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Title: Binding affinity models for Falcipain inhibition based on the Linear Interaction Energy method

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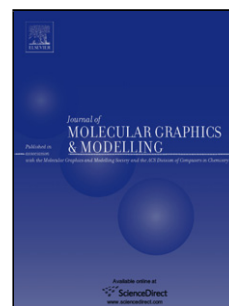
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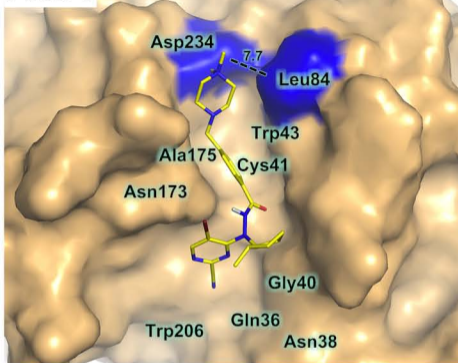
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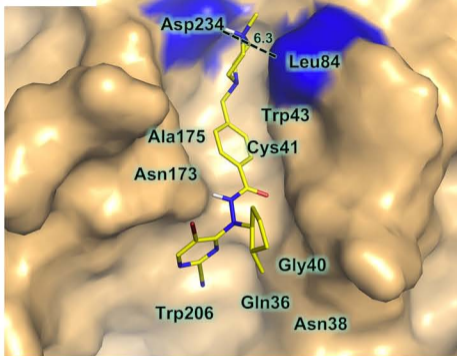
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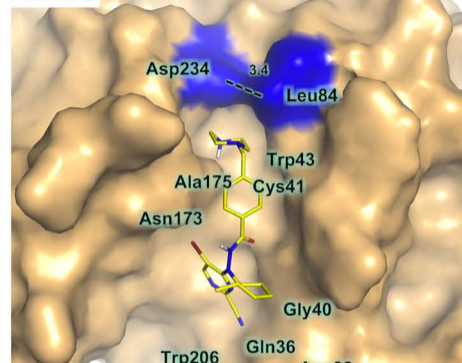
Pose 1



Pose 2



Pose 3



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

1.81 kcal/mol

1.65 kcal/mol

1.56 kcal/mol

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