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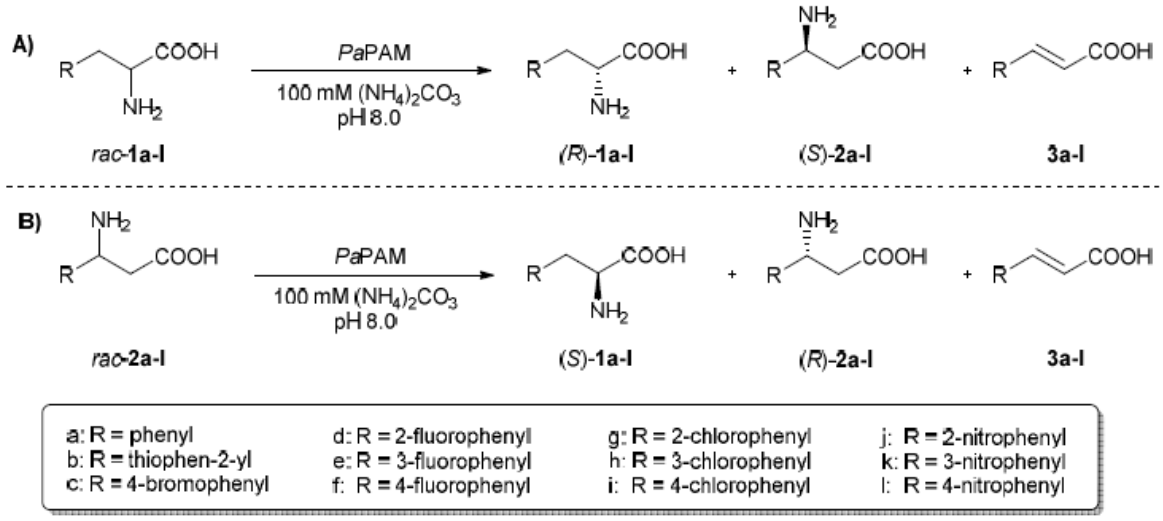
Influence of the aromatic moiety in α- and β-arylalanines on their biotransformation with phenylalanine 2,3-aminomutase from *Pantoea agglomerans*

A. Varga, G. Bánóczi, B. Nagy, L. C. Bencze, M. I. Toșa, Á. Gellért, F. D. Irimie, J. Rétey, L. Poppe, C. Paizs

Abstract

In this study enantiomer selective isomerization of various racemic α- and β-arylalanines catalysed by phenylalanine 2,3-aminomutase from *Pantoea agglomerans* (*Pa*PAM) was investigated. Both α- and β-arylalanines were accepted as substrates when the aryl moiety was relatively small, like phenyl, 2-, 3-, 4-fluorophenyl or thiophen-2-yl. While 2-substituted α-phenylalanines bearing bulky electron withdrawing substituents did not react, the corresponding substituted β-aryl analogues were converted rapidly. Conversion of 3- and 4-substituted α-arylalanines happened smoothly, while conversion of the corresponding β-arylalanines was poor or non-existent. In the range of 7-9 pH had no
significant influence on conversion of racemic α- or β-(thiophen-2-yl)alanines, whereas increasing the concentration of ammonia (ammonium carbonate from 50 to 1000 mM) inhibited the isomerization progressively and decreasing amount of the by-product, i.e. (*E*)-3-(thiophen-2-yl)acrylic acid, was detected. In all cases, the high *ee* values of the products indicated excellent enantiomer selectivity and stereospecificity of the isomerization except for (*S*)-2-nitro-α-phenylalanine (*ee* 92%) from the β-isomer. Substituent effects were rationalized by computational modelling revealing that one of the main factor controlling biocatalytic activity was the energy difference between the covalent regioisomeric enzymesubstrate complexes.



*Pa*PAM-catalysed transformation of (**A**) (±)-α-arylalanines *rac*-**1a-l** and (**B**) (±)-β-arylalanines *rac*-**2a-l**