

In Silico Fragmentation: MetFrag and MetFusion

Suggested Exercises

1. Perform a MetFrag search of this Orbitrap spectrum, 5 ppm error of the parent (M+H⁺) 207.138.
How many matches: **2 matches**
What do you think is the correct answer? **Ibuprofen**
Now perform the search using ChemSpider with the formula C₁₃H₁₈O₂, but don't do the fragmentation! How many matches do you get? **1748 hits!**
What happens if you do the same search with MetFusion? **Scores closer but wrong answer still on top. No similar compounds in the database ☹**
2. Perform a MetFrag search of this spectrum with ChemSpider using the parent mass 216.1012 (M+H⁺): **1551 hits!**
Try again with the formula C₈H₁₄ClN₅. How many structures? **16 hits.**
What do you think is the right answer? How did you decide? **Atrazine: look at the number of explained peaks**
Try this exact same search with MetFusion. What happens now? What is the right answer? What is the rank? **Atrazine is still the right answer, now ranked in place 1.**
3. Perform a MetFrag search of this spectrum with ChemSpider using the parent mass 214.1263 (M+H⁺). How many structures? **135 structures.**
What is the right answer? Why? **2-octylisothiazol-3(2H)-one (but not top rank)**
How many others would you consider if you don't really know the answer? **Anything between 2 and 6 could be right, depending what criteria you choose.**
Try this again with MetFusion. What happens now? **Correct answer is now the top rank.** How many would you consider if you don't really know the answer? **Still anything between 2 & 6.**
4. d. Precursor 223.0400 (M-H⁻) using MetFrag and MetFusion.
How many structures? **248 hits with ChemSpider and MetFrag.**
What is the right answer? **2-hydroxy-9,10-anthraquinone. ChemSpider ID 11303. Rank 37 or so with MetFrag.**