

Supplementary Material (ESI) for Journal of Environmental Monitoring
This journal is © The Royal Society of Chemistry 2009

Supplementary information:

Photochemical release of humic and fulvic acid-bound metals from simulated soil and streamwater

Petr Porcal, Aria Amirbahman, Jiří Kopáček, František Novák, Stephen A. Norton

¹³C NMR spectroscopy

Quantitative ¹³C liquid-state nuclear magnetic resonance (¹³C LS NMR) spectra of HA and FA dissolved in 0.1M sodium deuterioxide (Sigma-Aldrich) were measured on a Bruker Avance DRX 500 spectrometer operating at 125.75 MHz using the following parameters: recycle delay of 5 s, number of scans = 20,000, and inverse gated decoupling. The free induction decay was processed with line broadening of 20 Hz (Figure S1). The ¹³C chemical shifts were referenced to tetramethylsilane; quantification was achieved by instrumental integration of NMR peaks. The chemical shift regions 0 – 45, 45 – 110, 110 – 160 and 160 – 220 ppm were assigned to alkyl carbon (C), O-alkyl C, aromatic C, and carboxylic C, respectively ¹. We used the local minimum at 108 ppm as the border between aromatic and O-alkyl regions also. Aromaticity (f_a) was calculated as the ratio between aromatic and the sum of aromatic plus aliphatic (alkyl + O-alkyl) carbons ².

1. M. A. Wilson, NMR techniques and application in geochemistry and soil chemistry. Pergamon Press, Oxford, 1987
2. P. G. Hatcher, M. Schnitzer, L. W. Dennis, G. A. Maciel, Soil Sci. Soc. Am. J., 1981, 45, 1089 – 1094

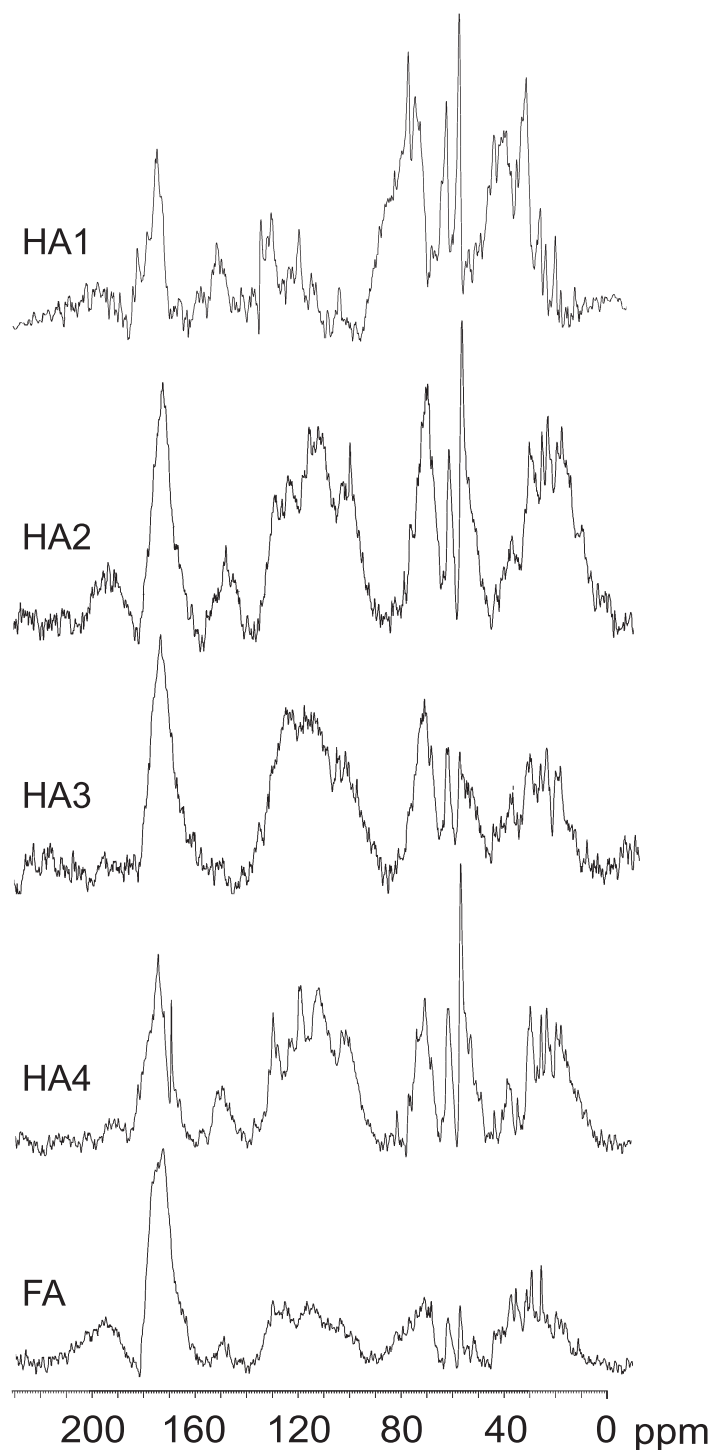


Figure S1: Quantitative solution state ^{13}C liquid-state nuclear magnetic resonance spectra of humic (HA1 – HA4) and fulvic (FA) acids dissolved in 0.1M NaOD, measured on Bruker Avance DRX 500 spectrometer operating at frequency of 125.75 MHz using the following parameters: recycle delay of 5 s, number of scans of 20,000, and inverse gated decoupling. The FID was processed with line broadening of 20 Hz. The ^{13}C chemical shifts were referenced to tetramethylsilane, quantitative analysis was achieved by instrumental integration of NMR peaks. The chemical shifts regions 0 – 45, 45 – 110, 110 – 160 and 160 – 220 ppm were assigned to alkyl carbon (C), O alkyl C, aromatic C, and carboxylic C, respectively.

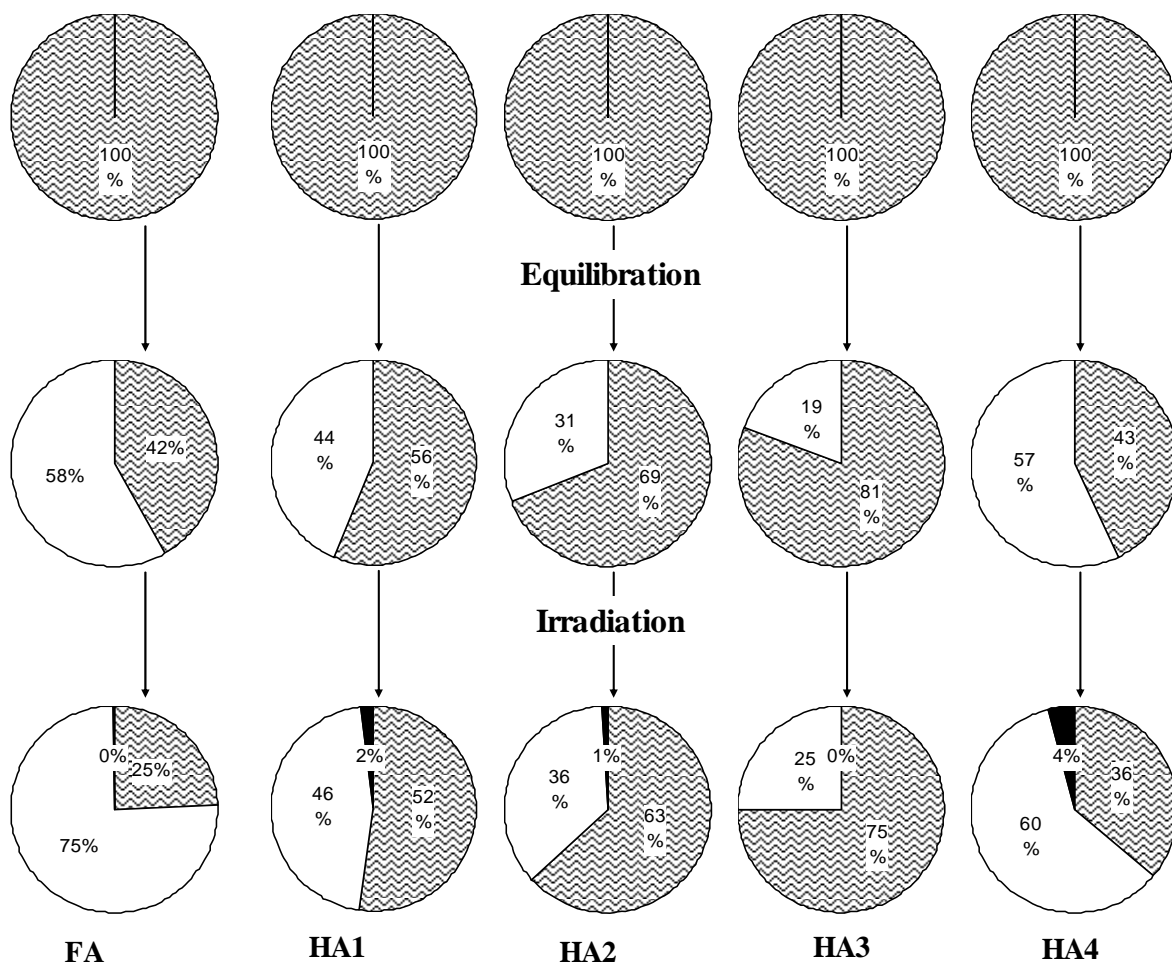


Figure S2: The changes in aluminum fractionation during the experiment. The equilibration represents the changes that occurred during the establishing of new equilibrium after passing the sample through the strong cation exchange resin. The irradiation represents changes induced by 2 hrs of irradiation at 350 nm.

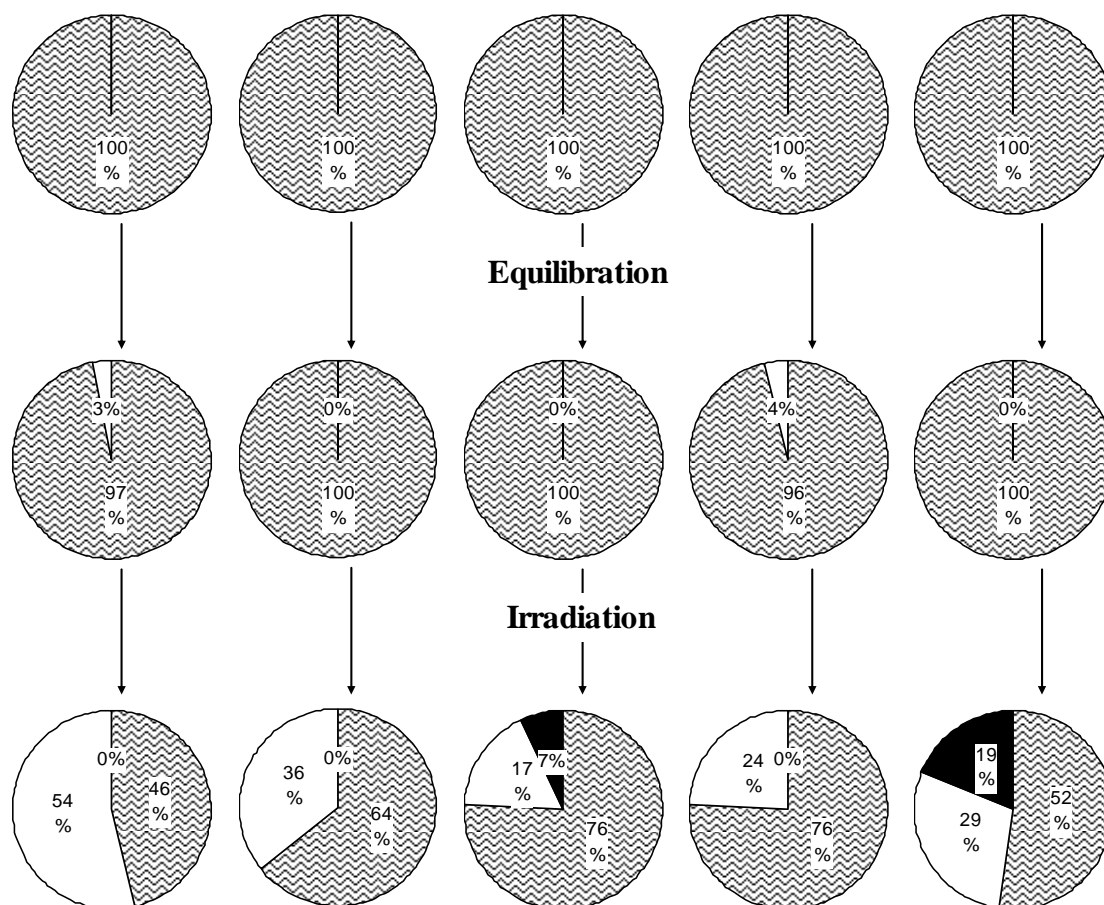


Figure S3: The changes of Fe fractions during the experiment. The equilibration represents the changes that occurred during the establishing of new equilibrium after passing the sample through the strong cation exchange resin. The irradiation represents changes induced by 2 hrs of irradiation at 350 nm.