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2, 4-Diaminobenzoic acid and its derivatives: Synthetic strategies, biological activities, and medicinal applications

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Keywords

2,4-Diaminobenzoic acid; anthranilic acid derivatives; synthetic strategies; medicinal chemistry; biological activities; structure–activity relationships; heterocyclic compounds; drug discovery; therapeutic potential.

Abstract

2,4-Diaminobenzoic acid (2,4-DABA) is an important multifunctional aromatic building block that has attracted increasing interest in synthetic and medicinal chemistry because of its two amino groups and carboxylic acid functionality, which provide versatile sites for structural modification and molecular diversification. The unique electronic and hydrogen-bonding characteristics of the 2,4-diaminobenzoic acid scaffold facilitate the synthesis of a wide range of substituted derivatives, heterocyclic systems, Schiff bases, amides, esters, and other structurally diverse molecules with potential pharmaceutical applications. This review provides a comprehensive overview of the synthetic strategies employed for the preparation and functionalization of 2,4-diaminobenzoic acid and its derivatives, with particular emphasis on approaches relevant to medicinal chemistry. The biological potential of reported derivatives is discussed with respect to their antimicrobial, anticancer, anti-inflammatory, antioxidant, analgesic, and other pharmacological activities, highlighting the influence of structural modifications on biological response. Where appropriate, structure–activity relationships and proposed mechanisms of action are examined to establish connections between molecular architecture and pharmacological properties. The review also discusses the versatility of 2,4-diaminobenzoic acid as a valuable intermediate for the synthesis of biologically relevant compounds and advanced chemical scaffolds. Finally, current challenges, unexplored structural possibilities, and future research opportunities are identified, with emphasis on the development of cost-effective synthetic methodologies and biologically active derivatives. This review aims to provide a focused perspective on the synthetic and medicinal significance of 2,4-diaminobenzoic acid and to support further exploration of this scaffold in drug discovery and pharmaceutical research.

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1. Introduction

Anthranilic acid derivatives are an important family of aromatic carboxylic acids containing amino and carboxylic acid functional groups attached to a benzene ring. 2,4-Diaminobenzoic acid (2,4-DABA) is a multifunctional derivative of the basic anthranilic acid, containing 2 amino groups and a carboxylic acid group. The functional groups found in 2,4-Diaminobenzoic acid offer flexibility for derivatization while the aromatic scaffold makes it attractive for organic synthesis as well as the preparation of structurally diverse derivatives. 2,4-Diaminobenzoic acid (figure 1) has been explored for natural product chemistry, analytical characterisation and biosynthetic studies. The compound has been identified as a natural product, as well as compounds based on its diaminobenzoic acid framework (see below). The natural presence of this amino acid underlines the chemical relevance of this scaffold. It was identified from the aerial parts of Daucus carota L. var. Boissieri, where the compound was identified by spectroscopic methods and found as part of the carotamine, a relatively unusual aromatic amide. The compound was also reported as a secondary metabolite of a microbial study of *Streptomyces flocculus*.

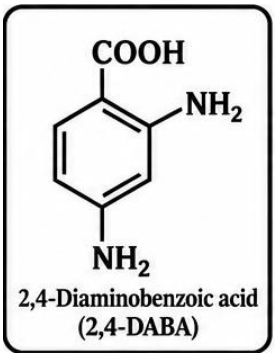


Figure 1: Chemical structure of 2-4 diaminobenzoic acid

The functional groups present on 2,4-diaminobenzoic acid mean its chemical properties can be modified. The proximity of the amino groups to the carboxylic acid in the 2,4-position lead to possible intramolecular hydrogen bonding, evidenced by spectroscopy that indicated the presence of a downfield, internal hydrogen-bonded proton resonance at approximately δ 12.7 ppm in DMSO-d_6. Therefore, the structural versatility and natural occurrence of this amino acid make it an interesting molecule for derivatization and synthesis and continued investigations of natural and synthetic 2,4-DABA derivatives are of interest to the fields of synthetic and medicinal chemistry.

2. Importance of 2, 4-diaminobenzoic acid

The role of 2,4-diaminobenzoic acid lies mainly in its multifunctional aromatic character and its incorporation into different chemical structures. The amino groups and carboxylic acid group can be used to give a complement of reactive functions and provide directional and selective synthesis through protection, reduction, acylation and derivatives. The natural occurrence of 2,4-DABA provides, on one hand, an interesting motivation for the synthesis of this family of

compounds. Its isolation from Daucus carota and its previous detection in Streptomyces flocculus show that this compound is not exclusive to the synthesis in vitro but can also be found in other natural sources. From the synthetic point of view, the compound can be synthesised through the transformation of suitable nitroanthranilic acids. In particular, the reduction of 4-nitroanthranilic acid would be a direct route to the 2,4-diamino pattern in the benzene ring (Valadbeigi et al. 2023; Kuwabara 2026). On the other hand, in addition to transformation, the possibility of protecting of the amino groups by means of derivatives to control their reactivity would be included into the synthesis of 2,4-DABA. Examples include derivatives of diaminobenzene rings (Mori et al. 1986). The concept of protected amino groups in the chemistry of diaminobenzoic acid was brought further by the chemistry of related positional isomers such as 3,4-diaminobenzoic acid, which has been used in peptide-related chemistry and in the synthesis of heterocyclic compounds (Chien et al. 2023; Kaplan et al. 2024) and 2,3-DABA, which has been found to crystallise as a derivative in a uranyl complex (Basha et al. 2022). However, these examples should be used as evidence for the scaffold rather than evidence for 2,4-DABA, as positional isomers may show different chemical behaviour, and even different bioactivity. In this context, a review of the literature on the thermal behaviour of diaminobenzoic acids shows that they may decarboxylate at high-temperature aqueous conditions producing phenylenediamines (Amaya-García et al. 2022), an important consideration that can be avoided by protecting the carboxyl group. In the presence of protected carboxyl group, known applications of diaminobenzoic acids are providing a range of molecular structures with different properties, even where amino groups are protected, which can be further used for the design of new molecular architectures with different ranges of biological activities.

3. Synthetic methods for 2,4-diaminobenzoic acid

Methods of preparing 2,4-diaminobenzoic acid and other diaminobenzoic acid derivatives (some by enzymatic or biosynthetic methods for homologous compounds) include chemical reduction, manipulation of functional groups, and enzymatic or biosynthetic methods for related compounds. Of the references reported in the available literature, 4-nitroanthranilic acid was identified as a key precursor for chemical synthesis of the 2,4-diamino substitution pattern (Figure 2).

3.1 Reduction of 4-nitroanthranilic acid

A straight forward, 2,4-diamino substitution pattern, involves a reduction of the nitro group of 4-nitroanthranilic acid. As per the literature reported in the Consensus report, reduction of the nitro group with sodium borohydride, in the presence of palladium (Pd/C), results in the formation of a 2, 4-diaminobenzoic acid and the required 2,4-diaminobenzoic acid 4 framework (Mori et al. 1986). The chemistry again also shows the need to control the reactivity of the amino groups, with reduction then optionally being followed by acetylation to afford protected derivatives, while different protection sequences afforded selectively protected amino derivatives. The addition of copper (Cu, II) acetate gave a route to selectively monoprotected derivatives via metal coordination.

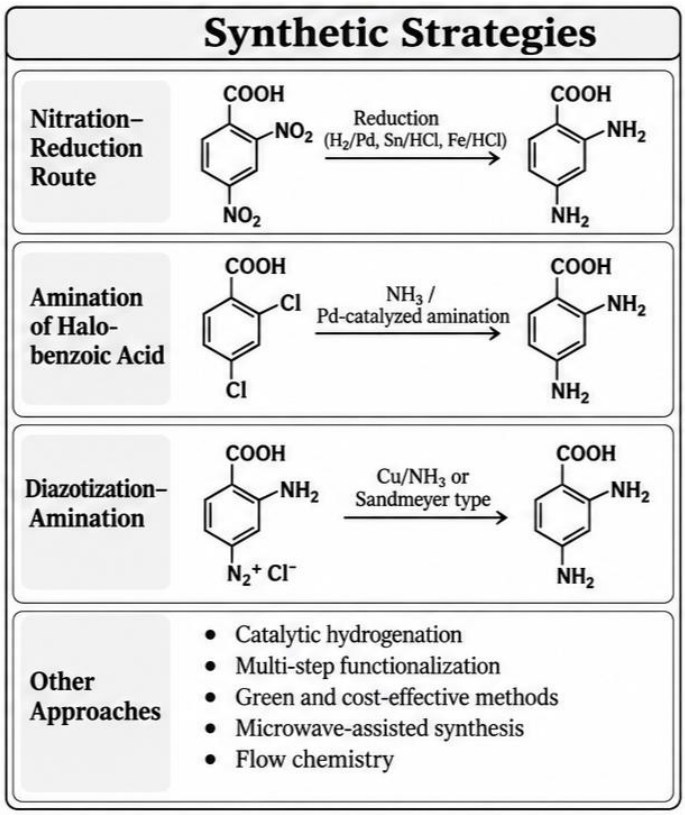


Figure 2: Different synthetic methods for 2,4-diaminobenzoic acid

This protection/deprotection chemistry can be of special interest to the synthesis of substituted 2,4-diaminobenzoic acid derivatives, where selective protection allows for different functionalization of the different amino groups.

3.2 Functionalization and derivatization

The molecule contains two amino groups and a carboxylic acid group, so they can be the substrates of functional-group transformations. The reports summarized in the papers, acetylation and protection methods are advanced strategies in control the chemical behavior of these multifunctional compounds. Other related diaminobenzoic acids have also been employed in the synthesis of more extended molecular architectures. 3,4-Diaminobenzoic acid has been used in peptide-related constructs and other derivatives in heterocyclic synthesis (Chien et al. 2023; Kaplan et al. 2024), illustrating the extensive synthetic utility of the diaminobenzoic acid framework, although these examples are not directly relevant to 2,4-DABA.

3.3 Enzymatic and biosynthetic strategies

This can lead to some recent efforts to expand the scope of enzymatic routes to substituted 2,4 diaminobenzoic acid derivatives. A 2026 publication disclosed an atypical nitrite-dependent aromatic amination to 2,4 diaminobenzoic acid product, 2,4-diamino-3-hydroxybenzoic acid, a close structural analogue. This is achieved by a combination of 3 enzymes, 2,4-diamino-3-hydroxybenzoic acid which were involved sequentially in diazotization, reduction, and aromatic amination reactions (Kuwabara et al. 2026).

While this compound is 2,4-diamino-3-hydroxybenzoic acid, and not 2,4-DABA, it may still be relevant to a forward-looking discussion because it shows that enzymatic aromatic amination can produce the following highly functionalized members of the 2,4-diamino-benzoic acid family.

4. Chemical characteristics relevant to derivative development

The geometric relationship between these groups results in well-defined spectroscopic and chemical behaviour. The proximity of the amino group and carboxylic acid groups enable the possibility for intramolecular hydrogen bonding, which has been linked to the downfield proton resonance at ~δ 12.7 ppm (DMSO-d_6).

-2- The degree of corrosiveness of diaminobenzoic acids is also strongly affected by temperature. A higher temperature aqueous treatment of some of the related diaminobenzoic acids can trigger decarboxylation to phenylenediamines and subsequent condensations resulting in heterocyclic products (Amaya-García et al. 2022). The report states that certain carboxylic acids being masked as esters, can prevent this type of degradation.

This information is important to consider when planning the synthesis of 2,4-DABA derivatives as the types of protection on groups, temperature of the reaction, and the reaction solutes can have an effect on product stability and selectivity.

5. Biological activities of 2,4-diaminobenzoic acid and its derivatives (Figure 3):

The biological activity of 2, 4-diaminobenzoic acid and its derivatives has been little studied and to date has remained relatively unexplored. The published literature can be generally summarized as regard to diaminobenzoic acid systems as being concerned with their physico-chemical and protonation properties, hydrogen bonding, and synthetic utility rather than any systematic approach to pharmacological evaluation. Published literature does not presently contribute an established biological activity for defined 2,4-DABA derivatives in disease models, enzyme assays, or animal experiments. However, biological information is available for far related diamino heterocycles and substituted benzoic acid derivatives.

5.1 Antimicrobial activity

Some diamino heterocyclic compounds with similar structures showed antimicrobial activity. The antimicrobials using were found for some members of this class of compounds under the study of proton-transfer complexes of 2, 4-diaminopyrimidine which showed its activity in opposites a several bacteria and fungi, as well as, was studied by an experiment for binding to DNA and molecular knock down and indication that was used as interaction with biological macromolecules (Basha et al. 2022).

These may be differentiated from information relating specifically to 2,4-DABA in that 2,4-Diaminopyrimidine is a heterocyclic compound and not a diaminobenzoic acid derivative and its activity is, therefore, likely to be supportive in terms of the wider biological activities of diamino containing scaffolds and not necessarily direct evidence for the activities of 2,4-DABA derivatives

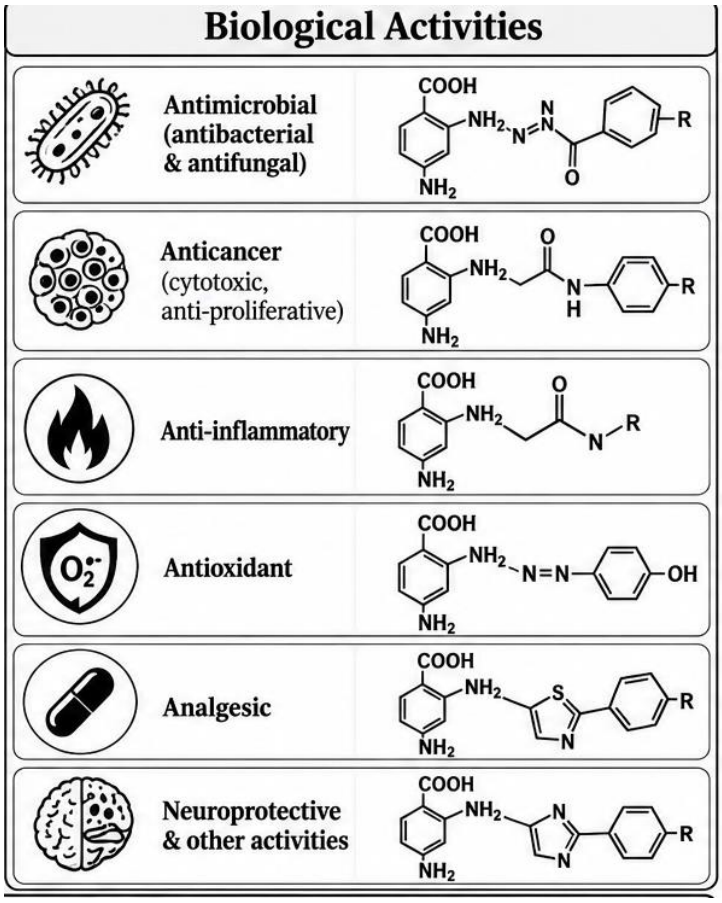


Figure 3: Biological activities of 2-4-diaminobezoic acid

Antimicrobial activity was similarly shown for other substituted benzoic acids alongside antioxidant and cytotoxic activity, providing evidence that substitution on this aromatic carboxylic acid scaffold can alter biological activity (Kalinowska et al. 2021). However, these structurally distinct compounds have somewhat different structures to 2,4-DABA and are therefore not indicative of the antimicrobial activity of this specific molecule. Overall, the evidence so far indicates that structured antimicrobial assessment of 2,4-DABA derivatives is a promising avenue to explore (Kalinowska et al. 2021).

5.2 Cytotoxic and antitumor activity

Another avenue of research that could be of value in the design of 2,4-DABA based molecules is that of the antitumor activity of related diamino compounds. A proton-transfer complex of 3,4-diaminopyridine was studied with regard to its DNA-binding and cytotoxic activity. The intercalative binding to DNA was confirmed and the compound was found to have a binding constant of around 4.6 x 10 4 M 1 and its cytotoxic activity was tested on A-549 and MCF-7 cancer cell lines (Alghanmi et al. 2024).

While these results do indeed show that diamino-substituted aromatic systems can have biological relevance in terms of DNA binding and cytotoxicity, the compound in this study is a 3,4-diaminopyridine proton-transfer complex rather than a 2,4-DABA derivative. As such, the results should be viewed as providing

evidence from a related scaffold rather than confirming the anticancer activity of 2,4-DABA derivatives.

Likewise, derivatives of hydroxybenzoic acids have been examined for their antioxidant, antimicrobial and cytotoxic activities; for example, activity against breast cancer cell lines such as MDA-MB-231 and MCF-7(Kalinowska et al. 2021). Again, these studies show that specific substitutions on the aromatic acid scaffold give rise to various biological responses. These results cannot be directly applied to 2,4-DABA derivatives without further experimental information.

5.3 DNA-binding potential

DNA binding Another biologically important activity seen for related series of diamino compounds was the interaction with DNA. Proton-transfer complexes of 2,4-diaminopyrimidine have been studied using DNA-binding experiments and molecular docking (Basha et al. 2022). Compound 3,4-diaminopyridine also a proton-transfer complex showed intercalative DNA binding and was cytotoxic for A-549 and MCF-7 cells (Alghanmi et al. 2024).

The potential to form hydrogen bonds, electrostatic and aromatic interactions of diamino groups may be involved in their reported binding to nucleic acids. However, direct DNA binding studies for 2,4-DABA and its derivatives were not located from the paper set searched for this review. Consequently, DNA interaction remains a possible avenue of research, rather than an established biological property of the 2,4-DABA framework.

5.4 Effect of substitution pattern and protonation

The biological activity of amino-aromatic compounds can also be affected by the compound's substitution pattern and state of protonation. Research into the isomers of diaminobenzoic acid has shown that the location of amino groups can affect the preference for a protonation site and intramolecular hydrogen bonding (Valadbeigi et al. 2023). This structural variation could alter charge distribution, conformation and hydrogen-bonding properties.

These considerations may be especially relevant for 2,4-DABA because the amino group connected to the carboxylic acid group can form intramolecular hydrogen bonds. Hydration and solvent effects may also influence the protonation state of amino-aromatic compounds (Kumar et al. 2020; Rana et al. 2025; Rana et al. 2025) and can thus alter interactions between molecules in a biological setting.

Therefore, in the synthesis of 2,4-DABA derivative, it would be wise to consider not only the type of the replaceable group to be inserted but also their impact on the basicity, hydrogen bonding, ionization, polarity and conformation of the molecules.

5.5 Structure-activity considerations

While no conclusive SAR has been established for 2,4-DABA derivatives at this time, there are several factors found in the literature that may aid in the direction of future medicinal-chemistry efforts. For instance, the location of amino groups has been shown to alter protonation and intramolecular hydrogen-bonding (Valadbeigi et al 2023). Likewise, substitution patterns in analogs of other benzoic acids have been related to observations of antioxidant, antimicrobial, and cytotoxic activity (Kalinowska et al. 2021).

The above observations appear to be promising

indicating that systematic modification of the 2,4-DABA 2 scaffold may serve as a good candidate to investigate changes in biological activity. The amino groups may be modified, the acid may be converted into an amide or ester derivative or added as a heterocyclic scaffold.

However, these are currently prospective medicinal-chemistry approaches rather than current SARs, as there is still, as yet, only limited biological datasets for a systematic series of 2,4-DABA analogues.

5.6 Current research gap and future biological potential

From the literature surveyed up to now, there exists a clear deficiency of biological testing of 2,4-DABA derivatives. The literature does not offer a one-step, strong profile of biological activity of this particular scaffold. The most profound biological evidence observed in the current literature was from similar diamino heterocycles - 2,4-diaminopyrimidine and 3,4-diaminopyridine derivates (Basha et al. 2022; Alghanmi et al. 2024).

These potential artifacts do not necessarily imply a state of biological inertness, but rather just that 2,4-DABA and its derivatives are not yet well studied pharmacologically. The scaffold's multitargeting characteristic opens avenues for chemical manipulation and screening.

Hence future studies could include the synthesis of different structurally bio-relevant 2,4-DABA derivatives and their subsequent evaluation of biological, antioxidant, antimicrobial, cytotoxic, etc. activities. The study of the mechanism of action by molecular docking, enzyme inhibitions, DNA-binding studies, SAR, etc. may provide insight into the biological aspects of the scaffolds.

In summary, the currently existing body of evidence seems to reinforce that 2,4-DABA is a hitherto unexploited lead with scope for drug discovery and that further experimental direct biological testing would be required before any particular therapeutic justification can be made.

6. 2, 4-Diaminobenzoic acid derivatives: structure-activity relationship

Potentailuse of the Structure activity relationship (SAR) analysis is an integral part of the medicinal chemistry process, as small differences in structure can have a large effect on the physicochemical and molecular recognition properties of a compound and as such, a compounds biological effect. SAR information is scarce for the class of compounds to be used here namely; 2,4 diaminobenzoic acid (2,4-DABA). The available literature can be used to make some assessment of the electronically related diamino acid and benzoic acid systems for their protonation, hydrogen bonding and biological activity can be used as a rough baseline for future interpretation of structures derivatives of 2,4-DABA (Valadbeigi et al. 2023; Valadbeigi et al. 2023; Kumar et al. 2020; Rana et al. 2025; Rana et al. 2025).

6.1 Effect of substitution pattern

Substituents on the aromatic ring are another critical factor influencing the physicochemical and biological properties of aromatic carboxylic acid derivatives. Examination of hydroxybenzoic acid derivatives suggests that even modifications in the number and positions of hydroxyl groups on the aromatic ring can give rise to significant differences in antioxidant activity

(Kalinowska et al. 2021). For example, in the one study directly comparing positional isomers with ortho and para related hydroxyls, activities differed while 2,5-dihydroxybenzoic acid was demonstrated to be more active than meta-oriented isomers such as 2,4- and 3,5-dihydroxybenzoic acids (Kalinowska et al. 2021).

Although it does not concern 2,4-DABA derivatives, this evidence is indicative of an overarching SAR concept: when tested around the benzoic acid structure, changing the location of the substituents can significantly alter the compound's biological properties. This is relevant in 2,4-DABA, because the amino groups are placed at specific locations in relation to the carboxylic acid and can affect both electron density and molecular interactions.

Research focusing on diaminobenzoic acid isomers clearly shows that amino substitution pattern influences preference for the protonation-site and intramolecular hydrogen bonds (Valadbeigi et al. 2023; Valadbeigi et al. 2023). Therefore, the changes in biological and physicochemical properties of the derivatives may be observed following positional modification of amino groups or doping with an extra substituent.

6.2 Role of amino-group position

On the aromatic ring, the positions of the two amino groups of 2,4-DABA are key features of the scaffold. These locations control the aromatic ring's overall electronic structure and affect the presence of hydrogen bonding and protonation of the molecules.

Researchers have used diaminobenzoic acid isomers that substituting the amino group to show how the basicity of the protonation site and the intramolecular hydrogen bonding can be influenced by the amino groups. The electronic influences from the amino substituents can have a marked influence on the electron density in the aromatic system (Valadbeigi et al. 2023).

The fact that the 2-amino group is ortho to the carboxylic acid is significant because the 2-amino group can intramolecularly hydrogen bond with the carboxyl group. This may have significant implications on conformation, the distribution of charge, and availability of functional groups. Therefore, selectively modifying or protecting one of the amino groups may be an advantageous approach in the manipulation of the physico-chemical properties of 2,4-DABA derivatives.

6.3 Effect of protonation state

Protonation state is another possible factor influencing the properties of 2,4-DABA derivatives. Amino-aromatic carboxylic acids can adopt multiple protonation states, and the relative stability of these is influenced by the structure of the molecules and their environments (Valadbeigi et al. 2023).

Similarly, analysis of aminobenzoic acid systems reveal that changes to a molecule's charge distribution in response to a different solvent or degrees of hydration can also alter the preference of the site of protonation (Kumar et al. 2020; Rana et al. 2025; Rana et al. 2025). *In vivo*these alterations could impact on a molecule's solubility, conformation, affinity for biological membranes, and interactions with other biological molecules.

Thus, with regard to 2,4-DABA derivatives, structural modifications that modulate the basicity of the amino groups or acidity of the carboxylic acid group are likely

to have an effect in biological setting. Protonation state must therefore be taken into account when trying to explain the differing biological activity of structurally related derivatives.

6.4 Hydrogen bonding within the molecule

Intramolecular hydrogen bonds could also play a role in the mode of activity of the 2,4-DABA derivatives. The location of the ortho-amino and carboxylic acid groups means it is possible to have intramolecular hydrogen-bonds. This could alter the conformation of the molecule.

Hydrogen bonding can stabilize some protonation states, and conformation of some amino-aromatic systems has been demonstrated (Buzásy et al. 2025; Hetmańczyk et al. 2024). These interactions can also alter the accessibility of functional groups to other molecules and thereby contribute to this recognition.

For 2, 4-DABA derivatives, alterations that enhance, reduce or remove intramolecular hydrogen bonding can induce conformational and physicochemical changes, which might be a useful consideration for future SARs.

6.5 Electronic effects of substituents

Electronic properties of the substituents should impact on the physicochemical properties of the 2,4-diaminobenzoic acids derivatives by manipulating the electron distribution across the aromatic ring and the acidic and amino functional groups. In the diaminobenzoic acid systems, the site preference of the amino groups to be protonated, the basicity and intramolecular hydrogen-bonding effects have been shown to depend on the position of the amino groups; that is, quite subtle structural variations can modify the electronic properties of the scaffold (Valadbeigi et al. 2023; Valadbeigi et al. 2023).

For 2, 4-diaminobenzoic acid derivatives, additional substituents may on the aromatic nucleus may impact factors such as protonation, hydrogen bonding, conformation and reactivity of the compound and thus alter bioavailability and interactions with biological targets. The current experimental data are insufficient to determine the effect that the addition of electron donating or withdrawing substituents may have on biological activity and so the influence of substituents on the electronic nature of 2,4-DABA derivatives as a SAR factor should be considered a hypothesis requiring further experimentation rather than an established SAR factor.

6.6 SAR insights from related diamino scaffolds

While no direct SAR of these 2,4-DABA derivatives is found in the current set of literature, certain structural observations can be made based on the following 2,4-diamino heterocycles. The complexes have been shown to form by interaction of protonated amino / nitrogen centersand acceptor groups. It has also exhibited antimicrobial activity. Similarly, 3,4-diaminopyridine was found to form a proton-transfer complex, exhibiting both DNA-intercalative activity (Alghanmi et al. 2024) and antitumor activity. These findings indicate that the number of donor/basic sites and their position can play a significant role in intermolecular recognition.

Nevertheless, these findings are scaffold-adjacent SAR evidence, and not SAR evidence directly related to 2,4-DABA. The nature of the chemical space of the pyrimidine, pyridine, and benzoic acid systems prevent such direct transfer of biological conclusions.

6.7 Potential sar parameters for future 2,4-DABA derivatives

Multiple structural and physicochemical parameters may be relevant in each 2,4-DABA derivative, such as amino-group position, substituents (additional substituents on the ring, and nature and position of all substituents), electronic effects, modification of the carboxylic acid and amino groups, free amino group(s), pKa/protonation, intramolecular hydrogen bonds, hydrogen-bond donor and acceptor count, lipophilicity and polarity, and three-dimensional molecular conformation. These factors may all together contribute to molecular recognition, physicochemical properties, and interactions with biological molecules (Valadbeigi et al. 2023; Valadbeigi et al. 2023).

Table: 1: Potential structural and physicochemical parameters relevant to SAR investigation of 2, 4-diaminobenzoic acid derivatives

Structural/physicochemical parameter	Potential influence on 2,4-DABA derivatives
Amino-group position	Protonation, electronic distribution, H-bonding
Ring substituent position	Molecular recognition and activity
Electronic effects	Basicity and charge distribution
Carboxylic acid modification	Lipophilicity, ionization, H-bonding
Amino-group modification	Selectivity and molecular interactions
Protonation state/pKa	Charge distribution and biological interactions
Intramolecular H-bonding	Conformation and functional-group accessibility
H-bond donor/acceptor properties	Target recognition
Lipophilicity/polarity	Solubility and membrane interaction
Molecular conformation	Binding orientation and molecular recognition

These factors could be explored in a systematic manner by synthesising a structurally varied series of 2,4-DABA derivatives and establishing correlation between their physico-chemical properties and the biological activity obtained experimentally.

Currently, however, these relationships should be considered tentative SAR hypotheses, as the available literature does not describe a clear biological series of 2,4-DABA derivatives from which concise SAR can be derived.

6.8 General SAR outlook

In general, the present data suggests that the substitution pattern, electronic factors, state of protonation, and intramolecular hydrogen-bonding may all be factors influencing the behaviour of 2,4-DABA derivatives. Shifts in the position of benzoic acid groups are known to influence biological activity, and as with diaminobenzoic acid isomers the position of amino groups influences protonation and hydrogen-bonding (Kalinowska et al. 2021; Valadbeigi et al. 2023).

However, SAR of 2,4-DABA derivatives has not yet been established. The most reasonable conclusion drawn

from the available data appears to be that these structural characteristics serve as guides for future medicinal-chemistry optimization, not as hard-and-fast rules.

Such an absence of systematic SAR data, however, might also be the opportunity for interesting research. With a systematic series of rationally designed 2,4-DABA derivatives, biophysical evaluation and computational studies may provide such a structure-physicochemical-target affinity-response relationships.

7. Medicinal applications and therapeutic potential

7.1 Current evidence and therapeutic capability

The pharmaceutical implications of 2,4-DABA derivatives are still in their infancy and there are, presently, no direct biological or medicinal evidence that this particular scaffold can be exploited. The existing literature is confined to physicochemical property profiling of the diaminobenzoic acid isomers, the synthetic use of its derivatives and the biological activity of apparently related diamino heterocyclic derivatives. Thus, at this point in time, the medicinal value of 2,4-DABA derivatives could be considered to be a developing research field, rather than a secure medicinal chemistry framework (Valadbeigi etg al. 2023; Chien et al. 2023).

Data from structurally similar compounds nonetheless offer useful guidance for subsequent work. Proton-transfer complexes of 2,4-diaminopyrimidine have shown activity against bacterial and fungal organisms as well as having been studied for their ability to bind DNA (Basha et al. 2022). Whilst these cannot be explicitly related to 2,4-DABA derivatives, they demonstrate the potential for aromatic diamino groups to be involved in biologically significant interactions involving hydrogen bonds and protonation-driven molecular recognition (Basha et al. 2022).

In the same vein, a proton-transfer complex of 3,4-diaminopyridine was also studied for DNA-intercalative interactions and antitumor activity on A-549 and MCF-7(Alghanmi et al. 2024). The DNA-binding constant and the calculated binding free energy indicate that diamino aro compounds are also able to interact with nucleic acids targets through specific molecular interactions (Alghanmi et al. 2024). Nonetheless, this indicates scaffold-adjacent evidence rather than direct evidence of the anticancer activity of 2, 4-DABA derivatives.

7.2 Medicinal chemistry aspects

The physicochemical properties of this 2,4-DABA scaffold suggest that there are various ways of applying medicinal chemistry optimization strategies. In particular, the substitution pattern of diaminobenzoic acid isomers modulates protonation-site preference, basicity and intramolecular hydrogen bonding (Valadbeigi et al. 2023). These properties are potentially key, given that variations in the ionization state may impact upon charge distribution, hydrogen-bonding pattern, solubility and molecular recognition.

Thus regio- and a-substitution patterns in future 2,4-DABA derivatives may be important parameters to consider in the design of our future compounds. Carboxylic acid positional isomers of hydroxybenzoic acids have demonstrated that modifications in ring substitution are able to modulate antioxidant, antimicrobial and cytotoxic activities (Kalinowska et al. 2021).

7.3 Potential therapeutic directions

Given the scaffold-adjacent evidence we have, we can suggest three possible areas to pursue future research on 2,4-DABA derivatives: anti-infective uses, anticancer/DNA targeting, and redox- or environmental-responsive molecular systems. These are based on biological findings on similar diamino heterocycles and aromatic amines, and not on the existing body of biological research on 2,4-DABA (Basha et al. 2022; Alghanmi et al. 2024; Buzasy et al. 2025).

In conclusion, 2,4-DABA is a flexible scaffold of structure and has drug-like properties, but there is limited direct evidence for therapeutic activity of derivatives. Therefore, targeted synthesis, biological screening and subsequent determination of physicochemical properties and molecular interactions of diverse derivatives, more specifically of derivatives with defined electronic, hydrogen-bonding and conformational properties, are needed to generate structure-activity relationships and to identify lead compounds (Valadbeigi et al. 2023).

8. Emerging trends and future perspectives

Recent advances in medicinal chemistry suggest that the present findings provide several new directions of application of diaminobenzoicacid-based scaffolds and derivatives, such as the fabrication of metal-coordination complexes, and the use of diaminobenzoic acid derivatives as antimicrobial substances and hetero cyclic derivatives as enzyme-inhibiting agents. Although these applications are mainly related to the associated diaminobenzoic acid isomers and scaffolds, this information may serve to guide future investigations concerning the exploration of 2,4-diaminobenzoic acid derivatives.

8.1 Metal containing derivatives and coordination chemistry

Another new method is to incorporate diaminobenzoicacid-based ligands into a metal coordination complex. Recent investigations of diamine-based Pt(IV) complexes have revealed their cytotoxic potential, as well as explored their physicochemical, ADME and molecular-docking properties (Majeed et al. 2025). In a series of compounds reported by the same research team, diamine-based metal complex showed activity against cancer cells, with some compounds showing an IC50 of 14.9 μg/mL against HeLa cells. Computational and mechanistic studies revealed interesting kinetically stable and good reduction behavior at physiological conditions (Majeed et al. 2025).

These data, however, do not necessarily constitute evidence of 2,4-DABA derivatives' antitumour activity, since the complexes reported here are based on 3,4-diaminobenzoic acid and related diamine scaffolds. Even so, they provide evidence for the possible use of diaminobenzoic acid derived functionalities as metals acting as ligands for metal-based therapeutic systems.

8.2 Antimicrobial uses

A further potential useful pathway is antimicrobial development. Several aromatic carboxylic acid derivatives and diaminobenzoic-acid-related structures have been reported to be active against Gram-positive and Gram-negative bacterial strains including Staphylococcus aureus, Escherichia coli and Klebsiella pneumoniae. For example, the diamine complexes of

Pt(IV) have been shown to produce inhibition zones of up to 23.6 mm for *S. aureus* and bisbenzimidazole derivatives based on diaminobenzoic acid precursors have exhibited antibacterial activity with a MIC of 0.195 mg mL-1(Majeed et al. 2025; Kaplan et al. 2024).

These data indicate that diaminobenzoic acid scaffolds may be modified with a variety of substituents, producing compounds with antimicrobial properties. However, for the time being, we can only conclude that significant SARs associated with antimicrobial activity have not yet been established for 2,4-DABA derivatives.

8.3 Heterocyclic derivatives and enzyme inhibition

Another novel application is the conversion of the diaminobenzoic acid scaffolds into heterocyclic molecules potentially active as enzyme inhibitors. The synthetic ability of diaminobenzoic acids as precursors to biologically active heterocycles including benzimidazoles was explored by Kaplan et al. (2024) who reported benzimidazole-derived coordination compounds having activity as cholinesterase inhibitors. Copper complexes reported by the same group showed experimental IC5o values of 0.51 mg/mL against both acetylcholinesterase and butyrylcholinesterase, and interaction with two targets of potential metabolic significance (including α-amylase) using in silico methods.

For 2,4-DABA, this indicates that a promising approach would be to employ the aromatic diamino acid as a final pharmacophore, along with a synthetic system to afford unique and interesting heterocyclic derivatives from a biologically active precursor that could greatly extend the derivatives that could be obtained from the parent scaffold.

8.4 Computationally guided derivative design

Computational methods are also gaining importance in the search of diaminobenzoic acid derived molecules. Docking studies and computational structure activity relationship studies have been conducted to explore these heterocyclic compounds with enzymes like α - amylase or acetylcholine esterase docking analysis has been compared with commonly used reference ligands (Kaplan et al. 2024).

However, for future 2,4-DABA research, to complement and enhance the synthesis and biological approaches, in silico methods can be employed to select derivatives for screening prior to in vitro testing. Specifically, computational methods such as molecular docking, molecular dynamics simulations, physicochemical property prediction and structure-activity relationship analysis can inform predicted substitution patterns and possible molecular targets.

8.5 The Research agenda going forward

Even with these developing paths, the medicinal chemistry of 2,4-DABA itself has been not enough investigated. Subsequent research should address the medicinal chemistry of 2,4-DABA towards systematically performed derivatizations of the molecules and in vitro biological screenings, target-oriented research, physicochemical testing and computational investigation. Specific consideration should be concentrated on the variation of amino-group, carboxylic acid derivates, substituents in ring, i.e., ring substitution, in addition to transformation of protatedacid and coordination with metals.

Thus, the literature to date appears to encourage the viewpoint that 2,4-DABA should be considered a novel

chemical 'scaffold', rather than an established pharmacophore. Further investigations, in silico, with combinatorial synthesis, biological evaluation and mechanistic studies, would provide more information on whether derivatives of 2,4-DABA are viable as anti-bacterial, anti-cancer, enzyme inhibitor or other biologically active molecules.

9. Obstacles and future outlooks

9.1 Difficulties in developing 2, 4-Diaminobenzoic Acid Derivatives

Most pharmacologically active diaminobenzoic acid derivatives present various synthetic, pharmacological, and translational hurdles. Significant shortcomings involve regioselective functionalization, purification issues, non-uniform conversion of biological activity to anticipated target-specific effects, pharmacological resistance, and pharmacokinetic limitations. These limitations limit the successful development of diaminobenzoic acid-derived compounds as therapeutic candidates (Chien et al. 2023; Huang et al. 2023; Brishty et al. 2021).

One synthetic challenge relates to the various types of reactivity exhibited by the amino groups of diaminobenzoic acid derivatives. The discrepancy in reactivity of amino groups can lead to partial or indiscriminate functionalization, side reactions and an early cyclisation in the course of coupling reactions. This issue of regioselectivity can introduce significant problems in the synthesis of well-defined derivatives and involve additional protection and deprotection (Chien et al. 2023).

Another important limitation is purification and isolation. Traditional synthetic routes include several chromatographies, which involve losses of solvent and time, since is necessary an additional effort for every purification step. In the report it is pointed out that low overall recovery in synthetic routes is an important practical limitation (Chien et al. 2023; Brishty et al. 2021).

Another issue is the lack of knowledge regarding the connection between observed biological activity and molecular target interaction. In vitro antiproliferative or other biological activity may not always directly relate to affinity for the target, complicating rational optimization and mechanistic understanding (Huang et al. 2023).

Another issue is that of therapeutic resistance, especially in the case of anti-microbial use. Microbial adaptation and target mutation could compromise the longevity of any anti-microbial compound, highlighting the importance of derivatives being able to remain active against resistant strains (Brishty et al. 2021; Ayyadurai et al. 2025; Sharma et al. 2026).

Of course, ADMET properties could also hinder further development. The report notes that some compounds, despite having promising activity, may not be advanced to clinical testing due to toxicity or low oral bioavailability (Brishty et al. 2021; Reyes-Vallejo et al. 2025).

9.2 Future outlook

The early development of 2,4-DABA derivatives should prioritize the enhancement of synthetic methods in terms of efficiency, selectivity and ecological compatibility. For example, one-pot reactions, microwave-assisted syntheses and more convenient isolation procedures would lead to a reduction in the

length of reaction times and time taken for isolation, whilst increasing the synthetic efficiency. Microwave assisted condensation and precipitation-based isolation are methods mentioned in this report that have led to improvements in the preparation of systems derived from related diaminobenzoic acids (Chien et al. 2023; Kaplan et al. 2024).

Direction two also involves rational structural modification and molecular hybridization. The exchange of fragments derived from diaminobenzoic acid molecules with other pharmacophore can lead to hybrid molecules with changed biological activity and provide insight into solutions to antimicrobial resistance or multi-target activity (Krátký et al. 2019; Huang et al. 2023; Ayyadurai et al. 2025).

Computer-aided drug design methods may also be used to accelerate the selection of interesting derivatives. In silico ADMET prediction and molecular docking could be used to rank compounds based on their predicted pharmacokinetic properties as well as interaction with selected target(s). In the report, there are examples of in silico studies of ALR2, PPAR-γ, and α-amylase as potential targets (Kaplan et al. 2024; Abdelmonsef et al. 2019; Reyes-Vallejo; Ayyadurai et al. 2025).

Metal coordination chemistry is also an option for future research. The design of heteronuclear coordination complexes and metal-chelating derivatives could be alternatives for modifying their biological activities and possibly overcoming tumor metabolism or drug resistance (Kaplan et al. 2024; Huang et al. 2023).

Addressing physicochemical and pharmacokinetic difficulties may also be possible by modifying the parent scaffold using prodrug techniques and/or hetero-fusion. These strategies have been recommended to enhance aqueous solubility, membrane permeability and systemic bioavailability (Brishty et al. 2021).

Overall, future development of diaminobenzoic acid-based molecules will be determined by successful addressing of regioselective synthesis problems, enhancement of synthesis efficiency, and combining molecular design with computational and biological considerations. Moving from exploratory chemistry to therapeutically valuable compounds is far from straightforward; it will necessitate systematic optimization of all three domains: structure, bioactivity, and pharmacokinetic properties. The report concludes that the key to successful development of diaminobenzoic acid derivatives towards therapeutic candidates lies in the solutions to regioselectivity problems, the incorporation of highly efficient one-pot synthesis strategies, and exploration of hybrid and prodrug approaches.

10. Conclusion

2, 4-Diaminobenzoic acid (2,4-DABA) is a privileged multi-decision, synthetically versatile aromatic scaffold that merits further investigation in the realms of synthetic and medicinal chemistry. The compound's two amino groups and carboxylic acid functionality are well suited to regioselective modification, leading to structural diversity and heterocyclic scaffolds. Additional elements of interest include the occurrence of 2,4-DABA as a natural product, the characteristic intramolecular hydrogen bonding, and inherent reactivity.

The synthetic review indicates that 2,4-DABA is readily prepared by reduction of suitably functionalised nitroanthranilic acid building blocks, and the protection

and subsequent manipulation of the remaining functional groups allows for further derivatisation of the molecule to be achieved. Functional groups also provide exciting opportunities for derivatisation, while related diaminobenzoic acid molecules illustrate the use of this class of scaffold in peptide, heterocycle and coordination chemistry.

Biological data, however, suggest that comparatively less work has been performed on 2,4-DABA and derivatives to date. Nonetheless, there is a relatively strong body of biological work on substituted diamino heterocycles and aromatic carboxylic acids bearing strong structural similarities with possible future directions involving the various substitution, charge state, electronic, hydrogen bonding, and conformation influences on biological interactions. This in turn provides an insight into the discrepancies and depth of our understanding that might be applied in future research directions.

Consequently, the SAR reported in this review product of the combination of all these factors, leading to an potentially tentative, rather than conclusive, picture of the structural factors that influence biological activity of 2,4-DABA derivatives. Thus, future investigations should determine the effects of amino-group position, ring substitution, electronic effects, carboxylic acid and amino-group modifications, protonation, intramolecular hydrogen bonding, lipophilicity, polarity and conformation on biological activity. Deriving experimentally validated correlations between these parameters and biological activity will be critical for optimal scaffold design.

In addition to the development of new derivatives, the above provides the scope for future directions in the field. Metal coordination, heterocyclic structures, molecular hybridisation, computer aided design of derivatives and the use of prodrugs all provide future avenues for the derivation of structures with enhanced biological activity and physicochemical properties. It should be noted that much of this evidence is derived from the approaches to other isomers of diaminobenzoic acids or related structures.

However, future progress will require solving major synthetic and translational hurdles such as regioselective functionalization, purification and isolation, minimal direct SAR data, target validation, resistance, and ADMET. Convergence of effective and more environmentally benign synthetic processes with computational drug design, systematic biological screening, mechanistic studies, and suitable pharmacokinetic assessment will likely pave a more rational road to promising derivatives.

In conclusion, 2,4-DABA should be viewed as a synthetically attractive and under-researched chemical scaffold with exciting potential for medicinal-chemistry research, rather than as an established therapeutic pharmacophore. The design, synthesis, and assay of more well-defined derivative libraries with appropriate biological and mechanistic studies will ultimately be decisive in establishing the true therapeutic potential of 2,4-DABA derivatives. Such studies may one day reveal whether rationally-designed 2, 4-DABA derivatives have useful roles to play in antibacterials, anticancer agents, enzyme-inhibitors, or other areas.

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