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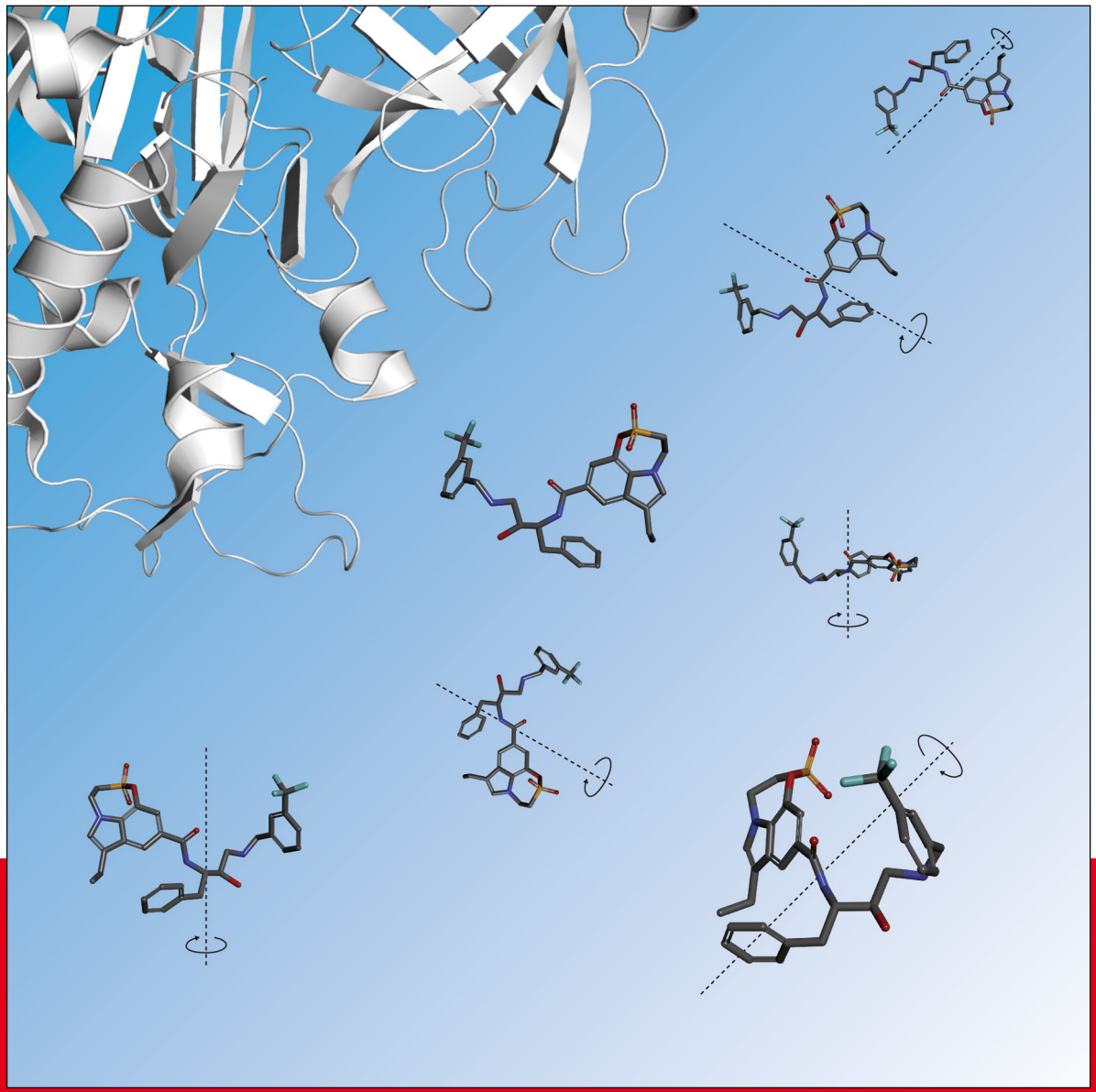

16/18
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Front Cover:
Won June Kim, Insung S. Choi et al.
Rotational Variance-Based Data Augmentation in 3D Graph Convolutional Network

WILEY-VCH

Data augmentation for 3D graph convolutional network (3DGCN) has been achieved, for the classification task of human β-secretase 1 (BACE-1)-ligand binding, by randomly rotating known active (1-labeled) ligands in the 3D Cartesian coordinate and assigning the rotated ones as label-0. The data augmentation improves the orientation-recognizing ability of 3DGCN significantly, suggesting the potential for identification of active ligands from a dataset, with rotation of candidates and evaluation of output sigmoid values. More information can be found in the Communication by Won June Kim, Insung S. Choi et al.

J. Kim, Y. Kim, Prof. E. K. Lee, Dr. C. H. Chae, Dr. K. Lee, Prof. W. J. Kim, Prof. I. S. Choi**

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