

Week 1

tentative program

Day	Time	Room	Speaker	Title
Mo 1-7	10.00-11.00	tbd	Prof. Dr. Jacob de Vlieg	Introduction to chemistry & eScience and general molecular informatics
	11.15-12.15	tbd	Dr. Scott Lusher	Nuclear receptors
	lunch			
	13.30-15.00	HG00.023		MOE introduction NEW
	15.15-17.00	HG00.023		Nuclear receptor functioning
Tu 2-7	9.00-10.30	tbd	Dr. Tina Ritschel	Overview SBDD
	11.00-12.30	tbd	Dr. Sander Nabuurs	Ligand docking
	lunch			
	13.30-15.00	HG00.023		In silico lead finding techniques: Virtual
	15.15-17.00	HG00.023		Structure based pharmacophore search
We 3-7	9.00-10.30	tbd	Dr. Tina Ritschel	Structure based pharmacophores
	11.00-12.30	tbd	Prof. Dr. Gert Vriend	Sequence alignment and homology modeling
	lunch			
	13.30-17.00	HG00.023	Prof. Dr. Gert Vriend	Target Protein Structure Analysis: Homology Modeling, Sequence Retrieval and Sequence Alignment Techniques
Th 4-7	9.00-10.30	tbd	Dr. Gijs Schaftenaar	QSAR
	11.00-12.30	tbd	Dr. Ross McGuire	Introduction to chemical databases and searching, PubChem
	lunch			
	13.30-15.00	HG00.023		In silico lead finding techniques: 2D/3D searches
	15.15-17.00	HG00.023		In silico lead finding techniques QSAR
Fr 5-7	9.30-18.00		Symposium	

Week 2

Day	Time	Room	Speaker	Title
Mo 8-7	9.00-10.30	tbd	Dr. Marijn Sanders / Wilco Fleuren	Literature text mining NEW
	11.00-12.30	tbd	Dr. Lars Ridder	Metabolomics NEW
	lunch			
	13.30-15.00	HG00.023	Dr. Marijn Sanders / Wilco Fleuren	Application of literature text mining in pharma and food research NEW
	15.15-17.00	HG00.023	Dr. Lars Ridder	Mass Spectrometry analysis using Magma NEW
Tu 9-7	9.00-10.30	tbd	Dr. Scott Lusher	The 4th paradigm in medicinal chemistry research
	11.00-12.30	tbd	Dr. Scott Lusher	Show case
	lunch			
	13.00-15.00	HG00.023		In silico lead optimization techniques: SBDD
	15.15-17.00	HG00.023	Dr. Tina Ritschel	Introduction group work
We-Th 10/11-7			Group work	
Fr 12-7	9.00-17.00	tbd	Group presentations	

lecture
symposium

practical
group work