Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Effective Estimation for Inhibitor Affinity of HIV-1 Protease via a Modified LIE Approach

Son Tung Ngo, [a,b,*] Nam Dao Hong[c], Le Huu Quynh Anh,[d] Dinh Minh Hiep,[e] and Nguyen Thanh Tung[f]

[a.] *Laboratory of Theoretical and Computational Biophysics, Ton Duc Thang University, Ho Chi Minh City, Vietnam*

[b.] *Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam*

[c.] *University of Medicine and Pharmacy at Ho Chi Minh City, Ho Chi Minh City, Vietnam*

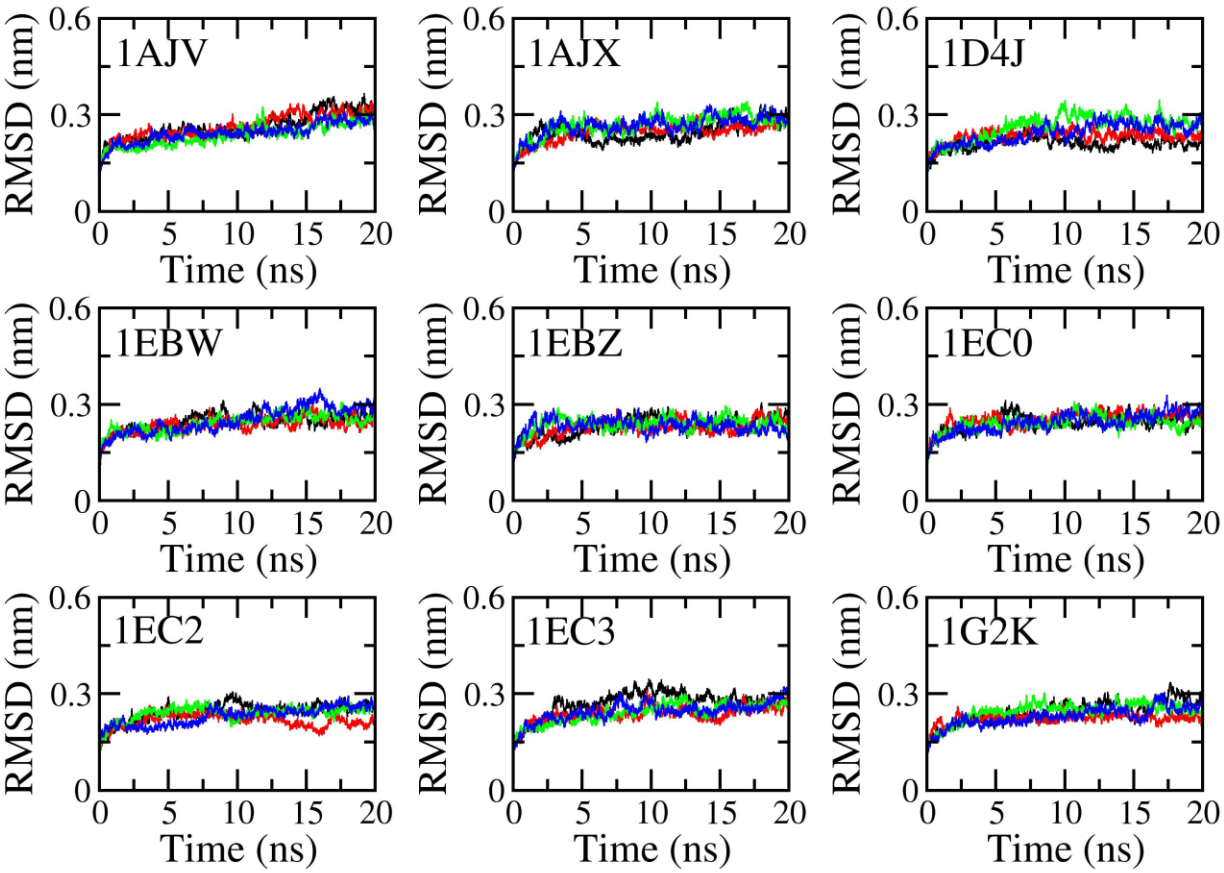
[d.] *Department of Climate Change and Renewable Energy, Ho Chi Minh City University of Natural Resources And Environment, Ho Chi Minh City, Vietnam*

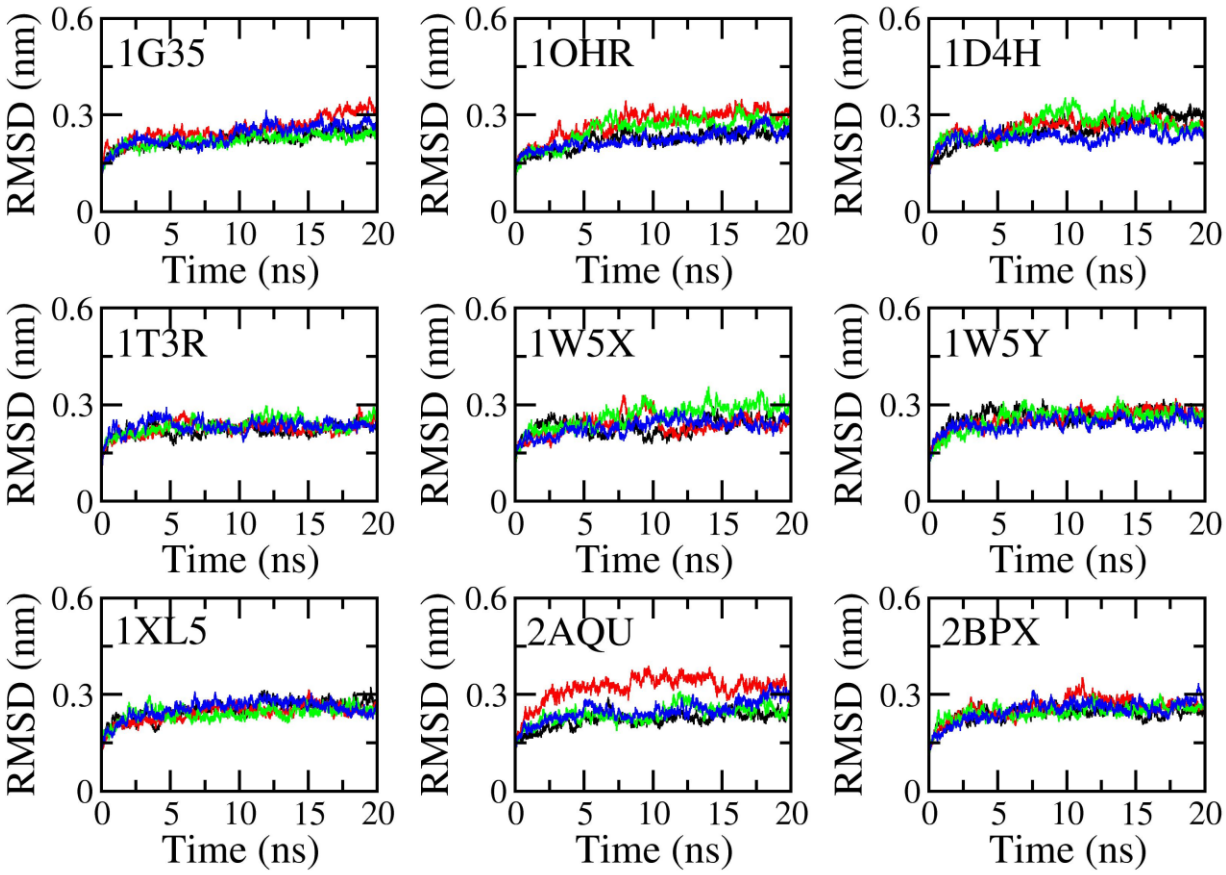
[e.] *Agricultural Hi-Tech Park, Ho Chi Minh City, Vietnam*

[f.] *Institute of Materials Science & Graduate University of Science and Technology, Vietnam Academy of Science and Technology, Hanoi, Vietnam*

*Email: ngosontung@tdtu.edu.vn

Figure S1. All-atom RMSD of HIV-1 PR + inhibitors over 4 independent MD trajectories with a length of 20 ns. The complexes almost reach equilibrium region after 5 ns.

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Time (ns)
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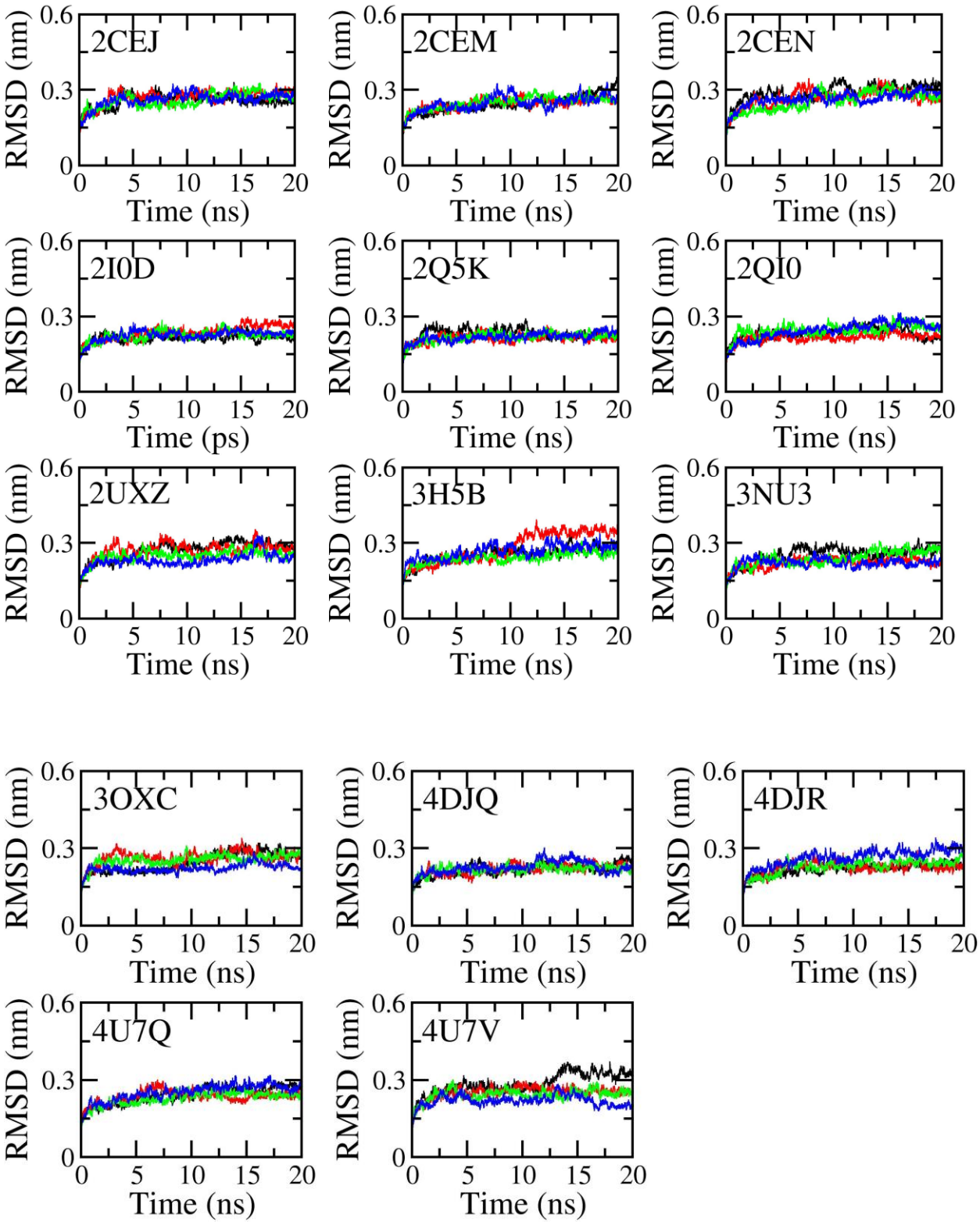
0.6
0
5
10
15
20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4DJQ
4DJR
4U7Q
4U7V
RMSD (nm)
Time (ns)
Time (ps)
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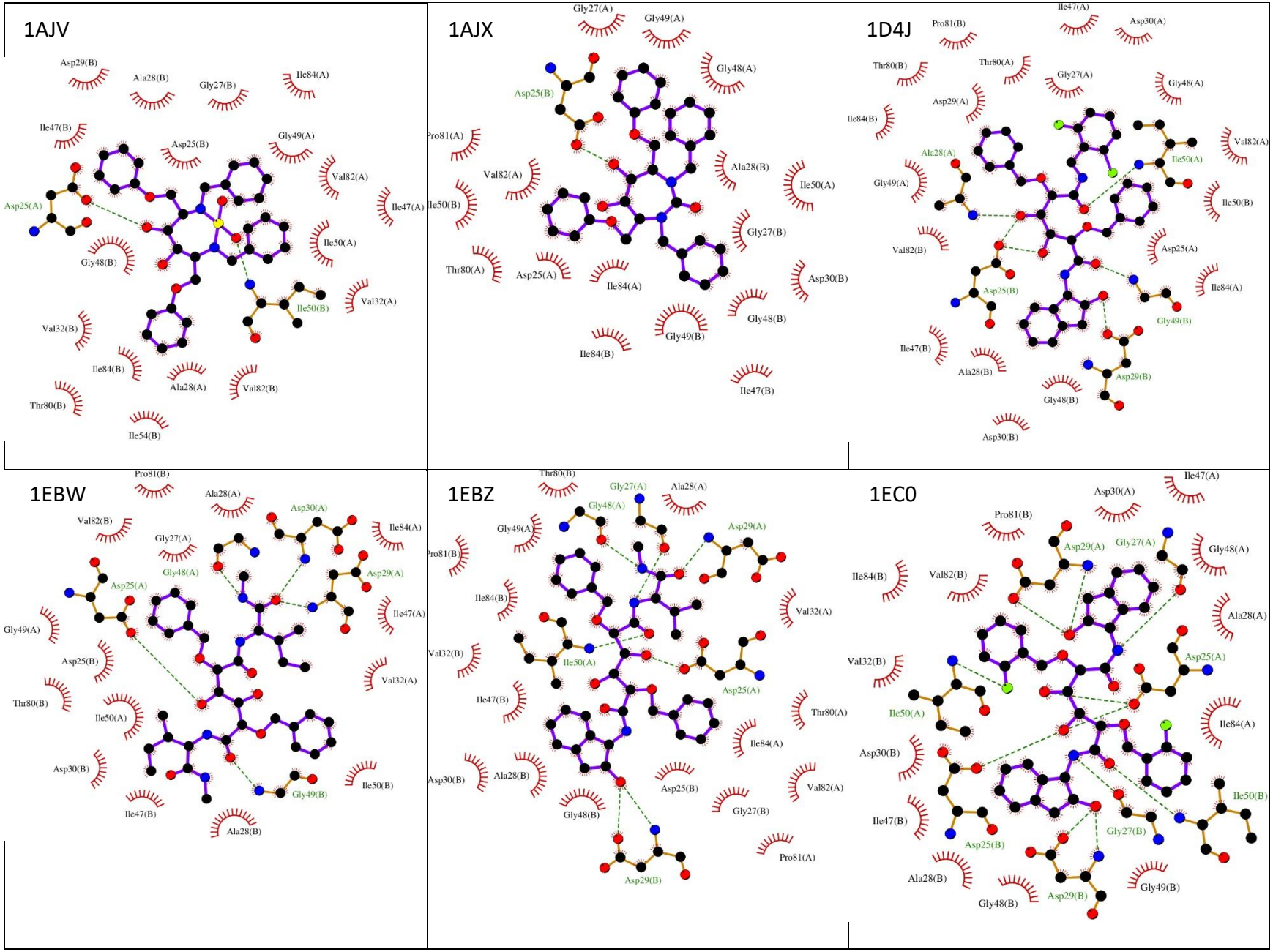
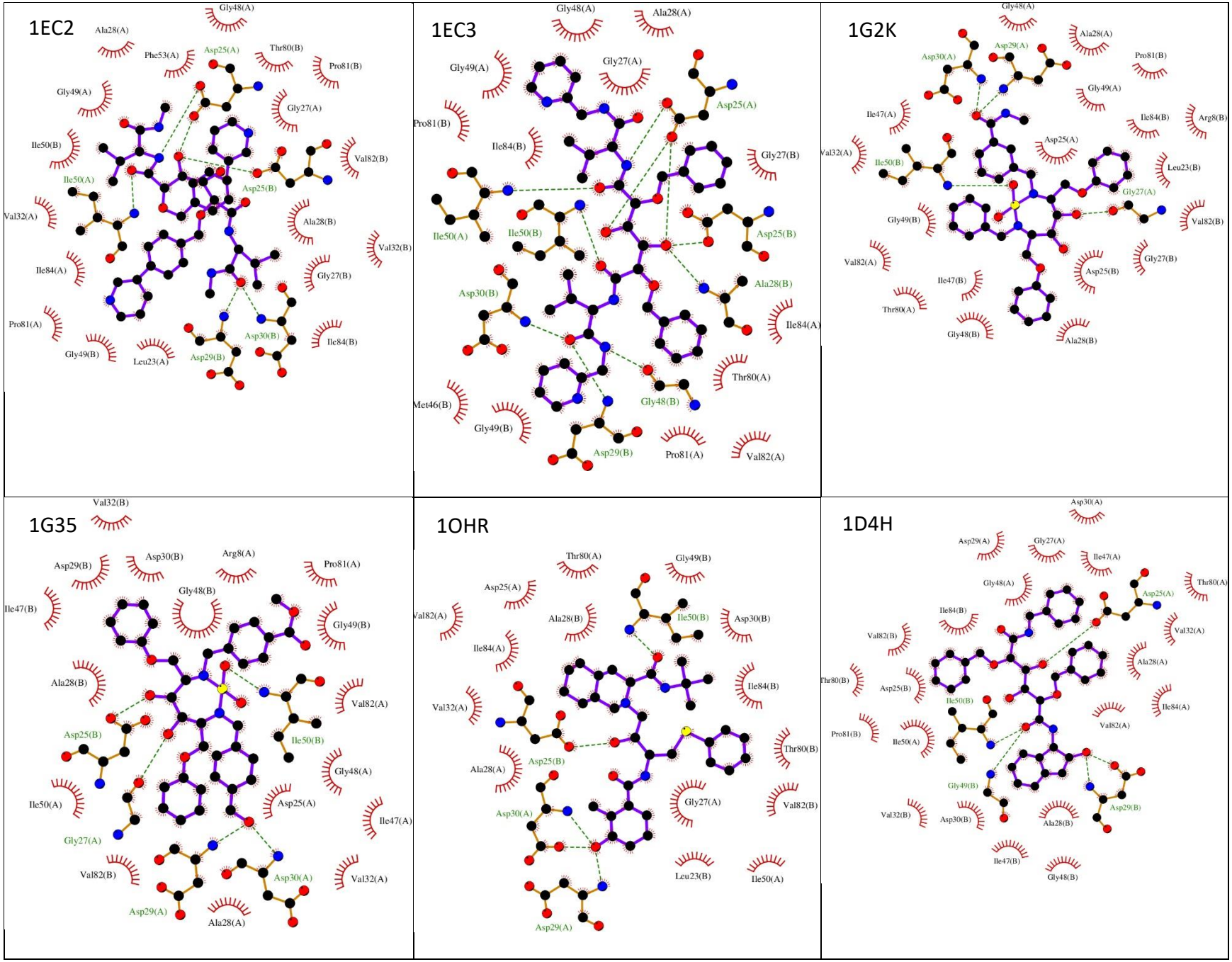
0.3
0.6
0 5 10 15 20

Figure S2. The two-dimensions protein-ligand interaction diagrams, which were prepared via LigPlot++.[1]

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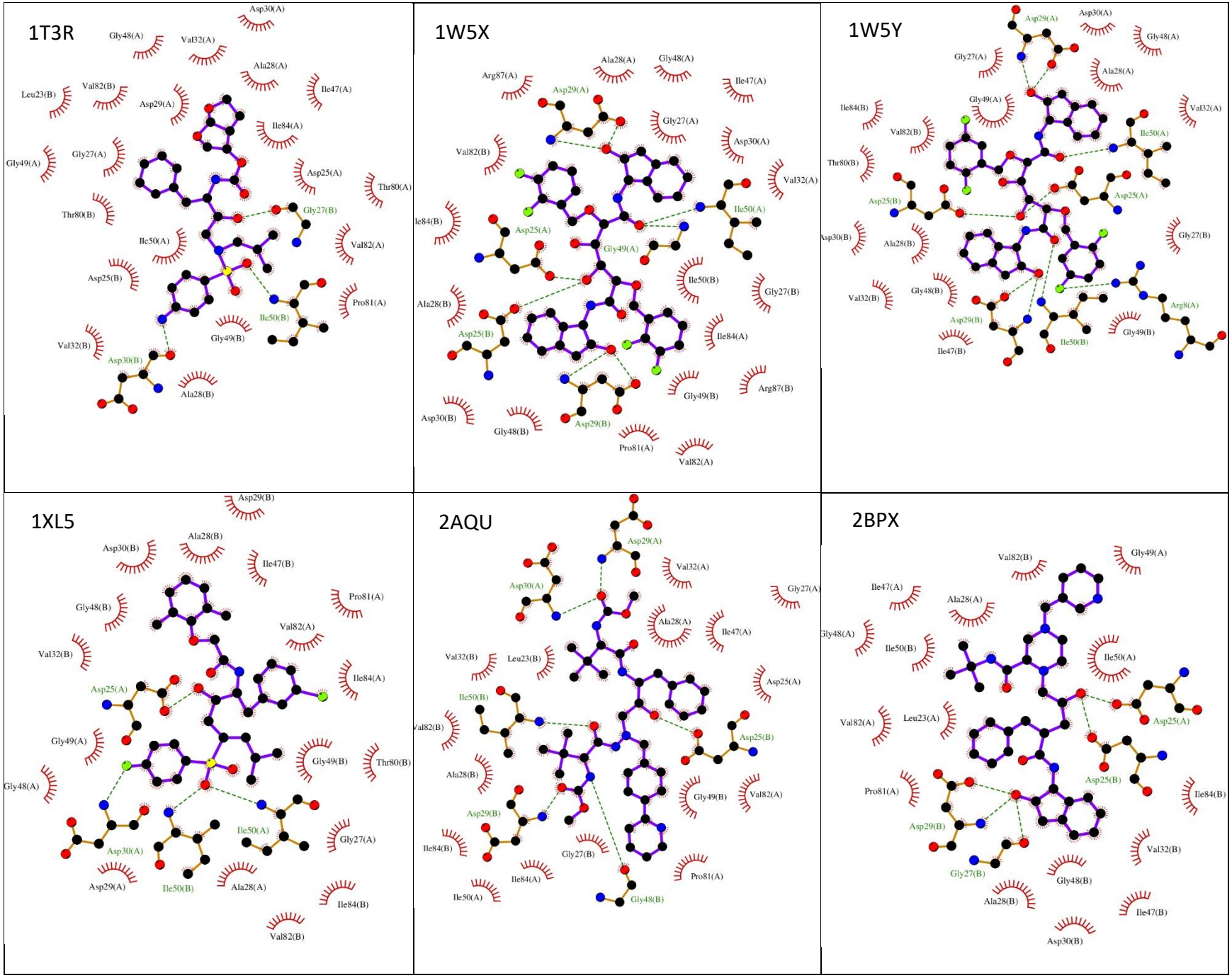
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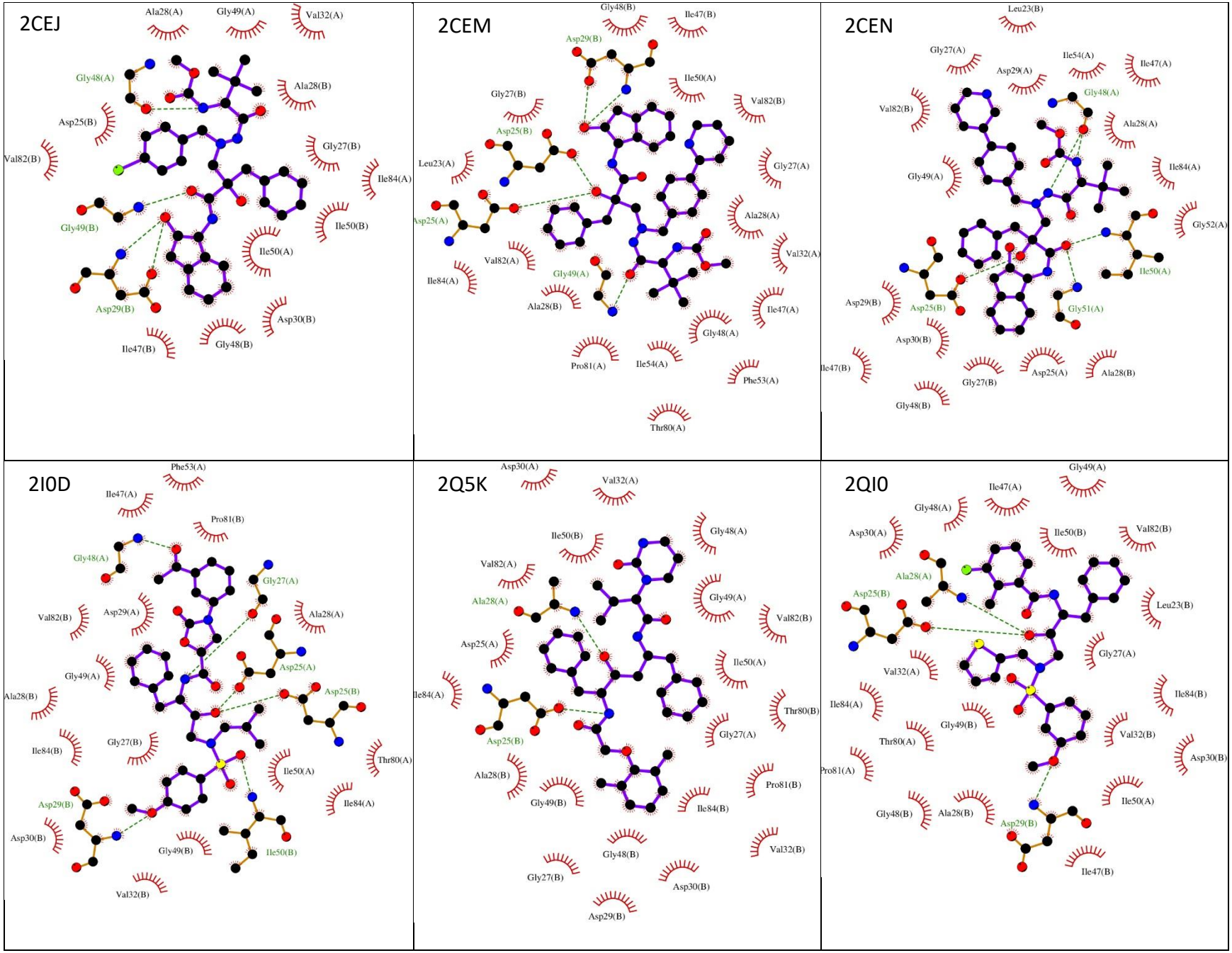
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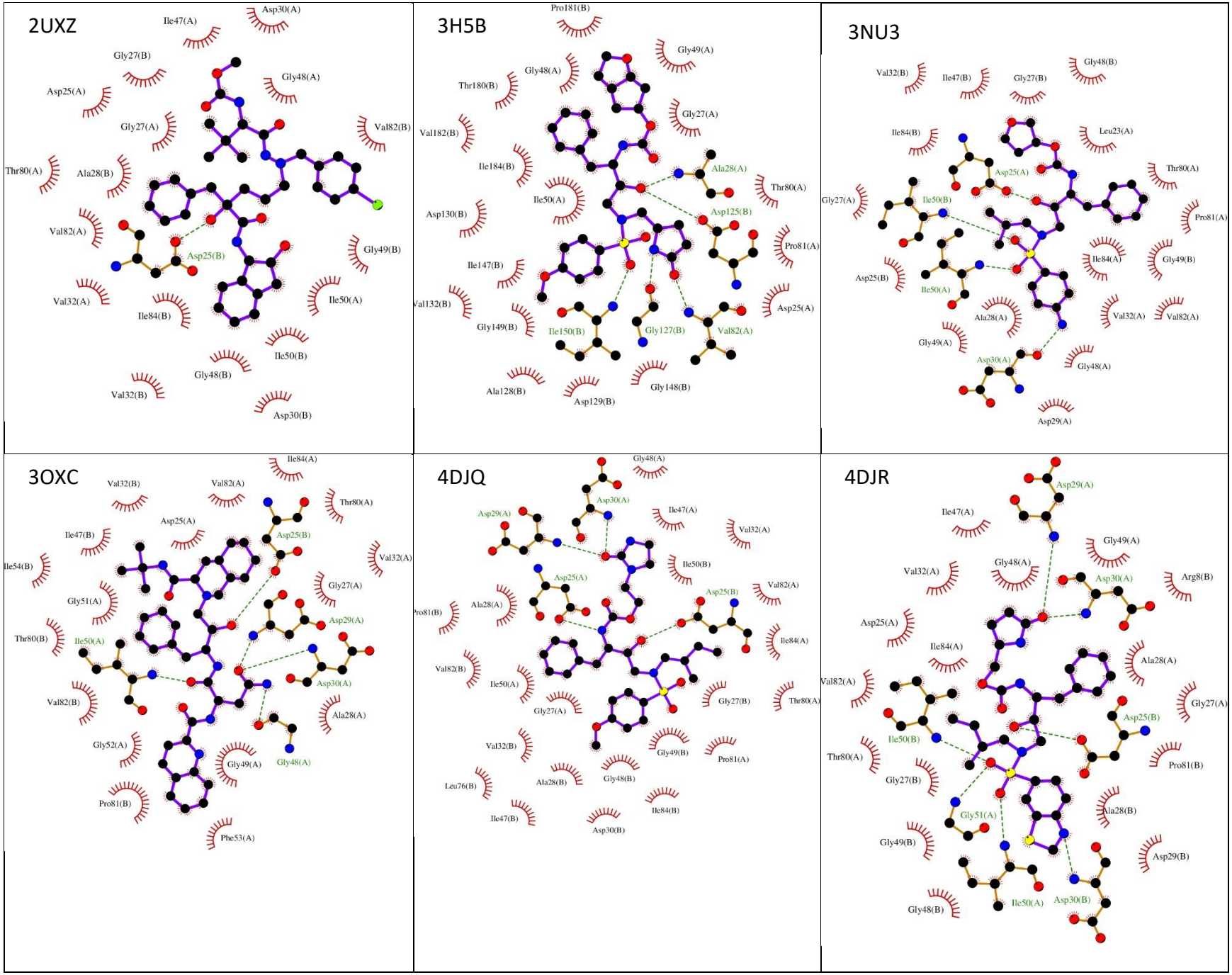
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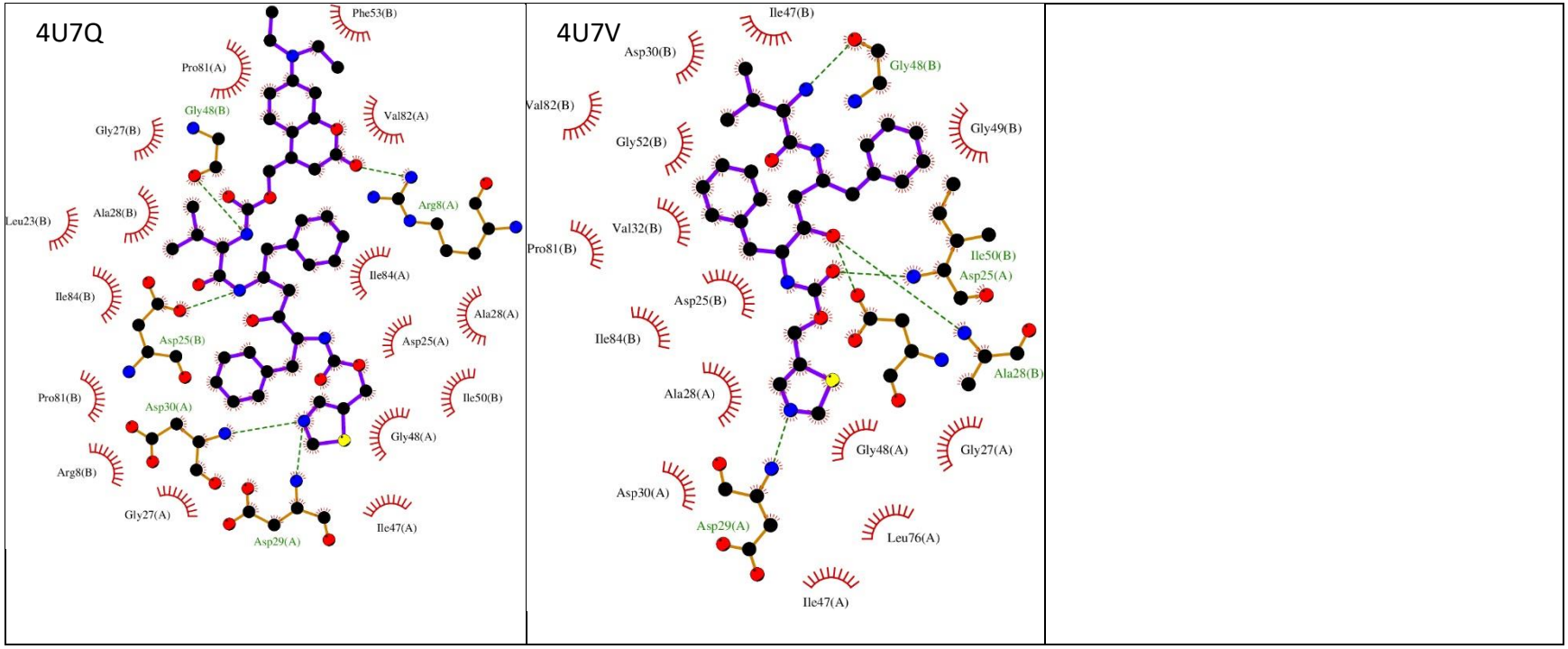

Reference

1. R. A. Laskowski and M. B. Swindells, *J. Chem. Inf. Model.*, 2011, **51**, 2778-2786.