ANNUAL REPORT

2007-2008



Indian Institute of Science Education and Research(IISER) Mohali

31, March 2008

Contents

1	Preface	3
2	Board of Governors	6
3	Senate	8
4	Administration	9
5	Academic Staff5.1Faculty	9 9 10 10
6	Progress made in 2007-086.1Milestones6.2New Campus6.3Facilities created6.3.1Computing Facility6.3.2Library6.3.3Teaching Labs6.3.4Lecture Rooms6.4.1Biology6.4.2Chemistry6.4.3Physics6.4.4Central Analytical Facility	10 10 11 11 11 12 12 12 12 12 12 14 15 17
7	Academic Programs Started7.1 Integrated MS in science7.2 Doctoral program in Science	17 17 17
8	Faculty Publications	17
9	 Meetings/Conferences/workshops organized 9.1 Workshop on Mathematics Education and Research in Punjab 9.2 Curriculum Committee Meeting for IISER Mohali 	18 18 18
10	Faculty Activity	19
11	Visits by Foreign Scientists	20

12	Sponsored Projects	20
13	Awards and honours received 13.1 Faculty	
14	13.2 Students	23 23
15	Accounts Statement	27
	15.1 Balance Sheet	28
	15.2 Receipts & Payments	29
	15.3 Income & Expenditure Account	
	15.4 Research & Development Account	33

1 Preface

The Indian Institutes of Science Education & Research (IISERs) were established by the Ministry of Human Resource Development (MHRD), Government of India, based on the recommendation of the Scientific Advisory Council to the Prime Minister. Currently, five IISERs have been created and are functioning at Pune, Kolkata, Mohali, Bhopal and Thiruvananthapuram. The IISERs have been patterned after the Indian Institute of Science (IISc) Bangalore in terms of high quality research in the basic sciences, but the IISERs in addition have a focus on high quality education in the basic sciences at the undergraduate as well as the postgraduate level. Each IISER is an autonomous institution and will award its own degrees. The financial outlay for each IISER is around Rs. 500 crores over a period of five years, with the aim to create state-of-the art research and teaching laboratories, library and computational facilities. The projected strength of each IISER in the next five years is around 2000 students (undergraduate as well as doctoral research fellows) and 200 faculty members in all core departments.

The basic mandate of the IISERs is to carry out research in frontier areas of science and to provide quality science education at the undergraduate and the postgraduate level. The major focus at IISER Mohali is to create a world class scientific institution with an intellectually alive research atmosphere.

IISER Mohali's transit campus is currently located at MGSIPAP Complex, Sector 26 Chandigarh, in space allocated by the State Government of Punjab. IISER Mohali's new fully residential campus will be developed on 125 acres of land in the Knowledge City at Sector 81 Mohali. The new campus is around 15Km from the center of Chandigarh city, and will be easily accessible from Mohali's envisaged international airport. Architectural plans for the new integrated campus include academic blocks, an administrative block, halls of residences for students, central computing and library buildings, central analytical facility, faculty and staff residential complex, sports & recreation facilities, institute guesthouse, and additional support infrastructure such as a health center, campus creche & childcare facilities, and a bank.

The 5 year MS (Int) program in Science at IISER Mohali admits students after 10+2. The course structure is interdisciplinary and research oriented in nature, with a focus on basic sciences. The curriculum provides comprehensive core courses in the first two years of the programs in all areas of basic sciences: chemical, physical, mathematical and biological sciences. After the first two core years, students can branch out to contemporary areas of interdisciplinary research of their choice. In addition to the basic courses, IISERs will also have courses in the interdisciplinary areas of earth, planetary and environmental sciences, computational sciences, humanities and social sciences. With a firm foundation in basic sciences and mathematics in the first two years, the students will be able (with counseling) to choose the subject in which they will major including interdisciplinary areas. An early exposure to research through summer training in other laboratories and institutions of the country, including industrial organizations, and counseling schemes for major R&D career opportunities are other attractive features of the program. To begin with, 25 students have been admitted to the integrated Masters program at IISER Mohali in the session that began on 16th August 2007. These students were admitted on basis of "Extended JEE List" of the IITs, KVPY and Indian National Olympiad selection. The 5-Yr MS(Int) graduates of IISER Mohali are expected to take up science as a career, although the diverse skills gained will equip them to pursue high-profile careers in any field, including industry.

Through liaison with research laboratories under the Department of Atomic Energy, Space, Science and Technology and Biotechnology, as well as the Council of Scientific & Industrial Research, opportunities will be created for job placement for students on the basis of campus interviews. The fifth year of the integrated Masters program will be devoted to full time research or to a technical project or to specialized training, in which the students will have to write a dissertation. The research component results in lowering of the average period for obtaining Ph.D. degree, for those students who pursue a doctoral program at IISER. Provisions for an accelerated development for truly deserving individuals will be a special feature of the program. The IISERs will maintain a high standard of education, training and scholarship, comparable to the best Indian institutes and international universities in various areas of learning. In addition to the integrated Masters program, the IISER will also have a post B. Sc. integrated Ph. D. program, as well as a doctoral program (post M. Sc.). All teaching activities will be based on a semester system accompanied by vigorous teacher-student contact through research, journal clubs, seminars and colloquia. Rigorous laboratory courses will be an essential part of the program.

IISER Mohali aims to be a "knowledge basin of attractor" in the northern region in India within the next decade. In this context, the institute plans on developing a synergetic network with other academic institutions both in India and abroad, and will hold regular conferences, seminars and symposia in research areas as well as workshops aimed at addressing fundamental issues in science education in India.

The doctoral program at IISER Mohali involves course work, a qualifying examination, thesis work and a thesis examination, leading to the award of a PhD degree. Besides research, scholars will be involved in several professional activities such as seminars, workshops and review meetings. The institute has provisions for a number of post-doctoral fellowships as well. Research infrastructure currently available at IISER Mohali includes a computing facility, an instrumentation facility and a modern library with access to many research journals and on-line databases. IISER Mohali aims to have a strong core faculty selected on a highly competitive basis and supported by attractive startup research grants. Young bright scientists including those wanting to return to India from abroad for teaching and research careers will be specially considered for faculty positions. Current faculty research at IISER Mohali spans a diverse spectrum ranging from theoretical chemistry, quantum information processing, metamaterials and spectroscopy to inorganic, physical chemistry, algebra, immunology and biophysics.

2 Board of Governors

- Professor P. Rama Rao (Chairman) Former Secretary, Department of Science and Technology, International Advanced Research Centre for Powder Metallurgy and New Materials (ARCI), Balapur P.O. Hyderabad 500005.
- Shri R P Agrawal IAS (Member) Secretary (HE), MHRD, Shastri Bhavan, New Delhi 110001.
- Shri Ramesh Inder Singh IAS (Member) Chief Secretary, Government of Punjab, Chandigarh 160 001.
- Dr. Anil Kakodkar (Member) Secretary, Department of Atomic Energy, Anushakti Bhavan, CSM Marg, Mumbai 400001.
- Dr. T. Ramasami (Member) Secretary, Department of Science and Technology, Technology Bhavan, New Mehrauli Road, New Delhi 110016.
- Dr. M. K. Bhan (Member) Secretary, Department of Biotechnology, CGO Complex, Lodi Road, New Delhi 110003.
- Professor P. Balaram (Member) Director, Indian Institute of Science, Bangalore 560012
- Professor Surendra Prasad (Member) Director, IIT Delhi Hauz Khas, New Delhi 110016.
- Professor K. N. Ganesh (Member) Director, IISER Pune,

900 NCL Innovation Park, Homi Bhabha Road, Pune 411008.

- Professor S. V. Kessar (Member) Department of Chemistry, Punjab University, Chandigarh 160014.
- Professor A. K. Sood (Member) Professor of Physics, Indian Institute of Science, Bangalore 560012.
- Professor Ashutosh Sharma (Member) Department of Chemical Engineering, IIT Kanpur Kanpur 208016
- Professor S. G. Dani (Member) School of Mathematics, TIFR, Homi Bhabha Road, Mumbai 400 005.
- Shri S. K. Ray (Member) Joint secretary & Financial Adviser, MHRD, Shastri Bhavan, New Delhi 110001.
- Professor Ramesh Kapoor (Member) IISER Mohali, MGSIPAP complex, Sector 26, Chandigarh 160019.
- Professor C.G. Mahajan (Member) IISER Mohali, MGSIPAP complex, Sector 26, Chandigarh 160019.
- Professor N. Sathyamurthy (Ex-officio) Director IISER Mohali, MGSIPAP complex, Sector 26, Chandigarh 160019.
- Shri J. P. Singh (Secretary) Registrar, IISER Mohali, MGSIPAP complex, Sector 26, Chandigarh 160019.

3 Senate

- Professor N. Sathyamurthy (Chairman) Director, IISER Mohali.
- Professor R. C. Sobti (Member) Vice-Chancellor, Panjab University Chandigarh-160 014
- Professor S. C. Laroiya (Member) Director N.I.T.T.R. Chandigarh -160 019
- Professor Vijay Gupta (Member) Vice-Chancellor, Lovely University Jalandhar.
- Dr. P. Rama Rao (Member) Director, NIPER Sector-67, SAS Nagar Mohali-160 062
- Professor Ashok Sahni (Member) Centre for Advanced Study in Geology, Panjab University, Chandigarh, 160014
- Prof. S. V. Kessar (Member)
 Department of Chemistry,
 Punjab University, Chandigarh, 160014
- Dr. A. K. Bachhawat, (Member) IMTECH Chandigarh-160 036
- Professor R. Kapoor (Member) Dean Academic, IISER Mohali
- Professor C. G. Mahajan (Member) Dean Students, IISER Mohali

- Professor I. B. S. Passi (Member) Honorary Professor IISER, Mohali
- Dr. Arvind (Member) Dean R&D, IISER Mohali
- Dr. Kavita Dorai (Member) IISER Mohali
- Mr. J. P. Singh (Secretary) Registrar, IISER Mohali

4 Administration

Director	Prof. N. Sathyamurthy
Dean (Academic)	Prof. R. Kapoor
Dean (Students)	Prof. C.G Mahajan
Dean (R&D)	Dr. Arvind
Registrar	Shri J.P. Singh
Coordinator	Dr. Jagdeep Singh (Punjab Government)
Warden	Dr. Manash Kumar Paul

5 Academic Staff

5.1 Faculty

- 1. Prof. N. Sathyamurthy (Prof Chemistry) Research area: Theoretical chemistry, Reaction dynamics
- 2. Prof. R. Kapoor (Prof Chemistry) Research area: Inorganic chemistry
- 3. Prof. C.G. Mahajan (Prof Physics) Research area: Optics
- 4. Dr. Arvind (Assoc Prof Physics) Research area: Quantum information theory, Quantum optics

- 5. Dr. Kavita Dorai (Asst Prof Physics) Research area: NMR methodology, Quantum computing
- Dr. Sanjay Singh (Asst Prof Chemistry) Research area: Inorganic synthetic chemistry, Gold chemistry
- 7. Dr. Tapan Mukherji (Asst Prof Biology) Research area: Molecular biology,Immunology
- 8. Dr. Manash Kumar Paul(Lecturer Biology) Research area: Cancer Biology

5.2 Honorary Faculty

- 1. Prof. I. B. S. Passi (Hon Prof Mathematics) Research area: Algebra
- 2. Prof. Anil Kumar (Hon Prof Physics) Research area: NMR Spectroscopy

5.3 Adjunct Faculty

- 1. Girish Sahni (Biology) Director IMTECH Chandigarh
- 2. C. S. Aulakh (Physics) Professor PU Chandigarh
- 3. A. K. Bachhawat (Biology) Scientist IMTECH Chandigarh
- 4. Jagdeep Singh (Biology) Punjab Govt.
- 5. P. Guptasarma (Biology) Scientist IMTECH Chandigarh
- 6. Alok Mandal (Biology) Scientist IMTECH Chandigarh

6 Progress made in 2007-08

6.1 Milestones

- Foundation stone laid on 27th Sept 2006 by the Prime Minister of India.
- Prof.N Sathyamurthy joined IISER Mohali as the first Director on 18th June 2007.

- The first meeting of the Board of Governors held on 18th July 2007.
- The first meeting of the Senate held on 02nd Aug 2007.
- The classes started on 16th Aug 2007.
- The computer facility inaugurated on 03rd Sept 2007 by Dr. T Ramasami (Secretary, DST)
- The transit campus inaugurated on November 13th 2007 by Sri Ramesh Inder Singh(IAS) Chief Secretary, Punjab.

6.2 New Campus

The master plan for IISER Mohali's new fully residential 125 acre campus coming up in the Knowledge City at Sector 81 Mohali has been finalized.

6.3 Facilities created

6.3.1 Computing Facility

A computing facility has been setup in IISER Mohali to cater to the research requirements of the faculty and as an educational resource. It is a Linux-based set of computers and the current CPU power will soon be augmented in order to create a parallel Linux cluster. Wireless LAN facility has also been setup and is available to the faculty. The computing facility was inaugurated on September 03rd 2007 by Dr. T. Ramasami (Secretary, DST)

6.3.2 Library

A library has been created with a large number of textbooks for undergraduate and postgraduate students. A large number of online research Journals and databases have been subscribed to.

6.3.3 Teaching Labs

Name	Number	Capacity
Biology Teaching Lab	1	30
Physics Teaching Lab	1	30
Chemistry Teaching Lab	1	30
Electronics Teaching Lab	1	30

6.3.4 Lecture Rooms

Name	Number	Capacity
Seminar Room	1	75
Conference Room	1	50
Class Room	1	50

6.4 Equipment Purchased

6.4.1 Biology

- S. No. Description
- 1. AICIL BOD Incubator
- 2. Horizontal Electrophoresis systm, Complete
- 3. Semi Dry Blotting systems
- 4. Vertical Electrophoresis systm
- 5. Gel Drying Systems
- 6. Gel Documentation Systems
- 7. Gradient Thermal Cycler
- 8. Pump with Filtration assembly
- 9. Refrigerated Table Top Multipurpose Centrifuge
- 10. Refrigerated Micro Centrifuge

- 11. High Speed Micro Centrifuge
- 12. UV-vis Spectrophotometer
- 13. Ice Flaker
- 14. Neo lab Water Bath Shaker
- 15. Refrigerator Shaking Incubator
- 16. CO_2 Incubator
- 17. Ultra Low Freezer
- 18. Water Bath Shaker Incubator
- 19. Gel Staining Shaker
- 20. NSW- 229 Autoclave
- 21. NSW-227 Vertical Autoclave
- 22. Micro Centrifuge, Sigma
- 23. Analytical Balance
- 24. Electronic Analytical Weighing Balance
- 25. Electronic Precision Balance
- 26. Water Bath
- 27. Magnetic stirrer, IKA
- 28. Microwave Oven, Samsung
- 29. Vertical Deep Freezer Stabilizer
- 30. Water Purification systm
- 31. Laminar Airflow, Godrej
- 32. Advance Binocular Microscope
- 33. Refrigerator Samsung, RT 31
- 34. PH Meter
- 35. Micro Centrifuge, Spin win
- 36. Spinix Vortex shaker

- 37. Magnetic Stirrer, 1L Remi
- 38. Magnetic stirrer 2L, without hot plate
- 39. do -, with hot plate
- 40. Water Bath Shaker
- 41. High Speed Refrigerated table top Centrifuge
- 42. Luminescence Spectrometer, Perkin Elmer
- 43. Air Purifier
- 44. Binocular Microscope, Labex
- 45. Magnetic Stirrer with heating

6.4.2 Chemistry

S. No.	Description
N: 110:	DODOLIDUIOI

- 1. PH/Conductivity Meter
- 2. Conductivity Meter
- 3. Melting Point Apparatus
- 4. Oil Free Vacuum Pump
- 5. Electronic Balance, 0.001g
- 6. Water Bath Rectangular
- 7. & High Pressor Water Bath
- 8. High Temperature Furnace
- 9. Analytical Balance, BT 2245
- 10. Magnetic Stirrer, IKA
- 11. Magnetic Stirrer with heating, white coated
- 12. IKA Rotary Evaporator with Magnetic Bars
- 13. MRC Aspirator
- 14. Ultrasonic Bath
- 15. Centrifugal Pump

- 16. 4 feet Fume-hood, Bench-type
- 17. Microwave Oven, Samsung
- 18. Magnetic Stirrer with hot plate
- 19. Micro pipette controller
- 20. Lab jack
- 21. Hot plate
- 22. Oil free Vacuum Pump
- 23. Electronic Balance, Analytical
- 24. Electronic Balance 0.01gm
- 25. PH/Conductivity Meter
- 26. Refrigerator, Samsung RT 31
- 27. Oven 350x350x350mm
- 28. Oven 600x600x600mm

6.4.3 Physics

- S No. Description
- 1. Diffraction Optical Bench
- 2. Phywe Equipments
- 3. Digital Trainer Board
- 4. Function Generator
- 5. Digital Gauss Meter
- 6. True RMS AC Multimeter
- 7. Tektronix Oscilloscope 60 MHz
- 8. Tektronix Oscilloscope 100 Mhz
- 9. Tektronix Function Generator
- 10. Pasco Equipments
- 11. Analog Oscilloscope

- 13. Screw Gauge 0-25mm
- 14. Standard Spectrometer
- 15. Research Spectrometer
- 16. 'g' by free fall apparatus
- 17. Young modulus brass
- 18. Torsion Pendulum
- 19. Maxwell Needle Brass
- 20. Kater's Pendulum
- 21. Compound Pendulum
- 22. Sodium Light Source
- 23. Crown Glass Prism
- 24. Extra Dense flint glass prism
- 25. Diffraction gratings
- 26. Spherometers
- 29. Digital stop watch
- 30. Spirit level, Bigger
- 31. Simple reading telescope
- 32. Bending of beam apparatus
- 33. Traveling microscope
- 34. Mercury light source
- 35. Stop watch module
- 37. Constant deviation spectrometer
- 38. Balance, 1kg
- 49. Electromagnetic Induction Apparatus
- 40. Function generator 2 Mhz

6.4.4 Central Analytical Facility

IISER Mohali has ordered two high-field high-resolution NMR spectrometers which will operate at proton frequencies of 600MHZ and 400MHZ. This will be an institute level facility to be used by scientists from all disciplines.

7 Academic Programs Started

7.1 Integrated MS in science

In August 2007, 42 students were admitted to the 5-Yr Integrated MS program in Science, of which 25 students joined the program. These students were admitted based on National Science Olympiad, KVPY and IIT JEE extended merit list.

7.2 Doctoral program in Science

Two students were admitted into the Doctoral program: one in Biology and one in Mathematics.

8 Faculty Publications

- 1. Hydrogen bonding in protonated water clusters: An atoms-in-molecules perspective, R. Parthasarathi, V. Subramanian and N. Sathyamurthy, J. Phys. Chem. A 111, 13287-13290(2007).
- 2. DTT abrogates the effect of Arsenic trioxide on normal rat mitochondria and human hepatocellular carcinoma cell line, M. K. Paul, R. Kumar & A. K. Mukhopadhyay, Toxicology and Applied Pharmacology 2008, 226:140-52.
- Book Review "Quantum Computing Back Action 2006, AIP Conference Proceedings Vol. 864, Debabrata Goswami (ed.)", Kavita Dorai, Current Science Vol. 94 No. 3,392-393 February 2008.
- 4. Presidential Address (General), I.B.S. Passi, Mathematics Student 75 (2006/07, 29-35.
- 5. Presidential Address (Technical): Homological and Combinatorial Methods in Group Rings, I.B.S. Passi, Mathematics Student 75 (2006/07), 37-63.
- Commutator subgroups of free nilpotent groups, N. Gupta and I.B.S.Passi, Int. J. Algebra Comp., 17 (2007), 1021-1031.

- Homology of centralizers, R. Mikhailov and I. B. S. Passi, Comm. Algebra, 35 (2007), 2191-2207.
- Group homology and extensions of groups, Homology, Homotopy and Applications, I. Emmanouil and I. B. S. Passi, 10 (2008), 237-257.

9 Meetings/Conferences/workshops organized

9.1 Workshop on Mathematics Education and Research in Punjab

The faculty of the Indian Institute of Science Education and Research, Mohali, organized on 15 February 2008 at the transit campus of the Institute - Mahatma Gandhi Institute of Public Administration Punjab Complex, Sector 26, Chandigarh - a one-day workshop on Mathematics Education and Research in Punjab. The workshop was inaugurated by Shri Ramesh Inder Singh(IAS), Chief Secretary, Government of Punjab, and attended by Vice-Chancellor, Panjab University, Professor R. C. Sobti, President of the Indian Mathematical Society, Professor R. B. Bapat, a number of mathematicians and senior officers of the Government of Punjab connected with various departments of education. The deliberations at the workshop focused on the status of mathematics education and research in the state with the aim of formulating recommendations for its improvement. The initiative for this activity was the result of the deep concern felt by the Chief Secretary for improving the interest in science among students of Punjab. The workshop was also motivated by the desire of the Director, Professor N. Sathyamurthy, and the faculty at IISER to explore possible ways of making contribution to the development of science in the region as a part of its overall objective of integrating science education with research so that undergraduate teaching as well as doctoral research work is carried out in symbiosis. The recommendations have been sent the Govt. of Punjab for implementation.

9.2 Curriculum Committee Meeting for IISER Mohali

- A National level Curriculum Committee was constituted by the Director, to draft the course structure for the five year Integrated MS program in Science.
- The committee met during 05-07th November 2007 at IISER Mohali and deliberated on all aspects of the course structure and curriculum for the MS program at IISER.

- The committee finalized the structure for the first two (core) years of the program.
- Based on the discussions that took place during the meeting, sub-committees were formed for different subjects to finalise the course structure and content for the five year Integrated MS program.

10 Faculty Activity

- 1. Dr. Arvind delivered an invited lecture at Govt. College for Women Amritsar, (27.10.07) on "From Classical to Quantum Physics".
- 2. Dr. Arvind delivered a set of two lectures in the refresher course of physics teachers at GNDU Amritsar during Dec.8-10 2008.
- 3. Dr. Kavita Dorai attended the 14th Meeting of NMRS, INMAS New Delhi Jan 16th-19th 2008 and delivered an invited talk on "Exploring the limits of eigenbase quantum computing".
- 4. Dr. Kavita Dorai delivered an invited talk in the Physics Department, Punjab University Chandigarh Jan 31st 2008 on "Perspectives in NMR Quantum Computing: Decompositions of the QFT using selective pulses".
- 5. Prof. N. Sathyamurthy delivered an invited talk in Indo-German Symposium, Indian Institute of Chemical Technology, Hyderabad, September 2007.
- 6. Prof. N. Sathyamurthy delivered an invited talk in JNC Frontier Lectures, Guru Nanak Dev University, Amritsar, October 24-26, 2007.
- 7. Prof. N. Sathyamurthy delivered an invited talk in Indo-German Symposium on Frontiers in Chemistry, IIT Kanpur Kanpur October 26-28, 2007.
- 8. Prof. N. Sathyamurthy delivered a colloquium an invited seminar at Physical Research Laboratory, Ahmedabad December 12, 2007.
- 9. Prof. N. Sathyamurthy delivered a talk organized by the INSA local chapter, Department of Chemistry, Panjab University, Chandigarh January 24, 2008.
- Prof. I. B. S. Passi attended the Anniversary General Meeting of the Indian National Science Academy held at the National Institute of Oceanography, Goa, 23-25 December 2007.

- 11. Prof. I. B. S. Passi attended the Annual Conference of Indian Mathematical Society held at the University of Pune, Pune, 27-30 December 2007.
- Prof. I. B. S. Passi delivered a A series of three talks on Homological Algebra in the Seminar on Algebra and Number Theory, Department of Mathematics, Panjab University Chandigarh [25 October, 1 November, and 22 November 2007].
- 13. Prof. I. B. S. Passi delivered Two talks on Theory of Groups at the Department of Mathematics, University of Delhi, Delhi, March 2008.

11 Visits by Foreign Scientists

- 1. During the period December 6-9th 2007, the eminent Czech quantum information theorist Prof Jozef Gruska visited IISER Mohali and delivered an institute colloquium. He had extensive academic discussions with the IISER faculty working in the areas of quantum information theory and quantum computing.
- 2. During the period January 28 February 07 2008, two Russian mathematicians Prof J Mostovoy (Mexico Univ) and Prof R Mikhailov (Moscow Univ), visited IISER Mohali for research collaborations and delivered talks. They held various research discussions with mathematics faculty.
- 3. Prof Tucker Carrington from Queen's university Kingston, Canada visited IISER Mohali during the period February 17-19 2008. He delivered seminar and held extensive discussions with the faculty working in the area of quantum computational chemistry.

12 Sponsored Projects

1. **Project Title:** "Conformational Dynamics of Model Tripeptides using NMR and Vibrational Spectroscopic Techniques"

Funding Agency	:	DST (Under Fast Track Scheme)
PI	:	Dr. Kavita Dorai (IISER Mohali)
Duration	:	2007-2010
Amount	:	5.7 Lakhs

Description:

This project seeks to undertake a conformational dynamics analysis of model tripeptides using NMR and vibrational spectroscopic techniques such as polarized Raman spectroscopy and compare the experimental results with those obtained from MD simulations. A combination of NMR, FTIR and Raman spectroscopic techniques is a powerful means of obtaining detailed information about the conformational properties and dynamics of biomolecules. Tripeptides are biomedically relevant as protease inhibitors, as taste receptors and for enzyme regulation. They also serve as a molecular scaffold for drug design and understanding their structural features is useful for the design of small bioactive peptides, using different experimental approaches to monitor their conformational stability in different biological environments. Such complementary methods will aid in understanding the relationship between structure, function and dynamics of proteins and peptides.

2. **Project Title:** "Studies of dissipative dynamics in quantum computers using NMR techniques"

Funding Agency	:	CSIR
PI	:	Dr. Kavita Dorai (IISER Mohali)
Co-PI	:	Dr. Arvind (IISER Mohali)
Duration	:	2007-2010
Amount	:	3.29Lakhs

Description:

The rapidly evolving field of quantum information processing is one of the most active areas of modern science and as such, attracts substantial funding with well-organized research programmes in countries like the United States, the European Union, Australia and other industrial nations. The race is on worldwide to develop viable and sufficiently complex quantum computing technologies that will be used as testbeds to explore architectural and algorithmic issues in quantum computer science. It is expected that there will be considerable synergy with other exciting fields such as communication and cryptography, nanotechnology and spintronics. The future of QIP is bright and will lead to unprecedented advances in fundamental scientific understanding and practical new technologies. In this project we plan to utilize our expertise in the field of NMR quantum computing to develop a consistent methodology to gain theoretical insights into the fundamental problems of quantum decoherence and develop experimental techniques to address problems of dissipation in physical realisations of quantum computers. In the long term, we wish to develop a research program to study quantum dissipation using NMR and to advance our understanding of fundamental aspects of quantum theory and quantum information processing.

3. **Project Title:** "Exploring biomolecular dynamics using cross correlated spin relaxation in NMR"

Funding Agency	: DBT
PI	: Dr. Kavita Dorai (IISER Mohali)
Co-I	: Dr. P. B. Sunil Kumar (IIT-Madras)
Duration	: 2008-2010
Amount	: Financial sanction awaited

Description:

This project seeks to undertake a detailed study of how various motional processes in biomolecules affect spin relaxation in NMR and how these processes can be related to experimentally measured cross-correlation relaxation rates. A more concrete understanding of biomolecular dynamics will be gained, by developing several experiments to exploit cross-correlated spin relaxation pathways and applying the pulse schemes to standard proteins. Cross correlation rates will be used to gain insight into phenomena such as the relative orientation of chemical bonds and to measure the extent of intramolecular mobility by characterising precisely the mobility of sidechains, the protein backbone and hydrogen bonds in proteins. The proposed study aims to develop a more complete theoretical description of the influence of biomolecular dynamics on different cross-correlation rates by using different motional models including anisotropic local motion. The expected outcome of the proposed study is a quantitative understanding of biomolecular dynamics using cross correlation relaxation experiments on model systems. Further, it is hoped that the study will shed some light on the bigger questions in molecular biology such as the influence of dynamics on biomolecular function.

13 Awards and honours received

13.1 Faculty

- 1. Appointment of Prof. N. Sathyamurthy, Director IISER Mohali, as Honorary Professor, JNCASR Bangalore.
- 2. A. V. Rama Rao Research Foundation lecture, JNCASR Bangalore to Prof. N. Sathyamurthy, Director IISER Mohali.

13.2 Students

 The CNR Rao Foundation has instituted a cash prize of Rs. 5000/- for the best student in each semester of the first year of MS programme at IISER Mohali. Mr. Sameep Chandel received the prize for the year 2007-08 I semester on Jan 26th 2008 from the Director IISER Mohali.

14 Colloquia and Technical Seminars held

- 1. 26, March 2008 (Wed 4pm) Prof. Narendra Nath (Kurukshetra) "Mysteries of the Universe- a perspective".
- 2. 25, March 2008 (Tue 4pm) Dr. Swarup Chattopadhyay (Ohio Univ. USA) "Biomimetic chemistry at Paramagnetic Nickel(II) center".
- 3. 18, March 2008 (Tue 4pm) Gautam Karan (Univ Utah USA) "Genetic association of Macular Degeneration with ELOVL4- a model approach".
- 4. 17, March 2008 (Mon 3pm) Arunika Mukhopadhaya (New York) "Dendritic cell mediated tolerization of autoreactive T cells: a novel therapeutic approach for Type 1 diabetes".
- 5. 17, March 2008 (Mon 2pm) Dr. Kausik Chattopadhyay (New York) "Structural basis of T-cell costimulation by GITR ligand".
- 6. 11, March 2008, Dr. Amreesh Chandra (Univ. of Surry UK) "Tailored Oxide Ceramics and their Polymer Composites"
- 7. 05, March 2008, Subhasish Banerjee (RRI Banglore) "Phase Distributions in open Quantum Systems"

- 8. 03, March 2008, Subhendu Rakshit (University of Dortmund) "Ice Fishing for NeutrinosIce Fishing for NeutrinosIce"
- 9. 28, Feburary 2008, Prof. Kankan Bhattacharyya (IACS Kolkata) "History of Raman Effect and Resurgence of Modern Science in India"
- 10. 27, Feburary 2008 Prof. Kankan Bhattacharyya (IACS Kolkata) "Femtosecond Laser: A new tool to study dynamics in biological systems"
- 11. 25, Feburary 2008 Dr. Rajneesh K Gaur "Structural and Biochemical insights on the mechanism of Ape enzyme"
- 25, Feburary 2008 Dr.Arulananda Babu (Osaka Univ, Japan) "An Emerging, Highly Efficient Metal in Synthetic Organic Chemistry"
- 13. 22, Feburary 2008 Dr. Jhumpa Mukherjee "Inorganic and bioinorganic perspectives of copper(II), cobalt (II) and iron (II) complexes"
- 14. 21, Feburary 2008 Dr. Kamal Kapoor (Jammu Univ) "Towards greener chemistry: Development of new methodologies and synthesis of heterocycles of biological significance"
- 15. 21, Feburary 2008 Dr. Gurunath (IITK) "Modelling the Green Fluorescence Protein Lumophore- interesting results and some intriguing application"
- 16. 20, Feburary 2008 Prof. Ajay Sood (IISc. Bangalore) "Nano-Carbon: Graphene and Nanotubes"
- 17. 20, Feburary 2008 Dr. S. Sinha (SNBCBS) "Ultracold atomic gases in optical lattice"
- 18. 19, Feburary 2008 Dr. S. Anantha Ramakrishna (IIT Kanpur) "Focusing the optical near-field using negative refractive index media"
- 19. 18, Feburary 2008 Tucker Carrington Jr. (McGill University Canada) "Vibrational spectrum of CH5+"
- 20. 30, January 2008 Prof. Ravi. S. Kulkarni (IIT Bombay) "Modular Group and its Subgroups"
- 21. 25, January 2008 Dr Boomi Sankar (Liverpool Univ UK) "From multi-anionic phosphazenates to multi-cationic phosphazenium ions: Versatile ligands for molecular assemblies"

- 22. 25, January 2008 Dr Kamal Singh (MPIKS Dresden Germany) "Femtosecond Photoionization of Atoms"
- 23. 23, January 2008 Dr Pratik Sen (Riken Japan) "Structure and Dynamics at Biological Interfaces: A Femtosecond Surface Sum Frequency Generation and Up-conversion study"
- 24. 18, January 2008 Kiran Kumar Maiti (Germany) "A challenge to explore structure and ultrafast dynamics of protein and peptide using 2D IR spectroscopy"
- 25. 15, January 2008 Dr Kausik Das (Univ of Toronto, Canada) "Surface Thermal Capacity: A New Property of Fluid-Fluid Interfaces"
- 26. 14, January 2008 Dr Sudip Mandal (UCLA,USA) "Regulation of cell cycle by mitochondrial signaling"
- 27. 14, January 2008 Dr Lolitika Mandal (UCLA,USA) "Drosophila as a model for hematopoietic development"
- 28. 09, January 2008 Dr Sanjay Singh (Cambridge UK) "Beta-Diketiminate Group 13 Complexes as Heterobimetallic Oxide Catalysts and Phospha(III)zane Based Inorganic Macrocycles"
- 29. 09, January 2008 Dr.Dinesh Khurana (PU Chandigarh) "Rings whose elements have some nice additive decompositions"
- 30. 02, January 2008 Abhijit Mitra (New York) "A new manifestation of Pi-Pi interaction"
- 31. 07, December 2007 Ashwini Kumar Sharma (TU Clausthal, Germany) "Midinfrared fiber-optic laser sensor for the detection of explosives"
- 32. 06, December 2007 Jozef Gruska (Masaryk Univ., Czech Republik) "Mysteries, puzzles and gold mines of quantum information processing"
- 33. 05, December 2007 A.K.Mallik (IIT, Kanpur) "The mathemagical black holes"
- 34. 26, November 2007 Sanjay Mandal (Clariant Corp., Florida USA) "Use of transition metal catalysts in organic synthesis"
- 35. 23, November 2007 U.P.Singh (Bath Univ, UK) "Enzymatic and structural characterization of amphinase a novel cytotoxic protein"

- 36. 16, November 2007 Samir K Maji (Salk Institute, La Jolla USA) "Amyloid aggregation: from dark side to novel therapeutics"
- 37. 15, November 2007 Ashwani Kumar Tiwari (TU Denmark, Copenhagen) "Laser control of molecular dynamics"
- 38. 07, November 2007 Navinder Singh (IOP, Bhubhaneswar) "Onsager-Machlup theory and work fluctuation theorem for a harmonically driven Brownian particle"
- 39. 17, October 2007 P.Sen, S.Ghosh, N.Sathyamurthy (IMTECH, IISER Mohali) "Special Session on the 2007 Nobel prizes in Medicine, Physics, and Chemistry"
- 40. 10, October 2007 J.S.Bagla (HRI, Allahabad) "Simulating formation of large scale structure in the universe"
- 41. 02, October 2007 R.V.Hosur (TIFR, Mumbai) "New Horizons in Protein NMR"
- 42. 19, September 2007 C. S. Aulakh (PU, Chandigarh) "Grand Unification Redux"
- 43. 04, September 2007 S Chandrasekaran (IISc, Bangalore) "Chemistry in Everyday Life"
- 44. 03, September 2007 T Ramasami (Secretary, DST) "Reflections of a Chemist"
- 45. 30, August 2007 Samrat Ghosh (Angstrom Power Inc., Vancouver) "Solution synthesis of functional materials"
- 46. 27, August 2007 Desh Deepak Singh (IIAR Gandhinagar) "Modern Biology: the great melting pot"
- 47. 23, August 2007 I. B. S. Passi (IISER Mohali) "Evariste Galois (1811-1832) and his Theory of Equations"

15 Accounts Statement

The Annual Statement of Accounts of IISER Mohali for the year 2007-08 was prepared in the month of April 2008 and the same has been approved by the Board of Governors in its meeting held on 19th April 2008. The Annual statement of Accounts includes the balance sheet, the Receipt and Payment Accounts and the Income and Expenditure Accounts. A copy of the Balance Sheet, Receipt and Payment Accounts and Income and Expenditure Accounts are enclosed herewith. The Government of India (MHRD) has released a sum of Rs.10,50,00000-/- as grant-in-aid to this Institute in the year 2007-08. In addition to the receipt of grant from the MHRD, the Institute has earned a sum of Rs.11.66 lakhs from student fee and Rs.15.30 lakhs as interest on fixed deposit. Some internal receipt to an extent of Rs.6690 has also been received. The Institute spent a sum of Rs.64.21 lakhs on salary component and Rs.179.20 lakhs on non-salary component and Rs.713.62 lakhs on creation of fixed assets, totally a sum of Rs.957.03 lakhs. The Annual Statement of Accounts of the Institute for the year 2007-08 has already been audited by the Principal Accountant General, Punjab & U.T. and the report is to be submitted before the Board of Governors for forwarding the same to the MHRD for laying before both the Houses of Parliament. In addition to the Plan grants received from MHRD, the Institute has also received Projects from DST, CSIR and DBT. A copy of the Research & Development Account is enclosed herewith.

15.1 Balance Sheet

LIABILITIES

S.N.	PARTICULARS	CURRENT	PREV. YEAR
		(As on 31/03/2008)	(As on 31/03/2008)
1	CORPUS/CAPITAL FUND		
	Opening Balance 01/04/07 Nil	Nil	Nil
	Add: Grant Received Rs .105000000.00		
	Less: Excess of expenditure over income Rs.	83200886.00	Nil
	21799114.00		
2	CURRENT LIABILITIES & PROVISIONS		
	a)Student Cautioned Money (Batch 2007-08)	100000.00	Nil
	b)Student fees A/c for the year 08-09 (re-	242125.00	Nil
	ceived on 2007-08)		
	TOTAL	83543011.00	Nil

<u>ASSETS</u>

S.N.	PARTICULARS	CURRENT	PREV. YEAR
		(As on 31/03/2008)	(As on 31/03/2007)
1	Fixed Assets	71362290.00	Nil
2	Investments	5000000.00	Nil
3	CURRENT ASSETS		
	a) Interest on FDR receivable (accrued but not received	180861.00	Nil
	b) KVPY Scholarship receivable	22742.00	Nil
	Bank Balance (Canara Bank, Sector 34, Chandigarh)	6977118.00	Nil
	TOTAL	83543011.00	Nil

15.2 Receipts & Payments

RECEIPT

Plan Grants		Amount (in Rs.)
Grant-in-Aid(By Santion order No.)		
(i) FN-21-2/2007-TS-1 dt.29/06/07	1000000.00	
(ii) FN-21-2/2007-TS-1 dt. 20/08/07	35000000.00	
(iii) FN-21-2/2007-TS-1 dt. $26/09/07$	30000000.00	
(iv) FN-21-2/2007-TS-1 dt. $20/02/08$	30000000.00	10500000.00
Student Fee Account		
Receipt from Student Fee	1260050.00	
Less Refunds	-93800.00	1166250.00
Interests on Fixed Deposits		1530157.00
Internal Receipt		
(i) Sale From the application forms	2450.00	
(ii) Receipt from Guest House	4240.00	6690.00
Other Receipt		
CNR Rao Award		5000.00

PAYMENT

Expenditure		(Amount in Rs.)
(A) Salary Components		
1.(a) Pay and Allowance	3644166.00	
(b) Traveling Allowance	1555397.00	
(c) LTC	42050.00	
(d) Outsourcing	1179020.00	6420633.00
(B) Non Salary Components		
2. Student Scholarship	545517.00	
3.(a) Administrative Expenditure	2534493.10	
(b) Departmental Expenditure	2540261.00	
(c) Advertisement	4219450.00	
4. Library Services(Online Journals)	6370426.00	

5. Computing Facilities	67371.00	
6. Student Support Services	74621.00	
7. Hall Subsidy & Hiring of hostels	633748.00	
8. Transport Subsidy	380311.00	
9. Health Services	5950.00	
10. Water & Electricity Charges	Nil	
11. House Keeping & Maintenance	548166.00	17920314.10
(C) Fixed Assets		
1. Purchase of Equipment	56799288.00	
2. Purchase of Furniture	8092387.00	
3. Purchase of Vehicle	647486.00	
4. Construction of Building	Nil	
5. Library Books	1248274.00	
6. Computers/Peripherals	4574855.00	71362290.00
(D) Other Expenditure		
(a) CNR Award	5000.00	
(b) KVPY Scholarship	22742.00	27742.00
(E) Investment		
Fixed Deposit No.2452401000469 $/1(598701)$		5000000.00
dt.03/10/07 in hand		
(F) Closing Balance		
As per cash book as on $31/03/2008$ Canara Bank		6977117.90
Grand Total		107708097.00
		0.100000.000

Income & Expenditure Account 15.3

S.N. PARTICULARS

S.N.	PARTICULARS	CURRENT	PREV. YEAR
		(As on 31/03/2008)	(As on 31/03/2007)
1	INCOME		
1.A	Income from Sales & Services	Nil	Nil
1.B	Grants/Subsidies (Utilized Part) (Other Grants)	Nil	Nil
1.C	Fees/Subscriptions (Student Fees)	824125.00	Nil
1.D	Income from Investment, interest (Excluding income from earmarked/endowment funds transferred to funds)	1711018.00	Nil
1.E	Income from Royalty/Publications, etc.	Nil	Nil
1.G	Other Income (internal receipt) (See R/P/ A/c)	6690.00	Nil
1.H	Increase/(Decrease) in Stock of Finished Goods & Work-in-Progress	Nil	Nil
	TOTAL (A)	2541833.00	Nil
2	EXPENDITURE		
2.A	(A) Salary Components		
	1(a) Pay and Allowance	3644166.00	Nil
	(b) Traveling Allowance	1555397.00	Nil
	(c) LTC	42050.00	Nil
	(d) Outsourcing	1179020.00	Nil
_	2 GPF/CPF	Nil	Nil
	TOTAL	6420633.00	Nil
2.B	(B) Non-Salary Components		
	3. Student Scholarship	545517.00	Nil
	4 (a) Administrative Expenditure	2534493.10	Nil
	(b) Departmental Expenditure	2540261.00	Nil
	(c) Advertisement	4219450.00	Nil
	5 Library Services		
	a)Online Journals	6370426.00	Nil
	6 Computer Software	67371.00	Nil

7. Student Support Services	74621.00	Nil
8. Hall Subsidy & Hiring of hostels	633748.00	Nil
9. Transport Subsidy	380311.00	Nil
10. Health Services	5950.00	Nil
11. Water & Electricity Charges	Nil	Nil
12. House Keeping & Maintenance	548166.00	Nil
TOTAL	17920314.10	Nil
GRAND TOTAL (B)	24340947.10	Nil
Excess of Expenditure over Income (B-A)	21799114.10	Nil
BALANCE BEING SURPLUS/(DEFICIT)		

CARRIED TO CORPUS/CAPITAL FUND

15.4 Research & Development Account

Opening Balance	Name of Project	Amount	Expenditure Amount
Grant received from DST-Project No.1 IISER (M) DST-07-0001	Conformational Dyn. of Model Tripeptides using NMR and Vibrational Spectro. Tech.	357000.00	DST Proj.(i) Equipt.116896.00(ii) CNC(R)5304.00DST Total122200.00
Grant received from CSIR Project No-2 IISER (M) CSIR-07-0002	Studies of Dissipative Dyn. in Quantum Comp. using NMR Tech.	329500.00	CSIR Proj.(i) T.A.4086.00(ii) CNC(R)4500.00(iii) Equipt.35677.00CSIR Total44263.00
Total		686500.00	Grand Total 166463.00
Closing Balance			520037.00