



COFFEE : every day at 10:30 and at 16:00

LUNCH : every day at 12:30

Monday 30

19:30 drink / dinner "Aux Artistes", 63, rue Falguière, 75015 Paris

Tuesday 1

AM

9:00 presentation of participants

11:00 Richard Lavery : historical perspective, force fields

PM

14:00 Valerie Daggett : molecular dynamics and energy minimisation, analysis

16:00 Tru Huynh: Intro to computing environment

16:30 Markwick / Blondel / Huynh: Practical Amber I : setup

EVENING : poster session / buffet dinner

Wednesday 2

AM

9:00 Richard Lavery : Monte Carlo, coarse grain models

11:00 Alan Mark : free energy calculations

PM

14:00 Markwick / Malliavin / Huynh: Practical Amber II : analysis

EVENING : poster session / buffet dinner

Thursday 3

AM

9:00 Alan Mark : research talk

11:00 Valerie Daggett : research talk

PM

14:00 Konrad Hinsen: normal modes, python programming + practical

EVENING : free

Friday 4

AM

9:00 Tom Simonson : electrostatics, implicit solvent

11:00 Adrian Mulholland: QMMM

PM

14:00 Mulholland: practical QMMM

EVENING : Pizza Flora, 113-117, rue de Cambronne, 75015 Paris

Saturday 5

AM

9:00 Michael Nilges: modelling with experimental data

11:00 Anna Tramontano : homology modelling

PM

14:00 Practical homology modelling

EVENING : free

Sunday 6

AM

9:00 Rebecca Wade: Brownian Dynamics

11:00 Phineus Markwick: accelerated dynamics

PM

14:30 Excursion "bateau mouche"

EVENING : free

Monday 7

AM

9:00 Leslie Kuhn: docking

11:00 Leslie Kuhn: practical docking

PM

14:00 Leslie Kuhn: practical docking continued

16:30 round table

EVENING : course dinner : L'Avel, 65, boulevard Pasteur