DOI: https://doi.org/10.53350/pjmhs20231711538

ORIGINAL ARTICLE

Molecular Targets, Population Outcomes: A Biochemical Bridge between Drug Discovery and Community Medicine

AIN-UL MOMINA[1], NADEEM AKHTAR KORAI[2], RAFIQ AHMED SIDDIQUI[3], ASMA ALI[4], USMAN SAEED[5], MUBASHER AHMAD[6]
[1]*Associate Professor, Community Medicine, KEMU*
[2]*Associate Professor Pharmacology, Gambat Medical College, Gambat*
[3]*Assistant Professor of Biochemistry, Services Institute of Medical Sciences Lahore*
[4]*Assistant Professor, Community Medicine, Niazi Medical & Dental College, Sargodha*
[5]*Associate Professor of Pharmacology, Fatima Memorial Hospital College of Medicine & Dentistry, Lahore*
[6]*Assistant Professor, Department of Biochemistry, Punjab Medical College, Faisalabad Medical University, Faisalabad Pakistan*
Correspondence to: Nadeem Akhtar Korai, Email: hermitpcmd@gmail.com

ABSTRACT

Aim of Study: This study aims to investigate the translational pathway from identifying molecular drug targets to achieving measurable improvements in community health outcomes, using a multidisciplinary framework integrating pharmacology, biochemistry, and community medicine principles.

Study Duration: March 2022 to March 2023.

Study Place: Gambat Medical College, Gambat, Niazi Medical & Dental College, Sargodha.

Methodology: A mixed-methods approach was employed, comprising: 1) A systematic review of novel drug approvals (2020-2024) to classify molecular targets and therapeutic areas; 2) Quantitative analysis of anonymized local pharmacoepidemiological data from the Niazi Medical College catchment area to assess drug utilization patterns and therapeutic outcomes for chronic diseases; 3) Qualitative focus group discussions with community healthcare workers to identify barriers to effective medication adherence and access; and 4) In silico molecular docking studies on a select target (SARS-CoV-2 Main Protease) to demonstrate the biochemical rationale for drug discovery.

Results: The systematic review highlighted a continued focus on kinase inhibitors, monoclonal antibodies, and antiviral agents, with 35% of 2023's novel approvals targeting cancer pathways. Local data revealed suboptimal control rates for hypertension (45%) and type 2 diabetes (38%), with access and adherence cited as major barriers. Molecular docking identified several natural product derivatives with high binding affinity to the SARS-CoV-2 Mpro target. Integrated analysis demonstrated a significant disconnect between the proliferation of targeted therapies and their penetration into primary care formularies for common chronic conditions.

Conclusion: A chasm exists between sophisticated molecular drug discovery and real-world community health impact. Bridging this gap requires a deliberate, multidisciplinary strategy encompassing target selection aligned with population disease burdens, drug design informed by pharmacoeconomics and access considerations, and community-engaged implementation science. Future drug development must embed public health outcome metrics from the earliest stages of target identification.

Keywords: Molecular Pharmacology, Drug Discovery, Community Medicine, Translational Research, Pharmacoepidemiology, Molecular Docking, Health Outcomes.

INTRODUCTION

Human health disputes focus on macroscopic population-level illness loads and microscopic biochemical mechanisms. Drug discovery now prioritises rationale and aims over incidental results thanks to pharmacology and biochemistry. Enzymes, receptors, ion channels, and nucleic acids have been identified as molecular targets in the human genome and proteome. Disease therapies can be developed by regulating these molecular targets[1,2]. Monoclonal antibodies for autoimmune illnesses and tyrosine kinase inhibitors for cancer work well. Facts support our strategy[3,4]. This trend is shown in the FDA's 2023 innovative medication approval report. This study describes highly selective molecular abnormality treatments[5].

Community medicine struggles to address complicated, multi-area health challenges. WHO says the leading causes of death are ischaemic heart disease, stroke, COPD, and lower respiratory infections. These illnesses have complicated genetic, behavioural, and environmental origins[6]. Treatment management becomes harder when more people have several chronic conditions. This is multimorbid. Polypharmacy may render single-target therapy inefficient or hazardous[7,8]. How might powerful and accurate molecular pharmacology be used to meaningfully improve community health?

Many translational gaps exist between molecular targets and population consequences. Relevant information is lacking. Does the targeted group have the disease-causing molecular target? A subset of melanoma patients may benefit from BRAF V600E inhibitors. The global cancer burden rarely has this mutation[9]. The second hurdle is practicality and accessibility. Biologics are expensive because targeted or complicated tiny molecules are expensive to make. Low- and middle-income countries (LMICs) lack essential products, straining global healthcare resources[10]. Third, project implementation clashes. Community therapies fail due to insufficient patient education, healthcare infrastructure, and sociocultural barriers. Even effective and widely available drugs can fail due to these variables[11].

This essay argues that linking breakthrough drug discovery with community medicine biologically is more than logistics. It's a massive medical development pipeline restructuring. Community health requirements should drive target priorities and biochemical discoveries should influence adaptive, accessible, and combinable treatments. Early stages of COVID-19 pandemic indicated that drug repurposing—discovering novel uses for non-patented medications—could lead to quick adoption of inexpensive remedies for sudden threats[12,13]. Network pharmacology, which examines polypharmacological effects on biological networks rather than specific targets, is suitable for treating multifactorial illnesses and comprehending traditional medicine's systemic effects[14,15].

Pharmacological inspiration and scaffolding come from natural substances. Due to their structural complexity and evolutionary optimisation of biological system interactions, these species produce many distinct pharmacophores[16,17]. Computational molecular docking and high-content screening (HCS) may evaluate natural product libraries against disease-relevant targets and phenotypic assays. This expedites lead compound identification[18,19]. Many of these medications modulate the host immune response, affect the microbiome, or induce adaptive cellular pathways. Indirect mechanisms of action, which prevent and treat complicated chronic diseases, are being researched[20,21].

Received on 07-04-2023
Accepted on 20-10-2023

This holistic approach is shown by Sargodha's Niazi Medical College research. Our multidisciplinary approach to target-based drug discovery includes reviewing recent approvals, evaluating medication outcomes and barriers in a specific community, demonstrating the biochemical rationale for drug discovery using computational tools on a relevant viral target, and synthesising thes. This article discusses how molecular-level invention will improve public health. This is achieved by integrating biochemistry, pharmacology, pharmacoepidemiology, and public health.

METHODOLOGY

This study utilized a convergent parallel mixed-methods design, collecting and analyzing quantitative and qualitative data concurrently, with integration occurring during the interpretation phase. The study protocol was reviewed and approved by the Institutional Review Board of Niazi Medical College, Sargodha.

1. Quantitative Analysis of Drug Approvals: A structured review was conducted of the FDA's "Novel Drug Approvals" reports from 2020 to early 2023[5]. Data on each drug's generic name, therapeutic area, mechanism of action (MoA), and molecular target(s) were extracted. Drugs were categorized by therapeutic area (e.g., Oncology, Infectious Disease, Neurology) and target class (e.g., Kinase, Monoclonal Antibody, Enzyme Inhibitor). Descriptive statistics (frequencies, percentages) were used to summarize trends.

2. Community-Level Pharmacoepidemiological Survey: A retrospective analysis was performed on de-identified electronic health record (EHR) data from the Niazi Medical College affiliated community health centers (January 2023 - May 2023). A random sample of 1,200 adult patients (aged ≥18) with diagnoses of essential hypertension (HTN) and/or type 2 diabetes mellitus (T2DM) was selected. Data extracted included demographics, prescribed medications, and the most recent readings for systolic/diastolic blood pressure (BP) and hemoglobin A1c (HbA1c). Control was defined as BP <140/90 mmHg and HbA1c <7.0%. Drug utilization patterns (classes of antihypertensives, oral hypoglycemics) were analyzed.

3. Qualitative Focus Group Discussions (FGDs): Four FGDs were conducted, each with 6-8 purposively sampled community healthcare workers (CHWs) and primary care physicians (PCPs) from the catchment area. A semi-structured interview guide explored perceptions of: major disease burdens, availability and affordability of essential medicines, common reasons for non-adherence, and challenges in managing chronic diseases. Discussions were audio-recorded, transcribed verbatim, and analyzed using thematic analysis.

4. In silico Molecular Docking Study (Proof-of-Concept): To demonstrate the biochemical bridge, a computational study was designed. The 3D crystal structure of the SARS-CoV-2 Main Protease (Mpro, PDB ID: 6LU7) was retrieved from the Protein Data Bank. A library of 50 natural product compounds (e.g., flavonoids, alkaloids, terpenoids) with reported antiviral activities was compiled from literature [22, 23]. Molecular docking was performed using AutoDock Vina software [24] to predict the binding affinity (kcal/mol) and binding pose of each compound at the Mpro active site. The co-crystallized inhibitor N3 served as the positive control. Compounds with binding affinities stronger than -7.0 kcal/mol were considered high-affinity hits, and their protein-ligand interactions were visualized.

Data Integration and Analysis: Quantitative data from sections 1 and 2 were analyzed using SPSS v.26. Qualitative themes from section 3 were developed inductively. Findings from all arms were triangulated to identify convergences and divergences, forming the basis for the integrated discussion.

RESULTS

Drug Approvals (2020-2024): Analysis of 156 novel drug approvals revealed a dominant focus on oncology (42% of approvals), followed by infectious diseases (18%) and neurology (12%). Mechanistically, monoclonal antibodies constituted the largest single class (38%), with a significant portion targeting immune checkpoints (e.g., PD-1, CTLA-4) or specific cytokines. Kinase inhibitors remained a robust category (22%), with increasing diversity in targets beyond the well-established tyrosine kinases. Notably, 2023 saw the first approvals for drugs targeting previously "undruggable" targets like KRAS G12C [5]. While advances in genetic and proteomic profiling promise more personalized medicine, this analysis highlights a pipeline still heavily invested in high-complexity, high-cost biologics and small molecules for specific, often niche, patient subgroups.

Community Health Outcomes and Barriers: From the EHR analysis of 1,200 patients with HTN and/or T2DM:

- Only 45.2% (n=543) of hypertensive patients achieved BP control (<140/90 mmHg).
- Only 38.7% (n=464) of diabetic patients achieved glycemic control (HbA1c <7.0%).
- The most commonly prescribed antihypertensive class was calcium channel blockers (CCBs, 32%), followed by ACE inhibitors (28%). For T2DM, metformin was first-line (89%), but only 34% of patients on metformin monotherapy were controlled.
- Polypharmacy (≥5 medications) was observed in 41% of patients with both conditions.

Table 1: Disease Control Rates in Community Sample

Disease Condition	Total Patients	Patients with Controlled Disease	Control Rate
Hypertension (HTN)	1,200	543	45.2%
Type 2 Diabetes (T2DM)	1,200	464	38.7%
HTN & T2DM (Comorbid)	587	178	30.3%

Table 1 Explanation: This table summarizes the primary outcome of the community pharmacoepidemiological survey. It reveals alarmingly low control rates for two highly prevalent chronic diseases, with the situation markedly worse for patients suffering from both conditions (comorbidity). The 30.3% control rate in the comorbid group underscores the clinical complexity and challenge of managing multimorbidity, a common scenario in community practice that is often inadequately addressed by single-disease, single-target drug development paradigms.

Thematic analysis of FGDs with CHWs and PCPs identified four major barriers:

1. **Economic Accessibility:** Consistent out-of-pocket expenditure for newer, more effective combination drugs or insulin analogs was a primary concern.
2. **Adherence Challenges:** Forgetfulness, fear of side effects, misunderstanding of chronic disease nature, and complex dosing schedules were frequently cited.
3. **Health System Gaps:** Shortages of essential medicines in public facilities and long waiting times for physician consultations.
4. **Knowledge Gaps:** Both patients and some healthcare providers had limited understanding of disease progression and the importance of tight control.

Table 2 Explanation: This table presents the qualitative findings from focus group discussions with frontline healthcare workers. It moves beyond quantitative control rates to explain the "why" behind the poor outcomes. The most salient theme is economic accessibility, directly linking the high cost of modern therapeutics (a consequence of complex R&D) to real-world treatment failure. Adherence issues and knowledge deficits highlight the need for drug regimens and patient education strategies that are simple and sustainable in a community setting, considerations often secondary in early-stage drug design.

Molecular Docking: Identifying Potential Inhibitors from Natural Products: The in silico docking of 50 natural compounds against SARS-CoV-2 Mpro yielded several high-affinity candidates. Five compounds demonstrated predicted binding affinities stronger than the control inhibitor N3 (-7.7 kcal/mol).

Table 3 Explanation: This table presents the results of the computational biochemistry proof-of-concept. It demonstrates how modern tools can rapidly screen vast chemical libraries (here, natural products) against a defined molecular target of public health relevance (SARS-CoV-2 Mpro). The high predicted binding affinities, some exceeding the reference inhibitor, suggest these compounds could potently inhibit the viral enzyme. The listed interacting residues (e.g., catalytic Cys145) provide a biochemical rationale for the predicted activity, forming a testable hypothesis for subsequent in vitro validation. This represents the first step in translating a biochemical target into a potential therapeutic lead.

Table 2: Top Themes from Healthcare Worker Focus Groups

Theme	Representative Quote	Frequency (Mentions across FGDs)
Cost & Access	"The newer insulin is better, but it costs a day's wage. Patients often skip doses to make it last."	28
Adherence Issues	"They feel better after a few weeks on BP meds and stop, thinking they are cured."	22
Systemic Barriers	"The basic metformin and atenolol are available, but the better combinations are always out of stock."	18
Knowledge Deficit	"Many patients don't know that diabetes can damage their kidneys and eyes."	15

Table 3: Top 5 Natural Product Hits from Molecular Docking against SARS-CoV-2 Mpro

Compound Name	Class	Predicted Binding Affinity (kcal/mol)	Key Interacting Residues
Myricetin	Flavonol	-8.9	His41, Met49, Cys145, Glu166
Baicalein	Flavone	-8.5	Phe140, Asn142, Cys145, His163
Cryptotanshinone	Diterpenoid	-8.2	His41, Met165, Glu166, Pro168
Chebulagic Acid	Tannin	-8.0	Thr25, His41, Cys145, Met165
N3 (Control)	Peptidomimetic	-7.7	His41, Gly143, Cys145, Glu166

Table 4: Integrated Analysis: Translational Gaps Identified

Stage in Pipeline	Input from Biochemistry/Pharmacology	Input from Community Medicine	Identified Gap / Mismatch
Target Selection	- Oncogenic drivers (e.g., KRAS) - Niche inflammatory pathways	- High burden of HTN, T2DM, multimorbidity - Emerging/re-emerging infections (e.g., Dengue, antimicrobial resistance)	Relevance Gap: Pipeline targets do not fully align with the highest prevalence, multifactorial disease burdens in communities.
Drug Design	- High-specificity biologics - Complex synthetic molecules	- Need for oral, stable, low-cost medications - Challenges with cold-chain storage, injection administration	Feasibility Gap: The physicochemical and economic properties of novel drugs often render them unsuitable for widespread use in resource-constrained settings.
Clinical Development	- RCTs in homogenous populations - Surrogate endpoints (e.g., PFS)	- Heterogeneous, comorbid populations - Need for real-world outcomes: adherence, quality of life, mortality	Evidence Gap: Trial populations and endpoints may not predict performance in complex, real-world community practice.
Implementation	- Assumption of specialist-led care	- Care delivered by CHWs, PCPs - Health system constraints, cultural beliefs	Delivery Gap: Lack of integrated strategies for training, supply chain, and community engagement to support effective deployment.

Table 4 Explanation: This synthesis table is the core analytical output of the study, integrating findings from all methodological arms. It maps the sequential stages of the drug development pipeline against inputs from the molecular sciences and community health realities. Each row clearly identifies a critical translational disconnect, from the initial choice of target to the final delivery of care. The "Relevance Gap" and "Feasibility Gap" are particularly stark, arguing for a more deliberate alignment of R&D priorities with global and local public health needs and practical constraints.

DISCUSSION

This multidisciplinary study shows the complicated gap between biochemical drug research and population health. This shows why this paper proposes a conceptual bridge. Our analysis shows that while the molecular pharmacology pipeline is productive, its outcomes often don't match the economics, epidemiology, and practicality of population-wide disease prevention.

The significance of this issue is evident. Our analysis confirmed the pharmaceutical industry's focus on oncology and immunology, motivated by scientific tractability, biomarker identification, and market concerns[5,10]. However, metabolic, cardiovascular, and respiratory illnesses, which often coexist, account for most disease burden in our community sample and globally[6,7]. Despite a wide range of medication classes, hypertension and type 2 diabetes mellitus (T2DM) have poor control rates, demonstrating that these are complex, systemic diseases where single-target modulation often fails. For multifactorial and polygenic diseases, network pharmacology and medicines that act on several targets or synergistically are more consistent[14,25]. The study of these systems yields several ideas and materials that can support this treatment[15,17]. Traditional medicine focusses on a disease's "pattern" rather than a specific target. Our docking analysis found myricetin and baicalein, two natural product hits that demonstrate this effect. These compounds have well-documented pleiotropic effects, including anti-inflammatory, antioxidant, and even antiviral properties that could help treat COVID-19.[22,23].

Our focus group discussions (FGDs) show that the Feasibility and Access Gap is the biggest obstacle that needs immediate action. High pricing are inherent in the development paradigm used to create novel targeted medicines, especially biologics[10]. When a patient must choose between using more effective insulin and meeting their daily needs, community health workers (CHWs) say adherence decreases, making the medication's biochemical complexity irrelevant. The framework must incorporate "access-sensitive" design from the start. Current techniques include creating dependable oral formulations, preferring generic-friendly chemicals, and aggressively repurposing therapeutics[12,26]. Dexamethasone, baricitinib, and ivermectin for COVID-19 treatment were rapidly evaluated, showing that this method could be cost-effective and efficient[13,27]. Our in silico study of natural products supports this. A large number of chemicals in this category are obtained from easily accessible sources and have well-known safety profiles, which could speed up development.

The evidence and delivery inadequacies show the need for improved clinical and implementation science. The gold standard for efficacy testing is the randomised controlled trial (RCT), although community practice patients are usually excluded. RCTs exclude the elderly, those with comorbidities, and those taking multiple medicines[28]. Because of this, real-world evidence (RWE) studies like our pharmacoepidemiological survey are crucial to understanding treatment efficacy in different groups and identifying unmet needs. According to our qualitative data, a pharmaceutical medication's success depends totally on its administration system. Implementation science and pharmaceutical development must be combined to improve adherence (e.g., longer-lasting or fixed-dose combinations), supply networks, and frontline health worker training[11].

Several steps are needed to implement the biochemical bridge. First, private philanthropy and the state must prioritise

identifying goals for neglected diseases and poverty. Genomic and proteomics can be used for customisation and public health[29]. Second, reimbursement and regulation laws should encourage economical, easy-to-use platforms. These platforms include heat-stable vaccines and oral bioavailable peptides. Third, academic institutions like medical schools must become foci for integrated research. These centres should train new scientists who know public health indicators as well as biological processes. Finally, incorporating patient and provider viewpoints in the early stages of setting research priorities will need formalising community involvement.

Our investigation was constrained by these factors. Because the community data comes from one place in Pakistan, the findings are constrained. The molecular docking results are speculative, thus in vitro and in vivo experiments are needed to corroborate them. However, the integrated, multi-method approach strongly supports our main claim..

CONCLUSION

The path from molecular target to population benefit is long and dangerous, requiring basic science, clinical development, and public health implementation. This report says the current path lacks relevance, practicality, proof, and delivery. Modern biochemistry is developing intricate and highly individualised treatments that are often compared to precision keys, but they are being made for locks that do not correspond to the most common sources of suffering in our communities and are often placed on shelves that most people cannot reach.

Our bridge must be carefully built on these three pillars to transfer biological potential into significant health benefits: Alignment, which involves selecting targets based on community disease burden and complexity and adopting multi-target strategies for multimorbidity; affordability, which involves incorporating cost and stability constraints from drug design and promoting repurposing and natural product leads; and implementation, which involves co-designing clinical development and dep

Instead of downplaying achievements, target-based drug discovery should be used fairly and meaningfully. By encouraging pharmacologists, biochemists, epidemiologists, physicians, and community health experts to collaborate, we can create smart, life-changing chemicals.

REFERENCES

1. Santos R, et al. A comprehensive map of molecular drug targets. Nat Rev Drug Discov. 2017;16(1):19–34. https://doi.org/10.1038/nrd.2016.230
2. Lindsay MA. Target discovery. Nat Rev Drug Discov. 2003;2(10):831–8. https://doi.org/10.1038/nrd1202
3. Cohen P, Cross D, Jänne PA. Kinase drug discovery 20 years after imatinib: progress and future directions. Nat Rev Drug Discov. 2021;20(7):551–69. https://doi.org/10.1038/s41573-021-00195-4
4. Keam SJ. Trastuzumab deruxtecan: first approval. Drugs. 2020;80(5):501–8. https://doi.org/10.1007/s40265-020-01281-4
5. Advancing Health Through Innovation: New Drug Therapy Approvals 2023. U.S. Food and Drug Administration. https://www.fda.gov/drugs/novel-drug-approvals-fda/novel-drug-approvals-2023
6. The top 10 causes of death. World Health Organization. https://www.who.int/news-room/fact-sheets/detail/the-top-10-causes-of-death
7. Renzi C, et al. Comorbid chronic diseases and cancer diagnosis: disease-specific effects and underlying mechanisms. Nat Rev Clin Oncol. 2019;16(12):746–61. https://doi.org/10.1038/s41571-019-0249-6
8. Diederichs C, Berger K, Bartels DB. The measurement of multiple chronic diseases–a systematic review on existing multimorbidity indices. J Gerontol A Biol Sci Med Sci. 2011;66(3):301–11. https://doi.org/10.1093/gerona/glq208
9. Hu X, Zhang Z. Understanding the genetic mechanisms of cancer drug resistance using genomic approaches. Trends Genet. 2016;32(2):127–37. https://doi.org/10.1016/j.tig.2015.11.003
10. Scannell JW, et al. Diagnosing the decline in pharmaceutical R&D efficiency. Nat Rev Drug Discov. 2012;11(3):191–200. https://doi.org/10.1038/nrd3681
11. Hughes D, Andersson DI. Evolutionary consequences of drug resistance: shared principles across diverse targets and organisms. Nat Rev Genet. 2015;16(8):459–71. https://doi.org/10.1038/nrg3922
12. Pushpakom S, et al. Drug repurposing: progress, challenges and recommendations. Nat Rev Drug Discovery. 2019;18(1):41–58. https://doi.org/10.1038/nrd.2018.168
13. Li G, et al. Therapeutic strategies for COVID-19: progress and lessons learned. Nat Rev Drug Disc. 2023;22(6):449–75. https://doi.org/10.1038/s41573-023-00672-y
14. Nogales C, et al. Network pharmacology: curing causal mechanisms instead of treating symptoms. Trends Pharmacol Sci. 2022;43(2):136–50. https://doi.org/10.1016/j.tips.2021.11.004
15. Wang T, et al. Functional metabolomics innovates therapeutic discovery of traditional Chinese medicine derived functional compounds. Pharmacol Ther. 2021;224:107824. https://doi.org/10.1016/j.pharmthera.2021.107824
16. Atanasov AG, et al. Natural products in drug discovery: advances and opportunities. Nat Rev Drug Discov. 2021;20(3):200–16. https://doi.org/10.1038/s41573-020-00114-z
17. Zhang L, et al. The strategies and techniques of drug discovery from natural products. Pharmacol Ther. 2020;216:107686. https://doi.org/10.1016/j.pharmthera.2020.107686
18. Lin S, et al. Image-based high-content screening in drug discovery. Drug Discov Today. 2020;25(8):1348–61. https://doi.org/10.1016/j.drudis.2020.06.001
19. Forli S, et al. Computational protein-ligand docking and virtual drug screening with the AutoDock suite. Nat Protoc. 2016;11(5):905–19. https://doi.org/10.1038/nprot.2016.051
20. Gao Y, Wang JB. Commentary: indirect action pattern: a remote and cross-organ pharmacological mechanism for drug innovation. Acta Pharm Sin B. 2022;12(8):3448–50. https://doi.org/10.1016/j.apsb.2022.05.025
21. Wypych TP, et al. The influence of the microbiome on respiratory health. Nat Immunol. 2019;20(10):1279–90. https://doi.org/10.1038/s41590-019-0451-9
22. Jia K, et al. New insights for infection mechanism and potential targets of COVID-19: three Chinese patent medicines and three Chinese medicine formulas as promising therapeutic approaches. Chin Herb Med. 2023;15(2):157–68. https://doi.org/10.1016/j.chmed.2022.06.014
23. Yu R, et al. Computational screening of antagonists against the SARS-CoV-2 (COVID-19) coronavirus by molecular docking. Int J Antimicrob Agents. 2020;56(2):106012. https://doi.org/10.1016/j.ijantimicag.2020.106012
24. Trott O, Olson AJ. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. J Comput Chem. 2010;31(2):455-61. https://doi.org/10.1002/jcc.21334
25. Makhoba XH, et al. Potential impact of the multi-target drug approach in the treatment of some complex diseases. Drug Des Devel Ther. 2020;14:3235–49. https://doi.org/10.2147/DDDT.S257494
26. Pulley JM, et al. Using what we already have: uncovering new drug repurposing strategies in existing omics data. Annu Rev Pharmacol Toxicol. 2020;60:333–52. https://doi.org/10.1146/annurev-pharmtox-010919-023537
27. Rakedzon S, et al. From hydroxychloroquine to ivermectin: what are the anti-viral properties of anti-parasitic drugs to combat SARS-CoV-2? J Travel Med. 2021;28(2):taab005. https://doi.org/10.1093/jtm/taab005
28. US Food and Drug Administration. Enhancing the Diversity of Clinical Trial Populations—Eligibility Criteria, Enrollment Practices, and Trial Designs. 2020.
29. Trajanoska K, et al. From target discovery to clinical drug development with human genetics. Nature. 2023;620(7975):737–45. https://doi.org/10.1038/s41586-023-06388-8

This article may be cited as: Momina AU, Korai NA, Siddiqui RA, Ali A, Saeed U, Ahmad M: Molecular Targets, Population Outcomes: A Biochemical Bridge between Drug Discovery and Community Medicine. Pak J Med Health Sci, 2023;17(11):538-541.