ERRATA

A Fuzzy ARTMAP Based Quantitative Structure−Property Relationship (QSPR) for Predicting Aqueous Solubility of Organic Compounds [*J. Chem. Inf. Comput. Sci. 41*, 1177−1207 (2001)] By Denise Yaffe, Yoram Cohen,* Gabriela Espinosa, Alex Arenas, and Francesc Giralt. Department of Chemical Engineering, University of California, Los Angeles, Los Angeles, California 90095-1592

Page 1177. The title should read A Fuzzy ARTMAP Based Quantitative Structure−Property Relationship (QSPR) for Predicting Aqueous Solubility of Organic Compounds.

Page 1177. The solubility range reported in the abstract was incorrectly reported as −11.62 to 4.31 logS. The correct range is −11.62 to 1.56 logS.

Page 1205. The average error was misreported in the second sentence of the last paragraph. The corrected sentence is as follows: "For the 287 compounds common with the study Katritzky et al.,[16] the present back-propagation QSPR model performed with average absolute and maximum absolute errors of 0.25 and 2.4 logS units, respectively, relative to the corresponding errors of 0.45 and 3.8 logS units for the Katritzky et al.[16] model."

Page 1179. The solubility range reported in the first sentence (i.e., $-5.82 \leq \log S \leq 5.45$) should be corrected to $-5.6 \leq \log S \leq 0.55$.

Pages 1180−1187. The reported -logS (S, mol/L) for a number of compounds in Table 1 (Molecular Descriptors and Experimental Aqueous Solubility Data at 25 °C) should be corrected as follows: −1.22 (acetic acid), −1.34 (formic acid), −1.22 (1-propanol), −0.26 (nitromethane), and +2.41 (4-*tert*-butylphenol).

Pages 1180−1187. In Table 1, the values of the molecular connectivity indices (χ^1, χ^2, χ^3, χ^4) for the first entry of diphenylmethane should be 4.98, 3.54, 2.60, 1.68, and the reported -logS value is 4.08. The second entry labeled as diphenylmethane should be replaced by diphenylethane with the values for the molecular connectivity indices (χ^1, χ^2, χ^3, χ^4) given as 4.53, 3.15, 2.09, 1.43, and the reported -logS value is 4.62.

Pages 1189−1196. In Table 2, the compound name diphenylmethane should be replaced by diphenylethane with the reported solubility value logS replaced by −4.62.

Pages 1189−1196 and pages 1199−1204. The logS (S, mol/L) values reported and estimated by FAM and Bk-Pro in Tables 2 and 5 should be corrected for a number of compounds as follows: acetic acid (1.22, 1.22, 1.41), formic acid (1.34, 1.31, 1.31), 1-propanol (1.22, 1.22, 1.08), and nitromethane (0.26, 0.26, −0.08), where the values in parentheses correspond to reported and estimated by FAM and Bk-Pro models, respectively.

Pages 1189−1196. In Table 2, the reported logS (S, mol/L) for 4-*tert*-butylphenol should be −2.41. The estimated logS values for the FAM and Bk-Pro should be −2.41 and −2.3, respectively, with the corresponding absolute logS errors of 0 and 0.11.

Pages 1199−1204. The reported average absolute logS errors in the fifth column in Table 5 (Comparison of Neural Network and Multilinear Regression Models for Predicting Aqueous Solubility of Selected Organic Compounds) should read 0.45 instead of 0.47. Also, the numerical columns that correspond to the last two rows (average absolute error and maximum absolute error) should be shifted one column to the right. Note that *n*-amyl acetate and *n*-pentyl acetate refer to the same compound. Also, *n*-pentylbenzene and pentylbenzene refer to the same compound.

Pages 1180−1187 and pages 1189−1196. The compound 3-ethylphenol is listed in error in Tables 1 and 2. It should be replaced by the compound 3-ethylpyridine with the descriptors no. of filled levels, dipole moment (debye), average polarizability (a.u.), resonance energy (EV), exchange energy (EV), E−N attraction (EV), N−N repulsion (EV), χ^1, χ^2, χ^3 and χ^4, having the values of 21, 2.37, 59.34, −224.15, −107.52, −8150.97, 4188.38, 2.83, 1.54, 0.85, 0.47, respectively, and logS (S in mol/L) = 0.54. Also, in Table 2, −logS = −0.54, and the FAM and Bk-Pro predictions for logS are 0.55 and 0.62 with the corresponding absolute logS errors of 0.01 and 0.08.

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