Manthos G. Papadopoulos

Title: Research Director
Institute of Biology, Pharmaceutical Chemistry and Biotechnology
Phone: +30210-7273892
Fax: +30210-7273831
E-mail: mpapad@eie.gr
Website: http://www.eie.gr/nhrf/institutes/iopc/cvs/cv-papadopoulos-gr.html

Education and qualifications

B. Sc in Chemistry, University of Patras, Greece (1971).
Ph. D in Theoretical Chemistry, University of Essex, U.K. (1976). The title of the thesis is: "Theoretical studies of NMR chemical shifts, susceptibilities and polarisabilities". The Ph. D work has been completed in three years (1972-1975), the first two of which were spent in Essex under the supervision of Dr R. Jones and the last in Cambridge under the guidance of Professor A. D. Buckingham.

Appointments

(a) A Postdoctoral fellowship was granted by the Science and Engineering Research Council, University of Bristol (1975-1977).
(b) Researcher at the National Hellenic Research Foundation since 1979.

Professional activities

(a) Development and application of methods for the computation of the linear and nonlinear optical properties of molecules, solids and liquids. Techniques for the calculation of the correlation, vibrational and relativistic contributions have been developed and applied.
(b) Design of novel photonic materials.
(c) Application of methods for the interaction between proteins and relatively small molecules (e.g. drugs).
(d) Analysis of the binding mechanisms of selected inhibitors.
(e) Discovery of drugs for a series of diseases (e.g. AIDS, hypertension).
(f) Toxicity studies of nanoparticles.

Recent highlights

The effect of the mutation I50V on the activity of 4 drugs for HIV-1PR. The emergence of HIV-1 drug-resistant mutations is the major problem against AIDS treatment. We employed molecular dynamics (MD) calculations and free energy (MM−PBSA and thermodynamic integration) analyses on wild-type and mutated HIV-1 protease (HIV-1 PR) complexes with darunavir, amprenavir, indinavir, and

saquinavir to clarify the mechanism of resistance due to the I50V flap mutation [155].

Analysis of the effect of 7 single mutatuions on the binding of saquinavir with HIV-1 PR. We examined L10I, G48V, L63P, A71V, G73S, V82A, and I84V single mutant HIV-1 PR strains in complexes with saquinavir to elucidate drug−protease interactions and dynamics. A comparative analysis of these mutations at the molecular level leads to a deeper understanding of saquinavir resistance [154].

Discovery of the linkage between AIDS, hypertension and diabetes. Dual inhinitors of HIV-1 PR and renin. Human immunodeficiency virus type 1 protease (HIV-1 PR) and renin are primary targets toward AIDS and hypertension therapies, respectively. Molecular mechanics Poisson−Boltzmann surface area (MM−PBSA) free-energy calculations and inhibition assays for canagliflozin, an antidiabetic agent verified its effective binding to both proteins. Moreover, drugs aliskiren (a renin inhibitor) and darunavir (an HIV-1 PR inhibitor) showed high affinity for HIV-1 PR and renin, respectively. This study suggests that canagliflozin, aliskiren, and darunavir may induce profound effects toward dual HIV-1 PR and renin inhibition. Since patients on highly active antiretroviral therapy (HAART) have a high risk of developing hypertension and diabetes, aliskiren-based or canagliflozin-based drug design against HIV-1 PR may eliminate these side-effects and also facilitate AIDS therapy [143].

Analysis of the binding mechanism, with HIV-1 PR, of darunavir. We have selected the potent drug darunavir and a weak inhibitor (fullerene analog) as HIV-1 PR substrates to compare protease's conformational features upon binding. Molecular dynamics (MD), molecular mechanics Poisson−Boltzmann surface area (MM−PBSA), and quantum-mechanical (QM) calculations indicated the importance of the stability of HIV-1 PR flaps toward effective binding: a weak inhibitor may induce flexibility to the flaps, which convert between closed and semiopen states. A water molecule in the darunavir−HIV-1 PR complex bridged the two flap tips of the protease through hydrogen bonding (HB) interactions in a stable structure, a feature that was not observed for the fullerene−HIV-1 PR complex [142].

Several novel fullerene-based inhibitors for HIV-1 PR have been proposed. A series of novel fullerene-based inhibitors for HIV-1 protease (HIV-1 PR) has been proposed, by employing two strategies that can also be applied to the design of inhibitors for any other target. This study has been performed by employing a docking technique, two 3D-QSAR models, MD simulations and the MM–PBSA method [136].

The effect of noble gas atoms on the diradicaloid character and the nonlinear optical properties.The electronic ground state of H-Ng-Ng-F , Ng= Ar, Kr, Xe has been studied theoretically by employing the ab initio complete active space valence bond (CASVB) and multistate complete active space perturbation theory (MS-CASPT2) methods. Both levels of theory confirm the diradicaloid character (DC) of the HNg_2F ground state, increasing in the order Ar > Kr > Xe. The very significant effect of the first and, even more, the second Xe atom on the (hyper)polarizabilities has been shown and interpreted. Thus, the present results demonstrate a mechanism for producing very large (hyper)polarizabilities [126].

A novel fullerene inhibitor for HIV-1 PR has been proposed. A database has been derived from recently reported [60]fullerene derivatives, and their binding scores

with HIV-1 PR have been computed using docking techniques. Computational methods have been used to predict which derivatives may have high binding affinities, and for these compounds biological tests have been performed with purified PR. Experimental results confirm the high binding scores of fullerene derivatives predicted from the docking calculations. Our measurements showed that one of our fullerene derivatives has about three times better inhibitory binding than the most active fullerene-based inhibitor currently available [117].

Computation of the linear and nonlinear optical properties of a series of fullerene derivatives and analysis of their potential for photonic applications. Using a wide variety of quantum-chemical methods we have analyzed in detail the linear and non-linear optical properties of [60]fullerene-chromophore dyads of different electron-donor character. The dyads are composed of [60]fullerene covalently linked with 2,1,3-benzothiadiazole and carbazole derivatives. Linear scaling calculations of molecular (hyper)polarizabilities were performed using wave function theory as well as density functional theory (DFT). Within the former approach, we used both semiempirical (PM3) and *ab initio* (Hartree-Fock and second-order Møller-Plesset perturbation theory) methods. Within the latter approach only the recently proposed long-range schemes successfully avoid a large overshoot in the value obtained for the first hyperpolarizability. Calculations on model fullerene derivatives establish a connection between this overshoot and the electron-donating capability of the substituent. Substitution of 2,1,3-benzothiadiazole by the triphenylamine group significantly increases the electronic first and second hyperpolarizabilities as well as the two-photon absorption cross section [114].

Committee memberships

(a) Member of the Executive Council of the National Hellenic Research Foundation (1994-1995).
(b) Member of the Advisory Council of the Institute of the Organic and Pharmaceutical Chemistrty.

Publications

1. Ellis, G. E., Jones, R. G., and Papadopoulos M.G. (1974) C-13 Nuclear Magnetic-Resonance Studies of Piperidine and Piperazine Compounds .2. Empirical Substituent Parameters for, and Shielding Anisotropy of, N-Nitroso-Group, J Chem Soc Perk T 2, 1381-1384.
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