

Negative Ion MS/MS Analysis of Drug-Like Compounds

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Research

Background

Rules For EI

- cleavage α to heteroatoms
- aromatic ions (77, 91, ...)
- alkyl cleavage (43, 57, 71...)
- re-arrangements (McLafferty, retro Diels-Alder)

• ***ODD*** \rightarrow ***EVEN ELECTRON RULE***

Rules for ESI

EVEN ELECTRON

Rules for ESI

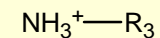
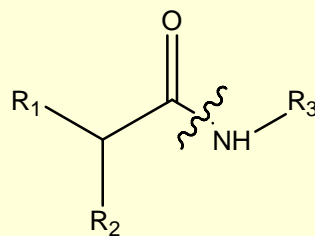
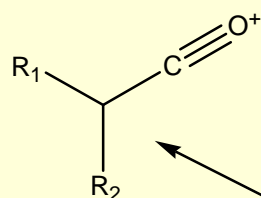
EVEN ELECTRON

- Mostly peptide chemistry
 - b and y'' ions

Rules for ESI

EVEN ELECTRON

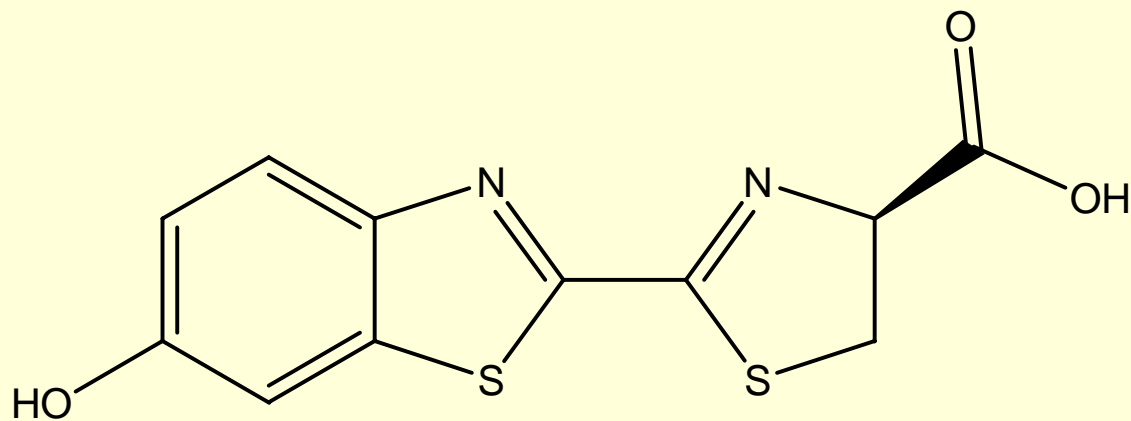
- Mostly peptide chemistry
 - b and y'' ions



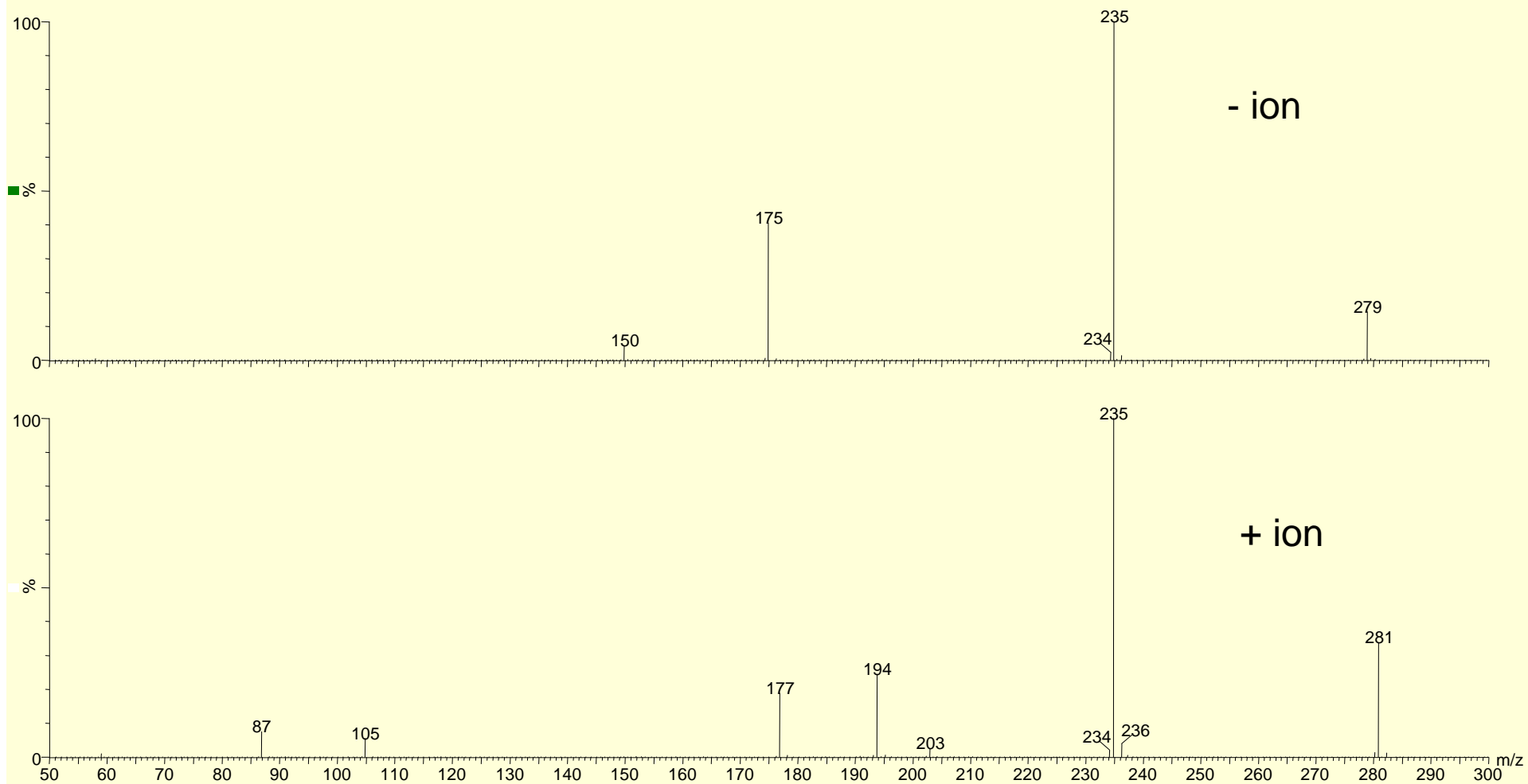
Compounds Analyzed

1. Firefly luciferin
2. Piroxicam
3. Cephalexin
4. Terfenadine
5. Bendroflumethiazide

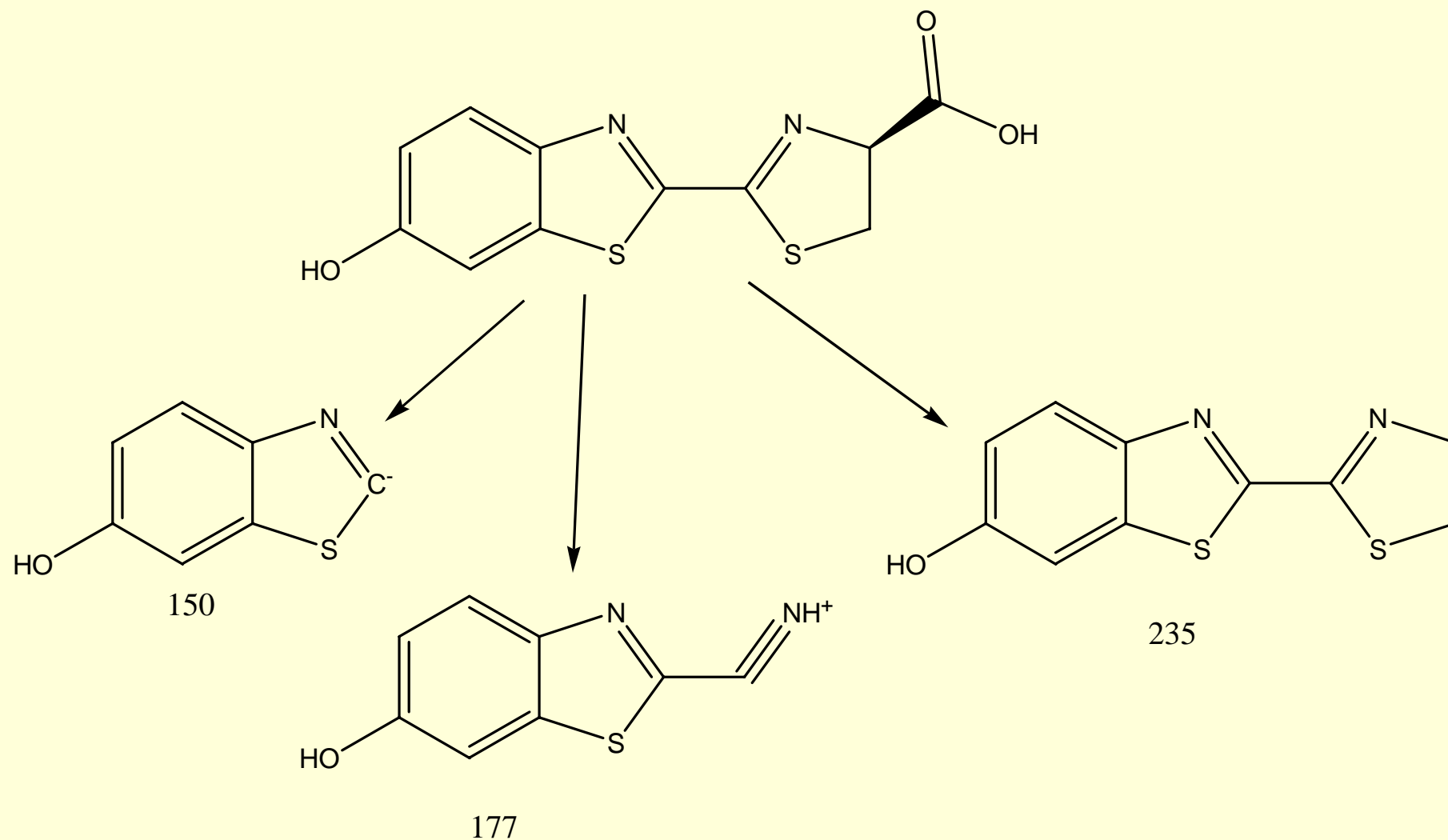
Structure of Luciferin



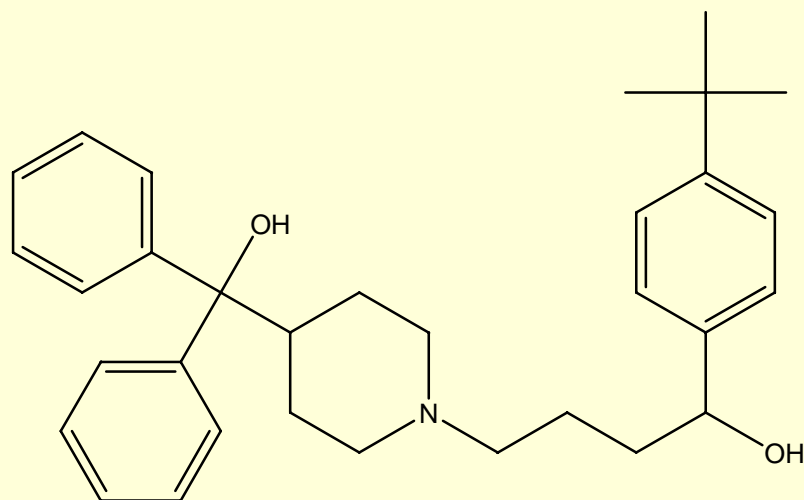
Luciferin



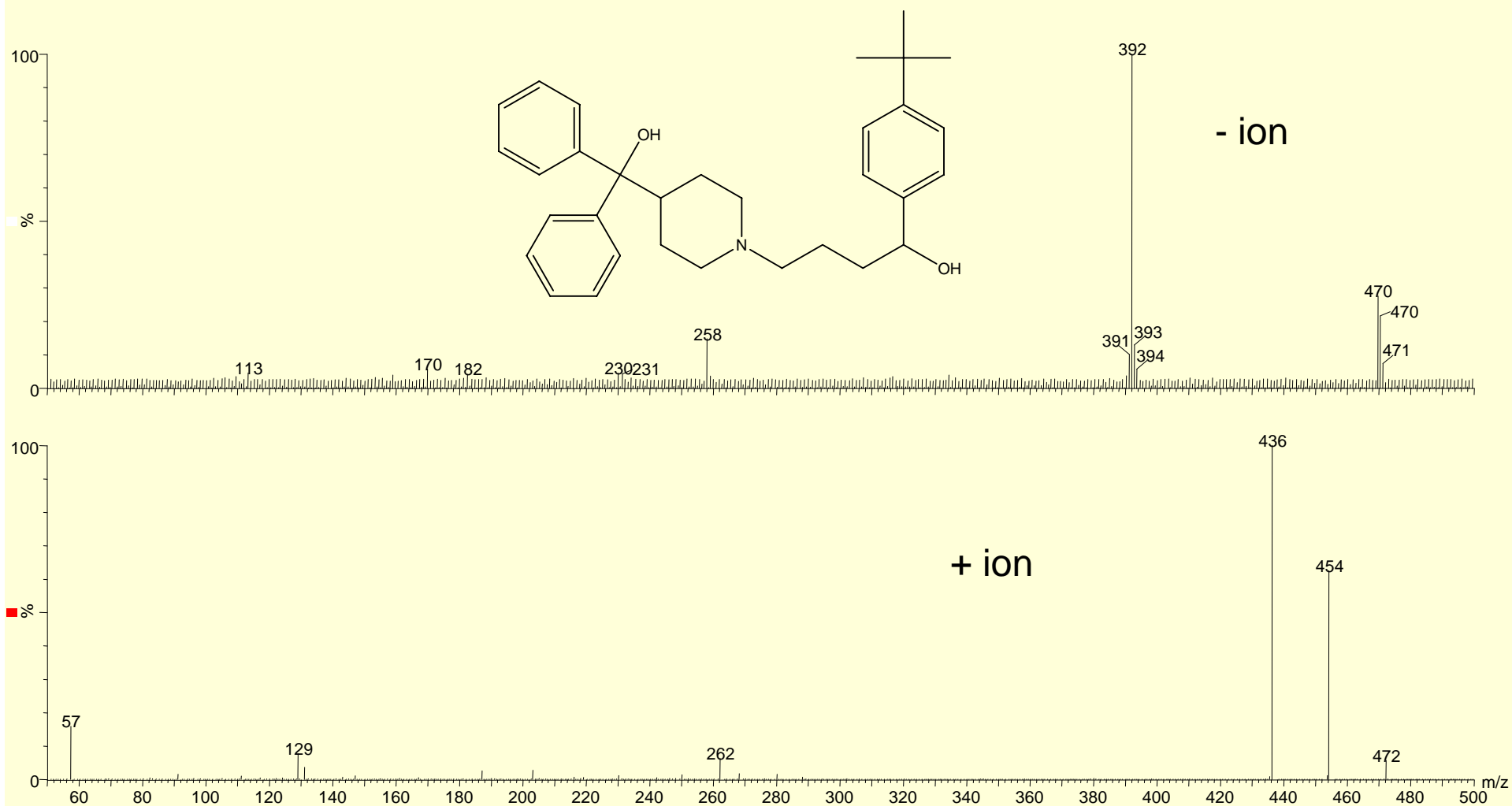
Fragmentation of Luciferin



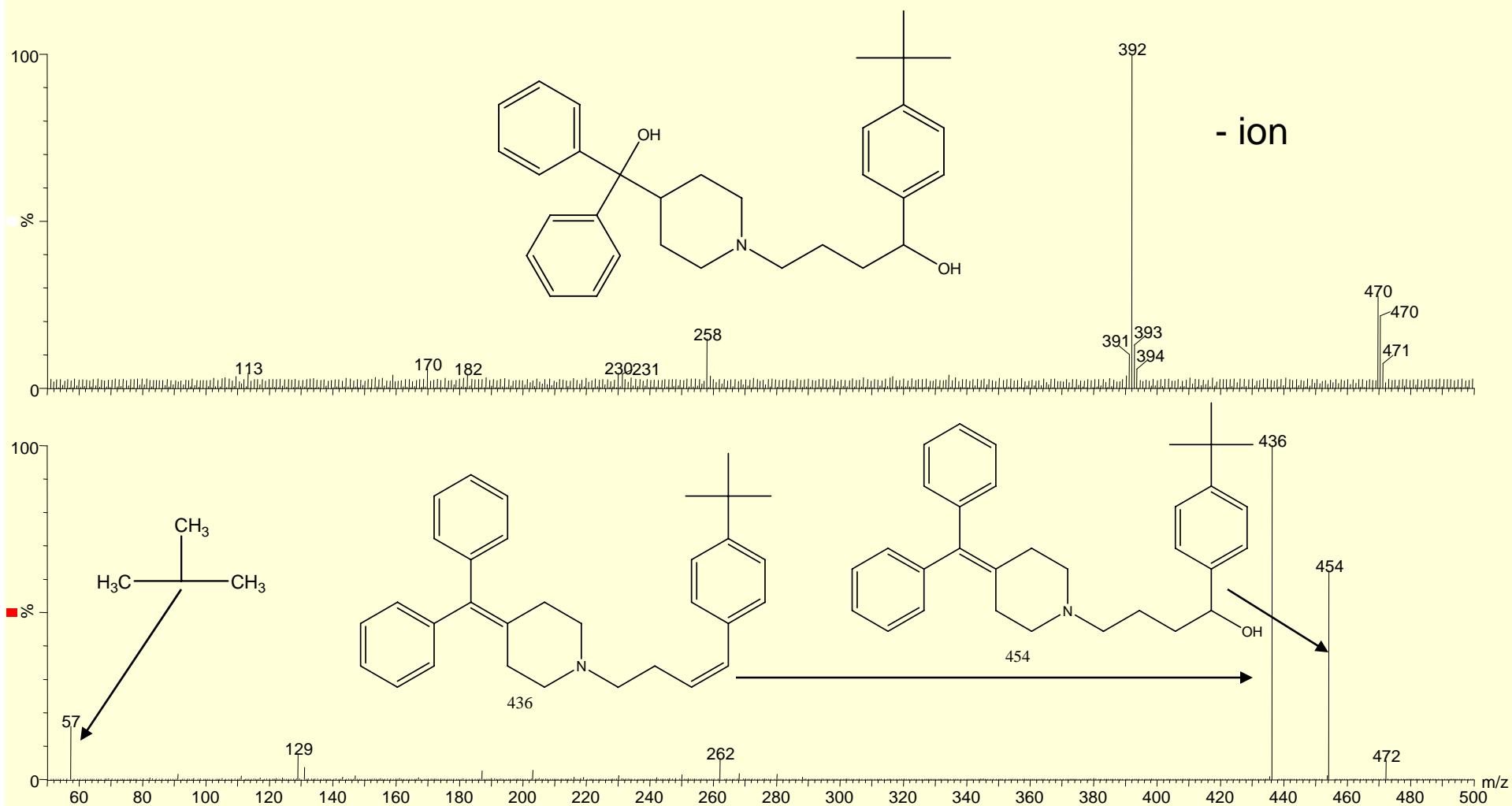
Terfenadine



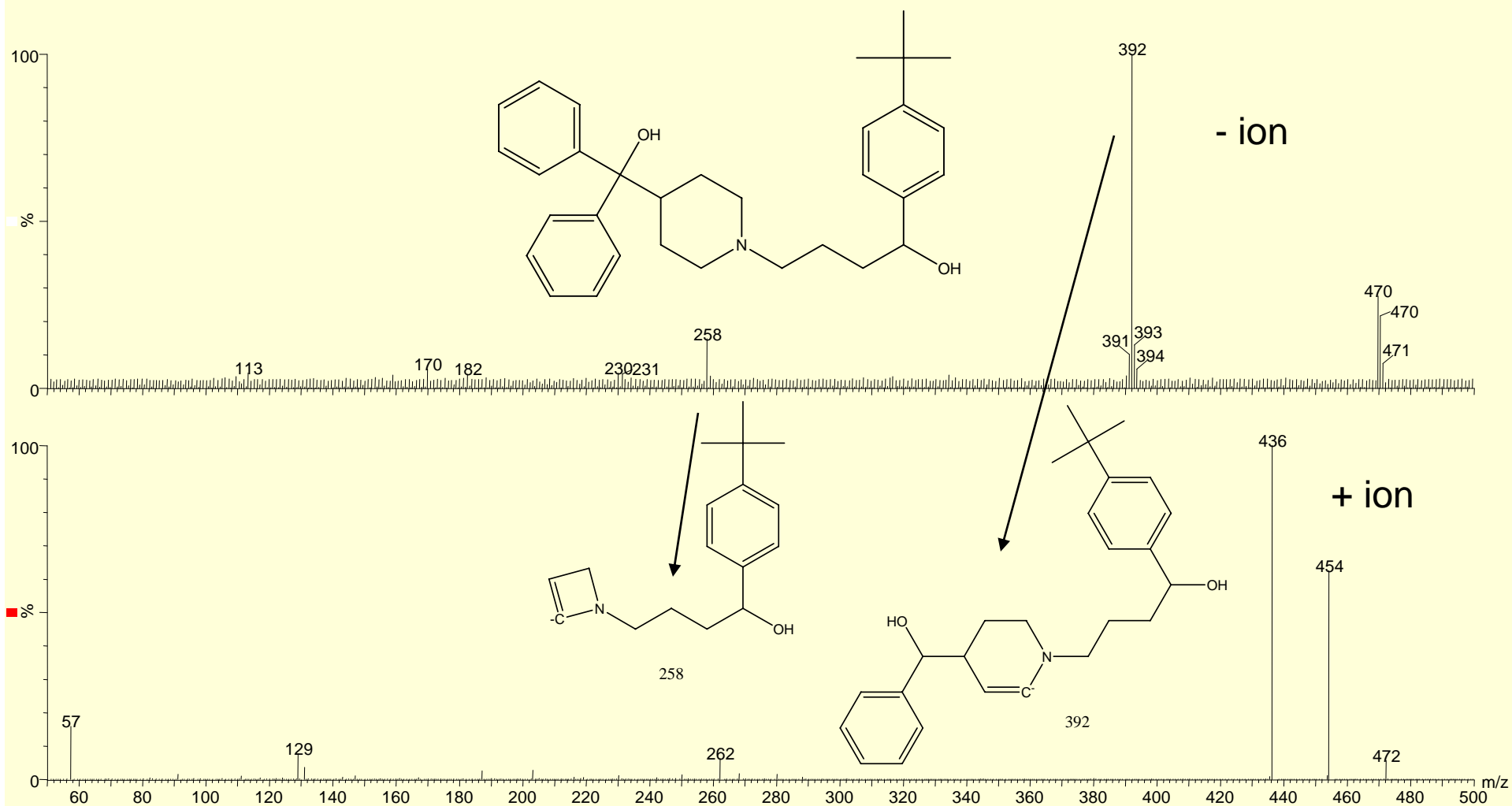
Terfenadine



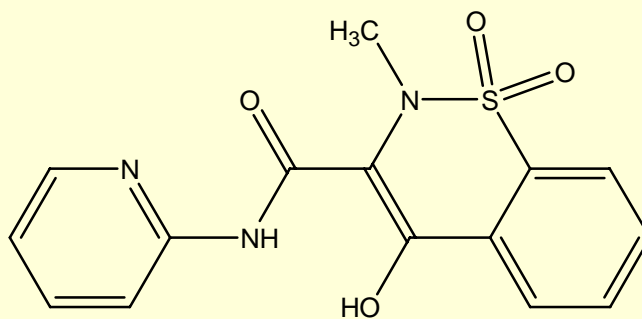
Terfenadine



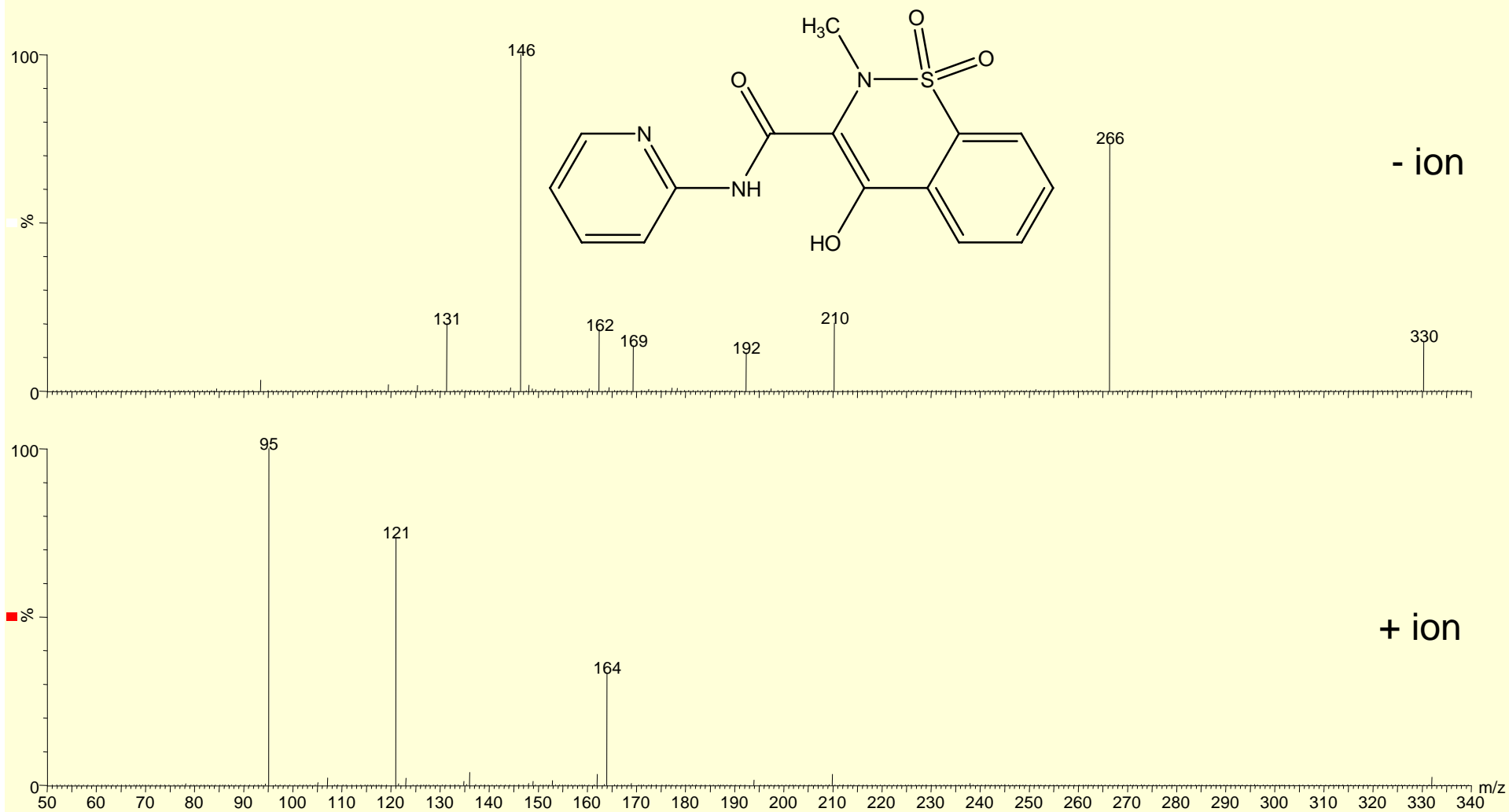
Terfenadine



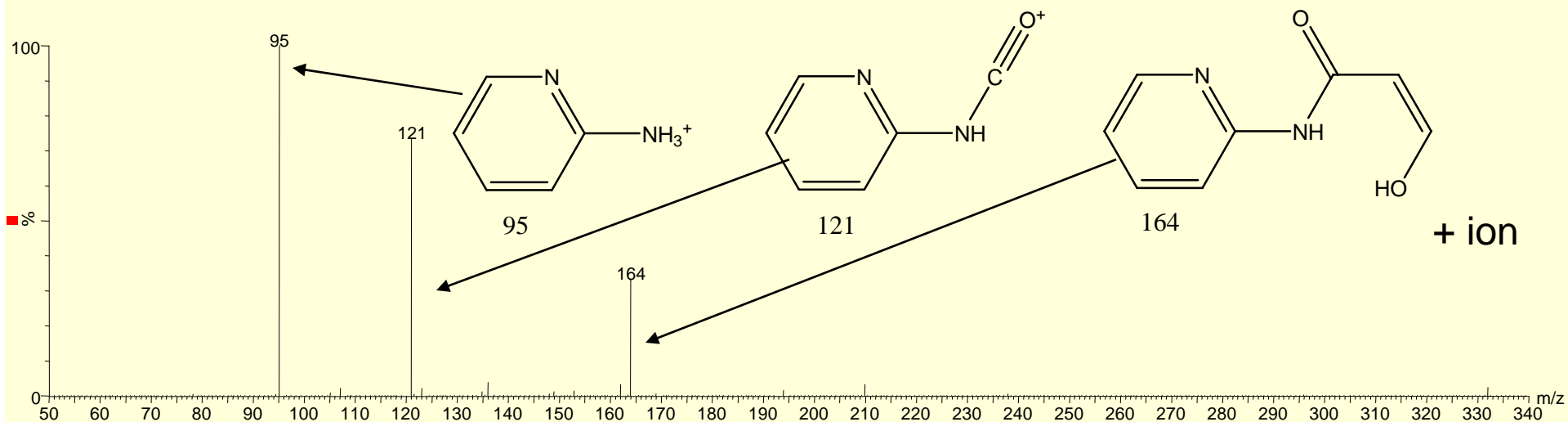
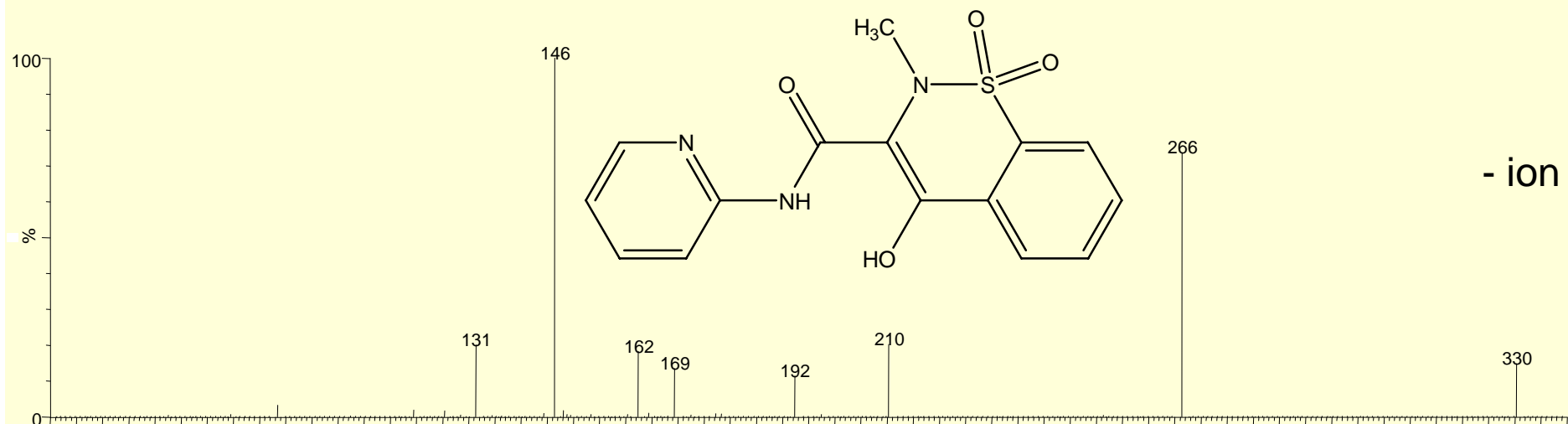
Piroxicam



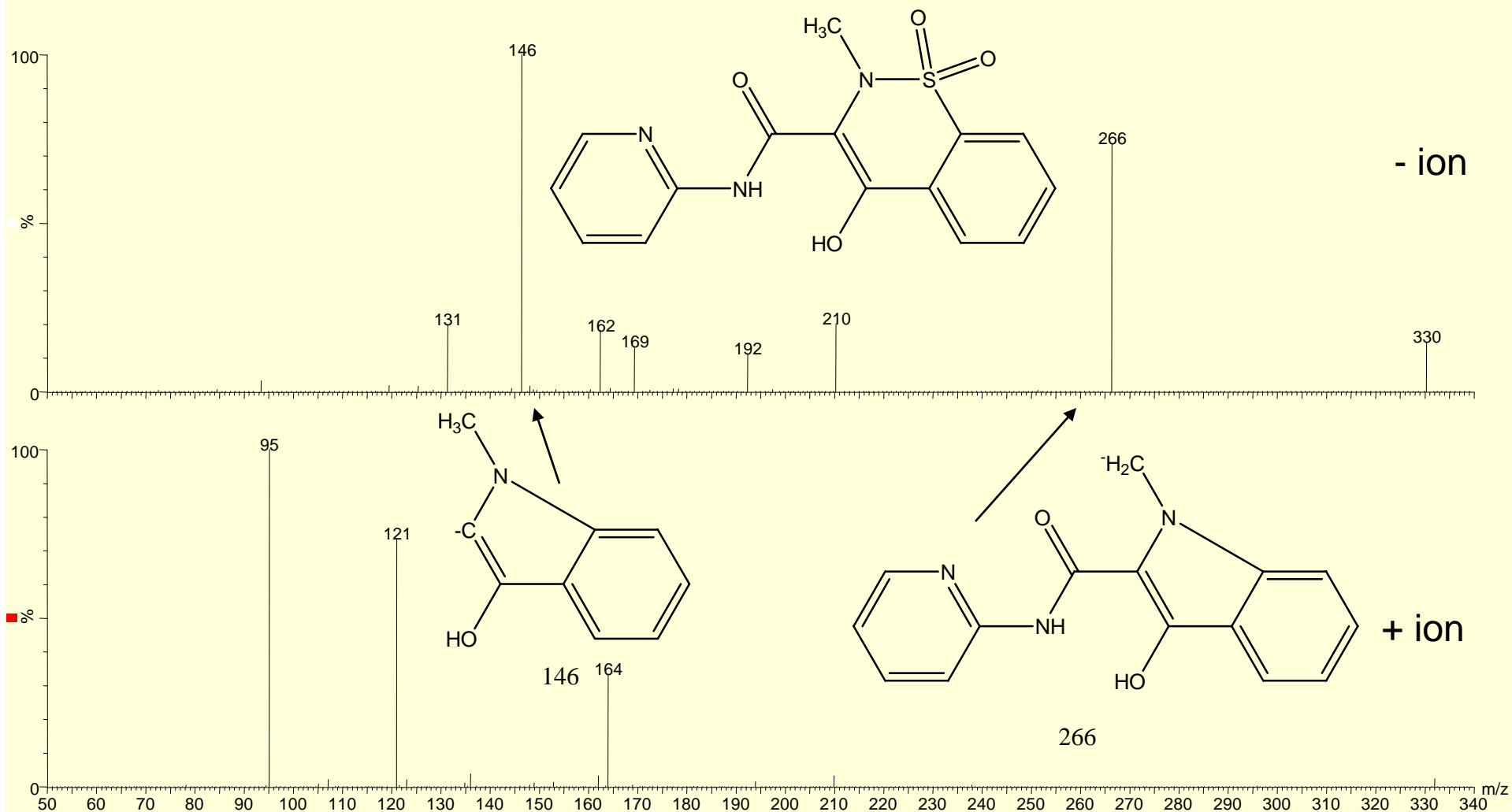
Piroxicam



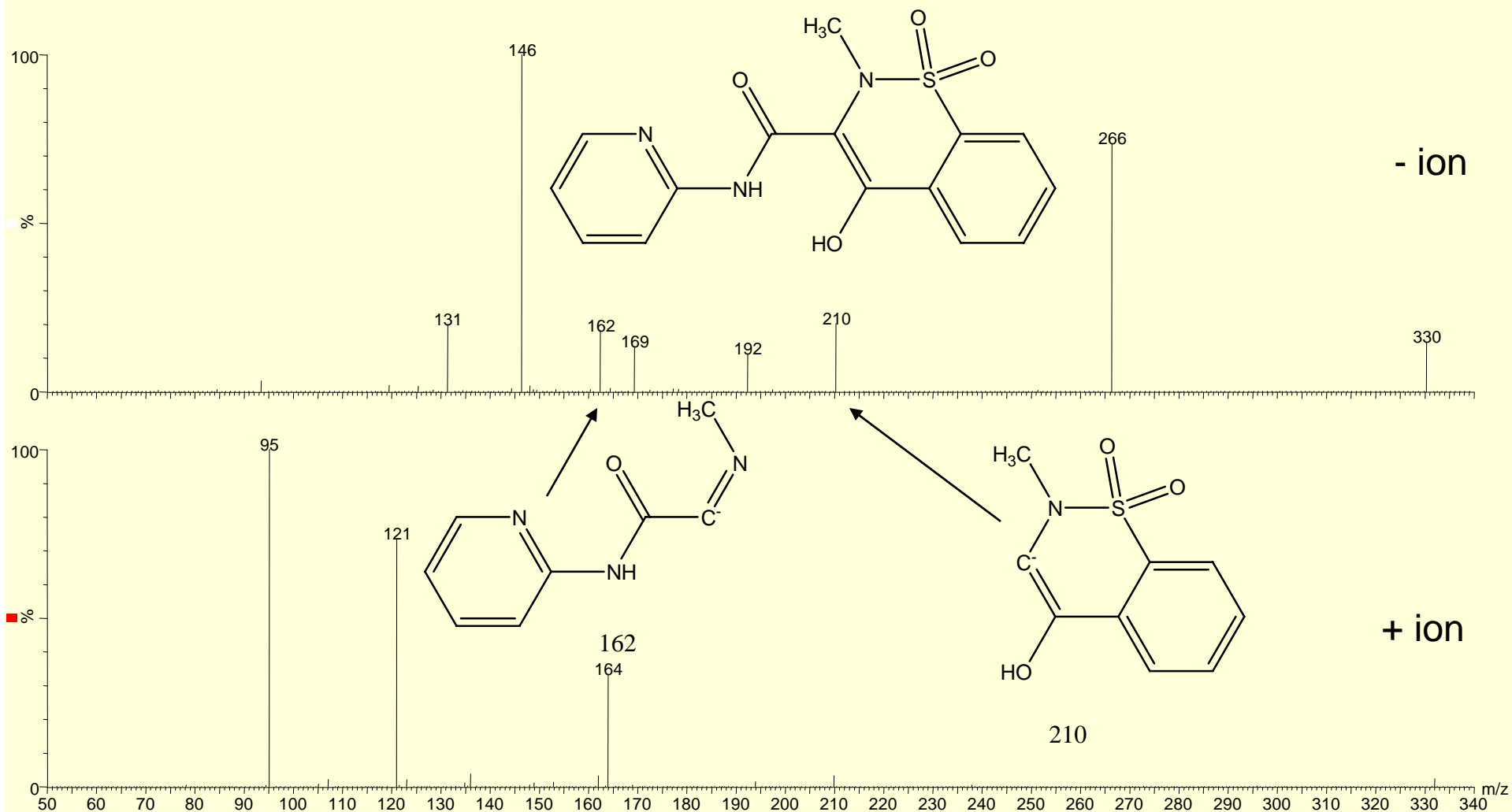
Piroxicam



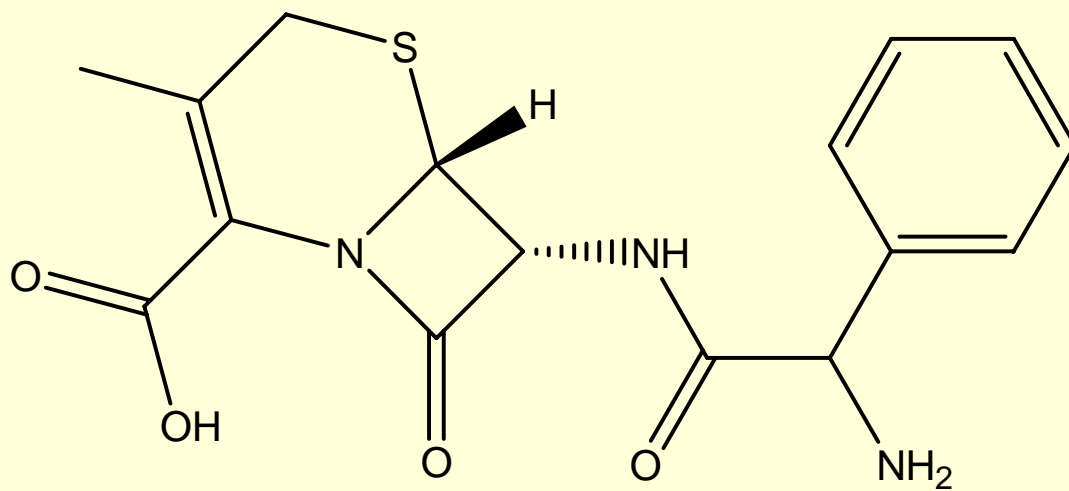
Piroxicam



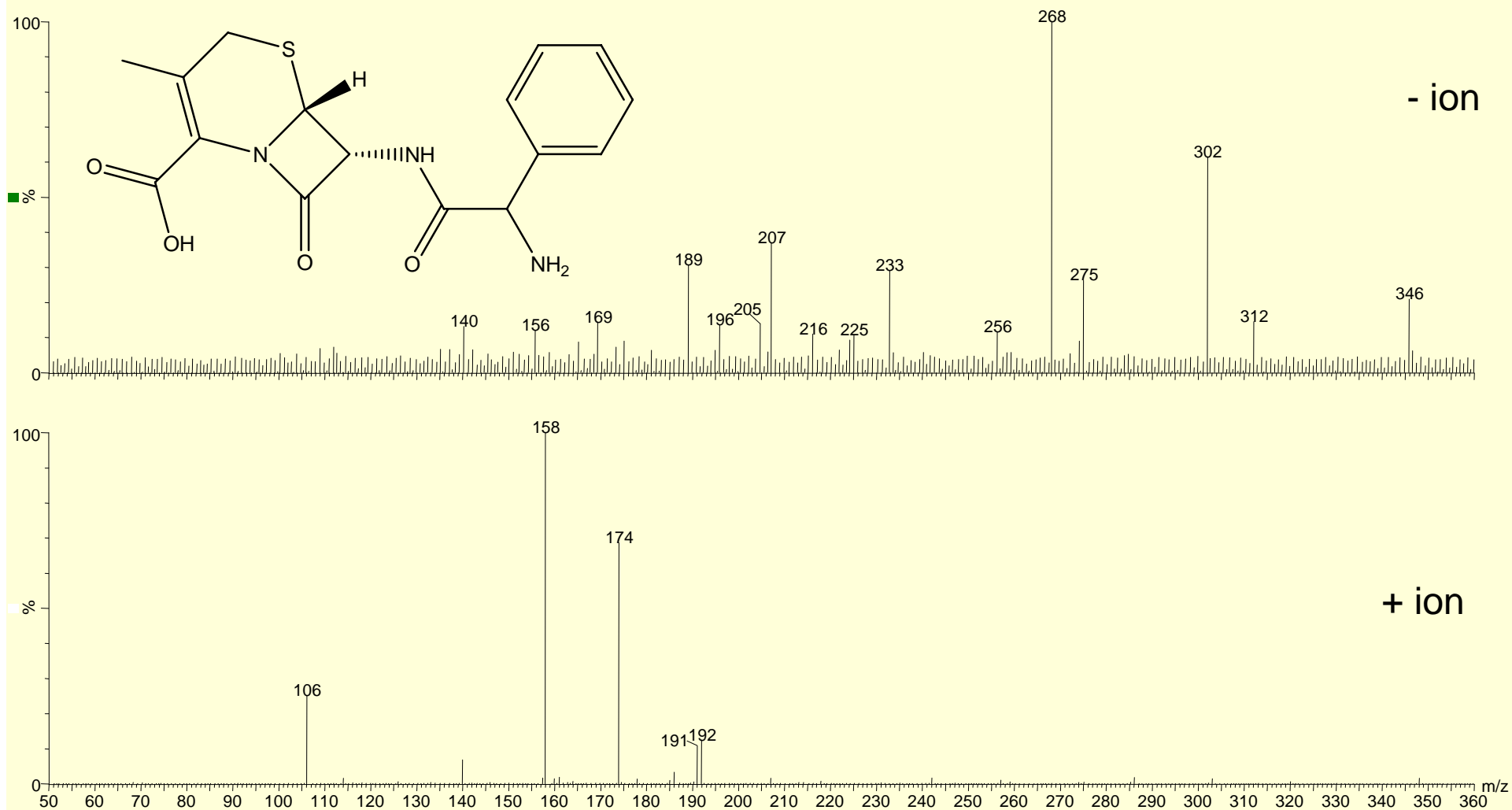
Piroxicam



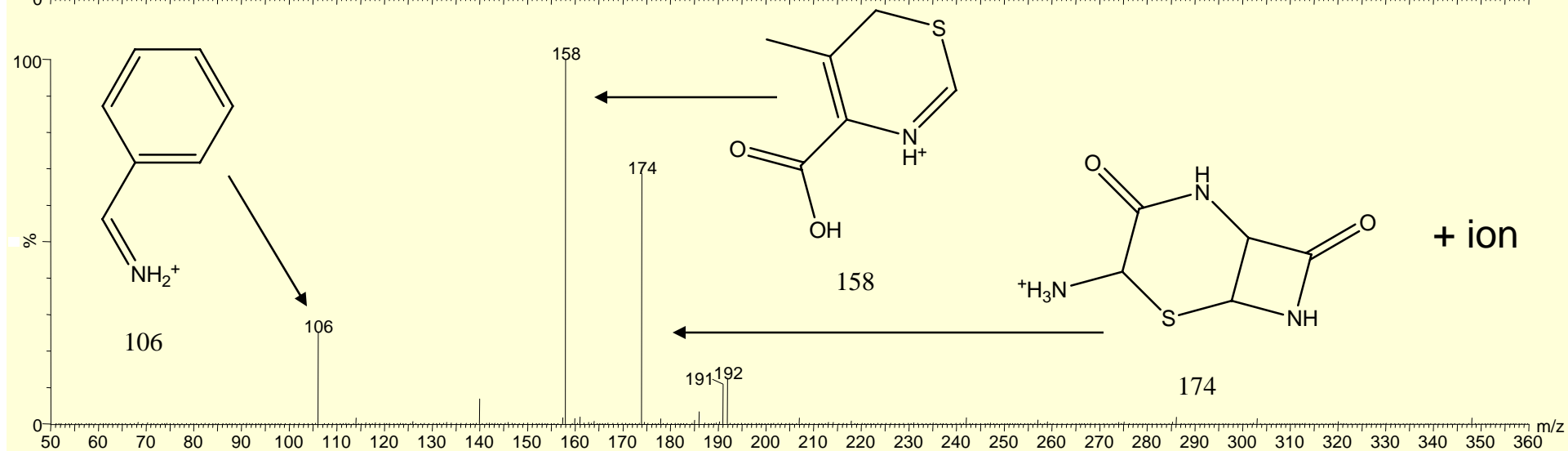
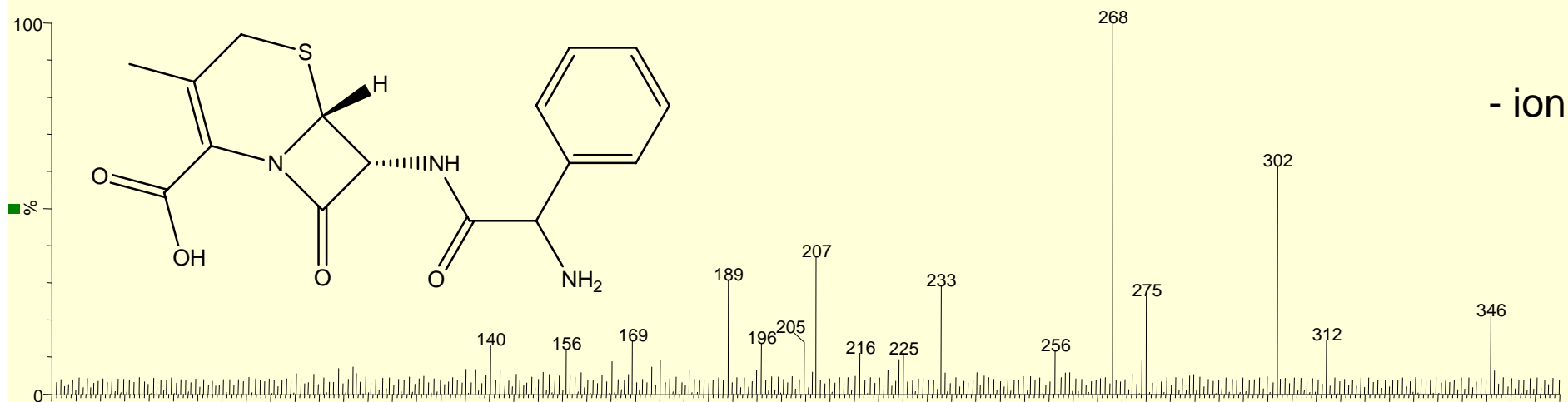
Cephalexin



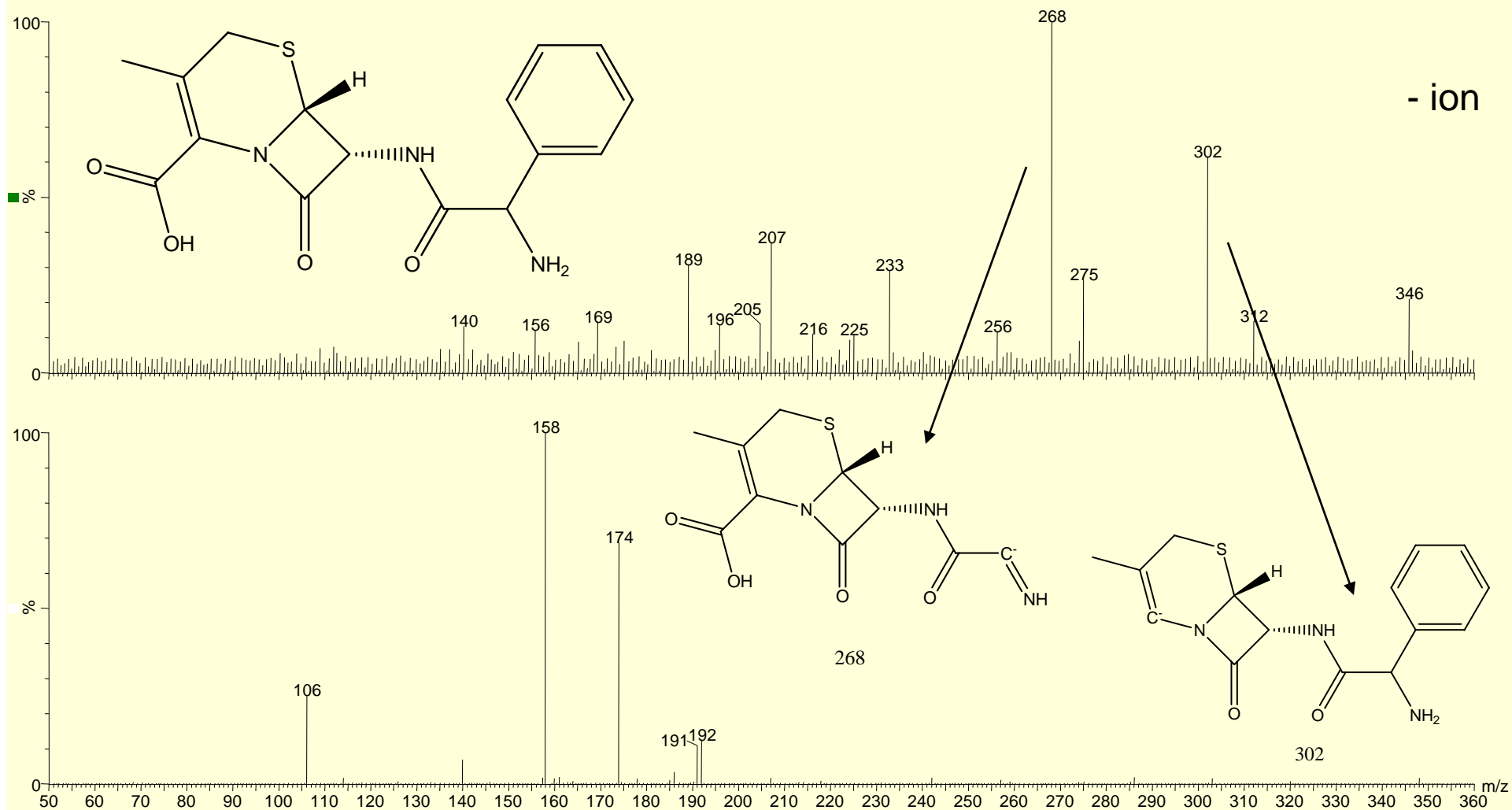
Cephalexin



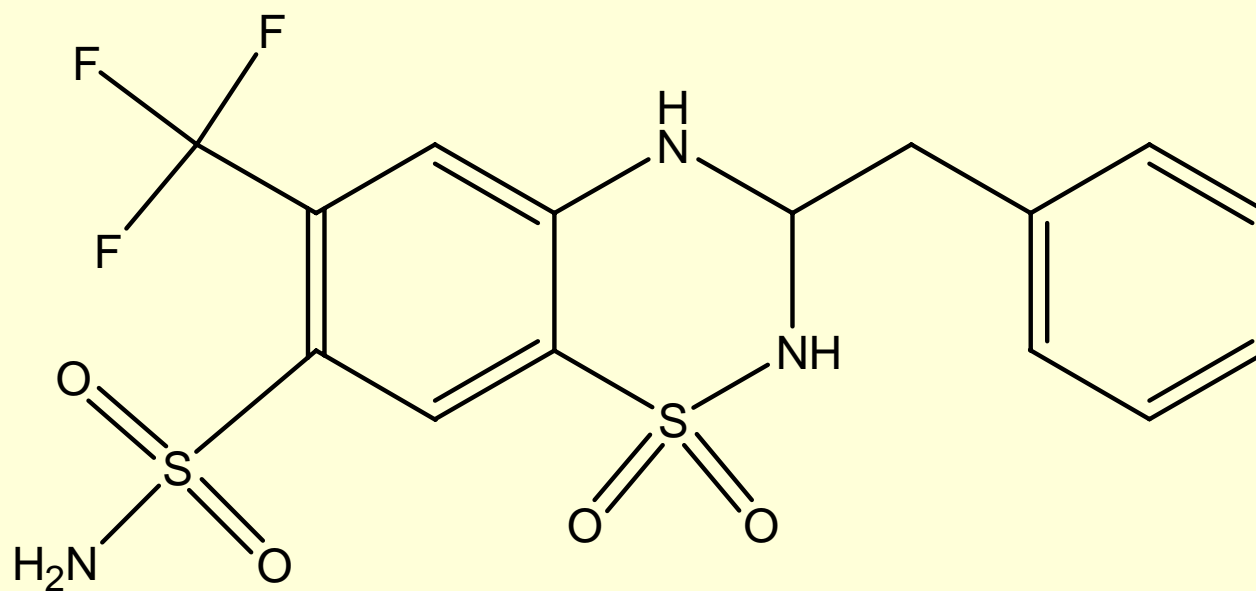
Cephalexin



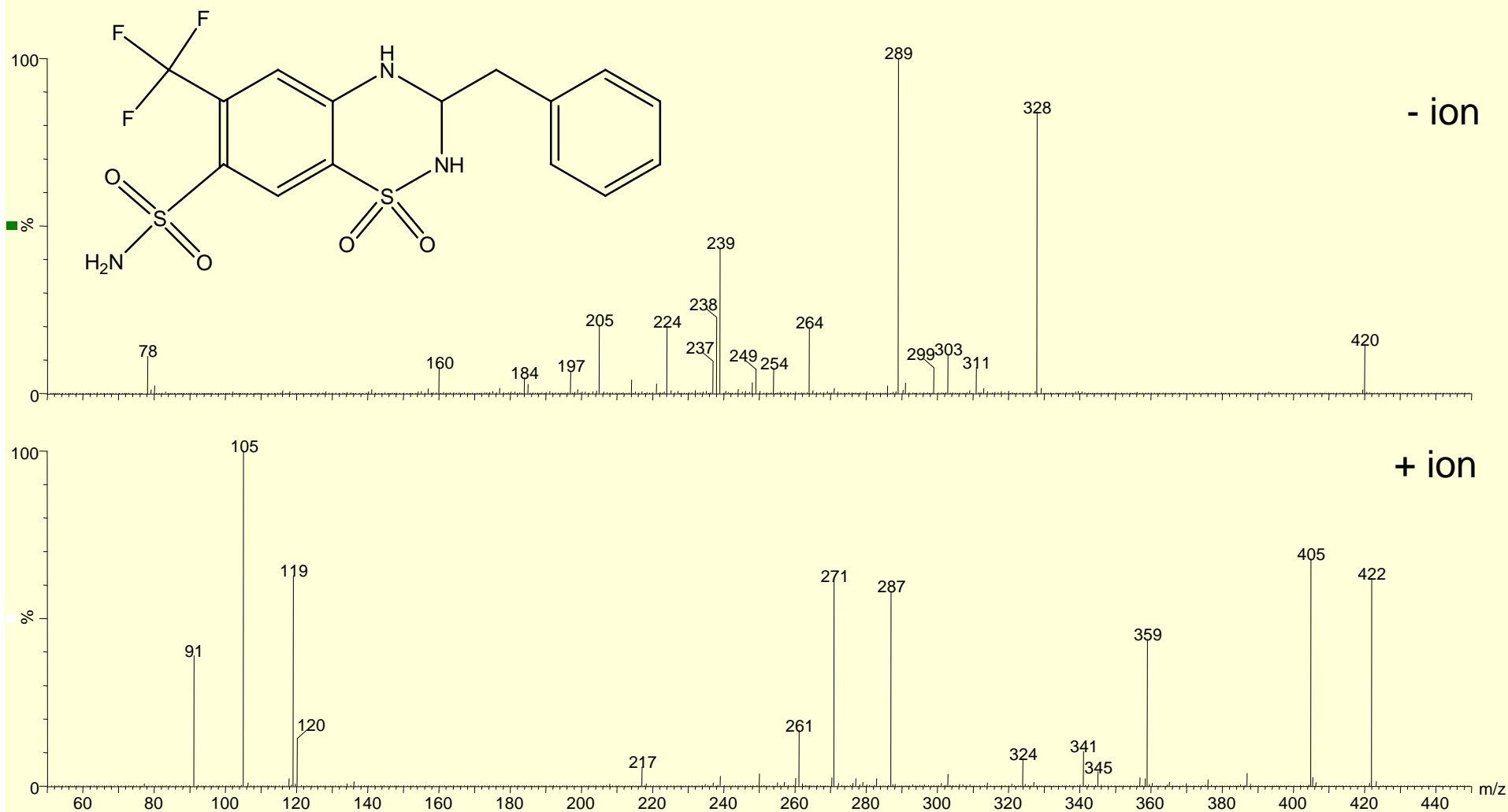
Cephalexin



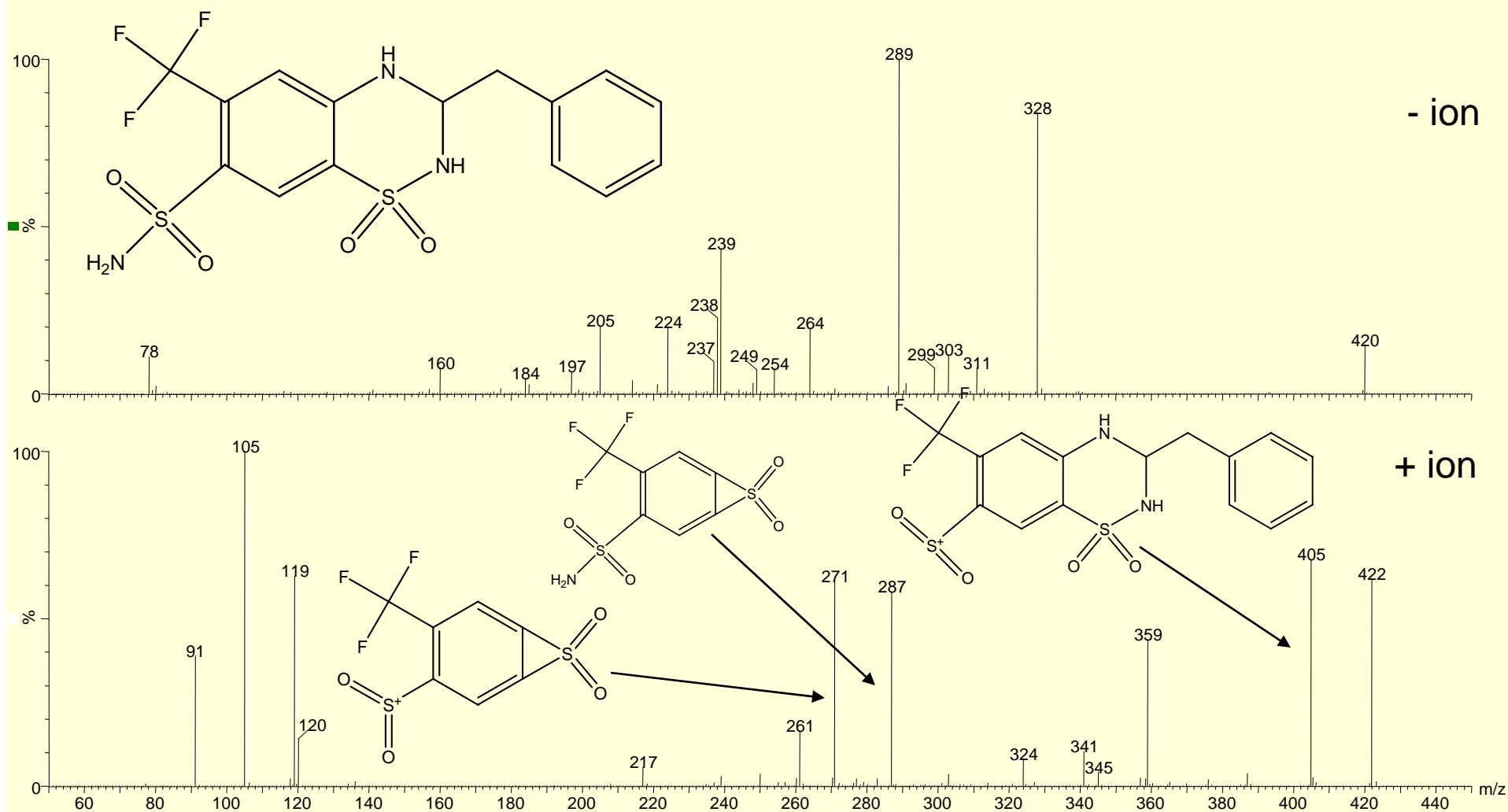
Bendroflumethiazide



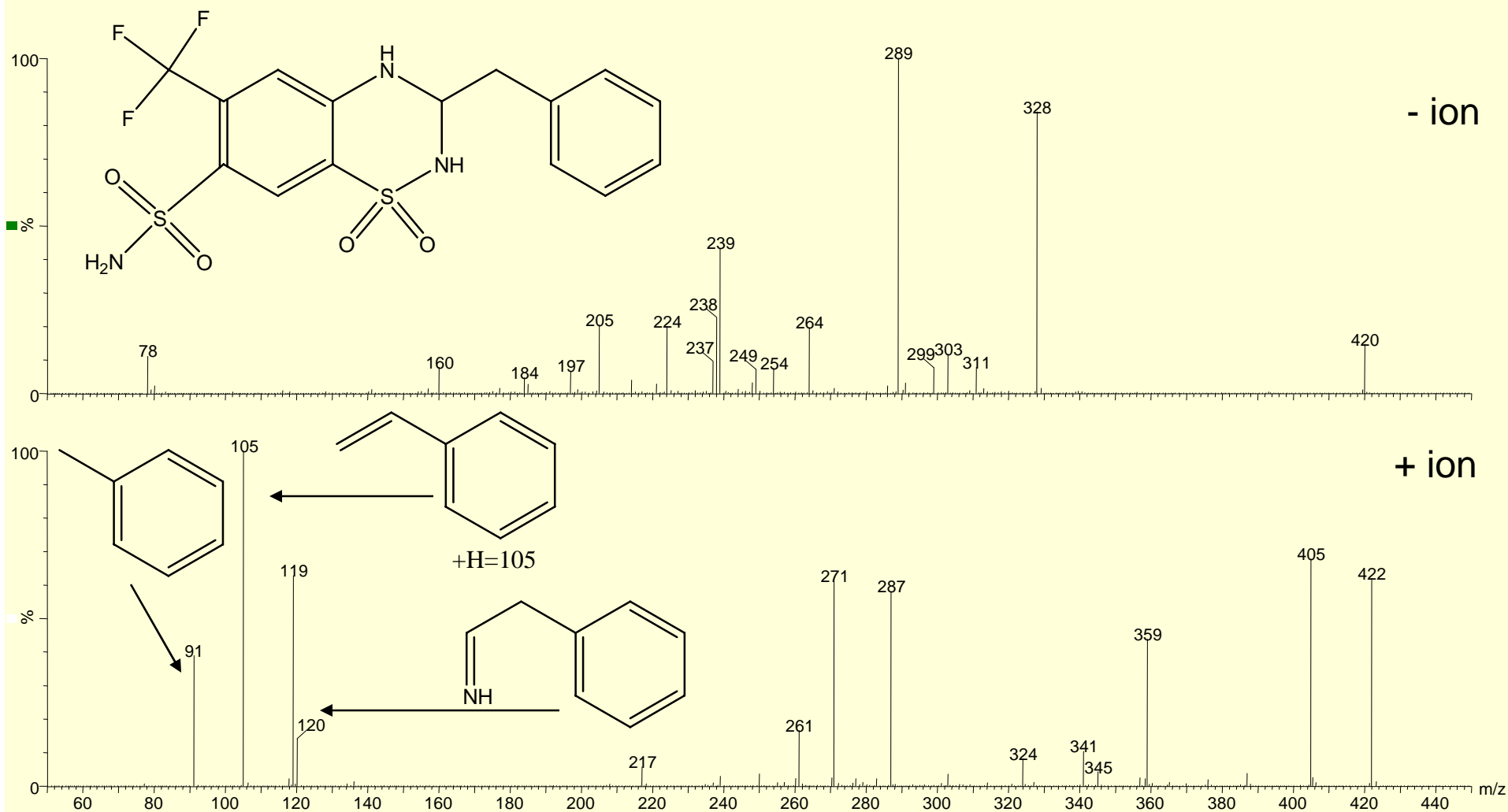
Bendroflumethiazide



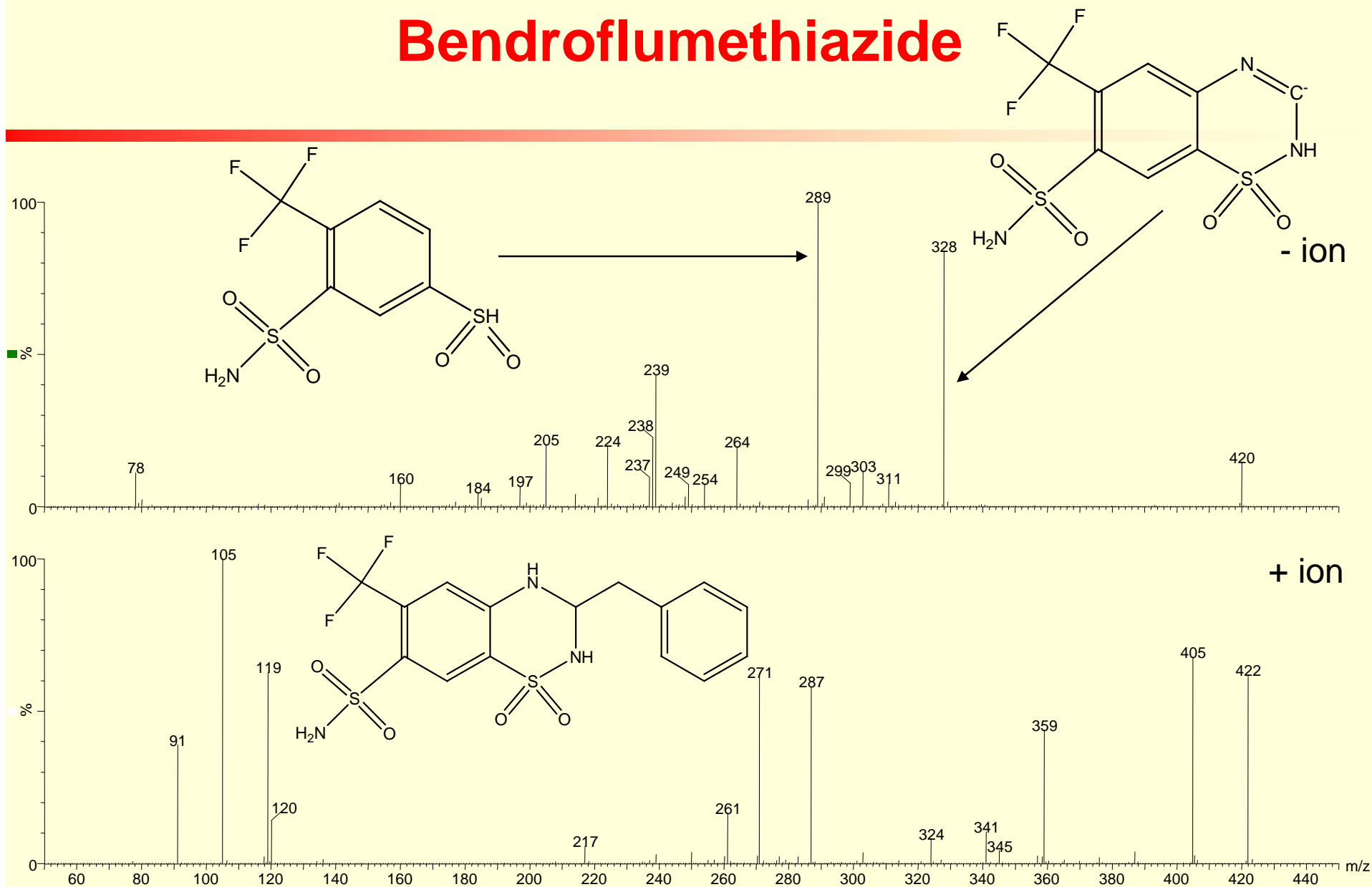
Bendroflumethiazide




Bendroflumethiazide



Bendroflumethiazide



Some Generalized Observations

y'' and  are consistent throughout

Conclusion

- Advantageous to always run both + and –
- Lots of structural information to be gained from - ion