

Final Programme Fall Meeting 2012:

“Dissecting and designing interactions”

Conference Chairs: **Prof. Dr. Alexandre Bonvin**, professor of Computational Structural Biology
Dr. Gerry Nicolaes, Cardiovascular Research Institute Maastricht

10:00 - 10:25 Arrival and coffee

10:25 - 10:30 Welcome

10:30 - 11:10 Keynote speaker: **Carlos Camacho** (Pittsburgh University, USA)

"Interactive and efficient discovery tool of small molecule protein-protein interaction antagonists"

11:10 - 11:30 **Ruben Vosmeer**, Margreet Terpstra, Mariëlvan Stee, Lovorka Perić-Hassler, Daan Geerke (Amsterdam)

"Fast and accurate prediction of substrate binding affinities for Cytochrome P450s"

11:30 - 11:50 **Adrien Melquiond**, Mikael Trelletand and Alexandre Bonvin (Utrecht)

"A unified conformational selection and induced fit approach to protein-peptide docking"

11:50 - 12:10 **Barbara Zarzycka**, Tom Seijkens, Mahesh Kulharia, Sander Nabuurs, Gert Vriend, Esther Lutgens and Gerry Nicolaes (Maastricht/Nijmegen/Amsterdam)

"CD40-TRAF6: structure-based virtual ligand screening for potential inhibitors of inflammation"

12:10 - 13:30 Lunch and Poster Session

13:30 - 14:10 Keynote speaker: **Siewert-Jan Marrink** (Rijksuniversiteit Groningen)

"Large scale modeling of membrane protein self-assembly"

14:10 - 14:30 **Markus Weingarh**, Alexander Prokofyev, Elwin van der Crujisen, Deepak Nand, Alexandre Bonvin, Olaf Pongsand and Marc Baldus (Utrecht/Homburg)

"Structural determinants and functional aspects of specific lipid binding to potassium channels as seen by coarse grained MD and solid state NMR"

14:30 - 14:50 **Floris van Eerden**, Djurre de Jong, Cezar Lopez, Alex de Vries, Xavier Periole and Siewert Marrink (Groningen)

"Lipid dynamics of the thylakoid membrane"

14:50 - 15:10 **Elisa Cilia**, Geerten Vuisterand Tom Lenaerts (Brussels/Leicester)

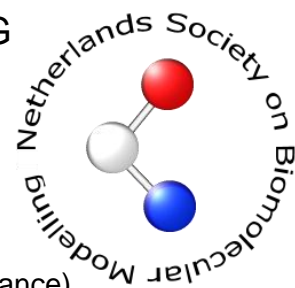
"Accurate prediction of peptide-induced dynamical changes within the 2nd PDZ domain of PTP1e"

15:10 - 15:30 Coffee and Tea

NETHERLANDS SOCIETY ON BIOMOLECULAR MODELLING

Fall Meeting - November 26th 2012

Venue: Academiegebouw, Kanunnikenzaal, Universiteit Utrecht
Domplein 29 Utrecht, NL



- 15:30 - 16:10 Keynote speaker: **Olivier Sperandio** (Université Paris Diderot, France)
"Toward the design of focused chemical libraries to modulate Protein-Protein Interactions: A Chemoinformatics approach"
- 16:10 - 16:30 **Wouter Touw**, Vincent Breukelsand Geerten Vuister (Nijmegen/Leicester)
"Solution structure of NCX3-CBD2-B"
- 16:30 - 16:50 **Jan Felix**, Jonathan Elegheert, Irina Gutsche, Alexander Shkumatov, Yurong Wen, Erwin Pannecoucke, Isabel Vandenberghe, Dmitri Svergun, Ewald Pauwels, Bjorn Vergauwen and Savvas Savvides (Ghent/Grenoble/Hamburg)
"Human IL-34 and CSF-1 establish structurally similar complexes with their common hematopoietic receptor"
- 16:50 - 17:00 Concluding remarks

Late Registration

Late registrations can be made free of charge via e-mail to science.secr.nmr@uu.nl with as subject line "NSBM meeting 2012". A lunch and coffee/tea breaks will be provided for.

Should a lack of funding be a hurdle for visiting the NSBM Fall Meeting, please contact prof. Gert Vriend at vriend@cmbi.ru.nl so that an arrangement can be made.

How to reach the "Academiegebouw"

By public transport

From Utrecht Central Station take bus 2, exit at Domplein.

By foot (10 minute walk from Utrecht Central Railway Station)

Follow directions to the 'Museumkwartier' (Museum Quarter). In the 'HoogCatharijne' shopping mall take the 'Godebaldkwartier' exit and continue left towards the Dom Tower. After passing right under the Dom Tower, cross over towards the right. The entrance to the University Hall is right in front of you.

By car

For up-to-date directions, please check your route planner. Information about road works in and around Utrecht is available from Utrecht bereikbaar.

Parking

The nearest car park is located at the Springweg, a ten-minute walk from the University Hall. On the motorway follow directions towards the city centre (Centrum), then look for signs to 'P Springweg'. After parking your car exit the car park at the 'Oudegracht' side and walk through the 'Strosteeg' towards the 'Oudegracht'. Cross the bridge and turn left. At the 'Wed' turn right, then cross the 'Lange Nieuwstraat'. The entrance to the University Hall is right in front of you.

