

## OSDD Chemistry OUTREACH Program (OSDDChem)

In the International Year of Chemistry (IYC), the Council of Scientific and Industrial Research (CSIR), New Delhi, has initiated a unique OUTREACH Program, under its Open Source Drug Discovery (OSDD) platform<sup>1</sup>, to impart practical training to a large number of M Sc chemistry students in various universities, IITs, IISERs and other academic institutes across the length and breadth of the country. The program will be coordinated by CSIR–Central Drug Research Institute (CSIR–CDRI), Lucknow.

The idea is that, as part of their practical classes, the students could undergo training in research, get to know how to carry out the modern synthetic reactions that they study in their courses and are encouraged to pursue their career in research. The age-old organic practical classes can be replaced by synthesis of small-molecule libraries using simple and easy-to-do reactions in 2–3 steps of modern synthetic methods in university postgraduate laboratories. Students will be encouraged to design their molecules, read about diseases like malaria, TB, drug discovery against these diseases and related subjects. Relevant study material can be provided by CSIR laboratories and OSDD community. Students can be helped in this exercise by their teachers and research scholars. The libraries and schemes can also be suggested by CSIR and OSDD community.

Each student, or a group of students, will make few compounds, learn their purification by chromatography and use NMR, mass spectroscopy (MS), etc. to characterize them. This can be part of their M Sc practical classes, last semester projects or summer projects. Many universities and institutes in the country now have NMR, MS and HPLC facilities that can be used to characterize these molecules and check their purity. Wherever these cannot be done, the samples can be sent to any nearby CSIR laboratory for the same.

The university departments designated for carrying out these studies can also be used to train other students from nearby colleges, who do not have any facility and would like to do summer projects in these representative universities. CSIR has also set up OSDD Chemistry OUTREACH centres in some of its laboratories, like CSIR–CDRI, CSIR–

NCL, CSIR–IICT, CSIR–NIIST, where at any given time students from nearby universities can carry out 2–6 months projects for creating new chemical entities for diseases like TB and malaria. Nodal scientists have been designated in these laboratories to coordinate the activities of this program in their respective regions.

All submissions will be based on the website<sup>2</sup> created especially for this program. Any registered member of OSDD can access the website for compound submission, viewing submissions or evaluation. The compounds should be registered first by the principal investigator (PI), a regular faculty of the university or institute, on the OSDDChem website. Next, the PI should submit a project for certain number of registered molecules. The OSDD community can view these molecules anytime, carry out *in silico* screening, give ratings, suggest better synthetic schemes, suggest modifications of structures based on docking studies, and so on. The projects will be evaluated within a short period of time and the sanctioned projects will be funded. SOPs for registering molecules – synthesized or to-be-synthesized virtual molecules, project submissions, evaluation and sanction are available on the website.

After the molecules are synthesized and all the requisite data are uploaded, these well-characterized pure molecules, each about 30 mg, are to be sent to CSIR–CDRI, where they will be screened for TB and malaria and the results will be promptly uploaded on the website. Each molecule submission will be adequately funded. Samples will also be stored at CSIR–CDRI repository under modern conditions with proper labelling, etc. These compounds can also be made available to OSDD community, whosoever wishes to screen them. Students will be able to see the biological screening data for their compounds in OSDD portal. Those who have done well will be given reward points or certificates. The research output can also lead to publications and that will be highly encouraged.

A new drug discovery program in the country requires large repository of small organic molecules which can be screened against various diseases. While India has a large pool of excellent organic chemists in various academic and research

institutes and universities in the country, their expertise remains largely untapped for any national initiative like creating a national repository of small molecules or screening these molecules against various diseases. Organic chemists have made commendable contributions toward India achieving a global leader status in the area of generics. The same success story can be recreated in transforming the country into an important hub for new drug discovery, especially in the area of neglected diseases. With nearly 900 deaths per day from TB and recent estimation of as many as 700–800 deaths from malaria in the country, we need a national initiative for combating these diseases.

OSDD, a brain-child of Samir K. Brahmachari (DG, CSIR), provides an ideal common platform to bring together not only chemists and biologists, but also other researchers interested in drug discovery. Started three years ago, this is not just another project but a movement, as Brahmachari says, that is attracting people from all over the world who are interested to work collectively in an atmosphere free of patent and IPR worries for a common cause and for the benefit of mankind. Many are yet not sure of how OSDD functions or can achieve its goal, but that does not deter them from joining this platform, and there is no lack of enthusiasm. As this movement gathers momentum, it will sweep away all the presently established drug discovery programs that are seriously suffering from stagnation and lack of new ideas.

CSIR–CDRI feels proud to be part of this unique movement and to have been entrusted the responsibility of spearheading two important components of the OSDD Program – the OSDD Malaria Program (OSDD $m$ )<sup>3</sup> and OSDDChem<sup>2</sup>. Established on 17 February 1951 to strengthen and advance the field of drug research and development in the country, CSIR–CDRI has been striving relentlessly in the pursuit of affordable drugs and healthcare for all. This year CSIR–CDRI has completed 60 years of its glorious existence. This is the only government-funded organization in the country today having all the infrastructural facilities for development of new drugs from conceptual to commercialization stage. Over the years CSIR–CDRI has deve-

veloped a large number of biological assays and screening protocols to carry out studies on the biological activity of compounds against various diseases<sup>4</sup>. The institute today wishes to invite all interested researchers in the country and from all over the world to participate in its drug discovery, delivery and development programs on collaborative/partnership modes. This is an appeal, especially to all those like-minded organic chemists who are genuinely interested to take their research to a higher level of practical application and want to work with a dedicated scientific community in

the translational mode of drug development without worrying too much about personal credits and royalties, not to let go a golden opportunity like this. With your active participation and cooperation, we can make it a real game changer for new drug discovery in the country. Let us join hands and work together to find ways and means to provide affordable healthcare to millions of underprivileged people in the world.

1. Open Source Drug Discovery; <http://www.osdd.net>

2. OSDD Chemistry Outreach Program; <http://crdd.osdd.net/osddchem>
3. OSDD Malaria Program; <http://malaria.osdd.net/home>
4. Biological assays available at CSIR-CDRI; <http://www.cdriindia.org/biologicalscr.htm>

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## Dengue and other unknown viral outbreaks in Warangal District, Andhra Pradesh, South India

All the villages and tribal hamlets of Warangal, Karimnagar, Khammam, Adilabad and neighbouring districts have been affected by viral outbreaks, with hospitals of various regions being flooded with patients suffering from viral fever. Most of the viral fever observed in these regions include dengue and other unknown viral pyrexia. Both male and female populations of all age groups have been severely affected. News reports from local media confirm death toll above 100 during the past two months, starting from the monsoon season with unknown fever and dengue.

This is the seventh consecutive year in which various viral outbreaks have hit these regions<sup>1</sup>. These areas experienced Japanese encephalitis<sup>1</sup> in 1979, HIV<sup>2</sup> in 2002, viral encephalitis (Chandipura virus)<sup>1</sup> in 2003, Chikungunya<sup>3</sup> in 2006, and endemic cases of dengue in 2009 and 2010, but these have now reached epidemic proportions.

Dengue virus was first isolated in Calcutta<sup>4</sup> in 1945. Since then, several outbreaks from different parts of the country have been reported during the last 50 years. Dengue virus belongs to the family Flaviviridae. It is spherical, 40–60 nm in diameter and contains an electron-dense core 30 nm in diameter. The genome is single-stranded RNA, about 11 kb in size. Three viral proteins are associated with the virion, the envelop, membrane and capsid. Dengue virus has four serotypes,

viz. DEN-1, DEN-2, DEN-3 and DEN-4. All four were recorded from India, but no serotypic information is available from this region.

Clinical manifestations of the patients from these region include high-grade fever ranging from 99°F to 102°F, platelet count 10,000 to 1 lakh, organomegaly, enlargement of gall bladder and liver, ascites, leucopenia, malalgia, headache, minimal right pleural effusion, free fluid in peritoneal cavity, nausea, vomiting, abdominal pain and gastroenteritis.

Some of the fevers were found to be positive for NS1 antigen, whereas some were positive for IgG and IgM antibodies of dengue. Rest of the samples was negative for the malaria, influenza and other known viral diseases.

Biochemistry of the patients' serum electrolytes (sodium, potassium, chlorides), liver SGPT, SGOT, bilirubin, blood picture, blood urea nitrogen and serum creatine was normal, except thrombocytopenia and leucopenia. Lungs were clear and cardiac profile was normal, no CNS involvement was observed.

Symptomatic treatment was initiated and thrombocytopenic patients were given single-donor platelet transfusion. Hospitalized and well-treated patients are surviving, but among the poor and rural communities mortality rate is increasing due to lack of proper medication. Now it is important to study why dengue and

other unknown viral outbreaks are rampant in this region.

Study should be directed towards serotyping of the virus strain prevailing in these regions for proper treatment. There is also a need to carry out research to find the etiological agent, its vector biology, environmental changes, rural and urban cycle, and reservoir host of the unknown viral agents of these regions by establishing at least a virology field laboratory.

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2. Radhakrishna, M., *J. Environ. Biol.*, 2007, **28**, 865–867.
3. Radhakrishna, M., Krishnareddy, M. and Ramreddy, S., *Curr. Sci.*, 2006, **91**, 570–571.
4. *Virology Bulletin*, National Institute of Virology, Pune, accessed on 22 September 2011.

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