



Supplementary Information

Predicting Partition Coefficients of Migrants in Food Simulant/Polymer Systems using Adaptive Neuro-Fuzzy Inference System

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Table S1. Experimental and calculated partition coefficients for both least square and ANFIS models in this QSAR study

System	Subset ^a	K _{Exp}	K _{Quadratic} ^b	K _{ANFIS}	System	Subset ^a	K _{Exp}	K _{Quadratic} ^b	K _{ANFIS}
111	A	0.1530	0.1553	0.1527	314	A	0.0592	0.0541	0.0590
211	A	0.1784	0.1453	0.1782	414	C	0.1588	0.1414	0.1588
311	B	0.1428	0.1519	0.1433	124	A	0.0310	0.0628	0.0310
411	A	0.0538	0.0541	0.0538	224	B	0.1292	0.0803	0.1292
121	C	0.1985	0.1676	0.1984	324	C	0.0494	0.0689	0.0493
221	A	0.1175	0.1576	0.1174	424	B	0.1362	0.1562	0.1362
321	A	0.1542	0.1642	0.1544	115	A	0.0357	0.0418	0.0349
421	B	0.0643	0.0664	0.0643	215	C	0.0567	0.0765	0.0561
112	C	0.0886	0.0605	0.0885	315	A	0.0426	0.0542	0.0440
212	A	0.0753	0.0349	0.0752	415	B	0.1557	0.1573	0.1557
312	C	0.0174	0.0512	0.0176	125	A	0.0474	0.0213	0.0471
122	A	0.0484	0.0516	0.0484	225	C	0.0598	0.0560	0.0596
222	C	0.0155	0.0260	0.0155	325	B	0.0429	0.0337	0.0434
322	B	0.0214	0.0423	0.0215	425	A	0.1213	0.1368	0.1213
113	A	0.2148	0.2477	0.2148	116	C	0.0217	0.0357	0.0228
213	A	0.0380	0.0060	0.0380	216	A	0.0174	0.0383	0.0182
313	C	0.1419	0.1622	0.1420	316	B	0.0385	0.0367	0.0366
123	B	0.4366	0.3924	0.4366	416	A	0.0216	0.0188	0.0216
223	A	0.0986	0.1384	0.0986	126	A	0.0349	0.0290	0.0353
323	A	0.3115	0.3069	0.3115	226	C	0.0413	0.0317	0.0416
114	A	0.0519	0.0480	0.0520	326	A	0.0428	0.0301	0.0421
214	B	0.0868	0.0655	0.0869	426	B	0.0143	0.0122	0.0143

^aSubsets: A (training), B (test) and C (prediction)

^bCalculated partition coefficients by Tehrani *et al.*⁸