WS-298

# Veltech Dr. RR & Dr. SR University

(Esd. u/s 3 of UGC Act, 1956)

## VEL TECH TECHNOLOGY INCUBATOR

(APPROVED BY DST)
CERTIFICATE OF REGISTRATION OF SOCIETIES
S. No. 438 of 2010

# EVENT REPORT

## HANDS ON TRAINING IN MOLECULAR DOCKING

**ORGANIZED BY**

**Vel Tech Technology Incubator**

**ON**

**26th October, 2017.**

0

Prof. Dr. E. Kannan
Registrar

Vel Tech
Rangarajan Dr. Sagunthala
R&D Institute of Science and Technology
(Deemed to be University Estd. u/s 3 of UGC Act, 1956)

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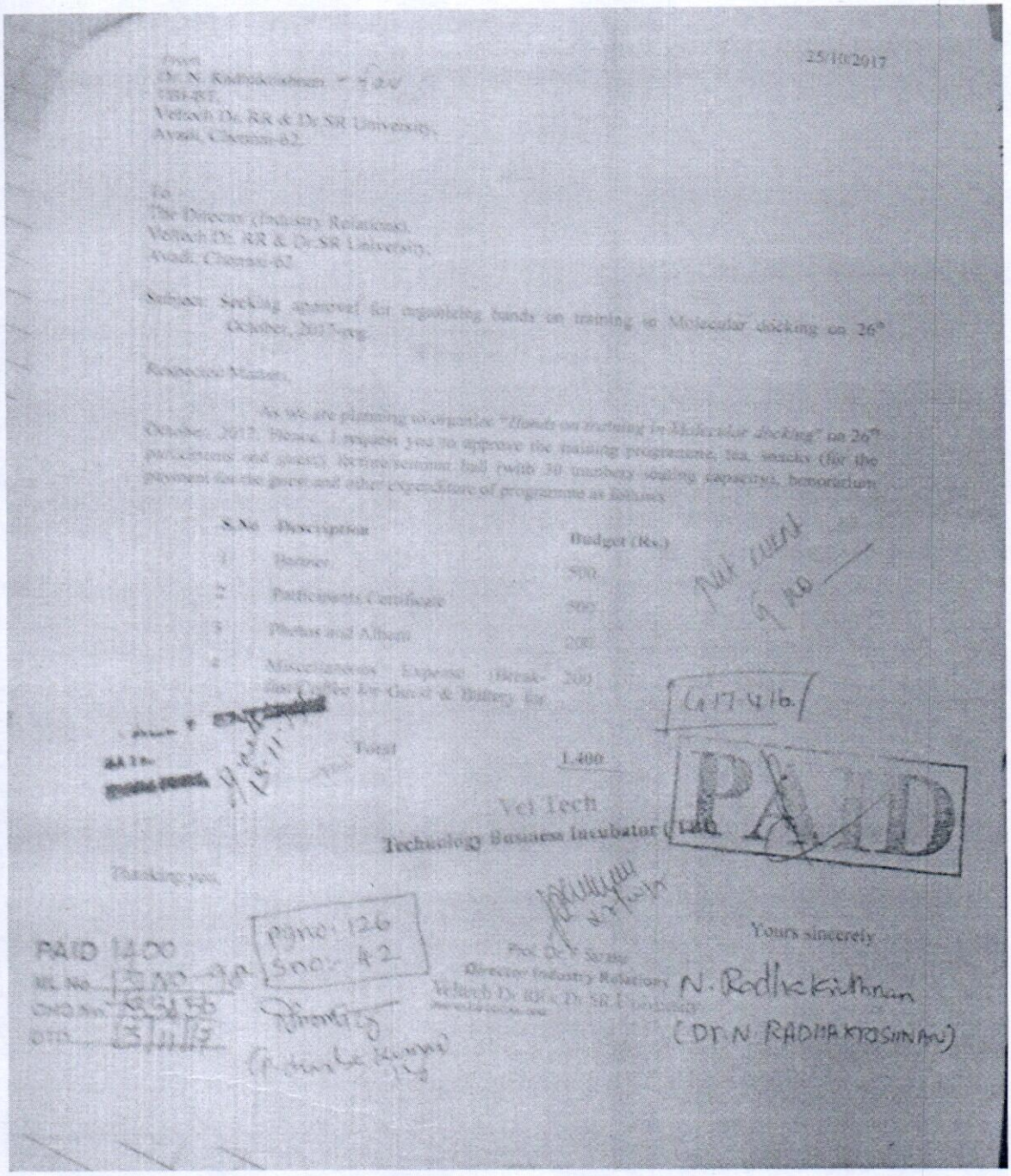

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Prof. Dr. E. Kannan
Registrar

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Rangarajan Dr. Sagunthala
R&D Institute of Science and Technology
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**Approval Letter**



25/10/2017

From
Dr. N. Radhakrishnan
CBCRT,
Vel tech Dr. RR & Dr SR University,
Avadi, Chennai-62.

To
The Director (Industry Relations),
Vel tech Dr. RR & Dr SR University,
Avadi, Chennai-62

Subject: Seeking approval for organizing hands on training in Molecular docking on 26th October, 2017 reg.

Respected Madam,

As we are planning to organize "*Hands on training in Molecular docking*" on 26th October, 2017. Hence, I request you to approve the training programme, tea, snacks (for the participants and guests), lecture/seminar hall (with 30 members seating capacities), honorarium payment for the guest and other expenditure of programme as follows.

| S.No | Description | Budget (Rs.) |
|---|---|---|
| 1 | Banner | 500 |
| 2 | Participants Certificate | 500 |
| 3 | Photos and Album | 200 |
| 4 | Miscellaneous Expense (Break-fast, Coffee for Guest & Battery for ... | 200 |
| | Total | 1,400 |

Vel Tech
Technology Business Incubator

PAID

Thanking you,

Yours sincerely

Prof. D.S. Suresh
Director-Industry Relations
Vel tech Dr. RR & Dr SR University

N. Radhakrishnan
(DR N. RADHAKRISHNAN)

PAID 1400
BL No. 1320
DHD No. 2554586
DTD. 13/11/17

Phone: 126
Soc: 82



Prof. Dr. E. Kannan
Registrar

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Rangarajan Dr. Sagunthala
R&D Institute of Science and Technology
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**Brochure**

# HANDS ON TRAINING IN MOLECULAR DOCKING

**October 26, 2017**

*Organised by*

## VEL TECH TECHNOLOGY INCUBATOR

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**S. No. 438 of 2010**

## Veltech Dr. RR & Dr. SR University

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**About Vel Tech Technology Incubator Center**

Vel Tech Technology Incubator Center at Veltech Dr. RR and Dr. SR University, Chennai was established in year 2010, in joining hands with Department of Science and Technology (DST), Government of India. It has seven thrust areas of research which includes Automobile; 3D printing; Embedded systems/VLSI; E-waste, Plastic waste and Bio-waste management; MAV/Robotics; IT/ITES Services and Renewable Energy. It also provides financial assistance to deserving Entrepreneurs to convert their innovative ideas into commercial viable products.

**About Bio Waste Management Laboratory**

Bio Waste Management Laboratory was established in year 2011 which functions under umbrella of Vel Tech Technology Incubator Center. More than, 25 research articles have been published by the Laboratory faculty members and organized four training programme so far. In addition, we also provide analytical services on charge basis for both internal and external researchers.

**About the training**

Computer-aided drug design (CADD) has been emerged as new field of modern drug discovery program. It represents computational methods and resources that are employed for facilitating the design and discovery of new potent therapeutic compounds. Especially the computational approaches like homology modeling, molecular docking, molecular dynamics and quantitative structure activity relationships (QSAR) are widely used to discover the new candidates for various therapeutic targets. Among these computational approaches, molecular docking is used to study the formation of intermolecular complexes of one smaller molecule (ligand/drug) with a larger molecule, which usually is a protein of known three-dimensional structure (drug target). Four different types of interactions between the molecules can be distinguished namely i) protein-protein; ii) protein-deoxyribonucleic acid (DNA); iii) deoxyribonucleic acid (DNA)-ligand and iv) protein-ligand. Molecular docking finds the following applications such as i) binding site identification (blind docking); ii) de-orphaning of a drug target; iii) drug discovery (lead optimization); iv) enzymatic reactions mechanisms; v) prediction of biological activity; vi) protein engineering; vii) structure-function studies and viii) virtual screening (hit identification).

**Objectives of the training:**

1. To teach and train the molecular docking tool to the researchers & students.
2. To adopt the molecular docking studies in their upcoming research programme.

**Training Program Schedule:**

Training program schedule includes two sessions:

- Introduction to Molecular Docking-Theory session and
- Hands on Training in Molecular Docking – Practical session.

**Eligibility**

The training programme is open to all students and researchers, who are all willing to learn the Molecular docking technique.

**Important dates:**

Last date for registration: **20.10.2017.**
Programme date: **26.10. 2017.**
**Venue**:

Research Park, Veltech Dr. RR and Dr. SR University.

**Programme fee Rs. 250/** (Cash/Deposit-Account no: **380401011000785,** Account name: **Vel Tech Technology Incubator**, Vijaya Bank, VTU Branch, Avadi, Chennai.

**About the Content delivering expert**

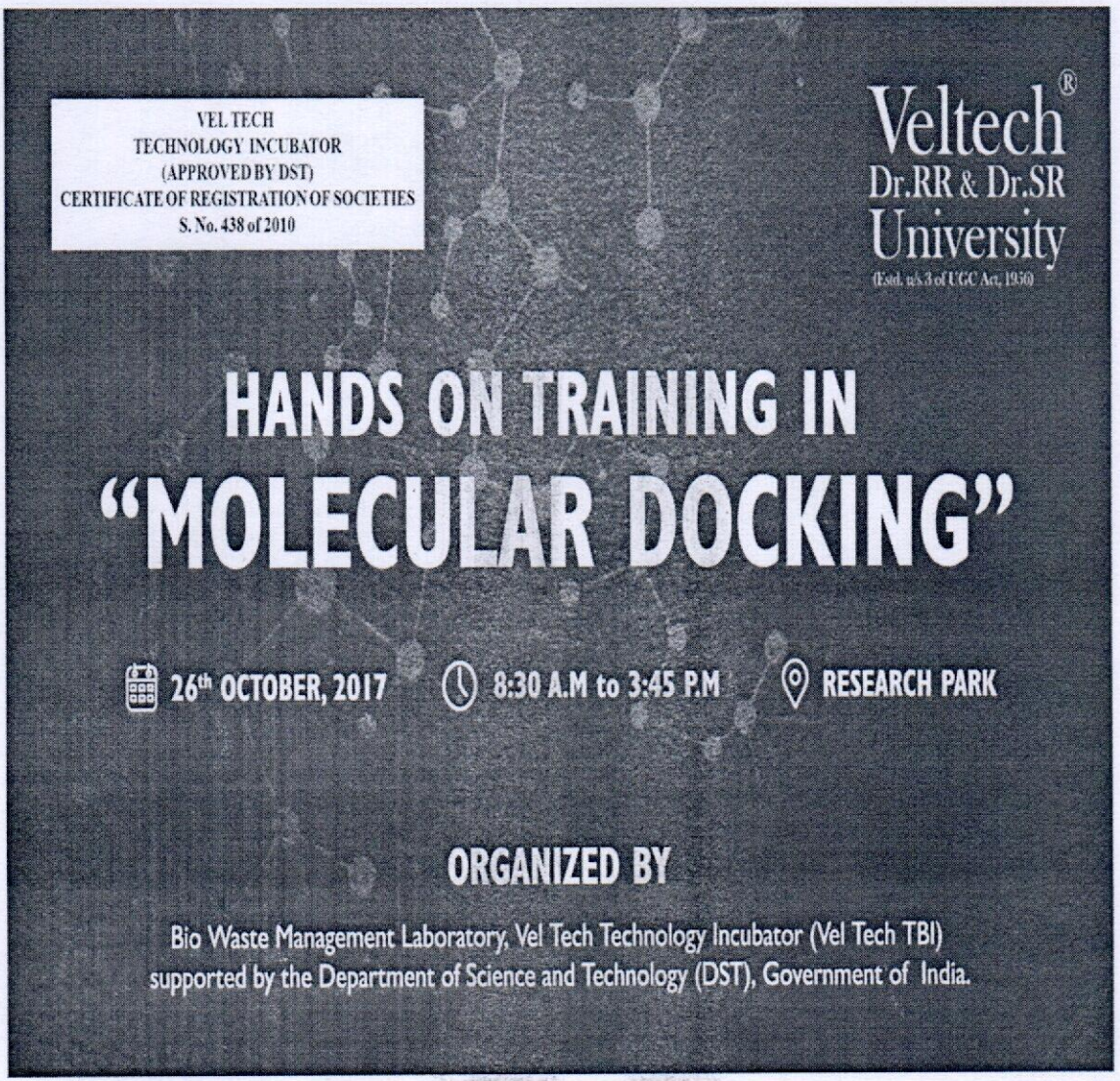
**Dr.Thirumurthy Madhavan, SRM University, Chennai**

He is currently working as Assistant Professor in Department of Genetic Engineering, School of Bioengineering, SRM University, Kattankulathur Campus, Chennai. Before joining SRM University, he had worked as Junior Executive in Orchid Chemicals & Pharmaceuticals Ltd, Chennai (from December 2002 to August 2006). His research interest are: Design of new bio-active molecules using molecular modelling techniques; Modelling of small organic molecules, proteins, and protein-ligand interactions; Ligand based and structure based pharmacophore design and Generation and screening of large virtual combinatorial compound libraries

**For more details contact**

Vel Tech TBI, Mobile no: 09600040254/08056573957 Email: veltechtbi@veltechuniv.edu.in

**Banner**


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HANDS ON TRAINING IN
"MOLECULAR DOCKING"
26th OCTOBER, 2017
8:30 A.M to 3:45 P.M
RESEARCH PARK
ORGANIZED BY
Bio Waste Management Laboratory, Vel Tech Technology Incubator (Vel Tech TBI)
supported by the Department of Science and Technology (DST), Government of India.

# Veltech Dr. RR & Dr. SR University

**HANDS ON TRAINING IN MOLECULAR DOCKING**

**ORGANIZED BY**

## Vel Tech Technology Incubator

**ON**

**Thursday, 26th October, 2017**

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### Programme Shedule

| S.No | Time | Topic | Resource Person | Venue |
|---|---|---|---|---|
| 1 | 08.30 | Registration | **Mr.Shaju/Mr.Thilipkumar** Vel Tech TBI | IBM Lab, 1st Floor, Research Park, VTU |
| 2 | 09.10-09.20 | Welcome Address | **Mr. Rajaram Venkataraman** CEO-NIDHI Centre of Excellence, Vel Tech TBI | IBM Lab, 1st Floor, Research Park, VTU |
| 3 | 09.20-10.20 | Introduction to Molecular docking | **Dr. Thirumurthy Madhavan,** Assistant Professor, SRM University | IBM Lab, 1st Floor, Research Park, VTU |
| 4 | 10.20-10.50 | Ligand preparation using ChemBiodraw & ChemBio3D software | **Dr. N. Radhakrishnan,** In-charge, Bio Waste Management Lab | IBM Lab, 1st Floor, Research Park, VTU |
| 5 | 10.50-11.20 | Protein preparation using UCSF Chimera software | | |
| 6 | 11.20-11.40 | Molecular descriptors calculation using Molinspiration online tool | | |
| 7 | 11.40-12.40 | Lunch Break | | |
| 8 | 12.40-01.10 | ADME analysis using SwissADME online tool | **Dr. N. Radhakrishnan,** In-charge, Bio Waste Management Lab | IBM Lab, 1st Floor, Research Park, VTU |
| 9 | 01.10-01.40 | PatchDock using online server | | |
| 10 | 01.40-02.40 | Docking result analysis using PyMol software | | |
| 11 | 02.40-03.10 | Introduction to Autodock | | |
| 12 | 03.10-03.45 | Lab Visit | **Mr.Shaju/Mr.Thilipkumar** Vel Tech TBI | Tinkering & Ewaste Lab |

## Participants Name List

| S. No | Name | Department | Institute |
|---|---|---|---|
| 1. | N. Srinivasan | Chemistry | VTU |
| 2. | V. Vijayakumar | Chemistry | VTU |
| 3. | S. Kavya | Chemistry | VTU |
| 4. | V.G. Prasanth | Chemistry | VTU |
| 5. | Uzbek Zaman | Biotech | VTU |
| 6. | Sushanto Das | Biotech | VTU |
| 7. | Steeve Shibu Chempolil | Biomed | VTU |
| 8. | Hima Manoj | Nanoscience & Technology | GKM College of Eng & Tech |
| 9. | V.R. Manoj | Biotech | VTU |
| 10. | N. Ravisankar | Chemistry | VTU |
| 11. | P.A. Vivekanand | Chemistry | VTU |
| 12. | R. Aarthi | Biotech | VTU |
| 13. | R. Nirmala Nithya | Biotech | VTU |
| 14. | Lovely Mathew | Biotech | VTU |
| 15. | CH. Madhavi | Biotech | VTU |
| 16. | M. Anandi | Biotech | VTU |
| 17. | L. Manjusri | Biomed | VTU |
| 18. | Pallab Kalita | Biotech | VTU |
| 19. | Shanuja Jakkala | Biotech | VTU |
| 20. | M. Subha lakshmi | Biomed | VTU |
| 21. | S. B. Sangeethan | Biotech | VTU |
| 22. | Abhishek Ram | Biotech | VTU |
| 23. | S. Deepeka | Biotech | VTHT |
| 24. | R. Mageshwari | Biotech | VTHT |
| 25. | R. Smruthi | Biotech | VTHT |
| 26. | A. Sumithra | Biotech | VTHT |

**Attendance Sheet**

# Veltech Dr. RR & Dr. SR University

HANDS ON TRAINING IN MOLECULAR DOCKING

ORGANIZED BY

**Vel Tech Technology Incubator**

ON

26th October, 2017

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**Attendance Sheet**

| S.no | Name of the Participant | Institute | Phone no | Signature |
|---|---|---|---|---|
| 01 | Pallab Kalita | Veltech University | 8402805279 | Pallab Kalita |
| 02 | SHANUJA JAKKALA | Veltech University | 7358164201 | |
| 03 | CH.MADHAVI | Veltech Chivesity | 8919530931 | |
| 04 | M. ANANDI | Veltech University | 8900903151 | |
| 05 | LOVELY MATHEW | Veltech Onivesity | 7397442535 | lovely |
| 06 | SUBHA LAKSHMI | Veltech University | 9677554677 | |
| 07 | L. MANJUSRI | Veltech university | 9626619779 | L. manjusri |
| 08 | M. Raman | Veltech University | 8721025974 | |
| 09 | Steeve Shibu | veltech Uni | 8778003774 | |
| 10 | Sangeethan .S.B. | veltech Univesty | 8939619540 | Sangeethan .S.B |
| 11 | Suhanto Das. | Veltech Univesity | 7397448965 | |
| 12 | D. VIVEKANAND | " | 7871753327 | |
| 13 | Hema Manoj | GRIMCET | 8939098466 | |
| 14 | Abhishek Ram | Veltech University | 8900923166 | |
| 15 | R. Smruti | Veltech Hightech | 9790933915 | R Smruti |
| 16 | A. Sumithra | Vel Tech High Tech | 7871824199 | A. Sumithra |

| | | | | |
|---|---|---|---|---|
| 17 | S. Deepika | Vel tech high tech | 9566201346 | |
| 18 | R. Magesheeswari | Vel tech high tech | 8148749748 | |
| 19 | V. Vijaya Kumar | VTU | 9715699714 | |
| 20 | S. H. KAVYA | VTU | 8682984825 | |
| 21. | Dr. R. Aarthi | VTU | 9535657778 | |
| 22. | Ms. R. Nirmala Nithya | VTU | 8754436468 | |
| 23. | Dr. V. R. Manoj. | VTU | 9176347263 | |
| 24. | Dr. N. Ramachandran | VTU | 9442023648 | |
| 25 | Dr. N. Srinivasan | " | 9787084069 | |
| 26 | Dr. V. G. Prasanth | VTU | 9030692929 | |

## Expert- Brief Biography




**Dr.Thirumurthy Madhavan**

Assistant Professor (Sr.G)
Bioinformatics Engineering
**Phone number**: 27417813, Extn: 1151
**E-mail**: thirumurthy.m@ktr.srmuniv.ac.in (mailto:thirumurthy.m@ktr.srmuniv.ac.in)
**Area**: Bioinformatics (Specialized in Structure based drug design)
**Affiliation:** Department of Genetic Engineering, School of Bioengineering, Faculty of Engineering & Technology, Kattankulathur Campus, SRM University.


**Education**

| | | |
|---|---|---|
| Ph.D. | Bioinformatics | Chosun University, South Korea, 2012 |
| M.Sc. | Bioinformatics | University of Madras (Guindy campus), Chennai, India, 2008 |
| B.Sc. | Chemistry | R.V Govt arts College, 2002 |

**Work in Progress**

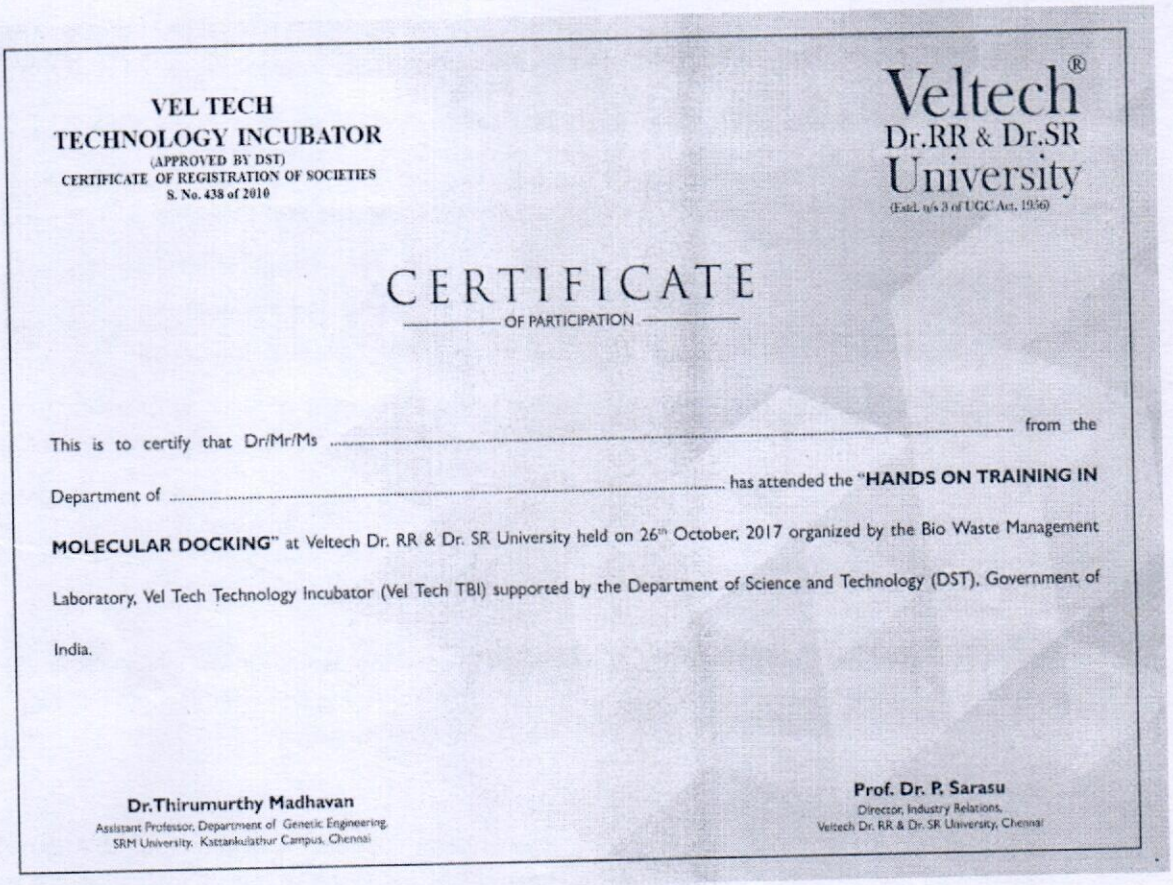
Ongoing project

- "Discovery and biological evaluation of a new class of selective Janus Kinase inhibitors: A combination of pharmacophore, 3D-QSAR based virtual screening and chemical optimization" funded by Department of Science and Technology, New Delhi (2014 onwards)

**Other Professional Experience**

- Junior Executive in Orchid Chemicals & Pharmaceuticals Ltd from December 2002 to August 2006
- Government Funded Project - Principal Investigator, Discovery and biological evaluation of a new class of selective janus kinase 2 inihibitors: A combination of pharmacophore, 3D-QSAR based virtual screening and chemical optimization, Scheme for Young Scientist, SERB, Government of India (From Jan 2014, 3 years, total grant: 21 Lakh)

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**Dr.Thirumurthy Madhavan**
Assistant Professor, Department of Genetic Engineering
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**Prof. Dr. P. Sarasu**
Director, Industry Relations,
Veltech Dr. RR & Dr. SR University, Chennai

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Director, Industry Relations,
Veltech Dr. RR & Dr. SR University, Chennai

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SRM University, Kattankulathur Campus, Chennai

**Prof. Dr. P. Sarasu**
Director, Industry Relations,
Veltech Dr. RR & Dr. SR University, Chennai

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**Dr.Thirumurthy Madhavan**
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SRM University, Kattankulathur Campus, Chennai

**Prof. Dr. P. Sarasu**
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**Prof. Dr. P. Sarasu**
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Assistant Professor, Department of Genetic Engineering,
SRM University, Kattankulathur Campus, Chennai

**Prof. Dr. P. Sarasu**
Director, Industry Relations,
Veltech Dr. RR & Dr. SR University, Chennai

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**Dr.Thirumurthy Madhavan**
Assistant Professor, Department of Genetic Engineering,
SRM University, Kattankulathur Campus, Chennai

**Prof. Dr. P. Sarasu**
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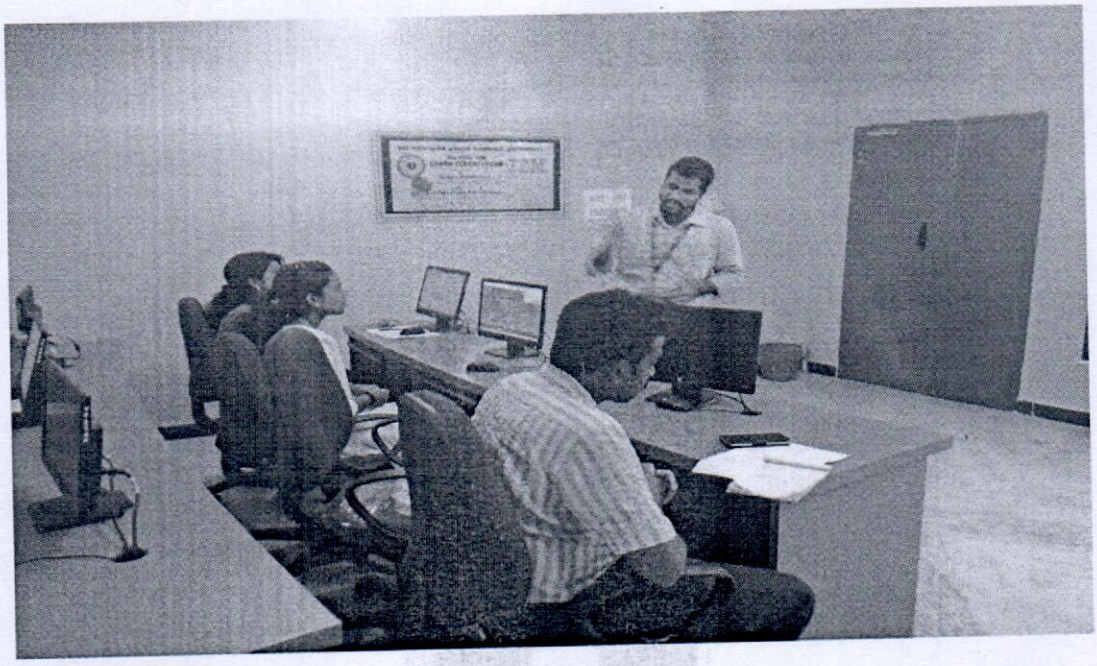
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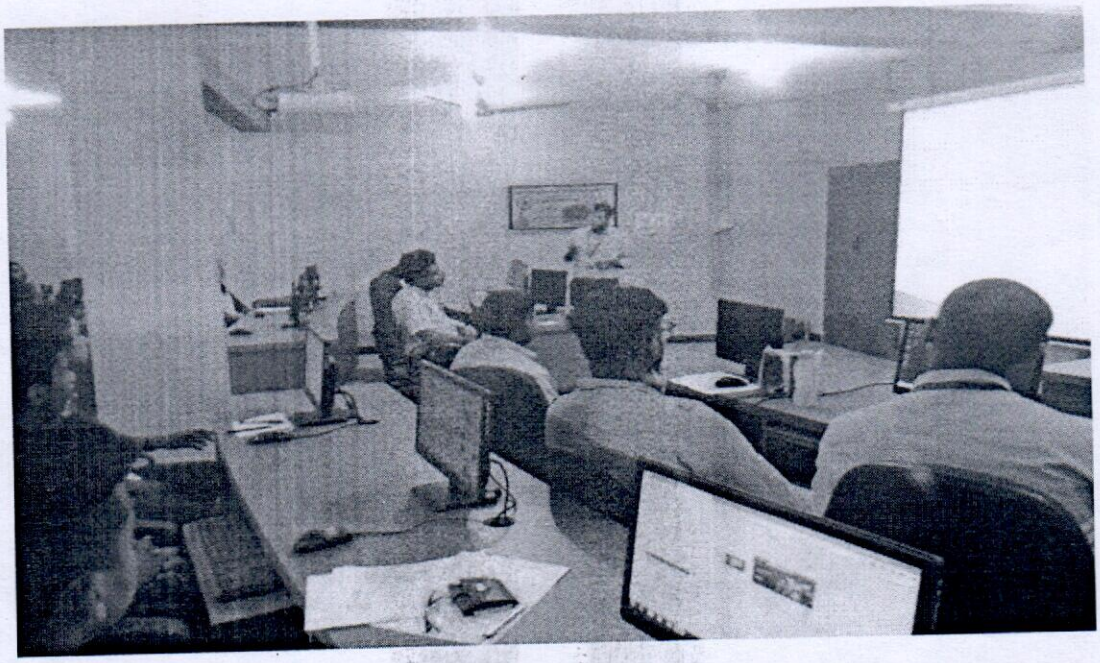
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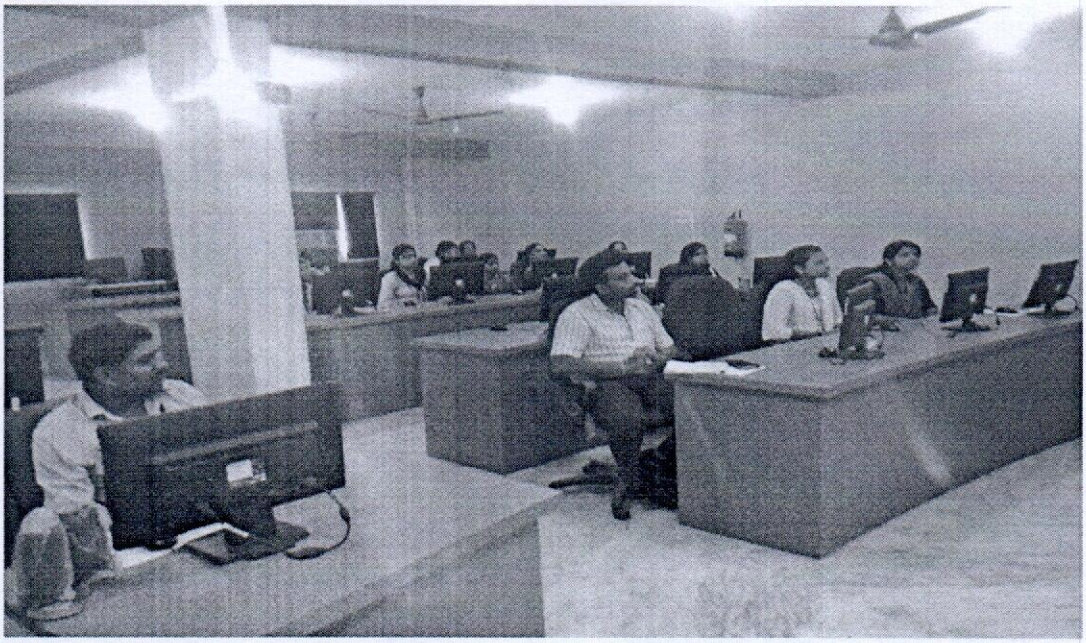
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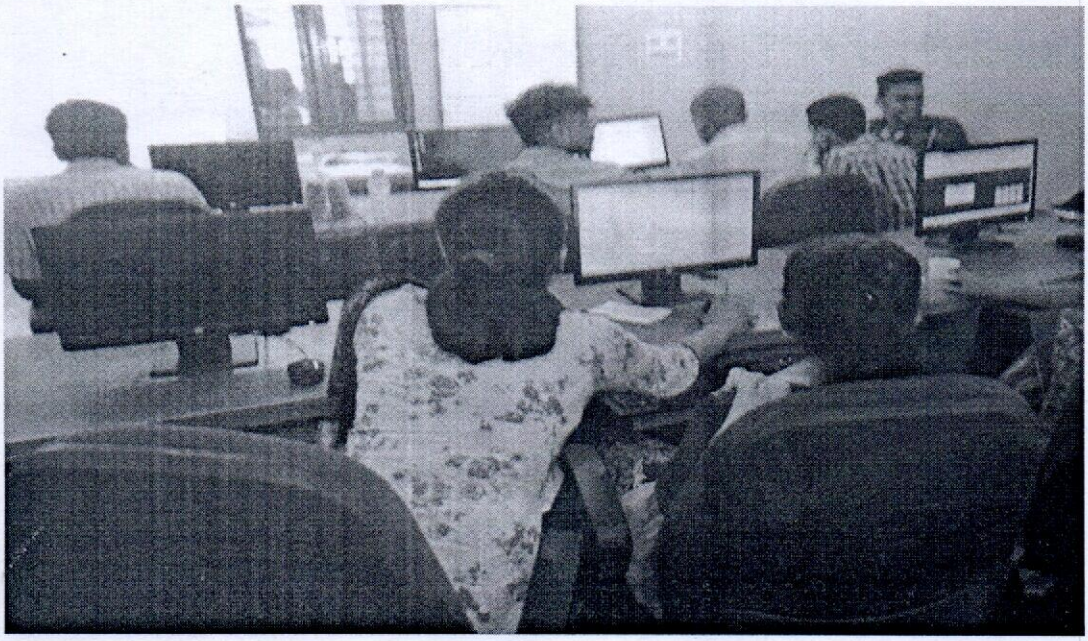
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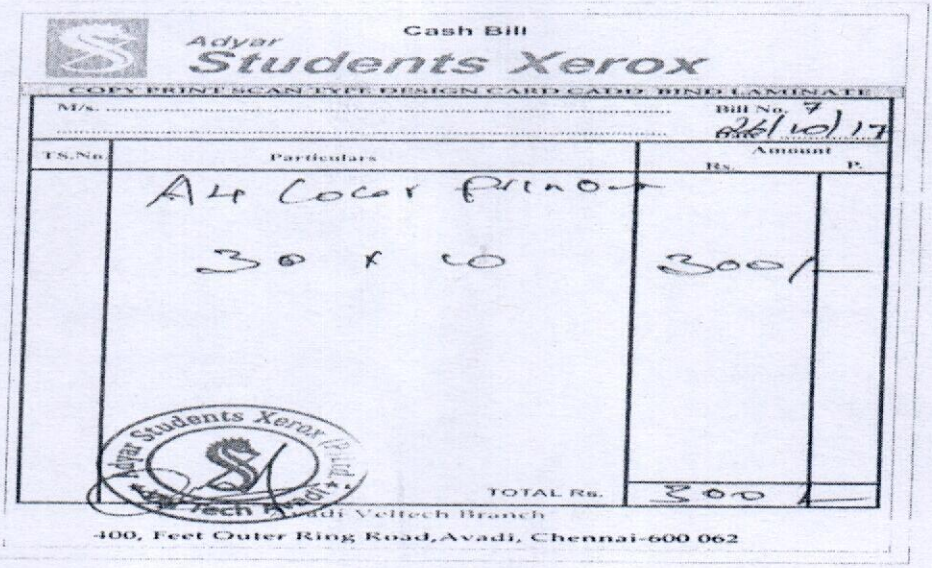








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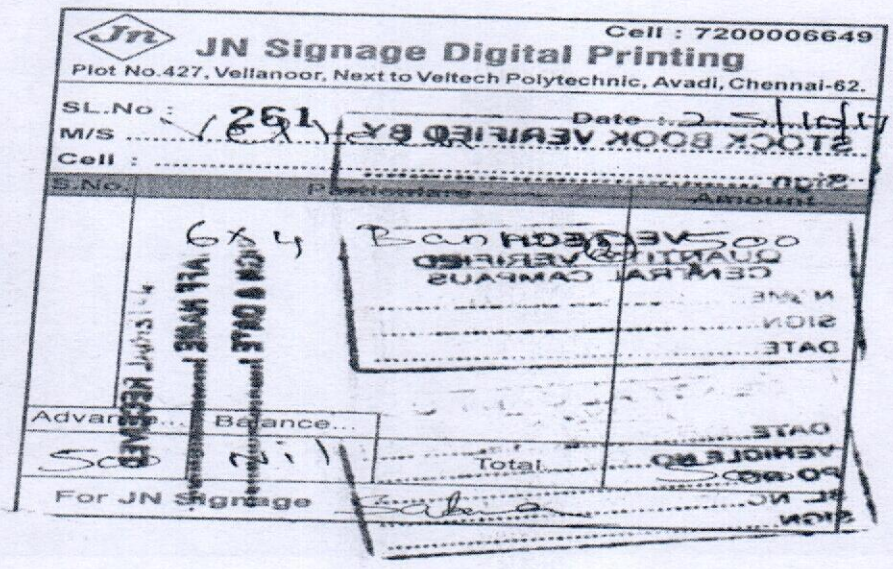
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नाम/Name VelTech Technology Incubator
रकम (अक्षरों में) रूपए Amount (in words) Rupees One thousand two hundred and fifty
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| जमा किए गए नकद / चेकों के विवरण Details of Cash/Cheques deposited | रकम (रू.) Amount (Rs) |
|---|---|
| Cash | 1250/- |
| | |
| | |
| कुल/Total | 1250/- |

प्राप्तकर्ता लिपिक
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Hands on training in Molecular docking

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दिनांक/Date: 20/10/17
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20 OCT 2017

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Hands on training in Molecular docking

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रकम (अक्षरों में) रूपए Amount (in words) Rupees TWO thousand two hundred and fifty only
नकद / चेक आदि / by cash /Cheque etc.

| जमा किए गए नकद / चेकों के विवरण Details of Cash/Cheques deposited | रकम (रू.) Amount (Rs) |
|---|---|
| 591333 dt 30/10/17 | 2250 |
| | |
| कुल/Total | 2250/- |

प्राप्तकर्ता लिपिक
Receiving Clerk
प्राधिकृत हस्ताक्षरी
Authorised Signatory
(नोट : चेक की वसूली होने की शर्त पर/Note : Cheques subject to realisation)

"AAS Training"

जमा खातों की जमापर्ची/प्रतिपर्णक 6-2
Paying-in-slip for
Deposit Accounts-Counter Foil

विजया बैंक VIJAYA BANK ..... शाखा Branch
VTU
दिनांक/Date : 23/8/17

खाते का स्वरूप : Nature of A/c .....

खाता सं A/c No. 3 8 0 4 0 1 0 1 1 0 0 0 7 8 5

नाम/Name VCL Tech Technology Incubator

(रकम अक्षरों में) रुपए/(Amount in words) Rupees Four thousand two hundred only

नकद/चेक/आदि/ by cash/cheque etc.

| जमा किए गए नकद/चेकों आदि के विवरण Details of cash/cheque deposited | रकम/Amount ₹ |
|---|---|
| | |
| | |
| | |
| कुल/Total | 4200/- |

विजया बैंक / VIJAYA BANK
Vel Tech Engg. College, Velloore, Chennai-62.

23 AUG 2017 CASH RECEIVED

प्राप्तकर्ता लिपिक
Receiving Clerk
(पूरा हस्ताक्षर/Full Signature)

प्राधिकृत हस्ताक्षरी
Authorised Signatory
(पूरा हस्ताक्षर/Full Signature)

(नोट : चेक आदि वसूली होने की शर्त पर)
(Note : Cheques etc. subject to realisation)

Income

"AAS Training"

जमा खातों की जमापर्ची/प्रतिपर्णक 6-2
Paying-in-slip for
Deposit Accounts-Counter Foil

विजया बैंक VIJAYA BANK ..... शाखा Branch
VTU
दिनांक/Date : 24/08/2017

खाते का स्वरूप : Nature of A/c .....

खाता सं A/c No. 3 8 0 4 0 1 0 1 1 0 0 0 7 8 5

नाम/Name VelTech Technology Incubator

(रकम अक्षरों में) रुपए/(Amount in words) Rupees three thousand only

नकद/चेक/आदि/ by cash/cheque etc.

| जमा किए गए नकद/चेकों आदि के विवरण Details of cash/cheque deposited | रकम/Amount ₹ |
|---|---|
| Cheque no: 591330 dt: 24/8/17 | 3000/- |
| कुल/Total | 3000/- |

प्राप्तकर्ता लिपिक
Receiving Clerk
(पूरा हस्ताक्षर/Full Signature)

प्राधिकृत हस्ताक्षरी
Authorised Signatory
(पूरा हस्ताक्षर/Full Signature)

(नोट : चेक आदि वसूली होने की शर्त पर)
(Note : Cheques etc. subject to realisation)

Income

"AAS Training"

विजया बैंक
VIJAYA BANK
(A GOVT. OF INDIA UNDERTAKING)
A friend you can bank upon

शाखा/Branch VTU
दिनांक/Date : 1 2 0 9 2 0 1 7

बबैंक/चाखा/ओड़ा/नत्र/आज/मीत्र खाता सं./क्रेडिट कार्ड सं.
SB / CA / OD / CC / RD / TL / DL / A/c. No. / Credit Card No.

3 8 0 4 0 1 0 1 1 0 0 0 7 8 5

नाम/Name : VelTech Technology Incubator

दूरभाष सं./मोबाईल सं.
Tel. No. / Mobile No. 8056573957

ईमेल आईडी
E-mail ID : nrrishnan@gmail.com

रुपए शब्दों में :
Rupees in words : three thousand only

| नकदी/चेक सं दिनांक व बैंक तथा शाखा का नाम Cash/Cheque No./Date/Name of Bank & Branch | ₹ | P. |
|---|---|---|
| 591332, Vijaya Bank, VTU | 3000 | 00 |
| | | |
| कुल/Total | 3000 | 00 |

अधिकारी/कैशियर/एसडब्ल्यूओ
Officer/Cashier/SWO

विजया बैंक VIJAYA BANK
टोल फ्री सं./Toll Free No.1800 124 5885

NMY-7-Lacs PADS 06-2017

"Hands on training in Molecular docking"
"Income from Bioanalytic Lab"

बचत खाता की जमापर्ची -प्रतिपर्ण 6-2
Paying-in-Slip for
Deposit Accounts - Counter Foil

विजया बैंक..... शाखा
VIJAYA BANK VTU Branch
दिनांक/Date : 25/10/17

खाते का स्वरूप : Nature of Account.....

खाता सं A/c No. 3 8 0 4 0 1 0 1 1 0 0 0 7 8 5

नाम/Name : VCL Tech Technology Incubator

रकम (अक्षरों में) रूपए Amount (in words) Rupees.....
one thousand only

नकद / चेक आदि / by cash / cheque etc.

| जमा किए गए नकद/चेकों के विवरण Details of Cash/Cheques deposited | रकम (केवल काउंटर के लिए) Amount (for Counters) |
|---|---|
| | |
| | |
| | |
| कुल/Total | 1000.00 |

VIJAYA BANK Vellore Chennai-62.
25 OCT 2017 CASH RECEIVED
खजांची/CASHIER

प्राप्तकर्ता लिपिक
Receiving Clerk

प्राधिकृत हस्ताक्षरी
Authorised Signatory

(नोट : चेक की वसूली होने की शर्त पर/Note : Cheques subject to realisation)

15-6

# Veltech Dr. RR & Dr. SR University

**HANDS ON TRAINING IN MOLECULAR DOCKING**

**ORGANIZED BY**

## Vel Tech Technology Incubator

**ON**

**Thursday, 26th October, 2017**

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**Budget Vs Expense Details**

| S.No | Description | Budget (Rs.) | Expense (Rs.) |
|---|---|---|---|
| 1 | Banner | 500 | 500 |
| 2 | Participants Certificate | 500 | 300 |
| 3 | Photos and Album | 200 | - |
| 4 | Miscellaneous Expense (Coffee for Guest & Battery for Mic) | 200 | - |
| Total | | 1,400 | 800 |

# Veltech Dr. RR & Dr. SR University

**HANDS ON TRAINING IN MOLECULAR DOCKING**

**ORGANIZED BY**

## Vel Tech Technology Incubator

**ON**

**Thursday, 26th October, 2017**

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**Income Vs Expense Details**

| S. No | Income (Rs.) | Expense (Rs.) |
|---|---|---|
| 1 | 26 Participants (26x 250) = 6,500 | 800 |

Profit (Income-Expense) = Rs. 5,700/-

**Profit = Rs. 5,700/-**