



## Chemical Structure Association Trust

### **Applications Invited for CSA Trust Grants for 2018.**

The Chemical Structure Association (CSA) Trust is an internationally recognized organization established to promote the critical importance of chemical information to advances in chemical research. In support of its charter, the Trust has created a unique Grant Program and is now inviting the submission of grant applications for 2018.

#### ***Purpose of the Grants:***

The Grant Program has been created to provide funding for the career development of young researchers who have demonstrated excellence in their education, research or development activities that are related to the systems and methods used to store, process and retrieve information about chemical structures, reactions and compounds. One or more Grants will be awarded annually up to a total combined maximum of ten thousand U.S. dollars (\$10,000). Grantees have the option of payments being made in U.S. dollars or in British Pounds equivalent to the U.S. dollar amount. Grants are awarded for specific purposes, and within one year each grantee is required to submit a brief written report detailing how the grant funds were allocated. Grantees are also requested to recognize the support of the Trust in any paper or presentation that is given as a result of that support.

#### ***Who is Eligible?***

Applicant(s), age 35 or younger, who have demonstrated excellence in their chemical information related research and who are developing careers that have the potential to have a positive impact on the utility of chemical information relevant to chemical structures, reactions and compounds, are invited to submit applications. Proposals from those who have not received a Grant in the past will be given preference. While the primary focus of the Grant Program is the career development of young researchers, additional bursaries may be made available at the discretion of the Trust. All requests must follow the application procedures noted below and will be weighed against the same criteria.

#### ***Which Activities are Eligible?***

Grants may be awarded to acquire the experience and education necessary to support research activities; e.g. for travel to collaborate with research groups, to attend a conference relevant to one's area of research (including the presentation of an already-accepted research paper), to gain access to special computational facilities, or to acquire unique research techniques in support of one's research. Grants will not be given for activities completed prior to the grant award date.

#### ***Application Requirements:***

Applications must include the following documentation:

1. A letter that details the work upon which the Grant application is to be evaluated as well as details on research recently completed by the applicant;
2. The amount of Grant funds being requested and the details regarding the purpose for which the Grant will be used (e.g. cost of equipment, travel expenses if the request is for financial support of meeting attendance, etc.). The relevance of the above-stated purpose to the Trust's objectives and the clarity of this statement are essential in the evaluation of the application);

3. A brief biographical sketch, including a statement of academic qualifications and a recent photograph;
4. Two reference letters in support of the application. Additional materials may be supplied at the discretion of the applicant only if relevant to the application and if such materials provide information not already included in items 1-4. A copy of the completed application document must be supplied for distribution to the Grants Committee and can be submitted via regular mail or e-mail to the Committee Chair (see contact information below).

***Deadline for Applications:***

Application deadline for the 2018 Grant is March 30, 2018. Successful applicants will be notified no later than May 9, 2018.

***Address for Submission of Applications:***

The application documentation can be mailed via post or emailed to: Bonnie Lawlor, CSA Trust Grant Committee Chair, 276 Upper Gulph Road, Radnor, PA 19087, USA. If you wish to enter your application by e-mail, please contact Bonnie Lawlor at [chescot@aol.com](mailto:chescot@aol.com) prior to submission so that she can contact you if the e-mail does not arrive.

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## Chemical Structure Association Trust: Recent Grant Awardees

### 2017

**Jesus Calvo-Castro:** University of Hertfordshire, England, was awarded a Grant to cover travel to present his work at the Fifth International Conference on Novel Psychoactive Substances to be held in Vienna, Austria from August 23-23, 2017. He works on the development of novel methodologies for the in-the-field detection of novel psychoactive substances (NPS), where chemical structure and information play a crucial role.

**Jessica Holien:** St. Vincent's Institute of Medical Research, Fitzroy, Victoria, Australia, was awarded a Grant to cover travel to present her work at the 2017 Computer-Aided Drug Design (CADD) Gordon Research Conference scheduled to take place July 16-21, 2017 in Mount Snow, VT, USA. She is a Postdoctoral researcher at St. Vincent's and is responsible for a range of computational molecular modelling including; compound database development, virtual screening, docking, homology modelling, dynamic simulations, and drug design.

### 2016

**Thomas Coudrat:** Monash University, Australia, was awarded a Grant to cover travel to present his work at three meetings in the United States: the Open Eye Scientific CUP XVI, The American Chemical Society Spring Meeting, and the Molsoft ICM User Group Meeting. His work is in ligand directed modeling.

**Clarisse Pean:** Chimie Paris Tech, France, was awarded a Grant to cover travel to give an invited presentation at the 2016 Pacific Rim Meeting on Electrochemical and Solid State Science later this year.

**Qian Peng:** University of Oxford, England, was awarded a Grant to attend the 23<sup>rd</sup> IUPAC Conference on Physical Organic Chemistry. His research is in the development of new ligands for asymmetric catalysis.

**Petteri Vainikka:** University of Turku, Finland, was awarded a Grant to spend the summer developing and testing new methods for modelling organic solvents in organic solutions with Dr. David Palmer and his group at the University of Strathclyde, Glasgow, Scotland.

**Qi Zhang:** Fudan University, China, was awarded a Grant to attend a Gordon Conference on Enzymes, coenzymes and metabolic pathways. His research is in enzymatic reactions.

### 2015

**Dr. Marta Encisco:** Molecular Modeling Group, Department of Chemistry, La Trobe Institute for Molecular Science, La Trobe University, Australia was awarded a Grant to cover travel costs to visit collaborators at universities in Spain and Germany and to present her work at the European Biophysical Societies Association Conference in Dresden, Germany in July 2015.

**Jack Evans:** School of Physical Science, University of Adelaide, Australia was awarded a grant to spend two weeks collaborating with the research group of Dr. Francois-Xavier Coudert (CNRS, Chimie Paris Tech).

**Dr. Oxelander Isayer:** Division of Chemical Biology and Medicinal Chemistry, UNC Eshelman School of Pharmacy, University of North Carolina at Chapel Hill, was awarded a Grant to attend summer classes at the Deep Learning Summer School 2015 (University of Montreal) to expand his knowledge of machine learning to include Deep Learning (DL). His goal is to apply DL to chemical systems to improve predictive models of chemical bioactivity.

**Aleix Gimeno Vives:** Cheminformatics and Nutrition Research Group, Biochemistry and Biotechnology Dept., Universitat Rovira I Virgili was awarded a Grant to attend the Cresset European User Group Meeting in June 2015 in order to improve his knowledge of the software that he is using to determine what makes an inhibitor selective for PTP1B.

### 2014

**Dr. Adam Madarasz:** Institute of Organic Chemistry, Research Centre for Natural Sciences, Hungarian Academy of Sciences. He was awarded a Grant for travel to study at the University of Oxford with Dr. Robert S. Paton, a 2013 CSA Trust Grant winner, in order to increase his experience in the development of computational methodology which is able to accurately model realistic and flexible transition states in chemical and biochemical reactions.

**Maria José Ojeda Montes:** Department of Biochemistry and Biotechnology, University Rovira i Virgili, Spain. She was awarded a Grant for travel expenses to study for four months at the Freie University of Berlin to enhance her experience and knowledge regarding virtual screening workflows for predicting therapeutic uses of Natural molecules in the field of functional food design.

**Dr. David Palmer:** Department of Chemistry, University of Strathclyde, Scotland. He was awarded a Grant to present a paper at the fall 2014 meeting of the American Chemical Society on a new approach to representing molecular structures in computers based upon ideas from the Integral Equation Theory of Molecular Liquids.

**Sona B. Warriar:** Departments of Pharmaceutical Chemistry, Pharmaceutical Biotechnology, and Pharmaceutical Analysis, NMIMS University, Mumbai. She was awarded a Grant to attend the International Conference on Pure and Applied Chemistry to present a poster on her research on inverse virtual screening in drug repositioning.

### **2013**

**Dr. Johannes Hachmann:** Department of Chemistry and Chemical Biology at Harvard University, Cambridge, MA. He was awarded the Grant for travel to speak on "Structure-property relationships of molecular precursors to organic electronics at a workshop sponsored by the Centre Européen de Calcul Atomique et Moléculaire (CECAM) that will take place October 22 – 25, 2013 in Lausanne, Switzerland. .

**Dr. Robert S. Paton:** University of Oxford, UK. He was awarded the Grant to speak at the Sixth Asian Pacific Conference of Theoretical and Computational Chemistry in Korea on July 11, 2013. Receiving the invitation for this meeting has provided Dr. Paton with an opportunity to further his career as a Principal Investigator.

**Dr. Aaron Thornton:** Material Science and Engineering at CSIRO in Victoria, Australia. He was awarded the Grant to attend the 2014 International Conference on Molecular and Materials Informatics at Iowa State University with the objective of expanding his knowledge of web semantics, chemical mark-up language, resource description frameworks and other on-line sharing tools. He will also visit Dr. Maciej Haranczyk, a prior CSA Trust Grant recipient, who is one of the world leaders in virtual screening.

### **2012**

**Tu C. Le:** CSIRO Division of Materials Science & Engineering, Clayton, VIC, Australia. She was awarded the Grant for travel to attend a Cheminformatics course at Sheffield University and to visit the Membrane Biophysics group of the Department of Chemistry at Imperial College London.

### **2011**

**J. B. Brown:** Kyoto University, Kyoto, Japan. J.B. was awarded the Grant for travel to work with Professor Ernst Walter-Knappe at the Freie University of Berlin and Professor Jean-Phillipe Vert of the Paris MinesTech to continue his work on the development of atomic partial charge kernels

### **2010**

**Noel O'Boyle:** University College Cork, Ireland. Noel was awarded the grant to both network and present his work on open source software for pharmacophore discovery and searching at the 2010 German Conference on Cheminformatics.

### **2009**

**Laura Guasch Pamies:** University Rovira & Virgili, Catalonia, Spain. Laura was awarded the Grant to do three months of research at the University of Innsbruck, Austria.

## **2008**

**Maciej Haranczyk:** University of Gdansk, Poland. Maciej was awarded the Grant to travel to Sheffield University, Sheffield, UK, for a 6-week visit for research purposes.

## **2007**

**Rajarshi Guha:** Indiana University, Bloomington, IN, USA. Rajarshi was awarded the Grant to attend the Gordon Research Conference on Computer Aided Design in August 2007.

## **2006**

**Krisztina Boda:** University of Erlangen, Erlangen, Germany. Krisztina was awarded the Grant to attend the 2006 spring National Meeting of the American Chemical Society in Atlanta, GA, USA.

## **2005**

**Dr. Val Gillet and Professor Peter Willett:** University of Sheffield, Sheffield, UK. They were awarded the Grant for student travel costs to the 2005 Chemical Structures Conference held in Noordwijkerhout, the Netherlands.

## **2004**

**Dr. Sandra Saunders:** University of Western Australia, Perth, Australia. Sandra was awarded the Grant to purchase equipment needed for her research.

## **2003**

**Prashant S. Kharkar:** Institute of Chemical Technology, University of Mumbai, Matunga, Mumbai. Prashant was awarded the Grant to attend the conference, Bioactive Discovery in the New Millennium, in, Lorne, Victoria, Australia (February 2003) to present a paper, The Docking Analysis of 5-Deazapteridine Inhibitors of Mycobacterium avium complex (MAC) Dihydrofolate reductase (DHFR).

## **2001**

**Georgios Gkoutos:** Imperial College of Science, Technology and Medicine, Dep. of Chemistry. London, UK. Georgios was awarded the Grant to attend the conference, Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, (CMTPI-2001) in Bordeaux, France, to present part of his work on internet-based molecular resource discovery tools.