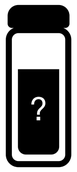
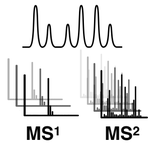
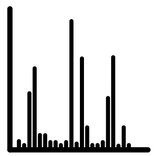
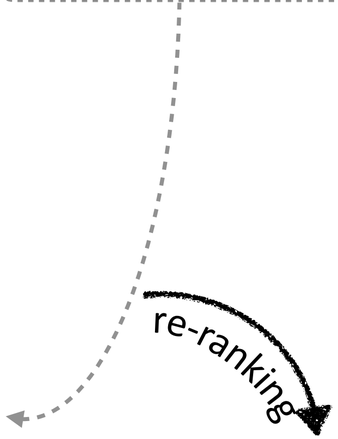




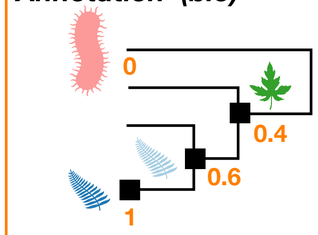
Metabolite annotation

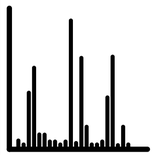
Optional MS¹-based annotation

Feature ID	Spectrum	Biological source	Candidate structure	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
...	...	...	...	...	...
1			INCHIKEY-9	0.00	9



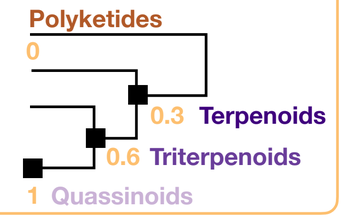
Taxonomically Informed Metabolite Annotation (bio)

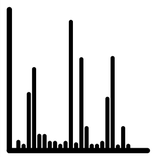
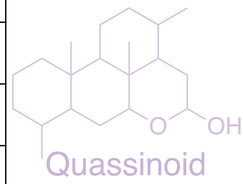


Feature ID	Spectrum	Biological source	Candidate structure	Score S_1	Initial rank	Candidate biological source	Score S_2	Combined score $(S_1 + S_2)$ /2	Final rank
1			INCHIKEY-4	**0.45**	**4**		1.00	**0.78**	**1**
			INCHIKEY-1	0.55	1		0.60	0.58	2
			INCHIKEY-2	0.53	2		0.40	0.47	3
			INCHIKEY-9	0.00	9		0.60	0.30	4
...	...	...	INCHIKEY-3	0.50	3		0.00	0.25	5

re-ranking

Taxonomically Informed Metabolite Annotation (chemo)



Feature ID	Spectrum	Biological source	Candidate structure	Score S_1	Initial rank	Candidate biological source	Score S_2	Combined score $(S_1 + S_2)$ /2	2nd rank	Attributed chemical class	Candidate chemical class	Score S_3	Combined score $(S_1 + S_2 + S_3)/3$	Final rank
1			INCHIKEY-4	**0.45**	**4**		1.00	**0.78**	**1**		Quassinoid	1.00	**0.82**	**1**
			INCHIKEY-1	0.55	1		0.60	0.58	2		Triterpenoids	0.60	0.58	2
			INCHIKEY-2	0.53	2		0.40	0.47	3		Terpenoids	0.30	0.41	3
			INCHIKEY-9	0.00	9		0.60	0.30	4		Terpenoids	0.30	0.30	4
...	...	...	INCHIKEY-3	0.50	3		0.00	0.25	5	...	Polyketides	0.00	0.17	5