EMDB

Javascript library for mass spectra analysis

www.chemcalc.org

Not Secure www.chemcalc.org

ChemCalc

Institute of chemical sciences and engineering ISIC

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Your Molecular Formula

HAla100OH

List of allowed groups

FWHM : 0.001

Resolution: 7121722

Apply Gaussian:

Submit

Reference version: 2013

FWHM = ΔM
(Peak Full Width at Half-Maximum)

Resolution = M / ΔM

HAla100OH

MF: C300H502N100O101
MW: 7125.817246
EM: 7121.72194
Unsat.: 100

Element	Count	Percent
C	300	50.566%
H	502	7.101%
N	100	19.656%
O	101	22.677%

Welcome to ChemCalc

If you are using our tools please don't forget to cite us:

ChemCalc: a building block for tomorrow's chemical infrastructure. Patiny, Luc; Borel, Alain
Journal of Chemical Information and Modeling **2013**. DOI: 10.1021/ci300563h

Cheat poster: Get HELP on how to use chemcalc !

What would you like to do ?

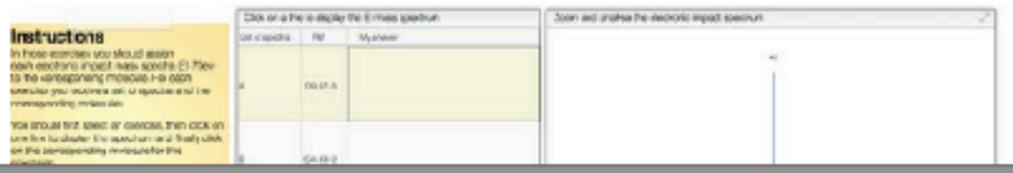
- Calculate molecular formula, molecular mass / molecular weight, exact mass (monoisotopic mass), elemental analysis and plots the isotopic distribution graph (isotopomers). Just enter a formula in the box on the left. Check the HELP.
- Find molecular formula from an accurate mass
- Calculate peptide fragmentation
- Integrate the tools in your website

Latest news ...

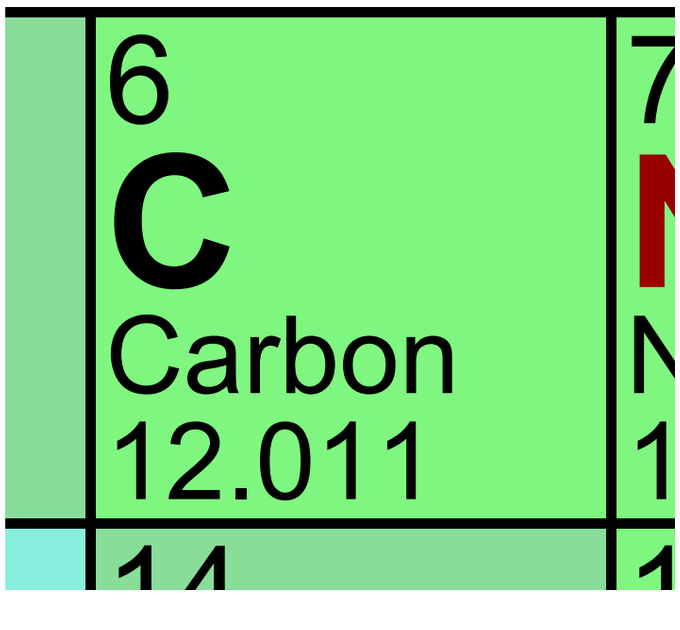
Tweets by @cheminformatics

Cheminfo
@cheminformatics

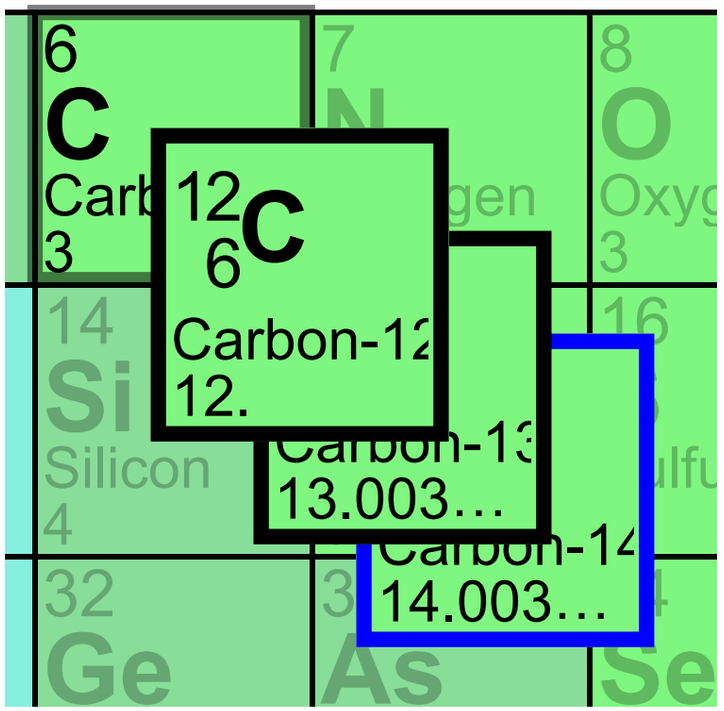
Are you teaching structural analysis (mass, IR or NMR) or just would like to make some exercises ? You could try the website we created for our teaching: cheminfo.org/flavor/structu... (using Google Chrome)



C_{10}

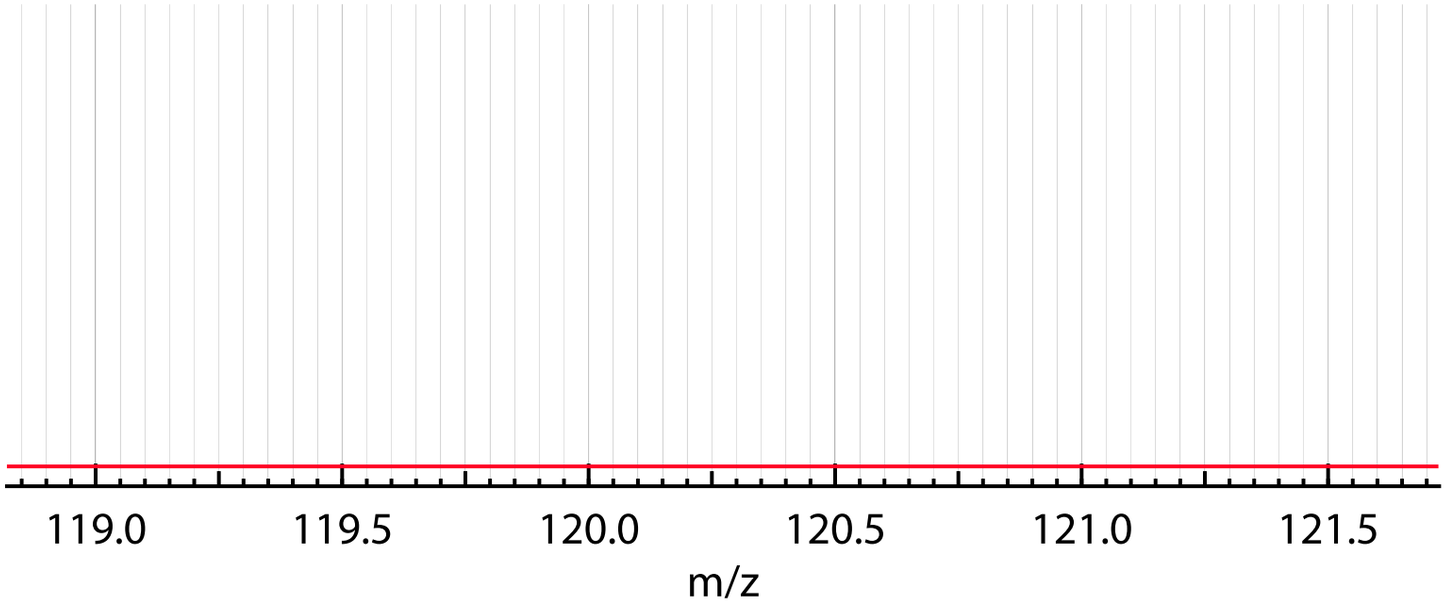


mw: 120.11



em: 120

C_{10} in the spectrometer

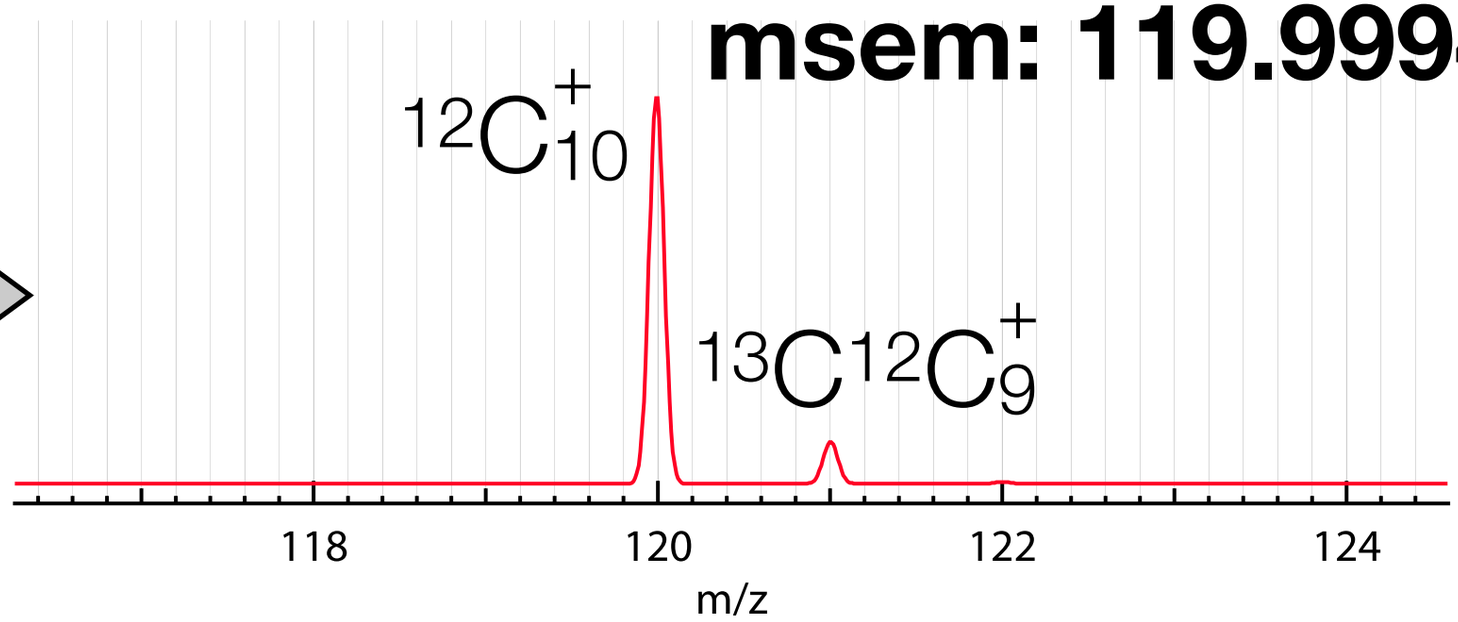


- e^-

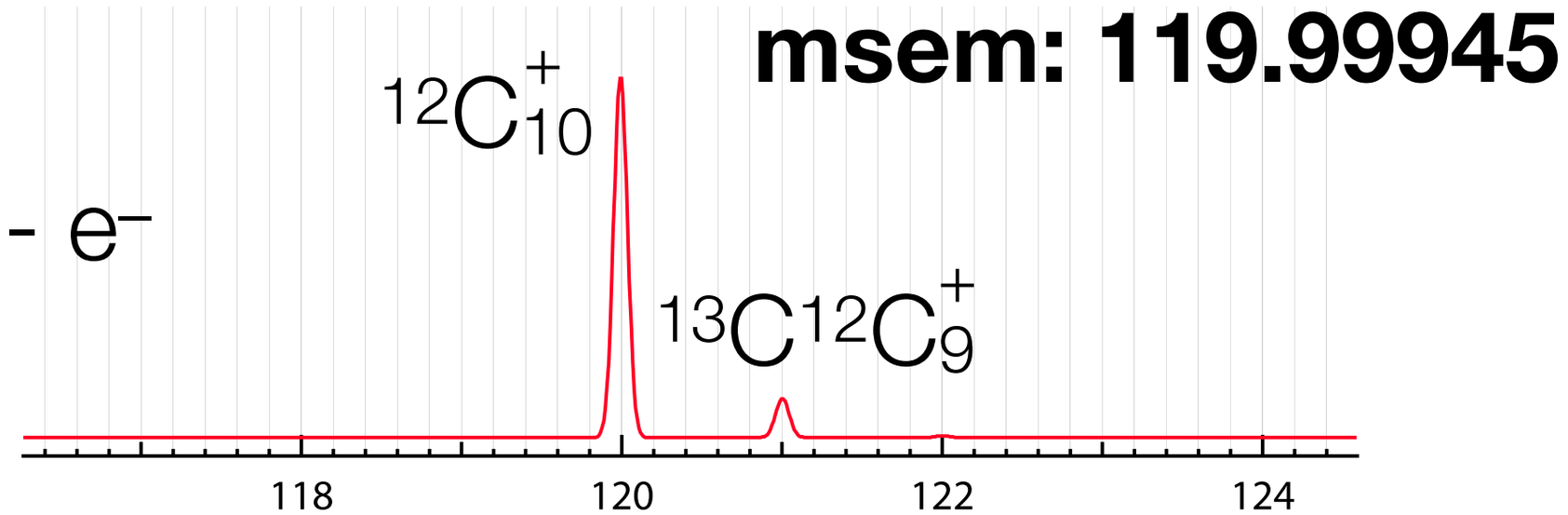
msem: 119.99945

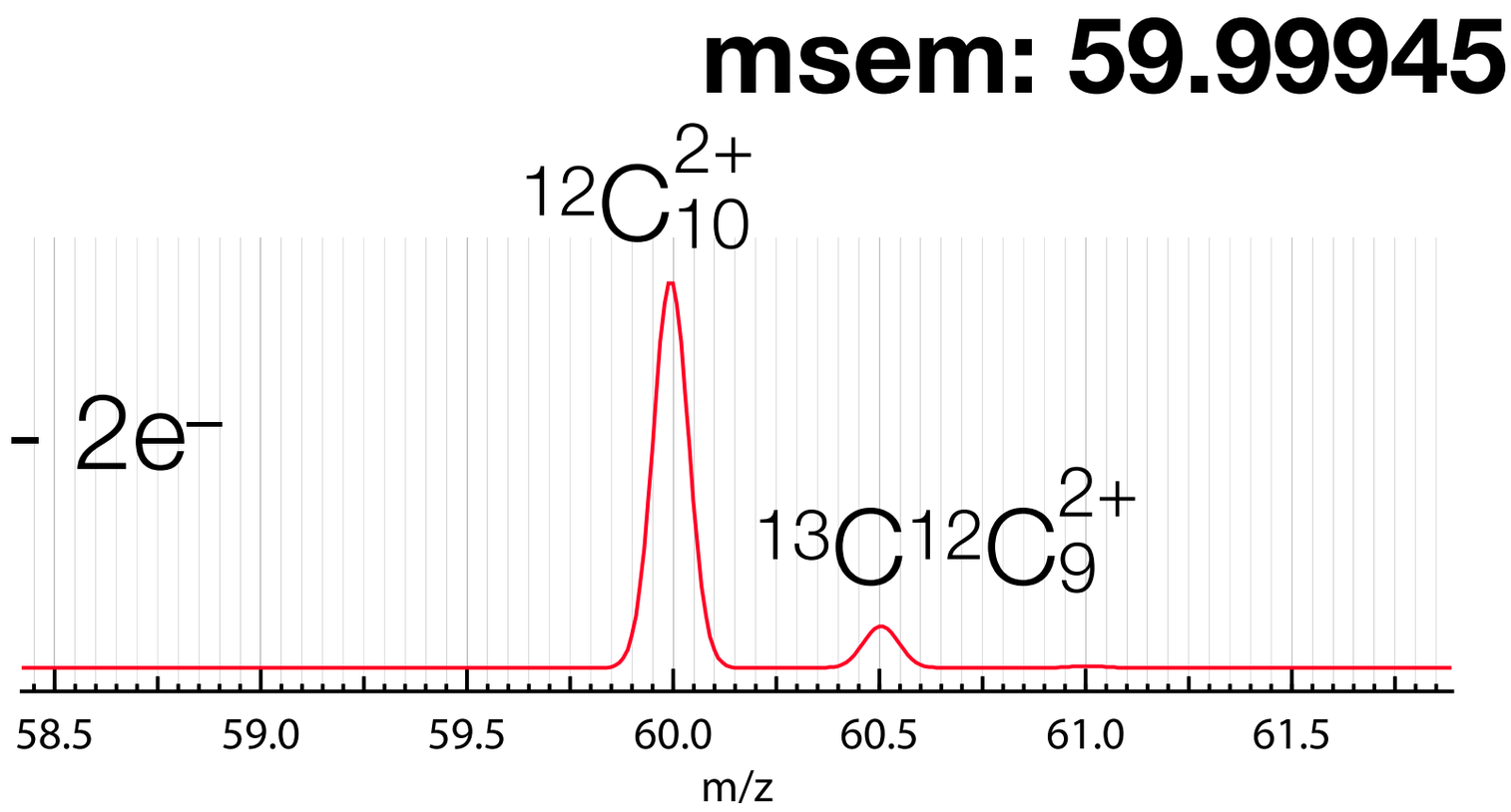
$^{12}C_{10}^+$

$^{13}C^{12}C_9^+$



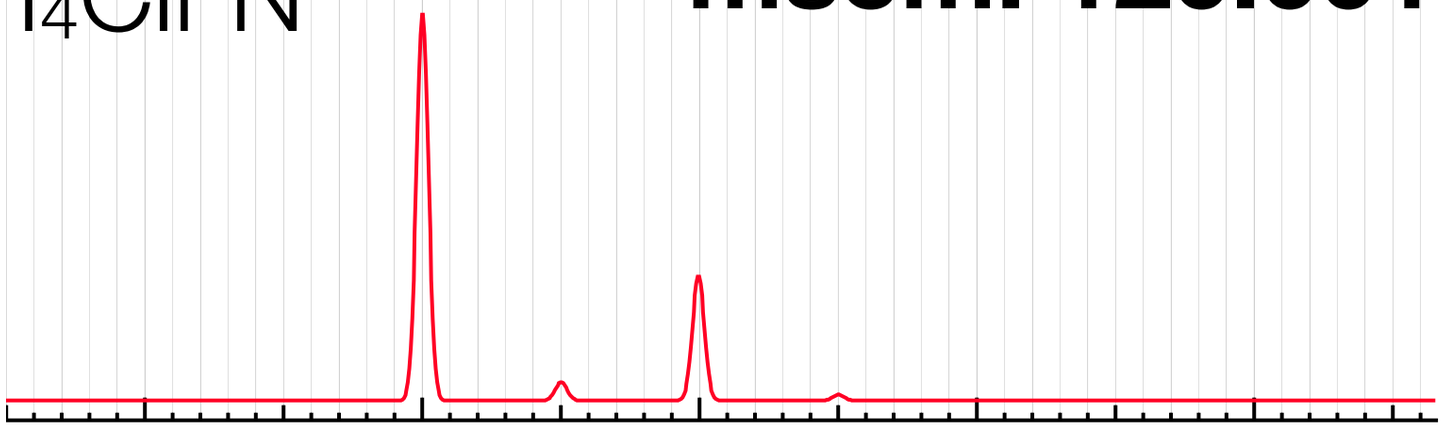
C_{10} and multiple charges



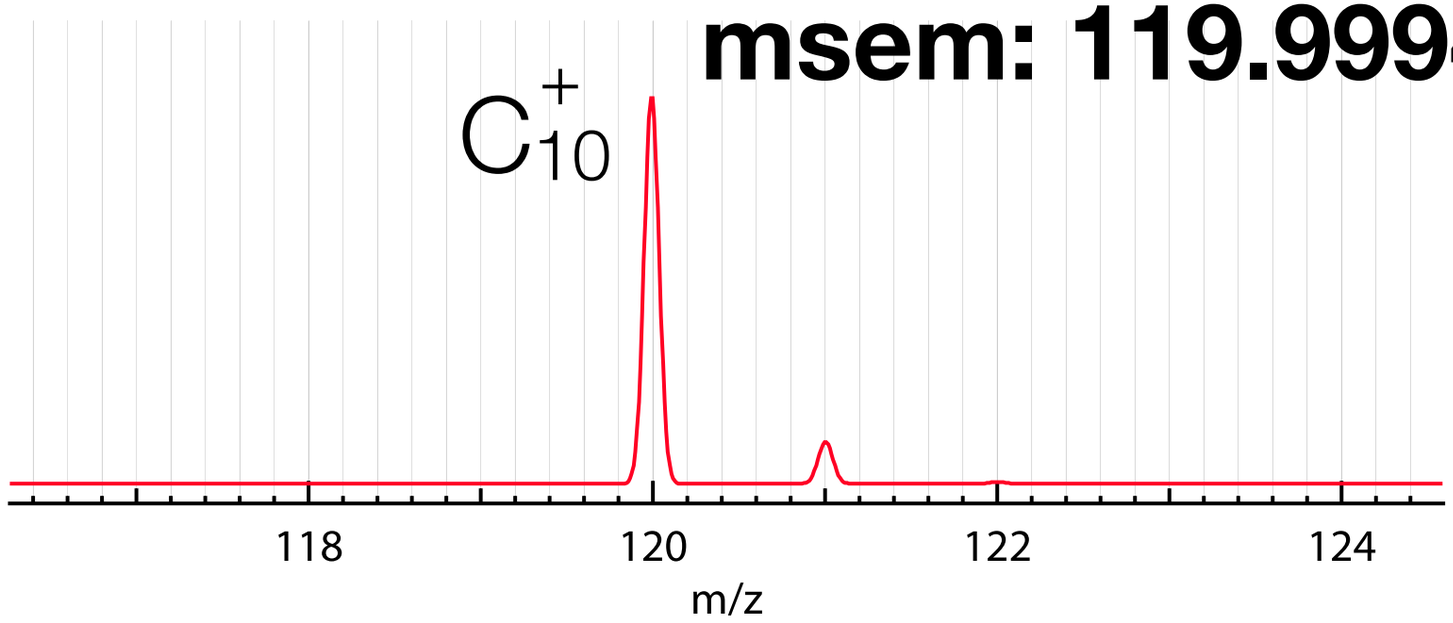


Monoisotopic mass

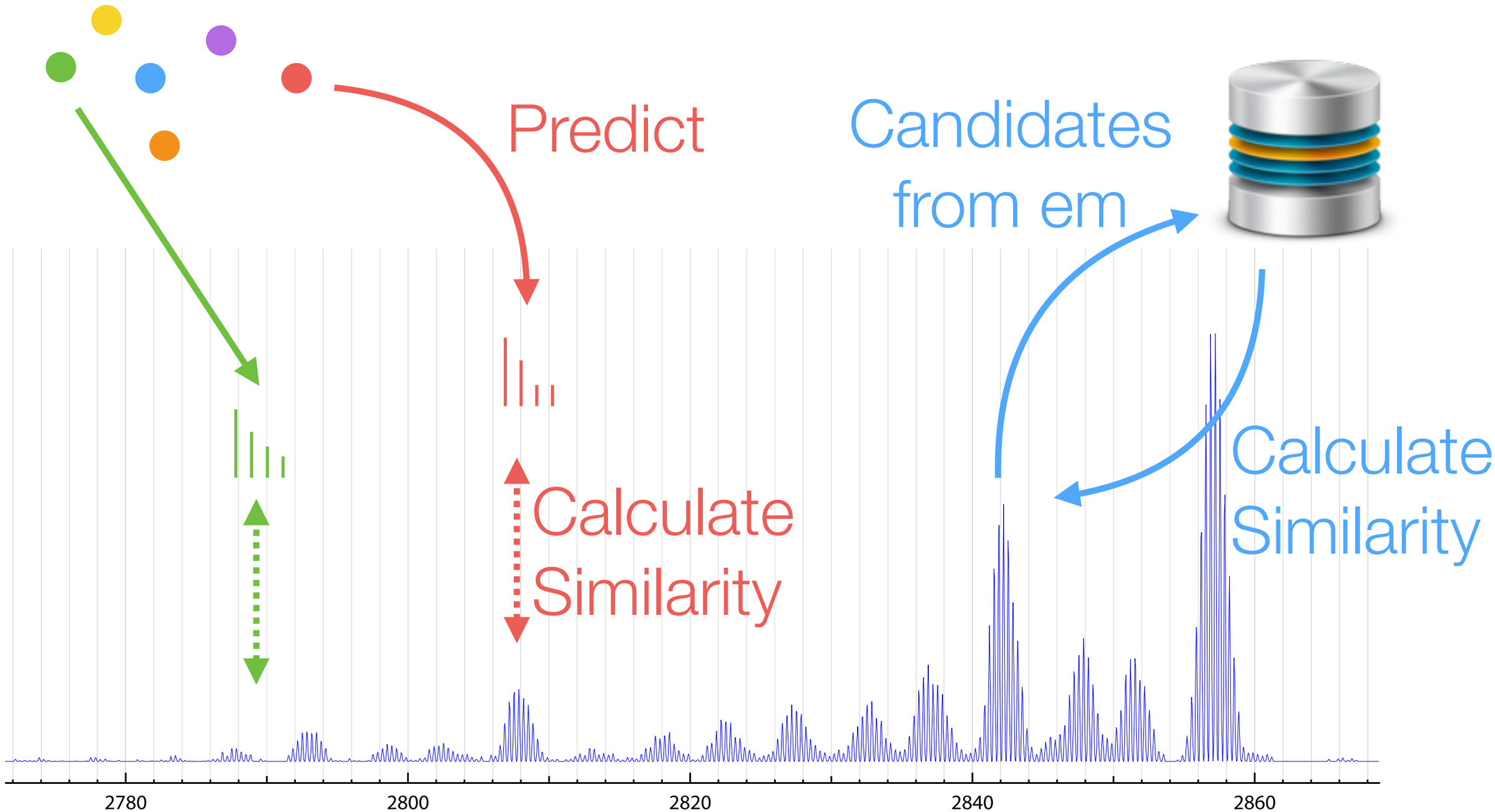
$C_4H_4ClFN^+$ **msem: 120.00108**



msem: 119.99945



Two possible workflow



Required tools

- Molecular formulas + ionizations
  - monoisotopic mass
  - isotopic distribution
- Monoisotopic mass + ionizations
  - possible molecular formulas
- Isotopic distribution similarity

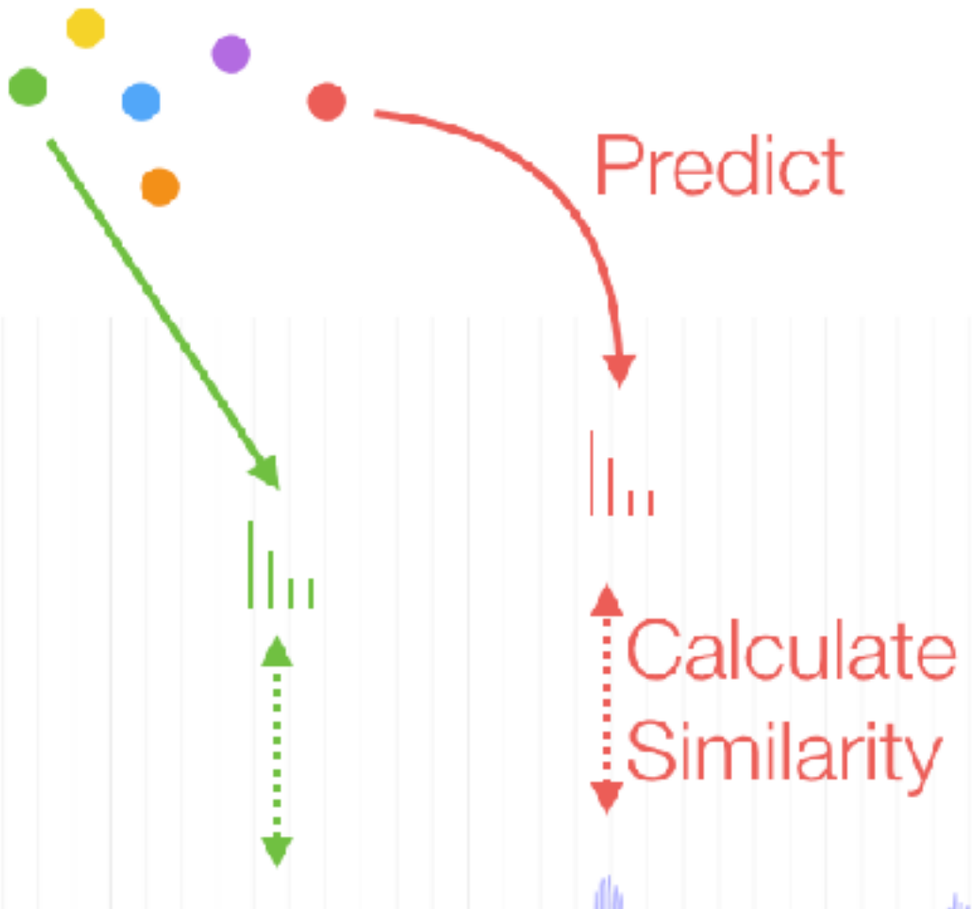
EMDB ?

Exact mass database

https://www.npmjs.com/package/emdb

- open-source MIT library
- javascript
- 3 important classes:
  - EMDB.Util.MF
  - EMDB.Util.IsotopicDistribution
  - EMDB

Information for a MF



```
const EMDB = require('emdb');

let mf = new EMDB.Util.MF('Et3N');

console.log( mf.getInfo() );
```

OUTPUT

```
{
    mass: 101.19022990269394,
    monoisotopicMass: 101.12044948788001,
    charge: 0,
    mf: 'C6H15N',
    atoms: { C: 6, H: 15, N: 1 },
    unsaturation: 0
}
```

```
const EMDB = require('emdb');

let dist = new EMDB.Util.IsotopicDistribution('Et3N', {
    ionizations: 'H+,Na+'
});

console.log( dist.getParts() );
```

OUTPUT

```
[
    {
        mf: 'C6H15N',
        mass: 101.19022990269394,
        monoisotopicMass: 101.12044948788001,
        charge: 0,
        ionization: { mf: 'H+', em: 1.00782503223, charge: 1 },
        ms: { ionization: 'H+', em: 102.12772594020095, charge: 1 }
    },
    {
        mf: 'C6H15N',
        mass: 101.19022990269394,
        monoisotopicMass: 101.12044948788001,
        charge: 0,
        ionization: { mf: 'Na+', em: 22.989769282, charge: 1 },
        ms: { ionization: 'Na+', em: 124.10967018997094, charge: 1 }
    }
]
```

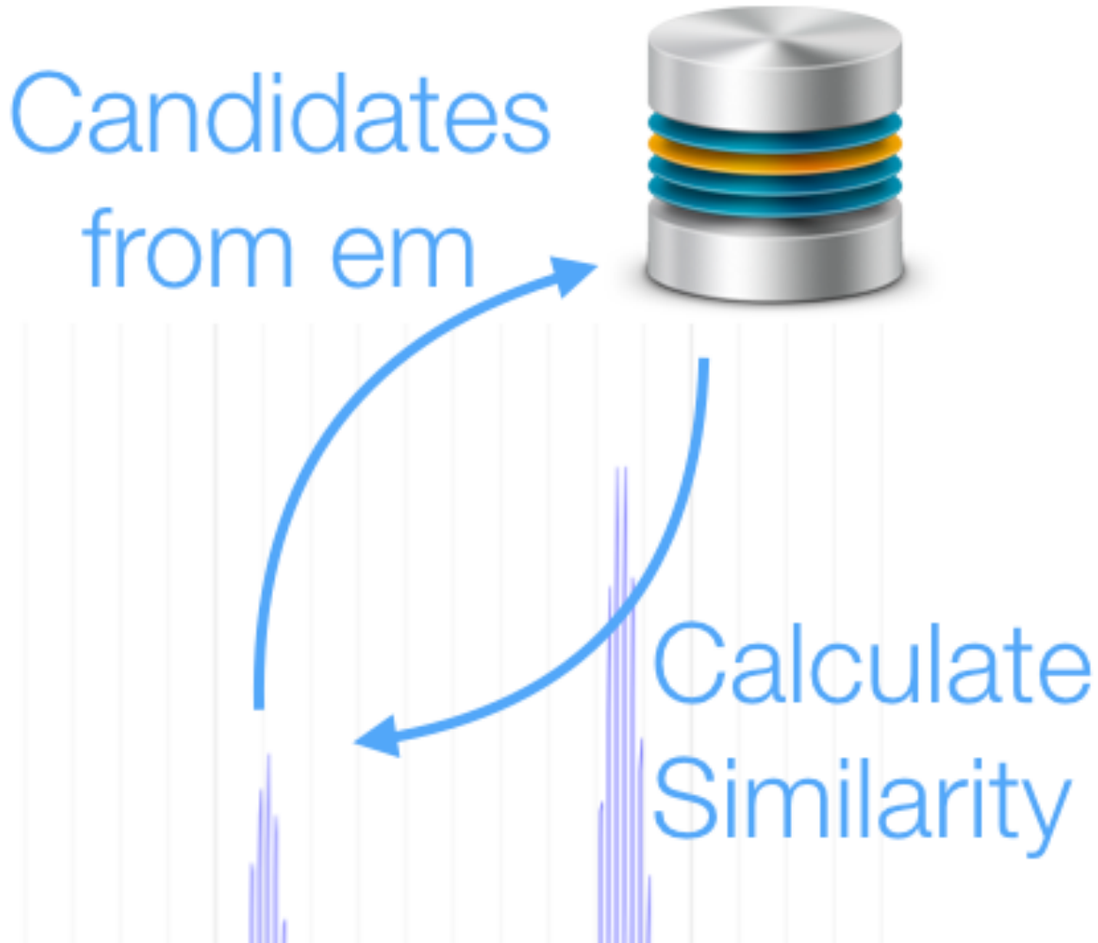
```
const EMDB = require('emdb');

let dist = new EMDB.Util.IsotopicDistribution('Et3N', {
    ionizations: 'H+,Na+'
});

console.log( dist.getDistribution() );
```

OUTPUT

```
[
    { x: 102.12772594020095, y: 0.9324705776936805 },
    { x: 103.1308239513846, y: 0.06552738010342345 },
    { x: 104.13387461619692, y: 0.0019688420812538 1 },
    { x: 105.13686740231948, y: 0.00003286617079521 77 },
    { x: 106.13974366256402, y: 3.289320912721756e-7 },
    { x: 124.10967018997094, y: 0.9324705776936805 },
    { x: 125.1127682011546, y: 0.06552738010342345 },
    { x: 126.11581886596692, y: 0.0019688420812538 1 },
    { x: 127.11881165208948, y: 0.00003286617079521 77 },
    { x: 128.121687912334, y: 3.289320912721756e-7 }
]
```

Demo

MF from monoisotopic mass



Database of monoisotopic mass

1. Create an in-memory database
2. (Search)
3. Show results

KnapSack

PubChem

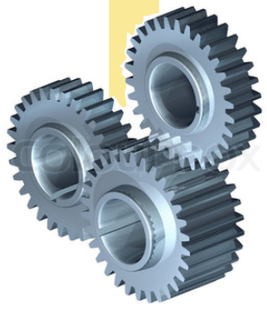
commercials

google sheet

EMDB

contaminants

array of MFs



monoisotopic mass

peptidic sequence

PubChem webservice

- Improved copy of PubChem
  - https://github.com/cheminfo/docker-pubchem
  - correct calculation MF (isotopes, charges, monoisotopic mass)
  - docker-compose project
- 96515520 molecules
- C H N O F Cl S: 452836 unique MFs

Monoisotopic Mass

```
emdb.fromMonoisotopicMass(300, {
  precision: 10,
  ranges: 'C0-50 H0-50 Cl0-50 O0-50 N0-50 Br0-50',
  ionizations: '(H+)2, K+',
  unsaturation: {
    min: 0,
    max: 10,
    integer: true,
    nonInteger: false
  }
});
```

- test over 5000000 MFs / s

From array

```
fromArray([
    '(CH2CH2O)0-9 H0-9 N0-9 O0-9',
    'F, Br, Cl, I, '
], {
  ionizations: 'H+, Na+, K+, (H+)2',
  filter: {
    minMSEM: 100,
    maxMSEM: 105
  }
});
```

- mw
- em
- msem
- charge
- unsaturation

Contaminants database

- Based on a google spreadsheet
- Over 1000 possibles contaminants
- Can be filtered depending the technique

Link

Demo

Conclusions

Conclusions

- Very flexible library for mass calculations
- Allows to solve complex mass problems
- Open-source in javascript