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- **P29** MILESI, Pietro — Development of MEK and AURKA drug inhibitors delivery systems for the treatment of metastatic melanoma tumour
- **P30** NADDEO, Simone — Multifunctional uses of furan derivatives: from fine chemicals to bio-based materials
- **P31** GUAITA, Lorenzo — Macrostructure control of bio-derived elastomeric polyesters
- **P32** DISPENZA, Clelia — Novel functional biomaterials from egg white protein irradiation
- **P33** MELCHIOR, Andrea — Adsorption of Cisplatin and Its Derivatives on Graphene
- **P34** PIROZZI, Pasqualina — Intermolecular interactions between quercetin and amorphous SiO_2 surface for drug delivery in biomedical applications
- **P35** ARONNE, Antonio — In Situ Modification of Hybrid Silica-Epoxy Flame Retardant Nanocomposites by Phosphorus via a Green Hydrolytic Sol-Gel Route
- **P36** FONTANA, Francesca — Azahelicenes as inherently chiral selectors for electrochemical enantiodiscrimination of biomolecules
- **P37** BERTOLOTTI, Benedetta — Preparation and characterization of a new hybrid heterohelicene
- **P38** GUIDOTTI, Giulia — Ad-hoc designed aliphatic random copolymers for cardiac differentiation of pluripotent stem cells
- **P39** TERRANEO, Giancarlo — Halogen-bonded Metal -Organic Frameworks
- **P40** ZAMBITO MARSALA, Massimo — Bionanocomposites based on a covalent network of chitosan and edge functionalized graphene layers
- **P41** CECCATO, Riccardo — Low temperature synthesis of bismuth-halogen perovskites for photoelectrochemical applications
- **P42** NATALI SORA, Isabella — X-Ray diffraction analysis of historic mortars of the Bergamo Walls
- **P43** DICHIARANTE, Valentina — Co-Crystal Strategy for Tuning the Properties of Amino Acid-based Hydrogels
- **P44** DI PIETRO, Maria Enrica — A deep dive into structure and dynamics of hydrophobic eutectics and eutectogels

Intermolecular interactions between quercetin and amorphous SiO_2 surface for drug delivery in biomedical applications

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The new generation of biomaterials able to incorporate drugs for in situ release after implantation is important in many pharmaceutical and biomedical applications. Several drugs show problems of diffusion through biological barriers [1] and the control of local administration is crucial to avoid cytotoxic effects.
Molecular Mechanics (MM) and Molecular Dynamics (MD) simulations are a useful tool to investigate drug and biomaterial surface interactions at atomistic level [2,3]. In this work the interaction between quercetin molecule, a flavonoid drug studied for its antioxidant and anticancer properties, and the amorphous SiO_2 surface terminated with silanol groups is studied using a simulation protocol proposed in previous work [3]. This protocol provides *i*) the initial energy minimization, *ii*) MD runs until the equilibrium state was achieved *iii*) final geometry optimizations of the final configuration assumed by the system at the end of MD run. These simulations are performed using the Consistent Valence Force Field (CVFF) [4] and Materials Studio packages [5]. At first the conformational study of quercetin single molecule was performed. The optimized geometry after MM and MD simulations lasting 2 ns at room temperature is reported in Figure 1.

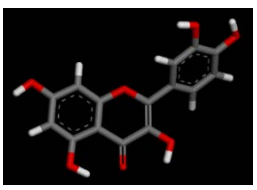

Figure 1. Optimized geometry of quercetin molecule after MD run. Color code: carbon atoms are in grey, oxygens in red, hydrogen atoms in white.

Afterwards, the adsorption process of quercetin molecule on the amorphous SiO_2 surface was studied starting from four different initial arrangements near the solid

surface in a simulation box of size equal to (85.53 × 85.53 × 250.0) Å considering the periodic boundary conditions. After the energy minimization of four different initial geometries and then four MD simulations at room temperature lasting 1 ns, quercetin molecules display favorable intermolecular interactions in the adsorption process during MD run due to H-bonds between drug and SiO_2 surface. These intermolecular interactions are weak. During the MD run, the adsorption and desorption process takes place, as reported in Figure 2, where the distance of the center of mass (c.o.m.) of the quercetin molecule and the best-fit plane of the SiO_2 surface, always fixed during MD run, is reported.

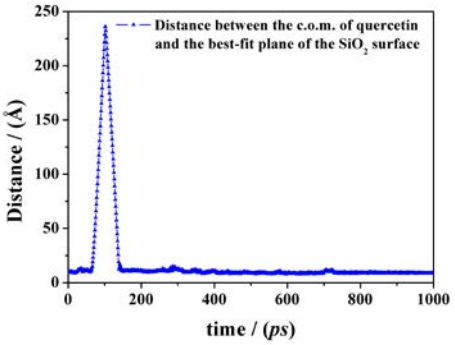

Figure 2. Distance between the c.o.m. of quercetin molecule and the best-fit plane of the silica surface calculated during a MD run lasting 1 ns.

The H-bonds between quercetin drug molecule and silica surface stabilize the adhesion on this solid surface. The H-bonds between the C–O and –OH quercetin groups with the hydroxyl groups and oxygen atoms exposed by silica surface stabilize the interactions drug-biomaterial, as in an optimized geometry after MD run reported in Figure 3 (see dashed blue lines). These preliminary theoretical results and the ongoing study at higher drug concentration will be compared to the experimental data from Fourier-Transform Infrared Spectroscopy (FT-IR) of quercetin molecules entrapped in a silica matrix obtained via the Sol-Gel methods studied by M. Catauro *et al*. [6].

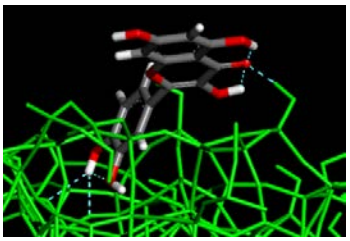

Figure 3. Optimized geometry of quercetin drug adsorbed on the amorphous SiO_2 surface terminated with silanol groups. Color code is the same of Figure 1, all silica surface atoms are in green for clarity. The H-bonds are in dashed blue lines.

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