ERRATUM

Erratum to: Design of chemical space networks using a Tanimoto similarity variant based upon maximum common substructures

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We have detected a small counting error in the routine to calculate similarity values according to the formula on page 940 of our paper. Re-calculation of all values revealed that differences from absolute values reported in the manuscript were small and deviations from reported percentage values were only 1–2 % (in some cases, there were no deviations). In addition, the re-generated graphs that were based upon similarity value distributions were very similar to the original figures and no qualitative differences

were observed. On the basis of the re-calculated values (i.e., in the presence of small numerical deviations), no changes to the manuscript text or any of the conclusions were required.

Independent of the similarity value calculations, we note that the schematic Fig. 2c on page 942 of the paper contained two drawing errors. The correct version of Fig. 2c is shown below. Accordingly, this figure should be described on page 943 as follows: “In addition, Fig. 2c shows substructure-based similarity relationships applying the MMP formalism. Here, compound A forms MMPs with compounds B, D, and F, thereby establishing three similarity relationships on the basis of six pairwise comparisons.”

The online version of the original article can be found under doi:[10.1007/s10822-015-9872-1](https://doi.org/10.1007/s10822-015-9872-1).

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Fig. 2 Comparison of similarity relationships. For a compound A and six related molecules B–G, similarity relationships are compared on the basis of **a** Tc_{MCS} values, **b** ECFP4 Tc values, and **c** MMP formation (i.e., binary yes/no similarity relationship). The *red cross* indicates the absence of a similarity relationship