

## Supporting Information

### **Synthesis and evaluation of novel F-18 labeled pyrimidine derivatives: Potential FAK inhibitors and PET imaging agents for cancer detection**

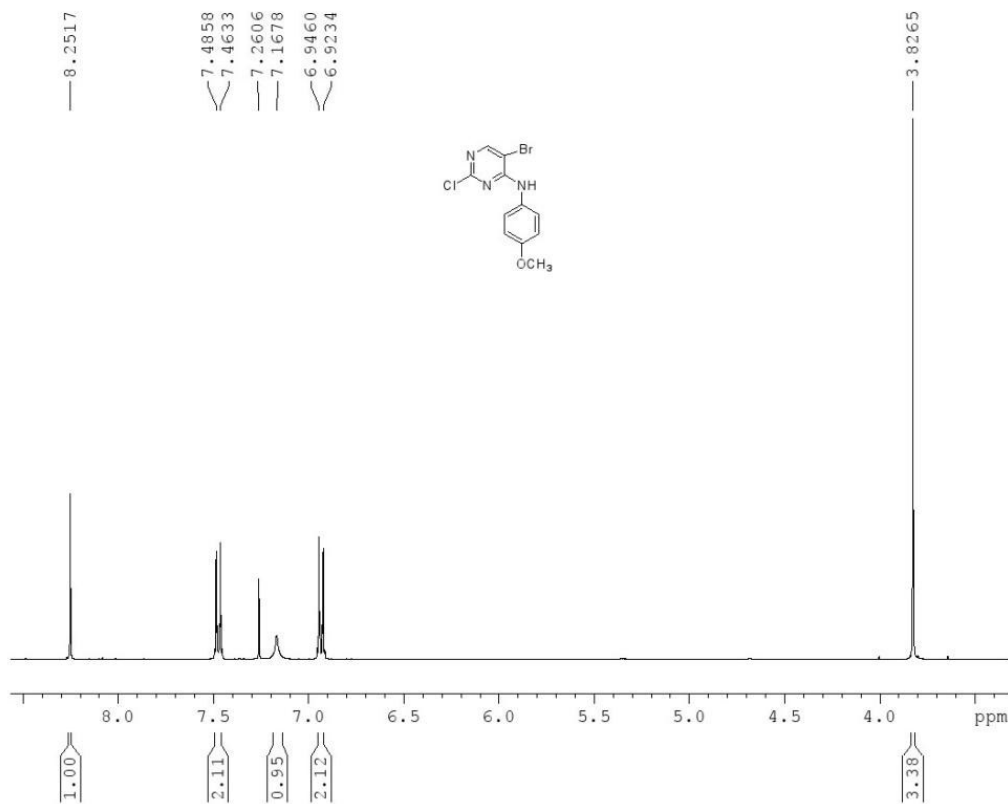
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Key Laboratory of Radiopharmaceuticals, Ministry of Education, College of Chemistry, Beijing  
Normal University, Beijing 100875, P. R. China.

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For H. Zhang: phone +86-10-58802012, E-mail [hbzhang@bnu.edu.cn](mailto:hbzhang@bnu.edu.cn).

<sup>1</sup>H NMR of 6a:



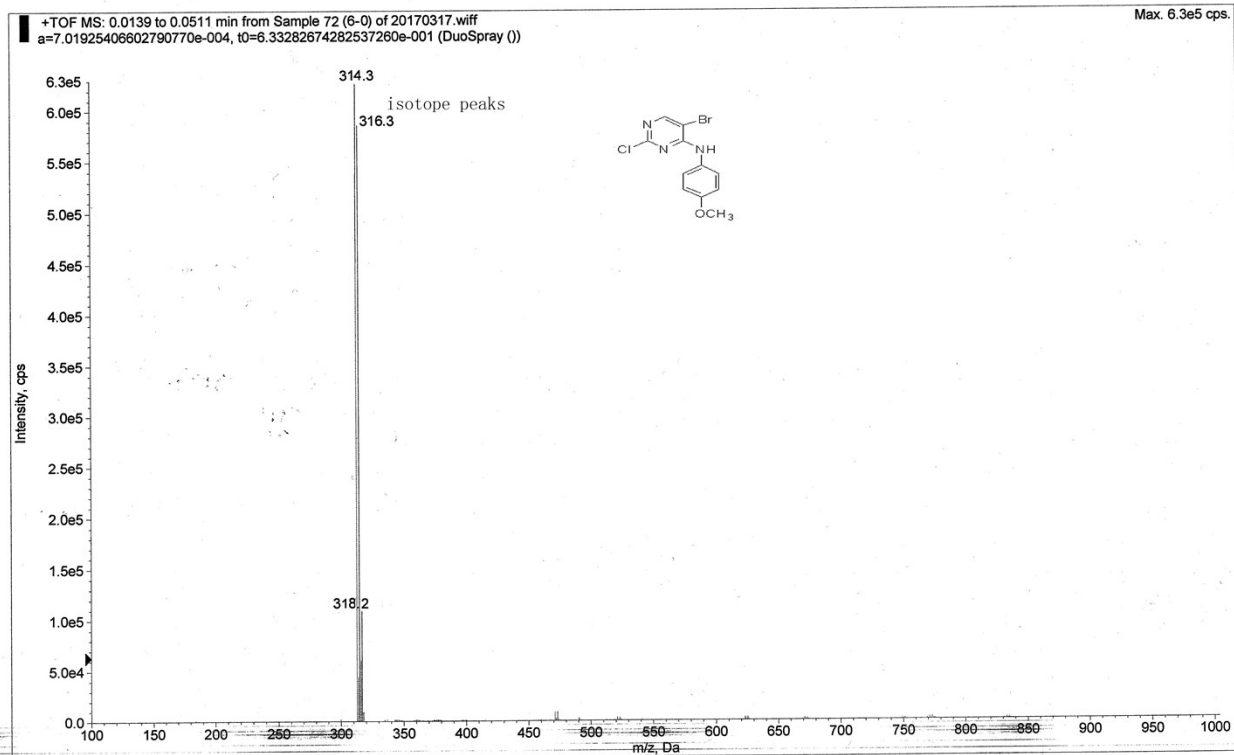
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PROCNO    1
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PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         22
DS         2
SWH        8222.605 Hz
FIDRES     0.125480 Hz
AQ         2.5286207 sec
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DE         6.50 usec
TE         300.0 K
D1         1.00000000 sec
TD0        1

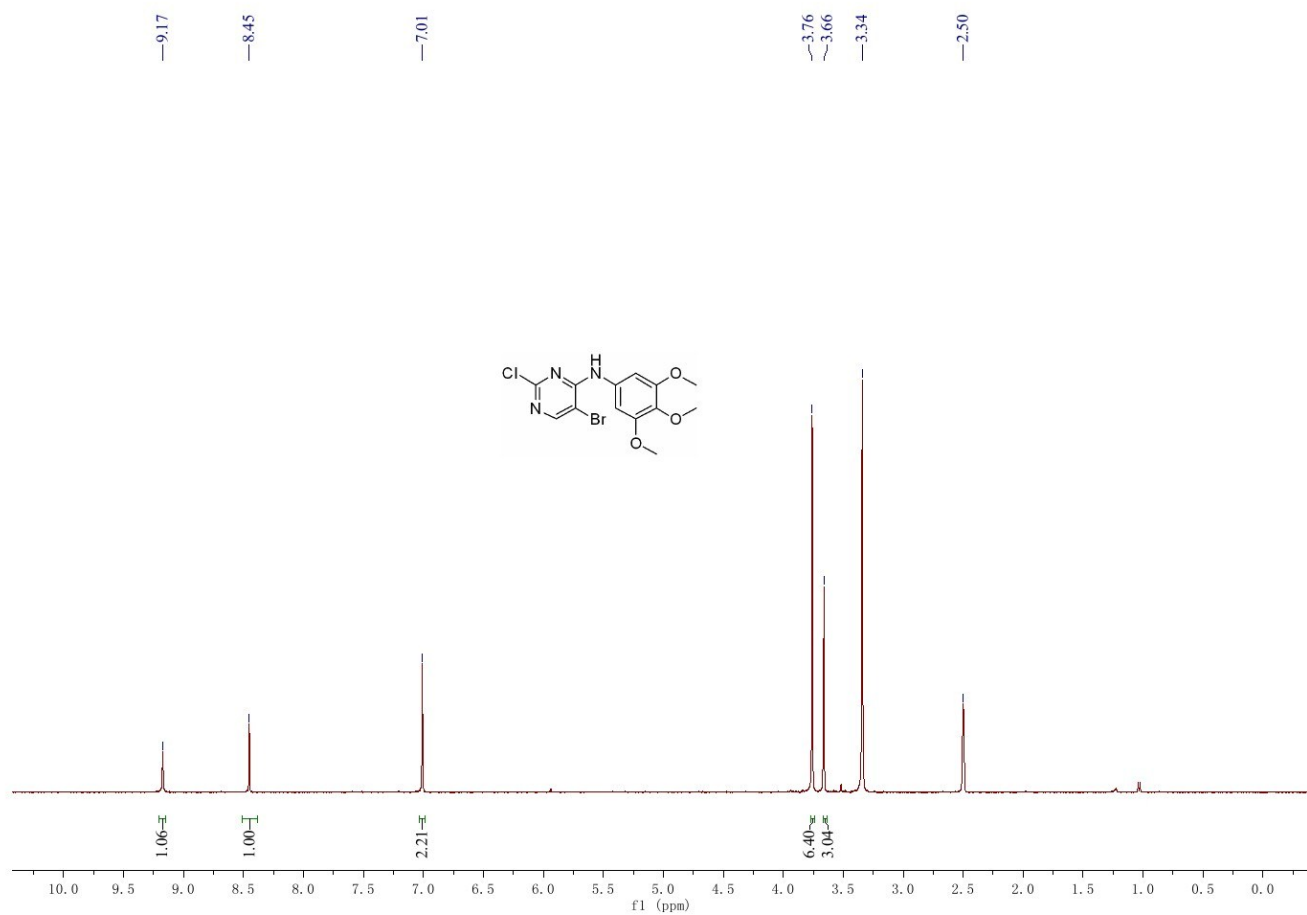
===== CHANNEL f1 =====
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P1         13.00 usec
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PL1W       1.00 dB
PL1W       13.18669786 W
SFO1       400.174412 MHz
SI         32768
SF         400.17000220 MHz
WDW        EM
SSB        0
LB         0.20 Hz
GB         0
PC         1.00
    
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# ESI-MS of 6a:

Acq. File: 20170317.wiff

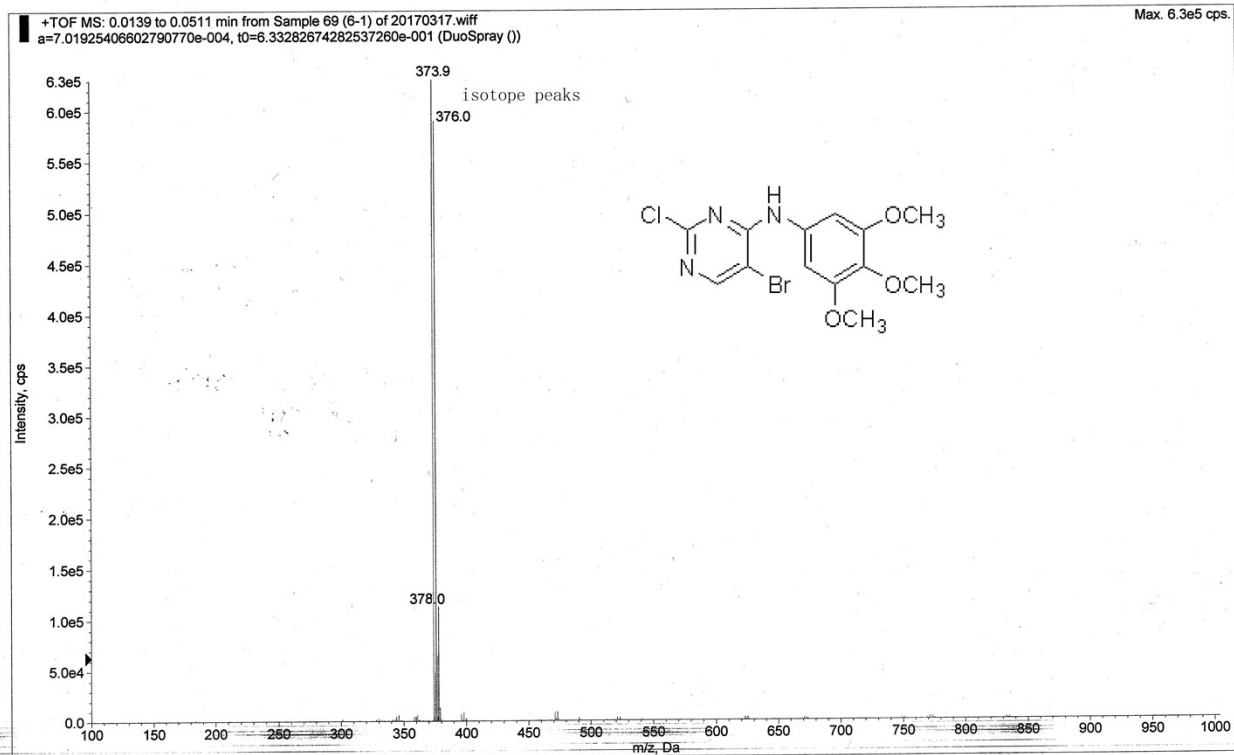


<sup>1</sup>H NMR of 6b:

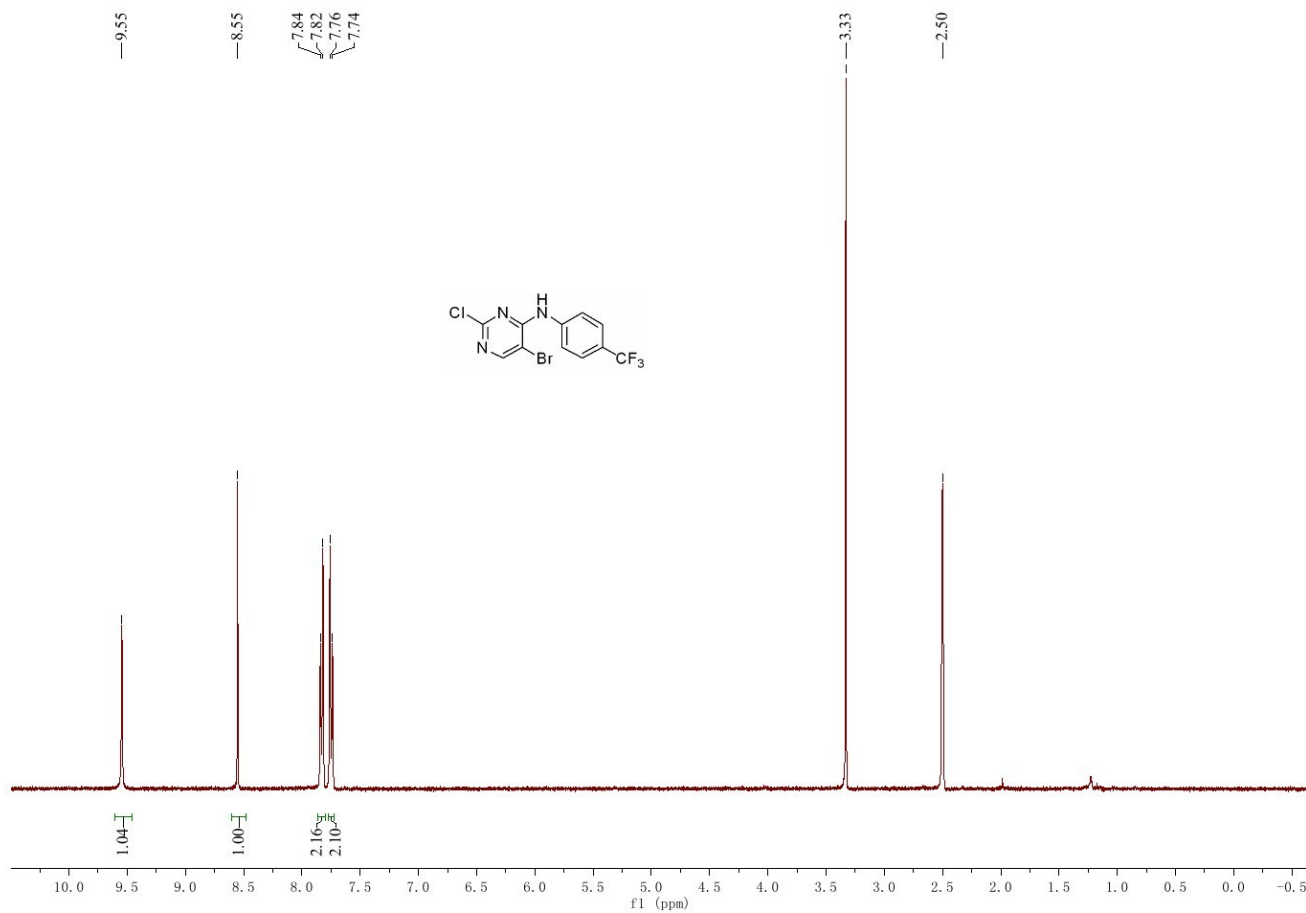


# ESI-MS of 6b:

Acq. File: 20170317.wiff

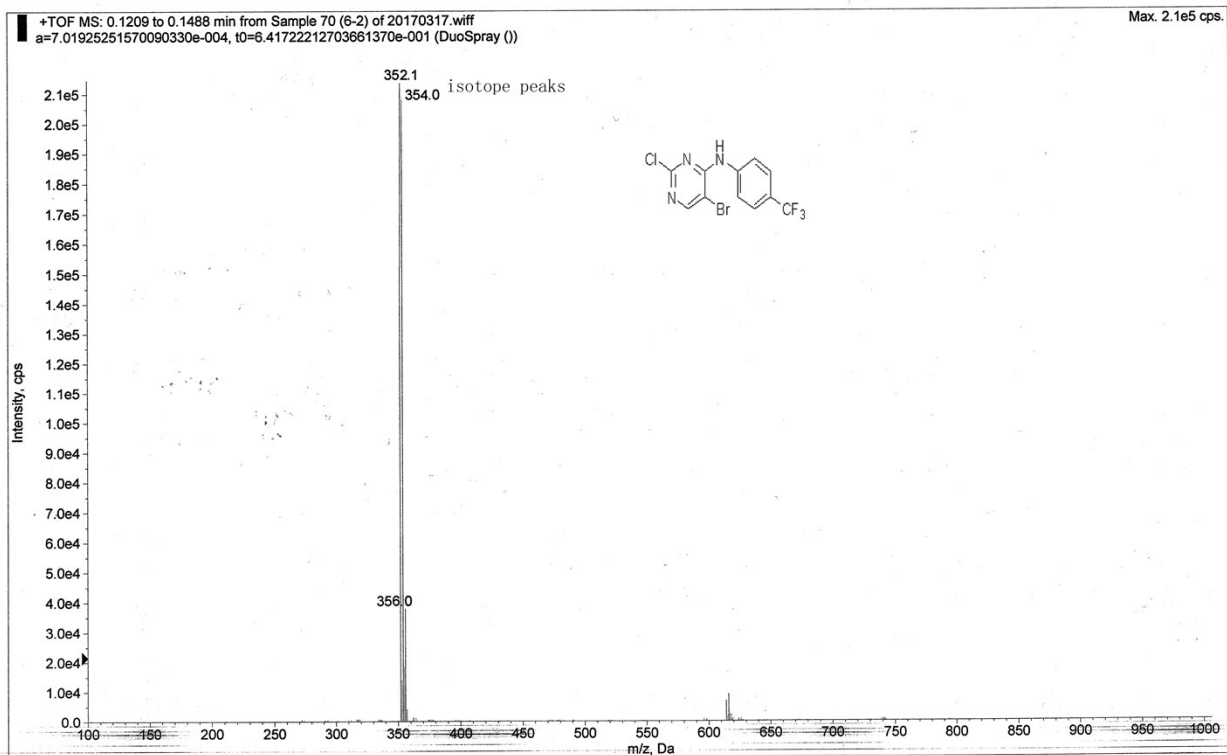


<sup>1</sup>H NMR of 6c:

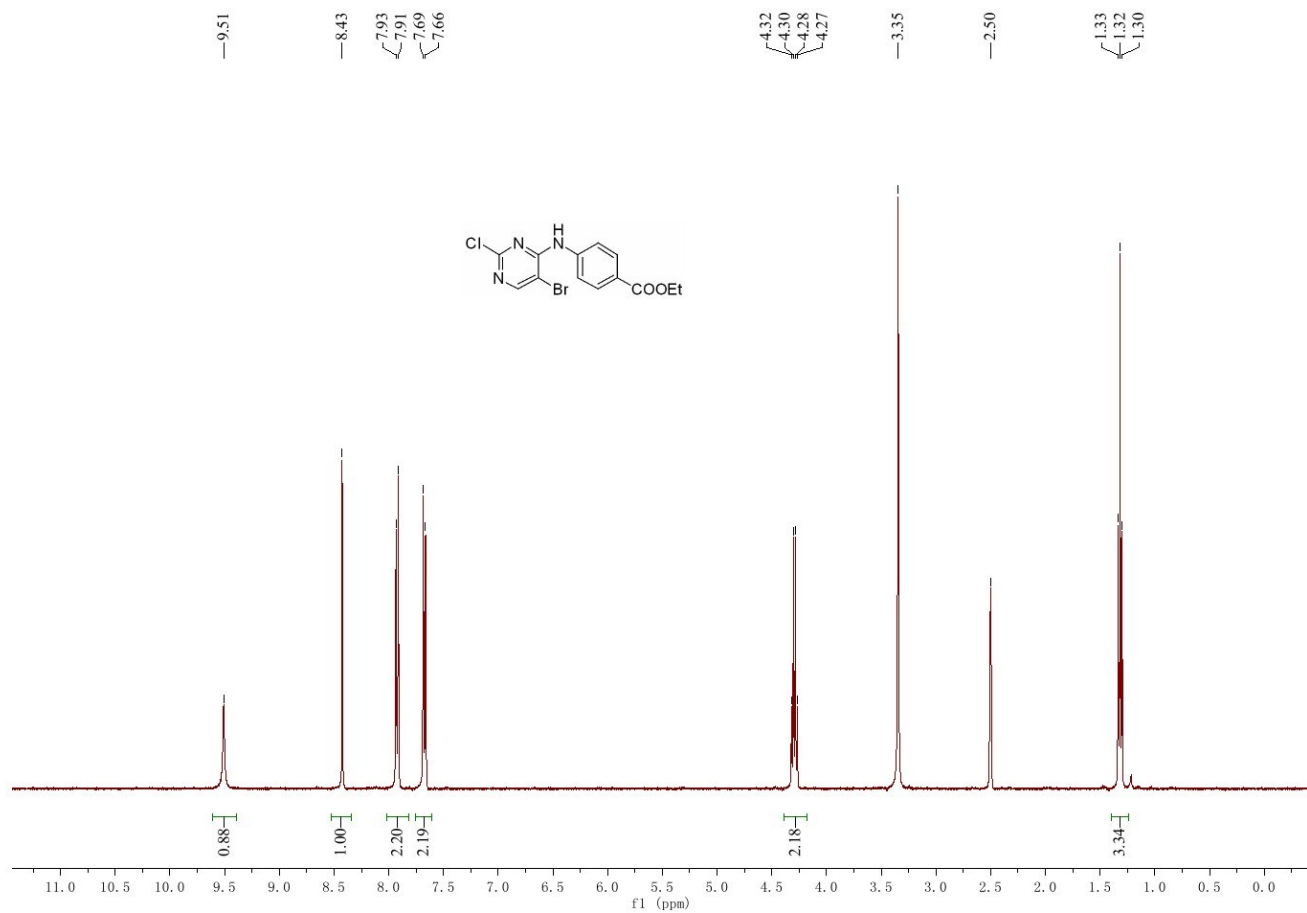


# ESI-MS of 6c:

Acq. File: 20170317.wiff



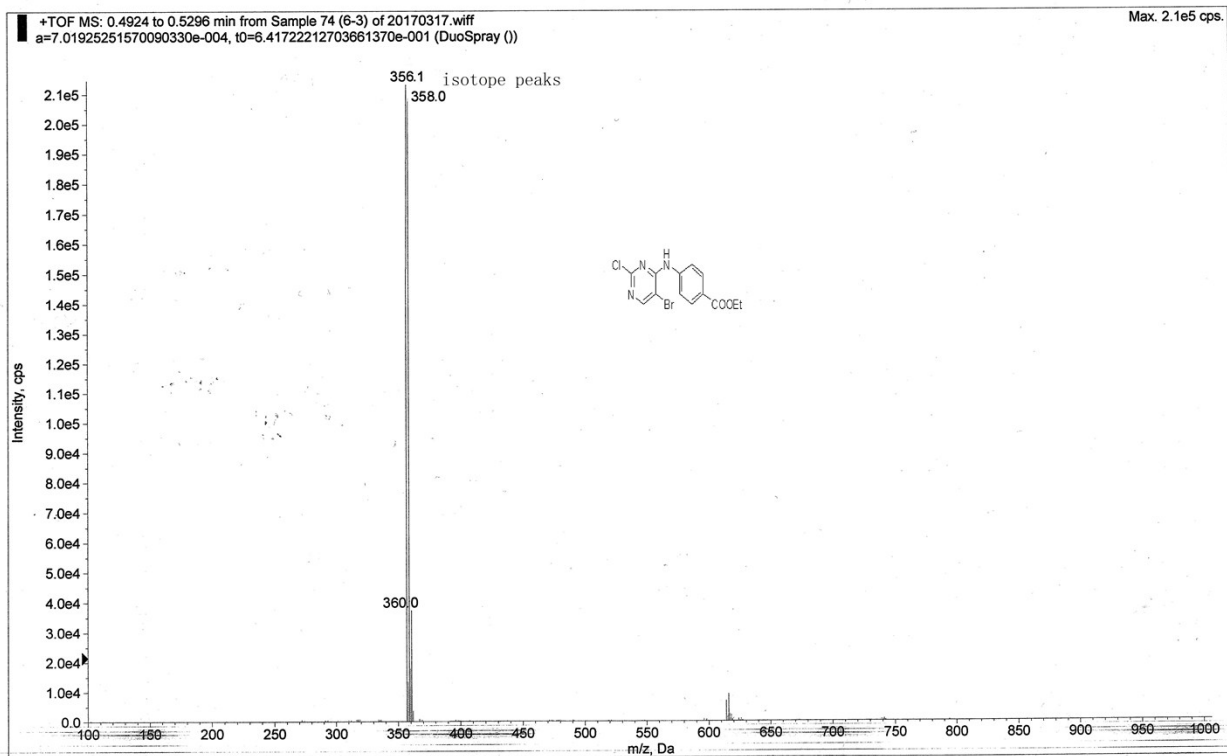
<sup>1</sup>H NMR of 6d:



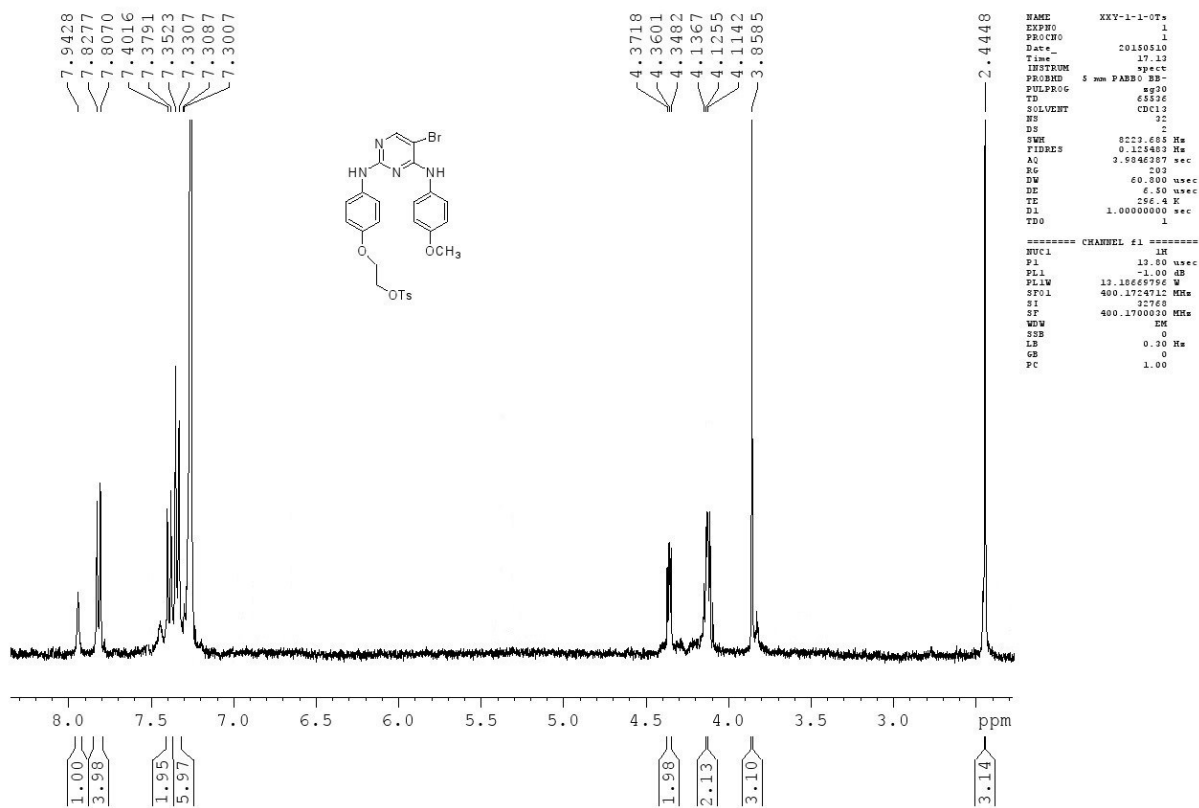


# ESI-MS of 6d:

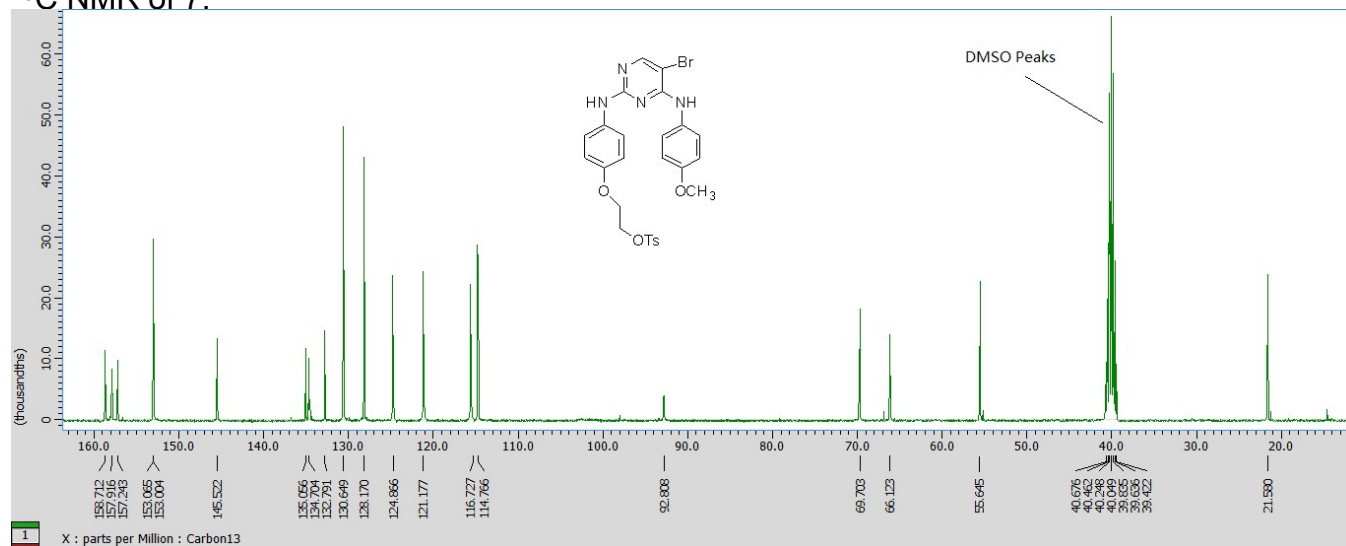
Acq. File: 20170317.wiff



<sup>1</sup>H NMR of 7:

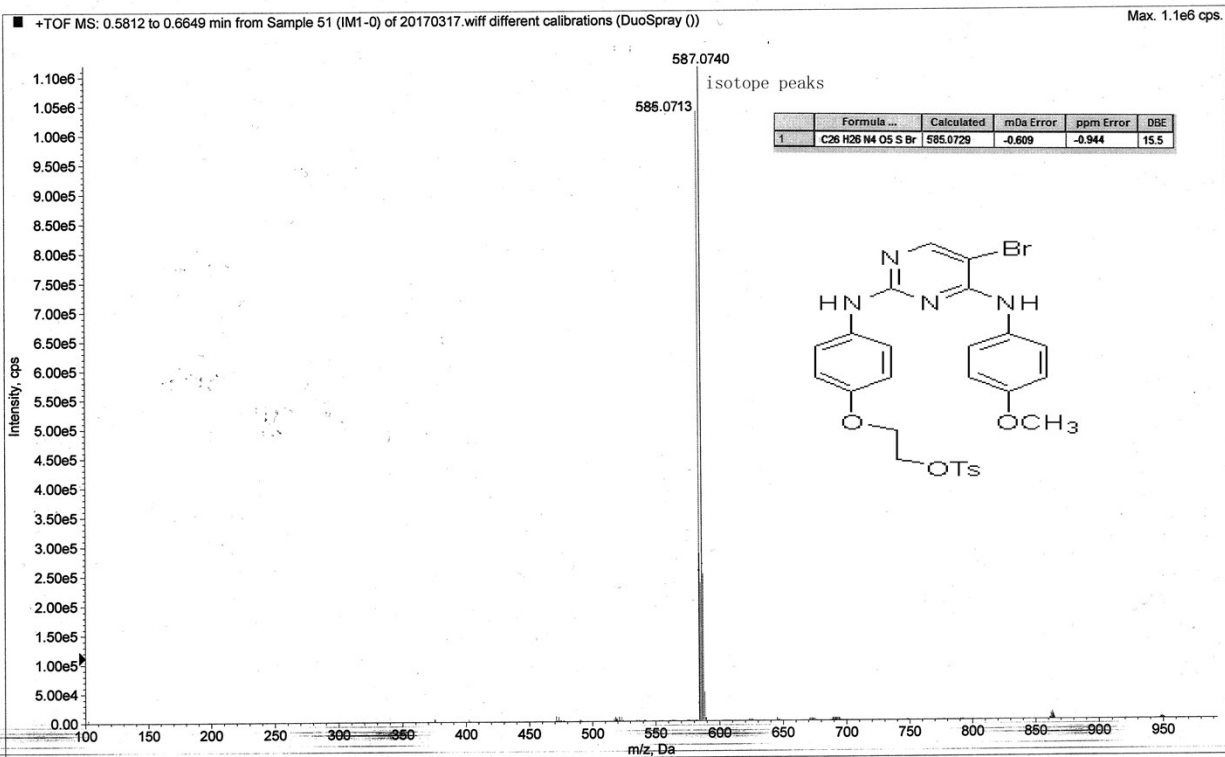


# <sup>13</sup>C NMR of 7:

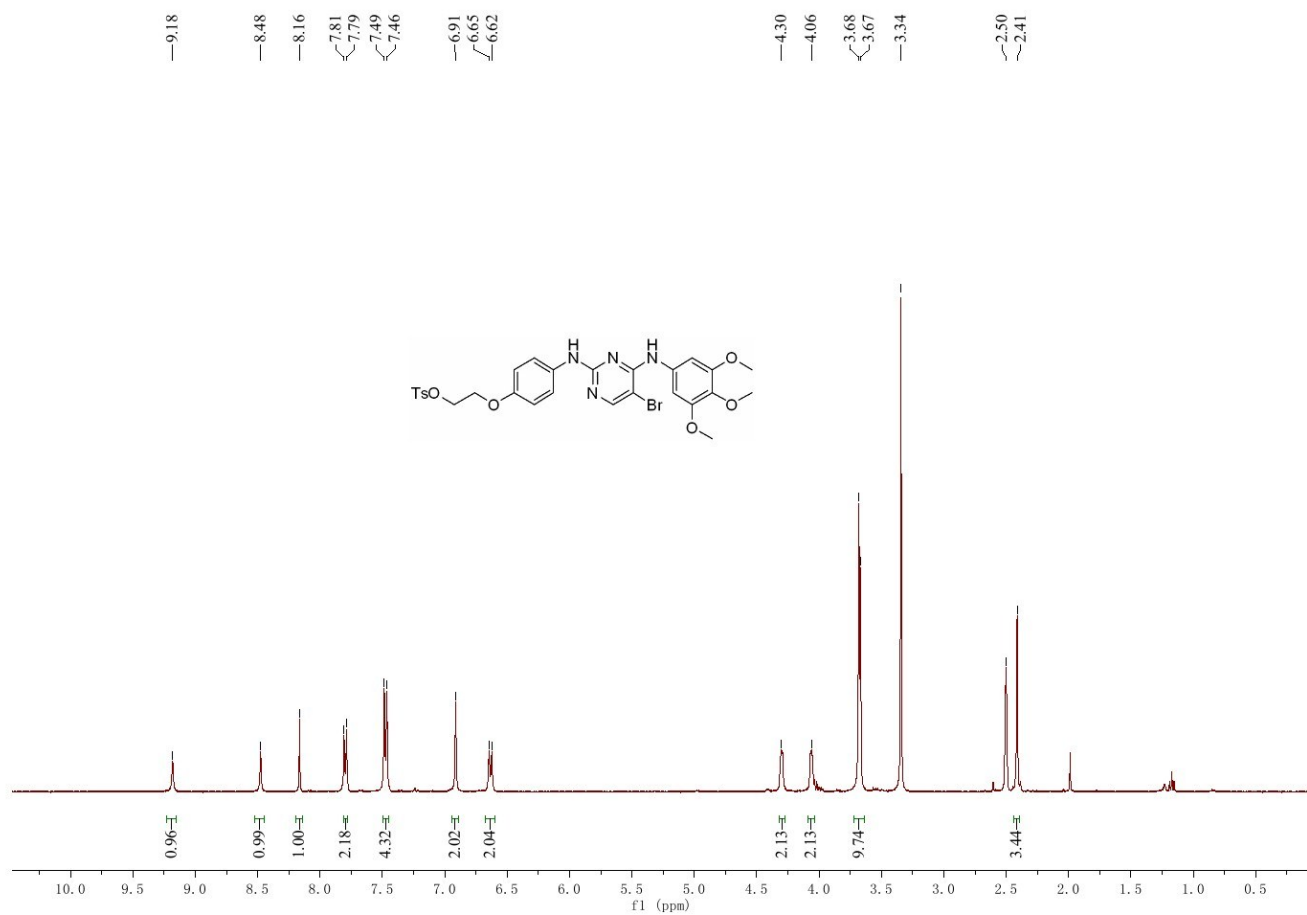


# HRMS (ESI) of 7:

Acq. File: 20170317.wiff



# <sup>1</sup>H NMR of 18a:



—9.18

—8.48

—8.16

~7.81

~7.79

~7.49

~7.46

—6.91

~6.65

~6.62

—4.30

—4.06

~3.68

~3.67

—3.34

~2.50

~2.41

0.96

0.99

1.00

2.18

4.32

2.02

2.04

2.13

2.13

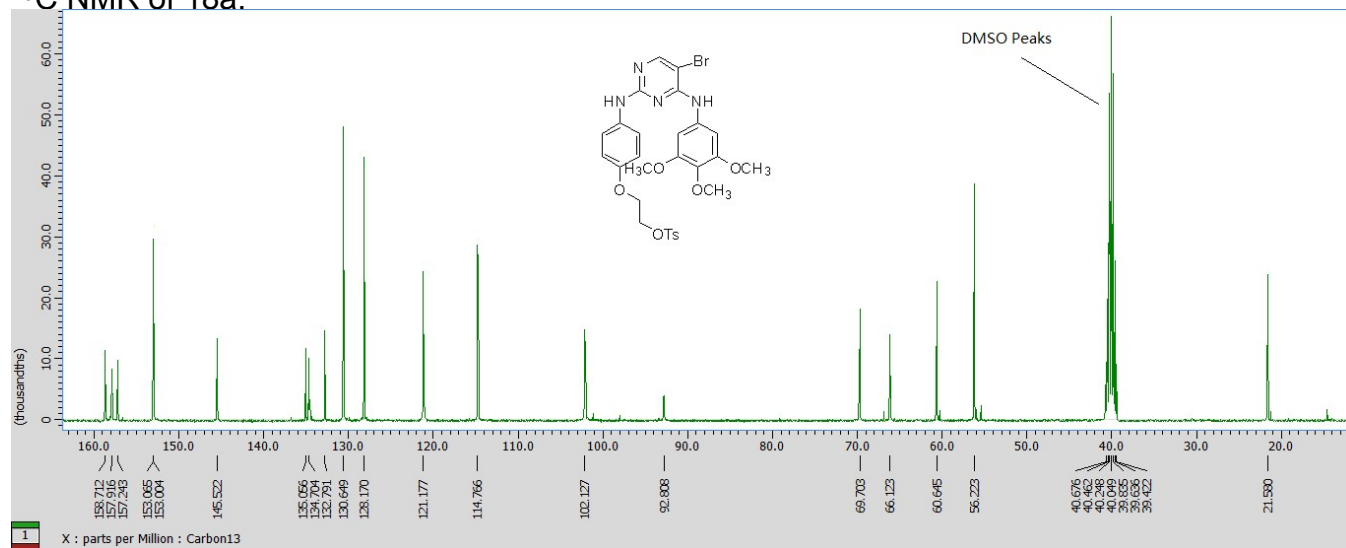
9.74

3.44

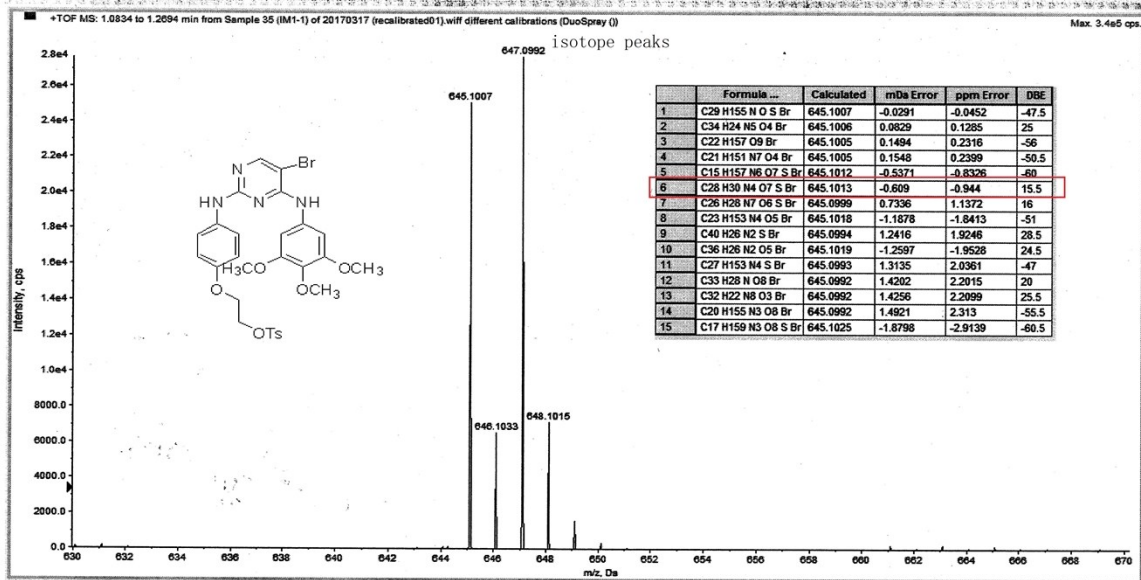
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

f1 (ppm)

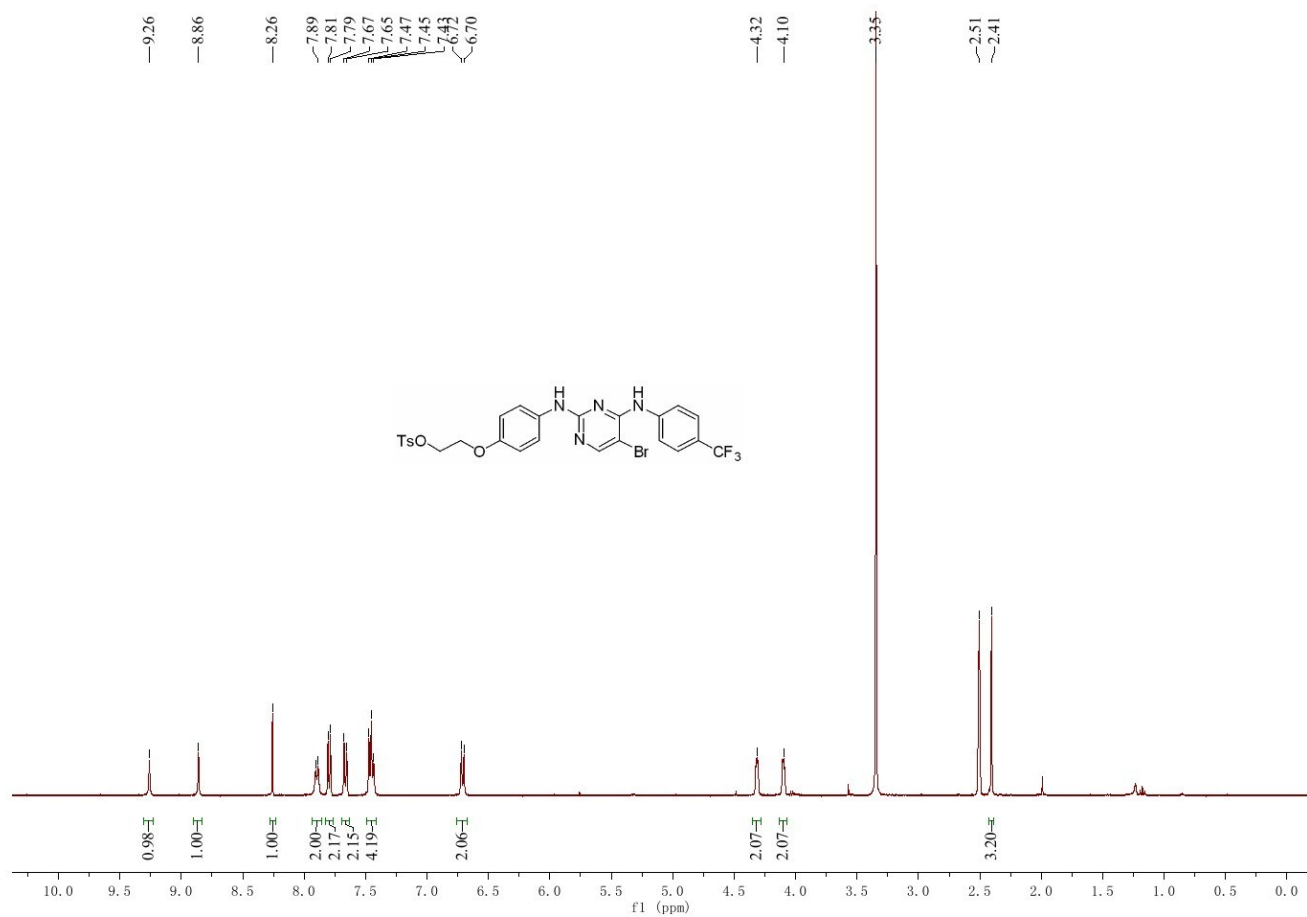
# <sup>13</sup>C NMR of 18a:



# HRMS (ESI) of 18a:

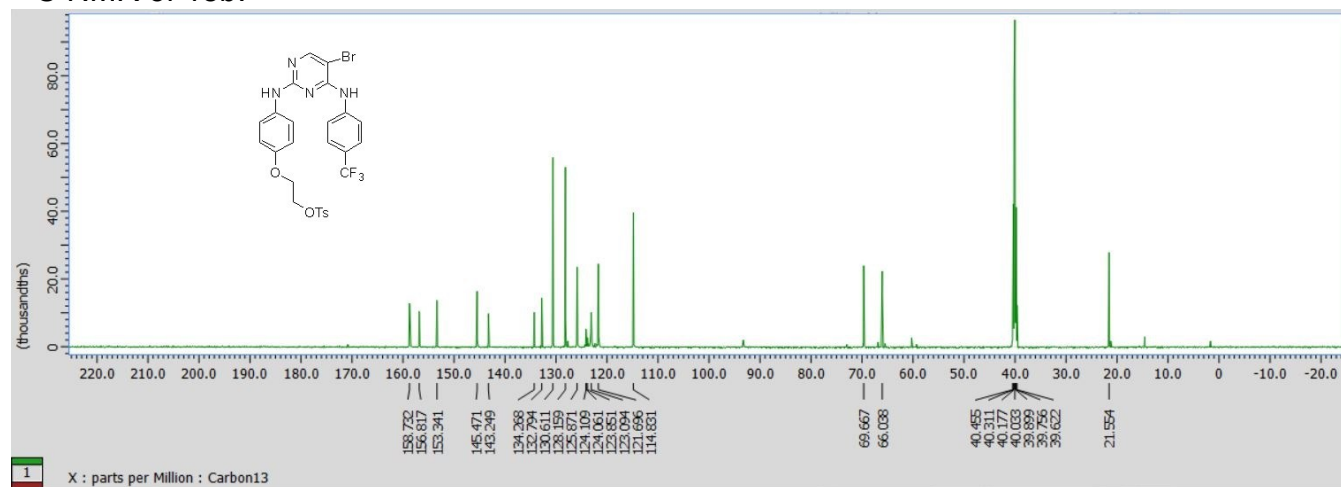


<sup>1</sup>H NMR of 18b:

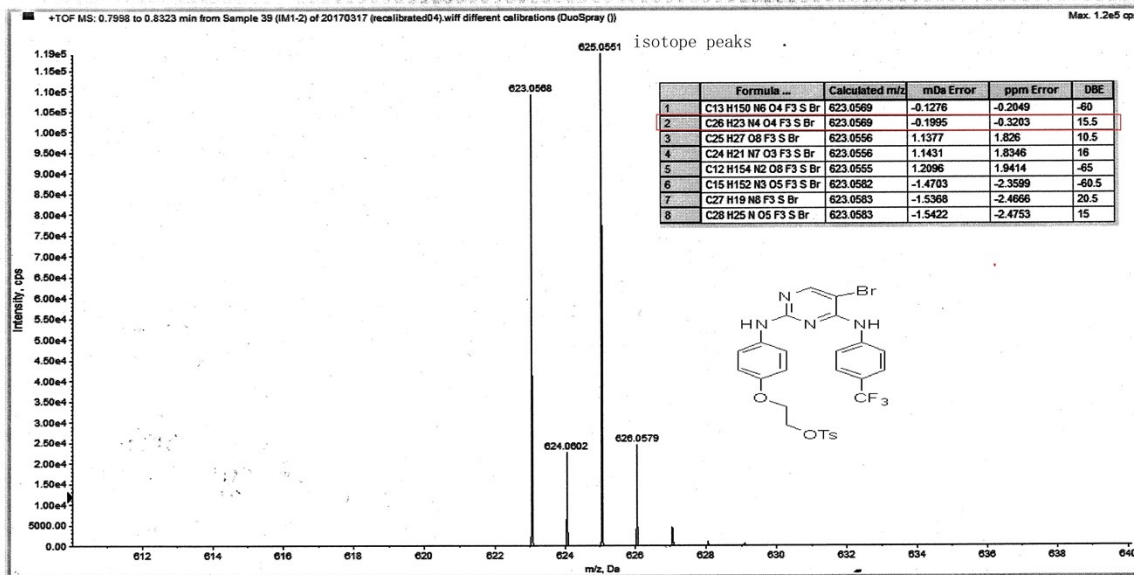




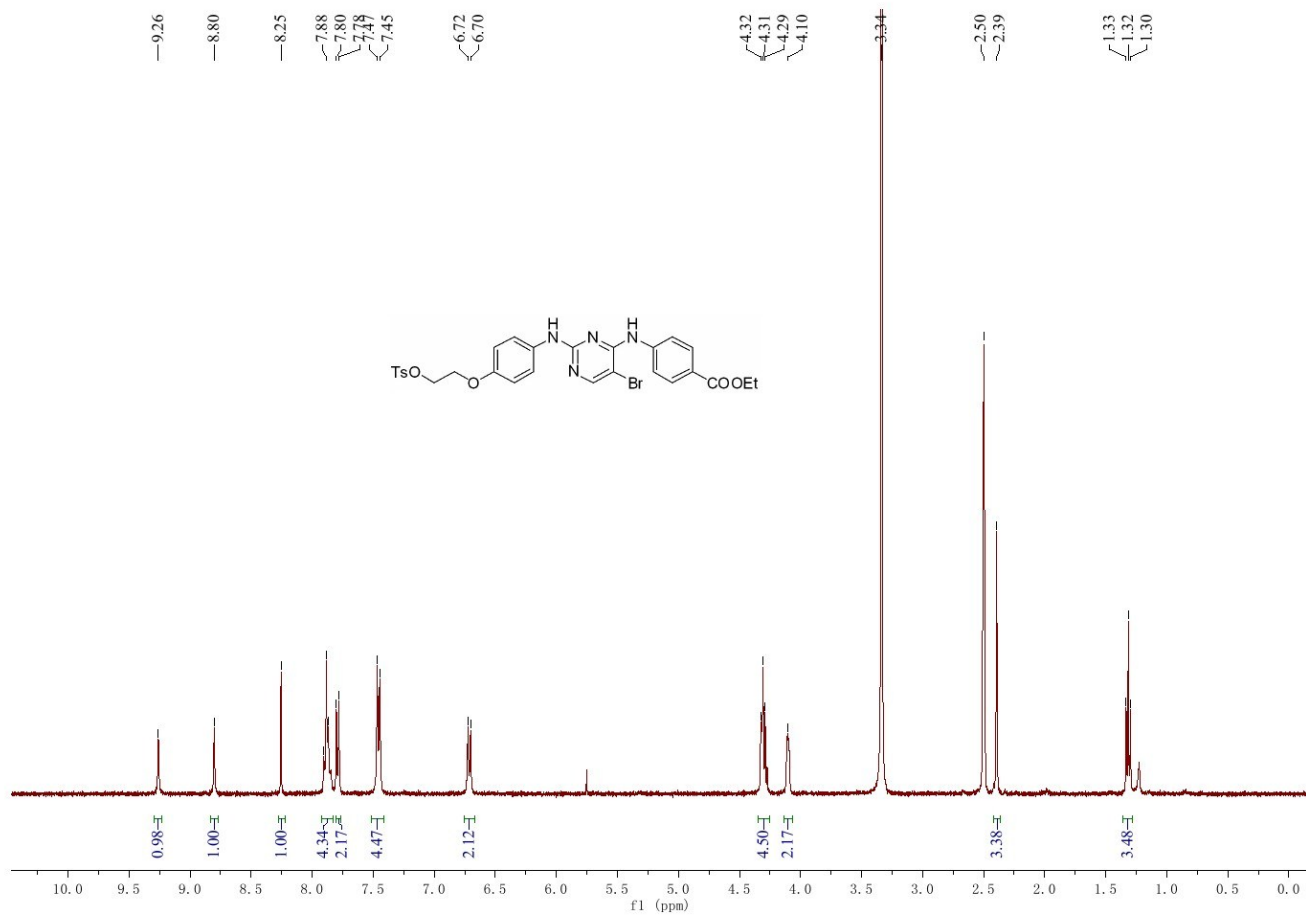
# <sup>13</sup>C NMR of 18b:



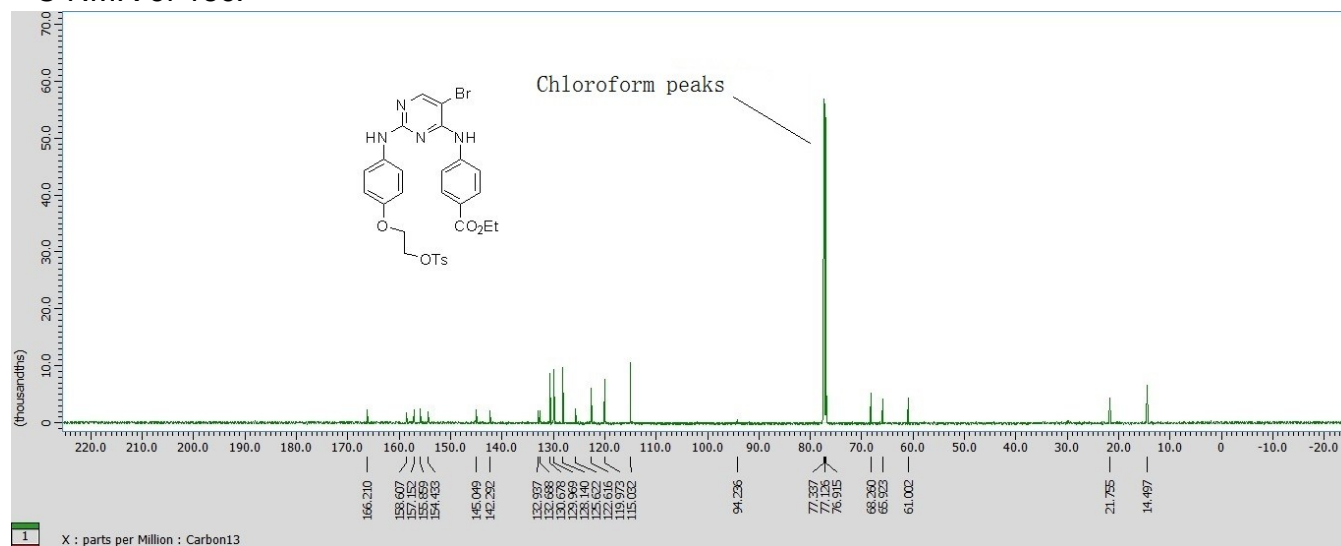
HRMS (ESI) of 18b:



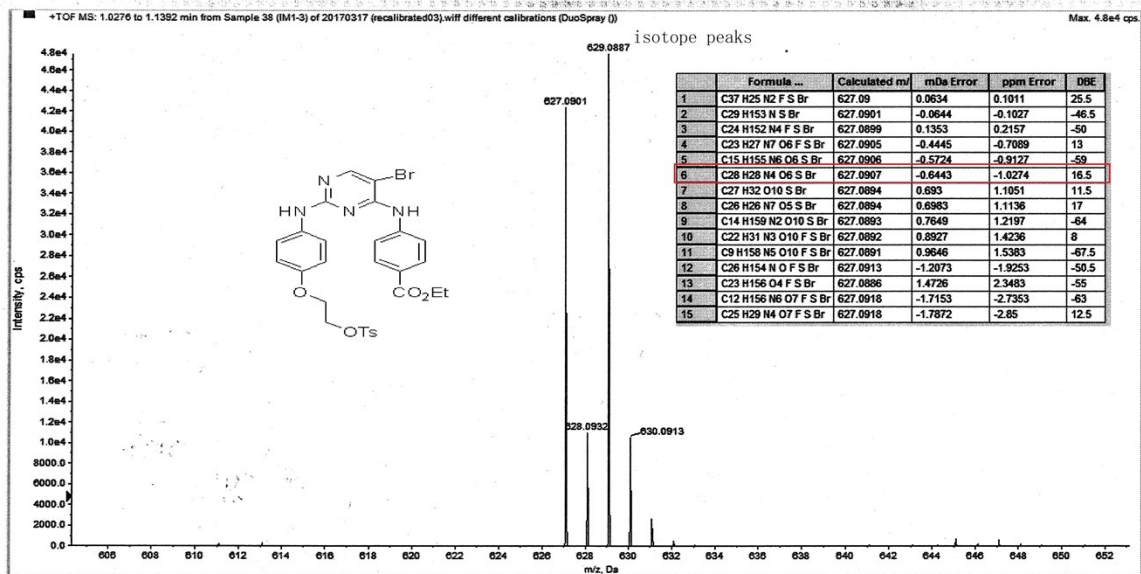
<sup>1</sup>H NMR of 18c:



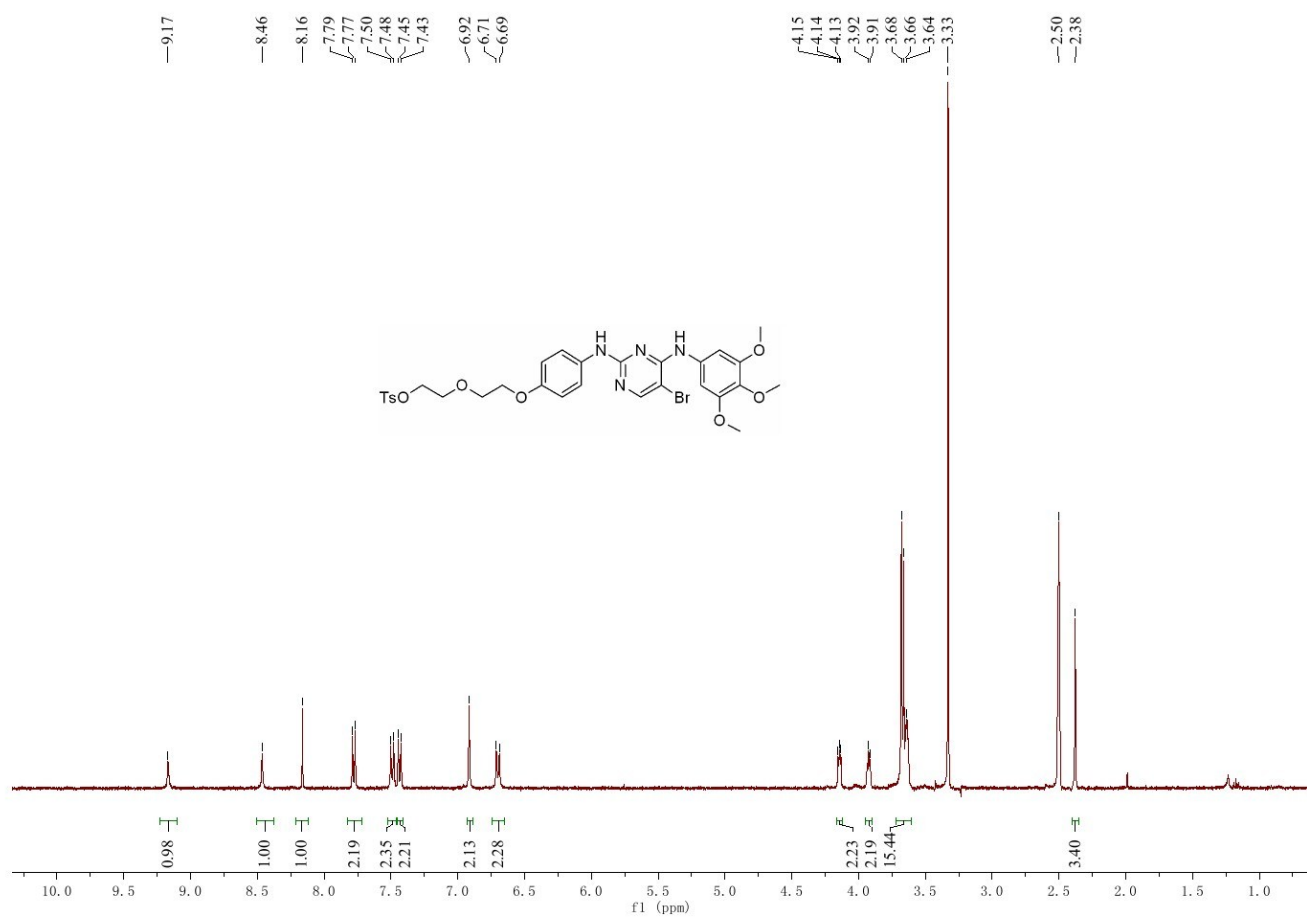
# <sup>13</sup>C NMR of 18c:



# HRMS (ESI) of 18c:



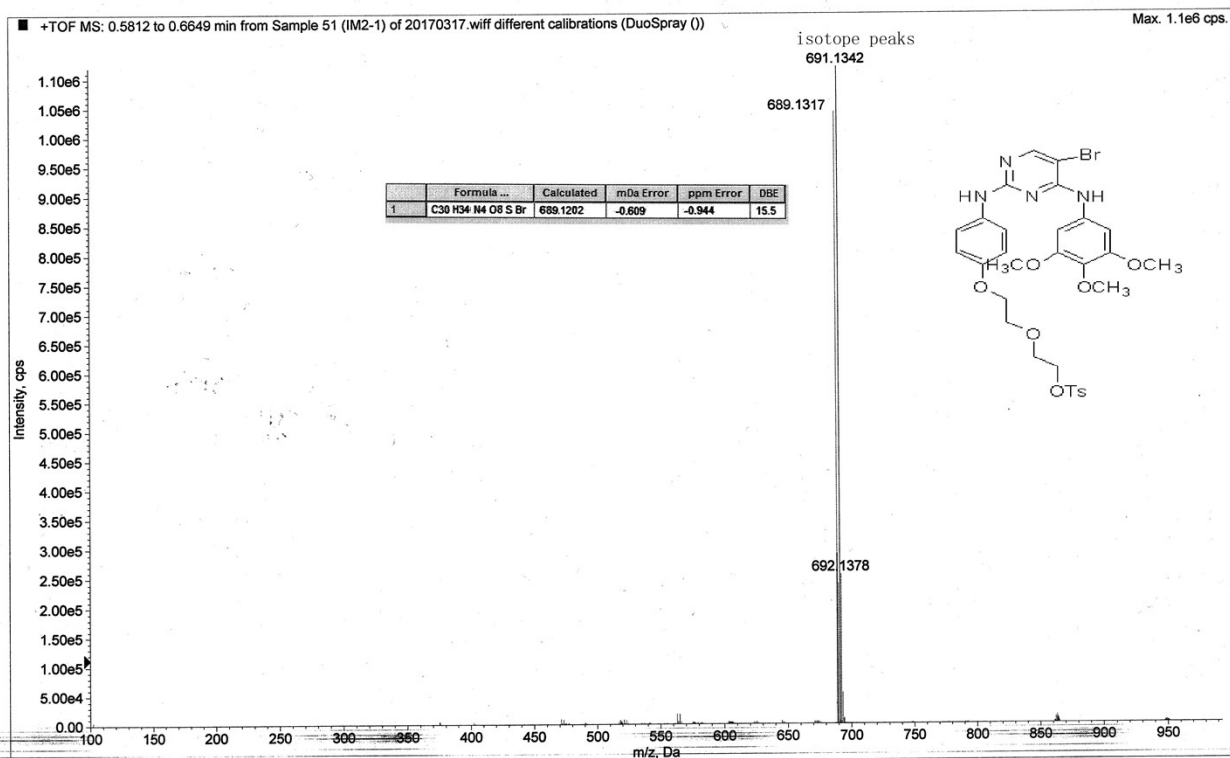
<sup>1</sup>H NMR of 18d:





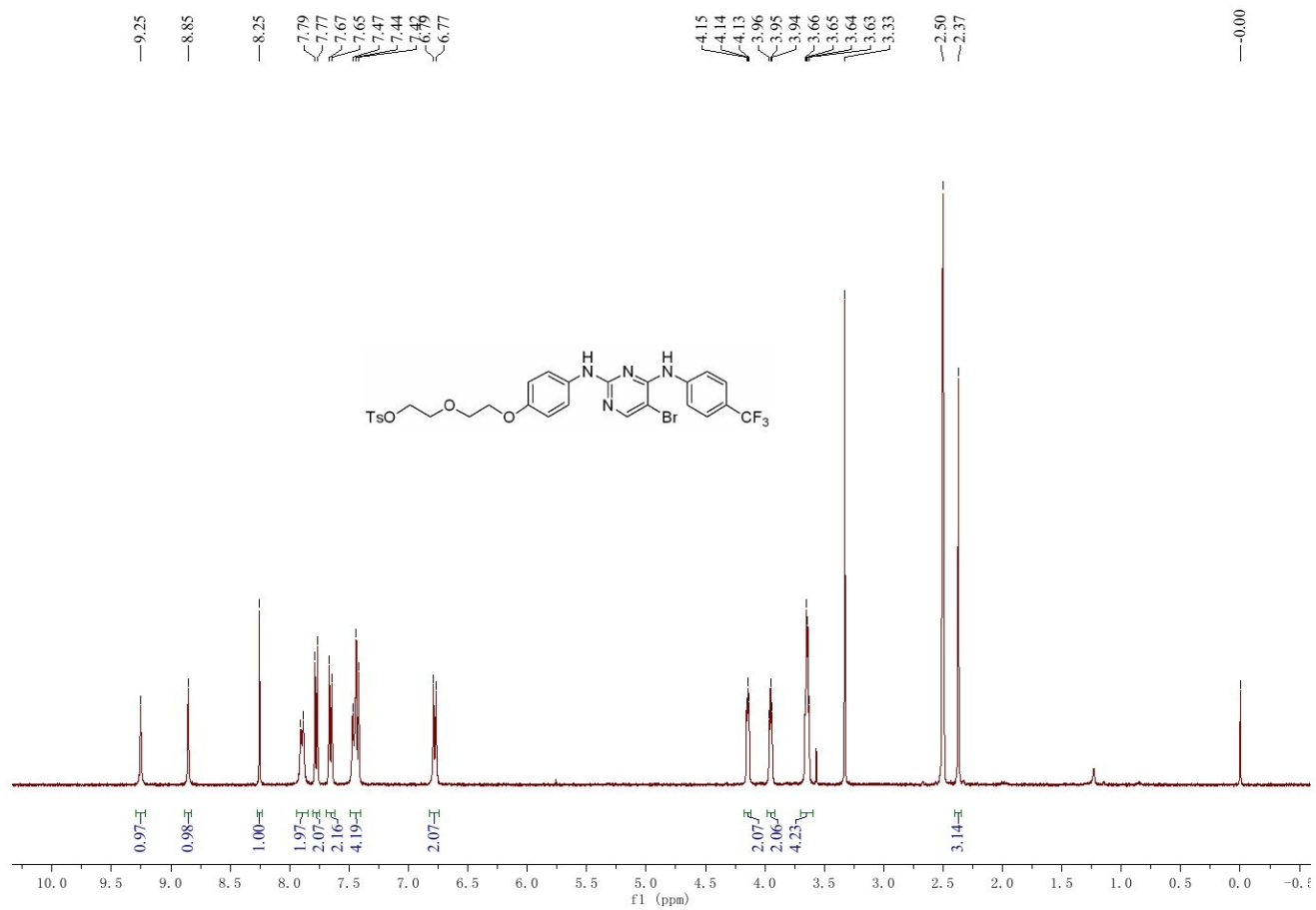
# HRMS (ESI) of 18d:

Acq. File: 20170317.wiff

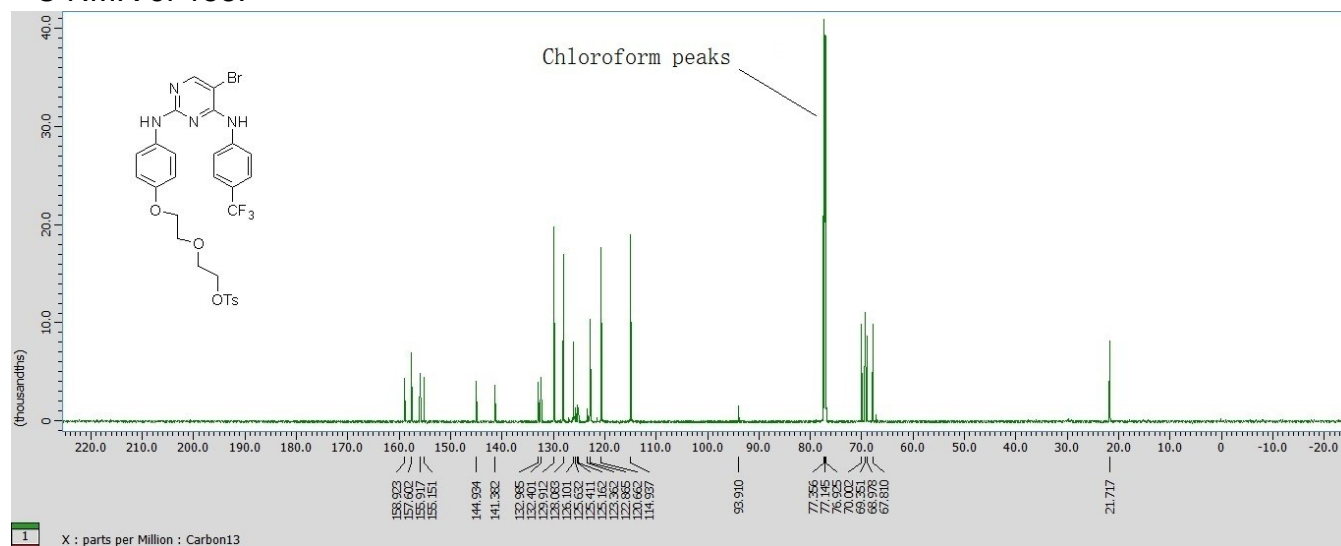




<sup>1</sup>H NMR of 18e:

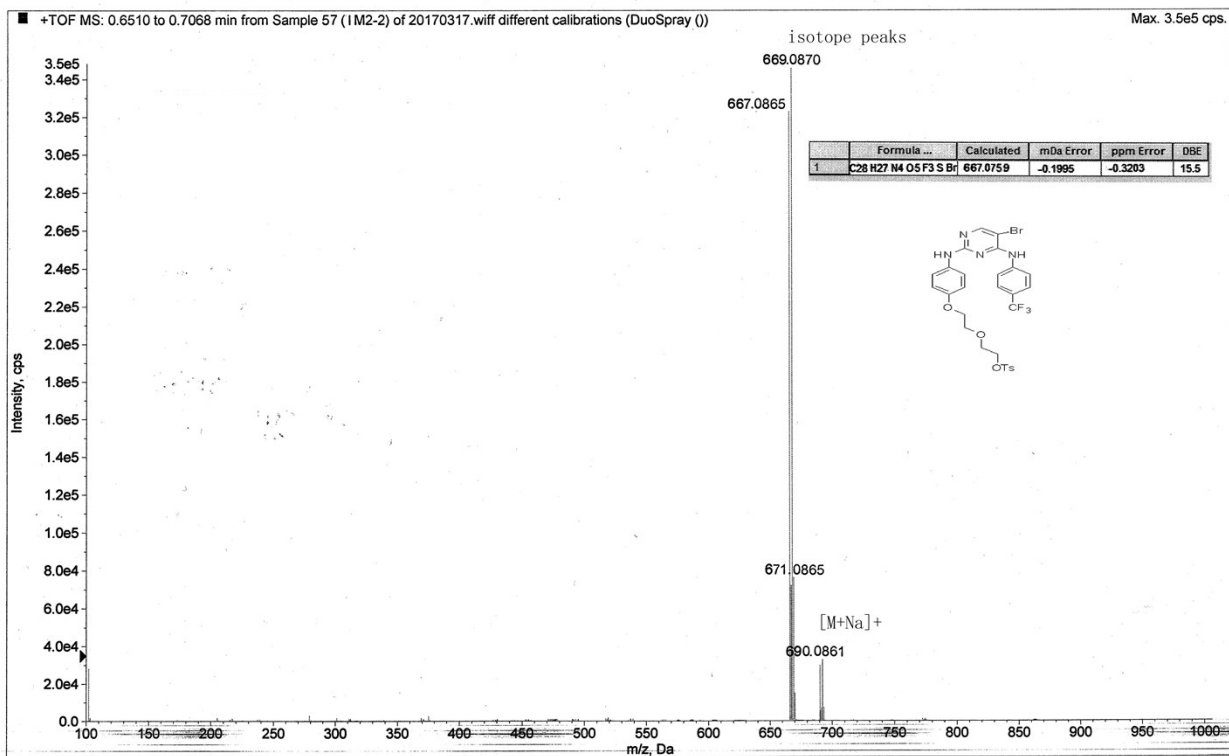


# <sup>13</sup>C NMR of 18e:



# HRMS (ESI) of 18e:

Acq. File: 20170317.wiff



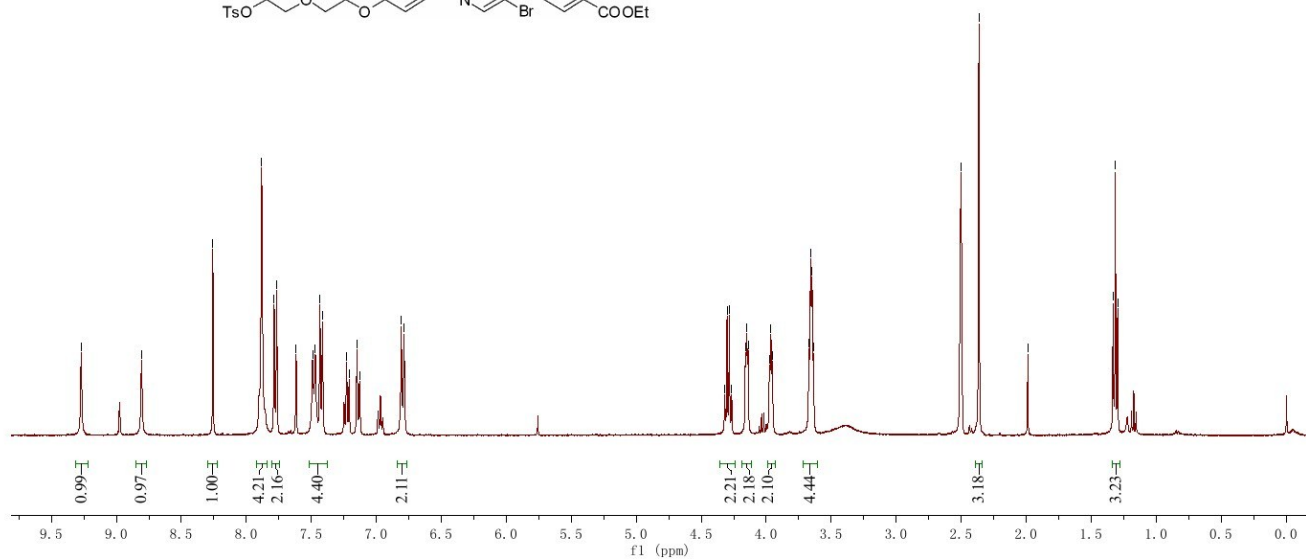
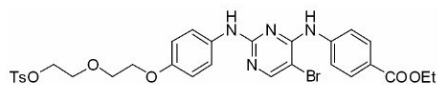
<sup>1</sup>H NMR of 18f:

—9.27  
—8.81  
—8.26  
7.88  
7.79  
7.77  
7.62  
7.47  
7.43  
7.41  
7.15  
6.81  
6.79

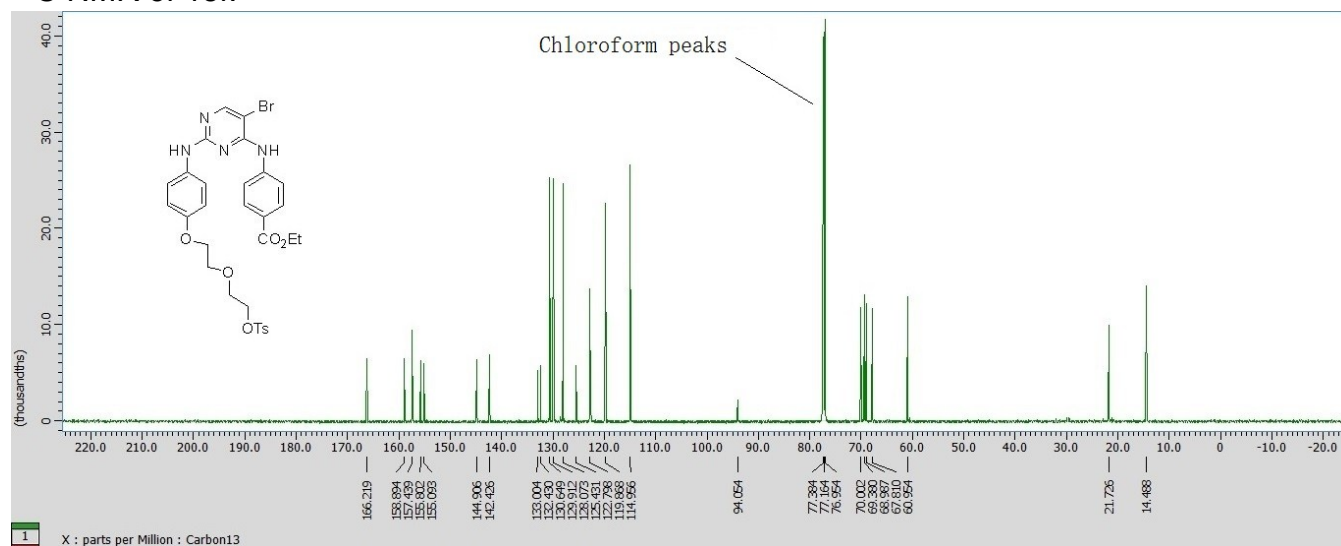
4.32  
4.30  
4.28  
4.27  
4.16  
4.15  
4.14  
3.97  
3.96  
3.95  
3.67  
3.66  
3.65  
3.64

—2.50  
—2.36  
—1.99

1.33  
1.31  
1.30

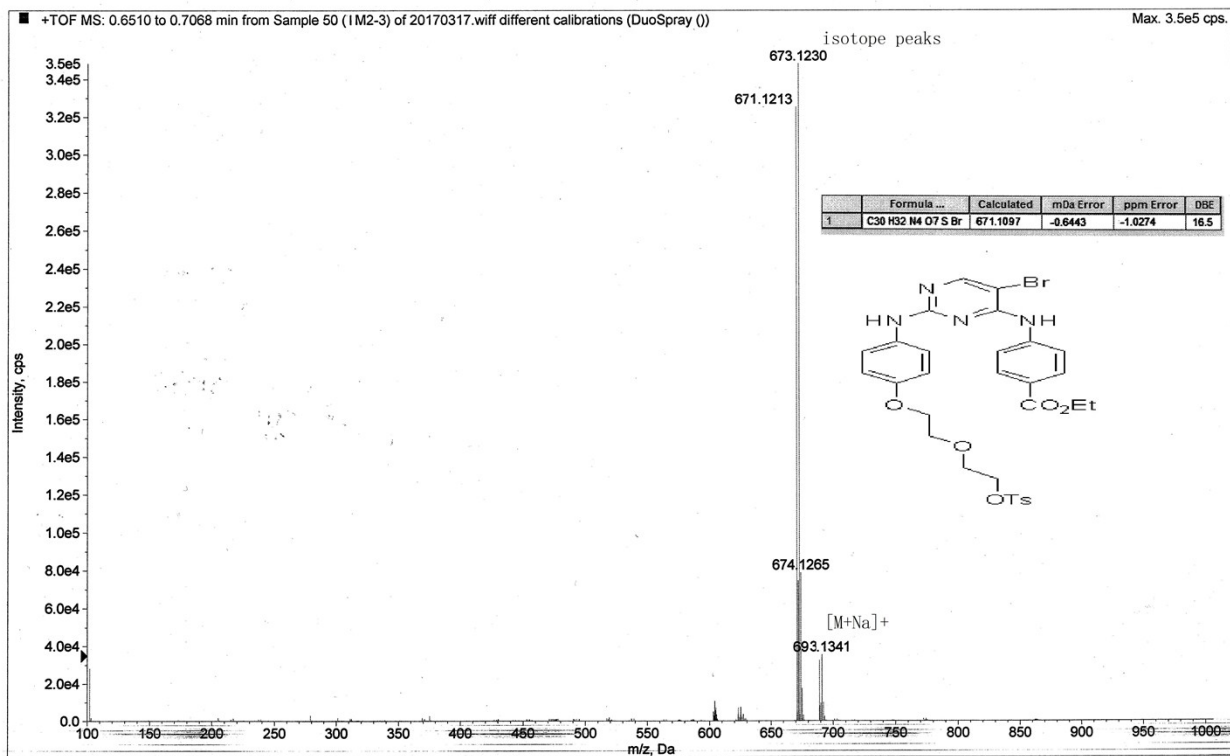


# <sup>13</sup>C NMR of 18f:

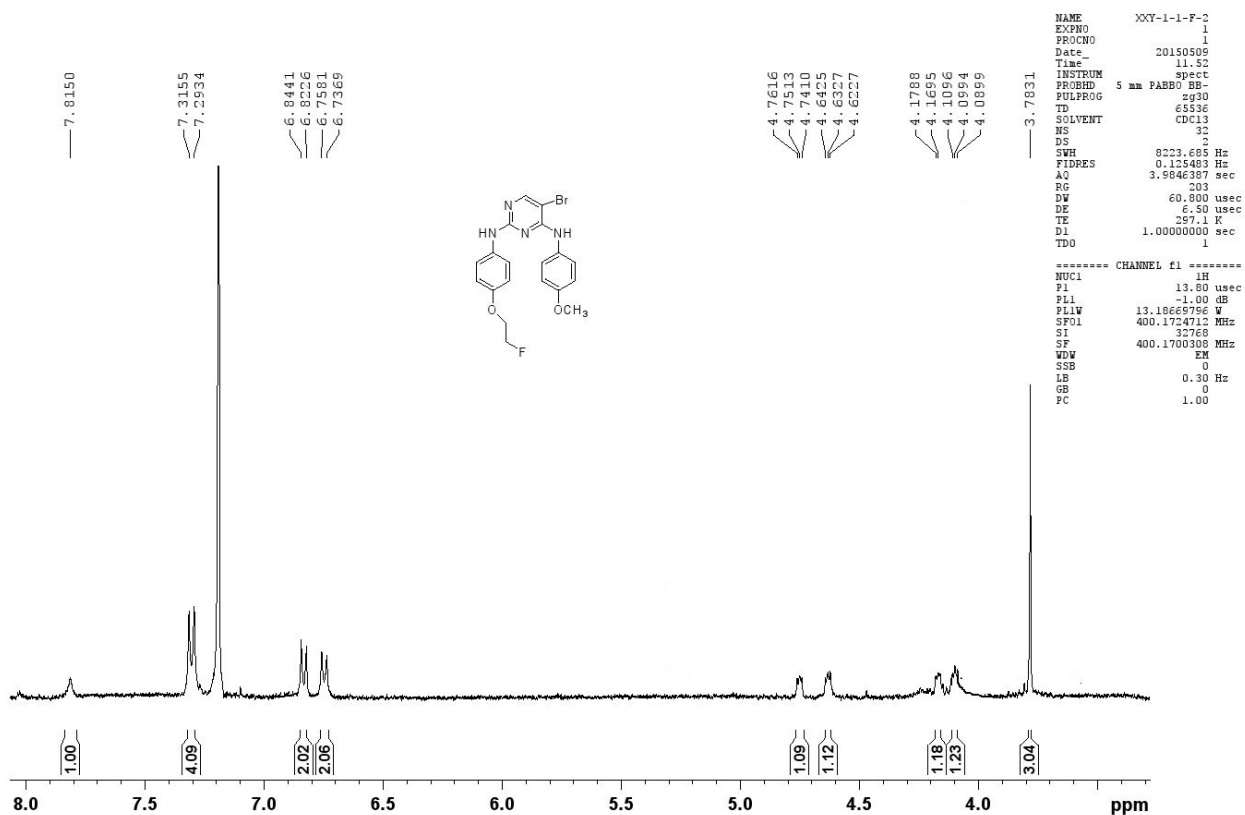


# HRMS (ESI) of 18f:

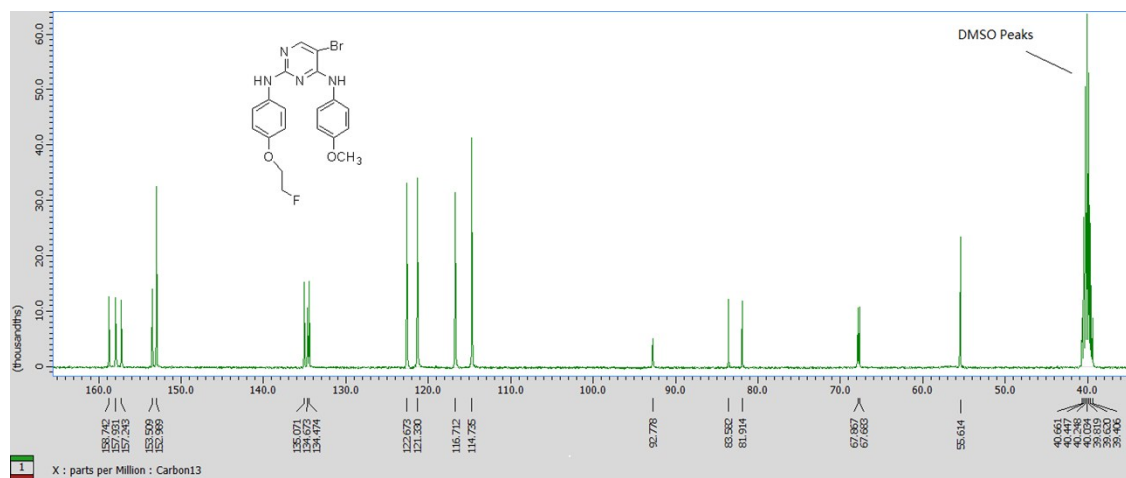
Acq. File: 20170317.wiff



<sup>1</sup>H NMR of 8a:

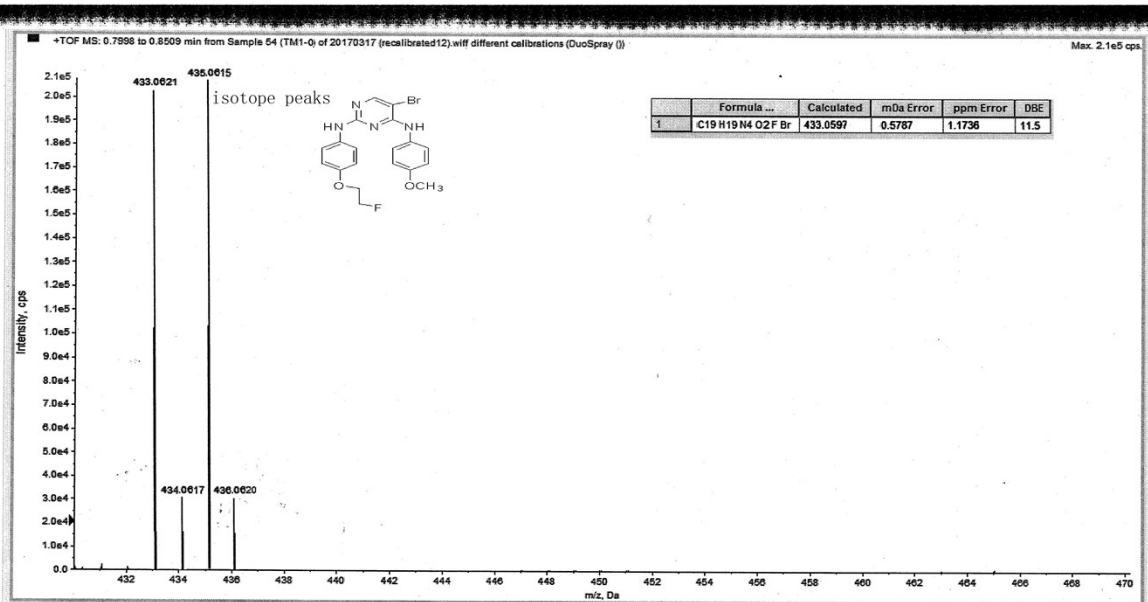


# <sup>13</sup>C NMR of 8a:

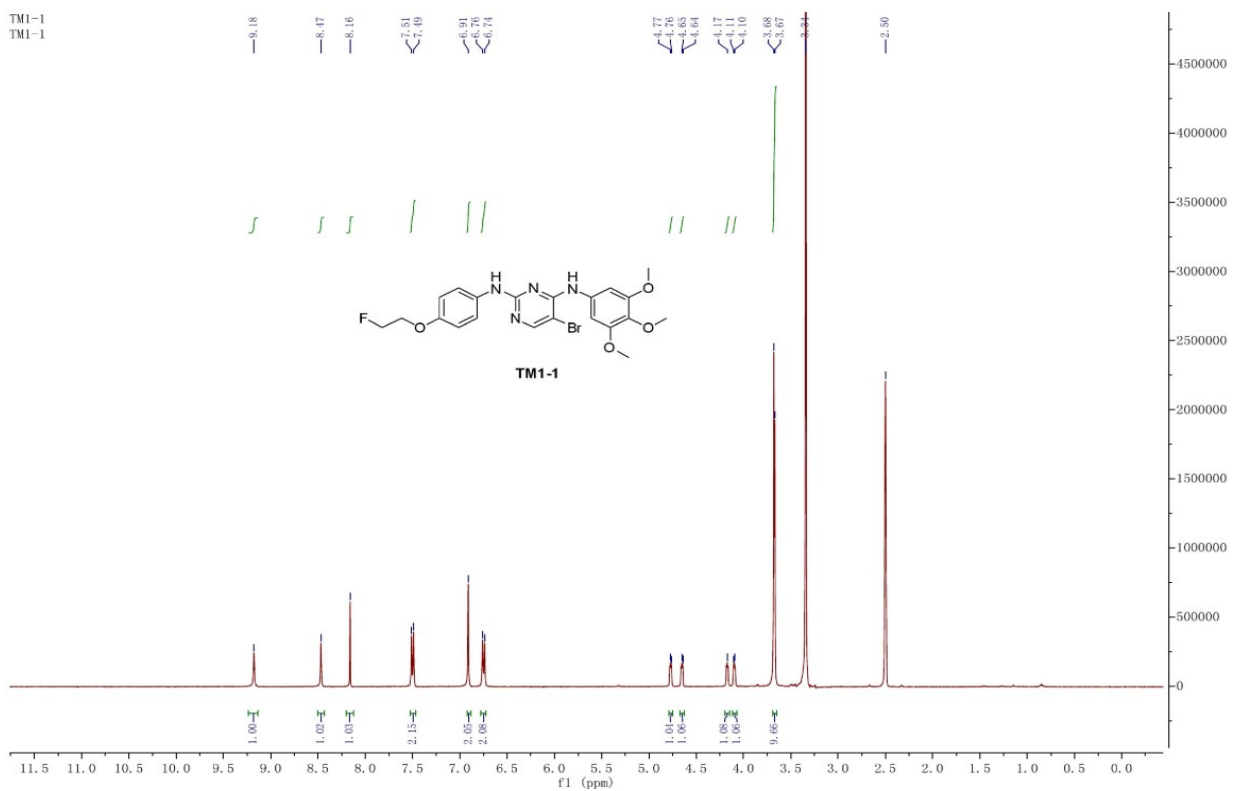




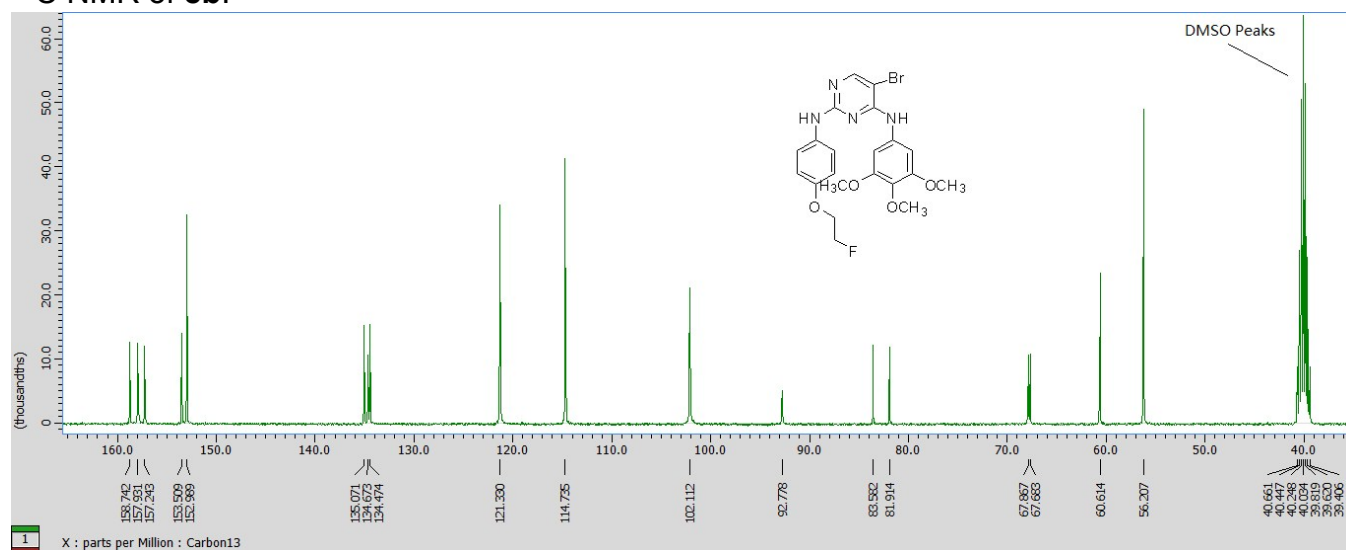
# HRMS (ESI) of 8a:



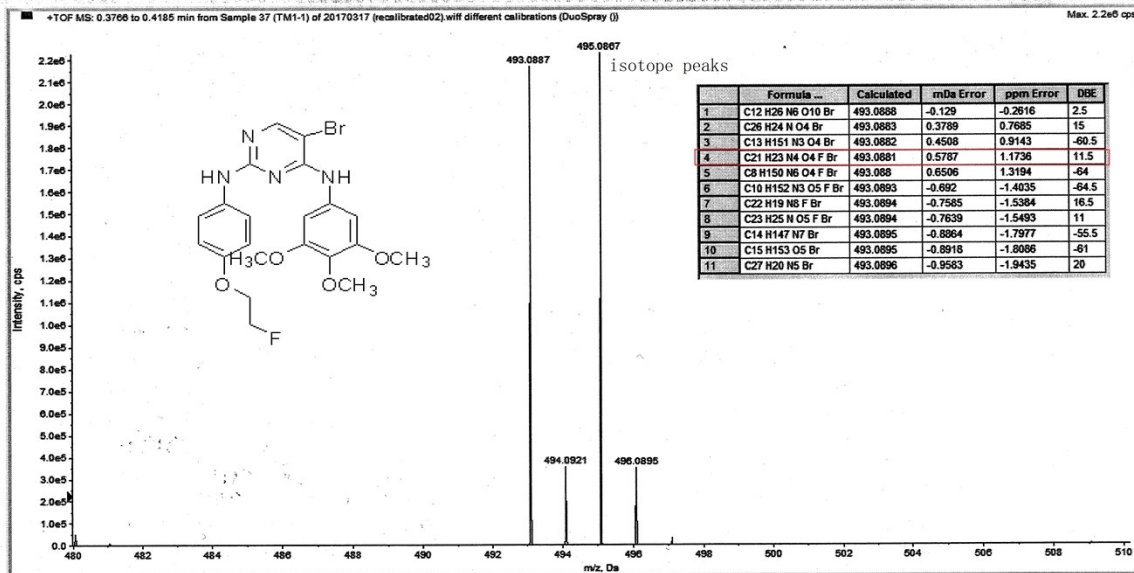
# <sup>1</sup>H NMR of 8b:



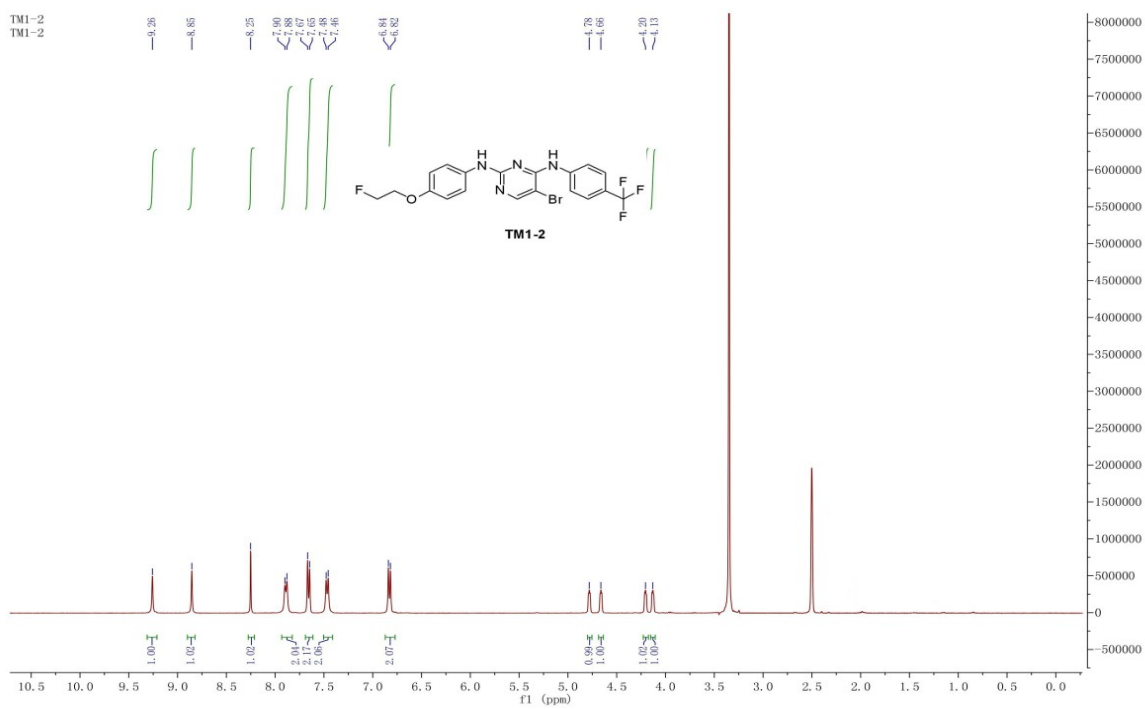
# <sup>13</sup>C NMR of 8b:



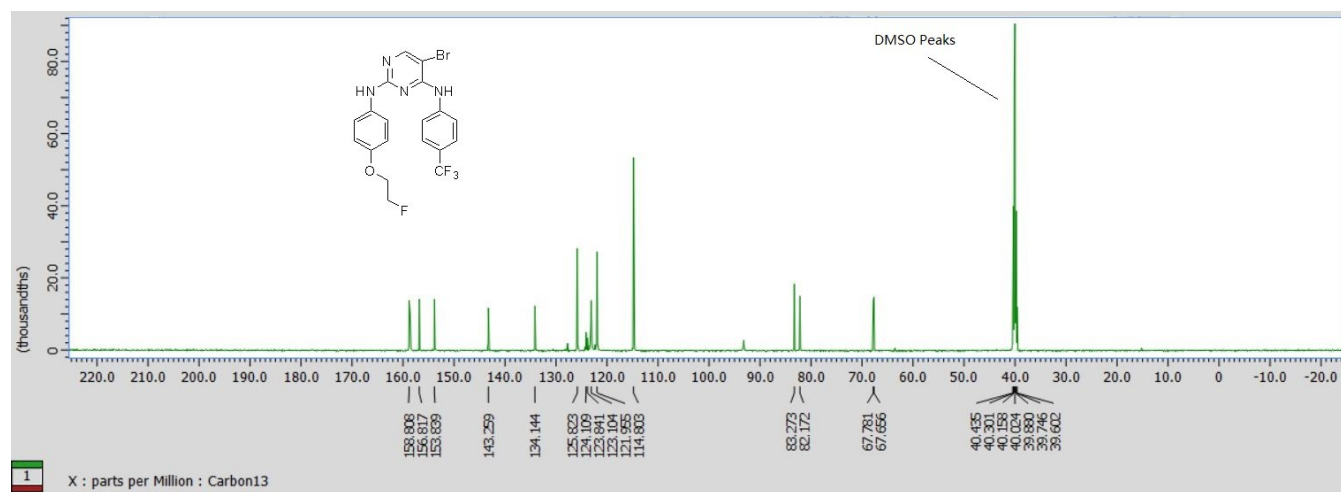
# HRMS (ESI) of 8b:



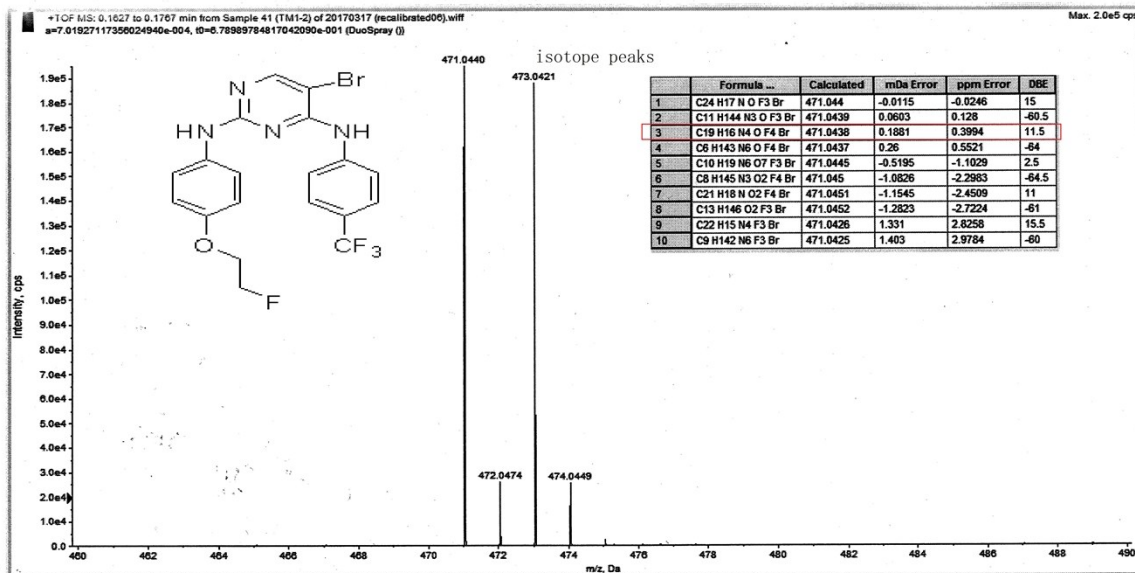
# <sup>1</sup>H NMR of 8c:



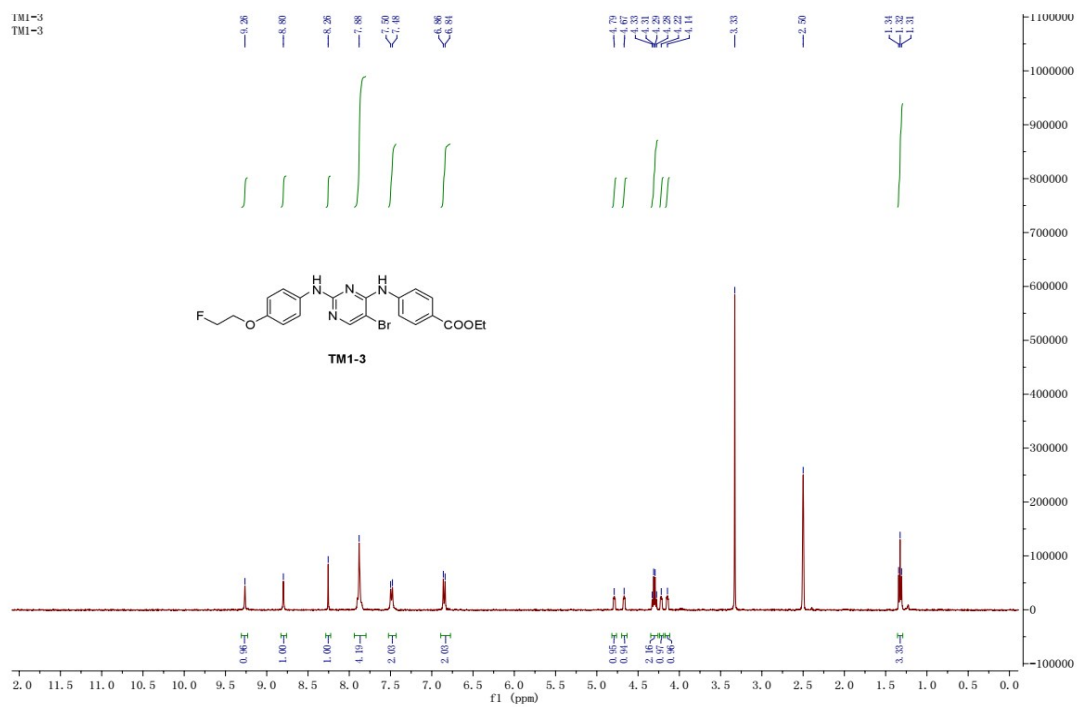
# <sup>13</sup>C NMR of 8c:



# HRMS (ESI) of 8c:

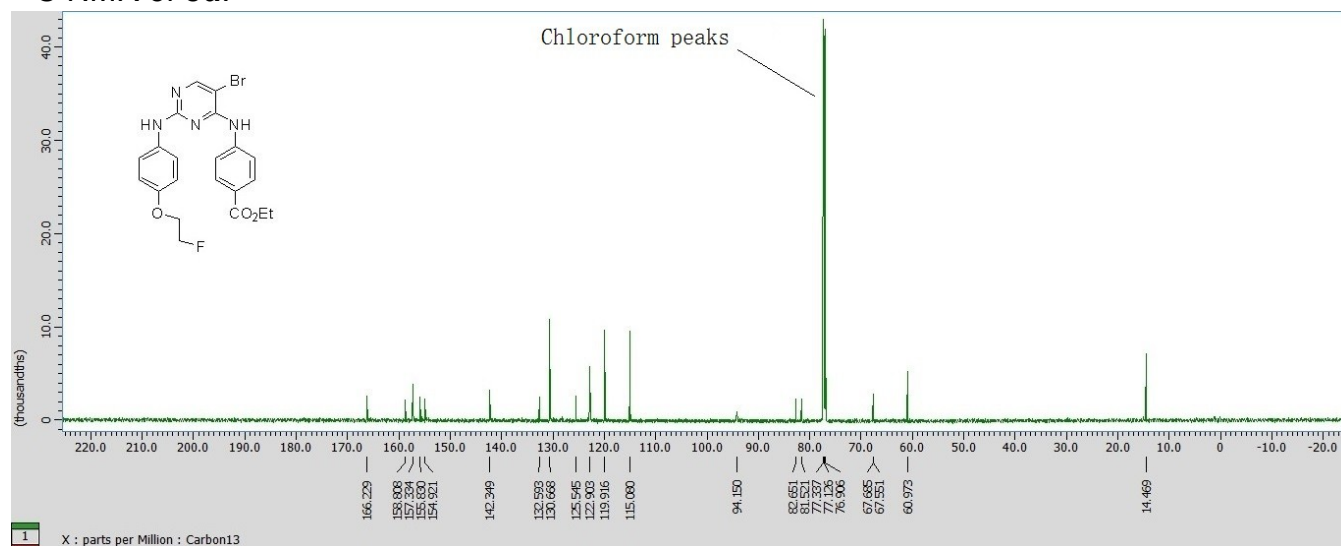


# <sup>1</sup>H NMR of 8d:

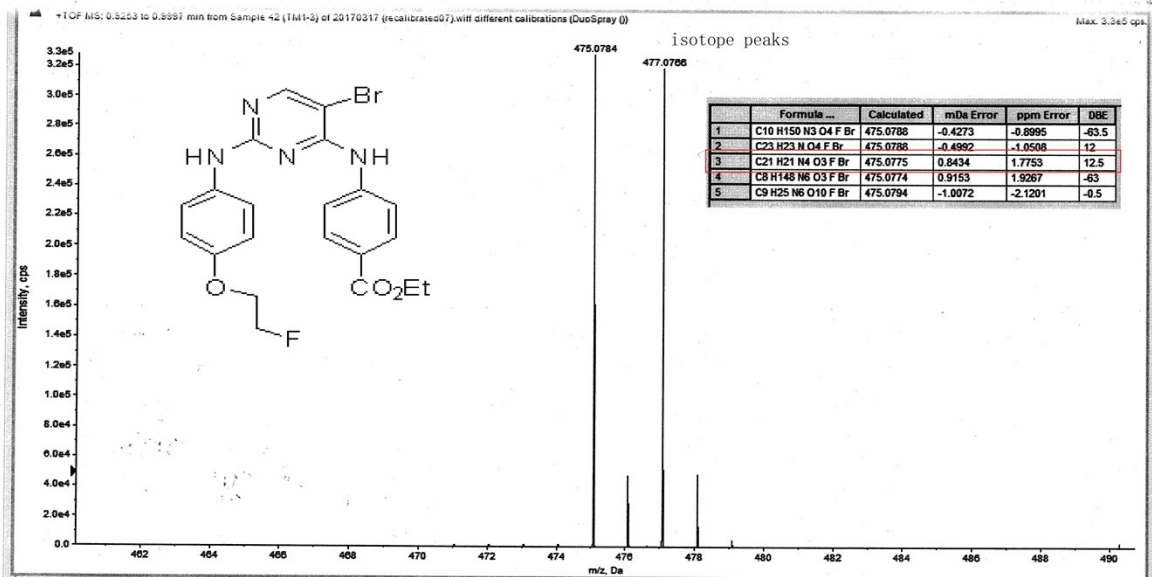




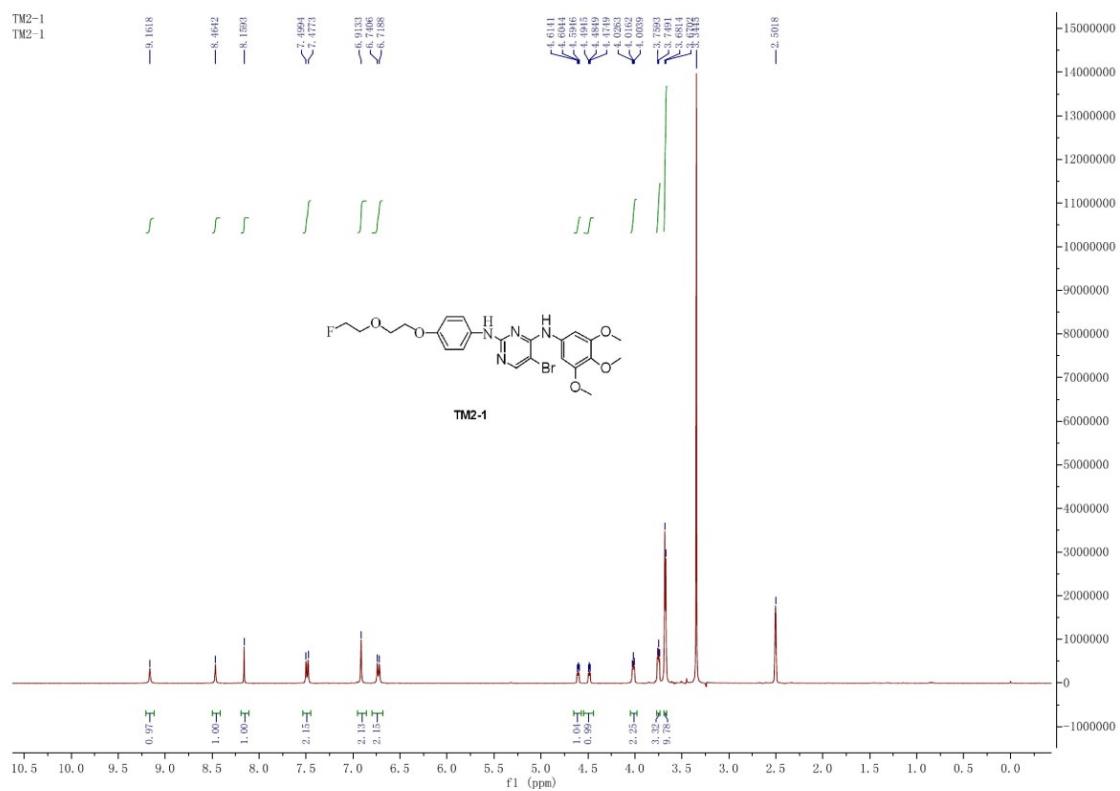
# <sup>13</sup>C NMR of 8d:



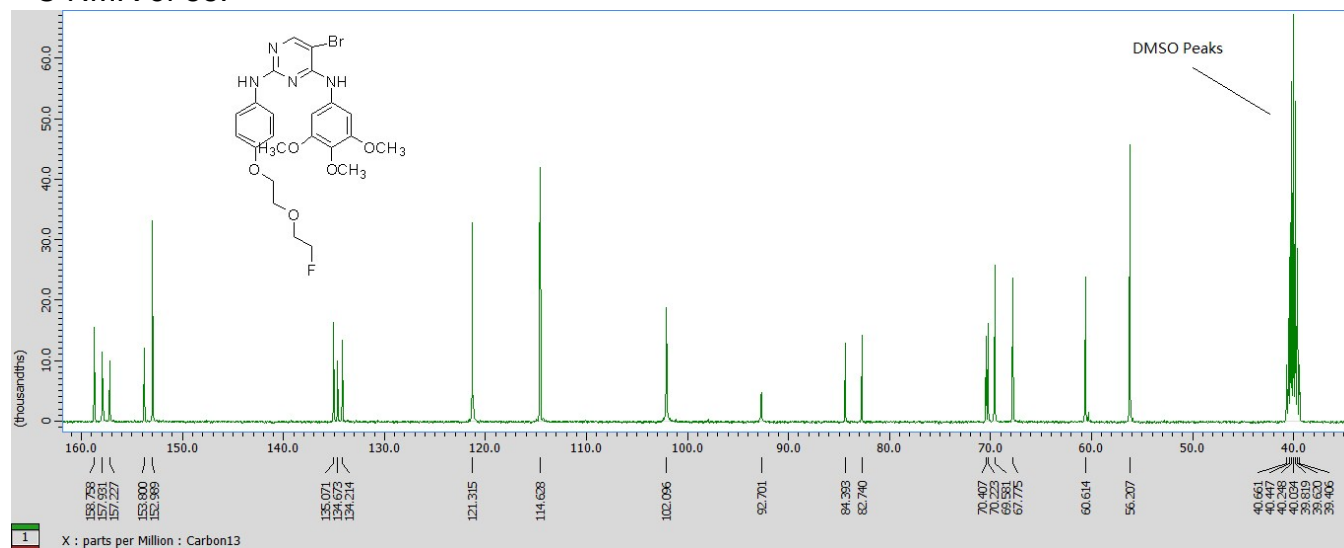
# HRMS (ESI) of 8d:



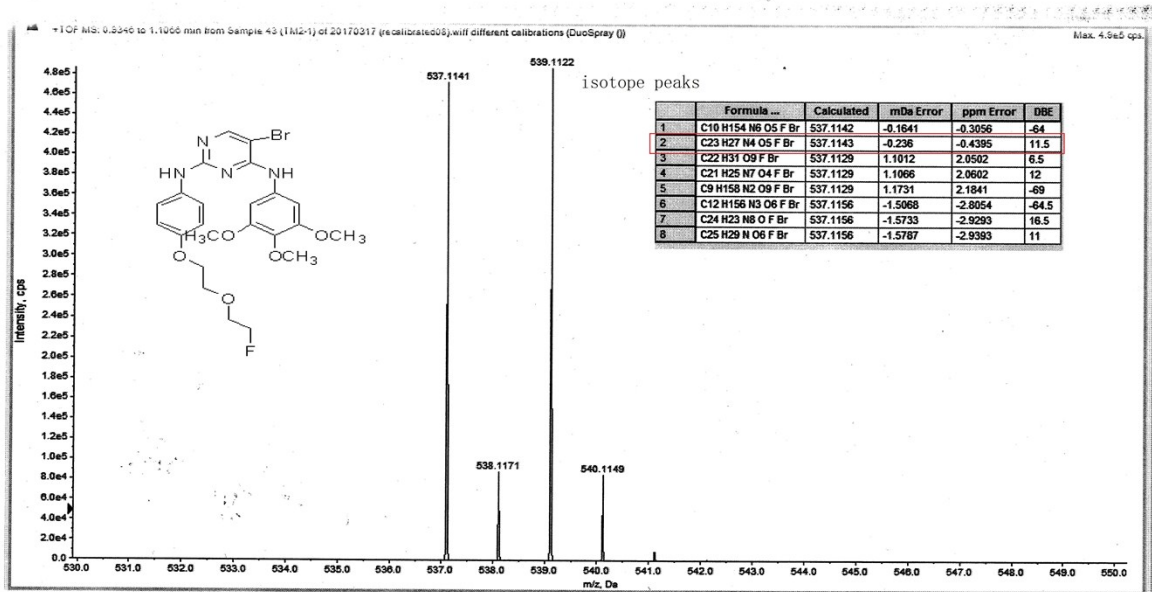
# <sup>1</sup>H NMR of 8e:



# <sup>13</sup>C NMR of 8e:

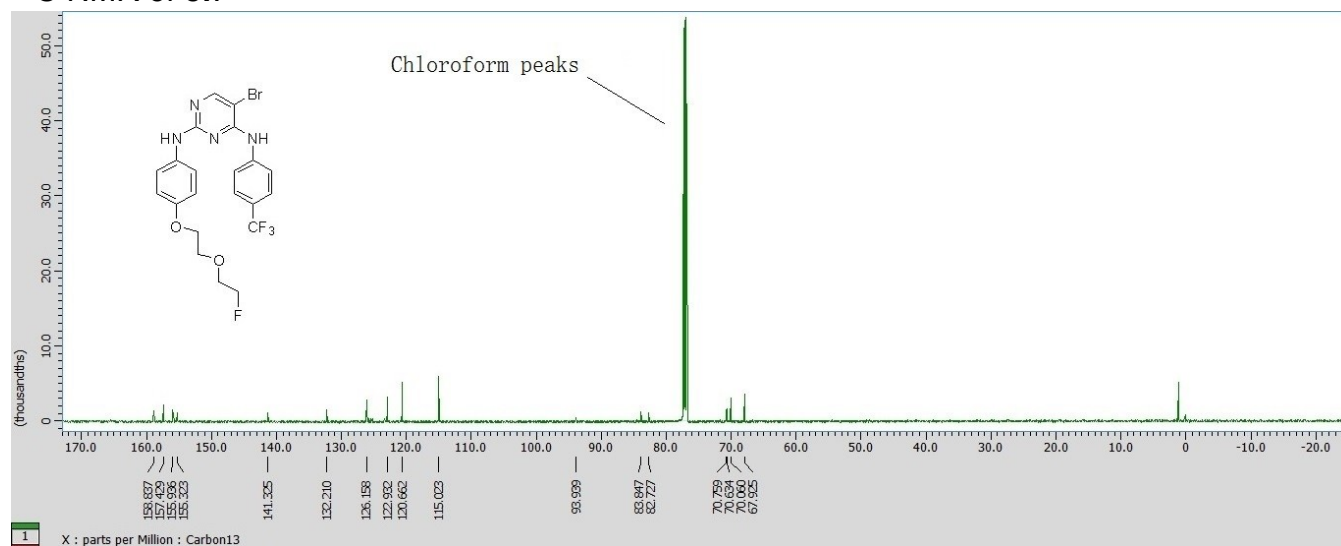


# HRMS (ESI) of 8e:

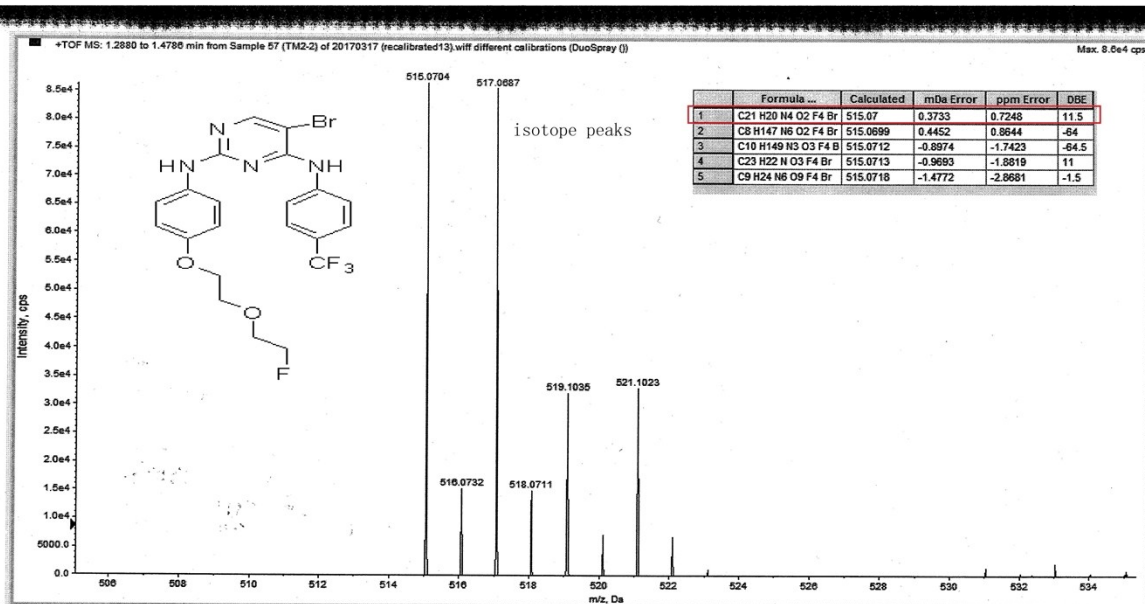




# <sup>13</sup>C NMR of 8f:

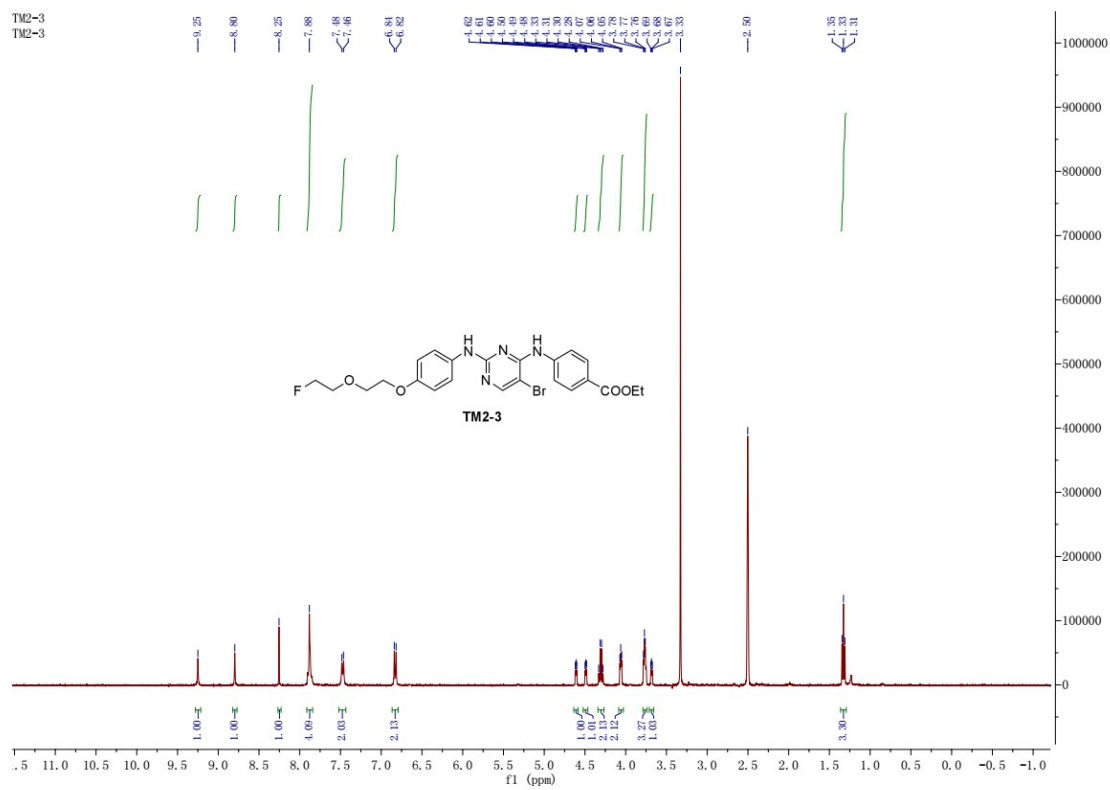


# HRMS (ESI) of 8f:

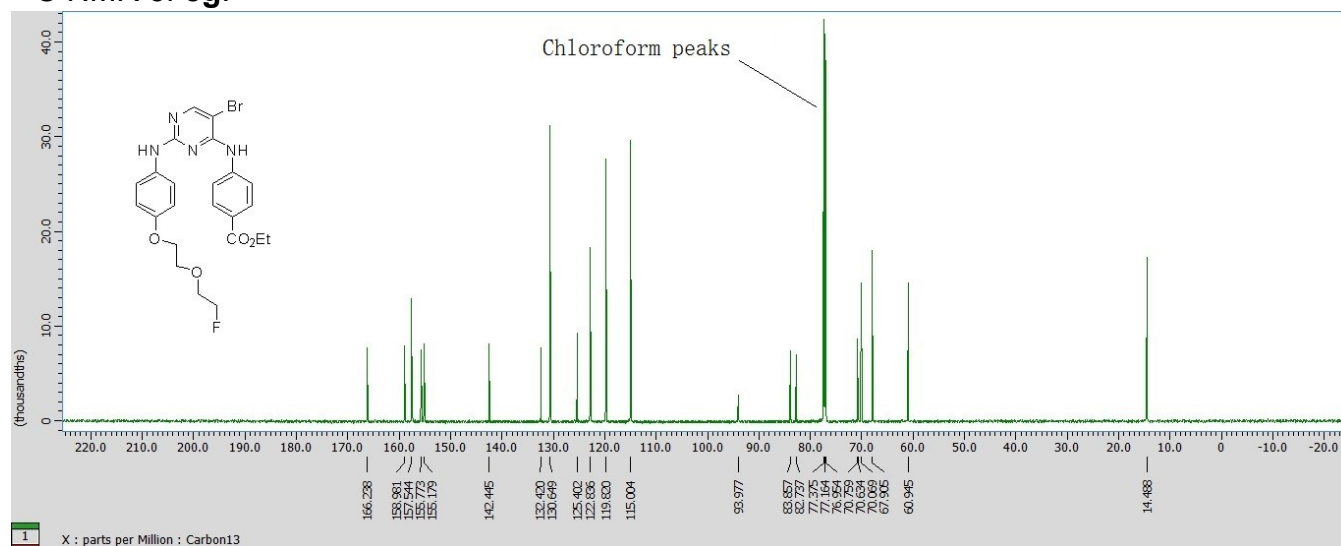




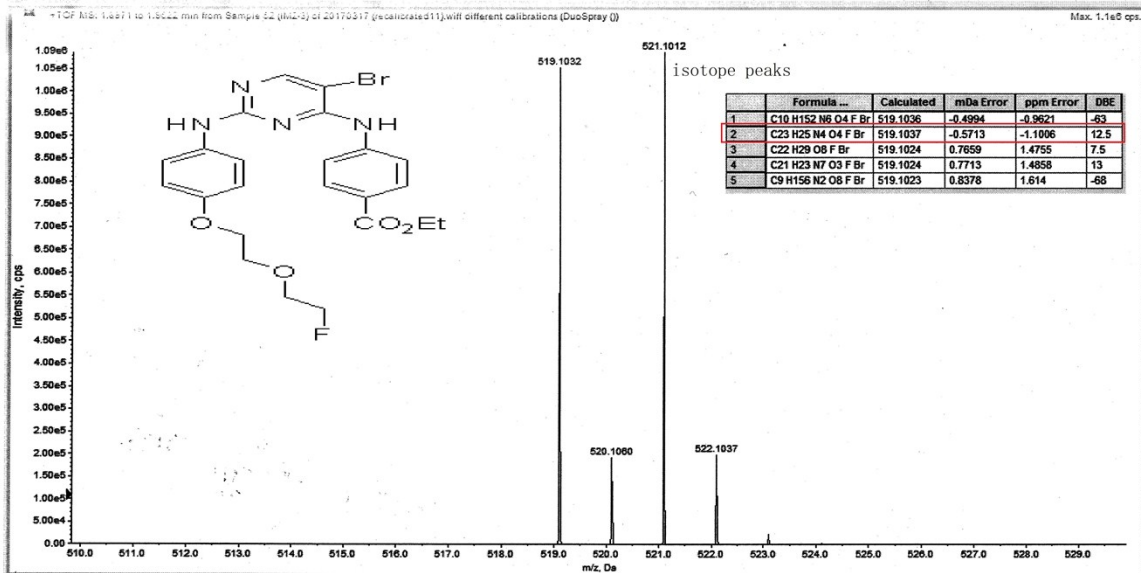
<sup>1</sup>H NMR of 8g:



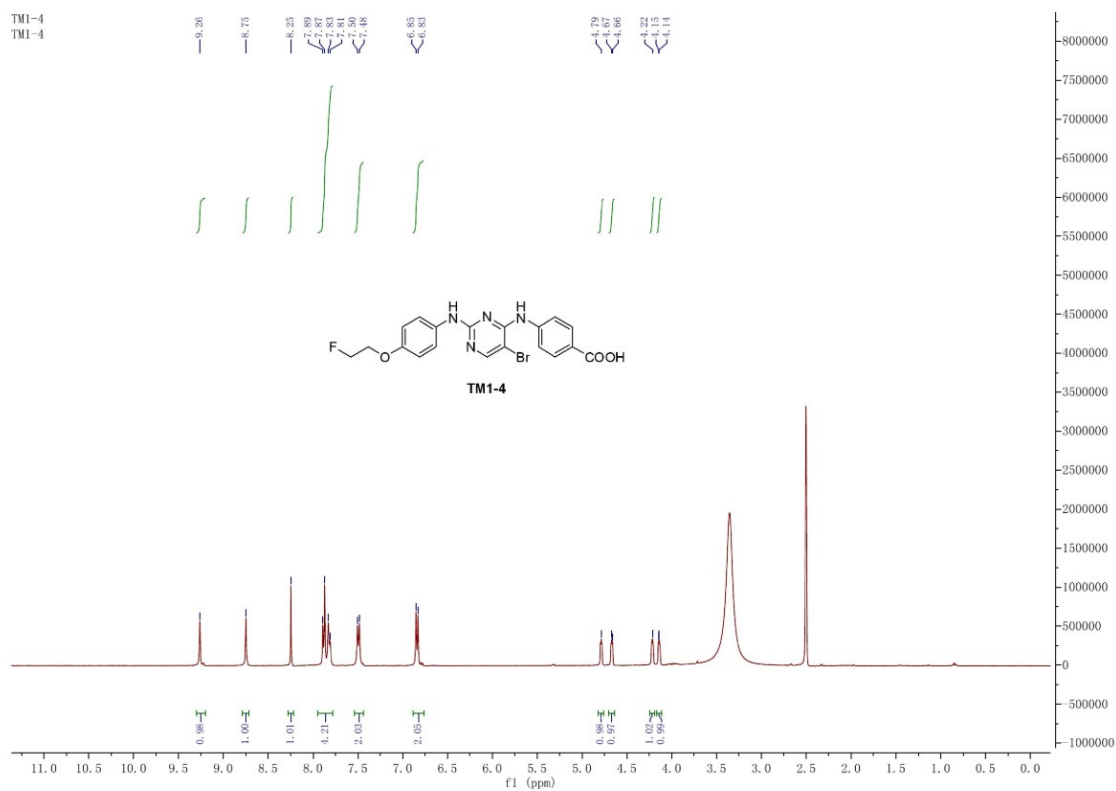
# <sup>13</sup>C NMR of 8g:



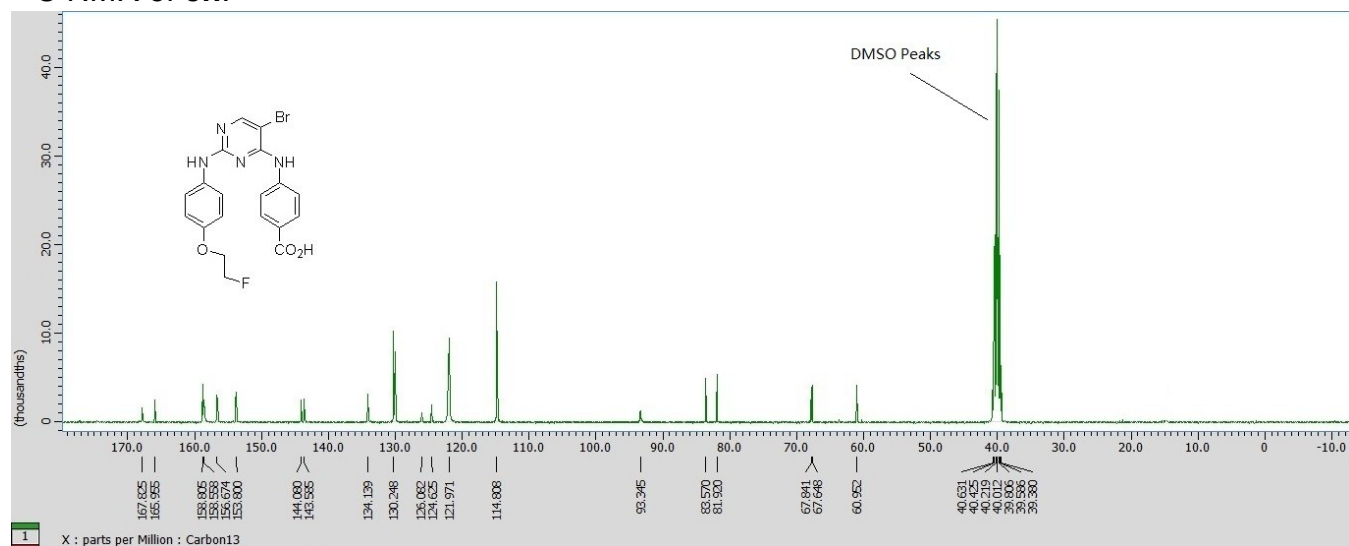
# HRMS (ESI) of 8g:



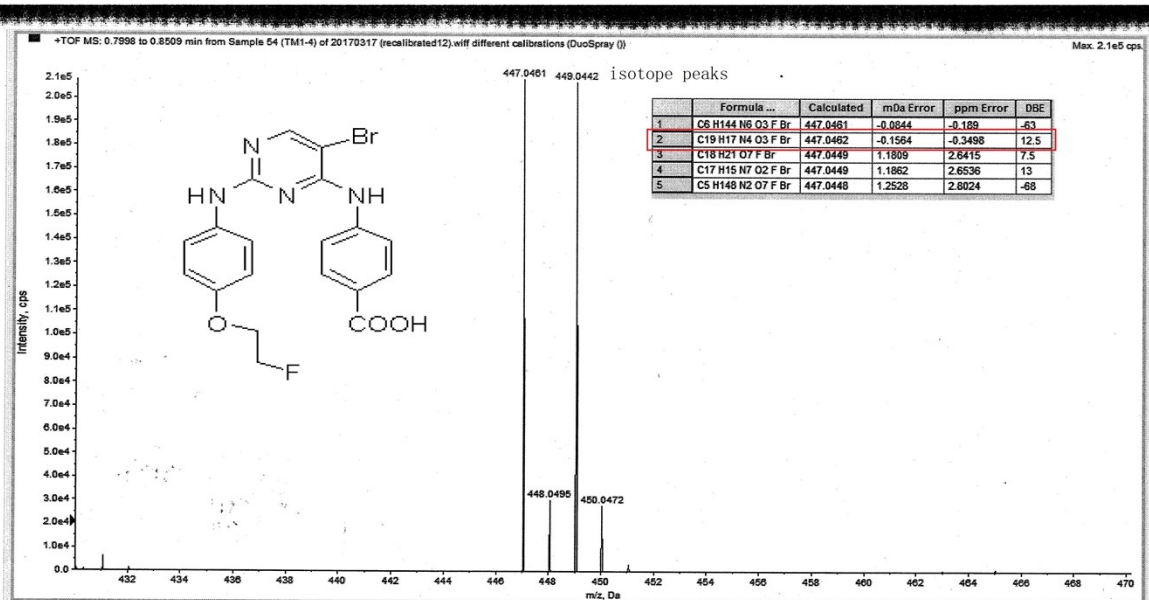
# <sup>1</sup>H NMR of 8h:



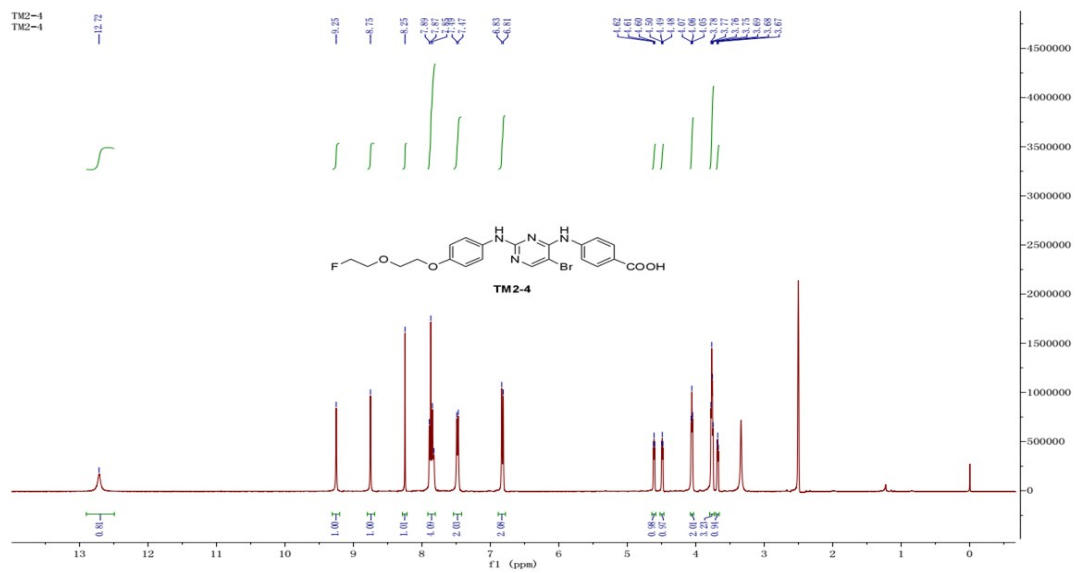
# <sup>13</sup>C NMR of 8h:



# HRMS (ESI) of 8h:



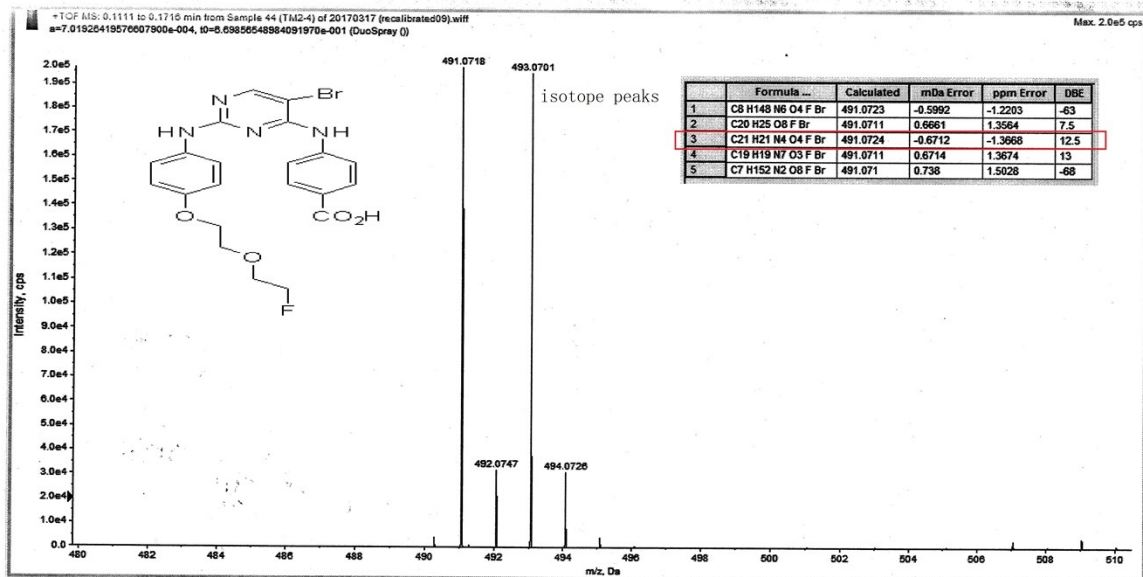
# <sup>1</sup>H NMR of 8i:







HRMS (ESI) of **8i**:

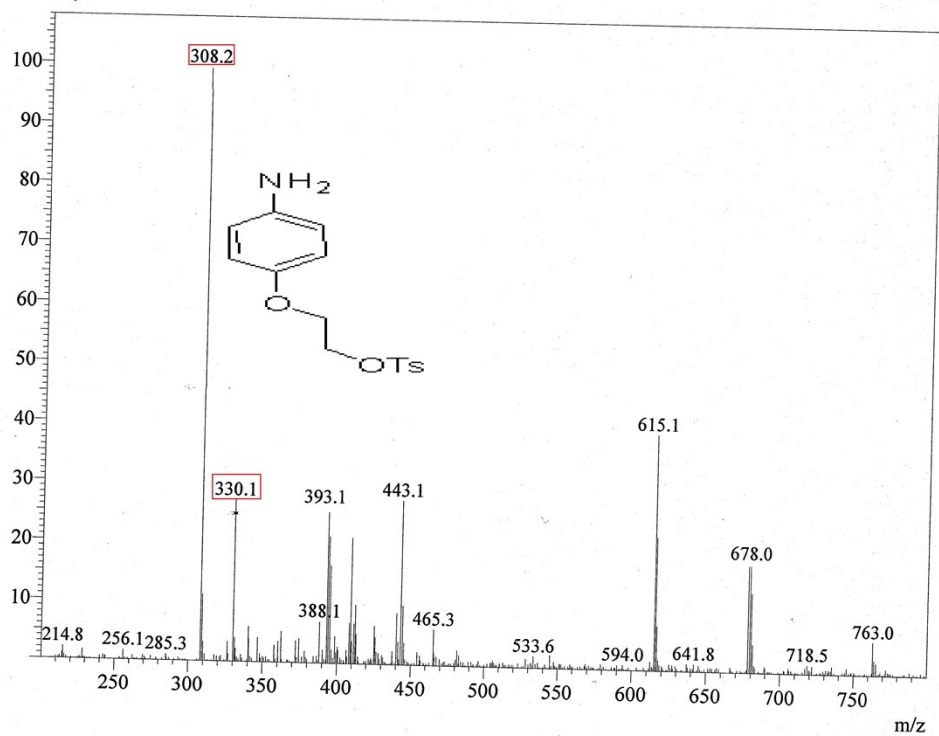


# ESI-MS of crude 3:

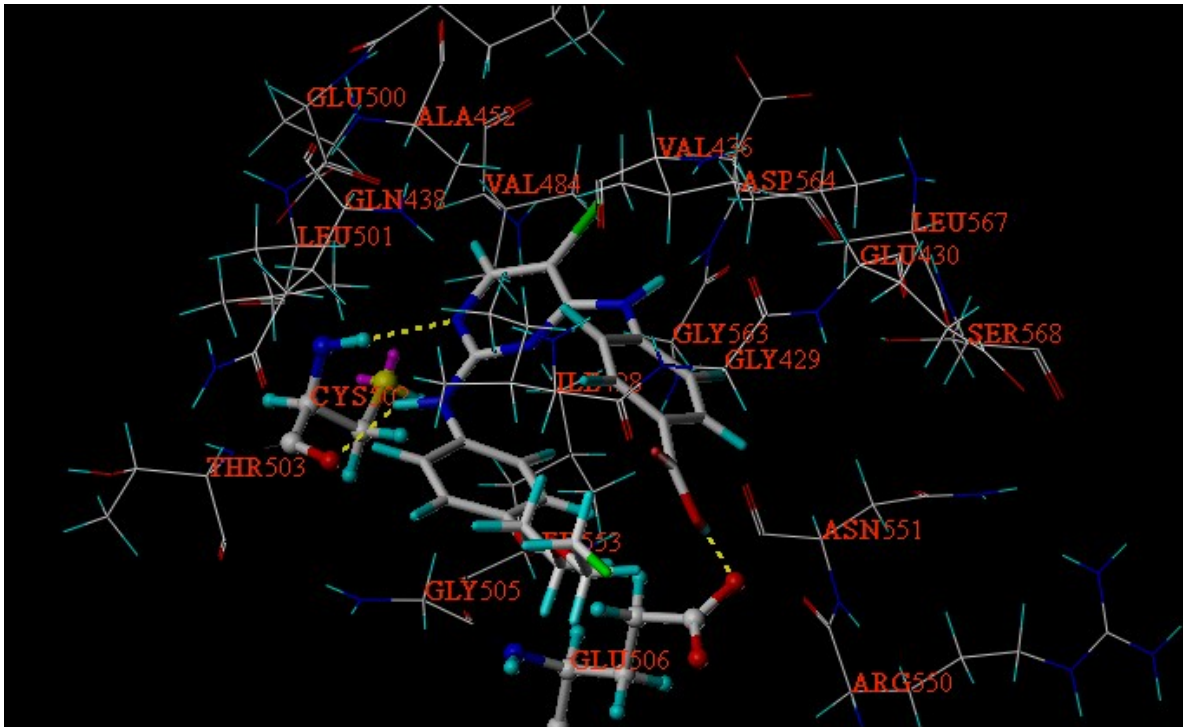
ESI-MS analysis of crude reaction mixture

ESI-MS Spectrum, 097-L-1-1

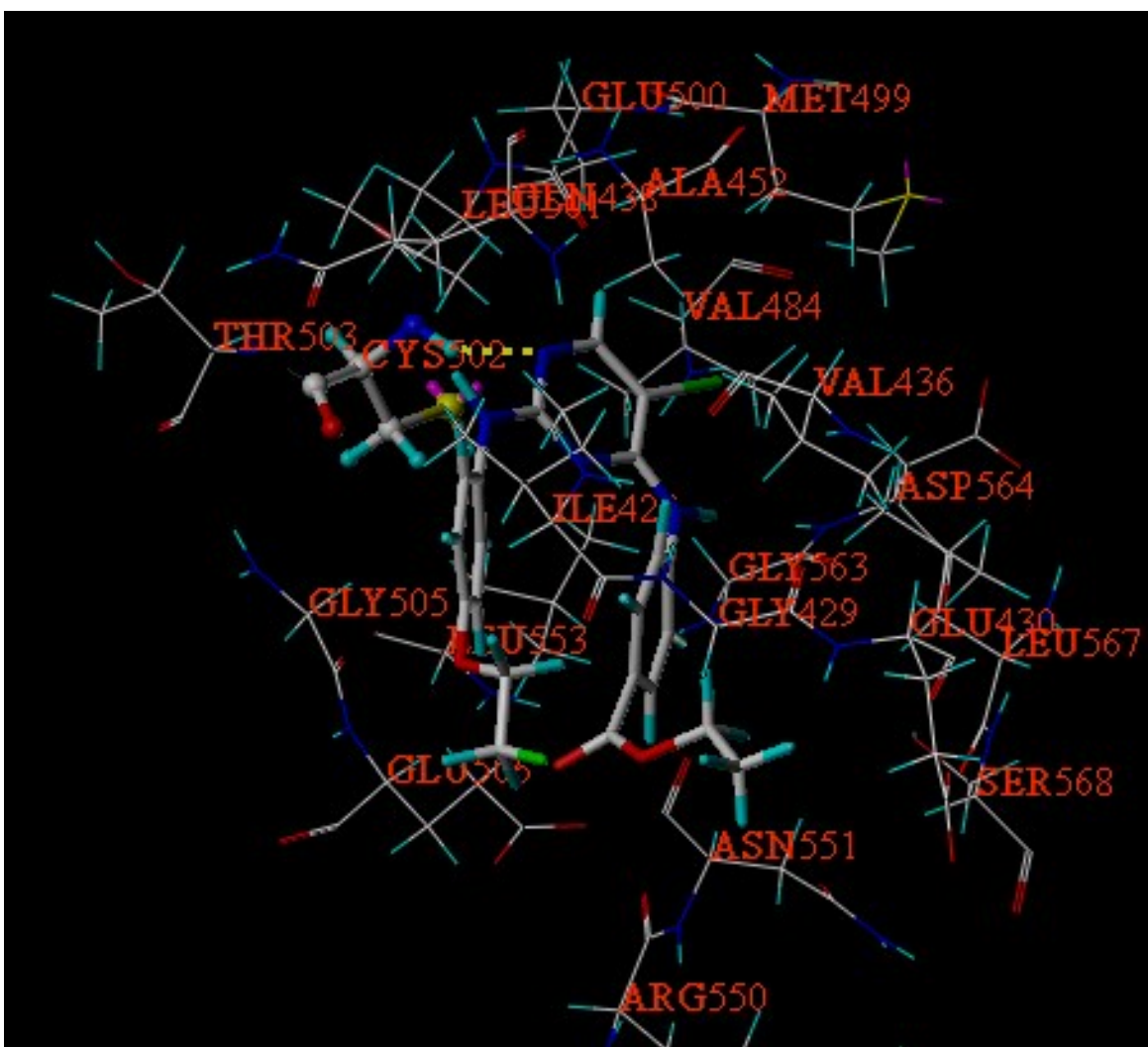
#1 Ret.Time:Averaged 1.280-1.733(Scan#:49-66)  
Mass Peaks:753 Base Peak:308.15(313072) Polarity:Pos Segment1 - Event1  
Intensity



Molecular docking of 8i:



Molecular docking of 8d:



Biodistribution of [<sup>18</sup>F]-8h in mice bearing S180 tumor

ID% (g <sup>-1</sup> )	Time (min)				
	5	15	30	60	120
Blood	0.17±0.02	0.14±0.02	0.19±0.03	0.07±0.01	0.13±0.01
Brain	0.15±0.03	0.08±0.02	0.09±0.01	0.13±0.02	0.11±0.01
Heart	1.13±0.03	0.35±0.04	0.27±0.02	0.26±0.02	0.40±0.03
Liver	3.17±0.12	1.30±0.22	0.65±0.14	0.31±0.02	0.43±0.02
Spleen	0.24±0.06	0.23±0.01	0.15±0.03	0.22±0.01	0.13±0.02
Lung	1.05±0.12	0.35±0.01	0.27±0.01	0.31±0.02	0.28±0.04
Kidney	1.03±0.20	0.26±0.03	0.04±0.02	0.18±0.04	0.20±0.04
Muscle	0.36±0.04	0.30±0.04	0.31±0.08	0.27±0.04	0.48±0.04
Bone	0.59±0.07	0.57±0.10	0.69±0.05	0.94±0.01	0.98±0.06
Intestine	2.49±0.36	1.44±0.06	1.80±0.34	1.23±0.12	0.34±0.06
Stomach	0.30±0.03	0.67±0.03	0.14±0.03	0.15±0.02	0.14±0.02
Tumor	0.52±0.03	0.67±0.01	0.90±0.02	0.64±0.09	0.74±0.04
Tumor/Muscle	1.44	2.23	2.90	2.37	1.54
Tumor/Bone	0.88	1.18	1.30	0.68	0.76
Tumor/Blood	3.06	4.79	4.74	9.14	5.69

Biodistribution of [<sup>18</sup>F]-8i in mice bearing S180 tumor

ID% (g <sup>-1</sup> )	Time (min)				
	5	15	30	60	120
Blood	0.79±0.10	0.60±0.11	0.37±0.01	0.37±0.03	0.28±0.09
Brain	0.32±0.10	0.17±0.02	0.26±0.05	0.17±0.03	0.20±0.01
Heart	1.41±0.25	0.53±0.04	0.54±0.09	0.50±0.07	0.47±0.06
Liver	12.77±0.16	6.51±0.47	2.46±0.22	1.14±0.11	0.83±0.07
Spleen	0.90±0.06	0.53±0.03	0.57±0.05	0.36±0.03	0.23±0.02
Lung	1.25±0.17	0.68±0.07	0.36±0.06	0.44±0.02	0.39±0.02
Kidney	4.39±0.15	2.63±0.29	2.52±0.18	0.96±0.13	0.35±0.05
Muscle	0.96±0.08	0.85±0.17	0.52±0.02	0.61±0.01	0.70±0.06
Bone	0.71±0.10	0.90±0.15	0.52±0.04	0.52±0.09	0.83±0.11
Intestine	0.79±0.11	3.90±0.53	0.98±0.15	0.52±0.07	0.58±0.04
Stomach	0.20±0.03	0.31±0.05	0.98±0.02	0.48±0.06	0.35±0.02
Tumor	1.35±0.18	1.82±0.05	1.22±0.12	1.08±0.06	0.67±0.09
Tumor/Muscle	1.41	2.14	2.35	1.77	0.96
Tumor/Bone	1.90	2.02	2.35	2.08	0.81
Tumor/Blood	1.71	3.03	3.30	2.92	2.39

Biodistribution of [<sup>18</sup>F]-8c in mice bearing S180 tumor

ID% (g <sup>-1</sup> )	Time (min)				
	5	15	30	60	120
Blood	3.59±0.03	3.40±0.13	3.62±0.12	4.45±0.08	4.34±0.05
Brain	2.92±0.13	2.79±0.08	2.20±0.11	2.87±0.14	2.95±0.08
Heart	4.96±0.36	3.22±0.48	2.51±0.19	3.25±0.17	3.72±0.26
Liver	10.36±0.30	11.62±0.69	9.35±0.28	5.59±0.39	4.62±0.09
Spleen	10.03±0.49	7.40±0.24	5.14±0.23	4.37±0.11	3.43±0.17
Lung	7.26±0.23	5.22±0.04	4.86±0.30	3.30±0.05	3.20±0.24
Kidney	4.50±0.32	3.04±0.16	2.69±0.22	2.87±0.15	2.46±0.08
Muscle	3.57±0.06	2.93±0.26	2.38±0.11	2.97±0.33	3.05±0.23
Bone	3.63±0.18	2.95±0.04	3.53±0.11	4.49±0.19	4.02±0.39
Intestine	0.45±0.03	0.62±0.06	0.31±0.02	0.39±0.01	0.36±0.06
Stomach	0.77±0.04	0.72±0.03	0.77±0.05	0.78±0.04	0.76±0.01
Tumor	3.54±0.23	3.22±0.38	3.73±0.08	4.57±0.54	4.46±0.51
Tumor/Muscle	0.99	1.10	1.57	1.54	1.46
Tumor/Bone	0.98	1.09	1.06	1.02	1.11
Tumor/Blood	0.99	0.95	1.03	1.03	1.03