

Actinomycete BGC ? Metabolomics Mini-Pipeline Report

Run Metadata

- Generated at: 2025-10-03T19:00:27.095345 UTC

Methods

Methods Documentation / ????

> ???

> English: This document will be referenced in the final report, detailing data sources, processing steps, scoring rules, and limitations.

Data Sources / ????

- TODO: antiSMASH / DeepBGC / PRISM ???????
- TODO: LC-MS/MS ???????
- TODO: NPAtlas/MIBiG ??????

Processing Steps / ????

- TODO: BGC ??????
- TODO: LC-MS/MS ?????
- TODO: ?????????
- TODO: ?????????
- TODO: ?????????
- TODO: ADMET ?????????

Parameters & Versions / ????

- TODO: ?????????????????????

Limitations & Future Work / ???????

- TODO: ?????????????????????

Top Candidates

Top Candidates

- ```
- **Rank 1** ? Compound CMP001 | Score: 0.760 | ADMET: Pass | Cluster: CLUSTER_001
- **Rank 2** ? Compound CMP002 | Score: 0.760 | ADMET: Pass | Cluster: CLUSTER_002
- **Rank 3** ? Compound CMP003 | Score: 0.760 | ADMET: Pass | Cluster: CLUSTER_003
- **Rank 4** ? Compound <NA> | Score: 0.400 | ADMET: Pass | Cluster: nan
```

## ## Figures

- cluster\_sizes.csv
- cluster\_summary.txt
- top\_scores.png

## ## Ranking Snapshot

| CompoundID                                               | EvidenceScore | EvidenceCount  | BGCUIDs                               |                 |                  |              |                |             |             |     |
|----------------------------------------------------------|---------------|----------------|---------------------------------------|-----------------|------------------|--------------|----------------|-------------|-------------|-----|
| FeatureIDs                                               | logP          | TPSA           | HBD                                   | HBA             | MW               | ToxicityFlag | RuleOfFivePass | ClusterID   | ClusterSize |     |
| Novelty                                                  | ADMETScore    | AggregateScore | Rank                                  | EvidenceSummary |                  |              |                |             |             |     |
| CMP001                                                   | 0.6           | 1              | SampleA_BGCUID_001                    |                 |                  |              |                |             |             |     |
| F001 F002 F003                                           | 1.00          | 48.0           | 4.0                                   | 8.0             | 166.0            | Low          | True           | CLUSTER_001 | 1.0         | 1.0 |
| 1.0                                                      | 0.76          | 1              | 1                                     | evidence links  |                  |              |                |             |             |     |
| CMP002                                                   | 0.6           | 2              | SampleA_BGCUID_001 SampleA_BGCUID_002 |                 |                  |              |                |             |             |     |
| F001 F002 F003                                           | 1.25          | 36.0           | 3.0                                   | 6.0             | 190.0            | Low          | True           | CLUSTER_002 | 1.0         |     |
| 1.0                                                      | 1.0           | 0.76           | 2                                     | 2               | evidence links   |              |                |             |             |     |
| CMP003                                                   | 0.6           | 1              | SampleA_BGCUID_001                    |                 |                  |              |                |             |             |     |
| F001 F002 F003                                           | 1.25          | 60.0           | 5.0                                   | 10.0            | 206.0            | Low          | True           | CLUSTER_003 | 1.0         | 1.0 |
| 1.0                                                      | 0.76          | 3              | 1                                     | evidence links  |                  |              |                |             |             |     |
|                                                          | NaN           |                |                                       |                 |                  | 0.5          |                |             |             | 9   |
| SampleA_BGCUID_001 SampleA_BGCUID_002 SampleB_BGCUID_001 |               |                |                                       |                 |                  |              |                |             |             |     |
| F001 F002 F003 F004 F005 F006                            | NaN           | NaN            | NaN                                   | NaN             | NaN              | NaN          | NaN            | NaN         | NaN         |     |
| NaN                                                      | 1.0           | 0.0            | 0.40                                  | 4               | 9 evidence links |              |                |             |             |     |