

Take Home Messages

- Path sampling is a powerful tool for gaining insight into biomolecular systems
- Path sampling gives insight into the oncogenic nature of K-Ras mutant Q61L by showing that a channel for opening closes off, keeping the protein active
- Path sampling can be used to study drug binding/unbinding
- New software (OpenPathSampling) and methods are making path sampling more accessible

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K-Ras



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OpenPathSampling



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