analytical chemistry

ADDITION/CORRECTION

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Correction to Computing Fragmentation Trees from Tandem Mass Spectrometry Data [*Analytical Chemistry* **2011**, *83*, 1243–1251. DOI: 10.1021/ac101825k]. Florian Rasche, Aleš Svatoš, Ravi Kumar Maddula, Christoph Böttcher, and Sebastian Böcker*

In the section Evaluation against Mass Frontier on page 1250, we evaluated results of our approach using the Mass Frontier software (Highchem, Bratislava, Slovakia). This section can be misinterpreted in the way that we wanted to compare the performance of our approach and Mass Frontier. To this end, we want to clarify the following: Mass Frontier computations were not carried out by us but by Hill et al.,[1] who kindly provided their data for our analysis. Details of these computations can be found in their paper; in particular, Hill et al. used version 4 of Mass Frontier for their analysis.[1] Comparison of the number of annotated peaks was not meant as a performance evaluation: It is rather number of *correctly* annotated peaks that is relevant. Furthermore, newer versions of Mass Frontier will likely annotate more peaks.

Our evaluation was intended to show the very high agreement (97.3%) of molecular formula annotations by Mass Frontier and our approach. Here, it is important that these two methods are based on orthogonal paradigms: If we had compared two methods both using the measured data as input, then an agreement of this strength might possibly be an artifact. In contrast, Hill et al. used molecular structures as input for Mass Frontier (but not the measured data),[1] whereas our approach used the measured data as input (but not the molecular structures). Therefore, our analysis indicates that the *matching* annotations are in fact correct. We also showed that by annotating peaks with the closest molecular formula, we reach a much smaller agreement (71.8%).

REFERENCES

(1) Hill, D. W.; Kertesz, T. M.; Fontaine, D.; Friedman, R.; Grant, D. F. *Anal. Chem.* **2008**, *80*, 5574–5582.

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