



$$k_d = 0.32 \mu mol/l$$











$[i:j]$



$[k : l]$

$$i-j$$

$$k-l$$

$$(i, j), \dots, (i + (k - 1), j - (k - 1))$$

$$p \in [i : j]$$

$$q \in [k : l]$$

$(i, j)$

$(p, q)$



$$i < p < j < q$$

$$p < i < q < j$$

$$E_{ij}$$

$$E_{ij} = \min \left[ \max_{(i,k) \in \{GC,CG,AU,UA,GU,UG\}} E_{ik}, \max_{(k,j) \in \{GC,CG,AU,UA,GU,UG\}} E_{kj} \right].$$

*e*

*kcal/mol*

*m*

$-5kcal/mol$



Q

$$G = -RT \cdot \log(Q)$$

$$q1k(k) = Q(1, k)$$

$$qln(l) = Q(l, n)$$

$$p(i,j) = S_i + S_j - p_{ij} * \ln(p_{ij})$$

$$\langle d(S) \rangle = \sum_{(i,j) \in S} (1 - p_{ij}) + \sum_{(i,j) \notin S} p_{ij}$$

$$p_{ij} > 0.5$$

$(i, j)$



$(k, l)$

$[i:j]$

$[i : k]$

$[l:j]$

$[k : l]$

$(l, j)$

$(i, k)$

$$(l, j - 1)$$



$$d < 0$$

$$d > 0$$

$$d == 0$$

$$\Delta G_{\text{SHAPE}}(i) = m \ln(\text{SHAPE reactivity}(i) + 1) + b$$



$q_i$

$$\Delta G_{\text{SHAPE}}(x,i) = \beta \left| x_i - q_i \right|$$









$$|x_i - q_i|$$



*dacal/mol*

$$1\text{d}acal/mol = 10cal/mol$$

$$\exp(-\hat{E}/kT)$$





*cal/mol*

$$\langle d \rangle = \sum_{a,b} p_a p_b d(S_a, S_b)$$

$p_i j$

$$\langle d \rangle = \sum_{ij} p_{ij} (1 - p_{ij})$$

$$(i+1, j-1)$$

$$p > \text{cutoff}$$



$$\geq 1$$





$$\Sigma = \{A, U, C, G\}$$

`strlen(sequence) + 1`

$$e^{-\Delta G/kT}$$

$$\Delta G$$

$$(n + m)$$

$$-kT \cdot \log(p)$$





$$10^{-2} * \text{kcal/mol}$$

$$N \times M$$

$N$

$M$

$X[100][5]$

$$A(S) = \sum_{(i,j) \in S} 2\gamma p_{ij} + \sum_{i \notin S} p_i^u$$



$$\exp(-E/(b \cdot kT))$$



$$\exp((-F/kT)/length)$$



$$\exp(-E/kT)$$



$$\hat{q}[i,j] = q[i,j]/s^{(j-i+1)}$$

$$s = \exp((sfact * MFE)/kT/length)$$

$$\exp(-\Delta G/kT)$$

$$e^{-E/(\alpha \cdot K \cdot T)}$$



$$F(\vec{\epsilon}) = \sum_{i=1}^n \frac{\epsilon_i^2}{\tau^2} + \sum_{i=1}^n \frac{(p_i(\vec{\epsilon}) - q_i)^2}{\sigma^2} \rightarrow \min$$

$$F(\vec{\epsilon}) = \sum_{i=1}^n \frac{|\epsilon_i|}{\tau^2} + \sum_{i=1}^n \frac{|p_i(\vec{\epsilon}) - q_i|}{\sigma^2} \rightarrow min$$

$$F(\vec{\epsilon}) = \sum_{\mu} \frac{\epsilon_{\mu}^2}{\tau^2} + \sum_{i=1}^n \frac{(p_i(\vec{\epsilon}) - q_i)^2}{\sigma^2} \rightarrow \min.$$

$P^t$

*rs*

$[0, 1]$

$$P_x^t[i] = X[i] * rs$$

$$P_y^t[i] = Y[i] * rs$$



$$1 \text{ } J = 1 \text{ } kg \cdot m^2 s^{-2}$$

$$1 \text{ kJ} = 1,000 \text{ J}$$

$$1\text{ cal}_{IT} = 4.1868\text{ J}$$

$$1 \text{ } d\text{acal}_{IT} = 10 \text{ } \text{cal}_{IT} = 41.868 \text{ } J$$

$$1\text{ kcal}_{IT} = 4.1868\text{ kJ}$$

$$1\text{ cal}_{th} = 4.184\text{ J}$$

$$1 \text{ } d\text{acal}_{th} = 10 \text{ } \text{cal}_{th} = 41.84 \text{ } J$$

$$1\text{ kcal}_{th} = 4.184\text{ kJ}$$



$$1\text{ g TNT} = 1,000\text{ cal}_{th} = 4,184\text{ J}$$

$$1\text{ kg TNT} = 1,000\text{ kcal}_{th} = 4,184\text{ kJ}$$

$$1\text{ t TNT} = 1,000,000\text{ kcal}_{th} = 4,184\text{ MJ}$$

$$1\text{ eV} = 1.602176565 \times 10^{-19}\text{ J}$$

$$1\text{ W} \cdot h = 1\text{ W} \cdot 3,600\text{ s} = 3,600\text{ J} = 3.6\text{ kJ}$$

$$1\text{ kW} \cdot h = 1\text{ kW} \cdot 3,600\text{ s} = 3,600\text{ kJ} = 3.6\text{ MJ}$$

$$[^{\circ}C] = [K] - 273.15$$

$$[^{\circ}F] = [K] \times \frac{9}{5} - 459.67$$



$$[{}^{\circ}R] = [K] \times \frac{9}{5}$$

$$[^{\circ}N] = ([K] - 273.15) \times \frac{33}{100}$$

$$[^{\circ}De] = (373.15 - [K])^{\frac{3}{2}}$$

$$[^{\circ}R\acute{e}] = ([K] - 273.15) \times \frac{4}{5}$$

$$[^\circ\mathrm{R}\phi] = ([K] - 273.15) \times \frac{21}{40} + 7.5$$

$$f(i, j)$$

$[i, j]$







$[i, j]$

$$1 \leq i < j \leq n$$



$$1 \leq i \leq n$$