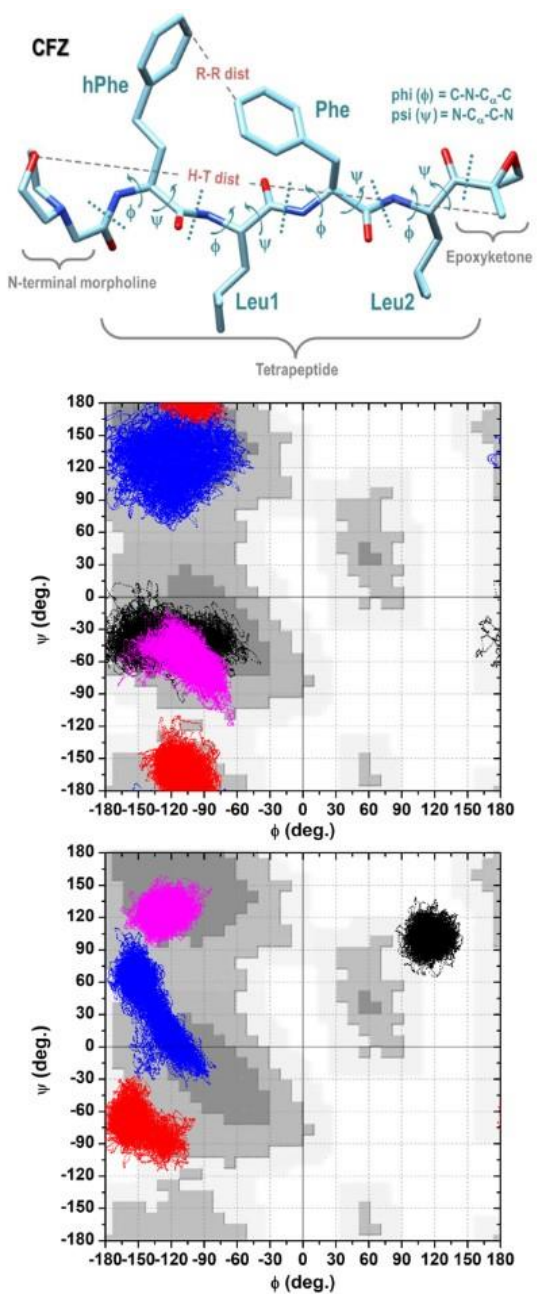
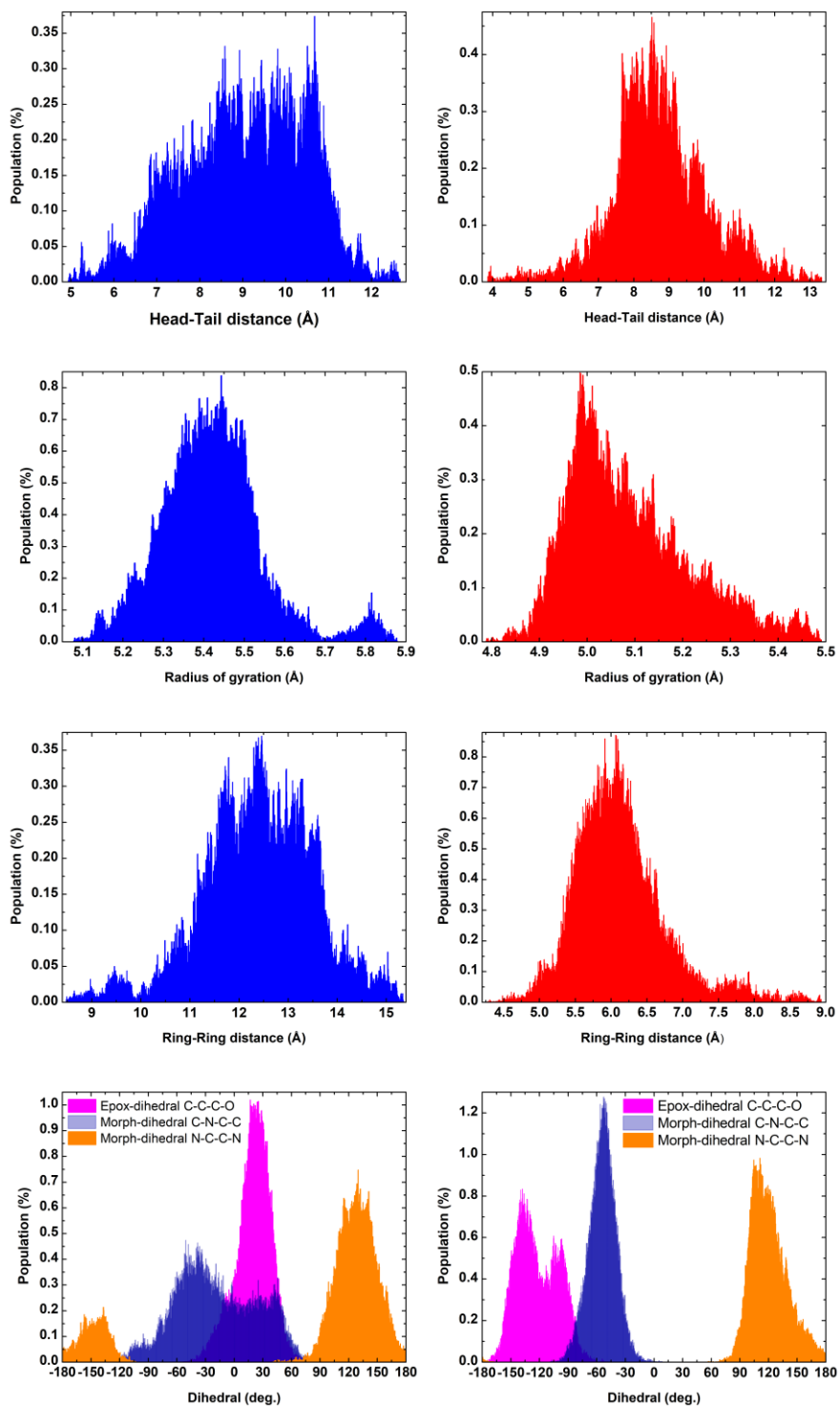


## Stability and potential degradation of the $\alpha',\beta'$ -Epoxyketone pharmacophore on ZnO nanocarriers: insights from reactive molecular dynamics and density functional theory calculations

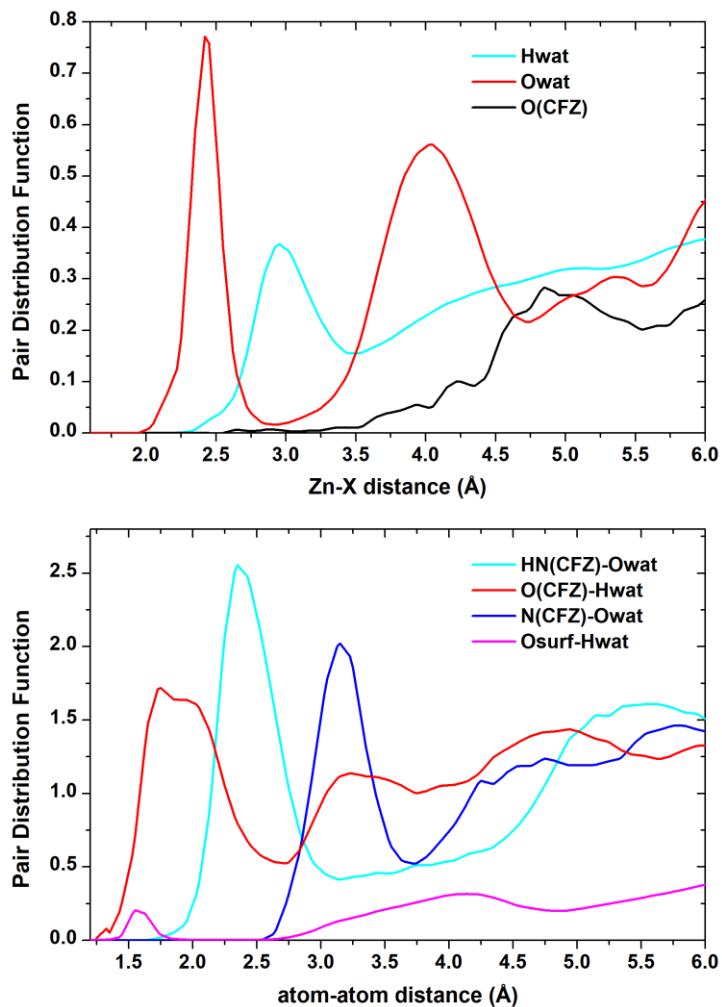
Cheherazade Trouki, Susanna Monti and Giovanni Barcaro



**Figure S1.** Ramachandran plots of the backbone torsional angles of the tetrapeptide CFZ adsorbed on the (0001)Zn-terminated (top) and (1010) (bottom) surfaces. Each aminoacid is identified by a color: Phe = red; Leu1 = magenta; hPhe = black; Leu2 = blue..



**Figure S2** Distributions of various geometrical descriptors of the last 50000 CFZ conformations sampled during the production RMD on the (0001)Zn-terminated (right) and (1010) (left) surfaces.



**Figure S3** Pair distribution functions obtained from the last 50000 configurations of the RMD simulations in water solution on the (0001)Zn-terminated surface.