

# Speeding-up the Substance Discovery to Commercialization Process: The SK-CC00-1A and SK-CC00-2A Catalysts for Cross-Coupling Reactions

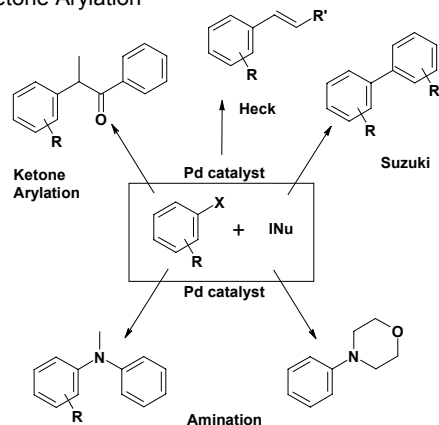
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## General

Pd catalyzed CC/CN cross coupling reactions are of highest importance in industrial processes. There is a major need for the discovery of highly active and versatile catalyst systems covering cross-coupling reactions like:

- Heck reaction
- Buchwald-Hardwig Amination
- Suzuki coupling
- Ketone Arylation



Picture 1 : Examples of cross-coupling reactions

## Application

Researchers at Solvias AG, by using a Chemspeed Automated Parallel Synthesizer have found, that the single component catalysts SK-CC00-1A and SK-CC00-2A efficiently activate aryl chlorides for a broad range of coupling reactions, incl. Buchwald-Hartwig amination, Heck-coupling, Suzuki-reactions and ketone arylations<sup>1,2</sup>.

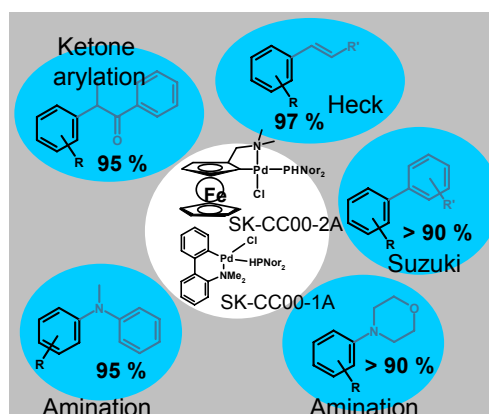


Picture 2 : Chemspeed's parallel reactor technology

## Results & Benefits

Two catalysts, SK-CC00-1A and SK-CC00-2A, have been selected to be commercialized after intensive characterization of their properties. These systems fulfill all the highly demanding requirements as:

- They activate aryl chlorides for most cross-coupling reactions
- They are single component catalysts
- They are highly active and yield in a high substrate/ligand ratios
- They are air, moisture and solution stable
- They give high yields under standard conditions



Picture 3 : Results of cross-coupling reactions

## Conclusion

Secondary phosphines were previously believed to be ineffective in these types of reaction. Two completely innovative, highly active, and extremely broad applicable catalysts for cross-coupling reactions were identified by an automated ligand screening program on a Chemspeed parallel synthesizer. SK-CC00-1A and SK-CC00-2A are beating even the best previously known catalyst (based on tertiary phosphine ligands). These catalysts are now commercially available on multi kg scale.

This example demonstrates the benefits of automation in catalysis research. Systematic screening allows the researchers to "think out of the box", and to discover innovative compounds, capable of even changing established dogmas in chemistry.

<sup>[1]</sup> Anita Schnyder, Thomas Aemmer, Adriano F. Indolese, Ulrich Pittelkow, Martin Studer; Adv.Synth.Catal., 2002, 344, 495-498.

<sup>[2]</sup> Anita Schnyder, Frédéric Naud, Marc Thommen, Hans-Ulrich Blaser; sp2, 2003, No. 9, 32-35.

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