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FULL PAPER

Astragaloside interaction of astragalus plant extract *(astragalus)* on adrenergic receptor alpha-2 as regulation of sympathetic nervous system activity

Rahadian Zainul[a,*] |Dony Novaliendry[b] |Agariadne Dwinggo Samala[b] |Budhi Oktavia[a] |Cheng-Hong Yang[c] |Devi Purnamasari[d] |Mirella Fonda Maahury[e] |Rollando[f] |Rismi Verawati[a] |Muhammad Arya Ghifari[g] |Muhammad Thoriq Albari[g] |Muhammmad Raffi Ghifari[g] |Putri Azhari[h] |Riso Sari Mandeli[i]

[a]*Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Negeri Padang, Padang, West Sumatra, Indonesia*

[b]*Department of Electronics Engineering, Faculty of Engineering, Universitas Negeri Padang, Indonesia*

[c]*Electronic Department, National Kaohsiung University of Science and Technology, Kaohsing, Taiwan*

[d]*Department of Radiology, Faculty Health, Universitas Awal Bros, Indonesia*

[e]*Department of Chemistry, Faculty of Mathemetics and Natural Sciences, Pattimura University, Indonesia*

[f]*Department of Pharmacy Program, Faculty of Health Sciences, Universitas Ma Chung, Malang, Indonesia*

[g]*Department of Information Technology, Faculty of Computer Sciences, Universitas Brawijaya, Malang, East Java, Indonesia*

[h]*Department of Agricultural Technology, Faculty of Agricultural Technology, Universitas Andalas, Padang, Indonesia*

[i]*Department of Environmental Science, Postgraduate Programme, Universitas Negeri Padang, Padang, West Sumatera, Indonesia*

***Corresponding Author:**
Rahadian Zainul
E-mail: rahadianzmsiphd@fmipa.unp.ac.id
Tel.:+ +62 812-6138-53

This research aims to study the interaction between astragaloside, astragalus plant extract, and adrenergic receptor alpha-2 as a regulation of sympathetic nervous system activity. The research methods used include the use of Pymol, Pyrex, Protein Plus, and Lipinski Rule software for molecular analysis and protein structure characterization. The results showed that astragaloside had a binding affinity of -6.4. In addition, RMSD was found to be 0, 2.515, and 2.703, which indicated the success of astragaloside in interacting with adrenergic receptor alpha-2. Analysis using Protein Plus showed an interaction between astragaloside and adrenergic receptor alpha-2. Lipinski analysis showed that astragaloside has a mass of 618, 10 hydrogen bond donors, 17 hydrogen bond recipients, a logP of -0.0197, and a molar reactivity of 127.710. These findings provide further understanding of the mechanism of astragaloside's interaction with adrenergic receptor alpha-2, which could potentially regulate sympathetic nervous system activity. This study contributes to the therapies development based on astragalus plant extracts for effective regulation of sympathetic nervous system function.

KEYWORDS

Astragaloside; astragalus; adrenergic receptor alpha-2 (ADRA2); sympathetic nervous system; molecular interactions.

Introduction

The sympathetic nervous system is one of the important components in the regulation of physiological activities of human body. Adrenergic receptor alpha-2 is one type of receptor involved in the regulation of the

sympathetic nervous system. *Astragalus*, a plant that has long been used in traditional medicine, is known to contain an active component called astragaloside. However, not much is known about the interaction of astragaloside with adrenergic receptor alpha-2 (ADRA2) and its potential as regulation of sympathetic nervous system activity [1-4].

Therefore, this study aims to investigate the interaction of astragaloside with adrenergic receptor alpha-2 and its impact on the regulation of sympathetic nervous system activity. This study may provide new insights into the use of astragalus as a potential therapy in effectively regulating sympathetic nervous system function, with relevant implications in the development of drugs and treatments based on Astragalus plant extracts [5-7].

Recent research in the field of molecular interactions between astragaloside, an astragalus plant extract, and adrenergic receptor alpha-2 has revealed a deeper understanding of the mechanisms of regulation of sympathetic nervous system activity. Several studies have shown that astragaloside has the ability to interact with adrenergic receptor alpha-2, indicating the potential of astragalus as a regulatory agent in the sympathetic nervous system [8, 9]. The use of molecular analysis software such as Pymol, Pyrex, Protein Plus, and Lipinski Rule has facilitated the structural understanding and characterization of proteins in this context [10,11].

In addition, Lipinski Rule analysis provided important information on the physicochemical characteristics of astragaloside, such as mass, hydrogen bond donor, hydrogen bond acceptor, logP, and molar reactivity. These findings provide a solid basis for further research in developing astragalus-based therapies to effectively regulate sympathetic nervous system activity and potentially contribute to the development of better medicines in this field [12,13].

This research has novelty and significant contribution in the field of molecular interaction between astragaloside and adrenergic receptor alpha-2 as regulation of sympathetic nervous system activity. This research expands our understanding of the interaction mechanism and the potential of astragalus as a regulator in the sympathetic nervous system. Using advanced molecular analysis and protein characterization methods, this study provides new insights into the physicochemical properties of astragaloside and the interaction pattern with adrenergic receptor alpha-2 [14-16].

The main contribution of this study is to provide a solid foundation for the development of astragalus-based therapies to effectively regulate sympathetic nervous system function. With a better understanding of these interactions, this research may pave the way for the development of potential new drugs in the treatment of sympathetic nervous system disorders, as well as provide a more natural and sustainable alternative in the medical field [17,18]. The aim of this study was to investigate the interaction between astragaloside, a plant extract of astragalus, with adrenergic receptor alpha-2 as a regulation of sympathetic nervous system activity and identify the potential of Astragalus as a potential therapy to effectively regulate sympathetic nervous system function.

Materials and methods

First, astragalus extracts containing astragaloside were collected. Extraction is carried out using a specific extraction method, such as solvent extraction method or maceration extraction method. afterwards, physicochemical analysis was conducted to identify the active components in the astragalus extract.

After the collection of astragalus extracts, molecular analysis was performed using Pymol and Pyrex software. Pymol is a software

used for visualization and analysis of molecular structures in biochemistry. In this study, Pymol was used to visualize the molecular structures of astragaloside and adrenergic receptor alpha-2. Application URL used https://pymol.org/.

Pyrex is software used for molecular analysis and docking. In this study, pyrex was used to analyze the interaction between astragaloside and adrenergic receptor alpha-2, including the observation of hydrogen bonding, electrostatic interaction, and hydrophobic interaction between the two. This software is used to visualize the molecular structure of astragaloside and adrenergic receptor alpha-2. In this analysis, the interactions between astragaloside and adrenergic receptor alpha-2 will be explored, including observations of hydrogen bonding, electrostatic interactions, and hydrophobic interactions between the two [19-21].

to understand more about the interaction of astragaloside with adrenergic receptor alpha-2, protein characterization was performed using Protein Plus software. Protein Plus is software used for protein characterization and structural analysis. Protein characterization involved secondary structure analysis, tertiary structure, and identification of key residues involved in the interaction with astragaloside [22-26].

In addition, Lipinski Rule analysis was performed to evaluate the physicochemical properties of astragaloside, such as mass, hydrogen bond donor, hydrogen bond acceptor, logP, and molar reactivity [27-29]. In this study, Protein Plus was used to characterize the protein structure of adrenergic receptor alpha-2 and identify key residues that interact with astragaloside.

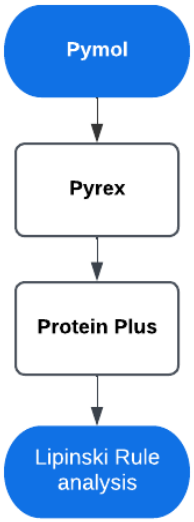


FIGURE 1 Flowchat of the reasearch

Results and discussion

This study makes an important contribution to the understanding of molecular interactions between astragaloside and adrenergic receptor alpha-2 in the regulation of sympathetic nervous system activity. The results of using Pymol and Pyrex software in molecular analysis showed significant interactions between astragaloside and adrenergic receptor alpha-2, including observations of hydrogen bonding, electrostatic interactions, and hydrophobic interactions. This information provides a deeper understanding of the mechanism of

regulation of sympathetic nervous system activity involving astragaloside.

Furthermore, protein characterization analysis using protein plus software revealed the secondary structure and tertiary structure of adrenergic receptor alpha-2. The identification of key residues that interact with astragaloside provides insight into the specific interactions between the molecules. This provides a strong foundation for understanding the regulatory mechanisms involved in these interactions and provides potential for the development of therapeutics based on Astragalus extracts [30-32]. Table 1 shows the binding affinity and RMSD results of astragaloside and ADRA2C.

TABLE 1 Binding affinity and RMSD results of astragaloside and ADRA2C

Ligand	Binding Affinity (Kcal/mol)	rmsd/ub (Å)	rmsd/lb (Å)
ADRA2C_Astragaloside	-6.4	0.0	0.0
ADRA2C_Astragaloside	-6.4	7.615	4.612
ADRA2C_Astragaloside	-6.4	5.204	2.515
ADRA2C_Astragaloside	-6.3	8.791	2.762
ADRA2C_Astragaloside	-6.2	13.229	9.982
ADRA2C_Astragaloside	-6.2	7.308	3.243
ADRA2C_Astragaloside	-6.1	8.971	3.165
ADRA2C_Astragaloside	-6.0	5.698	3.52
ADRA2C_Astragaloside	-6.0	8.665	2.703

In addition, Lipinski rule analysis provides important information on the physicochemical properties of astragaloside. characteristics such as mass, hydrogen bond donor, hydrogen bond acceptor, logP, and molar reactivity provide further understanding of the pharmacokinetic properties and stability of astragaloside. this information can be an important foundation in the development of astragalus-based drugs that can be used in regulating sympathetic nervous system function effectively and safely [33-35]. Table 2 presents the data from Lipinski and Figure 1 displays the interaction results of astragaloside and ADRA2C.

TABLE 2 Lipinski data

Mass	Hydrogen bond donor	Hydrogen bond acceptor	LOGP	Molar reactivity
618.000000	10	17	-0.019749	127.710968

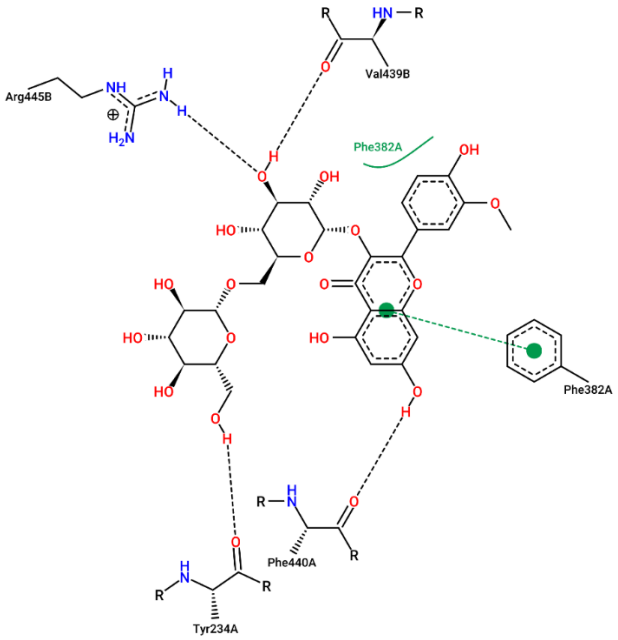


FIGURE 2 Result of the interaction between Astragaloside and ADRA2COverall, the analysis in this study provides significant insight into the molecular interaction of astragaloside with adrenergic receptor alpha-2 (ADRA2) and its potential as a regulator of sympathetic nervous system activity. These findings may form the basis for the development of novel therapeutics based on astragalus extracts and may provide a promising alternative in the effective treatment of sympathetic nervous system disorders [36,37].

The interaction between astragaloside, an astragalus plant extract, and adrenergic receptor alpha-2 in the regulation of sympathetic nervous system activity shows important potential in the development of therapies based on plant extracts. In this study, the utilization of molecular analysis software such as Pymol and Pyrex unveiled notable interactions between Astragaloside and the adrenergic receptor alpha-2 (ADRA2), encompassing hydrogen bonding, electrostatic, and hydrophobic interactions, as depicted in Figure 2. This suggests that astragaloside has a high affinity for adrenergic receptor alpha-2 (ADRA2), which could have potential in regulating sympathetic nervous system activity [38-40].

Protein characterization using Protein Plus software identified the secondary and tertiary structures of Adrenergic receptor alpha-2 as well as key residues that interact with astragaloside. This information provides further understanding of the molecular interaction mechanisms involved in the regulation of sympathetic nervous system activity. This provides a strong foundation for the therapies development that use Astragaloside as a selective regulator of sympathetic nervous system activity [41-43].

In addition, lipinski rule analysis provides an understanding of the physicochemical properties of astragaloside. Characteristics such as mass, hydrogen bond donor, hydrogen bond acceptor, logP, and molar reactivity provide important information on the stability and pharmacokinetic properties of Astragaloside. These findings strengthen the potential use of astragalus as a source of active ingredients in the development of drugs that can effectively regulate sympathetic nervous system activity [44-46].

Interpretation of this research reveals that astragaloside, an extract of the Astragalus plant, has the potential to regulate sympathetic nervous system activity through interaction with adrenergic receptor alpha-2

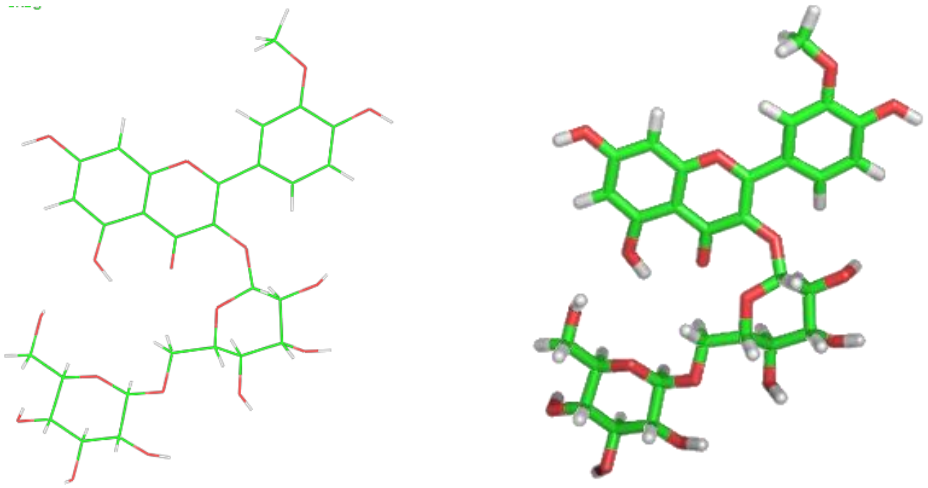
(ADRA2). The results of this study provide new insights into the molecular mechanisms involved and the physicochemical characteristics of astragaloside. These findings contribute to the development of therapies based on Astragalus extract in the treatment of sympathetic nervous system disorders [2-4,38].

In the perspective of previous scientific research, this study makes a significant contribution in expanding the understanding of the molecular interaction of astragaloside with adrenergic receptor alpha-2 (ADRA2). Several previous studies have investigated the effects of astragalus on the sympathetic nervous system, but this research focuses on understanding the molecular interactions involved in the regulation of sympathetic nervous system activity. Using a comprehensive molecular analysis and protein characterization approach, this study provides a deeper understanding of the mechanism and potential of Astragalus as a regulator in the sympathetic nervous system [3-5,48].

From a pharmacological perspective, this study provides an understanding of the physicochemical properties of Astragaloside and the molecular interaction characteristics with Adrenergic receptor alpha-2 [3, 4]. The lipinski rule analysis in this study provides important information on the pharmacokinetic properties of astragaloside, such as mass, hydrogen bond donor, hydrogen bond acceptor, logP, and molar reactivity. This can provide an important guidance in the development of astragalus-based drugs that can be effectively used in regulating sympathetic nervous system activity. From a pharmacology perspective, this research paves the way for the development of potential new therapies in the treatment of sympathetic nervous system disorders [33,48-50].

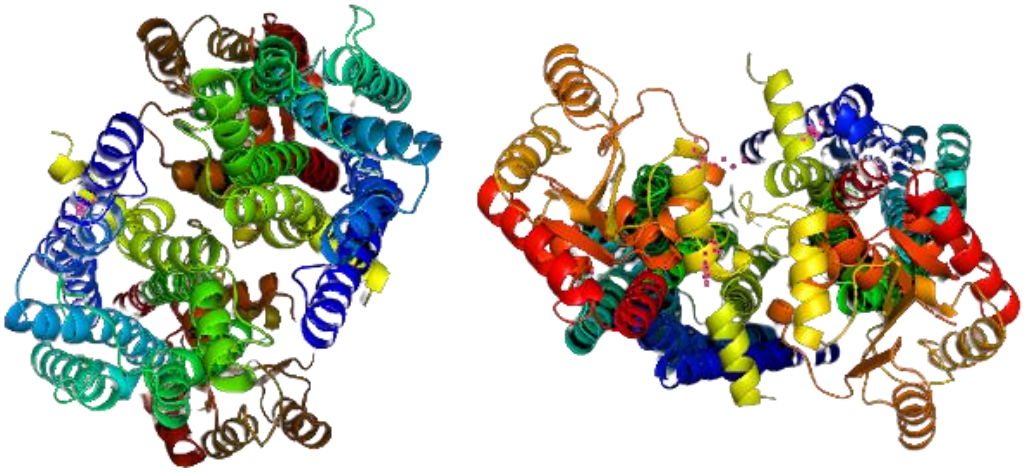
In terms of natural therapy development, this research contributes new knowledge about the potential use of astragalus as a regulator of sympathetic nervous system activity. As a plant that has long been used in traditional medicine, astragalus offers a promising natural alternative in the development of pharmaceuticals derived from plant sources. With further understanding of the molecular interaction of astragaloside with adrenergic receptor alpha-2 (ADRA2), this study may encourage the development of safer, effective, and sustainable therapies to regulate sympathetic nervous system function. Thus, this study provides an important perspective in the development of natural therapies that can provide significant health benefits [51-53].

This research provides important comparisons from various perspectives, including previous scientific research, pharmacological reviews, and the development of natural therapies. Through molecular analysis and protein characterization, this study provides a deeper understanding of the molecular interaction of astragaloside with adrenergic receptor alpha-2 (adra2). Thus, this study has the potential to encourage the development of therapies based on astragalus extracts in regulating sympathetic nervous system activity [54-55]. Figures 3 and 4 show astragaloside ligand and adrenergic receptor alpha-2 clean protein.



(a) (b)

FIGURE 3 (a) 2D Visualization of astragaloside ligand and (b) 3D Visualization of astragaloside ligand



(a) (b)

FIGURE 4 (a) Adrenergic receptor alpha-2 net protein and (b) Adrenergic receptor alpha-2 net protein P

Conclusion

This study concludes that astragaloside, an astragalus plant extract, has a significant interaction with adrenergic receptor alpha-2 (adra2), which has the potential to regulate sympathetic nervous system activity. Through molecular analysis and protein characterization, this study provides a deeper understanding of the molecular interaction mechanism of astragaloside with adrenergic receptor alpha-2 (adra2). The results of the lipinski rule analysis also provide important information about the physicochemical properties of astragaloside. With this understanding, this study makes an important contribution to the development of astragalus-based therapies that can be used to effectively regulate sympathetic nervous system activity. These findings provide an important foundation for the development of new, more natural, and sustainable therapies in the treatment of sympathetic nervous system disorders.

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Conflict of Interest

The authors declare that there is no conflict of interest.

Orcid:

Rahadian Zainul:
https://orcid.org/0000-0002-3740-3597
Dony Novaliendry:
https://orcid.org/0000-0003-2653-0467
Agariadne Dwinggo Samala:
https://orcid.org/0000-0002-4425-0605
Cheng-Hong Yang:
https://orcid.org/0000-0002-2741-0072
Mirella Fonda Maahury:
https://orcid.org/0000-0002-5119-4648
Rollando:
https://orcid.org/0000-0001-6210-6247
Rismi Verawati:
https://orcid.org/0009-0006-2143-0300
Muhammad Arya Ghifari:
https://orcid.org/0009-0009-3410-7694
Muhammad Thoriq Albari:
https://orcid.org/0009-0009-4074-2432
Muhammmad Raffi Ghifari:
https://orcid.org/0009-0006-4659-6091
Putri Azhari:
https://orcid.org/0009-0000-2966-9750
Riso Sari Mandeli:
https://orcid.org/0009-0004-4170-9582

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