

Computational Molecular Medicine: A minisymposium dedicated to Ruth Nussinov

10.22.2015, Konferenzraum MBP 026, building: Modulbau, Otto-blumenthal-Straße,
52064 Aachen (Melaten Campus)

10:00-10:20 – **Welcome**

10:20-10:30 – Paolo Carloni (RWTH-Aachen and FZJ, Germany) – *Introduction*

10:30-10:40 – Carsten Honerkamp (RWTH-Aachen and FZJ, Germany) – *The Physics department at
RWTH-Aachen*

10:40-11:20 – Ruth Nussinov (National Cancer Institute, Maryland, USA) ‘*Oncogenic K-Ras: the
undruggable protein*’

11:20-12:00 – Bernhard Lüscher (RWTH-Aachen, Germany) - TBA

12:00-12:40 – Giorgio Colombo (CNR, Milano, Italy)- ‘*Protein allostery and interactions:
computational studies with an eye to chemical biology*’

12:40-14:00 – **Lunch**

14:00-14:40 – Cristian Micheletti (SISSA, Trieste, Italy) - ‘*The knotted strands of life: physical knots in
proteins, DNA and RNA*’

14:40-15:20 - Giulia Rossetti (RWTH-Aachen and FZJ, Germany) - TBA

15:20-16:00 - Raffaello Potestio (Max Planck Institute for Polymer Research, Mainz, Germany)
- ‘*Building bridges: multi-scale computational methods in biophysics*’

16:00-16:30 – **Coffee Break**

16:30-17:10 – Alessandra Magistrato (CNR-IOM-Democritos and SISSA, Trieste, Italy) – ‘*Role of Mg²⁺
ions in RNA and Proteic Enzymes, insights from computational studies*’

17:20-18:00 – Marco De Vivo (IIT, Genova, Italy and FZJ, Germany) – “*Multiscale molecular
simulations to investigate pharmaceutically relevant metalloenzymes*”

18:00-18:10 *Concluding Remarks* - Paolo Carloni

18:10 – **Transfer to Pizza Dinner at L’Osteria**