***Guide to ViMMS: Thoughts***

* Two clear operations that can be performed by a user: **chemical generation** or **experiment simulation.** A potential 3rd individual component that is the **evaluator,** to be able to plot and visualise the results of a sim.
* Very extensive parameter lists for the experiment simulation, allowing for detailed customisation of re-simulation.
* Experiment simulation can be broken down into two components, either to run the entire experiment and produce an .mzML file to then perform evaluation on, or to use an existing .mzML file and bypass the need to re-sim the entire experiment and go straight to evaluation.
* Visualisation currently set up with matplotlib, will be good to look into how to make this interactive for the GUI.
* Connection to human metabolome DB could be good for sampling synthetically generated chemicals.

**Referring to Demos on ViMMS repo**

* **Chemical generation** has 3 separate methods: from an .mzML file, from HMDB, or by using the ChemicalMixtureGenerator class.
* **Simulation Algorithms:** We have 4 methods that are specific to ViMMS, and 3 that are controllers designed elsewhere. The 4 methods seem to be fairly straightforward, just loading the data with chosen parameters and then outputting the results to a specified .mzML file. TopNext doesn’t seem like too many more steps but AIF and SWATH mention an extra spectral deconvolution step that then goes on to refer to MS-DIAL.