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Computational Evaluation by *In-silico* Pharmacokinetics and Drug-likeness Prediction of 1,4-naphthoquinones Derivatives with [1,2,4]-triazole-3-thione Substitution as Potent Insecticidal agents

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ABSTRACT

Naphthoquinones are wide-spread phenolic compounds in nature. They are products of bacterial and fungal as well as high-plants secondary metabolism. Juglone, lawsone, and plumbagin are the most widespread compounds. Naphthoquinones display very significant pharmacological properties--they are cytotoxic, they have significant antibacterial, antifungal, antiviral, insecticidal, anti-inflammatory, and antipyretic properties. ADMET studies have also been performed using the SwissADME web tool to verify the pharmacological similarity of designed compounds. Hence, the present investigation studies will provide a new vision for the discovery of potent insecticidal agents.

Keywords: ADME studies, 1,4-naphthoquinones, [1,2,4]-triazole-3-thione, Pharmacokinetic properties, Drug-likeness, Insecticidal agents.

I. INTRODUCTION

Mythimna separata Walker (oriental armyworm) is a typical insect pest through crop-destruction. In the past decades of controling agricultural pests, the wanton use of synthetic agrochemicals has resulted in many problems such as pesticide-resistance, and environmental problems. Therefore, development of potential alternatives to efficiently control insect pests is becoming rather desirable[1]. Naphthoquinones are natural pigments that are widely distributed in nature and have important biological activities[2]. Lawsone (2-hydroxy-1,4-naphthoquinone) and its synthetic derivatives, and especially those containing nitrogen, have promising potential for the treatment of different diseases due to their antibacterial, antifungal, antiviral, antitumor and antiparasitic effects, and for pest control via their molluscicidal and insecticidal activities[3]. Their pharmacological activities and mechanisms of action are related to their oxide/reduction and acid/base properties, and can be modulated by directly adding a substituted to the 1,4-naphthoquinone ring. Due to this, naphthoquinones and their derivatives are at the

center of multiple areas of research[4-6]. As a result, scientists must design and discover new drug molecules as soon as possible, as this could provide some of the best chances for success in the current and future epochs[7]. However, a large number of pharmacologically active heterocyclic compounds are still used in clinical practise. Heterocyclic compounds are commonly distributed in nature and have a broad variety of synthetic applications and biological activity, which has assisted medicinal chemists in developing new approaches to drug development[8-9]. A lot more emphasis was given to the production of new methodologies like microwave synthesis for these heterocyclic compounds such as triazole, oxadiazole, benzimidazole and thiadiazole, triazine etc[10-18]. In the current investigation derivatives have previously been documented and synthesized in green chemistry. Microwave-assisted synthesis works by excitation of the material's dipoles in an external field using microwave electromagnetic radiations, and is typically used in combination with a well-known synthesis technique[19-28]. The interaction of electromagnetic waves with polar solvent molecules and/or ions in solution is the basis for microwave (MW) assisted synthesis[29-38]. High heating rates and homogeneous heating with high energy efficiency and shorter synthesis time are achieved by direct interaction of electromagnetic waves with the solution/reactants[39-47]. Since rapid forming of many seeds occurs due to local superheating, MW heating may produce smaller crystals. Because of the homogeneous heating, rapid kinetics, high phase purity, and high yield rate of products in a short amount of time, microwave (MW) and ultrasound synthetic routes have received a lot of attention. Fast crystallisation, uniform nucleation, easy morphology regulation, phase selectivity, reduction in particle size, and rapid warming are all advantages of the MW and US techniques[48-55]. Furthermore, one advantage of MW is the ability to monitor the particle size distribution, as shorter reaction times appear to have a narrower particle size distribution. Previously, MOF-5 was developed in larger quantities using the microwave irradiation method, and the effects of various synthetic parameters on the product crystallinity and morphology, such as microwave power level, irradiation time, temperature, solvent concentration, and substrate composition, were studied in depth[56-62]. In the synthesis of MOFs with smaller quantities, the irradiation time and power level of MW are also important factors. Larger crystals (20–25 m) benefit from increasing the MW irradiation time and power level. With the completion of the human genome project, an increasing number of new therapeutic targets for drug development have emerged. Simultaneously, high-throughput protein purification, crystallography, and nuclear magnetic resonance spectroscopy techniques have been developed, allowing researchers to learn more about the structure of proteins and protein–ligand complexes[63-68]. These advancements have enabled computational strategies to pervade all aspects of drug discovery today, including virtual screening (VS) techniques for hit detection and lead optimization methods as docking and ADME studies proved to be powerful study for *in-silico* study[69-72]. When a strong molecule is need to developed in this pandemic, i.e. coronavirus diseases. In pharmaceutical products, natural products, analytical reagents, agricultural products and dyes, heterocycles play a major role[73-74]. The prediction of ADMET properties plays an important role in the process of drug development because they account for approximately 60% failure of all drugs in the clinical phases. Where ADME tools were usually applied at the end of the drug development system, ADME is now being used in an early stages of drug development to extract from the drug development pipeline molecules with poor ADME properties and to save substantially in R & D costs. Over several years, the QSAR/QSPR group has developed models to predict the physicochemical properties of ADMET of interest (absorption,

distribution, metabolism, excretion, and toxicity). The coefficient of partition, aqueous solubility, absorption, and permeability, BBB-penetration, plasma protein binding, metabolism, hERG inhibition, elimination, P-GL (P-gp) efflux, modeling and toxicity on a physiological basis (PBPK). In addition, pharmacophore and homological modeling have of course also been carried out to allow improved metabolism and toxicity prediction[75]. At present, ADMET tests are low in performance and tend not to be sufficiently insightful or reliable to predict an effective drug, given the significant composite failure rate at all stages of its development[76]. Therefore, drug development companies aim to reorganize the ADMET mechanism to facilitate the early discovery chain. The goal is to predict at an early stage which compounds pass the test for a good medicine, maybe before the compounds are synthesized. Many software for the properties and toxicity of ADME-based species have been developed in recent years. Software is now available for BBB penetration, human gut absorption, oral bioavailability, jejunum permeability, Caco-2 or Madin–Darby canine cell permeability, serum protein binding, obvious delivery rate, blocking HERG potassium, P-gp efflux, human liver toxicity and carcinogenicity[77-78].

II. MATERIALS AND METHODS

In-silico ADMET screening, a software was used for the study of the total drug score and toxicity risks compared with the drugs available for chemical therapy to screen the synthesised drugs. For these molecules in humans, ADMET-properties were evaluated: water-solubility, blood brain barrier (BBB), plasma-protein binding, CYP2D6 binding, intestinal absorption, and hepatotoxicity. Further, the trust ellipses were plotted using AlogP98 and PSA 2D. The models used to predict the ADMET properties in this protocol are derived from a variety of experimental data sources and are catalogued in the product documentation. The online tool SwissADME from the Swiss Institute for Bioinformatics (http://www.sib.swiss) has been also utilized for the evaluation of individual ADME component comportments for pharmacokinetics and drug-like pharmacokinetics and drug-like predictions. In version 15.0 (Cambridge Software), 2D structure models were drawn, and each SMILES compound was molfile translated by an online SMILES translator and structure file generator in SwissADME online tool[79]. The mission to analyze the compounds inhibiting CYP450 (CYP) family isoforms such as CYP1A2 and CYP2D6 was carried out. The study was carried out[80]. Moreover, the drug-like forecast such as Lipinski, the Ghose and Veber rules and bioavailability score are used in pharmacokinetics (e.g. gastrointestinal absorption, P Glycoprotein and Blood brain Barrier). The druglikeness rules for Lipinski, Ghose and Veber were applied to predict whether a compound is possibly Bioactive in accordance with certain important parameters, such as molecular weight, logP, HPA number and HBD number. The Swiss ADME tool used vector machine algorithms (SVM) with broad data sets of known inhibitors as well as substrates/non-substrates, which were thoroughly refined[81-82].

Table 1: Test compounds used in study

Sr. no	Compound code	Name of compound
1	1a	2-chloro-3-{[3-(2-methylfuran-3-yl)-5-thioxo-1,5-dihydro-4H-1,2,4-triazol-4-yl]amino}naphthalene- 1,4-dione
2	1b	2-chloro-3-{[3-(3-methylfuran-2-yl)-5-thioxo-1,5- dihydro-4H-1,2,4-triazol-4-yl]amino}-naphthalene-1,4-dione
3	1c	2-{[4-amino-5-(2-methylfuran-3-yl)-4H-1,2,4-triazol-3-yl]sulfanyl}-3-chloronaphthalene-1,4-dione

III. RESULTS AND DISCUSSION

The SwissADME online version conducted a pharmacokinetic and drug-like prediction of test compounds and the data are shown in Table 3 and in the water solubility provision shown in Table 4. All compounds research showed modely soluble and soluble gastrointestinal absorption according to pharmacokinetic characteristics also show no BBB permeability, but a score of bioavailability was predicted for drug likeness.

Table 3 : Pharmacokinetics and drug-likeness prediction for test compounds (1a-c)

Sr No.	Compound code	Pharmacokinetics			Drug-likeness
		GI absorption	BBB permeability	Log Kp (skin permeation) cm/s	Bioavailability Score
1	1a	High	No	-2.49	0.22
2	1b	Low	No	-2.81	0.17
3	1c	High	No	-2.34	0.11

Table 4: Water solubility prediction for test compounds (1a-c)

Sr No.	Compound code	Log P	Water solubility		
		(Consensus Log P)	Log S (ESOL)	Log S (Ali)	Log S (SILICOS-IT)
1	1a	2.91	Moderately soluble	Moderately soluble	Moderately soluble
2	1b	2.43	Soluble	Soluble	Moderately soluble
3	1c	2.87	Soluble	Moderately soluble	Moderately soluble

IV. CONCLUSION

1,4-naphthoquinone and its derivatives are widely distributed in nature and have been used since ancient times in traditional medicine. Lawsone, one of the hydroxy derivatives of 1,4-naphthoquinone, has been used as a dye, and both its natural form and synthetic derivatives exhibit antibacterial, antifungal, antimalarial, antitumor, molluscicidal and antioxidant activity, among others. The online version of SwissADME carried out the pharmacokinetic characteristics and drug-like prediction of the eight test compounds. The Lipinski five rule states that it is more likely to absorb or permeate a molecule when molecular weight is less than 500 g/mol and log P is less than 5, and the molecule has 5 H-donors atoms. The Lipinski Five rule states that The Lipinski rule-of-five showed all the molecules a significant drug-liking (RO5). The BBB non-permeant (blood–brain barrier) in all molecules; this means no expected neurological adverse effects. All molecules displayed considerable bioavailability, implying that in case of use as a drug the molecules can be absorbed and delivered across the body. The molecules therefore were tested for ADMET and the molecules confirmed that they are acceptable drug-like molecules

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