

Supporting Information for the Manuscript “Effect of Ionic Composition on Partitioning of Organic Compounds in Octanol-Buffer Systems”

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Content:

Table S1: Coefficients a_{io} and b_{io} (eqn (1)) of the analysis of Collander linear relationships between distribution coefficients of drugs in all different octanol-buffer systems examined (NaPB – sodium phosphate buffer, pH 7.4; UB – universal buffer, pH 7.4, r is the regression coefficient, SD is the standard deviation and N is the number the number of compounds fitting the relationship).

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Reference		r^2	SD	b (\pm)	a (\pm)	N	N (outliers)	Outliers ID
0.01M NaPB	0.01M UB	0.9959	0.103	0.0(0.02)	1.05(0.01)	24	4	10,14,20,21
0.10M NaPB	0.10M UB	0.9945	0.157	0.02(0.04)	1.06(0.02)	19	10	2,3,5,10,15,17,20,25,26,27
0.01M NaPB	0.15M NaCl + 0.01M NaPB	0.9921	0.162	0.10(0.04)	1.06(0.02)	19	9	2,5,8,10,14,15,19,21,27
0.01M UB	0.15M NaCl + 0.01M NaPB	0.9947	0.137	0.09(0.03)	1.01(0.02)	18	10	2,8,10,14,17,19,20,21,22,27
0.01M NaPB	0.15M NaCl + 0.01M UB	0.9922	0.158	0.04(0.04)	1.04(0.02)	19	9	2,8,10,14,15,19,20,21,22
0.01M UB	0.15M NaCl + 0.01M UB	0.9953	0.122	0.03(0.03)	0.99(0.02)	19	9	2,5,8,10,14,17,19,22,27
0.01M UB	0.15M NaCl + 0.10M UB	0.9839	0.307	0.67(0.08)	1.32(0.05)	17	11	2,5,6,8,13,14,15,21,22,24,27
0.01M UB	0.15M NaCl + 0.10M NaPB	0.9946	0.132	0.37(0.04)	1.29(0.03)	12	16	2,3,4,5,6,8,10,12,13,14,15,17,21,22,24,27
0.01M NaPB	0.15M NaCl + 0.10M NaPB	0.9929	0.187	0.56(0.05)	1.25(0.03)	15	13	2,5,6,8,10,13,14,15,17,21,22,24,27
0.01M NaPB	0.15M NaCl + 0.10M UB	0.9855	0.271	0.78(0.07)	1.36(0.05)	15	13	2,3,5,6,8,13,14,15,17,21,22,24,27
0.15M NaCl + 0.01M UB	0.15M NaCl + 0.10M NaPB	0.9896	0.243	0.60(0.07)	1.19(0.04)	13	15	2,5,6,9,10,13,15,17,18,20,21,22,24,25,27
0.15M NaCl + 0.01M NaPB	0.15M NaCl + 0.10M NaPB	0.9897	0.237	0.48(0.06)	1.15(0.03)	17	12	2,5,6,10,13,15,17,18,21,22,24,27
0.15M NaCl +	0.10M NaPB	0.9904	0.233	0.68(0.07)	1.18(0.04)	12	16	2,5,6,9,10,12,13,15,17,18,

0.01M UB								20,21,22,24,25,27
0.15M NaCl + 0.01M NaPB	0.10M NaPB	0.9921	0.221	0.60(0.07)	1.13(0.03)	13	16	2,5,6,9,10,12,13,15,17,18, 20,21,22,24,25,27
0.15M NaCl + 0.01M NaPB	0.10M UB	0.9852	0.296	0.41(0.09)	1.39(0.05)	12	17	2,4,5,6,10,13,15,17,18,19, 20,21,22,24,25,26,27
0.15M NaCl + 0.01M UB	0.10M UB	0.9838	0.285	0.52(0.08)	1.41(0.05)	14	14	4,6,10,13,15,17,18,19,20,21, 22,24,25,27
0.15M NaCl + 0.01M NaPB	0.15M NaCl + 0.10M UB	0.9886	0.253	0.48(0.08)	1.42(0.05)	13	15	2,4,5,6,10,13,15,17,18,20, 21,22,24,25,27
0.15M NaCl + 0.01M UB	0.15M NaCl + 0.10M UB	0.9891	0.239	0.54(0.07)	1.44(0.04)	15	13	4,5,6,10,13,17,18,20,21,22, 24,25,27
0.15M NaCl + 0.10M NaPB	0.15M NaCl + 0.10M UB	0.9963	0.121	0.03(0.03)	1.06(0.02)	20	8	2,3,5,15,20,25,27,28
0.15M NaCl + 0.01M UB	0.15M NaCl + 0.01M NaPB	0.9992	0.048	0.05(0.01)	1.02(0.01)	22	6	2,5,19,20,21,22
0.15M NaCl + 0.10M UB	0.10M UB	0.9987	0.074	0(0.02)	1.01(0.01)	25	3	(<20%) 10,17,28
0.15M NaCl + 0.10M NaPB	0.10M UB	0.9962	0.136	0.00(0.03)	1.07(0.02)	19	10	2,3,5,10,17,19,20,25,26,27
0.15M NaCl + 0.10M NaPB	0.10M NaPB	0.9989	0.071	0.0(0.01)	1.01(0.01)	26	3	2,17,20
0.15M NaCl + 0.10M UB	0.10M NaPB	0.9923	0.183	0.06(0.05)	1.07(0.02)	21	7	2,3,5,15,20,25,27
0.01M UB	0.10M NaPB	0.9928	0.198	0.61(0.06)	1.15(0.03)	13	15	2,5,6,8,13,14,15,17,19,20, 21,22,24,25,27
0.01M UB	0.10M UB	0.9859	0.281	0.62(0.07)	1.29(0.04)	16	12	2,5,6,8,13,14,15,17,21,22, 24,27
0.01M NaPB	0.10M NaPB	0.9971	0.14	0.68(0.04)	1.26(0.02)	11	17	2,5,6,8,9,13,14,15,17,18,19, 20,21,22,24,25,27
0.01M NaPB	0.10M UB	0.996	0.148	0.74(0.04)	1.32(0.03)	13	15	2,3,5,6,8,10,13,14,15,17,20, 21,22,24,27