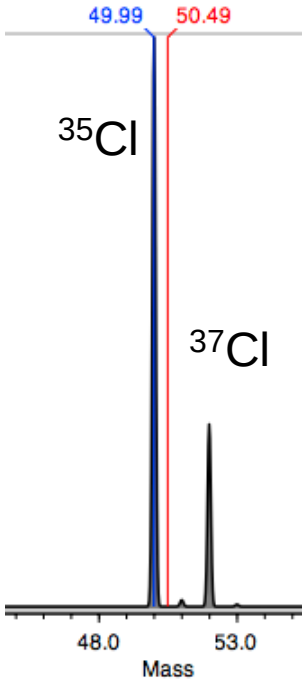
Mass Spectrometry

Lecturer: Shaymaa Adil Mohammed

4th Year

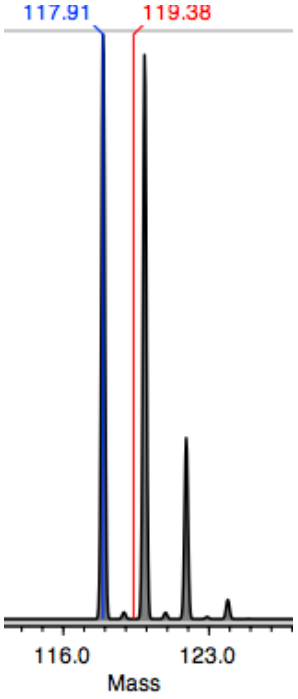
2020-2021

Using the Information in Ion Clusters--Halogens



CH_3Cl

One chlorine

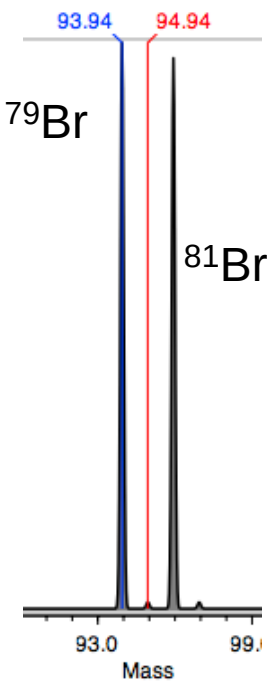


$CHCl_3$

Three chlorines

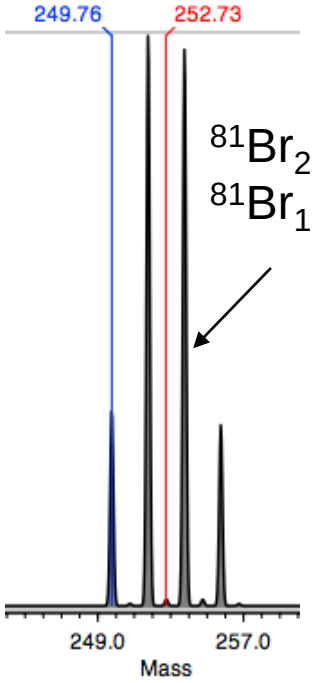
The paired appearance flags the ions as to the number of halogens

Fragment ions with the same halogen count preserve the pattern



CH_3Br

One bromine



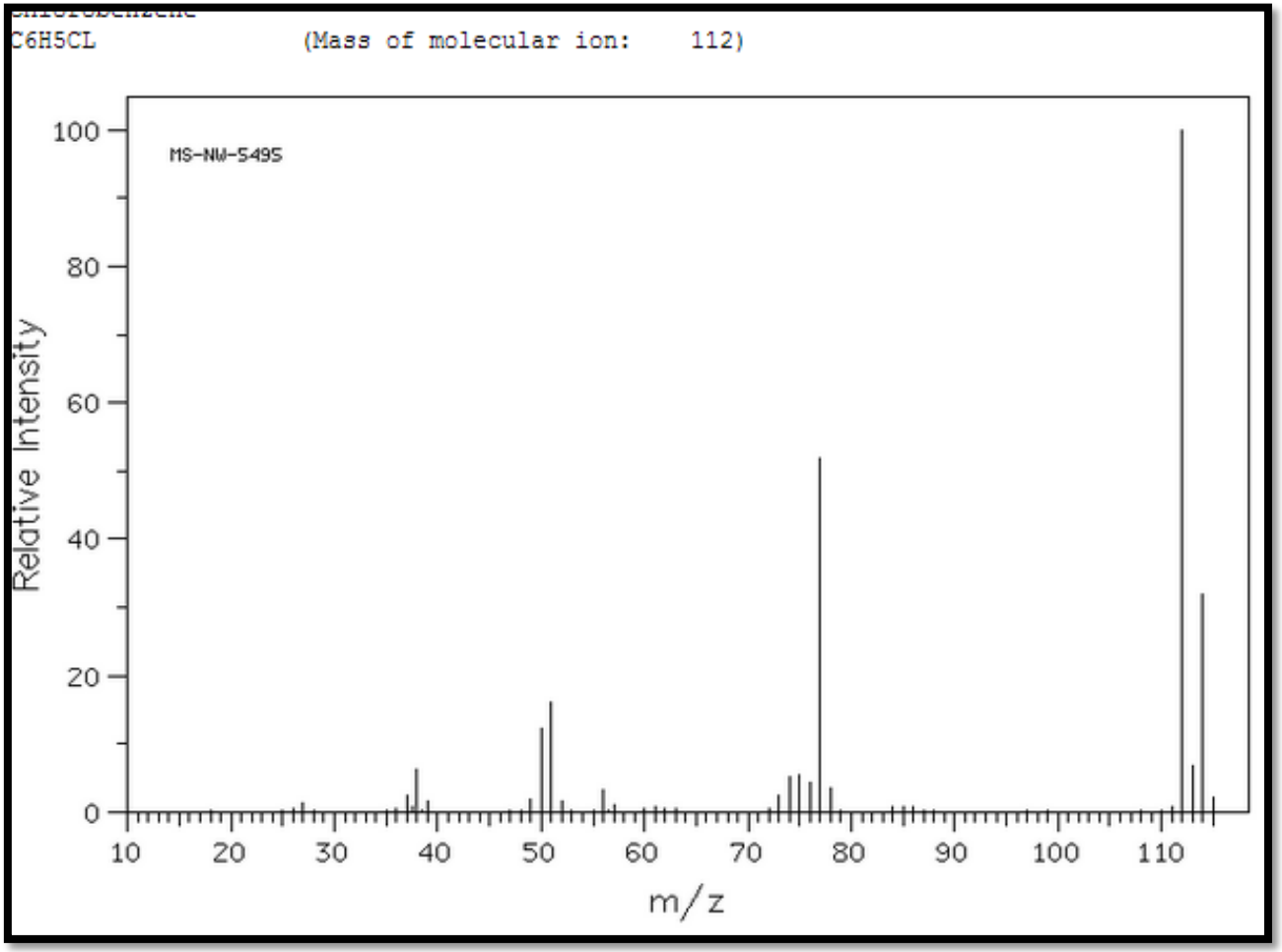
$CHBr_3$

Three bromines

Isotops

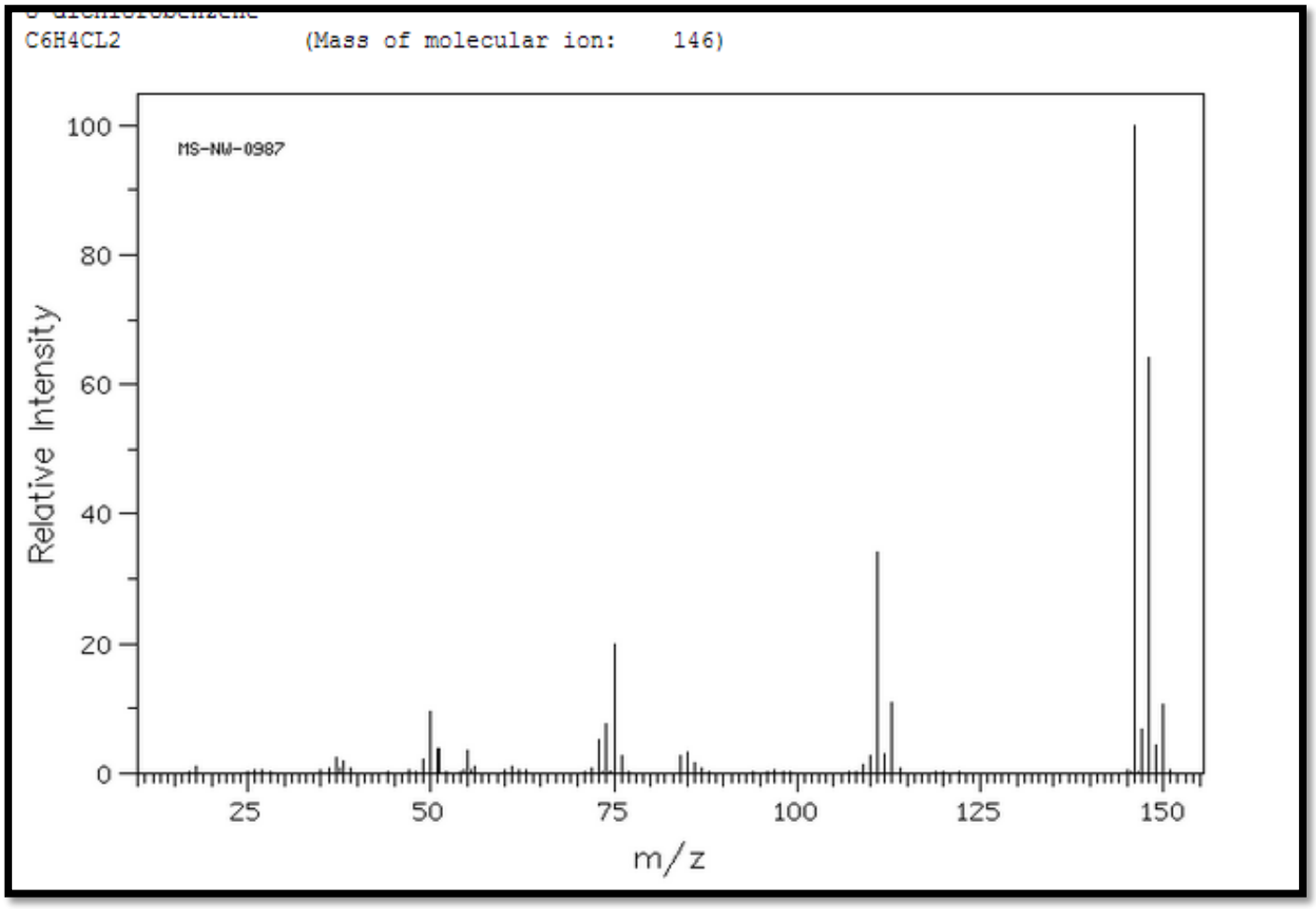
Element	Most Abundant Isotope	Secondary Isotope	Abundance/100 atoms of Primary Isotope
Hydrogen	^{1}H	^{2}H	0.015
Carbon	$^{1}2C$	^{13}C	1.080
Nitrogen	^{14}N	^{15}N	0.370
Oxygen	^{16}O	^{17}O	0.040
		^{18}O	0.200
Sulfur	^{32}S	^{33}S	0.800
		^{34}S	4.400
Chlorine	^{35}Cl	^{37}Cl	32.50
Bromine	^{79}Br	^{81}Br	98.00
Silicon	^{28}Si	^{29}Si	5.100
		^{30}Si	3.400

Chlorobenzene



27.0	1.2
37.0	2.5
38.0	6.2
39.0	1.7
49.0	1.9
50.0	12.3
51.0	16.0
52.0	1.5
56.0	3.3
57.0	1.0
73.0	2.3
74.0	5.2
75.0	5.3
76.0	4.3
77.0	52.0
78.0	3.5
112.0	100.0
113.0	6.8
114.0	31.8
115.0	2.2

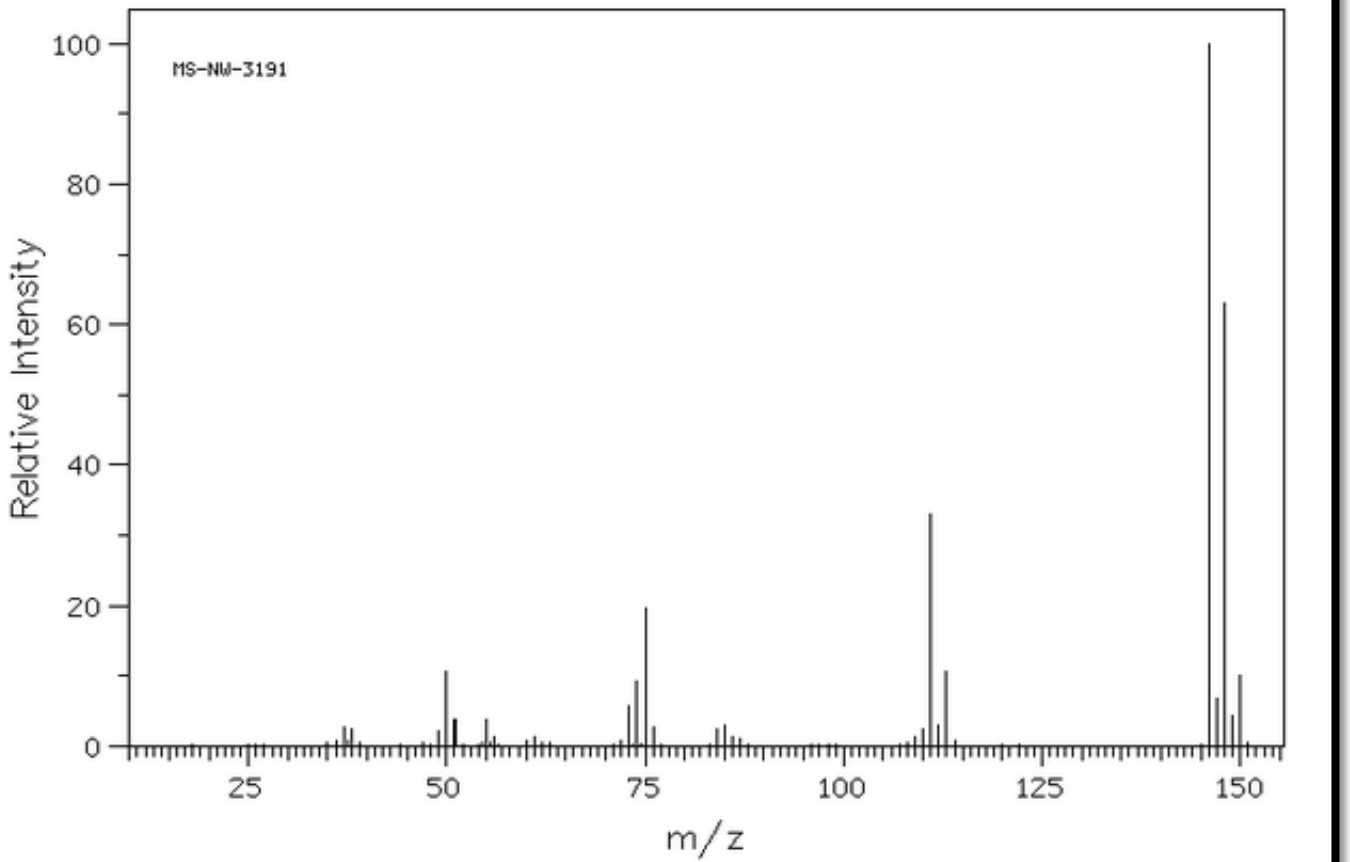
o-Dihlorobenzene



18.0	1.1
37.0	2.4
38.0	1.9
49.0	2.1
50.0	9.5
51.0	3.9
55.0	3.6
56.0	1.0
61.0	1.1
73.0	5.2
74.0	7.7
75.0	19.9
76.0	2.8
84.0	2.7
85.0	3.2
86.0	1.7
109.0	1.4
110.0	2.7
111.0	34.1
112.0	3.0
113.0	11.0
146.0	100.0
147.0	6.9
148.0	64.1
149.0	4.3
150.0	10.5

m-Dihlorobenzene

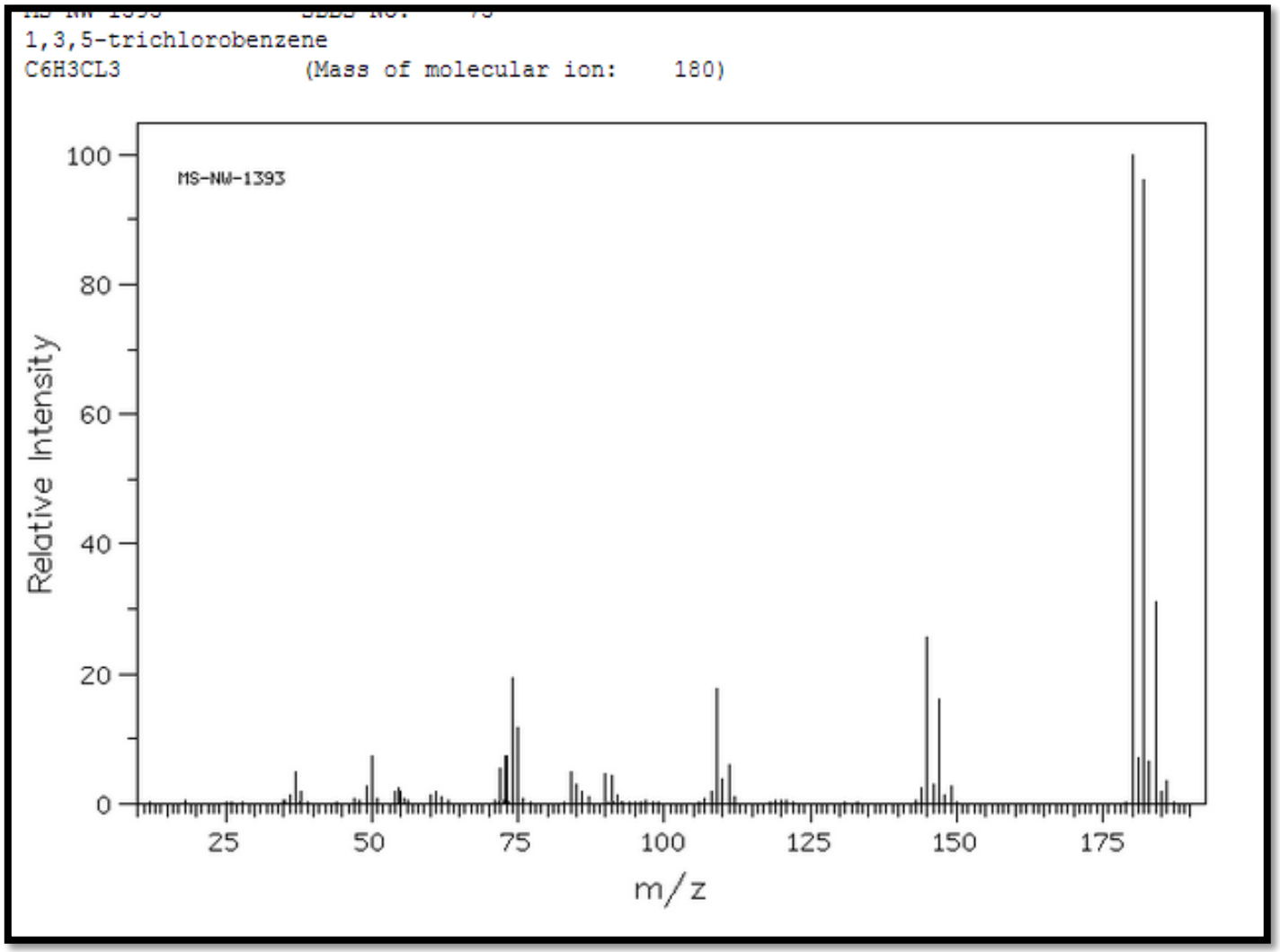
m-dichlorobenzene
C6H4CL2 (Mass of molecular ion: 146)



37.0	2.7
38.0	2.3
49.0	2.1
50.0	10.5
51.0	3.7
55.0	3.7
56.0	1.3
61.0	1.3
73.0	5.8
74.0	9.2
75.0	19.7
76.0	2.7
84.0	2.3
85.0	2.9
86.0	1.3
87.0	1.0
109.0	1.4
110.0	2.4
111.0	32.9
112.0	3.0
113.0	10.5
146.0	100.0
147.0	6.7
148.0	63.0
149.0	4.3
150.0	10.2

Trichlorobenzene

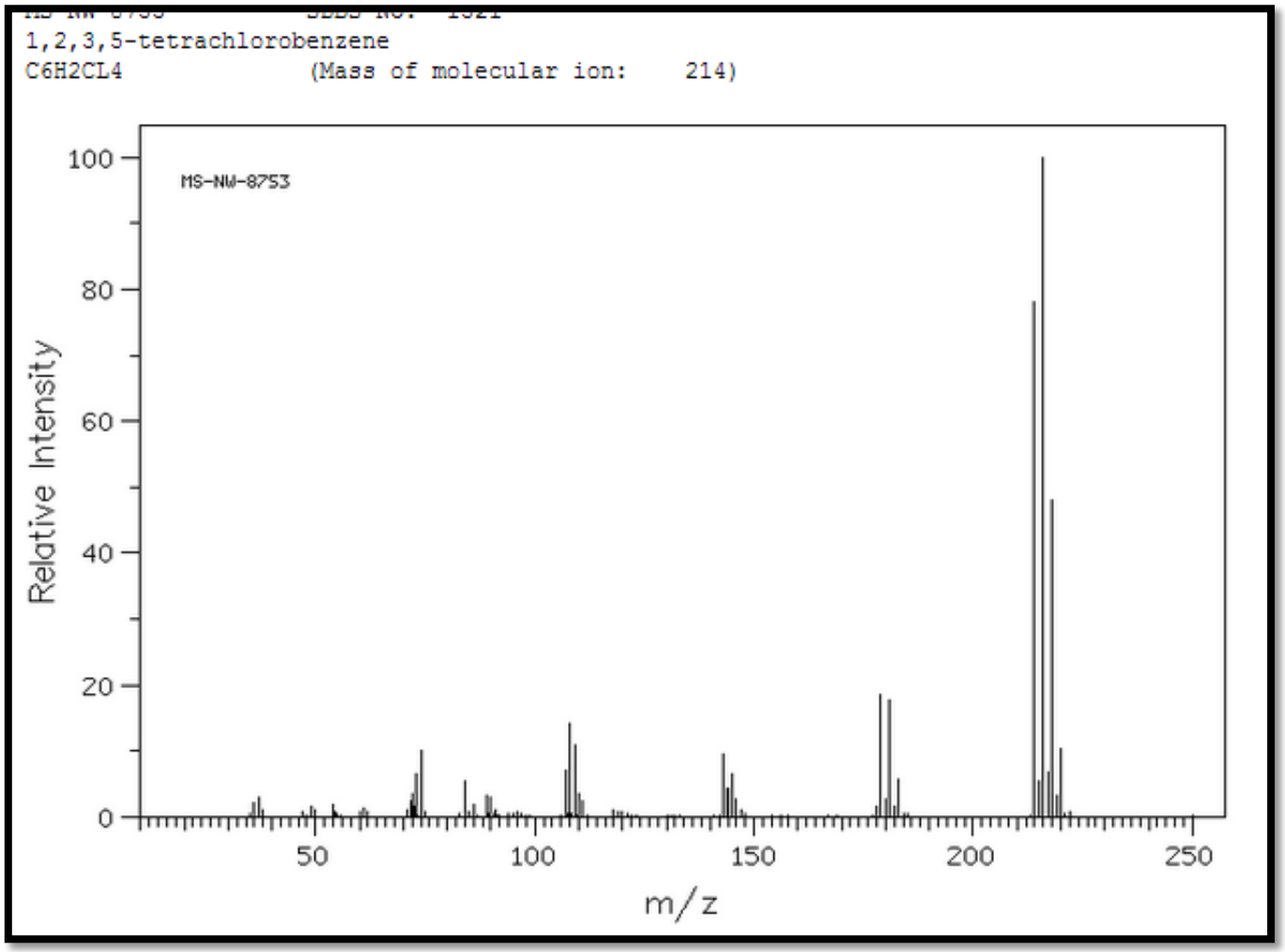
1,3,5-trichlorobenzene
C6H3CL3 (Mass of molecular ion: 180)



36.0	1.4
37.0	4.8
38.0	1.9
49.0	2.7
50.0	7.3
54.0	2.0
54.5	2.4
55.0	2.0
60.0	1.3
61.0	1.9
62.0	1.1
72.0	5.5
73.0	7.3
74.0	19.3
75.0	11.8
84.0	4.9
85.0	2.9
86.0	1.8
87.0	1.0
90.0	4.6
91.0	4.2
92.0	1.4
108.0	2.0
109.0	17.8
110.0	3.9
111.0	5.9
112.0	1.1
144.0	2.4
145.0	25.6
146.0	2.9
147.0	16.2
148.0	1.2
149.0	2.7
180.0	100.0
181.0	7.0
182.0	96.2
183.0	6.4
184.0	31.2
185.0	2.0
186.0	3.5

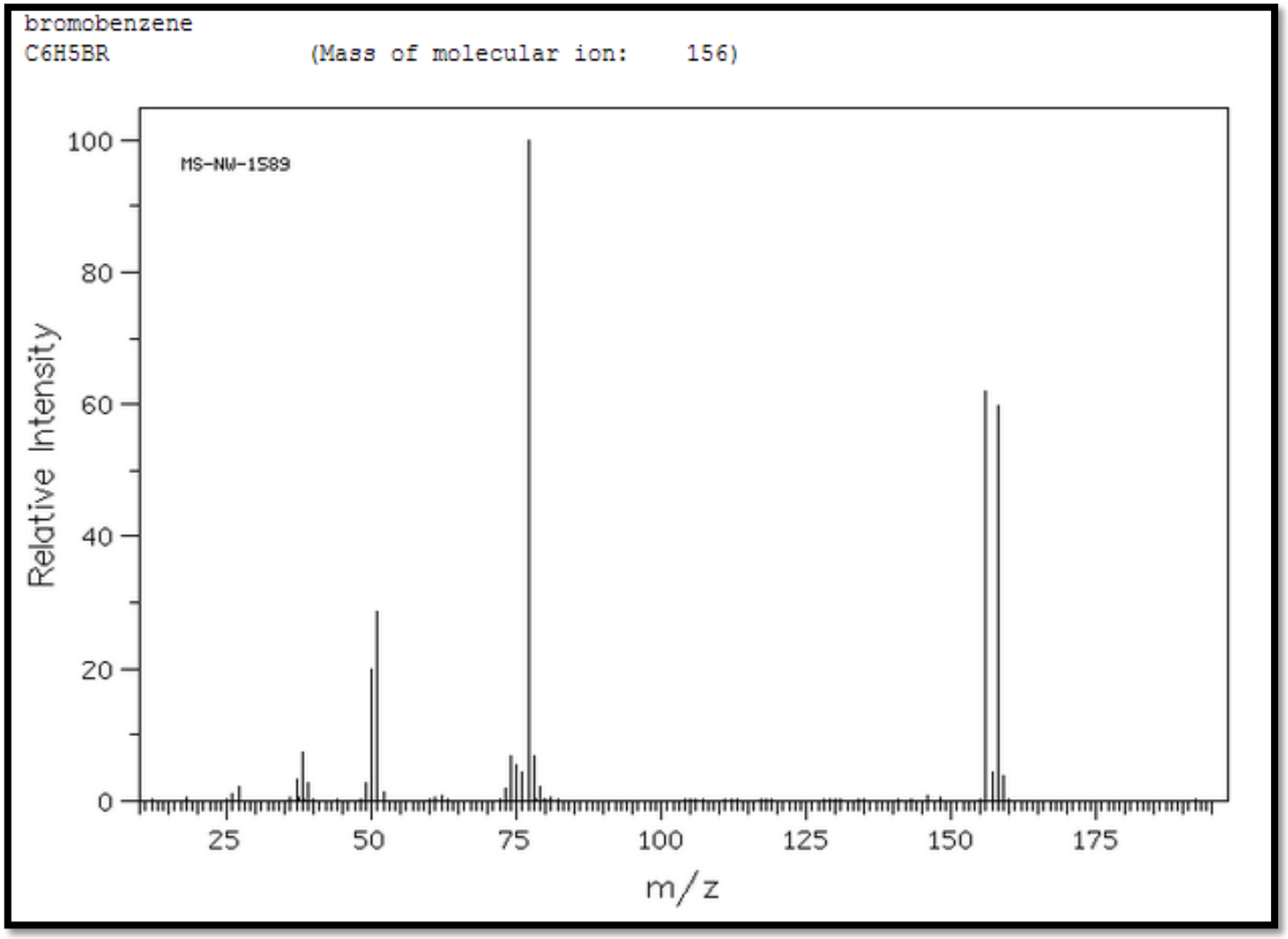
Tetrachlorobenzene

1,2,3,5-tetrachlorobenzene
C6H2CL4 (Mass of molecular ion: 214)



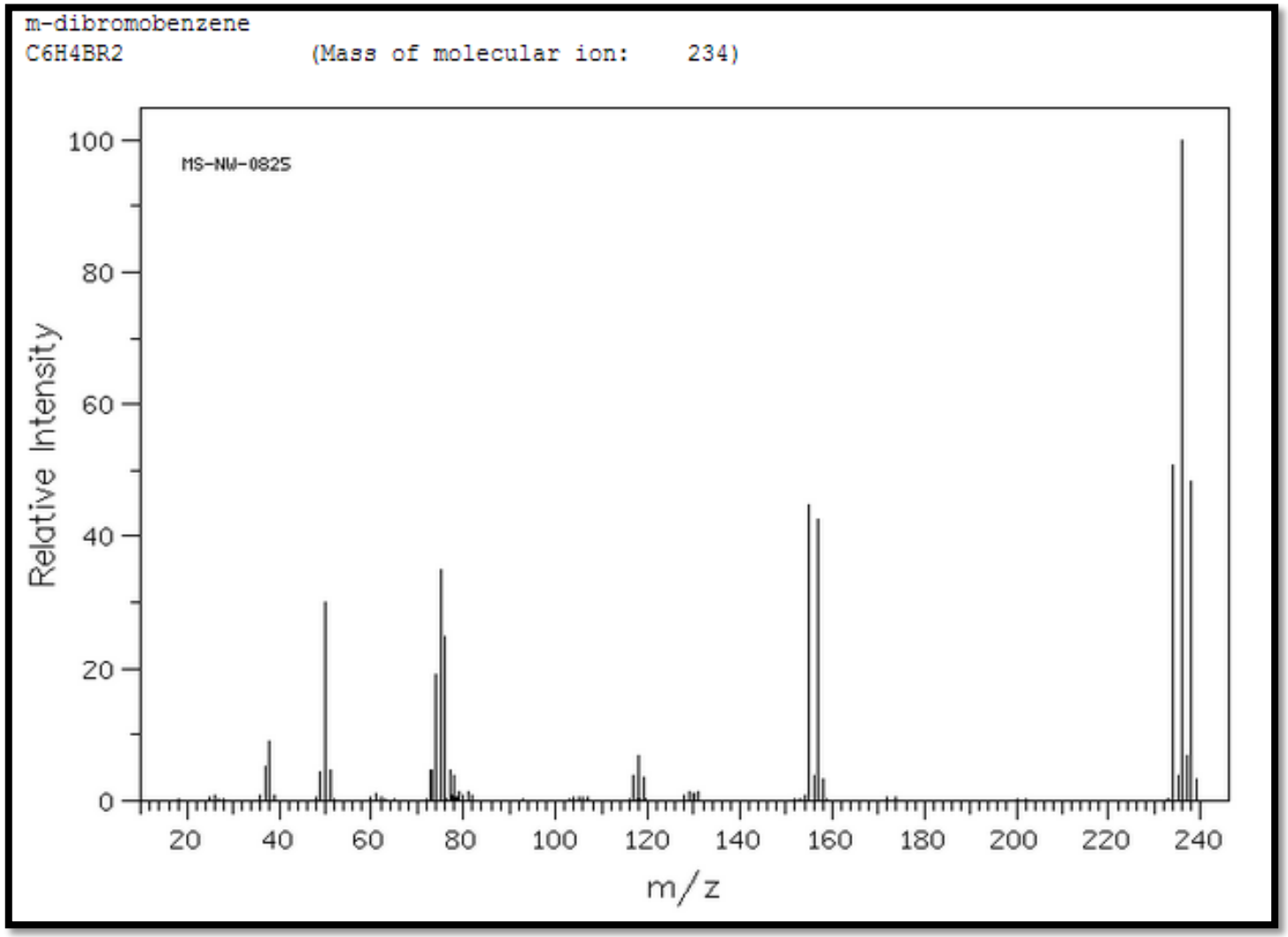
36.0	2.1
37.0	3.0
38.0	1.0
49.0	1.7
50.0	1.0
54.0	1.9
61.0	1.4
71.0	1.1
71.5	2.5
72.0	3.6
72.5	1.7
73.0	6.6
74.0	10.1
84.0	5.3
86.0	1.8
89.0	3.2
90.0	3.1
91.0	1.0
107.0	7.1
108.0	14.2
109.0	10.8
110.0	3.4
111.0	2.4
118.0	1.0
143.0	9.5
144.0	4.4
145.0	6.4
146.0	2.6
147.0	1.1
178.0	1.7
179.0	18.5
180.0	2.8
181.0	17.8
182.0	1.6
183.0	5.7
214.0	78.1
215.0	5.3
216.0	100.0
217.0	6.7
218.0	48.0
219.0	3.2
220.0	10.4

Bromobenzene



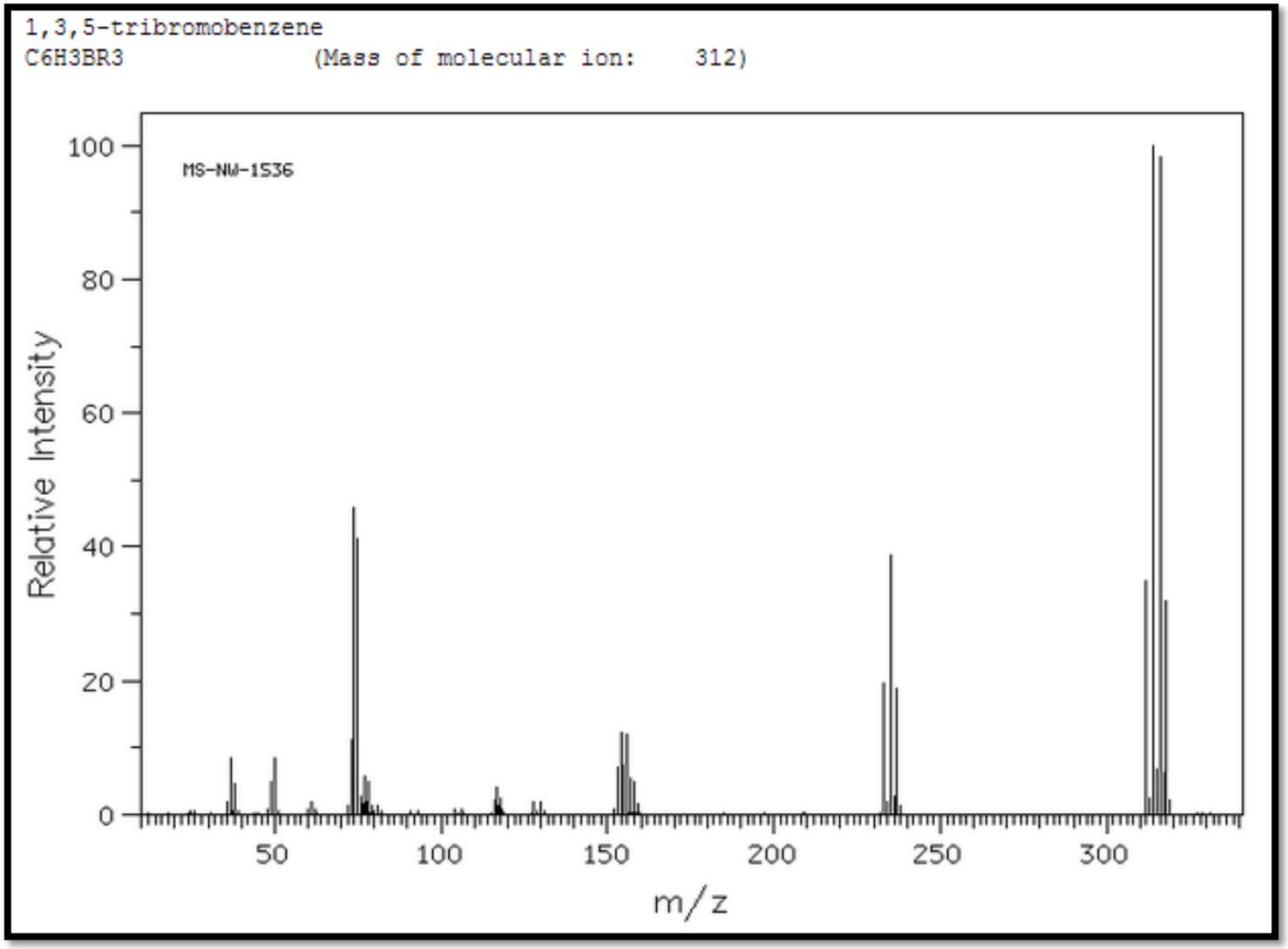
26.0	1.0
27.0	2.1
37.0	3.3
38.0	7.4
39.0	2.6
49.0	2.8
50.0	19.9
51.0	28.7
52.0	1.4
73.0	1.9
74.0	6.8
75.0	5.3
76.0	4.3
77.0	100.0
78.0	6.8
79.0	2.2
156.0	61.9
157.0	4.4
158.0	59.9
159.0	3.9

m-Dibromobenzene



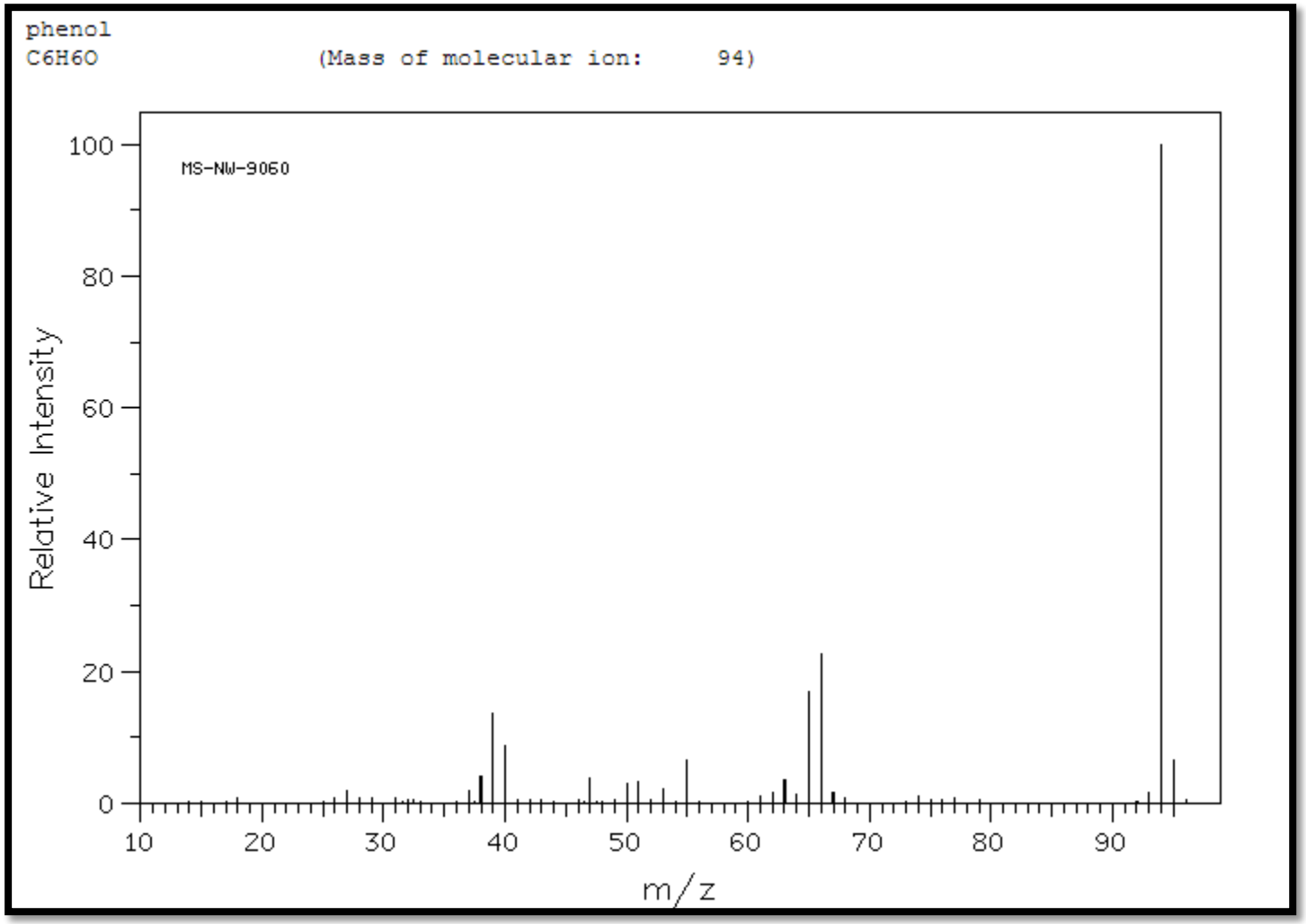
37.0	5.1
38.0	8.9
49.0	4.2
50.0	30.1
51.0	4.5
61.0	1.0
73.0	4.6
74.0	19.0
75.0	34.9
76.0	24.8
77.0	4.7
78.0	3.8
79.0	1.3
81.0	1.3
117.0	3.7
118.0	6.9
119.0	3.5
129.0	1.2
130.0	1.0
131.0	1.2
155.0	44.9
156.0	3.9
157.0	42.7
158.0	3.2
234.0	50.7
235.0	3.7
236.0	100.0
237.0	6.7
238.0	48.2
239.0	3.2

tribromobenzene



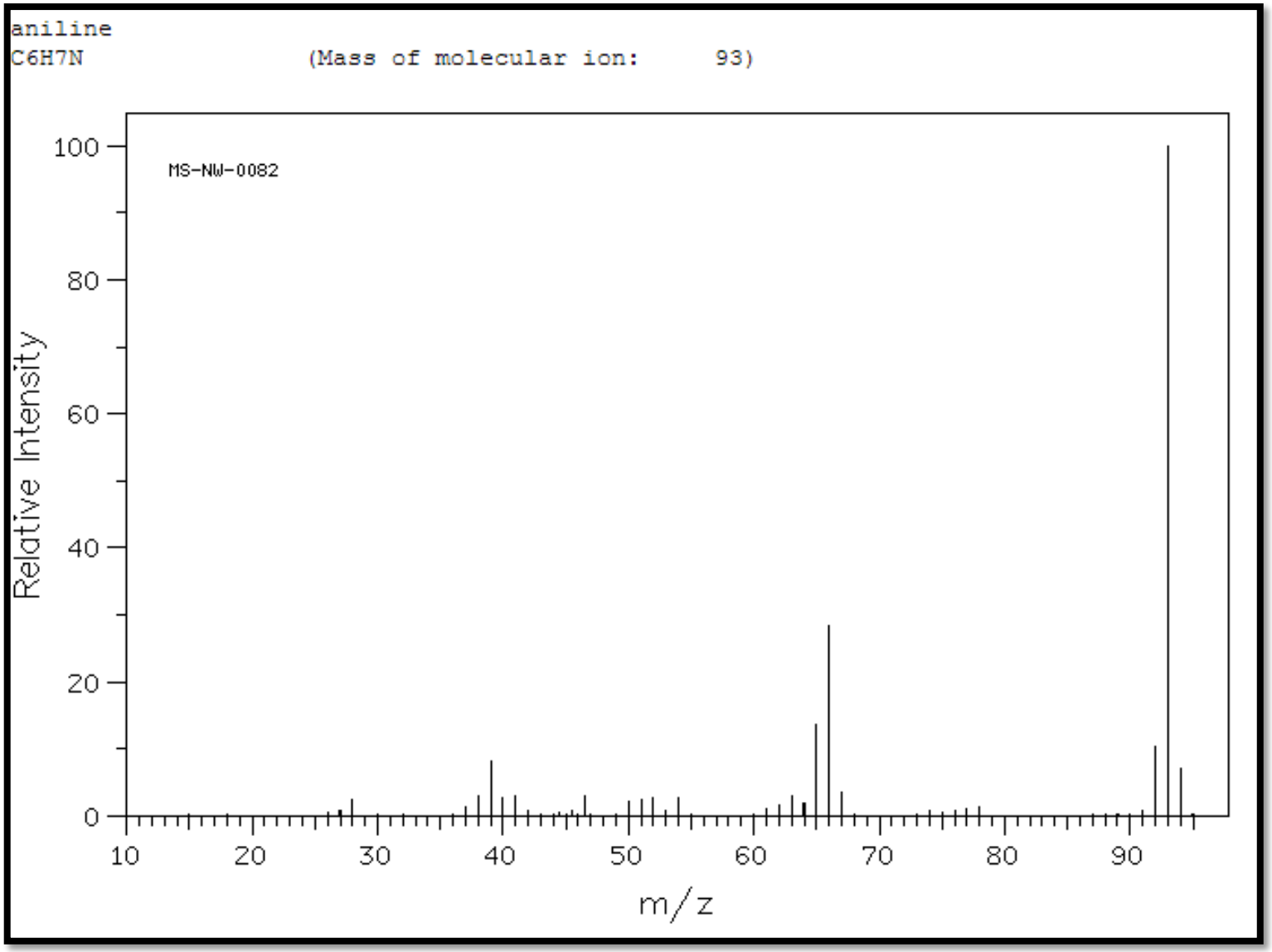
36.0	2.0
37.0	8.4
38.0	4.7
49.0	4.9
50.0	8.4
61.0	1.8
72.0	1.2
73.0	11.2
74.0	46.0
75.0	41.3
76.0	2.8
76.5	1.6
77.0	5.7
77.5	1.9
78.0	4.9
79.0	1.4
81.0	1.4
116.0	2.2
117.0	4.0
117.5	1.3
118.0	2.3
128.0	1.8
130.0	1.8
153.0	7.0
154.0	12.3
155.0	7.4
156.0	12.0
157.0	5.3
158.0	4.9
159.0	1.6
233.0	19.7
234.0	1.8
235.0	38.8
236.0	2.7
237.0	18.8
238.0	1.3
312.0	34.8
313.0	2.4
314.0	100.0
315.0	6.8
316.0	98.3
317.0	6.3
318.0	31.9
319.0	2.1

Phenol



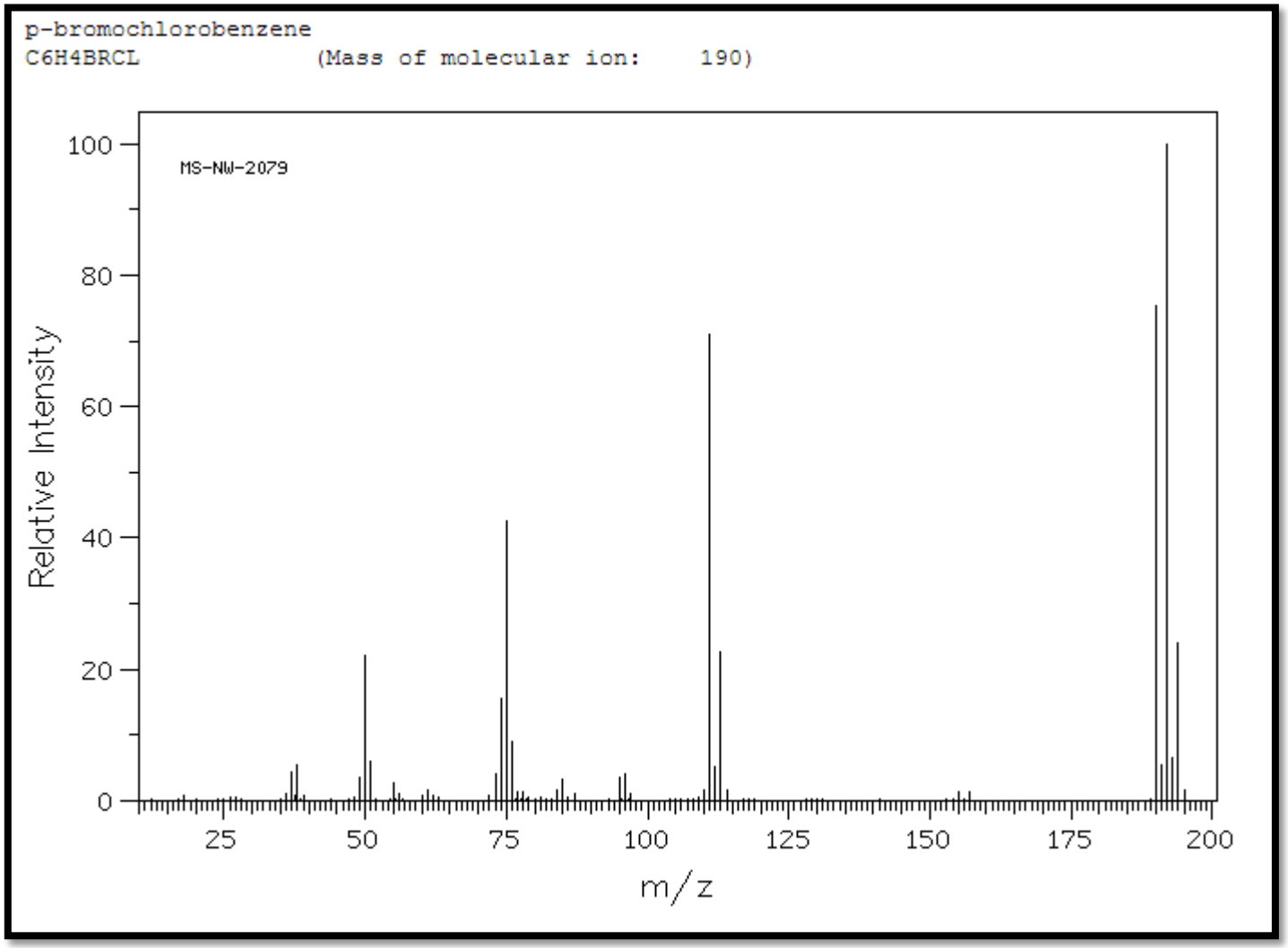
27.0	1.9
37.0	2.0
38.0	4.0
39.0	13.6
40.0	8.8
47.0	3.9
50.0	3.1
51.0	3.2
53.0	2.1
55.0	6.6
61.0	1.1
62.0	1.7
63.0	3.5
64.0	1.4
65.0	16.8
66.0	22.6
67.0	1.5
74.0	1.1
93.0	1.5
94.0	100.0
95.0	6.6

Aniline



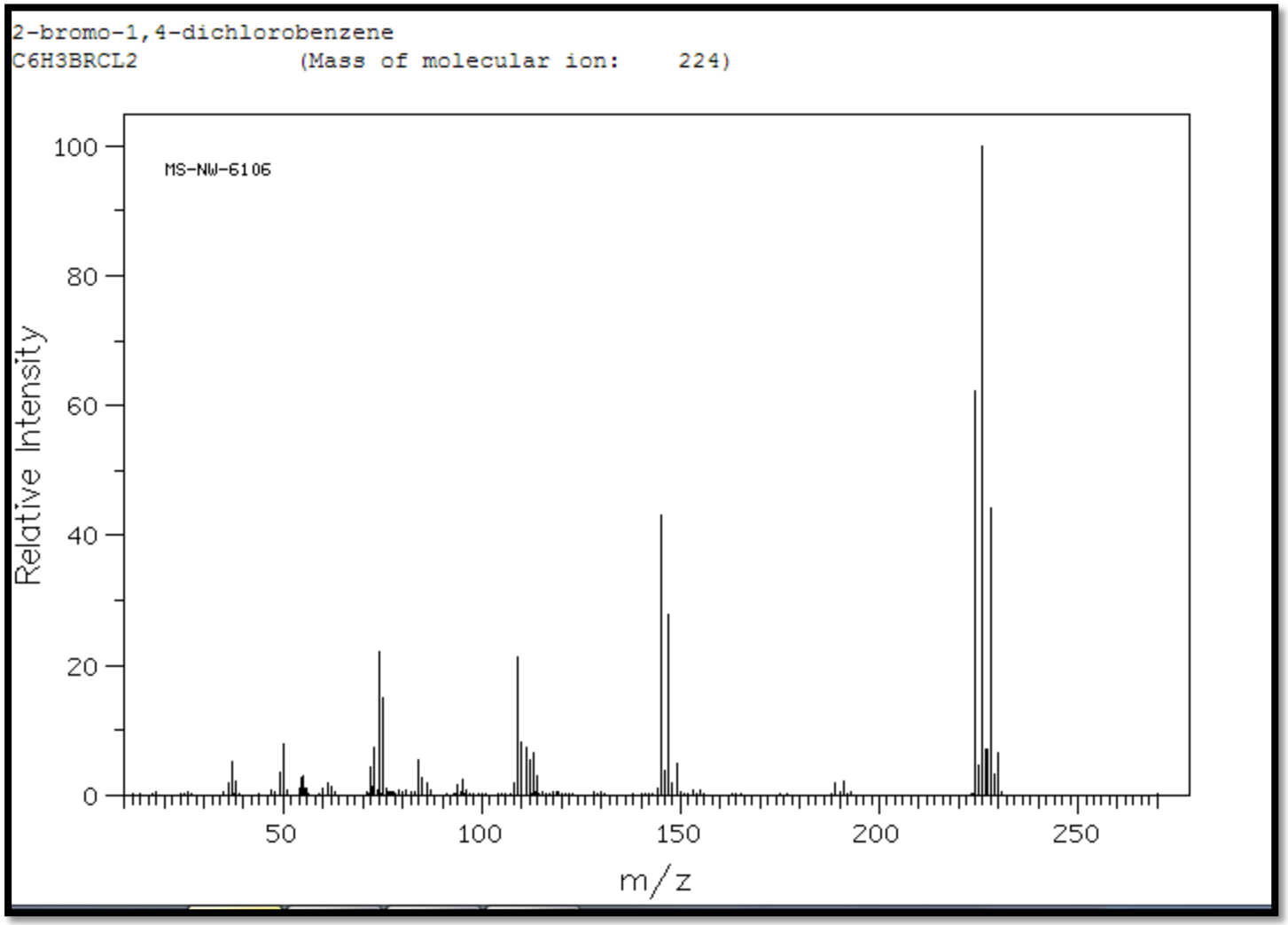
28.0	2.3
37.0	1.4
38.0	2.9
39.0	8.2
40.0	2.7
41.0	2.9
46.5	3.1
50.0	2.2
51.0	2.5
52.0	2.8
54.0	2.8
61.0	1.0
62.0	1.6
63.0	3.1
64.0	1.8
65.0	13.5
66.0	28.5
67.0	3.6
77.0	1.0
78.0	1.4
92.0	10.4
93.0	100.0
94.0	7.0

bromochlorobenzene



36.0	1.0
37.0	4.4
38.0	5.4
49.0	3.4
50.0	22.2
51.0	6.1
55.0	2.8
56.0	1.0
61.0	1.6
73.0	4.1
74.0	15.4
75.0	42.6
76.0	8.9
77.0	1.4
78.0	1.3
84.0	1.7
85.0	3.3
87.0	1.0
95.0	3.5
96.0	4.1
97.0	1.0
110.0	1.5
111.0	71.1
112.0	5.1
113.0	22.7
114.0	1.5
155.0	1.3
157.0	1.2
190.0	75.3
191.0	5.3
192.0	100.0
193.0	6.6
194.0	23.9
195.0	1.7

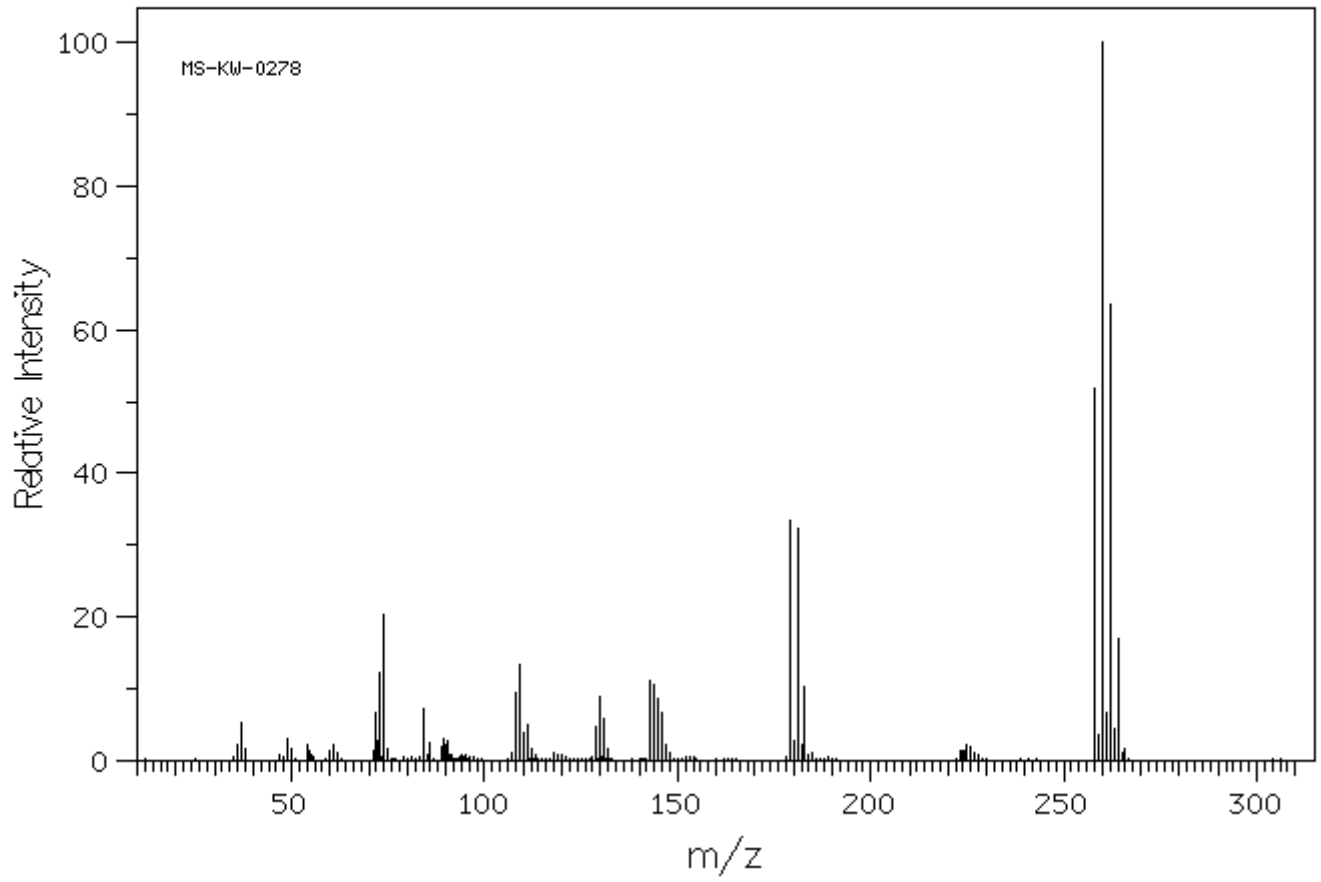
2-bromo-1,4-dichlorobenzene



36.0	1.9
37.0	5.1
38.0	2.1
49.0	3.5
50.0	8.0
54.0	1.0
54.5	2.7
55.0	3.1
55.5	1.1
56.0	1.0
60.0	1.1
61.0	1.8
62.0	1.2
72.0	4.4
72.5	1.2
73.0	7.3
74.0	22.2
75.0	15.0
76.0	1.1
84.0	5.5
85.0	2.7
86.0	2.0
94.0	1.7
95.0	2.4
108.0	1.8
109.0	21.4
110.0	8.2
111.0	7.3
112.0	5.4
113.0	6.4
114.0	3.1
144.0	1.0
145.0	43.1
146.0	3.7
147.0	27.9
148.0	2.0
149.0	5.0
189.0	1.8
191.0	2.2
224.0	62.2
225.0	4.6
226.0	100.0
227.0	7.1
228.0	44.3
229.0	3.2
230.0	6.4

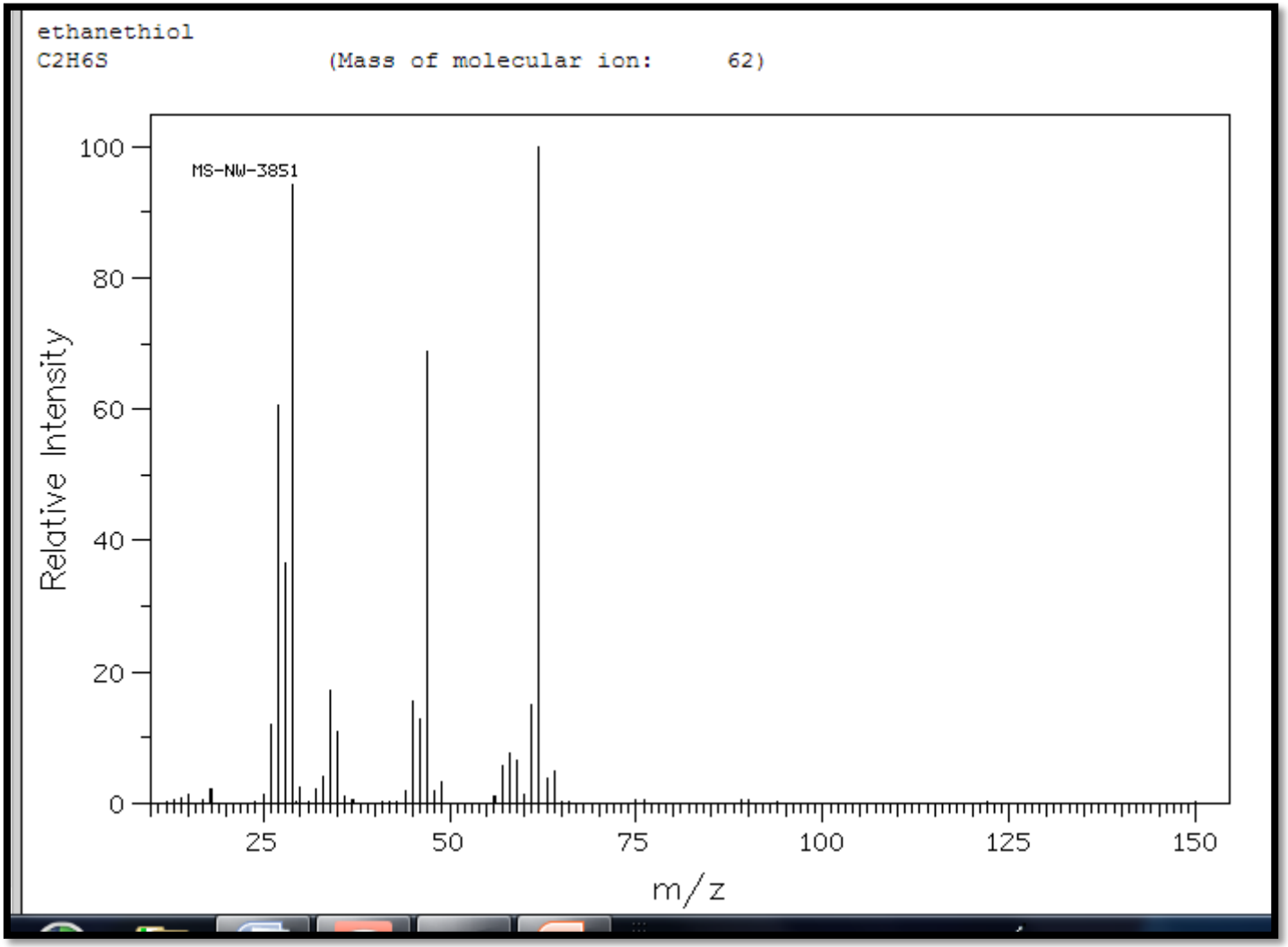
1-bromo-2,3,5-trichlorobenzene

1-bromo-2,3,5-trichlorobenzene
C6H2BRCL3 (Mass of molecular ion: 258)



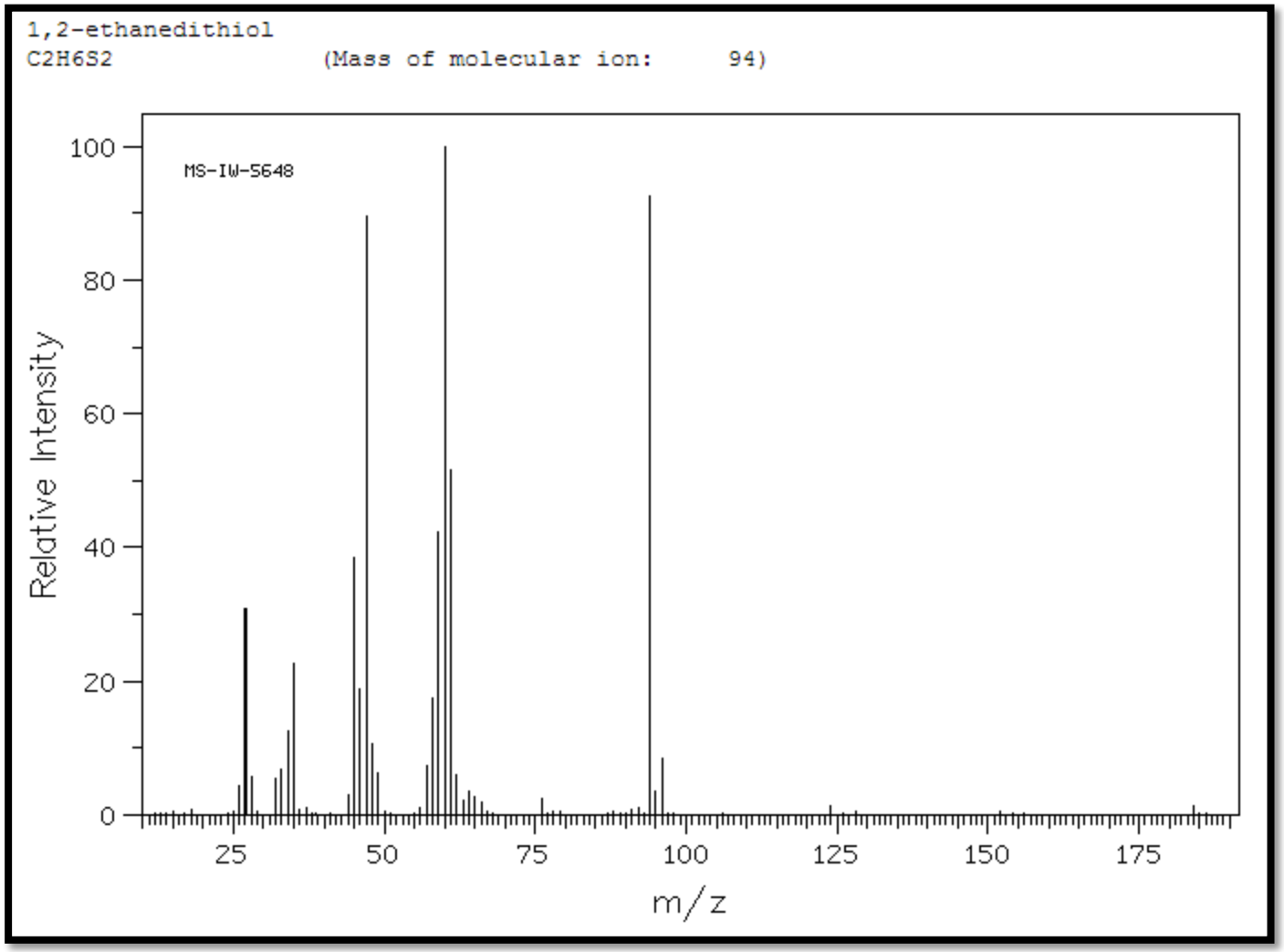
89.5	3.1
90.0	2.1
90.5	2.8
107.0	1.0
108.0	9.4
109.0	13.2
110.0	3.9
111.0	4.9
112.0	1.7
118.0	1.1
129.0	4.6
130.0	8.9
131.0	5.7
132.0	1.5
143.0	11.1
144.0	10.4
145.0	8.5
146.0	6.7
147.0	2.1
148.0	1.1
179.0	33.5
180.0	2.7
181.0	32.2
182.0	2.3
183.0	10.3
185.0	1.1
223.0	1.4
224.0	1.2
225.0	2.3
226.0	1.8
227.0	1.1
258.0	51.8
259.0	3.7
260.0	100.0
261.0	6.7
262.0	63.6
263.0	4.3
264.0	17.0
265.0	1.1
266.0	1.6

ethanethiol



15.0	1.4
18.0	2.2
25.0	1.4
26.0	12.1
27.0	60.6
28.0	36.6
29.0	94.2
30.0	2.3
32.0	2.2
33.0	4.0
34.0	17.3
35.0	10.9
36.0	1.0
44.0	2.0
45.0	15.5
46.0	12.8
47.0	68.7
48.0	1.9
49.0	3.2
56.0	1.1
57.0	5.6
58.0	7.5
59.0	6.6
60.0	1.3
61.0	14.9
62.0	100.0
63.0	3.7
64.0	4.9

1,2-ethanedithiol



26.0	4.4
27.0	30.8
28.0	5.8
32.0	5.5
33.0	6.8
34.0	12.5
35.0	22.7
37.0	1.0
44.0	3.0
45.0	38.4
46.0	18.9
47.0	89.7
48.0	10.6
49.0	6.2
56.0	1.1
57.0	7.3
58.0	17.4
59.0	42.4
60.0	100.0
61.0	51.6
62.0	6.1
63.0	2.2
64.0	3.5
65.0	2.7
66.0	2.0
76.0	2.3
92.0	1.1
94.0	92.6
95.0	3.6
96.0	8.5
124.0	1.3
184.0	1.2