



THE NEW CHEMICALIZE

Árpád Figyelmesei
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OVERVIEW

Original concept



Free demonstration and advertisement platform,
for non-commercial use only.



History

- 2008 Alpha release
- 2010 Calculation page
- 2011 Chemical search
- 2012 First million of structures



Current numbers

- 25k users monthly
- 1 million unique structures
- 1.5 million visited pages



COMING SOON

Vision

Preserve current values and make
Chemicalize the market-leader self-service
chemical calculation, web search and naming
technology platform.

- Improve reliability
- Extend functionality
- Know and understand users



General changes

chemicalize.org

- Free
- No login required
- Non-commercial only

Chemicalize



- Registration and login
- Free for non-commercial
- Pay-per-use commercial

Design concept

chemicalize.org

- Shiny
- Simple
- Fast

Chemicalize



- Practical
- Reliable
- Secure
- Scalable
- Shiny
- Simple
- Fast

Modules

Calculations

Names,
identifiers,
topological,
physicochemical
properties
Batch calculations
Report generation

Annotation

WEB pages,
PDF documents
Chemical
structures
recognition and
extraction
OSR

Search

Combined
chemical and text
search
Relevancy scoring
Hit highlighting
Alerting service
Report generation

+

Further modules

Compliance
Checker, Markush
and Reaction
enumeration,
Standardizer,
Markush
composer

THANK YOU