Geometric isomer discrimination capabilities of serine proteases

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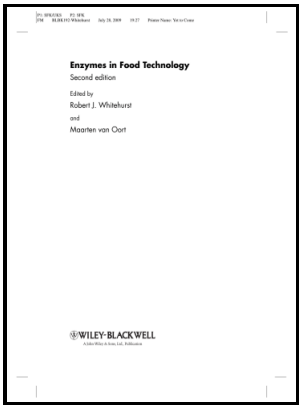

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The Lens

You must accept that these two structures represent the same molecule: But what happens if you have a carbon-carbon double bond - as in 1,2-dichloroeth ene? Thus, the energetic and physical behavior observed for hydrogen bonds in the oxyanion hole of KSI can be used to evaluate the active site environment.

Geometric Isomers

Refinement has been performed against structure factor amplitudes using PHENIX and five macrocycles in each refinement. This page explains what stereoisomers are and how you recognise the possibility of geometric isomers in a molecule. We then describe and implement a strategy to experimentally isolate and evaluate the effects of electrostatic complementarity on the reaction catalyzed by KSI.

Serine

The change in hydrogen bond strength accompanying charge rearrangement: Implications for enzymatic catalysis.

What are serine proteases?

Experimental evaluation of the effective dielectric constant of proteins.

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