Annual Report Year 1
Anticipating the Chemistry of Life (ACOL)

Marco Visani[1,2], Madleina Caduff[1,2], Daniel Wegmann[1,2], and Pierre-Marie Allard[1,2,3]

[1]Department of Biology, University of Fribourg, 1700 Fribourg, Switzerland
[2]Swiss Institute of Bioinformatics, 1700 Fribourg, Switzerland
[3]Corresponding author, pierre-marie.allard@unifr.ch

November 3, 2025

Contents

1 Introduction

2 Markov Random Field

2.1 WP 1

$$\mathbf{\Lambda}_c = \begin{pmatrix} -\alpha_c & \alpha_c \\ 1-\alpha_c & \alpha_c - 1 \end{pmatrix} \tag{1}$$

We changed from μ_0 and μ_1 to a single parameter α which is the change rate to go from 0 to 1.

$$\boldsymbol{P}(n) = \exp(\mathbf{\Lambda}_c \nu_c b(n)). \tag{2}$$

We now have an additional parameter ν_c which is the rate parameter of the clique.

$$\boldsymbol{P}_\infty = (1-\alpha_c, \alpha_c)\,. \tag{3}$$

$$\mathbb{P}(L_{ms}|\boldsymbol{x}(m,s),R_{ms}) = \begin{cases} \epsilon & \text{if } \boldsymbol{x}(m,s)=0, L_{ms}=1, \\ 1-\epsilon & \text{if } \boldsymbol{x}(m,s)=0, L_{ms}=0, \\ R_{ms} & \text{if } \boldsymbol{x}(m,s)=1, L_{ms}=1, \\ 1-R_{ms} & \text{if } \boldsymbol{x}(m,s)=1, L_{ms}=0. \end{cases} \tag{4}$$

Added an error rate ϵ in case a molecule was wrongly added to LOTUS.

$$R_{ms} = (1-e^{-\gamma_0 P_m})(1-e^{-\gamma_1 Q_s}) \tag{5}$$

Changed equation for research effort.

2.2 WP 2

Implementation still in discussion but we are planning to move from ViMMS [1] to just using outputs of annotation tools. We might use a combination of Sirius, Metfrag, CFM-ID and maybe weight these outputs.

2.3 Fake extract

Plate 3 was performed by a bachelor student, but results are weird, so we'll pass everything again. Plate 1 is done.

3 LOTUS Expanded

In silico chemical expansion of molecules in LOTUS. Produced $3 \cdot 10^6$ molecules.

4 EMI-Monorepo

Helped Luca on the Monorepo for a couple of crates.

5 Perspectives

I'd like to continue working with Luca in Rust as it is a skill that I want to master by the end of the PhD.

References

[1] J. Wandy et al. "ViMMS 2.0: A Framework to Develop, Test and Optimise fragmentation Strategies in LC-MS Metabolomics". In: *Journal of Open Source Software* 7.71 (30, 2022). DOI: 10.21105/joss.03990.