

Vertiefungsfach
Analytische Chemie

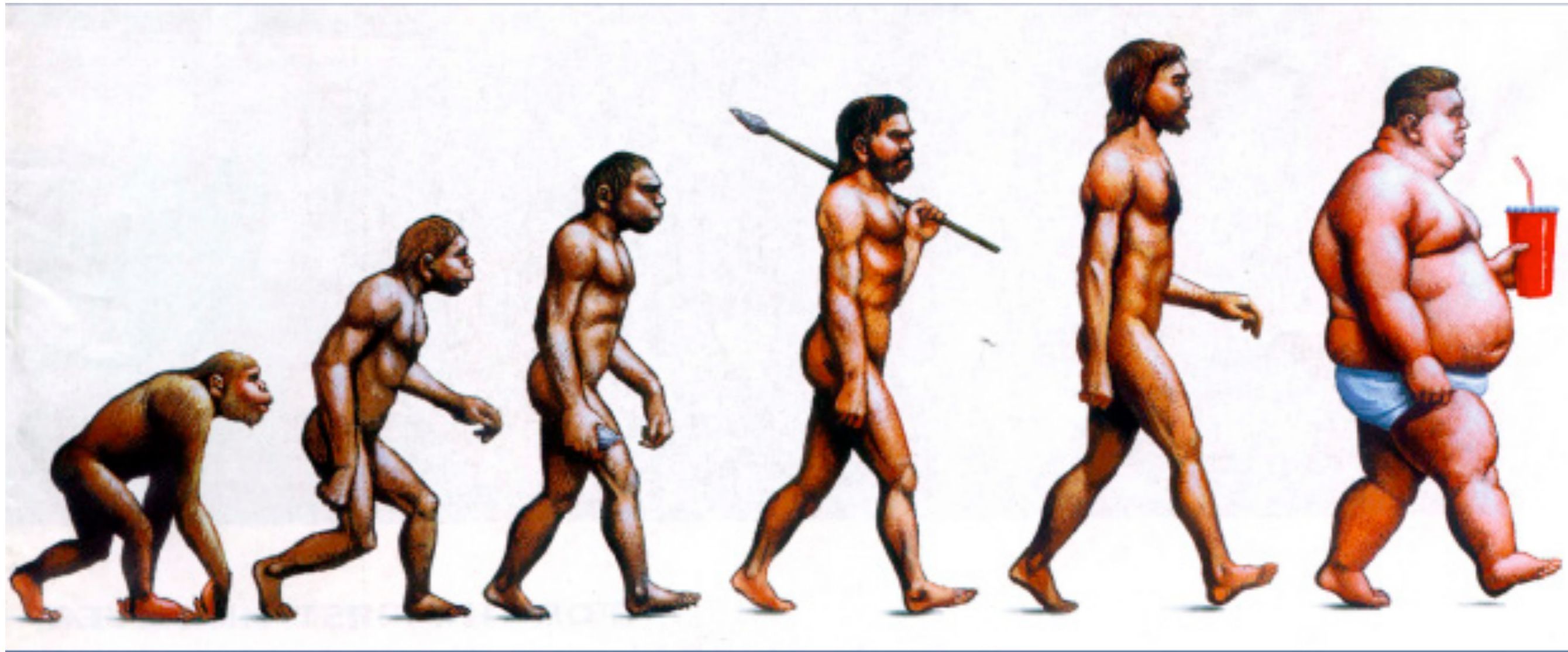
Multivariate Datenanalyse in Analytischer Organischer Chemie und Metabolomforschung

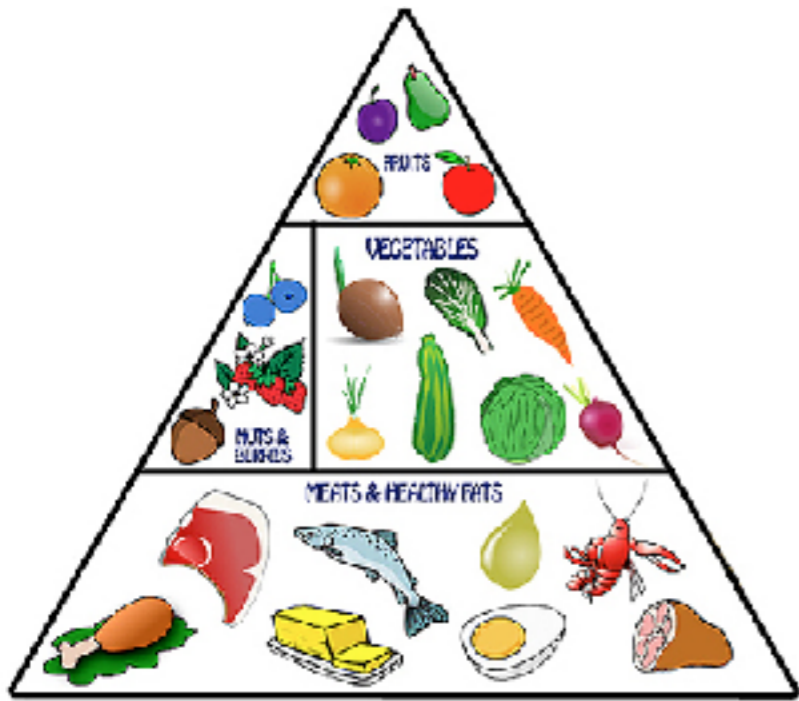
MC2.1.1

Analytische Chemie im Master, Teil 1

Prof. Dr. Christoph Steinbeck

Phänotypen verstehen





Nutrition



Disease



Exercise

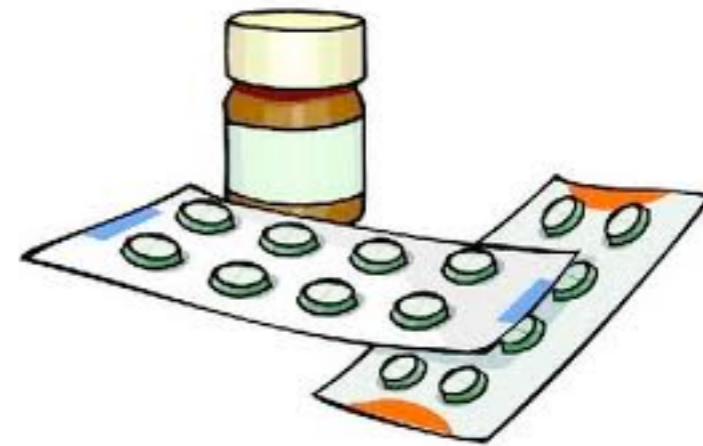
Phenome/ Exposome



Age



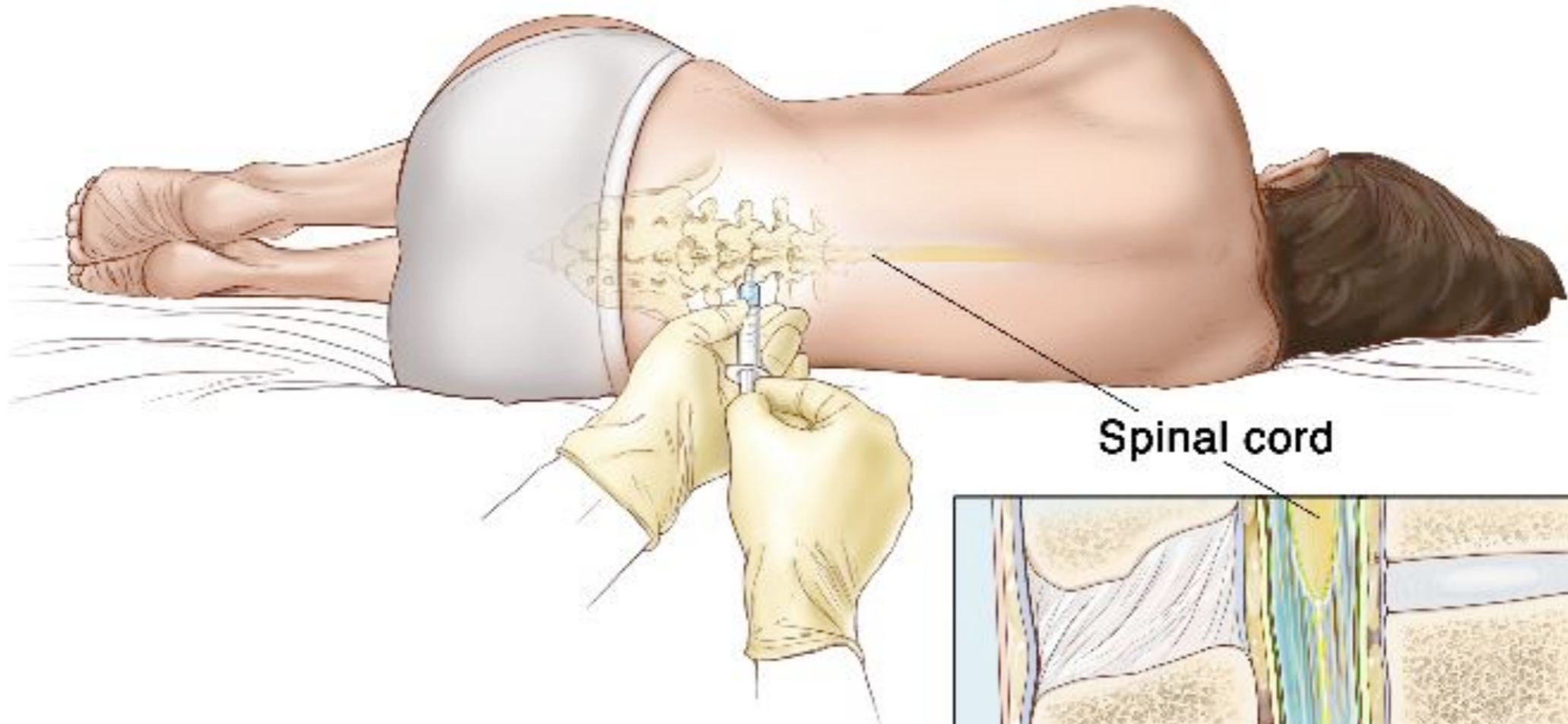
Environment



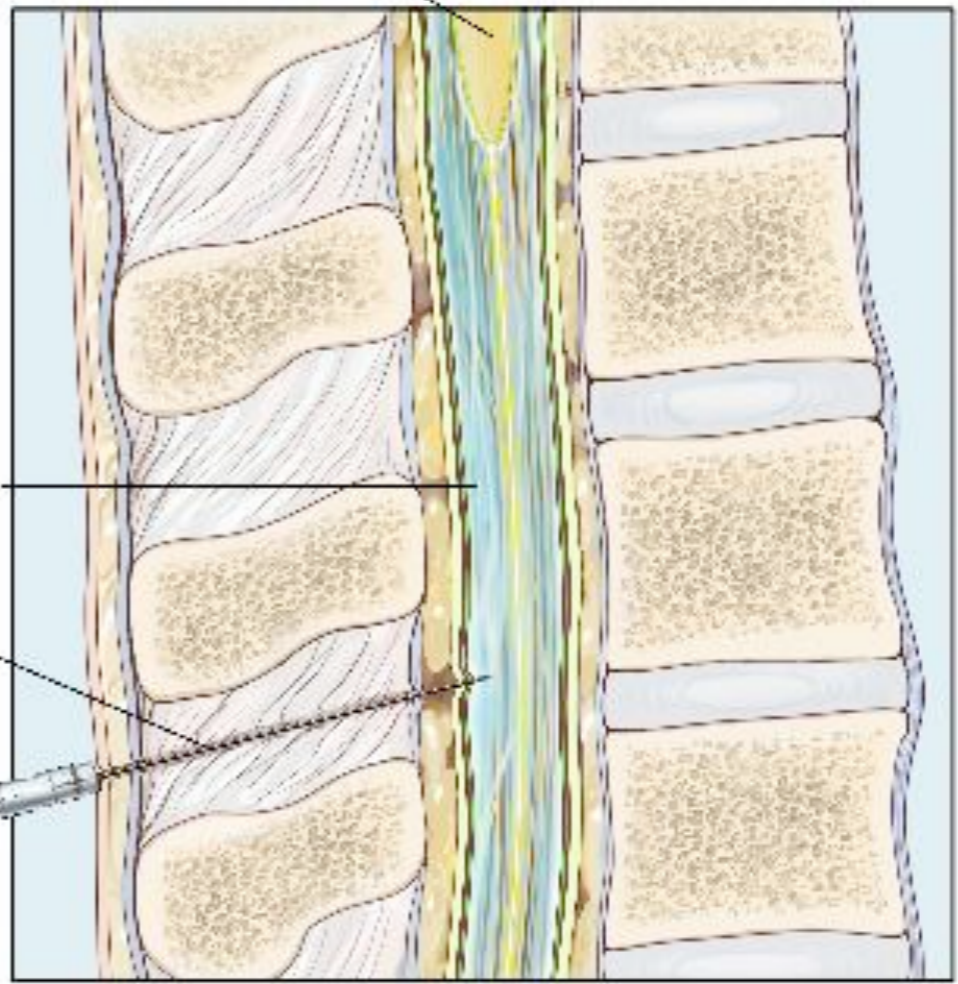
Drugs

Metabolomik

- Analytische Chemie “goes bio”
- Dritte Säule der großen Omics Felder
- Betrachtet so viele kleine Moleküle eines Organismus zur gleichen Zeit wie möglich



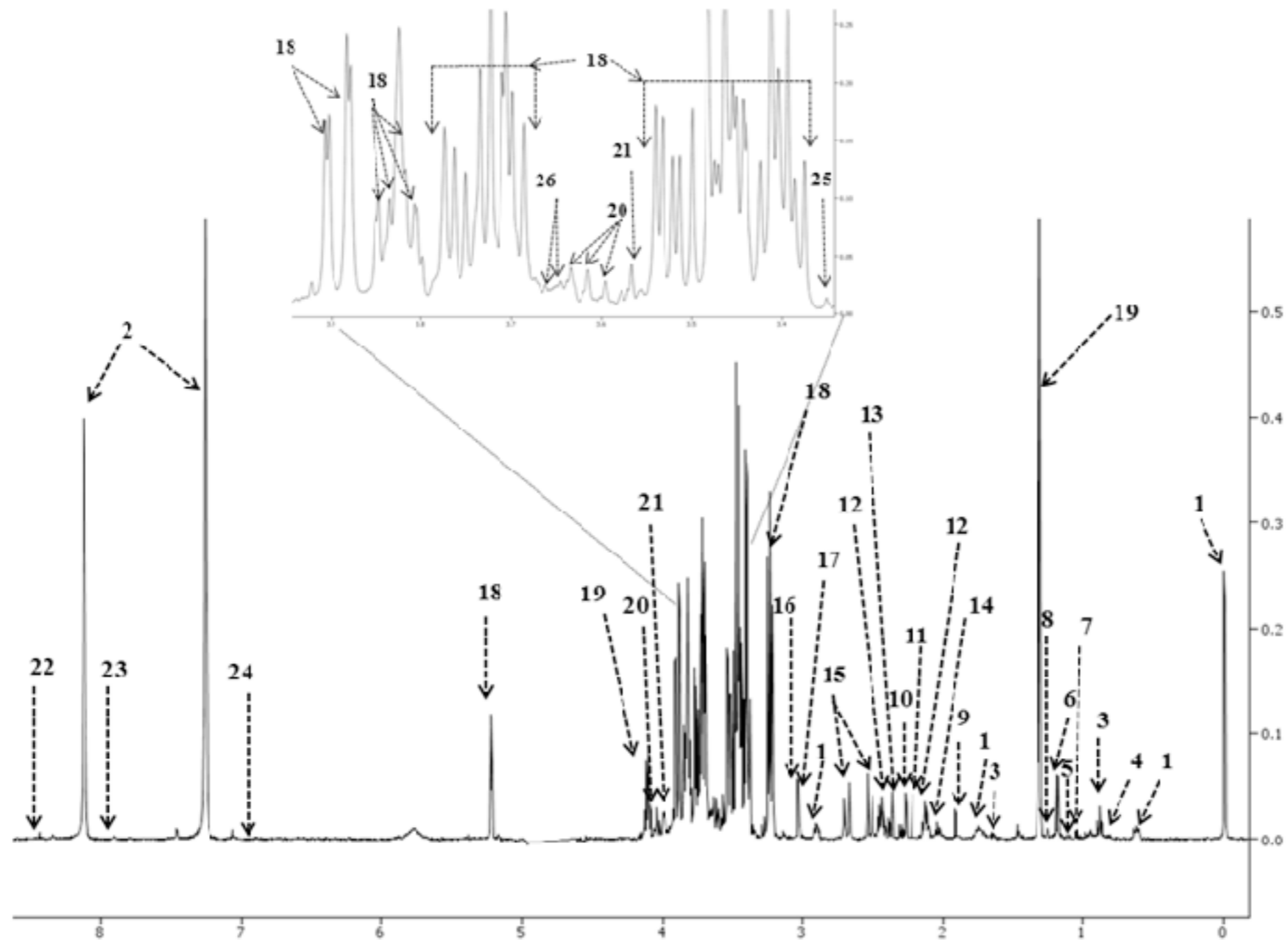
Spinal cord



Cerebrospinal fluid

Spinal needle



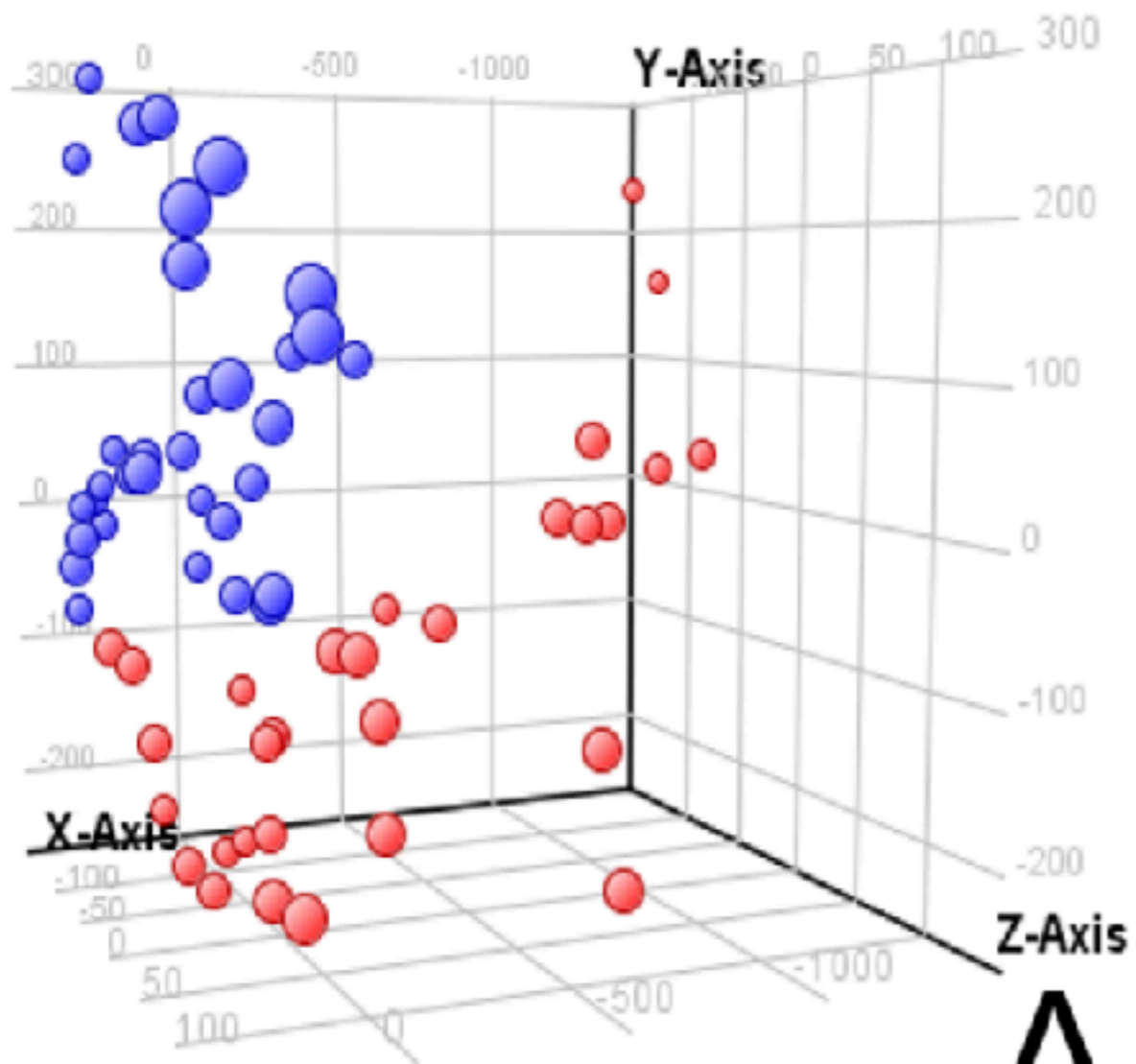


Typical 500 MHz ^1H -NMR spectrum of human cerebrospinal fluid. Numbers indicate the following metabolites:

1. DSS, 2. imidazole, 3. 2-hydroxybutyric acid, 4. 2-hydroxyisovaleric acid, 5. 2-oxoisovaleric acid, 6. 3-hydroxybutyric acid, 7. 3-hydroxyisobutyric acid, 8. 3-hydroxyisovaleric acid, 9. acetic acid, 10. acetoacetic acid, 11. acetone, 12. L-glutamine, 13. pyruvic acid, 14. L-glutamic acid, 15. citric acid, 16. creatinine, 17. creatine, 18. D-glucose, 19. lactic acid, 20. myo-inositol, 21. D-fructose, 22. formic acid, 23. L-histidine, 24. L-tyrosine, 25. methanol, 26. glycerol

Untargeted Metabolomics of Cerebrospinal Fluid

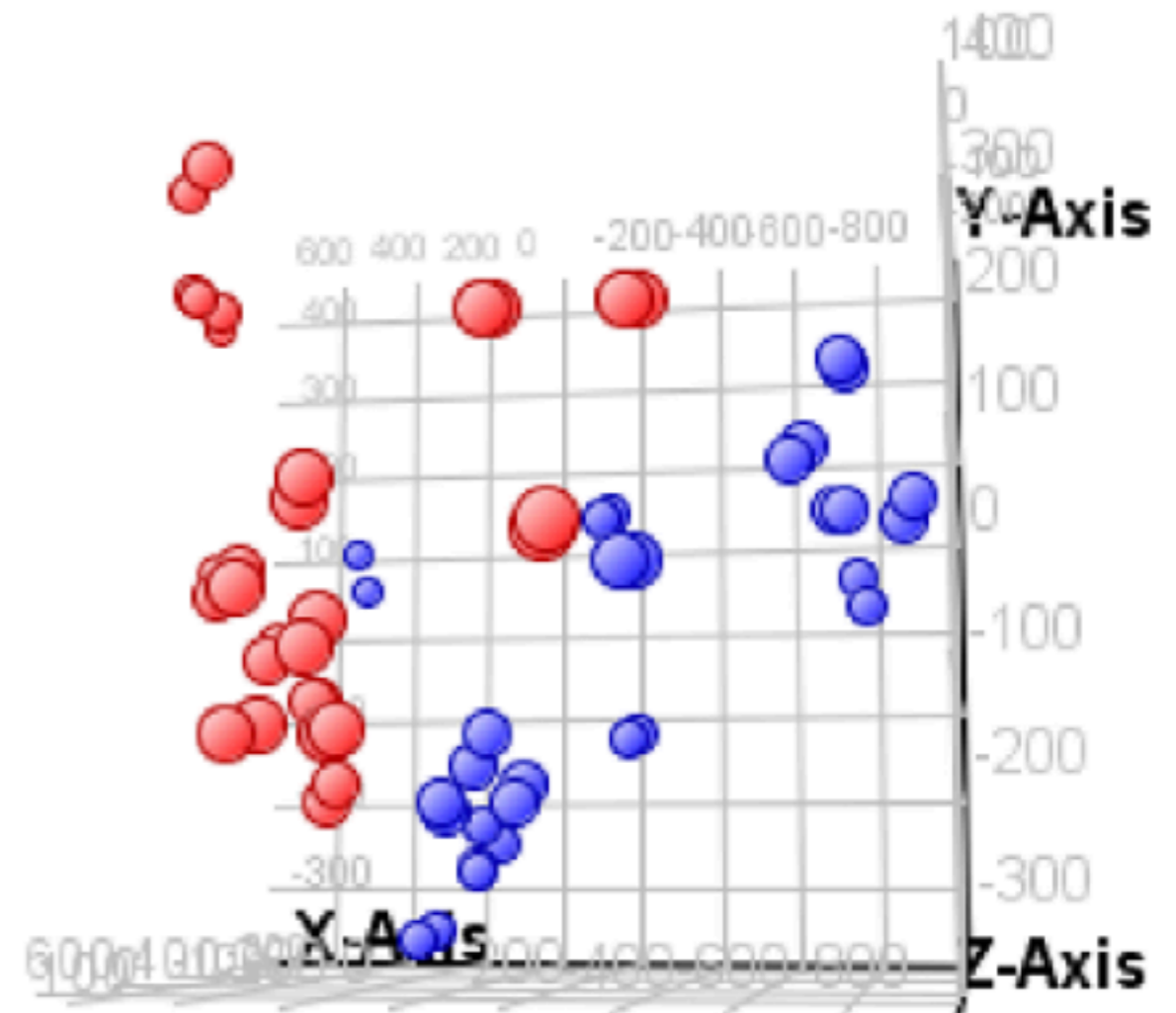
Plasma



AD = Red, CN = Blue

A

CSF



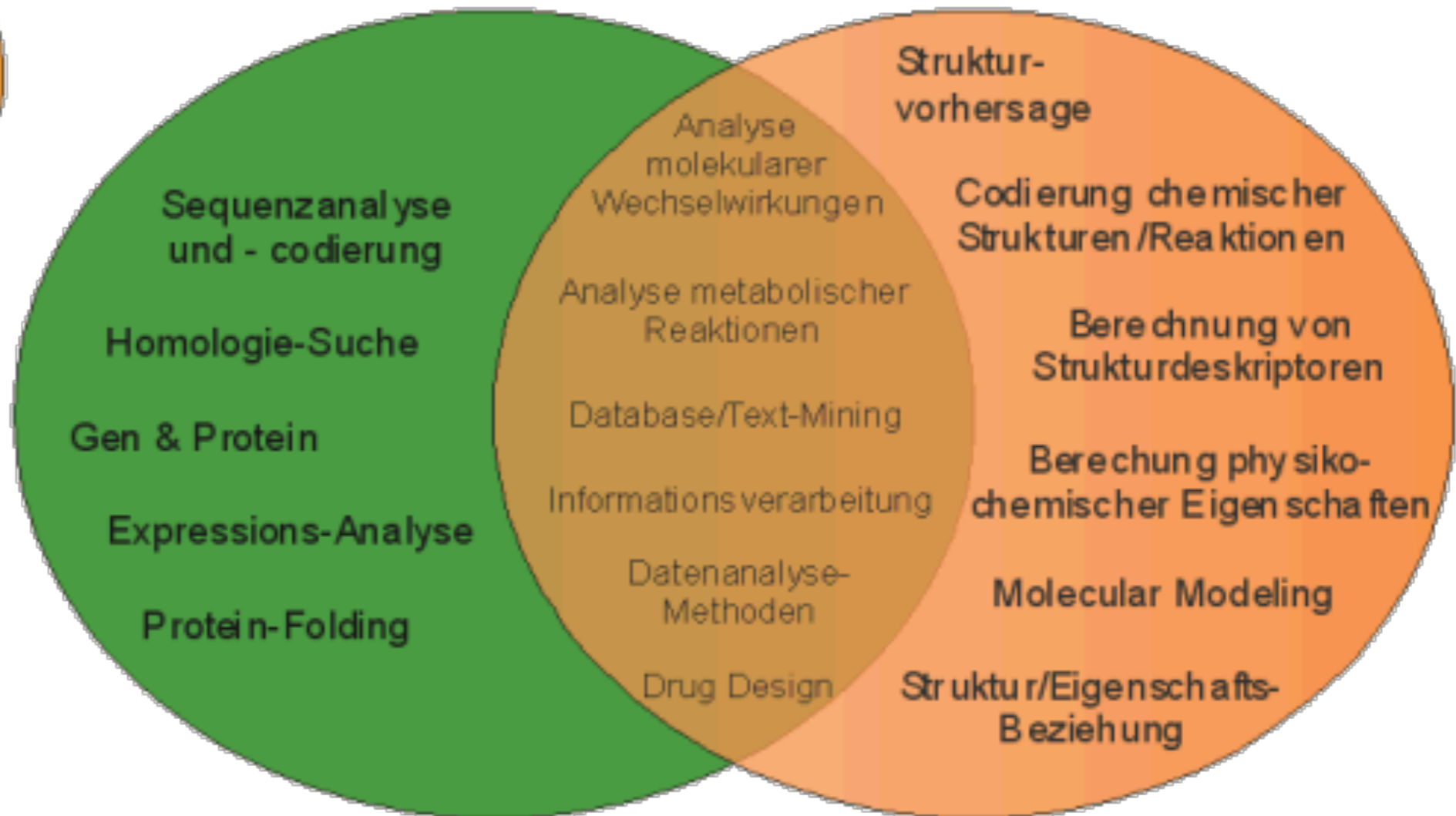
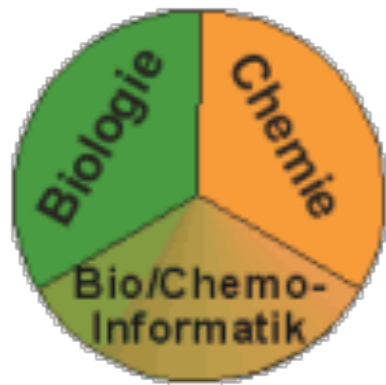
B

Struktur des Kurses

(Jeden Mittwoch, 9-11 Vorlesung, 11-12 Seminar, Blockpraktikum am Ende des Semesters)

- Experimentelles Design
- Datenprozessierung
 - Rauschunterdrückung, Baseline-Correction, Peak-Picking, Missing-Value-Imputation
- Multivariate Datenanalyse
 - PCA, PLSDA, Clustering, Maschinelles Lernen
- Alles begleitet von praktischen Übungen in R
- Blockpraktikum zur Datenanalyse mit Protokoll
- Mündliche Prüfung

MC 3.1.1. Chemoinformatik



- Struktur:
 - 2 SWS Vorlesung
 - 1 SWS Seminar
 - 16 SWS Praktikum als Forschungspraktikum in der Gruppe