

Supplementary Material (ESI) for Analyst
This journal is (C) The Royal Society of Chemistry 2007

The Analyst : Prepared Nov 15th 2007.

Supporting Information for:

**Direct ¹H NMR spectroscopy of Dissolved Organic
Matter in Natural Waters**

Buan Lam and André J. Simpson^{1*}

¹*Department of Chemistry, University of Toronto, Scarborough College, 1265 Military
Trail, Toronto, Ontario, M1C1A4.*

**Corresponding author. Tel: 1-416-287-7547; Fax: 1-416-287-7279; E-mail address:*

andre.simpson@utoronto.ca

This supporting Information contains 3 pages and 2 Figures.

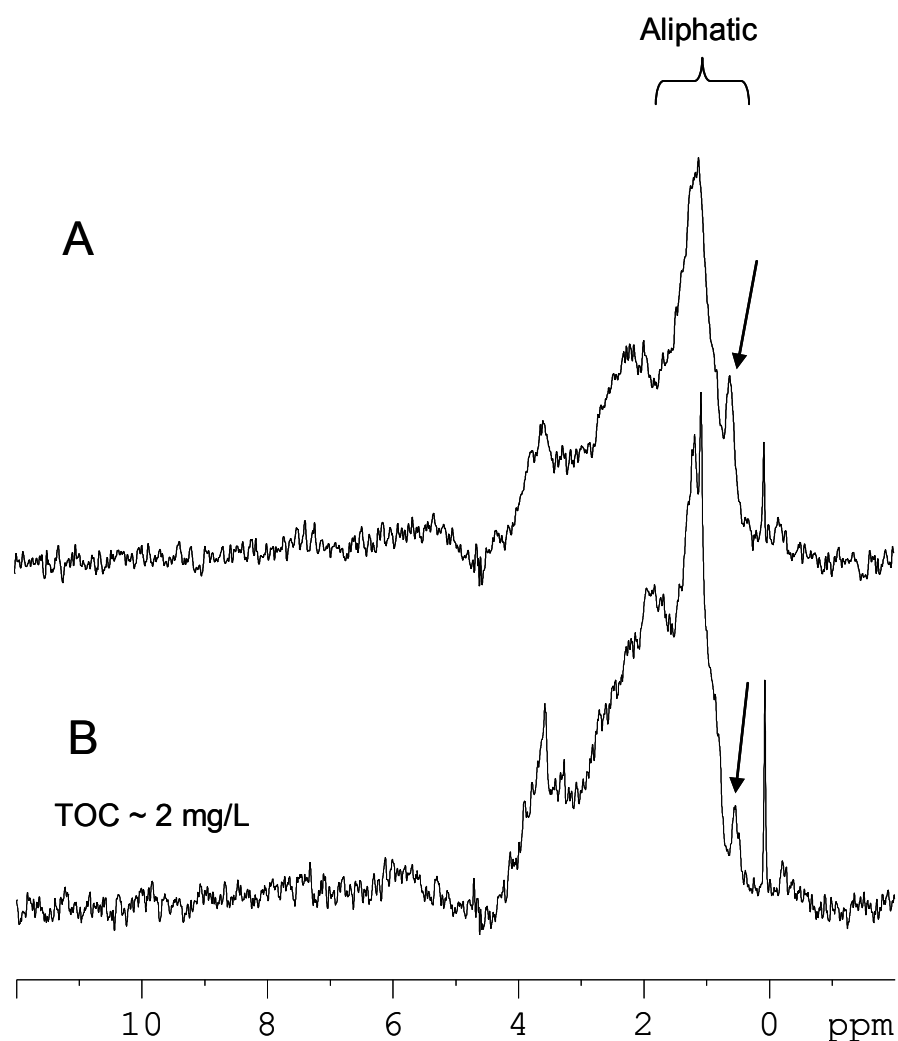


Figure S1 : Water from Lake Ontario (43°50' N, 78°57' W) collected in winter (Feb, 2007). A) sample analyzed without filtering, spectrum acquired using 49,152K scans B) sample filtered prior to analysis, spectrum acquired using 65,536K scans. The figure simply demonstrates that direct NMR analysis can be performed on filtered and/or unfiltered samples, as required. After normalization for the number of scans, the signal to noise is approximately 10% higher in the unfiltered spectrum. This is expected as filtering will remove many of the microbial species present. The signal labeled with an arrow is unusually low (~0.6 ppm) and is likely to result partially from proteins in microbial cells.¹ Additionally cellular lipids may also contribute to the additional intensity in the aliphatic region¹ in the non-filtered water. Interestingly the 0.6 ppm peak is not in the Lake Ontario sample collected in summer (see Figure 4C main paper). The winter sample was collected ~2 km west of the summer collection site, as extensive lake ice prevented safe sampling from the same beach location. Thus the difference between the summer and winter spectra may reflect the different populations of microbial species present at different times of the year and/or the different spatial populations.

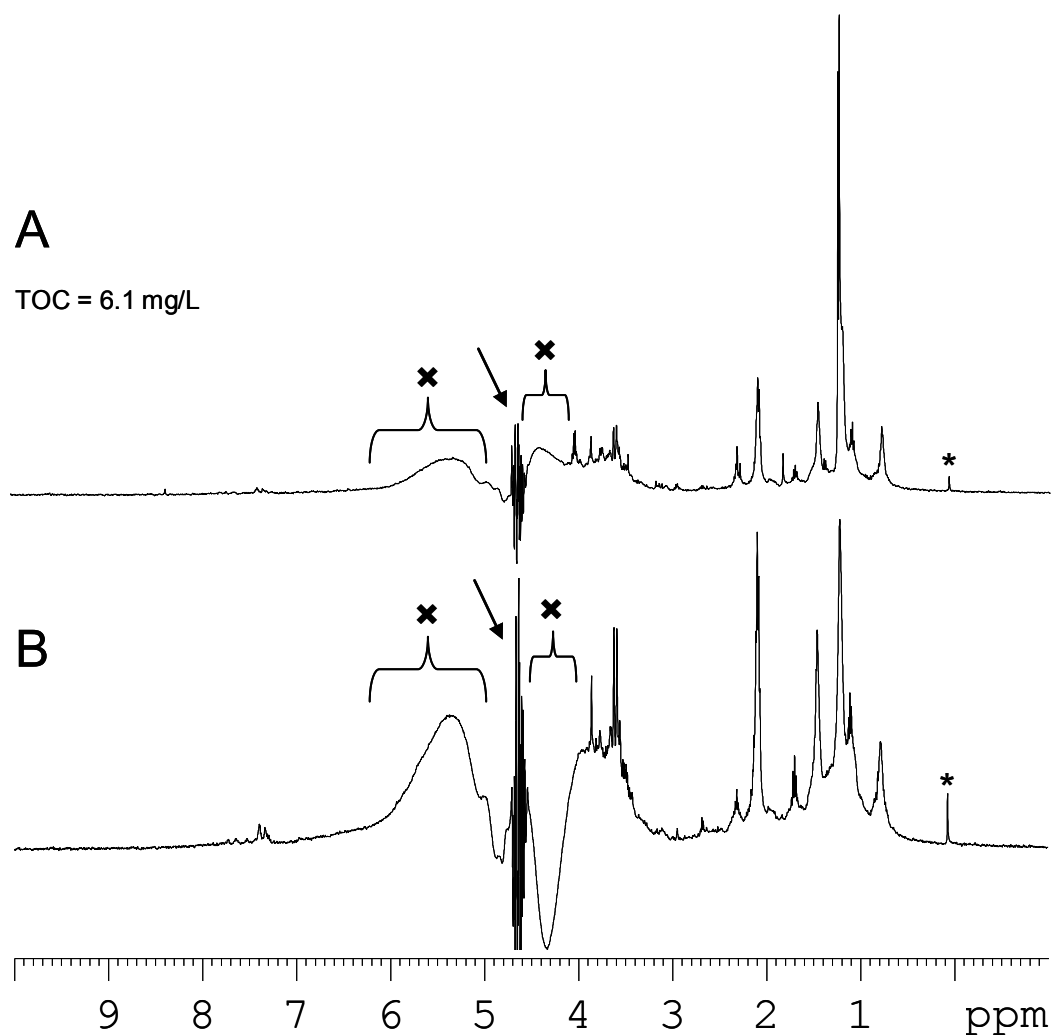


Figure S2 : Groundwater collected with a lysimeter at a depth of 100 cm from Highland Creek Valley, Toronto, Canada, (43°46' N, 79°11' W). Both samples were acquired using SPR-excitation sculpting and 16,384 scans. A) was acquired as soon as possible after collection (<1 hour before starting NMR acquisition), B) same sample re-acquired 24 hrs later. The sample was not filtered and thus will contain microbial species. Changes between the samples are most likely due to biological alteration with time. Thus, while analysis of unfiltered water is possible, utmost care should be taken to prevent biological alteration and preservative agents such as sodium azide may be required in unfiltered samples. ✕ indicates baseline distortions from the water suppression technique, the arrow indicates the central peak from residual water. Note, while this suppression is not as good as the SPR-W5-WATERGATE, it is much better than all other techniques tested, in which the residual water and baseline distortions are so large it is difficult to see any DOM signals (data not shown).

1. A. J. Simpson, M. J. Simpson, E. Smith and B. P. Kelleher, *Environ Sci Technol*, 2007, Published Online : 12-Oct-2007.