Bibliography

1. Nammalwar, B.; Bunce, R. A. Recent Syntheses of 1,2,3,4-Tetrahydroquinolines, 2,3-Dihydro-4(1*H*)-Quinolinones and 4(1*H*)-Quinolinones Using Domino Reactions. *Molecules* **2013**, *19* (1), 204–232. https://doi.org/10.3390/molecules19010204.
2. Al-Sha'alan, N. H. Antimicrobial Activity and Spectral, Magnetic and Thermal Studies of Some Transition Metal Complexes of a Schiff Base Hydrazone Containing a Quinoline Moiety. *Molecules* **2007**, *12* (5), 1080–1091. https://doi.org/10.3390/12051080.
3. Van Order, R. B.; Lindwall, H. G. Indole. *Chem. Rev.* **1942**, *30* (1), 69–96. https://doi.org/10.1021/cr60095a004.
4. Schenck, L. M.; Bailey, J. R. The Nitrogen Compounds in Petroleum Distillates. XXII. Isolation and Synthesis of 2,3-Dimethyl-4,8-Diethylquinoline (I) and 2,3-Dimethyl-4-Ethyl-8-n-Propylquinoline (II). *J. Am. Chem. Soc.* **1941**, *63* (5), 1365–1367. https://doi.org/10.1021/ja01850a066.
5. Bos, P. M., Gosens, I., Geraets, L., Delmaar, C., & Cassee, F. R. Pulmonary toxicity in rats following inhalation exposure to poorly soluble particles: The issue of impaired clearance and the relevance for human health hazard and risk assessment. *Regul. Toxicol. Pharmacol.*, **2019**, *109*, 104498. https://doi.org/10.1016/j.yrtph.2019.104498.
6. Troger, J.; Mueller, W. The Isomerization and Decomposition of Cusparine. *Arch. Pharm.* **1914**, *252* (1), 459–465. https://doi.org/10.1002/ardp.19112490303.
7. Spath, E.; Papaioanou, G. On phenol bases of Angostura bark: synthesis of galipolin. *Monatsh. Chem.* **1929**, *52* (1), 129–140. https://doi.org/10.1007/BF02715981.
8. Houghton, P. J., Woldemariam, T. Z., Watanabe, Y., & Yates, M. Activity against Mycobacterium tuberculosis of alkaloid constituents of Angostura bark, Galipea officinalis. *Planta medica*, **1999**, *65*(03), 250-254. DOI: 10.1055/s-1999-13988.
9. Xu, M.; Wagerle, T.; Long, J. K.; Lahm, G. P.; Barry, J. D.; Smith, R. M. Insecticidal Quinoline and Isoquinoline Isoxazolines. *Bioorg. Med. Chem. Lett.* **2014**, *24* (16), 4026–4030. https://doi.org/10.1016/j.bmcl.2014.06.004.
10. Senerovic, L.; Opsenica, D.; Moric, I.; Aleksic, I.; Spasić, M.; Vasiljevic, B. Quinolines and Quinolones as Antibacterial, Antifungal, Anti-Virulence, Antiviral and Anti-Parasitic Agents. *Adv. Microbiol. Infect. Dis. Public Health* **2020**, *14*, 37–69. https://doi.org/10.1007/5584_2019_428.

11. Foley, M.; Tilley, L. Quinoline Antimalarials: Mechanisms of Action and Resistance and Prospects for New Agents. *Pharmacol. Ther.* **1998**, *79* (1), 55–87. https://doi.org/10.1016/S0163-7258(98)00012-6.
12. Hayat, F.; Salahuddin, A.; Umar, S.; Azam, A. Synthesis, Characterization, Antiamoebic Activity, and Cytotoxicity of Novel Series of Pyrazoline Derivatives Bearing Quinoline Tail. *Eur. J. Med. Chem.* **2010**, *45* (10), 4669–4675. https://doi.org/10.1016/j.ejmech.2010.07.028.
13. Kumar Gupta, S.; Mishra, A. Synthesis, Characterization, and Screening for Anti-Inflammatory and Analgesic Activity of Quinoline Derivatives Bearing Azetidinones Scaffolds. *Anti-Inflamm. Anti-Allergy Agents Med. Chem.* **2016**, *15* (1), 31–43. DOI: 10.2174/1871523015666160210124545.
14. Ferlin, M. G.; Chiarelotto, G.; Antonucci, F.; Caparrotta, L.; Froldi, G. Mannich Bases of 3H-Pyrrolo[3,2-*f*]quinoline Having Vasorelaxing Activity. *Eur. J. Med. Chem.* **2002**, *37* (5), 427–434. https://doi.org/10.1016/S0223-5234(02)01355-7.
15. Nikookar, H.; Mohammadi-Khanaposhtani, M.; Imanparast, S.; Faramarzi, M. A.; Ranjbar, P. R.; Mahdavi, M.; Larijani, B. Design, Synthesis, and in Vitro α-Glucosidase Inhibition of Novel Dihydropyrano[3,2-c]quinoline Derivatives as Potential Anti-Diabetic Agents. *Bioorg. Chem.* **2018**, *77*, 280–286. https://doi.org/10.1016/j.bioorg.2018.01.025.
16. Singh, S.; Kaur, G.; Mangla, V.; Gupta, M. K. Quinoline and Quinolones: Promising Scaffolds for Future Antimycobacterial Agents. *J. Enzyme Inhib. Med. Chem.* **2015**, *30* (3), 492–504. https://doi.org/10.3109/14756366.2014.930454.
17. Afzal, O.; Kumar, S.; Haider, M. R.; Ali, M. R.; Kumar, R.; Jaggi, M.; Bawa, S. A Review on Anticancer Potential of Bioactive Heterocycle Quinoline. *Eur. J. Med. Chem.* **2015**, *97*, 871–910. https://doi.org/10.1016/j.ejmech.2014.07.044.
18. Kumar Gupta, S.; Mishra, A. Synthesis, Characterization, and Screening for Anti-Inflammatory and Analgesic Activity of Quinoline Derivatives Bearing Azetidinones Scaffolds. *Anti-Inflamm. Anti-Allergy Agents Med. Chem.* **2016**, *15* (1), 31–43. http://dx.doi.org/10.2174/1871523015666160210124545.
19. Muruganantham, N.; Sivakumar, R.; Anbalagan, N.; Gunasekaran, V.; Leonard, J. T. Synthesis, Anticonvulsant, and Antihypertensive Activities of 8-Substituted Quinoline Derivatives. *Biol. Pharm. Bull.* **2004**, *27* (10), 1683–1687. https://doi.org/10.1248/bpb.27.1683.

20. Ahmed, N.; Brahmbhatt, K. G.; Sabde, S.; Mitra, D.; Singh, I. P.; Bhutani, K. K. Synthesis and Anti-HIV Activity of Alkylated Quinoline 2,4-Diols. *Bioorg. Med. Chem.* **2010**, *18* (8), 2872–2879. https://doi.org/10.1016/j.bmc.2010.03.015.
21. Mathada, B. S. The Versatile Quinoline and Its Derivatives as Anti-Cancer Agents: An Overview. *Polycycl. Aromat. Compd.* **2023**, *43* (5), 4333–4345. https://doi.org/10.1080/10406638.2022.2089177.
22. Wang, C.; Chang, J.; Yang, S.; Shi, L.; Zhang, Y.; Liu, W.; Xing, D. Advances in Antitumor Research of CA-4 Analogs Carrying Quinoline Scaffold. *Front. Chem.* **2022**, *10*, 1040333. https://doi.org/10.3389/fchem.2022.1040333.
23. Guimaraes, C. R. W.; Boger, D. L.; Jorgensen, W. L. Elucidation of Fatty Acid Amide Hydrolase Inhibition by Potent α-Ketoheterocycle Derivatives from Monte Carlo Simulations. *J. Am. Chem. Soc.* **2005**, *127* (49), 17377–17384. https://doi.org/10.1021/ja055438j.
24. Bajaj, S.; Asati, V.; Singh, J.; Roy, P. P. 1,3,4-Oxadiazoles: An Emerging Scaffold to Target Growth Factors, Enzymes, and Kinases as Anticancer Agents. *Eur. J. Med. Chem.* **2015**, *97*, 124–141. https://doi.org/10.1016/j.ejmech.2015.04.051.
25. Das, B. C., Tang, X. Y., Rogler, P., & Evans, T. Design and synthesis of 3, 5-disubstituted boron-containing 1, 2, 4-oxadiazoles as potential combretastatin A-4 (CA-4) analogs. *Tetrahedron lett,*, **2012**, *53*(31), 3947-3950. https://doi.org/10.1016/j.tetlet.2012.02.110.
26. Nayak, G., Shrivastava, B., & Singhai, A. K. Azitidin-2-one fused quinoline analogues: Synthesis and Biological evaluation of some novel 2-chloro-3-formyl quinoline derivatives. *Int. J. Curr. Pharm. Res*, **2016**, *8*(3), 64-67. https://doi.org/10.1016/j.tetlet.2012.02.110.
27. Strekowski, L.; Czarny, A.; Lee, H. The Friedländer Synthesis of 4-Perfluoroalkylquinolines. *J. Fluorine Chem.* **2000**, *104* (2), 281–284.
28. Knorr, L. Synthetic experiments with aceto-acetic ester. *Chem. Eur.* **1886**, *236*, 69–115. https://doi.org/10.1002/jlac.18862360105.
29. Chongau, R. J.; Siddiqui, M. A.; Snieckus, V. Synthetic Connections to the Aromatic Directed Metalation Reaction. *Tetrahedron Lett.* **1986**, *27* (44), 5323–5326. https://doi.org/10.1016/S0040-4039(00)85201-6.
30. Pfitzinger, W. Quinoline derivatives from isatinic acid. *J. Prakt. Chem.* **1885**, *33* (1), 100–100. https://doi.org/10.1002/prac.18850330110.

31. Bondock, S.; Gieman, H. Synthesis, Antibacterial and Anticancer Evaluation of Some New 2-Chloro-3-Hetarylquinolines. *Res. Chem. Intermed.* **2015**, *41*, 8381–8403. https://doi.org/10.1007/s11164-014-1899-8.
32. Abd-El Maksoud, M. A.; Tawfik, H. A.; Maigali, S. S.; Soliman, F. M.; Moharam, M. E.; Dondeti, M. F. Synthesis, Antimicrobial, and Molecular Docking Evaluation of Some Heterocycles Containing Quinoline Moiety. *Der Pharma Chemica* **2016**, *8* (13), 291–301. ISSN 0975-413X CODEN (USA): PCHHAX.
33. Juddhawala, K. V.; Parekh, N. M. Design, Synthetic Approaches, Structure-Activity Relationship Strategy, and Antibacterial Evaluation for *N*-Alkylated Derivatives with Binding Mode of Chloroquinoline-Thiazolidinedione-Based Hybrids. *J. Chem. Sci.* **2024**, *63* (2), 218-233. https://doi.org/10.21203/rs.3.rs-5422836/v1.
34. Chavan, H. V.; Sirsat, D. M.; Mule, Y. B. An Environmentally Benign Synthesis of Aryl-Hydrazones with Aqueous Extract of Acacia Pods as a Natural Surfactant Type Catalyst. *Iranian Chem. Commun.* **2016**, *4* (4), 373-388.
35. Jaware, J., & Borhade, S. Synthesis and novel *N*-{[2-(morpholin-4-yl)-quinoline-3-yl] methyl} 2-[(4-aminopentyl)(ethyl) amino] ethanol derivatives. *Indo Am. J. Pharm. Res*, **2014**, *4*(5), 2496-2502.
36. Kattimani, P. P.; Kamble, R. R.; Dorababu, A.; Hunnur, R. K.; Kamble, A. A.; Devarajegowda, H. C. C5-Alkyl-1,3,4-Oxadiazol-2-ones Undergo Dealkylation upon Nitrogen Insertion to Form 2H-1,2,4-Triazol-3-ones: Synthesis of 1,2,4-Triazol-3-one Hybrids with Triazolothiadiazoles and Triazolothiadiazines. *J. Het. Chem.* **2017**, *54* (4), 2258-2265. https://doi.org/10.1002/jhet.2813.
37. Mandhane, P. G.; Joshi, R. S.; Nagargoje, D. R.; Gill, C. H. An Efficient Synthesis of 3,4-Dihydropyrimidin-2(1*H*)-ones Catalyzed by Thiamine Hydrochloride in Water under Ultrasound Irradiation. *Tetrahedron Lett.* **2010**, *51* (23), 3138-3140. https://doi.org/10.1016/j.tetlet.2010.04.037.
38. Riyadh, S. M., Abolibda, T. Z., Sayed, A. R., & Gomha, S. M. Synthetic utility of aminomercapto [1,2,4] triazoles in the preparation of fused triazoles. *Curr. Org. Chem.*, **2022**, *26*(7), 693-714. https://doi.org/10.2174/1385272826666220417131159.
39. Mandhane, P. G., Joshi, R. S., Mahajan, P. S., Nikam, M. D., Nagargoje, D. R., & Gill, C. H. Synthesis, characterization and antimicrobial screening of substituted quiazolinones derivatives. *Arab. Jour. Chem.*, **2015**, *8*(4), 474-479.

40. Hamama, W. S., Ibrahim, M. E., Gooda, A. A., & Zoorob, H. H. Recent advances in the chemistry of 2-chloroquinoline-3-carbaldehyde and related analogs. *RSC adv.*, **2018**, *8*(16), 8484-8515. DOI: 10.1039/C7RA11537G.
41. Zaheer, Z., Khan, F. A. K., Sangshetti, J. N., Patil, R. H., & Lohar, K. S. Novel amalgamation of phthalazine–quinolines as biofilm inhibitors: One-pot synthesis, biological evaluation and in silico ADME prediction with favorable metabolic fate. *Bioorg. Med. Chem. Lett.*, **2016**, *26*(7), 1696-1703. https://doi.org/10.1016/j.bmcl.2016.02.057.
42. Baruah, B.; Bhuyan, P. J. Synthesis of Some Complex Pyrano[2,3-*b*] and Pyrido[2,3-*b*] Quinolines from Simple Acetanilids via Intramolecular Domino Hetero Diels–Alder Reactions of 1-Oxa-1,3-Butadienes in Aqueous Medium. *Tetrahedron* **2009**, *65* (34), 7099-7104. https://doi.org/10.1016/j.tet.2009.06.036.
43. Bindu, P. J.; Mahadevan, K. M.; Satyanarayan, N. D.; Naik, T. R. Synthesis and DNA Cleavage Studies of Novel Quinoline Oxime Esters. *Bioorg. Med. Chem. Lett.* **2012**, *22* (2), 898-900. https://doi.org/10.1016/j.bmcl.2011.12.037.
44. Steeneck, C.; Kinzel, O.; Anderhub, S.; Hornberger, M.; Pinto, S.; Morschhaeuser, B.; Hoffmann, T. Discovery of Hydroxyamidine-Based Inhibitors of IDO1 for Cancer Immunotherapy with Reduced Potential for Glucuronidation. *ACS Med. Chem. Lett.* **2020**, *11* (2), 179-187. https://doi.org/10.1021/acsmedchemlett.9b00572.
45. Baucom, K. D.; Jones, S. C.; Roberts, S. W. 1,1′-Carbonyldiimidazole (CDI)-Mediated Coupling and Cyclization to Generate [1,2,4] Triazolo[4,3-*a*] Pyridines. *Org. Lett.* **2016**, *18* (3), 560-563. https://doi.org/10.1021/acs.orglett.5b03589.
46. Jivani, A.; Kapadiya, K.; Jainik, A.; Khunt, R. Efficacy of Binary Media and Gold Catalyst for the Synthesis of Conjugates with Cyclohexyl-Tetrazole-Alkyloxyphenyl-Benzenamine through Ugi 4-CC Reactions: Cytotoxic and Single-Crystal Studies. *Polycyclic Aromatic Compounds* **2024**, *44* (1), 403-417. https://doi.org/10.1080/10406638.2023.2174992.
47. Mohamed, M. S.; Awad, S. M.; Zohny, Y. M.; Mohamed, Z. M. New Theopyrimidine Derivatives of Expected Antiinflammatory Activity. *Pharmacophore* **2012**, *3* (1-2012), 62-75. ISSN 2229 – 5402.
48. Wang, Y.; Ai, J.; Wang, Y.; Chen, Y.; Wang, L.; Liu, G.; Geng, M.; Zhang, A. Synthesis and c-Met Kinase Inhibition of 3,5-Disubstituted and 3,5,7-Trisubstituted Quinolines. *J. Med. Chem.* **2011**, *54*, 2127-2142. https://doi.org/10.1021/jm101340q.
49. Muruganantham, N.; Sivakumar, R.; Anbalagan, N.; Gunasekaran, V.; Leonard, J. T. Synthesis, Anticonvulsant, and Antihypertensive Activities of 8-Substituted Quinoline

Derivatives. *Biol. Pharm. Bull.* **2004**, *27* (10), 1683-1687. https://doi.org/10.1248/bpb.27.1683.

50. Maguire, M. P.; Sheets, K. R.; McVety, K.; Spada, A. P.; Zilberstein, A. A New Series of PDGF Receptor Tyrosine Kinase Inhibitors: 3-Substituted Quinoline Derivatives. *J. Med. Chem.* **1994**, *37* (14), 2129-2137. https://doi.org/10.1021/jm00040a003.
51. Wilson, W. D.; Zhao, M.; Patterson, S. E.; Wydra, R. L.; Janda, L.; Strekowski, L.; Schinazi, R. F. Design of RNA Interactive Anti-HIV-1 Agents: Unfused Aromatic Intercalators. *ChemInform* **1992**, *23* (44). https://doi.org/10.1021/jm00101a022.
52. Palmer, K. J.; Holliday, S. M.; Brogden, R. N. Mefloquine: A Review of Its Antimalarial Activity, Pharmacokinetic Properties, and Therapeutic Efficacy. *Drugs* **1993**, *45*, 430-475. https://doi.org/10.2165/00003495-199345030-00009.
53. Kumar, A.; Srivastava, K.; Kumar, S. R.; Puri, S. K.; Chauhan, P. M. Synthesis and Bioevaluation of Hybrid 4-Aminoquinoline Triazines as a New Class of Antimalarial Agents. *Bioorg. Med. Chem. Lett.* **2008**, *18* (24), 6530-6533. https://doi.org/10.1016/j.bmcl.2008.10.049.
54. Lilienkampf, A.; Mao, J.; Wan, B.; Wang, Y.; Franzblau, S. G.; Kozikowski, A. P. Structure-Activity Relationships for a Series of Quinoline-Based Compounds Active Against Replicating and Nonreplicating *Mycobacterium tuberculosis*. *J. Med. Chem.* **2009**, *52* (7), 2109-2118. https://doi.org/10.1021/jm900003c.
55. Eswaran, S.; Adhikari, A. V.; Chowdhury, I. H.; Pal, N. K.; Thomas, K. D. New Quinoline Derivatives: Synthesis and Investigation of Antibacterial and Antituberculosis Properties. *Eur. J. Med. Chem.* **2010**, *45* (8), 3374-3383. https://doi.org/10.1016/j.ejmech.2010.04.022.
56. Goswami, B. N.; Kataky, J. C. S.; Baruah, J. N. Synthesis and Antibacterial Activity of 1□(2, 4□Dichlorobenzoyl)□4□Substituted Thiosemicarbazides, 1, 2, 4□Triazoles and Their Methyl Derivatives. *J. Hetero. Chem.* **1984**, *21*(4), 1225-1229. https://doi.org/10.1002/jhet.5570210460.
57. Cox, E.; Laessig, K. FDA Approval of Bedaquiline—The Benefit–Risk Balance for Drug-Resistant Tuberculosis. *N. Engl. J. Med.* **2014**, *371*(8), 689-691. DOI: 10.1056/NEJMp1314385**.**
58. Arshad, M.; Khan, T. A.; Khan, M. A. 1, 2, 4-Oxadiazole Nucleus with Versatile Biological Applications. *Int. J. Pharm. Sci. Res.* **2014**, *5*(7), 303-316. ISSN : 0975-9492.
59. Chandran, M., Renuka, J., Sridevi, J. P., Pedgaonkar, G. S., Asmitha, V., Yogeeswari, P., & Sriram, D. Benzothiazinone-piperazine derivatives as efficient Mycobacterium tuberculosis

DNA gyrase inhibitors. *Int. J. mycobacteriology*, **2015**, *4*(2), 104-115. https://doi.org/10.1016/j.ijmyco.2015.02.002.

60. Yempalla, K. R., Munagala, G., Singh, S., Magotra, A., Kumar, S., Rajput, V. S. & Singh, P. P. Nitrofuranyl methyl piperazines as new anti-TB agents: identification, validation, medicinal chemistry, and PK studies. *ACS Med. Chem. Lett.*, **2015**, *6*(10), 1041-1046. https://doi.org/10.1021/acsmedchemlett.5b00141.
61. Abad, N.; Sallam, H. H.; Al-Ostoot, F. H.; Khamees, H. A.; Al-Horaibi, S. A.; Khanum, S. A.; Ramli, Y. S. Synthesis, Crystal Structure, DFT Calculations, Hirshfeld Surface Analysis, Energy Frameworks, Molecular Dynamics, and Docking Studies of Novel Isoxazole Quinoxaline Derivative (IZQ) as Anti-Cancer Drug. *J. Mol. Struct.* **2021**, *1232*, 130004. https://doi.org/10.1016/j.molstruc.2021.130004.
62. Wang, C., Chang, J., Yang, S., Shi, L., Zhang, Y., Liu, W. & Xing, D. Advances in antitumor research of CA-4 analogs carrying quinoline scaffold. *Front. Chem.*, **2022**, *10*, 1040333.. https://doi.org/10.3389/fchem.2022.1040333.
63. Kumari, A.; Srivastava, S.; Manne, R. K.; Sisodiya, S.; Santra, M. K.; Guchhait, S. K.; Panda, D. C12, a Combretastatin-A4 Analog, Exerts Anticancer Activity by Targeting Microtubules. *Biochem. Pharmacol.* **2019**, *170*, 113663. https://doi.org/10.1016/j.bcp.2019.113663.
64. Ibrahim, T. S.; Hawwas, M. M.; Malebari, A. M.; Taher, E. S.; Omar, A. M.; Neamatallah, T.; Abdel-Samii, Z. K.; Safo, M. K.; Elshaier, Y. A. M. M. Discovery of Novel Quinoline-Based Analogues of Combretastatin A-4 as Tubulin Polymerisation Inhibitors with Apoptosis Inducing Activity and Potent Anticancer Effect. *J. Enzyme Inhib. Med. Chem.* **2021**, *36*(1), 802–818. https://doi.org/10.1080/14756366.2021.1899168.
65. Baykov, S.; Sharonova, T.; Shetnev, A.; Rozhkov, S.; Kalinin, S.; Smirnov, A. V. The First One-Pot Ambient-Temperature Synthesis of 1,2,4-Oxadiazoles from Amidoximes and Carboxylic Acid Esters. *Tetrahedron* **2017**, *73*(7), 945-951. https://doi.org/10.1016/j.tet.2017.01.007.
66. Zarei, M. A Mild and Efficient One□Pot Preparation of 1,2,4□Oxadiazoles from Nitriles and Carboxylic Acids Using Vilsmeier Reagent. *Chem. Sel.* **2018**, *3*(40), 11273-11276. https://doi.org/10.1002/slct.201801857.
67. Golushko, A. A.; Khoroshilova, O. V.; Vasilyev, A. V. Synthesis of 1,2,4-Oxadiazoles by Tandem Reaction of Nitroalkenes with Arenes and Nitriles in the Superacid TfOH. *J. Org. Chem.* **2019**, *84*(11), 7495-7500. https://doi.org/10.1021/acs.joc.9b00812.

68. Morelli, E.; Gemma, S.; Budriesi, R.; Campiani, G.; Novellino, E.; Fattorusso, C.; Specific Targeting of Peripheral Serotonin 5-HT3 Receptors. Synthesis, Biological Investigation, and Structure−Activity Relationships. *J. Med. Chem.* **2009**, *52*(11), 3548-3562. https://doi.org/10.1021/jm900018b.
69. Kala, P.; Khasim Sharif, S.; Murali Krishna, C. H.; Ramachandran, D. Design, Synthesis, and Anticancer Evaluation of 1,2,4-Oxadiazole Functionalized Quinoline Derivatives. *Med. Chem. Res.* **2020**, *29*, 136-144. https://doi.org/10.1007/s00044-019-02467-6.
70. Shruthi, T. G.; Eswaran, S.; Shivarudraiah, P.; Narayanan, S.; Subramanian, S. Synthesis, Antituberculosis Studies, and Biological Evaluation of New Quinoline Derivatives Carrying 1, 2, 4-Oxadiazole Moiety. *Bioorg. Med. Chem. Lett.* **2019**, *29*(1), 97-102. https://doi.org/10.1016/j.bmcl.2018.11.002.
71. El-Sayed, W. A.; El-Essawy, F. A.; Ali, O. M.; Nasr, B. S.; Abdalla, M. M.; Abdel-Rahman, A. A. H. Anti-HIV Activity of New Substituted 1,3,4-Oxadiazole Derivatives and Their Acyclic Nucleoside Analogues. *Z. Naturforsch. C* **2009**, *64*(11-12), 773-778. https://doi.org/10.1515/znc-2009-11-1203.
72. Kappe, C. O. Recent Advances in the Biginelli Dihydropyrimidine Synthesis. New Tricks from an Old Dog. *Acc. Chem. Res.* **2000**, *33*(12), 879-888. https://doi.org/10.1021/ar000048h.
73. Honnappa, N.; Mukhopadhyay, A.; Moorthy, J. N. Biginelli Reaction: An Overview. *Tetrahedron Lett.* **2006**, *57*(47), 5135-5149. https://doi.org/10.1016/j.tetlet.2016.09.047.
74. Jie-Ping, W.; Liu, Y. Synthesis of Dihydropyrimidinones and Thiones by Multicomponent Reactions: Strategies Beyond the Classical Biginelli Reaction. *Synthesis* **2010**, *2010*(23), 3943-3953. DOI: 10.1055/s-0030-1258290.
75. Patil, A. D.; Kumar, N. V.; Kokke, W. C.; Bean, M. F.; et al. Novel Alkaloids from the Sponge *Batzella* sp.: Inhibitors of HIV gp120-Human CD4 Binding. *J. Org. Chem.* **1995**, *60*, 1182-1188. https://doi.org/10.1021/jo00110a021.
76. Deshmukh, M. B.; Salunkhe, S. M.; Patil, D. R.; Anbhule, P. V. A Novel and Efficient One-Step Synthesis of 2-Amino-5-Cyano-6-Hydroxy-4-Aryl Pyrimidines and Their Anti-Bacterial Activity. *Eur. J. Med. Chem.* **2009**, *44*, 2651-2654. https://doi.org/10.1016/j.ejmech.2008.10.018.
77. Sondhi, S. M.; Jain, S.; Dinodia, M.; Shukla, R.; Raghubir, R. One-Pot Synthesis of Pyrimidine and Bispyrimidine Derivatives and Their Evaluation for Anti-Inflammatory and Analgesic Activities. *Bioorg. Med. Chem.* **2007**, *15*, 3334-3344. https://doi.org/10.1016/j.bmc.2007.03.028.

78. Balkan, A.; Ertan, M.; Burgemeister, T. Synthesis and Structural Evaluations of Thiazolo[3,2-a]Pyrimidine Derivatives. *Arch. Pharm. (Weinheim)* **1992**, *325*, 499-501. https://doi.org/10.1002/ardp.19923250809.
79. Sondhi, S. M.; Dinodia, M.; Rani, R.; Shukla, R.; Raghubir, R. Synthesis, Anti-Inflammatory and Analgesic Activity Evaluation of Some Pyrimidine Derivatives. *Indian J. Chem.* **2009**, *49b*, 273-281. http://nopr.niscpr.res.in/handle/123456789/3429.
80. Russowsky, D.; Canto, R. F. S.; Sanches, S. A. A.; D'Oca, M. G. M.; Synthesis and Differential Antiproliferative Activity of Biginelli Compounds against Cancer Cell Lines: Monastrol, Oxo-Monastrol, and Oxygenated Analogues. *Bioorg. Chem.* **2006**, *34*, 173-182. https://doi.org/10.1016/j.bioorg.2006.04.003.
81. Heys, L.; Moore, C. G.; Murphy, P. The Guanidine Metabolites of *Ptilocaulis spiculifer* and Related Compounds: Isolation and Synthesis. *Chem. Soc. Rev.* **2000**, *29*, 57–67. DOI: 10.1039/A903712H.
82. Woerly, E. The Biginelli Reaction: Development and Application. In *Organic chemistry seminar at the University of Illinois,* **2008**, (pp. 1-8).
83. Kappe, C. O. 100 Years of the Biginelli Dihydropyrimidine Synthesis. *Tetrahedron* **1993**, *49*, 6937–6963. DOI: 10.1016/S0040-4020(01)87971-0.
84. Jagir, S. S. Past, Present and Future of the Biginelli Reaction: A Critical Perspective. *ARKIVOC* **2012**, 66–133. DOI: 10.3998/ark.5550190.0013.103.
85. Maharramov, A. M., Ramazanov, M. A., Guliyeva, G. A., Huseynzada, A. E., Hasanova, U. A., Shikhaliyev, N. G. & Aghayev, M. M.. Synthesis, investigation of the new derivatives of dihydropyrimidines and determination of their biological activity. *Jour. Mol. Struc.*, **2017**, *1141*, 39-43. DOI: 10.1016/j.molstruc.2017.03.084.
86. Atwal, K. S.; Swanson, B. N.; Unger, S. E.; Floyd, D. M.; Moreland, S.; Hedberg, A.; O'Reilly, B. C. 3-Carbamoyl-4-aryl-1,2,3,4-tetrahydro-6-methyl-5-pyrimidinecarboxylic Acid Esters as Orally Effective Antihypertensive Agents. *J. Med. Chem.* **1991**, *34*, 806–811. https://doi.org/10.1021/jm00106a048.
87. Rovnyak, G. C., Kimball, S. D., Beyer, B., Cucinotta, G., DiMarco, J. D., Gougoutas, J. & McCarthy, J. P. Calcium Entry Blockers and Activators: Conformational and Structural Determinants of Dihydropyrimidine Calcium Channel Modulators. *J. Med. Chem.* **1995**, *38*(1), 119–129. DOI: 10.1021/jm00001a017.
88. Kappe, C. O.; Fabian, W. M. W.; Semones, M. A. Conformational Analysis of 4-aryl Dihydropyrimidine Calcium Channel Modulators: A Comparison of Ab Initio, Semiempirical,

and X-ray Crystallographic Studies. *Tetrahedron* **1997**, *53*(8), 2803–2816. DOI: 10.1016/S0040-4020(97)00022-7.

89. Collin, G.; Höke, H. Quinoline and Isoquinoline. In *Ullmann's Encyclopedia of Industrial Chemistry*; Wiley-VCH: 2000; pp 1–5. DOI: 10.1002/14356007.a22_465.
90. Ramachandran, V.; Arumugasamy, K.; Singh, S. K.; Edayadulla, N.; Ramesh, P.; Kamaraj, S. K. Synthesis, Antibacterial Studies, and Molecular Modeling Studies of 3,4-Dihydropyrimidinone Compounds. *J. Chem. Biol.* **2016**, *9*, 31–40. DOI: 10.1007/s12154-015-0142-4.
91. Abelman, M. M.; Smith, S. C.; James, D. R. Cyclic Ketones and Substituted α-Keto Acids as Alternative Substrates for Novel Biginelli-Like Scaffold Syntheses. *Tetrahedron Lett.* **2003**, *44*(24), 4559–4562. DOI: 10.1016/S0040-4039(03)00985-7.
92. Prakash, O.; Pannu, K.; Naithani, R.; Kaur, H. One□Pot Synthesis of Oxime Derivatives of 1,3□Diphenylpyrazole□4□Carboxaldehydes from Acetophenone Phenylhydrazones Using Vilsmeier–Haack Reagent. *Synth. Commun.* **2006**, *36*(23), 3479–3485. DOI: 10.1080/00397910600942941.
93. Trivedi, A. R.; Bhuva, V. R.; Dholariya, B. H.; Dodiya, D. K.; Kataria, V. B.; Shah, V. H. Novel Dihydropyrimidines as a Potential New Class of Antitubercular Agents. *Bioorg. Med. Chem. Lett.* **2010**, *20*(20), 6100–6102. DOI: 10.1016/j.bmcl.2010.08.046.
94. Agbaje, O. C.; Fadeyi, O. O.; Fadeyi, S. A.; Myles, L. E.; Okoro, C. O. Synthesis and In Vitro Cytotoxicity Evaluation of Some Fluorinated Hexahydropyrimidine Derivatives. *Bioorg. Med. Chem. Lett.* **2011**, *21*(3), 989–992. DOI: 10.1016/j.bmcl.2010.12.022.
95. Winter, C. A.; Risley, E. A.; Nuss, G. W. Carrageenin-Induced Edema in Hind Paw of the Rat as an Assay for Anti-Inflammatory Drugs. *Proc. Soc. Exp. Biol. Med.* **1962**, *111*(3), 544–547. https://doi.org/10.3181/00379727-111-27849.
96. Mohamed, M. S.; Awad, S. M.; Zohny, Y. M.; Mohamed, Z. M. New Theopyrimidine Derivatives of Expected Anti-Inflammatory Activity. *Pharmacophore* **2012**, *3*(1-2012), 62–75. ISSN: 2229-5402.
97. Wan, J. P.; Liu, Y. S. Synthesis of Dihydropyrimidinones and Thiones by Multicomponent Reactions: Strategies Beyond the Classical Biginelli Reaction. *Synthesis* **2010**, *2010*(23), 3943–3953. DOI: 10.1055/s-0030-1258290.
98. Ghannam, I. A.; Abd El-Meguid, E. A.; Ali, I. H.; Sheir, D. H.; El Kerdawy, A. M. Novel 2-Arylbenzothiazole DNA Gyrase Inhibitors: Synthesis, Antimicrobial Evaluation, QSAR and

Molecular Docking Studies. *Bioorg. Chem.* **2019**, *93*, 103373. DOI: 10.1016/j.bioorg.2019.103373.

99. Nayak, S. K.; Venugopala, K. N.; Chopra, D.; Govender, T.; Kruger, H. G.; Maguire, G. E.; Guru Row, T. N. Ethyl 4-(4-Chlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate. *Acta Crystallogr. Sect. E Struct. Rep. Online* **2009**, *65*(10), 2518. https://doi.org/10.1107/S1600536809037453.
100. Salem, M. A.; Behalo, M. S.; Elrazaz, E. Green Synthesis and 3D Pharmacophore Study of Pyrimidine and Glucoside Derivatives with In Vitro Potential Anticancer and Antioxidant Activities. *Med. Chem. Res.* **2019**, *28*, 1223–1234. DOI: 10.1007/s00044-019-02367-9.
101. Sujayev, A. S. Synthesis and Antimicrobial Properties of Some Tetra (Hexa) Hydropyrimidinethiones. *Am. Sci. J.* **2016**, *4*, 55–59.
102. Shafiq, N.; Ashraf, S.; Parveen, S.; Ali, B. A One-Pot Rapid Synthesis, Docking Study and Biological Evaluation of Some Tetrahydropyrimidine-5-carboxylates. *Indian J. Heterocycl. Chem.* **2019**, *29* (3), 249–253. ISSN : 2456-4311.
103. Braga, T. C.; Silva, T. F.; Maciel, T. M. S.; Silva, E. C. D.; Silva-Junior, E. F.; Modolo, L. V.; de Fatima, A. Ionic Liquid-Assisted Synthesis of Dihydropyrimidin (Thi) One Biginelli Adducts and Investigation of Their Mechanism of Urease Inhibition. *New J. Chem.* **2019**, *43* (38), 15187–15200. DOI https://doi.org/10.1039/C9NJ03556G.
104. Al-Sayed, E.; Hamid, H. A.; El Einin, H. M. A.; Ali, E.; Fahmy, Z. New Pyrimidine And Fused Pyrimidine Derivatives: Synthesis And Anti Hepatitis A Virus (Hav) Evaluation *Int. J. Pharm.* **2005**, *5* (1), 69–79. ISSN 2249-1848.
105. Huseynzada, A. E.; Jelsch, C.; Akhundzada, H. N.; Soudani, S.; Nasr, C. B.; Doria, F.; Freccero, M. Synthesis, Crystal Structure, and Antibacterial Properties of 6-Methyl-2-thio-4-(quinolin-2-yl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate. *J. Mol. Struct.* **2020**, *1219*, 128581. https://doi.org/10.1016/j.molstruc.2020.128581.
106. Arshad, U.; Ahmed, S.; Shafiq, N.; Ahmad, Z.; Hassan, A.; Akhtar, N.; Mehmood, T. Structure-Based Designing, Solventless Synthesis of 1,2,3,4-tetrahydropyrimidine-5-carboxylate Derivatives: A Combined *In Vitro* and *In Silico* Screening Approach. *Molecules* **2021**, *26* (15), 4424. https://doi.org/10.3390/molecules26154424.
107. Bakht, J.; Khan, S.; and Shafi, M. In Vitro Antimicrobial Activity of Allium Cepa (Dry Bulbs) Against Gram Positive and Gram-Negative Bacteria and Fungi. *Pak. J. Pharm. Sci.*, **2014**, *27*, 139-145. DOI: 10.1016/j.micpath.2018.08.008.

108. Trott, O.; Olson, A. J. Software News and Update Autodock Vina: Improving The Speed and Accuracy of Docking With A New Scoring Function. *Effic. Optim. Multithreading*, **2009**, *31*, 455-461. DOI: 10.1002/jcc.21334.

109. Dassault Systemes Biovia. *Discovery Studio Modeling Environment*, Release 2017; Dassault Systemes: San Diego, 2017.

110. Ali, I.; Lone, M. N.; Al-Othman, A.; Al-Warthan, A.; Sanagi, M. M. Heterocyclic Scaffolds: Centrality in Anticancer Drug Development. *Curr. Drug Targets* **2015**, *16* (7), 711–734. https://doi.org/10.2174/1389450116666150309115922.

111. Martorana, A.; Giacalone, V.; Bonsignore, R.; Pace, A.; Gentile, C.; Pibiri, I.; Palumbo Piccionello, A. Heterocyclic Scaffolds for the Treatment of Alzheimer's Disease. *Curr. Pharm. Des.* **2016**, *22* (26), 3971–3995. https://doi.org/10.2174/1381612822666160518141650.

112. Shiro, T.; Fukaya, T.; Tobe, M. The Chemistry and Biological Activity of Heterocycle-Fused Quinolinone Derivatives: A Review. *Eur. J. Med. Chem.* **2015**, *97*, 397–408. https://doi.org/10.1016/j.ejmech.2014.12.004.

113. Anand, P.; Singh, B. Pyrrolo-Isoxazole: A Key Molecule with Diverse Biological Actions. *Mini-Rev. Med. Chem.* **2014**, *14* (7), 623–627. https://doi.org/10.2174/1389557514999140728102737.

114. Barmade, A.; Murumkar, R.; Sharma, K.; Yadav, R. Medicinal Chemistry Perspective of Fused Isoxazole Derivatives. *Curr. Top. Med. Chem.* **2016**, *16* (26), 2863–2883. https://doi.org/10.2174/1568026616666160506145700.

115. Page, L. W.; Bailey, M.; Beswick, P. J.; Frydrych, S.; Gleave, R. J. The Acid-Mediated Intramolecular 1,3-Dipolar Cycloaddition of Derived 2-Nitro-1,1-Ethenediamines for the Synthesis of Novel Fused Bicyclic Isoxazoles. *Tetrahedron Lett.* **2010**, *51* (26), 3388–3391. https://doi.org/10.1016/j.tetlet.2010.04.098.

116. Firestone, R. A. Mechanism of 1,3-Dipolar Cycloadditions. *J. Org. Chem.* **1968**, *33* (6), 2285–2290. https://doi.org/10.1021/jo01270a023.

117. Huisgen, R. Mechanism of 1,3-Dipolar Cycloadditions. Reply. *J. Org. Chem.* **2002**, *33* (6), 2291–2297. https://doi.org/10.1021/jo01270a024.

118. Shaik, A.; Bhandare, R. R.; Palleapati, K.; Nissankararao, S.; Kancharlapalli, V.; Shaik, S. Antimicrobial, Antioxidant, and Anticancer Activities of Some Novel Isoxazole Ring Containing Chalcone and Dihydropyrazole Derivatives. *Molecules*, **2020**, *25*, 1047. DOI: 10.3390/molecules25051047.

119. Rodriguez, A. D.; Ramirez, C.; Rodriguez, I. I.; Gonzalez, E. Novel Antimycobacterial Benzoxazole Alkaloids, from The West Indian Sea Whip Pseudopterogorgia Elisabethae. *Org. Lett.*, **1999**, *1*(3), 527-530. DOI: 10.1021/ol9907116.

120. Mckee, M. L.; Kerwin, S. M. Synthesis, Metal Ion Binding, and Biological Evaluation of New Anticancer 2-(2′-Hydroxyphenyl)benzoxazole Analogs of UK-1. *Bioorg. Med. Chem.*, **2008**, *16*, 1775-1783. DOI: 10.1016/j.bmc.2007.11.019.

121. Zhang, H. Z.; Zhao, Z. L.; Zhou, C. H. Recent Advance in Oxazole-Based Medicinal Chemistry. *Eur. J. Med. Chem.*, **2018**, *144*, 444-492. DOI: 10.1016/j.ejmech.2017.12.044.

122. Stokes, N. R.; Baker, N.; Bennett, J. M.; Chauhan, P. K.; Collins, I.; Davies, D. T.; Haydon, D. J. Design, Synthesis and Structure – Activity Relationships of Substituted Oxazole–Benzamide Antibacterial Inhibitors of Ftsz. *Bioorg. Med. Chem.*, **2014**, *24*(1), 353-359. DOI: 10.1016/j.bmcl.2013.11.002.

123. Yamamuro, D.; Uchida, R.; Ohtawa, M.; Arima, S.; Futamura, Y.; Katane, Tomoda, H; Synthesis and Biological Activity of 5-(4-Methoxyphenyl)oxazole Derivatives. *Bioorg. Med. Chem.*, **2015**, *25*, 313-316. DOI: 10.1016/j.bmcl.2014.11.042.

124. Zhong, Z. J.; Zhang, D. J.; Peng, Z. G.; Li, Y. H., Shan; G. Z., Zuo; L. M.; Li, Z. R. Synthesis and Antiviral Activity of A Novel Class of (5-Oxazolyl)phenyl Amines. *Eur. J. Med. Chem.*, **2013**, *69*, 32-43. DOI: 10.1016/j.ejmech.2013.07.053.

125. Palleapati, K.; Kancharlapalli, V. R.; Shaik, A. B. Synthesis, Characterization and Antitubercular Evaluation of Some New Isoxazole Appended 1-Carboxamido-4,5-dihydro-1*H*-Pyrazoles. *J. Res. Pharm*, **2019**, *23*, 156-163. DOI: 10.12991/Jrp.2019.120.

126. Lee, H. K.; Yun, E.; Min, J. H.; Yoon, K. S.; Choung, D. H.; Lee, S. Convenient Synthesis of An Isoxazole Compound, KRIBB3, as An Anticancer Agent. *Synth. Commun.*, **2012**, *42*, 1890–1894. DOI: 10.1080/00397911.2010.546551.

127. Shakya, A. K.; Kaur, A.; Al-Najjar, B. O.; Naik, R. R. Molecular Modeling, Synthesis, Characterization and Pharmacological Evaluation of Benzo[*d*]oxazole Derivatives as Non-Steroidal Anti-Inflammatory Agents. *Saudi Pharm. J.*, **2016**, *24*, 616-624. DOI: 10.1016/j.jsps.2015.03.018.

128. Abdi, B.; Fekadu, M.; Zeleke, D.; Eswaramoorthy, R.; Melaku, Y. Synthesis and Evaluation of the Antibacterial and Antioxidant Activities of Some Novel Chloroquinoline Analogs. *J. Chem.*, **2021**, 1-13. DOI: 10.1155/2021/2408006.

129. Kumar Gupta, S.; Mishra, A. Synthesis, Characterization and Screening for Anti-Inflammatory and Analgesic Activity of Quinoline Derivatives Bearing Azetidinones Scaffolds. *Anti-*

Inflamm. Anti-Allergy Agents Med. Chem., **2016**, *15*, 31-43. DOI: 10.2174/1871523015666160210124545.

130. Goda, F. E.; Alaa, A. M.; Ghoneim, H. A. Synthesis and Biological Evaluation of Novel 6-Nitro-5-Substituted Aminoquinolines as Local Anaesthetic and Anti-Arrhythmic Agents: Molecular Modeling Study. *Bioorg. Med. Chem.*, **2005**, *13*, 3175-3183. DOI: 10.1016/j.bmc.2005.02.050.
131. Jin, H. G.; Sun, X. Y.; Chai, K. Y.; Piao, H. R.; Quan, Z. S. Anticonvulsant and Toxicity Evaluation of Some 7-Alkoxy-4,5-dihydro-[1,2,4]triazolo[4,3-*a*]quinoline-1(2*H*)-Ones. *Bioorg. Med. Chem.*, **2006,** *14*(20), 6868-6873. DOI: 10.1016/j.bmc.2006.06.044.
132. Zajdel, P.; Marciniec, K.; Maślankiewicz, A.; Grychowska, K.; Satała, G.; Duszynska, B; Pawłowski, M. Antidepressant and Antipsychotic Activity of New Quinoline and Isoquinoline-Sulfonamide Analogs of Aripiprazole Targeting Serotonin 5-HT1A/5-HT2A/5-HT7 and Dopamine D2/D3 Receptors. *Eur. J. Med. Chem.*, **2013**, *60*, 42-50. DOI: 10.1016/j.ejmech.2012.11.042.
133. Kumar, H.; Devaraji, V.; Joshi, R.; Jadhao, M.; Ahirkar, P.; Prasath, R.; Ghosh, S. K. Antihypertensive Activity of A Quinoline Appended Chalcone Derivative and Its Site Specific Binding Interaction With A Relevant Target Carrier Protein. *RSC Adv.*, **2015**, *5*, 65496-65513. DOI: 10.1039/C5RA08778C.
134. Muruganantham, N.; Sivakumar, R.; Anbalagan, N.; Gunasekaran, V.; Leonard, J. T. Synthesis, Anticonvulsant and Antihypertensive Activities of 8-Substituted Quinoline Derivatives. *Biol. Pharm. Bull.*, **2004**, *27*, 1683-1687. DOI: 10.1248/bpb.27.1683.
135. Deshmukh, A. R.; Dhumal, S. T.; Nawale, L. U.; Khedkar, V. M.; Sarkar, D.; Mane, R. A. Dicationic Liquid Mediated Synthesis of Tetrazoloquinolinyl Methoxy Phenyl 4-Thiazolidinones and Their Antibacterial and Antitubercular Evaluation. *Synth. Commu.*, **2019**, *49*(4), 587-601. DOI: 10.1080/00397911.2018.1564928.
136. Senerovic, L.; Opsenica, D.; Moric, I.; Aleksic, I.; Spasic, M.; Vasiljevic, B. Quinolines and Quinolones as Antibacterial, Antifungal, Anti-Virulence, Antiviral and Anti-Parasitic Agents. *Adv. Microbiol., Infect. Dis. Public Health* **2020**, *14*, 37–69. DOI: 10.1007/5584_2019_428.
137. Shaik, A.; Bhandare, R. R.; Palleapati, K.; Nissankararao, S.; Kancharlapalli, V.; Shaik, S. Antimicrobial, Antioxidant, and Anticancer Activities of Some Novel Isoxazole Ring Containing Chalcone and Dihydropyrazole Derivatives. *Molecules* **2020**, *25*, 1047. DOI: 10.3390/molecules25051047.

138. Fonseca-Berzal, C.; Arenas, D. R. M.; Bohorquez, A. R. R.; Escario, J. A.; Kouznetsov, V. V.; Gomez-Barrio, A. Selective Activity of 2,4-Diaryl-1,2,3,4-tetrahydroquinolines on *Trypanosoma cruzi* Epimastigotes and Amastigotes Expressing β-Galactosidase. *Bioorg. Med. Chem. Lett.* **2013**, *23*, 4851–4856. DOI: 10.1016/j.bmcl.2013.06.079.

139. Santos, M. R. A.; Duarte, Y. B.; Guiza, F. M.; Bohorquez, A. R. R.; Mendez-Sanchez, S. C. Effects of New Tetrahydroquinoline-Isoxazole Hybrids on Bioenergetics of Hepatocarcinoma Hep-G2 Cells and Rat Liver Mitochondria. *Chem. Biol. Interact.* **2019**, *302*, 164–171. DOI: 10.1016/j.cbi.2019.02.002.

140. Bokkala, K.; Bapuram, A. K.; Thirukovela, N. S.; Nukala, S. K. Synthesis of Fused Isoxazoles of Iodoquinol as in Vitro EGFR-Aiming Anticancer Agents. *Chem. Sel.* **2024**, *9*, e202302584. DOI: 10.1002/slct.202302584.

141. Galenko, E. E.; Novikov, M. S.; Bunev, A. S.; Khlebnikov, A. F. Acridine–Isoxazole and Acridine–Azirine Hybrids: Synthesis, Photochemical Transformations in the UV/Visible Radiation Boundary Region, and Anticancer Activity. *Molecules* **2024**, *29*, 1538. DOI: 10.3390/molecules29071538.

142. Guiza, F. M.; Duarte, Y. B.; Mendez-Sanchez, S. C.; Bohorquez, A. R. R. Synthesis and In Vitro Evaluation of Substituted Tetrahydroquinoline-Isoxazole Hybrids as Anticancer Agents. *Med. Chem. Res.* **2019**, *28*, 1182–1196. DOI: 10.1007/s00044-019-02363-z.

143. Akbari, J. D.; Tala, S. D.; Dhaduk, M. F.; Joshi, H. S.; Mehta, K. B.; Pathak, S. J. Synthesis of Some New Pyrazolo[3,4-*d*]pyrimidines and Thiazolo[4,5-*d*]pyrimidines and Evaluation of Their Antimicrobial Activities. *Phosphorus, Sulfur, Silicon Relat. Elem.* **2008**, *183*, 1471–1477. DOI: 10.1080/10426500701681581.

144. Thaker, K. M.; Ghetiya, R. M.; Tala, S. D.; Dodiya, B. L.; Joshi, K. A.; Dubal, K. L.; Joshi, H. S. Synthesis of Oxadiazoles and Pyrazolones as Antimycobacterial and Antimicrobial Agents. *Indian J. Chem. B* **2011**, *50B*, 738–744. DOI: http://nopr.niscpr.res.in/handle/123456789/11693.

145. Pellegrino, G.; Leonetti, F.; Carotti, A.; Nicolotti, O.; Pisani, L.; Stefanachi, A.; Catto, M. Solid Phase Synthesis of a Molecular Library of Pyrimidines, Pyrazoles, and Isoxazoles with Biological Potential. *Tetrahedron Lett.* **2010**, *51*, 1702–1705. DOI: 10.1016/j.tetlet.2010.01.089.

146. Lee, H. K.; Yun, E.; Min, J. H.; Yoon, K. S.; Choung, D.-H.; Lee, S. Convenient Synthesis of an Isoxazole Compound, KRIBB3, as an Anticancer Agent. *Synth. Commun.* **2012**, *42*, 1890–1894. DOI: 10.1080/00397911.2010.546551.

147. Burra, S.; Voora, V.; Rao, C. P.; Vijay Kumar, P.; Kancha, R. K.; Kru, D.; Padanam, G. L. Synthesis of Novel Forskolin Isoxazole Derivatives with Potent Anti-Cancer Activity Against Breast Cancer Cell Lines. *Bioorg. Med. Chem. Lett.* **2017**, *27*, 4314–4318. DOI: 10.1016/j.bmcl.2017.08.033.
148. Rouf, A.; Şahin, E.; Tanyeli, C. Divergent Synthesis of Polysubstituted Isoxazoles, Isoxazoline N-Oxides, and Dihydroisoxazoles by a One-Pot Cascade Reaction. *Tetrahedron* **2017**, *73*, 331–337. DOI: 10.1016/j.tet.2016.12.005.
149. Bommagani, M. B.; Yerrabelly, J. R.; Chitneni, M.; Thalari, G.; Vadiyala, N. R.; Boda, S. K.; Chitneni, P. R. Synthesis and Antibacterial Activity of Novel Cinnoline-Isoxazole Derivatives. *Chem. Data Collect.* **2021**, *31*, 100629. DOI: 10.1016/j.cdc.2020.100629.
150. Aleti, R. R.; Cherukupalli, S.; Dhawan, S.; Kumar, V.; Girase, P. S.; Mohite, S.; Karpoormath, R. A. Metal-Free Approach for in Situ Regioselective Synthesis of Isoxazoles Via 1,3-Dipolar Cycloaddition Reaction of Nitrile Oxide with Propargyl Bromide. *Chem. Pap.* **2022**, *76*, 3005–3010. DOI: 10.1007/s11696-021-02009-8.
151. Childers, M. C.; Daggett, V. Insights from Molecular Dynamics Simulations for Computational Protein Design. *Mol. Syst. Des. Eng.* **2017**, *2*, 9–33. DOI: 10.1039/C6ME00083E.
152. De Souza, O. N.; Ornstein, R. L. Effect of Warmup Protocol and Sampling Time on Convergence of Molecular Dynamics Simulations of a DNA Dodecamer using AMBER 4.1 and Particle-Mesh Ewald Method. *J. Bio. Struct. Dyn.* **1997**, *14*, 607–611. DOI: 10.1080/07391102.1997.10508160.
153. Wittig, G.; Geissler, G. Zur Reaktionsweise des Phenyl-lithiums. *Justus Liebigs Ann. Chem.* **1953**, *580*, 44–57. DOI: 10.1002/jlac.19535800105.
154. Byrne, P. A.; Gilheany, D. G. The Modern Interpretation of the Wittig Reaction Mechanism. *Chem. Soc. Rev.* **2013**, *42*, 6670–6696. DOI: 10.1039/C3CS60105F.
155. Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry: Part B: Reactions and Synthesis*, 5th ed.; Springer: New York, 2007.
156. Smith, M. B.; March, J. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6th ed.; Wiley: New York, 2007.
157. Parvatkar, P. T.; Torney, P. S.; Tilve, S. G. Recent Developments of Wittig Reaction in Organic Synthesis through Tandem or Sequential Processes. *Curr. Org. Synth.* **2013**, *10*, 288–317. DOI: 10.2174/1570179411310020005.

158. Ilia, G., Simulescu, V., Plesu, N., Chiriac, V., & Merghes, P. Wittig and Wittig–Horner Reactions under Sonication Conditions. *Molecules*, **2023**, *28*(4), 1958. https://doi.org/10.3390/molecules28041958.

159. Byrne, P. A.; Gilheany, D. G. The Modern Interpretation of the Wittig Reaction Mechanism. *Chem. Soc. Rev.* **2013**, *42*, 6670–6696. https://doi.org/10.1039/C3CS60105F.

160. Vedejs, E.; Peterson, M. J. Stereochemistry and Mechanism in the Wittig Reaction. *Topics Stereochem.* **1994**, *21*, 1–157. DOI: 10.1002/9780470147306.

161. Vedejs, E.; Marth, C. F. Mechanism of the Wittig Reaction: The Role of Substituents at Phosphorus. *J. Am. Chem. Soc.* **1988**, *110*, 3948–3958. https://doi.org/10.1021/ja00220a037.

162. Maryanoff, B. E.; Reitz, A. B.; Mutter, M. S.; Whittle, R. R.; Olofson, R. A. Stereochemistry and Mechanism of the Wittig Reaction: Diastereomeric Reaction Intermediates and Analysis of the Reaction Course. *J. Am. Chem. Soc.* **1986**, *108*, 7664–7678. https://doi.org/10.1021/ja00284a034.

163. Yang, H.; Zhang, J.; Zhang, S.; Xue, Z.; Hu, S.; Chen, Y.; Tang, Y. Chiral Bisphosphine-Catalyzed Asymmetric Staudinger/Aza-Wittig Reaction: An Enantioselective Desymmetrizing Approach to Crinine-Type Amaryllidaceae Alkaloids. *J. Am. Chem. Soc.* **2024**, *146*, 14136–14148. https://doi.org/10.1021/jacs.4c02755.

164. Rodríguez, A. D.; Ramírez, C.; Rodríguez, I. I.; González, E. Novel Antimycobacterial Benzoxazole Alkaloids, from the West Indian Sea Whip *Pseudopterogorgia elisabethae*. *Org. Lett.* **1999**, *1*, 527–530. DOI: 10.1021/ol9907116. https://doi.org/10.1021/ol9907116.

165. Zhang, H. Z.; Zhao, Z. L.; Zhou, C. H. Recent Advance in Oxazole-Based Medicinal Chemistry. *Eur. J. Med. Chem.* **2018**, *144*, 444–492. DOI: 10.1016/j.ejmech.2017.12.044.

166. Stokes, N. R.; Baker, N.; Bennett, J. M.; Chauhan, P. K.; Collins, I.; Davies, D. T.; Haydon, D. J. Design, Synthesis, and Structure–Activity Relationships of Substituted Oxazole–Benzamide Antibacterial Inhibitors of FtsZ. *Bioorg. Med. Chem.* **2014**, *24*, 353–359. DOI: 10.1016/j.bmcl.2013.11.002.

167. Yamamuro, D.; Uchida, R.; Ohtawa, M.; Arima, S.; Futamura, Y.; Katane, T.; Tomoda, H. Synthesis and Biological Activity of 5-(4-Methoxyphenyl)-Oxazole Derivatives. *Bioorg. Med. Chem.* **2015**, *25* (2), 313–316. https://doi.org/10.1016/j.bmcl.2014.11.042.

168. Zhong, Z. J.; Zhang, D. J.; Peng, Z. G.; Li, Y. H.; Shan, G. Z.; Zuo, L. M.; Li, Z. R. Synthesis and Antiviral Activity of a Novel Class of (5-Oxazolyl)Phenyl Amines. *Eur. J. Med. Chem.* **2013**, *69*, 32–43. https://doi.org/10.1016/j.ejmech.2013.07.053.

169. Palleapati, K.; Kancharlapalli, V. R.; Shaik, A. B. Synthesis, Characterization, and Antitubercular Evaluation of Some New Isoxazole-Appended 1-Carboxamido-4,5-Dihydro-1H-Pyrazoles. *J. Res. Pharm.* **2019**, *23* (2), 156–163. https://doi.org/10.12991/jrp.2019.120.

170. Semenyuta, I.; Kovalishyn, V.; Tanchuk, V.; Pilyo, S.; Zyabrev, V.; Blagodatnyy, N.; Metelytsia, L. 1,3-Oxazole Derivatives as Potential Anticancer Agents: Computer Modeling and Experimental Study. *Comput. Biol. Chem.* **2016**, *65*, 8–15. https://doi.org/10.1016/j.compbiolchem.2016.09.012.

171. Shakya, A. K.; Kaur, A.; Al-Najjar, B. O.; Naik, R. R. Molecular Modeling, Synthesis, Characterization, and Pharmacological Evaluation of Benzo[d]Oxazole Derivatives as Non-Steroidal Anti-Inflammatory Agents. *Saudi Pharm. J.* **2016**, *24* (5), 616–624. https://doi.org/10.1016/j.jsps.2015.03.018.

172. Karmacharya, U.; Guragain, D.; Chaudhary, P.; Jee, J. G.; Kim, J. A.; Jeong, B. S. Novel Pyridine Bioisostere of Cabozantinib as a Potent c-Met Kinase Inhibitor: Synthesis and Anti-Tumor Activity Against Hepatocellular Carcinoma. *Int. J. Mol. Sci.* **2021**, *22* (18), 9685. https://doi.org/10.3390/ijms22189685.

173. Ben-Baruch, N. E.; Bose, R.; Kavuri, S. M.; Ma, C. X.; Ellis, M. J. HER2-Mutated Breast Cancer Responds to Treatment with Single-Agent Neratinib, a Second-Generation HER2/EGFR Tyrosine Kinase Inhibitor. *J. Natl. Compr. Cancer Netw.* **2015**, *13* (9), 1061–1064. https://doi.org/10.6004/jnccn.2015.0131.

174. Yeates, C. Sitamaquine (GlaxoSmithKline/Walter Reed Army Institute). *Curr. Opin. Investig. Drugs* **2002**, *3* (10), 1446–1452. PMID: 12431016.

175. Somagond, M. S.; Kamble, R. R.; Kattimani, P. P.; Shaikh, S. K. J.; Dixit, S. R.; Joshi, S. D.; Devarajegowda, H. C. Design, Docking, and Synthesis of Quinoline-2*H*-1,2,4-Triazol-3(4*H*)-Ones as Potent Anticancer and Antitubercular Agents. *Chem. Sel.* **2018**, *3* (7), 2004–2016. https://doi.org/10.1002/slct.201702279.

176. Hong, D. S.; Rosen, P.; Lockhart, A. C.; Fu, S.; Janku, F.; Kurzrock, R.; Lee, P. A First-in-Human Study of AMG 208, an Oral MET Inhibitor, in Adult Patients with Advanced Solid Tumors. *Oncotarget* **2015**, *6* (21), 18693. https://doi.org/10.18632/oncotarget.4472.

177. Sebolt, J. S.; Scavone, S. V.; Pinter, C. D.; Hamelehle, K. L.; Von Hoff, D. D.; Jackson, R. C. Pyrazoloacridines, a New Class of Anticancer Agents with Selectivity Against Solid Tumors in Vitro. *Cancer Res.* **1987**, *47* (16), 4299–4304. PMID: 2440564.

178. Singh, R. P.; Patel, B.; Kallender, H.; Ottesen, L. H.; Adams, L. M.; Cox, D. S. Population Pharmacokinetics Modeling and Analysis of Foretinib in Adult Patients with Advanced Solid Tumors. *J. Clin. Pharmacol.* **2015**, *55* (10), 1184–1192. https://doi.org/10.1002/jcph.546.

179. Joint Formulary Committee (Ed.). *British National Formulary* (Vol. 64); Pharmaceutical Press: London, 2012; ISBN 9780857111562.

180. Horstmann, M. A.; Hassenpflug, W. A.; zur Stadt, U.; Escherich, G.; Janka, G.; Kabisch, H. Amsacrine Combined with Etoposide and High-Dose Methylprednisolone as Salvage Therapy in Acute Lymphoblastic Leukemia in Children. *Haematologica* **2005**, *90* (12), 1701–1703.

181. Wang, B.; Chu, D.; Feng, Y.; Shen, Y.; Aoyagi-Scharber, M.; Post, L. E. Discovery and Characterization of (8S, 9R)-5-Fluoro-8-(4-Fluorophenyl)-9-(1-Methyl-1*H*-1,2,4-Triazol-5-Yl)-2,7,8,9-Tetrahydro-3*H*-Pyrido[4,3,2-*d*,*e*]Phthalazin-3-One (BMN 673, Talazoparib), a Novel, Highly Potent, and Orally Efficacious Poly (ADP-Ribose) Polymerase-1/2 Inhibitor, as an Anticancer Agent. *J. Med. Chem.* **2016**, *59* (1), 335–357. https://doi.org/10.1021/acs.jmedchem.5b01498.

182. Dittrich, C.; Coudert, B.; Paz-Ares, L.; Caponigro, F.; Salzberg, M.; Gamucci, T.; Fumoleau, P. Phase II Study of XR 5000 (DACA), an Inhibitor of Topoisomerase I and II, Administered as a 120-H Infusion in Patients with Non-Small Cell Lung Cancer. *Eur. J. Cancer* **2003**, *39* (3), 330-334. https://doi.org/10.1016/S0959-8049(02)00559-2.

183. Seyrani, H.; Ramezanpour, S.; Vaezghaemi, A.; Kobarfard, F. A Sequential Ugi–Smiles/Transition-Metal-Free Endo-Dig Conia Ene Cyclization: The Selective Synthesis of Saccharin Substituted 2,5-Dihydropyrroles. *New J. Chem.* **2021**, *45* (34), 15647-15654. https://doi.org/10.1039/d1nj01159f.

184. Makowska, A.; Sączewski, F.; Bednarski, J.; Sączewski, J.; Balewski, L. Hybrid Molecules Composed of 2,4-Diamino-1,3,5-Triazines and 2-Imino-Coumarins and Coumarins: Synthesis and Cytotoxic Properties. *Molecules* **2018**, *23* (7), 1616. https://doi.org/10.3390/molecules23071616.

185. Shaveta, S.; Singh, P. Hybrid Molecules: The Privileged Scaffolds for Various Pharmaceuticals. *Eur. J. Med. Chem.* **2016**, *124*, 500-536. https://doi.org/10.1016/j.ejmech.2016.08.039.

186. Katariya, K. D.; Shah, S. R.; Reddy, D. Anticancer, Antimicrobial Activities of Quinoline-Based Hydrazone Analogues: Synthesis, Characterization, and Molecular Docking. *Bioorg. Chem.* **2020**, *94*, 103406. https://doi.org/10.1016/j.bioorg.2019.103406.

187. Patel, A. S.; Gandhi, S. A.; Modh, R. D.; Patel, U. H.; Naliapara, Y. T.; Kapuriya, N. P. Facile Synthesis of (*E*)-5-Styrylpyrimidines via Wittig Reaction Using Sodium Tripolyphosphate in Water. *Lett. Org. Chem.* **2021**, *18* (8), 634-639. https://doi.org/10.2174/1570178617999201012181526.

188. Dell'Erba, C.; Gabellini, A.; Novi, M.; Petrillo, G.; Tavani, C.; Cosimelli, B.; Spinelli, D. Ring Opening of 2-Substituted 4-Nitrothiophenes with Pyrrolidine: Access to New Functionalized Nitro-Unsaturated Building Blocks. *Tetrahedron* **2001**, *57* (38), 8159-8165. https://doi.org/10.1016/S0040-4020(01)00765-7.

189. Shet, J.; Desai, V.; Tilve, S. Domino Primary Alcohol Oxidation-Wittig Reaction: Total Synthesis of ABT-418 and (*E*)-4-Oxonon-2-Enoic Acid. *Synthesis* **2004**, *2004* (11), 1859-1863. https://doi.org/10.1055/s-2004-829123.

190. Dallanoce, C.; Magrone, P.; Matera, C.; Presti, L. L.; De Amici, M.; Riganti, L.; De Micheli, C. Synthesis of Novel Chiral Δ2-Isoxazoline Derivatives Related to ABT-418 and Estimation of Their Affinity at Neuronal Nicotinic Acetylcholine Receptor Subtypes. *Eur. J. Med. Chem.* **2010**, *45* (12), 5594-5601. https://doi.org/10.1016/j.ejmech.2010.09.009.

191. Sun, J.; Lin, C.; Qin, X.; Dong, X.; Tu, Z.; Tang, F.; Zhang, J. Synthesis and Biological Evaluation of 3,5-Disubstituted-4-Alkynylisoxazoles as a Novel Class of HSP90 Inhibitors. *Bioorg. Med. Chem. Lett.* **2015**, *25* (16), 3129-3134. https://doi.org/10.1016/j.bmcl.2015.06.009.

192. Purwono, B.; Smalley, R. K.; Porter, T. C. Isoxazolo [4,3-*c*] Quinoline Derivatives from o-Azidobenzonitrile Oxide by Sequential Carbanion Attack and Intramolecular Aza-Wittig Reaction. *Synlett* **1992**, *1992* (03), 231-232. DOI: 10.1055/s-1992-21323.

193. Sanghavi, K. N.; Sriram, D.; Kumari, J.; Kapadiya, K. M. Regioselective Pd-Catalyzed Suzuki–Miyaura Borylation Reaction for the Dimerization Product of 6-Bromoimidazo [1,2-*a*] Pyridine-2-Carboxylate: Mechanistic Pathway, Cytotoxic and Tubercular Studies. *Synlett* **2023**, *34* (09), 1049-1057. DOI: 10.1055/s-0042-1751404.

194. Al-Suwaidan, I. A.; Abdel-Aziz, N. I.; El-Azab, A. S.; El-Sayed, M. A. A.; Alanazi, A. M.; El-Ashmawy, M. B.; Abdel-Aziz, A. A. M. Antitumor Evaluation and Molecular Docking Study of Substituted 2-Benzylidenebutane-1,3-Dione, 2-Hydrazonobutane-1,3-Dione, and Trifluoromethyl-1H-Pyrazole Analogues. *J. Enzyme Inhib. Med. Chem.* **2015**, *30* (4), 679-687. https://doi.org/10.3109/14756366.2014.960863.

195. Artese, A.; Cross, S.; Costa, G.; Distinto, S.; Parrotta, L.; Alcaro, S.; Cruciani, G. Molecular Interaction Fields in Drug Discovery: Recent Advances and Future Perspectives. *Wiley Interdiscip. Rev.: Comput. Mol. Sci.* **2013**, *3* (6), 594–613. https://doi.org/10.1002/wcms.1143.

196. Taslimi, P.; Isik, M.; Turkan, F.; Durgun, M.; Turkeş, C.; Gulcin, I.; Beydemir, S. Benzenesulfonamide Derivatives as Potent Acetylcholinesterase, α-Glycosidase, and Glutathione S-Transferase Inhibitors: Biological Evaluation and Molecular Docking Studies. *J. Biomol. Struct. Dyn.* **2021**, *39* (15), 5449-5460. https://doi.org/10.1080/07391102.2020.1790422.

197. Selick, H. E.; Beresford, A. P.; Tarbit, M. H. The Emerging Importance of Predictive ADME Simulation in Drug Discovery. *Drug Discov. Today* **2002**, *7* (2), 109–116. https://doi.org/10.1016/S1359-6446(01)02194-2.

198. Lipinski, C. A.; Lombardo, F.; Dominy, B. W.; Feeney, P. J. Experimental and Computational Approaches to Estimate Solubility and Permeability in Drug Discovery and Development Settings. *Adv. Drug Deliv. Rev.* **2012**, *64*, 4-17. https://doi.org/10.1016/j.addr.2012.09.019.

199. Ghose, A. K.; Viswanadhan, V. N.; Wendoloski, J. J. Prediction of Hydrophobic (Lipophilic) Properties of Small Organic Molecules Using Fragmental Methods: An Analysis of ALOGP and CLOGP Methods. *J. Phys. Chem. A* **1998**, *102* (21), 3762-3772. https://doi.org/10.1021/jp980230o.

200. Veber, D. F.; Johnson, S. R.; Cheng, H. Y.; Smith, B. R.; Ward, K. W.; Kopple, K. D. Molecular Properties That Influence the Oral Bioavailability of Drug Candidates. *J. Med. Chem.* **2002**, *45* (12), 2615-2623. https://doi.org/10.1021/jm020017n.

201. Egan, W. J.; Lauri, G. Prediction of Intestinal Permeability. *Adv. Drug Deliv. Rev.* **2002**, *54* (3), 273-289. https://doi.org/10.1016/S0169-409X(02)00004-2.

202. Muegge, I.; Heald, S. L.; Brittelli, D. Simple Selection Criteria for Drug-Like Chemical Matter. *J. Med. Chem.* **2001**, *44* (12), 1841-1846. https://doi.org/10.1021/jm015507e.

203. Chen, X.; Li, H.; Tian, L.; Li, Q.; Luo, J.; Zhang, Y. Analysis of the Physicochemical Properties of Acaricides Based on Lipinski's Rule of Five. *J. Comput. Biol.* **2020**, *27* (9), 1397–1406. https://doi.org/10.1089/cmb.2019.0317.

204. Bojarska, J.; Remko, M.; Breza, M.; Madura, I. D.; Kaczmarek, K.; Zabrocki, J.; Wolf, W. M. A Supramolecular Approach to Structure-Based Design with a Focus on Synthons Hierarchy in Ornithine-Derived Ligands: Review, Synthesis, Experimental and In Silico Studies. *Molecules* **2020**, *25* (5), 1135. https://doi.org/10.3390/molecules25051135.

205. Prasad, S. K.; Pradeep, S.; Shimavallu, C.; Kollur, S. P.; Syed, A.; Marraiki, N.; Glossman-Mitnik, D. Evaluation of Annona Muricata Acetogenins as Potential Anti-SARS-CoV-2 Agents through Computational Approaches. *Front. Chem.* **2021**, *8*, 624716. https://doi.org/10.3389/fchem.2020.624716.

206. Kwofie, S. K.; Broni, E.; Asiedu, S. O.; Kwarko, G. B.; Dankwa, B.; Enninful, K. S.; Wilson, M. D. Cheminformatics-Based Identification of Potential Novel Anti-SARS-CoV-2 Natural Compounds of African Origin. *Molecules* **2021**, *26* (2), 406. https://doi.org/10.3390/molecules26020406.

207. Gaikwad, N. M.; Chaudhari, P. D.; Shaikh, K. S.; Chaudhari, S. Y.; Saleem, R. M.; Algahtani, M.; Abdel-Daim, M. M. Albendazole Repurposing on VEGFR-2 for Possible Anticancer Application: In-Silico Analysis. *PLoS One* **2023**, *18* (8), e0287198. https://doi.org/10.1371/journal.pone.0287198.

208. Choudhary, M. I.; Shaikh, M.; tul-Wahab, A.; ur-Rahman, A. In Silico Identification of Potential Inhibitors of Key SARS-CoV-2 3CL Hydrolase (Mpro) via Molecular Docking, MMGBSA Predictive Binding Energy Calculations, and Molecular Dynamics Simulation. *PLoS One* **2020**, *15* (7), e0235030. https://doi.org/10.1371/journal.pone.0235030.

209. Geerlings, P.; Fias, S.; Boisdenghien, Z.; De Proft, F. Conceptual DFT: Chemistry from the Linear Response Function. *Chem. Soc. Rev.* **2014**, *43* (14), 4989–5008. https://doi.org/10.1039/C4CS00057A.

210. Chakraborty, A.; Duley, S.; Giri, S.; Chattaraj, P. K. An Understanding of the Origin of Chemical Reactivity from a Conceptual DFT Approach. In *A Matter of Density: Exploring the Electron Density Concept in the Chemical, Biological, and Materials Sciences*; Elsevier, 2012; pp 157–201. https://doi.org/10.1016/B978-0-12-385219-8.00006-5.

211. Al-Khafaji, K.; Tok, T. T. Molecular Dynamics Simulation, Free Energy Landscape and Binding Free Energy Computations in Exploration the Anti-Invasive Activity of Amygdalin against Metastasis. *Comput. Methods Programs Biomed.* **2020**, *195*, 105660. https://doi.org/10.1016/j.cmpb.2020.105660.

212. Burley, S. K. Rcsb Protein Data Bank: Sustaining a Living Digital Data Resource that Enables Breakthroughs in Scientific Research and Biomedical Education. *Biophy.l Jour.*, **2019**, *116*(3), 329a. DOI: 10.1016/j.bpj.2018.11.1783.

213. O'Boyle, N. M.; Banck, M.; James, C. A.; Morley, C.; Vandermeersch, T.; Hutchison, G. R. Open Babel: An Open Chemical Toolbox. *J. Cheminf.* **2011**, *3*, 1-14. https://doi.org/10.1186/1758-2946-3-33.

214. Laskowski, R. A.; Swindells, M. B. LigPlot+: Multiple Ligand–Protein Interaction Diagrams for Drug Discovery. *J. Chem. Inf. Model.* **2011**, *51* (10), 2778-2786. https://doi.org/10.1021/ci200227u.

215. Frisch, M. J. *Gaussian 09, Revision D.01/Gaussian*, 2009.

216. Becke, A. D. A New Mixing of Hartree–Fock and Local Density-Functional Theories. *J. Chem. Phys.* **1993**, *98* (2), 1372-1377. https://doi.org/10.1063/1.464304.

217. Ahmad, I.; Khan, H.; Serdaroğlu, G. Physicochemical Properties, Drug Likeness, ADMET, DFT Studies, and In Vitro Antioxidant Activity of Oxindole Derivatives. *Comput. Biol. Chem.* **2023**, *104*, 107861. https://doi.org/10.1016/j.compbiolchem.2023.107861.

218. ProTox 3.0 - Prediction of Toxicity of Chemicals, https://tox new.charite.de/protox_II/index.php?site=home.

219. Ferreira, L. G.; Dos Santos, R. N.; Oliva, G.; Andricopulo, A. D. Molecular Docking and Structure-Based Drug Design Strategies. *Molecules* **2015**, *20* (7), 13384-13421. https://doi.org/10.3390/molecules200713384.

220. Issa, R. M.; Awad, M. K.; Atlam, F. M. DFT Theoretical Studies of Antipyrine Schiff Bases as Corrosion Inhibitors. *Mater. Corros.* **2010**, *61* (8), 709-714. https://doi.org/10.1002/maco.200905361.

221. Obot, I. B.; Kaya, S.; Kaya, C.; Tuzun, B. Density Functional Theory (DFT) Modeling and Monte Carlo Simulation Assessment of Inhibition Performance of Some Carbohydrazide Schiff Bases for Steel Corrosion. *Physica E: Low-Dimensional Syst. Nanostruct.* **2016**, *80*, 82-90. https://doi.org/10.1016/j.physe.2016.01.024.