

An Efficient New Pyrimidine Synthesis – A Pathway to Octupoles ¹⁾

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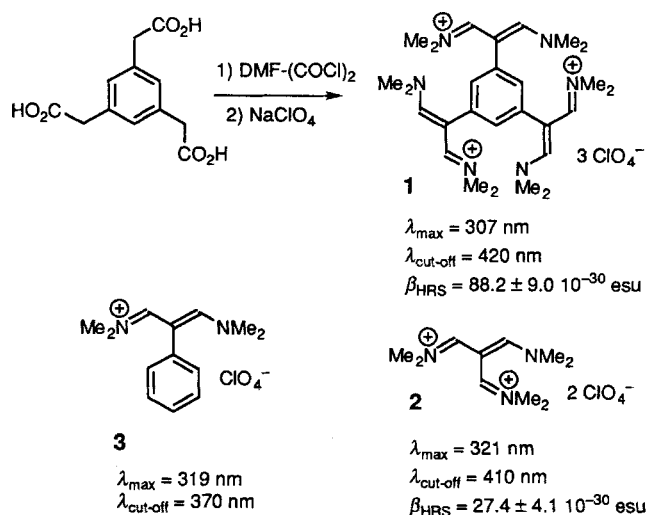
Abstract. The condensation of *N,N,N'*-tris(trimethylsilyl)-amidines (**6**, **11**, **22**) with vinamidinium salts (**1**, **7**) in the presence of potassium fluoride is the method of choice for the

synthesis of pyrimidines (**8**, **12**, **20**, **23**). Octupoles comprising 1,3,5-benzene (**8**) and triphenylamine (**12**, **20**) derivatives can be prepared in high yields.

Donor–acceptor substituted benzene derivatives such as 4-nitroaniline are solvatochromic and have nonlinear optical (NLO) properties, cf. [1]. For second harmonic generation (SHG) it is essential that the long-wavelength absorption of the compounds in question is ≤ 415 nm. Unfortunately, the hyperpolarizability β and the second-order nonlinear optical susceptibility $\chi^{(2)}$, respectively, of dipolar π -electron systems increases with a red-shift of λ_{\max} [2] (transparency-efficiency trade-off). An interesting possibility to escape the consequences of the transparency-efficiency trade-off, i.e., to obtain materials with λ_{\max} and $\lambda_{\text{cut-off}} \leq 415$ nm, having at same time high β values, are octupolar systems [3]. 1,3,5-Triamino-2,4,6-trinitrobenzene is one of the compounds studied in this regard [4, 5]. It absorbs at shorter wavelengths than 4-nitroaniline (PNA) and its β value is twice as high as that of PNA.

We have shown previously [7] that donor–acceptor substituted 2,5-diarylpyrimidines (diazaterphenyls) having interesting NLO properties (high β values at $\lambda_{\max} < 430$ nm) can readily be prepared by the condensation of amidines with vinamidinium salts. We wanted now to apply this method for the synthesis of octupoles. To this end, the trisvinamidinium salt **1** was prepared by reaction of 1,3,5-benzene triacetic acid [8] with the dimethylformamide–oxalyl chloride reagent (Scheme 1).

The X-ray analysis of **1** shows (Figure 1), that the planes formed by the dimethylamino groups of the vinamidinium moieties are twisted against one another by 18.18° . The plane formed by the carbon atoms of the vinamidinium moieties are twisted against the plane of the benzene ring by 70.77° . The strong steric inter-



Scheme 1

ence of the vinamidinium groups of **1**, an indication of which is the blue-shifted λ_{\max} , as compared to that of **2**, reduces the resonance interaction in the vinamidinium moieties and this implies that **1** is more reactive than **2**. This is born out by the reaction of **1** with 4-methoxybenzamidine to form 1,3,5-benzene-tris[2-(4-methoxyphenyl)-5-pyrimidine] **4** in 63% yield (Scheme 2). Besides being a novel type of octupole, **1** belongs to the class of star-shaped compounds that can be used as core-groups of dendrimers.

The hyperpolarizability β of **1** was measured [9] using the Hyper-Raleigh scattering (HRS) technique [10]. **1** can be viewed as a derivative of the trimethylenemeth-

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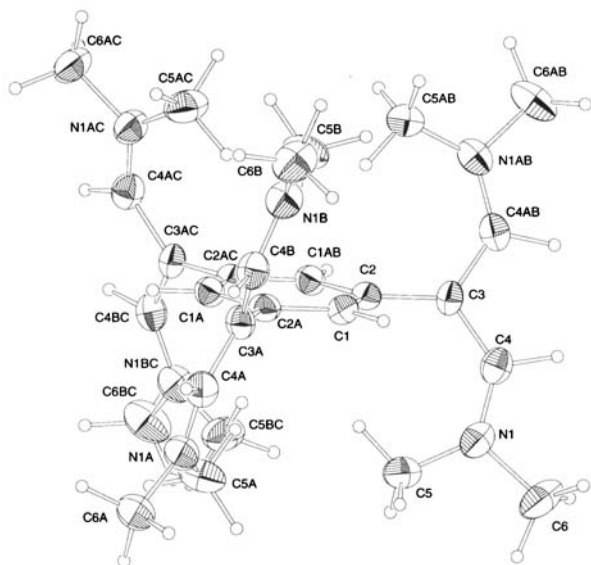
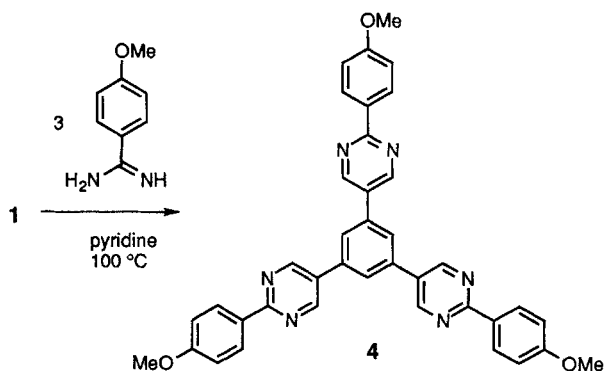


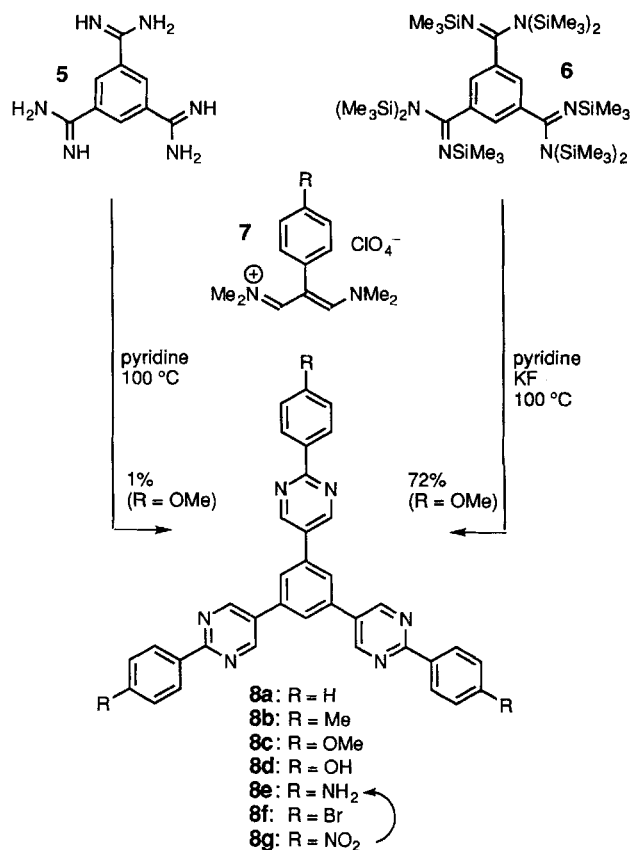
Fig. 1 Structure of **1** in the crystal (Ortep)



Scheme 2

ane dication salt **3** and as a derivative of the mesitylene trianion as well. Accordingly, the β value of **1** is roughly three times that of **3**.

Attempts to synthesize the isomer **8c** of **4** by condensation of 1,3,5-benzenetriscarboxamidine **5** with the corresponding vinamidinium salt **7c**, resulted in a frustratingly low yield of 1% (Scheme 3). Obviously, the vinamidinium salt **7c** is much less reactive than **1**. In order to overcome this problem we decided to use *N,N,N'*-tris(trimethylsilyl)amidines [11] for the condensation with vinamidinium salts. Thus, the reaction of **6** [11b] with **7c** in the presence of potassium fluoride provided **8** in 72% yield. This very good result demonstrates quite clearly, that the condensation of vinamidinium salts with *N,N,N'*-tris(trimethylsilyl)amidines is the method of choice for the synthesis of pyrimidines. Further compounds **8** could be prepared in the same way with 2-arylvinamidinium salts **7** as well as compounds **9** using 2-cyano- and 2-nitro-vinamidinium salts.



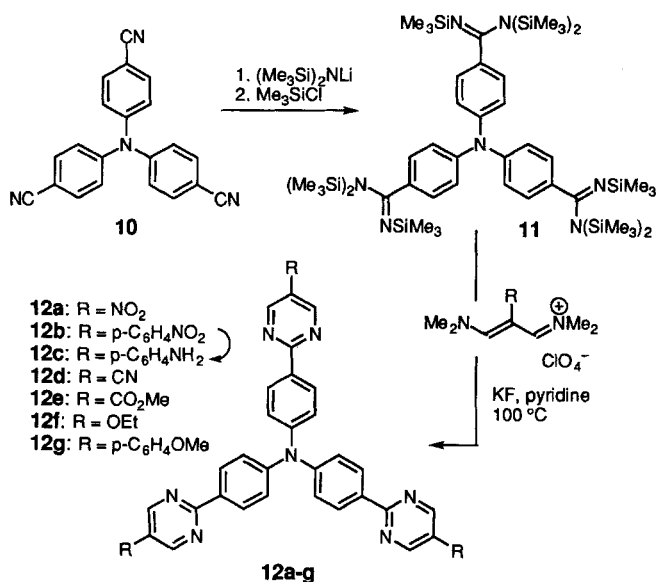
Scheme 3

Reduction of **8g** delivers the triamine **8e** which can be treated with triphenylpyrylium tetrafluoroborate to give rise to the tripyridinium salt **8h**.

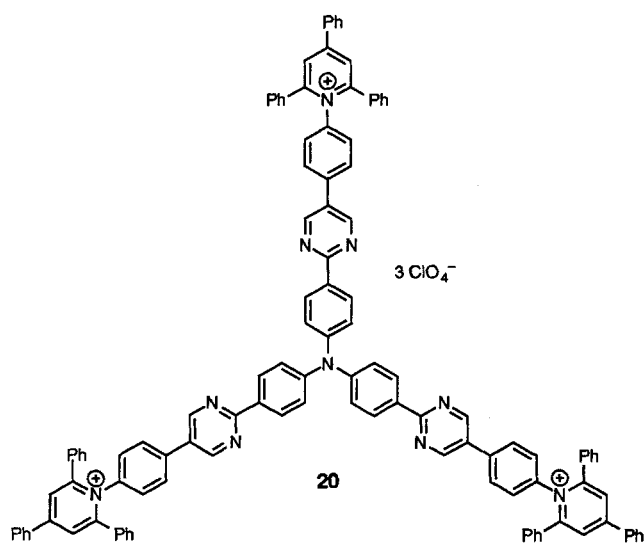
Starting from tricyanotriphenylamine **10** [12] (when prepared from triiodotriphenylamine [13] instead of tribromotriphenylamine with CuCN in DMF, there is no need to purify the compound through sublimation and chromatography) the per(trimethylsilyl)amidine **11** was prepared using the standard procedure. Its condensation with vinamidinium salts in the presence of potassium fluoride gave rise to 4,4',4''-tris(pyrimidin-2-yl)triphenylamines **12** in good yields (Scheme 4).

12b can be reduced with stannous dichloride to provide the corresponding triamino derivative **12c** which in turn can be treated with 2,4,6-triphenylpyrylium tetrafluoroborate to produce the tripyridinium salt **20**.

The dipolar diazaterphenyl derivative **14** absorbs at shorter wavelengths than the phenylpyrimidine derivative **13** ($\Delta\lambda = 46$ nm) and the same is true for the corresponding octupoles **12c** and **12a** (cf. Table 1). With related terphenyl and biphenyl derivatives the hypsochromic shift is much smaller ($\Delta\lambda = 12$ nm [2]). The fact that the octupolar compounds **12a**, **12b**, **12d** and **12e** have roughly the same λ_{max} as their dipolar analogues **13**–**16** but higher hyperpolarizabilities β shows that octupoles are promising candidates for SHG.

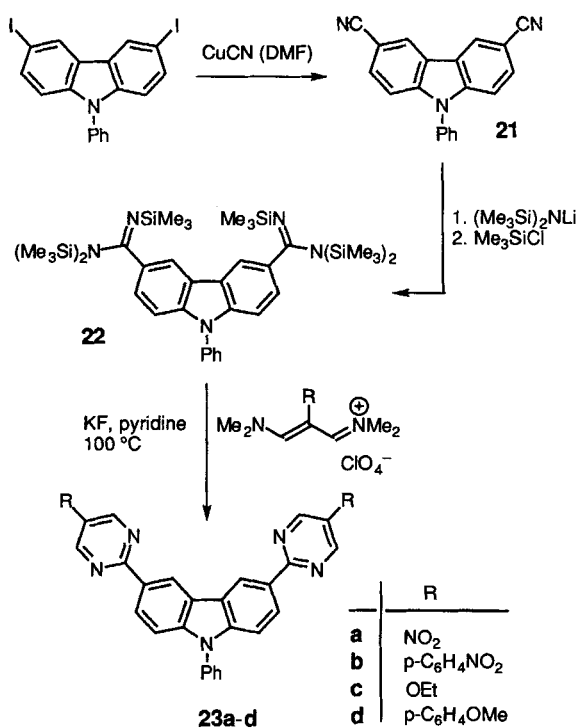


Scheme 4



In contrast to the situation with dipolar systems the donor substituted diazaterphenylderivative **18** absorbs at longer wavelengths than the phenylpyrimidine derivative **17**.

Another application of the new pyrimidine synthesis is the preparation of new carbazole derivatives. Starting material is 3,6-dicyano-*N*-phenylcarbazol **21**, prepared from 3,6-diiodo-*N*-phenylcarbazol [14] with CuCN in DMF, that can be transformed into *N*-phenylcarbazolyl-3,6-bis[*N,N,N'*-tris(trimethylsilyl)-carboxamide] **22** the in situ condensation of which with vinamidinium salts in the presence of KF gives rise to the carbazole derivatives **23** (Scheme 5).

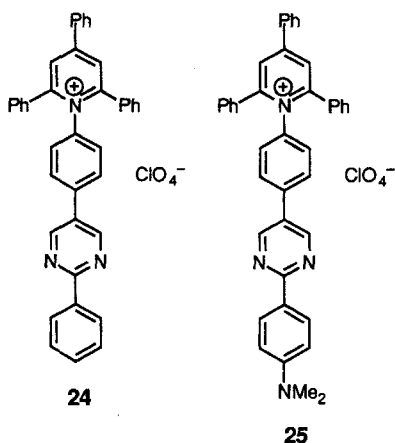


Scheme 5

Table 1 UV/VIS spectra ($\lambda_{\max}/\lambda_{\text{cutoff}}$ [nm], in DMSO) of dipolar (**13–19**) *vers.* corresponding octupolar compounds (**12a–g**)

13	14	15	16	17	18	19
448/595	402/495	394/484	388/458	335/380	362/415	429/435
12a	12b	12d	12e	12f	12g	12c
450/610	417/530	417/485	407/480	372/420	392/470	399/475

Cyclovoltammetric studies showed that **8h** can be irreversibly reduced at -0.81 V and reversibly/irreversibly oxidized at $4.48/0.91$ V. Since the reference compound **24** behaves similar ($0.37_{\text{rev}}/0.66_{\text{irrev}}$ V; -0.78_{irrev} V) it has to be assumed that in **8h** the 3 substructures are electronically independent.



12g can be quasireversibly reduced at -0.51 V and **12d** reversibly oxidized at 1.29 V. With **20** three irreversible reduction waves (-0.81 , -1.02 V) and one quasireversible oxidation wave (1.04 V) are detected. In contrast to **20**, **25** displays one quasi-reversible reduction wave (-1.33 V), two quasireversible oxidation waves (0.53 , 1.17 V) and one irreversible oxidation wave (0.98 V). Obviously, with **20** the 3 substructures interact electronically by way of the central nitrogen atom.

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Experimental

NMR spectra were recorded on a Bruker WP 80 (80MHz) and a Varian VXR 400 S (400 MHz); IR spectra on a Perkin-Elmer 125 and a Bruker IFS 45; UV/VIS spectra on a Zeiss DMR 10 and a Perkin-Elmer model Lambda 3; mass spectra on a AEJ, MS 902, and a MAT 95Q, Cs-Gun). Cyclovoltammetric measurement were performed with a Bioanalytical Systems CV-1B, using a Pt working electrode and an Ag/AgCl reference electrode (Bu_4NPF_6). Melting points were obtained on a Büchi SMP-20 and a Reichert Thermovar BHT apparatus.

Crystal data for **1**

$\text{C}_{27}\text{H}_{45}\text{N}_6 \times 3 \text{ClO}_4$, $M = 752.05$, rhomboedric, space group $R3_C$ (167), $a = 1224.8(3)$ pm, $\alpha = 19.16(2)(2)^\circ$, $V = 1.8373$ nm³, $Z = 2$, $D_c = 1.259$ g cm⁻³, $\mu = 3.100$ cm⁻¹, $F(000) = 792.00$, $2\Theta_{\text{max}} = 4-46^\circ$, ω -scan, crystal dimensions $7/30 \times 20/30 \times 24/30$ mm, maximum measuring time 180 s, graphite monochromated Mo- K_α radiation. 2829 measured (h, k, \pm I),

838 independent reflections, 762 classed as observed [$I > 3\sigma$ (I)]1; refined parameters: 75. Solution of structure: SHELXS-76, SIR. $R = 0.1255$, $R_w = 0.1115$; largest residual electron density $\rho = +0.575/-0.679$ e pm⁻³ 10⁶. Supplementary material on the X-ray structure determination may be obtained from the Fachinformationszentrum Karlsruhe, Gesellschaft für wissenschaftlich-technische Information mbH, D-76344 Eggenstein-Leopoldshafen 2, on quoting the depository number CSD, the names of the authors and the journal citation.

2,2',2''-(1,3,5-Benzene)-tris-(3-dimethylamino-*N,N*-dimethylpropene-2-eneiminium) triperchlorate (**1**)

1,3,5-benzenetriacetic acid (2.0 g, 7.9 mmol) was added to the reagent prepared from dimethylformamide (4.4 ml, 57.2 mmol) and oxalyl chloride (5 ml, 56.3 mmol) and the mixture refluxed for 2 days. After cooling, a solution of sodium perchlorate monohydrate (4.0 g, 28.5 mmol) in water (20 ml) was added dropwise (cooling with ice). The precipitate was collected by filtration, washed with water, stirred with a little methanol and dried in vacuo.

Colorless powder, m.p. 208°C , yield 2.0 g (34%). –

IR (KBr): $\nu = 3020$ cm⁻¹, 2990, 2942, 2810, 1597, 1490 1443, 1400, 1293, 1286, 1216, 1088, 825, 775, 625. – UV (DMSO): $\lambda_{\text{max}} = 307$ nm. – ¹H NMR ([D₆]DMSO): $\delta = 7.76$ (s, 6 H, vinyl-H), 7.29 (s, 3 H, benzene-H), 3.32 (d, 36 H, NMe₂). $\text{C}_{27}\text{H}_{45}\text{C}_{13}\text{N}_6\text{O}_{12}$ Calcd. C 43.12 H 6.03 N 11.17 (752.1) Found C 43.30 H 6.05 N 11.00

1,3,5-Benzene-tris[2-(4-methoxyphenyl)-5-pyrimidine (**4**)

A suspension of **1** (2.0 g, 2.66 mmol) and 4-methoxybenzamidinium chloride [x] in 50 ml of pyridine was heated to 100°C for 10 h. After cooling, the mixture was poured into water, the precipitate collected by filtration, dissolved in acetonitrile and deposited again by addition of water.

Colorless powder, m.p. 158°C , yield 1.06 g (63%). –

IR (KBr): $\nu = 3010$ cm⁻¹, 2965, 2940, 2840, 1606, 1582, 1539, 1515, 1456, 1423, 1384, 1334, 1255, 1168, 1028, 878, 846, 798, 709, 653. – UV (DMSO): $\lambda_{\text{max}} = 318$ nm. – ¹H NMR ([D₆]DMSO): $\delta = 9.20$ (s, 6 H, pyrimidine-H), 8.28 (d, 6 H, phenylene-H), 8.13 (s, 3 H, benzene-H), 6.95 (d, 6 H, phenylene-H), 3.76 (s, 9 H, OCH₃). – MS (70 eV): m/z (%) = 630.3 (100) [M⁺].

$\text{C}_{39}\text{H}_{30}\text{N}_6\text{O}_{33} \times 0.33\text{H}_2\text{O}$ Calcd. C 73.57 H 4.85 N 13.20 (636.7) Found C 73.67 H 5.00 N 13.17

1,3,5-Benzene-tris-(5-phenyl-2-pyrimidine) (**8a**)

General procedure for 8a–8d. 8f. 8g. 9a. 9b. 12a. 12b. 12d–12g. 23a–23d

7a [15] (2.4 g, 7.9 mmol) and potassium fluoride (1.5 g, 25.8 mmol) were added to a suspension of **6** (2.2 g, 2.6 mmol) in pyridine (50 ml) and the mixture stirred at 100°C for 6 h. After cooling, the product was poured into water (100 ml), the precipitate collected by filtration, washed with water and methanol and recrystallized from *N,N*-dimethylformamide.

Colorless powder, m.p. $>300^\circ\text{C}$, yield 0.98 g (70%). –

IR (KBr): $\nu = 3033$ cm⁻¹, 1581, 1563, 1443, 1417, 797 747, 697. – V (DMSO): $\lambda_{\text{max}} = 296.5$ nm. – ¹H NMR ([D₆]DMSO): $\delta = 9.60$ (s, 3 H, benzene-H), 9.15 (s, 6 H, pyrimidine-H), 7.76

(m, 6 H, phenyl-H), 7.43 (m, 9 H, phenyl-H). – MS (70 eV): m/z (%) = 540 (100) [M⁺].

C₃₆H₂₄N₆×H₂O Calcd. C 77.40 H 4.69 N 15.04
(558.6) Found C 77.09 H 4.60 N 14.92

1,3,5-Benzene-tris-[5-(4-tolyl)-2-pyrimidine] (8b)

With **7b** [15] (2.5 g, 7.9 mmol).

Colorless powder, m.p. 260 °C, yield 1.06 g (70%). – IR (KBr): ν = 3019 cm⁻¹, 2920, 1579, 1452, 1420, 1281, 817, 794. – UV (DMSO): λ_{max} = 303 nm. – ¹H NMR ([D₆]MSO): δ = 9.55 (s, 3 H, benzene-H), 9.10 (s, 6 H, pyrimidine-H), 7.55 (d, 6 H, phenylene-H), 7.30 (d, 6 H, phenylene-H), 2.38 (s, 9 H, CH₃).

C₃₉H₃₀N₆×0.33 H₂O Calcd. C 79.57 H 5.15 N 14.28
(588.7) Found C 79.81 H 5.36 N 14.41

1,3,5-Benzene-tris-[5-(4-methoxyphenyl)-2-pyrimidine] (8c)

With **7c** [15] (2.7 g, 8 mmol).

Colorless powder, m.p. 245 °C, yield 1.18 g (72%). – IR (KBr): ν = 3020 cm⁻¹, 3000, 2935, 2840, 1610, 1579, 1517, 1455, 1425, 1412, 1270, 1181, 1033, 830, 794, 720. – UV (DMSO): λ_{max} = 309 nm. – ¹H NMR ([D₆]DMSO): δ = 9.58 (s, 3 H, benzene-H), 9.10 (s, 6 H, pyrimidine-H), 7.70 (d, 6 H, phenylene-H), 7.03 (d, 6 H, phenylene-H), 3.20 (s, 9 H, OCH₃). – MS (70 eV): m/z (%) = 630.3 (100) [M⁺].

C₃₉H₃₀N₆O₃ Calcd. C 74.27 H 4.79 N 13.33
(630.7) Found C 74.26 H 4.86 N 13.15

1,3,5-Benzene-tris-[5-(4-hydroxyphenyl)-2-pyrimidine] (8d)

With **7d** [15] (2.6 g, 8.1 mmol).

Colorless powder, m.p. >300 °C, yield 0.68 g (45%). – IR (KBr): ν = 3424 cm⁻¹, 3020, 1653, 1610, 1589, 1417, 1273, 1177, 833, 792, 730. – UV (DMSO): λ_{max} = 327 nm. – ¹H NMR ([D₆]DMSO): δ = 9.50 (s, 3 H, benzene-H), 9.10 (s, 6 H, pyrimidine-H), 7.63 (d, 6 H, phenylene-H), 6.90 (d, 6 H, phenylene-H), 3.70 (s, broad, 3 H, OH). – MS (70 eV): m/z (%) = 588 (100) [M⁺].

C₃₆H₂₄N₆O₃×1.5 H₂O Calcd. C 70.23 H 4.42 N 13.65
(615.6) Found C 70.38 H 4.63 N 13.48

1,3,5-Benzene-tris-[5-(4-bromophenyl)-2-pyrimidine] (8f)

With **7f** [15] (3.0 g, 7.9 mmol).

Colorless powder, m.p. 200 °C, yield 1.43 g (71%). – IR (KBr): ν = 3022 cm⁻¹, 1581, 1534, 1453, 1420, 1281, 1075, 999, 824, 670. – UV (DMSO): λ_{max} = 365 nm. – ¹H NMR ([D₆]DMSO): δ = 9.74 (s, 3 H, benzene-H), 9.34 (s, 6 H, pyrimidine-H), 7.87 (d, 6 H, phenylene-H), 7.78 (d, 6 H, phenylene-H). – MS (70 eV): m/z (%) = 780 (36.89) [M⁺, 3 ⁸¹Br], 778 (99.8) [M⁺, ⁷⁹Br, 2 ⁸¹Br], 775.9 (100) [M⁺, ²⁷⁹Br, ⁸¹Br], 774 (31.44) [M⁺, ³⁷⁹Br].

C₃₆H₂₁N₆Br₃ Calcd. C 55.62 H 2.72 N 10.81 Br 30.84
(777.3) Found C 55.62 H 2.96 N 10.90 Br 30.34

1,3,5-Benzene-tris-[5-(4-nitrophenyl)-pyrimidine] (8g)

With **7g** [15] (2.80 g, 8 mmol).

Colorless powder, m.p. >300 °C, yield 1.40 g (80%). –

IR (KBr): ν = 3441 cm⁻¹, 3083, 1601, 1581, 1519, 1455, 1423, 1341, 1280, 850, 797. – UV (DMSO): λ_{max} = 324 nm. – ¹H NMR ([D₆]DMSO): δ = 9.77 (s, 3 H, benzene-H), 9.41 (s, 6 H, pyrimidine-H), 8.37 (d, 6 H, phenylene-H), 8.16 (d, 6 H, phenylene-H). – MS (70 eV): m/z (%) = 675 (100) [M⁺].

C₃₆H₂₁N₉O₆ Calcd. C 63.99 H 3.13 N 18.65
(675.6) Found C 63.95 H 3.47 N 18.30

1,3,5-Benzene-tris-(5-cyano-2-pyrimidine) (9a)

With 2-cyano-3-dimethylamino-*N,N*-dimethyl-prop-2-eneiminium perchlorate [16] (2.0 g, 7.9 mmol).

Colorless powder, m.p. >300 °C, yield 0.68 g (68%). – IR (KBr): ν = 2234 cm⁻¹, 1578, 1533, 1452, 1419, 1288, 1215, 925, 796, 762. – UV (DMSO): λ_{max} = 288 nm. – ¹H NMR ([D₆]DMSO): δ = 9.70 (s, 3 H, benzene-H), 9.40 (s, 6 H, pyrimidine-H).

C₂₁H₉N₉ Calcd. C 65.11 H 2.34 N 32.54
(387.4) Found C 65.34 H 2.34 N 32.38

1,3,5-Benzene-tris-(5-nitro-2-pyrimidine) (9b)

With 3-dimethylamino-*N,N*-dimethyl-2-nitroprop-2-eneiminium perchlorate [16] (2.17 g, 8 mmol).

Colorless powder, m.p. 325 °C, yield 0.87 g (75%). – IR (KBr): ν = 3080 cm⁻¹, 3040, 1604, 1582, 1563, 1517, 1415, 1347, 1283, 1148, 868, 831, 793. – UV (DMSO): λ_{max} = 314 nm. – ¹H NMR ([D₆]DMSO): δ = 9.66 (s, 3 H, benzene-H), 9.63 (s, 6 H, pyrimidine-H).

C₁₈H₉N₉O₆×0.33 DMF Calcd. C 48.38 H 2.42 N 27.72
(471.7) Found C 48.64 H 2.69 N 28.06

1,3,5-Benzene-tris-[5-(4-aminophenyl)-2-pyrimidine] (8e)

Stannous chloride dihydrate (10.0 g, 44.3 mmol) was added to the suspension of **8g** (2.0 g, 3 mmol) in conc. HCl (50 ml) and the mixture heated to 100 °C for 3 h. After cooling, the precipitate was collected by filtration, dried *in vacuo* and refluxed in DMF for 1 h. After filtration, the solvent was removed in *vacuo* and the residue recrystallized from acetonitrile. Pale yellow powder, m.p. >300 °C, yield 1.23 g (70%).

IR (KBr): ν = 3356 cm⁻¹, 3242, 3029, 1610, 1536, 1522, 1456, 1417, 1288, 1184, 828, 799. – UV (DMSO): λ_{max} = 365 nm. – ¹H NMR ([D₆]DMSO): δ = 9.43 (s, 3 H, benzene-H), 8.98 (s, 6 H, pyrimidine-H), 7.45 (d, 6 H, phenylene-H), 6.65 (d, 6 H, phenylene-H), 5.25 (s, broad, 6 H, NH₂). – MS (70 eV): m/z (%) = 585 (100) [M⁺].

C₃₆H₂₇N₉×2.1 H₂O Calcd. C 69.34 H 5.04 N 20.21
(623.5) Found C 69.04 H 4.57 N 20.10

1,3,5-Benzene-tris-[5-[4-(2,4,6-triphenyl-1-pyridinio)-phenyl]-2-pyrimidine] trisperchlorate (8h)

A suspension of **8e** (1.26 g, 2.15 mmol) and triphenylpyrylium tetrafluoroborate (2.6 g, 6.56 mmol) in pyridine (30 ml) was stirred at 100 °C for 2 d. After cooling and filtration a solution of sodium perchlorate monohydrate (0.4 g, 2.8 mmol) in water (10 ml) was added and the solvents removed by distillation *in vacuo* (not to complete dryness!). The residue was triturated in water and the undissolved material removed by filtration. A solution of sodium perchlorate monohydrate (1.0

g, 7.1 mmol) in water (10 ml) was added, the colorless precipitate collected by filtration, washed with water and recrystallized from acetonitrile-methanol. Colorless powder, m.p. 310 °C, yield 2.3 g (61%).

IR (KBr): $\nu = 3065 \text{ cm}^{-1}$, 1621, 1598, 1577, 1423, 1122, 1096, 850, 775, 771 624. – UV (DMSO): $\lambda_{\text{max}} = 315 \text{ nm}$. – $^1\text{H NMR}$ ($[\text{D}_6]$ DMSO): $\delta = 9.63$ (s, 3 H, benzene-H), 9.20 (s, 6 H, pyrimidine-H), 8.66 (d, 6 H, pyridinium-H), 8.44–8.25 (m, 6 H), 7.81–7.24 (m, 51 H).

$\text{C}_{105}\text{H}_{72}\text{C}_{13}\text{N}_9\text{O}_{12} \times 2 \text{ H}_2\text{O}$ Calcd. C 70.29 H 4.27 N 7.03 (1794.2) Found C 70.13 H 4.25 N 7.32

Triphenylamino-4,4,4"-tris-[N,N,N'-tris-(trimethylsilyl)-carboxamide] (11)

Lithium hexamethyldisilazene (2.5 g, 14.9 mmol) was added to a suspension of 1.5 g tricyanotriphenylamine (**10**) (1.5 g, 4.7 mmol) in 50 ml dry ether and the mixture stirred at room temperature for 12 h. The solvent was removed *in vacuo*, toluene (50 ml) and chlorotrimethylsilane (1.9 ml, 15 mmol) added to the residue and the mixture refluxed for 5 h. The solvent was distilled off *in vacuo* and the orange residue (yield 4.8 g) used according to the "general procedure" (cf. **8a**).

Tris-[4-(5-nitro-2-pyrimidinyl)-phenyl]-amine (12a)

With **11** (4.8 g, 4.7 mmol) and *N,N*-dimethyl-3-dimethylamino-2-nitroprop-2-eneiminium perchlorate [**16**] (4.2 g, 15.5 mmol).

Brickred powder, m.p. >300 °C, yield 2.05 g (71%). – IR (KBr): $\nu = 1585 \text{ cm}^{-1}$, 1560, 1420, 1342, 1316, 856, 798. – UV (DMSO): $\lambda_{\text{max}} = 450 \text{ nm}$; UV (toluene): $\lambda_{\text{max}} = 288 \text{ nm}$, 451. – $^1\text{H NMR}$ ($[\text{D}_6]$ DMSO): $\delta = 9.45$ (s, 6 H, pyrimidine-H), 8.39 (d, 6 H, phenylene-H), 7.23 (d, 6 H, phenylene-H). $\text{C}_{30}\text{H}_{18}\text{N}_{10}\text{O}_6$ Calcd. C 58.63 H 2.95 N 22.79 (614.5) Found C 59.07 H 3.20 N 22.55

Tris-[4-[5-(4-nitrophenyl)-2-pyrimidinyl]-phenyl]-amine (12b)

With **7g** [**15**] (5.4 g, 15.5 mmol).

Orange powder, m.p. 204 °C, yield 2.81 g (71%). – IR (KBr): $\nu = 1597 \text{ cm}^{-1}$, 1578, 1516, 1428, 1342, 1176, 855, 798. – UV (DMSO): $\lambda_{\text{max}} = 307 \text{ nm}$, 417; UV (toluene): $\lambda_{\text{max}} = 303 \text{ nm}$, 422. – $^1\text{H NMR}$ ($[\text{D}_6]$ DMSO): $\delta = 9.14$ (s, 6 H, pyrimidine-H), 8.36 (d, 6 H, phenylene-H), 8.25 (d, 6 H, phenylene-H), 8.00 (d, 6 H, phenylene-H), 7.18 (d, 6 H, phenylene-H).

$\text{C}_{48}\text{H}_{30}\text{N}_{10}\text{O}_6$ Calcd. C 68.40 H 3.59 N 16.62 (842.8) Found C 68.20 H 3.73 N 16.41

Tris-[4-(5-cyano-2-pyrimidinyl)-phenyl]-amine (12d)

With 2-cyano-*N,N*-dimethyl-3-dimethylaminoprop-2-eneiminium perchlorate [**16**] (3.7 g, 14.7 mmol). Chromatography on silica gel, eluent CHCl_3 .

Yellow powder, m.p. 275 °C (from DMF-acetonitrile), yield 1.77 g (68%). –

IR (KBr): $\nu = 2231 \text{ cm}^{-1}$, 1572, 1424, 1317, 1284, 1176, 798. – UV (DMSO): $\lambda_{\text{max}} = 417 \text{ nm}$; UV (acetonitrile): $\lambda_{\text{max}} = 410 \text{ nm}$; UV (toluene): $\lambda_{\text{max}} = 411 \text{ nm}$. – $^1\text{H NMR}$ ($[\text{D}_6]$ DMSO): $\delta = 9.24$ (s, 6 H, pyrimidine-H), 8.36 (d, 6 H, phenylene-H),

7.23 (d, 6 H, phenylene-H). – MS (70 eV): m/z (%) = 554 (100) [M^+].

$\text{C}_{33}\text{H}_{18}\text{N}_{10}$ Calcd. C 71.47 H 3.27 N 25.26 (554.6) Found C 71.33 H 3.52 N 24.97

Tris-[4-(5-methoxycarbonyl-2-pyrimidinyl)-phenyl]-amine (12e)

With 3-dimethylamino-2-methoxycarbonyl-*N,N*-dimethylprop-2-eneiminium perchlorate [**17**] (4.44 g, 15.6 mmol).

Yellow powder, m.p. 288 °C (from DMF-acetonitrile), yield 2.33 g (76%). –

IR (KBr): $\nu = 2960 \text{ cm}^{-1}$, 2935, 2865, 1730, 1577, 1422, 1285, 1177, 1133, 802, 756, 728. – UV (DMSO): $\lambda_{\text{max}} = 349 \text{ nm}$; UV (acetonitrile): $\lambda_{\text{max}} = 401 \text{ nm}$; UV (toluene): $\lambda_{\text{max}} = 414 \text{ nm}$. – $^1\text{H NMR}$ ($[\text{D}_6]$ DMSO): $\delta = 9.15$ (s, 6 H, pyrimidine-H), 8.36 (d, 6 H, phenylene-H), 3.85 (s, 9 H, CH_3). – MS (70 eV): m/z (%) = 653.2 (100) [M^+].

$\text{C}_{36}\text{H}_{27}\text{N}_7\text{O}_6 \times 0.5 \text{ H}_2\text{O}$ Calcd. C 65.25 H 4.26 N 14.80 (662.7) Found C 65.51 H 4.34 N 14.67

Tris-[4-(5-ethoxy-2-pyrimidinyl)-phenyl]-amine (12f)

With 3-dimethylamino-2-ethoxy-*N,N*-dimethylprop-2-eneiminium perchlorate [**18**] (4.20 g, 15.5 mmol). Chromatography on silica gel, eluent CHCl_3 .

Colorless powder, m.p. 168 °C (from THF), yield 1.15 g (40%). –

IR (KBr): $\nu = 3050 \text{ cm}^{-1}$, 2981, 2940, 2900, 1599, 1541, 1508, 1433, 1386, 1316, 1272, 1177, 1040, 847, 790, 736. – UV (DMSO): $\lambda_{\text{max}} = 265 \text{ nm}$, 372; UV (acetonitrile): $\lambda_{\text{max}} = 366 \text{ nm}$; UV (toluene): $\lambda_{\text{max}} = 378 \text{ nm}$. – $^1\text{H NMR}$ ($[\text{D}_6]$ DMSO): $\delta = 8.55$ (s, 6 H, pyrimidine-H), 8.23 (d, 6 H, phenylene-H), 7.15 (d, 6 H, phenylene-H), 4.23 (q, 2 H, OCH_2), 1.41 (t, 3 H, CH_3).

$\text{C}_{36}\text{H}_{33}\text{N}_7\text{O}_3 \times 0.5 \text{ H}_2\text{O}$ Calcd. C 69.66 H 5.52 N 15.79 (620.7) Found C 69.87 H 5.67 N 15.63

Tris-[4-[5-(4-methoxyphenyl)-2-pyrimidinyl]-phenyl]-amine (12g)

With **7c** [**15**] (5.20 g, 15.6 mmol).

Ochre powder, m.p. 170 °C, yield 2.58 g (69%). –

IR (KBr): $\nu = 2834 \text{ cm}^{-1}$, 1608, 1579, 1517, 1427, 1251, 1177, 828, 797. – UV (DMSO): $\lambda_{\text{max}} = 297 \text{ nm}$, 392; UV (acetonitrile): $\lambda_{\text{max}} = 386 \text{ nm}$; UV (toluene): $\lambda_{\text{max}} = 292 \text{ nm}$, 400. – $^1\text{H NMR}$ ($[\text{D}_6]$ DMSO): $\delta = 9.16$ (s, 6 H, pyrimidine-H), 8.43 (d, 6 H, phenylene-H), 7.80 (d, 6 H, phenylene-H), 7.29 (d, 6 H, phenylene-H), 7.11 (d, 6 H, phenylene-H), 3.84 (s, 9 H, OCH_3).

$\text{C}_{51}\text{H}_{39}\text{N}_7\text{O}_3$ Calcd. C 76.77 H 4.93 N 12.29 (797.9) Found C 76.67 H 5.14 N 12.42

Tris-[4-[5-(4-aminophenyl)-2-pyrimidinyl]-phenyl]-amine (12c)

Same procedure as for **8e** with **12b** (2.0 g, 2.4 mmol). The neutralized and dried precipitate was extracted (Soxhlet) with acetonitrile (200 ml) for 2 d.

Pale yellow powder, m.p. 220 °C, yield 0.9 g (50%). –

IR (KBr): $\nu = 3439 \text{ cm}^{-1}$, 3390, 3033, 1608, 1579, 1428, 1317, 1285, 1177, 827, 797. – UV (DMSO): $\lambda_{\text{max}} = 399 \text{ nm}$. – ^1H

NMR ($[D_6]DMSO$): δ = 8.96 (s, 6 H, pyrimidine-H), 8.33 (d, 6 H, phenylene-H), 7.48 (d, 6 H, phenylene-H), 7.18 (d, 6 H, phenylene-H), 6.68 (d, 6 H, phenylene-H), 4.25 (s, broad, 6 H, NH_2). – MS (70 eV): m/z (%) = 752 (12.64) $[M^+]$.
 $C_{48}H_{36}N_{10} \times 1.5 H_2O$ Calcd. C 73.92 H 5.04 N 17.96 (779.9) Found C 73.78 H 4.97 N 18.07

Tris-[4-[5-[4-(2,4,6-triphenyl-1-pyridinio)-phenyl]-phenyl]-amine trisperchlorate (20)

Same procedure as for **8h** with **12c** (1.0 g, 1.33 mmol). Yellow powder, m.p. 300 °C, yield 1.79 g (70%). – IR (KBr): ν = 3070 cm^{-1} , 1621, 1598, 1579, 1429, 1122, 1096, 847, 798. – UV (DMSO): λ_{max} = 308 nm 404. – 1H NMR ($[D_6]DMSO$): δ = 9.14 (s, 6 H, pyrimidine-H), 8.72 (s, 6 H, pyridinium-H), 8.38 (d, 12 H, phenylene-H), 7.80 (d, 6 H, phenylene-H), 7.72–7.38 (m, 51 H), 7.27 (d, 6 H, phenylene-H).
 $C_{117}H_{81}C_{13}N_{10}O_{12} \times 3 H_2O$ Calcd. C 70.99 H 4.43 N 7.08 (1979.4) Found C 70.87 H 4.33 N 7.28

2-(4-Dimethylaminophenyl)-5-nitropyrimidine (13)

N,N-Dimethyl-3-dimethylamino-2-nitroprop-2-eneiminium perchlorate [16] (1.55 g, 5.7 mmol) was added to a suspension of 4-dimethylaminobenzamidinium chloride [11c] (1.14 g, 5.7 mmol) in pyridine (30 ml) and the mixture heated to 100 °C for 10 h. The solvent was distilled off *in vacuo*, the residue triturated with water, the solid collected by filtration and washed with methanol.

Dark red powder, m.p. 298 °C (from acetonitrile), yield 0.90 g (65%). – IR (KBr): ν = 3070 cm^{-1} , 2910, 2870, 1606, 1534, 1422, 1367, 1343, 1326, 1188, 1149, 833, 791. – UV (DMSO): λ_{max} = 448 nm; UV (toluene): λ_{max} = 435 nm. – 1H NMR ($[D_6]DMSO$): δ = 9.23 (s, 2 H, pyrimidine-H), 8.23 (d, 2 H, phenylene-H), 6.75 (d, 2 H, phenylene-H), 3.00 (s, 6 H, $N(CH_3)_2$).
 $C_{12}H_{12}N_4O_2$ Calcd. C 59.00 H 4.95 N 22.93 (244.3) Found C 59.47 H 5.01 N 22.75

2-(4-Dimethylaminophenyl)-5-(4-nitrophenyl)-pyrimidine (14)

Lithium hexamethyldisilazene (2.4 g, 14.3 mmol) was added to a suspension of 4-dimethylaminobenzonitrile (2 g, 13.7 mmol) in dry ether (50 ml) and the mixture stirred at room temperature for 10 h. The solvent was removed *in vacuo*, toluene (50 ml) and chlorotrimethylsilane (1.9 ml, 15 mmol) were added and the mixture refluxed for 5 h. The solvent was distilled off *in vacuo* and **7g** [15] (4.76 g, 13.7 mmol), potassium fluoride (2.7 g, 46.5 mmol) and pyridine (50 ml) added to the residue and the mixture stirred at 100 °C for 6 h. After cooling, the product was poured into water (100 ml), the precipitate was collected by filtration and refluxed with DMF for 1 h. The solid material was collected by filtration and washed with methanol.

Red powder, m.p. 322 °C, yield 3.46 g (79%). – IR (KBr): ν = 3080 cm^{-1} , 2920, 2875, 2830, 1614, 1597, 1583, 1515, 1433, 1372, 1339, 1187, 866, 856, 825, 795. – UV (toluene): λ_{max} = 403 nm. – 1H NMR ($[D_6]DMSO$): δ = 9.05 (s, 2 H, pyrimidine-H), 8.20 (d, 4 H, phenylene-H), 7.93 (d, 2 H,

phenylene-H), 6.74 (d, 2 H, phenylene-H), 3.82 (s, 6 H, $N(CH_3)_2$).
 $C_{18}H_{16}N_4O_2 \times 0.25 H_2O$ Calcd. C 66.54 H 5.12 N 17.25 (324.9) Found C 66.25 H 5.16 N 17.25

5-Cyano-2-(4-dimethylaminophenyl)-pyrimidine (15)

Same procedure as for **13** with 2-cyano-*N,N*-dimethyl-3-dimethylaminoprop-2-eneiminium perchlorate [16] (2.2 g, 8.7 mmol).

Yellow powder, m.p. 217 °C, yield 1.22 g (74%). – IR (KBr): ν = 2920 cm^{-1} , 2875, 2820, 2222, 1808, 1580, 1535, 1515, 1433, 1368, 1183, 833, 793. – UV (DMSO): λ_{max} = 394.5 nm; UV (acetonitrile): λ_{max} = 387 nm; UV (toluene): λ_{max} = 390 nm. – 1H NMR ($[D_6]DMSO$): δ = 9.02 (s, 2 H, pyrimidine-H), 8.21 (d, 2 H, phenylene-H), 6.76 (d, 2 H, phenylene-H), 3.03 (s, 6 H, $N(CH_3)_2$).
 $C_{13}H_{12}N_4$ Calcd. C 69.61 H 5.39 N 24.98 (224.3) Found C 69.40 H 5.27 N 25.01

Methyl-2-(4-dimethylaminophenyl)-4-pyrimidinecarboxylate (16)

Same procedure as for **14** with 3-dimethylamino-2-methoxy-carbonyl-*N,N*-dimethyl-prop-2-eneiminium perchlorate [17] (3.90 g, 13.7 mmol).

Pale yellow powder, m.p. 214 °C, yield 2.82 g (80%). – IR (KBr): ν = 2910 cm^{-1} , 2820, 1723, 1710, 1611, 1581, 1422, 1366, 1288, 1191, 1134, 798. – UV (DMSO): λ_{max} = 303 nm, 388; UV (acetonitrile): λ_{max} = 380 nm; UV (toluene): λ_{max} = 383 nm. – 1H NMR ($[D_6]DMSO$): δ = 9.00 (s, 2 H, pyrimidine-H), 8.20 (d, 2 H, phenylene-H), 6.70 (d, 2 H, phenylene-H), 3.83 (s, 3 H, OCH_3), 2.98 (s, 6 H, $N(CH_3)_2$).
 $C_{14}H_{15}N_3O_2$ Calcd. C 65.35 H 5.88 N 16.33 (257.3) Found C 65.01 H 5.92 N 16.24

2-(4-Dimethylaminophenyl)-4-ethoxypyrimidine (17)

Same procedure as for **13** with 3-dimethylamino-2-ethoxy-*N,N*-dimethyl-prop-2-eneiminium perchlorate [18] (1.0 g, 3.7 mmol).

Colorless powder, m.p. 157 °C, yield 0.36 g (40%). – IR (KBr): ν = 2979 cm^{-1} , 2930, 2895, 2820, 1606, 1530, 1479, 1428, 1393, 1367, 1273, 1185, 1046, 829, 789. – UV (DMSO): λ_{max} = 335 nm; UV (acetonitrile): λ_{max} = 321 nm; UV (toluene): λ_{max} = 323 nm. – 1H NMR ($[D_6]DMSO$): δ = 8.44 (s, 2 H, pyrimidine-H), 8.08 (d, 2 H, phenylene-H), 6.74 (d, 2 H, phenylene-H), 4.17 (q, 2 H, OCH_2), 2.95 (s, 6 H, $N(CH_3)_2$).
 $C_{14}H_{17}N_3O$ Calcd. C 69.11 H 7.04 N 17.27 (243.3) Found C 69.32 H 7.26 N 17.07

2-(4-Dimethylaminophenyl)-4-(4-methoxyphenyl)-pyrimidine (18)

Same procedure as for **14** with **7c** [15] (4.60 g, 13.8 mmol). Pale yellow powder, m.p. 216 °C, yield 3.50 g (84%). – IR (KBr): ν = 3040 cm^{-1} , 2910, 2845, 2810, 1608, 1581, 1429, 1364, 1268, 1244, 1168, 1027, 840, 827, 796. – UV (DMSO): λ_{max} = 287 nm, 362; UV (acetonitrile): λ_{max} = 353 nm; UV (toluene): λ_{max} = 357 nm. – 1H NMR ($[D_6]DMSO$): δ = 8.84 (s, 2 H, pyrimidine-H), 8.13 (d, 2 H, phenylene-H), 7.59 (d, 2 H, phenylene-H), 6.95 (d, 2 H, phenylene-H), 6.69 (d, 2 H,

phenylene-H), 3.75 (s, 3 H, OCH₃), 2.94 (s, 6 H, N(CH₃)₂).
 C₁₉H₁₉N₃O Calcd. C 74.72 H 6.27 N 13.76
 (305.4) Found C 74.48 H 6.23 N 13.68

2-(4-Dimethylaminophenyl)-4-(4-aminophenyl)-pyrimidine (19)

Stannous chloride dihydrate (7.10 g, 31.5 mmol) was added to the suspension of **14** (2.0 g, 6.24 mmol) in conc. HCl (50 ml) and the mixture heated to 100 °C for 3 h. After cooling, the precipitate was collected by filtration and triturated with 5% aqueous NaHCO₃ (50 ml). The remaining solid material was filtered off, dried in vacuo and refluxed in DMF for 1 h. The solution was filtered and the filtrate was evaporated to dryness *in vacuo*.

Pale yellow powder, m.p. 235 °C (from acetonitrile), yield 1.10 g (61%). –

IR (KBr): $\nu = 3458\text{ cm}^{-1}$, 3387, 3040, 2900, 2865, 2815, 1610, 1582, 1530, 1431, 1361, 1191, 827, 794, 657. – UV (DMSO): $\lambda_{\text{max}} = 369\text{ nm}$. – ¹H NMR ([D₆]DMSO): $\delta = 9.90$ (s, 2 H, pyrimidine-H), 8.19 (d, 2 H, phenylene-H), 7.45 (d, 2 H, phenylene-H), 6.75 (d, 2 H, phenylene-H), 6.63 (d, 2 H, phenylene-H), 5.33 (s, 2 H, NH₂), 2.95 (s, 6 H, N(CH₃)₂).

C₁₈H₁₈N₄ × 0.33 H₂O Calcd. C 72.94 H 6.35 N 18.90
 (296.4) Found C 72.64 H 6.25 N 18.82

N-Phenylcarbazole-3,6-dicarbonitrile (21)

A suspension of 3,6-diiodo-N-phenylcarbazol [14] (4.0 g, 8.1 mmol) and cuprous cyanide (2.0 g, 22 mmol) in DMF (70 ml) was refluxed under nitrogen for 5 h. After addition of a solution ferric chloride hexahydrate (5.0 g, 18.5 mmol) in ethanol (60 ml) refluxing was continued for 5 min. The solvent was distilled off and the remaining solid material extracted 3 times with dichloromethane (600 ml each time). The combined dichloromethane phases were evaporated to dryness and the residue washed with methanol.

Colorless powder, m.p. 320 °C, yield 1.80 g (76%). –
 IR (KBr): $\nu = 3070\text{ cm}^{-1}$, 2219, 1633, 1596, 1502, 1482, 1368, 1294, 1244, 1187, 897, 817, 773, 698. – UV (DMSO): $\lambda_{\text{max}} = 281\text{ nm}$, 328, 344; UV (acetonitrile): $\lambda_{\text{max}} = 278\text{ nm}$, 293, 308, 328; UV (toluene): $\lambda_{\text{max}} = 284\text{ nm}$, 294, 329, 344. – ¹H NMR ([D₆]DMSO): $\delta = 8.93$ (s, 2 H, 4,5-carbazole-H), 7.89 (d, 2 H, carbazole-H), 7.73 (t, 2 H, phenyl-H), 7.65 (d, 3 H, phenyl-H), 7.43 (d, 2 H, carbazole-H).

C₂₀H₁₁N₃ Calcd. C 81.89 H 3.78 N 14.33
 (293.3) Found C 81.82 H 3.76 N 14.22

N-Phenylcarbazole-3,6-bis-[N,N,N'-tris-(trimethylsilyl)-carboxamide] (22)

Lithium hexamethyldisilazene (1.84 g, 11 mmol) was added to a suspension of **21** (1.5 g, 5.1 mmol) in dry ether (50 ml) and the mixture stirred at room temperature for 10 h. The solvent was removed *in vacuo*, toluene (50 ml) and chlorotrimethylsilane (1.5 ml, 12 mmol) were added and the mixture refluxed for 5 h. The solvent was distilled off *in vacuo* and the orange product (3.89 g) used according to the "general procedure" (cf. **8a**).

3,6-Bis-(5-nitro-2-pyrimidinyl)-N-phenylcarbazole (23a)

With **22** (3.89 g, 5.1 mmol) and 3-dimethylamino-2-nitro-N,N-

dimethyl-proeneiminium perchlorate [16] (2.9 g, 10.7 mmol). Orange powder, m.p. >300 °C, yield 1.60 g (64%). –

IR (KBr): $\nu = 1559\text{ cm}^{-1}$, 1512, 1417, 1338, 1291, 1231, 1132, 856, 798, 772, 699. – UV (DMSO): $\lambda_{\text{max}} = 270\text{ nm}$, 330, 405; UV (toluene): $\lambda_{\text{max}} = 322\text{ nm}$, 394. – ¹H NMR ([D₆]DMSO): $\delta = 9.58$ (s, 4 H, pyrimidine-H), 9.50 (s, 2 H, 4,5-carbazole-H), 8.66 (d, 2 H, carbazole-H), 7.80–7.62 (m, 5 H, phenyl-H), 7.53 (d, 2 H, carbazole-H).

C₂₆H₁₅N₇O₄ Calcd. C 63.80 H 3.09 N 20.03
 (489.5) Found C 63.95 H 3.32 N 20.06

3,6-Bis-[5-(4-nitrophenyl)-2-pyrimidinyl]-N-phenylcarbazole (23b)

With **7g** [15] (3.7 g, 10.6 mmol).

Yellow powder, m.p. >300 °C, yield 2.16 g (68%).

IR (KBr): $\nu = 1599\text{ cm}^{-1}$, 1581, 1517, 1424, 1345, 1293, 854, 798, 752, 695. – UV (DMSO): $\lambda_{\text{max}} = 290\text{ nm}$, 353, 379; UV (toluene): $\lambda_{\text{max}} = 335\text{ nm}$, 353, 383. – ¹H NMR ([D₆]DMSO): $\delta = 9.34$ (s, 2 H, 4,5-carbazole-H), 9.19 (s, 4 H, pyrimidine-H), 8.54 (d, 2 H, carbazole-H), 8.25 (d, 4 H, phenylene-H), 8.00 (d, 4 H, phenylene-H), 7.58 (s, 5 H, phenyl-H), 7.35 (d, 2 H, carbazole-H).

C₃₈H₂₃N₇O₄ × H₂O Calcd. C 69.19 H 3.82 N 14.86
 (659.7) Found C 69.15 H 4.16 N 14.76

3,8-Bis-(5-ethoxy-2-pyrimidinyl)-N-phenylcarbazole (23c)

With 3-dimethylamino-2-ethoxy-N,N-dimethyl-prop-2-eneiminium perchlorate [18] (2.9 g, 10.7 mmol).

Ochre powder, m.p. 242 °C, yield 0.55 g (22%). –

IR (KBr): $\nu = 1598\text{ cm}^{-1}$, 1543, 1502, 1429, 1396, 1274, 918, 899, 789, 698. – UV (DMSO): $\lambda_{\text{max}} = 300\text{ nm}$, 381, 408; UV (acetonitrile): $\lambda_{\text{max}} = 277\text{ nm}$, 297, 328; UV (toluene): $\lambda_{\text{max}} = 300\text{ nm}$, 335. – ¹H NMR ([D₆]DMSO): $\delta = 9.15$ (s, 2 H, 4,5-carbazole-H), 8.60 (s, 4 H, pyrimidine-H), 8.43 (d, 2 H, carbazole-H), 7.63 (s, 5 H, phenyl-H), 7.40 (d, 2 H, carbazole-H), 4.24 (q, 4 H, CH₂), 1.40 (t, 6 H, CH₃).

C₃₀H₂₅N₅O₂ × 0.33 H₂O Calcd. C 73.00 H 5.24 N 14.19
 (493.6) Found C 72.99 H 5.20 N 14.25

3,6-Bis-[5-(4-methoxyphenyl)-2-pyrimidinyl]-N-phenylcarbazole (23d)

With **7c** [15] (3.5 g, 10.5 mmol).

Ochre powder, m.p. >300 °C, yield 2.16 g (68%). –

IR (KBr): $\nu = 1606\text{ cm}^{-1}$, 1582, 1517, 1502, 1424, 1288, 1251, 1181, 1033, 828, 796. – UV (DMSO): $\lambda_{\text{max}} = 321\text{ nm}$, 362; UV (acetonitrile): $\lambda_{\text{max}} = 315\text{ nm}$, 354; UV (toluene): $\lambda_{\text{max}} = 307\text{ nm}$, 321, 350, 362. – ¹H NMR ([D₆]DMSO): $\delta = 9.39$ (s, 2 H, 4,5-carbazole-H), 9.20 (s, 4 H, pyrimidine-H), 8.61 (d, 2 H, carbazole-H), 7.83 (d, 4 H, phenylene-H), 7.75 (s, 5 H, phenyl-H), 7.52 (d, 2 H, carbazole-H), 7.13 (d, 4 H, phenylene-H), 3.85 (s, 6 H, OCH₃).

C₄₀H₂₉N₅O₂ Calcd. C 78.54 H 4.78 N 11.45
 (611.7) Found C 78.27 H 4.76 N 11.49

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