

Introduction

Drug Discovery organizations maintain novel chemical collections running into the hundreds of thousands or millions of chemicals. They will routinely synthesize and purchase chemicals which have or are aimed at having a biological effect.

In order to support this, reagent stores of chemicals, building blocks, standards and biological tool compounds are also maintained. These are often well known chemicals, but within screening become known via internal identifiers such as CMP-123456, with true origin and chemical name quickly lost in compound management systems

Given the vast numbers of chemicals under management it can often be difficult to track any regulatory or safety requirements that may go with these chemicals.

In addition, research chemicals are often shipped internationally requiring shipping information such Harmonized Tariff Codes (HS/HTS codes) and these codes vary depending on the chemical structure and class.

Scitegrity's Compliance Hub for Drug Discovery allows sample managers and medicinal chemists to automatically identify if chemicals (even if novel or proprietary) are regulated or pose safety risks. This allows appropriate controls or precautions to be put in place and the generation of shipping information such as tariff codes.

By working automatically in the background, examining the structure of each chemical Compliance Hub seamlessly provides extremely high levels of compliance and accuracy without the need for manual checks, lookups or matching names to regulatory lists.

Compliance Hub consists of a series of modules which we are constantly expanding and adding new capabilities too, making compliance to chemical regulations with Drug Discovery and the wider R&D industries much simpler and more robust. All Compliance Hub modules handle novel and proprietary chemicals and require no knowledge of chemistry or regulations to use

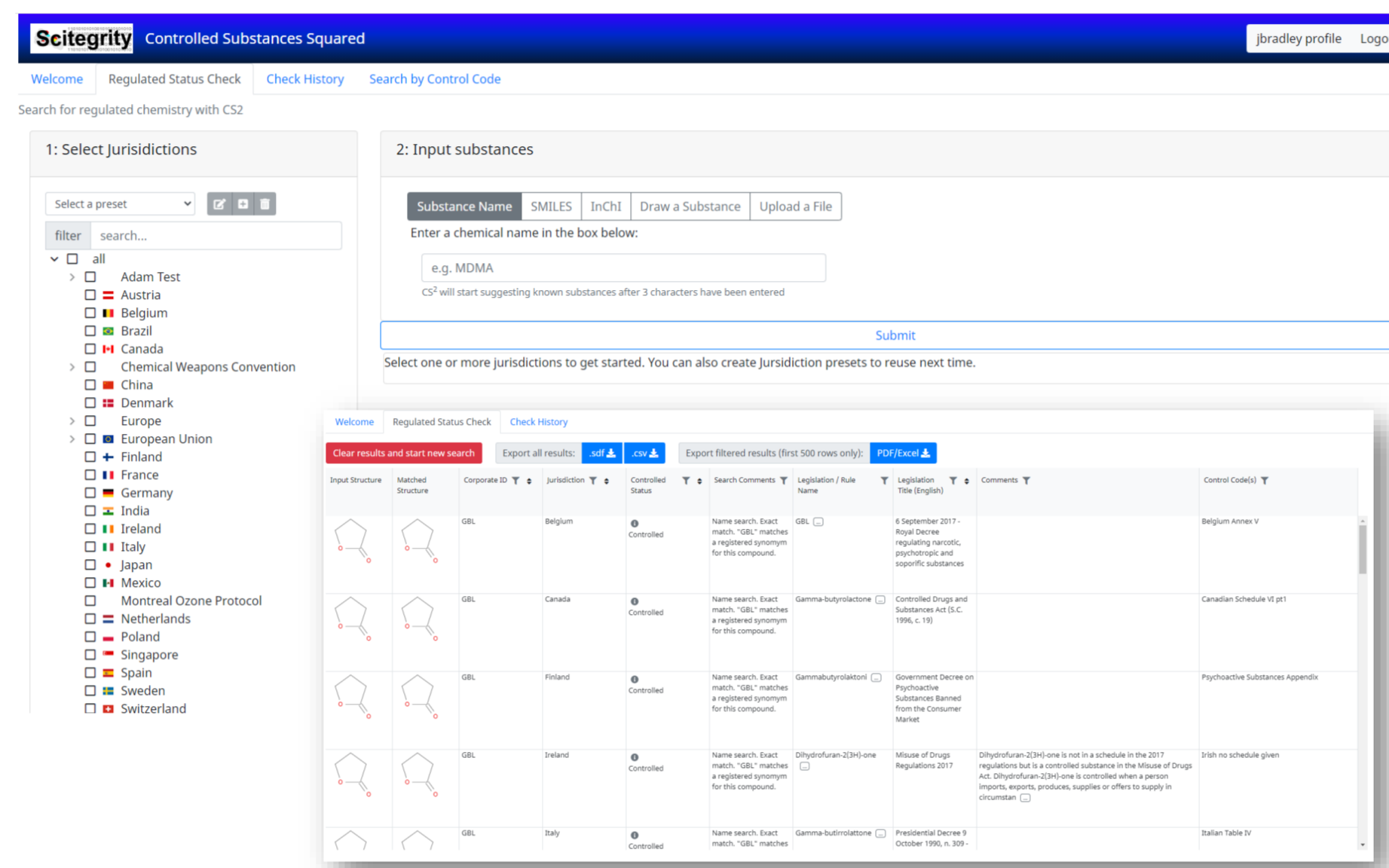
Are any of my chemicals regulated?

Within drug discovery we aim to synthesize chemicals with a biological effect. Some of these may affect the brain, by design or accident. As a result, many of the most relevant regulations globally for drug discovery chemical libraries relate to Controlled Drug legislation, which have very strong controls and penalties, even for milligram quantities and research use.

Controlled drug regulations control not just common 'named' drugs like Fentanyl or cocaine, but also all related chemical space and precursor chemicals that can be used to synthesize the main drug of abuse.

These laws and definitions differ significantly from country to country, even within Europe

Our Controlled Substances Squared module within Compliance Hub can automatically check all your chemicals against Controlled Drug laws in over 26 countries, including areas of controlled chemical space, in addition to International conventions such as the Chemical Weapon Convention, Montreal Ozone depleting protocol, PIC and strategic export control regulations



I need a HS/tariff code for shipping

To ship a chemical internationally you need to supply a HS or tariff code. Getting the correct HS code for a chemical requires detailed knowledge of both chemistry and international trade rules. With over 6000 HS codes for chemicals alone, each with different duty (tax) rates, its important to get the correct one to avoid under or overpaying import duties and risking fines.

Even if an organization has someone well versed in these rules, they may not be available to code a chemical leading to process delays

Our ExpediChem module simply and accurately generates the correct HS code to use for the USA, UK, EU, Switzerland and China. As with all Compliance Hub modules it handles novel and proprietary chemicals and requires no knowledge of chemistry or trade compliance rules.

Are any of my chemicals dangerous?

Within research we use a lot of novel and untested chemicals as well as reactive intermediates and chemical for synthesis. Although being used for research, international Dangerous Goods (DG) guidance and regulations on the safe storage and shipping of chemicals still applies if a chemical is potentially energetic, even if used on milligram scales (1 gram of an energetic chemical can still cause serious injury). These regulations require that appropriate packaging and labelling is used.

Our DG assessment module can identify chemicals likely to be classed as energetic allowing you to correctly label them and warn users.

The sensitivity (or threshold) can be adjusted, so untested chemicals used on bulk, such as process scale up can apply more rigorous filters than milligram quantities, given the greater risks which apply to bulk chemicals.

This module is also being expanded to cover other DG aspects such as toxicity and corrosives. This will provide useful information for better safety data sheet (SDS) generation, and a way to flag potentially dangerous chemicals that may unknowingly be in sample libraries, allowing scientists to take appropriate precautions.

Pre-clinical abuse liability

As chemicals move through the Discovery and Development funnel, the information requested by regulators such as the EMA and FDA increases. For CNS penetrant candidates this means pre-clinical assessments on whether there is an abuse liability. This includes *in vivo* and *in vitro* studies as well as assessing if the candidate is chemically similar to any known drugs of abuse or abuse liable chemical space.

Using our expertise, comprehensive data sets and algorithms of controlled chemical space and substances, we provide detailed quantitative report for regulatory submission. This robust assessment removes the subjective nature of assessing whether something is chemically 'similar' to known controlled substances, using data rather than opinion

Conclusion

Drug Discovery, chemical synthesis and sample management is a complex process. Those tasked with making it happen are also expected to have systems in place that comply with a vast array of complex and often hidden regulations.

Unfortunately, those managing chemicals are often the least well equipped to ensure compliance, despite being best placed to make it happen.

We have designed Compliance Hub to fill this gap, automatically flagging compliance issues with novel and proprietary chemicals, for actions to be taken through automated workflows in your own sample management, registration and eLN systems.

Compliance Hub is Cloud based, with powerful APIs to automate checks as well as intuitive user interfaces for those who don't wish to fully integrate. Compliance Hub also comes with regulatory workflow support and advice via e-mail.

It is used by 5 of the worlds top 10 Pharmaceutical companies at the enterprise level, plus dozens of CROs, chemical suppliers, pharma and regulators.

If you'd like to learn more, please contact us to discuss how we can solve your compliance issues and improve safety.