

2 Choose the tab according to the data you want to start with, e. g. Genomics data

Genomics -> Metabolomics

Metabolomics -> Genomics

3 Filter data using filters (optional)

Genomics filter

GCF ID



Type



Foldable tab

GCF ID



Enter one or more GCF IDs

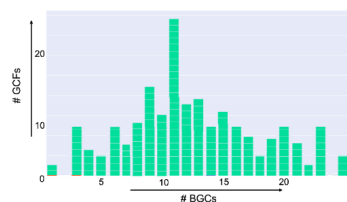


Type



Enter one or more compound types

4a Inspect the data (optional)



histogram or violin plot will be interactive, and it will be possible to identify GCFs corresponding to a certain number of BGCs

4b Select data

Data		2 GCFs selected
<input type="checkbox"/>	GCF ID	# BGC
<input checked="" type="checkbox"/>	1	3
<input type="checkbox"/>	2	1
<input type="checkbox"/>	3	10
<input checked="" type="checkbox"/>	4	6

Rows per page 20 <>

This format indicates hyperlinks

5 Set scoring methods and parameters (optional)

Scoring

Metcalf

☒ RAW ☐ STANDARDIZED

Cutoff

1

☒ Rosetta

Spectral score cutoff

0

BGC score cutoff

0

Logical operation between scoring methods

☐ AND ☒ OR

All cutoff forms display default value or valid value range

The operation option appears only when users set two or more scoring methods

6 Click to show the links found

Show spectra

Candidate Links

7 Inspect the results

Select columns

GCF ID	# links	Top 1 spectrum	Product	Score
1	300	100	xxx	0.8
4	20	20	yyy	0.6
3	400	45	zzz	0.5

Rows per page 3 <>

- ☒ GCF ID
- ☒ # links
- ☒ Top 1 Spectrum
- ☒ Product
- ☒ Score
- ☐ Predicted BGC class
- ☐ Taxonomy

Apply

GCF Viewer - When click or over

When click or over

Spectrum Viewer - When click or over

When click or over

GCF 1

GCF ID: 1
Class: PKS-NRP_Hybrids
Strains: Salinispora arenicola CNQ748
BigFam ID: xxx (if exists)

BGC name	Product	Hybrid?
BGC 1		
BGC 2		
BGC 3		

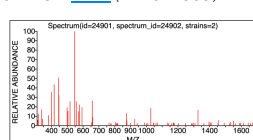
All links for GCF 1

Spectra	Product	Score
100		0.8
23		0.79
47		0.78

Rows per page 3 <>

Spectrum 100

Spectrum ID: 100
Precursor mz: 718.28
Parent mz: 717.27
Strains: Salinispora arenicola
GNPS hit: [link](#) (if exists)



Scores

Merged score: 0.6
Metcalf score: 0.45
Rosetta score: 0.52

Also NPClassScore will be here after having added it to the code-base

There will be a ranking algorithm for merging different scores values.

BGC table - When click or over

BGC name	Product	Hybrid?
BGC 1		
BGC 2		
BGC 3		

BGC 1, BGC 2, ... link to MiBig and/or BigFam, if any

2 Choose the tab according to the data you want to start with, e. g. Metabolomics data

Genomics -> Metabolomics

Metabolomics -> Genomics

3 Filter data using filters (optional)

Metabolomics filter

MF ID ☒Spectrum ID ☒

MF ID

Enter one or more Molecular Family IDs

+

Spectrum ID

Enter one or more Spectrum IDs

4 Select data

Data

2 MFs selected

<input type="checkbox"/>	MF ID	Spectrum ID
<input checked="" type="checkbox"/>	1	45
<input type="checkbox"/>	2	3
<input type="checkbox"/>	3	7
<input checked="" type="checkbox"/>	4	67

Rows per page 20 < >

5 Set scoring methods and parameters (optional)

Scoring

Metcalf

☒

RAW

☐

STANDARDIZED

Cutoff

1

+

Rosetta

Spectral score cutoff

0

BGC score Cutoff

0

Logical operation between scoring methods ☐ AND ☒ OR

6 Click to show the links found

Show GCFs

Candidate Links

7 Inspect the results

Select columns

MF ID	Spectrum ID	# links	Top 1 GCF	Product	Score
1	45	14	4	xxx	0.8
12	4	200	56	yyy	0.6
4	67	98	2	zzz	0.5

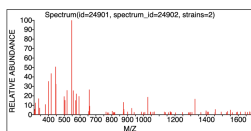
Rows per page 3 < >

Spectrum Viewer

GCF Viewer

Spectrum 45

Spectrum ID: 45
Precursor mz: 718.28
Parent mz: 717.27
Strains: *Salinispora arenicola*
GNPS hit: [link](#) (if exists)

All links for MF 1, [Spectrum 45](#)

GCF ID	Product	Score
4		0.8
10		0.79
12		0.78

Rows per page 3 < >

GCF 4

GCF ID: 4
Class: PKS-NRP_Hybrids
Strains: *Salinispora arenicola*
CNQ748
BigFam ID: xxx (if exists)

BGC name	Product	Hybrid?
BGC_1		
BGC_2		
BGC_3		

Scores

Merged score: 0.8
Metcalf score: 0.84
Rosetta score: 0.79