

EFEPR 2025 Summer School Handbook

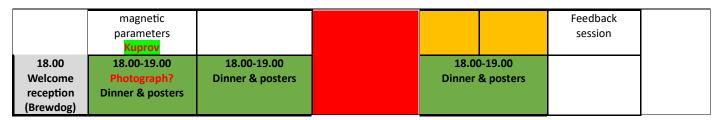


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Sunday 31 /08	Monday 1/09	Tuesday 2/09	Wednesday 3/09	Thursday 4/09		Friday 5/09	Saturday 6/09
·	09.00 Lecture 1: Basics of electron spin and cw EPR Klose 10.00 Lecture 2: Intro to the spin Hamiltonian di Valentin	09.00 Lecture 9: Basics of pulsed EPR Garcia-Rubio 10.00 Lecture 10: s-H: time dependent Schrodinger, density matrix, POF Timme	09.00 Lecture 16: Pulsed Dipolar Spectroscopy Theory and DEER/PELDOR Bordignon 10.00 Lecture 17: Dipolar modelling Lovett	09.00 Worksho p 1	09.00 Demonstr ation 1 10.00 Demonstr ation 2	09.00 Lecture 20: AWG Pulse shaping: why and how Jeschke 9.45 Lecture 21: Biology Pliotas 10.30 Lecture 22: Catalysis Richards	Departure
	11.00 coffee	11.00 coffee	11.00 coffee	11.00) coffee	11.15 coffee	
	11.30 Lecture 3: Interpretation of s- H parameters McInnes 12.30 Lecture 4: EasySpin 1: the spin system and CW EPR Stoll	11.30 Lecture 11: Relaxation: measurement & mechanisms Jeschke 12.30 Lecture 12: ESEEM methods Mitrikas	11.30 Lecture 18: Dipolar Methods: RIDME, CIDME, SIFTER/DQC Schiemann 12.30 Lecture 19: Lab safety briefing. On- line demo: pulsed set up, incl. Hahn echo, T _{1/2} Bowen	11.30 Worksho p 2	11.30 Demonstation 3 12.30 Demonstration 4	11.45 Lecture 23: QIS Ardavan 12.30 Lecture 24: Light-induced EPR (transient, pulsed) Richert	
	13.30 Lunch (IT Help)	13.30 Lunch (IT Help)	Free time (IT Help)	13.30) Lunch	13.15 Lunch	
	14.30 Lecture 5: CW instrumentation Kaminker 15.15 Lecture 6: Accessories to CW EPR Liao 15.45 Lecture 7: Multi- frequency EPR Collison	14.30 Lecture 13: Pulsed ENDOR methods Bennati 15.30 Lecture 14: EasySpin 2: pulsed hyperfine Stoll		14.30 Worksho p 3	14.30 Demonstr ation 5 15.30 Demonstr ation 6	14.15 Lecture 25: Paramagnetic NMR & links to EPR Novikov 15.00 Lecture 26: DNP Will 15.45 Lecture 27: EDMR Tait	
	16.30 Coffee	16.30 Coffee		16.00 Coffee	16.30 Coffee	16.30 Coffee??	
	17.00 Lecture 8: Electronic structure theory of	17.00 Lecture 15: Instrumentation: pulsed Kaminker		16.30 Worksho p 4	17.00 Demonstr ation 7	17:00 Lecture 28: open session on publishing 17.30	





Introduction from Organising Committee

- Welcome to the 10th EFEPR Summer School
- We hope you have a great time.
- So many institutions and countries...
- Foster collaboration/ideas/....

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Programme

Insert programme once confirmed



Sponsors

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Social Programme

Free afternoon on Wednesday

Manchester has many cultural, architectural, historic, sporting and leisure attractions – too many to list here. The city centre is only around 1 mile from the conference venue, so easily reachable by foot or bus.

Have a look at the following websites for suggestions:

Visit Manchester

The University of Manchester - City Guide

Free things to do in Manchester

The following are some of our favourite attractions:

The John Rylands Library: The historic University library holds one of the finest collections of rare books, manuscripts, and archives in the world. It is located on Deansgate, in the heart of the city centre, and worth visiting even for the building itself: one of the finest examples of neo-Gothic architecture in Europe.

<u>Manchester Museum</u>: The museum is a few minutes' walk from the conference venue, at the heart of the University's neo-Gothic buildings. It is the largest university museum in the UK, with extensive exhibits on archaeology, anthropology and natural history, including Stan the *T. Rex*.

Whitworth Art Gallery: Also a short walk from the conference venue, this University-owned gallery has collections of historic fine art, modern and contemporary art, prints and textiles. At the time of the conference there will be a special exhibition on the work of the artist J. M. W. Turner.

<u>Science and Industry Museum</u>: Well worth a visit if you enjoy your history of science, technology and industry, with a focus on Manchester's many contributions. It is located in the city centre.

Some other ideas

Imperial War Museum North, Salford Quays and MediaCityUK National Football Museum Old Trafford (Manchester United Football Club) Etihad Stadium (Manchester City Football Club)



Manchester Town Hall (unfortunately shut for refurbishment, but still a magnificent building) and Albert Square

Manchester Central Library, and St Peter's Square

The Northern Quarter and nearby areas (for hipster types and the best craft breweries in the land).

- Map of Manchester and general information
- AMBS map and how to get to labs (PSI, MIB and Michael Smith building)

Emergency Contact details

Adam Brookfield phone number: -

Liz Fleming phone number: - +441515293788

Email: firstname.secondname@manchester.ac.uk

EPR Service staff:

Prof David Collison (co-Director) – DC
Prof Eric McInnes (co-Director) – EJLM
Dr Alice Bowen (Dame Kathleen Ollerenshaw Fellow) - AMB
Dr Murali Shanmugam (SEO) - MS
Mr Adam Brookfield (RTP) – AdB
Mrs Elizabeth Fleming (Administrative Support) – LF

Other Useful Phone Numbers :-

AMBS Reception +44161 3056303 Campus Security +44161 306 9966 – they can be contacted 24/7 Emergency Services 999 (Police/Ambulance/Fire Brigade

Posters - include Abstracts

Probing Cgn Protein Complex Interactions by EPR Spectroscopy J.L. Wort, a K.P. Patel, b J. Koehnke, b C. Pliotas a*

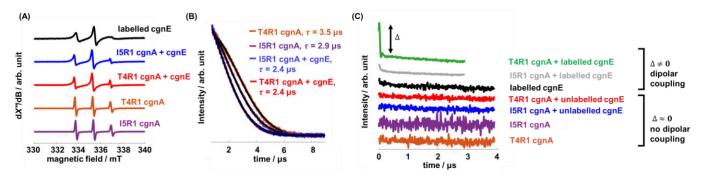


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Ribosomally synthesized and post-translationally modified peptides (RiPPs) are a diverse class of natural products, often with novel chemical modifications, which are appealing lead compounds towards therapeutic agents. One burgeoning class of RiPPs are the crocagins – first observed in the *cgn* biosynthetic gene cluster (BGC) of *Chondromyces Crocatus* – these pyrroloindoline alkaloids are synthesized from the immature peptide cgnA. Promisingly, crocagin A has demonstrated inhibitory activity for the carbon storage regulator CsrA, a global regulator of bacterial transcription, motivating a greater understanding of cgnA maturation into crocagin A. This process minimally involves several proteins (cgnB, cgnC, cgnE, and cgnD), in either a concerted (simultaneous) or sequential binding-mode, however the mechanism of biosynthesis is unclear.



EPR spectroscopy probes cgn protein interactions: (A) CW-EPR spectra of cgnA constructs ± unlabeled WT cgnE. (B) ESEEM measurements of cgnA constructs ± unlabeled cgnE. (C) PELDOR measurements of cgnA constructs and (un)labeled cgnE.

Using a suite of EPR methods, including continuous-wave (CW), electron spin echo envelope modulation (ESEEM), and pulse electron-electron double resonance (PELDOR) spectroscopy, we demonstrate that T4R1 and I5R1 cgnA constructs: (i) are competent to bind wildtype cgnE (via CW-EPR and ESEEM measurements), and (ii) bind monomeric cgnE with 1:1 stoichiometry (via PELDOR measurement modulation depths (Δ)). Additionally, PELDOR measurements of T4R1 cgnA and labeled wildtype cgnE (C160R1) provide agreement with *in-silico* distributions from a docked cgnA:cgnE structure. Taken together, these data provide a roadmap to investigate interactions of other *cgn* BGC members, characterize stoichiometry, and supply distance restraints for protein complex structural modelling.

References

- 1. K.J. Hetrick, and W.A. Van der Donk, *Curr. Opin. Chem. Biol.*, 2017, **38**, 36.
- 2. K. Viehrig, F. Surup, C. Volz, J. Herrmann, A. Abou Fayad, S. Adam, J. Köehnke, D. Trauner, and R. Müller, *Angew. Chem. Int. Ed.*, 2017, **56**, 7407.
- 3. S. Adam, D. Zheng, A. Klein, C. Volz, W. Mullen, S.L. Shirran, B.O. Smith, O.V. Kalinina, R. Müller, and J. Köehnke, *Nat. Chem.* 2023, **15**, 560.