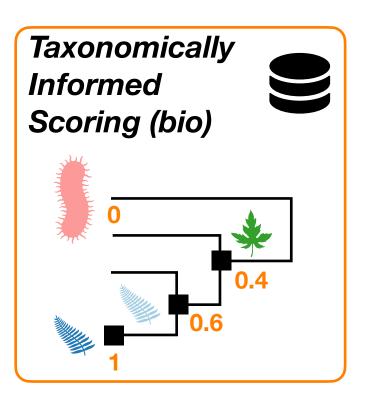


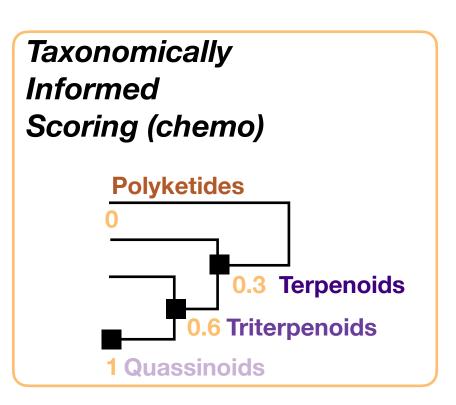
Feature ID	Spectrum	Biological source	Candidate structures	Score S ₁	Initial Rank	
	1 .	Λ.	INCHIKEY-1	0.55	1	
4	, , ,		INCHIKEY-2	0.53	2	
•			INCHIKEY-3	0.50	3	
	الساباسالسالس		INCHIKEY-4	0.45	4	





Feature ID	Spectrum	Biological source	Candidate structures	Score S ₁		Candidate biological source		Combined Score (S ₁ + S ₂) /2	Final Rank
1	1 1		INCHIKEY-4	0.45	4		1	0.78	1
			INCHIKEY-1	0.55	1		0.6	0.58	2
			INCHIKEY-2	0.53	2	*	0.4	0.47	3
			INCHIKEY-3	0.50	3	THE	0.0	0.25	4
•••	• • •			•••		• • •	•••		• • •





Feature	Spectrum	Biological	Candidate	Score	Initial	Candidate	Score	Combined Score	2nd	Attributed	Candidate	Score	Combined Score	Final
ID	Spectrum	source	structures	S ₁	Rank	biological source	S ₂	$(S_1 + S_2) / 2$	Rank	chemical class	chemical class	S ₃	$(S_1 + S_2 + S_3)/3$	Rank
1	1 .		INCHIKEY-4	0.45	4		1	0.78	1		Quassinoid	1	0.82	1
		INCHIKEY-1	0.55	1		0.6	0.58	2		Triterpenoids	0.6	0.58	2	
			INCHIKEY-2	0.53	2	*	0.4	0.47	3	OOO	Terpenoids	0.3	0.41	3
			INCHIKEY-3	0.50	3	Control March	0.0	0.25	4	Quassinoid	Polyketides	0.0	0.17	4
•••	•••					• • •							• • •	