Water and oil do mix: structure and dynamics of water in triglyceride oils

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The hydrogen-bond structure and dynamics of water in triglycerides triacetin, tributyrin and trioctanoin are studied using linear IR and 2D IR spectroscopy. We identify several stable (>20ps) water configurations: water clusters, waters with a single hydrogen bond to the triglyceride and waters with two hydrogen bonds to the triglyceride.

The essential role of water in biological systems is well-recognized [1]. Water is known to actively influence the structure and functioning of for example proteins, DNA and phospholipid membranes. However, the role of water has been somewhat neglected for a major class of biomolecules: the triglycerides. Triglycerides are crucial for metabolic functions and are used in daily life as foods, pharmaceuticals, cosmetics and biodiesel [2].
Here we study the hydrogen-bond (HB) dynamics of water in triglyceride oils using linear IR and femtosecond 2DIR spectroscopy of the water OD stretch vibration (fig. 1). We identify water clusters, waters with a strong HB to the triglyceride and waters with two weaker HBs to the triglyceride. While we observe cross-peaks between the symmetric and antisymmetric OD stretch vibrations, cross-peaks remain absent between the different water HB configurations (fig. 2), indicating that these do not interconvert on the 20 ps timescale of the experiment.

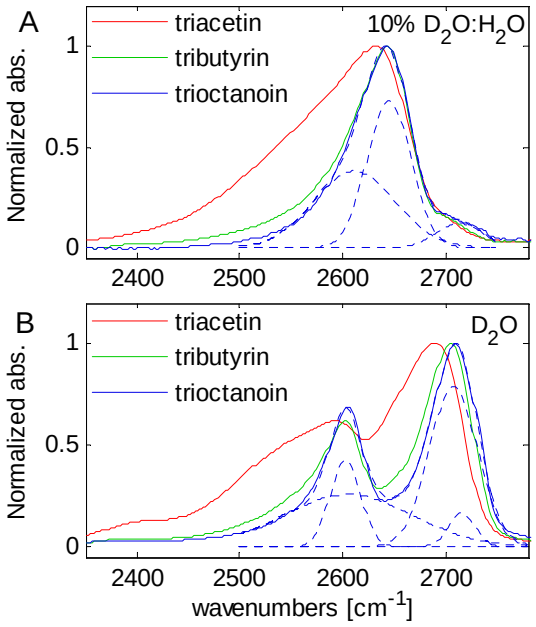

Fig.1. Linear IR spectra of saturated solutions of 10% D_2O:H_2O (A) and D_2O (B) in triacetin, tributyrin and trioctanoin. The spectra are corrected for H_2O in triglyceride background and normalized on peak intensity. The blue dotted lines represent a Gaussian fit.

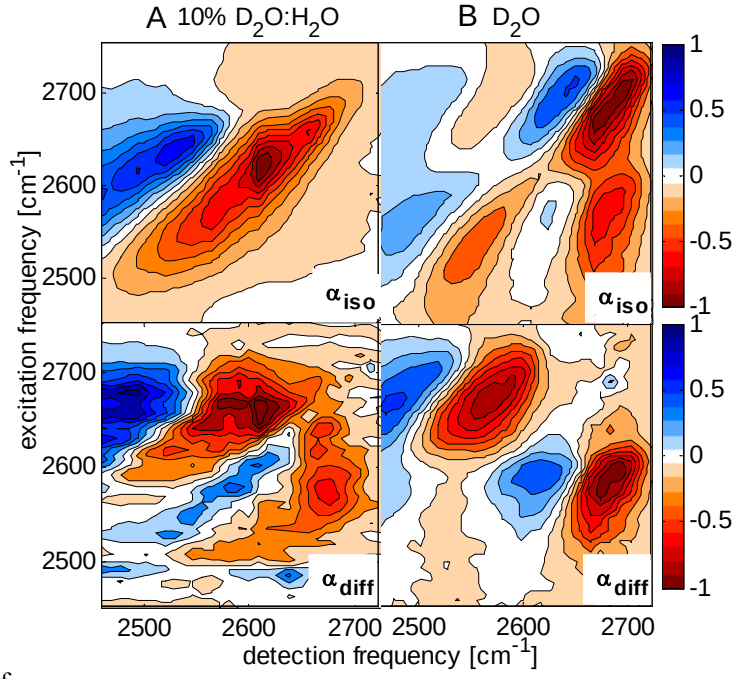

Fig. 2. 2DIR spectra of saturated solutions of 10%D_2O:H_2O (A) and D_2O (B) in triacetin, 0.4 ps after excitation. The top row shows the isotropic spectrum, $\alpha_{iso} = \frac{1}{3}(\alpha_{\parallel} + 2\alpha_{\perp})$, and the bottom row the difference spectrum (cross peaks only), $\alpha_{diff} = \alpha_{\parallel} - \alpha_{\perp} \cdot (\alpha_{\perp,max}/\alpha_{\parallel max})$. The spectra are normalized on peak intensity.

[1] P. Ball, Chemical Reviews **108**,1 (2008).
[2] M. Iwahashi and Y. Kasahara, Curr Opin Colloid In **16**, 359–366 (2011).