Pd(II) EnCat™

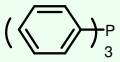
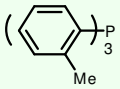
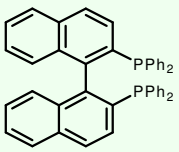
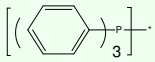
Encapsulated Palladium(II) Catalysts

Reaxa's Pd EnCat™ catalysts immobilise palladium acetate together with activating ligands within a robust porous polyurea matrix to allow easier, faster and cleaner processes to be developed

Contaminated crude Suzuki coupling product made with homogeneous Pd acetate catalyst system

Clean product made using Reaxa's Pd EnCat™ 30 catalyst with no extra purification

Cleaner products	typically less than 10 ppm Pd in crude product
Cleaner waste streams	reduced metal losses in Pd EnCat™ processes
Fast, efficient processes	the EnCat™ beads filter easily
No plant contamination	metal & ligands are trapped within the beads
Improved processes	high activity in many types of coupling reactions
Process intensification	can be used in batch & flow processes

Product	*Pd content %w/w*	*Co-encapsulated ligand*
Pd(II) EnCat™ 30	**4.3**	**none**
Pd(II) EnCat™ 40	**4.6**	**none**
Pd(II) EnCat™ TPP30	**4.7**	
Pd(II) EnCat™ TOTP30	**4.7**	
Pd(II) EnCat™ BINAP30	**4.7**	
Pd(II) EnCat™ polyTPP30	**4.6**	

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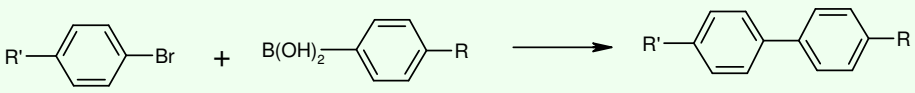
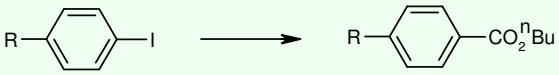
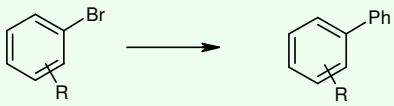
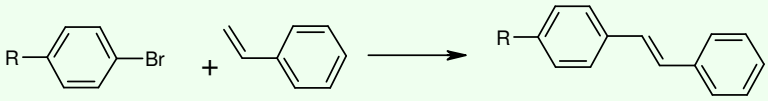
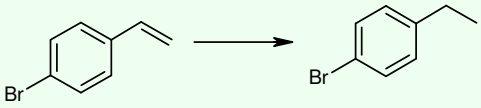
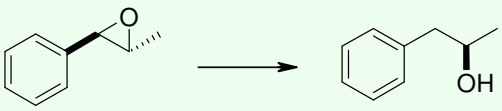
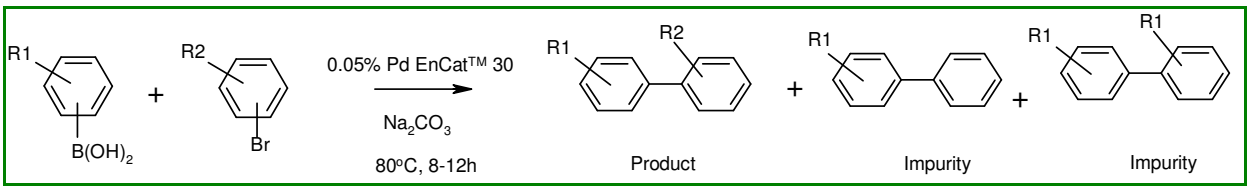
Pd EnCat™ Applications

Pd EnCat™ Chemistry Examples:

Suzuki	
Carbonylation	
Stille	
Heck	
Hydrogenation	
Transfer hydrogenation	

Process Scale Suzuki Coupling Example:



The client's process using 2.5 mol% Pd/C gave a 94% yield with impurities at 5% and 1% and a reaction time of 60 mins. Following extensive work-up and recrystallisation, Pd levels of > 50 ppm were present in the product. A switch to Pd(II) EnCat™ 30 at 0.25 mol% gave a dramatic improvement: after 30 mins the crude product was reproducibly obtained at >99% yield, with both impurities reduced to <1% and with Pd levels reduced to <10 ppm without recrystallisation, representing a significant cost saving for the client.

Selected References:

1. C.K.Y. LeeConnie, K.Y. Lee, A.B. Holmes, S.V. Ley, I.F. McConvey, B. Al-Duri, G.A. Leeke, R.C.D. Santos, J.P.K. Seville, *Chemical Communications*, 2005, **(16)**, 2175 – 2177.
2. I.R. Baxendale, C.M. Griffiths-Jones, S.V. Ley and G. Tranmer, *Chem. Eur. J.*, 2006, **12**, 4407-4416.
3. J. Gil-Molto, S. Karlstrom and C. Najera, *Tetrahedron,* 2005, **61,** 12168–76.

R&D quantities of Pd EnCat™ products are available from Sigma-Aldrich at: www.sigma-aldrich.com
For technical support, bulk quotations & information on Pd EnCat™ catalysts please contact: info@reaxa.com

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