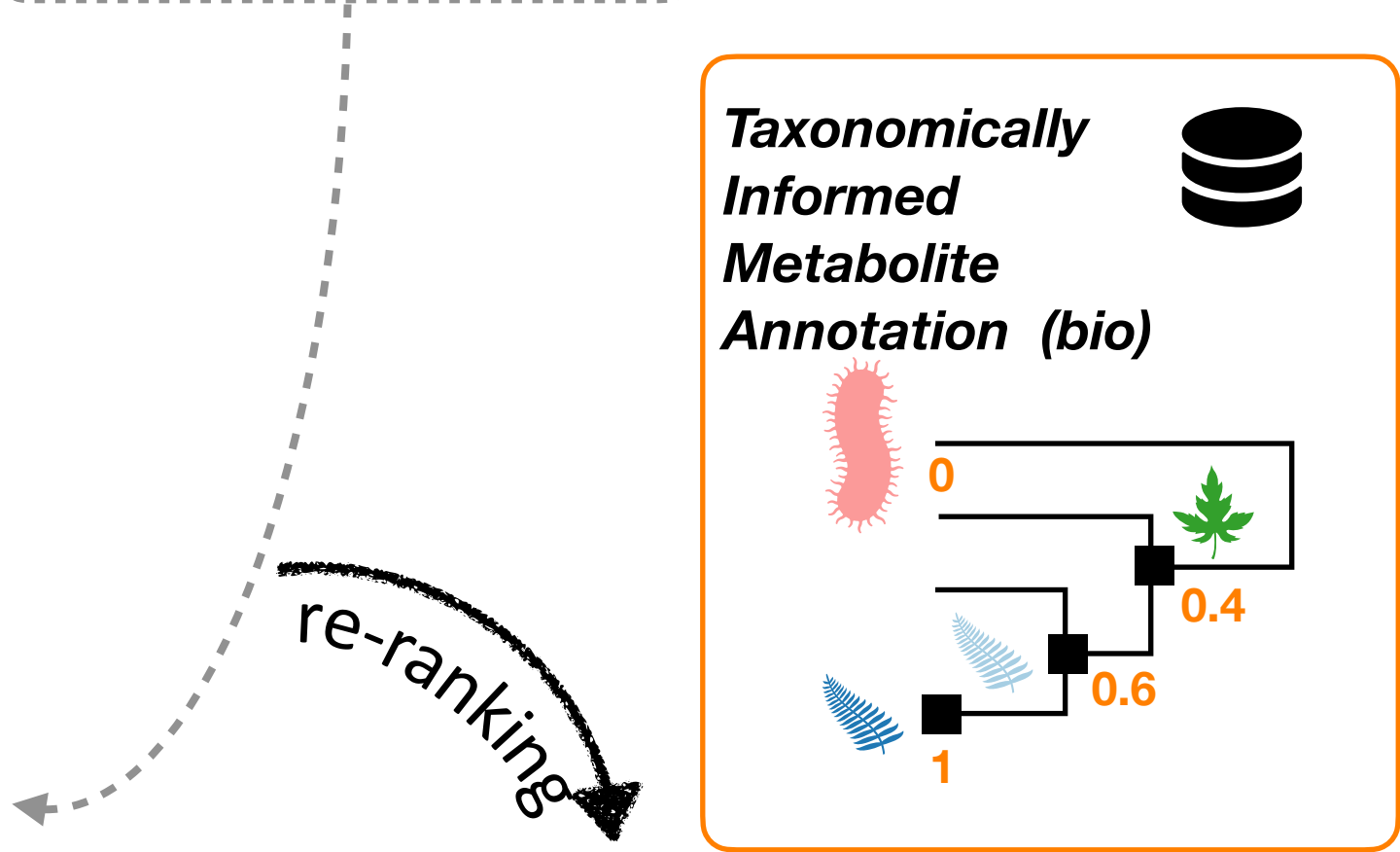


MS¹MS²

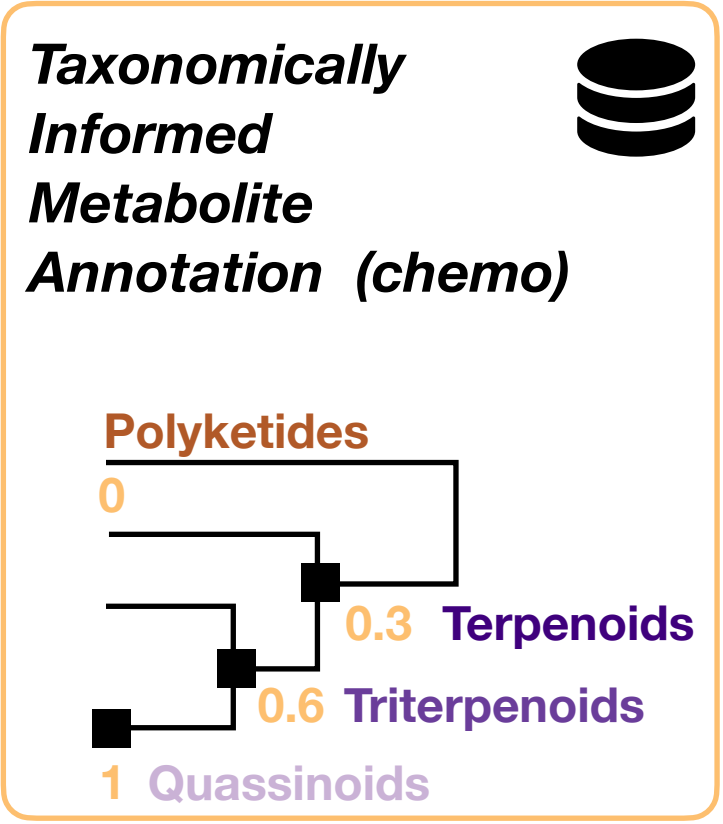
Metabolite annotation

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

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



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