

## Supplementary Information

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

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21-Aug-2017

10:58:07  
QUATTROZQUATTROZQ

1:B,7

WJ 70 (1.405) Cm (70:75)

1: Scan ES+  
1.20e6

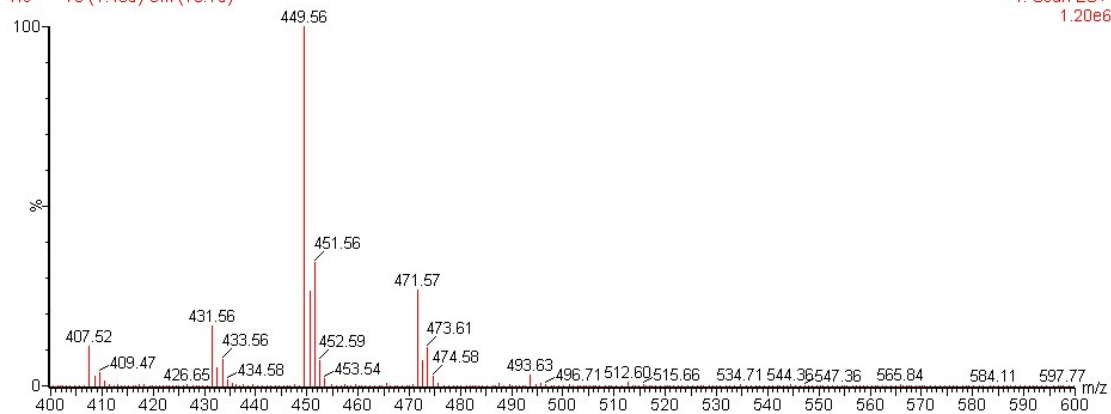


Fig. 1-1 MS spectrum of 9a

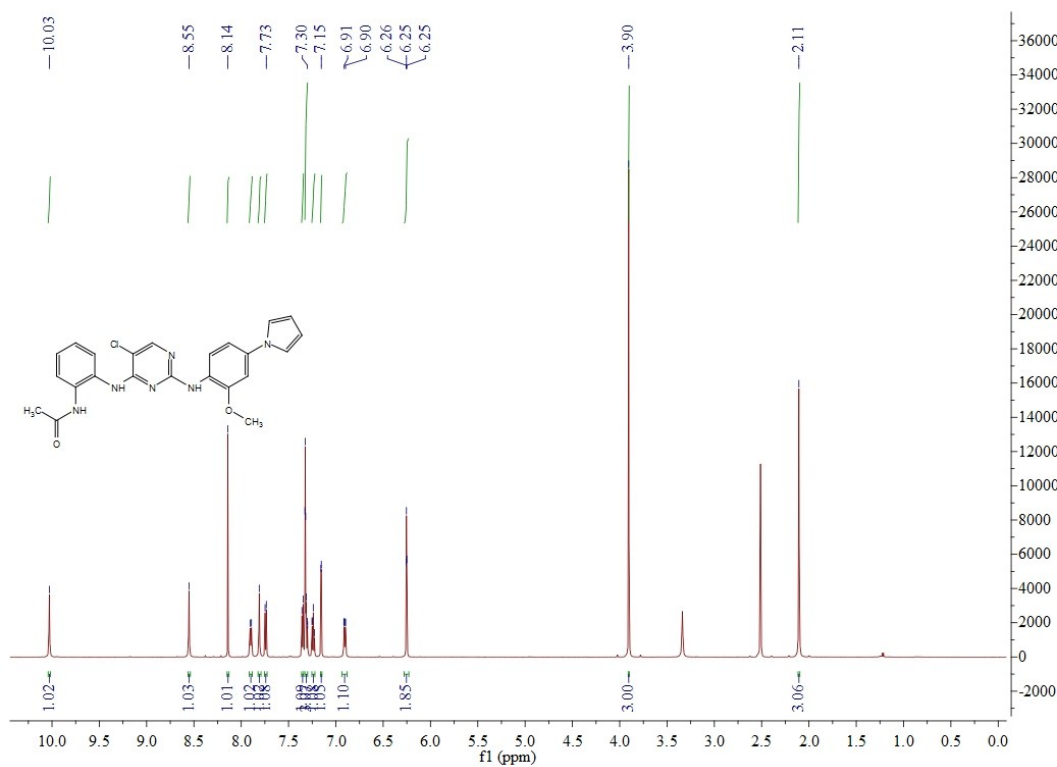


Fig. 1-2 <sup>1</sup>H-NMR spectrum of 9a

25-Aug-2017

12:56:50  
QUATTROZQUATTROZQ

1:D,7

WJ 246 (4.970) Cm (246:247)

2: Scan ES-  
2.82e4

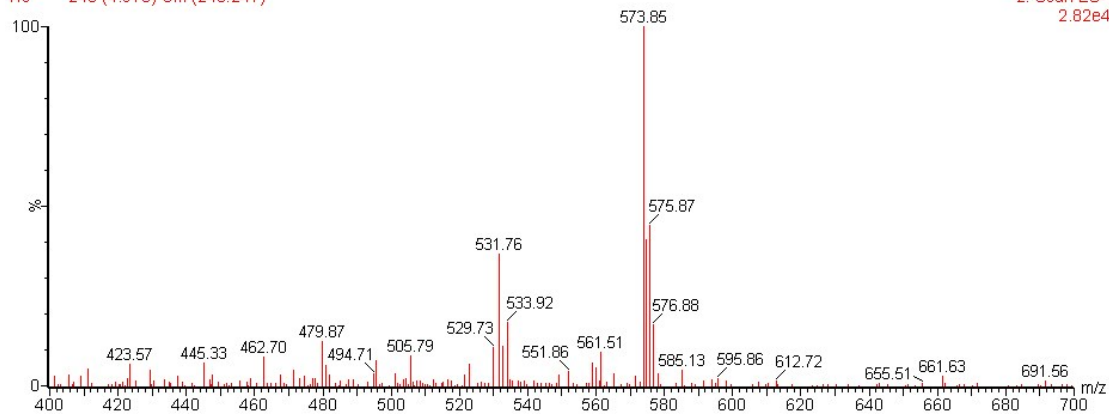


Fig. 2-1 MS spectrum of 9b

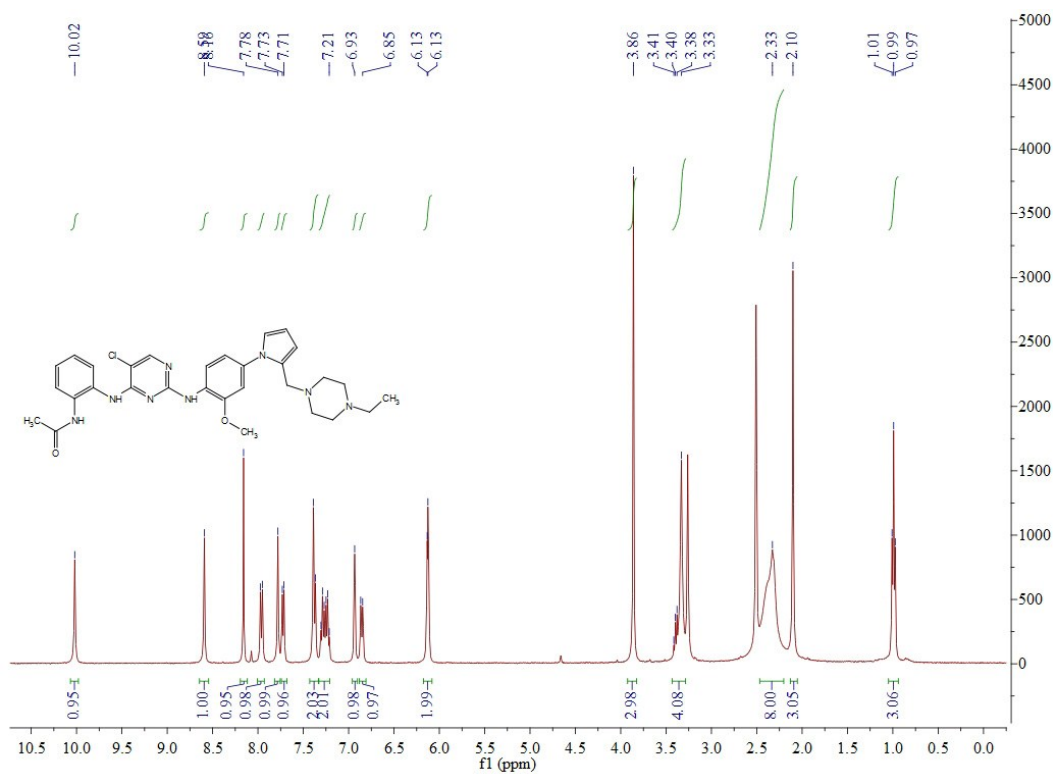


Fig. 2-2 <sup>1</sup>H-NMR spectrum of 9b

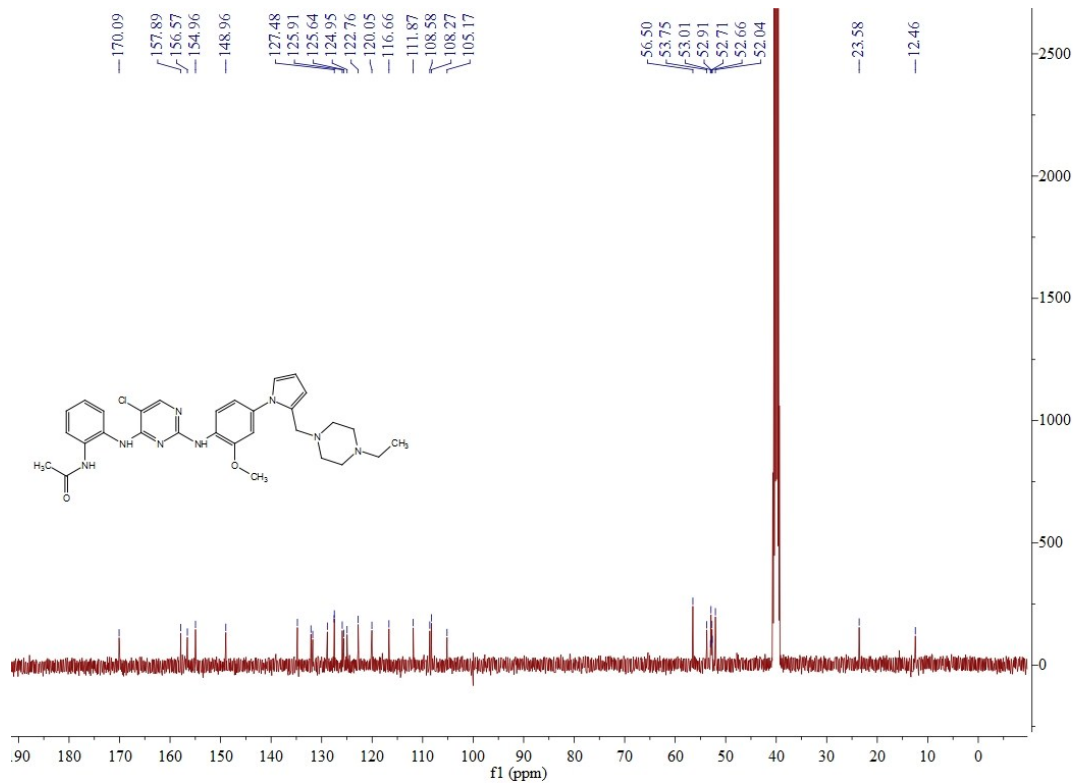


Fig. 2-3 <sup>13</sup>C-NMR spectrum of 9b

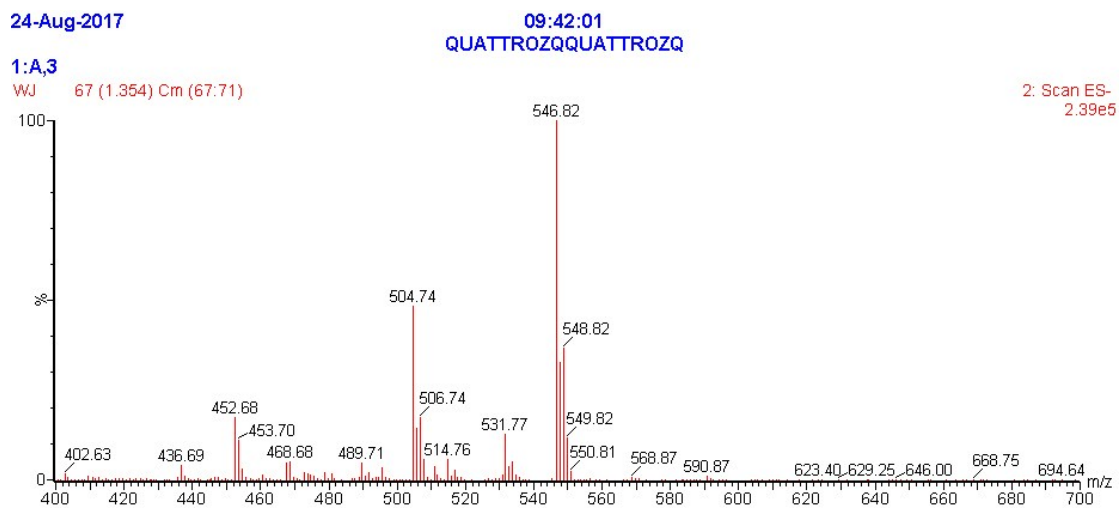


Fig. 3-1 MS spectrum of 9c

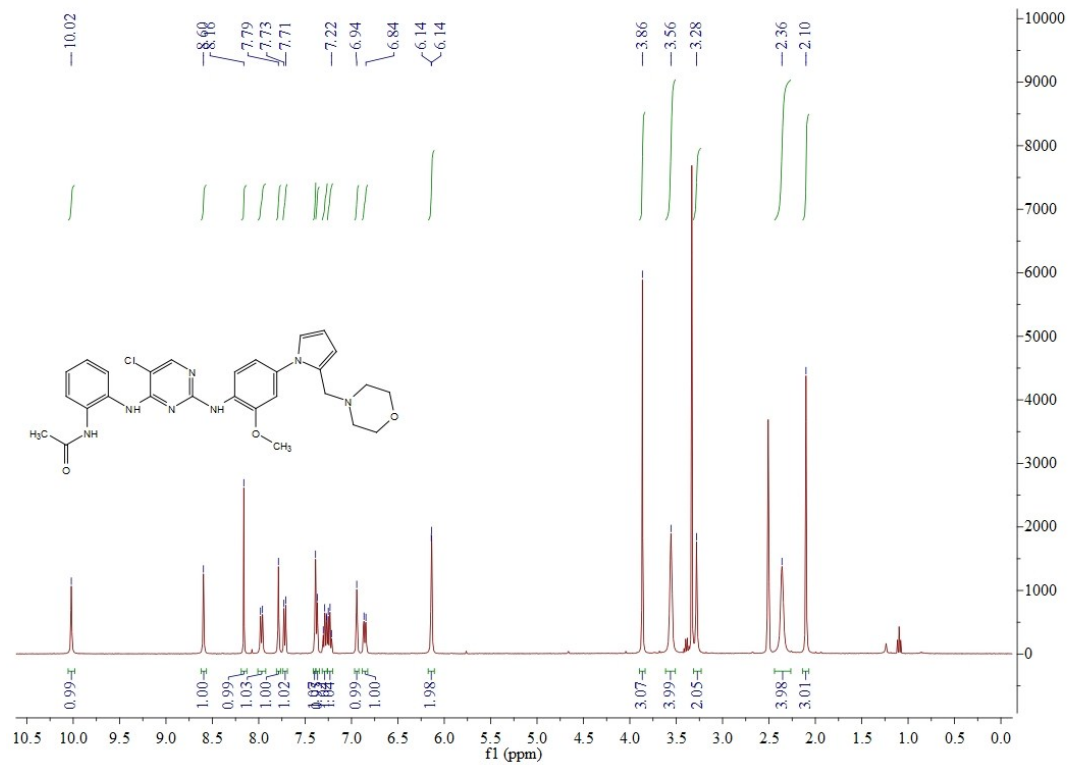


Fig. 3-2  $^1\text{H-NMR}$  spectrum of 9c

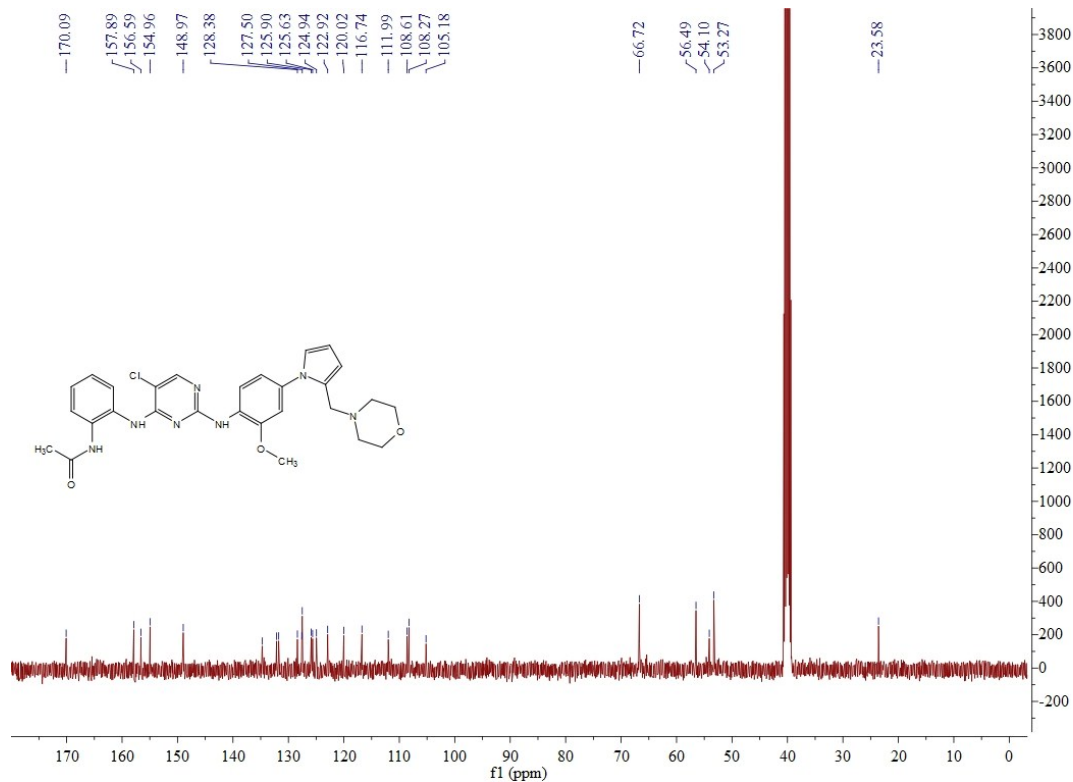


Fig. 3-3  $^{13}\text{C-NMR}$  spectrum of 9c

30-Mar-2018

11:56:55  
QUATTROZQUATTROZQ

1:D,3

J 90 (1.818) Cm (87:91)

2: Scan ES-  
7.89e5

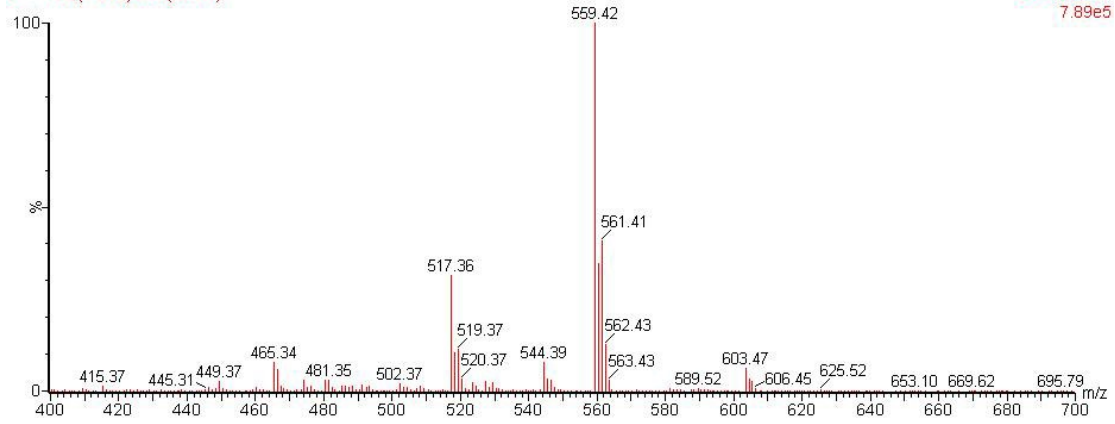


Fig. 4-1 MS spectrum of 9d

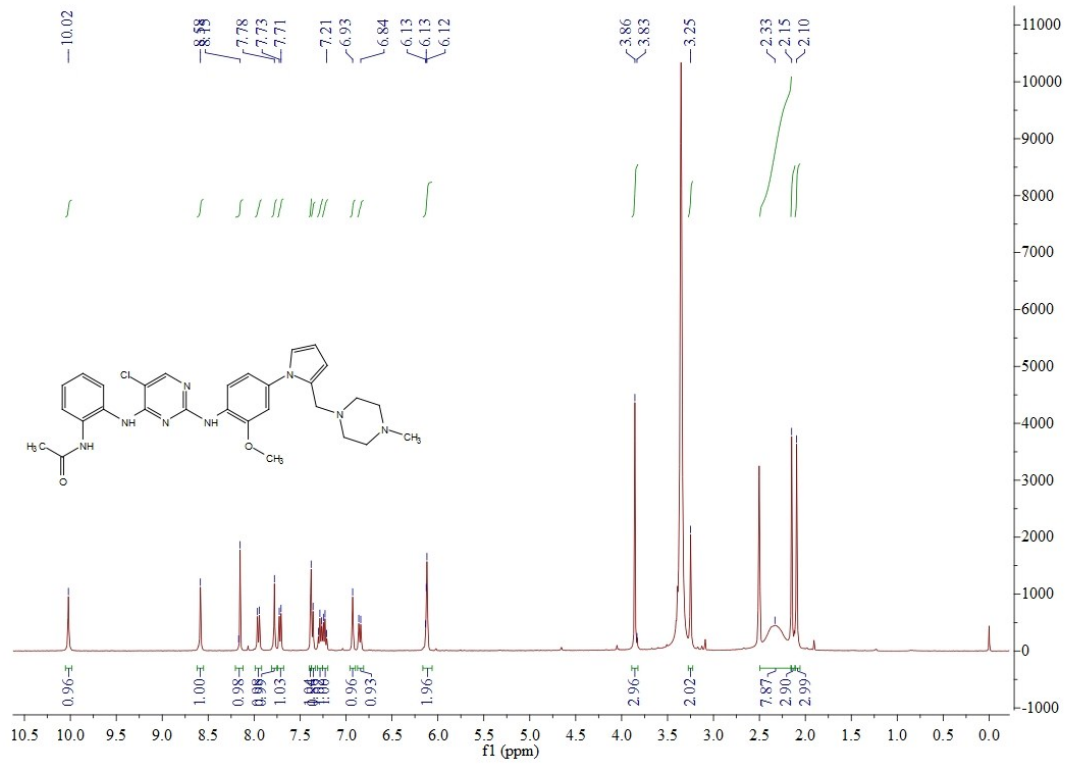


Fig. 4-2 <sup>1</sup>H-NMR spectrum of 9d

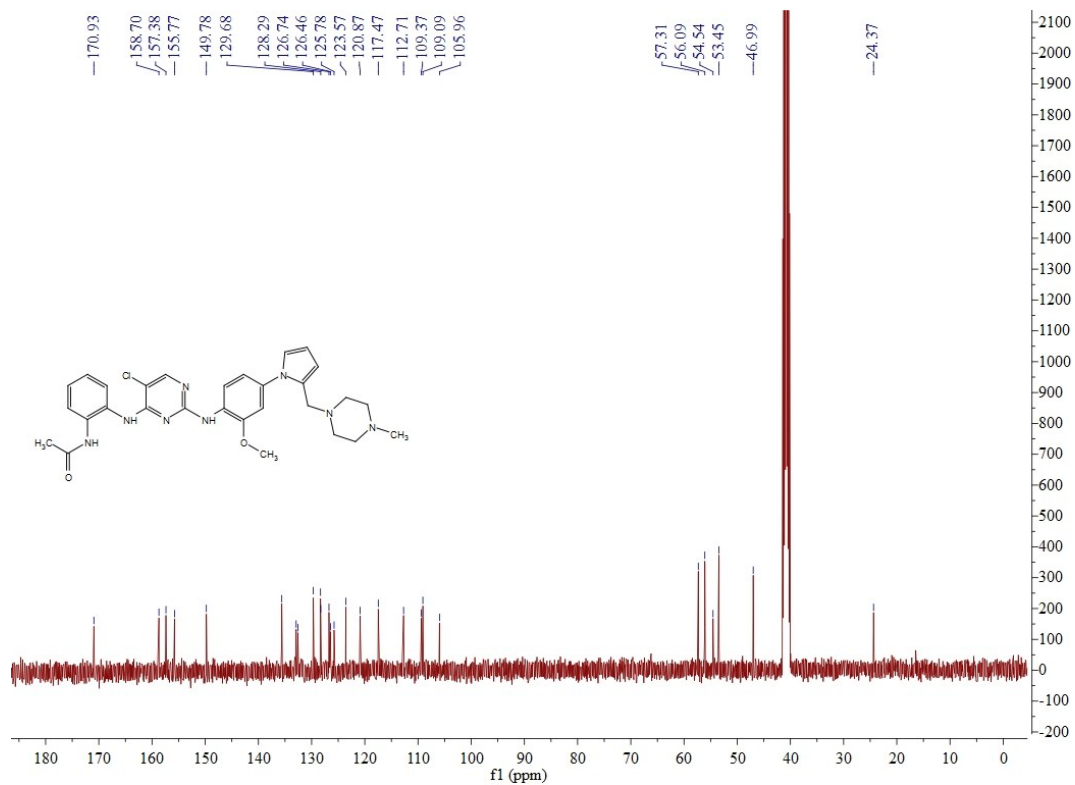


Fig. 4-3  $^{13}\text{C}$ -NMR spectrum of 9d

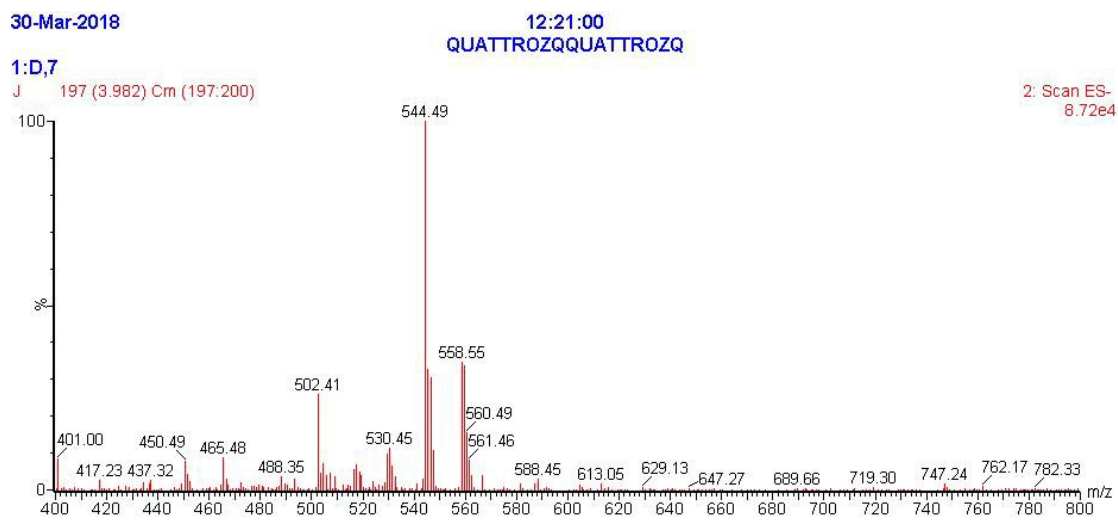


Fig. 5-1 MS spectrum of 9e

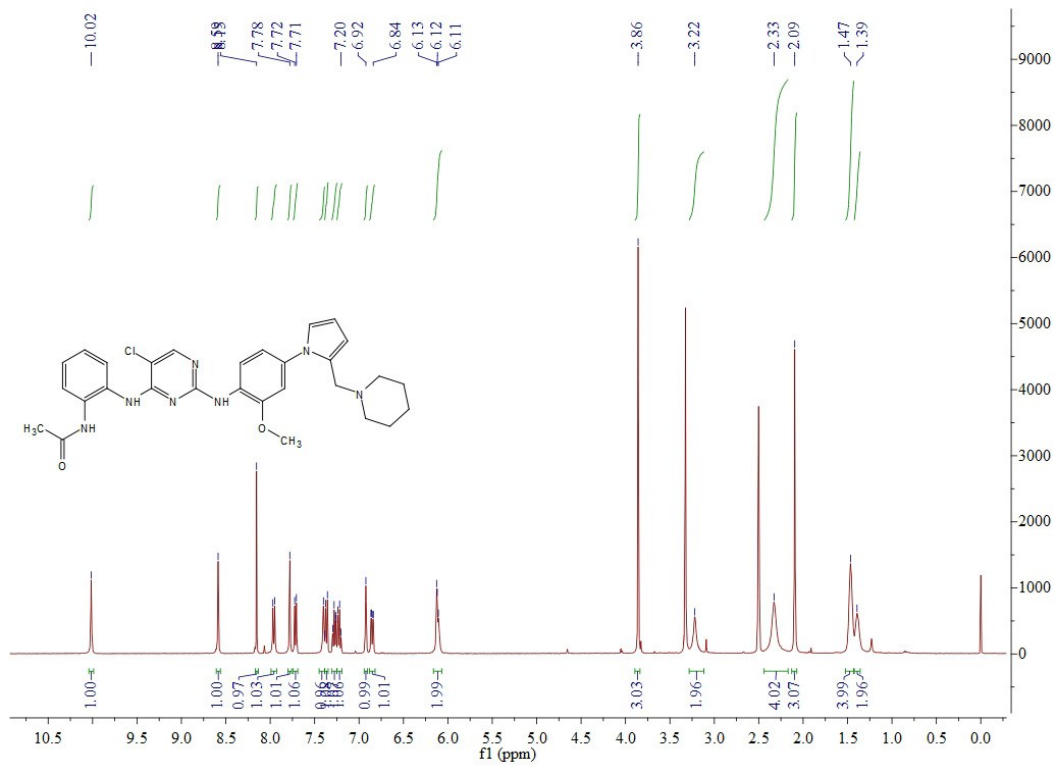


Fig. 5-2 <sup>1</sup>H-NMR spectrum of 9e

31-Mar-2018

11:12:22

QUATTROZQUATTROZQ

1:C,3

W 224 (4.524) Cm (219:224)

2: Scan ES-  
5.41e4

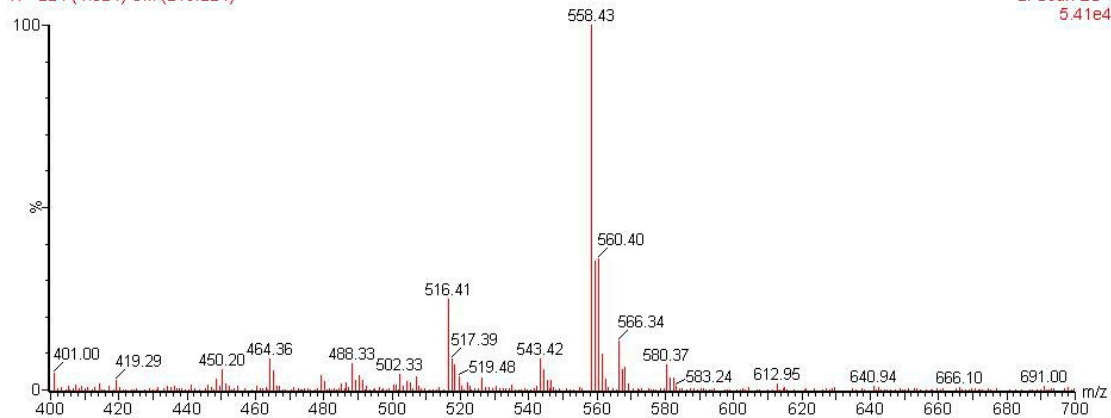


Fig. 6-1 MS spectrum of 9f



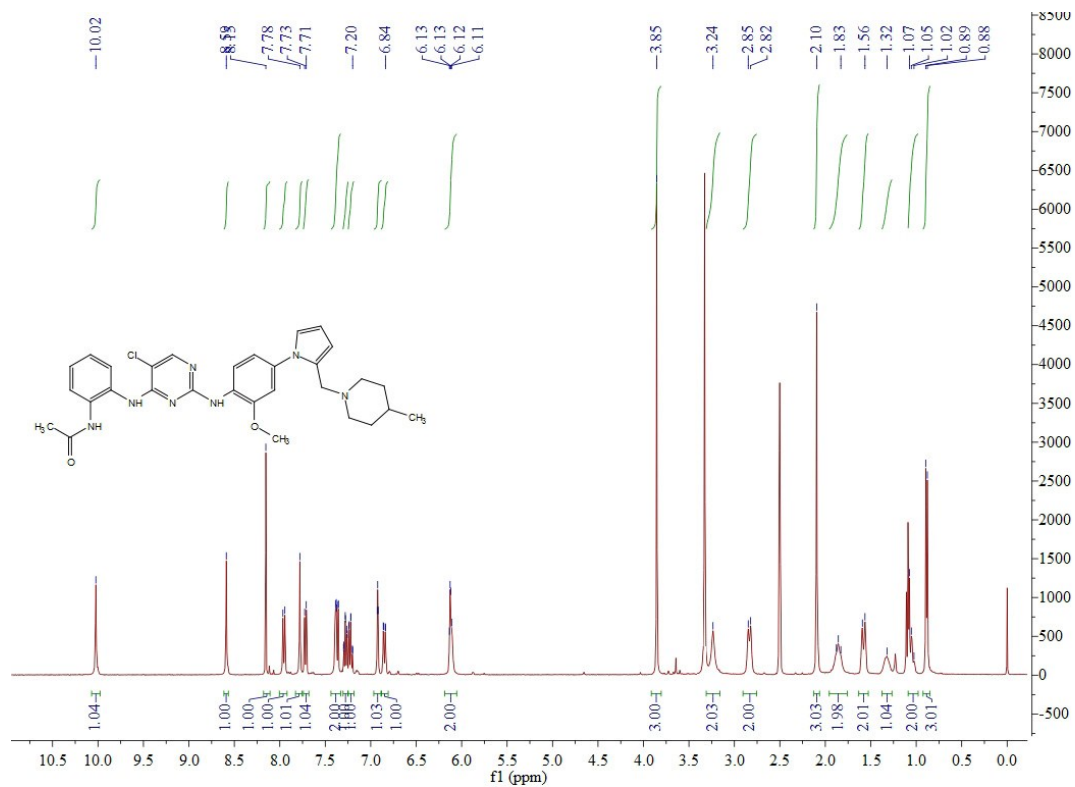


Fig. 6-2  $^1\text{H-NMR}$  spectrum of 9f

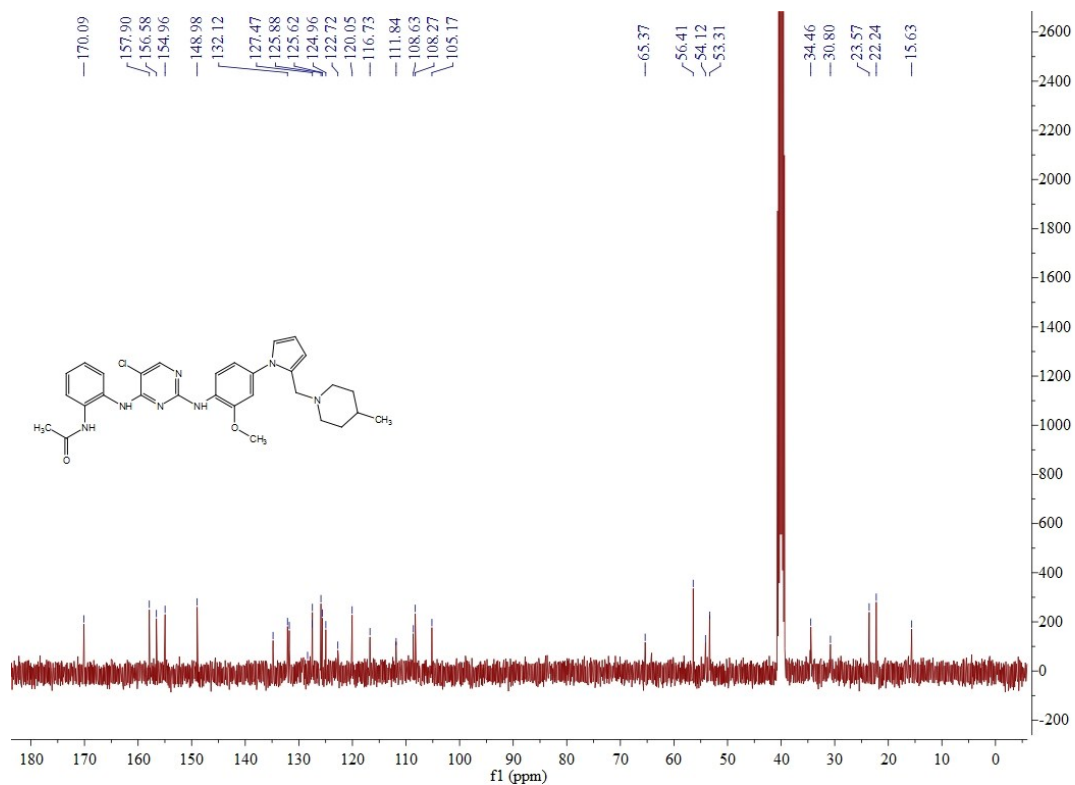


Fig. 6-3  $^{13}\text{C-NMR}$  spectrum of 9f

31-Mar-2018

11:24:23  
QUATTROZQUATTROZQ

1:C,5

W 99 (2.000) Cm (99.101)

2: Scan ES-  
4.24e4

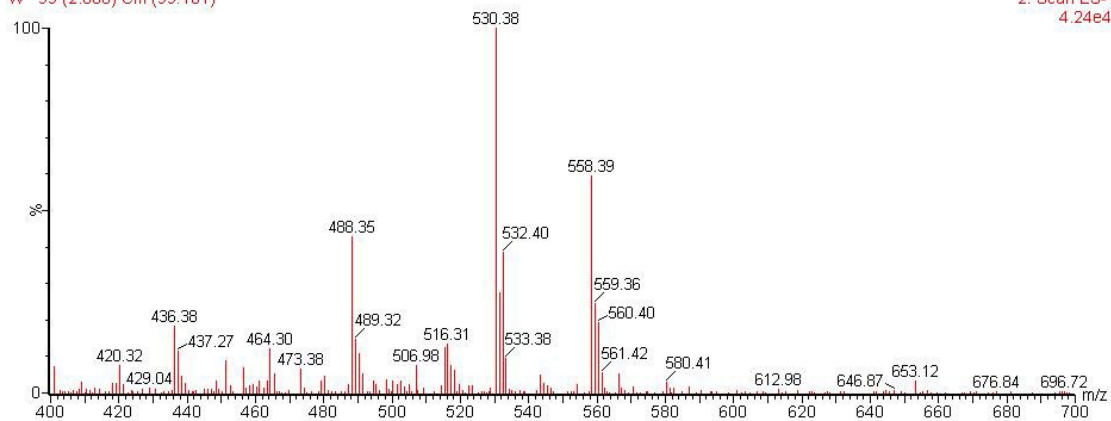


Fig. 7-1 MS spectrum of 9g

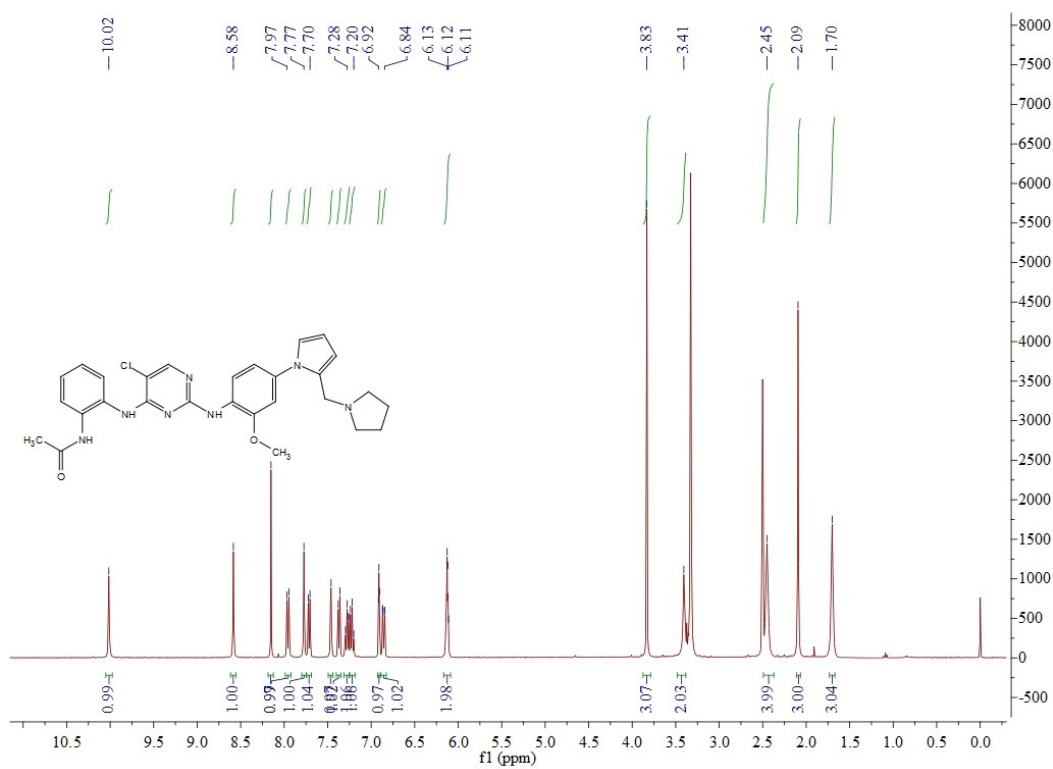


Fig. 7-2 <sup>1</sup>H-NMR spectrum of 9g

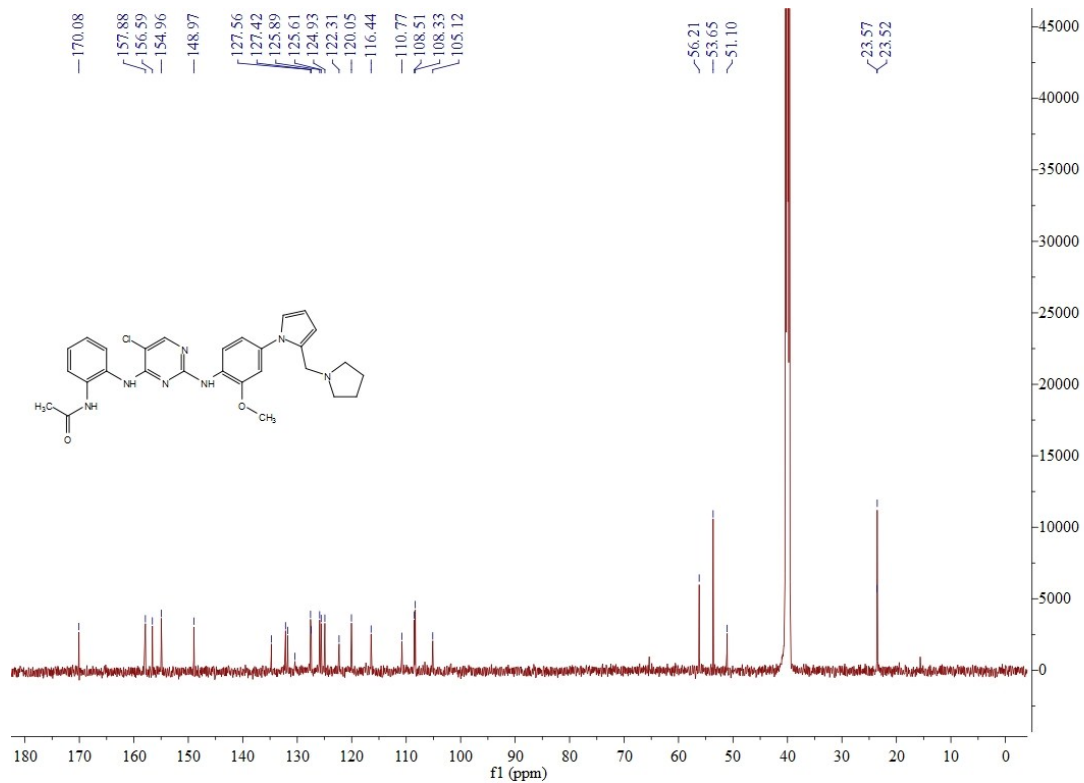


Fig. 7-3 <sup>13</sup>C-NMR spectrum of 9g

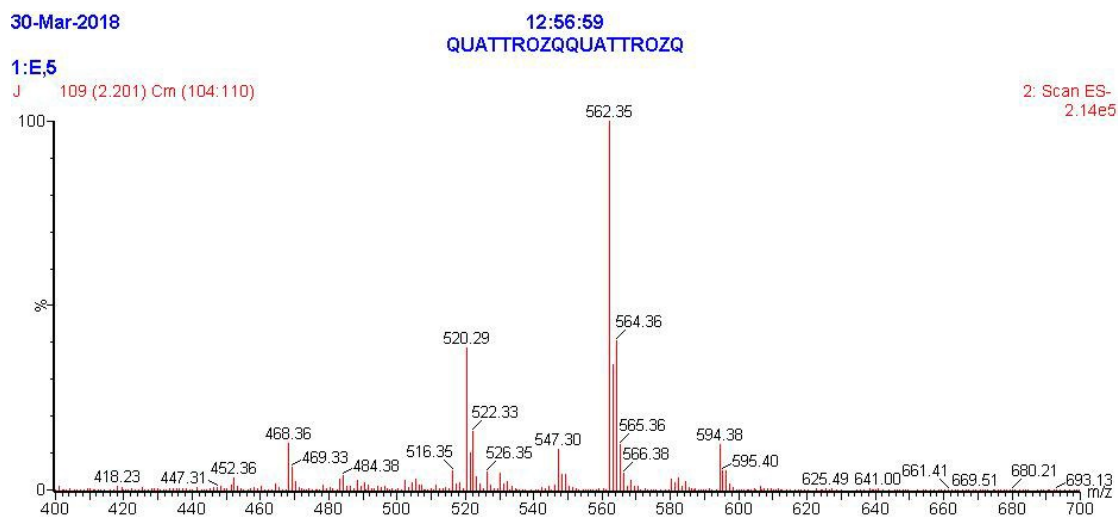


Fig. 8-1 MS spectrum of 9h

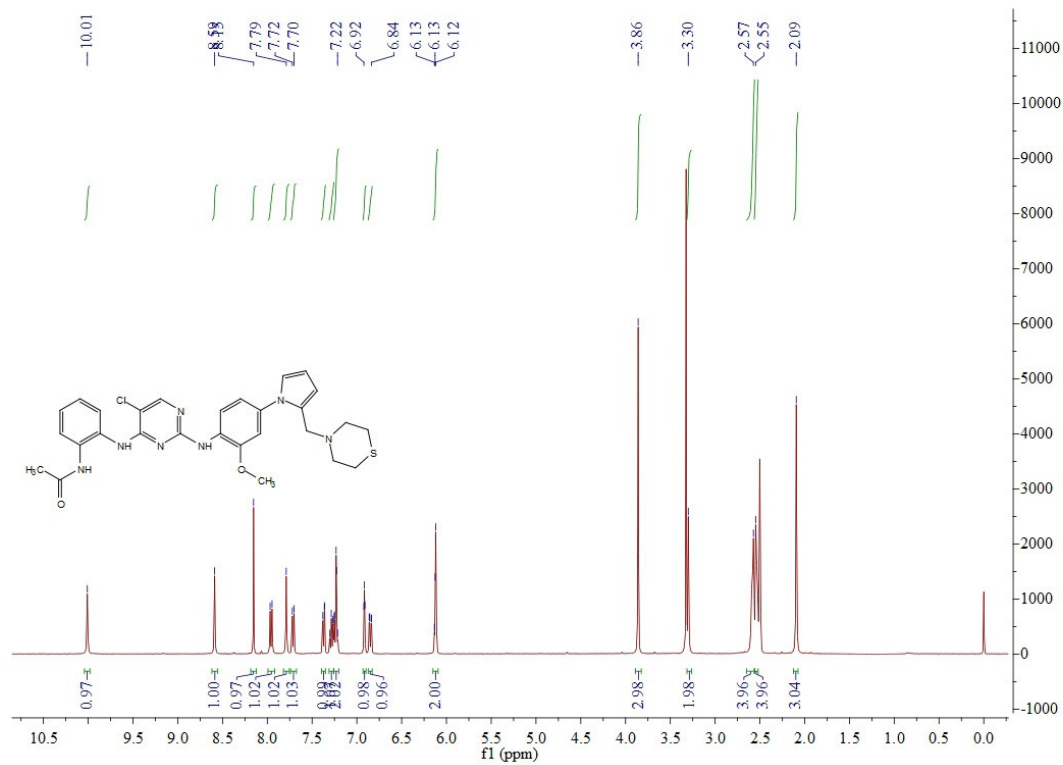


Fig. 8-2 <sup>1</sup>H-NMR spectrum of 9h

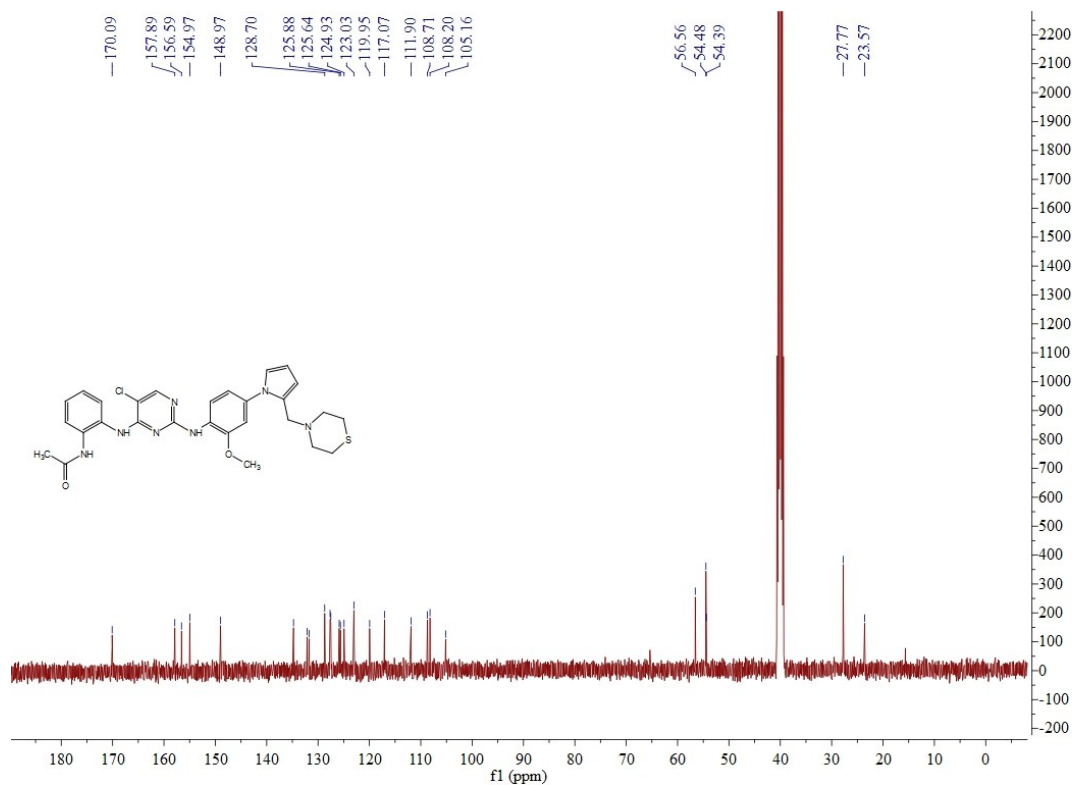


Fig. 8-3 <sup>13</sup>C-NMR spectrum of 9h

30-Mar-2018

13:02:57  
QUATTROZQUATTROZQ

1:E,6

J 16 (0.323) Cm (12:16)

2: Scan ES-  
1.99e5

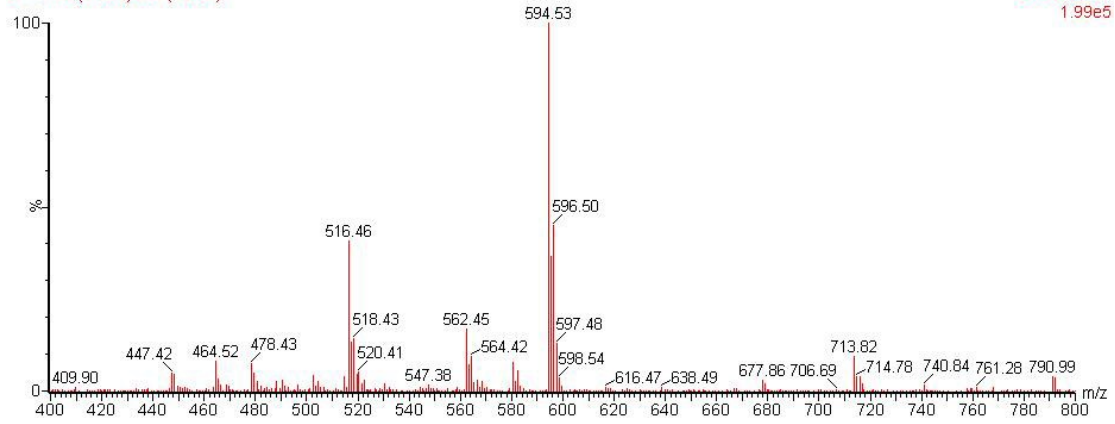


Fig. 9-1 MS spectrum of 9i

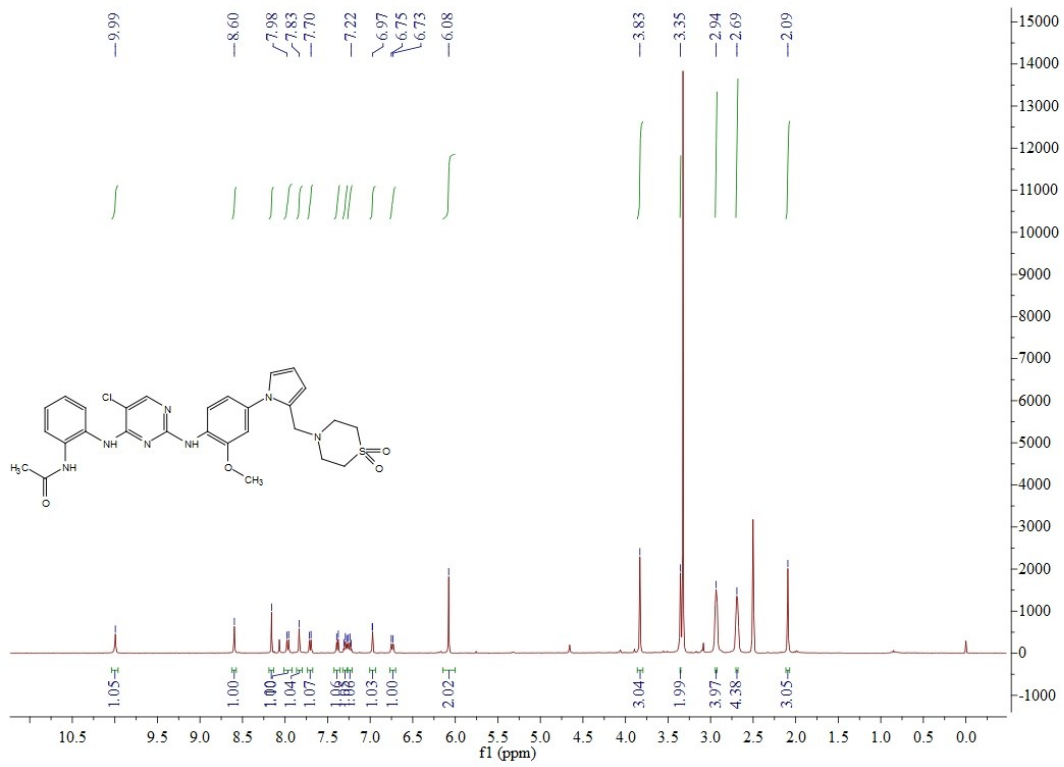


Fig. 9-2 <sup>1</sup>H-NMR spectrum of 9i

07-Sep-2017

12:54:10  
QUATTROZQUATTROZQ

1:C,2

WJ 142 (2.867) Cm (137:144)

2: Scan ES-  
8.37e4

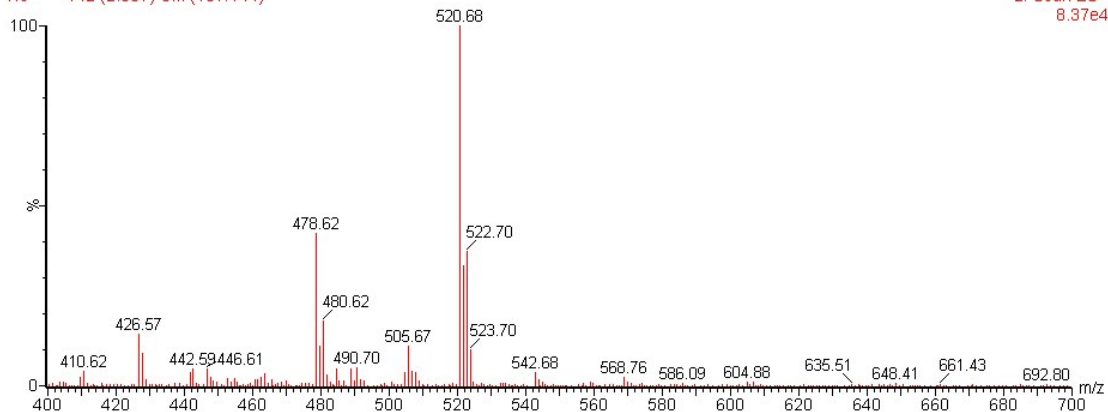


Fig. 10-1 MS spectrum of 9j

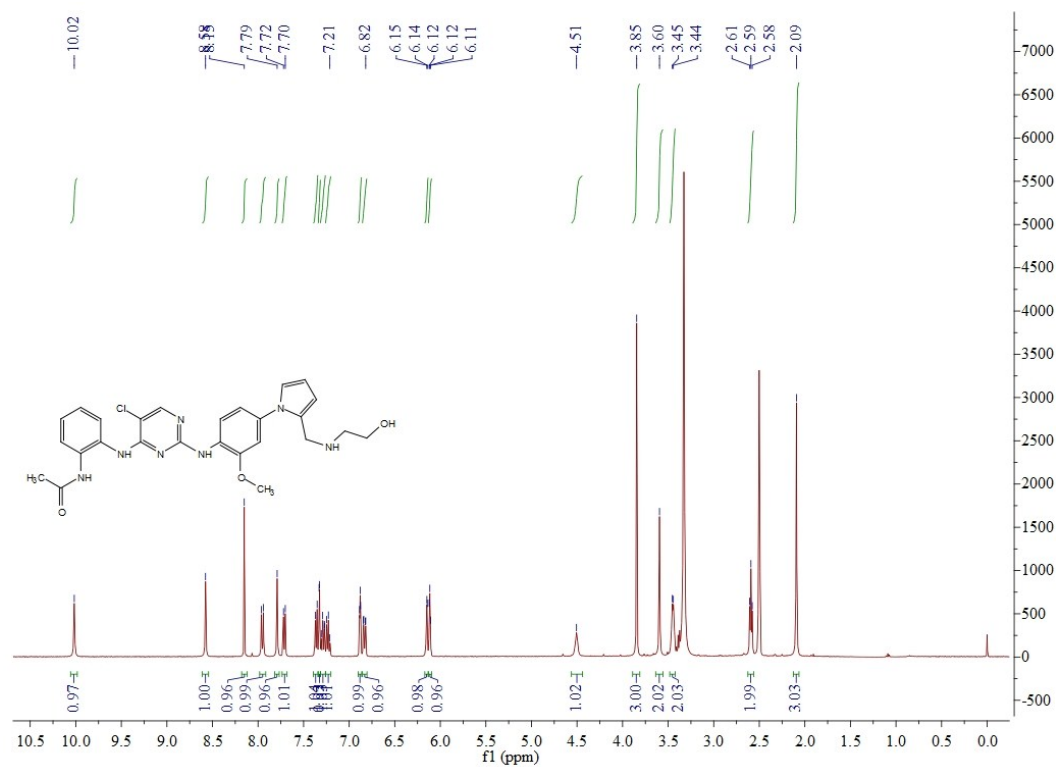


Fig. 10-2 <sup>1</sup>H-NMR spectrum of 9j

12-Sep-2017

17:08:24  
QUATTROZQUATTROZQ

1:B,6

WJ 232 (4.687) Cm (231:235)

2: Scan ES-  
1.71e5

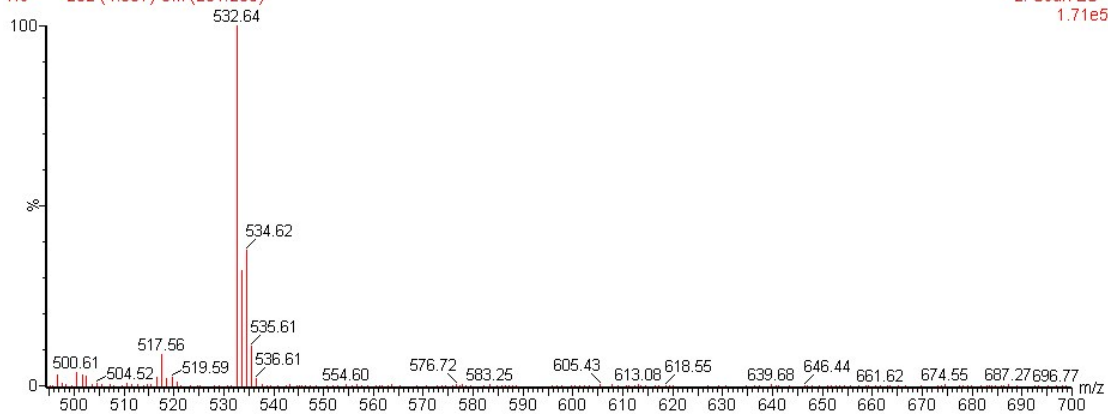


Fig. 11-1 MS spectrum of 9k

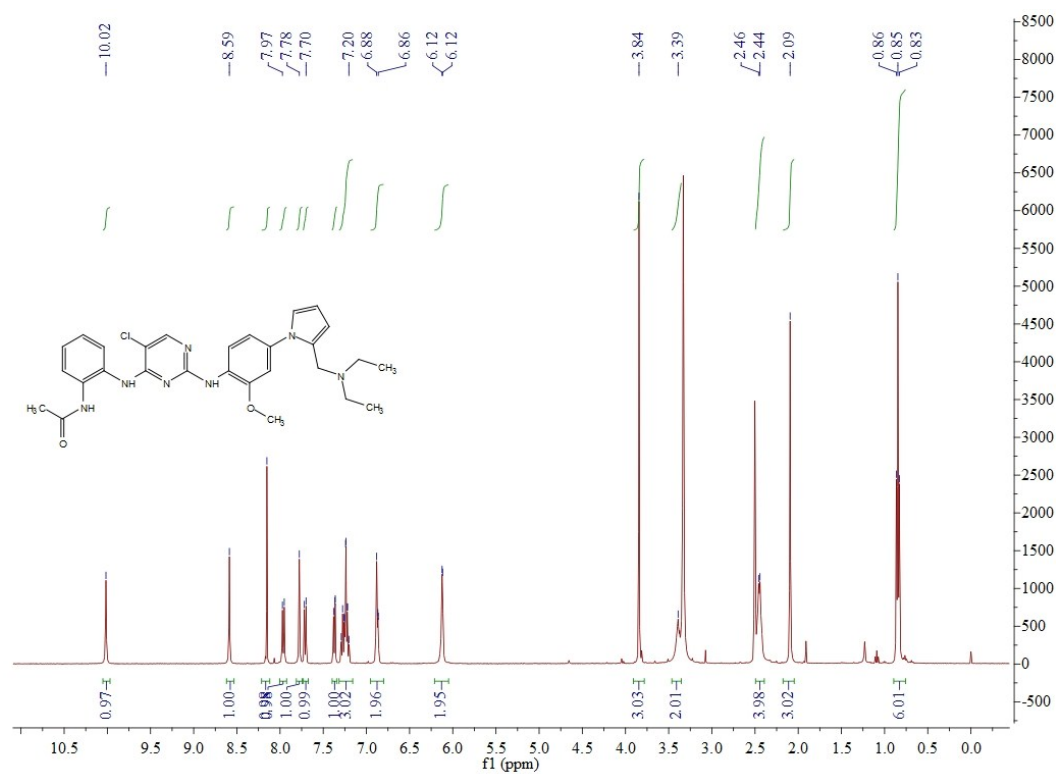


Fig. 11-2 <sup>1</sup>H-NMR spectrum of 9k

07-Sep-2017

16:33:37  
QUATTROZQUATTROZQ

1:E,4

WJ 160 (3.231) Cm (152:160)

2: Scan ES-  
4.63e4

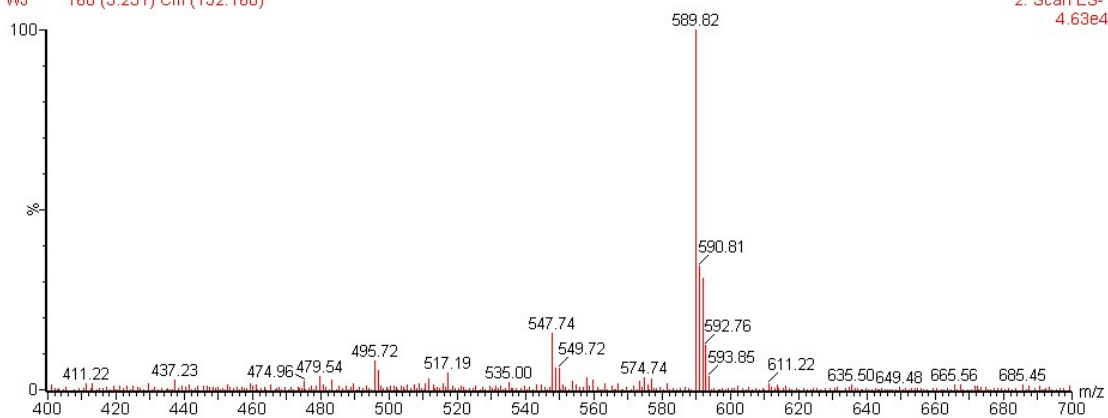


Fig. 12-1 MS spectrum of 9I

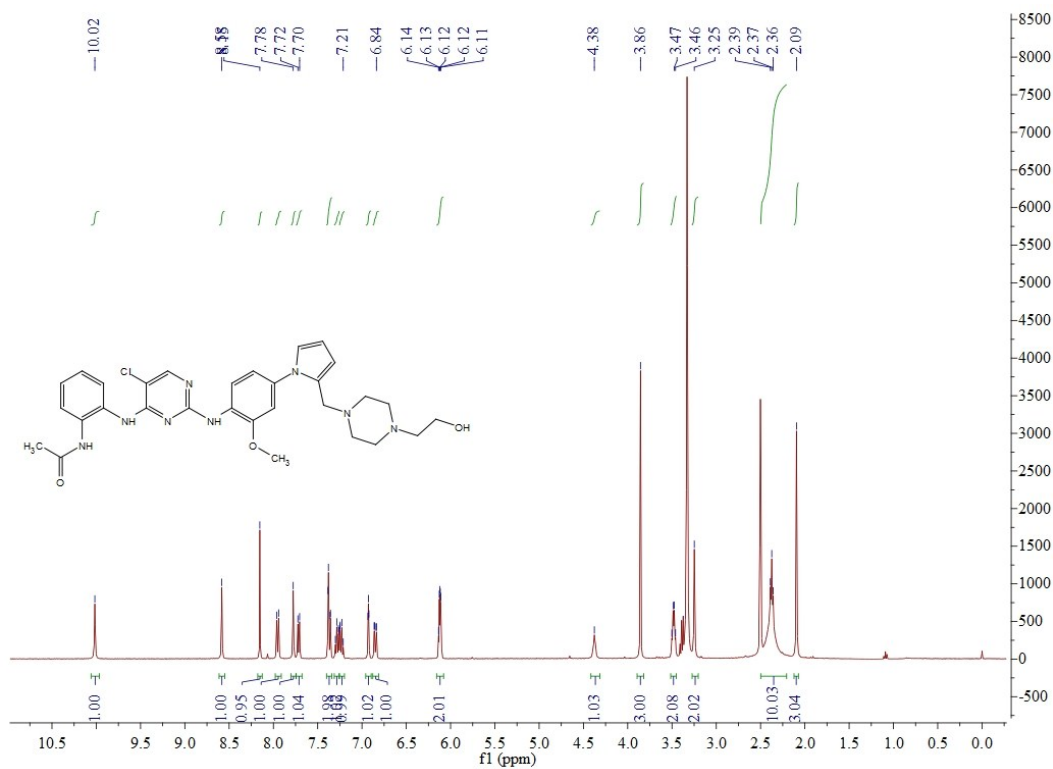


Fig. 12-2 <sup>1</sup>H-NMR spectrum of 9I



08-Sep-2017

16:12:51  
QUATTROZQUATTROZQ

1:C,4

WJ 172 (3.477) Cm (168:173)

2: Scan ES-  
5.24e4

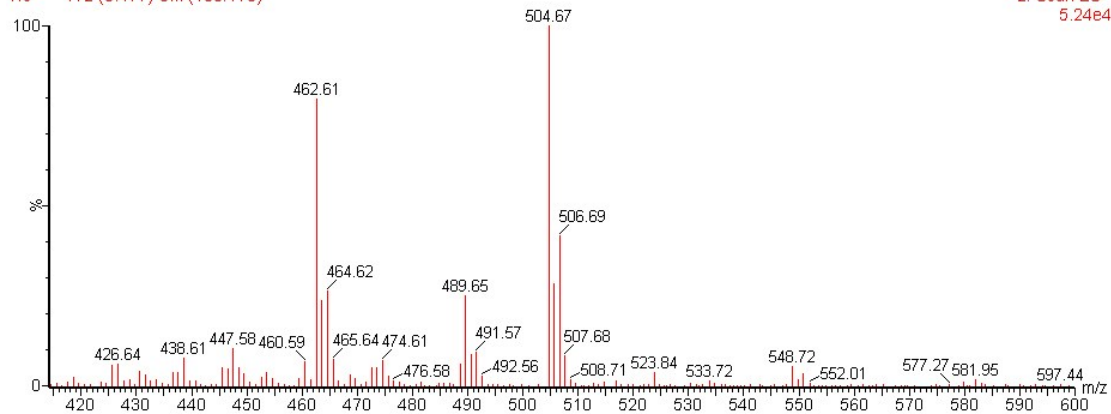


Fig. 13-1 MS spectrum of 9m

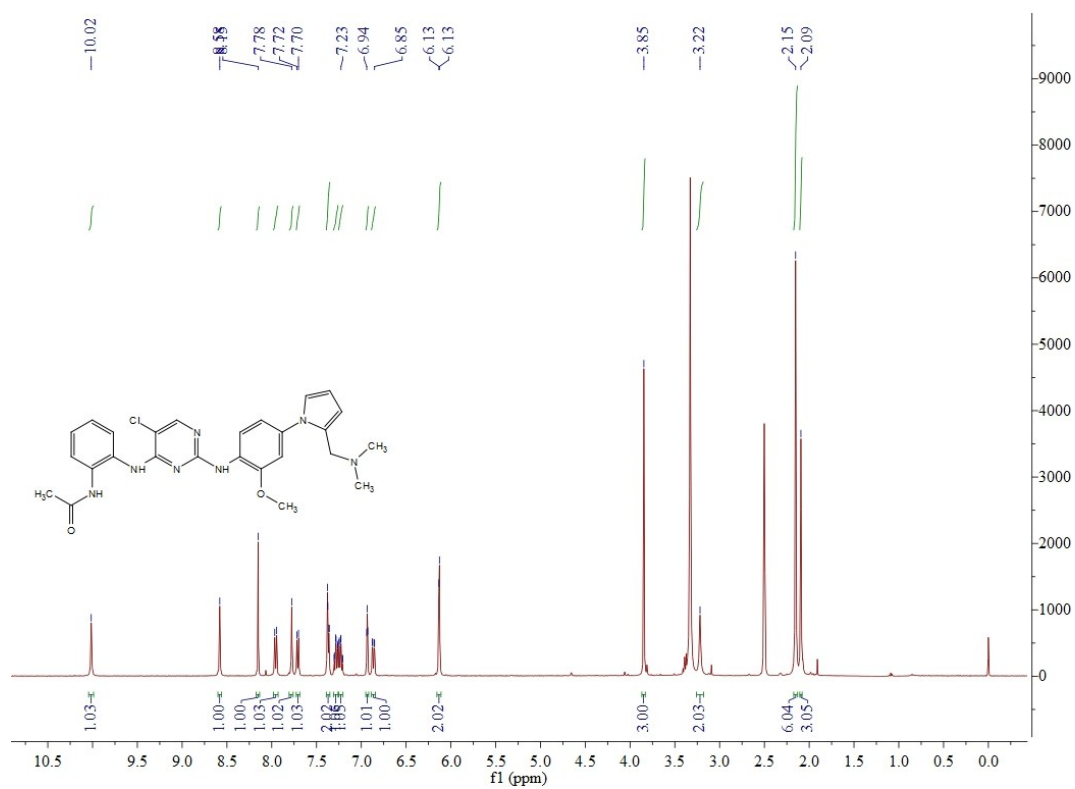


Fig. 13-2 <sup>1</sup>H-NMR spectrum of 9m

12-Sep-2017

17:08:24  
QUATTROZQUATTROZQ

1:B,6

WJ 127 (2.566) Cm (126:131)

2: Scan ES-  
3.58e5

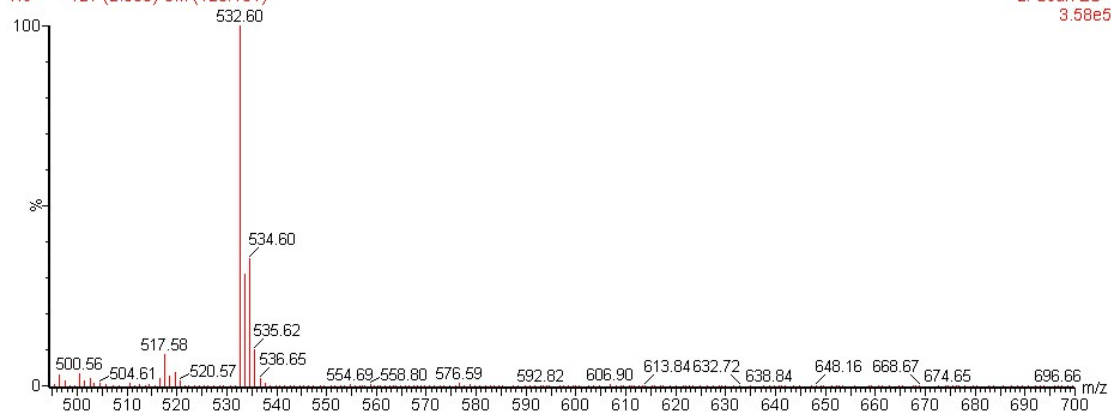


Fig. 14-1 MS spectrum of 9n

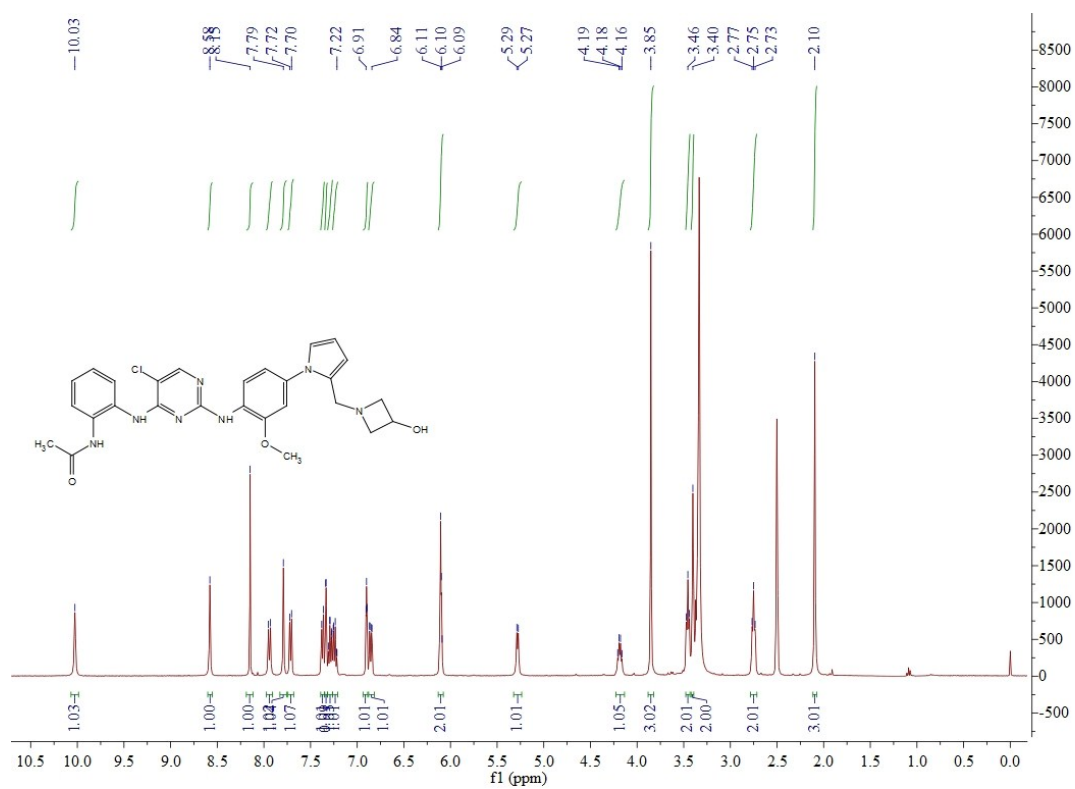


Fig. 14-2 <sup>1</sup>H-NMR spectrum of 9n

25-Aug-2017

09:25:07  
QUATTROZQUATTROZQ

1:A,3

WJ 71 (1.425) Cm (68.75)

1: Scan ES+  
6.51e6

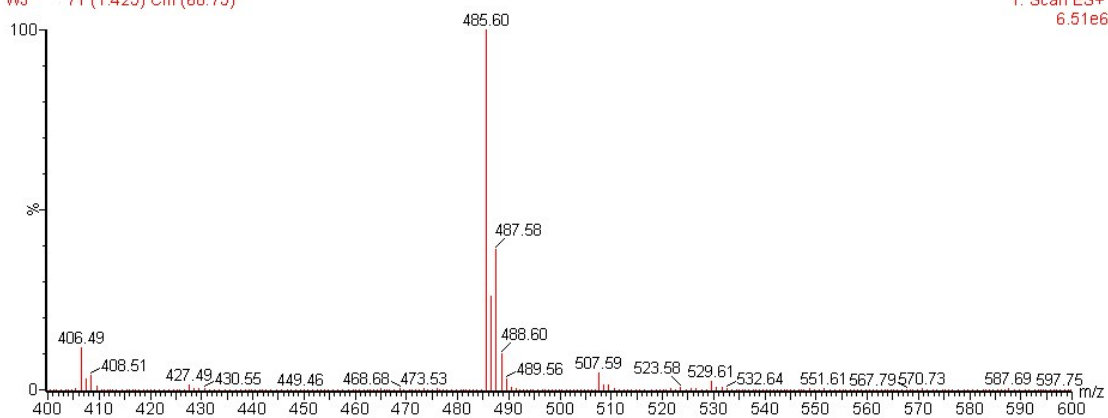


Fig. 15-1 MS spectrum of 10a

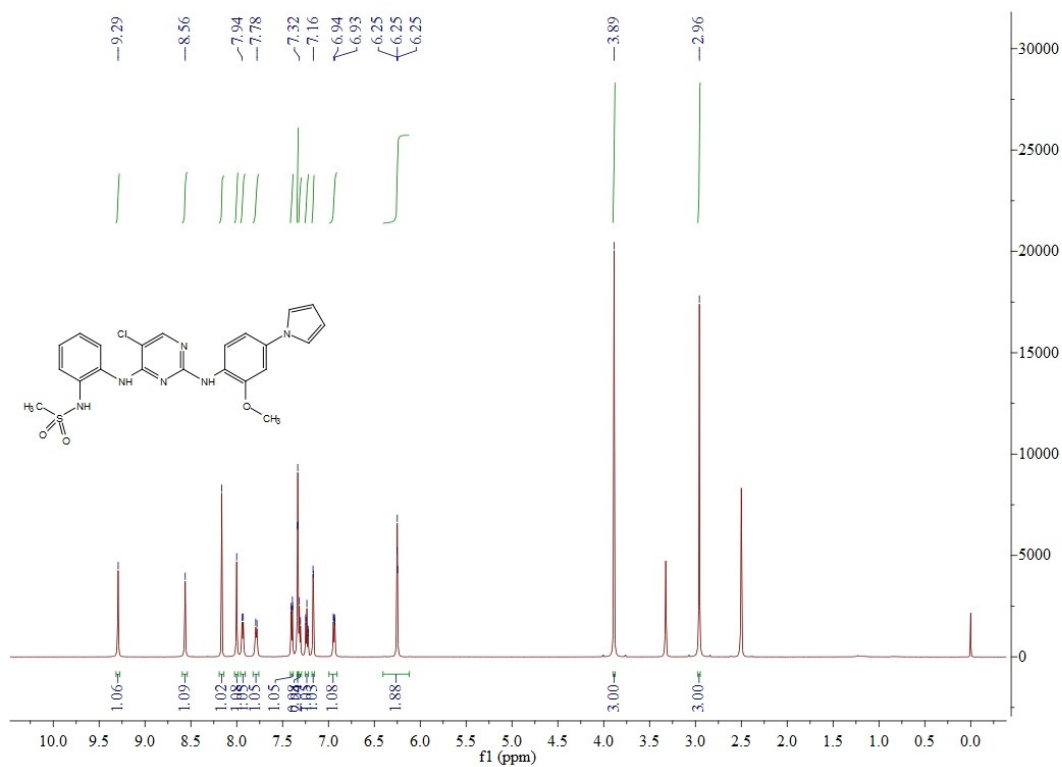


Fig. 15-2 <sup>1</sup>H-NMR spectrum of 10a

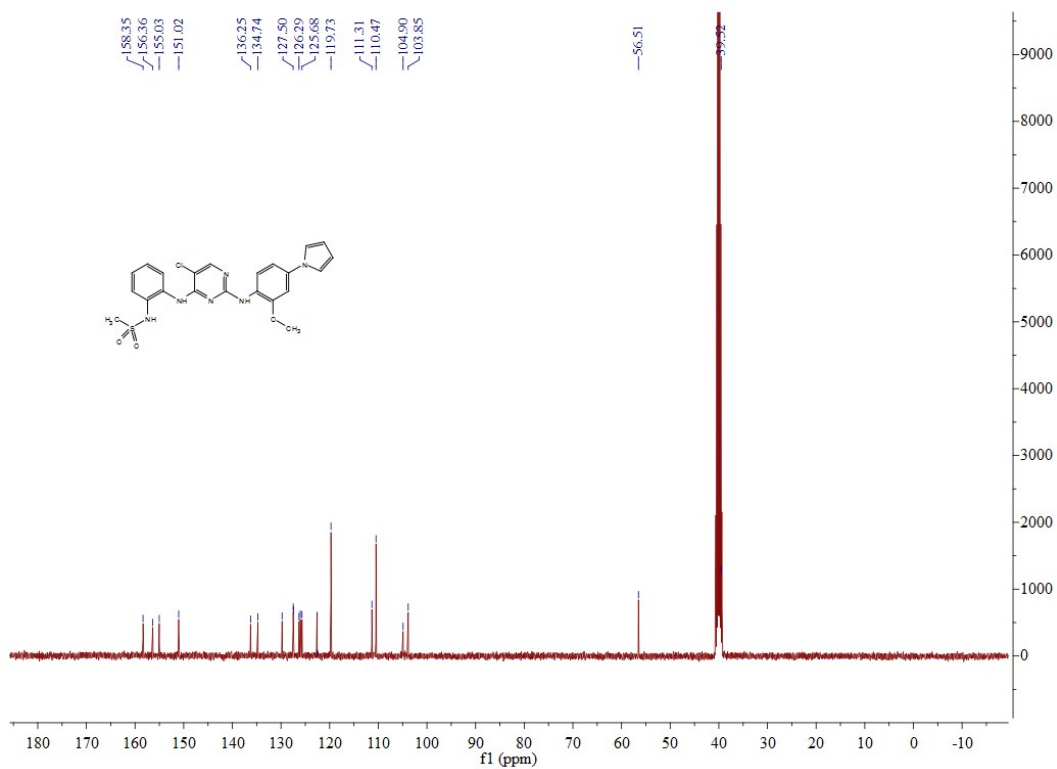


Fig. 15-3  $^{13}\text{C}$ -NMR spectrum of 10a

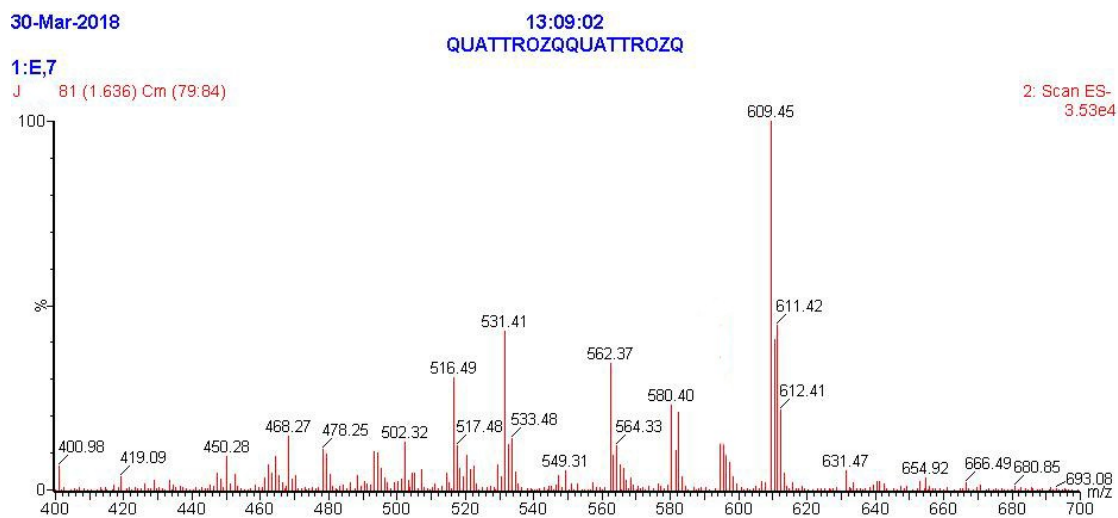


Fig. 16-1 MS spectrum of 10b

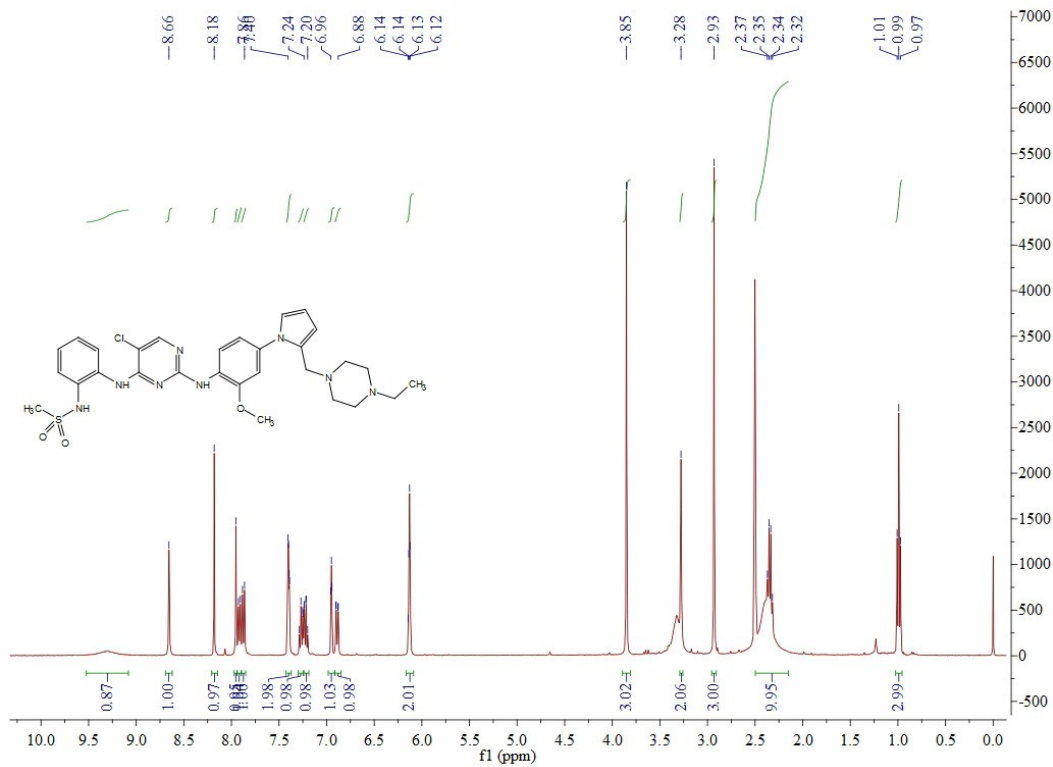


Fig. 16-2 <sup>1</sup>H-NMR spectrum of 10b

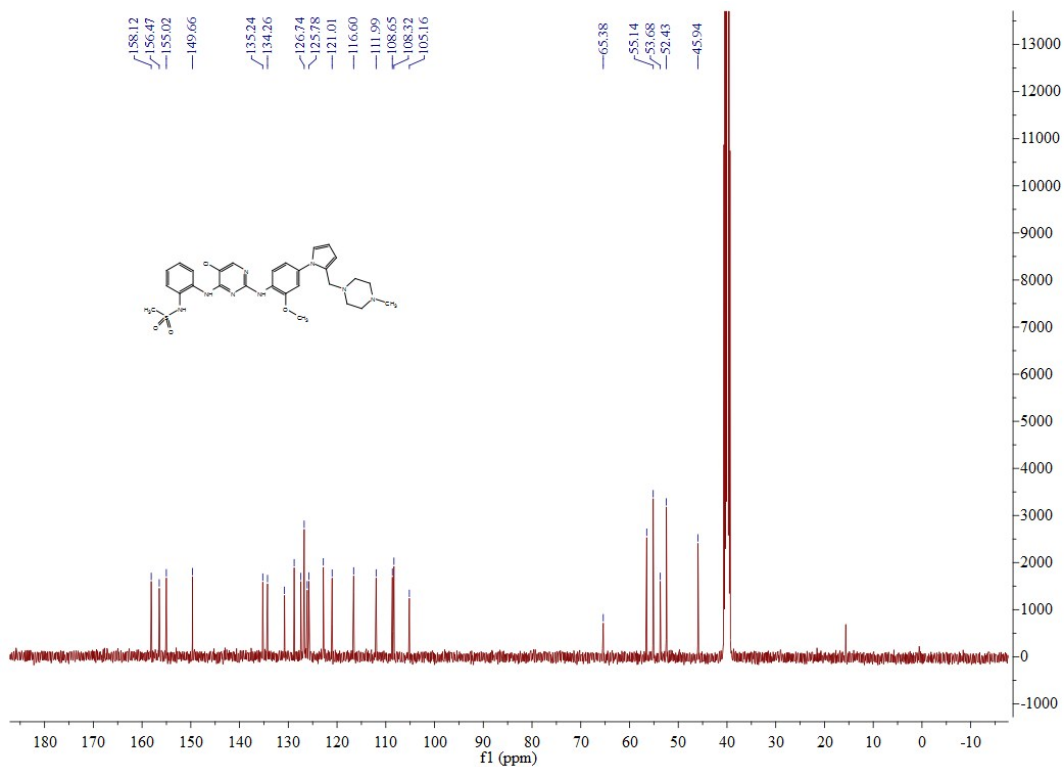


Fig. 16-3 <sup>13</sup>C-NMR spectrum of 10b

30-Mar-2018

12:51:02  
QUATTROZQUATTROZQ

1:E,4

J 78 (1.575) Cm (76.79)

2: Scan ES-  
1.91e5

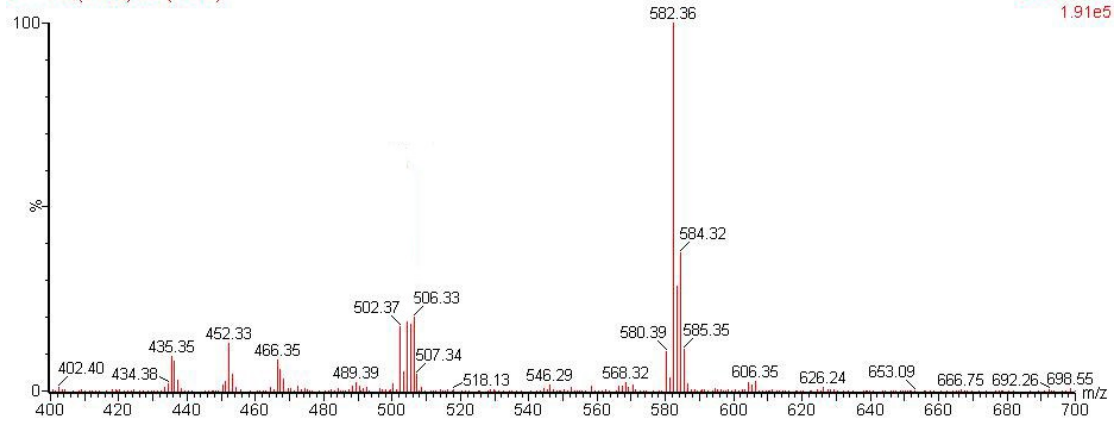


Fig. 17-1 MS spectrum of 10c

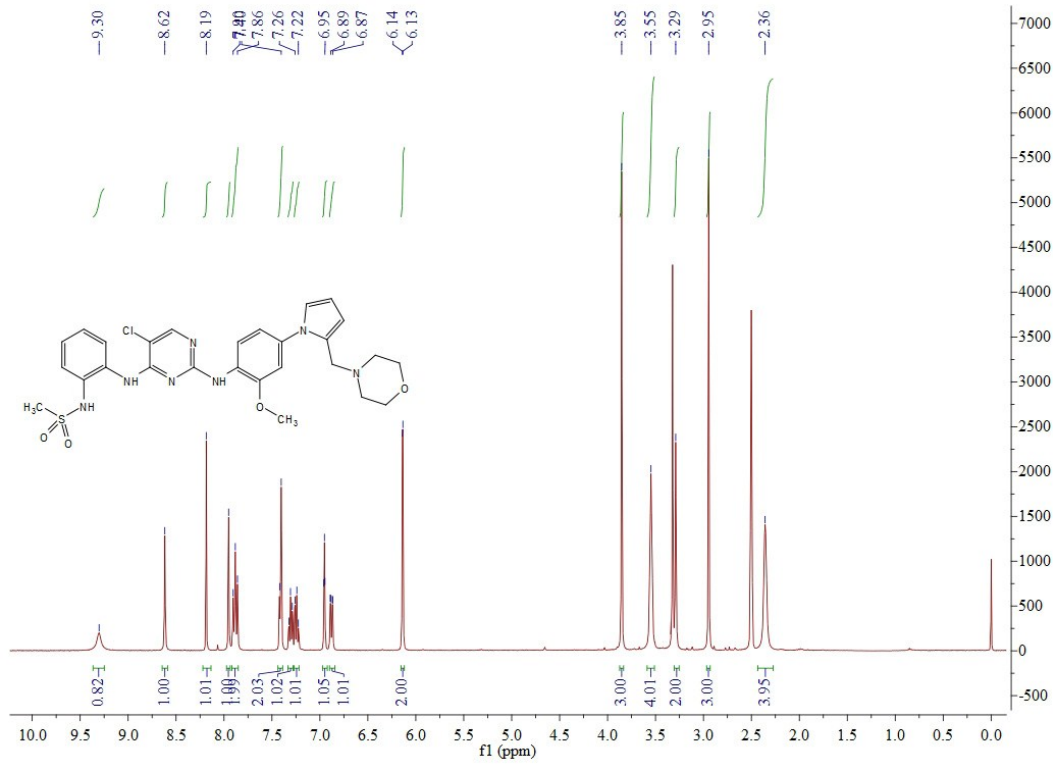


Fig. 17-2 <sup>1</sup>H-NMR spectrum of 10c

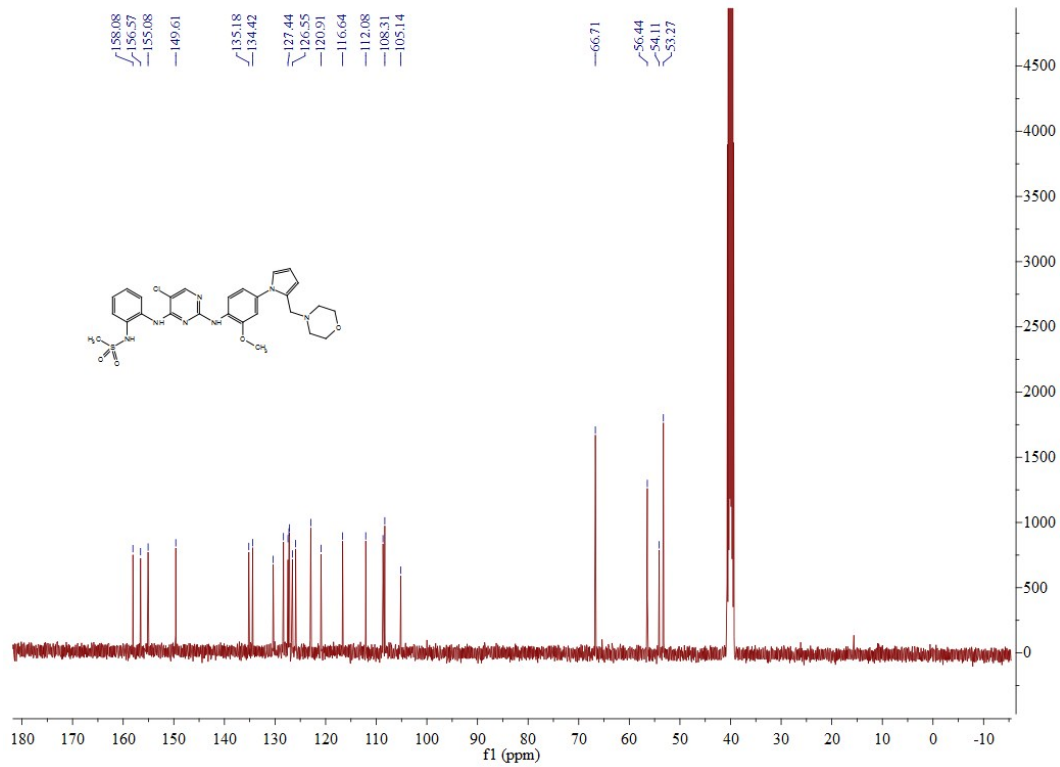


Fig. 17-3  $^{13}\text{C}$ -NMR spectrum of 10c

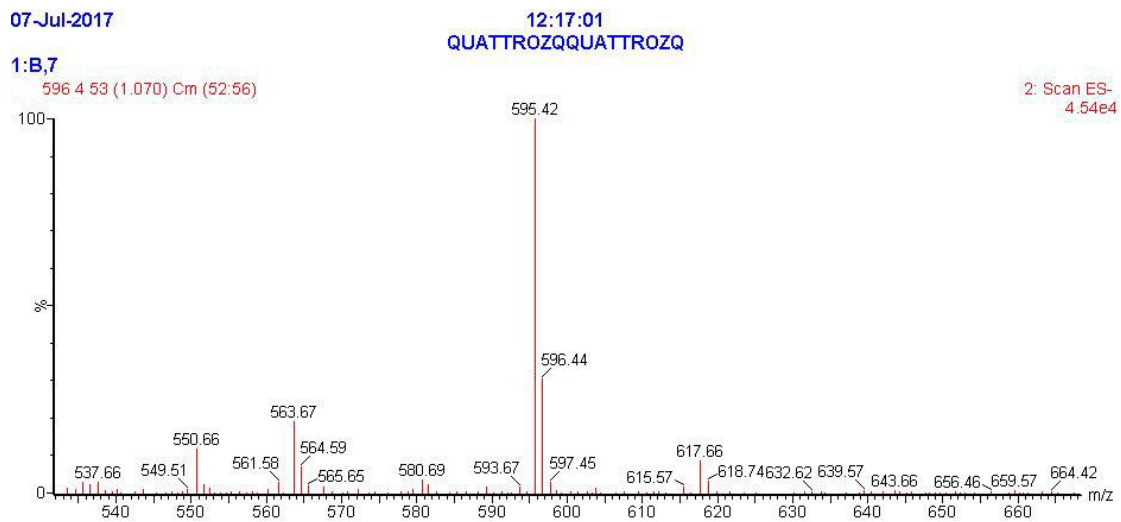


Fig. 18-1 MS spectrum of 10d

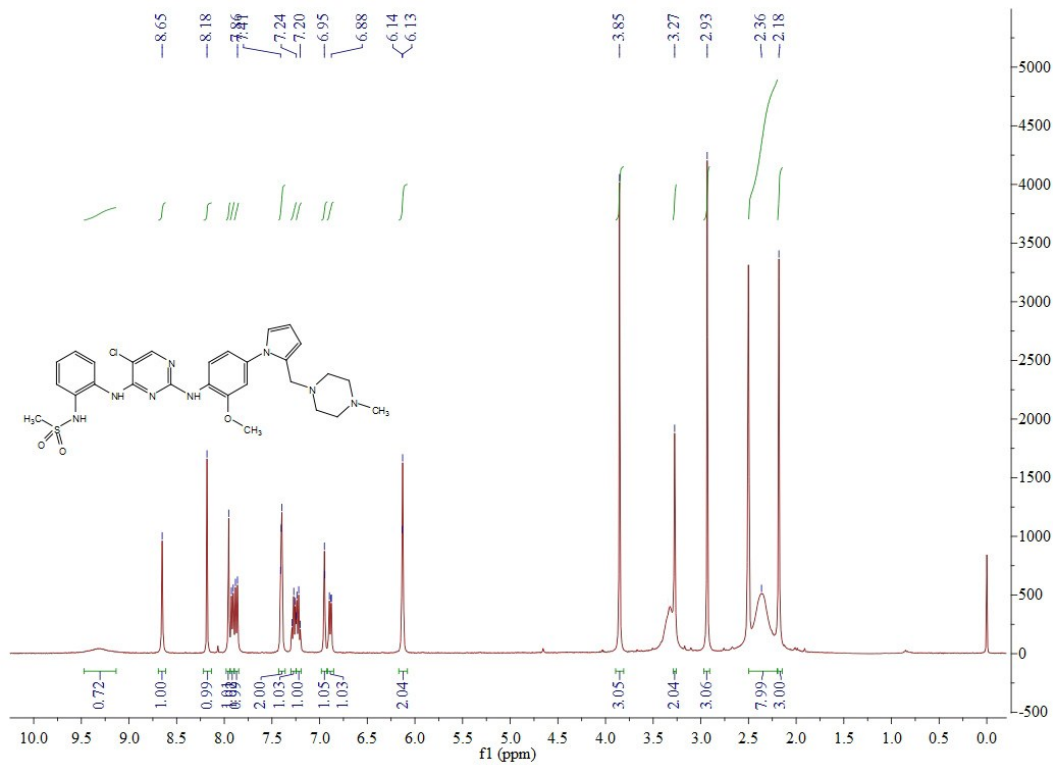


Fig. 18-2 <sup>1</sup>H-NMR spectrum of 10d

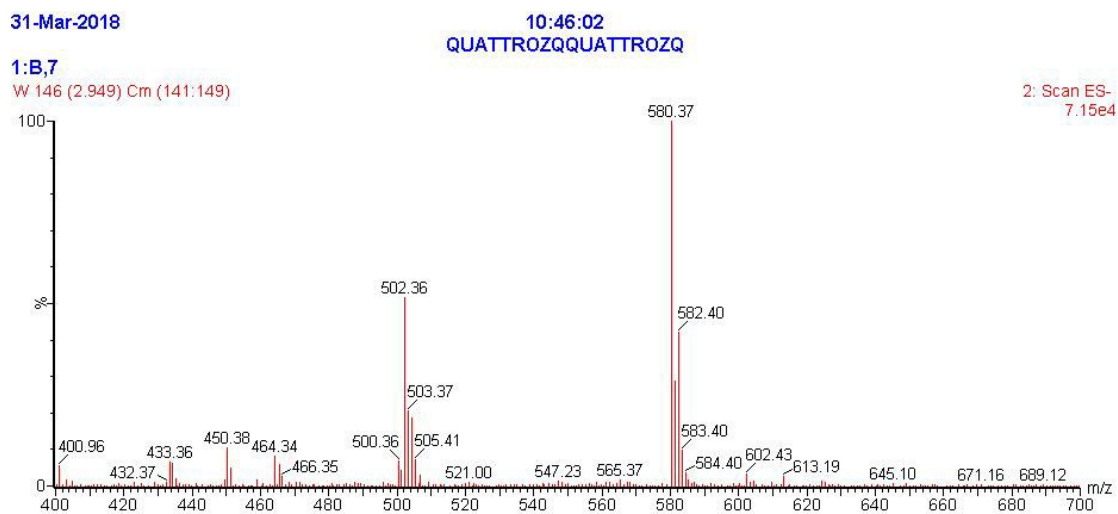


Fig. 19-1 MS spectrum of 10e



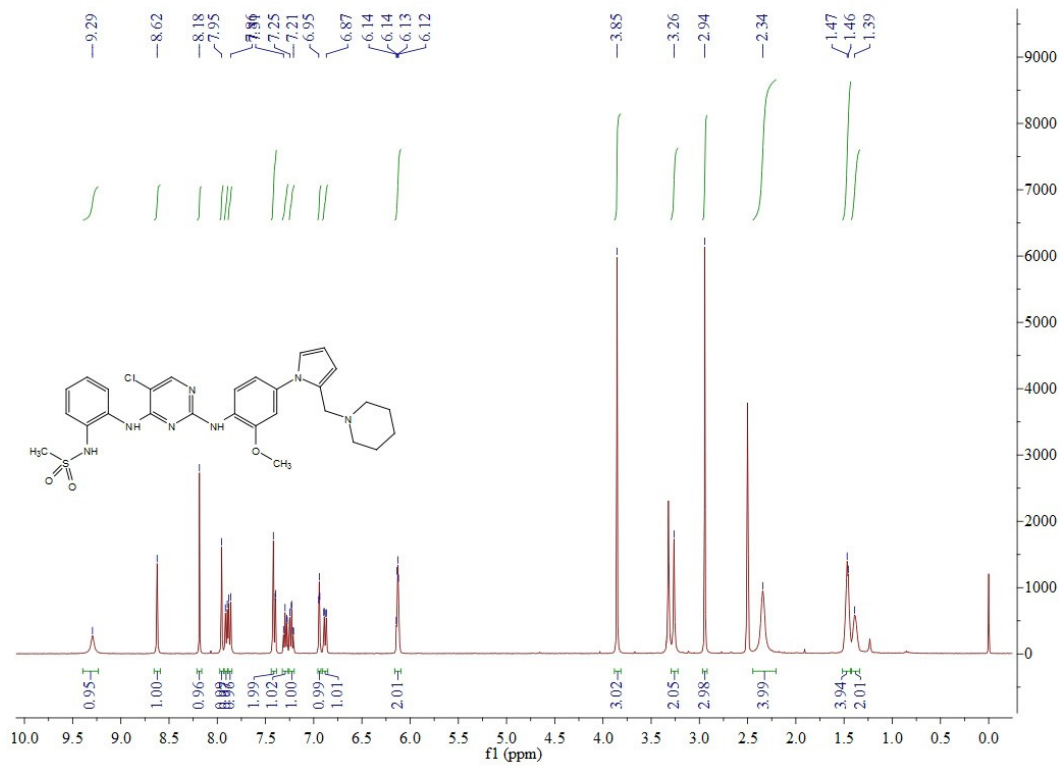


Fig. 19-2 <sup>1</sup>H-NMR spectrum of 10e

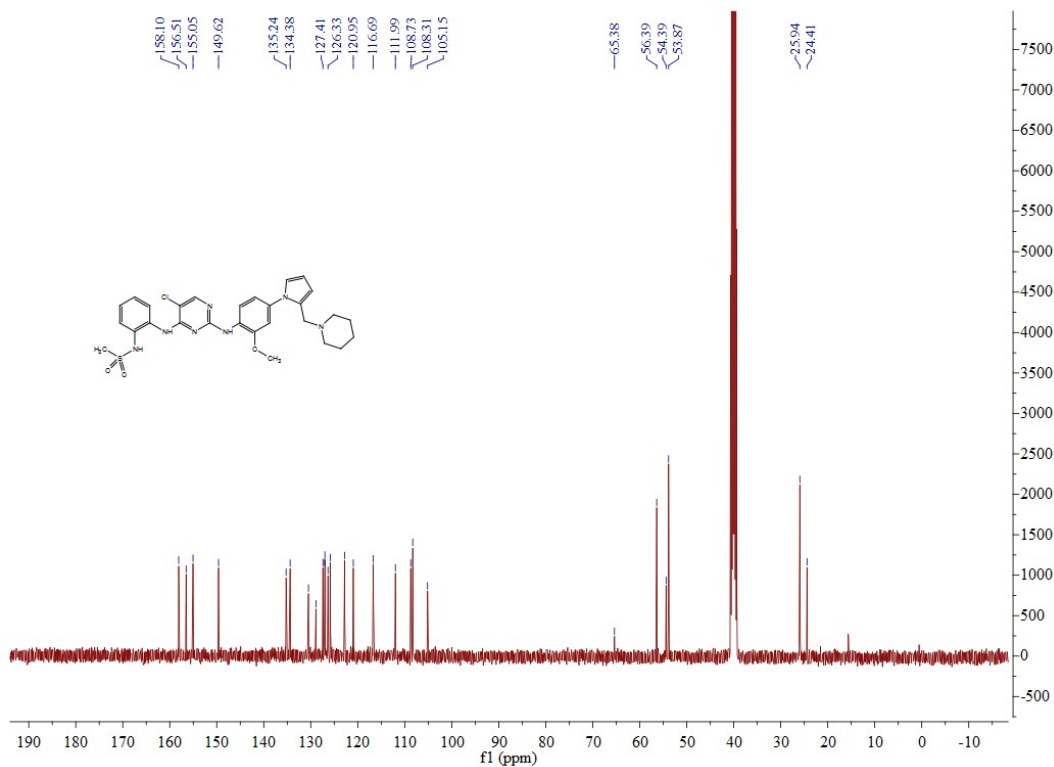


Fig. 19-3 <sup>13</sup>C-NMR spectrum of 10e

12-Jul-2017

16:30:32  
QUATTROZQUATTROZQ

1:E,5

W 238 (4.795) Cm (235:240)

1: Scan ES+  
8.72e5

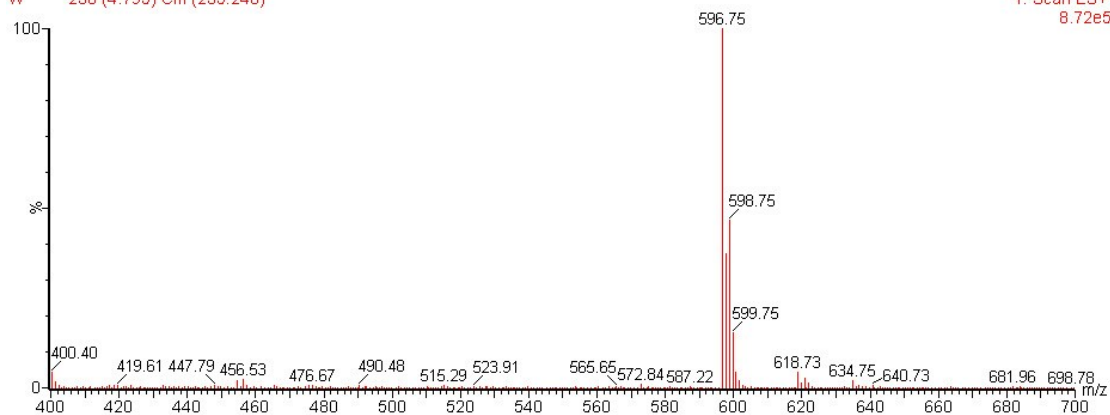


Fig. 20-1 MS spectrum of 10f

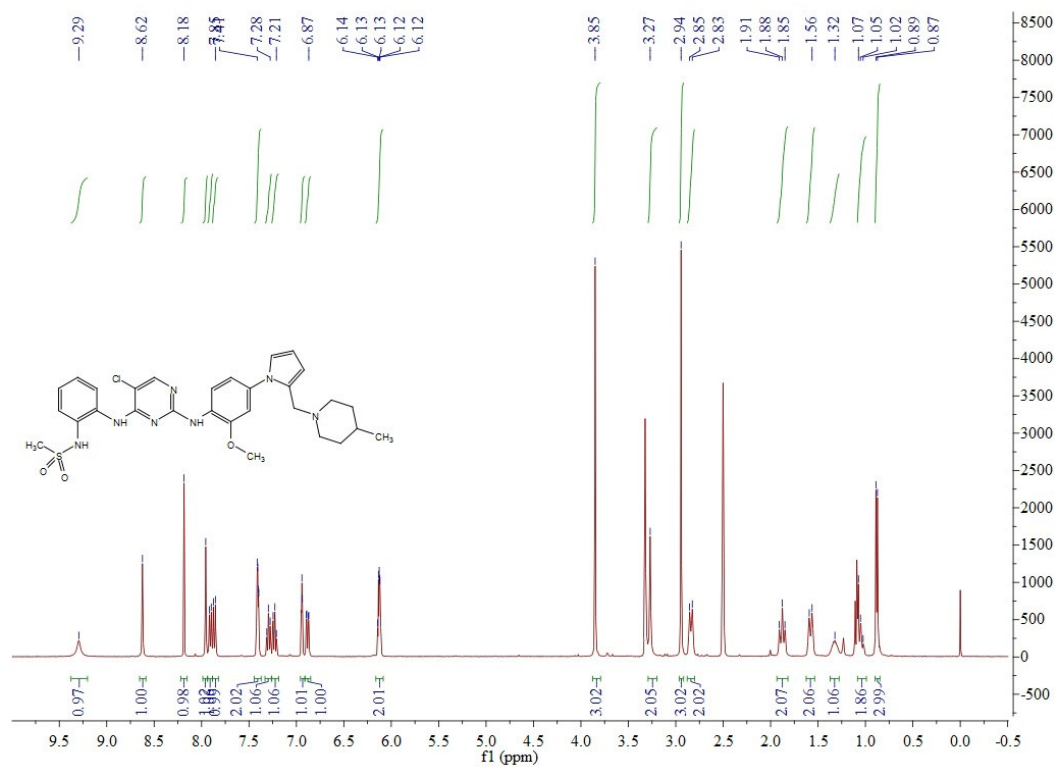


Fig. 20-2 <sup>1</sup>H-NMR spectrum of 10f

31-Mar-2018

11:00:28  
QUATTROZQUATTROZQ

1:C,1

W 144 (2.908) Cm (137:160)

2: Scan ES-  
3.13e4

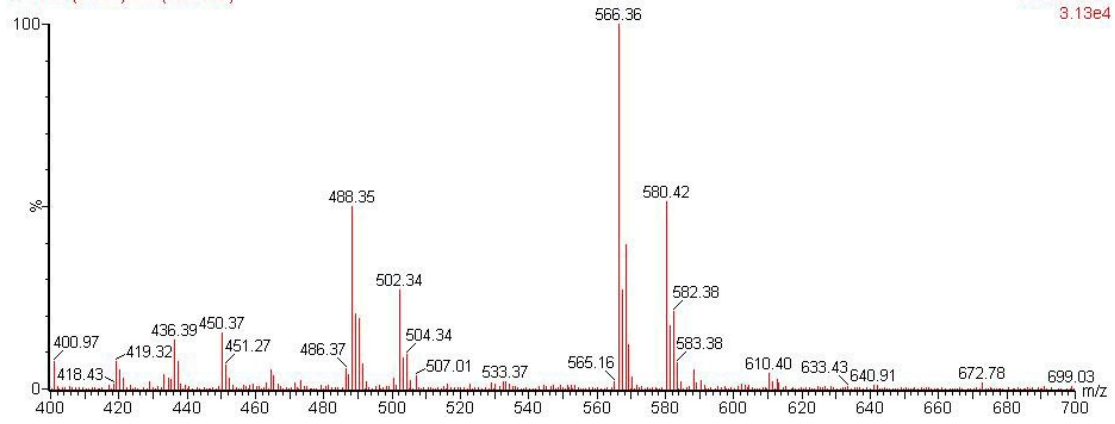


Fig. 21-1 MS spectrum of 10g

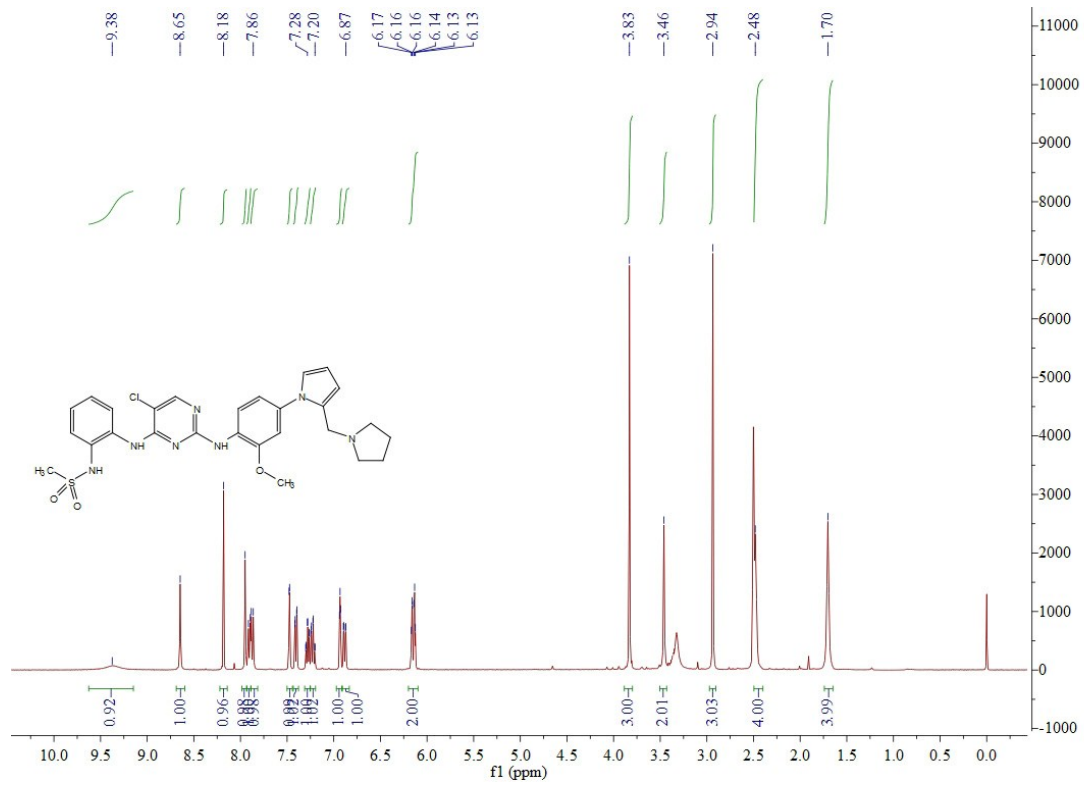


Fig. 21-2 <sup>1</sup>H-NMR spectrum of 10g

30-Mar-2018

12:27:05  
QUATTROZQUATTROZQ

1:D,8

J 105 (2.121) Cm (104:107)

2: Scan ES-  
1.20e5

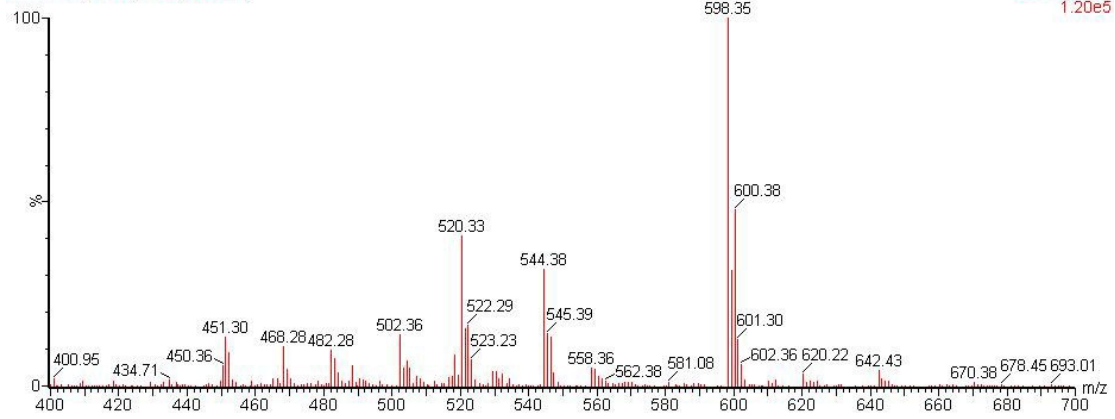


Fig. 22-1 MS spectrum of 10h

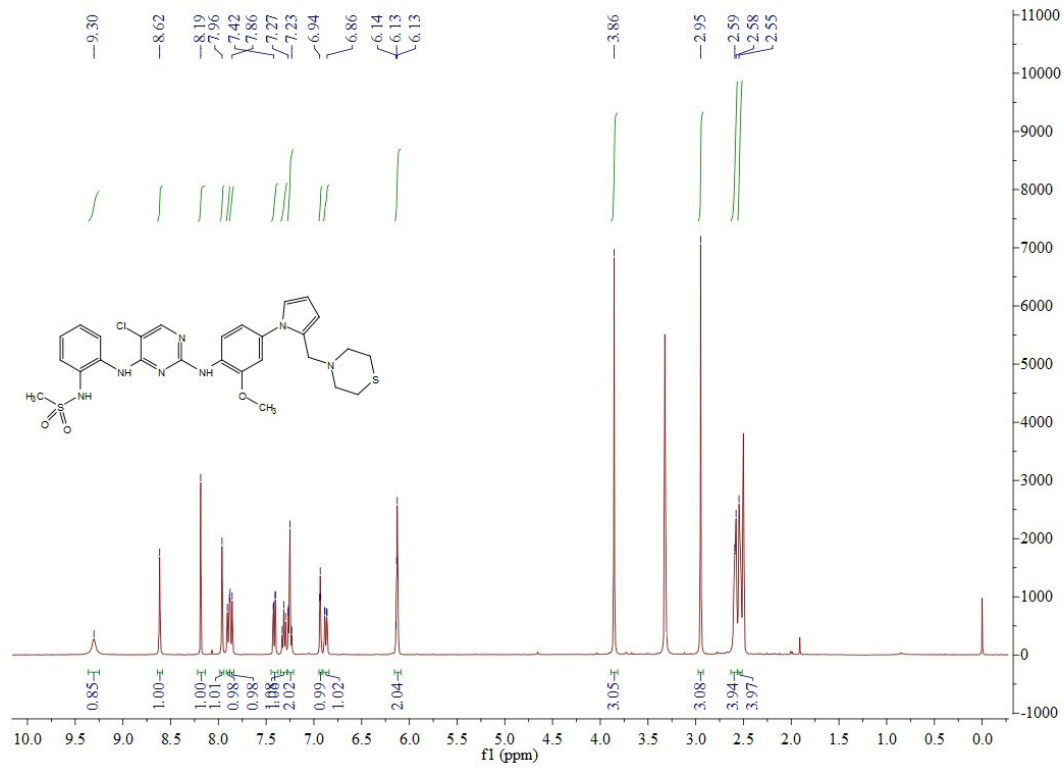


Fig. 22-2 <sup>1</sup>H-NMR spectrum of 10h

07-Sep-2017

11:57:42  
QUATTROZQUATTROZQ

1:B,6

WJ 44 (0.879) Cm (43:48)

1: Scan ES+  
2.30e6

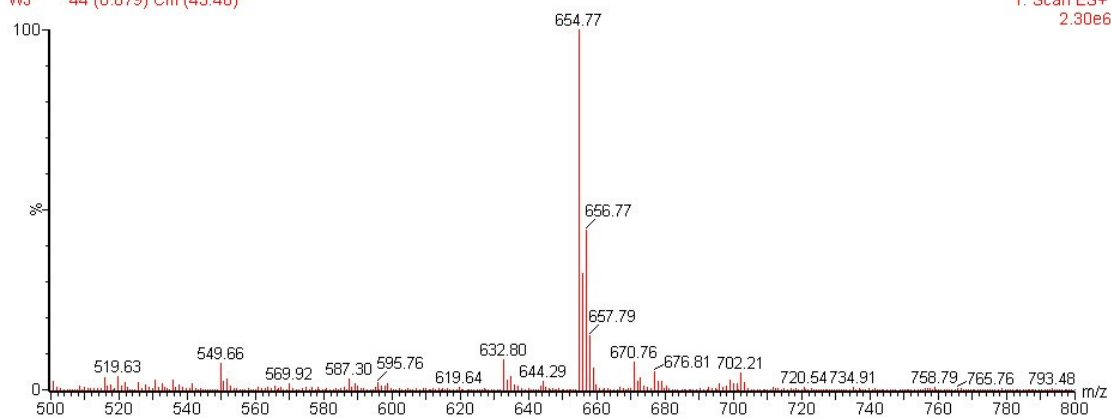


Fig. 23-1 MS spectrum of 10i

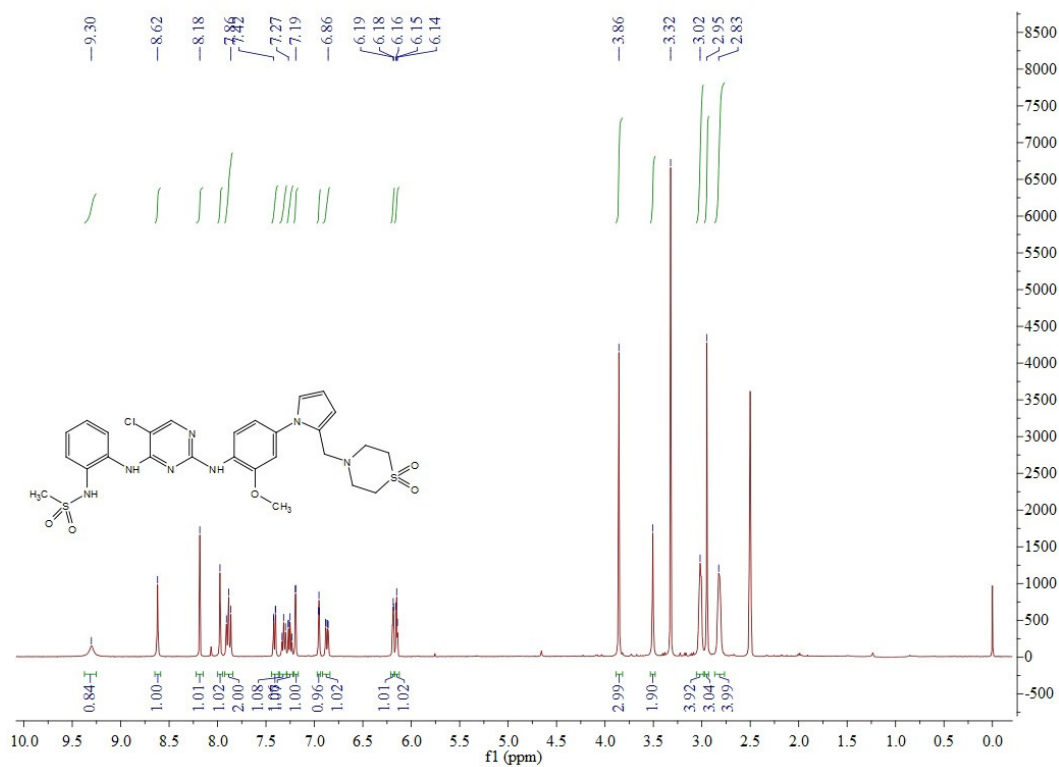


Fig. 23-2 <sup>1</sup>H-NMR spectrum of 10i

07-Sep-2017

12:09:51  
QUATTROZQUATTROZQ

1:B,8

WJ 80 (1.616) Cm (78.81)

2: Scan ES-  
1.28e5

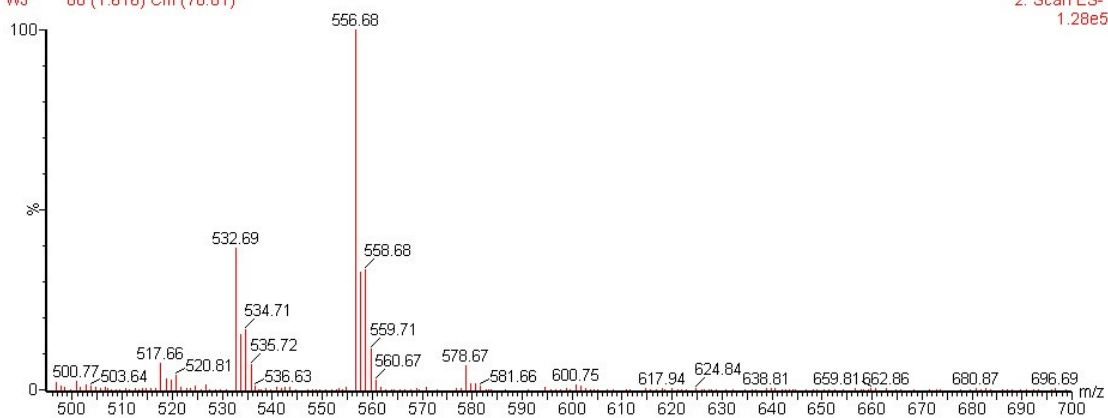


Fig. 24-1 MS spectrum of 10j

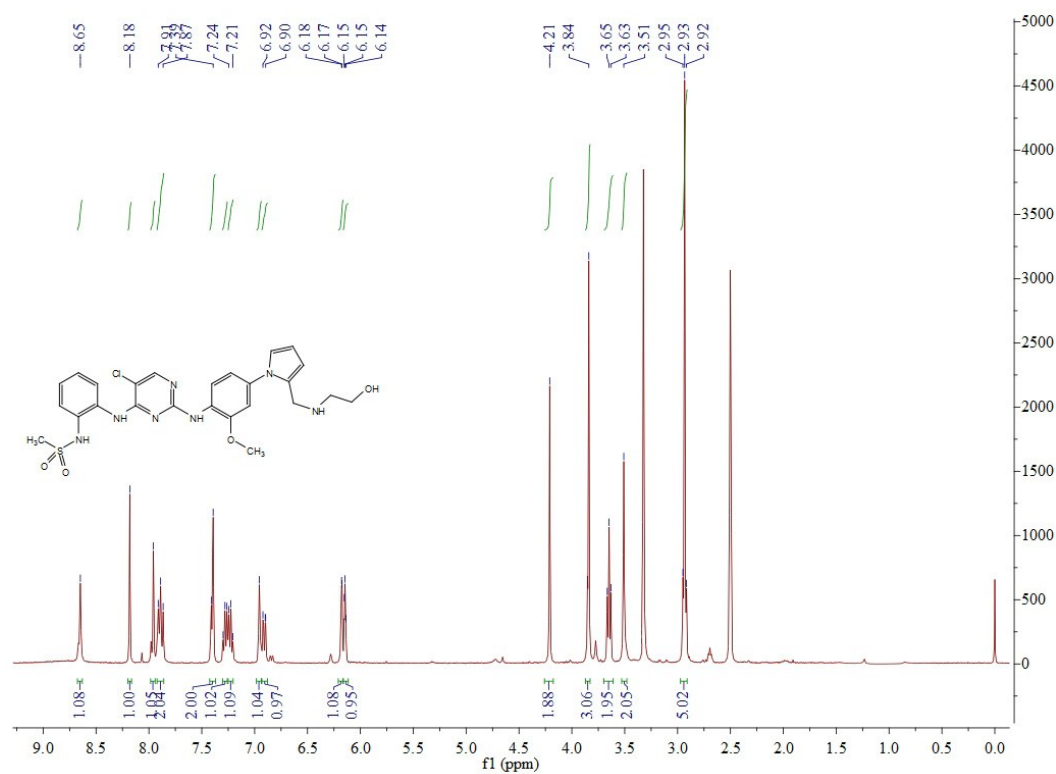


Fig. 24-2 <sup>1</sup>H-NMR spectrum of 10j

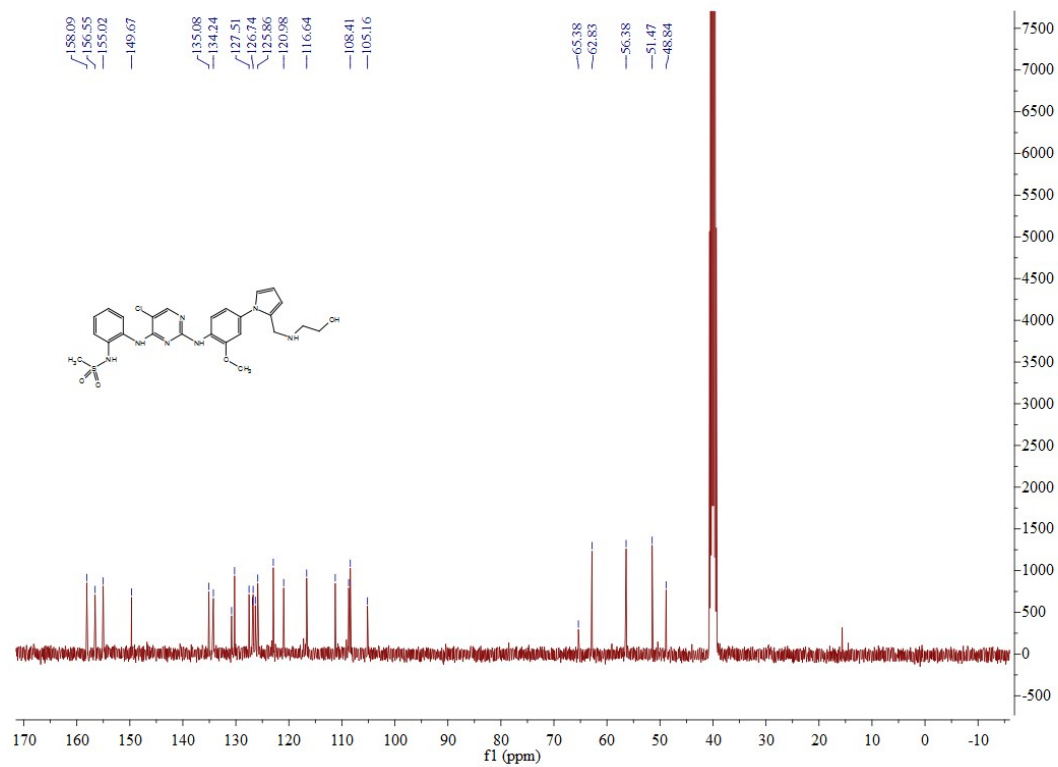


Fig. 24-3  $^{13}\text{C}$ -NMR spectrum of 10j

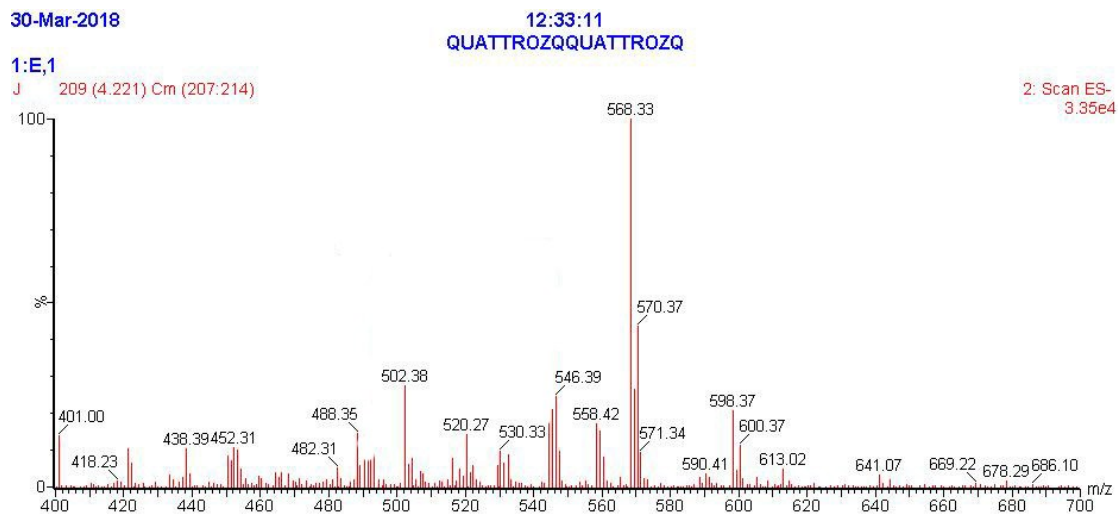


Fig. 25-1 MS spectrum of 10k

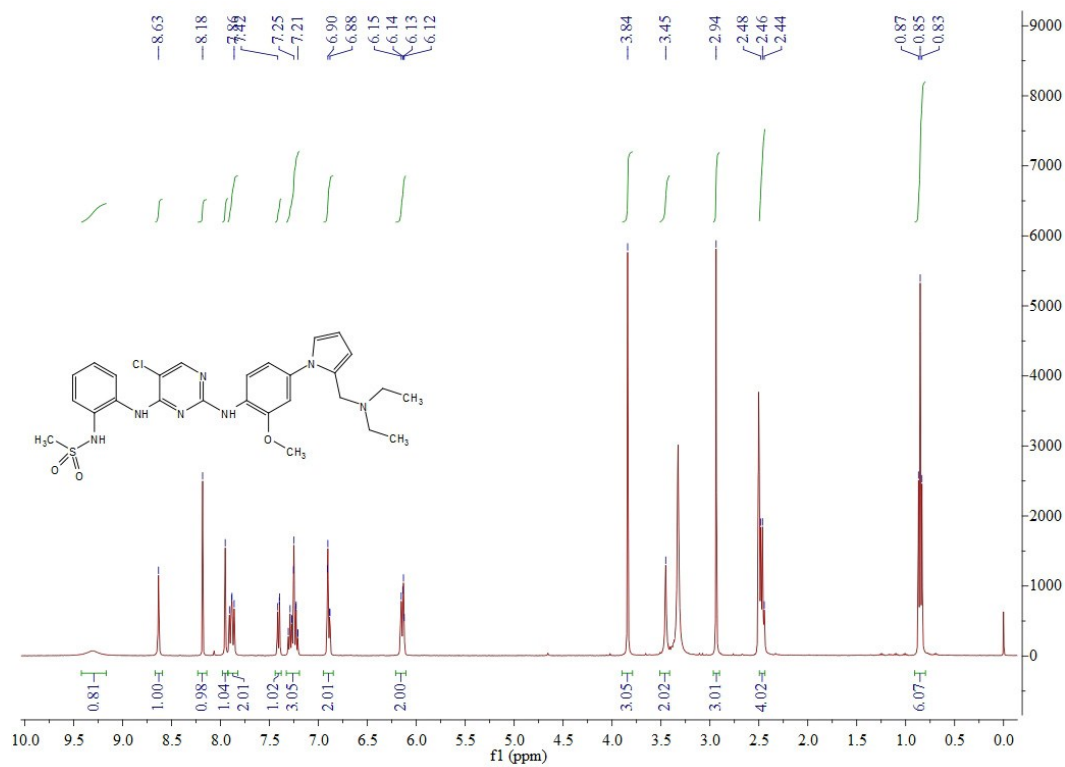


Fig. 25-2 <sup>1</sup>H-NMR spectrum of 10k

07-Sep-2017

16:39:43

QUATTROZQUATTROZQ

1:E,5

WJ 144 (2.907) Cm (140:144)

2: Scan ES-  
3.06e4

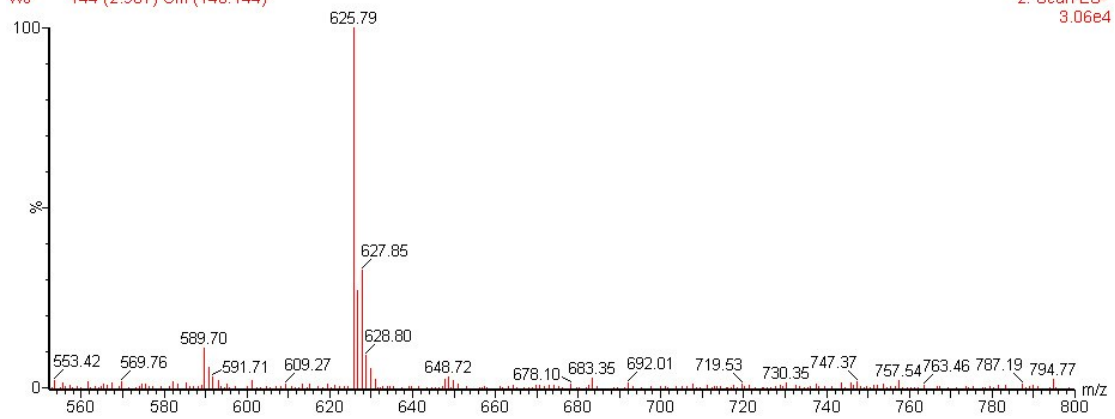


Fig. 26-1 MS spectrum of 10l



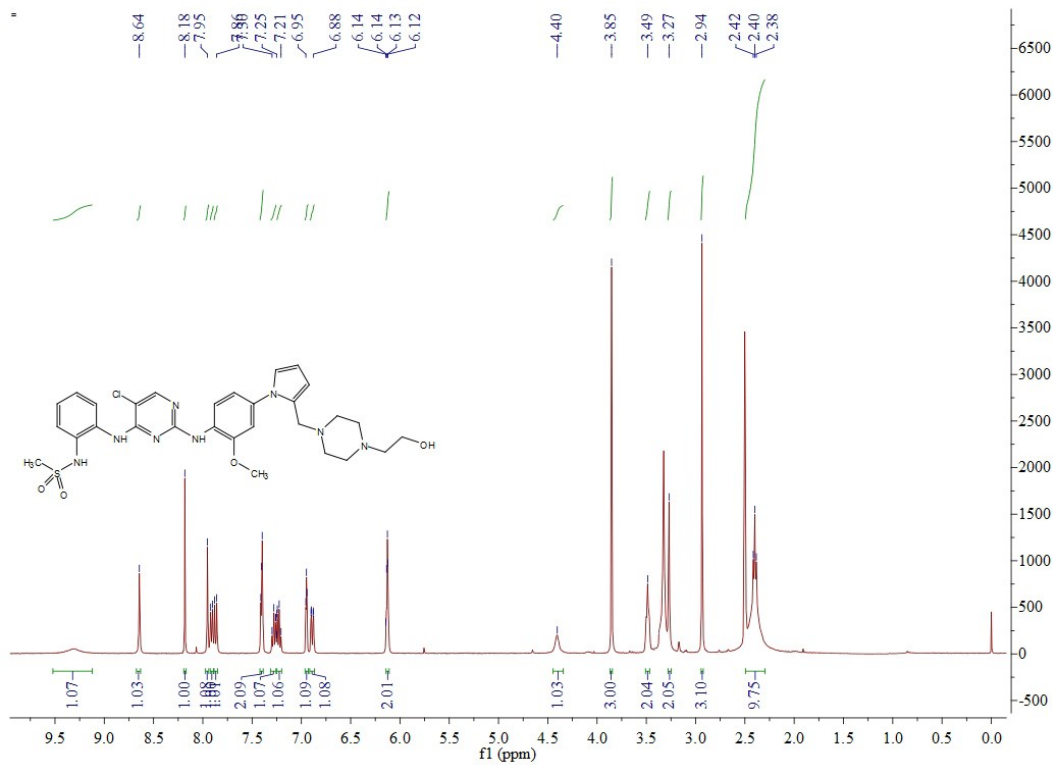


Fig. 26-2 <sup>1</sup>H-NMR spectrum of 101

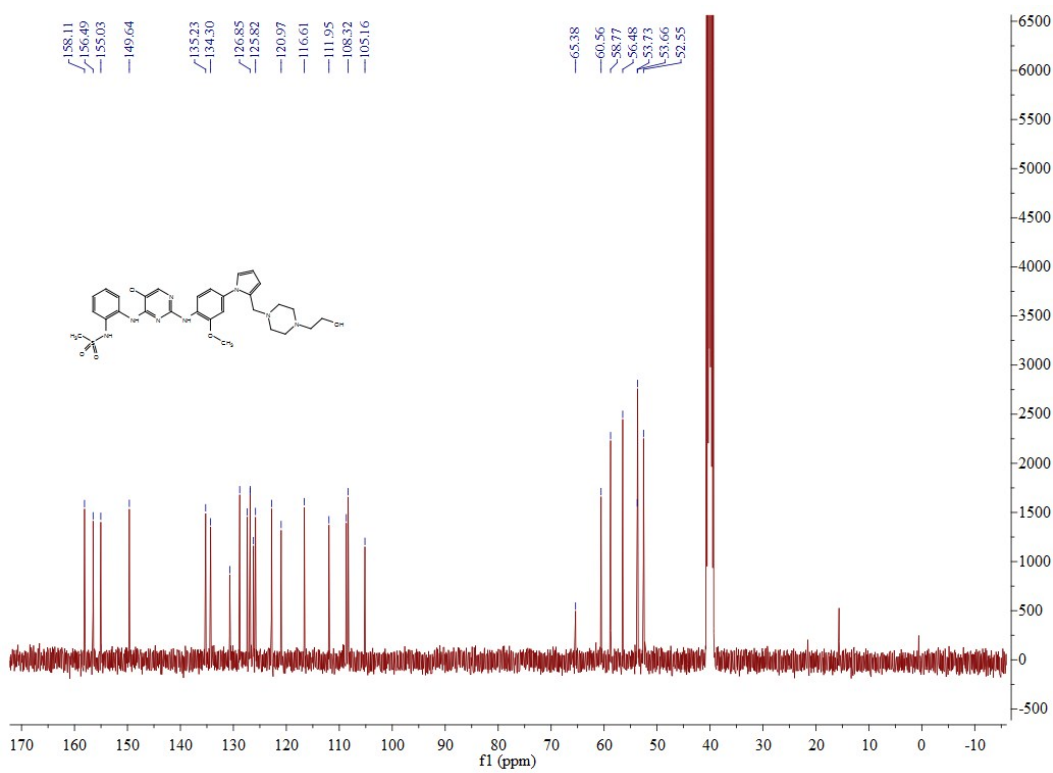


Fig. 26-3 <sup>13</sup>C-NMR spectrum of 101

08-Sep-2017

16:18:48  
QUATTROZQUATTROZQ

1:C,5

WJ 242 (4.886) Cm (239:243)

2: Scan ES-  
3.40e4

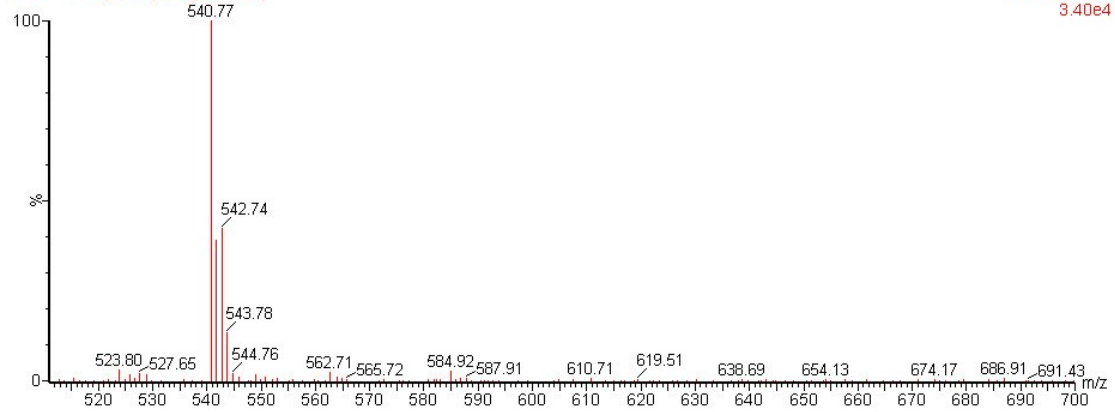


Fig. 27-1 MS spectrum of 10m

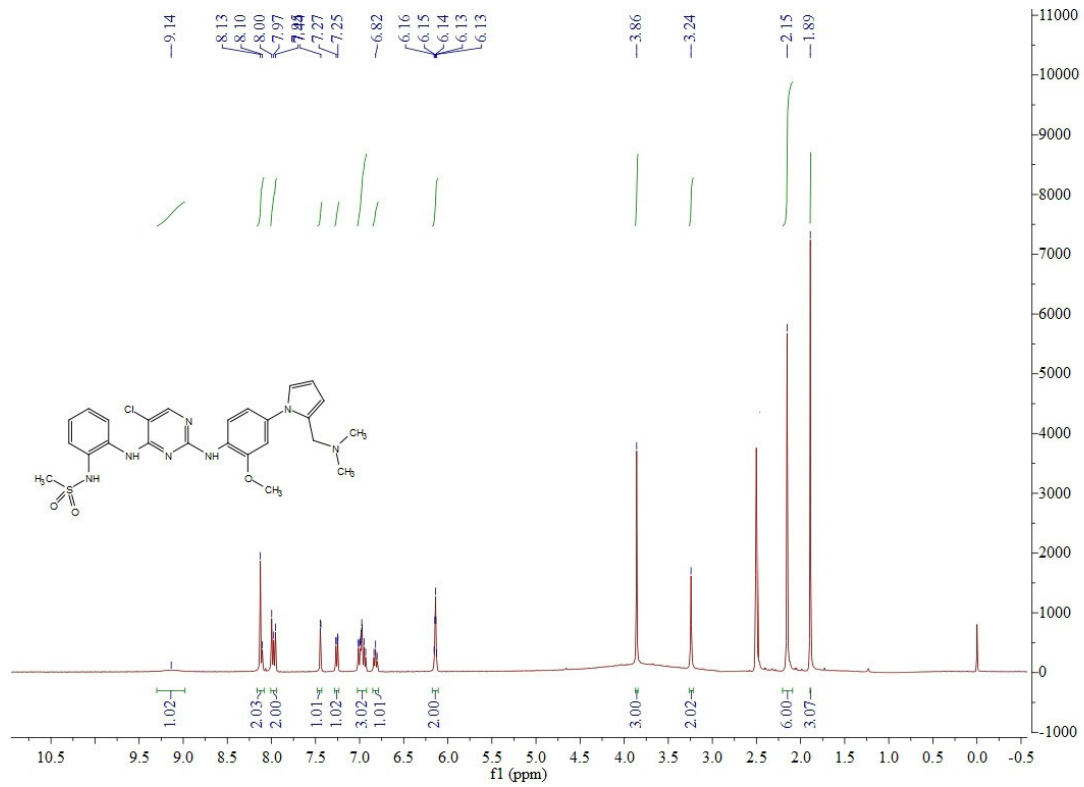


Fig. 27-2 <sup>1</sup>H-NMR spectrum of 10m

12-Sep-2017

17:14:21  
QUATTROZQUATTROZQ

1:B,7

WJ 137 (2.768) Cm (135:140)

2: Scan ES-  
3.16e5

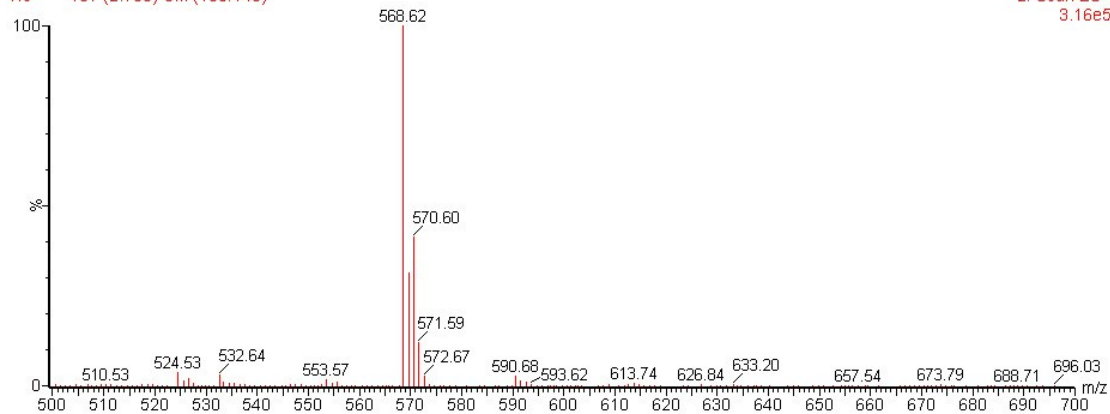


Fig. 28-1 MS spectrum of 10n

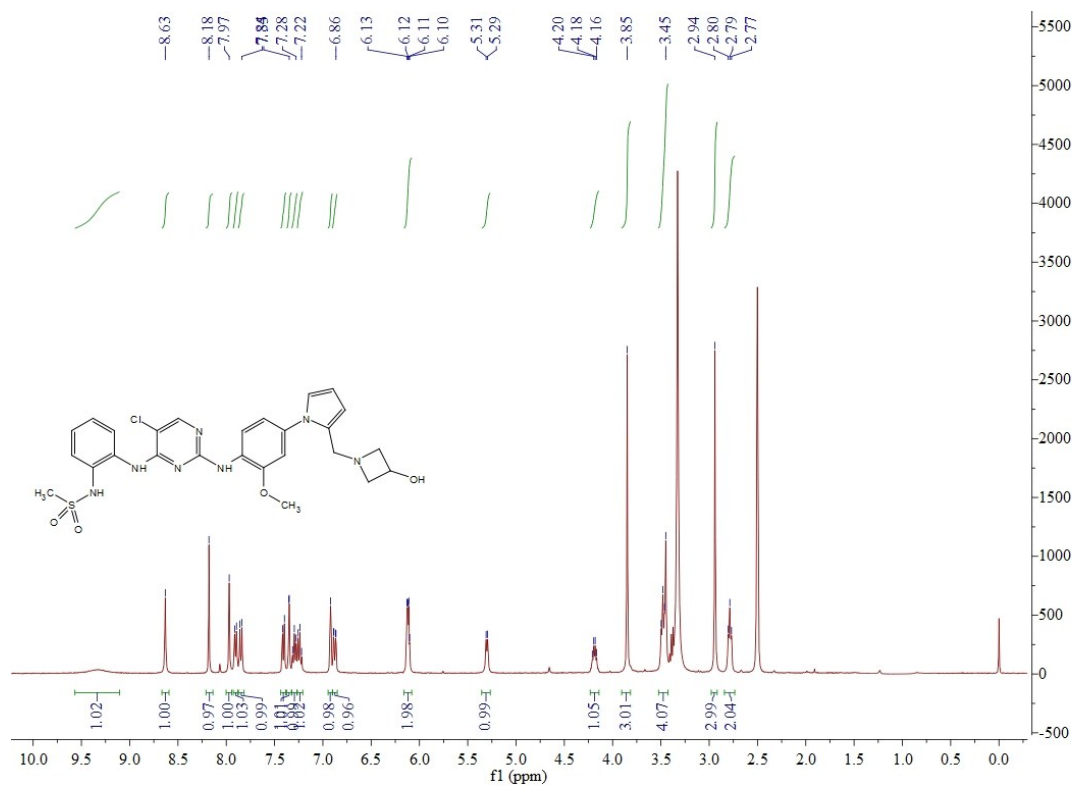


Fig. 28-2 <sup>1</sup>H-NMR spectrum of 10n