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Primer

Peptidomics

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Supplementary Information

Peptidomics

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Supplementary Table 1: Full list of databases and tools. Databases and tools marked with an asterisk are commercial platforms and maybe subject to licensing charges. DNA, deoxyribonucleic acid; RNA, ribonucleic acid; AA, amino acids; BGC, biosynthetic gene cluster

Databases:			
Database	**Use case**	**Data available**	**Key features**
EMBL-EBI	Biological sequences	DNA, RNA, AA	Repository of biological sequence data for model organisms
DDBJ	Biological sequences	DNA, RNA, AA	Repository of genomic sequence data
MIBiG	Biological sequences	BGCs	Repository containing biosynthetic gene clusters for natural products
VEuPathDB	Biological sequences	DNA, RNA, AA	Vector and host informatics resource
AntiBase*	Physico-chemical data	Spectra database	Database of over 48,000 natural products and their structures
Bactibase	Biological sequences	AA	Dedicated repository for bacteriocins
Conoserver	Biological sequences	DNA, AA	Dedicated repository for conotoxins
CyBase	Biological sequences	DNA, AA	Dedicated repository for circular peptides
Software:			
Tool	**Use case**	**Input data**	**Key Features**
EvoMining	RiPPs & NRPs	DNA	Phylogenetic genome mining
RODEO	RiPPs	Protein accession numbers	Gene neighborhood analysis on multiple RiPP clusters
BAGEL	RiPPs	DNA	Rule based detection of RiPPs
SPADA	sORFs	DNA	Identification of small, one or two exon genes
miPepid	sORFs	DNA/RNA	Identification of sORFs from DNA/RNA sequences
DeepCPP	sORFs	RNA	Novel feature selection for sORFS with good coverage
rAMPage	Antimicrobial peptides	RNA	Antimicrobial peptide detection in RNA-seq data
Comparative genomics tools:			
CoGE	Identification of homologs	DNA	Suite of various tools for comparative genomics
EDGAR	Identification of homologs	DNA	Comparative genomics and phylogenomics
Mapping to Genome tools:			

PoGo	PeptidoGenomic	Peptide seq + PSM	Fast mapping of peptides to genome coordinates
NERPA	NRPs	DNA + SMILES	Mapping of NRPs to biosynthetic gene clusters
BioCAT	NRPs	DNA + SMILES	Mapping of NRPs to biosynthetic gene clusters
Peptidogenetic pipelines:			
MetaMiner	RiPPs	DNA+LC-MS/MS data	Large scale screening for RiPP discovery (GNPS-framework)
DeepRiPP	RiPPs	DNA (ORF)	Classification, processing and spectral matching
Mass spectrometry analysis:			
Dereplicator+	RiPPs & NRPs	LC-MS/MS data	Natural product identification from MS spectra (GNPS-framework)
VarQuest	RiPPs & NRPs	LC-MS/MS data	Natural product identification from MS spectra (GNPS-framework)
MZmine3	MS data analysis	LC-MS/MS data	Visualisation and analysis of MS data
pacMass	Elemental composition	m/z, z, number of sulphur atoms	Prediction of elemental components for proteins and peptides
MS-FINDER	MS data analysis	EI-MS, GC-MS, MS/MS	Formula predictions, fragment annotations and structure elucidation
metaspace	MS data analysis	LC-MS/MS data	Metabolite annotation from high-resolution spectra
cyclobranch 2	NRPs	LC-MS, MSI, MS/MS	De-novo sequencing of NRPs from spectra
PEAKS Studio*	MS data analysis	MS data	De novo and database searching, post-translational modification assignment, protein quantitation
MaxQuant	Quantitative	MS data	Quantitative proteomics tool
TPP	MS data analysis	LC-MS/MS data	Data processing pipeline for large-scale proteomics/peptidomics, qualitative and quantitative
Skyline	MS data analysis	LC-MS/MS data	Open source platform for qualitative and quantitative peptide analysis
Spectronaut*	MS data analysis	LC-MS/MS data	Quantitative proteomics platform
DIA-NN	MS data analysis	LC-MS/MS data	DIA analysis using neural networks for signal selection, quantification, and interference correction
OpenSWATH	MS data analysis	LC-MS/MS data	Analysis platform for DDA/DIA proteomics data
MS-imaging tools:			
MassImager	MS data analysis	MS-imaging	MS-imaging platform with automatic pattern recognition