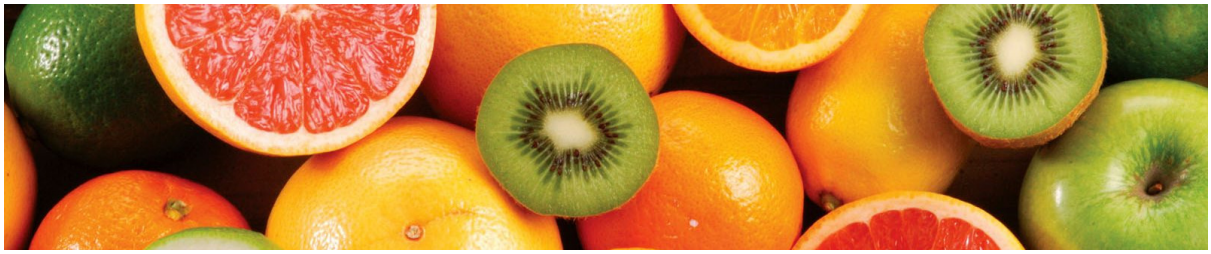

Limonene:
Interactions with water and in aqueous ethanol solutions

- Limonene is a small molecule found in the peels of citrus fruits and in other plants. It is a major component of citrus essential oils.
- Essential oils are volatile compounds – they smell!
- Plants produce essential oils to protect themselves against bacteria, fungi, insects & herbivores.
- Essential oils has been used in medicinal and cosmetic purposes for hundreds of years and dated back to Ancient Egyptians and Greeks. Essential oils are natural antimicrobial, anti-inflammatory and anti-fungal and even anti-cancer agents.
- Limonene is a curiously interesting molecule and is used in a range of commercial products from pharmaceutical & medicinal products, toothpaste, shower gels and cosmetics to insecticides and everyday household cleaning products.
- Experiments tell that limonene is hydrophobic – it is insoluble in water but soluble in alcohols.
- Atomistic molecular dynamic simulations confirm that limonene is insoluble in water – the limonene molecules placed in water box at random (Figure 1B) aggregate together in order to minimise their contacts with water (Figure 1C).
- Addition of ethanol, low-molecular weight alcohol, helps to dissolve limonene – simulations show that the limonene aggregate falls apart and all the molecules are perfectly dissolved in aqueous ethanol solution (Figure 1D).

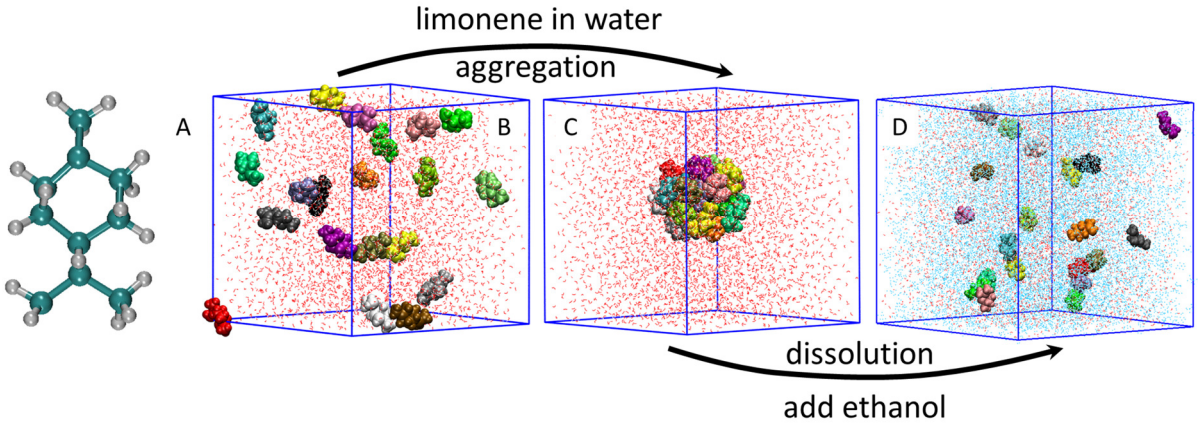

Figure 1. (A) All-atom model of limonene; (B) starting configuration for 20 limonene molecules in water; (C) aggregation of limonene molecules and (D) dissolution of limonene aggregate with ethanol. The limonenes are shown by different colours to visualise separate molecules, water is shown by thin red lines and ethanol is shown by cyan dots.