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Electronic Supplementary Information for

Inclusion complexes of propiconazole nitrate with substituted β-cyclodextrins. Synthesis, *in silico* and *in vitro* assessment of antifungal properties.

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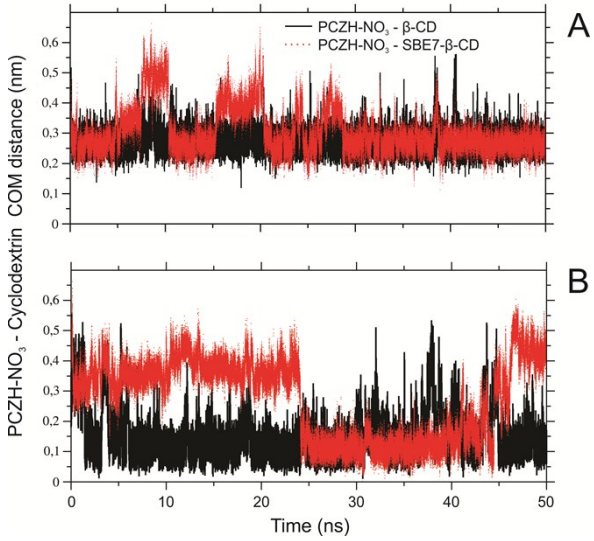
Computational studies

SI 1: PCZH-NO_3 – sugar ring center of mass (COM) distances plotted over the simulation time for the two analyzed modes of inclusion: with **[A]** the propyl group and **[B]** the dichlorophenyl group, respectively, inserted in the cyclodextrins central cavity. Graphs show no dissociation events, with COM distances below 0.7 nm in all cases. Higher fluctuations can be observed for SBE7-β-CD/PCZH-NO_3 complexes due to the higher flexibility of these assemblies.



SI 2: Molecular dynamics snapshots of the PCZH-NO_3 complexes for the two analyzed modes of inclusion. The first column represents ensembles of six equally time distributed conformations, fitted with respect of the sugar ring residues. The last column shows only the sugar ring residues ensembles. Higher flexibility can be observed for SBE7-β-CD/PCZH-NO_3 complexes. The fluctuations of the sugar ring conformations are higher for SBE7-β-CD/PCZH-NO_3 than for β-CD/PCZH- NO_3 inclusion compounds.