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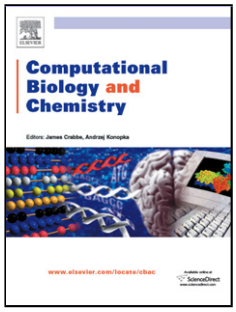

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Improving Virtual Screening Predictive Accuracy of Human Kallikrein 5 inhibitors using Machine Learning Models

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HighlightsSignature fingerprints with bond order information performs better in the QSAR study.

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