

Correction to "An Evolved Orthogonal Enzyme/Cofactor Pair"

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J. Am. Chem. Soc. 2016, 138, 12451-12458. DOI: 10.1021/jacs.6b05847

Supporting Information

Page 12456. In Table 2, the labeling for the stereochemical configuration of the *trans* enantiomers is swapped. The 1S,2S isomer is improperly labeled 1R,2R, and vice versa. In addition, the elution order of the ethyl 2-phenylcyclopropane-1-carboxylate isomers designated in Table 2 is incorrect. The *cis* diastereomers, while labeled correctly, have been inverted. In addition, the *trans* diastereomers (labeled incorrectly as stated above) have also been switched. As a result, Tabke 2 footnote b, describing calculation of ee cis, is incorrect and must be changed to (1S,2R) - (1R,2S). These same errors appear in Supplementary Figure S10. The corrected Table 2 is shown below, and the Supporting Information has been revised to include these corrections.

Table 2. Activities and Stereoselectivities of Biocatalysts for the Reaction of Styrene with Ethyl Diazoacetate

| Ph 🍆 | COOEt | 20 μM catalyst 5% EtOH 10 mM Na ₂ S ₂ O ₄ | 1S 2R EtOOC 3a Ph | 1R\(\frac{1}{2}S\) EtOOC\(\frac{1}{3}\) Th |
|-------------------|-------|--|-------------------------------|--|
| 1 30 mM | - 2 | 0.1 M KP _i , pH 8.0 | 1R\(\sigma_2R\) EtOOC'' 3c Ph | EtOOC 3d "Ph trans |

| catalyst | yield | TTN ^a | dr (cis:trans) | ee cis [%] ^b | ee trans [%] |
|-----------------------------------|-------|------------------|-------------------|----------------------------|--------------|
| heme | 7 | 35 | 16:84 | 0 | -11 |
| Fe-DPIX | 5 | 23 | 13:87 | 3 | -11 |
| BM3h T268A/heme | 57 | 284 | 1:99 | -6 | -9 7 |
| BM3h T268A/heme aerobic | 2 | 11 | 10:90 | -15 | -42 |
| WIVS-FM T268A/ Fe-DPIX | 44 | 221 | 12:88 | -51 | -46 |
| WIVS-FM T268A/ Fe-DPIX aerobic | 12 | 59 | 12:88 | -33 | -37 |

 $[^]a$ TTN = total turnover number. $^b(1S,2R) - (1R,2S)$. $^c(1R,2R) - (1S,2S)$. TTN and stereoselectivities determined by chiral GC analysis.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/jacs.6b10459.

Materials and methods including procedures for plasmid and library construction, protein expression and purification, HPLC assays, library screening, carbon monoxide binding assays, thermostability measurements, extinction coefficient determination, protein crystallography, cavity volume calculations, and cyclopropanation reactions (corrected) (PDF)

Published: October 19, 2016