

Computer simulation study of the interaction of RNA with montmorillonite clay

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We use molecular dynamics techniques, performed on international federations of supercomputing grids, to carry out large-scale simulations of various 25 nucleotide (nt) sequences of ribonucleic acid (RNA), in bulk water and with aqueous montmorillonite clay. Our method is similar to that which has been used in our previous studies on nucleic acid-clay systems [1, 2].

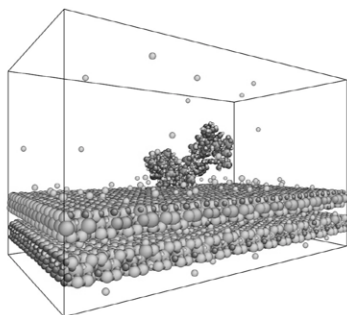


Figure 1: Image of a 25nt single stranded poly-adenine RNA molecule tethered to an aqueous montmorillonite clay surface, take after 30ns of simulation with water molecules hidden to aid viewing.

Our simulations are found to be in agreement with experimental observations pertaining to the relative adsorption of RNA on montmorillonite in the presence of charge balancing cations [3]. Over tens of nano-seconds, specific RNA sequences fold to characteristic secondary structural motifs when in the presence of the clay surface. Our simulations also show that, in aqueous Ca^{2+} environments, RNA can tether to the clay surface through a nucleotide base at the 5' end of the strand, providing a mechanism for the adsorption and elongation of RNA oligomers on clay surfaces. Our simulations demonstrate the importance of divalent cations in mediating the interactions between the surface and RNA.

- [1] Thyveetil *et al.* (2008) *J. Am. Chem. Soc.* **130**, 4742–4756.
[2] Thyveetil *et al.* (2008) *J. Am. Chem. Soc.* **130**, 12485–12495. [3] Franchi *et al.* (2003) *Orig. Life Evo. Bio.* **33**, 1–16.

A molecular biogeochemical study of a northern peatland ecosystem: the effects of substrate source on phenolic composition

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Peatlands contain about one third of the global soil carbon stocks. However, their response to increasing carbon dioxide levels and climate change are of great uncertainty. Phenolic compounds have been cited as playing an important role in the resistance to decomposition of organic carbon in peats [1].

This study compares the distributions and amounts of phenolics within peatland vascular plant and moss litter samples, including *Sphagnum* moss, using on-line thermally assisted hydrolysis and methylation (THM) in the presence of both unlabelled and ^{13}C -labelled tetramethylammonium hydroxide (TMAH). Phenolics specific to *Sphagnum* were identified using THM with unlabelled TMAH. THM in the presence of ^{13}C -TMAH allows the relative contribution of lignin, demethylated lignin and non-lignin phenolics, e.g. the hydrolysable tannins, to be assessed in the vascular plant species (cotton grass, heather and billberry).

It appears that phenolic acids including gallic acid, caffeic acid and protocatechuic acid are all significant components in peatland litter samples, which go undetected using unlabelled TMAH.

- [1] Freeman, Ostle & Kang (2001) *Nature* **409**, 149.