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Exploring the Interactions of EGFR with Phosphorylated Mig6 by
Molecular Dynamics Simulations and MM-PBSA Calculations

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Highlights

- A prior phosphorylation pathway on Y394 of Mig6-segment2 is proposed.
- The interactions of EGFR with phosphorylated Mig6-segment2 are explored.
- The L-shaped structure may be associated with Mig6 irreversible inhibition EGFR.

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