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# **Final Report**

**Workshop**

**on**

***"Combinatorial Chemistry and Technologies,  
Molecular Design and their  
Application to Exploit Biodiversity"***

National Chemical Laboratory

Pune, India

15 – 17 December 2006

**UNIDO Project No.: TE/GLO/04/105**

**UNIDO Contract Order No.: 16001309 ML/CZ**

## **International Workshop on Combinatorial chemistry and Technologies, Molecular Design and their Application to Exploit Biodiversity**

### **Summary:**

The National Chemical Laboratory, Pune, organized an ICS-UNIDO International Workshop on Combinatorial chemistry and Technologies, Molecular Design and their Application to Exploit Biodiversity during 15-17 December, 2006. The main focus of the workshop was on to build awareness and capacity as well as to strengthen the links between academy and industry in India and South East Asian countries with particular attention on application of CC/CT & MD techniques to explore the nearly virgin biodiversity in Asia. Fifty participants comprising scientists and technologists from Asian countries including Japan, Italy, China, Thailand, India and Vietnam, both from academia as well as industry participated in the workshop. Moreover, invited lecturers came also from Japan and Italy. Highly informative 22-lectures were delivered by 15-authoritative national/international speakers in six sessions, covering practically all aspects relevant to smartly explore the biodiversity using the combinatorial approach with a special visit to NCL's Combi-Chem Centre.

In the inaugural session, Dr. B. D. Kulkarni, Dy. Director, NCL, delivered his welcome address and very briefly explained the utility of combinatorial approach in the field of Chemical Engineering. Professor Stanislav Miertus, Chief of Pure and Applied Chemistry, ICS-UNIDO, Italy spoke on goals and programmes of ICS-UNIDO, on CC/CT/MD in India and South East Asian countries. Dr. M. K. Gurjar, Dy. Director, NCL, explained the essence of NCL programmes, present research activities and the futuristic plans. Dr. N. P. Argade, Scientist, NCL, discussed about the green therapy with an emphasis on conversion of leaf to capsule by reverse pharmacological approach using the rich *Indian Ayurvedic System of Medicine*.

Prof. Dr. Javed Iqbal, Vice President, Dr. Reddy's Research Foundation delivered the first talk highlighting the use of combinatorial chemistry approach both in academia and industries with several case studies. Prof. P. Seneci from Milan University and as an ICS-UNIDO expert talked about the use of CC/CT/MD in natural product research and their applications in diagnostics and biotechnology. Dr. G. Terstappen, Vice President, Sienabiotech from Italy gave two continuous lectures on High

Throughput Screening (HTS) in natural products research. Professor Kenji Mori from The Tokyo University gave a very authoritative multidimensional talk on natural product research and biodiversity. Dr. M. K. Gurjar gave a snap shot overview of research activities in OCS and OCT Divisions of NCL. Dr. Ganesh Pandey from NCL gave an elegant lecture on global strategies towards the total synthesis of complex bioactive natural products. Prof. K. N. Ganesh, Director, IISER, Pune talked on combinatorial oligonucleotides and applications. The participants from China, Thailand and Vietnam respectively, spoke about the diversity oriented synthesis, the status of bird-flu research in Thailand and why collaborations are essential. The researchers from Pune Prof. D. D. Dhavale, Dr. P. Tripathi, Dr. S. P. Chavan, Dr. S. Hotha and Dr. A. A. Natu discussed about the synthesis of bioactive natural and unnatural product scaffolds. Dr. K. K. Bhutani from NIPER talked about the unexplored rich biodiversity in the North-East region of India. Overall, a very healthy churning of combinatorial science covering identification of plant species, isolation of plant material, fractionation, high throughput screening, lead identification and optimization by the synthesis of focused combinatorial mini-libraries inclusive of pseudo natural products and natural product hybrids was successfully done to reach the conclusions very unanimously.

The work shop culminated with a round table discussion for further developing this field and enhancing cooperation between various participating countries. All agreed that the impact of natural products in Drug Discovery is an accepted reality and the genesis of ~ 50% drugs in the market is in Chemistry of Natural Products. Professor R. S. Mali and Professor Kenji Mori expressed the urgent need to scientifically explore the biodiversity in Asia to get new molecules with the better known and unknown bioactivities as a chemist's arsenal against the health problems of 21<sup>st</sup> century and CC/CT/MD have a great potential to accelerate the process of discovery of novel therapeutics. Professor Mori also added that the synthesis of focused pheromone libraries will be a meaningful exercise to challenge the Nature. The workshop also enabled the formation of a very useful network of scientists under the aegis of ICS-UNIDO which can act as a junction point and cooperate with each other to bring the results of their work into useful, sustainable and environment friendly products (For more details please see Aide-Memoire).

## **ORGANIZATION**

The Workshop on "Combinatorial Chemistry and Technologies, Molecular Design and their Application to Exploit Biodiversity" was jointly organized by the International Center for Sciences and High Technology of the United Nation Industrial Development Organization (ICS-UNIDO), with headquarters in Trieste, in collaboration with the National Chemical Laboratory, Pune, India. The following bodies took responsibility for the scientific and organizational aspects of the event:

### **Local Organizer:**

Dr. N. P. Argade (Scientist) and Dr. M. K. Gurgar (Head OCS and OCT), National Chemical Laboratory, Pune, India.

## **DATE AND SITE**

The Meeting was held on 15-17 December 2006 in National Chemical Laboratory, Pune, India. The final Agenda of the Workshop and list of participants are presented in the Annex I & II.

## **FUNDING**

The total expenses for the organization were **14979.82 €**, including the Local Organizer contribution

The planned contribution from ICS-UNIDO amounted to 15,000.00 €; however 10913.82 € was the real expenditure for the budget items specified in the terms of reference [i.e.: food charges (snaks and one lunch), conference materials, travel of key lecturers and participants, internal transport, ad-hoc DSA "pocket money", workshop materials).

The amount of 13,000.00 € has already been transferred by ICS-UNIDO to the local organizer. The remaining amount will be sent back to UNIDO account (€ **2,088.28** approx.).

**ITEMS TO BE COVERED WITH THE ICS-UNIDO BUDGET**

*(see also Annex III)*

|   |                   |
|---|-------------------|
| <b>ICS-UNIDO Contribution in EUR (TOTAL 15,000)</b>   |                   |
| Travel of 10 invited international lecturers  | 6905.65           |
| Travel of 3 invited national participants   | 838.68            |
| Daily Subsistence Allowance (ad hoc DSA) for 10 international lecturers   | 495               |
| Daily Subsistence Allowance (ad hoc DSA) for 3 invited national participants and lecturers  | 105               |
| Local transport and airport transfers<br>-local transport to and from the hotel to the Institute –<br>-coaches for the site visit –<br>-airport transfers                 | 947.15            |
| Workshop Materials (printed material, photocopies etc)  | 347.53            |
| Coffee breaks (2 x day x 3 days x 60 participants)  | 1274.81           |
| <b>Sub-Total ICS-UNIDO Contribution</b>   | <b>10913.82€</b>  |
| <b>Contributions of the hosting institution EUR (TOTAL 4066)</b><br>In kind and monetary contributions of the hosting institution (and other co-sponsoring organizations) |                   |
| Presentation projector, screen, memento   | 500               |
| Payment for accommodation, two meals and three dinners, educational visit to city of Pune and Pune University (cash contribution)   | 3066              |
| Room, Personnel, postal charges   | 500               |
| <b>Sub-Total Local Organizing Contribution</b>  | <b>4066</b>       |
| <b>GRAND TOTAL</b><br><b>(ICS contribution + Local contribution)</b>  | <b>14979.82 €</b> |

## **PARTICIPATION**

Fifty participants comprising scientists and technologists from six different countries including Japan, Italy, China, Thailand, India and Vietnam, both from academia as well as industry participated in the workshop. Highly informative 22-lectures were delivered by 15-authoritative national/international speakers in six sessions, covering practically all aspects relevant to smartly explore the biodiversity using the combinatorial approach with a special visit to NCL's Combi-Chem Centre.

## **WORKSHOP MATERIALS**

Each participant and lecturer obtained conference materials. The invitation containing the main objectives of the forum and some details on the organization was distributed by e-mail or regular mail.

At the registration and at the end of the workshop, the following materials were given to all of the registered participants:

Final Agenda of the workshop

The power point presentation of the contributions, published on compact disc

Office supplies with conference memento.

## **OPENING CEREMONY**

The opening ceremony was chaired by Dr. B. D. Kulkarny, Deputy Director of National Chemical Laboratory, Pune, India.

Welcome speeches were also delivered by:

Mr. Stanislav Miertus, Chief of Area of Pure and Applied Chemistry, ICS-UNIDO, Italy;

Mr. Pierfausto Seneci, ICS-UNIDO Scientific Advisor, University of Milan, Milan, Italy.

## **PROGRAMME**

Please refer to the attached final Agenda and time schedule (Annex I) for the details.

## **RESULTS AND PROPOSALS FOR FOLLOW UP ACTIVITIES**

The work shop culminated with a round table discussion for further developing this field and enhancing cooperation between various participating countries. All agreed that the impact of natural products in Drug Discovery is an accepted reality and the genesis of ~ 50% drugs in the market is in Chemistry of Natural Products. Professor R. S. Mali and Professor Kenji Mori expressed the urgent need to

scientifically explore the biodiversity in Asia to get new molecules with the better known and unknown bioactivities as a chemist's arsenal against the health problems of 21<sup>st</sup> century and CC/CT/MD have a great potential to accelerate the process of discovery of novel therapeutics. Professor Mori also added that the synthesis of focused pheromone libraries will be a meaningful exercise to challenge the Nature. The workshop also enabled the formation of a very useful network of scientists under the aegis of ICS-UNIDO which can act as a junction point and cooperate with each other to bring the results of their work into useful, sustainable and environment friendly products.

Participants also presented the country reports and were asked to submit new project proposals.



## Annex I

Friday, 15 December 2006

- 09:00 - 09:30 Registration of participants
- 09:30 - 10:00 Welcome address  
Dr. M. K. Gurjar, National Chemical Laboratory, India  
Dr. N. P. Argade, National Chemical Laboratory, India  
Prof. S. Miertus, Chief of Area of Pure and Applied Chemistry, ICS-UNIDO, Italy  
Dr. S. Sivaram, Director, National Chemical Laboratory, India  
Representative of UNIDO Regional Office
- 10:00 - 10:30 Goals and Programmes of ICS-UNIDO, Subprogramme on CC/CT/MD in India and South East Asian Countries (*S. Miertus, ICS-UNIDO, Italy*)
- 10:30 - 11:00 *Coffee and Tea Break*

### Session I: Intro on CC/CT/MD and Natural Product Research

(Chairman: S. Miertus)

- 11:00 - 11:45 Overview on CC/CT/MD (*Javed Iqbal, Reddys Laboratory, Hyderabad*)
- 11:45 - 12:15 Overview on CC/CT/MD in Natural Products Research (*P. Seneci, ICS-UNIDO, Italy*)
- 12:15 - 12:30 CC/CT/MD in Natural Products Research: Case Studies (*P. Seneci, ICS-UNIDO, Italy*)
- 12:30 - 13:00 Applications of CC/CT/MD in Diagnostics and Biotechnology (*G. Fassina/P. Seneci, ICS-UNIDO, Italy*)
- 13:00 - 14:00 *Lunch Break*

### Session II: Selected Topics in CC/CT/MD and Natural Product Research

(Chairman: K. Mori)

- 14:00 - 14:45 HTS in Natural Products Research (*G. Terstappen, Sienabiotech, Italy*)
- 14:45 - 15:15 HTS in Natural Products Research: Case Studies (*G. Terstappen, Sienabiotech, Italy*)
- 15:15 - 15:45 *Coffee and Tea Break*

### Session III: National Chemical Laboratory Activities

(Chairman: R. S. Mali)

|                      |  |
|----------------------|--|
| 15:45 - 16:15        | Introduction to NCL Programmes and Activities( <i>M.K. Gurjar, NCL Pune, India</i> )   |
| 16:15 - 16:45        | Global Strategy towards the Total Synthesis of Structurally Complex Biologically Active Alkaloids ( <i>Ganesh Pandey, NCL, Pune, India</i> ) |
| 16:45 - 17:05        | Combichem at NCL ( <i>A. A. Natu, NCL., Pune, India</i> )  |
| 17:05 - 17:25        | Synthesis of natural products and scaffolds ( <i>S.P. Chavan, NCL, Pune, India</i> )   |
| 17:25 - 18:00        | Discussion   |
| <b>19:30 - 21:30</b> | <b>DINNER</b>  |

**Saturday, 16 December 2006**

**Session IV: Synthesis and Biodiversity**

(Chairman: G. Pandey)

- 09:30 - 10:15 Natural Product Synthesis and Biodiversity (*K. Mori, University of Tokyo, Japan*)
- 10:15 - 10:45 The Progress of the Establishment of a Centre for Biodiversity and Modern Natural Products Research and Development in Thailand (*W. De-Eknamkul, Chulalongkorn University, Thailand*)
- 10:45 - 11:15 Diversity-oriented Solution and Solid-phase Synthesis of Bioactive Heterocycle Libraries (*Wei-Min Dai, China*)
- 11:15 - 11:30 Coffee and Tea Break
- 11:30 - 13:00 Visit to Combi-Chem Unit of NCL
- 13:00 - 14:30 *Lunch Break*
- 14:30 - 17:30 Hands on Instruments with Trial Experiments (15:30-16:00, Coffee and Tea)
- 19:30 - 21:30 **DINNER**

**Sunday, 17 December 2006**

**Session V: Project reports**

(Chairman: M. K. Gurjar)

- 09:00 - 09:30 Combinatorial oligonucleotides: Screening for new biomolecular functions via discovery of HIV Tat-NFKB DNA interactions (*K. N. Ganesh, I. I. S. E. R., Pune, India*)
- 09:30 - 10:00 High Throughput Screening (*Narayanswami, India*)
- 10:00 - 10:30 Enantioselective Total Synthesis of Biologically Active Natural Products (*Pradeep Kumar Tripathi, NCL, India*)
- 10:30 - 10:50 Mono- and bi-cyclic iminosugars: Synthesis and glycosidase inhibitory studies (*D. D. Dhavale, Pune University, Pune, India*)
- 10:50 - 11:20 Recent Experiences with Respect to Biodiversity of North-East Region of India and Role of Scientific Institutions for the Value Addition (*K. K. Bhutani, NIPER, India*)
- 11:20 - 11:40 *Coffee and Tea Break*

(Chairman: K. N. Ganesh)

- 11.40 - 12:00 Project report on CC/CT/MD and Natural Product Research (S. Hannongbua, Chulalongkorn University, Thailand)
- 12:00 - 12:20 The status of bird-flu research in Thailand (S. Hannongbua, Chulalongkorn University, Thailand)
- 12:20 - 12:40 Anti-HIV constituents of *Litsea verticillata* from Vietnam (Vu Dinh Hoang, Vietnam)
- 12:40 - 13:00 The Collaboration in the Region and on an International is Very Important and Necessary (Le Vien, Vietnam)
- 13:00 - 14:30 *Lunch Break*

**Session VI: Follow-up activities, common initiatives, recommendations and conclusions**

(Chairman: S. Miertus)

14:30 - 15:30 Round table discussions on selected topics for recommendations

15:30 - 16:30 Presentations of the Round Tables discussions

16:30 - 17:00 *Coffee and Tea Break*

17:00 - 17:45 Final discussion, recommendations and conclusions

**19:30 - 21:30 DINNER**

## Annex II

### LIST OF PARTICIPANTS

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## Annex III

### FINAL CALCULATIONS - ITEMS TO BE COVERED WITH THE ICS-UNIDO BUDGET

*Note:* The exchange rate applied (58.70 INR for 1 €) is the official exchange rate of State Bank of India the day advanced payment from ICS UNIDO was deposited into CC-BD Bank Account.

| No. | Items description   | Amount<br>(INR) | Amount<br>(Euro) |
|-----|---|-----------------|------------------|
| 1   | International Travel plus DA (3-Days) of Prof. Lursinsap Chidchanok           | 38248.00        | 651.58           |
| 2   | International Travel plus DA (3-Days) of Prof. Wei-Min Dai                    | 44021.00        | 749.93           |
| 3   | International Travel plus DA (4-Days) of Dr. Vu Dinh Hoang                    | 45446.00        | 774.20           |
| 4   | International Travel plus DA (5-Days) of Prof. Kenji Mori                     | 43444.00        | 740.10           |
| 5   | International Travel plus DA (3-Days) of Dr. Pornchai Rojsitthisak            | 38248.00        | 651.58           |
| 6   | International Travel plus DA (2-Days) of Prof. Hannongbua Supot               | 37360.00        | 636.46           |
| 7   | International Travel plus DA (3-Days) of Dr. Georg Terstappen                 | 65711.00        | 1119.44          |
| 8   | International Travel plus DA (3-Days) of Mr. Koobkokkrud Thongchai            | 38248.00        | 651.58           |
| 9   | International Travel plus DA (4-Days) of Mr. Le Vien                          | 45446.00        | 774.20           |
| 10  | International Travel plus DA (3-Days) of Prof. De-Eknamkul Wanchai            | 38248.00        | 651.58           |
| 11  | Hyderabad-Pune-Hyderabad air travel plus DA (1-Days) of Prof. Dr. Javed Iqbal | 17769.00        | 302.71           |
| 12  | Chandigarh-Pune-Chandigarh air travel plus DA (2-Days) of Prof. K. K. Bhutani | 29751.00        | 506.83           |
| 13  | Ahmednagar-Pune-Ahmednagar car travel plus DA (4-Days) of Dr. Vijay Khanna    | 7874.00         | 134.14           |
| 14  | Mumbai-Pune-Mumbai car travel of Prof. Kenji Mori                             | 10624.00        | 180.99           |
| 16  | Mumbai-Pune-Mumbai car travel of Prof. Wei-Min Dai                            | 6344.00         | 108.08           |
| 17  | Mumbai-Pune-Mumbai car travel of Dr. Georg Terstappen                         | 5699.00         | 97.09            |

|    |   |                  |                          |
|----|---|------------------|--------------------------|
| 18 | Mumbai-Pune-Mumbai car travel of two Vietnam participants                   | 6410.00          | 109.20                   |
| 19 | Mumbai-Pune-Mumbai car travel of five Thailand participants                 | 10550.00         | 179.73                   |
| 20 | Total local transport (14 to 17 Decmber, 2006)                              | 15970.00         | 272.06                   |
| 21 | Complete conference materials (55 number)                                   | 20400.00         | 347.53                   |
| 22 | Snacks, tea, coffee, juice etc (60 people, twice a day, three days)         | 36000.00         | 613.29                   |
| 23 | Partial food charges (lunch for 60 people, 15 <sup>th</sup> December, 2006) | 29000.00         | 494.04                   |
| 24 | Bottle water (60 people, three days)  | 9831.00          | 167.48                   |
|    | <b>Total</b>  | <b>640642.00</b> | <b>10913.82</b>          |
|    | <b>Total amount remaining (will be sent back to ICS-UNIDO)</b>              | <b>122582.00</b> | <b>2088.28 (Approx.)</b> |