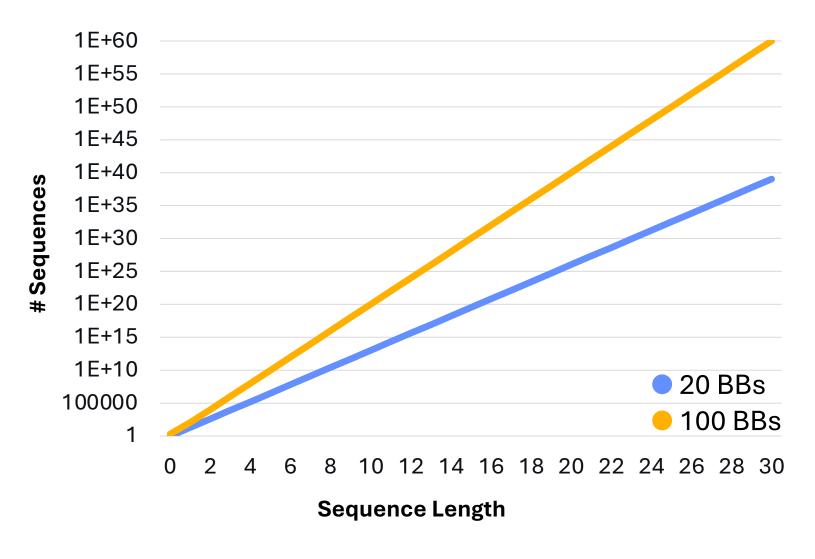
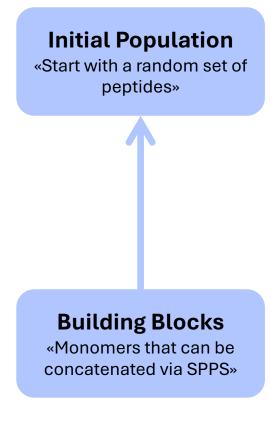
# Exploring Peptide Space with Genetic Algorithms

RDKit UGM 2024

#### Peptide space is vast

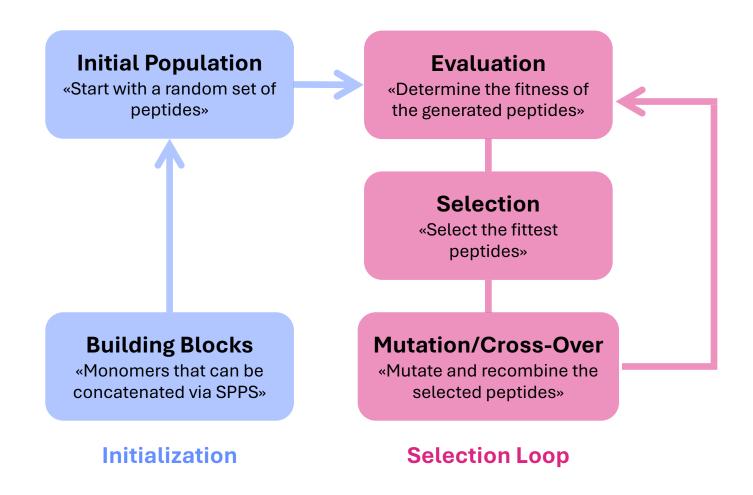


## Evolutionary search for peptides



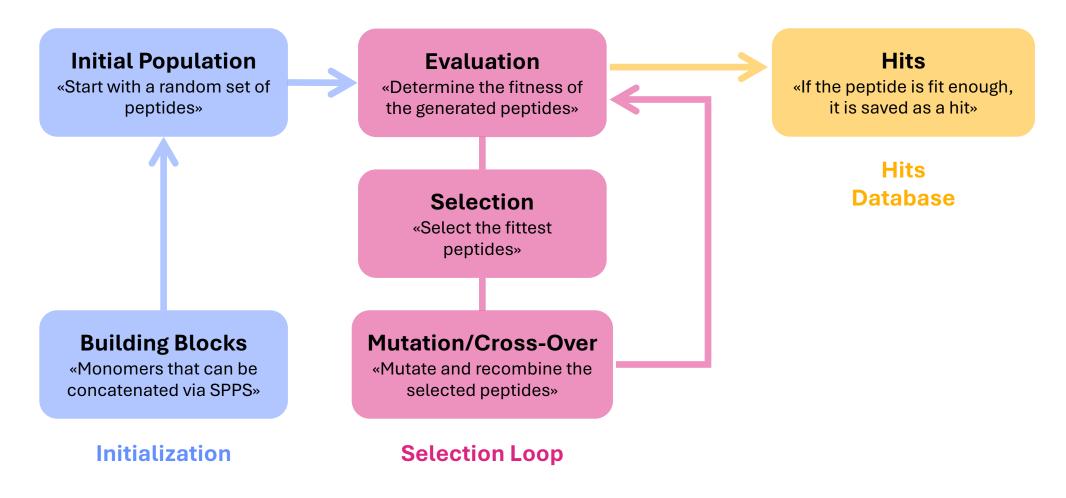
**Initialization** 

#### Evolutionary search for peptides



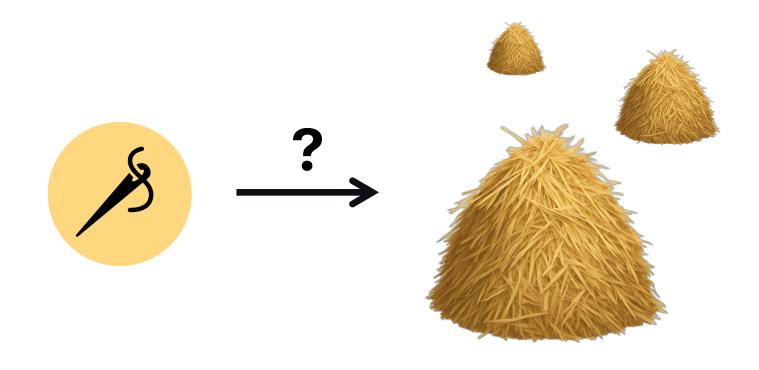
Orsi M. and Reymond J.-L. Navigating a 1E+60 Chemical Space of Peptide/Peptoid Oligomers, Molecular Informatics, 2024, accepted

#### Evolutionary search for peptides

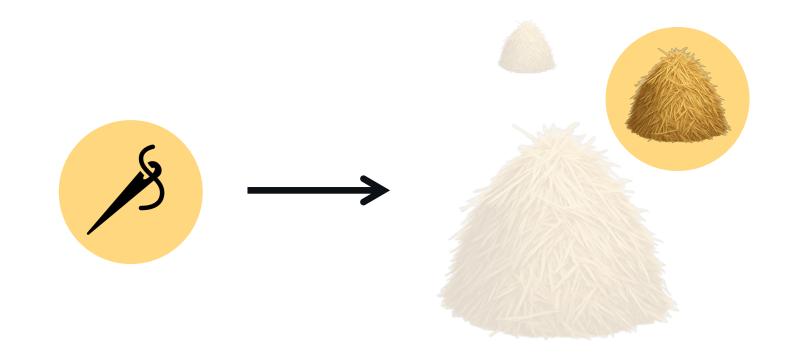


Orsi M. and Reymond J.-L. Navigating a 1E+60 Chemical Space of Peptide/Peptoid Oligomers, Molecular Informatics, 2024, accepted

## Will evolutionary search find the needle in the haystack(s)?



# Probably not – but it will find the haystack!



# Acknowledgements

Prof. Dr. Jean-Louis Reymond, the Cheminformatics Group and all the Reymond Group





UNIVERSITÄT BERN

Enter the first of the first of

Established by the European Commission







