




Supplementary Materials: Searching Hit Potential Antimicrobials in Natural Compounds Space Against Biofilm Formation

Roberto Pestana-Nobles ^{1,†} , Jorge A. Leyva-Rojas ^{1,†}  and Juvenal Yosa ^{1,†} *

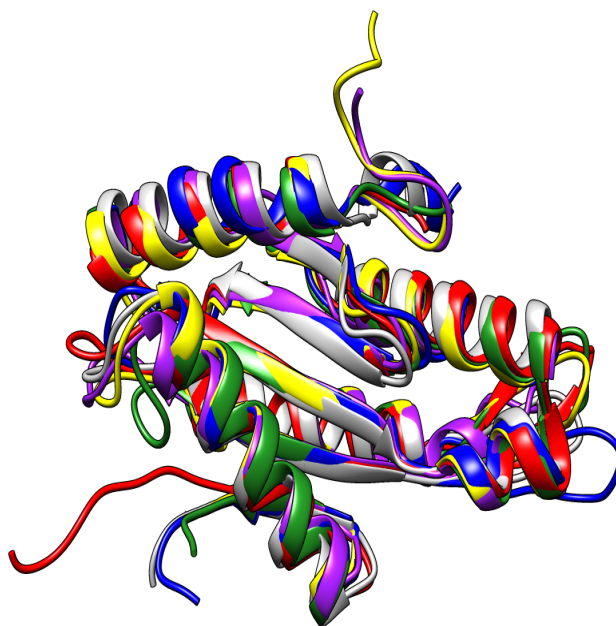


Figure S1. Alignment of five crystal structure of GGDEF domain compared with PleD for *Vibrio cholerae* (gray), *E. coli* DosC (blue), *Marinobacter aquaeolei* (yellow), *Pseudomonas aeruginosa* (green), and *P. fluorescens* (purple). All of them form a biofilm. As is shown the structural domain is well conserved. GTP has a high affinity for the active site of all GGDEF domain. Here, we assume that the active site for all the GGDEF domains in bacteria, binds GTP molecule similarly. In such a case, the hit that can be found in the natural products library the natural products library will be bind also similar to all GGDEF domains in bacteria. The RMSD between them is 0.915 Å, this structure was obtained using the Needleman-Wunsch matrix BLOSUM62 algorithm.

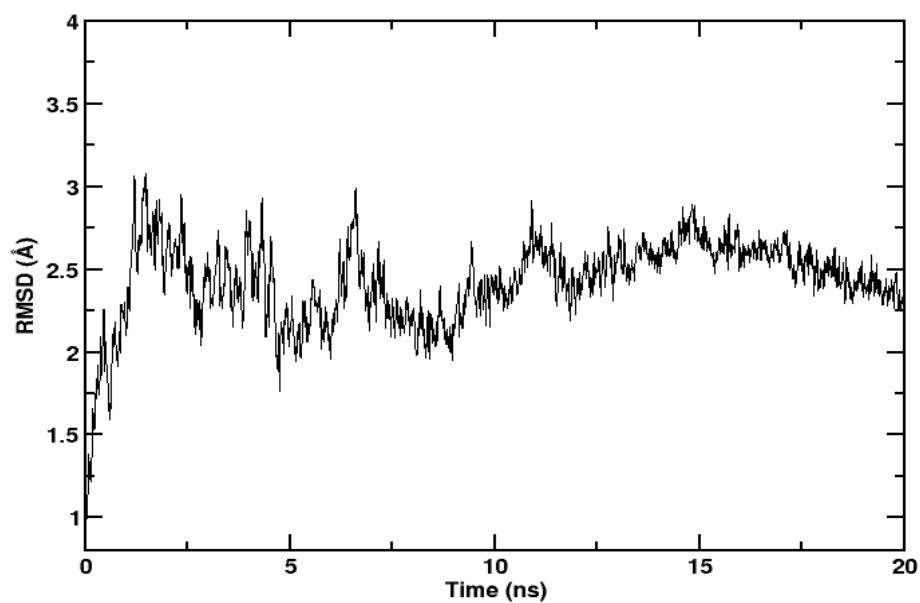


Figure S2. Root mean square deviation RMSD for the first 20 ns of MD simulation for average structure calculation.

Table S1. ICM energy score for the best 100 hit from virtual screening.

Begin of Table	
ZINC15 id	Score (kcal/mol)
GTP	-27.64327
ZINC04028703	-47.139771
ZINC38145808	-45.671547
ZINC19336068	-44.979202
ZINC19336068	-44.134228
ZINC14824069	-42.93782
ZINC72131066	-42.670437
ZINC19336068	-41.267788
ZINC01531039	-41.213696
ZINC61389537	-40.760124
ZINC13385611	-40.739395
ZINC08764797	-40.055969
ZINC85994780	-39.867146
ZINC15956889	-39.779278
ZINC20112504	-39.353798
ZINC20112501	-38.948174
ZINC70706013	-38.285667
ZINC19336068	-38.136402
ZINC08765165	-38.005142
ZINC70665805	-37.436745
ZINC04061910	-37.341373
ZINC04028701	-37.196304

Continuation of Table S1

ZINC15 id	Score
ZINC03870145	-37.095665
ZINC20112413	-36.982067
ZINC85489989	-36.273315
ZINC35365918	-36.247917
ZINC85509549	-35.961651
ZINC27558828	-35.729488
ZINC35363853	-35.638927
ZINC13783218	-35.60701
ZINC02154275	-35.538185
ZINC12890057	-35.364208
ZINC03984661	-35.360455
ZINC85568960	-35.339859
ZINC95099067	-35.153324
ZINC31156942	-34.981937
ZINC20112388	-34.671345
ZINC08214655	-34.58791
ZINC15957926	-34.518906
ZINC04501392	-34.423988
ZINC04501392	-34.37841
ZINC49543170	-34.348434
ZINC00895180	-34.218311
ZINC40312960	-34.154789
ZINC06624586	-34.142925
ZINC49543372	-34.080452
ZINC40312777	-33.969444
ZINC40312780	-33.945049
ZINC40312441	-33.902905
ZINC00895081	-33.780499
ZINC13460583	-33.716133
ZINC20611409	-33.608517
ZINC11867541	-33.59919
ZINC85507641	-33.556717
ZINC03870145	-33.400269
ZINC01628282	-33.386013
ZINC04029191	-33.353973
ZINC95913918	-33.329704
ZINC85506516	-33.233322
ZINC00895212	-33.085876
ZINC13548192	-33.034981
ZINC20112845	-33.005642
ZINC96222540	-32.85162
ZINC20112987	-32.810581
ZINC00895081	-32.805515
ZINC59777472	-32.789963
ZINC30726567	-32.767242
ZINC85541484	-32.749729
ZINC00057646	-32.733398
ZINC40312957	-32.714645

Continuation of Table S1

ZINC15 id	Score
ZINC98368979	-32.698872
ZINC00895081	-32.678986
ZINC04164596	-32.590797
ZINC38145807	-32.561115
ZINC00895081	-32.549793
ZINC36368084	-32.516823
ZINC12890057	-32.491215
ZINC85507538	-32.419991
ZINC49543329	-32.386856
ZINC40313216	-32.314423
ZINC20112385	-32.311005
ZINC09033627	-32.244923
ZINC06112681	-32.221901
ZINC59587150	-32.219753
ZINC20611262	-32.195625
ZINC40313128	-32.163731
ZINC95098987	-32.112232
ZINC38545590	-32.107368
ZINC12296571	-32.065216
ZINC00895081	-32.045967
ZINC85548977	-31.981853
ZINC95912584	-31.889652
ZINC85568565	-31.822807
ZINC08790482	-31.818468
ZINC70706327	-31.789642
ZINC96222502	-31.707294
ZINC95099065	-31.684559
ZINC20113196	-31.678776
ZINC20611063	-31.675303
ZINC96116292	-31.64535
ZINC12297114	-31.619473

End of Table

Table S2. Result of MM/PBSA calculation from the best 35 ligands from virtual screening from the 10 ns simulation.

Zinc15 id	ΔG
ZINC00895081	-99.4252
ZINC02154275	-26.0056
ZINC03870145	-103.3190
ZINC03984661	-19.7298
ZINC04028701	-119.6044
ZINC04028703	-86.3944
ZINC04061910	-65.4872
ZINC04501392	-121.3924
ZINC06624586	-22.4335
ZINC08764797	-19.9280
ZINC08765165	-37.7270
ZINC13460583	-30.0101
ZINC13783218	-53.0186
ZINC15956889	-12.8434
ZINC15957926	-15.4614
ZINC19336068	-107.8820
ZINC20112413	-86.6941
ZINC20112501	-78.3754
ZINC20112504	-76.4244
ZINC27558828	-101.0158
ZINC35363853	-13.7876
ZINC35365918	-17.0339
ZINC38145808	-42.6426
ZINC40312441	-37.3111
ZINC40312777	-49.1184
ZINC40312780	-34.0688
ZINC40312960	-46.9143
ZINC49543170	-42.5067
ZINC49543372	-32.4974
ZINC61389537	-31.3838
ZINC70665805	-16.5726
ZINC70706013	-48.3709
ZINC72131066	-19.3442
ZINC85509549	-32.3730
ZINC85568960	-55.4133
ZINC95099067	-33.2993