Name of laboratory
Laboratory of Computational Chemistry and Biochemistry (LCBC)

Name of professor
Prof. Ursula Röthlisberger

http
http://lcbc.epfl.ch/

@ ursula.roethlisberger@epfl.ch

General areas
(Description of the research area of the laboratory. Description of the main research topics where students could be involved during the Master thesis)
Computational Chemistry and Biochemistry

Research themes
Various possible projects (more information upon request)

Methodology of work/special instrumentation
(For example synthetic chemistry, wet chemistry, theoretical chemistry, simulation by computer, chemistry by Laser, mass spectrometry, NMR, etc.)
Computational work

Recent examples of MSc/PhD thesis

Vanni Stefano (PhD thesis)
“Exploring G-Protein Coupled Receptor Activation with Multiscale Molecular Simulations”
http://library.epfl.ch/theses/?nr=5005

Tapavicza Enrico Marko (PhD thesis)
“Development of a non-adiabatic ab initio molecular dynamics method and its application to photodynamical processes”
http://library.epfl.ch/theses/?nr=4115

Basile Curchod (MSc)
“Towards the binding of cisplatin to Cu,Zn superoxide dismutase: First steps of a theoretical study”

Pascal Baillod (PhD thesis)
“Solute energy based REMD : developments and applications to prion protein”
misfold predictions"
http://library.epfl.ch/theses/?nr=4103

Christian Gossens (PhD thesis)
“In silico DNA-binding and rational design of ruthenium-arene anticancer drugs”
http://library.epfl.ch/en/theses/?nr=3723