

Computational Competences @ D-CHAB

- Development of programming skills (basic and advanced)
- Knowledge of computational chemistry: (related) theory and methods
 - Quantum chemistry
 - Classical simulations
 - Computer-aided process engineering
 - Cheminformatics
 - Molecular representation
 - Database mining (searching, scripting)
 - Algorithmics
- Machine learning and data science in chemistry and medicine
 - Database management (including privacy issues, encryption)
- Use of software packages (commercial, open-source)
 - Typically combined with theory/methods in courses
- “Soft skills”:
 - LaTeX, creating graphics
 - Critical assessment of computational methods: potential and limitations

Computational Competences @ D-CHAB

Compulsory
Elective

Sem.	Chemistry		Biochemistry		Chemical Engineering		Pharmaceutical Sci.	
1.	Informatik I 529-0001-00	Prakt. Allg. Chemie 529-0011-04			Informatik I 529-0001-00	Prakt. Allg. Chemie 529-0011-04		
2.			Statistik I (D-MATH) 401-0643-00				Statistik I (D-MATH) 401-0643-00	
3.			Informatik I 529-0001-00	Statistik II (D-MATH) 401-0643-13			Grundl. Inform. (D-INFK) 252-0852-00	Statistik II (D-MATH) 401-0643-13
4.	Prakt. PC + AnalC 529-0054-00		Prakt. Anal. Biochem./phys. 529-0074-00		Prakt. PC + AnalC 529-0054-00		Prakt. PC (Pharm. Wiss.) 529-0430-00	
5.	APC 529-0002-00	Prakt. Spektroskopie 529-0449-00	Regular courses and block courses involving computational competencies		Stat. + Num. Methods 401-0675-00		Prakt. Med. Chemie 535-0239-00	
6.	Quantenchemie 529-0474-00				Modell. + Math. Methods 151-0940-00		Biopharmazie 535-0241-03	Prakt. Biopharmazie 535-0240-00
Msc	CSBMS 529-0004-01	Digital Chemistry 529-0150-00			Process Des. + Devel. 529-0643-01	Digital Chemistry 529-0150-00	Pharmaceut. Biostats. 511-0012-00	
	Adv. Quantum Chem. 529-0003-01				Proc. Sim. + Flowsheet. 529-0613-01		CADD 535-0022-00	
	Advanced Kinetics 529-0442-00				Case Studies Proc. Des. 529-0459-01			
					Chemometrics + ML 529-0017-00			

Computational Competences @ D-CHAB

Programming skills
Theory/software

Sem.	Chemistry	Biochemistry	Chemical Engineering	Pharmaceutical Sci.
1.	Informatik I 529-0001-00	Prakt. Allg. Chemie 529-0011-04	Informatik I 529-0001-00	Prakt. Allg. Chemie 529-0011-04
2.		Statistik I (D-MATH) 401-0643-00		Statistik I (D-MATH) 401-0643-00
3.		Informatik I 529-0001-00	Statistik II (D-MATH) 401-0643-13	Grundl. Inform. (D-INFK) 252-0852-00
4.	Prakt. PC + AnalC 529-0054-00	Prakt. Anal. Biochem./phys. 529-0074-00	Prakt. PC + AnalC 529-0054-00	Prakt. PC (Pharm. Wiss.) 529-0430-00
5.	APC 529-0002-00	Prakt. Spektroskopie 529-0449-00	Stat. + Num. Methods 401-0675-00	Prakt. Med. Chemie 535-0239-00
6.	Quantenchemie 529-0474-00		Modell. + Math. Methods 151-0940-00	Biopharmazie 535-0241-03
Msc	CSBMS 529-0004-01	Digital Chemistry 529-0150-00	Process Des. + Devel. 529-0643-01	Pharmaceut. Biostats. 511-0012-00
	Adv. Quantum Chem. 529-0003-01		Proc. Sim. + Flowsheet. 529-0613-01	CADD 535-0022-00
	Advanced Kinetics 529-0442-00		Case Studies Proc. Des. 529-0459-01	
			Chemometrics + ML 529-0017-00	

Programming Languages

- **Informatik I:** C(++) (and UNIX)
- **Praktikum Allgemeine Chemie, Phys.+Analyt. Chemie, Spektroskopie:** R
- **Algorithms and Programming in Chemistry (APC):** C++ (and Python)
- **Computer Simulation of BioMolecular Systems (CSBMS):** bash (and C++)
- **Digital Chemistry:** Python
- **Quantenchemie, Advanced Quantum Chemistry:** (Python)
- **Advanced Kinetics:** Python
- **Moderne Massenspektros., Analysenmethoden, Chemometrie:** Matlab

- **Modelling and Math. Methods in Process and Chemical Eng.:** Matlab
- **Statistical and Numerical Methods for Chemical Engineers:** Matlab
- **Chemometrics and ML for Chemical Engineers:** Matlab
- **Process Simulation and Flowsheeting:** Aspen Plus (software)
- **Process Design and Development:** GAMS and associated solvers
- **Case Studies in Process Design:** Aspen Plus (software)

- **Grundlagen der Informatik (D-INFK):** Python, Matlab
- **Statistik I + II (D-MATH):** R
- **Praktikum Phys. Chem. (Pharm. Wiss.):** R
- **Biopharmazie (lecture and practical):** R
- **Praktikum Medizinische Chemie:** R
- **Computer-Assisted Drug Design (CADD):** (Python)
- **Pharmaceutical Biostatistics:** R

Chemistry / Biochemistry

Chemical Engineering

Pharmaceutical Sciences

Databases

- Introduction into domain-specific databases is provided by Infozentrum Chemie, Biologie, Pharmazie
 - From a user perspective (access via GUI)
- **Chemistry / Biochemistry / Chemical Engineering:**
 - Part of practical “Organische und Anorganische Chemie I” (529-0230-00L, 2nd semester)
 - Reaxys, SciFinder (organic compounds, reactions), KnowItAll AnyWare (spectra)
 - Part of practical “Organische und Anorganische Chemie II” (529-0129-00L, 3rd semester)
 - Reaxys, SciFinder and hand books (metalorganic and inorganic compounds)
- **Chemical Engineering:**
 - Part of ”Case Studies in Process Design I” (529-0549-01L, 5th semester)
 - Effective database search (Detherm, SpringerMaterials, Scopus, Web of Science, SciFinder)
- **Pharmaceutical Sciences:**
 - Part of practical “Organische Chemie (für Biol./Pharm.Wiss.)” (529-0229-00L, 3rd semester)
 - Reaxys, SciFindern (organic compounds, reactions), KnowItAll AnyWare (spectra)