HETEROCYCLIC DERIVATIVES OF PURINES.

5.* NUCLEOPHILIC SUBSTITUTION IN SERIES OF IMIDAZO[1,2-f]PURINE DERIVATIVES

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The chlorination of 1,8-dimethyl-7-phenylimidazo[1,2-f]xanthine with an equimolar amount of PCl_5 in $POCl_3$ leads to 2,4-dichloro-8-methyl-7-phenylimidazo[1,2-f]-purine. The possibility of substitution of the halogen atoms in reactions with nucleophilic reagents to give various 4-amino and 2,4-diamino derivatives was studied.

We have previously described [2] the synthesis and some properties of the new imidazo-[1,2-f]purine heterocyclic system. The subject of the present research is the further study of the chemical properties and reactivity of this system.

One might have assumed that halo-substituted imidazo[1,2-f]purines would behave like thiazolo[2,3-f]purine derivatives, which are their isoelectronic analogs [3], with respect to nucleophilic reagents.

1,8-Dimethyl-7-phenyl-2-chloroimidazo[1,2-f]purine-4-one (II) is formed when 1,8-dimethyl-7-phenylimidazo[1,2-f]xanthine (I) is heated in phosphorus oxychloride; this was confirmed by the results of elementary analysis and physicochemical studies. An absorption band of stretching vibrations of a carbonyl group attached to the $C_{(4)}$ atom at 1675 cm^{-1} is present in the IR spectrum of II.

The reaction of chloro derivative II with piperidine in refluxing n-propyl alcohol leads to 1,8-dimethyl-7-phenyl-2-N-piperidinoimidazo[1,2-f]purin-4-one (III). Absorption of a carbonyl group is observed in the IR spectrum of III at a higher frequency (1700 cm^{-1}) as compared with starting II.

When III is heated in concentrated hydrochloric acid, it readily undergoes hydrolysis to starting I, which can also be obtained by hydrolysis of II in a solution of alkali or even in water at pH 7.

A mixture of di- and trichloro-substituted derivatives of imidazo[1,2-f]purine is formed in the chlorination of I with excess PCl_5 in $POCl_3$ [2]; however, only 8-methyl-2,4-dichloro-7-phenylimidazo[1,2-f]purine (IV) is formed when a strictly equivalent amount of phosphorus pentachloride is used.

The reaction of IV with amines (usually a twofold excess) at 80-100°C always leads to 4-amino(alkylamino or cycloalkylamino)-2-chloroimidazo[1,2-f]purines (VII, IX, X, XIII). However, 2,4-dialkylaminoimidazo[1,2-f]purines (XIV-XVI) were isolated when the reaction was carried out with a fourfold to tenfold excess of the amine in a sealed ampul or autoclave at 200-210°C. Thus heating IV with a fourfold excess of diethylamine under the given conditions leads to 8-methyl-7-phenyl-2,4-bis(N,N'-diethylamino)imidazo[1,2-f]purine (XV).

A molecular-ion peak (M^+) with m/z 391 is present in the mass spectrum of XV. The presence of fragment ions with m/z 77 ($[C_6H_5]^+$), 102 ($[C_6H_5C{\equiv}CH]^+$), 103 ($[C_6H_5C{\equiv}N]^+$), and 118 ($C_6H_5C{\equiv}N^+{-}CH_3$]) proves the presence and location of substituents in the imidazole part of the molecule. The presence of diethylamino substituents in responsible for the characteristic (for them) elimination processes involving the splitting out of methyl and ethyl radicals in the first step of the fragmentation of the M^+ ions and methylene and ethylene radicals in the second step of the fragmentation (m/z values given): 376 $[M{-}CH_3]^+$, 362 $[M{-}C_2H_5]^+$, 348 $[(M{-}C_2H_5){-}CH_2]^+$, 334 $[(M{-}C_2H_5){-}C_2H_4)]^+$ (A), 320 $[A{-}CH_2]^+$, 305 $[A{-}C_2H_5]^+$, 291 $[(A{-}C_2H_5){-}CH_2]^+$ [4].

*See [1] for Communication 4.

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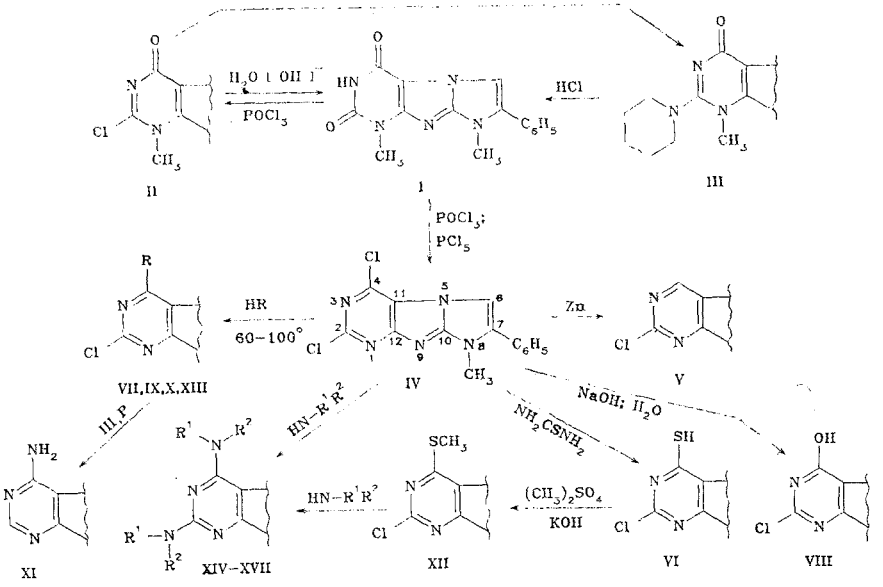
The UV spectrum of 5-alkylamino- and 5,7-bis(dialkylamino)imidazo[1,2-f]purines (VII, IX-XI, XIII, XVI) are characterized by the presence of two principal absorption maxima at 206-210 and 254-270 nm; this is characteristic for purine and its derivatives [5]. The presence of yet another absorption maximum in the long-wave region at 298-307 nm is extremely characteristic for 2,4-bis(dialkylamino) derivatives.

4-Mercapto- and 4-hydroxy-2-chloro-8-methyl-7-phenylimidazo[1,2-f]purines (VI, VIII), respectively, were obtained when IV was heated in alcohol or dioxane with thiourea or with aqueous alkali.

The alkylation of mercapto derivative VI with dimethyl sulfate leads to 4-dimethylmercapto derivative XII (see the scheme presented below). Simultaneous substitution of the methylmercapto group and the halogen atom by an amine residue to give the corresponding XIV-XVII occurs when XII is heated with secondary amines in an autoclave at 200-210°C.



VII R=N-piperidine ; IX R=$HNCH_2C_6H_5$; X R=NH_2; XIII R=$NHCH_3$; XIV $R^1=R^2=$ $=CH_3$; XV $R^1=R^2=C_2H_5$; XVI $R^1=H$, $R^2=CH_3$; XVII R^1, $R^2=-(CH_2)_5$

When IV is heated with an alcohol solution of ammonia or with ammonium carbonate in alcohol in a sealed ampul at 100-110°C, it is converted to 4-amino-2-chloro-8-methyl-7-phenylimidazo[1,2-f]purine (X), which is readily dehalogenated to give 8-methyl-7-phenylimidazo[1,2-f]-adenine (XI) when it is heated with concentrated hydriodic acid and red phosphorus. The following absorption bands are seen in the IR spectrum of XI: bands at 3375 and 3330 cm^{-1} (NH_2 and NH_2), a broad band at 3180 cm^{-1}, which constitutes evidence for the possibility of the existence of an imino form or an intermolecular hydrogen bond, a band at 3110 cm^{-1} (aromatic CH), and a band at 1655 cm^{-1} (primary amine NH) (scissors) [6].

A maximally intense M^+ peak with m/z 264, which corresponds to the molecular mass of the synthesized compound, is observed in the mass spectrum of X. The direct elimination of a CH_3 group from the M^+ ion indicates that it is attached to the N heteroatom in the imidazole (π-surplus) ring [7]. This fact is also confirmed by fragment ions with m/z 102 ($[HC\equiv C-C_6H_5]^+$), 103 ($[N\equiv C-C_6H_5]^+$), and 118 ($[CH_3-N=C-C_6H_5]^+$). The appearance of other fragment ions is associated with destruction of the pyrimidine ring in the investigated molecule: m/z 237 ($[M-HCN]^+$), 222 ($[M-NH_2CN]^+$) (ion A), and 195 ($[A-HCN]^+$). The high intensity of the peak of a doubly charged ion with m/z 132 emphasizes the aromatic character and the high π-donor character of the examined system. The action of zinc in acetic acid on IV leads to destruction of the molecule, evidently as a result of initial opening of the pyrimidine ring at the $C_{(2)}-N_{(1)}$ bond with subsequent decomposition of the molecule. An individual compound cannot be isolated from the reaction medium for this reason. Despite the high lability of the halogen in the 4 position, dehalogenation cannot be carried out by the action of zinc on IV in an alcohol medium. Only the action of zinc dust in refluxing demethylformamide (DMF) leads to 8-methyl-7-phenyl-2-chloroimidazo[1,2-f]purine (V).

Thus the set of data presented in this paper unambiguously confirms the individuality of the synthesized compounds and the scheme of chemical transformations presented above.

TABLE 1. Characteristics of the Synthesized Compounds IV-XVII

Compound	mp, °C	Found, %				Empirical formula	Calc., %				Yield, %
		C	H	Cl	N		C	H	Cl	N	
IV	203—205	52,6	3,2	21,8	21,8	$C_{14}H_9Cl_2N_5$	52,9	2,9	22,3	22,0	65
V	218—220	59,6	3,2	24,9	24,2	$C_{14}H_{10}ClN_5$	59,3	3,6	24,7	24,7	58
VI	>360	53,0	3,3	10,0	22,4	$C_{14}H_{10}ClN_5S$	53,3	3,2	10,2	22,2	78
VII	205—206	61,3	5,3	—	20,2	$C_{18}H_{19}ClN_5$	61,6	5,5	—	19,4	71
VIII	>360	55,8	3,1	11,7	23,1	$C_{14}H_{10}ClN_5O$	56,1	3,4	11,8	23,4	77
IX	119—121	64,7	4,2	—	21,4	$C_{21}H_{17}ClN_6$	64,9	4,4	—	21,6	47
X	>250	56,1	3,7	11,5	28,5	$C_{14}H_{11}ClN_6$	56,3	3,7	11,9	28,1	92
XI	350—352	63,5	4,2	—	31,1	$C_{14}H_{12}N_6$	63,6	4,6	—	31,8	45
XII	232—234	54,2	3,3	—	20,9	$C_{15}H_{12}ClN_5S$	54,6	3,7	—	21,2	78
XIII	262—264	57,4	4,6	—	26,3	$C_{15}H_{13}ClN_5$	57,6	4,2	—	26,9	71
XIV	218—219	64,5	6,3	—	29,2	$C_{18}H_{21}N_7$	64,2	6,1	—	29,6	76
XV	191—192	67,7	8,0	—	25,4	$C_{22}H_{29}N_7$	67,5	7,5	—	25,0	72
XVI	265—266	62,5	5,8	—	32,3	$C_{17}H_{16}N_7$	62,5	5,6	—	31,9	68
XVII	170—171	69,6	7,2	—	24,0	$C_{24}H_{29}N_7$	69,4	7,0	—	23,6	82

EXPERIMENTAL

The IR spectra of KBr pellets of the compounds were recorded with a UR-20 spectrometer. The electronic spectra of $(2-5)\cdot10^{-1}$ mole/liter solutions of the compounds in ethanol were recorded with a Specord UV-vis spectrophotometer. The PMR spectra of solutions of the compounds in d_6-DMSO, $CDCl_3$, and CF_3COOH were recorded with a Brucker WH-90 spectrometer with tetramethylsilane as the standard. The mass spectra were recorded with a Varian MAT-311A spectrometer with direct introduction of the samples into the ion source; the accelerating voltage was 3 kV, the cathode emission current was 300 μA, and the ionizing voltage was 70 eV. Thin layer chromatography (TLC) was carried out on Silufol UV-254 plates with development with iodine vapors.

1,8-Dimethyl-7-phenyl-2-chloroimidazo[1,2-f]purin-4-one (II). A 2.95-g (0.01 mole) sample of 1,8-dimethyl-7-phenylimidazo[1,2-f]xanthine (I) was refluxed in 100 ml of phosphorus oxychloride until it dissolved completely (3-4 h), after which the phosphorus oxychloride was removed by vacuum distillation to a small volume (20-30 ml). The residue was poured over 200 g of ice, and the mixture was neutralized at 0°C with solid sodium bicarbonate. The precipitate was removed by filtration, washed with water, and dried to give 1.75 g (56%) of a product with mp 271-272°C (ethanol) and R_f 0.18 [n-butyl alcohol—formic acid—water (77:10:13)]. Found: C 57.4; H 4.0; Cl 11.0; N 22.7%. $C_{15}H_{12}ClN_5O$. Calculated: C 57.5; H 3.8; Cl 11.3; N 22.3%.

1,8-Dimethyl-7-phenyl-2-N-piperidinoimidazo[1,2-f]purin-4-one (III). A 5-ml sample of piperidine was added to 3.14 g (0.01 mole) of 1,8-dimethyl-7-phenyl-2-chlorimidazo[1,2-f]-purin-4-one (II) in 30 ml of n-propyl alcohol, and the mixture was refluxed for 10-15 min. It was then cooled and poured into 100 ml of water. The precipitate was removed by filtration, washed with water, and dried to give 2.55 g (70.4%) of a product with mp 299-301°C (dec., from CH_3OH—acetone). Found: C 66.4; H 6.4; N 23.5%. $C_{20}H_{22}N_6O$. Calculated: C 66.3; H 6.1; N 23.2%.

1,8-Dimethyl-7-phenylimidazo[1,2-f]xanthine (I). A) A 3.14-g (0.01 mole) sample of II was refluxed for 30 min in 100 ml of 2 N sodium hydroxide solution, after which the mixture was cooled and made slightly acidic with hydrochloric acid, and the precipitate was removed by filtration and dried. The yield was quantitative.

B) A 0.01-mole sample of III was refluxed for 1 h in 100 ml of concentrated HCl, after which the mixture was cooled, and the precipitate was removed by filtration and washed with water to give the product in 55% yield.

No melting-point depression was observed for mixtures of samples of I obtained by methods A and B and a sample obtained by the method in [2].

8-Methyl-7-phenyl-2,4-dichloroimidazo[1,2-f]purine (IV). A 2.95-g (0.01 mole) sample of I was refluxed in 100-150 ml of phosphorus oxychloride for 4-5 h, after which the mixture was cooled to room temperature, 0.01 mole of phosphorus pentachloride was added, and the mixture was refluxed for another 6 h. The phosphorus oxychloride was removed by distillation to a small volume, and the residue was poured over 200 g of ice. The mixture was neutralized at 0°C with ammonium hydroxide. After 3-6 h, the precipitate was removed by filtration,

TABLE 2. Mass Spectra of the Synthesized Compounds

Compound	m/z values (intensities of the peaks in percent of the maximum peak)*
II	51 (5,15); 55 (14,9); 56 (8,17); 57 (26,0); 58 (3,27); 59 (5,9); 60 (10,6); 61 (14,5); 63 (3,0); 64 (4,2); 65 (11,8); 67 (7,3); 68 (3,2); 69 (9,25); 70 (5,3); 71 (11,8); 73 (6,3); 75 (3,4); 76 (3,4); 77 (10,9); 81 (4,2); 82 (3,4); 83 (6,1); 84 (4,2); 85 (6,9); 89 (3,9); 91 (100); 92 (8,5); 95 (3,2); 97 (4,6); 102 (5,4); 103 (4,4); 104 (5,2); 105 (6,3); 111 (5,8); 118 (4,0); 129 (3,4); 131 (3,07); 149 (11,5); 234 (9,4); 236 (3,6); 242 (3,6); 248 (10,8); 249 (72,7); 250 (16,5); 262 (3,6); 270 (23,8); 271 (3,4); 272 (16,0); 284 (3,4); 295 (3,28); 313 (7,49); 361 (6,2); 363 (4,5)
XI	51 (17,4); 55 (48,9); 57 (21,1); 59 (13,3); 63 (37,4); 71 (41,4); 77 (35,6); 81 (22,3); 83 (26,1); 89 (10,3); 91 (16,3); 102 (18,6); 103 (19,8); 118 (19,4); 119 (10,3); 132 (7,6); 149 (28,8); 157 (13,5); 167 (7,1); 195 (14,8); 222 (13,1); 237 (21,3); 249 (7,9); 263 (10,5); 264 (100,0); 265 (15,6)
XIV	41 (12,4); 42 (20,5); 44 (100,0); 56 (11,4); 57 (24,5); 67 (12,1); 71 (9,1); 77 (15,9); 91 (8,2); 102 (13,1); 103 (9,6); 105 (14,2); 118 (17,8); 124,5 (3,6); 138,5 (12,7); 145,5 (11,3); 146 (11,1); 153 (11,0); 159,5 (15,5); 160 (15,6); 167,5 (24,1); 173 (6,8); 209 (4,4); 221 (5,4); 222 (5,7); 223 (4,9); 235 (5,4); 236 (5,7); 248 (14,5); 249 (40,2); 250 (19,0); 262 (22,2); 263 (36,5); 276 (18,9); 277 (48,9); 291 (23,2); 292 (32,6); 306 (48,5); 307 (14,3); 320 (88,1); 321 (26,1); 334 (14,7); 335 (90,0); 336 (98,3)
XV	41 (17,3); 42 (8,2); 43 (65,6); 44 (100,0); 56 (17,4); 57 (45,8); 58 (16,1); 69 (7,3); 70 (5,8); 71 (14,3); 77 (8,5); 85 (7,0); 91 (5,1); 102 (3,8); 103 (3,0); 105 (21,0); 118 (4,4); 152,5 (5,1); 159,5 (10,5); 166,5 (8,3); 173,5 (9,0); 180,5 (7,2); 195,5 (13,9); 262 (7,9); 263 (7,8); 264 (6,0); 275 (3,0); 290 (3,0); 291 (13,4); 305 (3,2); 318 (9,2); 320 (9,1); 332 (6,8); 334 (3,8); 347 (3,6); 348 (33,3); 349 (8,1); 362 (80,0); 363 (25,7); 376 (14,6); 377 (3,8); 390 (4,5); 391 (42,9); 392 (10,7)
XVII	41 (15,8); 43 (21,8); 44 (100); 56 (19,1); 57 (48,0); 61 (6,9); 71 (16,7); 77 (5,0); 84 (5,7); 85 (6,2); 91 (3,5); 102 (3,2); 103 (3,0); 118 (3,7); 207,5 (13,9); 208 (5,8); 22 (7,6); 237 (6,1); 248 (6,6); 249 (17,3); 250 (7,7); 263 (7,3); 264 (8,4); 276 (5,9); 277 (7,5); 289 (8,3); 290 (3,6); 303 (6,3); 304 (7,3); 305 (3,2); 320 (3,0); 332 (48,5); 333 (13,8); 346 (3,7); 347 (3,9); 359 (9,9); 360 (15,3); 361 (3,3); 372 (11,1); 373 (6,7); 386 (35,7); 387 (12,6); 400 (4,0); 414 (9,4); 415 (49,9); 416 (13,4)

*The peaks with intensities greater than 3% are presented. The temperatures to which the input system were heated were 190°C for II, 80°C for XI, 215°C for XIV, 160°C for XV, and 200°C for XVII.

washed with water, and dried to give IV with R_f 0.83 [n-butyl alcohol—formic acid—water (77:10:13)]. The characteristics of IV-XVII are presented in Table 1.

8-Methyl-7-phenyl-2-chlorimidazo[1,2-f]purine (V). A mixture of 3.2 g (0.01 mole) of IV with 5.0 g of zinc dust was refluxed in 100 ml of DMF for 4 h, after which the hot mixture was filtered, and the filtrate was concentrated in vacuo to half its original volume. The resulting precipitate was removed by filtration, washed with water, and crystallized from aqueous DMF to give V. PMR spectrum (CF_3COOH): 8.42 (1H, s, C_6H), 8.85-9.07 (5H, m, aromatic protons), and 9.43 ppm (1H, s, C_4H).

4-Mercapto-2-chloro-8-methyl-7-phenylimidazo[1,2-f]purine (VI). A 1.5-g (5 mmole) sample of IV and 1.2 g (0.015 mole) of thioruea were refluxed in 50 ml of n-propyl alcohol for 6 h, after which the mixture was cooled, and the precipitate was removed by filtration, washed with water, and dried to give VI. The product was purified by reprecipitation from 250 ml of 20% sodium hydroxide solution by means of acetic acid (the yield after reprecipitation was 67.5%). The product was crystallized from DMSO. PMR spectrum (DMSO): 2.67 (1H, s, SH), 6.8 (1H, s, C_6H), and 6.28-6.37 ppm (5H, m, aromatic protons). UV spectrum, λ_{max} (log ε): 210 (4.47), 295 (4.3), and 352 nm (4.12).

4-Methylmercapto-2-chloro-8-methyl-7-phenylimidazo[1,2-f]purine (XII). A mixture of 3.15 (0.01 mole) of VI, 0.56 g (0.01 mole) of KOH, and 0.9 ml (0.01 mole) of dimethylsulfate in 100 ml of 50% aqueous n-propyl alcohol was refluxed for 1 h, after which it was cooled, and the precipitate was removed by filtration and crystallized from n-propyl alcohol. IR spectrum (KBr pellet): 2930, 1390 (CH_3); 3055, 3035 (CH, aromatic); 725, 715 cm^{-1} (C—Cl). PMR spectrum (CH_3COOH); 2.9 (3H, s, SCH_3), 3.77 [3H, s, $N_{(8)}—CH_3$], and 7.6 ppm (5H, s, aromatic protons).

2-Chloro-8-methyl-7-phenylimidazo[1,2-f]purin-4-one (VIII). A 3.2-g (0.01 mole) sample of IV and 0.8 g (0.02 mole) of sodium hydroxide in 100 ml of water was refluxed until a homo-

geneous solution formed, after which the solution was filtered, and the filtrate was cooled and made slightly acidic with acetic acid. The precipitated VIII was removed by filtration and crystallized from DMF. IR spectrum (KBr pellet): 3165 (NH) and 1695 cm^{-1} (C=O). UV spectrum, λ_{max} (log ε): 206 (4.35), 220 (4.32), and 270 nm (4.37). PMR spectrum (CF_3COOH): 3.83 [3H, s, $N_{(8)}-CH_3$] and 7.37-7.73 ppm (5H, m, aromatic protons).

4-Amino-, 4-Alkylamino-, and 4-Cycloalkylamino-2-chloro-8-methyl-7-phenylimidazo[1,2-f]-purines (VII, IX, X, XIII). A 0.01-mole sample of IV was heated with 0.02-0.1 mole of the corresponding amine in n-propyl alcohol for 0.5-1 h, after which the mixture was cooled and poured into 150-200 ml of water. The precipitate was removed by filtration and crystallized from alcohol. A saturated 20% alcohol solution of ammonia was used for the preparation of 4-amino-2-chloro-8-methyl-7-phenylimidazo[1,2-f]purine (X), or the reaction was carried out with excess ammonium carbonate (more than 2 moles) in alcohol by heating the ingredients in a sealed ampul for 1 h at 90-100°C (but no higher than 110°C). The constants of the compounds are presented in Table 1.

8-Methyl-7-phenylimidazo[1,2-f]adenine (XI). A 3.0-g sample of X was heated in 100 ml of concentrated hydriodic acid until it dissolved, after which 3.0 g of red phosphorus was added, and the mixture was refluxed for 1 h. The hot mixture was then filtered to remove the red phospnorus, and the filtrate was neutralized with 25% ammonium hydroxide. The precipitate was removed by filtration and crystallized from DMF. PMR spectrum (d_6-DMSO): 3.71 [3H, s, $N_{(8)}CH_3$], 6.96 (1H, c, C_6H), 7.3 (2H, broad s, NH_2), 7.58 (5H, m, aromatic protons), and 8.28 ppm (1H, s, C_2H) [8]. IR spectrum (KBr pellet): 1600 (C=C), 1530 (C=N) [9], and 1310 cm^{-1} (C=N).

2,4-Bis(alkylamino, dialkylamino)-8-methyl-7-phenylimidazo[1,2-f]purines (XIV-XVII). A mixture of 0.01 mole of 2,4-dichloro-8-methyl-7-phenylimidazo[1,2-f]purine (IV), 0.1-0.3 mole of the corresponding primary or secondary amine, 0.1 g of anhydrous copper sulfate, and 100 ml of alcohol (ethanol or methanol) was heated in an autoclave or sealed ampul at 200-210°C for 6 h, after which it was cooled and poured into 200-250 ml of water. The precipitate was removed by filtration and recrystallized from methanol.

8-Methyl-7-phenyl-2,4-bis-N-dimethylaminoimidazo[1,2-f]purine (XIV). Mass spectrum, m/z: 335 (M^+), 320 $(M-CH_3)^+$, 306 $[(M-CH_3)-CH_2]^+$, 292 $(M-CH_3CH_2N)^+$ (D), 291 $(M-CH_3NCH_3)^+$, 277 $(D-CH_3)^+$, 263 $[(D-CH_3)-CH_2]^+$, 249 $[(D-CH_3CH_2N)]^+$. IR spectrum (KBr pellet): 3480 (NH_2), 2965 (CH_3), 1640 (C=N), and 1560 cm^{-1} (C=C). PMR spectrum (CF_3COOH): 3.37 [6H, s, $(CH_3)_2N$], 3.62 [6H, s, $(CH_3)_2N$], 3.87 (3H, S, CH_3N_8), 7.5-7.75 (5H, m, aromatic protons), and 8.23 ppm (1H, s, C_6H).

8-Methyl-7-phenyl-2,4-di-N-piperidinoimidazo[1,2-f]purine (XVII). Mass spectrum, m/z: 415 $(M)^+$, 400 $(M-CH_3)^+$, 387 $(M-C_2H_4)^+$, 386 $(M-C_2H_5)^+$, 372 $(M-C_3H_7)^+$, 360 $(M-C_4H_7)^+$ (B), 332 $(B-H_2CN)^+$ or $(M-C_5H_9N)^+$ (C), 304 $(C-C_2H_4)^+$, 303 $(C-C_2H_5)^+$, 289 $(C-C_3H_7)^+$, 277 $(C-C_4H_7)^+$, 249 $[(C-C_4H_7)-H_2CN]^+$ or $(C-C_5H_9N)^+$. PMR spectrum (CF_3COOH): 1.52-1.85 (20H, m, CH_2), 3.71 (3H, s, CH_3N_8), 7.31 (1H, s, C_6H), and 7.55 ppm (5H, broad s, aromatic protons).

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