

Visualization and edition of polymers with non linear structures

Maude Pupin

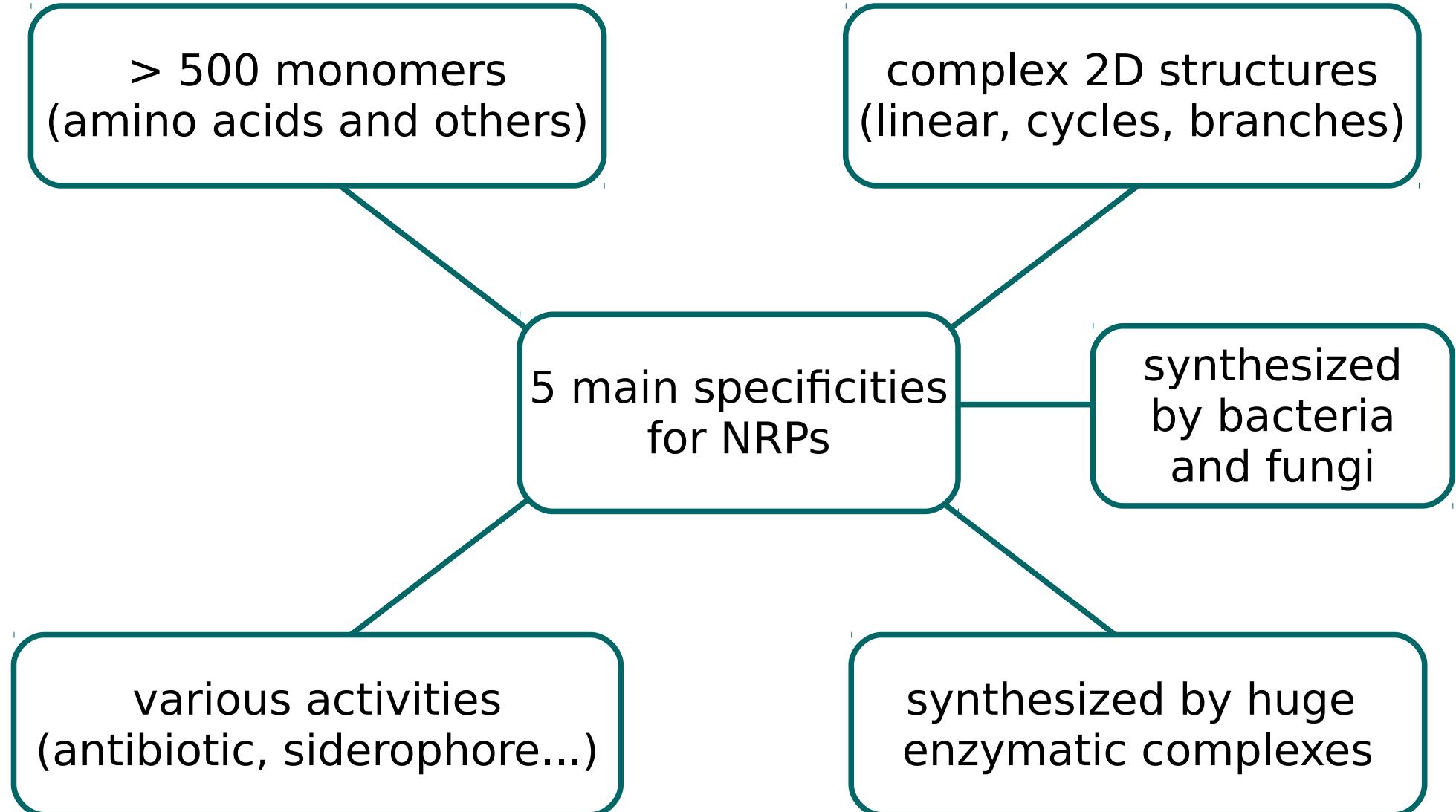
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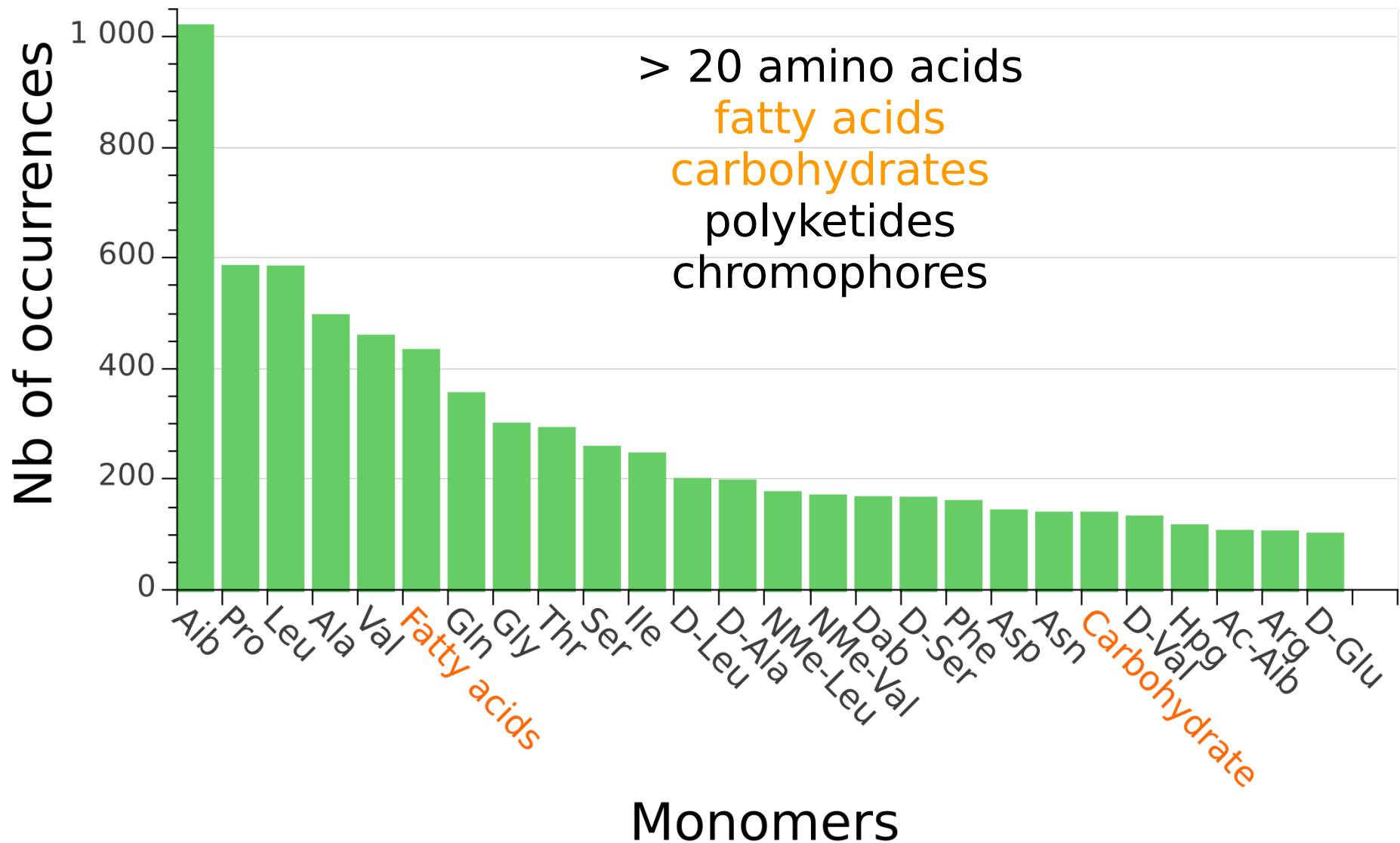
Outline

- Tool design for nonribosomal peptides
 - Extensible to any complex polymer
- Context
 - What are nonribosomal peptides ?
- Structure representations
- Tools
- Conclusion and future work

What are nonribosomal peptides ?

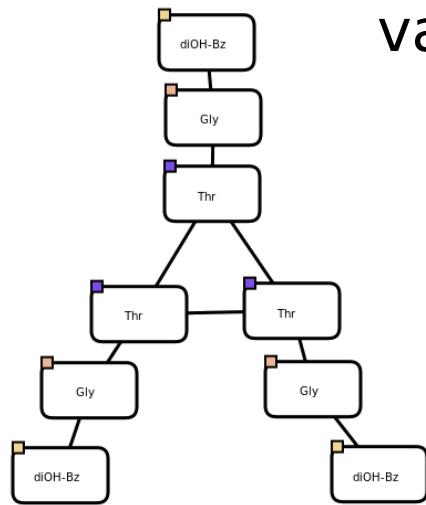


What are nonribosomal peptides ?



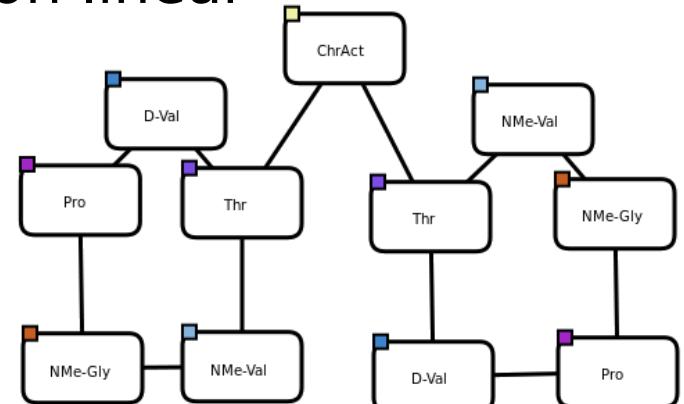
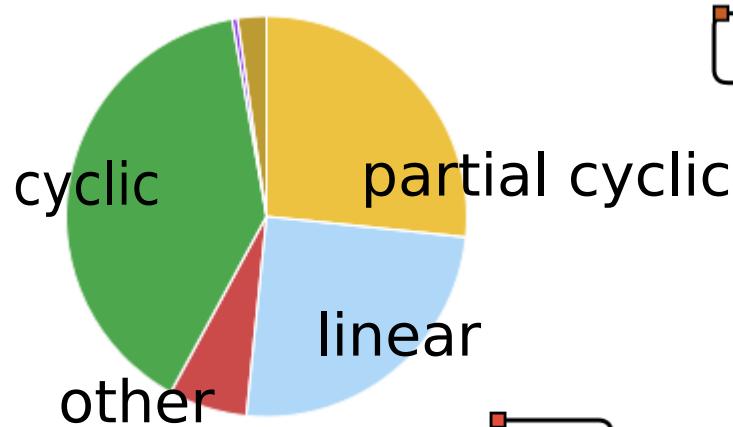
What are nonribosomal peptides ?

various 2D structures, mainly non linear

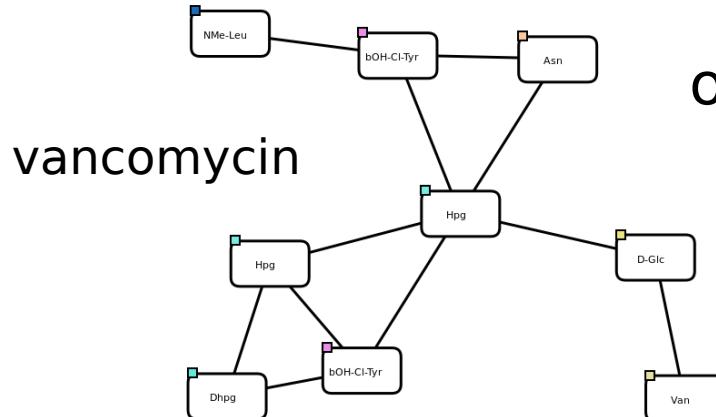


bacillibactin

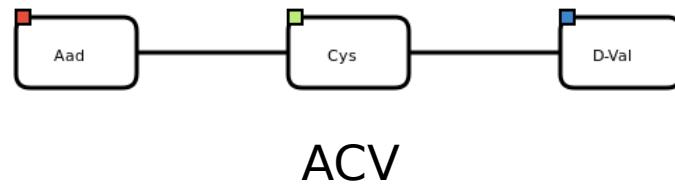
branched double cyclic



actinomycin D



vancomycin



ACV

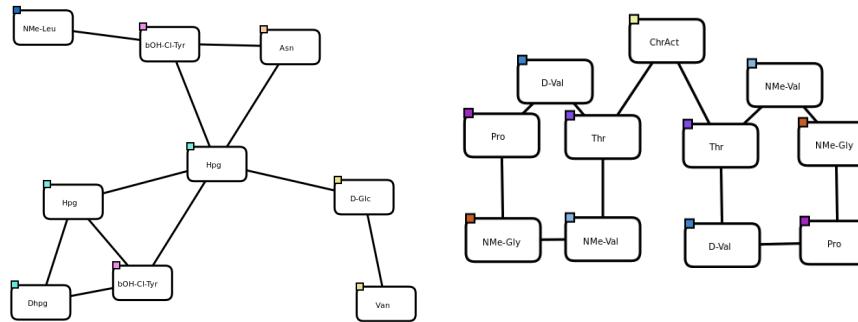
Specific needs for interesting peptides



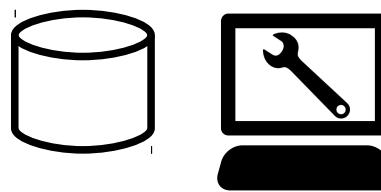
Biological interest:
unusual peptides



<http://bioinfo.lifl.fr/norine/>



Computer science interest:
need for specific algorithms

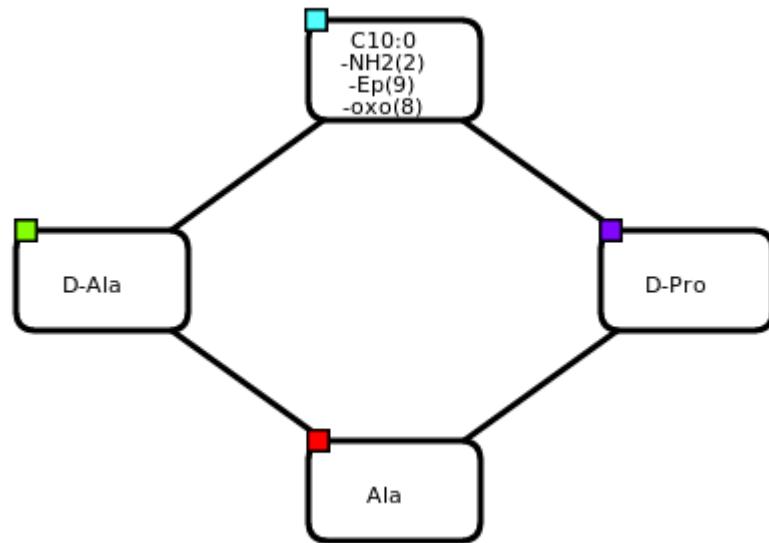


no existing
tools

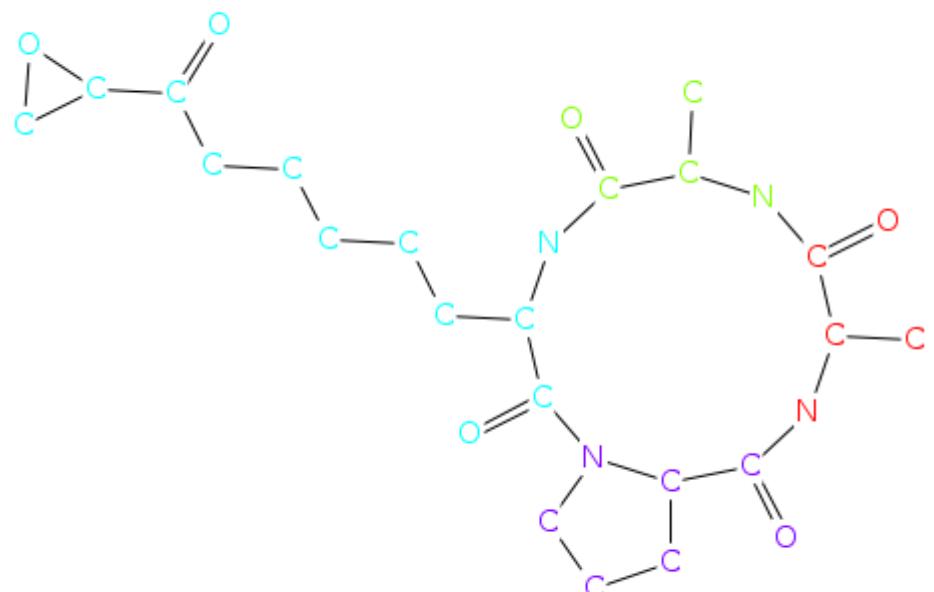


Norine: 4 structure representations

Monomeric structure



Atomic structure

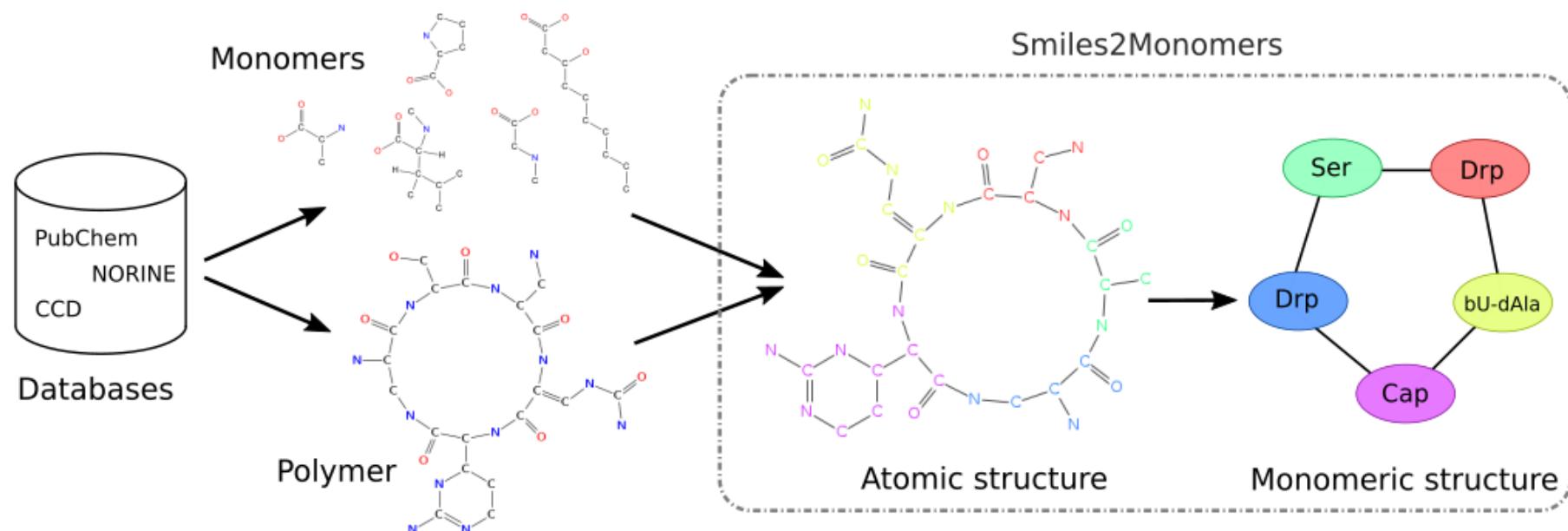


Textual representation for both structures

D-Pro, Ala, D-Ala, C10:0-NH2(2)-Ep(9)-oxo(8)@1,3@0,2@1,3@0,2
CC2NC(=O)C(C)NC(=O)C3CCCN3(C(=O)C(CCCCCC(=O)C1CO1)NC2(=O))

smiles2monomers

From the chemical structure to the monomeric structure



Monomeric editor

peptide(s) containing the structural pattern: Val,Orn,Leu,D-Phe,Pro@1@0,2@1,3@2,4@3

Open the graphical editor [?]

pro

- ▲ XPro
- ▲ Pro*
- 4oxo-Pro
- 4oxo-5Me-Pro
- 4Me-Pro
- D-Pro
- 5Me-Pro
- 4OH-Pro
- 3OH-Pro
- 3OH-5Me-Pro
- Ac-Pro
- 3Me-Pro
- Pro
- ProC
- NFo-Pro
- Cl2-Pro
- D-4OH-Pro

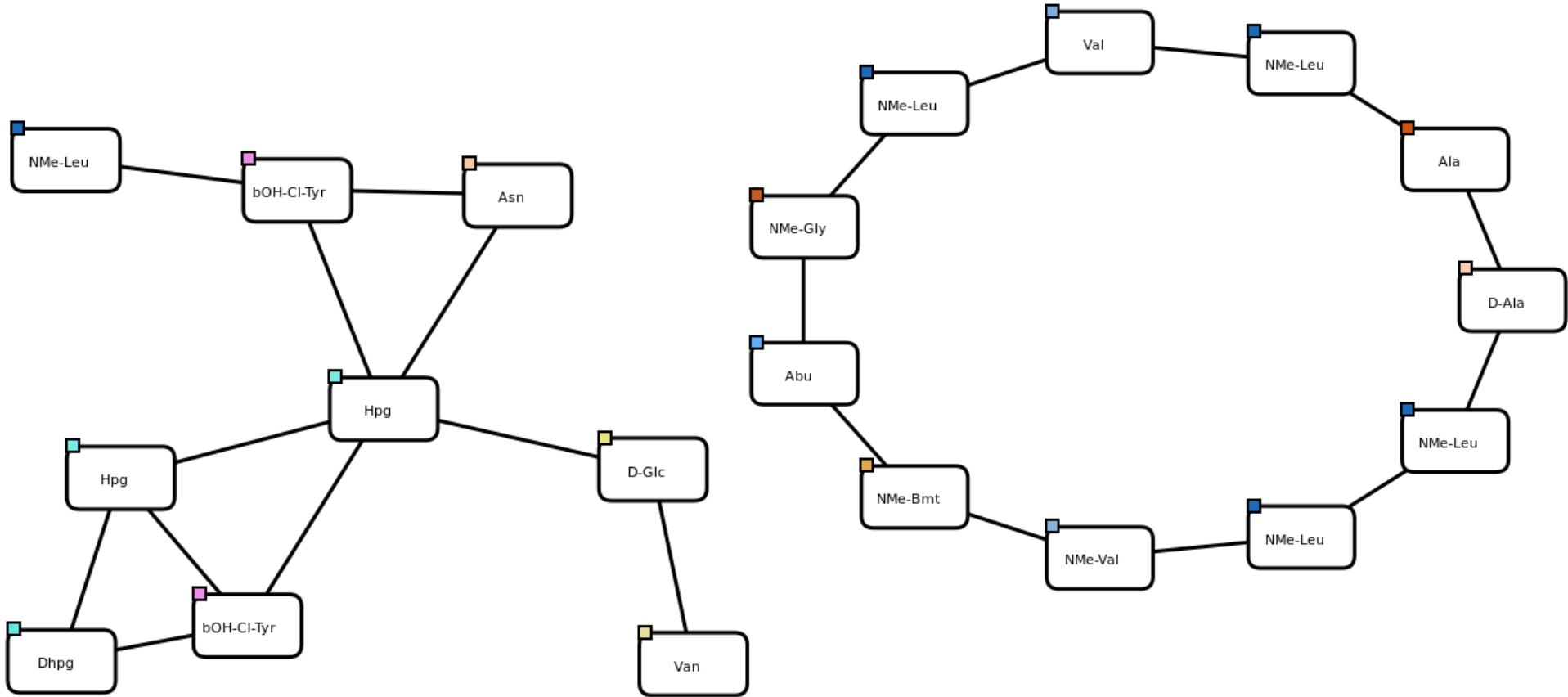
Clear

```
graph LR; Val[Val] --- Orn[Orn]; Orn --- Leu[Leu]; Leu --- D_Phe[D-Phe]; D_Phe --- Pro[Pro]
```

Redraw Clear

Val,Orn,Leu,D-Phe,Pro@1@0,2@1,3@2,4@3 Close

Monomeric visualisation



Algorithm for graph drawing
Specific strategies for simple structures

Conclusion and future work

- Visualization and edition of any polymers
- Source code available
 - <https://github.com/JurMich/EditORINE>
 - used in Norine
- Extension to edition of atomic structures drawn with monomers
- Interaction with HELM notation + Pistoia Alliance Public resources or BIRD (PDB peptides)



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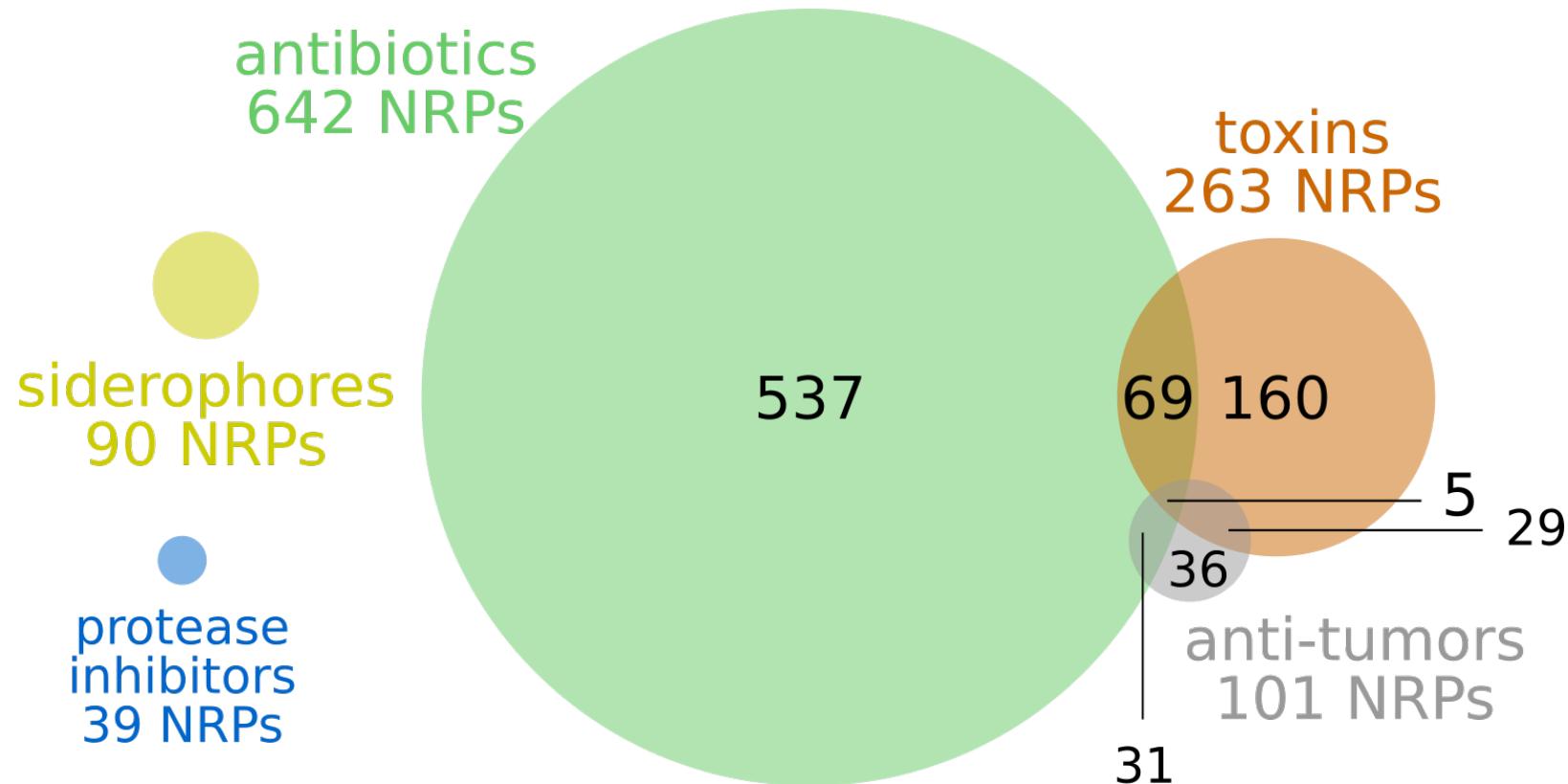


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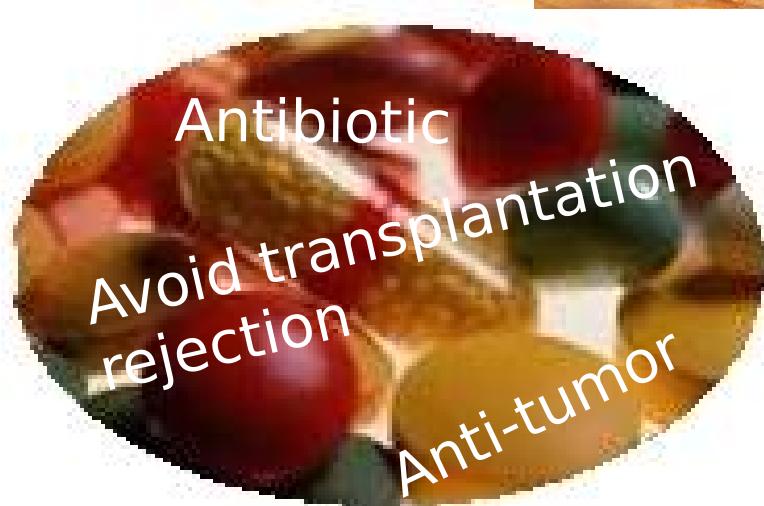
What are nonribosomal peptides ?

Various activities, several activities for some peptides

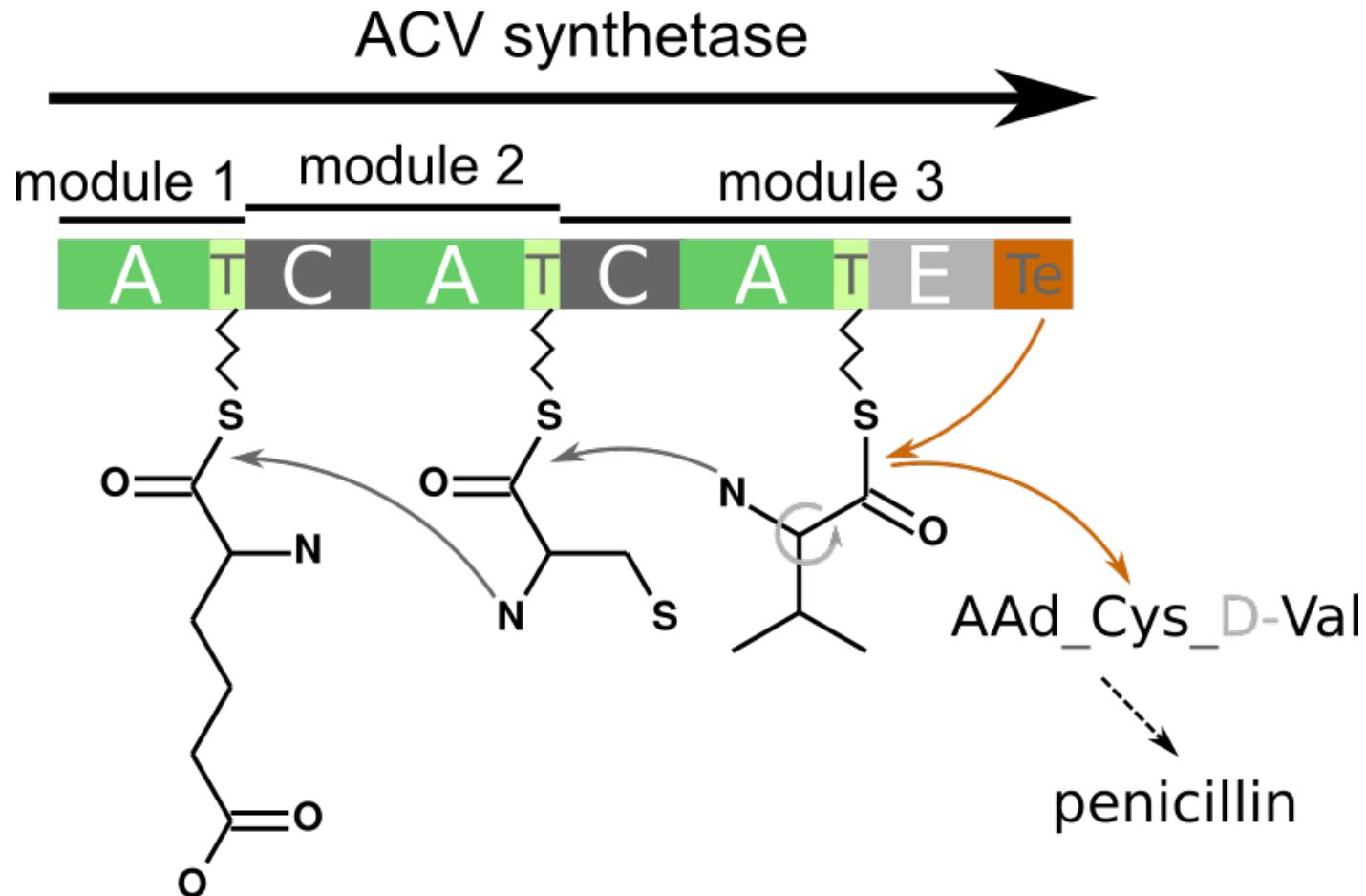


What are nonribosomal peptides ?

Diverse industrial applications



NRP synthesis: high specificity



a given
nonribosomal
peptide
synthetase

↓
a specific
nonribosomal
peptide