

SUPPORTING INFORMATION

for

Why a diaminopyrrolic tripodal receptor binds mannosides in acetonitrile but not in water?

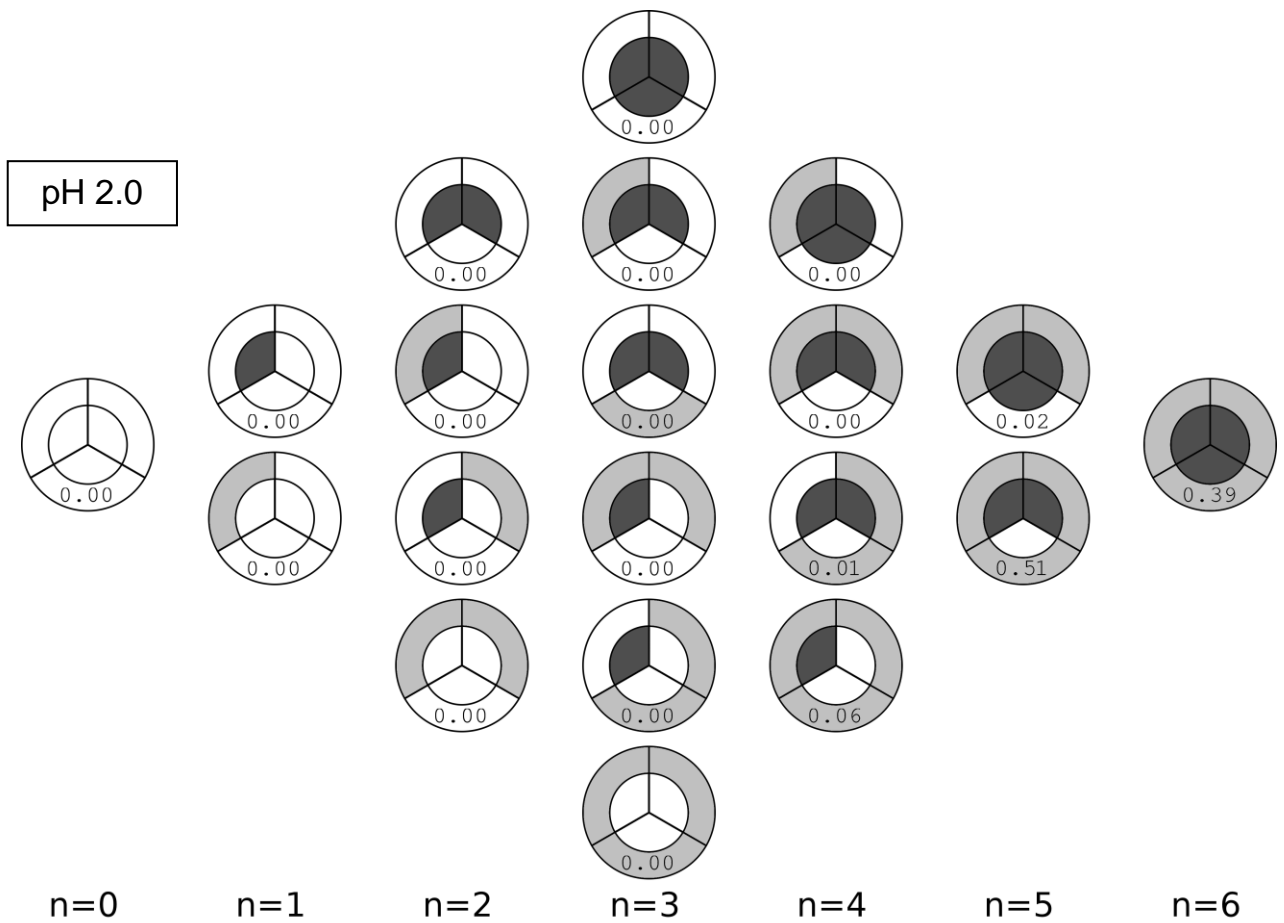
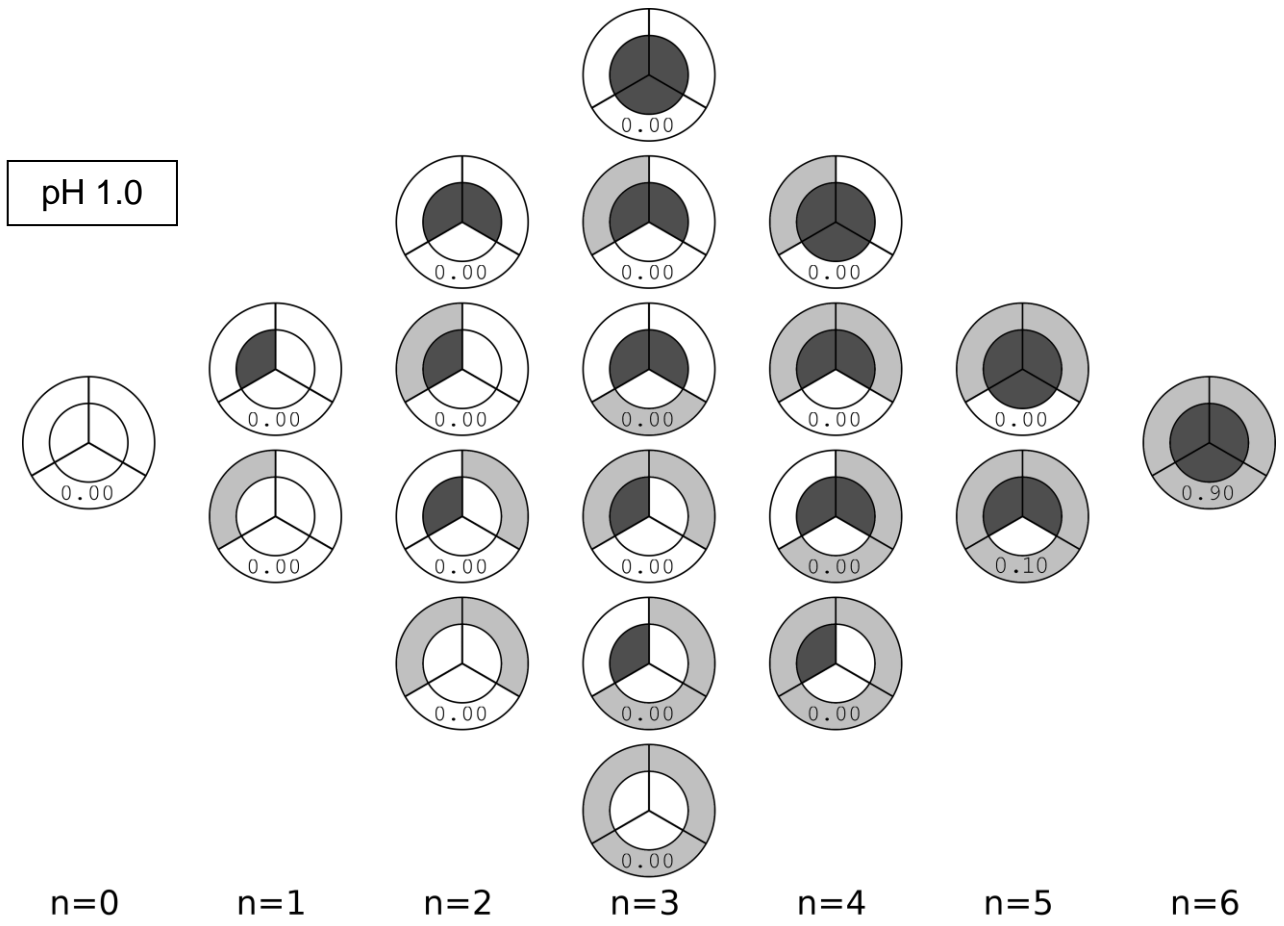
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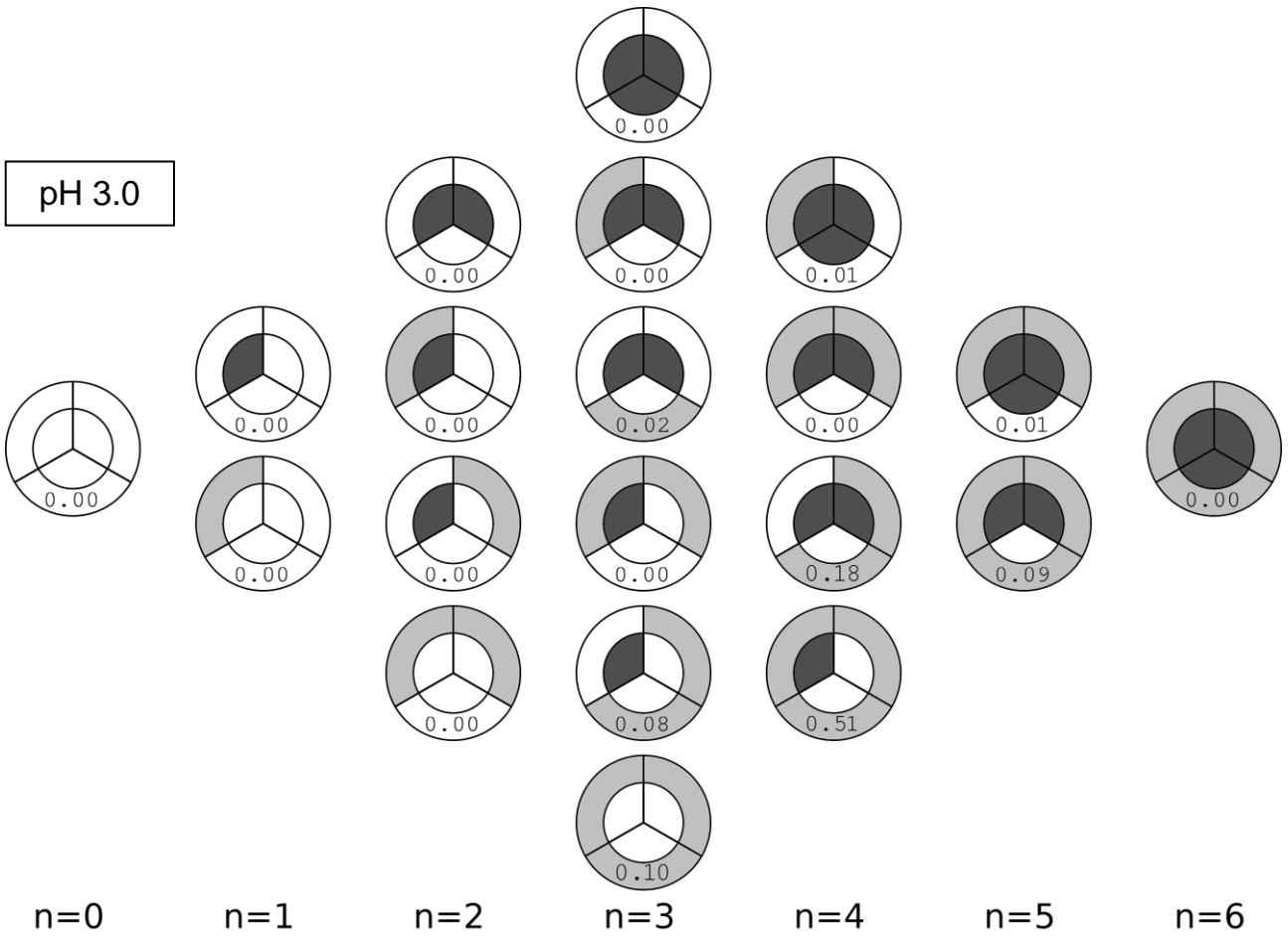
Email: Miguel Machuqueiro* - machuque@fc.ul.pt

*Corresponding author

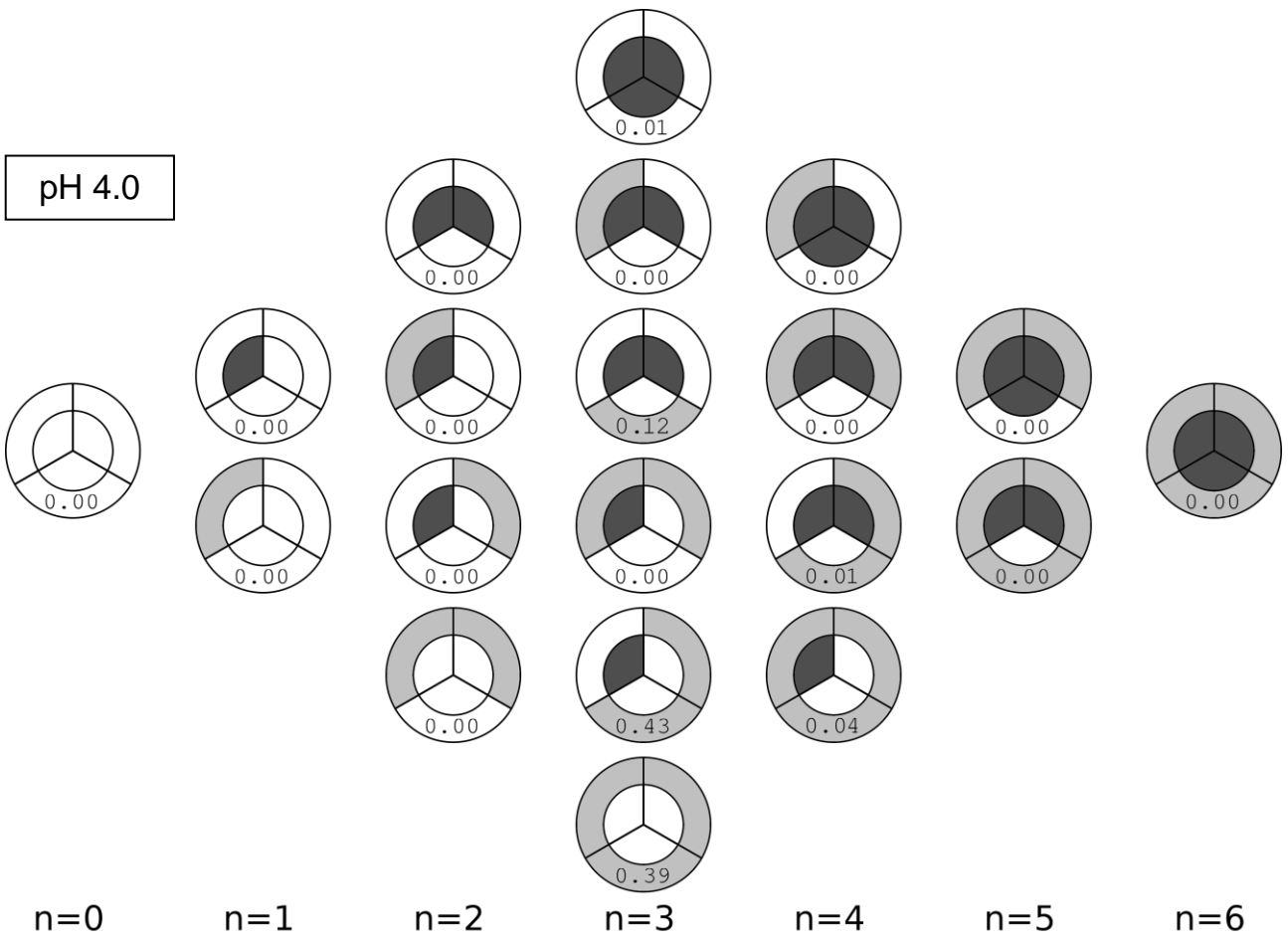
Diagrams representing the population of all microstates at all simulated pH values



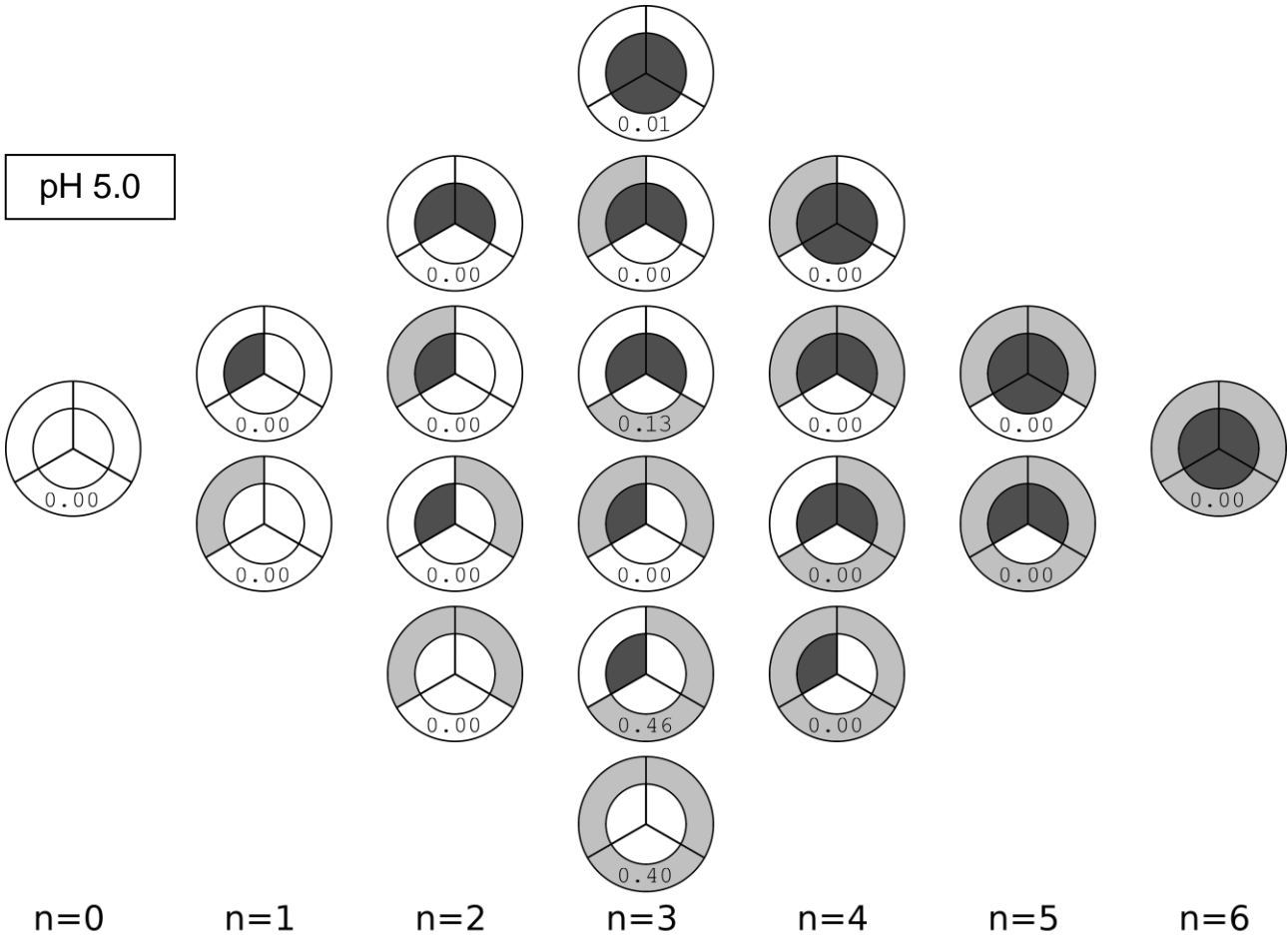
pH 3.0



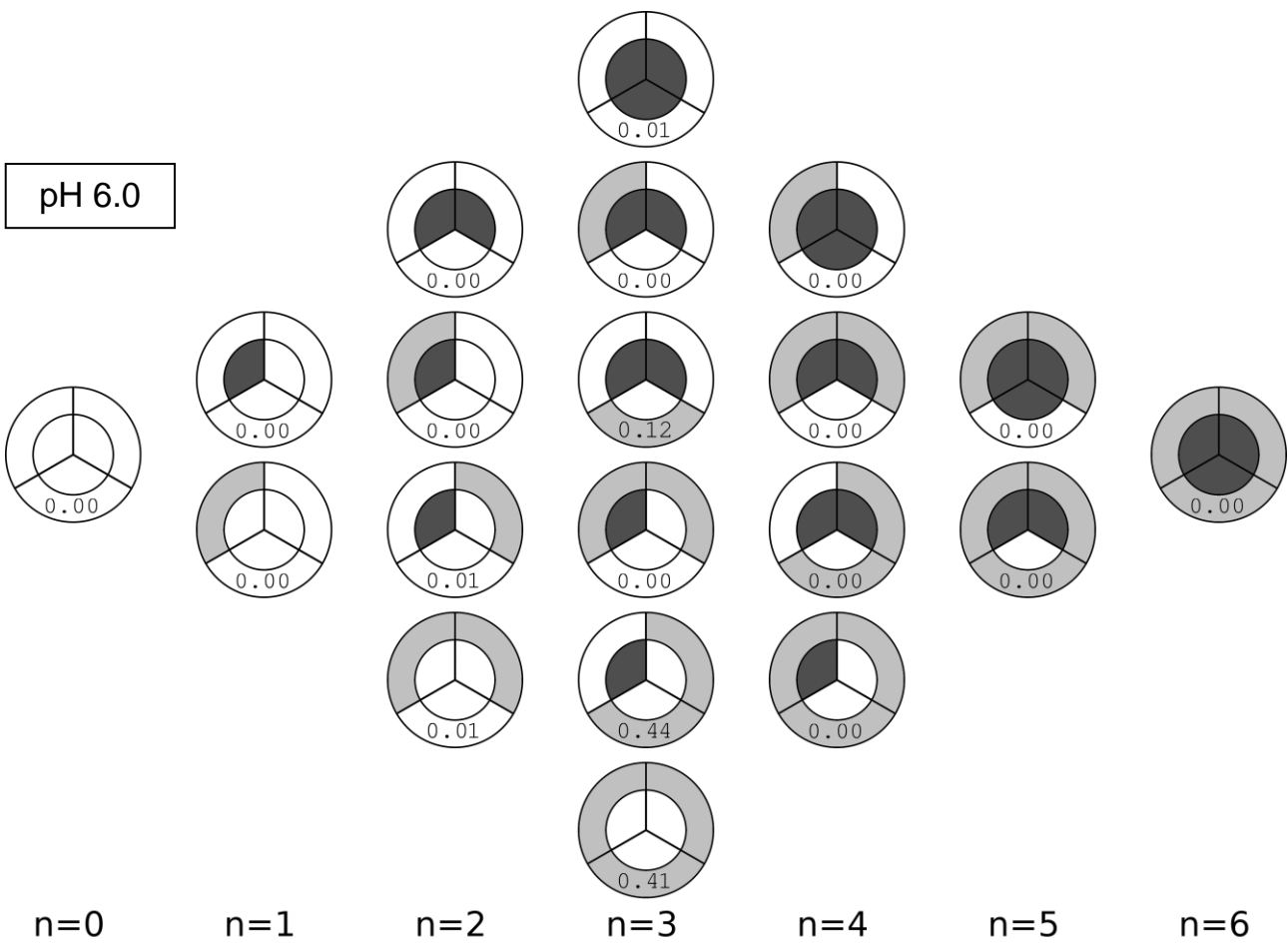
pH 4.0



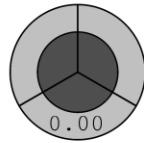
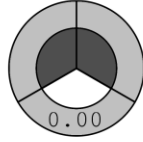
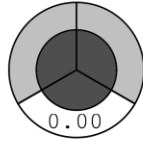
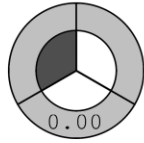
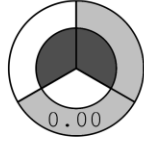
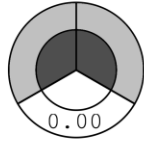
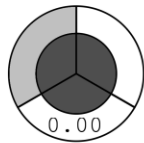
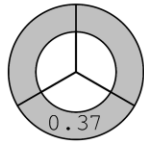
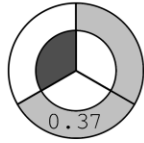
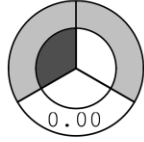
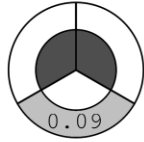
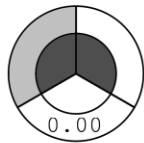
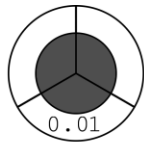
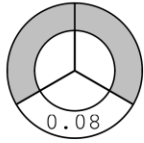
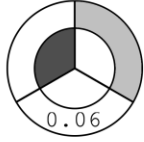
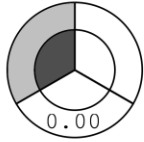
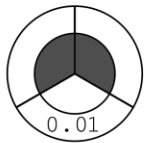
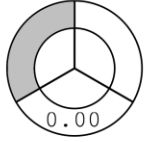
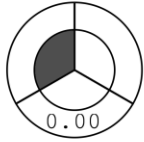
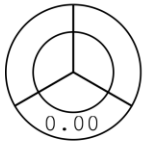
pH 5.0



pH 6.0



pH 7.0



n=0

n=1

n=2

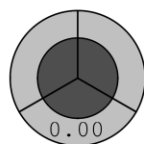
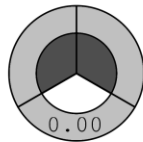
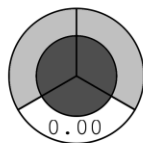
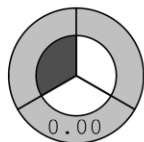
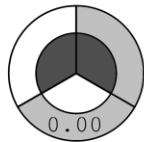
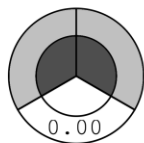
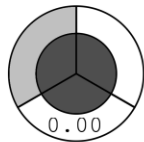
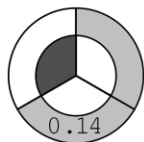
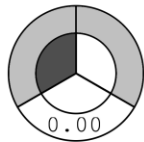
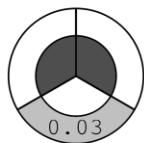
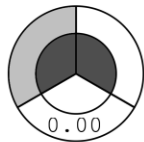
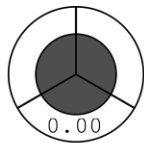
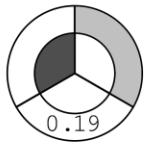
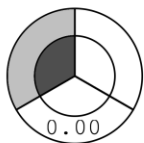
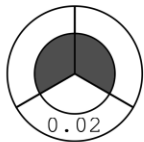
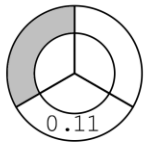
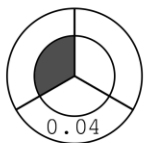
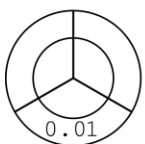
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n=4

n=5

n=6

pH 8.0



n=0

n=1

n=2

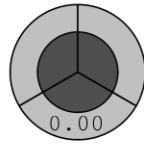
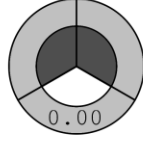
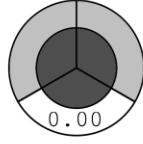
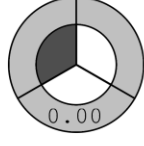
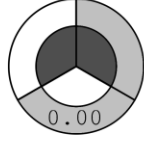
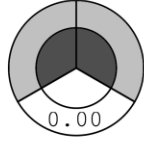
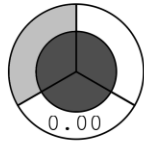
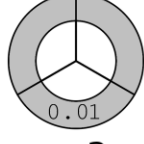
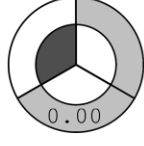
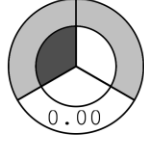
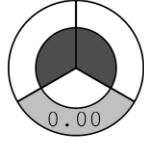
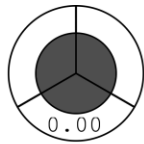
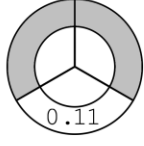
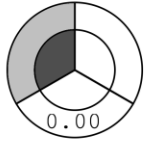
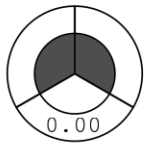
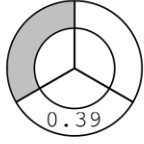
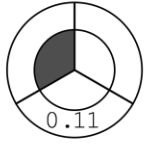
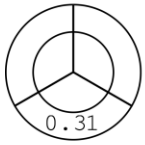
n=3

n=4

n=5

n=6

pH 9.0



n=0

n=1

n=2

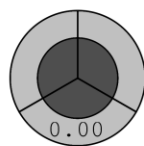
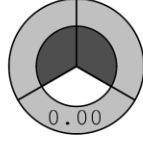
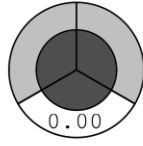
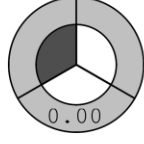
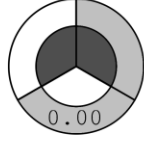
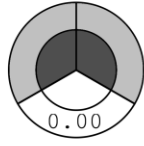
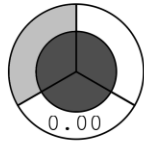
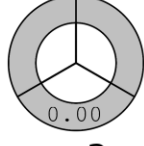
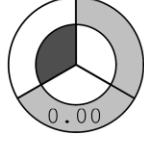
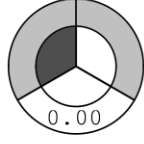
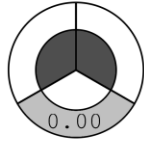
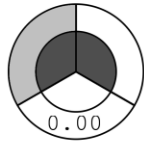
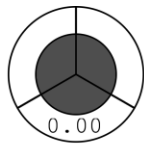
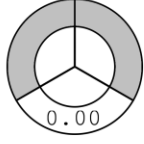
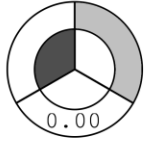
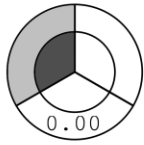
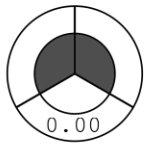
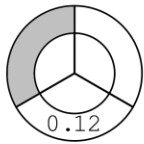
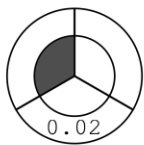
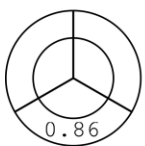
n=3

n=4

n=5

n=6

pH 10.0



n=0

n=1

n=2

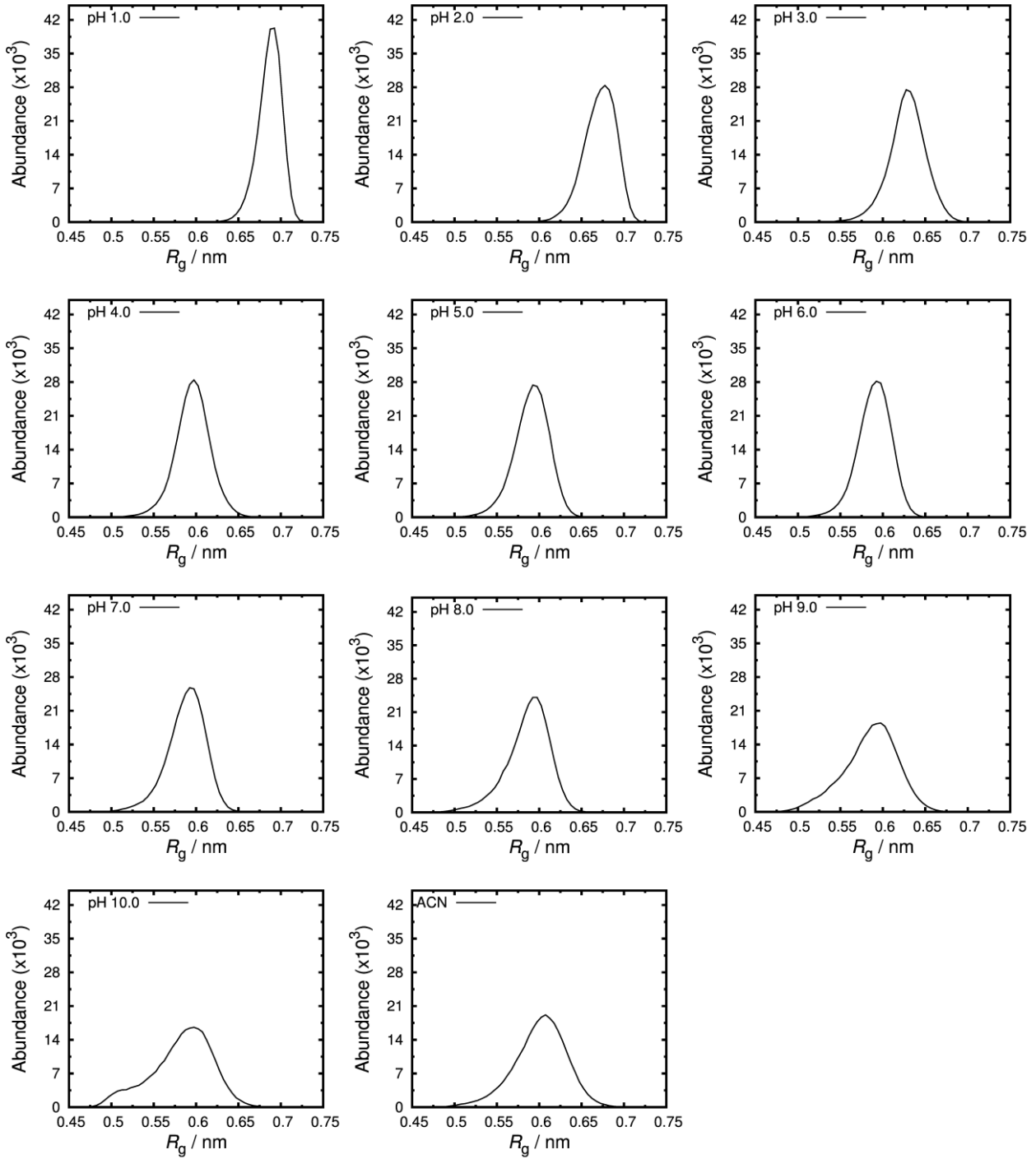
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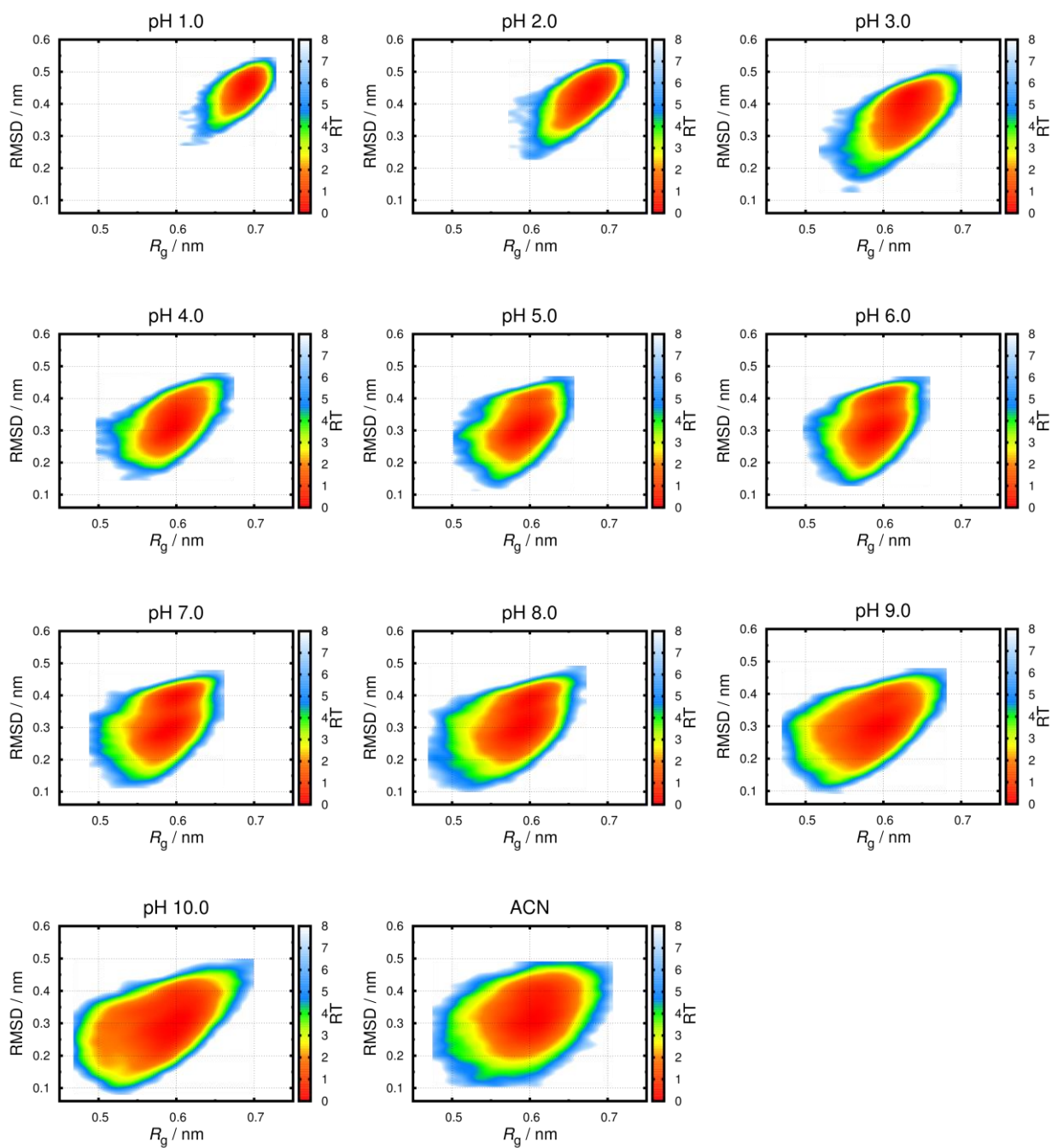
n=5

n=6

Radius of gyration (R_g) histograms for the receptor at all simulated pH values and acetonitrile (ACN)



Free energy profiles for the receptor at all simulated pH values and ACN using RMSD and R_g as structural coordinates



Schematic representation of the position of the arms of the receptor. Position of nitrogen atoms of the pyrrolic rings relative to the phenyl ring in 900 conformations at all simulated pH values and ACN.

