

## Microsymposium

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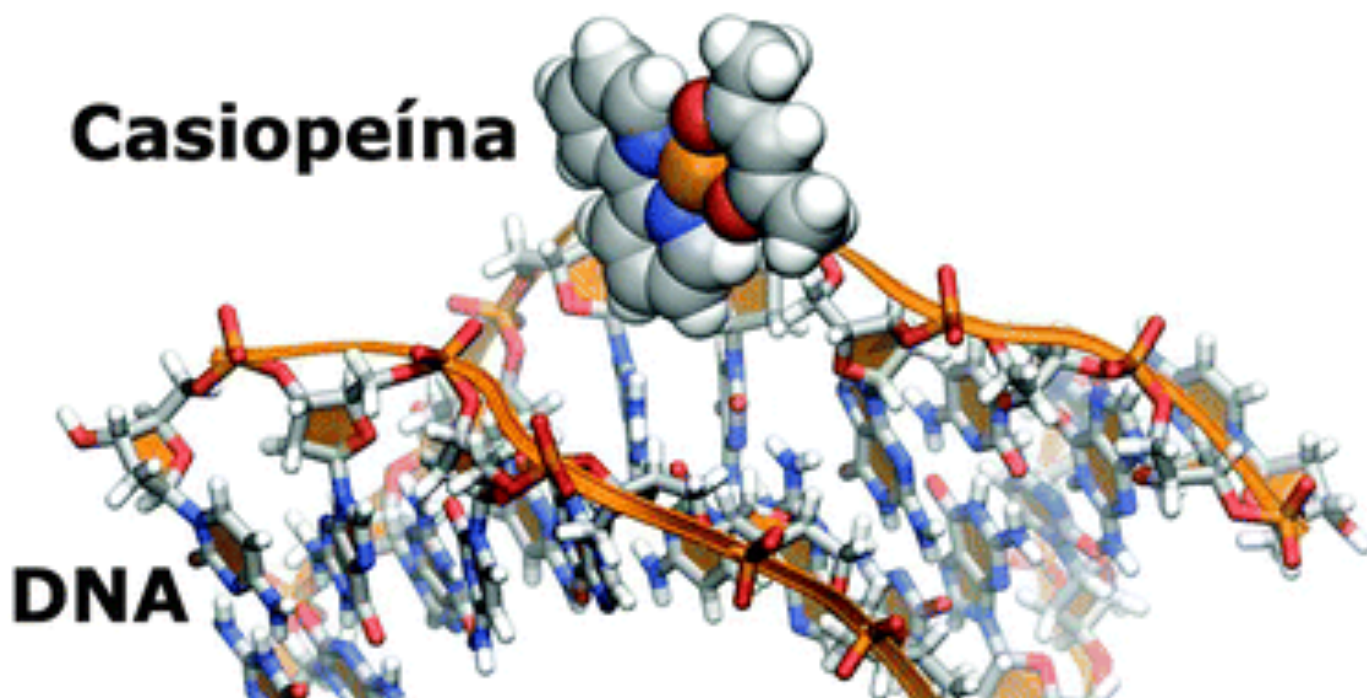
### *Intercalation process of anticancer copper (II) complexes in DNA*

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Ternary Copper (II) Complexes (TCC) have shown cytotoxic, genotoxic, and antineoplastic activity in vitro and in vivo. There are evidences that these compounds interact directly with DNA but it is not clear how deep TCC penetrates into the DNA double helix and their specific interactions have not been established. Recently, our group found that the deoxyribose-phosphate group is the specific recognition site of TCC in DNA. Here we report a crystallographic and theoretical study to determine each step of intercalation process of TCC in DNA with the recognition site as starting point. On the basis of crystal structures, Molecular Dynamics, DFT calculations and Electron Density Analysis we found that the family of analyzed TCC prefers the sequence Thymine-Adenine-Thymine to start the insertion. The intercalation process consists of an opening of a base pair as the complex intercalates within a succession of axial ligand exchange. The copper center migrates from phosphate to ribose then to thymine and finally to adenine. It is possible that the biological activity of TCC is related to its capability to evert base pairs and perform the necessary migrations from the recognition site to the complete intercalation

[1] Galindo-Murillo, Rodrigo; Ruiz, Lena; Moreno-Esparza, Rafael; Cortes-Guzman, Fernando. *Phys. Chem. Chem. Phys.*, 2012, 14, 15539-15546, [2] Galindo-Murillo R., Hernandez-Lima J., González-Rendón M., Cortés-Guzmán F., Ruiz-Azuara L., Moreno-Esparza R. *Phys. Chem. Chem. Phys.* 2011, 13 (32), 14510 – 14515, [3] Juan Carlos García-Ramos, Araceli Tovar-Tovar, Joseelyne Hernández-Lima, Fernando Cortés-Guzmán, Rafael Moreno-Esparza, Lena Ruiz-Azuara. *Polyhedron* 2011, 30, 2697-2703



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