VR-Enabled Process Chemistry: AI Avatars, Live Data Streams & On-Demand 3D Printing

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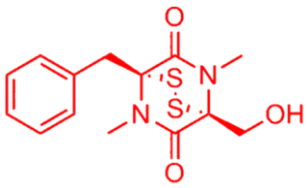
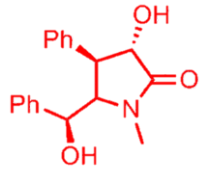
UCL SCHOOL OF PHARMACY
BRUNSWICK SQUARE

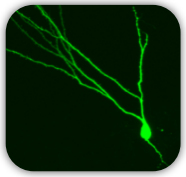
Research Overview

Medicinal Chemistry



Anti-Cancer Drug Discovery





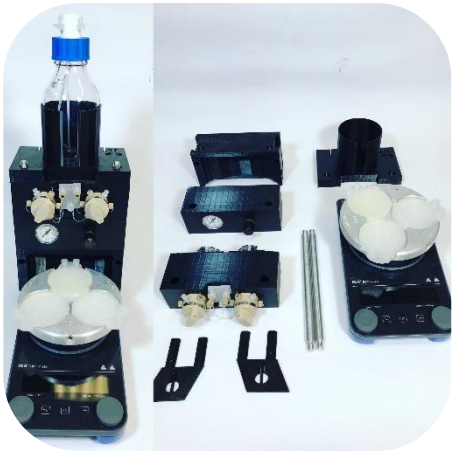
Neuroscience Drug Discovery

Cell Chemical Biology, **2018**, *25*, 1-9.
Molecular and Cellular Neuroscience, **2018**, *92*, 82-92.
European Journal of Organic Chemistry **2015**, *34,* 7438-7442.

3D Printing and Catalysis

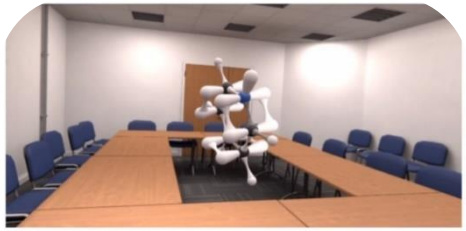
Reaction Chemistry and Engineering, **2020**, *5*, 853-858.
Reaction Chemistry and Engineering, **2023**, 752-757.
Journal of Organic Chemistry, **2023**, 16845-16853.

Continuous Flow Chemistry/Photo/Electro



ChemElectroChem, **2019**, *6*, 4144-4148.
European Journal of Organic Chemistry, **2019**, *23*, 3783-3787.
Journal of Flow Chemistry, **2021***, 11,* 19-29.

Virtual Reality/ 3DPrinting/ Robotics



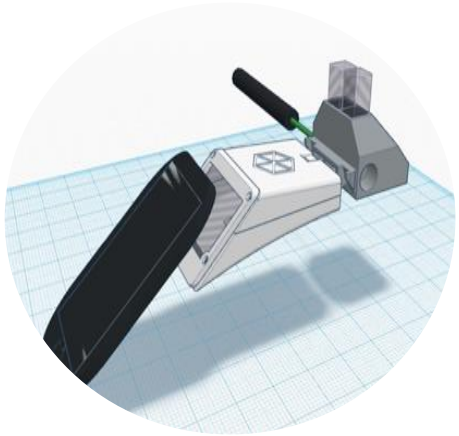
Journal of Chemical Education, **2017,** *94*, 1265-1271.
Nature Reviews Methods Primers, **2022**, *2*, 17.
Nature **2023**, Nature Spotlight.

Research Overview

Reactive Extrusion/ Equipment

European Journal of Organic Chemistry, **2019**, *23*, 3783-3787.
International Journal of Pharmaceutics **2015**, *494*, 651-656.
Journal of Applied Crystallography, **2019,** *52*, 171-174.

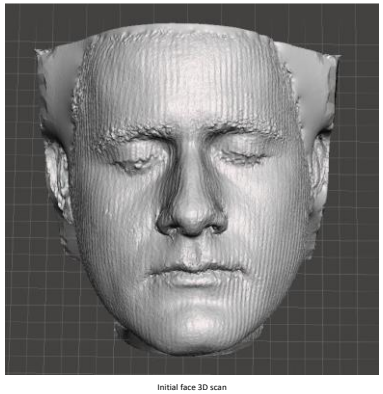
Point of Care Diagnostics

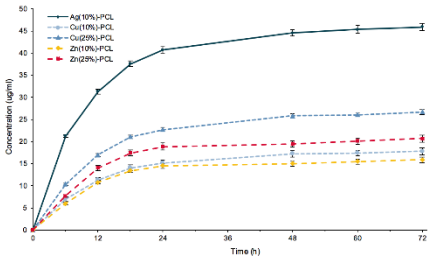


3D Printing and Internal/ External Drug Delivery

European Journal of Pharmaceutical Sciences **2018**,*123*, 217-227.
Pharmaceutics, **2019**, *11*, 250.

3DPrinting Personalized Therapy

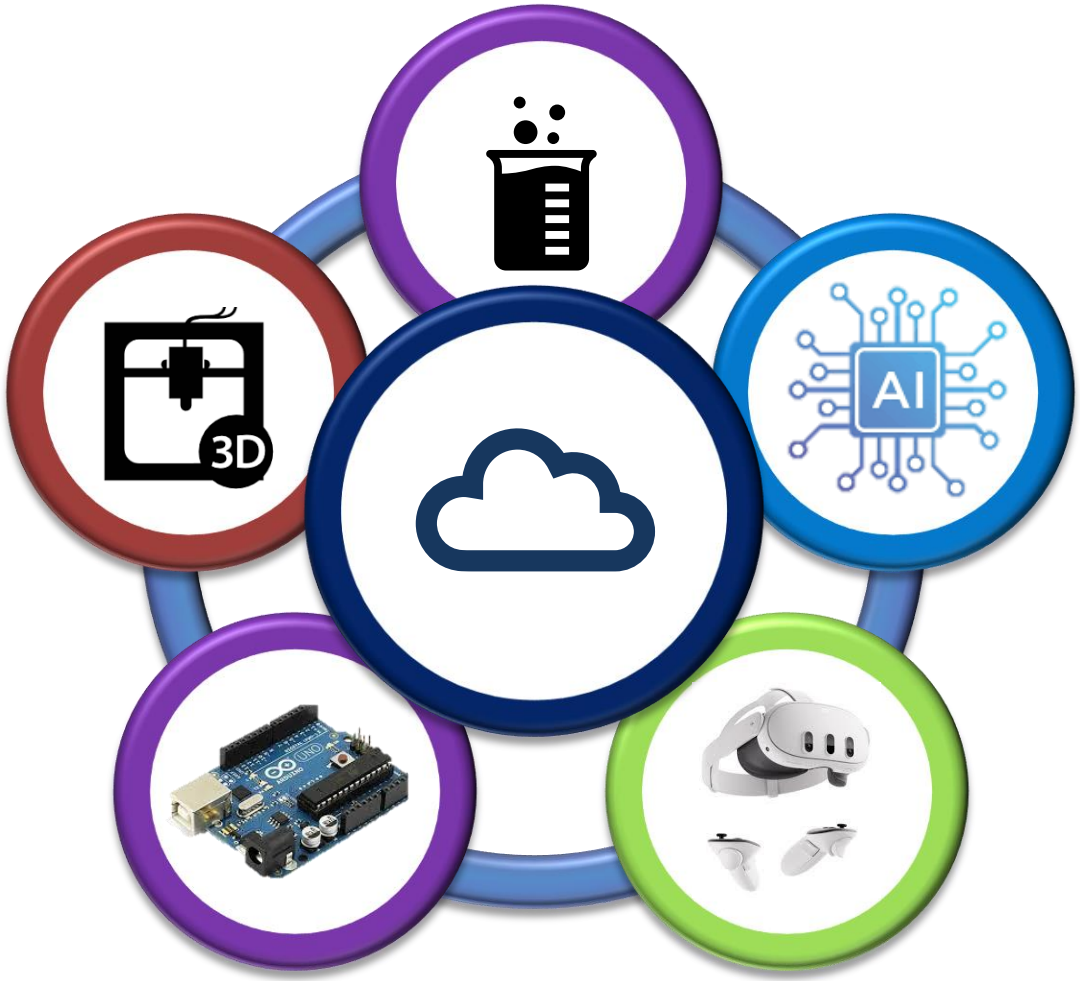

Initial face 3D scan



International Journal of Pharmaceutics **2017**, *527*, 161-170.
International Journal of Pharmaceutics **2022**, *613, 1213866.*

Our Laboratory 2023

2026 The Combined Laboratory



Nature, **2023,** *https://www.nature.com/articles/d41586-023-02688-1*
Nature Reviews Methods Primers, **2022**, *2*, 17.
ChemElectroChem, **2019**, *6*, 4144-4148.
European Journal of Organic Chemistry, **2019**, *23*, 3783-3787.
Journal of Flow Chemistry, **2021**, *11*, 19-29.
Reaction Chemistry and Engineering, **2020**, *5*, 853-858.
Reaction Chemistry and Engineering, **2022**, *early access*.
Journal of Flow Chemistry, **2023**, *13*, 435-442.
Digital Discovery, **2023**, *2, 1797 - 1805.*

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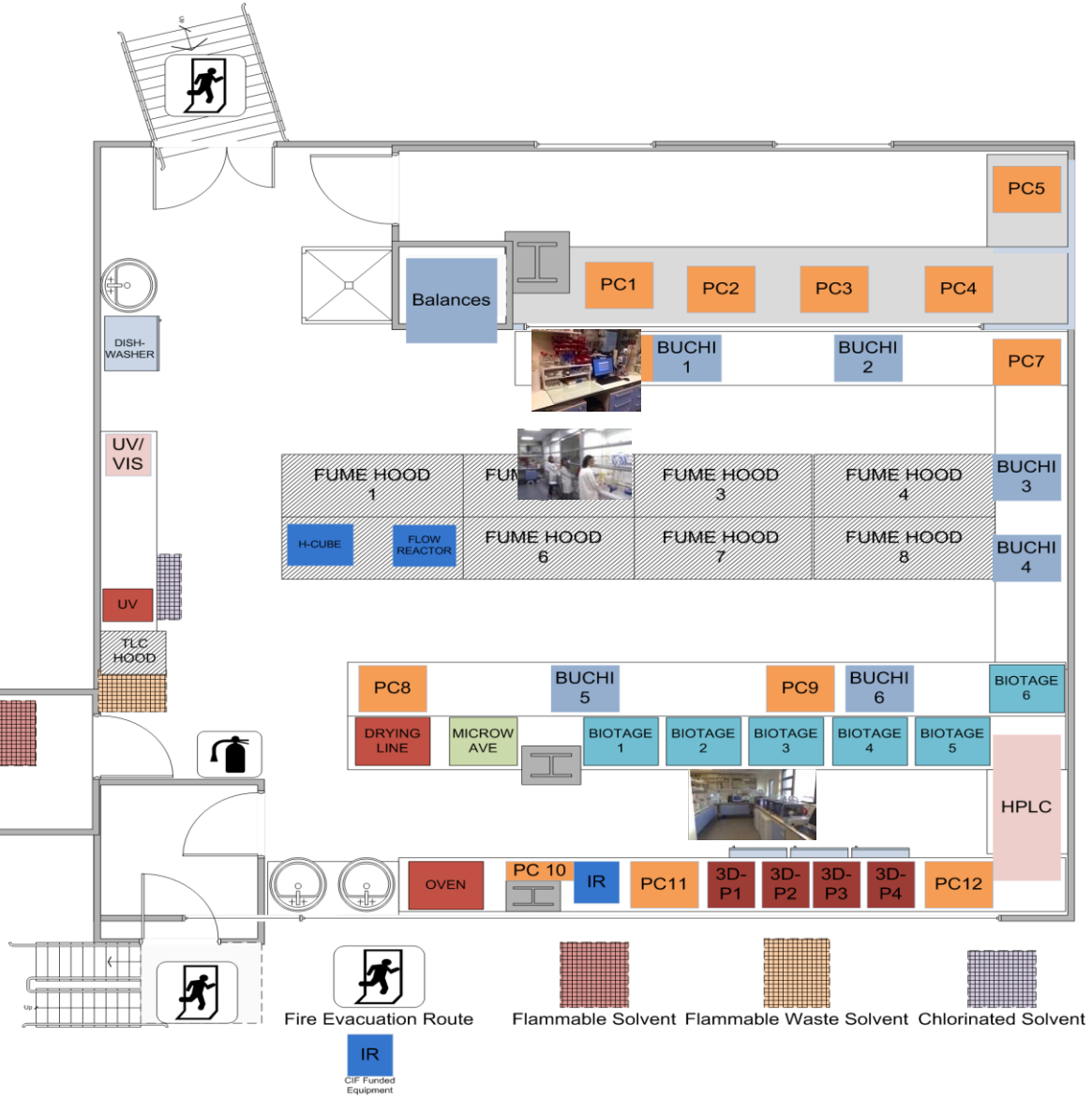
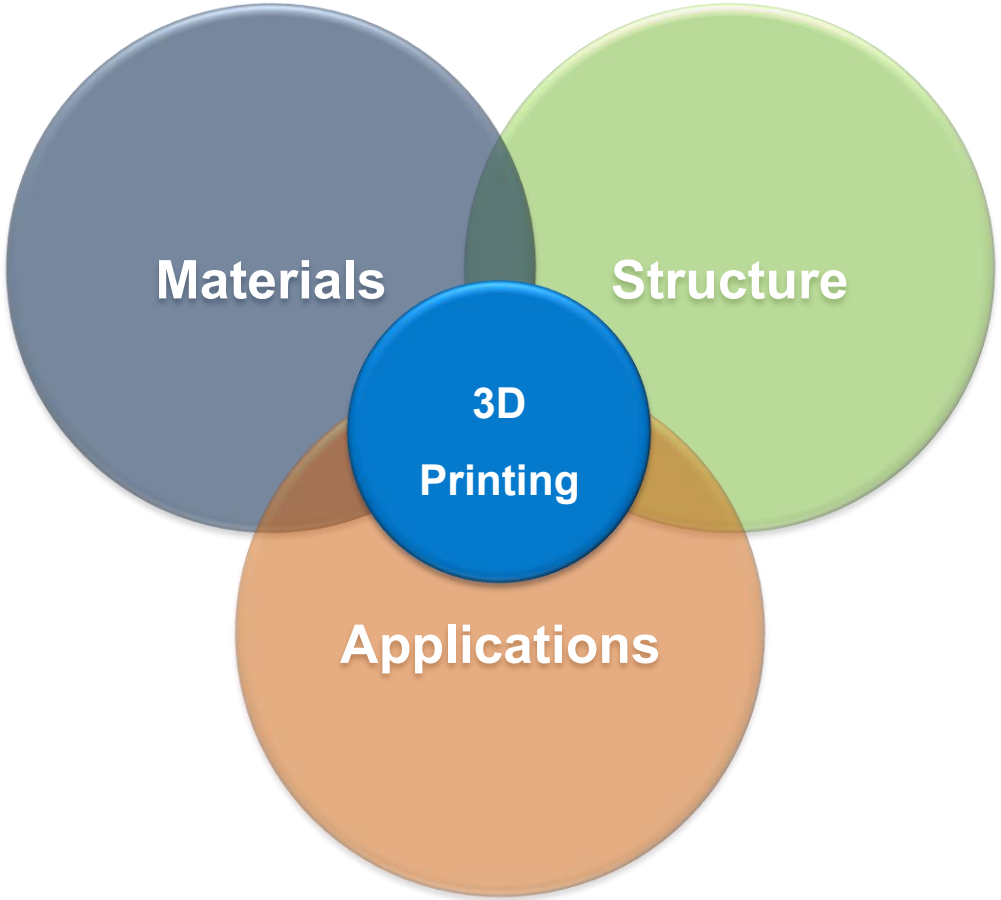
3D Printing and Infrastructure



Why 3D Printing?

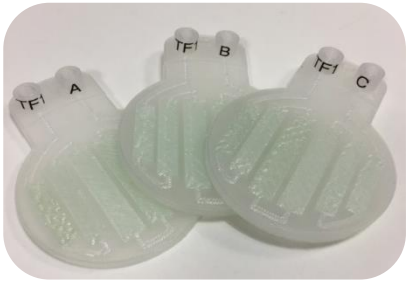
SLA

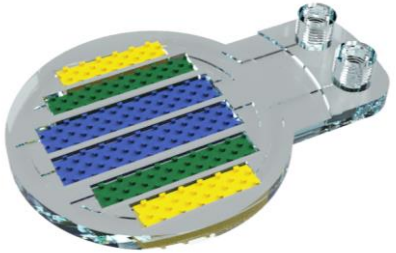
FDM



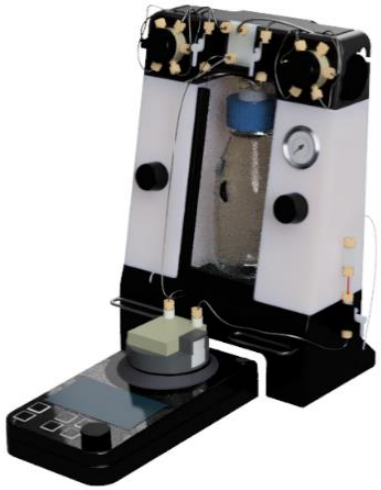
Why 3D Printing - Chemistry

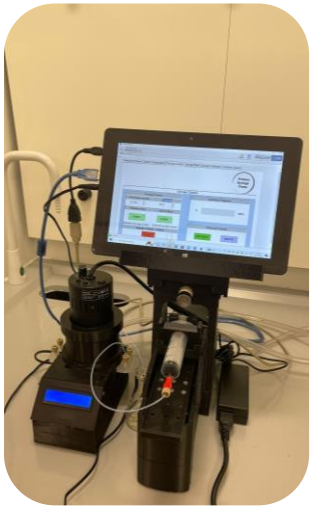
SLA





FDM





Global Laboratory Essentials

Internet

Manufacturing

VR

Knowledge

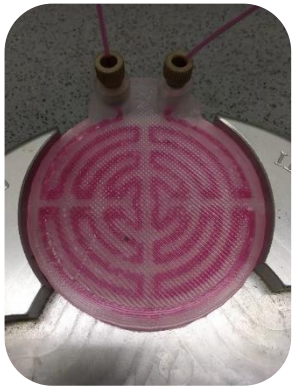
Telemetry

Computing

Total Cost: £5,500

Why 3D Printing - Savings

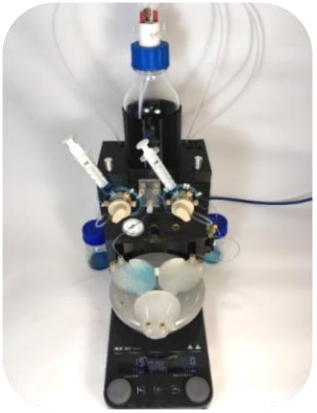
FDM



Flow Reactors: Total Savings:

£824,000 - £999,500

SLA



Flow Systems: Total Savings:

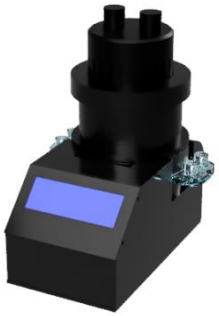
£631,500 - £1,293,000

Total Average Savings – £2,200,000

Savings – Other Items – VR Linked

Flow Systems:
Total Savings:

£35,745

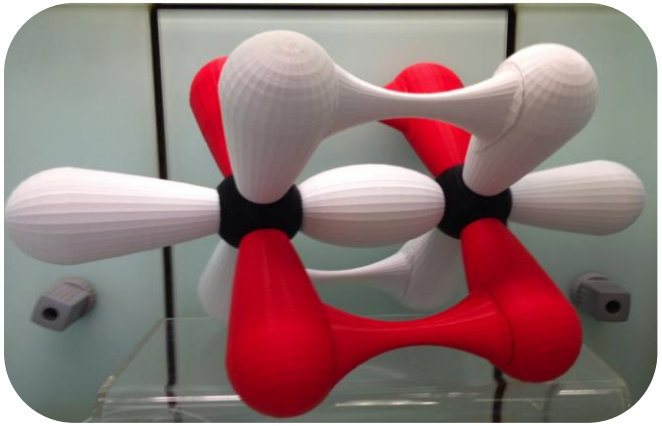


Flow Photochemistry

£75,000

Total Average Savings – £2,200,000

Savings – Other Items – VR Linked



3D Printed Models:
Hundreds of Objects

£15,000 including labour

Total Average Savings – £2,200,000

My Research Journey

My Research Journey

2016

My Research Journey

2016

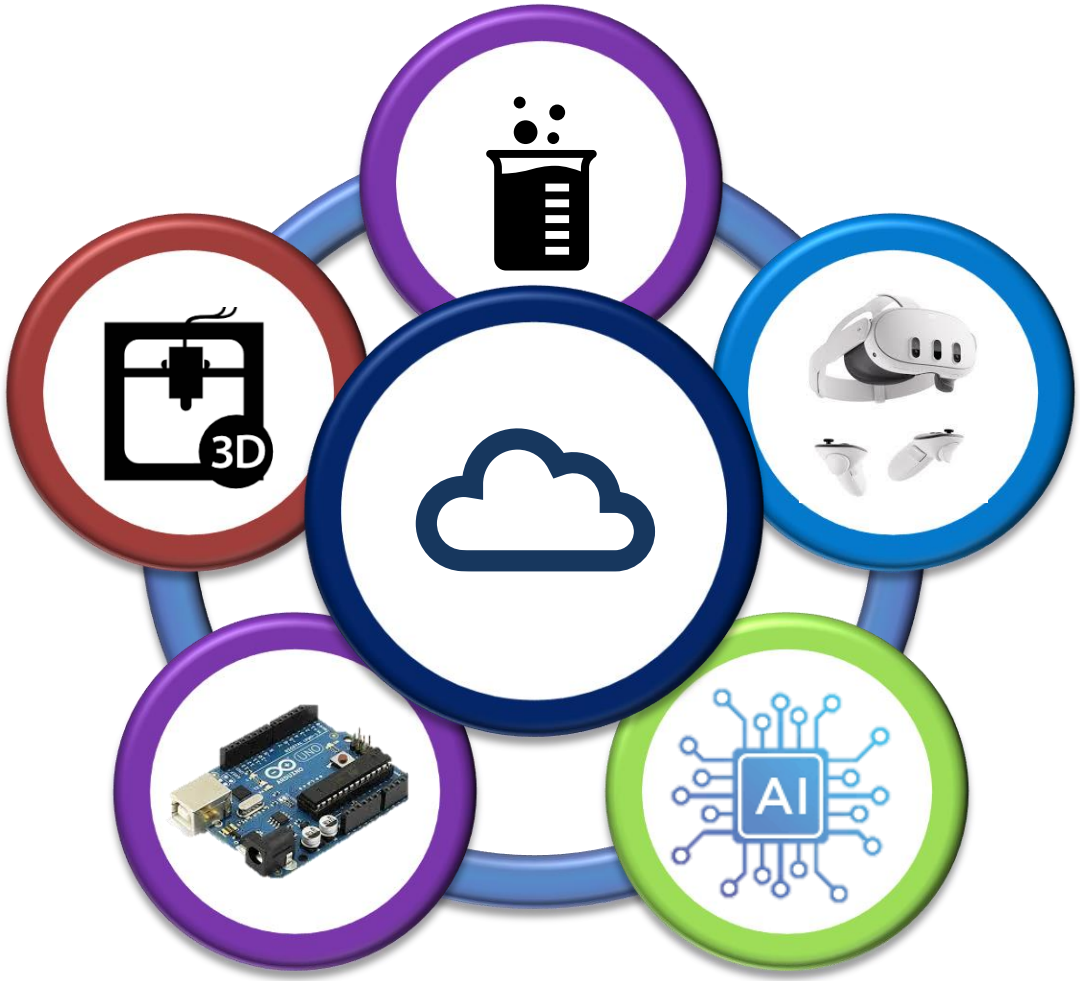
My Research Journey

2016

My Research Journey

2016

The Combined Laboratory



Nature, **2023,** *https://www.nature.com/articles/d41586-023-02688-1*
Nature Reviews Methods Primers, **2022**, *2*, 17.
ChemElectroChem, **2019**, *6*, 4144-4148.
European Journal of Organic Chemistry, **2019**, *23*, 3783-3787.
Journal of Flow Chemistry, **2021**, *11*, 19-29.
Reaction Chemistry and Engineering, **2020**, *5*, 853-858.
Reaction Chemistry and Engineering, **2022**, *early access*.
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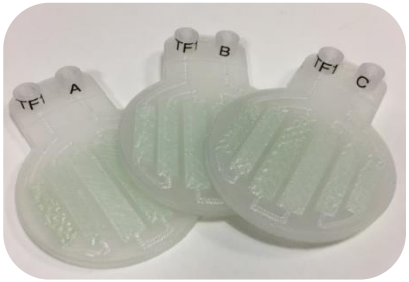
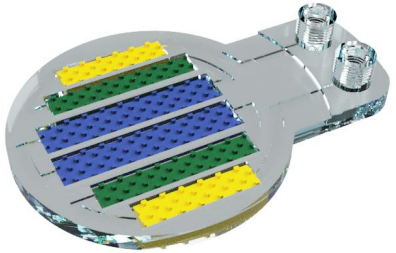
Digital Discovery, **2023**, *2, 1797 - 1805.*

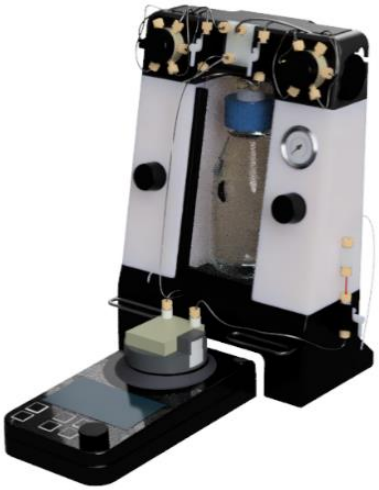
Why 3D Printing - Chemistry

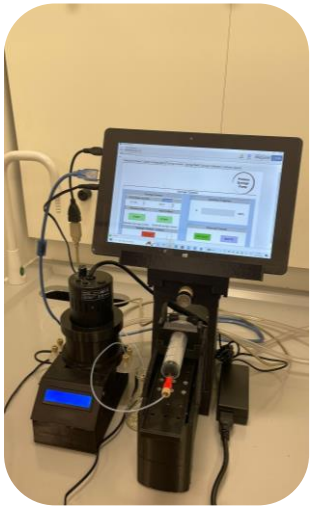
SLA





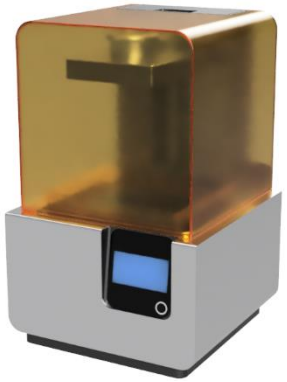
FDM

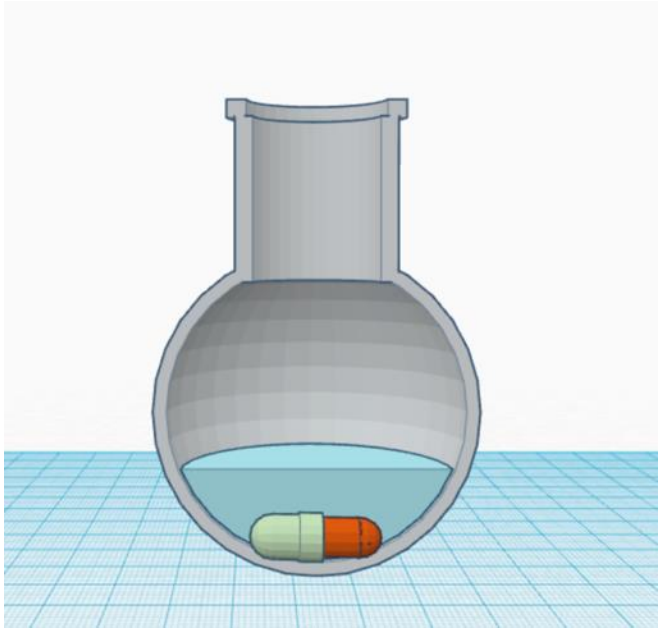


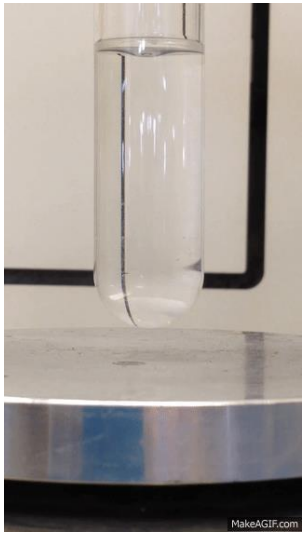


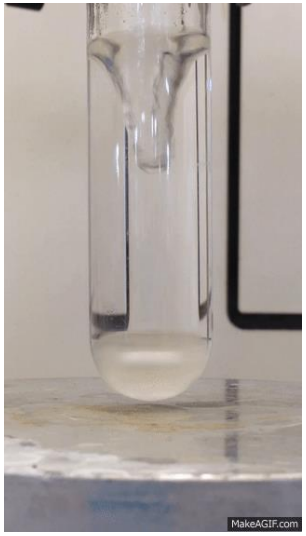
3D Catalytic Stirrer Beads

- SLA printing
- Shape maximises surface area and solvent mixing
- Catalyst loading between 5-10% (*w/v*)
- Resistant to nearly all solvents





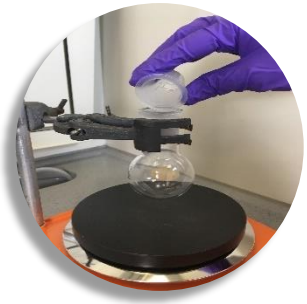




3D Catalytic Stirrer Beads



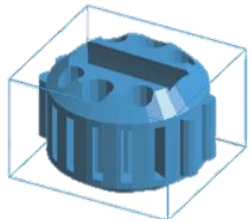

Reaction Setup **15 min** → Reaction **1-16 hours** → Clean-up **15-60 min** → Purification **1 hour**

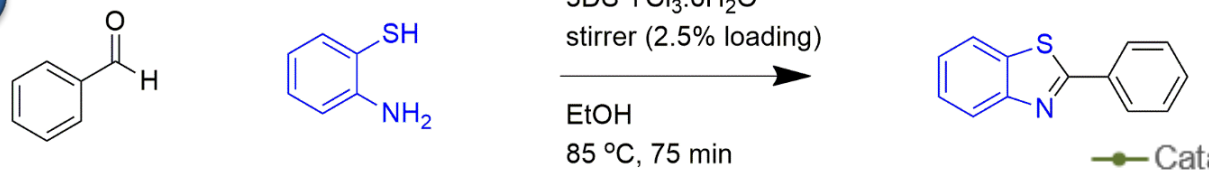


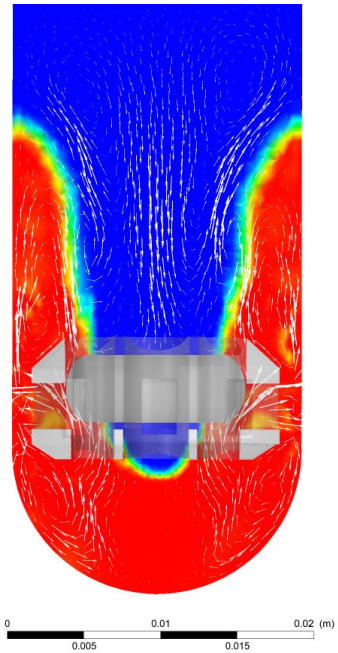
Setup **5 min** → Reaction **0.3- 8 hours** → Clean-up **1 min** → Purification **30 mins**

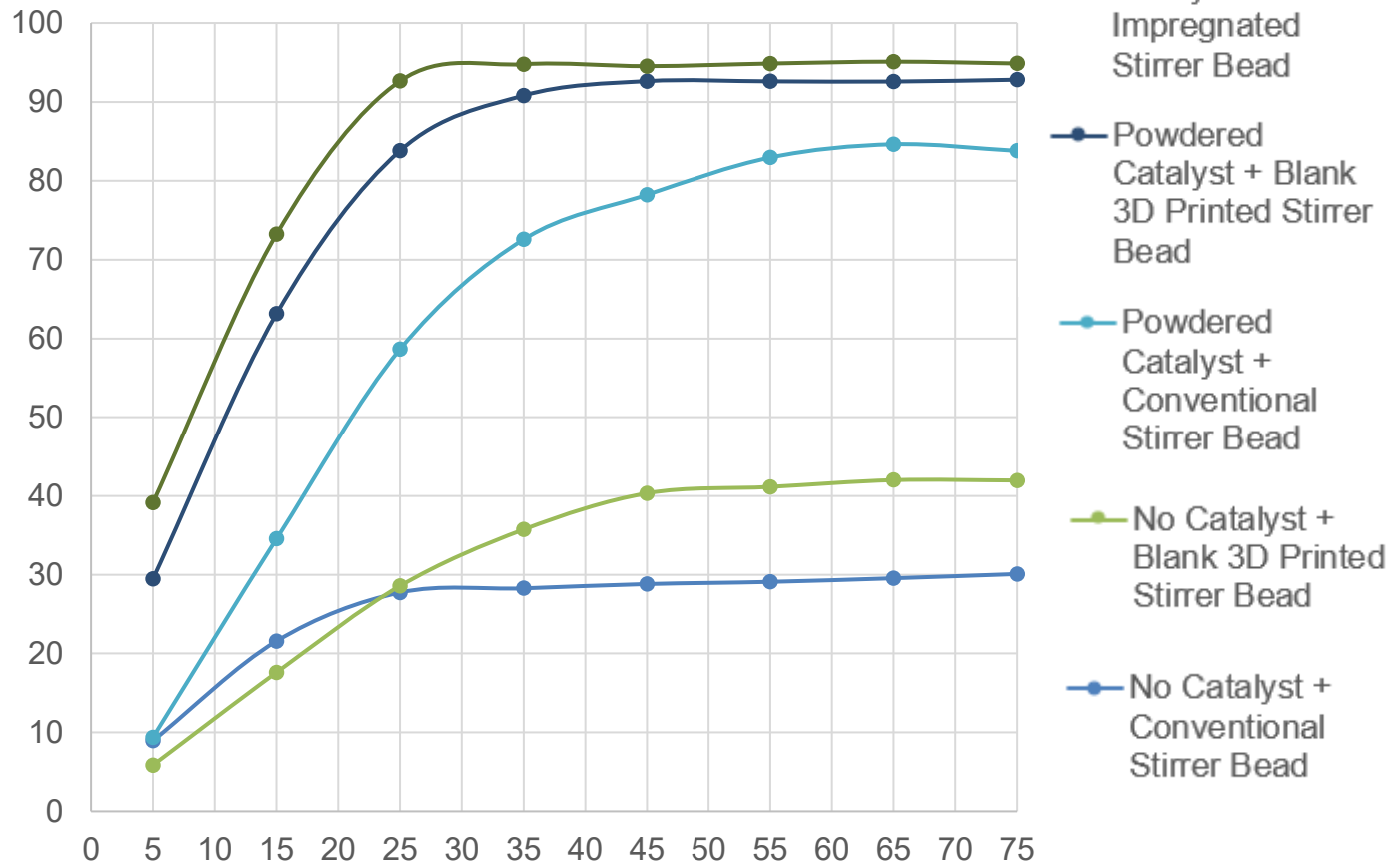
Heterocycle Formation

Heterocycle Formation



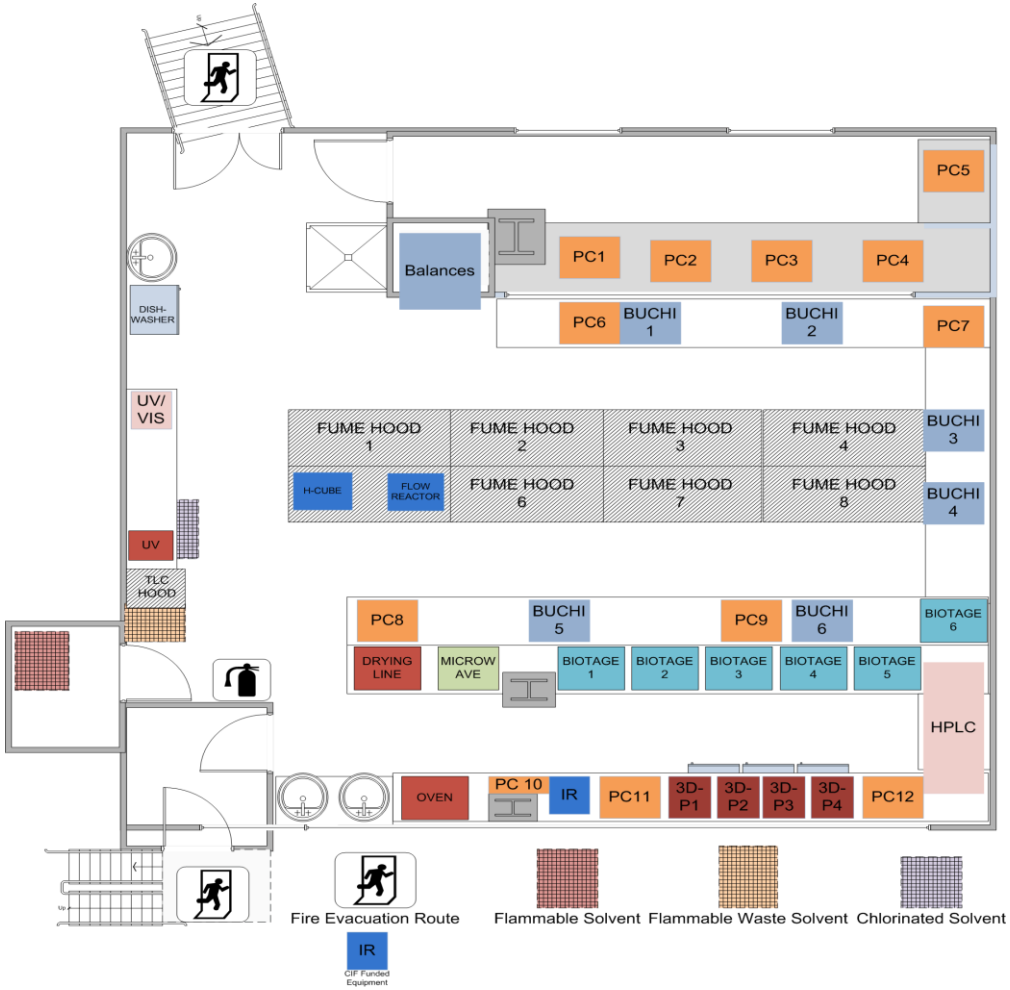






Journal of Organic Chemistry, **2023**, *88*, 16845-16853.

Low-Cost Continuous Flow



Key Barrier –
Flow chemistry is expensive:

£30-100 K per system
Locks out fume hood space

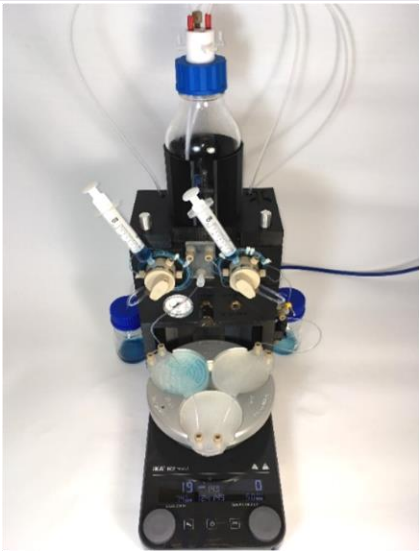
Flow Mixing Challenges

Designed to run off Compressed Air/ Nitrogen

Control of *pulseless* flow rate from

pressure control and resistance

capillary

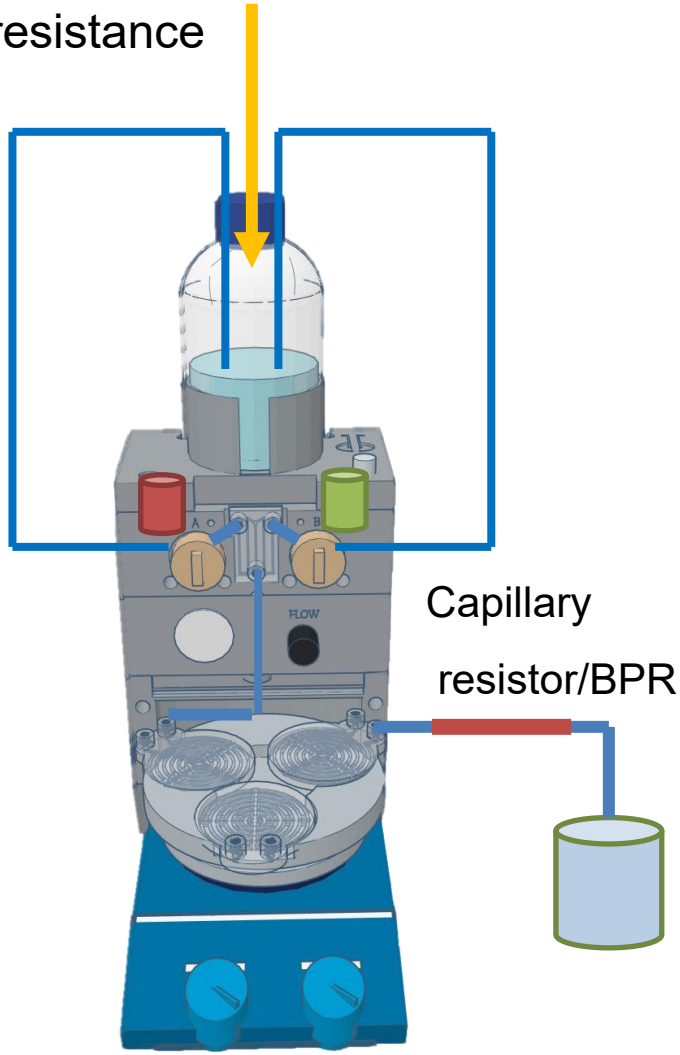


Solvent reservoir

Reagent Injection

Flow Control

Heating and residence time

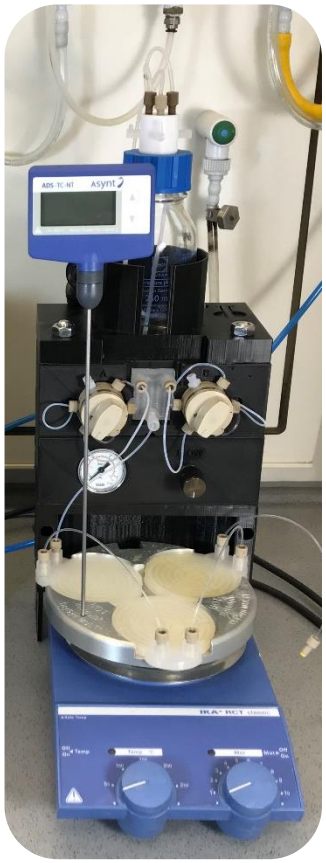


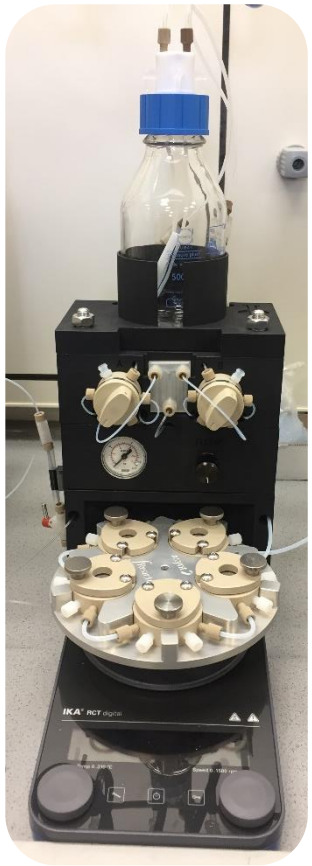
Capillary resistor/BPR

European Journal of Organic Chemistry, **2019**, *23*, 3783-3787.

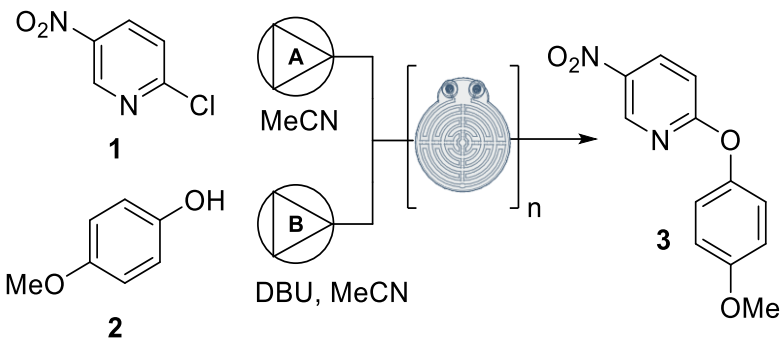
New Continuous Flow

Fits all types of Stirrer Hotplate
Ccompatible with the FReactor

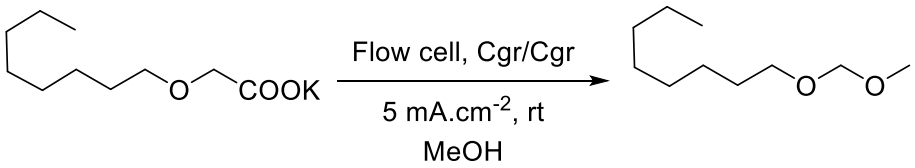




3D Printing and the IKA FLOW



European Journal of Organic Chemistry, **2019**, *23*, 3783-3787.



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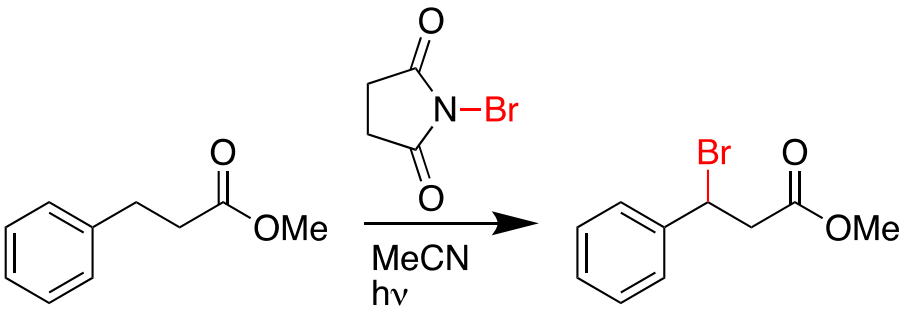
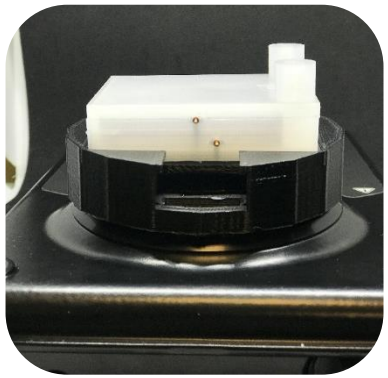
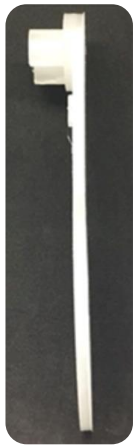
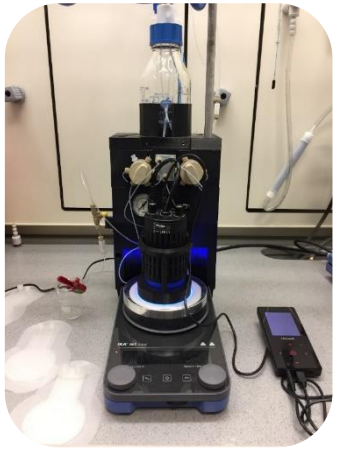
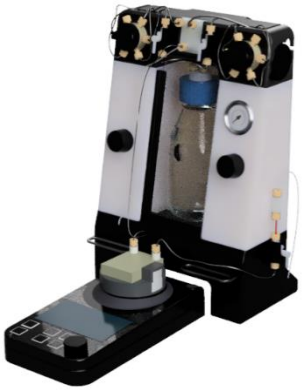


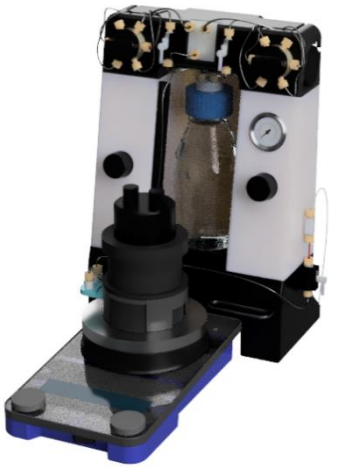
Journal of Flow Chemistry, **2023**, *13*, 435-442.



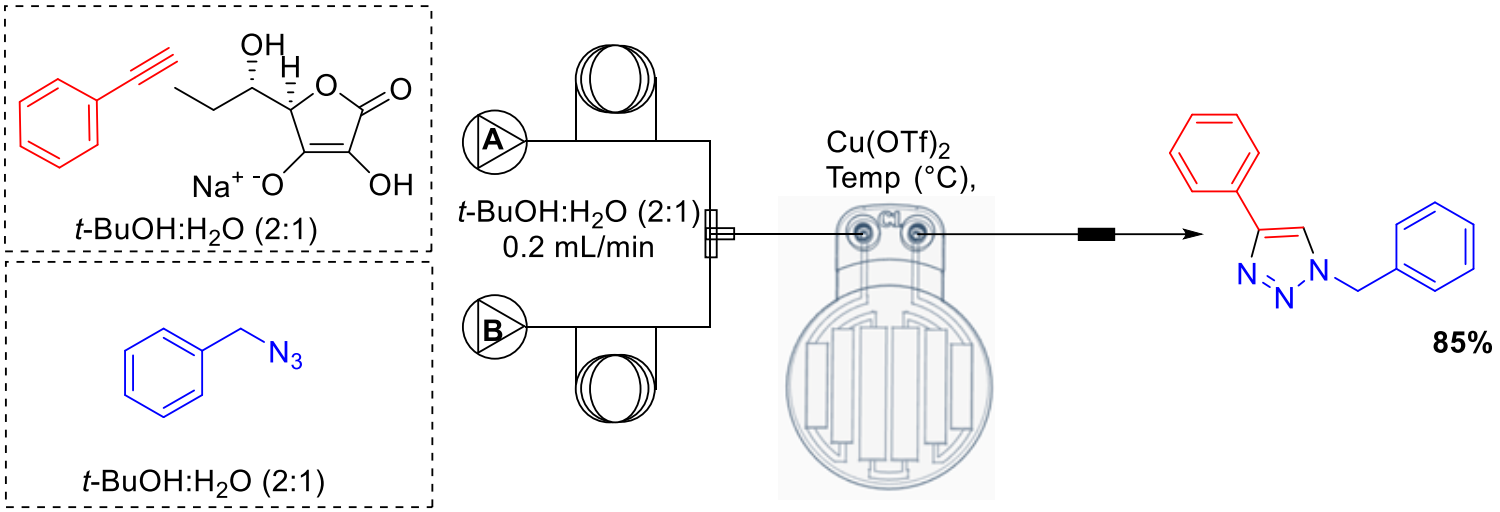


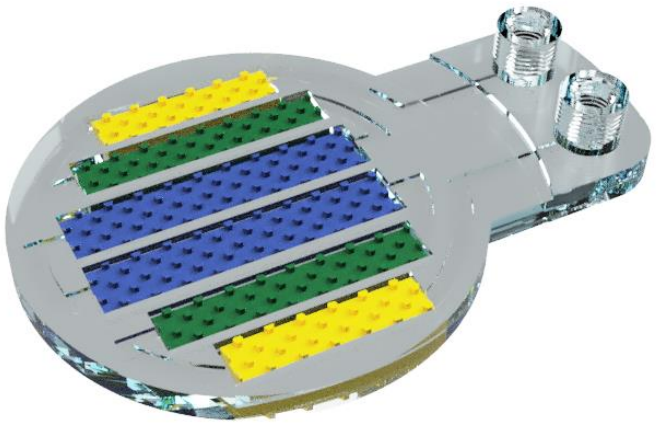


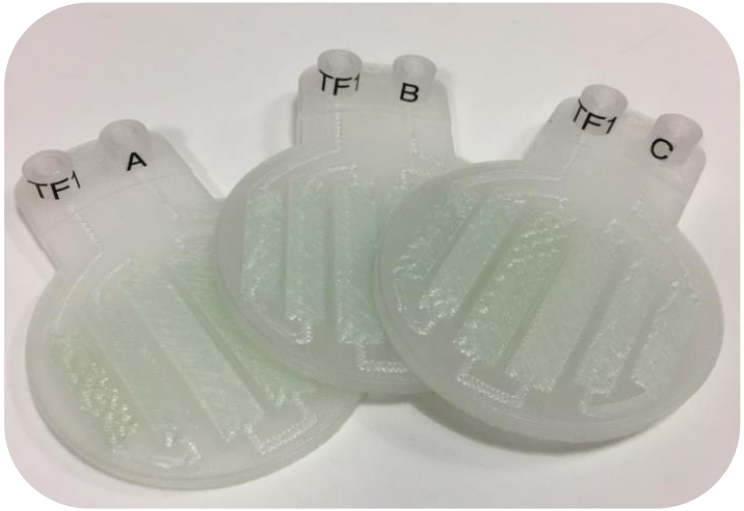




3D Printing – New Continuous Flow

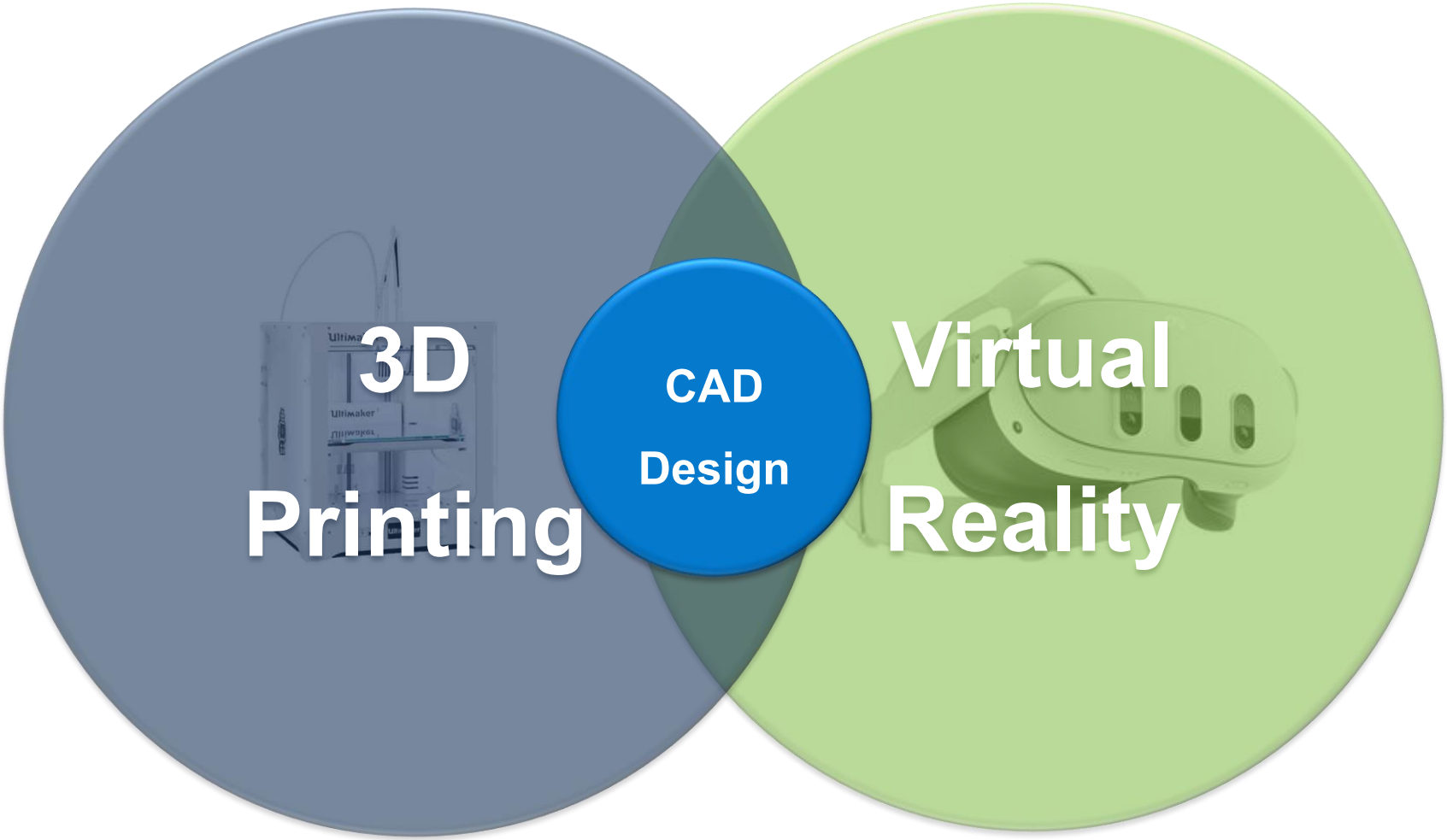






Polypropylene outer reactor with Cu catalyst embedded inserts

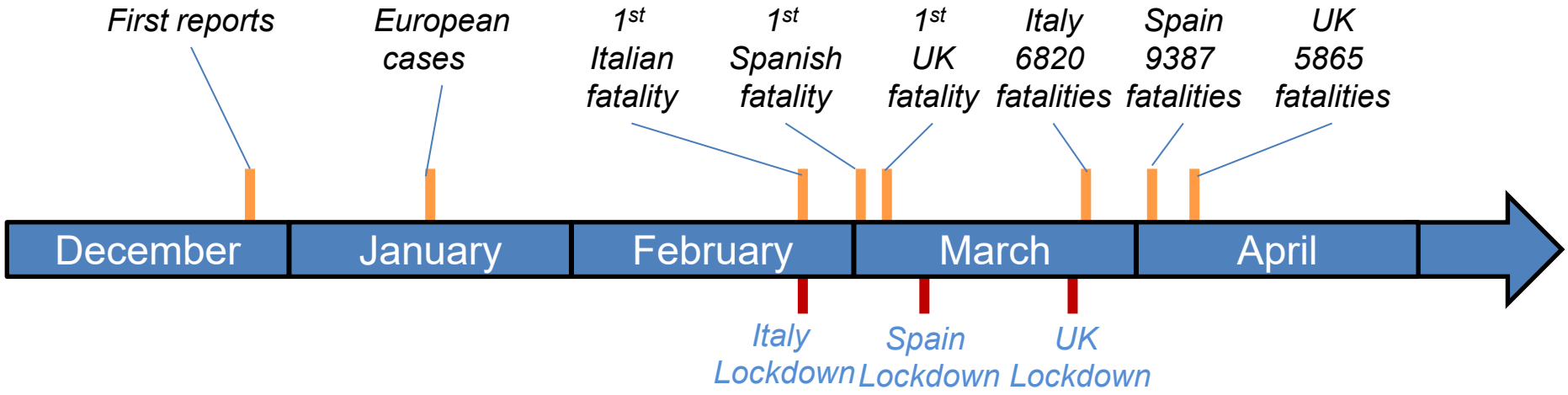
3D Printing and Virtual Reality



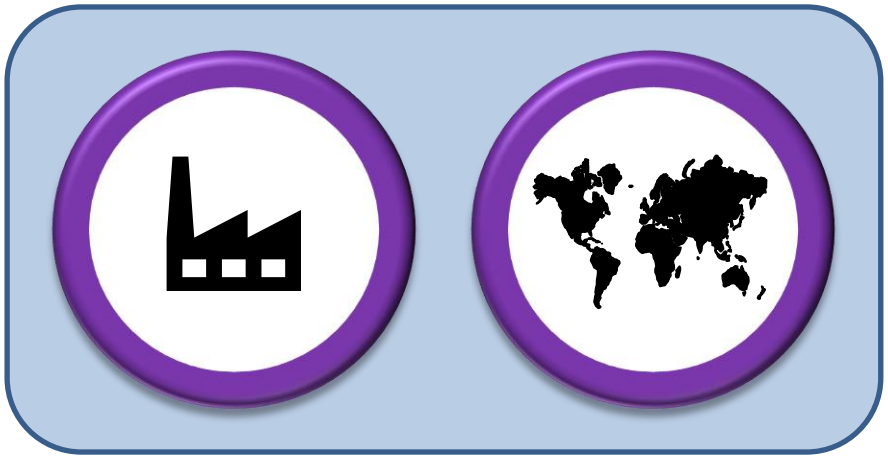
How did we get into Virtual Reality?

2) The pandemic

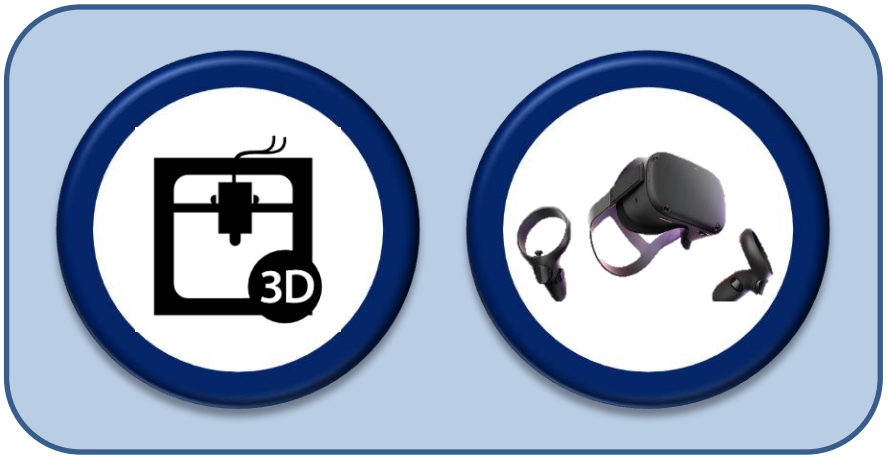
Covid-19 Timeline 2019/2020



Covid-19 Challenges

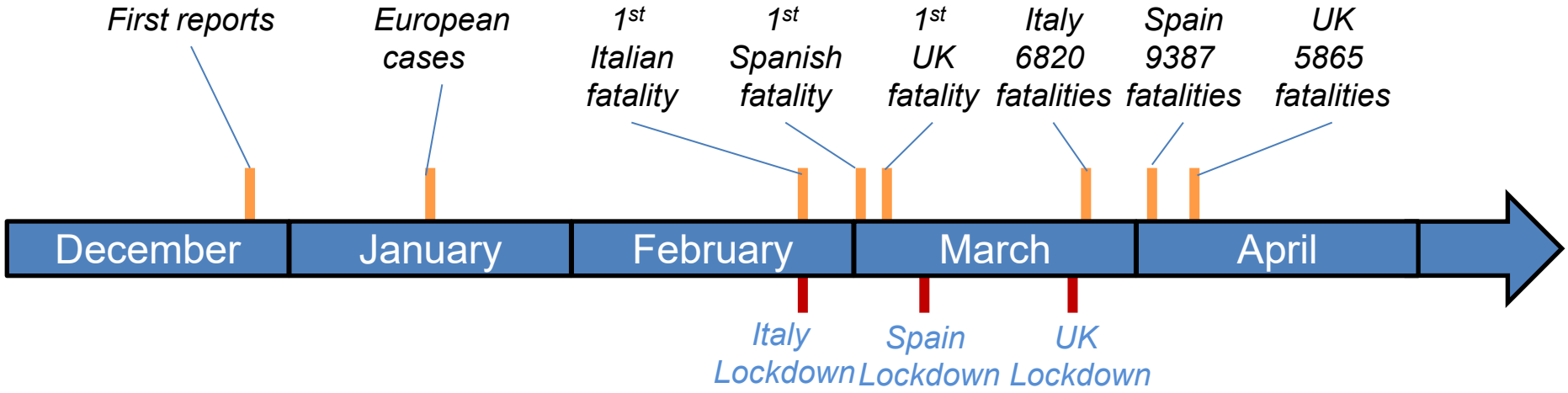


Covid-19 Solutions



3D Printed Covid-19 NHS Equipment

Covid-19 Timeline 2019/2020

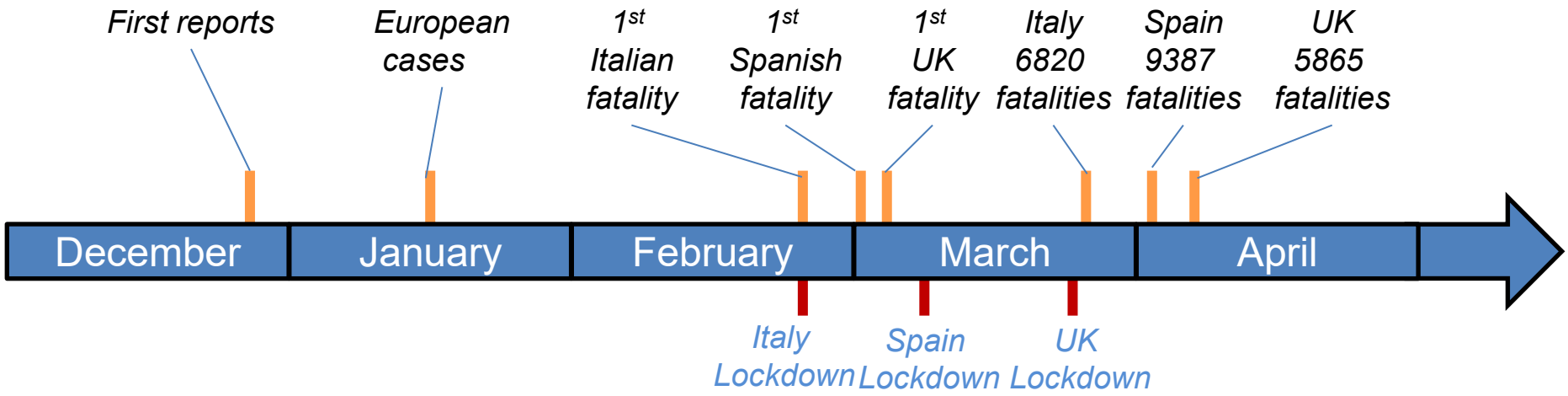


Personal Protective Equipment Shortages

Oxygen flow Equipment Shortages

3D Printed Covid-19 Face Shields

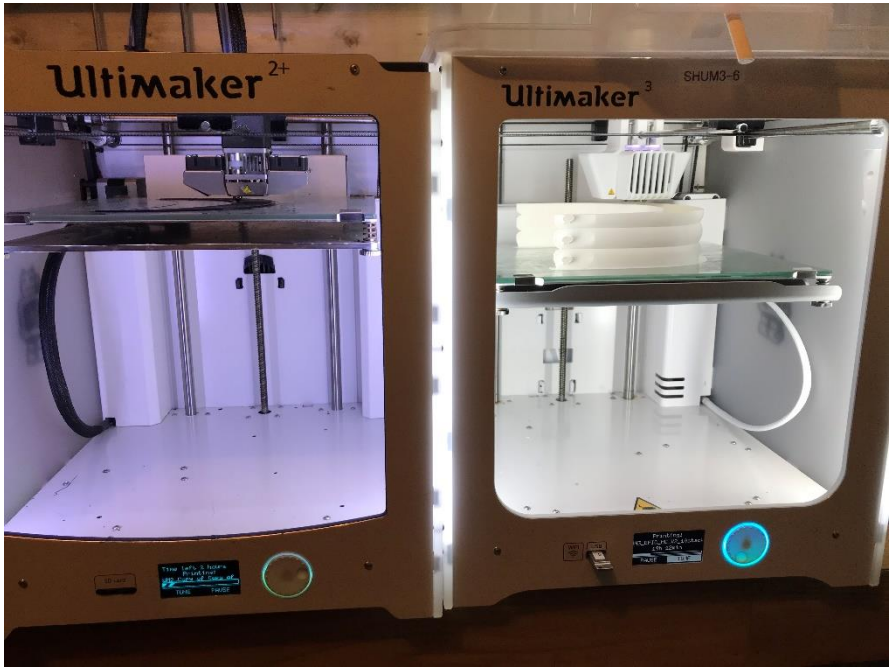
Covid-19 Timeline 2019/2020



Design Optimised to Print stack – 1.5 h per shield 21 g each

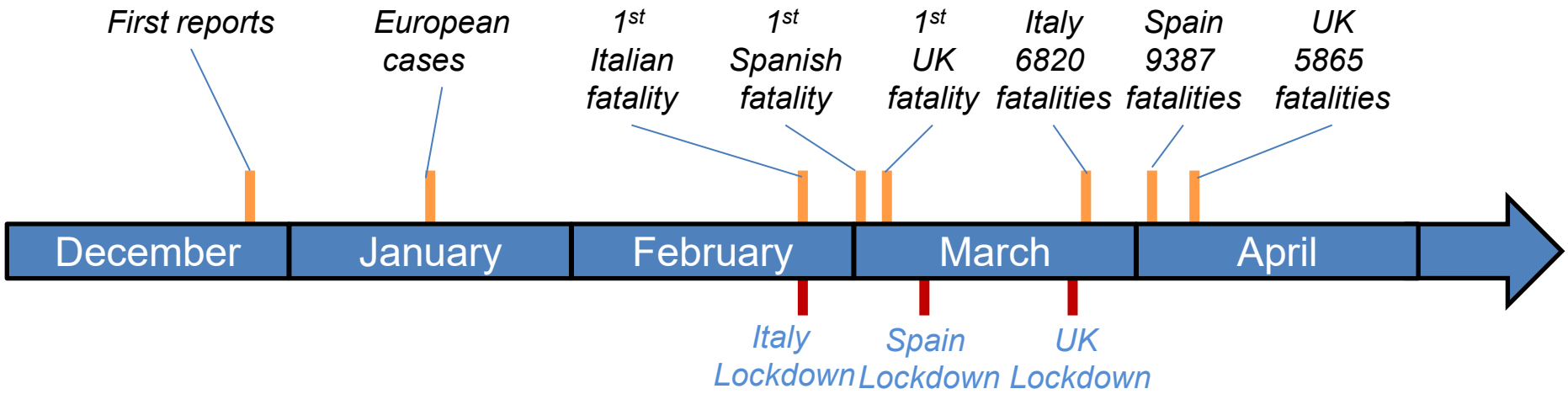
Stacks of 10 Printers across UCL Used for distributed Manufacturing

40 Printers running continuously Over 7000 distributed across London in 3-4 weeks



3D Printed Covid-19 NHS Equipment

Covid-19 Timeline 2019/2020



18th March - Printers and VR Sets at Home

Initial VR Approaches 2019/2020

Benefits:

1) ***Great Quality***

2) ***Understanding of VR***

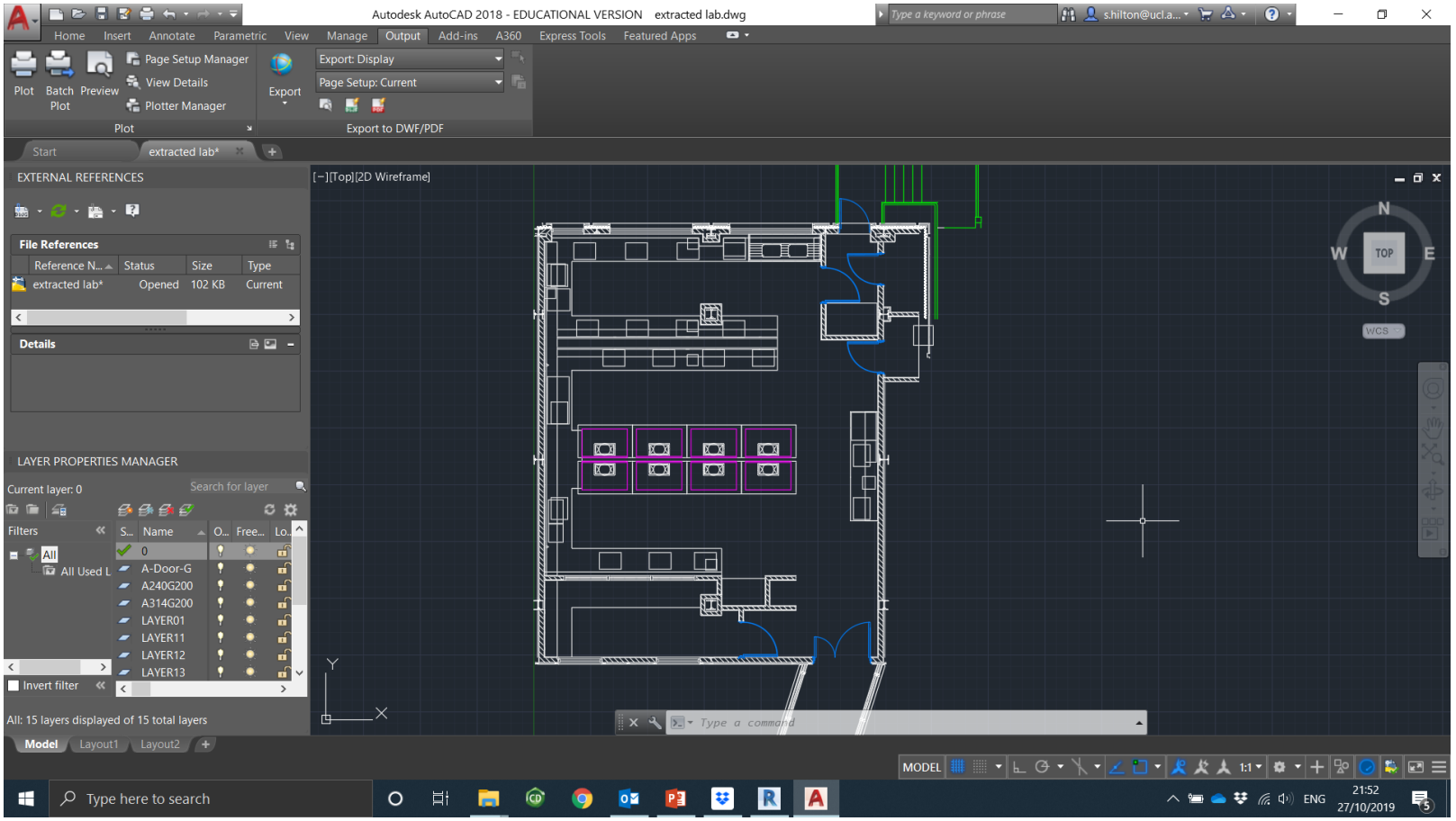
Challenges:

1) ***High Cost***

2) ***Static Builds***

3) ***Lack of modification possible***

Digital Twin Approach to VR



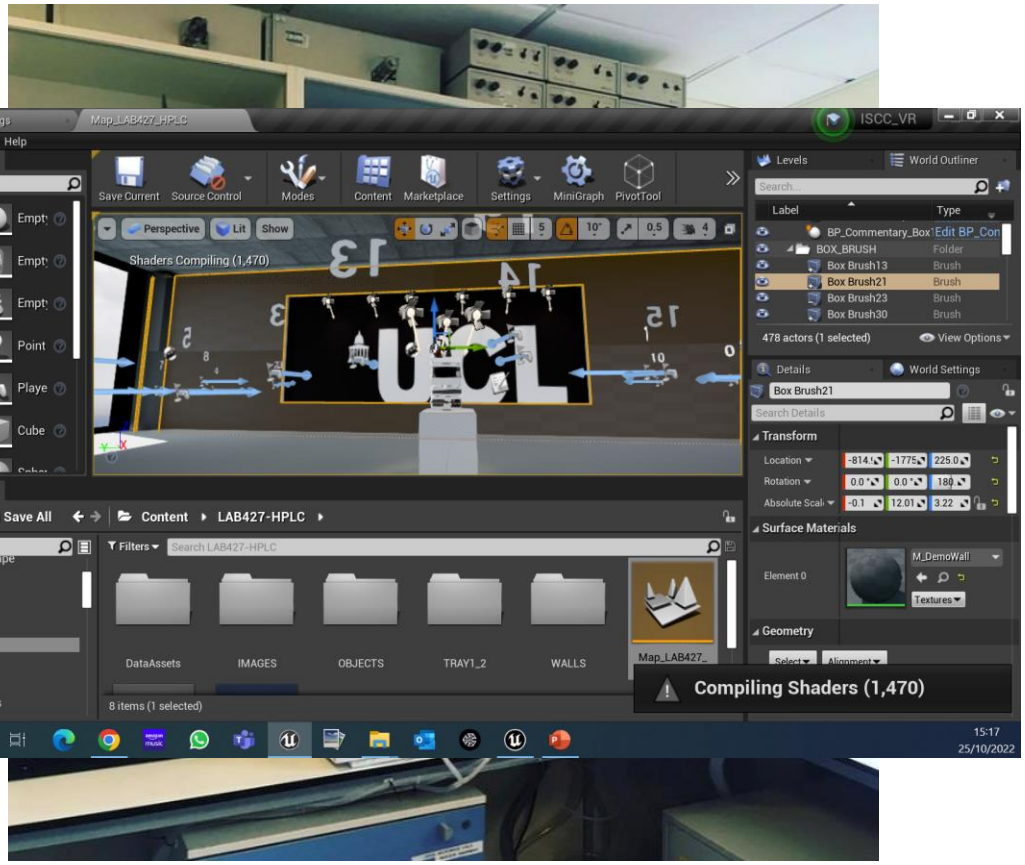
Digital Twin Approach to VR

Workflow - Reality to Virtual Reality

TINKERCAD

AUTODESK® FUSION 360™

UNREAL ENGINE



Initial VR Approaches – In-house

Virtual Reality Based Digital Education 2020

From Digital Designs to Physical Objects back to Digital Designs
or
"Back to the Future"

18th March - lab Locked Down

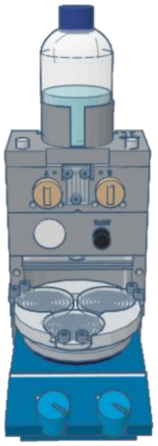
18th May - Virtual Laboratories

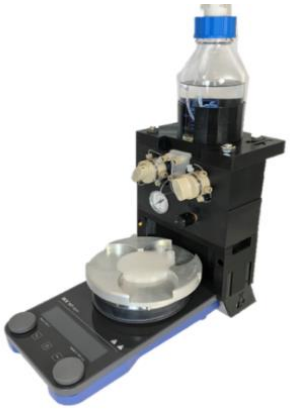
Digital Twin Approach to VR

Digital Twin Approach to VR

How did we get into Virtual Reality?

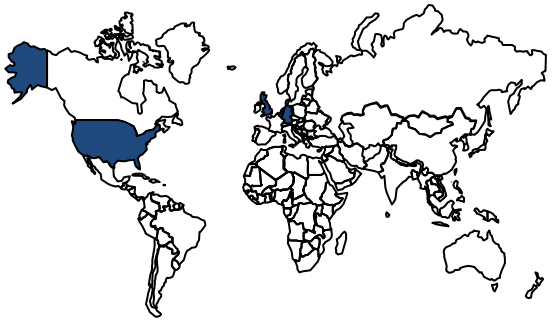
2) Development of the IKA FLOW 2019/2020

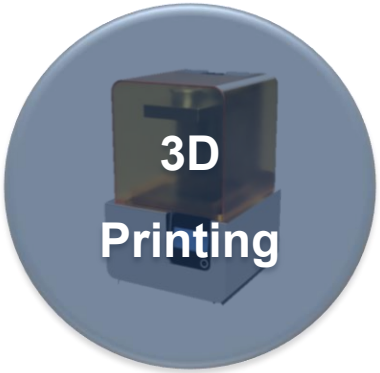




3D Printing and the IKA FLOW

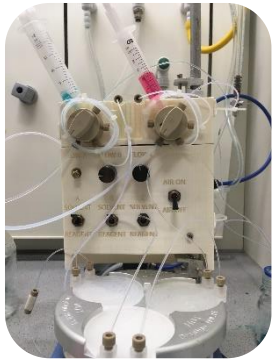
Development of the IKA FLOW 2019/2020





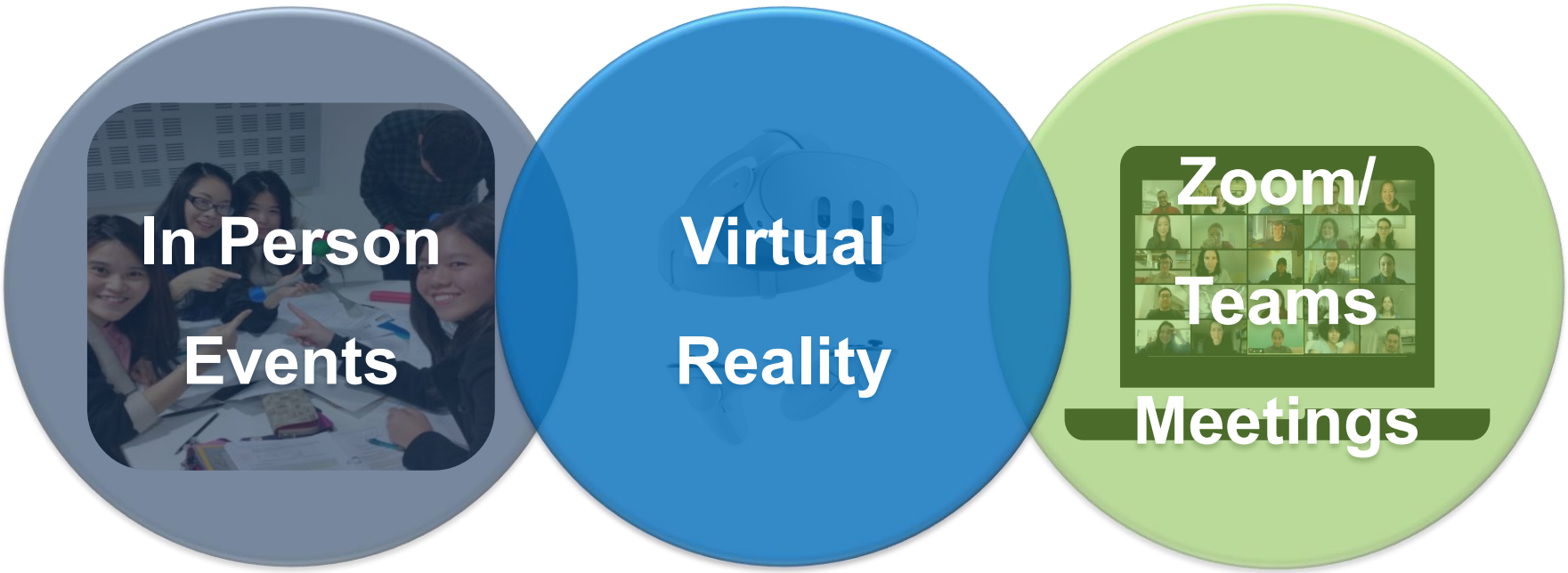
Two years from concept to product on the market.

August 2018	Feb 2019	March 2019	May 2020	Sep 2020



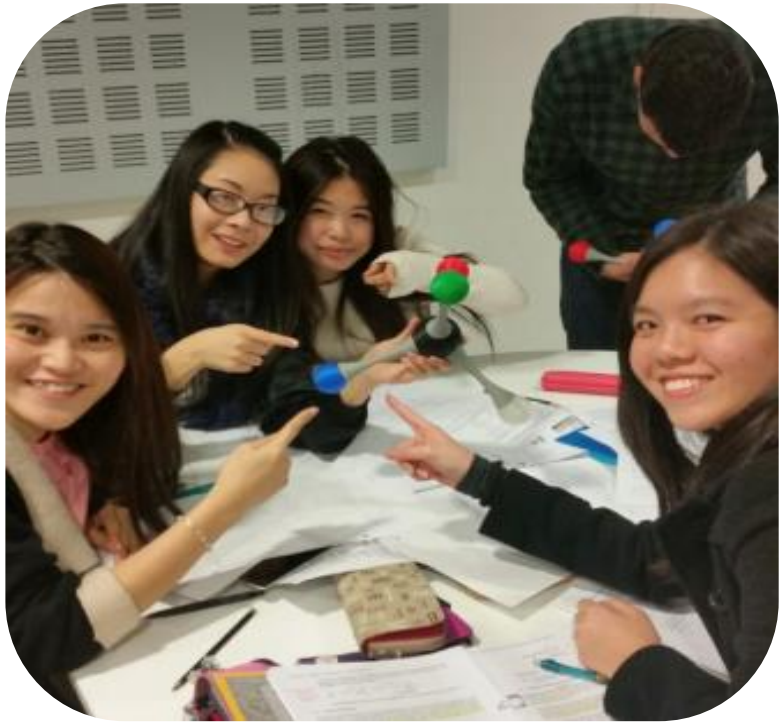
IKA®

VR in Training



3D Printing and Virtual Reality

3D Printing

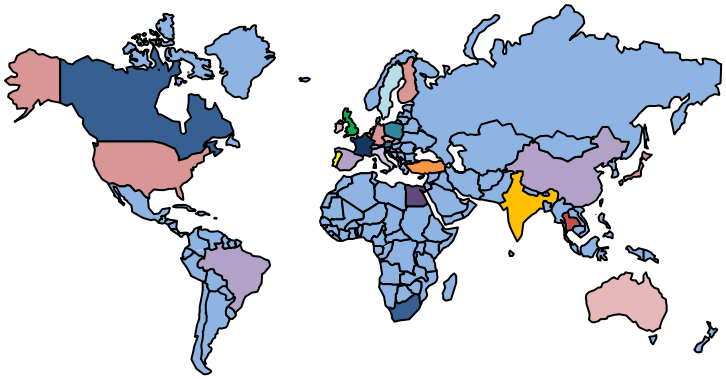


Virtual Reality

The Challenge

The Challenge:

Working together at the same standards **in multiple countries** and multiple time zones **is difficult** to maintain.



zoom

You Tube

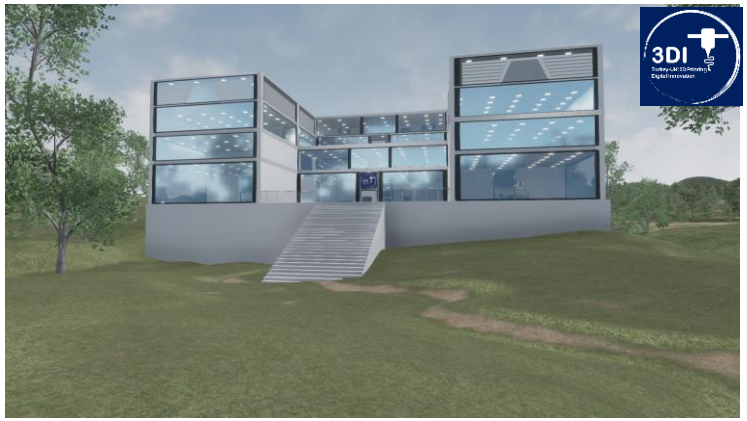
Virtual Reality and AI – the Solution

The Solution:

Working together at the same standards **in multiple countries** and multiple time zones **is easy.**

1

The solution:
Digital Virtual Centers



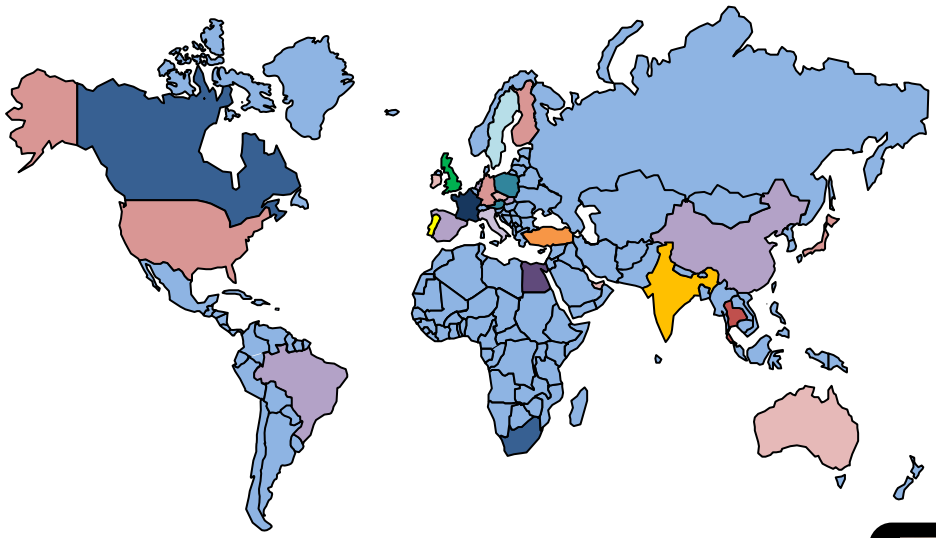
2

Comparable Training:
*Analogous **real time interaction***

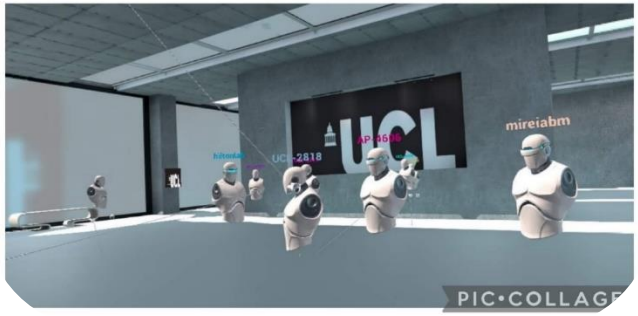
3

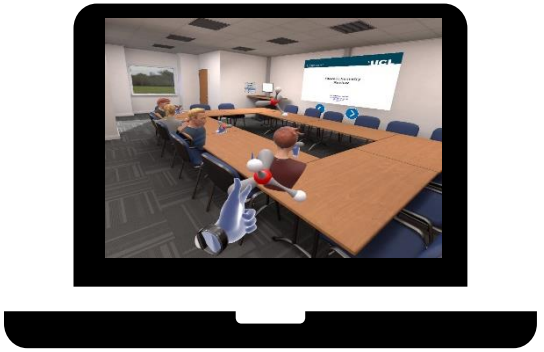
VR Based Collaboration:
Digitization of equipment and people in Virtual Reality **for 24/7 access** so *all scientists, receive comparative training and advice.*

LAB 427 VR Software Platform



Quest 2/3





PC Mode

The Solution – an Example

The Solution:

Working together at the same standards **in multiple countries** and multiple time zones **is easy – example UK- Thailand.**

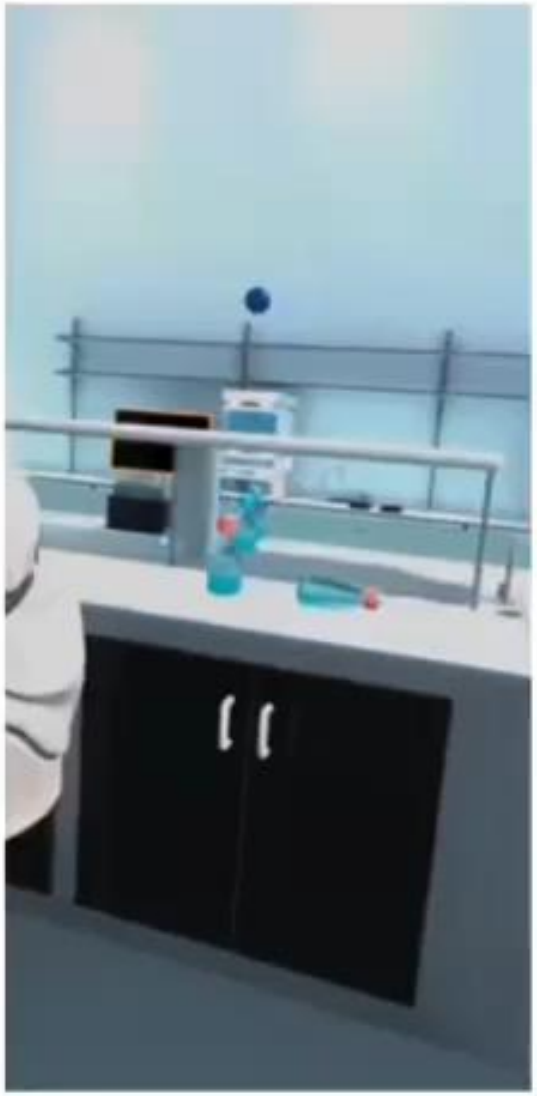
LAB 427 VR Software Platform

Virtual Reality HPLC Training

HPLC Training

Virtual Reality HPLC Training

HPLC Training

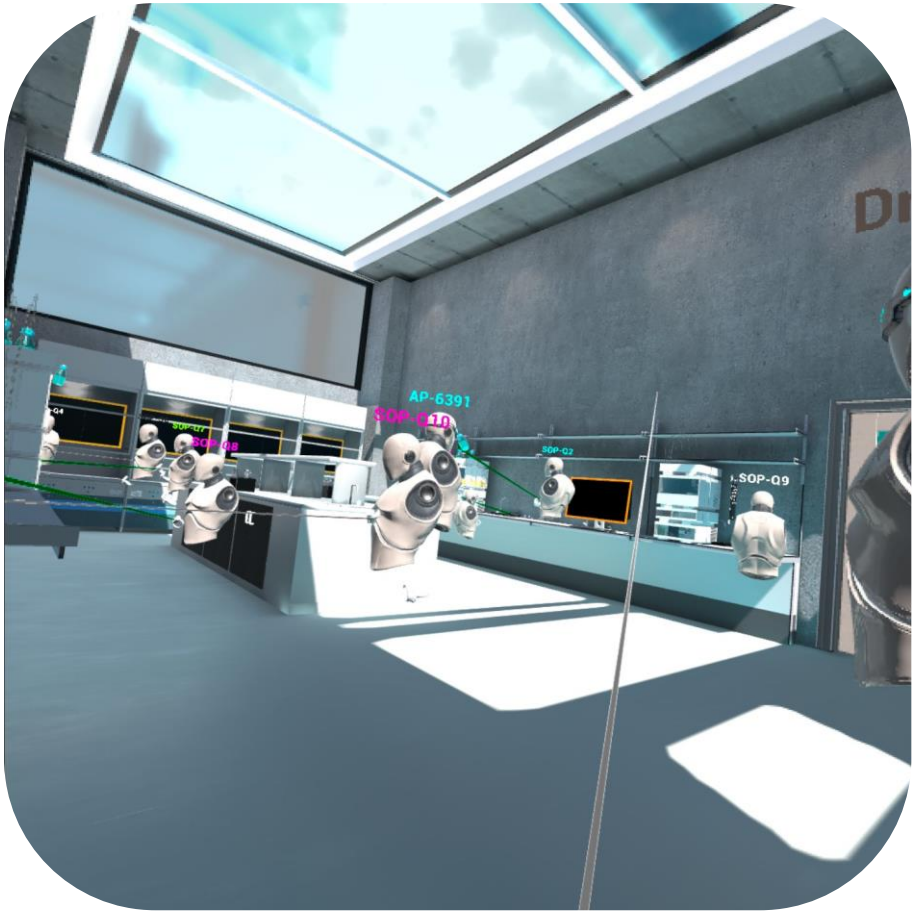


HPLC - VR Training

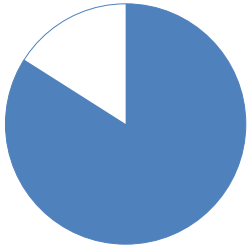
HPLC
Training

Virtual Reality Based Digital Education

Over 200 students in VR in one week

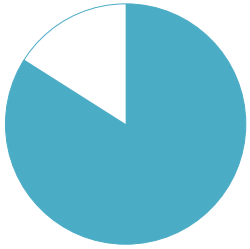


HPLC - VR Training



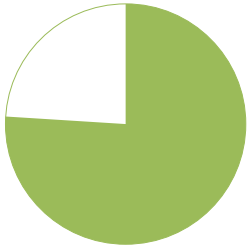
84%

I enjoyed the VR HPLC session



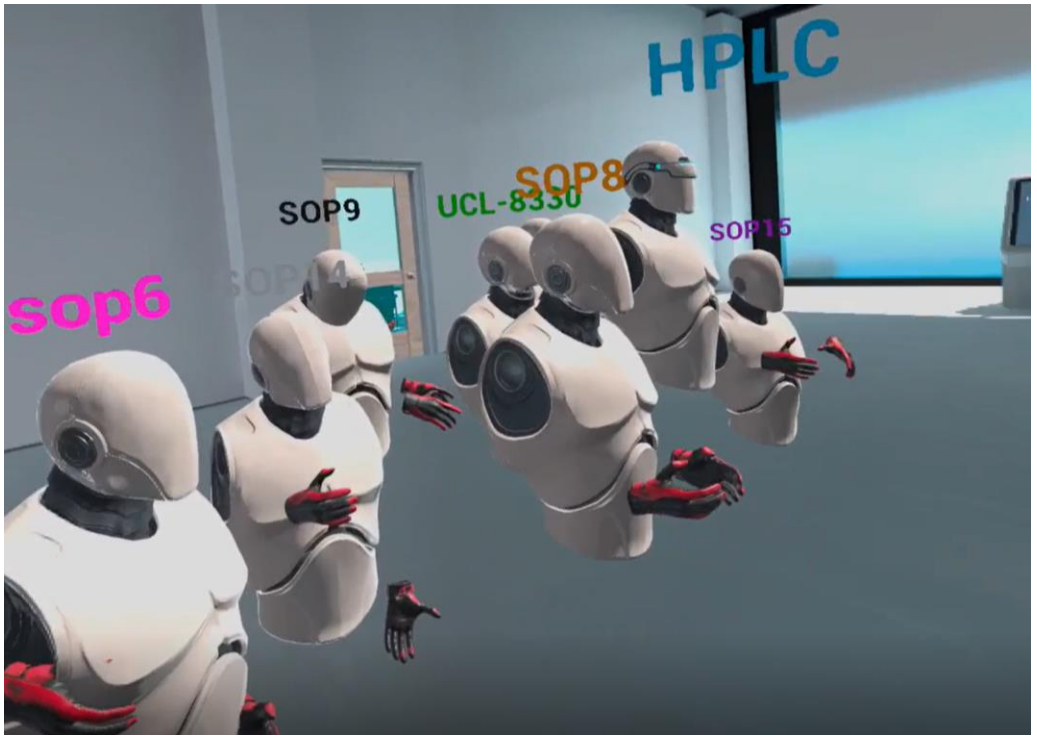
84%

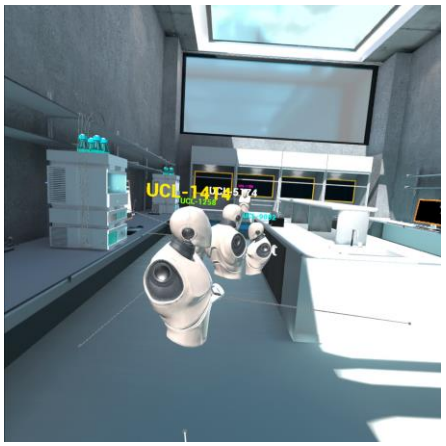
VR based practical's have good potential



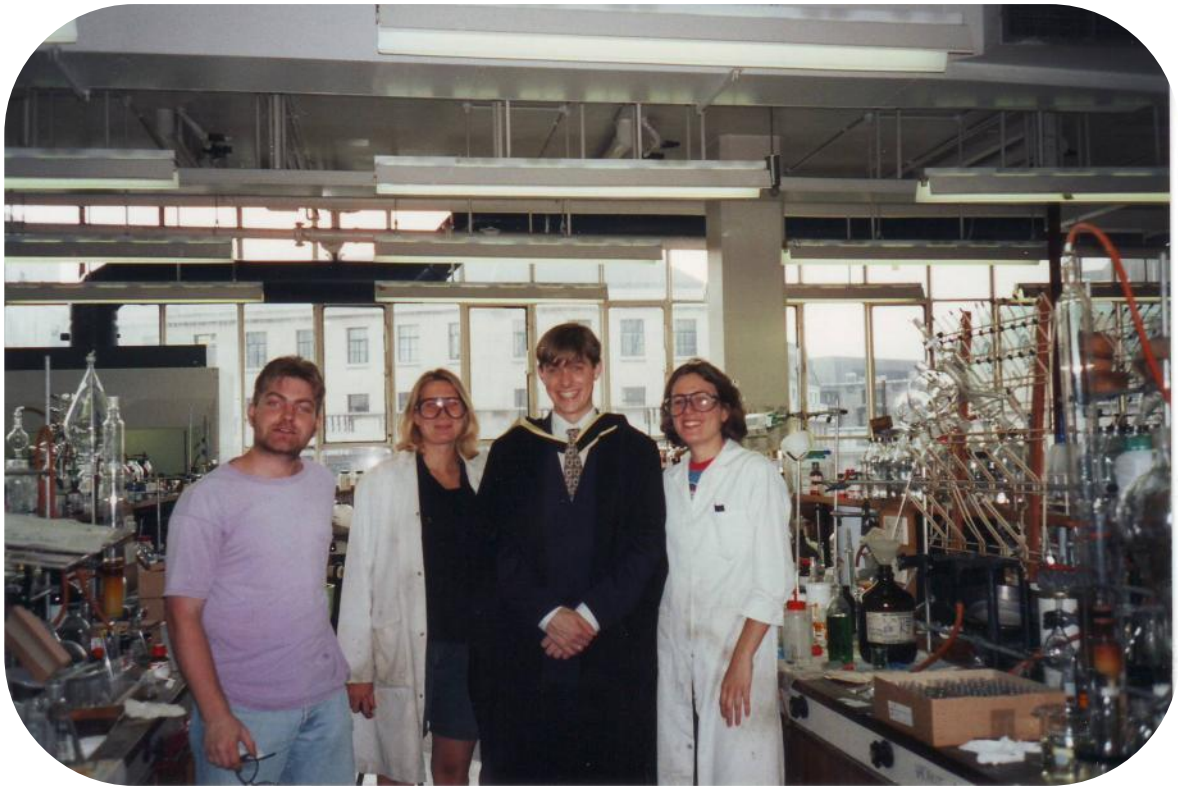
76%

The VR HPLC session taught me how the instrument is set up



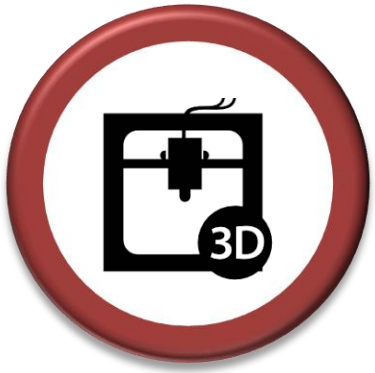


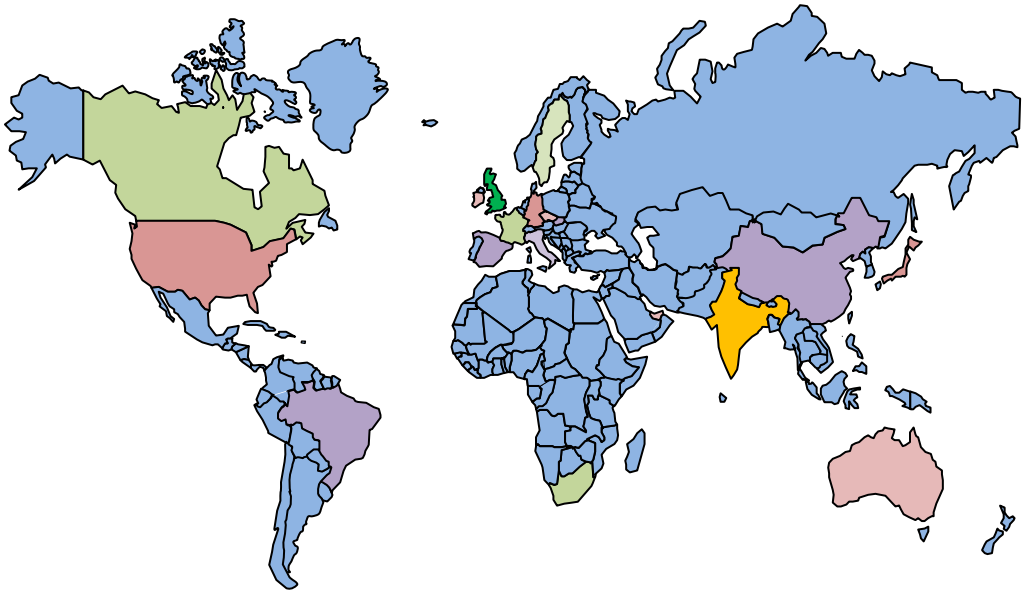
30 Years Ago..



1996

The Need for Conversational AI





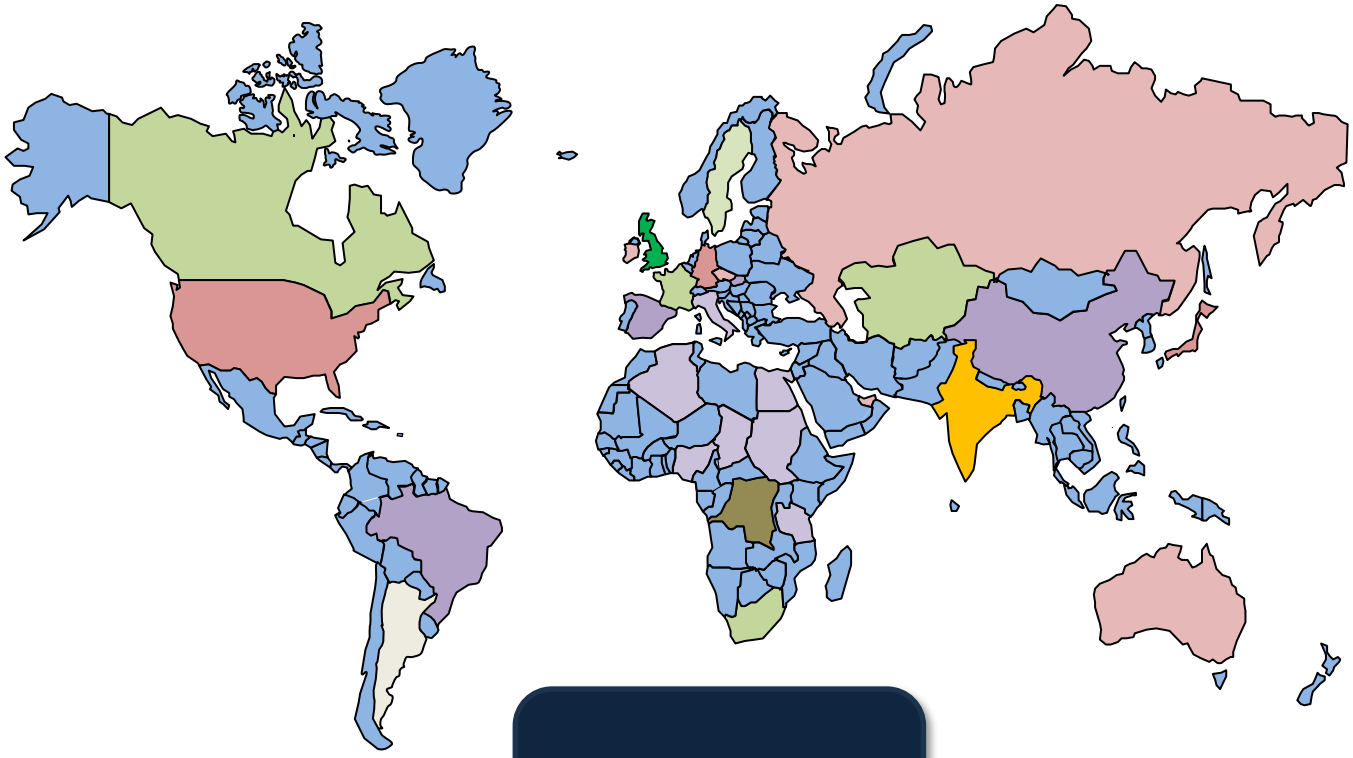
VR and Intelligent AI Incorporation

AI Co-pilots in the VR Centre

1. Sam is designed to help users in VR navigate chemical inventories for
2. experimental planning in VR.
3. Susan is designed as an on-hand health and safety expert for training.
4. Ingrid is designed for general laboratory navigation and queries regarding experimental set-up.

VR and Intelligent AI Incorporation

AI's Going Global



English

Arabic

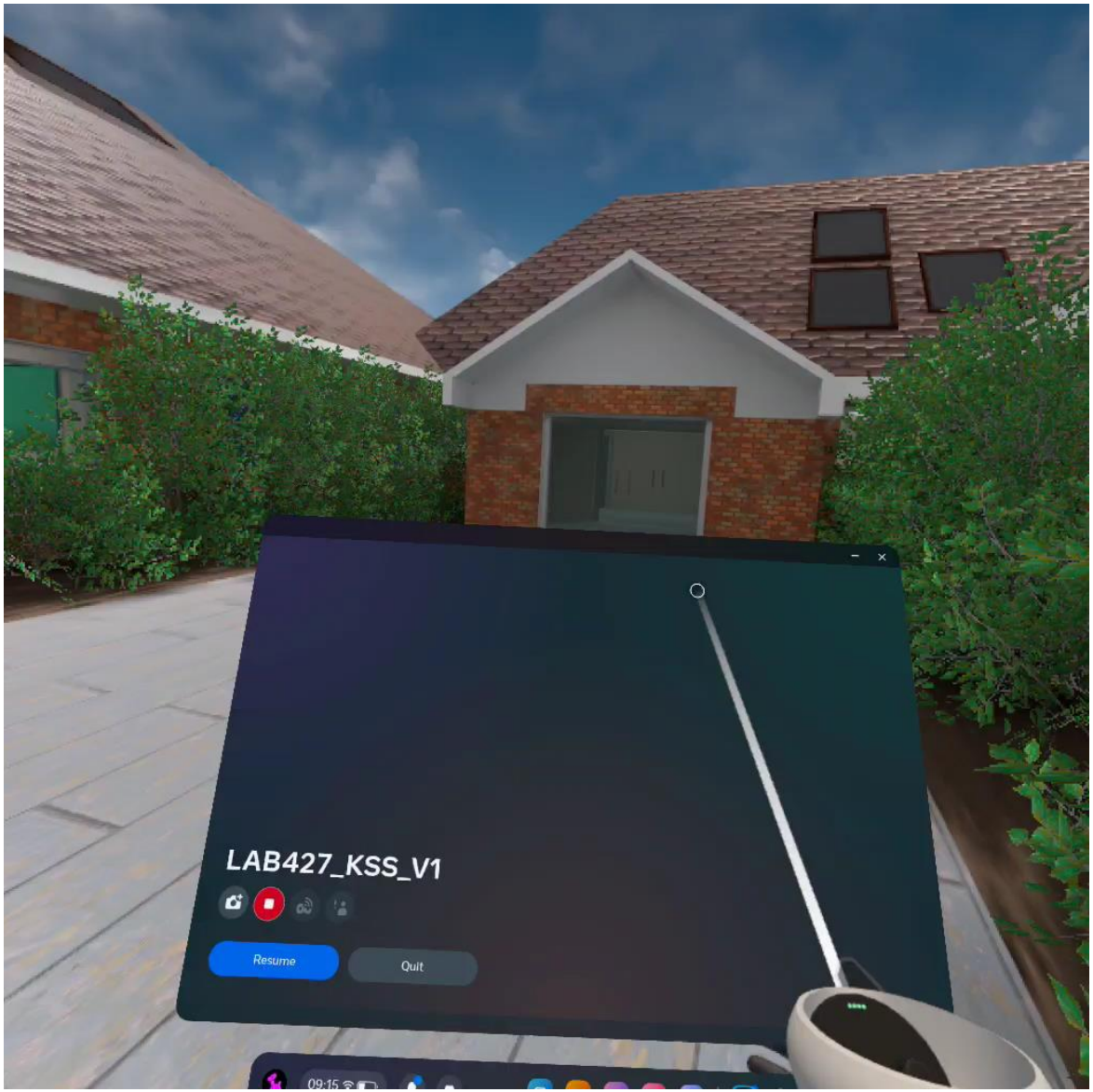
Italian

Hindi

Mandarin

AI's Going Global

Digital Twin Virtual Health Centers



Digital Twin Virtual Health Centers

VR and Intelligent AI Incorporation

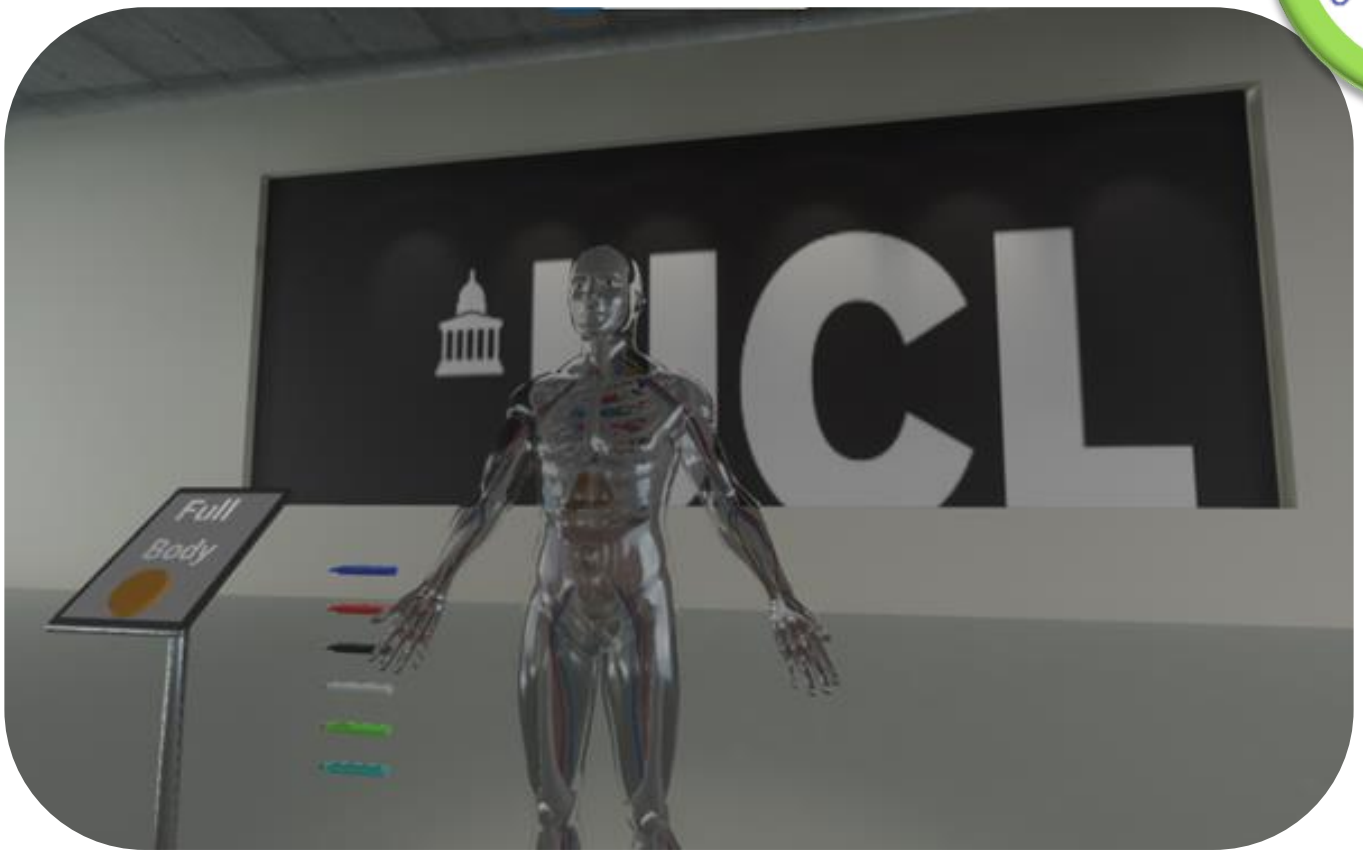
- The avatars are programmed with a customisable Knowledge Bank, meaning that we can create highly detailed training scenarios.

VR and Intelligent AI Incorporation

Designed to be run without any human educator

Anatomy Education

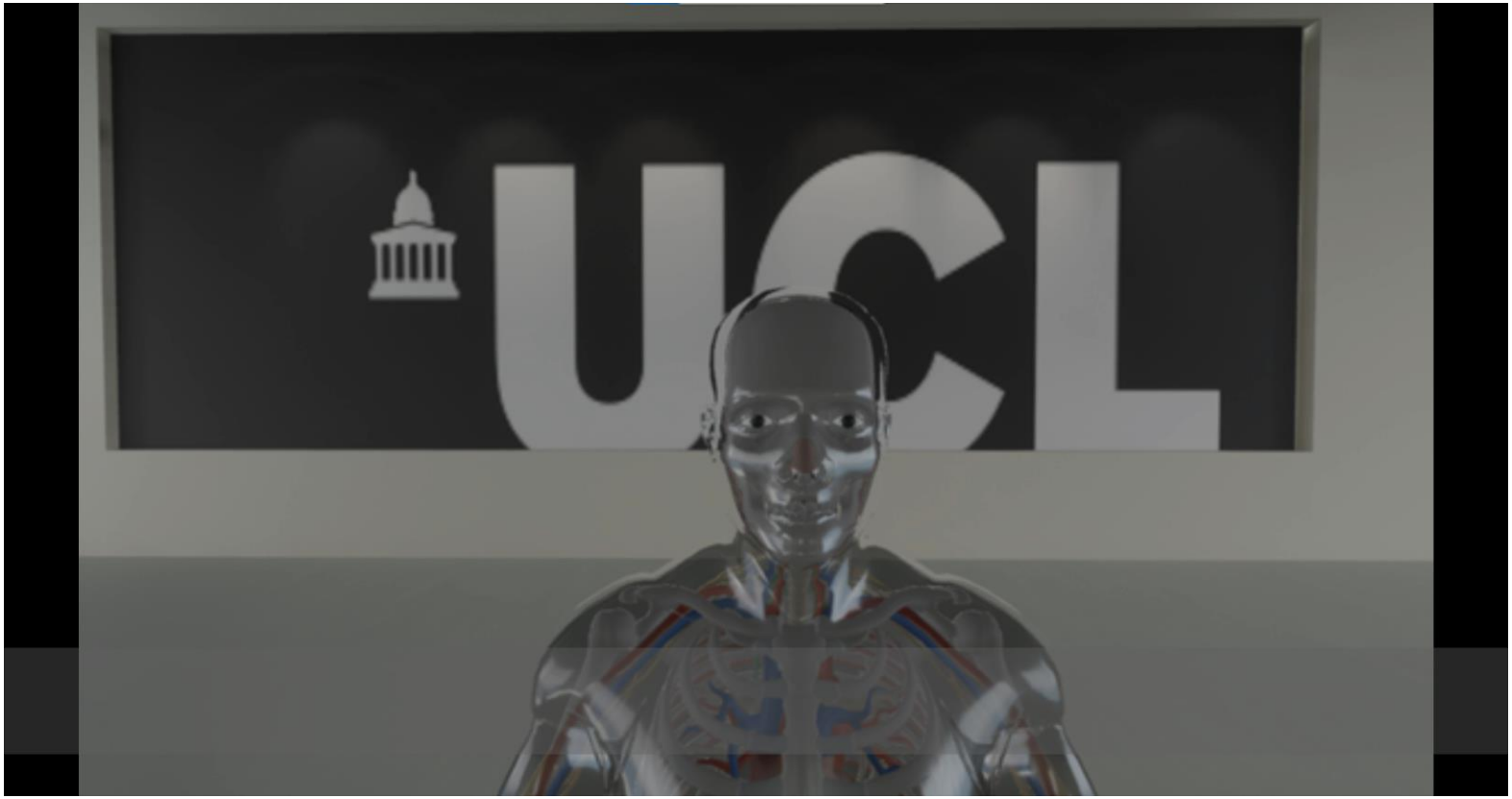
Designed to be run without any human educator



Pure AI Run Teaching

Designed to be run without any human educator

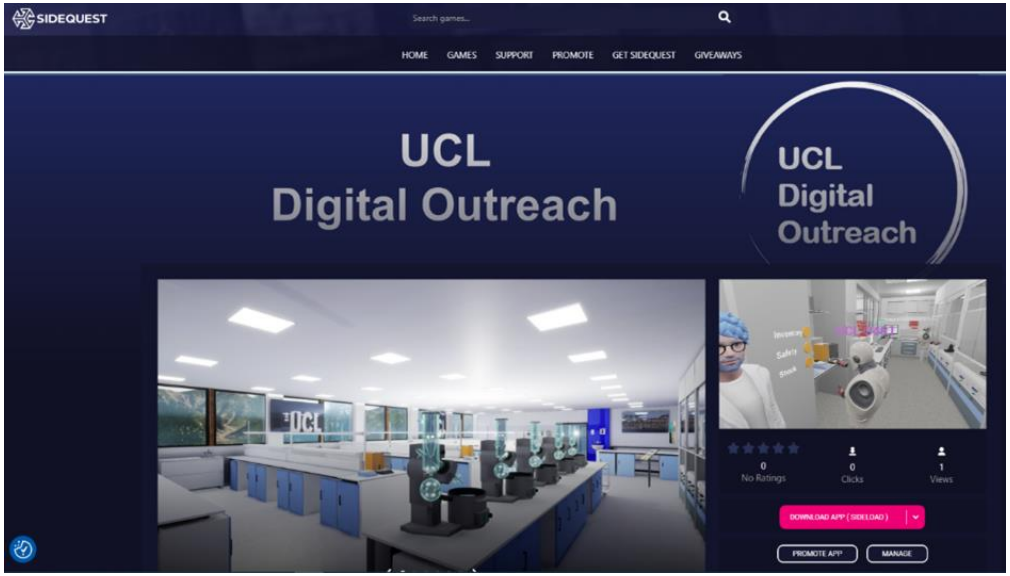
All communication purely with AI – no lecturer involved



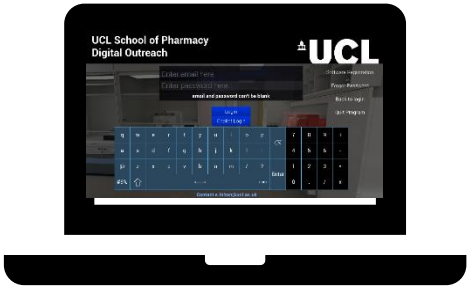
UCL Digital Outreach

Digital Outreach – A Global Approach to Science Education

Bridging Universities and Schools



Software is accessible via Quest 2/3 and PC for ease of access.



Virtual Outreach – Our Vision

Environments – reflective of the School:
Outreach environments cover real space, real people and extended environments - spaces can also be used for SoP Undergraduate training – anatomy.

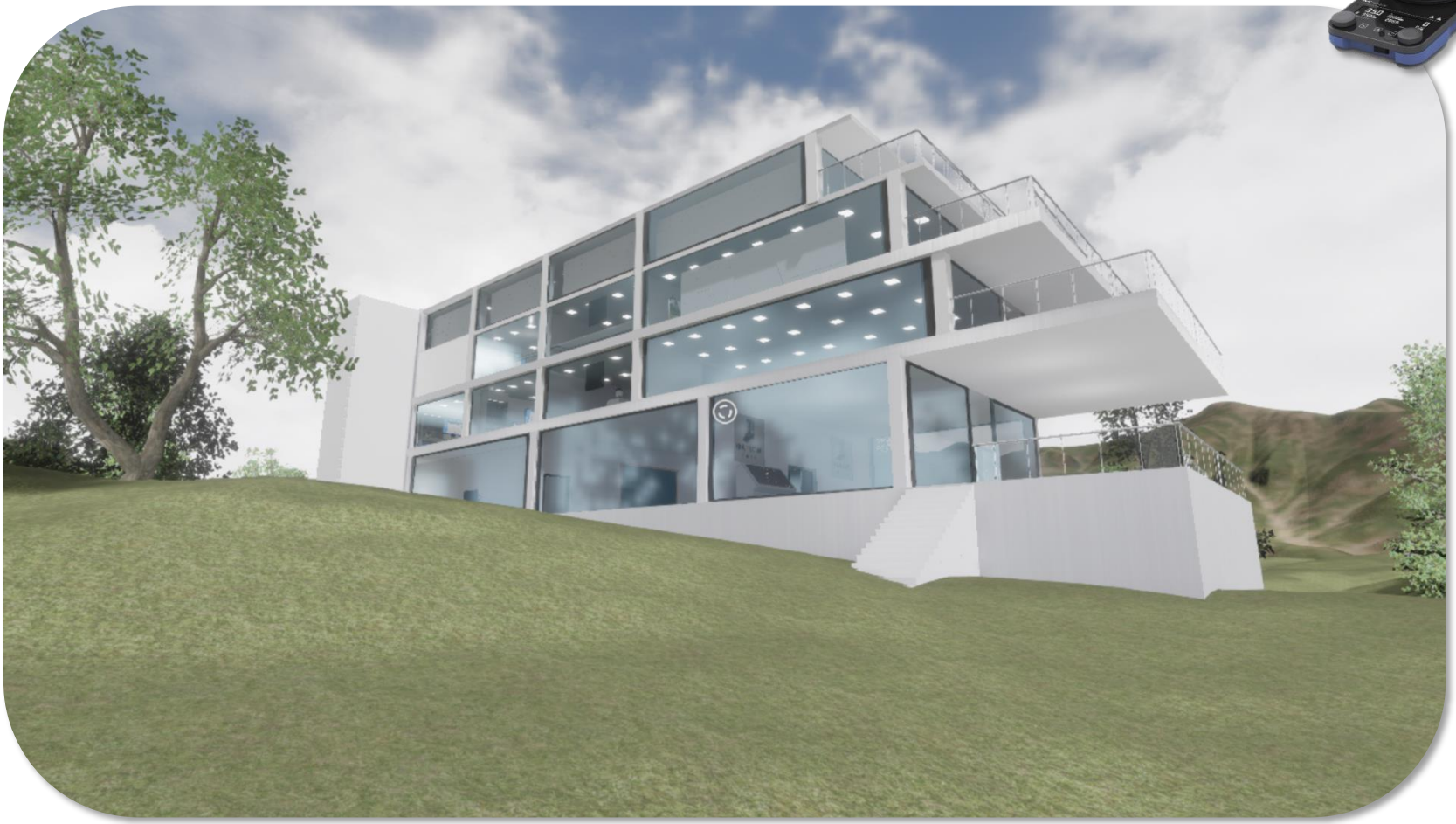
Digital Outreach

Wide Array of Education uses:

VR Flow Chemistry Training

FLOW Digital VR training Centre

- ***Global Flow Chemistry Digital Centre in VR***



VR Flow Chemistry Training

FLOW Digital VR training Centre

- ***Global Flow Chemistry Digital Centre in VR***

Flow Chemistry VR Training

IKA FLOW Digital VR training Centre

Conference room

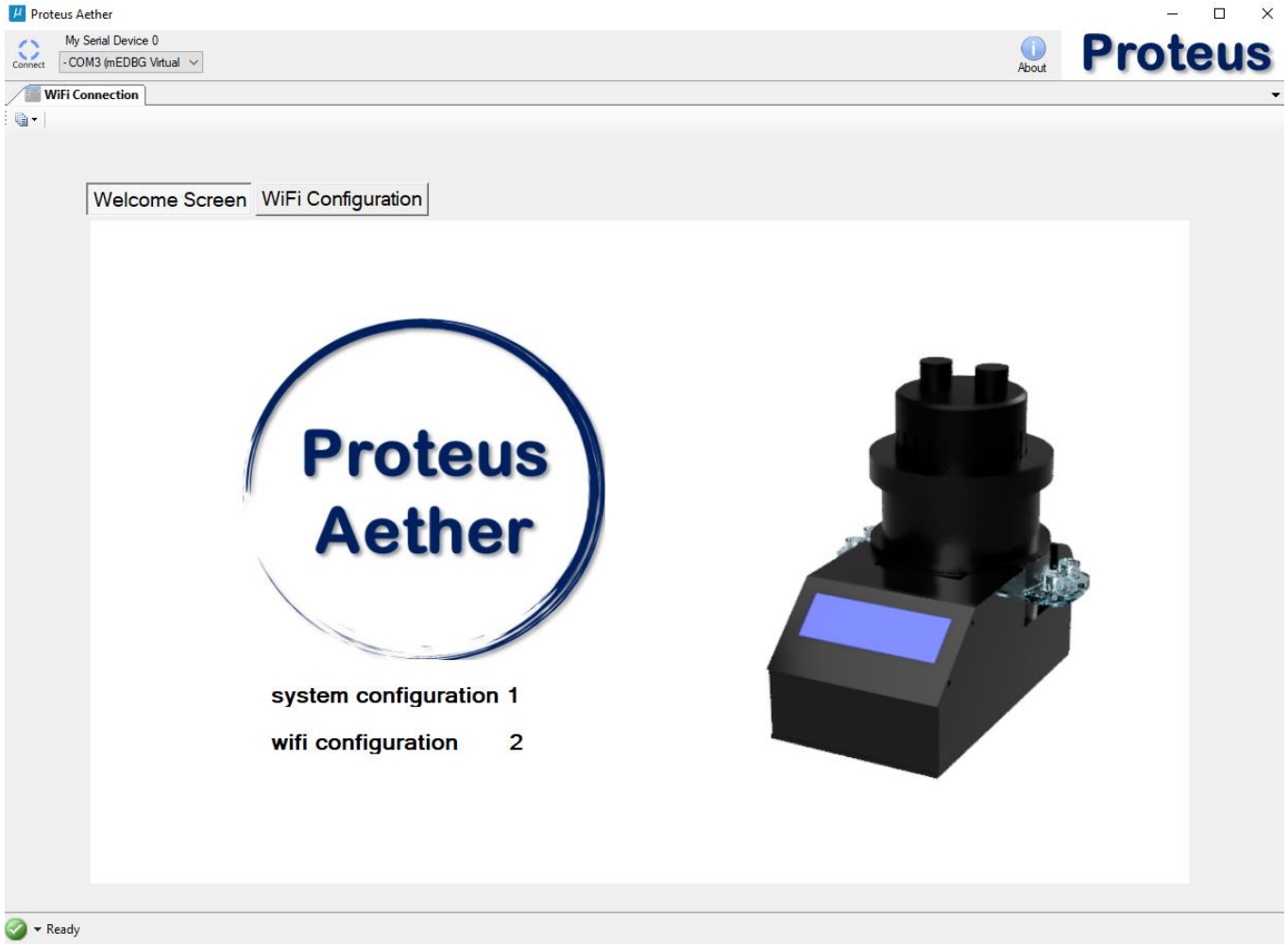
Meeting Rooms

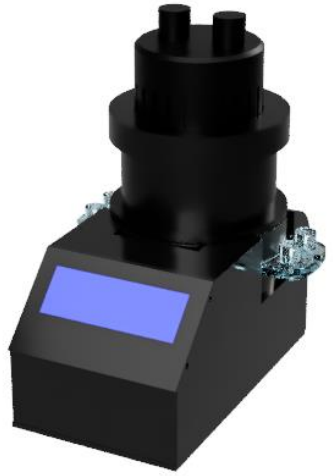
Training Rooms

Poster Space

VR & Digital Connected Laboratories

Proteus Aether – Digital connection to the Cloud via WiFi





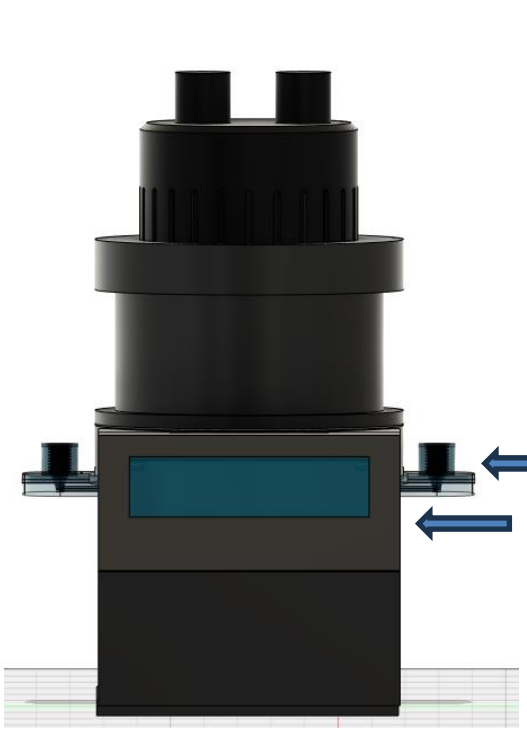
Proteus Aether Photoflow System

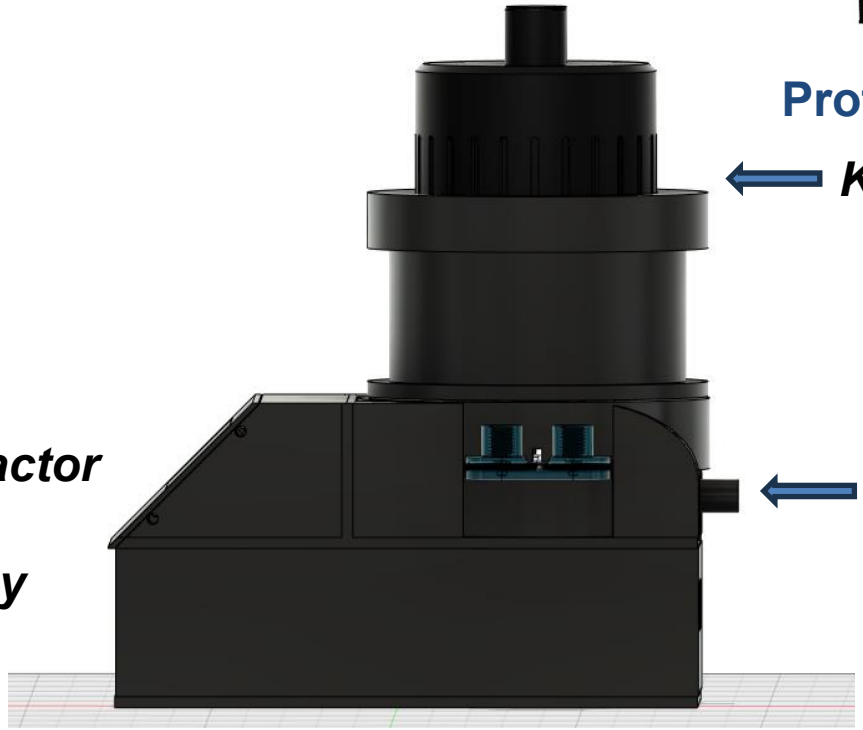
Proteus Aether

Designed to send data to the cloud for tracking via Wifi

Allows for parallel Photochemistry

Standardisation of Photoflow temperatures and telemetry





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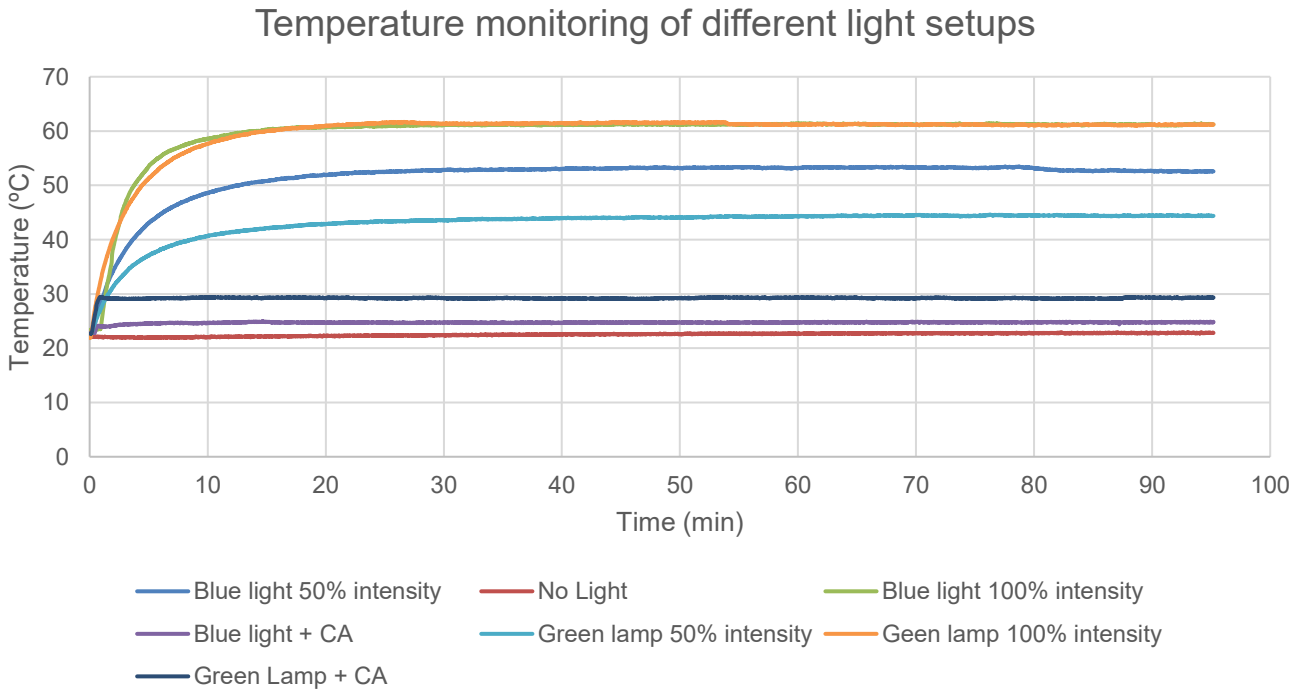
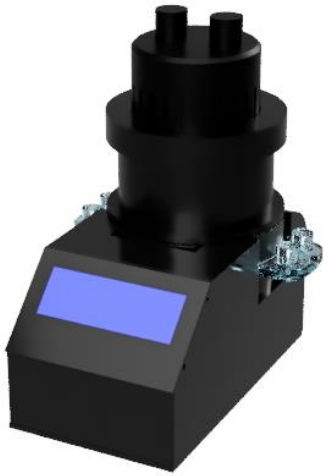


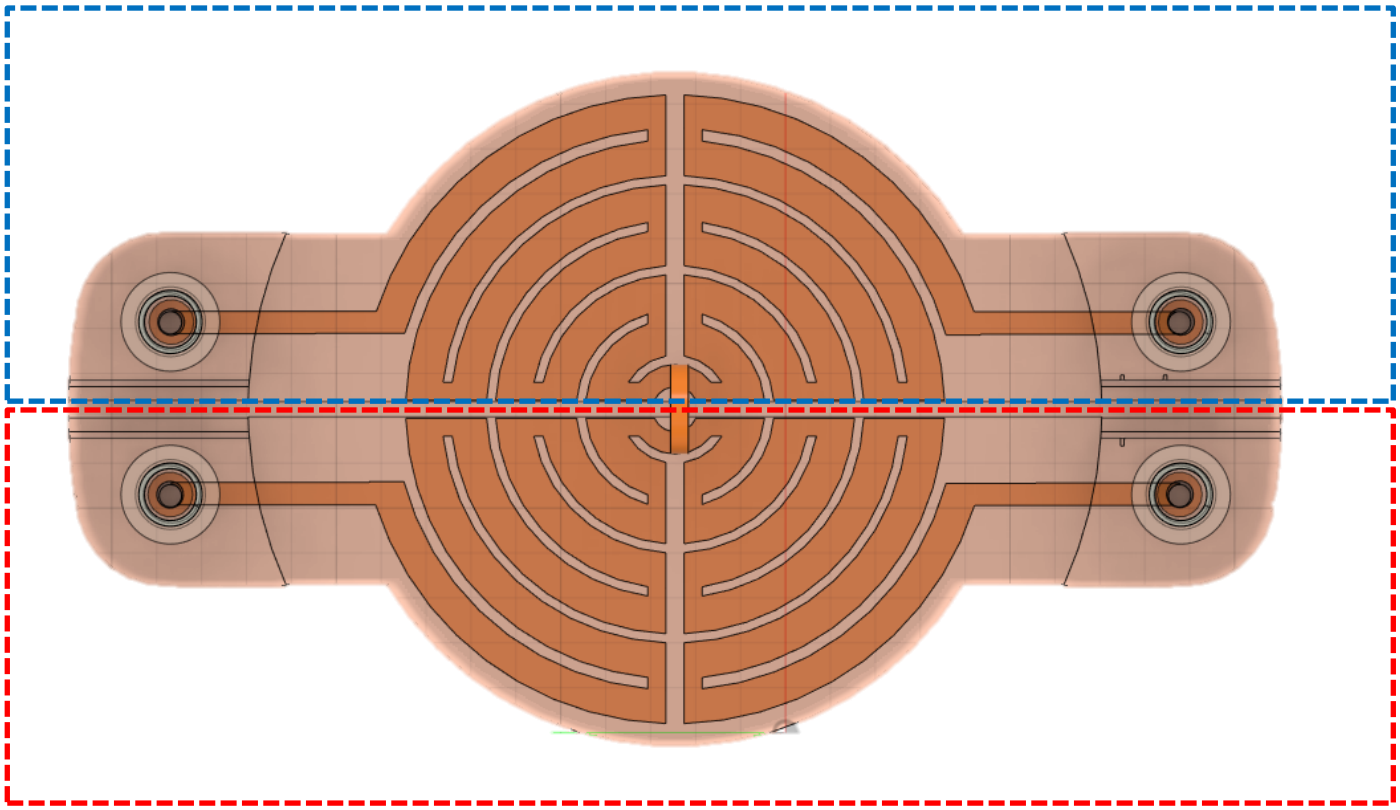


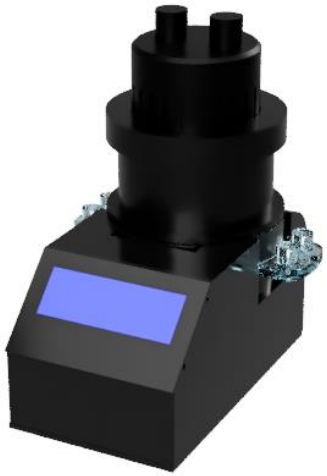
Proteus Aether Photoflow System

Proteus Aether

Reactors – Polypropylene – Used with Kessil lamps

Parallel reactions





Proteus Aether Photoflow System

Proteus Aether

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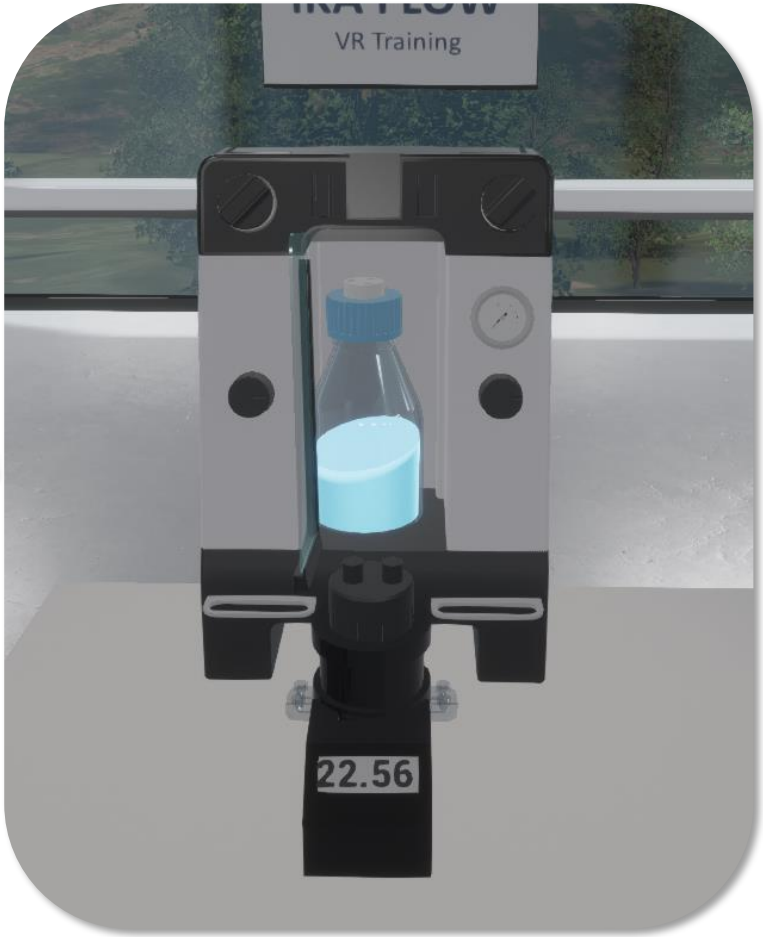
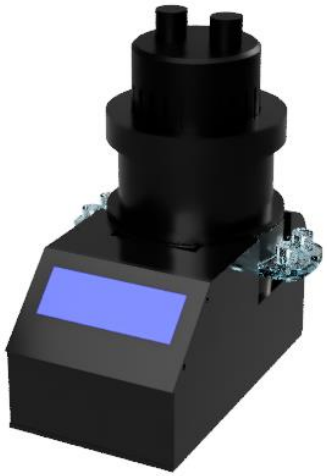


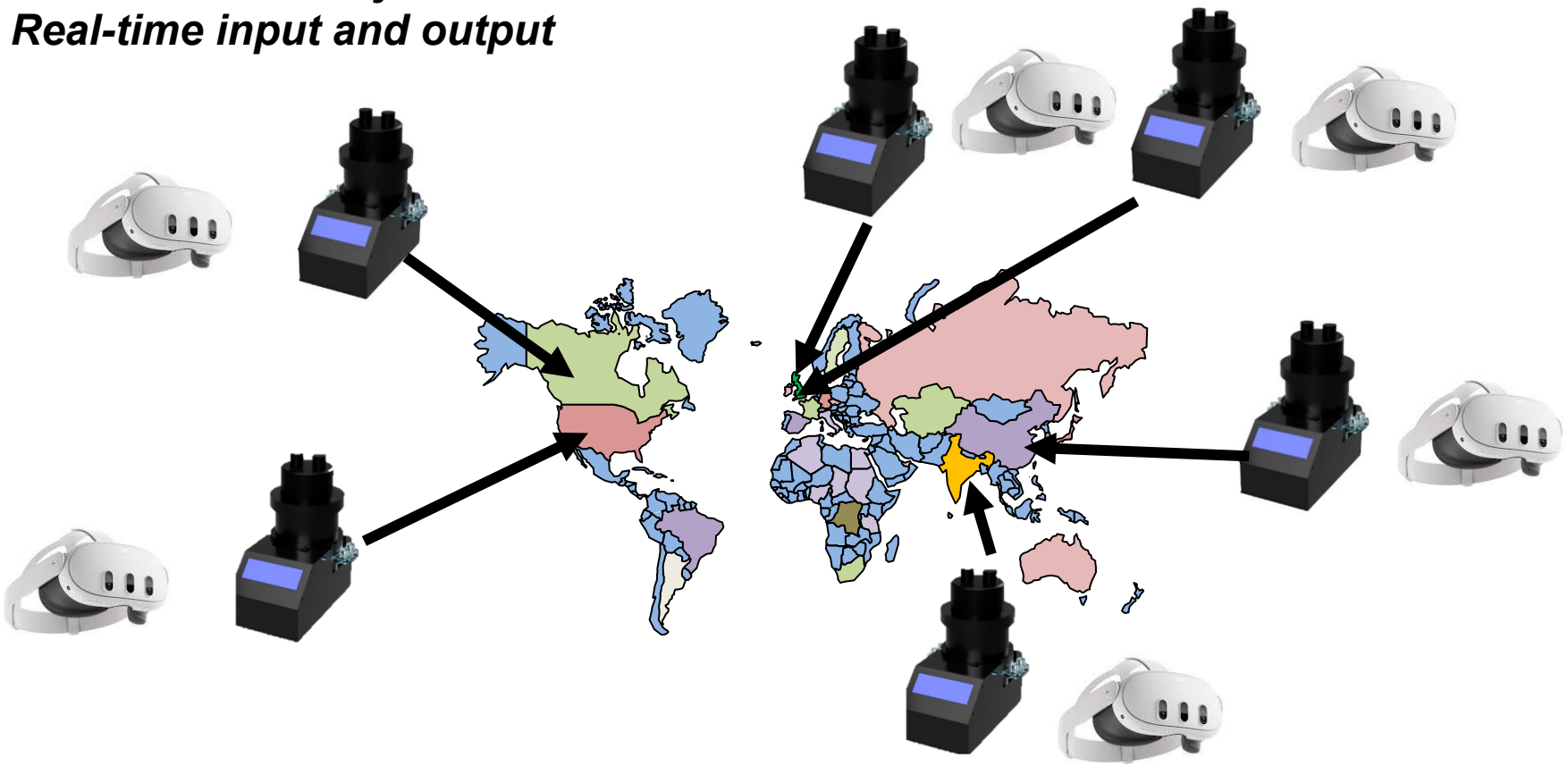


VR & Digital Connected Laboratories

Connecting multiple global laboratories

Visualise telemetry in real time

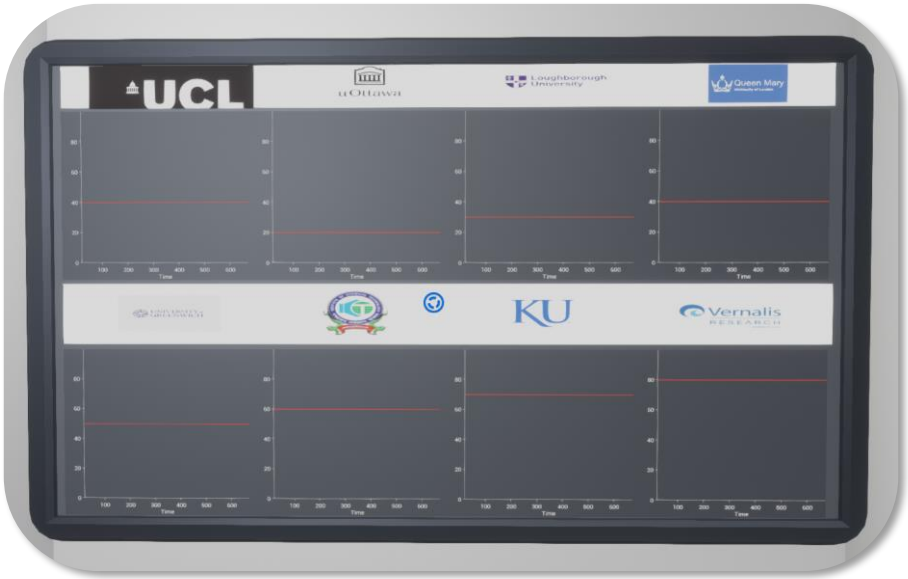
Real-time input and output



VR and Intelligent AI Incorporation

Multiple worldwide labs all linked together in VR

Collaboration Room



Live Global Telemetry

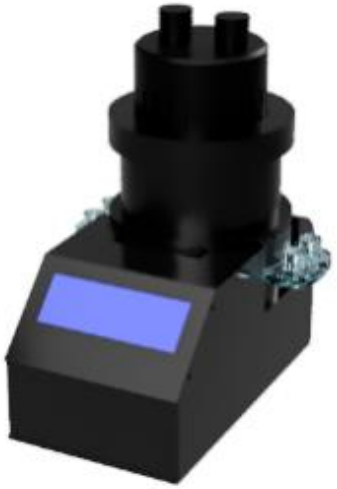
Digital Global Control

Jarvis

Meet Jarvis

- ***Jarvis knows all lab live data***
- ***Jarvis can speak with a user about this***
- ***Jarvis can then provide advice about the reaction or set temperatures via voice***
- ***Jarvis can also discuss and help optimise reactions in other laboratories***
- ***Ability to speak in multiple languages***

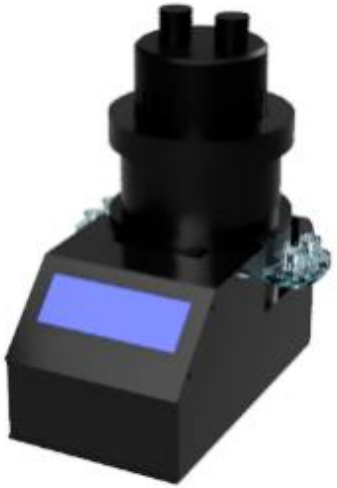
Jarvis



Python Read and Write Data


```python
import requests

def handle_event(data):
    # Get the target temperature from Convai
    temperature = data.get("val")

    # Your ThingSpeak channel + WRITE key
    CHANNEL_ID = "3167275"
    WRITE_KEY  = "6KFZJF50OJE5TRVY"

    # Build URL to write temperature into Field 5
    url = f"https://api.thingspeak.com/update?api_key={WRITE_KEY}&field5=
{temperature}"

    try:
        response = requests.get(url)
        response.raise_for_status()
        result = response.text  # ThingSpeak returns update ID or "0"
    except Exception as e:
        result = f"Error: {str(e)}"

    return {
        "message": f"Setting the hotplate to {temperature}°C (ThingSpeak: {result})"
    }
```

Jarvis



Python
Read and
Write Data

Discuss
User Data

Data Integration with Jarvis

Meet Jarvis

Jarvis

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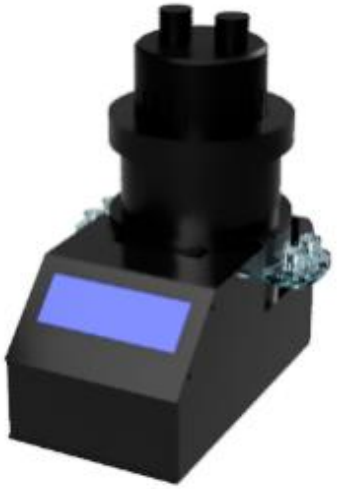
Jarvis



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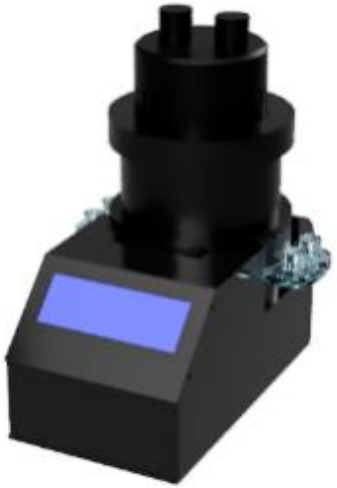
Jarvis



Python
Read and
Write Data

Discuss
User Data

Jarvis

set it to 48

10:48 AM

The temperature has been successfully set to 48°C, which is within the optimal range for your reaction. If you need any further adjustments or assistance, just let me know!

10:48 AM

7, temperature, 60.

10:48 AM

Setting the temperature to 60°C would exceed the optimal range for the reaction, which is between 35-50°C. This may negatively affect the reaction's efficiency. Would you like to adjust it to a more suitable temperature?

Proteus Aether Photoflow System

Proteus Aether

Reactors – Polypropylene – Used with Kessil lamps

Batch or CSTR reactions

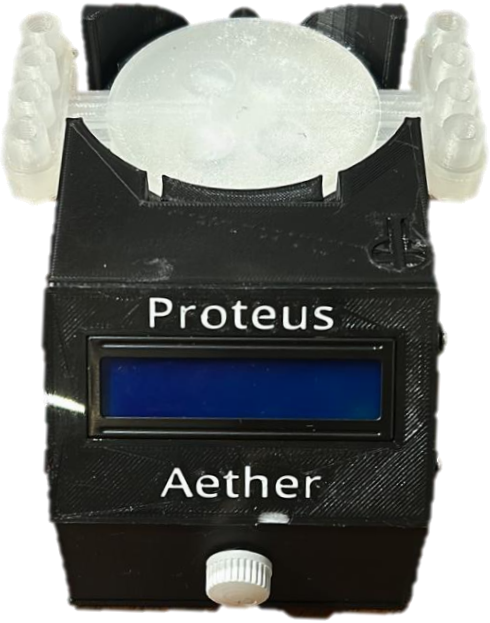
Data Integration with Jarvis

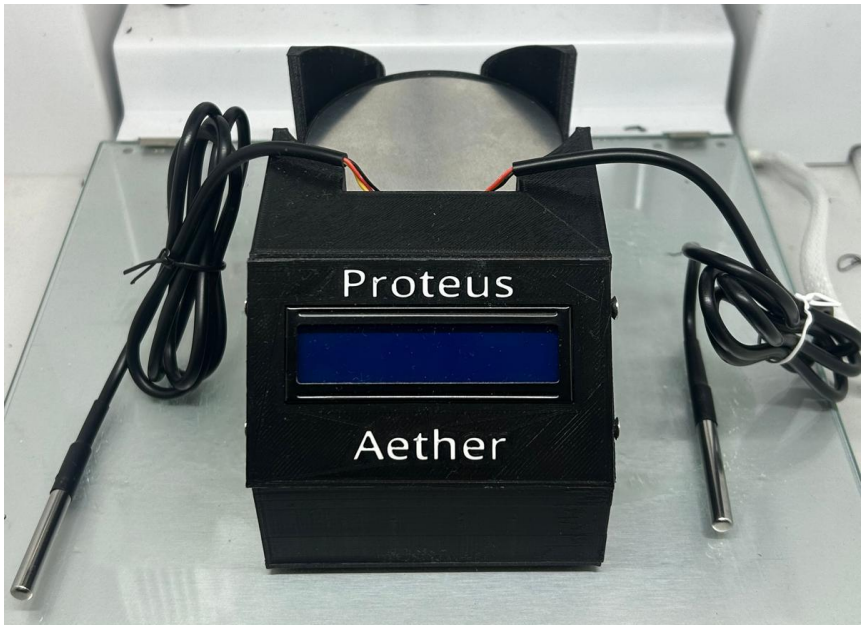
Proteus Devices

Integrated heating

Integrated Stirring

Cloud enabled Devices Linked to Jarvis





Global Collaboration

AETHERLINK

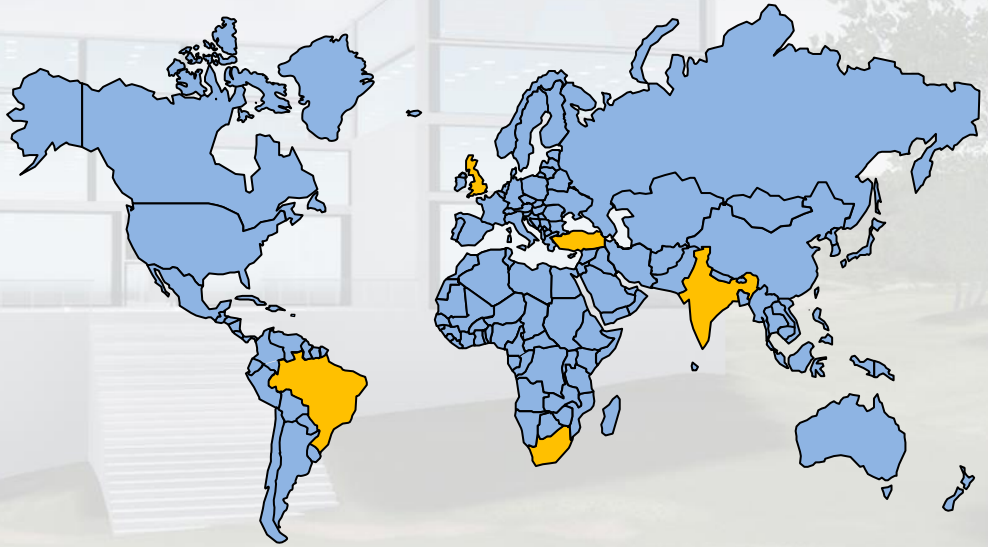
Science Without Borders

AETHERLINK

What is Aetherlink:

"*Aetherlink is a global Virtual Reality science network providing real-time training, research access, and AI-powered collaboration — anywhere, anytime.***"**

"Through immersive VR environments, multilingual AI avatars, and digital twins of real-world labs, Aetherlink breaks down barriers to scientific innovation, creating a sustainable and inclusive future for all"



AETHERLINK

Aetherlink Central:

"A *central building for scientists from across the globe to come together and train and collaborate. The central hub links to regional and global specialist centres"*

AETHERLINK

Science Without Borders

AETHERLINK

Aetherlink Central

"Through Aetherlink Central, users can join regional and specialist hubs"

ImmersaLab
Brazil Virutal Centre

ASI
Virtual Centre

TKD
Virtual Centre

ISCC
Virtual Centre

Equality Hub
Virtual Centre

Digital Outreach
Virtual Centre

Africa Science Institute

Virtual Centre

"Africa Science Institute: *Africa's gateway to sustainable science"*

AETHERLINK

Vision Statement:

"To position Africa as a leader in sustainable science innovation across Africa by providing 24/7 access to virtual laboratories, AI-powered training, and global research collaboration — enabling inclusive, high-impact science across the continent."

AETHERLINK

Science Without Borders

AETHERLINK

Vision:

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ASI Leads:
Professor Reinert Meijboom
and Dr Lungile Sitole

UCL SCHOOL OF PHARMACY
BRUNSWICK SQUARE

Come and Talk to Us

Acknowledgements

Group

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Erik Quall
Family

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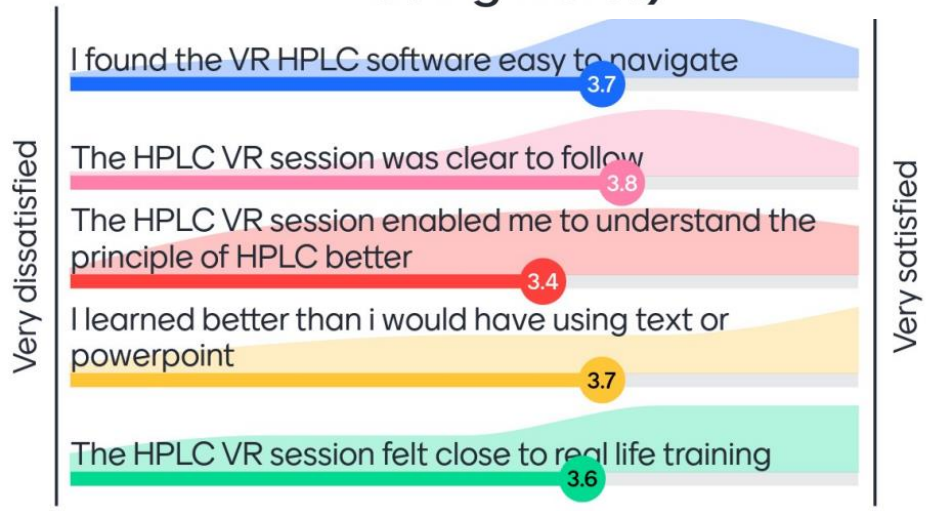
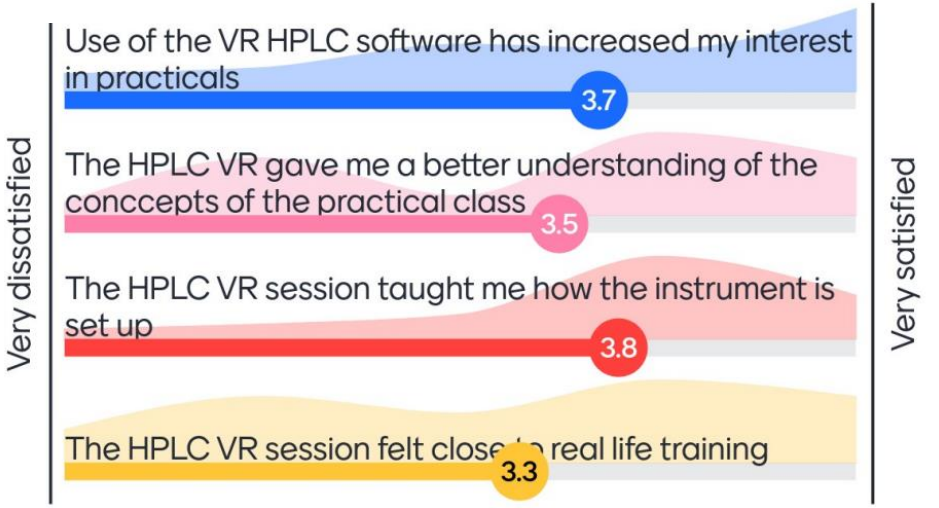
Department for Business, Energy & Industrial Strategy
Royal Society of Chemistry
IKA
Pancreatic Cancer Research Fund
The Royal Society Celebrating 350 Years
The Leverhulme Trust
GSK
EPSRC Engineering and Physical Sciences Research Council
FCT Fundação para a Ciência e a Tecnologia
LLR-G5
Petplan the pet people
FNSNF Fonds National Suisse Schweizerischer Nationalfonds Fondo Nazionale Svizzero Swiss National Science Foundation
UCLB
British Council
NHS Health Education England
LifeArc
Scott Bader Making a positive difference

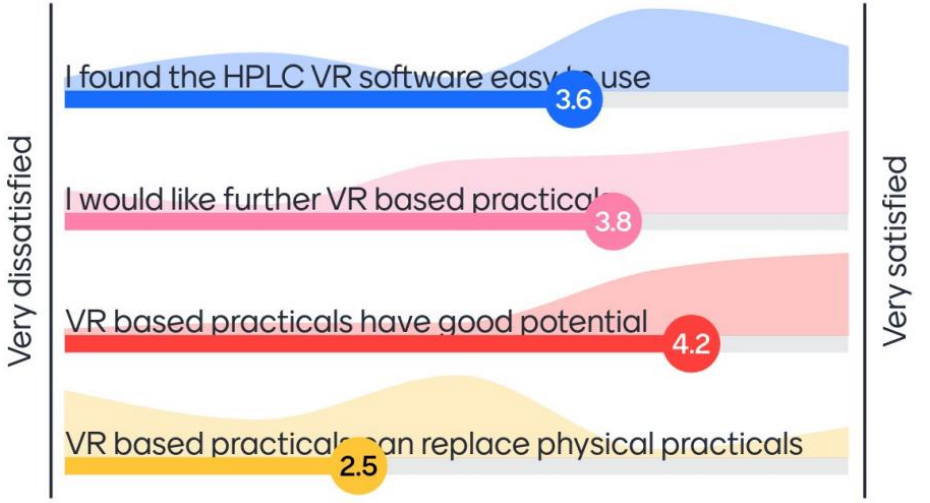
Where Next?

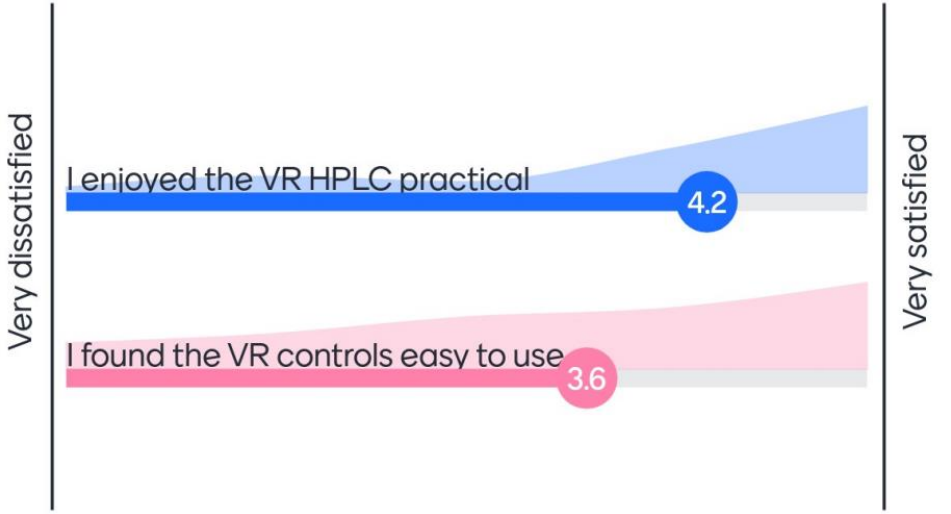
HPLC - VR Training

Please rate on a scale from 1-5 (5 being best and 1 being worst)



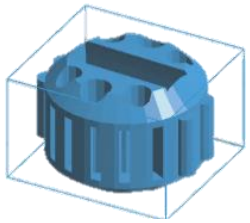


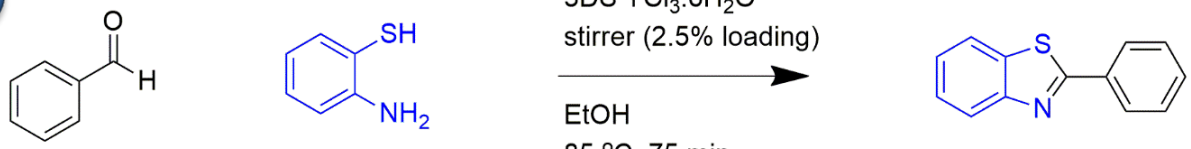


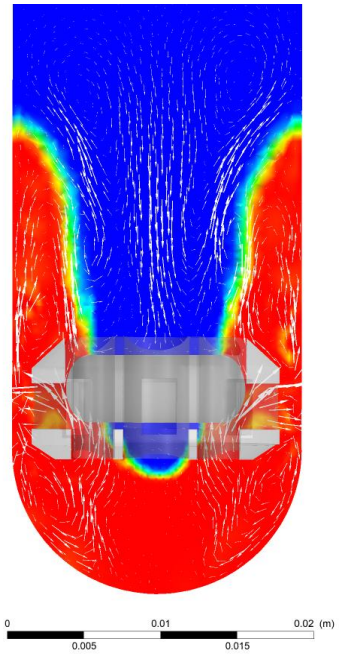


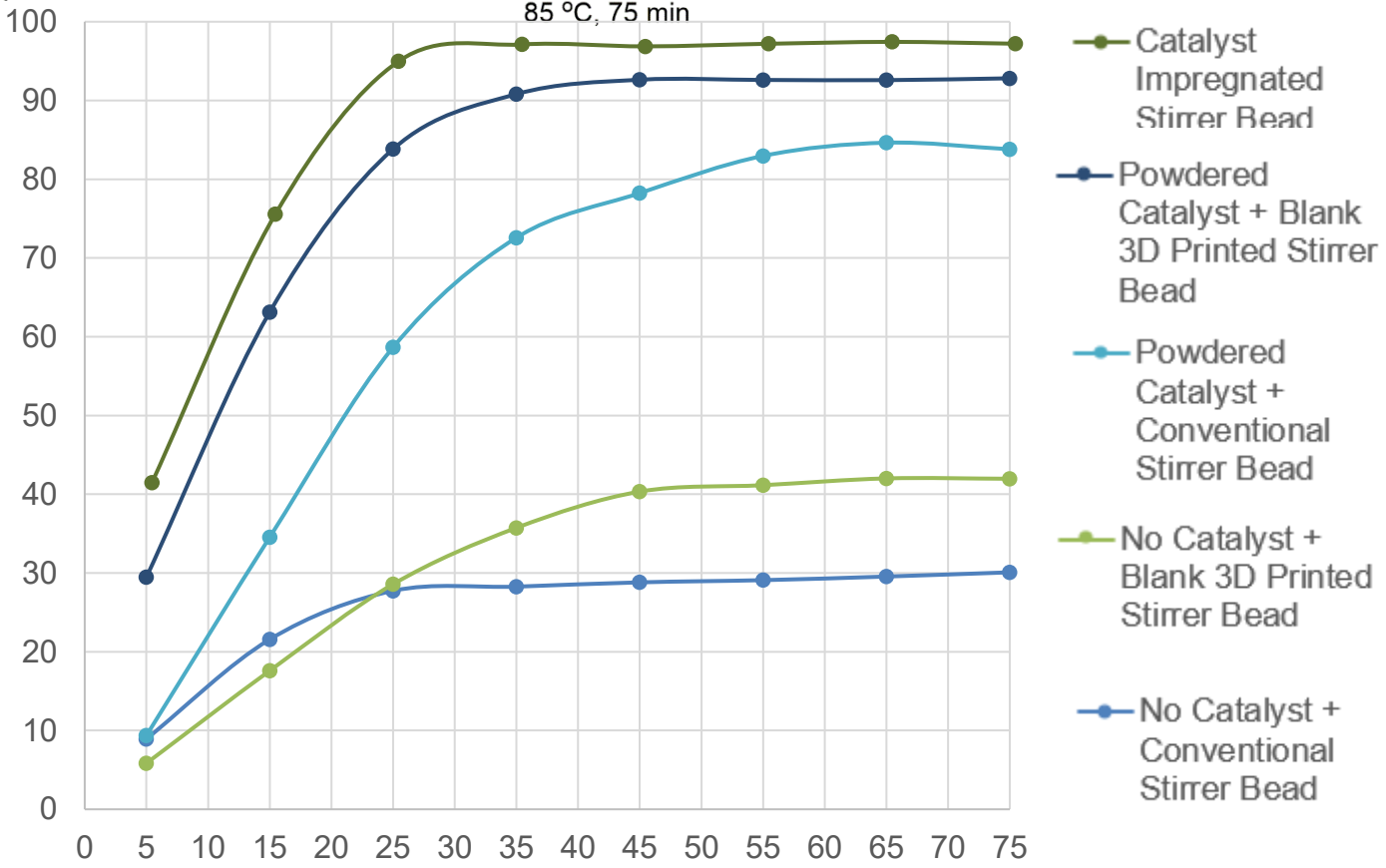
Heterocycle Formation

Heterocycle Formation









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