Integrated synthesis and purification of single enantiomers

Rendicontazione

Informazioni relative al progetto

INTENANT

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Progetto chiuso

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Questo progetto è apparso in...

Periodic Report Summary - INTENANT (Integrated synthesis and purification of single enantiomers)

Enantiomers are pairwise occurring molecules, which are non-superimposable mirror images one of the other. Due to homochirality of life, there is a large interest and need to produce pure enantiomers in the pharmaceutical, fine chemical, food and agrochemical industries. Their provision is a challenging task since standard non-selective chemical synthesis leads always to 50:50 mixtures which are difficult to separate. There is tremendous interest in the mentioned industries to develop innovative methods allowing for a faster access to pure enantiomers. The basic idea of the INTENANT project (INTegrated synthesis and purification of single ENANTiomers) is to combine efficiently the potential of the two rivalling approaches, namely the development of a) enantioselective synthesis methods and b) physical methods aiming to separate efficiently mixtures of the two enantiomers. Main goal of INTENANT is to demonstrate for several relevant target compounds the potential of such a new combined approach and to develop tools capable to evaluate innovative process schemes and to quantify their potential.
To achieve the described ambitious goal the INTENANT project was suggested by a consortium consisting of 7 academic institutions, 3 industrial partners and a research coordination society.
In a first work package (WP1) 18 compounds were chosen to be investigated in the different laboratories with different techniques. Hereby several compounds of industrial relevance were suggested by the three industrial partners. The SME MOLISA (MOL) suggested investigating the production of the alkaloid Noscapine (compound B1). AstraZeneca (AZ), a multi-national pharmaceutical company suggested to study 5 confidential compounds (C1-C5), which carry different prototypic features. Bayer Technology Services (BTS), the second multi-national company, brought with C6 another confidential compound of industrial interest into INTENANT.
In the first period of the INTENANT project it was an important task to deliver sufficient amounts of the pure compounds and racemic mixtures selected to the various labs in order to provide the basis to study the various unit operations. As planned this state was reached, in agreement with Milestone I, after month 12 (M12).
Systematic work was undertaken devoted to study synthesis (WP2) and racemization (WP5), as the two chemical methods, and chromatography (WP3) and crystallization (WP4), as the two most relevant separation methods. In these four work packages a large component specific data base was acquired, which is now available for all project partners on an internal website. In parallel to the experimentally oriented projects and in close cooperation with WP1-WP5 a theoretical framework and mathematical tools

were developed in WP6 (Process synthesis and optimization), which are capable to simulate and quantify the single unit operations considered and also several combinations. Achieving recently Milestone II which was due after M18, the consortium possesses now theoretical models and appropriate tools to study various options for the production of the different target components selected.
In the second part of the project (M18-M36) the consortium will proceed along the initial plan and will suggest new process routes to produce several target compounds. There is ongoing interest in developing an improved process regarding the production of Noscapine (MOL) and C6 (BTS). C1 and C3 are currently the leading AZ-compounds regarding the development of integrated processes, whereas C4 is a candidate for a novel chromatographic process design. It is further planned to evaluate the concept for a new AZ-compound (C7). The most promising process routes will be finally validated.
The INTENANT project is on a good track. It is expected that it will prove the general benefits of optimized combinations of the available chemical and physical methods to improve the production of single enantiomers.

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