VANDERBILT UNIVERSITY

UNIVERSITÄT LEIPZIG

Scientific and Methods Module “Molecular Modelling”

Module	HIGH THROGHPUT SCREENING IN DRUG DISCOVERY
Aims	Teach theoretical and practical aspects of drug discovery with a focus on computer-aided drug discovery and high throughput screening.
Basics	Biochemistry, amino acid structure, peptide bond, secondary structure, tertiary structure, small molecule binding, central dogma of molecular biology
Contents	The class will give an overview of drug discovery with a focus on computer-aided drug discovery and high throughput screening. Students will further learn the overall drug discovery process through the discussion of case studies.
Methods	High-throughput Screening in Drug Discovery, Experimental and Computational
Type	10 day block course, 05 – 16 December 2016
Work load	**MODULE: HIGH THROGHPUT SCREENING IN DRUG DISCOVERY** 30 hours presence / 60 hours self-study Each 3-hour session includes a lecture presented by one of the two instructors. Some sessions include a 90min discussion of a case study prepared and presented by one students.
Examination	Written Exam
Credit points	1
Responsible scientists	Prof. Dr. David Weaver (Vanderbilt University) Prof. Dr. Jens Meiler (Vanderbilt University) Prof. Dr. Annette Beck-Sickinger (Leipzig University)
Literature	Scientific papers will be assigned in class
Venue	Universität Leipzig, Fakultät für Biowissenschaften, Pharmazie und Psychologie, Institut für Biochemie, Brüderstraße 34, 04107 Leipzig

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Instructors:

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Schedule

HIGH THROGHPUT SCREENING IN DRUG DISCOVERY						
2016		**Dec 05**	**Dec 06**	**Dec 07**	**Dec 08**	**Dec 09**
LECTURES	09 – 12	**Topic** Course Overview and Introduction to the Drug Discovery Pipeline **Jens Meiler**	**Topic** An Introduction to High-throughput Screening **Charles David Weaver**	**Topic** HTS Assay Technologies: Strengths, Limitations, and Future Directions **Charles David Weaver**	**Topic** Technology-enabled Hits-to-Leads and Lead Optimization **Charles David Weaver**	**Topic** Practical uses of HTS for academic and industrial probe discovery and development **Charles David Weaver**

HIGH THROGHPUT SCREENING IN DRUG DISCOVERY						
2016		**Dec 12**	**Dec 13**	**Dec 14**	**Dec 15**	**Dec 16**
LECTURES	09 – 12	**Topic** Protein-Ligand-Docking **Jens Meiler**	**Topic** Structure-based Virtual Screening & Drug Design **Jens Meiler**	**Topic** Constitution, Configuration, & Conformation & Structure Generators **Jens Meiler**	**Topic** QSAR, Ligand-based Virtual Screening, and Pharmacophore mapping **Jens Meiler**	**Topic** Overflow, Conclusion, Exam **Jens Meiler**