



CSIR-CDRI Offers HPLC Service to OSDDChem

Offering a solution to the problem of HPLC data of the compounds, that is a mandatory requirement in the OSDDChem submissions, CDRI team from Lucknow has extended their hand of help to carry out HPLC analysis, to those who wish to submit molecules under the OSDD Chemistry Outreach Program but lack HPLC facility.



The HPLC at CDRI will be performed on a RP C-18 column (150 x 4.6 or 250 x 4.6 mm, 5µm particle size) with a linear gradient of acetonitrile (containing 0.01% TFA or HCO₂H) and water. The HPLC data shall be recorded at an absorbance of 220 or 254 nm. Submissions will require prior approval and each sample analysis will be charged Rs. two hundred fifty only (Rs. 250/-) to cover the cost of consumables and maintenance of the instrument. The analysis cost will have to be deposited with the samples in the form of a draft in the name of "Director, CDRI". The HPLC data will be communicated as PDF or JPEG files.

For details visit <http://groups.google.com/group/osddorganicchemistsforum>

New OSDD JSF Unit –Marthoma College, Kerala



OSDD is a youth movement extending across the nation with the objective of bringing generic medicines through a world knowledge platform which will bring the cost effective solution to medicare. OSDD Junior Scientist Forum aims at connecting together young brilliant minds from the remotest villages of India with peers to solve challenging problems in drug discovery. Numerous colleges across the country are already connected under this program and OSDD-JSF has received wide acceptance amongst the student community. A new addition to this growing research forum is the group from Marthoma College, Chungathara, Nilambur Kerala with the support and cooperation of the OSDD unit of Malabar Christian College. The forum being led by Mr Umesh C. V. has active participation of Mr Sumith P.S., Ms Soumya P.K., Ms Toncy Thomas and Ms Shilpa

OSDD Publications

Structural Annotation of Mycobacterium tuberculosis Proteome in PLoS One (2011)

Of the ~4000 ORFs identified through the genome sequence of *Mtb* H37Rv, experimentally determined structures are available for 312. Since knowledge of protein structures is essential to obtain a high-resolution understanding of the underlying biology, we seek to obtain a structural annotation for the genome, using computational methods.

Structural models were obtained and validated for ~2877 ORFs, covering ~70% of the genome. New algorithms for binding site detection and genome scale binding site comparison at the structural level, recently reported from the laboratory, were utilized. Read more at: <http://www.plosone.org/article/info%3Adoi%2F10.1371%2Fjournal.pone.0027044>

OSDD Authorship Policy

OSDD encourages the Principal Investigators (PI) to publish the results in peer reviewed publications. OSDD is a CSIR led team India consortium with global partnerships, a highly collaborative endeavor. OSDD Consortium, in keeping with the spirit of collaboration, has decided the following protocol for authorship of various papers. This pattern is adopted from the fundamental principles that were developed to guide the publications of the Indian Genome Variation Project of Institute of Genomics and Integrative Biology, a partnering CSIR laboratory of OSDD.

- All papers of OSDD would have OSDD Consortium as the last but one Author.

For example, if P1, P2...Pn are the PIs of the OSDD Consortium; S1, S2...Sn are the student researchers participating in the project, then the following authorship pattern may be followed: S1,S2...P1,P2, OSDD Consortium, Corresponding PI.

There may be projects where the Chief Mentor, Prof. Samir K. Brahmachari, has actively contributed and merits authorship. In such cases, his express consent should be taken to include him as an author. Where Prof. Samir K. Brahmachari is an author, his name will appear prior to that of the corresponding author, unless he is the corresponding author himself.

- As there are a large number of projects being pursued under OSDD, it is likely that there will be many publications. To avoid duplication and to ensure that the micro attribution system has been followed, the manuscript should be submitted to the Project Director who will then get this verification done and approve release of the manuscript.
- The Title, Abstract and Author List should be uploaded on the OSDD portal by the corresponding author before submission of the manuscript.

Acknowledging OSDD for funds received alone is not enough, as OSDD is not a mere funding agency; appropriate credits for all authors are mandatory. OSDD encourages publications in open access journals. All projects of OSDD are required to follow this authorship policy.



OPEN SOURCE DRUG DISCOVERY

A CSIR led Team India Consortium with Global Partnerships
www.osdd.net

Dr. Burrow discussed MMV's agenda to eradicate malaria and lectured that HTS screening of 6 million compounds resulted in more than 25,000 actives, out of which 400 actives have been submitted for community screening. Also, Dr. Burrow spoke about MMV's efforts to develop cheap and efficient Artemisinin combination therapy (ACT). The requirements for the new combination target product profile (TPP) were discussed in detail. He also informed the Open Box effort of MMV for discovery of new antimalarial. Prof. Rahul Jain from NIPER, Mohali spoke about "8-aminoquinolines as antimalarials". After introducing audience with various antimalarial 8-aminoquinolines such as quinocide, bulaquine, tefanoquine and sitamaquine, Dr. Jain discussed advantages and disadvantages associated with this class of antimalarials. He also discussed various strategies to develop new and more effective aminoquinolines to improve metabolic stability, decreased toxicity and increased blood-schizontocidal activity. Dr. Sanjay Batra, in his lecture titled "Antimalarials: CDRI's Perspective and Chemistry Outreach" talked about CDRI's facilities and the work carried out by various scientists of CSIR-CDRI for the discovery of antimalarials. Dr. Batra, a core team member of OSDD (Open Source Drug Discovery) introduced the audience with OSDD and the chemistry outreach program. He spoke about CSIR's initiative to open OSDD centers at many CSIR labs and initiatives to train college and university students in medicinal chemistry. He familiarized audience with the procedures for submission and screening of compounds at OSDD.



Dr. Steven Ward from Liverpool School of Tropical Medicine talked about tetraoxane class of antimalarials. He spoke about his team's efforts to design and develop a novel peroxide antimalarial candidate RKA182, which showed higher efficacy and superior PK profile than artesunate and artemisone. He also discussed various stages of RKA182 development from discovery to preclinical trials and finally the current stage i.e. phase I clinical trial. This molecule is once only antimalarial and is active against all stages of plasmodium. The topic of JNCASR scientist Prof. Hema Balaram's lecture was "Crosstalk between Purine Nucleotide Metabolism & Mitochondrial Pathways in Plasmodium falciparum" in which she discussed novel pathways and mechanisms to disrupt the lifecycle of malaria parasite.

CDRI Symposium Report- "Antimalarials: current approaches and new directions"



16/11/ 11: A one day symposium on Antimalarials: Current approaches and future directions under the aegis of OSDDm, OSDDChem Outreach and MMV was held at CSIR-CDRI on 16th November 2011. The said symposium was organized in the CSIR-IITR auditorium and was attended by researchers from India and speakers from abroad. The audience included scientists, faculty and students from CSIR-HQ (OSDD team), CLRI, Chennai, NIIST, Trivandrum, IIT, Kanpur and Guwahati, IISER, Mohali, Calcutta University, IITR, CIMAP and CDRI. The Director CSIR-CDRI Dr. T. K. Chakraborty initiated the meeting by welcoming the guests from India and abroad. Dr. Chakraborty emphasized on the role of the open science for the development of anti infectives and apprised the audience about the significance of different programs CSIR has initiated in the area.

Dr. Jeremy Burrow, Head Discovery, MMV, Geneva was the first speaker of the day. He gave a brief introduction about the functioning of the MMV, a virtual and "not-for-profit" foundation with the mission to discover, develop and deliver antimalarial drugs. Dr. Burrow informed that the funding for MMV comes from public, private donations and also from partner's contributions



Projects Submitted in OSDDChem

Along with submission of molecules to OSDDChem database, submissions of projects are also now being actively pursued under the OSDD Chemistry Outreach program. Projects on the synthesis and screening of interesting compounds have been submitted by Dr Palwinder, Guru Nanak Dev University, Punjab, Dr Nagaiah, Indian Institute of Chemical Technology, Hyderabad and Dr Dilip, University of Calcutta.

The feasibility and scope of the projects and the amount of the compounds that need to be sent for the purpose of screening are being discussed on the portal. For more details visit:

<http://crdd.osdd.net/osddchem/browse.php?f=project>

What OSDD Means to Us.....

I have had a thrilling experience with OSDD for the past 2 years and now I am ready to pursue my PHD at Indiana University. Thanks to OSDD team for support and mentoring - **Abhik Seal**

Thanks to OSDD, I was able to build up my profile with respect to Bioinformatics tools and techniques. The kind of research going on in OSDD is the one, which I might have dreamt of, during my graduation and post graduation to be a part of, and here I am with it. - **Rajdeep Poddar**

I am proud to be a part of the OSDD community. And encourage all youth to actively participate in it - **Yatindra Nath Yadav**

I am very thankful to the ones who bring this open source to us and who initiated the idea of open sourcing. It is really like a boon to me and will always keep working on it and I am going to contribute to the best I can all my life- **Swati Gandhi**



“OSDD Chemistry Outreach Program (OSDDChem)” Dr Tushar, Director, CDRI in Current Science

In the International Year Of Chemistry (IYC), the Council of Scientific and Industrial Research (CSIR), has initiated a unique OUTREACH program under it's Open Source Drug Discovery (OSDD) platform, to impart practical training to a large number of MSc Chemistry students in various universities ,IIT's , IISER's and and other academic institutions across the length and breadth of the country.The program will be coordinated by CSIR-Central Drug Research Institute (CSIR-CDRI) Lucknow

Read More at :

http://cstest.ias.ac.in/cs/Downloads/download_pdf.php?titleid=47500

Dr. Balaram discussed the pathways of purine and pyrimidine synthesis and the importance of fumarate incorporation in purine and pyrimidine bases in the parasitic cell. She also discussed the significance of purine nucleotide cycle (PNC) in the parasite and the strategies targeting these pathways to control the disease. The next speaker, Dr. Waterson from MMV, Geneva discussed in detail the MMV portfolio followed by the case histories of several recent antimalarial drug candidates belonging to spiroindoles, tetrahydro- β -carboline, imidazolopiperazine and oxaborole class of compounds. He spoke about MMV's future plans and also the OSDD initiative where after screening 50000000 compounds, 20000 hits were obtained out of which 200 drug like and 200 probe like molecules were selected. Dr. Amit Sharma from ICGEB, New Delhi kept the audience spellbound with his very interesting lecture on RNA based control of malarial parasite. He talked about AARS inhibitors and the RNA based mechanism of parasite control. Last but one lecture by Dr. K. M. Muralidharan titled “Antimalarial Peroxides: A Bird's Eye View” explained advantages and disadvantages of peroxide class of antimalarials and also compared artemisinin with artemisinone and other artemisinin analogues.Dr. Muraleedharan's talk mostly revolved around artemisinin including its numerous metabolic transformations and proposed hybrids and also Trojan horse approach and peroxide based new pharmacophores. The last speaker of the day Dr. Saman Habib introduced speakers with the operating principle, functions and procedures associated with OSDDm in detail. She introduced audience with the OSDDm website and the procedures for submission and monitoring of compounds in OSDD. Dr. Habib responded to various queries from audience related with data sharing, data reviewing and quality assurance on OSDD. She also briefed the audience about the monthly and annual monitoring of OSDDm projects by individual coordination teams. The symposium came to an end with Dr. Sanjay Batra's note of thank to the speakers and other guests.

This report is compiled by Dr. Namrata Rastogi, CDRI.