

Supporting information for:

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

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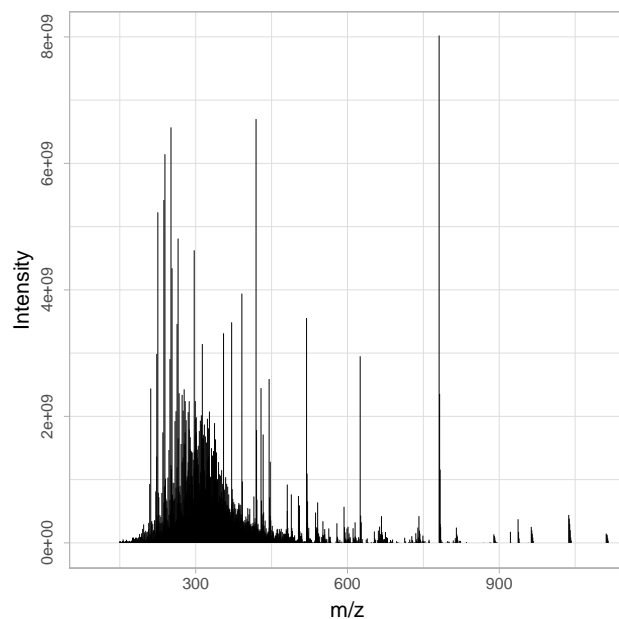


Figure S2: Mass spectrum created using the EICs extracted to be used for molecular assignments.

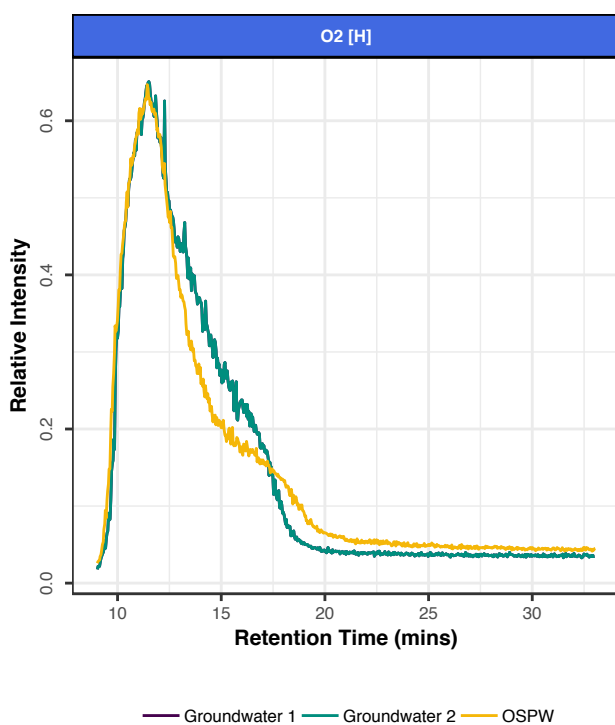


Figure S3: Comparison of the elution of the O<sub>2</sub>[H] class contribution between an OSPW and two Groundwater samples using a scan by scan resolution.

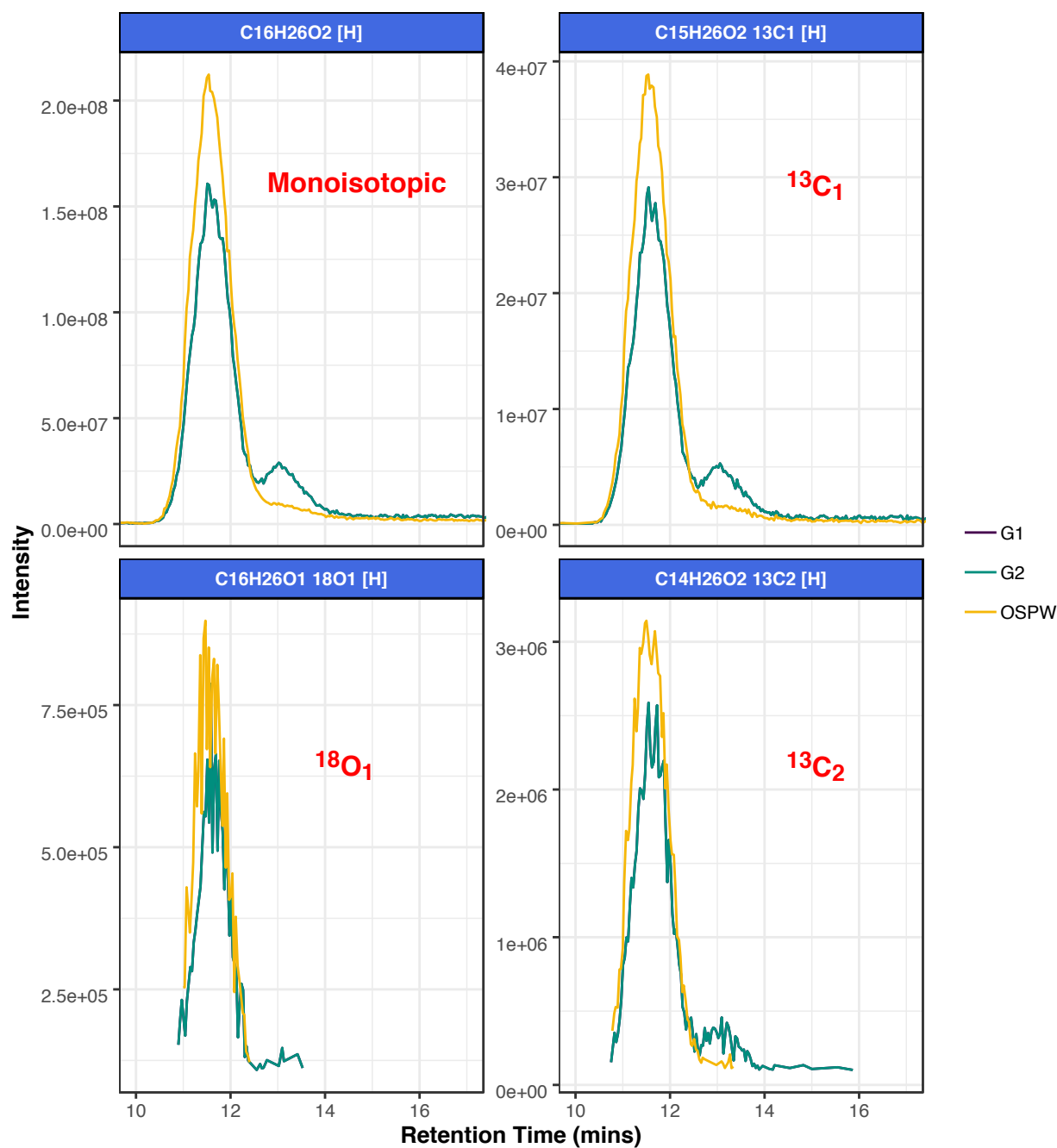


Figure S4: EICs for the monoisotopic form and isotopologues of  $C_{16}H_{26}O_2$  [H] for the G1, G2 and OSPW samples (G1 and G2 perfectly overlap). The same retention for the isotopologues is further evidence for the compositional assignment.

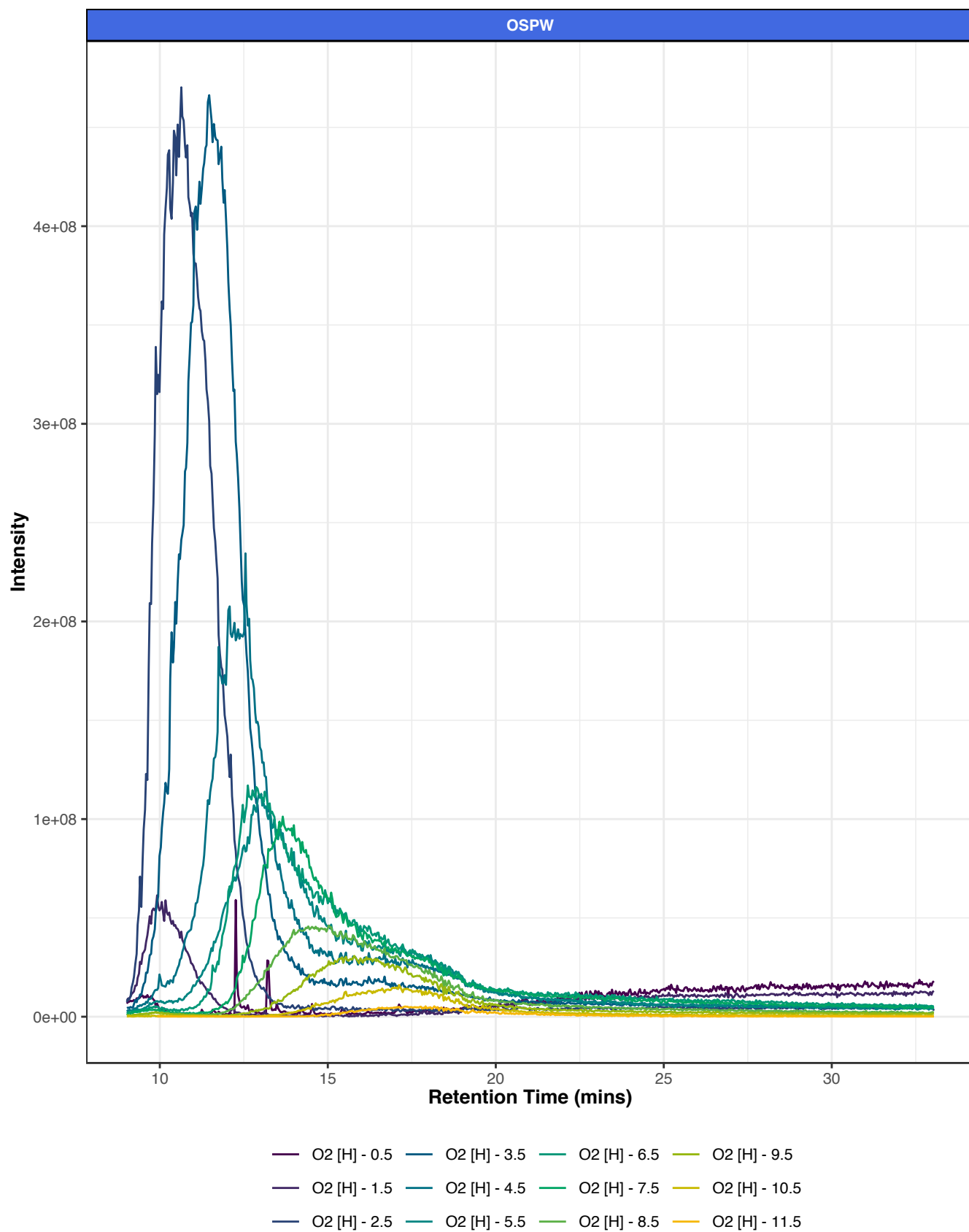


Figure S5: Elution of DBE series (homologous series) comprising the O<sub>2</sub>[H] class.

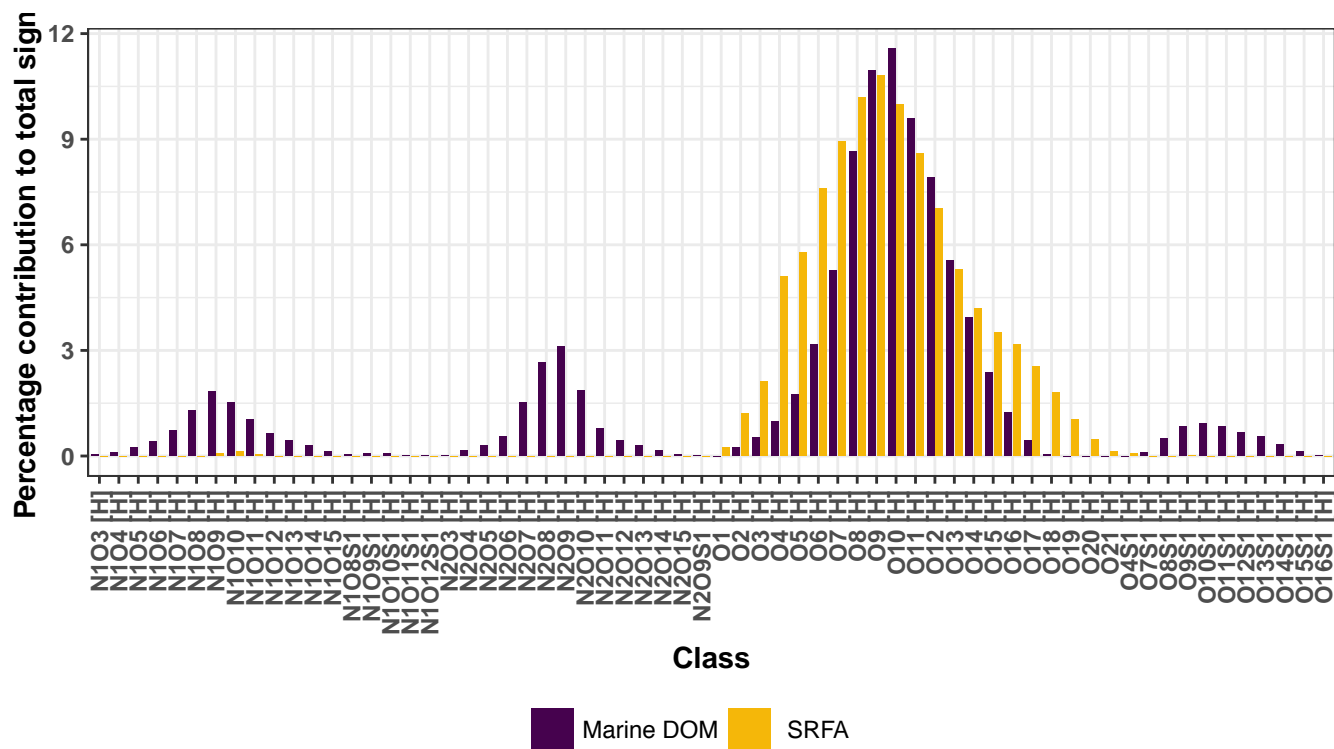


Figure S6: Percentage of contribution to the total signal, for all the classes identified in the SRFA and Marine DOM samples.

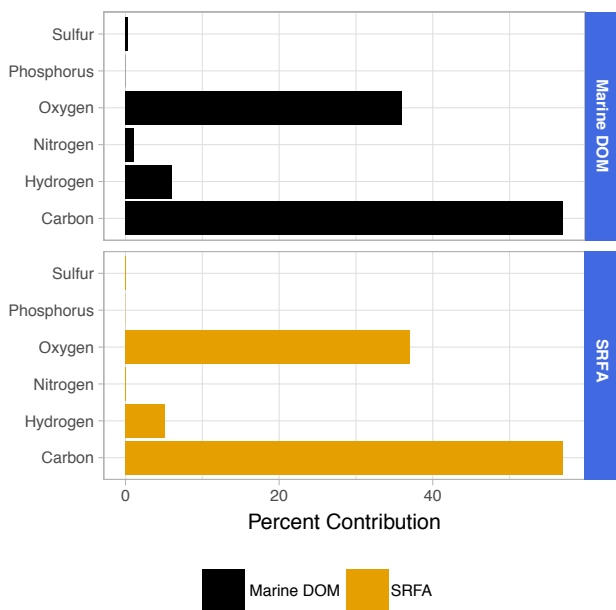


Figure S7: Elemental contributions for the samples SRFA and Marine DOM, based on all the assigned EICs.

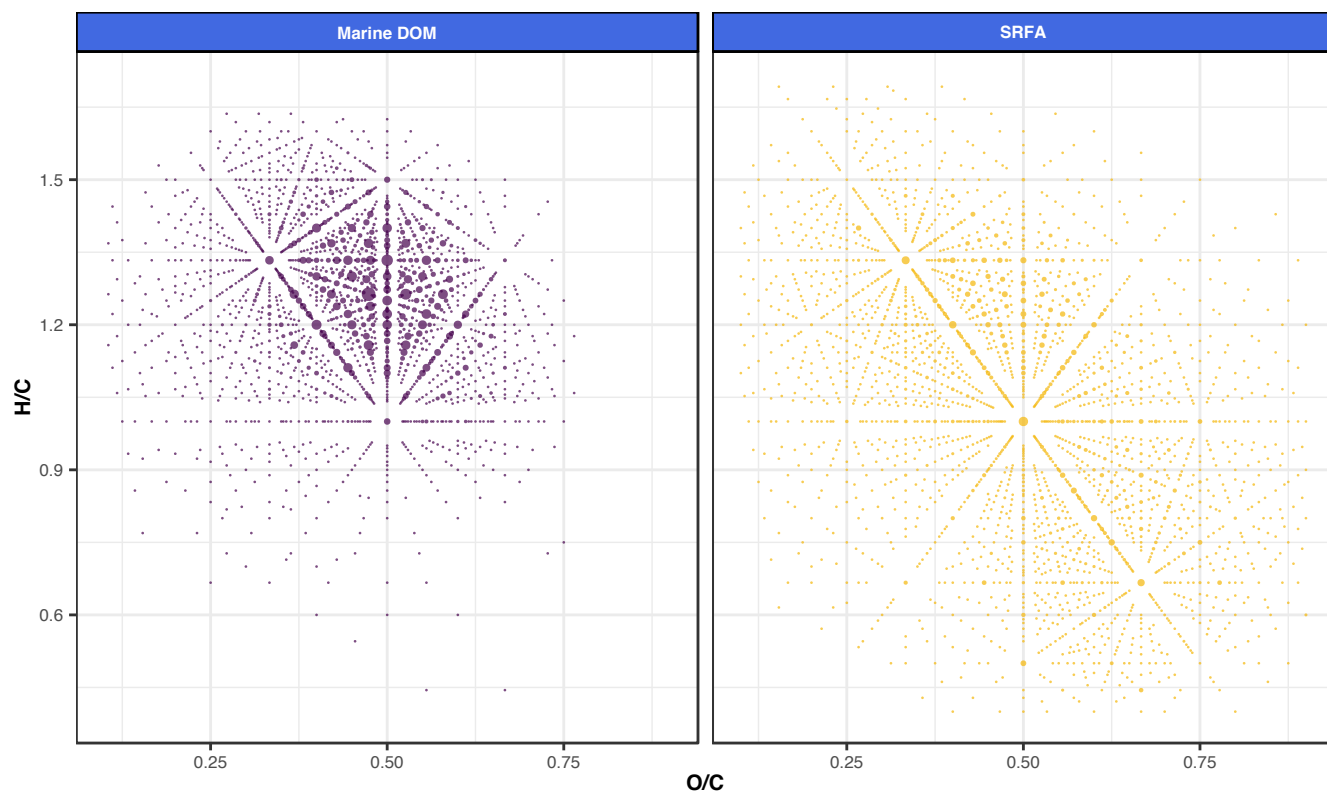


Figure S8: van Krevelen diagram of the  $H/C$  ratio vs  $O/C$  ratio for the Marine DOM and SRFA samples.

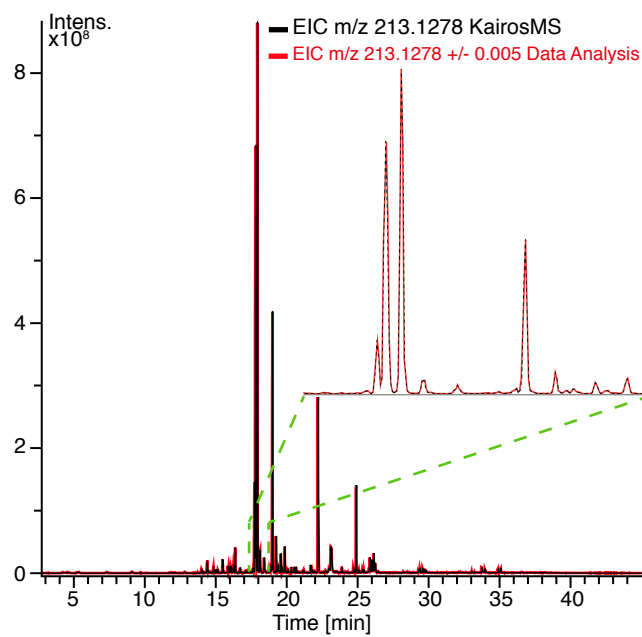


Figure S9: Comparison of the EIC of the same molecular assignment as seen in DA and KairosMS after peak picking at  $S/N$  1.

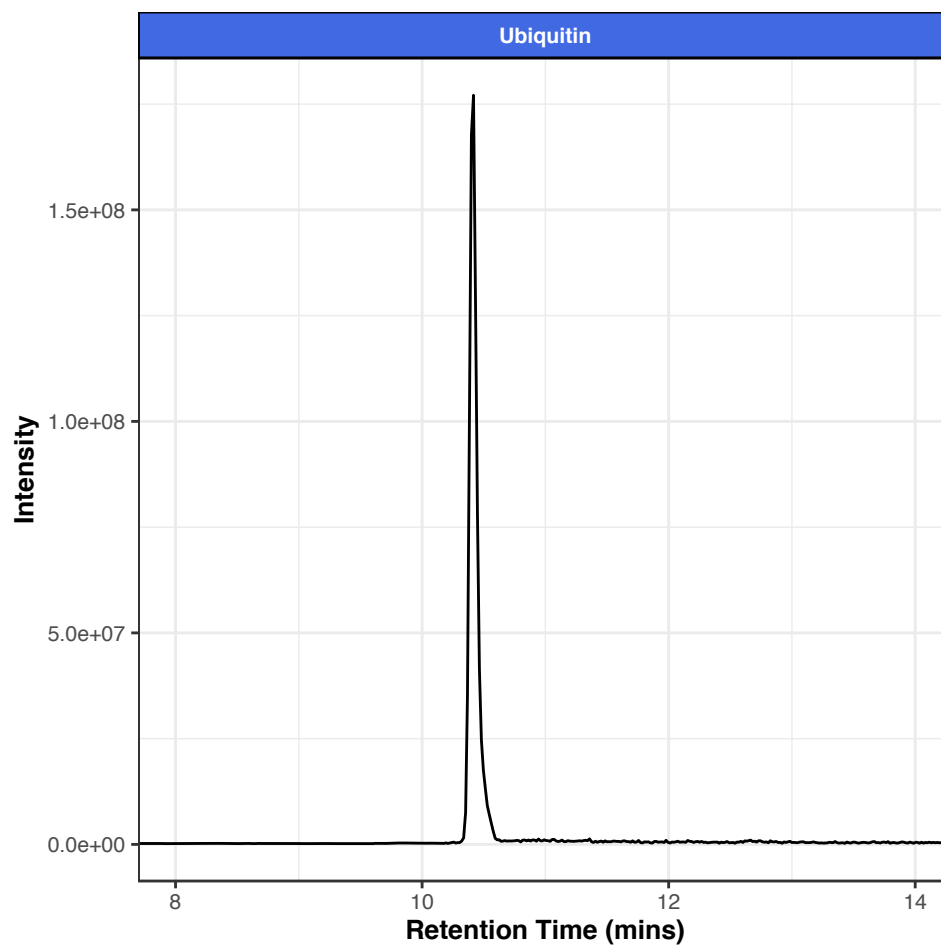


Figure S10: EIC from a peptide digest of ubiquitin analyzed by LC-FTICR MS.