

BULZ

#meetCXN

**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?

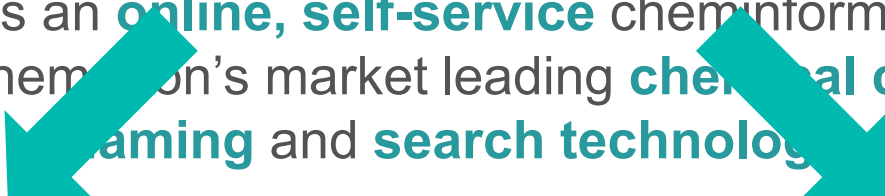
Who do I send the renewal request to?

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:

chemicalize.org^{alpha} Open All Close All Manage calculations Layout: Medicinal Chemist (4aS,6aR,6aS,6bR,8aR,1 Search

Molecule

Name
IUPAC name: (4aS,6aR,6aS,10R,11R,14bS)-10,11-dihydroxy-2,2,5a,6b,9,9,12a-heptamethyl-1,2,3,4,4a,5,5,9a,9b,7,8,8a,9,10,11,12,12a,12b,13,14b-tetrahydrocyclopene-4a-carboxylic acid
Traditional name: (4aS,6aR,6aS,10R,11R,14bS)-10,11-dihydroxy-2,2,5a,6b,9,9,12a-heptamethyl-1,3,4,5,6,7,8,8a,10,11,12,12b,13,14b-tetrahydrocyclopene-4a-carboxylic acid

Elemental Analysis
Formula: C₃₀H₄₈O₄
Isotope formula: C₃₀H₄₈O₄
Composition: C (76.23%), H (10.24%), O (13.54%)
Isotope composition: C (76.23%), H (10.24%), O (13.54%)
Mass: 472.6967
Exact mass: 472.355260024

Major Microspecies
Major microspecies at pH=7.4:

Geometry
Calculate Geometry

Lipinski-like filters
Lipinski's rule of five: no
Bioavailability: yes
Ghose filter: no
Lead likeness: no
Muegge filter: no
Veber filter: yes

Topology Analysis
Simple Ring Counts Path and distance
Atom count: 62
Bond count: 85
Cycloaromatic number: 5
Chain atom count: 12
Chain bond count: 12
Asymmetric atom count: 9
Rotatable bond count: 1

Polar Surface Area
Polar surface area: 77.75

Molecular Surface Area
Calculate Molecular Surface Area

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

- Calculations (single, batch)

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)" and buttons for DRAW, CALCULATE, and a credit indicator showing "2 credits".

The main content area is divided into two sections. The top section, titled "Basic properties", features a chemical structure of Viagra (sildenafil) and a table of its properties:

| Property | Value |
|-------------------------|---|
| 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 | ✓ |

The bottom section, titled "pKa", shows the same chemical structure with pKa values: -1.37 and 7.63. To the right is a graph of "Microspecies distribution" versus "pH". The graph shows three curves: a red curve (strongly acidic form) that is dominant at low pH, a blue curve (neutral form) that peaks around pH 7.63, and an orange curve (strongly basic form) that is dominant at high pH. The x-axis ranges from 0 to 14, and the y-axis ranges from 0 to 100. Below the graph are four small chemical structures representing the different microspecies of the molecule at different pH levels.

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 for 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. The main results area displays "More than 100 results for the query." and a grid of 20 chemical structures. On the left side of the results grid, there are filters for the number of results and their corresponding dates: "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. The browser address bar displays <https://chemicalize.com/#/document-search>. The navigation bar includes tabs for CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH (which is active), WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. A search bar at the top contains the text 'glycerol' and a green 'SEARCH' button. Below the search bar, a message states: 'More than 1000 results for query FULL:glycerol. Only the first 100 results are displayed.' The search results are presented in a list of cards. The first card is for 'Glycerol - Wikipedia', with a URL <https://en.wikipedia.org/wiki/Glycerol> and a snippet: '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.' The second card is for 'Piet Gros - Wikipedia', with a URL https://en.wikipedia.org/wiki/Piet_Gros and a snippet: '[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'. The third card is for 'US7569706B2 - Glycerol derivative', with a URL <https://patents.google.com/patent/US7569706B2> and a snippet: 'On the contrary to this, in the formula(I), 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.' The fourth card is for 'US9315440B2 - Process for obtaining acrolein by catalytic dehydration of glycerol or glycerin', with a URL <https://patents.google.com/patent/US9315440B2> and a snippet: ', 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.' The fifth card is for 'US9079841B2 - Process for preparing acrolein from glycerol or glycerin', with a URL <https://patents.google.com/patent/US9079841B2> and a snippet: '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'. A small orange smiley face icon is visible in the bottom right corner of the search results area.

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

CHEMICALIZE

The screenshot shows a web browser window with the URL <https://chemicalize.com/#/web-viewer>. The browser's address bar also shows <https://wikipedia.org/wiki/caffeine>. The page features a navigation bar with options: CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE, BATCH, DRAWING. A sidebar on the left contains a 'Structures' section with four chemical structures of caffeine (1,3,7-trimethylxanthine) and a 'WIKIPEDIA The Free Encyclopedia' logo. The main content area displays the Wikipedia article for 'Caffeine', including its chemical structure, a 3D ball-and-stick model, and a table of clinical data. The clinical data table lists pronunciation, synonyms, and other information.

| Clinical data | |
|---------------|---|
| Pronunciation | <i>ˈkæfˌeɪn</i> , <i>ˈkɔːfɪn</i> / <i>ˈkɔːfɪn</i> / |
| Synonyms | Guaranine Methyltheobromine 1,3,7-Trimethylxanthine |

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

CHEMICALIZE

The screenshot displays the Chemicalize web interface. At the top, the browser address bar shows the URL <https://chemicalize.com/#/compliance>. The navigation menu includes options like CALCULATION, STRUCTURE SEARCH, DOCUMENT SEARCH, WEB VIEWER, COMPLIANCE, BATCH, and DRAWING. The current search term is 'methamphetamine'. Below the search bar, there are buttons for 'DRAW', 'CHECK', and '5 credits'. The main content area features a 'Compliance Check Report' for 'methamphetamine'. On the left, there are two chemical structure diagrams: a small one and a larger one with stereochemistry. The report table lists various legislative controls across different countries.

| # | 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, Cn H2n-1 (n=3-5), acetyl, benzyl, methoxybenzyl, (CH2)n(n=4-6), cycloalkyl, haloalkyl, hydroxyalkyl, cyanoalkyl, cyclopropylmethyl, furylmethyl of methylendioxybenzyl, 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 methylendioxybenzyl. De amfetaminactien 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 de amino 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 meerdere substitues 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-EDI) Narcotics List A | Methamphetamine [(+)-isomer] |
| 6 | CN Incitant | metamfetamine (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 (which is active). The user's name is JOZSEF and they have 75 credits. The main workspace is titled "Name your structure" and contains a chemical drawing tool with a toolbar on the left and a central canvas. The canvas shows a chemical structure of a diester with a central hydroxyl group. The right sidebar has two sections: "PROPERTIES" and "IMAGE EXPORT". The "PROPERTIES" section is expanded to show "Basic properties":

| | |
|-------------------------|---|
| Molar mass | 206.194 g/mol |
| Exact mass | 206.079038171 Da |
| Formula | C ₈ 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 of the interface shows a status bar with icons for file operations and a small orange smiley face icon.

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



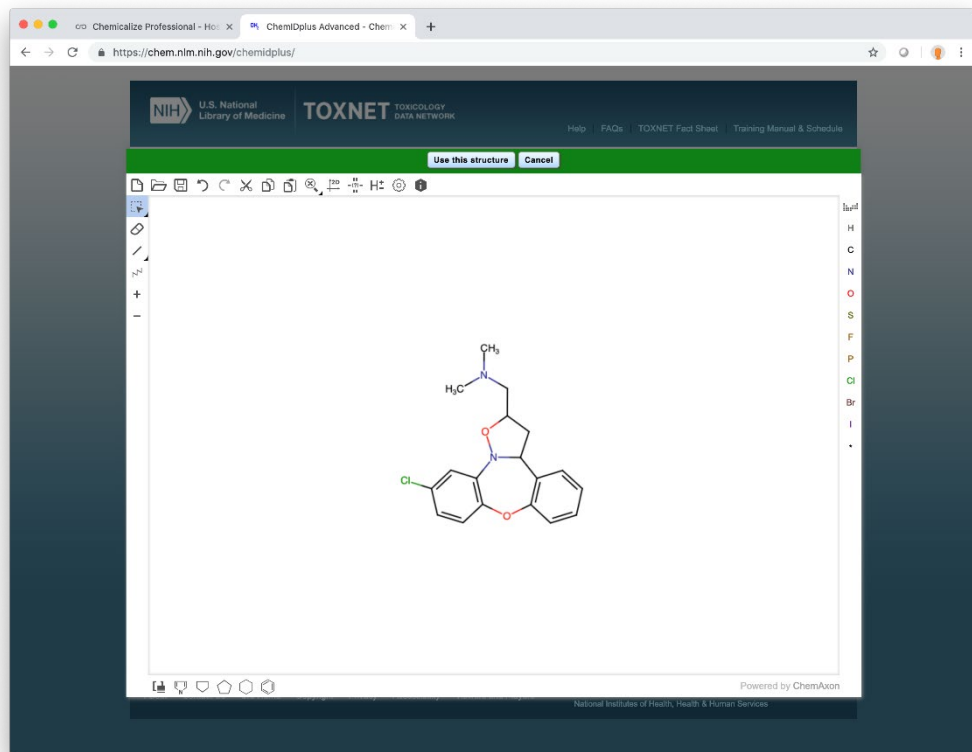
CHEMICALIZE PRO

CHEMICALIZE PRO

The screenshot displays the Chemicalize Pro web application interface. The browser address bar shows the URL <https://pro.chemicalize.com/api/search/demo>. The page 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 (CKN), and ADMIN. The main content area has a search bar containing the text "naphthalene". Below the search bar is a large canvas displaying a chemical structure of benzene. To the right of the canvas is a legend with colored circles corresponding to elements: H (white), C (grey), N (blue), O (red), S (yellow), F (green), P (orange), Cl (light blue), Br (dark blue), and I (purple). Below the canvas is a "Substructure search" input field with a "SEARCH" button. The search results are displayed in a grid of chemical structures, each with a numerical ID below it: 1001 (benzene), 1007 (indole), 1006 (N-methylphenethylamine), 1005 (4-(2-hydroxyethyl)phenylamine), 1002 (salicylic acid), and several other complex structures in the bottom row.

- Hosted catalog search

CHEMICALIZE PRO



- Hosted catalog search
- Hosted chemical drawing

CHEMICALIZE PRO

The screenshot displays the Chemicalize Pro web application interface. The browser address bar shows the URL `https://pro.chemicalize.com/app/cchecker/api`. The left sidebar contains navigation options: Dashboard, Hosted Search, Chemical Drawing, Compliance Checker, 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 endpoint 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 | ak_6e2630da33e44360a360a4a3d8d1ec07 |

The "Request body" section includes a "Request body example" with the following JSON structure:

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

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

CHEMICALIZE PRO

Chemicalize Pro

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**

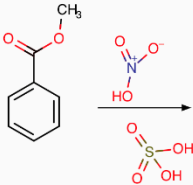
Chemicalize Professional - Ho...
https://www.liverpoolchirochem...
LIVERPOOL CHIROCHEM
Who We Are
STRUCTURE SEARCH
aspirin
No results for the query.

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?

CC(=O)c1ccccc1.O=[N+]([O-])O.OS(=O)(=O)O>>
- 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?

Marvin JS by ChemAxon

Powered by ChemAxon

CHECK ANSWER

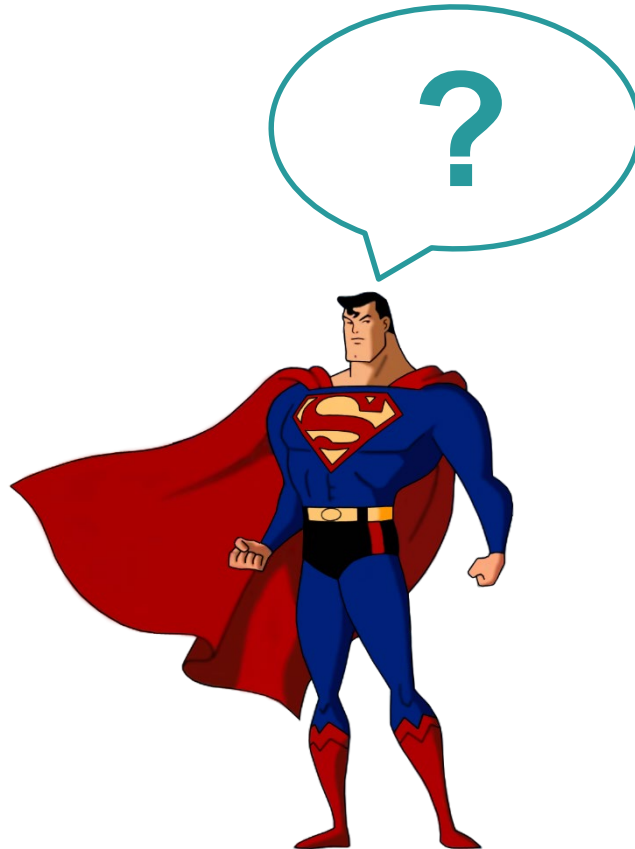
CURRENCY: USD MENU
ACCOUNT \$ 0.00+
SETTING UP AN ACCOUNT
Order, Payment & Shipping information
SEARCH



ARCHITECTURE

CHALLENGES AND SOLUTIONS

- High availability
- Maintainability
- Modifiability
- Scalability
- Security



CHALLENGES AND SOLUTIONS



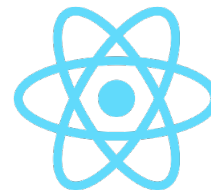
- Microservices (aws)
- Monitoring
- System logs
- Automatic backups
- Access management
- Release and upgrade management



Spring **Cloud**



Postgre**SQL**



React



mongo**DB**.
Atlas

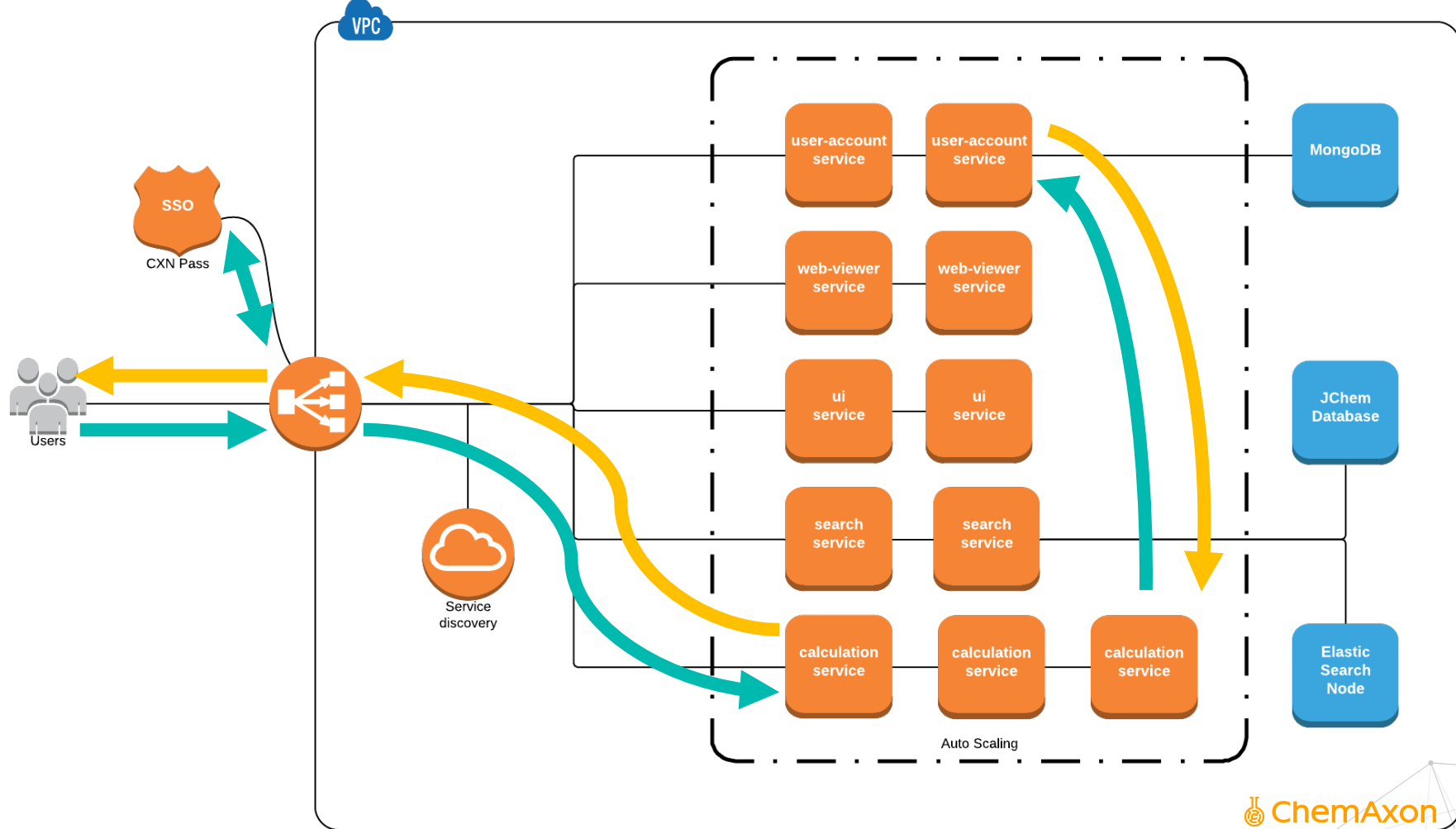


elastic

stripe



docker

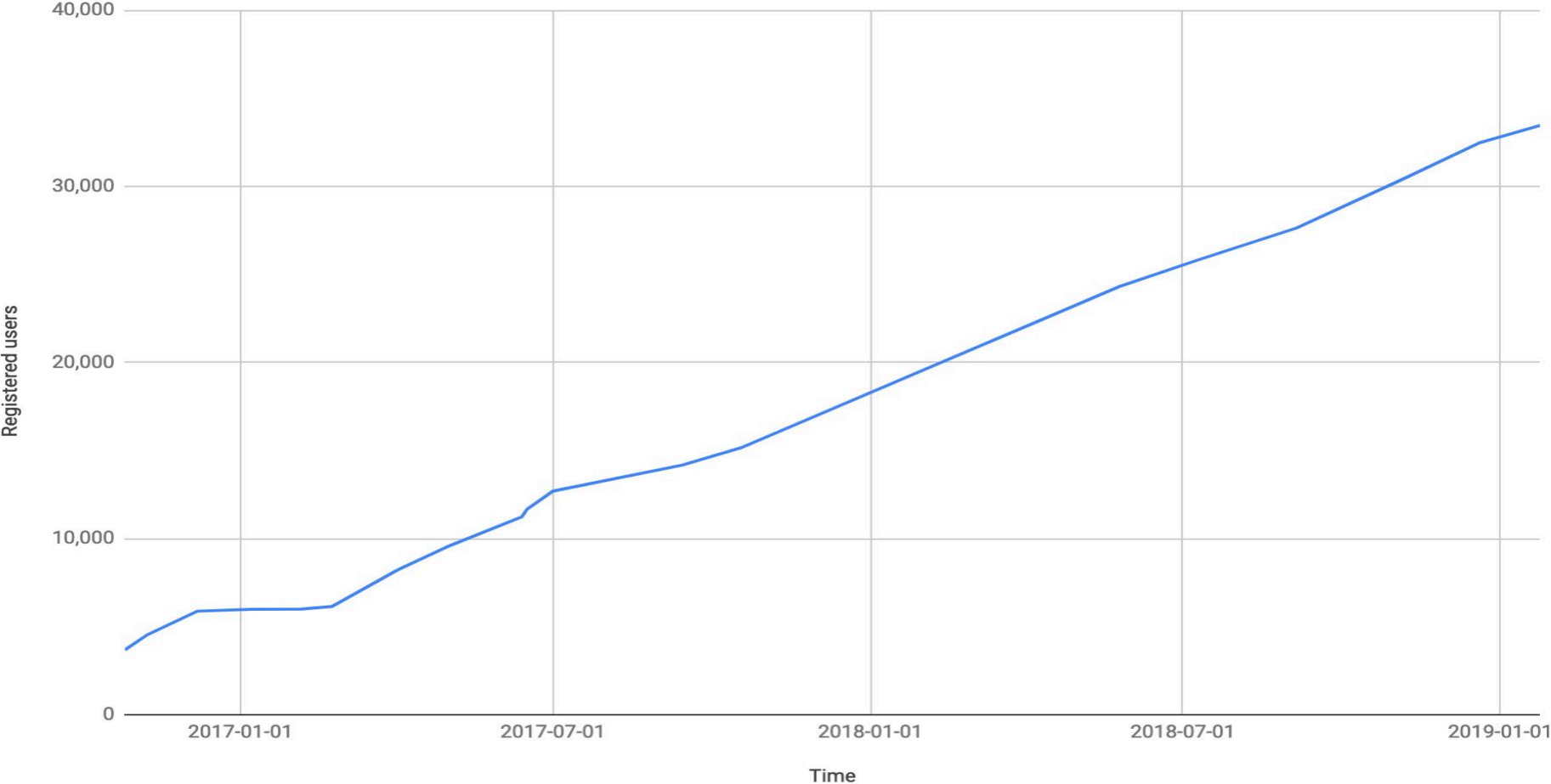




STATISTICS – DATA DRIVEN DEVELOPMENT

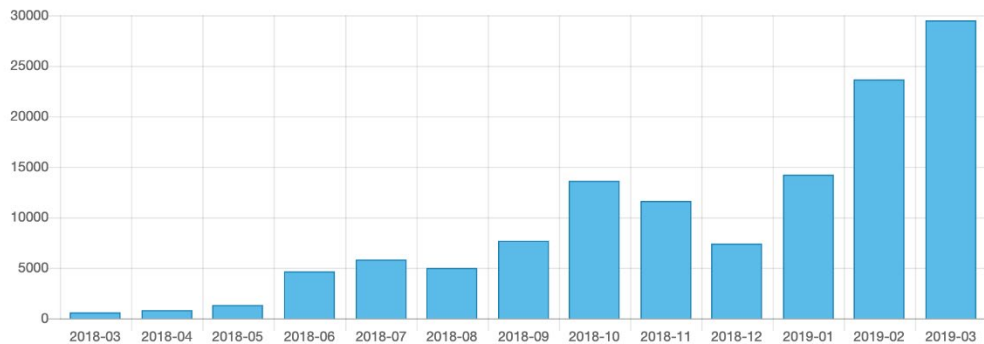


Chemicalize Users

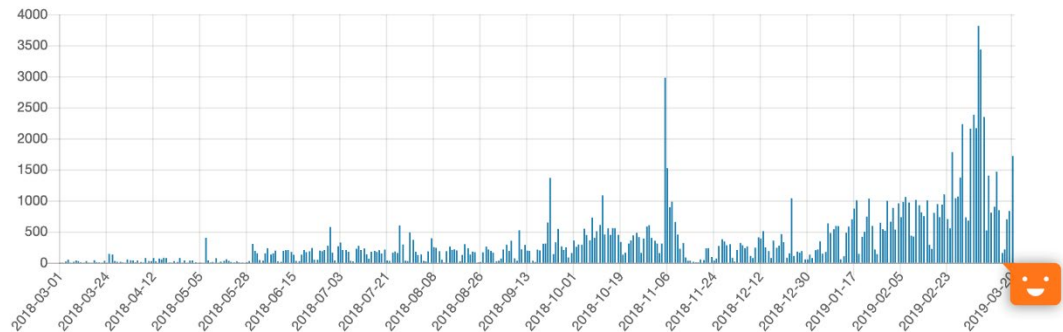


CHEMICALIZE PRO – HOSTED SEARCH

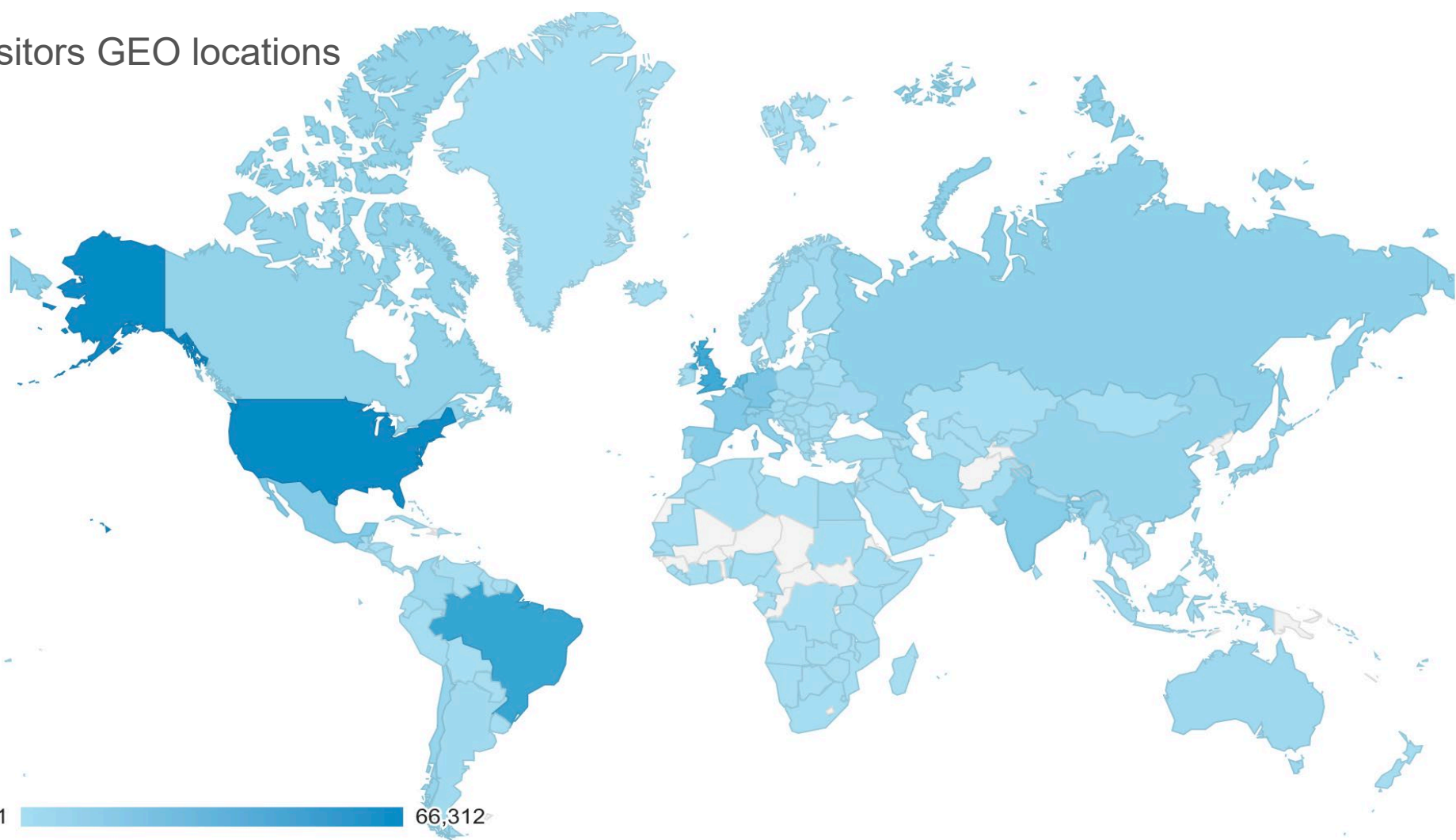
Monthly search count



Daily search count



Visitors GEO locations

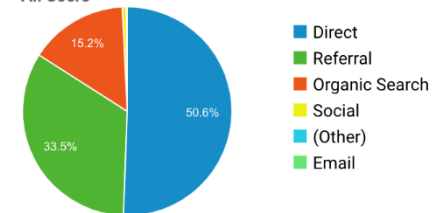


| Social Network | Sessions | % Sessions |
|-------------------|----------|------------|
| 1. reddit | 735 | 25.99% |
| 2. Twitter | 726 | 25.67% |
| 3. Facebook | 584 | 20.65% |
| 4. ResearchGate | 455 | 16.09% |
| 5. LinkedIn | 167 | 5.91% |
| 6. VKontakte | 80 | 2.83% |
| 7. Blogger | 58 | 2.05% |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

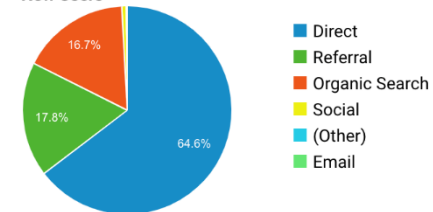
| Event Action | Total Events | % Total Events |
|-----------------------------|--------------|----------------|
| 1. CALCULATION/PRINT_PDF | 7,473 | 23.44% |
| 2. click | 7,302 | 22.90% |
| 3. CALCULATION/DOWNLOAD_ZIP | 6,331 | 19.86% |
| 4. DRAWING/EXPORT_IMAGE | 3,975 | 12.47% |
| 5. S_SEARCH/CALCULATION | 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

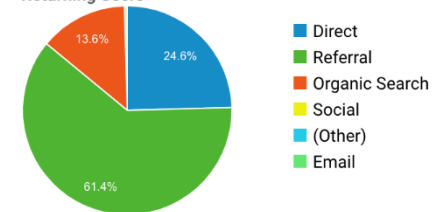
All Users



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](#)

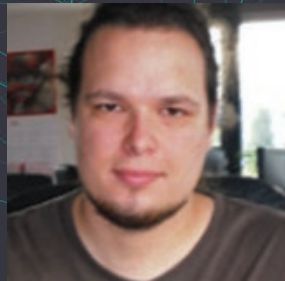
Chemical Drawing

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](#)



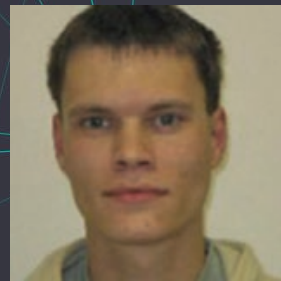
Arpad Figyelmese



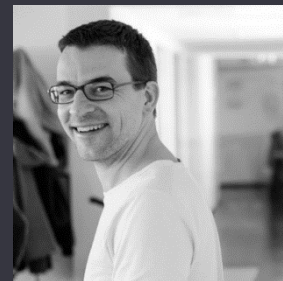
Gabor Botka



Peter Kovacs



Gabor Hornyak



Zsolt Varga

THANK YOU

Jozsef David