

# Supplementary Information to the manuscript: Inclusion complexes of the macrocycle nonactin with benchmark protonated amines: aniline and serine

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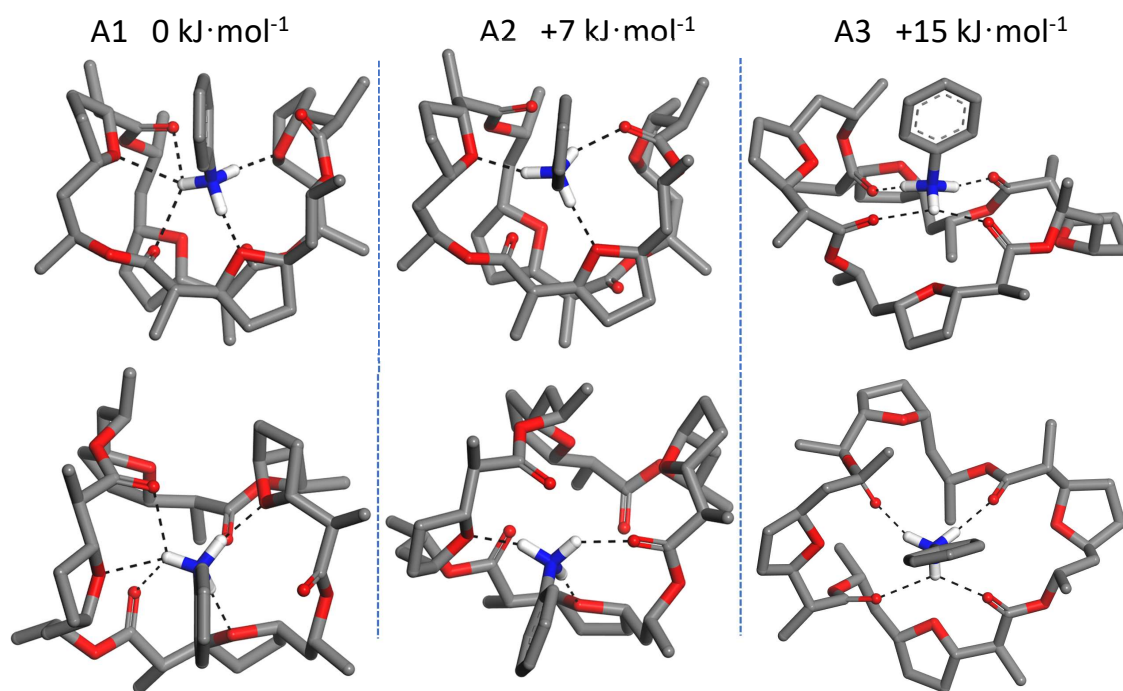


FIG. 1: Low-energy conformations found in this work for the Non-AniH<sup>+</sup> complex (side and top views). The H atoms of the nonactin macrocycle and of the phenyl side group of aniline are not shown for a better visualization of the host–guest coordination arrangement. Relative zero-point corrected electronic energies are provided for the conformers at the M06-2X/6-311++G(2df,2pd) level.

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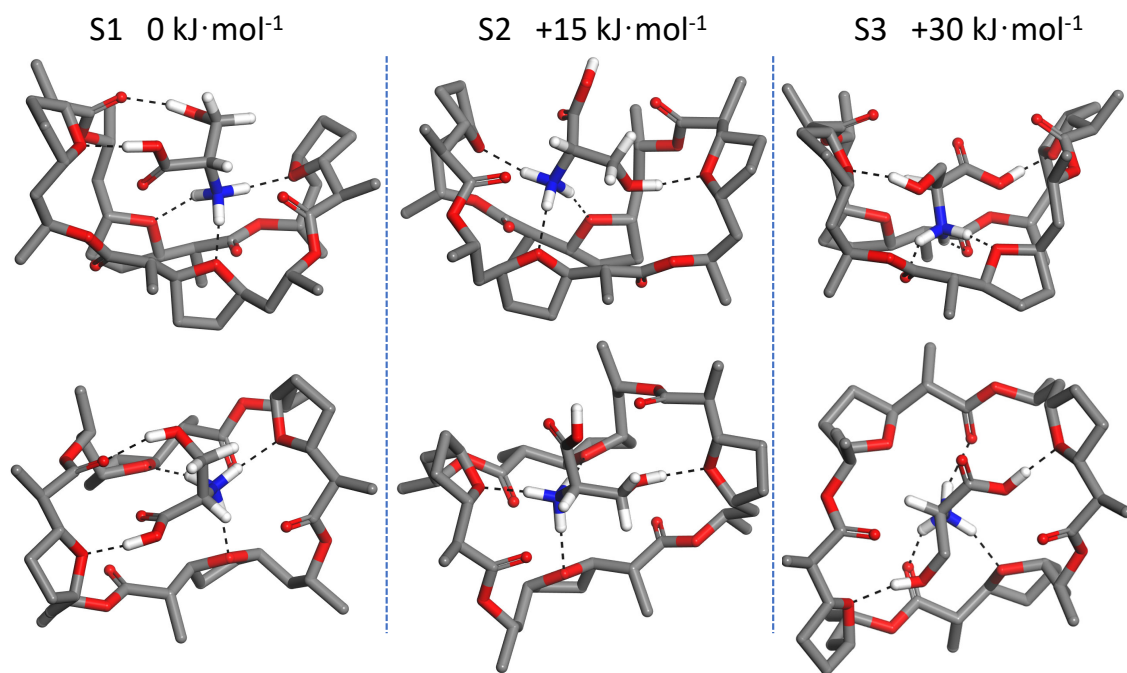


FIG. 2: Low-energy conformations found in this work for the Non-SerH<sup>+</sup> complex (side and top views). The H atoms of the nonactin macrocycle and of the phenyl side group of aniline are not shown for a better visualization of the host-guest coordination arrangement. Relative zero-point corrected electronic energies are provided for the conformers at the M06-2X/6-311++G(2df,2pd) level.