SUPPLEMENTARY MATERIAL

BIOFACQUIM: A Mexican compound database of natural products

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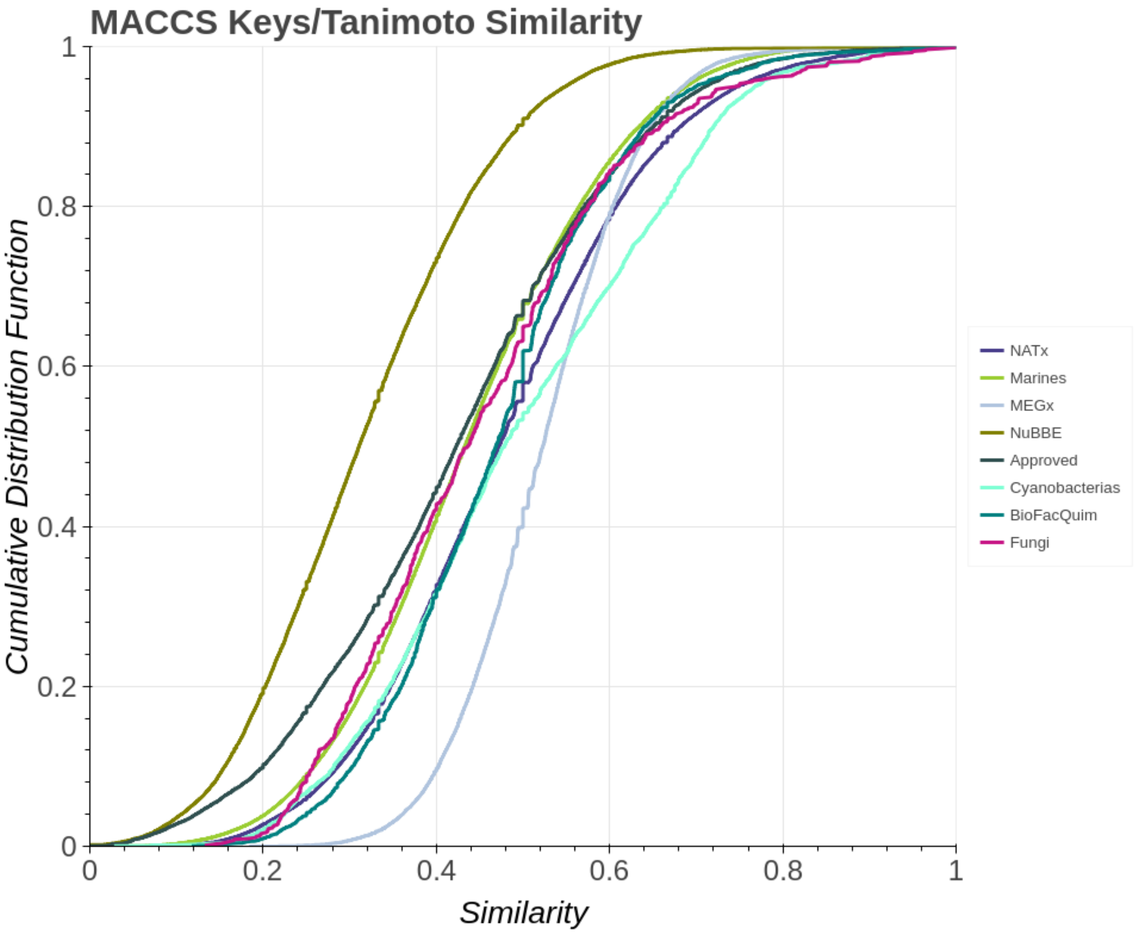
Table S1. Loadings for the first three principal components of the property space of eight databases

Principal Component	**PC1**	**PC2**	**PC3**
Eigenvalue	1.98	1.05	0.71
Cumulative eigenvalue (%)	65.58	83.85	92.15
SlogP	0.18	-0.86	0.23
TPSA	-0.49	0.04	0.21
MW	-0.45	-0.31	0.13
HBA	-0.45	-0.04	0.47
HBD	-0.44	0.23	-0.08
RB	-0.37	-0.33	-0.81



	NATx	Marines	MEGx	NuBBE	Approved	Cyanobacterias	BIOFACQUIM	Fungi
MIN	0.06	0.0	0.18	0.0	0.0	0.03	0.12	0.13
1Q	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MEDIAN	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0
MEAN	0.48	0.44	0.52	0.32	0.42	0.5	0.47	0.45
3Q	0.58	0.54	0.59	0.41	0.54	0.63	0.55	0.55
MAX	1.0	1.0	1	1.0	1.0	1.0	1.0	1.0
STD	0.15	0.14	0.1	0.13	0.17	0.17	0.13	0.16

Figure S1. Distribution of the pairwise similarity values calculated for BIOFACQUIM and the reference data sets computed with MACCS keys (166-bits) and the Tanimoto coefficient.

Table S2. Statistics of the cyclic system recovery curves for BIOFACQUIM and the reference data sets

DB	PCP	FP	Scaffold	Relative size
	EDmedian	Tmedian	AUC	
Approved	1.96	0.32	0.59	699
BIOFACQUIM	1.74	0.45	0.72	423
Cyanobacterias	2.64	0.50	0.74	473
Fungi	1.39	0.44	0.66	206
MEGx	2.28	0.43	0.60	1000
Marines	1.93	0.40	0.58	1500
NATx	3.04	0.51	0.55	2000
NuBBE	2.51	0.39	0.67	1000

Databases (DB), physicochemical diversity (PCP), Euclidean distance (ED), fingerprint (FP), Tanimoto coefficient (T), area under the curve (AUC).

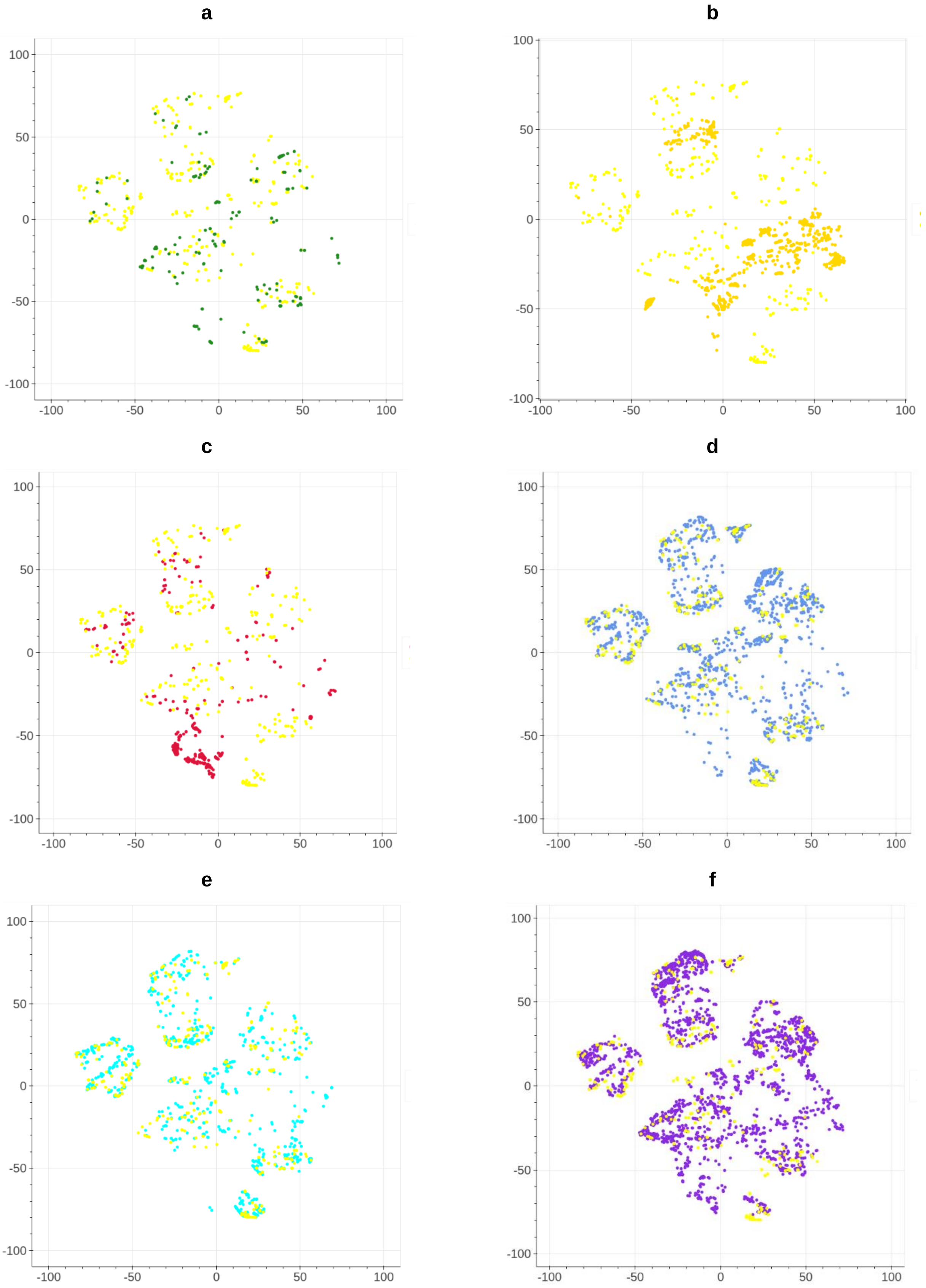


Figure S2. Visual representation of the chemical space of BIOFACQUIM compared with: **a**) Fungi, **b**) NATx, **c)** Cyanobacterias, **d)** MEGx, **e)** NuBBE$_{DB}$, **f**) Marines. Figure generated with t-SNE.

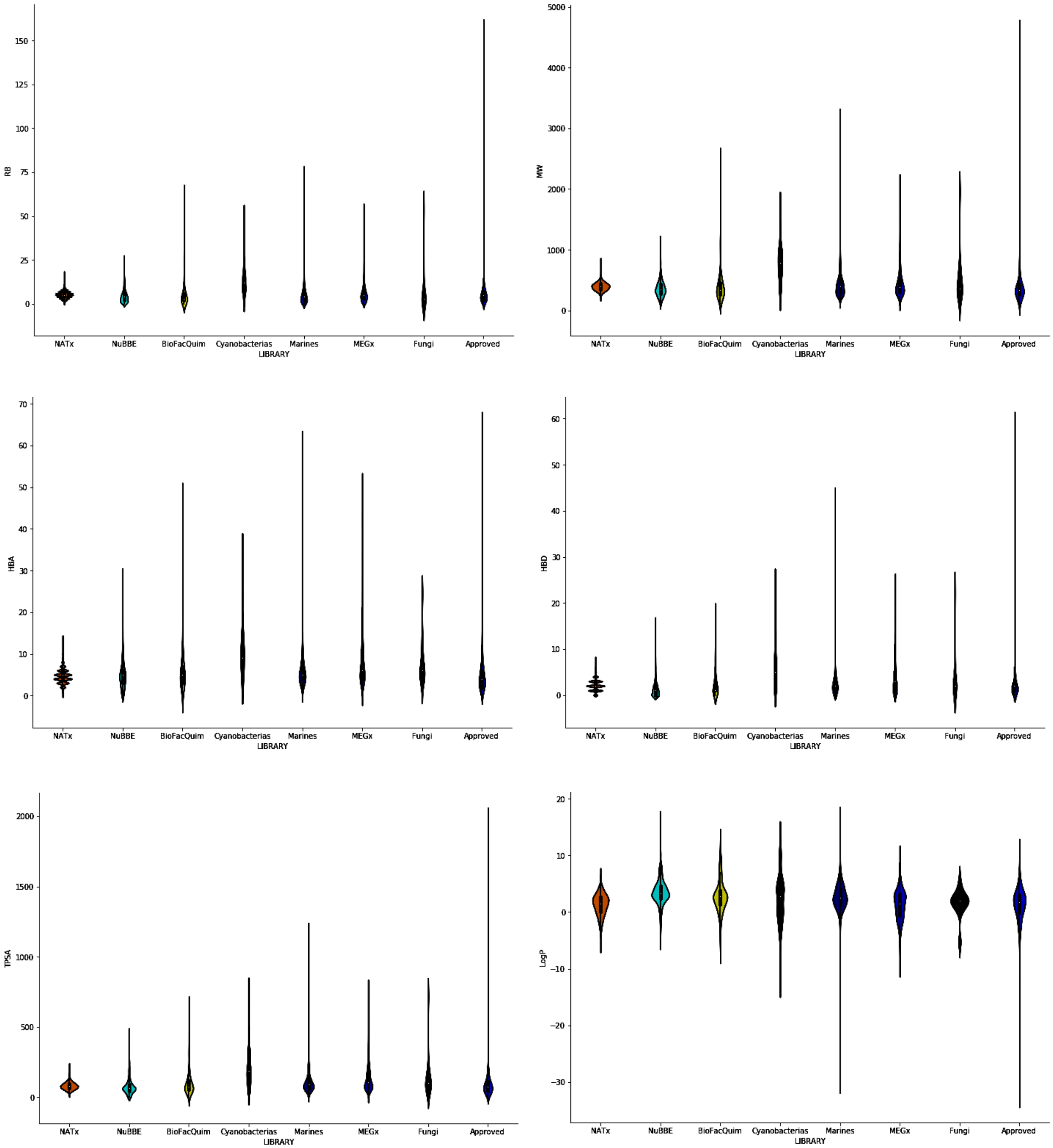


Figure S3. Violin plots for the physicochemical properties of BIOFACQUIM and reference data sets.