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Summary

Biography

Following my degree in medical biochemistry I gained a PhD in enzymology, both at Bristol University, with Professors John Holbrook and Anthony Clarke. I spent my first post-doc combining enzymology with structural biology and mutagenesis to further explore enzyme structure and function. I then moved into drug discovery programmes as a molecular modeller involving Trks A and B and the neurotrophins. This work was targeting pain management (in the periphery) and Alzheimer's disease (centrally). Following that I worked with the MRC Prion Unit and identified compounds capable of stabilizing the human prion protein with low micromolar affinity towards a treatment for Creutzfeld Jacob's disease. This was achieved using the Bristol University Docking Environment (BUDE) software written by Dr Richard Sessions, for which I had beta tested the release version and compiled tutorials and user manual. I then "side-lined" for a while setting up the beginnings of what I hope will lead to clinical trial to see whether targeting oral bacteria in the mouths of patients with mild Alzheimer's helps to slow disease progression. This was set up as a result of the compelling circumstantial evidence linking oral health to Alzheimer's. I myself and others had also found direct evidence of oral bacteria in samples taken post mortem from the brains of elderly donors.

I have now moved back into the arena of molcular modelling. In particular I am using atomistic molecular modelling methods to explore the sequence/structure relationships in nanoparticles including self-assembling peptide cages (SAGES).

Memberships

Organisations

School of Biochemistry

Other sites

- Brissynbio

Recent publications

- Oliveira, ASF, Shoemark, DK, Campello, HR, Wonnacott, S, Gallagher, T, Sessions, RB & Mulholland, AJ, 2019, 'Identification of the Initial Steps in Signal Transduction in the α4β2 Nicotinic Receptor: Insights from Equilibrium and Nonequilibrium Simulations'. *Structure*, vol 27., pp. 1171-1183.e3
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- Draper, GW, Shoemark, DK & Adams, JC, 2019, 'Modelling the early evolution of extracellular matrix from modern Ctenophores and Sponges'. *Essays in Biochemistry*, vol 63., pp. 389-405

- Shoemark, D, Ziegler, B, Watanabe, H, Strompen, J, Tucker, RP, Ozbek, S & Adams, J, 2019, 'Emergence of a Thrombospondin Superfamily at the Origin of Metazoans'. *Molecular Biology and Evolution*, vol 36., pp. 1220-1238
- Smith, A, Thomas, F, Shoemark, D, Woolfson, D & Savery, N, 2019, 'Guiding Biomolecular Interactions in Cells Using de Novo Protein - Protein Interfaces'. *ACS Synthetic Biology*, vol 8., pp. 1284-1293
- Campello, HR, Villar, SGD, Honraedt, A, Viñas, TM, Oliveira, S, Ranaghan, K, Shoemark, D, Bermudez, I, Gotti, C, Sessions, R, Mulholland, A, Wonnacott, S & Gallagher, T, 2018, 'Unlocking Nicotinic Selectivity via Direct C■H Functionalization of ()-Cytisine'. *Chem*, vol 4., pp. 1710-1725
- Lalaurie, CJ, Dufour, V, Meletiou, A, Ratcliffe, S, Harland, A, Wilson, O, Vamasiri, C, Shoemark, DK, Williams, C, Arthur, CJ, Sessions, RB, Crump, MP, Anderson, JL & Curnow, P, 2018, 'The de novo design of a biocompatible and functional integral membrane protein using minimal sequence complexity'. *Scientific Reports*, vol 8.
- Wyatt, R, Brigatti, C, Liberati, D, Grace, S, Gillard, B, Long, A, Marzinotto, I, Shoemark, D, Chandler, K, Achenbach, P, Gillespie, K, Piemonti, L, Lampasona, V & Williams, A, 2018, 'The first 142 amino acids of glutamate decarboxylase do not contribute to epitopes recognized by autoantibodies associated with Type 1 diabetes'. *Diabetic Medicine*, vol 35., pp. 954-963
- Shoemark, D, Sessions, R, Brancaccio, A & Bigotti, MG, 2018, 'Intraring allostery controls the function and assembly of a hetero-oligomeric class II chaperonin'. *FASEB Journal*, vol 32., pp. 2223-2234

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