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Chlorine and Chloramine Demand of Natural Organic Matter Surrogates

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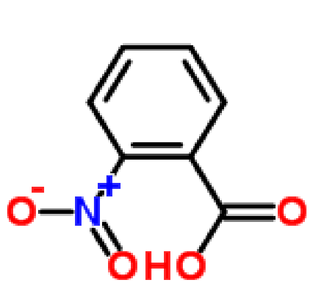
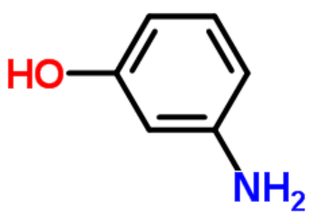
Introduction and Background

- The ability to predict chlorine and chloramine demand of natural organic matter (NOM) is important for being able to identify fractions which contribute significantly to the oxidant demand of water.
- There has been increased use of chloramines as secondary disinfectants over recent years (Seidel et al., 2005).
- NOM can be targeted during water treatment to minimise disinfection by product formation and optimised dosing of chlorine and chloramine can potentially lead to reduced chemical consumption.
- The twenty NOM surrogates tested were aromatic, which represent a large and reactive fraction of NOM.

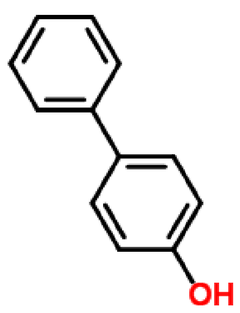
FIGURE 1: Selected NOM surrogates



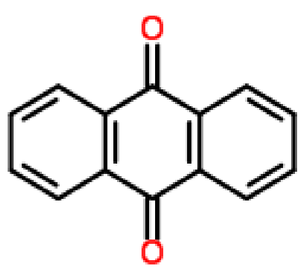
2-nitrobenzoic acid



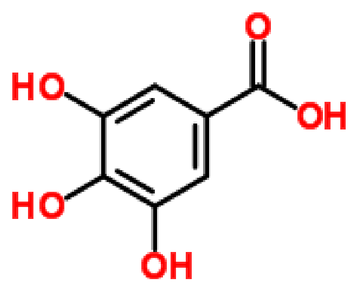
3-aminophenol



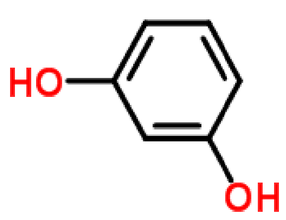
4-hydroxybiphenyl



Anthraquinone



Gallic Acid



Resorcinol

Experimental Procedure

- Humic substances were measured with the DPD-FAS titration method (APHA et al., 2005).
- The samples were stored for 24 hours in the dark at 20°C at pH 8.5.
- Blanks were also tested to account for natural degradation in the oxidant.

FIGURE 2: Experimental set up for DPD-FAS titration method

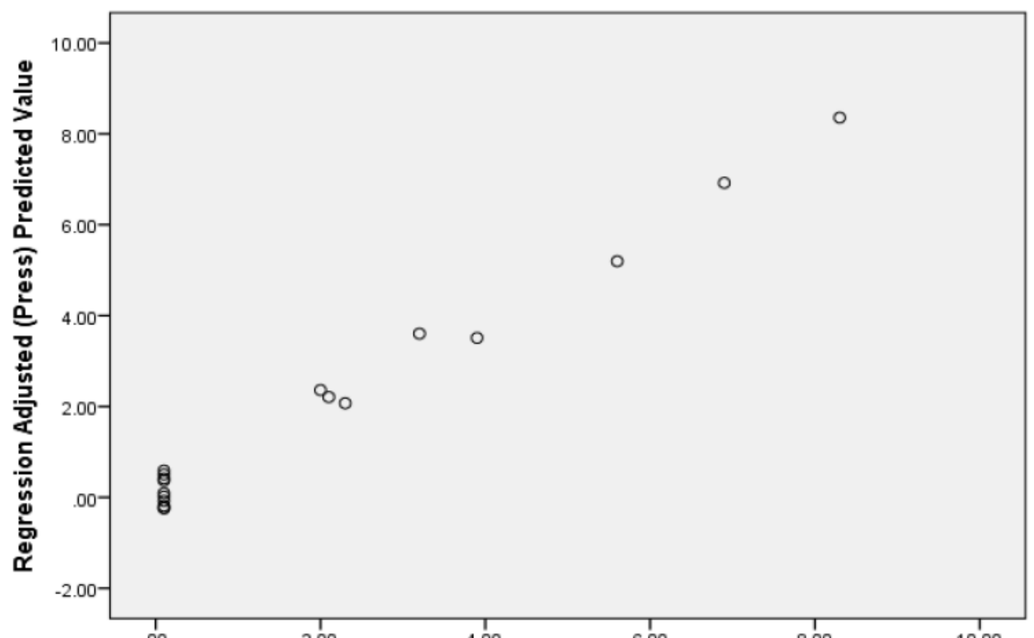
Quantitive Structure-Property Relationship (QSPR) Model

- The model chosen to predict oxidant demand was a QSPR, which is based on the multiple linear regression of various properties of the surrogates and has not been widely used in this area (Luilo & Cabaniss, 2010).
- The descriptors chosen include functional group counts, constitutional descriptors, molecular properties and indicators of molecular reactivity and stability.
- Quantum descriptors were calculated using the software Gaussian09 Revision D.01.

Table 1: Summary statistics for each of the models

Model	Adjusted R^2	Standard Error of Estimate
Chlorine	0.929	2.53
Chloramine	0.997	0.16
Chloramine with chlorine demand as a descriptor	0.990	0.33

Figure 3: Validation of monochloramine demand model



Conclusions

- With one exception, all NOM surrogates show higher chlorine demand than monochloramine demand
- The QSPR models created are reliable predictors of oxidant demand.
- Quantum descriptors are useful and should be further explored for use in this area.

Next steps…

- Gather more experimental data
  - For both chlorine and monochloramine demands
  - Extending to non-aromatic compounds
  - Potentially under a range of different conditions
    - pH, temperature, time
- Investigate more complex relationships between oxidant demand and descriptors – do not limit to the assumption of a simple linear relationship

ACKNOWLEDGEMENTS

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REFERENCES

Luilo, G. B. & Cabaniss, S. E. (2010) *Environmental Science & Technology.* 44 (7), 2503-2508.

Seidel, C. J., McGuire, M., Summers, R. S. & Via, S. (2005) *Journal of the American Water Works Association.* 97 (10).

APHA, AWWA, and WEF (2005) American Public Health Association, Washington, DC.