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Thermodynamic properties of isoprene- and monoterpene-derived organosulfates estimated with COSMO*therm*

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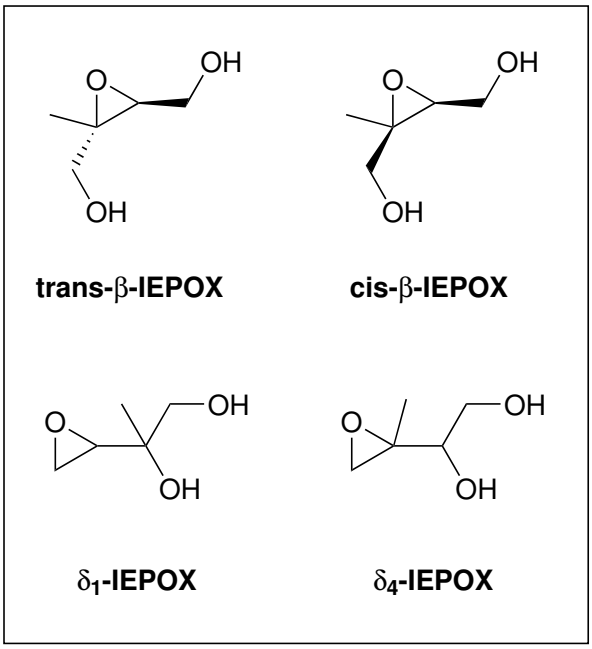

Figure S1: The isomers of IEPOX.

S1 Density calculation

COSMO*therm* estimates the density of a pure liquid using its corrected molar liquid volume $\widetilde{V}_i$:

$$\rho_i = \frac{MW_i}{\widetilde{V}_i(T) \cdot N_A}, \tag{S1}$$

where N_A is the Avogadro constant. The temperature dependent volume $\widetilde{V}_i$ is calculated from a quantitative-structure-property-relationship (QSPR):

$$\begin{aligned}\widetilde{V}_i(T) = c_1^T(T/T_{\text{room}} - 1) + c_2^T(T/T_{\text{room}} - 1)^2\widetilde{V}_i(T_{\text{room}}) + \\ c^T_{V_{\text{COSMO}}} V_i^{\text{COSMO}} + c^T_{M_2} M_{2_i} + c^T_{M_2^2} M_{2_i}^2 + c^T_{N_{\text{ring}}} N_i^{\text{ring}} + \\ c^T_{V_{C1}}(T/T_{\text{room}} - 1)V_i^{\text{COSMO}} + c^T_{V_{C2}} * (T/T_{\text{room}} - 1)^2 V_i^{\text{COSMO}} + \\ \sum_k^{elements} c^T_{A_k} A_i^k + c_0^T,\end{aligned} \tag{S2}$$

where

$$\widetilde{V}_i(T_{\text{room}}) = c_{V_{\text{COSMO}}} V_i^{\text{COSMO}} + c_{M_2} M_{2_i} + c_{M_2^2} M_{2_i}^2 + c_{N_{\text{ring}}} N_i^{\text{ring}} + \sum_k^{elements} c_{A_k} A_i^k + c_0, \tag{S3}$$

M is the second σ-moment of the compound, A_i^k is the area of surface if each atom k, N_{ring} is the number of ring atoms in the compound and c are parameters of the QSPR calculation.

For a mixture of multiple compounds, the density is calculated using the molar mass and the volume of the solution, MW_{solution} and $\widetilde{V}_{\text{solution}}$ respectively. Both are calculated as the weighted averages of the individual compounds in the solution:

$$MW_{\text{solution}} = \sum_i x_i MW_i \tag{S4}$$

$$\widetilde{V}_{\text{solution}}(T) = \sum_i x_i \widetilde{V}_i(T) \tag{S5}$$

where x_i is the mole fraction of compound i.

S2 Ions in COSMO*therm*

When salts are included in a system, COSMO*therm* treats the ions of the salt as separate entities and gives the mole fractions of each ion and neutral compound as normalized to one (for example in a binary mixture with water, $x'_{H_2O} + x'_{M^+} + x'_{X^-} = 1$). On the other hand, in experiments the salt is considered as a single compound ($x_{H_2O} + x_{MX} = 1$). This creates a difference between the calculation and the experimental framework for expressing non-measurable properties, such as activity coefficients, while keeping the activity in both frameworks equal. For example, the activity of compound i can equally be expressed using either the activity coefficient of the experimental (γ) or the calculation (γ') framework:

$$a_i = x_i \gamma_i = x'_i \gamma'_i \tag{S6}$$

The mole fraction in the experimental framework can be expressed using the calculation framework of COSMO*therm*:

$$x_i = \frac{x'_i}{1 - x'_{M^+}} \tag{S7}$$

assuming that the stoichiometry of the anion is 1 and of the cation is higher than or equal to 1. Combining Equations S6 and S7 allows us to calculate the activity coefficient in the experimental framework:

$$\gamma_i = \frac{x'_i}{x_i} \gamma'_i = (1 - x'_{M^+}) \gamma'_i \tag{S8}$$

Calculating solubilities as mole fractions, the different frame works have to be considered for both the solubility value and the mole fraction of the salt in the solvent. In calculating the solubility of a salt, COSMO*therm* allows for the definition of the solute as one salt entity, giving the result in the experimental framework. Figure S3 illustrates a ternary system (solvent containing one salt and one neutral compound) at the solubility limit using the mole fractions given by COSMO*therm* (x') to express the mole fraction of each component in the system. The solubility (in mole fraction) can be re-scaled to the experimental framework by

dividing with the new size of the system:

$$x_{\mathrm{SOL}} = \frac{x'_{\mathrm{SOL}}}{1 - (1 - x'_{\mathrm{SOL}}) \cdot x'_{\mathrm{M^+}}} \tag{S9}$$

Note that here $x'_{\mathrm{M^+}}$ is the mole fraction of the cation in the solvent as opposed to the whole solution, as in Equation (S8). Similarly, the mole fraction of salt in the solvent has to be calculated taking into account the new size of the solvent (again assuming that in the salt $\mathrm{M}_{\nu^+}\mathrm{X}_{\nu^-}$, $\nu^- = 1$ and $\nu^+ \geq \nu^-$):

$$x_{\mathrm{MX}} = \frac{x'_{\mathrm{X^-}}}{1 - x'_{\mathrm{M^+}}} \tag{S10}$$

Toure et al.[S1–S3] have studied the effect of hydrating strongly polar metallic mono-atomic ions in COSMO*therm* calculations. To use an appropriate hydration number for the sodium cation, we tested the effect of the number of water molecules on the relative solubilities of α-pinene-OS-1 in aqueous ammonium sulfate solutions. Considering the water molecules attached to the hydrated sodium ion of the solute ($\mathrm{Na} \cdot k\mathrm{H_2O}$) as part of the solvent, the mole fraction of the inorganic salt (MX) in the solvent needs to be calculated for each solubility value. Since the mole fraction of $\mathrm{H_2O}$ in the solvent changes by the addition of water molecules of the hydrated sodium ions, the mole fraction of the inorganic salt has to be scaled with the new solvent. The amount of solvent in the system at the solubility limit is originally $1 - x_{\mathrm{SOL}}$, and the additional water from the hydrated solute ($k \cdot x_{\mathrm{SOL}}$) is added to the original solvent ($1 - x_{\mathrm{SOL}} + k \cdot x_{\mathrm{SOL}}$). This is then used to divide the amount of inorganic salt.

$$x_{\mathrm{MX,dry}} = \frac{x_{\mathrm{MX}}(1 - x_{\mathrm{SOL}})}{1 + (k - 1) \cdot x_{\mathrm{SOL}}} \tag{S11}$$

The solubility used to calculate the mole fraction of inorganic salt in the solvent is the SLE solubility in 0.09 mole fraction of the inorganic salt scaled by the relative solubility from the relative screening calculation. All of the solubilities at this point are calculated using the hydrated sodium ion. Some of the relative solubilities are above one at low inorganic salt mole fractions, which leads to negative values for x_{MX} from Equation S11. In these cases,

the value of x_{MX} is set to 0.

In addition, the solubility needs to be re-calculated taking into account the increase in the mole fraction of the solvent caused by the dissociation of the hydrated solute ($\mathrm{NaOS} \cdot k\mathrm{H_2O}$). The final amount of solvent and solute in the system is the original 1 mole and an additional $k \cdot x_{\mathrm{SOL}}$ of water:

$$x_{\mathrm{SOL,dry}} = \frac{x_{\mathrm{SOL}}}{1 + k \cdot x_{\mathrm{SOL}}}, \tag{S12}$$

Using Equations S10 and S12, we obtain the relative solubilities seen in Figure S2. The mole fractions of the inorganic salt have not been re-scaled, since we only have the relative solubilities of the different hydrates, not the absolute solubilities. With a dry sodium cation ($k = 0$), COSMO*therm* predicts strong salting-in behavior at low ammonium sulfate concentrations. At $k = 4$, COSMO*therm* predicts salting-out through the whole ammonium sulfate concentration range and after $k = 5$ the relative solubility result has converged. We are using this fully hydrated sodium cation in our solubility calculations.

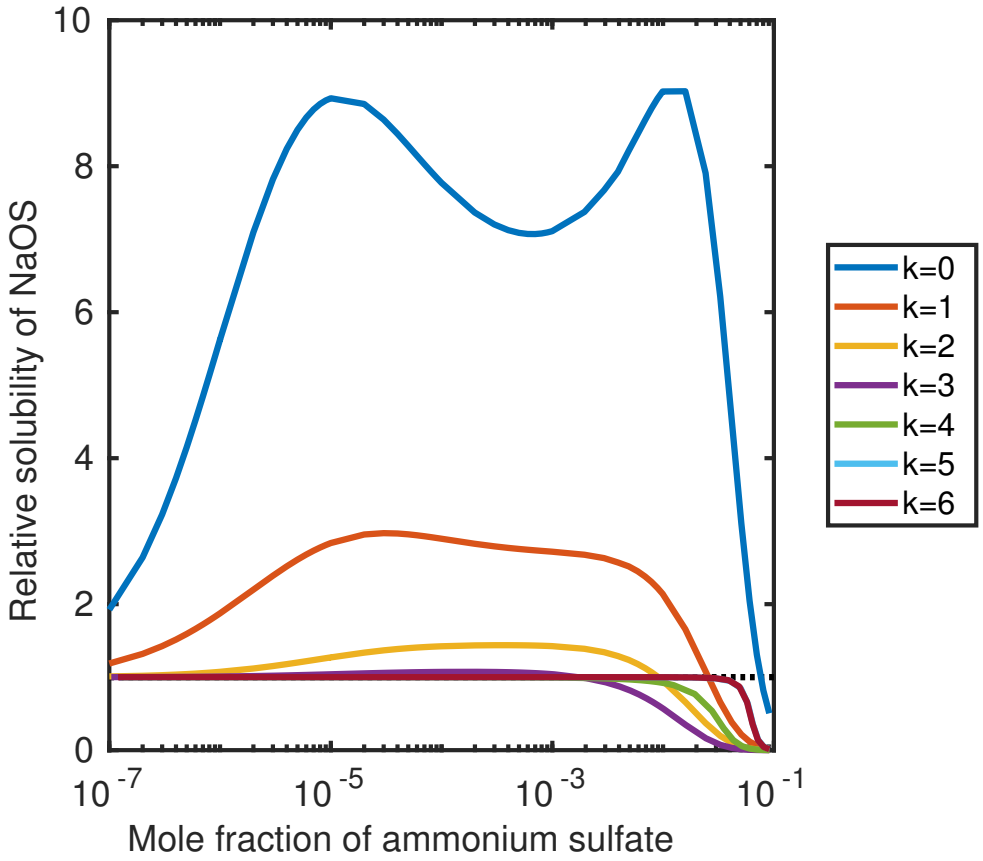

Figure S2: The relative solubilities ($x_{\mathrm{SOL}} = 1$ in pure water) of the sodium salt of α-pinene-OS-1 in $(NH_4)_2SO_4$ (aq) solutions ($T = 298.15$ K) estimated using the relative screening in COSMO*therm*. The hydrated sodium cation contains k water molecules.

For the $k = 5$, the absolute solubilities of the hydrated NaOS salts were calculated using the SLE solubilities in 0.09 mole fraction of each inorganic salt (AS and ABS) as a reference. Those solubility values were then used to calculate the corrected mole fraction of the inorganic salt for each of the organosulfate solutes. In Figure S8 the range of the ammonium sulfate varies depending on the absolute solubility of the solute, where the higher absolute solubility leads to a smaller mole fraction of the inorganic salt in the solvent.

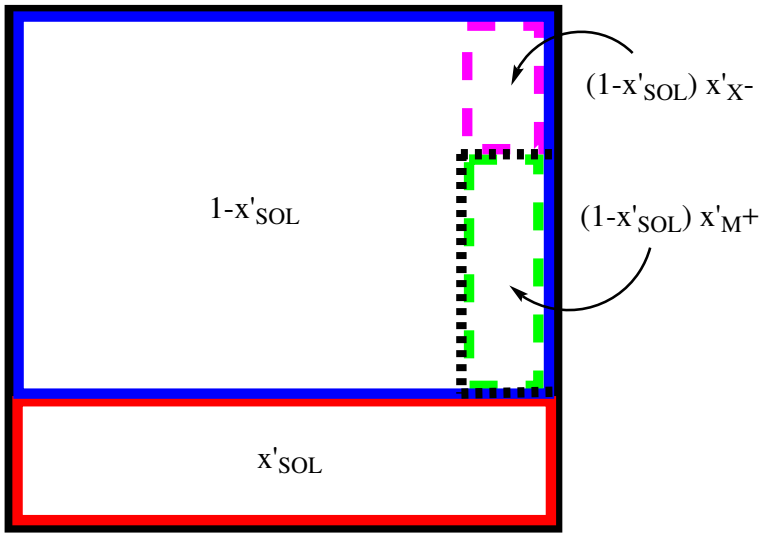

Figure S3: A ternary system at the solubility limit showing the mole fraction of each component in the system using the mole fractions given by COSMO*therm* for the solubility and the mole fractions of the salt ions in the solvent. Color coding: red = solute, blue = solvent, magenta = anion, green = cation.

S3 σ-profiles

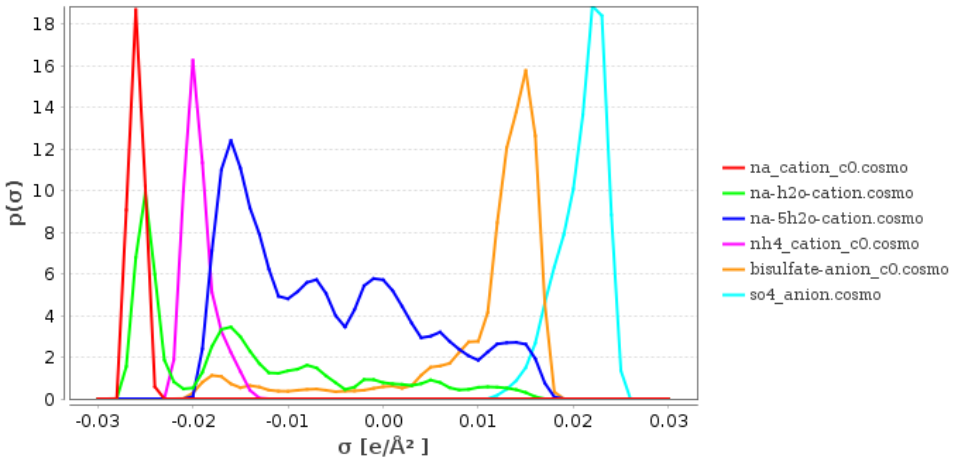

Figure S4: σ-profiles of the inorganic ions used in the COSMO*therm* calculations. Negative σ values (screening charge density) indicate a positive partial charge and positive σ values negative partial charge.

A sulfate group contains two double bonded oxygen atoms, one OH and one ether type oxygen. We have plotted the sigma surface (Fig. S5) and potential (Fig. S6) of SO_2H fragment of a sulfate group (corresponding to a carboxylic acid with the carbon replaced by sulfur), the whole sulfate group (OSO_3H) and a carboxylic acid (COOH). Comparing the σ-profiles of the sulfate group and the carboxylic acid group shows that the partial charges of the sulfate group (oxygens and hydrogen) are more positive than the charges of a carboxylic acid (see Fig. S6). The partial negative charge of the oxygen atoms of the sulfate group are slightly less negative but the charge covers a larger surface area than in the carboxylic acid oxygens. From the σ-potentials we can see that carboxylic acid is able to act as both a hydrogen bond acceptor and a donor, while sulfate is characterized only as a hydrogen bond donor. However, sulfate is a stronger hydrogen bond donor than carboxylic acid and carboxylic acid is a weaker H-bond acceptor than donor. Based on the σ-potentials, the negative partial charge of the sulfate group is too weak to be counted as H-bond acceptor in the σ-potential.

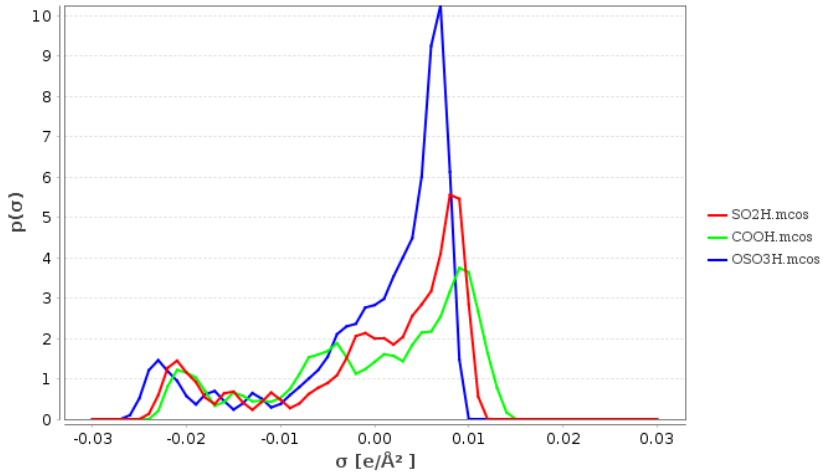

Figure S5: σ-profiles of the carboxylic acid group, sulfate group and SO_2H of the sulfate group (corresponding to a carboxylic acid group) of α-pinene-OS-5_c22. Negative σ values (screening charge density) indicate a positive partial charge and positive σ values negative partial charge.

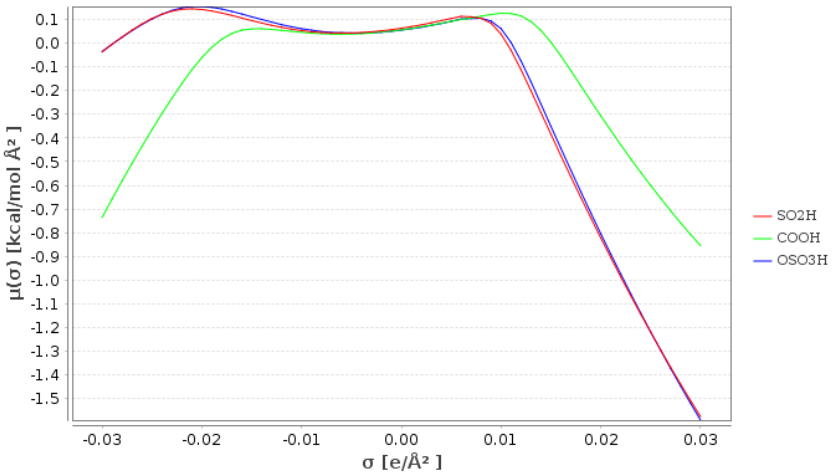

Figure S6: σ-potentials of the carboxylic acid group, sulfate group and SO_2H of the sulfate group (corresponding to a carboxylic acid group) of α-pinene-OS-5_c22. Negative $\mu(\sigma)$ values indicate favorable interaction with partial charges corresponding to the σ values on the x-axis. For example, all of the groups shown here are able to act as H-bond donors (interaction with negative partial charges).

Table S1: pK_a values of the organosulfates and sulfuric acid in water, at 298.15 K, estimated using COSMO*therm*. Literature values for methyl bisulfate -2.6 and for sulfuric acid -3.0 calculated by extrapolation. The solubilities (x_{SOL}) were calculated using the SLE solver and only conformers containing 0 intramolecular H-bonds. The dissociation corrected solubility (x^{DC}) was then calculated using Equation (11). For all of the compounds, the dissociation correction is approximate, as Equation (11) gives values >1.

	pK_a	x_{SOL}	x^{DC}	x_{MX}
α-pinene-OS-1	-3.19	$1.03 \cdot 10^{-3}$	1.00	$6.63 \cdot 10^{-2}$
α-pinene-OS-2	-3.19	$3.69 \cdot 10^{-3}$	1.00	$6.19 \cdot 10^{-2}$
α-pinene-OS-3	-2.42	$4.64 \cdot 10^{-3}$	1.00	-
α-pinene-OS-4	-3.12	$2.60 \cdot 10^{-3}$	1.00	-
α-pinene-OS-5	-4.23	$6.72 \cdot 10^{-3}$	1.00	-
α-pinene-OS-6	-4.58	$6.93 \cdot 10^{-3}$	1.00	-
β-pinene-OS-1	-4.24	$1.72 \cdot 10^{-3}$	1.00	$6.45 \cdot 10^{-2}$
β-pinene-OS-2	-2.98	$3.05 \cdot 10^{-3}$	1.00	$6.88 \cdot 10^{-2}$
limonene-OS-1	-3.00	$2.52 \cdot 10^{-3}$	1.00	$6.56 \cdot 10^{-2}$
limonene-OS-2	-2.90	$1.92 \cdot 10^{-3}$	1.00	$6.07 \cdot 10^{-2}$
limonene-OS-3	-3.17	$1.16 \cdot 10^{-3}$	1.00	-
limonene-OS-4	-3.64	$1.48 \cdot 10^{-3}$	1.00	-
isoprene-OS-1	-3.87	-	-	-
isoprene-OS-2	-4.49	-	-	-
isoprene-OS-3	-3.94	-	-	-
isoprene-OS-4	-2.37	-	-	-
Methyl bisulfate	-4.03	-	-	-
Sulfuric acid	-3.51	-	-	-

Table S2: LLE solubilities of the OS, AS and ABS, and SLE solubilities of NaOS. OS = organosulfate, NaOS = sodium salt of the organosulfate, AS = 0.09 mole fraction aqueous solution of ammonium sulfate, ABS = 0.09 mole fraction aqueous solution of ammonium bisulfate. Note that the actual concentration of the inorganic salt in the NaOS systems varies based on the solubility according to Equation S11.

Solvent	AS		ABS		OS	
Solute	OS	NaOS	OS	NaOS	AS	ABS
α-pinene-OS-1	$8.73{\cdot}10^{-7}$	$1.24{\cdot}10^{-3}$	$5.37{\cdot}10^{-5}$	$3.82{\cdot}10^{-2}$	0.973	0.884
α-pinene-OS-2	$4.52{\cdot}10^{-6}$	$1.21{\cdot}10^{-3}$	$2.78{\cdot}10^{-4}$	$3.52{\cdot}10^{-2}$	0.942	0.729
α-pinene-OS-3	$7.92{\cdot}10^{-6}$	$2.36{\cdot}10^{-3}$	$4.43{\cdot}10^{-4}$	$4.69{\cdot}10^{-2}$	0.677	0.493
α-pinene-OS-4	$2.58{\cdot}10^{-6}$	$1.64{\cdot}10^{-3}$	$2.17{\cdot}10^{-4}$	$3.92{\cdot}10^{-2}$	0.830	0.670
α-pinene-OS-5	$1.56{\cdot}10^{-5}$	$6.08{\cdot}10^{-3}$	$5.32{\cdot}10^{-4}$	$5.65{\cdot}10^{-2}$	0.694	0.546
α-pinene-OS-6	$1.87{\cdot}10^{-5}$	$4.82{\cdot}10^{-3}$	$6.07{\cdot}10^{-4}$	$5.11{\cdot}10^{-2}$	0.614	0.478
β-pinene-OS-1	$1.40{\cdot}10^{-6}$	$1.09{\cdot}10^{-3}$	$8.77{\cdot}10^{-5}$	$3.66{\cdot}10^{-2}$	0.984	0.890
β-pinene-OS-2	$4.50{\cdot}10^{-6}$	$2.13{\cdot}10^{-3}$	$2.69{\cdot}10^{-4}$	$4.66{\cdot}10^{-2}$	0.875	0.657
limonene-OS-1	$2.04{\cdot}10^{-6}$	$1.20{\cdot}10^{-3}$	$1.60{\cdot}10^{-4}$	$3.93{\cdot}10^{-2}$	0.935	0.742
limonene-OS-2	$1.38{\cdot}10^{-6}$	$8.07{\cdot}10^{-4}$	$1.12{\cdot}10^{-4}$	$3.05{\cdot}10^{-2}$	0.945	0.737
limonene-OS-3	$6.84{\cdot}10^{-7}$	$1.54{\cdot}10^{-3}$	$5.86{\cdot}10^{-5}$	$4.50{\cdot}10^{-2}$	0.980	0.852
limonene-OS-4	$1.23{\cdot}10^{-6}$	$1.71{\cdot}10^{-3}$	$1.00{\cdot}10^{-4}$	$4.83{\cdot}10^{-2}$	0.928	0.725
isoprene-OS-1	$1.03{\cdot}10^{-3}$	$1.42{\cdot}10^{-2}$	$9.78{\cdot}10^{-3}$	$5.40{\cdot}10^{-2}$	0.546	0.396
isoprene-OS-2	$1.04{\cdot}10^{-3}$	$9.09{\cdot}10^{-3}$	$9.61{\cdot}10^{-3}$	$4.95{\cdot}10^{-2}$	0.481	0.344
isoprene-OS-3	$3.20{\cdot}10^{-3}$	$1.60{\cdot}10^{-2}$	$4.83{\cdot}10^{-2}$	$5.63{\cdot}10^{-2}$	0.440	0.125
isoprene-OS-4	$2.95{\cdot}10^{-3}$	$1.04{\cdot}10^{-2}$	$5.87{\cdot}10^{-2}$	$5.02{\cdot}10^{-2}$	0.593	0.179
cis-β-IEPOX	$6.43{\cdot}10^{-3}$	-	-	-	0.900	-
trans-β-IEPOX	$6.34{\cdot}10^{-3}$	-	-	-	0.905	-
δ_1-IEPOX	$1.57{\cdot}10^{-2}$	-	-	-	0.903	-
δ_4-IEPOX	$6.71{\cdot}10^{-3}$	-	-	-	0.912	-
methyl bisulfate	$1.91{\cdot}10^{-2}$	$3.02{\cdot}10^{-2}$	$5.62{\cdot}10^{-2}$	$5.64{\cdot}10^{-2}$	0.441	0.320

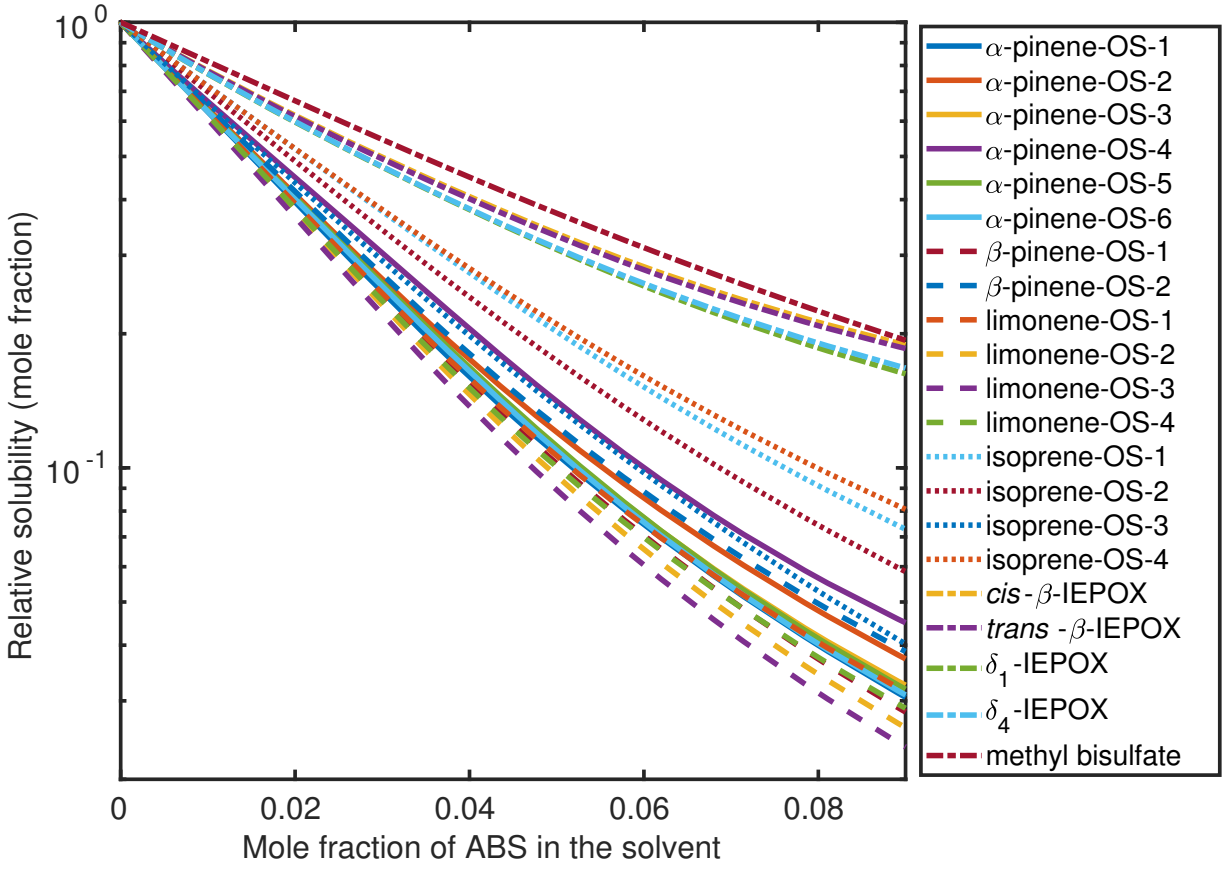

Figure S7: The relative solubilities of organosulfates in NH_4HSO_4 (aq) solutions ($T = 298.15$ K) estimated using the relative screening in COSMO*therm*.

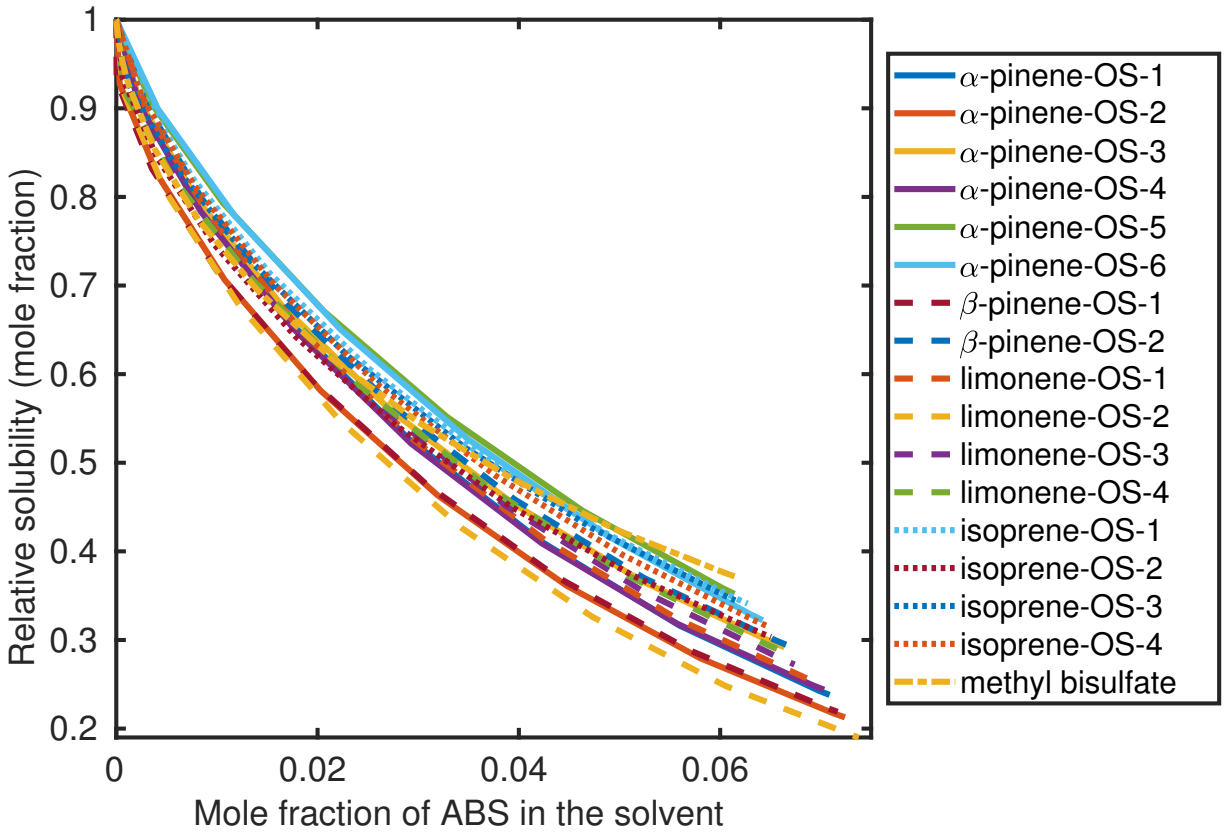

Figure S8: The relative solubilities of sodium salts of the organosulfates in NH_4HSO_4 (aq) solutions ($T = 298.15$ K) estimated using the relative screening in COSMO*therm*.

Table S3: Activity coefficients of the organics and water in stable binary solutions, at 298.15 K.

x(org)	$x(H_2O)$	$\ln \gamma^I$(org)	$\ln \gamma^I(H_2O)$
α-pinene-OS-1			
1.00E-08	1	6.24734649	0.00000007
2.06E-04	0.9998	6.22811677	0.00000205
4.12E-04	0.9996	6.20896327	0.00000798
6.17E-04	0.9994	6.18988691	0.00001782
8.23E-04	0.9992	6.17088756	0.00003155
1.03E-03	0.999	6.15196503	0.00004913
0.4825	0.5175	0.00161722	0.65774678
0.586	0.414	-0.01961669	0.67911130
0.6895	0.3105	-0.01786611	0.67203684
0.793	0.207	-0.01199478	0.64732295
0.8965	0.1035	-0.00436202	0.58261809
1	1.00E-08	0.00000000	0.40639492
α-pinene-OS-2			
1.00E-08	1	4.64148203	0.00000007
7.38E-04	0.9993	4.58852792	0.00001959
1.48E-03	0.9985	4.53627500	0.00007748
2.21E-03	0.9978	4.48471717	0.00017278
2.95E-03	0.997	4.43384673	0.00030453
3.69E-03	0.9963	4.38365661	0.00047181
0.3396	0.6604	-0.13905683	0.41166015
0.4717	0.5283	-0.14777537	0.41316214
0.6038	0.3962	-0.08022288	0.33168009

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
0.7358	0.2642	-0.02319357	0.21446242
0.8679	0.1321	-0.00099661	0.12409338
1	1.00E-08	0.00000000	0.10095576

α-pinene-OS-3

1.00E-08	1	3.34327061	0.00000007
9.27E-04	0.9991	3.27330652	0.00003256
1.86E-03	0.9981	3.20456294	0.00012857
2.78E-03	0.9972	3.13702604	0.00028597
3.71E-03	0.9963	3.07068090	0.00050267
4.64E-03	0.9954	3.00551141	0.00077663
0.2414	0.7586	-0.94679384	0.27242378
0.3931	0.6069	-0.80215482	0.19062734
0.5448	0.4552	-0.43626808	-0.14198733
0.6966	0.3034	-0.15397771	-0.60953333
0.8483	0.1517	-0.02555762	-1.05639976
1	1.00E-08	0.00000000	-1.42407901

α-pinene-OS-4

1.00E-08	1	4.80714672	0.00000007
5.20E-04	0.9995	4.77592096	0.00000817
1.04E-03	0.999	4.74487245	0.00003236
1.56E-03	0.9984	4.71400190	0.00007249
2.08E-03	0.9979	4.68330940	0.00012838
2.60E-03	0.9974	4.65279497	0.00019987
0.4378	0.5622	-0.47339566	0.57347139

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
0.5502	0.4498	-0.40747728	0.50420549
0.6627	0.3373	-0.25659803	0.26790042
0.7751	0.2249	-0.10843509	-0.10850990
0.8876	0.1124	-0.02388086	-0.51026669
1	1.00E-08	0.00000000	-0.85853086

α-pinene-OS-5

1.00E-08	1	3.40187659	0.00000007
1.35E-03	0.9987	3.31097218	0.00006137
2.69E-03	0.9973	3.22203769	0.00024188
4.03E-03	0.996	3.13508776	0.00053652
5.38E-03	0.9946	3.05012830	0.00094015
6.72E-03	0.9933	2.96715533	0.00144768
0.2268	0.7732	-0.55115713	0.25194749
0.3815	0.6185	-0.55708803	0.24183094
0.5361	0.4639	-0.33473359	0.04562307
0.6907	0.3093	-0.13044047	-0.28176504
0.8454	0.1546	-0.02507538	-0.63145548
1	1.00E-08	0.00000000	-0.93833312

α-pinene-OS-6

1.00E-08	1	2.76051800	0.00000007
1.39E-03	0.9986	2.66497968	0.00006594
2.77E-03	0.9972	2.57175691	0.00025950
4.16E-03	0.9958	2.48084905	0.00057464
5.54E-03	0.9945	2.39224474	0.00100533

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
6.93E-03	0.9931	2.30592136	0.00154561
0.21	0.79	-1.10577811	0.23036603
0.368	0.632	-1.06449898	0.19410079
0.526	0.474	-0.67829589	-0.13304361
0.684	0.316	-0.28410665	-0.74338900
0.842	0.158	-0.05869257	-1.45991421
1	1.00E-08	0.00000000	-2.10954675

β-pinene-OS-1

1.00E-08	1	5.68997377	0.00000007
3.45E-04	0.9997	5.65885767	0.00000545
6.90E-04	0.9993	5.62795753	0.00002150
1.03E-03	0.999	5.59727351	0.00004806
1.38E-03	0.9986	5.56680486	0.00008500
1.72E-03	0.9983	5.53655113	0.00013218
0.3907	0.6093	0.11356151	0.49383968
0.5126	0.4874	0.07498509	0.52450834
0.6344	0.3656	0.06057360	0.54605000
0.7563	0.2437	0.03750802	0.60512119
0.8781	0.1219	0.01099184	0.73598327
1	1.00E-08	0.00000000	0.92227144

β-pinene-OS-2

1.00E-08	1	4.45448952	0.00000007
6.11E-04	0.9994	4.40982444	0.00001369
1.22E-03	0.9988	4.36564937	0.00005415

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
1.83E-03	0.9982	4.32196049	0.00012091
2.44E-03	0.9976	4.27875342	0.00021339
3.05E-03	0.9969	4.23602351	0.00033106
0.3593	0.6407	-0.53198665	0.44250803
0.4875	0.5125	-0.50254423	0.40884389
0.6156	0.3844	-0.34573580	0.20206244
0.7437	0.2563	-0.16000620	-0.20423606
0.8719	0.1281	-0.03580048	-0.72346451
1	1.00E-08	0.00000000	-1.19208229

limonene-OS-1

1.00E-08	1	5.01896878	0.00000007
5.05E-04	0.9995	4.97944907	0.00001003
1.01E-03	0.999	4.94029114	0.00003968
1.51E-03	0.9985	4.90149379	0.00008867
2.02E-03	0.998	4.86305504	0.00015667
2.52E-03	0.9975	4.82497263	0.00024334
0.3724	0.6276	-0.16974861	0.46362004
0.4979	0.5021	-0.16297273	0.45411651
0.6235	0.3765	-0.09319285	0.36123235
0.749	0.251	-0.03195072	0.22383694
0.8745	0.1255	-0.00442394	0.10235441
1	1.00E-08	0.00000000	0.04181320

limonene-OS-2

1.00E-08	1	5.21158102	0.00000007

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
3.83E-04	0.9996	5.17811329	0.00000649
7.67E-04	0.9992	5.14489369	0.00002564
1.15E-03	0.9988	5.11192213	0.00005734
1.53E-03	0.9985	5.07919780	0.00010139
1.92E-03	0.9981	5.04671962	0.00015763
0.3625	0.6375	-0.19574436	0.44849806
0.49	0.51	-0.16781332	0.42309796
0.6175	0.3825	-0.08152360	0.31101061
0.745	0.255	-0.01489144	0.15945573
0.8725	0.1275	0.00704862	0.04119941
1	1.00E-08	0.00000000	0.00826903

limonene-OS-3

1.00E-08	1	5.87725874	0.00000007
2.32E-04	0.9998	5.85372965	0.00000280
4.64E-04	0.9995	5.83031494	0.00001095
6.96E-04	0.9993	5.80701536	0.00002448
9.28E-04	0.9991	5.78383069	0.00004332
1.16E-03	0.9988	5.76076064	0.00006743
0.3763	0.6237	-0.02139778	0.47099664
0.501	0.499	-0.01382572	0.46249432
0.6258	0.3742	0.01401673	0.42797760
0.7505	0.2495	0.01792621	0.42671848
0.8753	0.1247	0.00512185	0.50137643
1	1.00E-08	0.00000000	0.63305556

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
limonene-OS-4			
1.00E-08	1	5.35708475	0.00000007
2.96E-04	0.9997	5.33038275	0.00000402
5.92E-04	0.9994	5.30383423	0.00001581
8.88E-04	0.9991	5.27743972	0.00003535
1.18E-03	0.9988	5.25119877	0.00006255
1.48E-03	0.9985	5.22511068	0.00009732
0.3843	0.6157	-0.33421220	0.48362181
0.5074	0.4926	-0.28938819	0.43804153
0.6306	0.3694	-0.17284521	0.27478729
0.7537	0.2463	-0.06656310	0.02867420
0.8769	0.1231	-0.01158726	-0.21779401
1	1.00E-08	0.00000000	-0.40900861
isoprene-OS-1			
1.00E-08	1	1.38344406	0.00000007
0.05	0.95	0.32144684	0.02394751
0.15	0.85	-0.44833226	0.09927954
0.25	0.75	-0.61110043	0.13526486
0.35	0.65	-0.56239206	0.11117103
0.45	0.55	-0.43229078	0.02205117
0.55	0.45	-0.28567331	-0.12605092
0.65	0.35	-0.16027294	-0.31448215
0.75	0.25	-0.07273609	-0.51771424
0.85	0.15	-0.02285551	-0.71472290

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^{I}$(org)	$\ln \gamma^{I}$(H_2O)
0.95	0.05	-0.00226949	-0.89444067
1	1.00E-08	0.00000000	-0.97653593

isoprene-OS-2

1.00E-08	1	0.89819266	0.00000007
0.05	0.95	-0.22386930	0.02508034
0.15	0.85	-0.95177361	0.09612947
0.25	0.75	-1.02070596	0.10994303
0.35	0.65	-0.85545260	0.03694763
0.45	0.55	-0.60645970	-0.13095701
0.55	0.45	-0.36614515	-0.37269105
0.65	0.35	-0.18764655	-0.64098077
0.75	0.25	-0.07908318	-0.89396116
0.85	0.15	-0.02366416	-1.11422459
0.95	0.05	-0.00230280	-1.30150283
1	1.00E-08	0.00000000	-1.38373509

isoprene-OS-3

1.00E-08	1	-0.41196228	0.00000007
0.05	0.95	-0.97865783	0.01121896
0.15	0.85	-1.05947270	0.01414716
0.25	0.75	-0.81769233	-0.04704571
0.35	0.65	-0.54745110	-0.16424797
0.45	0.55	-0.32434986	-0.31680182
0.55	0.45	-0.16680632	-0.48174616
0.65	0.35	-0.06870731	-0.64167124

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
0.75	0.25	-0.01569136	-0.78758648
0.85	0.15	0.00589515	-0.91700462
0.95	0.05	0.00598847	-1.03085868
1	1.00E-08	0.00000000	-1.08259251

isoprene-OS-4

1.00E-08	1	0.21417729	0.00000007
0.05	0.95	-0.32793875	0.01206830
0.15	0.85	-0.63285155	0.03998876
0.25	0.75	-0.59936913	0.02921238
0.35	0.65	-0.47173317	-0.02627195
0.45	0.55	-0.33023171	-0.11994821
0.55	0.45	-0.20752311	-0.24043961
0.65	0.35	-0.11512777	-0.37509995
0.75	0.25	-0.05345091	-0.51310769
0.85	0.15	-0.01778959	-0.64712191
0.95	0.05	-0.00210553	-0.77323149
1	1.00E-08	0.00000000	-0.83280603

cis-β-IEPOX

1.00E-08	1	-0.06607103	0.00000007
0.05	0.95	-0.00540659	-0.00150073
0.15	0.85	0.02351606	-0.00346604
0.25	0.75	-0.01141428	0.00507173
0.35	0.65	-0.03779131	0.01526326
0.45	0.55	-0.04434317	0.01808982

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
0.55	0.45	-0.03768554	0.00965761
0.65	0.35	-0.02563953	-0.01036402
0.75	0.25	-0.01366817	-0.04050680
0.85	0.15	-0.00481492	-0.07864690
0.95	0.05	-0.00041435	-0.12262604
1	1.00E-08	0.00000000	-0.14619588

trans-β-IEPOX

1.00E-08	1	-0.11502697	0.00000007
0.05	0.95	-0.03167926	-0.00211193
0.15	0.85	0.01975114	-0.00674026
0.25	0.75	-0.01039226	0.00028072
0.35	0.65	-0.03770694	0.01073065
0.45	0.55	-0.04590063	0.01489269
0.55	0.45	-0.04017262	0.00816962
0.65	0.35	-0.02827853	-0.01013829
0.75	0.25	-0.01591409	-0.03864826
0.85	0.15	-0.00632601	-0.07518676
0.95	0.05	-0.00096277	-0.11751679
1	1.00E-08	0.00000000	-0.14022541

δ_1-IEPOX

1.00E-08	1	-0.96786087	0.00000006
0.05	0.95	-0.70766384	-0.00614888
0.15	0.85	-0.41478481	-0.03495589
0.25	0.75	-0.28853434	-0.06422185

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^I$(org)	$\ln \gamma^I$(H_2O)
0.35	0.65	-0.21401489	-0.09443639
0.45	0.55	-0.15579014	-0.13056960
0.55	0.45	-0.10680053	-0.17457643
0.65	0.35	-0.06689998	-0.22587768
0.75	0.25	-0.03657942	-0.28272363
0.85	0.15	-0.01564090	-0.34320634
0.95	0.05	-0.00328635	-0.40576005
1	1.00E-08	0.00000000	-0.43746403

δ_4-IEPOX

1.00E-08	1	-0.18735760	0.00000006
0.05	0.95	-0.05275575	-0.00291807
0.15	0.85	0.02779607	-0.00908656
0.25	0.75	0.00977799	-0.00428701
0.35	0.65	-0.01241106	0.00371545
0.45	0.55	-0.02154561	0.00732844
0.55	0.45	-0.02048365	0.00327313
0.65	0.35	-0.01453802	-0.00900165
0.75	0.25	-0.00773642	-0.02870865
0.85	0.15	-0.00250120	-0.05453296
0.95	0.05	-0.00003856	-0.08505944
1	1.00E-08	0.00000000	-0.10167232

methyl bisulfate

1.00E-08	1	0.55835039	0.00000002

Table S3 – continued from previous page

x(org)	x(H_2O)	$\ln \gamma^{I}$(org)	$\ln \gamma^{I}$(H_2O)
0.05	0.95	-0.14847044	0.01668245
0.15	0.85	-0.85943025	0.09005165
0.25	0.75	-1.14690289	0.15882766
0.35	0.65	-1.22465306	0.18952024
0.45	0.55	-1.15490370	0.13929634
0.55	0.45	-0.92841316	-0.09502714
0.65	0.35	-0.54918590	-0.67366264
0.75	0.25	-0.22800395	-1.41999653
0.85	0.15	-0.06108956	-2.07584590
0.95	0.05	-0.00447075	-2.56437274
1	1.00E-08	0.00000000	-2.71866247

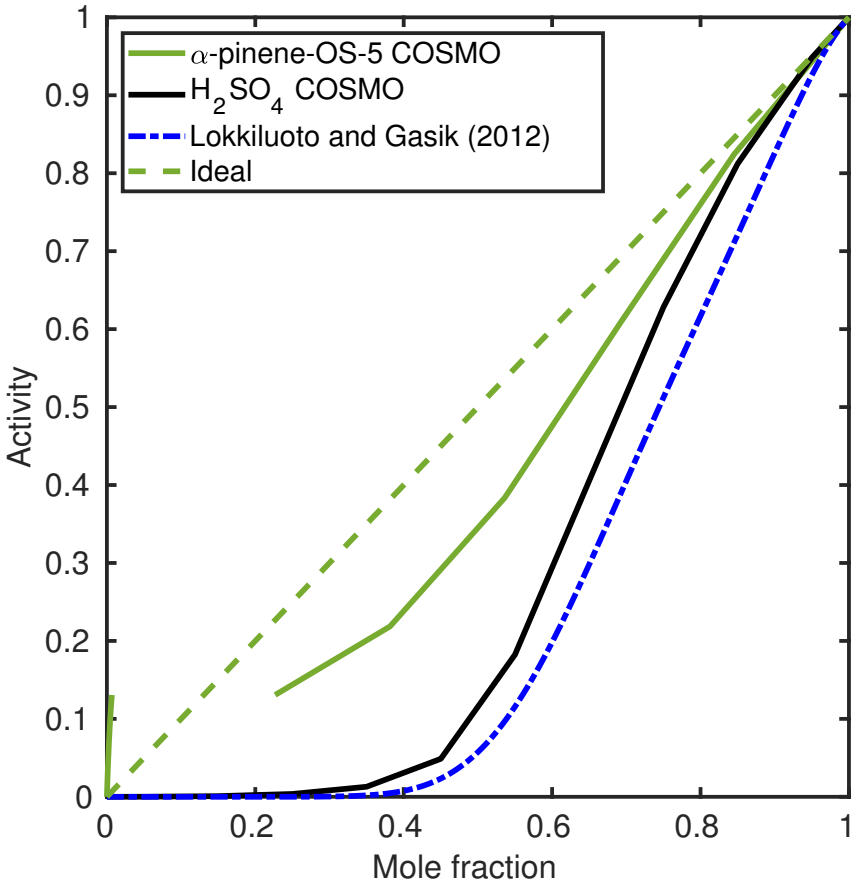

Figure S9: Comparison between COSMO*therm* calculated α-pinene-OS-5 and H_2SO_4 activities, and literature values[S4] of H_2SO_4 activities in pure water (T = 298.15 K). Note that the experimentally derived activity coefficients include the effects from the dissociation of sulfuric acid.

Table S4: Activity coefficients of the organics and water in ternary aqueous 0.09 mole fraction ammonium bisulfate solutions, at 298.15 K. Note that the mole fractions and activity coefficients are given in the COSMO*therm* framework, and should be converted using Equations S7 and S8, respectively. However, the activities can be calculated using either (Equation S6).

x'(org)	x'(H_2O)	$\ln \gamma^{I}$'(org)	$\ln \gamma^{I}$'(H_2O)
		α-pinene-OS-5	
0	0.8349	6.93440625	-0.07148410
9.76E-05	0.8348	6.92670895	-0.07172677
1.95E-04	0.8347	6.91901613	-0.07196911
2.93E-04	0.8346	6.91132789	-0.07221112
3.90E-04	0.8345	6.90364431	-0.07245278
4.88E-04	0.8345	6.89596540	-0.07269410
0.5244	0.3971	-0.08374992	-0.24283688
0.6195	0.3177	-0.05750087	-0.38050631
0.7146	0.2382	-0.02888838	-0.53204176
0.8098	0.1588	-0.00986429	-0.68085238
0.9049	0.0794	-0.00119644	-0.81753428
1	0	0.00000000	-0.93833314
		β-pinene-OS-1	
0	0.8349	9.34043829	-0.07148410
1.61E-05	0.8348	9.33892278	-0.07152657
3.22E-05	0.8348	9.33740746	-0.07156904
4.83E-05	0.8348	9.33589233	-0.07161149
6.44E-05	0.8348	9.33437740	-0.07165392
8.04E-05	0.8348	9.33286265	-0.07169634
0.8813	0.0991	0.03128335	0.58519254

Table S4 – continued from previous page

x'(org)	x'(H_2O)	$\ln \gamma^{I}$'(org)	$\ln \gamma^{I}$'(H_2O)
0.905	0.0793	0.02044998	0.64331224
0.9288	0.0595	0.01168913	0.70638528
0.9525	0.0397	0.00522123	0.77420323
0.9763	0.0198	0.00126136	0.84636938
1	0	0.00000000	0.92227145

limonene-OS-1

0	0.8349	8.56540801	-0.07148410
2.93E-05	0.8348	8.56303445	-0.07155621
5.86E-05	0.8348	8.56066103	-0.07162828
8.79E-05	0.8348	8.55828778	-0.07170033
1.17E-04	0.8348	8.55591474	-0.07177234
1.47E-04	0.8347	8.55354187	-0.07184432
0.7249	0.2297	0.04705734	0.01370163
0.7799	0.1838	0.03378174	-0.00986050
0.8349	0.1378	0.02178422	-0.02382205
0.8899	0.0919	0.01112840	-0.02276621
0.945	0.0459	0.00310955	-0.00184360
1	0	0.00000000	0.04181320

isoprene-OS-2

0	0.8349	3.82228285	-0.07148410
1.76E-03	0.8334	3.74309497	-0.07556788
3.53E-03	0.8319	3.66551171	-0.07953377
5.29E-03	0.8304	3.58950234	-0.08338449
7.06E-03	0.829	3.51504096	-0.08712259

Table S4 – continued from previous page

x'(org)	x'(H_2O)	$\ln \gamma^{I}$'(org)	$\ln \gamma^{I}$'(H_2O)
8.82E-03	0.8275	3.44209791	-0.09075080
0.3249	0.5636	-0.16419350	-0.31849729
0.4599	0.4509	-0.15632112	-0.52596279
0.5949	0.3382	-0.06944642	-0.79729730
0.73	0.2254	-0.01597782	-1.05299975
0.865	0.1127	-0.00093741	-1.24860285
1	0	0.00000000	-1.38373510

δ_1-IEPOX

0	0.8349	0.84847604	-0.07148410
0.05	0.7931	0.67644880	-0.13567635
0.15	0.7096	0.40802408	-0.22637132
0.25	0.6261	0.27811744	-0.28766514
0.35	0.5427	0.19334052	-0.33627708
0.45	0.4592	0.13230859	-0.37708178
0.55	0.3757	0.08579571	-0.41142791
0.65	0.2922	0.04971065	-0.43872772
0.75	0.2087	0.02273707	-0.45706549
0.85	0.1252	0.00512517	-0.46326792
0.95	0.0417	-0.00155910	-0.45214155
1	0	0.00000000	-0.43746404

Table S5: Activity coefficients of the organics and water in ternary aqueous 0.09 mole fraction ammonium sulfate solutions, at 298.15 K. Note that the mole fractions and activity coefficients are given in the COSMO*therm* framework, and should be converted using Equations S7 and S8, respectively. However, the activities can be calculated using either (Equation S6).

x'(org)	x'(H_2O)	$\ln \gamma^{I}$'(org)	$\ln \gamma^{I}$'(H_2O)
		α-pinene-OS-5	
0	0.7712	10.9746567	0.38650676
2.64E-06	0.7712	10.97425201	0.38648605
5.27E-06	0.7712	10.97384651	0.38646537
7.91E-06	0.7712	10.97344102	0.38644469
1.05E-05	0.7712	10.97303554	0.38642402
1.32E-05	0.7712	10.972627	0.38640318
0.6573	0.2643	0.15503718	-0.55855118
0.726	0.2113	0.11603024	-0.69706966
0.7945	0.1585	0.07475409	-0.81081242
0.863	0.1057	0.04004649	-0.89719833
0.9315	0.0528	0.01477921	-0.95353053
1	0	0	-0.93833314
		β-pinene-OS-1	
0	0.7712	13.62597811	0.38650676
2.38E-07	0.7712	13.62593646	0.3865048
4.76E-07	0.7712	13.62589411	0.38650287
7.14E-07	0.7712	13.62585176	0.38650093
9.52E-07	0.7712	13.6258094	0.386499
1.19E-06	0.7712	13.62576705	0.38649707
0.9809	0.0147	0.00350281	0.78810383

Table S5 – continued from previous page

x'(org)	x'(H_2O)	$\ln \gamma^I$'(org)	$\ln \gamma^I$'(H_2O)
0.9847	0.0118	0.00244294	0.80859989
0.9885	8.83E-03	0.00152435	0.83110332
0.9924	5.89E-03	0.0007718	0.85632922
0.9962	2.94E-03	0.00022908	0.88562421
1	0	0	0.92227145

limonene-OS-1

0	0.7712	13.21198231	0.38650676
3.46E-07	0.7712	13.21192412	0.38650385
6.92E-07	0.7712	13.2118652	0.38650097
1.04E-06	0.7712	13.21180627	0.38649809
1.38E-06	0.7712	13.21174735	0.3864952
1.73E-06	0.7712	13.21168843	0.38649232
0.9241	0.0585	0.02346932	-0.12346386
0.9393	0.0468	0.01707799	-0.11453178
0.9545	0.0351	0.0113298	-0.09987282
0.9697	0.0234	0.00631327	-0.07669965
0.9848	0.0117	0.00224958	-0.03853834
1	0	0	0.0418132

isoprene-OS-2

0	0.7712	6.36107283	0.38650676
1.76E-04	0.7711	6.34687248	0.38549488
3.52E-04	0.7709	6.33269604	0.38448634
5.28E-04	0.7708	6.31854383	0.3834811
7.04E-04	0.7706	6.30441632	0.38247916

Table S5 – continued from previous page

x'(org)	x'(H_2O)	$\ln \gamma^{I}$'(org)	$\ln \gamma^{I}$'(H_2O)
8.81E-04	0.7705	6.29027928	0.38147808
0.4399	0.432	0.07719509	-0.38817693
0.5517	0.3457	0.12851291	-0.70458111
0.6638	0.2593	0.13528186	-1.0211394
0.7759	0.1729	0.08662511	-1.26899869
0.8879	0.0864	0.03237511	-1.41924685
1	0	0	-1.3837351

δ_1-IEPOX

0	0.7712	4.57475479	0.38650676
2.68E-03	0.7691	4.50581095	0.37113771
5.35E-03	0.7671	4.43876863	0.35612251
8.03E-03	0.765	4.37353962	0.34144688
0.0107	0.7629	4.31003384	0.3270975
0.0134	0.7609	4.24765149	0.31294408
0.8874	0.0868	0.05339775	-0.64201559
0.91	0.0694	0.0386952	-0.63139267
0.9325	0.0521	0.02550655	-0.61443628
0.955	0.0347	0.01401898	-0.58730439
0.9775	0.0174	0.0047697	-0.54088997
1	0	0	-0.43746404

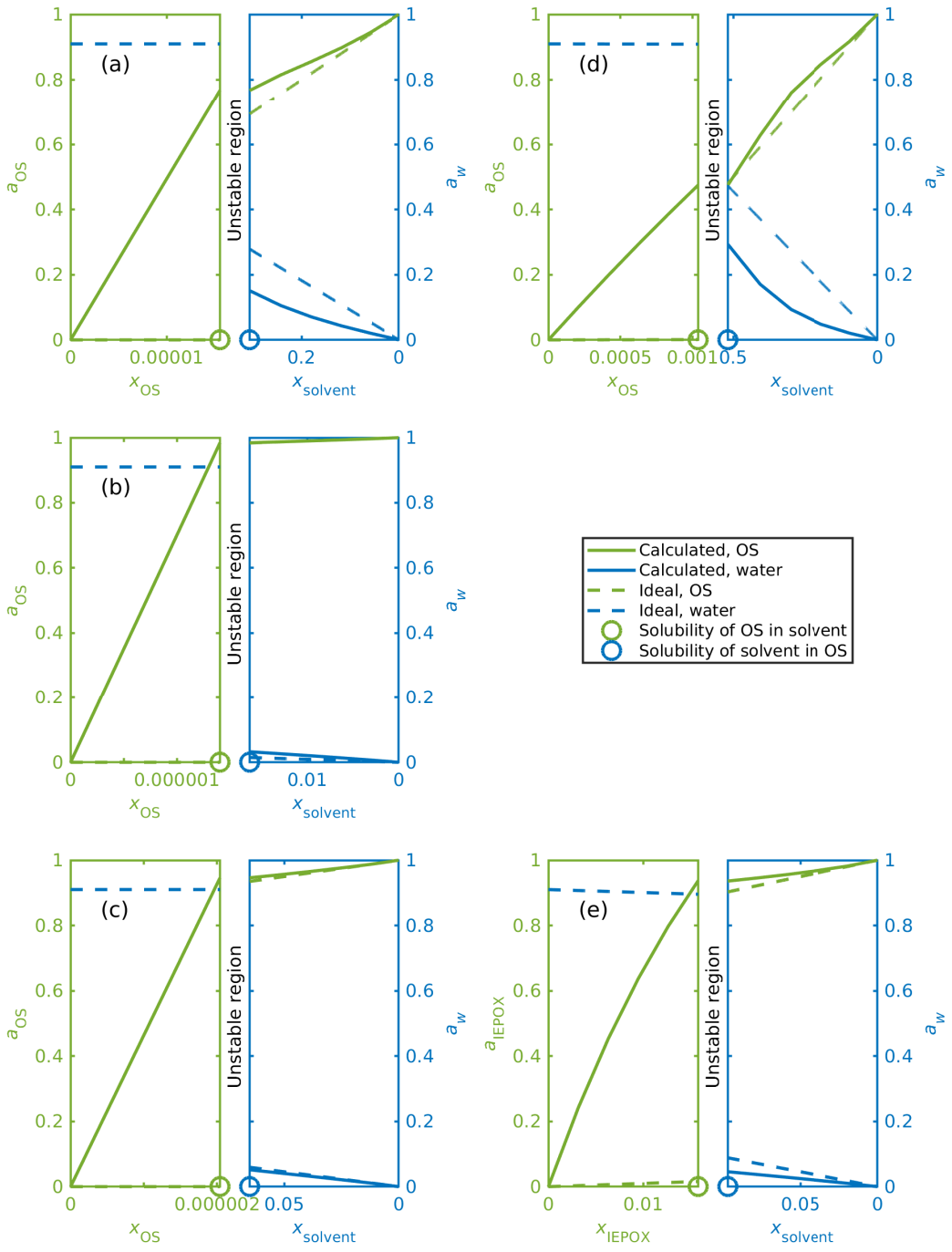

Figure S10: The activities of the OS and IEPOX, and water in ternary mixtures. The solvent is a 0.09 mole fraction ammonium sulfate and the ideal water activity is equal to the mole fraction of water. a) α-pinene-OS-5, b) β-pinene-OS-1, c) limonene-OS-1, d) isoprene-OS-2, e) δ_1-IEPOX. The left panel of each figure shows the solvent-rich phase and the right panel the organic-rich phase.The predicted activity of water in the solvent-rich phase is 1.14, which is outside the scale of the figures.

Table S6: Activity coefficients of the organic compounds in the infinite dilution of water ($\gamma^{\mathrm{I}}(0)$), free energies of solvation (G_{solv}) and Henry's law solubilities (H_{sol}) calculated with different methods. The free energies are given in units of kcal mol^{-1} and the Henry's law solubilities in mol m^{-3} Pa^{-1}.

solvent	H_2O				hexanoic acid	*cis*-pinonic acid
solute	H_{sol}^{LLE}	$\gamma^{\mathrm{I}}(0)$	G_{solv}	$H_{\mathrm{sol}}^{\infty}$	$H_{\mathrm{sol}}^{\infty}$	$H_{\mathrm{sol}}^{\infty}$
α-pinene-OS-1	$6.46{\cdot}10^{6}$	516.64	-14.36	$1.35{\cdot}10^{7}$	$8.82{\cdot}10^{8}$	$2.48{\cdot}10^{9}$
α-pinene-OS-2	$8.98{\cdot}10^{6}$	103.70	-14.76	$2.66{\cdot}10^{7}$	$3.37{\cdot}10^{8}$	$7.57{\cdot}10^{8}$
α-pinene-OS-3	$2.08{\cdot}10^{10}$	28.31	-19.99	$1.81{\cdot}10^{11}$	$4.91{\cdot}10^{11}$	$2.90{\cdot}10^{12}$
α-pinene-OS-4	$2.96{\cdot}10^{9}$	122.38	-18.3	$1.05{\cdot}10^{10}$	$5.29{\cdot}10^{10}$	$1.52{\cdot}10^{11}$
α-pinene-OS-5	$6.13{\cdot}10^{10}$	30.02	-20.39	$3.55{\cdot}10^{11}$	$1.09{\cdot}10^{12}$	$6.61{\cdot}10^{12}$
α-pinene-OS-6	$2.39{\cdot}10^{11}$	15.81	-21.56	$2.56{\cdot}10^{12}$	$3.70{\cdot}10^{12}$	$2.43{\cdot}10^{13}$
β-pinene-OS-1	$2.34{\cdot}10^{7}$	295.89	-15.15	$5.12{\cdot}10^{7}$	$2.04{\cdot}10^{9}$	$5.52{\cdot}10^{9}$
β-pinene-OS-2	$1.17{\cdot}10^{7}$	86.01	-15.14	$5.01{\cdot}10^{7}$	$3.74{\cdot}10^{8}$	$1.03{\cdot}10^{9}$
limonene-OS-1	$2.57{\cdot}10^{7}$	151.26	-15.38	$7.55{\cdot}10^{7}$	$1.35{\cdot}10^{9}$	$3.56{\cdot}10^{9}$
limonene-OS-2	$5.04{\cdot}10^{7}$	183.38	-15.82	$1.60{\cdot}10^{8}$	$3.91{\cdot}10^{9}$	$9.51{\cdot}10^{9}$
limonene-OS-3	$4.24{\cdot}10^{7}$	356.83	-15.62	$1.14{\cdot}10^{8}$	$7.04{\cdot}10^{9}$	$2.26{\cdot}10^{10}$
limonene-OS-4	$2.37{\cdot}10^{7}$	212.11	-15.44	$8.40{\cdot}10^{7}$	$1.97{\cdot}10^{9}$	$6.02{\cdot}10^{9}$
isoprene-OS-1	-	3.99	-18.16	$8.26{\cdot}10^{9}$	$3.67{\cdot}10^{9}$	$1.01{\cdot}10^{10}$
isoprene-OS-2	-	2.46	-16.94	$1.05{\cdot}10^{9}$	$5.11{\cdot}10^{8}$	$1.48{\cdot}10^{9}$
isoprene-OS-3	-	0.66	-21.73	$3.45{\cdot}10^{12}$	$2.21{\cdot}10^{11}$	$7.20{\cdot}10^{11}$
isoprene-OS-4	-	1.24	-21.46	$2.16{\cdot}10^{12}$	$3.20{\cdot}10^{11}$	$1.50{\cdot}10^{11}$
cis-β-IEPOX	-	0.89	-11.72	$1.59{\cdot}10^{5}$	$1.24{\cdot}10^{4}$	$1.45{\cdot}10^{4}$
trans-β-IEPOX	-	0.94	-12.00	$2.52{\cdot}10^{5}$	$1.37{\cdot}10^{3}$	$9.17{\cdot}10^{3}$
δ_1-IEPOX	-	0.38	-9.80	$6.20{\cdot}10^{3}$	$2.06{\cdot}10^{2}$	$2.36{\cdot}10^{2}$
δ_4-IEPOX	-	0.83	-11.70	$1.51{\cdot}10^{5}$	$6.40{\cdot}10^{3}$	$8.12{\cdot}10^{3}$
methyl bisulfate	-	1.75	-10.75	$3.04{\cdot}10^{4}$	$2.06{\cdot}10^{4}$	$1.33{\cdot}10^{5}$
sulfuric acid	-	$1.56{\cdot}10^{-3}$	-16.49	$4.91{\cdot}10^{8}$	-	-

Table S7: Molar weights (MW), and estimated densities (ρ) and volumes ($\widetilde{V}$) of the liquid phase compounds at 298.15 K. Experimentally determined density of pure sulfuric acid at 298.15 K is 1.8255 g cm^{-3}.[S5]

	MW(g mol^{-1})	ρ(g cm^{-3})	$\widetilde{V}$(Å^3)
α-pinene-OS-1	250.314	1.286	321.100
α-pinene-OS-2	250.314	1.284	322.023
α-pinene-OS-3	266.313	1.257	351.258
α-pinene-OS-4	280.296	1.251	363.253
α-pinene-OS-5	280.296	1.317	350.871
α-pinene-OS-6	280.296	1.313	353.888
β-pinene-OS-1	250.314	1.298	320.682
β-pinene-OS-2	250.314	1.299	318.565
limonene-OS-1	250.314	1.255	329.109
limonene-OS-2	250.314	1.249	331.035
limonene-OS-3	250.314	1.260	329.988
limonene-OS-4	250.314	1.254	329.435
isoprene-OS-1	198.195	1.391	234.832
isoprene-OS-2	198.195	1.385	237.445
isoprene-OS-3	216.211	1.427	249.176
isoprene-OS-4	216.211	1.446	244.129
cis-β-IEPOX	118.132	1.172	167.508
trans-β-IEPOX	118.132	1.173	167.626
δ_1-IEPOX	118.132	1.142	171.970
δ_4-IEPOX	118.132	1.163	171.575
methyl bisulfate	112.106	1.522	122.339
sulfuric acid	98.079	1.958	83.180

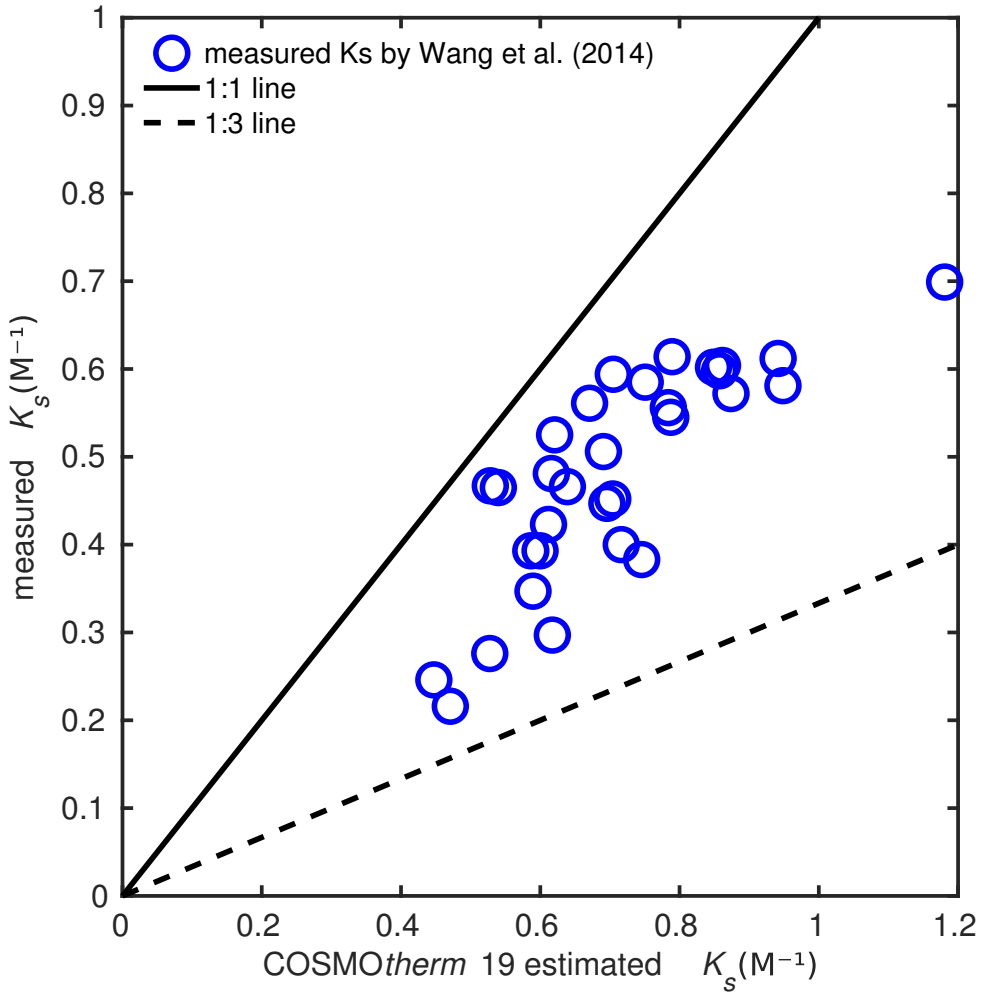

Figure S11: Comparison between measured[S6] and COSMO*therm*19 estimated Setschenow constants (K_s) using relative solubilities in $x_{\mathrm{AS}} = 0.007$.

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