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Research highlights

2019 – present

Building all-atom model of entire virus using cryo-EM data

Our work on building complete MD model of an entire bacteriophage MS2 in solution attracted interest from cryo-EM community [17] as the measured data is often of mixed resolution and reconstructing the atomistic structure is a non-trivial task; we have received a grant for working on the project (see [3] in table 1).

2020 – present

Molecular and cellular mechanisms of antitumour activity of Dioxadet

We have recently started a new collaborative project funded by Royal Society (see [5] in table 1) for experimental and computational investigation of a new anti-tumour drug "Dioxadet". Investigations of both cellular mechanisms and molecular details, using a collection of methods from biology, chemistry, and computer simulations are under way with the aim of reducing the drug's toxicity and increasing its effectiveness.

2018 – present

Developing drugs for tuberculosis to overcome antimicrobial resistance

We have started a new €730k project funded by Horizon2020 RISE scheme (see [8] in table 1) where I coordinate a consortium of 13 groups worldwide in experimental and theoretical research on drug development.

2010 – present

Hybrid multiscale atomistic/hydrodynamic theory of liquid systems

I, together with Dr Sergey Karabasov (QMUL), have developed the theory and implementation of a hybrid approach to modelling molecular systems at several space and time scales simultaneously, consistently combining classical atomistic (Molecular Dynamics) and macroscopic continuous (hydrodynamics) representations.

- key publications: [39, 40, 42, 43, 44, 45, 46];
- funding in excess of £1.2M included projects [23] and [18] among others (see table 1);
- we are developing a fundamentally new representation of matter, at the cutting edge of this field in the UK and worldwide: organised several research meetings (see page 4), member of UK Fluids Network - EPSRC Special Interest Group in Multiscale and Non-Continuum Flows;
- several postdoctoral researchers (Dr I Korotkin, Dr A Markensteijn, Dr Y Pavlov), PhD (Mr V Farafonov, Mr A Scukins) and MSc students (Mr Visencuk Visenko, Mr Pozhilenkov, Ms Bakumenko, Ms Berezovska) have been and still are actively involved in this work during a number of years.

2018 – present

Modelling graphene oxide – peptide co-assembly into nanofluidic structures

My group is part of an international team focused on the development of biocompatible nanodevices. We provide the Molecular Dynamics modelling side of the work.

- We have recently published a paper in *Nature Communications*: [26] (already cited 40 times). See also the review of our paper in 'news&views' at [A. Jain, R. Ulijn, Restoring order. *Nat. Chem.* **12**, 428-429 (2020). <https://doi.org/10.1038/s41557-020-0463-y>].

2013 – present

All-atom Molecular Dynamics simulation of whole viruses

My group is among very few in the world performing simulations of complete viruses at atomistic resolution.

- key publications: [28, 30, 31, 32, 34, 35];
- funding included several projects in collaboration with Japan (for example, projects [9, 10, 15, 20], table 1);
- we are the first who modelled all-atom virus using MD *together with the native genome*;
- access to the fastest in the world supercomputers in collaboration with Prof. Taiji group (RIKEN, Japan);
- my former PhD student Dr Tarasova is currently leading this line of research, she won a prestigious Fellowship (project [10], table 1) to work in Prof. Taiji group;
- we have recently published an invited perspective [32].

- 2000 – 2009 **Quantifying complexity of the dynamics of molecular systems**
 In Cambridge I established and led the Unilever Centre's (part of Chemistry Department) research in the field of complex dynamics of molecular systems where I applied modern abstract mathematical approaches in complex dynamics to molecular systems.
- key publications: [48, 52, 53, 56, 57, 60, 62, 63, 64, 67, 70, 77, 79, 81, 82];
 - I have initiated, prepared and informally lead a large EU project [24], table 1 (€1.2M budget) on the subject;
 - it has been a very successful project producing 77 publications and over 60 conference presentations; the consortium consisted of 8 research groups from 6 European countries, three major meetings were organised (~40 participants).

- 1998 – 2000 **Quantum Bohmian dynamics**
 I developed a novel method for quantum dynamics using trajectories-based Bohmian mechanics.
- The resulting publication [84] has been cited 45 times.

- 1991 – 1998 **Physical chemistry of electrolyte solutions**
 I experimentally measured and theoretically analysed vibrational spectra of non-aqueous electrolyte solutions, discovering a new molecular species in solution.
- key publications: [83, 85, 89, 90, 91].

Career

- 2013 – present Senior Lecturer, **Department of Mathematics, Aston University, UK**
- 2005 – present Visiting Scientist, **Center for Biosystems Dynamics Research, RIKEN, Japan**
- 2010 – 2013 Lecturer, **Department of Mathematics, Aston University, UK**
- 2005 – 2009 Senior Research Associate, **Department of Chemistry, Cambridge University, UK**
- 2000 – 2005 Research Associate, **Unilever Centre for Molecular Sciences Informatics, Department of Chemistry, Cambridge University, UK**
- 1998 – 2000 Research Associate, **Department of Chemistry, University of Nevada, Reno, USA**
- 1997 – 1998 Royal Society - NATO Fellow, **School of Chemistry, University of Leeds, UK**
- 1996 – 1997 Research Associate, **School of Chemistry, Kharkov State University, Ukraine**

Education

- 1993 – 1996 **PhD training** at the Department of Inorganic Chemistry, Kharkov State University, Ukraine
- PhD degree awarded on 1 Nov 1996;
 - thesis: "Interparticle interactions and dynamics of molecules in electrolyte solutions of n-hexanol and acetonitrile studied by vibrational spectroscopy".
- 1986 – 1994 **Master's degree in physical chemistry**, Kharkov State University, School of Chemistry (dates include 2 years of army service)

Teaching

Undergraduate and postgraduate teaching

- 2018 – present teaching MSc level course "Algorithmic and Computational Mathematics" as part of *Aston University* apprenticeship programme: online teaching with students located anywhere on the globe
- 2014 obtained PGCPP certificate; fellow of the HEA
- 2010 – present teaching second and third year courses "Vector Calculus", "Approximation Theory", "Mathematical Methods" (~80 students), MSc course "Algorithms and Computational Mathematics" at "Mathematics" teaching programme at *Aston University, UK*
- 2010 – 2013 teaching first year course "Mathematics for First Year Engineers" (~180 students) at *Aston University, UK*
- 2009 – 2011 supervising tutorials on theoretical chemistry at *Cambridge University, Department of Chemistry, UK*
- 2001 – 2010 teaching supervisions (a special arrangement of teaching in Cambridge that includes classes in groups and one-to-one) on the Natural Sciences Tripos Part II course (BA and MSc levels) "Molecular Spectroscopy", Part I course (first year level) including Introduction to Quantum Mechanics, Molecular Spectroscopy, Structure Determination, Symmetry and Bonding, Molecular Energy Levels, Thermodynamics, Introduction to Chemical Biology, *Department of Chemistry, Cambridge University, UK*
- 1996 – 1997 tutoring and lecturing at the MSc courses "General and Inorganic Chemistry", "Statistical Mechanics", *School of Chemistry, Kharkov State University, Ukraine*

Research Supervision: PhD and MSc students supervisions

PhD supervisions:

- 2024 – present Muhammad Shafiq (PhD), University of Karachi (co-supervision)

2022 – present	Josiah Shem Davis (PhD), Aston University
2023 – present	Maryna Bakumenko (PhD), Aston University
2019 – present	Alexey Pozhilenkov (PhD), Odessa National University, Ukraine (co-supervision)
2018 – 2022	Nizakat Ali (PhD), University of Karachi (co-supervision)
2017 – 2021	Hina Qaisar (PhD), visiting PhD student at Aston University (co-supervision), successful
2013 – 2016	Jutharath Voraprateep (PhD), Aston University, successful
2013 – 2017	Elvira Tarasova (PhD), Baltic Federal University, Kaliningrad, Russia, successful
2014 – 2018	Vladimir Farafonov (PhD), Kharkov National University, Ukraine (co-supervision), successful
2012 – 2014	Yongfang Zhu (PhD), Aston University, withdrawn for personal reasons
2011 – 2014	Arturs Scukins (PhD), Aston University, successful
2005 – 2008	Christian Jensen (PhD), Cambridge University (informal day to day supervision), successful
2002 – 2005	George Karvounis (PhD), Cambridge University (informal day to day supervision), successful
1996 – 1998	Sergey Yeremenko (PhD), Kharkov State University (informal day to day supervision), successful
	<i>MSc supervisions:</i>
2021 – 2022	Josiah Shem Davis (MSc), Aston University
2019 – 2020	Tatyana Kornilova (MSc), Odessa National University, Ukraine (co-supervision), successful
2019 – 2020	Anna Shokhina (MSc), Odessa National University, Ukraine (co-supervision), successful
2018 – 2019	Maryna Bakumenko (MSc), Kiev National University, Ukraine (co-supervision), successful
2017 – 2018	Yakov Yusypenko (MSc), Odessa National University, Ukraine (co-supervision), successful
2017 – 2018	Kateryna Malchyk (MSc), Odessa National University, Ukraine (co-supervision), successful
2017 – 2018	Alexey Pozhilenkov (MSc), Odessa National University, Ukraine (co-supervision), successful
2017 – 2018	Stanislav Bondarenko (MSc), Odessa National University, Ukraine (co-supervision), successful
2012 – 2013	Larry Godwin (MSc), Aston University, successful
2006 – 2008	Svitlana Ruzhitskaya (MSc), Goteborg Chalmers University (co-supervision), successful
1995 – 1996	Sergey Yeremenko (MSc), Kharkov State University (informal day to day supervision), successful

Administrative responsibilities:

I was responsible for 4 years for the placement programme at Mathematics. The programme consists of one year placements for all students at industry and other Universities abroad. I have organised a new type of placement that did not exist before at Aston: a research placement where the best students spend a year conducting real life research.

I have an administrative role at the University level. I am managing all aspects of Aston's participation in HPC midlands consortium, from creating accounts on the Athena machine to negotiating processing time allocation for Aston. I take part in regular meetings where I represent Aston and deal with all strategic and practical issues related to our use of HPC midlands. This work has already produced some very tangible results as the paper from my group reporting the calculations has been recently published by Nature.

Research

Main research interests



My research group in 2017-2018

- **Hybrid hydrodynamics/molecular dynamics multiscale, multiphysics modelling.** Modelling bio-molecular systems where fully atomistic and purely hydrodynamic representations coexist and smoothly transform into each other at different spatial locations.
- **All-atom molecular dynamics simulation of entire viruses.** Modelling whole viruses including surrounding water at atomistic resolution. High performance molecular dynamics is used for systems of 3-5 million atoms.
- **Kinetics of ligand binding.** Obtaining the rates of binding of small molecules to proteins from realistic full-atom molecular dynamics simulations. Developing approaches for calculating correct bio-molecular transformation rates, taking into account non-Markovian behaviour of states.
- **Self-organising molecular systems.** Adapting and evolving chemical systems. Applications to self-organising materials.
- **Complexity of dynamical systems.** Quantitative approaches to computing the complexity of physical systems. Informational contents of classical dynamics of molecular systems. Molecules as non-linear dynamical systems.
- **Protein folding.** Molecular Dynamics simulation of protein folding. Complexity of the dynamics of folding. "Controlled MD".
- **Bohmian quantum dynamics.** Application of Bohmian mechanics to realistic molecular systems. Developing methods for effective propagation of Bohmian quantum trajectories for multidimensional systems.

Applied research

- **Cardiac data analysis.** Statistical Complexity as diagnosis tool for heart failures.
- **Photonics.** Non-transient electrodynamics in photonic devices.
- **Specialised materials.** Thin films of C_{60} at low temperatures.

Previous fields of research

- **Vibrational and rotational dynamics of molecules.** Experimental: IR and Raman spectroscopy investigation of structure and dynamics of inter-particle interactions in liquids. Theoretical: vibrational spectra theories to obtain micro-dynamic parameters of liquid electrolyte solutions.
- Computational: **decomposition of experimental spectra** into individual bands of complex shape, the problem of line shape and obtaining parameters from spectra consisting of extensively overlapping bands.
- Methods of **global optimisation** in problems related to spectroscopy.

Publications

All publications and conference presentations are listed below (pages 9 - 17)

Publication metrics

I am aware that formal bibliographical metrics do not correctly quantify the quality of publications. I, personally, fully agree with the trend to not take them into account when evaluating researcher's productivity (such as in REF, for example). However, they are still in use and often informally considered. I, therefore, include them here.

- **total number of peer-reviewed publications:** 91
- **total citations:** 638 (Web of Science), 738 (Scopus), 1025 (Google Scholar), 852 (ResearchGate)
- **h-index:** 14 (Web of Science), 15 (Scopus), 19 (Google Scholar), 17 (ResearchGate)
- **impact factors** of journals: some of my papers are published in journals with high IF: Nat. Comm. (impact factor 11.9), J. Phys. Chem. Lett. (9.4), Colloids and Surfaces B: Biointerfaces (6.0), Scientific Reports (5.0), Faraday Discussions (4.6), J. Mol. Liq. (4.5), Optics Express (3.5), Phil. Tran. R. Soc. A (3.0), Comput. Phys. Comm. (3.1), J. Chem. Phys. (3.0), Interface Focus (3.1). During last 10 years **37** of 44 publications are in **Q1 journals**.

Grants

- **total number of grants:** 27
- **overall funding:** ~£5.3M
- all received grants are listed in table 1 (I am PI in all projects, unless explicitly indicated otherwise)

Most important projects

- I have recently received a grant from Horizon2020 for a RISE project "**Theoretical and computational investigation of tuberculosis antimicrobial resistance development based on extensive experimental library of mycobacterium strains**", the consortium includes 11 partners in UK, Spain, Italy, Russia, Ukraine, Ecuador, Japan; 58 secondments are planned for 159 person-months work, total budget €730k.
- I initiated the project, arranged the consortium, wrote and submitted the proposal for the €1.2M project "**Using next generation computers and algorithms for modelling the dynamics of large biomolecular systems**" funded by G8 Research Councils Initiative on Multilateral Research Funding in 2011. The UK teams received €697K of funding (€415K in Aston University and €282K in Cambridge University).
- I organised the consortium, prepared, submitted, and took part in the management of the €2.1M EU Framework 6 (NEST-2003-Path-1) project "**Emergent organisation in complex biomolecular systems**", EMBIO, one of 13 EU funded large scale initiatives. The consortium consisted of 8 research groups from 6 European countries. Three major meetings have been organised (~40 participants is a typical scale). The project resulted in 77 publications and over 60 conference presentations.

National and International recognition

Organised research meetings

- International CECAM workshop "Virus as a whole: meso- and macroscopic structure and dynamics at all atom resolution", Lausanne, Oct 2015
- Royal Society International Scientific Seminar "Multiscale systems: linking quantum chemistry, molecular dynamics, and microfluidic hydrodynamics", Kavli Centre, Jul 2013

Awards and fellowships

2016	Chartered Chemist
2009	Fellow of the Royal Society of Chemistry
2006	Member of the Royal Society of Chemistry
2005	Japan Society for the Promotion of Science Short-Term Award for 4 months visit to Genomic Sciences Centre, Yokohama RIKEN Institute, Japan (one of ten granted in the UK)
2004	College Research Associate at Clare College, Cambridge
2002	Senior member of Wolfson College, Cambridge
2000	RSC Journals Grant for International Authors
1994 – 1995	Participation in research project supported by International Science Foundation by J. Soros
1995	Soros postgraduate studentship award



Research leadership

at University level

- I was at the management board of several University level research Institutes (Systems Analytics Research Institute, Aston Institute for Materials Research, Aston Antimicrobial project)
- I was a member of UK Fluids Network - EPSRC Special Interest Group in Multiscale and Non-Continuum Flows

External examination of PhD and other refereeing

- Invited as an external examiner for Faizal Patel, the PhD viva at Leicester University is scheduled for Feb 2023.
- Served as an external examiner for Sarah Mapplebeck, successfully completed her PhD at Leeds University in Jun 2022.
- Served as an external examiner for V. Sergiievskiy, successfully completed his PhD at University of Strathclyde in Jan 2013.
- Served as an external referee for D. Babyuk DSc dissertation at Chernovtzy National University, Ukraine.
- Review manuscripts for international journals, approximately 5-10 high impact factor journals per year, including J. Chem. Phys., Phys. Chem. Chem. Phys., Angewandte Chemie, Chem. Phys. Lett. PLoS 1, and others.
- Review applications for national and international funding bodies, including EPSRC, Royal Society, Leverhulme Trust, Ministry of Education and Science of the Russian Federation (Grant Competition to attract leading scientists to Russian institutions, so-called).
- Review Horizon2020 project as external expert (the recent one was the mid-term review of the ITN project).
- Member of EPSRC Peer Review Associate College: reviewing research proposals and serving on an EPSRC Prioritisation Panel.
- Expert of Russian Academy of Science (identification number 2016-01-1666-4118): reviewing research proposals.

Nationality and languages

Nationality

- Great Britain
- Ukraine

Languages

I am fluent in **English, Russian, and Ukrainian**

References

- **Professor David Saad**, Department of Mathematics, Aston University, email: d.saad@aston.ac.uk
- **Professor Dmitry Shalashilin**, School of Chemistry, University of Leeds, Headingley Road, Leeds, LS2 9JT, email: D.Shalashilin@leeds.ac.uk
- **Professor Martha Clokie**, Department of Infection Immunity and Inflammation, Leicester University, University Road, Leicester, LE1 7RH, email: mrjc1@leicester.ac.uk

Table 1: Funded projects (I am PI in all projects, unless explicitly indicated otherwise)

	Funds source	Project title	Duration (months)	Starting Date	Total Value	Other holders	Comments
1	BBSRC, Flexible Talent Mobility Account	Characterising and modelling the Salmonella phage-flagella complex	5	Feb 2025	£17.6K	Michael Tadesse is the fellow, funding from Warwick University for the delivery of BBSRC-FTMA	The project is for measuring the atomistic structure of a phage-flagella complex using Dr Nerukh's collaboration at Osaka University and RIKEN, Japan
2	EPSRC, Exascale Computing ExCALIBUR programme	Establishing the Accessible Computational Regimes for Biomolecular Simulations at Exascale (ExaBioSim)	18	Jul 2023	£620K	A team of experts in biomolecular simulation using HPC, lead by Dr Sarah Harris, Leeds University	The aim of the project is to determine how Exascale computing can be employed to obtain dynamic information essential to understanding how biomacromolecules perform their functions
3	Horizon2020, MSCA Postdoctoral Fellowships	Atomistic reconstruction of large biomolecular systems from low-resolution cryo-electron microscopy data	24	Sep 2023	€221K	Dr Vladimir Farafonov	Fellowship for Vladimir to work in Aston and several other Universities in UK and Europe
4	EPSRC	Engineering bacteriophages for treating antimicrobial resistance using all-atom models of entire viruses	12	Dec 2021	N/A		Access to EPSRC Tier-2 Service for 500000 CPU hours of national supercomputer "Cirrus" time
5	Royal Society	Molecular and cellular mechanisms of antitumour activity of Dioxadet and its nanoforms	24	Dec 2020	£12K	Pavlov First Saint Petersburg State Medical University	Matching funds of ~£30K were granted by Russian Fund for Fundamental Research for experimental investigations of dioxadet and its anti-cancer activity
6	Erasmus+	International Credit Mobility - Research Students and Staff	12	2020	~€80K	N/A	Funds for 6 research students to work for 8 months each in Aston and several short term visits for research collaborators from and to Odessa, Kiev, and Kharkov Universities
7	Sasakawa Foundation	Hybrid modelling of biomolecules for AMR in tuberculosis	24	Sep 2019	£2K	N/A	Funds for 2 PhD students visit to Dr Taiji group in RIKEN, Japan
8	Horizon2020, RISE	Theoretical and computational investigation of tuberculosis antimicrobial resistance development based on extensive experimental library of mycobacterium strains	48	Feb 2019	€730K	A consortium of 9 partners	The consortium includes 9 partners in UK, Spain, Italy, Russia, Ukraine, Equador, Japan; 58 secondments are planned for 159 person-months work
9	JSPS, BRIDGE Fellowship	Multiscale molecular simulations using HPC	2	Oct 2018	~£10K		Senior Fellowship for developing collaboration with Japanese research groups
10	JSPS	International Fellowships for Research in Japan	12	Apr 2018	~£30K	Elvira Tarasova	Postdoctoral Fellowship for my PhD student to spend 1 year in one of the best research groups in the world on high performance computing; only 12 such fellowships were awarded worldwide and Elvira is the only recipient from Russia
11	Erasmus+	International Credit Mobility - Research Students and Staff	12	May 2017	€103K	N/A	Funds for 8 research students to work for 10 months each in Aston and several short term visits for research collaborators from and to Odessa, Kiev, and Kharkov Universities
12	EPSRC	ARCHER supercomputer time	6	Jan 2017	N/A	N/A	UK High-End Computing Consortium for Biomolecular Simulation

13	Erasmus+	International Credit Mobility - Research Students and Staff	12	Sep 2016	€85K	N/A	Funds for 5 research students to work for 10 months each in Aston and 5 short term visits for research collaborators from Odessa Universities
14	EPSRC	ARCHER supercomputer time	6	Jun 2016	N/A	N/A	UK High-End Computing Consortium for Bimolecular Simulation
15	Sasakawa Foundation	High performance simulation of biomolecular viruses	24	Jun 2014	£4K	N/A	Funds for 2 PhD students visit to Dr Taiji group in RIKEN, Japan
16	Wellcome Trust Biomedical Vacation Scholarships	All atom computer modelling of entire virus in water: structure and dynamics of pores for translocation of viral genome into the capsid	2	Aug 2015	£2K	N/A	Summer scholarship for a promising undergraduate student
17	CECAM-Lorentz Workshop	Virus as a whole: meso- and macroscopic structure and dynamics at all atom resolution	1 week	Oct 2015	€30K	Dr Sergey Karabasov, Queen Mary University of London	Complete funding for arranging a dedicated workshop at Centre Europeen de Calcul Atomique et Moleculaire, (Lausanne)
18	Royal Academy of Engineering/Leverhulme Trust Senior Research Fellowship	Personal supercomputer for modelling complete virus at all atom resolution	12	Oct 2014	£44K	N/A	The fellowship relieves Dr Nerukh from all teaching and administrative activities, allowing the concentration on research
19	Royal Society of Chemistry	JWT Jones Fellowship	3	Dec 2014	£3K	N/A	An extended visit to Dr Taiji for first hand experience of using MDGRAPE4
20	Royal Academy of Engineering, Distinguished Visiting Fellowship	High performance special purpose computers for scientific simulations: crossing the boundaries between atomistic and continuum representation of liquid systems	1	Jul 2013	£3K	Makoto Taiji, RIKEN Advanced Institute for Computational Science	Extended visit to Aston University for Dr Taiji
21	Royal Society International Scientific Seminars	Multiscale systems: linking quantum chemistry, molecular dynamics, and microfluidic hydrodynamics	0.1	Jul 2013	£5K	Dr Sergey Karabasov, Queen Mary University of London	A prestigious workshop for invited participants, followed by a special issue of Phil. Trans. A
22	Royal Society Research Grant	Hybrid molecular dynamics - hydrodynamics simulation framework for modelling the explicit kinetics of ligand binding at atomistic resolution	12	30 Apr 2012	£15K	None	The grant for equipment purchasing
23	G8 Research Councils Initiative on Multilateral Research Funding	Using next generation computers and algorithms for modelling the dynamics of large biomolecular systems	36	01 Jun 2011	€1.2M	Makoto Taiji, RIKEN Advanced Science Institute, Sergey Karabasov, University of Cambridge, Vassily Goloviznin, Moscow Institute of Nuclear Safety, Masahiro Ueda, Osaka University	Interdisciplinary Program on Application Software towards Exascale Computing for Global Scale Issues Leading PI: Makoto Taiji, UK PI: Dr Dmitry Nerukh.
24	EU Framework 6	Emergent organisation in complex biomolecular systems	42	1 Mar 2005	€2.1M	A Consortium of 8 Universities from 6 European Countries (see http://www.embio.ch.cam.ac.uk for details), DN has organised the Consortium, prepared, submitted, and took part in the management.	PI: Prof. Robert Glen.

25	MRC	Statistical complexity measure as a diagnosis tool for cardiac rhythms	12	17 Oct 2005	£42K	Prof. Robert Glen, Chemistry Dpt., Cambridge Univ., Dr Ian Wilkinson, Addenbrooke's Hospital, Cambridge University	PI: Prof. Robert Glen. 1 postdoc is funded.
26	Royal Society	Non-linear dynamics of emergent complexity in molecular systems	24	1 Dec 2006	£8K	Prof. Robert Glen, Chemistry Dpt., Cambridge Univ.; Prof. Vladimir Ryabov, Department of Complex Systems, Future University Hakodate, Japan	PI: Prof. Robert Glen. 4 bilateral UK-Japan visits
27	The Daiwa Anglo-Japanese Foundation	Chaos and complexity in the dynamics of molecular transitions during protein folding	12	1 Dec 2006	£10K	Dr Makoto Taiji, Yokohama RIKEN Institute; Prof. Vladimir Ryabov, Future University Hakodate; Prof. Tamiki Komatsuzaki, Kobe University	PI: Dr Dmitry Nerukh. 1 visit to and 3 visits from Japan
28	Royal Society of Chemistry	JWT Jones Fellowship	3	1 Sep 2009	£4K	None	PI: Dr Dmitry Nerukh. An extended visit to Dr Taiji for protein folding simulations is planned

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