First example of the Groebke MCR using hydoxybenzaldehydes and substituted 2-aminopyrimidines

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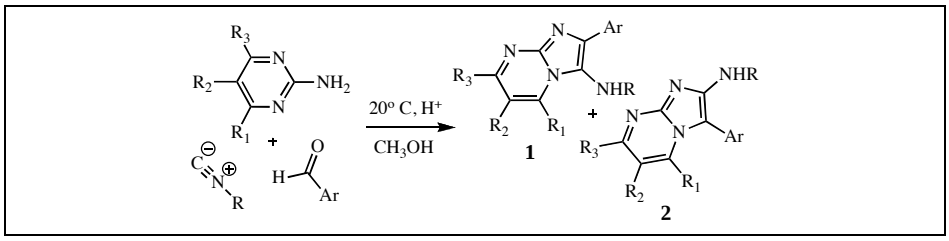

A three component condensation of 2-aminopyrimidines, isocyanides and 4-hydroxybenzaldehydes was studied. 3-Amino-2-(4-hydroxyphenyl)imidazo[1,2-*a*]pyrimidine derivatives were obtained in moderate yields. Using 4-hydroxy-3,5-dimethoxybenzaldehyde and 2-aminopyrimidine as starting materials in the condensation led to mixtures of isomeric 2- and 3-aminoimidazo[1,2-*a*]pyrimidines. It was demonstrated, that the regiospecificity of this reaction is mainly defined by the steric hindrance of substituents on the pyrimidine nucleus and the carbonyl activity of the corresponding aldehydes.

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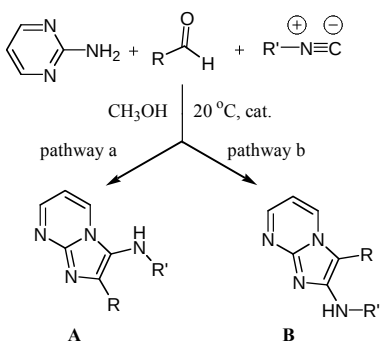
INTRODUCTION

Multi-component reactions (MCRs) are widely applied in the synthesis of compounds with high molecular diversity [1,2]. The three component, 'one-pot' condensation of 2-aminodiazines, aldehydes and isocyanides suggested in 1998 by Groebke enabled to obtain libraries of imidazo[1,2-*a*]azines [3-8]. Later the preparative variants of this reaction were elaborated both in solution and on solid support [9,10]. On further studying the Groebke reaction [8,11] it was shown that along with the desired 3-aminoimidazo[1,2-*a*]pyrimidines, the isomeric 2-aminoimidazo[1,2-*a*]pyrimidines were formed as by-products (Scheme 1).

Scheme 1



The available literature data points out that according to the Scheme 1, the Groebke reaction using 2-amino-pyrimidine leads towards two main products **A** ("normal") and **B**. However we failed finding any information on the reactivity of substituted 2-aminopyrimidines (2-amino-pyrimidines derivatives) in this MCR. Moreover, the usage of hydroxybenzaldehydes as carbonyl component in this reaction has not yet been described.

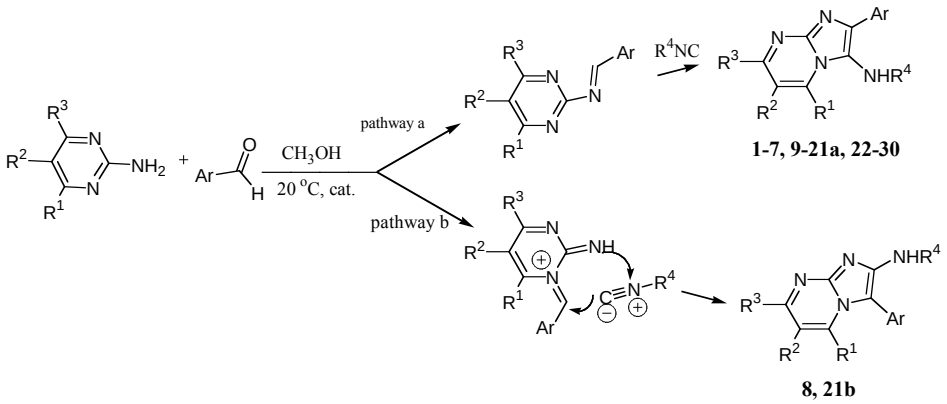
In spite of the reported possibility [11] to preclude the formation of isomer **B** by the use of NH_4Cl as a catalyst and aprotic solvent (toluene), more recent paper [12] reports on the concurrent formation of isomers **A** and **B** under the same reaction conditions . This information, along with the data on high stereoselectivity of this MCR in the case of 2-aminopyridine and 2-aminopyrazine [5,6] let us suppose that the amine basicity and spatial hindrance along with the reactivity of the carbonyl compound are the key factors in determining the reaction pathway.

In this context, we studied the reactions of 2-aminopyrimidine, 4-methyl-2-aminopyrimidine and 4,6-dimethyl-2-aminopyrimidine with various aromatic and cycloaliphatic isocyanides and hydroxy-substituted benzaldehydes.

RESULTS AND DISCUSSION

Imidazo[1,2-*a*]pyrimidines obtained by this MCR are representatives of 1,7-dideaza-5-azapurines, among which compounds with different substantial bioactivity were found [13]. The presence of a hydroxyl group in the target compounds could not only add one more point of diversity to the molecule core, but have a considerable influence on their pharmaceutical properties (metabolism, transportation, the influence on hypoxia and redox

Scheme 2



processes in biomembranes and inside of cells). The presence of hydroxyphenyl fragment is typical for many synthetic and natural antioxidants [14-16]. Since the pathogenetic role of active metabolites of oxygen and organic free radicals was identified for more than 100 diseases, we can expect the synthesis and screening of hydroxyl-containing aminoimidazo[1,2-*a*]azine derivatives as antioxidants to be expedient.

Out of all the catalysts described in the literature ($HClO_4$, $Sc(OTf)_3$, AcOH and NH_4Cl) we used acetic acid as catalyst of choice, since according to the previous data [8] it does not favor the formation of **B**.

Using acetic acid as a catalyst and carrying out the reaction at 20 ºC provided a high regiospecifity although it made the process longer (2-7 days). Moreover the mild reaction conditions diminished the decomposition of aromatic isocyanides. Yields of the recrystallized products did not exceed 25-30% (Scheme 2, Table 1).

For unsubstituted 2-aminopyrimidine almost all the reactions led to the formation of 2-alkyl(aryl)-3-aminoimidazo[1,2-*a*]pyrimidine derivatives **A** as the only isolated product of the reaction. The only exception was the MCR, involving 2-aminopyrimidine and 4-hydroxy-3,5-dimethoxybenzaldehyde, in this case the mixture of 2- and 3-aminoimidazopyridines (Table 1, compounds **7**, **8, 21a, 21b)** was formed (Scheme 2). Compounds **7** and **8** were isolated by column chromatography of the reaction mixture, whereas the attempts to separate compounds **21a** and **21b** failed and they were characterized as a mixture, 4:1, according to NMR data.

The structures of **7** and **8** were unambiguously elucidated on the base of the NOESY spectra. In the NOESY spectrum of compound **8** the intense NOE between 4-H and α-H was observed (Figure 1), whereas its absence in the spectrum of **7** was consistent with the offered structure. We refer the formation of two structural

Table 1

Imidazo[1,2-*a*]pyrimidines **1-30** yields and MP.

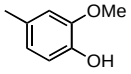
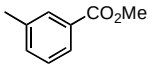
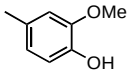
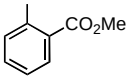
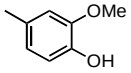
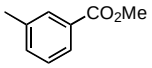
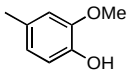
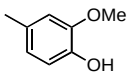
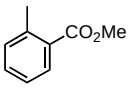
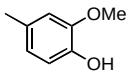
№№	R^1	R^2	R^3	R^4	Ar	Yield, %	melting point, °C
1	H	H	H			26	187-190
2	H	H	H			39	267-269
3	H	H	H			35	204-206
4	CH_3	H	CH_3			29	230-232
5	CH_3	H	CH_3			17	224-225
6[17]	CH_3	H	CH_3			*33*	*232-233*

Table 1 (continued)

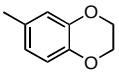
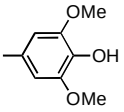
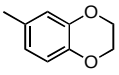
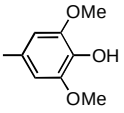
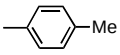
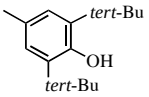
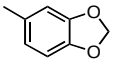
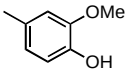
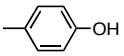
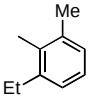
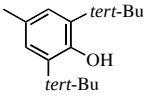
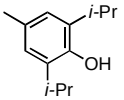
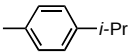
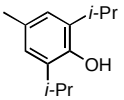
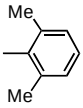
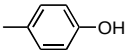
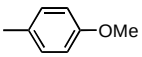
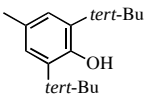
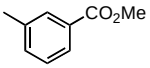
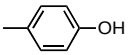
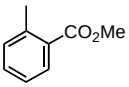
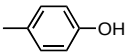
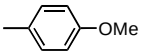
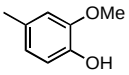
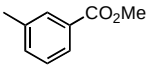
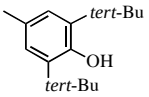
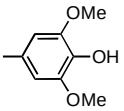
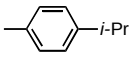
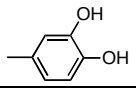
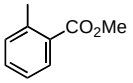
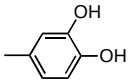
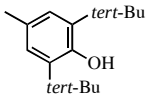
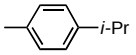
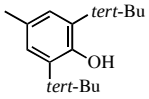
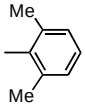
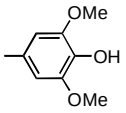
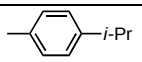
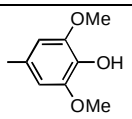
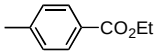
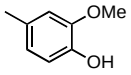
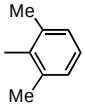
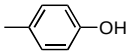
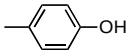
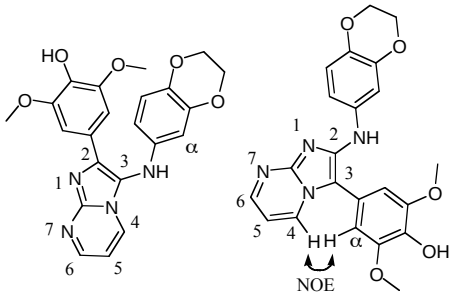
№№	R^1	R^2	R^3	R^4	Ar	Yield, %	melting point, °C
7[18]	H	H	H			34	250-252
8[19]	H	H	H			15	128-130
9[20]	H	H	CH_3			10	*260 (dec)*
10	H	H	H			*31*	*250-253*
11	H	H	H			28	227-229
12	H	H	H			16	211 (dec)
13	H	H	H			19	229 (dec)
14	H	H	H			23	263
15	H	H	H			36	257-259
16	H	H	H			28	274-278
17	H	H	H			30	270-273
18	H	H	H			27	258-260
19	CH3	H	CH3			24	271-274
20	H	H	H			27	236-237
21a and 21b	H	H	H			according to NMR a mixture of **21a** and **21b**, 1:4	-
22	H	H	H			29	273-275

Table 1 (continued)

№№	R^1	R^2	R^3	R^4	Ar	Yield, %	melting point, °C
23	H	H	H			46	254-256
24	H	H	H			25	247-249
25	H	H	H			27	280-284
26	H	H	H			49	266-268
27	CH_3	H	CH_3			31	145-146
28	H	H	H			43	229-231
29	CH_3	H	CH_3			27	275-277
30	H	H	H			39	248-249

isomers to the increased carbonyl activity of the starting aldehyde, making the C=O attack to the cyclic pyrimidine nitrogen possible.

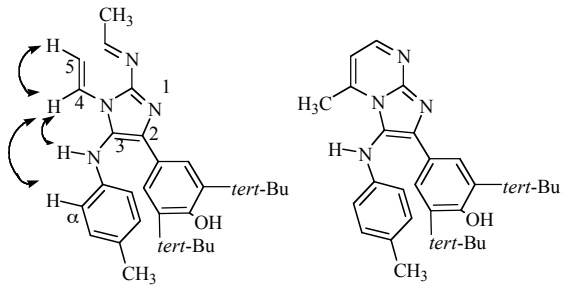


7 **8**

Figure 1

When 2-amino-4,6-dimethylpyrimidine was used instead of 2-aminopyrimidine in all the cases (including the reaction of 3,5-dimethoxy-4-hydroxybenzaldehyde), only the product **A** was isolated (Table 1, compounds **4**-**6**, **19**, **27**, **29**). Moreover, the NMR analysis of the reaction mixture showed the absence of the isomer **B**. This fact presumably can be explained by the steric hindrance caused by two Me groups, shielding the cyclic nitrogen atom thus disfavoring pathway b. (Scheme 2)

The use of 4-methyl-2-aminopyrimidine in this MCR always led to the formation of multi-component reaction mixtures, which we were unable to separate. The only exception was the condensation of 4-hydroxy-3,5-di-*tert*-butylbenzaldehyde, 4-methyl-2-aminopyrimidine and 4-methylphenylisocyanide where we were lucky to isolate the corresponding "normal" product **9** (Figure 2).



9

Figure 2

According to TLC and 1H NMR analysis only one isomer **9** is formed in the reaction. The structure of the product is confirmed by selective 1D ROESY with preirradiation saturation of 4-H. In the ROESY (standard software for Bruker DRX-500, mixing time 200 ms) only for compounds **9** spatial contacts between protons 4-H and N-H, 5-H, α-H of N-(4-methylphenyl) fragment are possible.

In conclusion we investigated the Groebke MCR of 4-hydroxybenzaldehydes and substituted 2-amino-pyrimidines. It was demonstrated, that the regiospecificity of this reaction is mainly defined by the steric hindrance of substituents on the pyrimidine nucleus and the carbonyl activity of the corresponding aldehydes. The antioxidant screening of the compounds synthesized is underway and will be reported in due course.

EXPERIMENTAL

Melting points are uncorrected. All solvents were distilled and dried before use. Column chromatography was performed with aluminium oxide. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ solutions, at 25 °C or in DMSO-d_6 solutions at 40 °C, using a 400 MHz NMR spectrometer operating at 400 and 100 MHz correspondingly, peak positions are given in parts per million (δ) with tetramethylsilane used as the internal standard. Mass-spectra were registered using ESI or EI techniques.

General procedure. A solution of aminopyrimidine (2.0 mmol), aldehyde (2.0 mmol) and acetic acid (4.0 mmol) in 20 mL of methanol was stirred for 20 min at 20 °C. The reaction mixture was cooled and at 0 °C and isocyanide (2.0 mmol) was added in one portion. Stirring was continued at 20 °C for additional 5-6 hours (TCL monitoring). The products crystallized from the reaction mixture or on adding several drops of water. The product was collected by filterration, washed with water (3×10 mL), dried and washed again with hexane (50 mL). The crude product was crystallized (methanol) or purified by column chromatography (CH_2Cl_2-CH_3OH, 15:5) to give crystalline compounds 1-30.

4-[3-(Cycloheptylamino)imidazo[1,2-*a*]pyrimidin-2-yl]-2-methoxyphenol (1). White powder. ^{1}H NMR: δ 9.14 (s, 1H, OH), 8.67 (d, *J* = 6.5 Hz, 1H, CH-Ar), 8.41 (s, 1H, CH-Ar), 7.82 (s, 1H, CH-Ar), 7.68 (d, *J* = 8.2 Hz, CH-Ar), 6.99 (dd, *J* = 4.2, 9.9 Hz, 1H, CH-Ar), 6.85 (d, *J* = 8.2 Hz, 1H, CH-Ar), 4.76 (d, *J* = 4.6 Hz, 1H, NH-CH), 3.86 (s, 3H, O-CH_3), 3.14 (m, 1H, NH-CH), 1.73 (m, 2H, CH_2), 1.59 (m, 2H, CH_2), 1.46 (m, 6H, 3xCH_2), 1.23 (m, 2H, CH_2) ppm. ^{13}C NMR: δ 148.5, 147.4, 146.2, 143.5, 136.6, 130.9, 125.4, 122.9, 119.9, 115.4, 110.9, 107.8, 57.9, 55.5, 34.7 (2C), 27.8 (2C), 23.3 (2C) ppm. IR (KBr) ν_{max}: 3343, 2937, 1611, 1523, 1362 cm^{-1}. EIMS. m/z (relative intensity): 352 (28), 255 (57), 228 (100), 213 (8), 79 (64), 55 (45), 41 (31). *Anal.* Calcd for $C_{20}H_{24}N_4O_2$: C, 68.16; H, 6.86; N, 15.90. Found: C, 68.46; H, 6.76; N, 15.60.

Methyl 3-{[2-(4-hydroxy-3-methoxyphenyl)imidazo[1,2-*a*]-pyrimidin-3-yl]amino}benzoate (2). Pale brown powder. ^{1}H NMR: δ 9.62 (s, 1H, OH), 9.08 (s, 1H, NH), 8.53 (s, 1H, CH-Ar), 8.41 (d, *J* = 6.8 Hz, 1H, CH-Ar), 7.93 (d, *J* = 7.0 Hz, 1H, CH-Ar), 7.55 (s, 1H, CH-Ar), 7.41 (d, *J* = 6.8 Hz, 1H, CH-Ar), 7.25 (t, *J* = 7.7 Hz, 1H, CH-Ar), 7.16 (s, 1H, CH-Ar), 7.02 (d, *J* = 7.0 Hz, 1H, CH-Ar), 6.78 (d, *J* = 8.4 Hz, 2H, CH-Ar), 3.92 (s, 3H, O-CH3), 3.58 (s, 3H, O-CH3) ppm. ^{13}C NMR: δ 166.2, 150.2, 147.9, 147.4, 146.9, 145.0, 139.3, 135.0, 131.5, 131.3, 124.2, 119.6, 118.1, 115.7, 114.8, 113.2, 112.1, 110.8, 108.7, 55.2, 51.9 ppm. IR (KBr) ν_{max}: 3506, 3332, 1711, 1673, 1509, 1466 cm^{-1}. ESIMS. m/z: 352 (M^+). *Anal.* Calcd for $C_{21}H_{18}N_4O_4$: C, 64.61; H, 4.65; N, 14.38. Found: C, 64.77; H, 4.64; N, 14.27.

Methyl 2-{[2-(4-hydroxy-3-methoxyphenyl)imidazo[1,2-*a*]-pyrimidin-3-yl]amino}benzoate (3). Yellow powder. 1H NMR: δ 9.25 (s, 1H, OH), 9.18 (s, 1H, NH), 8.57 (s, 1H, CH-Ar), 8.44 (d, *J* = 6.5 Hz, 1H, CH-Ar), 7.96 (d, *J* = 7.0 Hz, 1H, CH-Ar), 7.56 (s, 1H, CH-Ar), 7.45 (d, *J* = 6.8 Hz, 1H, CH-Ar), 7.26 (t, *J* = 4.8 Hz, 1H, CH-Ar), 7.02 (t, *J* = 5.0 Hz, 1H, CH-Ar), 6.80 (m, 2H, CH-Ar), 6.18 (d, *J* = 6.0 Hz, 1H, CH-Ar), 3.92 (s, 3H, O-CH_3), 3.61 (s, 3H, O-CH_3) ppm. ^{13}C NMR: δ 167.9, 150.1, 147.9, 147.4, 146.8, 144.9, 139.2, 135.0, 131.4, 131.2, 124.1, 119.7, 118.1, 115.6, 114.7, 113.1, 112.1, 110.5, 108.6, 55.0, 52.0 ppm. IR (KBr) ν_{max}: 3506, 3332, 1711, 1673, 1509, 1465 cm^{-1}. ESIMS. m/z: 391 $(M+1)^+$. *Anal.* Calcd for $C_{21}H_{18}N_4O_4$: C, 64.61; H, 4.65; N, 14.35. Found: C, 64.81; H, 4.45; N, 14.25.

Methyl 3-{[2-(4-hydroxy-3-methoxyphenyl)-5,7-dimethyl-imidazo[1,2-*a*]pyrimidin-3-yl]amino}benzoate (4). Pale yellow powder. ^{1}H NMR: δ 9.09 (s, 1H, OH), 8.33 (s, 1H, NH), 7.58 (s, 1H, CH-Ar), 7.47 (d, *J* = 6.8 Hz, 1H, CH-Ar), 7.30 (s, 2H, CH-Ar), 7.11 (s, 1H, CH-Ar), 6.77 (d, *J* = 7.4 Hz, 2H, CH-Ar), 6.72 (s, 1H, CH-Ar), 3.79 (s, 3H, O-CH_3), 3.62 (s, 3H, O-CH_3), 2.62 (s, 3H, CH_3), 2.48 (s, 3H, CH_3) ppm. ^{13}C NMR: δ 166.2, 159.6, 148.1, 147.3, 146.6, 145.9, 144.3, 139.6, 130.9, 130.0, 124.3, 119.7, 119.0, 117.5, 115.7, 115.5, 113.0, 110.8, 110.5, 55.1, 52.0, 23.9, 17.5 ppm. IR (KBr) ν_{max}: 3294, 2359, 1722, 1520 cm^{-1}. ESIMS. m/z: 419 $(M+1)^+$. *Anal.* Calcd for $C_{23}H_{22}N_4O_4$: C, 66.02; H, 5.30; N, 13.39. Found: C, 66.32; H, 5.10; N, 13.19.

4-[3-(Cycloheptylamino)-5,7-dimethylimidazo[1,2-*a*]pyr-imidine-2-yl]-2-methoxyphenol (5). White powder. ^{1}H NMR: δ=8.98 (s, 1H, OH), 7.73 (s, 1H, CH-Ar), 7.56 (d, *J* = 6.5 Hz, 1H, CH-Ar), 6.82 (d, *J* = 7.0 Hz, 1H, CH-Ar), 6.60 (s, 1H, CH-Ar), 4.40 (bs, 1H, *NH*-CH), 3.85 (s, 3H, O-CH_3), 3.08 (m, 1H, NH-*CH*), 2.92 (s, 3H, -CH_3), 2.52 (s, 3H, CH_3), 2.43 (s, 3H, CH_3), 1.40 (m, 12H, 6xCH_2) ppm. ^{13}C NMR: δ 157.9, 147.2, 146.0, 145.1, 144.8, 138.7, 125.9, 123.7, 120.3, 115.2, 111.5, 110.0, 59.2, 55.5, 34.0, 27.7 (2C), 23.7 (2C), 23.6 (2C), 18.6 ppm. IR (KBr) ν_{max}: 3328, 2479, 1619, 1519 cm^{-1}. ESIMS. m/z: 380 (M^+). *Anal.* Calcd for $C_{22}H_{28}N_4O_2$: C, 69.45; H, 7.42; N, 14.72. Found C, 69.75; H, 7.22; N, 14.52.

Methyl 2-{[2-(4-hydroxy-3-methoxyphenyl)-5,7-dimethyl-imidazo[1,2-*a*]pyrimidin-3-yl]amino}benzoate (6). Brown powder. ^{1}H NMR: δ 9.21 (s, 1H, OH), 9.03 (bs, 1H, NH), 7.94 (d, *J* = 6.5 Hz, 1H, CH-Ar), 7.51 (s, 1H, CH-Ar), 7.42 (d, *J* = 6.3 Hz, 1H, CH-Ar), 7.31 (t, *J* = 4.7 Hz, 1H, CH-Ar), 6.78 (m, 2H, CH-Ar), 6.70 (s, 1H, CH-Ar), 6.22 (d, *J* = 7.2 Hz, 1H, CH-Ar), 3.92 (s, 3H, O-CH_3), 3.59 (s, 3H, O-CH_3), 2.59 (s, 3H, CH_3), 2.52 (s, 3H, CH_3) ppm. ^{13}C NMR: δ 167.7, 159.3, 149.5, 147.2, 146.5, 146.0, 144.4, 139.1, 135.0, 131.3, 124.4, 119.6, 117.6, 115.4, 115.1, 114.1, 111.2, 110.5, 110.2, 54.9, 51.9, 23.9, 17.2 ppm. IR (KBr) ν_{max}: 3276, 1702, 1619, 1508 cm^{-1}. ESIMS. m/z: 419 $(M+1)^+$. *Anal.* Calcd for $C_{23}H_{22}N_4O_4$: C, 66.02; H, 5.30; N, 13.39. Found: C, 66.32; H, 5.10; N, 13.19.

4-[3-(2,3-Dihydro-1,4-benzodioxin-6-ylamino)imidazo[1,2-*a*]pyrimidin-2-yl]-2,6-dimethoxyphenol (7). Pale brown powder. ^{1}H NMR: δ 8.58 (s, 1H, OH), 8.55 (d, *J* = 6.8 Hz, 1H, CH-Ar), 8.47 (d, *J* = 6.9 Hz, 1H, CH-Ar), 7.92 (s, 1H, NH),

7.35 (s, 2H, CH-Ar), 7.04 (d, *J* = 6.4 Hz, 1H, CH-Ar), 6.67 (d, *J* = 7.4 Hz, 1H, CH-Ar), 6.08 (d, *J* = 7.2 Hz, 1H, CH-Ar), 5.99 (s, 1H, CH-Ar), 4.13 (t, *J* = 5.2 Hz, 2H, CH_2), 4.10 (t, *J* = 5.2 Hz, 2H, CH_2), 3.70 (s, 6H, 2xO-CH_3) ppm. ^{13}C NMR: δ 150.0, 147.9 (2C), 144.5, 143.9, 139.9, 138.5, 136.3, 135.8, 130.9, 123.1, 117.7, 117.2, 108.6, 106.2, 104.5 (2C), 101.5, 64.3, 63.7, 55.7 (2C) ppm. IR (KBr) ν_{max}: 3280, 2160, 1618, 1507 cm^{-1}. ESIMS. m/z: 421 $(M+1)^+$. *Anal.* Calcd for $C_{22}H_{20}N_4O_5$: C, 62.85; H, 4.80; N, 13.33. Found: C, 62.55; H, 4.90; N, 13.43.

4-[2-(2,3-Dihydro-1,4-benzodioxin-6-ylamino)-imidazo[1,2-*a*]pyrimidin-3-yl] (8). Dark green powder. 1H NMR: δ 8.67 (s, 1H, OH), 8.65 (s, 1H, NH), 8.32 (d, *J* = 7.2 Hz, 1H, CH-Ar), 7.99 (s, 1H, CH-Ar), 7.37 (s, 1H, CH-Ar), 7.04 (dd, *J* = 2.3, 6.9 Hz, 1H, CH-Ar), 6.96 (dd, *J* = 4.4, 7.5 Hz, 1H, CH-Ar), 6.80 (s, 2H, CH-Ar), 6.68 (d, *J* = 6.8 Hz, 1H, CH-Ar), 4.21 (t, *J* = 4.7 Hz, 2H, CH_2), 4.17 (t, *J* = 4.7 Hz, 2H, CH_2), 3.80 (s, 6H, 2xO-CH_3) ppm. ^{13}C NMR: δ 148.5, 145.8, 144.7, 142.9, 137.0, 136.7, 135.8, 129.3, 117.0, 116.2 (2C), 110.4, 108.3, 106.9 (2C), 105.8, 105.5, 64.2, 63.7, 56.0 (2C) ppm. IR (KBr) ν_{max}: 3275, 2366, 1619, 1508 cm^{-1}. ESIMS. m/z: 421 $(M+1)^+$. *Anal.* Calcd for $C_{22}H_{20}N_4O_5$: C, 62.85; H, 4.80; N, 13.33. Found: C, 62.55; H, 4.90; N, 13.43.

2,6-Di-*tert*-butyl-4-{7-methyl-3-[(4-methylphenyl)amino]-imidazo[1,2-*a*]pyrimidin-2-yl}phenol (9). Brown powder. ^{1}H NMR: δ 8.13 (d, *J* = 6.7 Hz, 1H, CH-Ar), 7.81 (s, 2H, OH, CH-Ar), 7.75 (s, 1H, NH), 6.87 (d, *J* = 8.1 Hz, 2H, 2xCH-Ar), 6.78 (d, *J* = 6.7 Hz, 1H,CH-Ar), 6.55 (s, 1H, CH-Ar), 6.42 (d, *J* = 8.1 Hz, 2H, 2xCH-Ar), 2.59 (s, 3H, CH_3), 2.21 (s, 3H, CH_3), 1.34 (s, 18H, 2xCH-(CH_3)$_3$) ppm. ^{13}C NMR: δ=159.1, 153.7, 144.6, 143.3 (2C), 138.9, 138.7, 130.2, 129.6 (2C), 126.8, 124.7, 123.6 (2C), 116.1, 112.9 (2C), 109.0, 34.4, 30.2 (6C), 24.3, 20.0, 15.1 ppm. IR (KBr) ν_{max}: 3615, 3236, 2956, 2159, 1619, 1515 cm^{-1}. ESIMS. m/z: 441 $(M+1)^+$. *Anal.* Calcd for $C_{28}H_{34}N_4O$: C, 75.98; H, 7.74; N, 12.66. Found: C, 75.68; H, 7.94; N, 12.86.

4-[3-(1,3-Benzodioxol-5-ylamino)imidazo[1,2-*a*]pyrimidin-2-yl]-2-methoxyphenol (10). Pale brown powder. 1H NMR: δ 9.14 (s, 1H, OH), 8.53 (s, 1H, CH-Ar), 8.39 (d, *J* = 6.3 Hz, 1H, CH-Ar), 7.97 (s, 1H, NH), 7.64 (s, 1H, CH-Ar), 7.53 (d, *J* = 8.3 Hz, 1H, CH-Ar), 7,02 (dd, *J* = 4.2, 6.2 Hz, 1H, CH-Ar), 6.81 (d, *J* = 8.3 Hz, 1H, CH-Ar), 6.68 (d, *J* = 8.3 Hz, 1H, CH-Ar), 6.23 (s, 1H, CH-Ar), 5.91 (d, *J* = 8.5 Hz, 1H, CH-Ar), 5.87 (s, 2H, 2xCH-Ar), 3.72 (s, 3H, CH_3) ppm. ^{13}C NMR: δ 149.8, 148.1, 147.4, 146.7, 144.6, 140.8, 139.9, 138.8, 130.9, 124.4, 119.8, 116.7, 115.5, 110.9, 108.8, 108.5, 104.3, 100.4, 95.7, 55.3 ppm. IR (KBr) ν_{max}: 3554, 3302, 1618, 1529, 1503 cm^{-1}. EIMS. m/z (relative intensity): 376 (19), 228 (18), 150 (12), 121 (6), 106 (10), 90 (6), 80 (100), 63 (23), 53 (47), 39 (18). *Anal.* Calcd for $C_{20}H_{16}N_4O_4$: C, 63.83; H, 4.29; N, 14.89. Found: C, 63.53; H, 4.49; N, 15.09.

4-[3-(Cycloheptylamino)imidazo[1,2-*a*]pyrimidin-2-yl]-phenol (11). White powder. ^{1}H NMR: δ 9.54 (s, 1H, OH), 8.64 (d, *J* = 6.5 Hz, 1H, CH-Ar), 8.41 (d, *J* = 1.7 Hz, 1H CH-Ar), 8.04 (d, *J* = 8.5 Hz, 2H, CH-Ar), 6.98 (dd, *J* = 4.6, 6.5 Hz, 1H, CH-Ar), 6.82 (d, *J* = 8.3 Hz, 2H, CH-Ar), 4.71 (d, *J* = 5.1 Hz, 1H, NH), 3.15 (m, 1H, NH-*CH*), 1.72 (m, 2H, CH_2), 1.58 (m, 2H, CH_2), 1.41 (m, 6H, 3xCH_2), 1.23 (m, 2H, CH_2) ppm. ^{13}C NMR: δ 156.9, 148.3, 143.5, 136.6, 130.8, 128.2 (2C), 125.0, 122.7, 115.1 (2C), 107.7, 57.7, 34.6 (2C), 27.9 (2C), 23.2 (2C) ppm. IR (KBr) ν_{max}: 3300, 2934, 1609, 1503 cm^{-1}. EIMS. m/z (relative intensity): 322 (44), 225 (83), 198 (100), 119 (11), 79 (99), 65 (10), 55 (62), 41 (42). *Anal.* Calcd for $C_{19}H_{22}N_4O$: C, 70.78; H, 6.88; N, 17.38. Found: C, 70.48; H, 6.98; N, 17.68.

2,6-Di-*tert*-butyl-4-{3-[(2-ethyl-6-methylphenyl)amino]imidazo[1,2-*a*]pyrimidin-2-yl}phenol (12). Brown powder. ^{1}H NMR: δ=8.47 (s, 1H, OH), 8.23 (d, *J* = 6.6 Hz, 1H, CH-Ar), 7.79 (s, 1H, NH), 7.14 (s, 2H, CH-Ar), 7.00 (m, 3H, CH-Ar), 6.84 (d, *J* = 7.0 Hz, 1H, CH-Ar), 6.72 (t, *J* = 7.4 Hz, 1H, CH-Ar), 2,51 (m, 2H, CH_2), 1,68 (s, 3H, CH_3), 1.32 (s, 18H, 2x(C-(CH_3)$_3$)), 1.02 (t, *J* = 7.3 Hz, 3H, CH_2-CH_3) ppm. ^{13}C NMR: δ 154.1, 149.2, 134.7, 140.6, 139.0, 135.3 (2C), 131.3, 131.1, 130.1, 127.6, 124.4, 124.8, 124.3 (2C), 120.4, 119.4, 108.6, 34.9 (2C), 30.6 (6C), 24.6, 18.8, 14.4 ppm. IR (KBr) ν_{max}: 3534, 2961, 1610, 1466 cm^{-1}. ESIMS. m/z: 456 (M^+). *Anal.* Calcd for $C_{29}H_{36}N_4O$: C, 76.28; H, 7.95; N, 12.27. Found: C, 76.48; H, 7.75; N, 12.37.

2,6-Diisopropyl-4-(3-(2-ethyl-6-methylphenyl)imidazo[1,2-*a*]pyrimidin-2-yl)phenol (13). Brown powder. ^{1}H NMR: δ=8.48 (dd, *J* = 1.8, 4.0 Hz, 1H, CH-Ar), 8.44 (dd, *J* = 1.8, 6.7 Hz, 1H, CH-Ar), 8.17 (s, 1H, OH), 7.54 (s, 2H, CH-Ar), 7,11 (s, 1H, NH), 7.02 (dd, *J* = 4.1, 6.7 Hz, 1H, CH-Ar), 6.97 (d, *J* = 7.0 Hz, 1H, CH-Ar), 6.84 (d, *J* = 7.0 Hz, 1H, CH-Ar), 6.71 (t, *J* = 7.4 Hz, 1H, CH-Ar), 3.23 (m, 2H, 2x*CH*-(CH_3)$_2$), 2.48 (m, 2H, CH_2-CH_3) 1.66 (s, 3H, CH_3), 1.04 (m, 15H, 2xCH-(CH_3)$_2$+CH_2-CH_3) ppm. ^{13}C NMR: δ 151.0, 149.3, 143.9, 140.9, 139.0, 135.2 (2C), 131.4, 131.1, 130.1, 127.5, 125.3, 124.7, 122.7 (2C), 120.2, 119.1, 108.6, 26.4 (2C), 24.4, 23.2 (4C), 18.8, 14.3 ppm. IR (KBr) ν_{max}: 3534, 2960, 1612, 1498 cm^{-1}. ESIMS. m/z: 428 $(M+1)^+$. *Anal.* Calcd for $C_{27}H_{32}N_4O$: C, 75.67; H, 7.53; N, 13.07. Found: C, 75.87; H, 7.33; N, 13.17.

2,6-Diisopropyl-4-{3-[(4-isopropylphenyl)amino]imidazo-[1,2-*a*]pyrimidin-2-yl}phenol (14). Brown powder. 1H NMR: δ 8.50 (m, 2H, CH-Ar), 8.12 (s, 1H, OH), 7.95 (s, 1H, NH), 7.66 (s, 2H, CH-Ar), 7.00 (m, 3H, CH-Ar), 6.45 (d, *J* = 8.4 Hz, 2H, CH-Ar), 3.28 (m, 2H, 2x*CH*-(CH_3)$_2$), 2.74 (m, 1H, *CH*-(CH_3)$_2$), 1.12 (d, *J* = 6.8 Hz, 6H, CH-(CH_3)$_2$), 1.04 (d, *J* = 6.8 Hz, 12H, 2xCH-(CH_3)$_2$) ppm. ^{13}C NMR: δ 151.2, 150.0, 145.0, 144.0, 139.9, 138.9, 135.3 (2C), 131.3, 127.5 (2C), 124.9, 122.7 (2C), 117.0, 113.6 (2C), 108.8, 33.0, 26.3 (2C), 24.6 (2C), 23.2 (4C) ppm. IR (KBr) ν_{max}: 3361, 3237, 2959, 1611, 1515 cm^{-1}. ESIMS. m/z: 429 $(M+1)^+$. *Anal.* Calcd for $C_{27}H_{32}N_4O$: C, 75.67; H, 7.53; N, 13.07. Found: C, 75.67; H, 7.53; N, 13.07.

4-{3-[(2,6-Dimethylphenyl)amino]imidazo[1,2-*a*]pyrimidin-2-yl}phenol (15): Pale brown powder. ^{1}H NMR: δ 9.45 (s, 1H, OH), 8.46 (s, 1H, CH-Ar), 8.18 (d, *J* = 6.2 Hz, 1H, CH-Ar), 7.83 (d, *J* = 8.4 Hz, 2H, CH-Ar), 7.10 (s, 1H, NH), 6.97 (dd, *J* = 4.6, 9.9 Hz, 1H, CH-Ar), 6.90 (d, *J* = 7.3 Hz, 2H, CH-Ar), 6.74 (d, *J* = 8.5 Hz, 2H, CH-Ar), 6.69 (t, *J* = 7.4 Hz, 1H, CH-Ar), 1.88 (s, 6H, 2xCH_3) ppm. ^{13}C NMR: δ 157.0, 148.7, 143.3, 140.6, 137.6, 130.4 (2C), 129.3 (2C), 128.4 (2C), 125.5, 124.2, 120.2, 118.9, 114.9 (2C), 108.2, 18.2 (2C) ppm. IR (KBr) ν_{max}: 3553, 3310, 1610, 1496, 1473 cm^{-1}. EIMS. m/z (relative intensity): 330 (70), 236 (16), 223 (14), 211 (48), 198 (60), 132 (25), 120 (38), 103 (9), 91 (10), 79 (100), 65 (18), 53 (45), 44 (8), 39 (26). ESIMS. m/z: 330 (M^+). *Anal.* Calcd for $C_{20}H_{18}N_4O$: C, 72.71; H, 5.49; N, 16.96. Found: C, 72.91; H, 5.29; N, 16.86.

2,6-Di-*tert*-butyl-4-{3-[(4-methoxyphenyl)amino]imidazo-[1,2-*a*]pyrimidin-2-yl}phenol (16): Brown powder. ^{1}H NMR: δ=8.60 (d, *J* = 4.6 Hz, 1H, CH-Ar), 8.31 (dd, *J* = 1.5, 5.8 Hz, 1H, CH-Ar), 8.03 (s, 1H, OH), 7.42 (d, *J* = 8.4 Hz, 2H, CH-Ar), 7.26 (s, 2H, CH-Ar), 7.14 (s, 1H, NH), 6.95 (dd, *J* = 4.5, 6.32 Hz, 1H, CH-Ar), 6.76 (d, *J* = 8.8 Hz, 2H, CH-Ar), 3.69 (s, 3H, O-CH_3), 1.41 (s, 18H, 2xC-(CH_3)$_3$) ppm. ^{13}C NMR: δ 153.5, 152.9, 145.9, 145.7, 144.8, 139.6 (2C), 136.5, 128.7, 125.1 (2C), 118.9, 118.1 (2C), 113.6 (2C), 108.4, 106.0, 55.1, 34.5 (2C),

30.1 (6C) ppm. IR (KBr) ν_{max}: 3554, 1620, 1571, 1511 cm^{-1}. EIMS. m/z (relative intensity): 444 (100), 429 (23), 222 (13), 79 (22), 57 (43), 41 (44). *Anal.* Calcd for $C_{27}H_{32}N_4O_2$: C, 72.95; H, 7.26; N, 12.60. Found: C, 72.75; H, 7.46; N, 12.70.

Methyl 3-{[2-(4-hydroxyphenyl)imidazo[1,2-*a*]pyrimidin-3-yl]amino}benzoate (17). Pale brown powder. ^{1}H NMR: δ 9.60 (s, 1H, OH), 8.55 (s, 1H, CH-Ar), 8.47 (s, 1H, NH), 8.39 (d, *J* = 6.4 Hz, 1H, CH-Ar), 7.89 (d, *J* = 8.4 Hz, 2H, CH-Ar), 7.34 (d, *J* = 7.5 Hz, 1H, CH-Ar), 7.27 (t, *J* = 7.7 Hz, 1H, CH-Ar), 7,16 (s, 1H, CH-Ar), 7.02 (dd, *J* = 4.3, 6.3 Hz, 1H, CH-Ar), 6.79 (d, *J* = 8.4 Hz, 2H, CH-Ar), 6.73 (d, *J* = 7.2 Hz, 1H, CH-Ar), 3.77 (s, 3H, CH_3) ppm. IR (KBr) ν_{max}: 3559, 1727, 1609, 1529, 1480 cm^{-1}. EIMS. m/z (relative intensity): 360 (100), 198 (72), 120 (8), 102 (7), 79 (40), 53 (16), 38 (8). *Anal.* Calcd for $C_{20}H_{16}N_4O_3$: C, 66.66; H, 4.48; N, 15.55. Found: C, 66.86; H, 4.28; N, 15.65.

Methyl 2-{[2-(4-hydroxyphenyl)imidazo[1,2-*a*]pyrimidin-3-yl]amino}benzoate (18). Pale brown powder. ^{1}H NMR: δ 9.61 (s, 1H, OH), 9.24 (s, 1H, NH), 8.54 (s, 1H, CH-Ar), 8.39 (d, *J* = 5.8 Hz, 1H, CH-Ar), 7.96 (d, *J* = 8.0 Hz, 1H, CH-Ar), 7.84 (d, *J* = 7.6 Hz, 2H, CH-Ar), 7.25 (t, *J* = 6.6 Hz, 1H, CH-Ar), 7.00 (s, 1H, CH-Ar), 6.80 (m, 3H, CH-Ar), 6.14 (d, *J* = 8.5 Hz, 1H, CH-Ar), 3.93 (s, 3H, O-CH_3) ppm. IR (KBr) ν_{max}: 3555, 3296, 1683, 1615, 1493 cm^{-1}. EIMS. m/z (relative intensity): 360 (96), 328 (67), 299 (75), 198 (75), 164 (13), 130 (12), 119 (12), 102 (13), 92 (8), 79 (100), 65 (12), 53 (35), 39 (16). *Anal.* Calcd for $C_{20}H_{16}N_4O_3$: C, 66.66; H, 4.48; N, 15.55. Found: C, 66.86; H, 4.28; N, 15.65.

2-Methoxy-4-{3-[(4-methoxyphenyl)amino]-5,7-dimethylimidazo[1,2-*a*]pyrimidin-2-yl}phenol (19): Brown powder. ^{1}H NMR: δ 9.07 (s, 1H, OH), 7.71 (s, 1H, NH), 7.61 (s, 1H, CH-Ar), 7.49 (d, *J* = 8.2 Hz, 1H, CH-Ar), 6.76 (m, 3H, CH-Ar), 6.66 (s, 1H, CH-Ar), 6.40 (d, *J* = 8.5 Hz, 2H, CH-Ar), 3.63 (s, 6H, 2xO-CH_3), 2.63 (s, 3H, CH_3), 2.46 (s, 3H, CH_3) ppm. IR (KBr) ν_{max}: 3522, 3396, 1620, 1509 cm^{-1}. EIMS. m/z (relative intensity): 390 (25), 256 (32), 214 (10), 134 (14), 108 (100), 93 (13), 77 (15), 67 (93), 53 (12), 42 (23). *Anal.* Calcd for $C_{22}H_{22}N_4O_3$: C, 67.68; H, 5.68; N, 14.35. Found: C, 67.88; H, 5.48; N, 14.45.

Methyl 3-{[2-(3,5-di-*tert*-butyl-4-hydroxyphenyl)imidazo-[1,2-*a*]pyrimidin-3-yl]amino}benzoate (20). Dark brown powder. ^{1}H NMR: δ 8.56 (s, 1H, OH), 8.49 (m, 2H, NH+CH-Ar), 7.82 (s, 2H, CH-Ar), 7.35 (d, *J* = 7.3 Hz, 1H, CH-Ar), 7.28 (t, *J* = 7.7 Hz, 1H, CH-Ar), 7.15 (s, 1H, CH-Ar), 7.08 (s, 1H, CH-Ar), 7.04 (m, 1H, CH-Ar), 6.77 (d, *J* = 6.8 Hz, 1H, CH-Ar), 3.77 (s, 3H, O-CH_3), 1.29 (s, 18H, 2xC-(CH_3)$_3$) ppm. ^{13}C NMR: δ 166.2, 154.1, 149.9, 146.0, 144.8, 139.9, 138.8 (2C), 130.9, 130.6, 129.7, 124.2, 123.6 (2C), 119.2, 117.6, 115.4, 113.3, 108.6, 51.9, 34.4 (2C), 30.1 (6C) ppm. IR (KBr) ν_{max}: 3629, 2951, 2360, 1719, 1605 cm^{-1}. ESIMS. m/z: 376 (M^+). *Anal.* Calcd for $C_{28}H_{32}N_4O_3$: C, 71.16; H, 6.83; N, 11.86. Found: C, 71.36; H, 6.93; N, 11.66.

Mixture of 4-[2-(o-tolylamino)imidazo[1,2-*a*]pyrimidin-3-yl]- and 4-[2-(o-tolylamino)imidazo[1,2-*a*]pyrimidin-2-yl]-2,6-dimethoxyphenols (21). Brown powder. Major compound ^{1}H NMR: δ 8.55 (m, 3H, OH+2CH-Ar), 7.54 (s, 1H, NH), 7.30 (s, 1H, CH-Ar), 7.12 (d, 1H, *J* = 7.3 Hz, CH-Ar), 7.04 (dd, 1H, *J* = 4.7, 6.07 Hz, 1H, CH-Ar), 6.83 (d, *J* = 7.6 Hz, 1H, CH-Ar), 6.68 (t, *J* = 7.4 Hz, 1H, CH-Ar), 5.93 (d, *J* = 7.4 Hz, 1H, CH-Ar), 3.66 (s, 6H, 2xO-CH_3), 2.49 (s, 3H, CH_3) ppm. Minor compound: ^{1}H NMR: δ 8.78 (d, *J* = 7.4 Hz, 1H, CH-Ar), 8.62 (s, 1H, OH), 8.38 (s, 1H, NH), 7.25 (s, 2H, CH-Ar), 7.21 (m, 3H, CH-Ar), 7.12 (d, *J* = 7.4 Hz, 1H, CH-Ar), 6.92 (t, *J* = 7.4 Hz, 1H, CH-Ar), 6.72 (t, *J* = 7.4 Hz, 1H, CH-Ar), 3.77 (s, 6H, 2xO-CH_3), 2.22 (s, 3H, CH_3) ppm.

4-{3-[(4-Isopropylphenyl)amino]imidazo[1,2-*a*]pyrimidin-2-yl}benzene-1,2-diol (22). Brown powder. ^{1}H NMR: δ 9.05 (s, 1H, OH), 8.94 (s, 1H, OH), 8.51 (dd, *J* = 1.6, 5.2 Hz, 1H, CH-Ar), 8.29 (d, *J* = 6.6 Hz, 1H, CH-Ar), 7.99 (s, 1H, NH), 7.59 (s, 1H, CH-Ar), 7.39 (d, *J* = 8.2 Hz, 1H, CH-Ar), 6.99 (m, 3H, CH-Ar), 6.73 (d, *J* = 8.2 Hz, 1H, CH-Ar), 6.43 (d, *J* = 8.2 Hz, 2H, CH-Ar), 2.74 (m, 1H, *CH*-(CH_3)$_2$), 1.13 (d, *J* = 6.8 Hz, 6H, CH-(CH_3)$_2$) ppm. IR (KBr) ν_{max}: 3221, 2959, 2361, 1607, 1535, 1514 cm^{-1}. ESIMS. m/z: 360 (M^+). *Anal.* Calcd for $C_{21}H_{20}N_4O_2$: C, 69.98; H, 5.59; N, 15.54. Found: C, 69.78; H, 5.79; N, 15.64.

Methyl 2-{[2-(3,4-dihydroxyphenyl)imidazo[1,2-*a*]pyrimidin-3-yl]amino}benzoate (23). Dark brown powder. ^{1}H NMR: δ 9.24 (s, 1H, OH), 9.09 (s, 1H, NH), 9.01 (s, 1H, OH), 8.53 (dd, *J* = 1.8, 3.9 Hz, 1H, CH-Ar), 8.36 (d, *J* = 6.6 Hz, 1H, CH-Ar), 7.97 (d, *J* = 6.9 Hz, 1H, CH-Ar), 7.52 (d, *J* = 1.66 Hz, 1H, CH-Ar), 7.30 (dd, *J* = 1.7, 8.4 Hz, 1H, CH-Ar), 7.24 (d, *J* = 7.2 Hz, 1H, CH-Ar), 6.99 (dd, *J* = 4.2, 6.22 Hz, 1H, CH-Ar), 6.81 (t, *J* = 7.4 Hz, 1H, CH-Ar), 6.71 (d, *J* = 8.2 Hz, 1H, CH-Ar), 6.13 (d, *J* = 8.3 Hz, 1H, CH-Ar), 3.93 (s, 3H, CH_3) ppm. IR (KBr) ν_{max}: 3499, 3286, 2360, 1683, 1617, 1583, 1493 cm^{-1}. ESIMS. m/z: 376 (M^+). *Anal.* Calcd for $C_{20}H_{16}N_4O_4$: C, 63.83; H, 4.29; N, 14.89. Found: C, 63.63; H, 4.49; N, 14.79.

2,6-Di-*tert*-butyl-4-{3-[(2-methylphenyl)amino]imidazo-[1,2-*a*]pyrimidin-2-yl}phenol (24). Brown powder. ^{1}H NMR: δ 8.70 (s, 1H, OH), 8.36 (s, 1H, NH), 7.42 (s, 1H, CH-Ar), 7.26 (s, 3H, CH-Ar), 7.14 (s, 1H, CH-Ar), 7.07 (d, *J* = 6.8 Hz, 1H, CH-Ar), 7.00 (d, *J* = 4.9 Hz, 1H, CH-Ar), 6.95 (m, 1H, CH-Ar), 6.75 (t, *J* = 7.2 Hz, 1H, CH-Ar), 2.22 (s, 3H, CH_3), 1.38 (s, 18H, 2xC-(CH_3)$_3$) ppm. IR (KBr) ν_{max}: 3410, 2959, 1619, 1502 cm^{-1}. ESIMS. m/z: 429 (M^+). *Anal.* Calcd for $C_{27}H_{32}N_4O$: C, 75.67; H, 7.53; N, 13.07. Found: C, 75.87; H, 7.33; N, 13.17.

2,6-Di-*tert*-butyl-4-{3-[(4-isopropylphenyl)amino]imidazo-[1,2-*a*]pyrimidin-2-yl}phenol (25): Brown powder. ^{1}H NMR: δ 8.53 (s, 1H, OH), 8.47 (d, *J* = 6.3 Hz, 1H, CH-Ar), 8.02 (s, 1H, NH), 7.79 (s, 1H, CH-Ar), 7.02 (m, 4H, CH-Ar), 6.45 (d, *J* = 7.6 Hz, 2H, CH-Ar), 2.74 (m, 1H, *CH*-(CH_3)$_2$), 1.29 (s, 18H, 2xC-(CH_3)$_3$), 1.12 (d, *J* = 6.0 Hz, 6H, CH-(CH_3)$_2$) ppm. IR (KBr) ν_{max}: 3623, 3225, 2959, 1511, 1513 cm^{-1}. ESIMS. m/z: 457 (M^+). *Anal.* Calcd for $C_{29}H_{36}N_4O$: C, 76.28; H, 7.95; N, 12.27. Found: C, 76.48; H, 7.75; N, 12.37.

2,6-Dimethoxy-4-{3-[(2,6-dimethylphenyl)amino]imidazo-[1,2-*a*]pyrimidin-2-yl}-phenol (26). Pale yellow powder. ^{1}H NMR: δ 8.50 (m, 2H, CH-Ar+OH), 8.46 (s, 1H, NH), 7.14 (m, 3H, CH-Ar), 7.05 (dd, *J* = 4.7, 6.0 Hz, 1H, CH-Ar), 6.91 (d, *J* = 7.4 Hz, 2H, CH-Ar), 6.67 (t, *J* = 7.4 Hz, 1H, CH-Ar), 3.61 (s, 6H, 2xO-CH_3), 1.87 (s, 6H, CH_3) ppm. IR (KBr) ν_{max}: 3336, 1613, 1510 cm^{-1}. ESIMS. m/z: 390 (M^+). *Anal.* Calcd for $C_{22}H_{22}N_4O_3$: C, 67.68; H, 5.68; N, 14.35. Found: C, 67.48; H, 5.88; N, 14.45.

2,6-Dimethoxy-4-{3-[(4-isopropylphenyl)amino]-5,7-dimethylimidazo[1,2-*a*]pyrimidin-2-yl}-phenol (27). Brown powder. ^{1}H NMR: δ 8.44 (s, 1H, OH), 7.90 (s, 1H, NH), 7.27 (s, 2H, CH-Ar), 7.02 (d, *J* = 8.1 Hz, 2H, CH-Ar), 6.69 (s, 1H, CH-Ar), 6.43 (d, *J* = 7.3 Hz, 2H, CH-Ar), 3.59 (s, 6H, 2xO-CH_3), 2.74 (m, 1H, *CH*-(CH_3)$_2$), 2.66 (s, 3H, CH_3), 2.47 (s, 3H, CH_3), 1.12 (d, *J* = 6.8 Hz, 6H, CH-(CH_3)$_2$) ppm. IR (KBr) ν_{max}: 3598, 3304, 2359, 1617, 1515 cm^{-1}. ESIMS. m/z: 432 (M^+). *Anal.* Calcd for $C_{25}H_{28}N_4O_3$: C, 69.42; H, 6.53; N, 12.95. Found: C, 69.22; H, 6.73; N, 12.75.

Ethyl 4-{[2-(4-hydroxy-3-methoxyphenyl)imidazo[1,2-*a*]-pyrimidin-3-yl]amino}benzoate (28). Yellow powder. ^{1}H NMR: δ 9.17(s, 1H, OH), 8.82 (s, 1H, NH), 8.56 (dd, *J* = 1.8, 4.0 Hz, 1H, CH-Ar), 8.43 (d, *J* = 6.6 Hz, 1H, CH-Ar), 7.77 (d, *J*

= 8.6 Hz, 2H, CH-Ar), 7.59 (s, 1H, CH-Ar), 7.48 (d, *J* = 8.2 Hz, 1H, CH-Ar), 7.04 (dd, *J* = 4.1, 6.6 Hz, 1H, CH-Ar), 6.80 (d, *J* = 8.2 Hz, 1H, CH-Ar), 6.62 (d, *J* = 8.1 Hz, 2H, CH-Ar), 4.23 (q, *J* = 7.0, 7.0 Hz, 2H, CH_2-CH_3), 3.68 (s, 3H, O-CH_3), 1.26 (t, *J* = 7.0 Hz, 3H, CH_2-CH_3) ppm. IR (KBr) ν_{max}: 3321, 1686, 1605, 1510 cm^{-1}. ESIMS. m/z: 404 (M^+). *Anal.* Calcd for $C_{22}H_{20}N_4O_4$: C, 65.34; H, 4.98; N, 13.85. Found: C, 65.54; H, 4.78; N, 13.95.

4-{3-[(2,6-Dimethylphenyl)amino]-5,7-dimethylimidazo-[1,2-*a*]pyrimidin-2-yl}phenol (29). Brown powder. ^{1}H NMR: δ 9.45 (s, 1H, OH), 7.71 (d, *J* = 8.6 Hz, 2H, CH-Ar), 7.02 (s, 1H, NH), 6.84 (d, *J* = 7.4 Hz, 2H, CH-Ar), 6.69 (d, *J* = 8.3 Hz, 3H ,CH-Ar), 6.54 (t, *J* = 7.4 Hz, 1H, CH-Ar), 2.66 (s, 3H, CH_3), 2.46 (s, 3H, CH_3), 1.83 (s, 6H, 2xCH_3) ppm. IR (KBr) ν_{max}: 3587, 3358, 2361, 1618, 1520 cm^{-1}. ESIMS. m/z: 358 (M^+). *Anal.* Calcd for $C_{22}H_{22}N_4O$: C, 73.72; H, 6.19; N, 15.63. Found: C, 73.82; H, 6.09; N, 15.83.

4-[3-(Cyclohexylamino)imidazo[1,2-*a*]pyrimidin-2-yl]phenol (30): White powder. ^{1}H NMR: δ 9.56 (s, 1H, OH), 8.84 (s, 1H, NH), 8.30 (d, *J* = 4.4 Hz, 1H, CH-Ar), 8.04 (d, *J* = 8.4 Hz, 2H, CH-Ar), 7.81 (d, *J* = 4.3 Hz, 1H, CH-Ar), 6.84 (d, *J* = 8.3 Hz, 2H, CH-Ar), 4.88 (d, *J* = 6.3 Hz, 1H, CH-Ar), 1.37 (m, 10H, 5xCH_2) ppm. IR (KBr) ν_{max}: 3299, 2922, 2852, 1611, 1496 cm^{-1}. ESIMS. m/z: 308 (M^+). Ana1. Calcd for $C_{18}H_{20}N_4O$: C, 70.11; H, 6.54; N, 18.17. Found: C, 70.31; H, 6.34; N, 18.27.

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