Towards designing environmentally safe ionic liquids: Influence of cation structure

Supplementary material 1.

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Table 1. Table representing correlation between descriptors and each of two Principle Components after PCA on both anions' and cations' indices. Values fulfilling Malinowski's rule are in bold.

Descriptor	Value for PC1	Value for PC2
L1u_a	**0.855**	0.097
L2u_a	**0.819**	0.149
L3u_a	**0.823**	0.125
P1u_a	**0.872**	0.081
P2u_a	-0.692	-0.045
G1u_a	-0.672	-0.148
G2u_a	**-0.834**	-0.143
G3u_a	-0.647	-0.139
E1u_a	**0.849**	0.146
E2u_a	**0.817**	0.137
E3u_a	0.665	0.132
L1m_a	**0.822**	0.114
L2m_a	**0.785**	0.174
L3m_a	**0.725**	0.102
P1m_a	**0.870**	0.065
P2m_a	**-0.713**	-0.006
G1m_a	-0.660	-0.165
G2m_a	**-0.822**	-0.144
G3m_a	-0.629	-0.137
E1m_a	**0.781**	0.116
E2m_a	0.631	0.137
E3m_a	0.417	0.093
L1e_a	**0.859**	0.099
L2e_a	**0.817**	0.153
L3e_a	**0.813**	0.122
P1e_a	**0.870**	0.075
P2e_a	-0.680	-0.031
G1e_a	-0.661	-0.166
G2e_a	**-0.818**	-0.143
G3e_a	-0.636	-0.139
E1e_a	**0.836**	0.137
E2e_a	**0.782**	0.145
E3e_a	0.618	0.125
L1p_a	**0.826**	0.105
L2p_a	**0.808**	0.152
L3p_a	**0.835**	0.127
P1p_a	**0.880**	0.088
P2p_a	**-0.721**	-0.054
G1p_a	-0.662	-0.165
G2p_a	**-0.820**	-0.140
G3p_a	-0.630	-0.135
E1p_a	**0.860**	0.146
E2p_a	**0.915**	0.138

E3p_a	**0.798**	0.134
L1i_a	**0.859**	0.094
L2i_a	**0.818**	0.148
L3i_a	**0.814**	0.124
P1i_a	**0.871**	0.079
P2i_a	-0.692	-0.043
G1i_a	-0.662	-0.159
G2i_a	**-0.830**	-0.139
G3i_a	-0.653	-0.134
E1i_a	**0.837**	0.139
E2i_a	**0.779**	0.136
E3i_a	0.612	0.126
Tu_a	**0.920**	0.118
Tm_a	**0.900**	0.136
Te_a	**0.923**	0.121
Tp_a	**0.896**	0.124
Ti_a	**0.922**	0.116
Au_a	**0.836**	0.129
Am_a	**0.830**	0.136
Ae_a	**0.845**	0.131
Ap_a	**0.809**	0.150
Ai_a	**0.838**	0.124
Gu_a	0.414	0.033
Gm_a	0.381	0.021
Ku_a	**0.872**	0.082
Km_a	**0.872**	0.068
Ke_a	**0.872**	0.078
Kp_a	**0.881**	0.088
Ki_a	**0.872**	0.080
Du_a	**0.830**	0.146
Dm_a	**0.727**	0.132
De_a	**0.796**	0.143
Dp_a	**0.921**	0.151
Di_a	**0.796**	0.142
Vu_a	**0.839**	0.143
Vm_a	**0.848**	0.150
Ve_a	**0.847**	0.145
Vp_a	**0.820**	0.163
Vi_a	**0.840**	0.138
L1u_k	-0.270	**0.886**
L2u_k	-0.179	0.544
L3u_k	-0.166	0.536
P1u_k	-0.215	0.572
P2u_k	0.163	-0.526
G1u_k	0.101	-0.311
G2u_k	-0.052	-0.210
G3u_k	0.049	-0.267
E1u_k	0.020	-0.147

E2u_k	0.194	-0.653
E3u_k	0.092	0.077
L1m_k	-0.270	**0.866**
L2m_k	-0.180	0.580
L3m_k	-0.200	0.562
P1m_k	-0.188	0.495
P2m_k	0.144	-0.445
G1m_k	0.147	-0.294
G2m_k	-0.050	-0.201
G3m_k	0.044	-0.239
E1m_k	-0.195	0.349
E2m_k	-0.090	0.182
E3m_k	-0.149	0.431
L1e_k	-0.270	**0.885**
L2e_k	-0.180	0.549
L3e_k	-0.172	0.544
P1e_k	-0.214	0.569
P2e_k	0.162	-0.522
G1e_k	0.112	-0.309
G2e_k	-0.053	-0.217
G3e_k	0.057	-0.286
E1e_k	-0.021	-0.073
E2e_k	0.176	-0.607
E3e_k	0.068	0.127
L1p_k	-0.270	**0.880**
L2p_k	-0.173	0.545
L3p_k	-0.156	0.521
P1p_k	-0.213	0.549
P2p_k	0.162	-0.507
G1p_k	0.135	-0.329
G2p_k	-0.040	-0.195
G3p_k	0.032	-0.279
E1p_k	-0.150	0.262
E2p_k	0.143	-0.467
E3p_k	0.077	0.153
L1i_k	-0.270	**0.886**
L2i_k	-0.181	0.545
L3i_k	-0.170	0.541
P1i_k	-0.215	0.574
P2i_k	0.162	-0.528
G1i_k	0.108	-0.307
G2i_k	-0.052	-0.214
G3i_k	0.058	-0.261
E1i_k	0.036	-0.189
E2i_k	0.184	-0.641
E3i_k	0.085	0.077
Tu_k	-0.277	**0.902**
Tm_k	-0.277	**0.887**

Te_k	-0.277	**0.902**
Tp_k	-0.276	**0.898**
Ti_k	-0.277	**0.903**
Au_k	-0.198	**0.865**
Am_k	-0.188	**0.851**
Ae_k	-0.198	**0.865**
Ap_k	-0.191	**0.858**
Ai_k	-0.199	**0.866**
Gu_k	0.036	-0.379
Gm_k	0.057	-0.383
Ku_k	-0.216	0.573
Km_k	-0.191	0.500
Ke_k	-0.215	0.571
Kp_k	-0.214	0.551
Ki_k	-0.216	0.576
Du_k	0.211	-0.442
Dm_k	-0.226	0.461
De_k	0.157	-0.324
Dp_k	0.044	-0.019
Di_k	0.203	-0.445
Vu_k	-0.187	**0.847**
Vm_k	-0.191	**0.849**
Ve_k	-0.188	**0.847**
Vp_k	-0.185	**0.845**
Vi_k	-0.188	**0.847**

Table 2. Table representing correlation between descriptors and each of two Principle Components after PCA on cations' indices only. Values fulfilling Malinowski's rule are in bold.

Descriptor	Value for PC1	Value for PC2
L1u_k	**0.926**	0.103
L2u_k	0.578	-0.696
L3u_k	0.563	-0.647
P1u_k	0.606	**0.774**
P2u_k	-0.545	**-0.774**
G1u_k	-0.326	-0.275
G2u_k	-0.183	0.170
G3u_k	-0.270	-0.024
E1u_k	-0.146	0.661
E2u_k	-0.680	-0.130
E3u_k	0.040	-0.090
L1m_k	**0.906**	0.122
L2m_k	0.612	-0.674
L3m_k	0.598	-0.646
P1m_k	0.524	**0.831**
P2m_k	-0.461	**-0.802**
G1m_k	-0.323	-0.256

G2m_k	-0.175	0.188
G3m_k	-0.243	0.041
E1m_k	0.386	0.397
E2m_k	0.203	-0.486
E3m_k	0.456	-0.542
L1e_k	**0.925**	0.103
L2e_k	0.584	-0.693
L3e_k	0.572	-0.645
P1e_k	0.603	**0.778**
P2e_k	-0.541	**-0.776**
G1e_k	-0.327	-0.263
G2e_k	-0.190	0.157
G3e_k	-0.290	-0.009
E1e_k	-0.064	0.695
E2e_k	-0.631	-0.153
E3e_k	0.095	-0.105
L1p_k	**0.920**	0.109
L2p_k	0.578	**-0.703**
L3p_k	0.546	-0.676
P1p_k	0.584	**0.791**
P2p_k	-0.527	**-0.789**
G1p_k	-0.353	-0.279
G2p_k	-0.172	0.152
G3p_k	-0.276	-0.025
E1p_k	0.292	0.667
E2p_k	-0.484	-0.503
E3p_k	0.121	-0.427
L1i_k	**0.926**	0.103
L2i_k	0.581	-0.694
L3i_k	0.569	-0.641
P1i_k	0.608	**0.772**
P2i_k	-0.546	**-0.773**
G1i_k	-0.324	-0.264
G2i_k	-0.187	0.168
G3i_k	-0.267	-0.005
E1i_k	-0.190	0.637
E2i_k	-0.666	-0.065
E3i_k	0.042	-0.031
Tu_k	**0.944**	-0.009
Tm_k	**0.929**	0.023
Te_k	**0.944**	-0.008
Tp_k	**0.940**	0.001
Ti_k	**0.945**	-0.009
Au_k	**0.889**	-0.375
Am_k	**0.872**	-0.396
Ae_k	**0.888**	-0.375
Ap_k	**0.880**	-0.387
Ai_k	**0.890**	-0.372

Gu_k	-0.371	-0.047
Gm_k	-0.382	0.018
Ku_k	0.609	**0.757**
Km_k	0.530	**0.822**
Ke_k	0.606	**0.761**
Kp_k	0.587	**0.775**
Ki_k	0.611	**0.755**
Du_k	-0.489	0.143
Dm_k	0.505	-0.058
De_k	-0.360	0.125
Dp_k	-0.033	-0.179
Di_k	-0.490	0.212
Vu_k	**0.868**	-0.408
Vm_k	**0.871**	-0.405
Ve_k	**0.868**	-0.409
Vp_k	**0.866**	-0.410
Vi_k	**0.869**	-0.407

Table 3. Table representing correlation between descriptors and each of two Principle Components after PCA on anions' indices only. Values fulfilling Malinowski's rule are in bold.

Descriptor	Value for PC1	Value for PC2
L1u_a	**0.861**	-0.351
L2u_a	**0.839**	0.124
L3u_a	**0.835**	0.283
P1u_a	**0.871**	-0.337
P2u_a	-0.676	0.393
G1u_a	**-0.704**	-0.007
G2u_a	**-0.863**	0.140
G3u_a	-0.677	-0.054
E1u_a	**0.858**	0.368
E2u_a	**0.828**	0.485
E3u_a	0.686	0.628
L1m_a	**0.826**	-0.348
L2m_a	**0.814**	0.168
L3m_a	**0.734**	0.315
P1m_a	**0.864**	-0.301
P2m_a	-0.690	0.400
G1m_a	-0.696	-0.031
G2m_a	**-0.852**	0.128
G3m_a	-0.657	-0.067
E1m_a	**0.792**	0.360
E2m_a	0.662	0.628
E3m_a	0.439	0.679
L1e_a	**0.863**	-0.350
L2e_a	**0.838**	0.142

L3e_a	**0.825**	0.295
P1e_a	**0.867**	-0.342
P2e_a	-0.660	0.405
G1e_a	-0.697	-0.029
G2e_a	**-0.848**	0.123
G3e_a	-0.665	-0.070
E1e_a	**0.845**	0.405
E2e_a	**0.798**	0.548
E3e_a	0.640	0.655
L1p_a	**0.834**	-0.374
L2p_a	**0.827**	0.052
L3p_a	**0.846**	0.192
P1p_a	**0.880**	-0.309
P2p_a	**-0.709**	0.370
G1p_a	-0.698	-0.029
G2p_a	**-0.846**	0.119
G3p_a	-0.660	-0.056
E1p_a	**0.866**	0.077
E2p_a	**0.925**	0.180
E3p_a	**0.820**	0.407
L1i_a	**0.864**	-0.349
L2i_a	**0.837**	0.139
L3i_a	**0.827**	0.308
P1i_a	**0.869**	-0.342
P2i_a	-0.675	0.396
G1i_a	-0.696	-0.024
G2i_a	**-0.861**	0.139
G3i_a	-0.681	-0.063
E1i_a	**0.846**	0.399
E2i_a	**0.791**	0.535
E3i_a	0.635	0.669
Tu_a	**0.929**	-0.221
Tm_a	**0.909**	-0.226
Te_a	**0.932**	-0.214
Tp_a	**0.908**	-0.279
Ti_a	**0.931**	-0.213
Au_a	**0.840**	-0.283
Am_a	**0.829**	-0.233
Ae_a	**0.847**	-0.274
Ap_a	**0.813**	-0.300
Ai_a	**0.842**	-0.277
Gu_a	0.411	0.676
Gm_a	0.375	0.669
Ku_a	**0.871**	-0.330
Km_a	**0.867**	-0.296
Ke_a	**0.870**	-0.334
Kp_a	**0.881**	-0.304
Ki_a	**0.869**	-0.335

Du_a	**0.843**	0.501
Dm_a	**0.752**	0.596
De_a	**0.811**	0.547
Dp_a	**0.931**	0.183
Di_a	**0.810**	0.547
Vu_a	**0.843**	-0.262
Vm_a	**0.845**	-0.227
Ve_a	**0.849**	-0.254
Vp_a	**0.826**	-0.286
Vi_a	**0.843**	-0.257

Following plots (fig. 1-8) are representing the projections of 375 ionic liquids in the space defined by two first principal components of all cations' and anions' WHIM descriptors. Each compound, with no toxicological data available, is represented by (**x**) symbol. Compounds with defined toxicity are represented by (**o**) symbols, coloured according to used scale (see manuscript for details).

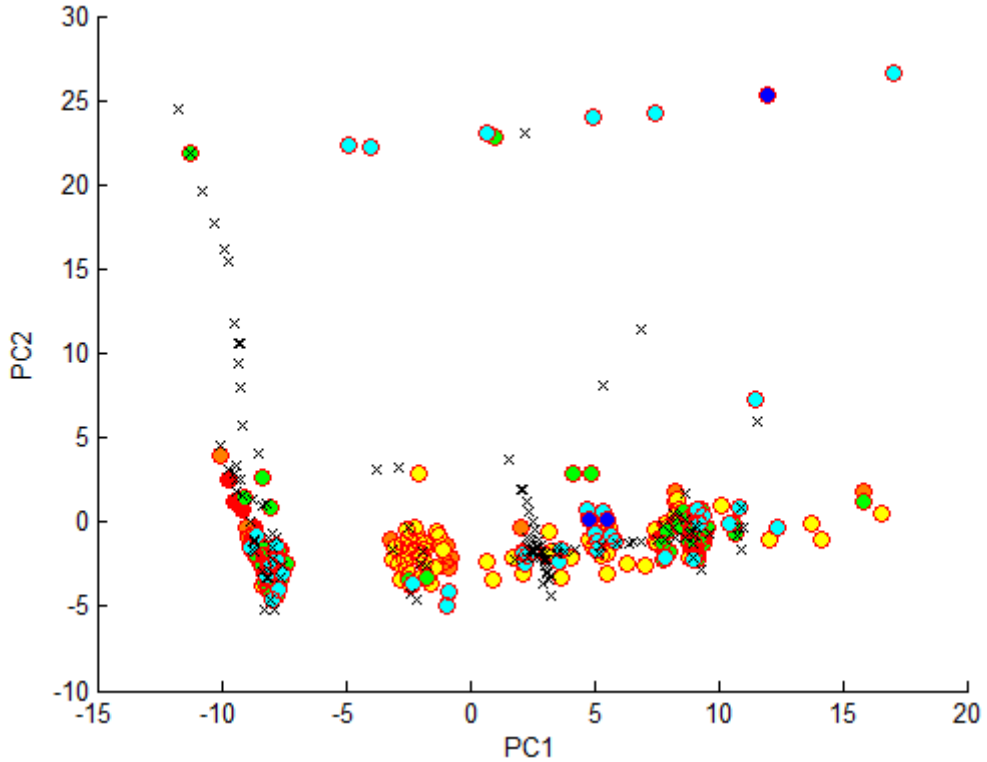

Figure 1. PCA analysis with marked ranges of the toxicity for Acetylcholine esterase

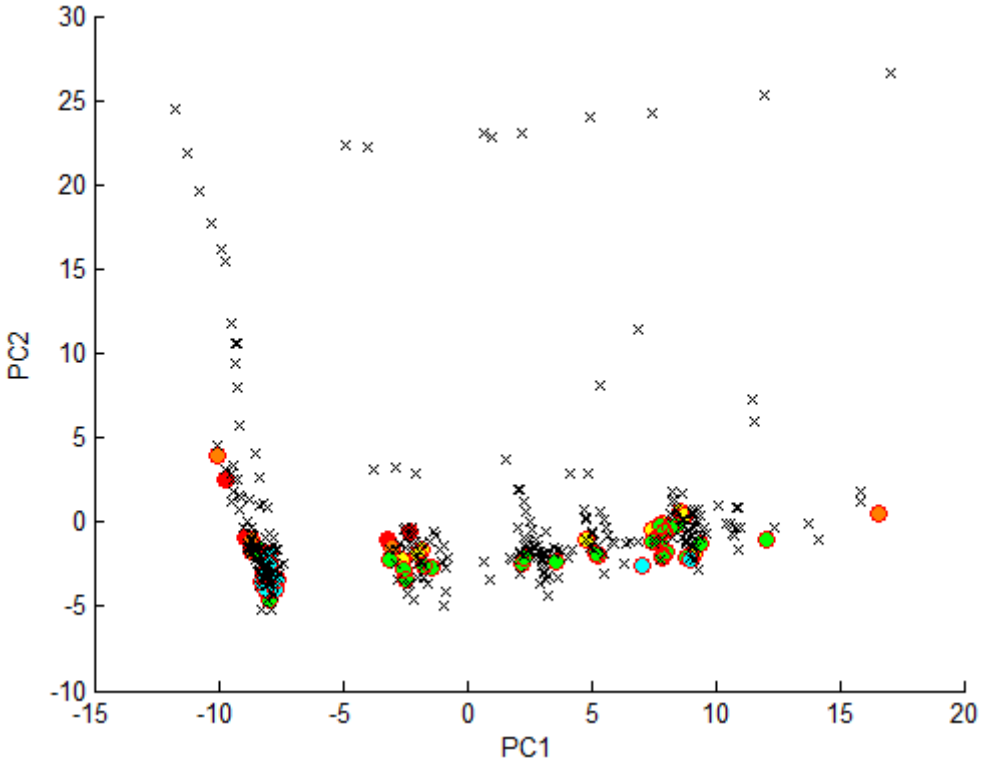

Figure 2. PCA analysis with marked ranges of the toxicity for Vibrio fischeri

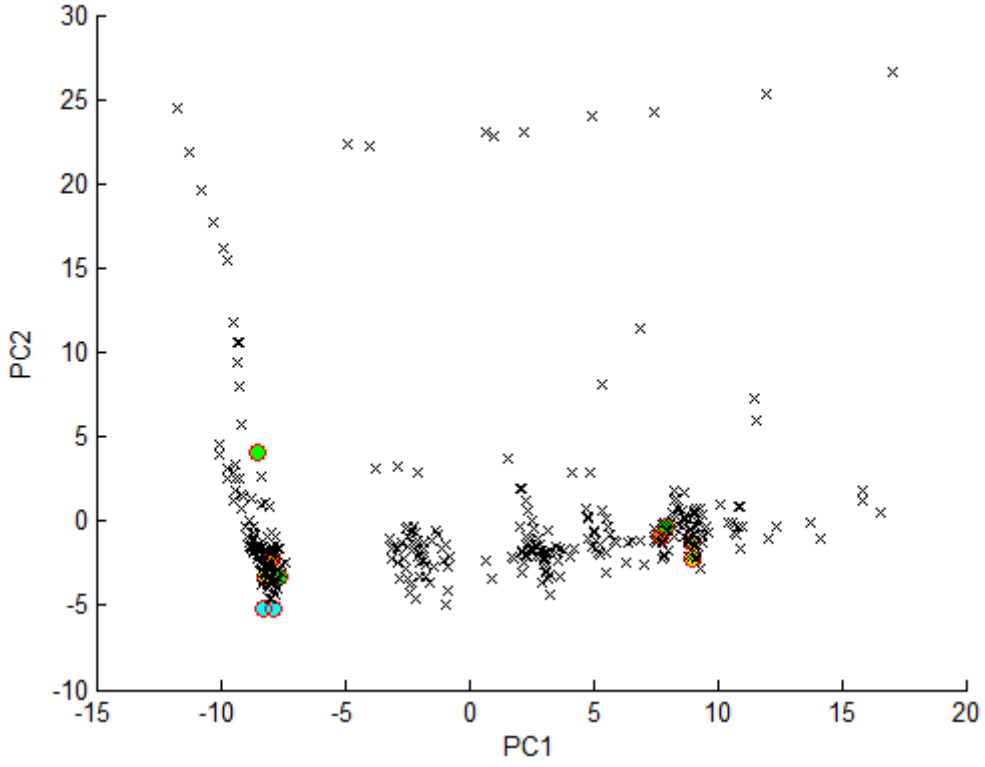

Figure 3. PCA analysis with marked ranges of the toxicity for Pseudokirchneriella subcapitata

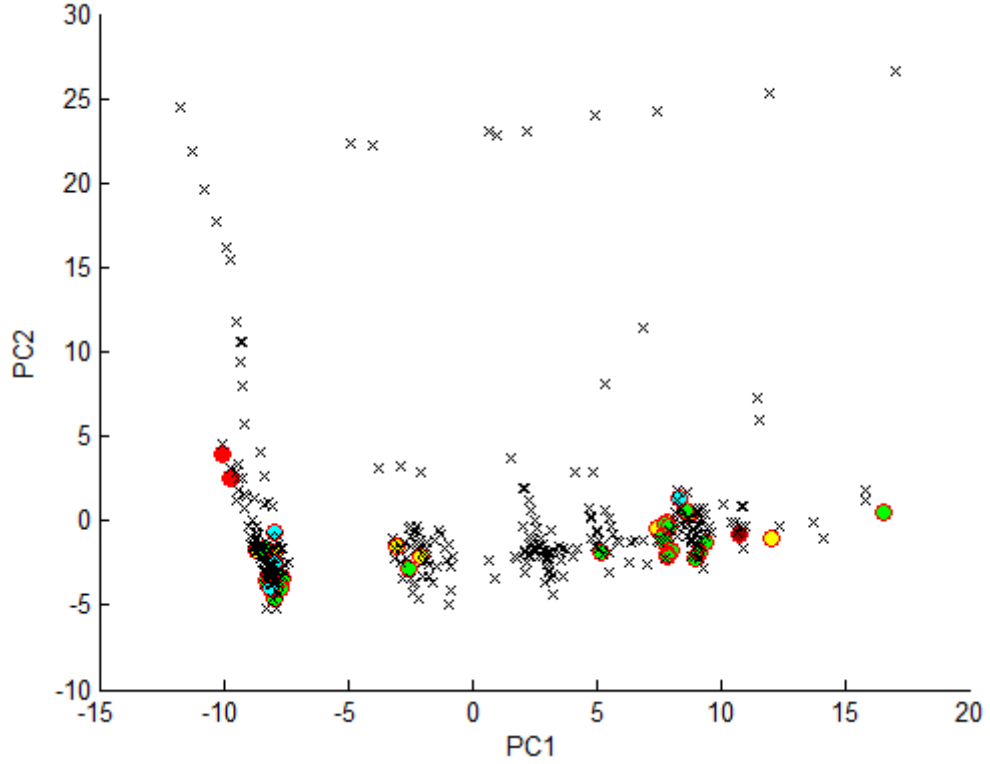

Figure 4. PCA analysis with marked ranges of the toxicity for Scenedesmus vacuolatus

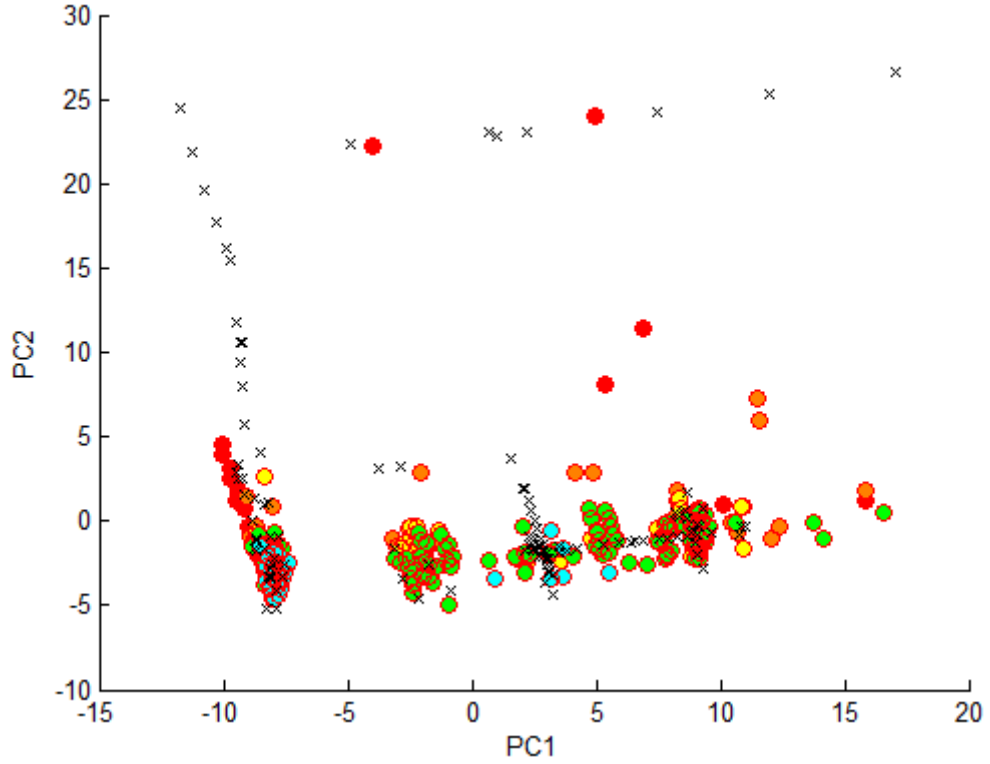

Figure 5. PCA analysis with marked ranges of the toxicity for Rat cell line IPC-81

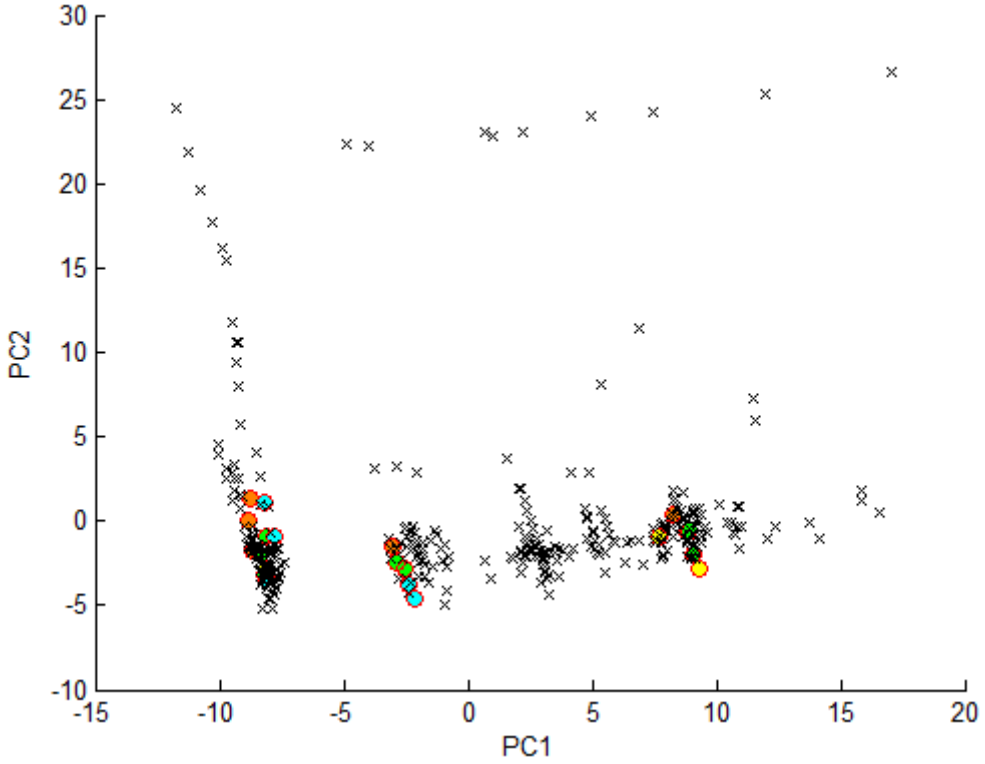

Figure 6. PCA analysis with marked ranges of the toxicity for Human cell line HeLa

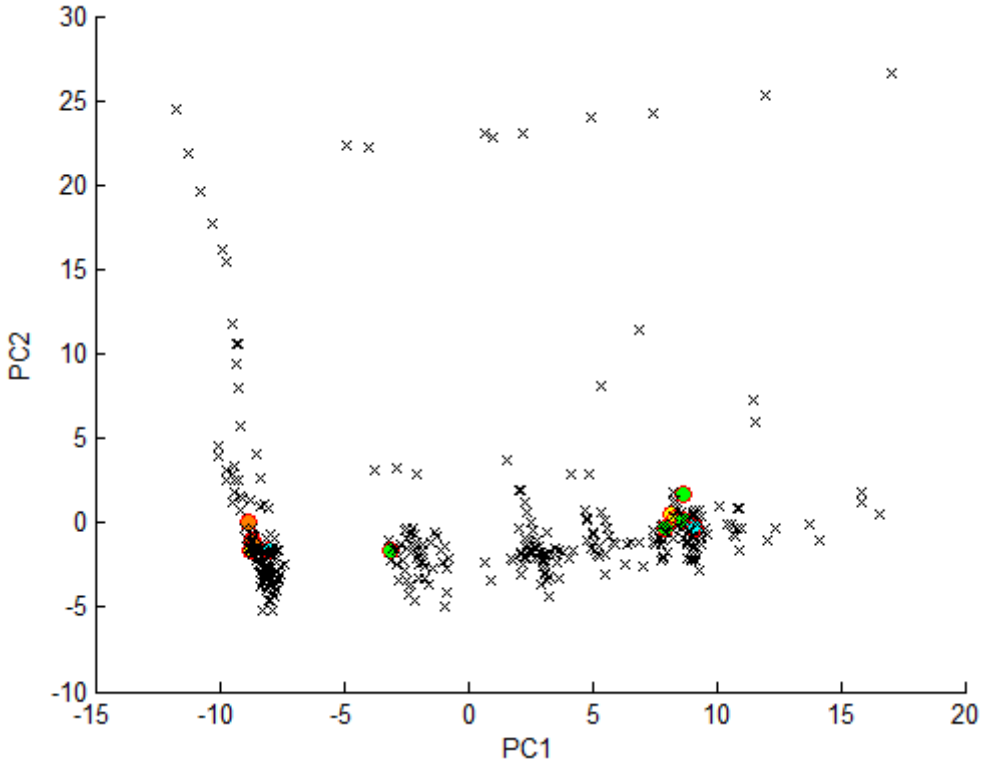

Figure 7. PCA analysis with marked ranges of the toxicity for Human cell line MCF7

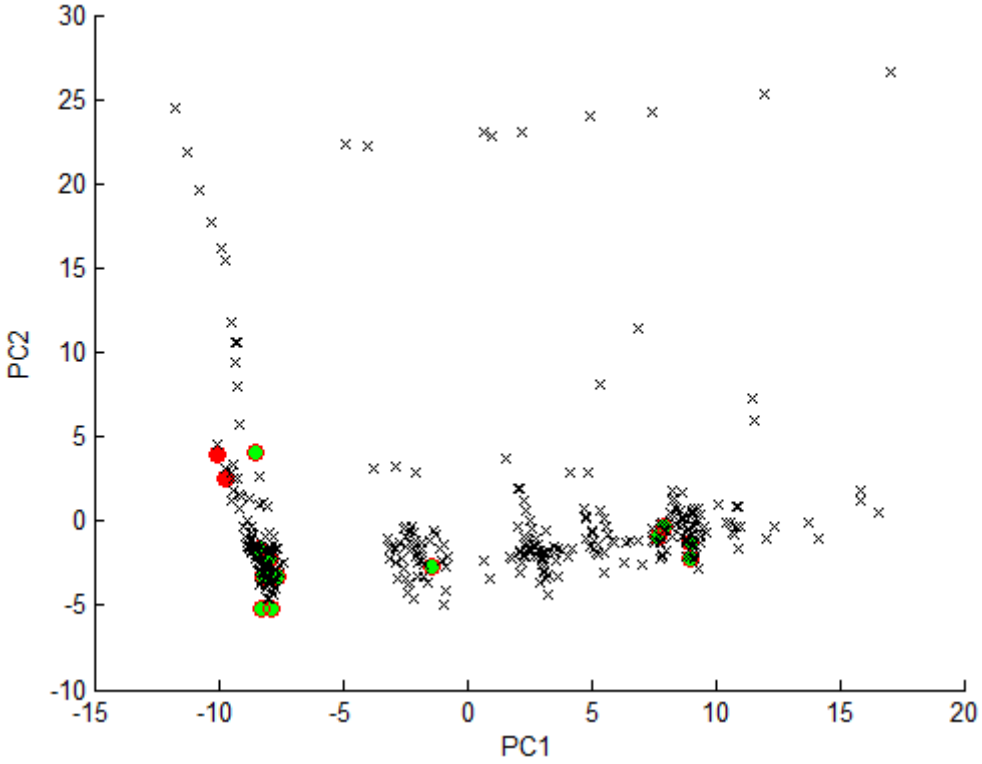

Figure 8. PCA analysis with marked ranges of the toxicity for Daphnia Magna

Following plots (fig. 9-16) are representing the projections of 375 ionic liquids in the space defined by two first principal components of cations' WHIM descriptors. Each compound, with no toxicological data available, is represented by (**x**) symbol. Compounds with defined toxicity are represented by (**o**) symbols, coloured according to used scale (see manuscript for details).

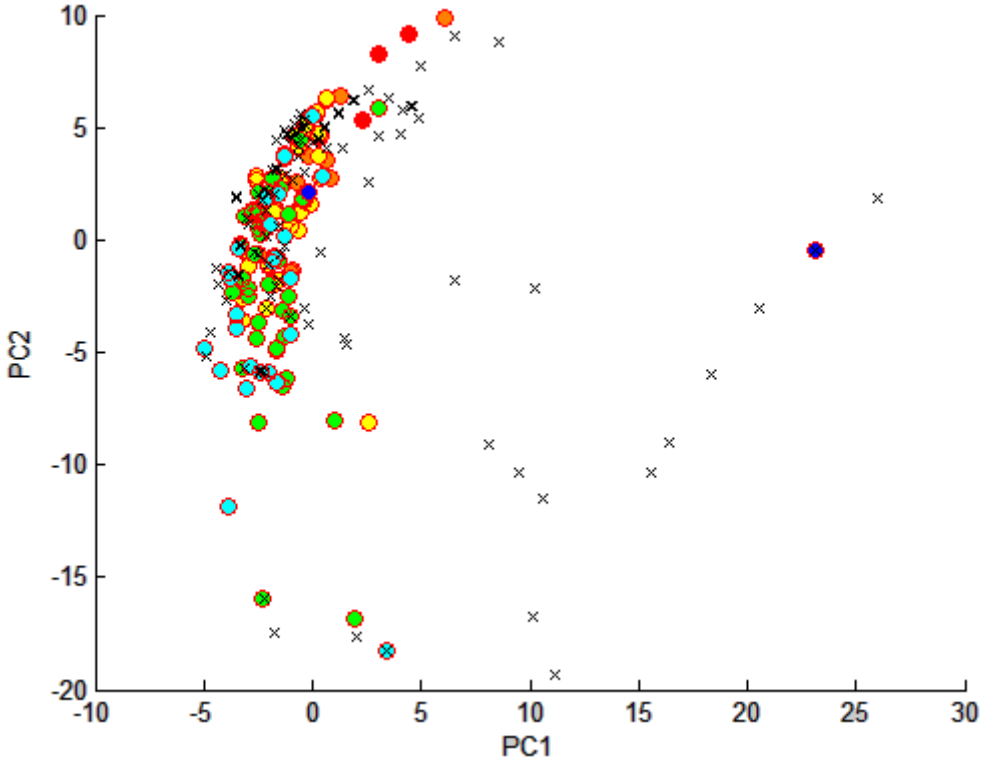

Figure 9. PCA analysis with marked ranges of the toxicity for Acetylcholine esterase

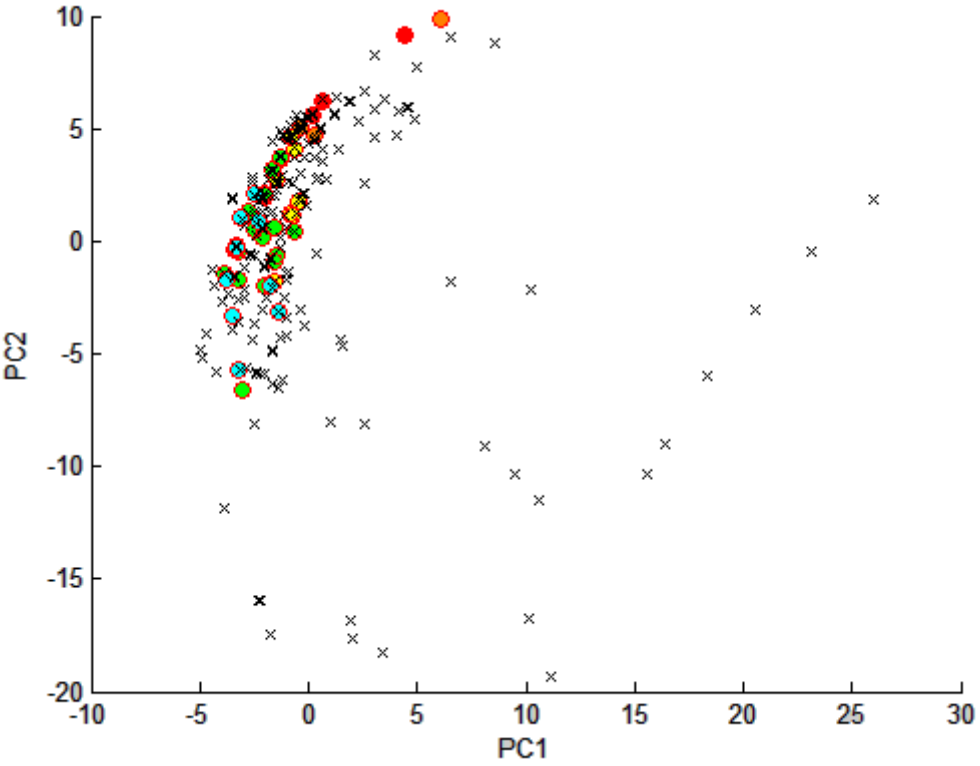

Figure 10. PCA analysis with marked ranges of the toxicity for Vibrio fischeri

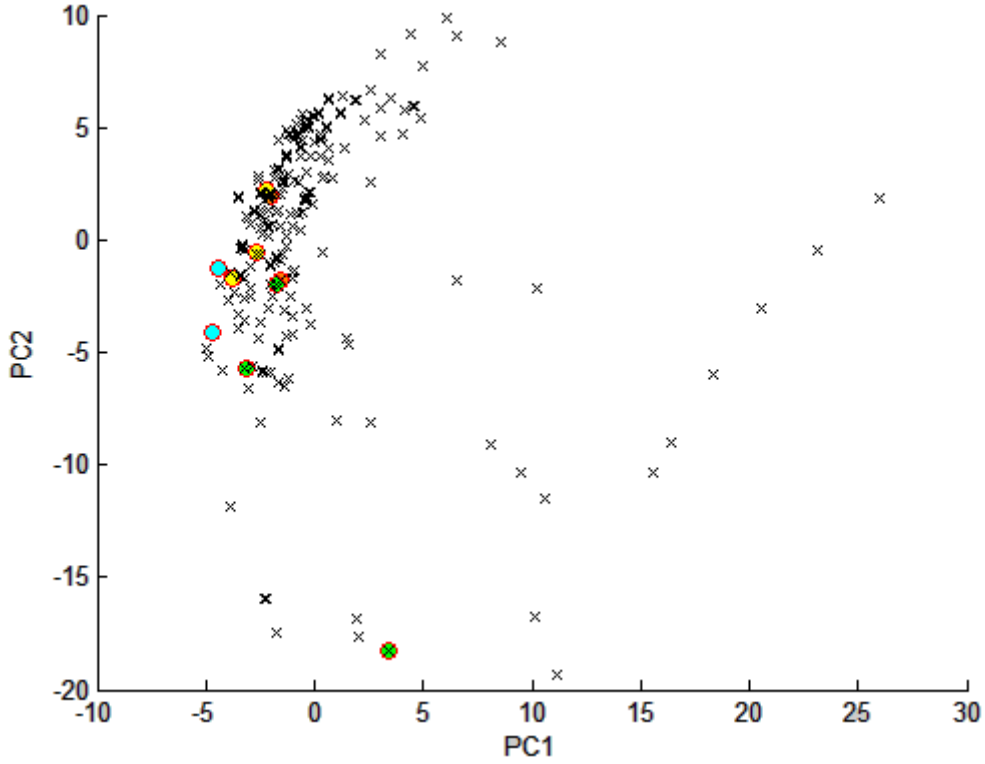

Figure 11. PCA analysis with marked ranges of the toxicity for Pseudokirchneriella subcapitata

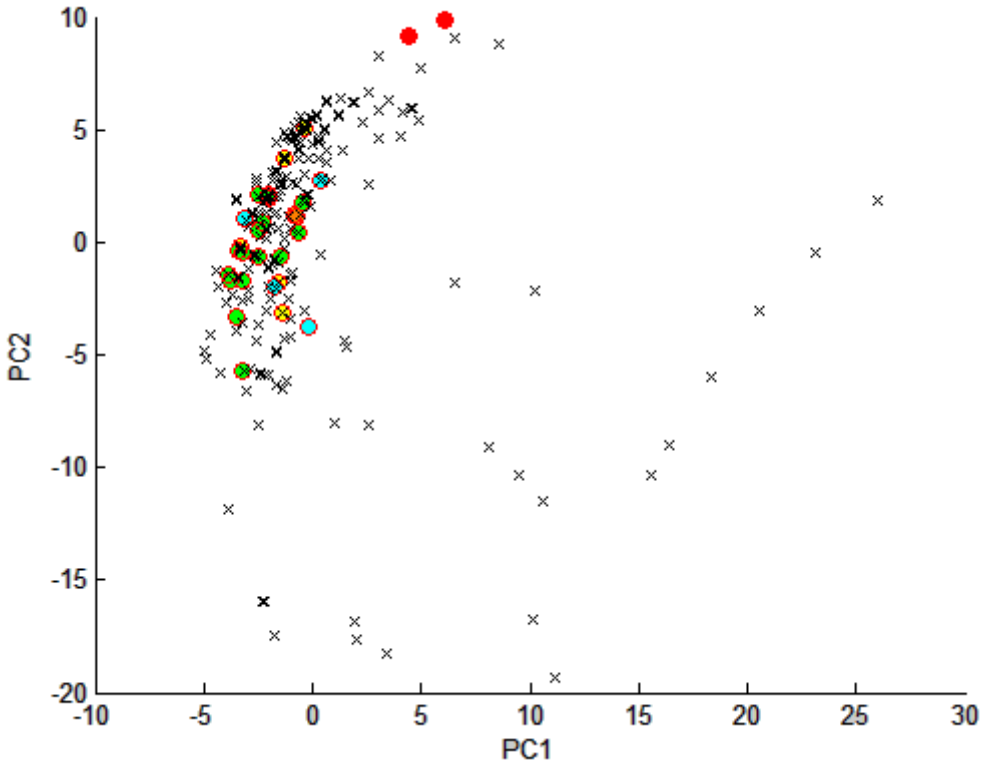

Figure 12. PCA analysis with marked ranges of the toxicity for Scenedesmus vacuolatus

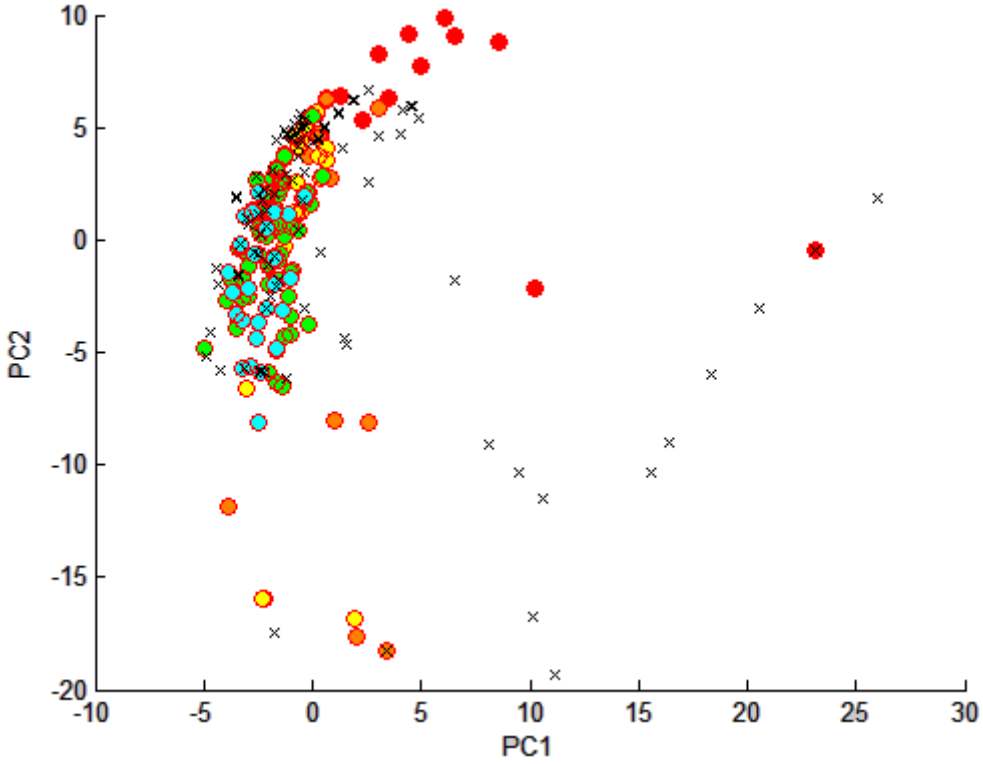

Figure 13. PCA analysis with marked ranges of the toxicity for Rat cell line IPC-81

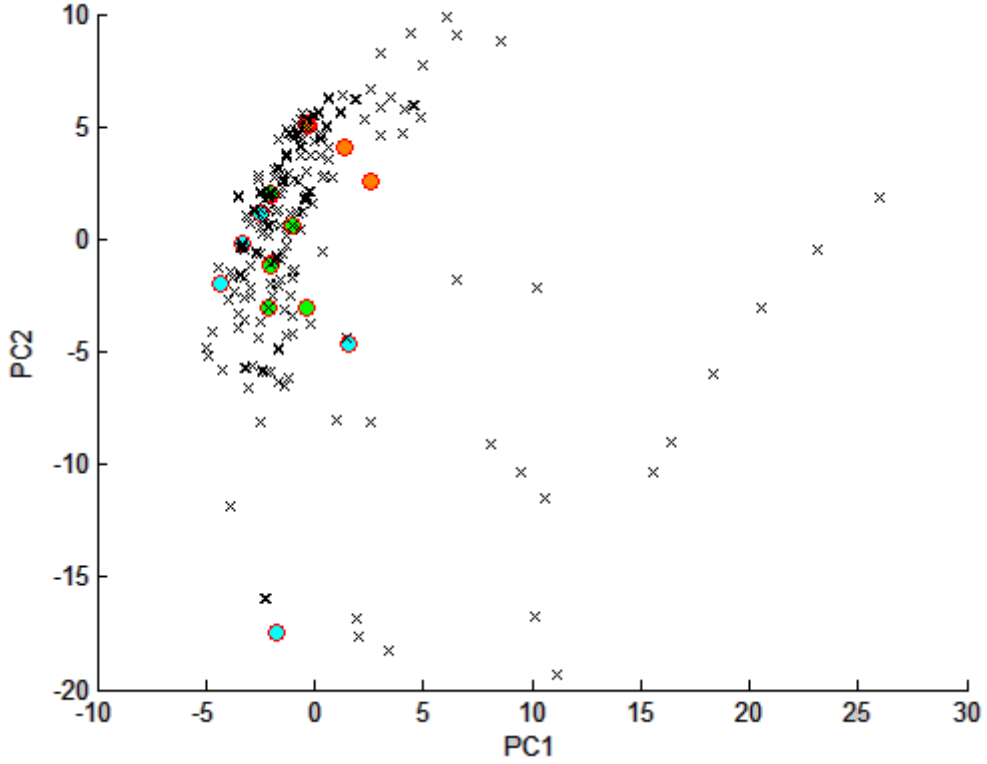

Figure 14. PCA analysis with marked ranges of the toxicity for Human cell line HeLa

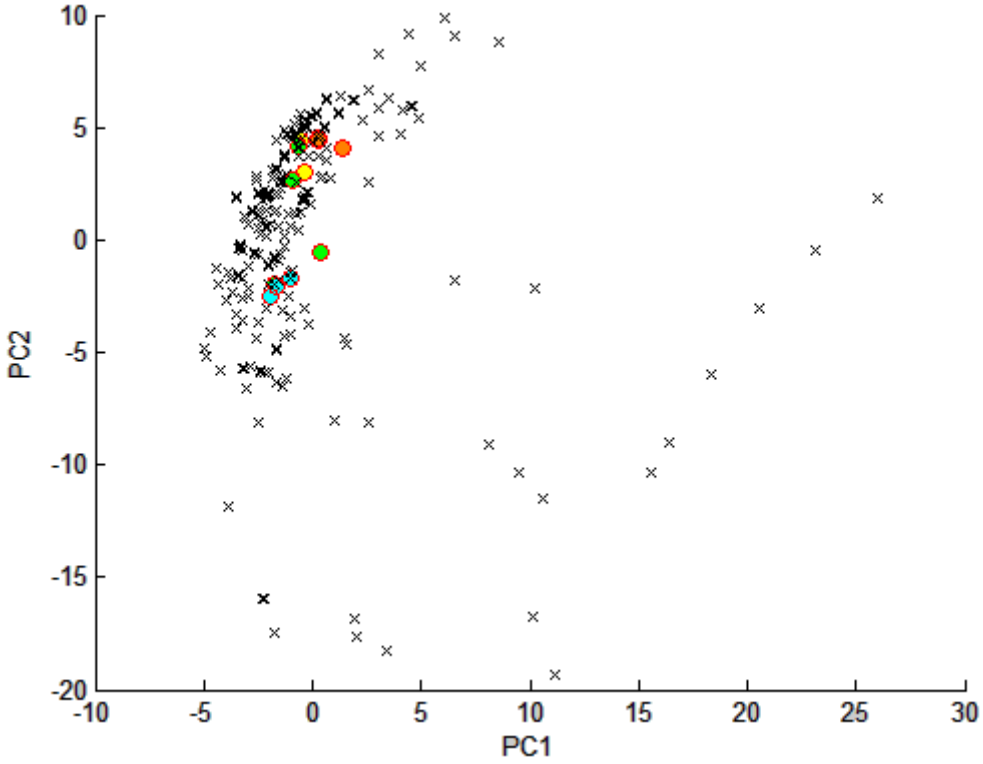

Figure 15. PCA analysis with marked ranges of the toxicity for Human cell line MCF7

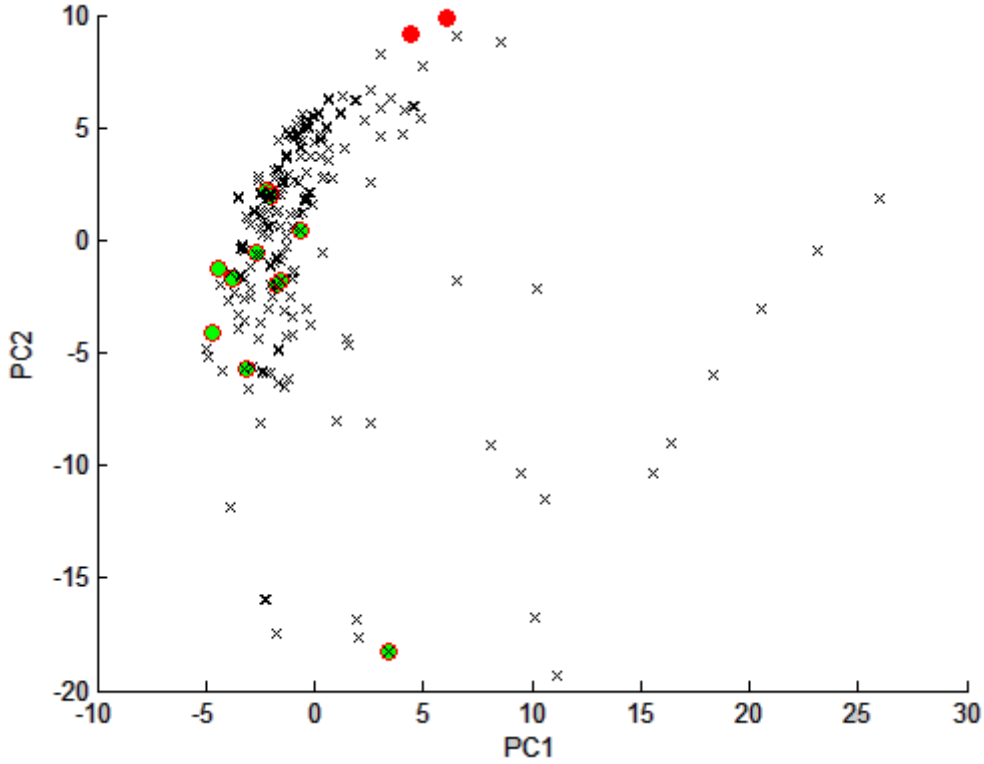

Figure 16. PCA analysis with marked ranges of the toxicity for Daphnia Magna

Following plots (fig. 17-24) are representing the projections of 375 ionic liquids in the space defined by two first principal components of anions' WHIM descriptors. Each

compound, with no toxicological data available, is represented by (**x**) symbol. Compounds with defined toxicity are represented by (**o**) symbols, coloured according to used scale (see manuscript for details).

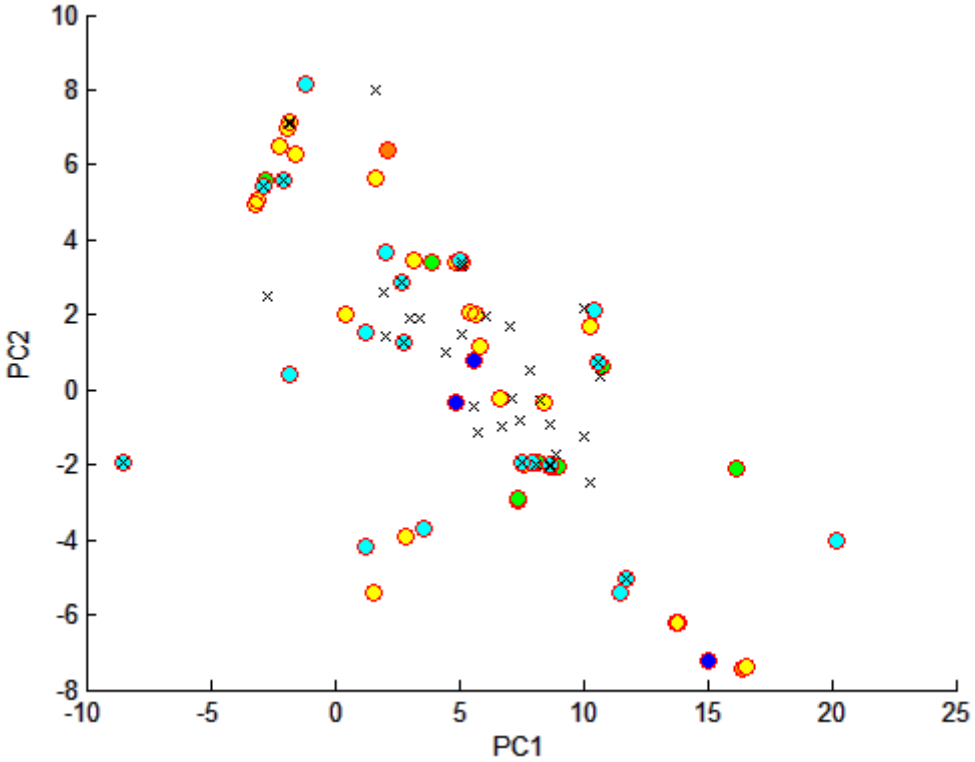

Figure 17. PCA analysis with marked ranges of the toxicity for Acetylcholine esterase

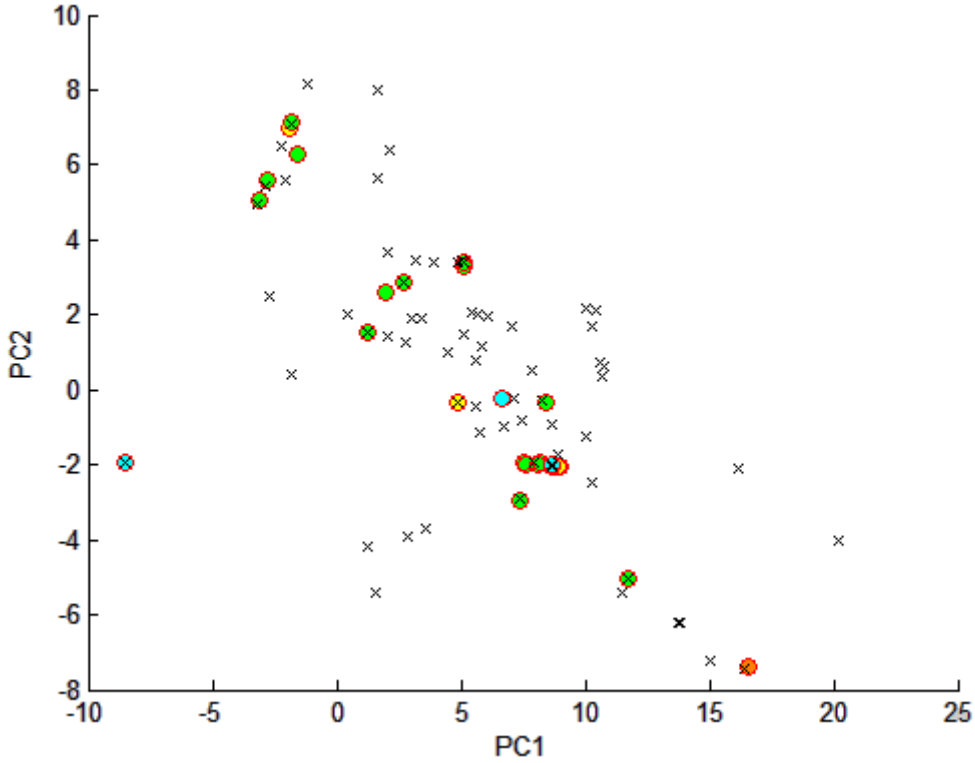

Figure 18. PCA analysis with marked ranges of the toxicity for Vibrio fischeri

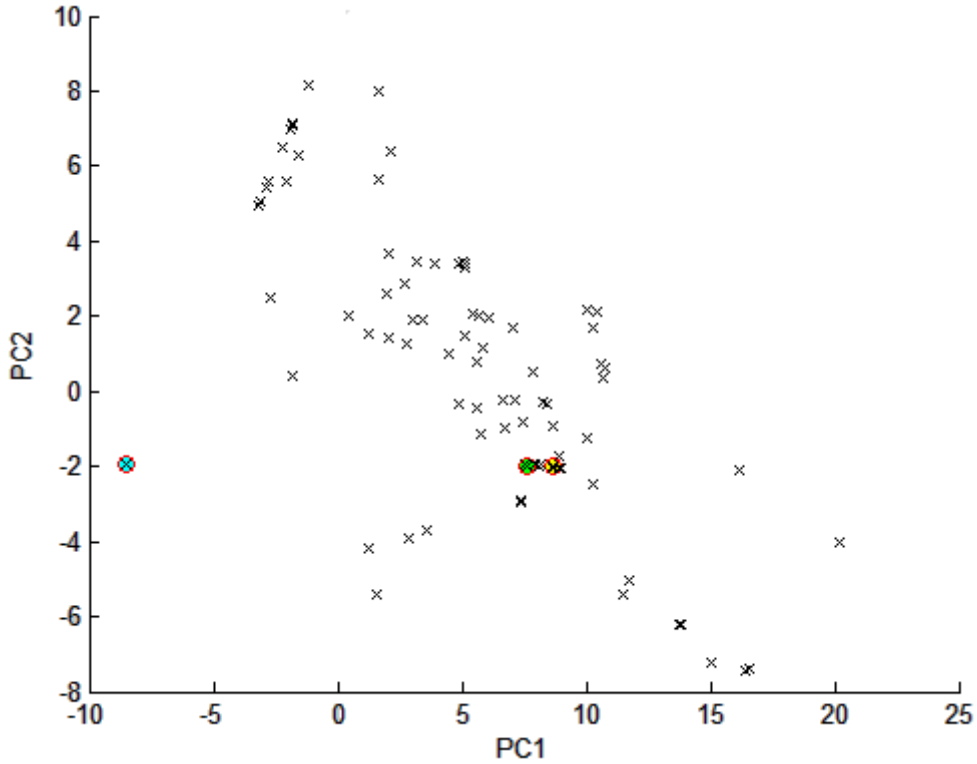

Figure 19. PCA analysis with marked ranges of the toxicity for Pseudokirchneriella subcapitata

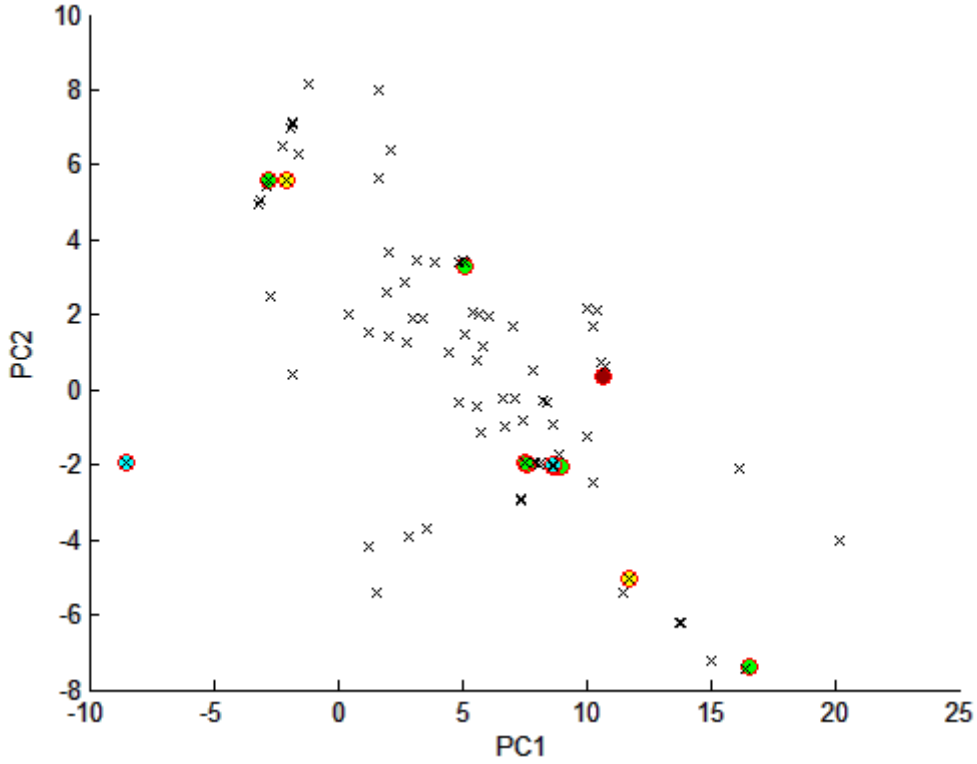

Figure 20. PCA analysis with marked ranges of the toxicity for Scenedesmus vacuolatus

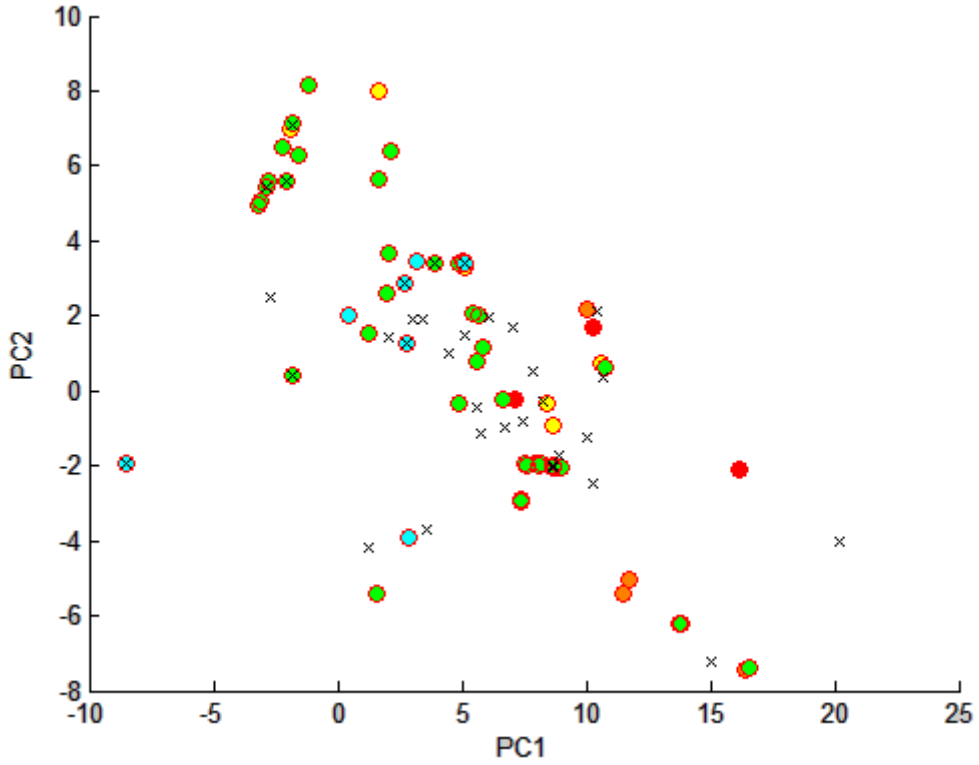

Figure 21. PCA analysis with marked ranges of the toxicity for Rat cell line IPC-81

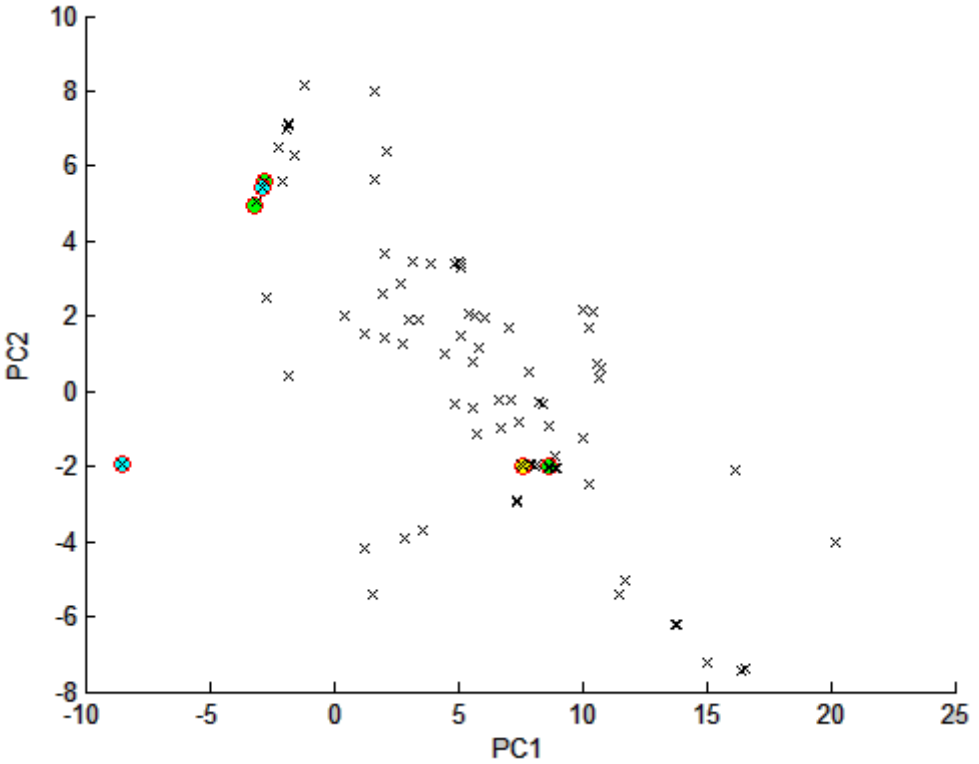

Figure 22. PCA analysis with marked ranges of the toxicity for Human cell line HeLa

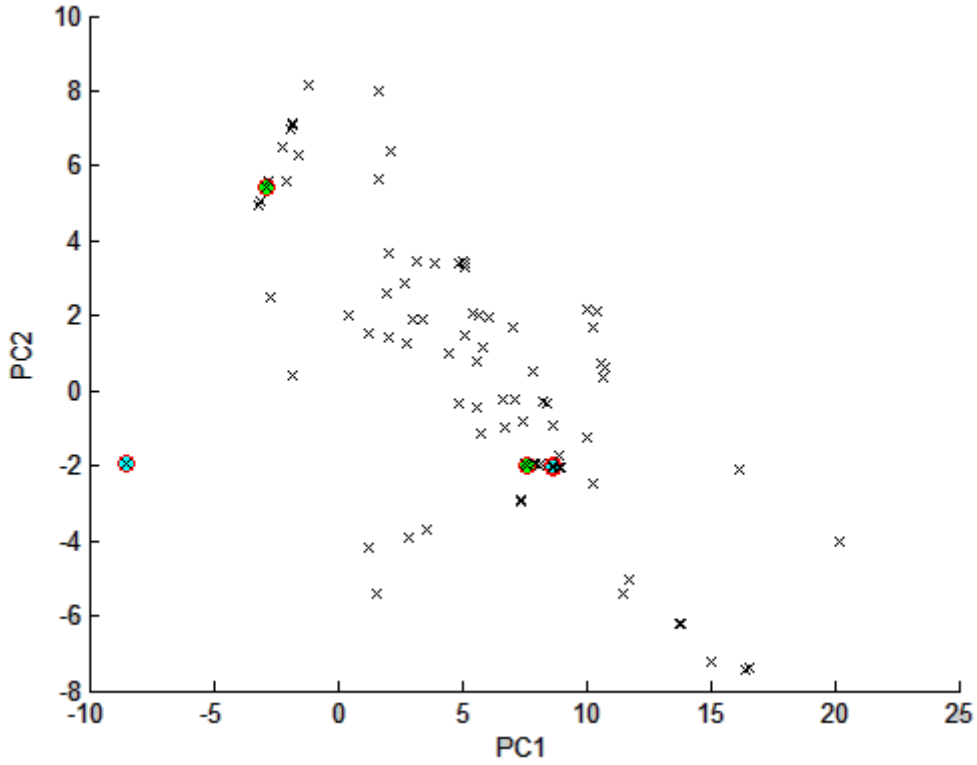

Figure 23. PCA analysis with marked ranges of the toxicity for Human cell line MCF7

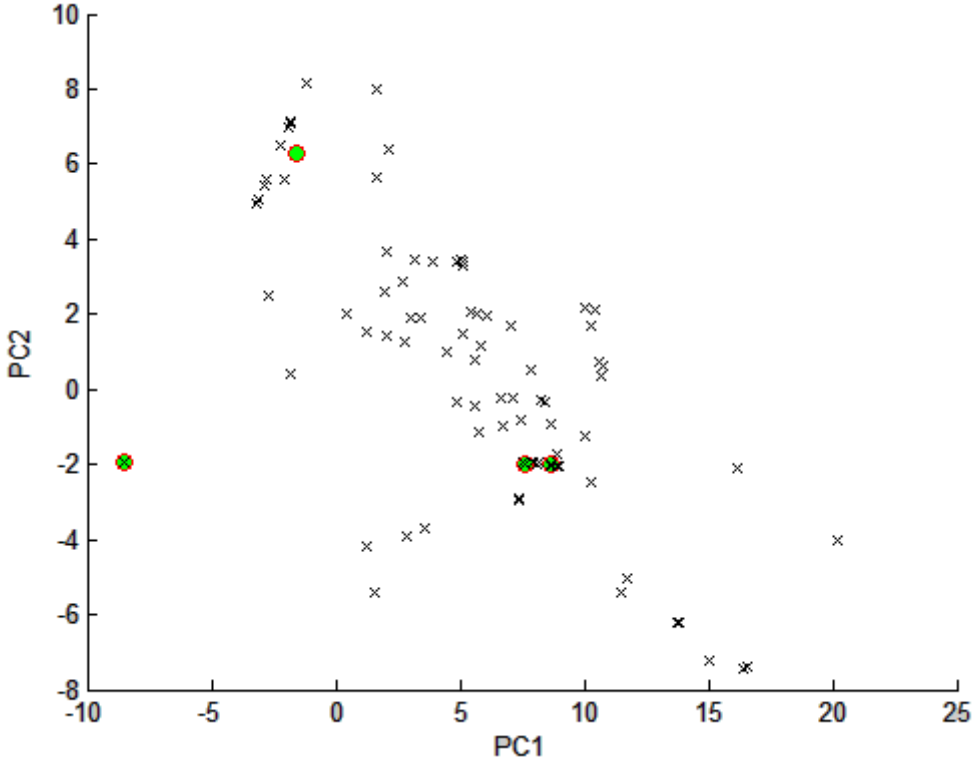

Figure 24. PCA analysis with marked ranges of the toxicity for Daphnia Magna

Following plots (fig. 25-29) are representing the projections of 375 ionic liquids in the space defined by two first principal components of anions' WHIM descriptors. Each

compound, with no toxicological data available, is represented by (**x**) symbol. Compounds with defined toxicity for the same cation are represented by (**o**) symbols, coloured according to used scale (see manuscript for details).

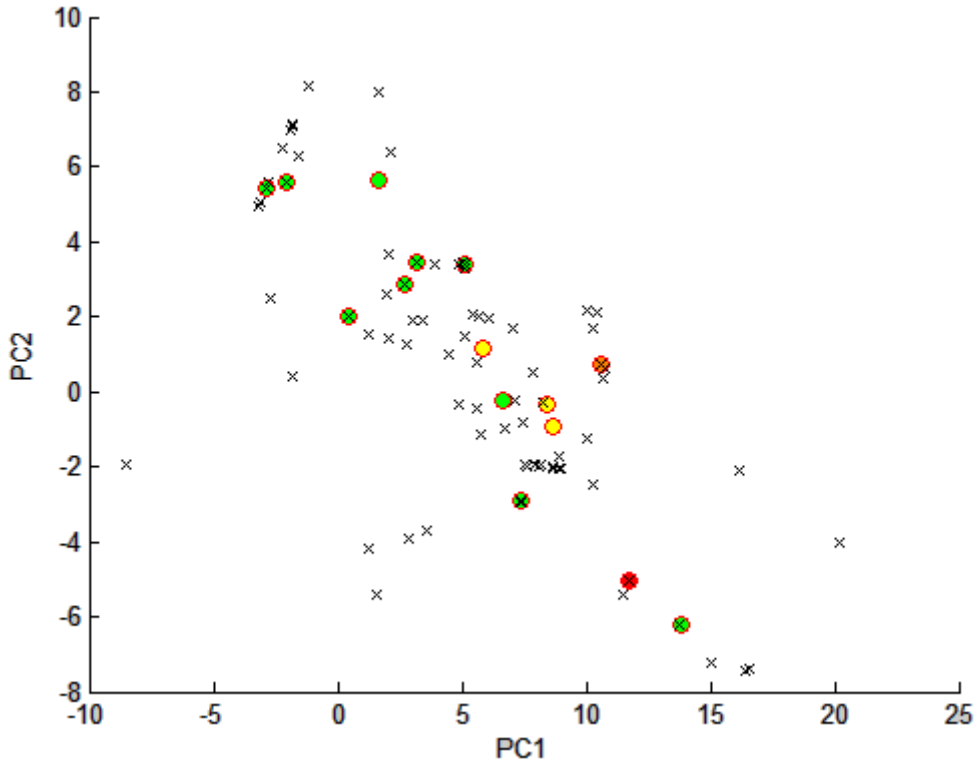

Figure 25. PCA analysis with marked ranges of the toxicity for Rat cell line IPC-81(cation: 1-butyl-3-methylimidazolium)

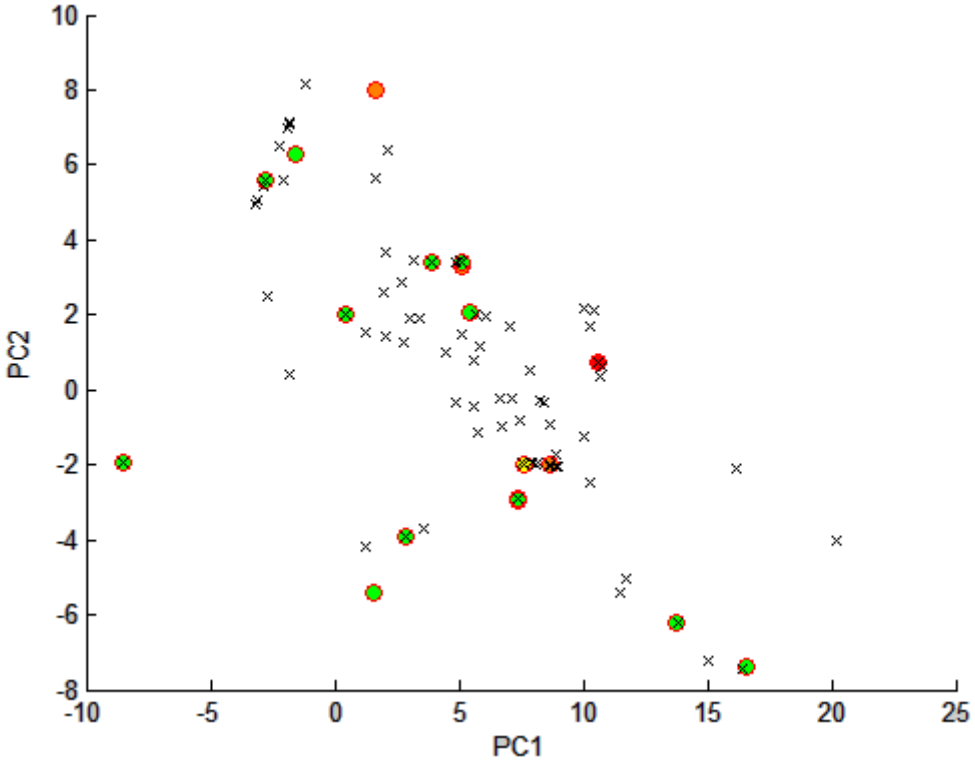

Figure 26. PCA analysis with marked ranges of the toxicity for Rat cell line IPC-81(cation: 1-ethyl-3-methylimidazolium)

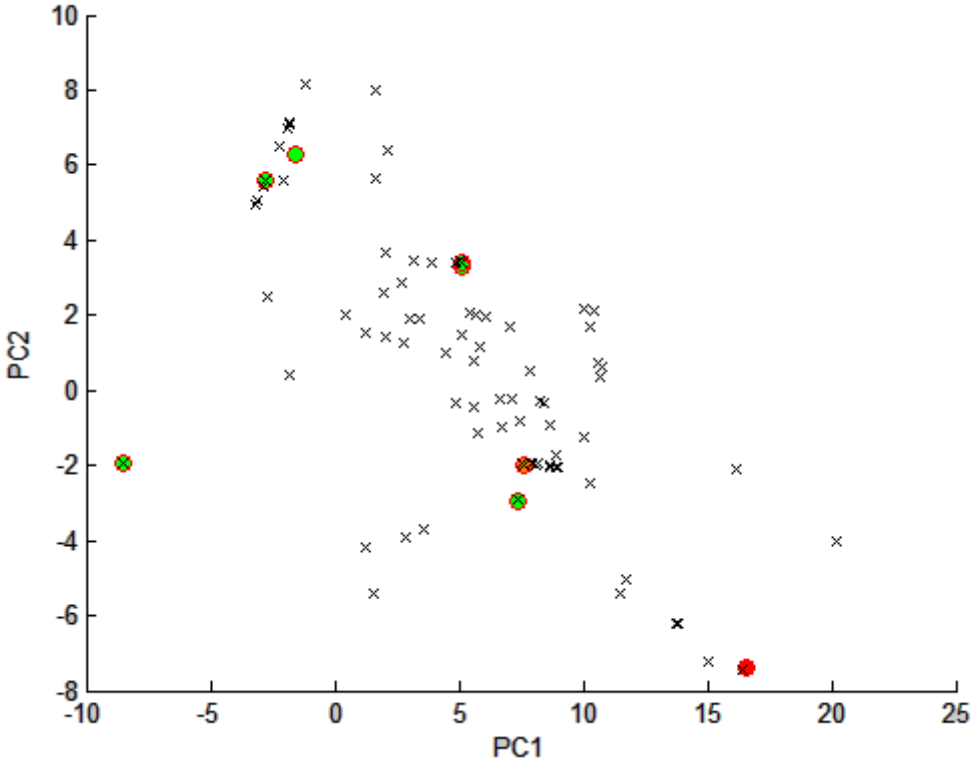

Figure 27. PCA analysis with marked ranges of the toxicity for Vibrio Fischeri (cation: 1-butyl-3-methylimidazolium)

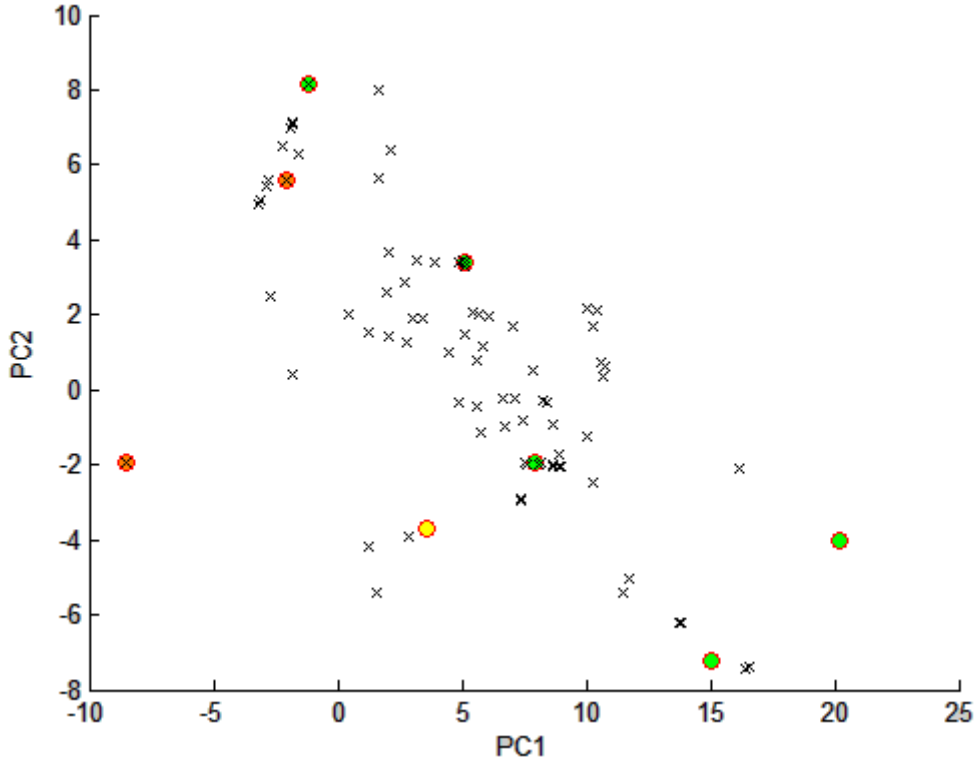

Figure 28. PCA analysis with marked ranges of the toxicity for Escherichia Coli (cation: trihexyltetradecylphosphinium)

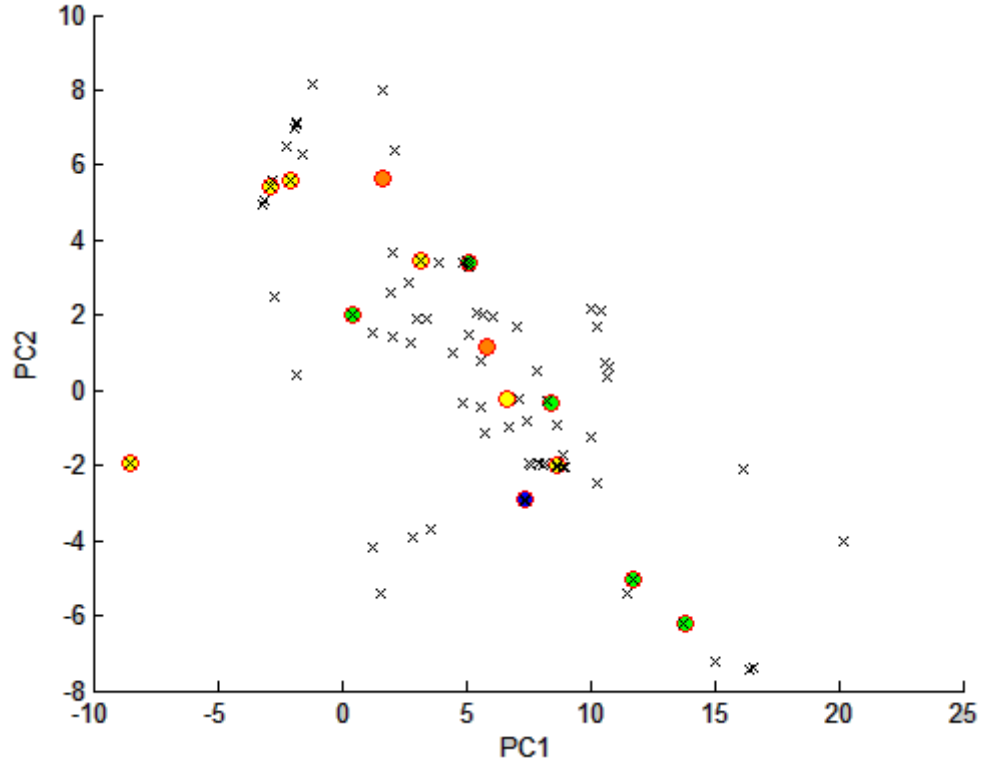

Figure 29. PCA analysis with marked ranges of the toxicity for Acetylcholine esterase (cation: 1-ethyl-3-methylimidazolium)