**Nhu CHH: Order of programs**

Updated: 5/3/22

1. RawConverter\_Formattingv2.py

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| --- | --- |
| **Input** | **Source** |
| Working directory | Choose folder |
| MS2 Path | .MS2 file from RawConverter |
| Trial number | User choice |

1. Precursor\_matching.py

Time: **Short**

|  |  |
| --- | --- |
| **Input** | **Source** |
| Spectra | Output from **Step 1** |
| Fragment list | User-provided list of fragments |
| Target list | User-provided list of targets |
| Final directory | Choose folder |

1. Fragment\_matching.py

Time: **Medium**

|  |  |
| --- | --- |
| **Input** | **Source** |
| Spectra | Output from **Step 1** |
| Fragment list | User-provided list of fragments |
| Precursor matches | Output from **Step 2** |
| Final directory | Choose folder |
| Sample name | User choice |
| Error precursor | User choice, in ppm |
| Error fragment | User choice, in Da |
| Precursor charges | User choice |
| Fragment charges | User choice |

1. CHH\_charge\_loop0\_2.py

|  |  |
| --- | --- |
| **Input** | **Source** |
| Spectra | Output from **Step 1** |
| Fragment list | User-provided list of fragments |
| Target list | User-provided list of targets |
| Final directory | User choice |
| Sample name | User choice |
| Error precursor | User choice, in ppm |
| Error fragment | User choice, in Da |
| Precursor charges | User choice |
| Fragment charges | User choice |

1. CHH\_charge\_loop0\_3.py

|  |  |
| --- | --- |
| **Input** | **Source** |
| Spectra | Output from **Step 1** |
| Fragment list | User-provided list of fragments |
| Target list | User-provided list of targets |
| Working directory | User choice |
| Final directory | User choice |
| Precursor matches | Output from **Step 5** |
| Sample name | User choice |
| Error precursor | User choice, in ppm |
| Error fragment | User choice, in Da |
| Precursor charges | User choice |

1. CHH\_charge\_loop0\_4.py

|  |  |
| --- | --- |
| **Input** | **Source** |
| Spectra | Output from **Step 1** |
| Fragment list | User-provided list of fragments |
| Target list | User-provided list of targets |
| Working directory | Same directory as in **Step 6** |
| Final directory | User choice |
| Precursor matches | Output from **Step 5** |
| Sample name | User choice |
| Error precursor | User choice, in ppm |
| Error fragment | User choice, in Da |
| Precursor charges | User choice |

1. Fragment\_combine.py

|  |  |
| --- | --- |
| **Input** | **Source** |
| Zero directory | Folder of fragment matches from **step 6** |
| Normal dataframe | Fragment matches from **step 4** |
| Output directory | User choice |
| Sample name | User choice |

1. Summary\_generate.py

|  |  |
| --- | --- |
| **Input** | **Source** |
| Fragment matches | Output from **step 7** |
| Final directory | User choice |
| Sample name | User choice |