Volume 3, Number 2, 2026
Pages 1198-1211
Bioscience Insights
ISSN: 3080-3489 (Print)
ISSN: 3080-3497 (Online)
BiosciInsights.com

VIRTUAL SCREENING AND MOLECULAR DOCKING OF PLANT-BASED ANTHELMINTIC COMPOUNDS AGAINST CATTLE NEMATODES: A SYSTEMATIC REVIEW

Nazish Nazir[1], Zahid Mustafa*[2], Abdul Manan[3], Muhammad Shah Jahan Bajoi[4], Irum manan[5]

[1]M. Phil Scholar, Casvab University of Balochistan
*[*2,3]Casvab University of Balochistan*
[4]Parasitology Department SAU Tandojam
[5]Department of Botany Sardar Bahadur khan women university Quetta Balochistan

[1]nazishnazir876@gmail.com, [*2]zunzah@gmail.com, [3]manan_haqyar@yahoo.com
[4]shahjahanbaloch638@gamil.com, [5]irummanan35@gmail.com

https://doi.org/10.5281/zenodo.23100312

Article Information

Article History

Received:	June 18, 2026
Revised:	August 18, 2026
Accepted:	September 05, 2026
Available Online:	September 30, 2026

Keywords:
Cattle gastrointestinal nematodes; anthelmintic resistance phytochemicals; plant-based anthelmintics. virtual screening; molecular docking. AutoDock Vina.β-tubulin; drug discovery

Copyright Author
Corresponding Author: *
Zahid Mustafa

Abstract

Gastrointestinal nematode infections are an important constraint on cattle health, productivity,and farm profitability. The supplied literature identifies Haemonchus, Trichostrongylus, Cooperia, Oesophagostomum, Trichuris, and Strongyloides among commonly reported intestinal nematodes and emphasizes the continuing challenge of anthelmintic resistance. Repeated use of conventional synthetic anthelmintics, together with factors such as underdosing and intensive treatment practices, has contributed to declining treatment efficacy. Plant-derived phytochemicals have therefore received increasing attention as potential sources of alternative anthelmintic agents. This review synthesizes the provided literature on the burden of bovine gastrointestinal nematodes, conventional control strategies, anthelmintic resistance, the chemical diversity and mechanisms of plant bioactives, and the application of virtual screening and molecular docking in anthelmintic discovery.Particular attention is given to condensed tannins, alkaloids, terpenes, flavonoids, and saponins, as well as molecular targets including β-tubulin, nicotinic acetylcholine receptors, glutamate-gated chloride channels,

glutathione S-transferase, Hsp90, and cytochrome c oxidase-related proteins. The reviewed material describes computational workflows involving target preparation, ligand-library curation, ADMET filtering, molecular docking, and, where appropriate, molecular dynamics simulation. Compounds including luteolin, ellagic acid, butein, silibinin, nigellicine, and Molport-039-195-358 are highlighted in the supplied literature as computationally promising candidates. However, docking predictions remain hypothesis-generating and require experimental validation. Overall, an integrated strategy combining phytochemical characterization, computational screening, in vitro assays, in vivo evaluation, pharmacokinetic assessment, and resistance monitoring may provide a rational pathway for identifying new plant-derived anthelmintic leads for cattle nematode control.

1. Introduction

Cattle production contributes substantially to agricultural livelihoods and food systems, but gastrointestinal helminth infections can reduce animal performance and increase production costs. (Ahmad, 2023 & Arsenopoulos et al., 2022). The supplied literature describes helminthiasis as a major constraint to cattle productivity and identifies gastrointestinal nematodes as particularly important livestock parasites.(Ademola et al., 2010). These parasitic worms belong to two major families: roundworms (phylum Nematoda) and flatworms (phylum Platyhelminthes) (Onyeyili, 2001). Among these parasites, gastrointestinal parasites pose a major threat to animal productivity. (Saddiqi and others, 2010). Infection has been associated with reduced feed intake and weight gain, impaired immunity and fertility, decreased milk production and work capacity, increased treatment costs, and mortality in severe cases. (Ademola et al., 2010 & Ahmed et al., 2023).

The major challenge in conventional control is the progressive development of anthelmintic resistance. The literature reviewed in the supplied manuscript indicates that resistance has been reported across several anthelmintic classes and geographic regions. (Afsheen et al., 2025; Arsenopoulos et al., 2022). Frequent treatment, underdosing, and mass-treatment practices are identified as contributors to selection for resistant parasite populations. These circumstances create a continuing need for new compounds and complementary control strategies. (Afsheen et al., 2025; Arsenopoulos et al., 2022).

Medicinal plants represent a diverse source of secondary metabolites with biological activity. Plant-derived compounds may provide structurally diverse starting points for anthelmintic

discovery, while computational methods can help prioritize candidates before experimental testing. Virtual screening and molecular docking are particularly relevant because they can evaluate large numbers of candidate molecules against selected molecular targets and provide predictions of binding mode and relative affinity. (Ahmed et al., 2023; Arsenopoulos et al., 2022).

2. Review Scope and Organization

This narrative review was developed from the supplied manuscript on plant-based anti-helminthic compounds, cattle nematodes, virtual screening, and molecular docking. The synthesis is organized around five connected themes: disease burden and economic consequences; conventional control and resistance; plant-derived bioactive compounds; computational approaches to anthelmintic discovery; and molecular targets and candidate phytochemicals. The review retains the studies and terminology cited in the supplied material and does not add unsupported bibliographic details.

3. Gastrointestinal Nematodes of Cattle and Their Impact

Gastrointestinal nematodes are widely recognized in the supplied literature as important parasites of cattle and other ruminants. The reviewed sources identify Haemonchus, Trichostrongylus, Cooperia, Oesophagostomum, Trichuris, and Strongyloides among prevalent intestinal nematode genera. Their distribution and prevalence vary with geographic location, management system, environmental conditions, season, temperature, and rainfall. (Grisi et al., 2014).The disease burden is not limited to overt clinical disease. Subclinical infection can reduce feed intake, nutrient utilization, growth, milk production, and feed efficiency. The supplied literature also describes substantial effects on the gastrointestinal tract. Ostertagia ostertagi is presented as an important model: larval and adult stages can damage the abomasal epithelium, contribute to protein and parietal-cell loss, alter acid secretion, increase abomasal pH, and affect physiological indicators such as gastrin and pepsinogen.(Ahmad, 2023).

The economic consequences described in the reviewed literature include lower milk yield, impaired weight gain, reduced carcass performance, increased treatment expenditure, and broader productivity losses. These effects establish gastrointestinal nematodes as both a veterinary-health problem and an agricultural-economic problem. (Arsenopoulos et al., 2022).

4. Potential of Plant-Based Bioactive Compounds as Anthelmintic Agents

The search for sustainable alternatives has become necessary due to the growing worldwide worry about anthelmintic resistance (Jamil et al., 2025). A potential, environmentally benign,

and biodegradable method of controlling parasites is the use of phytochemicals, which are a chemically varied variety of secondary metabolites (Rehman et al., 2021). These substances have clear advantages over traditional chemotherapy, such as decreased toxicity, a decreased risk of developing resistance, and the ability to operate as synergistic enhancers that boost the effectiveness of conventional anthelmintic treatments (Jamil et al., 2025).

5. Conventional Anthelmintic Control and the Emergence of Resistance

Chemotherapeutic treatment has historically been the principal method for controlling gastrointestinal nematodes in livestock. The supplied review identifies several important anthelmintic groups and compounds, including benzimidazoles, ivermectin and related macrocyclic lactones, moxidectin, levamisole, milbemycin oxime, doramectin, selamectin, abamectin, and eprinomectin. (Fissiha & Kinde, 2021).Anthelmintic resistance is described as a heritable reduction in parasite sensitivity to a treatment that was previously effective. The supplied literature indicates that resistance is geographically variable and differs among drug classes. Reported resistance ranges in European cattle varied substantially among benzimidazoles, macrocyclic lactones, moxidectin, and levamisole. A multinational assessment cited in the source manuscript also reported confirmed ivermectin and moxidectin resistance on a proportion of participating farms. (Afsheen et al., 2025)

The development of resistance is influenced by parasite genetic diversity and selection pressure. Frequent administration, inadequate dosing, and poorly timed mass treatments can accelerate this process. Consequently, sustainable control requires more than simply replacing one synthetic compound with another; it requires diversified and evidence-based control strategies, including improved diagnostics, selective breeding, vaccines where appropriate, sustainable use of existing products, and development of new active compounds. (Arsenopoulos et al., 2022

6. Plant-Derived Compounds as Potential Anthelmintic Agents

The therapeutic use of plants against parasitic infections has a long history, and the supplied literature presents medicinal plants as a potentially sustainable source of anthelmintic compounds. Plant extracts can contain multiple bioactive molecules, allowing activity through more than one biological pathway. However, crude extracts may vary in chemical composition and may not provide the target specificity required for rational drug development. (Ahmed et al., 2023)

Phytochemicals discussed in the supplied manuscript include condensed tannins, alkaloids, terpenes, flavonoids, and saponins. Their proposed activities are diverse. Condensed tannins are associated with effects on egg production and egg-to-larval development. Certain

alkaloids have been reported to exert neurotoxic effects. Terpenes may interfere with egg hatching and neurotransmission. Flavonoids have been associated with interference in parasite metabolism, whereas saponins may alter membrane permeability and mitochondrial function.

The source material also describes transcuticular absorption and diffusion through larval cuticles and eggshells as possible routes of action. Some compounds may affect somatic muscle receptors and induce paralysis, while others may interact with essential parasite proteins or deprive larvae of vital biological functions. Interactions among multiple phytochemicals may further broaden biological activity, although the precise contribution of individual constituents requires experimental characterization. (Ahmed et al., 2023).

7. Major Classes of Plant Bioactives

Phytochemical class	Potential anthelmintic action described in the source	Examples/notes
Condensed tannins	May inhibit egg production and interfere with egg-to-L3 development.	Plant secondary metabolites; effects require experimental confirmation.
Alkaloids	Some members show neurotoxic activity against helminths.	Benzo(c)phenanthridine and isoquinoline alkaloids are highlighted.
Terpenes	May affect egg hatching and neurotransmission, potentially causing flaccid paralysis.	Mechanistic effects are compound-dependent.
Flavonoids	May interfere with parasite metabolism, including phosphodiesterase and Ca-ATPase pathways.	Mechanisms may vary among compounds.
Saponins	May alter membrane permeability and mitochondrial function, producing membrane damage.	Activity depends on chemical structure and exposure.

8. In Silico Drug Discovery for Anthelmintic

The supplied literature positions in silico drug discovery as a means of reducing the time, cost, and experimental workload associated with early-stage drug discovery. Structure-based virtual screening involves evaluating compounds against a defined molecular target and ranking candidates according to predicted interactions and scoring functions. Molecular docking can then predict plausible ligand orientations within a binding site and estimate relative binding affinity. (Lionta et al., 2014)

This approach is particularly useful when the three-dimensional structure of a target is available or can be modeled. The computational workflow described in the source includes target-protein preparation, ligand-library curation, physicochemical and ADMET filtering, molecular docking, and, where appropriate, molecular dynamics simulations. Databases mentioned include PubChem, ZINC15, and IMPPAT, while SwissADME is identified as a platform for pharmacokinetic and drug-likeness assessment.

AutoDock Vina is identified in the supplied material as the docking platform for the proposed target-based investigation. The output of docking should be interpreted as a prioritization tool rather than direct proof of biological efficacy. Binding-energy values and interaction patterns can identify candidates for subsequent laboratory validation, but they do not by themselves establish potency, selectivity, bioavailability, safety, or therapeutic effectiveness. (Trott & Olson, 2010)

9. Virtual Screening and Molecular Docking in Anthelmintic Drug Discovery

Long development times and high prices are common obstacles to traditional drug research pipelines (Pathak & Kim, 2022). As a result, computational techniques—collectively referred to as "in silico drug design"—have become a crucial strategy for quickening the identification of lead compounds by accurately predicting receptor–ligand interactions (Liu et al., 2020; Pathak & Kim, 2022).

10. Molecular Targets Relevant to Nematode Control

Target selection is a central component of structure-based anthelmintic discovery. The supplied manuscript identifies several classes of nematode targets with established or proposed relevance to parasite survival and drug action. (Kaminsky et al., 2003)

11. β-Tubulin

β-Tubulin is described as a key target of benzimidazole anthelmintics and as an important structural protein involved in cellular organization. Because tubulin is already validated pharmacologically, it provides a rational target for screening new chemical scaffolds and exploring compounds that may retain activity where resistance to existing drugs has emerged.

12. Neuro-muscular Targets

Nicotinic acetylcholine receptors and glutamate-gated chloride channels are highlighted as neuro-muscular targets. Modulation of these proteins can disrupt parasite neuromuscular function and may lead to paralysis. Their inclusion in virtual screening therefore allows investigation of phytochemicals with mechanisms distinct from tubulin-directed compounds.

13. Metabolic and Stress-Response Targets

The source manuscript also identifies glutathione S-transferase, Hsp90, and cytochrome c oxidase-related proteins as targets associated with detoxification, stress responses, or energy metabolism. Targeting such proteins may provide alternative mechanisms for inhibiting parasite survival and may be useful in efforts to diversify anthelmintic chemotypes. (Arsenopoulos et al., 2022; Ahmad, 2023)

14. Computational Screening Pipeline

Stage	Purpose
Target preparation	Select an appropriate nematode protein structure from a structural database or construct and validate a model when an experimental structure is unavailable.
Ligand-library construction	Retrieve plant-derived compounds from databases such as PubChem, ZINC15, or IMPPAT and prepare chemically appropriate ligand structures.
Drug-likeness and ADMET filtering	Apply physicochemical criteria, Lipinski/Ghose-type filters, PAINS assessment where appropriate, and predicted pharmacokinetic/toxicity properties.
Molecular docking	Dock prioritized ligands into the selected target using a defined protocol such as AutoDock Vina and record binding scores and interaction patterns.
Post-docking analysis	Inspect hydrogen bonds, hydrophobic contacts, electrostatic interactions, and interactions with functionally important residues.

Molecular dynamics and validation	Where resources permit, evaluate complex stability computationally and then prioritize candidates for in vitro and in vivo testing.

15. Evidence for Promising Phytochemical Leads s

The supplied literature reports several computationally promising phytochemicals. Luteolin is described as showing favorable binding against β-tubulin in comparison with albendazole in the cited docking study. Ellagic acid is presented as a multi-target candidate with reported interactions involving glutamate-gated chloride channels, β-tubulin, and nicotinic acetylcholine receptors. The source also describes molecular-dynamics evidence for persistence of a luteolin–tubulin complex over a 250-ns simulation. (Boudou et al., 2025)

Molport-039-195-358 is described as a potential candidate interacting with tubulin isotype 1 and glutathione S-transferase. Specific residues, including Glu45 and Arg46 in β-tubulin isotype 1 and Leu99 and Asn100 in GST, are reported in the supplied material as part of the post-docking interaction analysis.

Butein, silibinin, and nigellicine are also highlighted following in silico filtering, with the supplied manuscript reporting favorable drug-likeness characteristics under Lipinski and Ghose criteria. These findings support prioritization for further study, but computational filtering alone cannot establish clinical efficacy or safety.

16.. Critical Synthesis of the Available Evidence

Taken together, the reviewed literature supports a coherent rationale for combining phytochemical discovery with structure-based computational screening. First, the continuing problem of anthelmintic resistance creates a need for new chemical matter. Second, plants provide chemically diverse secondary metabolites that can interact with biological targets through different mechanisms. Third, virtual screening can reduce the number of compounds requiring laboratory testing by prioritizing candidates according to predicted target interactions, drug-likeness, and pharmacokinetic properties. (Garcia-Bustos et al., 2019).

At the same time, several limitations should be recognized. Plant extracts are chemically complex, and activity observed for an extract cannot automatically be attributed to a single constituent. Docking scores are method-dependent and are not equivalent to experimentally measured affinity. Predicted ADMET properties are useful for prioritization but do not replace pharmacokinetic and toxicological experiments. Protein structures may contain uncertainties, and docking results can be affected by receptor flexibility, water molecules, protonation state, ligand preparation, scoring functions, and binding-site definition.

Therefore, the most defensible interpretation of a strong docking result is that a compound is a candidate for further investigation. Claims of anthelmintic efficacy should be reserved for candidates supported by experimental evidence, ideally progressing from biochemical or parasite assays to controlled animal studies.

17. Research Gaps and Future Directions

- Standardized characterization of plant extracts and purified phytochemicals is needed to link chemical composition with anthelmintic activity. (Garcia-Bustos et al., 2019).Target selection should combine validated parasite biology with structural information and, where possible, evidence from resistant parasite populations.
- Docking results should be complemented by molecular dynamics, binding assays, and parasite-based in vitro experiments.
- Promising compounds require assessment of selectivity toward nematode targets relative to cattle proteins and beneficial organisms.
- Pharmacokinetic, bioavailability, metabolism, and toxicity studies are essential before therapeutic claims can be made.
- Future studies should investigate combinations of phytochemicals and their possible synergy with conventional anthelmintics while monitoring resistance development.
- Field-relevant validation is needed because environmental conditions, parasite species, infection intensity, host physiology, and management systems can influence treatment outcomes.

18. Implications for Cattle Health and Sustainable Parasite Control

The literature reviewed here suggests that plant-derived compounds and computational drug-discovery approaches may contribute to a broader integrated strategy for gastrointestinal nematode control. The objective should not be viewed simply as replacing all synthetic anthelmintics with plant products. Rather, phytochemical discovery can expand the available chemical space and potentially provide compounds with alternative mechanisms of action. When combined with diagnostics, appropriate treatment practices, pasture and herd management, and resistance monitoring, such approaches may support more sustainable parasite-control programs. (Grisi et al., 2014)

19. Conclusion

Gastrointestinal nematodes remain an important constraint on cattle health and productivity, while resistance to conventional anthelmintics complicates long-term control. The supplied literature indicates that plant-derived phytochemicals offer a diverse source of candidate

molecules and that virtual screening and molecular docking provide a rational way to prioritize such compounds against biologically relevant nematode targets. β-Tubulin, neuromuscular receptors and channels, glutathione S-transferase, Hsp90, and related metabolic targets represent important avenues for investigation. Luteolin, ellagic acid, Molport-039-195-358, butein, silibinin, and nigellicine are among the candidates highlighted in the reviewed material. Nevertheless, computational predictions should be treated as an early discovery step. Robust validation through biochemical, parasitological, pharmacokinetic, toxicological, and in vivo studies is required before these compounds can be considered practical anthelmintic agents.

References

Ademola, I. O., & Eloff, J. N. (2010). In vitro anthelmintic activity of Combretum molle (R. Br. ex G. Don) (Combretaceae) against Haemonchus contortus ova and larvae. Veterinary Parasitology, 169(1–2), 198–203.

Afsheen, F., Srinivasan, M. R., Anbukumar, K., & Kumanan, V. (2025). Evaluation of *in silico* anthelmintic activity of Naaku Poochi Kolli Kudineer Chooranam, a Siddha formulation, against glutamate-gated chloride ion channel, β-tubulin, and nicotinic acetylcholine receptor, and ADMET profile. *Journal of Phytopharmacology, 14*(5), 335–34

Ahmed, H., Gunyakti Kilinc, S., Celik, F., Kaya Kesik, H., Simsek, S., Ahmad, K. S., Afzal, M. S., Farrakh, S., Safdar, W., et al. (2023). An inventory of anthelmintic plants across the globe. Pathogens, 12(1), 131.

Arsenopoulos, K. V., Katsarou, E. I., Mendoza Roldan, J. A., et al. (2022). Haemonchus contortus parasitism in intensively managed cross-Limousin beef calves: Effects on feed conversion and carcass characteristics and potential associations with climatic conditions. Pathogens, 11(9), 955.

Baumgard, L. H., Rhoads, R. P., Rhoads, M. L., Gabler, N. K., Ross, J. W., Keating, A. F., Boddicker, R. L., Lenka, S., & Sejian, V. (2012). Impact of climate change on livestock production. In Environmental stress and amelioration in livestock production (pp. 413–468). Springer.

Fissiha, W., & Kinde, M. Z. (2021). Anthelmintic resistance and its mechanism: A review. Infection and Drug Resistance, 14, 5403–5410.

Garcia-Bustos, J. F., Sleebs, B. E., & Gasser, R. B. (2019). An appraisal of natural products active against parasitic nematodes of animals. Parasites & Vectors, 12, 306

Geurden, T., Chartier, C., Fanke, J., Frangipane di Regalbono, A., Traversa, D., von Samson-Himmelstjerna, G., Demeler, J., Vanimisetti, H. B., Bartram, D. J., & Denwood, M. J. (2015). Anthelmintic resistance to ivermectin and moxidectin in gastrointestinal nematodes of cattle in Europe. International Journal for Parasitology: Drugs and Drug Resistance, 5(3), 163–171.

Grisi, L., Cerqueira Leite, R., de Souza Martins, J. R., de Barros, A. T. M., Andreotti, R., Duarte Cançado, P. H., Pérez de León, A. A., Pereira, J. B., & Silva Villela, H. (2014). Reassessment of the potential economic impact of cattle parasites in Brazil. Revista Brasileira de Parasitologia Veterinária, 23(2), 150–156.

Jin, Y., Sehgal, S. A., Hassan, F., & Liu, G. (2025). In silico identification of novel compounds as anthelmintics against Haemonchus contortus through inhibiting β-tubulin isotype 1 and glutathione S-transferase. Animals, 15(13), 1846.

Jones, B. P., van Vliet, A. H. M., LaCourse, E. J., & Betson, M. (2022). In silico docking of nematode β-tubulins with benzimidazoles points to gene expression and orthologue variation as factors in anthelmintic resistance. Frontiers in Tropical Diseases, 3, 898814.

Kaminsky, R. (2003). Drug resistance in nematodes: A paper tiger or a real problem? Current Opinion in Infectious Diseases, 16(6), 559–564

Karshima, S. N., Maikai, B.-V., & Kwaga, J. K. P. (2018). Helminths of veterinary and zoonotic importance in Nigerian ruminants: A 46-year meta-analysis (1970–2016) of their prevalence and distribution. Infectious Diseases of Poverty, 7, 52.

Lalthanpuii, P. B., & Lalchhandama, K. (2020). Phytochemical analysis and in vitro anthelmintic activity of Imperata cylindrica underground parts. BMC Complementary Medicine and Therapies, 20, 332.

Lesk, A. M. (2010). Introduction to protein science: Architecture, function, and genomics (2nd ed.). Oxford University Press.

Liu, M., Panda, S. K., & Luyten, W. (2020). Plant-based natural products for the discovery and development of novel anthelmintics against nematodes. Biomolecules, 10(3), 426. https://doi.org/10.3390/biom10030426

Mavrot, F., Hertzberg, H., & Torgerson, P. (2015). Effect of gastro-intestinal nematode infection on sheep performance: A systematic review and meta-analysis. Parasites & Vectors, 8, 557.

Oliveira, L. M. B., Bevilaqua, C. M. L., Costa, C. T. C., Macedo, I. T. F., Barros, R. S., Rodrigues, A. C. M., Camurça-Vasconcelos, A. L. F., Morais, S. M., Lima, Y. C., Vieira, L. S., & Navarro, A. M. C. (2009). Anthelmintic activity of Cocos nucifera L. against sheep gastrointestinal nematodes. Veterinary Parasitology, 159(1), 55–59.

Peña-Espinoza, M., Thamsborg, S. M., Desrues, O., Hansen, T. V. A., & Enemark, H. L. (2016). Anthelmintic effects of forage chicory (Cichorium intybus) against gastrointestinal nematode parasites in experimentally infected cattle. Parasitology, 143(10), 1279–1293.

Rastelli, G., & Pinzi, L. (2019). Refinement and rescoring of virtual screening results. Frontiers in Chemistry, 7, 498.

Rehman, T., Iqbal, K. J., Anwer, A., Abbas, R. Z., Babar, W., Ali, A., et al. (2021). In vitro anthelmintic efficacy of Citrullus colocynthis (L.) Schrad on Haemonchus contortus. Veterinarski Arhiv, 91(3), 309–318.

Saddiqi, H. A., Iqbal, Z., Khan, M. N., Sarwar, M., Muhammad, G., Yaseen, M., & Jabbar, A. (2010). Evaluation of three Pakistani sheep breeds for their natural resistance to artificial infection of Haemonchus contortus. Veterinary Parasitology, 168(1–2), 141–145.

Shaver, A. O., Wit, J., Dilks, C. M., Crombie, T. A., Li, H., Aroian, R. V., & Andersen, E. C. (2023). Variation in anthelmintic responses are driven by genetic differences among diverse C. elegans wild strains. PLoS Pathogens, 19(4), e1011285.

Taki, A. C., Kapp, L., Byrne, J. J., et al. (2025). Prediction and prioritisation of novel anthelmintic candidates from public databases using deep learning and available bioactivity data sets. International Journal of Molecular Sciences, 26(7), 3134.

Taylor, C. M., Wang, Q., Rosa, B. A., Huang, S. C.-C., Powell, K., Schedl, T., Pearce, E. J., Abubucker, S., & Mitreva, M. (2013). Discovery of anthelmintic drug targets and drugs using chokepoints in nematode metabolic pathways. PLoS Pathogens, 9(8), e1003505

Trott, O., & Olson, A. J. (2010). AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *Journal of Computational Chemistry, 31*(2), 455–461.

Vineer, H. R., Morgan, E. R., Hertzberg, H., Bartley, D. J., Bosco, A., Charlier, J., Chartier, C., Claerebout, E., de Waal, T., Hendrickx, G., Hinney, B., Höglund, J., Ježek, J., Kašný, M., Keane, O. M., et al. (2020). Increasing importance of anthelmintic resistance in European livestock: Creation and meta-analysis of an open database. Parasite, 27, 69.

Wadood, A., et al. (2013). Acute toxicity, brine shrimp cytotoxicity, anthelmintic and relaxant potentials of fruits of Rubus fruticosus Agg. BMC Complementary and Alternative Medicine, 13, 138.

Zajíčková, M., Nguyen, L. T., Skálová, L., Raisová Stuchlíková, L., & Matoušková, P. (2020). Anthelmintics in the future: Current trends in the discovery and development of new drugs against gastrointestinal nematodes. Drug Discovery Today, 25(2), 430–437

Zarlenga, D. S., Chute, M. B., Gasbarre, L. C., & Boyd, P. C. (2001). A multiplex PCR assay for differentiating economically important gastrointestinal nematodes of cattle. Veterinary Parasitology, 97(3), 199–209.

Zirintunda, G., Biryomumaisho, S., Kasozi, K. I., et al. (2022). Emerging anthelmintic resistance in poultry: Can ethnopharmacological approaches offer a solution? Frontiers in Pharmacology, 12, 774896.

Jamil, E., Saleem, Z., Godman, B., Ullah, M., Amir, A., Haseeb, A., ... & Almarzoky Abuhussain, S. S. (2025). Global variation in antibiotic prescribing guidelines and the implications for decreasing AMR in the future. Frontiers in Pharmacology, 16, 1600787.

Rehman, S. U., Kraus, S., Shah, S. A., Khanin, D., & Mahto, R. V. (2021). Analyzing the relationship between green innovation and environmental performance in large manufacturing firms. Technological forecasting and social change, 163, 120481.

Onyeyili, P. A., Nwosu, C. O., Amin, J. D., & Jibike, J. I. (2001). Anthelmintic activity of crude aqueous extract of Nauclea latifolia stem bark against ovine nematodes. Fitoterapia, 72(1), 12-21.

Saddiqi, H. A., Zafar Iqbal, Z. I., Khan, M. N., & Ghulam Muhammad, G. M. (2010). Comparative resistance of sheep breeds to Haemonchus contortus in a natural pasture infection.

Pathak, R. K., Seo, Y. J., & Kim, J. M. (2025). Vetinformatics approaches in veterinary medicine. In Bioinformatics in Veterinary Science: Vetinformatics (pp. 185-205). Singapore: Springer Nature Singapore.

Liu, J., Liao, X., Qian, S., Yuan, J., Wang, F., Liu, Y., ... & Zhang, Z. (2020). Community transmission of severe acute respiratory syndrome coronavirus 2, Shenzhen, China, 2020. Emerging infectious diseases, 26(6), 1320.