



**CERTΔINTY
DISCOVERY**

CERTARA[®] | Chemaxon

**Compliance? Anywhere, anytime:
Automated controlled
substance detection and tariff
classification at Merck KGaA**

Michael Hofmann

Merck KGaA

Ákos Papp

Chemaxon

A large, red, halftone-style portrait of a man with short hair, wearing a suit and tie, occupies the left side of the image. The portrait is composed of many small dots, creating a textured effect.

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Senior Product Manager



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Michael Hofmann – Merck KGaA
Ákos Papp - Chemaxon

November 5, 2025

CERTARA 

A little history from Frankfurt



Photo1: Bayer AG Archives / Historical press image, "Otto Bayer demonstrating polyurethane, 1952,"
Photo2: shroom360, Psilocybe azurescens 123020.jpg, licensed under CC BY-SA 3.0

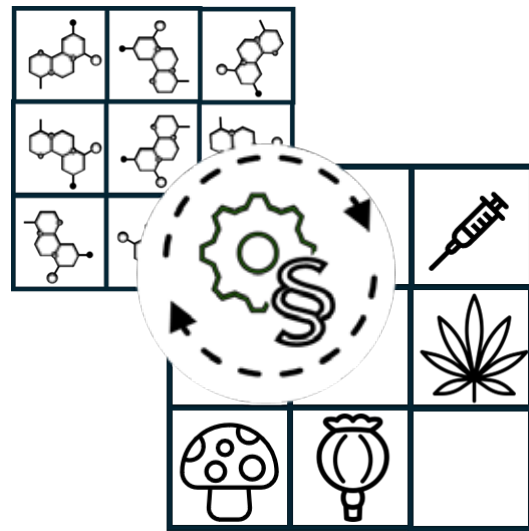


Compliance Checker

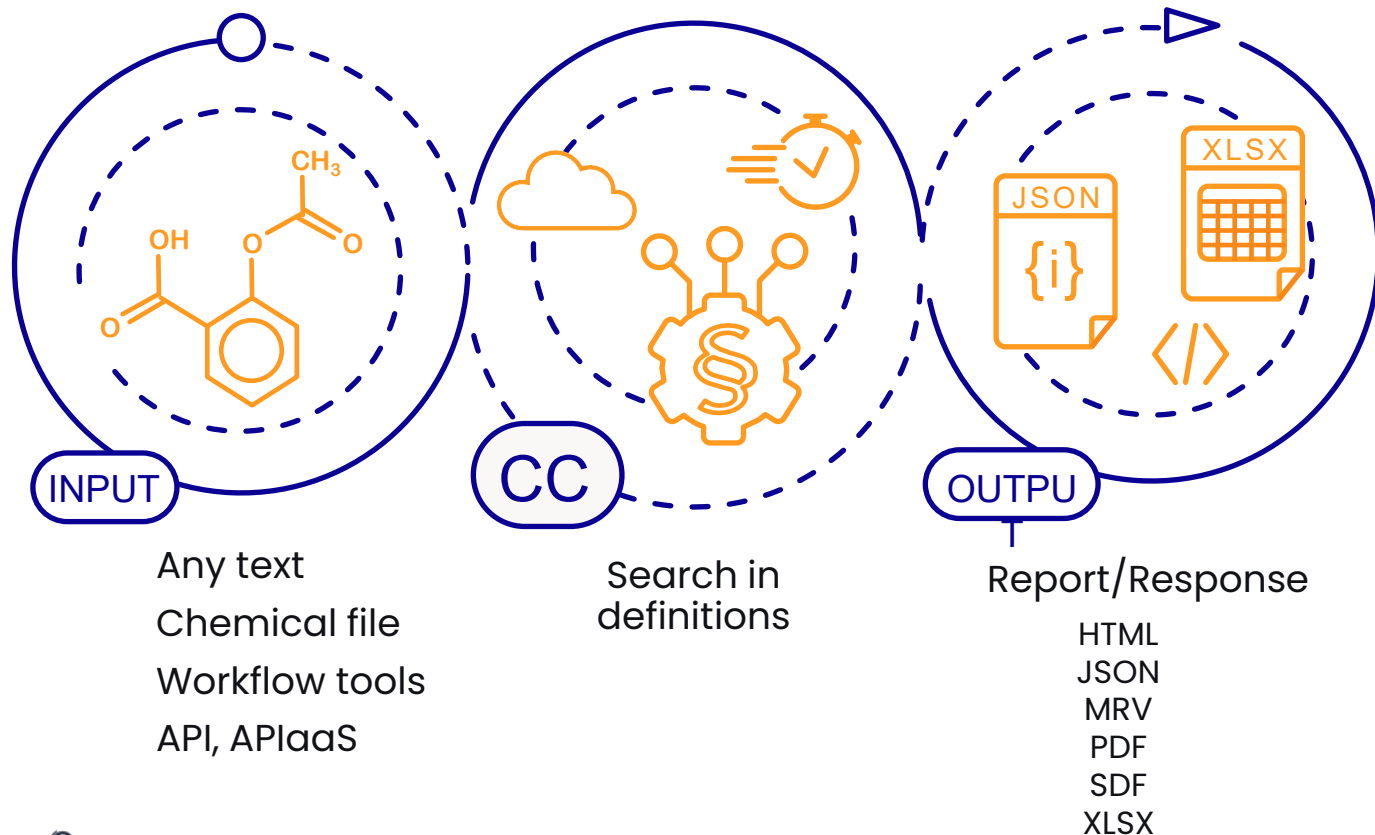
Akos Papp
PM of Compliance Checker and cHemTS

Product definition

Compliance Checker is a combination of a **software system and** a regularly updated **content package** providing a flexible tool to screen chemical structures efficiently against the controlling legislation **to identify controlled substances.**



Compliance Checker



Be compliant: Where?



Compound Design/Synthesis – decision making, licenses, proper destruction



Compound Management – safe storage, tracking samples



Compound Purchase – ensure that controlled substances are not inadvertently purchased



Compound Shipping – remove controlled substances or obtain shipping licenses

Key challenges

Frequent updates



Data management:

- Ensuring data is accurate across all platforms
- Magnitude

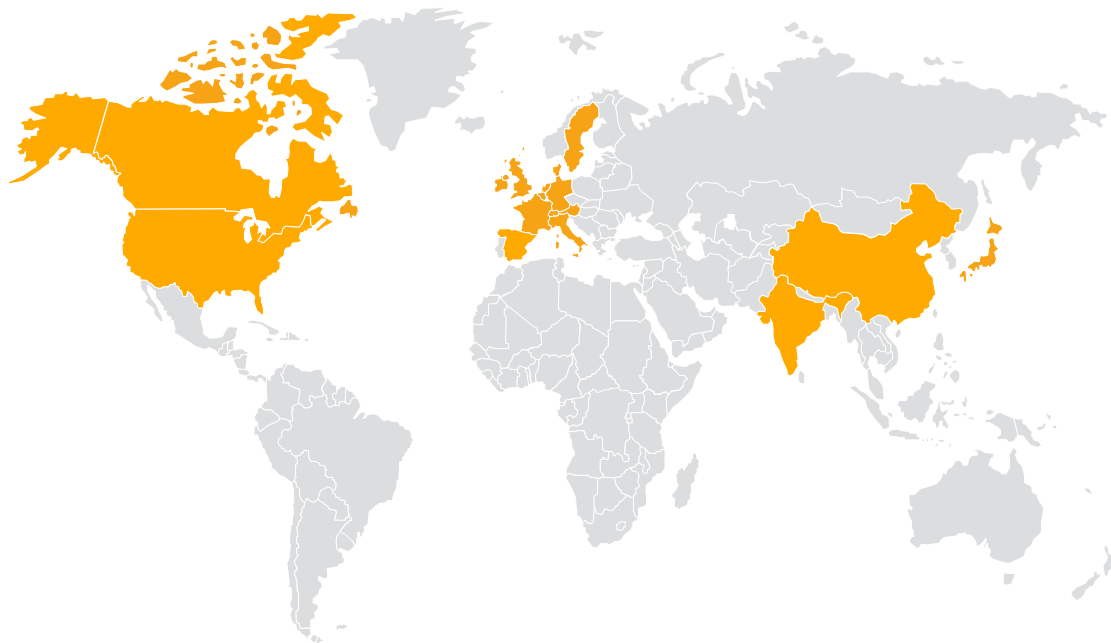


Regulatory complexity

- Generic definitions
- Analogue control



Coverage



EU



Rotterdam
Convention



Montreal
Protocol



OPCW
Convention on the
Use of Chemical Weapons



UN

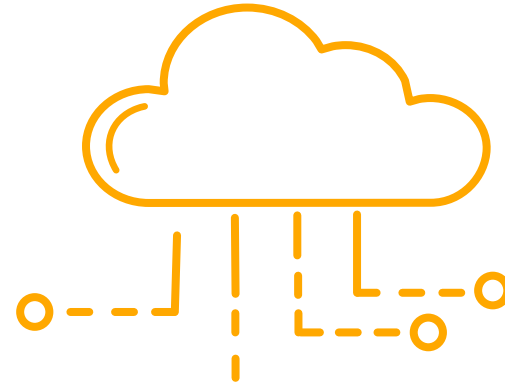
-  Austria
-  Belgium
-  Canada
-  China
-  Denmark
-  France
-  Germany
-  India
-  Ireland
-  Italy
-  Japan
-  Netherlands
-  Singapore
-  Slovenia
-  Spain
-  Sweden
-  Switzerland
-  United Kingdom
-  USA



Compliance Checker



on premise



Software as a Service

Integration API – performance

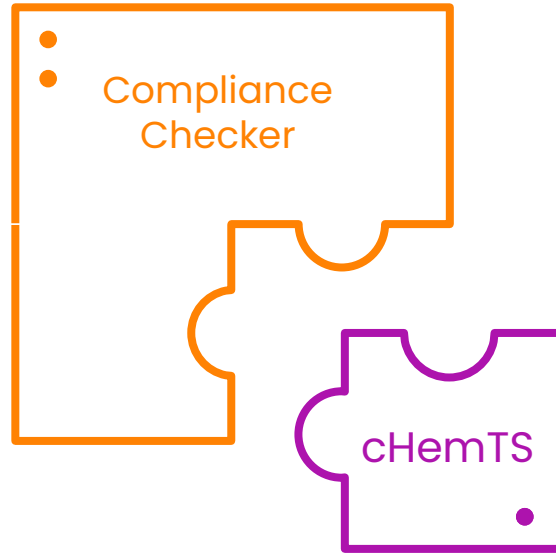


Compound
Database



Computation
AWS

Compliance Checker modular with cHemTS



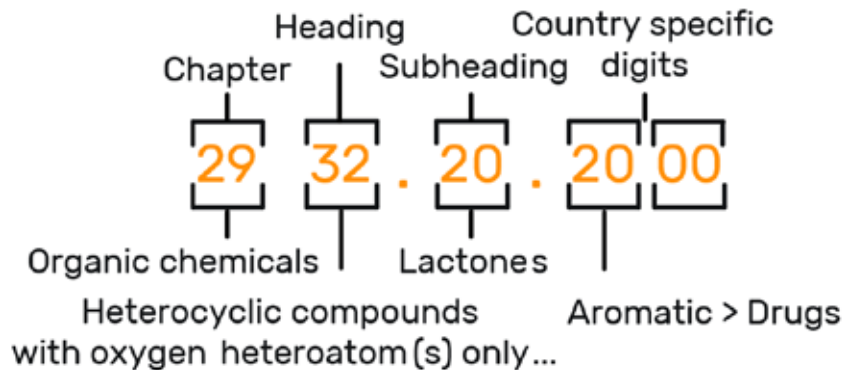
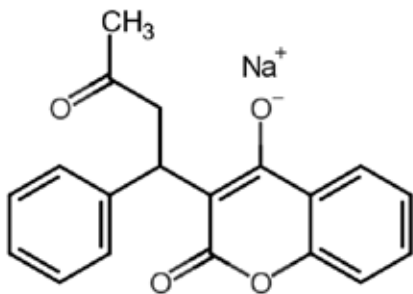


cHemTs

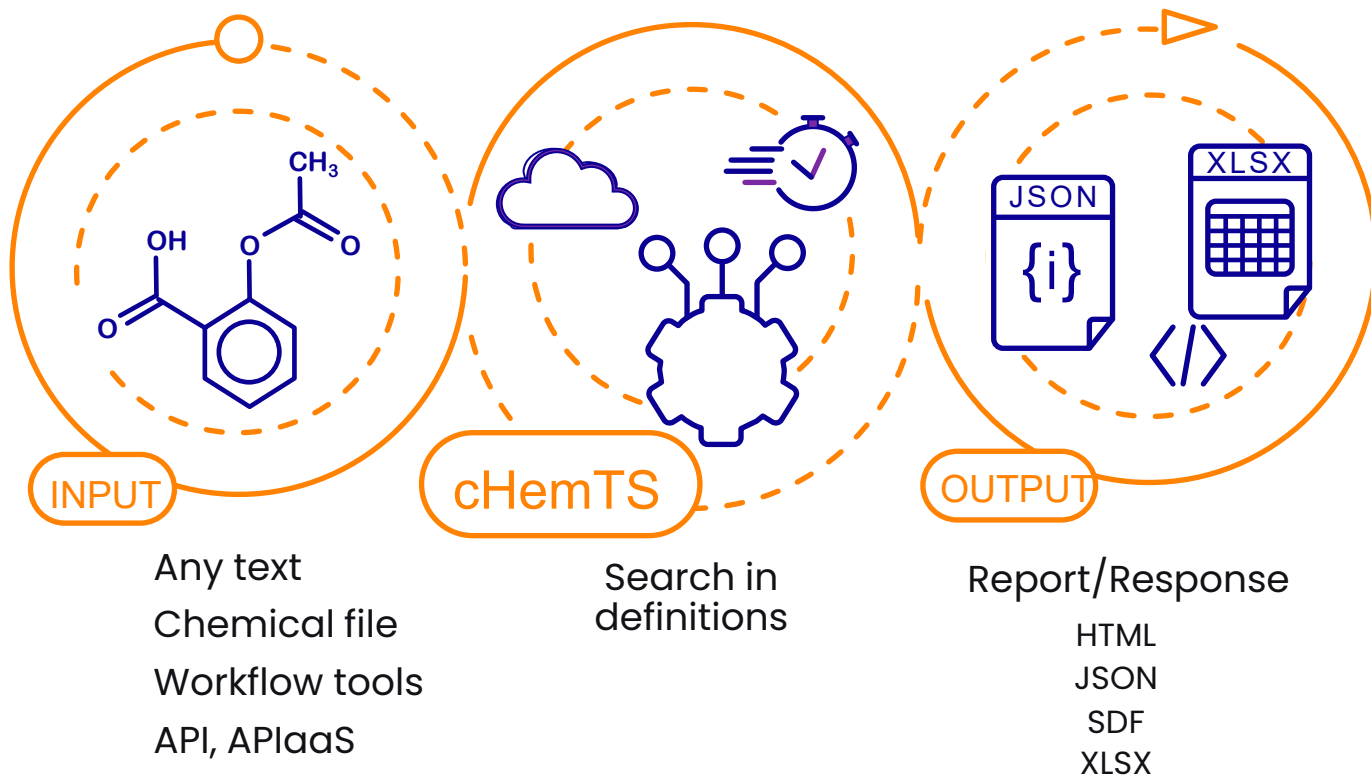
Product definition

cHemTS is a flexible, structure-based tool designed to assign **Harmonized (Tariff) System codes** for international shipping and accurately classify substances for global trade.

Warfarin's HTS code



cChemTS



cChemTS Content



Canada



China



European Union



India



Japan



Switzerland



United Kingdom



Germany



United States
including Schedule B

Pain Points in manual tariff coding



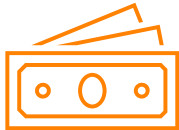
Risk of misclassification



Complexity of codes



Regular updates



Time and resource consuming

No time to assign the proper code for each structure

Benefits



Accurate and fast (JChem search)



Quick delivery of content updates (auto-monitoring)



Salts vs. mixtures proper classification

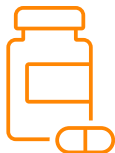


Enhanced support for Pharma

Enhanced support for Pharma



Lookups in country-specific Pharma Agreement



Structures found in Drugs@FDA or Green Book are automatically classified as Drugs



User-defined drugs

proper classification of your drugs in clinical and preclinical trials



User-defined flags

PGA HTS flags such as FD2 or DE1



Thank you

akos.pappcertara.com



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Michael Hofmann

Merck KGaA

Research Scientist &
System Consultant



compliance checker & CHEM TS

Certainty Discovery, Frankfurt, Nov. 2025

Michael Hofmann, Healthcare Digital, Data & IT R&D

AS one for patients

MERCK

Agenda



AS one for patients

- 01 Who we are
- 02 Compliance Checker
- 03 cHemTS
- 04 Acknowledgements
- 05 Questions



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we are **MERCK**

Every day, our +62,000 employees work in 65 countries to make a positive difference to millions of people's lives by creating more joyful and sustainable ways to live.



**EMD
SERONO**

**MILLIPORE
SIGMA**

**EMD
ELECTRONICS**

In the U.S. and Canada we operate as EMD Serono in the Healthcare business, MilliporeSigma in the Life Science business, and EMD Electronics in the high-tech materials business.

Merck KGaA, Darmstadt, Germany holds the rights to the name and trademark "MERCK" internationally, except for the United States and Canada

we are Healthcare Digital, Data & IT R&D

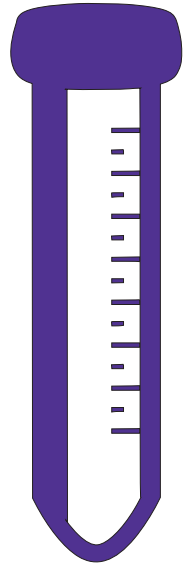
We support discovery and early development projects by managing the research data landscape and providing state-of-the-art solutions to capture, process, integrate, visualize and analyze internal and external scientific data.

We own and shape the Merck Healthcare Research Database as the core data and knowledge repository for discovery data containing millions of compounds and hundreds of millions measured data points characterizing them.

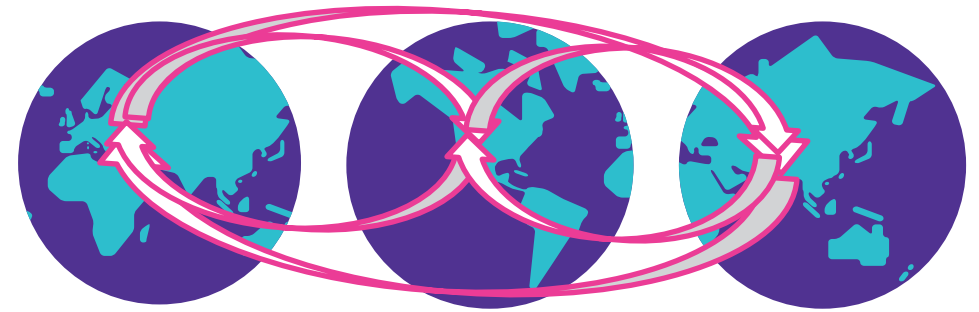
We deliver end to end scientific IT solutions for our users.



Today's talk



our compound world is global



Besides our internal resources, we have an increasing number of externalized activities:

Collaborations with **External Research Organizations** (ERO) for compound synthesis or assay testing require uni- or bi-directional compound exchange.

Effectiveness of compound shipment is crucial and besides the physical parts of the shipment process, legal aspects like **controlled substances** and **customs law** have to be considered.

Some statistics - Shipments from Darmstadt (Germany), our major research hub

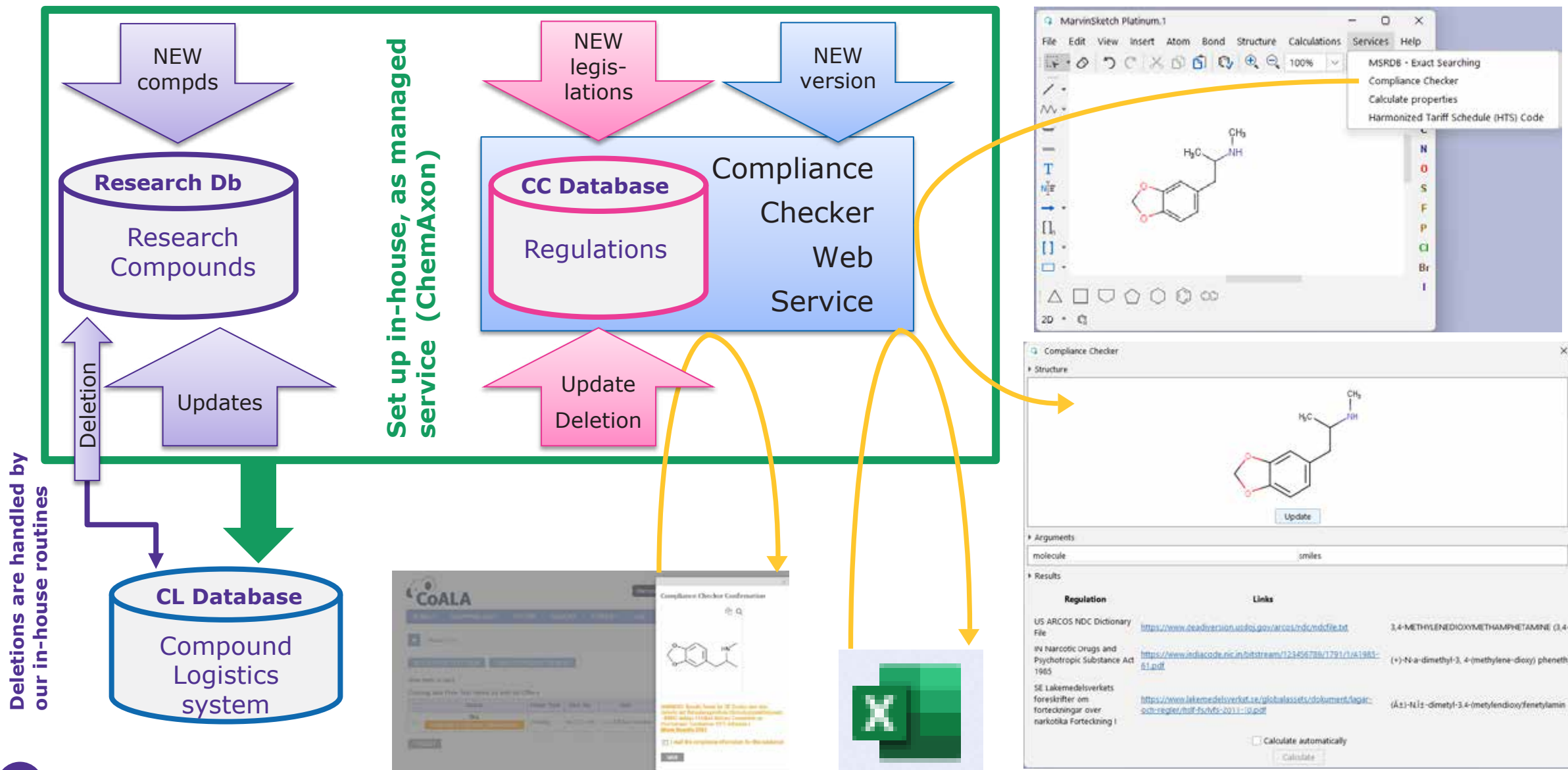
- More than 1.100 shipments per year
- to more than 30 countries

controlled substances / compliance checker

Merck decided on ChemAxons **Compliance Checker** in 2017 after evaluating

- **Accuracy**
test case: example data with a known number of expected hits
- **Scope:**
Percentage of countries relevant for us covered?
- **Modes of operation**
Should allow for automatic and interactive processing for both single and multiple compounds
- **Internal effort**
should be as minimal as possible for installation & run
- **Integrability**
integration into existing tools should be as easy as possible
Support of a wide range of chemical structure formats

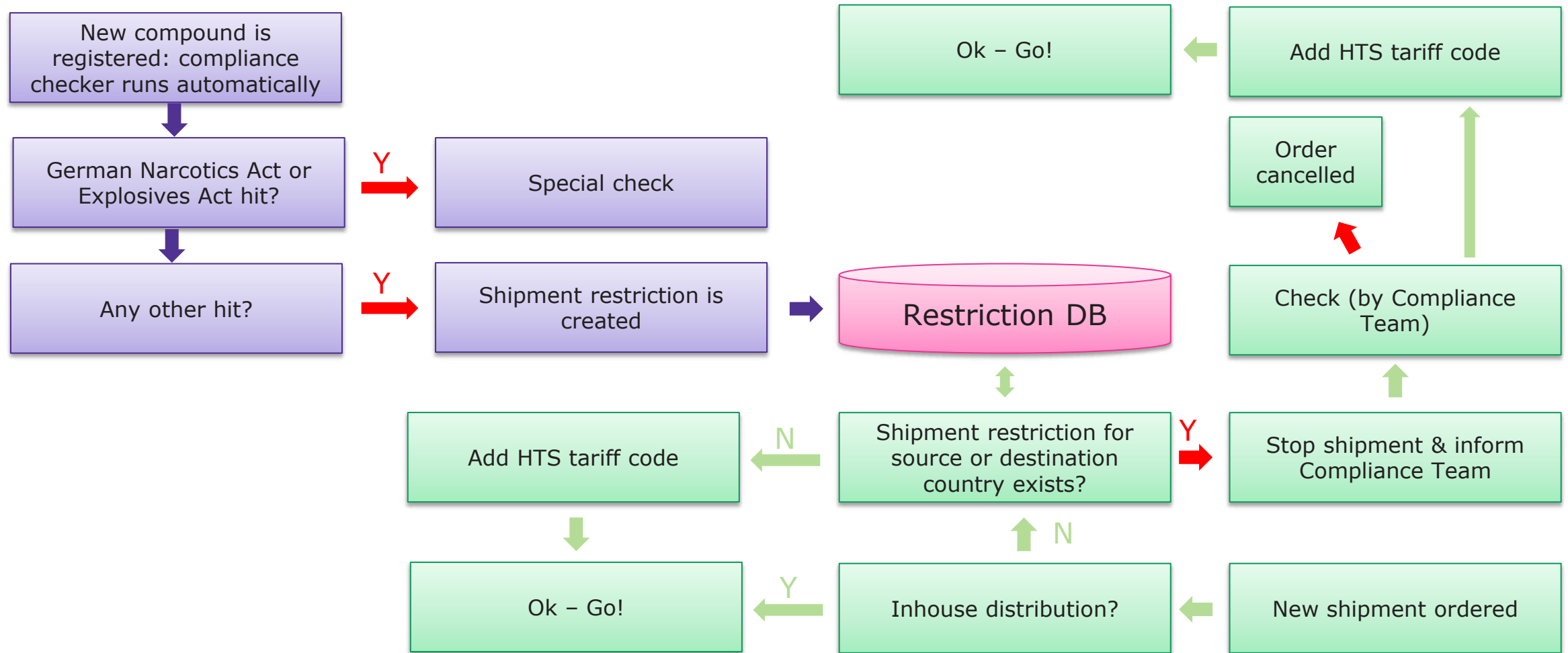
Compliance checker – Architecture & set up



COMPLIANCE CHECKER – WHERE WE ARE TODAY

- ChemAxon runs Compliance Checker as fully managed in-house web service (software updates, legislation updates)
- Merck used Compliance Checker to check all **internal compound stores**.
- Merck integrated Compliance Checker into Marvin for single interactive checks and into Excel for batch interactive checks
- Merck has integrated Compliance Checker into the Compound Shopping Tool to avoid buying in Germany controlled compounds (BTM, SprengG)
- ChemAxon developed a custom application for automated Research Database (RDB) check
 - Permanent check of new compounds
 - Complete re-check after knowledge base updates

compliance checker & compound logistics



restrictions in our compound logistics system

Restrictions

Restriction Name	Lock	Substance	Effect	Date
<input type="checkbox"/> CN Regulations on the Control of Anesthetic and Psychoactive Drugs	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> CN Regulations on the Control of Anesthetic and Psychoactive Drugs	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> CN Regulations on the Control of Anesthetic and Psychoactive Drugs The second class psychoactive drugs	Lock	Substance	Negotiate	11/13/2024
<input type="checkbox"/> CH Toxic Drugs for Medicinal Use	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> Community regime for the control of export, transfer, brokering and transit of dual-use items	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> Community regime for the control of export, transfer, brokering and transit of dual-use items	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> Community regime for the control of export, transfer, brokering and transit of dual-use items	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> Community regime for the control of export, transfer, brokering and transit of dual-use items	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> Community regime for the control of export, transfer, brokering and transit of dual-use items CATEGORY 0 NUCLEAR MATERIALS, FACILITIES, AND EQUIPMENT, OC Materials	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> Community regime for the control of export, transfer, brokering and transit of dual-use items CATEGORY 9 AEROSPACE AND PROPULSION, OC Materials	Lock	Substance	Negotiate	10/9/2020
<input type="checkbox"/> Compounds for	Lock	Sample Holder		
<input type="checkbox"/> Container Restriction on	Lock	Sample Holder		
<input type="checkbox"/> DJB BB	Lock	Substance		
<input type="checkbox"/> DG DMSO Shipment restriction - dual-use	Lock	Labware Item		
<input type="checkbox"/> DE Ausführungsverordnung zum Chemiewaffenübereinkommen (CWiV) Anhang 1	Lock	Substance		
<input type="checkbox"/> DE Ausführungsverordnung zum Chemiewaffenübereinkommen (CWiV) Anhang 1 Chemikalienliste 1	Lock	Substance		
<input type="checkbox"/> DE Ausführungsverordnung zum Chemiewaffenübereinkommen (CWiV) Anhang 1 Chemikalienliste 2	Lock	Substance		
<input type="checkbox"/> DE Ausführungsverordnung zum Chemiewaffenübereinkommen (CWiV) Anhang 2 Explosivstoffe	Lock	Substance		
<input type="checkbox"/> DE Gesetz über den Verkehr mit Arzneimitteln (Arzneimittelgesetz - AMG) Anhang I	Lock	Substance		
<input type="checkbox"/> DE Gesetz über den Verkehr mit Arzneimitteln (Arzneimittelgesetz - AMG) Anhang II	Lock	Substance		
<input type="checkbox"/> DE Gesetz über den Verkehr mit Arzneimitteln (Arzneimittelgesetz - AMG) Anhang III	Lock	Substance		
<input type="checkbox"/> DE Gesetz über den Verkehr mit Betäubungsmitteln (Betäubungsmittelgesetz - BtMG) Anlage I	Lock	Substance		
<input type="checkbox"/> DE Gesetz über den Verkehr mit Betäubungsmitteln (Betäubungsmittelgesetz - BtMG) Anlage II	Lock	Substance		
<input type="checkbox"/> DE Gesetz über den Verkehr mit Betäubungsmitteln (Betäubungsmittelgesetz - BtMG) Anlage III	Lock	Substance		
<input type="checkbox"/> DE Gesetz über die Kontrolle von Kriegswaffen	Lock	Substance		
<input type="checkbox"/> DE Gesetz über explosionsgefährliche Stoffe (Sprengstoffgesetz - SprengG)	Lock	Substance		
<input type="checkbox"/> DE Gesetz über explosionsgefährliche Stoffe (Sprengstoffgesetz - SprengG) Anlage III	Lock	Substance		

Restriction: DE Gesetz über den Verkehr mit Betäubungsmitteln (Betäubungsmittelgesetz - BtMG) Anlage I

[Edit Target Inventory](#) [Delete](#) [Show All Restrictions](#) [View Audit Trail](#)

RESTRICTION DETAILS

Name	DE Gesetz über den Verkehr mit Betäubungsmitteln (Betäubungsmittelgesetz - BtMG) Anlage I	Created By	
Active	<input checked="" type="checkbox"/>	Creation Date	10/9/2020
Applies To	Substance	Delete on Match	<input type="checkbox"/>
Type	Lock	Substance Owner	No special treatment
Form	Both	Zone	
Amount		Start Date	
Effect	Negotiate	End Date	
Despatch Warning	<input type="checkbox"/>		
Shipping	<input checked="" type="checkbox"/> Restriction only applies to orders that include shipping and source or destination locations are in selected countries: Germany		
Comment	Created from auto job 09-OCT-20; Externe Restriction ID:7161		

[Edit](#)

TARGET REQUESTORS

☐ Only: ☒ Everyone Except:

☐ User or Group ^

[Add User](#) [Add Group](#) [Remove](#)

EDITORS

☒ Only: ☐ Everyone Except:

☐ User or Group ^

[Add User](#) [Add Group](#) [Remove](#)

APPROVERS

☒ Only: ☐ Everyone Except:

☐ User or Group ^

☐ Controlled Substances approver

[Add User](#) [Add Group](#) [Remove](#)

Each hit in RDB is assigned to a restriction in our compound logistics system; new restrictions are created automatically as well



compound shipment tool

Ship4You - Test

Home

Ship4You

my Shipment Orders

prepare Mosaic Shipment

prepare Non-Mosaic Shipment

prepare Master Shipment

all Shipments

ORO Shipments

Data Management

created by

Shipment Temperature

Comment to Sample Shipment

Information for Recipient

Recipient

Country

Company

Create modified on

Packing List

Customer Invoice

stored Docs

New Customer Invoice (pdf)

New Customer Invoice (docx)

New Packing List (pdf)

New Packing List (docx)

last modified on

All shipments are handled here. Necessary shipment documents are automatically created. HTS Codes are added and custom value is calculated based on compound amount matrix.

David, Jiang (M104416)

Subcategory
Small molecules / Synthetic compounds

Description
Synthetic solid compound / Sample, Non-Hazardous small molecule for pharmaceutical Research

Trivial name

CAS number

Dangerous Goods Department

verified *
☐ Yes ☐ No

LPL-Number

additional remarks

last verified by

last modified by

HTS tariff code / cHEMTS

Evaluation in 2020 focused on

- **Accuracy**
test cases: from daily work
- **Modes of operation**
Should allow interactive processing for both single and multiple compounds
- **Internal effort**
should be as minimal as possible for installation & run
- **Integrability**
Integration into existing tools should be as easy as possible
Support of a wide range of chemical structure formats

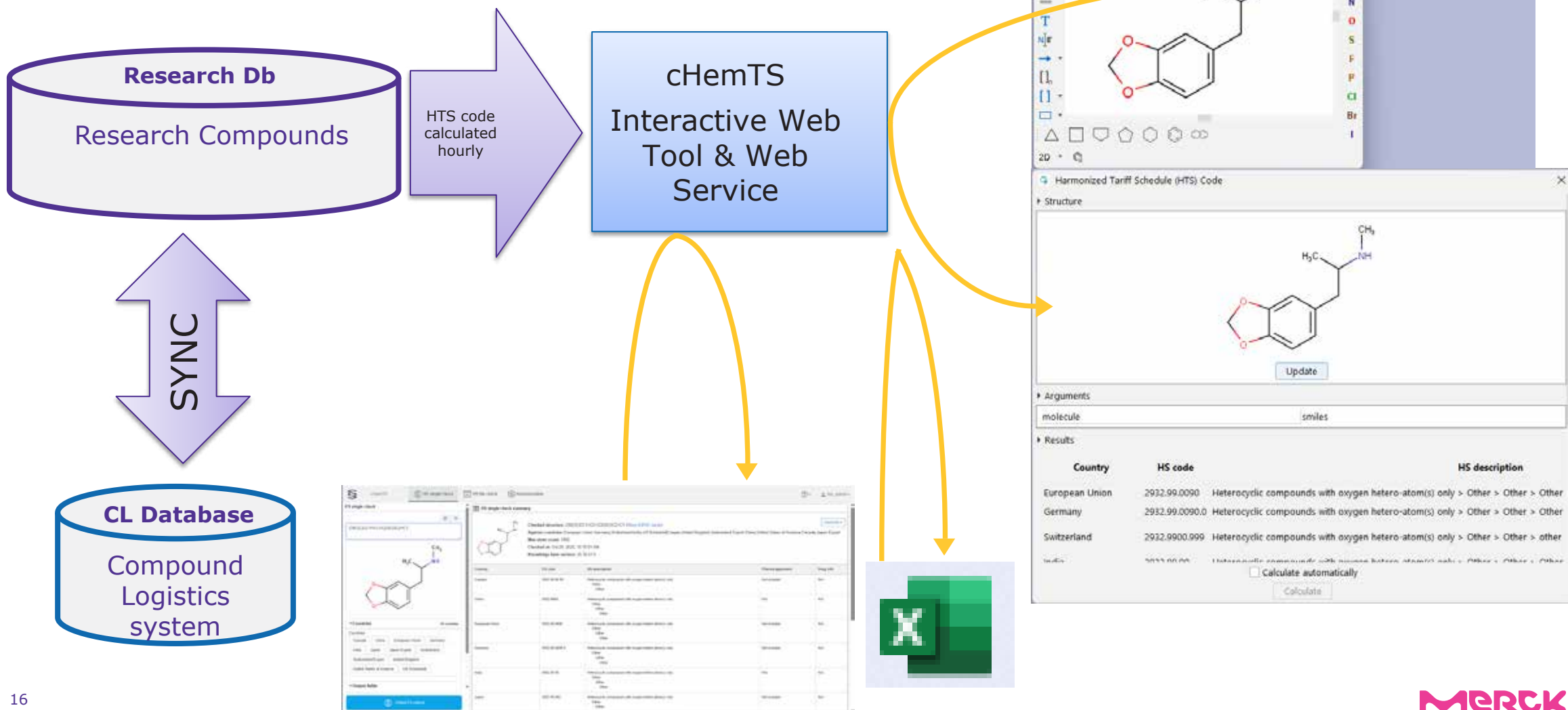
2021: based on positive feedback from users decision to add cHEMTS to our permanent application portfolio



HTS is used by over 200 countries, territories, or customs unions around the world to assign a number to each product to establish the appropriate duty that should be paid when goods are imported into a country.



CHEMITS - Architecture & set up



Compound Shipment Tool

Ship4You

Usage: Small molecules

Small amount of synthetic chemicals/simply small molecules / Created for the purpose of pharmaceutical research and development / For pharmaceutical (e.g. ONCOLOGY) Research only / Owned by Merck KGaA / Non-toxic / Not of human or animal origin / Do not contain any animal or cell culture derived product or additives such as albumin or Serum / Not for RE-SALE / The samples have no commercial value / The total value of this shipment is for customs purposes only

SQ Department

non-representative EU shipment

Remarks

verified: ☒ Yes ☐ No

set verified by: [input] on: [input]

set modified by: [input] on: 16.01.2025 08:27:54

HTS Codes

Valid	Country	HTS Code
Yes	Canada	2843900000
Yes	European Union	2845901000
Yes	Switzerland	2845900000
Yes	USA	2845900000
Yes	United Kingdom	2845901000
Yes	Japan	2845900000
Yes	China	2845900000
Yes	Germany	2845901000
Yes	India	2845900000

MSC Codes

Substance Code	MS Batch Code	MS Structure Code
4012381		
3636829		
3904462		
4018687		
3632969		
3283377		
3963754		
3975153		
3972179		
3979183		
3973817		
3975218		
3967225		
3966256		
3973346		

add HTS Codes

Back Save Article Print

Our Compound Shipment Tool takes HTS codes from the pre-calculated compound codes, or calculates them on-the-fly, if no pre-calculated codes are available.

Sender: Jörg Zissel
Direct Telephone: +49 6151 72-4235
Fax Number: +49 6151 72-914235
Email: Joerg.Zissel@merckgroup.com
Department: Biopharma, RD-XPA-1

Merck VAT-Reg.No.: DE811850788
Tax-No.: 00722565905

MERCK

Page 1 / 2

IT

Phone: [input]
E-mail: [input]

Our ref.: 07.10.2025 07:05:13 /
additional information for Recipient:

Customs Invoice No.: 19609 dated 07.10.2025

Item	No. of Units (PCC)	Description of Goods	EU Tariff Code	Tariff Code Import	Country of Origin	Total Customs Value (€)	Com-merciale Value (€)
1	2	Synthetic compound / Sample Non-Hazardous small molecule (heterocyclic compounds) for pharmaceutical Research. Not for sale. No commercial value. Value for customs only. 10131209 - 0.19 mg 10137291 - 0.18 mg	29341000		Germany	20	0
Total						20	0

Terms of Delivery: DDP

Manufacturer:
Merck KGaA, Frankfurter Str. 250, 64293 Darmstadt, Germany

99.9% of all shipments do not require manual corrections!

0.1% needs intervention of the compliance team.



cHemTS: beyond Healthcare

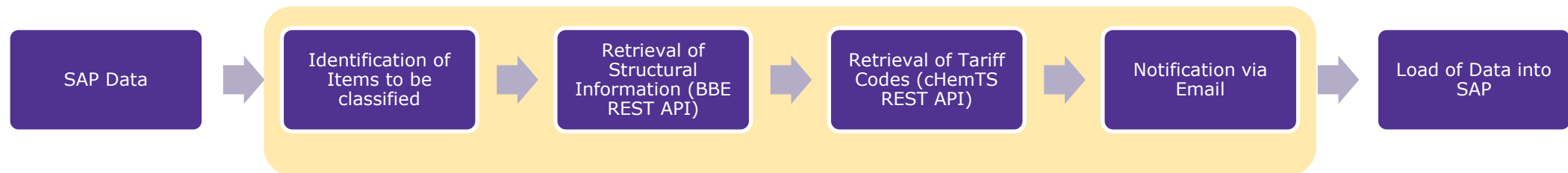
Surprisingly Merck functions from other sectors have an even stronger interest than Healthcare in the topic and play a big part in the usage now.

The team of **Corporate Sustainability, Quality and Trade Compliance** is responsible to create tariff codes for Building Block Explorer (BBE) items. In the past, this has been a manual process.

Now, the integration of cHemTS with the **Building Block Explorer** allows a fully automated approach.

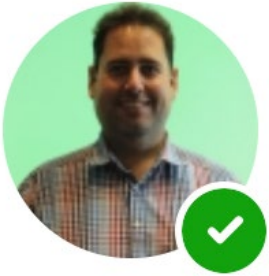
As automation platform, the **Palantir Foundry** was selected.

- SAP Data is synchronized daily and is the main data source.
- Palantir Foundry can perform API calls to external systems (here: BBE and cHemTS)
- Runs are scheduled, no manual trigger needed, and notifications upon runs are sent via E-Mail



Palantir Foundry

Acknowledgements



- Jörg Zissel

Compound Management

Biopharma | Discovery Technologies | Discovery Pharmacology



- Dr. Michael Franz

Product Compliance Europe

Corporate Sustainability, Quality and Trade Compliance | Export Control & Customs Regulations

Thanks for your attention

Any questions ?



AS ONE FOR PATIENTS

