**Supplementary Materials**

Integrating high-resolution mass spectral data, bioassays and computational models to annotate bioactives in botanical extracts: Case Study - analysis of *Centella asiatica* extract associates dicaffeoylquinic acids with protection against amyloid-β toxicity in an MC65 cell model.

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**Figure S1.** Fractionation scheme. 21 subfractions of CAW extract generated by solvent:solvent partitioning and LH-20 column chromatography. We analyzed each subfraction by flow-injection HRMS and correlated the features found with cytoprotective activity in an amyloid β-toxicity MC65 neuroblastoma cell model. In addition, CAW was analyzed by LC-HRMS/MS for obtaining precursor and fragment ion information for GNPS molecular network analysis. Relative polarity across fractions is indicated by “–“ and “+”.