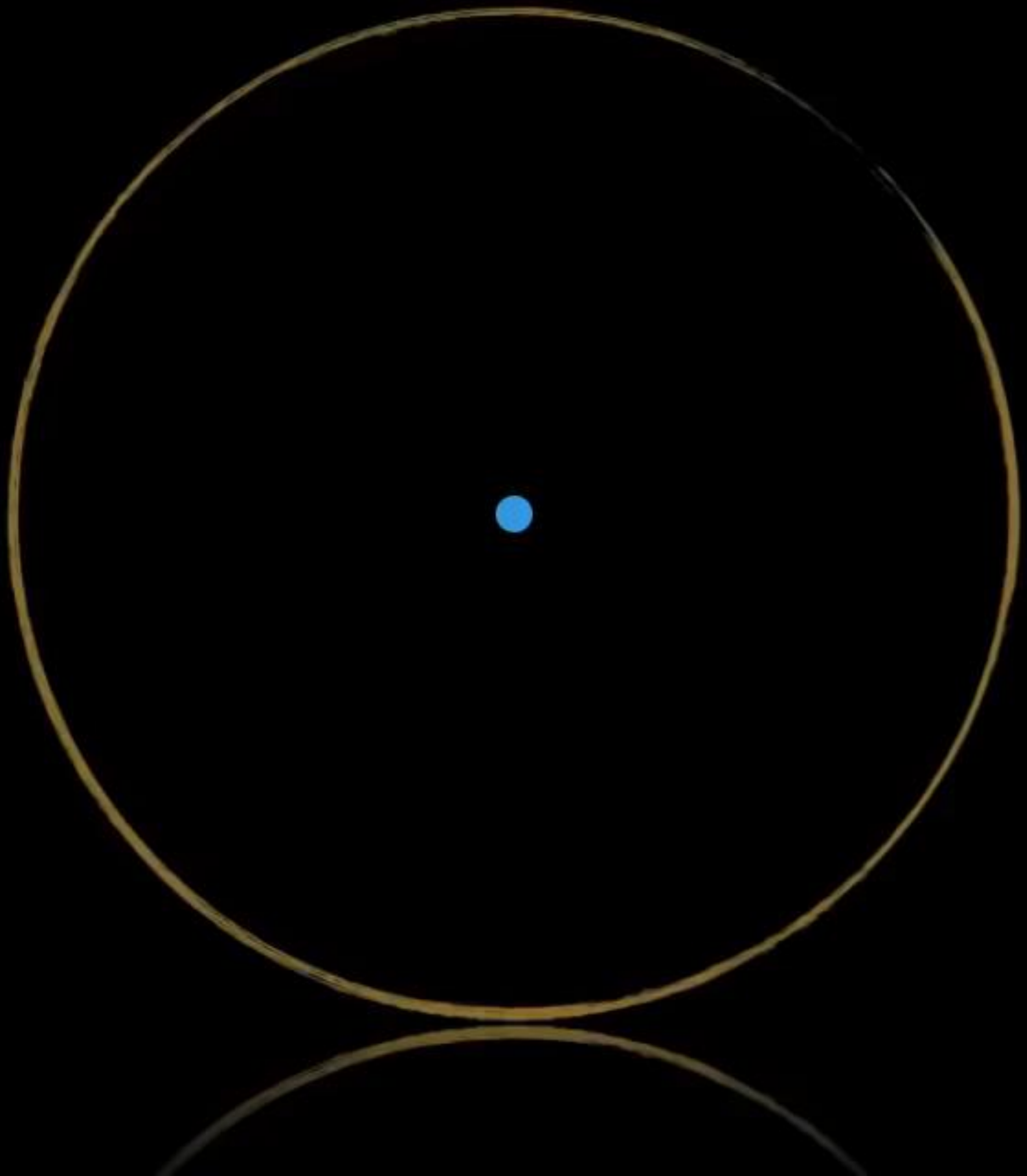
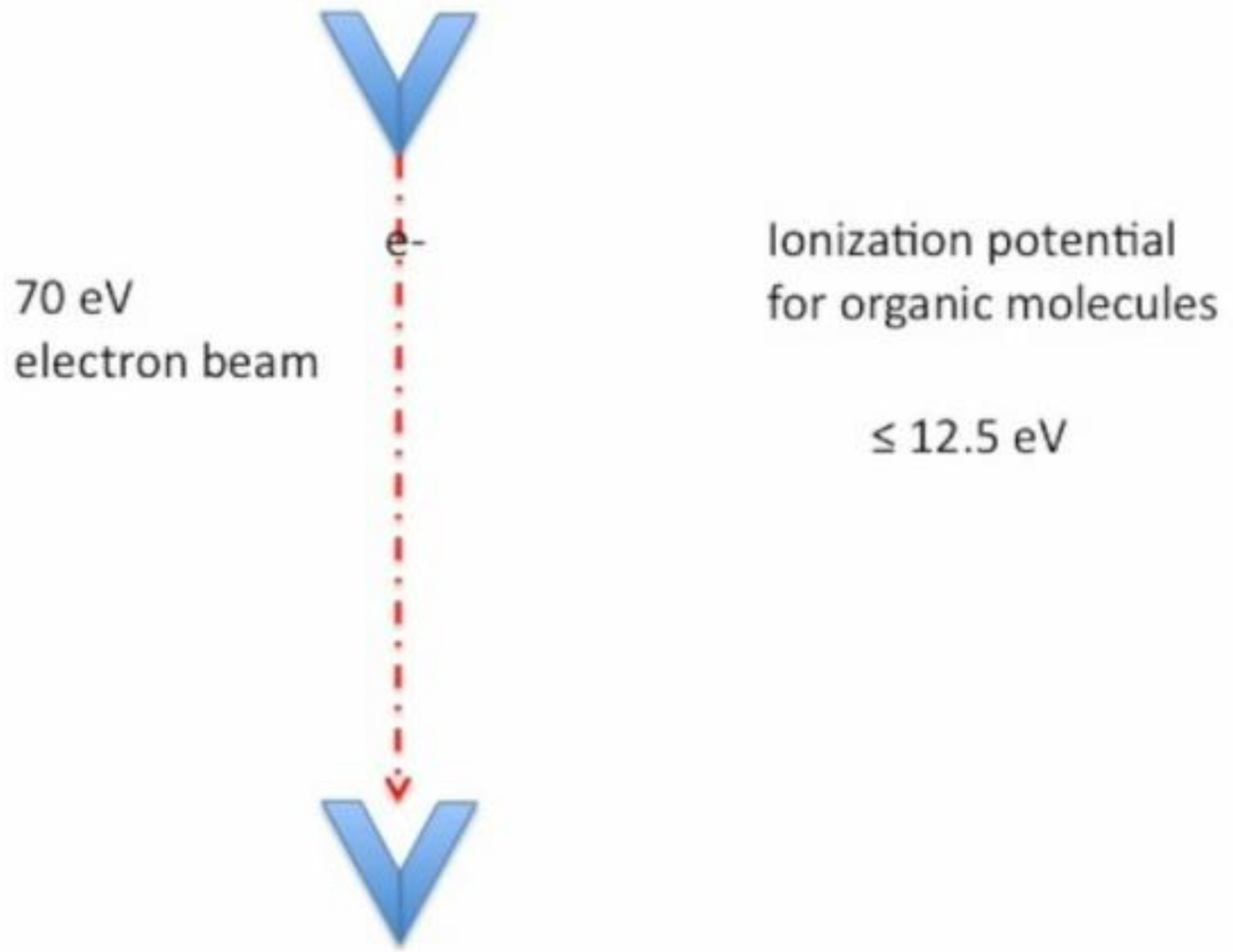
Mass Spectroscopy مطياف الكتلة

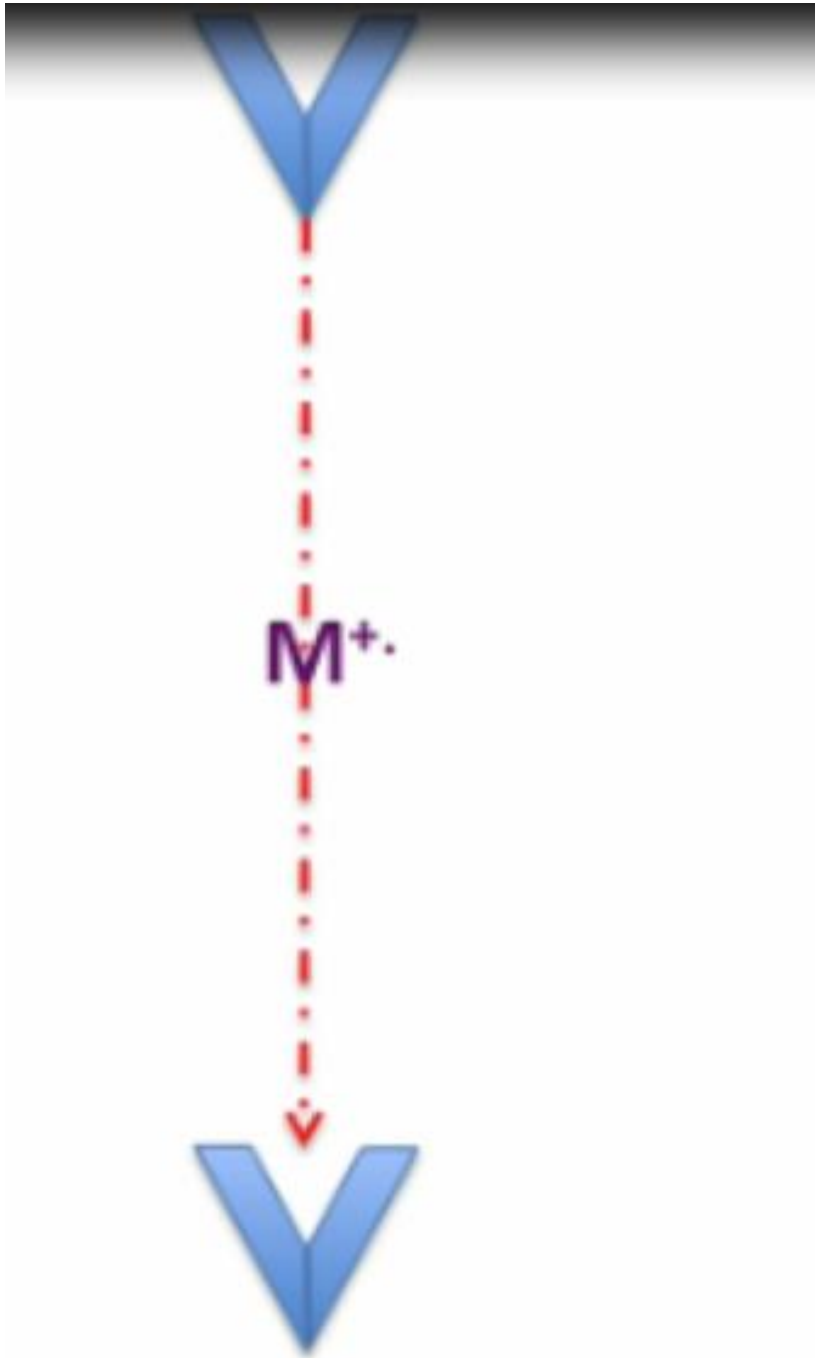
المحاضرة الرابعة

د. طه الملي




e-
70 eV
electron beam
Ionization potential
for organic molecules
≤ 12.5 eV


e-
M



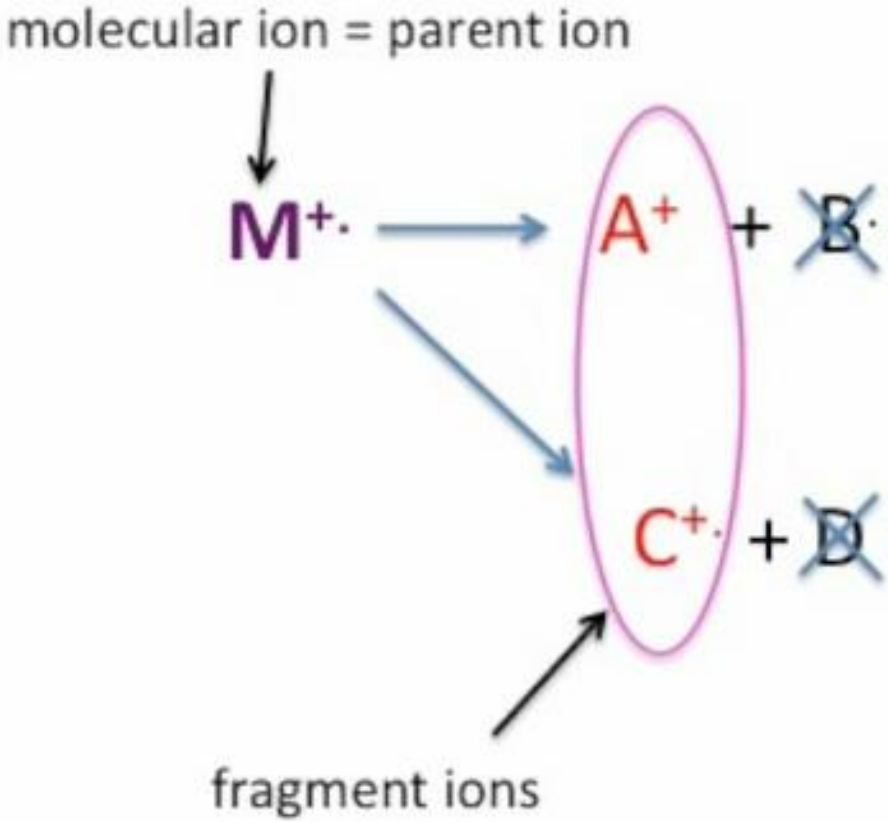
$M^{+\cdot}$

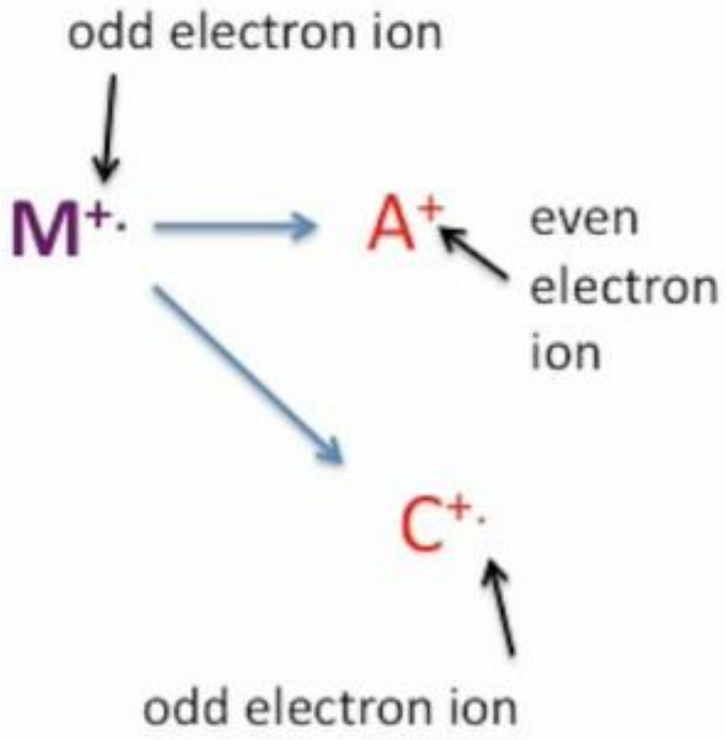
$M^{+\cdot}$

$$M^{+\cdot} \longrightarrow A^{+} + B^{\cdot}$$

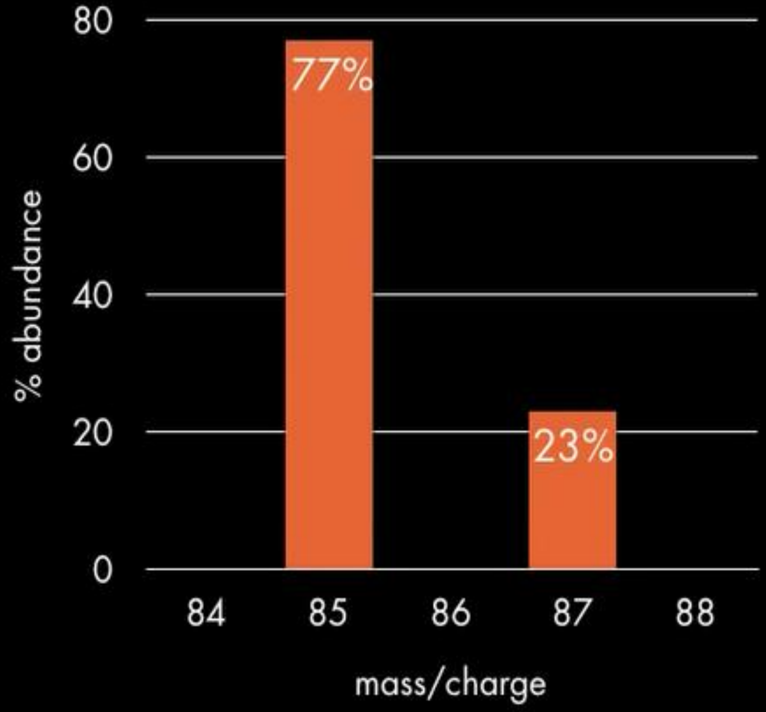
$$M^{+\cdot} \rightarrow A^{+} + B^{\cdot}$$

$$M^{+\cdot} \rightarrow C^{+\cdot} + D$$


molecular ion = parent ion
$M^{+\cdot}$
A^{+} + $B^{\cdot}$
$C^{+\cdot}$ + D
fragment ions

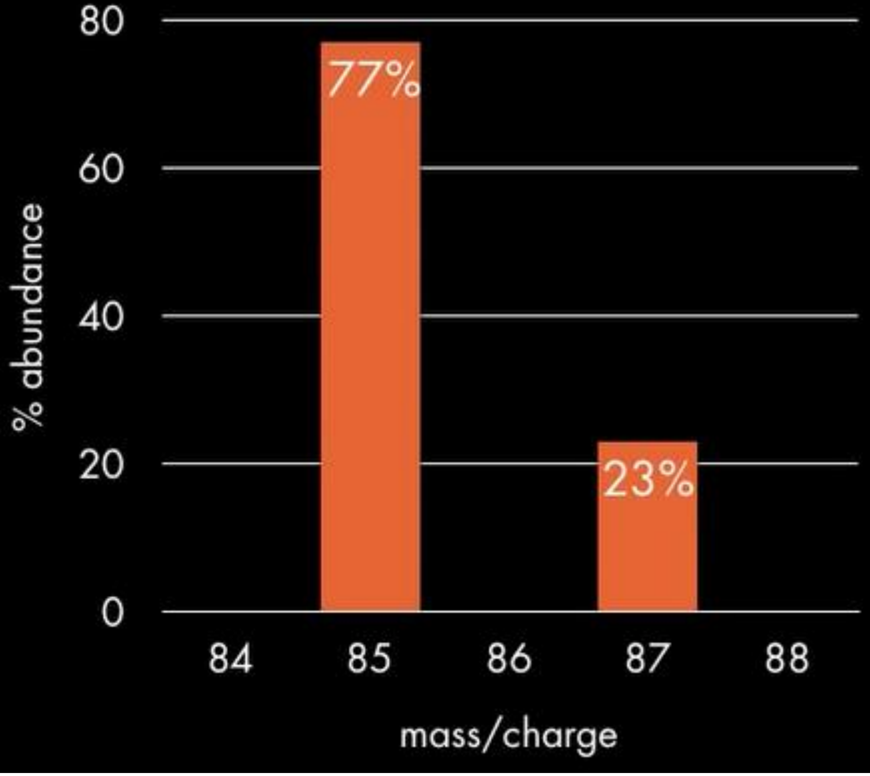

odd electron ion
M+·
A+
even electron ion
C+·
odd electron ion

Interpreting Mass Spec. Data



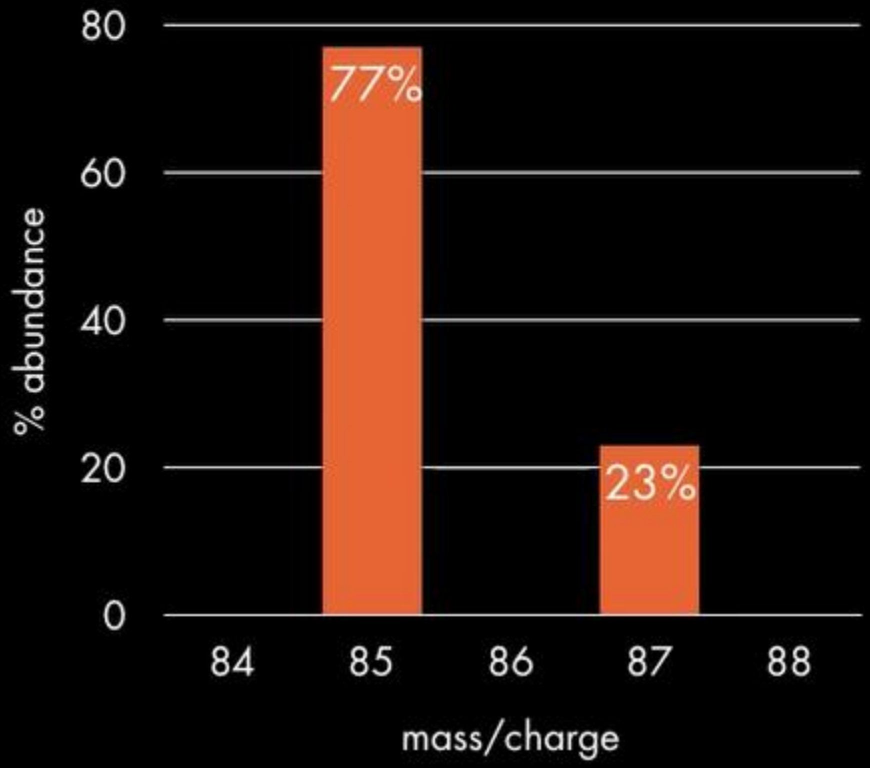
Interpreting Mass Spec. Data

$$
\begin{array}{r}
(77\% \times 85) \\
+\ (23\% \times 87) \\
\hline
=\quad 8546
\end{array}
$$

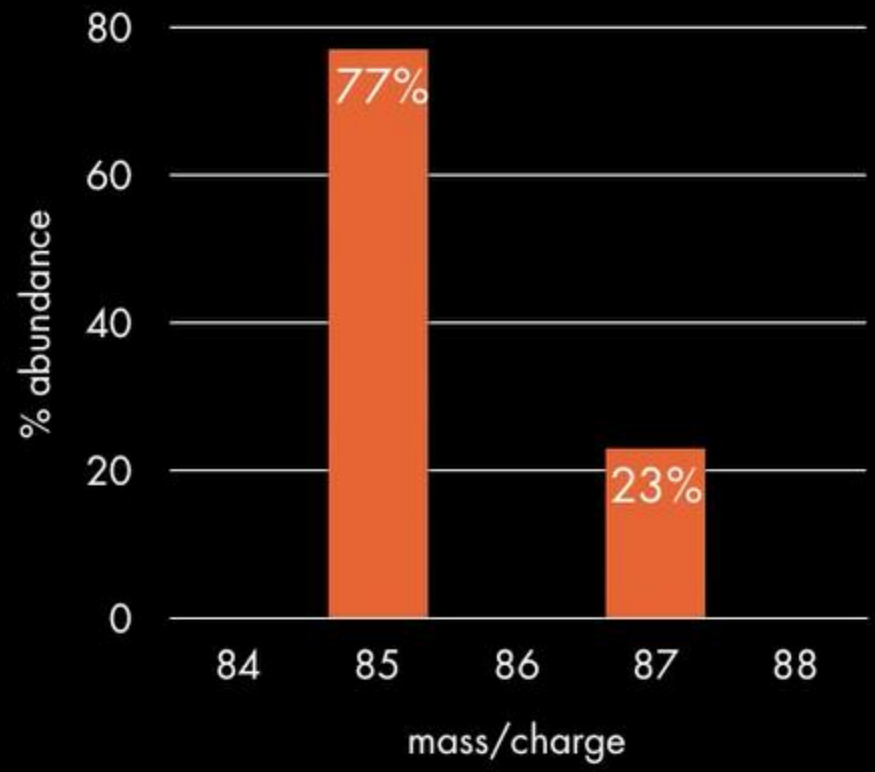


Interpreting Mass Spec. Data

8546
÷ 100
= *85.46*



Interpreting Mass Spec. Data



Calculating Isotope Abundancies

^{10}B

^{11}B

Calculating Isotope Abundancies

^{10}B

x

^{11}B

$100 - x$

100

Calculating Isotope Abundancies

^{10}B — x

^{11}B — $100 - x$

$$\frac{10x + (100 - x)11}{100} = 10.81$$

Calculating Isotope Abundancies

^{10}B

x

^{11}B

$100 - x$

$x = 19$

Calculating Isotope Abundancies

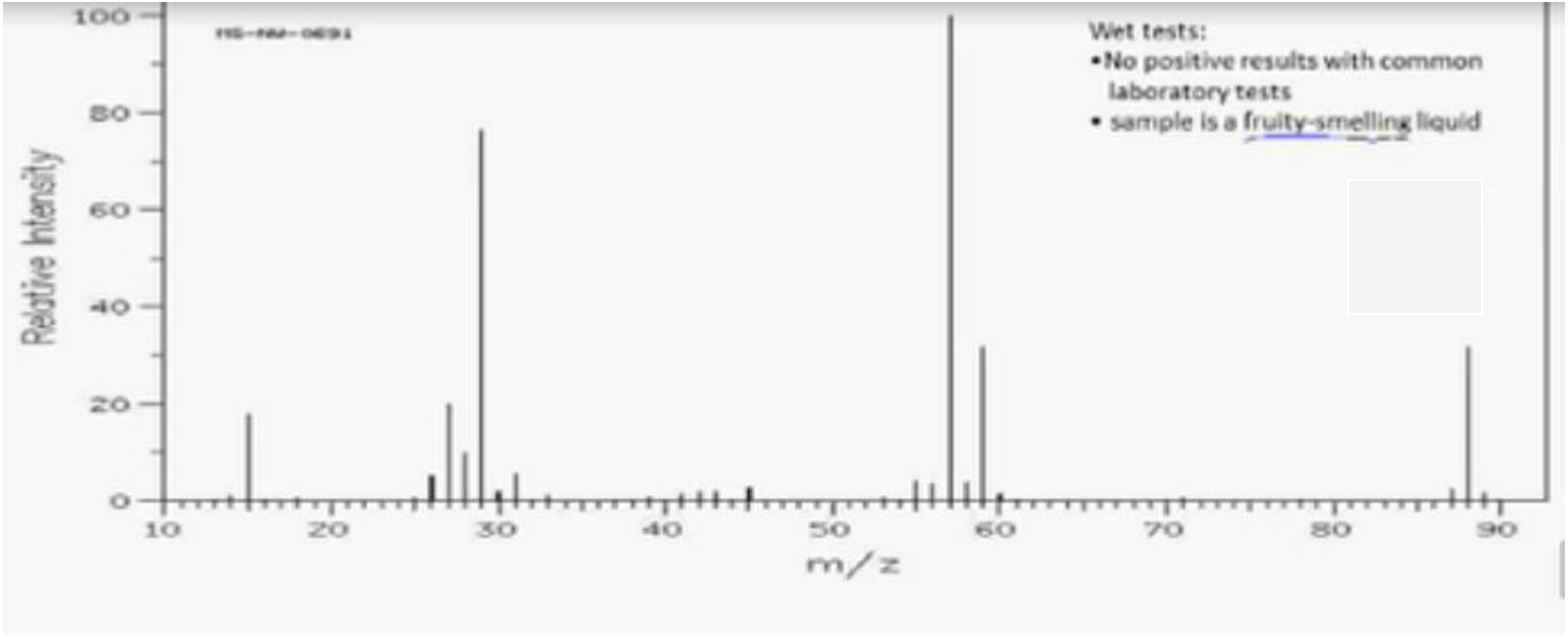
19% ^{10}B

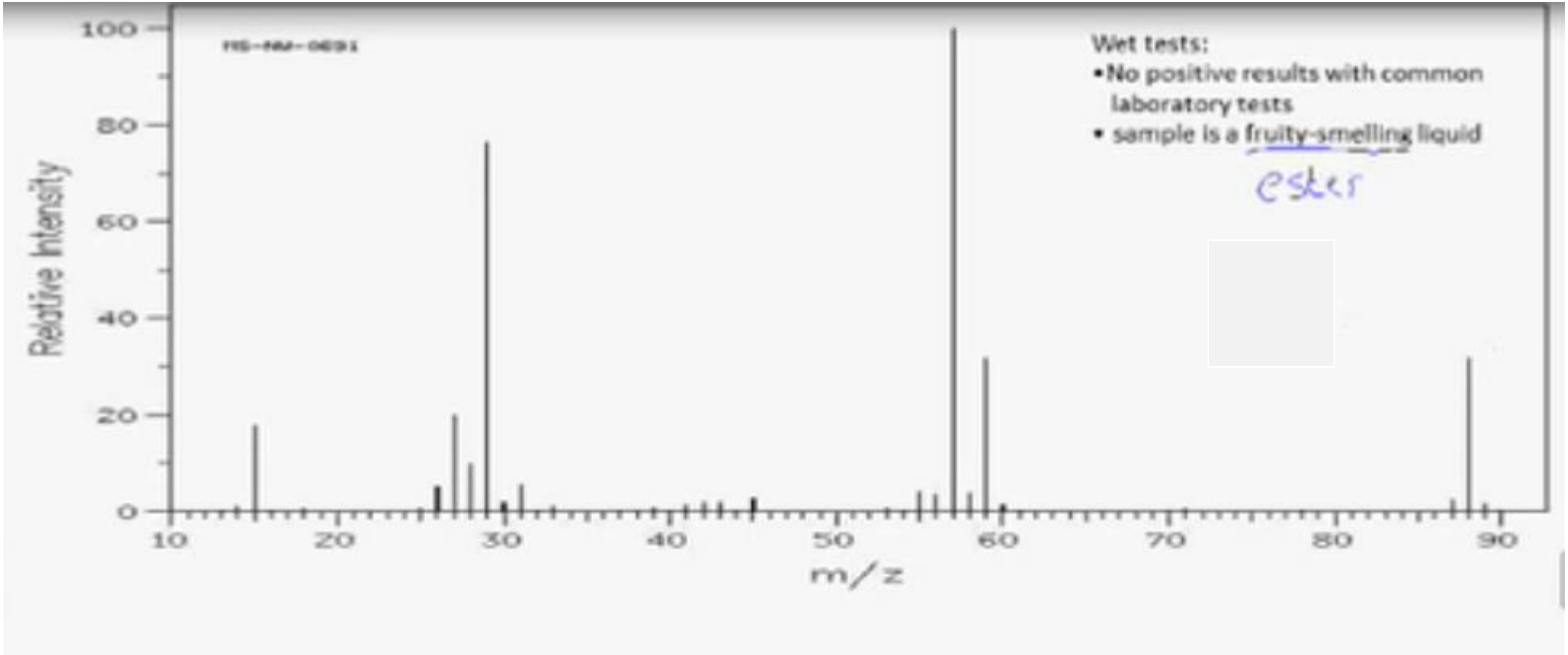
x

^{11}B *81%*

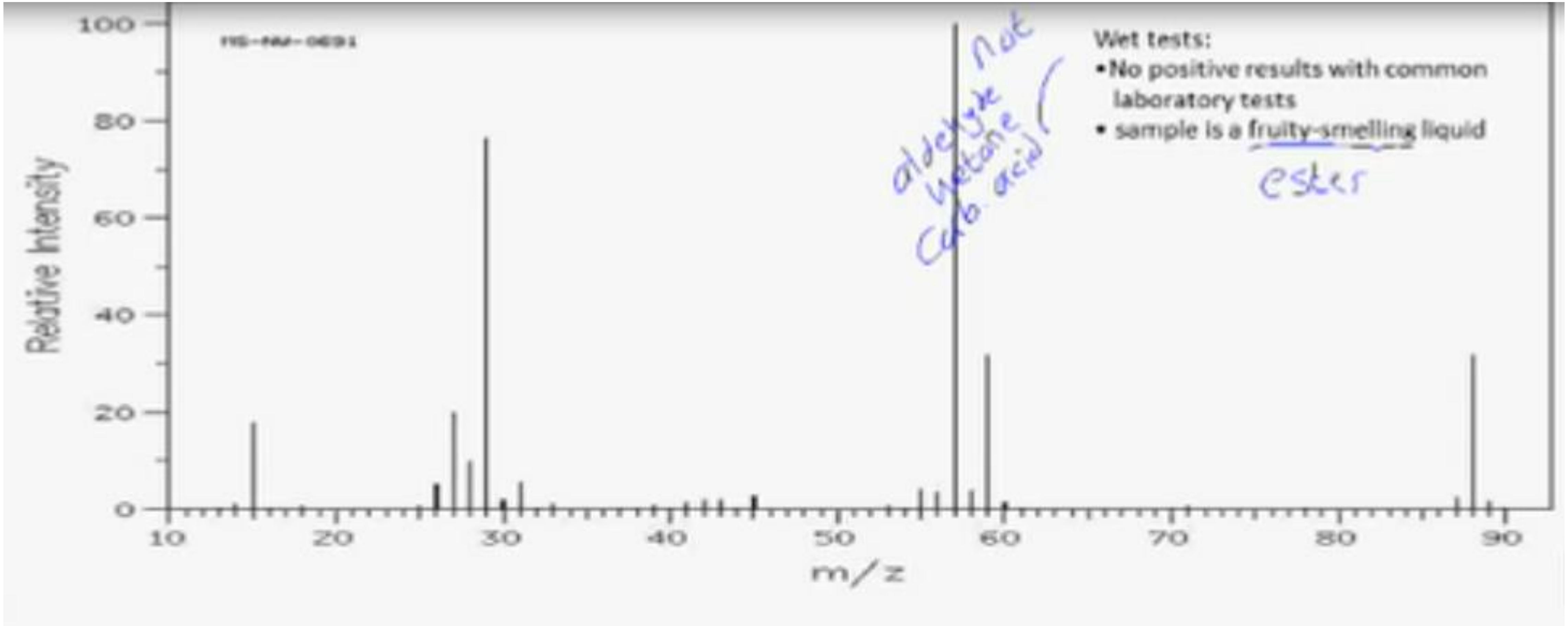
$100 - x$

$x = 19$

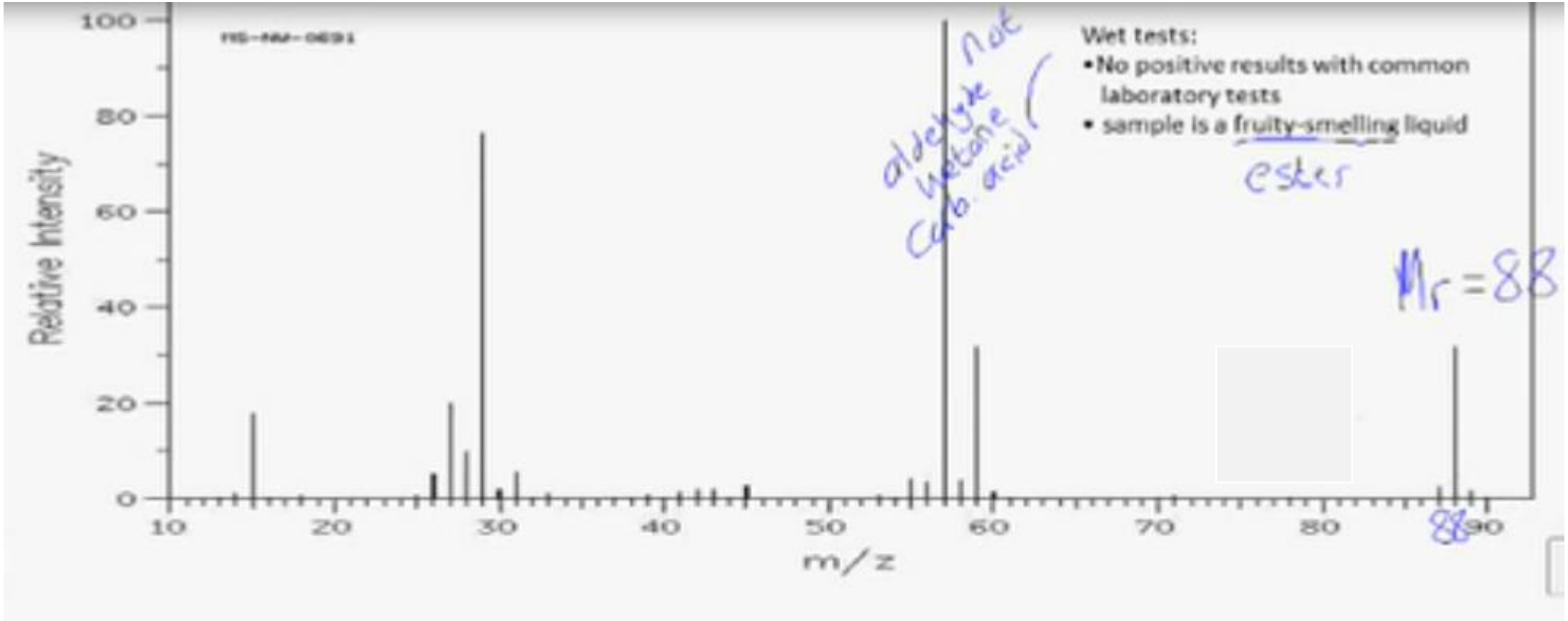

Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
Relative Intensity
100
80
60
40
20
0
10
20
30
40
50
60
70
80
90
m/z



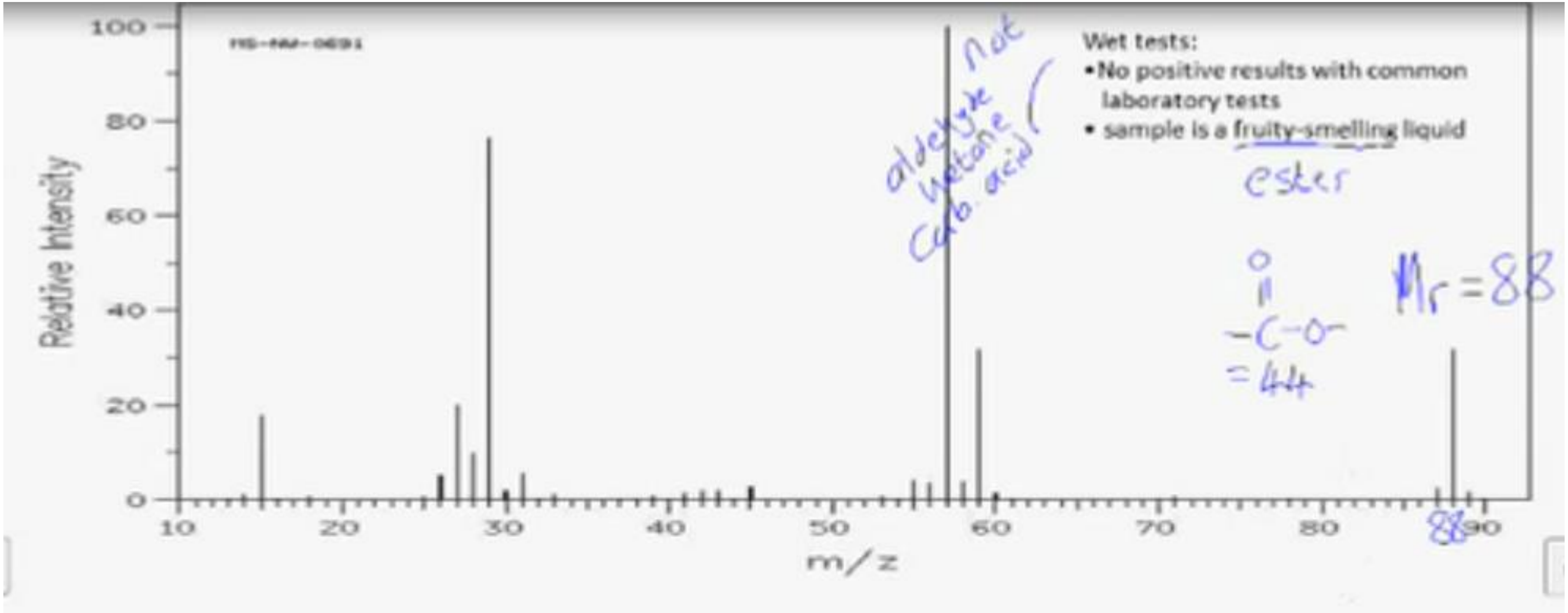
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
Relative Intensity
m/z



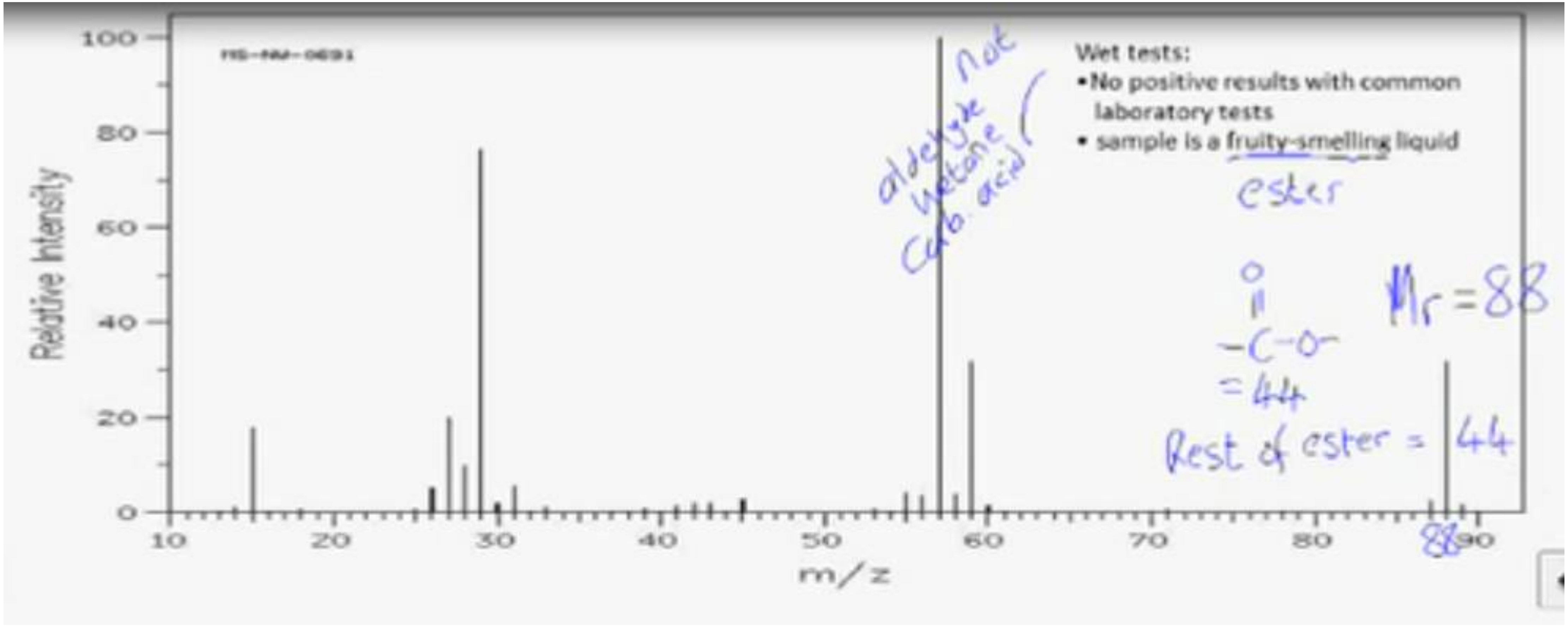
MS-NW-0691
Relative Intensity
100
80
60
40
20
0
10
20
30
40
50
60
70
80
90
m/z
Wet tests:
•No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
aldehyde
ketone
Carb. acid
not

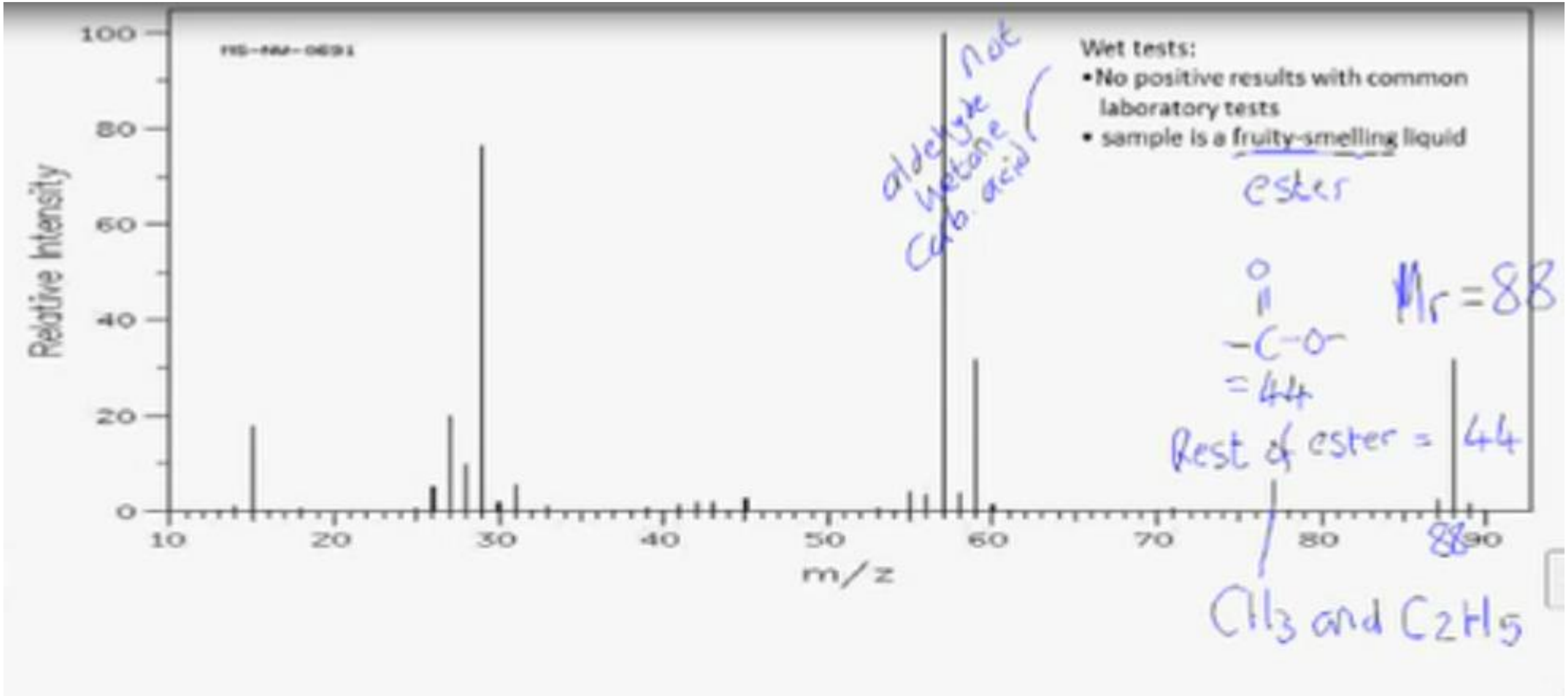


MS-NW-0691
Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
not aldehyde ketone carb. acid
Mr = 88
88

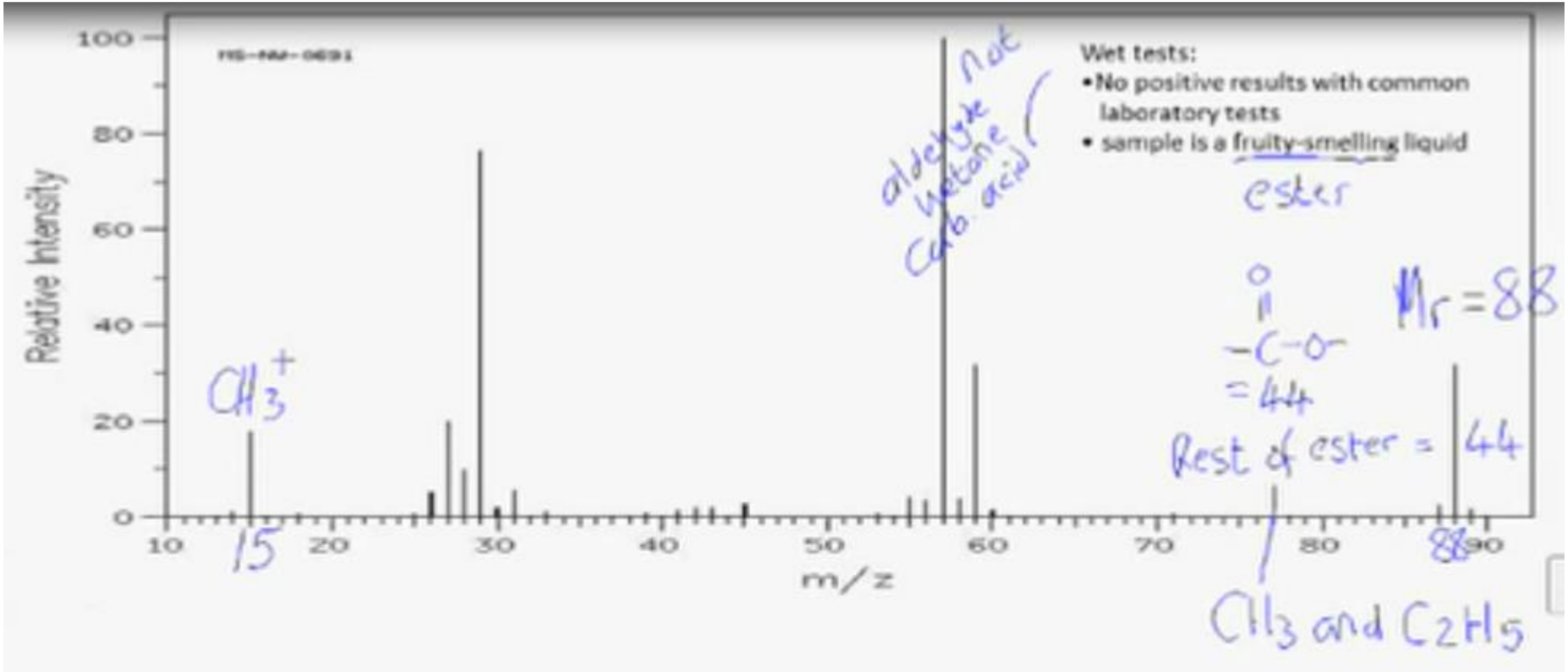


Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
aldehyde not ketone carb. acid
Mr = 88
=44
88

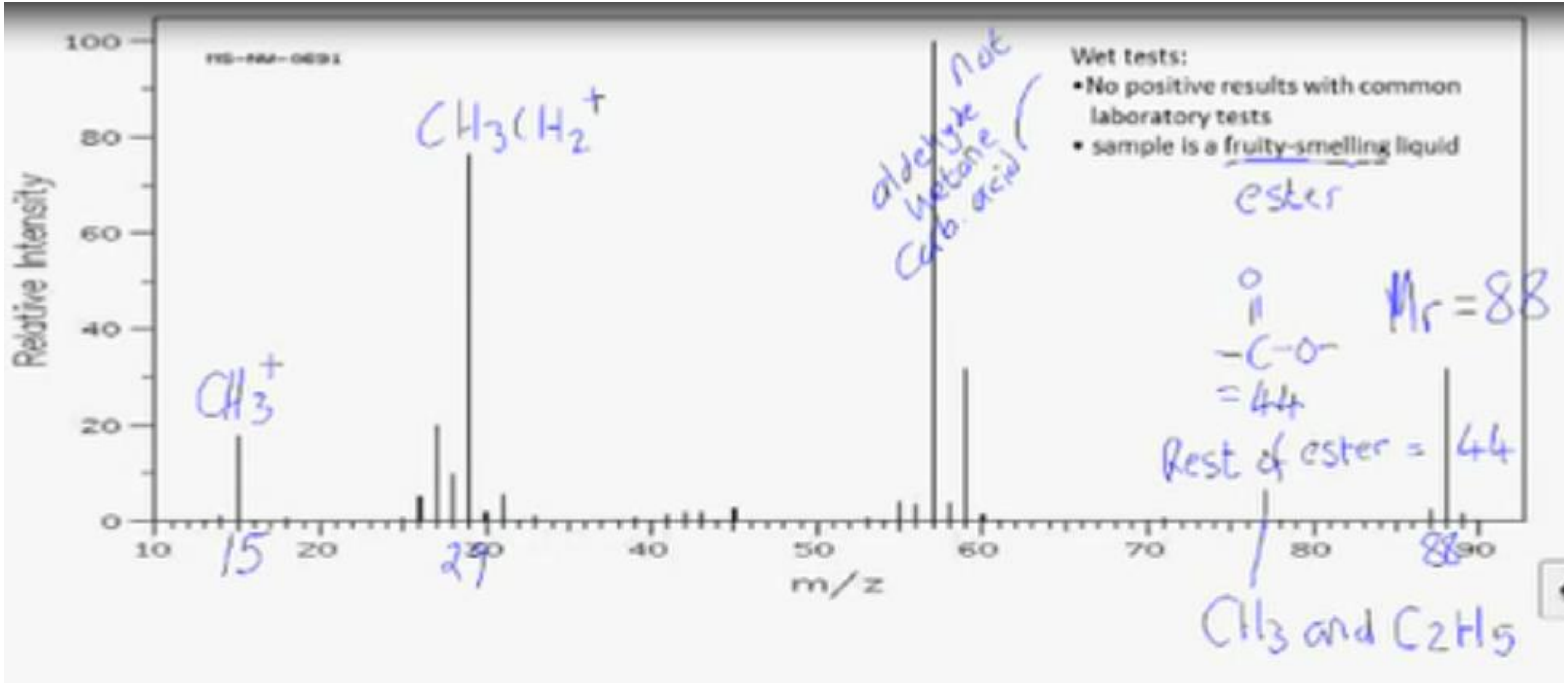

MS-NW-0691
Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
not aldehyde ketone carb. acid
Mr = 88
-C(=O)-O- = 44
Rest of ester = 44
88

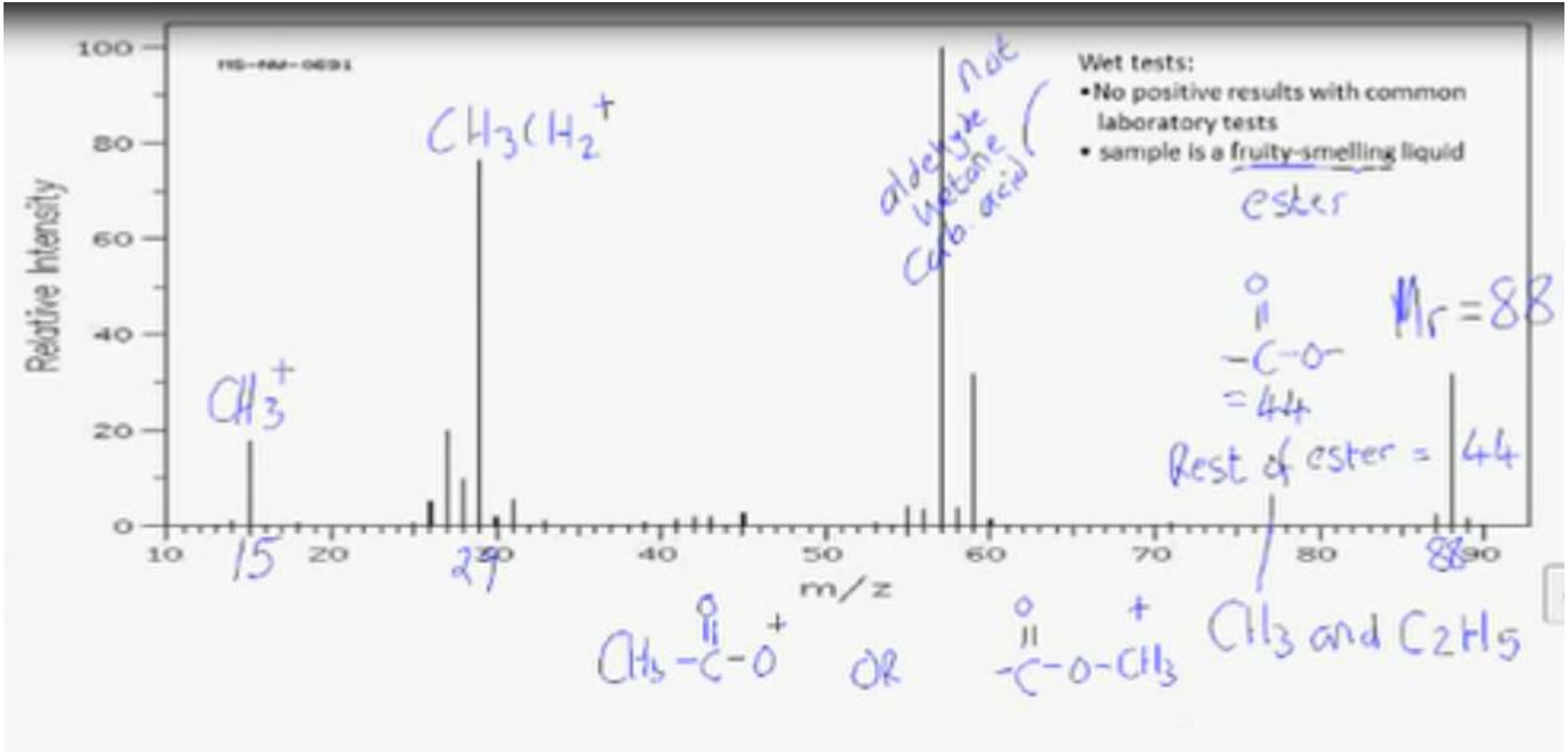


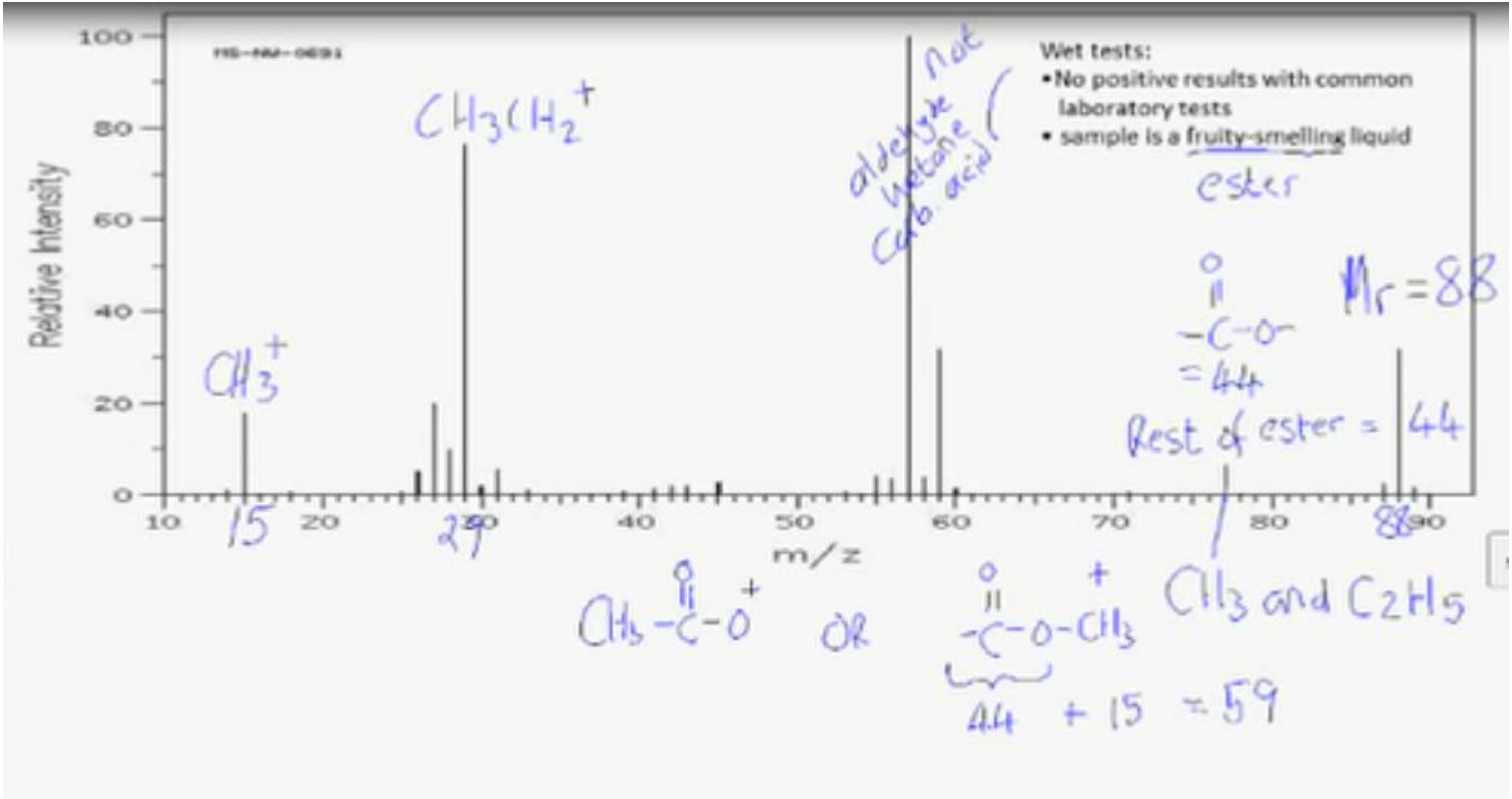
Relative Intensity
100
80
60
40
20
0
10
20
30
40
50
60
70
80
90
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
not aldehyde ketone carb. acid
Mr = 88
-C(=O)-O- = 44
Rest of ester = 44
88
CH3 and C2H5



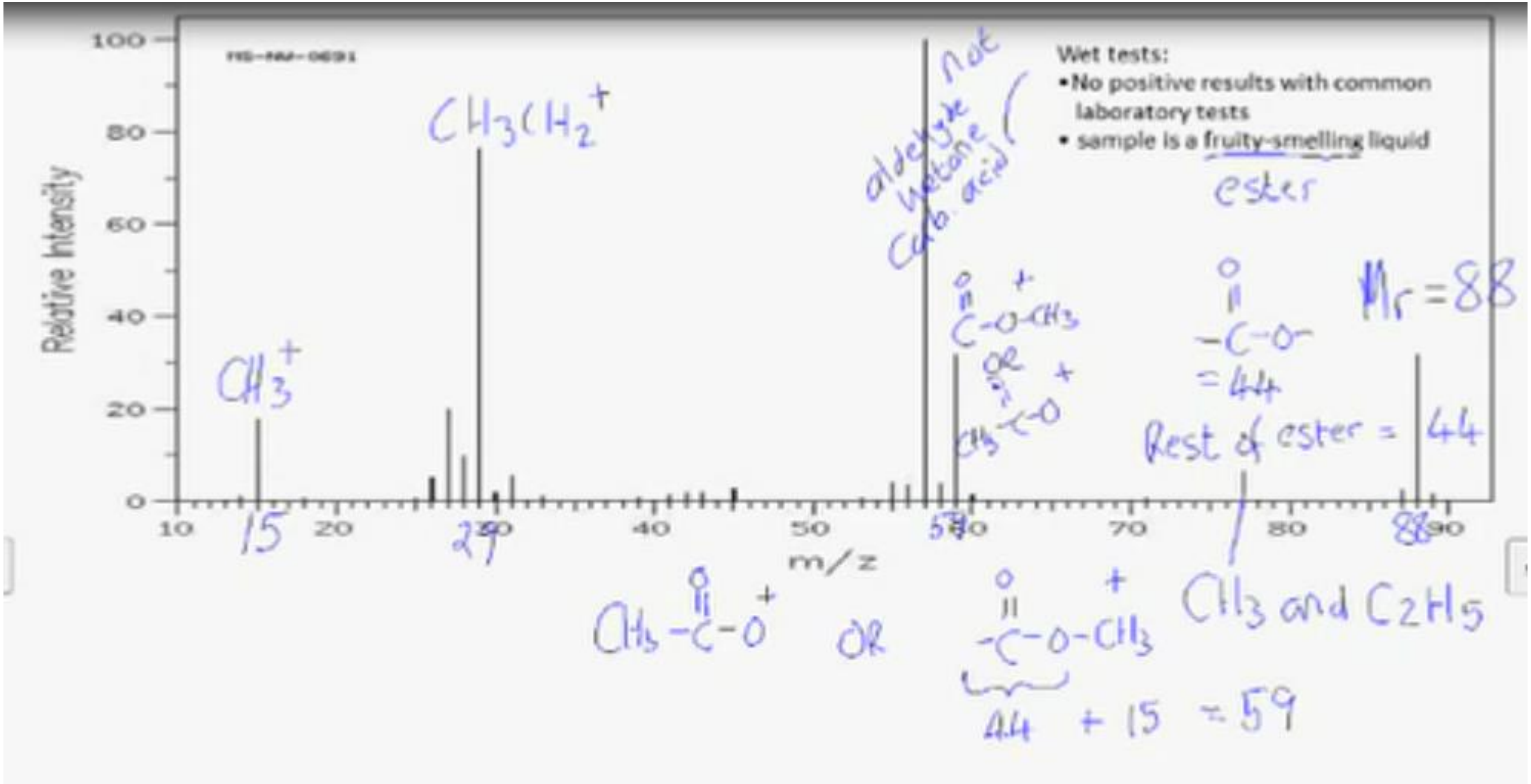
Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
aldehyde
ketone
carb. acid
not
CH_3^+
15
88
Mr = 88
-C(=O)-O- = 44
Rest of ester = 44
CH_3 and C_2H_5


Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
Relative Intensity
100
80
60
40
20
0
10
20
30
40
50
60
70
80
90
m/z
CH3CH2+
CH3+
15
29
aldehyde not
ketone
carb. acid
Mr = 88
-C-O-
= 44
Rest of ester = 44
88
CH3 and C2H5

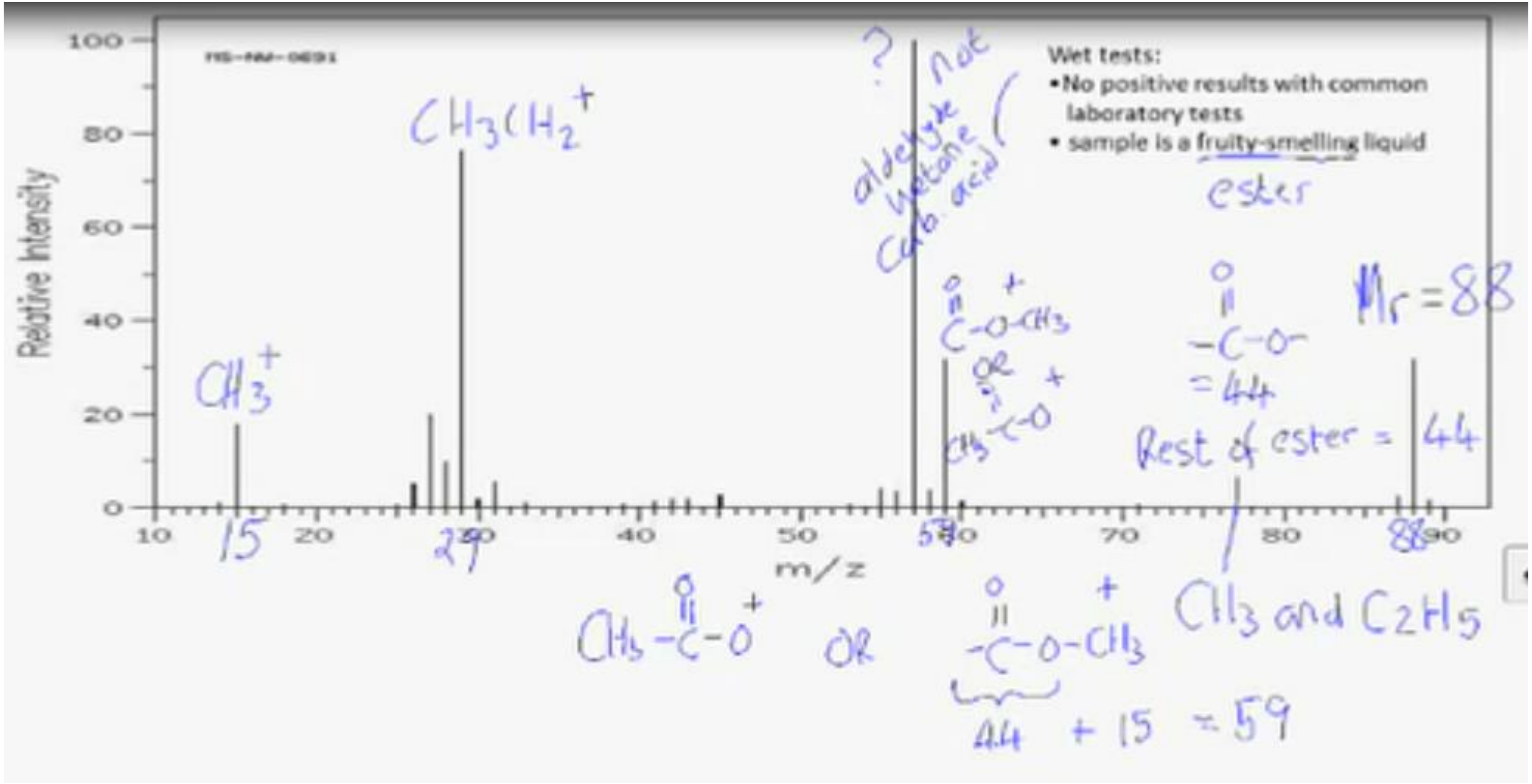

MS-NW-0691
Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
not aldehyde ketone carb. acid
$CH_3CH_2^+$
CH_3^+
15
29
88
$M_r = 88$
-C(=O)-O- = 44
Rest of ester = 44
CH_3 and C_2H_5
$CH_3-C(=O)-O^+$ OR $-C(=O)-O-CH_3^+$



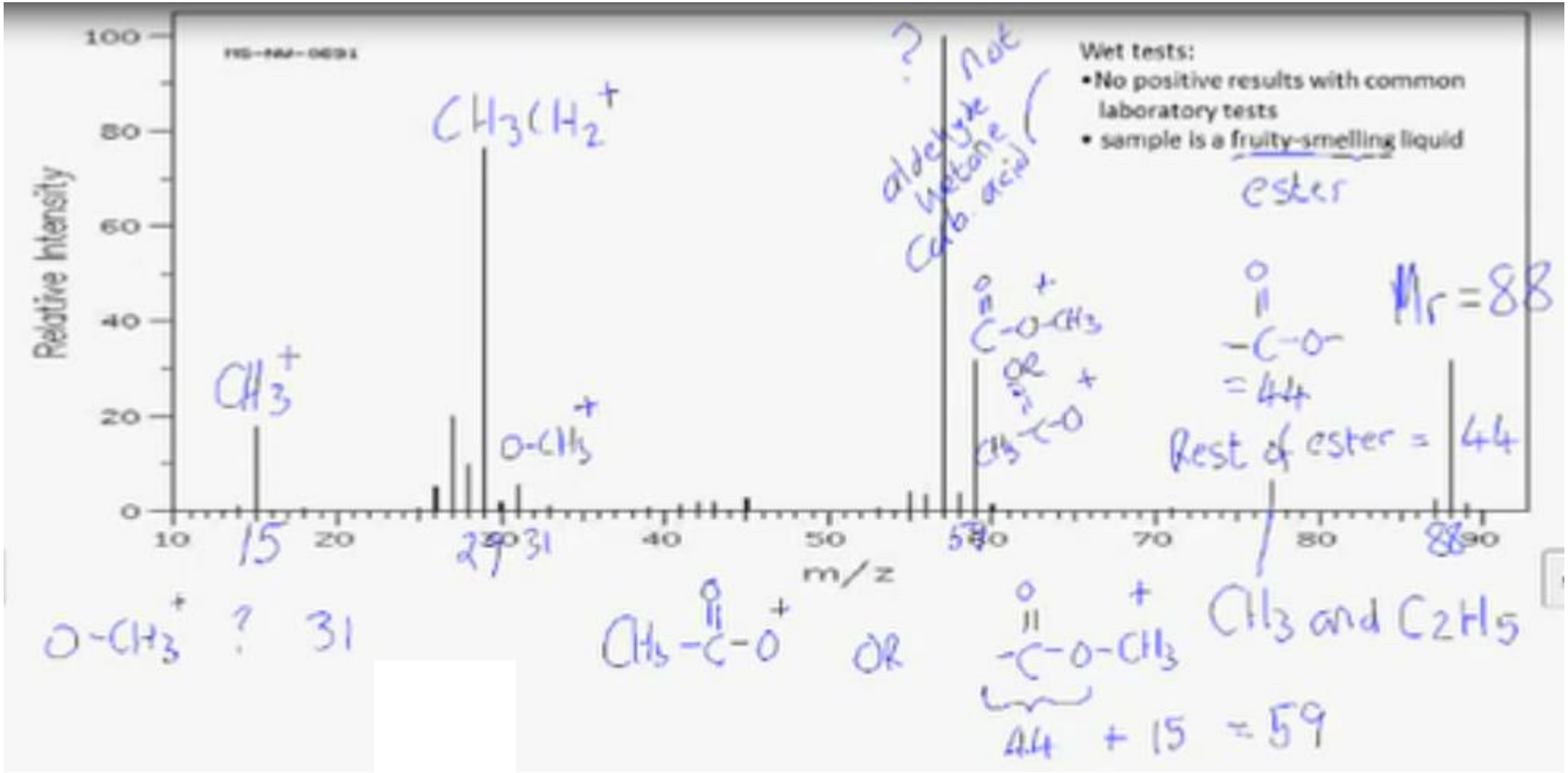
100
80
60
40
20
0
Relative Intensity
10
20
30
40
50
60
70
80
90
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
CH3CH2+
CH3+
15
29
not aldehyde ketone carb. acid
Mr = 88
88
-C(=O)-O- = 44
Rest of ester = 44
CH3 and C2H5
CH3-C(=O)-O+ OR -C(=O)-O-CH3 +
44 + 15 = 59



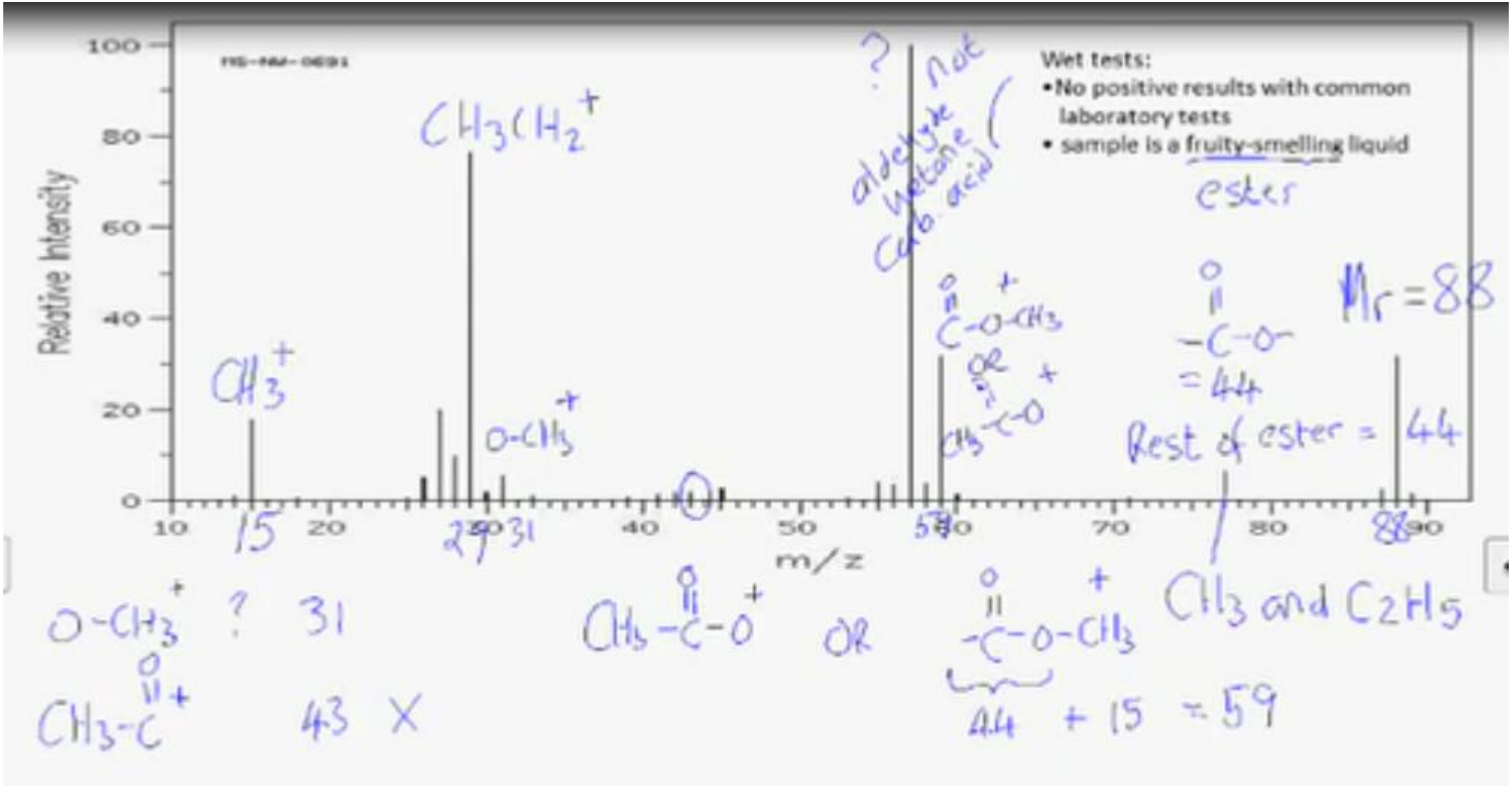
MS-NW-0691
Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
aldehyde not ketone carb. acid
CH3CH2+
CH3+
15
29
59
88
Mr = 88
Rest of ester = 44
CH3 and C2H5
44 + 15 = 59

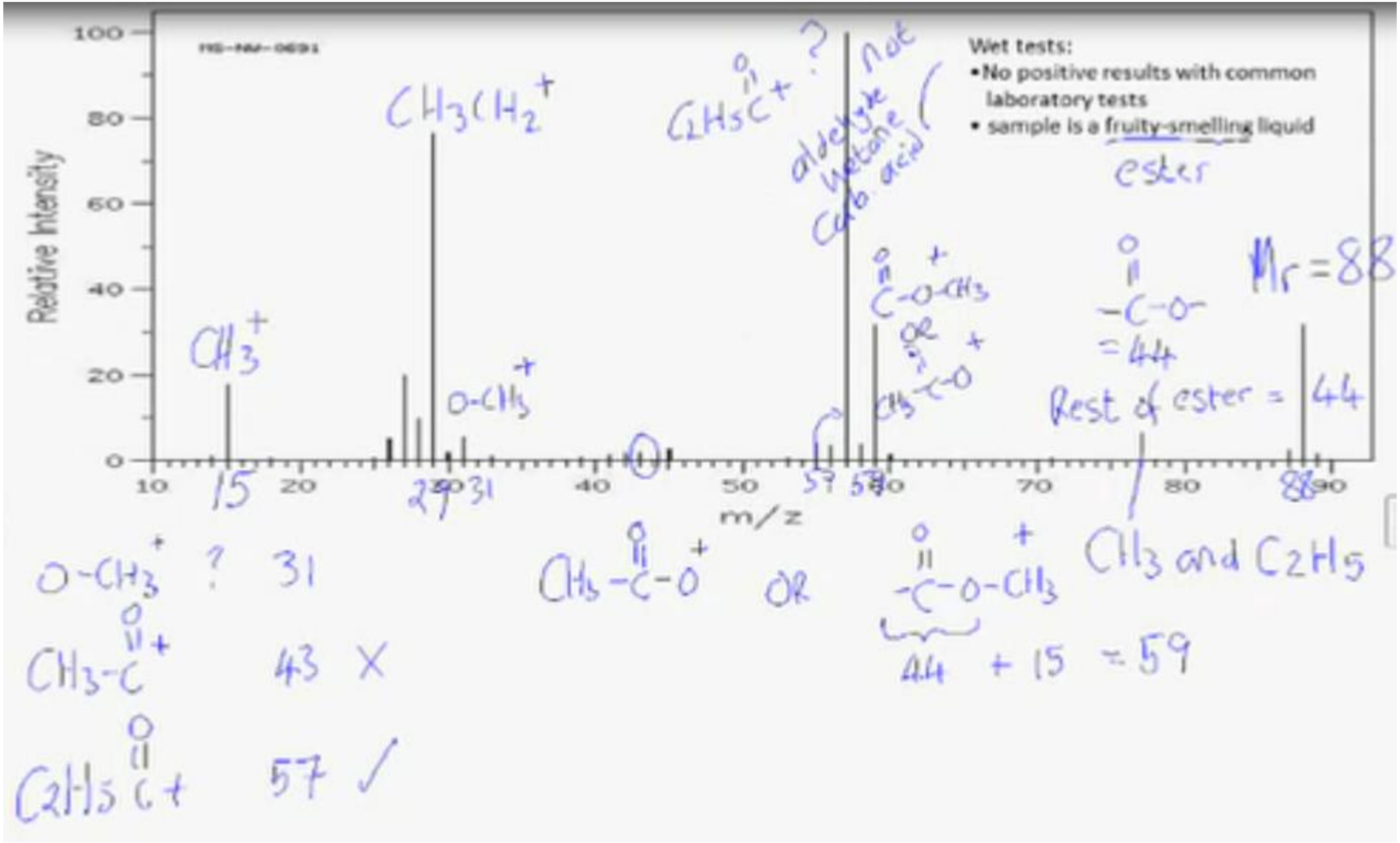


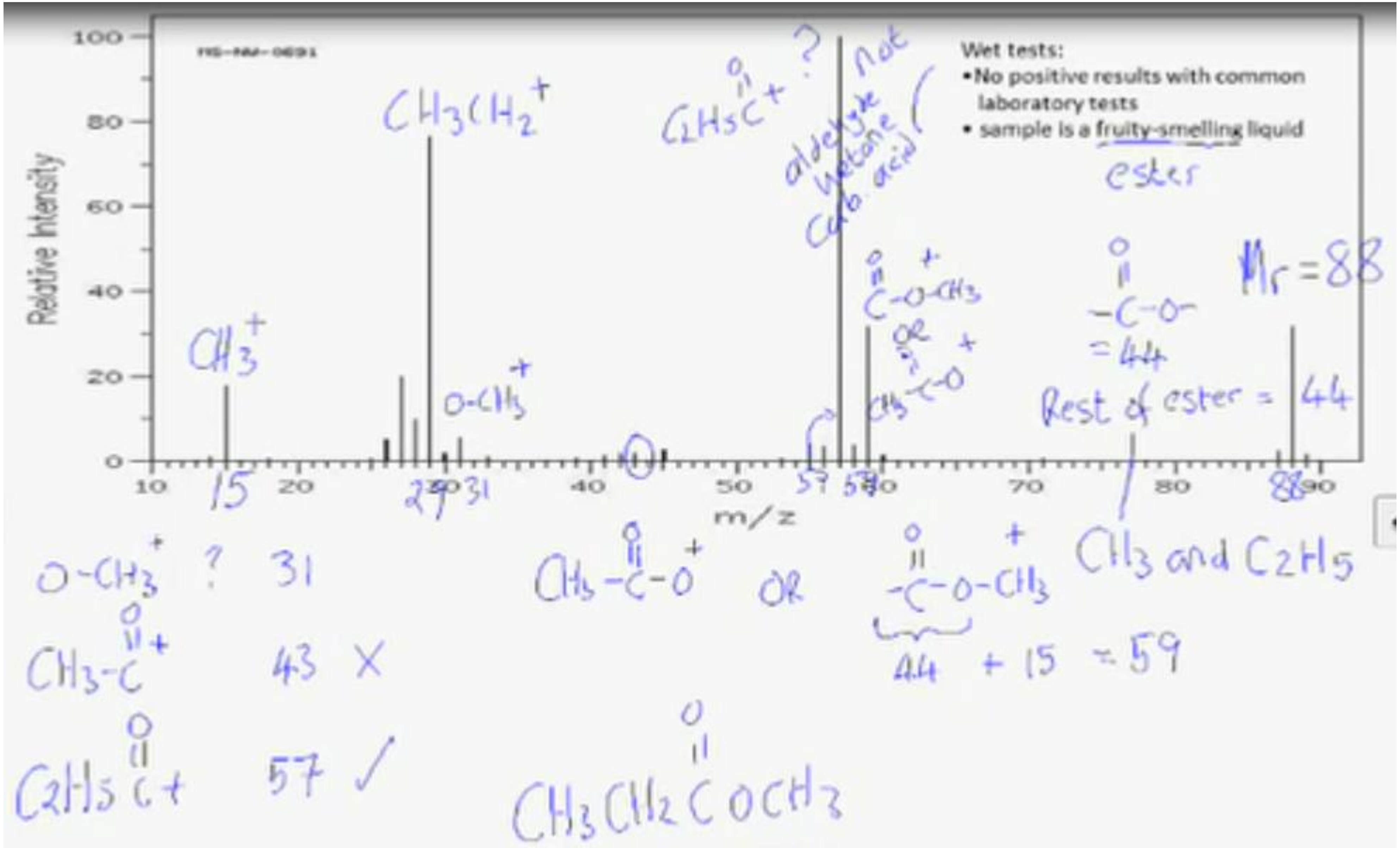
Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
not aldehyde ketone carb. acid
CH3CH2+
CH3+
15
29
59
88
Mr = 88
=44
Rest of ester = 44
CH3 and C2H5
44 + 15 = 59



MS-NW-0691
Relative Intensity
m/z
Wet tests:
•No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
Mr = 88
Rest of ester = 44
CH3 and C2H5
44 + 15 = 59


Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
CH3CH2+
CH3+
O-CH3+
aldehyde ketone carb. acid
? not
Mr = 88
=44
Rest of ester = 44
CH3 and C2H5
O-CH3+ ? 31
CH3-C+ 43 X
CH3-C-O+ OR -C-O-CH3
44 + 15 = 59

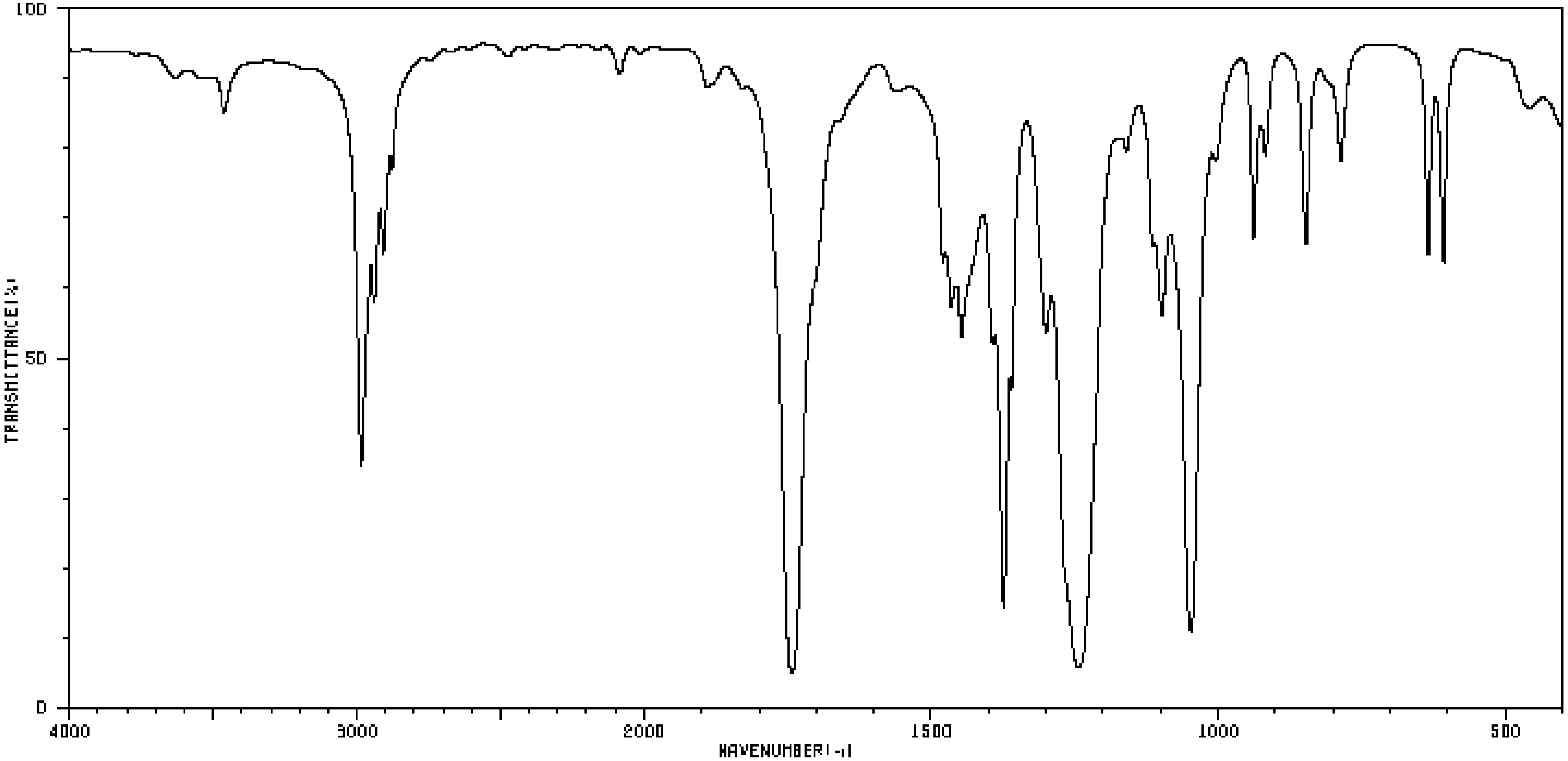

Relative Intensity
m/z
Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
$M_r = 88$
CH_3^+
$CH_3CH_2^+$
$O-CH_3^+$
$C_2H_5C^+$?
aldehyde ketone carb. acid not
Rest of ester = 44
CH_3 and C_2H_5
$O-CH_3^+$? 31
CH_3-C^+ 43 X
$C_2H_5C^+$ 57 ✓
CH_3-C-O^+ OR $-C-O-CH_3^+$
44 + 15 = 59
$-C-O-$ = 44


Wet tests:
• No positive results with common laboratory tests
• sample is a fruity-smelling liquid
ester
Relative Intensity
m/z
CH_3^+
$CH_3CH_2^+$
$O\text{-}CH_3^+$
$C_2H_5C^+$ (C=O) ?
not aldehyde ketone carb. acid
$M_r = 88$
$-C(=O)-O- = 44$
Rest of ester = 44
CH_3 and C_2H_5
$O\text{-}CH_3^+$? 31
$CH_3\text{-}C^+$ (C=O) 43 ✗
$C_2H_5C^+$ (C=O) 57 ✓
$CH_3\text{-}C(=O)\text{-}O^+$ OR $-C(=O)\text{-}O\text{-}CH_3^+$
44 + 15 = 59
$CH_3CH_2C(=O)OCH_3$

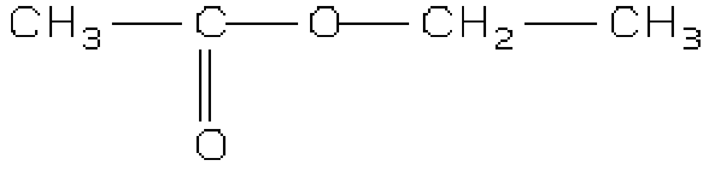
HIT-NO=1229	SCORE= ( )	SDBS-NO=889	IR-NIDA-01804 : LIQUID FILM

ETHYL ACETATE

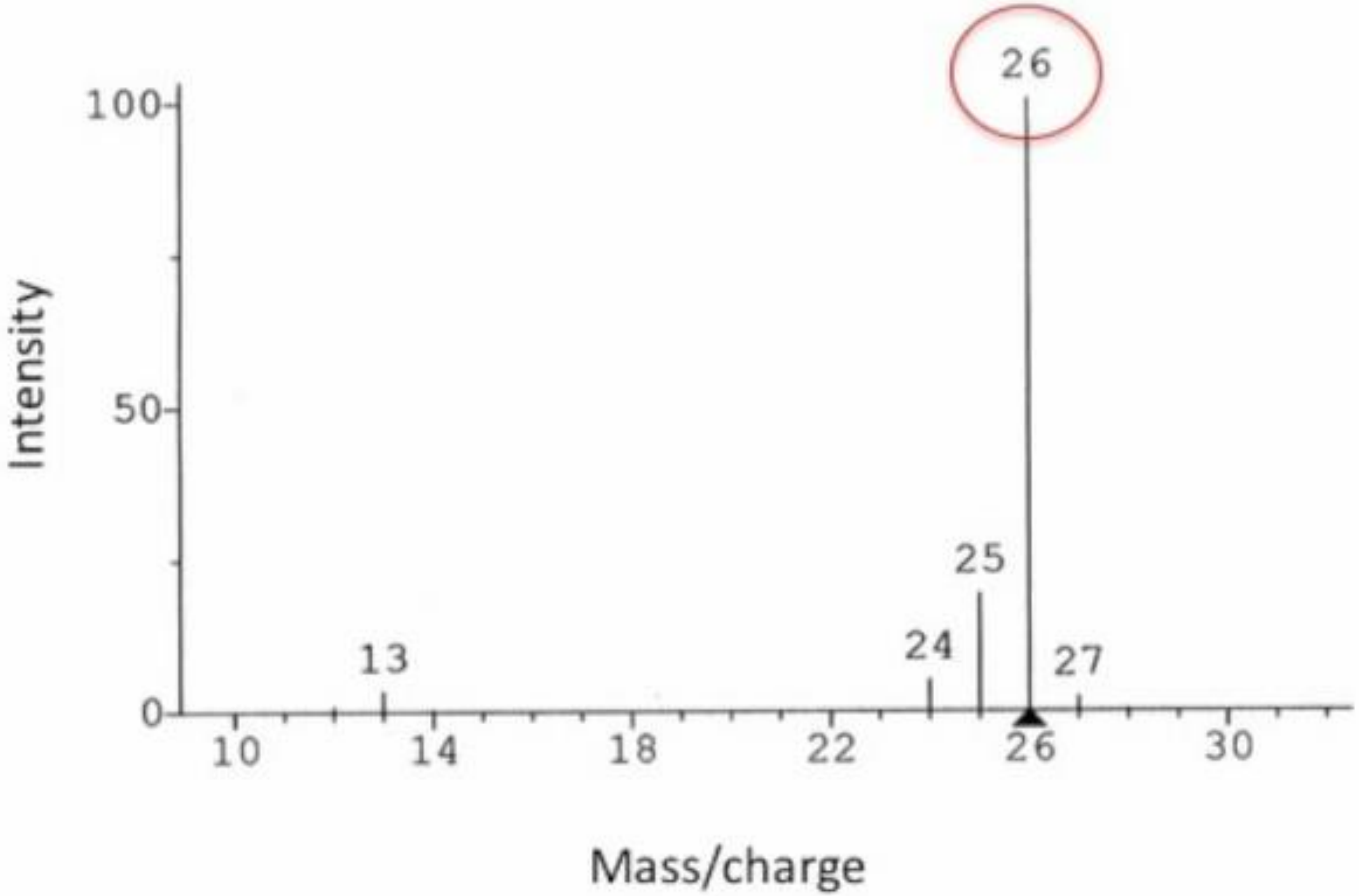
$C_4H_8O_2$



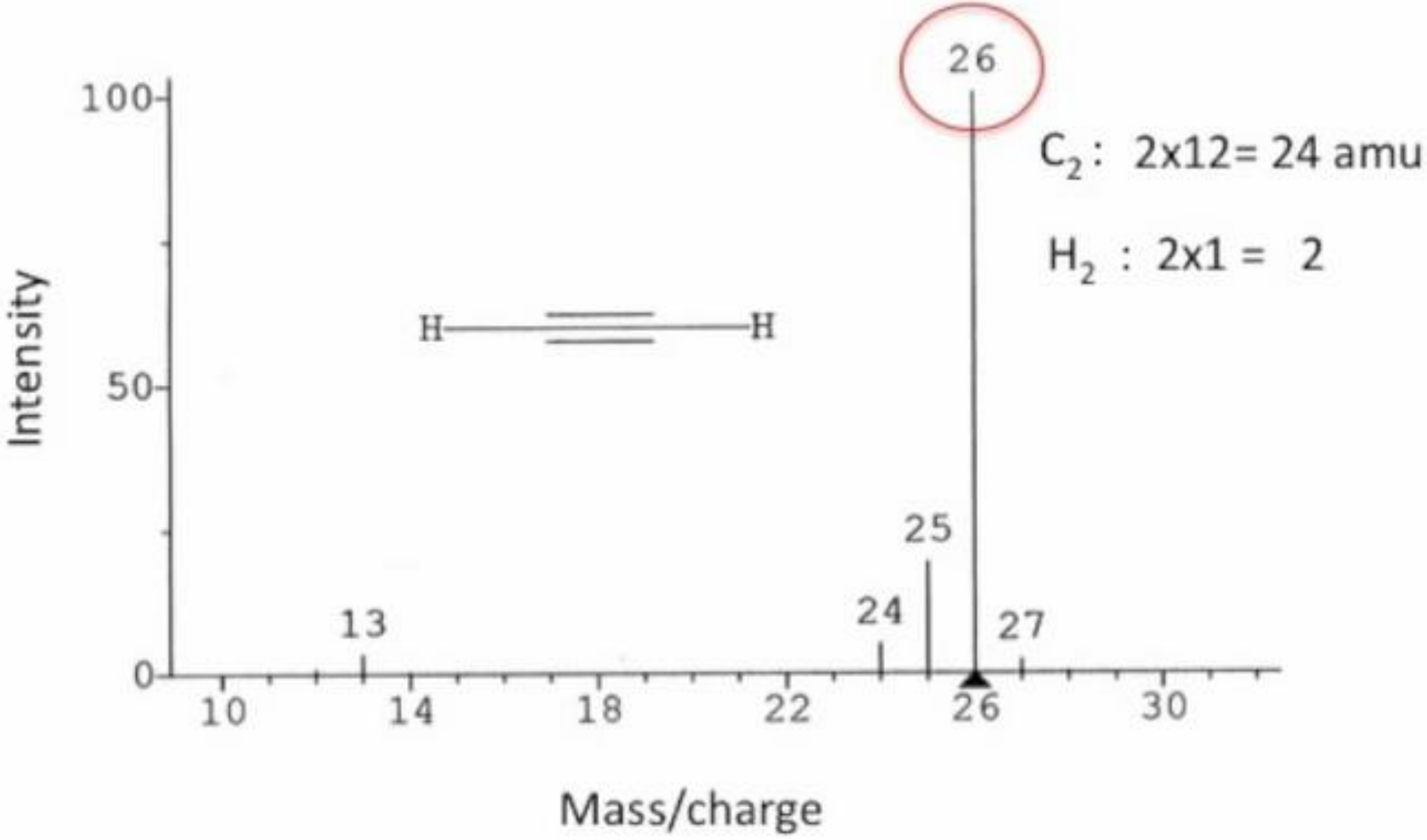
3462	81	1480	60	1243	6	847	64
2983	33	1466	55	1160	77	786	74
2940	55	1448	50	1111	84	634	62
2908	62	1393	60	1098	63	608	60
2877	74	1374	13	1048	10	457	81
1889	86	1360	45	939	84		
1743	4	1301	62	917	77		



Example 1

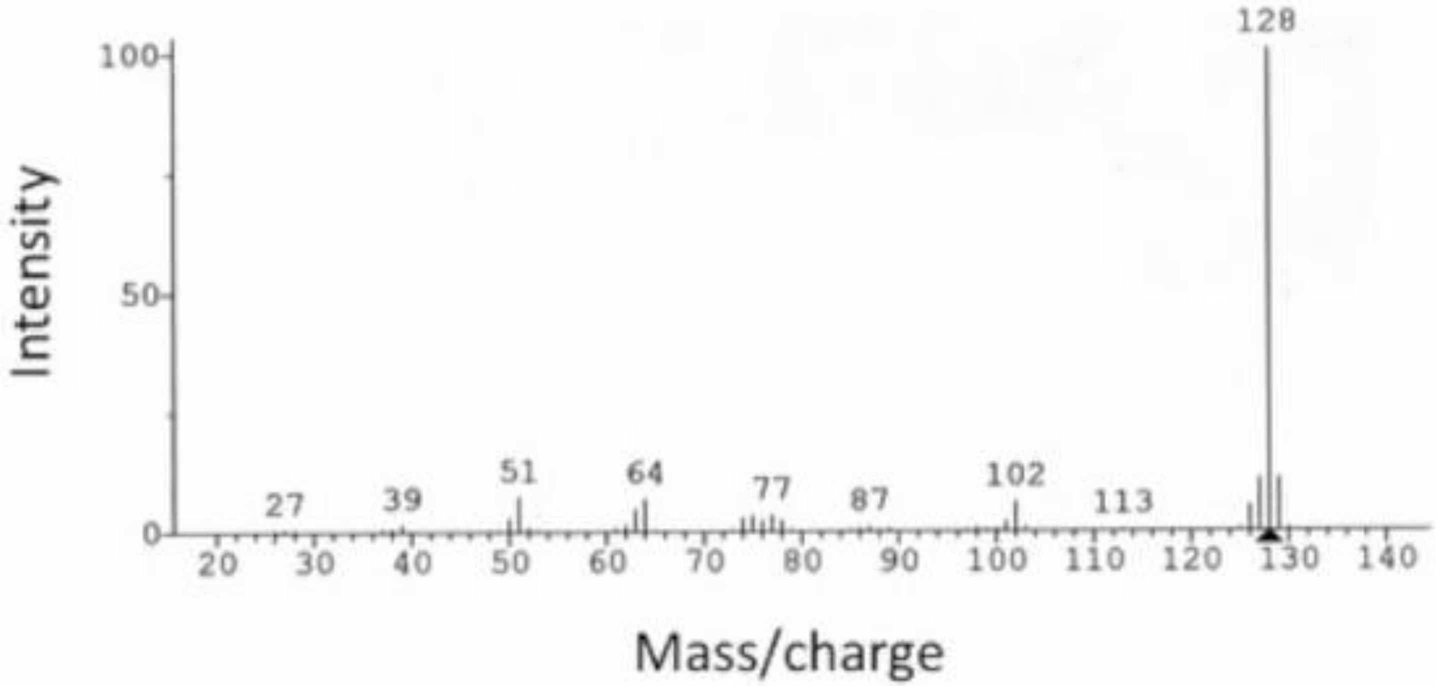


Example 1



26
100
50
0
Intensity
H
H
C_2: 2x12= 24 amu
H_2 : 2x1 = 2
25
24
13
27
10
14
18
22
26
30
Mass/charge

Example 2



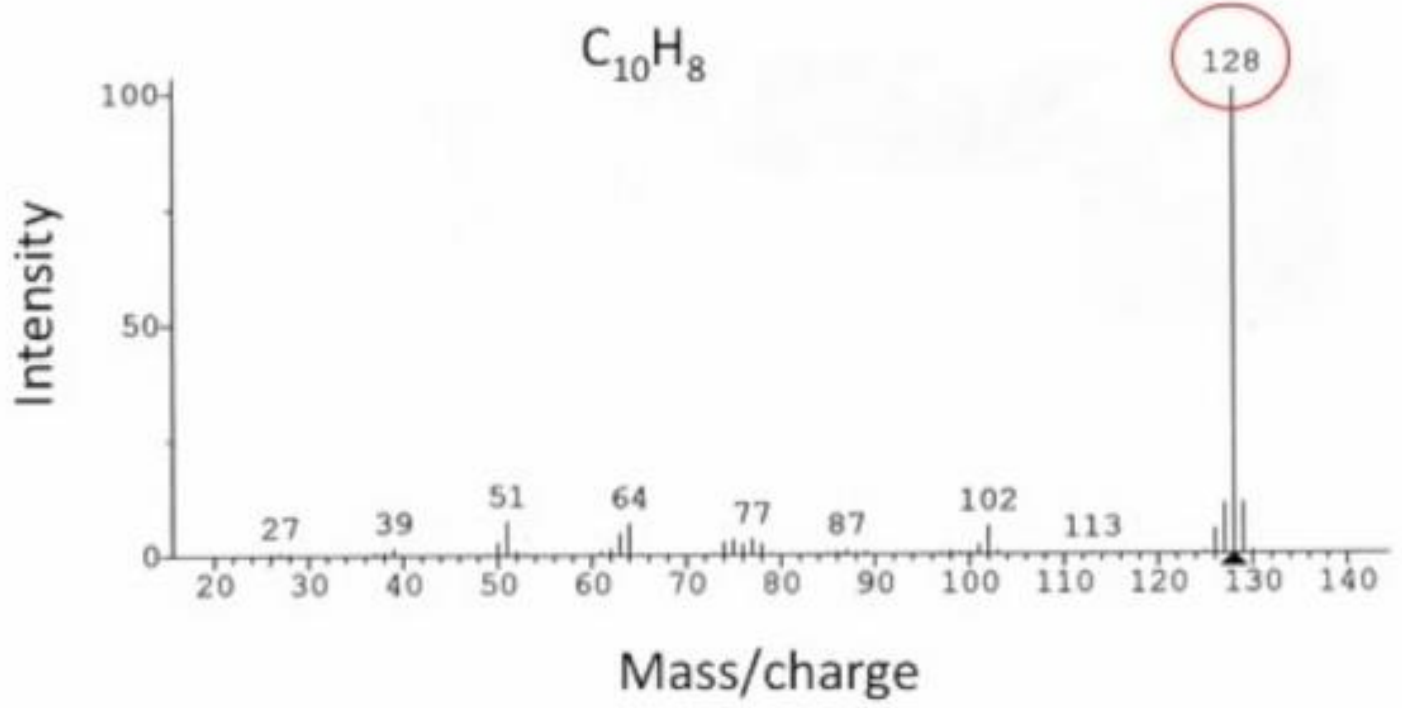
128
100
50
0
Intensity
27
39
51
64
77
87
102
113
20
30
40
50
60
70
80
90
100
110
120
130
140
Mass/charge

Example 2

Mol.wt. = 128

Assume 10 carbons ⟶ C_{10} : 10x12= 120 amu

8 amu ⟶ H_8

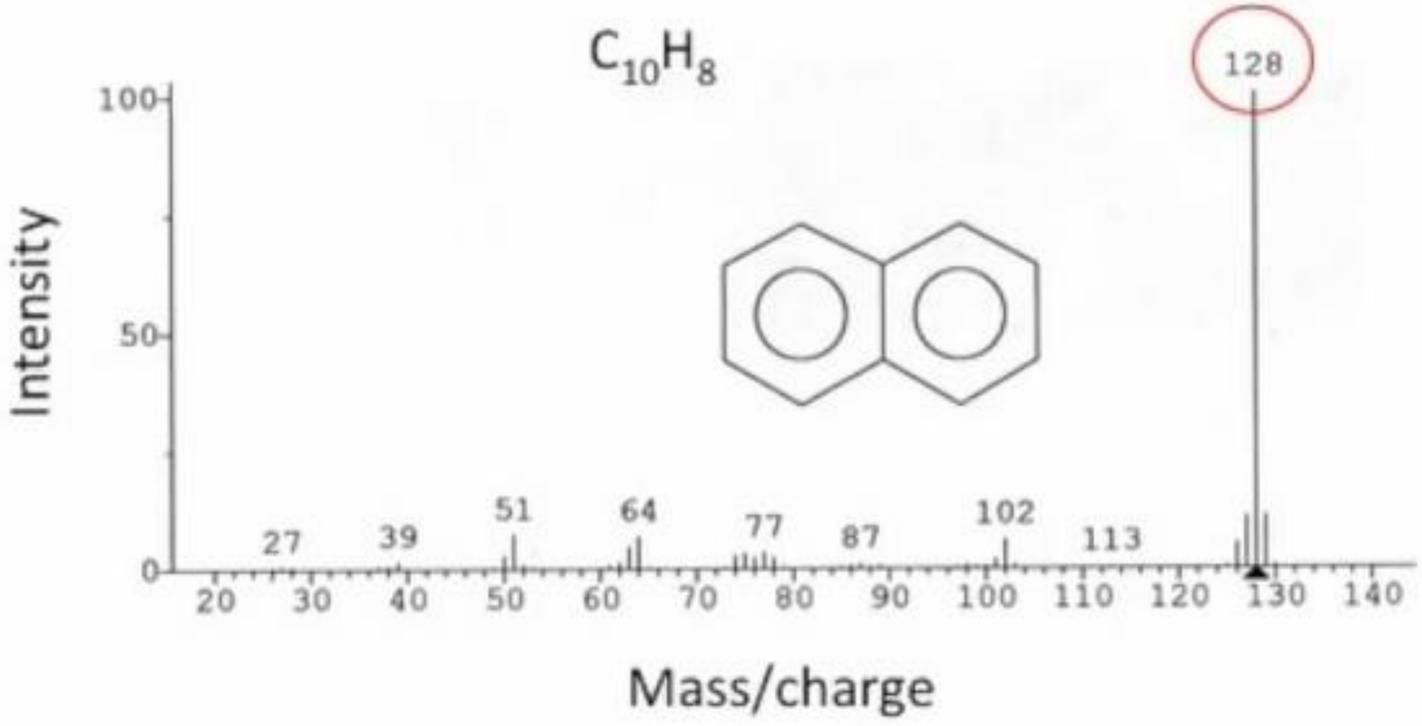


Example 2

Mol.wt. = 128

Assume 10 carbons ⟶ C_{10} : 10x12= 120 amu

8 amu ⟶ H_8

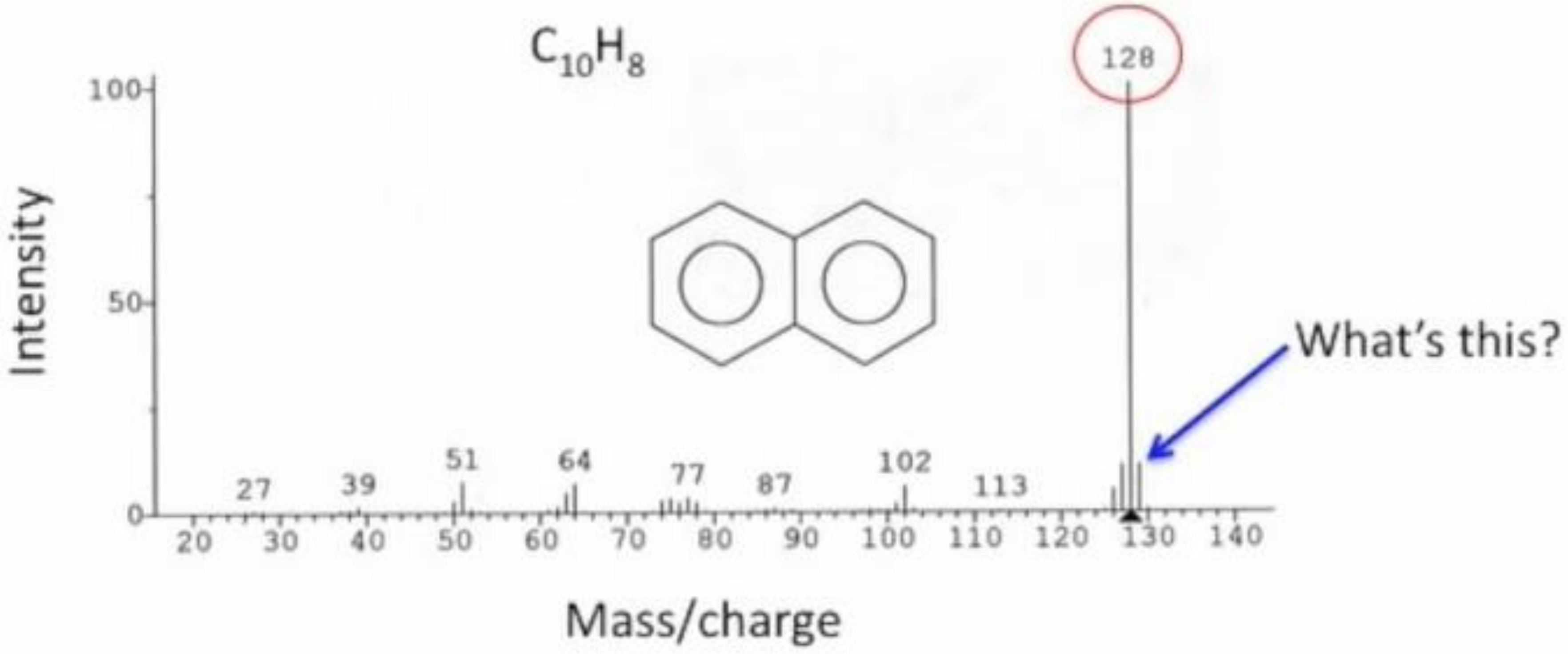


Example 2

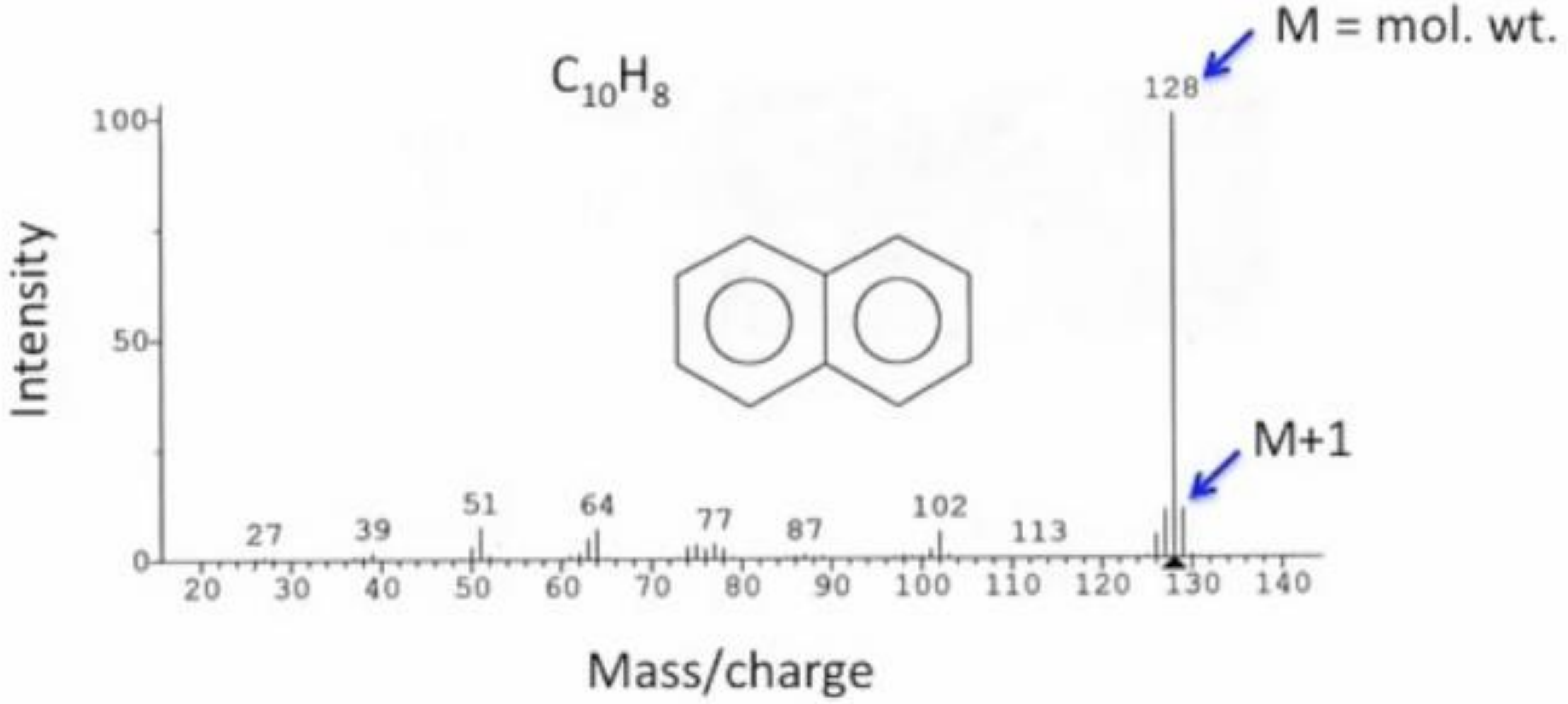
Mol.wt. = 128

Assume 10 carbons ⟶ C_{10} : 10x12= 120 amu

8 amu ⟶ H_8

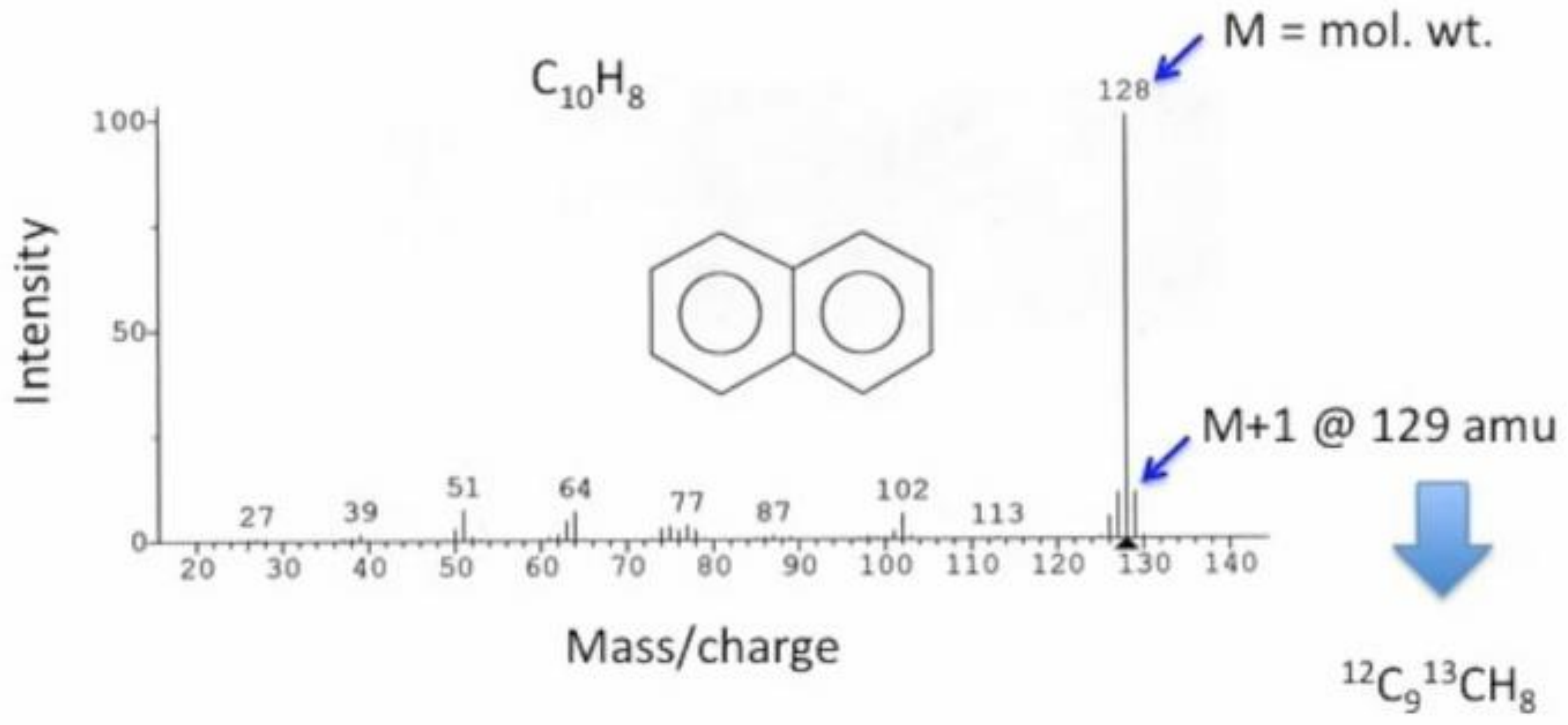


Example 2



$C_{10}H_8$
M = mol. wt.
128
M+1
100
50
0
27
39
51
64
77
87
102
113
20
30
40
50
60
70
80
90
100
110
120
130
140
Intensity
Mass/charge

Example 2


M = mol. wt.
$C_{10}H_8$
128
100
50
0
Intensity
27
39
51
64
77
87
102
113
20 30 40 50 60 70 80 90 100 110 120 130 140
Mass/charge
M+1 @ 129 amu
$^{12}C_9{}^{13}CH_8$

For every 100 atoms of ^{12}C there are ~ 1.1 atoms of ^{13}C

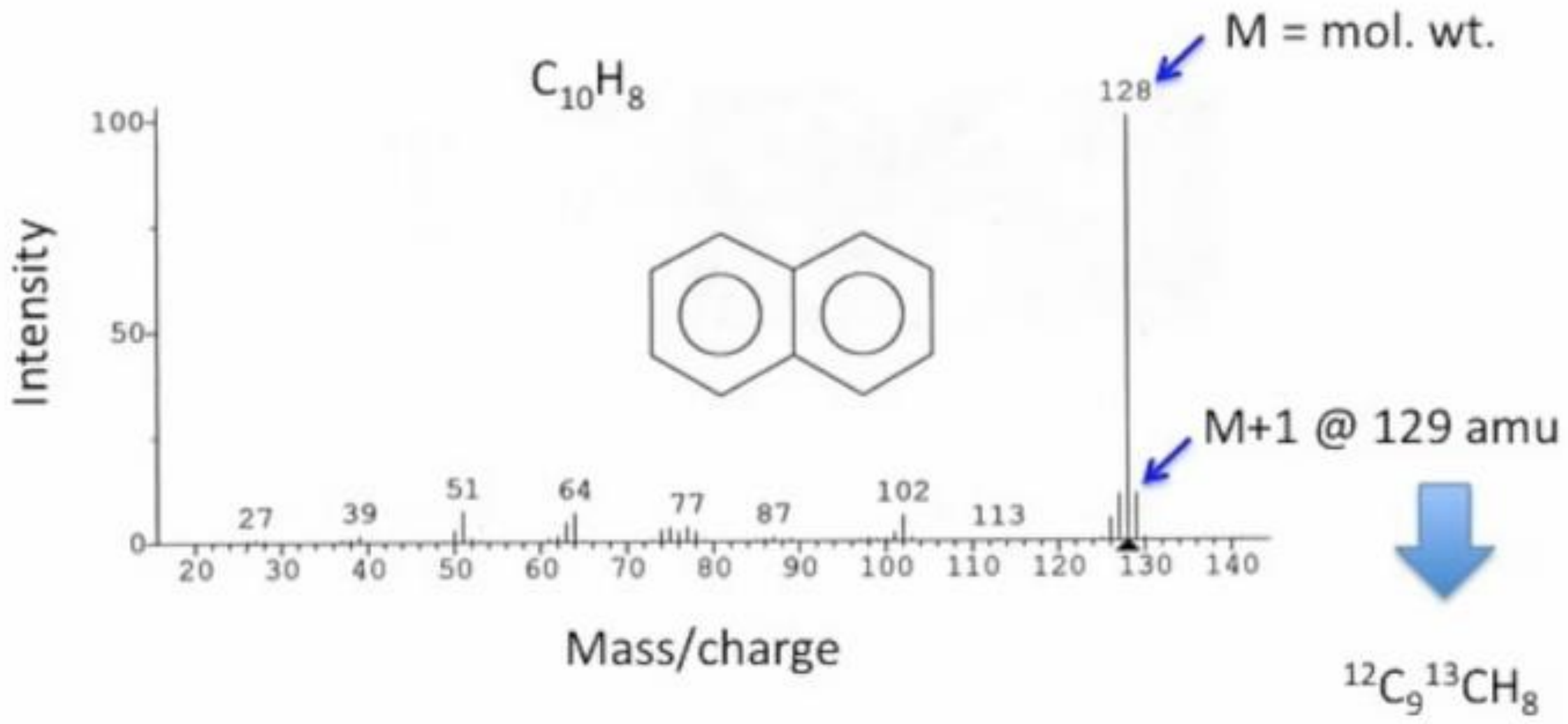
Element	Mass	%	1st Heavy Isotope Mass	%	2nd Heavy Isotope Mass	%
Hydrogen	^{1}H	100	^{2}H	0.015		
Carbon	^{12}C	100	^{13}C	1.1		
Nitrogen	^{14}N	100	^{15}N	0.37		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.4
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.80	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98.0
Iodine	^{127}I	100				

Molecular formula	Intensity of M+1 peak
CH_4	1.1 % as tall as molecular ion peak
C_2H_6	2.2 %
C_3H_8	3.3 %
C_4H_{10}	4.4 %
C_5H_{12}	5.5 %

$$\text{relative height of isotope peak} = \frac{[M+1]}{[M]}(100\%) = (1.1\%)(\#\,Carbons)$$

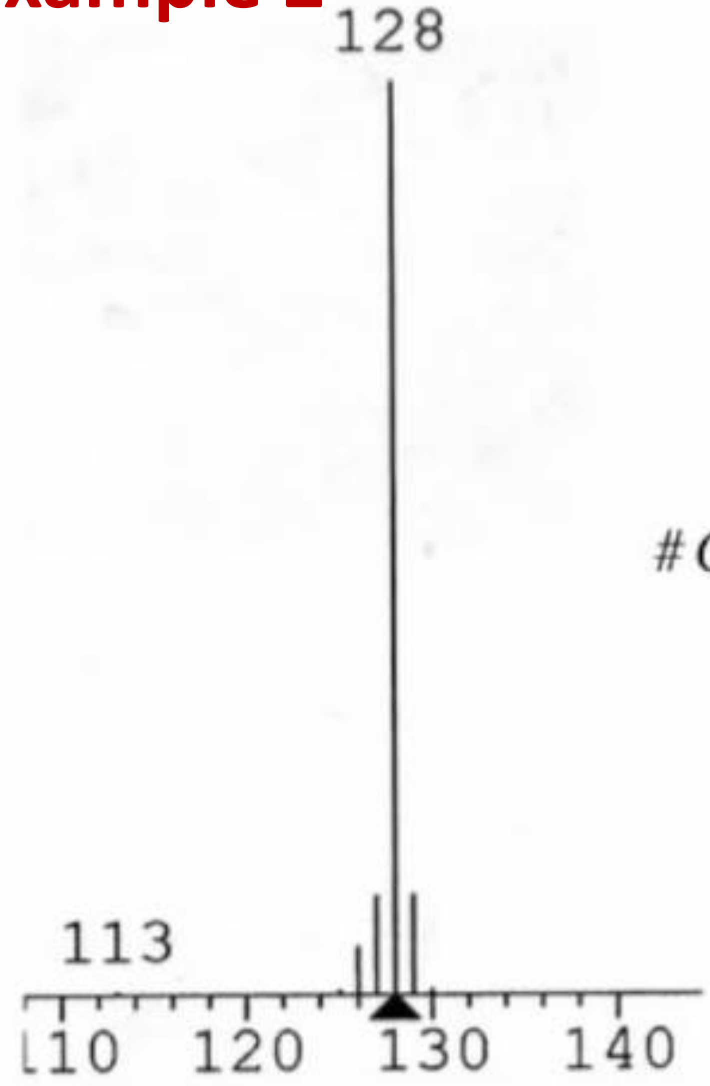
$$OR \quad \#\,Carbons = \frac{[M+1]}{[M]} \times \frac{100\%}{1.1\%}$$

Example 2



C10H8
M = mol. wt.
128
100
50
0
Intensity
27
39
51
64
77
87
102
113
20
30
40
50
60
70
80
90
100
110
120
130
140
Mass/charge
M+1 @ 129 amu
12C9 13CH8

Example 2



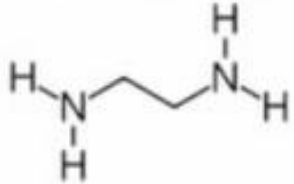
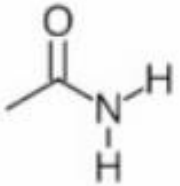
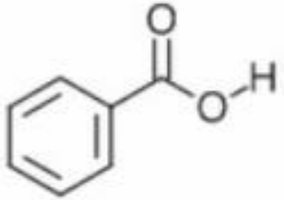
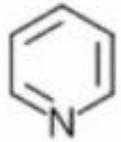
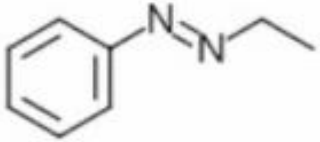
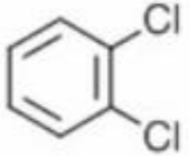
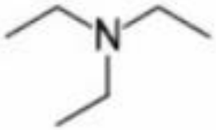
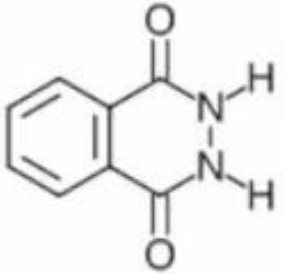
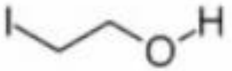
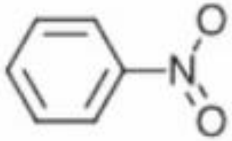
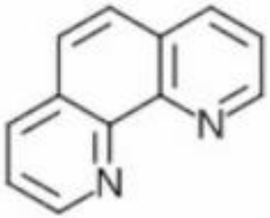
Mass/charge	Intensity	Identity
128	100	M
129	10.9	M+1

$$\# Carbons = \frac{[M+1]}{[M]} \times \frac{100\%}{1.1\%} = \frac{10.9}{100} \times \frac{100\%}{1.1} = 9_{.9}$$

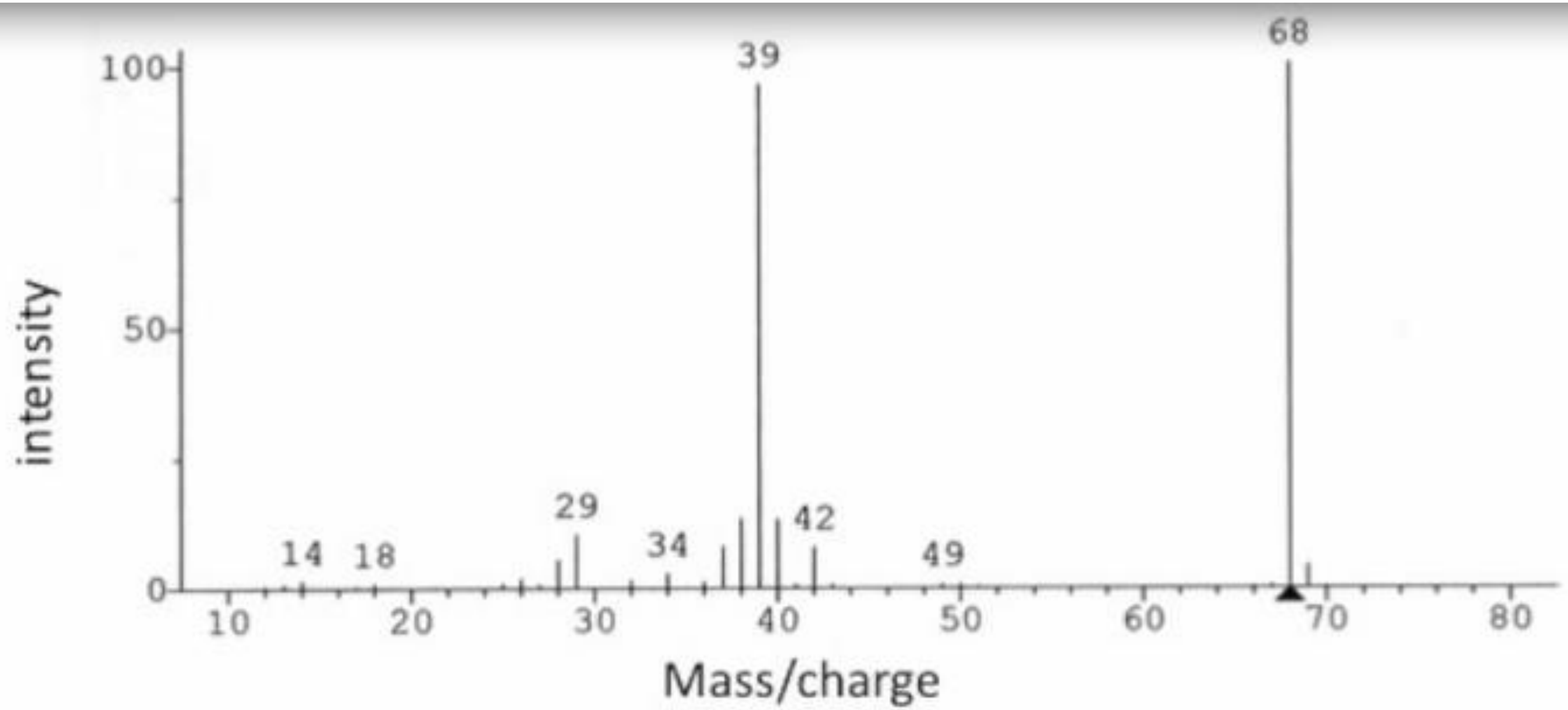
10 carbon atoms

Element	Mass	%	1st Heavy Isotope Mass	%	2nd Heavy Isotope Mass	%
Hydrogen	^{1}H	100	^{2}H	0.015		
Carbon	^{12}C	100	^{13}C	1.1		
Nitrogen	^{14}N	100	^{15}N	0.37		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.4
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.80	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98.0
Iodine	^{127}I	100				

Nitrogen rule: An odd molecular weight indicates an odd number of N atoms.

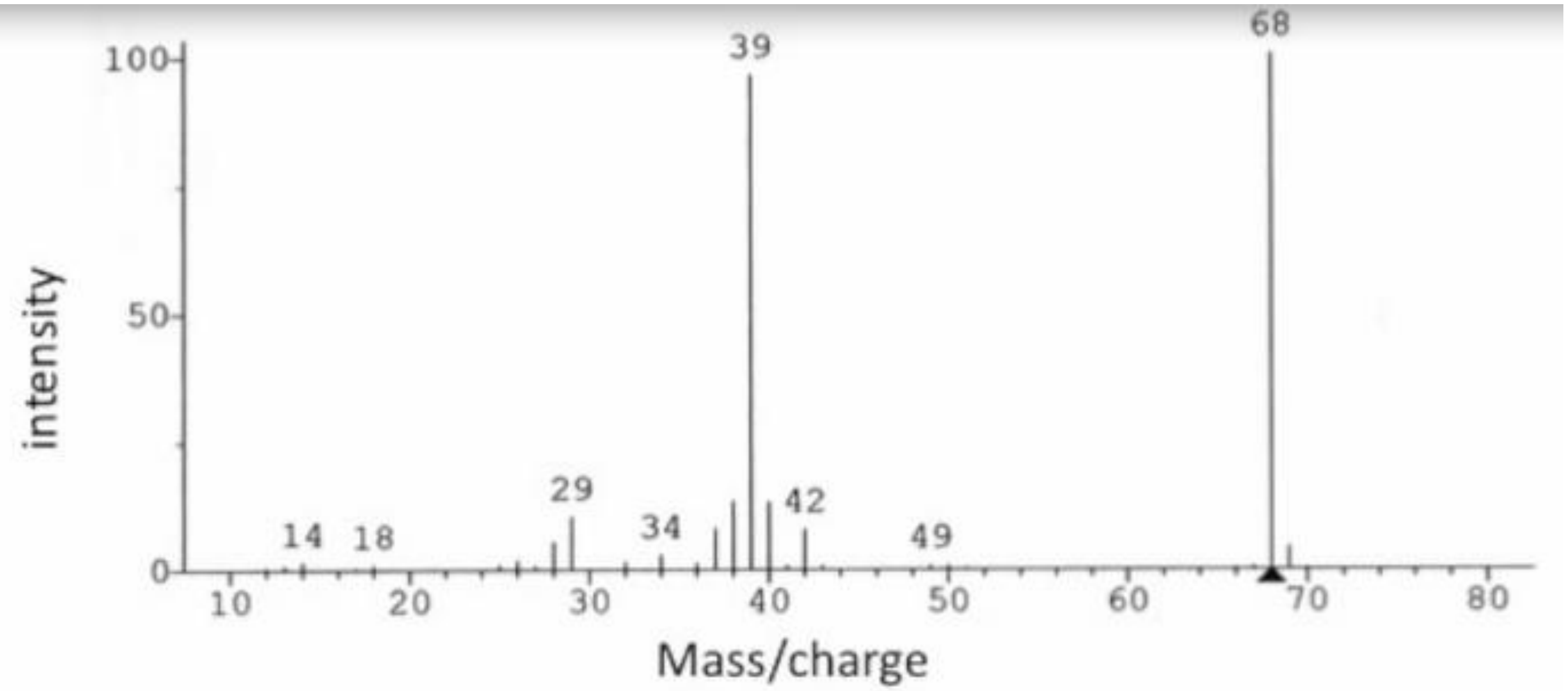
Compound	MW	Compound	MW	Compound	MW
CH_4	16	CH_3NH_2	31	NH_2-CH_2-NH_2	46
CH_3CO_2H	60		55		60
	78		59		68
	122		79		134
	146		101		162
	172		123		180

Example 3



	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

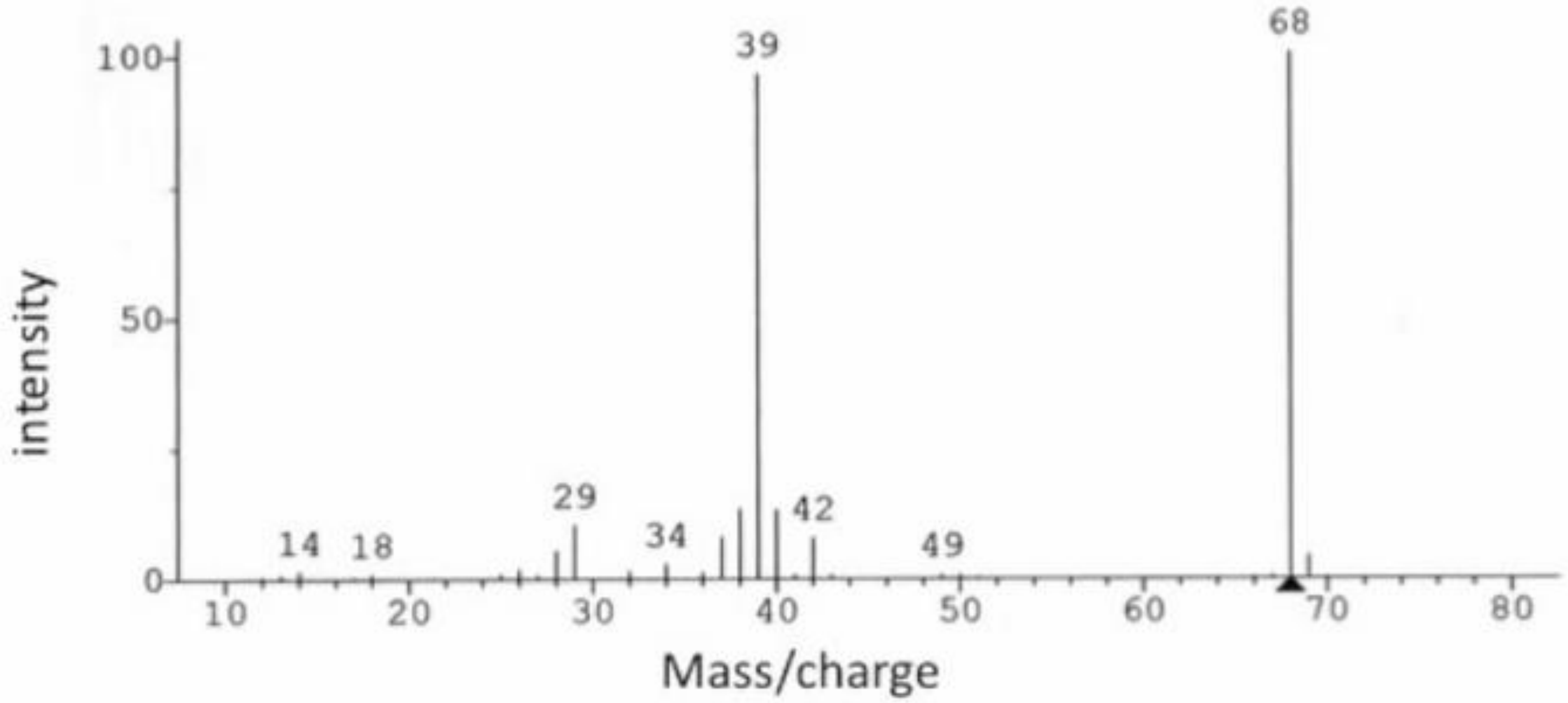
Example 3



	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4 \longrightarrow C_4$$

Example 3



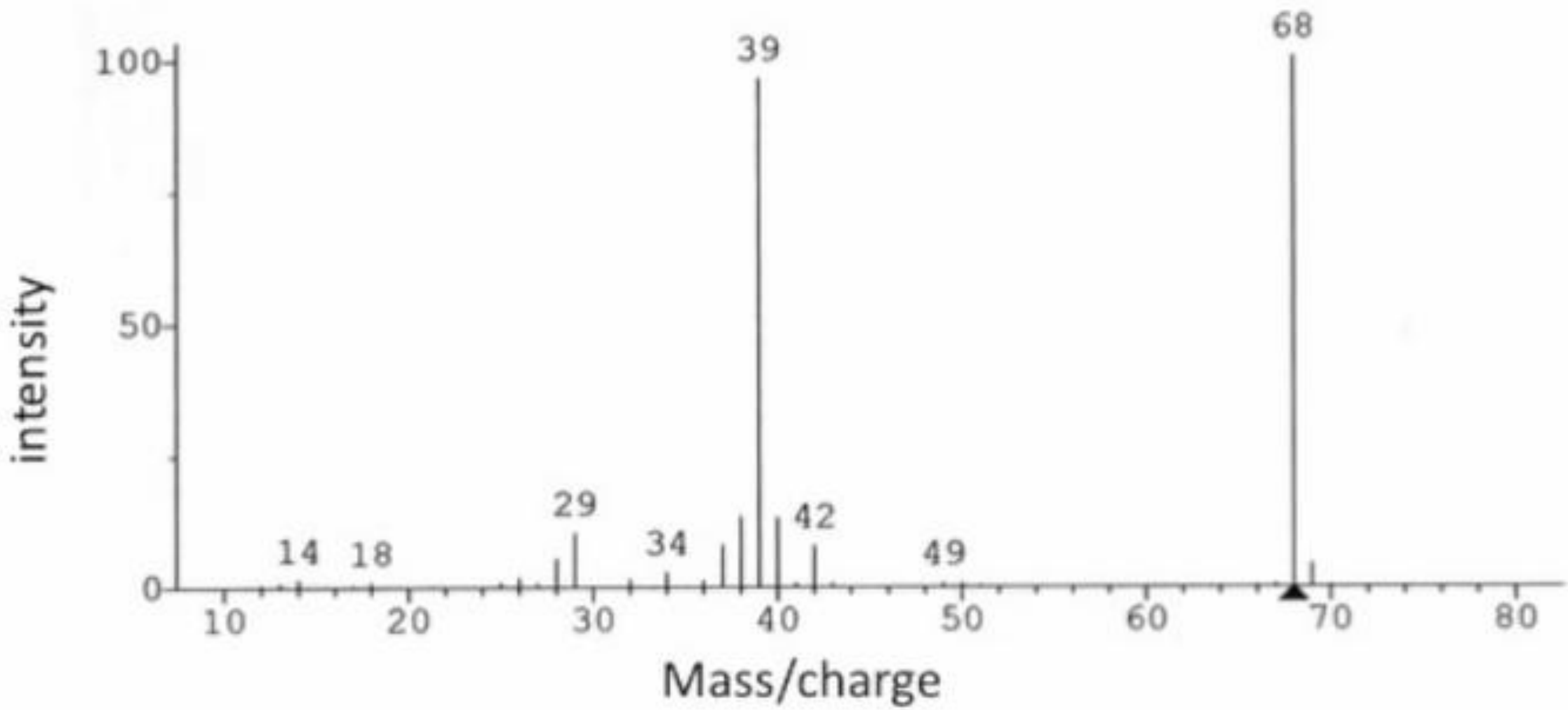
	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4$$

68 amu

-48 = 4x12 for C_4

Example 3



	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

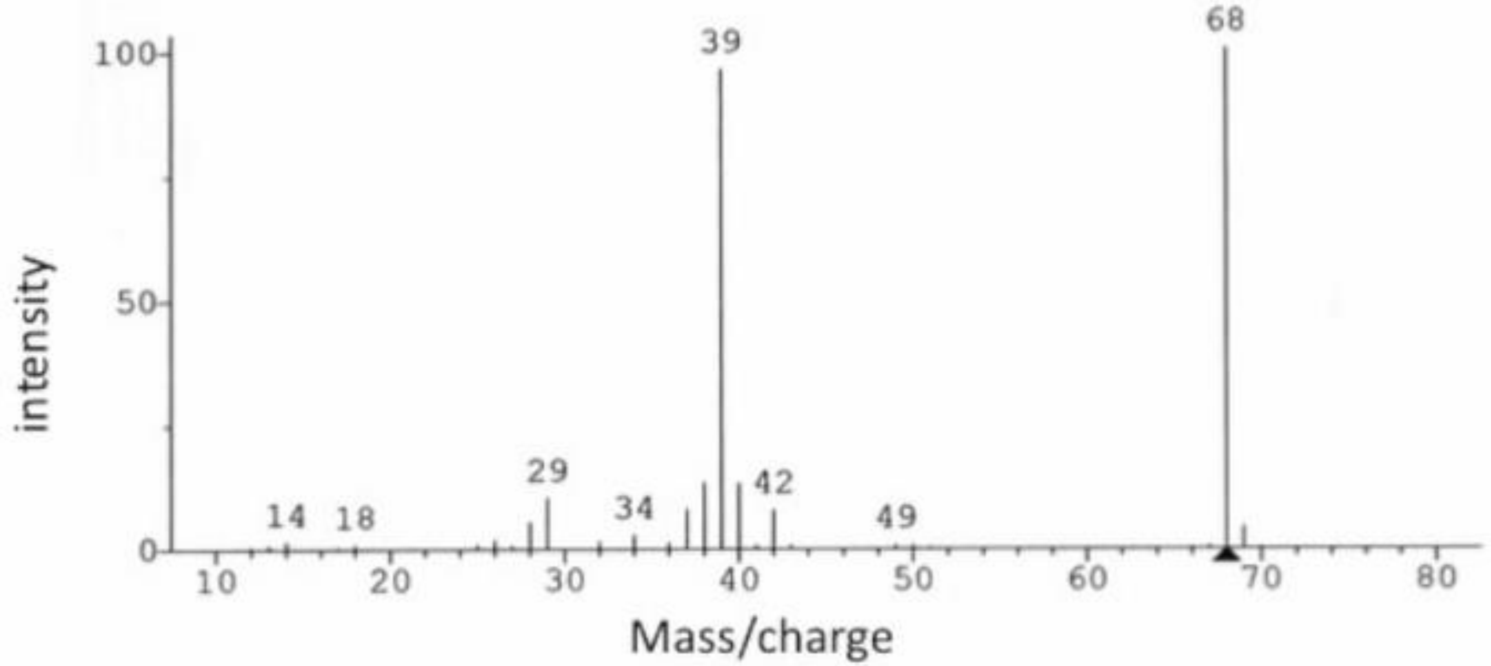
$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4$$

68 amu

-48 = 4x12 for C_4

20 amu

Example 3



	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4$$

68 amu

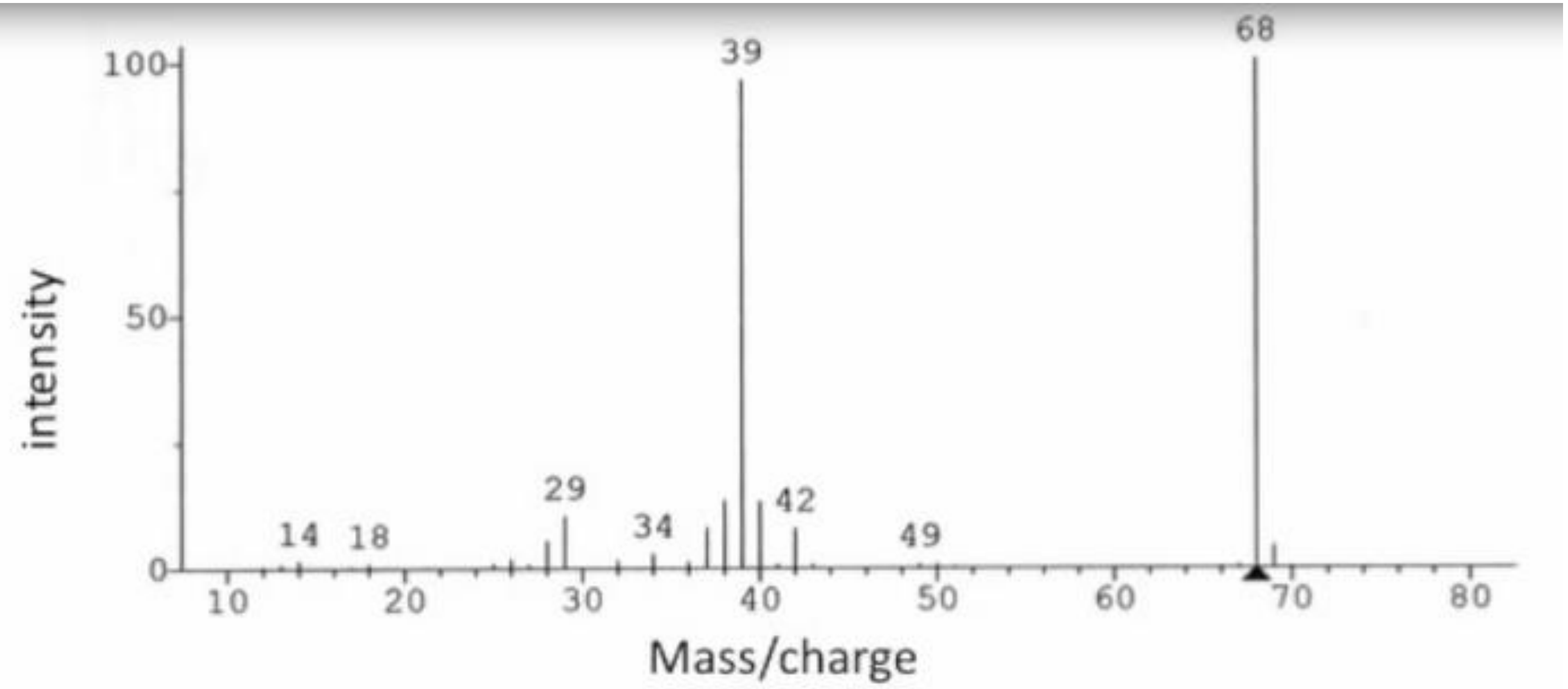
-48 = 4x12 for C_4

20 amu

-16 for O_1

4 amu

Example 3



	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4$$

68 amu

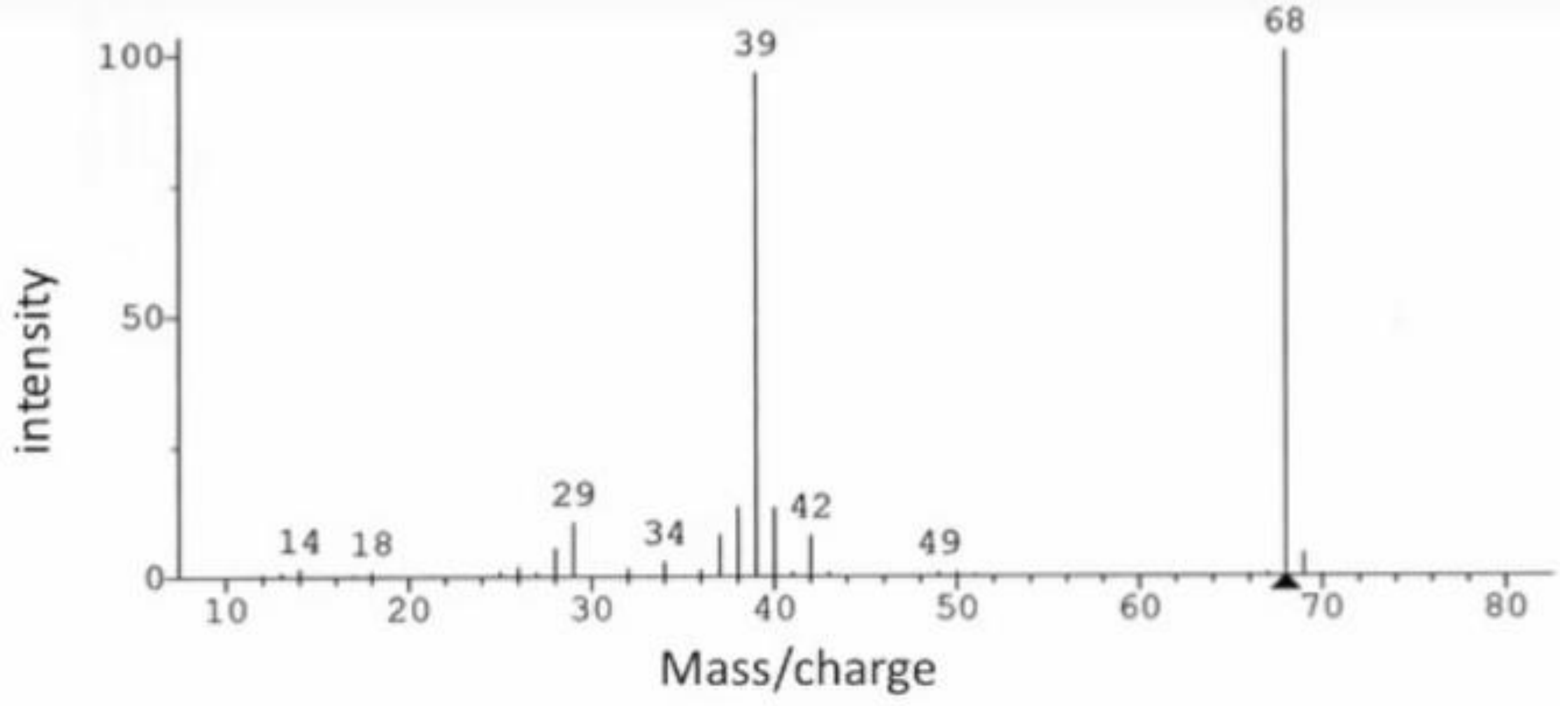
-48 = 4x12 for C_4

20 amu

-16 for O_1

4 amu ⟶ H_4

Example 3



	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4$$

68 amu

-48 = 4x12 for C_4

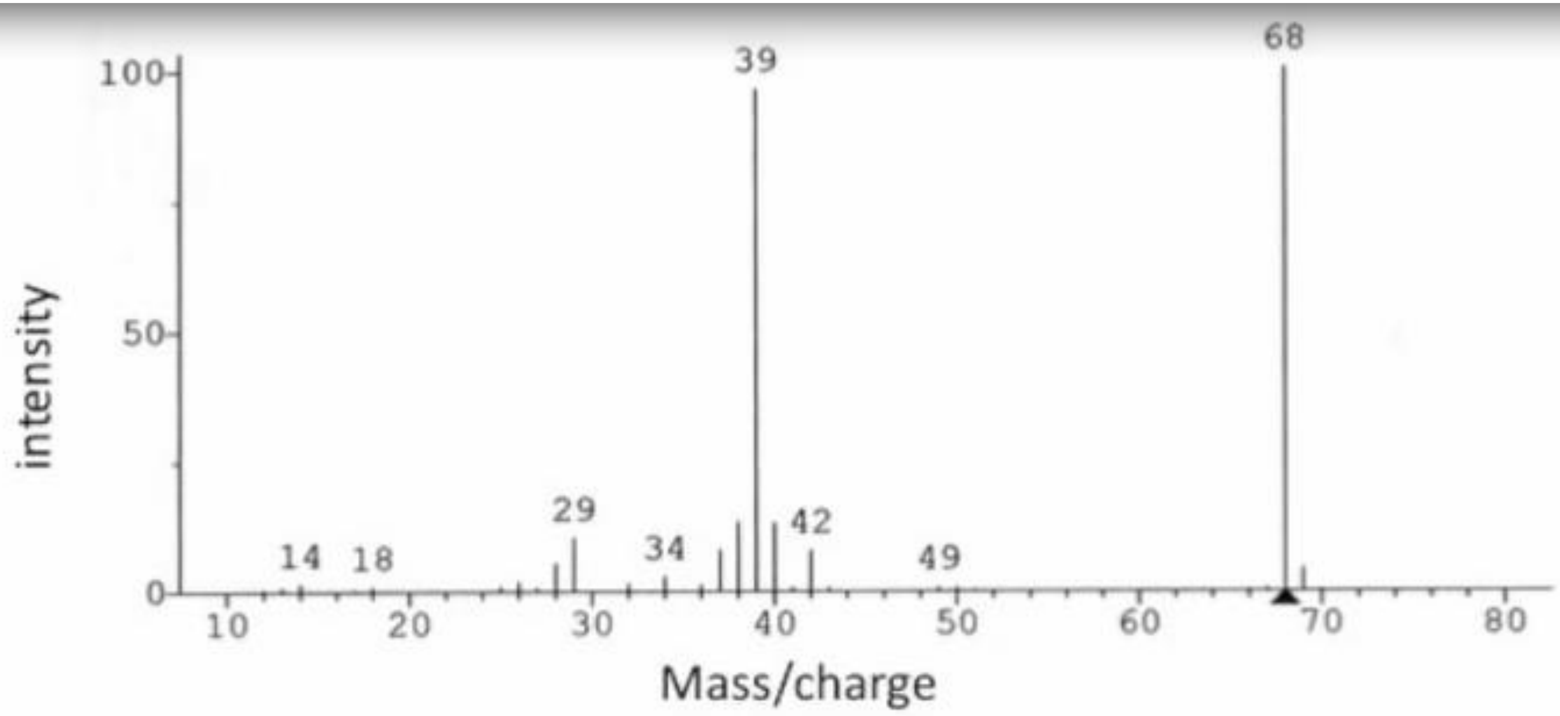
20 amu

-16 for O_1

4 amu ⟶ H_4

⇨ C_4H_4O

Example 3



Mass/charge	Intensity
67	0.5
M 68	100
M+1 69	4.2
70	0.1

$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4$$

C_4H_4O

68 amu

-48 = 4x12 for C_4

20 amu

-16 for O_1

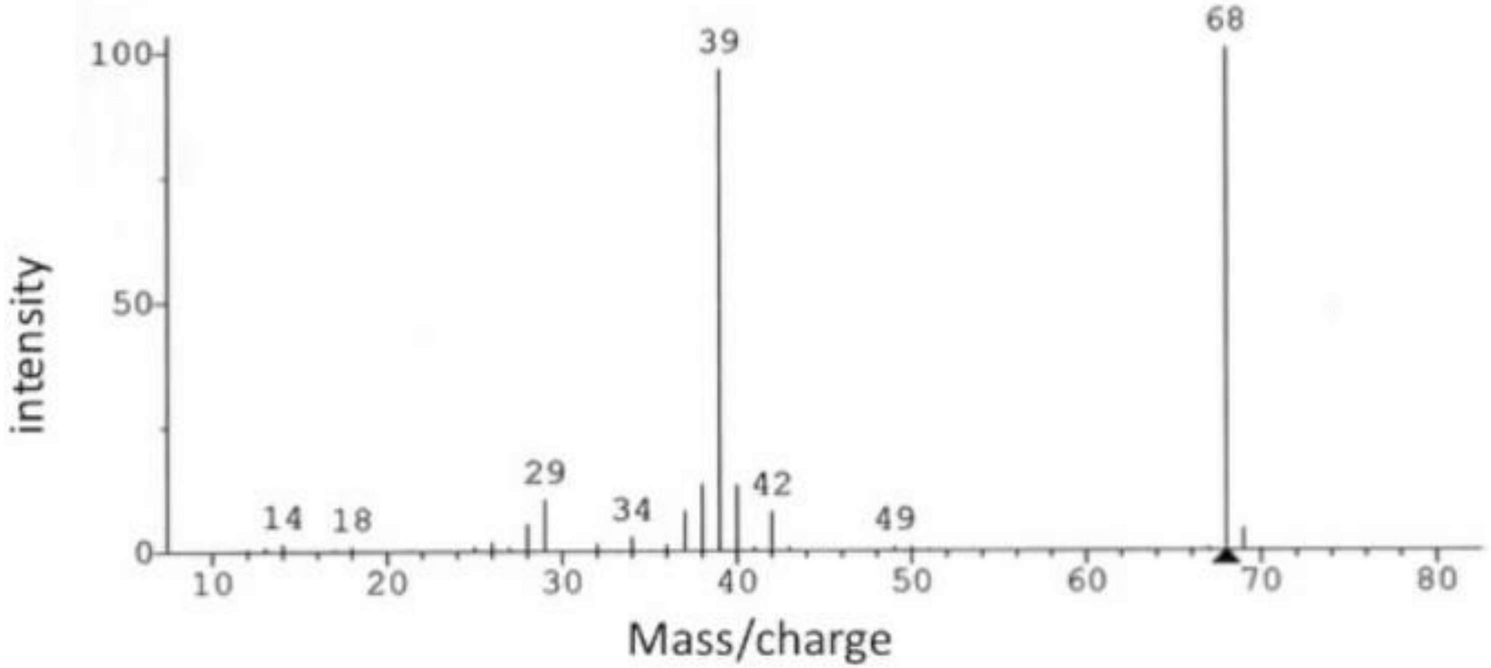
4 amu ⟶ H_4

Rings + double bonds

$$= DBE = C - \frac{H}{2} + \frac{N}{2} + 1$$

$$= 4 - \frac{4}{2} + \frac{0}{2} + 1$$

Example 3



	Mass/charge	Intensity
	67	0.5
M	68	100
M+1	69	4.2
	70	0.1

$$\#C = \frac{4.2}{100} \times \frac{100}{1.1} = 3.8 \sim 4$$

C_4H_4O

68 amu
-48 = 4x12 for C_4

20 amu
-16 for O_1

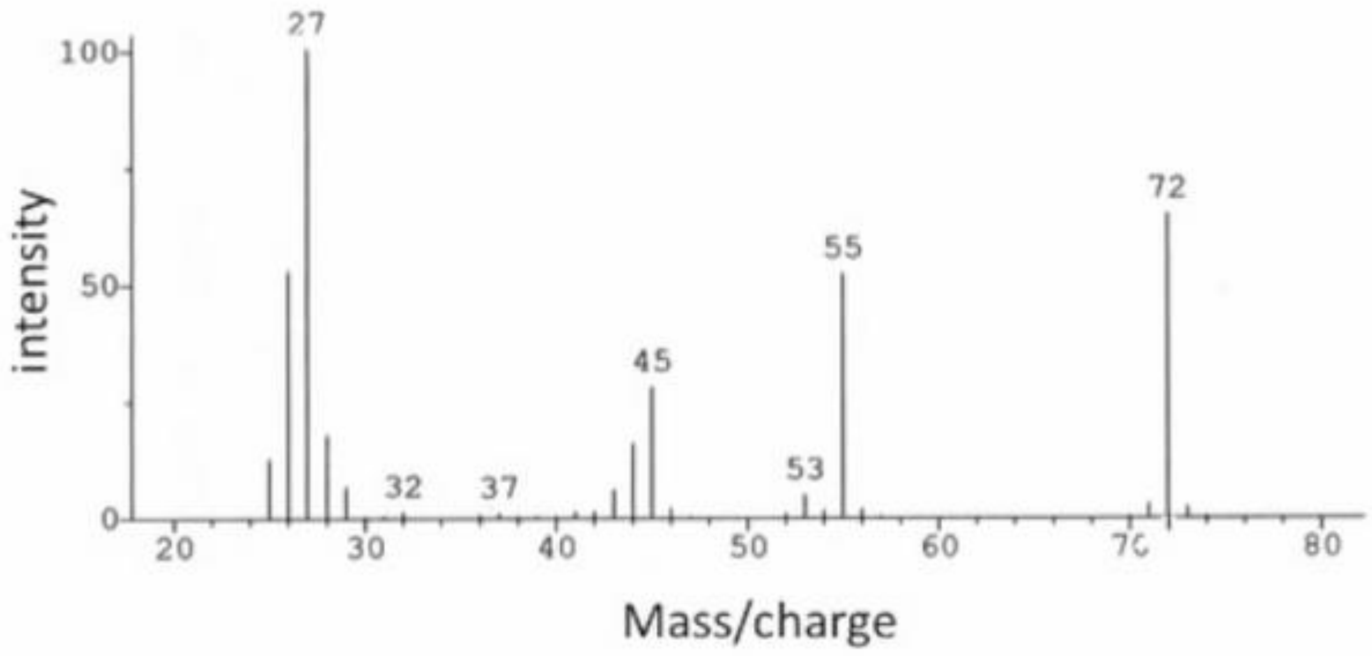
4 amu ⟶ H_4

Rings + double bonds

$$= \text{DBE} = C - \frac{H}{2} + \frac{N}{2} + 1$$

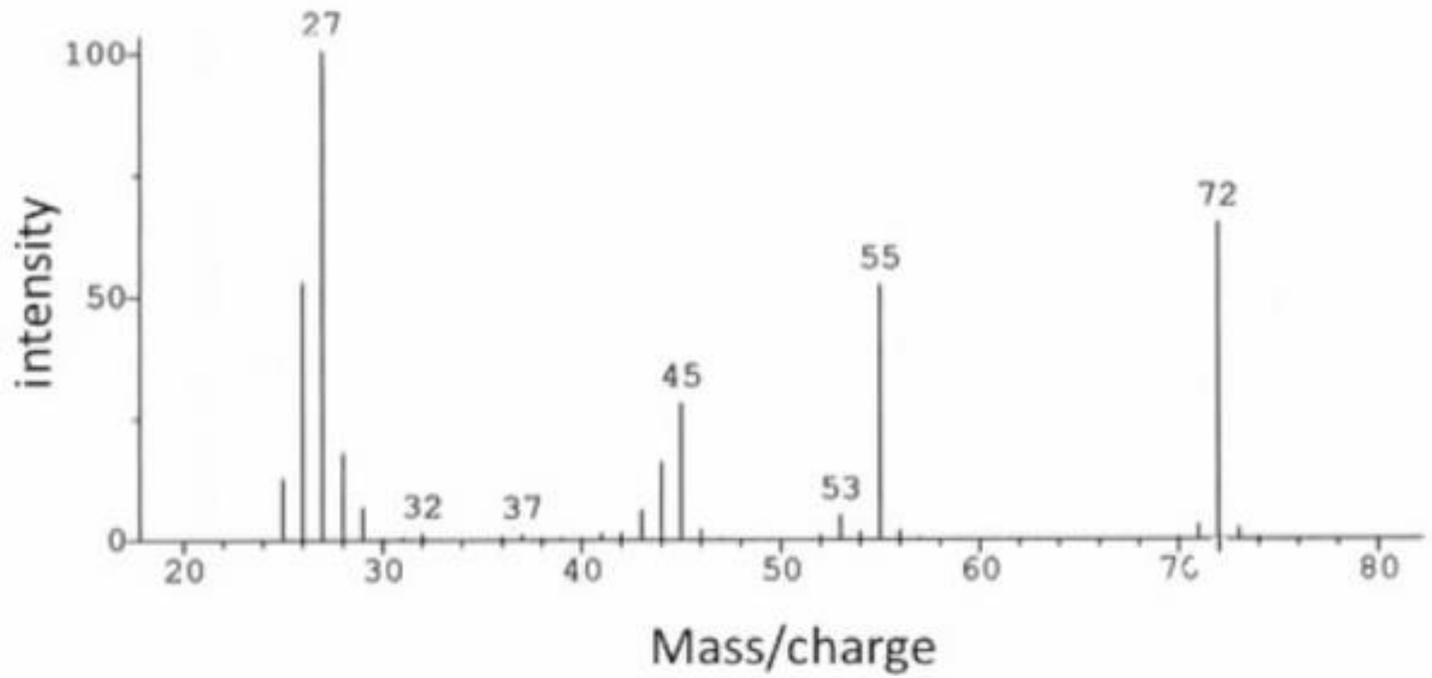
$$= 4 - \frac{4}{2} + \frac{0}{2} + 1 = 3$$

Example 4



	Mass/charge	Intensity
	71	3.2
M	72	64.6
M+1	73	2.2
	74	0.3

Example 4



	Mass/charge	Intensity
	71	3.2
M	72	64.6
M+1	73	2.2
	74	0.3

$$\# C = \frac{2.2}{64.6} \times \frac{100}{1.1} = 3.1 \sim 3$$

72 amu
-36 = 3x12 for C_3

36 amu
-32 for O_2

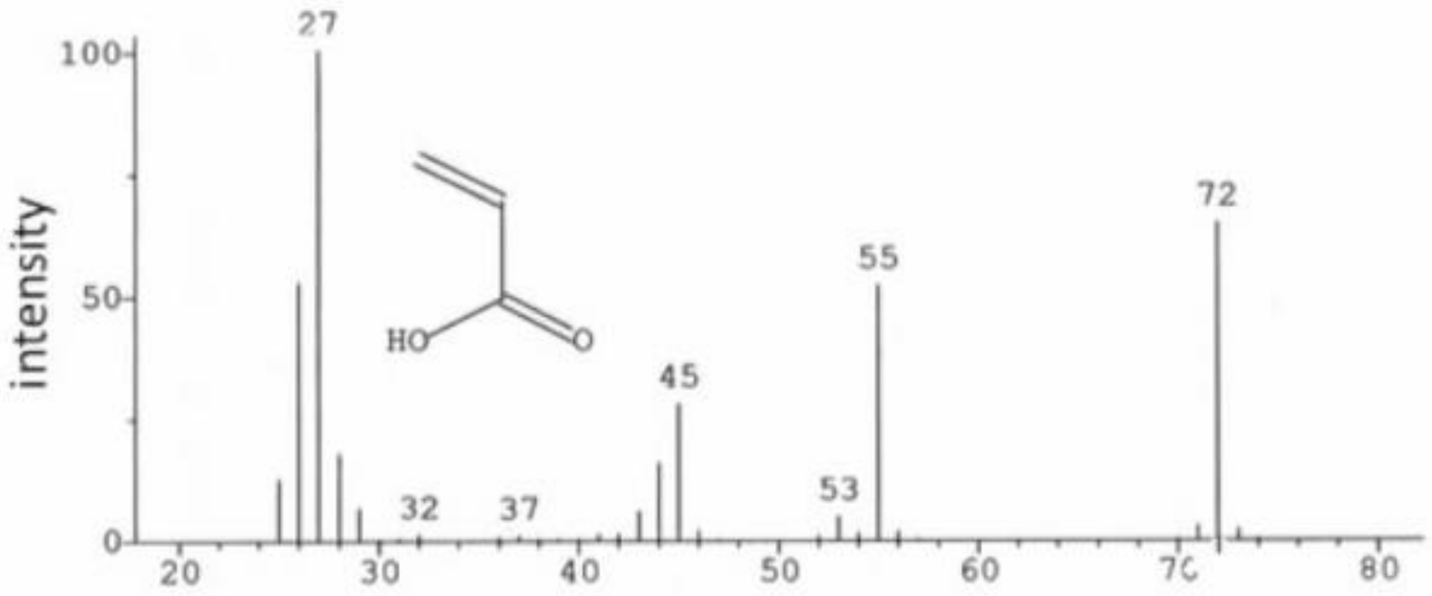
4 amu → H_4

$C_3H_4O_2$

$$\text{DBE} = 3 - \frac{4}{2} + \frac{0}{2} + 1$$

$$= 2$$

Example 4



	Mass/charge	Intensity
	71	3.2
M	72	64.6
M+1	73	2.2
M+2	74	0.3

$$\#C = \frac{2.2}{64.6} \times \frac{100}{1.1} = 3.1 \sim 3$$

72 amu
-36 = 3x12 for C_3

36 amu
-32 for O_2

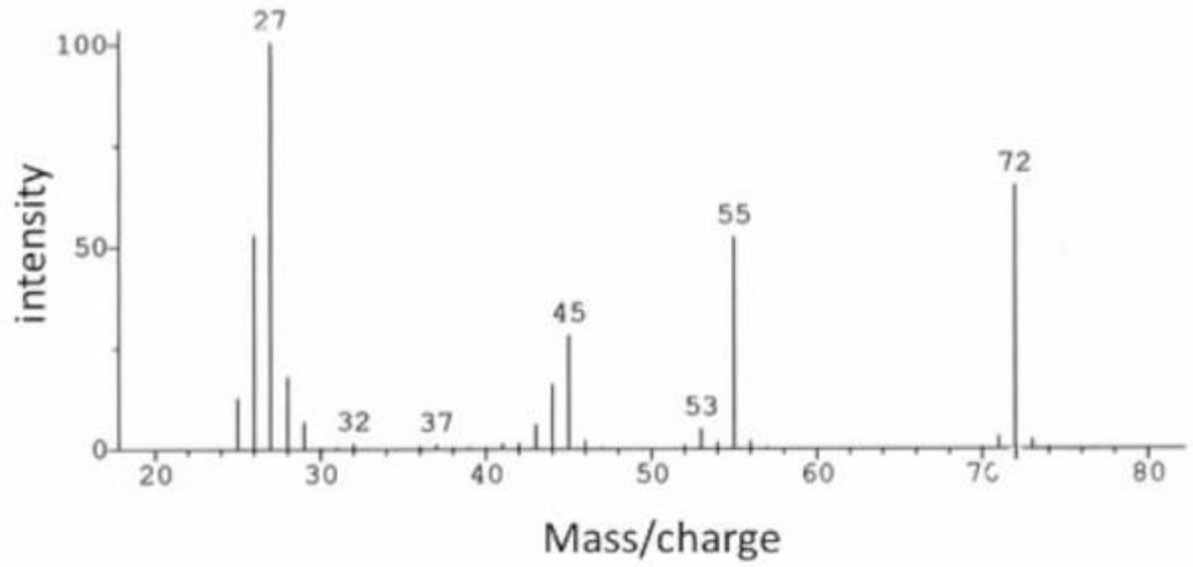
4 amu ⟶ H_4

$C_3H_4O_2$

$$\text{DBE} = 3 - \frac{4}{2} + \frac{0}{2} + 1$$

$$= 2$$

Example 4



	Mass/charge	Intensity
	71	3.2
M	72	64.6
M+1	73	2.2
M+2	74	0.3

$$\# C = \frac{2.2}{64.6} \times \frac{100}{1.1} = 3.1 \sim 3$$

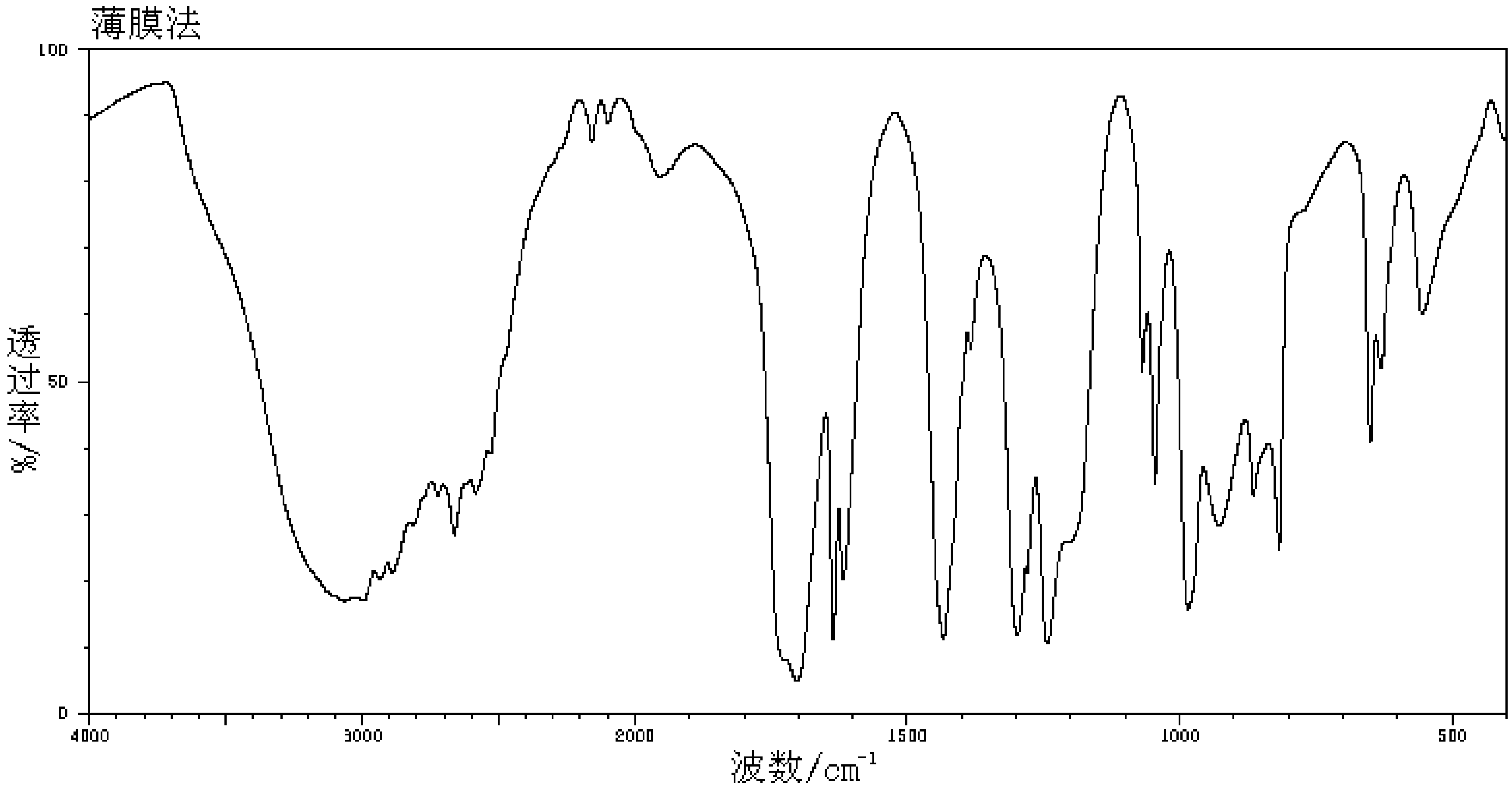
72 amu
-36 = 3x12 for C_3
36 amu
-28 for N_2
8 amu → H_8

$C_3H_8N_2$

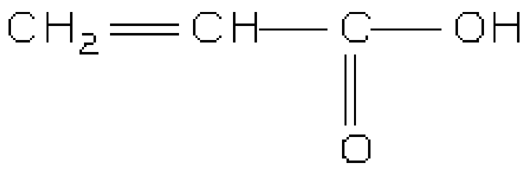
DBE $= 3 - \frac{8}{2} + \frac{2}{2} + 1$

$= 1$

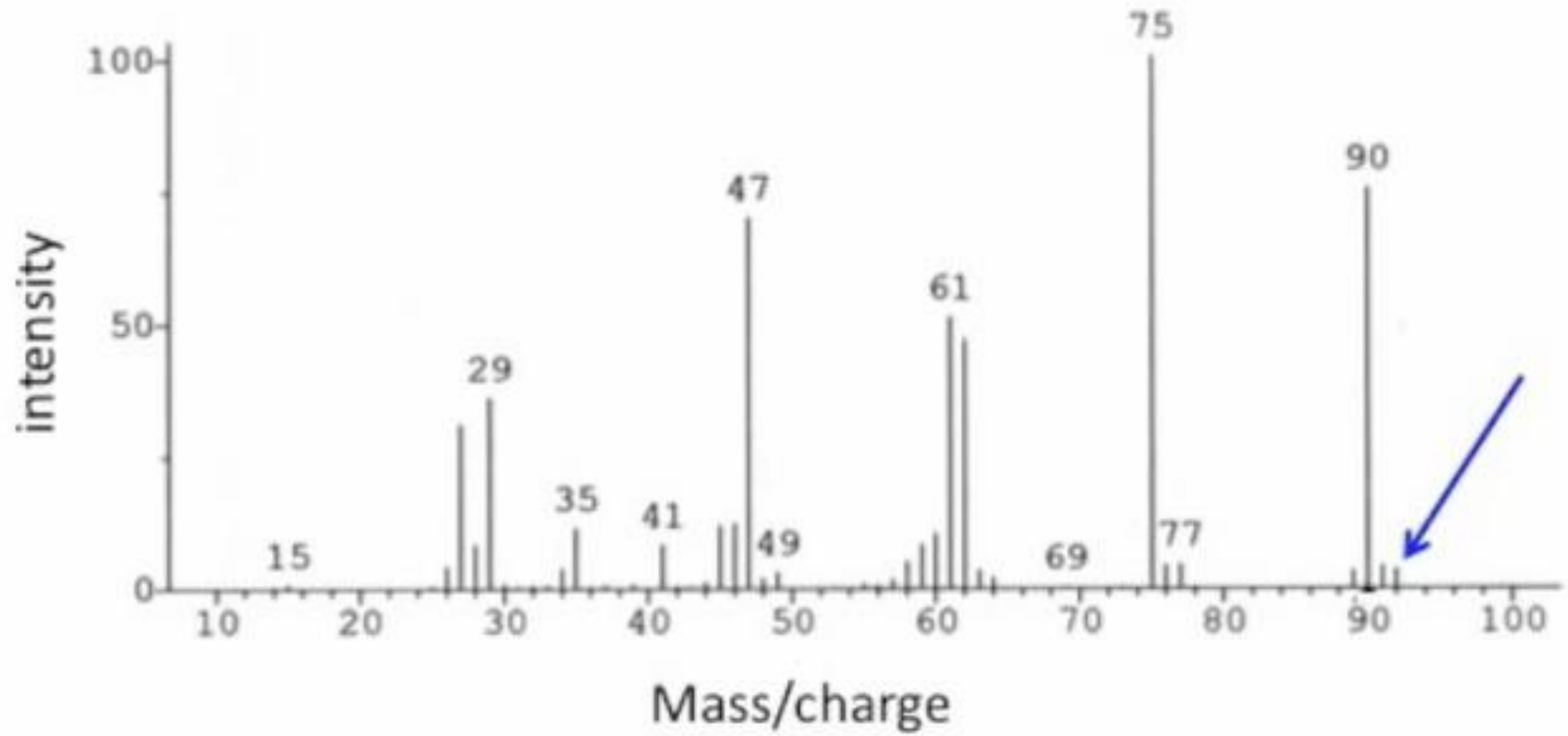
Acrylic Acid



2936	19	1964	77	1243	10	660	39
2889	20	1702	4	1069	49	630	50
2723	31	1637	10	1046	33	556	58
2661	26	1618	19	986	16	643	60
2585	32	1434	10	928	27		
2159	81	1384	59	865	31		
2099	86	1299	11	818	23		



Example 5



	Mass/charge	Intensity
	89	3.2
M	90	75.2
M+1	91	4.1
M+2	92	3.4

$$\#C = \frac{4.1}{75.2} \times \frac{100}{1.1} = 4.9_5 \sim 5$$

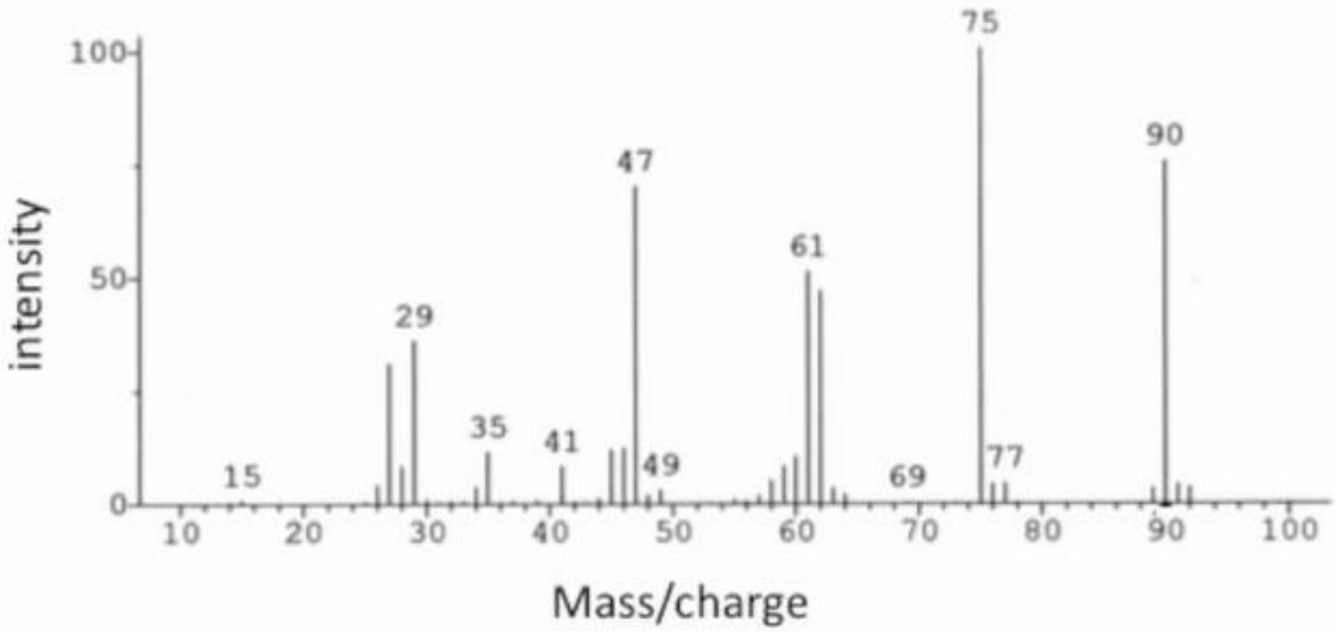
90 amu
-60 = 5x12 for C_5
30 amu

Element	Mass	%	1st Heavy Isotope Mass	%	2nd Heavy Isotope Mass	%
Hydrogen	^{1}H	100	^{2}H	0.015		
Carbon	^{12}C	100	^{13}C	1.1		
Nitrogen	^{14}N	100	^{15}N	0.37		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.4
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.80	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98.0
Iodine	^{127}I	100				

If sulfur is present, it contributed to the intensity for the M+1 peak as well as the M+2 peak.

Element	Mass	%	1st Heavy Isotope Mass	%	2nd Heavy Isotope Mass	%
Hydrogen	^{1}H	100	^{2}H	0.015		
Carbon	^{12}C	100	^{13}C	1.1		
Nitrogen	^{14}N	100	^{15}N	0.37		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.4
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.80	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98.0
Iodine	^{127}I	100				

4.4% of 75.2 = 3.3 **M+2**

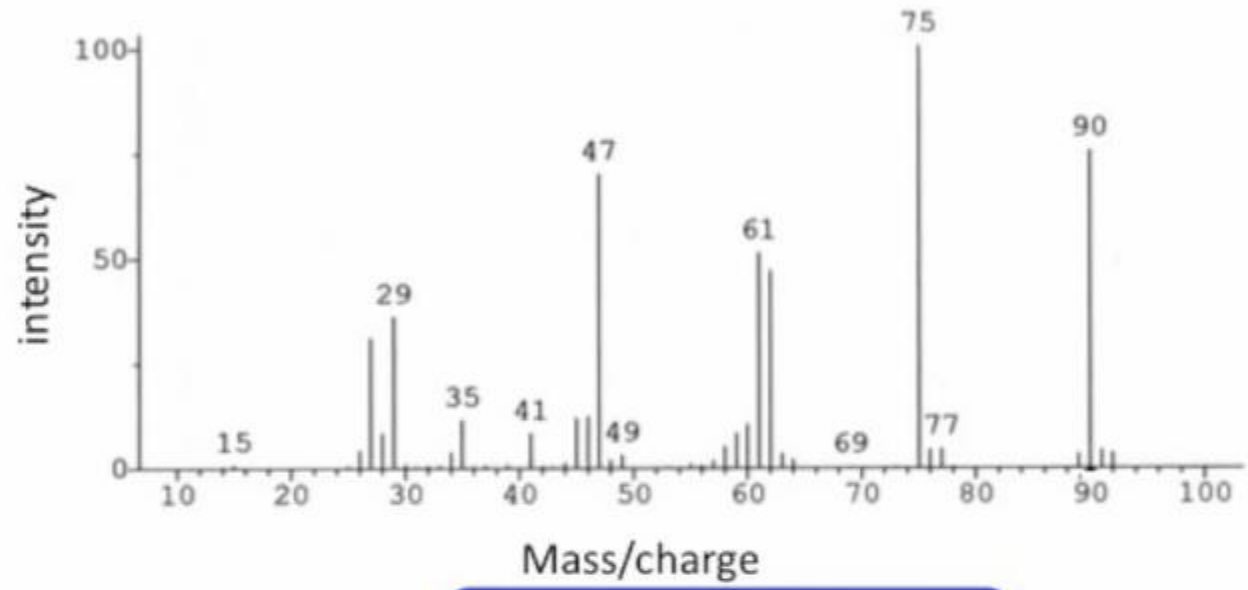


	Mass/charge	Intensity
	89	3.2
M	90	75.2
M+1	91	4.1
	92	3.4

$$\#C = \frac{4.1}{75.2} \times \frac{100}{1.1} = 4.9_5 \sim 5$$

90 amu
-60 = 5x12 for C_5
30 amu

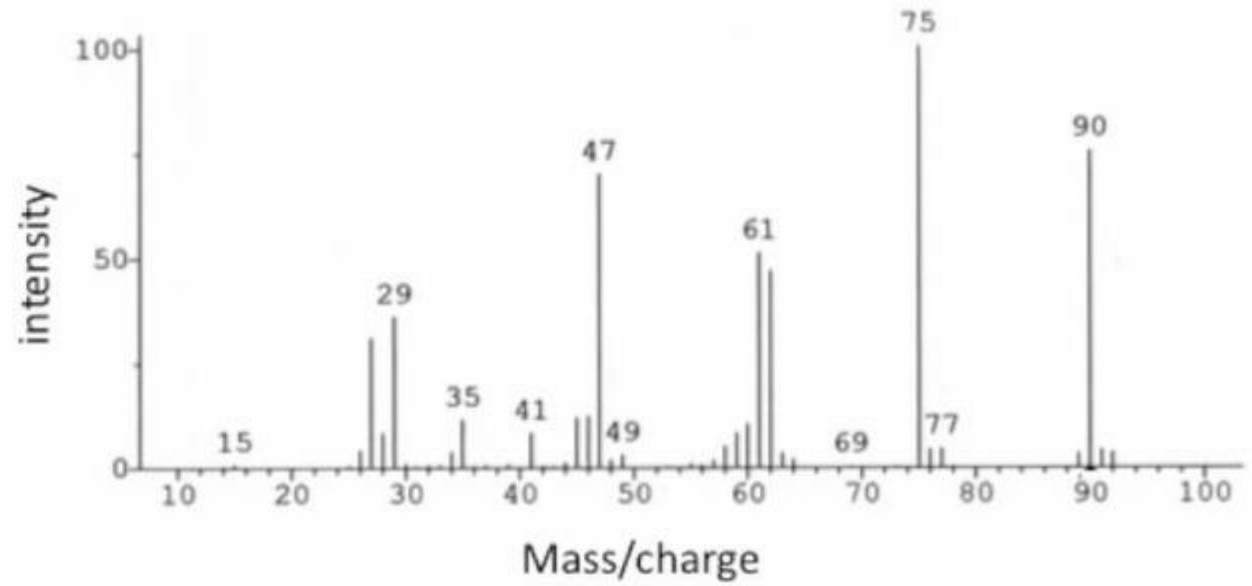
Example 5



	Mass/charge	Intensity
	89	3.2
M	90	75.2
M+1	91	4.1
	92	3.4

$$\#C = \frac{4.1-0.6}{75.2} \times \frac{100}{1.1} = 4.2_3 \sim 4$$

Example 5



	Mass/charge	Intensity
	89	3.2
M	90	75.2
M+1	91	4.1
	92	3.4

$$\#C = \frac{4.1-0.6}{75.2} \times \frac{100}{1.1} = 4.2_3 \sim 4$$

90 amu
-48 = 4x12 for C_4

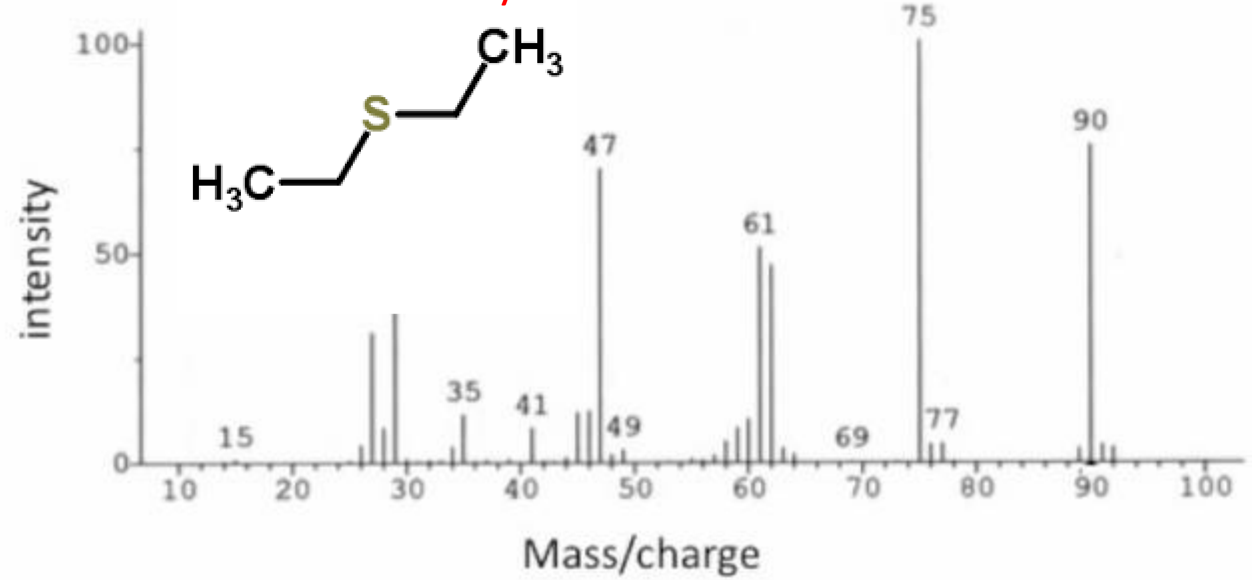
42 amu
-32 for S_1

10 amu ⟶ H_{10}

⇨ $C_4H_{10}S$

Example 5

Diethyl sulfide



	Mass/charge	Intensity
	89	3.2
M	90	75.2
M+1	91	4.1
	92	3.4

$$\#C = \frac{4.1-0.6}{75.2} \times \frac{100}{1.1} = 4.2_3 \sim 4$$

$C_4H_{10}S$

90 amu
-48 = 4x12 for C_4
42 amu
-32 for S_1
10 amu ⟶ H_{10}

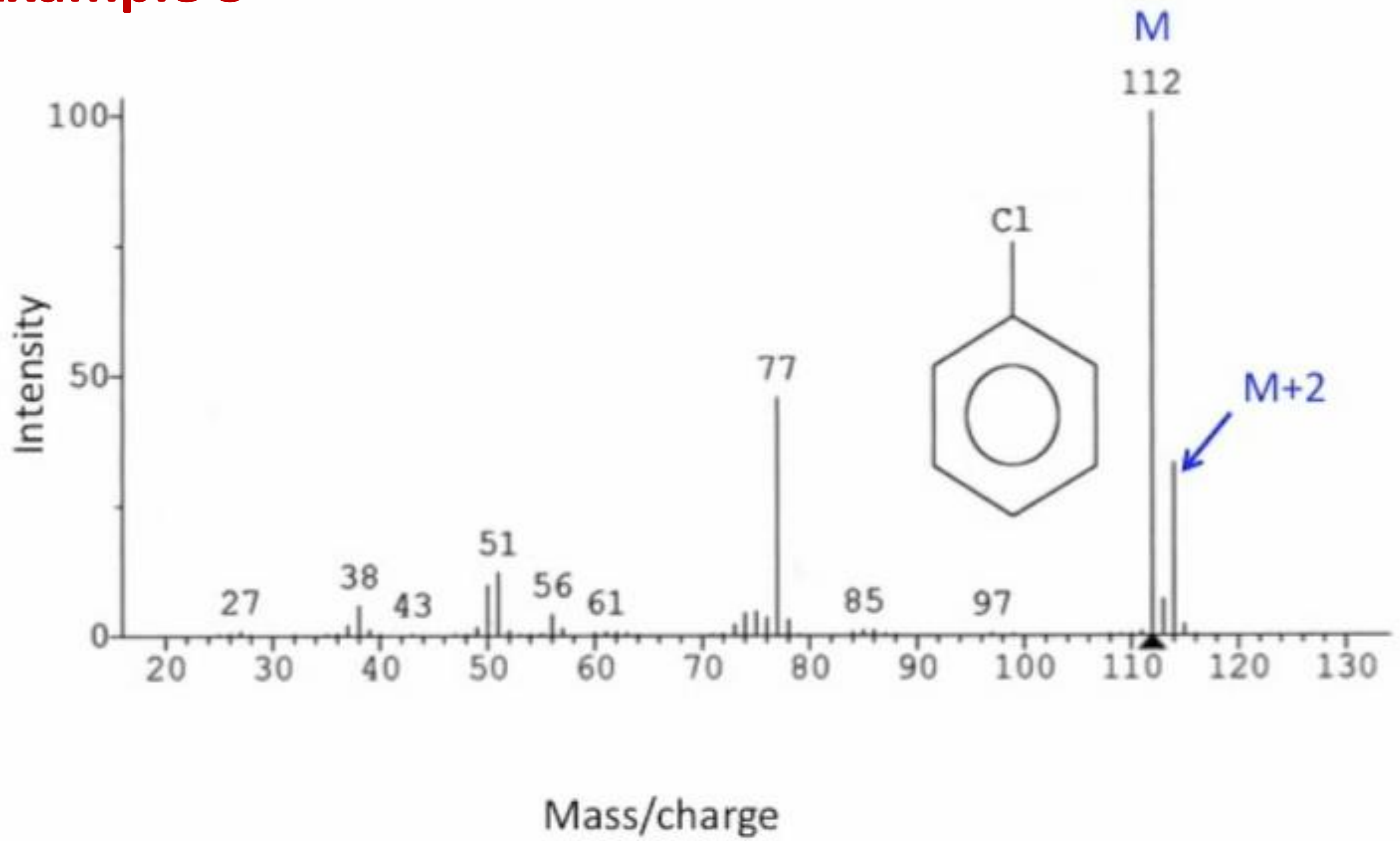
$$\text{DBE} = 4 - \frac{10}{2} + \frac{0}{2} + 1$$

$= 0$

Other isotpes

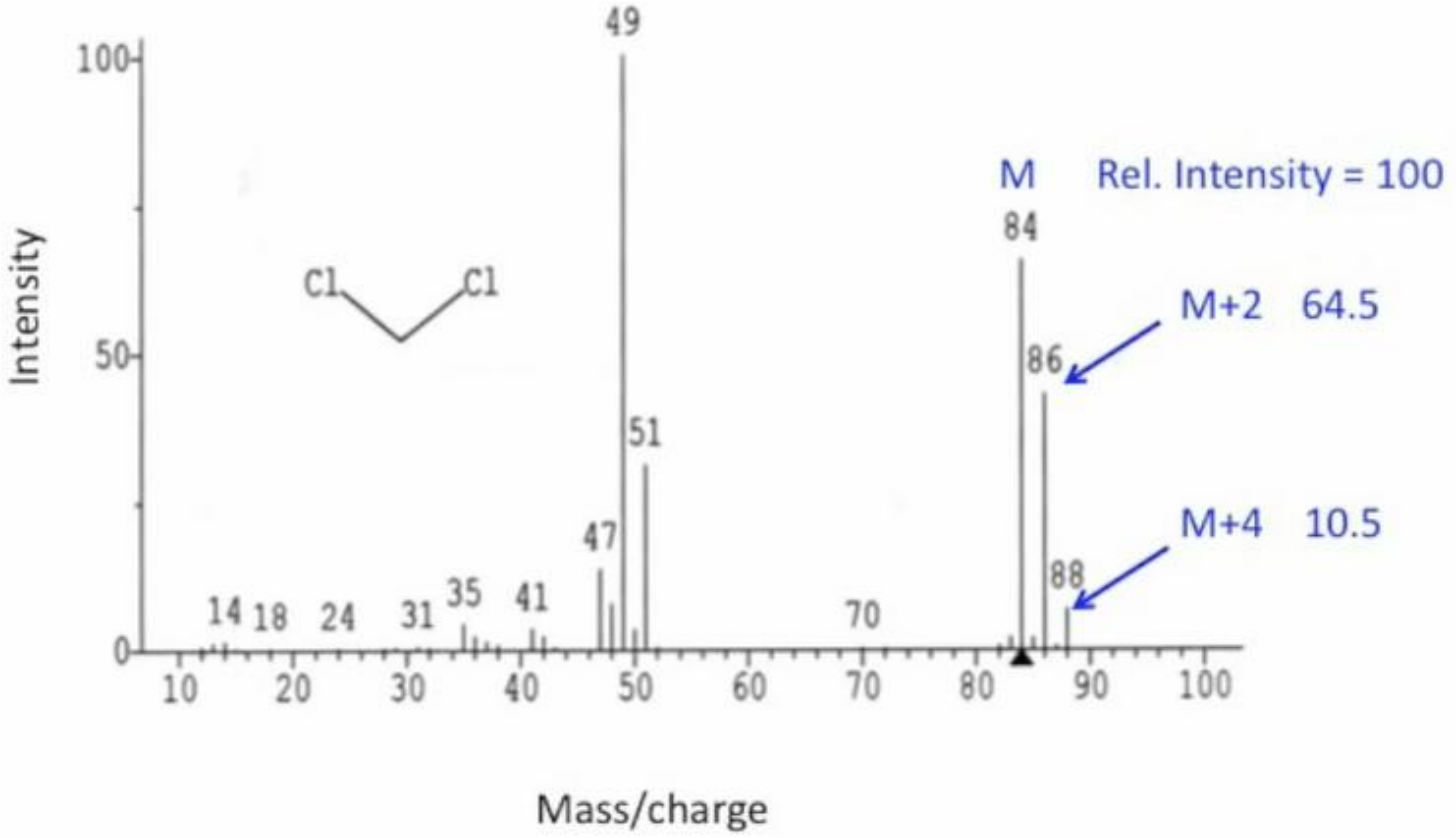
Element	Mass	%	1st Heavy Isotope Mass	%	2nd Heavy Isotope Mass	%
Hydrogen	^{1}H	100	^{2}H	0.015		
Carbon	^{12}C	100	^{13}C	1.1		
Nitrogen	^{14}N	100	^{15}N	0.37		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.4
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.80	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98.0
Iodine	^{127}I	100				

Example 3



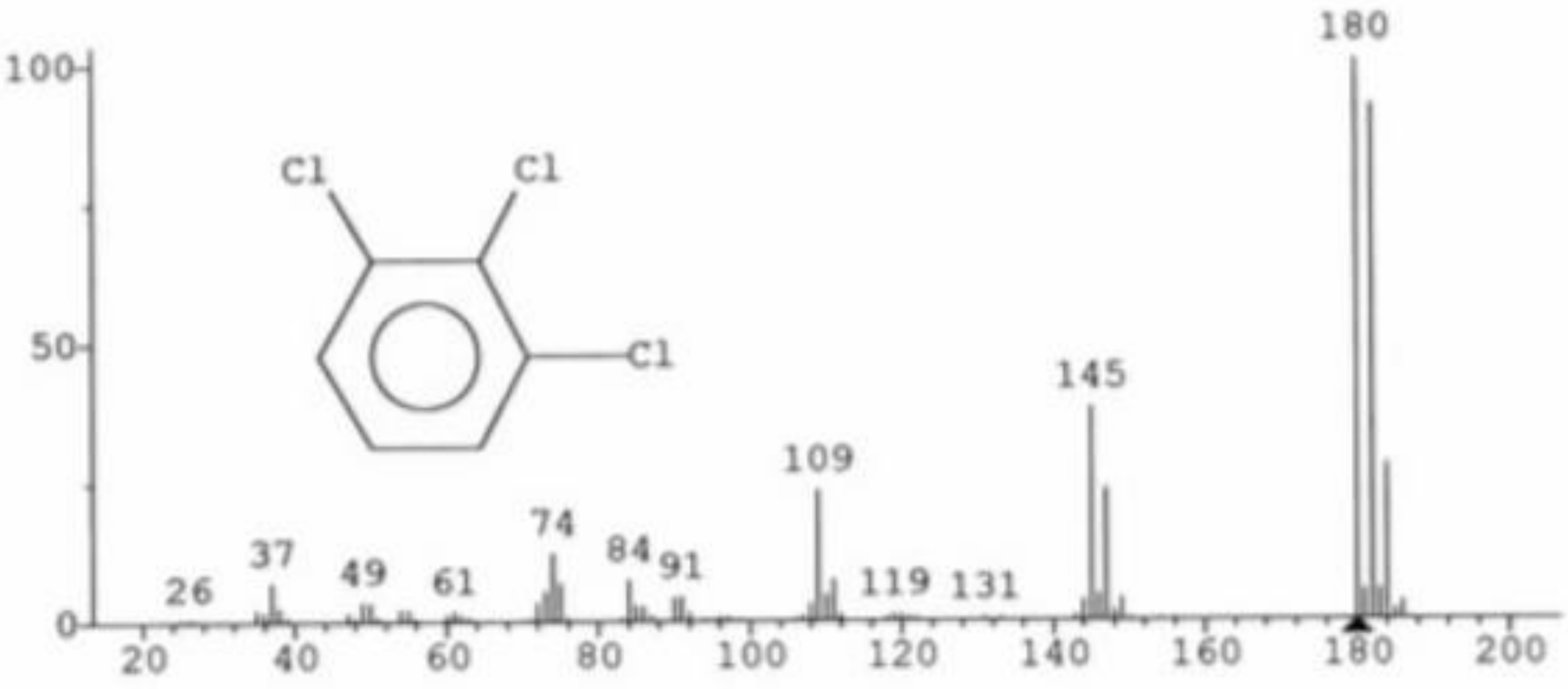
M
112
100
50
0
Intensity
Cl
77
M+2
27
38
43
51
56
61
85
97
20
30
40
50
60
70
80
90
100
110
120
130
Mass/charge

Example 4



Intensity
100
50
0
Cl
Cl
14
18
24
31
35
41
47
49
51
70
84
86
88
M
Rel. Intensity = 100
M+2 64.5
M+4 10.5
10
20
30
40
50
60
70
80
90
100
Mass/charge

Example 5



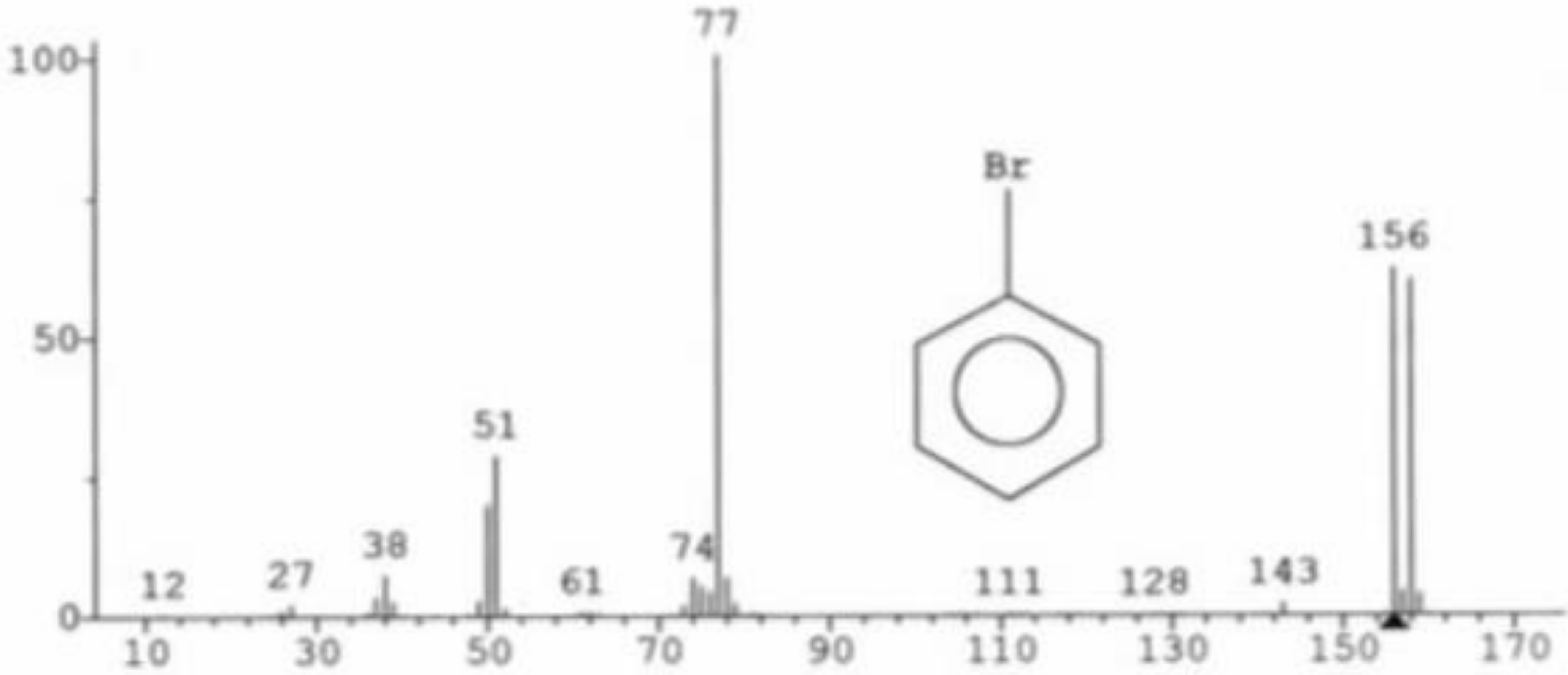
Cl
Cl
Cl
100
50
0
180
145
109
74
84
91
37
49
61
26
119
131
20
40
60
80
100
120
140
160
180
200

There are several websites that have free calculator programs where you can predict the distribution of isotope peaks for any given molecular formula. Here is a good link.

http://www.sisweb.com/mstools/isotope.htm

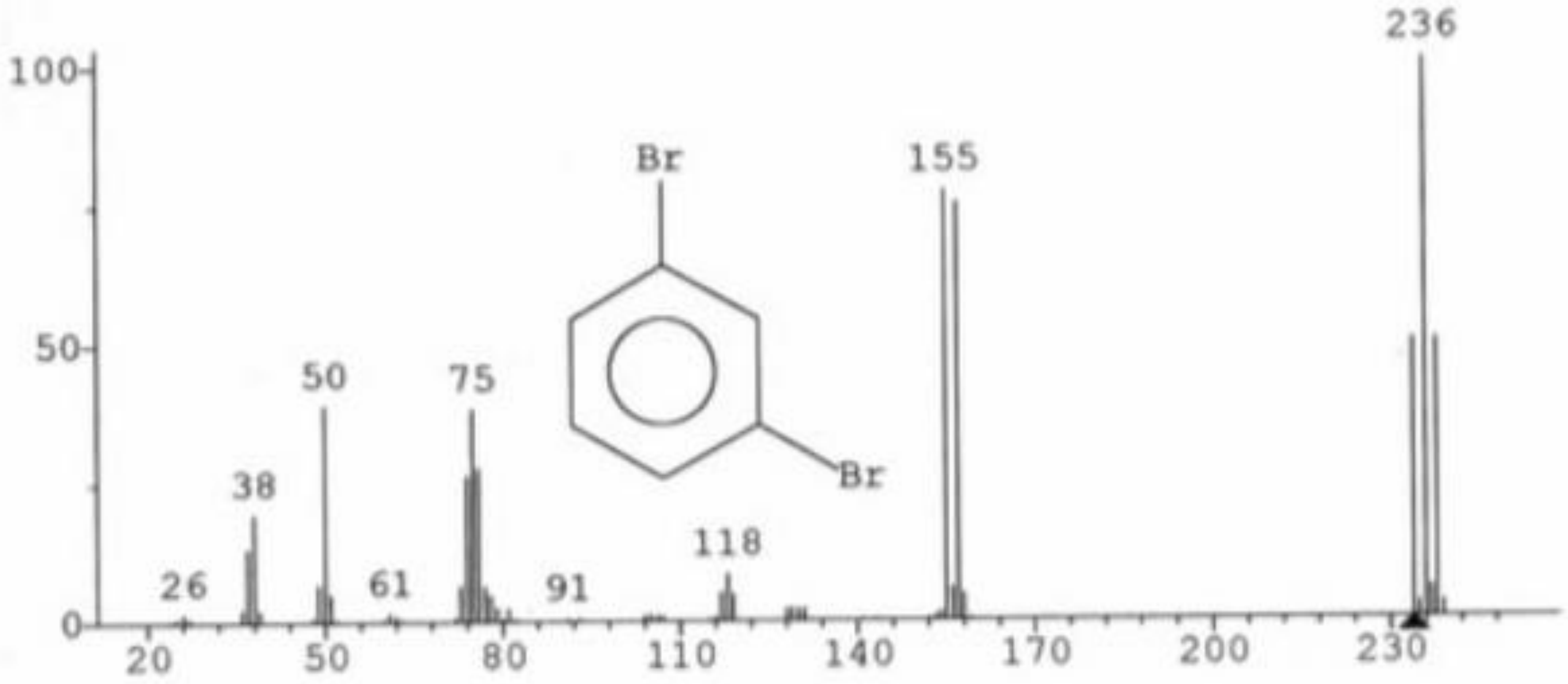
Element	Mass	%	1st Heavy Isotope Mass	%	2nd Heavy Isotope Mass	%
Hydrogen	^{1}H	100	^{2}H	0.015		
Carbon	^{12}C	100	^{13}C	1.1		
Nitrogen	^{14}N	100	^{15}N	0.37		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.4
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.80	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98.0
Iodine	^{127}I	100				

Example 6



77
100
50
0
51
38
74
12
27
61
111
128
143
156
Br
10
30
50
70
90
110
130
150
170

Example 7



100
50
0
236
155
Br
Br
50
75
38
26
61
91
118
20
50
80
110
140
170
200
230

Element	Mass	%	1st Heavy Isotope Mass	%	2nd Heavy Isotope Mass	%
Hydrogen	^{1}H	100	^{2}H	0.015		
Carbon	^{12}C	100	^{13}C	1.1		
Nitrogen	^{14}N	100	^{15}N	0.37		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.20
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.4
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.80	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98.0
Iodine	^{127}I	100				