Design and Screening of Chiral Metal Catalysts

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Phosphinooxazolines (PHOX ligands) have proven to be highly versatile, very efficient ligands for a variety of enantioselective catalytic reactions, such as hydrogenation, Heck reactions, allylic substitutions and conjugate additions of organozinc reagents to enones [1]. Recently, we have developed new classes of P,N-ligands derived from pyridine and quinoline, which gave promising results in the Ir-catalyzed hydrogenation and in Heck reactions [2].

$$(R^2)_2 P \qquad N \qquad (R^2)_2 P \qquad$$

Using Pd-catalyzed kinetic resolution of allylic esters as a test reaction, we have developed a new screening method for chiral catalysts [3]. The method is based on mass-labeled, pseudoenantiomeric substrates and electrospray mass spectrometry as an analytical tool. The enantioselectivity of chiral palladium catalysts in the kinetic resolution of allylic esters can be determined by mass spectrometric monitoring of allyl-Pd intermediates **A** and **B** derived from pseudoenantiomeric substrates **1a** and **1b**. In contrast to conventional screening methods, which are based on product analysis, simultaneous screening of catalyst mixtures in homogeneous solution is possible.

References

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