



## INTEGRATED GENOME MINING AND MALDI-TOF-MS FOR THE PROSPECTION OF BIOACTIVE METABOLITES OF *BACILLUS SP.*

***Maria José de Oliveira Pessoa***<sup>1\*</sup>, *Clara Detúlio Martins Cavalcante*<sup>1</sup>, *Júlia Firme Freitas*<sup>2</sup>,  
*Lucymara Fassarella Agnez-Lima*<sup>2</sup>, *Renata Mendonça Araujo*<sup>1</sup>

maria.pessoa.117@ufrn.rdu.br

*1-Lisco, Instituto de Química, CCET, UFRN, Campus Universitário, 59078-970, NATAL, RN, Brazil.*

*2-LBMG, Centro de Biociências, Campus Universitário, 59078-970, NATAL, RN, Brazil.*

*Bacillus* species are promising sources of bioactive secondary metabolites, particularly non-ribosomal lipopeptides and polyketides. In this study, genome mining performed using the AntiSMASH platform was integrated with MALDI-TOF-MS analyses to explore the metabolic potential of a *Bacillus sp.* strain isolated from petroleum-contaminated sand sediments. Genome mining of *Bacillus amyloliquefaciens* BG1 revealed biosynthetic gene clusters (BGCs), including those related to the production of non-ribosomal lipopeptides, ribosomal peptides, and polyketides, previously associated with antimicrobial and antifungal activities. The presence of multiple NRPS and PKS systems highlights the high biosynthetic potential of the strain investigated. Comparative analysis between AntiSMASH predictions and MALDI-TOF-MS spectra of the ethyl acetate extract revealed mass peaks consistent with genomically predicted metabolites.  $[M+H]^+$  ions were putatively annotated as compatible with aurantini B ( $m/z$  780.4732), surfactin ( $m/z$  1035.5732), surfactin C ( $m/z$  1021.5512), iturin A-7 ( $m/z$  1070.5092), iturin C/bacillomycin D ( $m/z$  1043.5292), and paenilarvin A ( $m/z$  1111.4652), corroborating the correlation between genomic predictions and metabolic expression. These findings demonstrate that the integration of genome mining with mass spectrometry represents a rapid and targeted strategy for the prospecting of secondary metabolites with potential biotechnological applications. The results highlight the *Bacillus* strain studied as a promising candidate for future purification, structural elucidation, and biological activity evaluation studies.

**Keywords:** *Bacillus*, Genome mining, Mass spectrometry, Bioactive metabolites, Peptide

**Acknowledgments:** Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Programa de Pós-graduação em Química (PPGQ-UFRN) Laboratório de Isolamento e Síntese de Compostos Orgânicos (LISCO-UFRN), Laboratório de Biologia Molecular e Genômica (LBGM-UFRN), and Central de Espectrometria de Massas de Micromoléculas Orgânicas (CEMMO-USP/Ribeirão Preto).

### References

Saiyam, D. *et al.* Lipopeptides from *Bacillus*: unveiling biotechnological prospects—sources, properties, and diverse applications. **Braz J Microbiol** 55, 281–295 (2024). <https://doi.org/10.1007/s42770-023-01228-3>

Wang, Z. *et al.* Analysis of antimicrobial biological activity of a marine *Bacillus velezensis* NDB. **Arch Microbiol** 206, 131 (2024). <https://doi.org/10.1007/s00203-024-03861-4>

