

**- Internship report -**  
**- Erwann Laplante -**

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## Introduction:

This internship took place in two parts, from September 28, 2023 until February 2, 2024 part-time, at 2 days per week, then from February 5, 2024 until June 7, 2024 full-time at ChemIntelligence.

# I - Context and team organisation

## 1. The company:

Deepmatter Group Ltd is a company focused on digitising chemistry.

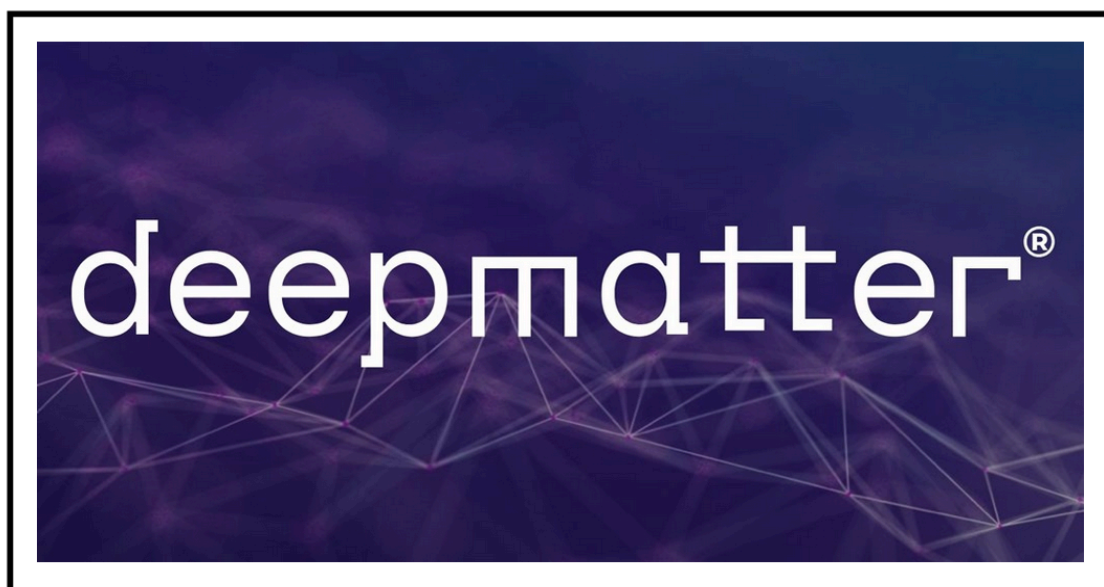


Figure 1: DeepMatter logo

The first company within this group is DeepMatter Ltd, based in Glasgow, which embarked on a transformative journey with its pioneering product, Digital Glassware, aimed at revolutionising laboratory practices. Recognising the prevalent issue of non-reproducibility in reactions across various laboratories, DeepMatter devised a proactive solution. By implementing real-time data collection during experiments and meticulously comparing results from different runs, they sought to enhance reproducibility and streamline processes. The benefits were profound, as the system provided invaluable insights into the efficacy of reactions, identifying successful methodologies while flagging ineffective approaches. Ultimately, DeepMatter's innovative approach not only optimised yields but also fostered a culture of continuous improvement within the scientific community.

The group has acquired InfoChem, headquartered in Munich. With over 30 years of expertise in cheminformatics, InfoChem is renowned for its proficiency in reaction and molecule handling, epitomised by its flagship software ICFSE. Moreover, they possess extensive data resources within a platform known as SPRESI. Notably, InfoChem has pioneered the concept of CASD (Computer Aided Synthesis Design) through their groundbreaking software ICSYNTH. This strategic acquisition not only

bolsters the group's technological capabilities but also underscores their commitment to advancing innovation in the field of chemistry.

In June 2022, ChemIntelligence, founded in August 2019 by Thomas GALEANDRO DIAMANT, was acquired by DeepMatter Group Plc, headquartered in Lyon, a move that significantly bolsters its capabilities in the field of chemistry. ChemIntelligence brings to the table its cutting-edge Chemassistant platform, renowned for its prowess in optimization and prediction within the chemical domain. This strategic integration enhances the group's ability to offer sophisticated solutions for chemical research and development. With Chemassistant's advanced features, including detailed optimization algorithms and predictive analytics, the group is poised to deliver even greater value to its clientele. The current chief executive officer of ChemIntelligence is Mark WARNE. This acquisition underscores the group's commitment to innovation and reinforces its position as a leader in the UK's chemical industry.

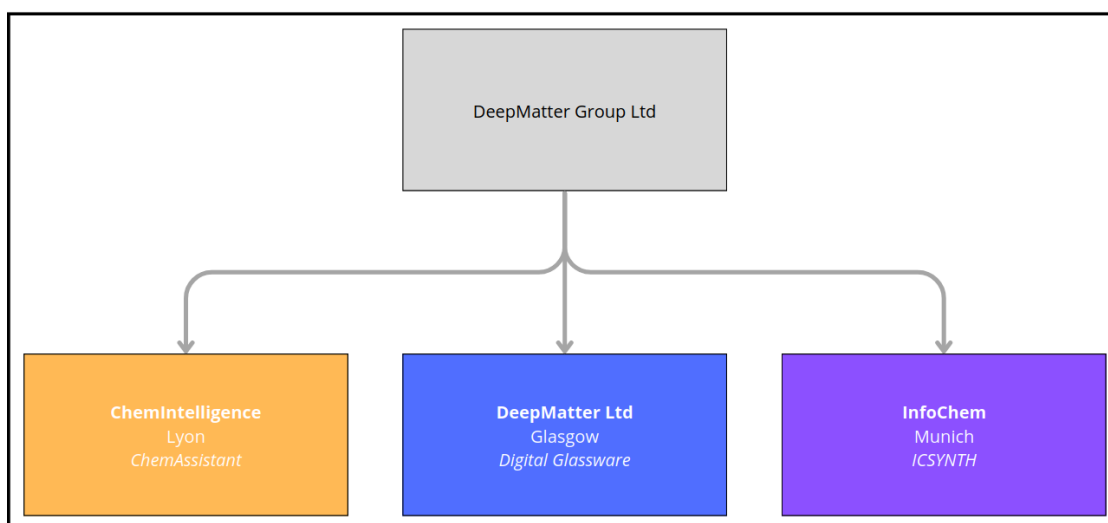


Figure 2: DeepMatter group organisation

DeepMatter is currently focused on amalgamating its acquired expertise into a singular platform known as SmartChemistry. This ambitious endeavour aims to consolidate the wealth of knowledge and capabilities from InfoChem and ChemIntelligence into a unified solution. SmartChemistry promises to revolutionise chemical research and development with its integrated approach and advanced functionalities.

As stated in the official DeepMatter website: “DeepMatter is a big-data and analysis company focused on enabling reproducibility and predictability in chemistry.”

Their vision is to provide the data that enables all medicines to be made in the best possible way.

They are a multidisciplinary team of big-data, software, chemistry and hardware engineers.

DeepMatter has been perfecting their technology platform over recent years and has been supported and advised by some of the best minds in the industry

According to the guidelines provided by DeepMatter website: “At DeepMatter, they are building a single platform that allows reaction data to be consumed from multiple data sources to provide a cleansed, harmonised and categorised repository for the exploitation of reaction data through APIs, search tools and machine learning or artificial intelligence learning.”

An Application Programming Interface, is a software interface that allows to «connect» a software or a service to another software or service in order to exchange data and functionalities.

According to the information presented on DeepMatter web portal: “DeepMatter is focused on SmartChemistry with machine learning powered products, SmartChemistry empowers chemists to design, experiment and understand their chemistry on an unprecedented scale. Utilising an advanced knowledge base that combines reaction data, real time sensor data and outcomes, SmartChemistry enables access to a higher level of experimentation in the chemistry laboratory.

DeepMatter has many partners such as: AstraZeneca, Springer Nature, American Chemical Society, University of Leeds, University of Nottingham, Thieme, BioIndustry Association, Tocris Bioscience, Pistoia Alliance.”



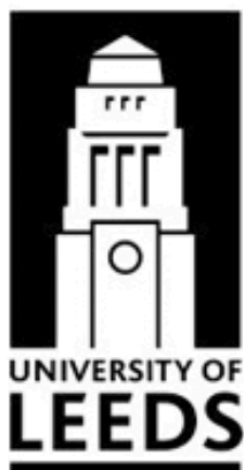
**TOCRIS**  
a biotechne® brand

**SPRINGER**  
**NATURE**

AstraZeneca 



 **Thieme**



  
Pistoia  
Alliance

**BIA**  
UK BioIndustry Association

Figure 3: DeepMatter partners logo

In the pharmaceutical industry, the molecules developed are often complex, which requires the use of multi-synthesis techniques to break down a target molecule into a series of synthetic intermediates to trace back to commercially available precursor molecules.

Retrosynthesis is often performed by chemists based on their knowledge of chemistry and intuition. However, the use of reaction databases or software specifically designed for retrosynthesis can accelerate the process of designing synthesis pathways, quickly proposing possible pathways based on known reactions.

ICSYNTH, InfoChem' synthesis planning software, is based on two proprietary algorithms. The first algorithm uses a database of more than 4.5 million reactions to generate "templates" of reactions, that is, rules. The second algorithm uses these templates to identify sequences of potential reactions to synthesise the target molecule from commercially available molecules. These synthesis pathways are then graphically presented to the user, who can choose the preferred pathway for further experimental testing.

SmartChemistry is the future fusion between ChemAssistant ICSYNTH, and probably Digital Glassware. The three software are not already merged and each one is still under development.

Mark WARNE serves as the chief executive officer, leading the strategic direction of the company, while Thomas GALEANDRO-DIAMANT, as the Chief Technical Officer, spearheads technological innovations. Meryem GUERSU, in her role as Chief Customer Officer, ensures customer satisfaction remains paramount. Jenny HAND, as the Chief of Staff, orchestrates seamless operations across departments. Kate ROWLEY, the Chief Business Officer, focuses on driving business growth and partnerships. Meanwhile, Tarik BOUMAZA, a Data Science Ph.D. Student, contributes expertise in data analytics, complemented by Flora DOMART, a Data Science Intern, who brings expertise in chemistry. Christoph OPPAWSKY, as Group Leader Applications and my direct supervisor, oversees the development of practical solutions. Lastly, as a Software Development Intern, I collaborate with the team to innovate and refine software solutions by debugging the application and working on small tasks to improve the software front-end.

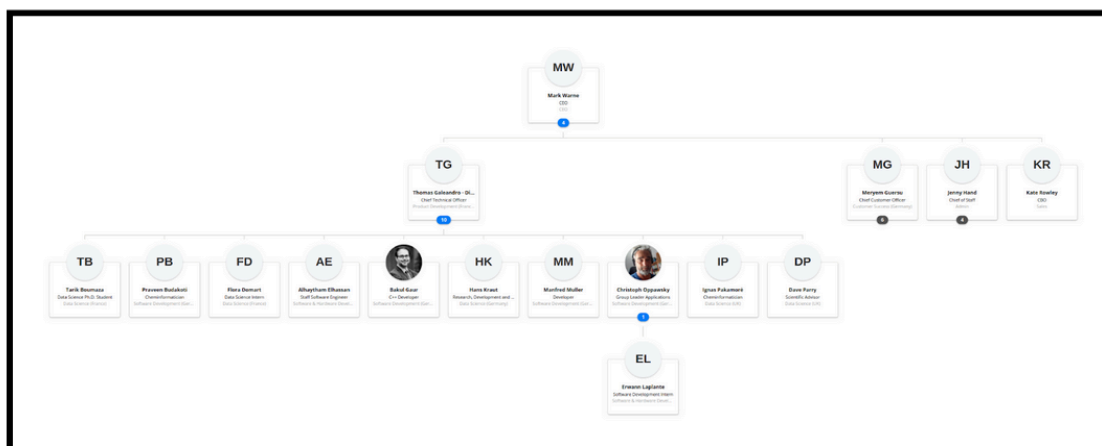


Figure 4: DeepMatter organisation charts

As documented in the official ChemIntelligence website: “They develop software that accelerates chemistry for materials research and development.

The development of new molecules, materials, formulations or chemical reactions requires many trial-and-error experiments and informed guesswork.

The software and the use of machine learning helps to reduce this number of experiments to a minimum, thereby saving customers time and money.

The main product from ChemIntelligence, which applies machine learning to optimise experimental parameters and thereby reduces the number of experiments by 25 to 80%.

The software enables the customer to be faster than the competition and analyse the data. Taking the failed experiments into account is a big plus as it helps the software to better guess what is right and what does not work.

ChemIntelligence platform learns from customers' research and development data and allows the customers to predict the properties of molecules, materials and formulations and also suggest the most relevant experiments to perform in order to obtain molecules, materials or formulations that meet chemist specifications.

This platform leverages both customers research and development data and customers domain expertise to allow customers to make more informed decisions for their research and development projects.

ChemIntelligence platform is easy to use, even for people who are not trained in machine learning. However, if customers do have machine learning skills, ChemIntelligence software allows them to tune the algorithms it uses.

This platform is continuously updated and upgraded in order to benefit from the latest advances in artificial intelligence. “

According to the information available on ChemIntelligence website: "If customers have specific needs, the ChemIntelligence team can even develop tailored software modules that will extend the company base platform in order to perfectly suit chemist use cases and customer data.

ChemIntelligence's proprietary artificial intelligence algorithms can learn relationships of any complexity from customer experiments, even when the underlying physics is not well-understood. It will benefit you even in complex research and development subjects.

They have developed proprietary machine learning algorithms by taking state-of-the-art machine learning algorithms and modifying/adapting them in order to fit the specificities of chemistry and material science research and development."

The chemist can test his experiments ideas with ChemIntelligence software before running them in the laboratory. It allows them to only run the most promising experiments and save time.

## 2. The project:

ChemIntelligence's main and only project is a web application for chemists called ChemAssistant.

### 2.1. ChemAssistant

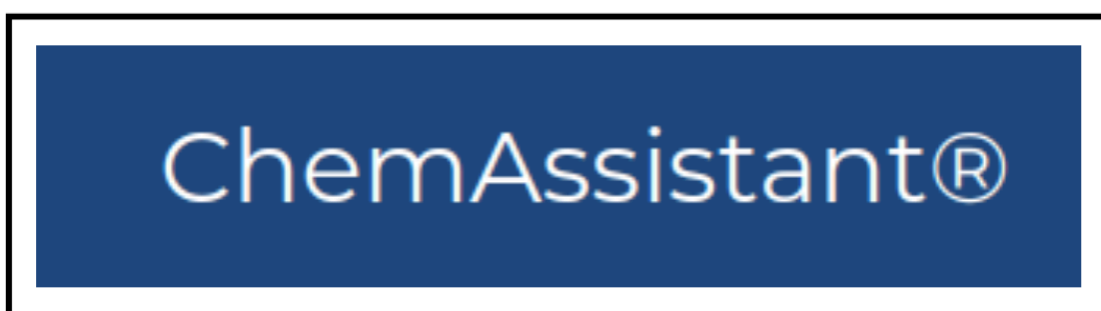


Figure 5: ChemAssistant logo

In ChemAssistant, the user can create, configure, manage, visualise, and analyse a dataset of chemical experiments. However, the main purpose of the software is the optimization and prediction tool. Based on the Bayesian Optimization method, it proposes to the user the experiments to perform in order to achieve some user-determined objectives in a minimum number of experiments.

Bayesian optimization is a method that allows one to find the best solution to a problem. It is very effective when the function to be optimised is complex and expensive to evaluate. It uses probabilistic models to effectively explore the space of possible solutions and find the one that maximises or minimises a given goal. Basically, it's like using probability-based assumptions to guide the search for the best solution.

#### 2.1.1. Overview

The following dataset is composed of parameters, properties and calculators.

ChemAssistant@ dataset\_example Edit Documentation Account Logout

Parameters, Properties & Calculators Data Optimization Visualization & Analysis Predictions Settings

### Parameters

Name	Type	Unit	
parameter 1	Numerical		Delete
parameter 2	Numerical		Delete
parameter 3	Categorical		Manage categories Delete

Group numerical parameters

Add numerical parameter Add categorical parameter Add text parameter

### Properties

Name	Type	Unit	Minimum	Maximum	
property 1	Numerical		0	100	Delete
property 2	Categorical	-	-	-	Delete

Add numerical property Add categorical property

### Calculators

Operators: + - \* / ( )

Parameters: parameter 1 parameter 2

Sum of all numerical parameters

Calculators: calculator 1

Properties: property 1

Numbers: Type a number

Drag a box to an expression

Name	Unit	Expression	Minimum	Maximum	
calculator 1		parameter 1 × × property 1 × × parameter 2 ×	0	100	Delete

Add calculator

Figure 6: ChemAssistant “Parameters, Properties & Calculators” tab

As written in the documentation of ChemAssistant®: “Parameters are the input variables of user experiments. They represent how each experiment has been performed. There are three types of parameters:

- Numerical (which can contain integers or real numbers, each numerical parameter can be assigned a unit and must be assigned a minimum value and a maximum value.)
- Categorical (which can be used to group together substances of the same type. Categorical parameters must contain at least one category. Chemists can add / modify / delete categories)
- Text (which are only informative and are neither used for building predictive models nor for optimization)

Properties are the output variables of user experiments. They represent the outcomes of chemists' experiments. Properties can be of two types:

- Numerical (contain integers or numbers. Each numerical property can be assigned a unit and must be assigned a minimum value and a maximum value)
- Categorical (can contain values of any type. Usually, they are qualitative and the categories cannot be ordered).

Calculators can create new data columns by performing arithmetic operations on parameters and / or properties (addition, subtraction, division and multiplication). Only numerical parameters and properties can be used in calculators.”

After the users have created their dataset, they need to create one or several optimisation objectives and they can add constraints for the optimisation.

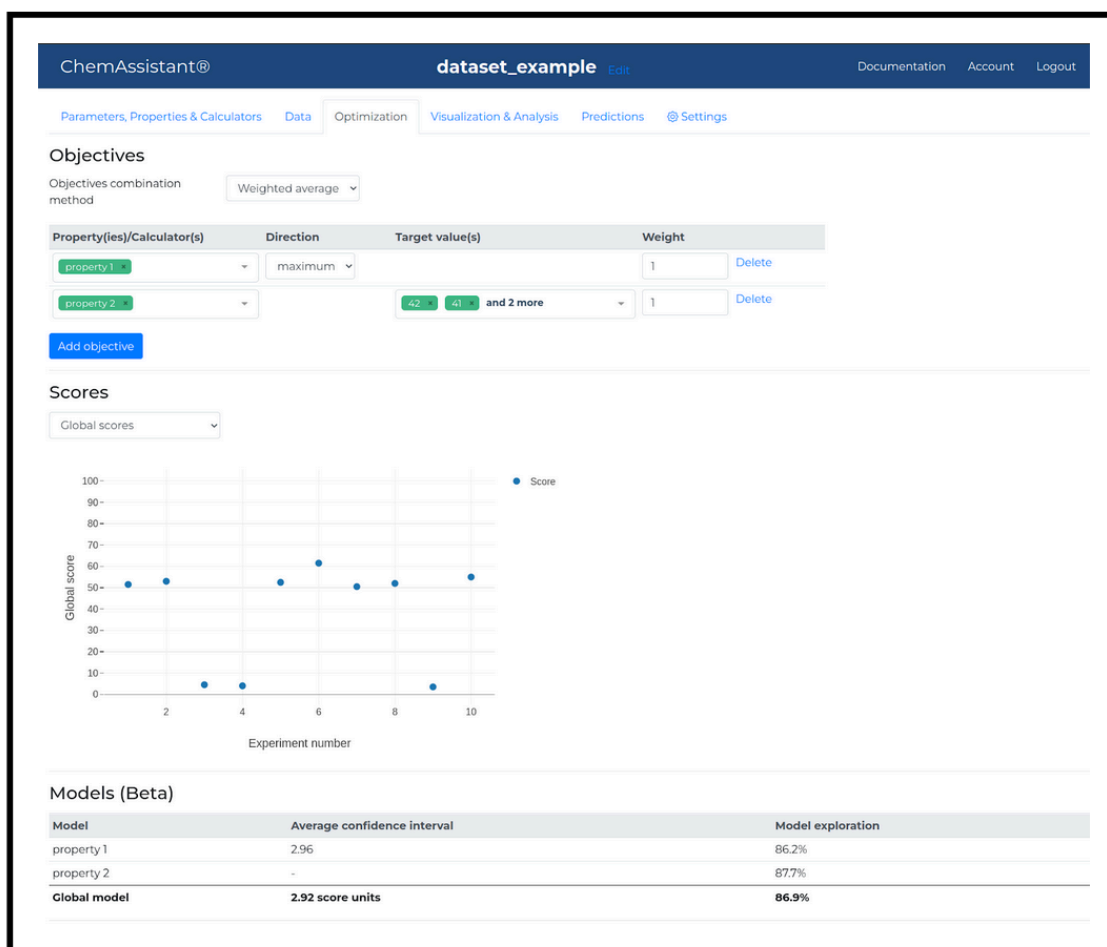


Figure 7: ChemAssistant “Optimization” tab

Constraints on numerical parameter groups

There are no numerical parameter groups yet.

Constraints on numerical parameters/attributes/calculators

Operators: +, -, \*, /, (, )

Parameters: parameter 1, parameter 2, parameter 3 - attribute 1

Calculators: Sum of all numerical parameters, calculator 1

Numbers: Type a number

Drag a box to the expressions to create a constraint

Expression	Operator	Value	
parameter 1	=	0	Delete
parameter 2	=	0	Delete

Add constraint

Conditional constraints

	Parameter	Value		Parameter	Value			
If	parameter 1	<	0	Then	parameter 2	>	0	Delete
and	parameter 3	=	category 2					
Add condition								
If	parameter 2	<	0	Then	parameter 3	=	category 1	Delete
Add condition								

Add conditional constraint

Figure 8: ChemAssistant "Constraints" part

### 2.1.2. Optimisation

Per the official ChemAssistant documentation: "The objectives set goals to reach for the properties, they are values for properties the user wants to achieve in the experiment. For example, the stickiness of adhesive at room temperature.

For an experiment, a score is calculated for each objective. This score ranges from 0 to 100 (100 meaning that the objective is reached). User can combine objectives by two methods:

- The weighted average method, which calculates the score of an experiment as the weighted average of the scores of the objectives.
- The hierarchical method, which calculates the score of an experiment according to the rank of each objective. This method ensures that the objectives with a higher rank are optimised before the objectives with a lower rank.

An objective is defined by six elements:

- The property to optimise.
- A direction, which sets the type of the objective.



- For categorical properties, a target category is set to define the category to reach if the category obtained is the same as the target category, the score is equal to 100, otherwise the score is equal to 0.
- For numerical properties, the objective can be the maximum, the minimum, equal, greater or lesser than a target value
- A target, which is the value the property should reach or exceed.
- A weight, which is the coefficient used to calculate the weighted average of the scores of each objective.
- A tolerance, which is the acceptable deviation from the targeted value.
- A rank, which is the position of an objective in the hierarchy of the objectives. The rank must be chosen between 1 and 20 with 1 the highest rank.”

### 2.1.3. Prediction

When the model is fully defined, ChemAssistant can suggest new experiments in order to reach these objectives. A Bayesian Optimisation based algorithm allows to reduce the number of experiments needed to achieve these objectives.

AI experiment suggestions

How many experiment suggestions do you want?

Exploration-exploitation balance

Mostly exploration   More exploration   **Balanced**   More exploitation   Mostly exploitation

[Suggest experiments](#)

Figure 9: ChemAssistant “experiment suggestions” part

As per the ChemAssistant technical documentation: “It includes a range of classification and regression models. Classification models can predict categorical variables, while regression models predict numerical variables.”

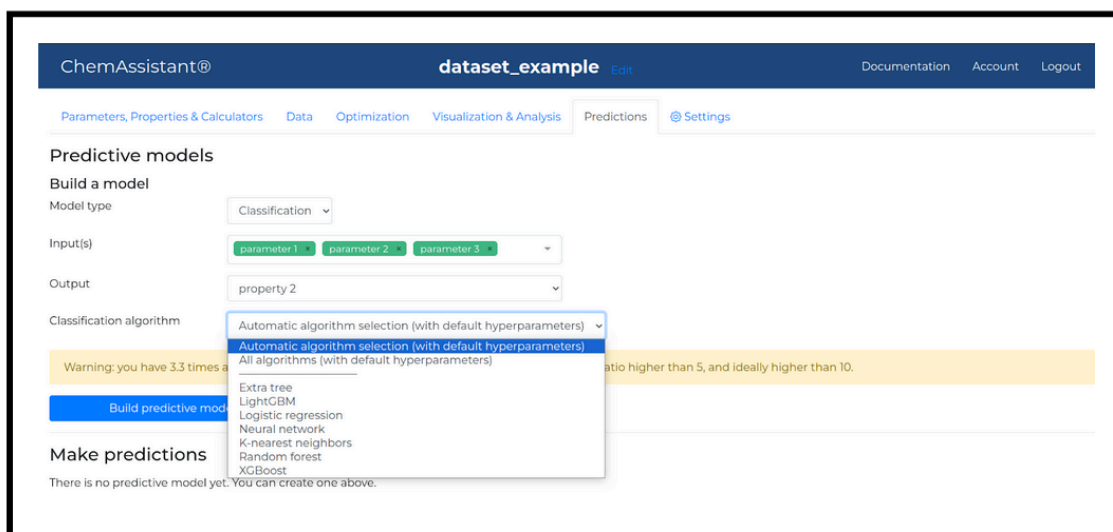


Figure 10: ChemAssistant classification predictions example

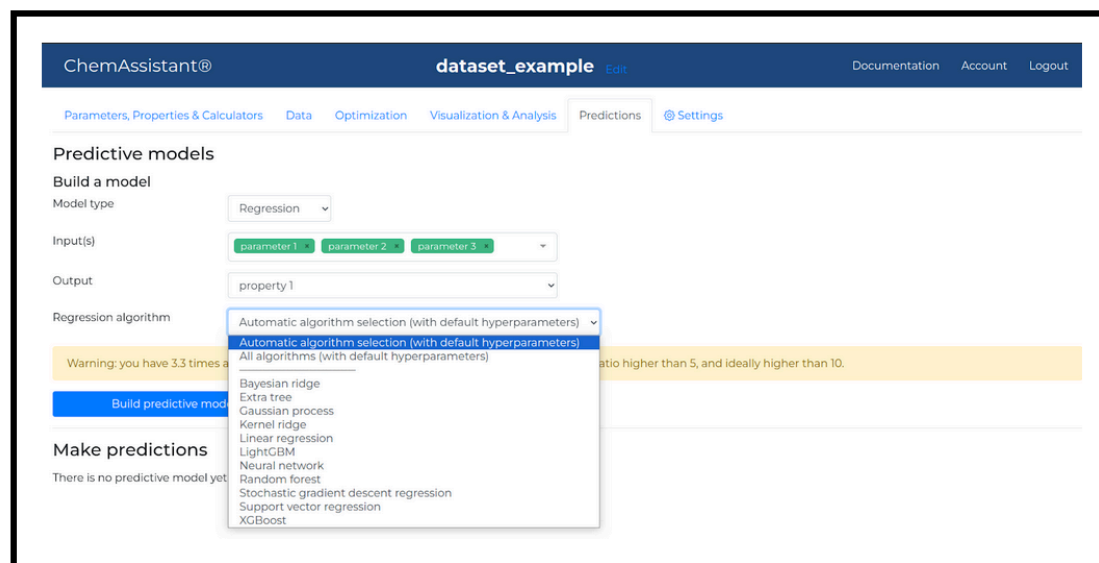


Figure 11: ChemAssistant regression predictions example

## 2.2. My mission

My mission was “to participate in the development of the SmartChemistry machine learning platform”.

ChemAssistant, ICSYNTH and DigitalGlassware are merging, I worked mostly on ChemAssistant and a small part of the merging.

I contributed to ChemAssistant by adding new functionalities and correcting some bugs.

### 2.2.1. The end to end test

On ChemAssistant, I added an end to end test, to verify that the API documentation is working well.

End to end tests are a testing technique that verifies the functionality and performance of an entire software application from start to finish by simulating a customer journey from the beginning to the end and replicating live data.

The purpose of this addition is to verify that the API documentation is still available even if the client does not have the right to access the API directly

### 2.2.2. Change API to export a dataset as excel file

I added the possibility to export the dataset in an excel file.

This task was in two parts, firstly I changed the API in the backend to have the possibility to export the dataset in an excel file based on the csv export .

Then I created the button to export and I linked it with the API entry point.

ChemAssistant® dataset\_example [Edit](#) [Documentation](#) [Account](#) [Logout](#)

Parameters, Properties & Calculators Data Optimization Visualization & Analysis Predictions Settings

#	parameter 1	parameter 2	parameter 3	property 1	property 2	calculator 1	Use   Select/unselect all
1	1	433	category 1	3	42	-430	<input checked="" type="checkbox"/>
2	2	5	category 2	6	41	7	<input checked="" type="checkbox"/>
3	3	8	category 3	9	3	19	<input checked="" type="checkbox"/>
4	4	95	category 2	8	12	-63	<input checked="" type="checkbox"/>
5	5	6	category 1	5	123	19	<input checked="" type="checkbox"/>
6	6	3	category 2	23	42	135	<input checked="" type="checkbox"/>
7	7	0	category 3	1	66	7	<input checked="" type="checkbox"/>
8	8	3	category 2	4	42	29	<input checked="" type="checkbox"/>
9	9	6	category 1	7	3	57	<input checked="" type="checkbox"/>
10	10	94	category 2	10	42	6	<input checked="" type="checkbox"/>
+							

Previous 1 Next

Select/Unselect all experiments ☒

[Export as Excel file](#) | [Export as CSV](#)

Figure 12: ChemAssistant dataset example

### 2.2.3. Prevent accumulation of unfinished reaction search jobs in database

The reaction search is a part of SmartChemistry, implemented in ChemAssistant, in which the chemist draws a chemical reaction, a process that involves rearrangement of the molecular or ionic structure of a substance, before ChemAssistant searches a similar reaction in a database with millions of chemical reactions.

A database is an organised collection of structured information, or data, typically stored electronically in a computer system.

The problem was that the search process took time to complete. Therefore, they run as jobs in a queue. Completed jobs should be removed from the queue once the result is retrieved. When the result is not retrieved or the job fails, it should not stay in the queue forever.

To fix this problem I added an expiration date to each job to check for deletable jobs and to delete expired jobs.

### 2.2.4. Display linear regression in 2D-Plots

A linear regression consists in determining a line passing as close as possible to the points of this cloud.

A point cloud graph in which the user defines which parameter, property or calculator he wants in x-axis and y-axis.

I've incorporated a linear regression line within the 2D plot, illustrating the trend. This regression analysis provides a clear depiction of the relationship between the x-axis and the y-axis, facilitating a deeper understanding of the experimental data and potentially aiding in predictive modelling or optimisation strategies within the chemical domain.

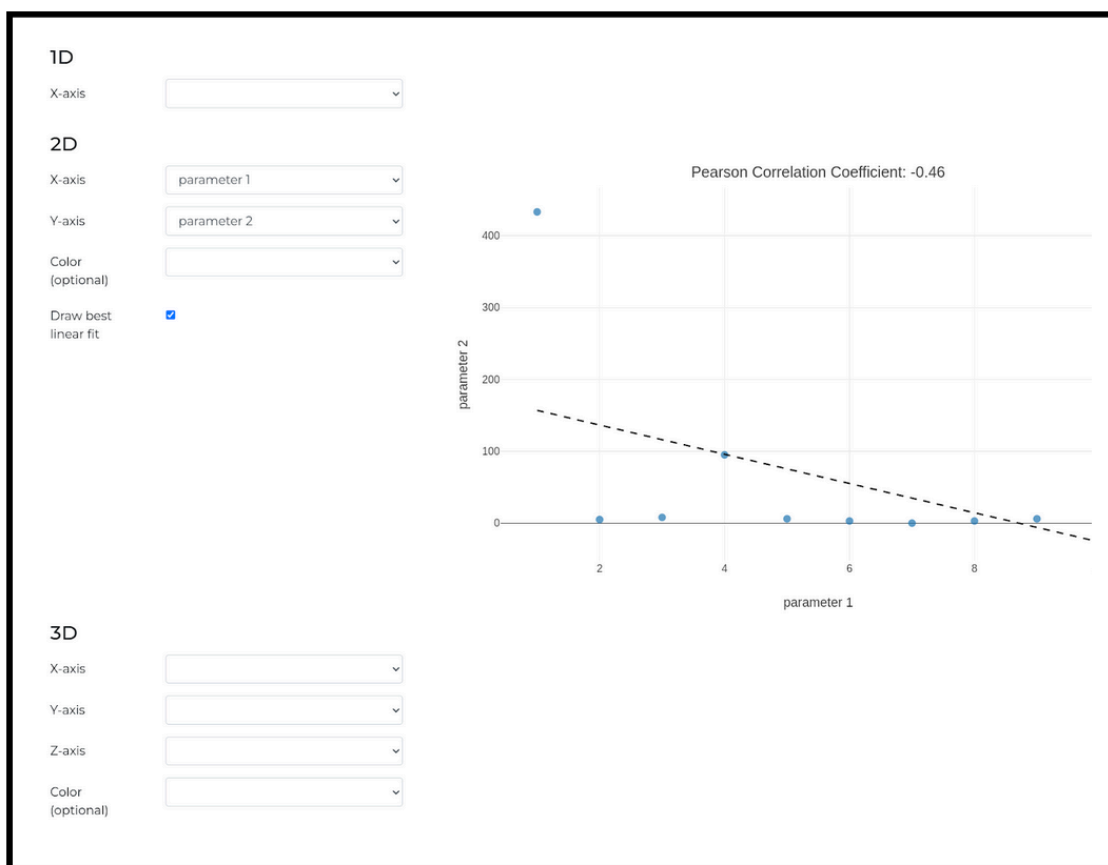


Figure 13: ChemAssistant 2D plot example

### 2.2.5. Bug fix in tooltips custom directives

The custom directive is defined as an object containing hooks. The hooks receive the element to which the directive is linked and act on it. Custom directives are mainly intended for reusing logic.

A tooltip is a message that appears above everything else when a cursor is positioned over an icon, image, hyperlink or other element in a graphical user interface.

I addressed an issue with custom tooltip directives where tooltips weren't properly hidden when necessary. The solution involved modifying the custom tooltip directives to remove the tooltip entirely instead of just hiding it. By implementing this adjustment, tooltips now adhere to expected behaviour, appearing and disappearing as intended based on user interactions. This enhancement ensures a smoother and

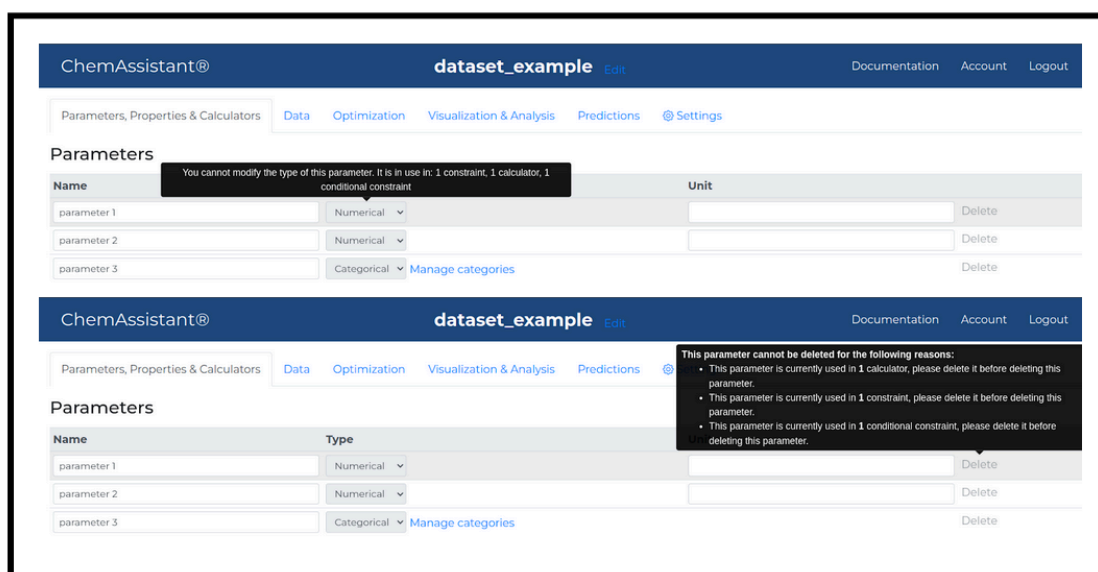
more intuitive user experience, eliminating any confusion or frustration caused by tooltips lingering when they should be hidden.

### 2.2.6. Block parameter type change or delete if in a conditional constraint

Conditional constraints are used to set the value of a parameter equal to a certain value if the value of one or more other parameters is equal to/greater than/less than one/more value(s) chosen by the user.

I tackled an issue where altering a parameter's type or deleting it would break conditional constraints, rendering them dysfunctional. The solution involved preventing parameter type changes or deletions when they are used in conditional constraints within the backend. In the frontend, I disabled buttons for changing types or deleting parameters and added tooltips explaining the issue. This approach ensures data integrity by safeguarding against inadvertent changes that could disrupt system functionality. Users are now guided effectively and prevented from actions that could compromise the integrity of conditional constraints, leading to a more robust and reliable system.

Figure 14: Example of type change and delete block



### 2.2.7. Add a marker on the y-axis of the score plot

The score graph displays the score of each experiment. The x-axis indicates the number of the experiment in the data table and the y-axis displays the score.

I implemented a feature to add a marker on the y-axis indicating the score of the data point when hovered over. This enhancement provides users with real-time feedback by displaying the exact score associated with each point as they interact with the graph. By visualising the score directly on the axis, users can quickly interpret the significance of each data point without the need for additional calculations or reference. This addition enhances the interpretability and usability of the graph, empowering users to make informed decisions based on the precise scoring information available at their fingertips.

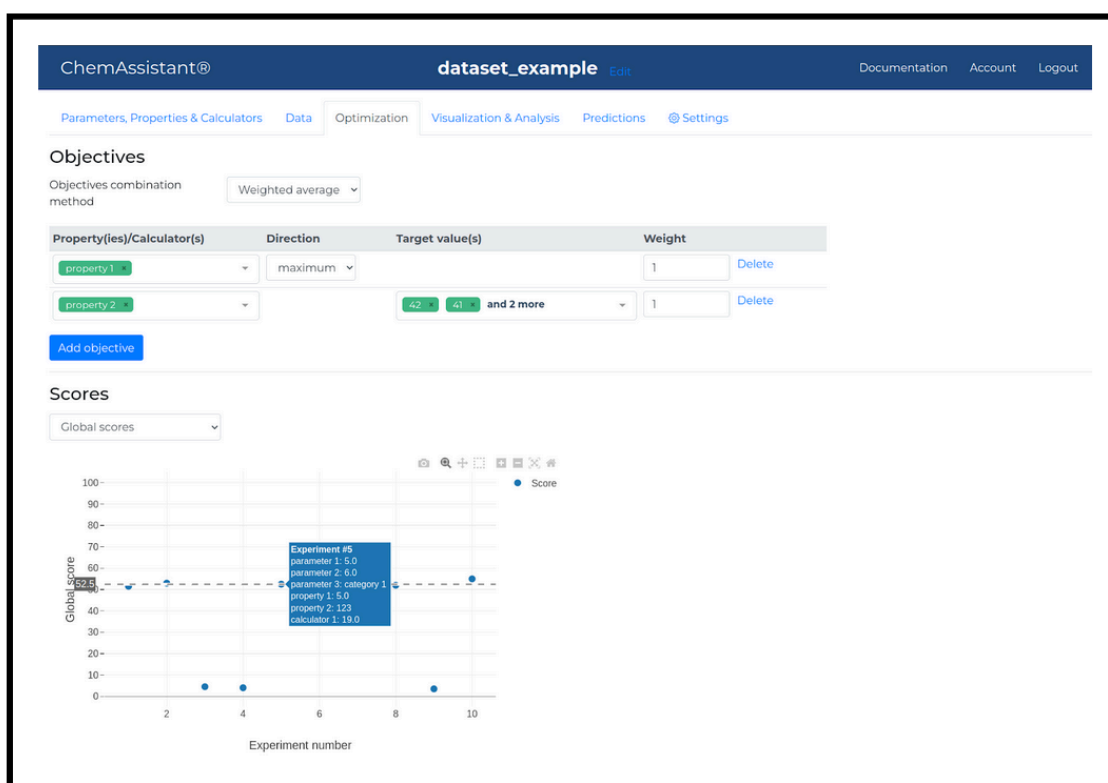


Figure 15: Score plot with Y-axis marker



### **3. The team organisation:**

In DeepMatter Group, all the teams are in three different offices. DeepMatter tech office is in Glasgow, the InfoChem office is in Munich. And the ChemIntelligence office is in Lyon.

There are also some people who work remotely, everywhere from Germany, from the United Kingdom or from Sweden.

Despite different countries, cities and offices, and even within the same office everyone uses teams and outlook to communicate

There are four people in the Lyon office: Thomas GALEANDRO - DIAMANT, Tarik BOUMAZA, Flora DOMART and me.

In the Lyon office, mutual help is very common, for example Flora helps Tarik and me for chemistry problems like chemical reaction. Tarik helps Flora for programming problems like git or docker. I help Tarik with technical advice on Gimp, Excel or for python issues.

When someone has a problem he can ask others to gather potential solutions or ideas for resolution. We can exchange ideas, on different points, on different points of view or on different subjects.

Between all the teams there are many meetings so that everyone is aware of what each one is doing. Each meeting has its own purpose, even if there are the same people in each meeting. For example, if someone is absent from a meeting, they can catch up with everyone's news at the next meeting.

Every four weeks, on Tuesday, there is a sprint review and retrospective to review the last sprint and analyse what was good and what was bad. A sprint is a short, time-boxed period when a team works to complete a set amount of work. Sprints are at the very heart of scrum and agile methodologies, and getting sprints right will help the agile team ship better software with fewer headaches.

Every two weeks, on Wednesday, there is a sprint planning to plan the new sprint and what everyone will do for the next two weeks. It is based on what everyone has done on the previous sprints to be sure that each developer will work on a task he likes and on a subject he already knows.

Every day, I had a daily meeting with Christoph, my internship mentor, to explain and show him what I had done the day before, ask him my questions, tell him my problems and what I will do on the day.

Sometimes, there is also a meeting organised by a developer who wants to learn, teach or make known something to other developers. These meetings are created by the developer and approved by his supervisor and are very useful because everyone knows something that others don't know.

The DeepMatter team works with tasks like many other teams. How does this task work and what is the organisation around them ?

A task is created if a bug is found, if it's a common client request or if the automated test doesn't work.

This task needs to have a clear title and a description of the addition to do or the bug to correct. Each task created has an automatically assigned number.

When this task is correctly defined, either someone takes it or it is distributed by Thomas to someone during sprint planning.

Thomas / ChemAssistant / Issues / #775

## Changing a parameter type shouldn't be allowed when it's used in a conditional constraint

Edit ⋮

🔒 Closed 📅 Issue created 2 months ago by Thomas

To reproduce the bug, create a dataset with two parameters, as shown below:

### Parameters

Name	Type	Unit	
X1	Categorical ▾		<a href="#">Manage categories</a> <a href="#">Delete</a>
X2	Numerical ▾		<a href="#">Delete</a>

Note: Also add a property, otherwise `conditional constraints` will not be active.

then create a conditional constraint involving both parameters, as shown below:

### Conditional constraints

	Parameter	Value		Parameter	Value	
If	X1 ▾	= 100.0 ▾	Then	X2 ▾	= ▾	0 <a href="#">Delete</a>
	<a href="#">Add condition</a>					

then change the type of parameter X1 from categorical to numerical:

### Parameters

Name	Type	Unit	
X1	Numerical ▾		<a href="#">Delete</a>
X2	Numerical ▾		<a href="#">Delete</a>

the conditional constraint is bugged, as shown below:

### Conditional constraints

	Parameter	Value		Parameter	Value	
If	X1 ▾	▾ [object Object]	Then	X2 ▾	= ▾	0 <a href="#">Delete</a>
	<a href="#">Add condition</a>					

Solution: don't allow changing the type of a parameter if it's used in a conditional constraint (or any other constraint type). FYI, there is already a mechanism to disallow a type change for any parameter that is used in a predictive model or experiment suggestions are displayed in the Optimization tab. You should extend that mechanism to conditional constraints.

Figure 16: Example of a task



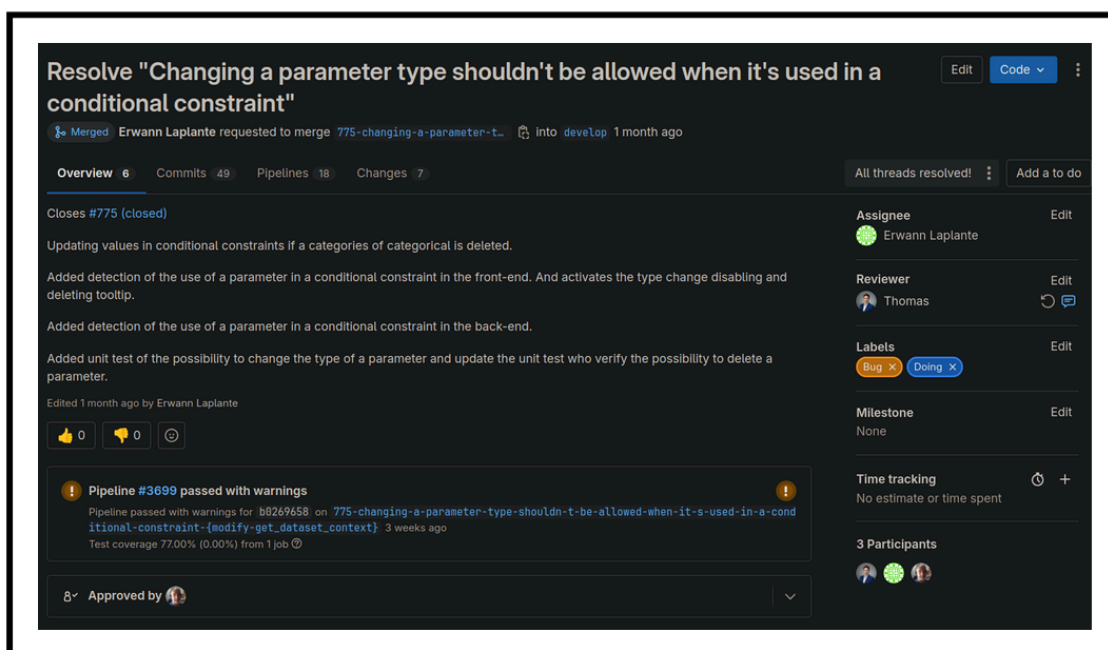


Figure 18: Example of a merge request

After this Thomas reviews the merge request if there are no merge conflicts. Conflicts usually occur when two people have edited the same lines in a file, or if one developer has deleted a file while another developer was editing it. In these cases, the correct version cannot be determined automatically. Conflicts only affect the developer who performs the merge, other team members are not aware of the conflict. The file will then be marked as conflicting and the merge process will be stopped. It is then up to the developer who created the merge request to resolve the conflict in order to share its edit version with the rest of the code .

The review of a merge request is to see if the new version works as desired. Then Thomas inspect the code that has been modified or added to check if there is no spelling error, if it meets the same criteria (same way of naming, same way of coding, etc ...) as the code that surrounds it. And if everything is fine and works, Thomas merges the task branch in the develop branch.

## II-Personal experience and results

SmartChemistry seems to be a very ambitious and very interesting project. Combining ChemAssistant which seem different but still so close, ICSYNTH and Digital Glassware, could be a revolution in the world of chemistry.

SmartChemistry is a very conspicuous project, ChemIntelligence and ICSYNTH being two highly developed software. The merge of the two will not be an easy and short task for the developers who will work on it, but that does not prevent me from wanting to be part of this team when the merger project is launched.

Working on SmartChemistry will allow me to discover ICSYNTH, its precise function and the way it was developed. Moreover, I think I would feel closer professionally to the people currently working on ICSYNTH.

Working on ChemAssistant, I have been in contact with everyone from ChemIntelligence (Thomas, Tarik and Flora) and Christoph from InfoChem. I think that working on SmartChemistry, if I have the opportunity, I will need to interact with many other people at InfoChem.

During this internship, I was able to add end-to-end tests in ChemAssistant, and every time I saved my work online I was running the pipeline. How would it be useful for me to work on SmartChemistry ?

For a project like SmartChemistry, or even smaller projects like ChemAssistant or ICSYNTH, pipeline setup and automated testing is very important.

A pipeline is the lead component of continuous integration, delivery, and deployment. It drives software development through building and testing. Pipelines are jobs, which define what will be done, such as compiling or testing code, as well as stages that spell out when to run the jobs. An example would be running tests after stages that compile the code.

A pipeline automates steps such as builds, tests, and deployments. When a team takes advantage of automated pipelines, they simplify the handoff process and decrease the chance of human error, creating faster iterations and better quality code. Everyone can see where code is in the process and identify problems long before they make it to production.

This allowed me to understand how automated testing works, how to create it, and to fix it when a bug occurs. If one day I have the chance to work on SmartChemistry.

Also, I work on the back-end of ChemAssistant, I really liked work on this part of the project and it is on these kinds of issues that I felt most comfortable. Whether

website, application or software, all have a back-end, so I have the opportunity to work on SmartChemistry. I would like to improve my knowledge and skills.

Having worked hard on the front-end of ChemAssistant, I now think I can understand how ChemAssistant works as a whole. This would allow me, if I work one day on SmartChemistry, to help create and understand it very quickly despite the addition of ICSYNTH functionality.

For example, to add a marker on the y-axis of the score plot when a point is hovered., I had to approach it from a different angle to avoid unnecessarily complicating the code, especially if there is a simpler method available. Additionally, opting for a simpler approach often enhances clarity for developers and anyone reviewing the code. Simplifying the solution not only streamlines the codebase but also improves its maintainability and readability, making it more accessible to future developers or collaborators. By prioritising simplicity without sacrificing functionality, the code becomes more intuitive and easier to comprehend, reducing the potential for errors and facilitating smoother collaboration within the development team. In essence, embracing simplicity in coding practices fosters a more efficient and effective development process, promoting better understanding and cooperation among team members. This shift in perspective underscores the importance of prioritising clarity and simplicity in problem-solving, ultimately leading to more robust and sustainable software solutions.

This way of solving problems keeps the code clear and comprehensible while solving the problem in a fairly simple way. I hope to bring this skill to the SmartChemistry project one day.

Problem-solving is at the core of my skill set, and I thrive when faced with complex challenges. Throughout my internship, I encountered numerous obstacles that required creative thinking and strategic problem-solving to overcome. I was able to identify solutions and implement them effectively. This ability to tackle challenges head-on will be instrumental in addressing any hurdles that arise during the SmartChemistry project.

My internship experience has honed my ability to adapt quickly to new technologies and environments. During my time at ChemIntelligence, I seamlessly transitioned between various tasks and projects, demonstrating my versatility and readiness to take on new challenges. This adaptability will be invaluable when integrating into the SmartChemistry project team, ensuring a smooth and efficient collaboration from the outset.



If I have the opportunity to do a new internship at ChemIntelligence or even within the DeepMatter Group, or if I had the opportunity to continue this internship at ChemIntelligence, I would be happy to contribute to the development of SmartChemistry.

Continuous learning is a core value of mine, and I am always seeking opportunities to expand my knowledge and skills. SmartChemistry presents a unique learning opportunity. By embracing this challenge, I aim to grow both personally and professionally, ultimately becoming a more well-rounded and versatile contributor.

Despite my primary passion lying in technology rather than chemistry, I find the SmartChemistry project incredibly compelling. My fascination with technology stems from its potential to revolutionise industries and improve lives. I am motivated by the prospect of leveraging technology to enhance chemical processes and drive innovation in the field. Embracing this opportunity would not only allow me to contribute my technique but also expand my horizons and deepen my understanding of chemistry's impact on technological advancements.

In conclusion, I am eager to be part of the SmartChemistry project and believe that my skills, experience, and passion make me a strong candidate. I am excited about the opportunity to collaborate with like-minded professionals in driving innovation forward.