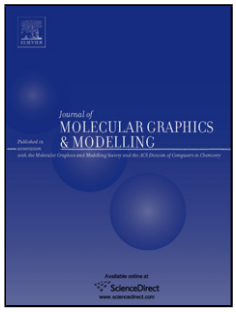

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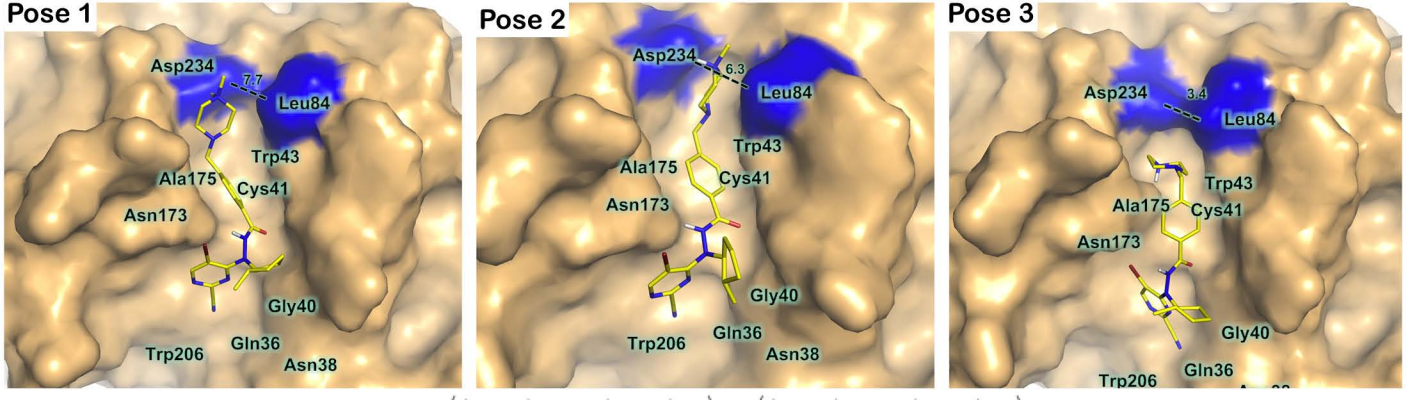
PII: S1093-3263(16)30102-4
DOI: http://dx.doi.org/doi:10.1016/j.jmgm.2016.06.008
Reference: JMG 6715

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 29-3-2016
Revised date: 6-6-2016
Accepted date: 15-6-2016

Please cite this article as: Vasanthanathan Poongavanam, Jacob Kongsted, Binding affinity models for Falcipain inhibition based on the Linear Interaction Energy method, Journal of Molecular Graphics and Modelling http://dx.doi.org/10.1016/j.jmgm.2016.06.008



$$\Delta G_{Bind} = \alpha\left(\left\langle U_{l-surr}^{vdw}\right\rangle_{bound} - \left\langle U_{l-surr}^{vdw}\right\rangle_{free}\right) + \beta\left(\left\langle U_{l-surr}^{el}\right\rangle_{bound} - \left\langle U_{l-surr}^{el}\right\rangle_{free}\right) + \gamma$$

1.81 kcal/mol **1.65 kcal.mol** **1.56 kcal/mol**