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PPDock-PortalPatch Dock (http://140.112.135.49/ppdock/) is a web server that focuses on the search of binding site(s) between the proteins and the drug molecules through docking simulations by applying the genetic programming algorithm (GP) and x-score scoring function. The target protein is at first regarded as a rigid body, whereas the drug molecule is allowed to be entirely flexible. As the starting step, one can obtain the coordinates file of the target protein from the PDB server (Protein Data Bank: http://www.rcsb.org/pdb/home/home.do; ".pdb" format) and then convert the coordinates of the drug molecule(s) to ".mol2" format by way of E-BABEL server (http://www.vcclab.org/lab/babel/). These two files will be used as the input files. For the docking results, the drug molecules will remain as .mol2 format and an Excel file consisting of the number of generations calculated with GP, the number of "evolution" trees, the values for score, the values for RMSD and the file names will be generated as the output file. All the results will be sent via e-mail. One can also check the results by visualizing the accomplished docking structures on line in 20 minutes.
During the test period, the server has been running for one month and accepted 120 inputs, including both from our group and about 10-15 individuals from outsides. For these trials, upon utilization of the X-Score as the scoring function, our PPDock software has produced an accuracy rate ranging from 66% to 76% in 100 protein-ligand complexes. In addition, a major purpose to add GP into the virtual screen system was to improve the search efficiency of docking. According to our results, the aforementioned trials were indeed faster than through other servers. It is reliable to use this virtual screen system to perform the docking simulations with both high accuracy and efficiency. Our new web service is now web-available and free for worldwide users in accelerating the development and design of new lead compounds.

Keywords: **Docking, Genetic Programming, X-score, Jmol**

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Crystal Structures and Radical-Scavenging Mechanism Investigation by X-Ray and Quantum Mechanical Methods of Antioxidant Triazolyl-Benzimidazole Derivatives.

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The three dimensional structures of triazolyl-benzimidazole derivatives were determined by X-ray diffraction method and structure-properties relationships were investigated using the molecular structure. Free DPPH$^{\cdot}$ radical scavenging mechanisms were clarified by density functional theory (DFT) on B3LYP/6-311+G (2D, 2P) level. According to the biological activity results all of the compounds were found to interact with DPPH$^{\cdot}$ strongly (78-88 %) at 10^{-3} M concentration [1]. It is well known that, there exist two mechanisms for an antioxidant to scavenge free DPPH$^{\cdot}$. The first one is a direct H-atom abstraction process, and the second one is a proton concerted electron-transfer process [2]. N-H bond dissociation enthalpies (BDEs) and ionization potentials (IPs) were calculated to find which mechanism of reaction's pathways is permitted. Our theoretical analysis indicates that free radical scavenging mechanisms of the compounds were direct H-atom abstraction processes rather than electron transfer. This mechanism will be helpful to elucidate the structure activity relationships for the novel antioxidants and to design novel compounds with better antioxidant properties.

[1] Ayhan-Kılcıgil G., Kus C., Coban T., Can-Eke B., Iscan M., Journal of Enzyme Inhibition and Medicinal Chemistry, 2004, 19(2), 129-135. [2] Litwinienko G., Ingold K.U., J. Org. Chem., 2003, 68, 3433-3438.

Keywords: antioxidant, DFT methods, DPPH$^{\cdot}$ radical scavenging mechanism

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CRYSTAL and CRYSCOR: two powerful tools for the ab-initio study of crystalline solids.

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CRYSTAL [1] (www.crystal.unito.it) is a general-purpose program for the study of crystalline solids. It computes the electronic structure of periodic systems (3D, 2D, 1D) within Hartree Fock, density functional or various hybrid approximations. The Bloch functions of the periodic systems are expanded as linear combinations of atom centered Gaussian functions. Powerful screening techniques are used to exploit real space locality. Space group symmetry is also fully exploited.
CRYSCOR [2] (www.cryscor.unito.it) is a program performing electronic structure calculations for 1D,- 2D- and 3D-periodic non-conducting systems at the correlated (presently local second order Møller-Plesset Perturbation Theory, LMP2) level. It uses the Hartree-Fock reference provided by CRYSTAL. It allows to obtain high quality results on total and cohesive energy, as well as the correlation-corrected density matrix, which can be used for the evaluation of diverse properties, like Compton profiles.
The new version of CRYSTAL, CRYSTAL09, and the first public version of CRYSCOR have been recently released.
In this poster the main features and capabilities of the two codes will be outlined, along with the most interesting and up to date applications to a variety of crystalline systems and properties, with a main focus on the newly implemented features.

[1] R. Dovesi, R. Orlando, B. Civalleri, C. Roetti, V.R. Saunders, C.M. Zicovich-Wilson Z. Kristallogr. 220, 571–573 (2005)
[2] C. Pisani, L. Maschio, S. Casassa, M. Halo, M. Schütz, D. Usvyat, J. Comput. Chem. 29 (13), 2113-2124 (2008)

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