



Data updates on Norine, the reference Non-Ribosomal Peptide knowledge base

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Data updates on Norine, the reference Non-Ribosomal Peptide knowledge base

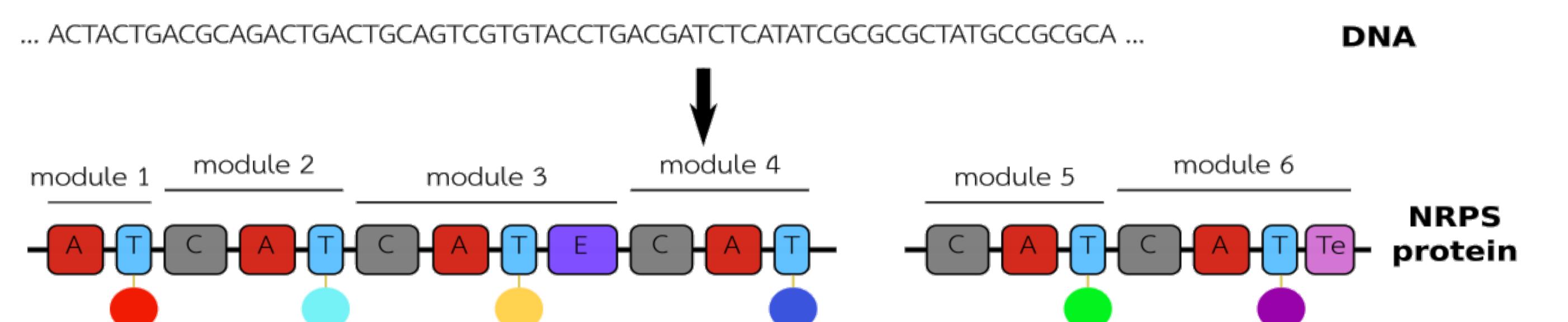
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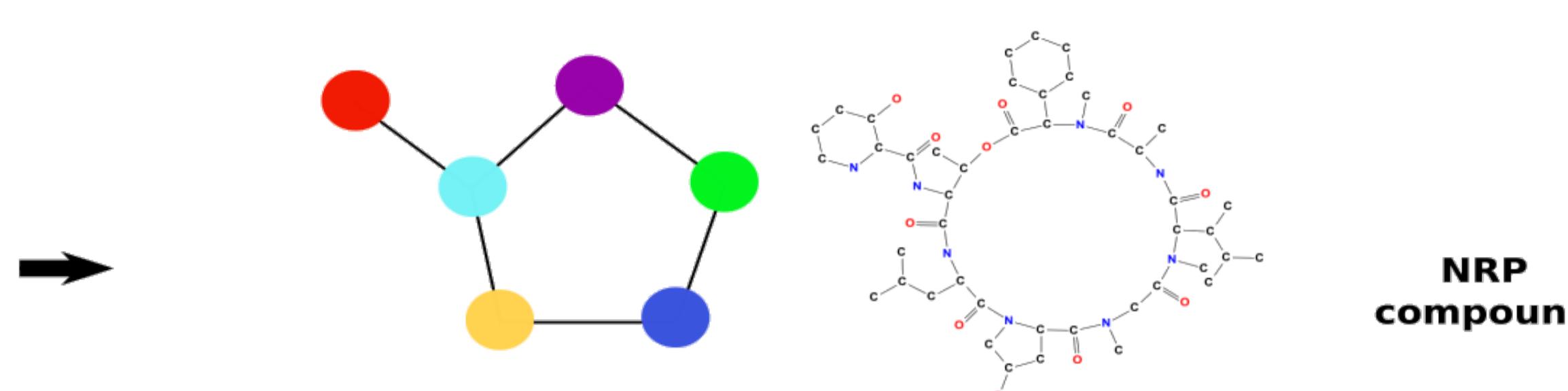
The Nonribosomal Peptides (NRP) pathway

Biological pathway



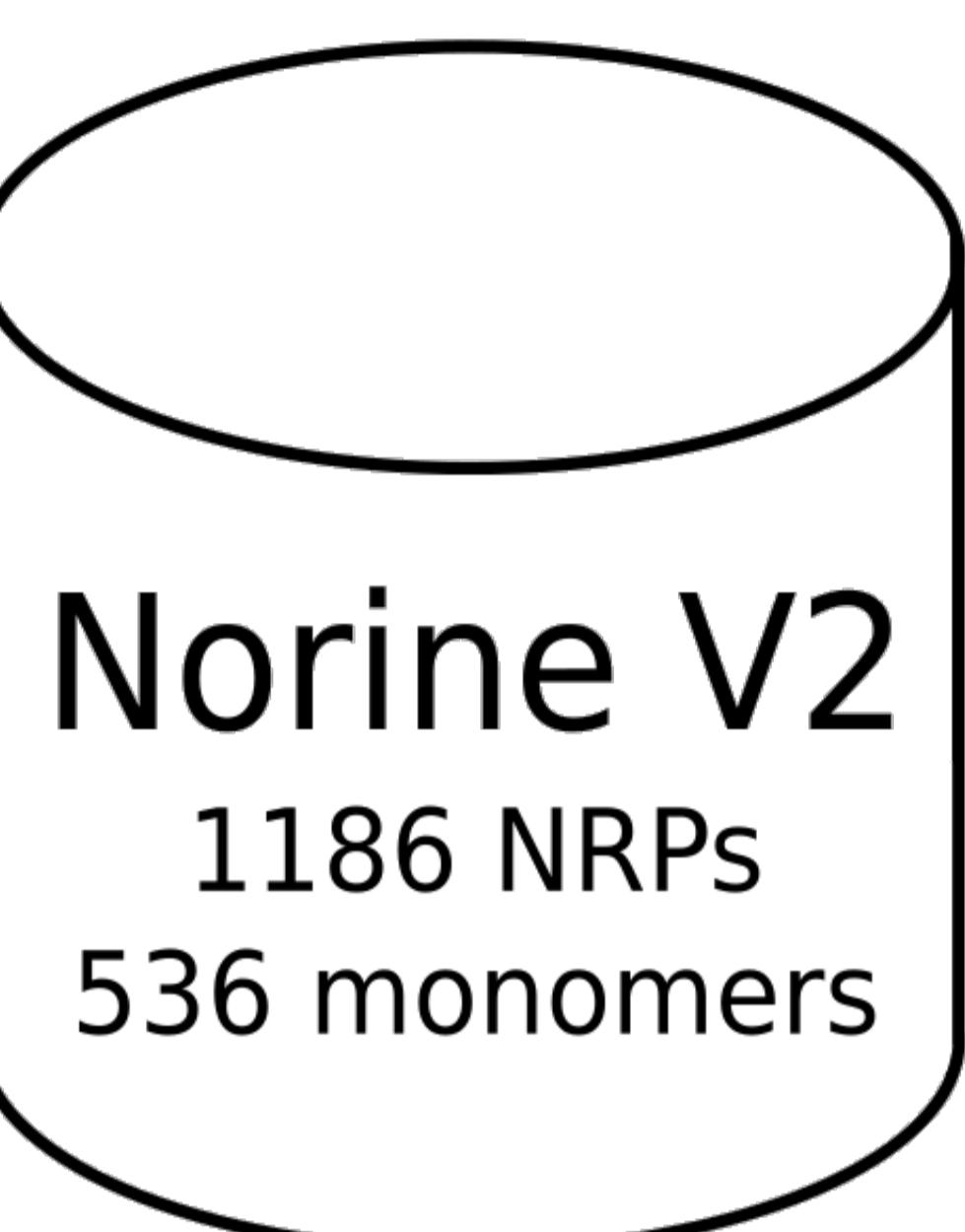
Non Ribosomal Peptides (NRP) are small polymers synthesised by enzymes. The enzymes (called Non Ribosomal Peptide Synthetases (NRPS)) are modular proteins grouped in complexes that select monomers and create NRP. One complex only creates one kind of NRP. The study of the proteic sequence of NRPS and the analysis of mass spectra led to discover hundreds of these molecules.

Compounds and interest



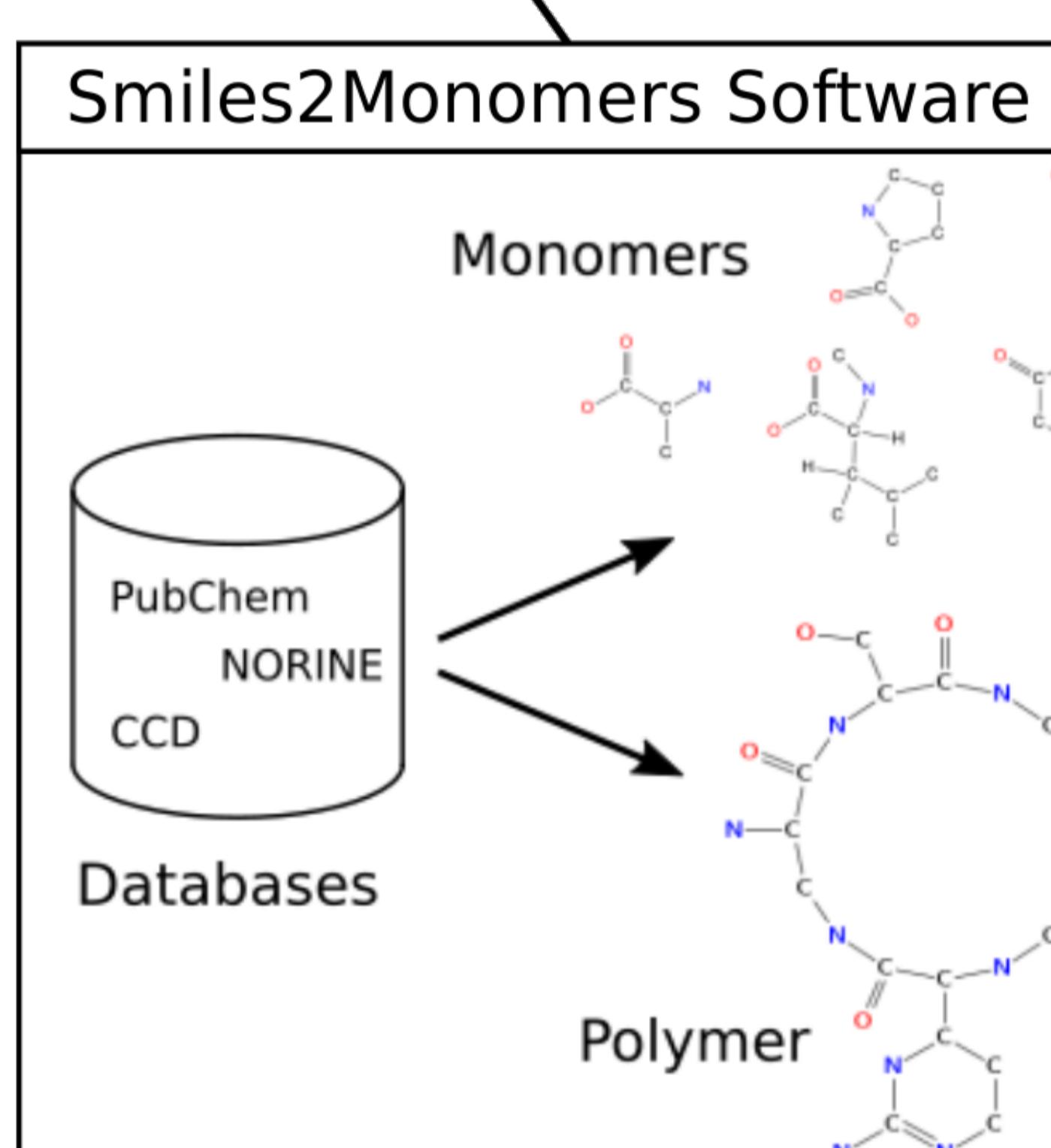
The NRPs are very interesting because of their particular structures and compositions. They are composed of many different monomers (more than 500) organized in various structure conformations (cycles, branches and mix of them). These particularities lend them many unique interesting activities.

Data update in Norine



Norine V2

- Reference knowledge-base for NRPs since 2009
- Manually curated annotations
- Open to expert sourcing by user-friendly forms
- But several NRPs are missing



109 detected
89 remaining
10 equivalences

Structure error detection

- 109 inconsistencies between the monomeric structures stored in Norine and the ones predicted by s2m from atomic structures.
- 20 have been manually corrected until now.

Automatic extraction from specialised databases

We develop scripts to extract known NRPs and fill up Norine

+472 NRP

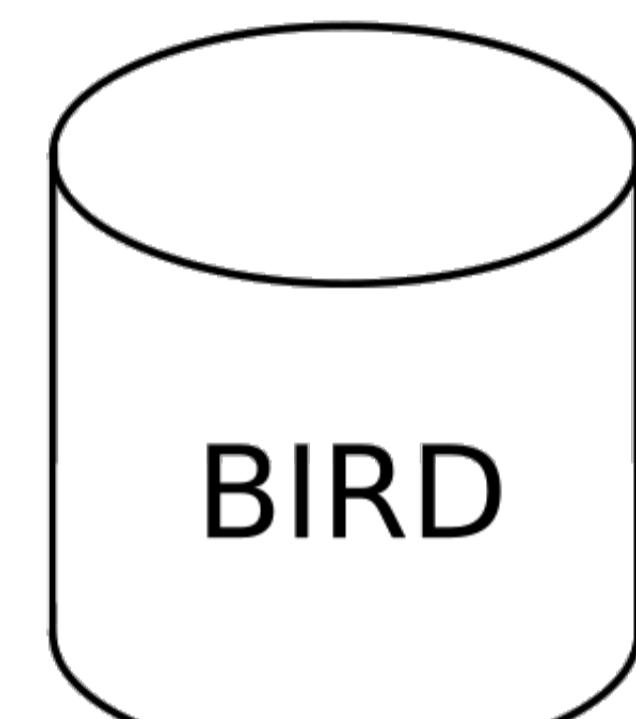
Third-party databases



Other databases store NRPs, among other molecules



PubChem
Information on the biological activities of small molecules

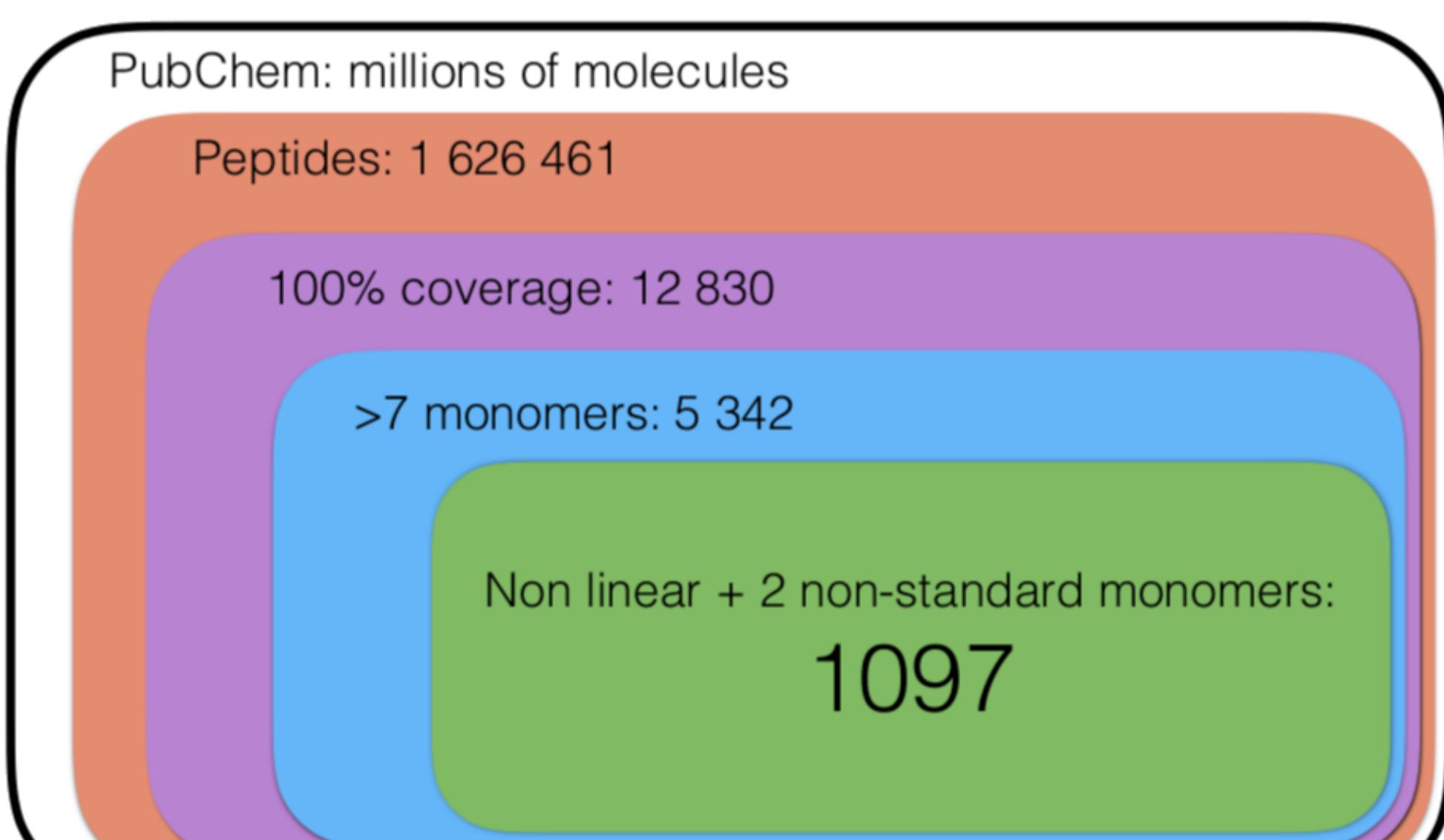


BIRD (wwPDB)
information about biologically interesting peptide-like antibiotic and inhibitor molecules in the PDB archive



Norine V3

- +30% NRP
- Better quality than ever
- s2m to correct error before its appended



Proof of concept to screen chemical databases

- PubChem contains many NRPs but they are not annotated
- We use s2m to annotate their structures and then detect NRP candidates

If I'm not in front of this poster and you want to contact me / you have questions :

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