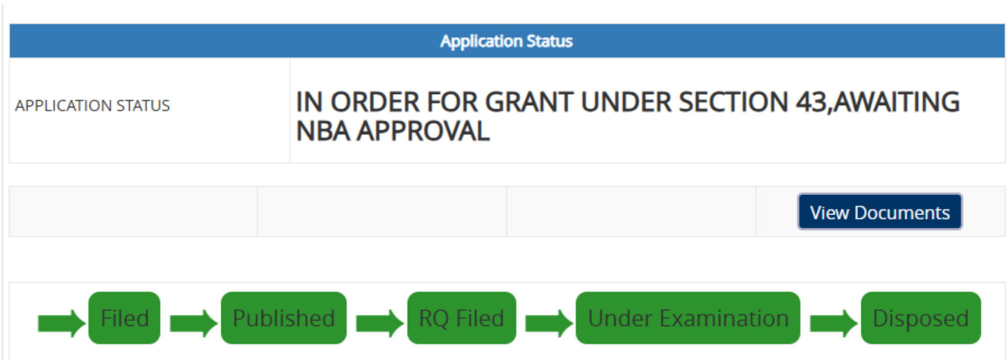
APPENDIX A

PATENTS AND PUBLICATIONS

PATENTS

- An Anti-leishmanial Steroidal Alkaloid Drug Compound (India) (Application No. 202211049337): Granted but waiting NBA approval before issue of certificate



PUBLICATIONS

- Naveena Menpadi, Pranjal Chandra, Vikash Kumar Dubey* (2025). Molecular mechanisms of cell death in *Leishmania donovani* induced by selected steroidal alkaloids. J. Basic Microbiol. Journal of Basic Microbiology. 65(3), e2400655 https://doi.org/10.1002/jobm.202400655
- Naveena Menpadi, Jay Prakash, Debanjan Kundu, Pranjal Chandra and Vikash Kumar Dubey* (2023). Integrated computational and experimental approach for novel anti-leishmanial molecules by targeting DPCK. Int. J. Biol. Macromol. 232, 31, 123441
- Naveena Menpadi, Pranjal Chandra, Vikash Kumar Dubey* (2025). Coenzyme A Biosynthesis in Protozoan Parasites: Dephospho-CoA Kinase (DPCK) as a Promising Drug Target. (submitted)
- Naveena Menpadi, Rajiv Kumar, Shyam Sundar, Pranjal Chandra, Vikash Kumar Dubey* Combating Miltefosine Unresponsiveness in *Leishmania donovani*: Synergistic Efficacy of Veratramine Co-Treatment. (submitted)

APPENDIX B

CONFERENCES ATTENDED

- **Poster Presentation** in the "2nd EFMC International Symposium on Chemical Biology" **(EFMC-ISCB 2025)**, Basel, Switzerland. (**International Travel Grant by ANRF**)
- **Best Oral Presentation** in the "International Conference on Advancements in Basic Science, Environmental Studies, and Traditional Medicine for Translational Drug Discovery and Development" **(TMT3D-2024)**, IMS, BHU, Varanasi, Uttar Pradesh, India
- **Oral Presentation** in the "65th Annual International Conference of the Association of Microbiologists of India" **(AMI-2024)**, GJUST, Hisar, Haryana, India
- **Poster Presentation** in the "International Conference on Drug Discovery, Delivery and Diagnostics" **(ICD4-2024)**, NIPER, Hyderabad, Telangana, India
- **Participation** in the "National Conference on Computational and Biochemical Drug Discovery-2021" **(NCCBDD-2021)**, IIT(BHU), Varanasi, India

REFERENCES

Abraham, M.J., Murtola, T., Schulz, R., Páll, S., Smith, J.C., Hess, B., Lindah, E., 2015. Gromacs: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. SoftwareX 1–2, 19–25. https://doi.org/10.1016/j.softx.2015.06.001

Altschup, S.F., Gish, W., Miller, W., Myers, E.W., Lipman, D.J., 1990. Basic Local Alignment Search Tool, J. Mol. Biol.

Antinarelli, L.M.R., de Oliveira Souza, I., Zabala Capriles, P.V., Gameiro, J., Britta, E.A., Nakamura, C.V., Lima, W.P., da Silva, A.D., Coimbra, E.S., 2018. Antileishmanial activity of a 4-hydrazinoquinoline derivative: Induction of autophagy and apoptosis-related processes and effectiveness in experimental cutaneous leishmaniasis. Exp Parasitol 195, 78–86. https://doi.org/10.1016/j.exppara.2018.10.007

Baranwal, A., Chiranjivi, A.K., Kumar, A., Dubey, V.K., Chandra, P., 2018. Design of commercially comparable nanotherapeutic agent against human disease-causing parasite, Leishmania. Sci Rep 8. https://doi.org/10.1038/s41598-018-27170-1

Barbosa, L.A., Fiuza, P.P., Borges, L.J., Rolim, F.A., Andrade, M.B., Luz, N.F., Quintela-Carvalho, G., Lima, J.B., Almeida, R.P., Chan, F.K., Bozza, M.T., Borges, V.M., Prates, D.B., 2018. RIPK1-RIPK3-MLKL-associated necroptosis drives Leishmania infantum killing in neutrophils. Front Immunol 9, 1–10. https://doi.org/10.3389/fimmu.2018.01818

Barritt, S.A., DuBois-Coyne, S.E., Dibble, C.C., 2024. Coenzyme A biosynthesis: mechanisms of regulation, function and disease. Nat Metab. https://doi.org/10.1038/s42255-024-01059-y

Basmaciyan, L., Berry, L., Gros, J., Azas, N., Casanova, M., 2018. Temporal analysis of the autophagic and apoptotic phenotypes in Leishmania parasites. Microbial Cell 5, 404–417. https://doi.org/10.15698/mic2018.09.646

Bateman, A., Martin, M.J., Orchard, S., Magrane, M., Agivetova, R., Ahmad, S., Alpi, E., Bowler-Barnett, E.H., Britto, R., Bursteinas, B., Bye-A-Jee, H., Coetzee, R., Cukura, A., da Silva, A., Denny, P., Dogan, T., Ebenezer, T.G., Fan, J., Castro, L.G., Garmiri, P., Georghiou, G., Gonzales, L., Hatton-Ellis, E., Hussein, A., Ignatchenko, A., Insana, G., Ishtiaq, R., Jokinen, P., Joshi, V., Jyothi, D., Lock, A., Lopez, R., Luciani, A., Luo, J., Lussi, Y., MacDougall, A., Madeira, F., Mahmoudy, M., Menchi, M., Mishra, A., Moulang, K., Nightingale, A., Oliveira, C.S., Pundir, S., Qi, G., Raj, S., Rice, D., Lopez, M.R., Saidi, R., Sampson, J., Sawford, T., Speretta, E., Turner, E., Tyagi, N., Vasudev, P., Volynkin, V., Warner, K., Watkins, X., Zaru, R., Zellner, H., Bridge, A., Poux, S., Redaschi, N., Aimo, L., Argoud-Puy, G., Auchincloss, A., Axelsen, K., Bansal, P., Baratin, D., Blatter, M.C., Bolleman, J., Boutet, E., Breuza, L., Casals-Casas, C., de Castro, E., Echioukh, K.C., Coudert, E., Cuche, B., Doche, M., Dornevil, D., Estreicher, A., Famiglietti, M.L., Feuermann, M., Gasteiger, E., Gehant, S., Gerritsen, V., Gos, A., Gruaz-Gumowski, N., Hinz, U., Hulo, C., Hyka-Nouspikel, N., Jungo, F., Keller, G., Kerhornou, A., Lara, V., Le Mercier, P., Lieberherr, D., Lombardot, T., Martin, X., Masson, P., Morgat, A., Neto, T.B., Paesano, S., Pedruzzi, I., Pilbout, S., Pourcel, L., Pozzato, M., Pruess, M., Rivoire, C., Sigrist, C., Sonesson, K., Stutz, A., Sundaram, S., Tognolli, M., Verbregue, L., Wu, C.H., Arighi, C.N., Arminski, L., Chen, C., Chen, Y., Garavelli, J.S., Huang, H., Laiho, K., McGarvey, P., Natale, D.A., Ross, K., Vinayaka, C.R., Wang, Q., Wang, Y., Yeh, L.S., Zhang, J., 2021. UniProt: the universal protein knowledgebase in 2021. Nucleic Acids Res 49, D480–D489. https://doi.org/10.1093/nar/gkaa1100

Bhalla, P., Sultana, S., Chiranjivi, A.K., Saikia, A.K., Dubey, V.K., 2018. Synthesis and Evaluation of Methyl 4-(7-Hydroxy-4,4,8-Trimethyl-3-Oxabicyclo[3.3.1]Nonan-2-yl)Benzoate as an Antileishmanial Agent and Its Synergistic Effect with Miltefosine.

Bhattacharya, P., Ghosh, S., Ejazi, S.A., Rahaman, M., Pandey, K., Ravi Das, V.N., Das, P., Goswami, R.P., Saha, B., Ali, N., 2016. Induction of IL-10 and TGFβ from CD4+CD25+FoxP3+ T Cells Correlates with Parasite Load in Indian Kala-azar Patients Infected with Leishmania donovani. PLoS Negl Trop Dis 10, 1–20. https://doi.org/10.1371/journal.pntd.0004422

Borkotoky, S., Banerjee, M., 2021. A computational prediction of SARS-CoV-2 structural protein inhibitors from Azadirachta indica (Neem). J Biomol Struct Dyn 39, 4111–4121. https://doi.org/10.1080/07391102.2020.1774419

Borkotoky, S., Banerjee, M., Modi, G.P., Dubey, V.K., 2021. Identification of high affinity and low molecular alternatives of boceprevir against SARS-CoV-2 main protease: A virtual screening approach. Chem Phys Lett 770. https://doi.org/10.1016/j.cplett.2021.138446

Bussi, G., Donadio, D., Parrinello, M., 2007. Canonical sampling through velocity rescaling. Journal of Chemical Physics 126. https://doi.org/10.1063/1.2408420

Butman, H.S., Kotzé, T.J., Dowd, C.S., Strauss, E., 2020. Vitamin in the Crosshairs: Targeting Pantothenate and Coenzyme A Biosynthesis for New Antituberculosis Agents. Front Cell Infect Microbiol 10, 1–33. https://doi.org/10.3389/fcimb.2020.605662

Calixto, S.L., Glanzmann, N., Xavier Silveira, M.M., da Trindade Granato, J., Gorza Scopel, K.K., Torres de Aguiar, T., DaMatta, R.A., Macedo, G.C., da Silva, A.D., Coimbra, E.S., 2018. Novel organic salts based on quinoline derivatives: The in vitro activity trigger apoptosis inhibiting autophagy in Leishmania spp. Chem Biol Interact 293, 141–151. https://doi.org/10.1016/j.cbi.2018.08.003

Campos-Salinas, J., León-Guerrero, D., González-Rey, E., Delgado, M., Castanys, S., Pérez-Victoria, J.M., Gamarro, F., 2013. LABCG2, a New ABC Transporter Implicated in Phosphatidylserine Exposure, Is Involved in the Infectivity and Pathogenicity of Leishmania. PLoS Negl Trop Dis 7. https://doi.org/10.1371/journal.pntd.0002179

Cavestro, C., Diodato, D., Tiranti, V., Di Meo, I., 2023. Inherited Disorders of Coenzyme A Biosynthesis: Models, Mechanisms, and Treatments. Int J Mol Sci 24. https://doi.org/10.3390/ijms24065951

Chakravarty, J., Sundar, S., 2019a. Current and emerging medications for the treatment of leishmaniasis. Expert Opin Pharmacother. https://doi.org/10.1080/14656566.2019.1609940

Chakravarty, J., Sundar, S., 2019b. Current and emerging medications for the treatment of leishmaniasis. Expert Opin Pharmacother. https://doi.org/10.1080/14656566.2019.1609940

Chakravarty, J., Sundar, S., 2010. Drug resistance in leishmaniasis. J Glob Infect Dis 2, 167. https://doi.org/10.4103/0974-777x.62887

Chaparro, V., Graber, T.E., Alain, T., Jaramillo, M., 2022. Transcriptional profiling of macrophages reveals distinct parasite stage-driven signatures during early infection by Leishmania donovani. Sci Rep 12, 1–13. https://doi.org/10.1038/s41598-022-10317-6

Chawla, B., Madhubala, R., 2010. Drug targets in Leishmania. Journal of Parasitic Diseases. https://doi.org/10.1007/s12639-010-0006-3

Ciucx, N., Peitsrh Urctrophuresis, M.C., 1997. SWISS-MODEL and the Swiss-PdbViewer: An environment for comparative protein modeling, IS.

Cortazzo da Silva, L., Aoki, J.I., Floeter-Winter, L.M., 2022. Finding Correlations Between mRNA and Protein Levels in Leishmania Development: Is There a Discrepancy? Front Cell Infect Microbiol 12. https://doi.org/10.3389/fcimb.2022.852902

Cortes, S., Bruno de Sousa, C., Morais, T., Lago, J., Campino, L., 2020. Potential of the natural products against leishmaniasis in Old World - a review of in-vitro studies. Pathog Glob Health. https://doi.org/10.1080/20477724.2020.1754655

Costa, C.H.N., Chang, K.P., Costa, D.L., Cunha, F.V.M., 2023. From Infection to Death: An Overview of the Pathogenesis of Visceral Leishmaniasis. Pathogens 12. https://doi.org/10.3390/pathogens12070969

Costa, M.S., Gonçalves, Y.G., Borges, B.C., Silva, M.J.B., Amstalden, M.K., Costa, T.R., Antunes, L.M.G., Rodrigues, R.S., Rodrigues, V. de M., de Faria Franca, E., Zoia, M.A.P., de Araújo, T.G., Goulart, L.R., Von Poelhsitz, G., Yoneyama, K.A.G., 2020. Ruthenium (II) complex cis-[RuII(ŋ2-O2CC7H7O2)(dppm)2]PF6-hmxbato induces ROS-mediated apoptosis in lung tumor cells producing selective cytotoxicity. Sci Rep 10, 1–21. https://doi.org/10.1038/s41598-020-72420-w

Croft, S.L., Sundar, S., Fairlamb, A.H., 2006. Drug resistance in leishmaniasis. Clin Microbiol Rev. https://doi.org/10.1128/CMR.19.1.111-126.2006

Daina, A., Michielin, O., Zoete, V., 2017. SwissADME: A free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci Rep 7. https://doi.org/10.1038/srep42717

Das, P., Saha, S., BoseDasgupta, S., 2021a. The ultimate fate determinants of drug induced cell-death mechanisms in Trypanosomatids. Int J Parasitol Drugs Drug Resist 15, 81–91. https://doi.org/10.1016/j.ijpddr.2021.01.003

Das, P., Saha, S., BoseDasgupta, S., 2021b. The ultimate fate determinants of drug induced cell-death mechanisms in Trypanosomatids. Int J Parasitol Drugs Drug Resist 15, 81–91. https://doi.org/10.1016/j.ijpddr.2021.01.003

Efstathiou, A., Smirlis, D., 2021. Leishmania protein kinases: Important regulators of the parasite life cycle and molecular targets for treating leishmaniasis. Microorganisms 9. https://doi.org/10.3390/microorganisms9040691

Fernandes, J.C.R., Zamboni, D.S., 2024. Mechanisms regulating host cell death during Leishmania infection. mBio 15, 1–11. https://doi.org/10.1128/mbio.01980-23

Fischer, E.R., Hansen, B.T., Nair, V., Hoyt, F.H., Dorward, D.W., 2012. Scanning electron microscopy, Current Protocols in Microbiology. https://doi.org/10.1002/9780471729259.mc02b02s25

Genheden, S., Ryde, U., 2015. The MM/PBSA and MM/GBSA methods to estimate ligand-binding affinities. Expert Opin Drug Discov. https://doi.org/10.1517/17460441.2015.1032936

Giri, S., Shaha, C., 2019. Leishmania donovani parasite requires Atg8 protein for infectivity and survival under stress. Cell Death Dis 10. https://doi.org/10.1038/s41419-019-2038-7

Goodsell, D.S., Morris, G.M., Olson, A.J., 1996. Automated Docking of Flexible Ligands: Applications of AutoDock, JOURNAL OF MOLECULAR RECOGNITION.

Gudkova, D., Panasyuk, G., Nemazanyy, I., Zhyvoloup, A., Monteil, P., Filonenko, V., Gout, I., 2012. EDC4 interacts with and regulates the dephospho-CoA kinase activity of CoA synthase. FEBS Lett 586, 3590–3595. https://doi.org/10.1016/j.febslet.2012.08.033

Guhe, V., Ingale, P., Tambekar, A., Singh, S., 2023. Systems biology of autophagy in leishmanial infection and its diverse role in precision medicine. Front Mol Biosci. https://doi.org/10.3389/fmolb.2023.1113249

Hess, B., Bekker, H., Berendsen, H.J.C., Fraaije, J.G.E.M., 1997. LINCS: A Linear Constraint Solver for Molecular Simulations, J Comput Chem. John Wiley & Sons, Inc.

Hess, B., Kutzner, C., Van Der Spoel, D., Lindahl, E., 2008. GRGMACS 4: Algorithms for highly efficient, load-balanced, and scalable molecular simulation. J Chem Theory Comput 4, 435–447. https://doi.org/10.1021/ct700301q

Irwin, J.J., Shoichet, B.K., 2005. ZINC-A Free Database of Commercially Available Compounds for Virtual Screening. https://doi.org/10.1021/ci049714

Journals, R., n.d. Synthetic and Natural Products Against Leishmaniasis A Review Related papers.

Karamysheva, Z.N., Guarnizo, S.A.G., Karamyshev, A.L., 2020. Regulation of translation in the protozoan parasite leishmania. Int J Mol Sci 21, 1–15. https://doi.org/10.3390/ijms21082981

Kayser, O., Kiderlen, A.F., Croft, S.L., 2002. Natural products as potential antiparasitic drugs. Studies in Natural Products Chemistry 26, 779–848. https://doi.org/10.1016/S1572-5995(02)80019-9

Keshav, P., Goyal, D.K., Kaur, S., 2021. GC–MS screening and antiparasitic action of Putranjiva roxburghii leaves against sensitive and resistant strains of Leishmania donovani. Journal of Parasitic Diseases 45, 1002–1013. https://doi.org/10.1007/s12639-021-01388-9

Kima, P.E., 2007. The amastigote forms of Leishmania are experts at exploiting host cell processes to establish infection and persist. Int J Parasitol 37, 1087–1096. https://doi.org/10.1016/j.ijpara.2007.04.007

Kirschning, A., 2021. Coenzymes and Their Role in the Evolution of Life Angewandte 6242–6269. https://doi.org/10.1002/anie.201914786

Ko, J., Park, H., Heo, L., Seok, C., 2012. GalaxyWEB server for protein structure prediction and refinement. Nucleic Acids Res 40. https://doi.org/10.1093/nar/gks493

Kumar, R., Tiwari, K., Dubey, V.K., 2017. Methionine aminopeptidase 2 is a key regulator of apoptotic like cell death in Leishmania donovani. Sci Rep 7, 1–10. https://doi.org/10.1038/s41598-017-00186-9

Kundu, D., Dubey, V.K., 2021. Potential alternatives to current cholinesterase inhibitors: an in silico drug repurposing approach. Drug Dev Ind Pharm 47, 919–930. https://doi.org/10.1080/03639045.2021.1952216

Lamont, E.A., Dillon, N.A., Baughn, A.D., 2020. The Bewildering Antitubercular Action of Pyrazinamide. Microbiology and Molecular Biology Reviews 84. https://doi.org/10.1128/mmbr.00070-19

Lee, N., Bertholet, S., Debrabant, A., Muller, J., Duncan, R., Nakhasi, H.L., 2002. Programmed cell death in the unicellular protozoan parasite Leishmania. Cell Death Differ 9, 53–64. https://doi.org/10.1038/sj.cdd.4400952

Leino, T.O., Turku, A., Yli-Kauhaluoma, J., Kukkonen, J.P., Xhaard, H., Wallén, E.A.A., 2018. Azulene-based compounds for targeting orexin receptors. Eur J Med Chem 157, 88–100. https://doi.org/10.1016/j.ejmech.2018.07.040

Leonardi, R., Zhang, Y.M., Rock, C.O., Jackowski, S., 2005. Coenzyme A: Back in action. Prog Lipid Res 44, 125–153. https://doi.org/10.1016/j.plipres.2005.04.001

Lu, S.H., Guan, J.H., Huang, Y.L., Pan, Y.W., Yang, W., Lan, H., Huang, S., Hu, J., Zhao, G.P., 2015. Experimental Study of Antiatherosclerosis Effects with Hederagenin in Rats. Evidence-based Complementary and Alternative Medicine 2015. https://doi.org/10.1155/2015/456354

Majester-Savornin, B., Elias, R., Diaz-Lanza, A.M., Balansard, G., Gasquet, M., Delmas, F., 1991. Saponins of the ivy plant, Hedera helix, and their Leishmanicidic activity. Planta Med 57, 260–262. https://doi.org/10.1055/s-2006-960086

Mendes, A., Armada, A., Cabral, L.I.L., Amado, P.S.M., Campino, L., Cristiano, M.L.S., Cortes, S., 2022a. 1,2,4-Trioxolane and 1,2,4,5-Tetraoxane Endoperoxides against Old-World Leishmania Parasites: In Vitro Activity and Mode of Action. Pharmaceuticals 15, 1–14. https://doi.org/10.3390/ph15040446

Mendes, A., Armada, A., Cabral, L.I.L., Amado, P.S.M., Campino, L., Cristiano, M.L.S., Cortes, S., 2022b. 1, 2, 4-trioxolane and 1, 2, 4, 5-tetraoxane endoperoxides against Old-World Leishmania parasites: in vitro activity and mode of action. Pharmaceuticals 15, 446.

Mendes, A., Armada, A., Cabral, L.I.L., Amado, P.S.M., Campino, L., Cristiano, M.L.S., Cortes, S., 2022c. 1,2,4-Trioxolane and 1,2,4,5-Tetraoxane Endoperoxides against Old-World Leishmania Parasites: In Vitro Activity and Mode of Action. Pharmaceuticals 15. https://doi.org/10.3390/ph15040446

Mendes, E.A., Desoti, V.C., Silva, S. de O., Ueda-Nakamura, T., Dias Filho, B.P., Yamada-Ogatta, S.F., Sarragiotto, M.H., Nakamura, C.V., 2016. C5 induces different cell death pathways in promastigotes of Leishmania amazonensis. Chem Biol Interact 256, 16–24. https://doi.org/10.1016/j.cbi.2016.06.018

Menpadi, N., Prakash, J., Kundu, D., Chandra, P., Dubey, V.K., 2023. Integrated computational and experimental approach for novel anti-leishmanial molecules by targeting Dephospho-coenzyme A kinase. Int J Biol Macromol 232, 123441. https://doi.org/10.1016/j.ijbiomac.2023.123441

Mignani, L., Gnutti, B., Zizioli, D., Finazzi, D., 2021. Coenzyme a biochemistry: From neurodevelopment to neurodegeneration. Brain Sci 11. https://doi.org/10.3390/brainsci11081031

Mishra, P.K., Park, P.K., Drueckhammer, D.G., 2001. Identification of yacE (coaE) as the structural gene for dephosphocoenzyme A kinase in Escherichia coli K-12. J Bacteriol 183, 2774–2778. https://doi.org/10.1128/JB.183.9.2774-2778.2001

Morris, G.M., Ruth, H., Lindstrom, W., Sanner, M.F., Belew, R.K., Goodsell, D.S., Olson, A.J., 2009. Software news and updates AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. J Comput Chem 30, 2785–2791. https://doi.org/10.1002/jcc.21256

Moulisha, B., Ashok Kumar, G., Kanti, H.P., 2010. Anti-leishmanial and Anti-cancer Activities of a Pentacyclic Triterpenoid Isolated from the Leaves of Terminalia arjuna Combretaceae, Tropical Journal of Pharmaceutical Research.

Naik, B., Gupta, N., Ojha, R., Singh, S., Prajapati, V.K., Prusty, D., 2020. High throughput virtual screening reveals SARS-CoV-2 multi-target binding natural compounds to lead instant therapy for COVID-19 treatment. Int J Biol Macromol 160, 1–17. https://doi.org/10.1016/j.ijbiomac.2020.05.184

Neto, R.L.M., Sousa, L.M.A., Dias, C.S., Filho, J.M.B., Oliveira, M.R., Figueiredo, R.C.B.Q., 2011. Morphological and physiological changes in Leishmania promastigotes induced by yangambin, a lignan obtained from Ocotea duckei. Exp Parasitol 127, 215–221. https://doi.org/10.1016/j.exppara.2010.07.020

Nkwenti Wonkam, A.K., Njanpa Ngansop, C.A., Njonte Wouamba, S.C., Jouda, J.B., Happi, G.M., Boyom, F.F., Sewald, N., Lenta, B.N., 2020. Rothmanniamide and other constituents from the leaves of Rothmannia hispida (K.Schum.) fagerl. (Rubiaceae) and their chemophenetic significance. Biochem Syst Ecol 93, 1–7. https://doi.org/10.1016/j.bse.2020.104137

Nurkanto, A., Imamura, R., Rahmawati, Y., Prabandari, E.E., Waluyo, D., Annoura, T., Yamamoto, K., Sekijima, M., Nishimura, Y., Okabe, T., Shiba, T., Shibata, N., Kojima, H., Duffy, J., Nozaki, T., 2022. Dephospho-Coenzyme A Kinase Is an Exploitable Drug Target against Plasmodium falciparum: Identification of Selective Inhibitors by High-Throughput Screening of a Large Chemical Compound Library. Antimicrob Agents Chemother. https://doi.org/10.1128/aac.00420-22

Nurkanto, A., Jeelani, G., Yamamoto, T., Hishiki, T., 2018a. Biochemical , Metabolomic , and Genetic Analyses of Dephospho Coenzyme A Kinase Involved in Coenzyme A Biosynthesis in the Human Enteric Parasite Entamoeba histolytica 9, 1–18. https://doi.org/10.3389/fmicb.2018.02902

Nurkanto, A., Jeelani, G., Yamamoto, T., Hishiki, T., Naito, Y., Suematsu, M., Hashimoto, T., Nozaki, T., 2018b. Biochemical, metabolomic, and genetic analyses of dephospho coenzyme a kinase involved in coenzyme a biosynthesis in the human enteric parasite entamoeba histolytica. Front Microbiol 9. https://doi.org/10.3389/fmicb.2018.02902

Nurkanto, A., Jeelani, G., Yamamoto, T., Hishiki, T., Naito, Y., Suematsu, M., Hashimoto, T., Nozaki, T., 2018c. Biochemical, metabolomic, and genetic analyses of dephospho coenzyme a kinase involved in coenzyme a biosynthesis in the human enteric parasite entamoeba histolytica. Front Microbiol 9. https://doi.org/10.3389/fmicb.2018.02902

O'Boyle, N.M., Banck, M., James, C.A., Morley, C., Vandermeersch, T., Hutchison, G.R., 2011. Open Babel: An Open chemical toolbox. J Cheminform 3. https://doi.org/10.1186/1758-2946-3-33

Papadopoulou, B., 1993. Mechanisms of Drug Resistance in Leishmania, Parasitology Today.

Peet, J., Selyutina, A., Bredihhin, A., 2016. Antiretroviral (HIV-1) activity of azulene derivatives. Bioorg Med Chem 24, 1653–1657. https://doi.org/10.1016/j.bmc.2016.02.038

Pérez-Victoria, F.J., Sánchez-Cañete, M.P., Seifert, K., Croft, S.L., Sundar, S., Castanys, S., Gamarro, F., 2006a. Mechanisms of experimental resistance of Leishmania to miltefosine: Implications for clinical use. Drug Resistance Updates 9, 26–39. https://doi.org/10.1016/j.drup.2006.04.001

Pérez-Victoria, F.J., Sánchez-Cañete, M.P., Seifert, K., Croft, S.L., Sundar, S., Castanys, S., Gamarro, F., 2006b. Mechanisms of experimental resistance of Leishmania to miltefosine: Implications for clinical use. Drug Resistance Updates 9, 26–39. https://doi.org/10.1016/j.drup.2006.04.001

Petersen, A.L. de O.A., Guedes, C.E.S., Versoza, C.L., Lima, J.G.B., de Freitas, L.A.R., Borges, V.M., Veras, P.S.T., 2012. 17-AAG Kills Intracellular Leishmania amazonensis while Reducing Inflammatory Responses in Infected Macrophages. PLoS One 7. https://doi.org/10.1371/journal.pone.0049496

Polonio, T., Efferth, T., 2008. Leishmaniasis: Drug resistance and natural products (review). Int J Mol Med. https://doi.org/10.3892/ijmm_00000020

Pushpakom, S., Iorio, F., Eyers, P.A., Escott, K.J., Hopper, S., Wells, A., Doig, A., Guilliams, T., Latimer, J., McNamee, C., Norris, A., Sanseau, P., Cavalla, D., Pirmohamed, M., 2018. Drug repurposing: Progress, challenges and recommendations. Nat Rev Drug Discov. https://doi.org/10.1038/nrd.2018.168

Roatt, B.M., de Oliveira Cardoso, J.M., De Brito, R.C.F., Coura-Vital, W., de Oliveira Aguiar-Soares, R.D., Reis, A.B., 2020. Recent advances and new strategies on leishmaniasis treatment. Appl Microbiol Biotechnol. https://doi.org/10.1007/s00253-020-10856-w

Robishaw, J., Neely, J.R., 1985. Coenzyme A metabolism. Am J Physiol Endocrinol Metab 11. https://doi.org/10.1152/ajpendo.1985.248.1.e1

Rodríguez-Hernández, D., Barbosa, L.C.A., Demuner, A.J., de Almeida, R.M., Fujiwara, R.T., Ferreira, S.R., 2016. Highly potent anti-leishmanial derivatives of hederagenin, a triperpenoid from Sapindus saponaria L. Eur J Med Chem 124, 153–159. https://doi.org/10.1016/j.ejmech.2016.08.030

Sabe, V.T., Ntombela, T., Jhamba, L.A., Maguire, G.E.M., Govender, T., Naicker, T., Kruger, H.G., 2021. Current trends in computer aided drug design and a highlight of drugs discovered via computational techniques: A review. Eur J Med Chem. https://doi.org/10.1016/j.ejmech.2021.113705

Salem, M.M., Werbovetz, K.A., 2006. Natural Products from Plants as Drug Candidates and Lead Compounds Against Leishmaniasis and Trypanosomiasis, Current Medicinal Chemistry.

Samuel Singh, N., 2019. A Review on Major Risk Factors and Current Status of Visceral Leishmaniasis in North India. American Journal of Entomology 3, 6. https://doi.org/10.11648/j.aje.20190301.12

Santos, D.M., Petersen, A.L.O.A., Celes, F.S., Borges, V.M., Veras, P.S.T., de Oliveira, C.I., 2014. Chemotherapeutic Potential of 17-AAG against Cutaneous Leishmaniasis Caused by Leishmania (Viannia) braziliensis. PLoS Negl Trop Dis 8. https://doi.org/10.1371/journal.pntd.0003275

Saudagar, P., Dubey, V.K., 2014. Molecular mechanisms of in vitro betulin-induced apoptosis of Leishmania donovani. American Journal of Tropical Medicine and Hygiene 90, 354–360. https://doi.org/10.4269/ajtmh.13-0320

Saudagar, P., Dubey, V.K., 2011. Cloning, expression, characterization, and inhibition studies on Trypanothione Synthetase, a drug target enzyme, from Leishmania donovani . Biol Chem. https://doi.org/10.1515/bc-2011-222

Scariot, D.B., Britta, E.A., Moreira, A.L., Falzirolli, H., Silva, C.C., Ueda-Nakamura, T., Dias-Filho, B.P., Nakamura, C. V., 2017. Induction of early autophagic process on Leishmania amazonensis by synergistic effect of miltefosine and innovative semi-synthetic thiosemicarbazone. Front Microbiol 8. https://doi.org/10.3389/fmicb.2017.00255

Schurigt, U., Schad, C., Glowa, C., Baum, U., Thomale, K., Schnitzer, J.K., Schultheis, M., Schaschke, N., Schirmeister, T., Moll, H., 2010. Aziridine-2,3-dicarboxylate-based cysteine cathepsin inhibitors induce cell death in Leishmania major associated with accumulation of debris in autophagy-related lysosome-like vacuoles. Antimicrob Agents Chemother 54, 5028–5041. https://doi.org/10.1128/AAC.00327-10

Seale, J.T., McDougal, O.M., 2022. Veratrum parviflorum: An Underexplored Source for Bioactive Steroidal Alkaloids. Molecules 27. https://doi.org/10.3390/molecules27165349

Seifert, K., Pérez-Victoria, F.J., Stettler, M., Sánchez-Cañete, M.P., Castanys, S., Gamarro, F., Croft, S.L., 2007. Inactivation of the miltefosine transporter, LdMT, causes miltefosine resistance that is conferred to the amastigote stage of Leishmania donovani and persists in vivo. Int J Antimicrob Agents 30, 229–235. https://doi.org/10.1016/j.ijantimicag.2007.05.007

Sengupta, S., Chowdhury, S., BoseDasgupta, S., Wright, C.W., Majumder, H.K., 2011. Cryptolepine-Induced Cell Death of Leishmania donovani Promastigotes Is Augmented by Inhibition of Autophagy . Mol Biol Int 2011, 1–12. https://doi.org/10.4061/2011/187850

Shadab, Md., Ali, N., 2011. Evasion of Host Defence by Leishmania donovani : Subversion of Signaling Pathways . Mol Biol Int 2011, 1–10. https://doi.org/10.4061/2011/343961

Shalev-Benami, M., Zhang, Y., Matzov, D., Halfon, Y., Zackay, A., Rozenberg, H., Zimmerman, E., Bashan, A., Jaffe, C.L., Yonath, A., Skiniotis, G., 2016. 2.8-Å Cryo-EM

Structure of the Large Ribosomal Subunit from the Eukaryotic Parasite Leishmania. Cell Rep 16, 288–294. https://doi.org/10.1016/j.celrep.2016.06.014

Shimosaka, T., Makarova, K.S., Koonin, E. V, Atomi, H., 2019a. Identification of Dephospho-Coenzyme A (Dephospho-CoA) Kinase in Thermococcus kodakarensis and Elucidation of the Entire CoA Biosynthesis Pathway in Archaea.

Shimosaka, T., Makarova, K.S., Koonin, E. V, Atomi, H., 2019b. Identification of dephospho-coenzyme A (dephospho-CoA) kinase in Thermococcus kodakarensis and elucidation of the entire CoA biosynthesis pathway in Archaea. mBio 10, e01146-19.

Sibon, O.C.M., Strauss, E., 2016. Coenzyme A: To make it or uptake it? Nat Rev Mol Cell Biol 17, 605–606. https://doi.org/10.1038/nrm.2016.110

Silva-Silva, J.V., Moragas-Tellis, C.J., Chagas, M.S.S., Souza, P.V.R., Moreira, D.L., Hardoim, D.J., Taniwaki, N.N., Costa, V.F.A., Bertho, A.L., Brondani, D., Zapp, E., De Oliveira, A.S., Calabrese, K.S., Behrens, M.D., Almeida-Souza, F., 2022. Carajurin Induces Apoptosis in Leishmania amazonensis Promastigotes through Reactive Oxygen Species Production and Mitochondrial Dysfunction. Pharmaceuticals 15. https://doi.org/10.3390/ph15030331

Singh, N., Mishra, B.B., Bajpai, S., Singh, R.K., Tiwari, V.K., 2014. Natural product based leads to fight against leishmaniasis. Bioorg Med Chem. https://doi.org/10.1016/j.bmc.2013.11.048

Singh, S., Kumari, E., Bhardwaj, R., Kumar, R., Dubey, V.K., 2017. Molecular events leading to death of Leishmania donovani under spermidine starvation after hypericin treatment. Chem Biol Drug Des 90, 962–971. https://doi.org/10.1111/cbdd.13022

Sundar, S., Rai, M., 2002. Laboratory diagnosis of visceral leishmaniasis. Clin Diagn Lab Immunol 9, 951–958. https://doi.org/10.1128/CDLI.9.5.951-958.2002

Thomé, M.P., Filippi-Chiela, E.C., Villodre, E.S., Migliavaca, C.B., Onzi, G.R., Felipe, K.B., Lenz, G., 2016. Ratiometric analysis of Acridine Orange staining in the study of acidic organelles and autophagy. J Cell Sci 129, 4622–4632. https://doi.org/10.1242/jcs.195057

Tiwari, N., Gedda, M.R., Tiwari, V.K., Singh, S.P., Singh, R.K., 2017. Limitations of Current Therapeutic Options, Possible Drug Targets and Scope of Natural Products in Control of Leishmaniasis. Mini-Reviews in Medicinal Chemistry 18. https://doi.org/10.2174/1389557517666170425105129

Uzcátegui, N.L., Carmona-Gutiérrez, D., Denninger, V., Schoenfeld, C., Lang, F., Figarella, K., Duszenko, M., 2007. Antiproliferative effect of dihydroxyacetone on Trypanosoma brucei bloodstream forms: Cell cycle progression, subcellular alterations, and cell death. Antimicrob Agents Chemother 51, 3960–3968. https://doi.org/10.1128/AAC.00423-07

Walia, G., Gajendar, K., Surolia, A., 2011. Identification of critical residues of the mycobacterial dephosphocoenzyme a kinase by site-directed mutagenesis. PLoS One 6. https://doi.org/10.1371/journal.pone.0015228

Walia, G., Kumar, P., Surolia, A., 2009. The role of UPF0157 in the folding of M. tuberculosis dephosphocoenzyme A kinase and the regulation of the latter by CTP. PLoS One 4, 1–16. https://doi.org/10.1371/journal.pone.0007645

Walia, G., Surolia, A., 2011. Insights into the regulatory characteristics of the Mycobacterial Dephosphocoenzyme a kinase: Implications for the universal CoA biosynthesis pathway. PLoS One 6. https://doi.org/10.1371/journal.pone.0021390

Wang, L., Li, W., Liu, Y., 2008. Hypotensive effect and toxicology of total alkaloids and veratramine from roots and rhizomes of Veratrum nigrum L. in spontaneously hypertensive rats. Pharmazie 63, 606–610. https://doi.org/10.1691/ph.2008.7873

Waterhouse, A., Bertoni, M., Bienert, S., Studer, G., Tauriello, G., Gumienny, R., Heer, F.T., De Beer, T.A.P., Rempfer, C., Bordoli, L., Lepore, R., Schwede, T., 2018. SWISS-MODEL: Homology modelling of protein structures and complexes. Nucleic Acids Res 46, W296–W303. https://doi.org/10.1093/nar/gky427

Wen, C., Wang, S., Huang, X., Liu, Z., Lin, Y., Yang, S., Ma, J., Zhou, Y., Wang, X., 2015. Determination and validation of hupehenine in rat plasma by UPLC-MS/MS and its application to pharmacokinetic study. Biomedical Chromatography 29, 1805–1810. https://doi.org/10.1002/bmc.3499

Wu, X., Chan, S. wan, Ma, J., Li, P., Shaw, P. chui, Lin, G., 2018. Investigation of association of chemical profiles with the tracheobronchial relaxant activity of Chinese medicinal herb Beimu derived from various Fritillaria species. J Ethnopharmacol 210, 39–46. https://doi.org/10.1016/j.jep.2017.08.027

Yang, J., Roy, A., Zhang, Y., 2013. Protein-ligand binding site recognition using complementary binding-specific substructure comparison and sequence profile alignment. Bioinformatics 29, 2588–2595. https://doi.org/10.1093/bioinformatics/btt447

Zhang, P., Li, J., Zhang, G., Pi, H., Zhang, Y., Ruan, H., Wu, J., 2008. Analysis of hupehenine in the total alkaloids from Fritillaria hupehensis by HPLC-ELSD. Journal of Huazhong University of Science and Technology - Medical Science 28, 118–120. https://doi.org/10.1007/s11596-008-0130-9

Zhang, S.X., Yang, G.B., Sun, J.Y., Li, Y.J., Yang, J., Wang, J.C., Deng, Y., 2025. Global, regional, and national burden of Visceral leishmaniasis, 1990–2021: findings from the global burden of disease study 2021. Parasites and Vectors 18. https://doi.org/10.1186/s13071-025-06796-x

Sengupta, S., Chowdhury, S., BoseDasgupta, S., Wright, C. W., and Majumder, H. K. (2011). Cryptolepine-induced cell death of Leishmania donovani promastigotes is augmented by inhibition of autophagy. Mol. Biol. Int., 2011, 187850–187912. doi:10. 4061/2011/187850

https://apps.who.int/neglected_diseases/ntddata/leishmaniasis/leishmaniasis.html