



OCCASION

This publication has been made available to the public on the occasion of the 50th anniversary of the United Nations Industrial Development Organisation.



DISCLAIMER

This document has been produced without formal United Nations editing. The designations employed and the presentation of the material in this document do not imply the expression of any opinion whatsoever on the part of the Secretariat of the United Nations Industrial Development Organization (UNIDO) concerning the legal status of any country, territory, city or area or of its authorities, or concerning the delimitation of its frontiers or boundaries, or its economic system or degree of development. Designations such as "developed", "industrialized" and "developing" are intended for statistical convenience and do not necessarily express a judgment about the stage reached by a particular country or area in the development process. Mention of firm names or commercial products does not constitute an endorsement by UNIDO.

FAIR USE POLICY

Any part of this publication may be quoted and referenced for educational and research purposes without additional permission from UNIDO. However, those who make use of quoting and referencing this publication are requested to follow the Fair Use Policy of giving due credit to UNIDO.

CONTACT

Please contact <u>publications@unido.org</u> for further information concerning UNIDO publications.

For more information about UNIDO, please visit us at www.unido.org

21883

15p. tables illus.

FINAL REPORT

TRAINING COURSE ON THE INDUSTRIAL APPLICATIONS OF STRUCTURE-BASED MOLECULAR DESIGN AND COMBINATORIAL CHEMISTRY UNIVERSITY OF MALAYA, KUALA LUMPUR JULY 28 -AUGUST 8 1997

OBJECTIVE

Molecular Modeling and Combinatorial Chemistry are unanimously considered as powerful tools for the development of a country's capabilities in pharmaceuticals, agrochemistry and new material/chemical industries. These capabilities are necessary in order to give developing countries the possibility of market competition. Furthermore, many developing countries have large potentials in terms of their natural resources which can be better developed using the technologies of structure-based molecular design and combinatorial chemistry. Therefore, the objectives of this training course are:

- to provide scientists and technologists participating in this course with the basic information and an up-to-date knowledge of the principles and fundamentals of structure-based molecular design and combinatorial chemistry and their applications in drug/material designs and synthesis. This would enable scientists and technologists from developing countries to apply such techniques in their respective areas resulting in lower investments and reduced development time,
- to identify regional R&D institutions in developing countries through contacts established with the participants in the training course,
- to give ICS the opportunity in identifying qualified centres to be considered for inclusion as focal points in the ICS Network.

VENUE AND DATE

The training course was held for two weeks, from July 28th to August 8th 1997. The first half of the training course was held at the CAD/CAM Centre, Faculty of Engineering, University of Malaya, Kuala Lumpur while the second half was held at the University Malaya Computer Service Centre. These centres were chosen due to the facilities that are required for the training course. Twenty five SGI workstations were made available by the CAD/CAM Centre while twenty Pentiums were provided by the Computer Service Centre for the purpose of the training course.

ORGANIZATION

The training course was jointly organised by the International Centre for Science and High Technology and the University of Malaya. The latter assumed the responsibility as the contractor and hosting institution. The local organising committee who are members of the University of Malaya constituted as follows:

Professor A. Hamid A. Hadi (Advisor)
Associate Professor Rauzah Hashim (Chairperson)
Associate Professor Noorsaadah Abd. Rahman (Secretariat)
Associate Professor Kamaliah Mahmood (Honorary Treasurer)
Associate Professor Chen Wei (Flight and Accommodation)
Dr. Sharifuddin Mohd. Zain (Technical)
Dr. Ibrahim Noorbatcha (Publication)
Associate Professor Zainudin Arifin (Social)
Mrs. Siti Puzlinda Salamat (Secretarial Assistant)

The organising committee operated following the guidelines and regulations specified by members of the Scientific Committee at the Scientific Planning and Co-ordination Meeting (SPCM) held at the International Centre of Science and High Technology (ICS) held in January 1997. The following persons constituted the Scientific Committee for this training course:

Professor Stanislav Miertus (ICS, Trieste, Italy)

Associate Professor Rauzah Hashim (University of Malaya, Kuala Lumpur, Malaysia)

Dr. G. Maggiora (Pharmacia & Upjohn, Kalamazoo, USA)

Dr. Radhey L. Singhal (Ranbaxy, New Delhi, India)

Dr. Vladimir Frecer (SAS, Bratislava, Slovakia Republic).

FUNDING

The training course was fully sponsored by ICS-UNIDO. Their contribution for the activity was USD 40000. The University of Malaya contributed by providing the premises for holding lectures and laboratories for handson session and facilities in terms of hardwares and audio-visual instruments. The CAD/CAM Centre provided 25 SGI INDY workstations at a subsidised rate of RM 2 000 while 20 Pentiums was provided by the Computer Centre without any fees. Technical support was provided by the staff of the CAD/CAM centre, Computer Centre, University of Malaya, Sime Darby Systems Malaysia and Silicon Graphics (M) Ltd while software support was provided by MSI and the Oxford Modeling Group. Full detail of expenditure for the training course is attached as Annex 1.

LECTURERS

A total of 16 lecturers were involved in training the participants in the area of structure-based molecular design and combinatorial chemistry. The origin of the lecturers is summarised in Table 1.

Country	No. of Lecturers		
USA	2		
Italy	3		
Slovakia] . 1		
Slovenia	1		
Malaysia	7		
India] 1		
Australia	1		

Table 1: Lecturer's Country of Origin

Lecturers were selected from both the industries and academic institutions. Since the participants are from a diverse scientific background, the lectures from the academic institutions were asked to deliver lectures on fundamental topics. This is done in the hope that the participants will be able to accustom themselves with the topics that are being covered so that they will be able to integrate and tie the new materials of the application of structure-based molecular design (SBMD) and combinatorial chemistry (CC) to their research work. In addition, lecturers from the industries and research centres were asked to provide case studies and examples from the industries where such techniques are being used. By doing so, it is believed that a more complete view, ranging from fundamentals to applied research to industrial application would be given. The lecturer's institutional distribution is shown in Table 2.

Table 2: L	ecturer's.	Institutional	Distribution
------------	------------	---------------	--------------

Country	No. of Lecturers				
Universities	· 9				
Research Centres	3				
Industries	4				

A complete list of lecturers is attached in Annex II.

PARTICIPANTS

Calls for application were done through circulation of flyers to institutions in developing countries all over the world. The selection of participants were made by ICS through evaluation of the application forms and the Curricula Vitae submitted by the candidates. All of the participants were either academic members and reserachers of the universities or researchers and technologists of industrial and applied research institutions. 25 participants were chosen taken into consideration their region of origin as well as their institution. The ratio of participants from the academic institutions to industry/research centres (applied based) is close to 1:1. Tables 3 and 4 show the geographical and institutional distribution of participants, respectively.

Table 3: Geographical Distribution of Participants

Country	Number of Participants
India	10
Hong Kong	1
Philippines	1
Malaysia	11
Egypt	2

Table 4: Institutional Distribution of Participants

Institution	Number of Participants
Academic	12
Research Centres	3
Industries	9

15 candidates were chosen to be fully sponsored by ICS-UNIDO. This means that the airfare, living allowances and accommodation was fully paid for. Those present (participants, lecturers and organisers) were provided with lunches, morning and afternoon teas throughout the training course. No registration fees were requested from any of the participants. Although 25 candidates were originally chosen to participate in the training course, finally 23 candidates turned up to participate at the training course.

The comprehensive list of participants and the institutions they come from is attached as Annex III.

Fully sponsored participants were accommodated at the Heritage Hotel in Kuala Lumpur which is about 5 km away from the University of Malaya. This hotel was chosen due to its central location. The hotel accommodation included breakfast which is served before the participants leave for the University. For the convenience of the participants transport to and from the University were provided for the participants, whenever possible. On days that transport from the hotel to the University were not available, participant were requested to take the commuter train to the nearest station to the University. Arrangements were made for pick-up of the participants from this station to the University.

MATERIAL DISTRIBUTED

Participants were provided with a bag consisting of the usual training course materials which include the programme, list of participants/lecturers/organising committee as well as hard copies of the lectures. A copy of the material distributed to the participants is enclosed in this report. Dr. David Gallagher from the Oxford Molecular Group provided each participant with a copy of CACHE Modeling CD version 2.1 to take back to their respective institutions for demonstration regarding the use of computational techniques to other members of their institutions. A booklet of the complete lecture materials handed out to the participant is enclosed.

PROGRAMME

Opening Ceremony

The training course was officially officiated by the Vice-Chancellor of the University of Malaya, Tan Sri Dato' Dr. Hj. Abdullah Sanusi Ahmad. The opening ceremony was held on the 28th July 1997 from 9:30 am to 11:00 am at the Rumah Universiti, University of Malaya. The programme for the Opening Ceremony was as follows:

- 9:45: Arrival of the Vice-Chancellor
- 9:55: Opening Remarks by Associate Professor Rauzah Hashim
- 10:10: Introduction to Activities of ICS-UNIDO by Professor Stanilav Miertus
- 10:30: Opening Speech by the Vice-Chancellor
- 10:45: Tea Break

Several reporters from within and outside the University were present at the opening ceremony. Report of this event will be published in the next issue of the *Berita UM*, the official newsletter for the University. *Budiman* and *Bulletin Kejuruteraan Komputer*, two latter newsletters will be reporting special edition of this event in their

later edition. Some pictures covering this event is enclosed in Annex IV.

Training Course Programme

A total of 33 hours lectures and 30 hours of hands-on training session were given at the course.

Lectures

Each lecture is designed for 45 minutes. The lectures were held mostly in the CAD/CAM Laboratories mainly due to the fact that most of the lecturers used the workstation to demonstrate the application of techniques. An extra 15 minutes were reserved for question and answer session at the end of each lecture.

Laboratory (Hands-on) Session.

The laboratory sessions were for 2 hours each with at least two lecturers involve in training the participants on the computer. Hands-on training session were done on SGI INDY workstation for 7 days and Pentium for 2 days of the course. For this session, each participant had access to one SGI INDY workstation while they were obliged to share one Pentium with another person due to the constraint of the CACHE software available.

A detailed programme is enclosed in Annex V.

VISITS

Three visits were carried out during the course:

• United Nations Development Programme (UNDP)

A meeting was held between Mr. Neil Buhne, Deputy Regional Representative and Dr. Selva Ramachandran, National Program Officer from UNDP with Professor Miertus and Associate Prof. Dr. Rauzah Hashim. The discussion carried out in order to:

- explore the activities of both organisations, i.e. UNDP and ICS-UNIDO;
- identify overlapping areas of activities in Malaysia;
- explore the possibilities of future co-operation on Projects in Malaysia.

Standards and Industrial Research Institute Malaysia (SIRIM) Ltd.

SIRIM is a government's corporate organisation with multitude activities. Amongst its activities is making sure that the standards set for Malaysian industries comply with the standards set by the International Organisation for Standardisation. SIRIM also performs industrial research to help improve the productivity of small/medium industries (SMI's) in Malaysia.

10 delegates from the training course was chosen for the visit to SIRIM Ltd. Considering the role of SIRIM in Malaysian industries, these delegates consists of mainly participants from the industries. The delegation, led by Professor Miertus, consists of the following persons: Associate Professor Rauzah Hashim, Dr. Sharifuddin Mohd. Zain, Dr. Vladimir Frecer, Dr. Giorgio Fassina, Dr. Janez Mavri, Dr. D.K. Dikshit, Dr. C. S. Choxi, Dr. S.K. Agarwal and Dr. Yenamandra Prabhakar. The delegates were warmly welcomed by Dr. Mohd. Shazali Othman, the Vice President of Engineering Services, SIRIM. During the visit, the delegates were first presented with the corporate video of SIRIM, Ltd followed by briefings by Dr. Mohd. Shazali on the role of SIRIM and by Dr. Zainal Abidin Yusuf, the General Manager of Chemical and Industrial Biotechnology Division. The delegates were also taken to the SIRIM's Exhibition Centre where the results of its activities were being exhibited. The delegates, mainly from the industries were very enthusiastic over the activities carried out in SIRIM. This led to a friendly and lively discussion between these delegates and some members of SIRIM, Ltd. Future links in some areas of research have also been implied.

National Scientific Council on Research and Development (MPKSN)

MPKSN is a government agency equivalent to the National Science Foundation in the U.S.A or the SERC in Britain. One of its role is to ascertain that the direction of research taken by scientists and industrialists is in line with the government's policy and vision. It provides inputs for science and technology policies and develops programmes for their implementation. MPKSN is also responsible for strengthening the nation's technological base through enhancement of R&D activities, promotion of science and formulation of comprehensive action plan for technological development. Due to this fact, delegates chosen for this visit consists of members from the local academic and research institutions. The delegates, Associate Professor Rauzah Hashim, Dr. Khozirah Shaari, Dr. Nornisah Mohamad, Associate Professor Zuriati Zakaria, Dr. Amir Feisal Merican and Dr. Awang Bono, was led by Professor Miertus to a discussion with the Director of Science and Technology Division, Professor Ishak Ismail.

Professor Miertus was interested in exploring the structure of the organisation and express the support for the setting up a focal point of activities which coincides with the wish of the delegates, i.e. to set up the National Computer-Aided Molecular Design (CAMD) Centre with biological, material and chemical applications. The delegates proposed to use such centre for high-level man-power training and reserach centre in order that the modeling and simulation technology being transferred effectively into the country and widely applied in the industries.

As a result of the discussion, Professor Ishak was able to suggest several mechanisms for setting up such centre including "top-down initiations" which may include the participation of ICS-UNIDO.

SOCIAL EVENTS

Several social events were organised to achieve better integration and enable a more informal discussions between participants and lecturers. The social events organised were:

- * a barbecue and steam-boat dinner at the lakeside Nelayan Restaurant, Shah Alam (some participants had the opportunity to visit the Shah Alam Mosque prior to the dinner).
- * Kuala Lumpur Country Tour on Saturday afternoon, 2/8/1997.
- * Malacca Historical City Tour, a city about 200 km away from Kuala Lumpur on Sunday, 3/8/1997.
- * A lunch picnic at the University's botanical garden, the *Rimba Ilmu* (The Forest of Knowledge).
- * Local food and fruits lunch.
- Special dinners for the lecturers and organisers.
- * A canopy walk and tour of the Forest Research Institute, Malaysia (FRIM) was organised for the participants who remained behind for a couple of days after the training course.

All the above events (except for the Malacca City Tour) were fully funded by the local organising committee.

RESULT

The training course has succeeded in its objective to create awareness amongst the participants regarding the application of SBMD and CC in their research work and in idustrial application. The course was also able to provide better interactions between scientists and industrialist in developing countries. It is hoped that the network and co-operation formed during this course will continue to develop, particularly in promoting the inter-disciplinary field of SBMD and CC in research and the industries.

FEED BACK

Reactions to the scientific contents and general organisation of the training course was sought by means of an anonymous and optional questionnaire distributed to the participants. Lecturers were not asked to give any evaluation regarding the training course since most of them did not stay throughout the whole two weeks of the course. 19 questionnaires representing 80% of participants were returned. A questionnaire template is attached in Annex VI. In general, participants were happy with the course content and general organisation of the training course and all of them feel that this course have benefited them in one way or another. Most of the participants will be going back to their respective institution and try to encourage their colleagues in using more of these techniques in their research. Participants also felt that the organisation of the programme was good, in particular to the organiser's response to the participant's need. All the responses received stated that they would encourage members of their institution to attend similar activities in the future.

Most participants feel that a two week course is a just right to cover the lecture materials. Some feel that this duration is too short since there are too many materials that need to be covered in too short a time span. Others feel that two weeks is a little too long since they feel that their concentration span begin to dwindle after one week. Most participants would like the course for combinatorial chemistry and structure-based molecular design be separated. They feel this will make the course much easier for them to follow and understand. Participants would like to have more time should be spend on laboratory or hands-on training since they feel that this will provide them with the experience and feel of the techniques and is the most beneficial part of the course.

A summary of the evaluation of the questionnaire is attached as Annex VII.

SUGGESTIONS AND COMMENTS

A few suggestions given by the participants sounded valid and if possible, should be looked into further:

- 1. Most participants suggested that the course be divided into two parts rather than be offered all in one go; i.e., one training course dedicated towards structure-based molecular design and another dedicated only for combinatorial chemistry. In this way, topics covered could be more comprehensive, given the length of two weeks for the course. Many participants suggested that laboratory training on combinatorial techniques should be included, which will be however the main topic of the Training Course in Naples this September.
- 2. Another suggestion that may be useful to adapt is to separate the two courses offered by a week or two, i.e., giving a week or two break between the two different topics offered in the course. This way, more participants from the industries will be able to attend. One reason given by the industries in the ASEAN region for not being able to attend is that two weeks is too long for them to leave their work place. If the courses offered were broken up into two parts, they could send in two different scientists or researches to take part in the training course without any expense to their company.
- 3. Some participants suggested that the fundamental topics be omitted from the course. This is, however, not feasible given the diverse background of the participants attending the course.

ANNEX 1

FINANCIAL REPORT

	RM	RM
 INCOME		
Total receipt		106,010
 UNIDO 1 (32,000 USD)	80,510	
UNIDO 2 (8,000 USD) (estimate)	20,000	
 Sime-Darby System and SGI (M) Ltd.	5,000	
Bibi-Saintifik	500	
 EXPENDITURE		
 Total Expenditure		105,959.39
 Airfare	39,571.55	
Local transport	5,241.80	
 Hotel	16,200	
 Per Diem and daily expenses	15,294.04	
 Printing	4,870	, <u>,</u>
 Mails and faxes	1,860	
Rental	2,000	
 Administration and clerical	10,400	
 Incidentals	6,123	
Honorarium	4,400	
 BALANCE		51.61

Note:

- 1. The local organiser received a total cash of RM106,010 (estimated), of which mostly was ICS-UNIDO's contribution. University of Malaya provided the facilities (the SGI-Lab and the Pentium Lab) at a very minimal charge to cover for the technical staff overtime.
- 2. The distribution of expenditure is shown in the table, Over 40% of expenditure was used to cover airfare, accomodation and per diems for sponsored participants and lecturers (from oversea). Daily expenses (about 10%) include cost of morning and afternoon teas, participants stationeries lunches, visits and social events both for lecturers and participants.
- 3. Apart from cash support, the organiser also received substantial technical help from MSI, Oxford Molecular Group, Sime-Darby System (M) Ltd. and Silicon Graphic (M) Ltd. The two software companies also provided for the two lecturers who attended the course while the organiser provided for their local expenses.

List of Lecturers:

Professor Miertus

Associate Area Coordinator

International Centre for Science and High Technology

Pure and Applied Chemistry

Via Grignano 9-34014, Trieste, Italy

Fax: 0039-40-224-575

Dr. Annaliese Palmer Molecular Simulations B2/4 Glen Street

Milsons Point NSW 2061,

Australia

Fax: 61-2-9954 4388 email: liese@msi.com

Dr. Susanna Monti ICQEM-CNR

Ins. Di Chimica Quantistica ed Energetica Molecolare,

Risorgimento 35 56126 Pisa, Italy

e-mail:susanna@hulk.icqem.pi.cnr.it

FAX +39-50-502270

Dr. R.L. Singhal

Ranbaxy Research Laboratories A-2, Phase 1, Okhla Industrial Area

New Delhi, 110 020 India

Fax: 91-044-681-3676/ 91-044-681-4111

Dr. Giorgio Fassina Technogen S.C.P.A.

1015 Piana di Monte Verna (CE), Italy

e-mail:fassina@technogen.it

Fax: +39-823-612-230

Dr.Karl M. Smith

College of Pharmacy

University of Texas

Austin, Texas 78712 USA

e-mail:smith@naphthyl.phr.utexas.edu

fax: 1-512-471-7474

Dr. Vladimir Frecer

POLY-BIOS Research Centre

Area Science Park

I-34012 Trieste, Italy

Fax: 39-40 922 0016

e-mail:Vlado@gloria.icc.trieste.it

Dr. David Gallagher

Oxford Molecular Group Inc. 13475 SW Karl Braun Drive

Beaverton, Oregon 97077, USA

Fax: 1-503-526-5099

e-mail:dgallagher@oxmol.com

Dr. Sharifuddin Mohd. Zain

Dept. Of Chemistry

University of Malaya

50603, Kuala Lumpur, Malaysia

Fax: (603) 759-4193

e-mail:zain@kimia.um.edu.my

Associate Professor Dr. Onn Hashim

Department of Biochemistry

University of Malaya

50603, Kuala Lumpur, Malaysia

Fax: (603) 755-7740

Associate Professor Dr. Wan Ahmad Tajuddin

Department of Physics

University of Malaya

50603, Kuala Lumpur, Malaysia

Fax: (603) 759-4146

Dr. Ibrahim Noorbatcha

Department of Chemistry

University of Malaya

50603, Kuala Lumpur, Malaysia

Fax: (603) 759-4193

e-mail:ibrahim@kimia.um.edu.my

Dr. Chen Wei

Department of Chemistry

University of Malaya

50603, Kuala Lumpur, Malaysia

Fax: (603) 759-4193

e-mail:chenwei@kimia.um.edu.

Dr. Janez Mavri

National Institute of Chemistry

Hajdrihova 19

1000 Ljubljana, Slovenia fax: +386-61-1259244

11 . 01 1 21

email: janez@kihp2.ki.si

Associate Professor Dr. Rauzah Hashim (Lab

Sessions)

Department of Chemistry

University of Malaya

50603 Kuala Lumpur, Malaysia

e-mail: rauzah@kimia.um.edu.my

Fax: (603)-759-4193

Associate Professor Dr. Noorsaadah Abd.

Rahman (Lab Sessions)

Department of Chemistry

University of Malaya

50603 Kuala Lumpur, Malaysia

e-mail: noor@kimia.um.edu.my

Fax: (603)-759-4193

Mr. R. Murugadoss
Dept. Of Chemistry
Bharathidasan University,
620 024 India
e-mail: physics@cmld.rect.ernet.in

Dr Yenamandra Prabhakar Central Drug Research Institute Lucknow, 226 001 India e-mail: root@cscdri@ren.nic.in

Dr. D. K. Dikshit Central Drug Research Institute Lucknow, 226 001 India e-mail: root@cscdri@ren.nic.in

Dr. S. K. Agarwal Wiockhardt Research Institute D-4, M.I.D.C. Chikalthana Aurangabad, 431 210 India Tel: INDIA 482590, 485498 Fax: INDIA 485242

Dr. J.A.R.P. Sarma Indian Institute of Chemical Technology Hyderabad, 500 007 India e-mail:jarps@hotmail.com

Dr. Ahsis Mukherjee Ranbaxy Research Laboratories A-2, Phase 1, Okhla Industrial Area New Delhi, 110 020 India Fax: 91-044-681-3676

Dr. Biswajit Das Ranbaxy Research Laboratories A-2, Phase 1, Okhla Industrial Area New Delhi, 110 020 India Fax: 91-044-681-3676 Dr. C. S. Choxi Cadila Helthcare Ltd Ghodasar, Mininagar Ahmedabad, 380008 India Tel: INDIA 5354852 Fax: INDIA (079) 5323659

Mr. S. Mustaffa Shikh Konel Malaysia Sumitomo Metal Mining Shah Alam, Selangor, Malaysia Fax: (603) 582 0779

Dr. Awang Bono School of Science and Technology University Malaysia Sabah KM19 Jalan Tuaran Kota Kinabalu, 88999 Sabah, Malaysia e-mail:awang@pc.jaring.my

Dr. Nomisah Mohamad School of Pharmaceutical Science Universiti Sains Malaysia Minden, 11800 Penang Malaysia e-mail:nornisah@usm.my

Dr. Khozirah Shaari Medicinal Plant Division Forest Research Institute Kepong, Kuala Lumpur, Malaysia e-mail:khozirah@frim.gov.my

Dr. Wan Jeffry Basirun Department of Chemistry University of Malaya 50603 Kuala Lumpur Malaysia e-mail:jeffry@kimia.um.edu.my Dr. Zuriati Zakaria Department of Chemistry National University Malaysia 43000 Bangi, Selangor, Malaysia e-mail: zuriz@skrisc.cc.ukm.my

Dr. Monir Mohmoud Kashef RPScherer Egypt Borg El-Arab City Alexandria, Egypt Tel: 20-3-974161 Fax: 20-3-974158/974159

Mr. Mohamed Beshr Abd. El-Hamid RPScherer Egypt Borg El-Arab City Alexandria, Egypt Tel: 20-3-974161 Fax: 20-3-974158/974159

Miss Cindy Qingli Shi Department of Biology Hong Kong Baptist University Kwoloon Tong, Hong Kong e-mail:c5403221@net1.hkbu.edu.hk

Mr. Roberto Roy Genora Institute of Chemistry University of the Philippines Los Banos College Laguna 4031, Philippines e-mail: rrlg@chem.uplb.edu.ph

Miss Zainab Ngaini Fakulti of Sains dan Teknologi Universiti Sarawak Malaysia 94300 Kota Samarahan Sarawak, Malaysia e-mail:nzainab@frst.unimas.my Mr. Karim Yaacob Palm Oil Research Institute Kajang, Selangor Malaysia Tel: (603)- 8255708

Dr. Amir Feisal Merican Dept. of Genetics & Cellular Biology University of Malaya 50603 Kuala Lumpur, Malaysia e-mail:merican@gene.um.edu.my

Dr. Khalijah Awang Dept. of Genetics & Cellular Biology University of Malaya 50603 Kuala Lumpur, Malaysia e-mail:khalijah@gene.um.edu.my

T. Kaliyyappan
Department of Chemistry
Anna University
Madras - 600 025
e-mail:muthu@giasmd01.vsnl.net.in
(Did not turn up)

Dr. Ajay Vanjara
Micro-Analytical Lab.
University Department of Chemical
Technology
Matunga, Mumbai
400 019 India
e-mail: ssd@udct.ernet.in
(late response, cannot come)

* A participant from Petronas Research, Malaysia did not turn up.









	9:00 - 9:45	10:00 - 10:45		11:15 - 12:00	12:00 - 13:00		14:30 - 15:15	15:15 - 16:15		16:45 - 17:30	17:30 -18:30	
Mon. 28/7	Ореп	ing Ceremony ing morning tea)		Introduction to SBMD and CC Prof. S. Miertus	Lunch		L5, L6: Molecul Similarity; Molec Dr. K.	ular Recognition	Tea	L3,L4,L5: Intro. To CC & CC Biological. Assay and Econ Aspects of CC. Dr. R.L. Singhal		
Tues. 29/7	L1, L2 : Handling (SGI), Intro. t (UNIX) and Dr. Sharifuddin,	o Info. Tech. Lab. Session	Tea	L8: Introduction to Molecular Modeling Dr. A. Palmer	L9: X-Ray Crystallography Dr. Chen Wei	Lunch	LAB: P1: Intro. To Molecular Modeling and CC Dr. A. Palmer, Dr. Noorsaadah Dr. Rauzah, Dr. Smith		Modeling and CC Tea Structur Dr. A. Palmer, Dr. Noorsaadah Dr. A. 1		Structure and S Dr. A. Palmer,	olecular Graphics Stereochemistry Dr. V. Frecer, Dr. Sharifuddin
Wed. 30/7	LAB: P4: Similar Descr Dr. K. Smith, D Dr. Sharifuddi	iptors or. Noorsaadah,	Tea	L10: Physical Basis for Modeling Dr. A. Palmer	L11: Conformational Searching Dr. A. Palmer	Lunch	L12: Quantum Mechanics I (Principles) Dr. Sharifuddin	L13: Molecular Dynamics/Mech Dr. A. Palmer, Dr. Noorsaadah	Tea	L14: Protein Chem. And Enzyme Funct. Dr. Onn Hashim		
Thurs. 31/7	L15: Quantum Mechanics II (Application) Dr. J. Mavri	L16: Docking, Structure-Based Molec. Design Dr. A. Palmer	Tea	LAB: P5, P6: PD Building Mad Dr. A. Palmer, I Dr. R	cromolecules Dr. Noorsaadah,	Lunch	Free Programme					
Fri. 1/8	L17: Neural Network Dr. Wan Ahmad Tajuddin	L18: Molecular Bioavailability Prediction Dr. V. Frecer	Tea	L19: Ab Initio, Semi-Empirical and MM Dr. Ibrahim	Lunch Brea (Friday Prayer Muslims)	rs for	LAB: P7: Application of Molecular Orbital in SBMD Dr. K. Smith, Dr. Sharifuddin		Tea	Free Energy Per	P9: QM/MM turbation Theory , Dr. Ibrahim	
Sat. 2/8 Sun.	9:30 am – 12:30 p Dr. Monti, Dr. R	Individual Train	•	on Sharifuddin, Dr. Smi	Fre	ee Program	nme	KL Country Site Tour Bus Pick Up at Hotel Lobby at 1:45 pm me				
3/8 Mon. 4/8	Application of Methods in Bior	22: Overview Combinatorial n. Ind. Research Fassina	Tea	1		Lunch	la Lumpur L24, L25: Methods in Library Generation and Screening (Chem. and Biol. Application) Dr. G. Fassina LAB: P10: Application Tea 3-D QSA Dr. S. Monti, Dr. N Dr. Rauzah, Dr.			QSAR		
Tues. 5/8	L26: Application of Combinatorial Technology Industry in Biomedical Section (Case Study) Dr. G. Fassina		Tea	LAB: P11: Receptor 3-D Screening, Docking Dr. Monti, Dr. Noorsaadah, Dr. Sharifuddin, Dr. Rauzah		Lunch	LAB: P12: Application CC and CT in Chem. Industry (Case Study) Dr. G. Fassina, Dr. Rauzah, Dr. Noorsaadah, Dr. Sharifuddin		Tea	and Va Dr. Monti, D	maco. Generation ilidation r. Noorsaadah, ı, Dr. Frecer	
Wed. 6/8	(Lecture and S	SAR & QSPR oftware Demo) Gallagher	Tea	CC in Ligand Pharmaceut	LAB: P14: Application SBMD & CC in Ligand Design and Pharmaceutical Industry Prof. S. Miertus, Dr. V. Frecer		LAB: P15: <i>De Novo</i> Protein Engineering Dr. S. Monti, Dr. Noorsaadah, Dr. Frecer		Tea	Properties, Vis Dr. D. C		
Thurs.		cal by Design Gallagher	Tea	(Sess Dr. D. Gallagher	mical by Design ion I) , Dr. Sharifuddin, ah, Dr. Ibrahim	Lunch	(Sess Dr. D. Gallagher	mical by Design ion II) , Dr. Noorsaadah, r. Sharifuddin	Tea	Evaluation of	1: f Programme Miertus	
Fri.8/8		END O	F PROGE	RAMME		Lunch	DEPARTURE OF PARTICIPANTS					

Annex VI

Evaluation Questionnaires:

A. 1.	Organisation: How did you obtain th	ne inform	ation abou	it the w	vorkshop/	course?				
2.	The information proce		□ very ge	ood	□ good		□ fair			
3.	The announcement an	d pre-cou □ excell		ial was □ very		□ good	, (fair		
4.	I found the scientific	programn excell		□ very	good	□ good	.5	fair		
4.1.	Applied Lecture/Wo	rkshop □ excell	ent	□ very	good	□ good	C	fair		
4.2.	Use of Small Working	ng Group: □ excell		□ very	good	□ good		fair		
4.3.	Case Studies	□ excell	ent	□ very	good	□ good		fair		
4.4.	The time spent by lea	cturers in		after cl □ very		ecific que		nples fair		
4.5.	Student scientific know	owledge v Balan		⊃ Unba	alanced					
1.	Duration of Programm Number of days Length of working day				□ just ri □ just ri		□ too long		☐ too short ☐ too short	
C. 1. 2. 3. 4.	Training facilities & H Lecture/Training Roo Breaks/Refreshments Hotel accommodation Meals at the hotel	ms))	□ excel □ excel □ cxcel □ excel	llent llent	□ very g □ very g □ very g □ very g	good [good good	000000000 000000000 000000000	fair fair
if	"fa	ir"		pl	ease		exp	lain		why
D.	Organiser's response		pant's nee		000 go	ood		fair		
E.	Overall programme or cap excell		n □□ very	good	000 go	ood		fair		
F.	Would you recommen ☐ Yes		rs from yo			untry to a	ittend a sim	ilar act	ivity in the future?	1
1.	Which part of the activ	vity did y	ou find m	ost use:	ful?					
2.	Which part of the activ	vity do yo	ou think sh	ould b	e expande	d?				

3. Which part of the activity do you think should be dropped?

4.	Any other suggestions for future improvements to the programme?							
5.	Do you think that the topics/tools you studied during the course could be used by industries in your country? If so, how? If not, why not?							
6.	Can you suggest any programme and future activities which ICS could pursue in order to help with the technological and scientific advancement of your country?							
7.	Do you think you have benefited from participation in this course/workshop? If so, how? And your institution?							
8.	How do you intend to disseminate the own country?	information you	have acquired duri	ng the activity once	back in your			
G. 1. fair	Evaluation of Lectures and Speakers Course materials	□ excellent	□ □ very good	□□□ good	0			
2.	Resident Lecture Presentation fair	□ excellent	□□ very good					
3. 4.	International Lecture Presentation fair	□ excellent	□□ very good	□□□ good				
5. 6. fair	Ability of lecturers to answer specific questions excellent very good good							
Any	comments:							
Tha	nank you for your collaboration							

Annex VII Summary of Analysis of Evaluation:

A. Organisation:

A. ORGANISATION	Excellent (%)	Very Good (%)	Good (%)	Fair (%)
The information process	15	40	30	15
The announcement and pre-course material	0	28	39	22
I found the scientific programme	21	47	.32	0
Applied Lecture/Workshop	21	42	32	5
Use of Small Working Group	17	33	44	5
Case Studies	5	53	42	0
The time spent by lecturers in class and after class on specific questions/examples	21	42	37	0
Organiser's response to participant's needs	32	32	37	0
Overall Programme Organisation	10	50	30	10

	Balanced	Not Balanced
	(%)	(%)
Student scientific knowledge	60	40

B. Duration of Programme	Just Right (%)	Too Long (%)	Too Short (%)
Number of days	60	30	10
Length of working days	65	35	0

D. Training Facilities and Hotel	Excellent (%)	Very Good (%)	Good (%)	Fair (%)
Lecture/ Training Rooms	37	37	26	0
Breaks/Refreshments	25	50	15	10
Hotel Accommodation (Applicable to only 13 participants)	9	27	64	0
Meals at the Hotel (Applicable to only 13 participants)	0	15	54	31

	Yes (%)	Maybe (%)	No (%)
Would you recommend to others from	your		
institution/country to attend a similar activity in the fu	ture 95	5	0

G. Evaluation of Lectures and Speakers	Excellent (%)	Very Good (%)	Good (%)	Fair (%)
Course Materials	30	45	25	0
Resident Lecture Presentation	15	45	40	0
International Lecture Presentation	20	60	20	0
Ability of lecturers to answer specific questions	21	68	11	0

.