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Synthesis of 4-(3-hydroxyalkyl)pyrimidines by ring transformation reactions of 2-alkylidenetetrahydrofurans with amidines

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Abstract—Domino reactions of amidines with 2-alkylidenetetrahydrofurans, prepared by cyclization of 1,3-dicarbonyl dianions or 1,3-bis-silyl enol ethers with various dielectrophiles, provided an efficient access to 4-(3-hydroxyalkyl)pyrimidines.

1. Introduction

Functionalized pyrimidines[1] play an important role as analgesic,[1a] antihypertensive,[1b] antipyretic,[1c] and anti-inflammatory drugs,[1d] as pesticides,[1e] herbicides,[1f] and plant growth regulators.[1g] For example, the naturally occurring L-lathyrine shows a wide range of biological activity, such as pollen growth inhibition, antitumor, and hypoglycaemic activity (Fig. 1).[2] Although pyrimidine syntheses are known for a long time,[3] the development of alternative and more efficient strategies is of considerable relevance.

2-Alkylidenetetrahydrofurans represent useful synthetic building blocks.[4–6] They are, for example, available by one-pot cyclizations of free and masked 1,3-dicarbonyl dianions with 1,2-dielectrophiles.[7] 2-Alkylidenetetrahydrofurans have been functionalized by lithiation and subsequent alkylation;[8] in addition, palladium(0) catalyzed cross-coupling reactions of 2′-bromo-2-alkylidenetetrahydrofurans have been reported.[9] Recently, we have reported the synthesis of 6-bromo-3-oxoalkanoates and functionalized benzofurans by reaction of 2-alkylidenetetrahydrofurans with boron tribromide (BBr_3).[10] Furans and benzofurans have been prepared based on elimination[11] or oxidation[12] reactions of 2-alkylideneterahydrofurans. Some years ago, Detty reported the synthesis of functionalized pyrazoles by reaction of 2-alkylidenetetrahydrofurans with hydrazine.[13] Herein, we report an efficient synthesis of functionalized 6-phenyl-4-(3-hydroxypropyl)pyrimidines by transformation reactions of 2-alkylidenetetrahydrofurans with amidines. The starting materials are readily available by one-pot cyclizations developed in our laboratory.

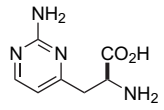
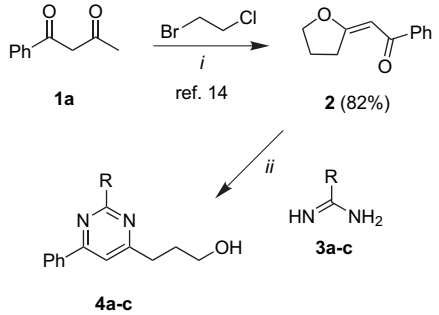


Figure 1. L-Lathyrine.

2. Results and discussion

2-(Benzoylmethylidene)tetrahydrofuran (**2**) was prepared, following our recently reported procedure,[14] by cyclization of the dianion of benzoylacetone (**1a**) with 1-bromo-2-chloroethane. The reaction of **2** with amidines **3a–c** (NEt_3, EtOH, reflux) afforded the 2-phenyl-, 2-methyl-, and 2-dimethylamino-4-(3-hydroxypropyl)pyrimidines **4a–c** (Scheme 1, Table 1).



Scheme 1. Synthesis of **4a–c**; i: (1) 2.3 equiv LDA, THF, 0 °C, 1 h, (2) $Br(CH_2)_2Cl$, −78 → 20 °C, 14 h, then reflux, 12 h; ii: NEt_3, EtOH, reflux, 12 h.

Keywords: Amidines; Heterocycles; Pyrimidines; Ring transformation; Tetrahydrofurans.
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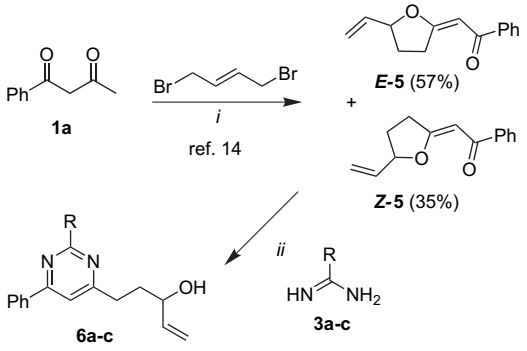
Table 1. Products and yields

4	R	% (4)[a]
a	Ph	60
b	Me	41
c	NMe_2	56

[a] Yields of isolated products.

The cyclization of dilithiated **1a** with 1,4-dibromo-2-butene gave, again following a known protocol,[14] the novel 5-vinyl-2-alkylidenetetrahydrofuran **5** as a separable mixture of *E*/*Z* diastereomers *E*-**5** and *Z*-**5**. The reaction of amidines **3a–c** with *E*-**5** afforded the functionalized pyrimidines **6a–c** (Scheme 2, Table 2).



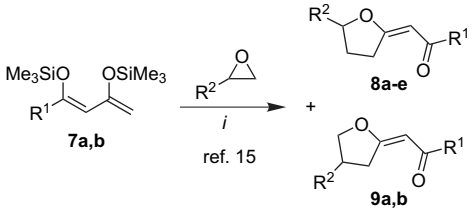
Scheme 2. Synthesis of **6a–c**; i: (1) 2.3 equiv LDA, THF, 0 °C, 1 h, (2) $BrCH_2CH{=}CHCH_2Br$, −78→20 °C, 14 h, then at 20 °C, 24 h; ii: NEt_3, EtOH, reflux, 12 h.

Table 2. Products and yields

6	R	% (6)[a]
a	Ph	76
b	Me	51
c	NMe_2	51

[a] Yields of isolated products.

The 5-alkyl- and 4-alkyl-2-alkylidenetetrahydrofurans **8a–d** and **9a**,**b** were prepared, following a recently reported procedure,[15] by $TiCl_4$ mediated cyclization of 1,3-bis-silyl enol ether **7a** (available from benzoylacetone) with various epoxides (Scheme 3, Table 3). The cyclization of **7** with 1,2-epoxypropane and 1,2-epoxybutane afforded the 4-methyl- and 4-ethyl-2-alkylidenetetrahydrofurans **9a** and **9b**, respectively; besides, a small amount of regioisomers **8a** and **8b** was isolated. The 5-chloromethyl- and 5-bromomethyl-2-alkylidenetetrahydrofurans **8c**,**d** were prepared from epichloro- and epibromohydrin, respectively. The $TiCl_4$ mediated cyclization of 1,3-bis-silyl enol ether **7b**, prepared from acetylacetone, with epibromohydrin afforded **8e**.



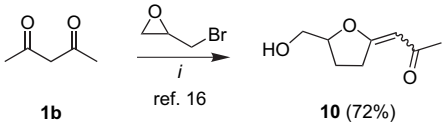
Scheme 3. Synthesis of **8a–e** and **9a**,**b**, i: $TiCl_4$ (2 equiv), CH_2Cl_2, −78→20 °C, 14 h, 20 °C, 3 h.

Table 3. Products and yields

8	9	R^1	R^2	% (8)[a]	% (9)[a]
a	**a**	Ph	Me	6	62[b]
b	**b**	Ph	Et	9[b]	65
c	**c**	Ph	CH_2Cl	54[b]	0
d	**d**	Ph	CH_2Br	56[b]	0
e	**e**	Me	CH_2Br	45	0

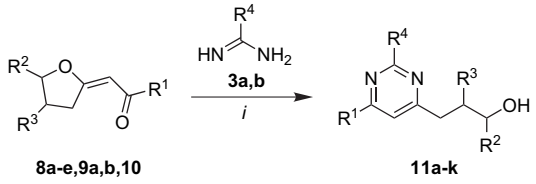
[a] Yields of isolated products.
[b] Known compound (Ref. 15)

The cyclization of dilithiated acetylacetone (**1b**) with epibromohydrin gave, following a known protocol,[16] the 5-hydroxymethyl-2-alkylidenetetrahydrofuran **10** as an inseparable mixture of *E*/*Z* diastereomers (Scheme 4).



Scheme 4. Synthesis of **10**, i: (1) NaH, *n*BuLi, THF, 0 °C, 1 h, (2) epibromohydrin, $LiClO_4$, −78→−40 °C, (3) −40 °C, 8 h, (4) −40→20 °C, (5) 20 °C, 10 h.

The reaction of 4- and 5-alkyl substituted 2-alkylidenetetrahydrofurans with amidines was studied next (Scheme 5, Table 4). The reaction of **8a** with benzamidine (**3a**) and acetamidine (**3b**) afforded the 2-phenyl- and 2-methyl-4-(3-hydroxyalkyl)pyrimidines **11a** and **11b**, respectively. Pyrimidine **11c** was prepared from **8b** and **3a**. The reaction of **3a** with **8c**,**d** gave the (4-halo-3-hydroxybutyl)pyrimidines **11d**,**e**. (3-Hydroxyalkyl)pyrimidines **11f–i** were prepared from **9a**,**b** and **3a**,**b**. The reaction of **8e** with **3a** afforded the (4-bromo-3-hydroxybutyl)pyrimidine **11j**. Likewise, pyrimidine **11k** was prepared by reaction of 5-hydroxymethyl-2-alkylidenetetrahydrofuran **10** with benzamidine (**3a**).



Scheme 5. Synthesis of **11a–k**, i: NEt_3, EtOH, reflux, 12 h.

Table 4. Products and yields

Substrate	11	R^1	R^2	R^3	R^4	% (11)[a]
8a	**a**	Ph	Me	H	Ph	45
8a	**b**	Ph	Me	H	Me	41
8b	**c**	Ph	Et	H	Ph	55
8c	**d**	Ph	CH_2Cl	H	Ph	85
8d	**e**	Ph	CH_2Br	H	Ph	79
9a	**f**	Ph	H	Me	Ph	50
9a	**g**	Ph	H	Me	Me	47
9b	**h**	Ph	H	Et	Ph	57
9b	**i**	Ph	H	Et	Me	42
8e	**j**	Me	CH_2Br	H	Ph	91
10	**k**	Me	CH_2OH	H	Ph	88

[a] Yields of isolated products.

In conclusion, we have reported an efficient synthesis of 4-(3-hydroxyalkyl)pyrimidines based on ring transformation reactions of amidines with 2-alkylidenetetrahydrofurans which are readily available by one-pot cyclization reactions of free and masked 1,3-dicarbonyl dianions.

3. Experimental

3.1. General

All solvents were dried by standard methods and all reactions were carried out under an inert atmosphere. For the ^{1}H and ^{13}C NMR spectra the deuterated solvents indicated were used. Chemical shifts δ are reported in parts per million relative to C*H*Cl$_3$ (^{1}H, 7.26 ppm) and CDCl$_3$ (^{13}C, 77.0 ppm) as internal standards. ^{13}C NMR spectral assignments are supported by DEPT analysis. Mass spectral data (MS) were obtained by electron ionization (EI, 70 eV), chemical ionization (CI, H_2O) or electrospray ionization (ESI). For preparative scale chromatography silica gel (60–200 mesh) was used. Melting points are uncorrected.

3.1.1. General procedure for the cyclization of 1,3-dicarbonyl dianions with 1-bromo-2-chloroethane and *trans*-1,4-dibromo-2-butene. A THF solution of LDA was prepared by addition of *n*BuLi (2.5 equiv) to a THF solution (10 mL/mmol) of diisopropylamine (2.5 equiv) at 0 °C. To the LDA solution was added the 1,3-dicarbonyl compound (1.0 equiv) at 0 °C and the solution was stirred at 0 °C for 1 h. To the solution was added 1-bromo-2-chloroethane (or *trans*-1,4-dibromo-2-butene) (1.2 equiv) at −78 °C. Subsequently, the temperature was allowed to rise to 20 °C during 14 h and the solution was stirred at 20 °C for 24 h. To the reaction mixture was added an aqueous solution of HCl (10%, 10 mL/mmol) and the mixture was extracted with diethylether (2×10 mL/mmol) and then dichloromethane (3×10 mL/mmol). The combined organic extracts were dried (Na_2SO_4), filtered, and the filtrate was concentrated in vacuo. The residue was purified by column chromatography (silica gel, *n*-hexane/EtOAc) to give 2-alkylidenetetrahydrofuran **2** (or **5**).

3.1.1.1. (Tetrahydrofuran-2(3*H*)-ylidene)acetophenone (2).[7a] Starting with benzoylacetone (2.50 g, 15.4 mmol), diisopropylamine (7.03 mL, 50 mmol), *n*BuLi (31.4 mL, 50 mmol, 15% in *n*-hexane), and 1-bromo-2-chloroethane (2.40 mL, 17 mmol) in THF (150 mL), **2a** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=75:1→1:1) as a yellow oil (2.367 g, 82%). ^{1}H NMR (CDCl$_3$, 300 MHz): δ=2.16 (quint, J=7.2 Hz, 2H, CH_2 at C-4), 3.29 (t, J=7.8 Hz, 2H, CH_2 at C-3), 4.30 (t, J=7.2 Hz, 2H, OCH_2 at C-5), 6.55 (s, 1H, HC=C), 7.40–7.52 (m, 3H, 3×CH of Ph), 7.86–7.92 (m, 2H, 2×CH of Ph). ^{13}C NMR (CDCl$_3$, 75 MHz): δ_C=23.5 (C-3), 31.2 (C-4, CH_2), 71.7 (C-5, OCH_2), 94.9 (H*C*=C–O), 127.4 (2C), 128.1 (2C), 131.5 (CH of Ph), 139.6 (C of Ph), 179.0 (O–*C*=CH), 189.9 (C=O). IR (neat, cm^{-1}): $\tilde{\nu}$=2985 (w), 2900 (w), 1656 (s), 1599 (s), 1588 (s), 1570 (s), 1447 (w), 1388 (m), 1363 (w), 1269 (w), 1283 (w), 1166 (s), 1054 (w), 1016 (m), 967 (s), 929 (m), 885 (w), 786 (w), 704 (s), 655 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=204 (4.21), 250 (3.93), 284 (4.26). MS (EI, 70 eV): *m*/*z* (%)=188 (M$^+$, 23), 77 (75), 70 (100). HRMS (ESI): calcd for $C_{12}H_{12}O_2$ [M$^+$]: 188.0832; found: 188.0822. Anal. Calcd for $C_{12}H_{12}O_2$ (188.226): C 76.57, H 6.43. Found: C 76.31, H 5.95.

3.1.1.2. (5-Vinyltetrahydrofuran-2(3*H*)-ylidene)acetophenone (5). Starting with benzoylacetone (1.622 g, 10 mmol), diisopropylamine (3.51 mL, 25 mmol), *n*BuLi (10 mL, 25 mmol, 2.5 M in *n*-hexane), and *trans*-1,4-dibromo-2-butene (2.781 g, 13 mmol) in THF (100 mL), *E*-**5** (1.221 g, 57%) and *Z*-**5** (0.747 g, 35%) were isolated after chromatography (silica gel, *n*-hexane/EtOAc=75:1→1:1) as a yellow solid and dark yellow oil, respectively (combined yield: 92%). *E*-**5**: mp=60.5 °C. ^{1}H NMR (CDCl$_3$, 300 MHz): δ=1.86–1.98 (m, 1H, CH_2 at C-4), 2.28–2.40 (m, 1H, CH_2 at C-4), 3.14–3.26 (m, 1H, CH_2 at C-3), 3.40–3.51 (m, 1H, CH_2 at C-3), 4.87–4.94 (m, 1H, OCH at C-5), 5.25–5.41 (m, 2H, CH_2=CH), 5.85–5.96 (m, 1H, C*H*=CH_2), 6.57 (m, 1H, C*H*=C), 7.40–7.52 (m, 3H, 3×CH of Ph), 7.86–7.92 (m, 2H, 2×CH of Ph). ^{13}C NMR (CDCl$_3$, 50 MHz): δ_C=29.7 (C-3), 31.4 (C-4, CH_2), 84.1 (C-5, OCH), 95.1 (H*C*=C–O), 117.6 (*C*H_2=CH), 127.6 (2C), 128.3 (2C, CH of Ph), 131.7 (*C*H=CH_2), 135.9 (CH of Ph), 139.8 (C of Ph), 178.5 (O–*C*=CH), 190.1 (C=O). IR (KBr, cm^{-1}): $\tilde{\nu}$=3059 (w), 2941 (w), 1640 (s), 1591 (s), 1566 (s), 1426 (w), 1382 (m), 173 (s), 997 (m), 974 (m), 932 (m), 900 (s), 841 (w), 790 (w), 705 (m). UV–vis (CH_3CN, nm): λ_{max} (log ε)=204 (4.16), 251 (3.92), 284 (4.27). MS (EI, 70 eV): *m*/*z* (%)=214 (M$^+$, 77), 160 (7), 146 (67), 137 (12), 129 (1), 120 (1), 108 (2), 105 (100), 77 (60). Anal. Calcd for $C_{14}H_{14}O_2$ (214.253): C 78.48, H 7.59; Found: C 78.33, H 7.63. *Z*-**5**: ^{1}H NMR (CDCl$_3$, 300 MHz): δ=1.85–2.01 (m, 2H, CH_2 at C-4), 2.59 (t, J=7.2 Hz, 2H, CH_2 at C-3), 4.18–4.25 (m, 1H, OCH at C-5), 5.14–5.31 (m, 2H, CH_2=CH), 5.84–5.95 (m, 1H, C*H*=CH_2), 6.20 (s, 1H, CH=C), 7.42–7.60 (m, 3H, 3×CH of Ph), 7.86–7.89 (m, 2H, 2×CH of Ph). ^{13}C NMR (CDCl$_3$, 75 MHz): δ_C=31.9 (C-3), 34.8 (C-4, CH_2), 71.3 (C-5, OCH), 95.8 (*C*H=C–O), 114.3 (*C*H_2=CH), 126.4 (2C), 128.1 (2C), 131.8 (CH of Ph), 134.0 (C of Ph), 140.2 (*C*H=CH_2), 181.8 (O–*C*=CH), 197.3 (C=O). IR (neat, cm^{-1}): $\tilde{\nu}$=3069 (w), 2979 (w), 2927 (w), 1716 (w), 1604 (s), 1572 (s), 1490 (m), 1456 (m), 1424 (m), 1360 (w), 1320 (w), 1298 (m), 1271 (m), 1181 (w), 1160 (w), 1150 (w), 1118 (w), 1055 (w), 1025 (w), 994 (m), 927 (m), 767 (m), 694 (m). UV–vis (CH_3CN, nm): λ_{max} (log ε)=246 (3.85), 299 (4.00). MS (EI, 70 eV): *m*/*z* (%)=214 (M$^+$, 100), 160 (7), 147 (81), 137 (10), 129 (1), 120 (1), 105 (99), 77 (82). HRMS (ESI): calcd for $C_{14}H_{14}O_2$ [M$^+$]: 214.0988; found: 214.0983.

3.1.2. General procedure for the [3+2] cyclization of 1,3-bis-silyl enol ethers with epoxides. To a CH_2Cl_2 solution (10 mL/mmol) of 1,3-bis-silyl enol ether **7a**,**b** (1.0 equiv) and the epoxide (1.2 equiv) [in the presence of molecular sieves (4 Å)], was added $TiCl_4$ (2.4 equiv) at −78 °C. Subsequently, the temperature was allowed to rise to 20 °C during 14 h and the solution was stirred for 3 h at 20 °C. The molecular sieves were filtered-off and washed with CH_2Cl_2. To the solution was added a saturated aqueous solution of $NaHCO_3$, the organic layer was separated and the aqueous layer was repeatedly extracted with CH_2Cl_2. The combined organic extracts were dried (Na_2SO_4), filtered, and the filtrate was

concentrated in vacuo. The residue was purified by column chromatography (silica gel, *n*-hexane/EtOAc) to give the 2-alkylidenetetrahydrofurans **8a–e** and **9a**,**b**.

Compounds **8a**,**9a**: Starting with **7a** (6.131 g, 20 mmol), propeneoxide (1.7 mL, 24 mmol) and $TiCl_4$ (5.3 mL, 48 mmol) in CH_2Cl_2 (200 mL), **9a** (2.487 g, 62%) and **8a** (0.232 g, 6%) were isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as light brown oils.

3.1.2.1. (4-Methyltetrahydrofuran-2(3*H*)-ylidene)acetophenone (9a).[15] ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.11 (d, J=6.6 Hz, 3H, CH_3), 2.45–2.56 (m, 1H, CH at C-4), 2.61–2.70 (m, 2H, CH_2 at C-3), 3.55–3.62 (m, 1H, OCH_2 at C-5), 4.07–4.15 (m, 1H, OCH_2 at C-5), 6.20 (d, J=1.8 Hz, 1H, CH=C), 7.43–7.54 (m, 3H, 3×CH of Ph), 7.87–7.91 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=17.4 (CH_3), 31.7 (C-4, CH), 39.4 (C-3, CH_2), 77.7 (C-5, OCH_2), 95.4 (*C*H=C-O), 127.6 (2C), 128.2 (2C), 131.6 (CH of Ph), 139.7 (C of Ph), 179.1 (O–*C*=CH), 190.2 (C=O). IR (neat, cm^{-1}): $\tilde{\nu}$=2967 (w), 1607 (s), 1457 (m), 1418 (m), 1267 (m), 845 (w), 766 (m), 694 (m). MS (EI, 70 eV): *m*/*z* (%)=202 (M^+, 70), 187 (100), 162 (13), 147 (20), 125 (22), 105 (45). Anal. Calcd for $C_{13}H_{14}O_2$ (202.249): C 77.20, H 6.98. Found: C 77.03, H 7.16.

3.1.2.2. (5-Methyltetrahydrofuran-2(3*H*)-ylidene)acetophenone (8a). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.57 (d, J=6.6 Hz, 3H, CH_3), 1.96–2.08 (m, 1H, CH_2 at C-4), 2.18–2.29 (m, 1H, CH_2 at C-4), 3.54–3.61 (m, 2H, CH_2 at C-3), 4.32–4.41 (m, 1H, OCH at C-5), 6.20 (d, J=1.8 Hz, 1H, CH=C), 7.38–7.54 (m, 3H, 3×CH of Ph), 7.87–7.91 (m, 2H, 2×CH of Ph). IR (neat, cm^{-1}): $\tilde{\nu}$=2967 (w), 1721 (w), 1681 (m), 1607 (s), 1453 (m), 1414 (m), 1269 (m), 1184 (w), 1079 (w), 1006 (w), 847 (w), 768 (m), 694 (m). MS (EI, 70 eV): *m*/*z* (%)=202 (M^+, 10), 187 (7), 162 (43), 147 (51), 105 (100), 91 (10), 77 (66), 69 (93). HRMS (ESI): calcd for $C_{13}H_{14}O_2$ [M^+]: 202.0988; found: 202.0994.

Compounds **8b**,**9b**: Starting with **7a** (6.131 g, 20 mmol), 1,2-epoxybutane (2.1 mL, 24 mmol) and $TiCl_4$ (5.3 mL, 48 mmol) in CH_2Cl_2 (200 mL), **9b** (2.792 g, 65%) and **8b** (0.402 g, 9%) were isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as light brown oils.

3.1.2.3. (4-Ethyltetrahydrofuran-2(3*H*)-ylidene)acetophenone (9b). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=0.86 (t, J=7.5 Hz, 3H, CH_2CH_3), 1.29–1.43 (m, 2H, CH_2CH_3), 1.75–1.89 (m, 1H, CH at C-4), 2.31–2.37 (m, 1H, CH_2 at C-3), 2.44–2.52 (m, 1H, CH_2 at C-3), 3.63–4.01 (dm, 2H, OCH_2 at C-5), 6.08 (d, J=1.8 Hz, 1H, CH=C), 7.30–7.44 (m, 3H, 3×CH of Ph), 7.74–7.78 (m, 2H, 2×CH of Ph). IR (neat, cm^{-1}): $\tilde{\nu}$=2964 (m), 2880 (w), 1721 (w), 1607 (s), 1457 (s), 1266 (s), 1184 (m), 1150 (w), 1080 (m), 1040 (m), 1006 (w), 925 (w), 847 (m), 767 (m), 694 (m). MS (EI, 70 eV): *m*/*z* (%)=216 (M^+, 10), 187 (100), 105 (72), 77 (70), 69 (91). HRMS (ESI): calcd for $C_{14}H_{16}O_2$ [M^+]: 216.1145; found: 216.1142.

3.1.2.4. (5-Ethyltetrahydrofuran-2(3*H*)-ylidene)acetophenone (8b).[15] ^{1}H NMR ($CDCl_3$, 300 MHz): δ=0.98 (t, J=7.5 Hz, 3H, CH_2CH_3), 1.43–1.55 (m, 2H, CH_2CH_3), 1.68–1.82 (m, 1H, CH_2 at C-4), 2.21–2.32 (m, 1H, CH_2 at C-4), 2.50 (dt, J=8.1, 0.6 Hz, 1H, CH_2 at C-3), 2.66–2.81 (m, 1H, CH_2 at C-3), 4.32–4.38 (m, 1H, OCH at C-5), 6.82 (d, J=1.8 Hz, 1H, CH=C), 7.34–7.50 (m, 3H, 3×CH of Ph), 7.81–7.85 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=9.7 (CH_2CH_3), 27.8 (CH_2CH_3), 28.6 (C-3), 31.8 (C-4, CH_2), 85.6 (C-5, OCH), 94.6 (*C*H=C-O), 127.4 (2C), 128.2 (2C), 131.5 (CH of Ph), 139.8 (C of Ph), 179.1 (O–*C*=CH), 190.2 (C=O). IR (neat, cm^{-1}): $\tilde{\nu}$=3084 (w), 3061 (w), 3030 (w), 2966 (s), 2933 (s), 2879 (m), 2855 (m), 1654 (s), 1587 (s), 1571 (m), 1456 (m), 1447 (m), 1386 (s), 1167 (s). MS (EI, 70 eV): *m*/*z* (%)=216 (M^+, 70), 201 (100), 176 (13), 161 (20), 139 (22), 119 (45). The exact molecular mass *m*/*z*=216.1150±2 ppm [M^+] for $C_{14}H_{16}O_2$ was confirmed by HRMS (EI, 70 eV). Anal. Calcd for $C_{14}H_{16}O_2$ (216.276): C 77.75, H 7.46. Found: C 77.48, H 7.60.

3.1.2.5. (5-Chloromethyltetrahydrofuran-2(3*H*)-ylidene)acetophenone (8c).[15] Starting with **7a** (6.131 g, 20 mmol), epichlorohydrin (1.9 mL, 24 mmol) and $TiCl_4$ (5.3 mL, 48 mmol) in CH_2Cl_2 (200 mL), **8c** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow oil (2.538 g, 54%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=2.00–2.12 (m, 1H, CH_2 at C-4), 2.30–2.41 (m, 1H, CH_2 at C-4), 3.19–3.31 (m, 1H, CH_2 at C-3), 3.43–3.55 (m, 1H, CH_2 at C-3), 3.69 (d, J=5.7 Hz, 2H, CH_2–Cl), 4.70–4.80 (m, 1H, OCH at C-5), 6.59 (t, J=1.5 Hz, 1H, CH=C), 7.40–7.53 (m, 3H, 3×CH of Ph), 7.89–7.92 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=26.6 (C-3), 31.2 (C-4, CH_2), 45.4 (CH_2–Cl), 82.1 (C-5, OCH), 95.3 (*C*H=C–O), 127.4 (2C), 128.2 (2C), 131.7 (CH of Ph), 139.4 (C of Ph), 177.7 (O–*C*=CH), 190.1 (C=O). IR (neat, cm^{-1}): $\tilde{\nu}$=3099 (w), 3083 (w), 3055 (w), 2984 (w), 2919 (w), 1663 (s), 1598 (s), 1583 (s), 1566 (s), 1383 (m), 1374 (m), 1167 (s). MS (EI, 70 eV): *m*/*z* (%)=236 (M^+, 100), 159 (52), 105 (46), 77 (33), 69 (48). The exact molecular mass *m*/*z*=236.0604±2 ppm [M^+] for $C_{13}H_{13}ClO_2$ was confirmed by HRMS (EI, 70 eV). Anal. Calcd for $C_{13}H_{13}ClO_2$ (236.694): C 65.97, H 5.54. Found: C 66.12, H 5.43.

3.1.2.6. (5-Bromomethyltetrahydrofuran-2(3*H*)-ylidene)acetophenone (8d).[15] Starting with **7a** (6.131 g, 20 mmol), epibromohydrin (2.0 mL, 24 mmol) and $TiCl_4$ (5.3 mL, 48 mmol) in CH_2Cl_2 (200 mL), **8d** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow oil (3.149 g, 56%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.98–2.11 (m, 1H, CH_2 at C-4), 2.34–2.45 (m, 1H, CH_2 at C-4), 3.19–3.30 (m, 1H, CH_2 at C-3), 3.43–3.52 (m, 1H, CH_2 at C-3), 3.53–3.57 (m, 2H, CH_2–Br), 4.69–4.78 (m, 1H, OCH at C-5), 6.58 (t, J=1.5 Hz, 1H, CH=C), 7.40–7.52 (m, 3H, 3×CH of Ph), 7.88–7.92 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=27.8 (C-3), 31.2 (C-4, CH_2), 33.4 (CH_2–Br), 81.9 (C-5, OCH), 95.3 (*C*H=C–O), 127.4 (2C), 128.2 (2C), 131.7 (CH of Ph), 139.4 (C of Ph), 177.6 (O–*C*=CH), 190.1 (C=O). IR (neat, cm^{-1}): $\tilde{\nu}$=3098 (w), 3054 (w), 3026 (w), 2981 (w), 2945 (w), 2917 (w), 1660 (s), 1596 (s), 1567 (s), 1457 (m), 1433 (m), 1380 (s), 1165 (s). MS (EI, 70 eV): *m*/*z* (%)=280 (M^+, 60), 203 (24), 180 (18), 147 (35), 122 (33), 105 (100). The exact molecular mass *m*/*z*=280.0099±2 ppm [M^+] for $C_{13}H_{13}BrO_2$ was

confirmed by HRMS (EI, 70 eV). Anal. Calcd for $C_{13}H_{13}BrO_2$ (281.145): C 55.54, H 4.66. Found: C 55.22, H 4.36.

3.1.2.7. 1-(5-Bromomethyldihydrofuran-2(3*H*)-ylidene)propan-2-one (8e). Starting with **7b** (7.334 g, 30 mmol), epibromohydrin (2.98 mL, 36 mmol) and $TiCl_4$ (7.91 mL, 72 mmol) in CH_2Cl_2 (150 mL), **8e** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a light brown oil (2.931 g, 45%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.92–2.05 (m, 1H, CH_2 at C-4), 2.14 (s, 3H, CH_3), 2.23–2.34 (m, 1H, CH_2 at C-4), 3.00–3.12 (m, 1H, CH_2 at C-3), 3.28–3.38 (m, 1H, CH_2 at C-3), 3.39–3.58 (m, 2H, CH_2–Br), 4.61–4.70 (m, 1H, OCH at C-5), 5.83 (t, J=1.5 Hz, 1H, CH=C). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=28.2 (C-3, CH_2), 31.3 (CH_3), 31.6 (C-4, CH_2), 34.0 (CH_2–Br), 82.1 (C-5, OCH), 99.4 (*C*H=C–O), 176.2 (O–*C*=CH), 198.4 (C=O). IR (neat, cm^{-1}): $\tilde{\nu}$=2960 (m), 2928 (m), 1704 (s), 1617 (s), 1591 (s), 1421 (s), 1365 (s), 1303 (s), 1252 (s), 1150 (s), 1086 (m), 1054 (m), 1020 (m), 979 (w), 951 (w), 662 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=260 (3.86). MS (EI, 70 eV): *m*/*z* (%)=220 (M^+ [^{81}Br], 9), 218 (M^+ [^{79}Br], 9), 205 (26), 203 (26), 139 (2), 123 (2), 95 (5), 85 (14), 69 (100). HRMS (ESI): calcd for $C_8H_{11}BrO_2$ [M^+]: 219.9916 (^{81}Br), 217.9937 (^{79}Br); found: 219.9921 (^{81}Br), 217.9942 (^{79}Br).

3.1.3. Cyclization of 1,3-dicarbonyl dianions with epibromohydrin: 1-(dihydro-5-(hydroxymethyl)furan-2(3*H*)-ylidene)propan-2-one (10). The synthesis of **10** has been previously reported.[16]

3.1.4. General procedure for synthesis of functionalized pyrimidines. To an ethanol (20 mL/mmol) solution of (tetrahydrofuran-2(3*H*)-ylidene)acetophenone (**2**, **5**, **8a**–**d**, **9a**,**b**, or **10**) (1 equiv) were added the amidine (**3a**–**c**) (10 equiv) and triethylamine (10 equiv) at 20 °C. The reaction mixture was heated and stirred for 12 h at 60 °C. After cooling, to the reaction mixture was added water (30 mL/mmol), and extracted with dichloromethane repeatedly. The combined organic extracts were dried (Na_2SO_4), filtered, and the filtrate was concentrated in vacuo. The residue was purified by column chromatography (silica gel, *n*-hexane/EtOAc) to give (6-phenylpyrimidin-4-yl) alcohols (**4a**–**c**, **6a**–**c** or **11a**–**k**).

3.1.4.1. 3-(2,6-Diphenylpyrimidin-4-yl)propan-1-ol (4a). Starting with **2** (0.100 g, 0.53 mmol), benzamidine hydrochloride monohydrate (**3a**) (0.928 g, 5.31 mmol) and NEt_3 (1.1 mL, 8.0 mmol) in ethanol (10 mL), **4a** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=20:1→1:1) as a pale yellow solid (0.92 g, 60%), mp=80.0 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ=2.13 (quint, J=6.45 Hz, 2H, CH_2), 3.05 (t, J=6.9 Hz, 2H, CH_2), 3.20 (br s, 1H, OH), 3.80 (t, J=6.0 Hz, 2H, CH_2OH), 7.46–7.55 (m, 7H, CH, 6×CH of Ph), 8.20–8.24 (m, 2H, 2×CH of Ph), 8.54–8.57 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 150 MHz): δ_C=31.0, 35.0 (CH_2), 62.2 (*C*H_2OH), 113.9 (*C*H=C–N), 127.4 (2C), 128.5 (2C), 128.7 (2C), 129.0 (2C), 130.8, 131.0 (CH of Ph), 137.2, 138.0 (C of Ph), 164.3 (*C*–Ph), 164.4 (N=C–N), 170.8 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3372 (br), 3088 (m), 3064 (m), 3038 (m), 3006 (w), 2933 (s), 2873 (m, C–H), 1770 (w), 1731 (m), 1598 (s), 1571 (s), 1533 (s), 1497 (m), 1445 (m), 1425 (m), 1400 (m), 1374 (s), 1317 (m), 1290 (m), 1221 (m), 1177 (m), 1061 (s), 1031 (s), 934 (m), 911 (w), 879 (w), 837 (w), 778 (w), 751 (s), 695 (s), 667 (w), 636 (m), 582 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=206 (4.52), 256 (4.52). MS (EI, 70 eV): *m*/*z* (%)=290 (M^+, 1), 273 (6), 259 (11), 246 (100), 219 (1), 205 (15), 164 (14), 103 (45), 77 (29). The exact molecular mass *m*/*z*=290.1419±2 ppm [M^+] for $C_{19}H_{18}N_2O$ was confirmed by HRMS (EI, 70 eV).

3.1.4.2. 3-(2-Methyl-6-phenylpyrimidin-4-yl)propan-1-ol (4b). Starting with **2** (0.100 g, 0.53 mmol), acetamidine hydrochloride (**3b**) (0.527 g, 5.3 mmol) and NEt_3 (1.1 mL, 8.0 mmol) in ethanol (10 mL), **4b** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=50:1→1:1) as a pale yellow oil (0.049 g, 41%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=2.02 (quint, J=6.3 Hz, 2H, CH_2), 2.77 (s, 3H, CH_3), 2.95 (t, J=6.9 Hz, 2H, CH_2), 3.74 (t, J=5.7 Hz, 2H, OCH_2), 7.40 (s, 1H, CH), 7.48–7.51 (m, 3H, 3×CH of Ph), 8.04–8.07 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=26.0 (CH_3), 31.0, 35.1 (CH_2), 62.1 (OCH_2), 113.1 (*C*H=C–N), 127.2 (2C), 128.2, 128.9 (2C, CH of Ph), 137.0 (C of Ph), 164.5 (*C*–Ph), 167.7 (N=C–N), 170.2 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3340 (s), 3065 (m), 2933 (s), 2870 (m), 1585 (s), 1535 (s), 1441 (s), 1396 (s), 1339 (m), 1285 (m), 1221 (w), 1179 (w), 1118 (w), 1063 (s), 1005 (w), 921 (w), 874 (w), 753 (m), 695 (s), 650 (w), 622 (w), 588 (w), 541 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=203 (4.40), 247 (3.97), 275 (4.07), 322 (3.50). MS (EI, 70 eV): *m*/*z* (%)=228 (M^+, 1), 211 (4), 197 (8), 184 (100), 128 (3), 114 (2), 102 (8), 77 (6). HRMS (ESI): calcd for $C_{14}H_{16}N_2O$ ([M+1]$^+$): 229.13409; found: 229.13331.

3.1.4.3. 3-(2-Dimethylamino-6-phenylpyrimidin-4-yl)-propan-1-ol (4c). Starting with **2** (0.100 g, 0.53 mmol), 1,1-dimethylguanidine sulfate (**3c**) (1.489 g, 5.3 mmol) and NEt_3 (1.84 mL, 13.3 mmol) in ethanol (10 mL), **4c** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=50:1→1:1) as a yellow oil (0.076 g, 56%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=2.00 (quint, J=6.0 Hz, 2H, CH_2), 2.85 (t, J=6.6 Hz, 2H, CH_2), 3.26 (s, 6H, 2×CH_3), 3.75 (t, J=6.0 Hz, 2H, CH_2OH), 6.82 (s, 1H, CH=C), 7.43–7.48 (m, 3H, 3×CH of Ph), 8.04–8.08 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=30.3, 35.4 (CH_2), 37.3 (2C, CH_3), 62.5 (OCH_2), 104.1 (*C*H=C–N), 127.1 (2C), 128.6 (2C), 130.3 (CH of Ph), 137.9 (C of Ph), 162.2 (N=C–N), 164.7 (*C*–Ph), 170.6 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3365 (br), 2927 (w), 1670 (w), 1645 (w), 1563 (s), 1494 (w), 1448 (m), 1408 (m), 1368 (m), 1326 (w), 1246 (w), 1223 (w), 1181 (w), 1149 (w), 1117 (w), 1066 (m), 1027 (w), 770 (w), 695 (w). MS (EI, 70 eV): *m*/*z* (%)=257 (M^+, 8), 242 (2), 227 (4), 213 (100), 198 (6), 184 (4), 170 (9), 128 (4), 114 (2), 114 (2), 105 (12), 77 (10).

3.1.4.4. 5-(2,6-Diphenylpyrimidin-4-yl)pent-1-en-3-ol (6a). Starting with **5** (0.100 g, 0.467 mmol), benzamidine hydrochloride monohydrate (**3a**) (0.815 g, 4.67 mmol), NEt_3 (0.7 mL, 4.67 mmol) in ethanol (10 mL), **6a** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a pale yellow solid (0.112 g, 76%), mp=85 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ=2.01–2.20 (m, 2H, CH_2), 3.00–3.11 (m, 2H, CH_2), 3.59 (br s,

1H, OH), 4.30 (q, J=6.0 Hz, 1H, OCH), 5.16 (dt, J=10.4, 1.5 Hz, 1H, CH_2=CH), 5.33 (dt, J=17.2, 1.5 Hz, 1H, CH_2=CH), 5.91–6.01 (m, 1H, CH=CH_2), 7.41 (s, 1H, CH), 7.43–7.57 (m, 6H, 6×CH of Ph), 8.19–8.23 (m, 2H, 2×CH of Ph), 8.54–8.56 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=33.8, 34.9 (CH_2), 72.0 (OCH), 113.6 (*C*H=C–N), 114.6 (*C*H_2=CH), 127.1 (2C), 128.3 (2C), 128.4 (2C), 128.8 (2C), 130.5, 130.7 (CH of Ph), 136.9, 137.7 (C of Ph), 140.8 (*C*H=CH_2), 163.9 (*C*–Ph), 164.0 (N=C–N), 170.6 (N–*C*=CH). IR (KBr, cm^{-1}): $\tilde{\nu}$=3343 (br), 3064 (w), 2921 (w), 1571 (s), 1535 (s), 1373 (s), 926 (m), 752 (m), 697 (s). UV–vis (CH_3CN, nm): λ_{max} (log ε)=204 (4.56), 256 (4.54). MS (EI, 70 eV): *m*/*z* (%)=316 (M$^+$, 12), 299 (10), 285 (3), 271 (1), 259 (28), 246 (100), 103 (54), 77 (80). HRMS (ESI): calcd for $C_{21}H_{20}N_2O$ [M$^+$]: 315.1492; found: 315.1491. Anal. Calcd for $C_{21}H_{20}N_2O$ (316.402): C 79.72, H 6.37, N 8.85. Found: C 79.73, H 6.57, N 8.50.

3.1.4.5. 5-(2-Methyl-6-phenylpyrimidin-4-yl)pent-1-en-3-ol (6b). Starting with **5** (0.100 g, 0.467 g), acetamidine hydrochloride (**3b**) (0.465 g, 4.67 mmol) and NEt_3 (0.7 mL, 4.67 mmol) in ethanol (100 mL), **6b** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a pale yellow solid (0.061 g, 51%), mp=61.9 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.94–2.06 (m, 2H, CH_2), 2.77 (s, 3H, CH_3), 2.95 (dd, J=7.2, 1.5 Hz, 2H, CH_2), 4.19 (br s, 1H, OH), 4.21–4.27 (m, 1H, OCH), 5.13 (dt, J=10.5, 1.5 Hz, 1H, CH_2=CH), 5.30 (dt, J=17.1, 1.5 Hz, 1H, CH_2=CH), 5.87–5.99 (m, 1H, CH=CH_2), 7.39 (s, 1H, CH), 7.46–7.51 (m, 3H, 3×CH of Ph), 8.03–8.06 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=26.0 (CH_3), 33.9, 35.2 (CH_2), 72.0 (OCH), 113.1 (*C*H=C–N), 114.6 (*C*H_2=CH), 127.2 (2C), 128.9 (2 C), 130.7 (CH of Ph), 137.0 (C of Ph), 140.9 (*C*H=CH_2), 164.4 (*C*–Ph), 167.7 (N=C–N), 170.2 (N–*C*=CH). IR (KBr, cm^{-1}): $\tilde{\nu}$=3253 (br), 3091 (w), 3065 (w), 2921 (w), 2853 (w), 1583 (s), 1539 (s), 1497 (w), 1446 (m), 1404 (s), 1368 (m), 1326 (w), 1122 (m), 1055 (w), 998 (m), 925 (m), 862 (w), 785 (w), 743 (w), 692 (m), 624 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=204 (4.48), 249 (4.02), 255 (4.03), 275 (4.20). MS (EI, 70 eV): *m*/*z* (%)=254 (M$^+$, 9), 237 (6), 225 (2), 209 (5), 197 (25), 184 (100), 128 (5), 114 (3), 77 (6). Anal. Calcd for $C_{16}H_{18}N_2O$ (254.332): C 75.56, H 7.13, N 11.02. Found: C 75.61, H 7.18, N 10.89.

3.1.4.6. 5-(2-Dimethylamino-6-phenylpyrimidin-4-yl)-pent-1-en-3-ol (6c). Starting with **5** (0.100 g, 0.467 mmol), 1,1-dimethylguanidine sulfate (**3c**) (1.311 g, 4.67 mmol) and NEt_3 (0.7 mL, 4.67 mmol) in ethanol (10 mL), **6c** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a pale yellow oil (0.067 g, 51%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.89–1.98 (m, 1H, CH_2), 1.99–2.11 (m, 1H, CH_2), 2.79–2.93 (m, 2H, CH_2), 3.27 (s, 6H, 2×NCH_3), 4.25–4.28 (m, 1H, OCH), 5.13 (dt, J=10.5, 1.5 Hz, 1H, CH_2=CH), 5.31 (dt, J=17.1, 1.5 Hz, 1H, CH_2=CH), 5.87–5.98 (m, 1H, CH=CH_2), 6.82 (s, 1H, CH), 7.44–7.48 (m, 3H, 3×CH of Ph), 8.04–8.06 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=34.0, 34.6 (CH_2), 37.3 (NCH_3), 72.2 (OCH), 104.1 (*C*H=C–N), 114.3 (*C*H_2=CH), 127.1 (2C), 128.6 (2C), 130.3 (CH of Ph), 137.9 (C of Ph), 141.2 (*C*H=CH_2), 162.1 (N=C–N), 164.6 (*C*–Ph), 170.6 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3403 (br), 2926 (m), 2859 (w), 1680 (w), 1645 (w), 1562 (s), 1497 (w), 1445 (w), 1408 (m), 1368 (m), 1320 (w), 1245 (w), 1223 (w), 1180 (w), 1117 (w), 1067 (w), 1026 (w), 995 (w), 922 (w), 770 (w), 694 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=254 (4.27), 337 (3.45). MS (EI, 70 eV): *m*/*z* (%)=283 (M$^+$, 15), 226 (9), 213 (100), 198 (5), 184 (2), 105 (40), 77 (34). HRMS (ESI): calcd for $C_{17}H_{21}N_3O$ [M$^+$]: 283.16846; found: 283.16879.

3.1.4.7. 4-(2,6-Diphenylpyrimidin-4-yl)-butan-2-ol (11a). Starting with **8a** (0.100 g, 0.49 mmol), benzamidine hydrochloride monohydrate (**3a**) (0.857 g, 4.9 mmol) and NEt_3 (0.67 mL, 4.9 mmol) in ethanol (5 mL), **11a** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow oil (0.067 g, 45%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.28 (d, J=6.6 Hz, 3H, CH_3), 1.92–2.03 (m, 2H, CH_2), 2.93–3.07 (m, 2H, CH_2), 3.90–3.99 (m, 1H, OCH), 7.41–7.55 (m, 7H, CH=C, 6×CH of Ph), 8.20–8.24 (m, 2H, 2×CH of Ph), 8.53–8.57 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=23.1 (CH_3), 34.0, 37.0 (CH_2), 66.6 (OCH), 113.1 (*C*H=C–N), 126.2 (2C), 127.9 (2C), 128.0 (2C), 128.3 (2C), 130.1, 130.5 (CH of Ph), 136.7, 137.7 (C of Ph), 163.2 (*C*–Ph), 163.7 (N=C–N), 169.2 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3336 (br), 3061 (w), 2956 (m), 2927 (m), 2873 (w), 1633 (w), 1575 (s), 1536 (s), 1498 (w), 1451 (m), 1374 (s), 1276 (w), 1177 (w), 1112 (m), 1077 (m), 1033 (m), 753 (m), 697 (s). UV–vis (CH_3CN, nm): λ_{max} (log ε)=207 (4.48), 256 (4.52). MS (EI, 70 eV): *m*/*z* (%)=304 (M$^+$, 1), 287 (5), 272 (4), 259 (15), 245 (100), 231 (19), 227 (1), 143 (7), 128 (6), 114 (7), 104 (26), 77 (14). Anal. Calcd for $C_{20}H_{20}N_2O$ (304.391): C 78.92, H 6.62, N 9.20. Found: C 78.83, H 6.49, N 9.12.

3.1.4.8. 4-(2-Methyl-6-phenylpyrimidin-4-yl)-butan-2-ol (11b). Starting with **8b** (0.100 g, 0.49 mmol), acetamidine hydrochloride (**3b**) (0.488 g, 4.9 mmol) and NEt_3 (0.67 mL, 4.9 mmol) in ethanol (5 mL), **11b** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=50:1→EtOAc), as a pale yellow oil (0.049 g, 41%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.24 (d, J=6.3 Hz, 3H, CH_3), 1.70–1.79 (m, 1H, CH_2), 1.97–2.10 (m, 1H, CH_2), 2.35–2.49 (m, 2H, CH_2), 2.77 (s, 3H, CH_3), 3.83–3.93 (m, 1H, OCH), 7.40 (s, 1H, CH=C), 7.48–7.51 (m, 3H, 3×CH of Ph), 8.04–8.08 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=20.4, 25.4 (CH_3), 32.5, 36.8 (CH_2), 66.0 (OCH), 112.6 (*C*H=C–N), 126.7 (2C), 127.7, 128.3 (2C, CH of Ph), 136.3 (C of Ph), 163.7 (*C*–Ph), 167.0 (N=C–N), 170.8 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3339 (br), 3063 (w), 2965 (m), 2932 (m), 2878 (w), 1606 (s), 1531 (s), 1452 (m), 1421 (m), 1377 (m), 1326 (s), 1287 (s), 1180 (w), 1119 (w), 1075 (m), 1041 (m), 741 (s), 698 (m), 649 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=242 (3.96), 325 (4.18). MS (EI, 70 eV): *m*/*z* (%)=242 (M$^+$, 98), 227 (1), 225 (2), 210 (2), 197 (5), 183 (100), 169 (17), 148 (5), 105 (14), 77 (19), 57 (22). Anal. Calcd for $C_{15}H_{18}N_2O$ (242.316): C 74.35, H 7.49, N 11.56. Found: C 73.95, H 7.21, N 11.16.

3.1.4.9. 1-(2,6-Diphenylpyrimidin-4-yl)pentan-3-ol (11c). Starting with **8b** (0.100 g, 0.46 mmol), benzamidine hydrochloride monohydrate (**3a**) (0.808 g, 4.6 mmol) and NEt_3 (0.64 mL, 4.6 mmol) in ethanol (5 mL), **11c** was

isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow oil (0.081 g, 55%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.25 (t, J=7.2 Hz, 3H, CH_3), 1.51–1.63 (m, 2H, CH_2), 1.92–2.05 (m, 2H, CH_2), 2.92 (t, J=7.8 Hz, 2H, CH_2), 3.81–3.91 (m, 1H, OCH), 7.37–7.53 (m, 7H, CH=C, 6×CH of Ph), 8.19–8.22 (m, 2H, 2×CH of Ph), 8.57–8.60 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=23.5 (CH_3), 24.8, 37.8, 38.6 (CH_2), 67.7 (OCH), 113.4 (*C*H=C–N), 127.1 (2C), 128.3 (2C), 128.4 (2C), 128.8 (2C), 130.4, 130.6 (CH of Ph), 137.2, 138.1 (C of Ph), 163.7 (*C*–Ph), 164.2 (N=C–N), 171.1 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3382 (br), 3064 (w), 2974 (s), 2931 (m), 2865 (s), 2810 (w), 1721 (m), 1575 (s), 1532 (s), 1493 (m), 1451 (m), 1375 (s), 1314 (m), 1309 (m), 1278 (s), 1172 (m), 1118 (s), 1077 (m), 1029 (w), 921 (w), 841 (w), 746 (s), 697 (s), 637 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=256 (4.41). MS (EI, 70 eV): *m*/*z* (%)=318 (M^+, 1), 273 (16), 259 (14), 146 (100), 233 (2), 216 (31), 202 (5), 174 (28), 158 (5), 143 (6), 133 (16), 128 (5), 120 (17), 114 (9), 106 (14), 104 (83), 91 (6), 77 (41). Anal. Calcd for $C_{21}H_{22}N_2O$ (318.418): C 79.21, H 6.96, N 8.89. Found: C 78.99, H 7.01, N 8.64.

3.1.4.10. 1-Chloro-4-(2,6-diphenylpyrimidin-4-yl)-butan-2-ol (11d). Starting with **8c** (0.100 g, 0.42 mmol), benzamidine hydrochloride monohydrate (**3a**) (0.725 g, 4.2 mmol) and NEt_3 (0.6 mL, 4.2 mmol) in ethanol (5 mL), **11d** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow solid (0.120 g, 85%), mp=62.6 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ=2.28–2.36 (m, 2H, CH_2), 3.02–3.12 (m, 2H, CH_2), 3.81 (dd, J=14.7, 7.2 Hz, 1H, CH_2–Cl), 4.22 (dd, J=14.7, 9.6 Hz, 1H, CH_2–Cl), 4.87–4.94 (m, 1H, OCH), 7.37–7.54 (m, 5H, 5×CH), 7.93–7.96 (m, 2H, 2×CH), 8.19–8.22 (m, 2H, 2×CH), 8.58–8.62 (m, 2H, 2×CH). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=33.7, 34.0 (CH_2), 60.0 (CH_2–Cl), 79.2 (OCH_2), 113.5 (*C*H=C–N), 127.1 (2C), 128.1, 128.2 (2C), 128.3, 128.4 (2C), 128.8 (2C, CH of Ph), 137.1, 138.0 (C of Ph), 163.9 (*C*–Ph), 164.2 (N=C–N), 169.9 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3064 (w), 2970 (w), 2931 (w), 2865 (w), 1648 (m), 1575 (s), 1534 (s), 1495 (w), 1448 (w), 1374 (s), 1260 (w), 1174 (w), 1116 (m), 1072 (m), 1028 (w), 778 (m), 750 (m), 695 (s). UV–vis (CH_3CN, nm): λ_{max} (log ε)=256 (4.44). MS (EI, 70 eV): *m*/*z* (%)=302 ([M–Cl]$^+$, 15), 261 (30), 257 (14), 233 (4), 215 (100), 195 (5), 169 (3), 159 (24), 141 (4), 128 (13), 119 (3), 117 (21), 91 (22), 86 (20), 84 (37), 79 (4), 77 (16). Anal. Calcd for $C_{20}H_{19}ClN_2O$ (338.837): C 70.90, H 5.65, N 8.27. Found: C 71.17, H 6.11, N 8.25.

3.1.4.11. 1-Bromo-4-(2,6-diphenylpyrimidin-4-yl)-butan-2-ol (11e). Starting with **8d** (0.100 g, 0.36 mmol), benzamidine hydrochloride monohydrate (**3a**) (0.629 g, 3.6 mmol) and NEt_3 (0.49 mL, 3.6 mmol in ethanol (5 mL), **11e** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow solid (0.109 g, 79%), mp=111.3 °C. ^{1}H NMR ($CDCl_3$, 300 MHz): δ=2.27–2.35 (m, 2H, CH_2), 3.01–3.14 (m, 2H, CH_2), 3.80 (dd, J=14.7, 7.2 Hz, 1H, CH_2–Br), 4.21 (dd, J=14.7, 9.6 Hz, 1H, CH_2–Br), 4.84–4.91 (m, 1H, OCH), 7.36–7.54 (m, 5H, 5×CH), 7.92–7.95 (m, 2H, 2×CH), 8.19–8.22 (m, 2H, 2×CH), 8.58–8.62 (m, 2H, 2×CH). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=33.7, 33.9 (CH_2), 60.0 (CH_2–Br), 79.2 (OCH), 113.5 (*C*H=C–N), 127.1 (2C), 128.0 (2C), 128.2 (2C), 128.27, 128.34, 128.7 (2C, CH of Ph), 137.1, 137.9 (C of Ph), 163.8 (*C*–Ph), 164.2 (N=C–N), 169.9 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3063 (w), 2944 (w), 1647 (s), 1572 (s), 1533 (s), 1495 (w), 1447 (m), 1424 (w), 1373 (s), 1327 (m), 1285 (w), 1258 (m), 1176 (w), 1082 (m), 1066 (m), 1027 (m), 991 (w), 920 (w), 909 (w), 868 (w), 779 (w), 748 (m), 694 (s). UV–vis (CH_3CN, nm): λ_{max} (log ε)=255 (4.54). MS (EI, 70 eV): *m*/*z* (%)=302 ([M–Br]$^+$, 3), 300 (11), 285 (18), 284 (68), 283 (27), 271 (21), 259 (30), 246 (100), 234 (2), 232 (1), 142 (7), 128 (4), 117 (15), 104 (30), 77 (30).

3.1.4.12. 3-(2,6-Diphenylpyrimidin-4-yl)-2-methyl-propan-1-ol (11f). Starting with **9a** (0.500 g, 2.5 mmol), benzamidine hydrochloride monohydrate (**3a**) (4.370 g, 25 mmol) and NEt_3 (3.4 mL, 25 mmol) in ethanol (25 mL), **11f** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow oil (0.381 g, 50%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.03 (d, J=6.9 Hz, 3H, CH_3), 2.28–2.37 (m, 1H, CH_2), 2.82–2.89 (m, 1H, CH_2), 2.93–2.99 (m, 1H, CH_2), 3.48 (dd, J=11.1, 6.9 Hz, 1H, OCH_2), 3.63 (dd, J=11.1, 5.1 Hz, 1H, OCH_2), 7.35–7.53 (m, 7H, CH=C, 6×CH of Ph), 8.15–8.22 (m, 2H, 2×CH of Ph), 8.52–8.60 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=17.9 (CH_3), 35.4 (CH), 41.8 (CH_2), 66.9 (OCH_2), 114.4 (*C*H=C–N), 127.2 (2C), 128.2 (2C), 128.5 (2C), 128.8 (2C), 130.6, 130.8 (CH of Ph), 137.0, 137.7 (C of Ph), 163.7 (*C*–Ph), 164.0 (N=C–N), 169.6 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3338 (br), 3064 (w), 2966 (m), 2926 (m), 2872 (w), 1632 (w), 1574 (s), 1533 (s), 1498 (w), 1451 (m), 1374 (s), 1278 (w), 1176 (w), 1111 (m), 1075 (m), 1035 (m), 751 (m), 695 (s), 636 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=256 (4.47). MS (EI, 70 eV): *m*/*z* (%)=303 (M^+, 1), 289 (1), 287 (4), 273 (3), 259 (12), 246 (100), 143 (7), 128 (4), 114 (5), 104 (23). Anal. Calcd for $C_{20}H_{20}N_2O$ (304.391): C 78.92, H 6.62, N 9.20. Found: C 78.73, H 6.59, N 9.15.

3.1.4.13. 2-Methyl-3-(2-methyl-6-phenylpyrimidin-4-yl)propan-1-ol (11g). Starting with **9a** (0.708 g, 3.5 mmol), acetamidine hydrochloride (**3b**) (3.483 g, 35 mmol) and NEt_3 (4.9 mL, 35 mmol) in ethanol (35 mL), **11g** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→EtOAc), as a pale yellow oil (0.395 g, 47%). ^{1}H NMR ($CDCl_3$, 300 MHz): δ=1.01 (d, J=6.6 Hz, 3H, CH_3), 2.01–2.14 (m, 1H, CH), 2.46 (dd, J=12.9, 5.7 Hz, 1H, CH_2), 2.76 (s, 3H, CH_3), 2.85 (dd, J=18.3, 5.7 Hz, 1H, CH_2), 3.48 (dd, J=10.5, 6.6 Hz, 1H, OCH_2), 3.61 (dd, J=10.8, 4.5 Hz, 1H, OCH_2), 7.38–7.44 (m, 4H, CH=C, 3×CH of Ph), 7.85–7.88 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=16.4, 25.8 (CH_3), 35.2 (CH), 40.3 (CH_2), 66.2 (OCH_2), 113.8 (*C*H=C–N), 126.8 (2C), 127.0, 128.0 (2C, CH of Ph), 136.6 (C of Ph), 164.1 (*C*–Ph), 167.3 (N=C–N), 169.3 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3346 (br), 3065 (w), 2963 (m), 2927 (m), 2874 (w), 1604 (s), 1529 (s), 1450 (m), 1419 (m), 1375 (m), 1325 (s), 1286 (s), 1182 (w), 1123 (w), 1074 (m), 1040 (m), 743 (s), 696 (m), 648 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=244 (3.99), 277 (3.89), 325 (4.03). MS (EI, 70 eV): *m*/*z* (%)=242 (M^+, 100), 197 (5), 184 (93), 173 (20), 148 (5), 105 (14), 77 (19), 57 (22). HRMS (ESI): calcd for $C_{15}H_{18}N_2O$ [M^+]: 241.1335; found: 241.1332.

3.1.4.14. 2-(2,6-Diphenylpyrimidin-4-ylmethyl)butan-1-ol (11h). Starting with **9b** (0.200 g, 0.92 mmol), benzamidine hydrochloride monohydrate (**3a**) (1.616 g, 9.2 mmol) and NEt_3 (1.3 mL, 9.2 mmol) in ethanol (10 mL), **11h** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→1:1) as a yellow oil (0.166 g, 75%). ^1H NMR ($CDCl_3$, 300 MHz): δ=1.01 (t, J=7.2 Hz, 3H, CH_3), 1.37–1.48 (m, 2H, CH_2), 1.51–1.61 (m, 1H, CH), 2.93–3.08 (m, 2H, CH_2), 3.55 (dd, J=11.4, 6.6 Hz, 1H, OCH_2), 3.71 (dd, J=11.4, 4.5 Hz, 1H, OCH_2), 7.44–7.56 (m, 7H, CH=C, 6×CH of Ph), 8.20–8.24 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=11.5 (CH_3), 24.0, 39.6 (CH_2), 42.0 (CH), 64.4 (OCH_2), 114.3 (*C*H=C–N), 127.1 (2C), 128.1 (2C), 128.4 (2C), 128.7 (2C), 130.5, 130.7 (CH of Ph), 136.8, 137.6 (C of Ph), 163.8 (*C*–Ph), 163.9 (N=C–N), 169.7 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3398 (br), 3064 (w), 2966 (m), 2928 (m), 2870 (m), 1627 (w), 1574 (s), 1534 (s), 1495 (w), 1452 (m), 1374 (s), 1175 (w), 1114 (m), 1072 (m), 1035 (w), 927 (w), 751 (m), 695 (s), 636 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=204 (4.53), 256 (4.52). MS (EI, 70 eV): *m*/*z* (%)=317 (M^+, 1), 301 (3), 300 (3), 289 (3), 287 (2), 285 (2), 273 (3), 272 (3), 271 (12), 259 (7), 246 (100), 167 (2), 143 (3), 128 (3), 114 (3), 104 (15), 77 (7). Anal. Calcd for $C_{21}H_{22}N_2O$ (318.418): C 79.21, H 6.96, N 8.80. Found: C 79.19, H 6.82, N 8.68.

3.1.4.15. 2-(2-Methyl-6-phenylpyrimidin-4-ylmethyl)-butan-1-ol (11i). Starting with **9b** (0.075 g, 0.347 mmol), acetamidine hydrochloride (**3b**) (0.328 g, 3.47 mmol) and NEt_3 (0.48 mL, 3.47 mmol) in ethanol (7 mL), **11i** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=50:1→1:1) as a pale yellow oil (0.037 g, 42%). ^1H NMR ($CDCl_3$, 300 MHz): δ=0.98 (t, J=7.5 Hz, 3H, CH_3), 1.33–1.45 (m, 2H, CH_2), 1.92–2.01 (m, 1H, CH), 2.76 (s, 3H, CH_3), 2.91 (dd, J=8.4, 8.4 Hz, 2H, CH_2), 3.50 (dd, J=11.1, 6.3 Hz, 1H, OCH_2), 3.66 (dd, J=11.1, 4.2 Hz, 1H, OCH_2), 7.39 (s, 1H, CH), 7.47–7.51 (m, 3H, 3×CH of Ph), 8.05–8.08 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=11.8 (CH_3), 24.4 (CH_2), 26.1 (CH_3), 40.1 (CH_2), 42.1 (CH), 64.8 (OCH_2), 113.9 (*C*H=C–N), 127.3 (2C), 128.9 (2C), 130.8 (CH of Ph), 137.0 (C of Ph), 164.6 (*C*–Ph), 167.6 (N=C–N), 169.4 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3376 (w), 2963 (m), 2928 (m), 2873 (m), 1654 (w), 1583 (s), 1540 (s), 1492 (w), 1449 (m), 1391 (m), 1382 (m), 1311 (w), 1250 (w), 1170 (m), 1116 (w), 1047 (m), 1000 (w), 974 (w), 789 (w), 756 (w), 696 (m). UV–vis (CH_3CN, nm): λ_{max} (log ε)=249 (3.94), 255 (3.93), 276 (4.07). MS (EI, 70 eV): *m*/*z* (%)=256 (M^+, 1), 241 (1), 239 (3), 225 (4), 211 (4), 197 (9), 184 (100). HRMS (ESI): calcd for $C_{16}H_{20}N_2O$ ($[M-H]^+$): 255.14879; found: 255.14974.

3.1.4.16. 1-Bromo-4-(6-methyl-2-phenylpyrimidin-4-yl)butan-2-ol (11j). Starting with **8e** (0.100 g, 0.46 mmol), benzamidine hydrochloride monohydrate (**3a**) (0.735 g, 4.6 mmol) and NEt_3 (0.64 mL, 4.6 mmol) in ethanol (5 mL), **11j** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=100:1→3:1) as a light brown oil (0.135 g, 91%). ^1H NMR ($CDCl_3$, 300 MHz): δ=2.17–2.31 (m, 2H, CH_2), 2.53 (s, 3H, CH_3), 2.87–3.03 (m, 2H, CH_2), 3.77 (dd, J=14.7, 7.5 Hz, 1H, CH_2–Br), 4.19 (dd, J=14.7, 9.6 Hz, 1H, CH_2–Br), 4.80–4.88 (m, 1H, OCH), 6.94 (s, 1H, CH=C), 7.37–7.49 (m, 3H, 3×CH of Ph), 8.42–8.47 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=24.1 (CH_3), 33.2, 33.8 (CH_2), 59.7 (CH_2–Br), 79.2 (OCH), 117.4 (*C*H=C–N), 128.1 (2C), 128.3 (2C), 130.3 (CH of Ph), 137.9 (C of Ph), 164.0 (N=C–N), 167.0 (*C*–CH_3), 168.8 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3066 (br, w), 2935 (m), 2868 (w), 1646 (s), 1584 (s), 1543 (m), 1445 (m), 1371 (s), 1316 (w), 1260 (m), 1073 (m), 1030 (w), 696 (s). UV–vis (CH_3CN, nm): λ_{max} (log ε)=254 (4.17). MS (EI, 70 eV): *m*/*z* (%)=322 (M^+ [^{81}Br], 11), 320 (M^+ [^{79}Br], 11), 304 (3), 289 (3), 242 (35), 228 (41), 198 (19), 184 (100). HRMS (ESI): calcd for $C_{15}H_{17}BrN_2O$ [M^+]: 322.0504 (^{81}Br), 320.0524 (^{79}Br); found: 322.0509 (^{81}Br), 320.0529 (^{79}Br). Anal. Calcd for $C_{15}H_{17}BrN_2O$ (321.212): C 56.09, H 5.33, N 8.72. Found: C 55.95, H 5.62, N 8.68.

3.1.4.17. 4-(6-Methyl-2-phenylpyrimidin-4-yl)butane-1,2-diol (11k). Starting with **10** (0.100 g, 0.64 mmol), benzamidine hydrochloride monohydrate (**3a**) (1.023 g, 6.4 mmol) and NEt_3 (0.89 mL, 6.4 mmol) in ethanol (5 mL), **11k** was isolated after chromatography (silica gel, *n*-hexane/EtOAc=50:1→EtOAc) as a light brown oil (0.145 g, 88%). ^1H NMR ($CDCl_3$, 300 MHz): δ=1.87–1.98 (m, 2H, CH_2), 2.55 (s, 3H, CH_3), 2.94–2.98 (m, 2H, CH_2), 3.52 (dd, J=11.1, 6.6 Hz, 1H, CH_2–OH), 3.66 (dd, J=11.1, 3.3 Hz, 1H, CH_2–OH), 3.76–3.84 (m, 1H, OCH), 6.95 (s, 1H, CH=C), 7.43–7.49 (m, 3H, 3×CH of Ph), 8.35–8.39 (m, 2H, 2×CH of Ph). ^{13}C NMR ($CDCl_3$, 75 MHz): δ_C=24.1 (CH_3), 31.2, 33.6 (CH_2), 66.5 (CH_2–OH), 71.5 (OCH), 117.7 (*C*H=C–N), 128.1 (2C), 128.5 (2C), 130.4 (CH of Ph), 137.6 (C of Ph), 163.9 (N=C–N), 167.4 (*C*–CH_3), 169.5 (N–*C*=CH). IR (neat, cm^{-1}): $\tilde{\nu}$=3375 (br, s), 2929 (m), 2867 (w), 1663 (m), 1586 (s), 1539 (s), 1442 (m), 1376 (s), 1099 (m), 1043 (w), 698 (w). UV–vis (CH_3CN, nm): λ_{max} (log ε)=256 (4.12). MS (EI, 70 eV): *m*/*z* (%)=258 (M^+, 12), 241 (3), 224 (5), 210 (37), 197 (39), 183 (45), 169 (100). HRMS (ESI): calcd for $C_{15}H_{18}N_2O_2$ [M^+]: 258.13683; found: 258.13678. Anal. Calcd for $C_{15}H_{18}N_2O_2$ (258.316): C 69.74, H 7.02, N 10.84. Found: C 69.91, H 6.83, N 10.68.

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