New Approaches to the Synthesis of 4-(2-Aminophenyl)-1,3-dihydro-2*H*-imidazol-2-ones and 3-Ureidoindoles and a Study of Their Interconversion

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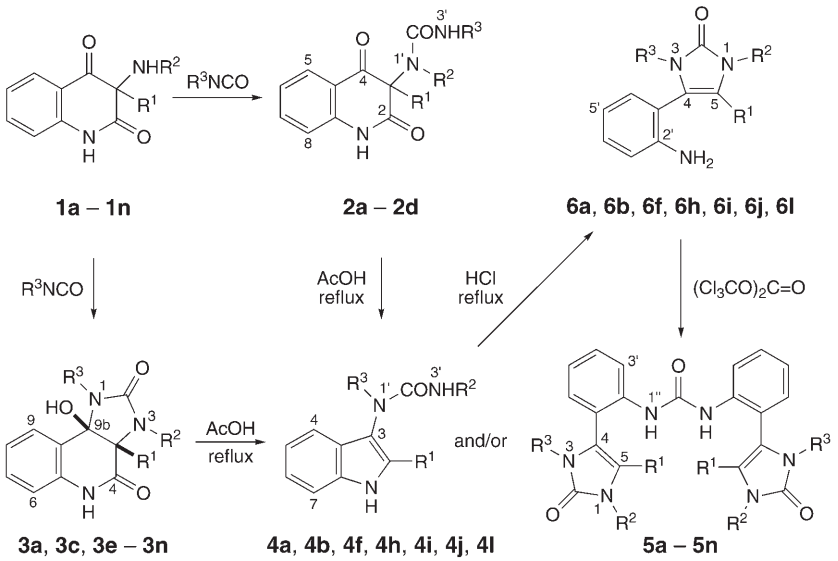
Dedicated to Professor *Vojeslav Štěrba* on the occasion of his 85th birthday

3-Alkyl/aryl-3-ureido-1*H*,3*H*-quinoline-2,4-diones (**2**) and 3a-alkyl/aryl-9b-hydroxy-3,3a,5,9b-tetrahydro-1*H*-imidazo[4,5-*c*]quinoline-2,4-diones (**3**) react in boiling concentrated HCl to give 5-alkyl/aryl-4-(2-aminophenyl)-1,3-dihydro-2*H*-imidazol-2-ones (**6**). The same compounds were prepared by the same procedure from 2-alkyl/aryl-3-ureido-1*H*-indoles (**4**), which were obtained from the reaction of 3-alkyl/aryl-3-aminoquinoline-2,4(1*H*,3*H*)-diones (**1**) with 1,3-diphenylurea or by the transformation of 3a-alkyl/aryl-9b-hydroxy-3,3a,5,9b-tetrahydro-1*H*-imidazo[4,5-*c*]quinoline-2,4-diones (**3**) and 5-alkyl/aryl-4-(2-aminophenyl)-1,3-dihydro-2*H*-imidazol-2-ones (**6**) in boiling AcOH. The latter were converted into 1,3-bis[2-(2-oxo-2,3-dihydro-1*H*-imidazol-4-yl)phenyl]ureas (**5**) by treatment with triphosgene. All compounds were characterized by ^{1}H- and ^{13}C-NMR and IR spectroscopy, as well as atmospheric pressure chemical-ionisation mass spectra.

1. Introduction. – In our laboratory, much attention has been paid to study the reactivity of 3-alkyl/aryl-3-hydroxy-quinoline-2,4(1*H*,3*H*)-diones and their 3-amino analogues **1** [1–9]. Both types of compounds readily rearrange into other heterocyclic systems. In the case of the 3-hydroxy derivatives, thermally induced rearrangement produces dioxindoles or 3,1-benzoxazin-2-ones [1][2], rearrangement in an alkaline environment produces dioxindoles and 2-hydroxyindoxyls [3]. 3-Amino derivatives rearrange, when treated with urea in boiling AcOH, to yield imidazo[1,5-*c*]quinazoline-3,5-diones [4] or 3-ureidoindolin-2-ones [5]. The reaction of 3-aminoquinoline-2,4-diones **1** with nitrourea in dioxane was successful in preparing anticipated reaction intermediates of this rearrangement [6][7], whereas the reaction with isocyanates yielded 3′-substituted 3-ureidoquinoline-2,4-diones **2** or their cyclic isomers **3** [8]. These compounds rearrange in boiling AcOH to give either mixtures of 3-ureidoindoles **4** and 1,3-disubstituted ureas **5**, or merely 1,3-disubstituted ureas **5** (*Scheme 1*) [9]. Refluxing compounds **4** in conc. HCl changes the indole system into imidazolinone, and compounds **6** prepared in this manner provide compounds **5** by a reaction with triphosgene [9].

The discovery that the addition products of 3-aminoquinoline-2,4-diones and isocyanates (**2** and **3**) rearrange to indole and imidazolinone derivatives, opens up a

Scheme 1



	a	b	c	d	e	f	g	h	i	j	k	l	m	n
R^1	Bu	Bu	Ph	Ph	Bu	Bu	Bu	Bu	Bu	Bu	Ph	Ph	Ph	Ph
R^2	H	H	H	H	Me	Me	Bu	Bu	$PhCH_2$	$PhCH_2$	Bu	Bu	$PhCH_2$	$PhCH_2$
R^3	Bu	Ph	Bu	Ph	Bu	Ph	Bu	Ph	Bu	Ph	Bu	Ph	Bu	Ph

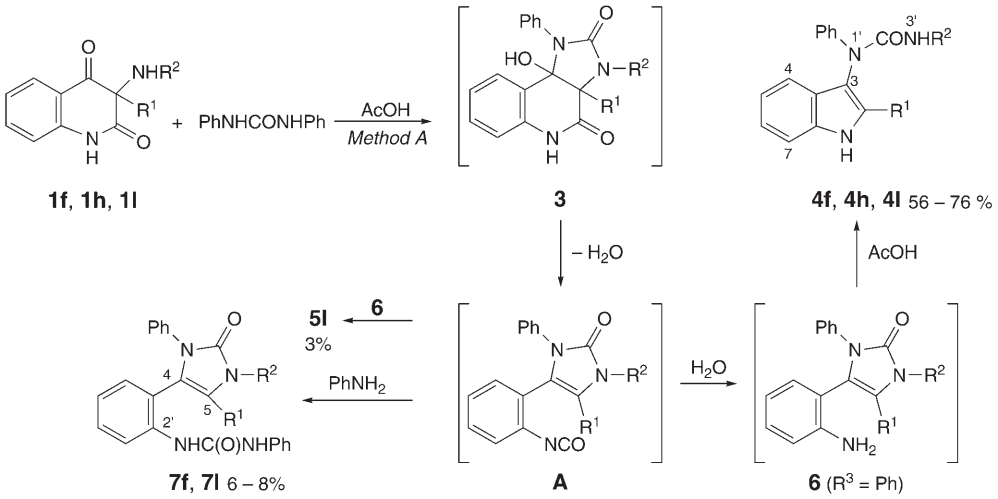
path for the preparation of new compounds of type **4**, **5**, and **6**, which may be interesting structures for studying biological activity. For example, 2-phenyl-3-semicarbazidoindoles, which have a structure similar to **4**, display antimicrobial and antihistaminic activity [10][11]; interesting biological activity is described for many imidazolin-2-ones [12], and a number of 1,3-diarylureas act as anti-cytokinine agents [13].

Transformation of compounds **2** and/or **3** to compounds **4** occurs only in rather low yield, and the main or even sole product in most cases are 1,3-disubstituted ureas **5** [9]. Another difficulty is, that mixtures of **4** and **5** can be separated only with great difficulty. For that reason, we tried to find reaction conditions where 3-ureidoindoles **4** or imidazolinones **6** arise, while the formation of compounds **5** is limited. This paper describes the results achieved in this matter so far.

2. Results and Discussion. – Our first aim was to find reaction conditions that would enable us to prepare 3-ureidoindoles **4** directly from α-amino ketones **1**. In one of our earlier papers [6], we described that 3-aminoquinoline-2,4-diones **1** in boiling AcOH yield products of molecular rearrangement not only in the reaction with urea but also in reactions with monosubstituted or 1,1-disubstituted ureas (butylurea, phenylurea, 1,1-dibenzylurea). Under the given reaction conditions, monosubstituted or 1,1-disubstituted ureas split into the respective amine and isocyanic acid, which reacts with 3-aminoquinoline-2,4-diones **1** giving rise to intermediates analogous to **2** and **3**

($R^3 = H$), subject of molecular rearrangement. This fact led to the idea that, under similar reaction conditions, 1,3-disubstituted ureas could produce the corresponding amine and isocyanate that would react with **1** to yield intermediates **2** and/or **3**, which subsequently rearrange to the products **4**. This assumption was confirmed, and from the reaction of 3-aminoquinolones **1f**, **1h**, and **1l** with 1,3-diphenylurea in boiling AcOH (*Scheme 2*) the rearranged compounds **4f**, **4h**, and **4l** were isolated as the main products (*Table 1*, *Method A*).

Scheme 2



As a side product, acetanilide was isolated. Additionally, in one single case, the diarylurea **5l** was obtained in negligible quantities. Other side products, which exhibited a molecular peak of even *m*/*z* values in the mass spectra were obtained in two cases (starting from **1f** and **1l**). Their molecular peaks split into two primary fragments, which differ by a value of *m*/*z* 26. Such splitting of the molecular ion is typical for 1,3-disubstituted ureas [9] and, therefore, we propose structure **7** for the side products of the reaction of compounds **1f** and **1l** with 1,3-diphenylurea (*Scheme 2*). This proposal was confirmed by synthesizing **7** from **6** and phenyl isocyanate. The formation of compounds **7f** and **7l** may be explained by a reaction mechanism analogous to that of the transformation of compounds **2** and **3** into **4** and **5** *via* an intermediate **A** [9] (*Scheme 2*). The reaction of amines **1** with diphenylurea (*Table 1*, *Method A*) gives generally lower yields of **4** than the reaction of **2** or **3**, which are transformed to **4** in boiling AcOH [9]; but the formation of 1,3-diarylureas is limited in every case. However, the disadvantage of the direct transformation of **1** into **4** (*Method A*) is its limitation to 3-ureidoindoles **4** that bear a Ph group in position 1′ ($R^3 = Ph$). When compounds **1** were reacted with 1,3-dibutylurea, we merely obtained inseparable mixtures of products. A further disadvantage of the direct transformation of **1** to **4** is the difficult chromatographic separation of **4** from the reaction mixture containing considerable quantities of unreacted 1,3-diphenylurea and acetanilide. A considerable proportion of compounds displaying a polar character also arose, and these could not

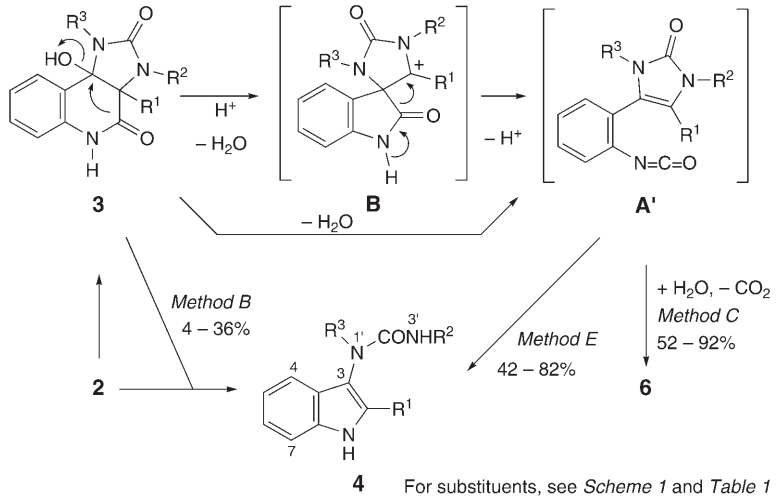
Table 1. *Preparation of 3-Ureidoindoles* **4** *from Compounds* **1** (*Method A*), **2** (*Methods B* and *E*), **3** (*Methods B* and *E*), *and* **6** (*Method D*)

Entry	Starting compound				Method	Reaction time [h]	Products (Yield [%])
		R^1	R^2	R^3			
1	**2a**	Bu	H	Bu	*E*	1 + 1.5	**4a** (68)
2	**2a**	Bu	H	Bu	*B*	1.5	**4a** (18), **5a** (67)
3	**3a**	Bu	H	Bu	*B*	1.5	**4a** (31), **5a** (53)
4	**6a**	Bu	H	Bu	*D*	3	**4a** (45)
5	**6a**	Bu	H	Bu	*D*	1.5	**4a** (30)
6	**6b**	Bu	H	Ph	*D*	1	**4b** (31)
7	**3c**	Ph	H	Bu	*E*	1 + 1.5	**4c** (82)
8	**6c**	Ph	H	Bu	*D*	1	**4c** (67)
9	**2d**	Ph	H	Ph	*E*	1 + 1.5	**4d** (65)
10	**6d**	Ph	H	Ph	*D*	1	**4d** (65)
11	**3e**	Bu	Me	Bu	*E*	1 + 1.5	**4e** (42), **6e** (31)
12	**6e**	Bu	Me	Bu	*D*	2	**4e** (28)
13	**1f**	Bu	Me	Ph	*A*	1.5	**4f** (21), **7f** (8)
14	**1f**	Bu	Me	Ph	*A*	2	**4f** (29), **7f** (6)
15	**6f**	Bu	Me	Ph	*D*	1	**4f** (76)
16	**6g**	Bu	Bu	Bu	*D*	3	**4g** (86)
17	**1h**	Bu	Bu	Ph	*A*	4.5	**4h** (33)
18	**3h**	Bu	Bu	Ph	*B*	0.5	**4h** (36), **5h** (28)
19	**6h**	Bu	Bu	Ph	*D*	4	**4h** (56)
20	**6i**	Bu	$PhCH_2$	Bu	*D*	3.5	**4i** (53)
21	**6j**	Bu	$PhCH_2$	Ph	*D*	2.5	**4j** (36)
22	**3k**	Ph	Bu	Bu	*E*	1 + 1.5	**4k** (67)
23	**6k**	Ph	Bu	Bu	*D*	1	**4k** (43), **8k** (16), **6k** (7)
24	**1l**	Ph	Bu	Ph	*A*	6	**4l** (47), **5l** (3), **7l** (8)
25	**6l**	Ph	Bu	Ph	*D*	3	**4l** (58)
26	**3m**	Ph	$PhCH_2$	Bu	*E*	1 + 1.5	**4m** (53), **6m** (12), **8m** (9)
27	**3m**	Ph	$PhCH_2$	Bu	*B*	0.5	**4m** (4), **5m** (51), **6m** (12)
28	**6m**	Ph	$PhCH_2$	Bu	*D*	5	**4m** (14), **6m** (25), **8m** (21)
29	**3n**	Ph	$PhCH_2$	Ph	*B*	0.5	**4n** (4), **5n** (34), **6n** (32)
30	**3n**	Ph	$PhCH_2$	Ph	*E*	1 + 1.5	**4n** (77)
31	**6n**	Ph	$PhCH_2$	Ph	*D*	1.5	**4n** (21), **8n** (16), **6n** (32)
32	**6n**	Ph	$PhCH_2$	Ph	*D*	3	**4n** (16), **8n** (25), **6n** (32)

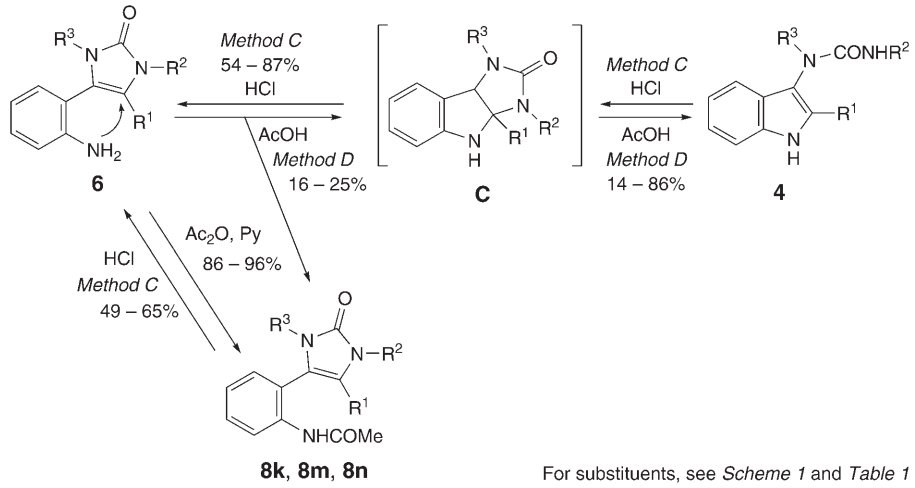
be separated by chromatography. For this reason, we abandoned this path for preparing 3-ureidoindoles **4** and sought for other possibilities.

We propose a reaction mechanism with a rearrangement of compounds **2** and **3** in boiling AcOH to **4** and **5** (or **5** only) *via* the formation of an intermediate **A′** (*Scheme 3*) [9]. This intermediate partly hydrolyses to give **6**, which is transformed to **4** as indicated in *Scheme 4*. However, at the same time, **A′** reacts with **6** to yield the disubstituted urea **5**. It can be assumed that, in the presence of excess H_2O, compounds **4** should arise as the sole products. Therefore, we carried out the rearrangement of compounds **2a** and **3a**, **3h**, **3m**, and **3n** in aqueous AcOH (*Method B*). However, the results of these experiments (*Table 1*, *Entries 2*, *3*, *18*, *27*, and *29*) show that even under these reaction conditions, intermediate **A′** reacts with the amino group of **6**, and mixtures of **4** and **5**

Scheme 3



Scheme 4



arise. In cases where $R^1 = Ph$, compounds **6** are obtained as well (*Table 1*, *Entries 27* and *29*). This finding is in accordance with the fact that, in these cases, the tendency for intramolecular addition of the amino group in **6** is lowered [9]. Because the use of *Method B* does not lead to satisfactory results, these experiments were discontinued.

Compounds **6** are also possible sources for the preparation of 3-ureidoindoles **4**. As already described [9], compounds **6** are unstable in polar solvents, and some of them were converted back to compounds **4** during NMR spectra collection in (D_6)DMSO. This conversion is particularly easy when $R^2 = H$. However, there is a question how **6**

can be easily prepared. We have described the transformation of 3-ureidoindoles **4a**, **4b**, **4f**, **4h**, **4i**, **4j**, and **4l** to imidazolones **6a**, **6b**, **6f**, **6h**, **6i**, **6j**, and **6l** (*Scheme 1*) by boiling compounds **4** in HCl [9]. Compounds **4c**, **4d**, **4e**, **4g**, **4k**, **4m**, and **4n** have not been available earlier, because only 1,3-disubstituted ureas **5** were isolated from the corresponding reaction mixtures after reacting the corresponding compounds **2** or **3** with urea in AcOH. However, the easy transformation of 3-ureidoindoles **4** into imidazolinones **6** led us to reason that compounds **6** could also be formed by direct transformation of ureidoquinolinediones **2** or their cyclic isomers **3** in strongly acidic aqueous environments. This assumption was fully confirmed, and the corresponding dihydroimidazolones **6** were isolated in high yields from the reactions of **2a**–**2d** or **3c**, **3e**–**3n** with conc. HCl (*Table 2*, *Method C*). Acid-catalyzed rearrangement of **2** or **3** (*Scheme 3*) gives rise to carbocation **B**, followed by the opening of the indolone ring under formation of intermediate **A′**. The latter immediately hydrolyses in a strongly acidic aqueous environment to give dihydroimidazolone **6** and, therefore, formation of disubstituted ureas **5** cannot take place.

Table 2. *Preparation of Dihydroimidazolones* **6**, *from Compounds* **2**, **3**, **4**, *and* **8** *under Reflux in conc. HCl* (*Method C*)[a])[b])

Entry	Starting compound	Reaction time [h]	Product (Yield [%])	*Entry*	Starting compound	Reaction time [h]	Product (Yield [%])
1	**2a**	2	**6a** (80)	*16*	**4g**	1	**6g** (83)
2	**2a**	1	**6a** (54)	*17*	**3h**	0.5	**6h** (66)
3	**3a**	4	**6a** (76)	*18*	**3h**	2	**6h** (52)
4	**2b**	1	**6b** (74)	*19*	**3i**	2	**6i** (72)
5	**2c**	1	**6c** (79)	*20*	**3j**	2	**6j** (50)
6	**3c**	1	**6c** (78)	*21*	**3k**	1	**6k** (85)
7	**4c**	1	**6c** (68)	*22*	**4k**	1	**6k** (75)
8	**2d**	0.5	**6d** (83)	*23*	**8k**	1	**6k** (65)
9	**4d**	2.5	**6d** (79)	*24*	**3l**	1.5	**6l** (78)
10	**3e**	2	**6e** (75)	*25*	**3m**	1	**6m** (72)
11	**4e**	0.5	**6e** (80)	*26*	**4m**	1	**6m** (79)
12	**3f**	1.5	**6f** (83)	*27*	**8m**	1	**6m** (49)
13	**3f**	2	**6f** (73)	*28*	**3n**	0.5	**6n** (73)
14	**3f**	3	**6f** (63)	*29*	**4n**	2.5	**6n** (54)
15	**3g**	1	**6g** (92)	*30*	**8n**	1	**6n** (53)

[a]) For substituents, see *Table 1*. [b]) Conversion of compounds **4a**, **4b**, **4f**, **4h**, **4i**, **4j**, and **4l** to the corresponding compounds **6** has been described in [9].

Now we found that reconversion of **6** into ureidoindoles **4** may be successfully executed in boiling AcOH (*Table 1*, *Method D*). In a weakly acidic environment, compounds **6** undergo an intramolecular nucleophilic addition of the amino group to form intermediate **C**. The intermediate's imidazolidinone ring is opened, and ureidoindoles **4** are formed (*Scheme 4*).

The anticipated intermediates **C** are aza-analogues of hexahydropyrrolo[2,3-*b*]indole alkaloids, which are cyclic analogues of *N*-acylated derivatives of tryptophane. It is well-known, that these alkaloids and their synthetic analogues arise from *N*-acylated tryptophane derivatives in a strongly acidic environment but, under weakly

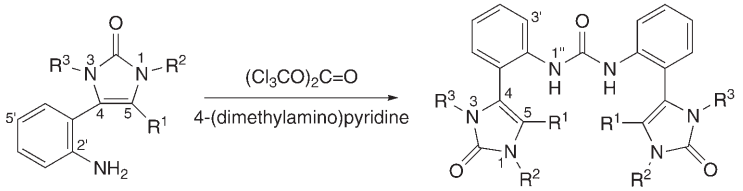
acidic conditions, they reconvert into acyclic tautomers [14–18]. The transformation of **6** to **4** *via* the intermediate **C** bears a certain distant analogy to the conversions of hexahydropyrrolo[2,3-*b*]indoles. Despite all efforts, we did not succeed in our earlier work [9] and have not yet succeeded in isolating or trapping anticipated intermediates **C**. In a majority of cases, heating **6** in AcOH to reflux merely provided the corresponding compounds **4** (*Table 1*, *Method D*). However, the reaction of **6k**, **6m**, and **6n** in AcOH gave, apart from the corresponding products **4k**, **4m**, and **4n** and unreacted **6k**, **6m**, and **6n**, other side products (**8k**, **8m**, and **8n**). These compounds revert to **6** in boiling conc. HCl (*Table 2*, *Method C*). Hence, **6k**, **6m**, and **6n**, which differ from other compounds **6** by the presence of a Ph group at C(5) of the imidazolone nucleus, obviously convert only slowly into indole derivatives **4** by heating in AcOH, and a competitive transformation into acetylated compounds **8** occurs (*Scheme 4*). The structure of **8** was confirmed by its synthesis from **6** and Ac_2O. The reason why this transformation from **6** to **8** does not take place in the case of **6l**, which bears a Ph group at C(5) like **6k**, **6m**, and **6n**, is an issue we failed to resolve.

Rearrangement of compounds **2** or **3** in conc. HCl (*Table 2*, *Method C*) offers high yields of imidazolinones **6** (mostly in a 74–92% range). In a number of cases, however, the following transformation of **6** into ureidoindoles **4** (*Table 1*, *Method D*) shows substantially lower yields (28–86%). If the target products are compounds **4**, it is much more favorable to prepare them from compounds **2** or **3** by performing a two-stage reaction without isolating an intermediate (*Scheme 3*, *Table 1*, *Method E*). Compounds **4a**, **4c**, **4d**, **4k**, and **4n** were prepared from **2a**, **3c**, **2d**, **3k**, and **3n** in this manner with yields of 65–82% (*Table 1*). In the cases of **3e** and **3m**, compounds **6** were obtained additionally to **4** (*Table 1*).

In our previous work [9], we described the preparation of **5a**, **5f**, **5h**, **5i**, **5j**, and **5l** by a reaction of the corresponding dihydroimidazolones **6** with triphosgene (bis(trichloromethyl) carbonate). The other compounds of type **5** could not be prepared because ureidoindoles **4** were not available from the reactions of **2** and/or **3** in AcOH, thus dihydroimidazolones **6** could not be prepared either. But now, having in hand the relevant compounds **6** from the reaction of **2** and/or **3** in conc. HCl, we attempted to prepare the remaining **5c**, **5d**, **5e**, **5g**, **5k**, **5m**, and **5n**. As in our previous work [9], we found that compounds **6** react with triphosgene at room temperature in CH_2Cl_2 very slowly, even though this procedure has been currently employed by other groups [19][20]. The disubstituted ureas **5e**, **5g**, **5k**, **5m**, and **5n** were obtained by performing the reaction in boiling benzene and in the presence of a catalytic quantity of 4-(dimethylamino)pyridine (*Scheme 5*). Preparation failed only in cases where **6** is not substituted at C(1) ($R^2 = H$). Similar to our previous work [9], where compound **5a** was prepared in only 6% yield and preparation of **5b** was not possible, we obtained **5c** in only 12% yield and failed to prepare **5d**.

In conclusion, we would like to emphasise that the elaborated methods enable us to prepare 3-ureidoindoles **4** and/or dihydroimidazolones **6** from 3-aminoquinolinediones **1** *via* the intermediates **2** or **3** in high yields. The unprecedented mutual transformation of **4** and **6** is not merely of theoretical importance but enables, through a simple procedure, a targeted preparation of new types of compounds suitable for biological testing as well as for studying further transformations, particularly in the case of dihydroimidazolones **6** bearing a reactive aniline fragment.

Scheme 5



6c, **6d**, **6e**, **6g**, **6k**, **6m**, **6n**
For substituents, see *Scheme 1* and *Table 1*

5c, **5d**, **5e**, **5g**, **5k**, **5m**, **5n**
yield 12 – 78%

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Experimental Part

1. *General.* Reactions, as well as the course of separation and also the purity of substances, were monitored by TLC (elution systems benzene/AcOEt, 4:1 (solvent system *S3*), $CHCl_3$/EtOH, 9:1 (*S4*) and/or 19:1 (*S5*), and $CHCl_3$/AcOEt, 7:3 (*S6*)) on *Alugram® SIL G/UV$_{254}$* foils (*Macherey-Nagel*). Column chromatography (CC) was carried out on silica gel (*Merck*, grade *60*, 70–230 mesh), using $CHCl_3$, and then successive mixtures of $CHCl_3$/EtOH (99:1 to 8:2, solvent system *S1*) or benzene, and then successive mixtures of benzene/AcOEt (99:1 to 8:2, solvent system *S2*). M.p.: *Kofler* block or *Gallencamp* apparatus. IR (KBr) Spectra: *Mattson 3000* spectrophotometer. NMR Spectra were recorded on a *Bruker Avance* spectrometer (500.13 MHz for ^{1}H and 125.76 MHz for ^{13}C) in (D_6)DMSO. ^{1}H and ^{13}C chemical shifts are given on the δ scale (in ppm) and are referenced to internal TMS. All 2D experiments (gradient-selected (gs)-COSY, NOESY, gs-TOCSY, gs-HMQC, gs-HMBC) were performed using the manufacturer's software. ^{1}H-NMR Spectra were assigned using gs-COSY. Protonated C-atoms were assigned by gs-HMQC. Quaternary C-atoms were assigned by gs-HMBC. The positive-ion atmospheric pressure chemical ionization (APCI) mass spectra were measured on an ion trap analyzer *Esquire 3000* (*Bruker Daltonics*) within the mass range *m/z* 50–500. Samples were dissolved in MeCN and analyzed by direct infusion at the flow rate of 50 µl/min. The ion-source temp. was 350°, the APCI probe temp. was 300°, the flow rate and the pressure of N_2 were 4 l/min and 45 psi, resp. For MS/MS measurements, the isolation width of precursor ions was 4 *m/z* and the collision amplitude was 1 V. Elemental analyses (C, H, N): *EA 1108 Elemental Analyzer* (*Fisons Instrument*).

Starting compounds **2** and **3** were prepared from the corresponding compounds **1** according to the protocol described in [8]. Yields of products **4**, **6**, and **8** are given in *Tables 1* and *2*.

2. *General Procedures for the Preparation of (1*H*-Indol-3-yl)ureas* **4** *and 4-(2-Acetamidophenyl)-1,3-dihydroimidazol-2-ones* **8**. *Method A.* A soln. of **1** (0.5 mmol) and 1,3-diphenylurea (117 mg, 0.55 mmol) in AcOH (2 ml) was heated to reflux for the time given in *Table 1.* After cooling, the precipitated crystals were filtered off with suction and recrystallized from an appropriate solvent. In cases when crystallization failed, the mixtures were evaporated *in vacuo* to dryness, and the residue was crystallized from an appropriate solvent. In some cases, mother liquors were chromatographed on silica gel using solvent systems *S1* or *S2*.

Method B. A soln. of **2** or **3** (0.5 mmol) in aq. AcOH (70% *v/v*, 6 ml) was heated to reflux for the time given in *Table 1*. After cooling, the solvent was evaporated *in vacuo* to dryness, and the residue was crystallized from an appropriate solvent. In some cases, mother liquors were worked up by CC on silica gel.

Method D. A soln. of **6** (0.5 mmol) in AcOH (6 ml) was heated to reflux for the time given in *Table 1*. Following treatment of the reaction mixture, workup was carried out as described in *Method B.*

Method E. A soln. of compound **2** or **3** (0.5 mmol) in conc. HCl (5 ml) was heated to reflux for 1 h. After cooling, the soln. was evaporated *in vacuo* to dryness, the residue was dissolved in pyridine (5 ml), anh. K_2CO_3 (350 mg) was added, and the mixture was stirred for 1 h. Insoluble material was filtered off, the filtrate was evaporated do dryness, dissolved in AcOH (5 ml), and the mixture was heated to reflux for 1.5 h. After cooling, the solvent was evaporated *in vacuo* to dryness, and the residue was crystallized from an appropriate solvent. In some cases, mother liquors were separated by CC on silica gel.

2.1. *1-Butyl-1-(2-butyl-1*H*-indol-3-yl)urea* (**4a**). Prepared from **2a** (*Methods B* (besides **5a**) and *E*), **3a** (*Method B*), and **6a** (*Method D*). Colorless crystals. M.p. 136–141° (benzene/hexane), identical in all respects to authentic **4a** of m.p. 135–142°, prepared from **2a** and **3a** [9].

2.2. *1-(2-Butyl-1*H*-indol-3-yl)-1-phenylurea* (**4b**). Prepared from **6b** (*Method D*). Colorless crystals. M.p. 205–208° (AcOEt), identical in all respects to authentic **4b** of m.p. 204–208°, prepared from **2b** [9].

2.3. *1-Butyl-1-(2-phenyl-1*H*-indol-3-yl)urea* (**4c**). Prepared from **3c** (*Method E*) and **6c** (*Method D*). Colorless crystals. M.p. 212–215° (benzene). IR: 3445, 3306, 3218, 3195, 3064, 2952, 2932, 2869, 1641, 1581, 1491, 1464, 1453, 1427, 1379, 1356, 1339, 1309, 1279, 1231, 1179, 1036, 1115, 1074, 1028, 1008, 965, 921, 764, 739, 697, 630, 614, 564. ^{1}H- and ^{13}C-NMR: see *Table 3*. APCI-MS (pos.): 308 (28, $[M+H]^+$), 291 (100, $[M+H-NH_3]^+$), 263 (36, $[M+H-NH_3-CO]^+$). APCI-MS/MS (pos.) of *m/z* 308: 291 (100, $[M+H-NH_3]^+$). APCI-MS (neg.): 306 (100, $[M-H]^-$), 261 (18, $[M-H-COOH]^-$), 233 (4, $[M-H-BuNH_2]^-$). APCI-MS/MS (neg.) of *m/z* 306: 263 (43, $[M-H-NHCO]^-$), 249 (75, $[M-H-Bu]^-$), 206 (100, $[M-H-Bu-NHCO]^-$). Anal. calc. for $C_{19}H_{21}N_3O$ (307.39): C 74.24, H 6.89, N 13.67; found: C 74.32, H 6.92, N 13.51.

2.4. *1-Phenyl-1-(2-phenyl-1*H*-indol-3-yl)urea* (**4d**). Prepared from **2d** (*Method E*) and **6d** (*Method D*). Colorless crystals. M.p. 250–256° (benzene). IR: 3458, 3394, 3318, 3190, 3061, 1659, 1579, 1492, 1453, 1404, 1340, 1264, 1239, 1198, 1148, 1073, 1030, 829, 763, 741, 693, 637, 616, 564, 519. ^{1}H- and ^{13}C-NMR: see *Table 3*. APCI-MS (pos.): 328 (67, $[M+H]^+$), 311 (55, $[M+H-NH_3]^+$), 283 (100, $[M+H-COOH]^+$), 206 (3, $[M+H-COOH-Ph]^+$). APCI-MS/MS (pos.) of *m/z* 328: 311 (100, $[M+H-NH_3]^+$), 284 (5, $[M+H-NH_2CO]^+$), 209 (6, $[M+H-PhNCO]^+$). APCI-MS (neg.): 326 (100, $[M-H]^-$), 282 (94, $[M-H-NH_2CO]^-$). APCI-MS/MS (neg.) of *m/z* 326: 283 (100, $[M-H-NH_2CO]^-$). Anal. calc. for $C_{21}H_{17}N_3O$ (327.38): C 77.04, H 5.23, N 12.84; found: C 77.14; H 5.36, N 12.69.

2.5. *1-Butyl-1-(2-butyl-1*H*-indol-3-yl)-3-methylurea* (**4e**). Prepared from **3e** (*Method E*, besides **6e**) and from **6e** (*Method D*). Colorless crystals. M.p. 127–130° (hexane). IR: 3348, 3249, 2959, 2930, 2872, 2745, 1613, 1523, 1458, 1409, 1383, 1292, 1227, 1185, 1144, 1124, 1011, 924, 768, 743, 715, 646, 568, 521. ^{1}H- and ^{13}C-NMR: see *Table 3*. APCI-MS (pos.): 302 (100, $[M+H]^+$), 271 (45, $[M+H-MeNH_2]^+$), 243 (50, $[M+H-MeNH_2-CO]^+$), 215 (22, $[M+H-MeNH_2-butene]^+$), 172 (79, $[M+H-MeNH_2-butene-NHCO]^+$). APCI-MS/MS (pos.) of *m/z* 302: 271 (100, $[M+H-MeNH_2]^+$), 243 (72, $[M+H-MeNH_2-CO]^+$), 215 (37, $[M+H-MeNH_2-butene]^+$), 172 (79, $[M+H-MeNH_2-butene-NHCO]^+$). APCI-MS (neg.): 300 (100, $[M-H]^-$), 269 (3, $[M-H-MeNH_2]^-$). APCI-MS/MS (neg.) of *m/z* 300: 243 (100, $[M-H-Bu]^-$), 186 (45, $[M-H-2\,Bu]^-$), 170 (5, $[M-H-Bu-BuNH_2]^-$). Anal. calc. for $C_{18}H_{27}N_3O$ (301.43): C 71.72, H 9.03, N 13.94; found: C 71.62, H 9.14, N 13.79.

2.6. *1-(2-Butyl-1*H*-indol-3-yl)-3-methyl-1-phenylurea* (**4f**). Prepared from **1f** (*Method A*) and from **6f** (*Method D*). Colorless crystals. M.p. 208–214° (AcOEt), identical in all respects to authentic **4f** of m.p. 204–208°, prepared from **3f** [9]. In a small quantity (8 and 6%, resp.), a side-product with m.p. 229–234° (benzene/hexane), identical in all respects to synthetic **7f** (*Section 6.1*), was isolated from the reactions of **1f** with diphenylurea (*Method A*).

2.7. *1,3-Dibutyl-1-(2-butyl-1*H*-indol-3-yl)urea* (**4g**). Prepared from **6g** (*Method D*). Yellowish oil. IR: 2958, 2929, 2870, 1708, 1639, 1586, 1517, 1458, 1379, 1330, 1287, 1225, 1178, 1148, 1128, 1014, 924, 845, 767, 743, 624, 522. ^{1}H- and ^{13}C-NMR: see *Table 3*. APCI-MS (pos.): 344 (100, $[M+H]^+$), 271 (13, $[M+H-BuNH_2]^+$), 243 (12, $[M+H-BuNHCOH]^+$), 215 (5, $[M+H-BuNH_2-butene]^+$). APCI-MS/MS (pos.) of *m/z* 344: 271 (85, $[M+H-BuNH_2]^+$), 243 (100, $[M+H-BuNHCOH]^+$), 215 (32, $[M+H-BuNH_2-butene]^+$), 172 (54, $[M+H-BuNH_2-butene-NHCO]^+$). APCI-MS (neg.): 342 (100,

Table 3. *^{1}H- and ^{13}C-Chemical Shifts* (δ [ppm]) *of Compounds* **4** *in (D_6)DMSO*

Position	**4c**		**4d**		**4e**		**4g**		**4k**		**4m**		**4n**	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	11.62	–	11.75	–	11.10	–	11.13	–	11.64	–	11.66	–	11.78	–
2	–	131.3	–	131.1	–	137.4	–	137.2	–	133.0	–	133.3	–	133.8
3	–	114.9	–	114.9	–	113.1	–	112.9	–	114.2	–	114.1	–	113.8
3a	–	126.0	–	125.9	–	125.1	–	124.8	–	126.0	–	126.3	–	126.0
4	7.40	117.7	7.40	117.6	7.26	116.9	7.26	116.7	7.35	117.6	7.39	117.8	7.40	117.6
5	7.12	119.8	7.12	120.1	7.01	119.2	7.01	119.1	7.10	119.9	7.11	119.9	7.02	120.0
6	7.21	122.2	7.21	123.6	7.09	120.8	7.09	120.7	7.20	122.4	7.21	122.4	7.23	123.5
7	7.47	111.9	7.47	112.0	7.35	111.4	7.35	111.4	7.47	112.0	7.47	112.0	7.52	112.0
7a	–	134.9	–	134.9	–	134.5	–	134.4	–	135.0	–	135.0	–	135.0
NH*C*ONH	–	158.5	–	157.2	–	158.4	–	157.6	–	157.7	–	158.4	–	156.5
CON*H*R^2	5.62	–	6.11	–	5.30	–	5.25	–	5.72	–	6.44	–	6.95	–
1′ (R^1)	–	132.6	–	133.2	2.62, 2.59	24.8	2.62, 2.59	24.8	–	131.3	–	133.2	–	131.0
2′ (R^1)	7.83	126.5	7.88	126.3	1.76, 1.66	31.2	1.74, 1.69	30.4	7.79	126.5	7.78	126.6	7.85	126.8
3′ (R^1)	7.51	128.8	7.52	128.9	1.39	22.3	1.39	22.3	7.52	128.9	7.50	128.6	7.52	128.9
4′ (R^1)	7.41	127.9	7.42	128.1	0.96	14.1	0.96	13.8	7.40	128.0	7.42	128.1	7.42	128.1
1′ (R^2)	–	–	–	–	2.51	27.4	3.03, 2.91	39.6	3.01, 2.96	39.8	4.21, 4.19	43.6	4.27, 4.21	43.6
2′ (R^2)	–	–	–	–	–	–	1.28	32.3	1.26	32.4	–	141.5	–	140.8
3′ (R^2)	–	–	–	–	–	–	1.16	19.4	1.13	19.4	7.17	127.0	7.24	126.8
4′ (R^2)	–	–	–	–	–	–	0.83	13.9	0.72	13.9	7.25	128.1	7.20	128.2
5′ (R^2)	–	–	–	–	–	–	–	–	–	–	7.21	126.4	7.20	126.3
1′ (R^3)	3.73, 3.22	48.1	–	143.6	3.59, 3.52	48.2	3.58, 3.51	48.1	3.72, 3.24	48.4	3.76, 3.28	48.6	–	143.7
2′ (R^3)	1.36, 1.18	30.8	7.27	124.0	1.39	30.5	1.39	31.0	1.35, 1.26	31.0	1.39, 1.27	31.0	7.30	123.8
3′ (R^3)	1.14	19.7	7.21	128.2	1.28	19.8	1.28	19.7	1.13	19.9	1.16	19.9	7.11	128.0
4′ (R^3)	0.73	13.8	7.24	122.5	0.87	13.9	0.85	13.8	0.80	13.9	0.73	13.9	7.23	122.5

$[M-H]^-$), 241 (3, $[M-H-PhNHCOH]^-$). APCI-MS/MS (neg.) of *m/z* 342: 285 (19, $[M-H-Bu]^-$), 243 (100, $[M-H-PhNCO]^-$), 186 (94, $[M-H-PhNCO-Bu]^-$), 143 (7, $[M-H-PhNCO-Bu-NHCO]^-$). Anal. calc. for $C_{21}H_{33}N_3O$ (343.51): C 73.43, H 9.68, N 12.23; found: C 73.31, H 9.75, N 12.13.

2.8. *3-Butyl-1-(2-butyl-1*H*-indol-3-yl)-1-phenylurea* (**4h**). Prepared from **1h** (*Method A*), **3h** (*Method B*, besides **5h**), and **6h** (*Method D*). Colorless crystals. M.p. 166–169° (benzene/hexane), identical in all respects to authentic **4h** of m.p. 168–171°, prepared from **3h** [9].

2.9. *3-Benzyl-1-butyl-1-(2-butyl-1*H*-indol-3-yl)urea* (**4i**). Prepared from **6i** (*Method D*). Colorless crystals. M.p. 135–140° (benzene/hexane), identical in all respects to authentic **4i** of m.p. 137–142°, prepared from **3i** [9].

2.10. *3-Benzyl-1-(2-butyl-1*H*-indol-3-yl)-1-phenylurea* (**4j**). Prepared from **6j** (*Method D*). Colorless crystals. M.p. 152–156° (cyclohexane), identical in all respects to authentic **4j** of m.p. 153–157°, prepared from **3j** [9].

2.11. *1,3-Dibutyl-1-(2-phenyl-1*H*-indol-3-yl)urea* (**4k**). Prepared from **3k** (*Method E*) and from **6k** (*Method D*, besides **8k** and unreacted **6k**). Colorless crystals. M.p. 150–153° (benzene/hexane). IR: 3426, 3185, 2956, 2929, 2870, 1632, 1585, 1518, 1455, 1383, 1335, 1285, 1227, 1147, 1113, 1032, 1007, 916, 764, 744, 695, 633, 613, 563. ^{1}H- and ^{13}C-NMR: see *Table 3*. APCI-MS (pos.): 364 (100, $[M+H]^+$), 291 (10, $[M+H-BuNH_2]^+$). APCI-MS/MS (pos.) of *m/z* 364: 291 (100, $[M+H-BuNH_2]^+$), 265 (51, $[M+H-BuNCO]^+$), 235 (9, $[M+H-BuNH_2-butene]^+$). APCI-MS (neg.): 362 (100, $[M-H]^-$), 261 (4, $[M-H-BuNHCOH]^-$). APCI-MS/MS (neg.) of *m/z* 362: 305 (12, $[M-H-Bu]^-$), 263 (52, $[M-H-BuNCO]^-$), 206 (100, $[M-H-BuNCO-Bu]^-$). Anal. calc. for $C_{23}H_{29}N_3O$ (363.50): C 76.00, H 8.04, N 11.56; found: C 75.88, H 8.15, N 11.39.

2.12. *4-(2-Acetamidophenyl)-1,3-dibutyl-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one* (= N-*[2-(1,3-Dibutyl-2-oxo-5-phenyl-2,3-dihydro-1*H*-imidazol-4-yl)phenyl]acetamide*; **8k**). Prepared from **6k** (*Method D*, besides **4k** and unreacted **6k**). Colorless crystals. M.p. 135–137° (hexane). IR: 3290, 3074, 2956, 2936, 2871, 1679, 1604, 1580, 1526, 1454, 1443, 1406, 1372, 1296, 1257, 1209, 1115, 1074, 1009, 944, 869, 769, 760, 703, 677, 649, 597, 550, 535. ^{1}H- and ^{13}C-NMR: see *Table 4*. APCI-MS (pos.): 406 (100, $[M+H]^+$), 364 (3, $[M+H-NCO]^+$). APCI-MS/MS (pos.) of *m/z* 406: 364 (100, $[M+H-NCO]^+$), 332 (7, $[M+H-butene]^+$), 307 (15, $[M+H-NCO-Bu]^+$), 291 (11, $[M+H-NCO-BuNH_2]^+$), 265 (42, $[M+H-NCO-BuNCO]^+$). APCI-MS (neg.): 404 (100, $[M-H]^-$). APCI-MS/MS (neg.) of *m/z* 404: 362 (5, $[M-H-NCO]^-$), 348 (32, $[M-H-butene]^-$), 306 (100, $[M-H-butene-NCO]^-$), 263 (16, $[M-H-NCO-BuNCO]^-$), 206 (8, $[M-H-NCO-BuNCO-Bu]^-$). Anal. calc. for $C_{25}H_{31}N_3O_2$ (405.53): C 74.04, H 7.70, N 10.36; found: C 74.18, H 7.56, 10.29.

2.13. *3-Butyl-1-phenyl-1-(2-phenyl-1*H*-indol-3-yl)urea* (**4l**). Prepared from **1l** (*Method A*) and from **6l** (*Method D*). Colorless crystals. M.p. 230–232° (AcOH), identical in all respects to authentic **4l** of m.p. 226–230°, prepared from **3l** [9]. Two side products were isolated besides **4l** from the reaction of **1l** with diphenylurea: compound of m.p. 224–229° (benzene/hexane), identical in all respects to synthetic **7l** (*Section 6.2*) and compound of m.p. 260–265°, identical in all respects to authentic **5l**, prepared from **3l** [9].

2.14. *3-Benzyl-1-butyl-1-(2-phenyl-1*H*-indol-3-yl)urea* (**4m**). Prepared from **3m** (*Method E*, besides **6m** and **8m** and *Method B*, besides **5m** and **6m**) and from **6m** (*Method D*, besides **6m** and **8m**). Colorless crystals. M.p. 164–166° (benzene/hexane). IR: 3419, 3061, 2955, 2928, 2969, 1638, 1603, 1584, 1512, 1452, 1418, 1383, 1333, 1296, 1227, 1167, 1113, 1027, 965, 827, 763, 738, 719, 693, 612, 563. ^{1}H- and ^{13}C-NMR: see *Table 3*. APCI-MS (pos.): 398 (100, $[M+H]^+$), 381 (3, $[M+H-NH_3]^+$), 291 (25, $[M+H-NH_3-MeC_6H_3]^+$). APCI-MS/MS (pos.) of *m/z* 398: 381 (33, $[M+H-NH_3]^+$), 291 (100, $[M+H-NH_3-MeC_6H_3]^+$), 235 (17, $[M+H-NH_3-MeC_6H_3-butene]^+$), 193 (4, $[M+H-NH_3-MeC_6H_3-butene-NCO]^+$). APCI-MS (neg.): 396 (100, $[M-H]^-$), 261 (9, $[M-H-C_6H_6-Bu]^-$), 233 (7, $[M-H-C_6H_6-Bu-CO]^-$). APCI-MS/MS (neg.) of *m/z* 396: 339 (17, $[M-H-Bu]^-$), 295 (18, $[M-H-BuNHCOH]^-$), 263 (77, $[M-H-Bu-C_6H_6]^-$), 206 (100, $[M-H-2\,Bu-C_6H_6]^-$). Anal. calc. for $C_{26}H_{27}N_3O$ (397.51): C 78.56, H 6.85, N 10.57; found: C 78.41, H 6.94, N 10.41.

2.15. *4-(2-Acetamidophenyl)-1-benzyl-3-butyl-5-phenyl-1,3-dihydro-2*H*-imidazol-2-one* (= N-*[2-(1-Benzyl-3-butyl-2-oxo-5-phenyl-2,3-dihydro-1*H*-imidazol-4-yl)phenyl]acetamide*; **8m**). Prepared from **6m** (*Method D*, besides **4m** and **6m**). Colorless crystals. M.p. 120–121° (hexane). IR: 3410, 3315, 3063, 3032,

Table 4. *^{1}H- and ^{13}C-Chemical Shifts* (δ [ppm]) *of Compounds* **7** *and* **8** *in (D$_6$)DMSO*

Position	**7f**		**7l**		**8k**		**8m**		**8n**	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
2	–	152.5	–	152.2	–	152.9	–	153.1	–	152.5
4	–	113.9	–	115.8	–	116.5	–	117.3	–	117.0
5	–	122.7	–	123.0	–	121.1	–	121.2	–	122.4
1′	–	118.2	–	117.8	–	121.1	–	121.4	–	120.4
2′	–	138.9	–	138.8	–	137.8	–	137.9	–	137.9
3′	8.06	119.6	7.90	119.6	7.79	123.7	7.76	124.0	7.66	122.9
4′	7.27	129.1	7.21	129.1	7.35	129.4	7.35	129.1	7.17	129.3
5′	6.95	121.8	6.85	121.6	7.12	124.0	7.14	124.2	6.91	123.5
6′	7.11	132.0	7.13	132.5	7.24	132.4	7.26	132.4	7.03	132.1
1′ (R^1)	2.42	22.8	–	128.8	–	129.0	–	129.1	–	128.9
2′ (R^1)	1.50	30.1	[a])	129.4	7.29	127.2	7.12	126.5	[b])	[b])
3′ (R^1)	1.23	21.6	[a])	128.5	7.34	128.4	7.32	128.4	[b])	[b])
4′ (R^1)	0.74	13.4	[a])	128.5	7.34	127.9	7.24	127.0	[b])	[b])
1′ (R^2)	3.34	27.7	3.86, 3.60	40.1	3.73, 3.60	40.7[c])	4.97, 4.78	44.5	5.02, 4.84	44.7
2′ (R^2)	–	–	1.52	30.9	1.38	30.8[c])	–	138.2	–	137.9
3′ (R^2)	–	–	1.23	19.4	1.15	19.2[c])	7.23	128.2	[b])	[b])
4′ (R^2)	–	–	0.81	13.5	[d])	13.4[c])	7.18	128.4	[b])	[b])
5′ (R^2)	–	–	–	–	–	–	7.23	127.9	[b])	[b])
1′ (R^3)	–	135.4	–	135.2	3.56, 3.31	40.7[c])	3.62, 3.32	41.0	–	135.5
2′ (R^3)	7.12	126.4	[a])	126.8	1.38	30.8[c])	1.41	30.8	[b])	[b])
3′ (R^3)	7.23	128.4	[a])	128.5	1.15	19.2[c])	1.14	19.2	[b])	[b])
4′ (R^3)	7.16	126.5	[a])	126.9	[d])	13.4[c])	0.75	13.4	[b])	[b])
C(2′)–NHCO	9.14	152.1	9.03	151.9	8.96	168.3	9.10	168.3	9.09	167.6
N*H*Ph	7.85		7.84							
NH*Ph* or NH*Me*	–	139.6	–	139.6	1.96	23.6	1.98	23.6	1.86	23.7
	7.44	118.3	7.42	118.5						
	7.29	128.9	7.33	128.9						
	7.02	122.0	7.03	122.0						

[a]) Strong overlap of ^{1}H resonances ($\delta(^1H) = 7.16–7.35$). [b]) Strong overlap of ^{1}H and ^{13}C resonances of three Ph groups, $\delta(^1H) = 7.16–7.36$ (*m*, 15 H), $\delta(^{13}C) = 129.9$, 128.5, 128.4, 127.0, 126.9, 126.7. [c]) ^{13}C Resonances of appropriate pairs in two Bu group signals differ maximally in 0.04 ppm. [d]) $\delta(^1H) = 0.77$ or 0.72.

2957, 2930, 2871, 1678, 1606, 1580, 1530, 1497, 1451, 1402, 1368, 1299, 1252, 1209, 1030, 975, 941, 764, 752, 724, 701, 659, 598, 550. ^{1}H- and ^{13}C-NMR: see *Table 4*. APCI-MS (pos.): 440 (100, $[M + H]^+$). APCI-MS/MS (pos.) of *m/z* 440: 422 (10, $[M + H - H_2O]^+$), 398 (9, $[M + H - NCO]^+$), 349 (100, $[M + H - MeC_6H_4]^+$), 332 (6, $[M + H - MeC_6H_4 - NH_3]^+$), 307 (21, $[M + H - MeC_6H_4 - NCO]^+$). APCI-MS (neg.): 438 (100, $[M - H]^-$). APCI-MS/MS (neg.) of *m/z* 438: 382 (5, $[M - H - Bu]^-$), 347 (43, $[M - H - MeC_6H_5]^+$), 304 (100, $[M - H - MeC_6H_5 - NHCO]^+$), 291 (4, $[M - H - MeC_6H_5 - butene]^+$), 262 (5, $[M - H - MeC_6H_5 - NCO]^+$). Anal. calc. for $C_{28}H_{29}N_3O_2$ (439.55): C 76.51, H 6.65, N 9.56; found: C 76.35, H 6.69, N 9.39.

2.16. *3-Benzyl-1-phenyl-1-(2-phenyl-1*H*-indol-3-yl)urea* (**4n**). Prepared from **3n** (*Method B*, besides **5n** and **6n** or *Method E*), and from **6n** (*Method D*, besides **8n** and **6n**). Colorless crystals. M.p. 222–224° (benzene/hexane). IR: 3427, 3342, 3061, 3027, 2949, 1669, 1620, 1584, 1512, 1491, 1454, 1374, 1321, 1284, 1244, 1151, 1113, 1075, 1028, 918, 741, 696, 632, 562, 517. ^{1}H- and ^{13}C-NMR: see *Table 3*. APCI-MS

(pos.): 418 (100, $[M+H]^+$), 401 (3, $[M+H-NH_3]^+$), 311 (11, $[M+H-NH_3-MeC_6H_3]^+$), 283 (51, $[M+H-NH_3-MeC_6H_3-CO]^+$). APCI-MS/MS (pos.) of *m/z* 418: 401 (52, $[M+H-NH_3]^+$), 375 (8, $[M+H-NHCO]^+$), 311 (100, $[M+H-NH_3-MeC_6H_3]^+$), 285 (54, $[M+H-C_6H_5CH_2NCO]^+$). APCI-MS (neg.): 416 (100, $[M-H]^-$), 282 (41, $[M-H-Ph-Bu]^-$), 255 (3, $[M-H-Ph-Bu-HCN]^-$). APCI-MS/MS (neg.) of *m/z* 416: 283 (100, $[M-H-Ph-butene]^-$). Anal. calc. for $C_{28}H_{23}N_3O$ (417.50): C 80.55, H 5.55, N 10.06; found: C 80.42, H 5.67, N 10.11.

2.17. *4-(2-Acetamidophenyl)-1-benzyl-3,5-diphenyl-1,3-dihydro-2*H-*imidazol-2-one* (= N-*[2-(1-Benzyl-2-oxo-3,5-diphenyl-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]acetamide*; **8n**). Prepared from **6n** (*Method D*, besides **4n** and **6n**). Colorless crystals. M.p. 237–241° (benzene/hexane). IR: 3341, 3335, 3061, 2953, 1677, 1595, 1579, 1520, 1493, 1453, 1383, 1296, 1253, 1231, 1158, 1125, 1042, 1015, 957, 887, 820, 781, 763, 747, 736, 710, 700, 651, 592, 519, 502. ^{1}H- and ^{13}C-NMR: see *Table 4*. APCI-MS (pos.): 460 (100, $[M+H]^+$), 416 (15, $[M+H-NCO]^+$). APCI-MS/MS (pos.) of *m/z* 460: 442 (50, $[M+H-H_2O]^+$), 418 (32, $[M+H-NCO]^+$), 401 (9, $[M+H-NCO-NH_3]^+$), 369 (100, $[M+H-MeC_6H_4]^+$), 352 (12, $[M+H-MeC_6H_4-NH_3]^+$), 327 (48, $[M+H-MeC_6H_4-NCO]^+$), 309 (11, $[M+H-MeC_6H_4-NCO-H_2O]^+$). APCI-MS (neg.): 458 (100, $[M-H]^-$), 416 (5, $[M-H-NCO]^-$). APCI-MS/MS (neg.) of *m/z* 458: 416 (12, $[M-H-NCO]^-$), 325 (55, $[M-H-C_6H_5CH_2NCO]^-$), 282 (100, $[M-H-C_6H_5CH_2NCO-NCO]^-$). Anal. calc. for $C_{30}H_{25}N_3O_2$ (459.54): C 78.41, H 5.48, N 9.14; found: C 78.29, H 5.62, N 9.09.

3. *General Procedure for the Preparation of 4-(2-Aminophenyl)-1,3-dihydro-2*H-*imidazol-2-ones* (**6**) *from Compounds* **2**, **3**, **4**, *and* **8** (*Method C*). A soln. of respective starting compound **2**, **3**, **4**, and **8** (2.5 mmol) in conc. HCl (25 ml) was heated to reflux for the time given in *Table 2*. If necessary, AcOH was added to dissolve poorly soluble starting compound. After cooling, the soln. was evaporated *in vacuo* to dryness. The residue was dissolved in pyridine (5 ml), anh. K_2CO_3 (350 mg) was added and the mixture was stirred for 1 h. The insoluble material was filtered off, the filtrate was evaporated to dryness, and the residue was crystallized from an appropriate solvent or separated by CC on silica gel.

3.1. *5-(2-Aminophenyl)-1,4-dibutyl-1,3-dihydro-2*H-*imidazol-2-one* (**6a**). Prepared from **2a** and **3a**. Colorless crystals. M.p. 134–139° (benzene/cyclohexane), identical in all respects to authentic **6a** of m.p. 135–140°, prepared from **4a** [9].

3.2. *5-(2-Aminophenyl)-4-butyl-1-phenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6b**). Prepared from **2b**. Colorless crystals. M.p. 134–140° (without recrystallization), identical in all respects to authentic **6b** of m.p. 138–141°, prepared from **4b** [9].

3.3. *5-(2-Aminophenyl)-1-butyl-4-phenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6c**). Prepared from **2c**, **3c**, and **4c**. Colorless crystals. M.p. 167–169° (benzene/hexane). IR: 3457, 3345, 3142, 3057, 2959, 2933, 2871, 1675, 1615, 1604, 1574, 1506, 1490, 1453, 1403, 1376, 1361, 1310, 1264, 1158, 1115, 1077, 1031, 969, 935, 908, 751, 693, 665, 520, 498. ^{1}H- and ^{13}C-NMR: see *Table 5*. APCI-MS (pos.): 308 (100, $[M+H]^+$), 291 (59, $[M+H-NH_3]^+$), 263 (28, $[M+H-COOH]^+$). APCI-MS/MS (pos.) of *m/z* 308: 291 (100, $[M+H-NH_3]^+$), 265 (15, $[M+H-NHCO]^+$), 252 (21, $[M+H-butene]^+$), 235 (22, $[M+H-NH_3-butene]^+$), 209 (29, $[M+H-BuNCO]^+$). APCI-MS (neg.): 306 (100, $[M-H]^-$), 261 (11, $[M-H-COOH]^-$), 233 (4, $[M-H-BuNH_2]^-$). APCI-MS/MS (neg.) of *m/z* 306: 263 (82, $[M-H-NHCO]^-$), 249 (92, $[M-H-Bu]^-$), 206 (100, $[M-H-Bu-NHCO]^-$). Anal. calc. for $C_{19}H_{21}N_3O$ (307.39): C 74.24, H 6.89, N 13.67; found: C 74.29, H 6.98, N 13.53.

3.4. *5-(2-Aminophenyl)-1,4-diphenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6d**). Prepared from **2d** and **4d**. Colorless crystals. M.p. 297–309° (benzene/dioxane). IR: 3432, 3333, 3134, 3061, 3030, 2978, 2878, 2762, 1674, 1622, 1596, 1492, 1454, 1392, 1309, 1256, 1151, 1072, 1030, 915, 853, 776, 764, 747, 709, 693, 664, 649, 549, 504. ^{1}H- and ^{13}C-NMR: see *Table 5*. APCI-MS (pos.): 328 (100, $[M+H]^+$), 311 (4, $[M+H-NH_3]^+$), 283 (99, $[M+H-COOH]^+$), 208 (3, $[M+H-COOH-C_6H_3]^+$). APCI-MS/MS (pos.) of *m/z* 328: 311 (82, $[M+H-NH_3]^+$), 285 (78, $[M+H-NHCO]^+$), 235 (48, $[M+H-NH_3-C_6H_4]^+$), 209 (100, $[M+H-NHCO-C_6H_4]^+$), 182 (51, $[M+H-NHCO-C_6H_4\text{-}HCN]^+$). APCI-MS (neg.): 326 (66, $[M-H]^-$), 282 (100, $[M-H-NH_2CO]^-$), 255 (31, $[M-H-NH_2CO-HCN]^-$). APCI-MS/MS (neg.) of *m/z* 326: 283 (100, $[M-H-NHCO]^-$). Anal. calc. for $C_{21}H_{17}N_3O$ (327.38): C 77.04, H 5.23, N 12.84; found: C 76.85, H 5.35, N 12.71.

3.5. *4-(2-Aminophenyl)-3,5-dibutyl-1-methyl-1,3-dihydro-2*H-*imidazol-2-one* (**6e**). Prepared from **3e** and **4e**. Colorless crystals. M.p. 74–78° (hexane). IR: 3401, 3337, 3226, 3028, 2957, 2931, 2866, 1668, 1632,

Table 5. *^{1}H- and ^{13}C-Chemical Shifts* (δ [ppm]) *of Compounds* **6** *in (D_6)DMSO*[a])

Position	**6c**		**6d**		**6e**		**6g**		**6k**		**6m**		**6n**	
	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C	δ_H	δ_C
1	10.72	–	11.00	–	–	–	–	–	–	–	–	–	–	–
2	–	153.5	–	153.0	–	153.1	–	152.9	–	152.9	–	153.2	–	152.7
4	–	117.8	–	117.9	–	115.4	–	115.6	–	117.7	–	118.2	–	118.0
5	–	117.3	–	118.6	–	119.8	–	119.3	–	120.6	–	120.8	–	122.2
1′	–	113.2	–	113.3	–	112.8	–	113.0	–	112.7	–	112.4	–	112.5
2′	–	148.1	–	148.2	–	148.0	–	147.8	–	148.3	–	148.3	–	148.1
3′	6.82	114.8	6.65	114.5	6.76	114.5	6.76	114.5	6.68	114.5	6.70	114.5	6.50	114.3
4′	7.21	130.3	7.34	130.0	7.14	129.6	7.13	129.6	7.07	128.9	7.08	129.9	6.92	128.4
5′	6.55	116.1	6.45	115.8	6.61	115.7	6.62	115.8	6.52	115.7	6.52	115.7	6.37	115.4
6′	7.03	132.1	7.04	132.3	6.96	132.1	6.97	132.1	6.97	132.7	6.98	132.7	6.96	132.8
NH_2	5.05	–	5.18	–	4.91	–	4.86	–	4.97	–	5.05	–	5.08	–
1′ (R^1)	–	130.2	–	130.0	2.32, 2.23	22.8	2.33, 2.25	22.7	–	129.8	–	129.4	–	129.1
2′ (R^1)	7.26	124.4	7.28	124.9	1.40	30.6	[b])	[b])	7.33	128.3	7.11	126.6	[c])	[c])
3′ (R^1)	7.22	128.3	7.27	128.4	1.27	21.5	[b])	[b])	7.33	129.5	7.31	128.4	[c])	[c])
4′ (R^1)	7.13	126.0	7.22	126.6	0.78	13.5	[d])	[d])	7.30	127.7	7.25	127.7	[c])	[c])
1′ (R^2)	–	–	–	–	3.19	27.2	3.58	40.5	3.67, 3.60	40.7	4.93, 4.78	44.6	4.99, 4.82	44.8
2′ (R^2)	–	–	–	–	–	–	1.62	[b])	1.38	30.9	–	138.4	–	138.0
3′ (R^2)	–	–	–	–	–	–	[b])	[b])	1.15	19.2	7.23	128.2	[c])	[c])
4′ (R^2)	–	–	–	–	–	–	[d])	[d])	0.76	13.4	7.18	129.5	[c])	[c])
5′ (R^2)	–	–	–	–	–	–	–	–	–	–	7.23	127.0	[c])	[c])
1′ (R^3)	3.44, 3.26	39.9	–	135.5	3.44, 3.27	40.4	3.44, 3.26	40.3	3.55, 3.30	40.5	3.62, 3.34	42.4	–	135.6
2′ (R^3)	1.37	30.9	7.35	127.4	1.31	30.9	[b])	[b])	1.38	30.9	1.41	31.0	[c])	[c])
3′ (R^3)	1.15	19.3	7.27	128.2	1.09	19.2	[b])	[b])	1.15	19.2	1.16	19.3	[c])	[c])
4′ (R^3)	0.76	13.4	7.19	126.5	0.72	13.4	[d])	[d])	0.76	13.4	0.78	13.5	[c])	[c])

[a]) Numbering as indicated in *Scheme 1*. This numbering does not match with the systematic names given in the *Exper. Part* for compounds **6c** and **6d**. [b]) Strong overlap of ^{1}H resonances of CH_2 groups, $\delta(^1H) = 1.07–1.40$ (*m*, 10 H), $\delta(^{13}C) = 31.1, 30.9, 21.6, 19.6, 19.5$. [c]) Strong overlap of ^{1}H resonances of three Ph groups, $\delta(^1H) = 7.16–7.36$ (*m*, 15 H), $\delta(^{13}C) = 129.6$ (2 C), 128.4 (2 C), 128.3 (2 C), 128.2 (2 C), 128.1, 127.0, 126.9 (2 C), 126.8 (2 C), 125.7. [d]) Resonances of three Me groups: $\delta(^1H) = 0.96$, 0.77 and 0.74, $\delta(^{13}C) = 13.8$, 13.5 and 13.4.

1567, 1493, 1457, 1401, 1370, 1317, 1265, 1152, 1081, 1023, 950, 940, 825, 749, 656, 599, 552. ^{1}H- and ^{13}C-NMR: see *Table 5*. APCI-MS (pos.): 302 (100, $[M + H]^+$), 256 (7, $[M + H - HCOOH]^+$). APCI-MS/MS (pos.) of *m/z* 302: 284 (10, $[M + H - H_2O]^+$), 258 (100, $[M + H - NH_2CO]^+$), 246 (98, $[M + H - butene]^+$), 201 (85, $[M + H - NH_2CO - Bu]^+$), 189 (78, $[M + H - butene - Bu]^+$), 172 (97, $[M + H - butene - Bu - NH_3]^+$). APCI-MS (neg.): 300 (100, $[M - H]^-$). APCI-MS/MS (neg.) of *m/z* 300: 257 (3, $[M - H - NHCO]^-$), 243 (100, $[M - H - Bu]^-$), 199 (13, $[M - H - Bu - NH_2CO]^-$), 186 (15, $[M - H - 2\ Bu]^-$). Anal. calc. for $C_{18}H_{27}N_3O$ (301.43): C 71.72, H 9.03, N 13.94; found: C 71.52, H 9.14, N 13.87.

3.6. *4-(2-Aminophenyl)-5-butyl-1-methyl-3-phenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6f**). Prepared from **3f**. Colorless crystals. M.p. 155–160° (benzene/hexane), identical in all respects to authentic **6f** of m.p. 154–162°, prepared from **4f** [9].

3.7. *4-(2-Aminophenyl)-1,3,5-tributyl-1,3-dihydro-2*H-*imidazol-2-one* (**6g**). Prepared from **3g** and **4g**. Yellowish oil. IR: 3464, 3331, 2957, 2932, 2871, 1676, 1640, 1573, 1494, 1457, 1412, 1368, 1310, 1260, 1157, 1112, 939, 749, 653, 555. ^{1}H- and ^{13}C-NMR: see *Table 5*. APCI-MS (pos.): 344 (100, $[M + H]^+$), 298 (41, $[M + H - HCOOH]^+$), 271 (6, $[M + H - BuNH_2]^+$), 243 (9, $[M + H - BuNHCOH]^+$). APCI-MS/MS (pos.) of *m/z* 344: 300 (4, $[M + H - NH_2CO]^+$), 288 (4, $[M + H - butene]^+$), 271 (20, $[M + H - BuNH_2]^+$), 243 (100, $[M + H - BuNHCOH]^+$). APCI-MS (neg.): 342 (100, $[M - H]^-$), 312 (18, $[M - H - CH_2O]^-$), 241 (11, $[M - H - BuNHCOH]^-$). APCI-MS/MS (neg.) of *m/z* 342: 285 (12, $[M - H - Bu]^-$), 243 (100, $[M - H - BuNCO]^-$), 186 (92, $[M - H - BuNCO - Bu]^-$). Anal. calc. for $C_{21}H_{33}N_3O$ (343.51): C 73.43, H 9.68, N 12.23; found: C 73.52, H 9.59, N 12.37.

3.8. *4-(2-Aminophenyl)-1,5-dibutyl-3-phenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6h**). Prepared from **3h**. Colorless crystals. M.p. 115–121° (benzene/hexane), identical in all respects to authentic **3h** of m.p. 115–122°, prepared from **4h** [9].

3.9. *4-(2-Aminophenyl)-1-benzyl-3,5-dibutyl-1,3-dihydro-2*H-*imidazol-2-one* (**6i**). Prepared from **3i**. Colorless crystals. M.p. 98–104° (hexane), identical in all respects to authentic **6i** of m.p. 98–105°, prepared from **4i** [9].

3.10. *4-(2-Aminophenyl)-1-benzyl-5-butyl-3-phenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6j**). Prepared from **3j**. Colorless crystals. M.p. 87–93° (hexane), identical in all respects to authentic **6j** of m.p. 88–94°, prepared from **4j** [9].

3.11. *4-(2-Aminophenyl)-1,3-dibutyl-5-phenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6k**). Prepared from **3k**, **4k**, and **8k**. Colorless crystals. M.p. 77–81° (hexane). IR: 3466, 3424, 3336, 3229, 3059, 2953, 2930, 2867, 1663, 1625, 1602, 1573, 1491, 1457, 1406, 1366, 1312, 1262, 1209, 1159, 1114, 1077, 1027, 938, 805, 749, 701, 664, 651, 624, 550, 513. ^{1}H- and ^{13}C-NMR: see *Table 5*. APCI-MS (pos.): 364 (100, $[M + H]^+$), 318 (15, $[M + H - HCOOH]^+$), 263 (10, $[M + H - BuNHCOH]^+$). APCI-MS/MS (pos.) of *m/z* 364: 346 (8, $[M + H - H_2O]^+$), 308 (38, $[M + H - butene]^+$), 291 (9, $[M + H - BuNH_2]^+$), 263 (100, $[M + H - BuNHCOH]^+$). APCI-MS (neg.): 362 (100, $[M - H]^-$), 206 (26, $[M - H - BuNCO - Bu]^-$). APCI-MS/MS (neg.) of *m/z* 362: 306 (45, $[M - H - butene]^-$), 263 (100, $[M - H - BuNCO]^-$), 206 (71, $[M - H - BuNCO - Bu]^-$). Anal. calc. for $C_{23}H_{29}N_3O$ (363.50): C 76.00, H 8.04, N 11.56; found: C 75.87, H 7.87, N 11.42.

3.12. *4-(2-Aminophenyl)-1-butyl-3,5-diphenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6l**). Compound was prepared from **3l**. Colorless crystals. M.p. 65–73° (without recrystallization), identical in all respects to authentic compound of m.p. 54–57°, prepared from **4l** [9].

3.13. *4-(2-Aminophenyl)-1-benzyl-3-butyl-5-phenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6m**). Prepared from **3m**, **4m**, and **8m**. Colorless crystals. M.p. 114–115° (benzene/hexane). IR: 3451, 3325, 3203, 3063, 3029, 2954, 2932, 2872, 1672, 1622, 1600, 1572, 1489, 1448, 1398, 1356, 1308, 1265, 1155, 1075, 1028, 951, 921, 775, 749, 702, 831, 577, 501. ^{1}H- and ^{13}C-NMR: see *Table 5*. APCI-MS (pos.): 398 (100, $[M + H]^+$), 352 (10, $[M + H - HCOOH]^+$). APCI-MS/MS (pos.) of *m/z* 398: 381 (25, $[M + H - NH_3]^+$), 355 (25, $[M + H - NHCO]^+$), 307 (100, $[M + H - MeC_6H_4]^+$), 263 (29, $[M + H - MeC_6H_4 - NH_2CO]^+$), 208 (33, $[M + H - MeC_6H_4 - BuNCO]^+$). APCI-MS (neg.): 396 (100, $[M - H]^-$). APCI-MS/MS (neg.) of *m/z* 396: 340 (31, $[M - H - butene]^-$), 263 (100, $[M - H - butene - C_6H_5]^-$), 219 (15, $[M - H - butene - C_6H_5 - NH_2CO]^-$), 206 (42, $[M - H - butene - C_6H_5Bu]^-$). Anal. calc. for $C_{26}H_{27}N_3O$ (397.51): C 78.56, H 6.85, N 10.57; found: C 78.41, H 6.94, N 10.39.

3.14. *4-(2-Aminophenyl)-1-benzyl-3,5-diphenyl-1,3-dihydro-2*H-*imidazol-2-one* (**6n**). Prepared from **3n**, **4n**, and **8n**. Colorless crystals. M.p. 209–212° (benzene/hexane). IR: 3465, 3366, 3061, 3028, 2926,

1687, 1615, 1600, 1572, 1498, 1453, 1427, 1386, 1370, 1310, 1241, 1157, 1130, 1072, 1026, 953, 917, 824, 784, 763, 745, 701, 660, 587, 544, 520. ^{1}H- and ^{13}C-NMR: see *Table 5*. APCI-MS (pos.): 418 (100, $[M + H]^+$), 373 (16, $[M + H-COOH]^+$). APCI-MS/MS (pos.) of *m/z* 418: 401 (11, $[M + H - H_2O]^+$), 375 (12, $[M + H-NHCO]^+$), 327 (100, $[M + H-MeC_6H_4]^+$), 283 (52, $[M + H-MeC_6H_4-NH_2CO]^+$). APCI-MS (neg.): 416 (100, $[M - H]^-$). APCI-MS/MS (neg.) of *m/z* 416: 325 (100, $[M - H-MeC_6H_4]^-$), 283 (48, $[M - H-MeC_6H_4-NH_2CO]^-$). Anal. calc. for $C_{28}H_{23}N_3O$ (417.50): C 80.55, H 5.55, N 10.06; found: C 80.41, H 5.67, 10.12.

4. *General Procedure for the Preparation of 4-(2-Acetamidophenyl)-5-phenyl-1,3-dihydro-2*H-*imidazol-2-ones* (**8**). A mixture of **6** (0.1 mmol), Ac_2O (1 ml), and pyridine (1 ml) was left at r.t. for 4 h, evaporated to dryness *in vacuo*, and the residue was crystallized from an appropriate solvent. The following compounds **8**, identical in all respects to those described in *Sect. 3.2*, were prepared: **8k** (86% yield), **8m** (92 % yield), and **8n** (96% yield).

5. *General Procedure for the Preparation of 1,3-Bis[2-(2-oxo-2,3-dihydro-1*H-*imidazol-4-yl)-phenyl]ureas* (**5**). Compounds **5c**, **5e**, **5g**, **5k**, **5m**, and **5n** were prepared from the corresponding compounds **6** and triphosgene according to the same procedure as was reported for preparation of compounds **5a**, **5f**, **5h**, **5i**, **5j**, and **5l** [9].

5.1. *1,3-Bis[2-(3-butyl-2-oxo-5-phenyl-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]urea* (**5c**). Prepared from **6c** in 12% yield. Colorless crystals. M.p. 176–186° (AcOEt/hexane), identical in all respects to authentic **6c** of m.p. 173–179°, prepared from **3c** [9].

5.2. *1,3-Bis[2-(3,5-dibutyl-1-methyl-2-oxo-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]urea* (**5e**). Prepared from **6e** in 18% yield. Yellowish oil, identical in all respects to authentic **5e** prepared from **3e** [9].

5.3. *1,3-Bis[2-(1,3,5-tributyl-2-oxo-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]urea* (**5g**). Prepared from **6g** in 55% yield. Yellowish oil, identical in all respects to authentic **5g** prepared from **3g** [9].

5.4. *1,3-Bis[2-(1,3-dibutyl-2-oxo-5-phenyl-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]urea* (**5k**). Prepared from **6k** in 65% yield. Colorless crystals. M.p. 173–176° (hexane), identical in all respects to authentic **5k** of m.p. 154–164°, prepared from **3k** [9].

5.5. *1,3-Bis[2-(1-benzyl-3-butyl-2-oxo-5-phenyl-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]urea* (**5m**). Prepared from **6m** in 68% yield. Colorless crystals. M.p. 94–98° (hexane), identical in all respects to authentic **5m** of m.p. 95–100°, prepared from **3m** [9].

5.6. *1,3-Bis[2-(1-benzyl-2-oxo-3,5-diphenyl-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]urea* (**5n**). Prepared from **6n** in 78% yield. Colorless crystals. M.p. 242–248°, identical in all respects to authentic **5n** of m.p. 227–232°, prepared from **3n** [9].

6. *General Procedure for the Preparation of Ureas* **7** *from Dihydroimidazolones* **6**. Phenylisocyanate (0.03 ml, 0.28 mmol) was added under stirring at r.t. to the soln. of **6** (0.25 mmol) in $CHCl_3$ (2 ml). The mixture was stirred for 2.5 h at r.t., evaporated *in vacuo* to dryness, and the residue was crystallized from benzene/hexane (1:1, *v/v*).

6.1. *1-[2-(5-Butyl-1-methyl-2-oxo-3-phenyl-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]-3-phenylurea* (**7f**). Prepared from **6f** in 91% yield. Colorless crystals. M.p. 235–237° (benzene/hexane). IR: 3335, 3298, 2957, 2932, 2868, 1709, 1670, 1645, 1600, 1584, 1554, 1530, 1500, 1443, 1396, 1294, 1259, 1229, 1198, 889, 753, 684, 633, 535, 506. ^{1}H- and ^{13}C-NMR: see *Table 4*. APCI-MS (pos.): 441 (100, $[M + H]^+$), 348 (38, $[M + H-PhNH_2]^+$), 322 (37, $[M + H-PhNCO]^+$). APCI-MS/MS (pos.) of *m/z* 441: 397 (13, $[M + H-NH_2CO]^+$), 348 (37, $[M + H-PhNH_2]^+$), 322 (98, $[M + H-PhNCO]^+$), 265 (21, $[M + H-PhNCO-Bu]^+$), 203 (7, $[M + H-2\,PhNCO]^+$), 172 (100, $[M + H-PhNCO-PhNH_2-Bu]^+$). APCI-MS (neg.): 439 (42, $[M - H]^-$), 346 (9, $[M - H-PhNH_2]^-$), 320 (100, $[M - H-PhNCO]^-$). APCI-MS/MS (neg.) of *m/z* 439: 320 (100, $[M - H-PhNCO]^-$). Anal. calc. for $C_{27}H_{28}N_4O_2$ (440.54): C 73.61, H 6.41, N 12.72; found: C 73.52, H 6.24, N 12.67.

6.2. *1-[2-(1-Butyl-2-oxo-3,5-diphenyl-2,3-dihydro-1*H-*imidazol-4-yl)phenyl]-3-phenylurea* (**7l**). Prepared from **6l** in 79% yield. Colorless crystals. M.p. 221–228° (benzene/hexane). IR: 3342, 3302, 3057, 2957, 2932, 2861, 1713, 1672, 1599, 1582, 1527, 1497, 1446, 1395, 1292, 1258, 1229, 1192, 1094, 755, 695, 656, 505. ^{1}H- and ^{13}C-NMR: see *Table 4*. APCI-MS (pos.): 503 (100, $[M + H]^+$), 410 (28, $[M + H-PhNH_2]^+$), 384 (31, $[M + H-PhNCO]^+$). APCI-MS/MS (pos.) of *m/z* 503: 410 (100, $[M + H-PhNH_2]^+$), 384 (52, $[M + H-PhNCO]^+$), 354 (9, $[M + H-PhNH_2-\text{butene}]^+$), 285 (25, $[M + H-PhNCO-BuNCO]^+$). APCI-MS (neg.): 501 ($[M - H]^-$), 382 ($[M - H-PhNCO]^-$). APCI-MS/

MS (neg.) of *m*/*z* 501: 382 (100, $[M-H-PhNCO]^-$). Anal. calc. for $C_{32}H_{30}N_4O_2$ (502.61): C 76.47, H 6.02, N 11.15; found: C 76.57, H 6.19, N 11.02.

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