Sunday, June 19th

9:50 City Walk (only for registered participants)
13:30 – 15:30 Registration
15:00 Welcome snack
15:20 Meeting opening

Session: Nucleic Acids I - Chair: Tom Cheatham

15:30 **Modesto Orozco**
Simulating DNA from the electron to the chromosome
16:10 **Montgomery Pettitt**
DNA confined: Advantages of non-linear behavior
16:50 Coffee break
17:10 **Mahdi Bagherpoor Helabad**
The role of Protein-DNA interactions in the DNA binding specificity of hormone receptors
17:30 **Lennart Nilsson**
Triplex forming oligonucleotides and gene therapy
18:10 **Vlad Cojocaru**
From decoding dynamics to tailoring cooperativity in protein-DNA interactions
19:00 Dinner at Terminus hotel (only for registered participants)

Monday, June 20th

Session: Nucleic Acids II - Chair: Lennart Nilsson

8:30 **Thomas E. Cheatham III**
Challenges and successes in modeling RNA structure, dynamics and interactions with ions.
9:10 **Joanna Trylska**
Interactions of aminoglycoside antibiotics with RNA
9:30 **Filip Lankas**
Modelling allosteric effects in DNA

9:50 Coffee break

Session: protein-lipid interactions - Chair: Michele Cascella

10:10 **Carmen Domene**
Computational approaches to the molecular thermometers of the human body
10:50 **Syma Khalid**
Molecular simulations that put the chemical complexity into model bacterial membranes
11:30 **Stefano Vanni**
Taking advantage of membrane diversity in intracellular trafficking pathways
11:50 **Michael Schauperl**
Explaining the recognition process of ice binding proteins

12:10-13:30 Lunch Break

Session: ISQBP awards talks - Chair: Alex MacKerell

13:30 **Rebecca Wade** - ISQBP Award in Computational Biology
In silico prediction of biomolecular recognition

14:30 **Marta Filizola** - ISQBP Loew Lectureship
New Challenges and Opportunities in G Protein-Coupled Receptor Drug Discovery

15:30 Coffee Break and **Poster session**

17:40 Recommended departure to Welcome ceremony (by foot)
18:00 Welcome ceremony by the City of Bergen (at the University Aula, Cf. map)

Tuesday, June 21st

Session: Drug design I - Chair: Annick Dejaegere

8:30 **William L.Jorgensen**
Design and Discovery of Potent Enzyme Inhibitors

9:10 **Daniel Cappel**
Rigorous Free Energy Calculations Applied to Protein Homology Models

9:30 **Elsa Sánchez-Garcia**
Supramolecular Ligands as Regulators of Biomolecular Interactions

9:50 Coffee Break

Session: Drug design II - Chair: Bjørn Olav Brandsdal

10:10 **Carmay Lim**
Using an old drug to target a new drug site

10:50 **Sanja Zivanovic**
Multi-level strategy for analysis of bioactive drug conformations

11:10 **Chandra Verma**
Stapled diets: tackling resistance

11:30 ISQBP General Assembly
12:00-13:30 Lunch Break

Session: Methodological Advances I - Chair: William L. Jorgensen

13:30 **Alex MacKerell**
Overview of the Classical Drude Oscillator Polarizable Force Field for Biomolecules

14:10 **Charles L.Brooks III**
High-throughput, free energy based ligand discovery and optimization using multi-site λ-dynamics

14:50 **Hima Bindu Kolli**
Hybrid Particle-Field Approach with Electrostatics for Mesoscale Biomolecular Simulations

15:10 **Iain Bethune**

Molecular Integration Simulation Toolkit - interfacing novel integrators with Molecular Dynamics codes.

15:30 Coffee Break

18:30 Recommended departure from Grand Hotel Terminus (by foot, Cf. map)
19:00 Boat departure to *Cornelius på Holmen*, Conference Dinner, sponsored by the Journal of Chemical Theory and Computation (JCTC)

Wednesday, June 22nd

Session: Methodological Advances II – chair: Vlad Cojocaru

8:50 **Thomas Gaillard**
Computational Protein Design with an MMGBSA Energy Function
9:10 **Kwangho Nam**
Development and acceleration of multiscale QM/MM methods for simulations of complex biomolecular systems
9:30 **Xabier Lopez**
Aluminum and bioligand interactions with phosphate containing groups.

9:50 Coffee Break

Session: Enzyme and protein dynamics – chair: Nathalie Reuter

10:10 **Annick Dejaegere**
Structural dynamics and signalling mechanisms in nuclear retinoid receptors
10:50 **Carol Post**
An unusual allosteric mechanism for regulating protein interactions of Syk tyrosine kinase
11:30 **Natacha Gillet**
Understanding Charge Transfer in Cryptochromes and Photolyases via QM/MM Simulations: Application to PhrB Protein
11:50 **Thibault Tubiana**
Norovirus Capsid Assembly

12:10 Closing remarks
12:30 Lunch