

# Comment on “Determination of diffusion coefficient of organic compounds in water using a simple molecular-based method [Gharagheizi, Ind. Eng. Chem. Res. 2012, 51, 2797-2803]”

Sierra Rayne<sup>a,\*</sup>

<sup>a</sup>*Chemologica Research, 318 Rose Street, PO Box 74, Mortlach, Saskatchewan, Canada, S0H 3E0*

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In his article, Gharagheizi [1] states that “a new simple three-parameter equation is presented for calculation / prediction of the diffusion coefficient of nonelectrolyte organic compounds in water at infinite dilution. The model variables include three molecular-based descriptors.” In contrast to these claims, many of the compounds investigated in ref. [1] are indeed electrolytes in pure water at infinite dilution. For example, Gharagheizi’s dataset in the Supporting Information of ref. [1] includes a large number of compounds with carboxylic acid (see, e.g., compounds 11, 70, 83, 135, 144, 170, 204, 217, 219, 246, 282, 346, 351, 386, 391, 410, 426, 430, 433, 441, 444, 448, 451, 462, 473, 479, 484, 501, 529, 549, 663, 725, 817, 835, 842, 850, 940, 1013, 1031, 1076, 1084, 1091, 1133, 1184, 1236, 1286, 1368, 1467, 1518, 1614, 1676, 1684, 1697, 1785, 1845, 1940, 2172, 2195, 2285, 2337, 2675, 3224, 3455, 3515, 3652, 3678, 3774, 3845, 4014, 4026, 4062, 4262, and 4292) and basic amine groups (see, e.g., compounds 8, 58, 65, 69, 94, 125, 132, 188, 197, 221, 273, 292, 309, 323, 343, 447, 454, 467, 528, 598, 662, 665, 679, 680, 684, 685, 688, 695, 696, 697, 699, 700, 703, 704, 720, 726, 727, 734, 736, 773, 776, 1036, 1050, 1072, 1106, 1134, 1147, 1188, 1209, 1213, 1214, 1224, 1237, 1238, 1242, 1244, 1245, 1246, 1256, 1258, 1269, 1278, 1279, 1320, 1623, 1646, 1653, 1675, 1682, 1683, 1685, 1691, 1695, 1700, 1719, 1744, 1750, 1773, 1798, 1810, 1811, 1813, 1825, 1831, 1846, 1854, 1867, 1891, 1898, 2188, 2230, 2287, 2288, 2290, 2298, 2306, 2604, 2622, 2632, 2635, 2638, 2671, 2684, 2690, 2694, 2974, 2998, 3002, 3018, 3021, 3131, 3167, 3441, 3478, 3480, 3485, 3494, 3518, 3662, 3663, 3686, 3687, 3689, 3690, 3691, 3693, 3765, 3766, 3769, 3770, 3775, 3837, 3846, 3848, 3849, 3850, 3852, 3853, 3921, 3924, 3926, 3927, 3929, 3931, 3936, 3990, 3991, 3992, 3993, 3998, 3999, 4034, 4061, 4063, 4065, 4070, 4071, 4126, 4134, 4135, 4137, 4139, 4143, 4147, 4207, 4216, 4218, 4222, 4225, 4265, 4266, 4272, 4274, 4281, 4283,

4313, 4314, 4315, 4316, 4318, 4321, 4346, 4348, 4349, 4350, 4351, 4353, 4374, 4375, 4376, 4377, 4379, 4398, 4399, 4400, 4401, 4404, 4405, 4407, 4420, 4421, 4423, 4425, 4427, 4441, 4442, 4443, 4444, 4446, 4448, 4461, 4462, 4463, 4464, 4465, 4467, 4481, 4482, 4483, 4484, 4485, 4487, 4501, 4502, 4503, 4504, 4506, 4520, 4521, 4522, 4523, 4524, 4525, 4540, 4541, 4542, 4543, 4545, 4556, 4559, 4560, 4561, 4563, 4565, 4574, 4577, 4578, 4582, 4583, 4585, 4595, 4596, 4597, 4598, 4603, 4605, 4613, 4616, 4617, 4622, 4623, 4633, 4634, 4635, 4636, 4638, 4642, 4645, 4653, 4655, 4656, 4658, 4663, 4669, 4672, 4673, 4674, 4677, 4683, 4688, 4689, 4690, 4694, 4695, 4703, 4707, 4711, and 4715) - as well as acidic moieties such as sulfonic acids (compound 52), thioacetic acid (compound 117), phenols with electron withdrawing groups (compounds 767, 802, and 818), and thiophenols (compounds 878, 879, 890, 1354, 1360, 1366, 1367, 1376, 1381, 1382, 1383, and 1384) - that will be effectively entirely, dominantly, or significantly ionized in pure water at infinite dilution. Consequently, the molecular modeling efforts conducted by Gharagheizi [1] on the non-ionized molecular speciation of each compound were - in many cases - conducted on species that would not be dominantly present under the experimental conditions the modeling efforts are being developed against.

## References

- [1] F. Gharagheizi, Determination of diffusion coefficient of organic compounds in water using a simple molecular-based method, Industrial and Engineering Chemistry Research 51 (2012) 2797–2803.

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\*Corresponding author. Tel.: +1 306 690 0573. E-mail address: sierra.rayne@live.co.uk (S. Rayne).