Supplementary Materials

1. Calculation of dielectric constant (ε_m) of solvent mixtures

The calculation of ε_m for a solvent mixture [1,2] was done on the basis of ε of every solvent contained in the mixture by using the following equation:

$$\varepsilon_m = \sum_i^t \varepsilon_i \varphi_i \text{ , } i = 1, 2, 3$$

where ε_i is dielectric constant of a solvent, and φ_i is a volume fraction of a solvent in the mixture.

Dielectric constants of the used solvents at 80 ºC (353.15 K) were calculated by using following equations [3]:

$$\varepsilon_{(T)} = a - b \times T + c \times (T)^2$$

Ethanol: $\varepsilon_{(353.15)} = 151.45 - 0.87020 \times 353.15 + 0.001957 \times (353.15)^2$

$\varepsilon_{(353.15)} = 88.21$

Acetone: $\varepsilon_{(353.15)} = 88.157 - 0.34300 \times 353.15 + 0.00038925 \times (353.15)^2$

$\varepsilon_{(353.15)} = 15.57$

Water: $\varepsilon_{(353.15)} = 249.21 - 0.79069 \times 353.15 + 0.00072997 \times (353.15)^2$

$\varepsilon_{(353.15)} = 61.02$

2. Calculation of relative polarity (RP_m) of solvent mixtures

The calculation of RP_m for a solvent mixture was done on the basis of relative polarity of every solvent contained in the mixture on the basis of the following equation [4]:

$$RP_m = \sum_i^t RP_i \varphi_i \text{ , } i = 1, 2, 3$$

where RP_i is a relative polarity of a solvent and φ_i is a volume fraction of a solvent in the mixture.

RP (ethanol) = 0.654, RP (acetone) = 0.355, RP (water) = 1.000 [5]

3. Calculation of density (ρ_m) of solvent mixtures

The calculation of ρ_m of a solvent mixture was done on the basis of density of every solvent contained in the mixture by using the following equation [2]:

$$\rho_m = \sum_i^t \rho_i \varphi_i \text{ , } i = 1, 2, 3$$

where ρ_i is density of a solvent, and φ_i is a volume fraction of a solvent in the mixture.

ρ (ethanol, 80 ºC) = 725.634 g/dm^3, ρ (acetone, 80 ºC) = 720.761 g/dm^3, ρ (water, 80 ºC) = 962.029 g/dm^3 [6]

4. Calculation of polarity index (P') of solvent mixtures

Polarity index (P') of a solvent mixture was calculated on the basis of polarity index of every solvent contained in the mixture. The calculation of P'_m of a solvent mixture was done on the basis of the following equation [7,2]:

$$P'_m = \sum_1^t P'_i \varphi_i , \; i = 1, 2, 3$$

where P'_i is polarity index of a solvent, and φ_i is a volume fraction of a solvent in the mixture.

P' (ethanol) = 5.2, P' (acetone) = 5.4, P' (water) = 9.0 [8]

References:

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4. C. Diaz, L. Barrio, J. Catalan, Characterization of ternary solvent mixtures: the methanol/ethanol/aceton mixture, *Chem. Phys. Lett.* **371** (2003) 645-654.

5. C. Reichardt, *Solvents and solvent effects in organic chemistry,* Wwiley Verlag GmbH & Co. KgaA, Weinheim, Germany, 2003.

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7. C. F. Poole, S. K. Poole, *Chromatography Today,* Elsevier, Amsterdam, Netherlands, 1991.

8. L. B. Kier, Quantitation of solvent polarity based on molecular structure, *J. Pharm. Sci.* **70** (1981) 930-933.

Table S1. The normalized data used in the SRD analysis of extraction experiments.

Experiment	Solvent volume fraction (v/v)			ε_m	RP_m	$\rho_m(g/dm^3)$	P'_m	T_{Car} (mg/100 ml)
	Ethanol	**Acetone**	**Water**					
1	0.7940	0.0100	0.9900	0.9166	0.9900	0.9900	0.8196	0.0112
2	0.0100	0.7940	0.9900	0.1326	0.3533	0.9167	0.9900	0.5683
3	0.0100	0.7940	0.9900	0.1326	0.3533	0.9167	0.9900	0.5354
4	0.2060	0.5980	0.9900	0.3286	0.5125	0.9351	0.9474	0.2431
5	0.4020	0.4020	0.9900	0.5246	0.6717	0.9534	0.9048	0.1082
6	0.5980	0.2060	0.9900	0.7206	0.8308	0.9717	0.8622	0.0456
7	0.7940	0.0100	0.9900	0.9166	0.9900	0.9900	0.8196	0.0100
8	0.4020	0.4020	0.9900	0.5246	0.6717	0.9534	0.9048	0.0933
9	0.9900	0.0100	0.0100	0.9900	0.8058	0.1016	0.0100	0.7633
10	0.0100	0.9900	0.0100	0.0100	0.0100	0.0100	0.2230	0.4509
11	0.0100	0.9900	0.0100	0.0100	0.0100	0.0100	0.2230	0.4474
12	0.2550	0.7450	0.0100	0.2550	0.2090	0.0329	0.1698	0.8067
13	0.5000	0.5000	0.0100	0.5000	0.4079	0.0558	0.1165	0.8157
14	0.7450	0.2550	0.0100	0.7450	0.6069	0.0787	0.0633	0.9900
15	0.9900	0.0100	0.0100	0.9900	0.8058	0.1016	0.0100	0.7601
16	0.5000	0.5000	0.0100	0.5000	0.4079	0.0558	0.1165	0.8997
Opt	0.6333	0.3667	0.0100	0.6333	0.5161	0.0682	0.0875	0.9282

Table S2. The input matrix used in the SRD modeling

Experiment	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	*Opt**	Read**
Ethanol	0.7940	0.0100	0.0100	0.2060	0.4020	0.5980	0.7940	0.4020	0.9900	0.0100	0.0100	0.2550	0.5000	0.7450	0.9900	0.5000	0.6333	0.4510
Acetone	0.0100	0.7940	0.7940	0.5980	0.4020	0.2060	0.0100	0.4020	0.0100	0.9900	0.9900	0.7450	0.5000	0.2550	0.0100	0.5000	0.3667	0.4510
Water	0.9900	0.9900	0.9900	0.9900	0.9900	0.9900	0.9900	0.9900	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.5000
ε_m	0.9166	0.1326	0.1326	0.3286	0.5246	0.7206	0.9166	0.5246	0.9900	0.0100	0.0100	0.2550	0.5000	0.7450	0.9900	0.5000	0.6333	0.5123
RP_m	0.9900	0.3533	0.3533	0.5125	0.6717	0.8308	0.9900	0.6717	0.8058	0.0100	0.0100	0.2090	0.4079	0.6069	0.8058	0.4079	0.5161	0.5398
ρ_m	0.9900	0.9167	0.9167	0.9351	0.9534	0.9717	0.9900	0.9534	0.1016	0.0100	0.0100	0.0329	0.0558	0.0787	0.1016	0.0558	0.0682	0.5046
P'_m	0.8196	0.9900	0.9900	0.9474	0.9048	0.8622	0.8196	0.9048	0.0100	0.2230	0.2230	0.1698	0.1165	0.0633	0.0100	0.1165	0.0875	0.5107
T_{Car}	0.0112	0.5683	0.5354	0.2431	0.1082	0.0456	0.0100	0.0933	0.7633	0.4509	0.4474	0.8067	0.8157	0.9900	0.7601	0.8997	0.9282	0.4718

*in the first step of the SRD analysis the *Opt* column was not considered
**average row values are calculated on the basis of the data for experiments 1–16