

COMPLIANCE CHECKER

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The Revamped Compliance Checker

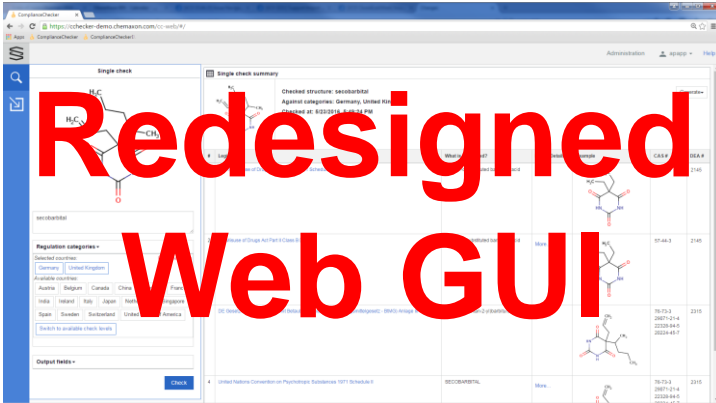
1.0
Released

RESTful Web Service

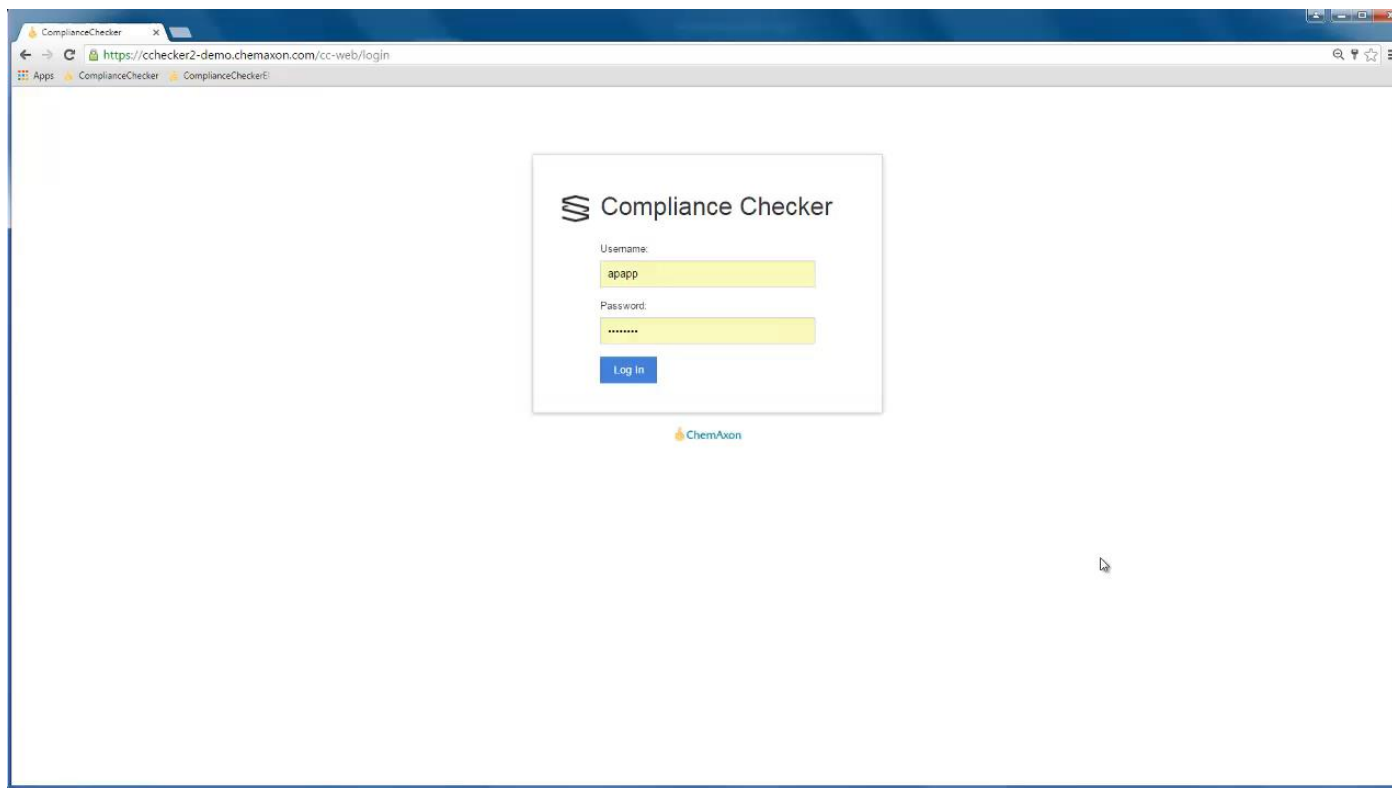
Powerful API

60x
faster

**Redesigned
Web GUI**



Single Check



Batch Check

The screenshot displays the 'Batch check from file' interface in the ComplianceChecker application. The left sidebar contains navigation icons for home, search, and a document icon. The main content area is divided into two sections: a configuration panel on the left and a table of uploaded files on the right.

Batch check from file

Check multiple molecules at once by uploading a source file. A report of the molecules and corresponding legislations will then be created and added to the table.

[Choose file](#)

Regulation categories ▾

Selected countries:

All (click on the buttons to specify countries)

Available countries:

Austria Belgium Canada China Denmark France

Germany India Ireland Italy Japan Netherlands

Singapore Spain Sweden Switzerland

United Kingdom United States of America

[Switch to available check levels](#)

Report formats ▾

Report contains ▾

Description (optional) ▾

[Check](#)

Uploaded files

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First Previous 1 Next Last

Uploaded file name	Download last reports	#Input	#Hit	#Passed	Started at	Progress	Actions
random.smiles	PDF	1000	34	966	5/23/2016, 4:36:54 PM	Done(7 s)	
Maybridge_HitDiscover.sdf	MRV	52160	151	52009	5/11/2016, 4:14:03 PM	Done(598 s)	
nci100000.smiles	PDF	100000	3820	96180	5/11/2016, 3:52:14 PM	Done(567 s)	
nci10000.smiles	PDF	10000	382	9518	5/11/2016, 1:56:41 PM	Done(98 s)	
CSCS Confirmed Test Set 2015_02_28.sdf	PDF MRV XLSX	306	212	94	5/11/2016, 1:55:10 PM	Done(17 s)	
100.smiles	SDF XLSX	100	1	99	5/11/2016, 1:53:01 PM	Done(1 s)	
40_mols.mrv	PDF	40	1	39	5/11/2016, 1:52:35 PM	Done(0 s)	

Administration page

The screenshot shows a web browser window with the URL `https://cchecker-demo.chemaxon.com/cc-web/#/`. The page is titled "ComplianceChecker" and has a navigation bar with "Exit administration", a user profile "apapp", and a "Help" link. The main content area is divided into two sections: "Category editor" and "User defined levels".

Category editor
Create or edit categories

Montreal Protocol on Substances that Deplete the Ozone Layer	MPO
Rotterdam Convention on the Prior Informed Consent Procedure for Certain Hazardous Chemicals and Pesticides in International Trade	RCT
The Convention on the prohibition of the development, production, stockpiling, and use of chemical weapons and on their destruction	CWC
United Nations	UN

User defined levels:

Chemical weapons	USR4
Dual-use Items transport	USR3
European Union	USR5

Close

UK only

This settings contains the following legislations:

Id	Name	URLs
709	UK Misuse of Drugs Act Part I Class A Drugs	\$\$\$\$
710	UK Misuse of Drugs Act Part II Class B Drugs	\$\$\$\$\$\$
729	UK Misuse of Drugs Act Part III Class C Drugs	\$\$\$\$
981	UK The Misuse of Drugs Regulations 2001 Schedule I	\$\$\$\$\$\$\$\$\$\$\$\$
1038	UK The Misuse of Drugs Regulations 2001 Schedule II	\$\$\$\$\$\$\$\$\$\$
1040	UK The Misuse of Drugs Regulations 2001 Schedule IV	\$\$\$\$\$

Integration API

Swagger UI

https://cchecker2-demo.chemaxon.com/cc-bigdata/#/integration/checkListRestrictionUsingPOST_1

integration

: Service for integrating ComplianceChecker functionalities in other softwares.

Show/Hide | List Operations | Expand Operations

- GET** /integration/categories Returns the available countries
- GET** /integration/categories/simple Returns all the available categories, including countries and check levels
- GET** /integration/check Checks a single molecule. The molecule is passed as a Get variable
- POST** /integration/check Checks a single molecule. The molecule is passed as a Post message
- POST** /integration/check/list Checks a list of molecules.

Response Class (Status 200)

Model | Model Schema

```
{
  "categoryLabel": "string",
  "checkTime": {},
  "simpleResponses": [
    "List"
  ]
}
```

Response Content Type: application/json

Parameters

Parameter	Value	Description	Parameter Type	Data Type
request	<pre>{ "categories": ["string"], "input": ["string"] }</pre>	The list of sources of molecules as a JSON List of Strings	body	Model Model Schema

```
{
  "categories": [
    "string"
  ],
  "input": [
    "string"
  ]
}
```

Performance

- 100 compounds per second
 - on a single medium-type Amazon server (m4.xlarge)
- Almost linear scale up with increasing the
 - Performance of the server
 - The number of computation servers

Accuracy

Country	Pass Rate
Canada	100%
France	100%
USA	99%
UK	99.7%
Sweden	100%
Switzerland	100%



Coverage

Austria	Belgium	Canada	China	Denmark	
France	Germany	India	Ireland	Italy	Japan
Netherlands	Singapore	Spain	Sweden	Switzerland	
United Kingdom	United States of America				

Community regime for the control of export, transfer, brokering and transit of dual-use items	CDU
European Union	EU
Montreal Protocol on Substances that Deplete the Ozone Layer	MPO
Rotterdam Convention on the Prior Informed Consent Procedure for Certain Hazardous Chemicals and Pesticides in International Trade	RCT
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Roadmap

- Integration into Plexus
- Pay-per-view services
 - Integration into Chemicalize
 - Standalone pay-per-view site
- Hosted solutions

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Tamás
Varga

Krisztina
Vajda

Ádám
Villei



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