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Comparison of the surface structure of RuBisCO surrounding the bound xylulose biphosphate.

Homology model of vulcanus RuBisCO was constructed by MOE homology modeling tool using the crystal structure of 6301 RuBisCO with xylulose biphosphate as the template. And the model of the vulcanus RuBisCO was refined by amber8. Tobacco RuBisCO with three Pi (PDB code 1EJ7) was bound with etidronate virtually by ASEDock in MOE.

Red and green spheres show oxygen and carbon atoms, respectively. Blue surface shows nitrogen of 326K. Yellow spheres show a cluster of 8 etidronates with highest binding energy calculated by ASEDock. Binding positions of xylulose biphosphate against model were determined by superimposing the models on the crystal structure of 6301 RuBisCO with the ligand.

Related article: Iwaki, T., Shiota, K., Al-Taweel, K., Kobayashi, D., Kobayashi, A., Suzuki, K., Yui, T., and Wadano, A., "Inhibition of RuBisCO cloned from *Thermosynechococcus vulcanus* and expressed in *Escherichia coli* with compounds predicted by molecular operation environment (MOE)", *J. Biosci. Bioeng.*, vol. 105, 26-33 (2008).

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