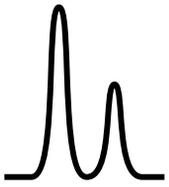
Taxonomic distance

A score, inversely proportional to the taxonomic distance between the biological source of the annotated compound and the biological source of the candidate structures.

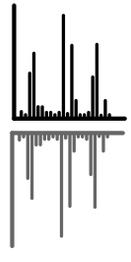


Physico-chemical consistency

A score, proportional to the closeness of physico-chemical properties measured or calculated between the annotated compound and the candidate structures. Typically: retention time, retention order, collisional cross section.

$$S_{tot} = w_1S_1 + w_2S_2 + w_3S_3 + w_4S_4$$

Spectral similarity score



exp

e.g. GNPS or ISDB-DNP approach

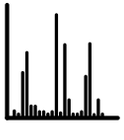
exp. or in-silico

Structural DB

Fingerprint similarity score

1000111010101010

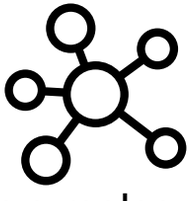
1100101011101110



exp

e.g. Sirius approach

Structural consistency



When annotating spectrally organised data (i.e a molecular network), a structural consistency is expected between nodes of a cluster. A structural similarity distance is calculated among all annotations of the cluster. If a validated annotation is present within the cluster, remaining annotations are reranked so that the distance between this validated annotation and the remaining annotations is kept minimal. If no validated annotations are present, the annotations are reranked in order to obtain maximal structural consistency at rank 1.