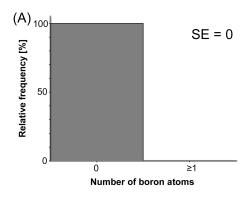
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Correction to Identification of Descriptors Capturing Compound Class-Specific Features by Mutual Information Analysis [Journal of Chemical Information and Modeling 2010, 50, 1935–1940]. Anne Mai Wassermann, Britta Nisius, Martin Vogt, and Jürgen Bajorath*



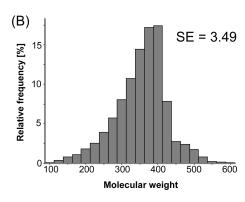
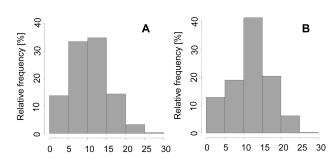


Figure 1

1. Calculation of histograms for databases A and B

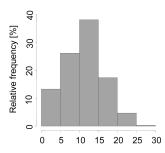


2. Calculation of class specific entropies

$$H_{A}(D) = 2.05$$

$$H_B(D) = 2.10$$

3. Calculation of the combined histogram



4. Calculation of SE for combined histogram

$$\mathsf{H}_{\mathsf{AB}}(D) = 2.09$$

5. Calculation of DSE

$$DSE(D) = 2.09 - ((2.05 + 2.10) / 2) = 0.015$$

Figure 3



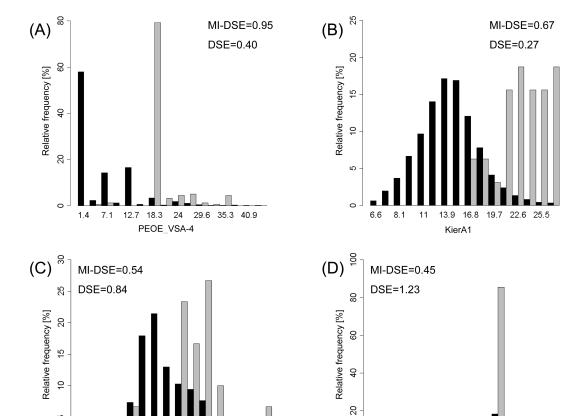


Figure 5

Page 1939: Typographical sign errors have occurred in eqs 7 and 9. The corrected equations are listed below

$$MI(D, C) = H(D) - \frac{(H_A(D) + H_B(D))}{2}$$
with MI(D, C) \le H(C) = 1 (7)

-3.7 -3.5 -3.2

$$MI\text{-DSE}(D) = H_{norm}(D) - \frac{H_A(D) + H_B(D)}{2} \qquad (9)$$

Pages 1936-1939: We have noticed plotting/labeling errors in individual histograms in Figures 1, 3, and 5. The corrected figures are provided.

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2.22 2.33 2.44 2.55 2.66 2.77 2.88 2.99

BCUT_SLOGP_3

-2.6 -2.4 -2.2

-3 -2.8

BCUT_SLOGP_0