Here we use a mixture of 10 nM Fe-desferrichrome, 10 nM Fe-desferrioxamine E, and 10 nM Ga-desferrioxamine E as an example. The LC-ICPMS data is in the xlsx file and is plotted as the eps file.

The CMA-T filter is named peakpick\_isotopelogue\_v1, which calls three functions: multiMSalignGa, rawEIC, and Accumulation

The CMA-C filter is named peakpick\_isotopelogue\_13C\_annotated, which calls two functions: multiMSalignGa, and rawEIC

Due to the size restriction by GitHub, the mzXML file could not be uploaded. Instead, we uploaded the two mat files, which are generated after mzXML file import, and spectra alignment. Furthermore, the mat files attached here are only a subset of the raw mat files, in terms of retention time. All the scans beyond 30-60 min (our interested time window) have been discarded, to generate mat files of smaller size. The code to cut the dataset is shown in line 58-64 of peakpick\_isotopelogue\_v1