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Biologically active sulphur rich volatiles of *Allium stracheyi* and their molecular docking studies against 5IBS

Balam Singh Bisht*[1], Darshan Singh[2], Gunjan Karki[1], Mahesh Chandra Vishwakarma[3] & Himanshu Rawat[4]
[1]*Himalayan Medicinal & Aromatic Plants Research Centre (HIMARC), Berinag, Pithoragarh Uttarakhand*
[2]*Department of Chemistry, Government Postgraduate College, Bazpur, US Nagar Uttarakhand*
[3]*Department of Chemistry, Government Postgraduate College, Berinag, Pithoragarh Uttarakhand*
[4]*ARIES, Devasthal, Nainital Uttarakhand*
**Email: bbbantychem@gmail.com*

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Abstract

Allium stracheyi, an endemic species of the Himalayan region, is part of the diverse *Allium* genus, known for its medicinal, nutritional, and aromatic properties. This research investigates the volatile constituents of *Allium stracheyi*, which contribute to its characteristic aroma, flavor, and potential therapeutic properties. Gas chromatography-mass spectrometry (GC-MS), was used to identify and characterize the volatile organic compounds (VOCs) present in this species. Sulphur-containing compounds, especially trisulfide dipropyl, tetrasulfide dipropyl, dipropyl disulfide and trisulfide methyl propyl were the predominant constituents, accompanied by several aldehydes, alcohols, and hydrocarbons.

To assess the potential bioactivity of these compounds, molecular docking studies were carried out using the 5IBS protein (chain A), a crystal structure of a target enzyme involved in a biological pathway. The 5IBS protein was selected for its relevance to inflammatory and microbial processes. The docking results demonstrated significant binding affinities of the sulphur-containing volatiles to the active site of the 5IBS A chain, indicating a possible inhibitory mechanism. 1-allyl-2-isopropyldisulfane and disulfide, 1-(1-propenylthio) propyl propyl exhibited a notable docking score of -3.5 kcal/mol.

This study suggests that sulphur-rich compounds from *Allium stracheyi* could serve as promising candidates for the development of natural antimicrobial and anti-inflammatory agents. Further *in vitro* and *in vivo* studies are warranted to explore these bioactivities and understand the therapeutic potential of these volatiles.

Keywords: *Allium stracheyi*, volatile organic compounds, sulphur, GC-MS, thiosulfinates, Himalayan flora, antimicrobial property

Introduction

In Uttarakhand, India, spices play a crucial role in food, medicine, the economy and culture of the area. Through sustainable farming techniques, they serve as a major source of income for farmers and contribute significantly to Ayurveda and local medical practices. They enhance the flavour and nutritional value of traditional cuisines. Furthermore, spices support the regional biodiversity and are integral to its cultural heritage, playing a key role in celebrations, rituals and the transmission of traditional knowledge (Srinivasan, 2005). Overall, spices play a fundamental role in Uttarakhand Himalayan life, representing the distinct fusion of local customs and environment. Their significance may be seen from multiple perspectives, such as their role in enhancing the flavour of Uttarakhand cuisines (Viuda-Martos *et al*., 2011). Many spices used in Uttarakhand are also valued in Ayurveda for their healing properties. Spices like Timur and Jakhiya are used in local medicine to treat various ailments, from digestive issues to respiratory problems (Srinivasan, 2014). The cultivation and sale of spices provide a significant source of income for local farmers. This is particularly important in the hilly terrain where large-scale farming is challenging. These spices are a staple in local markets, contributing to the local economy and supporting small businesses (Meghwal, *et al.,* 2012). Traditional farming of spices often involves sustainable practices that help in preserving the ecological balance of the Himalayan region. The variety of spices grown contributes to the biodiversity of the region, which is crucial for maintaining ecological stability. The use of spices is deeply rooted in the cultural heritage of Uttarakhand. Knowledge about their cultivation, culinary applications and medicinal properties is passed down through generations and is used in various cultural and religious festivals, where they are considered as ingredients of special dishes and offerings. Spices of Indian Himalayan Region (IHR) often contain essential nutrients, antioxidants, and vitamins (Bisht *et al*., 2018). To achieve chemical standardization of these aromatic spices we have taken *Allium stracheyi* for the determination of its essential oil composition and flavour constituents.

The *Allium* genus, encompassing over 900 species, includes widely known species like garlic (*Allium sativum*) and onion (*Allium cepa*), which are cultivated worldwide for their culinary and medicinal uses. Among these, *Allium stracheyi*, commonly known as Jambu, Faran and Sekua (Maikhuri *et al*., 2017) is native to the Himalayan region

along with neighbouring countries such as Pakistan and Nepal (Kuniyal *et al*., 2018). Despite its historical and ethnobotanical significance, it remains understudied. Traditionally used in folk medicine and local cuisines, *Allium stracheyi* exhibits a strong aromatic profile, which suggests the presence of bioactive volatile compounds. The volatile organic compounds (VOCs) in this species are responsible for its characteristic pungency and potential therapeutic effects. Commercial production of these spices is also reported (Maikhuri *et al*., 2017; Kuniyal *et al*., 2018; Nautiyal *et al*., 2001). *Allium stracheyi* is useful as a stimulant, cordial, cardioactive, and diaphoretic, carminative, expectorant, curing stomach troubles and in treating constipation. Only a few studies have assessed the flavour constituents of this species (Singh *et al.,* 2009, Mathela *et al*., 2005). Sulphur-containing compounds have emerged as significant players in the development of anticancer agents, particularly through their incorporation into heterocyclic structures. These compounds exhibit diverse mechanisms of action, targeting various cancer-specific pathways and proteins. Compounds such as benzothiazole, thiazole, and thiophene have shown promising anticancer activity by inhibiting critical signaling pathways involved in tumor growth (Maji *et al.* 2024, Kaur *et al.,* 2022). Sulphur-containing nucleosides have demonstrated significant antitumor activity in various cancer cell lines (Hao *et al.* 2024). Thiazole-based polyamides have been synthesized, showing enhanced solubility and anticancer activity against breast and colon carcinoma cells (Kritika *et al.,* 2021; Kaur *et al.,* 2022). This study aims to explore the chemical composition of the volatile constituents of *Allium stracheyi* using gas chromatography-mass spectrometry (GC-MS) and their molecular docking analysis against 5IBS protein. By identifying its volatile profile, this research will enhance our understanding of the biological and pharmacological potential of this species.

Materials and methods

Collection and identification of plant material

Fresh leaves of *Allium stracheyi* were collected from Kuti village (Dharchula), Pithoragarh district of Uttarakhand (India), the high-altitude regions of the Western Himalayas at an elevation of approximately 3,500 meters. The plant samples were authenticated based on morphological characteristics by a taxonomist specializing in Himalayan flora. Voucher No.: HIMARC/BSB/JB/2024 was deposited in the Himalayan Medicinal & Aromatic Plants Research Centre (HIMARC), Berinag, Pithoragarh (Uttarakhand) for future reference. The fresh plant material was immediately transported to the laboratory for analysis.

Extraction of essential oil

The plant material (150 gm) was subjected to steam distillation. The distillates were saturated with NaCl and extracted with n-hexane and dichloromethane. The organic phase was dried over anhydrous sodium sulphate and the solvents were distilled off. The essential oil was extracted by

hydrodistillation following the method reported previously (Adams 2001; Mathela *et al*., 2005).

Gas Chromatography (Gc-Fid) and Gas Chromatography-Mass Spectrometry (Gc-Ms) analysis

Gas chromatography-Mass spectrometry (GC-MS) analysis (A.I.R.F. (J.N.U), New Delhi, India) with GCMS-QP 2010 Ultra DB-5 and GCMS-QP 2010 Ultra Rtx-5MS column (30 m x 0.25 mm i.d., 0.25 m) was used to determine the phytochemical makeup of both essential oils with a split ratio of 10.0 and a flow rate of 1.21 mL/min. Helium was used as the carrier gas, with a temperature gradient of 3 °C/min up to 210 °C (an isotherm for 2 min) and subsequently 6 °C/min up to 280 °C. The GC oven temperature program was 50–280 °C. By comparing the mass spectrum fragmentation patterns and relative retention index (RI) values of essential oils with the MS library (NIST14.lib, FFNSC2.lib, WILEY8.LIB) and comparing the spectra with literature, the components of these oils were determined.

Compound identification

The identification was done on the basis of Linear Retention Index (LRI), determined with reference to homologous series of *n*-alkanes (C_9-C_{24}, Polyscience Corp., Niles IL under identical experimental condition), co-injection with standard (Sigma and Aldrich), MS Library search (NIST and WILLEY), by comparing with the MS literature data[11] and by NMR (^1H, ^{13}C NMR) of major isolates. The relative amounts of individual components were calculated based on the GC peak area (FID response). without using correction factor (Adams 2001; Mathela *et al*., 2005).

Molecular docking study

The crystal structure of the cancer-associated phosphatase SHP2 mutant (PDB ID: 5IBS) was obtained from the Protein Data Bank (https://www.rcsb.org). The preparation of the protein structure (PDB ID: 5IBS) using Discovery Studio involves a series of steps to ensure that the structure is suitable for molecular docking and other computational studies. Below is a detailed outline of the preparation process:

1. Importing the protein structure

- The crystal structure of 5IBS was downloaded in PDB format from the Protein Data Bank (https://www.rcsb.org).
- The structure was imported into Discovery Studio for preprocessing and optimization.

2. Protein cleanup

- ***Water molecules:*** Water molecules were analyzed for their relevance to the binding site. Non-essential water molecules were removed, while those mediating crucial interactions in the active site were retained.
- ***Heteroatoms and ligands:*** The native ligands, cofactors, and ions were assessed. Unrelated ligands and ions were removed to eliminate potential interference.

3. Assigning force field and charges

- The CHARMm force field was applied to the protein structure to assign proper atom types and charges.
- Any issues related to bond orders and atomic connectivity were corrected.

4. Energy minimization

- The structure underwent energy minimization to relieve steric clashes and optimize geometry. This step ensured that the protein maintained its biological relevance while being structurally stable.

5. Defining the binding site

- The active site of 5IBS was defined using automated binding site prediction tools or manual selection based on known active site residues.

6. Validation of the prepared structure

- The prepared structure was validated to ensure that no steric clashes or geometric distortions were present and all the critical residues in the binding site were intact and properly oriented.

The prepared structure of 5IBS was now optimized and ready for downstream molecular docking or simulation studies. In a molecular docking study using PyRx with the protein 5IBS (a structure commonly associated with a viral enzyme or a receptor protein), sulphur compounds were docked into the active site to analyze binding interactions and affinities. PyRx, a virtual screening tool, utilizes AutoDock Vina to perform docking simulations, ranking ligands based on binding energies and poses within the receptor's binding pocket. The grid box center values were set to X: 0.2387, Y: 0.8439, and Z: 5.4112. When docking a potential inhibitor or ligand, such as a small molecule or drug candidate, to 5IBS, the study focused on identifying key interactions, such as hydrogen bonding, hydrophobic interactions, and π-π stacking, between the ligand and specific active site residues. This information helps assess the ligand's potential as a therapeutic agent by considering its binding affinity and the stability of its interactions with essential residues, such as those involved in catalysis or substrate recognition in 5IBS. The evaluation of the docked compound relied on the lowest binding energy. Discovery studio 2024 was employed for 2D depiction of the docked complexes (Ngalang *et al*., 2024).

Results and discussion

Volatile profile of *Allium stracheyi*

The GC-MS analysis revealed the presence of a wide array of volatile organic compounds in *Allium stracheyi* (Fig 1). The most abundant compounds identified were sulphur-containing compounds, characteristic of the *Allium* genus. These compounds contribute to the pungent aroma and potential health benefits associated with the plant (Table 1).

Dominance of sulphur compounds

Sulphur-containing compounds such as trisulfide dipropyl, tetrasulfide dipropyl, dipropyl disulfide and trisulfide methyl propyl were the most prominent constituents, collectively representing over 53.94% of the total volatile content (Fig. 2).

These compounds are known to contribute significantly to the characteristic pungency and are associated with various biological activities, including antimicrobial, antioxidant, and anticancer properties (Mohan *et al*., 2019; Shah *et al*., 2014). sulphur compounds, particularly thiosulfinates, are responsible for the reactive nature of *Allium* species' volatiles. When the plant tissue is disrupted, these compounds are formed enzymatically, contributing to the defensive and therapeutic properties of *Allium stracheyi* (Dobhal, 2015; Tiwari *et al*., 2014, Ranjan *et al*., 2010, Kumar *et al*., 2015).

The presence of sulphur compounds can vary based on the region where the plant is grown. Higher altitudes (1800-3000 meters above sea level) from Kumaon region of Uttarakhand contained higher concentrations of allicin and diallyl disulfide (Dobhal, 2015; Tiwari *et al*., 2014; Ranjan *et al*., 2010; Kumar *et al*., 2015) while Garhwal region was found rich in allicin, methyl cysteine sulfoxide, and propyl disulfide (Kumar *et al*., 2015; Samal *et al*., 2010, Block, 2010). Our investigation found the presence of trisulfide dipropyl, tetrasulfide dipropyl, dipropyl disulfide and trisulfide methyl propyl as major sulphur compounds. Following factors can be attributed for this variation in the sulphur constituents of *Allium stracheyi*.

- Altitude: Higher altitudes generally lead to increased sulphur compound concentration, particularly allicin, due to the stress conditions such as cold temperatures and lower oxygen levels, which can stimulate the synthesis of these compounds.
- Soil composition: The mineral content and pH of the soil significantly affect the sulphur uptake by plants. Regions with sulphur-rich soils may produce *Allium stracheyi* with higher sulphur compound content.
- Climate: Cooler temperatures at higher altitudes can enhance the flavor intensity by preserving the sulphur compounds, while warmer climates might lead to their degradation or lower accumulation.
- Cultivation practices: Traditional cultivation methods and the use of organic fertilizers in certain regions can also impact the sulphur compound profile in *Allium stracheyi*.

This variation affects both the culinary uses and the potential health benefits of the plant, making the regional selection important for specific purposes in cooking and traditional medicine

Contribution of aldehydes and alcohols

Apart from sulphur compounds, aldehydes like 2,4-dimethyl-5,6-dithia-2,7-nonadienal were detected. These compounds are known for their grassy and fruity aromas, adding complexity to the overall volatile profile of *Allium stracheyi*. The presence of patchouli alcohol, an alcohol with a sweet odor, further diversified the aroma profile, indicating that both sulphur and non-sulphur compounds contribute to the sensory characteristics of this plant.

Biological significance of volatile compounds

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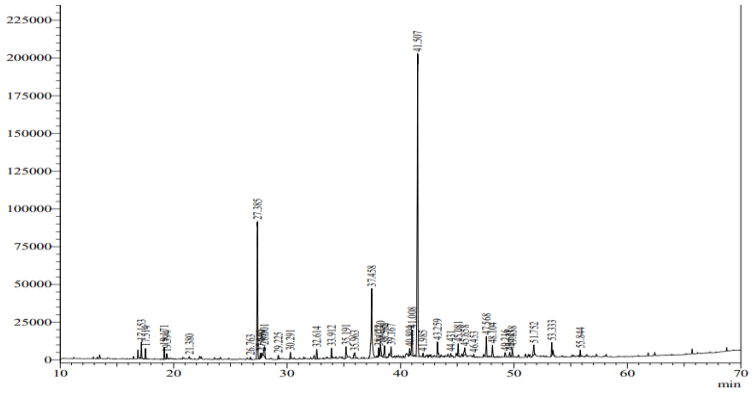

Fig. 1. Gas chromatogram of *Allium stracheyi* essential oil

Contribution of aldehydes and alcohols

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Biological significance of volatile compounds

Biogenesis of sulphur volatiles

The primary sulphur-containing compounds in *Allium* species, such as γ-glutamylcysteine peptides and S-alk(en)yl cysteine sulfoxides (ACSOs), undergo enzymatic conversion by the enzyme alliinase when plant cells are disrupted. This conversion leads to the formation of sulfenic acids, which spontaneously rearrange to produce various sulphur volatiles, including thiosulfinates (e.g., allicin) and polysulfides (e.g., diallyl disulfide) (Miron *et al*., 2000; Griffiths *et al*., 2002; Iciek *et al*., 2009, Banerjee *et al., 2003*).

Antimicrobial activity

Sulphur volatiles from *Allium* species have demonstrated significant antimicrobial activity against a wide range of pathogens, including bacteria, fungi, and viruses. Allicin, in particular, exhibits broad-spectrum antimicrobial properties by inhibiting the thiol-containing enzymes in microorganisms, thereby disrupting essential metabolic processes (Miron *et al*., 2000; Griffiths *et al*., 2002; Iciek *et al*., 2009; Banerjee *et al., 2003*).

Antioxidant properties

The antioxidant activity of sulphur volatiles is well-documented, with these compounds scavenging free radicals and enhancing the body's antioxidant defense systems. Diallyl disulfide and diallyl trisulfide are particularly noted for their ability to upregulate antioxidant enzymes like superoxide dismutase (SOD) and glutathione peroxidase (Miron *et al*., 2000; Griffiths *et al*., 2002; Iciek *et al*., 2009; Banerjee *et al., 2003*).

Table 1. Volatile constituents of *Allium stracheyi* essential oil

S. no.	Compound name	RI	%	Mode of identification
1.	1-Allyl-2-isopropyldisulfane	1045	1.03	a, b
2.	4-Methyl-1,2,3-trithiolane	1084	0.65	a, b
3.	Dipropyl Disulfide	1110	3.39	a, b
4.	Trisulfide, methyl propyl	1171	3.26	a, b
5.	2-isothiocyanato-2-methylpropane	-	0.23	a, b
6.	5-Methyl-1,2,3,4-tetrathiane	1345	2.01	a, b
7.	Trisulfide, dipropyl	1370	21.69	a, b
8.	(E)-1-(Prop-1-en-1-yl)-3-propyltrisulfane	1378	2.11	a, b
9.	S-prop-1-en-1-yl propane-1-sulfonothioate	1383	0.42	a, b
10.	2-Methyloxane-2-carbohydrazide	1486	0.70	a, b
11.	(-)-Globulol	1530	1.51	a, b
12.	2,4-Dimethyl-5,6-dithia-2,7-nonadienal	1535	0.79	a, b
13.	Phenol, 3,5-bis(1,1-dimethylethyl)-	1555	1.38	a, b
14.	1,4-Dimethyl-7-(prop-1-en-2-yl) decahydroazulen-4-ol	1601	3.16	a, b
15.	Disulfide, 1-(1-propenylthio) propyl propyl	1612	0.23	a, b
16.	Humulene epoxide II	1613	1.13	a, b
17.	Tetrasulfide, dipropyl	1621	15.06	a, b
18.	Patchouli alcohol	1668	36.50	a, b
19.	3,4-Dimethyl-2-(propyldisulfanyl)thiophene	1674	0.73	a, b
20.	Disulfide, 1-(1-propenylthio) propyl propyl	1863	2.36	a, b
	% sulphur Compounds		53.94	
	% other Volatile Compounds		44.37	
	% Total		98.31	

RI= Retention Index, a= GC, b=GC-MS

Anticancer potential

Sulphur volatiles from *Allium* species are also recognized for their anticancer properties. These compounds modulate multiple molecular pathways involved in carcinogenesis, including apoptosis, cell cycle regulation, and angiogenesis. Allicin, for example, induces apoptosis in cancer cells by activating caspase enzymes and altering mitochondrial membrane potential (Maji *et al.,* 2024; Kaur *et al.,* 2022; Kritika *et al., 2021;* Miron *et al*., 2000).

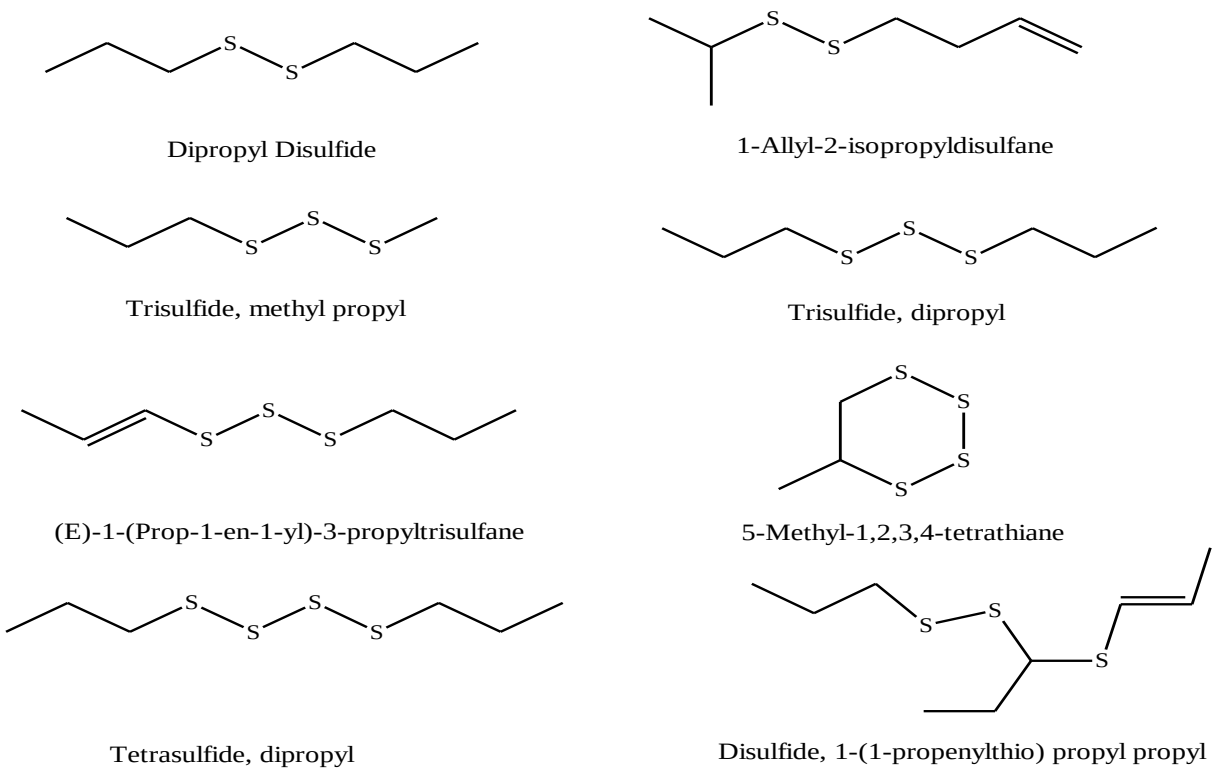

Fig. 2. Structures of major sulphur containing volatile constituents from *Allium stracheyi*

Cardiovascular benefits

Regular consumption of *Allium* species has been linked to reduced risk of cardiovascular diseases, largely due to the bioactive sulphur volatiles. These compounds have been shown to improve lipid profiles, reduce blood pressure, and inhibit platelet aggregation, thus providing a protective effect against atherosclerosis and related conditions (Miron *et al*., 2000; Griffiths *et al*., 2002; Iciek *et al*., 2009; Banerjee *et al., 2003*).

Applications in food and medicine

The bioactive properties of sulphur volatiles from *Allium* species have significant implications for both food preservation and the development of novel therapeutics. In food science, these compounds can be used as natural preservatives due to their antimicrobial and antioxidant properties. In medicine, their potential to prevent and treat various diseases, including infections, cancer, and cardiovascular disorders, is being increasingly recognized (Miron *et al*., 2000; Griffiths *et al*., 2002; Iciek *et al*., 2009; Banerjee *et al., 2003*).

Molecular docking analysis

The molecular docking analysis revealed important insights into *Allium stracheyi* essential oil major sulphur containing components interaction with cancer-associated mutation of the

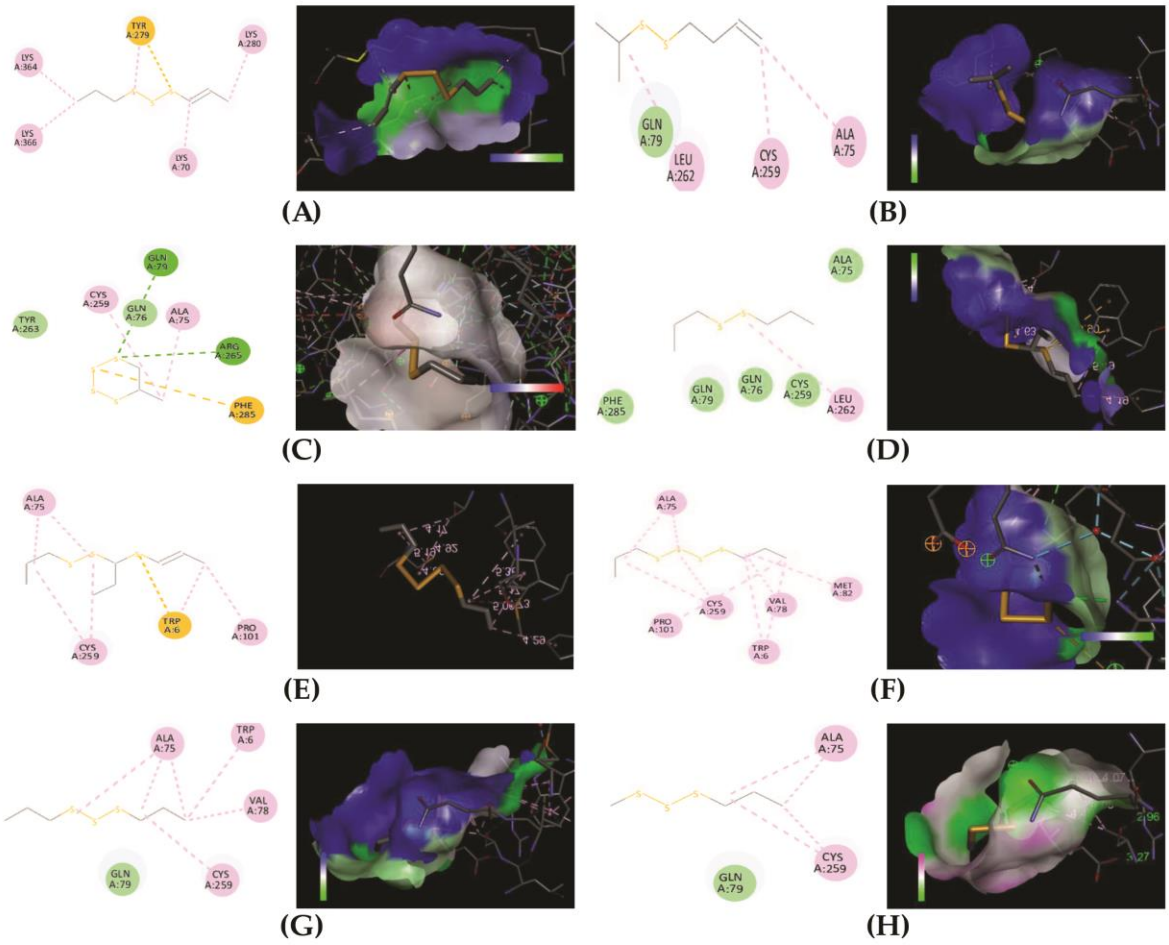

Fig. 3. 2D binding of sulphur constituents of *Allium stracheyi* with 5IBS and their position inside the binding pocket (**A**=(E)-1-(Prop-1-en-1-yl)-3-propyltrisulfane, **B**=1-Allyl-2-isopropyldisulfane, **C**=5-Methyl-1,2,3,4-tetrathiane, **D**=Dipropyl disulfide, **E**= Disulfide, 1-(1-propenylthio) propyl propyl, **F**= Trisulfide, dipropyl, **G**=Tetrasulfide, dipropyl, **H**=Trisulfide, methyl propyl)

oncogenic phosphatase SHP2 (PDB ID: 5IBS), elucidating its binding affinity and potential effect against it (Fig. 3). 1-Allyl-2-isopropyldisulfane (Fig. 3B) and disulfide, 1-(1-propenylthio) propyl propyl (Fig. 3E) exhibited a notable docking score of -3.5 kcal/mol, revealing robust interaction within the receptor's binding pocket, engaging with hydrogen bonding, π-sulphur, π-alkyl and alkyl interactions. The 1-Allyl-2-isopropyldisulfane and disulfide, 1-(1-propenylthio) propyl propyl appears to interact with a diverse set of amino acids, suggesting a complex binding pocket. The presence of both polar (GLN) and non-polar (LEU, ALA) residues indicates a mix of hydrophilic and hydrophobic interactions. The cysteine residue (CYS) could be significant, potentially involved in disulfide interactions or as a nucleophilic site. The presence of both polar (CYS) and non-polar

(ALA, PRO) residues indicates a mix of hydrophilic and hydrophobic interactions. TRP (tryptophan) could be involved in aromatic or π-interactions. Residues like GLN often engage in hydrogen bonding through their polar side chains. This interaction stabilizes ligands by forming specific directional bonds critical for high binding affinity. Residues such as LEU, with non-polar aliphatic side chains, contribute via van der Waals interactions, which enhance the ligand's fit into the binding pocket without strong directional preferences. If aromatic residues are involved (e.g., PHE, TYR), they might establish π-π stacking with aromatic rings in the sulphur-rich ligand. Residues like CYS could potentially form covalent bonds with reactive groups in sulphur-rich ligands, stabilizing their binding. Docking studies might indicate competitive or allosteric inhibition based on where the compounds bind. For instance, active site binding suggests that the compound acts as a competitive inhibitor, directly interfering with the enzyme's activity and allosteric binding indicates modulation of the enzyme's activity indirectly.

Conclusion

This study provides a comprehensive analysis of the volatile constituents of Himalayan *Allium stracheyi*, identifying sulphur-containing compounds as the dominant group. These volatile compounds contribute to the plant's distinct aroma and are likely responsible for its biological activities, including antimicrobial and antioxidant properties. The 5IBS protein is associated with specific molecular interactions, and docking studies with sulphur-rich volatiles from *Allium stracheyi* have provided insights into the binding affinities and potential biological activities of these compounds. The docking results highlight how well these volatiles interact with the 5IBS A chain, which could be an enzyme or a protein involved in significant biological processes like inflammation or oxidative stress. The results suggest that the sulphur-rich compounds have strong binding affinities with the active sites of the 5IBS A chain, indicating possible therapeutic applications. These applications could include developing new drugs for combating diseases related to oxidative stress, inflammation, or microbial infections. The study likely emphasizes the importance of validating traditional knowledge scientifically, as *Allium stracheyi* has been used in local medicinal practices. Further *in vivo* or *in vitro* studies are needed to explore the bioactivity of these compounds, validating their effectiveness as therapeutic agents. Additionally, deeper analysis into other molecular targets beyond 5IBS could reveal broader implications of the sulphur-rich volatiles.

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