ChemAxon

Jozsef David

CHEMISTRY AS A SERVICE - CHEMICALIZE

What is Chemicalize?

Current status

The journey

Values and features

Architecture

Statistics

WHAT IS CHEMICALIZE?

What to do with the license files?

How to integrate your tools?

Do you have an API?

Can you make it cheaper?

Who do I send the renewal request to?

Can I access it faster?

Can you make it easier to use?

How to get updates?

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Chemicalize is an **online, self-service** cheminformatics **platform** based on Chem[illegible]on's market leading **chemical calculations**, **naming** and **search technolog**[illegible]

Chemicalize

Provides UI for users

Chemicalize PRO

Provides hosted services and API access for integrators

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CURRENT STATUS

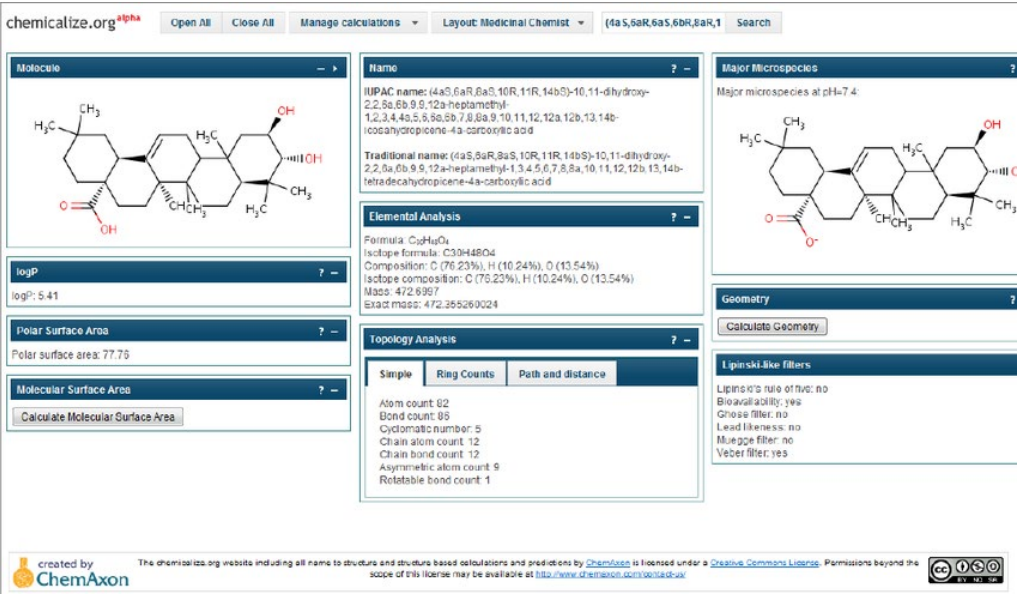
CURRENT STATUS

- **36k** registered users
- **120k** visitors
- **475k** page views
- **1.5k** feedback (daily 2-3)
- Automatic **credit card payment** option
- Reached **new user segments**
- Offering ChemAxon's **chemistry as online service**
- **High availability** cloud architecture

THE JOURNEY

THE JOURNEY

Started 11 years ago with:



- 2008 Alpha release
- 2009 Webpage annotation
- 2010 Property calculation
- 2011 Chemical and web search
- 2016 New Chemicalize
- 2018 Chemicalize PRO

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VALUES

VALUES AND BENEFITS

- Popular features of ChemAxon
- Always the latest and greatest versions available
- No IT and operation costs
- Pay as you go
- Minimal learning curve
- Easy integration
- Scalability and security

Chemicalize	Chemicalize PRO
FEATURES	
Simple end users applications	Embeddable web components and hosted backend services
SEGMENTS	
Individual users, small companies, academia	Catalog companies, third party SaaS providers, resource groups
USERS	
Students, teachers, consultants, researchers	Web developers, KNIME users, site administrators

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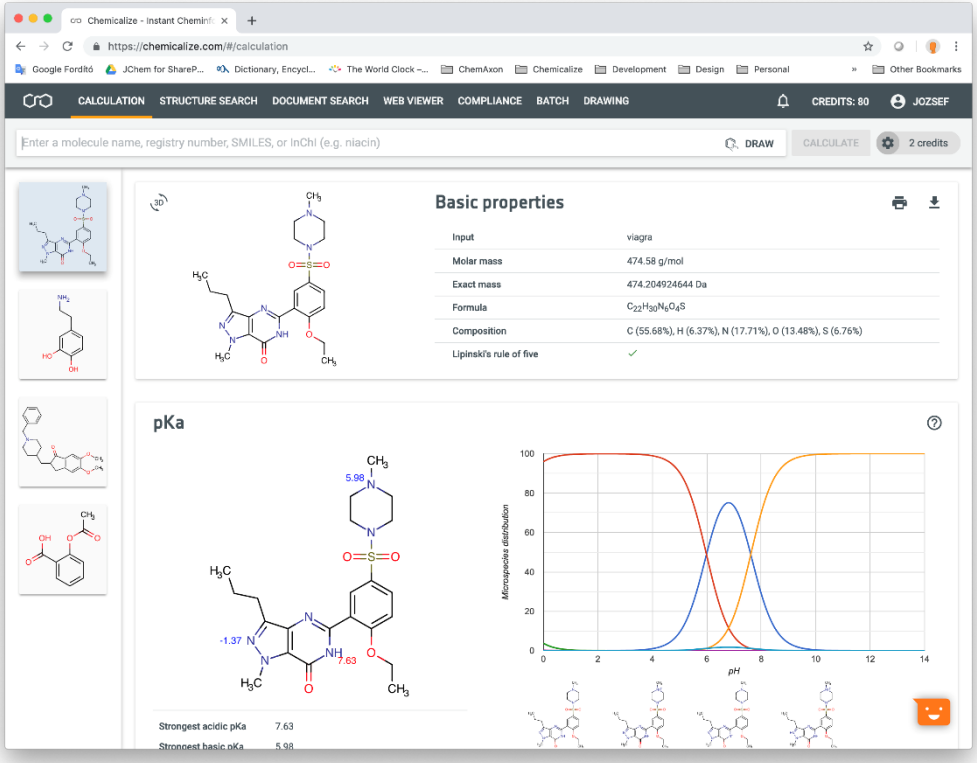
CHEMICALIZE

CHEMICALIZE



- Calculations (single, batch)

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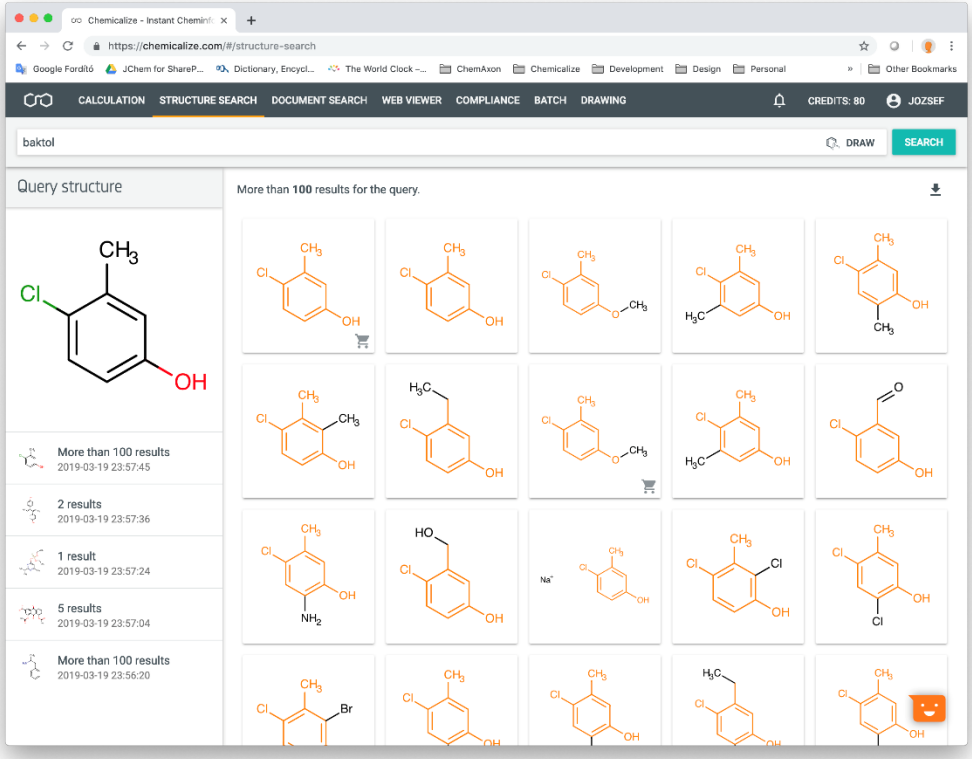
CHEMICALIZE



- Calculations (single, batch)
- Chemical structure search

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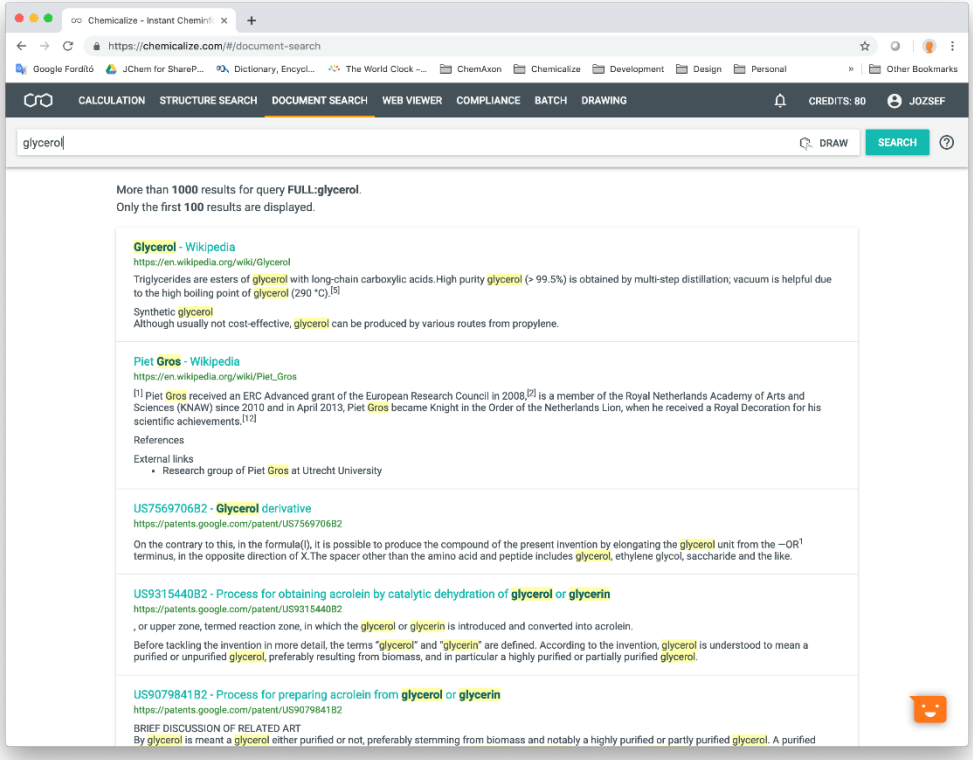
CHEMICALIZE



- Calculations (single, batch)
- Chemical structure search
- Document search

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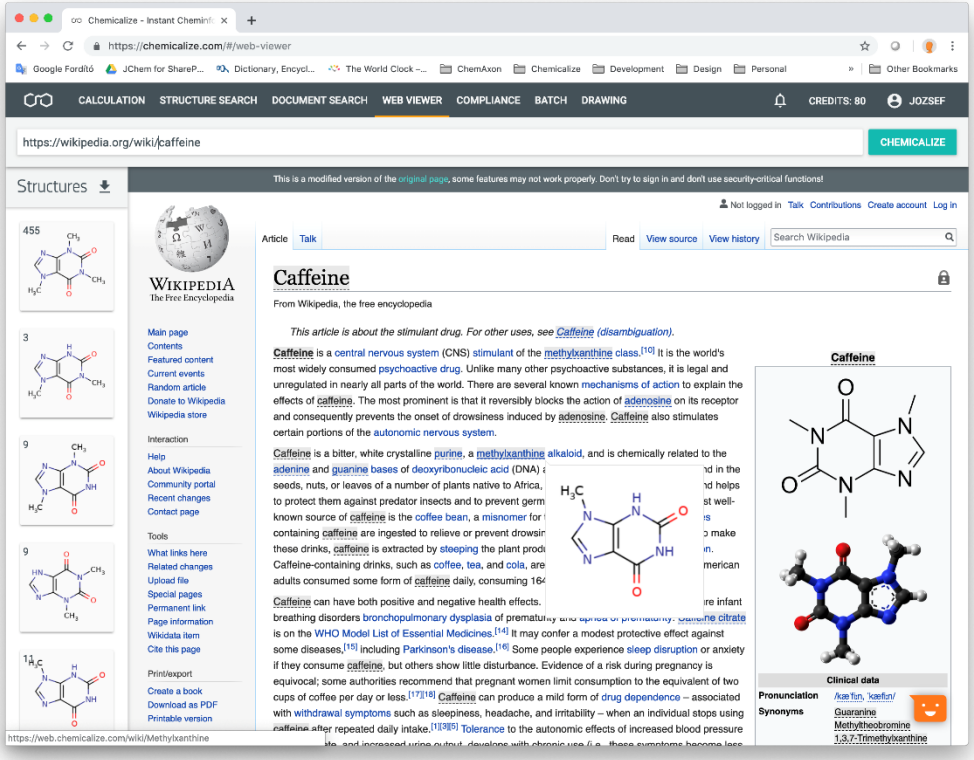
CHEMICALIZE



- Calculations (single, batch)
- Chemical structure search
- Document search
- Web viewer/annotator

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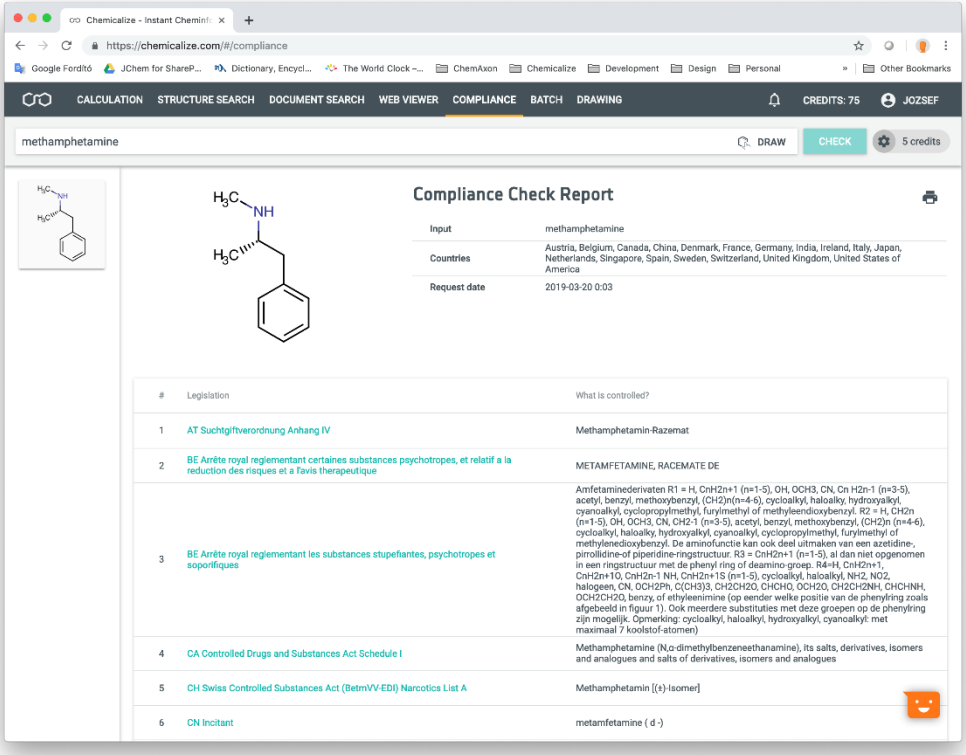
CHEMICALIZE



- Calculations (single, batch)
- Chemical structure search
- Document search
- Web viewer/annotator
- Compliance checking

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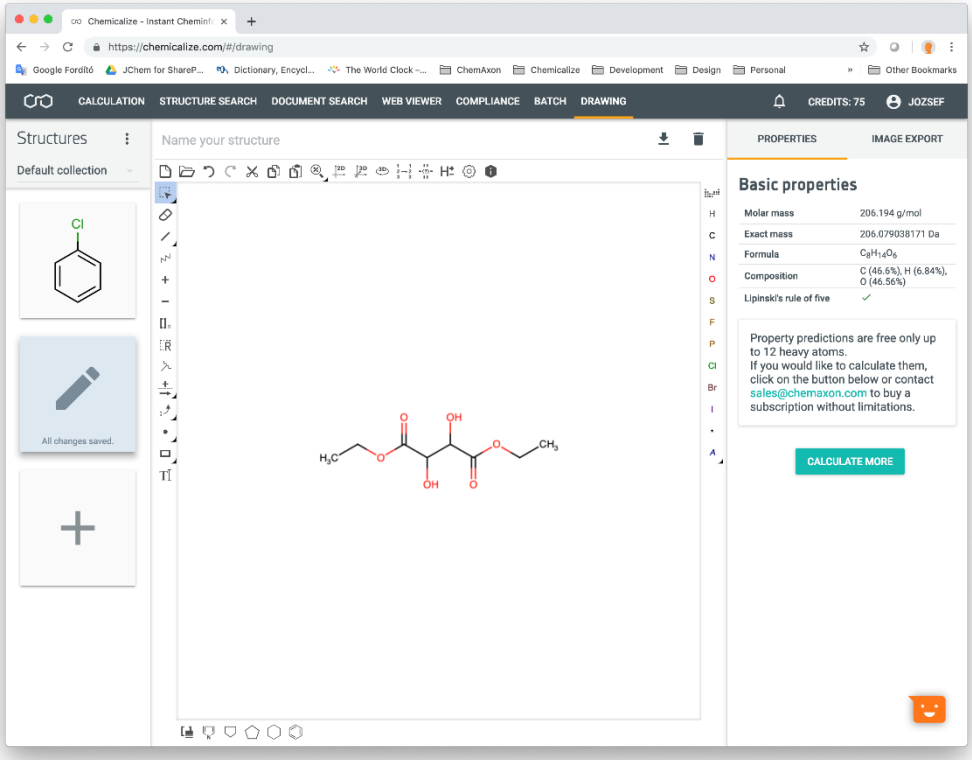
CHEMICALIZE



- Calculations (single, batch)
- Chemical structure search
- Document search
- Web viewer/annotator
- Compliance checking
- Chemical drawing

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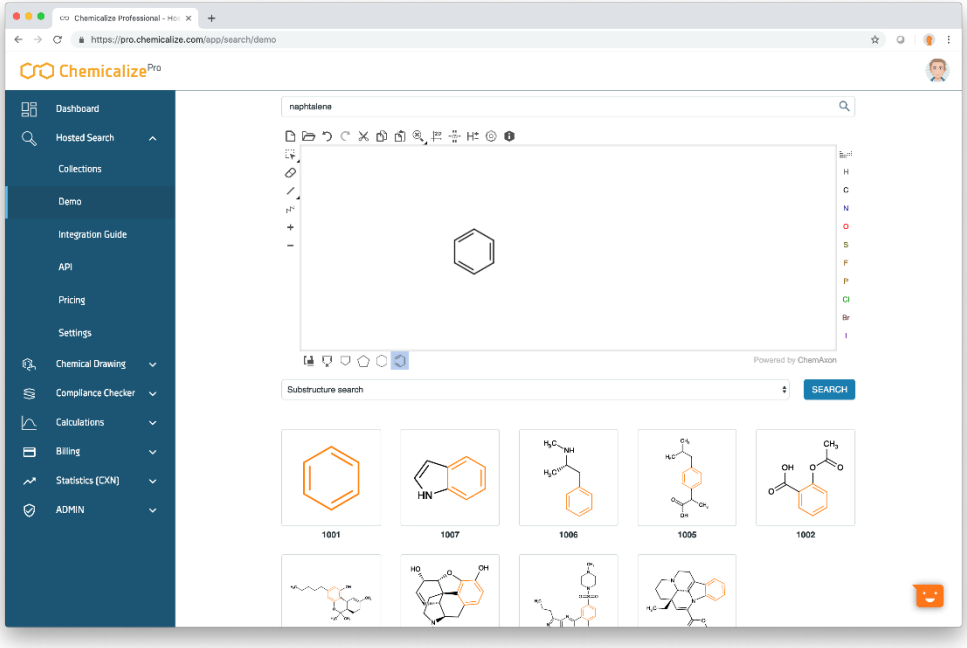
CHEMICALIZE PRO

CHEMICALIZE PRO



- Hosted catalog search

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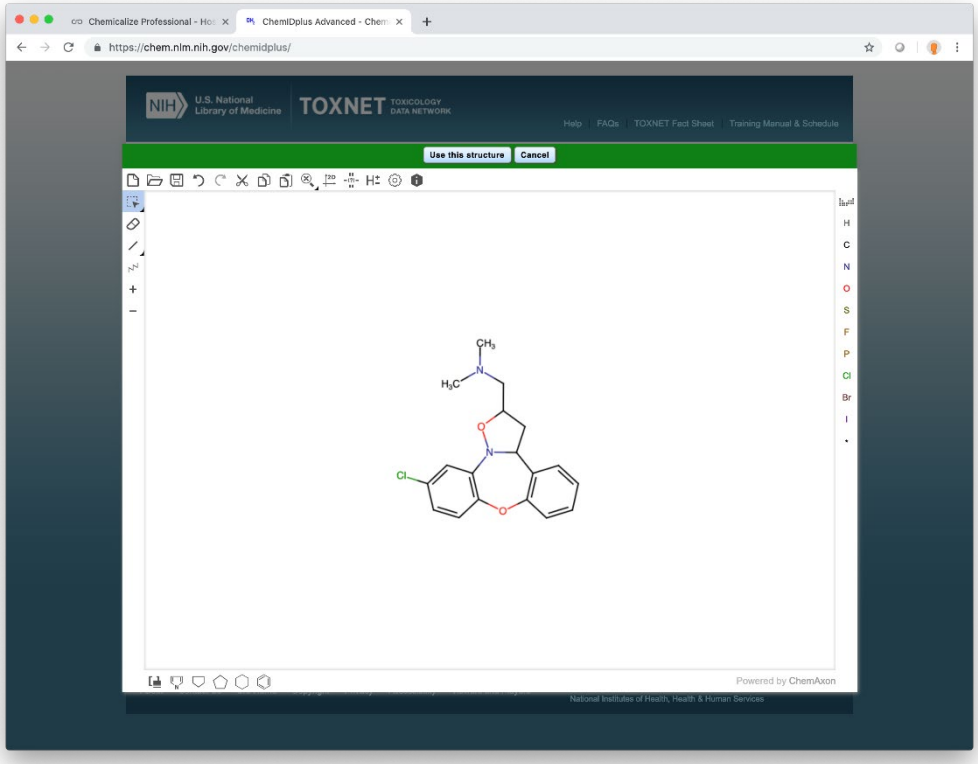
CHEMICALIZE PRO



- Hosted catalog search
- Hosted chemical drawing

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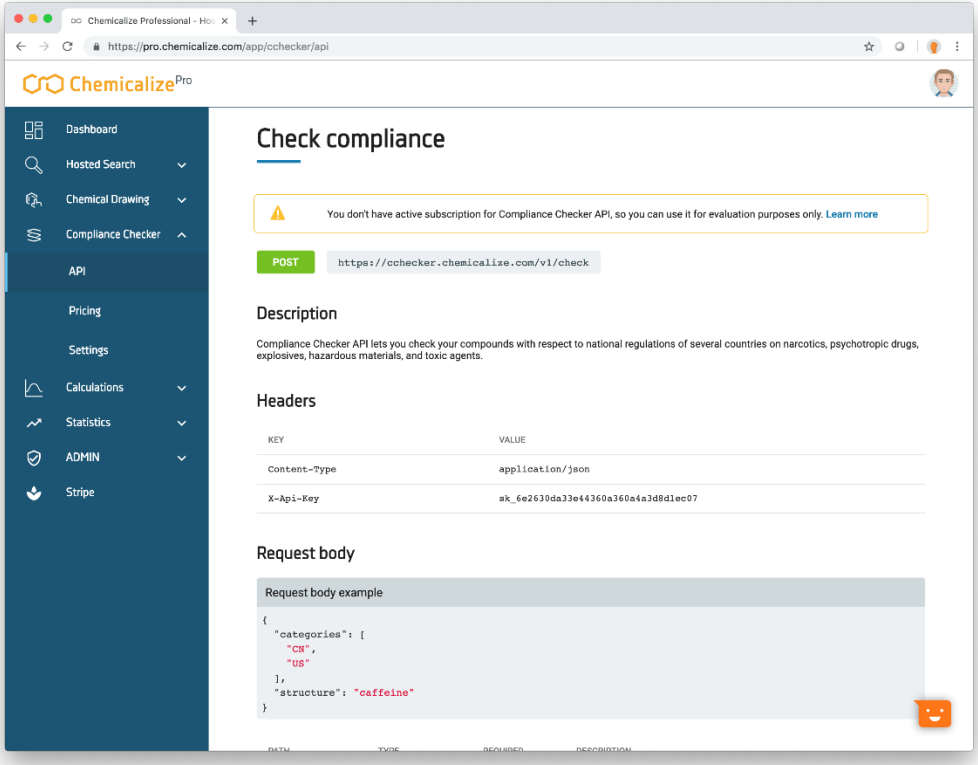
CHEMICALIZE PRO



- Hosted catalog search
- Hosted chemical drawing
- Compliance checking API

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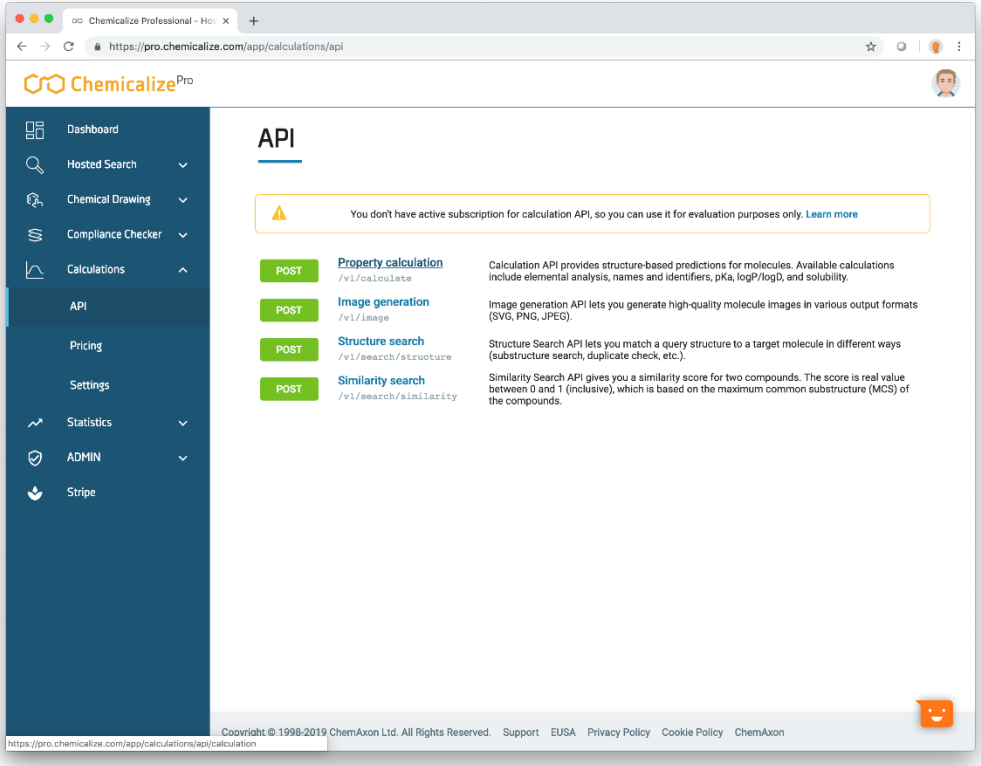
CHEMICALIZE PRO



- Hosted catalog search
- Hosted chemical drawing
- Compliance checking API
- Calculation API

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Chemicalize Professional - Ho

Zosimos

https://zosimos.io/fill-a-studyset/5c725aacb82b3700264320cd/5c9271de4d05f2002659af7b

Zosimos | Study Sets | Submissions | Study Groups | J

Aromatic electrophilic and nucleophilic substitution reactions

Score

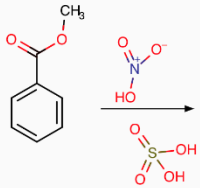
0/30

Exercises

1. What is the product in the following reaction?
2. What is the final product if you react phenol with excess of bromine in aqueous solution?
3. Your task is to prepare propylbenzene from benzene in 2 steps. What molecule would you prepare in the first step?
4. What is the product in the following reaction?
5. What is the main product in the following reaction? Use the known SEAr directing rules!
6. What is/are the product(s)in the following reaction?
7. Draw up the structure of the rmediate in the previous tion?

What is the product in the following reaction?

1/3 attempts



Marvin JS by ChemAxon

Powered by ChemAxon

CHECK ANSWER

LCC LIVERPOOL CHIROCHEM

Who We Are

STRUCTURE SEARC

aspirin

Substructure search

No results for the query.

CURRENCY: USD | MENU | ACCOUNT | $ 0.00 *

SETTING UP AN ACCOUNT

Order, Payment & Shipping information

SEARCH

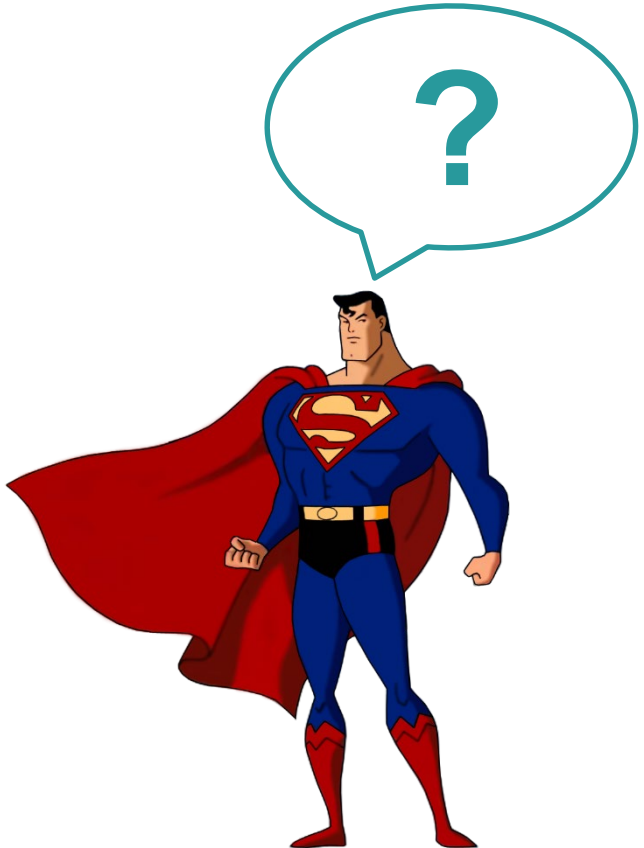
Accept

ChemAxon

ARCHITECTURE

CHALLENGES AND SOLUTIONS

- High availability
- Maintainability
- Modifiability
- Scalability
- Security



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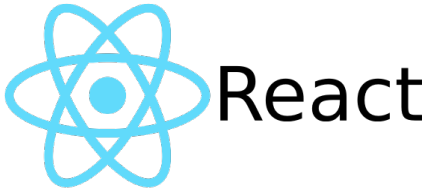
CHALLENGES AND SOLUTIONS

- Microservices (aws)
- Monitoring
- System logs
- Automatic backups
- Access management
- Release and upgrade management

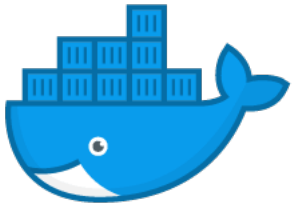

amazon
web services


Spring Cloud

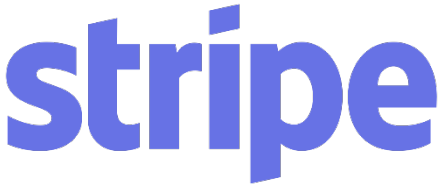

React


mongoDB.
Atlas

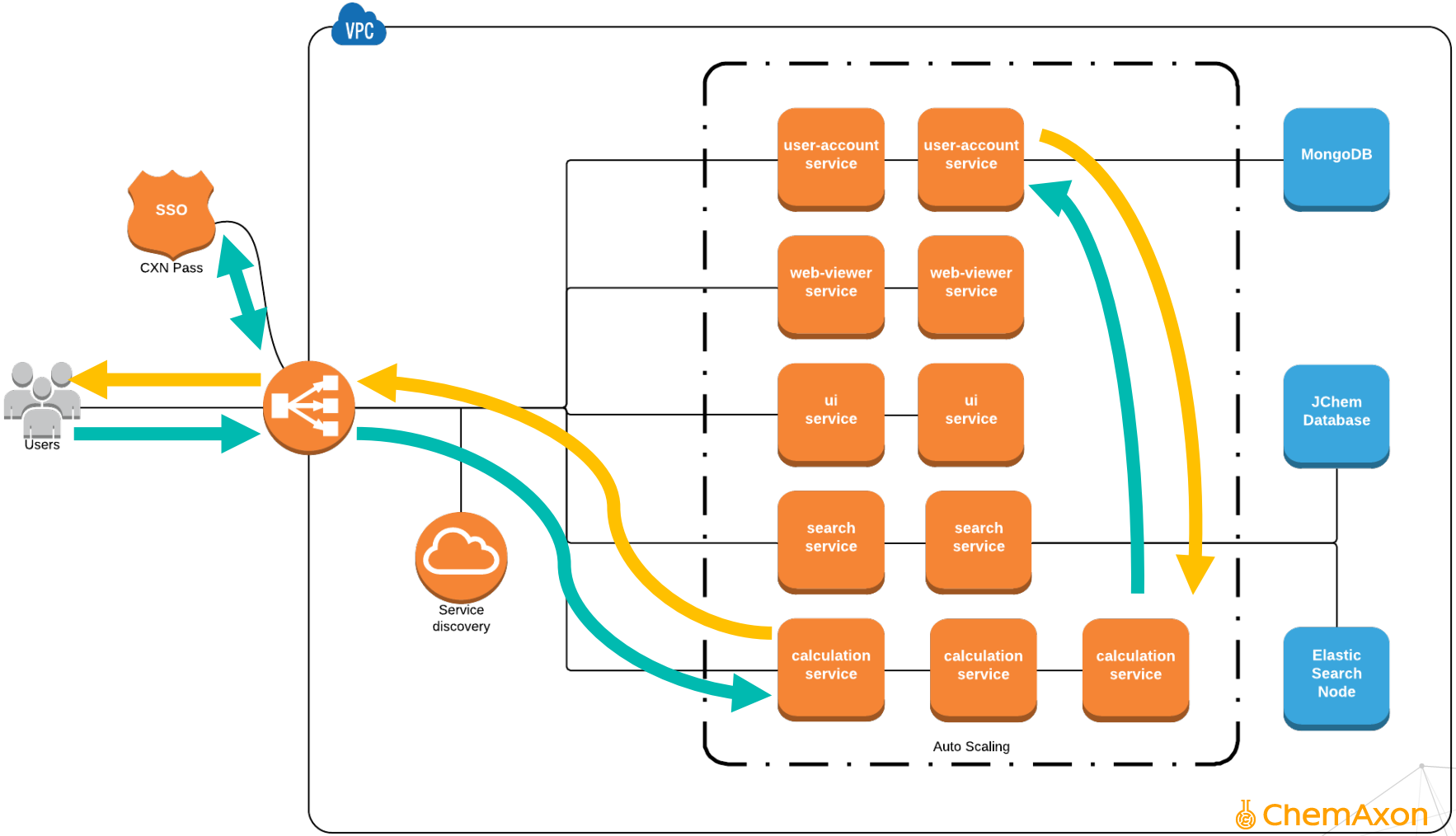

PostgreSQL




elastic

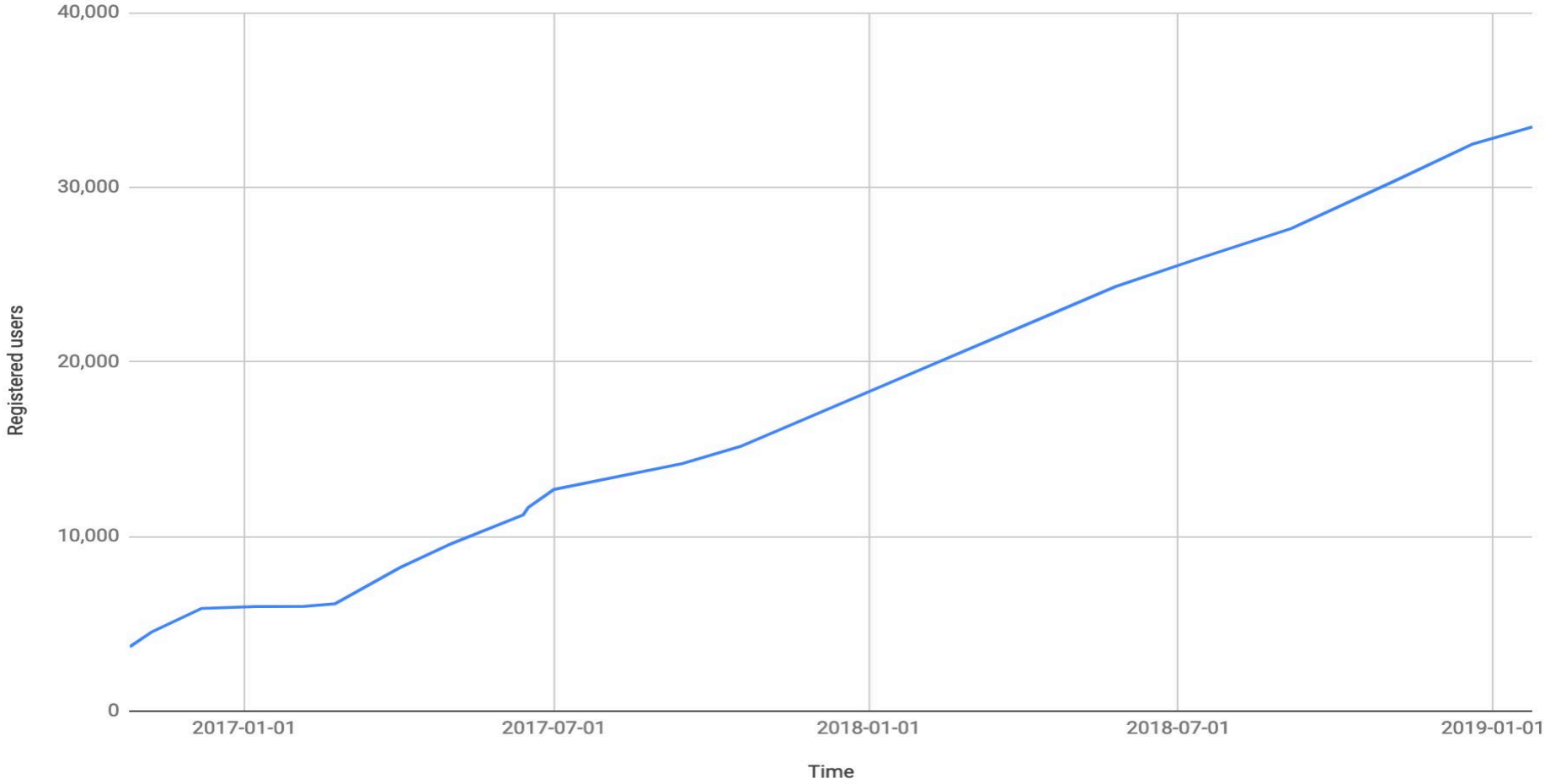

stripe


docker


VPC
SSO
CXN Pass
Users
Service discovery
user-account service
user-account service
web-viewer service
web-viewer service
ui service
ui service
search service
search service
calculation service
calculation service
calculation service
Auto Scaling
MongoDB
JChem Database
Elastic Search Node
ChemAxon

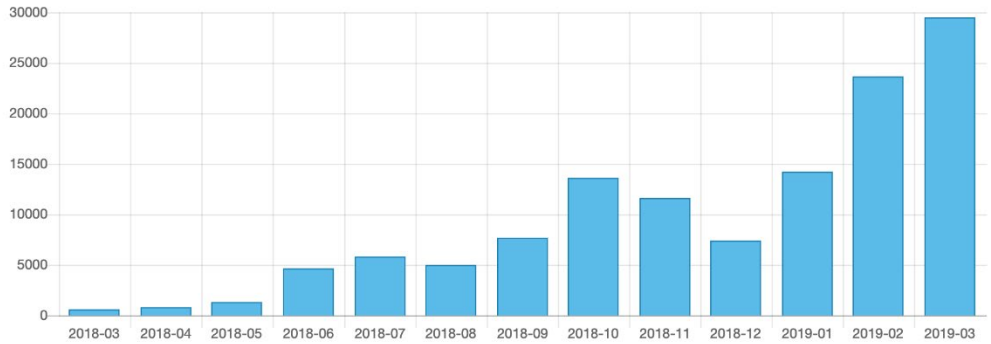
STATISTICS – DATA DRIVEN DEVELOPMENT

Chemicalize Users

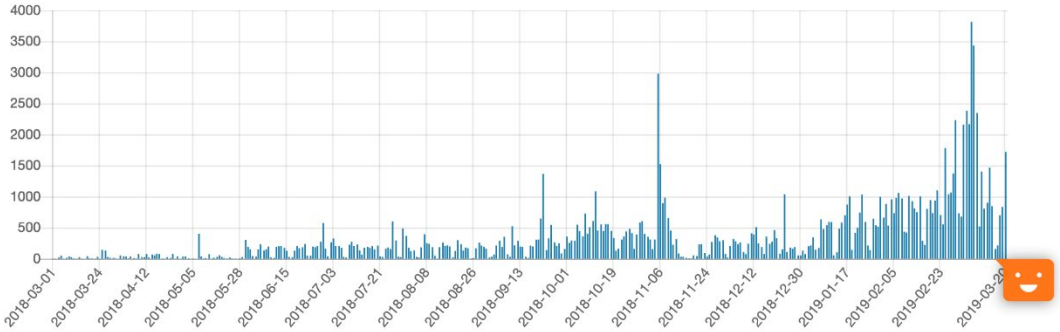


CHEMICALIZE PRO – HOSTED SEARCH

Monthly search count



Daily search count



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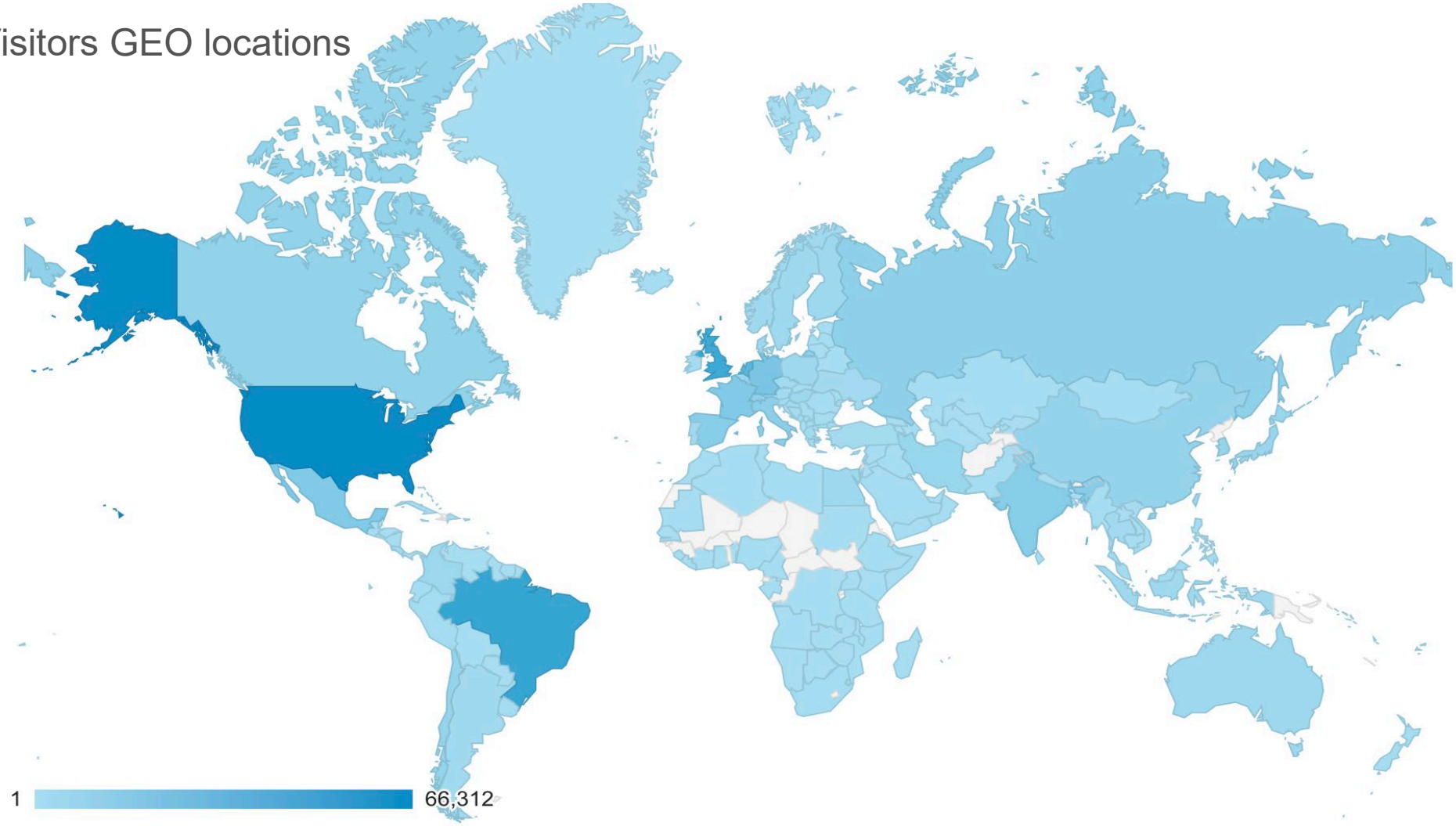
Visitors GEO locations

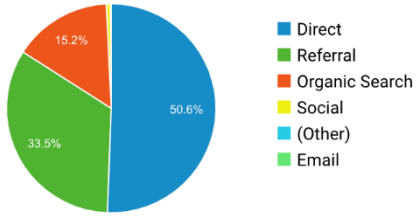


	Social Network	Sessions	% Sessions
1.	reddit	735	25.99%
2.	Twitter	726	25.67%
3.	Facebook	584	20.65%
4.	ResearchGate	455	16.09%
5.	LinkedIn	167	5.91%
6.	VKontakte	80	2.83%
7.	Blogger	58	2.05%
8.	Google+	7	0.25%
9.	Stack Exchange	4	0.14%
10.	SlideShare	3	0.11%

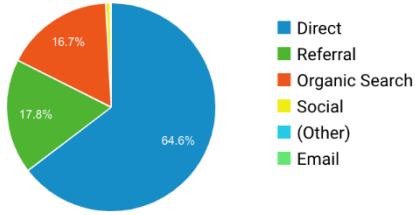
	Event Action	Total Events	% Total Events
1.	CALCULATION/PRINT_PDF	7,473	23.44%
2.	click	7,302	22.90%
3.	CALCULATION/DOWNLOAD_ZIP	6,331	19.86%
4.	DRAWING/EXPORT_IMAGE	3,975	12.47%
5.	S_SEARCH/CALCULATION	2,800	8.78%
6.	CALCULATION/SHOW_IN_3D	2,708	8.49%
7.	S_SEARCH/DOCUMENT_SEARCH	990	3.11%
8.	WEB_VIEWER/ANNOTATE	121	0.38%
9.	CALCULATION/VIEW_CATALOG	114	0.36%
10.	test action	37	0.12%

Top Channels

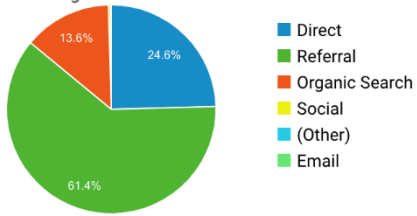
All Users



New Users



Returning Users



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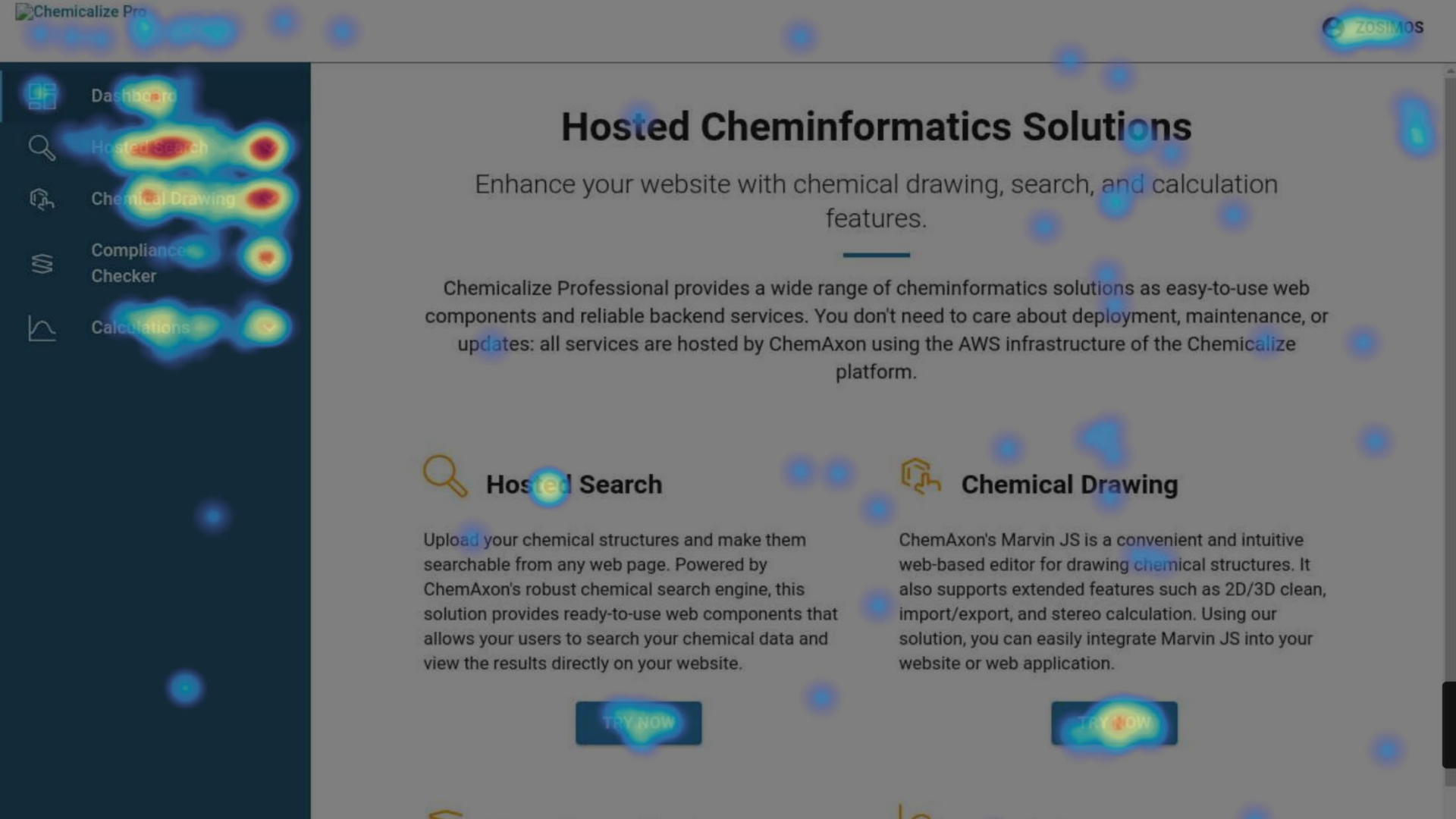
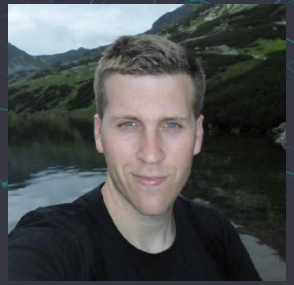
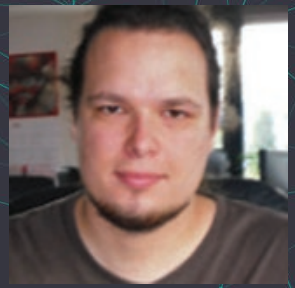

Chemicalize Pro
ZOSIMOS
Dashboard
Hosted Search
Chemical Drawing
Compliance Checker
Calculations
Hosted Cheminformatics Solutions
Enhance your website with chemical drawing, search, and calculation features.
Chemicalize Professional provides a wide range of cheminformatics solutions as easy-to-use web components and reliable backend services. You don't need to care about deployment, maintenance, or updates: all services are hosted by ChemAxon using the AWS infrastructure of the Chemicalize platform.
Hosted Search
Upload your chemical structures and make them searchable from any web page. Powered by ChemAxon's robust chemical search engine, this solution provides ready-to-use web components that allows your users to search your chemical data and view the results directly on your website.
TRY NOW
Chemical Drawing
ChemAxon's Marvin JS is a convenient and intuitive web-based editor for drawing chemical structures. It also supports extended features such as 2D/3D clean, import/export, and stereo calculation. Using our solution, you can easily integrate Marvin JS into your website or web application.
TRY NOW



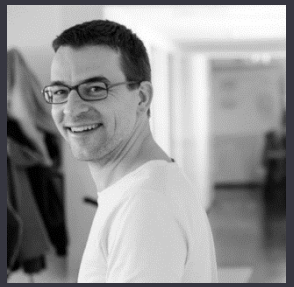
Arpad Figyelmesi



Gabor Botka

Peter Kovacs

Gabor Hornyak



Zsolt Varga

THANK YOU

Jozsef David

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