



Off the shelf, quick to start & easy to use data management solution for SMEs

Cloud Solution for Early Drug Discovery Data Management

Webinar December 6th 2018

Presented by Lenka Cardova & Csaba Peltz

Who we are



Lenka Cardova

IT Business Analyst
ChemAxon



Csaba Peltz

Product Owner of Cloud Solutions
ChemAxon

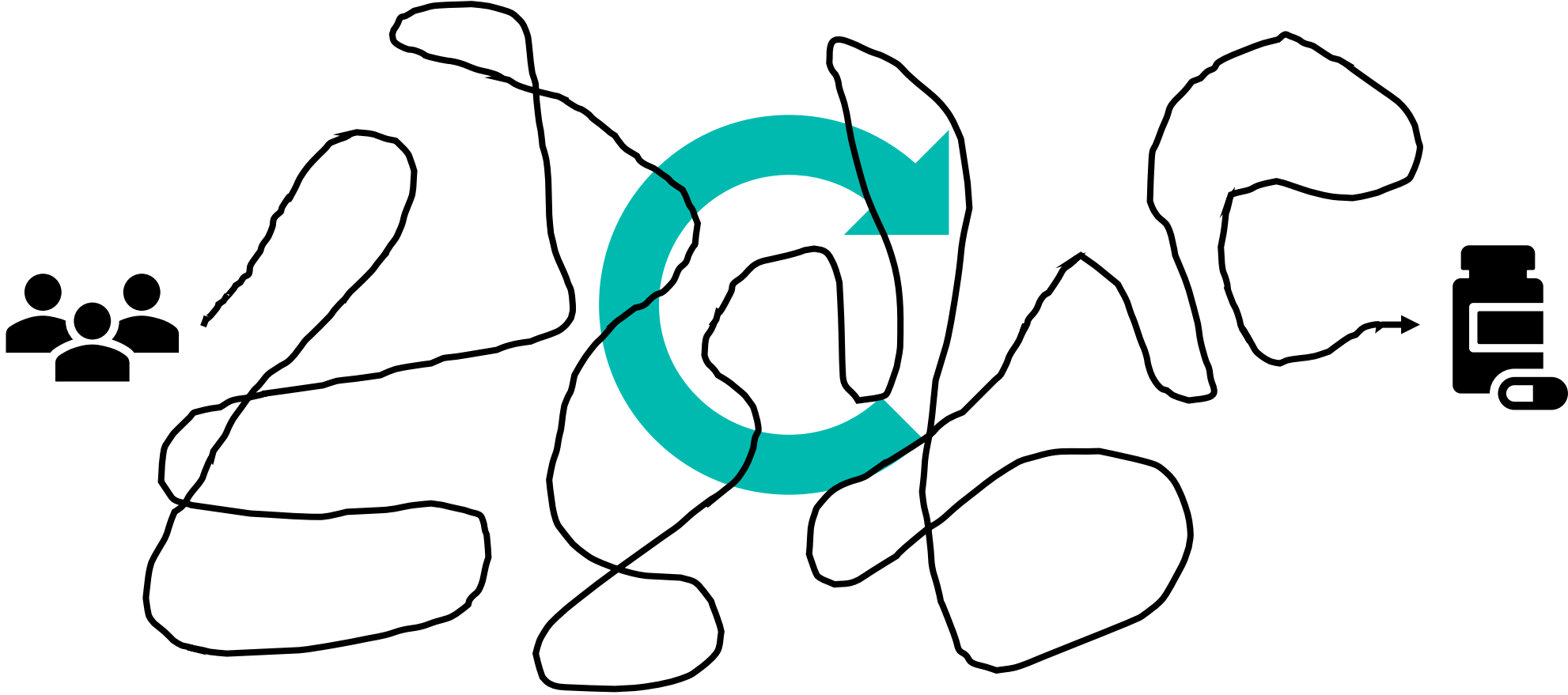
Objective

To encourage you to step into the world of ChemAxon's cloud solutions.

How does the discovery process look like?







Agenda

Integrated Compound and Assay Data Management



Compounds

Assay

SAR analysis

Library of Congress (USA)



1800

6 487



16 000 000

How do you store data?



Stuttgart City Library (DE)



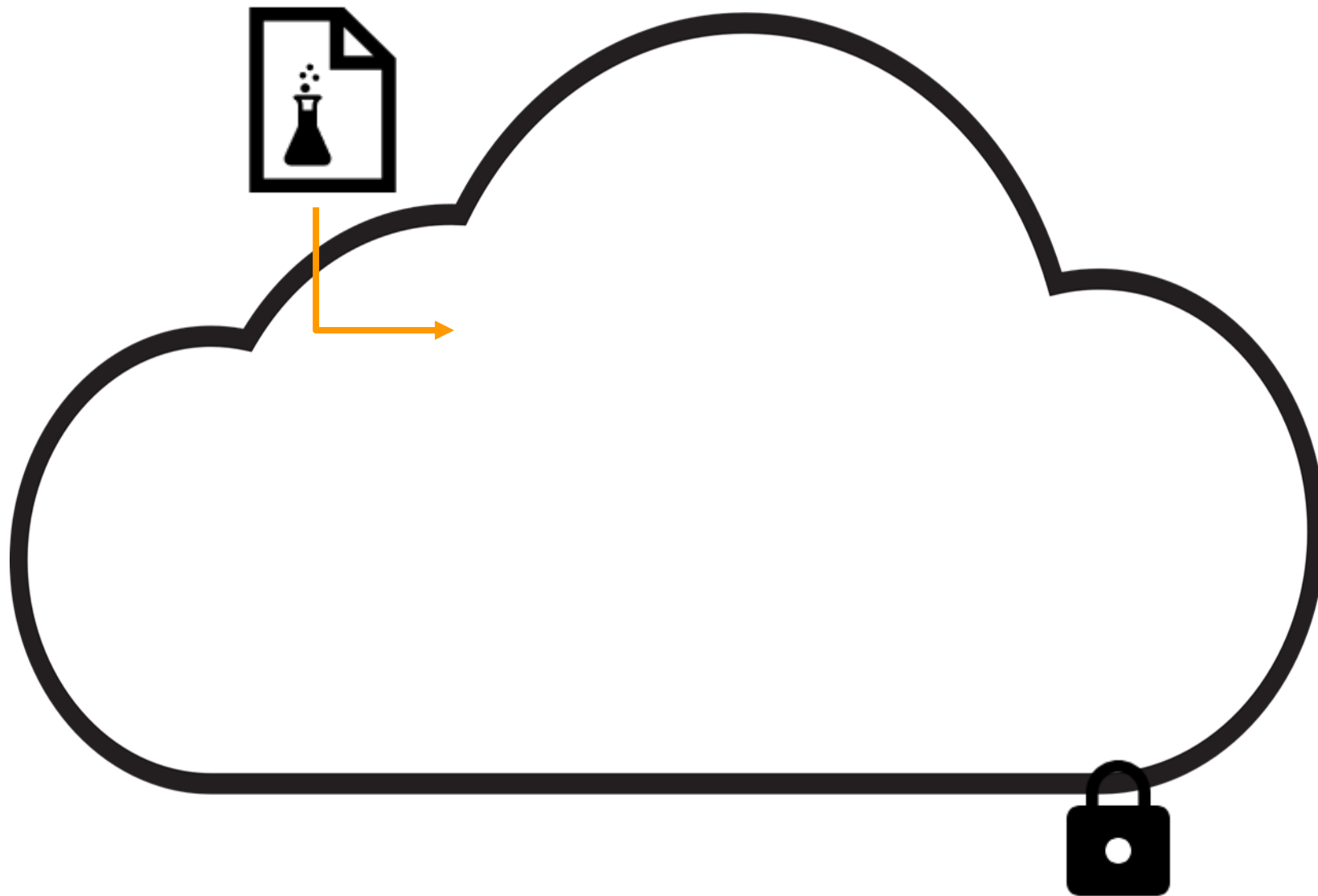
What is the purpose of a library?



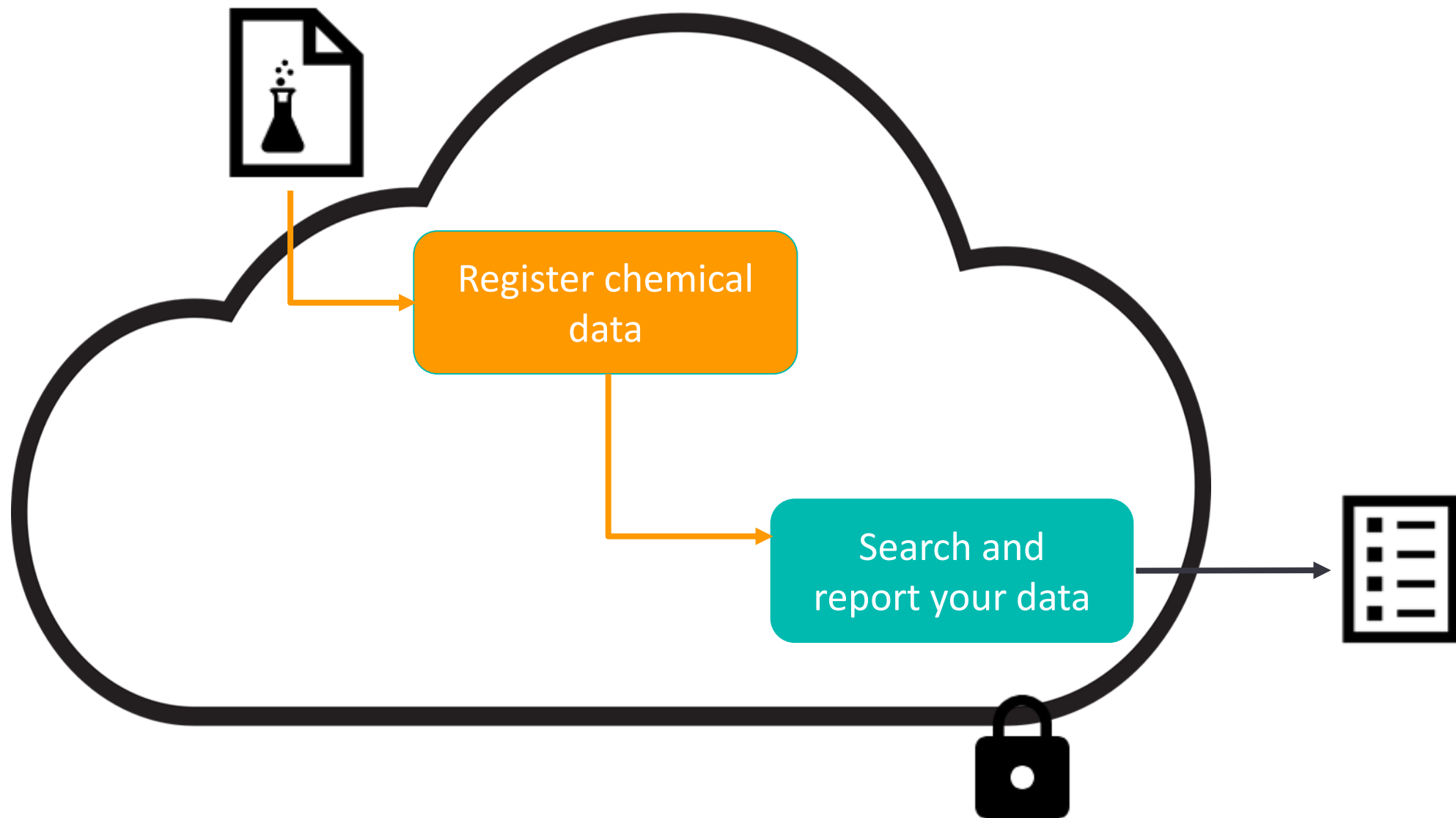
What better fits your needs & budget?



Integrated Compound and Assay Data Management



Integrated Compound and Assay Data Management



Register chemical data

Registration Upload Staging Search lcardova@chemaxon.com

My Recent Registration Statistics

80
TOTAL

FAILED

SUCCESSFUL

Recently Failed Submissions

Assigned to me

LNBREF	CREATED ON
--	2018-10-11 09:24:10
--	2018-10-11 09:24:11
--	2018-10-11 09:24:11

More detailed list of submissions can be found in staging.

Recent Successful Registrations

LNBREF	PCN	CREATED ON
P1234	CXN4	2018-10-11 09:31:32
CXN7-001	CXN7	2018-10-11 09:24:12
CXN8-001	CXN8	2018-10-11 09:24:11
CXN9-001	CXN9	2018-10-11 09:24:11
CXN5-001	CXN5	2018-10-11 09:24:11
CXN6-001	CXN6	2018-10-11 09:24:10
CXN2-003	CXN2	2018-10-11 09:24:10
T123	CXN4	2018-10-11 09:18:33
W1610	CXN3	2018-10-11 09:00:40
W1016	CXN3	2018-10-11 08:39:56
CXN38-002	CXN38	2018-10-10 15:33:42
CXN39-002	CXN39	2018-10-10 15:33:41

My Latest Bulk Uploads

Silychristin_analogues.sdf 📅 2018-10-11 09:24:10 👤 lcardova@chemaxon.com	DONE
combretafuranone_analogues.sdf 📅 2018-10-10 15:33:39 👤 lcardova@chemaxon.com	DONE

Register chemical data

Registration workflow



Set QA



Structure upload

Interactive

Interactive

Bulk

Interactive

Bulk

Integrated

Register chemical data

Registration workflow



Set QA



Structure upload



View & Update

Register chemical data

Registration workflow



Set QA



Structure upload



View & Update



Integration

Downstream service

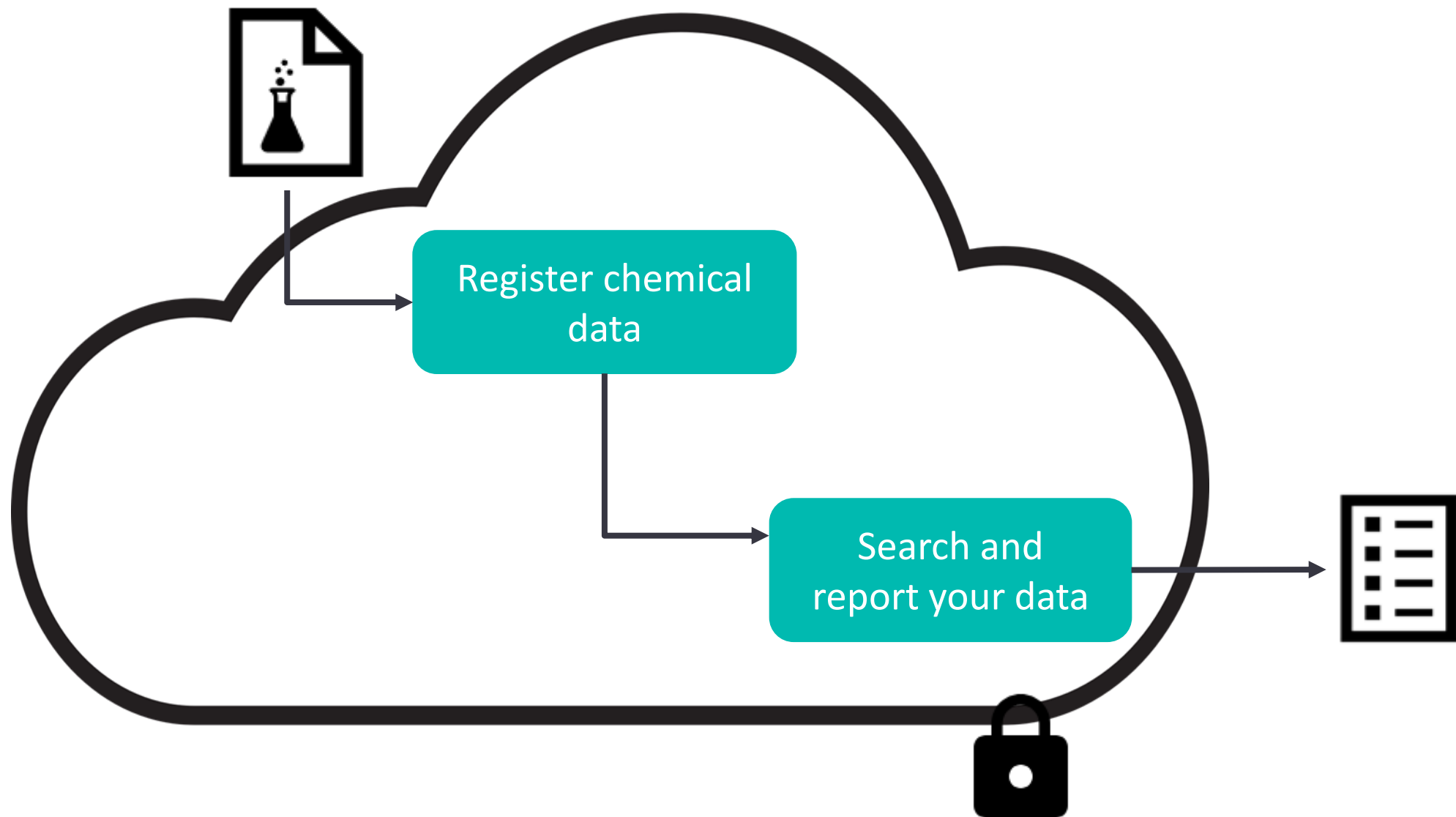
Downstream service

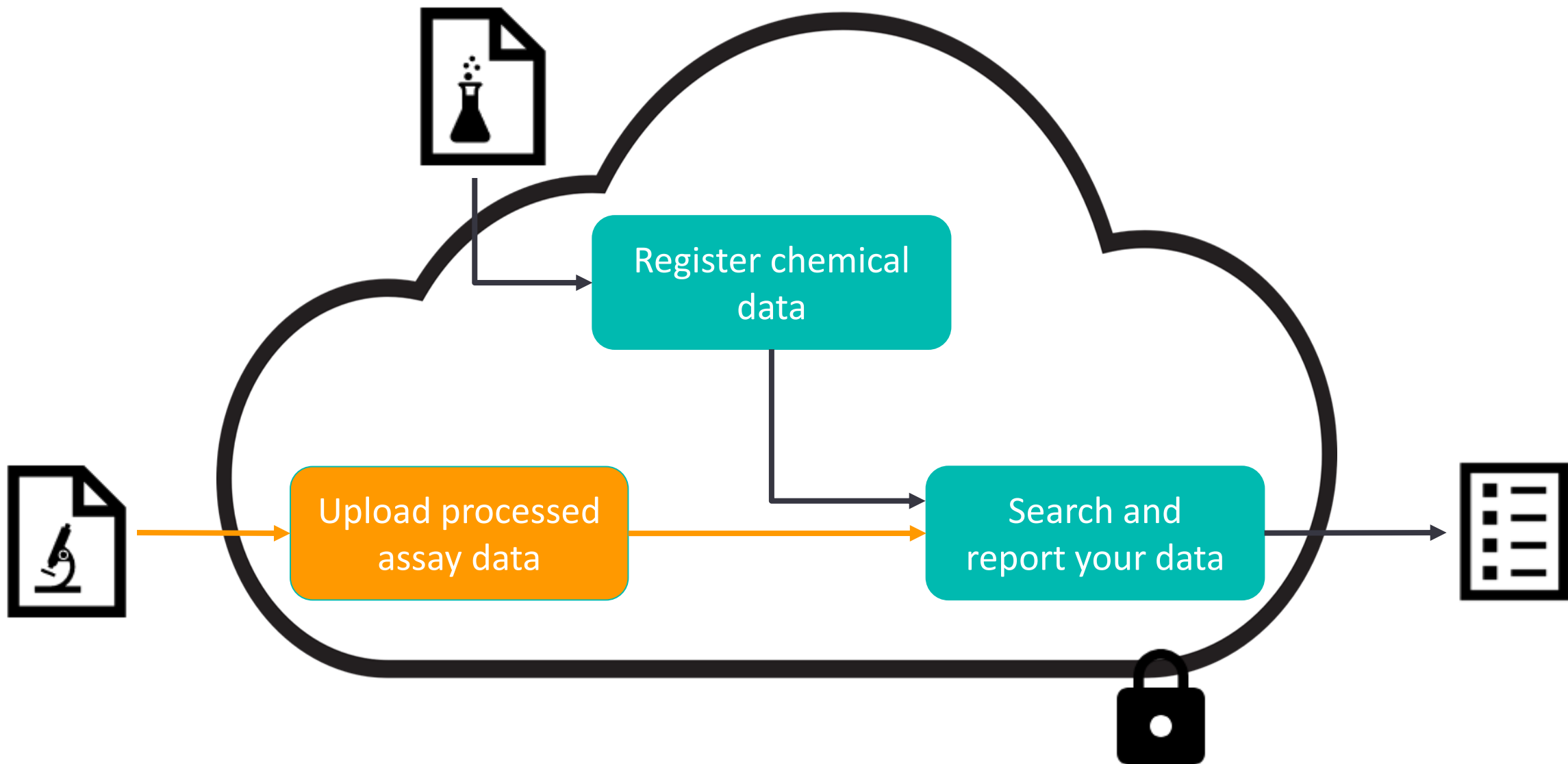
Web services

Downstream service

Web services

Upstream service





Assay data upload

Plexus Processed Data Capture Upload Parameter Types Procedures Tasks Processed Data Icardova@chemaxon.com Help

Tasks 6 items

Project Title	Task Title	Procedure	User	Date	Status
Silychristin: Skeletal Alterations and Biological...	T-0 Screening results of Silychristin analogues	Processed data upload	Icardova@chemaxon.com	11-Oct-2018	OPEN
Project 1	1st run, 1st batch	Processed data upload	ajakab@chemaxon.com	11-Oct-2018	CONFIRMED
Silychristin: Skeletal Alterations and Biological...	T-2 Screening results of Silychristin analogues	Processed data upload	ajakab@chemaxon.com	11-Oct-2018	CONFIRMED
Silychristin: Skeletal Alterations and Biological...	T-3 Screening results of Silychristin analogues	Processed data upload	ajakab@chemaxon.com	10-Oct-2018	CONFIRMED
Silychristin: Skeletal Alterations and Biological...	T-10 Screening results of Silychristin analogues	Processed data upload	Icardova@chemaxon.com	10-Oct-2018	CONFIRMED
Silychristin: Skeletal Alterations and Biological...	T-1 Screening results of Silychristin analogues	Processed data upload	Icardova@chemaxon.com	10-Oct-2018	CONFIRMED

Feedback

Upload assay data

UPLOAD workflow



SOPs



File upload

Semi-automated

Semi-automated

Automated

Semi-automated

Automated

Interactive

Upload assay data

UPLOAD workflow



SOPs



File upload



Data viewer

Upload assay data

UPLOAD workflow



SOPs



File upload



Data viewer

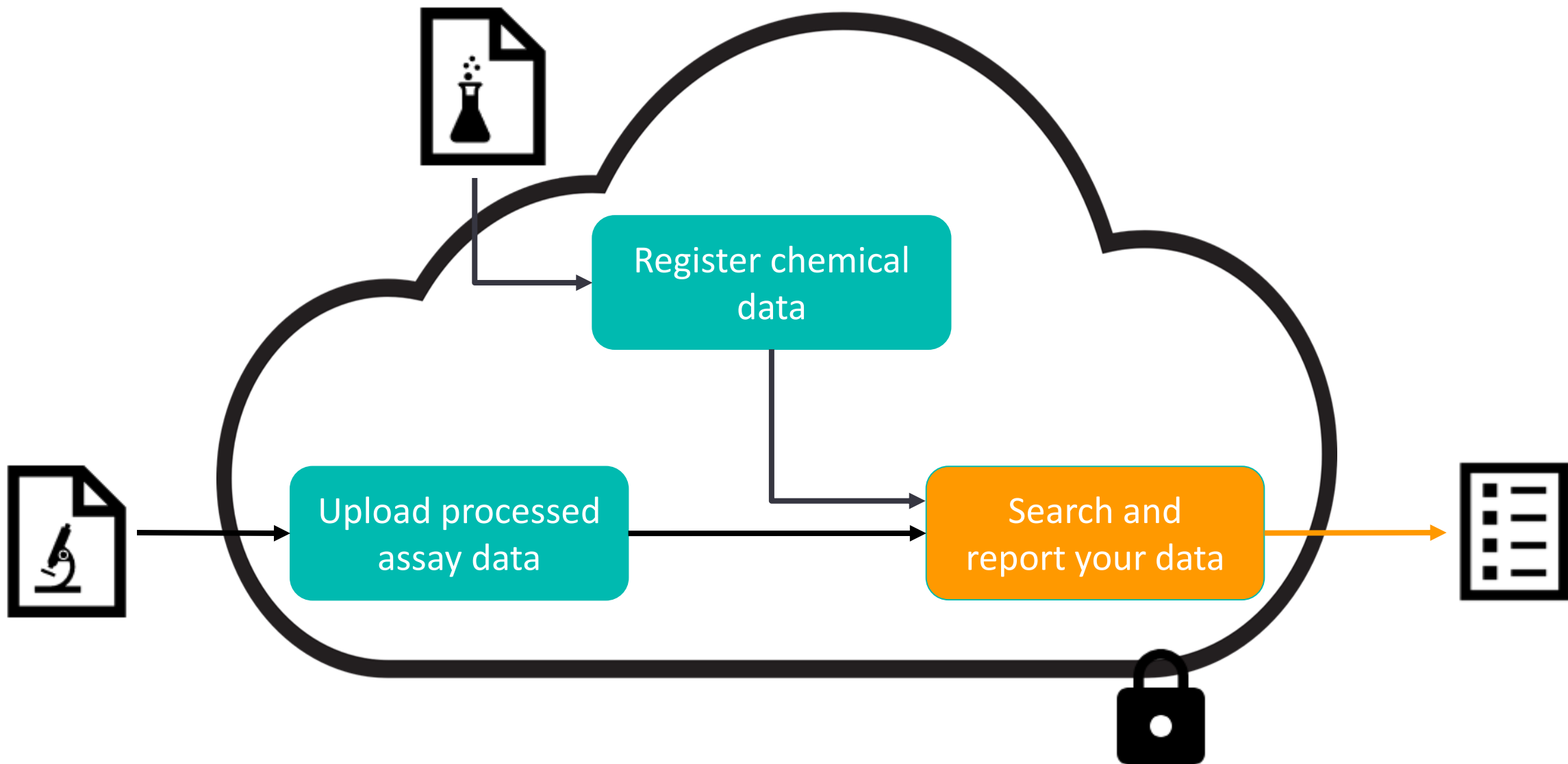


Integration

Downstream service

Downstream service

Web services



Search and report



Reporting Workflow



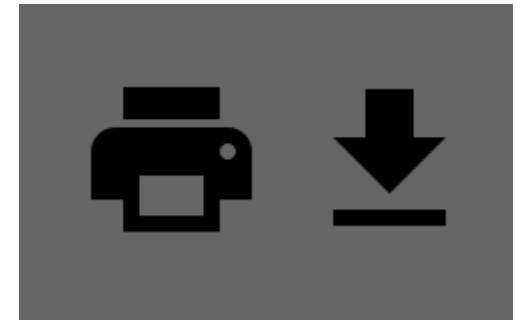
Customize
your workspace



Search, Filter
& Analyse



Save & Share







Print & Export

Search and report





Connect lcardova@chemaxon.com ▾

Filters Lists Charts Views Workspaces Export

Views

-  Assay - Compound view
-  Compound - Assay view
-  Assay grid view
-  Compound grid view

Recent Views

-  Assay - Compound view
-  Compound - Assay view
-  Compound grid view
-  Assay grid view

CRO workflow support



Poll question



Why cloud?



Why cloud?



Why cloud?

Needs

Quick & cheap launch

Guaranteed availability

Accessibility

Scalability

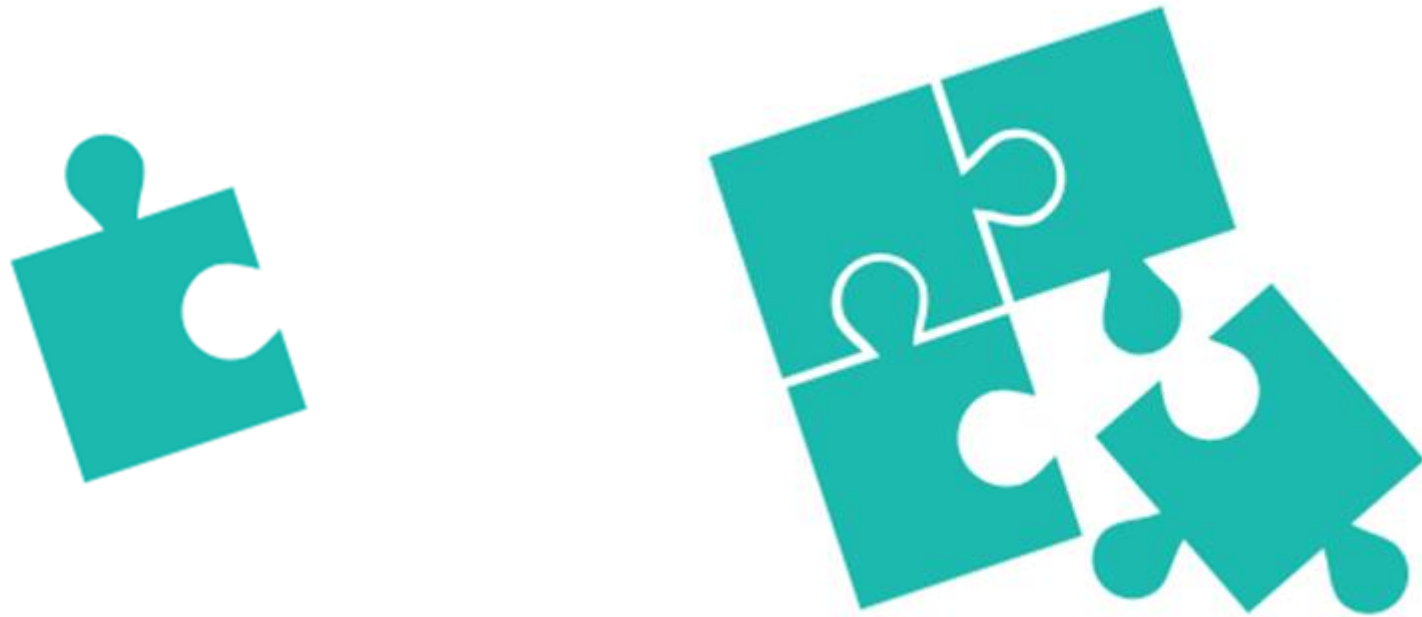
Up-to-date HW & SW

Zero maintenance

Solution

Software as a Service (SaaS)


Integration




Integration

ChemAxon Synergy lcardova@chemaxon.com


- Applications
- Team Members
- Groups
- Projects



Assay Processed Data Uploader




Compound Registration




Plexus Connect


A complete array of web applications




Normalize and register unique compounds



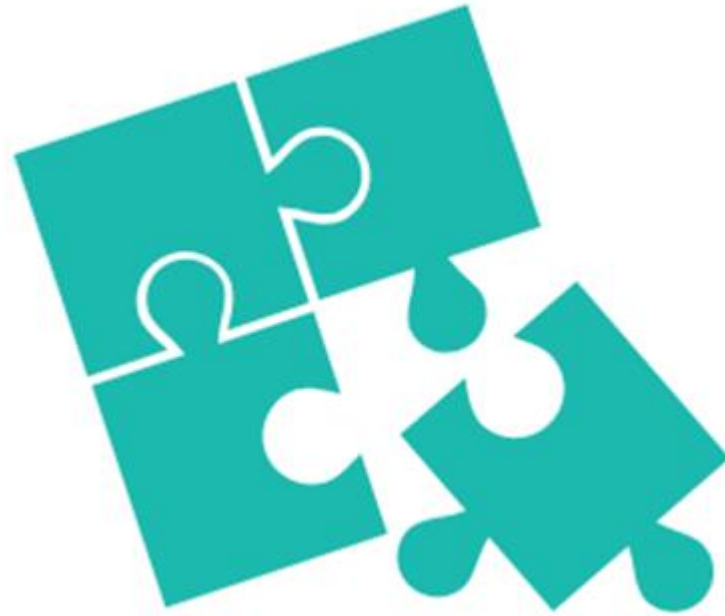
Central idea repository for project teams



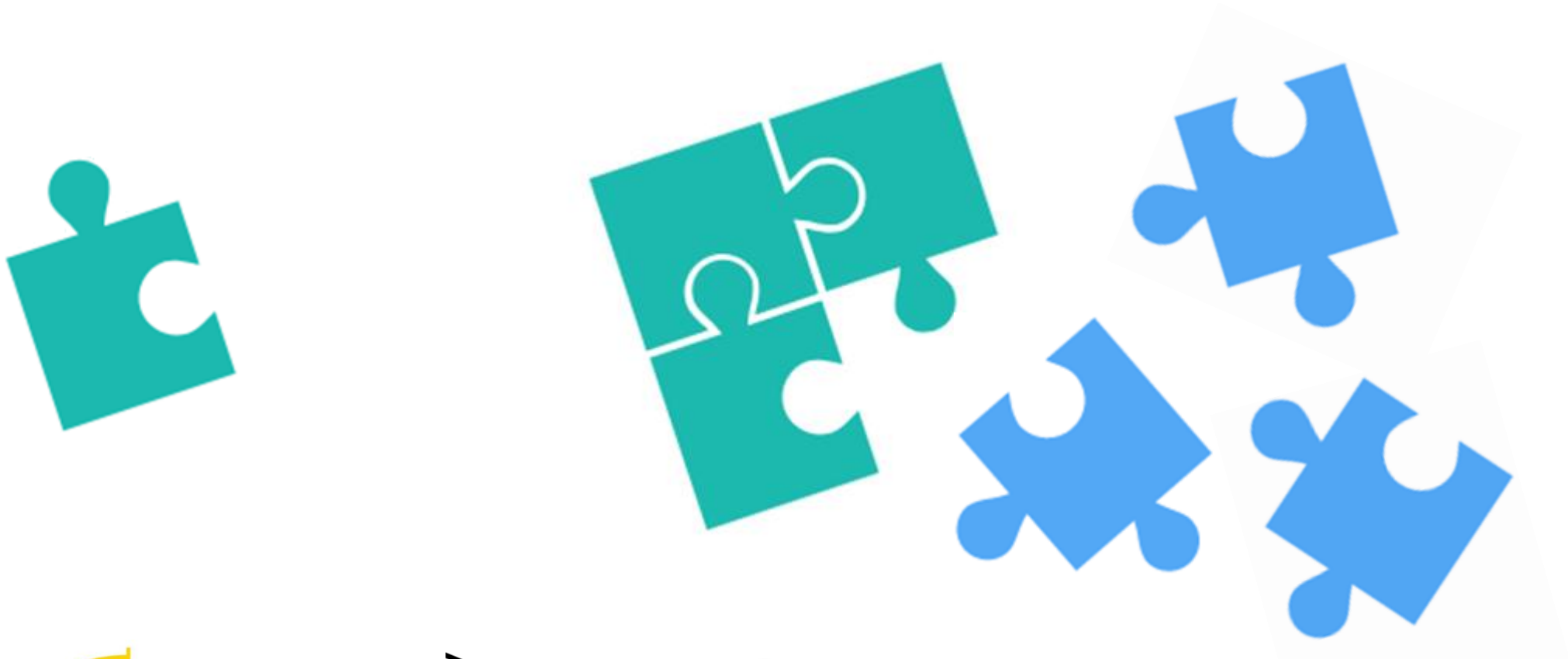
Easily upload compound assay data

 **Questions? Get in touch!**

Integration



Integration



amazon

idbs

accenture

titian

A^{Rx} Arxspan

KNIME

... and others

Follow us

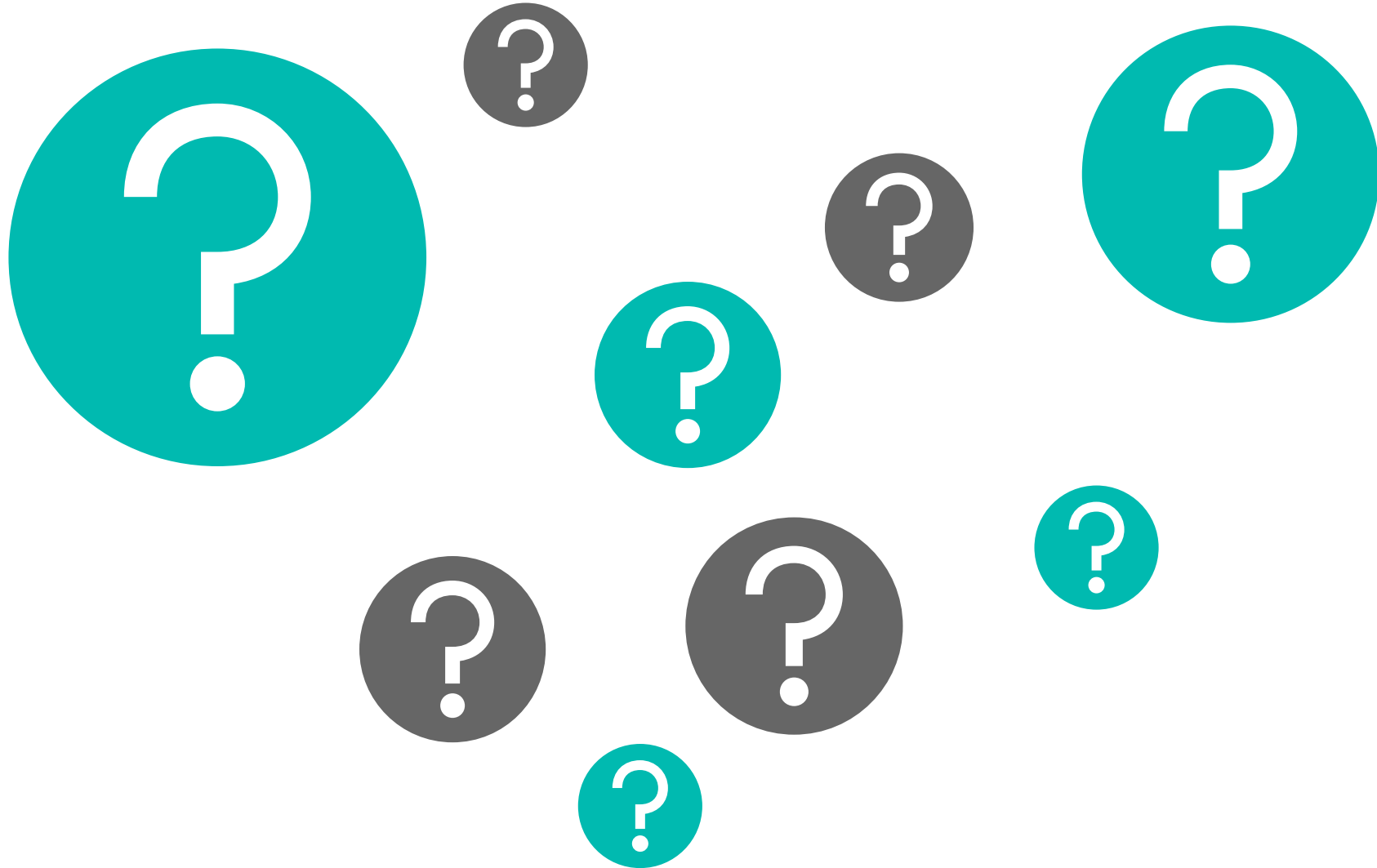


The image shows a navigation menu for ChemAxon. At the top left is the ChemAxon logo. To its right are navigation links: PRODUCTS, SOLUTIONS (which is underlined), SUPPORT, COMPANY, and LOGIN. A search icon is located at the far right of the top bar. Below the navigation bar are four circular icons, each with a corresponding text label below it:

-  Biopolymer Informatics
-  Chemical and Assay Data Management
-  Chemical Compliance Legislation
-  Chemical Innovation



Questions





THANK YOU

Write us at sales@chemaxon.com

Feel free try out at <https://synergy.cxn.io/>