Retention times MLC

Table A 1: Exemplary retention data for MLC measurements at 20°C, retention time for KI (dead volume) and the solutes phenol, 3-methoxyphenol and vanillin

TritonX-100 (wt%)	flow (ml/min)	KI (min)	phenol (min)	3-methoxyphenol (min)
0.05	1.0	0.90	16.30	25.86
0.10	1.0	0.88	16.02	24.37
0.20	1.0	0.89	15.36	22.09
0.30	1.0	0.86	14.41	19.88
0.40	1.0	0.86	13.80	19.11
0.50	1.0	0.85	13.24	17.57
			vanillin (min)	
0.10	0.5	1.84	26.84	
0.20	0.5	1.82	26.01	
0.30	0.5	1.77	24.06	
0.40	0.5	1.76	23.26	
0.50	0.5	1.74	22.24	

Table A 2: Exemplary retention data for MLC measurements at 50°C, retention time for KI (dead volume) and the solutes phenol, 3-methoxyphenol and vanillin

TritonX-100 (wt%)	flow (ml/min)	KI (min)	phenol (min)	3-methoxyphenol (min)	vanillin (min)
0.05	1.0	0.87	11.68	15.15	8.30
0.10	0.5	1.74	23.31	29.74	15.76
0.20	0.5	1.71	22.60	28.52	14.82
0.30	0.5	1.69	22.07	27.51	14.24
0.40	0.5	1.68	21.50	26.47	13.69
0.50	0.5	1.67	20.90	25.45	13.18

Composition of the phases used for the predictions with COSMO-RS

Table A 3: predicted distribution of ethanol between micelles and water at 85°C, data used as input for calculation of the partition coefficient of the solutes

	overall concentration (wt%)	composition aqueous phase (mol/mol)	composition surfactant aggregates (mol/mol)
water	96.00	1.000	0.000
TritonX-100	4.00	$4.51 \cdot 10^{-06}$	1.000
n-butanol	0.00	0.000	0.000
water	94.52	0.997	0.000
TritonX-100	4.00	$4.56 \cdot 10^{-06}$	0.723
n-butanol	1.48	0.003	0.277
water	93.04	0.993	0.000
TritonX-100	4.00	$4.62 \cdot 10^{-06}$	0.546
n-butanol	2.96	0.007	0.454
water	91.55	0.990	0.000
TritonX-100	4.00	$4.67 \cdot 10^{-06}$	0.428
n-butanol	4.45	0.010	0.572
water	90.07	0.986	0.000
TritonX-100	4.00	$4.73 \cdot 10^{-06}$	0.350
n-butanol	5.93	0.014	0.650
water	88.59	0.983	0.000
TritonX-100	4.00	$4.80 \cdot 10^{-06}$	0.298
n-butanol	7.41	0.017	0.702

Table A 4: predicted distribution of butanol between micelles and water at 85°C, data used as input for calculation of the partition coefficient of the solutes

	overall concentration (wt%)	composition aqueous phase (mol/mol)	composition surfactant aggregates (mol/mol)
water	96.00	1.000	0.000
TritonX-100	4.00	$4.51 \cdot 10^{-06}$	1.000
ethanol	0.00	0.000	0.000
water	95.08	0.996	0.000
TritonX-100	4.00	$4.48 \cdot 10^{-06}$	0.963
ethanol	0.92	0.004	0.037
water	94.16	0.992	0.000
TritonX-100	4.00	$4.47 \cdot 10^{-06}$	0.930
ethanol	1.84	0.008	0.070
water	93.24	0.989	0.000
TritonX-100	4.00	$4.45 \cdot 10^{-06}$	0.902
ethanol	2.76	0.011	0.098
water	92.31	0.985	0.000
TritonX-100	4.00	$4.43 \cdot 10^{-06}$	0.877
ethanol	3.69	0.015	0.123
water	91.39	0.980	0.000
TritonX-100	4.00	$4.41 \cdot 10^{-06}$	0.855
ethanol	4.61	0.020	0.145

Prediction of the influence of different alcohols on the partition coefficient

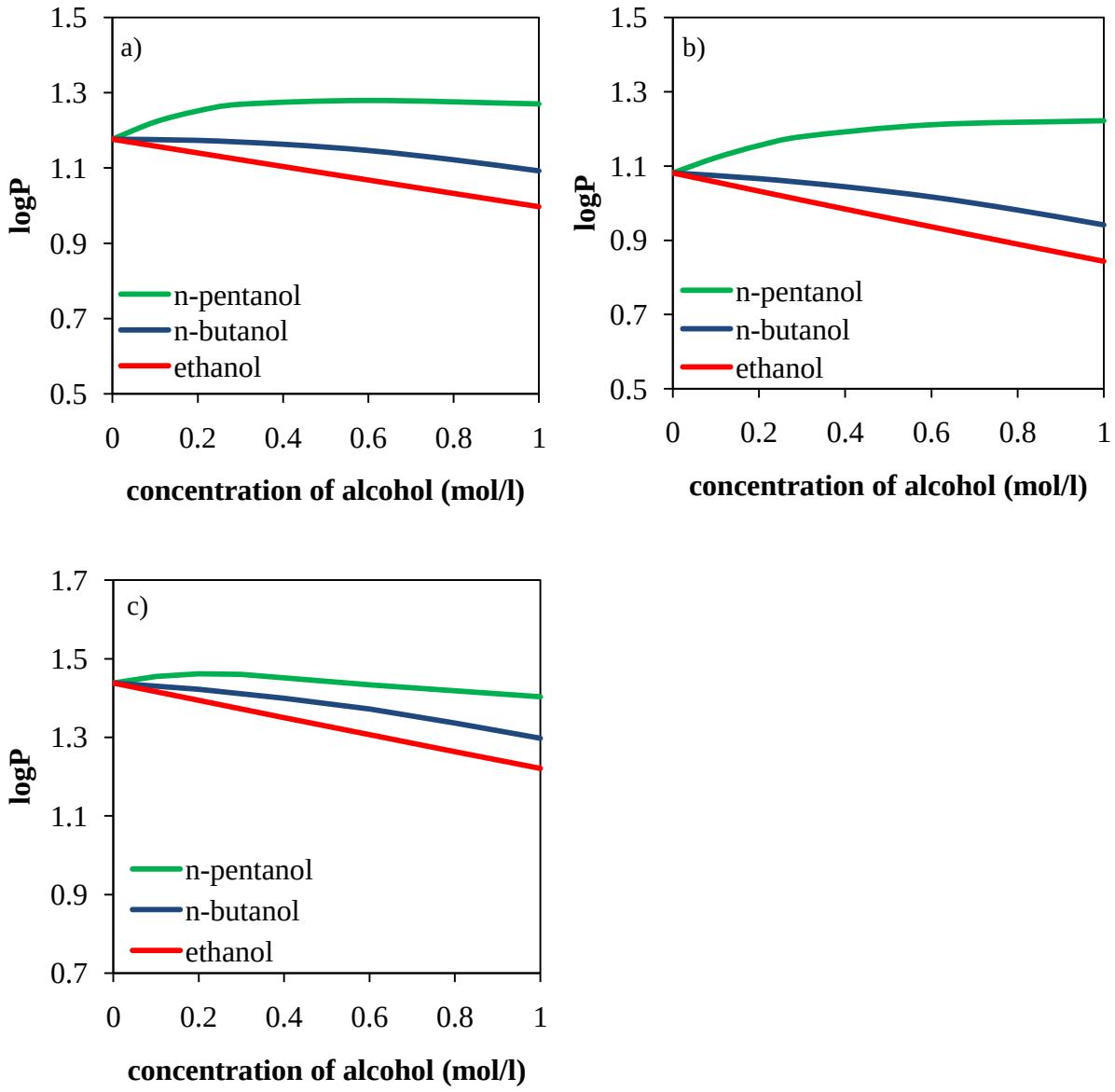

Figure A 1: influence of different alcohols on the partition coefficient of a) phenol, b) vanillin and c) 3-methoxyphenol between TritonX-100 micelles and water at 85°C as predicted by the model COSMO-RS