

0368330 - Basics of mathematical simulation models in endothelial research	
Ort	ZOM Anästhesie, A2-3 Besprechungsraum
Wochentag, Uhrzeit	Wöchentl. 17:00 bis 19:15
Erste Veranstaltung	April (Termine nach Vereinbarung)
Letzte Veranstaltung	Mai (Termine nach Vereinbarung)
Verantw. Dozent	Dr.med. Sergey Shityakov Ph.D
Anwesenheitspflicht	Nein
Prüfungstermin	keiner
Prüfungsform	keine
Scheinausgabe	Siehe Sb@Home
Veranstaltungsinhalte	
Termin ab April (Termine nach Vereinbarung)	<p>Thema</p> <ol style="list-style-type: none"> 1) In silico, in vitro, and in vivo methods used in the blood-brain barrier (BBB) research to analyze drug-like chemical compounds: An overview 2) Molecular docking methods in the BBB research: An overview 3) Molecular dynamics methods in the BBB research: An overview 4) Mathematical models based on differential equations and dose-response logistic functions used in the BBB research and biomedicine (MATLAB, Maple programming) 5) Molecular descriptor methods to predict blood-brain barrier permeation for drug-like chemical compounds 6) 3D-QSAR (three-dimensional quantitative structure-activity relationship) approach in the BBB research.
Maximal Teilnehmer	10
Links/Literatur	<ol style="list-style-type: none"> 1) Shityakov, S*, Salvador, E, Förster, C*, 2013, In silico, in vitro and in vivo methods used in pharmaceutical research to analyse drug permeation through the blood-brain barrier, OA Anaesthetics 2013 Jul 01;1(2):13. 2) Salvador, E, Shityakov, S, Foerster, C*, 2013, Glucocorticoids and endothelial cell barrier function, Cell Tissue Res, PMID:24352805 3) Shityakov, S*, Foerster, C*, 2013, Pharmacokinetic delivery and metabolizing rate of nocardipine incorporated in hydrophilic and hydrophobic cyclodextrins using two-compartment model, The Scientific World Journal, 01/2013; 2013:55-58 4) Shityakov, S*, Foerster, C*, 2013, Multidrug resistance protein P-gp interaction with nanoparticles (fullerenes and carbon nanotube) to assess their drug delivery potential: a molecular docking study, Int. J. Computational Biology and Drug Design, Vol. 6, No. 4, pp. 343-357. 5) Shityakov, S*, Broscheit, J., Foerster, C*, 2012. Beta-Cyclodextrin dimer complexes of dopamine and levodopa derivatives to assess drug delivery to the central nervous system: ADME and molecular docking studies. International Journal of Nanomedicine, Vol 7: 1-9. 6) Shityakov, S*, Neuhaus, W., Dandekar, T., Foerster, C*, 2012. Analyzing molecular polar surface descriptors to predicts blood-brain barrier permeation, Journal of Computational Biology and Drug Design, 6(1-2): 146-56.