

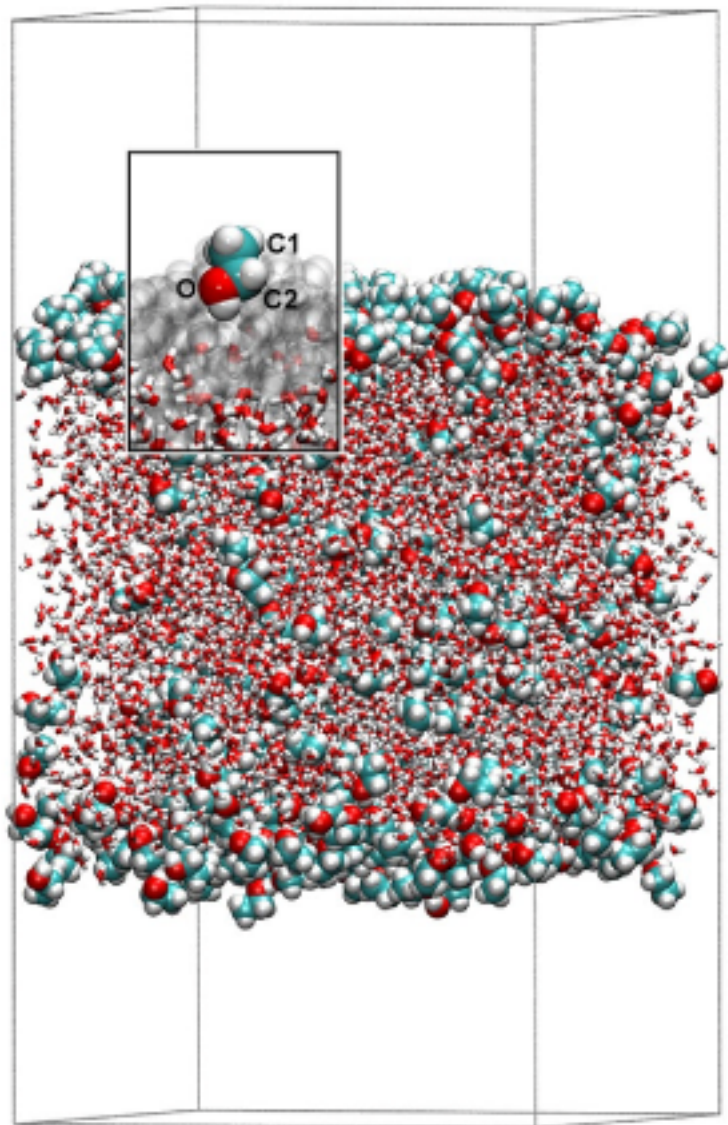
Molecular Dynamics

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Scotch Whisky

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Dilution of whisky – the molecular perspective

Björn C. G. Karlsson^{1,3} & Ran Friedman^{2,3}

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Whisky is distilled to around 70% alcohol by volume (vol-%) then diluted to about 40 vol-%, and often drunk after further slight dilution to enhance its taste. The taste of whisky is primarily associated with amphipathic molecules, such as guaiacol, but why and how dilution enhances the taste is not well understood. We carried out computer simulations of water-ethanol mixtures in the presence of guaiacol, providing atomistic details on the structure of the liquid mixture. We found that guaiacol is preferentially associated with ethanol, and, therefore, primarily found at the liquid-air interface in mixtures that contain up to 45 vol-% of ethanol. At ethanol concentrations of 59 vol-% or higher, guaiacol is increasingly surrounded by ethanol molecules and is driven to the bulk. This indicates that the taste of guaiacol in the whisky would be enhanced upon dilution prior to bottling. Our findings may apply to other flavour-giving amphipathic molecules and could contribute to optimising the production of spirits for desired tastes. Furthermore, it sheds light on the molecular structure of water-alcohol mixtures that contain small solutes, and reveals that interactions with the water may be negligible already at 89 vol-% of ethanol.