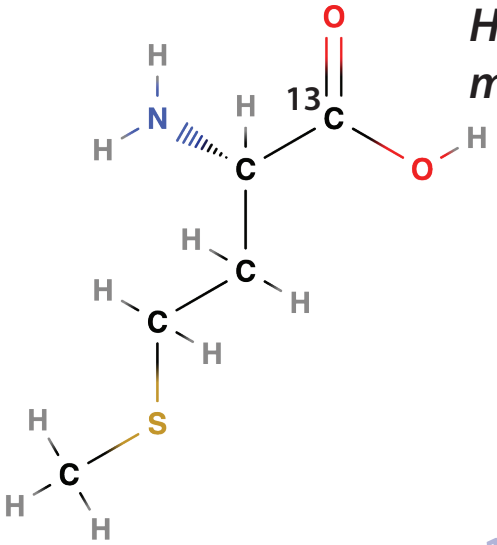
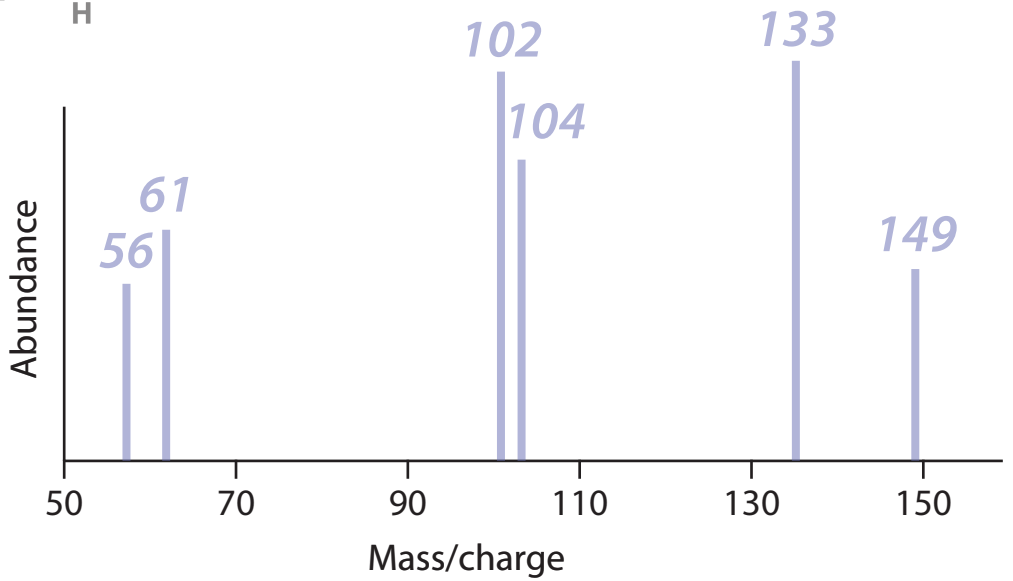
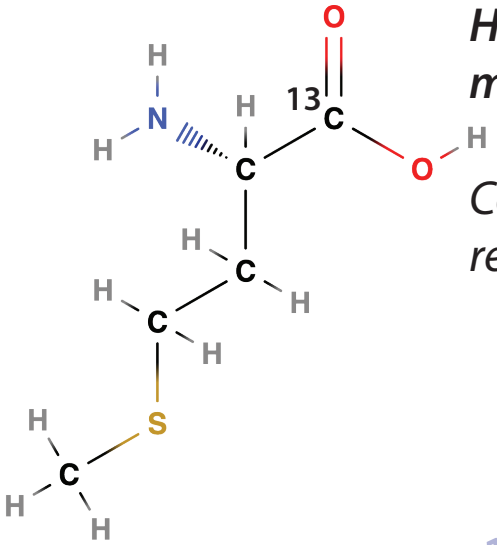
How does a ^{13}C substitution change the methionine mass spectrum ?

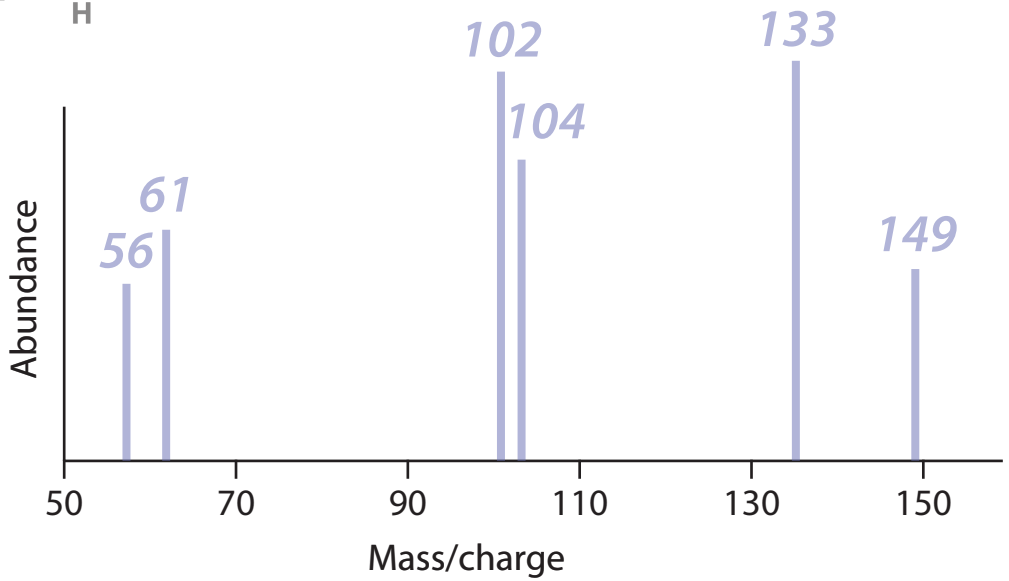


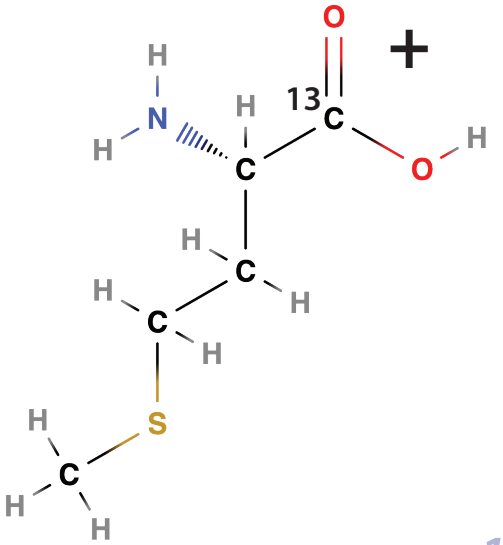




How does a ^{13}C substitution change the methionine mass spectrum ?

Consider the same fragmentation reactions as before...




O
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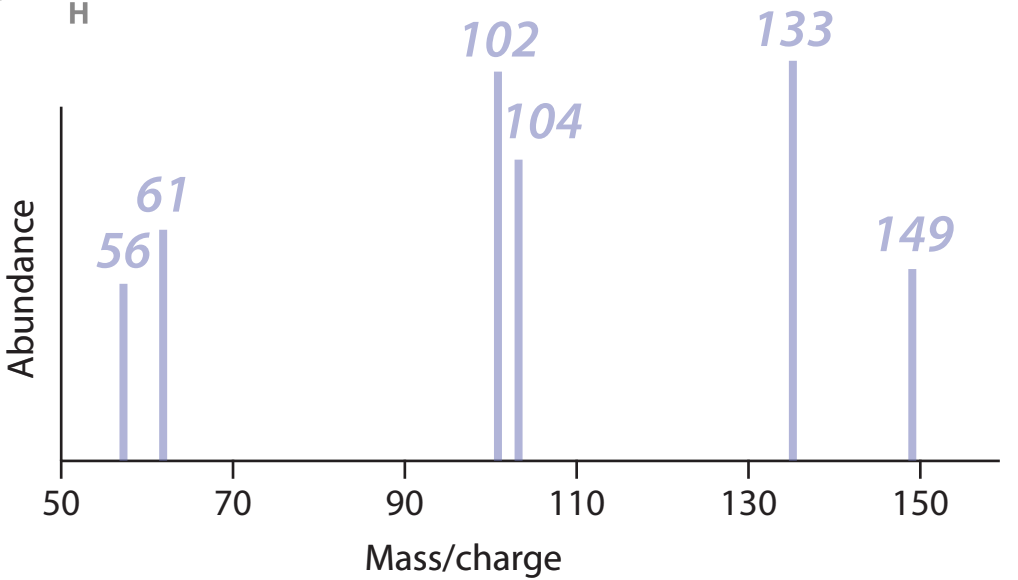
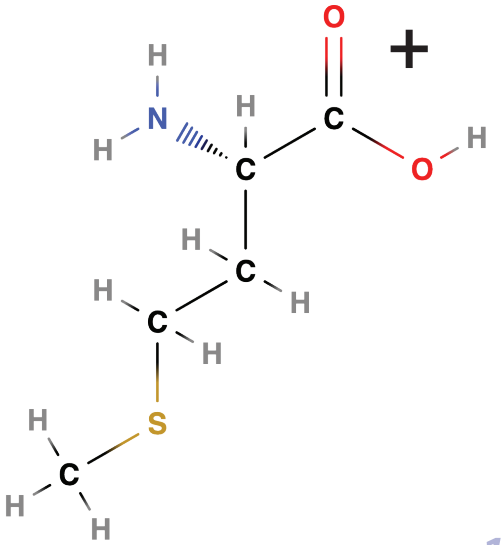

102
133
104
61
56
149
Abundance
50
70
90
110
130
150
Mass/charge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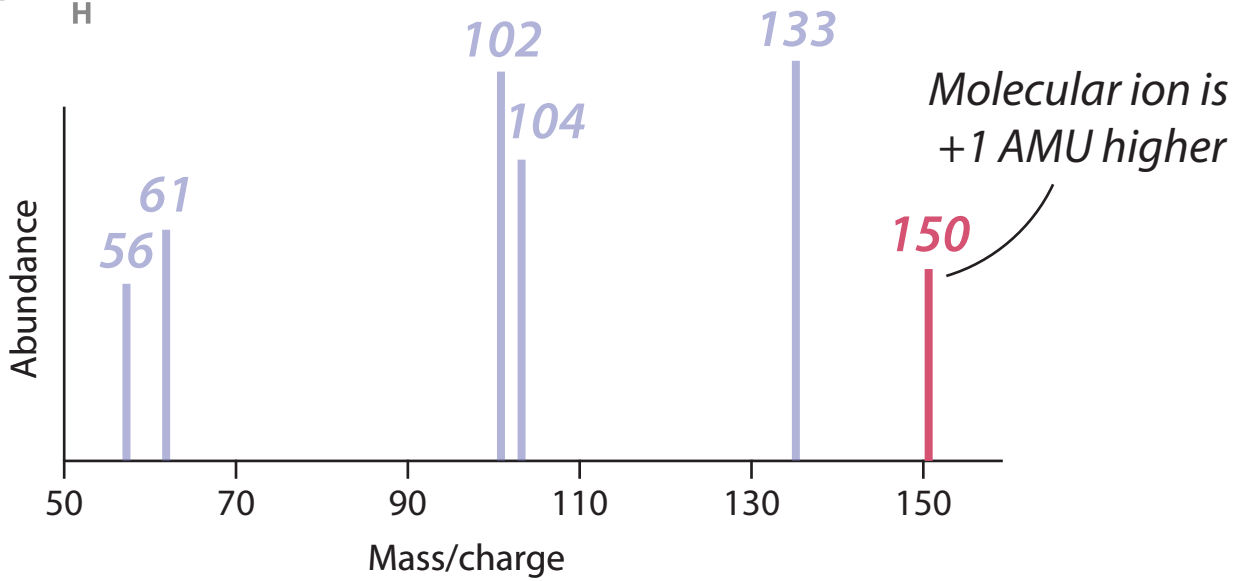
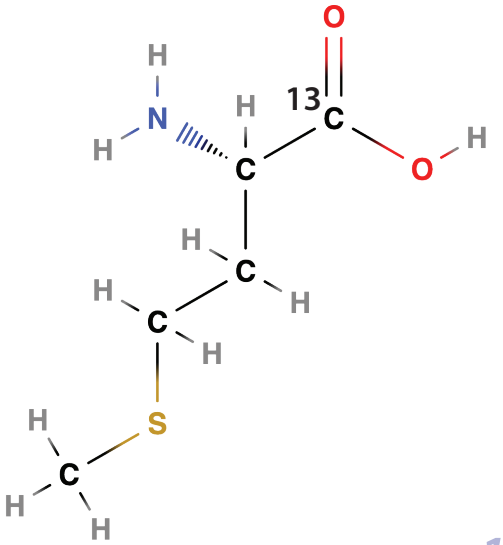

102
133
104
Molecular ion is
+1 AMU higher
61
56
150
Abundance
50
70
90
110
130
150
Mass/charge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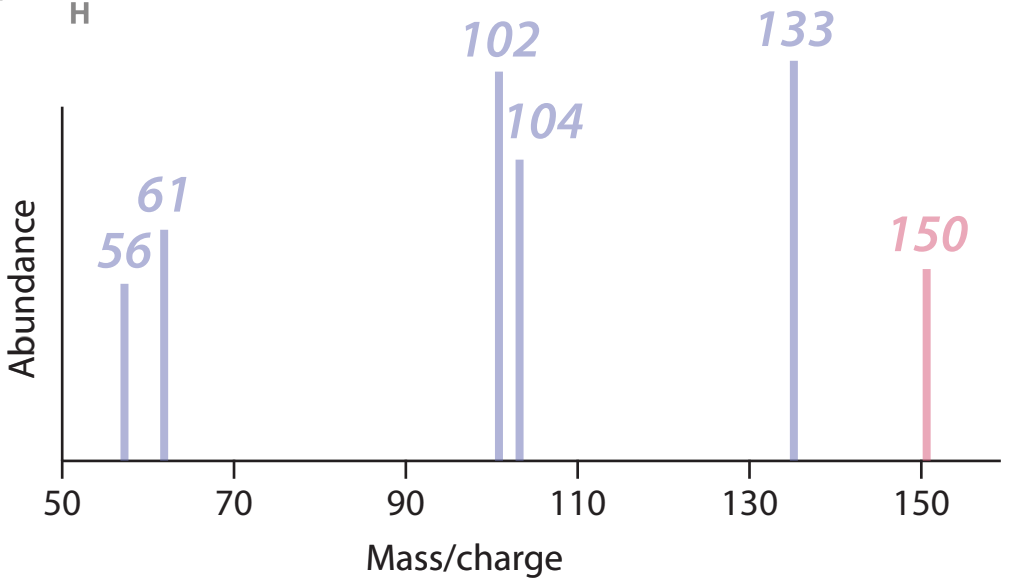
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Abundance
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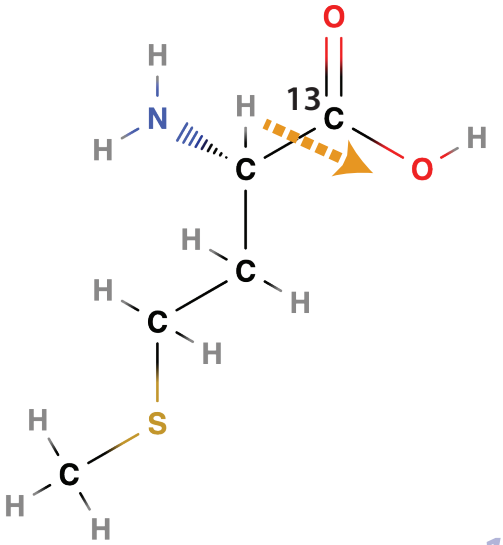
150
Mass/charge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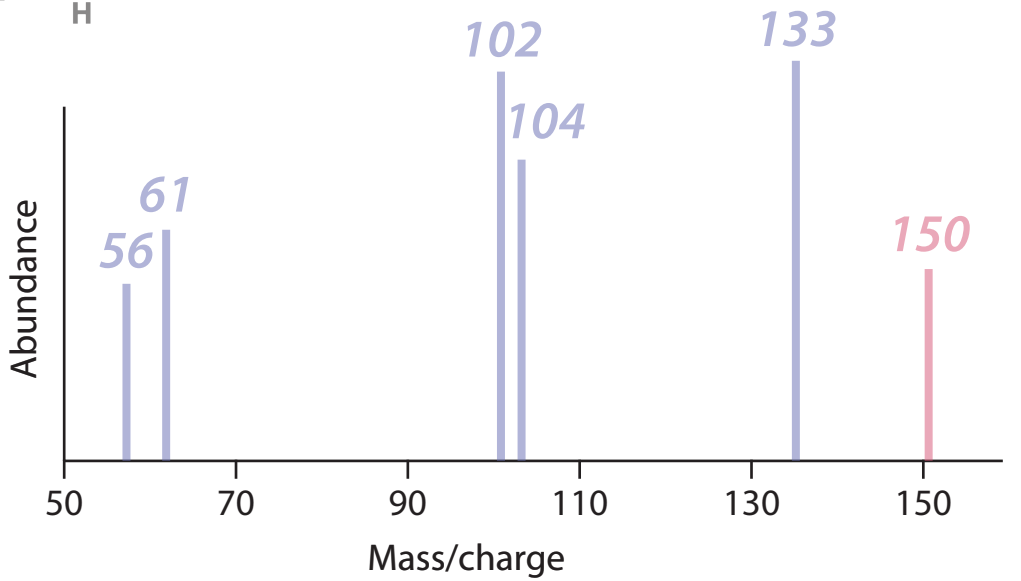
102
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Abundance
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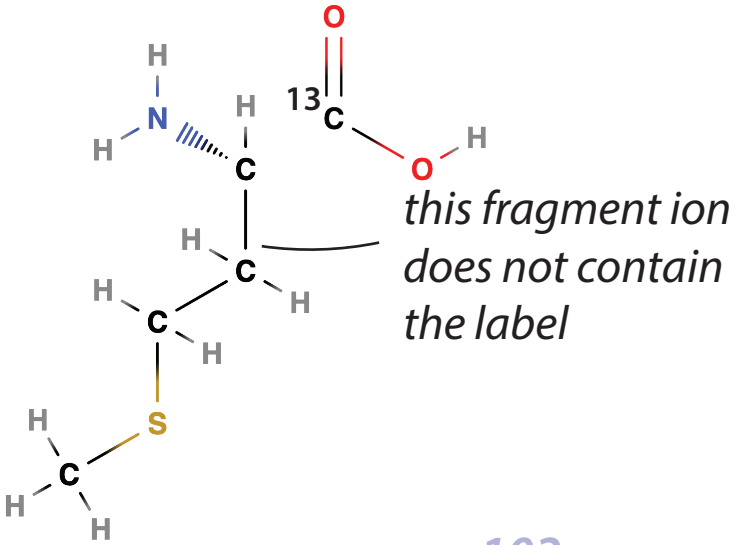
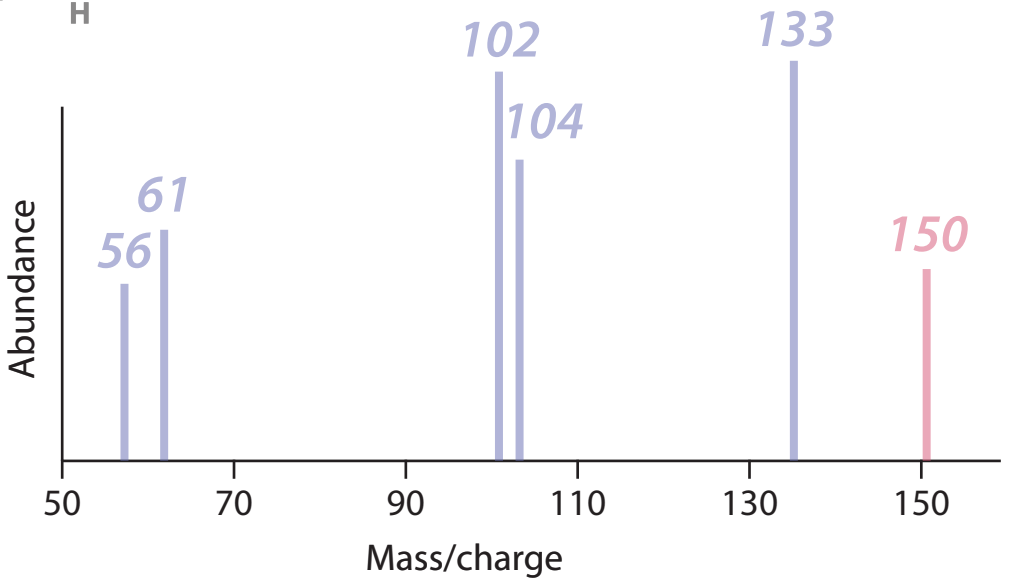
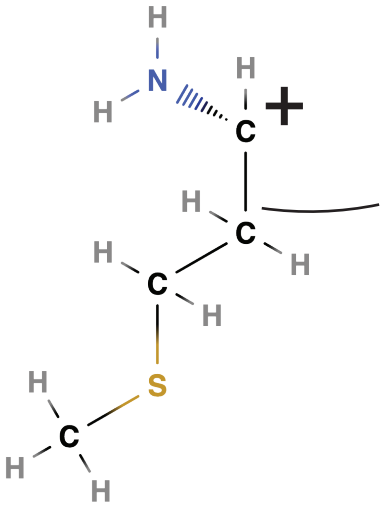
130
150
Mass/charge

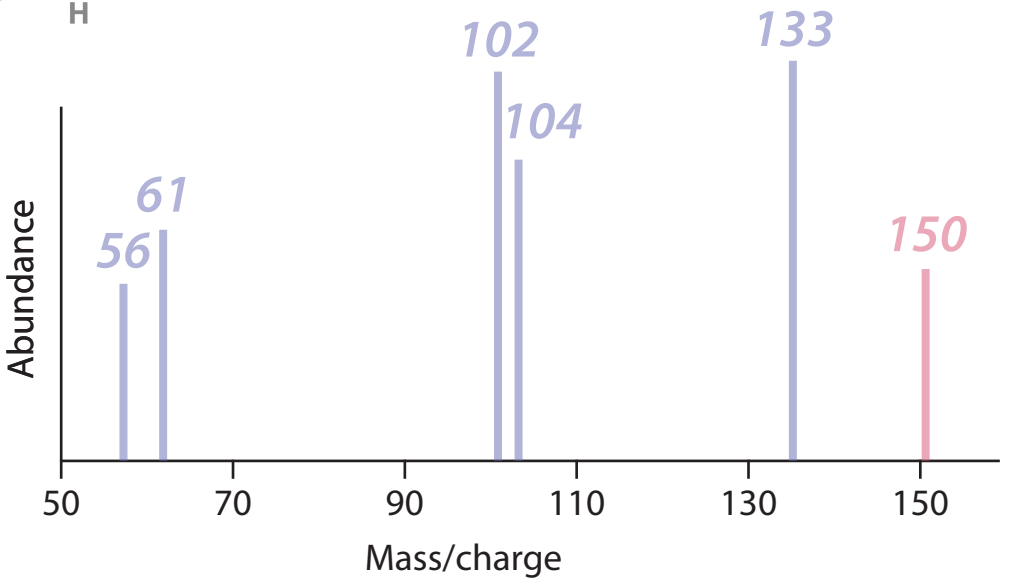


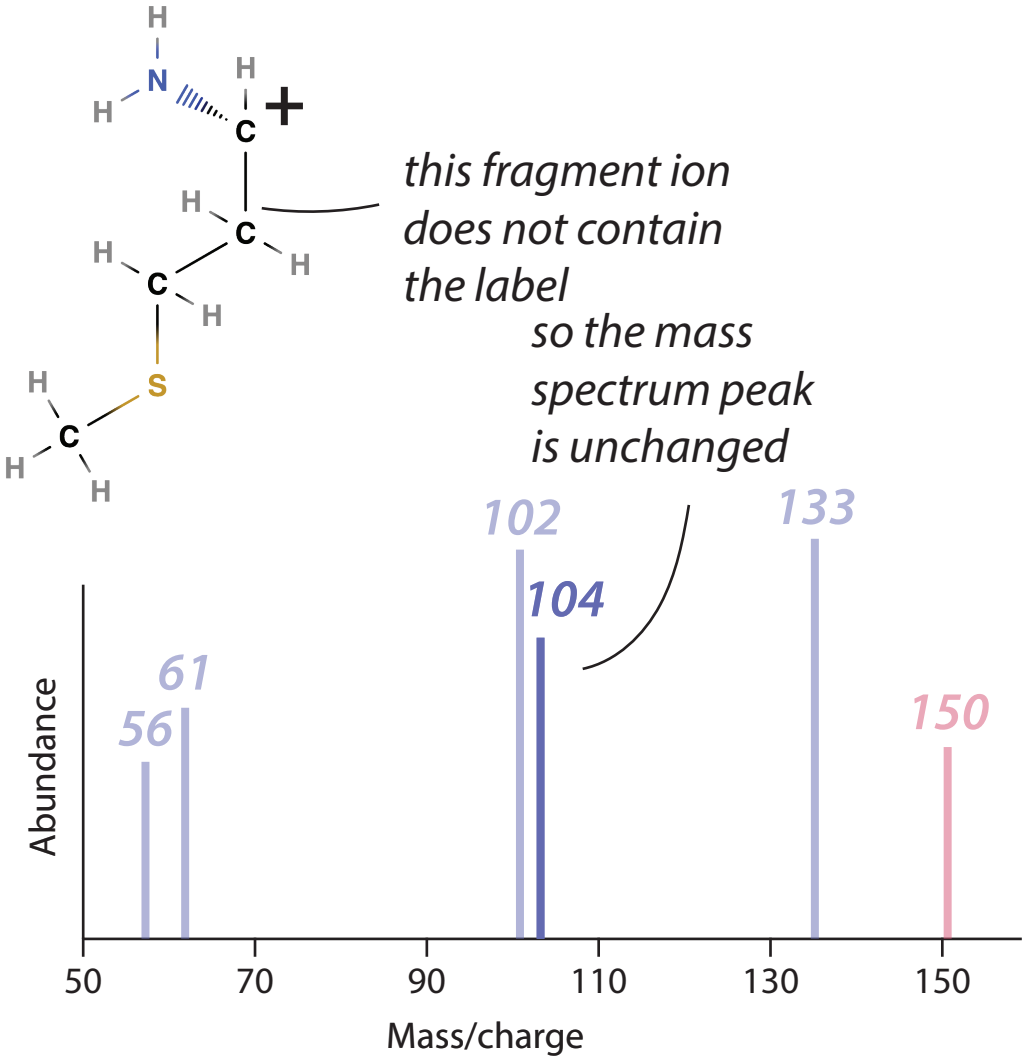
this fragment ion does not contain the label





this fragment ion does not contain the label




this fragment ion
does not contain
the label
so the mass
spectrum peak
is unchanged
102
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56
150
Abundance
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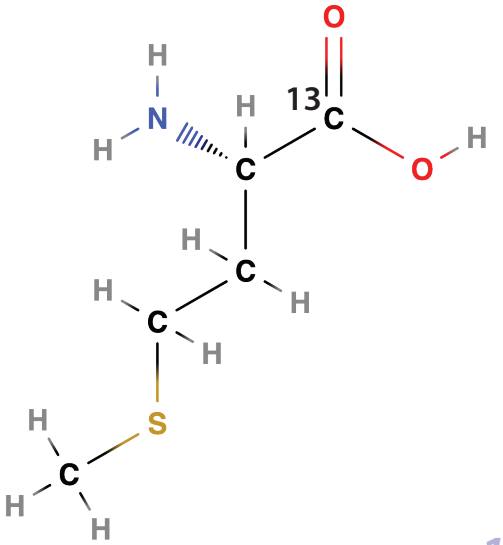
90
110
130
150
Mass/charge


O
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H
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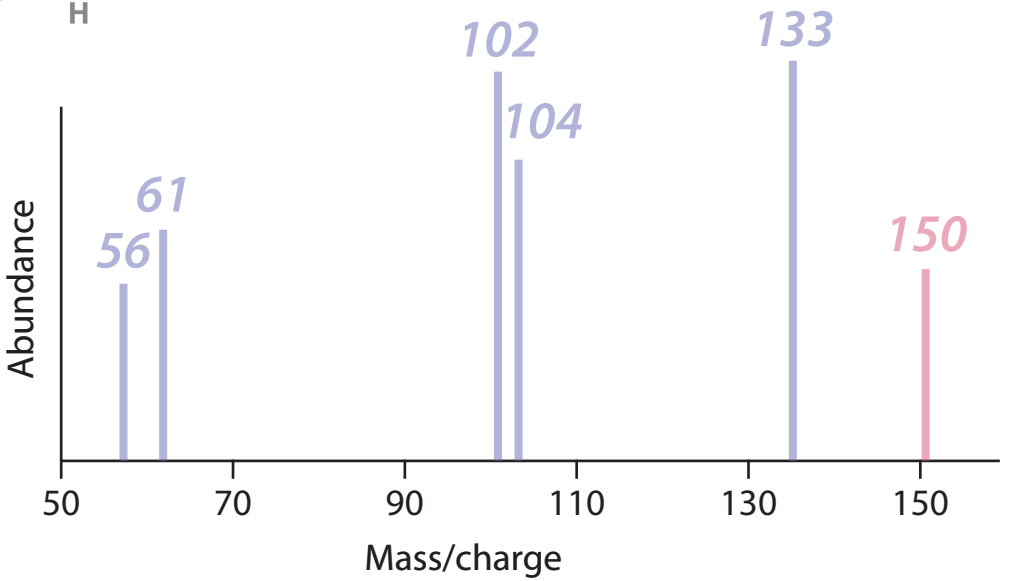
H


102
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133
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Abundance
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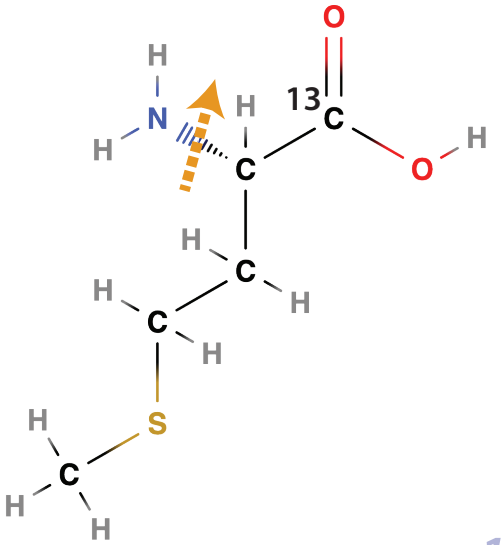
Mass/charge


O
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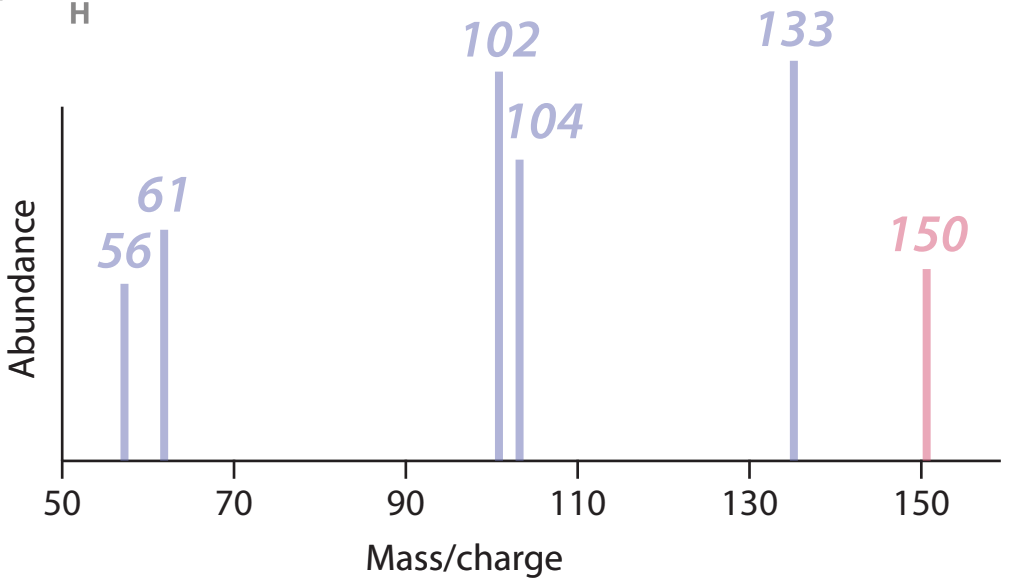
102
133
104
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56
150
Abundance
50
70
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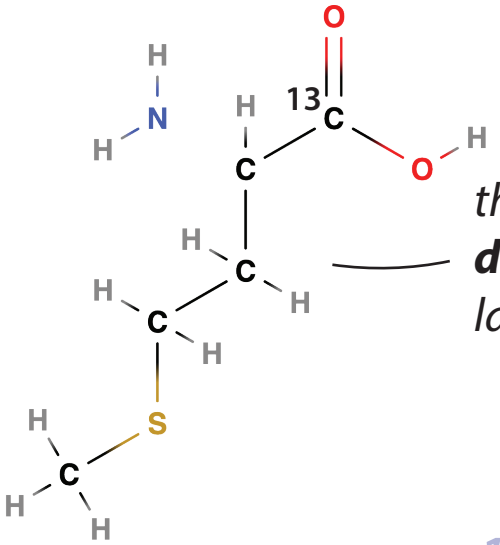
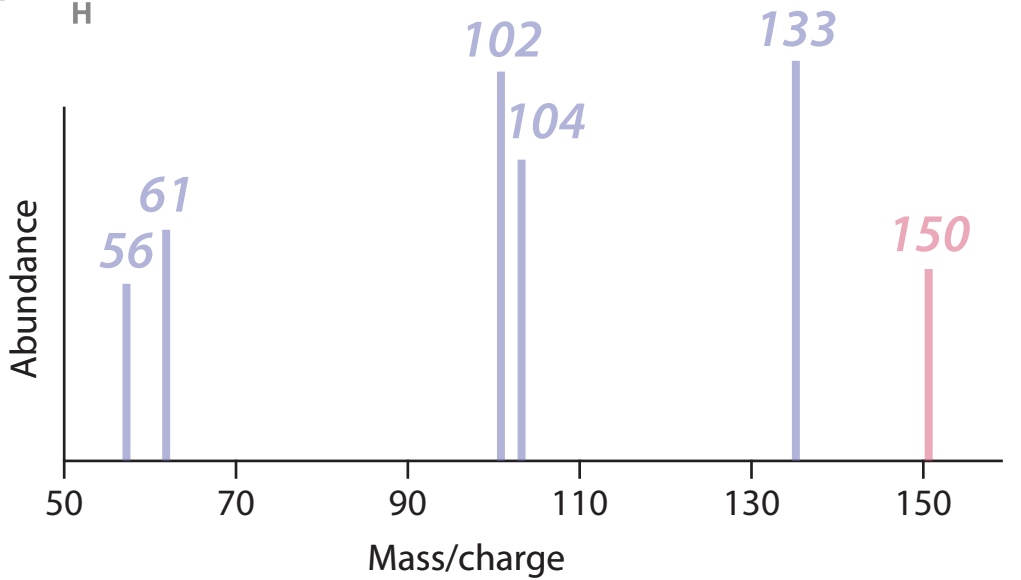
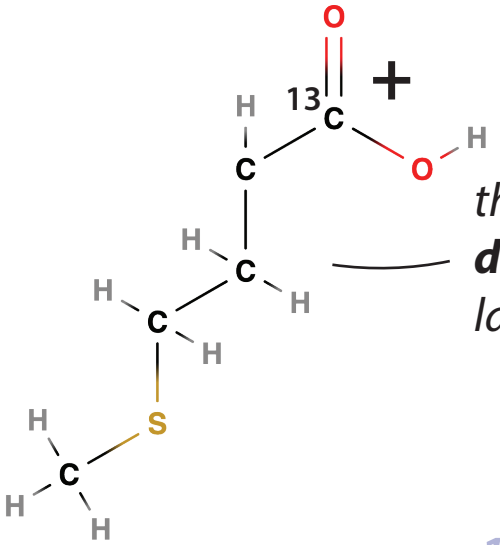
110
130
150
Mass/charge

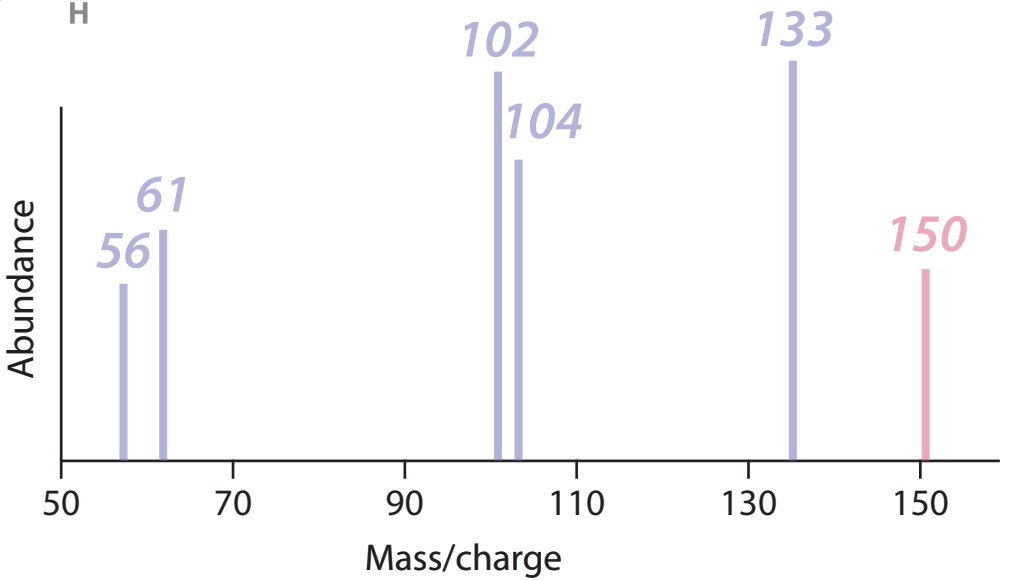


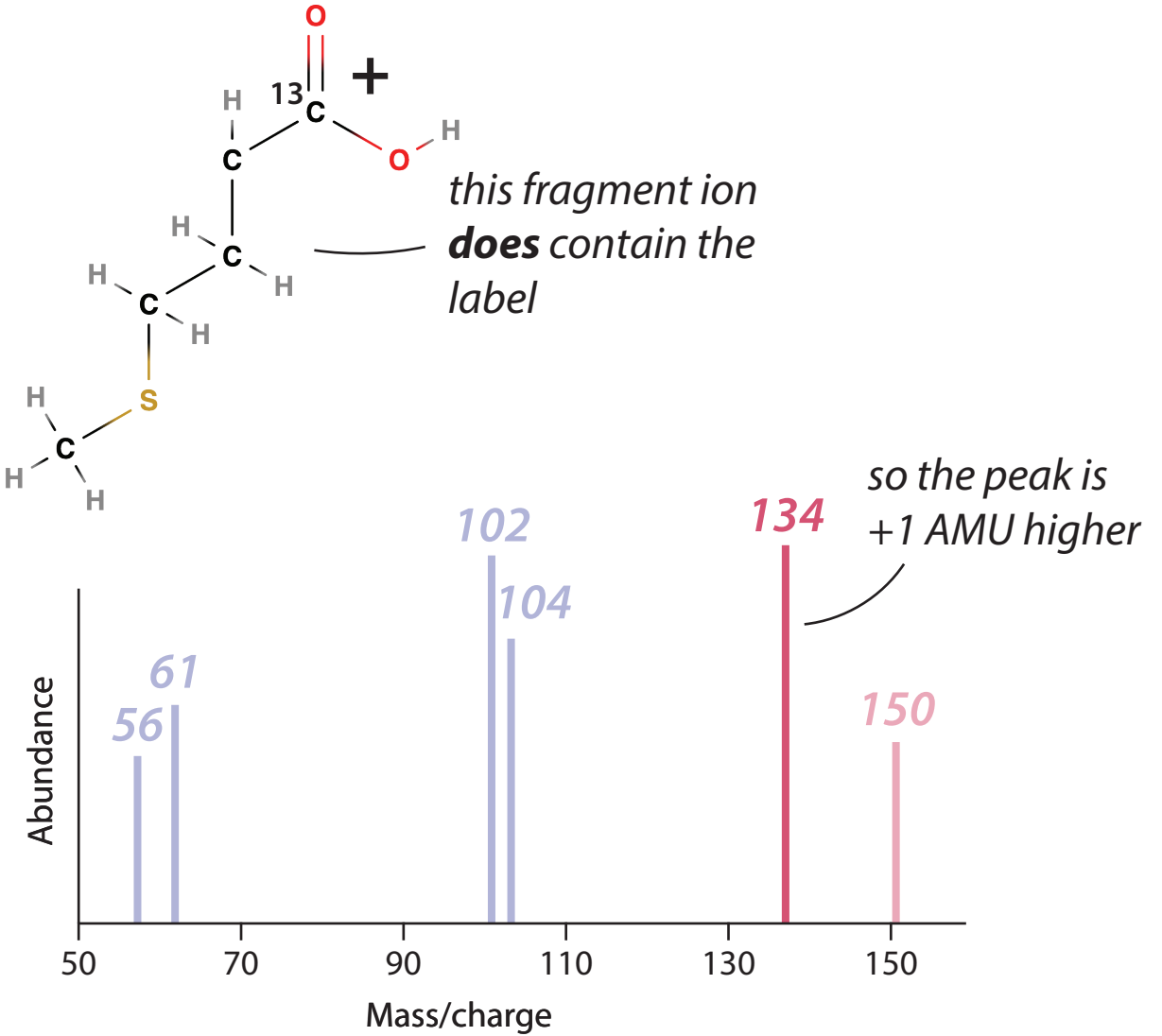
*this fragment ion **does** contain the label*





*this fragment ion **does** contain the label*




O
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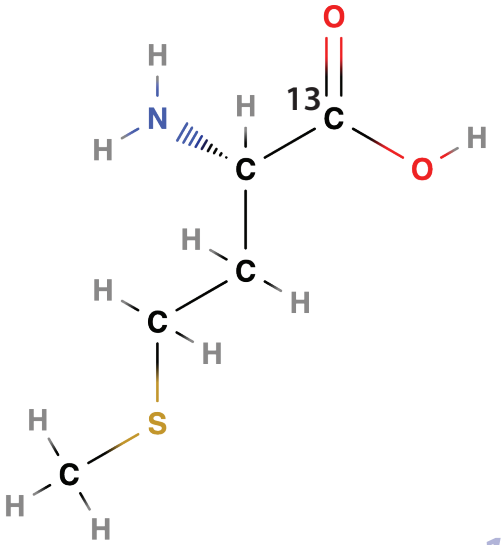
H
this fragment ion
does contain the
label
so the peak is
+1 AMU higher
102
104
134
61
56
150
Abundance
50
70
90
110
130
150
Mass/charge


O
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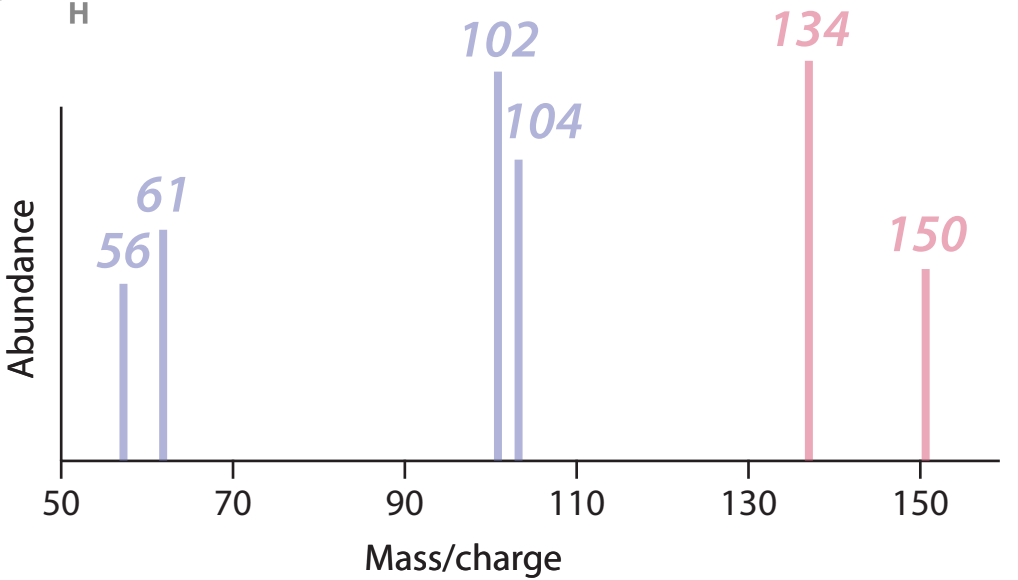
102
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Abundance
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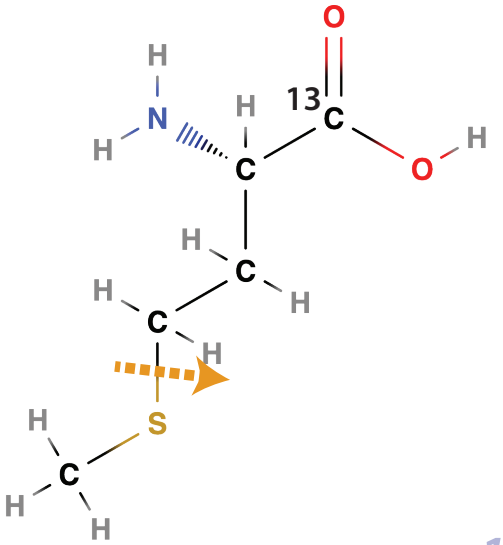
Mass/charge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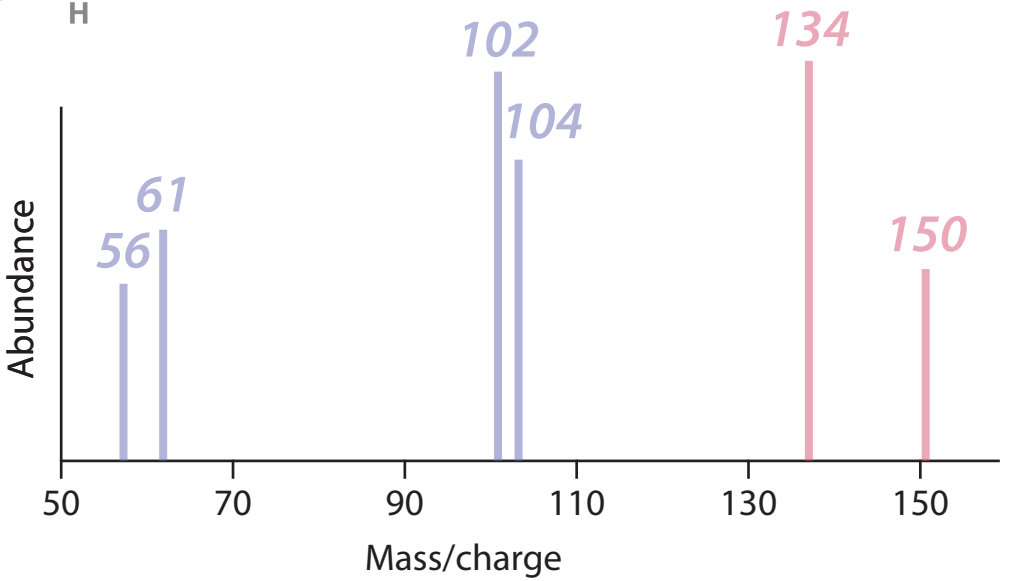
102
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Abundance
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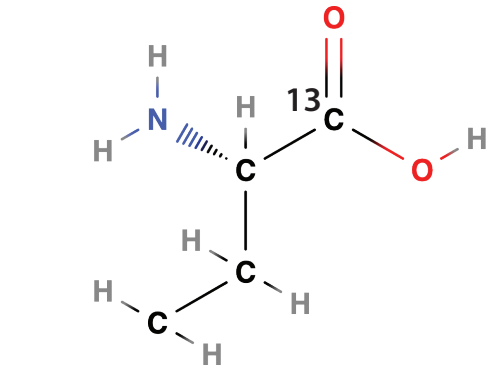
Mass/charge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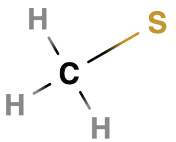
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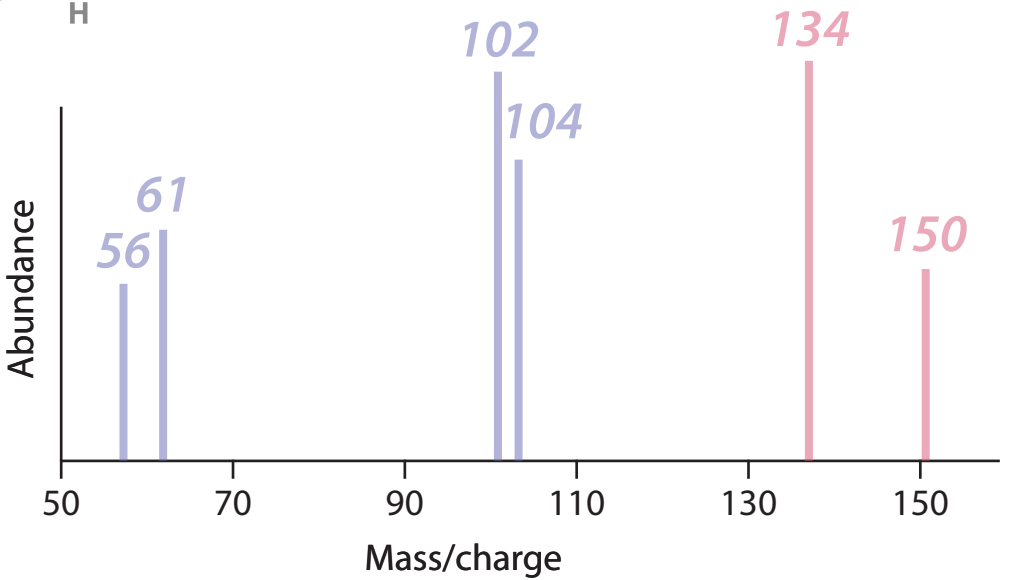
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Abundance
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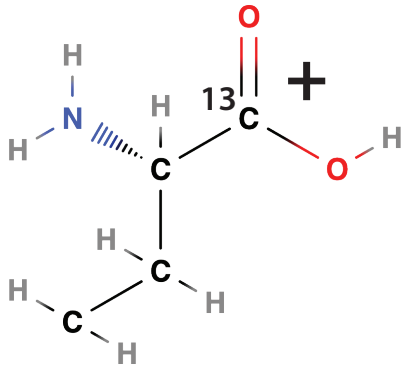
Mass/charge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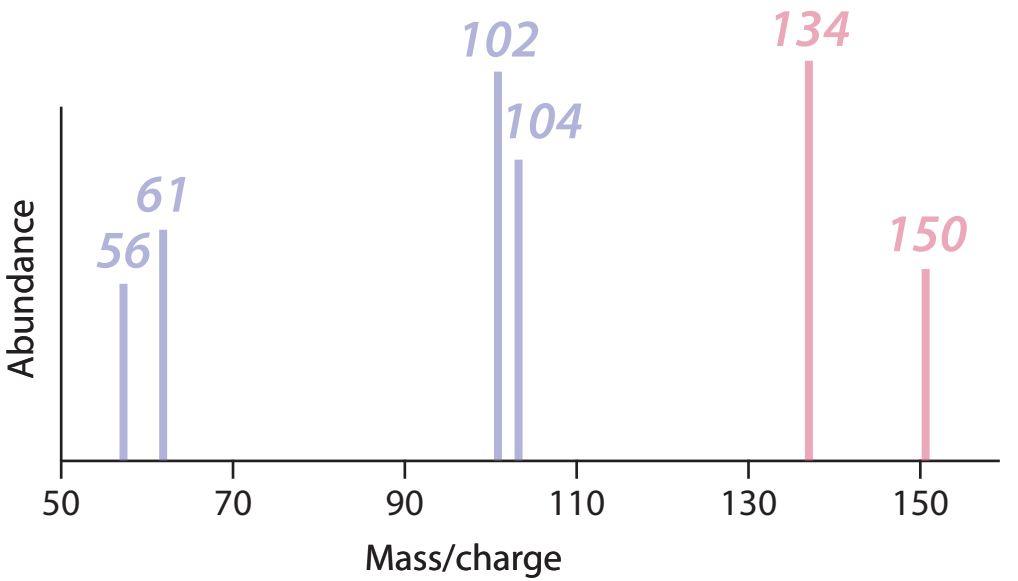
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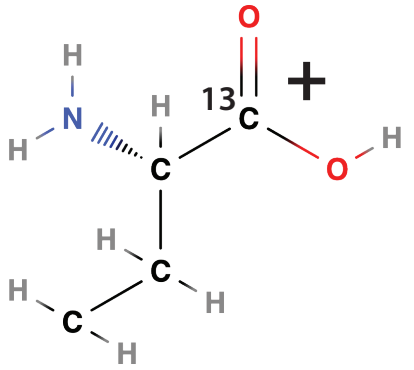
Mass/charge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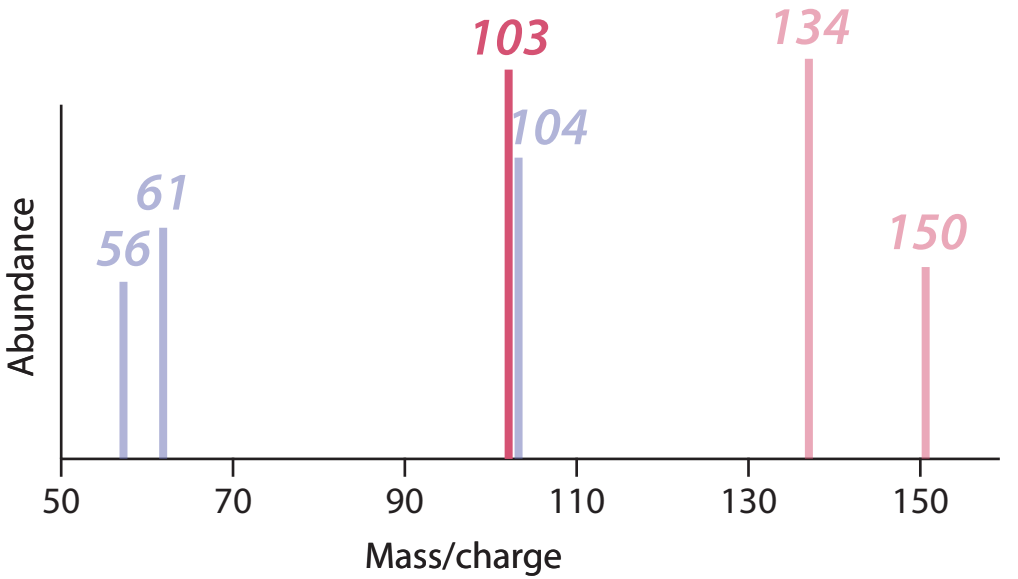
103
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Abundance
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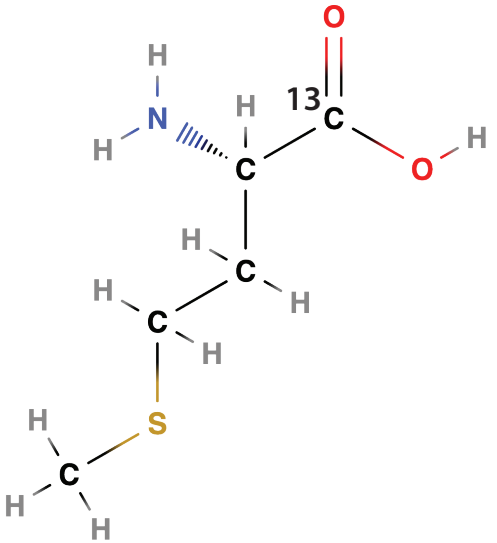
Mass/charge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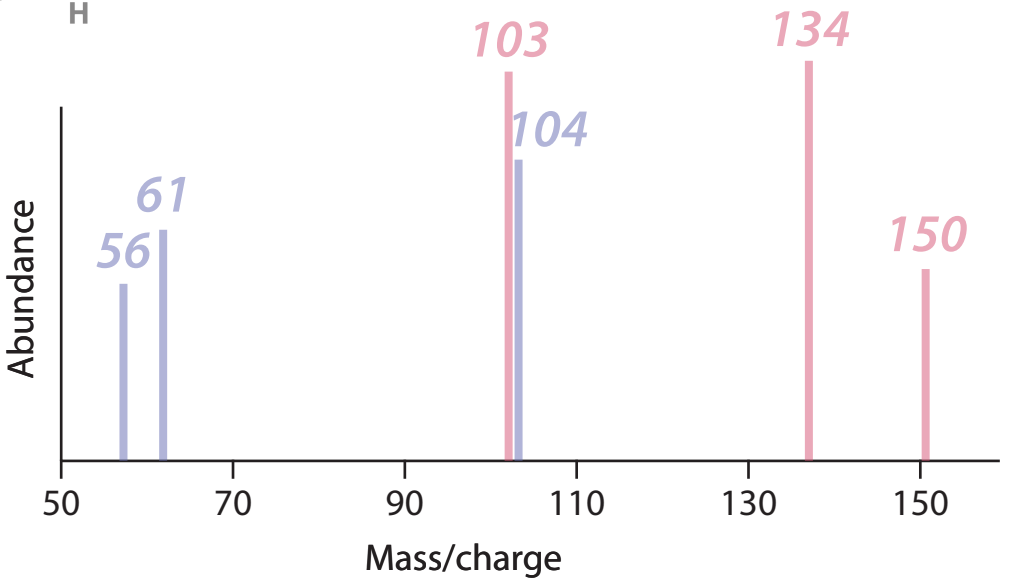
103
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Abundance
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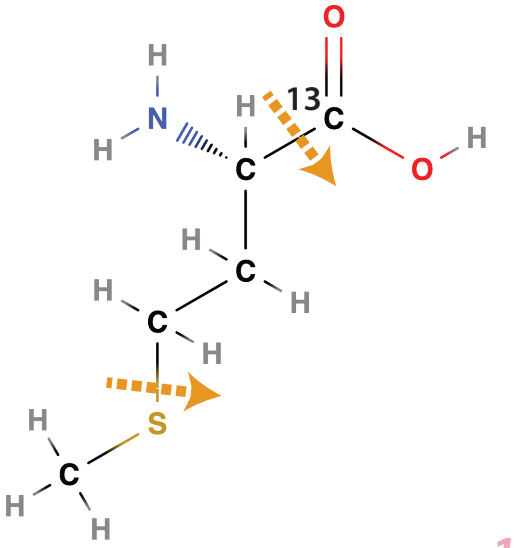
Mass/charge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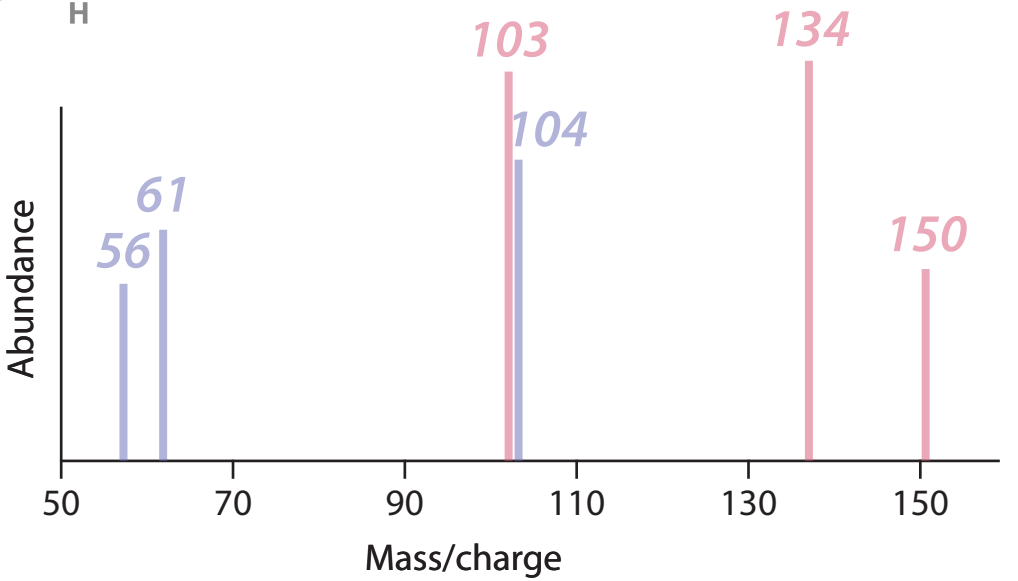
103
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Abundance
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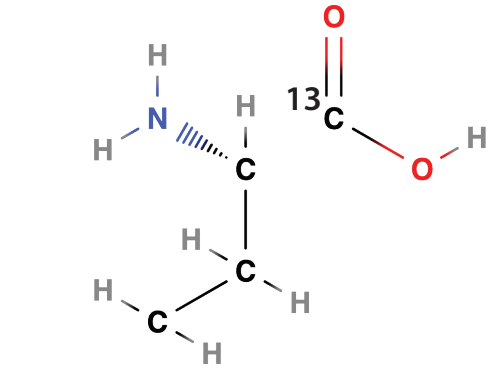
150
Mass/charge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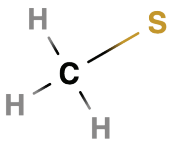
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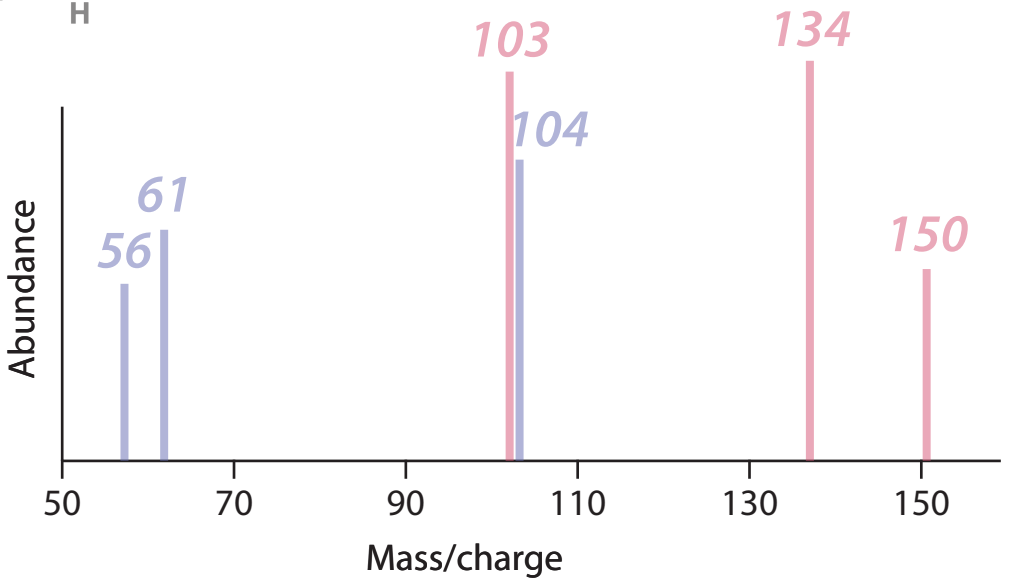
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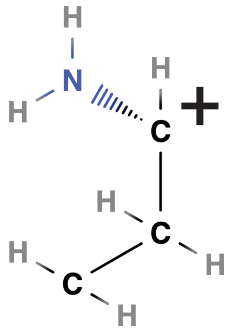
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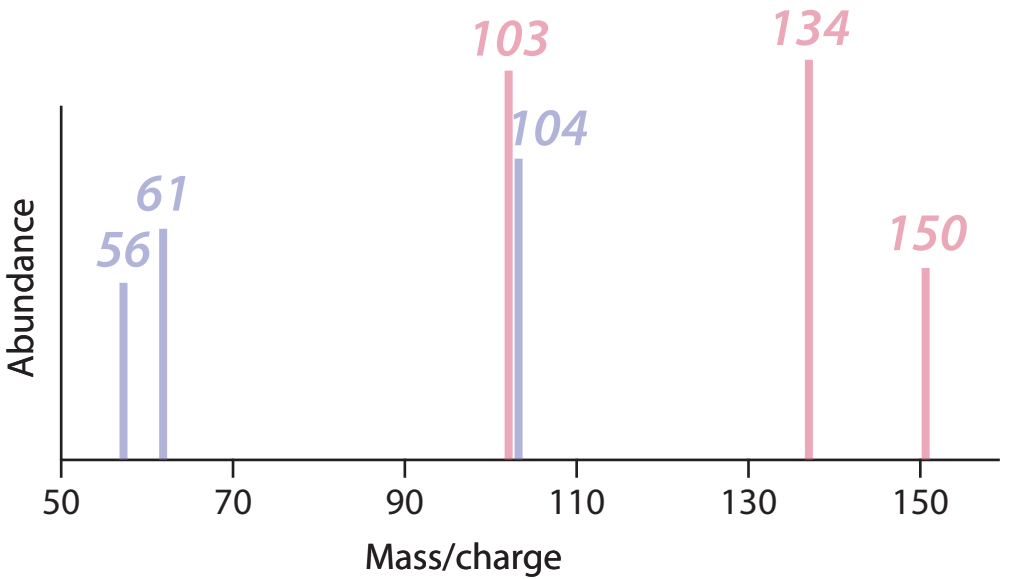
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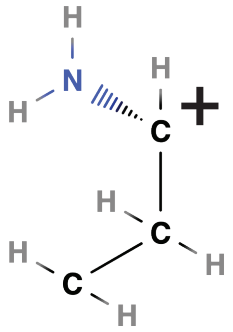
Mass/charge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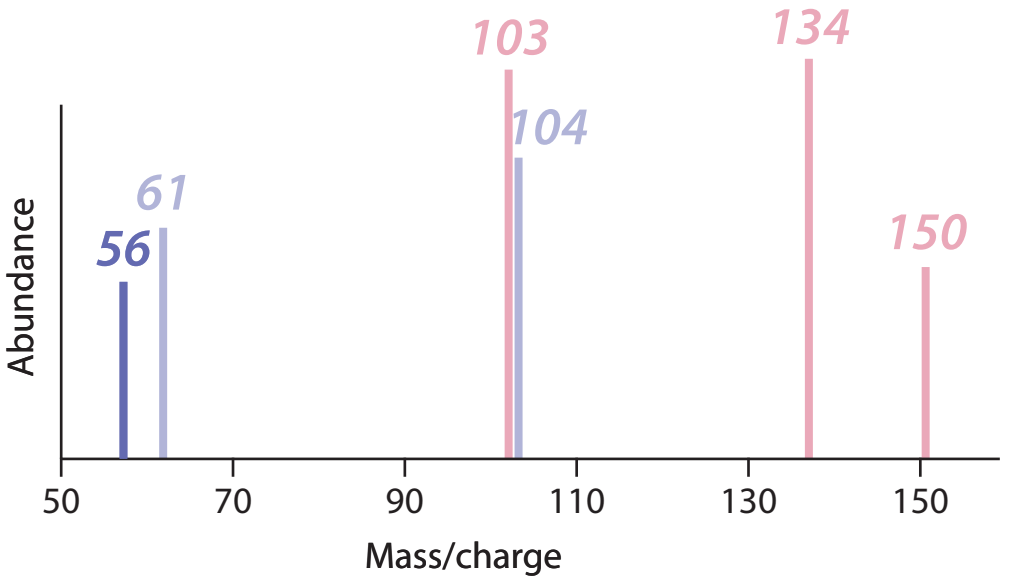
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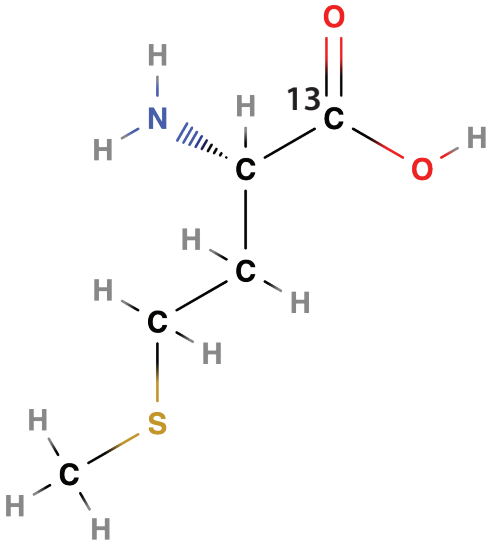
Mass/charge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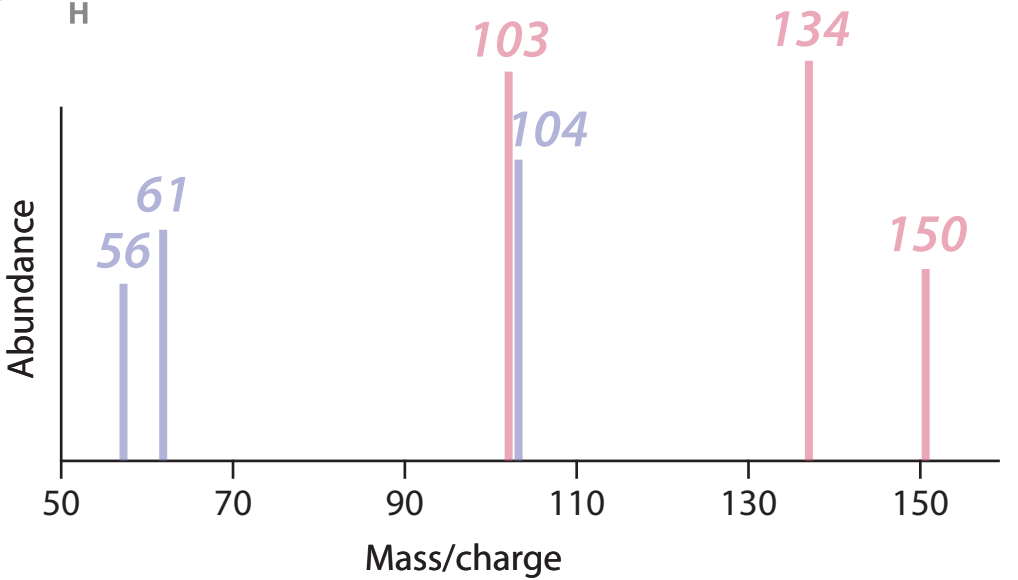
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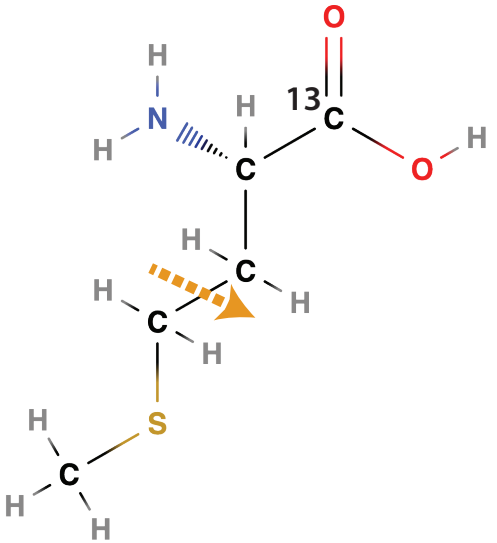
Mass/charge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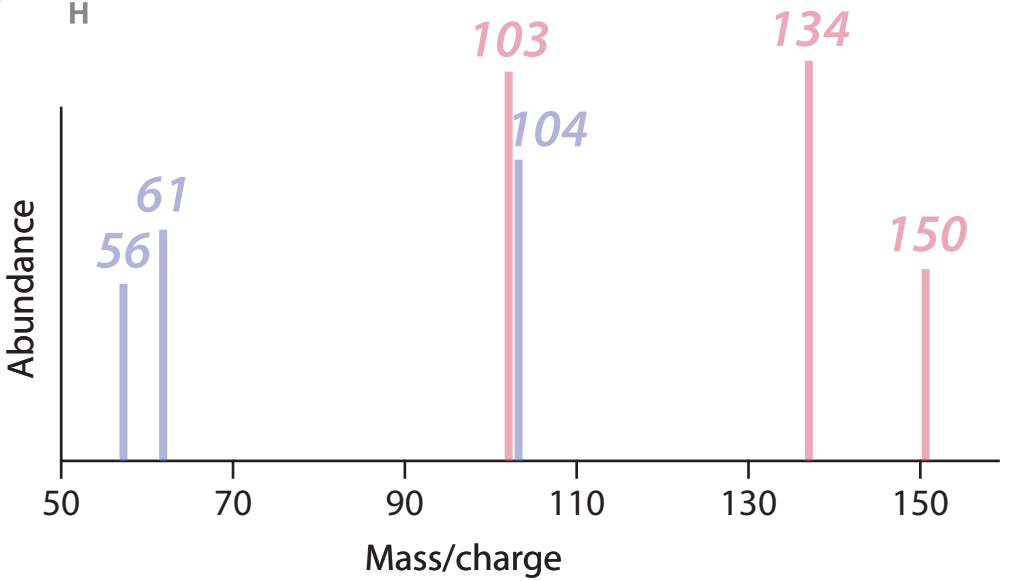
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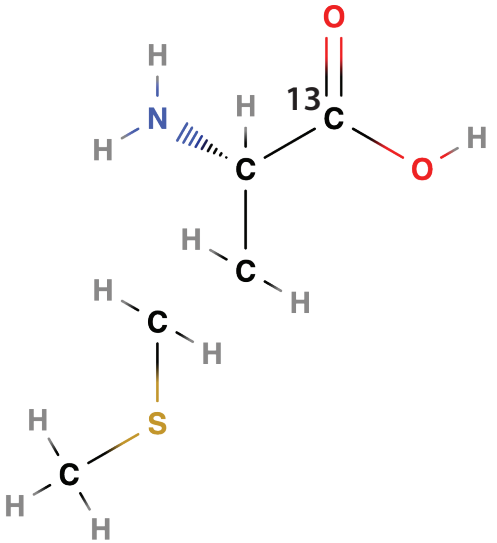
Mass/charge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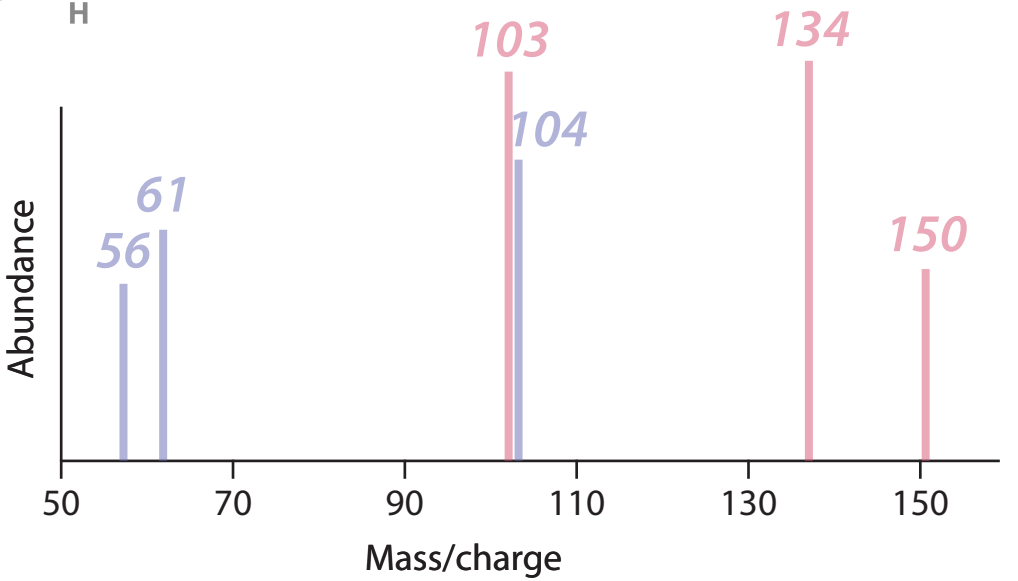
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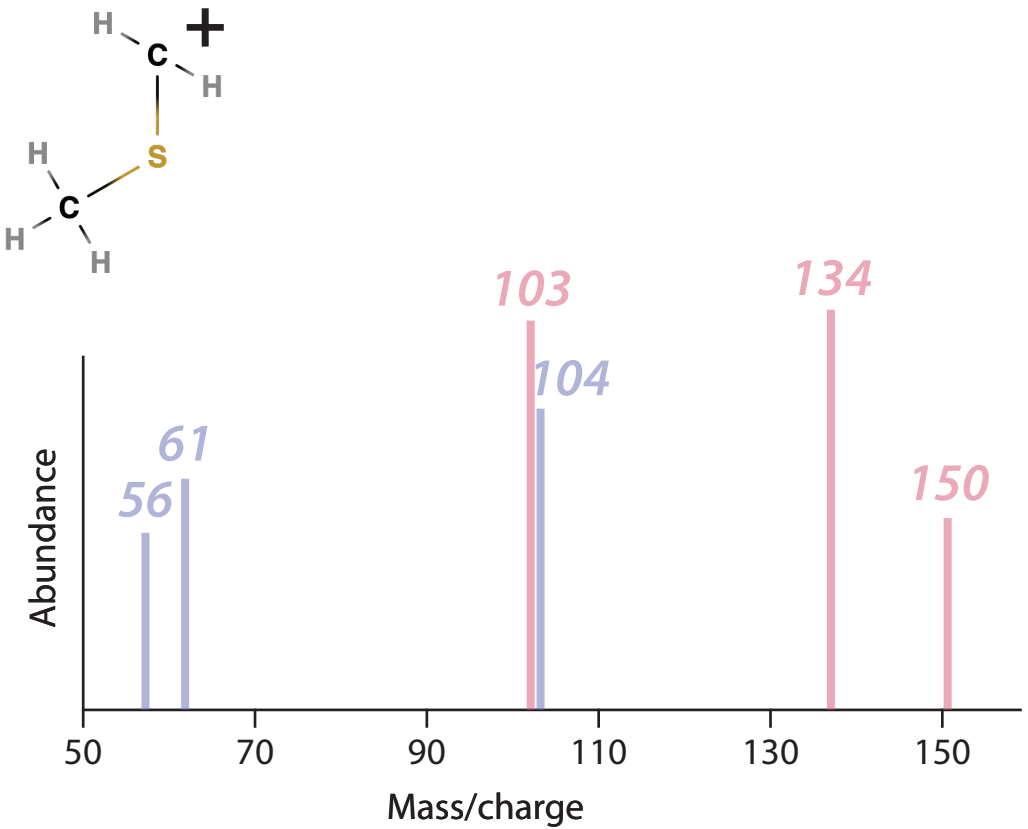
Mass/charge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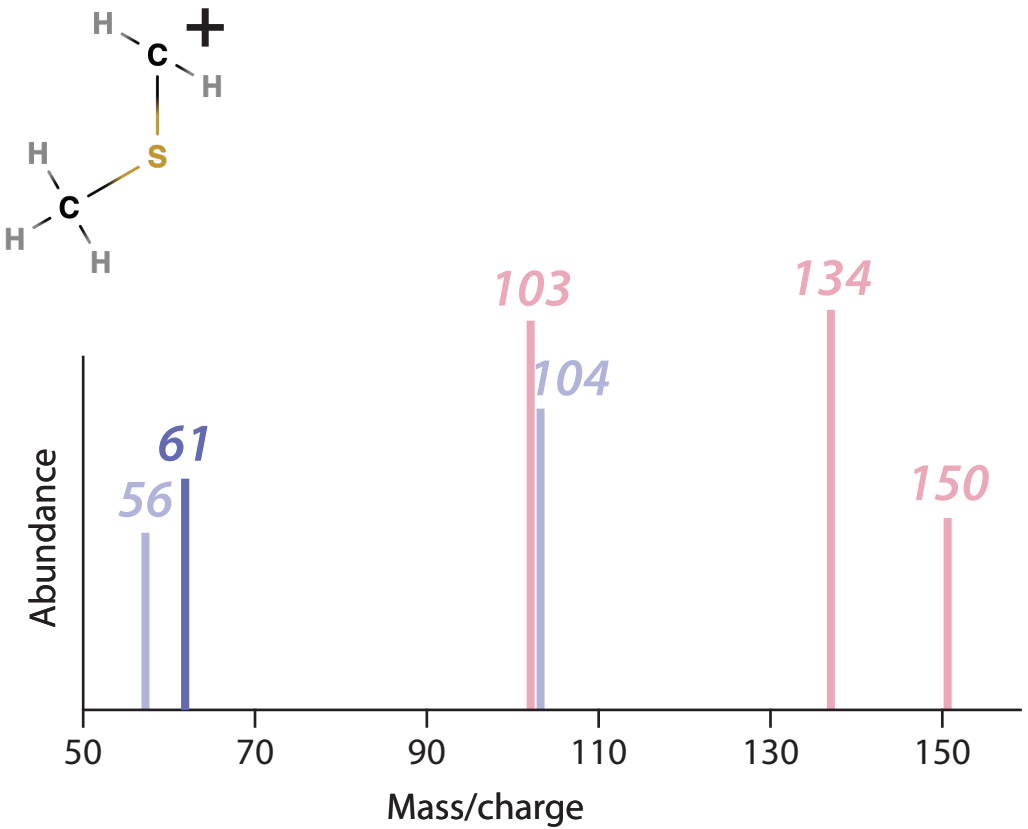
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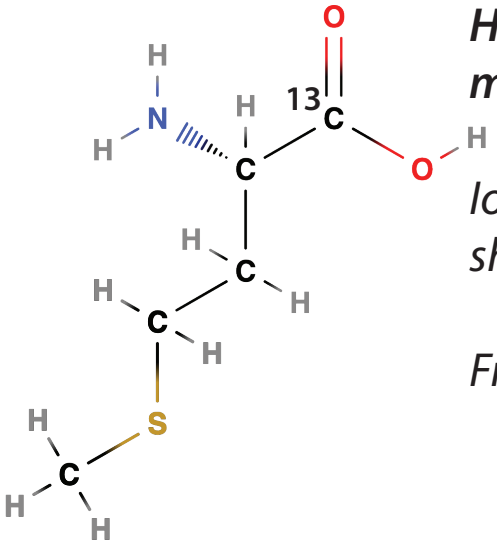
Mass/charge



How does a ^{13}C substitution change the methionine mass spectrum ?

Ion peaks that contain the substitution are shifted (red).

Fragment ions that do not are not (blue).