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Sorption of Aldrich humic acids onto hematite:
Insights into fractionation phenomena by
ElectroSpray Ionization with Quadrupole Time-Of-
Flight Mass Spectrometry

Supplementary Information

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This section contains 6 pages, 1 table and 5 figures.

The following supplement gives complementary information about the experimental conditions used throughout the study, the values of absorbance at 203 and 253 nm and evolution of the ratio A_{253}/A_{203} , the absorbance spectra obtained for the initial PAHA sample and of supernatants from sorption experiments.

Complementary ESI mass spectra are also given:

- verification of the influence of concentration on ESI mass spectra for a given sample;
- intermediate mass spectra of the supernatants that were not essential to the discussion;
- the evolution of number-averaged ($\bar{I}_n$) and weight-averaged ($\bar{I}_w$) mean molecular intensities.

Table S1: initial PAHA concentration and pH of the sorption experiments and absorbance values of the initial sample and supernatant: $[\alpha\text{-Fe}_2\text{O}_3] = 500 \text{ mg/L}$.

[PAHA] ^o (mg/L)	pH	A_{253}	A_{203}	A_{253}/A_{203}
Initial sample				
11	7.14	0.4263	0.6350	0.67
Supernatant				
3.3	7.19	0.0153	0.0507	0.30
7.7	7.03	0.1194	0.2238	0.53
11	7.10	0.2134	0.3148	0.68
22	7.02	0.6161	0.8767	0.70
33	7.00	1.0619	1.4872	0.71
55	7.07	1.9327	2.6268	0.74
111 ^a	7.13	-	-	-

^a not analysed due to saturation of the UV-Visible detector

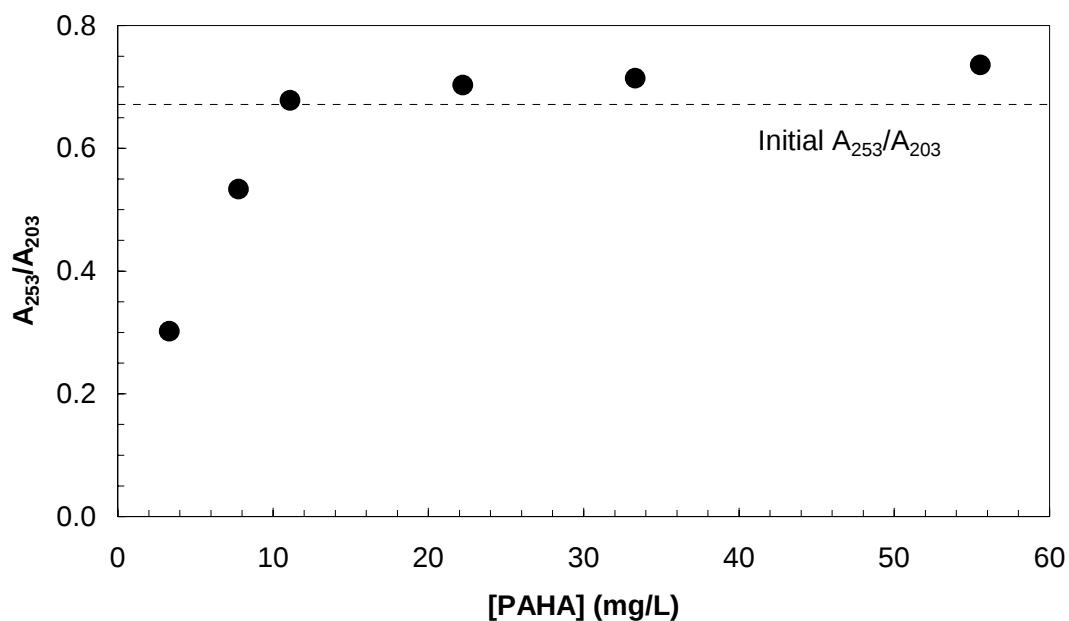


Figure S1: Variation of A_{253}/A_{203} ratios of supernatant samples (from Table S1) after PAHA retention by 500 mg/L hematite at $\text{pH} \approx 7$.

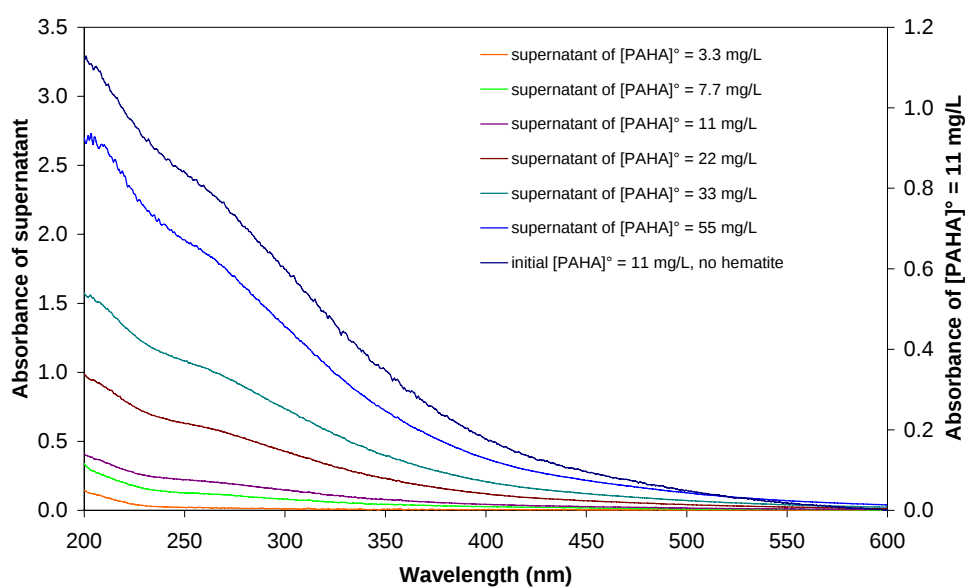


Figure S2: Absorbance spectra of initial PAHA and of supernatant from sorption experiment onto 500 mg/L hematite at $\text{pH} \approx 7$ (see table S1).

ESI QToF mass spectra of PAHA at 25 mg/L and 11 mg/L have been compared on Figure S3. No difference in the shape of the mass spectra can be evidenced under our conditions and for this particular humic extract.

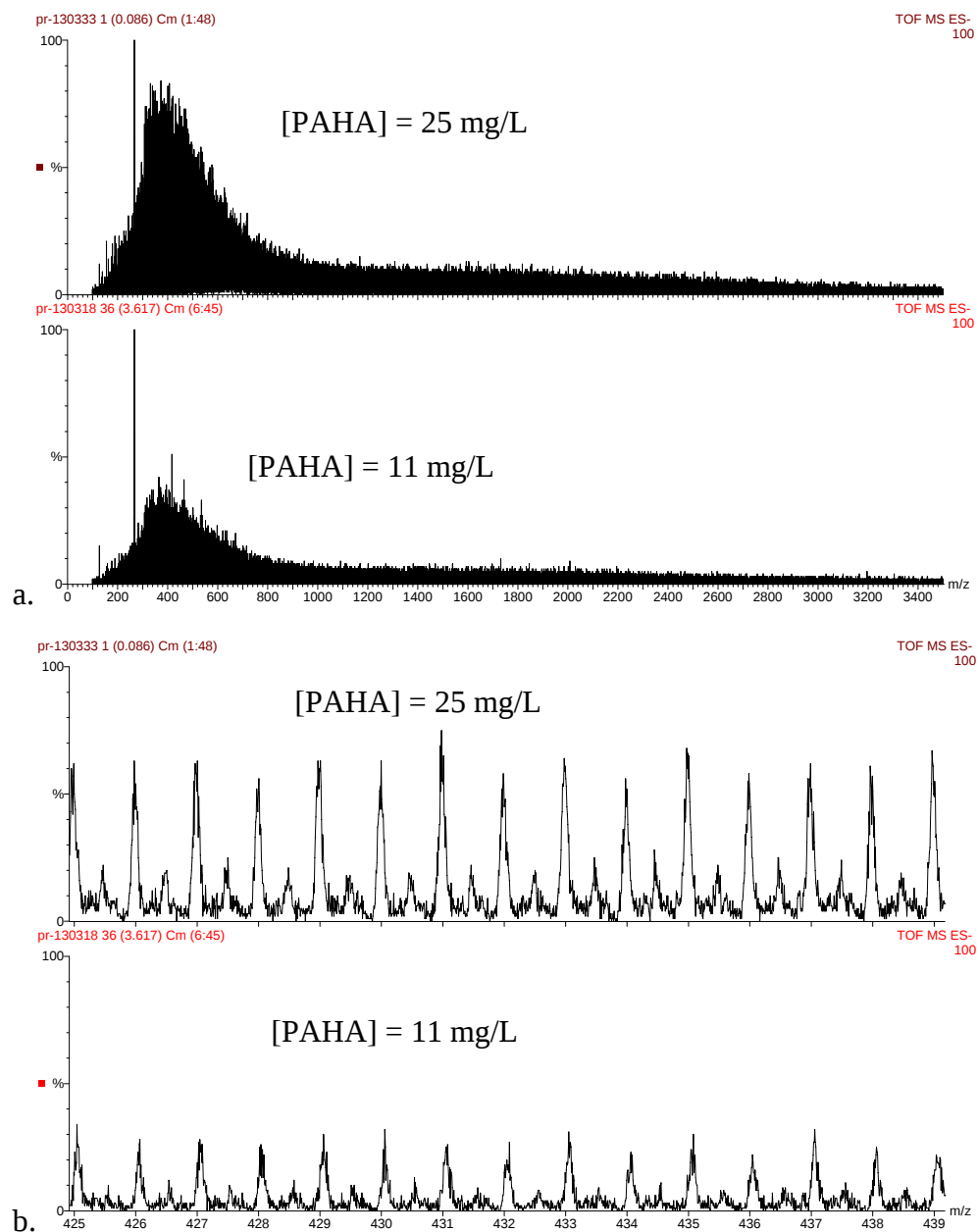
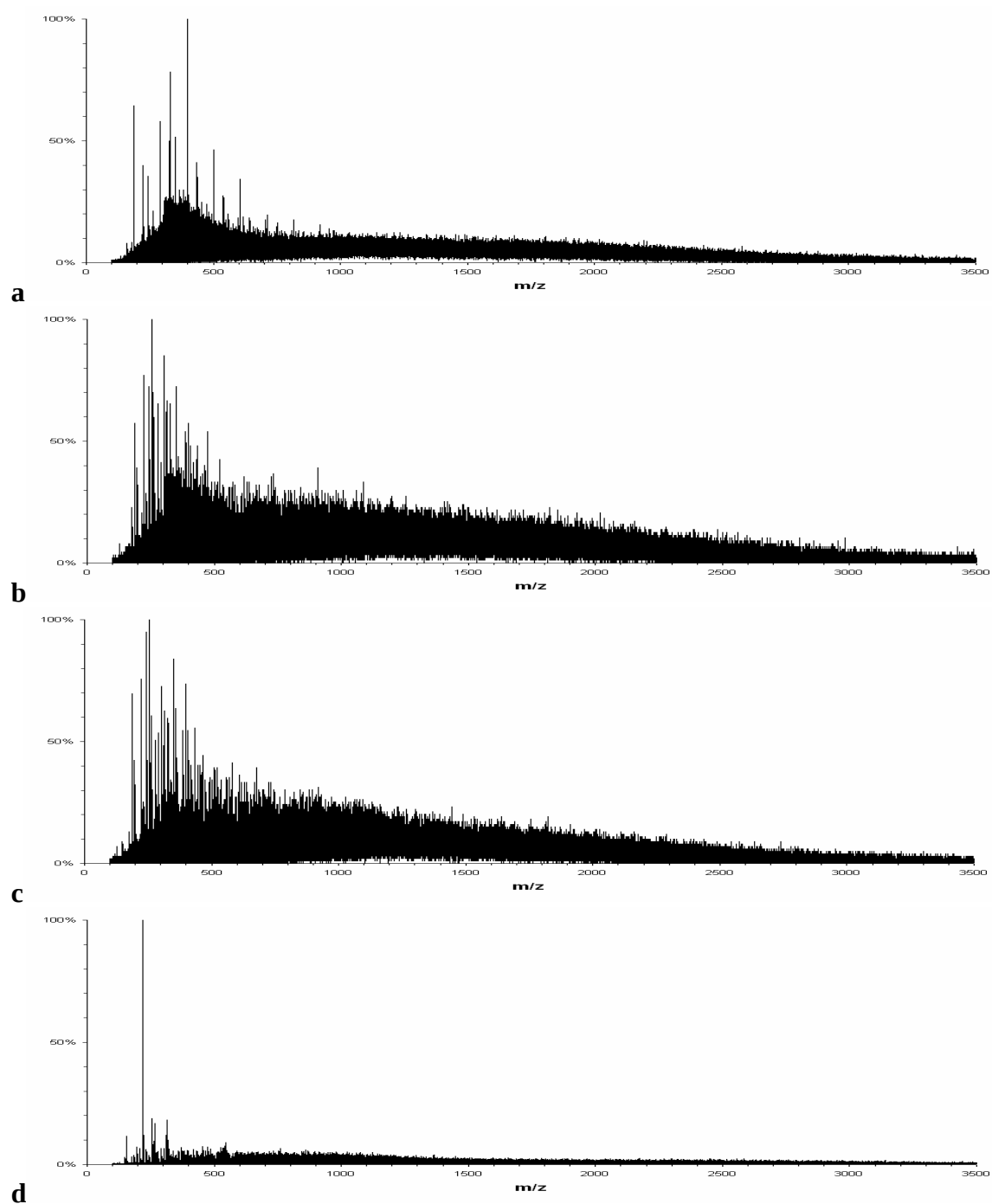


Figure S3: Comparison between ESI Q-ToF negative ion mass spectra of PAHA obtained at two different concentration at cone 55V, a. [PAHA] = 25 ppm and [PAHA] = 11 ppm in the range 100-3500 Da; b. detail in the range 425-439 Da.



d Figure S4: ESI Q-ToF negative ion mass spectra of PAHA (a) before sorption: 11 mg/L at pH ≈ 7 ; (b-d) after sorption at pH ≈ 7 , $[\alpha\text{-Fe}_2\text{O}_3] = 500$ mg/L, under varying initial [PAHA] : (a) 111 mg/L, (b) 55 mg/L (c) 22 mg/L, (d) 7.7 mg/L.

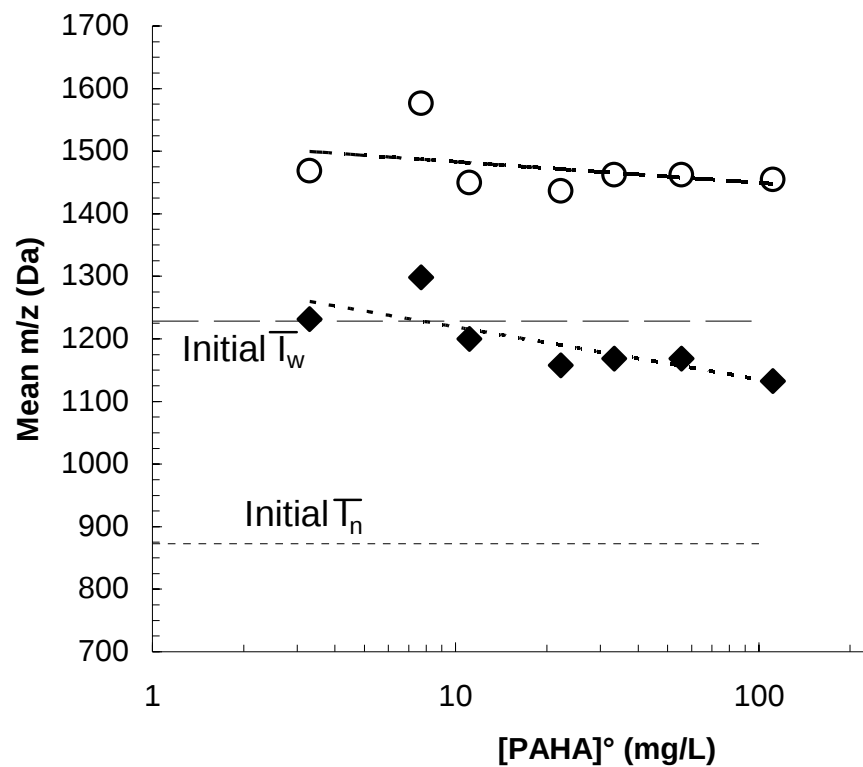


Figure S5: Influence of PAHA sorption onto hematite on the mean molecular intensity calculated from supernatants ESI mass spectra compared to the initial solution at pH $\approx$ 7: m/z interval between 100 and 2535 Da; black diamonds $\bar{I}_n$, white circles $\bar{I}_w$; Horizontal dotted and dashed lines are the values of the initial PAHA at pH $\approx$ 7 sample before retention for $\bar{I}_w$ and $\bar{I}_n$ respectively.