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CORRECTION

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Correction: A structure–activity relationship study of the toxicity of ionic liquids using an adapted Ferreira–Kiralj hydrophobicity parameter

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Correction for 'A structure–activity relationship study of the toxicity of ionic liquids using an adapted Ferreira–Kiralj hydrophobicity parameter' by Eduardo Borges de Melo *et al.*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 4516–4523.

In the original work,[1] a hydrophobicity descriptor based in the Ferreira–Kiralj hydrophobicity parameter[2] W_c, named W_cAdap, was proposed using a simple adaptation of the type of polar carbon atoms included in the calculations to explore the possibility of its use in quantitative structure–activity relationship (QSAR) studies of ionic liquids (ILs). However, the author found an inaccuracy in the parameter N_H (number of hydrogen atoms). Using the correct values, the study was carried out again. The methods used were the same. The basic results have not changed, and the corrected W_cAdap parameter was able to generate a new model **A** with virtually the same statistical quality as the original. RmSquare overall metrics show that the new model is still superior to model **B**, obtained using Crippen log *P*. Below the new model and its statistical parameters:

$\log EC_{50} = 5.492 - 0.054*(nAromBond) - 0.162*(nAtomLAC) - 0.079*(nRotBt) - 1.767*(W_cAdap)$ (**A**)

$\log EC_{50} = -0.191*(nAromBond) - 0.538*(nAtomLAC) - 0.410*(nRotBt) - 0.293*(W_cAdap)$ (**A, autoscaled coefficients**)

$R^2 = 0.819$; RMSEC = 0.373; $F = 173.907$; $Q_{LOO}^2 = 0.798$; RMSEV = 0.394; average r_m^2(LOO)-scaled = 0.711; delta r_m^2(LOO)-scaled = 0.169; cumulated information: 70.599% (LV1: 40.098%; LV2: 30.501%)

Robustness-Average $Q_{LNO}^2 = 0.797$; R^2 *vs.* $r(y_0,y_r) = -0.030$; Q_{LOO}^2 *vs.* $r(y_0,y_r) = -0.158$

$R_{pred}^2 = 0.780$; RMSEP = 0.530; average r_m^2(pred)-scaled = 0.643; delta r_m^2(pred)-scaled = 0.184; $k = 0.944$; $k' = 1.030$; $|R_0^2 - R_0'^2| = 0.084$

Average r_m^2(overall)-scaled = 0.678; delta r_m^2(overall)-scaled = 0.180

Descriptors:

nAromBond: number of aromatic bonds; nAtomLAC: number of atoms in the longest aliphatic chain; nRotBt: number of rotatable bonds, including terminal bonds.

The correct values of molecular descriptors are presented in Table 1.

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Table 1 Values of N_C^{hyd}, N_C^{hyd}Adap, A, N_H, and W_cAdap

Sample	N_C^{hyd}	N_C^{hyd}Adap	A	N_H	W_c	W_cAdap
1	12	9	38	23	0.800	0.600
2	8	5	26	15	0.727	0.455
3	20	17	62	40	0.909	0.773
4	9	6	29	17	0.750	0.500
5	11	8	35	21	0.786	0.571
6	13	10	41	25	0.813	0.625
7	8	5	26	15	0.727	0.455
8	11	8	35	21	0.786	0.571
9	8	5	26	15	0.727	0.455
10	11	8	39	21	0.611	0.444
11	6	3	24	11	0.462	0.231
12	12	9	42	23	0.632	0.474
13	7	4	27	13	0.500	0.286
14	12	9	39	23	0.750	0.563
15	12	9	30	15	0.800	0.600
16	11	8	39	21	0.611	0.444
17	11	8	31	13	0.611	0.444
18	7	4	24	13	0.636	0.364
19	4	1	26	14	0.333	0.083
20	13	10	48	26	0.591	0.455
21	7	4	27	11	0.438	0.250
22	10	7	40	15	0.400	0.280
23	14	11	52	23	0.483	0.379
24	7	4	26	11	0.467	0.267
25	7	4	27	14	0.538	0.308
26	9	6	29	14	0.600	0.400
27	10	7	28	16	0.833	0.583
28	11	7	37	24	0.846	0.538
29	13	9	43	28	0.867	0.600
30	13	9	51	24	0.481	0.333
31	10	7	33	17	0.625	0.438
32	9	6	25	14	0.818	0.545
33	10	7	32	16	0.625	0.438
34	10	7	32	14	0.556	0.389
35	12	9	38	18	0.600	0.450
36	9	6	25	14	0.818	0.545
37	12	9	34	20	0.857	0.643
38	12	9	34	20	0.857	0.643
39	12	9	38	20	0.667	0.500
40	7	4	20	10	0.700	0.400
41	8	5	23	12	0.727	0.455
42	10	7	32	16	0.625	0.438
43	14	11	44	24	0.700	0.550
44	11	8	35	18	0.647	0.471
45	12	9	42	16	0.462	0.346
46	10	7	36	12	0.417	0.292
47	10	7	28	16	0.833	0.583
48	10	7	28	16	0.833	0.583
49	9	4	31	18	0.692	0.308
50	11	6	45	18	0.407	0.222
51	11	8	40	14	0.423	0.308
52	11	7	46	20	0.423	0.269
53	10	6	35	22	0.769	0.462
54	11	8	40	14	0.423	0.308
55	23	19	67	42	0.920	0.760
56	13	10	35	16	0.684	0.526
57	13	10	31	16	0.867	0.667
58	14	10	43	23	0.700	0.500
59	10	6	44	18	0.385	0.231
60	10	6	44	18	0.385	0.231
61	11	7	47	20	0.407	0.259
62	10	6	44	18	0.385	0.231
63	11	7	47	20	0.407	0.259
64	11	7	46	20	0.423	0.269
65	11	7	45	20	0.440	0.280
66	12	8	49	22	0.444	0.296
67	11	7	46	20	0.423	0.269
68	12	8	48	22	0.462	0.308
69	11	7	46	20	0.423	0.269
70	11	7	46	20	0.423	0.269

Table 1 (*continued*)

Sample	N_C^{hyd}	N_C^{hyd}Adap	A	N_H	W_c	W_cAdap
71	12	8	49	22	0.444	0.296
72	10	6	43	18	0.400	0.240
73	10	5	40	15	0.400	0.200
74	9	5	32	20	0.750	0.417
75	10	6	35	22	0.769	0.462
76	8	4	29	18	0.727	0.364
77	11	8	31	18	0.846	0.615
78	9	5	31	7	0.375	0.208
79	7	3	17	7	0.700	0.300
80	10	6	34	22	0.833	0.500
81	14	11	44	27	0.824	0.647
82	10	7	32	19	0.769	0.538
83	6	3	20	11	0.667	0.333
84	13	10	45	25	0.650	0.500
85	9	6	33	17	0.563	0.375
86	9	6	33	17	0.563	0.375
87	9	6	33	15	0.500	0.333
88	12	9	46	19	0.444	0.333
89	10	7	34	15	0.526	0.368
90	7	4	28	14	0.500	0.286
91	14	11	40	24	0.875	0.688
92	7	4	19	10	0.778	0.444
93	8	3	26	15	0.727	0.273
94	19	15	55	34	0.905	0.714
95	15	12	41	20	0.714	0.571
96	9	4	38	13	0.360	0.160
97	10	7	41	15	0.385	0.269
98	9	4	37	13	0.375	0.167
99	11	7	37	24	0.846	0.538
100	8	5	30	15	0.533	0.333

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

1 E. B. de Melo, *Phys. Chem. Chem. Phys.*, 2015, **17**, 4516.
2 M. M. C. Ferreira and R. Kiralj, *J. Chemom.*, 2004, **18**, 242.