

3: Criteria for Selection of the Synthetic Route

Once a Target Molecule is chosen for synthesis, one could sit down and devise several routes for its synthesis. On what criteria do you select a Target and how do you arrive at a synthetic route? The answer depends on the overall goal of your project.

For a natural product chemist, he might have isolated and determined the structure of a new molecule. He may need to synthesize the molecule to prove the structure. While working on structure elucidation, the route chosen for synthesis should unambiguously establish the part of the structure you are working on. Each step is chosen on this structure-criterion alone. Here the length of the route and the cost of the chemicals are not important.

An elegant (enantiopure) synthesis of some complex structure is the dream of an academician working in the university laboratory. He is often more concerned with developing new routes, new reactions and new mechanistic principles. His concern is to develop new horizons and give good training to the young chemists. He is seldom worried about the cost of his research. He has time at his command and hopefully enough money to pursue his passion. He is judged by the quality (and quantity) of his research publications and the quality of training he has imparted to the students. Having a patent is an added feather to his cap.

A pharmaceutical chemist and a material chemist are more interested in developing versatile and fast synthetic routes for a chosen molecule. Their efforts are directed towards the synthesis of a large number of closely related molecules, within a short time. Such a chemist is looking into Structure-Activity Studies, aimed at developing new drug molecules or molecules with special properties. He is often judged by the number of such active molecules that he has discovered and patents held in his name and not just by the number of new molecules synthesized by him or the elegance of the synthetic route. A publication to his credit is an added feather to his cap. In his endeavours, the cost and the efficiency of the synthetic routes are not the criteria for research. He believes that once the 'right molecule' is discovered, more efficient routes could always be generated at a suitable date. His art is directed towards fast discovery of molecules with the right properties.

An industrial chemist is most concerned with the 'cost' of synthesis of the molecule. His efforts are directed towards development of economical synthetic procedures, which includes not only the cost of the chemicals but also the cost of waste treatment, recycling and environmental cleaning. He selects the molecules on the basis of their economic value (net profit for his company). He should be concerned about eco-friendly reactions and procedures. In general, a development chemist in an industrial R&D laboratory looks at very large-scale (typically several kilogram batch) reactions, their reproducibility, safety and cost parameters. His focus is on the commercial value of his product, the profitability and the patents.

Therefore, the target molecule and the route chosen depend of the hat the chemist is wearing. We do have examples of amazing chemists who efficiently juggle with more than one hat at the same time. We take our proverbial hats off for those versatile and multifaceted chemists. This is because, for an efficient operation, different tasks demand different skill-sets and use of different sets of databases. Nonetheless, the underlying chemistry is same in all these activities. Of course, occasionally one could be creative, versatile and cost-effective at the same time. In the following pages we would look into the broad principles governing the art of organic syntheses. We have already discussed some 'rules' that govern synthesis. We would now explore guidelines that concern the logic of organic syntheses. We would then discuss several interesting syntheses to illustrate these principles.

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