# FUNCTIONAL CHARACTERIZATION OF BIOSYNTHETIC CLASSES THROUGH ACCESSORY MODULES OF BGCs

Example for the Atacama Desert and perspectives for the ocean



## EXAMPLE FOR THE TALABRE-LEJÍA TRANSECT, ANDEAN ATACAMA DESERT



#### 23°50'S 67°69'W

Supplementary Figure 1. Talabre-Lejía transect geographical information. (González, M. et al. (unpublished)).













Biosynthetic class

terpene

T1PKS

T2PKS

T3PKS

hglE-KS







**Figure 4.** Sequence similarity networks of GCFs with at least two members as delivered by BiG-SCAPE.

**Figure 3.** Hierarchical clustering of genomes with antiSMASH results (n=42) based on presence or absence of core specialized capabilities (n=22) over 133 observations. Sites are coloured if relative abundance was above 0.1%.

### Functional characterization of biosynthetic classes through accessory modules of BGCs

biological

function

#### Comments:

Terpenes harbor two different domains related to iron transport, and another one to arsenic regulation.

Regarding carbon metabolism, L-arabinose has been described to inhibit lactose and gluconate mechanisms in E. coli and V. cholerae, respectively. Specifically, when AraC is bounded to its cognate-sugar and CRP is so to cAMP, catabolite repression of other unpreferred non-glucose carbon source occurs. We hypothesize that different regulation triggers among hybrids and terpenes might account for the antagonist way these sugars are consumed.

Periplasmic and extracellular binding proteins cluster with transposases, describing hybrids and bacteriocins.

The only transposase smCOG related to RiPPs in this dataset distinguishes from those in group I with the annotation: IS407A.





#### Figure 5.

Hierarchical clustering of sm-COGs (n=46) assigned to accessory genes based on their presence or absence in BGCs according to their biosynthetic classes (n=6) over 88 observations.



### PERSPECTIVES FOR THE OCEAN Questions we could answer:

- Do specialized metabolites have distinct patterns in the ocean?
- If so, which are common to other environments? Which are specific to our data?
- Is there functional overlap between layers? Which one shows more plasticity?
- What functional signatures serve to separate SRF from DCM samples?
- Which functional signatures can be interpreted as indicators of a healthy ocean? Can we use them to track key environmental shifts?
- Are terpenes related to metal homeostasis in marine bacteria?
- Are bacteriocins and hybrid BGCs related to transposase domains? Where? Are these samples correlated with viral abundancy or diversity?
- What transporters and/or regulators can be found adjacent to specific types of core biosynthetic capabilities in the ocean? Which are widespread in these matters?
- Can we say something about antibiotics? About signalling and sensing? About mechanisms to cope with environmental stresses?
- But first... What do we wanna know?

### PERSPECTIVES FOR THE OCEAN

Article

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### **Biosynthetic potential of the global ocean** microbiome

https://doi.org/10.1038/s41586-022-04862-3	Lucas Paoli <sup>1</sup> , Hans-Joachim Ruscheweyh <sup>1,18</sup> , Clarissa C. Forneris <sup>238</sup> , Florian Hubrich <sup>2,18</sup>					
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Published online: 22 June 2022	Ahmed A. Zayed <sup>9</sup> , Dylan R. Cronin <sup>9</sup> , Silvia G. Acinas <sup>8</sup> , Peer Bork <sup>20,11</sup> , Chris Bowler <sup>12,13</sup> , Tom O. Delmont <sup>13,14</sup> , Josen M. Gasol <sup>8</sup> , Alvar D. Gossert <sup>15</sup> , André Kables <sup>4,5,6</sup>					
Open access	Matthew B. Sullivan <sup>8,16</sup> , Patrick Wincker <sup>13,14</sup> , Georg Zeller <sup>7</sup> , Serina L. Robinson <sup>2,17</sup>					
Check for updates	Jörn Piel <sup>2™</sup> & Shinichi Sunagawa <sup>1™</sup>					

nature climate change

ARTICLES https://doi.org/10.1038/s41558-022-01314-8

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#### Restructuring of plankton genomic biogeography in the surface ocean under climate change

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Actinobacteriota Proteobacteria

Firmicutes

Cyanobacteria

Bacteroidota

Chloroflexota Verrucomicrobiota Planctomycetota

REFs/SAGs only

REFs/SAGs and MAGs

Thermoplasmatota Marinisomatota







Heatmaps for relative abundances of TGs according to the TFs they are regulated by per layer: SRF DCM MES



#### SHAPIRO

### ANOVA

	LAYERS			
*	*	*		
rejected	rejected	rejected		
**	rejected	***		
rejected	*	rejected		
*	rejected	*		
rejected	**	*		
*	rejected	*		
	LAYERS			
BirA	FabR	LiuR		
TyrR		MetR		
	GulR			
LexA		NsrR		
	FUR	NagC		
PhnF		SahR_SamR		

	SRF.DCM					
rejected	*	rejected				
rejected	rejected rejected					
rejected	*** rejected					
*	rejected	rejected				
rejected	***	rejected				
rejected	*	**				
rejected	*	rejected				
	SRF.DCM					
	FabR					
	HrcA					
FadR						
	PurR:rejected					
	FUR:rejected	NagC				
	GntR					

TUKEY

	SRF						
BirA	FabR	LiuR		DCM			
TyR	GulR	MetR					
LexA	FUR	NsrR					
PhnF	SahR	NagC					
						MES	
						WE3	



## COMPARATIVE APPROACHES AND CATEGORICAL VARIABLES: TODAY'S KEYS TOWARDS FUNCTIONAL CHARACTERIZATION

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Keller-Costa *et al. Microbiome* (2021) 9:72 https://doi.org/10.1186/s40168-021-01031-y

#### RESEARCH

#### Microbiome Open Access

### Metagenomic insights into the taxonomy, function, and dysbiosis of prokaryotic communities in octocorals

T. Keller-Costa<sup>1\*</sup>, A. Lago-Lestón<sup>2\*</sup>, J. P. Saraiva<sup>3</sup>, R. Toscan<sup>3</sup>, S. G. Silva<sup>1</sup>, J. Gonçalves<sup>4</sup>, C. J. Cox<sup>4</sup>, N. Kyrpides<sup>5</sup>, U. Nunes da Rocha<sup>3</sup> and R. Costa<sup>1,4,5</sup>









## FUNCTIONAL CHARACTERIZATION: **EXAMPLE OF ECOLOGICAL INSIGHTS**

# 

Community-

weighted trait

Genome size CRISPR

Coding density

No till

Till

BGCs

rrn

www.nature.com/ismecomm Geodermatophilaceae Plant Check for updates ARTICLE **OPEN** Sphingomonas association Chthoniobacter Ecological insights into soil health according to the genomic KD4-96 Gaiella traits and environment-wide associations of bacteria in Ca. Udaeobacter Associated with bulk soil agricultural soils Associated with **lower** disturbance В Roland C. Wilhelm<sup>1<sup>™</sup></sup>, Joseph P. Amsili<sup>1</sup>, Kirsten S. M. Kurtz<sup>1</sup>, Harold M. van Es<sup>1</sup> and Daniel H. Buckley<sup>1</sup> © The Author(s) 2023 Biological Physical Disturbance Active ACE Org. carbon protein matter lealth Water cap. Agg. stabil. Surf. hard. Sub. hard DNA Respir score -0.444 -0.302 -0.218 -0.195 -0.306 -0.141 -0.192 -0.165 -0.322 -0.337 -0.149 -0.3 -0.199 -0.31 -0.316 -0.165 Associated with higher disturbance -0.146 -0.316 -0.316 Associated with conservation practices 0.126 -0.152 0.16 gei Health score rrn copy number Genome size r = -0.44; p < 0.001 mean (Mb) \*\*\* Siz Veighted Management gei (Mb) Associated with conventional practices 250 750 1000 125 -1.0-0.5 0.5 1.0 n Total active carbon (mg C · kg<sup>-1</sup> of soil) ndicator statistic No till Till No till Till

Associated with rhizosphere

## FUNCTIONAL CHARACTERIZATION: EXAMPLE OF EVOLUTIONARY INSIGHTS



## FUNCTIONAL CHARACTERIZATION: CAPITALIZATION OF PUBLIC DATABASES









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