

antiSMASH 4.0 — Improvements in Chemistry Prediction and Gene Cluster Boundary Identification.

Blin K, Wolf T, Chevrette M, Lu X, Schwalen C, Kautsar S, Suarez Duran, H, de los Santos E, Kim HU, Nave M, Dickschat J, Mitchell D, Shelest E, Breitling R, Takano E, Lee SY, Weber T, Medema M (2017) antiSMASH 4.0 — Improvements in Chemistry Prediction and Gene Cluster Boundary Identification. *Nucleic Acids Res* 45(W1), W36-W41.

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Abstract

Many antibiotics, chemotherapeutics, crop protection agents and food preservatives originate from molecules produced by bacteria, fungi or plants. In recent years, genome mining methodologies have been widely adopted to identify and characterize the biosynthetic gene clusters encoding the production of such compounds. Since 2011, the 'antibiotics and secondary metabolite analysis shell-antiSMASH' has assisted researchers in efficiently performing this, both as a web server and a standalone tool. Here, we present the thoroughly updated antiSMASH version 4, which adds several novel features, including prediction of gene cluster boundaries using the ClusterFinder method or the newly integrated CASSIS algorithm, improved substrate specificity prediction for non-ribosomal peptide synthetase adenylation domains based on the new SANDPUMA algorithm, improved predictions for terpene and ribosomally synthesized and post-translationally modified peptides cluster products, reporting of sequence similarity to proteins encoded in experimentally

characterized gene clusters on a per-protein basis and a domain-level alignment tool for comparative analysis of trans-AT polyketide synthase assembly line architectures. Additionally, several usability features have been updated and improved. Together, these improvements make antiSMASH up-to-date with the latest developments in natural product research and will further facilitate computational genome mining for the discovery of novel bioactive molecules.

Involved units

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