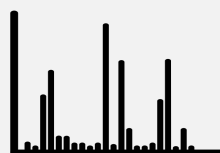


## SPECTRA

(66,646 experimental MS/MS spectra + metadata)



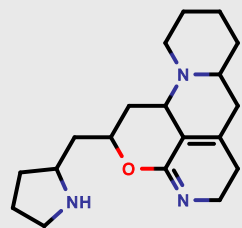
at least 6 fragments  
max 500 fragments  
100 Da < mass < 1500 Da  
[M+H]<sup>+</sup> adduct filtering



(40,138 experimental MS/MS spectra + metadata)

[GNPS lib\\_structural.tsv](#)

## STRUCTURES



SMILES / InChI



**ZDXXWMFBNIKKDB**

Short InChIKey  
standardized 2D structures

## BIOLOGICAL SOURCES

Raw text fields :

“Alkaloid from *Brunfelsia hopeana*”



gnfinder

- text recognition
- match and resolved against the Catalogue of Life

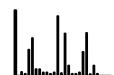
<http://globalnames.org>

Kingdom	Phylum	Class	Order	Family	Genus	Species
Plantae	Tracheophyta	Magnoliopsida	Solanales	Solanaceae	Brunfelsia	<i>Brunfelsia uniflora</i>

## Benchmarking dataset

**2107 unique entries**

SPECTRA ↔ STRUCTURE ↔ BIOLOGICAL SOURCE



[benchmarking\\_dataset\\_spectral.mgf](#)



[benchmarking\\_dataset\\_metadata.tsv](#)