Unraveling the hydrolysis mechanism of chemical warfare agents with *ab initio* molecular dynamics simulations

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After World War II, the Baltic Sea was contaminated by dumping unused chemical warfare agents (CWA), which now constitutes a huge environmental hazard. We use both experimental and theoretical methods to understand the reactivity of selected CWA in water, in particular the hydrolysis, which is one of the chemical reactions leading to the neutralization of CWA.

We perform *ab initio* molecular dynamics simulations in explicit water solution at finite temperature to study the relative occurrence and stability of various CWA conformers in water. The mechanism of hydrolysis was studied by gas chromatography-mass spectrometry (GC-MS/MS) experiments and umbrella sampling simulations to obtain the activation energy, free energy barrier and to provide an atomistic view of the reaction process.

References:
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