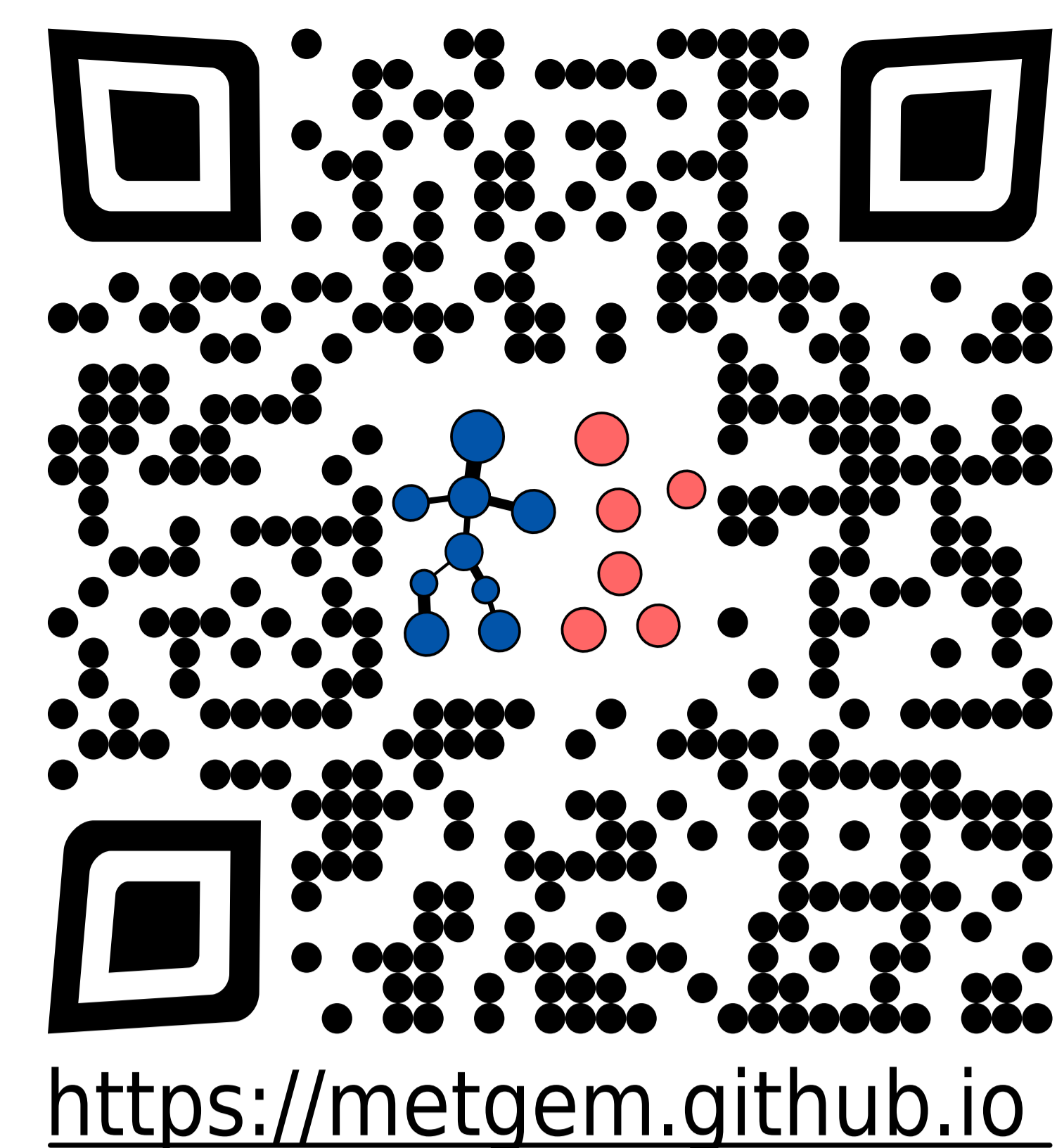


MetGem Software for the Generation of Molecular Networks Based on the t-SNE Algorithm

Nicolas Elie, Florent Olivon, Gwendal Grelier, Fanny Roussi, Marc Litaudon and David Touboul

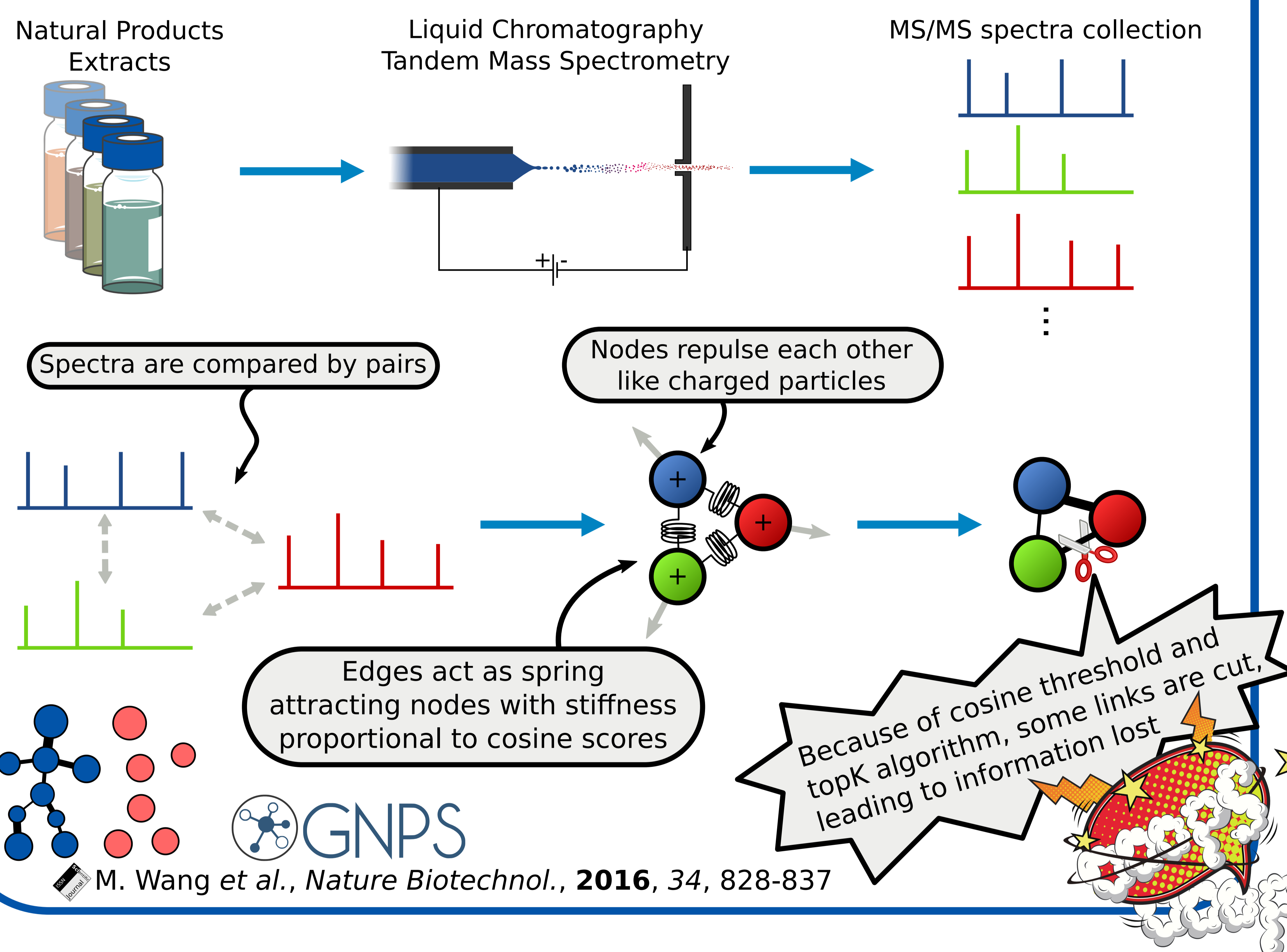
Institut de Chimie des Substances Naturelles, CNRS UPR 2301, Université Paris-Sud, Université Paris-Saclay, Gif-sur-Yvette, France.

F. Olivon, N. Elie *et al.*, *Anal. Chem.*, **2018**, 90 (23), pp 13900–13908, DOI: 10.1021/acs.analchem.8b03099

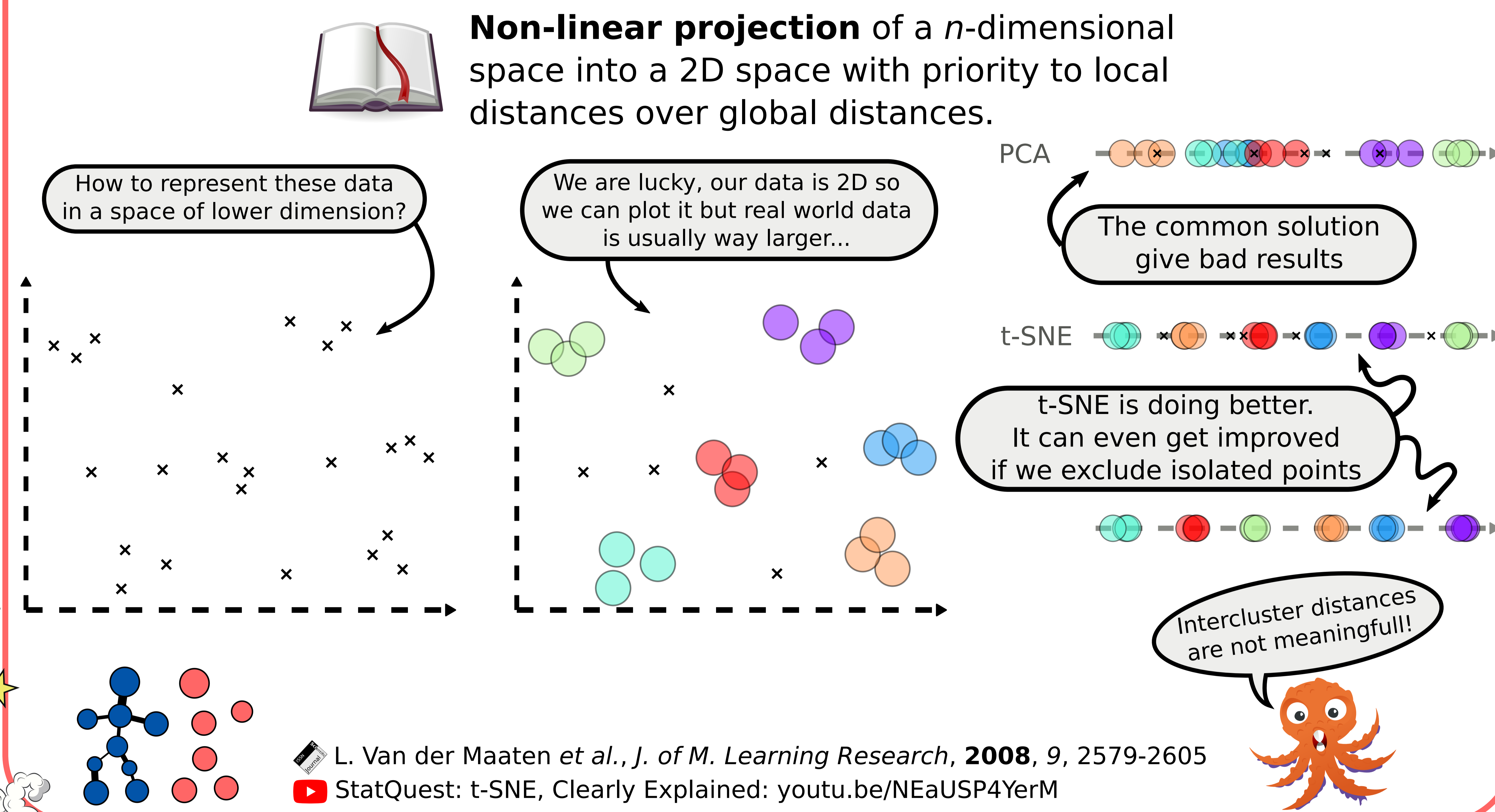


<https://metgem.github.io>

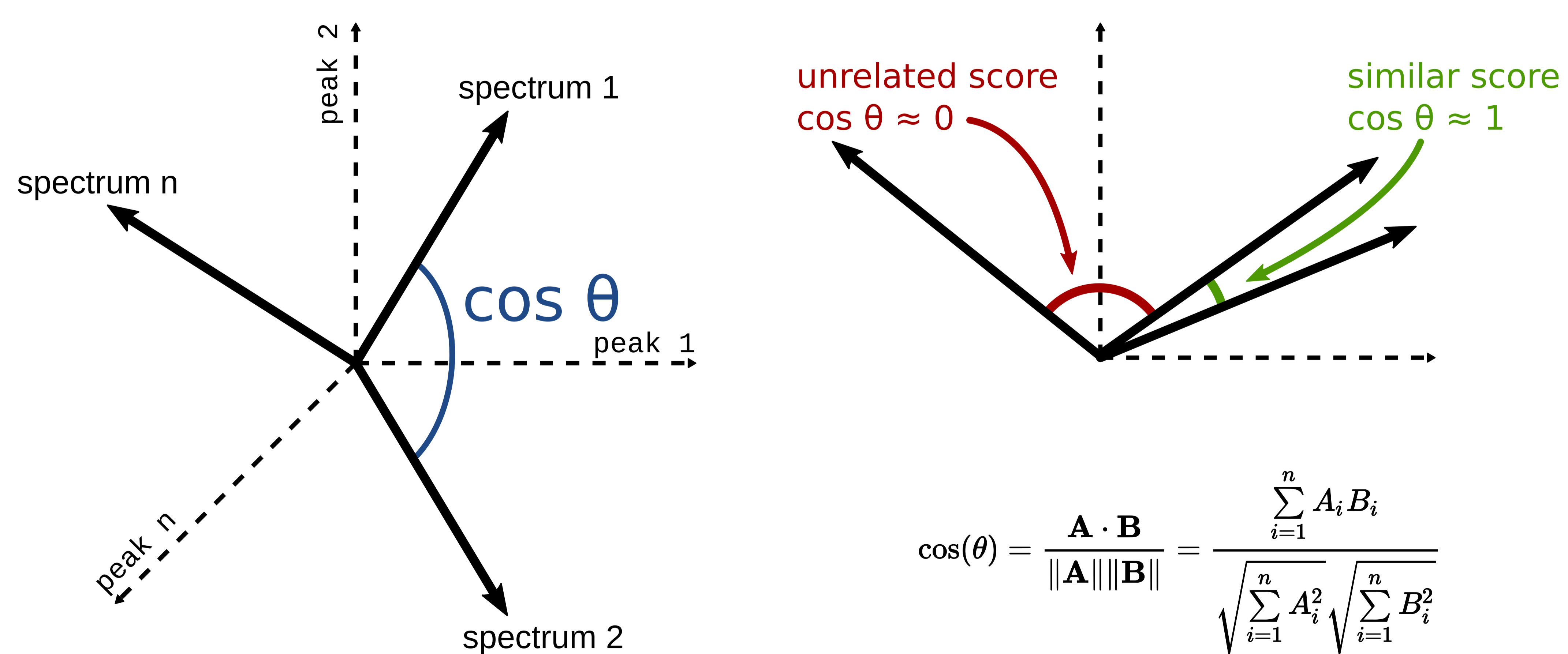
Molecular Networks



t-SNE



Cosine scores



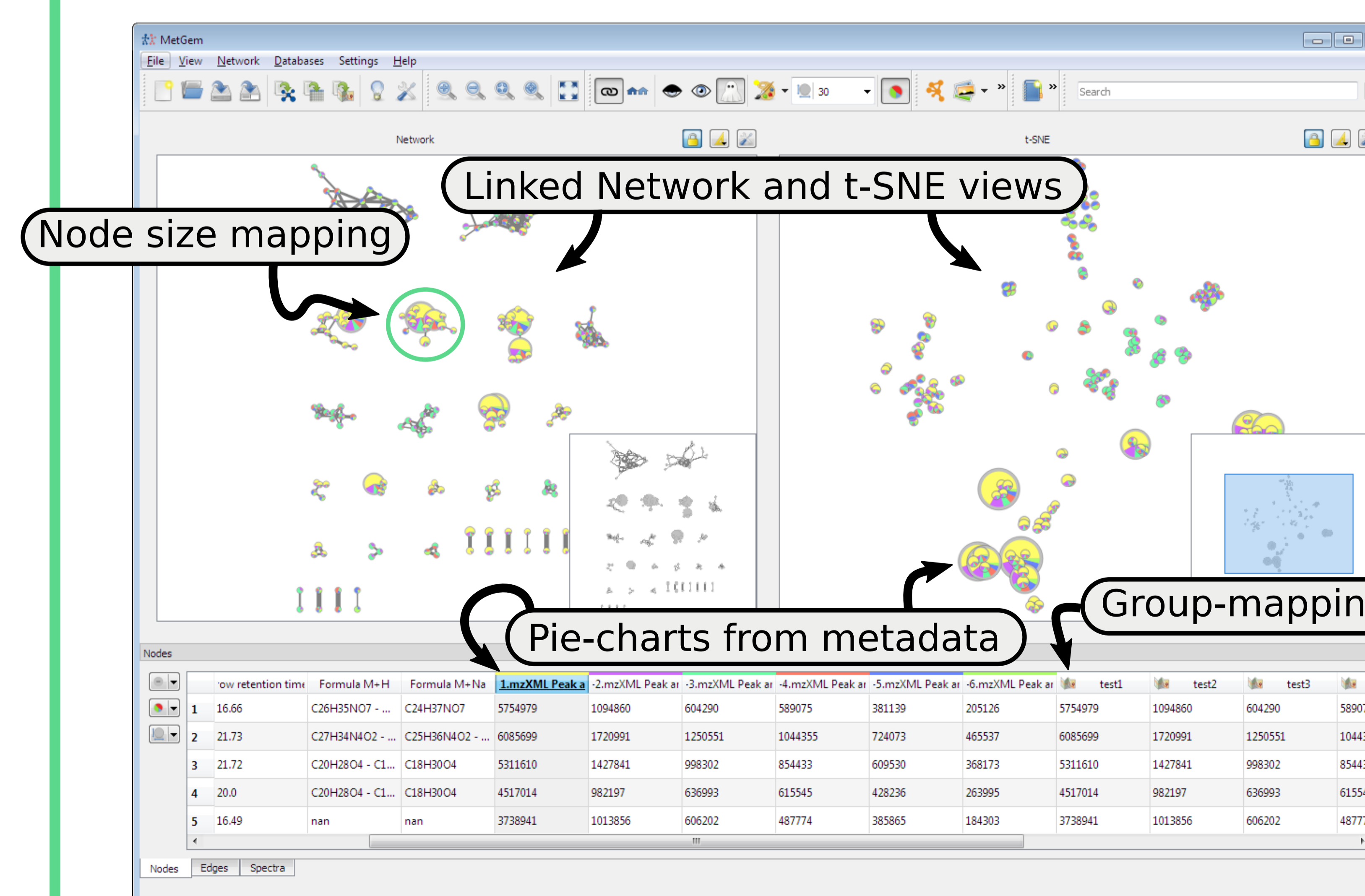
Free software: contributions, suggestions are welcome!



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<https://github.com/metgem/metgem>
Source code repository

Key features



- ✓ Quickly and easily tune parameters
- ✓ Fast generation of molecular networks
- ✓ No internet connection required
- ✓ Read data from: MGF files exported by **MZmine 2**
MSP files (**NIST** file format)
- ✓ Use databases from different sources
MS-Dial, GNPS, ISDB
- ✓ Plugins can be easily created to add new databases
- ✓ One-click import of user databases
- ✓ Export both views to cytoscape
- ✓ Cross-platform (Linux, Windows, macOS)

MetGem is powered by

