



MetFrag - Query Chemical Structure Databases and Match Predicted Fragments with Mass Spectra

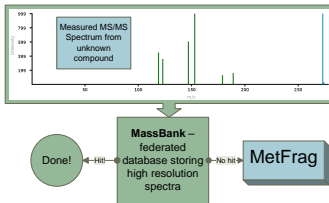
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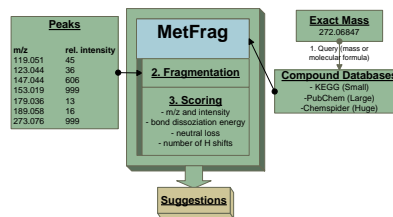


Introduction

- Mass Spectrometry is an important analysis technology
- New automated instruments with several fragmentation steps generate large amounts of data
- Interpretation is non trivial and time consuming
- MetFrag helps identifying the measured molecule using compound databases.



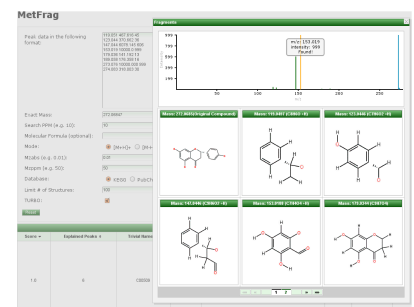
Workflow



Results

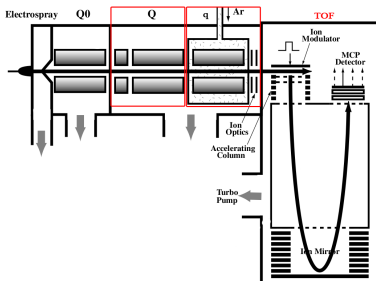
- TODO: maybe allow 2000 hits in pubchem
- TODO TODO TODO.... mit neuen Erweiterungen!

Webinterface



- <http://msbi.ipb-halle.de/MetFrag>
- Tomcat6, JSF, RichFaces

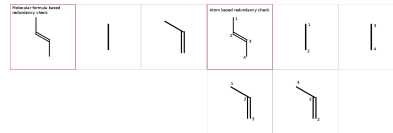
Tandem Mass Spectrometry (MS/MS)



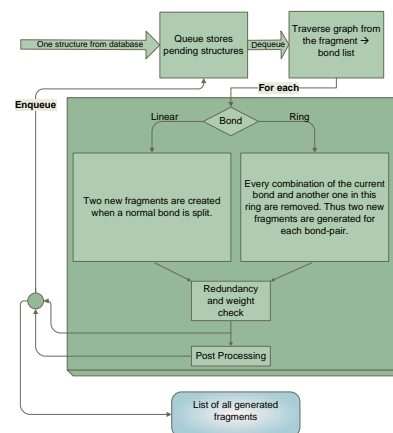
- Mass-to-charge ratio of charged particles
- Two stages of mass analysis
- Q - Quadrupole mass analyzer - isolate precursor ion
- q - Radio frequency collision quadrupole
- TOF - Time-of-flight mass analyzer
- Helps to identify the chemical composition of a compound

Heuristics

- Fragments have to heavier than the smallest peak
- Compute until a given tree depth is reached
- Molecular formula and atom based redundancy check



Fragmentation Algorithm



- Post processing:
 - Create a new tree node when fragment mass - neutral loss mass explains peak

Further Research

- Improve identification rate
 - Improve Scoring (characteristic fragments) - User feedback
 - Fragment energy/stability
 - Assign peaks molecular formulas [SIRIUS]
- Precompute database entries
- Format for exchanging annotated spectra (mzAnnotate)
- Create a MetFrag BioMoby webservice and integrate into workflows

Representation of Molecules

- Molecules are represented as a labeled graph $G=(V,E)$:
 - V ... set of vertices \rightarrow atoms
 - E ... set of edges \rightarrow bonds
- Chemistry Development Kit is used as API
 - Java library for structural chemo- and bioinformatics

Acknowledgements

- Matthias Müller-Hannemann
- Stephan Schmidt

References