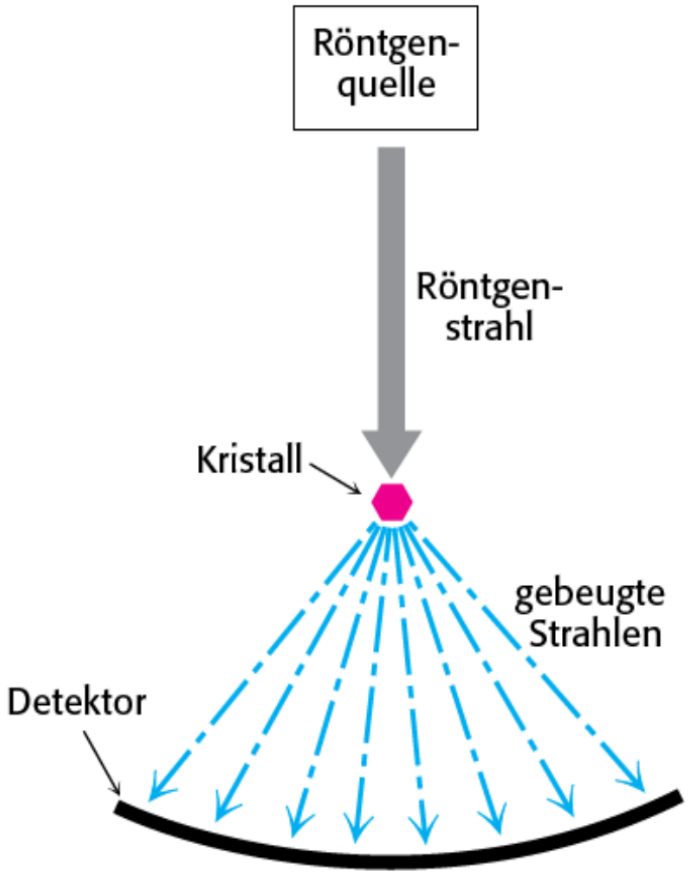
Genauigkeit

AST Übung

Röntgenstrukturanalyse

Experiment

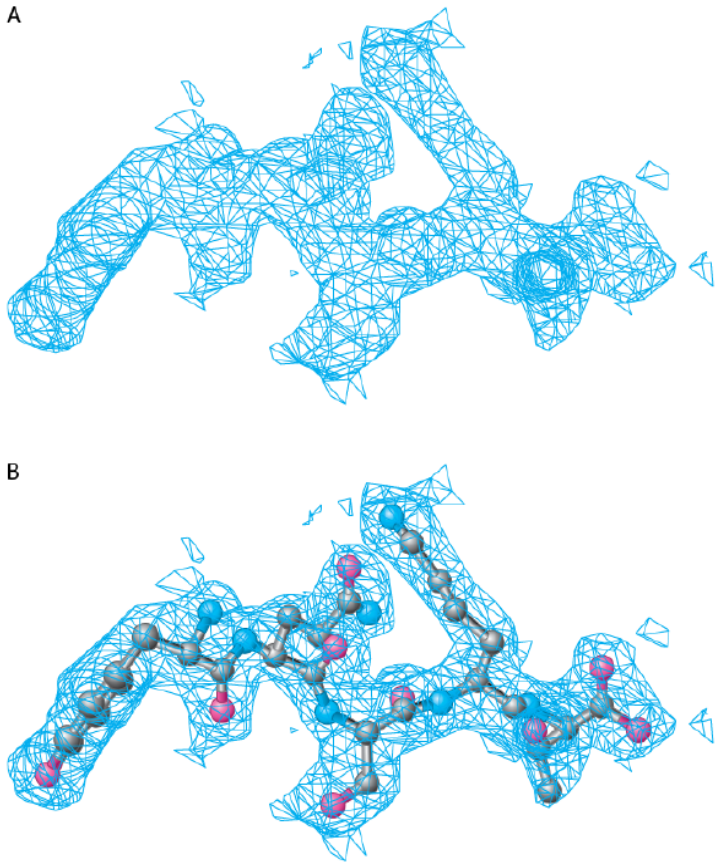


Jeremy M Berg, Lubert Stryer, and John L Tymoczko. *Stryer biochemie*. Springer-Verlag, 2015.

Rohdaten

Jeremy M Berg, Lubert Stryer, and John L Tymoczko. *Stryer biochemie*. Springer-Verlag, 2015.

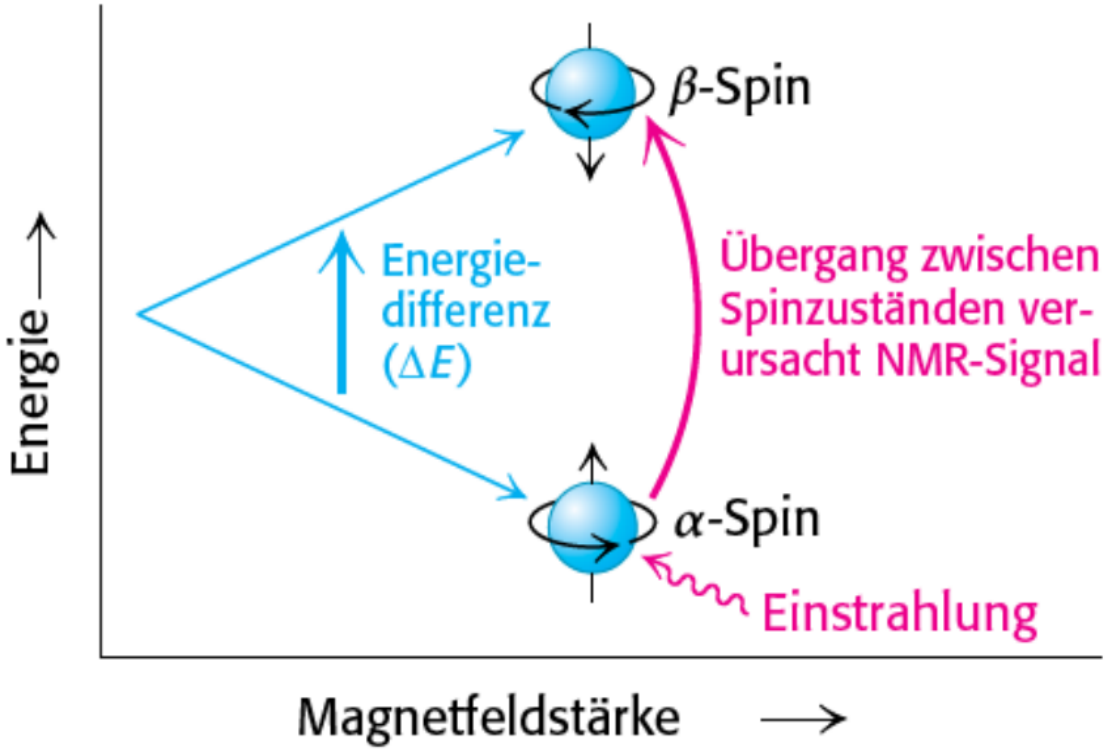
Elektronendichte



Jeremy M Berg, Lubert Stryer, and John L Tymoczko. *Stryer biochemie*. Springer-Verlag, 2015.

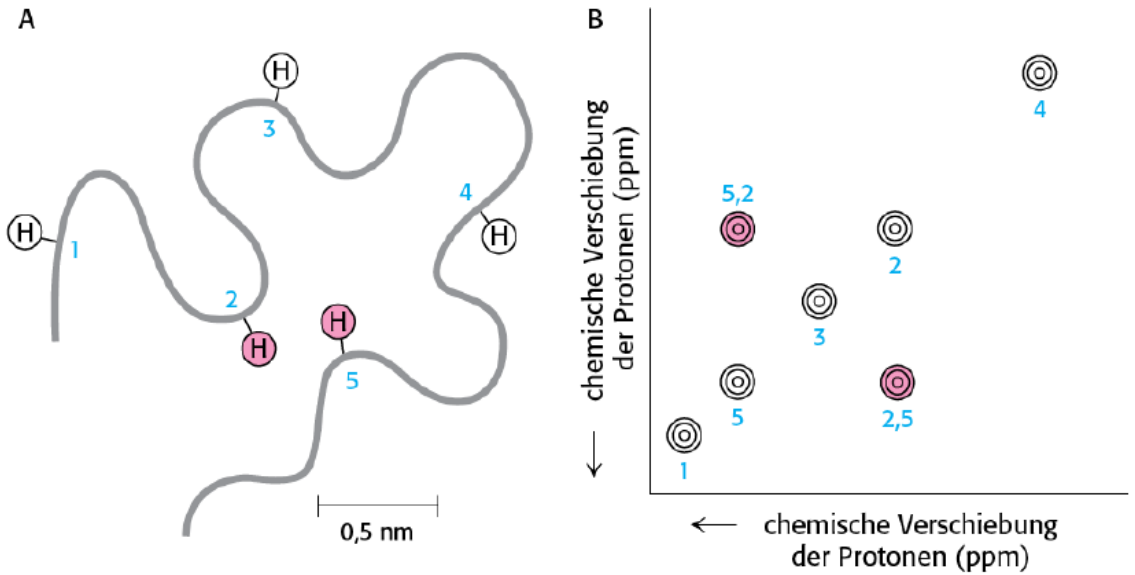
Kernspinresonanzspektroskopie

Experiment



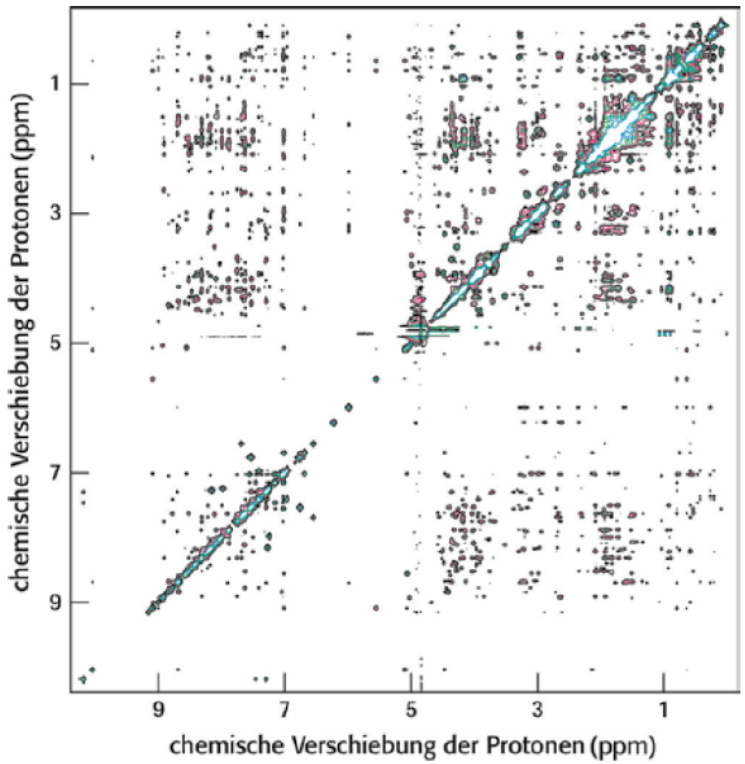
Jeremy M Berg, Lubert Stryer, and John L Tymoczko. *Stryer biochemie*. Springer-Verlag, 2015.

Messung



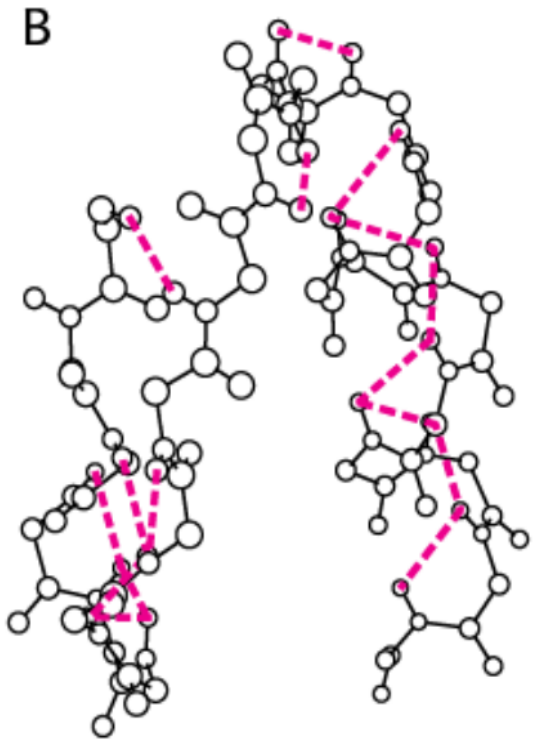
Jeremy M Berg, Lubert Stryer, and John L Tymoczko. *Stryer biochemie*. Springer-Verlag, 2015.

Rohdaten



Jeremy M Berg, Lubert Stryer, and John L Tymoczko. *Stryer biochemie*. Springer-Verlag, 2015.

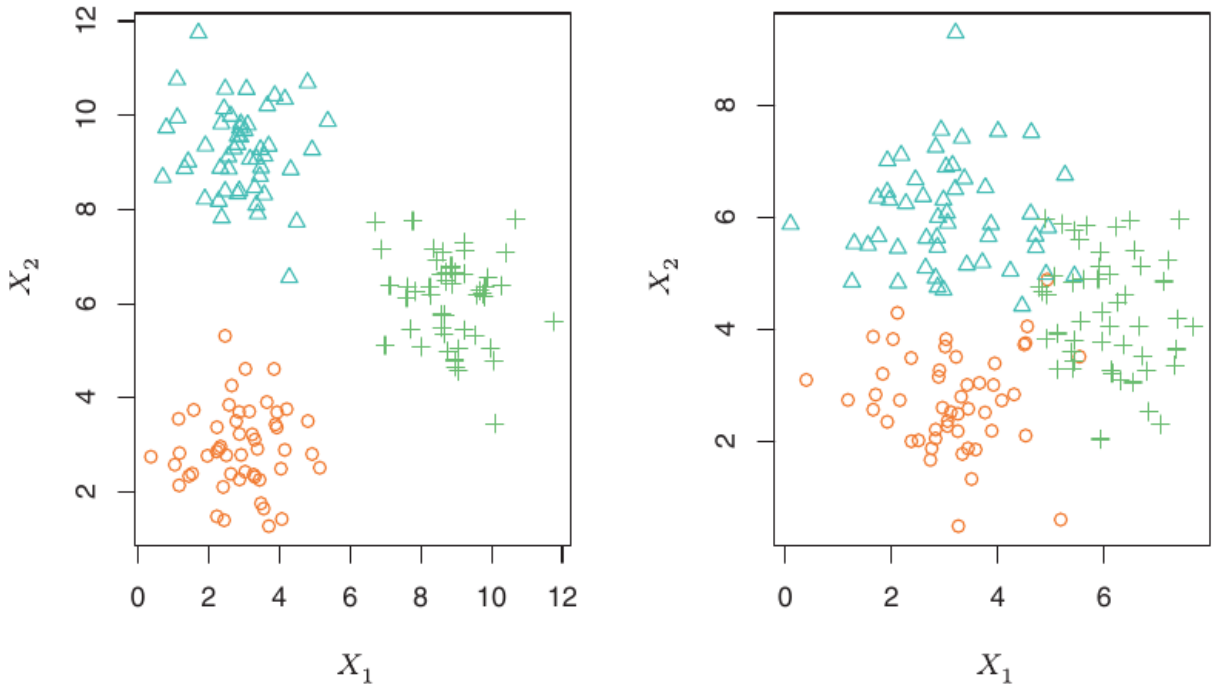
Distanzgeometrie



Jeremy M Berg, Lubert Stryer, and John L Tymoczko. *Stryer biochemie*. Springer-Verlag, 2015.

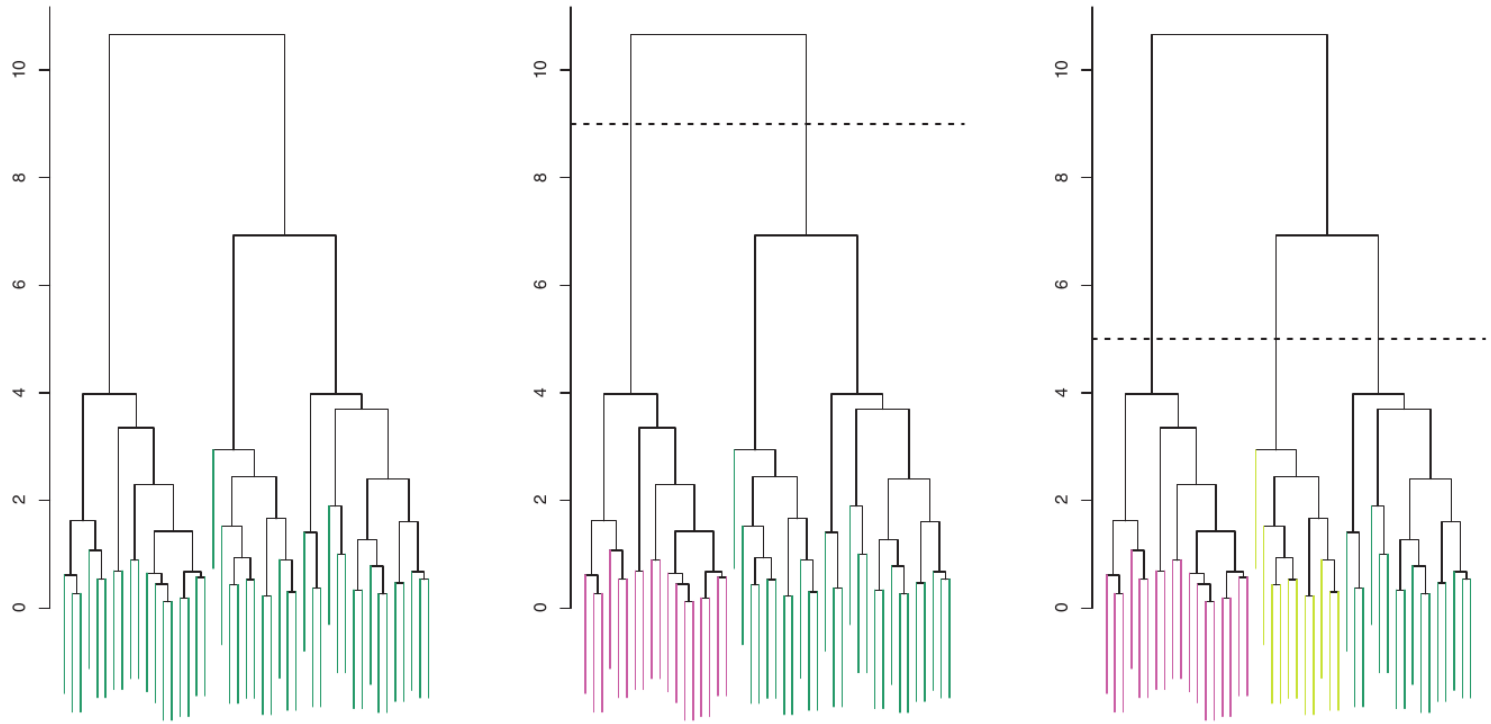
Clustering

Clustering



Gareth James et al. *An introduction to statistical learning*. Vol. 112. Springer, 2013.

Dendrogram



Gareth James et al. *An introduction to statistical learning*. Vol. 112. Springer, 2013.

Algorithmus

Algorithm 10.2 *Hierarchical Clustering*

1. Begin with n observations and a measure (such as Euclidean distance) of all the $\binom{n}{2} = n(n-1)/2$ pairwise dissimilarities. Treat each observation as its own cluster.

2. For $i = n, n-1, \ldots, 2$:

   (a) Examine all pairwise inter-cluster dissimilarities among the i clusters and identify the pair of clusters that are least dissimilar (that is, most similar). Fuse these two clusters. The dissimilarity between these two clusters indicates the height in the dendrogram at which the fusion should be placed.

   (b) Compute the new pairwise inter-cluster dissimilarities among the $i-1$ remaining clusters.

Gareth James et al. *An introduction to statistical learning*. Vol. 112. Springer, 2013.