RESULTS

Determine Elemental Composition

Perform chemical database search

Map fragment structures

Figure 2.  Determination of elemental composition.

Figure 3.  Improved determination of elemental composition

Figure 4.  Similarity Search Result Display - Mass Frontier 5.0 software

Figure 5.  Fragmentation analysis available on mzCloud

Figure 6. Example of mzLogic result for glycyl-prolyl-glutamic acid

Positive elemental composition, calculated from the accurate mass [M+H]⁺, can be refined through chemical database searching and spectral library similarity search. The confident assignment of molecular formula (Figure 3) is further supported by the matching of the fragment structure highlighted in the image. The mzLogic algorithm screens through the positive 200+ chemical database(s) looking for a substructure matching to the observed elemental composition. In this case, the candidate (natural toxin) is in the mzCloud database.

In this case the similarity hit selected was a natural toxin, the matching explained fragments are shown in the image. The mzLogic algorithm screens through the putative chemical database candidates (Figure 5) as a confirmation that the overlapping substructure observed in the database candidate is seen in common with observed fragmentation. Because of this, the implementation also considers the structural match – how much of the compound database hit is matching to the known fragmentation structure from the mzCloud library, which has extensive annotation of fragments.

Another example of the mzLogic sorting capability can be seen with a more complex example. The data was from rosmarinic acid, another compound not present in the reference spectral library. Another example of the mzLogic sorting capability can be seen with a more complex example. The data was from rosmarinic acid, another compound not present in the reference spectral library. The mzLogic algorithm screens through the putative chemical database candidates (Figure 5) as a confirmation that the overlapping substructure observed in the database candidate is seen in common with observed fragmentation. Because of this, the implementation also considers the structural match – how much of the compound database hit is matching to the known fragmentation structure from the mzCloud library, which has extensive annotation of fragments. The mzLogic algorithm screens through the putative chemical database candidates (Figure 5) as a confirmation that the overlapping substructure observed in the database candidate is seen in common with observed fragmentation. Because of this, the implementation also considers the structural match – how much of the compound database hit is matching to the known fragmentation structure from the mzCloud library, which has extensive annotation of fragments.

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