Supporting information for: KairosMS: A new solution for the processing of hyphenated ultrahigh resolution mass spectrometry data

Remy Gavard,† Hugh E. Jones,‡ Diana Catalina Palacio Lozano,‡ Mary J. Thomas,† David Rossell,¶§ Simon E. F. Spencer,† and Mark P. Barrow*,‡

MAS CDT, University of Warwick, Coventry, CV4 7AL, United Kingdom, Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom, Department of Statistics, University of Warwick, Coventry, CV4 7AL, United Kingdom, and Department of Economics & Business, Universitat Pompeu Fabra, Barcelona, 08005, Spain

E-mail: M.P.Barrow@warwick.ac.uk

*To whom correspondence should be addressed
†MAS CDT, University of Warwick, Coventry, CV4 7AL, United Kingdom
‡Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom
¶Department of Statistics, University of Warwick, Coventry, CV4 7AL, United Kingdom
§Department of Economics & Business, Universitat Pompeu Fabra, Barcelona, 08005, Spain
Figure S1: Screenshot presenting KairosMS interface.
Figure S2: Mass spectrum created using the EICs extracted to be used for molecular assignments.

Figure S3: Comparison of the elution of the O$_2$[H] class contribution between an OSPW and two Groundwater samples using a scan by scan resolution.
Figure S4: EICs for the monoisotopic form and isotopologues of $C_{16}H_{26}O_2$ [H] for the G1, G2 and OSPW samples (G1 and G2 perfectly overlap). The same retention for the isotopologues is further evidence for the compositional assignment.
Figure S5: Elution of DBE series (homologous series) comprising the O$_2$[H] class.
Figure S6: Percentage of contribution to the total signal, for all the classes identified in the SRFA and Marine DOM samples.

Figure S7: Elemental contributions for the samples SRFA and Marine DOM, based on all the assigned EICs.
Figure S8: van Krevelen diagram of the $H/C$ ratio vs $O/C$ ratio for the Marine DOM and SRFA samples.

Figure S9: Comparison of the EIC of the same molecular assignment as seen in DA and KairosMS after peak picking at $S/N$ 1.
Figure S10: EIC from a peptide digest of ubiquitin analyzed by LC-FTICR MS.