

Supplementary Data

**Accurate Molecular Weight Measurements of Cystine  
Derivatives on FAB-MS**

Mihoyo Fujitake<sup>a,\*</sup> and Shinya Harusawa<sup>b</sup>

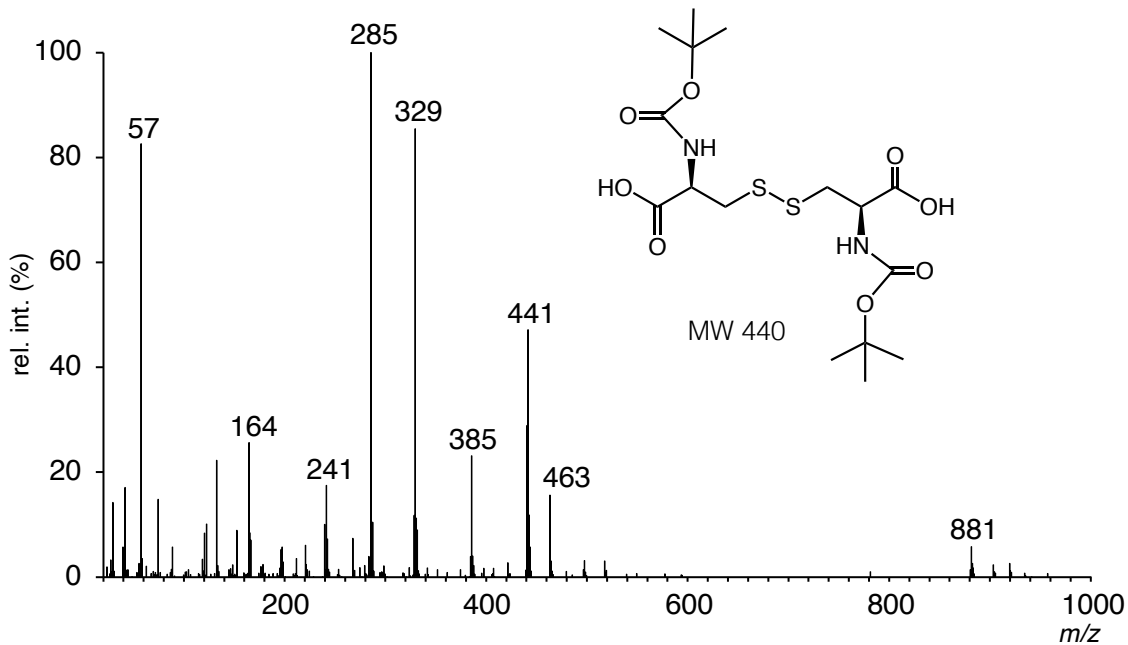
<sup>a</sup> *Department of MS analysis at Center for Pharmaceutical Research & Development, Faculty of Pharmacy, Osaka Medical and Pharmaceutical University, 4-20-1 Nasahara, Takatsuki, Osaka 569-1094, Japan;* <sup>b</sup> *Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Osaka Medical and Pharmaceutical University, 4-20-1 Nasahara, Takatsuki, Osaka 569-1094, Japan.*

**FAB-MS using DTDE**

compounds <b>2</b> and <b>3</b>	.....	S-1
compounds <b>4</b> and <b>5</b>	.....	S-2
compounds <b>6</b> and <b>7</b>	.....	S-3
compounds <b>8</b> and <b>9</b>	.....	S-4
compounds <b>10</b> and <b>11</b>	.....	S-5
compounds <b>12</b> and <b>13</b>	.....	S-6
compounds <b>14</b> and <b>15</b>	.....	S-7
compounds <b>16</b> and <b>17</b>	.....	S-8
compound <b>18</b>	.....	S-9
<b>EI-MS of diphenyl disulfide</b>	.....	S-9
<b>EI-MS of didodecyl disulfide</b>	.....	S-10

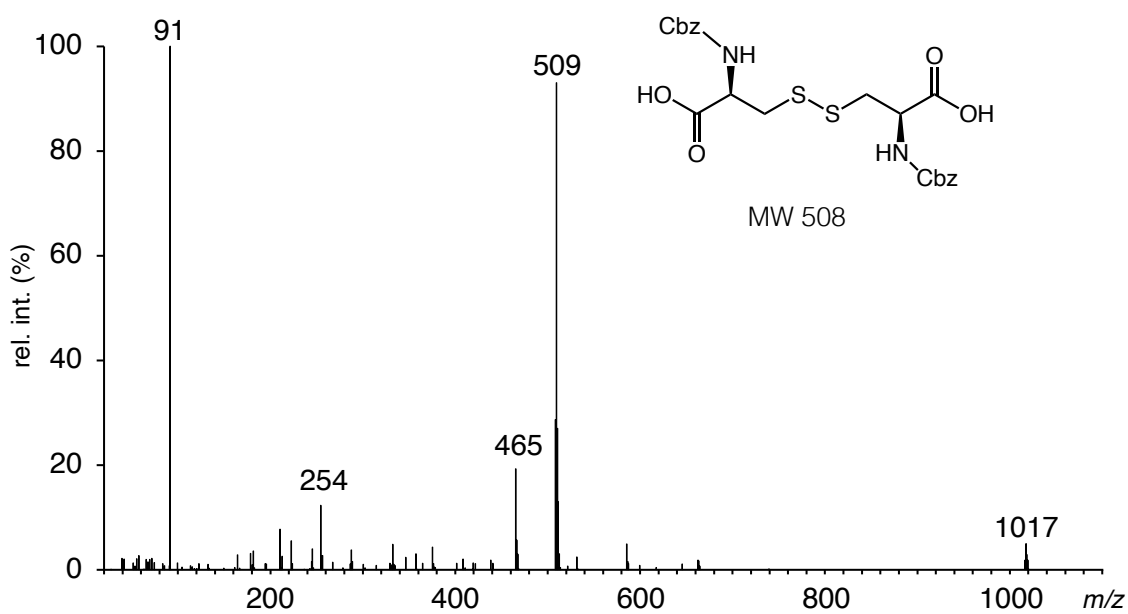
## FAB-MS of compound 2 (*N*-Boc-cystine)

[ Mass Spectrum ]  
Sample : *N*-Boc  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(35,45)



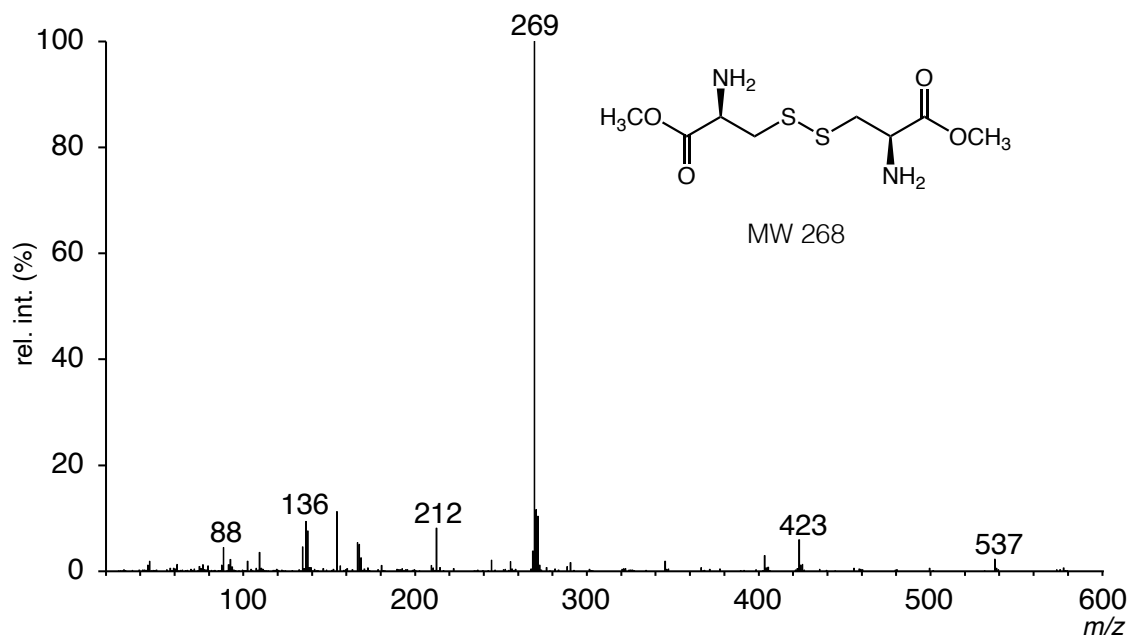
## FAB-MS of compound 3 (*N*-Cbz)

[ Mass Spectrum ]  
Sample : *N*-Cbz  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(35,45)



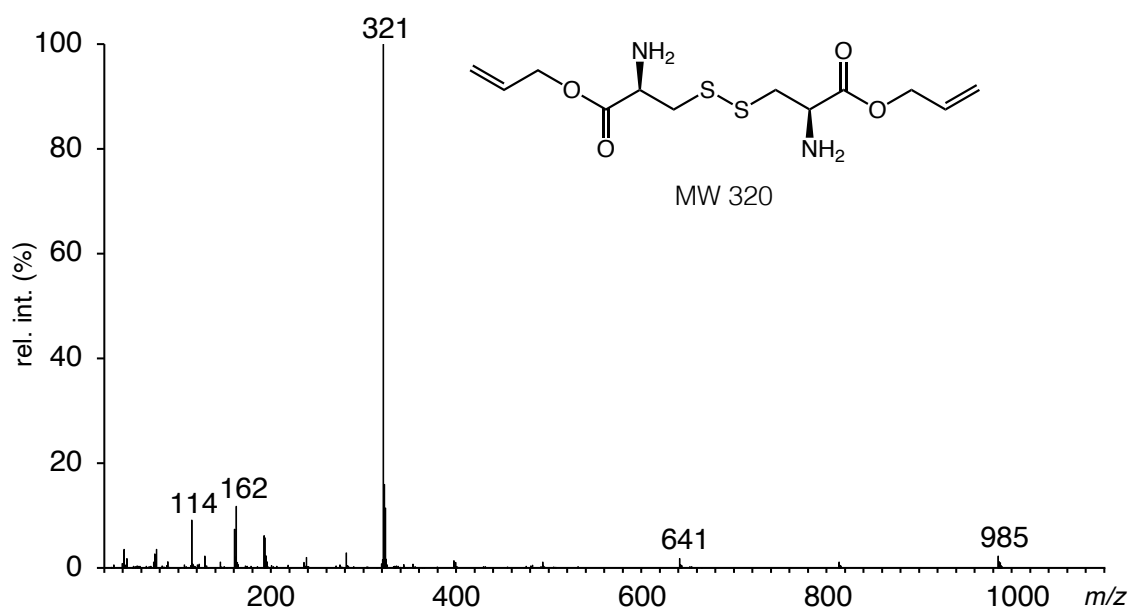
### FAB-MS of compound 4 (C-Me)

[ Mass Spectrum ]  
Sample : C-Me  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(30,40)



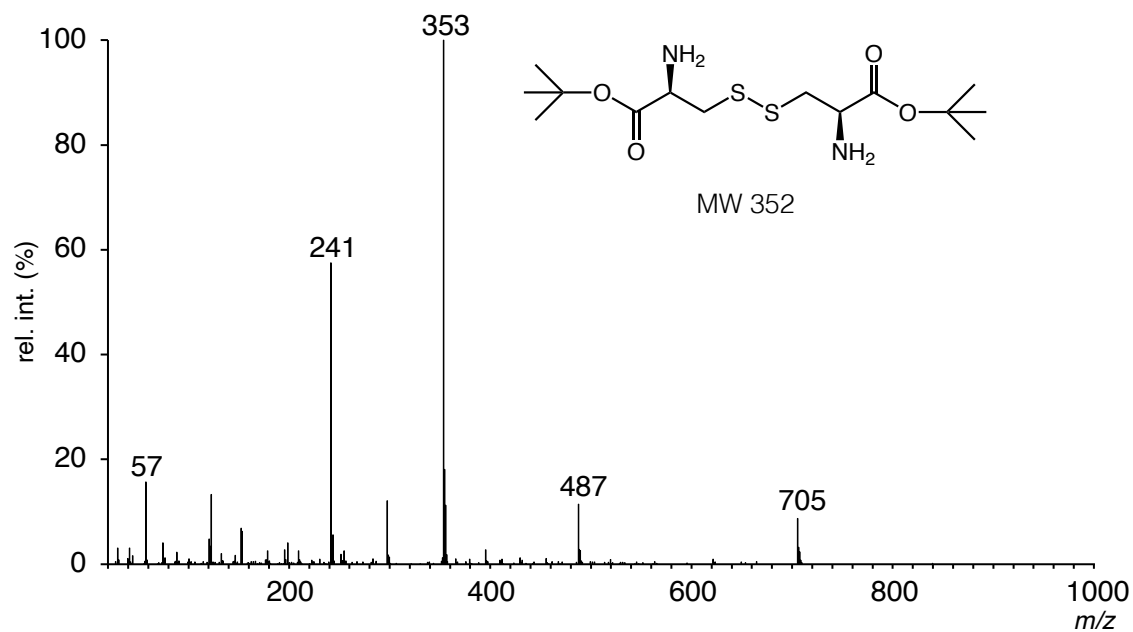
### FAB-MS of compound 5 (C-allyl)

[ Mass Spectrum ]  
Sample : C-allyl. 2p-tosylate  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(30,40)



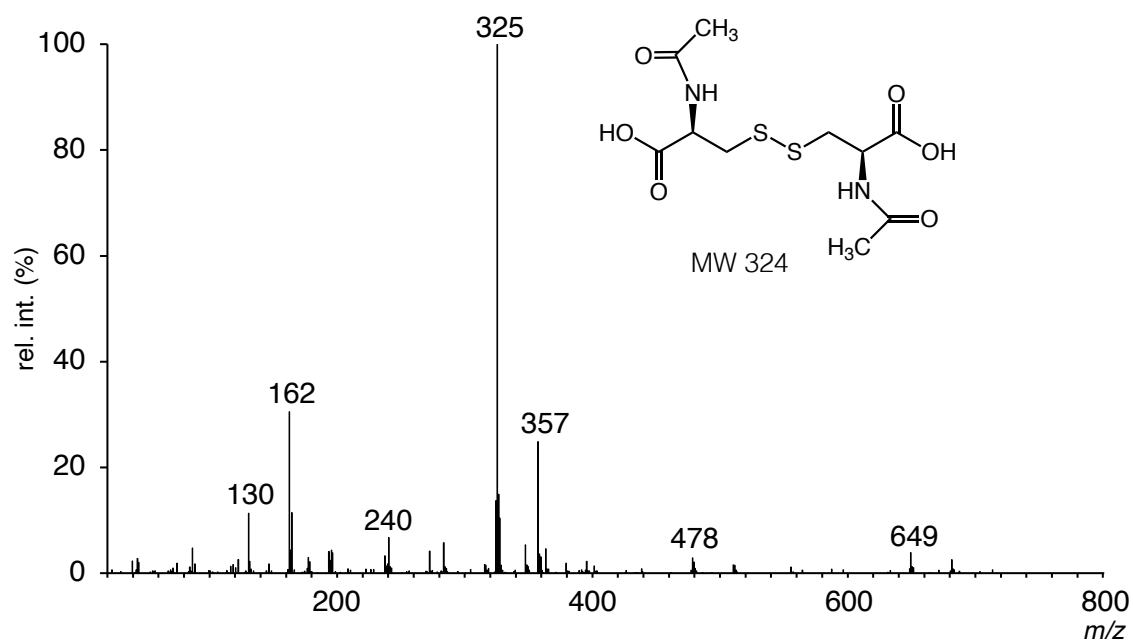
## FAB-MS of compound 6 (C-'Bu)

[ Mass Spectrum ]  
Sample : C-'Bu. 2HCl  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(30,40)



## FAB-MS of compound 7 (DiNAC)

[ Mass Spectrum ]  
Sample : DiNAC  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(35,45)



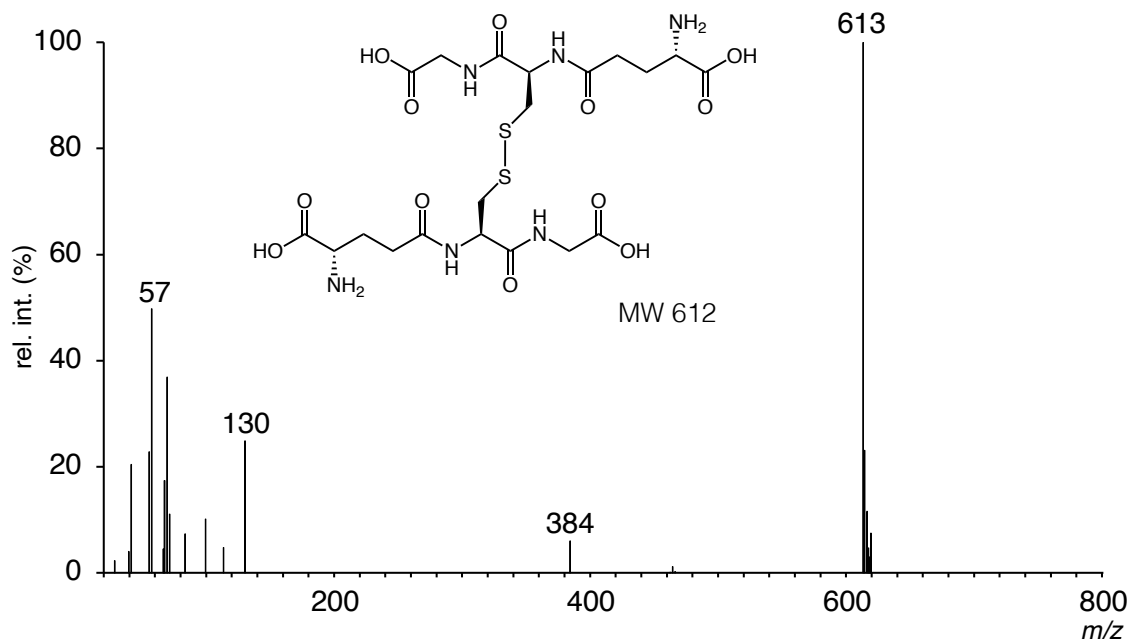
FAB-MS of compound **8** (GSSG)

[ Mass Spectrum ]

Sample : GSSG

Ion Mode : FAB+ (matrix:DTDE)

Scan : (75,85)-(55,65)



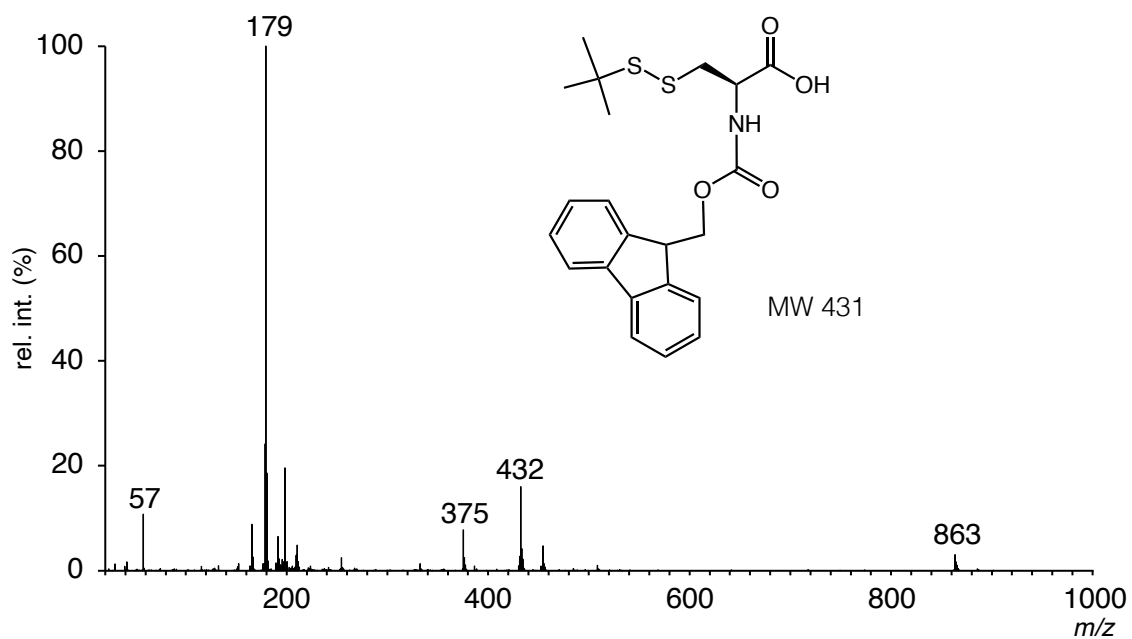
FAB-MS of compound **9** [FmocCys('BuS)OH]

[ Mass Spectrum ]

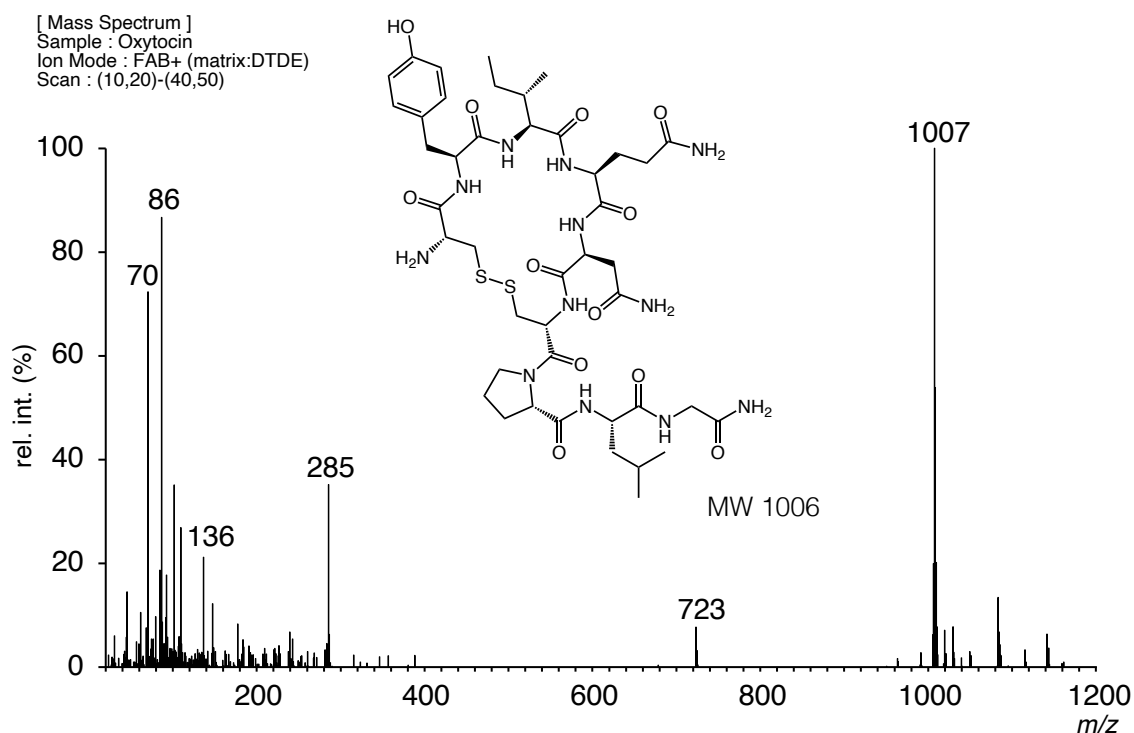
Sample : FmocCys('BuS)OH

Ion Mode : FAB+ (matrix:DTDE)

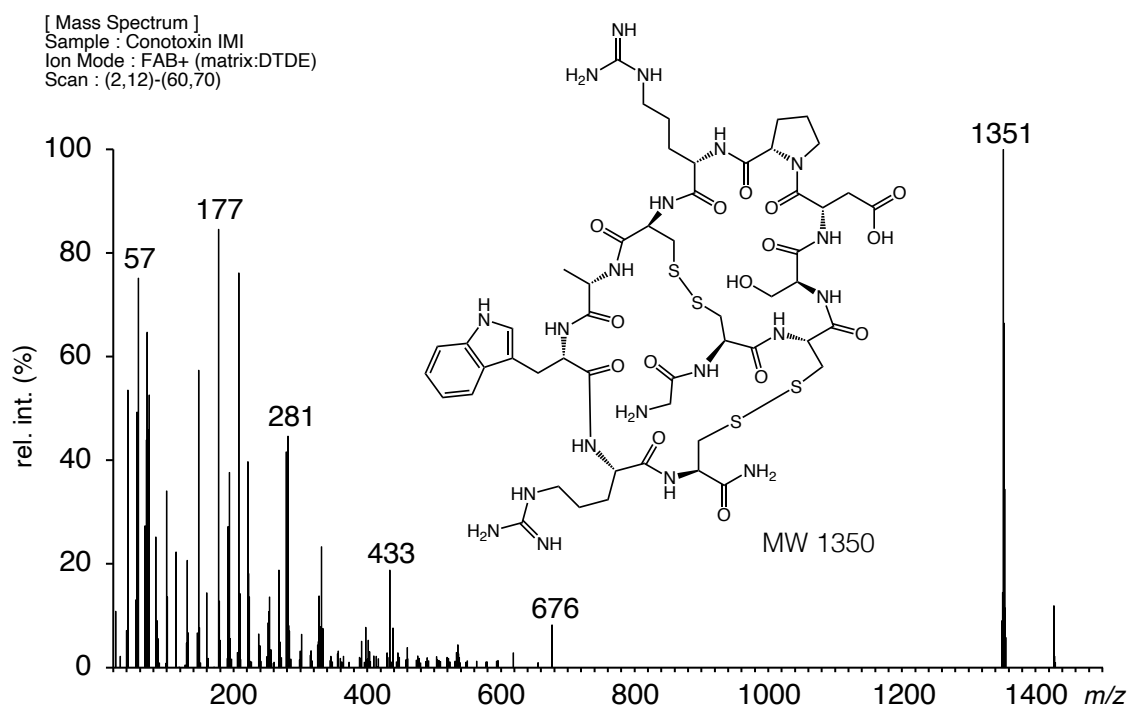
Scan : (10,20)-(30,40)



FAB-MS of compound **10** (Oxytocin)

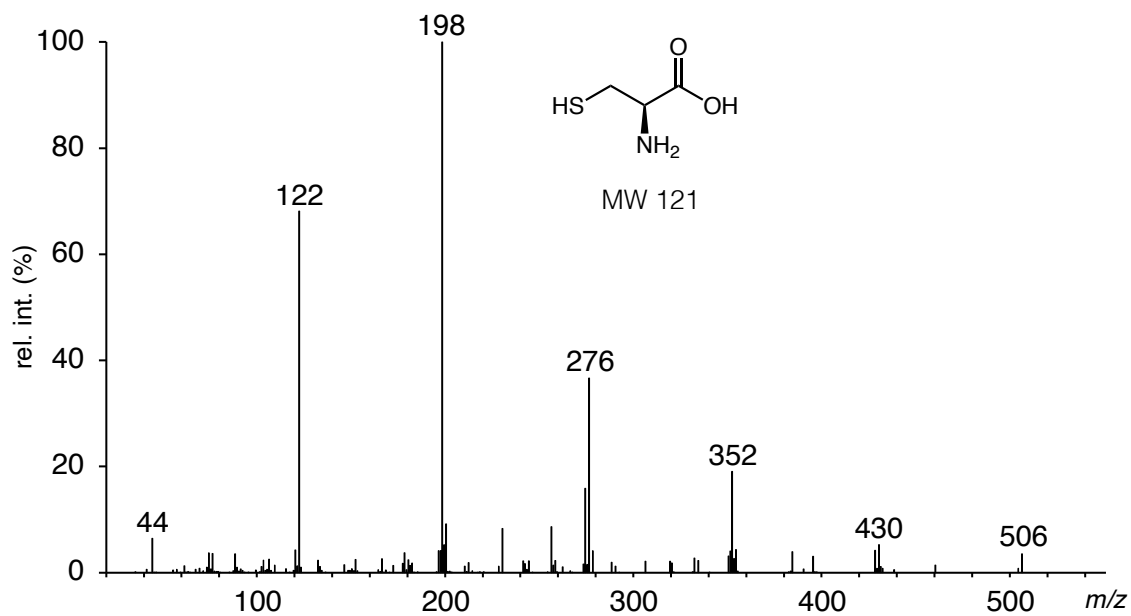


FAB-MS of compound **11** (Conotoxin)



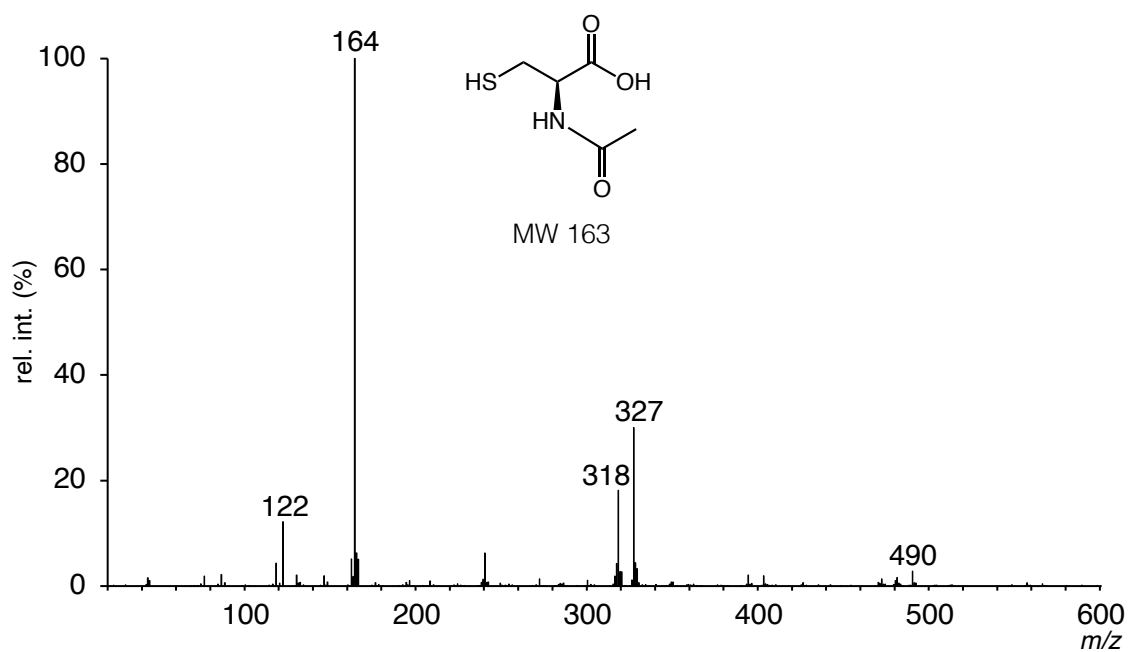
### FAB-MS of compound **12** (Cys)

[ Mass Spectrum ]  
Sample : L-Cysteine  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(45,55)



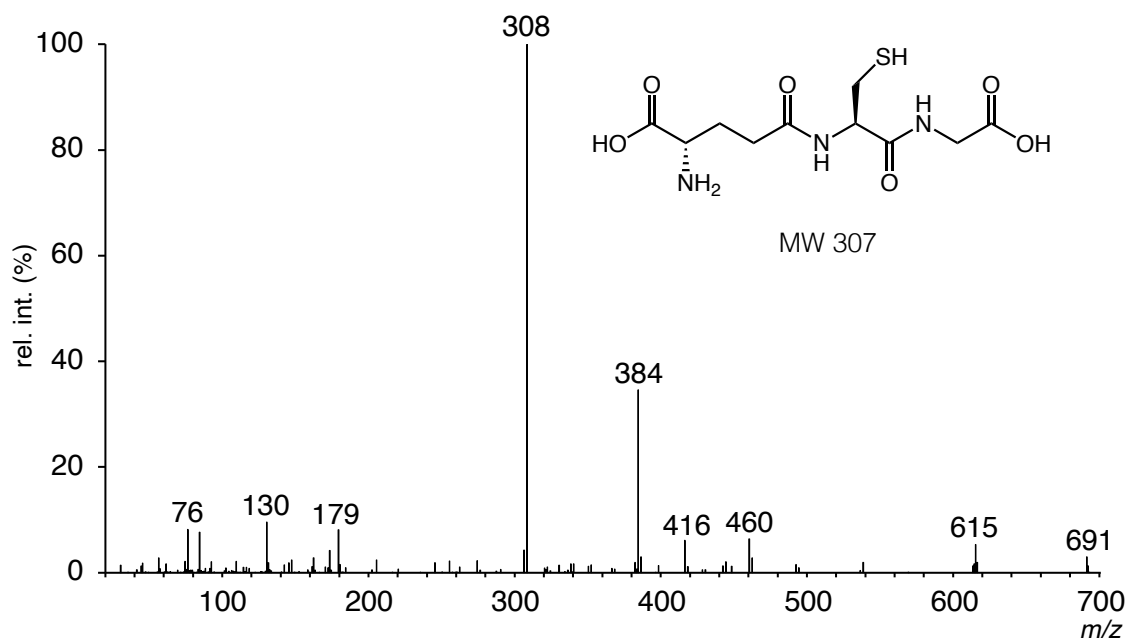
### FAB-MS of compound **13** (NAC)

[ Mass Spectrum ]  
Sample : N-Acetyl-L-cysteine (NAC)  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(30,40)



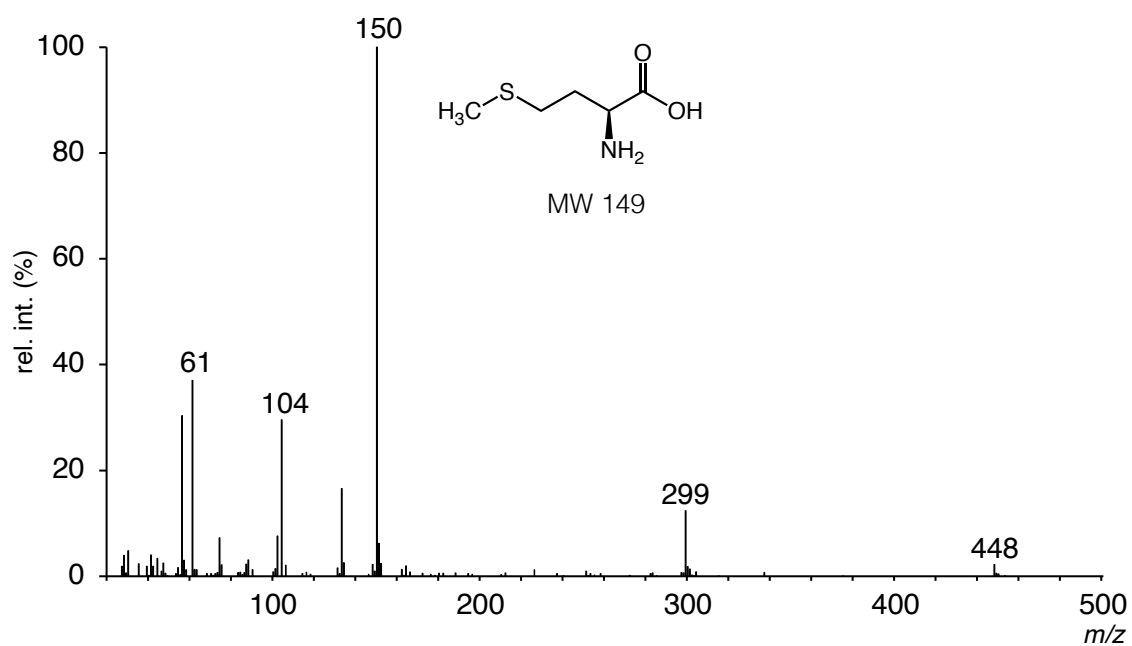
## FAB-MS of compound **14** (GSH)

[ Mass Spectrum ]  
Sample : GSH  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (15,25)-(65,75)



## FAB-MS of compound **15** (Met)

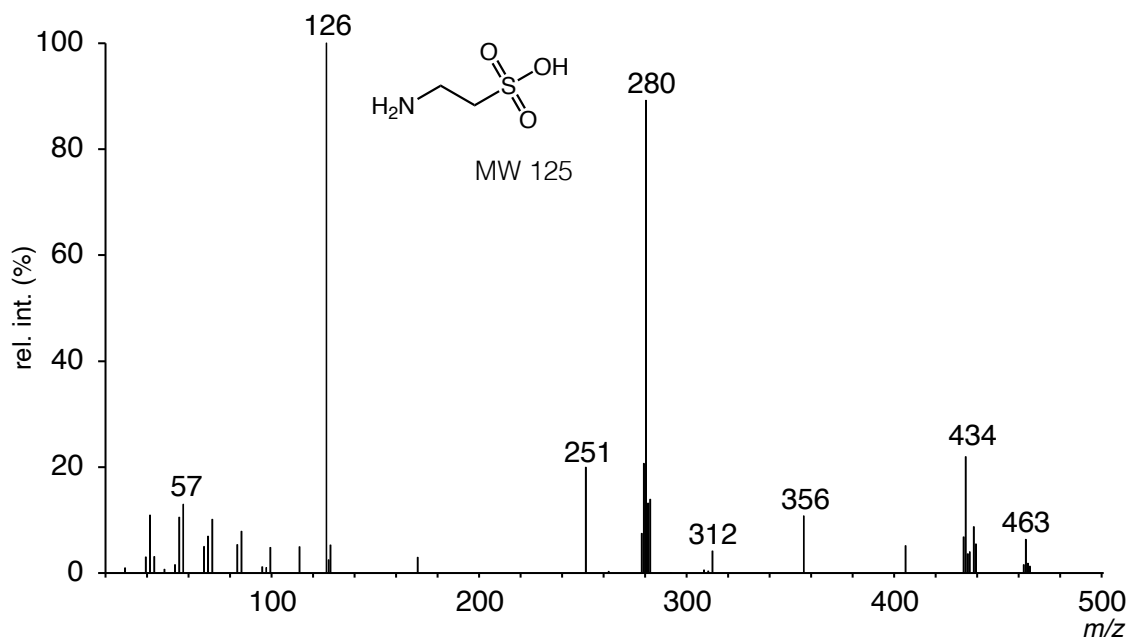
[ Mass Spectrum ]  
Sample : L-Methionine  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (10,20)-(30,40)





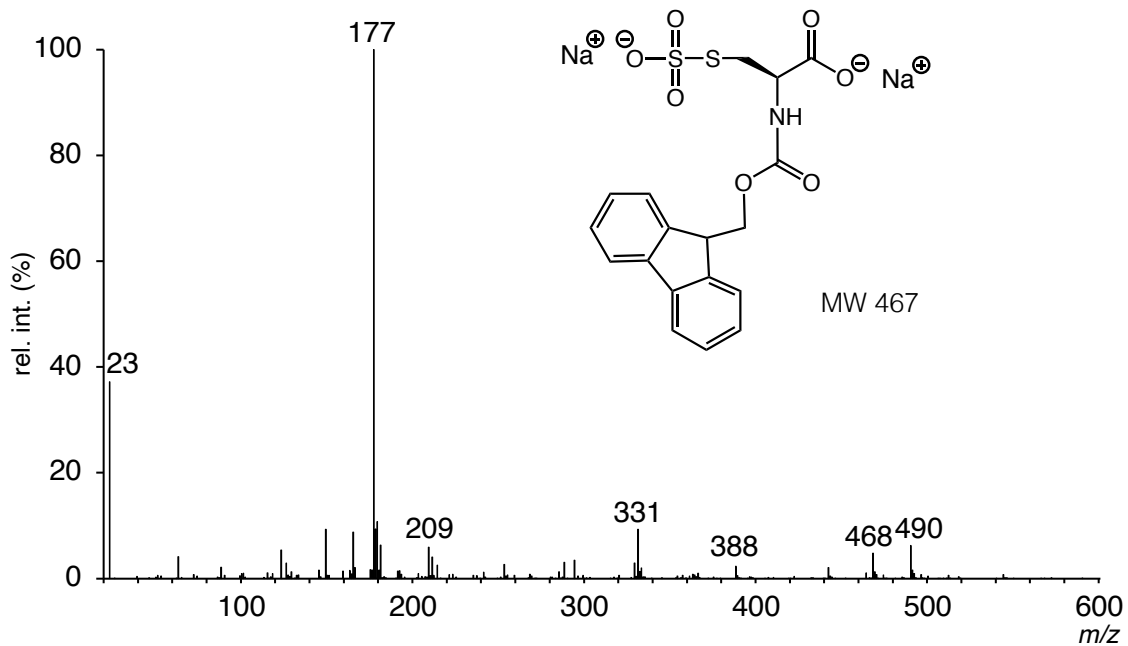
### FAB-MS of compound **16** (Taurine)

[ Mass Spectrum ]  
Sample : Taurine  
Ion Mode : FAB+ (matrix:DTDE)  
Scan : (3,7)-(26,31)



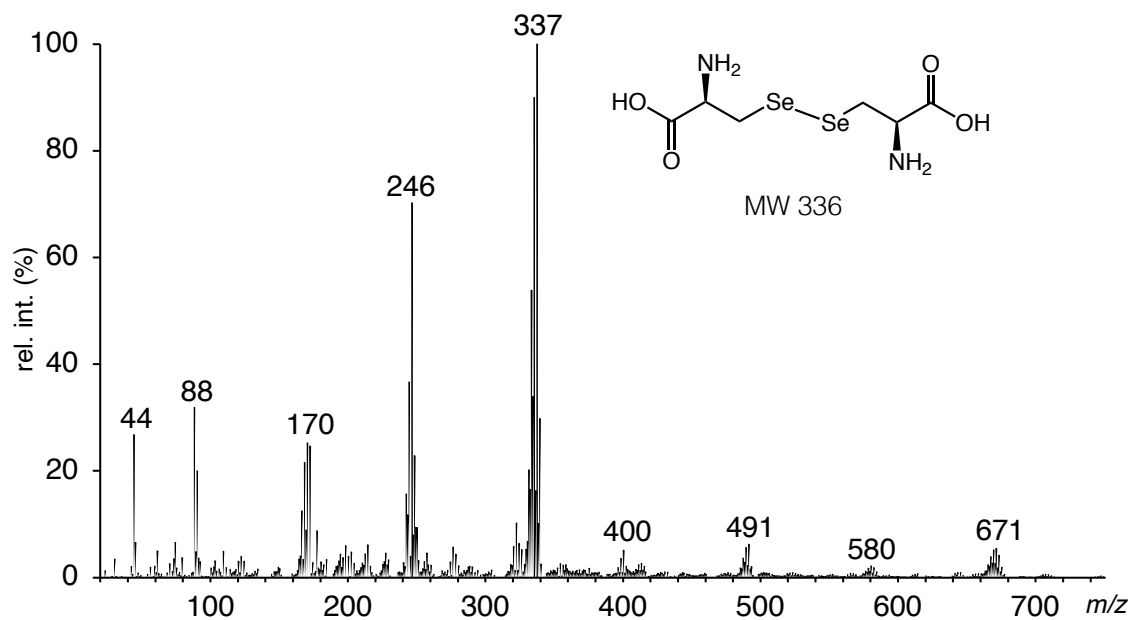
### FAB-MS of compound **17** [FmocCys(SO<sub>3</sub>H)OH]

[ Mass Spectrum ]  
Sample : FmocCys(SO<sub>3</sub>H)OH. 2Na  
Ion Mode : FAB+ (matrix: DTDE)  
Scan : (3,13)-(40,50)



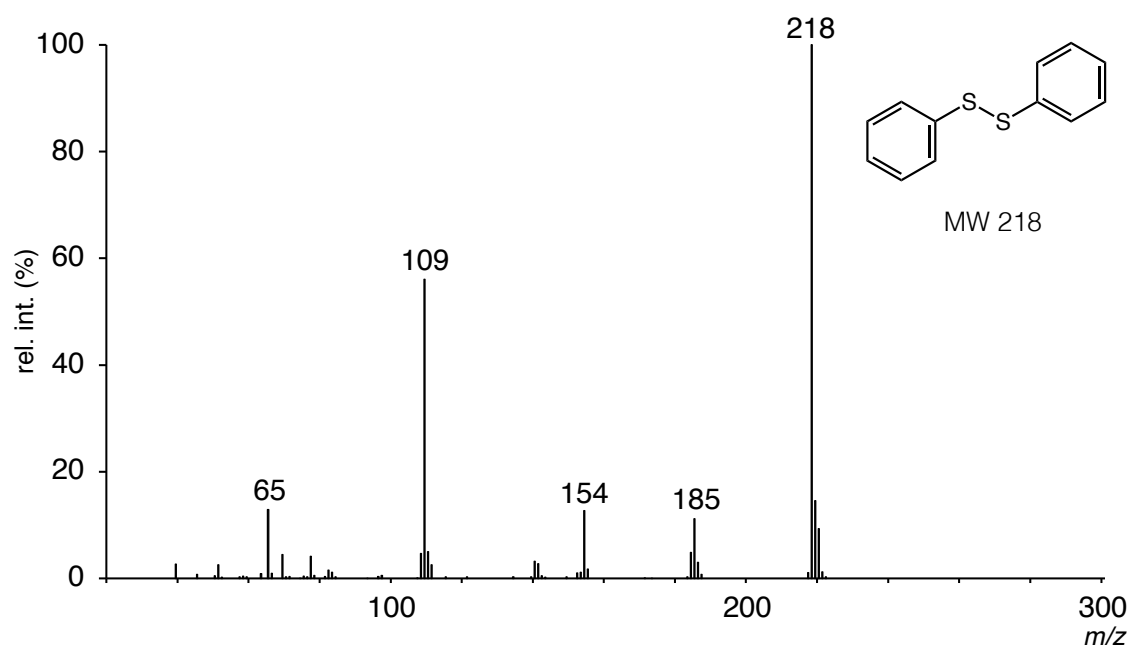
## FAB-MS of compound **18** (SeCys)<sub>2</sub>

[ Mass Spectrum ]  
Sample : L-Selenocystine  
Ion Mode : FAB+ (matrix: DTDE)  
Scan : (3,13)-(30,40)



## EI-MS of diphenyl disulfide

[ Mass Spectrum ]  
Sample : Diphenyl disulfide  
Ion Mode : EI+  
Scan : (17,22)



# EI-MS of didodecyl disulfide

[ Mass Spectrum ]  
Sample : Didodecyl disulfide  
Ion Mode : EI+  
Scan : (40,45)

