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Research Article

In-Silico Characterization, Admet Prediction, And Molecular Docking Studies of *Tephrosia Purpurea* Against *Mycobacterium Leprae*

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ABSTRACT

Leprosy is a tropical illness that affects millions of people. The current therapy for leprosy comprises a variety of antibacterial medications, including dapsone, clofazimine, and rifampicin, which are identified as bound to *Mycobacterium leprae*'s dihydropteroate synthase. Dapsone is an expensive antibacterial medication with a number of side effects. It is necessary to develop a natural alternative to dapsone and it has fewer to no side effects and less expensive to produce. *M. leprae* dihydropteroate synthase's three-dimensional protein structure is unknown. Methods: Protein algorithm runs of the target molecule was conducted, as well as protein sequence validation and energy minimization. Phytochemicals with antileprosy properties that were mentioned in the literature were analysed The one's who cleared Therapeutical screens on absorbing, distributed, metabolic, elimination, and toxicology (ADMET) qualities also were submitted to comparing in computational molecular docking studies with dapsone. AutoDock Vina was used for preliminary docking analysis, and the results were confirmed using AutoDock 4.2.6 and SwissDock. Results: Glabratephirin and pongamol It was projected that it would be 10 times safer to administer than dapsone. Glabratephirin and pongamol used to have higher binding affinity than dapsone and formed a stable binding protein, according to in silico docking results. Van der Waals residues containing TYR A:182 and LYS A:181 are valuable binding site byproducts. Conclusion: In silico studies are also needed to prove glabratephirin's antileprosy capabilities over the medication clofazimane..


INTRODUCTION

Neglected tropical diseases (NTDs) are a group of infective illnesses that impact over one billion

individuals worldwide, primarily in developing nations, tropical and subtropical areas. NTDs can be deadly or cause lifelong handicap, wrecking

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havoc on patients' physical, social, and economic well-being. NTDs are more frequent in persons from Economically disadvantaged categories who lack adequate hygiene are unable to afford basic safety measures to prevent interaction to worms or hazardous pathogens. Because individuals in poor areas can hardly afford to exist, when they become infected They pursue an inefficient and expensive localized cure for any one of the NTDs, which generally comprises of extraction generated from trees and shrubs. Many phytoconstituents contain phytochemicals, which seem to be essential for such tree's medicinal properties. The present research is focused upon leprosy, an instance of NTD. *Tephrosia purpurea* Linn. (Leguminosae), Sharapunkha, as it is known in Sanskrit, is a densely branching, sub-erect, herbaceous perennial plant. This plant is also known as "Sarwa wranvishapaka" in Ayurveda literature, which signifies claims it really is capable of healing all types of infections [1]. It is a large element of certain formulations was using to treat liver problems, including such "Tephroli" as well as "Yakrifit." [2]. The roots as well as seed pods are utilized as a souring agent and have antiparasitic and piscicidal properties. These roots are additionally believed to be beneficial in treating leprosy wounds and there own liquid with preventing skin eruptions [3]. For diabetic animals, a extract showed of seedlings demonstrated considerable throughout vivo hypoglycemic action [4]. *Tephrosia purpurea* ethanolic extracts exhibited antibacterial action. Total flavanoids were isolated from a plant that was discovered to have antibacterial action [5]. All through our review of the literature, we determined that this herb has more medicinal potential. We attempted to outline the research findings conducted for scientific authentication of the species and its preparations in this study. This review will surely help the scholars who are studying this plant.

Geographical Distribution

Tephrosia purpurea is a flowering plant species found in wastelands that belongs It belongs toward the pea family and has a tropical and subtropical regions distributionIt really is grown as little more than a biomass source in a number of places. The plant *T. purpurea* may be widespread throughout the globe. It is indigenous to Africa, Southeast Asia, Australia, the western Pacific, China, Sri Lanka, and India. It is prevalent in the Indian regions of Andhra Pradesh, Haryana, Rajasthan, among Tamil Nadu.[6]

Common Names [7,8]

English: Fish poison, Wild indigo

Hindi: Sarphonk, Sarpunkha

Hawaiian: Auhuhu, Auhola, Hola

Gujarati: Unnali

Rajasthani: Masa

Punjabi: Jhojro

Marathi: Untoali

Malayalam: Kattamari, Kozhinjil

Taxonomic Classification[9]

Kingdom - Plantae (Plants)

Division - Magnoliophyta

Class-Magnoliopsida

Order - Fabales

Family – Fabaceae

Genus - *Tephrosia*

Species – *purpurea*

Synonyms: *Cracca purpurea*, *Tephrosia piscatorial*



Figure 1 :- *Tephosuria Purpurea* Linn

Botanical Description

Tephrosia purpurea is a little sapling that really can spread to just be 1.5 meters high. The leaves are starting and running, with 7 to 15 leaflet as well as a solitary final leaflet. The leaves have lengths ranging from 10 to 32 millimeters, and their widths vary from 5 to 11 mm. Flower have colors that range from white to purple and are clustered in inflorescences upwards to 25 centimeters Long Beach flower corollas approximately between 2 and 3 mm in length. With dimensions varying from 20 to 45 mm and diameters ranging from 3 to 5 mm, these pods are straighter or up slightly curled just at terminal end. Whenever the pods are dry, they separate along two valves, revealing 2 to 9 black rectangular seeds approximately 2.5 to 5 mm in length and 1.8 to 3 mm in width.^[10,11]

Traditional uses

The plant is well documented in numerous conventional medical systems to treat various illness problems, e.g. The roots of *Tephrosia purpurea* are utilized to treat viral infections, wounds, acne, blisters, irritation, gastrointestinal issues, asthmatic, snake bite gastroenteritis, as well as kidney problems are all possible.^[12] At first when rats bites, seeds are thrown at them to poison them. The leaves are utilized for the treatment of respiratory disorders, digestive issues, gonorrhoea, piles, as well as syphilis. The whole plant was utilized to treat asthma, ulcers, leprosy, blood purifier, piles, as well as dental treatments. Coughs and colds, as well as renal disorders, are treated using rhizome and petals^[13].

Pharmacological Activities

Tephrosia purpurea It can be utilized to treating various different percutaneous lesions of various types^[14] and gastro-duodenal disorders. The trees It has also been reported to be effective in treating renal, hepatic, spleen, heart, and blood disorders. The dried herbs are employed to treat viral infections, bile fever outbreaks, boils, pimples, and bleeding piles, as well as as tonic laxatives and

diuretics^[15]. An analgesics and anti-inflammatory extraction of pod can be utilized to cure vomiting-like symptoms, and its infusion is employed to cure nausea. Traditional medical systems recommend a *T. Purpurea* infusion again for treatment of a variety of illnesses. In vitro, an ethyl acetate extract plant extract was proven to exhibit anticancer activity versus KB-cell cultures^[16]. The decoction of seeds exhibits tremendous anti-diabetic activity in vivo.^[17] and ethanol extract have been demonstrated to have antibacterial property^[18]. Additionally, its roots extract is reported to be beneficial in the treatment of Dysphagia, prolonged diarrhea, severe spasm are all symptoms. Furthermore, flavonoid has been shown to be antimicrobial.^[19] Roots are used to treat dyspepsia and persistent diarrhea^{[20],[21]}. In Ayurvedic medical operation The plant's constituents are employed to cure insufficiency, asthma, diarrhoea, syphilis, arthritis, ulcers, as well as other disorders, urinary, and cancers., leprosy, and bronchitis^[22].

Chemical Constituents

Phytochemical investigation of the plants showed the existence of highest abundance, isoflavones, flavan-3-ols, chalcones, sterols, flavanones, and flavonoids. Karanjin (1), purpurin (2), pongamol (3), lanceolatin B (4), purpuritenin (5), and purpuretimethide are all found in the seeds Their roots contain flavonoid, apollinine, semiglabin, semiglabinol, tephroglabin, tepurindiol, pongamol, international organization for standardization, O-methylpongamol, lanceolatins A and B, as well as other constituents.^[23] Among several other substances, the leaves have included the flavonoids quercetin, the sesquiterpene luteolin, as well as the sterol -sitosterol. The flavonoids (+)-tephrorins A and B, as well as (+)-tephrosone, are found throughout the plant, as is an isoflavone 7, 4'-dihydroxy-3', 5'-dimethoxyisoflavone, and a chalcone (+)-tephropurpurin^[24]. *T. purpurea* aerial components



extraction was reinvestigated, while three chemicals, an aromatic esters, a sesquiterpene with both the unusual rotundane structure, as well as a prenylated flavonoids, were isolated as structurally elucidated for the inaugural time from in this plant. Some recently discovered chemicals include 4-isopropyl-1, 8-dimethyl-decahydro-azulene-5, 8, 9-triol (**6**), 2-propenoic acid, 3'-(4'-(acetyloxy)-3'-methoxyphenyl)-3-(4-acetyloxy)-3-methoxyphenyl)-2-propenyl ester (**7**), and the prenylated flavonoid (**8**). Chemical analysis of *T. purpurea* aerial parts produced the unusual prenylated flavonoids tephropurpulin A (**9**) and isoglabratephrin (**10**), as well as glabratephrin, a previously discovered flavonoid. Three new flavonoids were isolated from *T. purpurea*: (+)-tephrorins A (**11**), tephrorin B (**12**), and (+)-tephrosone (**13**), and The Mosher ester method was used to determine their relative configuration [20]. Flavonoids having a tetrahydrofuran molecule include molecules 11 and 12 Using a cell-based quinone reductase induction test, compounds 1113 were investigated for their potential cancer chemopreventive activities.

Botanical Description And Varieties

T. purpurea is indeed an annual or brief permanent species that stands erect or spreads, up to 1.5 m tall, with a thinAt the bottom, its stem can indeed be upright or decumbent. Complex (imparipinnate) leaflets with triangle free transverse sepals, rachis up to 14.5 cm long, leaflet 525 mm in length, orbicular to broadly elliptic, terminal leaf (728) mm (211) mm, sharp at base, apex round to emarginate, venation repeated measures design unicostate, venation tightly coiled unicostate. Inflorescence of racemose. Blooms in 46 fascicles, with a pedicel 26 mm long and a

flower 48.5 mm long, purple to white, bisexual, symmetrically zygomorphic, and hypogynous. Calyx-bell shaped gamosepalous, persistent, unequally 4toothed, pubescent teeth on the interior. Corolla papillon-like (i.e., multipetaled irregular corolla), typical broadly ovate posterior petals ((3.5–7.3) mm × (5–10) mm), two lateral petals clawed, 2 Anterior petals very small, slightly united at base, keel or keel ((2.2–4.5) mm × (2–3) mm), stamens 10, stamen diadelphus united, stamen tube long 4–6 mm, ovary upper, style up to 4.5 mm long, upper half glabrous. *T. purpurea*'s pod is dry dehiscent (Legume), flat, linear, (24.5) cm (35) mm, and slightly up-curved towards the end. Seeds are rectangular to transversely ellipsoid, (2.55) mm (1.83) mm, pale to dark brown to black, and occasionally speckled. *T. purpurea* has three primary kinds, according to the Indian Materia Medica Rakta Sarpunkha, Sveta Sarapunkha, and Kantaki Sarapunkha. They are comparable to their current equivalents as continues to follow: *T. procumbens*/*T. candida* Sveta Sarapunkha Kantaki Sarapunkha *T. villosa* Rakta Sarapunkha unexplained.^[25]

Leprosy

Mycobacterium leprae produces leprosy, an extremely infectious infectious Disease. This harmful bacterium bacteria affects the skin surface, nerves, and upper airways because it demands an ideal temperature of 27°C-30°C.^[26] Worldwide, 215,656 new cases of leprosy were recorded in 2013, 213,899 new cases in 2014, and 211,973 cases in 2015.^[27] In 2017, 211,009 cases of leprosy was detected in tropical nations, the majority of which were undeveloped or developing, including Brazil, Africa, and East Asia.^[28]





Figure 2 :- Leprosy Affected Human Being

Since infection with the microbial species, this same clinical features of the disease occurs throughout five forms: opposite poles shapes of tuberculoid (paucibacillary) as well as people can be affected (multibacillary) leprosy and 3 sub - types of transitional stage leprosy - borderline tuberculoid (BT), midborderline (BB), and borderline lepromatous (BL), and this classification is done based just on microbial infection, immune status, and amount of lesions upon this screen. Tuberculoid leprosy occurs when the host's immune system reacts strongly to the infection, As a consequence, leprosy becomes weaker and much more confined. Only one or a few macules or papules-shaped skin lesions will emerge. Lepromatous leprosy occurs whenever the host's immunological responses towards the sickness is insufficient. This causes the condition to become generalized or broad, resulting in multiple reddishbrown Skin or nerve abnormalities are common. The lesions would be symmetrical, and foot oedema could occur at this stage. Unidentified leprosy is asymptomatic and seldom identified because there aren't any evident signs apart having hyperpigmentation erythematous merely over body. That period might endure for many years is usually misunderstood as the other skin conditions; this infection may progress to some other variety of leprosy dependent on host immune system. This grade would be further broken down into three groups:

The three kinds of leprosy are BT syphilis, BB syphilis, and BL syphilis.^[29]

1. MATERIALS AND METHODS

Programs and software for the ligand compounds were drawn using Chemscketch, a chemical molecular drawing tool ^[30]. The .mol file was converted to .pdb format using Avogadro software^[31]. Autodock 4.0 is a new version of Autodock^[32]. The semi-flexible protein-ligand docking Investigations were conducted utilizing a preliminary docking program. The chemical properties of the molecule were studied using the Molinspiration online property calculator^[33]. [PDB: 2ntv] was the pdb code for the crystalline structure of receptors that were downloaded from the protein database. This will be the focus of computational research. For the virtual screening of a library of derivatives, more software was used^[34]. For molecular interaction and visualization, Discovery Studio 3.5 ^[35] and Maestro 12.7 ^[36] were employed.

2.1 Preparation of Ligand

These molecules' combined library of ligands, which was selected, has the best affinity for binding to the target. To create the ligand structures, chemsketch software was utilized, then the clean structure tool was used to tidy them up. The working directory received the structure as an a.mol file. The structure was optimized using the optimization tool after all ligands were entered into the Avogadro program using control. The

ligands then are generated through finding the torsional root, modifying the torsional angles, distributing charged, and optimizing to use the UFF (Universal force field), before even being saved in pdb file in the creating file.

2.2 Preparation of Receptor

PDB ID: 2ntv from the Protein Data Bank (<http://www.swissadme.ch/>) was used for an in silico analysis of the crystal structure. To form a homodimer, the 2ntv protein has two chains, B and C. The Go Loco motif proteins that bind to the inhibiting Gi subtype of G-protein alpha subunit, causing the releasing of binding GDP to be postponed. This interaction is believed to be essential for asymmetrical cellular division, neuro-epithelium, as well as the development of epithelial progenitors. Unwanted chain residues, bound ligand fragments of the receptor, and water molecules were also eliminated. Furthermore, charges were added to the protein and its energy was decreased using Autodock Vina in the open-source program PyRx before the protein was converted to pdbqt format.

2.3 Identification of Receptor-Ligand Interaction:-

Using Docking Autodock v4.0, binding postures and associated binding energies were detected. The conformation with the greatest binding energy is less stable since energy and stability are inversely correlated. The software's default settings have been applied, which are equivalent to other places' usage of the protocol. To score energy, a Lamarckian Genetic Algorithm (LGA)

was built at coordinates X = 65.7709, Y = 56.6367, and Z = 62.2641 with 0.375 angstroms grid point spacing with default atomic salvation parameters 126 (x, y, and z) grid boxes in the ratio of (60:60:60). The receptor's active location was carefully considered to be surrounded by a 3D grid box that was centered on its active ligand binding site location.

2.4 Physicochemical Properties

Each compound's SMILES structure was swissADME (<http://www.swissadme.ch/>) and Lipinski's rule were implemented to computer was used to assess their physicochemical properties and predict their drug-like attributes.

3. RESULT & DISCUSSION

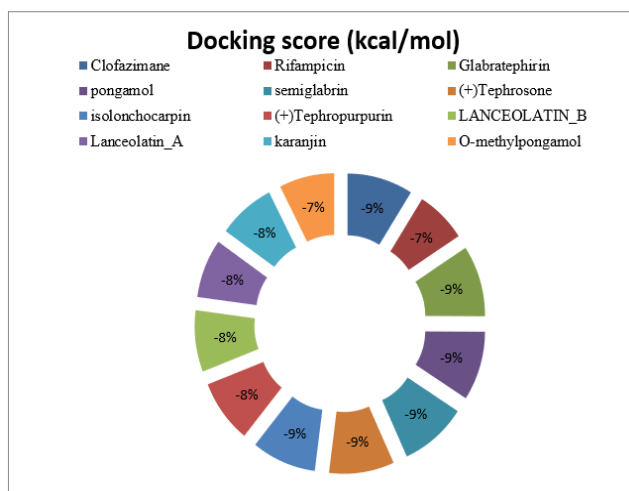
The outcomes of the molecular docking analysis using AutoDock Vina showed what the chosen medications' and reference molecules' binding energies were (Table 1). In addition, SwissDock's findings were contrasted with these ones. The method was divided into many steps, first with the FACTS-based creation of as many binding modes as feasible, then the clustering evaluation. The best full fitness (FF) rating belongs to Cluster "0." Protein and phytochemical samples were provided in separate packages. The output clusters of each docking run was detected, and the single creates two different The clustering that featured the most beneficial complex formation and the most detrimental FF score has been recommended for any further investigation since it provided the best outcome.

Table 1. Ligand with their binding energy and Lipinski rule parameter from the PDB for 2ntv from *Mycobacterium leprae* receptors

Sr. No.	Ligand	Docking score (kcal/mol)	MW (g/mol)	Rotatable bonds	H-bond acceptors	H-bond donors	TPSA ⁰ A	Follow Lipinski	Violations
1	Clofazimane	-10.5	473.4	4	4	1	40 ⁰ A	Yes	1
2	Rifampicin	-8.1	822.9	4	15	5	222 ⁰ A	No	0
3	Glabratephirin	-11	420.41	3	7	0	92.04 ⁰ A	Yes	1
4	pongamol	-10.7	362.42	7	4	0	105.51 ⁰ A	Yes	1
5	semiglabin	-10.7	392.4	3	6	0	71.1 ⁰ A	Yes	1
6	(+)Tephrosone	-10.4	352.4	3	5	2	76 ⁰ A	Yes	1



7	isolonchocarpin	-10.3	306.4	1	3	0	35.5 ⁰ A	Yes	1
8	(+)Tephropurpurin	-9.8	424.4	6	7	1	91.3 ⁰ A	Yes	1
9	LANCEOLATIN-B	-9.5	262.26	1	3	0	39.4 ⁰ A	Yes	1
10	Lanceolatin-A	-9.1	336.4	4	4	1	55.8 ⁰ A	Yes	1
11	karanjin	-9.1	292.3	2	4	0	48.7 ⁰ A	Yes	1
12	O-methylpongamol	-8.8	308.3	5	4	0	48.7 ⁰ A	Yes	1



The Clofazimane forms a van der waals with TYR A:182, LYS A: 181, SER A: 140, with the lowest binding energy (-10.5 kcal/mol), indicating that it interacts with the catalytic residues.

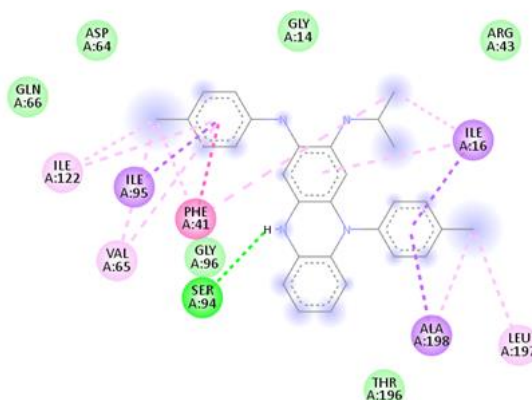


Figure 3 : Interaction after docking 2ntv from *Mycobacterium leprae* receptors with Clofazimane 2D image.

The pongamol forms a van der waals with TYR A:182 and LYS A: 181, with the lowest binding energy (-10.7 kcal/mol), indicating that it interacts with the catalytic residues.

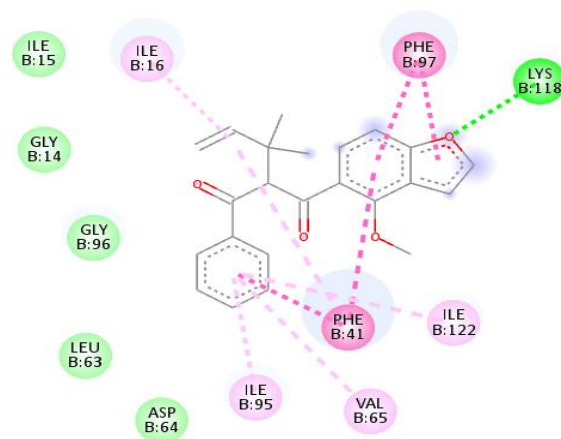


Figure 4: Interaction after docking 2ntv from *Mycobacterium leprae* receptors with Pongamol 2D image.

The pongamol forms a van der waals with ASN B:231 and SER A: 140, with the lowest binding energy (-10.7 kcal/mol), indicating that it interacts with the catalytic residues.

3.1 Physicochemical Characterization

To predict the pharmacokinetics of the drugs, the physicochemical properties of the compounds were also examined using Lipinski's rule. Lipinski's guidelines state that A molecular weight

(MW) of 500 Da or less, an octanol-water partition coefficient (Log P) of 5 or less, a polar surface area (PSA) of 150 A0 or less, several hydrogen bond donors (HBDs) of 5 or less, several hydrogen bond acceptors (HBAs) of 10 or less, and several rotatable bonds (RBs) of 10 or less are required for orally active drug compounds. Lipinski's values are shown in Table 1 for each chemical.

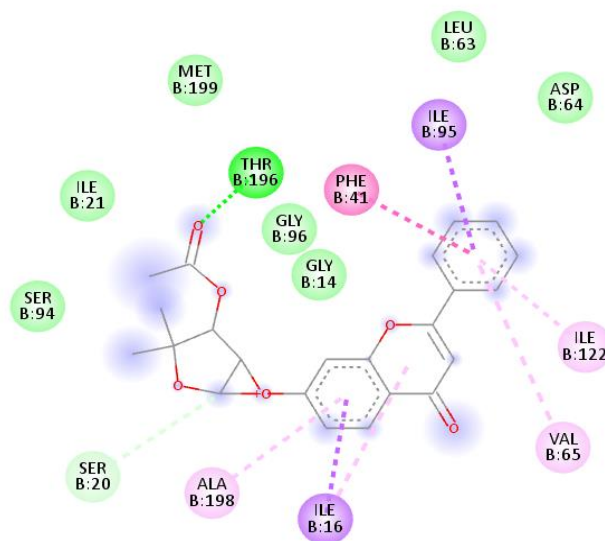
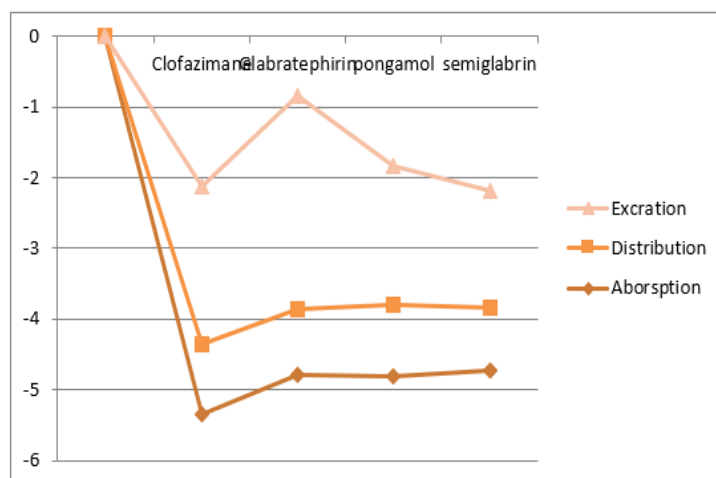


Figure 5: Interaction after docking 2ntv from *Mycobacterium leprae* receptors with semiglabin 2D image.

Sr. No.	Active compound	Absorption Caco-2	Distribution (PPB)	Excretions	Toxicity
1.	Clofazimane	-5.340	99.253%	2.222	0.62
2.	Glabratephirin	-4.776	91.435%	3.009	0.54
3.	pongamol	-4.798	99.698%	1.971	-

4.	semiglabin	-4.725	89.034%	1.647	-
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Conflict of Interest Statement

"The authors claimed that they had no conflicts of interest."

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