

## Supplementary Material

### **Rare earth elements binding humic acids: NICA–Donnan modelling**

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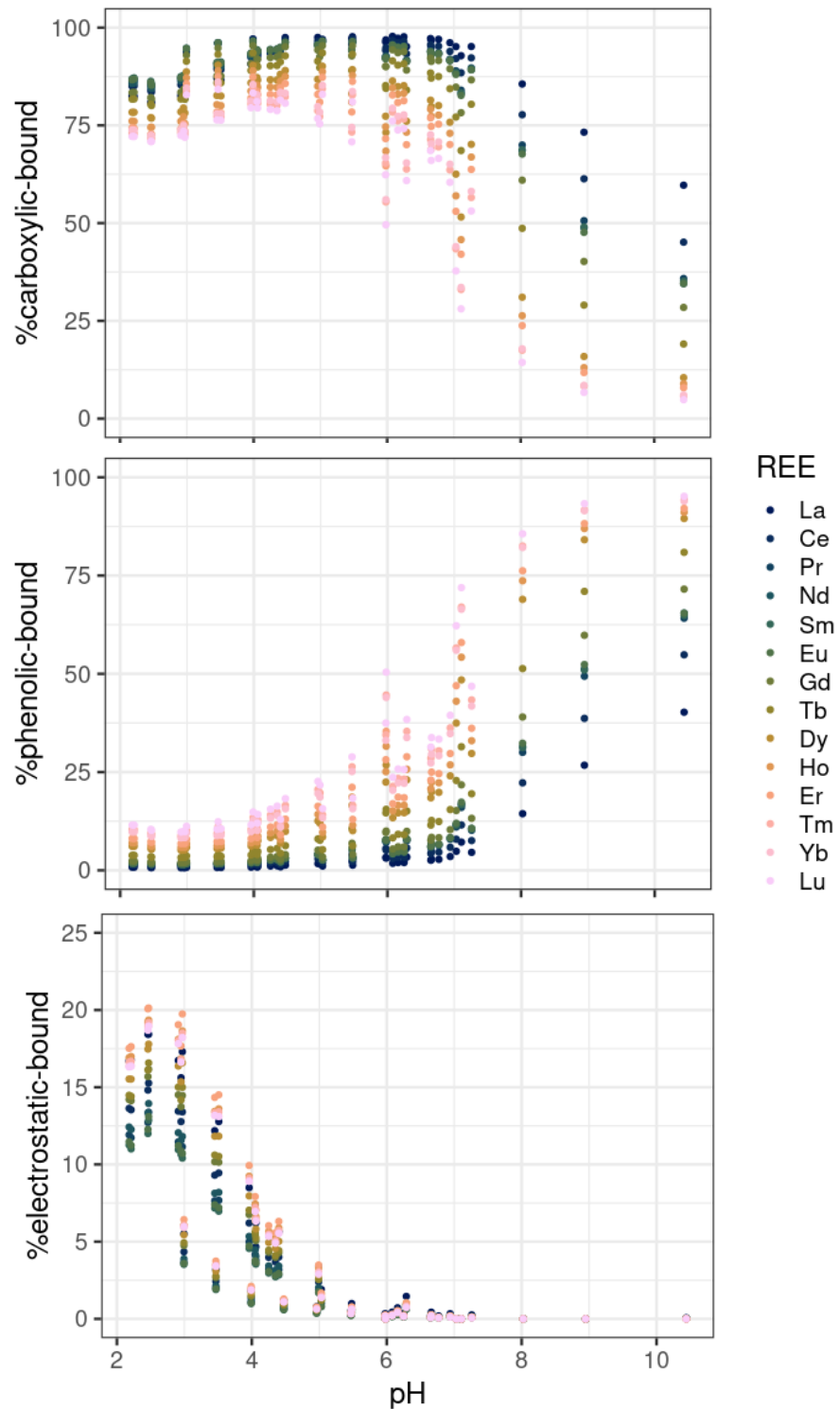
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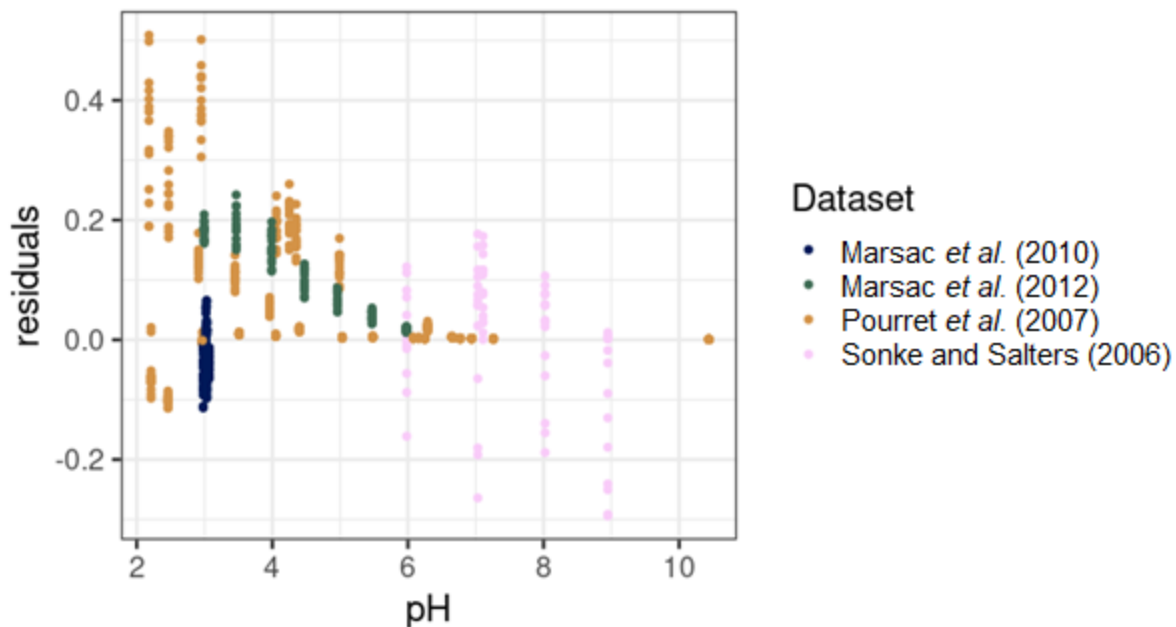
**Table S1.** NICA–Donnan binding parameters obtained in the literature modelled for generic HA, for proton and competitor metals.

Ion	H <sup>+</sup>	Fe <sup>3+</sup>		Al <sup>3+</sup>		Cu <sup>2+</sup>
Parameter	Generic	Generic	Adapted from LFER	Generic	Adapted from LFER	Generic
b	0.49					
Q <sub>max,1</sub> (eq/kg)	3.15					
Q <sub>max,2</sub> (eq/kg)	2.55					
p <sub>1</sub>	0.62					
p <sub>2</sub>	0.41					
log $\tilde{K}_{i,1}$	2.93	3.5	3.95	-1.05	2.09	2.23
log $\tilde{K}_{i,2}$	8.00	17.5		8.89	9.07	6.85
n <sub>i,1</sub>	0.81	0.30		0.40		0.56
n <sub>i,2</sub>	0.63	0.25		0.30		0.34

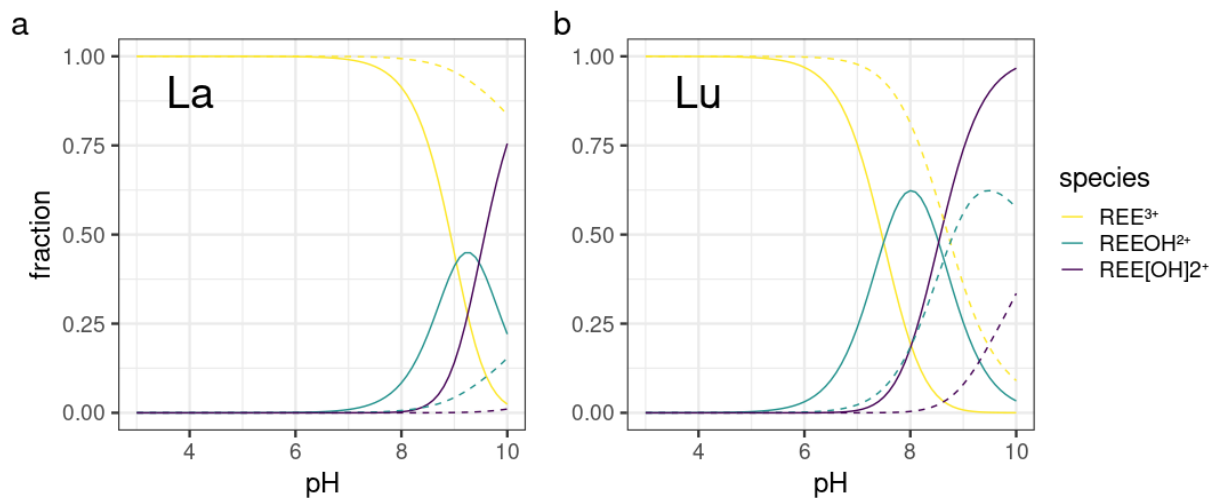
Sources: H<sup>+</sup>, Fe<sup>3+</sup>, Al<sup>3+</sup> and Cu<sup>2+</sup> Generic are from Milne *et al.* (2003); Fe<sup>3+</sup> and Al<sup>3+</sup> Adapted from LFER (this study)



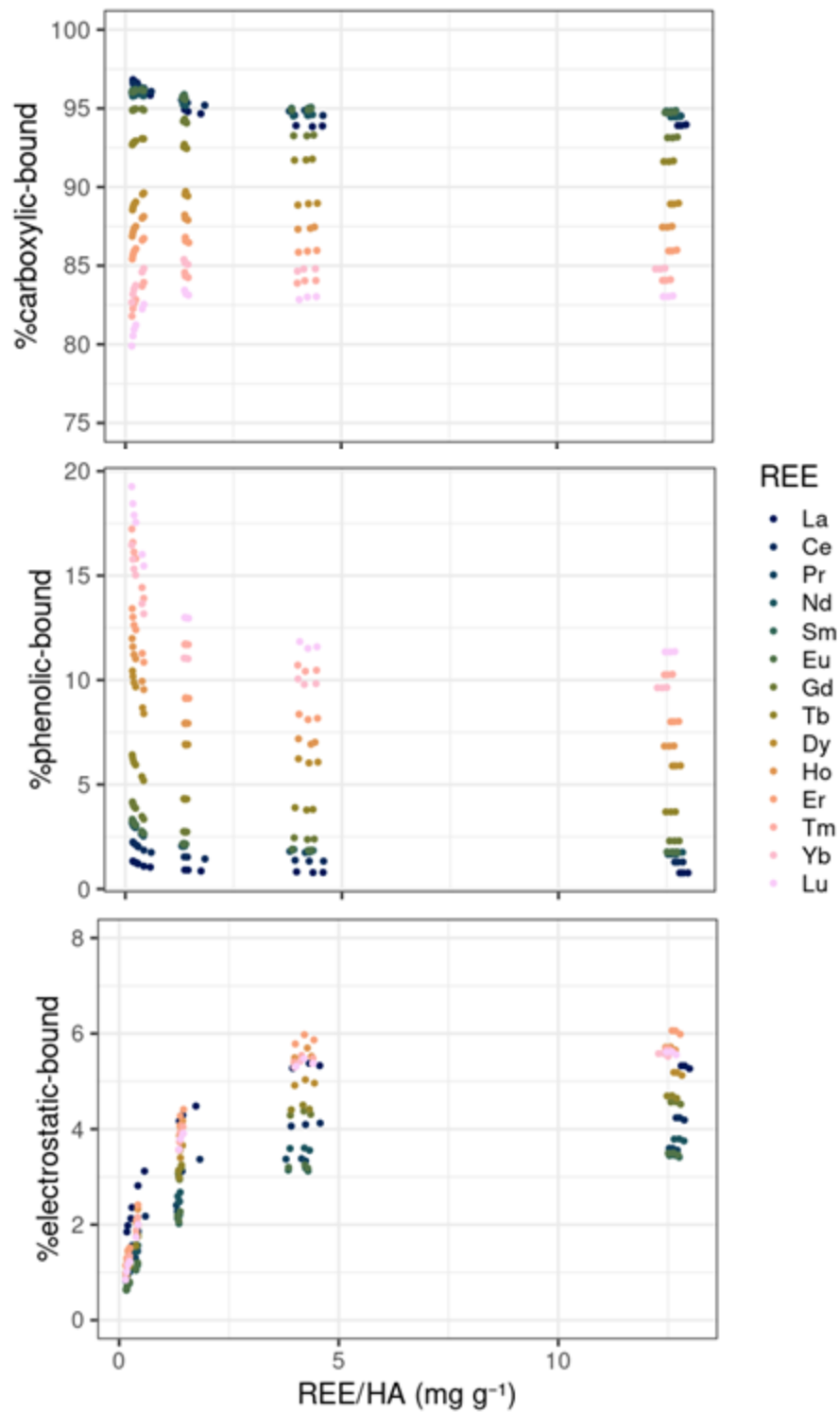
**Fig. S1.** Predicted speciation of REEs bound to HA as a function of pH. Marsac *et al.* (2010) dataset was excluded from the plot for the sake of clarity, due to the limited pH range of these experiments, performed in different conditions.



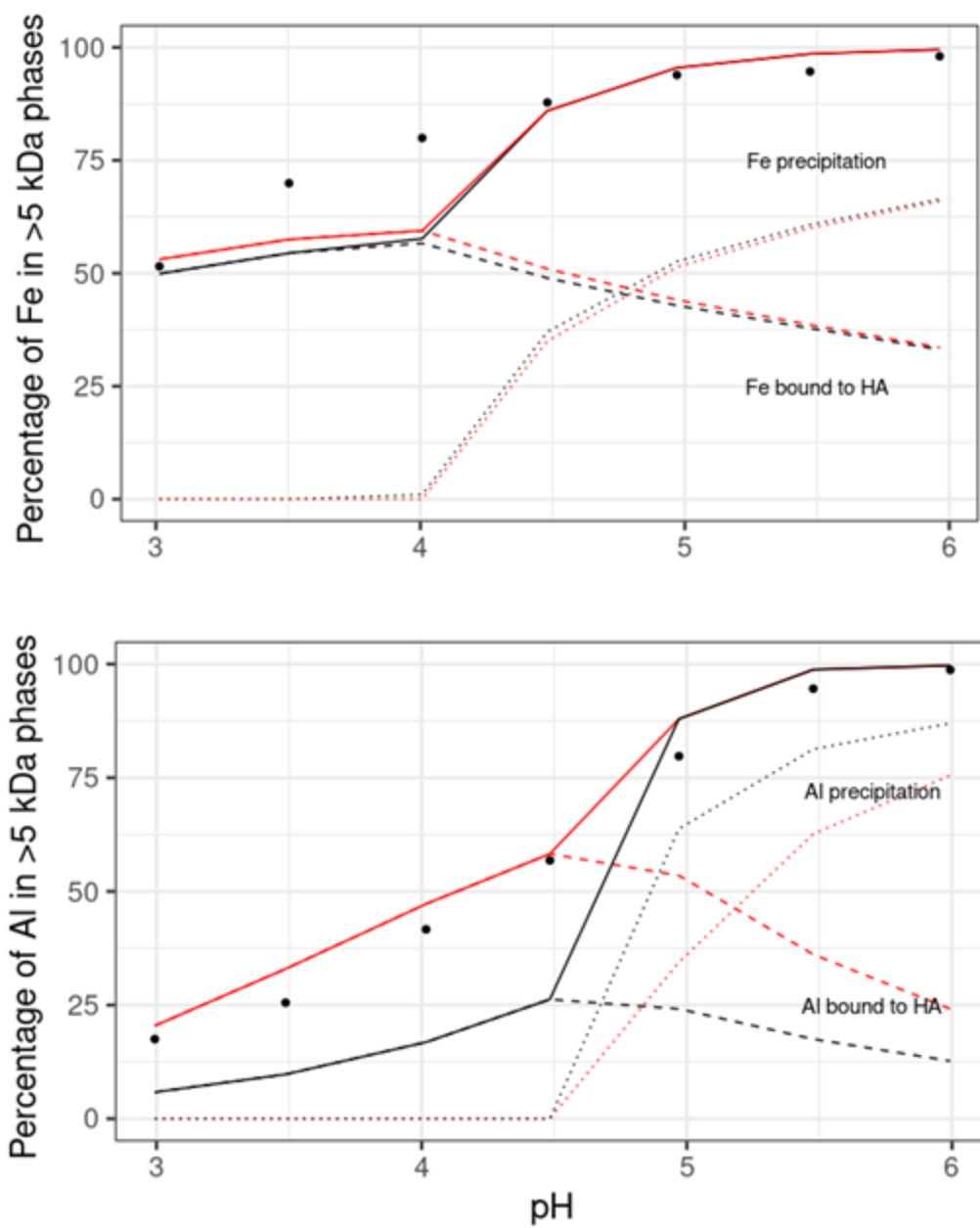
**Fig. S2.** Residuals distribution of parameterization dataset as a function of solution pH and original dataset.



**Fig. S3.** Calculated speciation of La (a) and Lu (b) in bulk solution (solid lines) and in the Donnan volume (dashed lines) using generic HA binding parameters.



**Fig. S4.** Predicted speciation of REEs bound to HA as a function of REE/HA ratio for the Marsac *et al.* (2010) dataset.



**Fig. S5.** Percentage of  $\text{Fe}^{\text{III}}$  (top) or  $\text{Al}^{\text{III}}$  (bottom) retained by a 5-kDa filter *v.* pH in presence of REE, as experimentally determined (symbols) or calculated (lines) for  $[\text{HA}] = 12 \text{ mg L}^{-1}$ ,  $\sum[\text{REE}] = [\text{Al}/\text{Fe}] = 10 \text{ }\mu\text{M}$  in 0.01 M NaCl. Black lines correspond to default generic parameters, red lines to Fe/Al parameters adapted according to the LFER given in Fig. 4.

## References

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