

CHEMISTRY AS A SERVICE - CHEMICALIZE

What is Chemicalize?

Current status

The journey

Values and features

Architecture

Statistics

A man in a dark suit and tie is standing in front of a whiteboard. He is holding a black marker in his right hand and has just finished writing the word 'Agenda' in a large, white, cursive font. The background is a plain, light-colored wall.

Agenda

1

2

3

4

5

6



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?

Chemicalize is an **online, self-service** cheminformatics **platform** based on ChemAxon's market leading **chemical calculations, machine learning and search technologies**.

Chemicalize

Provides UI for users

Chemicalize PRO

Provides hosted services and API access for integrators



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:

The screenshot displays the ChemAxon chemicalize.org interface for a complex polycyclic molecule. The main window shows the chemical structure with various methyl groups (CH₃) and hydroxyl groups (OH) highlighted. The interface includes several panels:

- Molecule:** Displays the chemical structure and a "Calculate Molecular Surface Area" button.
- Name:** Lists IUPAC and Traditional names for the compound.
- Elemental Analysis:** Provides the formula (C₃₉H₄₈O₄), composition, and isotopic data.
- Topology Analysis:** Shows ring counts, path and distance data, and atom counts.
- Major Microspecies:** Shows the structure at a specific pH.
- Geometry:** Includes a "Calculate Geometry" button.
- Lipinski-like filters:** Lists various filter criteria such as molecular weight, aromaticity, and hydrogen bond donors.

At the bottom, there is a footer with the ChemAxon logo and a Creative Commons license: CC BY-NC-ND 4.0.

2008

Alpha release

2009

Webpage annotation

2010

Property calculation

2011

Chemical and web search

2016

New Chemicalize

2018

Chemicalize PRO



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



CHEMICALIZE

Chemicalize

The screenshot displays the Chemicalize web application interface. At the top, there is a navigation bar with tabs for CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. Below this is a search bar with the text "Enter a molecule name, registry number, SMILES, or InChI (e.g. niacin)". To the right of the search bar are buttons for DRAW, CALCULATE, and a gear icon for settings, along with a "2 credits" indicator.

The main content area is divided into two sections:

- Basic properties:** This section shows the chemical structure of the molecule (a complex heterocyclic compound with a piperazine ring, a sulfonamide group, and a pyridine ring). To the right of the structure is a table of properties:

Input	viagra
Molar mass	474.58 g/mol
Exact mass	474.204924644 Da
Formula	C ₂₂ H ₃₀ N ₄ O ₄ S
Composition	C (55.68%), H (6.37%), N (17.71%), O (13.48%), S (6.76%)
Lipinski's rule of five	✓
- pKa:** This section shows the same chemical structure with pKa values highlighted: -1.37, 7.63, and 5.98. To the right is a graph of "Microspecies distribution" versus "pH". The graph shows three curves representing different ionization states of the molecule. The x-axis ranges from 0 to 14, and the y-axis ranges from 0 to 100. The curves are color-coded: red (dominant at low pH), blue (dominant at intermediate pH), and orange (dominant at high pH). Below the graph are four small chemical structures representing the different microspecies.

- Calculations (single, batch)

Chemicalize

The screenshot displays the Chemicalize web application interface. At the top, the browser address bar shows the URL <https://chemicalize.com/#/structure-search>. The navigation menu includes options like CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. The search bar contains the query 'baktol' and a 'SEARCH' button. Below the search bar, the 'Query structure' section shows a chemical structure of 3-chloro-4-methylphenol. To the right, a grid of search results is displayed, with the text 'More than 100 results for the query.' and a download icon. The grid contains various chemical structures, including substituted phenols and alcohols. On the left side of the grid, there are filters for different categories, such as 'More than 100 results' (2019-03-19 23:57:45), '2 results' (2019-03-19 23:57:36), '1 result' (2019-03-19 23:57:24), '5 results' (2019-03-19 23:57:04), and 'More than 100 results' (2019-03-19 23:56:20).

- Calculations (single, batch)
- Chemical structure search

Chemicalize

The screenshot shows the Chemicalize web application interface. At the top, there is a navigation bar with tabs for CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH (which is active), WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. Below the navigation bar is a search input field containing the text 'glycerol' and a green 'SEARCH' button. The main content area displays search results for the query 'FULL:glycerol'. A message states 'More than 1000 results for query FULL:glycerol. Only the first 100 results are displayed.' The results are listed in a vertical stack, each with a title, a URL, and a brief description. The first result is 'Glycerol - Wikipedia', followed by 'Piet Gros - Wikipedia', 'US7569706B2 - Glycerol derivative', 'US9315440B2 - Process for obtaining acrolein by catalytic dehydration of glycerol or glycerin', and 'US9079841B2 - Process for preparing acrolein from glycerol or glycerin'. A small orange smiley face icon is visible in the bottom right corner of the results area.

More than 1000 results for query FULL:glycerol.
Only the first 100 results are displayed.

Glycerol - Wikipedia
<https://en.wikipedia.org/wiki/Glycerol>
Triglycerides are esters of glycerol with long-chain carboxylic acids. High purity glycerol (> 99.5%) is obtained by multi-step distillation; vacuum is helpful due to the high boiling point of glycerol (290 °C).^[6]
Synthetic glycerol
Although usually not cost-effective, glycerol can be produced by various routes from propylene.

Piet Gros - Wikipedia
https://en.wikipedia.org/wiki/Piet_Gros
^[1] Piet Gros received an ERC Advanced grant of the European Research Council in 2008.^[2] is a member of the Royal Netherlands Academy of Arts and Sciences (KNAW) since 2010 and in April 2013, Piet Gros became Knight in the Order of the Netherlands Lion, when he received a Royal Decoration for his scientific achievements.^{[1][2]}
References
External links
• Research group of Piet Gros at Utrecht University

US7569706B2 - Glycerol derivative
<https://patents.google.com/patent/US7569706B2>
On the contrary to this, in the formula(), it is possible to produce the compound of the present invention by elongating the glycerol unit from the -OR¹ terminus, in the opposite direction of X. The spacer other than the amino acid and peptide includes glycerol, ethylene glycol, saccharide and the like.

US9315440B2 - Process for obtaining acrolein by catalytic dehydration of glycerol or glycerin
<https://patents.google.com/patent/US9315440B2>
, or upper zone, termed reaction zone, in which the glycerol or glycerin is introduced and converted into acrolein.
Before tackling the invention in more detail, the terms "glycerol" and "glycerin" are defined. According to the invention, glycerol is understood to mean a purified or unpurified glycerol, preferably resulting from biomass, and in particular a highly purified or partially purified glycerol.

US9079841B2 - Process for preparing acrolein from glycerol or glycerin
<https://patents.google.com/patent/US9079841B2>
BRIEF DISCUSSION OF RELATED ART
By glycerol is meant a glycerol either purified or not, preferably stemming from biomass and notably a highly purified or partly purified glycerol. A purified

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

Chemicalize

The screenshot displays the Chemicalize web viewer interface. At the top, a navigation bar includes options like CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. The address bar shows the URL https://chemicalize.com/#/web-viewer. Below this, a secondary navigation bar lists various tools and a 'CHEMICALIZE' button. The main content area displays a Wikipedia article for Caffeine, with the URL https://wikipedia.org/wiki/caffeine. The article text is partially visible, discussing caffeine's role as a CNS stimulant and its chemical properties. On the left side, there is a sidebar with 'Structures' and a list of chemical structures, including caffeine (455), theophylline (3), and theobromine (9). The bottom of the page shows the URL https://web.chemicalize.com/wiki/Methylxanthine.

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

Chemicalize

The screenshot displays the Chemicalize web interface. At the top, there's a navigation bar with tabs for CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE (selected), BATCH, and DRAWING. Below this is a search bar containing 'methamphetamine' and buttons for DRAW, CHECK, and a gear icon for settings (5 credits). The main content area is titled 'Compliance Check Report' and features a chemical structure of methamphetamine (1-(1S)-amino-3-phenylpropan-1-ol) with a 3D wedge-dash representation. Below the structure is a table with 6 rows of legislation details.

#	Legislation	What is controlled?
1	AT Suchtgiftverordnung Anhang IV	Methamphetamin-Razemat
2	BE Arrêté royal réglementant certaines substances psychotropes, et relatif à la réduction des risques et à l'avis thérapeutique	METAMFETAMINE, RACEMATE DE
3	BE Arrêté royal réglementant les substances stupefiantes, psychotropes et soporifiques	Amfetaminederivaten R1 = H, CnH2n+1 (n=1-5), OH, OCH3, CN, CnH2n-1 (n=3-5), acetyl, benzyl, methoxybenzyl, (CH2)n(n=4-6), cycloalkyl, haloalkyl, hydroxyalkyl, cyanoalkyl, cyclopropylmethyl, furylmethyl of methyleendioxybenzyl, R2 = H, CH2n (n=1-5), OH, OCH3, CN, CH2-1 (n=3-5), acetyl, benzyl, methoxybenzyl, (CH2)n (n=4-6), cycloalkyl, haloalkyl, hydroxyalkyl, cyanoalkyl, cyclopropylmethyl, furylmethyl of methyleendioxybenzyl. De amfetamicten kan ook deel uitmaken van een azetidine-, piperidine- of piperidine-ringstructuur. R3 = CnH2n+1 (n=1-5), al dan niet opgenomen in een ringstructuur met de phenyl ring of deamino-groep. R4=H, CnH2n+1, CnH2n+1O, CnH2n-1 NH, CnH2n+1S (n=1-5), cycloalkyl, haloalkyl, NH2, NO2, halogeen, CN, OCH2Ph, C(CH3)3, CH2CH2O, CHCHO, OCH2O, CH2CH2NH, CHCHNH, OCH2CH2O, benzyl, of ethyleenimine (op eender welke positie van de phenylring zoals afgebeeld in figuur 1). Ook nweidere substituties met deze groepen op de phenylring zijn mogelijk. Opmerking: cycloalkyl, haloalkyl, hydroxyalkyl, cyanoalkyl: met maximaal 7 koolstof-atomen)
4	CA Controlled Drugs and Substances Act Schedule I	Methamphetamine (N,G-dimethylbenzeethanamine), its salts, derivatives, isomers and analogues and salts of derivatives, isomers and analogues
5	CH Swiss Controlled Substances Act (BetmVV-ED) Narcotics List A	Methamphetamine [(±)-isomer]
6	CN Incitant	metamfetamin (d -)

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

Chemicalize

The screenshot displays the Chemicalize web application interface. The browser address bar shows the URL <https://chemicalize.com/#/drawing>. The application has a dark navigation bar with tabs for CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. The DRAWING tab is active. On the left, there is a 'Structures' panel with a 'Default collection' and a 'Name your structure' input field. Below this is a toolbar with various drawing tools, including a benzene ring and a pencil icon. The main workspace shows a chemical structure of a diester with a central hydroxyl group. On the right, the 'PROPERTIES' panel is visible, showing 'Basic properties' for the structure. The properties include:

Molar mass	206.194 g/mol
Exact mass	206.079038171 Da
Formula	C ₁₄ H ₁₄ O ₆
Composition	C (46.6%), H (6.84%), O (46.56%)
Lipinski's rule of five	✓

Below the table, there is a message: 'Property predictions are free only up to 12 heavy atoms. If you would like to calculate them, click on the button below or contact sales@chemaxon.com to buy a subscription without limitations.' A 'CALCULATE MORE' button is located below the message. The bottom right corner of the interface features a small orange smiley face icon.

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



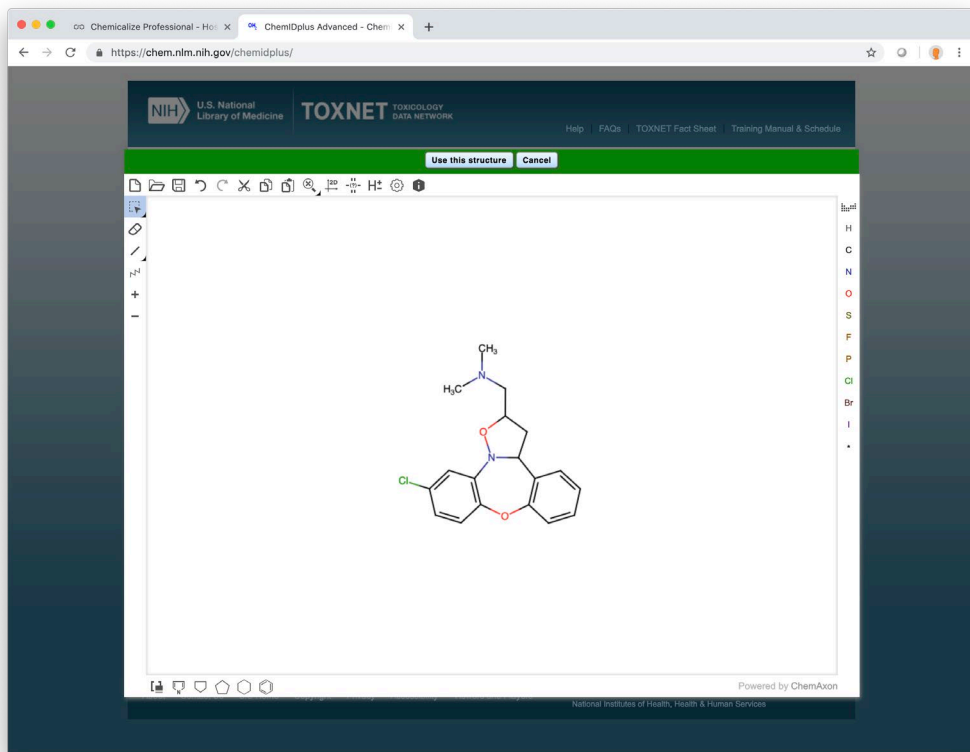
CHEMICALIZE PRO

Chemicalize PRO

The screenshot displays the Chemicalize PRO web application interface. The browser address bar shows the URL <https://pro.chemicalize.com/app/search/demo>. The application features a dark blue sidebar on the left with navigation options: Dashboard, Hosted Search, Collections, Demo, Integration Guide, API, Pricing, Settings, Chemical Drawing, Compliance Checker, Calculations, Billing, Statistics (CXN), and ADMIN. The main content area has a search bar containing the text "naphthalene". Below the search bar is a large canvas for chemical drawing, currently showing a benzene ring. To the right of the canvas is a legend for chemical elements: H, C, N, O, S, F, P, Cl, Br, I. Below the canvas is a "Substructure search" input field with a "SEARCH" button. The search results are displayed as a grid of chemical structures, each with a numerical ID: 1001 (benzene), 1007 (indole), 1006 (N-methylphenethylamine), 1005 (serotonin), 1002 (salicylic acid), and several other complex structures in the second row.

- Hosted catalog search

Chemicalize PRO



- Hosted catalog search
- Hosted chemical drawing

Chemicalize PRO

The screenshot shows the Chemicalize PRO web interface. The left sidebar contains navigation options: Dashboard, Hosted Search, Chemical Drawing, Compliance Checker (expanded), API, Pricing, Settings, Calculations, Statistics, ADMIN, and Stripe. The main content area is titled "Check compliance" and features a warning message: "You don't have active subscription for Compliance Checker API, so you can use it for evaluation purposes only. [Learn more](#)". Below this, a green "POST" button is next to the URL "https://cchecker.chemicalize.com/v1/check". The "Description" section states: "Compliance Checker API lets you check your compounds with respect to national regulations of several countries on narcotics, psychotropic drugs, explosives, hazardous materials, and toxic agents." The "Headers" section contains a table with the following data:

KEY	VALUE
Content-Type	application/json
X-API-Key	sk_6e2630da33e44360a360a4a3d8d1ec07

The "Request body" section shows a "Request body example" in a code block:

```
{
  "categories": [
    "CN",
    "US"
  ],
  "structure": "caffeine"
}
```

At the bottom of the interface, a table header is partially visible with columns: PATH, TYPE, REQUIRED, and DESCRIPTION.

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

Chemicalize PRO

Chemicalize Professional - Ho: X
https://pro.chemicalize.com/app/calculations/api

API

Warning: You don't have active subscription for calculation API, so you can use it for evaluation purposes only. [Learn more](#)

- POST** **Property calculation**
`/v1/calculate`
Calculation API provides structure-based predictions for molecules. Available calculations include elemental analysis, names and identifiers, pKa, logP/logD, and solubility.
- POST** **Image generation**
`/v1/image`
Image generation API lets you generate high-quality molecule images in various output formats (SVG, PNG, JPEG).
- POST** **Structure search**
`/v1/search/structure`
Structure Search API lets you match a query structure to a target molecule in different ways (substructure search, duplicate check, etc).
- POST** **Similarity search**
`/v1/search/similarity`
Similarity Search API gives you a similarity score for two compounds. The score is real value between 0 and 1 (inclusive), which is based on the maximum common substructure (MCS) of the compounds.

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

Chemicalize Professional - Home

https://www.liverpoolchirochem.com

Who We Are

STRUCTURE SEARCH

aspirin

Substructure search

No results for the query.

Chemicalize Professional - Home

Zosimos

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

Zosimos Study Sets Submissions Study Groups

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 intermediate in the previous reaction?

What is the product in the following reaction? 1/3 attempts

Marvin JS by ChemAxon

Powered by ChemAxon

CHECK ANSWER

CURRENCY: USD MENU

ACCOUNT \$ 0.00*

SETTING UP AN ACCOUNT

Order, Payment & Shipping information

SEARCH

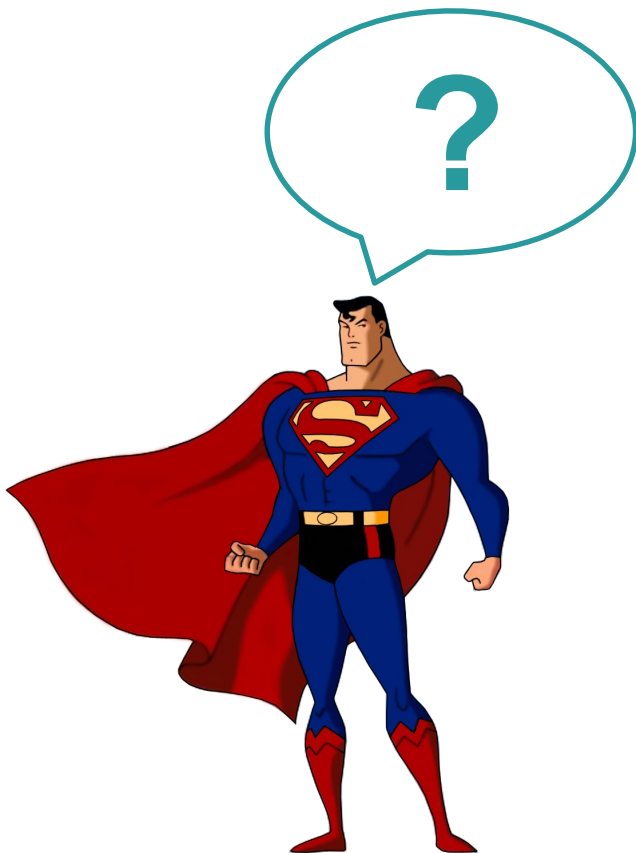
Accept



ARCHITECTURE

CHALLENGES AND SOLUTIONS

- High availability
- Maintainability
- Modifiability
- Scalability
- Security



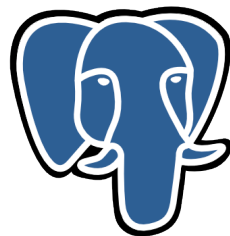
CHALLENGES AND SOLUTIONS



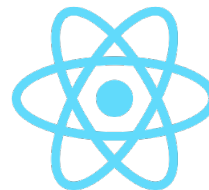
- Microservices (aws)
- Monitoring
- System logs
- Automatic backups
- Access management
- Release and upgrade management



Spring **Cloud**



Postgre**SQL**



React

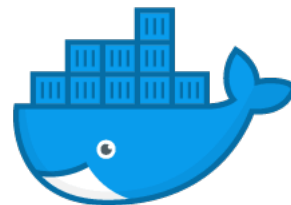


mongo**DB**.
Atlas

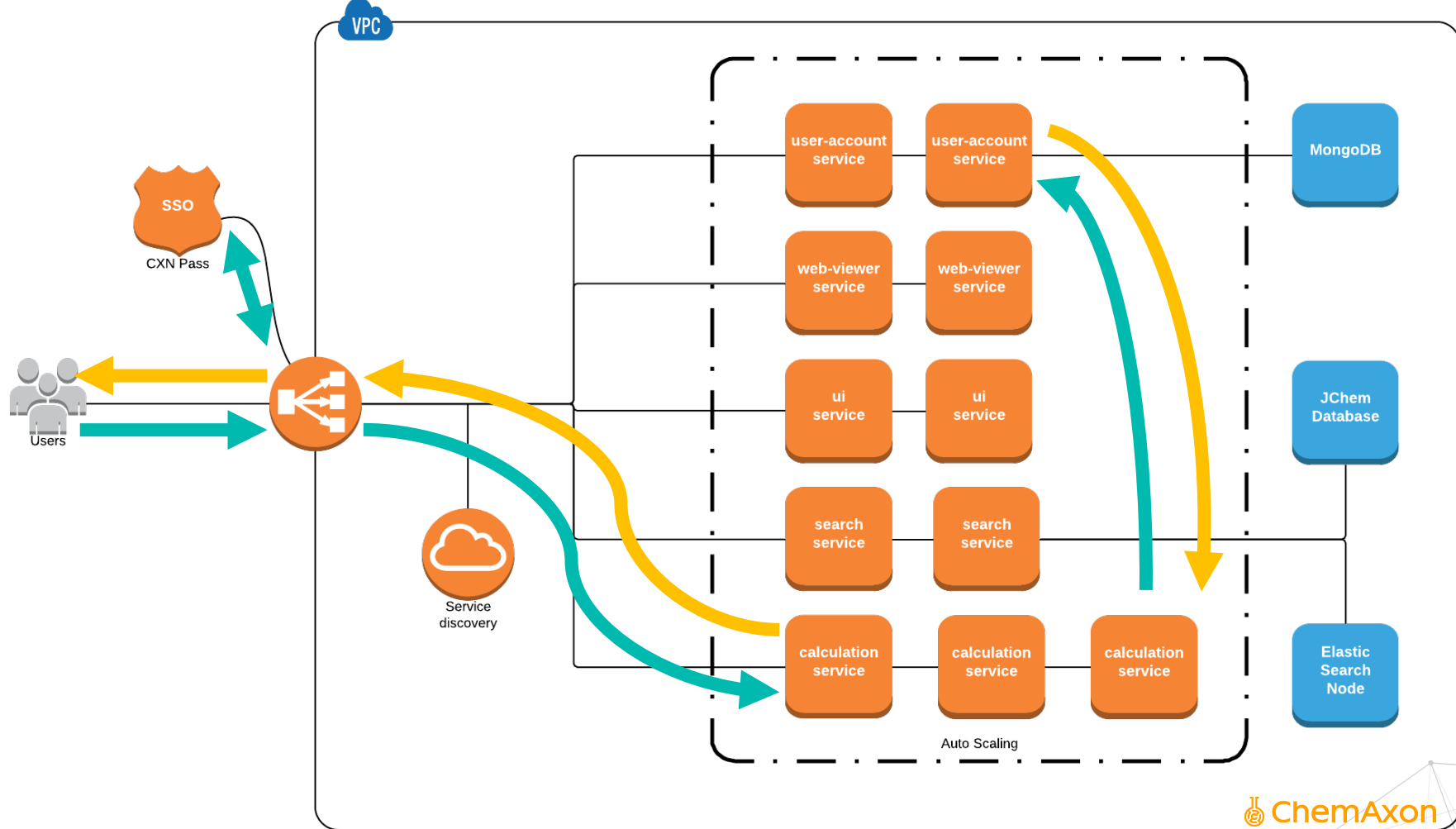


elastic

stripe



docker



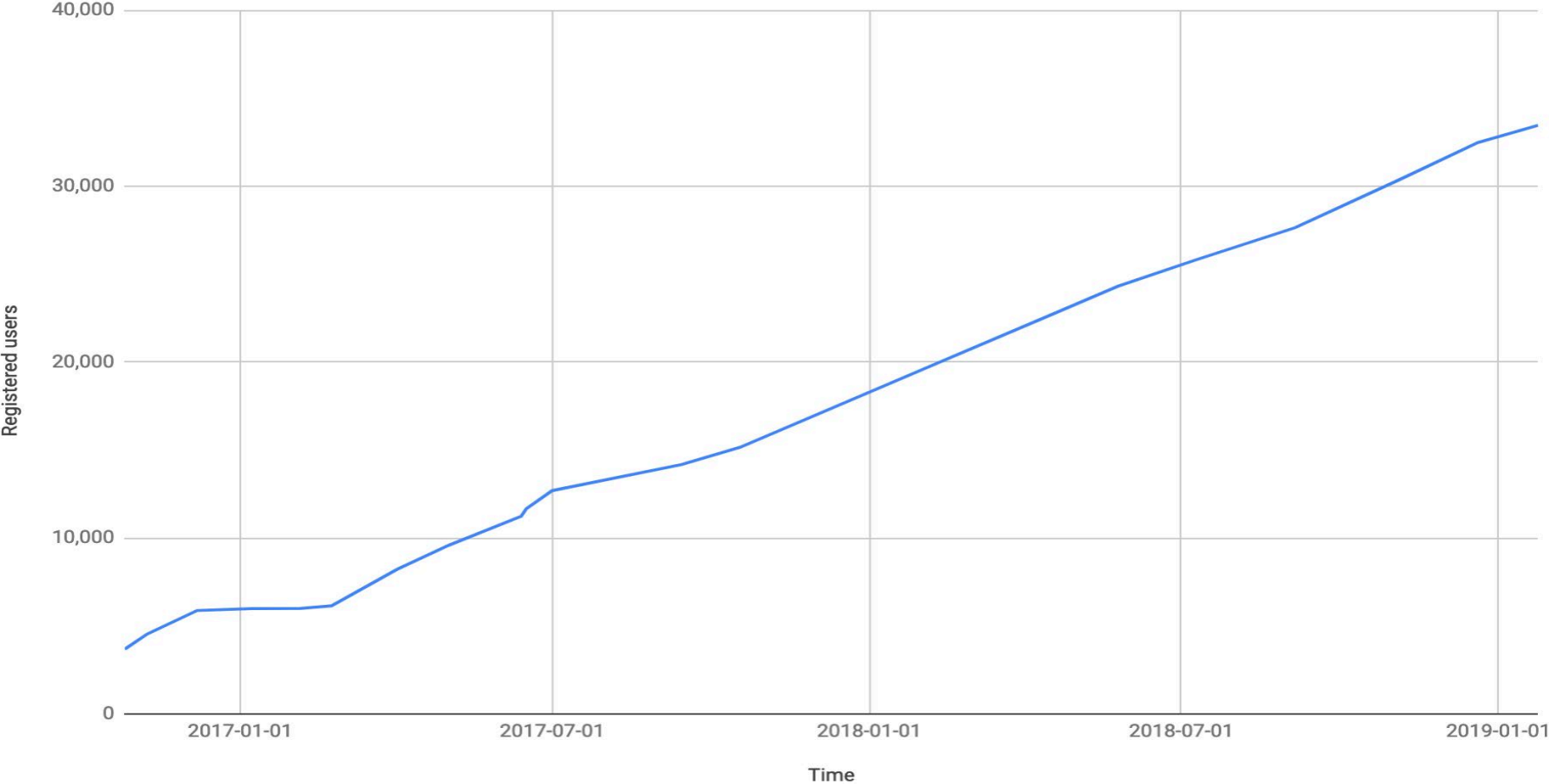


STATISTICS

Data driven development

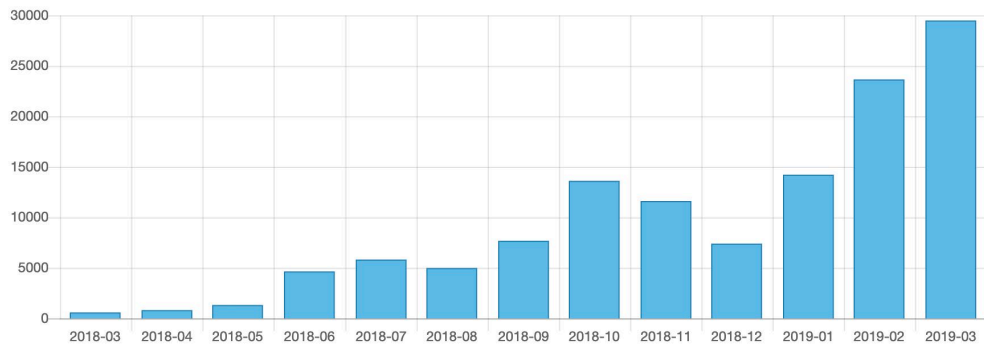


Chemicalize Users

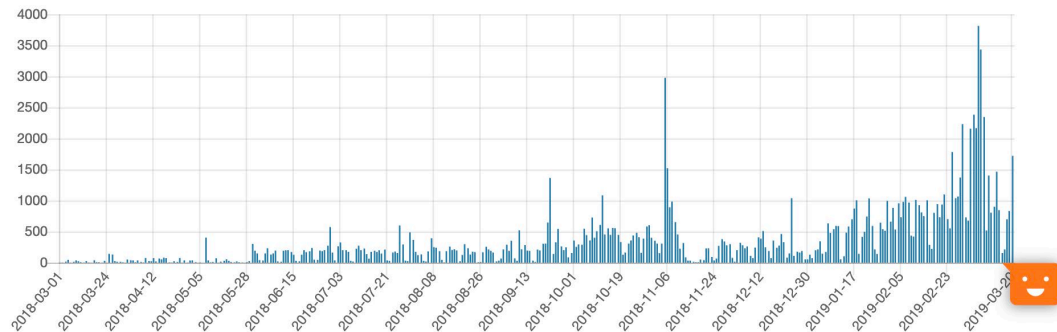


Chemicalize PRO – Hosted search

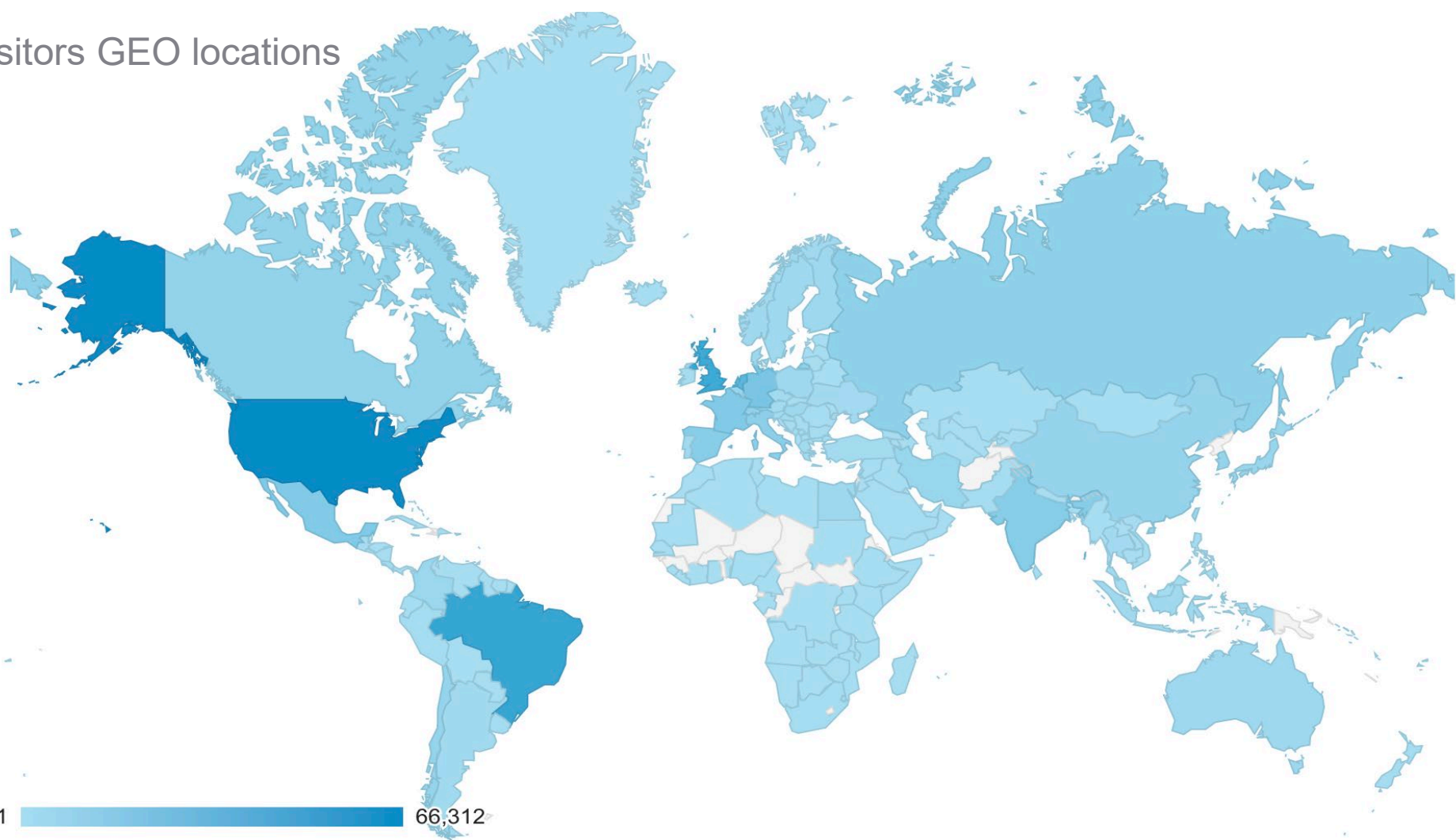
Monthly search count



Daily search count



Visitors GEO locations

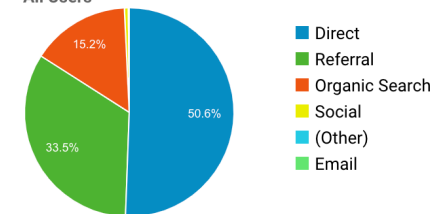


Social Network	Sessions	% Sessions
1. reddit	735	25.99%
2. Twitter	726	25.67%
3. Facebook	584	20.65%
4. ResearchGate	455	16.09%
5. LinkedIn	167	5.91%
6. VKontakte	80	2.83%
7. Blogger	58	2.05%
8. Google+	7	0.25%
9. Stack Exchange	4	0.14%
10. SlideShare	3	0.11%

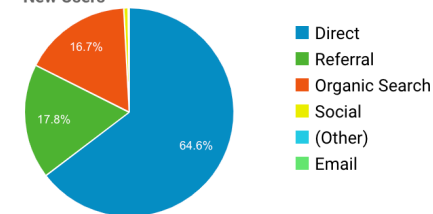
Event Action	Total Events	% Total Events
1. CALCULATION/PRINT_PDF	7,473	23.44%
2. click	7,302	22.90%
3. CALCULATION/DOWNLOAD_ZIP	6,331	19.86%
4. DRAWING/EXPORT_IMAGE	3,975	12.47%
5. S_SEARCH/CALCULATION	2,800	8.78%
6. CALCULATION/SHOW_IN_3D	2,708	8.49%
7. S_SEARCH/DOCUMENT_SEARCH	990	3.11%
8. WEB_VIEWER/ANNOTATE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

Top Channels

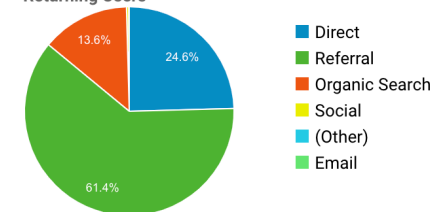
All Users



New Users



Returning Users





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](#)

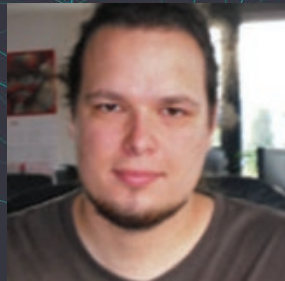
Chemical Drawing

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](#)



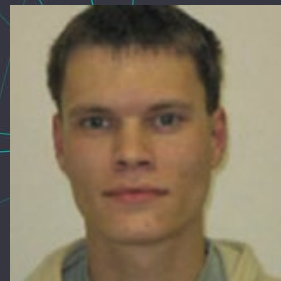
Arpad Figyelmese



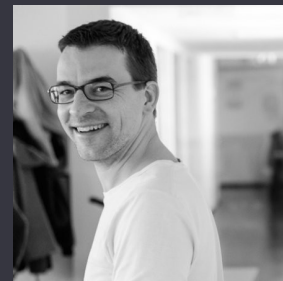
Gabor Botka



Peter Kovacs



Gabor Hornyak



Zsolt Varga

THANK YOU

Jozsef David