Electronic Supplementary Material (ESI) for RSC Advances.

Harnessing the power of natural deep eutectic solvents (choline chloride/sucrose) and polypropylene glycol in the formation of aqueous biphasic systems and the application of these systems in drug extraction

Fariba Ghaffari, Mohammed Taghi Zafarani-Moattar,* Hemayat Shekaari

Department of Physical Chemistry, University of Tabriz, Tabriz, Iran

*Corresponding author. Tel: +98 4133393135 Fax: 98 4133340191.
E-mail addresses: zafarani47@yahoo.com.

Table S1

The values of parameters of Eq. 10, Eq. 11 and 12 along with the standard deviation of the models, *sd*, from the experimental values of partition coefficients for the {PPG400 + ChCl(HBA) +sucrose(HBD) + H_2O} at 298.15 K and atmospheric pressure (≈ 85 kPa).

HBA:HBD	Diamond-Hsu (Eq. 10)			
	A	$10^3 \cdot B$		$100.sd^a$
		Diclofenac potasium		
2:1	0.0907	-0.8209		0.49
1:1	0.0917	-0.9239		0.38
		Salicylic acid		
2:1	0.092	-0.8639		0.30
1:1	0.0899	-0.8975		0.30
		Acetaminophen		
2:1	0.1415	-1.7571		0.59
1:1	0.1669	-2.4408		0.17
	Modified Diamond-Hsu (Eq. 11)			
	A_1	B_1	$10^4 \cdot C_1$	$100.sd$
		Diclofenac potasium		
2:1	4.4090	-0.0385	1.1532	0.11
1:1	3.8590	-0.0325	63.1330	0.12
		Salicylic acid		
2:1	3.3914	-0.0075	-1.4389	0.02
1:1	2.9721	-0.0058	-1.373	0.13
		Acetaminophen		
2:1	-4.9348	0.2861	-0.0028	0.41
1:1	2.6239	0.0824	-18.0000	0.40
	Polynomial Equation (Eq. 12)			

	A_2	B_2	$10^4 \cdot C_2$	100.*sd*
		Diclofenac potasium		
2:1	5.3917	-0.2759	55.6320	0.14
1:1	5.5045	-0.3118	64.3750	0.08
		Salicylic acid		
2:1	4.6506	-0.1868	25.2990	0.16
1:1	4.6038	-0.2137	37.8300	0.10
		Acetaminophen		
2:1	2.9866	0.1712	-0.0153	0.45
1:1	12.1332	-0.8287	95.8130	0.22

[a] $sd = (\sum_{i=1}^{N} (K^{cal} - K^{\exp})^2 / N)^{0.5}$ where K and N represented the partition coefficients and number of partition coefficient data, respectively.

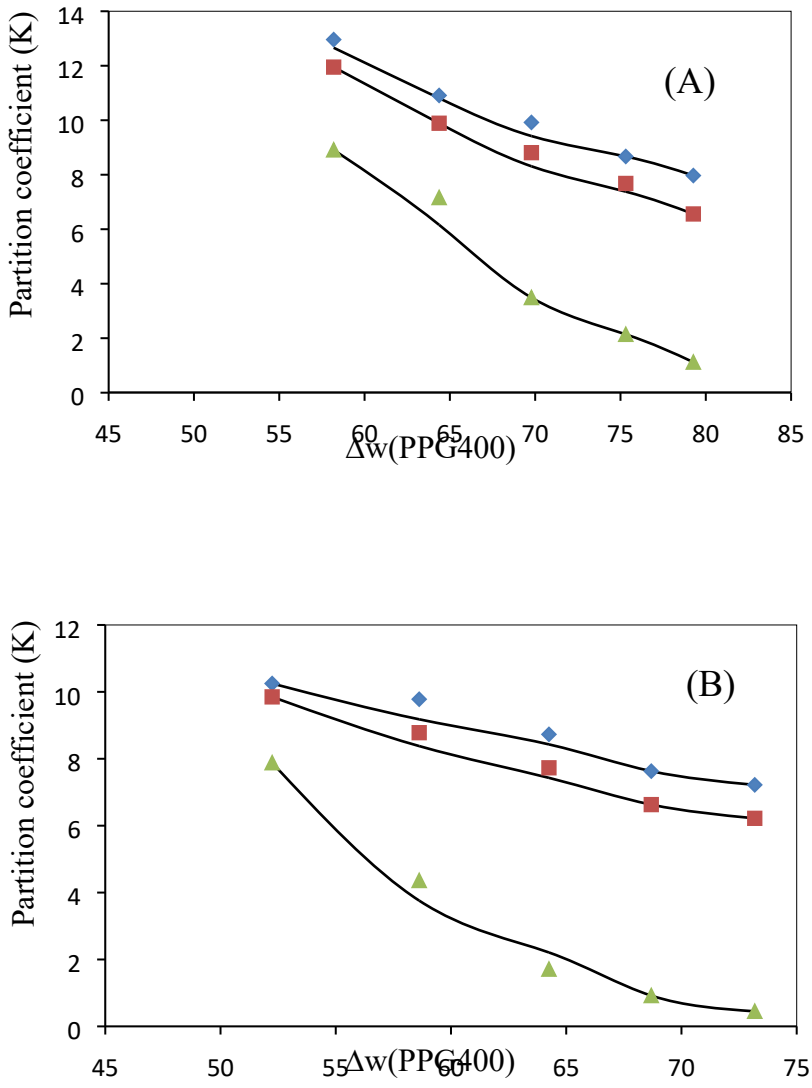

Fig. S1. Partition coefficient, *K*, as a function of the mass fraction difference of PPG400 in the top and bottom phases for each studied drug in ABS {NADES [ChCl : sucrose] + PPG400 + H_2O} at different ChCl:sucrose molar ratios: (A) 2:1; (B) 1:1. Diclofenac potassium: (◆); Salicylic acid: (■); Acetaminophen: (▲): (–); calculated partition coefficient, *K*, from Eq. 10.

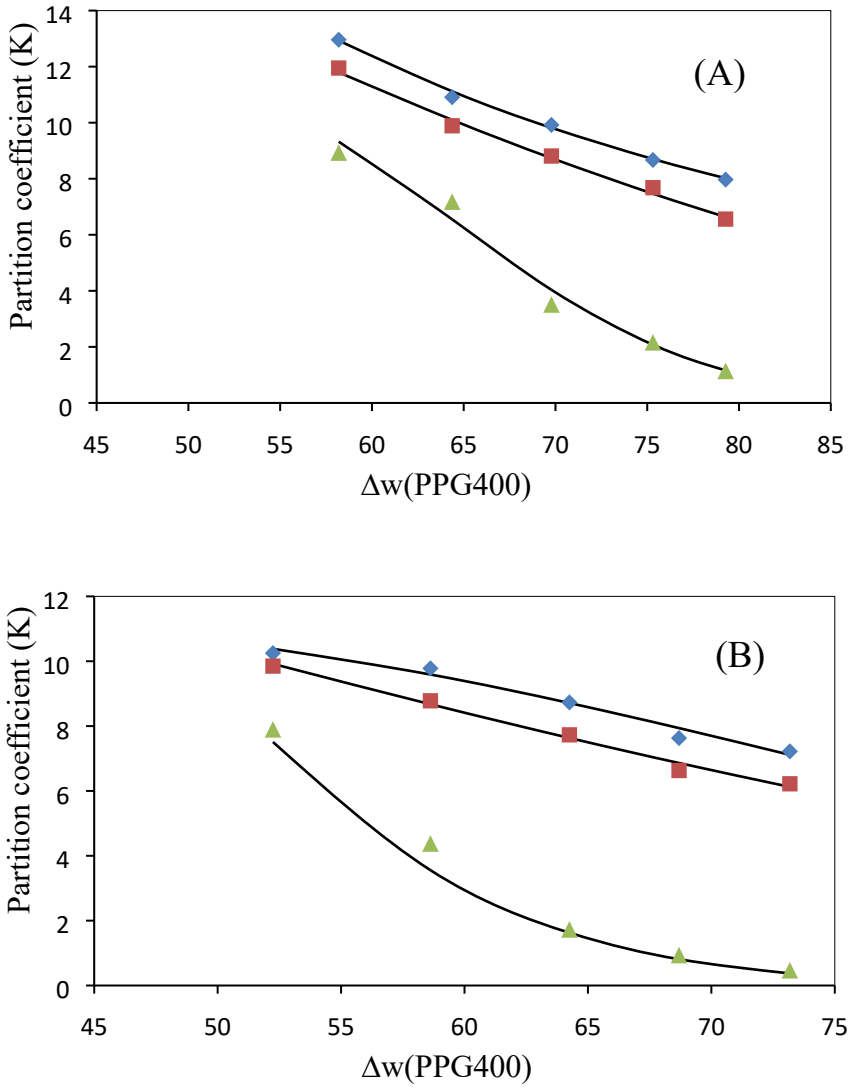

Fig. S2. Partition coefficient, *K*, as a function of the mass fraction difference of PPG400 in the top and bottom phases for each studied drug in ABS {NADES [ChCl : sucrose] + PPG400 + H_2O} at different ChCl:sucrose molar ratios: (A) 2:1; (B) 1:1. Diclofenac potassium: (◆); Salicylic acid: (■); Acetaminophen: (▲): (–); calculated partition coefficient, *K*, from Eq. 11.

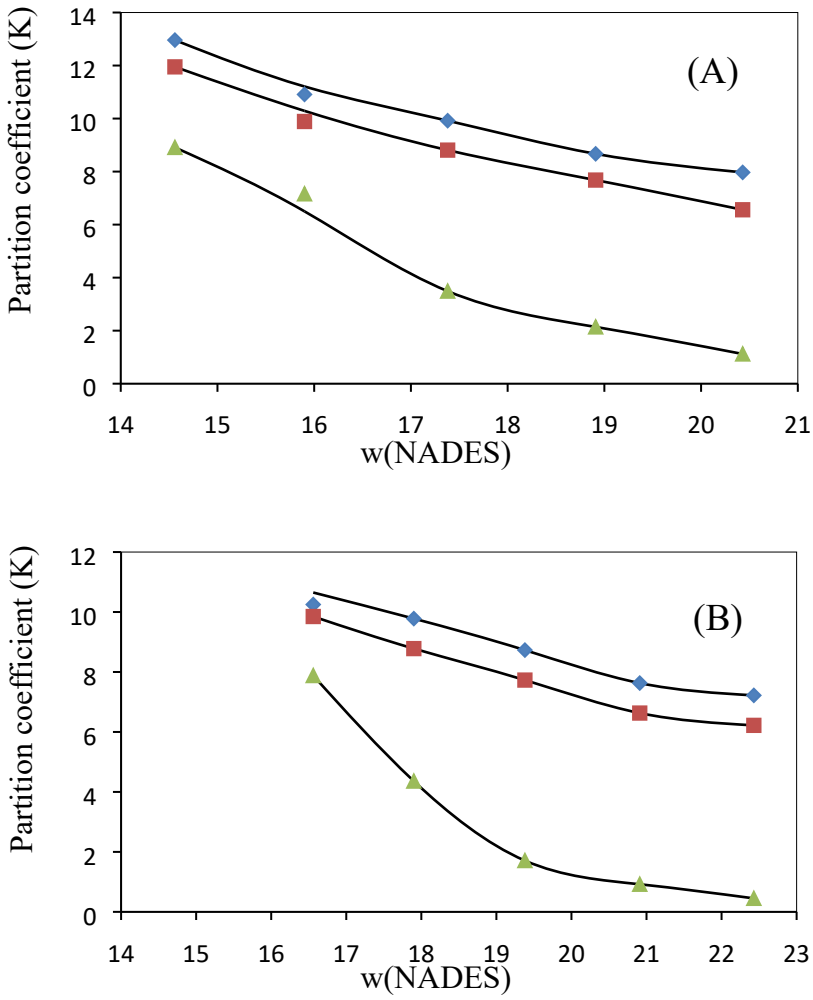

Fig. S3. Partition coefficient, *K*, as a function of the overall composition of NADES for each studied drug in ABS {NADES [ChCl : sucrose] + PPG400 + H_2O}at different ChCl: sucrose molar ratios: (A) 2:1; (B) 1:1. Diclofenac potassium: (◆); Salicylic acid: (■); Acetaminophen: (▲): (–); calculated partition coefficient, *K*, from Eq. 12.