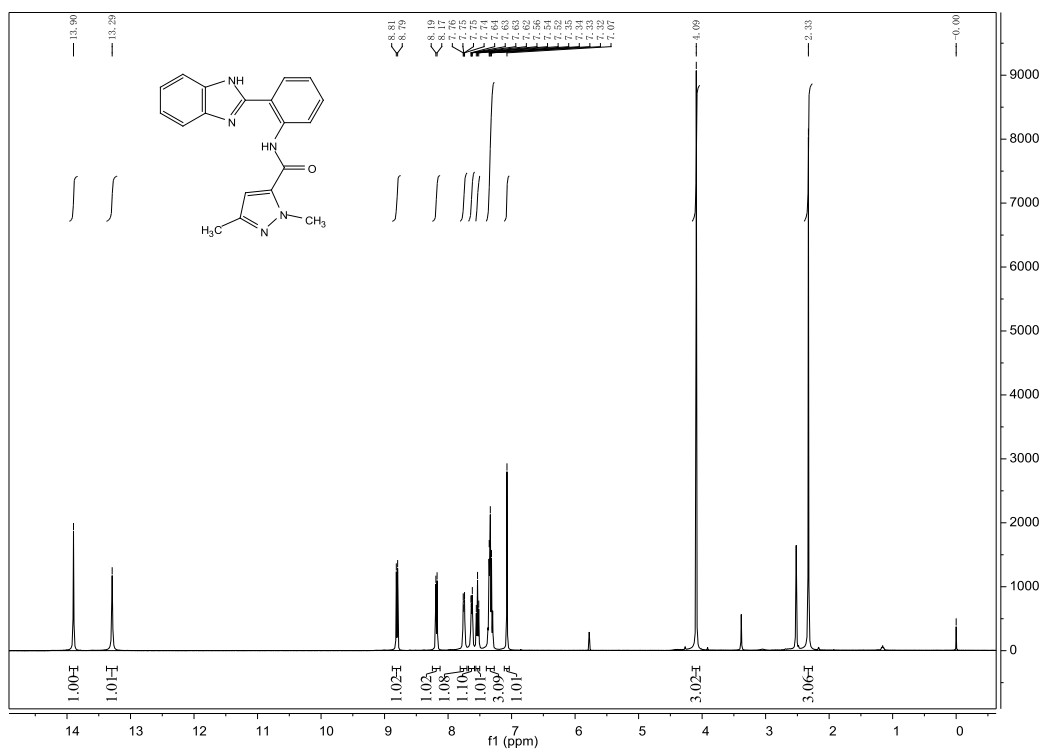
$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T6**

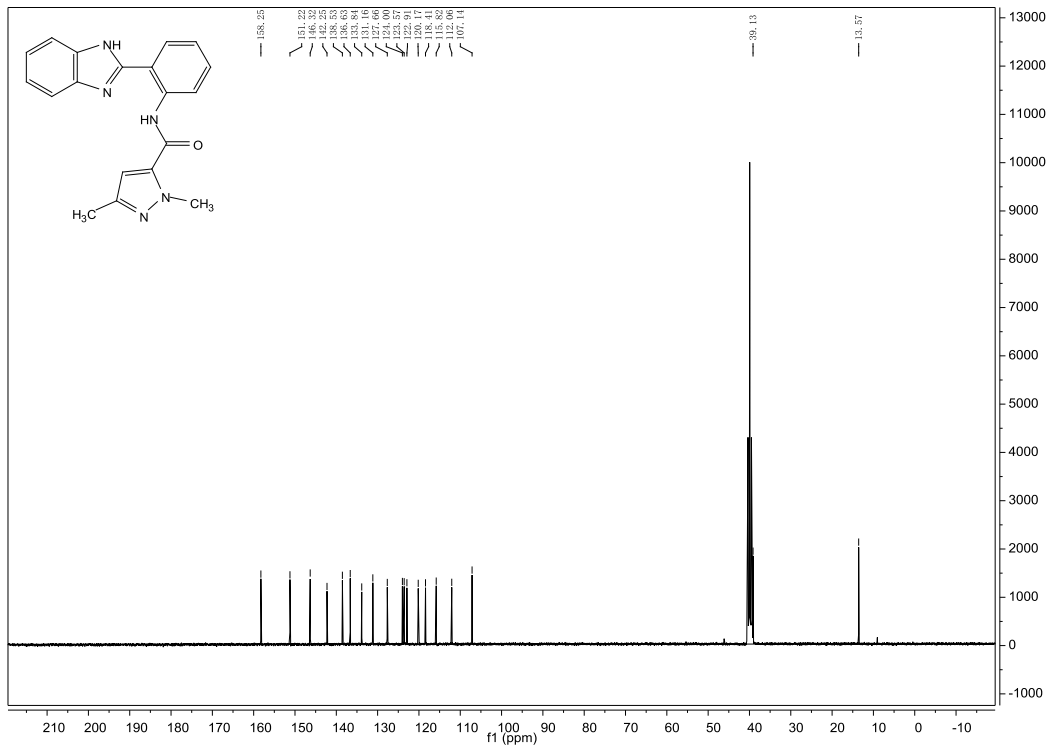


B49 #33-34 RT: 0.44-0.45 AV: 2 NL: 3.37E6  
T: FTMS {1,1} + p ESI Full ms [100.00-1000.00]

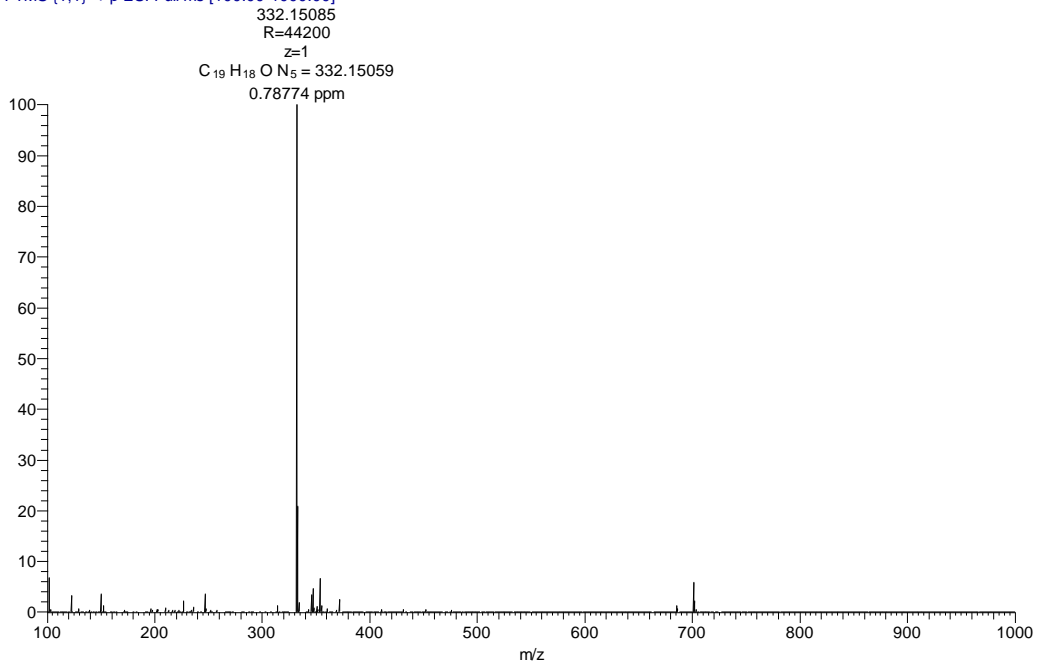


<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound **T7**

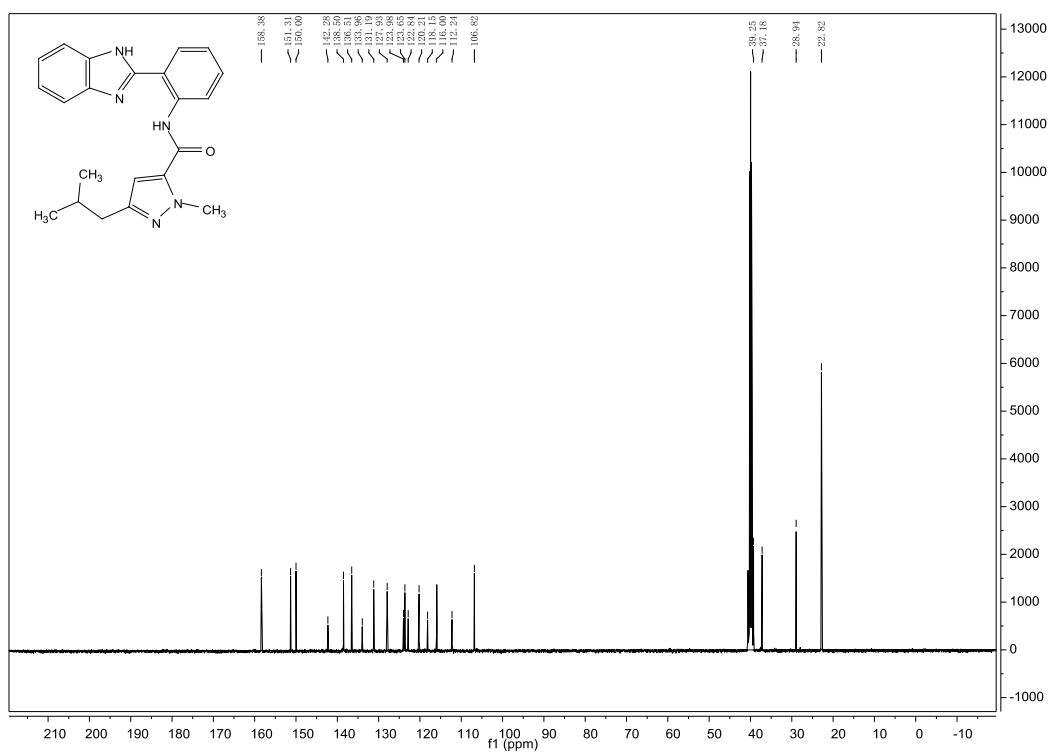
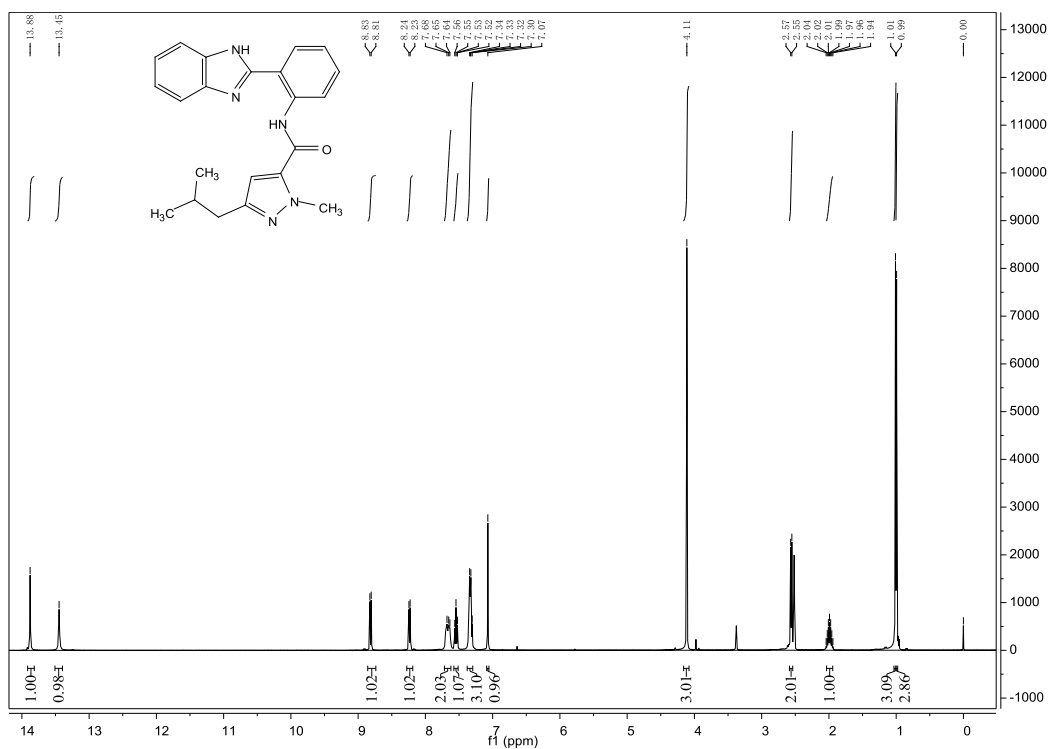




B34 #17 RT: 0.26 AV: 1 NL: 2.71E6  
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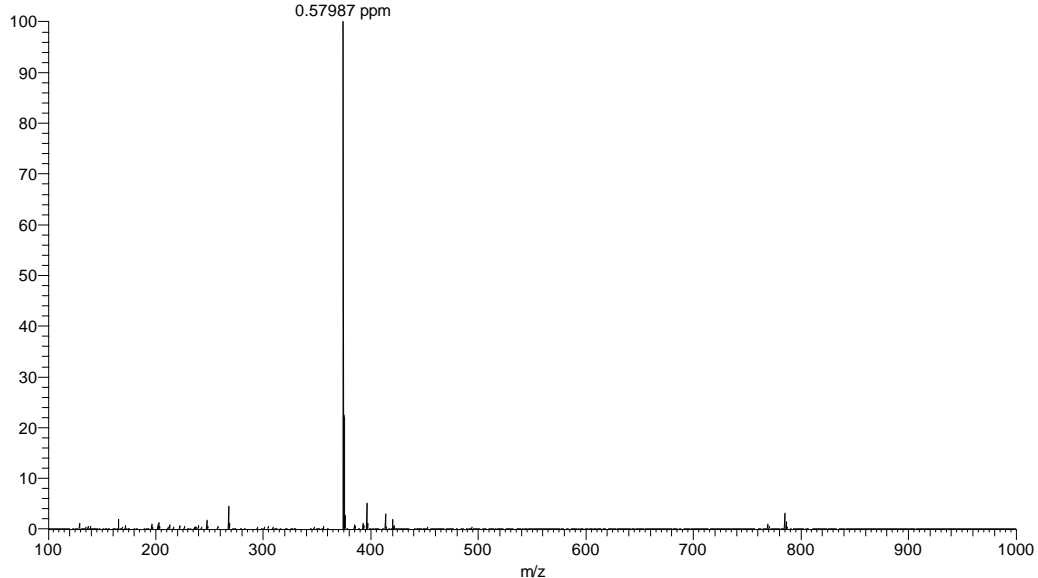


$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T8**

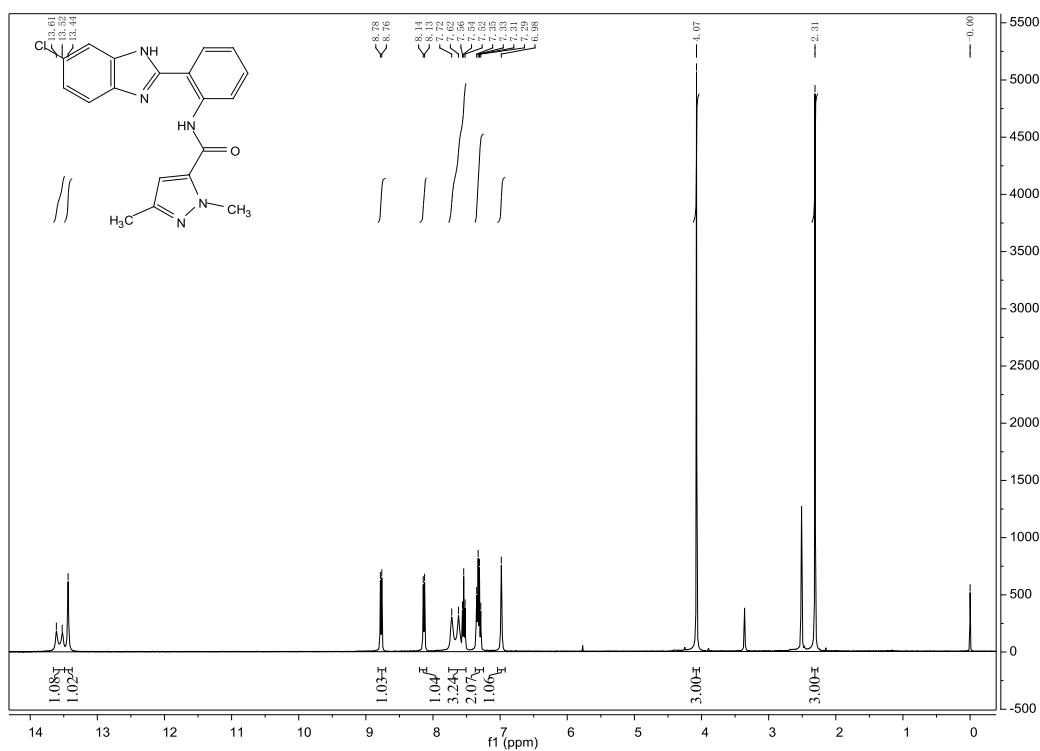


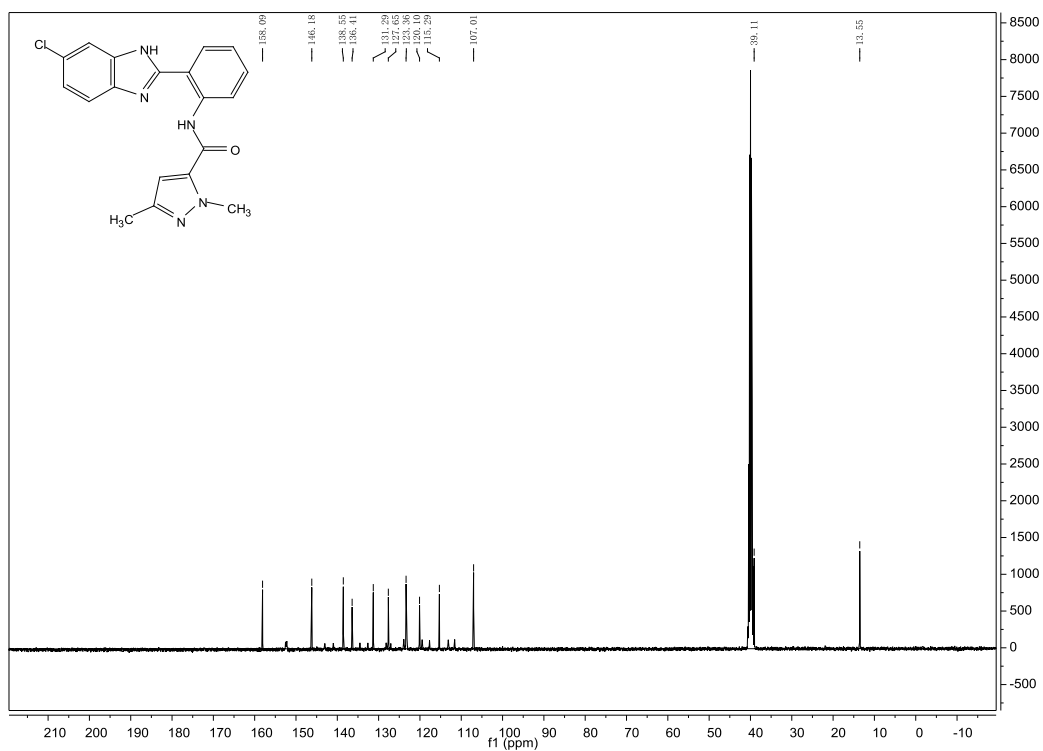
B37 #25 RT: 0.37 AV: 1 NL: 2.14E6  
T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]

374.19775  
R=42500  
z=1  
C<sub>22</sub>H<sub>24</sub>O N<sub>5</sub> = 374.19754  
0.57987 ppm

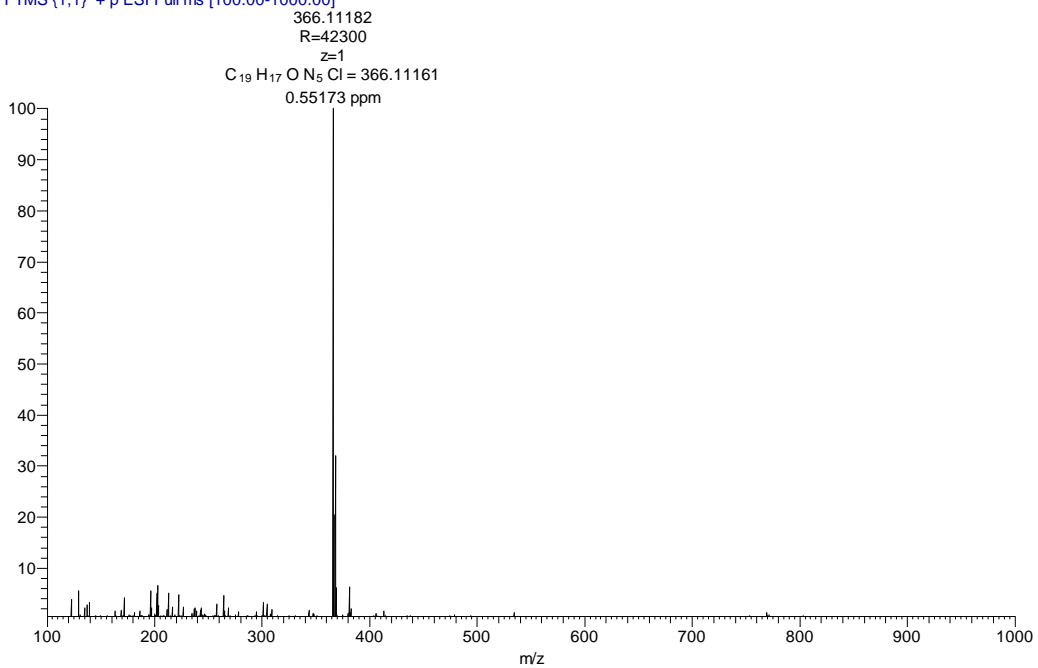


### <sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound T9





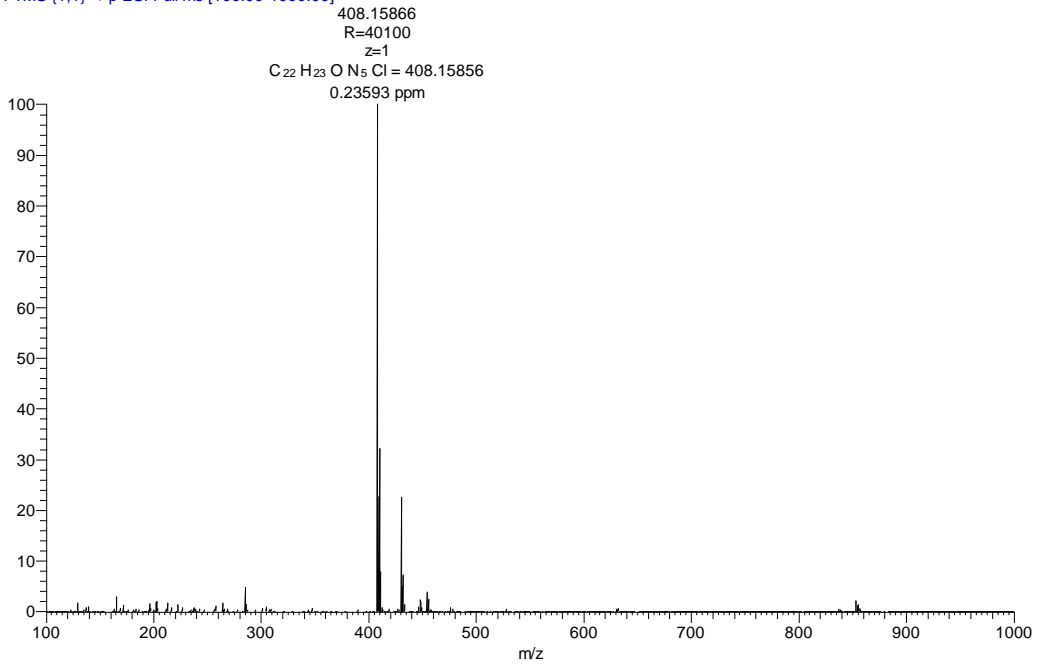
B41 #27 RT: 0.44 AV: 1 NL: 2.96E5  
 T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]



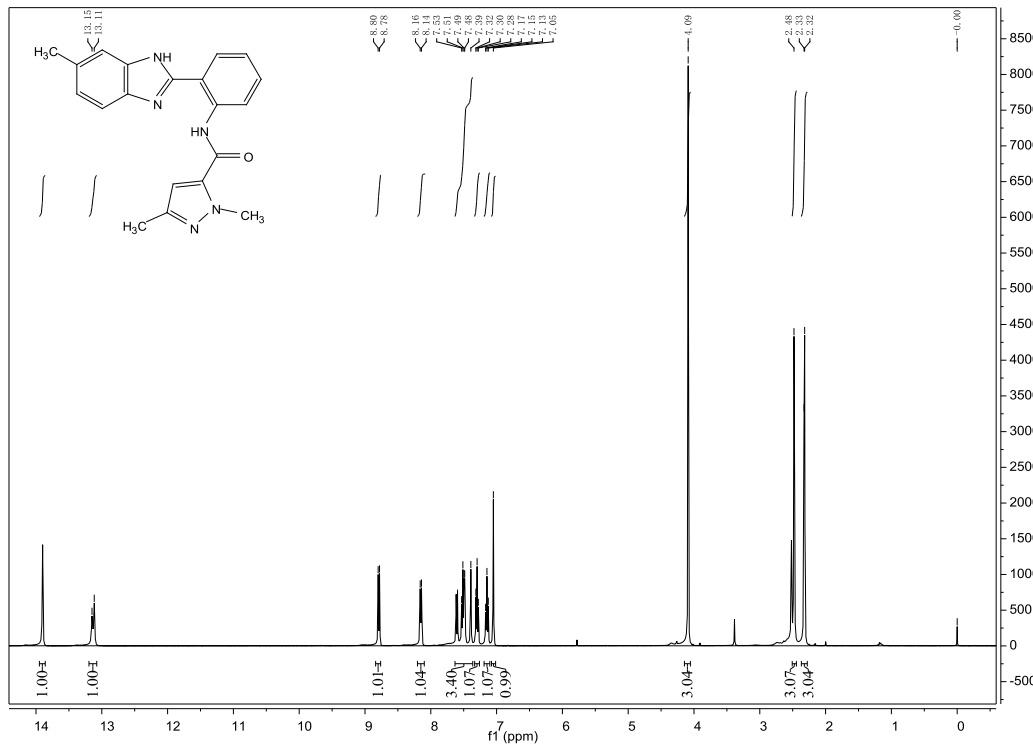


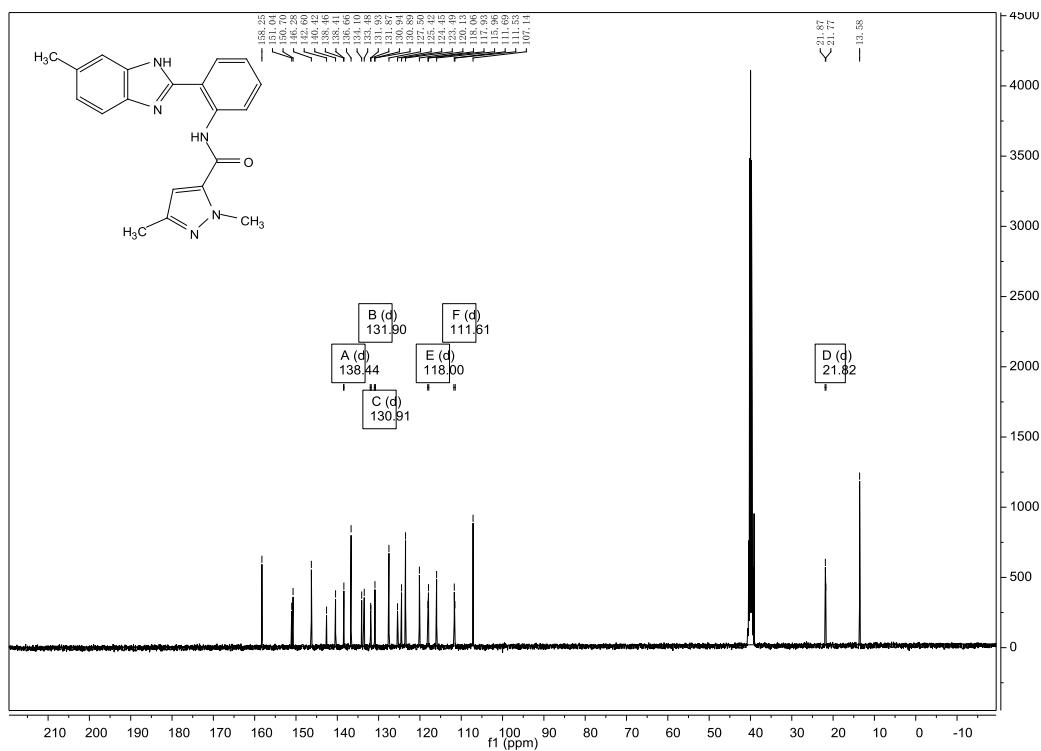


B44 #25 RT: 0.38 AV: 1 NL: 1.07E6  
T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]



<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound **T11**





B47 #21 RT: 0.31 AV: 1 NL: 3.33E6

T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]

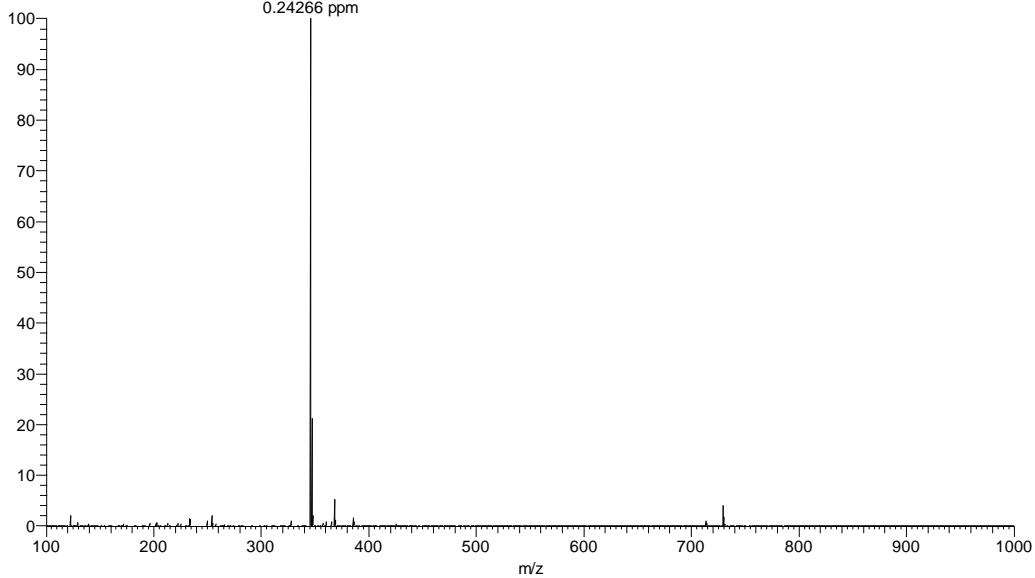
346.16632

R=43800

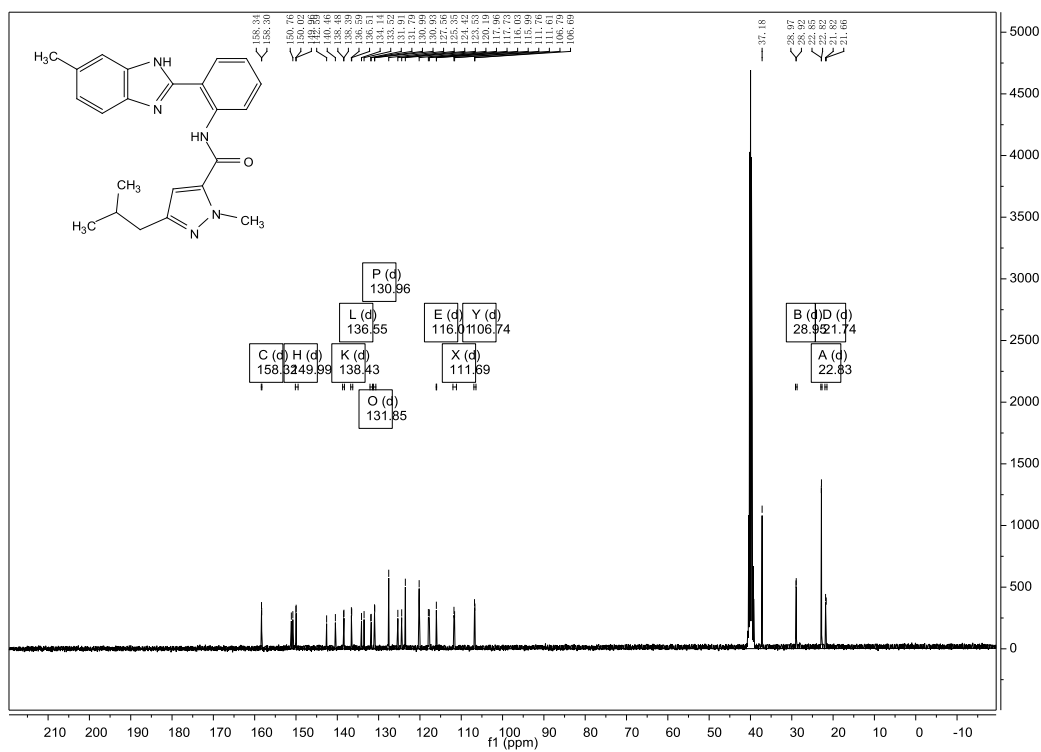
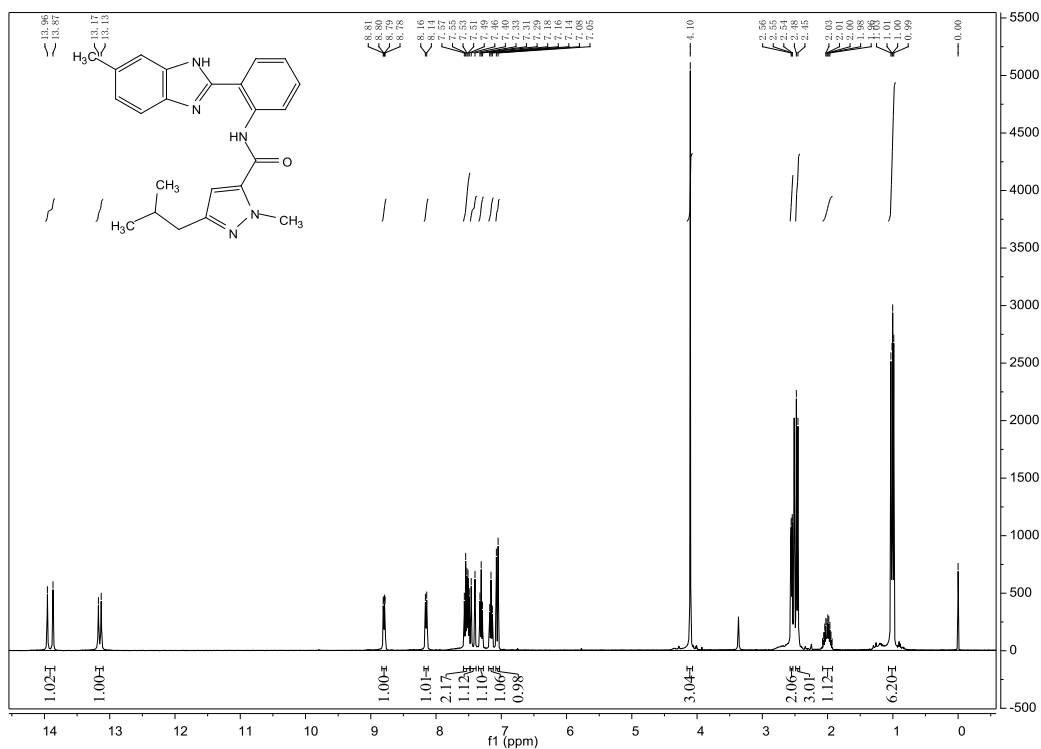
z=1

C<sub>20</sub>H<sub>20</sub>O N<sub>5</sub> = 346.16624

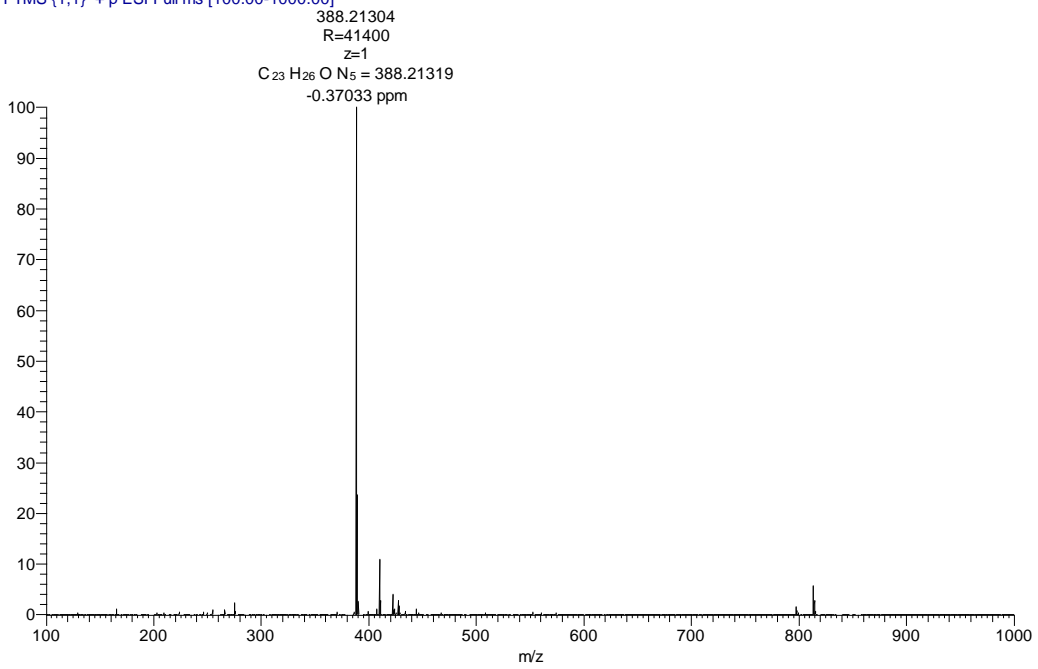
0.24266 ppm



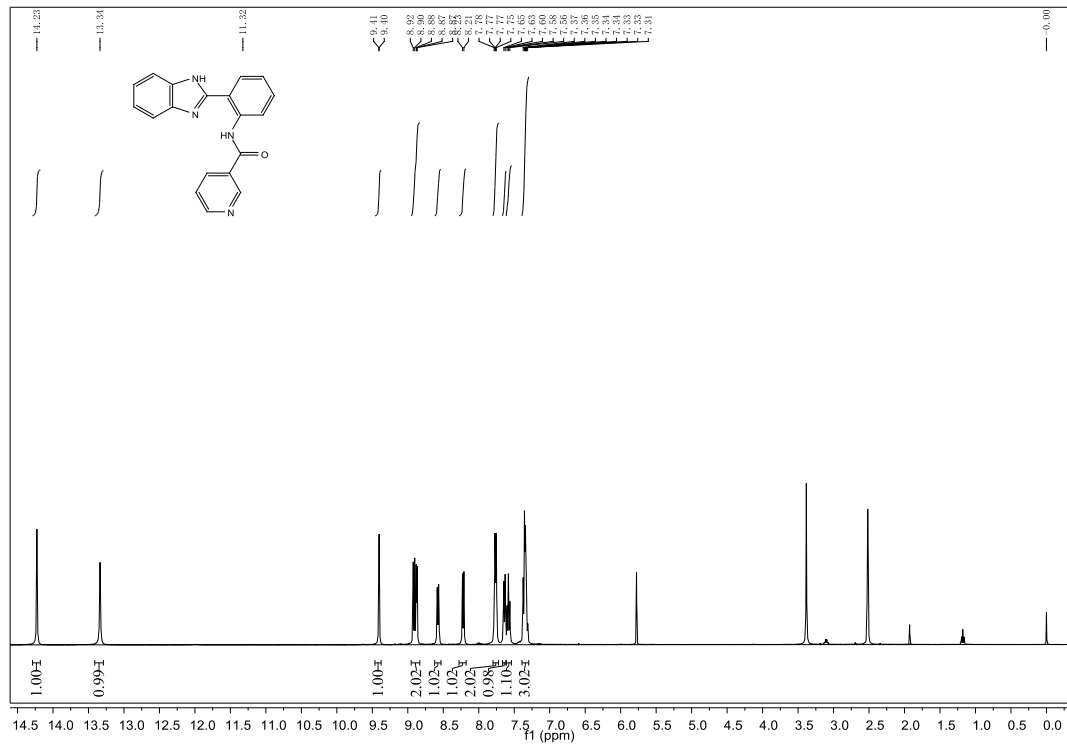
$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T12**

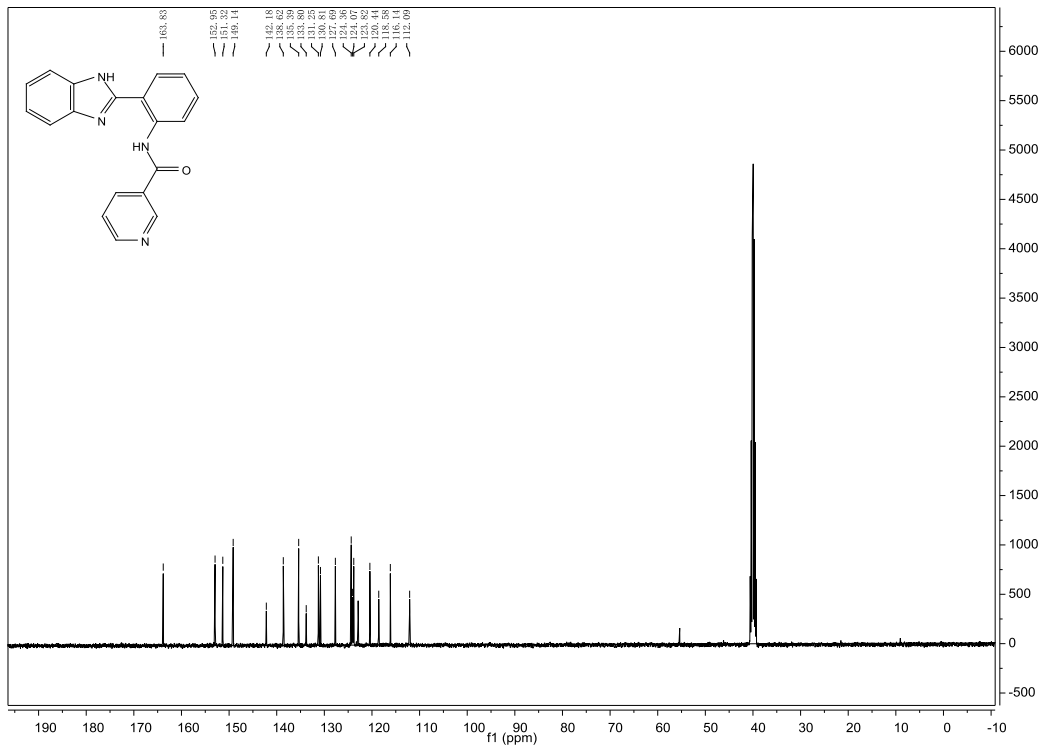


B50 #31 RT: 0.42 AV: 1 NL: 4.84E6  
T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]



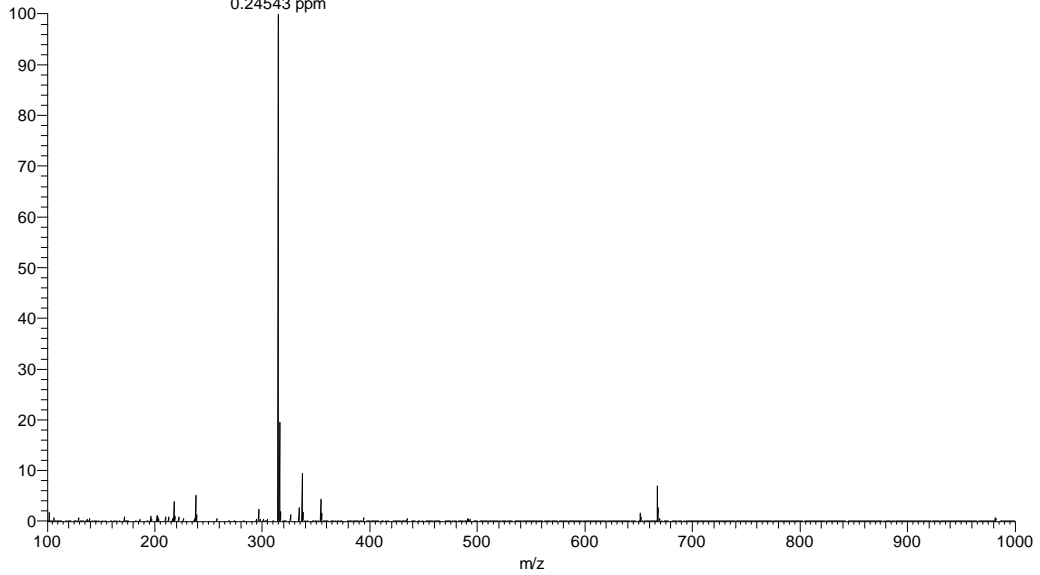
<sup>1</sup>H NMR, <sup>13</sup>C NMR spectra of the compound **T13**



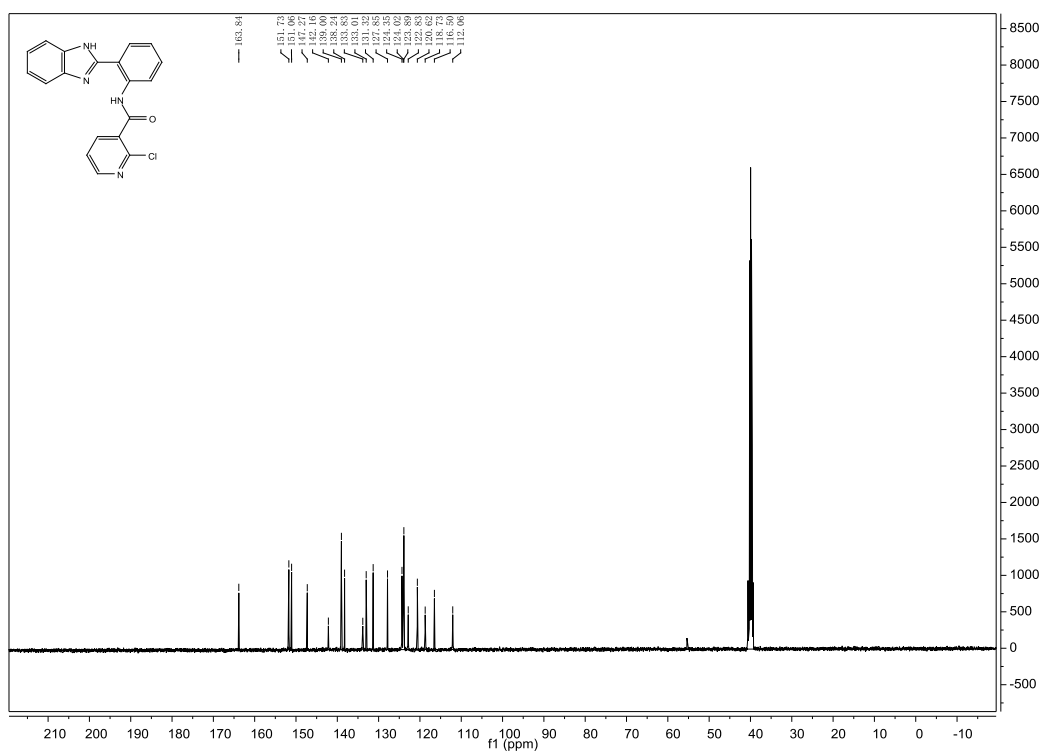
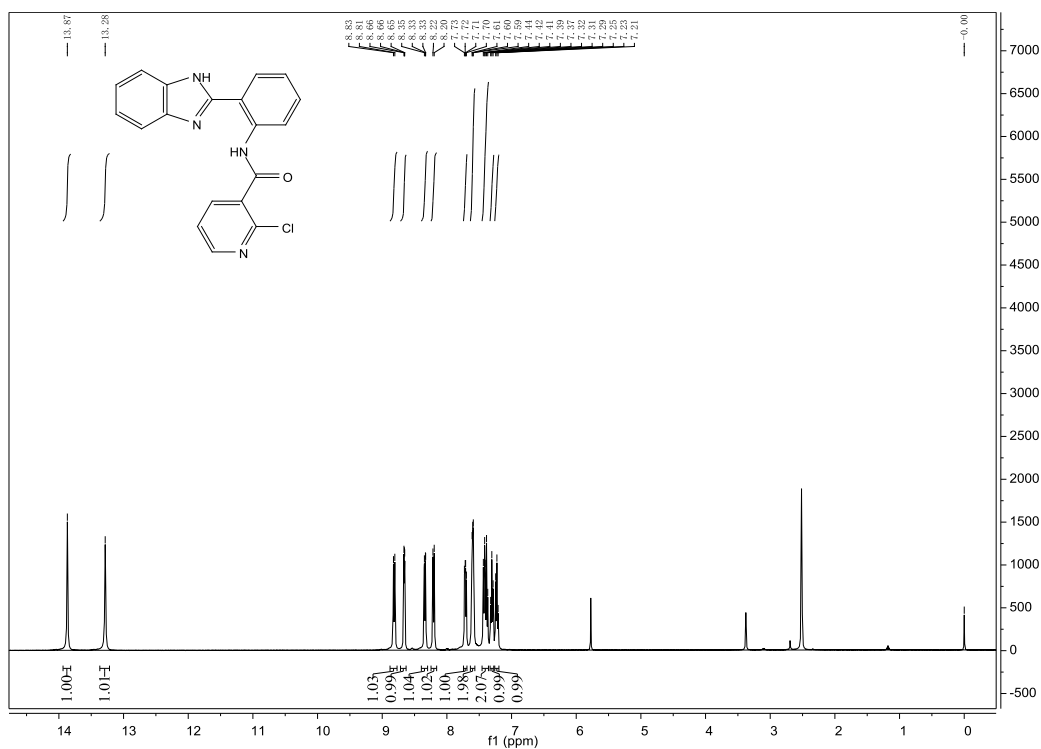


B31 #21 RT: 0.32 AV: 1 NL: 1.98E6  
 T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]

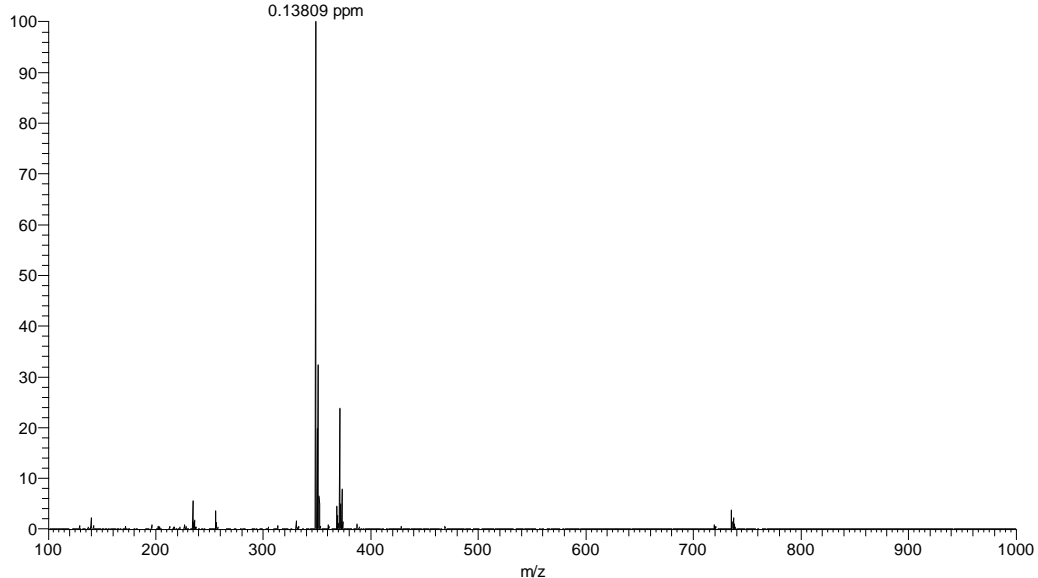
315.12411  
 R=46200  
 z=1  
 C<sub>19</sub>H<sub>15</sub>O<sub>4</sub>N<sub>4</sub> = 315.12404  
 0.24543 ppm



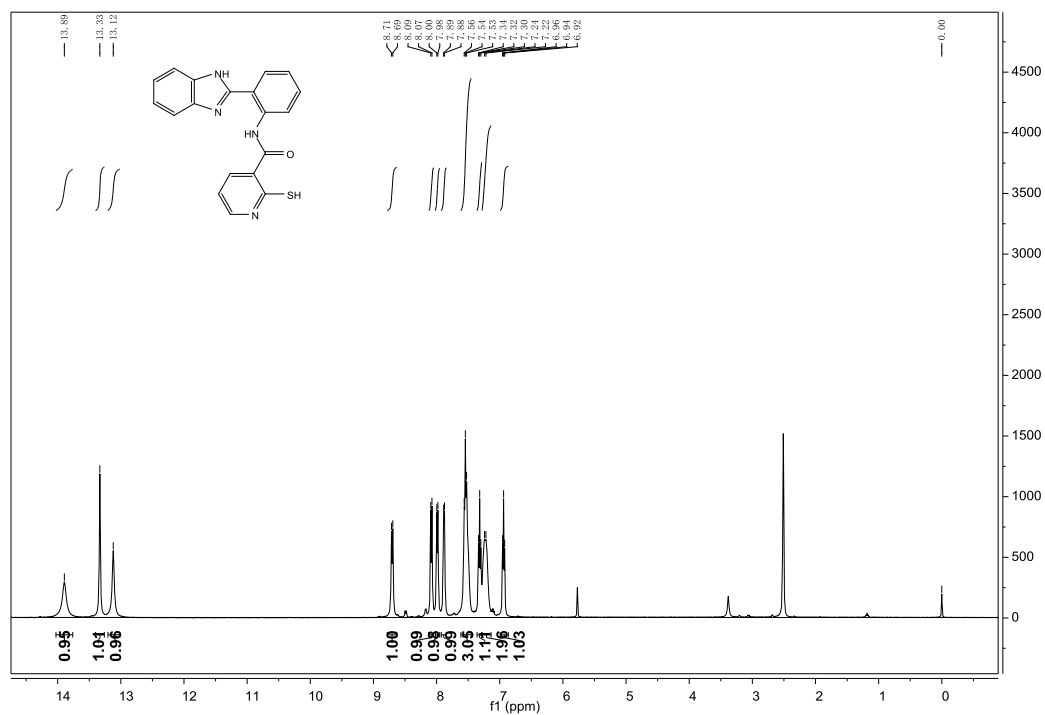
$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T14**

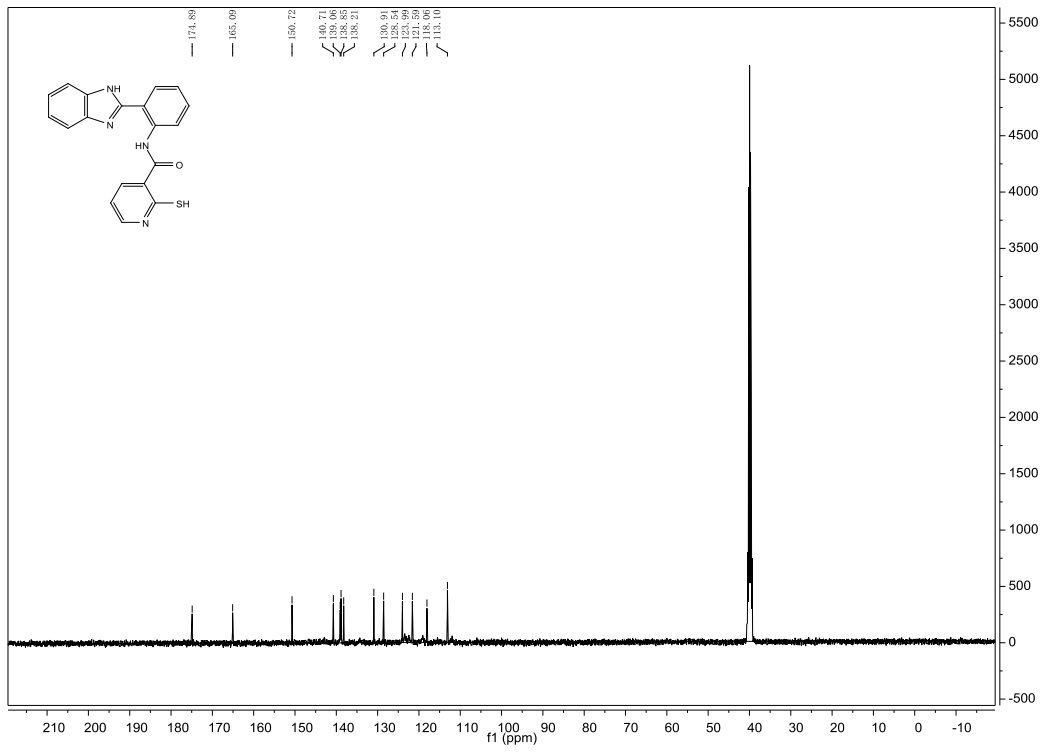


B32 #33 RT: 0.45 AV: 1 NL: 2.81E6  
 T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]  
 349.08511  
 R=44000  
 Z=1  
 C<sub>19</sub> H<sub>14</sub> O N<sub>4</sub> Cl = 349.08507  
 0.13809 ppm



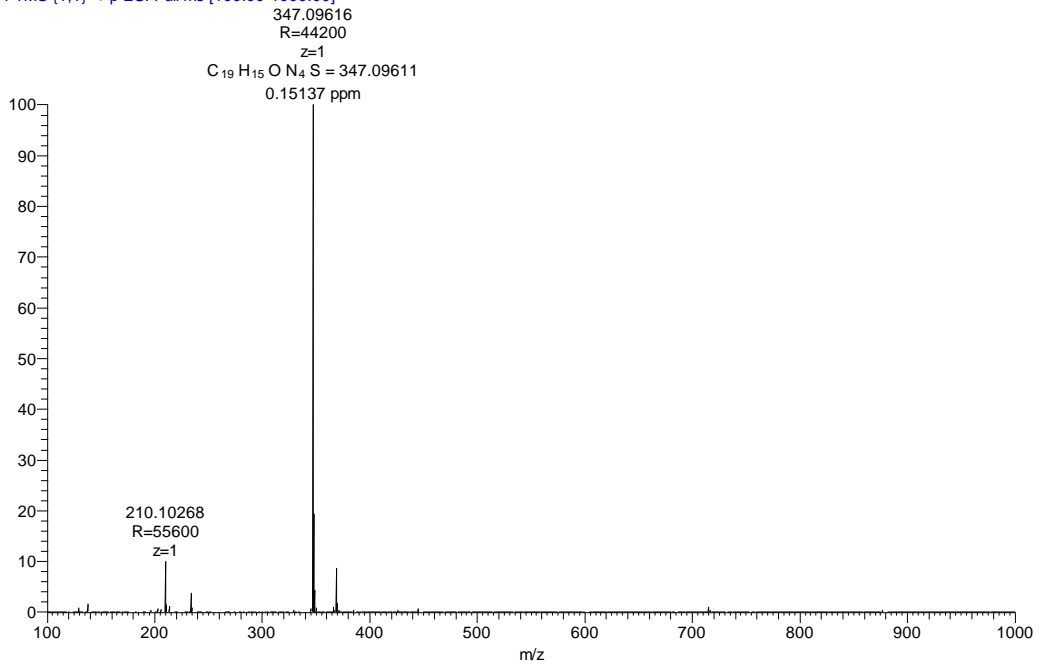
<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound **T15**





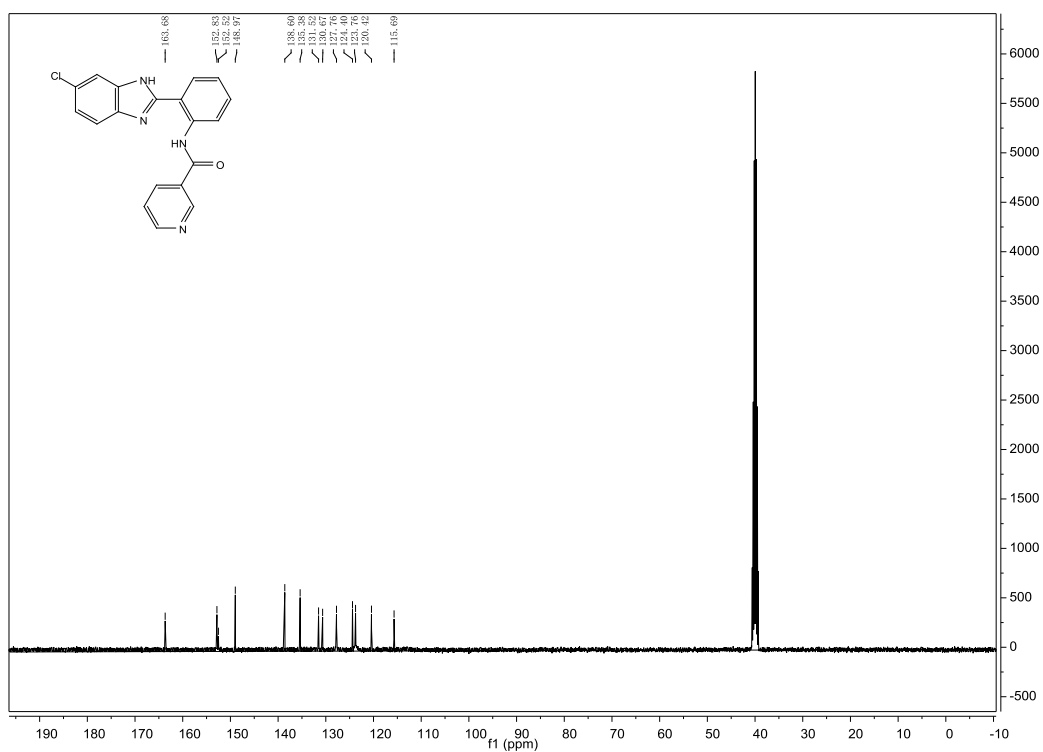
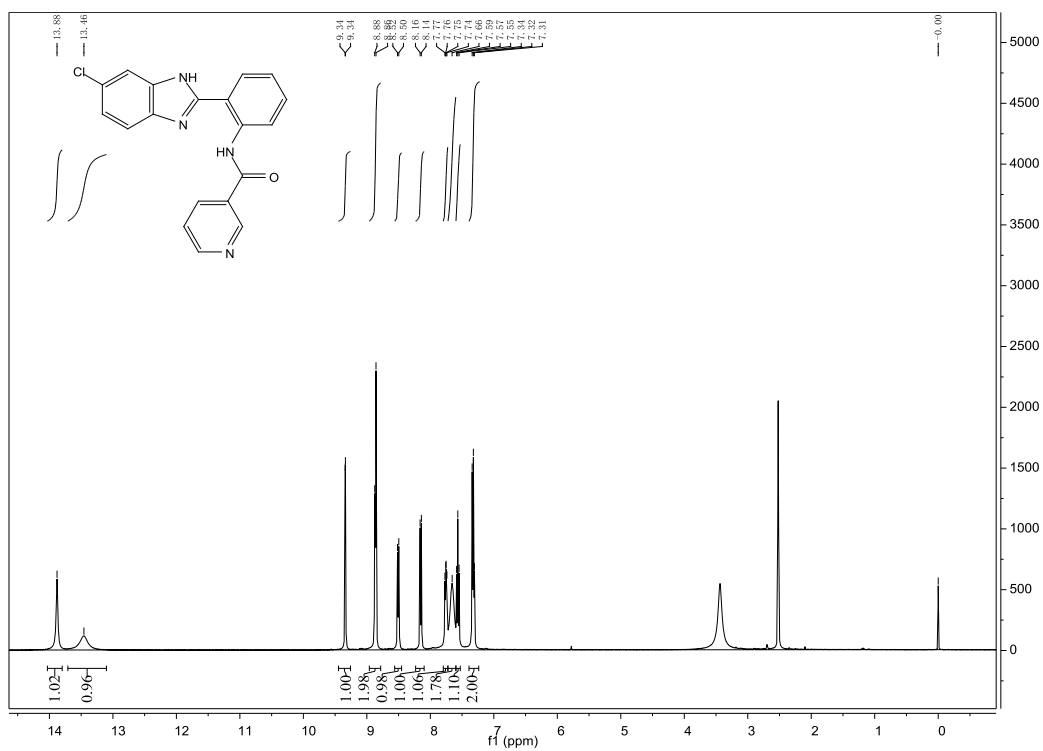
B33 #23 RT: 0.35 AV: 1 NL: 4.43E6

T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]

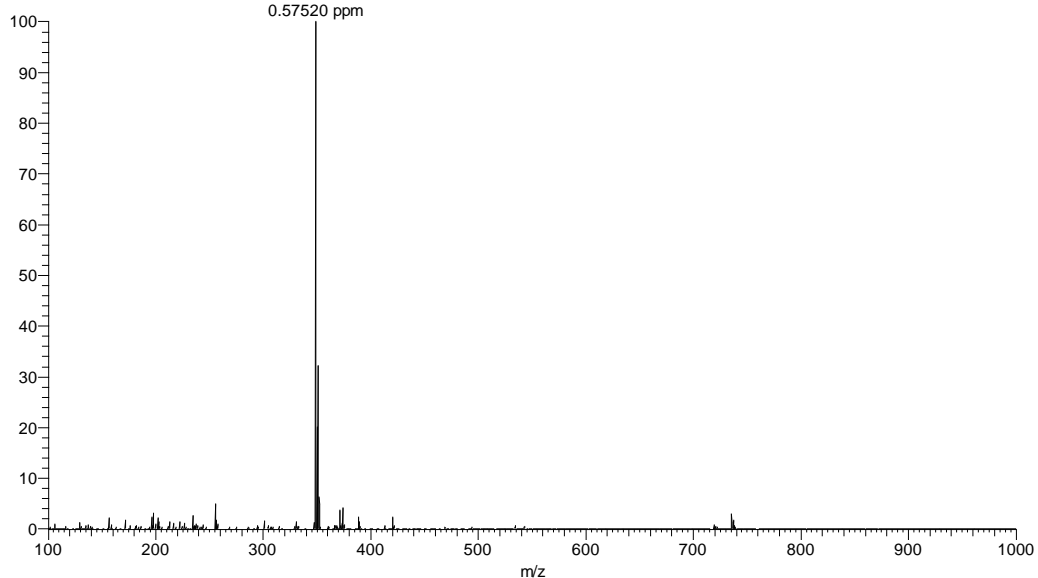




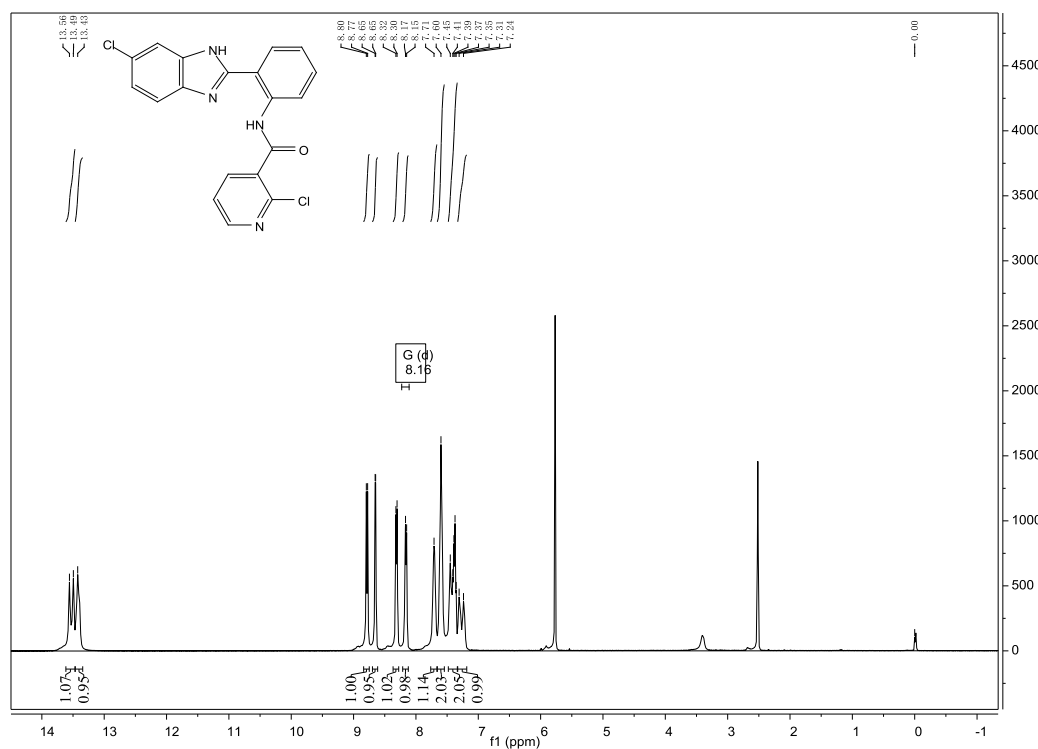
$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T16**

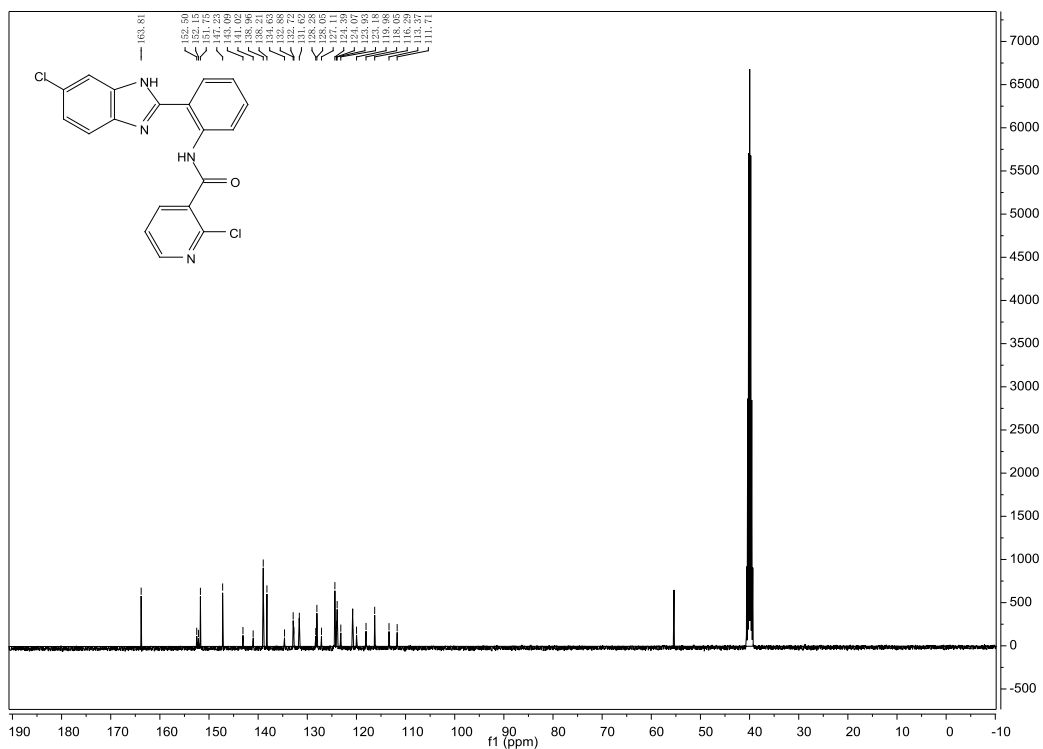


B38 #13 RT: 0.21 AV: 1 NL: 9.26E5  
 T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]  
 349.08527  
 R=43900  
 Z=1  
 C<sub>19</sub> H<sub>14</sub> O N<sub>4</sub> Cl = 349.08507  
 0.57520 ppm

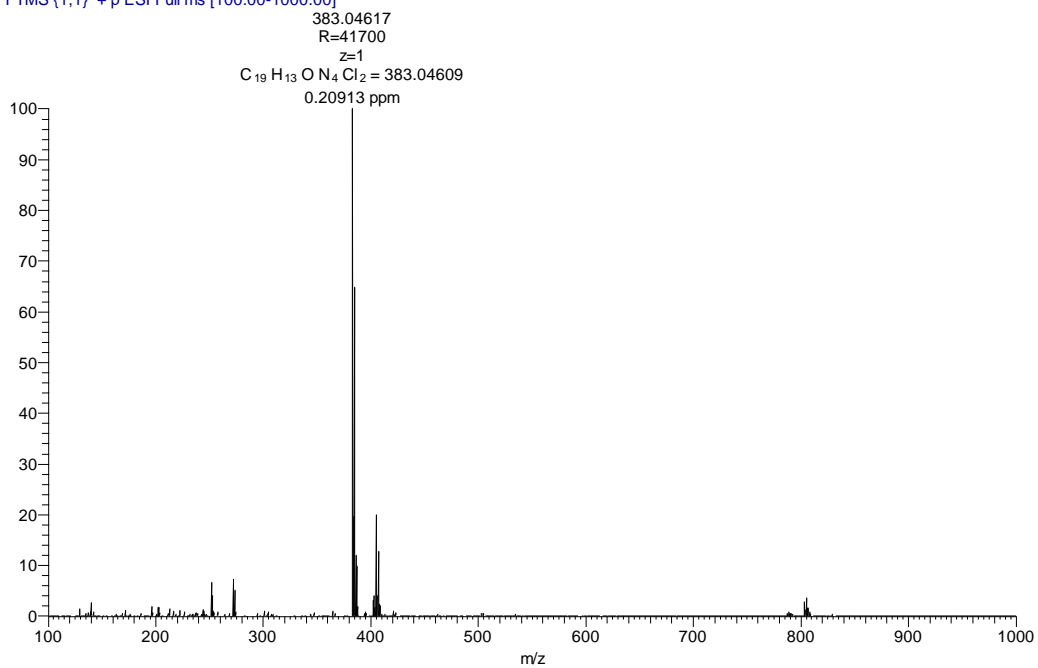


<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound **T17**

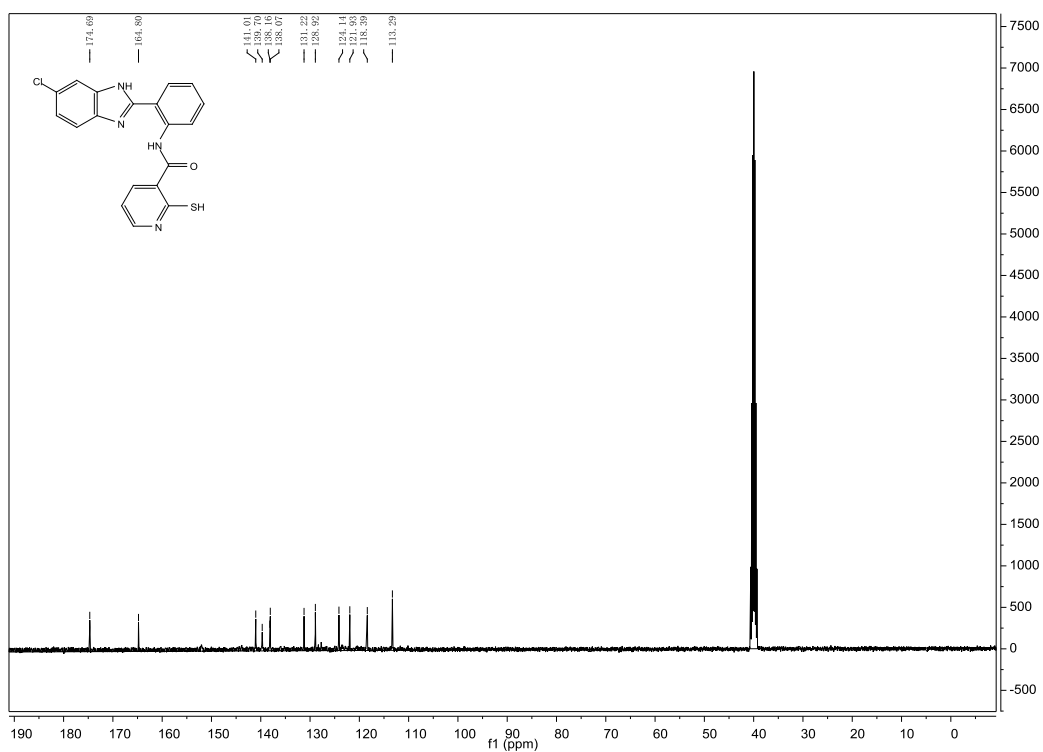
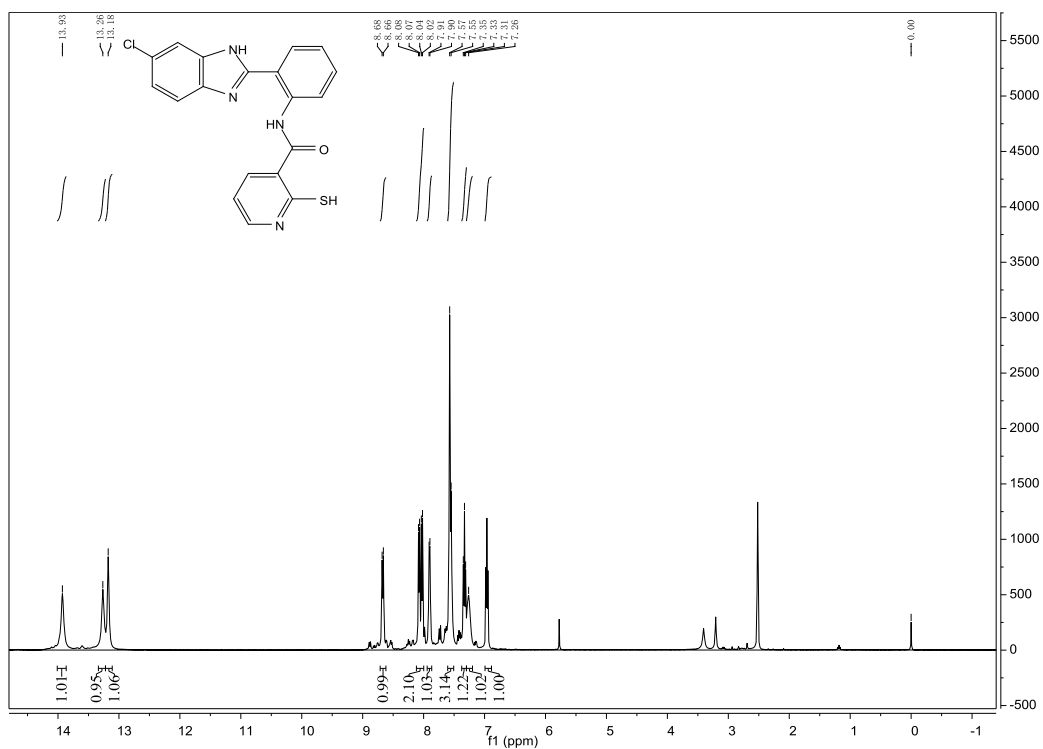




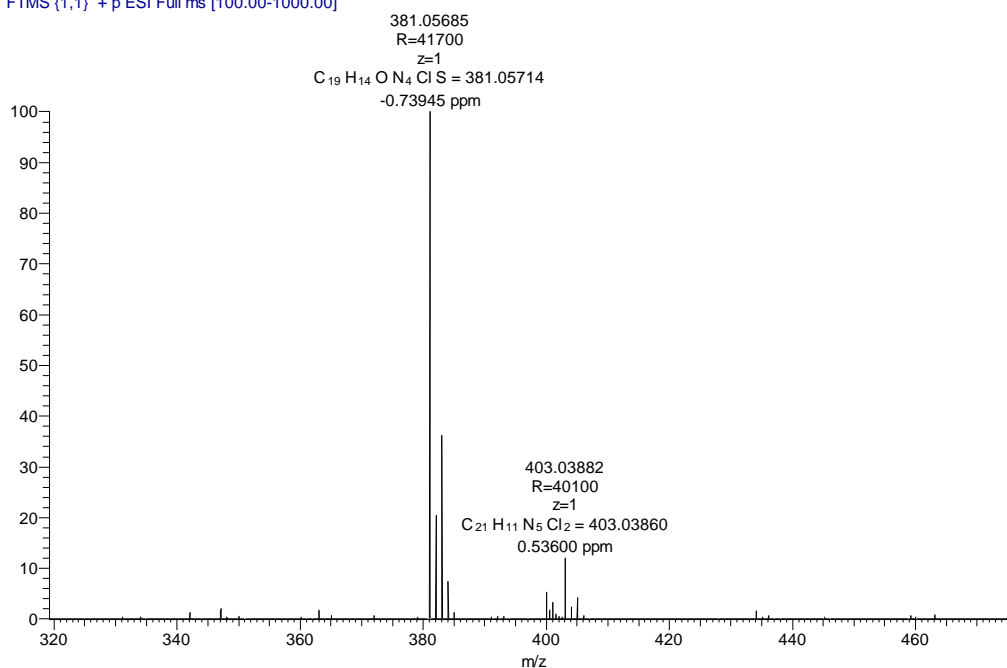
B39 #25 RT: 0.37 AV: 1 NL: 1.28E6  
 T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]



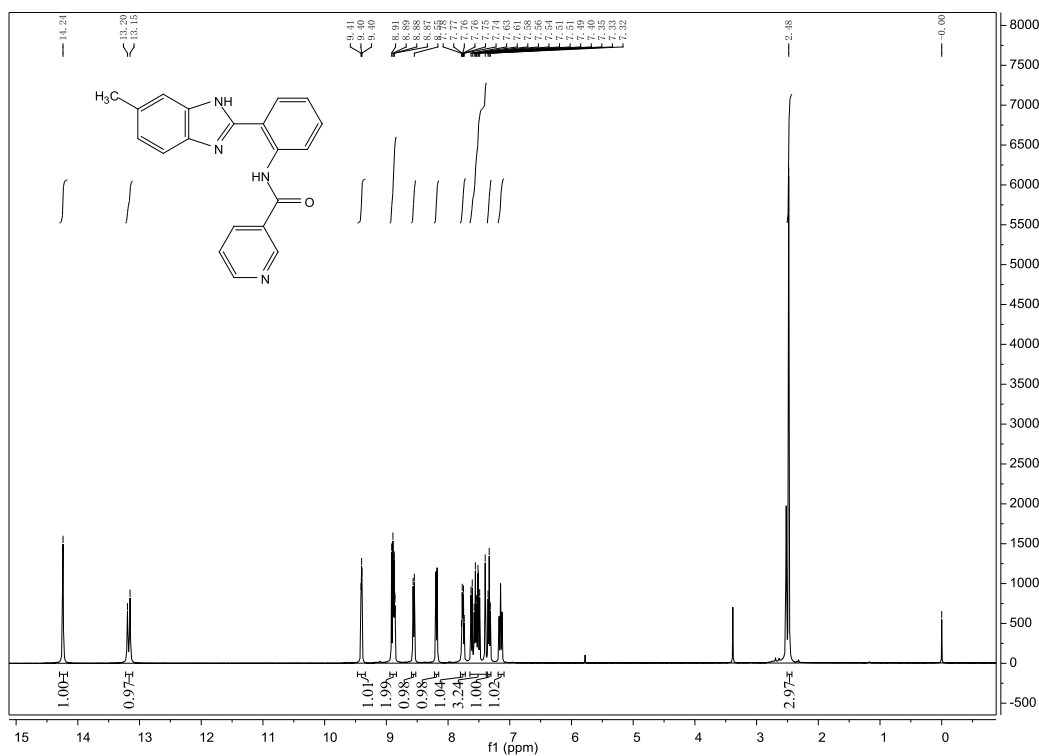
$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T18**

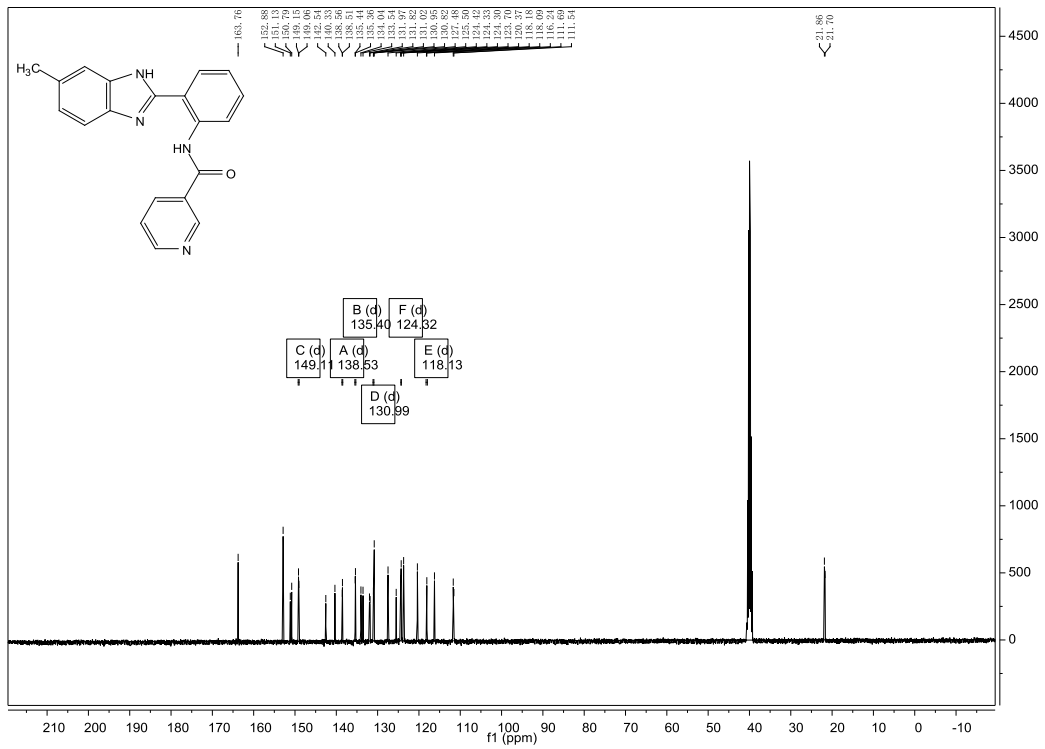


B40 #11 RT: 0.16 AV: 1 NL: 1.81E7  
T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]



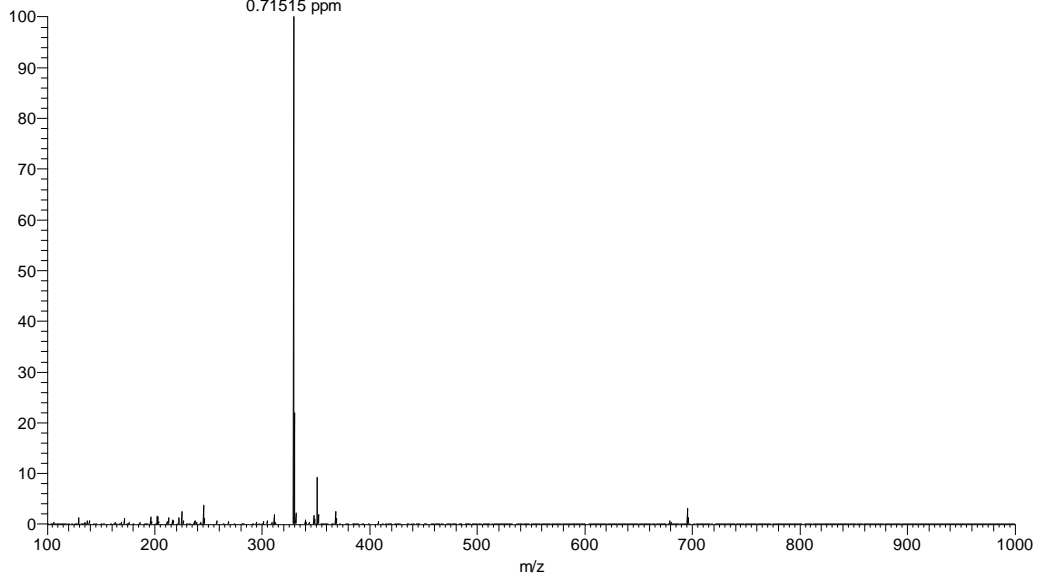
<sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of the compound T19



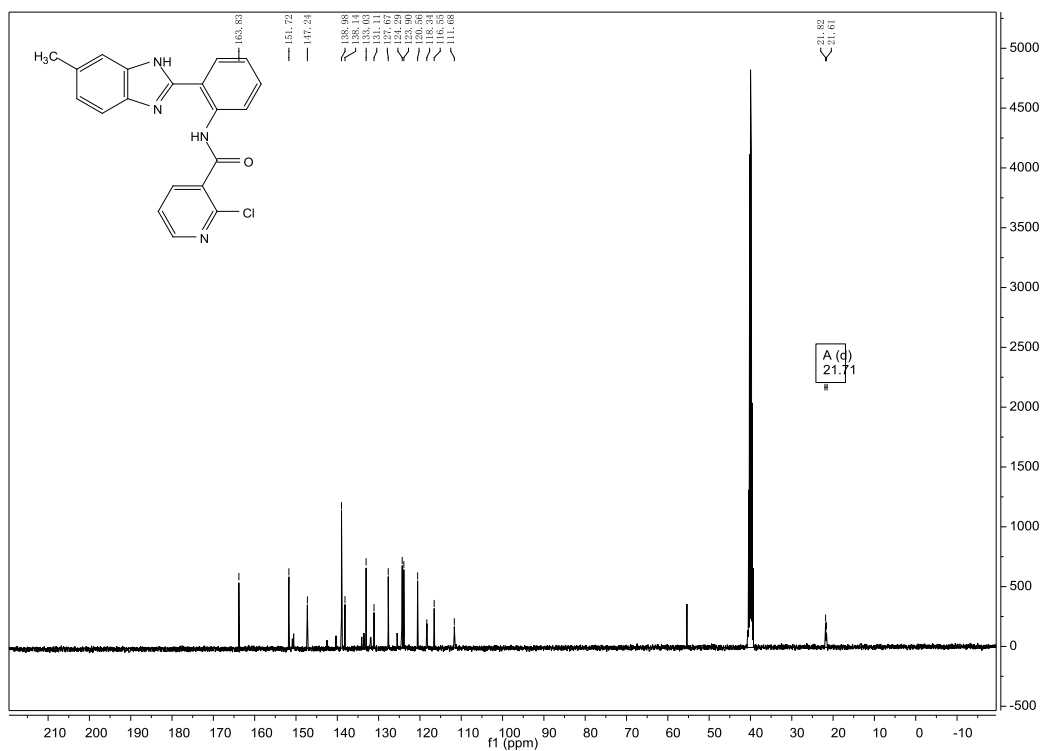
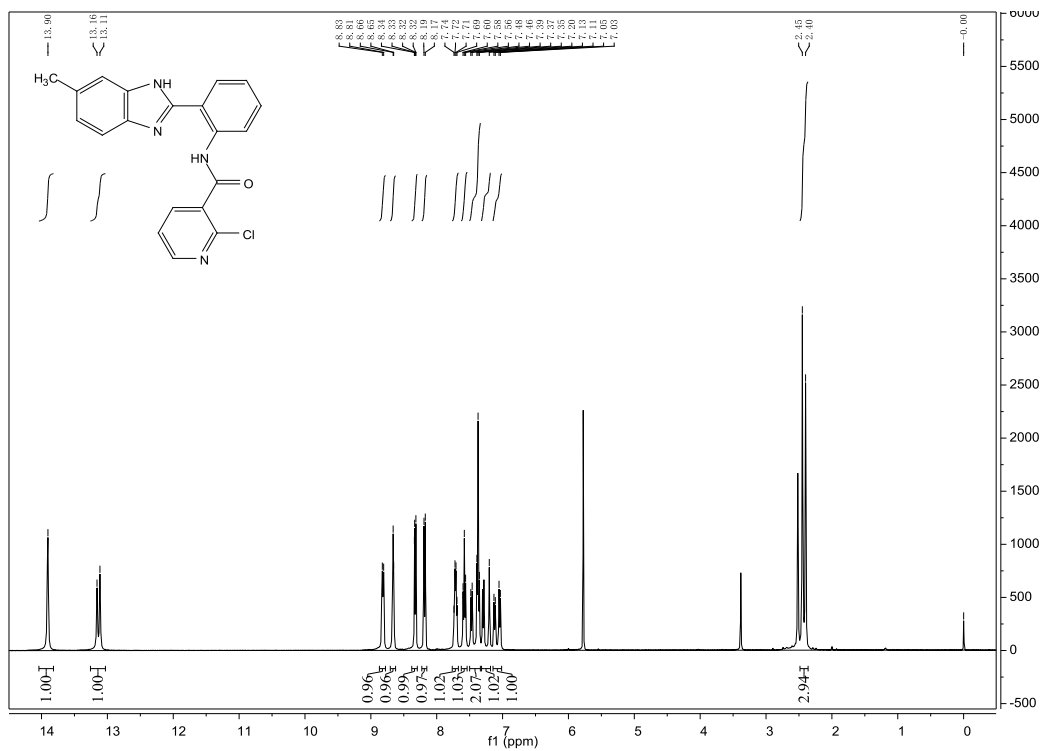


B45 #21 RT: 0.34 AV: 1 NL: 1.49E6  
 T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]

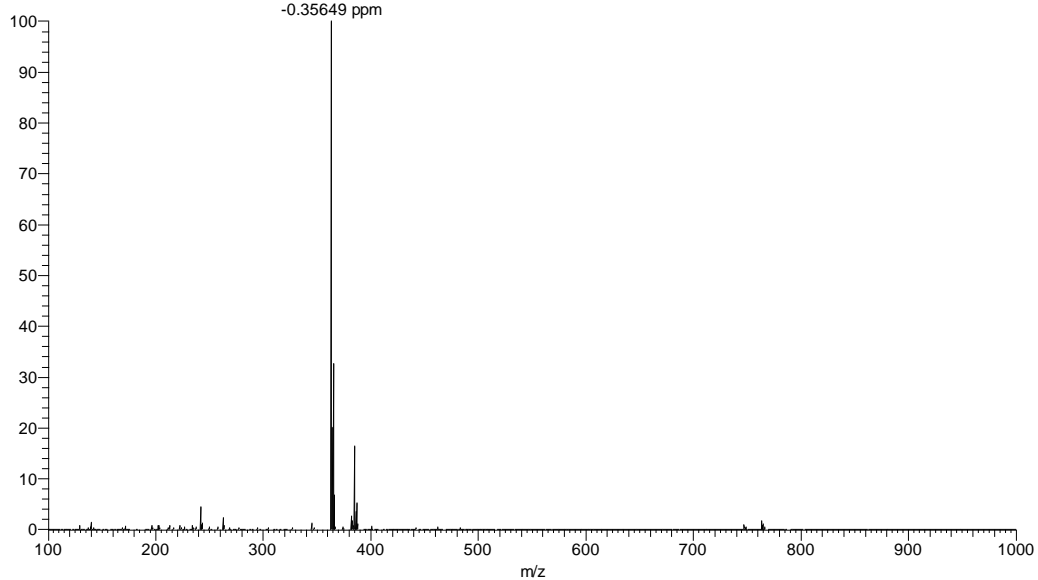
329.13992  
 R=44400  
 z=1  
 C<sub>20</sub>H<sub>17</sub>O N<sub>4</sub> = 329.13969  
 0.71515 ppm



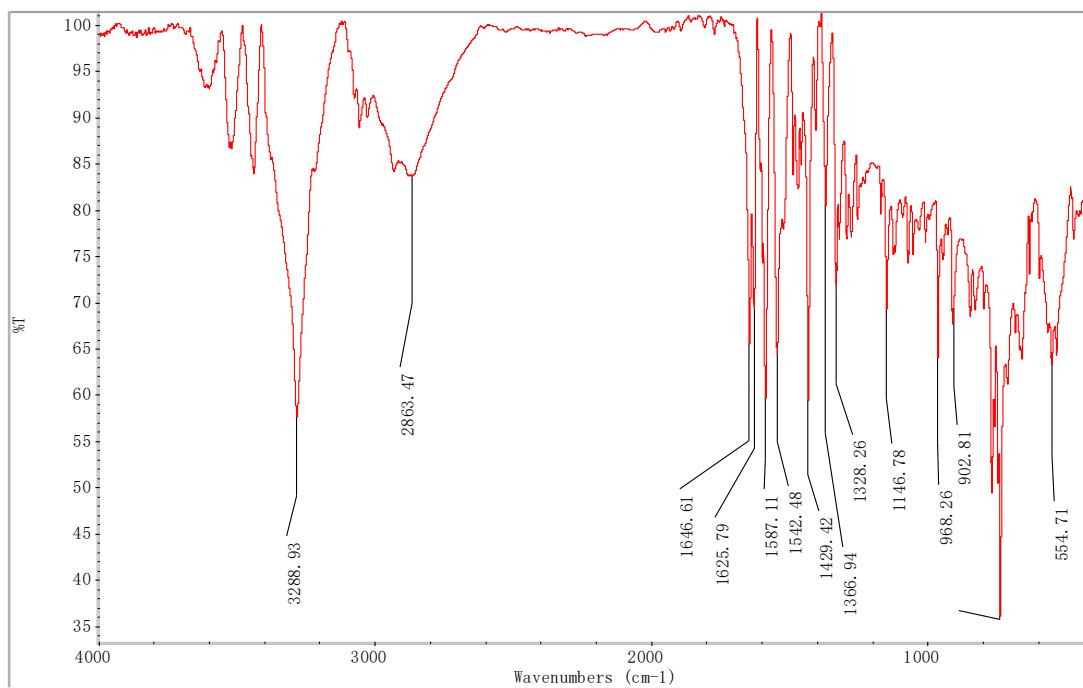
$^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and HRMS spectra of the compound **T20**



B46 #29 RT: 0.41 AV: 1 NL: 2.53E6  
T: FTMS (1,1) + p ESI Full ms [100.00-1000.00]  
363.10059  
R=43000  
z=1  
C<sub>20</sub>H<sub>16</sub>O N<sub>4</sub>Cl = 363.10072  
-0.35649 ppm

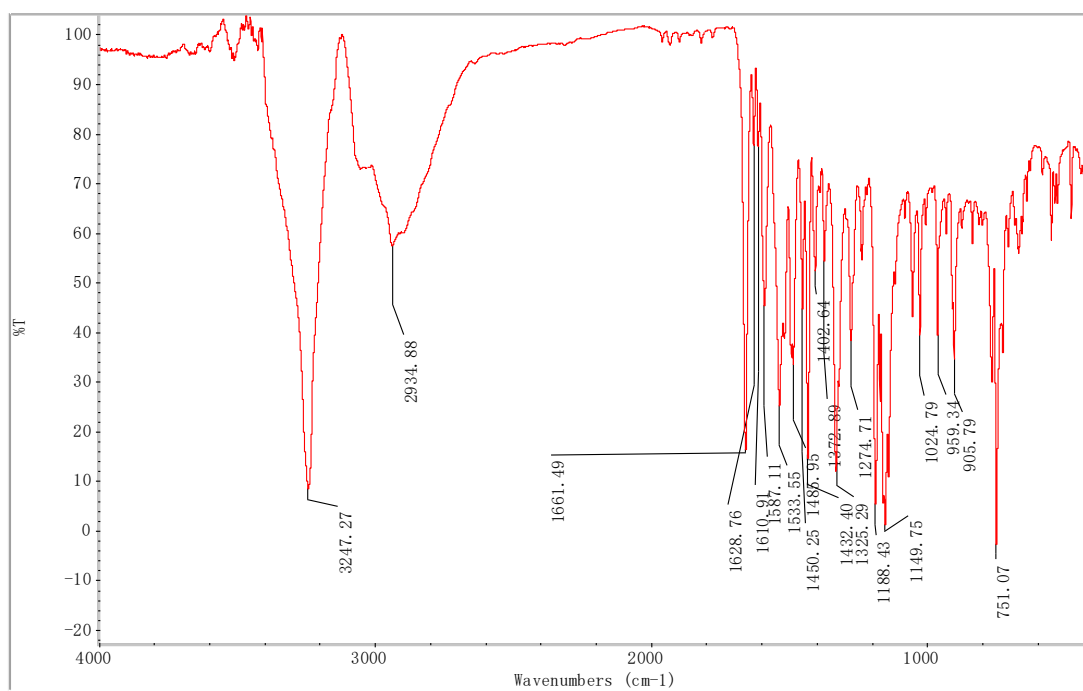


### FTIR spectra of the compound T1

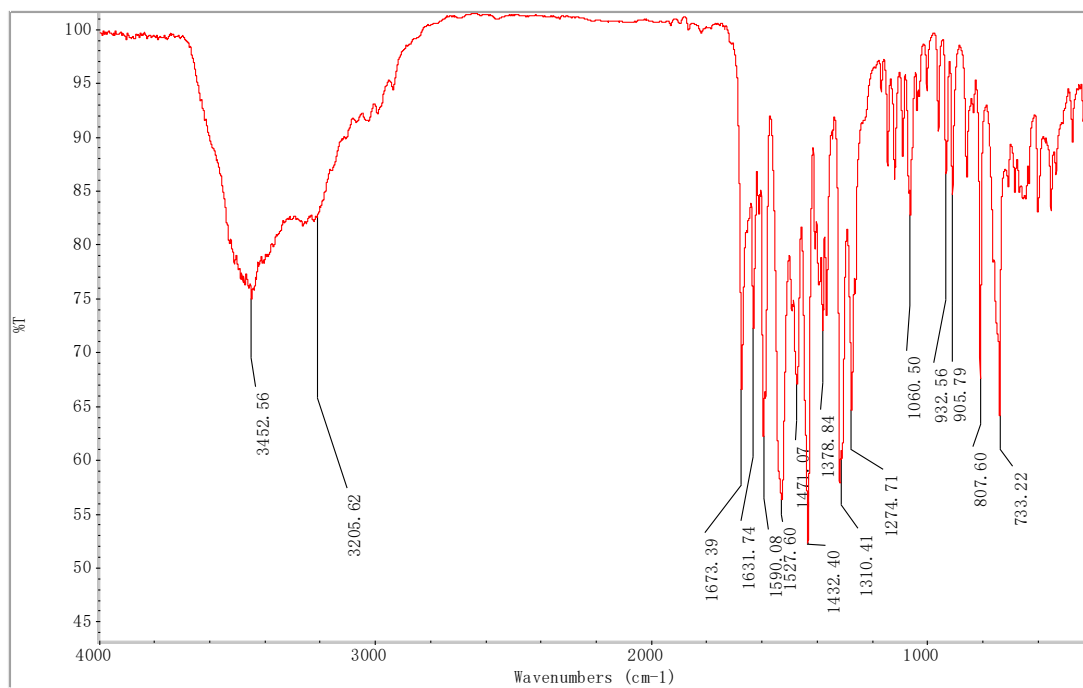




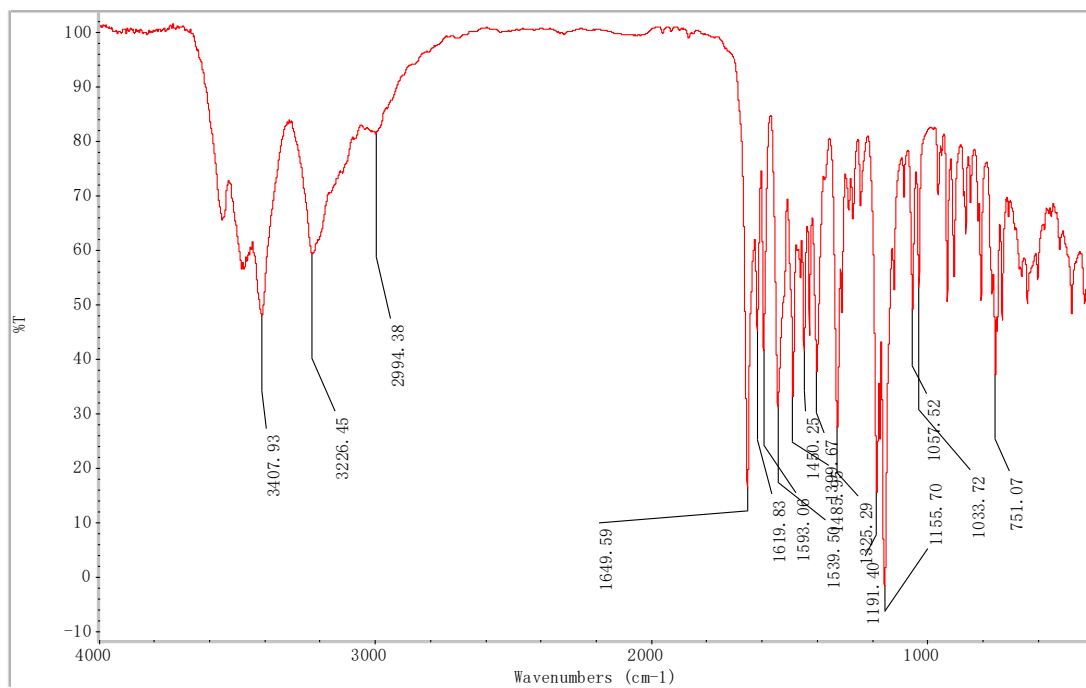
### FTIR spectra of the compound T2



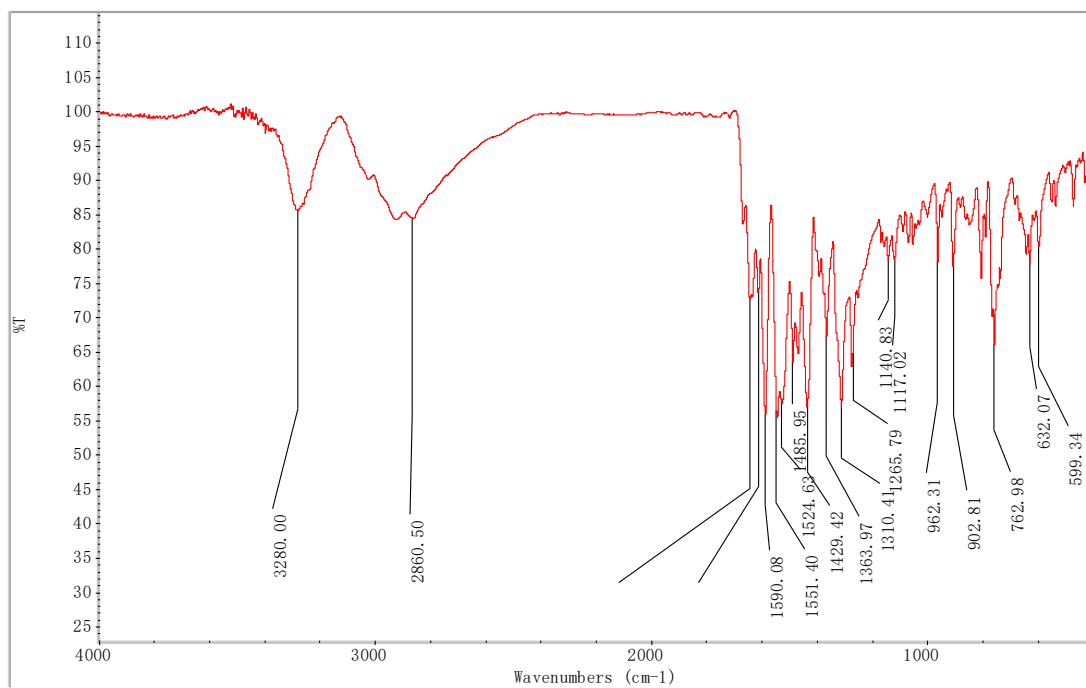
### FTIR spectra of the compound T3



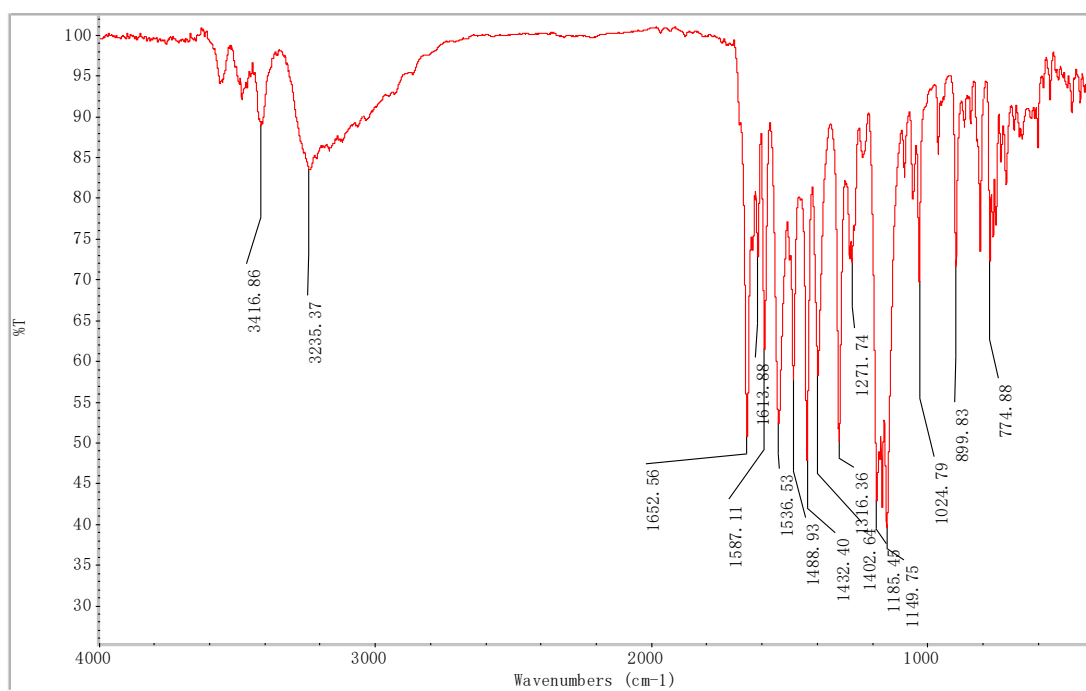
### FTIR spectra of the compound T4



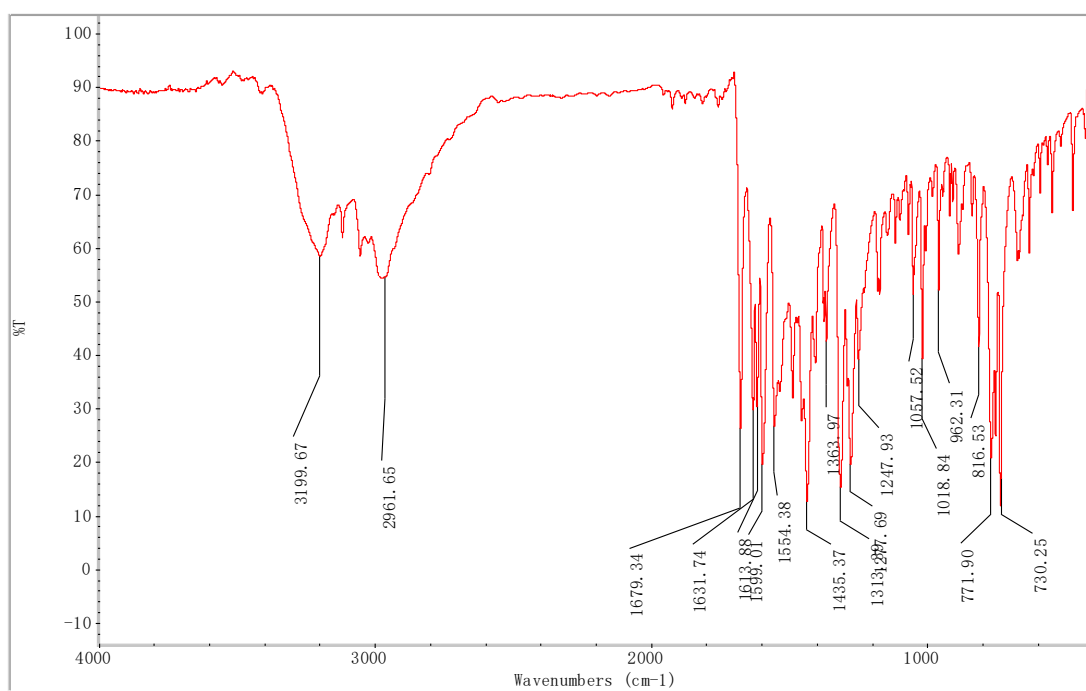
### FTIR spectra of the compound T5



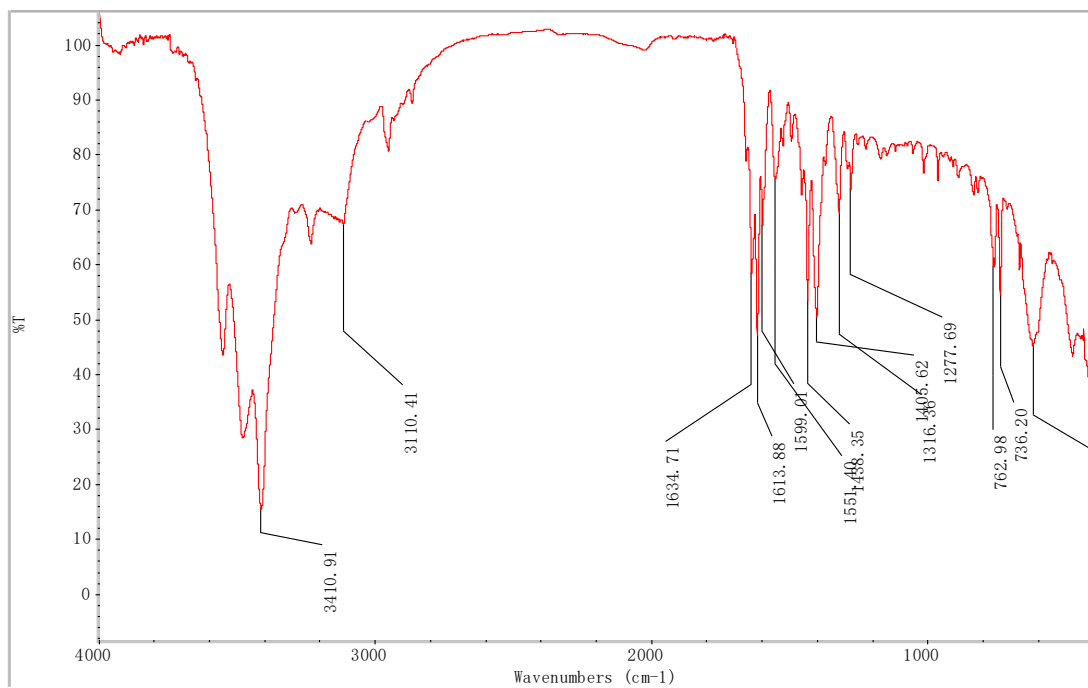
### FTIR spectra of the compound T6



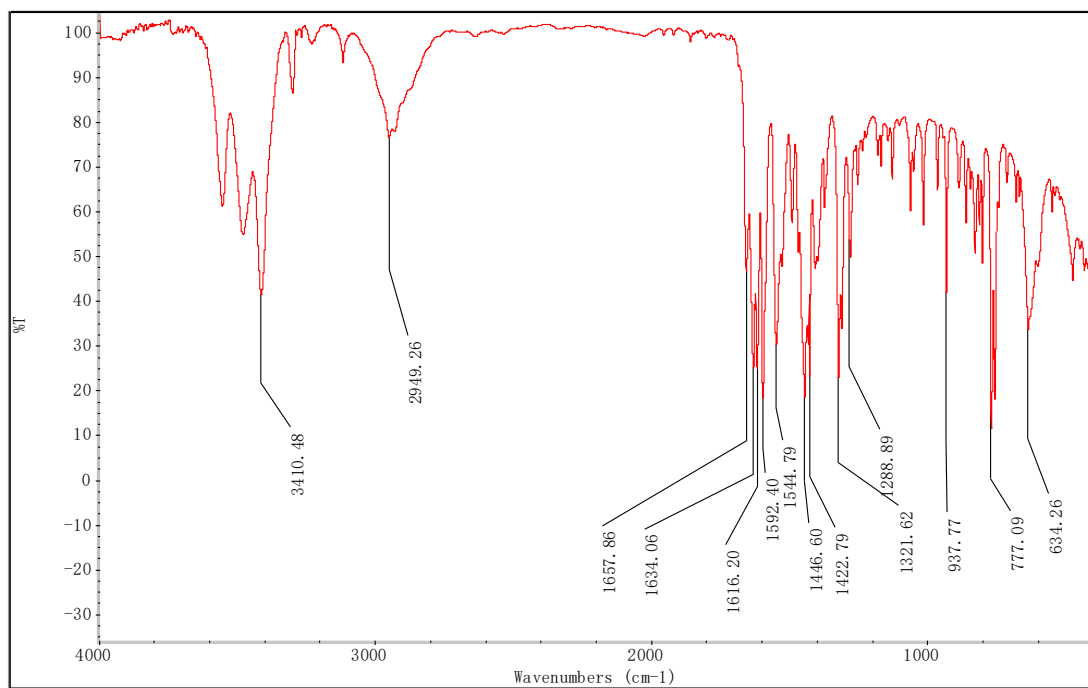
### FTIR spectra of the compound T7



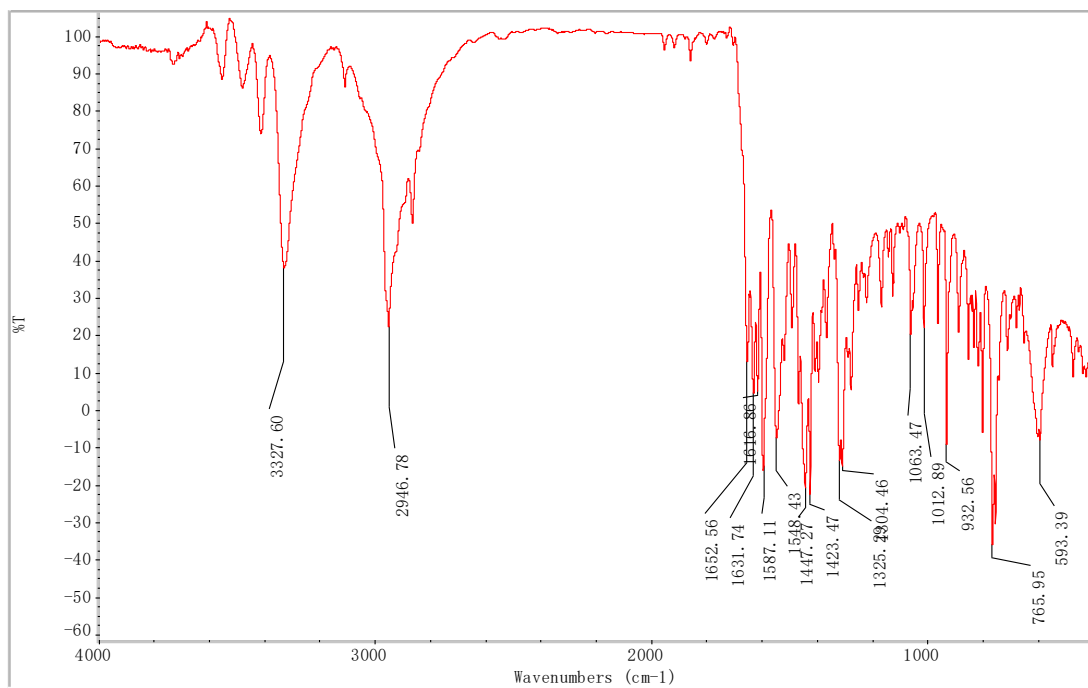
FTIR spectra of the compound T8



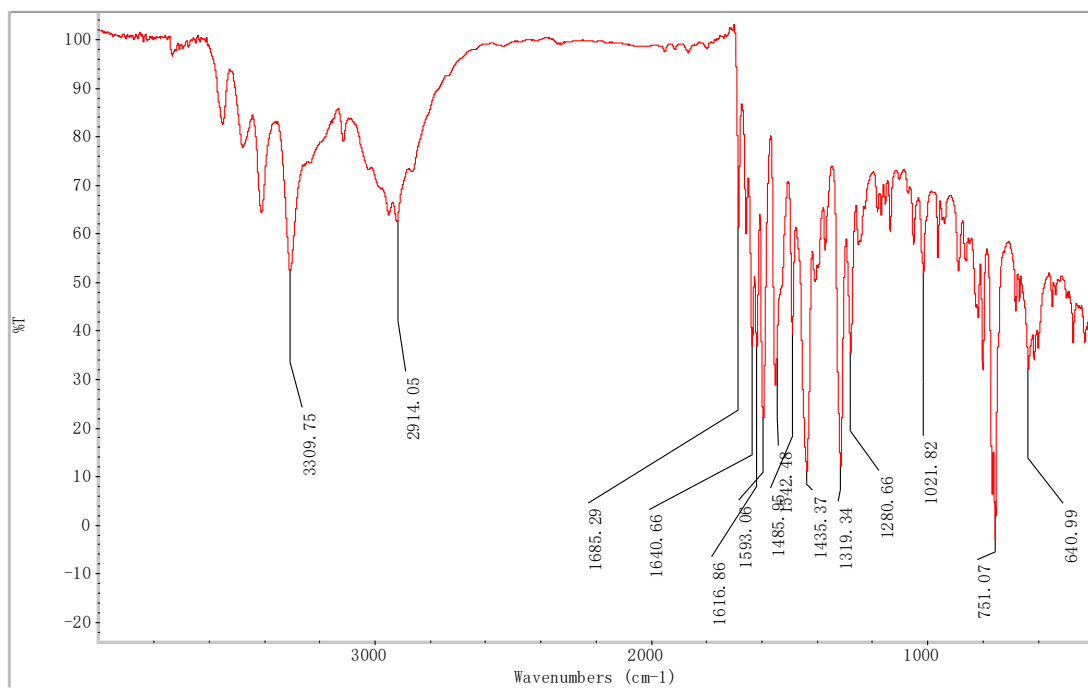
FTIR spectra of the compound T9



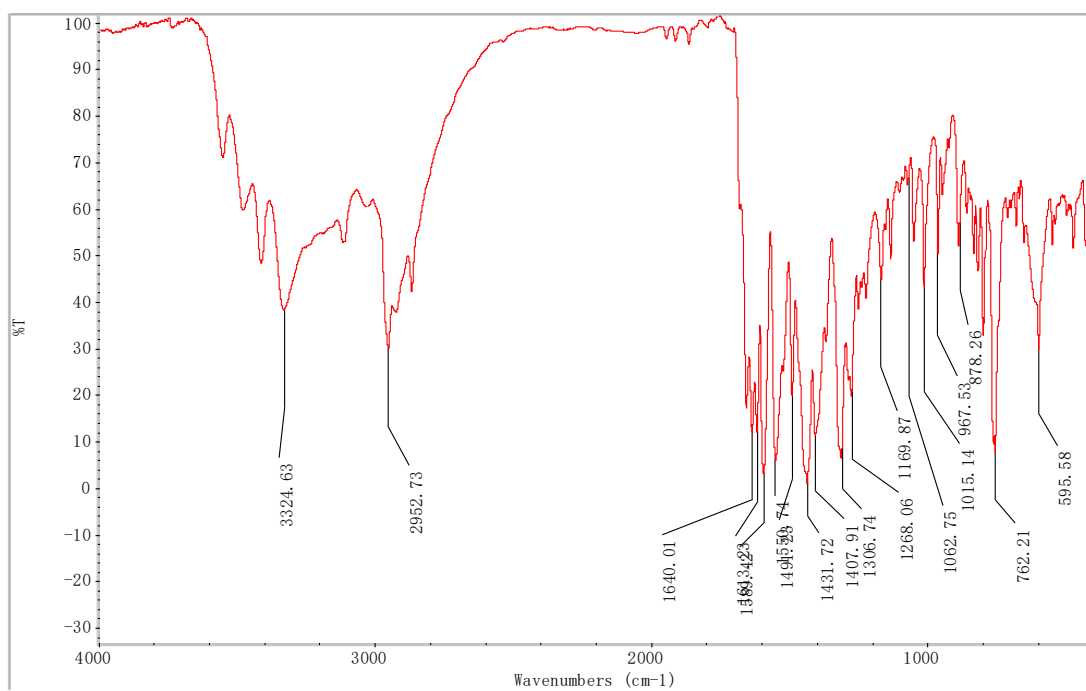
### FTIR spectra of the compound T10



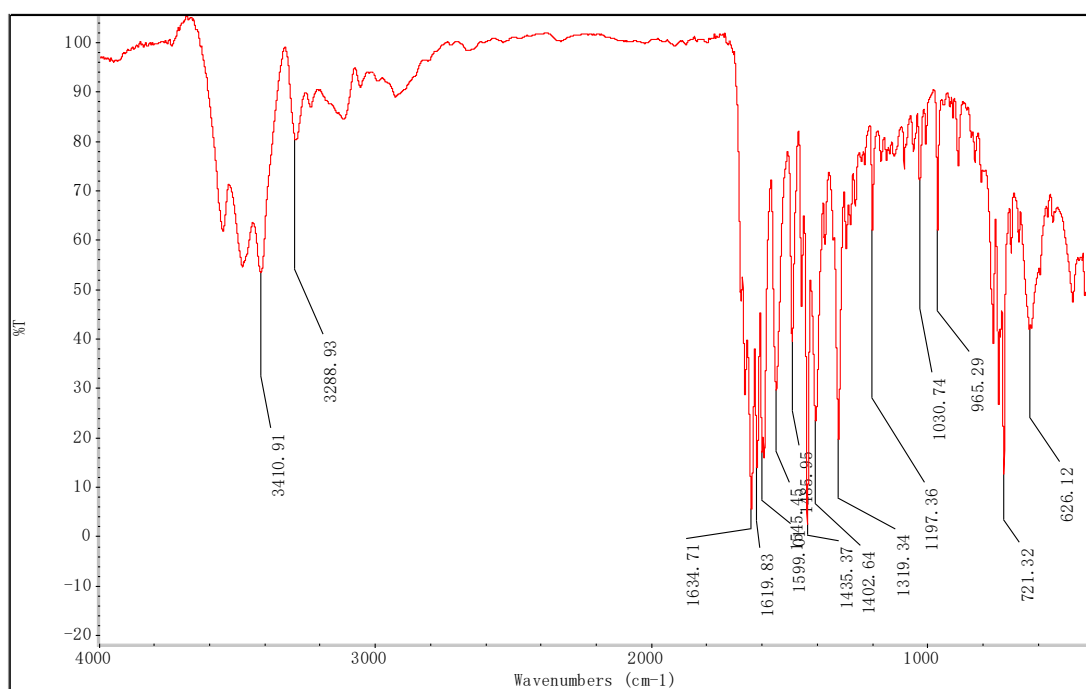
### FTIR spectra of the compound T11



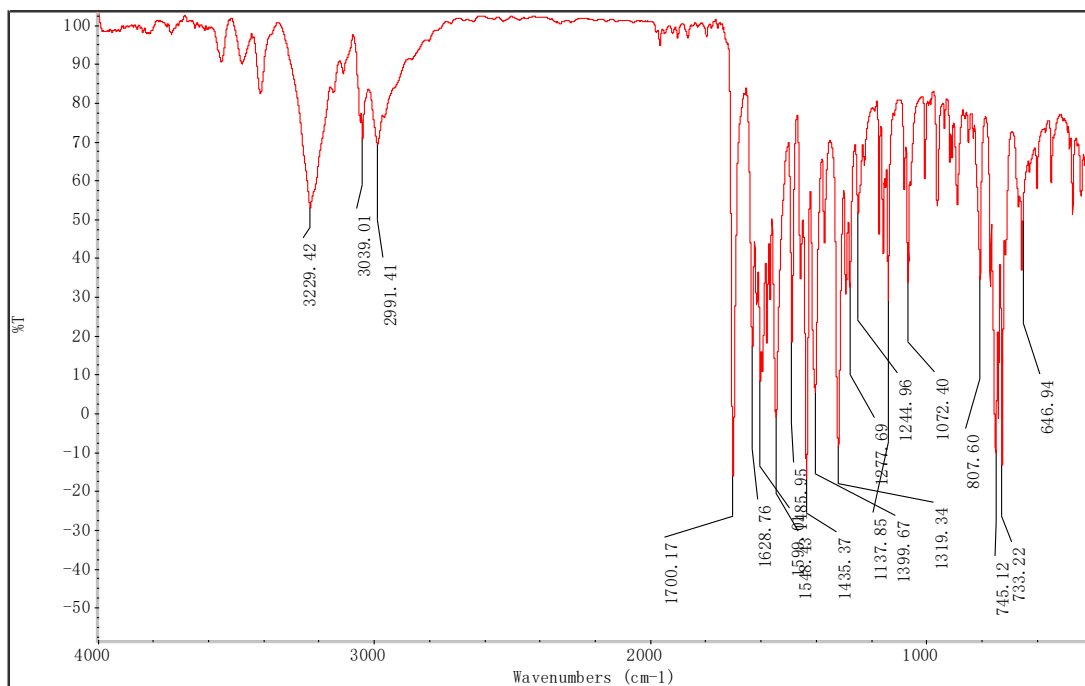
### FTIR spectra of the compound T12



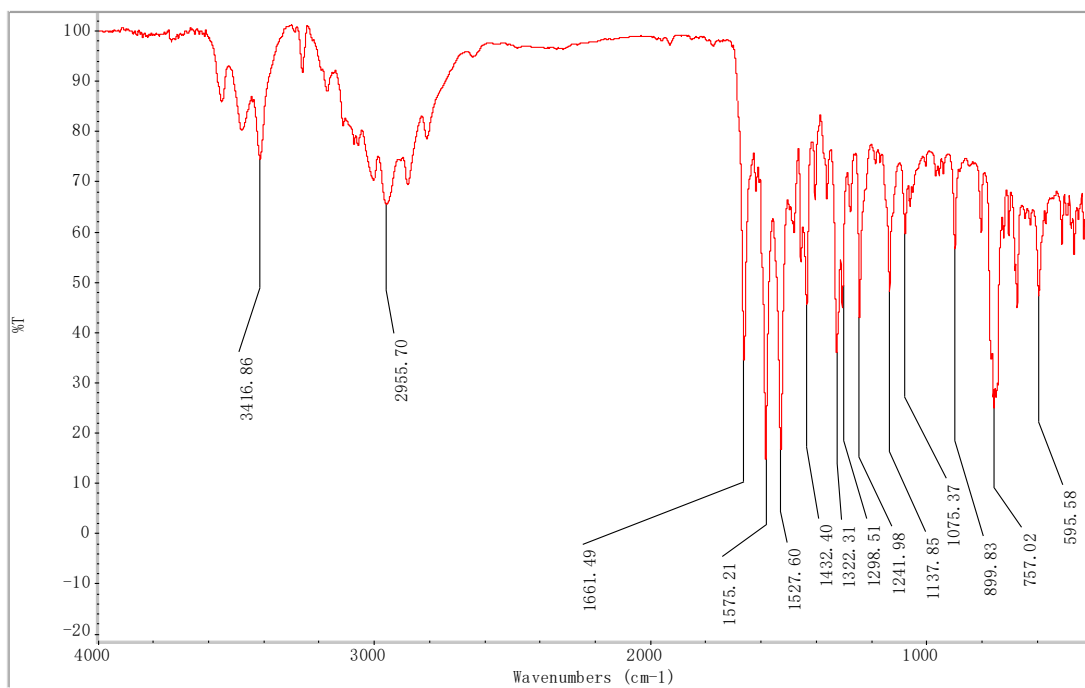
### FTIR spectra of the compound T13



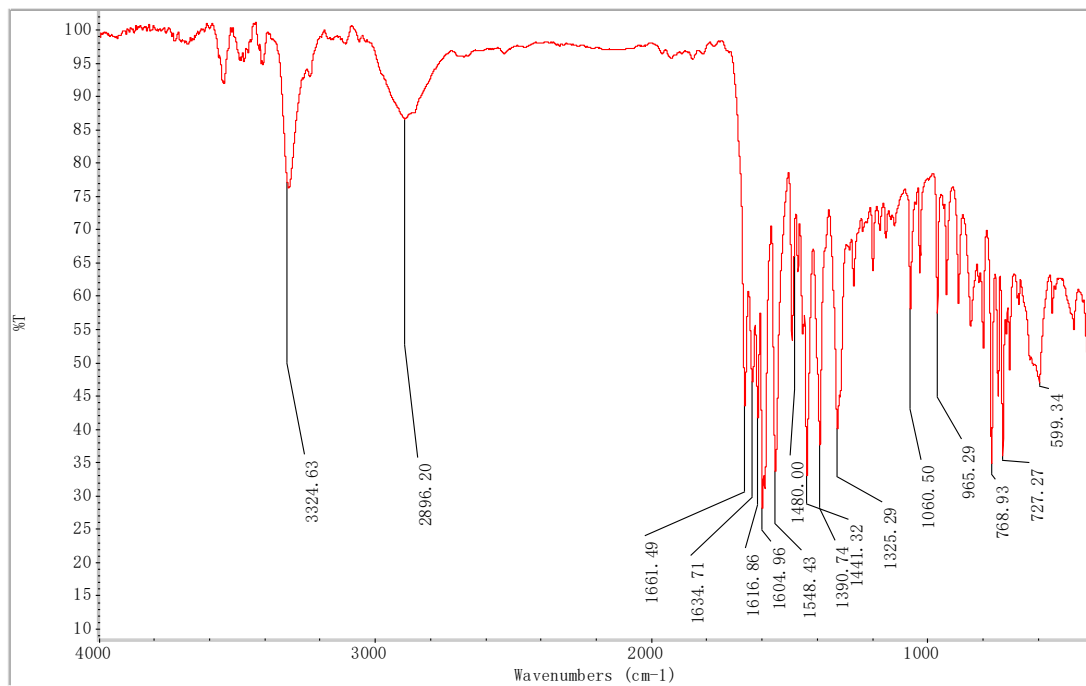
### FTIR spectra of the compound T14



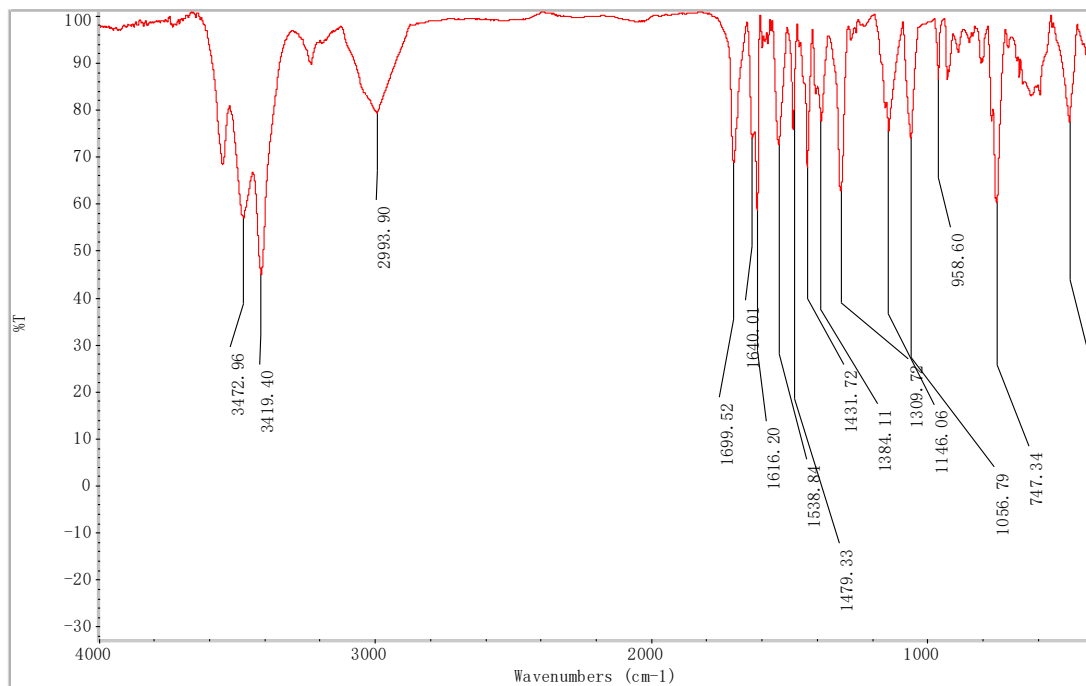
### FTIR spectra of the compound T15



FTIR spectra of the compound **T16**

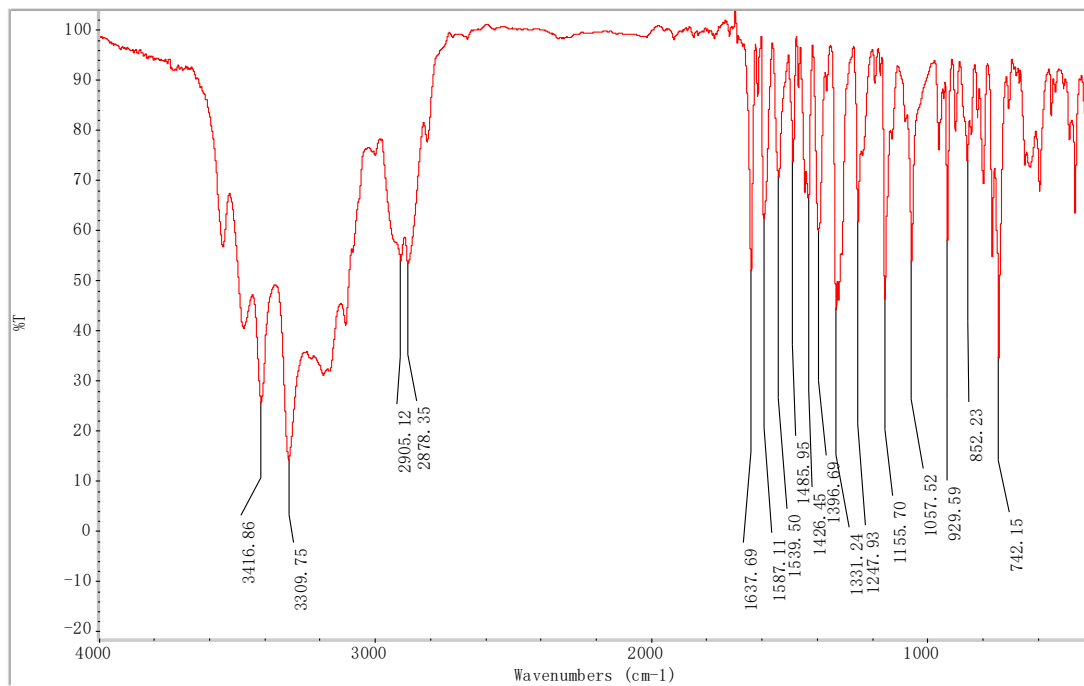


FTIR spectra of the compound **T17**

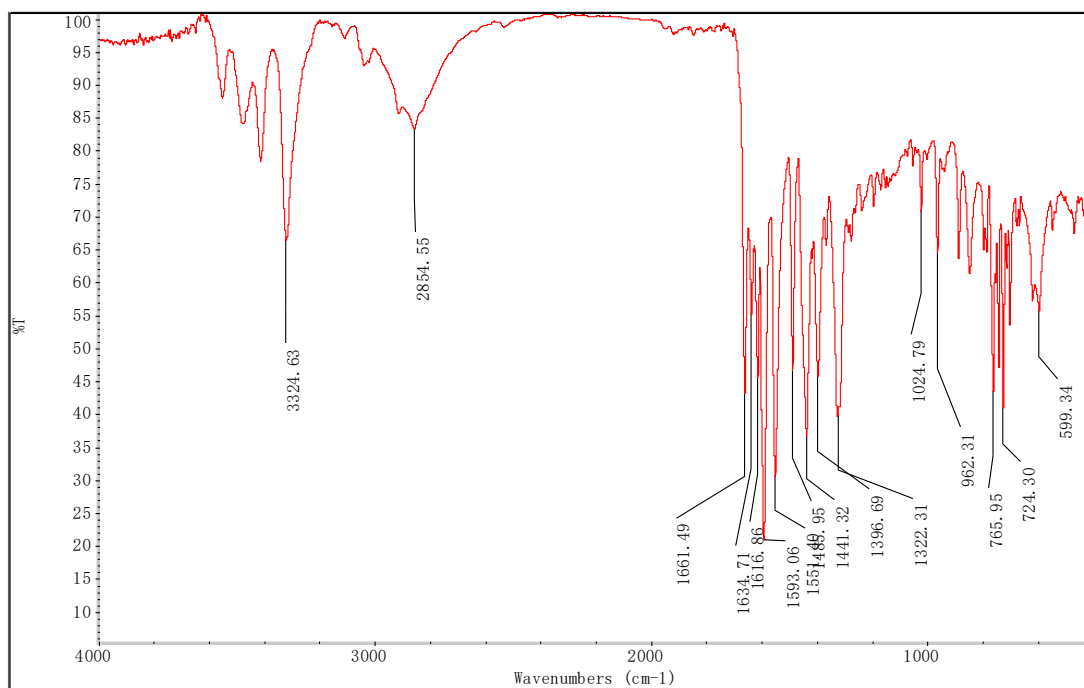




### FTIR spectra of the compound T18



### FTIR spectra of the compound T19



# FTIR spectra of the compound T20

