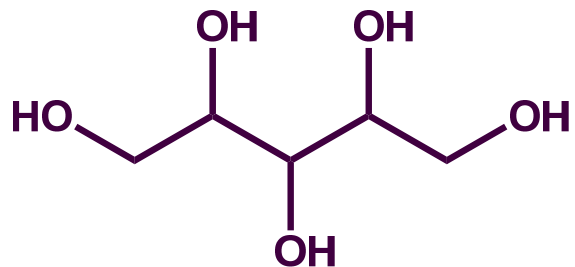


COMPARISON OF MS/MS SPECTRA USING DIFFERENT INSTRUMENTS

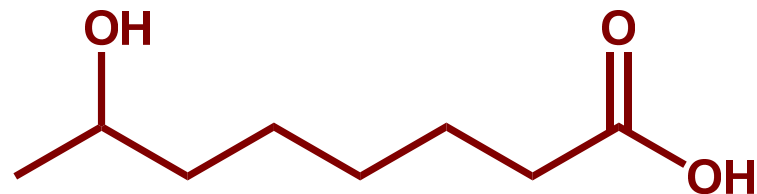
HMDB Meeting
Nov 3, 2008

Avalyn Lewis

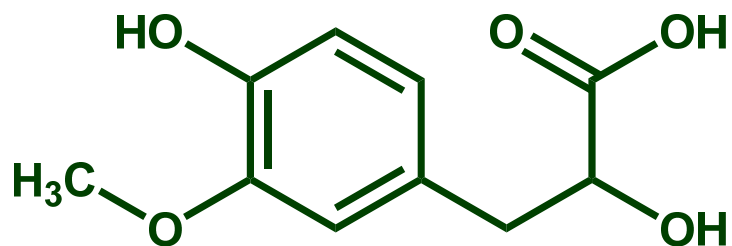
Compounds studied



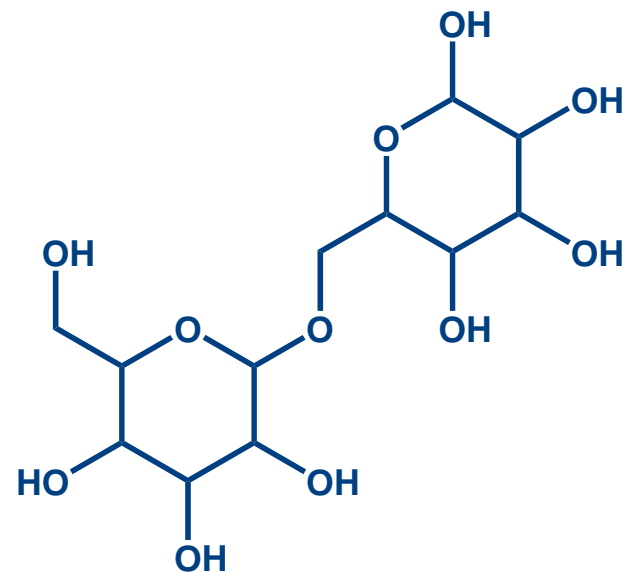
HMDB 002917 - Xylitol



HMDB 00486 – 7-hydroxyoctanoic acid



HMDB 00913 - Vanillic acid



HMDB 02923 - Isomaltose

Instrumentation



Micromass Quattro



API QStar Pulsar



AB 4000 Q TRAP[®] System

Workflow



Sample dissolved in 50/50
MeOH, 0.1% formic acid



Direct infusion into MS



10



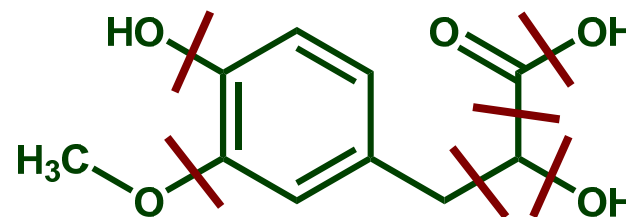
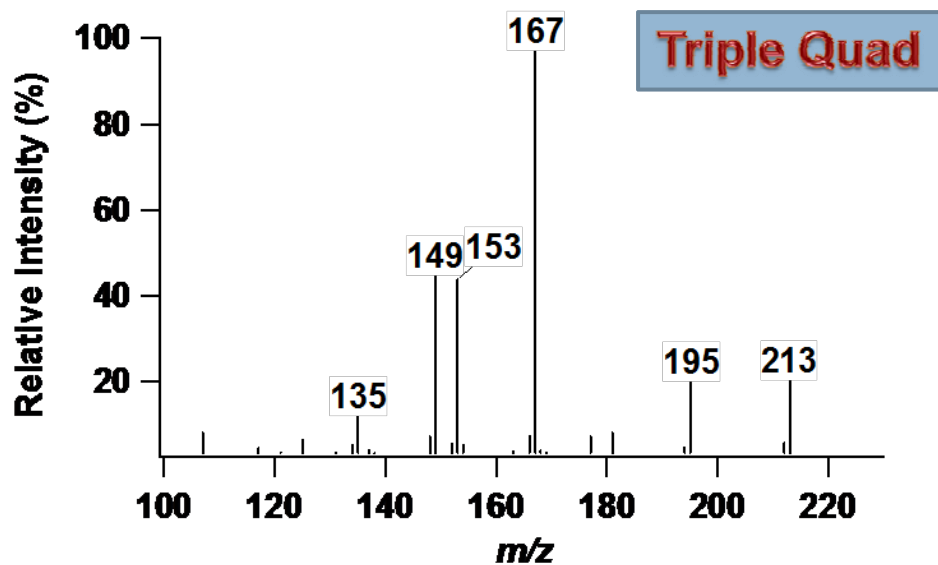
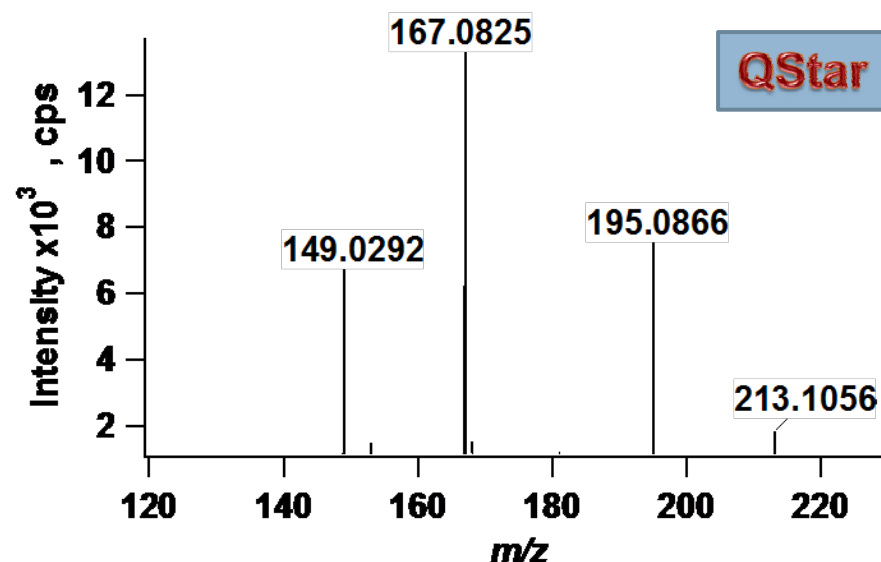
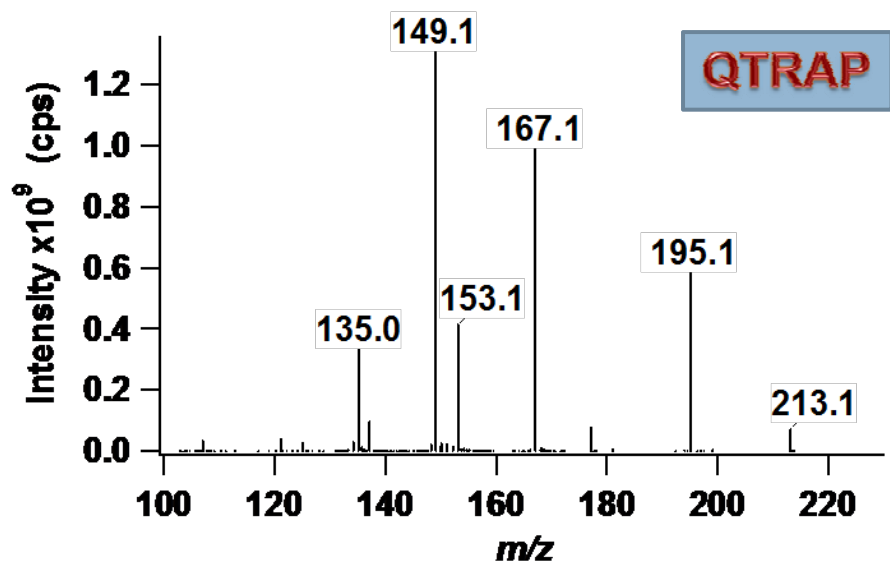
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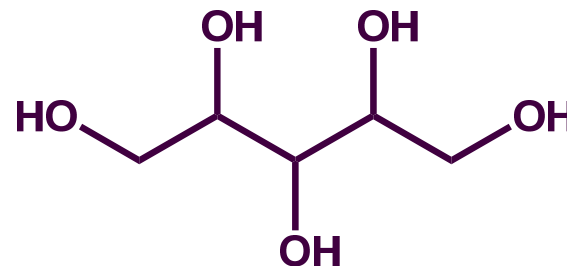
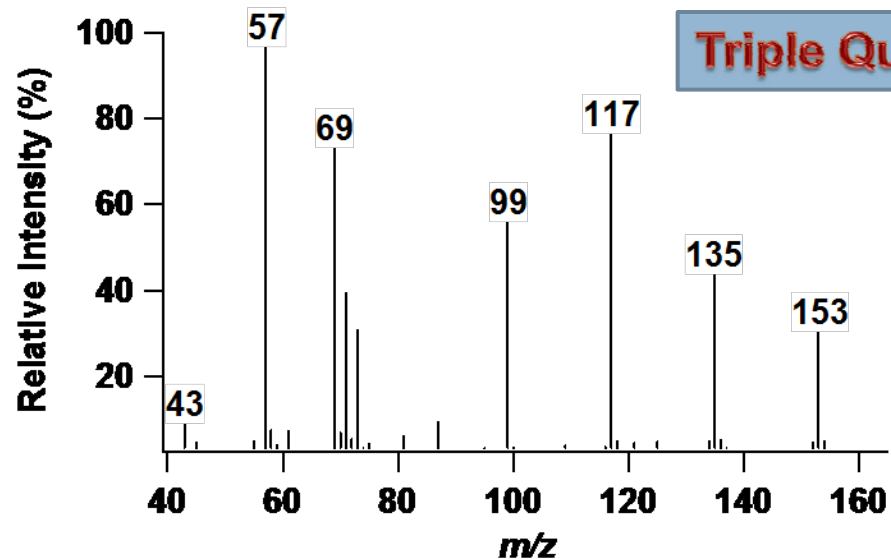
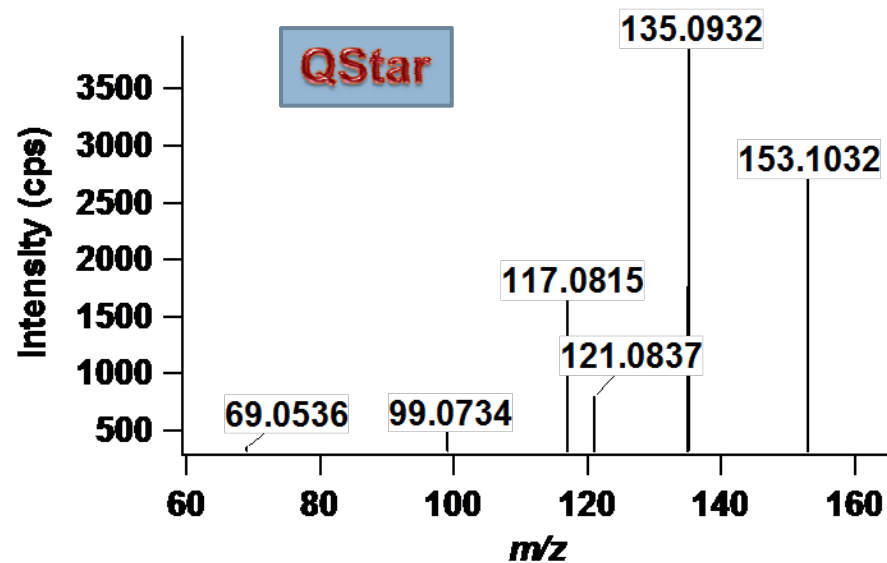
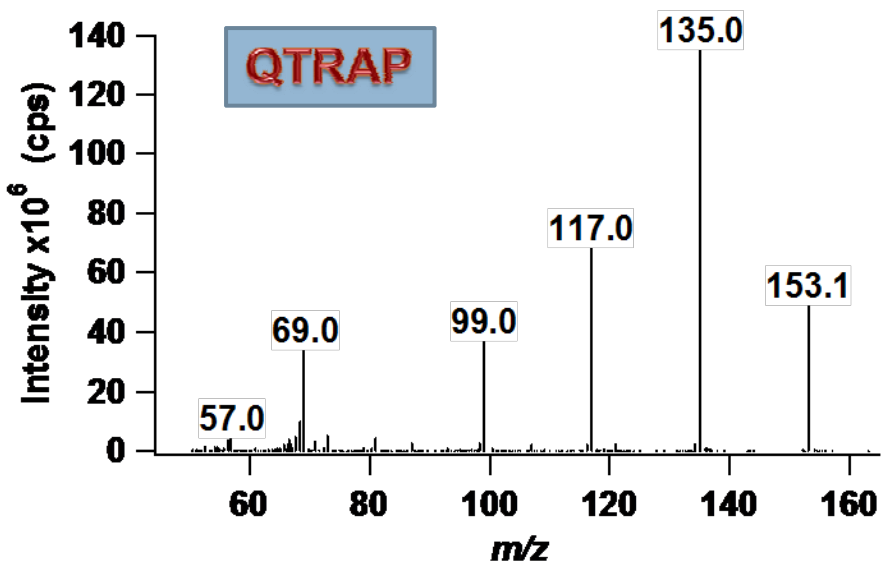
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Collision energy

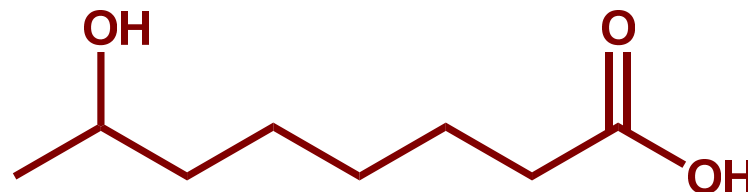
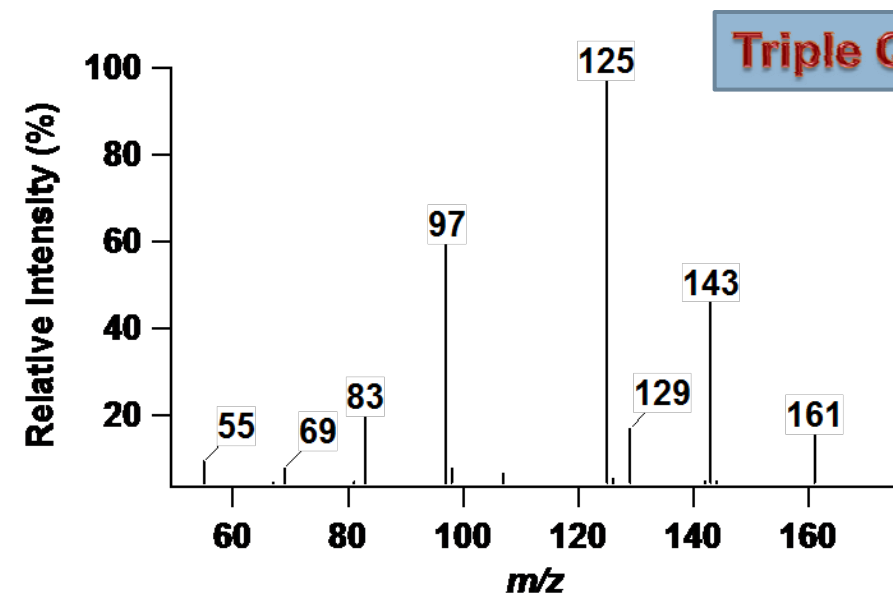
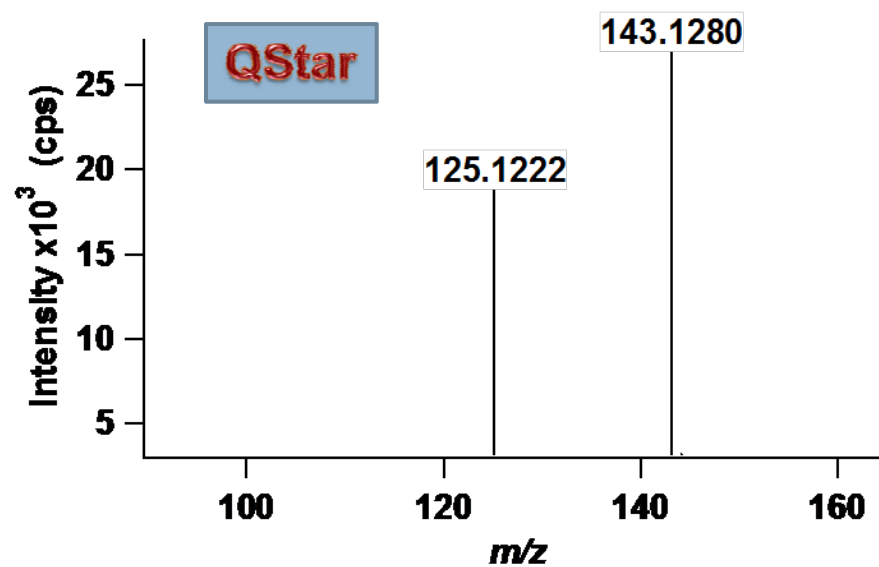
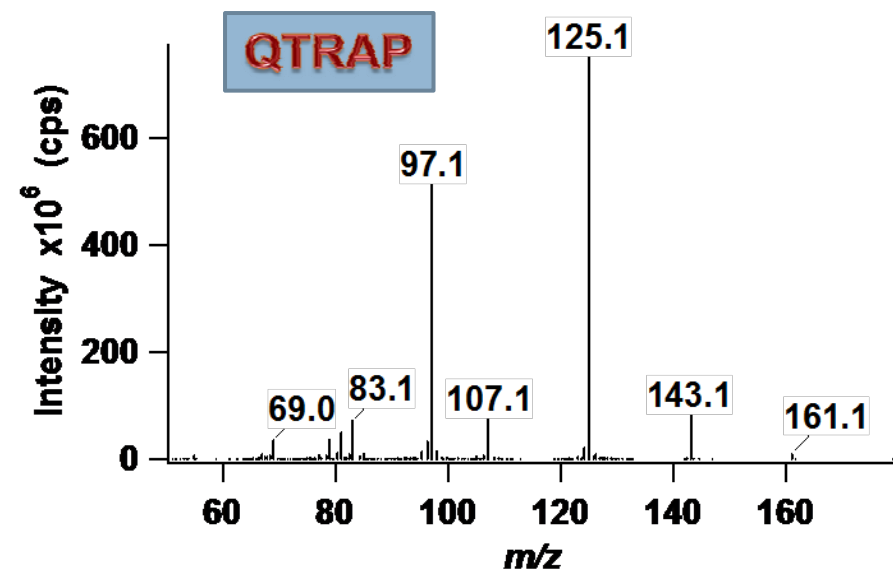
HMDB 00913



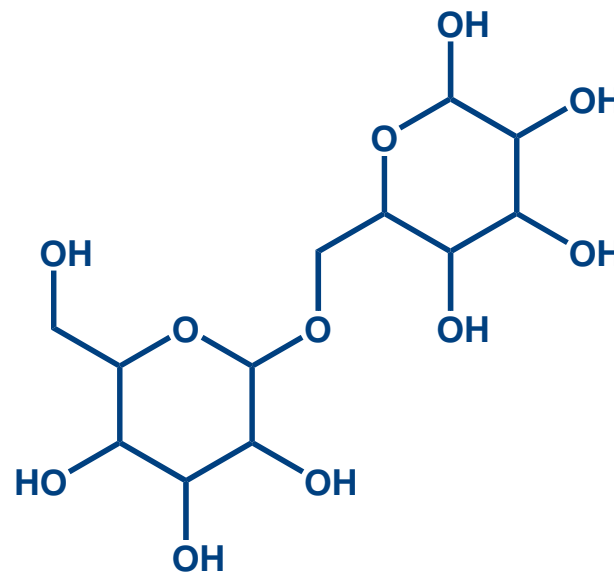
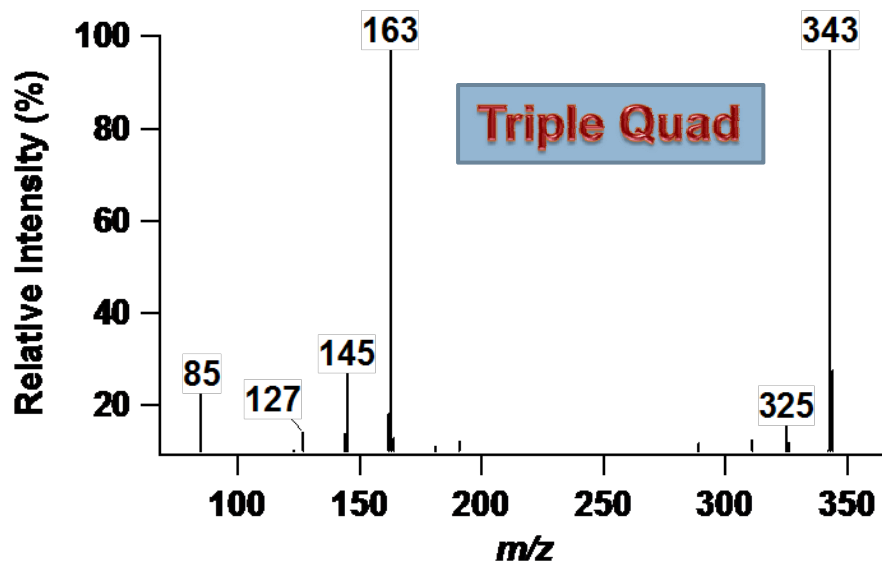
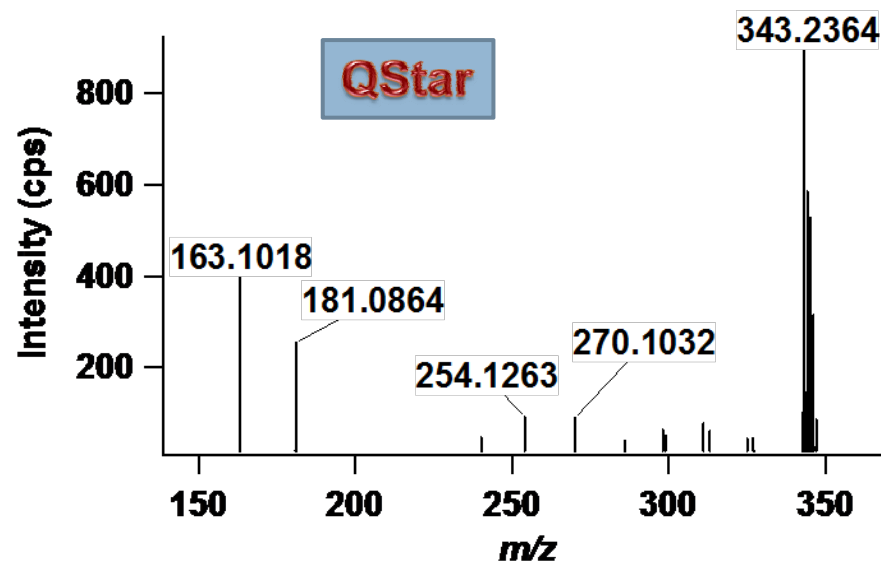
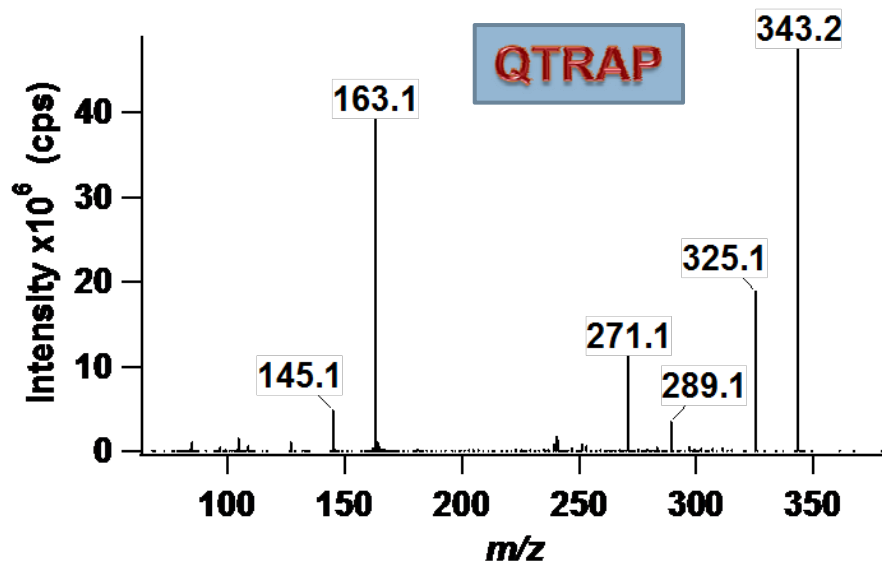
HMDB 02917



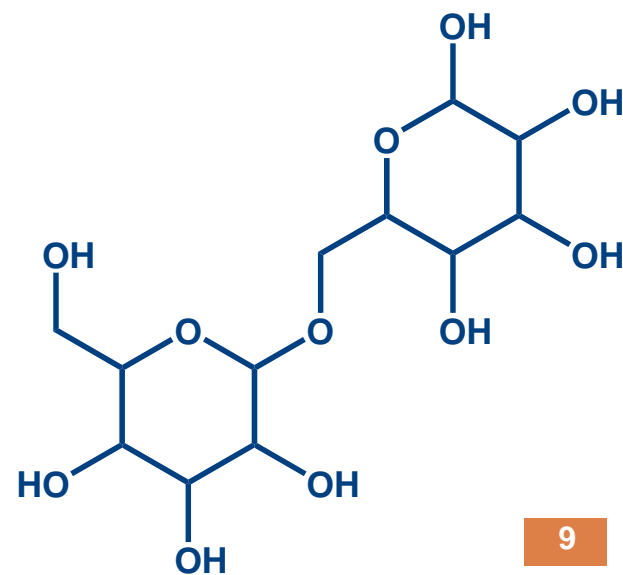
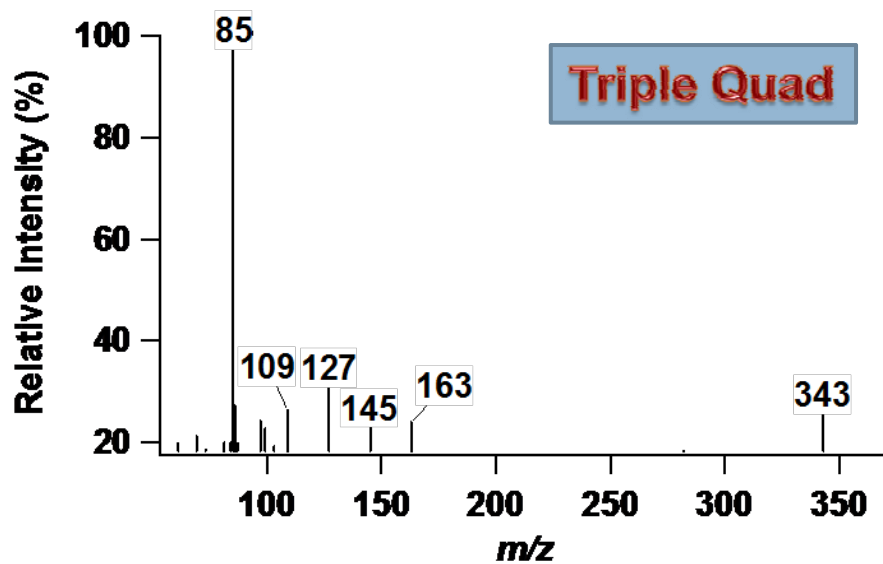
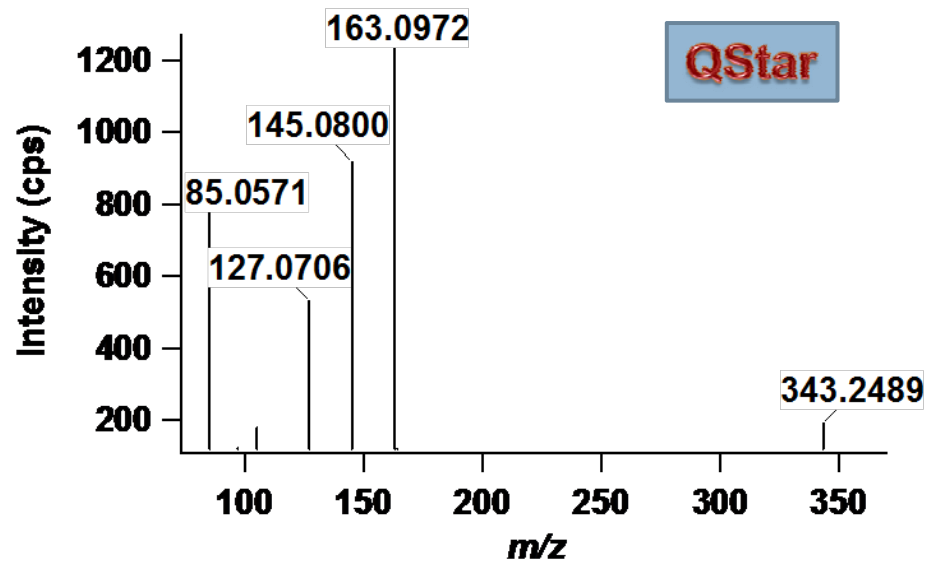
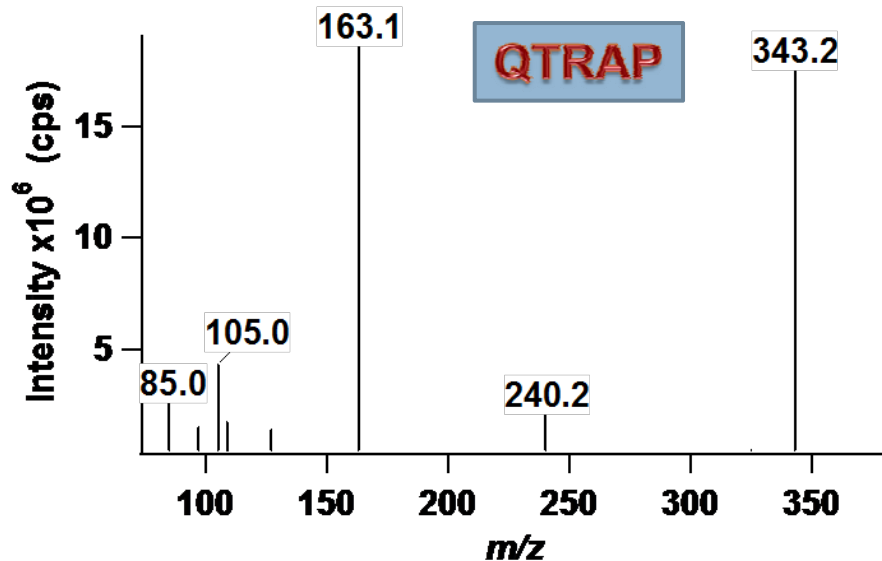
HMDB 00486



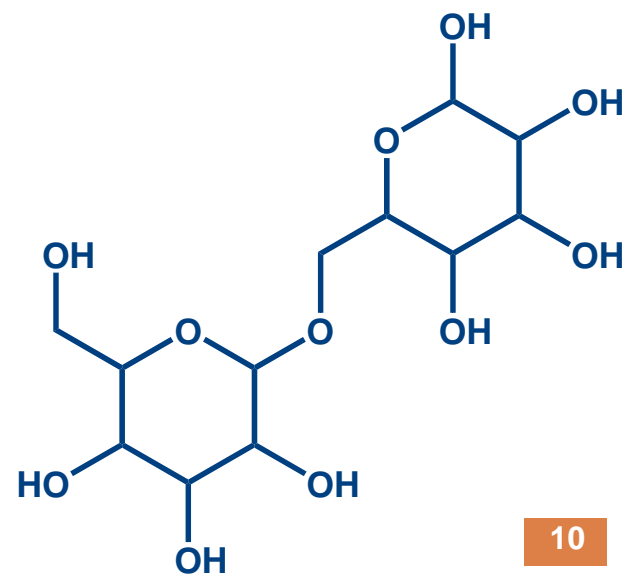
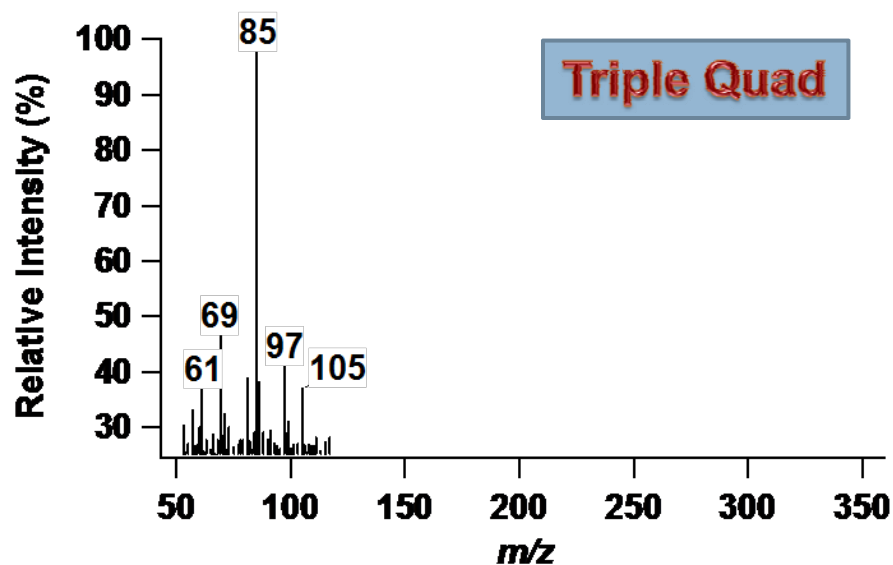
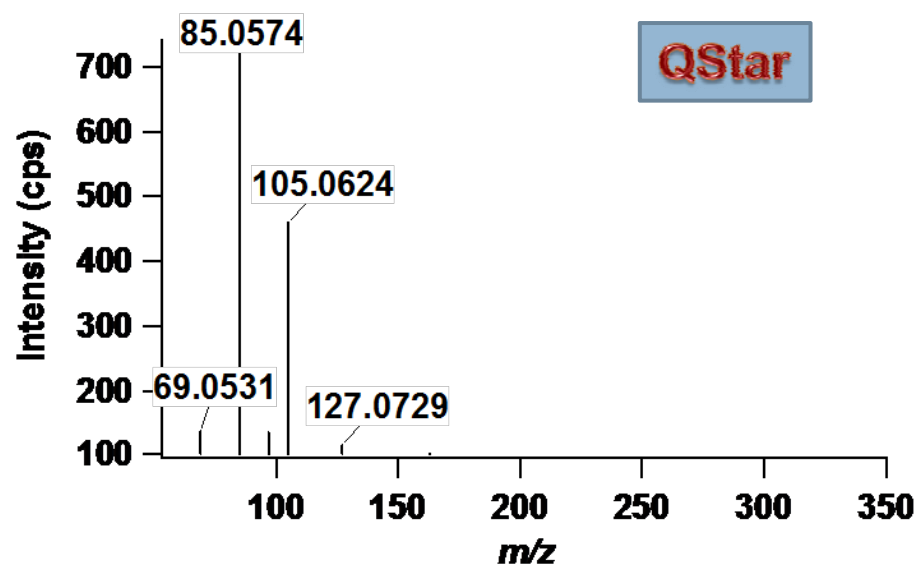
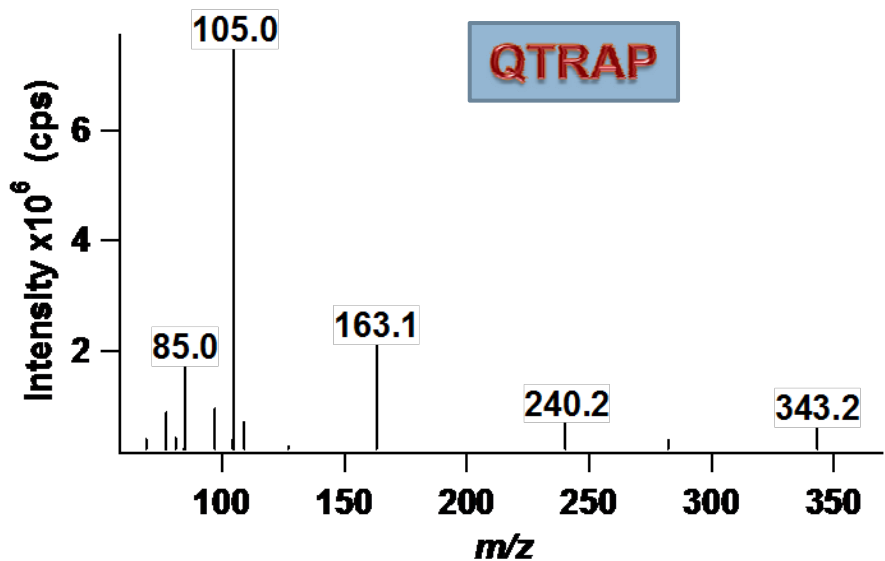
HMDBB 02923 – Low Energy



HMDBB 02923 – Medium Energy



HMDB 02923 – High Energy



Comparison of techniques

- Significant differences in relative intensities.
- Significant differences in the degree of fragmentation.
- Some fragments may be absent but there are no new or unique fragments.
- Similar fragments observed for the QTRAP and the triple quadrupole instruments.

Conclusions

- For searching algorithms, maybe higher weight should be placed on m/z values rather than relative intensities.
- Choose characteristic peaks as criteria for good fit in library search.

Thank you for your attention

Any Questions?

