Réseau moléculaire massif pour l'annotation en lipidomique

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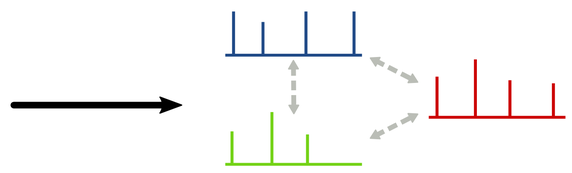
Lipidblast

~5× 10^5 *in silico* lipids spectra



Comparison of spectra by pairs

t-SNE projection

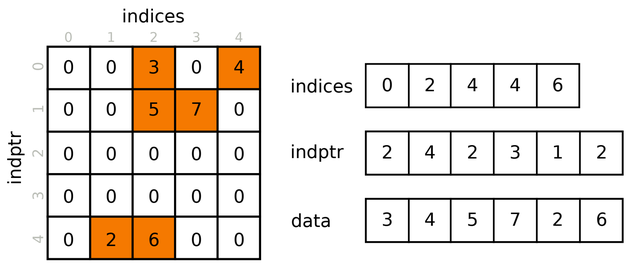
Polarity	Positive	Negative
Perplexity	100	200
Learning Rate	200	30000
Early exaggeration	12	12
# iterations	1000	1000

t-SNE parameters

Operating System: KUbuntu 20.04
Processors: 32 × Intel® Xeon® CPU E5-2650 0 @ 2.00GHz
Memory: **128 GiB** + 184 GiB of swap

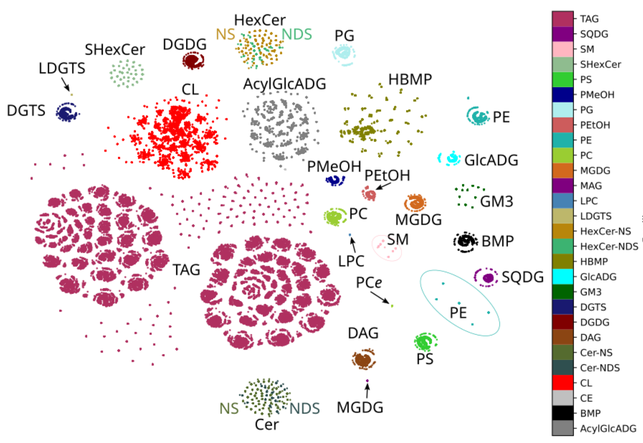
MetGem

To handle such a large dataset, libmetgem library has been updated to store similiarity scores in sparse matrices (Compressed Sparse Row format)

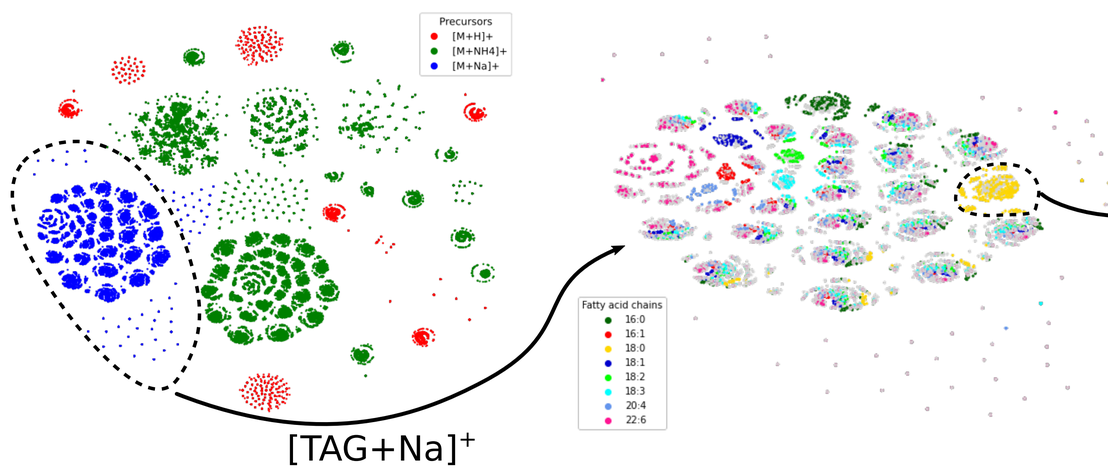


Positive

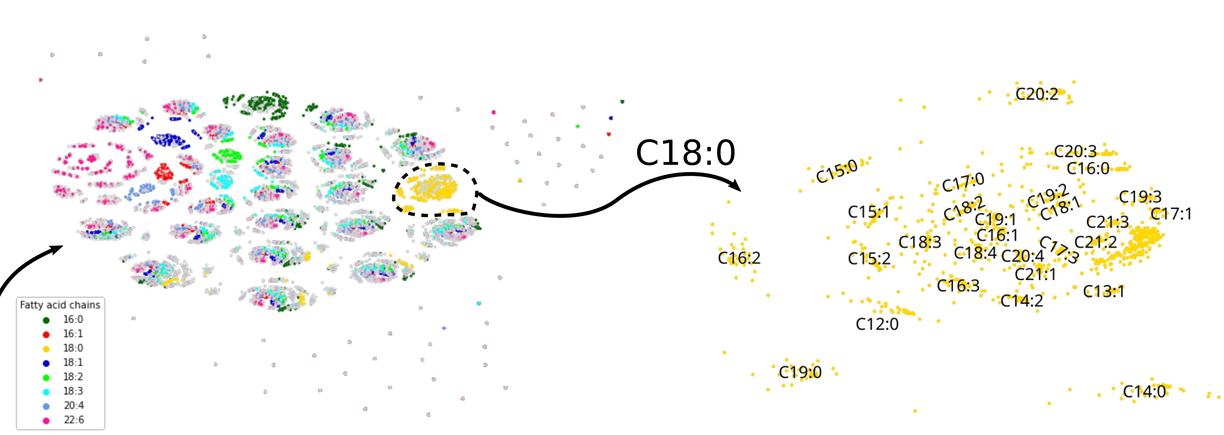
Families



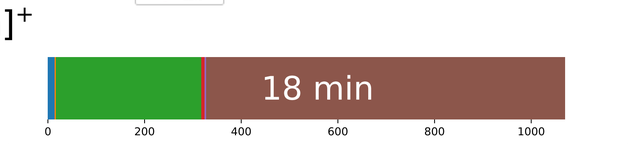
Precursors



Fatty acid chains

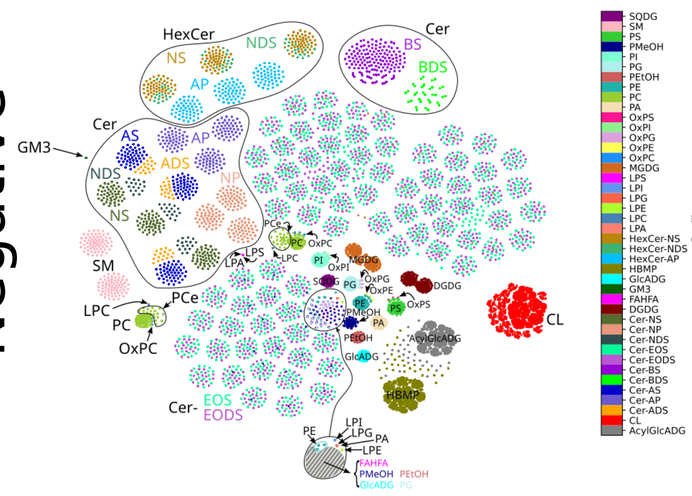


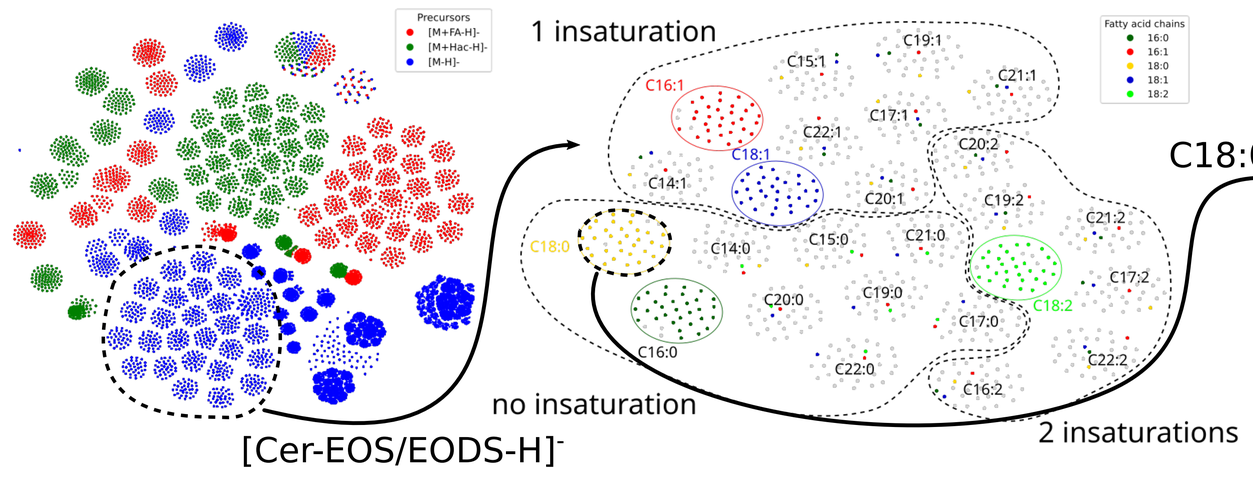
1.4×10^5 spectra 28 lipid families



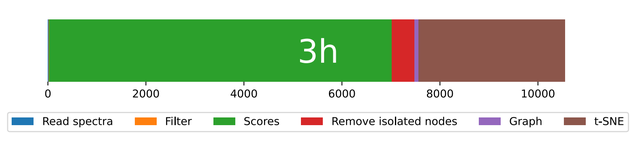
Dense matrix: 76 GiB
Sparse matrix: 3 GiB

Negative



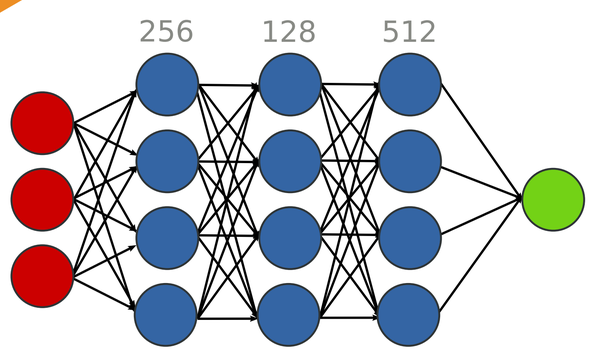


3.4×10^5 spectra 42 lipid families



Dense matrix: 440 GiB
Sparse matrix: 4 GiB

Could we use Deep Learning to predict position of new points?



MultiLayer Perceptron

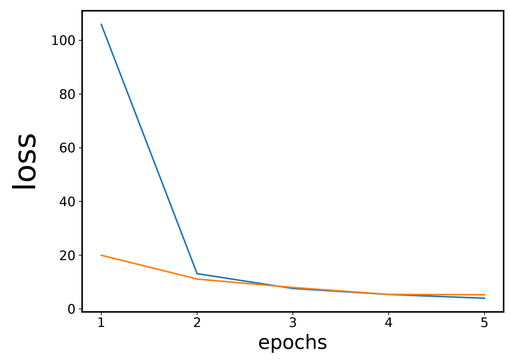
Dataset was split in 3 subsets

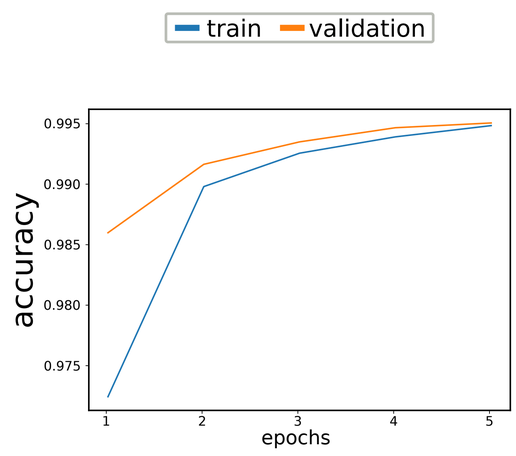
Training set 60 %
Test set 20 %
Validation set 20 %

Accuracy on validation

99.45%

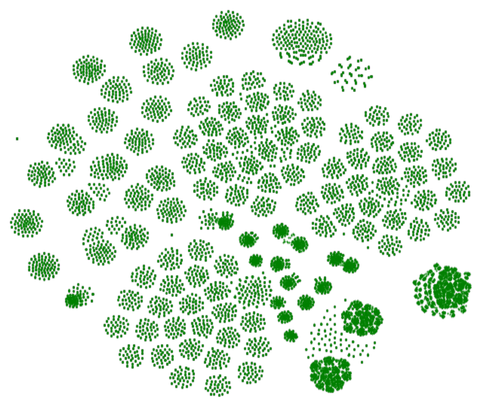
Parameter	Value
Loss	mse
Metrics	accuracy
# epochs	5





train validation

t-SNE projection of test set



Model predictions