

## DAFTAR PUSTAKA

- Adamo, C. and Barone, V., 1998, Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models, *J. Chem. Phys.*, 108, 664–675.
- Adamo, C. and Barone, V., 1999, Toward reliable density functional methods without adjustable parameters: The PBE0 model, *J. Chem. Phys.*, 110, 6158–6170.
- Aguiar, A.C.C., da Rocha, E.M., de Souza, N.B., França, T.C., and Krettli, A.U., 2012, New approaches in antimalarial drug discovery and development - A Review, *Mem. Inst. Oswaldo Cruz*, 107, 831–845.
- Alkorta, I., Perez, J.J., and Villar, H.O., 1994, Molecular polarization maps as a tool for studies of intermolecular interactions and chemical reactivity, *J. Mol. Graph.*, 12, 3–13.
- Austin, A., Petersson, G.A., Frisch, M.J., Dobek, F.J., Scalmani, G., and Throssell, K., 2012, A Density Functional with Spherical Atom Dispersion Terms, *J. Chem. Theory Comput.*, 8, 4989–5007.
- Autschbach, J., 2014, Relativistic calculations of magnetic resonance parameters : background and some recent developments, *Philos. Transactions R. Soc. A*, 372, 1–39.
- Becke, A.D., 1993, Density functional thermochemistry. III. The role of exact exchange, *J. Chem. Phys.*, 98, 5648–5652.
- Bhagat, S., Gahlawat, A., and Bharatam, P. V, 2019, *Structure-Based Drug Design of PfDHODH Inhibitors as Antimalarial Agents*. In Mohan, C.G., *Structural Bioinformatics: Applications in Preclinical Drug Discovery Process*. Springer, Cham.
- BIOVIA, D.S., 2019, Discovery Studio Visualizer.
- Boechat, N., Pinheiro, L.C.S., Silva, T.S., Aguiar, A.C.C., Carvalho, A.S., Bastos, M.M., Costa, C.C.P., Pinheiro, S., Pinto, A.C., Mendonça, J.S., Dutra, K.D.B., Valverde, A.L., Santos-Filho, O.A., Ceravolo, I.P., and Krettli, A.U., 2012, New Trifluoromethyl Triazolopyrimidines as Anti-Plasmodium falciparum Agents, *Molecules*, 17, 8285–8302.
- Brandão, G.C., Missias, F.C.R., Arantes, L.M., Soares, L.F., Roy, K.K., Doerksen, R.J., de Oliveira A.B., Pereira, G.R., 2017, Antimalarial naphthoquinones. Synthesis via click chemistry, *in vitro* activity, docking to PfDHODH and SAR of lapachol-based compounds, *Eur. J. Med. Chem.*, 145, 191–205.
- Cárdenas-Jirón, G.I., Gutiérrez-Olivía, S., Melin, J., and Toro-Labbé, A., 1997, Relations between Potential Energy, Electronic Chemical Potential, and

- Hardness Profiles, *J. Phys. Chem. A*, 101, 4621–4627.
- Caron, S. and McInturff, E., 2020, *Nucleophilic Aromatic Substitution*. In Caron, S. (ed.), *Practical Synthetic Organic Chemistry*, Wiley, Hoboken, 231–246.
- Chai, J. and Head-Gordon, M., 2008, Systematic optimization of long-range corrected hybrid density functionals, *J. Chem. Phys.*, 128, 081061-081075.
- Chattaraj, P.K. and Duley, S., 2010, Electron Affinity, Electronegativity, and Electrophilicity of Atoms and Ions, *J. Chem. Eng. Data*, 55, 1882–1886.
- Chattaraj, P.K. and Giri, S., 2009, Electrophilicity index within a conceptual DFT framework, *Annu. Reports Sect. "C" Physical Chem.*, 105, 13–39.
- Chattaraj, P.K., Sarkar, U., and Roy, D.R., 2006, Electrophilicity Index, *Chem. Rev.*, 106, 2065–2091.
- Chauhan, K., Sharma, M., Saxena, J., Singh, S.V., Trivedi, P., Srivastava, K., Puri, S.K., Saxena, J.K., Chaturvedi, V., and Chauhan, P.M.S., 2013, Synthesis and biological evaluation of a new class of 4-aminoquinoline-rhodanine hybrid as potent anti-infective agents, *Eur. J. Med. Chem.*, 62, 693–704.
- Chen, Y.-C., 2015, Beware of docking!, *Trends Pharmacol. Sci.*, 36, 78–95.
- Clayden, J., Greeves, N., and Warren, S., 2012, *Organic Chemistry*, 2nd edition, Oxford University Press, Oxford.
- Coslédan, F., Fraisse, L., Pellet, A., Guillou, F., Mordmüller, B., Kreamsner, P.G., et al., 2008, Selection of a trioxaquine as an antimalarial, *PNAS USA*, 105, 17579–17584.
- Cremer, D. and Gräfenstein, J., 2007, Calculation and analysis of NMR spin–spin coupling constants, *Phys. Chem. Chem. Phys.*, 9, 2791–2816.
- Deligkaris, C. and Rodriguez, J.H., 2012, Correction to DFT interaction energies by an empirical dispersion term valid for a range of intermolecular distances, *Phys. Chem. Chem. Phys.*, 14, 3414–3424.
- Dennington, R.D., Keith, T.A., and Millam, J.M., 2008, GaussView 5.0.8.
- Deshpande, S. and Kuppast, B., 2016, 4-aminoquinolines: An Overview of Antimalarial Chemotherapy, *Med. Chem.*, 6, 1–11.
- Dodson, G. and Wlodawer, A., 1998, Catalytic triads and their relatives, *Trends Biochem. Sci.*, 23, 347–352.
- Dominguez, J.N., Leon, C., Rodrigues, J., de Dominguez, N.G., Gut, J., and Rosenthal, P.J., 2009, Chemistry Synthesis of chlorovinyl sulfones as structural analogs of chalcones and their antiplasmodial activities, *Eur. J. Med. Chem.*, 44, 1457–1462.
- Dunnington, B.D. and Schmidt, J.R., 2012, Generalization of Natural Bond Orbital Analysis to Periodic Systems: Applications to Solids and Surfaces via Plane-

- Wave Density Functional Theory, *J. Chem. Theory Comput.*, 8 (6), 1902–1911.
- Fehr, A.R. and Perlman, S., 2015, Coronaviruses: An Overview of Their Replication and Pathogenesis, *Coronaviruses*, 1282, 1–23.
- Ferreira, L.G., dos Santos, R.N., Oliva, G., and Andricopulo, A.D., 2015, Molecular Docking and Structure-Based Drug Design Strategies, *Molecules*, 20, 13384–13421.
- Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Jr., Scalmani, G., Barone, V., Petersson, G.A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A., Bloino, J., Janesko, B.G., Gomperts, R., Mennucci, B., Hratchian, H.P., Ortiz, J. V., Izmaylov, A.F., Sonnenberg, J.L., Williams-Young, D., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V.G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery, J.A., Jr., Peralta, J.E., Ogliaro, F., Bearpark, M., Heyd, J.J., Brothers, E., Kudin, K.N., Staroverov, V.N., Keith, T., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J.C., Iyengar, S.S., Tomasi, J., Cossi, M., Millam, J.M., Klene, M., Adamo, C., Cammi, R., Ochterski, J.W., Martin, R.L., Morokuma, K., Farkas, O., and Foresman, J.B., Fox, D.J., 2013, Gaussian09.
- Fukui, K., 1982, Role of Frontier Orbitals In Chemical Reactions. *Science*, 218, 747–754.
- Glendening, E.D., Landis, C.R., and Weinhold, F., 2012, Natural bond orbital methods, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2 (1), 1–42.
- Glendening, E.D., Reed, A.E., Carpenter, J.E., and Weinhold, F., 2003, NBO Version 3.1.
- Goerigk, L., 2017, *A Comprehensive Overview of the DFT-D3 London-Dispersion Correction*. In de la Roza, A.O. and DiLabio, G.A., *Non-covalent Interactions in Quantum Chemistry and Physics*, Elsevier, Amsterdam.
- Goerigk, L. and Grimme, S., 2011, A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions, *Phys. Chem. Chem. Phys.*, 13, 6670–6688.
- Goerigk, L. and Grimme, S., 2014, Double-hybrid density functionals *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 4, 576–600.
- Goerigk, L. and Mehta, N., 2019, A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User, *Aust. J. Chem.*, 72, 563–573.
- Gralinski, L.E. and Menachery, V.D., 2020, Return of of the the Coronavirus: 2019-nCov, *Viruses*, 12, 1–8.

- Grimme, S., 2004, Accurate Description of van der Waals Complexes by Density Functional Theory Including Empirical Corrections, *J. Comput. Chem.*, 25, 1463–1473.
- Grimme, S., 2006, Semiempirical hybrid density functional with perturbative second-order correlation, *J. Chem. Phys.*, 124, 03451081–03451097.
- Grimme, S., 2011, Density functional theory with London dispersion corrections. *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 1, 211–228.
- Grimme, S., Antony, J., Ehrlich, S., and Krieg, H., 2010, A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, *J. Chem. Phys.*, 132, 154104–(1–19).
- Hadanu, R., Mustofa, and Nazudin, 2012, Synthesis and Antiplasmodial Activity of 2-(4-Methoxyphenyl)-4-Phenyl-1,10-Phenanthroline Derivative Compounds, *Makara J. Sci.*, 16, 101–109.
- Hamada, Y. and Kiso, Y., 2012, The application of bioisosteres in drug design for novel drug discovery: focusing on acid protease inhibitors, *Expert Opin. Drug Dis.*, 7, 903–922.
- Hanna, M.W., 1969, *Quantum Mechanics in Chemistry*, 2nd edition. W.A. Benjamin, Inc., Menlo Park.
- Helgaker, T., Coriani, S., Jørgensen, P., Kristensen, K., Olsen, J., and Ruud, K., 2012, Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations, *Chem. Revs.*, 112, 543–631.
- Heyd, J., Scuseria, G.E., and Ernzerhof, M., 2003, Hybrid functionals based on a screened Coulomb potential, *J. Chem. Phys.*, 118, 8207–8215.
- Hohenberg, P.C. and Kohn, W., 1964, Inhomogeneous Electron Gas, *Phys. Rev.*, 136, B864–B871.
- Horowitz, S. and Trievel, R.C., 2012, Carbon-Oxygen Hydrogen Bonding in Biological Structure and Function, *J. Biol. Chem.*, 287, 41576–41582.
- Hosteny, R.P., Gilman, R.R., Dunning Jr., T.H., and Pipano, A., 1970, Comparison of Slater and Contracted Gaussian Basis Sets in SCF and CI Calculations on H<sub>2</sub>O, *Chem. Phys. Lett.*, 7, 325–328.
- Huang, S.-Y. and Zou, X., 2010, Advances and Challenges in Protein-Ligand Docking, *Int. J. Mol. Sci.*, 11, 3016–3034.
- Huey, R., Morris, G.M., Olson, A.J., and Goodsell, D.S., 2007, A Semiempirical Free Energy Force Field with Charge-Based Desolvation, *J. Comput. Chem.*, 28, 1145–1152.
- Hurt, D.E., Widom, J., and Clardy, J., 2006, Structure of Plasmodium falciparum dihydroorotate dehydrogenase with a bound inhibitor, *Acta Crystallogr. Sect. D Biol. Crystallogr.*, 62, 312–323.

- Ingle, R.A., 2011, Histidine Biosynthesis, In *The Arabidopsis Book*, American Society of Plant Biologists.
- Islam, R., Parves, M.R., Paul, A.S., Uddin, N., Rahman, M.S., Al Mamun, A., Hossain, M.N., Ali, M.A., Halim, M.A., 2020, A molecular modeling approach to identify effective antiviral phytochemicals against the main protease of SARS-CoV-2, *J. Biomol. Struct. Dyn.*, 1–12.
- Jain, A., 2017, Computer aided drug design, *The 1<sup>st</sup> Physics and Technologies in Medicine and Dentistry Symposium*, 15<sup>th</sup>-16<sup>th</sup> July 2017, Depok.
- Jambrina, P.G. and Aldegunde, J., 2016, Computational Tools for the Study of Biomolecules, In *Computer Aided Chemical Engineering*, Elsevier, 583–648.
- Jin, Z., Du, X., Xu, Y., Deng, Y., Liu, M., Zhao, Y., Zhang, B., Li, X., Zhang, L., Peng, C., Duan, Y., Yu, J., Wang, L., Yang, K., Liu, F., Jiang, R., Yang, X., You, T., Liu, X., Yang, X., Bai, F., Liu, H., Liu, X., Guddat, L.W., Xu, W., Xiao, G., Qin, C., Shi, Z., Jiang, H., Rao, Z., and Yang, H., 2020, Structure of Mpro from COVID-19 virus and discovery of its inhibitors, *Nature*, 1–28.
- St. John, S.E., Tomar, S., Stauffer, S.R., and Mesecar, A.D., 2015, Targeting zoonotic viruses: Structure-based inhibition of the 3C-like protease from bat coronavirus HKU4 — The likely reservoir host to the human coronavirus that causes Middle East Respiratory Syndrome (MERS), *Bioorg. Med. Chem.*, 23, 6036–6048.
- Kohn, W. and Sham, L.J., 1965, Self-Consistent Equations Including Exchange and Correlation Effects, *Phys. Rev.*, 140, A1133–A1138.
- Kouznetsov, V.V. and Gómez-Barrio, A., 2009, Recent developments in the design and synthesis of hybrid molecules based on aminoquinoline ring and their antiplasmodial evaluation, *Eur. J. Med. Chem.*, 44, 3091–3113.
- Kramer, B., Rarey, M., and Lengauer, T., 1999, Evaluation of the FLEXX Incremental Construction Algorithm for Protein–Ligand Docking, *Proteins Struct. Funct. Genet.*, 37, 228–241.
- Krivdin, L.B., 2019, Computational <sup>1</sup>H NMR: Part 1. Theoretical background, *Magn. Reson. Chem.*, 57, 897–914.
- Krungkrai, S.R. and Krungkrai, J., 2016, Insights into the pyrimidine biosynthetic pathway of human malaria parasite *Plasmodium falciparum* as chemotherapeutic target, *Asian Pac. J. Trop. Med.*, 9, 525–534.
- Kubinyi, H., 1998, Similarity and Dissimilarity: A Medicinal Chemist's View, *Perspect. Drug Discov. Des.*, 9, 225–252.
- Kubinyi, H., 2002, Chemical Similarity and Biological Activities, *J. Braz. Chem. Soc.*, 13, 717–726.
- Kumagai, Y., Butler, K.T., Walsh, A., and Oba, F., 2017, Theory of ionization potentials of nonmetallic solids, *Phys. Rev. B*, 95, 1253091-1253100.

- Kumar, S., Singh, R.K., Patial, B., Goyal, S., and Bhardwaj, T.R., 2016, Recent advances in novel heterocyclic scaffolds for the treatment of drug-resistant malaria, *J. Enzyme Inhib. Med. Chem.*, 31, 173–186.
- Laskowski, R.A. and Swindells, M.B., 2011, LigPlot+: Multiple Ligand-Protein Interaction Diagrams for Drug Discovery, *J. Chem. Inf. Model.*, 51, 2778–2786.
- Leung, K., Wu, J.T., Liu, D., and Leung, G.M., 2020, First-wave COVID-19 transmissibility and severity in China outside Hubei after control measures and second-wave scenario planning: a modelling impact assessment, *Lancet*, 395, 1382–1393.
- Liu, J., Cao, R., Xu, M., Wang, X., Zhang, H., Hu, H., Zhong, W., and Wang, M., 2020, Hydroxychloroquine, a less toxic derivative of chloroquine, is effective in inhibiting SARS-CoV-2 infection in vitro, *Cell Discov.*, 6, 6–9.
- Luo, J., Wei, W., Waldispühl, J., and Moitessier, N., 2019, Challenges and current status of computational methods for docking small molecules to nucleic acids, *Eur. J. Med. Chem.*, 168, 414–425.
- Malmquist, N.A., Gujjar, R., Rathod, P.K., and Phillips, M.A., 2008, Analysis of Flavin Oxidation and Electron-Transfer Inhibition in *Plasmodium falciparum* Dihydroorotate Dehydrogenase, *Biochemistry*, 47, 2466–2475.
- Manohar, S., Rajesh, U.C., Khan, S.I., Tekwani, B.L., and Rawat, D.S., 2012, Novel 4-Aminoquinoline-Pyrimidine Based Hybrids with Improved in Vitro and in Vivo Antimalarial Activity, *ACS Med. Chem. Lett.*, 3, 555–559.
- Manohar, S., Tripathi, M., and Rawat, D.S., 2014, 4-Aminoquinoline based molecular hybrids as antimalarials: An Overview, *Curr. Top. Med. Chem.*, 14, 1706–1733.
- Masecar, A.D. and CSGID, 2020, Structure of COVID-19 main protease bound to potent broad-spectrum non-covalent inhibitor X77.
- Meanwell, N.A., 2011, Synopsis of Some Recent Tactical Application of Bioisosteres in Drug Design, *J. Med. Chem.*, 54, 2529–2591.
- Meng, X.-Y., Zhang, H.-X., Mezei, M., and Cui, M., 2011, Molecular Docking : A Powerful Approach for Structure-Based Drug Discovery, *Curr. Comput. Aided. Drug Des.*, 7, 146–157.
- Momma, K. and Izumi, F., 2011, VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data, *J. Appl. Crystallogr.*, 44, 1272–1276.
- Morris, G.M., Huey, R., Lindstrom, W., Sanner, M.F., Belew, R.K., Goodsell, D.S., and Olson, A.J., 2010, AutoDock4 and AutoDockTools4: Automated Docking with Selective Receptor Flexibility, *J. Comput. Chem.*, 30, 2785–2791.
- Murray, J.S. and Politzer, P., 2017, Molecular electrostatic potentials and

- noncovalent interactions, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 7, 1–10.
- Nqoro, X., Tobeka, N., and Aderibigbe, B.A., 2017, Quinoline-Based Hybrid Compounds with Antimalarial Activity, *Molecules*, 22, 1–22.
- O’Boyle, N.M., Banck, M., James, C.A., Morley, C., Vandermeersch, T., and Hutchison, G.R., 2011, OpenBabel: An open chemical toolbox, *J. Cheminform*, 1–14.
- Paloque, L., Ramadani, A.P., Puijalon, O.M., Augereau, J.M., and Vical, F.B., 2016, *Plasmodium falciparum*: multifaceted resistance to artemisinins, *Malar. J.*, 1–12.
- Papajak, E. and Truhlar, D.G., 2010, Density Functional Theory, *J. Chem. Theory Comput.*, 6, 597–601.
- Parija, S.C. and Praharaj, I., 2011, Drug resistance in malaria, *Indian J. Med. Microbiol.*, 29, 243–248.
- Parr, R.G. and Pearson, R.G., 1983, Absolute Hardness: Companion Parameter to Absolute Electronegativity, *J. Am. Chem. Soc.*, 105, 7512–7516.
- Patani, G.A. and LaVoie, E.J., 1996, Bioisosterism: A Rational Approach in Drug Design. *Chem. Rev.*, 96, 3147–3176.
- Pavia, D.L., Lampman, G.M., Kriz, G.S., and Vyvyan, J.R., 2015, *Introduction to Spectroscopy*, 5th ed., Cengage Learning, Stamford.
- Pearson, R.G., 2005, Chemical hardness and density functional theory, *J. Chem. Sci.*, 117, 369–377.
- Perdew, J.P., 1986, Density-functional approximation for the correlation energy of the inhomogeneous electron gas, *Phys. Rev. B*, 33, 8822–8824.
- Perdew, J.P., Burke, K., and Ernzerhof, M., 1996, Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett.*, 77, 3865–3868.
- Perdew, J.P., Tao, J., Staroverov, V.N., and Scuseria, G.E., 2004, Meta-generalized gradient approximation: Explanation of a realistic nonempirical density functional, *J. Chem. Phys.*, 120, 6898–6911.
- Petterson, E.F., Goddard, T.D., Huang, C.C., Couch, G.S., Greenblatt, D.M., Meng, E.C., and Ferrin, T.E., 2004, UCSF Chimera — A Visualization System for Exploratory Research and Analysis, *J. Comp.*, 25, 1605–1612.
- Phillips, M.A. and Rathod, P.K., 2010, Plasmodium dihydroorotate dehydrogenase: a promising target for novel anti-malarial chemotherapy, *Infect. Disord. - Drug Targets*, 10, 226–239.
- Politzer, P., 1981, Relationships between the energies of atoms and molecules and the electrostatic potentials at their nuclei. In Politzer, P. and Truhlar, D.G. (eds), *Chemical Applications of Atomic and Molecular Electrostatic*

*Potentials*, Elsevier, New York, 7–28.

Pierrefixe, S.C.A.H. and Bickelhaupt, F.M., 2007, Aromaticity: Molecular-Orbital Picture of an Intuitive Concept, *Chem. Eur. J.*, 13 (22), 6321–6328.

Politzer, P., 1981, Relationships between the energies of atoms and molecules and the electrostatic potentials at their nuclei. In Politzer, P. and Truhlar, D.G. (eds), *Chemical Applications of Atomic and Molecular Electrostatic Potentials*, Elsevier, New York, 7–28.

Politzer, P., Abu-Awwad, F., and Murray, J.S., 1998, Comparison of Density Functional and Hartree-Fock Average Local Ionization Energies on Molecular Surfaces, *Int. J. Quantum Chem.*, 69, 607–613.

Reddy, P.L., Khan, S.I., Ponnan, P., Tripathi, M., and Rawat, D.S., 2017, Design, synthesis and evaluation of 4-Aminoquinoline-purine hybrids as potential antiplasmodial agents, *Eur. J. Med. Chem.*, 126, 675–686.

Ren, J., Zhao, J., Zhou, Y.-S., Liu, X.-H., Chen, X., and Hu, K., 2013, Synthesis and antitumor activity of novel 4-aminoquinoline derivatives, *Med. Chem. Res.*, 22, 2855–2861.

Ribas, J., Cubero, E., Luque, F.J., and Orozco, M., 2002, Theoretical Study of Alkyl- $\pi$  and Aryl- $\pi$  Interactions. Reconciling Theory and Experiment, *J. Org. Chem.*, 67, 7057–7065.

Rojas Ruiz, F.A., García-sánchez, R.N., Villabona, S., Gómez-barrio, A., Torres, D.F., Pérez-Solórzano, B.M., Nogal-Ruiz, J.J., Martínez-Fernández, A.R., and Kouznetsov, V.V., 2011, Synthesis and antimalarial activity of new heterocyclic hybrids based on chloroquine and thiazolidinone scaffolds, *Bioorg. Med. Chem.*, 19, 4562–4573.

Satish, P.V. V and Sunita, K., 2017, Antimalarial efficacy of *Pongamia pinnata* (L) Pierre against *Plasmodium falciparum* (3D7 strain) and *Plasmodium berghei* (ANKA), *BMC Complement Altern. Med.*, 17, 1–26.

Schneider, W.B. and Auer, A.A., 2014, Constant chemical potential approach for quantum chemical calculations in electrocatalysis., *Beilstein J. Nanotechnol.*, 55, 668–676.

Shafee, T., 2013, Evolvability of a Viral Protease: Experimental Evolution of Catalysis, Robustness and Specificity, *Dissertation*, Department of Biochemistry and Gonville and Caius College, University of Cambridge, Cambridge.

Shalini, A., Tandon, H., and Chakraborty, T., 2017, Molecular Electrophilicity Index—A Promising Descriptor for Predicting Toxicological Property, *J. Bioequiv. Availab.*, 9, 518–527.

Shang, J., Ye, G., Shi, K., Wan, Y., Luo, C., Aihara, H., Geng, Q., Auerbach, A., and Li, F., 2020, Structural basis of receptor recognition by SARS-CoV-2.

*Nature*, 1–8.

- Shereen, M.A., Khan, S., Kazmi, A., Bashir, N., and Siddique, R., 2020, COVID-19 infection: Origin, transmission, and characteristics of human coronaviruses, *J. Adv. Res.*, 24, 91–98.
- Singh, A., Maqbool, M., Mobashir, M., and Hoda, N., 2017, Dihydroorotate dehydrogenase: An inevitable drug target for the development of antimalarials, *Eur. J. Med. Chem.*, 125, 640–651.
- Singh, A.K., Singh, A., Shaikh, A., Singh, R., and Misra, A., 2020, Chloroquine and hydroxychloroquine in the treatment of COVID-19 with or without diabetes: A systematic search and a narrative review with a special reference to India and other developing countries, *Diabetes Metab. Syndr. Clin. Res. Rev.*, 14, 241–246.
- Sjoberg, P. and Politzer, P., 1990, Use of the Electrostatic Potential at the Molecular Surface, *J. Phys. Chem.*, 94, 3959–3961.
- Sousa, S.F., Fernandes, P.A., and Ramos, M.J., 2007, General Performance of Density Functionals, *J. Phys. Chem. A*, 111, 10439–10452.
- Spitznagel, G.W., Clark, T., von Rague Schleyer, P., and Hehre, W.J., 1987, An Evaluation of the Performance of Diffuse Function-Augmented Basis Sets for Second Row Elements, Na-Cl, *J. Comput. Chem.*, 8, 1109–1116.
- Su, N.Q. and Xu, X., 2019, Insights into Direct Methods for Predictions of Ionization Potential and Electron Affinity in Density Functional Theory, *J. Phys. Chem. Lett.*, 10, 2692–2699.
- Sureshkumar, B., Mary, Y.S., Panicker, C.Y., Armakovič, S.J., Suma, S., Armakovič, S., et al., 2020, Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study, *Arab. J. Chem*, 13, 632–648.
- Sureshkumar, B., Mary, Y.S., Resmi, K.S., Suma, S., Armakovič, S., Armakovič, S.J., Van Alsenoy, C., and Sobhana, D., 2018, Spectroscopic characterization of hydroxyquinoline derivatives with bromine and iodine atoms and theoretical investigation by DFT calculations, MD simulations and molecular docking studies, *J. Mol. Struct.*, 1167, 95–106.
- Takahashi, O., Kohno, Y., and Nishio, M., 2010, Relevance of Weak Hydrogen Bonds in the Conformation of Organic Compounds and Bioconjugates: Evidence from Recent Experimental Data and High-Level *ab initio* MO Calculations, *Chem. Rev.*, 110, 6049–6076.
- Tandon, H., Chakraborty, T., and Suhag, V., 2019, A New Scale of The Electrophilicity Index Invoking The Force Concept and Its Application in Computing the Internuclear Bond Distance, *J. Struct. Chem.*, 60, 1725–1734.
- Torrent-Sucarrat, M., De Proft, F., Ayers, P.W., and Geerlings, P., 2010, On the

- applicability of local softness and hardness, *Phys. Chem. Chem. Phys.*, 12, 1072–1080.
- Ulusoy, I.S. and Nest, M., 2011, Correlated Electron Dynamics: How Aromaticity Can Be Controlled, *J. Am. Chem. Soc.*, 133 (50), 20230–20236.
- Vieth, M., Hirst, J.D., Kolinski, A., and Brooks III, C.L., 1998, Assessing Energy Functions for Flexible Docking, *J. Comput. Chem.*, 19, 1612–1622.
- Vincent, M.J., Bergeron, E., Benjannet, S., Erickson, B.R., Rollin, P.E., Ksiazek, T.G., Seidah, N.G., and Nichol, S.T., 2005, Chloroquine is a potent inhibitor of SARS coronavirus infection and spread, *Virology*, 2, 1–10.
- Vyas, V.K., Qureshi, G., Ghate, M., Patel, H., and Dalai, S., 2016, Identification of novel *PfDHODH* inhibitors as antimalarial agents via pharmacophore-based virtual screening followed by molecular docking and in vivo antimalarial activity, *SAR-QSAR Environ. Res.*, 27, 427–440.
- Walls, A.C., Park, Y.-J., Tortorici, M.A., Wall, A., McGuire, A.T., Veesler, D., 2020, Structure, Function, and Antigenicity of the SARS-CoV-2 Spike Glycoprotein, *Cell*, 181, 281–292.
- Wang, J., Guo, Z., Fu, Y., Wu, Z., Huang, C., Zheng, C., Shar, P.A., Wang, Z., Xiao, W., and Wang, Y., 2017, Weak-binding molecules are not drugs?—toward a systematic strategy for finding effective weak-binding drugs, *Brief. Bioinform.*, 18, 321–332.
- Wang, M., Cao, R., Zhang, L., Yang, X., Xu, M., Shi, Z., Hu, Z., Zhong, W., and Xiao, G., 2020, Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro, *Cell Res.*, 30, 269–271.
- Wang, W., Li, Q., Wei, Y., Xue, J., Sun, X., Yu, Y., Chen, Z., Li, S., and Duan, L., 2017, Novel carbazole aminoalcohols as inhibitors of b-hematin formation: Antiplasmodial and antischistosomal activities, *Int. J. Parasitol. Drugs Drug Resist.*, 7, 191–199.
- Weinhold, F. and Landis, C.R., 2005, Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective, Cambridge University Press, Cambridge.
- Weinhold, F., Landis, C.R., and Glendening, E.D., 2016, What is NBO analysis and how is it useful?, *Int. Rev. Phys. Chem.*, 35, 399–440.
- WHO, 2016, Global technical strategy for malaria 2016–2030.
- WHO, 2019, World malaria report 2019.
- Yanai, T., Tew, D.P., and Handy, N.C., 2008, A new hybrid exchange – correlation functional using the Coulomb-attenuation method (CAM-B3LYP), *Chem. Phys. Lett.*, 393, 51–57.
- Yesselman, J.D., Horowitz, S., Brooks III, C.L., and Trievel, R.C., 2015, Frequent

side chain methyl carbon-oxygen hydrogen bonding in proteins revealed by computational and stereochemical analysis of neutron structures, *Proteins*, 83, 403–410.

Yi, J., Thomas, L.M., and Richter-Addo, G.B., 2011, Structure of human R-state aquomethemoglobin at 2.0 Å resolution, *Acta Crystallogr. Sect. F*, 67, 647–651.

Young, D.C., 2001, *Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems*, John Wiley and Sons, Inc., New York.

Yu, W. and MacKerell Jr., A.D., 2018, Computer-Aided Drug Design Methods, *Methods Mol. Biol.*, 1520, 85–106.

Zhang, L., Lin, D., Sun, X., Curth, U., Drosten, C., Sauerhering, L., Becker, S., Rox, K., and Hilgenfeld, R., 2020, Crystal structure of SARS-CoV-2 main protease provides a basis for design of improved  $\alpha$ -ketoamide inhibitors, *Science*, 3405, 1–9.

Zhu, N., Zhang, D., Wang, W., Li, X., Yang, B., Song, J., Zhao, X., Huang, B., Shi, W., Lu, R., Niu, P., Zhan, F., Ma, X., Wang, D., Xu, W., Wu, G., Gao, G.F., and Tan, W., 2020, A Novel Coronavirus from Patients with Pneumonia in China, 2019, *N. Engl. J. Med.*, 382, 727–733