- This week (45) we will discuss algorithms for finding the K shortest paths (resp. hyperpaths) in graphs (resp. hypergraphs).

  After that we will start with Analytic Combinatorics, a powerful and generic technique for counting, analysing, and sampling combinatorial objects. While the techniques are well established in the area of algorithm analysis (e.g., in order to infer the average runtime of an algorithm), their use in chemistry is limited.

- Mandatory Reading (K shortest path finding):

  – The slides

- Recommended Reading:

  – Rolf Fagerberg, Christoph Flamm, Rojin Kianian, Daniel Merkle, and Peter F. Stadler: *Finding the K best synthesis plans*. J Cheminform. 2018; 10: 19.