

NMR based methods in drug design

Göran Karlsson
Svenskt NMR-centrum
Göteborgs Universitet

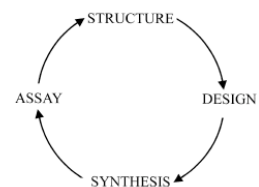


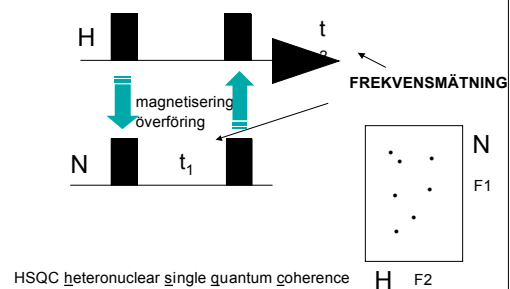
Fig. 1. Outline of the structure-based drug design process.

Tekniker

Förändringar i kemiskt skift
Isotop-filtrering och selektering
Vätebindningsutbyte
Kartläggning av ytor
Joniserbara grupper
Proteindynamik

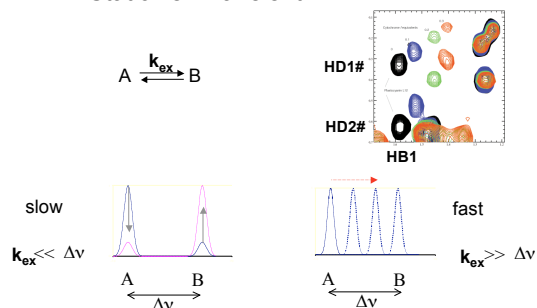
Trosy-tekniker
Gradient-NMR
Prober

Heteronukleär NMR

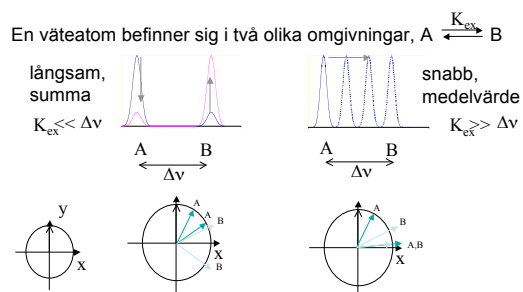


HSQC heteronuclear single quantum coherence

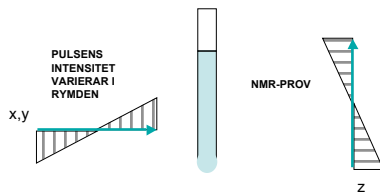
Static vs. Transient



Utbyte (Exchange)

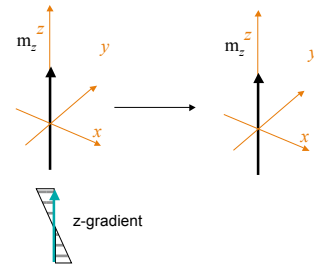


GRADIENTPULS

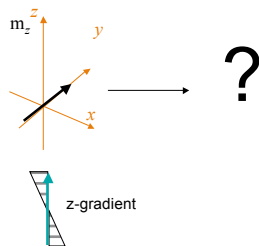


Används för att ta bort "icke önskvärd" magnetisering, eller för att selektera en viss koherens.

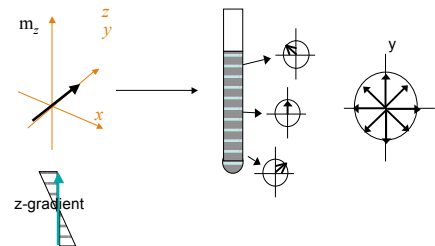
GRADIENT-PULS



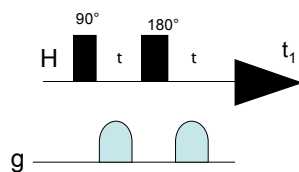
GRADIENT-PULS



GRADIENT-PULS



GRADIENT-SELEKTION



DIFFUSION?