

mp 161°; ir (potassium bromide): 3400 and 3300 (m), 1630 and 1605 cm^{-1} (s); ^1H nmr (dimethyl sulfoxide- d_6): δ 4.76 (s, 2H, CH_2), 6.7 (br, 2H, NH_2), 7.6 (s, 5H, Ph), 8.66 (s, 1H, $\text{CH}=\text{N}$); ^{13}C nmr (dimethyl sulfoxide- d_6): δ 45.2 (CH_2), 117.7 (CN), 125.3 (C-4), 143.3 (C-5), 123.9, 129.0, 129.7 and 134.6 (Ph), 158.8 ($\text{CH}=\text{N}$, $^1J_{\text{CH}} = 160$ Hz).

Anal. Calcd. for $\text{C}_{11}\text{H}_{10}\text{N}_6$ (mol wt 226): C, 58.40; H, 4.46. Found: C, 58.33; H, 4.52.

Synthesis of the 5-Aminotriazoles **5f,g**.

Equimolar amounts (2.6 mmoles) of **1** (0.5 g) and amine were allowed to react in ethanol (20 ml) at room temperature for 15 minutes. After removal of the solvent at room temperature, the residue was crystallized (without heating!) from chloroform/ether.

5-Amino-1-phenyl-4-(*N*-phenyl)iminomethyl-1,2,3-triazole (**5f**).

This compound was obtained in 18% yield, mp 124°; ir (potassium bromide): 3460 and 3300 (m), 1630 cm^{-1} (br, s); ^1H nmr (deuteriochloroform): δ 5.9 (br, 2H, NH_2), 7.0-7.5 (m, 5H, =NPh), 7.6 (s, 5H, Ph), 8.8 (s, 1H, $\text{CH}=\text{N}$); ^{13}C nmr (deuteriochloroform): δ 120.8, 123.6, 129.4 and 151.2 (=NPh), 123.8, 130.2, 130.0 and 134.4 (Ph), 127.6 (C-4), 142.4 (C-5), 153.4 ($\text{CH}=\text{N}$, $^1J_{\text{CH}} = 162$ Hz).

Anal. Calcd. for $\text{C}_{15}\text{H}_{13}\text{N}_5$ (mol wt 263): C, 68.43; H, 4.98. Found: C, 68.26; H, 4.93.

5-Amino-4-(*N*-*p*-methoxyphenyl)iminomethyl-1-phenyl-1,2,3-triazole (**5g**).

This compound was obtained in 39% yield, mp 191°; ir (potassium bromide): 3460 and 3320 (m), 1630 cm^{-1} (br, s); ^1H nmr (deuteriochloroform): δ 3.8 (s, 3H, OCH_3), 6.9 and 7.2 (two d, 4H, anisyl), 7.5 (s, 5H, Ph), 8.8 (s, 1H, $\text{CH}=\text{N}$); ^{13}C nmr (deuteriochloroform): δ 55.0 (OCH_3), 113.9, 121.5, 143.8 and 158.0 (anisyl), 123.3, 128.5, 129.4 and 134.7 (Ph), 126.7 (C-4), 142.8 (C-5), 150.0 ($\text{CH}=\text{N}$, $^1J_{\text{CH}} = 161$ Hz).

Anal. Calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_5\text{O}$ (mol wt 293): C, 65.52; H, 5.15. Found: C, 65.48; H, 5.06.

Synthesis of the 4-Amidinotriazoles **6a-h**.

A solution of **4** (0.5 g, 2.6 mmoles) and amine (two equivalents of ethylamine, isopropylamine, *t*-butylamine, benzylamine and aniline, and one equivalent of aminoacetonitrile, *p*-methoxyaniline and *p*-chloroaniline) in ethanol (20 ml) was refluxed for 2 hours. Compounds **6d,e,g,h** precipitated from the solutions and were filtered off, washed with *n*-hexane and crystallized from alcohol. In the other cases, **6a,b,c,f**, the solvent was removed and the residue was crystallized from the appropriate solvent.

1-Ethyl-4-(*N*-phenyl)amidino-1,2,3-triazole (**6a**).

This compound was obtained in 90% yield, mp 143° (benzene); ir (potassium bromide): 3365 and 3180/3140 (m), 1635/1615 cm^{-1} (s); ^1H nmr (deuteriochloroform): δ 1.6 (t, 3H, CH_3), 4.5 (q, 2H, CH_2), 5.5 (br, 2H, NH_2), 7.0-7.4 (two m, 5H, Ph), 8.2 (s, 1H, triazole H); ^{13}C nmr (deuteriochloroform): δ 15.4 and 45.6 (Et), 121.7, 123.2, 129.5 and 148.6 (Ph), 122.9 (C-5), 144.5 (C-4), 147.8 (C=N).

Anal. Calcd. for $\text{C}_{11}\text{H}_{13}\text{N}_5$ (mol wt 215): C, 61.38; H, 6.09. Found: C, 61.26; H, 6.00.

1-Isopropyl-4-(*N*-phenyl)amidino-1,2,3-triazole (**6b**).

This compound was obtained in 76% yield, mp 120° (chloroform/ether); ir (potassium bromide): 3470 and 3320 (m), 1630 cm^{-1} (s); ^1H nmr (deuteriochloroform): δ 1.6 (d, 6H, two Me), 4.9

(septet, 1H, CH), 5.5 (br, 2H, NH_2), 6.9-7.5 (two m, 5H, Ph), 8.2 (s, 1H, triazole H); ^{13}C nmr (deuteriochloroform): δ 22.9 and 53.3 (*i*-Pr), 121.7, 123.2, 129.4 and 148.5 (Ph), 121.1 (C-5), 144.1 (C-4), 147.9 (C=N).

Anal. Calcd. for $\text{C}_{12}\text{H}_{15}\text{N}_5$ (mol wt 229): C, 62.86; H, 6.59. Found: C, 62.79; H, 6.48.

1-*t*-Butyl-4-(*N*-phenyl)amidino-1,2,3-triazole (**6c**).

This compound was obtained in 93% yield, mp 157° (ether); ir (potassium bromide): 3480 and 3340 (m), 1630 cm^{-1} (s); ^1H nmr (deuteriochloroform): δ 1.7 (s, 9H, *t*-Bu), 5.4 (br, 2H, NH_2), 6.9-7.5 (two m, 5H, Ph), 8.2 (s, 1H, triazole H); ^{13}C nmr (deuteriochloroform): δ 30.0 and 59.9 (*t*-Bu), 121.8, 123.2, 129.5 and 148.5 (Ph), 121.0 (C-5), 143.6 (C-4), 148.2 (C=N).

Anal. Calcd. for $\text{C}_{13}\text{H}_{17}\text{N}_5$ (mol wt 243): C, 64.17; H, 7.04. Found: C, 64.00; H, 7.00.

1-(Cyanomethyl)-4-(*N*-phenyl)amidino-1,2,3-triazole (**6d**).

This compound was obtained in 66% yield, mp 136° (methanol); ir (potassium bromide): 3450 and 3300 (m), 2210 (m), 1640 cm^{-1} (s); ^1H nmr (dimethyl sulfoxide- d_6): δ 5.97 (s, 2H, CH_2), 6.4 (br, 2H, NH_2), 6.9-7.5 (two m, 5H, Ph), 8.77 (s, 1H, triazole H); ^{13}C nmr (dimethyl sulfoxide- d_6): δ 37.6 (CH_2), 114.8 (C=N), 121.5, 122.1, 129.0 and 148.8 (Ph), 125.7 (C-5, $^1J_{\text{CH}} = 203.4$ Hz), 144.6 (C-4), 146.9 (C=N).

Anal. Calcd. for $\text{C}_{11}\text{H}_{10}\text{N}_6$ (mol wt 226): C, 58.40; H, 4.46. Found: C, 58.26; H, 4.54.

1-Benzyl-4-(*N*-phenyl)amidino-1,2,3-triazole (**6e**).

This compound was obtained in 95% yield, mp 216° (ethanol); ir (potassium bromide): 3470 and 3320 (m), 1630 cm^{-1} (s); ^1H nmr (deuteriochloroform): δ 5.45 (br, 2H, NH_2), 5.54 (s, 2H, CH_2), 6.9-7.45 (three m, 10 H, two Ph), 8.05 (s, 1H, triazole H); ^{13}C nmr (deuteriochloroform): δ 54.6 (CH_2), 121.6, 123.3, 129.5 and 148.5 (=NPh), 128.4, 129.0, 129.2 and 133.8 (Ph), 123.5 (C-5), 144.8 (C-4), 147.7 (C=N).

Anal. Calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_5$ (mol wt 277): C, 69.30; H, 5.45. Found: C, 69.28; H, 5.54.

1-Phenyl-4-(*N*-phenyl)amidino-1,2,3-triazole (**6f**).

This compound was obtained in 91% yield, mp 151° (benzene); ir (potassium bromide): 3480 and 3340 (m), 1630 cm^{-1} (s); ^1H nmr (deuteriochloroform): δ 5.6 (br, 2H, NH_2), 7.0-7.8 (four m, 10 H, two Ph), 8.65 (s, 1H, triazole H); ^{13}C nmr (deuteriochloroform): δ 121.6, 123.3, 129.5 and 148.4 (=NPh), 120.5, 129.1, 129.8 and 136.6 (Ph), 121.7 (C-5, $^1J_{\text{CH}} = 198$ Hz), 145.0 (C-4), 147.5 (C=N).

Anal. Calcd. for M^+ : 263.1171. Found: 263.1167. **Note:** No satisfactory elemental analysis could be obtained (Calcd. C, 68.43; H, 4.98. Found: C, 67.42; H, 5.09).

1-(*p*-Methoxyphenyl)-4-(*N*-phenyl)amidino-1,2,3-triazole (**6g**).

This compound was obtained in 83% yield, mp 183° (ethanol); ir (potassium bromide): 3480 and 3345 (m), 1625 cm^{-1} (s); ^1H nmr (deuteriochloroform): δ 3.9 (s, 3H, OMe), 5.5 (br, 2H, NH_2), 7.0-7.7 (three m, 9 aromatic H), 8.55 (s, 1H, triazole H); ^{13}C nmr (deuteriochloroform): δ 55.0 (OMe), 121.7, 123.3, 129.5 and 148.6 (Ph), 114.9, 122.2, 130.1 and 160.1 (anisyl), 121.8 (C-5, $^1J_{\text{CH}} = 198$ Hz), 144.9 (C-4), 147.5 (C=N).

Anal. Calcd. for $\text{C}_{16}\text{H}_{15}\text{N}_5\text{O}$ (mol wt 293): C, 65.52; H, 5.15. Found: C, 65.42; H, 5.17.

1-(*p*-Chlorophenyl)-4-(*N*-phenyl)amidino-1,2,3-triazole (**6h**).

This compound was obtained in 87% yield, mp 206° (ethanol); ir (potassium bromide): 3480 and 3340 (m), 1642 cm⁻¹ (s); ¹H nmr (dimethyl sulfoxide-d₆): δ 3.5 (br, 2H, NH₂), 6.9-8.0 (four m, 9 aromatic H), 9.2 (s, 1H, triazole H); ¹³C nmr (dimethyl sulfoxide-d₆): δ 121.5, 122.4, 129.5 and 148.7 (Ph), 121.3, 128.9, 133.3 and 135.0 (p-ClC₆H₄), 122.0 (C-5), 145.0 (C-4), 147.0 (C=N).

Anal. Calcd. for C₁₅H₁₂ClN₅ (mol wt 297): C, 60.51; H, 4.06. Found: C, 60.45; H, 4.07.

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