Supplementary material

Free-energy calculations on potential A_3 adenosine receptors inhibitors

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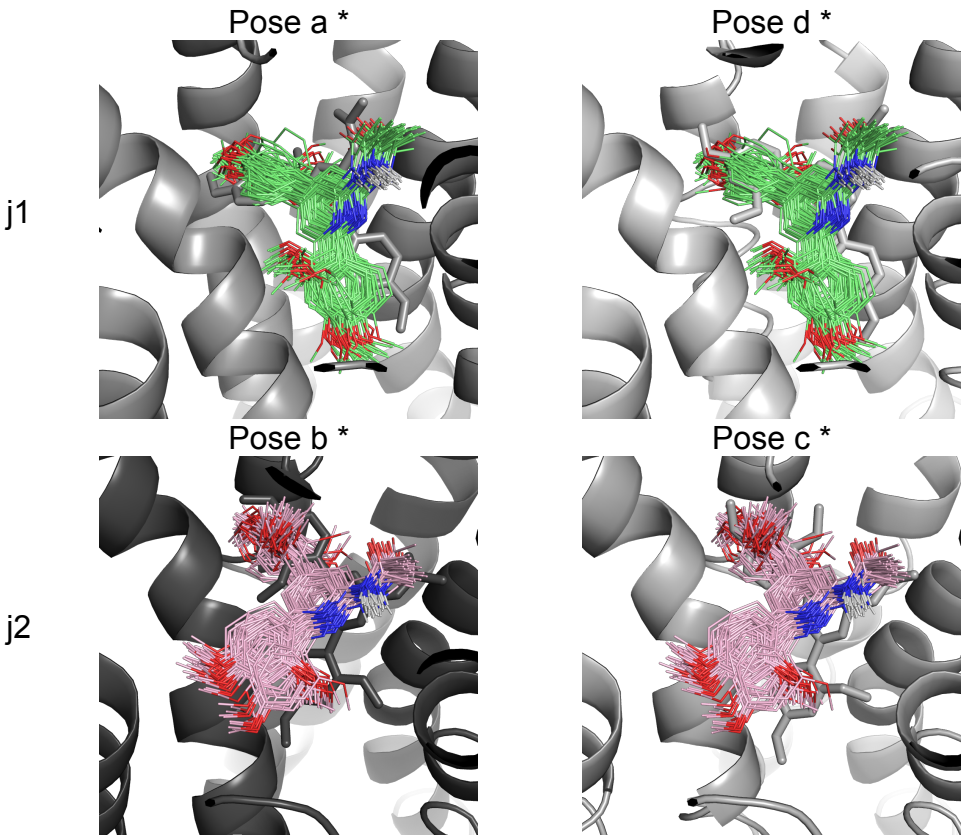

Figure S1: Overlay of trajectory snapshots of 2j1>3j1 and 2j2>3j2 with ligand in lines with poses from Azuaje et al. in grey sticks.

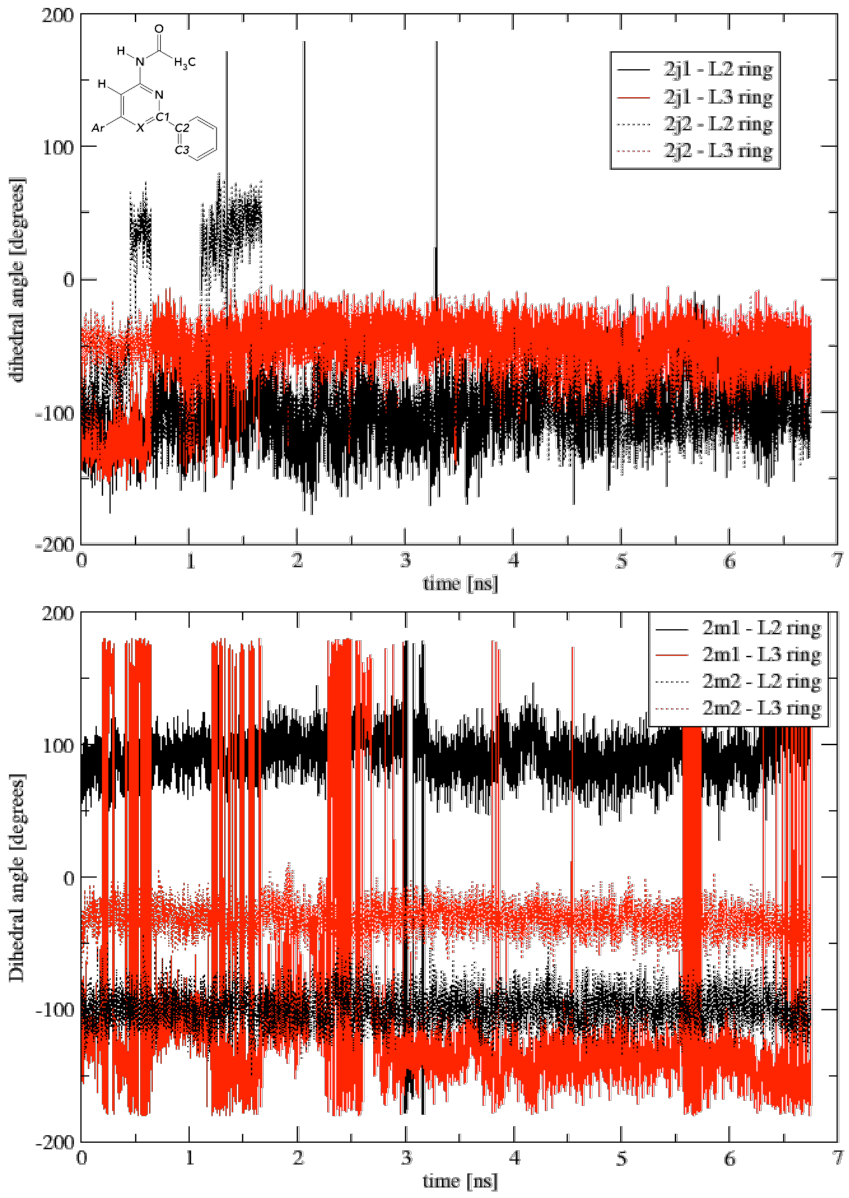

Figure S2: Time series of dihedral angles between X-C1-C2-C3 on both L2 and L3 rings for **m** and **j** compounds in starting poses 1 and 2.