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Direct incorporation of prior phase information in macromolecular model refinement

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TIE ISTÉ 2. DERIVÁCIE AKO NA PRŮCH. STRANĚ, LEN S IMIT. OČNĚ
(KVŮ IMPLEMENTÁCI) (INDEXY KL. BUDŮ ZAHNENÉ ZA P, Q A M, N ZA

2. DERIV. 1. FCIE

$$\frac{\partial(-\ln P)}{\partial D_{pq} \partial D_{kl}} = -\frac{\partial}{\partial D_{kl}} \left(\frac{1}{K} \frac{\partial K}{\partial D_{pq}} \right) - \frac{\partial^2 E}{\partial D_{pq} \partial D_{kl}} - \frac{F_1^2}{R} \frac{\partial R}{\partial D_{pq} \partial D_{kl}} \left(\frac{I_0(B)}{I_0(B)} - \frac{\frac{1}{2} I_0(B)}{I_0^2(B)} - \frac{I_0(B)}{I_0^2(B)} \right) - \frac{I_0(B)}{I_0(B)}$$

$$\frac{\partial}{\partial D_{kl}} \left(\frac{1}{K} \frac{\partial K}{\partial D_{pq}} \right) = 2k_{pq} \left[\operatorname{Re} \left(\frac{\partial^2 \sigma_{pq}}{\partial D_{pq} \partial D_{kl}} \right) (c_{pq} - a_{pq}) + \operatorname{Re} \left(\frac{\partial^2 \sigma_{pq}}{\partial D_{pq} \partial D_{kl}} \right) \left(\frac{\partial c_{pq}}{\partial D_{kl}} - \frac{\partial a_{pq}}{\partial D_{kl}} \right) + \operatorname{Im} \left(\frac{\partial^2 \sigma_{pq}}{\partial D_{pq} \partial D_{kl}} \right) \left(\frac{\partial c_{pq}}{\partial D_{kl}} + \frac{\partial a_{pq}}{\partial D_{kl}} \right) \right]$$

$$\frac{\partial^2 E}{\partial D_{pq} \partial D_{kl}} = -F_1^2 \frac{\partial^2 a_{11}}{\partial D_{pq} \partial D_{kl}} - \sum_{i=2}^N \left\{ F_i^2 \left(\frac{\partial^2 a_{ii}}{\partial D_{pq} \partial D_{kl}} - \frac{\partial^2 c_{ii}}{\partial D_{pq} \partial D_{kl}} \right) + \sum_{j=i+1}^N 2F_i F_j \left[\left(\frac{\partial^2 a_{ij}}{\partial D_{pq} \partial D_{kl}} - \frac{\partial^2 c_{ij}}{\partial D_{pq} \partial D_{kl}} \right) S_{ij} \right] \right\}$$

$$\frac{\partial^2 R}{\partial D_{pq} \partial D_{kl}} = \sum_{i=2}^N \left\{ 2F_i^2 \left(\frac{\partial^2 a_{ii}}{\partial D_{pq} \partial D_{kl}} + a_{ii} \frac{\partial a_{ii}}{\partial D_{pq} \partial D_{kl}} + \frac{\partial^2 a_{ii}}{\partial D_{pq} \partial D_{kl}} + b_{ii} \frac{\partial b_{ii}}{\partial D_{pq} \partial D_{kl}} \right) + \sum_{j=i+1}^N 2F_i F_j \left[\left(\frac{\partial^2 a_{ij}}{\partial D_{pq} \partial D_{kl}} a_{ij} + \frac{\partial a_{ii}}{\partial D_{pq} \partial D_{kl}} \frac{\partial a_{ij}}{\partial D_{kl}} + \frac{\partial^2 b_{ii}}{\partial D_{pq} \partial D_{kl}} b_{ij} + \frac{\partial b_{ii}}{\partial D_{pq} \partial D_{kl}} \frac{\partial b_{ij}}{\partial D_{kl}} \right) C_{ij} + \left(\frac{\partial^2 a_{ij}}{\partial D_{pq} \partial D_{kl}} b_{ii} + \frac{\partial a_{ij}}{\partial D_{pq} \partial D_{kl}} \frac{\partial b_{ii}}{\partial D_{kl}} + a_{ij} \frac{\partial^2 b_{ii}}{\partial D_{pq} \partial D_{kl}} \right) S_{ij} \right] \right\}$$

2. DERIV. 2. FCIE

$$\frac{\partial(-\ln P)}{\partial D_{pq} \partial D_{kl}} = -\frac{\partial}{\partial D_{kl}} \left(\frac{1}{K} \frac{\partial K}{\partial D_{pq}} \right) - \frac{\partial^2 E}{\partial D_{pq} \partial D_{kl}} + \frac{1}{I^2} \frac{\partial I}{\partial D_{pq} \partial D_{kl}} I \frac{\partial I}{\partial D_{pq} \partial D_{kl}}$$

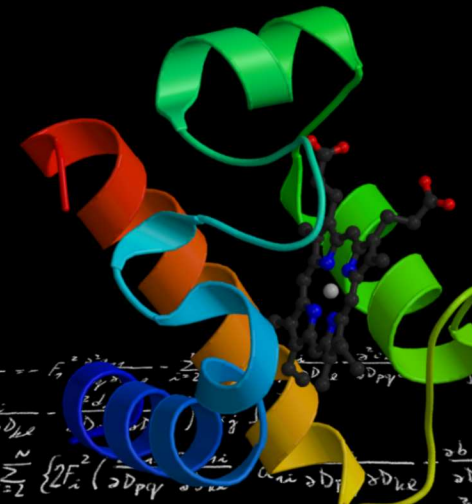
$$\frac{\partial}{\partial D_{kl}} \left(\frac{1}{K} \frac{\partial K}{\partial D_{pq}} \right) \text{ má formulu } + \text{var rovnaké ako pri 1. fcii}$$

$$\frac{\partial^2 E}{\partial D_{pq} \partial D_{kl}} = -F_1^2 \frac{\partial^2 a_{11}}{\partial D_{pq} \partial D_{kl}} - F_2^2 \frac{\partial^2 a_{22}}{\partial D_{pq} \partial D_{kl}} - \sum_{i=3}^N \left\{ F_i^2 \left(\frac{\partial^2 a_{ii}}{\partial D_{pq} \partial D_{kl}} - \frac{\partial^2 c_{ii}}{\partial D_{pq} \partial D_{kl}} \right) + \sum_{j=i+1}^N 2F_i F_j \left[\left(\frac{\partial^2 a_{ij}}{\partial D_{pq} \partial D_{kl}} - \frac{\partial^2 c_{ij}}{\partial D_{pq} \partial D_{kl}} \right) S_{ij} \right] \right\}$$

$$\frac{\partial^2 I}{\partial D_{pq} \partial D_{kl}} = \int_0^{\infty} \exp(-E_2) \left\{ \left[\frac{\partial E_2}{\partial D_{pq} \partial D_{kl}} + \frac{\partial^2 E_2}{\partial D_{pq} \partial D_{kl}} + \frac{F_1^2}{R} \frac{\partial R}{\partial D_{pq} \partial D_{kl}} \right] I_0(B) + \frac{F_2}{\sqrt{R}} \left[\frac{\partial E_2}{\partial D_{pq} \partial D_{kl}} + \frac{\partial E_2}{\partial D_{kl} \partial D_{pq}} - \frac{1}{R} \frac{\partial R}{\partial D_{pq} \partial D_{kl}} + \frac{\partial^2 R}{\partial D_{pq} \partial D_{kl}} \right] I_1(B) \right\} d\lambda$$

$$\frac{\partial^2 E_2}{\partial D_{pq} \partial D_{kl}} = - \sum_{i=3}^N 2F_i F_j \left(\frac{\partial^2 a_{ii}}{\partial D_{pq} \partial D_{kl}} C_{ii} - \frac{\partial^2 b_{ii}}{\partial D_{pq} \partial D_{kl}} S_{ii} \right)$$

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$$\frac{\partial^2 E}{\partial D_{pq} \partial D_{kl}} = -F_1^2 \frac{\partial^2 a_{11}}{\partial D_{pq} \partial D_{kl}} - \sum_{i=2}^N \left\{ F_i^2 \left(\frac{\partial^2 a_{ii}}{\partial D_{pq} \partial D_{kl}} - \frac{\partial^2 c_{ii}}{\partial D_{pq} \partial D_{kl}} \right) + \sum_{j=i+1}^N 2F_i F_j \left[\left(\frac{\partial^2 a_{ij}}{\partial D_{pq} \partial D_{kl}} a_{ij} + \frac{\partial a_{ii}}{\partial D_{pq} \partial D_{kl}} \frac{\partial a_{ij}}{\partial D_{kl}} + \frac{\partial^2 b_{ii}}{\partial D_{pq} \partial D_{kl}} b_{ij} + \frac{\partial b_{ii}}{\partial D_{pq} \partial D_{kl}} \frac{\partial b_{ij}}{\partial D_{kl}} \right) C_{ij} + \left(\frac{\partial^2 a_{ij}}{\partial D_{pq} \partial D_{kl}} b_{ii} + \frac{\partial a_{ij}}{\partial D_{pq} \partial D_{kl}} \frac{\partial b_{ii}}{\partial D_{kl}} + a_{ij} \frac{\partial^2 b_{ii}}{\partial D_{pq} \partial D_{kl}} \right) S_{ij} \right] \right\}$$

Pavol Skubák

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Pavol Skubák

Uitnodiging

De openbare verdediging
van dit proefschrift vindt

plaats op donderdag

10 januari 2007

om 16.15 uur

op de Lokhorstkerk,

Pieterskerkstraat 1

te Leiden.

Na afloop van de promotie

zal een receptie

plaatsvinden.

Omdat de wachtruimte

beperkt is worden

de gasten verzocht

niet eerder dan 15 minuten

voor de aanvang

van de verdediging

aanwezig te zijn.