

# Workshop

## Structure, dynamics, and function of proteins

ITQB, September, 17–19, 2008

ITQB – Technical University of Berlin/ UNICAT –  
Unifying Concepts in Catalysis

| <b>Wednesday, September 17, 2008</b> |                                     |            |   |
|--------------------------------------|-------------------------------------|------------|---|
| <i>Metalloenzymes</i>                |                                     |            |   |
| 16:00                                | José M. Simões<br>Peter Hildebrandt | ITQB<br>TU | Opening and Introductory Remarks  |
|                                      | Chair: Inez Weidinger               |            |   |
| 16:20                                | Miguel Teixeira                     | ITQB       | Flavodiiron NO/O <sub>2</sub> <sup>-</sup> reductases, and O <sub>2</sub> <sup>-</sup> reductases |
| 16:45                                | Marta Justino                       | ITQB       | A novel repair system for iron sulfur proteins  |
| 17:00                                | <i>Coffee break</i>                 |            |   |
|                                      | Chair: Filipa Sousa                 |            |   |
| 17:30                                | Susana Lobo                         | ITQB       | Enzymes of Haem biosynthesis  |
| 17:45                                | Olga Iranzo                         | ITQB       | Modelling and designing metal centers   |
| 18:10                                | Pedro Matias                        | ITQB       | Hydrogenases  |
| 18:35                                | <b>End of day 1</b>                 |            |   |
| <b>Thursday, September 18, 2008</b>  |                                     |            |   |
| <i>Metalloenzymes (Cont.)</i>        |                                     |            |   |
|                                      | Chair: Miguel Saggiu                |            |   |
| 9:15                                 | Lígia O. Martins                    | ITQB       | Structure-function studies in multicopper-oxidases  |

| <b><i>Theoretical Methods</i></b>         |                            |      |  |
|---|----------------------------|------|--|
| 9:40                                      | Claudio M. Soares          | ITQB | Molecular modelling of hydrogenases  |
| 10:05                                     | Bruno Victor               | ITQB | Molecular Modelling of NO/O <sub>2</sub> <sup>-</sup> flavodiiron reductases |
| 10:20                                     | <b><i>Coffee break</i></b> |      |  |
| <b><i>Experimental Methods</i></b>        |                            |      |  |
|   | Chair: Susana Lobo         |      |  |
| 10:50                                     | Uwe Kuhlmann               | TU   | Vibrational spectroscopies   |
| 11:15                                     | Jui-Ju Feng                | TU   | Novel devices for SER spectroscopy   |
| 11:40                                     | Diego Millo                | TU   | Electrochemistry of redox proteins   |
| <b><i>Respiratory enzymes</i></b>         |                            |      |  |
| 12:05                                     | Manuela Pereira            | ITQB | Respiratory enzymes - Introduction   |
| 12:30                                     | <b><i>Lunch break</i></b>  |      |  |
| <b><i>Respiratory enzymes (Cont.)</i></b> |                            |      |  |
|   | Chair: Diego Millo         |      |  |
| 14:00                                     | Filipa Sousa               | ITQB | Heme copper oxygen reductases  |
| 14:15                                     | Patrícia Refojo            | ITQB | Novel Quinol:acceptor oxido reductases                                       |
| 14:30                                     | Smilja Todorovic           | ITQB | Resonance Raman spectroscopy of multi-heme enzymes                           |
| 14:55                                     | Inês C. Pereira            | ITQB | Respiratory Complexes from anareobes   |
| 15:20                                     | <b><i>Coffee break</i></b> |      |  |
| <b><i>Metalloproteins</i></b>             |                            |      |  |
|   | Chair: Catarina Paquete    |      |  |
| 15:50                                     | Célia Romão                | ITQB | Iron storage proteins, a look to BFr and Dps                                 |
| 16.:15                                    | David Turner               | ITQB | How do cytochromes <i>c</i> <sub>3</sub> work in solution?                   |
| 16:50                                     | Miguel Saggi               | TU   | EPR Spectroscopy of metalloenzymes   |
| 17:25                                     | Ingo Zebger                | TU   | SEIRA spectroscopy of redox proteins   |

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| 17:50   | <b>End of day 2</b>        |      |  |
| <b>Friday, September 19, 2008</b>                     |                            |      |  |
| <b><i>Theoretical Methods</i></b>                     |                            |      |  |
|   | Chair: Steve Kaminski      |      |  |
| 9:15  | Antonio Baptista           | ITQB | Modeling the protonation and reduction equilibrium in proteins   |
| 9:40  | Miguel Machuqueiro         | ITQB | The coupling between conformation, reduction and protonation in cytochrome c <sub>3</sub>                        |
| 9:55  | Tillmann Utesch            | TU   | MD simulations of immobilised proteins   |
| <b><i>Photoreceptors</i></b>                          |                            |      |  |
| 10:10   | Patrick Scheerer           | TU   | Crystal structure of the ligand-free G-protein-coupled receptor opsin in its G protein-interacting conformation. |
| 10:35   | <b><i>Coffee break</i></b> |      |  |
|   | Chair: Bruno Victor        |      |  |
| 11:00   | David von Stetten          | TU   | Introduction to phytochromes   |
| 11:25   | Steve Kaminski             | TU   | QM/MM methods – Introduction and application to phytochrome  |
| 12:00   | Francisco Velasquez        | TU   | Resonance Raman spectroscopy of phytochrome Cph1   |
| 12:15   | Matthias Schenderlein      | TU   | Spectroscopy of carotenes  |
| 12:30   | <b><i>Lunch break</i></b>  |      |  |
| <b>Voltage-clamp / spectroscopy and ion transport</b> |                            |      |  |
|   | Chair: David von Stetten   |      |  |
| 14:00   | Ana P. Baptista            | ITQB | Sodium transport by Complex I  |
| 14:15   | Jacek Kozuch               | TU   | Vibrational spectroscopy of proteins in oocytes  |
| 14:40   | Yann Astier                | ITQB | Nanopores: an emerging technology for molecular interaction studies  |

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|--|---------------------------|------|---|
| 15:05  | <i>Coffee break</i>       |      |   |
| <b><i>Electron Transfer of cytochromes</i></b> |                           |      |   |
|  | Chair: Miguel Machuqueiro |      |   |
| 15:35  | Inez Weidinger            | TU   | Electron transfer of Cytochrome c immobilised on electrodes:<br>objectives and approaches                           |
| 16:00  | Anja Kranich              | TU   | Re-orientation of cytochrome c  |
| 16:15  | Murat Sezer               | TU   | Gated electron transfer of iso-1-cytochrome c from yeast  |
| 16:30  | Khoa Ly                   | TU   | Electron transfer dynamics of covalently bound cytochrome c   |
| 16:45  | Ricardo Louro             | ITQB | Characterization of multiheme cytochromes by NMR  |
| 17:10  | Catarina Paquete          | ITQB | Detailed kinetic characterization of multicentre proteins:<br>application to tetraheme cytochromes c <sub>3</sub> . |
| 17.25  | Miguel Teixeira           | ITQB | Concluding Remarks  |
|  | Peter Hildebrandt         | TU   |   |
| 20:00  | <i>Workshop dinner</i>    |      |   |