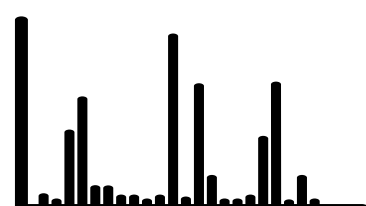


## SPECTRA

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

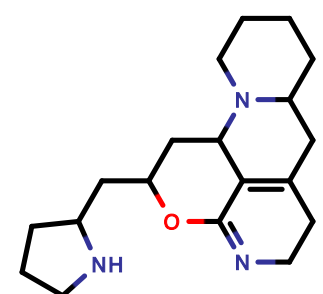


at least 6 fragments  
max 500 fragments  
100 Da < mass < 1500 Da  
[M+H]<sup>+</sup> adduct filtering



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

## STRUCTURES



SMILES  
InChI



chemical translation  
and sanitization

## BIOLOGICAL SOURCES

“Alkaloid from *Brunfelsia hopeana*”



<http://globalnames.org>

text recognition  
matching and  
resolving against the  
Catalogue of Life

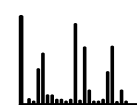
**ZDXXWMFBNIKKDB**

Short InChIKey  
standardized 2D structures

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

# 2107 unique entries

SPECTRA



STRUCTURE

BIOLOGICAL SOURCE

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

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