

In Silico Fragmentation: MetFrag and MetFusion

Suggested Exercises

1. Perform a MetFrag search of this spectrum using KEGG (too many matches using ChemSpider!):

```
105.0701 12973 433
119.0857 19630.1 656
161.1323 29891.9 999
```

<http://msbi.ipb-halle.de/MetFrag/>

This is an Orbitrap spectrum, 5 ppm error of the parent (M+H⁺) 207.138. How many matches?

What do you think is the correct answer?

Now perform the search using ChemSpider with the formula C₁₃H₁₈O₂, but don't do the fragmentation! How many matches do you get?

What happens if you do the same search with MetFusion?

2. Perform a MetFrag search of this spectrum with ChemSpider using the parent mass 216.1012 (M+H⁺). Again, don't do the fragmentation! How many structures?

```
61.9792 41017.8 1
68.0244 925017.5 35
71.0604 126421.1 4
79.0058 866817.4 33
96.0557 1626824.6 62
104.0011 1661710.4 63
110.0461 33191.5 1
132.0324 1330284.9 50
138.0775 412263.8 15
138.1028 229978.4 8
146.0229 934598 35
146.048 188498.9 7
174.0544 26094636.3 999
180.1245 109076.8 4
188.0697 166563.2 6
216.1012 22558671.7 863
```

Try again with the formula C₈H₁₄ClN₅. How many structures? Now you can perform the fragmentation!

What do you think is the right answer? How did you decide?

Try this exact same search with MetFusion. What happens now? What is the right answer? What is the rank?

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3. Perform a MetFrag search of this spectrum with ChemSpider using the parent mass 214.1263 (M+H+). How many structures?

```
57.0698 112137.4 17
71.0855 135308.2 21
102.0008 3397360.7 529
214.1261 6413030.2 999
```

Perform the in silico fragmentation with MetFrag (this may take ~5 min). What is the right answer? Why? How many others would you consider if you don't really know the answer?

Try this again with MetFusion. What happens now? How many would you consider if you don't really know the answer? What does the matrix look like?

4. If you still have time try a few more things:
- Change databases from KEGG to PubChem to ChemSpider on MetFrag and MetFusion
 - Change the mass spectral database on MetFusion
 - Change the fragmentation parameters. What happens? (do this on one of the quick examples!)
 - Have a go at this spectrum:
195.0454 46286.9 999
223.0402 19359.1 417
With precursor 223.0400 (M-H-), using MetFrag and MetFusion. Watch your settings!!!
What is it?

If you want more examples: pick random spectra from MassBank and try to see if you can identify it, even if you know the answer...