References

Adler S, Ber M. 1941. Transmission of *Leishmania tropica* by the bite of Phlebotomus papatasii [5]. Nature 148(3747):227.

Ali R, Tabrez S, Akand SK, Rahman F, Husein A, Arish M, Alqahtani AS, Ahmed MZ, Husain M, Rub A. 2021. Sesamol Induces Apoptosis-Like Cell Death in *Leishmania donovani.* Front Cell Infect Microbiol 11:1–11.

Antwi CA, Amisigo CM, Adjimani JP, Gwira TM. 2019. In vitro activity and mode of action of phenolic compounds on *leishmania donovani.* PLoS Negl Trop Dis 13(2):1–22.

Are S, Gatreddi S, Jakkula P, Qureshi IA. 2020. Structural attributes and substrate specificity of pyridoxal kinase from *Leishmania donovani*. Int J Biol Macromol 152(June):812–827.

Arenas R, Torres-Guerrero E, Quintanilla-Cedillo MR, Ruiz-Esmenjaud J. 2017. Leishmaniasis: A review. F1000Research 6:1–15.

Aruleba RT, Carter KC, Brombacher F, Hurdayal R. 2020. Can we harness immune responses to improve drug treatment in leishmaniasis? Microorganisms 8(7):1–20.

Auger C, Lemire J, Cecchini D, Bignucolo A, Appanna VD. 2011. The metabolic reprogramming evoked by nitrosative stress triggers the anaerobic utilization of citrate in pseudomonas fluorescens. PLoS One 6(12).

Azam SS, Abro A, Raza S, Saroosh A. 2014. Structure and dynamics studies of sterol 24-C-methyltransferase with mechanism-based inactivators for the disruption of ergosterol biosynthesis. Mol Biol Rep 41(7):4279–4293.

Bhat SY, Qureshi IA. 2021. Structural and Functional Basis of Potent Inhibition of Leishmanial Leucine Aminopeptidase by Peptidomimetics. ACS Omega 6(29):19076–19085.

Bhowmik D, Jagadeesan R, Rai P, Nandi R, Gugan K, Kumar D. 2020. Evaluation of potential drugs against leishmaniasis targeting catalytic subunit of *Leishmania donovani* nuclear DNA primase using ligand-based virtual screening, docking, and molecular dynamics approaches. J

Biomol Struct Dyn 39(5):1838- 1852.

Bloxham DP, Parmelee DC, Kumar S, Wade RD, Ericsson LH, Neurath H, Walsh KA, Titani K. 1981. Primary structure of porcine heart citrate synthase. Proc Natl Acad Sci U S A 78(9 II):5381–5385.

Boelaert M, Meheus F, Sanchez A, Singh SP, Vanlerberghe V, Picado A, Meessen B, Sundar S. 2009. The poorest of the poor: A poverty appraisal of households affected by visceral leishmaniasis in Bihar, India. Trop Med Int Heal 14(6):639–644.

Bortoleti BT da S, Gonçalves MD, Tomiotto-Pellissier F, Contato VM, Silva TF, Matos RLN de, Detoni MB, Rodrigues ACJ, Carloto AC, Lazarin DB, Arakawa NS, Costa IN, Conchon-Costa I, Miranda-Sapla MM, Wowk PF, Pavanelli WR. 2021. Solidagenone acts on promastigotes of *L. amazonensis* by inducing apoptosis-like processes on intracellular amastigotes by IL-12p70/ROS/NO pathway activation. Phytomedicine 85:153536.

Broni E, Kwofie SK, Asiedu SO, Iii WAM, Wilson MD. 2021. A Molecular Modeling Approach to Identify Potential Antileishmanial Compounds Against the Cell Division Cycle (cdc) -2-Related Kinase 12 (CRK12) Receptor of *Leishmania donovani* 11(3):458.

Butt F, Yasinzai M, Malik SI, Munir A. 2020. Isolation and Characterization of Leishmanial Adenine Aminohydrolase as a Drug Target. Curr Comput Aided Drug Des 17(7):905–915.

Chapman ADM, Cortés A, Dafforn TR, Clarke AR, Brady RL. 1999. Structural basis of substrate specificity in malate dehydrogenases: Crystal structure of a ternary complex of porcine cytoplasmic malate dehydrogenase, α-ketomalonate and tetrahydoNAD. J Mol Biol 285(2):703–712.

Corona SP, Generali D. 2018. Abemaciclib: A CDK4/6 inhibitor for the treatment of HR+/HEeR2- advanced breast cancer. Drug Des Devel Ther 12:321–330.

Croft SL, Sundar S, Fairlamb AH. 2006. Drug resistance in leishmaniasis. Clin Microbiol Rev 19(1):111–126.

Das R, Roy A, Dutta N, Majumder HK. 2008. Reactive oxygen species and imbalance of calcium homeostasis contribute to curcumin-induced programmed cell death in *Leishmania donovani*. Apoptosis 13(7):867–882.

Dashty M. 2013. A quick look at biochemistry: Carbohydrate metabolism. Clin Biochem 46(15):1339–1352.

Davidson RN, Boer M den, Ritmeijer K. 2009. Paromomycin. Trans R Soc Trop Med Hyg 103(7):653–660.

Davies CR, Reithinger R, Campbell-Lendrum D, Feliciangeli D, Borges R, Rodriguez N. 2000. The epidemiology and control of leishmaniasis in Andean countries. Cad saúde pública / Ministério da Saúde, Fundação Oswaldo Cruz, Esc Nac Saúde Pública 16(4):925–950.

Dorlo TPC, Balasegaram M, Beijnen JH, vries PJ de. 2012. Miltefosine: A review of its pharmacology and therapeutic efficacy in the treatment of leishmaniasis. J Antimicrob Chemother 67(11):2576–2597.

Dutta A, Ghoshal A, Mandal D, Mondal NB, Banerjee S, Sahu NP, Mandal C. 2007. Racemoside A, an anti-leishmanial, water-soluble, natural steroidal saponin, induces programmed cell death in *Leishmania donovani*. J Med Microbiol 56(9):1196–1204.

Flynn JP, Gerriets V. 2024. Imatinib 1–10.

Freitas-Junior LH, Chatelain E, Kim HA, Siqueira-Neto JL. 2012. Visceral leishmaniasis treatment: What do we have, what do we need, and how to deliver it? Int J Parasitol Drugs Drug Resist 2:11–19.

Freitas PG, Castilho TE, Almeida L De, Maciel-Rezende CM, Costa LT, Viegas C, Marques MJ, Santos MH Dos, Silveira NJF Da. 2018. An in silico study of benzophenone derivatives as potential non-competitive inhibitors of *trypanosoma cruzi* and *Leishmania amazonensis* cysteine proteinases. J Braz Chem Soc 29(3):515–527.

Frías L, Leles D, Araújo A. 2013. Studies on protozoa in ancient remains - A review. Mem Inst

Oswaldo Cruz 108(1):1–12.

Ganesan A, Coote ML, Barakat K. 2017. Molecular dynamics-driven drug discovery: leaping forward with confidence. Drug Discov Today 22(2):249–269.

Ge YD, Hou SL, Jiang LL, Su FZ, Wang P. 2019. Expression and characterization of thermostable citrate synthase from *Microcystis aeruginosa* PCC7806. FEMS Microbiol Lett 366(19).

Gibson ME. 1983. The identification of kala azar and the discovery of *Leishmania donovani*. Med Hist 27(2):203–213.

Good A. 2006. Virtual screening. Compr Med Chem II 4:459–494.

Guney Eskiler G, Deveci Ozkan A, Haciefendi A, Bilir C. 2022. Mechanisms of abemaciclib, a CDK4/6 inhibitor, induced apoptotic cell death in prostate cancer cells *in vitro*. Transl Oncol 15(1).

Haldar AK, Sen P, Roy S. 2011. Use of Antimony in the Treatment of Leishmaniasis: Current Status and Future Directions. Mol Biol Int 2011:1–23.

Hendrickx S, Maes L, Croft SL, Caljon G. 2018. The challenges of effective leishmaniasis treatment. Drug Resist Leishmania Parasites Consequences, Mol Mech Possible Treat 193–206.

Herowati R, Widodo GP. 2014. Molecular Docking Studies of Chemical Constituents of *Tinospora cordifolia* on Glycogen Phosphorylase. Procedia Chem 13:63–68.

Hillar M, Lott V, Lennox B. 1975. Correlation of the effects of citric acid cycle metabolites on succinate oxidation by rat liver mitochondria and submitochondrial particles. J Bioenerg 7(1):1–15.

Iacobazzi V, Infantino V. 2014. Citrate-new functions for an old metabolite. Biol Chem 395(4):387–399.

Ilaghi M, Sharifi I, Sharififar F, Sharifi F, Oliaee RT, Babaei Z, Meimamandi MS, Keyhani A,

Bamorovat M. 2021. The potential role and apoptotic profile of three medicinal plant extracts on *Leishmania tropica* by MTT assay, macrophage model, and flow cytometry analysis. Parasite Epidemiol Control 12: e00201.

Islamuddin M, Ali A, Afzal O, Ali A, Ali I, Altamimi ASA, Alamri MA, Kato K, Parveen S. 2022. Thymoquinone Induced Leishmanicidal Effect via Programmed Cell Death in *Leishmania donovani*. ACS Omega 7(12):10718–10728.

Jakkula P, Narsimulu B, Qureshi IA. 2021. Biochemical and structural insights into 6-phosphogluconate dehydrogenase from *Leishmania donovani*. Appl Microbiol Biotechnol 105(13):5471–5489.

Jamshaid H, Din F ud, Khan GM. 2021. Nanotechnology-based solutions for anti-leishmanial impediments: a detailed insight. J Nanobiotechnology 19(1):1–51.

Jardim A, Hardie DB, Boitz J, Borchers CH. 2018. Proteomic Profiling of *Leishmania donovani* Promastigote Subcellular Organelles. J Proteome Res 17(3):1194–1215.

Johnson JD, Muhonen WW, Lambeth DO. 1998. Characterization of the ATP- and GTP-specific succinyl-CoA synthetases in pigeon: The enzymes incorporate the same α-subunit. J Biol Chem 273(42):27573–27579.

Kanamori E. 2015. Biophysics and Physicobiology morphogenesis. Biophys Physicobiology 12:13–20.

Keshav P, Goyal DK, Kaur S. 2023. *In vitro* and *in vivo* therapeutic antileishmanial potential of ellagic acid against *Leishmania donovani* in murine model. Med Microbiol Immunol 212(1):35–51.

Khan JM, Qadeer A, Ahmad E, Ashraf R, Bhushan B, Chaturvedi SK, Rabbani G, Khan RH. 2013. Monomeric Banana Lectin at Acidic pH Overrules Conformational Stability of Its Native Dimeric Form. PLoS One 8(4).

J.M. Khan, A. Qadeer, E. Ahmad, R. Ashraf, B. Bhushan, S.K. Chaturvedi, G. Rabbani, R.H.

Khan, Monomeric banana lectin at acidic pH overrules conformational stability of its native dimeric form, PLoS One. 8 (2013).

Kuldeep J, Karthik R, Kaur P, Goyal N, Siddiqi MI. 2020. Identification of potential anti-leishmanial agents using computational investigation and biological evaluation against trypanothione reductase. J Biomol Struct Dyn 1102.

Kumar A, Pandey SC, Samant M. 2018. Slow pace of antileishmanial drug development. Parasitol Open 4.

Kumar Mahto K, Prasad P, Kumar M, Ali I, Vohra V, Kumar Arya D. 2023. Visceral Leishmaniasis: An Overview and Integrated Analysis of the Current Status, Geographical Distribution and Its Transmission. Leishmania Parasites- Epidemiology, Immunopathology and hosts 1–16.

Lainson R. 2010. The Neotropical Leishmania species: a brief historical review of their discovery, ecology, and taxonomy. Rev Pan-Amazônica Saúde 1(2):13–32.

Lamba J, Paul S, Hasija V, Aggarwal R, Chaudhuri TK. 2009. Monitoring protein folding and unfolding pathways through surface hydrophobicity changes using fluorescence and circular dichroism spectroscopy. Biochem 74(4):393–398.

Lee N, Bertholet S, Debrabant A, Muller J, Duncan R, Nakhasi HL. 2002. Programmed cell death in the unicellular protozoan parasite Leishmania. Cell Death Differ 9(1):53–64.

Lee SH, Son HF, Kim KJ. 2019. Structural insights into the inhibition properties of archaeon citrate synthase from *Metallosphaera sedula*. PLoS One 14(2):1–16.

Légaré D, Richard D, Mukhopadhyay R, Stierhof YD, Rosen BP, Haimeur A, Papadopoulou B, Ouellette M. 2001. The Leishmania ATP-binding Cassette Protein PGPA is an Intracellular Metal-Thiol Transporter ATPase. J Biol Chem 276(28):26301–26307.

Leishman BY, Ross BMR. 1903. 1903.1.

Liao KH, Chen KB, Lee WY, Sun MF, Lee CC, Chen CYC. 2014. Ligand-based and structure-

based investigation for Alzheimer's disease from traditional Chinese medicine. Evidence-based Complement Altern Med 2014.

Lipinski CA. 2004. Lead- and drug-like compounds: The rule-of-five revolution. Drug Discov Today Technol 1(4):337–341.

Lloyd SJ, Lauble H, Prasad GS, Stout CD. 2008. The mechanism of aconitase: 1.8 Å resolution crystal structure of the S642A: citrate complex. Protein Sci 8(12):2655–2662.

M V V., Dubey VK, Ponnuraj K. 2018. Identification of two natural compound inhibitors of *Leishmania donovani* Spermidine Synthase (SpdS) through molecular docking and dynamic studies. J Biomol Struct Dyn 36(10):2678–2693.

Maroli M, Feliciangeli MD, Bichaud L, Charrel RN, Gradoni L. 2013. Phlebotomine sandflies and the spreading of leishmaniases and other diseases of public health concern. Med Vet Entomol 27(2):123–147.

Marquis N, Gourbal B, Rosen BP, Mukhopadhyay R, Ouellette M. 2005. Modulation in aquaglyceroporin AQP1 gene transcript levels in drug-resistant Leishmania. Mol Microbiol 57(6):1690–1699.

Martínez-Chávez A, Tibben MM, Jong KAM de, Rosing H, Schinkel AH, Beijnen JH. 2021. Simultaneous quantification of abemaciclib and its active metabolites in human and mouse plasma by UHPLC–MS/MS. J Pharm Biomed Anal 203:1–25.

McConville MJ, Saunders EC, Kloehn J, Dagley MJ. 2015. Leishmania carbon metabolism in the macrophage phagolysosome- feast or famine? F1000Research 4:1–11.

Mettler M. 2001. Visceral leishmaniasis in a German child who had never entered a known endemic area: Case report and review of the literature. Clin Infect Dis 32(2):302–306.

Michel G, Ferrua B, Lang T, Maddugoda MP, Munro P, Pomares C, Lemichez E, Marty P. 2011. Luciferase-expressing *Leishmania infantum* allows the monitoring of amastigote population size *in vivo*, *ex vivo,* and *in vitro*. PLoS Negl Trop Dis 5(9):1–7.

Moreira D, Rodrigues V, Abengozar M, Rivas L, Rial E, Laforge M, Li X, Foretz M, Viollet B, Estaquier J, Cordeiro da Silva A, Silvestre R. 2015. *Leishmania infantum* Modulates Host Macrophage Mitochondrial Metabolism by Hijacking the SIRT1-AMPK Axis. PLoS Pathog 11(3):1–24.

Moslehi M, Namdar F, Esmaeilifallah M, Hejazi SH, Sokhanvari F, Siadat AH, Hosseini SM, Iraji F. 2019. Evaluation of Different Concentrations of Imatinib on the Viability of *Leishmania major*: An In Vitro Study. Adv Biomed Res 8(1):61.

Moslehi M, Namdar F, Esmaeilifallah M, Iraji F, Vakili B, Sokhanvari F, Hosseini SM, Khamesipour F, Sebghatollahi Z, Hejazi SH. 2020. Study of therapeutic effect of different concentrations of imatinib on balb/c model of cutaneous leishmaniasis. AIMS Microbiol 6(2):152–161.

Murad H, Hawat M, Ekhtiar A, AlJapawe A, Abbas A, Darwish H, Sbenati O, Ghannam A. 2016. Induction of G1-phase cell cycle arrest and apoptosis pathway in MDA-MB-231 human breast cancer cells by sulfated polysaccharide extracted from *Laurencia papillosa*. Cancer Cell Int 16(1):1–11.

Murakami M, Kouyama T. 2016. Crystal Structures of Two Isozymes of Citrate Synthase from *Sulfolobus tokodaii* Strain 7. Biochem Res Int 2016:10–14.

Murtas G, Marcone GL, Peracchi A, Zangelmi E, Pollegioni L. 2021. Biochemical and biophysical characterization of recombinant human 3-phosphoglycerate dehydrogenase. Int J Mol Sci 22(8).

Muthuvel SK, Elumalai E, Girija K, Hemalatha K. 2018. Molecular docking and dynamics studies of 4-anilino quinazolines for epidermal growth factor receptor tyrosine kinase to find potent inhibitor. J Recept Signal Transduct 38(5–6):475–483.

Narsimulu B, Qureshi R, Jakkula P, Are S, Qureshi IA. 2022. Biophysical and Structural Characterization of Ribulose-5-phosphate Epimerase from *Leishmania donovani*. ACS Omega

7(1):548–564.

Nesic De Freitas LSF, Silva CF Da, Intagliata S, Amata E, Salerno L, Soeiro MDNC. 2023. *In vitro* and *in silico* analysis of imatinib analogues as anti-*Trypanosoma cruzi* drug candidates. Parasitology 150(4):359–364.

Nieto J, Alvar J, Mullen AB, Carter KC, Rodríguez C, San Andrés MI, San Andrés MD, Baillie AJ, González F. 2003. Pharmacokinetics, toxicities, and efficacies of sodium stibogluconate formulations after intravenous administration in animals. Antimicrob Agents Chemother 47(9):2781–2787.

Oeggl R, Neumann T, Gätgens J, Romano D, Noack S, Rother D. 2018. Citrate as Cost-Efficient NADPH Regenerating Agent. Front Bioeng Biotechnol 6:1–12.

Opperdoes FR, Michels P a M. 2008. The metabolic repertoire of Leishmania and implications for drug discovery. Leishmania 123–158.

Ortiz-Ramírez P, Hernández-Ochoa B, Ortega-Cuellar D, González-Valdez A, Martínez-Rosas V, Morales-Luna L, Arreguin-Espinosa R, Castillo-Rodríguez RA, Canseco-ávila LM, Cárdenas-Rodríguez N, la Cruz VP de, Montiel-González AM, Gómez-Chávez F, Gómez-Manzo S. 2022. Biochemical and Kinetic Characterization of the Glucose-6-Phosphate Dehydrogenase from *Helicobacter pylori* Strain 29CaP. Microorganisms 10(7).

Oryan A, Akbari M. 2016. Worldwide risk factors in leishmaniasis. Asian Pac J Trop Med 9(10):925–932.

Owen OE, Kalhan SC, Hanson RW. 2002. The key role of anaplerosis and cataplerosis for citric acid cycle function. J Biol Chem 277(34):30409–30412.

Paixão VG da, Pita SS da R. 2019. In silico identification and evaluation of new *Trypanosoma cruzi* trypanothione reductase (TcTR) inhibitors obtained from natural products database of the Bahia semi-arid region (NatProDB). Comput Biol Chem 79:36–47.

Panigrahi GC, Qureshi R, Jakkula P, Kumar KA, Khan N, Qureshi IA. 2020. Leishmanial

aspartyl-tRNA synthetase: Biochemical, biophysical and structural insights. Int J Biol Macromol 165(December):2869–2885.

Pape P Le. 2008. Development of new antileishmanial drugs - Current knowledge and future prospects. J Enzyme Inhib Med Chem 23(5):708–718.

Petillo A, Abruzzese V, Koshal P, Ostuni A, Bisaccia F. 2020. Extracellular Citrate Is a Trojan Horse for Cancer Cells. Front Mol Biosci 7(November):1–9.

Picado A, Ostyn B, Singh SP, Uranw S, Hasker E, Rijal S, Sundar S, Boelaert M, Chappuis F. 2014. Risk factors for visceral leishmaniasis and asymptomatic *Leishmania donovani* infection in India and Nepal. PLoS One 9(1):1–8.

Pietrocola F, Galluzzi L, Bravo-San Pedro JM, Madeo F, Kroemer G. 2015. Acetyl coenzyme A: A central metabolite and second messenger. Cell Metab 21(6):805–821.

Pires DEV, Blundell TL, Ascher DB. 2015. pkCSM: Predicting small-molecule pharmacokinetic and toxicity properties using graph-based signatures. J Med Chem 58(9):4066–4072.

Piscopo T V., Azzopardi CM. 2007. Leishmaniasis. Postgrad Med J 83(976):649–657.

Raina PM, Parmar M. 2024. Bazedoxifene belongs to the category of SERMs and is a member of the cytokine family known 1–9.

Raj S, Saha G, Sasidharan S, Dubey VK, Saudagar P. 2019a. Biochemical characterization and chemical validation of Leishmania MAP Kinase-3 as a potential drug target. Sci Rep 9(1):1–11.

Raj S, Sasidharan S, Dubey VK, Saudagar P. 2019b. Identification of lead molecules against potential drug target protein MAPK4 from *L. donovani*: An *in-silico* approach using docking, molecular dynamics, and binding free energy calculation. PLoS One 14(8):1–12.

Rakotomanga M, Blanc S, Gaudin K, Chaminade P, Loiseau PM. 2007. Miltefosine affects lipid metabolism in *Leishmania donovani* promastigotes. Antimicrob Agents Chemother

51(4):1425–1430.

Ramos H, Valdivieso E, Gamargo M, Dagger F, Cohen BE. 1996. Amphotericin B kills unicellular leishmanias by forming aqueous pores permeable to small cations and anions. J Membr Biol 152(1):65–75.

Rani A, Khanikar S, Dutta M, Katiyar S, Qamar T, Seth A, Agnihotri PK, Guha R, Vishwakarma JN, Kar S. 2022. Quinolinyl β-enaminone derivatives exhibit leishmanicidal activity against *Leishmania donovani* by impairing the mitochondrial electron transport chain complex and inducing ROS-mediated programmed cell death. J Antimicrob Chemother 2–5.

Ranjan P, Dubey VK. 2023a. Krebs cycle enzymes for targeted therapeutics and immunotherapy for anti-leishmanial drug development using: Pathways, potential targets, and future perspectives. Life Sci 322: 121314.

Ranjan P, Dubey VK. 2023b. Novel chemical scaffold as a potential drug against *Leishmania donovani*: Integrated computational and experimental approaches. J Cell Biochem 124(9):1404–1422.

Remington SJ. 1992. Structure and Mechanism of Citrate Synthase. Curr Top Cell Regul 33(C):209–229.

Rose IA. 1998. How fumarase recycles after the malate → Fumarate reaction. Insights into the reaction mechanism. Biochemistry 37(51):17651–17658.

Róycki B, Cieplak M. 2014. Citrate synthase proteins in extremophilic organisms: Studies within a structure-based model. J Chem Phys 141(23).

Ruiz-postigo JA, Jain S, Ruiz-postigo JA, Jain S. 2023. Global leishmaniasis surveillance , 2022 : assessing trends over the past 10 years Surveillance mondiale de la leishmaniose , 2022 : évaluation des tendances des 10 dernières années.

Ryan DG, O'Neill LAJ. 2020. Krebs Cycle Reborn in Macrophage Immunometabolism. Annu Rev Immunol 38:289–313.

Samuel Singh N. 2019. A Review on Major Risk Factors and Current Status of Visceral Leishmaniasis in North India. Am J Entomol 3(1):6.

Sangshetti JN, Kalam Khan FA, Kulkarni AA, Arote R, Patil RH. 2015. Antileishmanial drug discovery: Comprehensive review of the last 10 years. RSC Adv 5(41):32376–32415.

Sasidharan S, Saudagar P. 2021. Leishmaniasis: where are we and where are we heading? Parasitol Res 120(5):1541–1554.

Saudagar P, Dubey VK. 2014. Molecular mechanisms of in vitro betulin-induced apoptosis of *Leishmania donovani.* Am J Trop Med Hyg 90(2):354–360.

Saudagar P, Saha P, Saikia AK, Dubey VK, Saha P, Saikia AK, Dubey VK. 2013. Molecular mechanism underlying antileishmanial effect of oxabicyclo[3.3.1]nonanones: inhibition of key redox enzymes of the pathogen.Eur. J. Pharm. Biopharm. 85 (3): 569-577.

Saunders EC, McConville MJ. 2020. Immunometabolism of *Leishmania granulomas*. Immunol Cell Biol 98(10):832–844.

Saunders EC, Ng WW, Chambers JM, Ng M, Naderer T, Krömer JO, Likić VA, McConville MJ. 2011. Isotopomer profiling of *Leishmania mexicana* promastigotes reveals important roles for succinate fermentation and aspartate uptake in Tricarboxylic Acid Cycle (TCA) anaplerosis, glutamate synthesis, and growth. J Biol Chem 286(31):27706–27717.

Saunders EC, Ng WW, Kloehn J, Chambers JM, Ng M, McConville MJ. 2014. Induction of a Stringent Metabolic Response in Intracellular Stages of *Leishmania mexicana* Leads to Increased Dependence on Mitochondrial Metabolism. PLoS Pathog 10(1).

Saunders EC, Souza DP De, Naderer T, Sernee MF, Ralton JE, Doyle MA, MacRae JI, Chambers JL, Heng J, Nahid A, Likic VA, McConville MJ. 2010. Central carbon metabolism of Leishmania parasites. Parasitology 137(9):1303–1313.

Sen R, Bandyopadhyay S, Dutta A, Mandal G, Ganguly S, Saha P, Chatterjee M. 2007. Artemisinin triggers induction of cell-cycle arrest and apoptosis in *Leishmania donovani*

promastigotes. J Med Microbiol 56(9):1213–1218.

Siddaramaiah M, Kapaettu S, Rao BSS, Roy S, Chandra S, Mahato KK. 2017. Identification of protein secondary structures by laser-induced autofluorescence: A study of urea and GnHCl induced protein denaturation. Spectrochim Acta - Part A Mol Biomol Spectrosc 174:44–53.

Silva Rodrigues JH da, Miranda N, Volpato H, Ueda-Nakamura T, Nakamura CV. 2019. The antidepressant clomipramine induces programmed cell death in *Leishmania amazonensis* through a mitochondrial pathway. Parasitol Res 118(3):977–989.

Singh N, Kumar M, Singh RK. 2012. Leishmaniasis: Current status of available drugs and new potential drug targets. Asian Pac J Trop Med 5(6):485–497.

Singh OP, Singh B, Chakravarty J, Sundar S. 2016. Current challenges in treatment options for visceral leishmaniasis in India: A public health perspective. Infect Dis Poverty 5(1).

Singh R, Kashif M, Srivastava P, Manna PP. 2023. Recent Advances in Chemotherapeutics for Leishmaniasis: Importance of the Cellular Biochemistry of the Parasite and Its Molecular Interaction with the Host. Pathogens 12(5).

Sood D, Kumar N, Singh A, Sakharkar MK, Tomar V, Chandra R. 2018. Antibacterial and Pharmacological Evaluation of Fluoroquinolones: A Chemoinformatics Approach. Genomics Inform 16(3):44–51.

Srere A. 1966. Citrate-condensing enzyme-oxalacetate binary complex studies on its physical and chemical properties, J. Biol. Chem.241:9.

Steverding D. 2017. The history of leishmaniasis. Parasites and Vectors 10(1):1–10.

Sudhakar R, Adhikari N, Pamnani S, Panda A, Bhattacharjee M, Rizvi Z, Shehzad S, Gupta D, Sijwali PS. 2022. Bazedoxifene, a Postmenopausal Drug, Acts as an Antimalarial and Inhibits Hemozoin Formation. Microbiol Spectr 10(3):1–13.

Sundar S, Chakravarty J, Rai VK, Agrawal N, Singh SP, Chauhan V, Murray HW. 2007. Amphotericin B treatment for Indian visceral leishmaniasis: Response to 15 daily versus

alternate-day infusions. Clin Infect Dis 45(5):556–561.

Taketa K, Sarngadharan MG, Watanabe A, Aoe H, Pogell BM. 1971. Reversible inactivation of rabbit liver fructose 1,6-diphosphatase by adenosine triphosphate and adenosine diphosphate. J Biol Chem 246(18):5676–5683.

Tantry US, Bliden KP, Chaudhary R, Novakovic M, Rout A, Gurbel PA. 2020. Vorapaxar in the treatment of cardiovascular diseases. Future Cardiol 16(5):373–384.

Taylor WM, Halperin ML. 1973. Regulation of pyruvate dehydrogenase in muscle. Inhibition by citrate. J Biol Chem 248(17):6080–6083.

Teixeira BVF, Teles ALB, Silva SG da, Brito CCB, Freitas HF de, Pires ABL, Froes TQ, Castilho MS. 2019. Dual and selective inhibitors of pteridine reductase 1 (PTR1) and dihydrofolate reductase-thymidylate synthase (DHFR-TS) from *Leishmania chagasi*. J Enzyme Inhib Med Chem 34(1):1439–1450.

Teodoro JS, Rolo AP, Palmeira CM. 2013. The NAD ratio redox paradox: Why does too much reductive power cause oxidative stress? Toxicol Mech Methods 23(5):297–302.

Tielens AGM, Hellemond JJ van. 2009. Surprising variety in energy metabolism within Trypanosomatidae. Trends Parasitol 25(10):482–490.

Vargas JAR, Lopez AG, Piñol MC, Froeyen M. 2018. Molecular docking study on the interaction between 2-substituted-4,5-difuryl Imidazoles with different protein targets for antileishmanial activity. J Appl Pharm Sci 8(3):14–22.

Voli LA, Mamyrbékova JA, Bazureau J-P. 2020. Abemaciclib, a Recent Novel FDA-Approved Small Molecule Inhibiting Cyclin-Dependant Kinase 4/6 for the Treatment of Metastatic Breast Cancer: A Mini-Review. Open J Med Chem 10(03):128–138.

K. Batumalaie, E Khalili, N A Mahat, F Huyop, R A. Wahab. 2018. Biophysical characterization of a recombinant lipase KV1 from *Acinetobacter haemolyticus* in relation to pH and temperature, 152:198-210.

Wamai RG, Kahn J, McGloin J, Ziaggi G. 2020. Visceral leishmaniasis: a global overview. J Glob Heal Sci 2(1):1–22.

Wang B, Rao YH, Inoue M, Hao R, Lai CH, Chen D, McDonald SL, Choi MC, Wang Q, Shinohara ML, Yao TP. 2014. Microtubule acetylation amplifies p38 kinase signalling and anti-inflammatory IL-10 production. Nat Commun 5.

Wang Z, Tan K, Cai J, Hou S, Yue, Wang, Jiang P, Liang M. 2019. Pt Pt Sc. Colloids Surfaces A Physicochem Eng Asp 561:388–394.

Wiegand G, Remington SJ. 1986. Citrate synthase: structure, control, and mechanism. Annu Rev Biophys Biophys Chem 15:97–117.

Williams NC, O'Neill LAJ. 2018. A role for the Krebs cycle intermediate citrate in metabolic reprogramming in innate immunity and inflammation. Front Immunol 9:1–11.

Wortmann G, Miller RS, Oster C, Jackson J, Aronson N. 2002. A randomized, double-blind study of the efficacy of a 10- or 20-day course of sodium stibogluconate for treatment of cutaneous leishmaniasis in United States military personnel. Clin Infect Dis 35(3):261–267.

Wu M, Han J, Liu Z, Zhang Y, Huang C, Li J, Li Z. 2020. Identification of novel CDK 9 inhibitors based on virtual screening, molecular dynamics simulation, and biological evaluation. Life Sci 258.

Zara V, Assalve G, Ferramosca A. 2022. Multiple roles played by the mitochondrial citrate carrier in cellular metabolism and physiology. Cell Mol Life Sci 79(8).

Zhong Y, Lee K, He JC. 2018. SIRT1 is a potential drug target for the treatment of diabetic kidney disease. Front Endocrinol (Lausanne) 9:1–6.

APPENDIX A

LIST OF PUBLICATION

Preeti Ranjan, Manash Sarma and Vikash Kumar Dubey, (**2024**) "Biochemical and biophysical characterization of *Leishmania donovani* citrate synthase." **Journal of Biological Macromolecules**, 279(3): 135400.

Manash Sarma, Kushal Bora, **Preeti Ranjan** and Vikash Kumar Dubey, (**2024**), "Identification of novel anti-leishmanials targeting glutathione synthetase of the parasite: a drug repurposing approach." **FEBS Letters**.

Preeti Ranjan and Vikash Kumar Dubey, **(2024)** "Identification of potential antileishmanial compounds from natural sources against citrate synthase enzyme using structure-based drug designing." **Journal of Molecular Structure**,136556.

Preeti Ranjan and Vikash Kumar Dubey, **(2023)** "Novel chemical scaffold as a potential drug against *Leishmania donovani*: Integrated computational and experimental approaches." **Journal of Cellular Biochemistry**, 124(9): 1404-1422.

Preeti Ranjan and Vikash Kumar Dubey, **(2023)** "Krebs cycle enzymes for targeted therapeutics and immunotherapy for anti-leishmanial drug development using: pathways, potential targets, and future perspectives." (Review), **Life Sciences,** 322:121314**.**

PATENT

A thrombin receptor antagonist for management of leishmaniasis. (Application no. 202211067169: 22-11-22). Inventor: Vikash Kumar Dubey and **Preeti Ranjan (Status: Filed)**

APPENDIX B

CONFERENCES & WORKSHOPS

Participated and presented a poster **Preeti Ranjan** and Vikash Kumar Dubey on the topic "**Drug Repurposing Screening for Potential Antileishmanial Agents Targeting *Leishmania donovani* Citrate Synthase." in Biomolecular Horizons 2024 Congress** organized by the International Union of Biochemistry and Molecular Biology (IUBMB), the Federation of Asian & Oceanian Biochemists & Molecular Biologists (FAOBMB) and ComBio in Melbourne, Australia from 22nd – 26th September, 2024.

Participated and presented a paper **Preeti Ranjan** and Vikash Kumar Dubey on the topic **"Exploring Citrate Synthase of *Leishmania donovani* for Potential Drugs Against Leishmaniasis."** in **Biosangum 2024: 6th International Conferences on "Bio-Technological Intervention for Health, Agriculture and Circular Economy."** Organized by MNIT, Allahabad, India from 23rd – 25th February, 2024. (Oral presentation).

Participated in **"4th Online International Flow Cytometry Courses"** organized by Trust for Education and Training in Cytometry (TETC), India from 22nd – 24th September, 2023.

Participated in **"One-day Training on Application of Flow Cytometry"** jointly organized by the School of Biochemical Engineering, IIT (BHU) and Beckman Coulter India Pvt. Ltd on 12th May, 2022.

Participated in two days online conferences on **"National Conference on Computational and Biochemical Drug Discovery"** jointly organized by DST-funded I-DAPT HUB Foundation IIT(BHU), Varanasi and School of Biochemical Engineering, IIT(BHU) Varanasi during 11th and 12th September, 2021.

Participated in Short-term courses with hands-on training on **"Advances in Medical Imaging"** organized by DST DST-funded I-DAPT HUB Foundation at IIT(BHU) Varanasi from 15th to 19th March, 2021.

Participated in Short-term courses with hands on training on **"Computer Aided Drug Design and Protein Analysis"** organised by DST-funded I-DAPT HUB Foundation at IIT(BHU) Varanasi from 22nd Feb to 26th Feb, 2021.

Participated in INDO-US conference on **"Bioengineering & Regenerative Medicine (ICBR 2020)"** organized by the School of Biochemical Engineering, IIT(BHU) Varanasi from 27th to 29th February, 2020.