Comparison of molecular dynamics of cyclosporin A and cyclosporin E

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P01-09 (F-2)

Activation Pathway of IL-2-inducible T cell kinase Explored by Tree-Search Molecular Dynamics

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MDContactCom: A tool to identify differences of protein molecular dynamics from two MD simulation trajectories in terms of residue-residue contacts

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Dynamic FMO analysis for RNA sequence specificity in inhibitor recognition of translation initiation factor complex

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Design and Implementation of New Methods for Odor Molecule Generation

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P03-08 (F-4)

Development of a Prediction Method for Protein Cryptic Sites Using Machine Learning

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Interaction Analysis of GPCR in the Presence of Lipid Bilayer Using Fragment Molecular Orbital (FMO) Method

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Yusuke Kawashima  
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Koji Okuwaki  
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Takayuki Furuishi  
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Etsuo Yonemochi  
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Inhibitor discovery targeting UHRF1 by MD simulations and biochemical analyses

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P13-01 (F-7)

In silico-guided design of growth factor mutants with varied physicochemical parameters

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