List of 10 best papers

1. Computational pharmacology profiling of borapetoside C against melanoma, J. Biomol. Struct. Dyn. 0 (2023) 1–16. https://doi.org/10.1080/07391102.2023.2213333

The main discoveries from the article are:

Borapetoside C, a phytoconstituent found in Tinospora crispa, has been identified as having antistress properties. Through network pharmacology and molecular docking, it was found that borapetoside C may target MMP9 and EGFR, two proteins involved in melanoma development.

The study identified eight targets associated with melanoma through network pharmacology and KEGG pathway analysis. Among these targets, borapetoside C showed a strong binding affinity with MAP2K1, MMP9, and EGFR, suggesting its potential as a therapeutic agent for melanoma.

Molecular dynamics simulations confirmed the stability of the borapetoside C complex with MMP9 and EGFR. These findings suggest that borapetoside C from a natural source could be explored as a novel treatment option for melanoma.

2. Systems and in vitro pharmacology profiling of diosgenin against breast cancer, Front. Pharmacol. 13 (2023) 1–25. https://doi.org/10.3389/fphar.2022.1052849

The main discovery of this study on diosgenin against breast cancer is:

Diosgenin, a compound found in plants, was shown to impact multiple signaling pathways involved in breast cancer progression, including FoxO, PI3K-Akt, p53, Ras, and MAPK signaling.

Molecular docking and dynamics simulations revealed that diosgenin formed stable complexes with key proteins IGF1R, MDM2, and SRC, indicating its strong binding affinity towards these targets.

Diosgenin exhibited significant cytotoxicity against MCF7 cell lines, with the lowest inhibitory constant in oxidative stress conditions induced by H2O2.

Diosgenin also demonstrated the potential to counter the Warburg effect, particularly in non-cancer Vero cell lines, and inhibited cell proliferation in SKBR3 cell lines.

Overall, these findings suggest that diosgenin has promising anti-breast cancer properties through its modulation of signaling pathways, formation of stable protein complexes, cytotoxicity against cancer cells, and reversal of the Warburg effect.

3. Multi-Epitope Vaccine Design against Monkeypox Virus via Reverse Vaccinology Method Exploiting Immunoinformatic and Bioinformatic Approaches. Vaccines 2022, 10, 2010. https://doi.org/10.3390/vaccines10122010

The main discoveries of this study on developing a potential vaccine against the monkeypox virus are:

A multiepitope vaccine was successfully constructed using B-cell and T-cell epitopes from the MPXVgp181 strain, along with adjuvants and linkers.

The constructed vaccine was predicted to be antigenic, non-allergenic, and non-toxic, making it safe for use. It also exhibited excellent global population coverage and showed satisfactory immune response in silico.

Expression analysis and cloning studies confirmed the successful production of the vaccine in E. coli, indicating its suitability for large-scale production in the pharmaceutical industry.

This research provides a promising foundation for the development of a globally effective vaccine against the monkeypox virus. Further in vitro and in vivo studies are necessary to validate its efficacy and safety.

The use of bioinformatics and immunoinformatics in vaccine development offers a valuable approach for combating the monkeypox virus and potentially other viral diseases.

4. In silico screening, TLC bioautography and in vivo studies of Zanthoxylum armatum DC (Indian Prickly Ash) extract as a potential neuroprotective agent. South African J Bot 2022;150:997–1010. https://doi.org/10.1016/j.sajb.2022.09.009

The main discoveries from this study on Zanthoxylum armatum extract and its neuro-protective potential are:

Three bioactive phytoconstituents, b-sitosterol, stigmasterol, and lupeol, were isolated from the extract, and molecular docking studies showed that stigmasterol had the strongest binding affinity with acetylcholinesterase.

In vivo studies demonstrated that pre-treatment with the extract improved memory retention, reduced acetylcholinesterase activity in the brain, and exhibited antioxidant properties against scopolamine-induced cognitive impairment.

The extract showed promising effects as a neuroprotective agent, possessing anticholinesterase and antioxidant properties, making it a potential nootropic drug.

These findings support the traditional use of Zanthoxylum armatum as a remedy for digestive and nervous system disorders, and further research on extracts and isolated compounds is needed to strengthen the scientific evidence for its traditional uses.

The study highlights the potential of Zanthoxylum armatum as a source for natural nootropics and emphasizes the importance of additional scientific investigations to validate and expand its therapeutic applications.

5. In silico discovery of 3 novel quercetin derivatives against papain-like protease, spike protein, and 3C-like protease of SARS-CoV-2. J Genet Eng Biotechnol. 2022;7. https://doi.org/10.1186/s43141-022-00314-7

The main discoveries from this study are:

Forty bioactive compounds derived from quercetin were identified, showing positive drug-likeness scores and regulating pathways associated with antiviral activity and immune modulation.

Through molecular docking and dynamics simulations, three lead molecules were identified with high binding affinities to potential coronavirus targets: quercetin 3-O-arabinoside 7-O-rhamnoside (binding affinity with PLpro), quercetin 3-[rhamnosyl-(1- > 2)-alpha-L-arabinopyranoside] (binding affinity with spike protein receptor-binding domain), and quercetin-3-neohesperidoside-7-rhamnoside (binding affinity with 3CLpro).

The identified lead molecules exhibited stronger binding affinities compared to the standard antiviral drug remdesivir in docking studies.

Normal mode analysis confirmed the stability of the protein-ligand complexes formed by the lead molecules.

These findings suggest the potential of quercetin derivatives, particularly the identified lead molecules, as promising candidates for further investigation as immune modulators and antiviral agents against COVID-19.

6. Development and validation of stability-indicating UPLC method for the determination of gliclazide and its impurities in pharmaceutical dosage forms. *Futur J Pharm Sci* 7, 95 (2021). https://doi.org/10.1186/s43094-021-00248-w

The important discoveries from the study on the development of a UPLC method for gliclazide and its impurities are:

A stability-indicating UPLC method was successfully developed for the quantitative determination of gliclazide and its potential impurities.

Separation of gliclazide and impurities was achieved using an isocratic elution mode with a specific mobile phase composition and on an Acquity CSH 18 column.

The developed method demonstrated the ability to separate degradation products from the analyte peak, indicating its stability-indicating nature.

The method was validated following the guidelines of the International Conference on Harmonization, ensuring its suitability in terms of precision, accuracy, specificity, sensitivity, linearity, and robustness.

The UPLC method provides a reliable, accurate, and efficient analytical approach for the quantification of gliclazide and its impurities, offering potential applications in pharmaceutical analysis and quality control.

7. Evaluation of a novel melatonin-loaded gelatin sponge as a wound dressing, J. Vasc. Nurs. (2021). https://doi.org/10.1016/j.jvn.2021.09.004

The main points from the study on the formulation of a Melatonin sponge for wound healing are:

Melatonin, a neuroendocrine hormone, influences angiogenesis and cell proliferation, making it a potential candidate for wound healing applications.

A gelation-based Melatonin sponge crosslinked with fructose was formulated using surfactant foaming and freeze-drying methods, with the objective of studying its characteristics for wound healing.

The formulated gelatin sponge exhibited favorable characteristics such as abundant and uniform pores, good mechanical properties, water uptake, water retention capacities, and high drug entrapment efficiency.

Animal experiments demonstrated that wounds covered by the Melatonin-loaded gelatin sponge healed quickly, as observed through histological and macroscopic observations.

The formulated sponge showed promise as a wound healing material due to its suitable physical and mechanical properties, as well as biocompatibility, highlighting its potential application in wound care.

8. Pharmacoscintigraphic evaluation and antidiabetic efficacy of gliclazide-loaded 99mTc-labelled mucoadhesive microspheres. *Futur J Pharm Sci* 7, 229 (2021). https://doi.org/10.1186/s43094-021-00376-3

The important points from the study on Musa balbisiana starch-based mucoadhesive microspheres for oral delivery of gliclazide are:

Musa balbisiana starch was evaluated for its potential application in formulating mucoadhesive microspheres for enhanced oral delivery of gliclazide, aiming to improve its bioavailability and duration of action for better glycemic control.

The formulation of the microspheres was optimized using response surface methodology and 32 full factorial designs, resulting in an optimum formulation coded as F8.

Characterization studies confirmed the compatibility of the drug and excipient, the occurrence of spherical microspheres with a smooth surface, and an initial burst release followed by sustained release in vitro.

Pharmacokinetic studies demonstrated a 2.7-fold enhancement in gliclazide bioavailability with the prepared microspheres, and gamma scintigraphy studies indicated gastro-retentive properties with a retention time of over 4 hours.

The antidiabetic efficacy of the optimized microsphere formulation was confirmed in a streptozotocin-induced diabetic rat model, highlighting its potential for improved glycemic control.

9. Phytochemical screening and anthelmintic activity of Artocarpus altilis extract. Res. J. Pharm. Technol. 14, 640–644. https://doi.org/10.5958/0974-360x.2021.00114.1

The important points from the study are:

Helminthiasis, or worm infection, is a parasitic disease caused by helminths, which are parasitic worms that infect humans and animals.

The development of alternative medicines for helminthiasis has garnered significant interest, particularly in screening phytochemicals with antihelminthic properties.

The present study focuses on Artocarpus altilis, a plant species, and aims to provide phytochemical screening and evaluate the antihelminthic activity of its leaves extract using dichloromethane-methanol as the extraction solvent.

Previous research has not explored the combination of solvents for extracting the leaves of Artocarpus altilis or evaluated its anthelmintic activity.

In vitro tests conducted on the Indian adult earthworm Pheretima posthuma demonstrated promising anthelmintic activity of the dichloromethane-methanol leaves extract of Artocarpus altilis, surpassing the standard albendazole.

10. Development and Validation of a RP-UHPLC Method for estimation of Gliclazide loaded Microsphere, Res. J. Pharm. Technol. 15 (2022) 773–778. https://doi.org/10.52711/0974-360X.2022.00129.

Important points regarding the RP-UHPLC method for the determination of Gilcazide in a microsphere formulation:

The objective of this work was to develop and validate a reliable and reproducible RP-UHPLC method for the quantification of Gilcazide in a microsphere formulation.

The chromatographic analysis was performed using a Thermo Scientific (Dionex Ultra 3000plus) UHPLC system with a stainless steel YMC C8 column, utilizing an isocratic elution mode with a phosphate buffer pH 3.4 and acetonitrile as the eluent.

The method demonstrated a linear dynamic range from 2-10 μg/mL, and the percentage recovery ranged from 94% to 98%, indicating the accuracy and reliability of the developed UHPLC method.

The retention time for Gilcazide was observed at 1.9 minutes, allowing for efficient analysis.

The validation parameters of the method were performed according to ICH guidelines, and the % Drug Entrapment Efficiency of the Gilcazide loaded microsphere formulation was determined to be satisfactory at 93.72%.