Example of conformational entropy calculation

Contribution to a helix nucleation transition within a « net » substructure

123 Soz (=> 504 5 513 -Acli²-Acslis chushlis chushlis e -e -e - p Fitz 6 Aus blor 1 if Angliloz=0 30 14 000 C = (Son + S13) (Sus 514 (Sun + S24 S34 (Sou + S14)) + Sor Siz (Sou + Site) (Su + Szu) : $A_{1} = \frac{5}{24} \frac{5}{34} \frac{5}{54} \frac{5}{54} + \frac{5}{502} + \frac{5}{13} + \frac{5}{524} + \frac{5}{34} \frac{30}{504} \frac{25}{54} + \frac{5}{504} \frac{5}{513} + \frac{5}{54} \frac{5}{504} \frac{5}{513} + \frac{5}{504} \frac{5}{513} + \frac{5}{514} \frac{5}{502} \frac{5}{503} + \frac{5}{514} \frac{5}{503} \frac{5}{503} + \frac{5}{514} \frac{5}{503} \frac{5}{503} + \frac{5}{514} \frac{5}{503} \frac{5}{503} + \frac{5}{514} \frac{5}{503} \frac{5}{503} \frac{5}{513} + \frac{5}{514} \frac{5}{503} \frac{5}{513} + \frac{5}{514} \frac{5}{513} \frac{5}$ A23 = Sou S14 (S24 + S34 + So2 + S3) + (Sou+S4) [S24 S34 + So2 S3 + S24 S3 Airs = Sou Sig (Sig + Sig) + Sig (Sou + Sig) + Siz Sig + Siz Sog Sig 89

(scanned from the original notebook)

dridez de AFL $\int \int \left(e^{-\frac{\Gamma_{u}}{L}} \left(\frac{1}{S_{u}} + \frac{1}{S_{1}} + \frac{1}{S_{2}} + \frac{1}{S_{2}} \right) + 2\Gamma_{u}} \left(\frac{\Gamma_{1}}{S_{1}} + \frac{\Gamma_{u}}{S_{1}} + \frac{S_{1}}{S_{1}} + \frac{S_{1}}{S_{1}} \right) \right)$ $\rho = \frac{F_1^{\perp}}{S_{14}} = \frac{F_2^{\perp}\left(\frac{1}{S_{22}} + \frac{1}{S_{24}}\right) = \frac{F_3^{\perp}}{S_{24}} = \left(\frac{F_3 - F_1}{S_{24}}\right)^2$) / 11 > S() hdri 1 () / 40- 42 - 42 Cm $\int e^{-T_{4}} \left(\frac{1}{S_{04}} + \frac{1}{S_{14}} + \frac{1}{S_{24}} + \frac{1}{S_{34}} \right) + 2T_{4} - \left(\frac{T_{1}}{S_{14}} + \frac{T_{2}}{S_{14}} + \frac{T_{3}}{S_{34}} \right)$ dr. $= \sqrt{\frac{1}{11} + \frac{1}{5_{14}} + \frac{1}{5_{14}} + \frac{1}{5_{14}} + \frac{1}{5_{14}}} \sqrt{\frac{1}{5_{14}} + \frac{1}{5_{14}} + \frac{1$

 $\left[\frac{1}{S_{34}} + \frac{1}{S_{13}} - \frac{1}{S_{4}^{2}\left(\frac{1}{S_{64}} + \frac{1}{S_{14}} + \frac{1}{S_{24}} + \frac{1}{S_{55}}\right)\right]$ $= \frac{\frac{1}{S_{04}} + \frac{1}{S_{14}} + \frac{1}{S_{24}}}{\frac{1}{S_{24}} + \frac{1}{S_{24}} + \frac{1}{S_{24}} + \frac{1}{S_{24}} + \frac{1}{S_{24}}} + \frac{1}{S_{24}}$ $= \frac{c_{04} S_{14} + S_{14} S_{24} + S_{04} S_{24}}{S_{04} S_{14} S_{24} + S_{34} \left(S_{04} S_{14} + S_{14} S_{24} + S_{34} + \frac{1}{5_3}\right)} + \frac{1}{5_3}$ (Su+S13)() + Su Su Su S13[Sou Su Su + S34 ()] C)

W. [e - lis C - 2 A las 600 \$ F2- BF1] 2x lis hadde
 [Lis C - 2 A las 600 \$ F2- BF1] 2x lis hadde
 [Lis Cis - 40 \$ dde
 [Lis Cis - 40 \$ dde
]
]
]
]
]
]
]
]
]
 [Lis Cis - 40 \$ dde
]
]
]
]
]
]
 [Lis Cis - 40 \$ dde
]
]
]
]
]
]
]
]
 [Lis Cis - 40 \$ dde
]
]
]
]
]
]
]
 [Lis Cis - 40 \$ dde
]
]
]
]
]
]
 [Lis Cis - 40 \$ dde
]
]
 [Lis Cis - 40 \$ dde
]
]
 [Lis Cis - 40 \$ dde
]
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 [
]
 $= \frac{l_{13}c}{2} \cdot \frac{2Al_{13}\left[\overline{r_2} - B\overline{r_1}\right] - 2Al_{13}\left[\overline{r_2} - B\overline{r_1}\right]}{4\frac{14}{7}Al_{13}\left[\overline{r_2} - B\overline{r_1}\right]}$ $\int \frac{-\frac{\Gamma_{1}^{2}}{S_{14}} - (\overline{S_{2}} - 8\overline{r_{1}} + 8\overline{r_{1}})^{2} (\frac{1}{S_{22}} + \frac{1}{S_{24}})}{(\frac{1}{S_{24}} + \frac{1}{S_{14}} + \frac{1}{S_{14$ $e^{-\left(\overline{r_2} - 8r_1 + 8r_1\right)^2} \frac{1}{\sqrt{s_1}} - \left(\overline{r_2} - 8r_1 + (8-1)r_1\right)^2 \frac{1}{\sqrt{s_2}}$ e lise @ 2Alis [FI-BFI] e - 2Alis [FI-BFI] e. _ _ dri dli-bij 4 A las 1/2 - 8 FT)

 $\rightarrow \left[\frac{A \cdot (2)}{2} = Ans \right]$

$$\begin{array}{c} \underbrace{(5)}_{1} \\ \underbrace{(5)}_{2} \\ \underbrace{(5)}_{2}$$

$$A = \frac{1}{S_{B}} + \frac{\frac{1}{S_{0_{L}}} + \frac{1}{S_{1_{L}}}}{S_{3L_{L}}\left(\frac{1}{S_{0_{L}}} + \frac{1}{S_{1_{L}}} + \frac{1}{S_{1_{L}}} + \frac{1}{S_{2_{L}}}\right)}$$

$$AB = \frac{1}{S_{13}} + \frac{\frac{1}{S_{14}}}{S_{14}} \left(\frac{1}{S_{14}} + \frac{1}{S_{14}} + \frac{1}{S_{24}} + \frac{1}{S_{24}} \right)$$

$$(2) = \frac{1}{5_{22}} + \frac{1}{5_{13}} + \frac{1}{(\frac{1}{5_{24}} + \frac{1}{5_{34}})(\frac{1}{5_{64}} + \frac{1}{5_{14}})}{\frac{1}{5_{64}} + \frac{1}{5_{24}} + \frac{1}{5_{24}} + \frac{1}{5_{54}}}$$

Ð $\frac{O + 1}{(1)} = A + \frac{1}{O} \qquad \left(\frac{1}{S_{13}} + \frac{1}{S_{14}} + \frac{1}{S_{14}} + \frac{1}{S_{14}} - \frac{1}{S_{14}} \right).$ $A \begin{bmatrix} J \\ J \end{bmatrix} = \frac{\frac{1}{S_{13}} \begin{pmatrix} \end{pmatrix} + \frac{1}{S_{34}} \begin{pmatrix} \frac{1}{S_{34}} + \frac{1}{S_{44}} \end{pmatrix}}{\begin{pmatrix} \end{pmatrix}} \frac{r_{13}^{+} \begin{pmatrix} \end{pmatrix} + \frac{1}{s_{44}} \begin{pmatrix} \frac{1}{S_{44}} + \frac{1}{s_{44}} \end{pmatrix}}{\begin{pmatrix} \end{pmatrix}}$ (_____ $\left(\frac{1}{5_{2}}+\frac{1}{5_{13}}\right)\left(\frac{1}{5}\right)+\left(\frac{1}{5_{0l_{1}}}+\frac{1}{5_{1}}\right)\left(\frac{1}{5_{1l_{1}}}+\frac{1}{5_{3}}\right)$ $+ \underbrace{EJ}_{=} \begin{bmatrix} \frac{1}{5\eta} () + \frac{1}{5\eta} (\frac{1}{5\eta} + \frac{1}{5\eta}) \end{bmatrix} \begin{bmatrix} \frac{1}{5\eta} () + \frac{1}{5\eta} (\frac{1}{5\eta} + \frac{1}{5\eta}) \end{bmatrix}$ $AB = \frac{\frac{1}{5}}{5} \left(\begin{array}{c} \\ \end{array} \right) + \frac{1}{5} \frac{1}{5} \frac{1}{5} \left(\begin{array}{c} \\ \end{array} \right)$ $Ab - A \overline{51} = - \left[\frac{1}{573} \left(\right) + \frac{1}{524} \left(\frac{1}{504} + \frac{1}{514} \right) \right] \left[\frac{1}{513} \left(\right) + \frac{1}{514} \left(\frac{1}{544} + \frac{1}{514} \right) \right]$ $+\left[\frac{1}{S_{13}}\left(\begin{array}{c}\right)+\frac{1}{S_{14}}\frac{1}{S_{24}}\right]\left[\left(\frac{1}{4z}+\frac{1}{S_{13}}\right)\left(\begin{array}{c}\right)+\left(\frac{1}{S_{04}}+\frac{1}{S_{14}}\right)\left(\frac{1}{S_{04}}+\frac{1}{S_{14}}\right)\right]$ () for the

$$\frac{(3)}{(3)} = \frac{1}{5\pi} \frac{1}{5\pi} (1)^{2}$$

$$\frac{1}{5\pi} (1) \left\{ \frac{1}{5\pi} \frac{1}{5\pi} \frac{1}{5\pi} (1)^{2} - \frac{1}{5\pi} \frac{1}{5\pi} \frac{1}{5\pi} \frac{1}{5\pi} (1)^{2} + \frac{1}{5\pi} \frac{1}$$

$$C = (So_{2} + Si_{3}) \left\{ Si_{4} Si_{4} Si_{4} + So_{4} Si_{4$$

