

# Publications

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## 2025

Harms, C., **Nash, A.**, et al. The collagen substrate changes matrix metalloprotease-1 dynamics and ligand binding affinity – bioRxiv 2025.02.08. 637235.

**Under review with Biophysical Journal**

## 2024

Harlow, C. E., **Nash, A.**, et al. GWAS of Extended Prescription Analgesic Use Identifies Novel Genetic Loci in Chronic Pain - medRxiv 2024.12.

**Second review after reply to Reviewers. Nature Communications**

## 2022

Kamboj, S., Harms, C., Wright, D., **Nash, A.**, et al. Identification of allosteric fingerprints of alpha-synuclein aggregates in matrix metalloprotease-1 and substrate-specific virtual screening with single molecule insights. 2022. Scientific Reports 12 (1), 5764.

## 2021

**Nash, A.**, et al. Lysine-arginine advanced glycation end-product cross-links and the effect on collagen structure: A molecular dynamics study. 2021. Proteins: Structure, Function, and Bioinformatics 89 (5), 521-530.

Kamboj, S., Harms, C., Wright, D., **Nash, A.**, et al. Quantification of allosteric communications in matrix metalloprotease-1 on alpha-synuclein aggregates and substrate-dependent virtual screening. 2021. BioRxiv.

**Nash, A.**, et al. Rdrugtrajectory: An R Package for the Analysis of Drug Prescriptions in Electronic Health Care Records. 2021. BioRxiv.

## 2020

**Nash, A.**, et al. Concurrent comorbidities substantially alter long-term health behaviours and outcomes of headache patients. 2020. MedRxiv.

**Nash, A.**, et al. Extraction of CPRD additional clinical data using R. 2020. F1000Research 9 (1124), 1124.

Kumar, L., **Nash, A.**, et al. Allosteric communications between domains modulate the activity of matrix metalloprotease-1. 2020. Biophysical Journal 119 (2), 360-374

Pokhilko, A., **Nash, A.**, et al. Common transcriptional signatures of neuropathic pain. 2020. Pain 161 (7), 1542-1554.

Noh, S. Y., **Nash, A.**, et al. The aggregation of striped nanoparticles in mixed phospholipid bilayers. 2020. Nanoscale 12 (8), 4868-4881.

## 2019

**Nash, A.**, et al. Glucosepane is associated with changes to structural and physical properties of collagen fibrils. 2019. *Matrix Biology Plus* 4 (100013).

**Nash, A.**, et al. Using longitudinal real-world electronic healthcare records to study long-term outcomes in headache sufferers. 2019. *Cephalgia* 39, 43-43.

Shrestha, R., Khatiwada, R., **Nash, A.** A molecular dynamics study in structural dynamics of a V717I substitution in the Amyloid precursor. 2019. Proceedings of the first international conference on advances in nanomaterials and devices for energy and environment.

**Nash, A.**, et al. A P system model of swarming and aggregation in a Myxobacterial colony. 2019. *Journal of Membrane Computing*, 1-9.

Collier, T. A., **Nash, A.**, et al. Relative orientation of collagen molecules within a fibril: a homology model for homo sapiens type I collagen. 2019. *Journal of Biomolecular Structure and Dynamics* 37 (2), 537-549.

## 2018

Richards, L., **Nash, A.**, et al. A Molecular Dynamics Study of Plasticiser Migration in Nitrocellulose Binders. 2018. *New Journal of Chemistry* 42, 17420-17428.

**Nash, A.**, et al. MARDY: Mycology Antifungal Resistance Database. 2018. *Bioinformatics* 34 (18), 3233-3234.

**Nash, A.**, et al. Headache and type 2 diabetes association: a US national ambulatory case-control study. 2018. *BioRxiv*.

**Nash, A.**, et al. Simulations of CYP51A from Aspergillus fumigatus in a model bilayer provide insights into triazole drug resistance. 2018. *Medical Mycology* 56 (3), 361-373.

Collier, T. A., **Nash, A.**, et al. Effect on the mechanical properties of type I collagen of intra-molecular lysine-arginine derived advanced glycation end-product cross-linking. 2018. *Journal of Biomechanics* 67, 55-61.

Farrer, R. A., **Nash, A.**, et al. Genome sequencing reveals infection mechanisms for two amphibian-infecting chytrid species. 2018. *Medical Mycology* 56 (suppl. 2), S7-S7.

Richards, L. A., **Nash, A.**, et al. Modelling water diffusion in plasticizers: development and optimisation of a force field for 2,4-dinitroethylbenzene and 2,4,6-trinitroethylbenzene. 2018. *RSC Advances* 8 (11), 5728-5739.

**Nash, A.**, et al. ForceGen: atomic covalent bond value derived for Gromacs. 2018. *Journal of Molecular Modeling* 24 (5).

## 2017

Ahmed, T., **Nash, A.**, et al. Combining nano-physical and computational investigations to understand the nature of “ageing” in dermal collagen. 2017. *International Journal of Nanomedicine* 12, 3303-3314.

**Nash, A.**, et al. Parameterisation of advanced glycation end-products and a thermodynamic exploration of glucosepane cross-linked collagen packing. 2017. Autumn Meeting of the British-

Society-for-Matrix-Biology (BSMB) - The Art of Communication-Signalling Cascades in Mechano transduction.

**Nash, A.**, et al. Mapping Intermolecular Interactions and Active Site Conformations: from Human MMP-1 Crystal Structure to Molecular Dynamics Free Energy Calculations. 2017. Journal of Biomolecular Dynamics 35 (3), 564-573.

## 2016

**Nash, A.**, et al. A toolset for the parameterisation of advanced glycation end-products: a thermodynamic investigation of cross-linked collagen packing. 2016. Spring Meeting of the British-Society-for-Matrix-Biology (BSMB) on Grey Area-Age and the Extracellular Matrix.

Collier, T. A., **Nash, A.**, et al. A comparison of preferential sites for glucosepane and DOGDIC formation in fibrillar type I collagen - an all-atom molecular dynamics study. 2016. Spring Meeting of the British-Society-for-Matrix-Biology (BSMB) on Grey Area-Age and the Extracellular Matrix.

Collier, T. A., **Nash, A.**, et al. Intra-molecular Lysine-Arginine derived Advanced Glycation End-product cross-linking in Type I collagen: A molecular dynamics simulation study. 2016. Biophysical Chemistry 218, 42-46.

**Nash, A.**, et al. Computational study of glucosepane-water hydrogen bond formation: an electron topology and orbital analysis. 2016. Journal of Biomolecular Structure and Dynamics 35 (5), 1127-1137.

## 2015

Collier, T. A., **Nash, A.**, et al. Preferential sites for intramolecular glucosepane cross-link formation in type I collagen: a thermodynamic study. 2015. Matrix Biology 48, 78-88.

**Nash, A.**, et al. De novo design of transmembrane helix-helix interactions and measurement of stability in a biological membrane. 2015. Biochimica et Biophysica Acta (BBA)-Biomembrane 1848 (5), 1248-1257.

Collier, T. A., **Nash, A.**, et al. The thermodynamics identification of glucosepane cross-linking in type I collagen - an all-atom molecular dynamics study. 2015. International Journal of Experimental Pathology 96 (2), A11-A12.

**Nash, A.**, et al. The thermodynamic characterisation of glucosepane cross-linking in the extra cellular matrix: a density functional theory study. 2015. International Journal of Experimental Pathology 96 (2), A13-A13.

## 2014

Hall, V., **Nash, A.**, et al. SSNN, a method for neural network protein secondary structure fitting using circular dichroism data. 2014. Analytical Methods 6 (12), 6721-6726.

## 2013

Hall, V., **Nash, A.**, et al. Elucidating protein secondary structure with circular dichroism and a neural network. 2013. Journal of Computational Chemistry 34 (32), 2774-2786.

Thake, T. H. F., Webb, J. R., **Nash, A.**, et al. Permeation of polystyrene nanoparticles across model lipid bilayer membranes. 2013. Soft Matter 9 (43), 10265-10274.

## 2012

Beever, A. J., Nash, A., et al. Effects of the Oncogenic V664E Mutation on the Membrane Insertion, Structure, and Sequence-Dependent Interactions of the Neu Transmembrane Domains in Micelles. 2012. *Biochemistry* 51 (12), 2558-2568.

## 2009

Nash, A., et al. A framework proposition for cellular locality in Dictyostelium modelled in Pi-Calculus. 2009. *CoSMoS*, 83.