Chemical activity of anticancer compounds : computational studies on the mechanism of bleomycin and the recognition of flavonoids

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Propositions

Belonging to the thesis entitled:
"Chemical Activity of Anticancer Compounds:
Computational studies on the mechanism of bleomycin
and the recognition of flavonoids"

1. The first step in the bleomycin activity is the homolytic cleavage of the O-O bond.
   Chapter 5 and 6 of this thesis
2. The selectivity of the activated bleomycin action depends directly on the formed hydrogen bond facilitating the homolytic O-O bond cleavage.
   Chapter 5 and 6 of this thesis
3. It is proposed that degradation of the double stranded DNA by activated bleomycin is due to the formation of the BLM-Fe(IV)=O complex.
   Chapter 6 of this thesis
4. Quantum mechanical calculations are complementary to other tools used in the "pipeline" of the drug discovery process and play there an increasingly important role.
   This thesis
5. The multi-scale metadynamics represents a computational solution to the protein folding problem.
6. The real goal of university education is the development of personalities who will be unique in their thinking and action.
   Compare with R. R. Ernst "The responsibility of scientists, a European view" Angew. Chem. Int. Ed. ***42*** *(2003) 4434-4439*
7. In our highly specialized world a scientific development of the researcher requires interdisciplinary knowledge and efficient communication between open-mind researchers.
8. To be a mother helps to be a good scientist but not the other way around.
9. A PhD project is like exploring the landscape of a free energy surface. It is not trivial to find an optimal pathway.