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Correction: How to develop a sustainable palladium-catalyzed cross-coupling reactions for active ingredient manufacture

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KEYWORDS

palladium, cross-coupling, turnover, catalysis, metrics, workflow

A Correction on
How to develop a sustainable palladium-catalyzed cross-coupling reactions for active ingredient manufacture

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There was a mistake in Table 1 as published. A table cell contains 2 separate equations, but their present juxtaposition in the published version means it is not clear that they are in fact separate. The corrected Table 1 appears below, where the existence of two separate equations has been made more clear. The equations themselves have been additionally modified slightly to clarify their meaning.

$TOF(t) = \frac{1}{[Cat](t)} \cdot \frac{d[Prod]}{dt}$,
$TOF_0 = \frac{1}{[Cat]_0} \cdot \left(\frac{d[Prod]}{dt}\right)_0$

The original article has been updated.

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TABLE 1 Metrics relevant to the development of a high turnover palladium-catalyzed cross-coupling.

Metric	Comment	Formula
Process mass intensity	Simple	$\frac{\text{mass of all input materials (including water)}}{\text{mass of product corrected for assay}}$
	Used by non-technical stakeholders	
	Does not account for input material preparation or waste destruction	
Catalyst loading	≤0.1 mol/mol% for a highly active catalyst	$\frac{\text{moles of catalyst}}{\text{moles of limiting reactant}} \cdot 100\%$
	<0.5 mol/mol% API production (pharmaceutical commercialisation)	
	<2 mol/mol% (late pharmaceutical development)	
	<5 mol/mol% (early pharmaceutical development)	
	<0.1 mol/mol% fine chemical and agrochemical production	
Turnover frequency (TOF)	Catalyst productivity[a,b]	$TOF(t) = \frac{1}{[Cat](t)} \cdot \frac{d[Prod]}{dt}$ $TOF_0 = \frac{1}{[Cat]_0} \cdot \left(\frac{d[Prod]}{dt}\right)_0$
	Reaction time ≤12 h to avoid bottlenecking process	
Turnover number (TON)	Time integral of TOF equating to total number of turnovers the catalyst can achieve until its total decay[b]	$TON = \int_0^{\infty} TOF(t) \cdot \frac{[Cat](t)}{[Cat]_0} dt$ $TON = (initial\ TOF) \cdot \frac{(catalyst\ half-life)}{ln\,2}$ where catalyst deactivation is (pseudo)first order

[a]When quoted alongside the temperature, solvent and concentration, a useful proxy for catalyst productivity is: $\frac{\text{moles of substrate converted to product}}{(\text{moles of catalyst used})(\text{time})}$

[b]The calculation of TOF, or TON, is most meaningful for the initial rate region before catalyst degradation can make an impact, and when product formation is pseudo-linear with time (Kozuch and Martin, 2012). Rather than being considered solely in isolation, they are better applied as part of the evaluation of very similar conditions side by side, as with the effect of changing the ligand. There are standard conditions (1 M for limiting reactant, 0 °C) whose use simplifies reporting requirements.