

SUPPORTING INFORMATION

8-Amino-5,6,7,8-tetrahydroquinoline in iridium(III) biotinylated Cp* complex as artificial imine reductase

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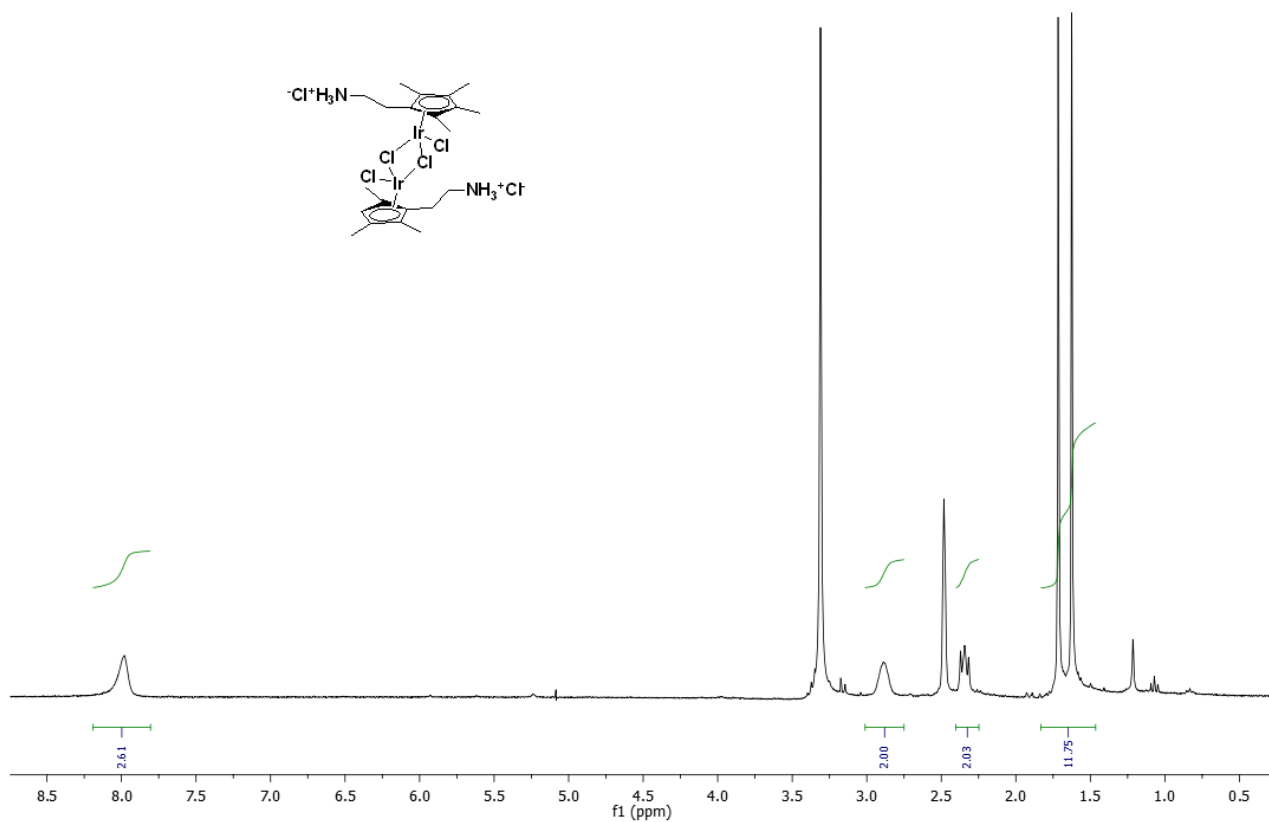
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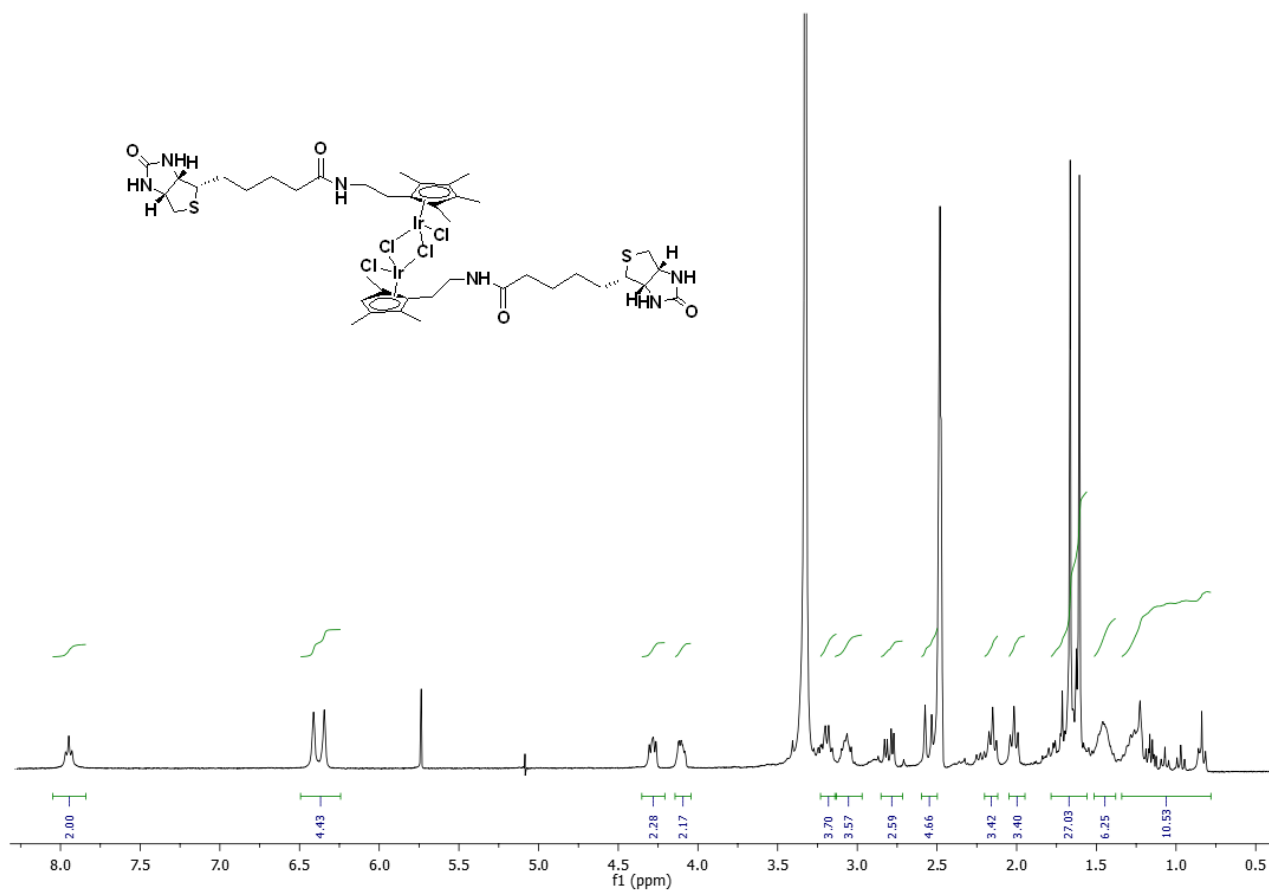
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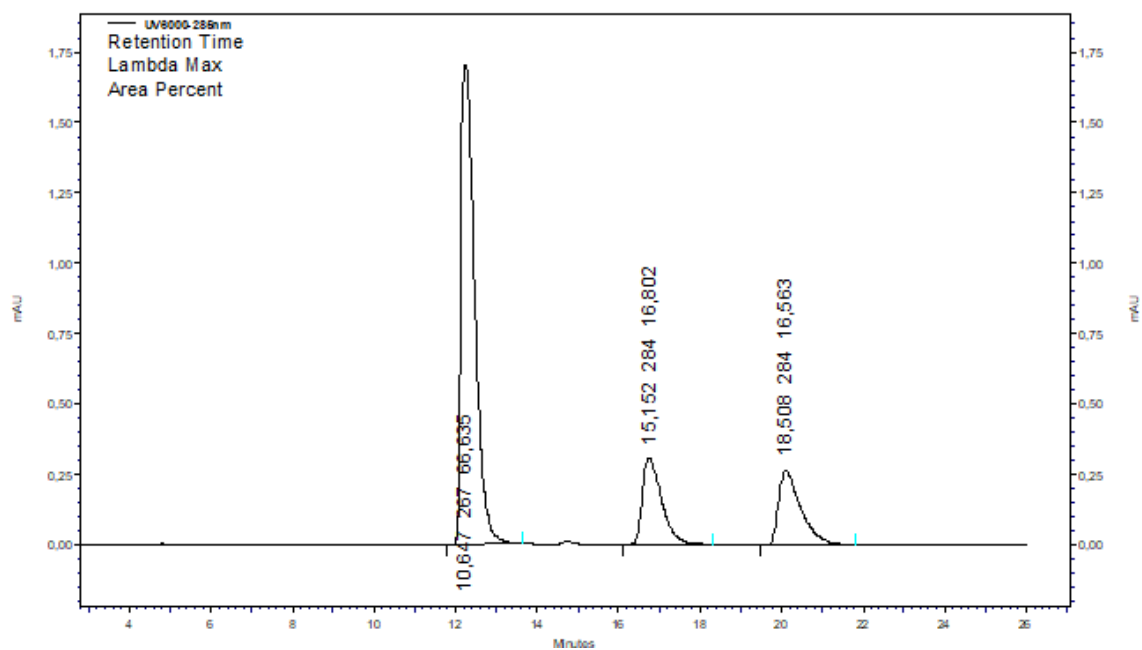
$^1\text{H-NMR}$ spectrum of $[\eta^5\text{-}(2\text{-}(2,3,4,5\text{-tetramethylcyclopentadienyl)ethylamine hydrochloride})\text{IrCl}_2]_2 \cdot \delta \text{H}$ (300 MHz, DMSO) 7.98 (br, 3H), 2.89 (m, 2H), 2.37-2.32 (m, 2H), 1.72 (s, 6H), 1.63 (s, 6H).¹

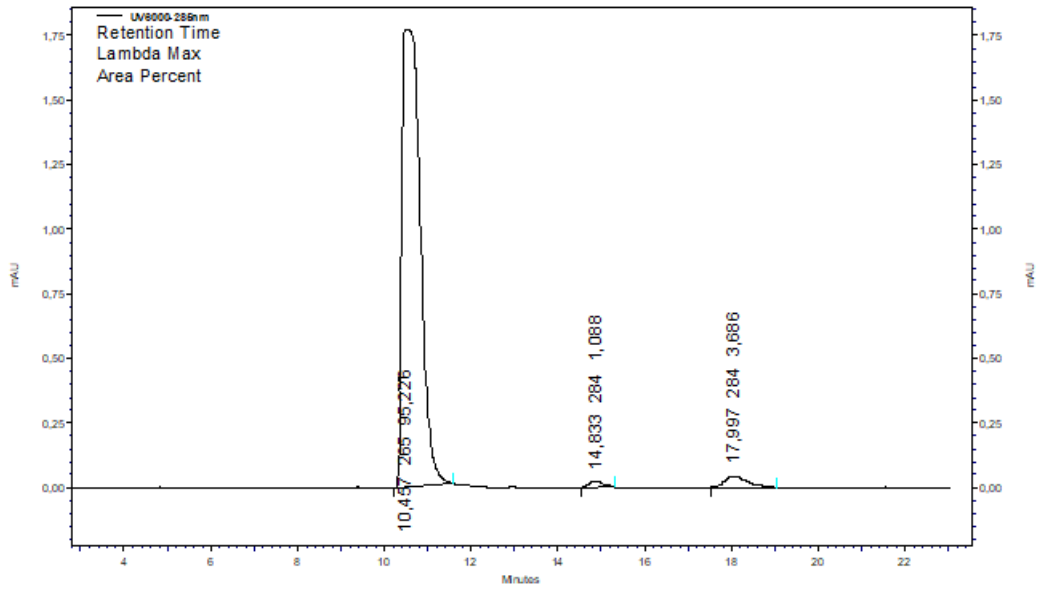


$^1\text{H-NMR}$ spectrum of $[\eta^5\text{-}(\text{Biot-2-(2,3,4,5\text{-tetramethylcyclopentadienyl)ethylamine})\text{IrCl}_2]_2$: δ_{H} (300 MHz, DMSO) 7.95 (t, $J=6.0$ Hz, 2H), 6.41 (s, 2H), 6.34 (s, 2H), 4.30-4.26 (m, 2H), 4.12-4.10 (m, 2H), 3.24-3.20 (m, 4H), 3.16-3.04 (m, 2H), 2.82 (dd, $J=12.5, 5.1$ Hz, 2H), 2.57 (d, $J=12.3$ Hz, 2H), 2.15 (t, $J=6.5$ Hz, 4H), 2.02 (t, $J=7.5$ Hz, 4H), 1.76 (s, 12H), 1.66 (s, 12H), 1.63-1.17 (m, 12H).

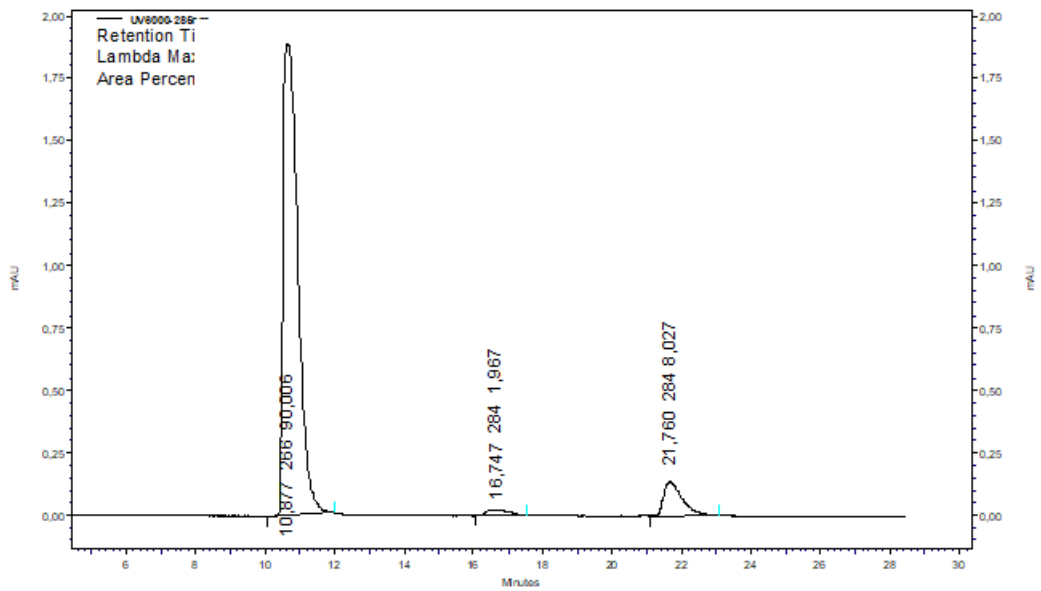


HPLC conditions for 6,7-dimethoxy-1-methyl-3,4-dihydroisoquinoline: eluent hexane/ethanol/DEA=95/5/0.1; $\lambda=285$ nm; flow=1.0 mL/min; retention time for substrate 10.7 min; for two enantiomers of the product: $t_s=15.1$ min; $t_R=18.5$ min. Conversion was obtained by HPLC using correction factor of 1.32.²

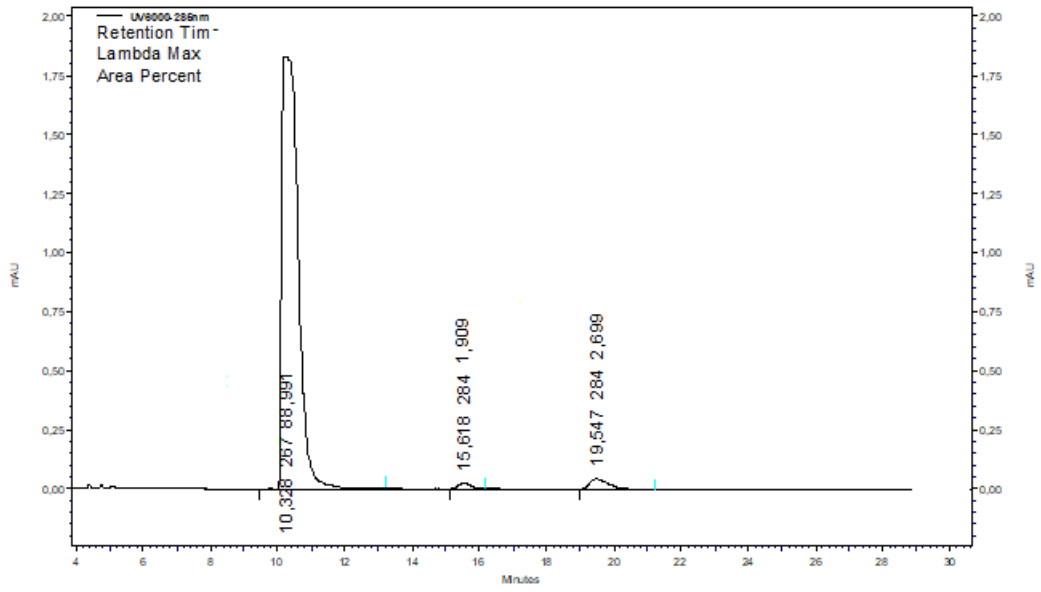




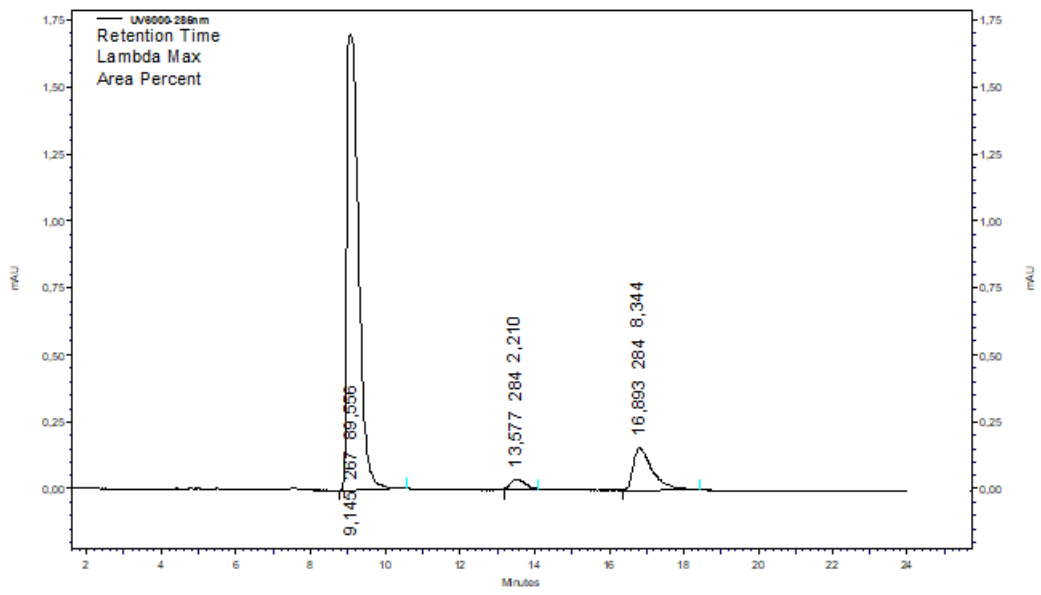
Entry 1, Table 3: conversion 7 %, e.e. 53 %.



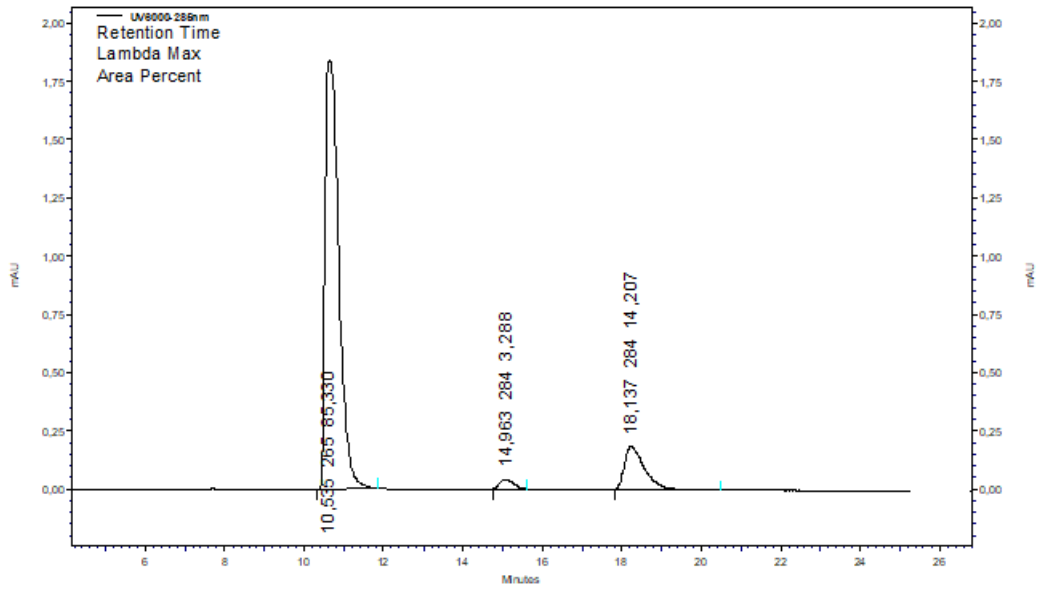
Entry 2, Table 3: conversion 13 %, e.e. 60 %.



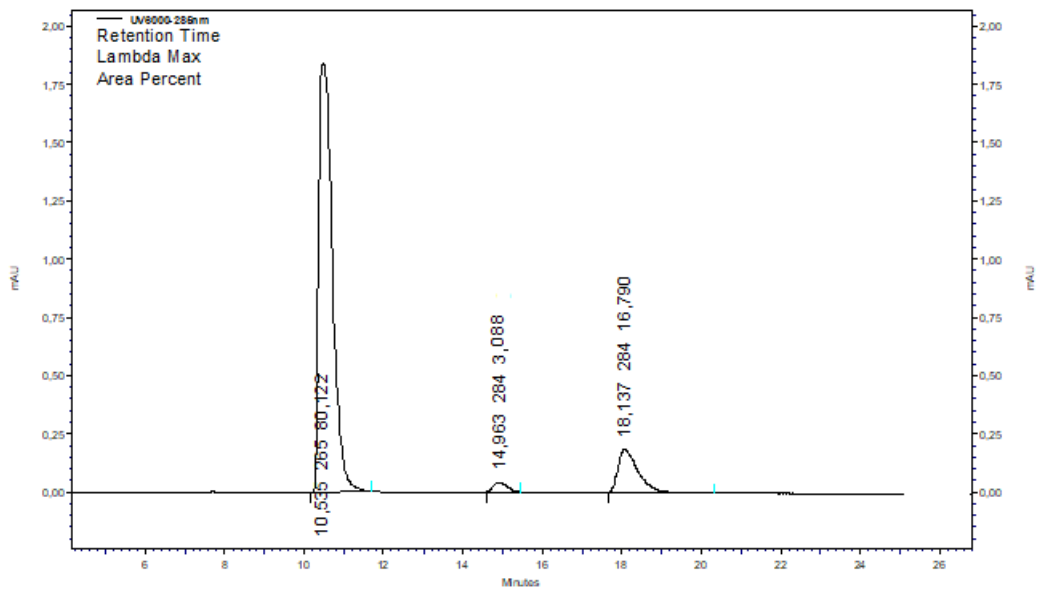
Entry 3, Table 3: conversion 7 %, e.e. 17 %.



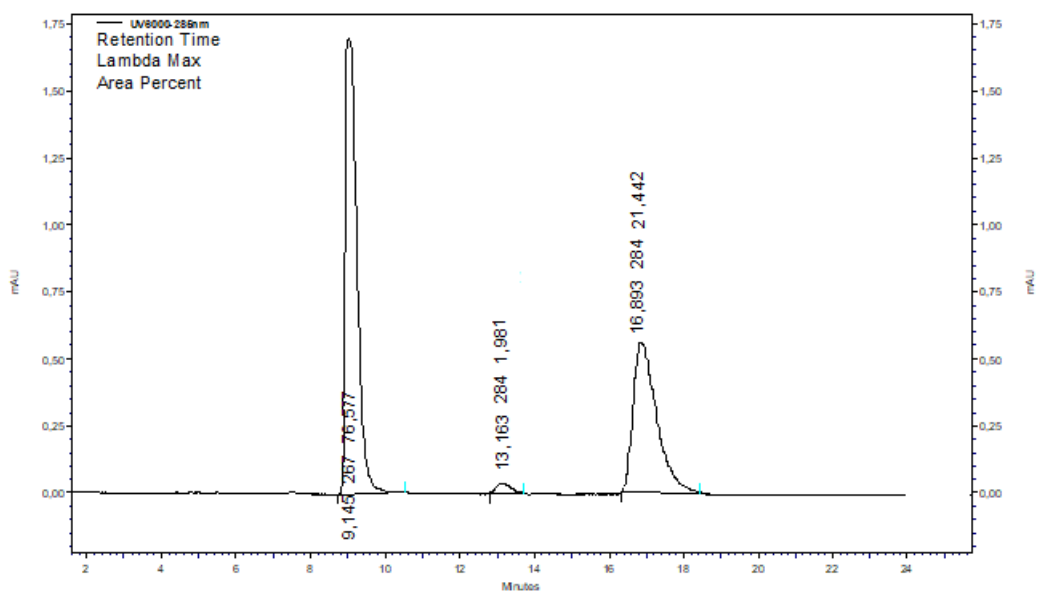
Entry 4, Table 3: conversion 14 %, e.e. 59 %.



Entry 5, Table 3: conversion 23 %, e.e. 62 %.



Entry 6, Table 3: conversion 27 %, e.e. 68 %.



Entry 7, Table 3: conversion 32 %, e.e. 83 %.

References

1. Zimbron JM, Heinisch T, Schmid M, Hamels D, Nogueira ES, Schirmer T, et al. A Dual Anchoring Strategy for the Localization and Activation of Artificial Metalloenzymes Based on the Biotin–Streptavidin Technology. *J Am Chem Soc* 2013 2013/04/10;135(14):5384-88.
2. Pellizzoni M, Facchetti G, Gandolfi R, Fusè M, Contini A, Rimoldi I. Evaluation of Chemical Diversity of Biotinylated Chiral 1,3-Diamines as a Catalytic Moiety in Artificial Imine Reductase. *ChemCatChem* 2016;8(9):1665-70.