



molbank

IMPACT
FACTOR
0.3

CITESCORE
0.9

Communication

Crystal Structure of 1,1-Dimethyl-3-(quinolin-2-yl)urea and 3-(Isoquinolin-1-yl)-1,1-dimethylurea

Svetlana O. Baykova, Sergey V. Baykov, Vadim P. Boyarskiy and Nadezhda A. Bokach



<https://doi.org/10.3390/M2231>

Communication

Crystal Structure of 1,1-Dimethyl-3-(quinolin-2-yl)urea and 3-(Isoquinolin-1-yl)-1,1-dimethylurea

Svetlana O. Baykova ¹, Sergey V. Baykov ^{1,2} , Vadim P. Boyarskiy ¹  and Nadezhda A. Bokach ^{1,*} 

¹ Institute of Chemistry, Saint Petersburg State University, Universitetskaya Nab. 7/9, Saint Petersburg 199034, Russia

² Institute of Experimental Medicine, 12 Academician Pavlov Str., Saint Petersburg 197022, Russia

* Correspondence: n.bokach@spbu.ru

Abstract

The crystal structures of two isomeric urea derivatives—1,1-dimethyl-3-(quinolin-2-yl)urea (**1**) and 3-(isoquinolin-1-yl)-1,1-dimethylurea (**2**)—have been investigated by single-crystal X-ray diffraction. These compounds differ in the relative position of the heterocyclic nitrogen atom and the urea substituent. A structural study revealed that the compounds exhibit distinct molecular conformations. In **1**, the molecule exists predominantly in a ureide form with a single C–N bond between the quinoline fragment and urea moiety. The ureide group is out of the plane of the quinoline ring, forming an *anti*-conformation. In contrast, **2** adopts an exocyclic C=N configuration with an intramolecular hydrogen bond between the heterocyclic NH group and ureide oxygen, resulting in a *syn*-conformation. The supramolecular organization of the compounds also differs: **1** forms one-dimensional chains through N–H⋯O hydrogen bonds, which further assemble into two-dimensional layers via C–H⋯O interactions; in **2**, the molecules form dimers through intermolecular C–H⋯O hydrogen bonds. Thus, subtle structural differences between isomeric urea derivatives can lead to distinct molecular conformations, tautomeric forms, and supramolecular organizations.

Keywords: quinoline; isoquinoline; urea; tautomers; X-ray diffraction; supramolecular organization

1. Introduction

Quinoline and isoquinoline derivatives containing a urea (carbamide) moiety constitute a large class of heterocyclic compounds that are actively studied in both fundamental and applied chemistry. Quinoline and isoquinoline themselves are considered “privileged” heterocyclic scaffolds in medicinal chemistry, serving as the basis for numerous pharmaceutical agents [1–5]. Hetaryl ureas with varying positions of the ureide substituent within the heterocyclic fragment frequently exhibit antimicrobial [6–9], anticancer [10], and anti-inflammatory properties [11], along with other types of biological activities [12]. Pyridyl- and quinolinyl ureas are of interest for organic synthesis [13], as they can act as masked isocyanates [14] and be employed to construct pharmaceutically relevant polynuclear heterocyclic systems [15]. Ureas can display ligand properties; when combined with a heteroaromatic ring (quinoline/isoquinoline), such molecules can function as bidentate or polydentate ligands, forming stable metal complexes that are used in the development of catalysts, luminescent materials, and medicinal agents [16–19]. The ability of urea groups to form strong hydrogen bonds enables the design of supramolecular assemblies, gels,



Academic Editor: Kristof Van Hecke

Received: 23 August 2026

Revised: 10 September 2026

Accepted: 15 September 2026

Published: 16 September 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

and porous structures. The presence of the heteroaromatic fragment additionally provides the possibility of π -stacking interactions, thereby expanding the scope of supramolecular design [17].

Derivatives in which the urea moiety is located in close proximity to a heteroatom within the ring (Figure 1) are of particular interest as potential bi-/polydentate ligands and tectons for supramolecular assembly [20], as well as model systems for studying tautomeric equilibria and proton transfer—which is important for fundamental research into reaction mechanisms. In such compounds, the urea fragment is capable of tautomeric transformations and proton transfer, while the presence of a heteroatom in the ring (the N atom in quinoline/isoquinoline) can influence the acid–base properties and the dynamics of these processes.

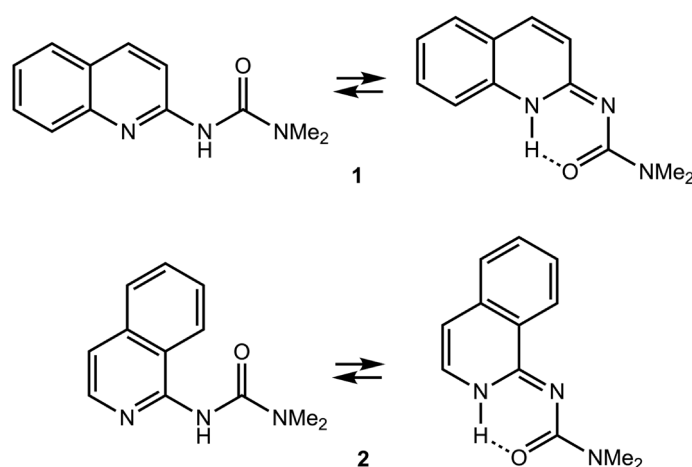


Figure 1. The tautomeric forms of isomeric compounds **1** and **2**.

In this work, the structures of two isomeric compounds—1,1-dimethyl-3-(quinolin-2-yl)urea (**1**) and 3-(isoquinolin-1-yl)-1,1-dimethylurea (**2**)—were studied by single-crystal X-ray diffraction (XRD). These compounds differ in the relative positioning of the heterocyclic nitrogen atom and the urea substituent. The interest in these compounds stems from the fact that, despite their similar overall structures, they exhibit different chemical properties and reactivity [21]. This study revealed that, in the crystalline phase, these substituted ureas exist as different tautomeric forms. The structural features of the compounds are discussed in the following sections.

2. Results

2.1. XRD Analysis and the Structures of Compounds **1** and **2**

Suitable crystals of compounds **1** and **2** were grown from 1,2-dichloroethane at room temperature and studied by XRD.

Compound **1** crystallizes in the *Pbca* space group within the orthorhombic crystal system. The crystal contains one molecule of **1** as the crystallographically independent unit (Figure 2). The labile hydrogen atom in the structure is localized on the nitrogen atom of the amide group. Selected bond lengths and bond angles are listed in Table 1. Analysis of the bond lengths in the heterocyclic fragment reveals a similarity to the parameters of an analogous fragment in structurally related compounds, such as 1-(1*H*-indol-7-yl)-3-quinolin-2-yl urea (CCDC code CIGSES) [22] or 1-quinolin-2-yl-3-quinolin-8-yl urea (CIDGIH) [22]. The bond lengths in the peripheral ureide fragment (Table 1) indicate its existence in carbamide form, with a relatively short C–O bond (1.2371(15) Å) and elongated C–N bonds (1.3868(15) and 1.3539(15) Å), which is typical for substituted ureas—for example, in CLPHUR01 [23] or in ureas with a quinoline substituent (CIGSES [22] and

CIDGIIH [22]). The C1–N2 bond (1.3986(15) Å) between the quinoline fragment and the urea moiety is essentially single in character (ca. 1.40 Å, compared to 1.34–1.42 Å [24] for a single bond). The carbamide group is out of the plane of the quinoline fragment (the torsion angle N1–C1–N2–C10 is 147.91(11)°; the twist angle between the planes of the quinoline fragment C₉N and the ureide N₂CO is 134.41(4)°), indicating negligible or no conjugation between these two fragments. The quinoline fragment (C1N1) and the urea substituent are located on opposite sides of the C1–N2 bond, forming an *anti*-conformation.

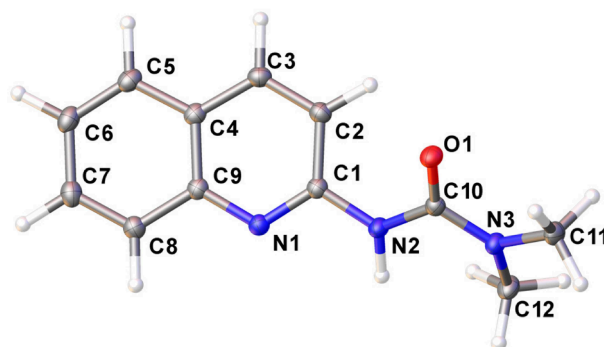


Figure 2. The molecular structure of compound 1 is shown with thermal ellipsoids drawn at the 50% probability level.

Table 1. Selected bond lengths and bond angles in compounds 1 and 2.

Atoms	Distance, Å	Atoms	Angle, °
1			
O1–C10	1.2371(15)	N1–C1–N2	115.21(10)
N1–C1	1.3171(16)	C1–N2–C10	124.08(10)
N1–C9	1.3699(15)	O1–C10–N2	122.71(11)
N2–C1	1.3986(15)	O1–C10–N3	122.59(11)
N2–C10	1.3868(15)	N3–C10–N2	114.70(10)
N3–C10	1.3539(15)	C10–N3–C11	119.32(10)
N3–C11	1.4549(15)	C10–N3–C12	123.79(10)
N3–C12	1.4595(16)	C11–N3–C12	116.35(10)
2			
O1–C1	1.2547(15)	N1–C1–N2	124.66(11)
N1–C1	1.3628(16)	C1–N2–C10	119.32(10)
N1–C2	1.3766(17)	O1–C10–N2	126.26(11)
N2–C1	1.3215(16)	O1–C10–N3	120.10(11)
N2–C10	1.3813(16)	N3–C10–N2	113.63(11)
N3–C10	1.3556(17)	C10–N3–C11	119.94(11)
N3–C11	1.4540(16)	C10–N3–C12	123.21(11)
N3–C12	1.4557(17)	C11–N3–C12	116.72(11)
O1A–C1A	1.2584(15)	N1A–C1A–N2A	124.42(11)
N1A–C1A	1.3593(15)	C1A–N2A–C10A	119.58(10)
N1A–C2A	1.3748(16)	O1A–C10A–N2A	126.41(11)
N2A–C1A	1.3257(16)	O1A–C10A–N3A	119.76(11)
N2A–C10A	1.3808(15)	N3A–C10A–N2A	113.82(10)
N3A–C10A	1.3607(16)	C10A–N3A–C11A	120.97(10)
N3A–C11A	1.4530(15)	C10A–N3A–C12A	124.10(10)
N3A–C12A	1.4525(15)	C11A–N3A–C12A	114.87(10)

Compound **2** crystallizes in the $P2_1/c$ space group within the monoclinic crystal system. The structure comprises two types of crystallographically independent molecules of **2** (Figure 3). In both molecule types, the labile hydrogen atom is localized on the isoquinoline nitrogen atom, which exhibits an amide-like character. Bond lengths and bond angles for both molecule types are presented in Table 1; the corresponding parameters for the two molecules differ only slightly (within 3σ). For the heterocyclic fragment in **2**, an alternating pattern of bond lengths is observed, characteristic of structurally similar substituted N-protonated isoquinolines—for example, in ethoxy(isoquinolinium-1-ylimino)methanethiolate (JEKTID) [25].

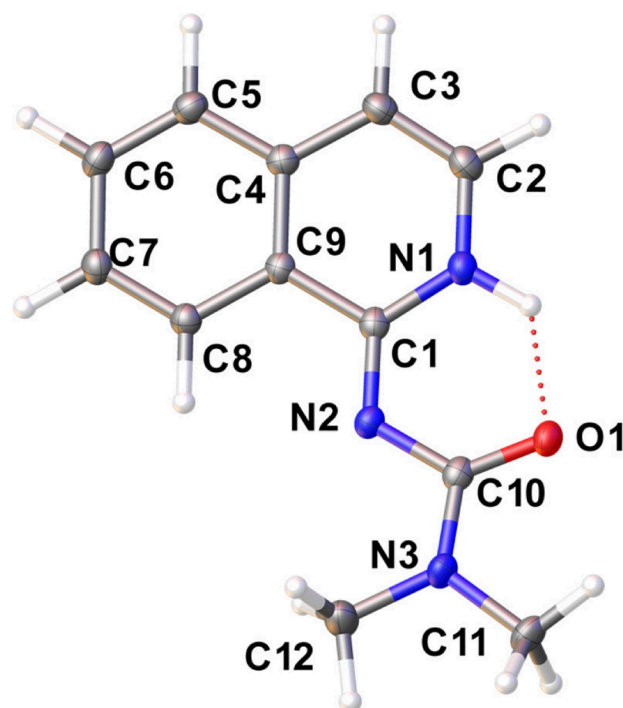


Figure 3. Molecular structure of compound **2**; one of the two crystallographically independent molecules is depicted, with thermal ellipsoids shown at the 50% probability level. The intramolecular hydrogen bond is indicated by a dotted line.

The bond lengths in the ureide fragment of **2** differ from those in compound **1**. Thus, the C1–N2 (and C1A–N2A) bond becomes notably shorter (1.3215(16) Å and 1.3257(16) Å in **2** vs. 1.3986(15) Å in **1**), while the O1–C1 bond slightly elongates (1.2547(15) Å and 1.2584(15) Å in **2** vs. 1.2371(15) Å in **1**). Furthermore, the C1–N1 bond in the heterocyclic fragment (1.3628(16) Å and 1.3593(15) Å) is elongated compared to that in **1** (1.3171(16) Å). All these observations indicate a different distribution of electron density in molecules **1** and **2**. This, in turn, suggests the presence of a different tautomer in the case of **2**, characterized by a distinct proton position relative to **1** and a different bond-order pattern (Figure 1).

The C1–N2 bond between the quinoline fragment and the urea moiety is of double-bond character (ca. 1.32 Å, compared to 1.28–1.32 Å [24] for a double bond). The ureide group and the isoquinoline fragment are nearly coplanar (the torsion angle N1–C1–N2–C10 is 0.31(14)° and 0.93(15)°; the twist angle between the planes of the isoquinoline fragment C₉N and the ureide N₂CO is 0.23(4)° and 7.91(4)°). The isoquinoline fragment and the urea substituent are located on the same side of the C1–N2 group, forming a *syn*-configuration (Figure 3). This configuration is stabilized by an intramolecular hydrogen bond N–H···O (Figure 3, Table 2). Similar examples of Resonance-Assisted Hydrogen Bonds have been

repeatedly observed in cyclic H–N–C=N–C=O fragments and have been studied using various methods, including XRD and computational techniques [26,27].

Table 2. Hydrogen bonds in the structures of compounds **1** and **2**.

Contact X–D···A	Distance, D–A, Å	Distance, X–A, Å	Angle X–D–A, °	Assignment
1				
N2–H2–O1	2.0504(8)	2.9947(13)	153.90(6)	intermolecular
C5–H5–O1	2.3621(8)	3.4189(15)	164.21(7)	intermolecular
2				
C1–H1–O1	1.8214(9)	2.5700(13)	127.21(8)	intramolecular
C1A–H1A–O1A	1.8195(9)	2.5762(13)	128.01(7)	intramolecular
C2A–H2A–O1	2.3656(9)	3.1170(16)	124.97(7)	intermolecular
C2–H2–O1A	2.4387(8)	3.2000(15)	126.07(7)	intermolecular

2.2. Intermolecular Interactions and Supramolecular Organization of Compounds **1** and **2**

In the structure of **1**, two prominent intermolecular hydrogen bonds are formed: N–H···O and C–H···O (Table 2, Figure 4). The former interactions assemble molecules of **1** into extended one-dimensional chains; these chains, with the participation of the second type of hydrogen bond, are further connected into two-dimensional pseudo-layers.

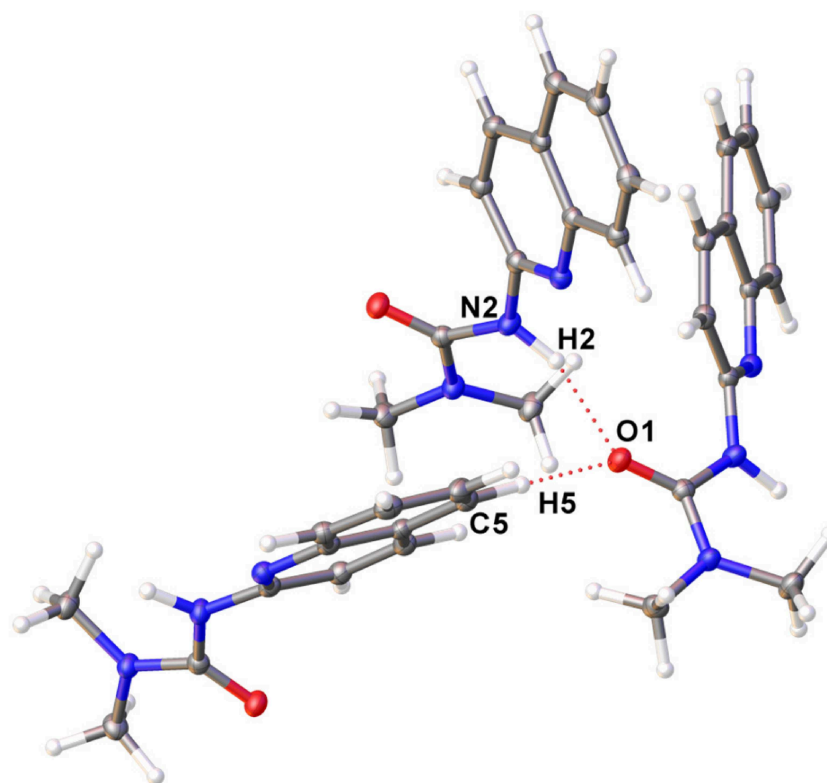


Figure 4. A fragment of the molecular structure of compound **1**, demonstrating the formation of intermolecular hydrogen bonds.

In addition to the short intramolecular hydrogen bond, the structure of **2** features two longer intermolecular C–H···O hydrogen bonds (Table 2, Figure 5). These interactions cause the molecules of **2** to assemble into dimers. Moreover, adjacent, parallel-oriented molecules of **2** exhibit a π -stacking interaction between the phenylene and ureide fragments, with an inter-plane distance of approximately 3.3 Å.

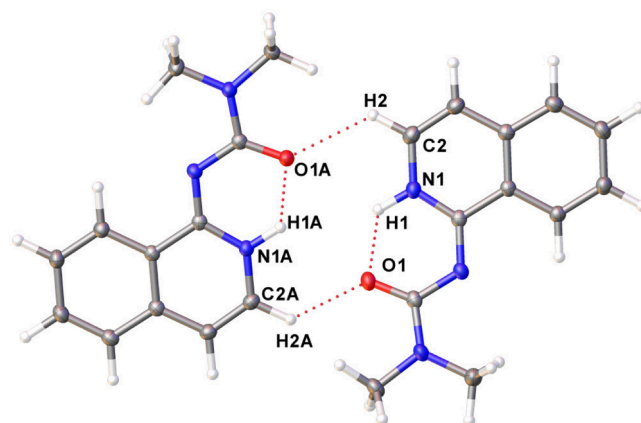


Figure 5. A fragment of the molecular structure of compound **2**, demonstrating the formation of dimers via intermolecular hydrogen bonds.

3. Discussion

The structural study of two isomeric urea derivatives with a heterocyclic fragment (compounds **1** and **2**) by single-crystal XRD revealed that different tautomeric forms are stabilized in the solid state (Figure 6). This likely also occurs in solution, which explains some fundamental differences in the ^1H and ^{13}C NMR spectra that we observed earlier [18]. Thus, in CDCl_3 solution, compound **1** exhibits a single signal for the NMe_2 group in both the ^1H and ^{13}C NMR spectra, whereas the corresponding spectra of compound **2** display two signals for the NMe_2 group [18]. This observation is consistent with the hetarylureide form of compound **1** and with the scenario in which the other NH bond competes with the NMe_2 group for interaction with the $\text{C}=\text{O}$ bond. This competition weakens the interaction of the NMe_2 group with $\text{C}=\text{O}$, thereby enabling rapid rotation around the $\text{C}-\text{NMe}_2$ bond and resulting in the equivalence of the two methyl groups. In contrast, compound **2** features an intramolecular hydrogen bond and an exocyclic $\text{C}=\text{N}$ bond, which do not engage in the same type of competition as in compound **1**. Consequently, the interaction between the NMe_2 group and the $\text{C}=\text{O}$ bond is strengthened. In this case, the free rotation of the NMe_2 group is restricted.

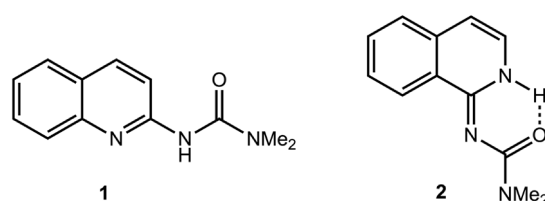


Figure 6. Structures of compounds **1** and **2**.

Such tautomerism is typical for amino derivatives of azaheterocycles [28]. Topological charge stabilization plays an important role in this process [29]. 1- And 2-aminoquinolines preferably exist in the form of amines [29,30], although the energy difference between the amine and imine forms for these condensed heterocycles is much smaller than for 2-amino pyridine. However, when switching to acylamine derivatives, the situation may change [31], and in this case, non-covalent interactions begin to play a significant role, which will be very different for 1- and 2-substituted systems. Therefore, it is not surprising that in our case, compounds **1** and **2** exhibit different crystalline structures.

The existence of different tautomers for compounds **1** and **2** can be explained by the difference in the electronic structure between the quinoline and isoquinoline fragments, which leads to changes in the basicity and reactivity of their derivatives. Thus, unsubsti-

tuted isoquinoline is slightly more basic than quinoline (pK_a of quinoline is about 4.9, while that of isoquinoline is about 5.4) [32,33]. The higher basicity of the isoquinoline fragment increases the stability of the tautomer with a protonated heterocyclic nitrogen atom and the resulting exocyclic C=N bond in compound **2**, compared to compound **1**. The lower basicity of the quinoline fragment favors the ureide form for compound **1**. Another explanation for the structural difference may be a greater preference for the *syn*-configuration (relative to the C1=N2 bond) over the *anti*-configuration for compound **2**. The latter configuration is unfavorable due to steric hindrance arising from the close proximity of the ureide group and the phenylene fragment. The *syn*-configuration, in turn, is geometrically favorable for proton transfer from the ureide nitrogen atom to the heterocyclic nitrogen atom, leading to the formation of a planar six-membered ring stabilized by an intramolecular hydrogen bond. For compound **1**, there are no significant obstacles to the formation of either the *syn*- or *anti*-conformation (relative to the C1–N2 bond). It is likely that the *anti*-conformation of **1** is realized in the solid state as the more favorable one in terms of packing effects.

The differences in the structures of the isomeric compounds **1** and **2** determine their distinct supramolecular organization in the solid state. In compound **1**, intermolecular N–H...O hydrogen bonds drive the assembly of one-dimensional chains; these chains are then linked via C–H...O hydrogen bonds into two-dimensional pseudo-layers. In the structure of **2**, the ureide group is involved in forming an intramolecular N–H...O hydrogen bond, while mutual C–H...O interactions between two molecules lead to the formation of supramolecular dimers.

The obtained results demonstrate the fundamental importance of studying tautomeric transformations of urea derivatives with heterocyclic fragments. The revealed structural differences between isomeric compounds **1** and **2** open up new opportunities for designing supramolecular assemblies with tailored structures and properties.

4. Materials and Methods

Compounds **1** and **2** were synthesized by us earlier [18]; the description of their synthesis is available in the Supplementary Materials. Crystals of **1** and **2** were grown by the slow evaporation of their solutions in 1,2-dichloroethane in air at RT. X-ray diffraction data were collected at 100(2) K on a Rigaku XtaLAB Synergy diffractometer (Rigaku Corporation, Akishima, Tokyo, Japan) with Cu-K α radiation ($\lambda = 1.54184$ Å). Data reduction was performed using CrysAlisPro 1.171.40.71a software (Rigaku Oxford Diffraction, Abingdon, UK, 2020). The structures were solved with the ShelXT [34] structure solution program using Intrinsic Phasing and refined with the ShelXL [35] refinement package incorporated in the OLEX2 program package [36] using full-matrix least-squares method for non-hydrogen atoms. All hydrogen atoms were placed in ideally calculated positions determined according to neutron diffraction statistical data [37] and refined as riding atoms with fixed isotropic displacement parameters. Crystal data and structure-refinement details for both structures are summarized in Table S1, Supplementary Materials.

Supplementary crystallographic data have been deposited at Cambridge Crystallographic Data Centre: 2579605 (**1**) and 2579606 (**2**). They can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif (accessed on 11 August 2026).

Supplementary Materials: The following supporting information can be downloaded online. Table S1: Crystal data and structure refinement for **1** and **2**; preparation of compounds **1** and **2**.

Author Contributions: Conceptualization, S.V.B. and V.P.B.; methodology, S.O.B. and S.V.B.; investigation, S.O.B.; resources, V.P.B.; data curation, S.V.B. and N.A.B.; writing—original draft preparation, S.V.B. and N.A.B.; writing—review and editing, S.V.B., V.P.B. and N.A.B.; visualization, N.A.B.;

supervision, S.V.B.; project administration, V.P.B.; funding acquisition, V.P.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Saint Petersburg State University (project No. 126022017742-6).

Data Availability Statement: The original contributions presented in this study are included in the article/Supplementary Material. Supplementary crystallographic data have been deposited at Cambridge Crystallographic Data Centre: 2579605 (1) and 2579606 (2). They can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif (accessed on 11 August 2026).

Acknowledgments: All physicochemical studies were performed at the Center for XRD Studies, the Center for Magnetic Resonance, and the Center for Chemical Analysis and Materials Research (all belonging to Saint Petersburg State University).

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Ajani, O.O.; Iyaye, K.T.; Ademosun, O.T. Recent advances in chemistry and therapeutic potential of functionalized quinoline motifs—A review. *RSC Adv.* **2022**, *12*, 18594–18614. [[CrossRef](#)] [[PubMed](#)]
2. Vijayakumar, A.; Manod, M.; Krishna, R.B.; Mathew, A.; Mohan, C. Diversely functionalized isoquinolines and their core-embedded heterocyclic frameworks: A privileged scaffold for medicinal chemistry. *RSC Med. Chem.* **2023**, *14*, 2509–2534. [[CrossRef](#)] [[PubMed](#)]
3. Mao, Y.; Soni, K.; Sangani, C.; Yao, Y. An Overview of Privileged Scaffold: Quinolines and Isoquinolines in Medicinal Chemistry as Anticancer Agents. *Curr. Top. Med. Chem.* **2020**, *20*, 2599–2633. [[CrossRef](#)] [[PubMed](#)]
4. Yadav, V.; Reang, J.; Sharma, V.; Majeed, J.; Sharma, P.C.; Sharma, K.; Giri, N.; Kumar, A.; Tonk, R.K. Quinoline-derivatives as privileged scaffolds for medicinal and pharmaceutical chemists: A comprehensive review. *Chem. Biol. Drug Des.* **2022**, *100*, 389–418. [[CrossRef](#)] [[PubMed](#)]
5. Kirad, S.; Deepa, P.R.; Sankaranarayanan, M. Greener alternatives for synthesis of isoquinoline and its derivatives: A comparative review of eco-compatible synthetic routes. *RSC Adv.* **2025**, *15*, 30231–30275. [[CrossRef](#)] [[PubMed](#)]
6. Panchaud, P.; Bruyère, T.; Blumstein, A.-C.; Bur, D.; Chambovey, A.; Ertel, E.A.; Gude, M.; Hubschwerlen, C.; Jacob, L.C.; Kimmerlin, T.; et al. Discovery and Optimization of Isoquinoline Ethyl Ureas as Antibacterial Agents. *J. Med. Chem.* **2017**, *60*, 3755–3775. [[CrossRef](#)] [[PubMed](#)]
7. Han, M.I.; Dengiz, C.; Doğan, Ş.D.; Gündüz, M.G.; Köprü, S.; Özkul, C. Isoquinolinedione-urea hybrids: Synthesis, antibacterial evaluation, drug-likeness, molecular docking and DFT studies. *J. Mol. Struct.* **2022**, *1252*, 132007. [[CrossRef](#)]
8. Moodley, R.; Mashaba, C.; Rakodi, G.H.; Ncube, N.B.; Maphoru, M.V.; Balogun, M.O.; Jordan, A.; Warner, D.F.; Khan, R.; Tukulula, M. New Quinoline–Urea–Benzothiazole Hybrids as Promising Antitubercular Agents: Synthesis, In Vitro Antitubercular Activity, Cytotoxicity Studies, and In Silico ADME Profiling. *Pharmaceuticals* **2022**, *15*, 576. [[CrossRef](#)] [[PubMed](#)]
9. Bala, I.A.; Al Sharif, O.F.; Asiri, A.M.; El-Shishtawy, R.M. Quinoline: A versatile bioactive scaffold and its molecular hybridization. *Results Chem.* **2024**, *7*, 101529. [[CrossRef](#)]
10. Khasawneh, M.A.; AlKaabi, A.; Samadi, A.; Antony, P.; Vijayan, R.; Al-Keridis, L.A.; Saadeh, H.A.; Abutaha, N. Synthesis and biological applications of some novel 8-Hydroxyquinoline urea and thiourea derivatives. *Arab. J. Chem.* **2022**, *15*, 103905. [[CrossRef](#)]
11. Gomtsyan, A.; Bayburt, E.K.; Schmidt, R.G.; Zheng, G.Z.; Perner, R.J.; Didomenico, S.; Koenig, J.R.; Turner, S.; Jinkerson, T.; Drizin, I.; et al. Novel transient receptor potential vanilloid 1 receptor antagonists for the treatment of pain: Structure-activity relationships for ureas with quinoline, isoquinoline, quinazoline, phthalazine, quinoxaline, and cinnoline moieties. *J. Med. Chem.* **2005**, *48*, 744–752. [[CrossRef](#)] [[PubMed](#)]
12. Genç, H.; Zengin, M.; Yavuz, E.; Genç, N.; Arslan, O. Synthesis and tyrosinase inhibitory properties of novel isoquinoline urea/thiourea derivatives. *Artif. Cells Nanomed. Biotechnol.* **2014**, *42*, 178–185. [[CrossRef](#)] [[PubMed](#)]
13. Baykova, S.O.; Baykov, S.V.; Boyarskiy, V.P. Pyridyl-Substituted Ureas and Carbamates: Synthesis and Application (A Review). *Russ. J. Gen. Chem.* **2024**, *94*, S60–S90. [[CrossRef](#)]
14. Baykova, S.O.; Baykov, S.V.; Solodyankina, O.V.; Boyarskiy, V.P. Access to 4-((Pyridin-2-yl)amino)quinazolinones via Annulation of 2-Aminobenzonitriles with N'-(Pyridin-2-yl)-N,N-dimethyl Ureas. *J. Org. Chem.* **2024**, *89*, 12094–12103. [[CrossRef](#)] [[PubMed](#)]
15. Baykova, S.O.; Geyl, K.K.; Baykov, S.V.; Boyarskiy, V.P. Synthesis of 3-(Pyridin-2-yl)quinazolin-2,4(1H,3H)-diones via Annulation of Anthranilic Esters with N-pyridyl Ureas. *Int. J. Mol. Sci.* **2023**, *24*, 7633. [[CrossRef](#)] [[PubMed](#)]
16. Kumar, R.; Thakur, A.; Sachin; Chandra, D.; Kumar Dhiman, A.; Kumar Verma, P.; Sharma, U. Quinoline-based metal complexes: Synthesis and applications. *Coord. Chem. Rev.* **2024**, *499*, 215453. [[CrossRef](#)]

17. Braga, D.; d'Agostino, S.; D'Amen, E.; Grepioni, F.; Genovese, D.; Prodi, L.; Sgarzi, M. A quest for supramolecular gelators: Silver(i) complexes with quinoline-urea derivatives. *Dalton Trans.* **2013**, 42, 16949–16960. [[CrossRef](#)] [[PubMed](#)]
18. Dobrynin, M.V.; Kasatkina, S.O.; Baykov, S.V.; Savko, P.Y.; Antonov, N.S.; Mikherdov, A.S.; Boyarskiy, V.P.; Islamova, R.M. Deprotonated diaminocarbene platinum complexes for thermoresponsive luminescent silicone materials: Both catalysts and luminophores. *Dalton Trans.* **2021**, 50, 14994–14999. [[CrossRef](#)] [[PubMed](#)]
19. Geyl, K.K.; Baykov, S.V.; Kalinin, S.A.; Bunev, A.S.; Troshina, M.A.; Sharonova, T.V.; Skripkin, M.Y.; Kasatkina, S.O.; Presnukhina, S.I.; Shetnev, A.A.; et al. Synthesis, Structure, and Antiproliferative Action of 2-Pyridyl Urea-Based Cu(II) Complexes. *Biomedicines* **2022**, 10, 461. [[CrossRef](#)] [[PubMed](#)]
20. Baykov, S.V.; Katlenok, E.A.; Semenov, A.V.; Baykova, S.O.; Boyarskiy, V.P.; Bokach, N.A.; Kukushkin, V.Y. Different Stacking Types in a Single Hybrid Cocrystal System: $\pi\cdots\pi$ - and π -Hole-Based Organic–Inorganic Planar Assemblies. *Inorg. Chem.* **2025**, 64, 4005–4016. [[CrossRef](#)] [[PubMed](#)]
21. Kasatkina, S.O.; Geyl, K.K.; Baykov, S.V.; Boyarskaya, I.A.; Boyarskiy, V.P. Catalyst-free synthesis of substituted pyridin-2-yl, quinolin-2-yl, and isoquinolin-1-yl carbamates from the corresponding hetaryl ureas and alcohols. *Org. Biomol. Chem.* **2021**, 19, 6059–6065. [[CrossRef](#)] [[PubMed](#)]
22. Olivari, M.; Caltagirone, C.; Garau, A.; Isaia, F.; Light, M.E.; Lippolis, V.; Montis, R.; Scorciapino, M.A. Non-symmetric substituted ureas locked in an (E,Z) conformation: An unusual anion binding via supramolecular assembly. *New J. Chem.* **2013**, 37, 663–669. [[CrossRef](#)]
23. Gilon, C.; Cohen, S.; Siderer, Y. The crystal structure of the photosynthetic inhibitors DCMU and DTPU. *Biopolymers* **1986**, 25, 1615–1621. [[CrossRef](#)]
24. Allen, F.H.; Kennard, O.; Watson, D.G.; Brammer, L.; Orpen, A.G.; Taylor, R. Tables of bond lengths determined by X-ray and neutron diffraction. Part 1. Bond lengths in organic compounds. *J. Chem. Soc. Perkin Trans. 2* **1987**, 16, S1–S19. [[CrossRef](#)]
25. Yu, Y.; Lin, L.-R.; You, J.; Huang, R.-B.; Zheng, L.-S. CCDC 605047: *Experimental Crystal Structure Determination*; Cambridge Crystallographic Data Centre (CCDC): Cambridge, UK, 2006. [[CrossRef](#)]
26. Zarie-Moghaddam, E.; Zahedi-Tabrizi, M. QAIM, NBO, and NMR studies of hydrogen bonds in capecitabine. *Monatsh. Chem.* **2019**, 150, 1267–1274. [[CrossRef](#)]
27. Gilli, P.; Bertolasi, V.; Ferretti, V.; Gilli, G. Evidence for Intramolecular N–H $\cdots$ O Resonance-Assisted Hydrogen Bonding in β -Enaminones and Related Heterodienes. A Combined Crystal-Structural, IR and NMR Spectroscopic, and Quantum-Mechanical Investigation. *J. Am. Chem. Soc.* **2000**, 122, 10405–10417. [[CrossRef](#)]
28. Katritzky, A.R.; Jug, K.; Oniciu, D.C. Quantitative Measures of Aromaticity for Mono-, Bi-, and Tricyclic Penta- and Hexatomic Heteroaromatic Ring Systems and Their Interrelationships. *Chem. Rev.* **2001**, 101, 1421–1450. [[CrossRef](#)] [[PubMed](#)]
29. Hatanaka, M. Role of Topological Charge Stabilization in Protomeric Tautomerism. *J. Phys. Chem. A* **2015**, 119, 1074–1086. [[CrossRef](#)] [[PubMed](#)]
30. Cook, M.J.; Katritzky, A.R.; Linda, P.; Tack, R.D. Aromaticity and tautomerism. Part II. The 4-pyridone, 2-quinolone, and 1-isoquinolone series. *J. Chem. Soc. Perkin Trans. 2* **1973**, 2, 1080–1086. [[CrossRef](#)]
31. Rybczyński, P.; Kaczmarek-Kędziera, A.; Iglesias-Reguant, A.; Plažuk, D.; Ośmiałowski, B. Tautomeric Equilibrium in 1-Benzamidoisoquinoline Derivatives. *Molecules* **2023**, 28, 1101. [[CrossRef](#)] [[PubMed](#)]
32. Joule, J.A. *Heterocyclic Chemistry*, 3rd ed.; CRC Press: Boca Raton, FL, USA, 1995.
33. Hosmane, R.S.; Liebman, J.F. Paradoxes and paradigms: Why is quinoline less basic than pyridine or isoquinoline? A classical organic chemical perspective. *Struct. Chem.* **2009**, 20, 693–697. [[CrossRef](#)]
34. Sheldrick, G.M. SHELXT—Integrated space-group and crystal-structure determination. *Acta Crystallogr. A* **2015**, 71, 3–8. [[CrossRef](#)] [[PubMed](#)]
35. Sheldrick, G. Crystal structure refinement with SHELXL. *Acta Crystallogr. C* **2015**, 71, 3–8. [[CrossRef](#)] [[PubMed](#)]
36. Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. OLEX2: A complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **2009**, 42, 339–341. [[CrossRef](#)]
37. Allen, F.H.; Bruno, I.J. Bond lengths in organic and metal-organic compounds revisited: X–H bond lengths from neutron diffraction data. *Acta Crystallogr. B* **2010**, 66, 380–386. [[CrossRef](#)] [[PubMed](#)]

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.