Comment on "Representation and Prediction of Molecular Diffusivity of Nonelectrolyte Organic Compounds in Water at Infinite Dilution Using the Artificial Neural Network-Group Contribution Method [Gharagheizi et al., J. Chem. Eng. Data 2011, 56, 1741-1750]"

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In their article, Gharagheizi et al. [1] claim to develop a model to predict the molecular diffusivity of "nonelectrolyte organic compounds" in water using an artificial neural network-group contribution method. The Supporting Information in ref. [1] lists the compounds considered by Gharagheizi et al. [1]. Many of these compounds have ionizable functionalities with pK_a values that result in either substantial or effectively complete ionization in water (making them electrolytes, in contrast to the claims made in the title for ref. [1]).

For example, Gharagheizi et al. [1] include large numbers of compounds such as carboxylic acids (see, e.g., compounds 13, 56, 74, 87, 124, 142, 153, 180, 215, 228, 230, 258, 295, 366, 371, 410, 415, 434, 450, 454, 457, 465, 468, 472, 475, 487, 498, 504, 510, 527, 555, 575, 689, 752, 844, 862, 869, 877, 969, 1043, 1061, 1108, 1116, 1124, 1166, 1218, 1272, 1322, 1405, 1505, 1556, 1652, 1715, 1723, 1737, 1825, 1885, 1980, 2212, 2236, 2329, 2381, 2724, 3275, 3506, 3566, 3692, 3706, 3732, 3829, 3900, 4071, 4083, 4119, 4204, 4256, 4329, 4362, 4365, 4394, and 4452), acidic phenols with electron withdrawing groups and thiophenols (see, e.g., compounds 794, 829, 845, 905, 906, 917, 1403, 1404, 1413, 1418-1421), basic aliphatic and aromatic amines (see, e.g., compounds 10, 62, 69, 73, 98, 132, 139, 157, 198, 207, 232, 285, 309, 328, 343, 363, 471, 478, 492, 554, 624, 688, 691, 705-706, 710-711, 714, 721-723, 725-726, 729-730, 747, 753-754, 761, 763, 800, 803, 1066, 1081, 1104, 1139, 1167, 1180, 1222, 1244, 1248-1249, 1259, 1273-1274, 1278, 1280-1282, 1305, 1314-1315, 1356, 1661, 1669, 1685, 1692, 1714, 1721-1722, 1724, 1731, 1735, 1740, 1759, 1784, 1790, 1813, 1838, 1850-1851, 1853, 1865, 1871, 1886, 1894, 1907, 1931, 1938, 2228, 2273, 2331-2332, 2334, 2342, 2350, 2650, 2668, 2679, 2682, 2685-2686, 2719, 2733, 2739, 2743, 3025, 3049, 3053, 3069, 3072, 3182, 3218, 3492, 3529, 3531, 3536, 3545, 3569, 3716-3717, 3740-3741, 3743-3745, 3747, 3820-3821, 3824-3825, 3830, 3892, 3901, 3903-3905, 3907-3908, 3976, 3979, 3981-3982, 3984, 3986, 3991, 4046-4049, 4054-4055, 4091, 4118, 4120, 4122, 4127-4128, 4186, 4195-4196, 4198, 4200, 4205, 4209, 4233, 4274, 4283, 4285, 4289, 4292, 4332-4333, 4339, 4341, 4350, 4352, 4385-4388, 4390, 4393, 4425, 4427-4430, 4432, 4456-4459, 4461, 4484-4487, 4490-4491, 4493, 4508-4509, 4511, 4513, 4515, 4529-4532, 4534, 4536, 4553-4557, 4560, 4575-4579, 4581, 4596-4599, 4601, 4617-4622, 4624, 4639-4642, 4644, 4655, 4658-4660, 4662, 4664, 4673, 4677-4678, 4682-4683, 4685, 4695-4698, 4703, 4705, 4713, 4716-4717, 4724-4725, 4735-4738, 4740, 4744, 4747, 4755, 4757-4758, 4760, 4765, 4771, 4774-4776, 4779, 4785, 4791-4793, 4797-4798, 4807, 4811-4814, 4822, 4831, 4835, 4838, and 4840-4843), and other acidic/basic moieties whose speciation would be either effectively entirely, dominantly, or significantly as the ionized form under the conditions in which the experimental data was obtained.

Consequently, the model developed and applied by Gharagheizi et al. [1] does not computationally model the actual speciation(s) of each compound expected to be present under the experimental conditions for which the underlying data has been obtained and erroneously classifies many organic compounds as non-electrolytes.

References

[1] F. Gharagheizi, A. Eslamimanesh, A. H. Mohammadi, D. Richon, Representation and prediction of molecular diffusivity of nonelectrolyte organic compounds in water at infinite dilution using the artificial neural network-group contribution method, Journal of Chemical and Engineering Data 56 (2011) 1741–1750.

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