**WEBSITE TEMPLATE**

**1. RESEARCH THEME/s; PRP; GI:**

Material and Advanced Technologies for Healthcare

Developing future therapies

**2. PI DETAILS (Name, Pure Link, Twitter Handle & Photo)**

**Irina Tikhonova,**

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Email: i.tikhonova@qub.ac.uk

**3. Research focus (80 words max)**The focus of our research efforts is to facilitate understanding biomolecule interactions and function employing computational tools and, using the gained knowledge, to develop novel computer-aided drug design strategies and design new small molecule ligands. The current targets of our interest include G protein-coupled receptors (GPCRs).

**4. Research opportunities** 40 words max

We offer PhD study in cutting-edge computational approaches in computer simulations, data collection, mining, and analysis at the interface of chemistry and biology as well as state-of-the art functional assays, facilitating skills development in drug design research applicable in academia and industry.

**5. Research students**

Name: Abdul-Akim Guseinov
PhD title: Understanding allosteric and biased GPCR signaling from computer simulations and mutagenesis
Years of Study: 2021-2024
Country: Russia

Name: Tianyi Ding
PhD title: Computer simulations of a chemokine receptor family to map allosteric sites.

Years of Study: 2020-2023
Country: China

Name: Ramya Nuti
PhD title: Targeting glycans as an anti-viral strategy
Years of Study: 2021-2024
Country: India

Name: Mathew Skinner
PhD title: Exploiting stem cell receptors for parasite control
Years of Study: 2022-2024
Country: Northern Ireland

**6. Alumni - where are they now? (3 Max)**

Name: Dr. Balaji Selvam

PhD title: Bioaminergic Receptors: The Role of a Dynamic Conformational Ensemble in Molecular Recognition, Activation and Drug Design

Years of Study: 2010-2014
Country: India
Current position: Computational chemist at Ferring Pharmaceuticals, San Diego

Name: Dr. Daniel Moore
PhD title: The role of dynamic conformational ensembles in substrate recognition, mechanism of inhibition and drug design against the malaria M1 aminopeptidase
Years of Study: 2014-2017
Country: Northern Ireland
Current position: Lead Data Scientist at Liberty IT, Belfast

Name: Aaron Maguire

PhD Title: Understanding the conformational dynamics of the genetic variants of the human FKBPL

Years of Study: 2016-2019

Country: Northern Ireland

Current Position: Lecturer in Science, at Northwest Reginal College, Derry City

**7. Public Outreach/ other achievements** (media links; DNA innovation links etc; other press)

<https://www.youtube.com/watch?app=desktop&v=nItoq3t7WOs&feature=youtu.be>

<https://www.sciencedaily.com/releases/2021/10/211027121951.htm>

<https://www.digitalhealthnews.eu/research/6555-new-computer-modelling-could-boost-drug-discovery>

**8. Key words**

Drug design, molecular modelling, pharmacology, data mining