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# From mass to structure: an aromaticity index for high-resolution mass data of natural organic matter

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For the calculation of the Aromaticity Index (AI) all functional groups that potentially contribute Double Bond Equivalents (DBE) through bonds between carbon and heteroelements are subtracted from the original molecular formula. $DBE_{AI}$ is the DBE of the resulting molecular core, and $C_{AI}$ is the respective number of carbon atoms. AI is the $DBE_{AI}$ to $C_{AI}$ ratio.

By mistake, in Eqn. (3), the number of N and P is not adjusted, as done in the correct way in Table 1 (compound d) of the original publication. This error is only relevant for molecular formulae that contain N and P, and in these cases it leads to a slight overestimation of $DBE_{AI}$ and consequently of AI. The corrected Eqn. (3) should read (the corrections are printed in bold red):

$$DBE_{AI} = 1 + \frac{1}{2}(2(C - O - N - S - P) - (H - N - P) + N - \mathbf{N} + P - \mathbf{P}) \quad (3)$$

The error propagates into Eqns. (4) and (6) and the equation in Fig. 5. The corrected equations are:

$$DBE_{AI} = 1 + C - O - S - \frac{1}{2}(N + P + H) \quad (4)$$

$$AI = \frac{DBE_{AI}}{C_{AI}} = \frac{1 + C - O - S - \frac{1}{2}(N + P + H)}{C - O - N - S - P} \quad (6)$$

$$AI_{mod} = \frac{DBE_{AI}}{C_{AI}} = \frac{1 + C - \frac{1}{2}O - S - \frac{1}{2}(N + P + H)}{C - \frac{1}{2}O - N - S - P} \quad (\text{Fig. 5})$$

This error in Eqn. (3) does not affect the figures, interpretations and conclusions.

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