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Supplement of

Using the chemical equilibrium partitioning space to explore factors influencing the phase distribution of compounds involved in secondary organic aerosol formation

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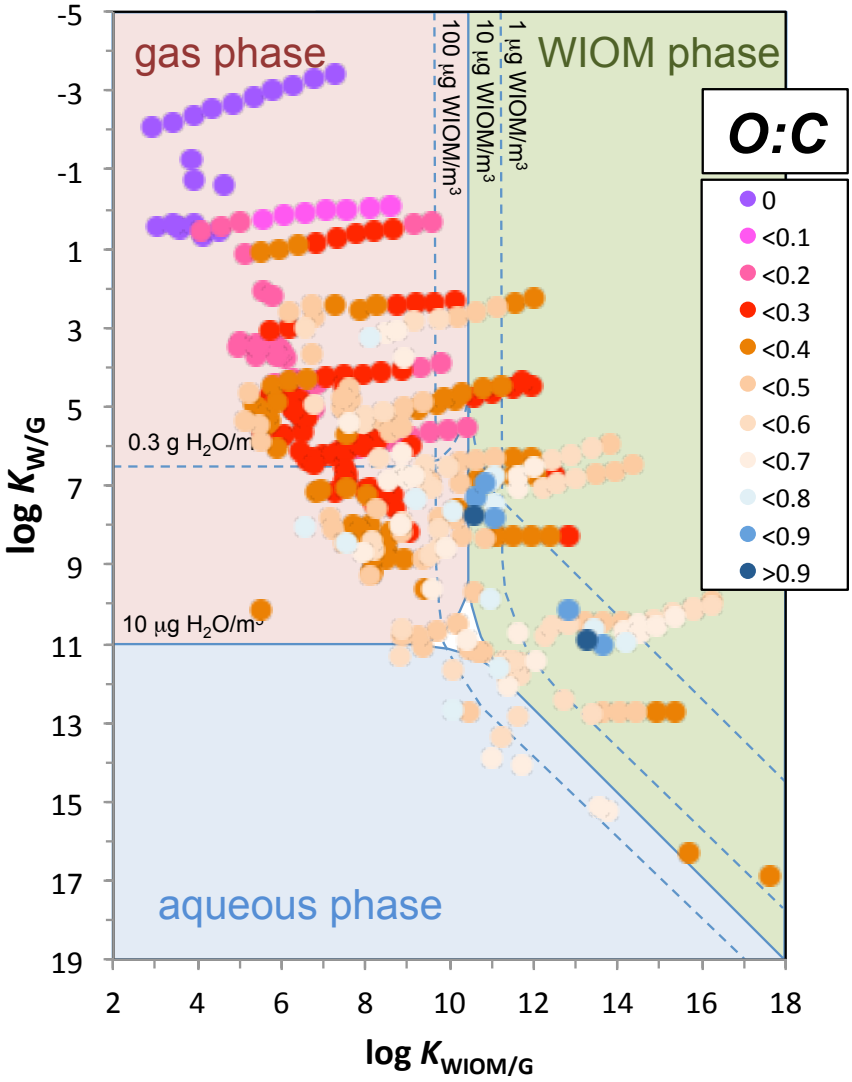

Figure S1 Placement of the selected oxidation products of *n*-alkanes, biogenic terpenes and mono-aromatic hydrocarbons in the partitioning space. $K_{WIOM/G}$ and $K_{W/G}$ at 15 °C and 0 M salt of the compounds was estimated using SPARC assuming the solvation properties of WIOM can be approximated by those of structure B. The markers are coloured based on a chemical's oxygen to carbon ratio (*O:C*).

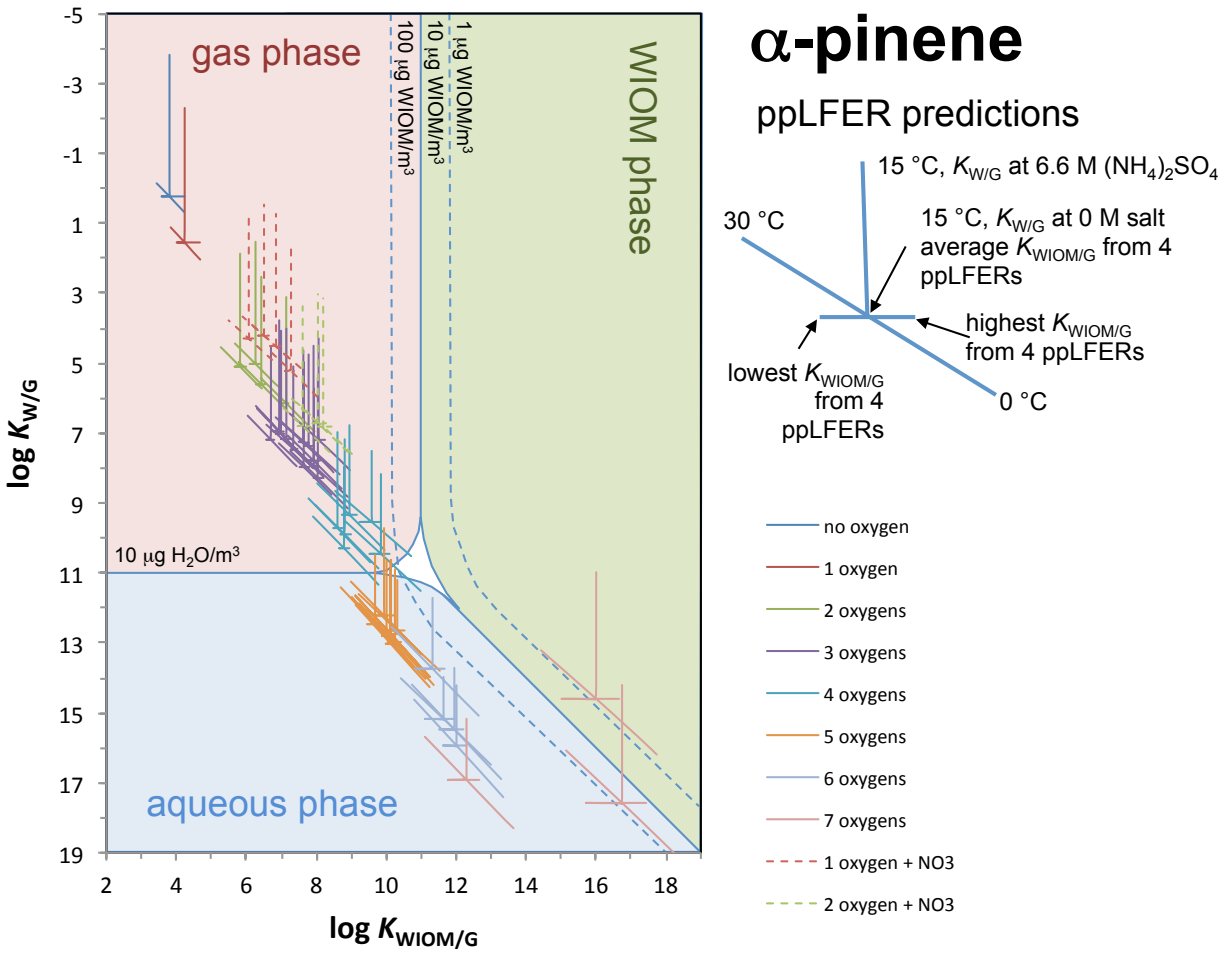

Figure S2 Placement of α-pinene and some of its oxidation products in the chemical partitioning space based on predictions with ppLFERs. Each chemical is represented by three lines, which account for the influence of temperature variations between 0 and 30 °C (diagonal line), the salting-out effect by 6.6 M $(NH_4)_2SO_4$ (vertical line) and ppLFERs for four different aerosol samples (horizontal line).

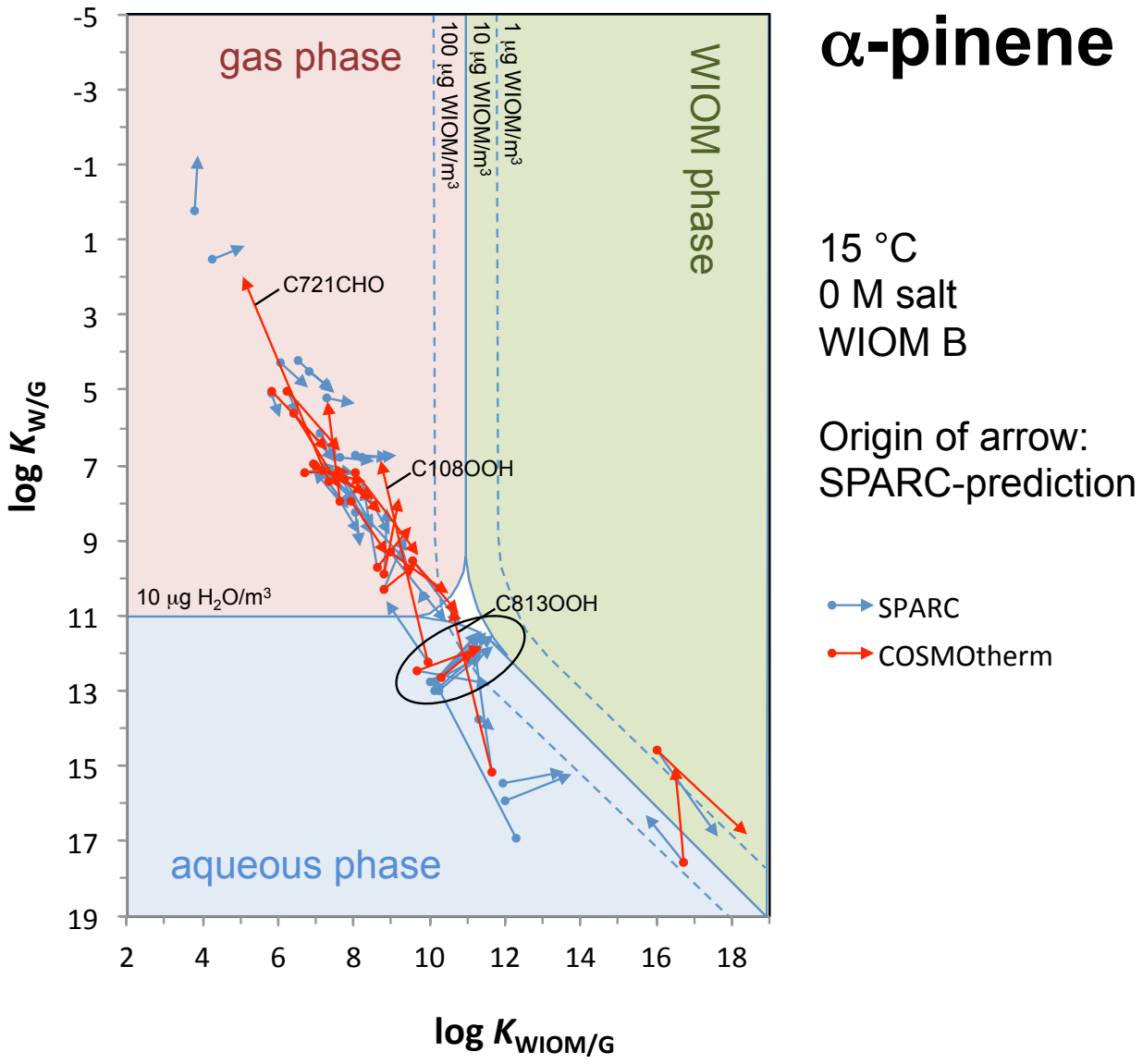

Figure S3 Arrows indicating the uncertainty of the placement of α-pinene oxidation products in the partitioning space based on the discrepancy of $K_{WIOM/G}$ and $K_{W/G}$ predictions made with SPARC (origin of arrows), ppLFERs (tip of blue arrows) and COSMOtherm (tip of red arrows). For some compounds, no COSMOtherm predictions are available. The black oval identifies oxidation products with 5 oxygens. Log red arrows indicate large discrepancies in the $K_{W/G}$ prediction for C108OOH, C813OOH and C721CHO using ppLFER and COSMOtherm.

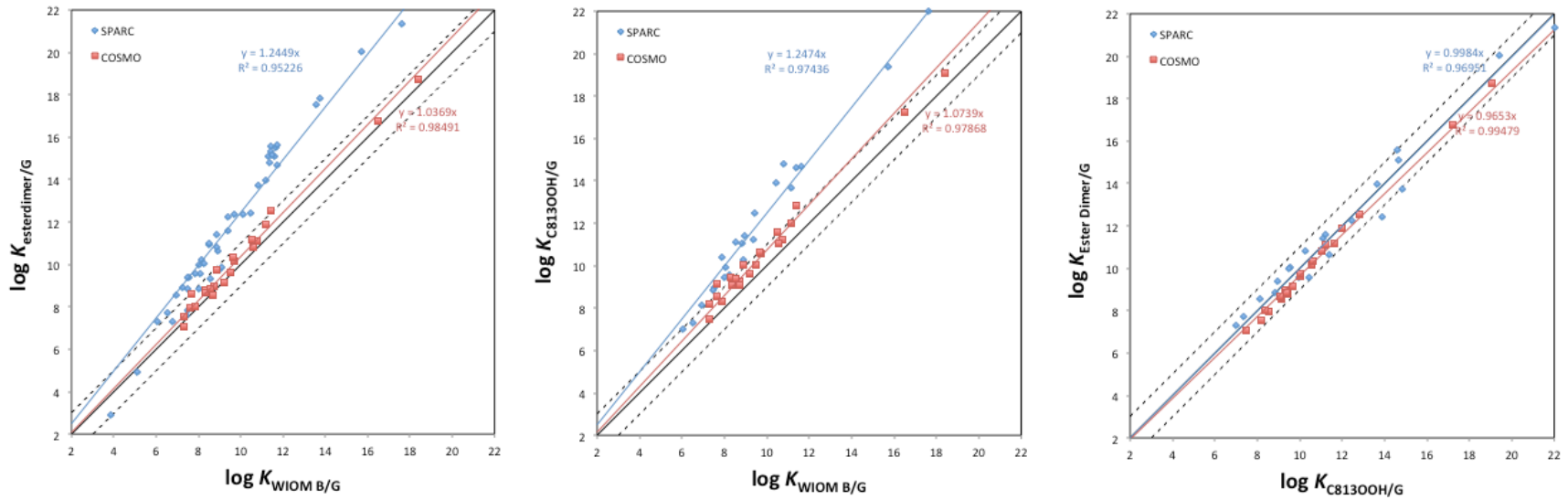

Figure S4 Comparison of the equilibrium partitioning coefficients between three different surrogates for water insoluble organic matter (structure B (Kalberer et al., 2004), ESTER_dimer (Zuend and Seinfeld, 2012), C813OOH (Valorso et al., 2011) and the gas phase $K_{X/G}$ predicted by SPARC (blue markers) and COSMOtherm (red markers).

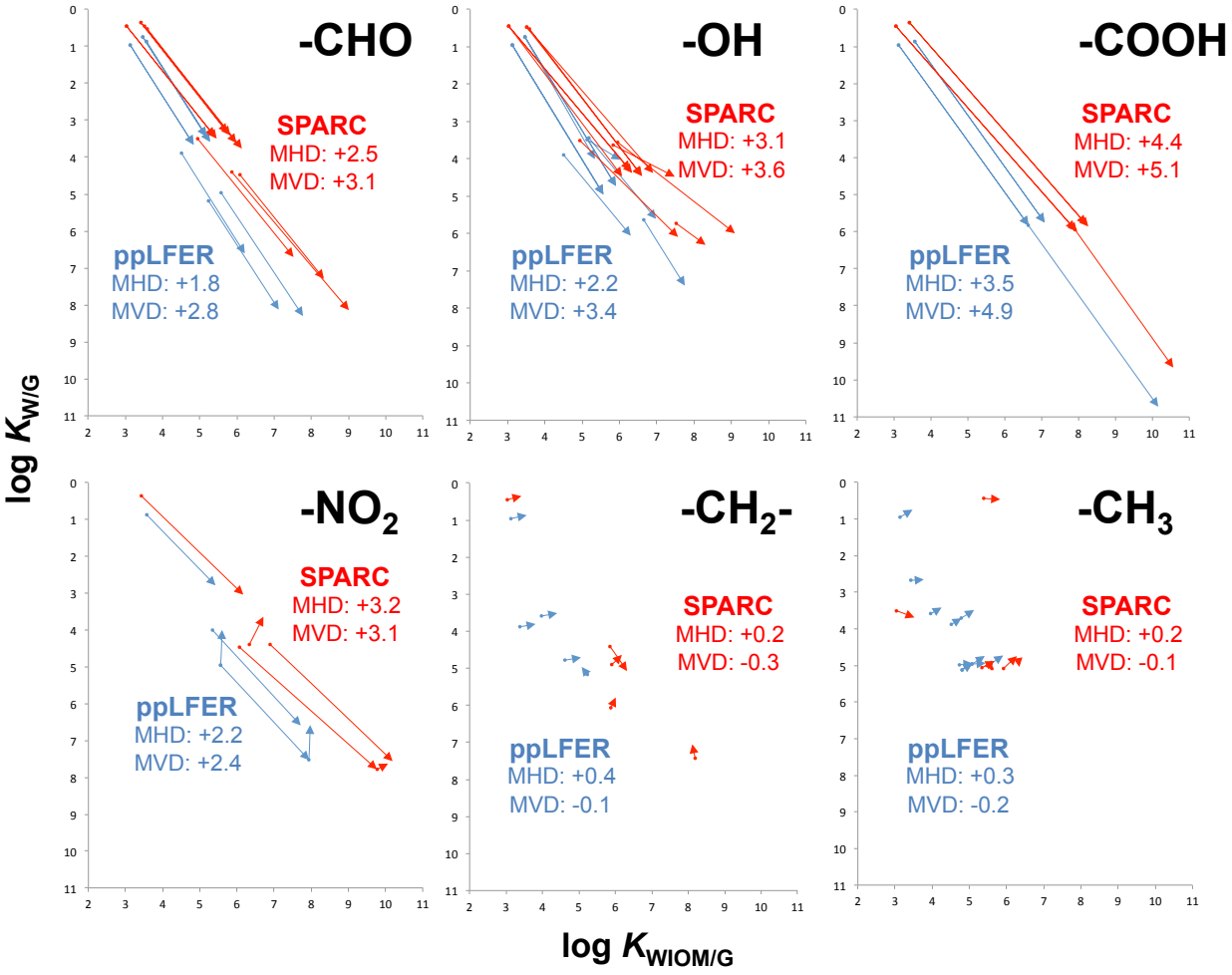

Figure S5 Displacement in the chemical partitioning space occurring upon the addition of functional groups to a mono-aromatic hydrocarbon, as predicted by SPARC at 15 °C and using structure B for WIOM (red arrows) or ppLFER (blue arrows). Outliers were not included in the calculation of mean vertical displacement (MVD) and mean horizontal displacement (MHD).