This folder contains a series of .csv files which contain the data used to create the mass spectra and iso-abundance plots presented in the manuscript “Molecular Characterization of Strongly- and Weakly-interfacially Active Asphaltenes by High-Resolution Mass Spectrometry”.

The files are named as descriptively as possible, with WA, RA and IAA being the full-spectra analysis of these samples. The precursor and fragment data is labelled accordingly for both *m/z* 450 and 650. Finally, the extrography fractions are named ‘RA’ or ‘IAA’ followed by the solvent used for the extraction. The following list shows the file names corresponding to each figure:

**Figure 1** = WA.csv, RA.csv, IAA.csv

**Figure 2** = RA.csv, IAA.csv

**Figure 3** = RA.csv, IAA.csv (even / odd columns)

**Figure 4** = RA\_precursors\_650mz.csv, IAA\_precursors\_650mz.csv

**Figure 5** = RA\_precursors\_650mz.csv, IAA\_precursors\_650mz.csv

**Figure 6** = RA\_TolTHFMeOH.csv, IAA\_TolTHFMeOH.csv, RA\_HepTol.csv, RA\_Acetone.csv, IAA\_Acetone.csv

**Figure 7** = n/a

**Figure S1** = WA.csv, RA.csv, IAA.csv

**Figure S2** = WA.csv, RA.csv, IAA.csv

**Figure S3** = WA.csv, RA.csv, IAA.csv

**Figure S4** = WA.csv, RA.csv, IAA.csv

**Figure S5** = WA.csv, RA.csv, IAA.csv

**Figure S6** = WA.csv, RA.csv, IAA.csv

**Figure S7** = WA.csv, RA.csv, IAA.csv

**Figure S8** = WA.csv, RA.csv, IAA.csv

**Figure S9** = RA\_TolTHFMeOH.csv, IAA\_TolTHFMeOH.csv, RA\_HepTol.csv, RA\_Acetone.csv, IAA\_Acetone.csv

**Figure S10** = RA\_TolTHFMeOH.csv, IAA\_TolTHFMeOH.csv, RA\_HepTol.csv, RA\_Acetone.csv, IAA\_Acetone.csv

**Figure S11** = RA\_TolTHFMeOH.csv, IAA\_TolTHFMeOH.csv, RA\_HepTol.csv, RA\_Acetone.csv, IAA\_Acetone.csv

**Figure S12** = RA\_TolTHFMeOH.csv, IAA\_TolTHFMeOH.csv, RA\_HepTol.csv, RA\_Acetone.csv, IAA\_Acetone.csv

**Figure S13** = RA\_precursors\_450mz.csv, IAA\_precursors\_450mz.csv

**Figure S14** = RA\_precursors\_450mz.csv, IAA\_precursors\_450mz.csv

**Figure S15** = RA\_precursors\_650mz.csv, IAA\_precursors\_650mz.csv