

# **The 2<sup>nd</sup> Opatija Meeting On Computational Solutions in the Life Sciences**

## **List of Invited Speakers (to be confirmed)**

**Walter Thiel, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr**

**Gerhard Klebe, Philipps-Universität Marburg, Marburg**

**Ursula Röthlisberger, Ecole Polytechnique Federale de Lausanne, Lausanne**

**Rebecca Wade, EML Research gGmbH, Heidelberg**

**Paolo Carloni, International School for Advanced Studies, Trieste**

**Siewert-Jan Marrink, University of Groningen, Groningen**

**Jack Leunissen, Wageningen University, Wageningen**

**Helmut Grubmüller, Max-Planck-Institute for Biophysical Chemistry, Göttingen**

**Eivind Hovig, Institute for Cancer Research, The Norwegian Radium Hospital, Oslo**

**Dušanka Janežič, National Institute of Chemistry, Ljubljana**

**Rob Russell, European Molecular Biology Lab, Heidelberg**

**Hendrik Zipse, Ludwig-Maximilians-Universität, München**

**Janez Mavri, National Institute of Chemistry, Ljubljana**

**Oliver Kühn, Freie Universität Berlin, Berlin**

**Milan Hodošček, National Institute of Chemistry, Ljubljana**

**Rudi Podgornik, University of Ljubljana, Ljubljana**

**Vlasta Bonačić-Koutecký, Humboldt-Universität zu Berlin, Berlin**

**Snežana Zarić, University of Belgrade, Belgrade**

**Wolfgang Domcke, Technische Universität München, Garching**

**Davor Juretić, University of Split, Split**

**Max Holthausen, Johann Wolfgang Goethe-Universität Frankfurt am Main**

**Ana Smith, Universität Stuttgart, Stuttgart**

**Leif Eriksson, Örebro University, Örebro**

**Anna Tramontano, University of Rome, Rome**

**Danica Agbaba, University of Belgrade, Belgrade**

**Igor Weber, Ruđer Bošković Institute, Zagreb**

## Tentative program

### **Tuesday, 4. September 2007**

12 <sup>00</sup> -15 <sup>00</sup>	<b><i>Registration</i></b>
15 <sup>00</sup> -16 <sup>00</sup>	<b><i>Welcome snack and introductory remarks</i></b>
16 <sup>00</sup> -16 <sup>50</sup>	<b>Students meeting – formation of groups for the hands on sessions</b>
17 <sup>00</sup> -17 <sup>50</sup>	<b>The first 'hands on' sessions-Part I</b>
17 <sup>50</sup> -18 <sup>05</sup>	<b><i>Coffee Discussion</i></b>
18 <sup>05</sup> -18 <sup>55</sup>	<b>The first 'hands on' sessions-Part II</b>

### **Wednesday, 5. September 2007**

10 <sup>00</sup> - 10 <sup>50</sup>	<b>The second 'hands on' sessions-Part I</b>
10 <sup>50</sup> -11 <sup>05</sup>	<b><i>Coffee Discussion</i></b>
11 <sup>05</sup> -11 <sup>55</sup>	<b>The second 'hands on' sessions-Part II</b>
12 <sup>00</sup> -14 <sup>30</sup>	<b>Lunch</b>
15 <sup>00</sup> - 15 <sup>50</sup>	<b>The third 'hands on' sessions-Part I</b>
15 <sup>50</sup> -16 <sup>05</sup>	<b><i>Coffee Discussion</i></b>
16 <sup>05</sup> -16 <sup>55</sup>	<b>The third 'hands on' sessions-Part II</b>

**Short presentations** (students will present their work)  
(Chairman Boris Kovačević)

16 <sup>55</sup> -17 <sup>15</sup>	<b><i>Coffee Discussion</i></b>
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$17^{15}$ - $19^{00}$       **7 lectures (15 minutes each)**

**Thursday, 6. September 2007**

**Macromolecules in Cell** (Chairman S. Tomić)

$09^{00}$ - $09^{20}$       **2 lectures**

$10^{20}$ - $10^{50}$       ***Coffee Discussion***

$10^{50}$ - $11^{30}$       **1 lecture**

$12^{00}$ - $13^{30}$       ***Lunch***

$14^{00}$ - $20^{00}$       ***Excursion***

**Friday, 7. September 2007**

**Bioinformatics & Molecular Simulation of Macromolecules** (Chairman D. Smith)

$9^{00}$ - $10^{45}$       **3 lectures**

$10^{45}$ - $11^{15}$       ***Coffee Discussion***

$11^{15}$ - $12^{25}$       **2 lectures**

$12^{30}$ - $14^{00}$       ***Lunch***

**Structure-based Drug Design** (Chairman D. Babić)

$14^{00}$ - $15^{45}$       **3 lectures**

$15^{45}$ - $16^{15}$       ***Coffee Discussion***

16<sup>15</sup>-18<sup>30</sup>      **3 lectures**  
19<sup>00</sup>-20<sup>00</sup>      *Dinner*  
20<sup>00</sup>-21<sup>30</sup>      **Poster session**

### Saturday, 8. September 2007

#### **Quantum Chemistry QM/MM** (Chairman M. Hodošček)

9<sup>00</sup>- 10<sup>45</sup>      **3 lectures**  
10<sup>45</sup>-11<sup>15</sup>      *Coffee Discussion*

#### **Quantum Dynamical Study of Biomolecules** (Chairman N. Došlić)

11<sup>15</sup>-12<sup>25</sup>      **2 lectures**  
12<sup>30</sup>-14<sup>00</sup>      *Lunch*

#### **Quantum Chemical Study of Biomolecules** (Chairman V. Mirčeski)

14<sup>00</sup>-15<sup>45</sup>      **3 lectures**  
15<sup>45</sup>-16<sup>15</sup>      *Coffee Break*  
16<sup>15</sup>-19<sup>00</sup>      **Poster session**  
19<sup>30</sup>-      *Conference dinner*

### Sunday, 9. September 2007

#### **Quantum Chemical Study of Biomolecules** (Chairman M. Ramek)

9<sup>30</sup>-10<sup>40</sup>      **2 lectures**

$10^{40}$ - $11^{10}$       *Coffee Break*

**Short presentations (QM/MM and Quantum Chemical Study of Biomolecules)**  
(Chairman F. Babani)

$11^{10}$ - $12^{00}$       **3 lectures (15 minutes each)**

$12^{15}$ - $13^{00}$       *Wrap Up*