Supplementary Information: Finding suitable biobased solvents for extractions from water

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Figure S1. Molecular structures of the benchmark solutes: water, acetamide, methanol, ethanol, tetrahydrofuran, methanethiol, aniline, phenol, ethane, benzene, cyclohexane, and hexane. The solutes were selected because of their broad dynamic range and relatively even spacing of hydrophobicity, which is a necessary requirement for the regression analysis.

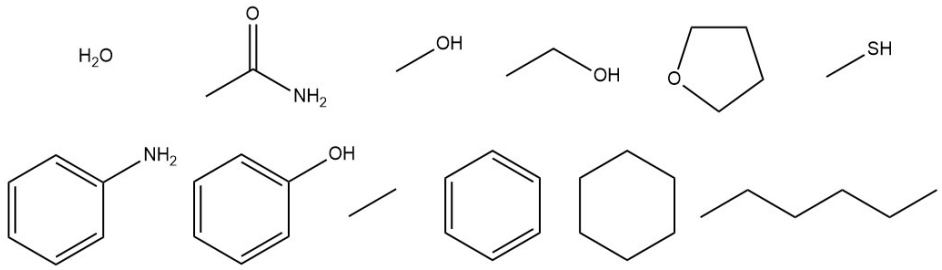

Figure S2. 1D-NMR spectrum of the employed aqueous medium.

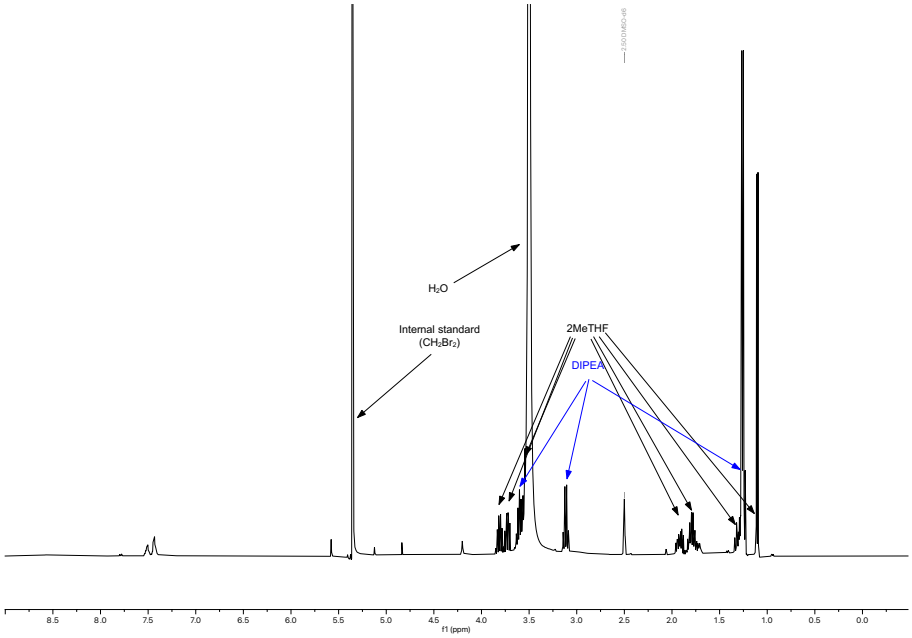

Figure S3. qNMR of the aqueous solution after the extractions with the corresponding green solvent. Spectra are shown for cyclopentanol (CP), ethyl acetate (EA), 1-butanol (BU), 2-pentanol (2P), 2-methyl tetrahydrofuran (2T), 1-pentanol (1P), cyclopentyl methyl ether (CM), butyl methyl ether (BM), butyl acetate (BA), 1-octanol (OC), methyl oleate (MO), as well as the original waste water (WW) before the extraction. Spectra are normalized with respect to the CH_2Br_2 internal standard.

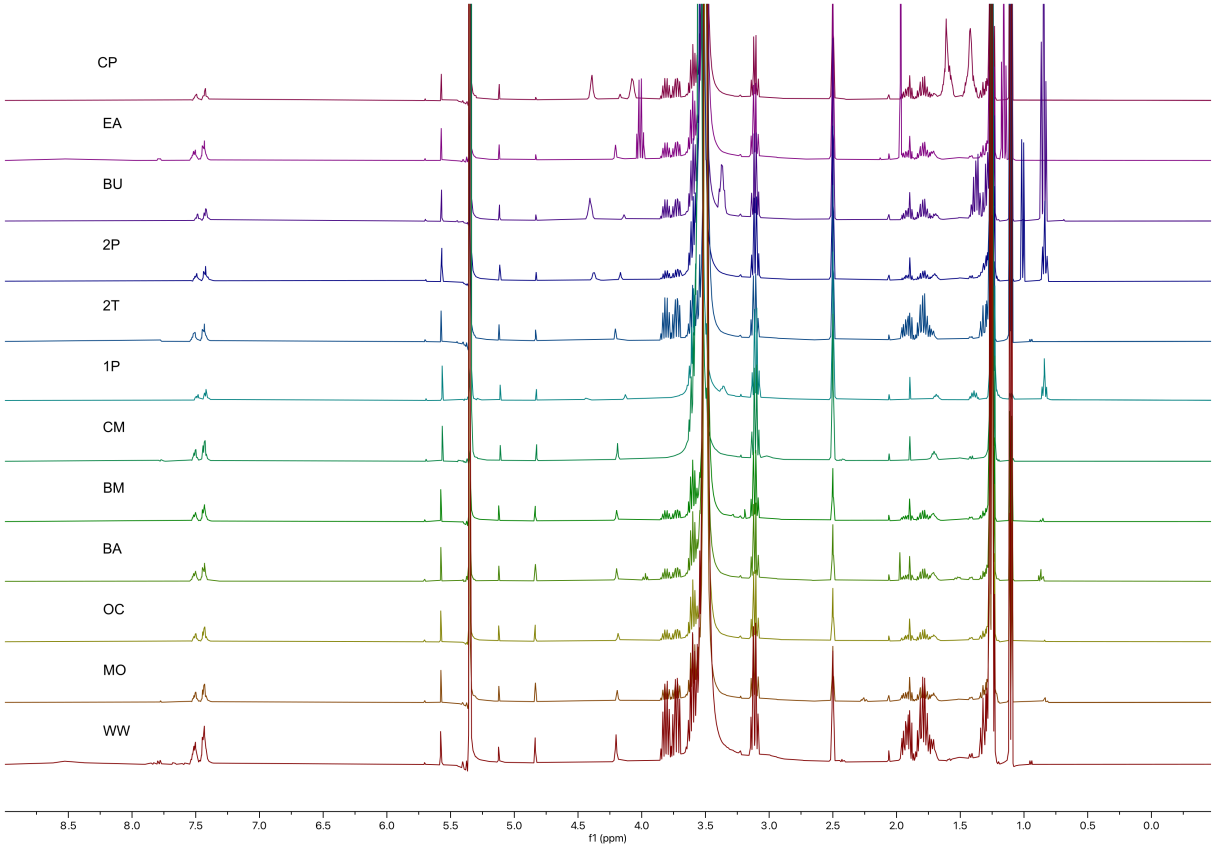

Table S1: Simulated and experimental densities (ρ) of the employed green solvents.

ρ (g/l)	Simulation	Experiment[a]	Difference
Cyclopentanol	949	927	2.3 %
Ethyl acetate	900	877	2.5 %
1-Butanol	810	797	1.6 %
2-Pentanol	809	793	2.0 %
2-Methyl tetrahydrofuran	855	830	2.9 %
1-Pentanol	814	802	1.5 %
Butyl methyl ether	740	722	2.5 %
Cyclopentyl methyl ether	863	851	1.4 %
Butyl acetate	883	860	2.7 %
1-Octanol	826	817	1.1 %
Methyl oleate	874	871	0.3 %
Average Error			2.1%

[a] Experimental densities from Ref. 1

Table S2: Simulated and experimental partition coefficients of water between aqueous solution and the employed solvents.

Molecule	$\log \mathrm{P}_{\mathrm{solv}}^{\mathrm{Sim}\,a}$	$\log \mathrm{P}_{\mathrm{solv}}^{\mathrm{Exp}\,b}$
Cyclopentanol	0.80 ± 0.09	0.77[c]
Ethyl acetate	1.12 ± 0.06	1.54[d]
1-Butanol	0.79 ± 0.08	0.77[e]
2-Pentanol	1.16 ± 0.08	1.03[c]
2-Methyl tetrahydrofuran	1.62 ± 0.10	1.50[f]
1-Pentanol	1.16 ± 0.06	1.08[c]
Cyclopentyl methyl ether	-2.76 ± 0.08	-2.59[g]
Butyl methyl ether	2.45 ± 0.08	2.18[h]
Butyl acetate	1.50 ± 0.07	1.99[i]
1-Octanol	1.50 ± 0.08	1.42[j]
Methyl oleate	2.33 ± 0.07	2.84[k]
MSE[l]	0.07	
RMSE[m]	0.28	

[a] Simulated partition coefficients of water between aqueous solution and corresponding the wet solvent. Standard deviations were calculated by separating the simulations into ten blocks.
[b] Experimental partition coefficients of water between aqueous solution and corresponding the wet solvent, as calculated from the densities and water solubility data.
[c] Ref. 2 [d] Ref. 3 [e] Ref. 4 [f] Ref. 5 [g] Ref. 6 [h] Ref. 7 [i] Ref. 8 [j] Ref. 9 [k] Ref. 10
[l] Mean signed error with respect to experimental values
[m] Root mean square error with respect to experimental values

Table S3: Comparison of the simulated and available experimental partition coefficients between water and 1-octanol ($\mathrm{LogP}^{\mathrm{Sim}}_{\mathrm{ocoh}}$ and $\mathrm{LogP}^{\mathrm{Exp}}_{\mathrm{ocoh}}$), as well as 1-butanol ($\mathrm{LogP}^{\mathrm{Sim}}_{\mathrm{buoh}}$ and $\mathrm{LogP}^{\mathrm{Exp}}_{\mathrm{buoh}}$), for the selected twelve simple solutes.

Molecule	$\mathrm{LogP}^{\mathrm{Sim}}$ [a]	$\mathrm{LogP}^{\mathrm{Exp}}$	$\log \mathrm{P}^{\mathrm{Sim}}_{\mathrm{buoh}}$ [a]	$\log \mathrm{P}^{\mathrm{Exp}}_{\mathrm{buoh}}$
Water	-1.50 ± 0.10	-1.42[b]	-0.79 ± 0.10	-0.77[c]
Acetamide	-0.42 ± 0.20	-1.09[d]		
Methanol	-0.65 ± 0.13	-0.77[d]	-0.19 ± 0.10	-0.28[e]
Ethanol	-0.07 ± 0.13	-0.31[d]	0.20 ± 0.12	0.34[e]
Tetrahydrofuran	0.70 ± 0.13	0.47[d]		
Methanethiol	1.47 ± 0.08	0.65[f]		
Aniline	0.87 ± 0.15	0.90[g]		
Phenol	1.63 ± 0.14	1.50[g]	1.81 ± 0.14	1.14[e]
Ethane	1.69 ± 0.08	1.81[f]		
Benzene	2.18 ± 0.12	2.13[g]	2.14 ± 0.11	1.92[h]
Cyclohexane	3.55 ± 0.13	3.44[g]		
Hexane	4.02 ± 0.15	4.00[g]		
MSE[i]	**0.18**		**0.16**	
RMSE[j]	**0.35**		**0.33**	

[a] Simulated partition coefficients. Standard deviations were calculated by separating the simulations into ten blocks.
[b] Calculated from Ref. 9 [c] Calculated from Ref. 4 [d] Ref. 11 [e] Ref. 12 [f] Ref. 13 [g] Ref. 14 [h] Ref. 15
[i] Mean signed error with respect to experimental values
[j] Root mean square error with respect to experimental values

Table S4: Simulated and experimental partition coefficients between water and 1-octanol ($LogP^{Sim}_{ocoh}$ and $LogP^{Exp}_{ocoh}$) of the selected green solvent molecules.

Molecule	$LogP^{Sim\,a}$	$LogP^{Exp}$
Water	-1.50 ± 0.10	-1.39[b]
Cyclopentanol	1.11 ± 0.18	0.71[c]
Ethyl acetate	0.51 ± 0.16	0.73[c]
1-Butanol	0.98 ± 0.20	0.88[c]
2-Pentanol	1.28 ± 0.18	1.19[c]
2-Methyl tetrahydrofuran	1.33 ± 0.15	1.26[d]
1-Pentanol	1.57 ± 0.16	1.56[c]
Cyclopentyl methyl ether	2.08 ± 0.21	1.59[e]
Butyl methyl ether	1.98 ± 0.14	1.66[f]
Butyl acetate	1.79 ± 0.21	1.78[c]
1-Octanol	3.26 ± 0.29	3.07[c]
Methyl oleate	8.35 ± 0.35	7.45[g]
MSE[h]	0.19	
RMSE[i]	0.35	

[a] Simulated partition coefficients. Standard deviations were calculated by separating the simulations into ten blocks.
[b] Calculated from densities and water solubility data in 1-octanol reported in Ref. 16
[c] Ref. 13 [d] Ref. 17 [e] Ref. 6 [f] Ref. 11 [g] Ref. 18
[h] Mean signed error with respect to experimental values
[i] Root mean square error with respect to experimental values

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