

## **Supporting Information:**

# **Prediction of Toluene/Water Partition Coefficients of SAMPL9 compounds: Comparison of the molecular dynamics force fields GAFF/RESP and GAFF/IPolQ-Mod+LJ-fit**

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## Visualization of the planes of the plane projection analysis and solvent orientation

In this section we provide figures illustrating the cutting plane for the plane projection analysis of the components Mol12, Mol2, Mol5, Mol3, Mol4 and Mol11. Also shown is the internal vector in toluene that was chosen to define the orientation of the solvent

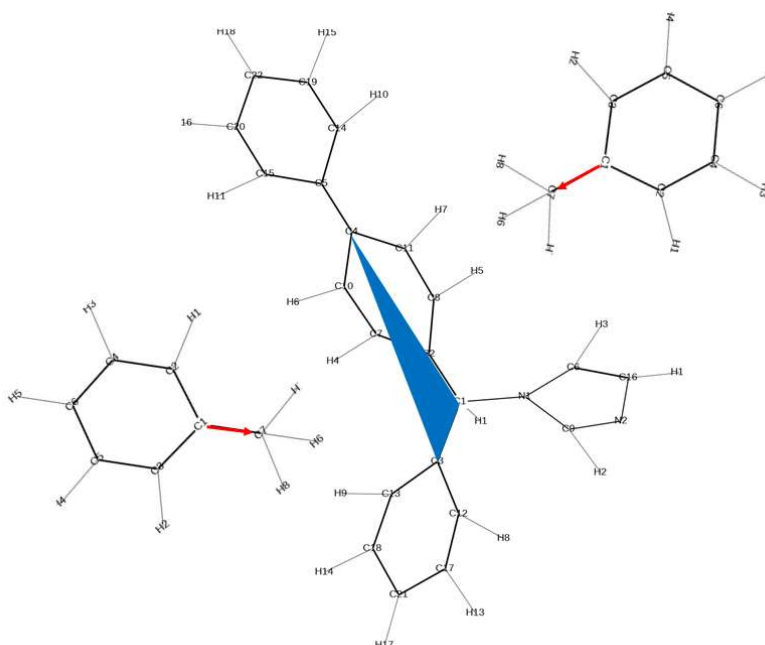


Figure S1: Mol12 in toluene: the blue triangle indicates the plane of the plane projection analysis and the red array indicates the direction of the solvent toluene in the vector field.

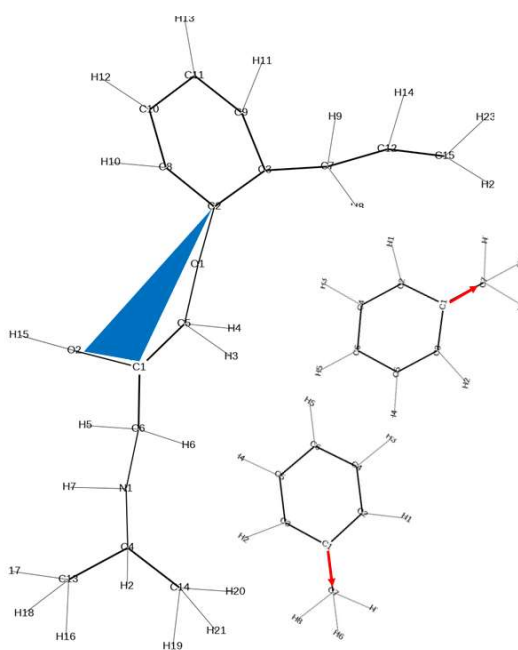


Figure S2: Mol2 in toluene: the blue triangle indicates the plane of the plane projection analysis and the red array indicates the direction of the solvent toluene in the vector field.

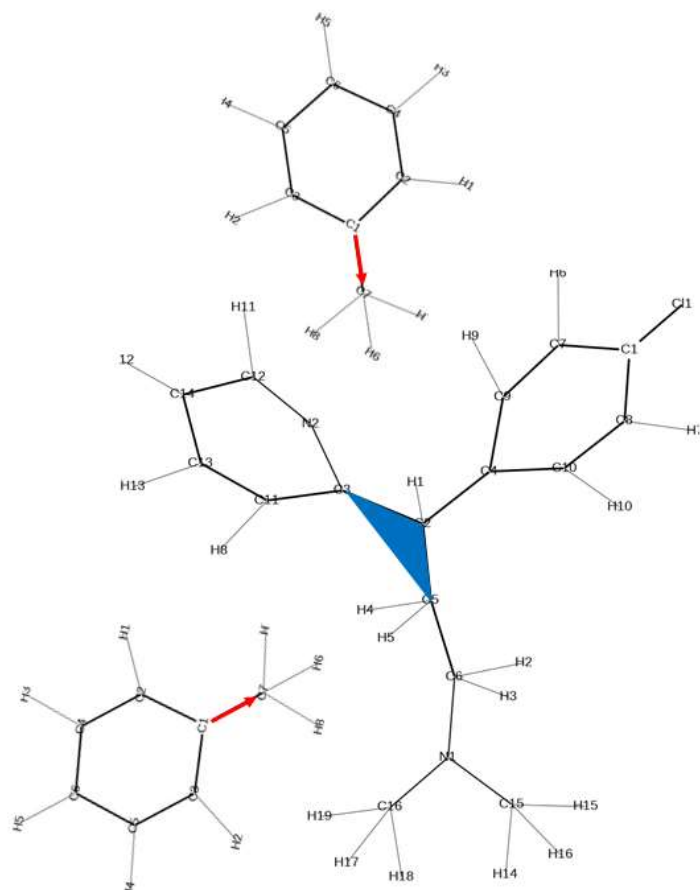


Figure S3: Mol5 in toluene: the blue triangle indicates the plane of the plane projection analysis and the red array indicates the direction of the solvent toluene in the vector field.

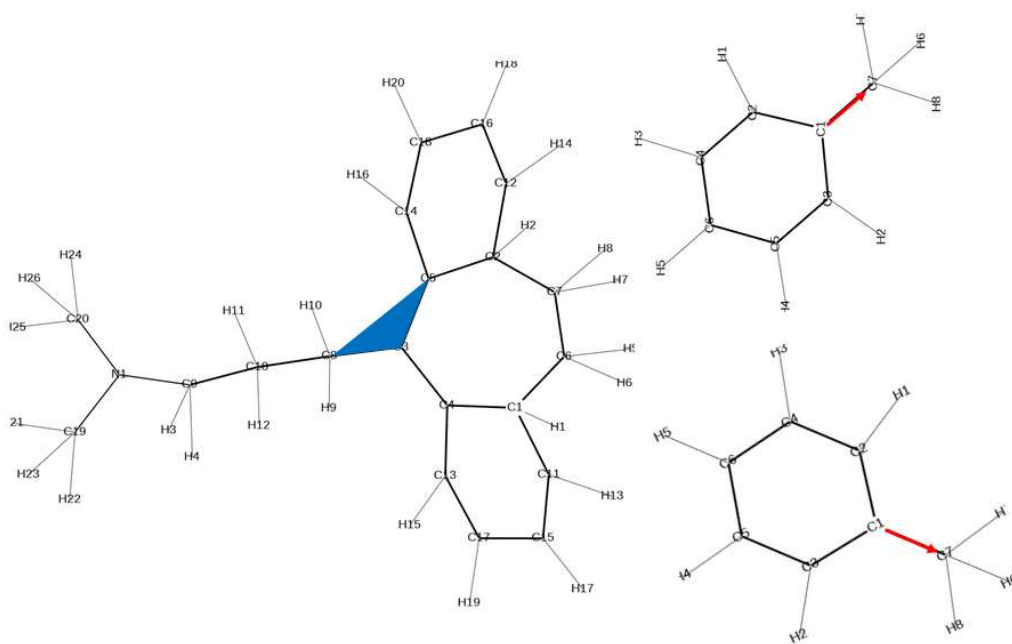


Figure S4: Mol3 in toluene: the blue triangle indicates the plane of the plane projection analysis and the red array indicates the direction of the solvent toluene in the vector field.

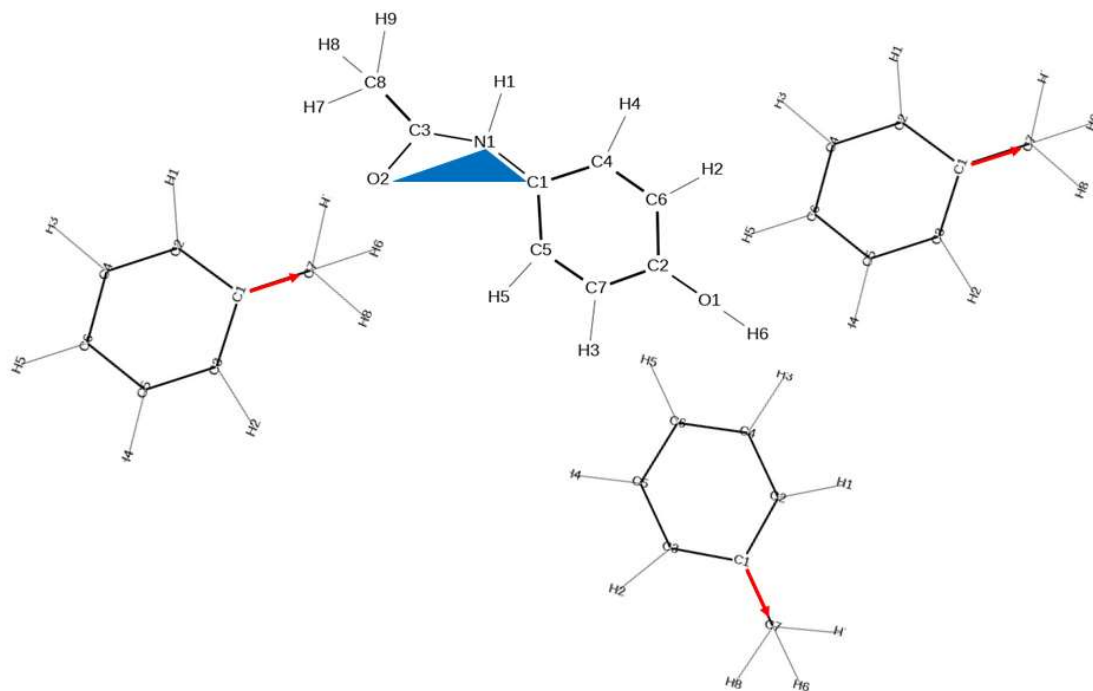


Figure S5: Mol4 in toluene: the blue triangle indicates the plane of the plane projection analysis and the red array indicates the direction of the solvent toluene in the vector field.

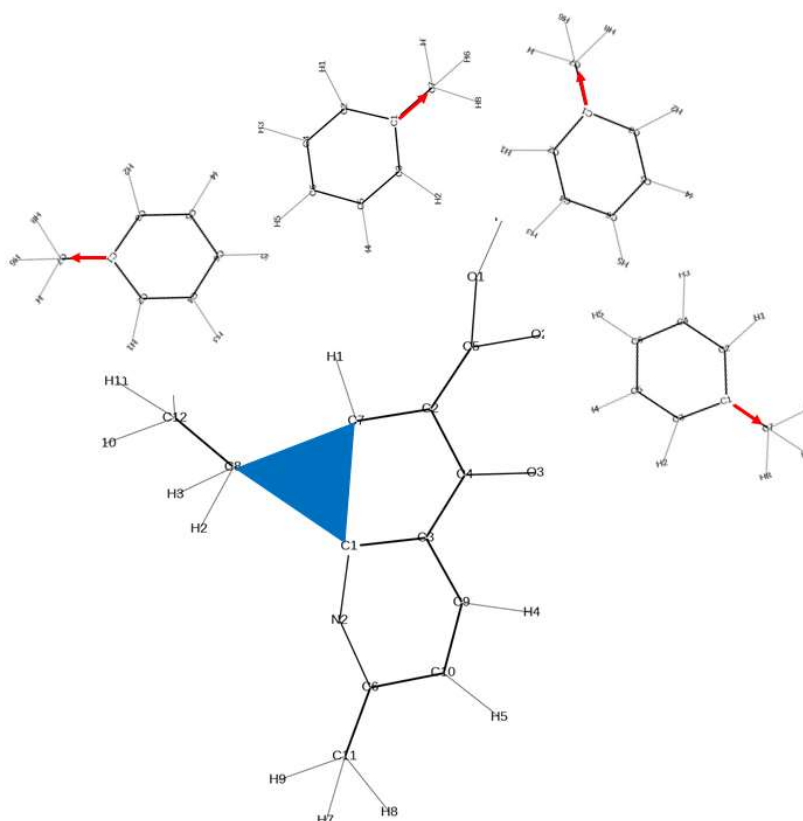


Figure S6: Mol11 in toluene: the blue triangle indicates the plane of the plane projection analysis and the red array indicates the direction of the solvent toluene in the vector field.