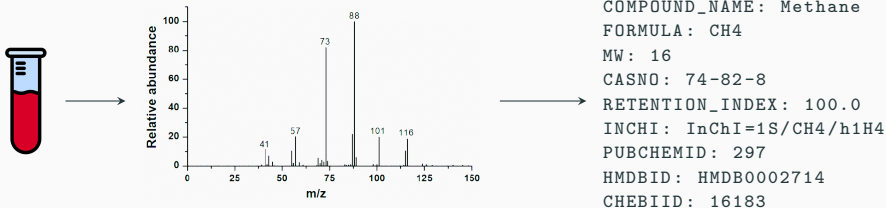# MSMetaEnhancer: A Galaxy Tool for Mass Spectra Metadata Annotation

Matej Troják, Helge Hecht, Martin Čech, and Elliott James Price

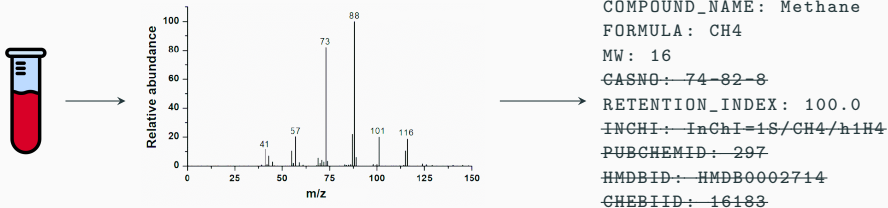RECETOX, Masaryk University, Czech republic

- identify unknown compounds in a sample
- spectrum associated with metadata containing identifiers


```
COMPOUND_NAME: Methane
FORMULA: CH4
MW: 16
CASNO: 74-82-8
RETENTION_INDEX: 100.0
INCHI: InChI=1S/CH4/h1H4
PUBCHEMID: 297
HMDBID: HMDB0002714
CHEBIID: 16183
```

Mass spectrometry

- identify unknown compounds in a sample
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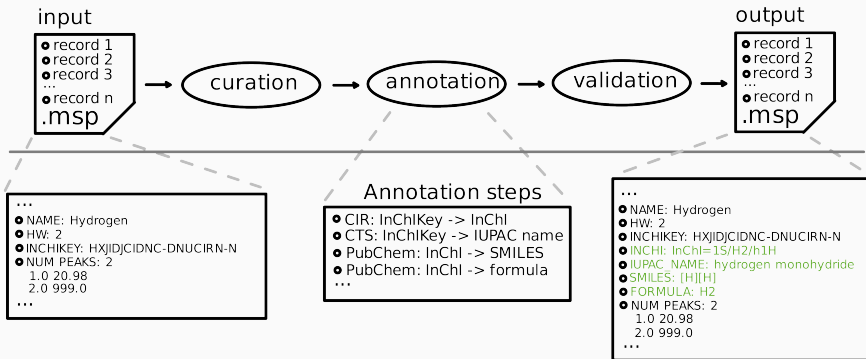~~PUBCHEMID: 297~~
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Mass spectrometry

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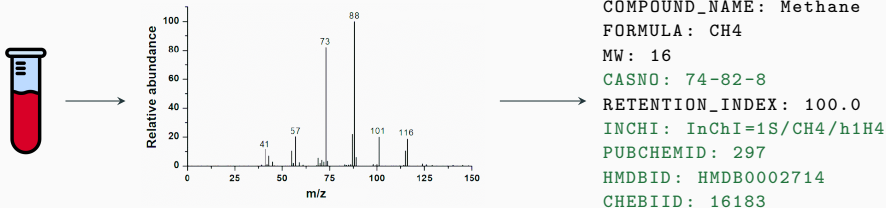
MSMetaEnhancer

- customisable annotation process (semi-automatic)
  - conversion: `service: source → target`
  - defined vs. arbitrary order
- support for web services (via API) and compute engines (CIR, CTS, IDSM, PubChem, BridgeDB, ...)
- supported identifiers (InChI, InChIKey, SMILES, IUPAC chemical name, CAS number, many database-specific IDs, ...)
- iterative annotation with asynchronous approach (service limitations)
- additional curation (input data) and validation (obtained data) steps

Galaxy wrapper

- select single conversion in repeat mode

Ordered conversions

| 1: Ordered conversions | 🗑 |

Available conversions

| PubChem: compound_name -> inchi | ▾ |

| 2: Ordered conversions | 🗑 |

Available conversions

| IDSM: inchi -> inchikey | ▾ |

| 3: Ordered conversions | 🗑 |

Available conversions

| CTS: compound_name -> inchikey | ▾ |

+ Insert Ordered conversions

- select multiple conversions

Other conversions

☐ Select/Unselect all

| × RDKit: smiles -> mw | × BridgeDB: pubchemid -> chemspiderid | × BridgeDB: pubchemid -> hmdbid |

MSMetaEnhancer

https://github.com/RECETOX/MSMetaEnhancer

https://toolshed.g2.bx.psu.edu/view/recetox/msmetaenhancer

http://bioconda.github.io/recipes/msmetaenhancer

Demo – Wednesday @ 10:20 AM

Thank you for your attention!