

Creation of a Broad-Range and Highly Stereoselective D-Amino Acid Dehydrogenase for the One-Step Synthesis of D-Amino Acids

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Supporting Information

The following table contains the chromatography conditions used to analyze the enantioselectivity of the mutant D-amino acid dehydrogenase (BC621).

| D-Amino acid product | Column | Retention time (min) | Method |
|-----------------------------------|--------|----------------------|--|
| D-Alanine (D-2-aminopropionate) | T | L: 8.3 D: 9.6 | 40% methanol 60% water (0.2% TEAA, pH 3.8) |
| D-2-Aminobutyrate | T | L: 8.8 D: 9.9 | 20% acetonitrile 80% water (0.2% TEAA, pH 3.8) |
| D-Norvaline (D-2-aminopentanoate) | R | L: 7.5 D: 11.2 | 20% acetonitrile 80% water (0.2% TEAA, pH 3.8) |
| D-Norleucine (D-2-aminohexanoate) | T | L: 8.7 D: 17.1 | 40% methanol 60% water (0.2% TEAA, pH 3.8) |
| D-2-Aminoheptanoate | T | L: 9.7 D: 17.3 | 40% methanol 60% water (0.2% TEAA, pH 3.8) |
| D-2-Aminooctanoate | T | L: 11.5 D: 21.3 | 40% methanol 60% water (0.2% TEAA, pH 3.8) |
| D-Valine | T | L: 9.37 D: 10.5 | 20% acetonitrile 80% water (0.2% TEAA, pH 3.8) |
| D-Isoleucine | T | L: 7.8 D: 12.5 | 40% methanol 60% water (0.2% TEAA, pH 3.8) |
| D-Leucine | T | L: 11.0 D: 13.5 | 20% acetonitrile 80% water (0.2% TEAA, pH 3.8) |
| D-Cyclopentylglycine | T | L: 9.3 D: 13.2 | 40% methanol 60% water (0.2% TEAA, pH 3.8) |
| D-Cyclohexylalanine | T | L: 7.9 D: 8.9 | 50% methanol 50% water (0.1% each TEA, acetic acid) |
| D-Methionine | T | L: 8.2 D: 17.0 | 40% methanol 60% water (0.2% TEAA, pH 3.8) |
| D-Phenylalanine | T | L: 5.6 D: 7.3 | 80% methanol 20% water (0.2% TEAA, pH 3.8) |
| D-Tyrosine | T | L: 5.1 D: 6.3 | 80% methanol 20% water (0.2% TEAA, pH 3.8) |
| D-4-Fluorophenylalanine | T | L: 5.4 D: 6.7 | 80% methanol 20% water (0.2% TEAA, pH 3.8) |
| D-4-Chlorophenylalanine | T | L: 5.7 D: 7.2 | 80% methanol 20% water (0.2% TEAA, pH 3.8) |

Notes:

- T: Chirobiotic T (Astec, Inc.), 250 x 4.6 mm, 5 μ m particle size
- R: Chirobiotic R (Astec, Inc.), 250 x 4.6 mm, 5 μ m particle size
- The flow rate was 1 ml/min in all cases and all runs were performed isocratic conditions.

- TEAA was made by adding triethylamine to water at the given concentration and adjusting to the given pH with acetic acid.
- All amino acid, except for the aromatic amino one, were labeled with Fmoc for UV visualization at 265 nm. The aromatic amino acids were observed directly at 254 nm.