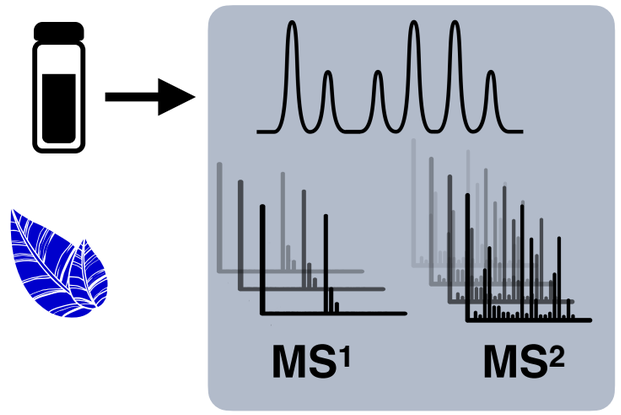
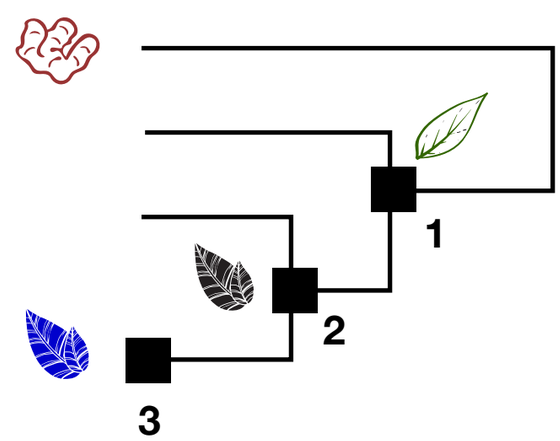


metabolite annotation

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
...									