



Engineering and Physical Sciences Research Council



MoSMed CDT Newsletter

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Notes from the Editors

As the summer months approach, 2022 has seen a busy start to the year for all of our Doctoral Reseachers. Our newest cohort (cohort 3) are in full swing into their PhD studies, our first Mini MBA has taken place, recruitment for our 4th cohort is near completion and we have lots more to update you on from across the CDT. Following the postponement of the Annual MoSMed Conference in December due to Covid, we are pleased to announce that the Conference will now take place on the 12th and 13th July in Durham. Despite the ongoing challenges of Covid restrictions, our Doctoral Researchers are rising to the challenge yet again and a big congratulations goes to Toni Pringle on securing not one but two opportunities to deliver presentations at esteemed academic gatherings! Also congratulations to Jess Graham on her poster prize win! Scroll down to read more about what Toni and Jess have been up to. We hope that you enjoy reading about the activities and achievements taking place across the CDT. A special thanks goes to Olivia Gittins for her hard work in pulling together this edition of the newsletter, whilst juggling many work commitments alongside her third year of PhD study.

Olivia Gittins, Abbey Butler, Selina McCarthy & Emma Worden.



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MoSMed Annual Conference Rescheduled

Despite having to postpone the third MoSMed Annual Conference which was set to take place in December 2021, we are delighted that we are able to reschedule the Conference to Tuesday 12th and Wednesday 13th July in Durham. The Conference will be held at the Calman Learning Centre at Durham University and will include a Conference Dinner at the Radisson Blu hotel in Durham City. Watch this space for further details!

Cohort 3 - Foundations of Science Course

Cohort 3 (our first-year researchers) have so far undertaken three sessions of their Foundations of Science course at Durham University with Ehmke Pohl (Durham University). Due to the easing of Covid restrictions we were able to run these events in a hybrid model where most of the students were able to join in person and the others joined virtually.

Our researchers have enjoyed and benefitted hugely from the opportunity to be able to build their cohort and interact across institutions and lab groups while exploring a wide range of topics in the full-day workshops 'The Theory and Practice of Science' (22nd October), Responsible Innovation: Teamwork and Ethics (26th November) and Science Communication (21st January).

The 'Responsible Innovation' session included talks from Simon Rees (Durham Centre for Academic Development) on 'Creative Chemistry' and Mike Waring (Newcastle University) on 'Data analysis and decision making in drug discovery'. In addition to exploring the concepts presented, participating in discussions in these sessions our Researchers have worked in small groups to research, prepare and present their work on Fraud Squad cases. Presentations have included analysis of the Surgisphere Scandal, the controversy surrounding Andrew Wakefield's



Above: Cohort 3 in their Foundations of Science workshop

allegations of the links between the MMR vaccine and autism.

The session on 'Science Communication' included presentations on scientific publications as well as a talk on Outreach projects by Lara Small (Durham University). Students also presented their group work on one example of unethical behaviour of a company with significant societal consequences highlighting the notorious Thalidomide case by Gruenenthal which led to the stringent FDA test regime for new pharmaceuticals in place today. Researcher feedback has indicated that the students have enjoyed these opportunities to work as a group and to practice their presenting skills especially in light of the expectation of delivering a 3 minute flash presentation at the MoSMed Conference.

One student's thoughts on the course:

"I really enjoyed the latest session because it felt directly relatable to where we are all currently at the start of our career, especially the 'how to write a paper' presentation. No one ever actually teaches you how to write so for you to go through it step by step like that is really helpful!"

Our Cohort 3 Researchers have recently taken part in a Computational training session on 18th February at Durham. This addressed Computational Matters with Matteo Degiacomi (Durham University) and Agnieszka Bronowska (Newcastle University). Looking ahead we are awaiting confirmation whether a collaborative two day Statistics Workshop led by Procter & Gamble can go ahead later this year with the SOFI CDT (Durham University). In addition there will be a further one day session on ED&I to be delivered by experts in the field again at Durham University.



Launch of the MoSMed Podcast

By Kenneth Zhi Jian Tan (Cohort 2 Doctoral Researcher and MoSMed Comms Rep)

The MoSMed CDT communications working group are dipping their toes into podcasting as a new outreach platform! We hope to use the podcast as a means of sharing information about the CDT in a more casual style, be it about research projects, science in general, or life and events in the CDT.

A pilot episode was recorded on 11th October 2021 with our very own CDT Directors Mike and Ehmke, who gave us some insights into their research career and their goals for the CDT. The pilot episode will be available on the MoSMed website soon. We hope to record more episodes this year. If you have a topic that you would like to share with the CDT community, feel free to come by for a chat.



Guest Speaker: Dr Craig Johnstone – Evotec MoSMed talk and meet & greet!

On Thursday 20th January MoSMed CDT were thrilled to welcome Dr Craig Johnstone, COO of one of our industrial partners Evotec, to give a talk on "Creating conditions for recurring innovation".

Craig was appointed Chief Operating Officer of Evotec in 2019 after joining the company in 2012 as Head of Innovation Efficiency. He served in various roles during combining scientific drug discovery that time, leadership with operational effectiveness improvements within Global Chemistry and Global Drug Discovery functions. He is based in Toulouse, France, where he is the Site Head of one of Evotec's main integrated drug discovery sites, 750 hosting researchers.

Following the fantastic talk, Craig was kind enough to hold a Q&A session with MoSMed Doctoral



Researchers. This prompted some great discussion, such as navigating confidentiality and contractual obligations through Evotec's many collaborations while also trying to drive innovation through the coming together of new ideas. Craig also shared his experience of heading up the Toulouse site for Evotec back in 2015 and the expansion of the site over the following years.



New MoSMed Advisory Board Member! Introducing Anju Massey-Brooker

By Selina McCarthy – MoSMed CDT Manager (Newcastle University)

Professor in Practice Anju Massey-Brooker (FRSC)

MoSMed Advisory Board Member (EDI)

1) Can you tell us a bit about yourself and your professional background?

I am professional technologist and business leader with 28 years of experience in the Fast Moving Consumer Goods sector. This involved leading numerous product and technology innovation programmes, impacting several billion dollars of sales around the world and enabled Procter & Gamble's expansion into new markets, eg. Central and Eastern Europe and South American geographies.

Some of my acheivements throughout my career include:

- Winner of multiple innovation awards and listed as an Inventor on over 50 patents protecting these innovations.
- Over 20 peer reviewed publications.
- Winner and Project Coordinator for numerous multi-million €/£ Industry-Academia collaboration programmes.
- Immediate past, member of the EPSRC strategic Advisory Team for Physical Sciences and Strategic Advisory Network for Circular Economy.
- Previous Co-Leader of Equality Diversity & Inclusion European forum and several Community of Practice organisations within Procter & Gamble.

Since retirement in May 2021, I have been appointed to several Honorary positions, Professor in Practice at Durham University, Senior Research Fellow at University of Birmingham, E&I Advisor to EPSRC and have appointed Fellow of Royal Society of Chemistry. I now also work part time for the Royal Society of Chemistry leading a 15 member cross Industrial Task Force for Sustainable Polymers in Formulated Products.

2) You have recently joined the MoSMed Advisory Board to provide strategic advice in relation to Equality, Diversity and Inclusion (EDI). What does EDI mean to you?

Becoming a voice of influence and change for better for those who are marginalised, underrepresented and vulnerable.

3) What do you see as the big EDI challenges/opportunities within research and scientific communities?

- Support and Empowerment of underrepresented groups.
- Equal opportunities for everyone
- Inclusion of everyone as Agent of Change for a Better and Inclusive society and workplace

4) What are you most looking forward to in your new role on the MoSMed Advisory Board?

- Becoming a voice of Influence for does individuals and demographic groups most marginalised
- Bringing my experience as a BAME scientist to support, role model to encourage younger aspiring BAME student to have successful and fulling careers in STEM.
- Making E&I an organisational and Instituational Strategy for a more inclusive and fairer environment to work and flourish in.
- Sharing my nearly 30 years of E&I experience, some in leadership roles to guide equal opportunities for everyone.

Thank you to Anju for telling us a bit about herself, and welcome to MoSMed CDT - we're thrilled to have you!





Good News Stories!

Toni Pringle delivers presentations at two esteemed academic gatherings in December



MoSMed Doctoral Researcher Toni Pringle (third-year, Cohort 1) secured two highly esteemed and competitive opportunities to present her work on development of а dual-labelled antibody

imaging agent that is capable of selectively targeting sarcoma cells in vivo.

The first of these oral presentations took place on the 2nd December at the 'Bridging Chemical Biology and Cancer Research' conference which was jointly held by the RSC Chemical Biology & Bio-organic Group and the British Association for Cancer Research. Her talk outlined her exciting research focused on the development of new PET/NIR probes for imaging sarcoma. Toni was one of only 4 PGRs to present her work at this two-day event that featured a star-studded line up of distinguished experts in chemical biology and cancer research. Among the other speakers at the event were MoSMed supervisors Professor Akane Kawamura and Dr Kate Madden.

In addition, on 10th December, Toni was invited to give an oral presentation at the RSC Biological & Medicinal Chemistry postgraduate symposium.

We asked Toni to tell us about her experience of speaking at these events:

"It was a great experience being able to present my most recent work alongside some truly great speakers and feel a sense of community within Med Chem/ Chem Bio. I am really looking forward to potentially attending some in person conferences in the near future!"



Pictured left: Graphical abstract of Toni's talk. To find out more about Toni's work or contact her about her talk, visit her student profile page on the MoSMed website:

https://research.ncl.ac.uk/m osmed/people/students/coh ort12019-

present/tonialexandrapringl e.html



Jessica Graham wins poster prize at RSC BMCS Postgrad Symposium



Congratulations are also in order Jessica Graham (third-year, Cohort 1) who won the 'People's Choice' poster award at the 15th Royal Society of Chemistry Biological and Medicinal Chemistry Postgraduate Symposium!

The virtual meeting featured oral and poster presentations from PhD students and postdoctoral workers researching in biological or medicinal chemistry, as well as talks by invited keynote speakers from industry and academia. We asked Jess how she found the experience:

"I had a great time presenting my research at the RSC BMCS postgraduate symposium in December. This was the first time I've presented at an external conference and it was an excellent showcase of some fantastic research that is ongoing across the field of biological and medicinal chemistry. I had some really interesting discussions with people from a variety of backgrounds, who had some refreshing insights into my current and future work."

Highly Efficient Buchwald-Hartwig Coupling of Arylamines for DNA-Encoded Library Synthesis



Pictured left: Introductory section of Jess' poster. To view the whole poster/chat to Jess about her work please see the email address provided on her poster or visit Jess' student profile page on the MoSMed website: https://research.ncl. ac.uk/mosmed/peop le/students/cohort12 019present/jessicagrah am.html

Double Success!

Katie Gristwood and Toni Pringle have each won Travel Awards to present their research at the International Symposium on Radiopharmaceutical Sciences (ISRS) being held in Nantes, France this summer. The ISRS is a high-profile international conference that



brings together experts in radiochemistry, imaging, and clinical translation. Katie and Toni are working with Dr James Knight to develop new oncological radiotracers for positron emission tomography and secondary Cerenkov-induced fluorescence imaging.

Congratulations to you both! We look forward to hearing about your experiences at the conference in the summer.



Recent Publications from MoSMed

Riemannian Geometry and Molecular Surfaces I: Spectrum of the Laplacian

Daniel J. Cole, Stuart J. Hall, Rachael Pirie (Pre-print, available at:

https://www.researchgate.net/publication/35779 1355 Riemannian Geometry and Molecular Surfaces_I_Spectrum_of_the_Laplacian)



Figure 3: Key steps involved in the computation of our shape descriptor using Sildenafil as an example.

Abstract: Ligand-based virtual screening aims to reduce the cost and duration of drug discovery campaigns. Shape similarity can be used to screen large databases, with the goal of predicting potential new hits by comparing to molecules with known favourable properties. This paper presents the theory underpinning RGMoISA, a new alignment-free and mesh-free surface-based molecular shape descriptor derived from the mathematical theory of Riemannian geometry. The treatment of a molecule as a series of intersecting spheres allows the description of its surface geometry using the Riemannian metric, obtained by considering the spectrum of the Laplacian. This gives a simple vector descriptor constructed of the weighted surface area and eight non-zero eigenvalues, which capture the surface shape. We demonstrate the potential of our method by considering a series of PDE5 inhibitors that are known to have similar shape as an initial test case. RGMoISA displays promise when compared to existing shape descriptors and in its capability to handle different molecular conformers.

Micellar Buchwald–Hartwig Coupling of Aryl and Heteroarylamines

for the Synthesis of DNA-Encoded Libraries

Jessica S. Graham, James H. Hunter, and Michael J. Waring The Journal of Organic Chemistry 2021 86 (23), 17257-17264 DOI: 10.1021/acs.joc.1c02325

Abstract: DNA-encoded libraries are a verv efficient means of identifying ligands for protein targets in high throughput. To fully maximize their use, it is essential to be able to carry out efficient reactions on **DNA-conjugated** substrates. Arylamines are privileged motifs in druglike molecules, and methods for their incorporation into DNA-encoded libraries are highly desirable. One of the preferred methods for their preparation, the Buchwald-Hartwig coupling, does not perform well on DNA conjugates using current approaches. We report the application of our recently developed micellar technology for on-DNA chemistry to the Buchwald-Hartwig reaction. Optimization of conditions led to a robust, high-yielding method for the synthesis of DNA-conjugated aryl and heteroarylamines, which is broad in substrate scope for both the arylamine and the DNA-conjugated aryl halide and is fully compatible with DNA-encoding and decoding procedures. This method will enable the preparation of diverse, high-fidelity libraries of biarylamines.



Be featured in our next issue!

We want to promote all of the fantastic work being carried out by CDT Doctoral Researchers, academics and industrial partners. Email <u>mosmed.cdt@ncl.ac.uk</u> with your news!



On-DNA Transfer Hydrogenolysis and Hydrogenation for the Synthesis of DNA-Encoded Chemical Libraries

Harriet. A. Stanway-Gordon, Jessica. S. Graham, Michael. J. Waring Angewandte Chemie. 2022, 61 (3) DOI: https://doi.org/10.1002/anie.202111927

Graphical Abstract:

A catalytic hydrogen transfer reaction using Pd/C, HCONH4 and the micelle-forming surfactant, TPGS-750-M for hydrogenolysis of Cbz-protected amines and benzyl protected alcohols and hydrogenation of alkenes, alkynes, nitros, nitriles, halides and aldehydes of DNA-conjugated substrates is described. The methodology is fully compatible with DNA-amplification and sequencing, demonstrating its applicability to DEL synthesis. This method will enable synthetic DEL sequences using orthogonal protecting groups



Abstract: DNA-encoded libraries (DELs) are an increasingly popular approach to finding small molecule ligands for proteins. Many DEL synthesis protocols hinge on sequential additions of monomers using split-pool combinatorial methods. Therefore, compatible protecting group strategies that allow the unmasking of reactive functionality (e.g. amines and alcohols) prior to monomer coupling, or the removal of less desirable functionality (e.g., alkenes and alkynes) are highly desirable. Hydrogenation/hydrogenolysis procedures would achieve these ends but have not been amenable to DEL chemistry. We report a catalytic hydrogen transfer reaction using Pd/C, HCONH4 and the micelle-forming surfactant, TPGS-750-M, which gives highly efficient conversions for hydrogenolysis of Cbzprotected amines and benzyl protected alcohols and hydrogenation of nitros, halides, nitriles, aldehydes, alkenes and alkynes. Application to multicycle synthesis of an encoded compound was fully compatible with DNA-amplification and sequencing, demonstrating its applicability to DEL synthesis. This method will enable synthetic DEL sequences using orthogonal protecting groups.

Scope of on-DNA nucleophilic aromatic substitution on weakly-activated heterocyclic substrates for the synthesis of DNA-encoded libraries

Isaline F.S.F. Castan, Andrew Madin, Garry Pairaudeau, Michael J. Waring Bioorganic & Medicinal Chemistry. 2022, 116688 DOI: https://doi.org/10.1016/j.bmc.2022.116688

Graphical Abstract:



Abstract:

DNA-Encoded Libraries (DEL) represent a promising hit finding strategy for drug discovery. Nonetheless, the available DNAcompatible chemistry remains of limited scope. Nucleophilic aromatic substitution (SNAr) has been extensively used in DEL synthesis but has generally been restricted to highly activated (hetero)arenes. Herein, we report an optimised procedure for of the SNAr reaction through the use of factorial experimental design (FED) on-DNA using 15% THF as a cosolvent. This method gave conversions of > 95% for pyridine and pyrazine scaffolds for 36 secondary cyclic amines. This analysis provides a new DNA-compatible SNAr reaction to produce high yielding libraries. The scope of this reaction on other amines is described. This work identifies challenges for the further development for DNA-compatible SNAr reactions.



Fig. 1. Schematic representation of a DNAencoded library synthesis.

Structure and assembly of the S-layer in C. difficile

Lanzoni-Mangutchi, P., Banerji, O., Wilson, J. et al. Nat Commun (2022) 13, 970. DOI: https://doi.org/10.1038/s41467-022-28196-w

Abstract: Many bacteria and archaea possess a two-dimensional protein array, or S-layer, that covers the cell surface and plays crucial roles in cell physiology. Here, we report the crystal structure of SIpA, the main S-layer protein of the bacterial pathogen Clostridioides difficile, and use electron microscopy to study S-layer organisation and assembly. The SlpA crystal lattice mimics S-laver assembly in the cell. through tiling of triangular prisms above the cell wall, interlocked by distinct ridges facing the environment. Strikingly, the array is very compact, with pores of only ~10 Å in diameter, compared to other S-layers (30-100 Å). The surface-exposed flexible ridges are partially dispensable for overall structure and assembly, although a mutant lacking this region becomes susceptible to lysozyme, an important molecule in host defence. Thus, our work gives insights into S-layer organisation and provides a basis for development of C. difficile-specific therapeutics.



Image created by Newcastle-based science Artist and Science Communicator, Dr. Lizah van der Aart.

This work by MoSMed supervisor Dr Paula Salgado's group based at Newcastle University, in collaboration with researchers from several other institutions, provided an exciting breakthrough in understanding how the S-layer, could contribute to C. difficile antibiotic and immune resistance. As such it has received a lot of media attention:

https://www.newscientist.com/article/2309517antibiotic-resistant-superbug-has-a-proteincoat-like-chain-mail/#ixzz7NcCgrmrm

Dr Salgao also wrote a blog post about their publication which you can read here: https://salgadolab.org/blog/3_slayer_ps/

International Womens Day Celebrations!

8th March 2022 marked International Womens Day, and what better way to celebrate women in science in particular than to hear from our very own Professor Akana Kawamura about her experiences and career as an esteemed female academic. Akane's talk promted some great discussions around navigating life as an academic and a mum, the importance of having a good support network around you and having the confidence to embrace opportunities no matter how scary they may seem! A big thank you to Akane for a fantastic and thought provoking session.

(Pictured below are Akane's group (left) and the MoSMed cohorts and management (right) showing support for the 'Break the Bias' campaign)



Molecular Sciences for Medicine Newsletter 9



MoSMed Book and Film Club

Recently a 'Book and Film Club' channel was added to the MoSMed Cohort Teams page. This allows our doctoral researchers and management board members to share thoughts or recommendations on anything from TV Series' and Films to books and podcasts. So far this has promtped some really great reviews and discussions, so we thought why not share some of those here in the Newsletter!

Book: Vaxxers – Professor Sarah Gilbert and Dr Catherine Green *Recommended by: Emma Worden (CDT Manager – Durham)*

"This gives a fascinating insight into the process behind the development and distribution of the vaccine as well as the human element of the individuals involved in the process in responding to the inevitable highs and lows of such a unique situation when politics, science and economics collide."





Documentary Film: Picture a Scientist

Recommended by: Isaline Castan (Cohort 1 Doctoral Researcher)

"Definitely a great documentary on women in science and easy to watch too!"

This recommendation from Isaline prompted other cohort members to watch and share their thoughts....

"Finally got around to watching picture a scientist! Thanks for the recommendation Isaline. Very eye opening as a woman in science and would love to hear what others thought about it (men and women)!" – *Jess Graham*

"I also watched the Picture A Scientist documentary recently. I thought it was a great documentary, but like Jess said it was very eye opening to see that women in science were not just overlooked but were also targeted for abuse too. I liked that the documentary ended on a more positive note by looking at the wave of change that is already happening. As a guy, it made me want to strive to more to actively combat these attitudes in academia." – *Alex Hallatt*





DeepMind: The Podcast

Recommended by: Olivia Gittins (Cohort 1 Doctoral Researcher)

"I binged the first season of this podcast and am currently hooked on the second! I would highly recommend for anyone who is interested in Artificial Intelligence but doesn't have a computational background. Not only do you learn about advances in AI in an accessible way, the podcast also challenges you to consider how the world will look as AI research continues to advance."



MoSMed Christmas Social!

By Jess Graham (Cohort 1 Doctoral Researcher and Social Rep)

In December, we were delighted to be able to arrange the first in person social for the MoSMed doctoral researchers. Despite some last minute venue changes due to a certain storm, it was great to get the majority of students together at Fab's bar in Durham. This coincided with Durham DJ society having a session at Fab's, so we were lucky to be serenaded with their music for the evening. The evening was a fab excuse to get the three cohorts together for the first time, topped off with a yummy selection of pizzas and pastas. We're hoping to get the next one arranged in Newcastle soon, so keep your eyes peeled for what we get up to then!



New Modalities in Modern Chemical Biology Seminar Series

A new MoSMed seminar series in underway, organised by Dr Chiara Maniaci (BBSRC discovery fellow based within the School of Natural and Environmental sciences, Newcastle University) and assisted by Siddique Amin (Cohort 2 Doctoral Researcher).

The series, entitled 'New Modalities in Modern Chemical Biology' has so far featured several excellent talks including;

- Professor Ben Cravatt from the Scripps Research Institute, California: "Development of activity based probes and their applications"
- Prof Stuart Conway from University of Oxford: "Publishing process from the perspective of an Editor"
- Professor Alessio Ciulli from the University of Dundee: "Targeted protein degradation (PROTACs)"

Following each seminar is a "Meet the Speaker" informal gathering where MoSMed students have the opportunity to network and learn more from top academics. The series has been an enormous success so far – a big thanks to Dr Maniaci for organising this!



Pictured above: Meet the speaker session at the Crows Nest pub on Newcastle University campus.



News and Updates



Current trends in macromolecular model refinement and validation

5th-7th January

Cohort 3 Doctoral Researcher **Victoria Burge** put together a brilliant account of her expereince of the CCP4 Study Weekend as a 1st year PhD student for her Lab's blog.

"The talk that inspired me most was 'Picture a programmer' where Prof. Kevin Cowtan explored equality, diversity and inclusion (EDI) within research and the barriers to inclusion through social stereotypes that many hadn't considered." Check out the full blog post here:

https://salgadolab.org/blog/ccp4sw2022_vic/

EDI Feedback session

MoSMed doctorial researchers across all cohorts were invited to participate in an EDI Feedback Session at Newcastle University, giving them the opportunity to share ideas about and experiences of the MoSMed CDT. The session prompted some excellent discussions around research culture and values, career goals and advancement, and wellbeing support. Feedback from this session will help ensure continuous development of the CDT. We would encourage all MoSMed students to look out for future opportunities to take part in EDI related activities and feedback sessions.

MoSMed recuitment for the 4th cohort of CDT doctoral researchers!

Since January we have been busy recruiting our fourth Cohort of Doctoral Researchers to start in September/ October 2022. We have 15 fully funded studentships at Newcastle and Durham Universities. We have two projects still out to advert, please help to promote these opportunities to anyone that may be interested. For details visit: <u>PhD Studentships | MoSMed CDT | Newcastle University (ncl.ac.uk)</u>

Exciting Training Opportunity

Mini MBA course:

The MiniMBA course took place at Durham University from 28th March until 8th April. This course was led by Peter Allen who is an MBA programme director from the Durham Business School. This exciting training opportunity was offered to our second and third year Researchers. The two week full time course featured an innovation challenge whereby our researchers worked in small teams to develop and test a business idea to respond to the healthcare challenges of a post-pandemic world. These business ideas were then pitched to a panel of experts at the end of the two week period of interactive workshops. Having completed the training and challenge activities our researchers have now been offered the opportunity to undertake assessment for a Level 7 Award from the Chartered Institute of Management in 'Strategic Management and Leadership Practice'. We look forward to sharing the highlights of this course with you in the next edition of our Newsletter.

Find us online: www.research.ncl.ac.uk/mosmed Follow us on Twitter: @MosmedC Follow us on Instagram: @mosmed.cdt Please get in touch with any feedback and suggestions to: mosmed.cdt@ncl.ac.uk







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