CHEMIJA. 2012. Vol. 23. No. 1. P. 61–67

Synthesis of novel 2,4,6-triarylpyrimidines

Sigitas Tumkevičius[1]*,

Andžejus Voitechovičius[1],

Povilas Adomėnas[2]

[1] *Department of Organic Chemistry, Faculty of Chemistry, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania*

[2] *Institute of Applied Research, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania*

A series of new 2,4,6-triarylpyrimidines bearing π-conjugated aryl units in positions 4 and 6 of the pyrimidine ring were synthesized by palladium-catalyzed cross-coupling reaction of 2-(4-ethylphenyl)- and 2-(4-dimethylaminophenyl)-4,6-dichloropyrimidines with arylboronic acids in the presence of $Pd(PPh_3)_2Cl_2$ / K_3PO_4 as a catalyst system. The structure of the synthesized compounds was established by spectral and elemental analysis data. The synthesized 2,4,6-triarylpyrimidines were found to exibit UV-blue fluorescence.

Key words: Suzuki reaction, 4,6-dichloropyrimidines, arylboronic acids, fluorescence

INTRODUCTION

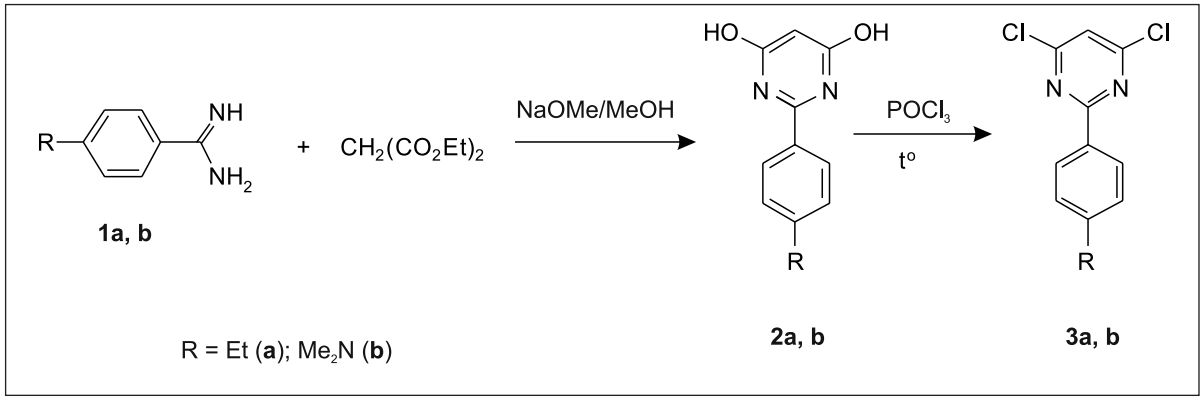
Over recent years, organic molecules with a π-conjugated backbone have attracted an increasing interest due to their numerous applications in various fields. They are attractive candidates as components of organic light-emitting devices (OLEDs) for display and lighting [1], field-effect transistors (FETs) [2], single molecular electronics [3] and non-linear optical materials [4]. An incorporation of a π-deficient heterocycle such as pyridine [5], pyrazine [6], pyrimidine [7], s-triazine [8], or quinoxaline [9] in the centre of the backbone of such molecules often leads to a significant enhancement of some of their physical properties such as mesomorphism, fluorescence and solvatochromism. In view of the growing importance of highly efficient light-emitting materials in biological, chemical and materials science and continuing our work on the construction of heterocyclic core containing fluorescent molecules [10], we report herein on the synthesis of novel non-linear oligoarylenes of pyrimidine series. For construction of these molecules the Suzuki reaction has been chosen. The choice was made because of several reasons: boronic acids used in the Suzuki reaction are non-toxic and ecologically acceptable; the reactions often give good results even with chloroarenes and heteroarenes; the Suzuki reaction provides a short synthetic route to the desired aromatics or heteroaromatics with conjugated aryl branches [11].

RESULTS AND DISCUSSION

For the synthesis of 2,4,6-triarylpyrimidines the corresponding 2-aryl-4,6-dichloropyrimidines **3a, b** were used as starting materials. Compounds **3a, b** were synthesized by cylocondensation reaction of the corresponding benzamidines **1a, b** with malonic ester in the precence of sodium methoxide and the following reaction of the obtained 4,6-dihydroxypyrimidines **(2a, b)** with phosphorous oxychloride (Scheme 1).

Taking into account our earlier results on the synthesis of 4,6-diarylpyrimidines bearing various substituents in

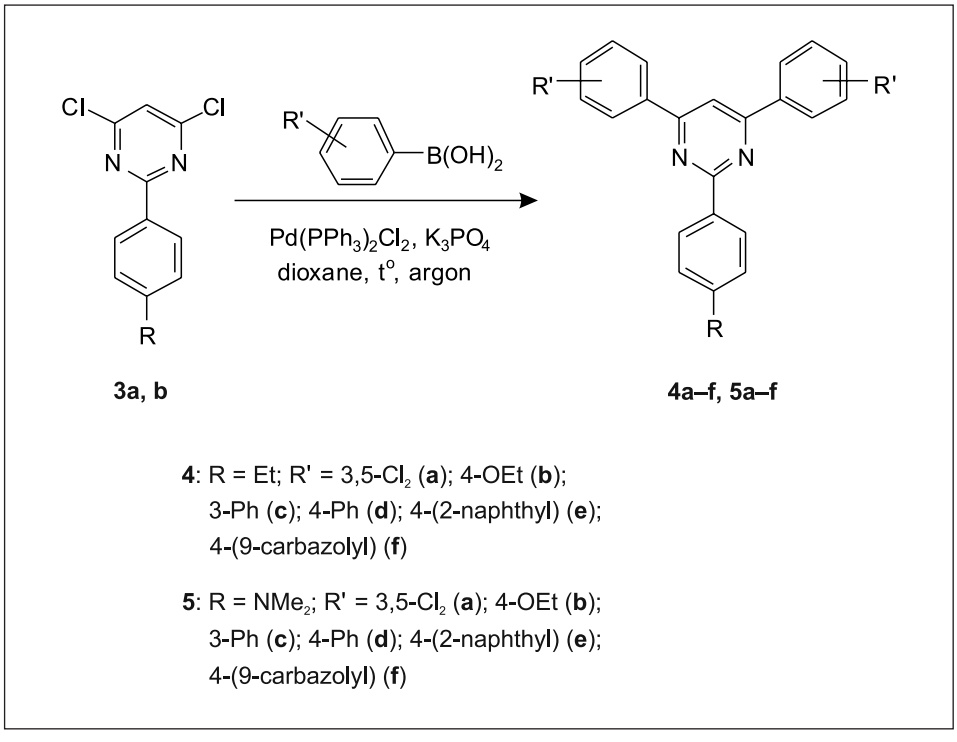
* Corresponding author. E-mail: sigitas.tumkevicius@chf.vu.lt



Scheme 1

positions 2 and 5 of the pyrimidine ring by the Suzuki reaction [12], $Pd(PPh_3)_2Cl_2$ / K_3PO_4 as a catalyst system was chosen in the present investigation. Thus, 4,6-dichloropyrimidines **3a**, **b** reacted with a slight excess of the corresponding arylboronic acids in the presence of 2.5 mol% of $Pd(PPh_3)_2Cl_2$ to give the corresponding 4,6-diarylpyrimidines **4a–f**, **5a–f** in moderate yields (Scheme 2, Table). Lower yields of compounds **4e**, **5b, c** were obtained, presumably because of more complex purification by column chromatography (Table, entries 5, 8, 9) and formation of homo-coupling products of boronic acids in reasonable amounts. All the reactions were carried out by reflux in anhydrous dioxane under argon atmosphere. The reaction time depending on the nature of arylboronic acids varied from 4 to 10 hours (Table). The structure of the obtained compounds **4a–f** and **5a–f** was consistent with their ^1H and ^{13}C NMR spectra and elemental analysis data.

The synthesized pyrimidine derivatives **4a–f**, **5f** were subjected to optical absorption and fluorescence studies in tetrahydrofuran solutions. A preliminary investigation of photophysical properties of the synthesized compounds has shown that they exhibit strong absorption with their absorption maxima in the range 237–344 nm and UV-blue fluorescence with emission maxima located in the range 345–436 nm. The compound **4f** bearing carbazolylphenyl units in positions 4 and 6 of the pyrimidine moiety exhibits strong fluorescence in tetrahydrofuran at λ_{em} = 436 nm with fluorescence quantum yield 60%. A more detailed study of the photophysical properties of the synthesized compounds and further variations of oligoarylene branches at the pyrimidine nucleous are currently in progress and the results will be reported in due course.



Scheme 2

Table. **Data of cross-coupling reaction of 3a, b with arylboronic acids**

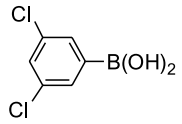
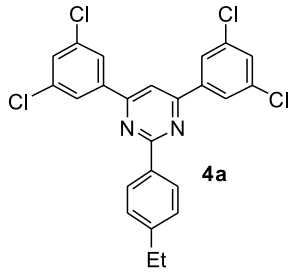
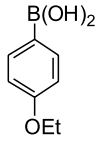
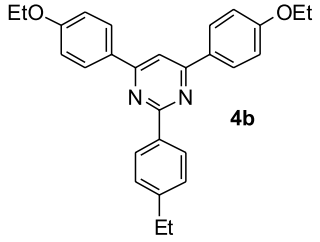
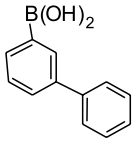
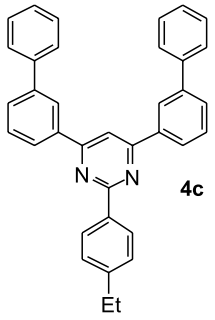
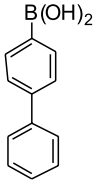
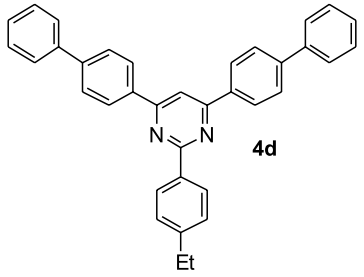
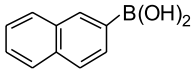
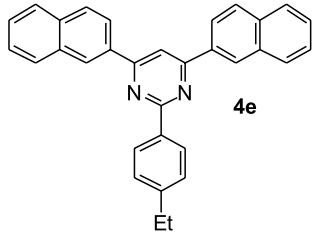
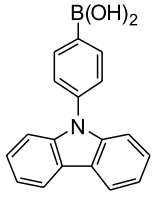
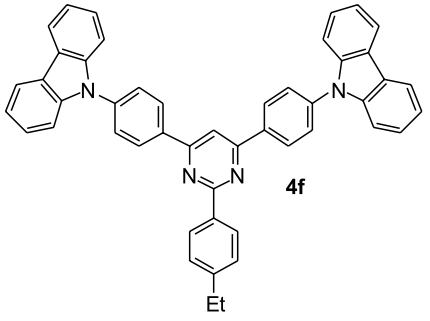
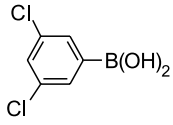
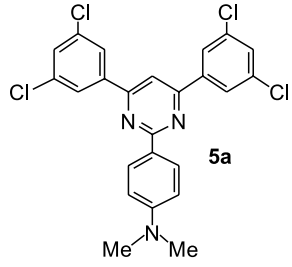
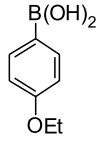
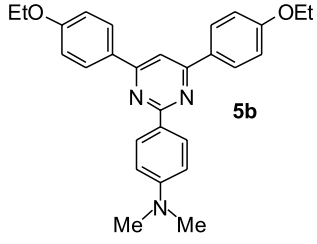
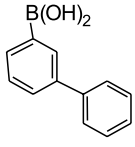
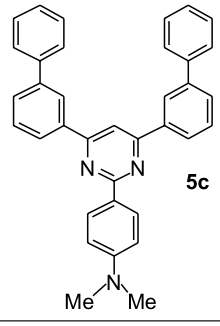
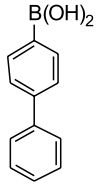
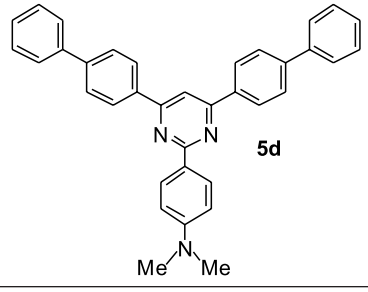
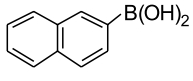
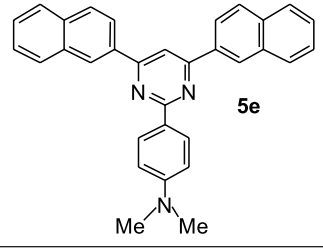
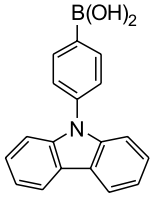
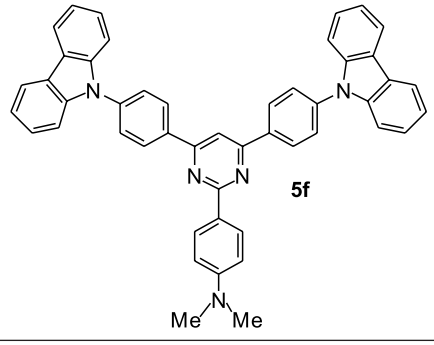
Entry	Compd. 3	Arylboronic acid	Reaction time, h	Product 4, 5	Yield, %
1	**3a**		8	 **4a**	53
2	**3a**		5	 **4b**	65
3	**3a**		10	 **4c**	43
4	**3a**		4	 **4d**	91
5	**3a**		7	 **4e**	25
6	**3a**		7	 **4f**	76

Table **(continued)**

Entry	Compd. 3	Arylboronic acid	Reaction time, h	Product 4, 5	Yield, %
7	**3b**		7	 **5a**	64
8	**3b**		6	 **5b**	25
9	**3b**		9	 **5c**	30
10	**3b**		4	 **5d**	42
11	**3b**		5	 **5e**	49
12	**3b**		10	 **5f**	64

EXPERIMENTAL

Melting points were determined in open capillaries with a digital melting point IA9100 series apparatus (ThermoFischer Scientific) and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a Varian INOVA spectrometer (300 MHz and 75 MHz respectively) using residual solvent peaks as an internal standard. Column chromatography was performed using Silica gel 60 (0.040–0.063 mm) (Merck). All reactions and the purity of the synthesized compounds were monitored by TLC using Silica gel 60 F_{254} aluminium plates (Merck). Visualization was accomplished by UV light. The absorption spectra were recorded on a Perkin-Elmer UV-VIS spectrophotometer Lambda 20 in THF solutions. Fluorescence of the sample solutions was excited by a 320 nm wavelength light-emitting diode and measured using a back-thinned CCD spectrometer (Hamamatsu PMA-11). The fluorescence quantum yield of the solutions was estimated by comparing the wavelength-integrated fluorescence intensity of the solution with that of the reference. Quinine sulfate dissolved in 0.1 M H_2SO_4 has been used as a reference.[13] Absorbance of the reference and the sample solutions was ensured to be below 0.05 to avoid reabsorption effects. The estimated quantum yield was verified by using an alternative method of an integrating sphere (Sphere Optics)[14] which was coupled to the CCD spectrometer by an optical fiber. Fluorescence transients of the sample solutions were measured using the time-correlated single photon counting system (PicoQuant PicoHarp 300).

4,6-Dihydroxy-2-(4-substituted phenyl)pyrimidines (2a, b). To a solution of sodium methoxide in methanol prepared before the reaction from sodium (34.5 g, 1.5 mol) and methanol (1 000 mL), the corresponding benzamidine hydrochloride (0.5 mol) was added at room temperature. Then ethyl malonate (80 g, 0.5 mol) was added, and the reaction mixture was stirred at 60 °C for 6 h. The solid obtained was filtered off, dissolved in water, the obtained solution acidified with hydrochloric acid to pH = 5. The resulting solid was filtered off, washed several times with water to pH = 7 to give compounds **2a, b**.

Compound **2a**: Yield 86%, mp > 320 °C (dec.). ^{1}H NMR (DMSO-D_6), δ, ppm: 1.21 (t, J = 7.5 Hz, 3H), 2.64 (q, J = 7.5 Hz, 2H), 5.32 (s, 1H), 7.28 (d, J = 8.1 Hz, 2H), 8.02 (d, J = 8.1 Hz, 2H), 11.85 (br s, 2H). ^{13}C NMR (DMSO-D_6), δ, ppm: 15.91, 28.74, 88.88, 128.53, 128.74, 130.30, 148.73, 158.14, 168.06.

Compound **2b**: Yield 26%, mp > 310 °C (dec.). ^{1}H NMR (DMSO-D_6), δ, ppm: 3.05 (s, 6H), 6.80 (d, J = 9.0 Hz, 2H), 7.65 (s, 1H), 8.12 (s, J = 9 Hz, 2H). ^{13}C NMR (DMSO-D_6), δ, ppm: 40.35, 112.17, 117.32, 121.59, 130.59, 153.70, 161.77, 165.71.

4,6-Dichloro-2-(4-substituted phenyl)pyrimidines (3a, b). Phosphorous oxychloride (206 g, 1.5 mol) was added dropwise to a round-bottom flask containing the corresponding compound **2a, b** (0.43 mol). The reaction mixture was refluxed for 4 h. Then an excess of phosphorous oxychloride was removed under the reduced pressure, and the residue was poured onto ice. The obtained solution was extracted several times with dichloromethane, solvent evaporated, the residue recrystallized to give compounds **3a, b**, respectively.

Compound **3a**: Yield 78%, mp 73–75 °C (from hexane). ^{1}H NMR ($CDCl_3$), δ, ppm: 1.30 (t, J = 7.5 Hz, 3H), 2.74 (q, J = 7.5 Hz, 2H), 7.25 (s, 1H), 7.32 (d, J = 8.1 Hz, 2H), 8.36 (d, J = 8.1 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.52, 29.18, 118.60, 128.57, 129.23, 132.68, 149.40, 162.11, 166.10. Anal. calcd. for ($C_{12}H_{10}Cl_2N_2$): C, 56.94; H, 3.98. Found: C, 56.71; H, 3.64.

Compound **3b**: Yield 70%, mp 173–175 °C. Lit. [15]: Yield 20%, mp 174–175 °C.

4,6-Diaryl-2-substituted pyrimidines (4a–f, 5a–f) (General procedure). A mixture of 4,6-dichloro-2-(4-substituted phenyl)pyrimidine **(3a, b)** (3.9 mmol), the corresponding arylboronic acid (9.88 mmol), $Pd(PPh)_3Cl_2$ (0.069 g, 0.098 mmol), and anhydrous K_3PO_4 (8 g, 38 mmol) in an anhydrous 1,4-dioxane (60 ml) was refluxed under argon atmosphere for 4–10 h. After cooling to room temperature, the reaction mixture was poured into water, the water solution was stirred for 30 min and then extracted with dichloromethane. The extract was filtered through a layer of silica gel, dichloromethane evaporated to dryness, and the residue recrystallized from a mixture of toluene and isopropanol (1 : 2) to give the corresponding compounds **4a–f** and **5a–f**.

4,6-Di(3,5-dichlorophenyl)-2-(4-ethylphenyl)pyrimidine (4a). Mp 141–143 °C. UV-vis (THF) λ, nm (ε, l mol^{-1} cm^{-1}): 265 (4.25 × 10^4), 332 (6.56 × 10^3). ^{1}H NMR ($CDCl_3$), δ, ppm: 1.35 (t, J = 7.5 Hz, 3H), 2.79 (q, J = 7.5 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.55 (s, 2H), 7.81 (s, 1H), 8.14 (s, 4H), 8.58 (d, J = 8.4 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.67, 29.18, 110.08, 125.96, 128.47, 128.87, 131.01, 134.87, 136.05, 140.28, 148.26, 162.78, 165.35. Anal. calcd. for $C_{24}H_{16}Cl_4N_2$: C, 60.79; H, 3.40. Found: C, 60.99; H, 3.57.

4,6-Di(4-ethoxyphenyl)-2-(4-ethylphenyl)pyrimidine (4b). Mp 127–130 °C. ^{1}H NMR ($CDCl_3$), δ, ppm: 1.34 (t, J = 7.5 Hz, 3H), 1.50 (t, J = 6.9 Hz, 6H), 2.77 (q, J = 7.5 Hz, 2H), 4.15 (q, J = 6.9 Hz, 4H), 7.06 (d, J = 8.4 Hz, 4H), 7.37 (d, J = 8.1 Hz, 2H), 7.89 (s, 1H), 8.26 (d, J = 8.4 Hz, 4H), 8.63 (d, J = 8.1 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.04, 15.78, 29.14, 63.89, 108.53, 114.94, 128.18, 128.76, 129.02, 130.22, 136.16, 147.19, 161.48, 164.12, 164.51. Anal. calcd. for $C_{28}H_{28}N_2O_2$: C, 79.22; H, 6.65. Found: C, 79.38; H, 6.41.

4,6-Di(3-biphenyl)-2-(4-ethylphenyl)pyrimidine (4c). Mp 180–182 °C. UV-vis (THF) λ, nm (ε, l mol^{-1} cm^{-1}): 257 (8.08 × 10^4), 326 (8.88 × 10^3). ^{1}H NMR ($CDCl_3$), δ, ppm: 1.35 (t, J = 7.5 Hz, 3H), 2.78 (q, J = 7.5 Hz, 2H), 7.43 (m, 5H), 7.55 (t, J = 7.8 Hz, 2H), 7.65 (m, 3H), 7.74 (m, 6H), 8.11 (s, 1H), 8.29 (d, J = 7.8 Hz, 2H), 8.53 (s, 2H), 8.68 (d, J = 8.1 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.76, 29.18, 110.65, 126.44, 126.51, 127.63, 127.89, 128.31, 128.5, 128.86, 129.17, 129.6,

129.8, 135.92, 138.51, 141.17, 142.32, 147.5, 165.01. Anal. calcd. for $C_{36}H_{28}N_2$: C, 88.49; H, 5.78. Found: C, 88.02; H, 5.73.

4,6-Di(4-biphenyl)-2-(4-ethylphenyl)pyrimidine (4d). Mp 190–193 °C. UV-vis (THF) λ, nm (ε, l mol^{-1} cm^{-1}): 295 (6.32 × 10^4), 333 (3.24 × 10^4). ^{1}H NMR ($CDCl_3$), δ, ppm: 1.36 (t, *J* = 7.8 Hz, 3H), 2.80 (q, *J* = 7.8 Hz, 2H), 7.42 (m, 8H), 7.51 (m, 4H), 7.72 (m, 4H), 7.82 (d, *J* = 8.4 Hz, 2H), 8.09 (s, 1H), 8.41 (d, *J* = 8.4 Hz, 2H), 8.70 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.78, 29.18, 110.00, 127.30, 127.46, 127.63, 127.84, 128.00, 128.10, 129.18, 136.05, 136.78, 140.65, 143.76, 147.44, 164.51, 164.96. Anal. calcd. for $C_{36}H_{28}N_2$: C, 88.49; H, 5.78. Found: C, 88.70; H, 5.98.

2-(4-Ethylphenyl)-4,6-di(2-naphthyl)pyrimidine (4e). Mp 148–150 °C. ^{1}H NMR ($CDCl_3$), δ, ppm: 1.37 (t, *J* = 7.8 Hz, 3H), 2.81 (q, *J* = 7.8 Hz, 2H), 7.44 (t, *J* = 8.7 Hz, 2H), 7.60–7.63 (m, 4H), 7.95 (t, *J* = 6.9 Hz, 2H), 8.05–8.12 (m, 4H), 8.30 (s, 1H), 8.46 (d, *J* = 6.9 Hz, 2H), 8.73 (d, *J* = 8.4 Hz, 2H). 8.86 (s, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.80, 29.21, 110.73, 124.60, 126.83, 127.58, 127.76, 128.06, 128.34, 128.91, 128.94, 129.34, 133.59, 134.90, 135.09, 135.92, 147.55, 164.82, 164.93. Anal. calcd. for $C_{32}H_{24}N_2$: C, 88.04; H, 5.54. Found: C, 87.80; H, 5.78.

4,6-Di[4-(9-carbazolyl)phenyl]-2-(4-ethylphenyl) pyrimidine (4f). Mp 234–236 °C. UV-vis (THF) λ, nm (ε, l mol^{-1} cm^{-1}): 237 (1.16 × 10^5), 256 (7.7 × 10^4), 281 (4.47 × 10^4), 291 sh (4.03 × 10^4), 343 (3.65 × 10^4). ^{1}H NMR ($CDCl_3$), δ, ppm: 1.35 (t, *J* = 7.5 Hz, 3H), 2.84 (q, *J* = 7.5 Hz, 2H), 7.37 (m, 4H), 7.49 (m, 6H), 7.60 (d, *J* = 8.4 Hz, 4H), 7.84 (d, *J* = 8.4 Hz, 4H), 8.20 (m, 5H), 8.60 (d, *J* = 8.4 Hz, 4H), 8.74 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.73, 29.19, 110.10, 110.18, 120.61, 120.69, 123.97, 126.40, 127.48, 128.42, 128.91, 129.20, 135.68, 136.55, 140.76, 140.83, 147.83, 164.28, 165.22. Anal. calcd. for $C_{48}H_{34}N_4$: C, 86.46; H, 5.14. Found: C, 86.84; H, 5.15.

2-(4-Dimethylaminophenyl)-4,6-di(3,5-dichlorophenyl) pyrimidine (5a). Mp 141–143 °C. ^{1}H NMR ($CDCl_3$ + CF_{3-}COOD), δ, ppm: 3.13 (s, 6H), 6.83 (d, *J* = 9.0 Hz, 2H), 7.54 (s, 2H), 7.69 (s, 1H), 8.13 (s, 4H), 8.54 (d, *J* = 9.0 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 47.54, 111.82, 120.56, 126.09, 131.45, 131.71, 136.39, 139.19, 144.21, 160.38, 162.94, 163.57. Anal. calcd. for $C_{24}H_{17}Cl_4N_3$: C, 58.92; H, 3.50. Found: C, 58.66; H, 3.41.

4,6-Di(4-ethoxyphenyl)-2-(4-dimethylaminophenyl)pyrimidine (5b). Mp 164–166 °C. ^{1}H NMR ($CDCl_3$), δ, ppm: 1.50 (t, *J* = 6.9 Hz, 6H), 3.10 (s, 6H), 4.12 (q, *J* = 6.9 Hz, 4H), 6.87 (d, *J* = 8.7 Hz, 2H), 7.05 (d, *J* = 8.7 Hz, 4H), 7.79 (s, 1H), 8.25 (d, *J* = 8.7 Hz, 4H), 8.62 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 15.07, 40.76, 63.86, 107.48, 112.03, 114.85, 128.91, 128.94, 130.62, 146.24, 153.16, 161.25, 163.91, 164.69. Anal. calcd. for $C_{28}H_{29}N_3O_2$: C, 76.51; H, 6.65. Found: C, 76.39; H, 6.63.

4,6-Di(3-biphenyl)-2-(4-dimethylaminophenyl)pyrimidine (5c). Mp 203–205 °C. ^{1}H NMR ($CDCl_3$), δ, ppm: 3.12 (s, 6H), 6.91 (d, *J* = 6.4 Hz, 2H), 7.6 (m, 14H), 8.00 (s, 1H), 8.27 (d, *J* = 7.2 Hz, 2H), 8.53 (s, 2H), 8.68 (d, *J* = 6.4 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 40.73, 109.53, 112.08, 126.43, 126.49, 127.64, 127.85, 128.43, 129.17, 129.54, 129.62, 130.14, 138.82, 141.25, 142.22, 152.40, 164.80, 165.15. Anal. calcd. for $C_{36}H_{29}N_3$: C, 85.85; H, 5.80. Found: C, 85.86; H, 6.06.

4,6-Di(4-biphenyl)-2-(4-dimethylaminophenyl)pyrimidine (5d). Mp 261–263 °C. ^{1}H NMR ($CDCl_3$), δ, ppm: 3.13 (s, 6H), 6.93 (d, *J* = 6.9 Hz, 2H), 7.5 (m, 6H), 7.72 (d, *J* = 6.9 Hz, 4H), 7.81 (d, *J* = 8.4 Hz, 4H), 7.99 (s, 1H), 8.39 (d, *J* = 8.4 Hz, 4H), 8.68 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 40.86, 108.95, 112.17, 127.46, 127.64, 127.79, 127.97, 128.05, 129.11, 127.17, 130.11, 137.10, 141.73, 143.55, 164.28, 165.06. Anal. calcd. for $C_{36}H_{29}N_3$: C, 85.85; H, 5.80. Found: C, 85.65; H, 5.65.

2-(4-Dimethylaminophenyl)-4,6-di(2-naphthyl)pyrimidine (5e). Mp 245–248 °C. ^{1}H NMR ($CDCl_3$), δ, ppm: 3.14 (s, 6H), 6.93 (d, *J* = 8.4 Hz, 2H), 7.61 (m, 4H), 8.03 (m, 6H), 8.19 (s, 1H), 8.45 (d, *J* = 8.4 Hz, 2H), 8.74 (d, *J* = 9.0 Hz, 2H), 8.84 (s, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 40.77, 109.60, 112.06, 124.68, 126.74, 127.40, 127.55, 128.05, 128.81, 129.30, 130.14, 133.60, 134.80, 135.58, 138.11, 152.50, 164.61, 165.17. Anal. calcd. for $C_{32}H_{25}N_3$: C, 85.11; H, 5.58. Found: C, 85.29; H, 5.68.

4,6-Di[4-(9-carbazolyl)phenyl]-2-(4-dimethylaminophenyl)pyrimidine (5f). Mp 267–268 °C. UV-vis (THF) λ, nm (ε, l mol^{-1} cm^{-1}): 237 (4.79 × 10^4), 282sh (1.72 × 10^4), 291sh (1.71 × 10^4), 344 (2.98 × 10^4). ^{1}H NMR ($CDCl_3$), δ, ppm: 3.15 (s, 6H), 6.93 (d, *J* = 7.5 Hz, 2H), 7.48 (m, 12H), 7.83 (d, *J* = 8.4 Hz, 4H), 8.08 (s, 1H), 8.21 (d, *J* = 7.5 Hz, 4H), 8.58 (d, *J* = 8.4 Hz, 4H), 8.73 (d, *J* = 8.7 Hz, 2H). ^{13}C NMR ($CDCl_3$), δ, ppm: 40.71, 109.03, 110.13, 112.03, 120.56, 120.71, 123.92, 126.40, 127.43, 129.15, 130.19, 136.99, 140.20, 140.84, 152.50, 164.04, 165.38. Anal. calcd. for $C_{48}H_{35}N_5$: C, 84.55; H, 5.17. Found: C, 84.76; H, 5.17.

CONCLUSIONS

In summary, a simple and general procedure of the synthesis of 2,4,6-triarylpyrimidines by the Suzuki reaction of the corresponding 2-aryl-4,6-dichloropyrimidines with arylboronic acids was elaborated and a series of new fluorescent materials were synthesized.

ACKNOWLEDGEMENTS

Authors wish to express their gratitude to L. Skardžiūtė, Dr. K. Kazlauskas and prof. S. Juršėnas (Institute of Applied Research of Vilnius University) for fluorescence measure-

ments. The Research Council of Lithuania is also greatly acknowledged for financial support of this investigation (Project No. MIP-65/2010).

Received 5 December 2011
Accepted 18 January 2012

References

1. A. Kraft, A. C. Grimsdale, A. B. Holmes, *Angew. Chem. Int. Ed.*, **37**, 402 (1998); U. Mitschke, P. Bäuerle, *J. Mater. Chem.*, **10**, 1471 (2000); J. H. Borroughes, D. D. C. Bradley, A. R. Brown, et al., *Nature*, **347**, 539 (1990); S.-C. Lo, P. L. Burn, *Chem. Rev.*, **107**, 1097 (2007).
2. D. Fichou, *J. Mater. Chem.*, **10**, 571 (2000); D. H. Kim, Y. D. Park, Y. Jang, et al., *Adv. Funct. Mater.*, **15**, 77 (2005); M. Funahashi, F. Zhang, N. Tamaoki, *Adv. Mater.*, **19**, 353 (2007).
3. J. M. Tour, *Acc. Chem. Res.*, **33**, 791 (2000); J. M. Tour, *Chem. Rev.*, **96**, 537 (1996); C. Wang, A. S. Batsanov, M. R. Bryce, I. Sage, *Org. Lett.*, **6**, 2181 (2004); M. Elbing, R. Ochs, M. Koentopp, et al., *PNAS*, **102**, 8815 (2005); A. Blaszczyk, M. Chadim, C. Von Hänisch, M. Mayor, *Eur. J. Org. Chem.*, 3809 (2006).
4. M. Albota, D. Beljonne, J.-L. Brédas, et al., *Science*, **281**, 1653 (1998); A. Hayek, F. Bolze, J.-F. Nicoud, P. L. Baldeck, Y. Mély, *Photochem. Photobiol. Sci.*, **5**, 102 (2000); F. Cherioux, A.-J. Attias, H. Maillotte, *Adv. Funct. Mater.*, **12**, 203 (2002); J. Wang, M. Lu, Y. Pan, Z. Peng, *J. Org. Chem.*, **67**, 7781 (2002).
5. W.-B. Zhang, W.-H. Jin, X.-H. Zhou, J. Pei, *Tetrahedron*, **63**, 2907 (2007); A.-J. Attias, C. Cavalli, B. Donnio, D. Guillon, P. Hapiot, J. Malthete, *Chem. Mater.*, **14**, 375 (2002).
6. R. Cristiano, E. Westphal, I. H. Bechtold, A. J. Bortoluzzia, H. Gallardo, *Tetrahedron*, **63**, 2851 (2007).
7. K. Itami, D. Yamazaki, J. Yoshida, *J. Am. Chem. Soc.*, **126**, 15396 (2004); L. Pascal, J. J. Vanden Eynde, Y. Van Haverbeke, et al., *J. Phys. Chem. B*, **106**, 6442 (2002); K.-T. Wong, C. C. Hsu, *Org. Lett.*, **3**, 173 (2001); K.-T. Wong, T. S. Hung, Y. Lin, et al., *Org. Lett.*, **4**, 513 (2002); C. C. Wu, Y. T. Lin, H. H. Chiang, et al., *Appl. Phys. Lett.*, **81**, 577 (2002); S. Achelle, Y. Ramondenc, G. Dupas, N. Ple, *Tetrahedron*, **64**, 2783 (2008); S. Achelle, Y. Ramondenc, F. Marsais, N. Ple, *Eur. J. Org. Chem.*, 3129 (2008); R. Gompper, H. Mair, K. Polborn, *Synthesis*, 696 (1997).
8. H. Meier, E. Karpuk, H. C. Holst, *Eur. J. Org. Chem.*, 2609 (2006); H. Meier, H. C. Holst, A. Oehlhof, *Eur. J. Org. Chem.*, 4173 (2003); S. J. Lee, J. Y. Chang, *Tetrahedron Lett.*, **44**, 7493 (2003); H. Lee, D. Kim, H.-K. Lee, et al., *Tetrahedron Lett.*, **45**, 1019 (2004).
9. J.-Y. Jaung, *Dyes Pigments*, **71**, 245 (2006).
10. S. Tumkevicius, J. Dodonova, K. Kazlauskas, V. Masevicius, L. Skardziute, S. Jursenas, *Tetrahedron Lett.*, **51**, 3902 (2010); S. Tumkevicius, J. Dodonova, *Synlett*, 1705 (2011).
11. A. R. Gholap, K. S. Toti, F. Shirazi, M. V. Deshpande, K. V. Srinivasan, *Tetrahedron*, **64**, 10214 (2008); J. Li, X. Zhang, Y. Xie, *Synlett*, 1897 (2005); J. Yin, M. P. Rainka, X. Zhang, S. L. Buchwald, *J. Am. Chem. Soc.*, **124**, 1163 (2002); S. Kotha, K. Lahiri, D. Kashinath, *Tetrahedron*, **58**, 9633 (2002); N. Miyaura, A. Suzuki, *Chem. Rev.*, **95**, 2457 (1995); A. Suzuki, *J. Organomet. Chem.*, **576**, 147 (1999); F. Bellina, A. Carpita, R. Rossi, *Synthesis*, 2419 (2004); S. Schroter, C. Stock, T. Bach, *Tetrahedron*, **61**, 2245 (2005); I. J. S. Fairlamb, *Chem. Soc. Rev.*, **36**, 1036 (2007).
12. S. Tumkevicius, J. Dodonova, I. Baskirova, A. Voitechovicius, *J. Heterocycl. Chem.*, **46**, 960 (2009).
13. M. J. Adams, J. G. Highfield, G. F. Kirkbright, *Anal. Chem.*, **49**, 1850 (1977).
14. J. C. Mello, H. F. Wittmann, R. H. Friend, *Adv. Mater.*, **9**, 230 (1997).
15. J. Rojo, F. J. Romero-Salguero, J.-M. Lehn, G. Baum, D. Fenske, *Eur. J. Inorg. Chem.*, 1421 (1999).

Sigitas Tumkevičius, Andžejus Voitechovičius, Povilas Adomėnas

NAUJŲ 2,4,6-TRIARILPIRIMIDINŲ SINTEZĖ

Santrauka

Panaudojant paladžiu katalizuojamą kryžminio jungimo reakciją tarp 2-(4-etilfenil)- bei 2-(4-dimetilaminofenil)-4,6-dichlorpirimidinų ir arilboro rūgščių, esant katalitinei sistemai $Pd(PPh_3)_2Cl_2$ / K_3PO_4, paruoštas paprastas 2,4,6-triarilpirimidinų, turinčių 4-oje ir 6-oje pirimidino žiedo padėtyse π-konjuguotas aromatines sistemas, sintezės metodas. Susintetinti junginiai pasižymi mėlynos spalvos fluorescencija.