# H2020 Marie Skłodowska-Curie Innovative Training Network CORE www.coreitn.eu

# **Introductory Week**

Glasgow, Monday 30 January – Friday 3 February 2017 University of Strathclyde [Google map]



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## 1 Welcome

#### About the network

Industries are in need of highly skilled academically trained experts and powerful sets of tools enabling the design, control & prediction of optimized & efficient production process of future high-value products such as chiral pharmaceuticals. The CORE Network will in parallel train 15 ESRs and develop tools, approaches and methods within the area of Continuous Resolution (CORE), the process to obtain enantiopure molecules of chiral compounds.

CORE brings together 8 beneficiary partners (academic and industrial) and 7 associate partners (industrial) across 6 European countries resulting in an unparalleled combination of chirality, synthesis and crystallization training and research covering the areas of Chemical Engineering, Chemistry and Applied Physics.



Figure 1: Beneficiary partner countries

This booklet will give you an overview of the CORE training network, and the Introductory event being held in the University of Strathclyde and an overview on helpful practical information for the organisation of your stay in Glasgow.

# 2 Overview of the training programme

This event will be the first of nine network wide event, which are the main meeting events of our Innovative Training Network. Before getting into programme details it might be helpful to give you a brief reminder of the key elements of the training and research programme.

	Main Training Events & Conferences	EC	Lead	Month
1	CORE Introduction period	2	USTRATH	4
2	Summerschool Crystallization	2	RUN	8
3	Workshop Solid State Properties	2	TC	14
4	Summerschool Process Analytical Tools	2	UM	19
5	Workshop Resolution Fundamentals	2	UR	23
6	Conference Chirality & Resolution		UR/USTRATH	23
7	Summerschool Continuous Resolution	2	OVGU/MPI	31
8	Workshop Chiral Synthesis	2	SYNCOM	35
9	Conference Chirality & Resolution		USTRATH	48

**Figure 2:** Main Network-Wide Training Events, Conferences and Contribution of Beneficiaries. ECTS = European Credit Transfer and Accumulation System.

The training objective of the CORE network is to deliver a CORE skills toolbox of **knowledge**, **personal**, **organizational and impact skills** to a core of multi-disciplinary scientists and engineers in the interdisciplinary and cross-sectional field of Continuous Resolution. Each ESR obtains dedicated training through their **research project**, **network events**, **webinar course**, **management involvement and an academic & industrial secondment**.

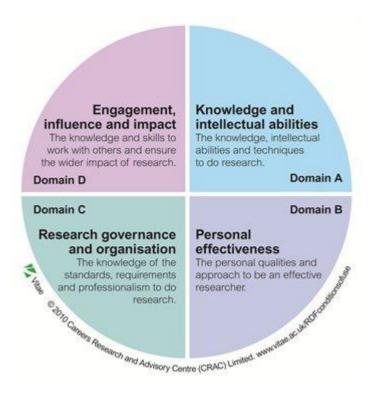
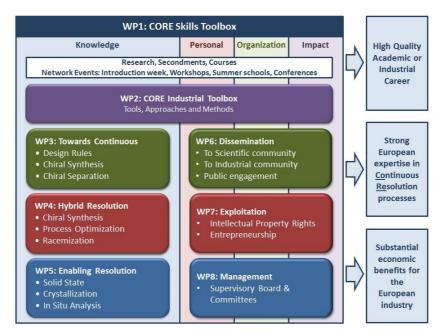


Figure 3: Core skills toolbox - knowledge, personal, organizational and impact skills

#### **Research Work Packages**

The research objective of the CORE Network is to jointly construct a **CORE Industrial Toolbox on Continuous Resolution that provides next generation tools, approaches and methods to industry for the development continuous resolution processes.** The strongly involved industrial partners will ensure that the CORE Industrial Toolbox fulfils their requirements in the skills gap areas Towards Continuous, Hybrid Resolution and Enabling Resolution.



**Figure 4:** Each ESR will develop, validate and deliver a tool, approach or method within WP3-5 to be integrated in the CORE Industrial Toolbox (WP2)

See <u>Figure 6</u> below for the relation between WP and individual ESR projects. Through WP2 the ESRs will be trained to work in an international multidisciplinary team on a joint target where the synergy between the ESRs will be responsible for an intensified training in both knowledge and transferable skills. Expertise areas that will be covered by the network are: Continuous Manufacturing, Chiral Resolution, Chiral Synthesis, Crystallization Fundamentals, Process Analytical Tools and Process Modelling & Design.

WP	WP Title	Lead	Start Month	End month	Activity Type	Lead Participant	ESRs
1	CORE Skills Toolbox	6	1	48	T	UM/TV	All
2	CORE Industrial Toolbox	1	1	48	R	USTRATH/JtH	All
3	Towards Continuous Processes	2	1	48	R	OVGU/ASM	1-4
4	Hybrid Resolution	4	1	48	R	RUN/EV	5-9
5	Enabling Resolution	3	1	48	R	UR/GC	10-15
6	Dissemination	4	1	48	D	RUN/EV	All
7	Exploitation	5	1	48	Е	SYNCOM/RK	All
8	Management	1	1	48	M	USTRATH/JtH	All

**Figure 5:** Work Package (WP) List. Activity types: R – Research, T – Training, D – Dissemination & public engagement, E – Exploitation, IPR & Entrepreneurship, M – Management

#### **ESR Projects**

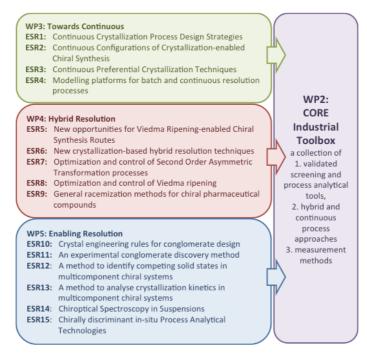


Figure 6: Relationship between WP and individual ESR projects

#### **Management Involvement**

Each ESR will be a member of the Training Committee, CORE Industrial Toolbox Committee, Dissemination Committee, Exploitation Committee or the Supervisory Board. In each of these committees 3 ESRs will be positioned. This will help the ESRs to develop management and organization skills while developing detailed strategies on e.g., dissemination.

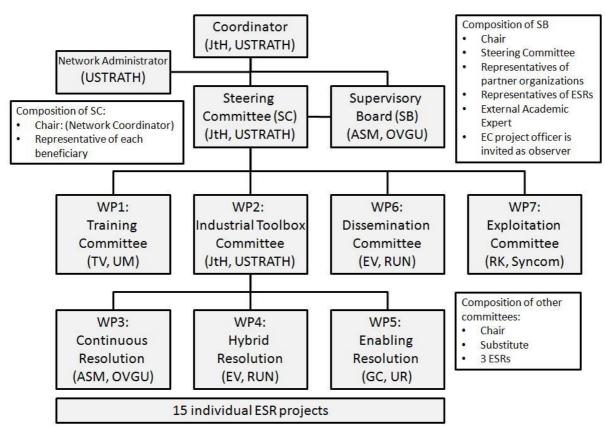


Figure 7: CORE management structure

Supervis	Supervisory Board (Chair: Prof Andreas Andreas Seidel-Morgenstern)							
2	Johannes Hoffmann	USTRATH						
8	Francesca Breveglieri	ETH						
9	Carola Tortora	UEN						
WP1: Tr	WP1: Training Committee (Chair: Thomas Vetter, Deputy Chair: Prof Joop ter Horst)							
3	not yet recruited	OVGU						
12	Lina Harfouche	UR						
15	Gufrhan ur Rehman	UM						
WP2: Industrial Toolbox (Chair: Prof Joop ter Horst, Deputy Chair: Prof Andreas Seidel-Morgenstern)								
1	Shashank Bhandari	OVGU						
7	Ryusei Oketani	UR						
10	Jan Joris Devogelaer	RUN						
WP6: Dis	ssemination Committee (Chair: Prof Elias Vli	eg, Deputy Chair: Prof Svetlana Tsogoeva)						
5	not yet recruited	RUN						
11	Aliou Mbodji	UR						
13	Sudhansu Sekhar Jena	USTRATH						
WP7: Ex	WP7: Exploitation Committee (Chair: Prof Richard Kellogg, Deputy Chair: Prof Joop ter Horst)							
4	not yet recruited	ETH						
6	Guilio Valenti	Syncom						
14	Raghunath Venkatramanan	USTRATH						

Figure 8: ESR allocation to CORE committees

#### Academic & Industrial Secondment

All ESRs visits/secondments are planned at the secondary supervisor institute (2 months), at an academic partner (3-5 months) as well as at an industrial partner (3-5 months), please see the Gantt Chart. Additional minor secondments at other academic or industrial partners may be arranged for the ESR to acquire additional specific skills to be added to the CORE Skills Toolbox.

		ESR													
	WP3: Towards Continuous WP4: Hybrid Resolution							WP5: Reso	lution Funda	amentals					
ESR	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Н	OVGU	USTRATH	ovgu	ETH	RUN	SYNCOM	UR	ETH	FAU	RUN	UR	UR	USTRATH	USTRATH	UM
2	ETH	OVGU	UR	OVGU	USTRATH	USTRATH	ETH	UM	RUN	UR	RUN	USTRATH	FAU	UR	MPI
S1	USTRATH	RUN	ETH	MPI	FAU	UR	RUN	USTRATH	UM	MPI	UM	OVGU	UR	OVGU	ETH
S2	PCAS	SYNCOM	MERCK	CORBION	TC	ETH	MERCK	SYNCOM	cc	PCAS	TC	PSE	PSE	CORBION	cc

**Figure 9:** Planned secondments of the ESRs within the CORE Network.

H - Host institute; 2 - Second supervisor visit; S1 - Academic secondment; S2 - Industrial Secondment.

The ESR will define a short research project in cooperation with the primary and secondary supervisor to perform during the secondary supervisor visit. The second supervisor will thus provide complementary expertise and, if beneficial, can also provide access to additional equipment, analysis techniques and transferable skills training.

The academic partners will host the **academic secondments**. The ESR in cooperation with the academic secondment supervisor and the primary supervisor will define the academic research project to be performed during the 3-5 month academic secondment. The secondment at the academic partner is targeting a specific skill needed to develop the tool, approach or method for the CORE Toolbox. The aim of the visit will be to come to a joint scientific paper on the defined project.

The industrial participants will host and supervise the **industrial secondments**. The ESR in cooperation with the industrial secondment supervisor and the primary supervisor will define the industrial project to be performed during the 3-5 month industrial secondment. The secondment at the industrial partner is targeting the viability of the developed tool, approach or method for the CORE Toolbox.

#### The Introductory week

The CORE introductory week and kick-off meetings will take place from 30 January until 3 February 2017 in Glasgow. During the kick-off meeting, the newly recruited Early Stage Researchers (ESRs) and their supervisors, together with representatives of the partner organisations, and the project manager will meet to discuss the start-up of the CORE project.

On Monday 30 January 2017, 09:00hrs ESR participants will meet for the first time at the Introduction to the Network in the Lord Hope Building (Room LH228), University of Strathclyde. Supervisors and partners can participate on a voluntary basis. This will be followed throughout the week by lectures, lab sessions and classes. Some of these sessions will be conducted jointly with the <a href="CMAC DTC">CMAC DTC</a> (Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, Doctoral Training School).

ESRs will be provided with information on the Marie Sklodowska Curie Actions (MSCA) and the CORE training framework. The main network research objective of constructing the toolbox will be introduced, explained and discussed by the WP2 Lead Beneficiary, Professor Joop ter Horst (University of Strathclyde). They will receive training on Crystallization and Chirality, as well as general training for example project management.

The kick-off meetings will take place on Wednesday 1 February, with the first face to face meeting of the Steering Committee for beneficiary partners and on Thursday 2 February, the first meeting of the network Supervisory Board for beneficiary and associate partners will take place, this will be followed by a visit to Glengoyne Distillery and dinner at Ross Priory on the banks of Loch Lomond.

Further, the social programme will provide an opportunity for informal interaction between the participating ESRs and partners, as well as with other PhD students within <u>CMAC</u>.

The full programme is outlined in section 3 on the following pages.

## 3 Programme

This CORE Introductory event will take place across <u>five buildings in University Strathclyde</u> each venue is linked to a map and there is also a map in Appendix 3, p19 or you can download the mobile app <a href="https://www.strath.ac.uk/studywithus/mobileapp/">https://www.strath.ac.uk/studywithus/mobileapp/</a> and we have also created a google map <a href="https://drive.google.com/open?id=1EdDVL1KD5tj-6I6g6wkDcTTYwPU&usp=sharing">https://drive.google.com/open?id=1EdDVL1KD5tj-6I6g6wkDcTTYwPU&usp=sharing</a>

Building Code: LH - Lord Hope Building (141 St James Road, G4 0LT)

Building Code: TIC Technology and Innovation Centre (99 George Street, G1 1RD)

Building Code: CW - <u>Strathclyde Business School- Cathedral Wing</u> (100 Cathedral St, G4 0QU) Building Code: SW - <u>Strathclyde Business School- Stenhouse Wing</u> (173 Cathedral St, G4 0QU)

Building Code: LT - Livingstone Tower (26 Richmond Street, G1 1XH)

#### Sunday 29 January 2017

ESR Participants arrive in Glasgow: recommended accommodation Premier Inn. George Square

#### Monday 30 January 2017

Venue: University of Strathclyde, Lord Hope Building (141 St James Road, G4 OLT)

09:00-10:45 Introduction to the CORE Network and Industrial Toolbox (room: LH228)

Professor Joop ter Horst, University of Strathclyde

Claire Lynch, University of Strathclyde

10:45-11:00 Coffee break (room: LH228)

11:00-12:30 **Introduction to Industrial Crystallization** (room: LH228)

Professor Joop ter Horst, University of Strathclyde

Venue: Ad Lib Merchant City (33 Ingram Street, G1 1HA)

12:30-14:00 Lunch – Ad Lib Merchant City

Venue: <u>University of Strathclyde, Lord Hope Building</u> (141 St James Road, G4 0LT)

14:00-15:30 **Stereochemistry in Synthesis & Crystallization** (room: LH228)

Dr Réne Steendam, University of Strathclyde

15:30-15:45 Coffee break

Venue: <u>University of Strathclyde, Technology and Innovation Centre</u> (99 George Street, G1 1RD)

16:00-17:30 **Lab Tour** (room: TIC Level 6 Lab)

Professor Joop ter Horst and Dr Réne Steendam, University of Strathclyde

Venue: <u>Babbity Bowsters</u> (16-18 Blackfriars Street, G1 1PE)

17:30-18:30 Drink Reception - Meet the CMAC DTC PhD students (Babbity Bowsters)

### Tuesday 31 January 2017

Venue: <u>University of Strathclyde, Business School-</u> <u>Cathedral Wing</u> (100 Cathedral St, G4 0QU)

09:00-10:00 **Crystal shape engineering** (room: CW507a and b)

Professor Marco Mazzotti, ETH Zurich (Swiss Federal Institute of Technology in Zurich),

Switzerland

10:00-12:30 **Introduction to Process Analytical Technology** (room: CW506a)

Dr Alison Nordon, University of Strathclyde

Venue: Amore restaurant (30 Ingram Street, G1 1EZ)

12:30-14:00 Lunch - Amore

Venue: <u>University of Strathclyde, Technology and Innovation Centre</u> (99 George Street, G1 1RD)

14:00-17:30 **Lab Session** (room: TIC Level 6 Lab)

Venue: <u>Drygate</u> (85 Drygate, G4 0UT)

17:30 Evening event – Drygate [this is cash bar event with all CMAC DTC PhD students]

Meeting in TIC Reception at 17:30

#### Wednesday 1 February 2017

Venue: <u>University of Strathclyde</u>, <u>Business School- Cathedral Wing</u> (100 Cathedral St, G4 0QU)

09:00-10:45 **Industrial Partner Lectures** (room: CW506b)

Dr Sean Bermingham, Process System Enterprise/ Professor Richard Kellogg, Syncom

10:45-11:15 Coffee (room: CW506b)

11:15-12:30 **Committee Chairs meet with relevant ESRs** – see figure 8 (room: CW506b)

12:30-13:30 Lunch CW506b

13:30-17:00 <u>In parallel:</u>

**Solid State Science – <u>for ESRs</u>** (room: CW506b) Professor Alastair Florence, University of Strathclyde

13:30-17:30 **CORE Steering Committee -** for Full Beneficiary Partners only (room: SW109)

Venue: Gandolfi Fish Restaurant (84-86 Albion Street, G1 1NY)

19:00 Dinner with CORE members – Gandolfi Fish

#### Thursday 2 February 2017

Venue: <u>University of Strathclyde</u>, <u>Business School-</u> <u>Cathedral Wing</u> (100 Cathedral St, G4 0QU)

09:00-10:00 **CORE Network Lecture - Processes to separate enantiomers** (room: CW507a/b)

Professor Andreas Seidel-Morgenstern, Otto von Guericke University and Max Planck

Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

10:00-10:45 "Speed Networking" Coffee with PhD students, Supervisors and Industrial partners

(Room: CW506a)

10:45-12:30 **Supervisory Board Meeting (room: CW404b)** 

Venue: <u>University of Strathclyde, Technology and Innovation Centre (TIC)</u> (99 George Street, G1 1RD)

12:45-13:45 **Lab Tours for Partners** (room: TIC Level 6 Lab)

Dr Thomas McGlone, University of Strathclyde

13:45-14:00 Paper bag lunch to eat on the bus – available from TIC reception

14:00 Bus departs for Glengoyne from outside TIC

Venue: Glengoyne Distillery and Ross Priory

14:00 Excursion to Glengovne Distillery & Dinner (Ross Priory) with CMAC DTC

21:00 Bus returns to Glasgow

#### Friday 3 February 2017

Venue: <u>University of Strathclyde, Lord Hope Building</u> (141 St James Road, G4 0LT)

09:30-12:30 Introduction to Managing Your PhD Project and Supervisor Relationship (room:

LH229a)

Dr Fraser Roberston, Fistral Training and Consultancy Ltd.

Venue: <u>Dakhin</u> (89 Candleriggs, G1 1NP)

12:30-14:00 Lunch - <u>Dakhin</u>

Venue: <u>University of Strathclyde, Livingstone Tower</u> (26 Richmond Street, G1 1XH)

14:00-17:00 **Introduction to Mathematics II** (room: LT901)

Dr Cameron Brown and Dr Alison Nordon, University of Strathclyde

More information about the social programme can be found in Annex 3.

# Timetable

	Мо	Tue	We	ed	Thu	Fri		
	30 January 2017	31 January 2017	01 Februa	ary 2017	02 February 2017	03 February 2017		
09:00 - 10:00 10:00 - 11:00	L1: Prof Joop ter Horst/ Claire Lynch - Introduction to the CORE Network and Industrial Toolbox (room: LH228)	Prof Marco Mazzotti Crystal shape engineering (room: CW507a and b)	Dr Sean Bermingham, PSE/ Prof Richard Kellogg, Syncom Industrial Partner Lectures (room: CW506b)		Richard Kellogg, Syncom Industrial Partner Lectures (room:		Prof Andreas Seidel-Morgenstern Processes to separate enantiomers (room: CW507a and b)  "Speed Networking" Coffee with PhD students, Supervisors and Industrial partners (Room: CW506b)	Dr Fraser Robertson (Fistral) Introduction to Managing Your PhD
11:00 - 12:00	Coffee L2: Prof Joop ter Horst	Dr Alison Nordon Introduction to PAT (room: CW506a)			Supervisory Board Meeting (room:	Project and Supervisor Relationship (room: LH229a)		
12:00 - 13:00	Introduction to Industrial Crystallization (room: LH228)	(100111101111)	Committee Chairs (room: C		CW404b)			
13:00 - 14:00	lunch - Ad Lib	lunch - Amore	Lunch - tbc  Beneficiary		Lab tour for partners (TIC level 6) and Paper bag lunch for everyone	lunch - Dakhin		
14:00 - 15:00	Dr Réne Steendam Stereochemistry in Synthesis &		<u>For ESRs</u> : Prof Alastair	Partners: Steering Committee (room:		Dr Cameron Brown and Dr Alison		
15:00 - 16:00	Crystallization (room: LH228)  Coffee	, , , , , , , , , , , , , , , , , , , ,		SW109) Coffee Break	Excursion to Glengoyne Distillery & Dinner (Ross Priory) with CMAC DTC	Nordon Introduction to Mathematics II		
16:00 - 17:00	Prof Joop ter Horst / Dr Dr Réne Steendam		(Room: CW506b)	Steering Committee (room:	- bus returns to Glasgow 21:00	(room: LT901)		
17:00 - 18:00	Lab tour (TIC level 6)			SW109)		Closure		
Evening	Meet the CMAC DTC PhD students (venue: Babbity Bowsters)	Informal Evening Event - cash bar (venue: Drygate)	Dinner with the CORE members (venue: Gandolfi Fish)					

Building codes/floor plans:	http://www.strath.ac.uk/estates/ad
	min/roombooking/buildingcodes/
Room Key:	TIC Level 6 - Technology & Innovation
	Centre
	LH228/ LH229a - Lord Hope Building
	CW506a and b/CW404b /CW507a
	and b - Business School, Cathedral
	Wing (SBS)
	SW109 - Business School, Stenhouse
	Wing (SBS)
	LT901 - Livingstone Tower

CORE Network
Crystallization
Chirality
General Training
Lab Sessions
Organization
Social Activities

## 4 Class Outlines

Session marked with an \*\* will be audio recorded for those who are not able to attend and will be made available on the members area of the core web-site.

#### Monday 30 January 2017

# **Introduction to the CORE Network and Industrial Toolbox** (room: LH228) \*\* Professor Joop ter Horst and Claire Lynch, University of Strathclyde

This session will include short ice breaker to give ESRs an opportunity to meet each other. It will provide an overview of the Marie Skłodowska-Curie actions and the CORE network, and the training and research within each of the different work packages.

## Introduction to Industrial Crystallization (room: LH228) \*\*

Professor Joop ter Horst, University of Strathclyde

Industrial crystallization is a separation technology that exploits the first-order phase transition between a liquid and a solid. It is a highly selective technology resulting in a very pure solid particulate product in a single process step, making it a highly efficient technique in e.g., chiral resolution processes. The particulate product crystals have a specific form, size, shape, and purity. Customer and manufacturer demands for a crystalline product can usually be traced back to these four product quality aspects. The industrial crystallization techniques are defined by the way supersaturation is created. Even on industrial scales with large production rates, crystallization generally remains a molecular-level process which is complex to control. The increasing complexity and molecular size of future products relies on the development of new and innovative crystallization approaches.

# **Stereochemistry in Synthesis & Crystallization** (room: LH228) \*\* Dr Réne Steendam, University of Strathclyde

Stereochemistry is an important discipline in chemistry that studies the spatial arrangement of molecules. Chiral molecules or enantiomers in particular are the topic of ongoing interest as there is an increasing demand for enantiopure pharmaceutical drugs. Both synthesis and crystallization are effective means to manufacture enantiopure compounds.

This lecture provides an introduction to stereochemistry with an emphasis on chirality and resolution. The assignment, measurement and quantification of chiral molecules will be addressed. The main challenge in chirality is to obtain one of the two chiral forms of a compound, which can be achieved through synthesis or crystallization. A short introduction on crystallization-based resolution will be given.

From its discovery onwards, Viedma ripening has shown to be an easy and powerful means to deracemize enantiomers in crystal suspensions. Viedma ripening was recently combined with synthesis to give an integrated process. Viedma ripening, its mechanism and its applications will be discussed in detail. The topics addressed in this presentation will also be covered throughout the Horizon2020 innovative training network CORE.

## Lab Tour (room: TIC Level 6 Lab)

## Professor Joop ter Horst and Dr Réne Steendam, University of Strathclyde



 World class facilities for forming, processing and analysing particles and particulate systems

 Pilot scale manufacturing capability supporting global

partners

• Inspiring researchers and enabling breakthroughs in medicines manufacture

Vision: To support a world class manufacturing research facility, inspiring researchers, supporting innovation

Mission: To provide cost effective access and support to all users within a safe, well managed and collaborative environment

The CMAC National Facility aims to deliver world class research, training and knowledge exchange on a global scale as well as operating as a National Facility supporting users from both academia and industry. Our advanced pharmaceutical manufacturing research facilities will be easily accessible by academics and businesses in the UK and internationally.

The National Facility has the additional benefit of co-locating multidisciplinary teams of academic and industry researchers within the state of the art Technology and Innovation Centre (TIC) at the University of Strathclyde.

The facility is equipped using £11.4 m funding awarded by the Higher Education Funding Council for England (HEFCE)'s UK Research Partnership Investment Fund (UKRPIF) and supported with £22.8 m industry and charity contributions. The National Facility features world class capabilities in:

- Primary Processing
- Secondary Processing
- PAT/Spectroscopy
- X-ray Diffraction
- Surface Analysis
- Materials Characterisation

The National Facility is working towards end-to-end continuous manufacturing and crystallisation research capability under one roof. This capability features key items of equipment:

- Modular skid-mounted crystallisation platforms (batch and continuous)
- Pilot scale filtration and drying
- Secondary processing including spray drying, hot melt extrusion (HME), granulation and tableting
- ToF-SIMS
- Atomic force microscopy (AFM)
- Nuclear magnetic resonance (NMR) spectroscopy
- World class X-ray suite including single crystal, powder (crystalline & amorphous), small angle scattering (SAXS) and nano computed tomography (CT).



**CORE Network Lecture – Crystal Shape Engineering** (room: CW507a/b) \*\*
Professor Marco Mazzotti, ETH Zurich (Swiss Federal Institute of Technology in Zurich),
Switzerland

The importance of crystallization in the pharmaceutical, food and fine chemical industries stems from its ability to yield highly pure solid products. Beside the final chemical purity, however, the solid state form,



the size and the shape of the resulting particles are of paramount importance for the product quality, because they determine characteristics such as filterability, tabletability, flowability and even bioavailability. Practitioners in these industries are well aware of the fact that crystals can take on a variety of shapes, even for the same chemical substance. Any form of control over particle size and especially shape should allow for the design of improved processes. Until recently, however, the optimization of crystallization processes in terms of particle size and shape has been hindered by a major obstacle: the lack of reliable, fast and quantitative measurement devices, which made online monitoring impossible, hence modelling and optimization unfeasible.

The lecture complements the module devoted to Process Analytical Technology (PAT) by providing insight on how to measure and monitor particles size and shape distributions during crystallization processes.

The lecture will be structured in three parts. The first will be devoted to the introduction of the key concepts about how to deal with size and shape of an ensemble of crystals. The second part will focus on the experimental platform developed and used at ETH Zurich to measure particle size and shape distributions; the pleasures and sorrows of applying this technique will be illustrated with examples. Finally, in the third part we will discuss a possible process to tune the crystal size and shape of crystals in seeded cooling crystallization, using a combination of cooling, milling and heating steps. Also in this case examples will be provided, using both simulations and experiments to assess the process performance.

A short list of key references is provided below:

- Schorsch S., T. Vetter, M. Mazzotti, Measuring multidimensional particle size distributions during crystallization, Chem. Eng. Sci. 77 (2012) 130-142
- Schorsch S., D.R. Ochsenbein, T. Vetter, M. Morari, M. Mazzotti, High accuracy online measurement of multidimensional particle size distributions during crystallization, Chem. Eng. Sci. 105 (2014) 155-168
- de Albuquerque I., D. Ochsenbein, M. Mazzotti, M. Morari, Effect of needle-like crystal shape on measured particle size distributions, AIChE Journal 62 (2016) 2974-2985

## **Lab Session** (room: TIC Level 6 Lab)

There will be five different lab demo setups, ESRs will be split into small groups of 3 and 4 with the CMAC DTC students and spend 30-45 minutes at each station on a rotation.

## Wednesday 1 February 2017

#### Industrial Partner Lectures (room: CW506b) \*\*

Dr Sean Bermingham, Process System Enterprise/ Professor Richard Kellogg, Syncom

**PSE** is the world's leading supplier of Advanced Process Modelling technology and related model-based engineering and innovation services to the process industries. Operations are based in the UK (head office), USA, Switzerland, Japan and Korea, and agencies in China, Taiwan and the UAE.

**Syncom BV** is a small/medium sized company (115 employees in total) that does contract work chiefly for the major pharmaceutical industries. The majority of the work is organic synthetic. This work is carried out by 100 research chemists about half of whom have PhDs and the others have master degrees. Synthetic projects include candidate structure for drug development as well as the synthesis of isotopically labelled compounds and metabolites. Considerable work is also done on the synthesis of organic compounds with unusual properties. Work is also carried out on process improvement. A specialty of Syncom is chirality including diastereomeric resolutions, deracemizations and chiral synthesis. An example of a typical synthetic project will be given. Syncom has also always been very active in fundamental research on chirality and some examples of this work will be shown and explained. Finally some new Syncom research on the organic aspects of gene therapy will be discussed.

#### **Solid State Science** (room: CW506b)

Professor Alastair Florence, University of Strathclyde

Professor Alistair Florence is Director of the EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation (CMAC) and associated 45 PhD Doctoral Training Centre. Leads the new world-class CMAC National Facility within the Technology and Innovation Centre (TIC) at the University of Strathclyde offering access to academic and industrial users to state-of-the art processing, analysis and characterisations facilties and support. Expertise in crystallisation and physical form control and characterisation of pharmaceuticals spanning polymorphism, solvate, co-crystal and salt formation and studies of amorphous systems. Extensive experience in the formation of pharmaceutical particles in continuous processes using a range of technologies as part of the CMAC programme. Interests also in the development and application of new technologies to control and monitor crystallisation and pharmaceutical solids.

Approaches for the characterisation of particles are also widely used and physical analysis of crystalline pharmaceuticals with a focus on the influence of crystallisation processes on structure and critical pharmaceutically relevant attributes that dictates product performance. Exploitation of X-ray powder diffraction techniques for phase identification, structure determination from powder diffraction data and in-situ phase surveys including local order using variable-temperature X-ray powder diffraction are key areas.

Has published over 120 peer reviewed research papers in these areas and currently supervises a large multidisciplinary research group including pharmacists, chemists and chemical engineers.

#### Thursday 2 February 2017

**CORE Network Lecture - Processes to separate enantiomers** (room: CW507a/b) \*\*
Professor Andreas Seidel-Morgenstern, Otto von Guericke University and Max Planck
Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

In the pharmaceutical, fine chemical, food and agrochemical industries, due to the homochirality of life, there is a large interest in producing pure enantiomers. This is a challenging task since highly enantioselective synthesis methods are difficult to develop. Conventional chemical synthesis is non-selective and leads to 50:50 (racemic) mixtures, creating a need in efficient enantioselective separation processes. Chromatography and crystallization are currently the most powerful methods. Recently it could be demonstrated, that an optimized joint application of these two methods can provide efficient overall processes.

The lecture will first introduce essential thermodynamic properties required for a rational development of enantioselective separation processes, in particular the different types of phase diagrams of chiral compounds. Since the occurence of conglomerates is very limited and most frequently racemic compounds are formed, successful crystallization processes require enriched feed solutions. This enrichment can be provided either by a partially selective synthesis or by a suitable first separation process.

The presentation will describe several case studies devoted to design and apply preparative chromatography in combination with subsequent selective crystallization. The possibility to directly combine continuously performed synthesis reactions and separation processes as well as the incorporation of racemizing the counter-enantiomer within yield increasing recycling concepts will be also discussed. Several of these aspects will be in the next four years intensively investigated within the Horizon2020 Innovative Training Network "Continuous resolution and deracemization of chiral components by crystallization (CORE)".

#### Friday 3 February 2017

# **Introduction to Managing Your PhD Project and Supervisor Relationship** (room: LH229)

Dr Fraser Roberston, Fistral Training and Consultancy Ltd.

This 3-hour session provides a high-level introduction to Project Management as well as guidance on managing your supervisor. This session provides a brief overview of the process of managing projects and the key tools to assist in planning and tracking progress. It introduces useful, applicable tools and techniques that will assist the planning and management of your research. It will also present considerations for managing, understanding and appreciating one of the most important relationships of your research project - your supervisory relationship.

#### **Introduction to Mathematics II** (room LT901)

Dr Cameron Brown and Dr Alison Nordon, University of Strathclyde

Calculations, processing and interpretation of data are common place in crystallisation research. This module highlights some of the common mathematical tools that you might encounter in your research. This will include overviews of gCrystal for population balance modelling and COMSOL multiphysics for computational fluid dynamics. Practical assignments cover "Less known but useful Excel function" and "Basic introduction to Matlab".

\*\* Introduction to Mathematics I will be available as an audio recording.

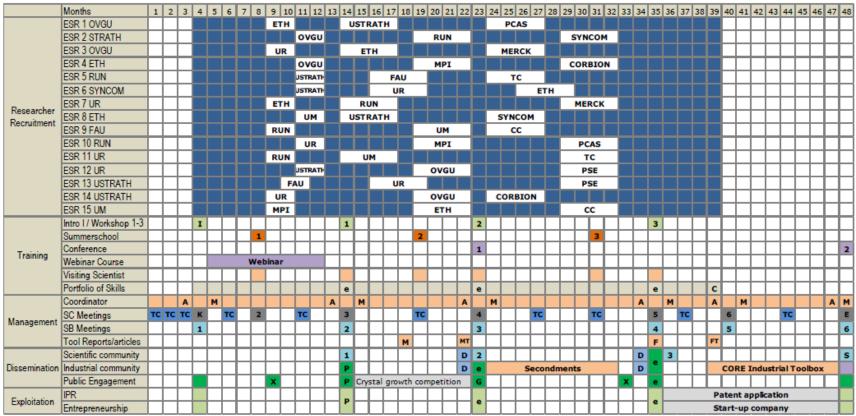
# **Appendices**

# **Appendix 1 – Introductory Event Participants**

Category:	First Name:	Family Name:	Organisation:
AP	Sean	Bermingham	PSE
ESR	Shashank	Bhandari	OVGU
ESR	Francesca	Breveglieri	ETH Zurich
FP	Pascal	Cardinael	Université de Rouen
ESR	Jan-Joris	Devogelaer	Radboud University Nijmegen
EXT	Neil	George	Syngenta
ESR	Lina	Harfouche	Université de Rouen
ESR	Johannes	Hoffmann	University of Strathclyde
AP	Alex	Kalbasenka	Corbion
FP	Richard	Kellogg	Syncom BV
EXT	Tom	Leyssens	UCL
FP	Claire	Lynch	University of Strathclyde
FP	Marco	Mazzotti	ETH Zurich
AP	Claus-Peter	Niesert	Merck
ESR	Ryusei	Oketani	Université de Rouen
AP	Mihaela	Pop	TeraCrystal
ESR	Ghufran ur	Rehman	University of Manchester
FP	Andreas	Seidel- Morgenstern	Max Planck Institute Magdeburg
FP	Joop	ter Horst	University of Strathclyde
ESR	Carola	Tortora	Friedrich-Alexander-Universität Erlangen- Nürnberg
FP	Svetlana	Tsogoeva	Friedrich-Alexander Universität Erlangen- Nürnberg, Germany
ESR	Giulio	Valenti	Syncom
FP	Thomas	Vetter	University of Manchester
FP	Elias	Vlieg	Radboud University

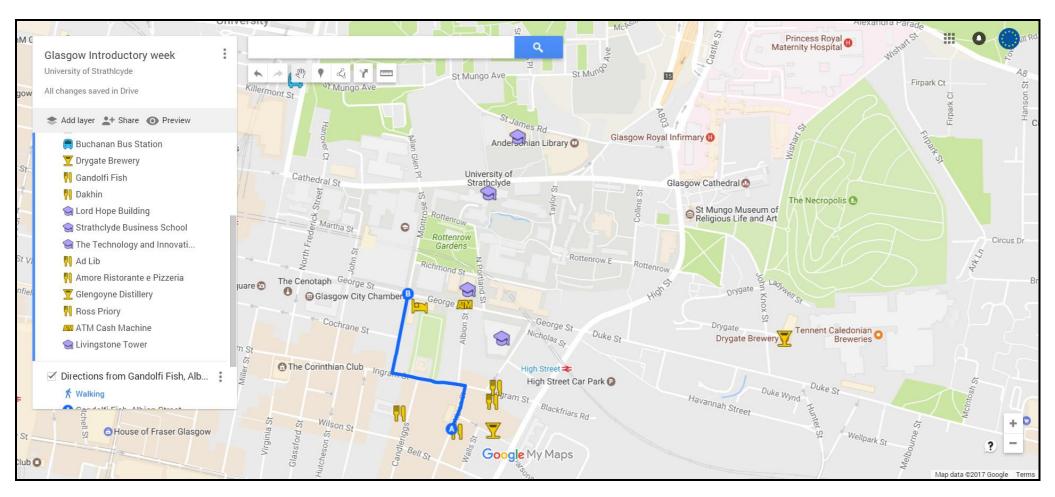
# **Appendix 2 – Gantt Chart**

Table 10: Gantt Chart. K: Kick-off meeting, E: End of project meeting, TC: Telephone Conference, M: Midterm report ESRs, MT: Midterm report on CORE Industrial Toolbox, F: ESR final tool article, FT: Final review article on CORE Industrial Toolbox, C: Skills Portfolio Certified, A: SB Agenda, M: SB Minutes, G: Midterm conference high school crystal picture competition, X: European Researchers' Night/Exploration, P: Plan for dissemination, public engagement, exploitation. e: Evaluation/adjustment of plan/PDP.



The start of all ESR projects is envisaged in month 4. Small differences in start date for the ESRs might arise due to regulations and university procedures in different countries. The ESR projects and the project planning in the Gant chart are sufficiently flexible to cope with these small differences. For all ESR projects, time periods for the secondary supervisor group visit and the Academic and Industrial Secondment are indicated. These periods for visit (ESR first year), academic secondment (second year) and industrial secondment (third year) are to some extend flexible and will be finalized by the ESR in cooperation with the supervisory team. The final secondment plans will be reported to the Training and Steering Committee for formal approval. Care will be taken that visit/secondment stimulate inter-ESR contact.

# **Appendix 3 – Practical Information**



[view Google map]

#### Venues

This CORE Introductory event will take place across <u>five buildings in University Strathclyde</u> each venue is linked to a map and there is also a campus map in <u>Appendix 4</u> or you can download the mobile app <a href="https://www.strath.ac.uk/studywithus/mobileapp/">https://www.strath.ac.uk/studywithus/mobileapp/</a>

Building codes/floor plans: http://www.strath.ac.uk/estates/admin/roombooking/buildingcodes/

Building Code: LH - Lord Hope Building (141 St James Road, G4 0LT)

Building Code: TIC Technology and Innovation Centre (99 George Street, G1 1RD)

Building Code: CW - <u>Strathclyde Business School- Cathedral Wing</u> (100 Cathedral St, G4 0QU) Building Code: SW - <u>Strathclyde Business School- Stenhouse Wing</u> (173 Cathedral St, G4 0QU)

Building Code: LT - Livingstone Tower (26 Richmond Street, G1 1XH)

#### Using the wireless network as a visitor to Strathclyde

#### **Eduroam**

If you are visiting Strathclyde from an institution that participates in the Eduroam scheme you can connect to the "eduroam" wireless network name to gain basic Internet connectivity. Your device will require to be configured in advance before you arrive. To log in you should use the credentials supplied by your home institution.

#### WiFi Guest

Alternatively, for customers who do not have access to Eduroam, we deploy a free wireless service across the campus. To connect, look for a network named "WiFi Guest" and follow the instructions. There is a first-time registration process, which requires users to provide an email address and set a password.

http://www.strath.ac.uk/it/services/wireless/

#### **Transport**

You can use the route planner to plan your journey by public transport in Glasgow http://www.travelinescotland.com/welcome.do

#### **Arrival Transport**

Getting from the Airport to Premier Inn Hotel

Glasgow is served by two airports:

Glasgow International Airport - being just a few miles outside the city centre is the main airport for transatlantic and worldwide flights. There is a regular bus service (500) into the city centre (George Square, North Frederick Street Bus Stop which is three minutes walk to the Premier Inn) costing around £7.50 which can be purchased on board using cash or credit card, alternatively a taxi from the airport to the Premier Inn will cost around £25 and are available outside the arrivals hall.

http://www.glasgowairport.com/im-departing/getting-here

Glasgow Prestwick International Airport is approximately 30 miles away from Glasgow city centre and is a smaller airport mainly used by low cost airlines offering domestic and European flights. Prestwick Airport is connected to a train station which is accessed via a covered walkway and journey time between the airport and Glasgow city centre is approximately 50 minutes. Passengers are entitled to a 50% discount on the train fare if they show their flight ticket/confirmation (the fare is approximately £6 with discount). The Premier Inn hotel is around a ten minute walk from Glasgow Central railway station or a short taxi journey (the fare is approximately £5).

http://www.glasgowprestwick.com/to-and-from-prestwick/

Getting from Central Train station to Premier Inn Hotel

The Premier Inn hotel is around a ten minute walk from Glasgow Central railway station or a short taxi journey (the fare is approximately £5).

#### http://www.networkrail.co.uk/glasgow-central-station/departures-arrivals/

Getting from Premier Inn to University of Strathclyde

The Premier Inn hotel is located a short 5 minute walk from the University buildings.

#### **Getting around in Glasgow**

The city centre itself is quite small and is easy to get around without needing to use public transport. The University's campus is located just a few minutes' walk from the main city centre square (George Square) and the two main train stations (Glasgow Central and Queen Street). If you do get lost, just ask someone – they will be happy to help!

There are 4 forms of public transport in the city; buses, trains, underground and public bikes.

#### Buses

The main bus operator is First Bus which covers the whole city, with smaller, localised operators covering certain routes. Major bus routes have services which run from early morning to late at night and a frequent service during peak hours. There are several ticket types. For current ticket and pricing information please visit First Bus.

#### **Trains**

Train services operate to the suburbs of Glasgow and further a field. Glasgow Central is the main station for train services to London and the south as well as southern and western suburbs of Glasgow, whilst Queen Street is the main station for services to Edinburgh, the East and North of Scotland as well as northern suburbs of Glasgow. Fares vary greatly depending on distance travelled, but are generally more expensive than travelling by bus. Timetables and prices are available from railway stations or by visiting <a href="Scotrail">Scotrail</a>.

#### **Underground/Subway Railway**

Glasgow Underground/Subway has a circular route, serving the city centre and western suburbs. Trains are frequent and fast and travel information is available from most Subway /underground ticket offices. Current pricing information can be found at <u>SPT</u>.

#### **Next Bike**

Next Bikes are available to rent 24/7 from any nextbike station. Renting a bike is easy using the free app, the on-bike computer, or by phoning the nextbike hotline. http://www.nextbike.co.uk/en/glasgow/

#### **Social Programme**

A social programme has been put together to allow time to informally meet with others from the CORE network and within CMAC.

#### Monday 30 January 2017: Drinks Reception, Babbity Bowsters

A drinks reception has been organised in Babbity Bowster (<a href="http://babbitybowster.com/">http://babbitybowster.com/</a>) to meet with the CMAC DTC students.

#### Tuesday 31 January 2017: Informal drinks (cash bar), Drygate

This will be an opportunity to meet all of the CMAC PhD students in Drygate (<a href="http://drygate.com/">http://drygate.com/</a>). We will meet at the TIC reception at 17:30. Please note that this event will be a cash bar.

#### Wednesday 1 February 2017: Network Dinner, Gandolfi Fish

This will take place in Gandolfi Fish restaurant (<a href="http://www.cafegandolfi.com/gandolfi-fish/">http://www.cafegandolfi.com/gandolfi-fish/</a>), 84-86 Albion Street, Glasgow G1 1NY, Tel: +44 (0)141 552 9475 at 19:00 – the restaurant is located 5 minutes walk from the Premier Inn hotel.



Thursday 2 February 2017: Social activity and dinner, Glengoyne Whisky Distillery and Ross Priory

The final social event of the introductory week will be a tour of Glengoyne Whisky Distillery (<a href="http://www.glengoyne.com/visit-us/distillery-tours/wee-">http://www.glengoyne.com/visit-us/distillery-tours/wee-</a>

<u>tasting-tour</u>) followed by dinner at Ross Priory (<a href="https://www.strath.ac.uk/rosspriory/">https://www.strath.ac.uk/rosspriory/</a>).

Glengoyne is said to be one of Scotland's most beautiful distilleries located just under 40 minutes from Glasgow. During the tour you will discover the process of whisky making and savour a wee dram. You will then be transferred to Ross Priory which is situated in an unrivalled position on the banks of Loch Lomond with stunning views of Ben Lomond and the surrounding hills, Ross Priory is a secluded and unusual venue enhanced by magnificent gardens. Dating back to 1693, Ross Priory is one of the finest examples of Gothic architecture in Scotland. The historic building was bought by



the University of Strathclyde in 1971 and is used extensively for a variety of events.

The buses will depart from outside the TIC Building at 14:00 and return at 21:00. There will be a paper bag lunch available from 13:45 in the reception of TIC which you can take on the bus.

#### **Glasgow**

Glasgow is Scotland's largest city and is renowned for its culture, style and the friendliness of its people.

Glasgow offers a blend of internationally-acclaimed museums and galleries, stunning architecture, vibrant nightlife, fantastic shopping and a diverse array of restaurants and bars.

Vibrant and energetic, Glasgow enjoys a year-round buzz with an arts scene that regularly produces cuttingedge productions and attracts high-profile exhibitions that led to the city being crowned European City of Culture in 1990.

Glasgow was also the UK's City of Architecture and Design in 1999 and its architecture is an attraction in itself. The city centre has countless impressive Victorian structures and then there are the unique masterpieces of one of the city's most celebrated sons, the legendary architect and designer Charles Rennie Mackintosh.

The city has a long-standing reputation for its live music scene and is very well off too in terms of city parks.

More information can be found at http://www.visitscotland.com/info/towns-villages/glasgow-p237531

#### Internet

Glasgow was the first Scottish city to offer free city wide wifi. For free internet access, users should simply switch on Wi-fi in your device settings. The device will search the airwaves and find which hotspots are in range and the strength of the signal. Users can then select **GlasgowCC WiFi** and go online.

#### Climate and weather

January and February are generally the coldest months in Scotland, with the daytime maximum temperatures averaging around 5 °C (41 °F) to 7 °C (45 °F).

As the old Scottish saying goes, "there's no such thing as bad weather, only the wrong clothes!" So even though Scotland isn't blessed with year-round sunshine and tropical temperatures, that doesn't mean to say that our weather gets in the way.

#### Currency

The currency is the British Pound /GBP (1 EUR = 0.83 GBP on 16 Dec 2016). For the international currency converter please click <a href="http://www.xe.com">http://www.xe.com</a>

In the UK, all major credit cards are generally widely accepted throughout the country in shops, restaurants, hotels etc.

ATMs (automatic cash machines) or 'cash machines' as they are called in Scotland are accessible 24h a day at banks, airports and train stations and give instructions in different languages.

#### **Electricity**

Electrical current in the UK is 240 volts. Adaptors for any electrical appliances you may bring with you are available to buy in airport shops and in many shops in Glasgow city centre e.g. Boots or WH Smith for approximately £3 to £5.

#### **Emergency numbers**

999 – Ambulance Service, Police, Fire Service

#### Some other useful information:

http://www.strath.ac.uk/visiting/

#### **Medical services**

Citizens of the EU receive free or reduced-cost state-provided health care cover with the European Health Insurance Card (EHIC) for medical treatment that becomes necessary while in UK: <a href="http://ec.europa.eu/social/main.jsp?catId=559">http://ec.europa.eu/social/main.jsp?catId=559</a>

#### **Telephone**

The international access code for the UK is +44.

#### **Time Zone**

The UK is in the Western Europe Time Zone which is Greenwich Mean Time Zone (GMT) is 1 hour ahead of Central European Time (CET-1).

#### **Tipping**

Prices shown in bars and restaurants always include tax. However, if you have appreciated the service, you may wish to leave a tip. This is usually around 10%.

#### **Tourist information**

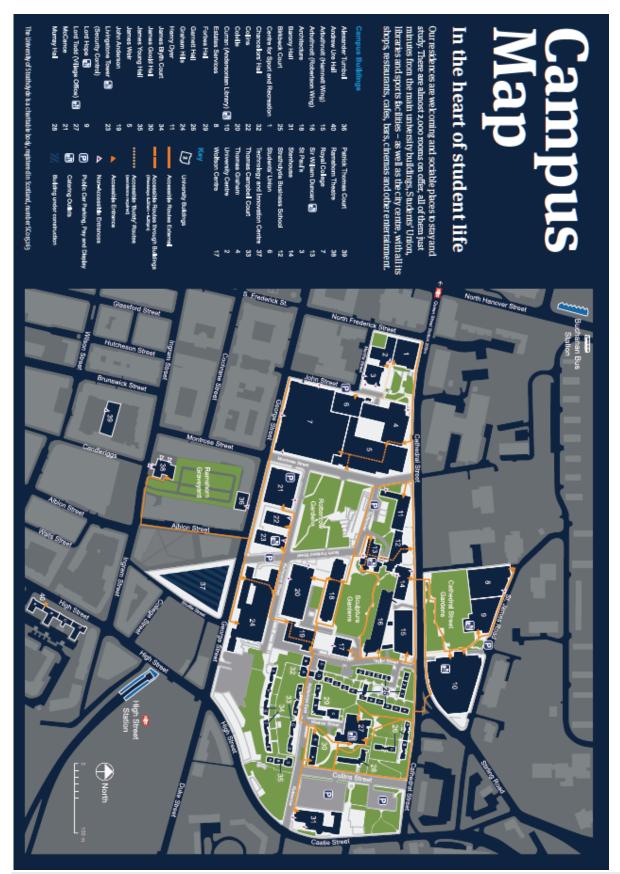
Tourist information can be found in the following location amongst others:

Glasgow Tourist Information Centre 10 Sauchiehall Street, Glasgow, G2 3GF info@visitscotland.com

Opening hours: Monday – Saturday: 9:00 am – 5:00 pm and Sunday 9:00am to <a href="http://www.visitscotland.com/info/services/glasgow-information-centre-p332751">http://www.visitscotland.com/info/services/glasgow-information-centre-p332751</a>

# **Appendix 4 - Campus Map**

You can download the mobile app version of the campus map: <a href="https://www.strath.ac.uk/studywithus/mobileapp/">https://www.strath.ac.uk/studywithus/mobileapp/</a> or print a PDF version: <a href="http://www.strath.ac.uk/media/stockmedia/maps/pdf/A4">http://www.strath.ac.uk/media/stockmedia/maps/pdf/A4</a> download map.pdf



# **Appendix 5 - Contact Details**

#### **CORE Network Coordinator:**

Prof. Joop H. ter Horst

**Industrial Crystallisation** 

EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation (CMAC)

Strathclyde Institute of Pharmacy and Biomedical Sciences (SIPBS)

Technology and Innovation Centre Level 6

University of Strathclyde

99 George Street, Glasgow G1 1RD, U.K.

Phone: +44 141 548 2858

Email: joop.terhorst@strath.ac.uk

#### **CORE Project Manager:**

Claire Lynch

EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation (CMAC)

Strathclyde Institute of Pharmacy and Biomedical Sciences (SIPBS)

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University of Strathclyde

99 George Street, Glasgow G1 1RD, U.K.

Phone: +44 141 444 7198 Email: <a href="mailto:claire.lynch@strath.ac.uk">claire.lynch@strath.ac.uk</a>

#### **CORE Social Platforms**



@coreitn



**CORE Innovative Training Network** 



**CORE Innovative Training Network** 



https://www.youtube.com/channel/UCDt01AAPIwIhFyv\_ng-LBMA



https://www.researchgate.net/project/CORE-European-Training-Network-on-Continuous-Resolution-and-Deracemization-of-Chiral-Compounds-by-Crystallization

We wish you a pleasant stay in Glasgow!

www.coreitn.eu