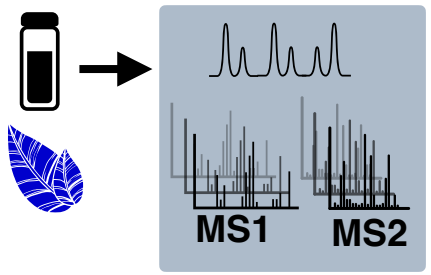
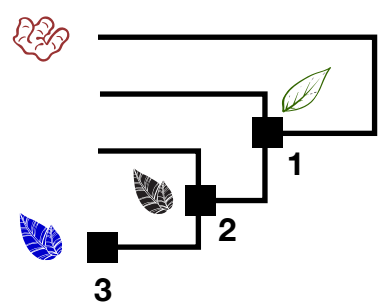



**metabolite annotation**

| Spectral ID | Spectra | Query Biological source | Candidate structures | Score $S_1$ | Initial Rank |
|---|---|---|---|---|---|
| 1 | | | INCHIKEY-1 | 0.55 | 1 |
| | | | INCHIKEY-2 | 0.53 | 2 |
| | | | INCHIKEY-3 | 0.50 | 3 |
| | | | INCHIKEY-4 | 0.45 | 4 |
| | | | INCHIKEY-5 | 0.42 | 5 |
| | | | INCHIKEY-6 | 0.41 | 6 |
| ... | | | | | |

re-ranking

***taxonomically informed scoring***




| Spectral ID | Spectra | Query Biological source | Candidate structures | Score $S_1$ | Candidate Biological source | Taxonomical Score $S_2$ | Combined Score $S_1 + S_2$ | Initial Rank | Final Rank |
|---|---|---|---|---|---|---|---|---|---|
| 1 | | | INCHIKEY-6 | **0.41** | | **3** | **3.41** | **6** | **1** |
| | | | INCHIKEY-1 | 0.55 | | 2 | 2.55 | 1 | 2 |
| | | | INCHIKEY-4 | 0.45 | | 1 | 1.45 | 4 | 3 |
| | | | INCHIKEY-5 | 0.42 | | 1 | 1.42 | 5 | 4 |
| | | | INCHIKEY-2 | 0.53 | | 0 | 0.53 | 2 | 5 |
| | | | INCHIKEY-3 | 0.50 | | 0 | 0.50 | 3 | 6 |
| ... | | | | | | | | | |