Supporting Information

Design, Synthesis, and Biological Evaluation of AT_1 Angiotensin II Receptor Antagonists Based on the Pyrazolo[3,4-*b*]pyridine and Related Heteroaromatic Bicyclic Systems

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Contents: Experimental details for the synthesis and the characterization of **7** and **8** and related compounds (chemistry, NMR, MS, crystallography, and analytical data).

Experimental Section

Chemistry

All chemicals used were of reagent grade. Yields refer to purified products and are not optimized. Melting points were determined in open capillaries on a Gallenkamp apparatus and are uncorrected. Microanalyses were carried out by means of a Perkin-Elmer 240C or a Perkin-Elmer Series II CHNS/O Analyzer 2400. Merck silica gel 60 (230-400 mesh) was used for column chromatography. Merck TLC plates, silica gel 60 F_{254} were used for TLC. ^{1}H-NMR spectra were recorded with a Bruker AC 200 spectrometer in the indicated solvents (TMS as internal standard): the values of the chemical shifts are expressed in ppm and the coupling constants (*J*) in Hz. Mass spectra were recorded on either a Varian Saturn 3 spectrometer or a ThermoFinnigan LCQ-Deca.

General Procedure for the Deprotection of Triphenylmethyltetrazole Derivatives 17a-m,p, 22, 34a,b, 39a-c, 44d-g, 48 (Deprotection Procedure).

A mixture of the appropriate triphenylmethyl-protected tetrazole derivative (**17a-m,p**, **22**, **34a**,**b**, **39a-c**, **44d-g**, **48,** 1.0 mmol) in CH_2Cl_2 (8 mL) with formic acid (12 mL) was stirred at room temperature overnight. The solvent was then removed under reduced pressure and the residue was purified by washing with diethyl ether-ethyl acetate to give the expected tetrazole derivative (**7a-m,p**, **8a-g**, **18**, **35a**,**b**, **45**).

2,3-Dihydro-2-propyl-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7a).

The title compound was obtained from **17a** by means of the "deprotection procedure" and was further purified by recrystallization from methanol to give compound **7a** as off-white crystals (yield 43%, mp 152-154 °C). ^{1}H-NMR ($CDCl_3$): 0.83 (t, *J* = 7.3, 3H), 1.64 (m, 2H), 3.80 (t, *J* = 7.0, 2H),

5.17 (s, 2H), 6.85-7.57 (m, 8H), 7.95 (d, *J* = 6.7, 1H), 8.08 (d, *J* = 7.6, 1H), 8.62 (d, *J* = 4.3, 1H). MS(ESI): *m/z* 412 ($M+H^+$).

2-*iso*-Butyl-2,3-dihydro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7b).

The title compound was prepared from **17b** by means of the "deprotection procedure" to obtain a white solid (yield 79%, mp 174-176 °C). ^{1}H-NMR ($CDCl_3$): 0.85 (d, *J* = 6.7, 6H), 2.08 (m, 1H), 3.69 (d, *J* = 7.4, 2H), 5.18 (s, 2H), 6.85-7.57 (m, 8H), 7.96 (d, *J* = 7.8, 1H), 8.08 (d, *J* = 7.9, 1H), 8.61 (d, *J* = 4.9, 1H). MS(ESI, negative ions): *m/z* 424 ($M-H^+$).

2-Butyl-2,3-dihydro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7c).

The title compound was prepared from **17c** by means of the "deprotection procedure" to obtain a white solid (yield 73%, mp 180-182 °C). ^{1}H-NMR ($CDCl_3$): 0.86 (t, *J* = 7.2, 3H), 1.22 (m, 2H), 1.60 (m, 2H), 3.84 (t, *J* = 7.1, 2H), 5.19 (s, 2H), 6.87-7.00 (m, 4H), 7.13 (m, 1H), 7.32 (m, 1H), 7.51 (m, 2H), 7.96 (m, 1H), 8.07 (m, 1H), 8.60 (d, *J* = 4.5, 1H). MS(ESI): *m/z* 426 ($M+H^+$).

2,3-Dihydro-2-*iso*-pentyl-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7d).

The title compound was prepared from **17d** by means of the "deprotection procedure" to obtain a white solid (yield 70%, mp 179-180 °C). ^{1}H-NMR ($CDCl_3$): 0.87 (d, *J* = 5.9, 6H), 1.46 (m, 3H), 3.88 (t, *J* = 7.1, 2H), 5.18 (s, 2H), 6.87-7.00 (m, 4H), 7.13 (m, 1H), 7.32 (m, 1H), 7.51 (m, 2H), 7.87 (d, *J* = 8.7, 1H), 8.07 (d, *J* = 7.9, 1H), 8.60 (d, *J* = 4.9, 1H). MS(ESI, negative ions): *m/z* 438 ($M-H^+$).

2,3-Dihydro-2-pentyl-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7e).

The title compound was prepared from **17e** by means of the "deprotection procedure" to obtain an off-white solid (yield 60%, mp 167-169 °C). ^{1}H-NMR ($CDCl_3$): 0.84 (t, *J* = 6.8, 3H), 1.25 (m, 4H), 1.64 (m, 2H), 3.85 (t, *J* = 7.2, 2H), 5.19 (s, 2H), 6.87-7.01 (m, 4H), 7.12 (m, 1H), 7.33 (m, 1H), 7.52 (m, 2H), 8.00 (m, 1H), 8.09 (m, 1H), 8.62 (m, 1H). MS(ESI, negative ions): *m/z* 438 ($M-H^+$).

2-Benzyl-2,3-dihydro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7f).

The title compound was prepared from **17f** by means of the "deprotection procedure" to obtain a white solid (yield 82%, mp 102-104 °C). ^{1}H-NMR ($CDCl_3$): 5.05 (s, 2H), 5.14 (s, 2H), 6.86-7.61 (m, 13H), 8.07 (m, 1H), 8.17 (m, 1H), 8.60 (m, 1H). MS(ESI, negative ions): *m/z* 458 ($M-H^+$).

2,3-Dihydro-2-ethyl-6-methyl-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7g).

The title compound was prepared from **17g** by means of the "deprotection procedure" to obtain compound **7g** as a white solid (yield 22 %, mp 180-182 °C). ^{1}H-NMR ($CDCl_3$): 1.11 (t, *J* = 7.1, 3H), 2.62 (s, 3H), 3.79 (q, *J* = 6.9, 2H), 5.15 (s, 2H), 6.86-6.99 (m, 5H), 7.36 (m, 1H), 7.48 (m, 2H), 7.88 (m, 2H). MS(ESI, negative ions): *m/z* 410 ($M-H^+$).

2,3-Dihydro-6-methyl-2-propyl-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7h).

The title compound was prepared from **17h** by means of the "deprotection procedure" to obtain compound **7h** as a white solid (yield 47 %, mp 206 °C). ^{1}H-NMR ($CDCl_3$): 0.80 (t, *J* = 7.3, 3H), 1.62 (m, 2H), 2.64 (s, 3H), 3.76 (t, *J* = 7.0, 2H), 5.16 (s, 2H), 6.85-6.99 (m, 5H), 7.35-7.53 (m, 3H), 7.94 (m, 2H). MS(ESI, negative ions): *m/z* 424 ($M-H^+$).

2-Butyl-2,3-dihydro-6-methyl-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7i).

This compound was prepared from **17i** by means of the "deprotection procedure" to obtain compound **7i** as a white solid (yield 68 %, mp 218-219 °C). ^{1}H-NMR ($CDCl_3$): 0.87 (t, *J* = 7.2, 3H), 1.22 (m, 2H), 1.61 (m, 2H), 2.65 (s, 3H), 3.82 (t, *J* = 7.0, 2H), 5.17 (s, 2H), 6.86-7.00 (m, 5H), 7.33 (m, 1H), 7.52 (m, 2H), 7.92-8.02 (m, 2H). MS(ESI, negative ions): *m/z* 438 ($M-H^+$).

2-Butyl-6-chloro-2,3-dihydro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7j).

The title compound was prepared from **17j** by means of the "deprotection procedure" to obtain a white solid (yield 45%, mp 207-208 °C). ^{1}H-NMR ($CDCl_3$): 0.87 (t, *J* = 7.1, 3H), 1.23 (m, 2H), 1.58 (m, 2H), 3.83 (t, *J* = 7.1, 2H), 5.18 (s, 2H), 6.95 (d, *J* = 8.0, 2H), 7.04 (d, *J* = 8.0, 2H), 7.11 (d, *J* = 8.2, 1H), 7.36 (m, 1H), 7.53 (m, 2H), 8.01 (m, 2H). MS(ESI): *m/z* 460 ($M+H^+$).

2-Butyl-6-chloro-2,3-dihydro-5-fluoro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7k).

The title compound was prepared from **17k** by means of the "deprotection procedure" to obtain a white solid (yield 40%) melting at 189-190 °C. ^{1}H-NMR ($CDCl_3$): 0.86 (t, *J* = 7.1, 3H), 1.19 (m, 2H), 1.58 (m, 2H), 3.84 (t, *J* = 7.0, 2H), 5.14 (s, 2H), 6.95 (d, *J* = 7.9, 2H), 7.04 (d, *J* = 7.8, 2H), 7.37 (m, 1H), 7.53 (m, 2H), 7.78 (d, *J* = 6.6, 1H), 7.97 (m, 1H). MS(ESI): *m/z* 500 ($M+Na^+$).

2-Butyl-2,3-dihydro-5-fluoro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7l).

The title compound was prepared from **17l** by following the "deprotection procedure" to obtain a white solid (yield 71%) melting at 190-193 °C. ^{1}H-NMR ($CDCl_3$): 0.89 (t, *J* = 7.2, 3H), 1.23 (m, 2H), 1.64 (m, 2H), 3.88 (t, *J* = 7.1, 2H), 5.15 (s, 2H), 6.91 (d, *J* = 8.0, 2H), 7.02 (d, *J* = 8.0, 2H), 7.35 (d, *J* = 7.5, 1H), 7.51 (m, 2H), 7.75 (m, 1H), 8.06 (m, 1H), 8.52 (s, 1H). MS(ESI): *m/z* 444 ($M+H^+$).

2-Butyl-5-chloro-2,3-dihydro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7m).

The title compound was prepared from **17m** by means of the "deprotection procedure" to obtain compound **7m** as a white solid (yield 70%) melting at 237-238 °C. ^{1}H-NMR ($CDCl_3$): 0.90 (t, *J* = 7.3, 3H), 1.25 (m, 2H), 1.63 (m, 2H), 3.89 (t, *J* = 7.2, 2H), 5.18 (s, 2H), 7.03 (m, 4H), 7.36 (m, 1H), 7.54 (m, 2H), 8.06 (m, 2H), 8.57 (d, *J* = 2.5, 1H). MS(ESI, negative ions): *m/z* 458 ($M-H^+$).

2-Butyl-2,3-dihydro-6-morpholino-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7p).

The title compound was prepared from **17p** by means of the "deprotection procedure" to obtain a white solid (yield 64%) melting at 210-211 °C. ^{1}H-NMR ($CDCl_3$): 0.85 (t, *J* = 7.2, 3H), 1.12-1.28 (m, 2H), 1.48-1.63 (m, 2H), 3.68-3.75 (m, 6H), 3.82 (t, *J* = 4.4, 4H), 5.04 (s, 2H), 6.42 (d, *J* = 8.8, 1H), 6.93 (d, *J* = 8.0, 2H), 6.99 (d, *J* = 8.0, 2H), 7.37 (m, 1H), 7.51 (m, 2H), 7.78 (d, *J* = 8.8, 1H), 8.00 (m, 1H). MS(ESI): *m/z* 511 ($M+H^+$).

1-Butyl-2,3-dihydro-2-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (8a).

The title compound was prepared from **39a** by means of the "deprotection procedure". Compound **8a** was obtained as a white solid (yield 64%, mp 216-218 °C). ^{1}H-NMR ($CDCl_3$): 0.77 (t, *J* = 6.8,

3H), 1.07-1.24 (m, 4H), 3.93 (t, *J* = 6.8, 2H), 5.06 (s, 2H), 7.01-7.62 (m, 8H), 7.98 (d, *J* = 7.3, 1H), 8.10 (d, *J* = 6.7,1H), 8.52 (d, *J* = 3.7, 1H). MS(ESI, negative ions): *m/z* 424 ($M-H^+$).

1-Butyl-2,3-dihydro-6-methyl-2-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (8b).

The title compound was prepared from **39b** by means of the "deprotection procedure". Compound **8b** was obtained as a white solid (yield 69%, mp 239-241 °C). ^{1}H-NMR ($CDCl_3$): 0.76 (t, *J* = 6.9, 3H), 0.96-1.24 (m, 4H), 2.54 (s, 3H), 3.88 (t, *J* = 6.9, 2H), 4.99 (s, 2H), 6.86 (d, *J* = 7.9, 1H), 7.09-7.61 (m, 7H), 7.90-7.96 (m, 2H). MS (ESI, negative ions): *m/z* 438 ($M-H^+$).

1-Butyl-6-chloro-2,3-dihydro-2-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (8c).

The title compound was prepared from **39c** by means of the "deprotection procedure". Compound **8c** was obtained as a white solid (yield 49%, mp 206-208 °C). ^{1}H-NMR ($CDCl_3$): 0.79 (t, *J* = 6.9, 3H), 1.01-1.40 (m, 4H), 3.91 (t, *J* = 7.1, 2H), 5.04 (s, 2H), 7.00-7.55 (m, 8H), 8.02 (m, 2H). MS (ESI, negative ions): *m/z* 458 ($M-H^+$).

6,7-Dihydro-6-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (8d).

The title compound was prepared from **44d** by means of the "deprotection procedure" and was purified by recrystallization from ethyl acetate-ethanol. Compound **8d** was obtained as a light brown solid (yield 81%, mp 210-214 °C). ^{1}H-NMR ($CDCl_3$): 4.36 (s, 2H), 4.78 (s, 2H), 7.19-7.63 (m, 8H), 8.08 (m, 2H), 8.67 (d, *J* = 4.8, 1H). MS(ESI): *m/z* 391 ($M+Na^+$).

6,7-Dihydro-7-ethyl-6-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (8e).

The title compound was prepared from **44e** by means of the "deprotection procedure" and was purified by washing with ethyl ether. Compound **8e** was obtained as a white solid (yield 84%, mp 191-193 °C). ^{1}H-NMR($CDCl_3$): 0.48 (t, *J* = 7.3, 3H), 1.90-2.35 (m, 2H), 4.16 (d, *J* = 15.0, 1H), 4.46 (m, 1H), 5.24 (d, *J* = 15.2, 1H), 7.15-7.62 (m, 8H), 7.98-8.06 (m, 2H), 8.67 (d, *J* = 4.8, 1H). MS(ESI, negative ions): *m/z* 395 ($M-H^+$).

6,7-Dihydro-7-propyl-6-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (8f).

The title compound was prepared from **44f** by means of the "deprotection procedure" and was purified by flash chromatography with ethyl acetate-methanol (85:15) as the eluent. Compound **8f** was obtained as a colorless glassy solid (yield 70%). ^{1}H-NMR ($CDCl_3$): 0.76-1.21 (m, 5H), 1.82-2.35 (m, 2H), 4.23 (d, *J* = 15.1, 1H), 4.47 (m, 1H), 5.24 (d, *J* = 13.9, 1H), 7.18-7.62 (m, 8H), 8.05 (m, 2H), 8.69 (d, *J* = 3.5, 1H). MS(ESI, negative ions): *m/z* 409 ($M-H^+$).

7-Butyl-6,7-dihydro-6-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (8g).

The title compound was prepared from **44g** by means of the "deprotection procedure" and was purified by washing with diethyl ether. Compound **8g** was obtained as a white solid (yield 78%, mp 159-162 °C). ^{1}H-NMR (DMSO-d_6): 0.50-0.69 (m, 4H), 0.81-1.12 (m, 3H), 1.81-2.13 (m, 2H), 4.40-4.50 (m, 2H), 4.71 (d, *J* = 15.4, 1H), 7.02-7.26 (m, 4H), 7.46-7.64 (m, 5H), 8.09 (d, *J* = 7.6, 1H), 8.74 (d, *J* = 4.7, 1H). MS(ESI, negative ions): *m/z* 423 ($M-H^+$).

2-Butyl-2,3-dihydro-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-indazol-3-one (18).

The title compound was prepared from **22** by means of the "deprotection procedure" and was purified by washing with diethyl ether. Compound **17** was obtained as a white solid (yield 64%, mp

240-242 °C). ^{1}H-NMR ($CDCl_3$): 0.82 (t, *J* = 7.2, 3H), 1.09-1.30 (m, 2H), 1.56 (m, 2H), 3.81 (t, *J* = 7.2, 2H), 4.77 (s, 2H), 6.88-6.98 (m, 4H), 7.05-7.16 (m, 2H), 7.25-7.52 (m, 4H), 7.62 (d, *J* = 7.3, 1H), 7.72 (d, *J* = 7.7, 1H). MS(ESI, negative ions): *m/z* 423 ($M-H^+$).

1-Propyl-3-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methoxy]-1*H*-pyrazolo[3,4-*b*]pyridine (35a).

This compound was prepared from **34a** by means of the "deprotection procedure" and was purified by washing with diethyl ether. Compound **35a** was obtained as a white solid (yield 43%, mp 87-89 °C). ^{1}H-NMR($CDCl_3$): 0.87 (t, *J* = 7.1, 3H), 1.85 (m, 2H), 4.23 (t, *J* = 7.0, 2H), 5.36 (s, 2H), 6.99-7.57 (m, 8H), 8.00-8.15 (m, 2H), 8.38 (m, 1H). MS(ESI, negative ions): *m/z* 410 ($M-H^+$).

1-Butyl-3-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methoxy]-1*H*-pyrazolo[3,4-*b*]pyridine (35b).

The title compound was prepared from **34b** by means of the "deprotection procedure" and was purified by washing with diethyl ether. Compound **35b** was obtained as a white solid (yield 39%, mp 69-70 °C). ^{1}H-NMR($CDCl_3$): 0.90 (t, *J* = 7.2, 3H), 1.26-1.39 (m, 2H), 1.82 (m, 2H), 4.28 (t, *J* = 7.3, 2H), 5.45 (s, 2H), 6.97-7.61 (m, 8H), 8.03 (m, 1H), 8.14 (m, 1H), 8.39 (m, 1H). MS(ESI, negative ions): *m/z* 424 ($M-H^+$).

7-Butyl-7,8-dihydro-5-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methoxy]pyrido[2,3-*d*]pyridazin-8-one (45).

The title compound was prepared from **48** and was crystallized from ethyl acetate to give white crystals (yield 87 %, mp 180-181 °C). ^{1}H-NMR ($CDCl_3$): 0.95 (t, *J* = 7.3, 3H), 1.30-1.48 (m, 2H), 1.79 (m, 2H), 4.13 (t, *J* = 7.1, 2H), 5.26 (s, 2H), 7.01 (d, *J* = 7.8, 2H), 7.20-7.43 (m, 3H), 7.54 (m, 2H), 7.75 (m, 1H), 7.92 (m, 1H), 8.72 (m, 1H), 8.80 (m, 1H). MS(ESI): *m/z* 454 ($M+H^+$).

2-Butyl-2,3-dihydro-6-methoxy-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7n).

A mixture of **17j** (0.10 g, 0.14 mmol) in MeOH (10 mL) with 0.15 mL of a 30% solution of MeONa/MeOH was refluxed for 6 h. The resulting mixture was neutralized with 3N HCl and concentrated under reduced pressure; the residue obtained was partitioned between chloroform and water. The organic layer was dried over sodium sulfate, and concentrated under reduced pressure. Purification of the residue by washing with diethyl ether gave compound **7n** as a white solid (0.030 g, yield 47 %, mp 237-238 °C).^{1}H-NMR ($CDCl_3$): 0.87 (t, *J* = 7.4, 3H), 1.22 (m, 2H), 1.58 (m, 2H), 3.77 (t, *J* = 7.1, 2H), 4.03 (s, 3H), 5.12 (s, 2H), 6.52 (d, *J* = 8.1, 1H), 6.91 (d, *J* = 7.8, 2H), 7.00 (d, *J* = 7.9, 2H), 7.35 (m, 1H), 7.51 (m, 2H), 7.88 (d, *J* = 8.6, 1H), 7.99 (m, 1H). MS(ESI, negative ions): *m/z* 454 ($M\text{-}H^+$).

2-Butyl-2,3-dihydro-6-methylamino-1-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (7o).

A mixture of **7j** (0.030 g, 0.065 mmol) in absolute EtOH (5 mL) with a large excess of a 33% solution of CH_3NH_2 in EtOH (5 mL) was refluxed overnight. The resulting mixture was concenrated under reduced pressure, the residue obtained was partitioned between chloroform and water. The organic layer was dried over sodium sulfate and concentrated under reduced pressure. Purification of the residue by recrystallization from diethyl ether gave compound **7o** as a pale yellow solid (yield 68%, mp 228-230 °C).^{1}H-NMR (DMSO-d_6): 0.78 (t, *J* = 6.9, 3H), 1.09 (m, 2H), 1.42 (m, 2H), 3.76 (t, *J* = 6.4, 2H), 3.94 (s, 3H), 5.08 (s, 2H), 6.52 (d, *J* = 8.4, 1H), 6.94-7.07 (m, 4H), 7.43-7.60 (m, 4H), 7.89 (d, *J* = 8.3, 1H). MS(ESI, negative ions): *m/z* 453 ($M\text{-}H^+$).

6,7-Dihydro-6-propyl-7-[[2'-(2*H*-tetrazol-5-yl)-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (7q).

A mixture of **26** (0.10 g, 0.14 mmol) in 10 mL of ethanol with 4.2 mL of 0.1N NaOH was refluxed for 1 h. The cooled reaction mixture was neutralized with 0.1N HCl and the mixture was concentrated under reduced pressure. The residue was partitioned between water and ethyl acetate and the organic layer was dried and evaporated under reduced pressure. The residue was treated with diethyl ether to obtain **7q** as a white solid (yield 61%). ^{1}H-NMR (DMSO-d_6): 0.77 (t, *J*= 7.4, 3H), 1.40-1.61 (m, 2H), 3.06-3.42 (m, 3H), 3.69-3.77 (m, 1H), 4.99 (t, *J* = 4.4, 1H), 6.65-6.83 (m, 4H), 7.13-7.45 (m, 5H), 7.89 (d, *J* = 7.5, 1H), 8.75 (d, *J* = 4.7, 1H). MS(EI): *m/z* 410 (M^+, 5).

General Procedure for the Preparation of Compounds 17a-m,p, 22, 26, 34a,b, 48 (Coupling Procedure).

A mixture of the appropriate derivative (**16a-m,p, 21, 25, 30, 31, 47,** 1.0 mmol) in dry DMF (7 mL) with NaH (0.036 g, 1.5 mmol) was stirred at room temperature until the evolution of hydrogen ceased. A solution of 5-[4'-(bromomethyl)biphenyl-2-yl]-2-(triphenylmethyl)-2*H*-tetrazole[1] (1.0 mmol) in dry DMF (10 mL) was added and the resulting mixture was stirred at room temperature overnight, poured into ice-water, neutralized with 1N HCl and extracted with chloroform. The organic layer was dried under sodium sulfate and evaporated under reduced pressure. Purification of the residue by flash chromatography with the appropriate eluent gave the expected compound (**17a-m,p, 22, 26, 34a,b, 48**).

2,3-Dihydro-2-propyl-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17a).

The title compound was prepared from **16a** by means of the "coupling procedure" and was purified by flash chromatography with *n*-hexane-ethyl acetate (65:35) as the eluent to give a brown solid (yield 40%) melting at 189-190 °C. ^{1}H-NMR ($CDCl_3$): 0.80 (t, *J* = 7.4, 3H), 1.51-1.66 (m, 2H), 3.77 (t, *J* = 7.2, 2H), 5.05 (s, 2H), 6.79-7.49 (m, 23H), 7.88 (m, 1H), 8.12 (m, 1H), 8.58 (m, 1H). MS(ESI): *m/z* 676 ($M+Na^+$).

2-*iso*-Butyl-2,3-dihydro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl] -1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17b).

The title compound was prepared from **16b** by means of the "coupling procedure" and was purified by flash chromatography with ethyl acetate-*n*-hexane (7:3) as the eluent to give a brown solid (yield 37%) melting at 179-180 °C. ^{1}H-NMR ($CDCl_3$): 0.84 (d, *J* = 6.7, 6H), 2.03 (m, 1H), 3.67 (d, *J* = 7.6, 2H), 5.06 (s, 2H), 6.73-7.50 (m, 23H), 7.88 (m, 1H), 8.13 (m, 1H), 8.60 (m, 1H). MS(ESI): *m/z* 690 ($M+Na^+$).

2-Butyl-2,3-dihydro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17c).

The title compound was prepared from **16c** by means of the "coupling procedure" and was purified by flash chromatography with *n*-hexane-ethyl acetate (65:35) as the eluent to give a white solid (yield 12%) melting at 168-171 °C. ^{1}H-NMR ($CDCl_3$): 0.85 (t, *J* = 7.1, 3H), 1.23 (m, 2H), 1.55 (m, 2H), 3.81 (t, *J* = 7.0, 2H), 5.06 (s, 2H), 6.76 (d, *J* = 7.9, 2H), 6.87-6.98 (m, 8H), 7.09 (m, 1H), 7.17-7.62 (m, 12H), 7.88 (m, 1H), 8.12 (d, *J* = 8.4, 1H), 8.59 (m, 1H). MS(ESI): *m/z* 690 ($M+Na^+$).

2,3-Dihydro-2-*iso*-pentyl-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17d).

The title compound was prepared from **16d** by means of the "coupling procedure" and was purified by flash chromatography with ethyl acetate-*n*-hexane (7:3) as the eluent to give a off-white solid (yield 42%) melting at 151-153 °C. ^{1}H-NMR ($CDCl_3$): 0.87 (d, *J* = 5.8, 6H), 1.46-1.55 (m, 3H), 3.82 (t, *J* = 7.2, 2H), 5.06 (s, 2H), 6.76-7.46 (m, 23H), 7.90 (m, 1H), 8.12 (m, 1H), 8.59 (m, 1H). MS(ESI): *m/z* 704 ($M+Na^+$).

2,3-Dihydro-2-pentyl-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17e).

The title compound was prepared from **16e** by means of the "coupling procedure" and was purified by flash chromatography with ethyl acetate-*n*-hexane (7:3) as the eluent to give a glassy solid (yield 60%). ^{1}H-NMR ($CDCl_3$): 0.83 (t, *J* = 6.8, 3H), 1.22 (m, 4H), 1.57 (m, 2H), 3.80 (t, *J* = 7.1, 2H), 5.06 (s, 2H), 6.75-7.50 (m, 23H), 7.89 (m, 1H), 8.13 (d, *J* = 8.1, 1H), 8.59 (d, *J* = 5.1, 1H). MS(ESI): *m/z* 704 ($M+Na^+$).

2-Benzyl-2,3-dihydro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17f).

The title compound was prepared from **16f** by means of the "coupling procedure" and was purified by flash chromatography with ethyl acetate-*n*-hexane (7:3) as the eluent to give a glassy solid (yield 58%). ^{1}H-NMR ($CDCl_3$): 5.00 (s, 2H), 5.04 (s, 2H), 6.70-7.52 (m, 28H), 7.92 (m, 1H), 8.21 (m, 1H), 8.59 (m, 1H). MS(ESI): *m/z* 724 ($M+Na^+$).

2,3-Dihydro-2-ethyl-6-methyl-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17g).

The title compound was prepared from **16g** by means of the "coupling procedure" and was purified by flash-chromatography with ethyl acetate as the eluent to give a off-white solid (yield 46%) melting at 175-177 °C. ^{1}H-NMR ($CDCl_3$): 1.11 (t, *J* = 7.0, 3H), 2.62 (s, 3H), 3.78 (q, *J* = 7.1, 2H), 5.04 (s, 2H), 6.74-6.98 (m, 10H), 7.21-7.50 (m, 13H), 7.88 (m, 1H), 7.99 (d, *J* = 7.9, 1H). MS(ESI): *m/z* 676 ($M+Na^+$).

2,3-Dihydro-6-methyl-2-propyl-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17h).

The title compound was prepared from **16h** by means of the "coupling procedure" and was purified by flash chromatography with ethyl acetate as the eluent to give yellow crystals (yield 35%) melting at 145-147 °C. ^{1}H-NMR ($CDCl_3$): 0.78 (t, *J* = 7.5, 3H), 1.58 (m, 2H), 2.62 (s, 3H), 3.73 (t, *J* = 7.0, 2H), 5.04 (s, 2H), 6.73-6.97 (m, 10H), 7.20-7.48 (m, 13H), 7.88 (m, 1H), 8.00 (d, *J* = 7.9, 1H). MS(ESI): *m/z* 690 ($M+Na^+$).

2-Butyl-2,3-dihydro-6-methyl-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17i).

The title compound was prepared from **16i** by means of the "coupling procedure" and was purified by flash chromatography with dichloromethane-ethyl acetate (8:2) as the eluent to give a glassy solid (yield 47%). ^{1}H-NMR ($CDCl_3$): 0.84 (t, *J* = 7.2, 3H), 1.20 (m, 2H), 1.53 (m, 2H), 2.63 (s, 3H), 3.77 (t, *J* = 7.0, 2H), 5.05 (s, 2H), 6.72-6.98 (m, 10H), 7.29-7.47 (m, 13H), 7.89 (m, 1H), 8.00 (d, *J* = 7.9, 1H). MS(ESI): *m/z* 704 ($M+Na^+$).

2-Butyl-6-chloro-2,3-dihydro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17j).

The title compound was prepared from **16j** by means of the "coupling procedure" and was purified by flash chromatography with *n*-hexane-ethyl acetate (65:35) as the eluent and then by washing with ether to give a white solid (yield 40%) melting at 155-156 °C. ^{1}H-NMR ($CDCl_3$): 0.84 (t, *J* = 7.2, 3H), 1.19 (m, 2H), 1.53 (m, 2H), 3.78 (t, *J* = 7.1, 2H), 5.03 (s, 2H), 6.76 (d, *J* = 8.0, 2H), 6.90 (d, *J* = 7.5, 6H), 6.98 (d, *J* = 7.9, 2H), 7.08 (d, *J* = 8.0, 1H), 7.22-7.51 (m, 12H), 7.92 (m, 1H), 8.05 (d, *J* = 8.0, 1H). MS(ESI): *m/z* 724 ($M+Na^+$).

2-Butyl-6-chloro-2,3-dihydro-5-fluoro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17k).

The title compound was prepared from **16k** by means of the "coupling procedure" and was purified by flash chromatography with n-hexane-ethyl acetate (65:35) as the eluent to give a pale yellow solid (yield 43%) melting at 170-171 °C. ^{1}H-NMR ($CDCl_3$): 0.85 (t, *J* = 7.1, 3H), 1.19 (m, 2H), 1.55 (m, 2H), 3.80 (t, *J* = 7.0, 2H), 4.98 (s, 2H), 6.75 (d, *J* = 7.9, 2H), 6.90 (d, *J* = 7.5, 6H), 6.99 (d, *J* = 7.8, 2H), 7.19-7.49 (m, 12H), 7.85 (d, *J* = 6.8, 1H), 7.93 (m, 1H). MS(ESI): *m/z* 742 ($M+Na^+$).

2-Butyl-2,3-dihydro-5-fluoro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17l).

The title compound was prepared from **16l** by means of the "coupling procedure" and was purified by flash chromatography with n-hexane-ethyl acetate (65:35) as the eluent to obtain a pale yellow thick oil which crystallized on standing (yield 45%, mp 165-168 °C). ^{1}H-NMR ($CDCl_3$): 0.86 (t, *J* = 7.3, 3H), 1.25 (m, 2H), 1.57 (m, 2H), 3.84 (t, *J* = 7.1, 2H), 5.02 (s, 2H), 6.78 (d, *J* = 8.2, 2H), 6.90-7.00 (m, 8H), 7.19-7.51 (m, 12H), 7.84 (m, 1H), 7.92 (m, 1H), 8.47 (m, 1H). MS(ESI): *m/z* 708 ($M+Na^+$).

2-Butyl-5-chloro-2,3-dihydro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17m).

The title compound was prepared from **16m** by means of the "coupling procedure" and was purified by flash chromatography with *n*-hexane-ethyl acetate (65:35) as the eluent and then by washing with ether to give a white solid (yield 24%) melting at 201-203 °C. ^{1}H-NMR ($CDCl_3$): 0.86 (t, *J* = 7.2, 3H), 1.22 (m, 2H), 1.57 (m, 2H), 3.82 (t, *J* = 7.1, 2H), 5.04 (s, 2H), 6.77 (d, *J* = 8.0, 2H), 6.88-6.93 (m, 6H), 6.99 (d, *J* = 8.0, 2H), 7.19-7.52 (m, 12H), 7.91 (m, 1H), 8.08 (d, *J* = 2.6, 1H), 8.51 (d, *J* = 2.0, 1H).

2-Butyl-2,3-dihydro-6-morpholino-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (17p).

The title compound was prepared from **16p** by means of the "coupling procedure" and was purified by flash chromatography with *n*-hexane-ethyl acetate (7:3) as the eluent. Compound **17p** was recrystallized from ethyl acetate to give white needles (yield 18%, mp 150-151 °C). ^{1}H-NMR ($CDCl_3$): 0.82 (t, *J* = 7.2, 3H), 1.18 (m, 2H), 1.48 (m, 2H), 3.64-3.79 (m, 10H), 4.91 (s, 2H), 6.40 (d, *J* = 8.8, 1H), 6.82-7.01 (m, 10H), 7.19-7.51 (m, 12H), 7.86 (m, 2H). MS(ESI): *m/z* 775 ($M+Na^+$).

2-Butyl-2,3-dihydro-1-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-indazol-3-one (22).

The title compound was prepared from **21** by means of the "coupling procedure" and was purified by flash chromatography with *n*-hexane-ethyl acetate (65:35) as the eluent to give a white solid (yield 19%) melting 186-188 °C. ^{1}H-NMR ($CDCl_3$): 0.88 (t, *J* = 7.2, 3H), 1.26 (m, 2H), 1.62 (m, 2H), 3.85 (t, *J* = 7.2, 2H), 4.68 (s, 2H), 6.84-7.51 (m, 25H), 7.81-7.92 (m, 2H). ME(ESI): *m/z* 689 ($M+Na^+$).

6,7-Dihydro-6-propyl-7-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (26).

The title compound was prepared from **25** by means of the "coupling procedure" (dry THF was used in place of dry DMF) and was purified by flash chromatography with dichloromethane-ethyl acetate (8:2) as the eluent to give a glassy solid (yield 21%). ^{1}H-NMR ($CDCl_3$): 0.97 (t, J = 7.1, 3H), 1.68 (m, 2H), 3.18-3.85 (m, 7H), 6.38-7.54 (m, 23H), 7.79 (m, 1H), 8.07 (m, 1H), 8.64 (m, 1H).

1-Propyl-3-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methoxy]-1*H*-pyrazolo[3,4-*b*]pyridine (34a).

The title compound was prepared from **30** by means of the "coupling procedure" and was purified by flash chromatography with *n*-hexane-ethyl acetate (65:35) as the eluent to give a colorless glassy solid (yield 39%). ^{1}H-NMR ($CDCl_3$): 0.95 (t, *J* = 7.0, 3H), 1.95 (m, 2H), 4.34 (t, *J* = 6.9, 2H), 5.32 (s, 2H), 6.88-6.98 (m, 7H), 7.14-7.33 (m, 13H), 7.39-7.51 (m, 3H), 7.83-7.98 (m, 2H), 8.47 (m, 1H).

1-Butyl-3-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methoxy]-1*H*-pyrazolo[3,4-*b*]pyridine (34b).

The title compound was prepared from **31** by means of the "coupling procedure" and was purified by flash chromatography with ethyl acetate as the eluent to give a colourless oil (yield 31%). ^{1}H-NMR ($CDCl_3$): 0.98 (t, *J* = 7.1, 3H), 1.39 (m, 2H), 1.93 (m, 2H), 4.41 (t, *J* = 7.0, 2H), 5.36 (s, 2H), 6.92-6.98 (m, 7H), 7.16-7.40 (m, 13H), 7.42-7.54 (m, 3H), 7.87 (d, *J* = 7.8, 1H), 7.98 (m, 1H), 8.48 (m, 1H). MS(ESI): *m/z* 690 ($M+Na^+$).

7-Butyl-7,8-dihydro-5-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methoxy]pyrido[2,3-*d*]pyridazin-8-one (48).

The title compound was prepared from **47** by means of the "coupling procedure" and was purified by flash chromatography (ethyl acetate as the eluent) to obtain a yellow oil which crystallized on standing (yield 20%, mp 168-169 °C). ^{1}H-NMR ($CDCl_3$): 0.93 (t, *J* = 7.2, 3H), 1.22-1.46 (m, 2H), 1.70-1.85 (m, 2H), 4.12 (t, *J* = 7.0, 2H), 5.35 (s, 2H), 6.90 (m, 6H), 7.12-7.51 (m, 16H), 7.67 (m, 1H), 7.90 (m, 1H), 8.68 (m, 1H), 9.07 (m, 1H). MS(ESI): *m/z* 718 ($M+Na^+$).

General procedure for the Preparation of Compounds 16a-k,m.

A mixture of the hydrazide intermediate (**15a-k,m,** 2.0 mmol) in 1-pentanol (20 mL) with Na_2CO_3 (0.212 g, 2.0 mmol) was refluxed for 18-24 h under argon. The reaction mixture was allowed to

cool to room temperature and was acidified with glacial acetic acid up to pH 6. The solvent was removed under reduced pressure and the residue was purified by flash chromatography.

2,3-Dihydro-2-propyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16a).

The title compound was obtained from **15a** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent (yield 82%). Recrystallization of **16a** from ethyl acetate/diethyl ether gave red prisms melting at 85-87 °C. ^{1}H-NMR ($CDCl_3$): 0.97 (t, *J* = 7.4, 3H), 1.80-1.91 (m, 2H), 3.96 (t, *J* = 7.2, 2H), 7.04-7.10 (m, 1H), 8.21 (d, *J* = 7.7, 1H), 8.43 (d, *J* = 4.9, 1H). MS(EI): *m/z* 177 (M^+, 58).

2-*iso*-Butyl-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16b).

The title compound was prepared from **15b** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent to obtain **16b** (yield 72%). ^{1}H-NMR ($CDCl_3$): 1.01 (d, *J* = 6.8, 6H), 2.14-2.34 (m, 1H), 3.80 (d, *J* = 7.7, 2H), 7.13 (m, 1H), 8.23 (m, 1H), 8.45 (d, *J* = 4.9, 1H).

2-Butyl-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16c).

The title compound was prepared from **15c** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent (yield 55%, mp 108-110 °C). Recrystallization of **16c** from diethyl ether gave colourless needles suitable for X-ray diffraction studies. ^{1}H-NMR ($CDCl_3$): 0.86 (t, *J* = 7.3, 3H), 1.23-1.42 (m, 2H), 1.70-1.85 (m, 2H), 3.99 (t, *J* = 7.2, 2H), 6.97 (dd, *J* = 5.0, 7.5, 1H), 8.18 (dd, *J* = 1.2, 7.6, 1H), 8.37 (dd, *J* = 1.3, 4.9, 1H), 10.78 (br s, 1H). MS(ESI): *m/z* 192 ($M+H^+$).

2,3-Dihydro-2-*iso*-pentyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16d).

The title compound was prepared from **15d** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent to obtain pure **16d** (yield 29%). ^{1}H-NMR ($CDCl_3$): 0.97 (d, *J* =

6.0, 6H), 1.57-1.73 (m, 3H), 3.99 (t, *J* = 7.5, 2H), 7.10-7.17 (m, 1H), 8.21 (m, 1H), 8.49 (d, *J* = 4.9, 1H).

2,3-Dihydro-2-pentyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16e).

The title compound was prepared from **15e** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent to obtain **16e** (yield 48%) as a white solid melting at 119-121 °C. ^{1}H-NMR ($CDCl_3$): 0.89 (m, 3H), 1.32-1.40 (m, 4H), 1.74-1.85 (m, 2H), 3.95 (t, *J* = 7.2, 2H), 7.14 (m, 1H), 8.20 (m, 1H), 8.49 (m, 1H). MS(ESI): *m/z* 206 ($M+H^+$).

2-Benzyl-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16f).

The title compound was prepared from **15f** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent to obtain **16f** (yield 57%) as a pink solid melting at 195-198 °C (literature[2] mp: 188-189 °C). ^{1}H-NMR ($CDCl_3$): 5.10 (s, 2H), 7.02 (m, 1H), 7.36 (s, 5H), 7.90 (m, 1H), 8.19 (d, *J* = 8.4, 1H). MS(ESI): *m/z* 248 ($M+Na^+$).

2,3-Dihydro-2-ethyl-6-methyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16g).

This compound was prepared from **15g** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent (yield 38%); **16g** was obtained as a red solid melting at 184-186 °C. ^{1}H-NMR ($CDCl_3$): 1.35 (t, *J* = 7.2, 3H), 2.57 (s, 3H), 3.98 (q, *J* = 7.2, 2H), 5.79 (br s, 1H), 6.93 (d, *J* = 8.1, 1H), 8.07 (d, *J* = 7.9, 1H). MS(ESI): *m/z* 178 ($M+H^+$).

2,3-Dihydro-6-methyl-2-propyl-1*H*-pyrazolo[3,4-b]pyridin-3-one (16h).

The title compound was prepared from **15h** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent (yield 25%); **16h** was obtained as an orange solid melting at 111-113 °C. ^{1}H-NMR ($CDCl_3$): 0.91 (t, *J* = 7.4, 3H), 1.79 (m, 2H), 2.56 (s, 3H), 3.90 (t, *J* = 7.1, 2H), 6.88 (d, *J* = 7.9, 1H), 8.07 (d, *J* = 7.9, 1H). MS(ESI): *m/z* 192 ($M+H^+$).

2-Butyl-2,3-dihydro -6-methyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16i).

The title compound was obtained from **15i** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent (yield 59%); **16i** was obtained as a pale red solid melting at 144-146 °C. ^{1}H-NMR ($CDCl_3$): 0.93 (t, *J* = 7.2, 3H), 1.36 (m, 2H), 1.75 (m, 2H), 2.59 (s, 3H), 3.93 (t, *J* = 7.0, 2H), 6.96 (d, *J* = 7.9, 1H), 8.07 (d, *J* = 7.9, 1H). MS(ESI): *m/z* 228 ($M+Na^+$).

2-Butyl-6-chloro-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16j).

The title compound was prepared from **15j** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent; pure **16j** was obtained as a white solid after washing with ethyl acetate (yield 68%, mp 195-198 °C). ^{1}H-NMR ($CDCl_3$): 0.94 (t, *J* = 7.1, 3H), 1.37 (m, 2H), 1.78 (m, 2H), 3.99 (t, *J* = 7.2, 2H), 7.13 (d, *J* = 8.0, 1H), 8.17 (d, *J* = 8.0, 1H), 9.23 (s, 1H). MS(ESI): *m/z* 226 ($M+H^+$).

2-Butyl-6-chloro-2,3-dihydro-5-fluoro -1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16k).

This compound was prepared from **15k** and was purified by flash chromatography with ethyl acetate as the eluent to obtain pure **16k** (yield 28%) as a white solid melting at 179-180 °C. ^{1}H-NMR ($CDCl_3$): 0.95 (t, *J* = 7.2, 3H), 1.39 (m, 2H), 1.75 (m, 2H), 3.92 (t, *J* = 7.2, 2H), 7.92 (d, *J* = 6.7, 1H). MS(ESI): *m/z* 244 ($M+H^+$).

2-Butyl-5-chloro-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16m).

The title compound was prepared from **15m** and was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent to obtain pure **16m** (yield 66%) as a white solid melting at 175-176 °C. ^{1}H-NMR ($CDCl_3$): 0.96 (t, *J* = 7.3, 3H), 1.41 (m, 2H), 1.75 (m, 2H), 3.92 (t, *J* = 7.1, 2H), 8.13 (d, *J* = 1.9, 1H), 8.49 (d, *J* = 2.0, 1H). MS(ESI, negative ions): *m/z* 224 ($M-H^+$).

2-Butyl-2,3-dihydro-5-fluoro-1*H*-pyrazolo[3,4-*b*]pyiridin-3-one (16l).

A mixture of **16k** (0.24 g, 0.98 mmol) in EtOH (30 mL) with Na_2CO_3 (0.10 g, 0.94 mmol) and 0.05 g of 10% Pd on carbon was hydrogenated at atmospheric pressure and at room temperature for 24 h. The catalyst was filtered off and the filtrate was evaporated under reduced pressure. The residue was purified by flash chromatography with ethyl acetate as the eluent to give 0.16 g of **16l** as a yellow solid (yield 79%). ^{1}H-NMR (CD_3OD): 0.93 (t, *J* = 7.3, 3H), 1.34 (m, 2H), 1.79 (m, 2H), 4.04 (t, *J* = 7.2, 2H), 7.65 (dd, *J* = 3.0, 8.3, 1H), 8.14 (t, *J* = 2.5, 1H). MS(ESI, negative ions): *m/z* 208 ($M-H^+$).

2-Butyl-2,3-dihydro-6-morpholino-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (16p).

A mixture of **16j** (0.11 g, 0.48 mmol) in morpholine (30 mL) was refluxed for 2 h under an argon atmosphere. The solvent was removed under reduced pressure and the residue was purified by flash chromatography with ethyl acetate-methanol (9:1) as the eluent to give 0.11 g of **16p** as a white solid (yield 83%). ^{1}H-NMR ($CDCl_3$): 0.93 (t, *J* = 7.3, 3H), 1.35 (m, 2H), 1.69 (m, 2H), 3.63 (m, 4H), 3.79 (m, 6H), 6.44 (d, *J* = 8.8, 1H), 7.87 (d, *J* = 8.8, 1H). MS(ESI): *m/z* 277 ($M+H^+$).

General procedure for the Preparation of Compounds 15a-k,m.

A mixture of the appropriate 2-chloronicotinic acid (3.0 mmol) (**10-13**) (or 2- hydroxynicotinic acid, **14**) in $SOCl_2$ (20 mL) and a catalytic amount of anhydrous DMF was refluxed overnight. The $SOCl_2$ excess was azeotropically removed under reduced pressure with toluene. The resulting acid chloride was dissolved in CH_2Cl_2 (20 mL) and added to a mixture of the appropriate hydrazine oxalate (3.0 mmol) into CH_2Cl_2 (20 mL) with NaOH (0.48 g, 12 mmol) and water (3 mL). The reaction mixture was refluxed for 15 min and diluted with water (20 mL). The organic layer was dried over sodium sulfate and evaporated under reduced pressure. Purification of the residue by flash chromatography with the suitable eluent gave compounds **15a-k,m**, which were rapidly used in the next step.

2-Chloro-*N*-propylnicotinohydrazide (15a).

The title compound was prepared from **10** and propylhydrazine oxalate to obtain a colourless oil after purification by flash chromatography with ethyl acetate as the eluent (yield 76 %). The ^{1}H NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H NMR ($CDCl_3$): 0.76 (t, J = 7.4), 1.00 (t, J = 7.4), 1.55-1.81 (m), 3.20 (br s), 3.67 (t, J = 7.3), 3.81 (s), 4.47 (br s), 7.21-7.32 (m), 7.60-7.65 (m), 8.33-8.44 (m). MS(EI): *m/z* 213 (M^+, 52).

2-Chloro-*N*-isobutylnicotinohydrazide (15b).

The title compound was prepared from **10** and isobutylhydrazine oxalate to obtain a pale yellow oil after purification by flash chromatography with ethyl acetate as the eluent (yield 44 %). The ^{1}H NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.98 (d, J = 6.7), 2.27 (m), 3.05 (br s), 3.50 (d, J = 7.5), 3.84 (s), 4.48 (s), 7.26 (m), 7.60 (m), 8.32 (d, J = 4.8), 8.41 (d, J = 4.7).

2-Chloro-*N*-butylnicotinohydrazide (15c).

The title compound was prepared from **10** and butylhydrazine oxalate to obtain a colourless oil which crystallized on standing (yield 80 %, mp 91-93 °C). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.77 (t, J = 7.2), 0.95 (t, J = 7.2), 1.06-1.24 (m), 1.30-1.49 (m), 1.50-1.73 (m), 3.21 (t, J = 6.5), 3.68 (t, J = 7.2), 3.83 (br s), 4.46 (br s), 7.20-7.31 (m), 7.61 (m), 8.31-8.42 (m). MS(ESI): *m/z* 250 ($M+Na^+$).

2-Chloro-*N*-isopentylnicotinohydrazide (15d).

The title compound was prepared from **10** and isopentylhydrazine oxalate to obtain a pale yellow oil after purification by flash chromatography with ethyl acetate as the eluent (yield 64 %). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.76 (d, *J* = 6.1), 0.99 (d, *J* = 6.2), 1.32-1.81 (m), 3.23 (br s), 3.71-3.82 (m), 4.48 (s), 7.27-7.35 (m), 7.65 (m), 8.37 (m), 8.47 (m).

2-Chloro-*N*-pentylnicotinohydrazide (15e).

The title compound was prepared from **10** and pentylhydrazine oxalate to obtain a pale yellow oil after purification by flash chromatography with ethyl acetate as the eluent (yield 70%). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.78-1.01 (m), 1.14-1.44 (m), 1.48-1.73 (m), 3.23 (br s), 3.70 (t, *J* = 7.6), 3.83 (s), 4.47 (s), 7.23-7.33 (m), 7.64 (m), 8.36 (m), 8.45 (m). MS(ESI, negative ions): *m/z* 240 ($M-H^+$).

***N*-Benzyl-2-chloronicotinohydrazide (15f).**[2]

The title compound was prepared from **10** and benzylhydrazine oxalate to obtain a white solid after purification by flash chromatography with ethyl acetate as eluent (yield 55%). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 3.66 (s), 4.48 (m), 4.90 (s), 7.12-7.38 (m), 7.65 (m), 8.35 (m), 8.45 (m).

2-Chloro-*N*-ethyl-6-methylnicotinohydrazide (15g).

The title compound was prepared from **11** and ethylhydrazine oxalate to obtain a colorless oil after purification by flash chromatography with ethyl acetate as the eluent (yield 53%). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the

sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 1.18 (t, *J* = 6.9), 1.28 (t, *J* = 7.3), 2.54 (s), 2.56 (s), 3.31 (q, *J* = 7.0), 3.71-3.84 (m), 4.46 (br s), 7.09-7.16 (m), 7.50-7.56 (m).

2-Chloro-6-methyl-*N*-propylnicotinohydrazide (15h).

The title compound was prepared from **11** and propylhydrazine oxalate to obtain a colorless oil after purification by flash chromatography with ethyl acetate as the eluent (yield 60%). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.78 (t, *J* = 7.5), 1.00 (t, *J* = 7.7), 1.56-1.79 (m), 2.54 (s), 2.56 (s), 3.22 (t, *J* = 7.1), 3.68 (t, *J* = 7.0), 3.82 (s), 4.46 (s), 7.09-7.16 (m), 7.50-7.56 (m).

***N*-Butyl-2-Chloro-6-methylnicotinohydrazide (15i).**

The title compound was prepared from **11** and butylhydrazine oxalate to obtain a glassy yellow solid after purification by flash chromatography with ethyl acetate as the eluent (yield 76%). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.80 (t, *J* = 7.1), 0.96 (t, *J* = 7.4), 1.06-1.25 (m), 1.31-1.74 (m), 2.52 (s), 2.54 (s), 3.23 (t, *J* = 7.2), 3.69 (t, *J* = 7.4), 3.83 (s), 4.45 (br s), 7.07-7.14 (m), 7.48-7.54 (m).

***N*-Butyl- 2,6-dichloronicotinohydrazide (15j).**

The title compound was prepared from **12** and butylhydrazine oxalate and was purified by flash chromatography with dichloromethane-ethyl acetate (8:2) as the eluent to obtain a yellow oil which crystallized on standing (yield 72%, mp 78-81 °C). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.82 (t, *J* = 7.3), 0.97 (t, *J* = 7.1), 1.08-1.27 (m),

1.32-1.50 (m), 1.53-1.75 (m), 3.23 (t, *J* = 7.0), 3.70 (t, *J* = 7.1), 3.82 (br s), 4.42 (br s), 7.35 (m), 7.58 (d, *J* = 7.9). MS(ESI): *m/z* 262 ($M+H^+$).

_N_-Butyl-2,6-dichloro-5-fluoronicotinohydrazide (15k).

The title compound was prepared from **13** and butylhydrazine oxalate and purified by flash chromatography with petroleum ether-ethyl acetate (65:35) as the eluent to obtain a colourless oil which crystallized on standing (yield 97%, mp 84-85 °C). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.85 (t, *J* = 7.2), 0.99 (t, *J* = 7.2), 1.12-1.30 (m), 1.33-1.48 (m), 1.56-1.76 (m), 3.26 (t, *J* = 7.1), 3.71 (t, *J* = 7.3), 3.92 (br s), 4.43 (br s), 7.45 (m). MS(ESI): *m/z* 280 ($M+H^+$).

_N_-Butyl-2,5-dichloronicotinohydrazide (15m).

The title compound was prepared from **14** and butylhydrazine oxalate and purified by flash chromatography with petroleum ether-ethyl acetate (65:35) as the eluent to obtain a colorless oil (yield 70%). The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.86 (t, *J* = 6.9), 0.97 (t, *J* = 7.0), 1.11-1.32 (m), 1.36-1.51 (m), 1.55-1.75 (m), 3.26 (t, *J* = 6.8), 3.70 (t, *J* = 7.2), 3.84 (br s), 4.45 (br s), 7.60 (m), 8.26 (d, *J* = 2.9), 8.37 (d, *J* = 2.7). MS(ESI): *m/z* 284 ($M+Na^+$).

_N_-Butyl-2-iodobenzohydrazide (20).

A mixture of 2-iodobenzoic acid (**19**, 1.00 g, 4.0 mmol) in 15 mL of CH_2Cl_2 with $SOCl_2$ (3.0 mL) was refluxed for 2 h. The volatile material was removed under reduced pressure and the residue was diluted with 10 mL of dichloromethane and added to a mixture of butylhydrazine oxalate (0.71 g, 4.0 mmol) in 10 mL of CH_2Cl_2 with 0.64 g (16 mmol) of NaOH and water (1.0 mL). The

resulting mixture was refluxed for 30 min and partitioned between CH_2Cl_2 and water. The organic layer was washed with water, dried over sodium sulfate, and evaporated under reduced pressure. The residue was purified by flash-chromatography with ethyl acetate as the eluent to obtain 0.71 g of **20** (yield 56%) as a light brown oil, which was promptly used in the subsequent step. The ^{1}H-NMR spectrum of this compound shows the presence of two different rotamers in equilibrium. For the sake of simplification the integral intensities have not been given. ^{1}H-NMR ($CDCl_3$): 0.73 (t, *J* = 7.3), 0.90 (t, *J* = 7.2), 1.02-1.20 (m), 1.31-1.68 (m), 3.14 (t, *J* = 6.6), 3.62 (t, *J* = 7.4), 4.01 (br s), 6.96-7.05 (m), 7.11-7.15 (m), 7.25-7.35 (m), 7.68-7.77 (m). MS(ESI): *m/z* 319 ($M+H^+$).

2-Butyl-2,3-dihydro-1*H*-indazol-3-one (21).[3]

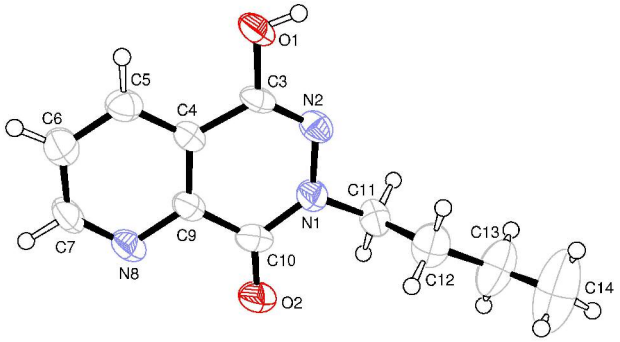
A mixture of **20** (0.47 g, 1.48 mmol) in 20 mL of EtOH with 0.48 g of NaOH (12 mmol) and 10 mg of $Pd(dppf)_2Cl_2$ (0.012 mmol) was refluxed for 3 h. The solvent was removed under reduced pressure and the residue was diluted with water, neutralized with 1N HCl, and extracted with chloroform. The organic layer was dried over sodium sulfate and evaporated under reduced pressure to give **21** as a brown glassy solid (0.26 g, yield 92%). ^{1}H-NMR ($CDCl_3$): 0.83 (t, *J* = 7.2, 3H), 1.26 (m, 2H), 1.71 (m, 2H), 3.87 (t, *J* = 7.2, 2H), 7.07 (t, *J* = 7.4, 1H), 7.18 (d, *J* = 8.2, 1H), 7.41 (t, *J* = 7.7, 1H), 7.70 (d, *J* = 7.9, 1H), 9.51 (br s).

7-Butyl-5-hydroxy-7,8-dihydropyrido[2,3-*d*]pyridazin-8-one (47).

A mixture of 2,3-pyridinedicarboxylic anhydride (**46**, 0.15 g, 1.0 mmol) in EtOH (30 mL) with triethylamine (1.0 mL) and butylhydrazine oxalate (0.18 g, 1.0 mmol) was refluxed for 45 min under argon. The volatile material was then removed under reduced pressure and the residue was partitioned between $CHCl_3$ and water. The organic layer was washed with water, dried over sodium sulfate and concentrated under reduced pressure. The residue was recrystallized from $CHCl_3$ by slow evaporation of the solvent to give 0.18 g of white crystals suitable for X-ray diffraction studies (yield 82%, mp 186-187° C). ^{1}H-NMR ($CDCl_3$): 0.96 (t, *J* = 7.3, 3H), 1.44 (m, 2H), 1.82 (m, 2H),

4.14 (t, *J* = 7.3, 2H), 7.74 (dd, *J* = 4.8, 7.9, 1H), 8.40 (dd, *J* = 1.6, 8.0, 1H), 9.17 (m, 1H). MS(ESI): *m/z* 220 ($M+H^+$).

Figure 1S. Crystal structure of compound **47**. Ellipsoids enclose 50% probability.



Preparation of Pyrazolo[3,4-*b*]pyridines 30-33.

A mixture of the appropriate ester (**27-29**) (26 mmol) in ethanol (30 mL) and TEA (20 mL) with butylhydrazine oxalate (or propylhydrazine oxalate) (39 mmol) was refluxed for 22 h. The solvent was then removed under reduced pressure and the residue was partitioned between CH_2Cl_2 and water. The organic layer was dried over sodium sulfate and evaporated under reduced pressure. The residue was purified by flash-chromatography with the appropriate eluent to give compounds **30-33**.

2,3-Dihydro-1-propyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (30).

The title compound was prepared from ester **27** and propylhydrazine oxalate and was purified by flash chromatography with ethyl acetate as the eluent to obtain a white solid (yield 74% mp 132-134 °C). Recrystallization of **30** from ethyl acetate by slow evaporation gave colorless needles suitable for X-ray diffraction studies. ^{1}H-NMR ($CDCl_3$): 0.95 (t, *J* = 7.2, 3H), 1.95 (m, 2H), 4.33 (t, *J* = 6.9, 2H), 7.03 (m, 1H), 8.10 (m,1H), 8.53 (m, 1H).

1-Butyl-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (31).

The title compound was prepared from **27** and butylhydrazine oxalate and was purified by washing with diisopropyl ether to obtain a pale-orange solid (yield 86%, mp 97-99 °C). ^{1}H-NMR ($CDCl_3$): 0.92 (t, J = 7.3, 3H), 1.31 (m, 2H), 1.88 (m, 2H), 4.34 (t, J = 7.0, 2H), 7.01 (m, 1H), 8.08 (d, J = 7.8, 1H), 8.51 (m, 1H). MS(ESI): *m/z* 192 ($M+H^+$).

1-Butyl-2,3-dihydro-6-methyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (32).

The title compound was prepared from **28** and butylhydrazine oxalate and was purified by flash chromatography with CH_2Cl_2-ethyl acetate (1:1) as the eluent to give a pale yellow solid (yield 89%, mp 156-158 °C). Recrystallization of **32** from ethyl acetate gave glasslike crystals suitable for X-ray diffraction studies. ^{1}H-NMR ($CDCl_3$): 0.93 (t, J = 7.2, 3H), 1.33 (m, 2H), 1.86 (m, 2H), 2.65 (s, 3H), 4.32 (t, J = 7.2, 2H), 6.88 (d, J = 8.0, 1H), 7.97 (d, J = 8.0, 1H). MS (ESI): *m/z* 206 ($M+H^+$).

1-Butyl-6-chloro-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (33).

The title compound was prepared from **29** and purified by flash chromatography with CH_2Cl_2-ethyl acetate (8:2) as the eluent to obtain a white solid (yield 73%, mp 175-177 °C). ^{1}H-NMR ($CDCl_3$): 0.95 (t, J = 7.3, 3H), 1.34 (m, 2H), 1.87 (m, 2H), 4.30 (t, J = 7.0, 2H), 7.02 (d, J = 8.8, 1H), 8.00 (d, J = 7.9, 2H). MS(ESI, negative ions): *m/z* 224 ($M-H^+$).

Preparation of *t*-Butyldimethylsilylether Derivatives 36a-c.

To a mixture of the appropriate pyrazolo[3,4-*b*]pyridine derivative (**31**-**33**) (7.4 mmol) in anhydrous THF (20 mL), DIPEA (10 mmol) and *t*-butyldimethylsilyl trifluoromethanesulfonate (TBDMS-OTf) (7.6 mmol) were added in sequence and the resulting mixture was stirred at room temperature for 20 min. The solvent was removed under reduced pressure and the residue was partitioned between CH_2Cl_2 and water. The organic layer was dried over sodium sulfate and concentrated under

reduced pressure. Purification of the residue by flash chromatography with the suitable eluent gave the expected silylether derivative (**36a**-**c**), which was promptly used in the subsequent synthetic step.

1-Butyl-3-(*tert*-butyldimethylsilyl)oxy-1*H*-pyrazolo[3,4-*b*]pyridine (36a).

The title compound was prepared from **31** and purified by flash chromatography with chloroform as the eluent to obtain a colorless thick oil (yield 92%). ^{1}H-NMR ($CDCl_3$): 0.30 (s, 6H), 0.83-1.00 (m, 12H), 1.31 (m, 2H), 1.82 (m, 2H), 4.30 (t, *J* = 7.8, 2H), 6.93 (m, 1H), 7.88 (m, 1H), 8.40 (m, 1H). MS(ESI): *m/z* 306 ($M+H^+$).

1-Butyl-3-(*t*-butyldimethylsilyl)oxy-6-methyl-1*H*-pyrazolo[3,4-*b*]pyridine (36b).

The title compound was prepared from **32** and purified by flash chromatography with dichloromethane as the eluent to obtain a colorless thick oil (yield 89 %). ^{1}H-NMR ($CDCl_3$): 0.30 (s, 6H), 0.85-1.00 (m, 12H), 1.30 (m, 2H), 1.85 (m, 2H), 2.60 (s, 3H), 4.28 (t, *J* = 7.0, 2H), 6.81 (d, *J* = 8.0, 1H), 7.74 (d, *J* = 8.0, 1H). MS (ESI): *m/z* 320 ($M+H^+$).

1-Butyl-3-(*t*-butyldimethylsilyl)oxy-6-chloro-1*H*-pyrazolo[3,4-*b*]pyridine (36c).

The title compound was prepared from **33** and purified by flash chromatography with chloroform as the eluent to give a colorless thick oil (yield 73%). ^{1}H-NMR ($CDCl_3$): 0.30 (s, 6H), 0.91 (t, *J* = 7.3, 3H), 1.00 (s, 9H), 1.32 (m, 2H), 1.82 (m, 2H), 4.25 (t, *J* = 7.2, 2H), 6.94 (d, *J* = 8.8, 1H), 7.80 (d, *J* = 8.8, 1H). MS (ESI): *m/z* 340 ($M+H^+$).

Preparation of Bromobenzyl Derivatives 37a-c.

To an ice-cooled mixture of 4-bromobenzyl bromide (12 mmol) and the appropriate silylether derivative (**36a**-**c**) (6.0 mmol) in anhydrous THF (13 mL) a 1M solution of tetrabutylammonium fluoride in THF (6.0 mmol) was added. The reaction mixture was stirred at room temperature for 15

min. The solvent was removed under reduced pressure and the residue was partitioned between diethylether and water. The organic layer was dried over sodium sulfate and evaporated under reduced pressure. The residue was purified by flash-chromatography with the suitable eluent to give compounds **37a-c**.

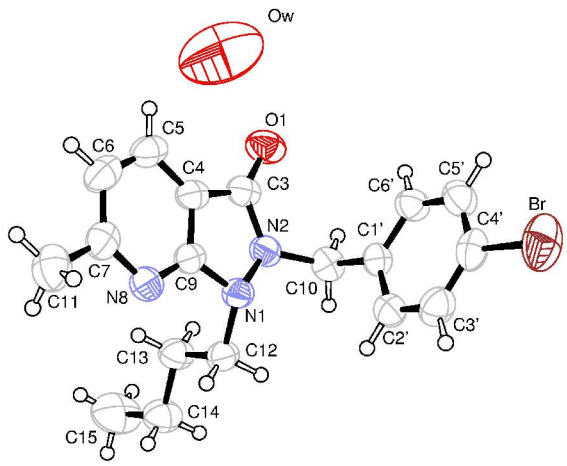
2-(4-Bromobenzyl)-1-butyl-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (37a).

The title compound was prepared from **36a** and purified by flash chromatography with diethyl ether-ethyl acetate (8:2) as the eluent to give a colorless thick oil (yield 13%). ^{1}H-NMR ($CDCl_3$): 0.77 (t, J = 7.0, 3H), 1.00-1.32 (m, 4H), 3.90 (t, J = 7.3, 2H), 5.04 (s, 2H), 7.02-7.14 (m, 3H), 7.40 (d, J = 8.6, 2H), 8.15 (d, J = 7.9, 1H), 8.51 (d, J = 5.0, 1H). MS(ESI): *m/z* 382 ($M+Na^+$).

2-(4-Bromobenzyl)-1-butyl-2,3-dihydro-6-methyl-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (37b).

The title compound was prepared from **36b** and purified by flash chromatography with CH_2Cl_2-ethyl acetate (9:1) as the eluent to obtain a white solid (yield 18%). Recrystallization of **37b** from diethyl ether by slow evaporation gave colourless prisms (mp 88-90 °C) suitable for X-ray diffraction studies. ^{1}H-NMR ($CDCl_3$): 0.79 (t, J = 6.9, 3H), 1.00-1.33 (m, 4H), 2.58 (s, 3H), 3.89 (t, J = 7.3, 2H), 5.02 (s, 2H), 6.92 (d, J = 7.9, 1H), 7.11 (d, J = 8.1, 2H), 7.39 (d, J = 8.6, 2H), 8.01 (d, J = 7.9, 1H). MS (ESI): *m/z* 396 ($M+Na^+$).

Figure 2S. Crystal structure of compound **37b·H_2O**. Ellipsoids enclose 50% probability.



2-(4-Bromobenzyl)-1-butyl-6-chloro-2,3-dihydro-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (37c).

The title compound was obtained from **36c** and purified by flash chromatography with CH_2Cl_2-ethyl acetate (8:2) as the eluent to obtain an off-white solid (yield 13%, mp 107-109 °C). ^{1}H-NMR ($CDCl_3$): 0.81 (t, *J* = 7.0, 3H), 1.03-1.39 (m, 4H), 3.89 (t, *J* = 7.4, 2H), 5.04 (s, 2H), 7.02-7.12 (m, 3H), 7.42 (d, *J* = 8.4, 2H), 8.06 (d, *J* = 7.9, 1H). MS (ESI): *m/z* 416 ($M+Na^+$).

3-(4-Bromobenzyloxy)-1-butyl-1*H*-pirazolo[3,4-*b*]pyridine (38a).

This compound was obtained from the purification by flash chromatography of **37a** (CH_2Cl_2 as the eluent, colourless oil, yield 81%). ^{1}H-NMR ($CDCl_3$): 0.92 (t, *J* = 7.3, 3H), 1.31 (m, 2H), 1.85 (m, 2H), 4.34 (t, *J* = 7.2, 2H), 5.36 (s, 2H), 6.96 (m, 1H), 7.36-7.53 (m, 4H), 7.98 (d, *J* = 7.8, 1H), 8.44 (m, 1H). MS(ESI): *m/z* 360 ($M+H^+$).

6-(4-Bromobenzyl)-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (40).

A mixture of ethyl 2-methylpyridine-3-carboxylate (**23**) (0.50 g, 3.0 mmol) in 10 mL of CCl_4 with *N*-bromosuccinimide (0.59 g, 3.3 mmol) and dibenzoyl peroxide (0.073 g, 0.30 mmol) was refluxed for 3 h. The reaction mixture was concentrated under reduced pressure to half of the

initial volume and the insoluble succinimide was filtered-off. The solvent was evaporated under reduced pressure and the residue obtained was dissolved into ethanol (10 mL) and added to an homogeneous mixture of 4-bromobenzylamine hydrochloride (1.34 g, 6.06 mmol) in ethanol (10 mL) and triethylamine (0.8 mL, 5.7 mmol). The resulting mixture was refluxed for 1 h, the solvent was removed under reduced pressure and the residue obtained was partitioned between CH_2Cl_2 and water. The organic layer was dried over sodium sulfate and concentrated under reduced pressure. Purification of the residue by flash-chromatography with ethyl acetate as the eluent gave compound **40** as a white solid (yield 40%, mp 110-113 °C). ^{1}H-NMR ($CDCl_3$): 4.32 (s, 2H), 4.77 (s, 2H), 7.19 (m, 2H), 7.36-7.49 (m, 3H), 8.11 (m, 1H), 8.70 (m, 1H). MS(ESI): *m/z* 325 ($M+Na^+$).

6,7-Dihydro-6-propyl-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (24).

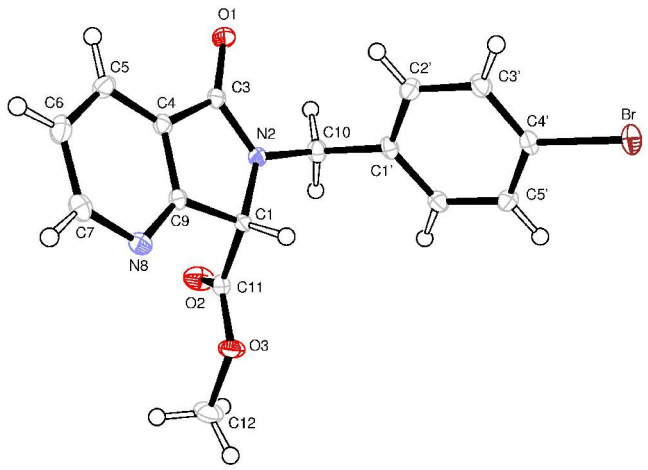
This compound was prepared from **23** by following the procedure used for the synthesis of **40** except for the fact that propylamine (3 equivalents) was used in the place of 4-bromobenzylamine hydrochloride. Compound **24** was purified by flash-chromatography with ethyl acetate as the eluent to obtain a thick oil (yield 62%), which was promptly used in the next synthetic step.^{1}H-NMR ($CDCl_3$): 0.88 (t, *J* = 7.4, 3H), 1.63 (m, 2H), 3.52 (t, *J* = 7.4, 2H), 4.34 (s, 2H), 7.29 (m, 1H), 8.00 (d, *J* = 7.9, 1H), 8.60 (d, *J* = 4.9, 1H). MS(ESI): *m/z* 177 ($M+H^+$).

Methyl 6-(4-Bromobenzyl)-6,7-dihydro-5-oxo-5*H*-pyrrolo[3,4-*b*]pyridine-7-carboxylate (41).

A mixture of **40** (1.0 g, 3.3 mmol) in dimethyl carbonate (50 mL) and anhydrous DMF (15 mL)with sodium hydride (0.40 g, 16.7 mmol) was refluxed for 3 h and poured into ice-water. The precipitate was extracted with dichloromethane and the organic layer was dried over sodium sulfate and evaporated under reduced pressure. Purification of the residue by flash chromatography with dichloromethane-ethyl acetate (1:1) as the eluent gave **41** as a white solid (yield 67%). An analytical sample recrystallized from diethyl ether (colorless plates) melted at 138-140 °C. ^{1}H-NMR

($CDCl_3$): 3.64 (s, 3H), 4.20 (d, *J* = 15.0, 1H), 4.92 (s, 1H), 5.17 (d, *J* = 15.1, 1H), 7.06 (m, 2H), 7.35 (m, 3H), 8.05 (d, *J* = 7.6, 1H), 8.61 (d, *J* = 4.7, 1H). MS(ESI): *m/z* 383 ($M+Na^+$).

Figure 3S. Crystal structure of compound **41**. Ellipsoids enclose 50% probability.



Methyl 6,7-Dihydro-5-oxo-6-propyl-5*H*-pyrrolo[3,4-*b*]pyridine-7-carboxylate (25).

This compound was prepared from **24** by following the procedure used for the synthesis of **41** and purified by flash-chromatography with ethyl acetate as the eluent to obtain a colorless thick oil (yield 43%), which was promptly used in the next synthetic step. ^{1}H-NMR ($CDCl_3$): 0.93 (t, *J* = 7.1, 3H), 1.65 (m, 2H), 3.17 (m, 1H), 3.80-4.04 (m, 4H), 5.19 (s, 1H), 7.39 (m, 1H), 8.11 (m, 1H), 8.69 (m, 1H). MS(ESI): *m/z* 257 ($M+Na^+$).

Procedure for the Preparation of Compounds 42e-g (Alkylation Procedure).

To a solution of the ester (**41**, 0.36 g, 1.0 mmol) in dry DMF (12 mL) cooled to -25 °C, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (1.56 mL, 11 mmol) was slowly added. After 20 min, to the red-coloured solution the appropriate iodide (13 mmol) was slowly added until the complete decoloration of the solution. The resulting mixture was stirred for 20 min at room temperature, poured into ice, and extracted with diethyl ether. The organic layer was washed with water, dried

over sodium sulfate and evaporated under reduced pressure. Purification of the residue by flash chromatography with the appropriate eluent gave pure compounds **42e-g.**

Methyl 6-(4-Bromobenzyl)-6,7-dihydro-7-ethyl-5-oxo-5*H*-pyrrolo[3,4-*b*]pyridine-7-carboxylate (42e).

The title compound was prepared from **41** according to the alkylation procedure and purified by flash chromatography with dichloromethane-ethyl acetate (8:2) as the eluent to obtain a pale yellow thick oil (yield 72%). ^{1}H-NMR ($CDCl_3$): 0.24 (t, J = 7.4, 3H), 2.18-2.66 (m, 2H), 3.17 (s, 3H), 4.33 (d, J = 15.4, 1H), 4.85 (d, J = 15.0, 1H), 7.21-7.41 (m, 5H), 8.10 (d, J = 8.2, 1H), 8.67 (m, 1H). MS(ESI): *m/z* 411 ($M+Na^+$).

Methyl 6-(4-Bromobenzyl)-6,7-dihydro-5-oxo-7-propyl-5*H*-pyrrolo[3,4-*b*]pyridine-7-carboxylate (42f).

The title compound was prepared from **41** according to the general alkylation procedure and purified by flash chromatography with dichloromethane-ethyl acetate (9:1) (yield 40%). An analytical sample recrystallized from diethyl ether melted at 97-100 °C. ^{1}H-NMR ($CDCl_3$): 0.31-0.86 (m, 5H), 2.19 (m, 1H), 2.53 (m, 1H), 3.25 (s, 3H), 4.46 (d, J = 15.2, 1H), 4.81 (d, J = 15.2, 1H), 7.25-7.44 (m, 5H), 8.14 (d, J = 8.1, 1H), 8.71 (m, 1H). MS(ESI): *m/z* 425 ($M+Na^+$).

Methyl 6-(4-Bromobenzyl)-7-butyl-6,7-dihydro-5-oxo-5*H*-pyrrolo[3,4-*b*]pyridine-7-carboxylate (42g).

The title compound was prepared from **41** according to the general alkylation procedure and purified by flash chromatography with dichloromethane-ethyl acetate (9:1) as the eluent. Recrystallization from diethyl ether gave **42g** as yellow crystals (yield 51%, mp 126-128 °C). ^{1}H-NMR ($CDCl_3$): 0.17-1.54 (m, 7H), 2.20 (m, 2H), 2.54 (m, 2H), 3.28 (s, 3H), 4.46 (d, J = 15.2, 1H), 4.80 (d, J = 15.2, 1H), 7.23-7.43 (m, 5H), 8.11 (m, 1H), 8.72 (m, 1H). MS(ESI): *m/z* 439 ($M+Na^+$).

Procedure for the Preparation of Compounds 43e-g (Hydrolysis-Decarboxylation Procedure).

To an ice-cooled mixture of the appropriate ester (**42e-g**) (0.5 mmol) in ethanol (10 mL), a 3N sodium hydroxide solution (5 mL) was added and the resulting mixture was stirred at 0 °C for 15 min. The organic solvent was the removed under reduced pressure, and the residue was diluted with water (20 mL). The basic solution was extracted with dichloromethane and the organic extracts were discarded, while the aqueous solution was acidified with 3N HCl and extracted with dichloromethane. The organic layer was dried over sodium sulfate and evaporated under reduced pressure to obtain pure compounds **43e-g**.

6-(4-Bromobenzyl)-6,7-dihydro-7-ethyl-5*H*-pyrrolo[3,4-*b*]pyridine-5-one (43e).

The title compound was obtained from **42e** by means of the "hydrolysis-decarboxylation procedure" as a thick colourless oil (yield 93%), which was used in the next step without further purification. ^{1}H-NMR ($CDCl_3$): 0.45 (t, *J* = 7.4, 3H), 1.81-2.28 (m, 2H), 4.09 (d, *J* = 15.2, 1H), 4.37 (m, 1H), 5.22 (d, *J* = 15.1, 1H), 7.11-7.39 (m, 5H), 8.05 (d, *J* = 8.0, 1H), 8.64 (d, *J* = 4.8, 1H). MS(ESI): *m/z* 353 ($M+Na^+$).

6-(4-Bromobenzyl)-6,7-dihydro-7-propyl-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (43f).

The title compound was obtained from **42f** by means of the "hydrolysis-decarboxylation procedure" as a thick colorless oil (yield 97%), which was used in the next step without further purification. ^{1}H-NMR ($CDCl_3$): 0.65-1.13 (m, 5H), 1.79 (m, 1H), 2.04 (m,1H), 4.10 (d, *J* = 15.2, 1H), 4.33 (m, 1H), 5.16 (d, *J* = 15.1, 1H), 7.08-7.35 (m, 5H), 8.01 (d, *J* = 7.7, 1H), 8.59 (d, *J* = 4.8, 1H). MS(ESI): *m/z* 367 ($M+Na^+$).

6-(4-Bromobenzyl)-7-butyl-6,7-dihydro-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (43g).

The title compound was obtained from **42g** by means of the "hydrolysis-decarboxylation procedure" as a pale yellow oil (yield 89%), which was used in the next step without further purification. ^{1}H-NMR ($CDCl_3$): 0.52-1.24 (m, 7H), 1.93 (m, 1H), 2.18 (m, 1H), 4.18 (d, *J* = 15.1, 1H), 4.44 (m, 1H), 5.27 (d, *J* = 15.2, 1H), 7.11-7.38 (m, 5H), 8.06 (d, *J* = 7.3, 1H), 8.64 (d, *J* = 4.8, 1H). MS(ESI): *m/z* 381 ($M+Na^+$).

General Procedure for the Preparation of Compounds 39a-c and 44d-g (Suzuki Cross-Coupling Procedure).

To a degassed solution of triphenylphosphine (0.030 g, 0.11 mmol) in anhydrous THF (2.5 mL) $Pd(OAc)_2$ (6.0 mg, 0.027 mmol) was added. The resulting mixture was degassed again under nitrogen purge, heated at 60 °C for 30 min, and cooled to room temperature.

A mixture of 5-(2'-boronophenyl)-2-(triphenylmethyl)-2*H*-tetrazole[4] (1.2 g, 2.8 mmol) in degassed DEM (10 mL) was stirred at room temperature for 30 min. Water (0.13 mL, 6.9 mmol) was added and the resulting mixture was stirred at room temperature for 30 min. Powdered K_2CO_3 (0.80 g, 5.8 mmol) and the appropriate aryl bromide (**37a-c**, **40**, **43e-g**; 2.3 mmol) were added sequentially. The mixture was degassed again and the palladium catalyst solution in THF was added. The reaction mixture was refluxed overnight and the solvent was removed under reduced pressure. The residue obtained was partitioned between ethyl acetate and water and the organic layer was dried over sodium sulfate and concentrated under reduced pressure. Purification of the residue by flash chromatography with the suitable eluent gave target compounds **39a-c** and **44d-g**.

1-Butyl-2,3-dihydro-2-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (39a).

The title compound was obtained from **37a** by means of the "Suzuki cross-coupling procedure" and was purified with dichloromethane-ethyl acetate (8:2) as the eluent. Compound **39a** was obtained as a pale yellow glassy solid (yield 56%). ^{1}H-NMR ($CDCl_3$): 0.77 (t, *J* = 6.9, 3H), 0.98-1.30 (m, 4H),

3.84 (t, *J* = 7.3, 2H), 5.00 (s, 2H), 6.88-7.50 (m, 23H), 7.91 (m, 1H), 8.18 (d, *J* = 8.0, 1H), 8.51 (d, *J* = 5.0, 1H). ME(ESI): *m/z* 690 ($M+Na^+$).

1-Butyl-2,3-dihydro-6-methyl-2-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (39b).

The title compound was obtained from **37b** by means of the "Suzuki cross-coupling procedure" and was purified with dichloromethane-ethyl acetate (9:1) as the eluent. Compound **39b** was obtained as a white crystalline solid (yield 47%) melting at 88-90 °C. ^{1}H-NMR ($CDCl_3$): 0.77 (t, *J* = 6.9, 3H), 0.98-1.28 (m, 4H), 2.56 (s, 3H), 3.81 (t, *J* = 7.2, 2H), 4.98 (s, 2H), 6.84-7.49 (m, 23H), 7.91 (m, 1H), 8.03 (d, *J* = 7.9, 1H). MS (ESI): *m/z* 704 ($M+Na^+$).

1-Butyl-6-chloro-2,3-dihydro-2-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-1*H*-pyrazolo[3,4-*b*]pyridin-3-one (39c).

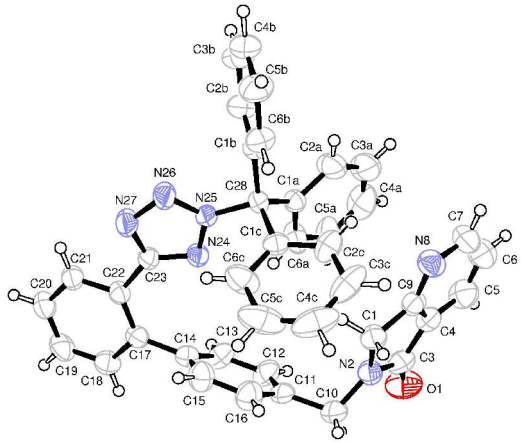
The title compound was obtained from **37c** by means of the "Suzuki cross-coupling procedure" and was purified with dichloromethane-ethyl acetate (9:1) as the eluent. Compound **39c** was obtained as a pale yellow solid (yield 11%) melting at 83-85 °C. ^{1}H-NMR ($CDCl_3$): 0.79 (t, *J* = 7.0, 3H), 1.03-1.25 (m, 4H), 3.80 (t, *J* = 7.4, 2H), 5.00 (s, 2H), 6.88-7.47 (m, 23H), 7.95 (m, 1H), 8.08 (d, *J* = 8.0, 1H). MS (ESI): 724 ($M+Na^+$).

6,7-Dihydro-6-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (44d).

The title compound was obtained from **40** by means of the "Suzuki cross-coupling procedure" and was purified by flash chromatography with CH_2Cl_2-ethyl acetate (1:1) as the eluent. A subsequent recrystallization from ethyl acetate gave **44d** (yield 49%, mp 174-177 °C) as light brown prisms suitable for X-ray diffraction studies. ^{1}H-NMR ($CDCl_3$): 4.14 (s, 2H), 4.70 (s, 2H), 6.84 (m, 6H),

7.04-7.51 (m, 17H), 7.98 (m, 1H), 8.14 (d, *J* = 8.1, 1H), 8.66 (d, *J* = 4.9, 1H). MS(ESI): *m/z* 633 ($M+Na^+$).

Figure 4S. Crystal structure of compound **44d**. Ellipsoids enclose 50% probability.



6,7-Dihydro-7-ethyl-6-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (44e).

The title compound was obtained from **43e** by means of the "Suzuki cross-coupling procedure" and was purified by flash chromatography with dichloromethane-ethyl acetate (8:2) as the eluent. Compound **44e** was obtained as a pale yellow glassy solid (yield 42 %). ^{1}H-NMR ($CDCl_3$): 0.48 (t, *J* = 7.3, 3H), 1.88-2.26 (m, 2H), 3.98 (d, *J* = 15.1, 1H), 4.30 (m, 1H), 5.35 (d, *J* = 14.9, 1H), 6.87 (m, 6H), 7.03-7.48 (m, 17H), 7.96 (m, 1H), 8.12 (m, 1H), 8.67 (d, *J* = 4.9, 1H). MS(ESI): *m/z* 661 ($M+Na^+$).

6,7-Dihydro-7-propyl-6-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (44f).

The title compound was obtained from **43f** by means of the "Suzuki cross-coupling procedure" and was purified with dichloromethane-ethyl acetate (8:2) as the eluent. Compound **44f** was obtained as a colorless glassy solid (yield 46%). ^{1}H-NMR ($CDCl_3$): 0.66-1.21 (m, 5H), 1.87 (m, 1H), 2.11 (m,

1H), 4.02 (d, *J* = 15.2, 1H), 4.30 (m, 1H), 5.30 (d, *J* = 14.9, 1H), 6.87 (m, 6H), 7.03-7.47 (m, 17H), 7.96 (m, 1H), 8.12 (d, *J* = 6.9, 1H), 8.67 (m, 1H). MS(ESI): *m/z* 675 ($M+Na^+$).

7-Butyl-6,7-dihydro-6-[[2'-[2-(triphenylmethyl)-2*H*-tetrazol-5-yl]-1,1'-biphenyl-4-yl]methyl]-5*H*-pyrrolo[3,4-*b*]pyridin-5-one (44g).

The title compound was obtained from **43g** by means of the "Suzuki cross-coupling procedure" and was purified with dichloromethane-ethyl acetate (8:2) as the eluent. Compound **44g** was obtained as a colorless glassy solid (yield 34%). ^{1}H-NMR ($CDCl_3$): 0.53-1.27 (m, 7H), 1.88 (m, 1H), 2.15 (m, 1H), 4.01 (d, *J* = 14.9, 1H), 4.32 (m, 1H), 5.29 (d, *J* = 14.9, 1H), 6.86 (m, 6H), 7.03-7.47 (m, 17H); 7.95 (m, 1H), 8.12 (d, *J* = 7.8, 1H), 8.68 (d, *J* = 4.8, 1H). MS(ESI): *m/z* 689 ($M+Na^+$).

Table 1S. Crystal data and structure refinement for **7a, 16a·H_2O**, **16c**, **30**, **32**, **37b·H_2O**, **41**, **44d**, **47**.

Compound 7a Empirical formula	$C_{23}H_{21}N_7O$
Formula weight	411.47
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a=8.284(2), b=10.341(2), c=12.716(3)Å, α=90.96(2), β=106.24(2), γ=99.07(2)deg
Volume	1030.6(4) $Å^3$
Z, Calculated density	2, 1.326 Mg/m^3
Absorption coefficient	0.087 mm^{-1}
F(000)	432
Theta range for data collection	2.52 to 24.99 deg.
Limiting indices	$-1 \le h \le 9$, $-12 \le k \le 12$, $-15 \le l \le 14$
Reflections collected / unique	3529 / 2839 [R(int)=0.0681]
Completeness to theta=24.99	78.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2839 / 0 / 282
Goodness-of-fit on F^2	0.972
Final R indices [I>2sigma(I)]	R1=0.0863, wR2=0.1440
R indices (all data)	R1=0.2453, wR2=0.2039
Largest diff. peak and hole	0.209 and -0.193 e.$Å^{-3}$

Compound 16a·H_2O	
Empirical formula	$C_9H_{11}N_3O \cdot H_2O$
Formula weight	195.22
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a=10.167(3), b=22.864(3), c=8.702(2)Å, β=100.22(3) deg.
Volume	1990.8(8) $Å^3$
Z, Calculated density	8, 1.303 Mg/m^3
Absorption coefficient	0.095 mm^{-1}
F(000)	832
Theta range for data collection	1.78 to 25.01 deg.
Limiting indices	$-12 \le h \le 12$, $-27 \le k \le 1$, $-1 \le l \le 10$
Reflections collected / unique	4476 / 3512 [R(int)=0.0276]
Completeness to theta=25.01	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3512 / 4 / 278
Goodness-of-fit on F^2	1.103
Final R indices [I>2sigma(I)]	R1=0.0740, wR2=0.1719
R indices (all data)	R1=0.1529, wR2=0.2099
Extinction coefficient	0.0056(13)
Largest diff. peak and hole	0.537 and -0.297 e.$Å^{-3}$

Compound 16c

Empirical formula	$C_{10}H_{13}N_3O$
Formula weight	191.23
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a=11.530(7), b=7664(2), c=11.708(4)Å, β=90.04(3)deg
Volume	1034.6(8) $Å^3$
Z, Calculated density	4, 1.228 Mg/m^3
Absorption coefficient	0.083 mm^{-1}
F(000)	408
Theta range for data collection	3.18 to 24.99 deg.
Limiting indices	-13≤h≤13, -9≤k≤1, -1≤l≤13
Reflections collected / unique	2427 / 1814 [R(int)=0.0548]
Completeness to theta=24.99	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1814 / 0 / 144
Goodness-of-fit on F^2	0.911
Final R indices [I>2sigma(I)]	R1=0.0708, wR2=0.1205
R indices (all data)	R1=0.1864, wR2=0.1471
Largest diff. peak and hole	0.166 and -0.175 $e.Å^{-3}$

Compound 30 Empirical formula	$C_9H_{11}N_3O$
Formula weight	177.21
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a=10.686(3), b=5.578(2), c=15.286(3)Å, β=96.51(2) deg.
Volume	905.3(4) $Å^3$
Z, Calculated density	4, 1.300 Mg/m^3
Absorption coefficient	0.089 mm^{-1}
F(000)	376
Theta range for data collection	2.21 to 25.00 deg.
Limiting indices	-12≤h≤12, 0≤k≤6, -18≤l≤18
Reflections collected / unique	3068 / 1548 [R(int)=0.0555]
Completeness to theta=25.00	96.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1548 / 0 / 128
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1=0.0485, wR2=0.1167
R indices (all data)	R1=0.0714, wR2=0.1291
Largest diff. peak and hole	0.161 and -0.158 $e.Å^{-3}$

Compound 32 Empirical formula	$C_{11}H15N_3O$
Formula weight	205.26
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a=10.2050(6), b=13.4670(7), c=8.6000(7)Å, β=104.730(5) deg.
Volume	1143.06(13) $Å^3$
Z, Calculated density	4, 1.193 Mg/m^3
Absorption coefficient	0.079 mm^{-1}
F(000)	440
Theta range for data collection	2.56 to 24.99 deg.
Limiting indices	-12≤h≤11, -16≤k≤1, -1≤l≤10
Reflections collected / unique	2627 / 1994 [R(int) = 0.0149]
Completeness to theta = 24.99	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1994 / 4 / 159
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0564, wR2 = 0.1411
R indices (all data)	R1 = 0.0922, wR2 = 0.1609
Largest diff. peak and hole	0.242 and -0.116 e.$Å^{-3}$

Compound 37b·H_2O

Empirical formula	$C_{18}H_{20}BrN_3O·H_2O$
Formula weight	392.29
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a=9.122(2), b=10.432(4), c=11.009(2)Å, α=67.77(2), β=77.580(10), γ=69.37(5) deg.
Volume	903.5(4) $Å^3$
Z, Calculated density	2, 1.435 Mg/m^3
Absorption coefficient	2.290 mm^{-1}
F(000)	400
Theta range for data collection	2.01 to 25.00 deg.
Limiting indices	-1≤h≤10, -11≤k≤11, -12≤l≤13
Reflections collected / unique	3662 / 3050 [R(int)=0.0105]
Completeness to theta=25.00	95.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3050 / 0 / 226
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1=0.0637, wR2=0.1700
R indices (all data)	R1=0.0824, wR2=0.1854
Extinction coefficient	0.048(16)
Largest diff. peak and hole	0.929 and -0.904 e.$Å^{-3}$

Compound 41 Empirical formula	$C_{16}H_{13}BrN_2O_3$
Formula weight	361.19
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a=6.0444(2), b=7.80770(10), c=15.7658(4)Å, α=83.670(2), β=84.1440(10), γ=78.886(2) deg.
Volume	723.14(3) $Å^3$
Z, Calculated density	2, 1.659 Mg/m^3
Absorption coefficient	2.857 mm^{-1}
F(000)	364
Theta range for data collection	1.30 to 27.55 deg.
Limiting indices	-7≤h≤7, -10≤k≤9, -20≤l≤20
Reflections collected / unique	16715 / 3318 [R(int)=0.0347]
Completeness to theta=27.55	99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3318 / 0 / 212
Goodness-of-fit on F^2	1.172
Final R indices [I>2sigma(I)]	R1=0.0269, wR2=0.0752
R indices (all data)	R1=0.0355, wR2=0.0880
Largest diff. peak and hole	0.342 and -0.587 e.$Å^{-3}$

Compound 44d Empirical formula	$C_{40}H_{30}N_6O$
Formula weight	610.70
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a=11.4080(10), b=11.871(2), c=23.993(2)Å, β=103.090(10)deg.
Volume	3164.8(7) $Å^3$
Z, Calculated density	4, 1.282 Mg/m^3
Absorption coefficient	0.079 mm^{-1}
F(000)	1280
Theta range for data collection	1.84 to 25.00 deg.
Limiting indices	-1≤h≤13, -1≤k≤14, -28≤l≤28
Reflections collected / unique	7149 / 5572 [R(int)=0.0263]
Completeness to theta=25.00	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5572 / 0 / 424
Goodness-of-fit on F^2	1.010
Final R indices [I>2sigma(I)]	R1=0.0524, wR2=0.1159
R indices (all data)	R1=0.0971, wR2=0.1372
Largest diff. peak and hole	0.249 and -0.210 e.$Å^{-3}$

Compound 47 Empirical formula	$C_{11}H_{13}N_3O_2$
Formula weight	219.24
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a=4.9110(10), b=23.418(6), c=9.7070(10)Å, β=93.010(10)deg
Volume	1114.8(4) $Å^3$
Z, Calculated density	4, 1.306 Mg/m^3
Absorption coefficient	0.093 mm^{-1}
F(000)	464
Theta range for data collection	1.74 to 24.98 deg.
Limiting indices	$-1 \le h \le 5$, $-1 \le k \le 27$, $-11 \le l \le 11$
Reflections collected / unique	1435 / 1357 [R(int)=0.0082]
Completeness to theta=24.98	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1357 / 2 / 147
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1=0.0605, wR2=0.1367
R indices (all data)	R1=0.1049, wR2=0.1608
Absolute structure parameter	-1(4)
Largest diff. peak and hole	0.212 and -0.191 $e.Å^{-3}$

Table 2S. Åtomic coordinates for non-hydrogen atoms ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **7a, 16a·H_2O**, **16c**, **30**, **32**, **37b·H_2O**, **41**, **44d**, **47**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Compound 7a

	x	y	z	U(eq)
N(1)	7145(9)	3394(6)	6168(5)	47(2)
N(2)	6379(9)	2487(6)	5229(5)	43(2)
C(3)	4737(11)	2623(7)	4756(6)	44(2)
O(1)	3864(7)	2053(5)	3857(4)	54(2)
C(4)	4310(11)	3495(7)	5492(6)	41(2)
C(5)	2878(11)	3990(7)	5527(6)	53(2)
C(6)	2992(12)	4852(7)	6382(7)	55(2)
C(7)	4552(14)	5186(8)	7193(7)	61(3)
N(8)	6009(10)	4734(6)	7203(5)	50(2)
C(9)	5799(11)	3923(7)	6324(6)	40(2)
C(10)	7443(10)	1958(7)	4615(6)	56(2)
C(11)	7248(11)	493(7)	4646(6)	58(2)
C(12)	8148(10)	-46(8)	3859(7)	67(3)
C(13)	8552(10)	3080(7)	7051(6)	52(2)
C(14)	9321(10)	-2905(7)	8555(6)	40(2)
C(1')	8158(10)	1798(7)	7567(5)	40(2)
C(2')	6555(10)	1248(7)	7619(6)	44(2)
C(3')	6285(10)	97(7)	8142(6)	49(2)
C(4')	7633(10)	-526(7)	8646(5)	38(2)
C(5')	9263(10)	2(7)	8599(5)	39(2)
C(6')	9494(10)	1169(7)	8059(5)	46(2)
C(1")	7362(10)	-1752(7)	9250(5)	38(2)
C(2")	6196(11)	-1770(8)	9884(6)	56(3)
C(3")	5976(11)	-2851(8)	10508(6)	59(3)
C(4")	6860(11)	-3853(8)	10530(6)	55(2)
C(5")	8010(10)	-3848(7)	9901(5)	51(2)
C(6")	8186(9)	-2783(7)	9254(5)	37(2)
N(14)	10830(9)	-3302(7)	8866(5)	66(2)
N(15)	11341(10)	-3370(8)	7941(7)	76(2)
N(16)	10205(10)	-3029(7)	7099(6)	69(2)
N(17)	8893(8)	-2733(5)	7452(5)	46(2)

Compound 16a·H_2O

	x	y	z	U(eq)
OW1	7379(2)	8022(1)	1489(3)	76(1)
OW2	7037(2)	7041(1)	-429(3)	73(1)
N(1A)	10221(3)	5477(1)	3304(4)	59(1)
N(2A)	9216(3)	5850(1)	2544(4)	53(1)
C(3A)	8362(4)	5611(2)	1351(4)	43(1)
O(1A)	7404(3)	5875(1)	520(3)	54(1)
C(4A)	8808(3)	5013(2)	1306(4)	38(1)
C(5A)	8418(4)	4531(2)	430(5)	48(1)
C(6A)	9143(4)	4018(2)	763(5)	53(1)
C(7A)	10235(4)	4005(2)	1935(5)	54(1)
N(8A)	10640(3)	4476(1)	2797(4)	52(1)
C(9A)	9953(4)	4989(2)	2531(5)	48(1)
C(10A)	9153(4)	6437(2)	3154(6)	68(1)
C(11A)	10427(4)	6773(2)	3214(8)	110(2)
C(12A)	10424(6)	7357(2)	3972(7)	98(2)

Table 2 ctd.

N(1B)	4431(4)	9546(2)	-2811(4)	72(1)
N(2B)	5181(4)	9170(1)	-1741(4)	64(1)
C(3B)	6252(4)	9419(2)	-823(5)	45(1)
O(1B)	7057(3)	9154(1)	219(3)	55(1)
C(4B)	6188(4)	10022(2)	-1316(4)	39(1)
C(5B)	6936(4)	10507(2)	-905(5)	52(1)
C(6B)	6551(4)	11024(2)	-1713(5)	62(1)
C(7B)	5438(4)	11035(2)	-2853(5)	59(1)
N(8B)	4700(3)	10562(1)	-3263(4)	53(1)
C(9B)	5058(4)	10043(2)	-2531(5)	47(1)
C(10B)	4600(9)	8585(3)	-1562(8)	52(2)
C(11B)	4673(14)	8252(4)	-3033(11)	84(4)
C(10C)	5254(11)	8522(4)	-2100(20)	50(5)
C(11C)	3871(11)	8308(7)	-2750(30)	71(7)
C(12B)	3954(6)	7656(2)	-2982(7)	95(2)

Compound 16c

	x	y	z	U(eq)
N(1)	3270(3)	3716(5)	1063(3)	55(1)
N(2)	3951(3)	2952(5)	1926(2)	51(1)
C(3)	3331(3)	2606(5)	2875(3)	44(1)
O(1)	3762(2)	2111(4)	3795(2)	60(1)
C(4)	2136(3)	2985(5)	2560(3)	44(1)
C(5)	1078(4)	2821(6)	3113(3)	60(1)
C(6)	118(4)	3275(7)	2488(4)	68(1)
C(7)	224(4)	3807(6)	1373(4)	63(1)
N(8)	1229(3)	3998(5)	816(3)	56(1)
C(9)	2153(3)	3574(5)	1451(3)	45(1)
C(10)	5218(3)	3101(7)	1871(3)	57(1)
C(11)	5741(3)	2063(7)	907(3)	55(1)
C(12)	7056(3)	2182(7)	890(4)	67(1)
C(13)	7585(4)	1238(10)	-120(4)	92(2)

Compound 30

	x	y	z	U(eq)
N(1)	7379(1)	2875(3)	4794(1)	50(1)
N(2)	6249(1)	1691(3)	4841(1)	48(1)
C(3)	5399(2)	2810(3)	4301(1)	46(1)
O(1)	4184(1)	2162(3)	4173(1)	61(1)
C(4)	5925(2)	4757(3)	3878(1)	45(1)
C(5)	5516(2)	6531(4)	3273(1)	55(1)
C(6)	6413(2)	8104(4)	3047(1)	63(1)
C(7)	7659(2)	7883(4)	3424(1)	62(1)
N(8)	8097(2)	6237(3)	4005(1)	57(1)
C(9)	7207(2)	4710(3)	4216(1)	46(1)
C(10)	8538(2)	1949(4)	5267(1)	57(1)
C(11)	8546(2)	2007(5)	6249(2)	74(1)
C(12)	8485(3)	4456(6)	6622(2)	103(1)

Table 2 ctd.

Compound 32

	x	y	z	U(eq)
N(1)	6600(2)	757(2)	2736(2)	64(1)
N(2)	5867(2)	327(1)	3706(2)	62(1)
C(3)	5559(2)	-578(2)	3140(3)	61(1)
C(4)	6058(2)	-769(2)	1786(3)	62(1)
C(5)	6058(3)	-1528(2)	702(3)	76(1)
C(6)	6719(3)	-1362(2)	-467(3)	85(1)
C(7)	7376(3)	-455(3)	-559(3)	80(1)
N(8)	7392(2)	298(2)	452(2)	75(1)
C(9)	6730(2)	113(2)	1583(3)	62(1)
O(1)	4851(2)	-1214(1)	3802(2)	81(1)
C(10)	8116(4)	-290(3)	-1852(4)	114(1)
C(11)	7062(3)	1777(2)	3007(3)	77(1)
C(12A)	8182(3)	1927(4)	4502(4)	80(2)
C(13A)	9482(4)	1418(5)	4365(8)	108(2)
C(12B)	8552(5)	1907(13)	3749(17)	115(6)
C(13B)	9141(16)	1355(11)	5319(14)	101(5)
C(14)	10630(4)	1592(4)	5880(6)	165(2)

Compound 37b·H_2O

	x	y	z	U(eq)
N(1)	811(4)	6630(4)	10263(3)	47(1)
N(2)	921(4)	8073(4)	9779(3)	50(1)
C(3)	2379(5)	8085(5)	9925(4)	51(1)
O(1)	2831(4)	9166(4)	9430(4)	68(1)
C(4)	3152(5)	6617(5)	10702(4)	50(1)
C(5)	4592(5)	5909(6)	11219(5)	58(1)
C(6)	4916(6)	4450(6)	11910(5)	63(1)
C(7)	3821(5)	3719(5)	12079(4)	57(1)
N(8)	2417(4)	4386(4)	11585(4)	51(1)
C(9)	2152(5)	5791(5)	10899(4)	47(1)
C(10)	8(6)	9129(5)	8680(4)	54(1)
C(11)	4177(7)	2133(6)	12799(6)	77(2)
C(12)	-718(5)	6461(5)	10960(4)	51(1)
C(13)	-1166(6)	6874(6)	12198(5)	59(1)
C(14)	-2728(6)	6688(6)	12893(6)	69(1)
C(15)	-3142(9)	7014(10)	14168(8)	108(2)
C(1')	554(5)	8743(4)	7439(4)	45(1)
C(2')	33(6)	7748(5)	7234(5)	55(1)
C(3')	568(6)	7354(6)	6121(5)	63(1)
C(4')	1608(6)	7948(5)	5204(5)	59(1)
Br	2336(1)	7404(1)	3665(1)	94(1)
C(5')	2142(6)	8947(6)	5366(5)	61(1)
C(6')	1599(5)	9332(5)	6490(5)	54(1)
OW	4183(13)	10738(14)	10298(16)	250(5)

Table 2 ctd.

Compound 41

	x	y	z	U(eq)
C(1)	-2621(4)	4060(3)	12944(1)	13(1)
N(2)	-4121(3)	3237(2)	12522(1)	14(1)
C(3)	-6205(4)	4252(3)	12423(1)	15(1)
O(1)	-7669(3)	3923(2)	12021(1)	20(1)
C(4)	-6252(4)	5838(3)	12872(1)	14(1)
C(5)	-7940(4)	7285(3)	12990(2)	19(1)
C(6)	-7385(4)	8587(3)	13416(2)	21(1)
C(7)	-5237(4)	8388(3)	13694(2)	20(1)
N(8)	-3575(3)	6979(2)	13582(1)	17(1)
C(9)	-4159(4)	5753(3)	13172(1)	14(1)
C(10)	-3338(4)	1631(3)	12097(2)	17(1)
C(11)	-1756(4)	2961(3)	13747(1)	16(1)
O(2)	-2613(3)	1836(2)	14152(1)	26(1)
C(1')	-1805(4)	1878(3)	11289(1)	14(1)
C(2')	-2608(4)	2975(3)	10581(2)	18(1)
C(3')	-1202(4)	3202(3)	9841(2)	18(1)
C(4')	1008(4)	2311(3)	9817(1)	16(1)
Br	2971(1)	2581(1)	8807(1)	21(1)
C(5')	1849(4)	1211(3)	10506(2)	18(1)
C(6')	422(4)	1015(3)	11240(2)	17(1)
O(3)	107(3)	3471(2)	13929(1)	21(1)
C(12)	1080(5)	2687(4)	14715(2)	27(1)

Compound 44d

	x	y	z	U(eq)
C(1)	6303(2)	6520(2)	2339(1)	50(1)
N(2)	7113(2)	7430(2)	2575(1)	51(1)
C(3)	7305(2)	7522(2)	3157(1)	54(1)
O(1)	7937(2)	8231(2)	3451(1)	80(1)
C(4)	6611(2)	6611(2)	3339(1)	50(1)
C(5)	6465(3)	6298(3)	3874(1)	69(1)
C(6)	5720(3)	5407(3)	3893(1)	76(1)
C(7)	5169(3)	4865(3)	3396(1)	67(1)
N(8)	5297(2)	5138(2)	2870(1)	57(1)
C(9)	6020(2)	6019(2)	2866(1)	46(1)
C(10)	7601(2)	8192(2)	2211(1)	58(1)
C(11)	6646(2)	8903(2)	1834(1)	48(1)
C(12)	6107(2)	9769(2)	2063(1)	58(1)
C(13)	5222(2)	10432(2)	1726(1)	57(1)
C(14)	4817(2)	10213(2)	1147(1)	44(1)
C(15)	5365(3)	9348(2)	917(1)	60(1)
C(16)	6272(3)	8709(2)	1254(1)	61(1)
C(17)	3855(2)	10928(2)	790(1)	42(1)
C(18)	4131(2)	12040(2)	683(1)	57(1)
C(19)	3285(3)	12750(2)	360(1)	59(1)
C(20)	2135(3)	12375(2)	138(1)	53(1)
C(21)	1834(2)	11288(2)	245(1)	46(1)
C(22)	2676(2)	10556(2)	567(1)	39(1)
C(23)	2236(2)	9422(2)	671(1)	37(1)
N(24)	2682(2)	8759(2)	1110(1)	40(1)
N(25)	1935(2)	7882(2)	1023(1)	36(1)
N(26)	1083(2)	7973(2)	550(1)	56(1)

Table 2 ctd.

N(27)	1256(2)	8954(2)	324(1)	58(1)
C(28)	2179(2)	6796(2)	1353(1)	36(1)
C(1A)	2527(2)	7040(2)	2005(1)	40(1)
C(2A)	2153(3)	6320(3)	2380(1)	71(1)
C(3A)	2530(3)	6448(4)	2967(1)	88(1)
C(4A)	3268(3)	7315(3)	3192(1)	83(1)
C(5A)	3689(3)	8017(3)	2827(1)	82(1)
C(6A)	3347(3)	7860(2)	2240(1)	63(1)
C(1B)	1014(2)	6097(2)	1179(1)	38(1)
C(2B)	-19(2)	6433(2)	1345(1)	54(1)
C(3B)	-1062(2)	5802(3)	1204(1)	64(1)
C(4B)	-1093(3)	4828(3)	894(1)	64(1)
C(5B)	-90(2)	4496(3)	720(1)	64(1)
C(6B)	959(2)	5124(2)	862(1)	51(1)
C(1C)	3244(2)	6231(2)	1169(1)	41(1)
C(2C)	3817(2)	5334(2)	1486(1)	55(1)
C(3C)	4764(3)	4791(3)	1344(2)	76(1)
C(4C)	5185(3)	5133(3)	889(2)	87(1)
C(5C)	4624(3)	6011(3)	561(2)	93(1)
C(6C)	3640(3)	6561(2)	696(1)	68(1)

Compound 47

	x	y	z	U(eq)
N(1)	2656(10)	5806(2)	1810(5)	41(1)
N(2)	1176(11)	5484(2)	2703(5)	39(1)
C(3)	1720(11)	4947(3)	2771(5)	36(2)
O(1)	353(10)	4607(2)	3607(4)	49(1)
C(4)	3684(13)	4661(2)	1959(7)	32(1)
C(5)	4204(13)	4081(3)	2030(6)	44(2)
C(6)	6084(16)	3859(3)	1168(7)	54(2)
C(7)	7354(15)	4222(3)	292(6)	48(2)
N(8)	6983(11)	4775(2)	213(5)	42(1)
C(9)	5125(12)	4995(3)	1058(6)	37(1)
C(10)	4649(13)	5611(3)	977(6)	42(2)
O(2)	5898(9)	5935(2)	246(4)	52(1)
C(11)	1825(14)	6392(2)	1734(6)	47(2)
C(12)	3069(17)	6747(3)	2908(8)	66(2)
C(13)	2220(20)	7360(3)	2877(9)	88(3)
C(14)	3230(30)	7696(4)	4047(13)	159(6)

Table 3S. Bond lengths [Å] and angles [deg] for non-hydrogen atoms **7a, 16a·H_2O**, **16c**, **30**, **32**, **37b·H_2O**, **41**, **44d**, **47**.

Compound 7a

N(1)-C(9)	1.376(9)	O(1)-C(3)-C(4)	130.8(8)
N(1)-N(2)	1.435(8)	N(2)-C(3)-C(4)	106.3(7)
N(1)-C(13)	1.457(9)	C(5)-C(4)-C(9)	117.6(8)
N(2)-C(3)	1.356(9)	C(5)-C(4)-C(3)	136.1(9)
N(2)-C(10)	1.486(8)	C(9)-C(4)-C(3)	106.3(8)
C(3)-O(1)	1.248(8)	C(6)-C(5)-C(4)	118.6(9)
C(3)-C(4)	1.440(10)	C(5)-C(6)-C(7)	118.9(9)
C(4)-C(5)	1.375(10)	N(8)-C(7)-C(6)	125.3(8)
C(4)-C(9)	1.385(9)	C(9)-N(8)-C(7)	112.0(8)
C(5)-C(6)	1.367(10)	N(8)-C(9)-N(1)	120.8(8)
C(6)-C(7)	1.398(11)	N(8)-C(9)-C(4)	127.6(8)
C(7)-N(8)	1.359(10)	N(1)-C(9)-C(4)	111.6(7)
N(8)-C(9)	1.341(9)	N(2)-C(10)-C(11)	110.7(6)
C(10)-C(11)	1.500(9)	C(10)-C(11)-C(12)	109.4(6)
C(11)-C(12)	1.548(9)	N(1)-C(13)-C(1')	114.9(6)
C(13)-C(1')	1.520(8)	N(14)-C(14)-N(17)	109.6(6)
C(14)-N(14)	1.333(8)	N(14)-C(14)-C(6")	126.1(6)
C(14)-N(17)	1.368(8)	N(17)-C(14)-C(6")	124.1(7)
C(14)-C(6")	1.480(9)	C(6')-C(1')-C(2')	117.6(6)
C(1')-C(6')	1.375(10)	C(6')-C(1')-C(13)	118.1(7)
C(1')-C(2')	1.379(9)	C(2')-C(1')-C(13)	124.3(7)
C(2')-C(3')	1.391(8)	C(1')-C(2')-C(3')	121.7(8)
C(3')-C(4')	1.384(9)	C(4')-C(3')-C(2')	120.7(7)
C(4')-C(5')	1.392(10)	C(3')-C(4')-C(5')	118.8(6)
C(4')-C(1")	1.512(8)	C(3')-C(4')-C(1")	121.1(7)
C(5')-C(6')	1.412(8)	C(5')-C(4')-C(1")	120.0(7)
C(1")-C(6")	1.353(9)	C(4')-C(5')-C(6')	119.1(8)
C(1")-C(2")	1.419(9)	C(1')-C(6')-C(5')	122.2(7)
C(2")-C(3")	1.400(9)	C(6")-C(1")-C(2")	119.1(6)
C(3")-C(4")	1.356(10)	C(6")-C(1")-C(4')	124.9(7)
C(4")-C(5")	1.405(10)	C(2")-C(1")-C(4')	116.0(7)
C(5")-C(6")	1.400(8)	C(3")-C(2")-C(1")	118.1(8)
N(14)-N(15)	1.362(8)	C(4")-C(3")-C(2")	121.8(8)
N(15)-N(16)	1.308(9)	C(3")-C(4")-C(5")	120.6(7)
N(16)-N(17)	1.360(8)	C(6")-C(5")-C(4")	117.4(8)
C(9)-N(1)-N(2)	103.9(6)	C(1")-C(6")-C(5")	123.0(7)
C(9)-N(1)-C(13)	124.5(7)	C(1")-C(6")-C(14)	123.2(6)
N(2)-N(1)-C(13)	119.7(6)	C(5")-C(6")-C(14)	113.8(7)
C(3)-N(2)-N(1)	110.9(6)	C(14)-N(14)-N(15)	105.7(6)
C(3)-N(2)-C(10)	123.0(6)	N(16)-N(15)-N(14)	110.5(7)
N(1)-N(2)-C(10)	120.9(7)	N(15)-N(16)-N(17)	108.1(6)
O(1)-C(3)-N(2)	122.9(8)	N(16)-N(17)-C(14)	106.2(6)

Compound 16a·H_2O

N(1A)-C(9A)	1.305(5)	N(2A)-C(3A)-C(4A)	104.1(3)
N(1A)-N(2A)	1.404(4)	C(5A)-C(4A)-C(9A)	120.3(3)
N(2A)-C(3A)	1.346(4)	O(1B)-C(3B)-C(4B)	131.4(3)
N(2A)-C(10A)	1.447(5)	N(2B)-C(3B)-C(4B)	103.7(3)
C(3A)-O(1A)	1.260(4)	C(5B)-C(4B)-C(9B)	120.7(3)
C(3A)-C(4A)	1.443(5)	C(5B)-C(4B)-C(3B)	135.2(3)
C(4A)-C(5A)	1.360(5)	C(9B)-C(4B)-C(3B)	104.1(3)
C(4A)-C(9A)	1.433(5)	C(4B)-C(5B)-C(6B)	117.7(4)
C(5A)-C(6A)	1.387(5)	C(7B)-C(6B)-C(5B)	120.3(4)
C(6A)-C(7A)	1.368(5)	N(8B)-C(7B)-C(6B)	122.3(4)
C(7A)-N(8A)	1.334(5)	C(7B)-N(8B)-C(9B)	119.4(3)
N(8A)-C(9A)	1.365(4)	N(1B)-C(9B)-N(8B)	126.1(3)
C(10A)-C(11A)	1.4998(11)	N(1B)-C(9B)-C(4B)	114.4(3)
C(11A)-C(12A)	1.488(6)	N(8B)-C(9B)-C(4B)	119.5(3)
N(1B)-C(9B)	1.304(5)	N(2B)-C(10B)-C(11B)	106.7(7)
N(1B)-N(2B)	1.391(4)	C(10B)-C(11B)-C(12B)	109.0(7)
N(2B)-C(3B)	1.355(4)	C(11C)-C(10C)-N(2B)	108.6(11)
N(2B)-C(10B)	1.483(8)	C(10C)-C(11C)-C(12B)	107.6(10)
N(2B)-C(10C)	1.519(9)	C(11C)-C(12B)-C(11B)	34.2(5)
C(3B)-O(1B)	1.263(4)	C(5A)-C(4A)-C(3A)	136.2(3)
C(3B)-C(4B)	1.442(5)	C(9A)-C(4A)-C(3A)	103.5(3)
C(4B)-C(5B)	1.357(5)	C(4A)-C(5A)-C(6A)	118.5(3)
C(4B)-C(9B)	1.417(5)	C(7A)-C(6A)-C(5A)	120.3(4)
C(5B)-C(6B)	1.396(5)	N(8A)-C(7A)-C(6A)	122.0(4)
C(6B)-C(7B)	1.366(5)	C(7A)-N(8A)-C(9A)	120.0(3)
C(7B)-N(8B)	1.329(5)	N(1A)-C(9A)-N(8A)	126.4(4)
N(8B)-C(9B)	1.365(4)	N(1A)-C(9A)-C(4A)	114.7(3)
C(10B)-C(11B)	1.5017(11)	N(8A)-C(9A)-C(4A)	118.9(3)
C(11B)-C(12B)	1.551(11)	N(2A)-C(10A)-C(11A)	113.2(4)
C(10C)-C(11C)	1.5017(11)	C(12A)-C(11A)-C(10A)	113.9(4)
C(11C)-C(12B)	1.509(18)	C(9B)-N(1B)-N(2B)	102.8(3)
C(9A)-N(1A)-N(2A)	102.1(3)	C(3B)-N(2B)-N(1B)	115.0(3)
C(3A)-N(2A)-N(1A)	115.6(3)	C(3B)-N(2B)-C(10B)	127.6(4)
C(3A)-N(2A)-C(10A)	126.5(3)	N(1B)-N(2B)-C(10B)	116.5(4)
N(1A)-N(2A)-C(10A)	117.9(3)	C(3B)-N(2B)-C(10C)	117.8(5)
O(1A)-C(3A)-N(2A)	125.1(3)	N(1B)-N(2B)-C(10C)	120.3(6)
O(1A)-C(3A)-C(4A)	130.8(3)	C(10B)-N(2B)-C(10C)	34.5(5)
		O(1B)-C(3B)-N(2B)	125.0(3)

Compound 16c

N(1)-C(9)	1.371(4)	C(3)-N(2)-C(10)	125.5(3)
N(1)-N(2)	1.407(4)	N(1)-N(2)-C(10)	119.4(3)
N(2)-C(3)	1.348(4)	O(1)-C(3)-N(2)	124.2(3)
N(2)-C(10)	1.466(5)	O(1)-C(3)-C(4)	131.1(3)
C(3)-O(1)	1.245(4)	N(2)-C(3)-C(4)	104.7(3)
C(3)-C(4)	1.456(5)	C(9)-C(4)-C(5)	119.0(3)
C(4)-C(9)	1.375(5)	C(9)-C(4)-C(3)	106.9(3)
C(4)-C(5)	1.387(5)	C(5)-C(4)-C(3)	134.1(3)
C(5)-C(6)	1.372(5)	C(6)-C(5)-C(4)	115.9(4)
C(6)-C(7)	1.373(5)	C(5)-C(6)-C(7)	120.7(4)
C(7)-N(8)	1.337(4)	N(8)-C(7)-C(6)	125.0(4)
N(8)-C(9)	1.339(4)	C(7)-N(8)-C(9)	113.1(3)
C(10)-C(11)	1.507(5)	N(8)-C(9)-N(1)	123.0(3)
C(11)-C(12)	1.519(5)	N(8)-C(9)-C(4)	126.3(3)
C(12)-C(13)	1.515(6)	N(1)-C(9)-C(4)	110.7(3)
C(9)-N(1)-N(2)	104.7(3)	N(2)-C(10)-C(11)	113.0(3)
C(3)-N(2)-N(1)	112.2(3)	C(10)-C(11)-C(12)	112.2(3)
		C(13)-C(12)-C(11)	112.6(4)

Compound 30

N(1)-C(9)	1.350(2)	N(2)-N(1)-C(10)	120.16(15)
N(1)-N(2)	1.386(2)	C(3)-N(2)-N(1)	106.53(15)
N(1)-C(10)	1.457(2)	N(2)-C(3)-O(1)	123.50(17)
N(2)-C(3)	1.314(2)	N(2)-C(3)-C(4)	111.75(16)
C(3)-O(1)	1.340(2)	O(1)-C(3)-C(4)	124.74(16)
C(3)-C(4)	1.412(2)	C(5)-C(4)-C(9)	118.50(17)
C(4)-C(5)	1.391(3)	C(5)-C(4)-C(3)	137.71(17)
C(4)-C(9)	1.408(2)	C(9)-C(4)-C(3)	103.79(15)
C(5)-C(6)	1.372(3)	C(6)-C(5)-C(4)	116.51(19)
C(6)-C(7)	1.395(3)	C(5)-C(6)-C(7)	120.1(2)
C(7)-N(8)	1.326(3)	N(8)-C(7)-C(6)	125.9(2)
N(8)-C(9)	1.344(2)	C(7)-N(8)-C(9)	113.22(18)
C(10)-C(11)	1.501(3)	N(8)-C(9)-N(1)	126.15(17)
C(11)-C(12)	1.484(4)	N(8)-C(9)-C(4)	125.84(17)
C(9)-N(1)-N(2)	109.90(14)	N(1)-C(9)-C(4)	108.01(15)
C(9)-N(1)-C(10)	129.68(16)	N(1)-C(10)-C(11)	113.41(17)
		C(12)-C(11)-C(10)	114.1(2)

Compound 32

N(1)-C(9)	1.349(3)	N(2)-C(3)-O(1)	122.5(2)
N(1)-N(2)	1.382(2)	N(2)-C(3)-C(4)	111.8(2)
N(1)-C(11)	1.451(3)	O(1)-C(3)-C(4)	125.7(2)
N(2)-C(3)	1.320(3)	C(5)-C(4)-C(9)	117.2(2)
C(3)-O(1)	1.338(3)	C(5)-C(4)-C(3)	138.9(2)
C(3)-C(4)	1.409(3)	C(9)-C(4)-C(3)	103.8(2)
C(4)-C(5)	1.383(3)	C(6)-C(5)-C(4)	117.4(3)
C(4)-C(9)	1.404(3)	C(5)-C(6)-C(7)	121.1(3)
C(5)-C(6)	1.364(4)	N(8)-C(7)-C(6)	123.4(2)
C(6)-C(7)	1.405(4)	N(8)-C(7)-C(10)	116.3(3)
C(7)-N(8)	1.334(4)	C(6)-C(7)-C(10)	120.3(3)
C(7)-C(10)	1.511(4)	C(7)-N(8)-C(9)	114.0(2)
N(8)-C(9)	1.341(3)	N(8)-C(9)-N(1)	125.1(2)
C(11)-C(12A)	1.5015(10)	N(8)-C(9)-C(4)	126.8(2)
C(11)-C(12B)	1.5021(10)	N(1)-C(9)-C(4)	108.08(19)
C(12A)-C(13A)	1.5242(10)	N(1)-C(11)-C(12A)	114.2(3)
C(13A)-C(14)	1.533(7)	N(1)-C(11)-C(12B)	115.5(7)
C(12B)-C(13B)	1.5247(10)	C(12A)-C(11)-C(12B)	32.0(6)
C(13B)-C(14)	1.507(16)	C(11)-C(12A)-C(13A)	111.2(3)
C(9)-N(1)-N(2)	110.11(18)	C(12A)-C(13A)-C(14)	111.0(4)
C(9)-N(1)-C(11)	129.6(2)	C(11)-C(12B)-C(13B)	116.6(9)
N(2)-N(1)-C(11)	120.22(19)	C(14)-C(13B)-C(12B)	108.6(8)
C(3)-N(2)-N(1)	106.20(18)	C(13B)-C(14)-C(13A)	37.3(4)

Compound 37b·H_2O

N(1)-C(9)	1.380(6)	N(1)-N(2)-C(10)	117.7(3)
N(1)-N(2)	1.428(5)	O(1)-C(3)-N(2)	123.3(5)
N(1)-C(12)	1.475(6)	O(1)-C(3)-C(4)	131.4(4)
N(2)-C(3)	1.379(6)	N(2)-C(3)-C(4)	105.2(4)
N(2)-C(10)	1.467(6)	C(5)-C(4)-C(9)	117.6(4)
C(3)-O(1)	1.227(5)	C(5)-C(4)-C(3)	135.0(4)
C(3)-C(4)	1.442(7)	C(9)-C(4)-C(3)	107.3(4)
C(4)-C(5)	1.383(7)	C(6)-C(5)-C(4)	117.5(4)
C(4)-C(9)	1.397(6)	C(5)-C(6)-C(7)	120.8(4)
C(5)-C(6)	1.373(8)	N(8)-C(7)-C(6)	122.7(5)
C(6)-C(7)	1.402(7)	N(8)-C(7)-C(11)	116.1(5)
C(7)-N(8)	1.343(6)	C(6)-C(7)-C(11)	121.1(5)
C(7)-C(11)	1.487(8)	C(9)-N(8)-C(7)	115.0(4)
N(8)-C(9)	1.330(6)	N(8)-C(9)-N(1)	122.9(4)
C(10)-C(1')	1.503(6)	N(8)-C(9)-C(4)	126.4(4)
C(12)-C(13)	1.514(6)	N(1)-C(9)-C(4)	110.7(4)
C(13)-C(14)	1.505(7)	N(2)-C(10)-C(1')	112.3(3)
C(14)-C(15)	1.507(8)	N(1)-C(12)-C(13)	114.1(3)
C(1')-C(6')	1.370(6)	C(14)-C(13)-C(12)	113.1(4)
C(1')-C(2')	1.387(6)	C(13)-C(14)-C(15)	113.5(5)
C(2')-C(3')	1.375(7)	C(6')-C(1')-C(2')	117.9(4)
C(3')-C(4')	1.353(7)	C(6')-C(1')-C(10)	121.5(4)
C(4')-C(5')	1.375(7)	C(2')-C(1')-C(10)	120.6(4)
C(4')-Br	1.900(5)	C(3')-C(2')-C(1')	120.9(5)
C(5')-C(6')	1.383(7)	C(4')-C(3')-C(2')	119.9(5)
C(9)-N(1)-N(2)	104.7(3)	C(3')-C(4')-C(5')	121.0(4)
C(9)-N(1)-C(12)	118.5(3)	C(3')-C(4')-Br	119.7(4)
N(2)-N(1)-C(12)	115.6(3)	C(5')-C(4')-Br	119.3(4)
C(3)-N(2)-N(1)	111.2(4)	C(4')-C(5')-C(6')	118.6(5)
C(3)-N(2)-C(10)	122.6(4)	C(1')-C(6')-C(5')	121.7(4)

Compound 41

C(1)-N(2)	1.456(3)	C(1)-N(2)-C(10)	122.77(18)
C(1)-C(9)	1.518(3)	O(1)-C(3)-N(2)	126.1(2)
C(1)-C(11)	1.528(3)	O(1)-C(3)-C(4)	128.2(2)
N(2)-C(3)	1.366(3)	N(2)-C(3)-C(4)	105.74(18)
N(2)-C(10)	1.462(3)	C(9)-C(4)-C(5)	120.0(2)
C(3)-O(1)	1.220(3)	C(9)-C(4)-C(3)	108.96(19)
C(3)-C(4)	1.487(3)	C(5)-C(4)-C(3)	130.9(2)
C(4)-C(9)	1.382(3)	C(4)-C(5)-C(6)	116.1(2)
C(4)-C(5)	1.384(3)	C(5)-C(6)-C(7)	119.8(2)
C(5)-C(6)	1.387(3)	N(8)-C(7)-C(6)	124.5(2)
C(6)-C(7)	1.388(3)	C(9)-N(8)-C(7)	114.22(19)
C(7)-N(8)	1.353(3)	N(8)-C(9)-C(4)	125.3(2)
N(8)-C(9)	1.331(3)	N(8)-C(9)-C(1)	125.43(19)
C(10)-C(1')	1.514(3)	C(4)-C(9)-C(1)	109.28(18)
C(11)-O(2)	1.197(3)	N(2)-C(10)-C(1')	113.44(18)
C(11)-O(3)	1.332(3)	O(2)-C(11)-O(3)	125.4(2)
C(1')-C(6')	1.383(3)	O(2)-C(11)-C(1)	125.9(2)
C(1')-C(2')	1.399(3)	O(3)-C(11)-C(1)	108.75(19)
C(2')-C(3')	1.387(3)	C(6')-C(1')-C(2')	118.8(2)
C(3')-C(4')	1.381(3)	C(6')-C(1')-C(10)	120.3(2)
C(4')-C(5')	1.383(3)	C(2')-C(1')-C(10)	120.9(2)
C(4')-Br	1.904(2)	C(3')-C(2')-C(1')	120.8(2)
C(5')-C(6')	1.384(3)	C(4')-C(3')-C(2')	118.5(2)
O(3)-C(12)	1.449(3)	C(3')-C(4')-C(5')	122.0(2)
N(2)-C(1)-C(9)	101.83(17)	C(3')-C(4')-Br	119.47(17)

N(2)-C(1)-C(11)	112.77(18)	C(5')-C(4')-Br	118.52(17)
C(9)-C(1)-C(11)	110.93(17)	C(4')-C(5')-C(6')	118.5(2)
C(3)-N(2)-C(1)	113.96(17)	C(1')-C(6')-C(5')	121.3(2)
C(3)-N(2)-C(10)	122.28(18)	C(11)-O(3)-C(12)	117.16(19)

Compound 44d

C(1)-N(2)	1.451(3)	C(5)-C(6)-C(7)	119.9(3)
C(1)-C(9)	1.496(3)	N(8)-C(7)-C(6)	125.2(3)
N(2)-C(3)	1.366(3)	C(9)-N(8)-C(7)	113.2(2)
N(2)-C(10)	1.453(3)	N(8)-C(9)-C(4)	125.7(2)
C(3)-O(1)	1.223(3)	N(8)-C(9)-C(1)	124.7(2)
C(3)-C(4)	1.465(4)	C(4)-C(9)-C(1)	109.6(2)
C(4)-C(9)	1.375(3)	N(2)-C(10)-C(11)	112.73(19)
C(4)-C(5)	1.382(4)	C(12)-C(11)-C(16)	117.6(2)
C(5)-C(6)	1.364(4)	C(12)-C(11)-C(10)	120.5(2)
C(6)-C(7)	1.376(4)	C(16)-C(11)-C(10)	121.9(3)
C(7)-N(8)	1.344(3)	C(11)-C(12)-C(13)	121.6(2)
N(8)-C(9)	1.334(3)	C(14)-C(13)-C(12)	120.8(3)
C(10)-C(11)	1.506(3)	C(15)-C(14)-C(13)	117.5(2)
C(11)-C(12)	1.375(4)	C(15)-C(14)-C(17)	122.3(2)
C(11)-C(16)	1.380(4)	C(13)-C(14)-C(17)	120.2(2)
C(12)-C(13)	1.387(3)	C(14)-C(15)-C(16)	121.3(2)
C(13)-C(14)	1.385(3)	C(11)-C(16)-C(15)	121.2(3)
C(14)-C(15)	1.381(3)	C(18)-C(17)-C(22)	117.7(2)
C(14)-C(17)	1.494(3)	C(18)-C(17)-C(14)	118.4(2)
C(15)-C(16)	1.385(4)	C(22)-C(17)-C(14)	123.8(2)
C(17)-C(18)	1.395(3)	C(19)-C(18)-C(17)	121.5(2)
C(17)-C(22)	1.402(3)	C(20)-C(19)-C(18)	120.3(2)
C(18)-C(19)	1.380(4)	C(19)-C(20)-C(21)	119.3(2)
C(19)-C(20)	1.373(4)	C(20)-C(21)-C(22)	121.3(2)
C(20)-C(21)	1.374(3)	C(21)-C(22)-C(17)	119.8(2)
C(21)-C(22)	1.393(3)	C(21)-C(22)-C(23)	116.4(2)
C(22)-C(23)	1.477(3)	C(17)-C(22)-C(23)	123.8(2)
C(23)-N(24)	1.322(3)	N(24)-C(23)-N(27)	111.2(2)
C(23)-N(27)	1.353(3)	N(24)-C(23)-C(22)	126.4(2)
N(24)-N(25)	1.331(2)	N(27)-C(23)-C(22)	122.4(2)
N(25)-N(26)	1.322(2)	C(23)-N(24)-N(25)	102.93(17)
N(25)-C(28)	1.505(3)	N(26)-N(25)-N(24)	112.99(17)
N(26)-N(27)	1.318(3)	N(26)-N(25)-C(28)	122.26(18)
C(28)-C(1C)	1.537(3)	N(24)-N(25)-C(28)	123.52(16)
C(28)-C(1B)	1.541(3)	N(27)-N(26)-N(25)	106.06(18)
C(28)-C(1A)	1.552(3)	N(26)-N(27)-C(23)	106.79(18)
C(1A)-C(2A)	1.378(3)	N(25)-C(28)-C(1C)	106.69(17)
C(1A)-C(6A)	1.379(3)	N(25)-C(28)-C(1B)	105.91(16)
C(2A)-C(3A)	1.384(4)	C(1C)-C(28)-C(1B)	112.13(18)
C(3A)-C(4A)	1.361(5)	N(25)-C(28)-C(1A)	110.10(17)
C(4A)-C(5A)	1.372(5)	C(1C)-C(28)-C(1A)	109.37(17)
C(5A)-C(6A)	1.388(4)	C(1B)-C(28)-C(1A)	112.42(18)
C(1B)-C(6B)	1.376(3)	C(2A)-C(1A)-C(6A)	116.9(2)
C(1B)-C(2B)	1.385(3)	C(2A)-C(1A)-C(28)	119.8(2)
C(2B)-C(3B)	1.382(4)	C(6A)-C(1A)-C(28)	122.6(2)
C(3B)-C(4B)	1.370(4)	C(1A)-C(2A)-C(3A)	121.7(3)
C(4B)-C(5B)	1.362(4)	C(4A)-C(3A)-C(2A)	120.5(3)
C(5B)-C(6B)	1.386(3)	C(3A)-C(4A)-C(5A)	118.8(3)
C(1C)-C(6C)	1.372(3)	C(4A)-C(5A)-C(6A)	120.5(3)
C(1C)-C(2C)	1.383(3)	C(1A)-C(6A)-C(5A)	121.3(3)
C(2C)-C(3C)	1.365(4)	C(6B)-C(1B)-C(2B)	117.7(2)
C(3C)-C(4C)	1.351(5)	C(6B)-C(1B)-C(28)	122.0(2)
C(4C)-C(5C)	1.373(5)	C(2B)-C(1B)-C(28)	120.3(2)

C(5C)-C(6C)	1.397(4)	C(3B)-C(2B)-C(1B)	121.0(3)
N(2)-C(1)-C(9)	101.92(19)	C(4B)-C(3B)-C(2B)	120.4(3)
C(3)-N(2)-C(1)	113.5(2)	C(5B)-C(4B)-C(3B)	119.3(3)
C(3)-N(2)-C(10)	124.7(2)	C(4B)-C(5B)-C(6B)	120.5(3)
C(1)-N(2)-C(10)	121.7(2)	C(1B)-C(6B)-C(5B)	121.1(2)
O(1)-C(3)-N(2)	125.6(3)	C(6C)-C(1C)-C(2C)	118.1(2)
O(1)-C(3)-C(4)	128.5(3)	C(6C)-C(1C)-C(28)	122.9(2)
N(2)-C(3)-C(4)	105.9(2)	C(2C)-C(1C)-C(28)	118.9(2)
C(9)-C(4)-C(5)	119.3(3)	C(3C)-C(2C)-C(1C)	121.9(3)
C(9)-C(4)-C(3)	109.1(2)	C(4C)-C(3C)-C(2C)	120.4(3)
C(5)-C(4)-C(3)	131.6(3)	C(3C)-C(4C)-C(5C)	119.1(3)
C(6)-C(5)-C(4)	116.6(3)	C(4C)-C(5C)-C(6C)	121.1(3)
		C(1C)-C(6C)-C(5C)	119.4(3)

Compound 47

N(1)-C(10)	1.379(8)	N(2)-N(1)-C(11)	113.4(5)
N(1)-N(2)	1.384(6)	C(3)-N(2)-N(1)	116.8(5)
N(1)-C(11)	1.432(7)	N(2)-C(3)-O(1)	120.2(5)
N(2)-C(3)	1.286(7)	N(2)-C(3)-C(4)	124.7(5)
C(3)-O(1)	1.342(6)	O(1)-C(3)-C(4)	115.1(5)
C(3)-C(4)	1.442(9)	C(5)-C(4)-C(9)	118.9(6)
C(4)-C(5)	1.384(7)	C(5)-C(4)-C(3)	123.8(6)
C(4)-C(9)	1.394(8)	C(9)-C(4)-C(3)	117.3(5)
C(5)-C(6)	1.379(9)	C(6)-C(5)-C(4)	117.9(6)
C(6)-C(7)	1.375(9)	C(7)-C(6)-C(5)	118.9(6)
C(7)-N(8)	1.310(7)	N(8)-C(7)-C(6)	125.5(6)
N(8)-C(9)	1.360(7)	C(7)-N(8)-C(9)	115.8(6)
C(9)-C(10)	1.463(8)	N(8)-C(9)-C(4)	123.0(6)
C(10)-O(2)	1.225(7)	N(8)-C(9)-C(10)	116.9(6)
C(11)-C(12)	1.513(9)	C(4)-C(9)-C(10)	120.1(6)
C(12)-C(13)	1.494(9)	O(2)-C(10)-N(1)	121.8(6)
C(13)-C(14)	1.447(12)	O(2)-C(10)-C(9)	123.8(6)
C(10)-N(1)-N(2)	126.8(5)	N(1)-C(10)-C(9)	114.3(6)
C(10)-N(1)-C(11)	119.8(5)	N(1)-C(11)-C(12)	112.7(6)
		C(13)-C(12)-C(11)	114.4(7)
		C(14)-C(13)-C(12)	115.0(8)

Table 4S. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **7a, 16a·H_2O**, **16c**, **30**, **32**, **37b·H_2O**, **41**, **44d**, **47**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka^*b^*U_{12}]$

Compound 7a

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	50(5)	45(4)	46(4)	12(4)	10(4)	9(4)
N(2)	49(5)	42(4)	40(4)	7(3)	14(4)	12(4)
C(3)	51(6)	50(5)	31(4)	12(4)	9(5)	16(5)
O(1)	65(4)	63(4)	36(3)	2(3)	9(3)	26(3)
C(4)	55(6)	32(4)	42(5)	7(4)	18(5)	13(4)
C(5)	75(7)	43(5)	50(5)	14(4)	30(5)	13(5)
C(6)	81(8)	43(5)	58(5)	6(5)	39(6)	20(5)
C(7)	95(8)	41(5)	51(6)	8(5)	33(7)	7(6)
N(8)	75(6)	40(4)	34(4)	8(3)	11(4)	10(4)
C(9)	53(6)	32(4)	35(4)	9(4)	12(5)	6(4)
C(10)	74(7)	49(5)	61(5)	9(4)	42(5)	13(5)
C(11)	62(6)	58(5)	66(6)	18(5)	21(5)	39(5)
C(12)	58(6)	72(6)	78(6)	-6(5)	16(6)	39(5)
C(13)	57(7)	54(5)	42(5)	14(4)	5(5)	15(5)
C(14)	44(6)	43(5)	38(4)	10(4)	13(4)	22(4)
C(1')	34(5)	45(5)	34(4)	12(4)	-3(4)	7(4)
C(2')	45(6)	42(5)	47(5)	11(4)	14(5)	13(4)
C(3')	40(6)	62(5)	52(5)	22(5)	21(5)	15(5)
C(4')	43(6)	44(5)	25(4)	-1(4)	7(4)	7(4)
C(5')	36(5)	51(5)	27(4)	0(4)	1(4)	17(4)
C(6')	48(6)	44(5)	40(5)	4(4)	14(5)	-7(4)
C(1")	56(6)	35(4)	26(4)	-2(4)	12(4)	9(4)
C(2")	68(7)	58(5)	54(5)	8(5)	32(5)	20(5)
C(3")	60(7)	74(6)	50(5)	18(5)	28(5)	5(5)
C(4")	67(7)	51(5)	56(5)	21(4)	29(5)	12(5)
C(5")	55(6)	55(5)	39(4)	8(4)	5(5)	10(5)
C(6")	48(6)	39(4)	30(4)	8(4)	14(4)	15(4)
N(14)	72(6)	83(5)	60(5)	25(4)	30(5)	42(5)
N(15)	75(7)	95(6)	85(6)	12(5)	48(6)	46(5)
N(16)	74(6)	87(6)	61(5)	18(4)	36(5)	31(5)
N(17)	64(5)	44(4)	43(4)	-1(3)	36(4)	14(4)

Compound 16a·H_2O

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
OW1	125(3)	47(2)	50(2)	5(2)	-2(2)	-5(2)
N(1A)	61(2)	44(2)	58(2)	-5(2)	-24(2)	9(2)
N(2A)	54(2)	36(2)	59(2)	-7(2)	-15(2)	9(2)
C(3A)	41(2)	40(2)	43(2)	0(2)	-7(2)	-4(2)
O(1A)	48(2)	37(2)	67(2)	-1(1)	-21(2)	5(1)
C(4A)	37(2)	39(2)	34(2)	-1(2)	-3(2)	-4(2)
C(5A)	46(2)	46(2)	46(2)	-1(2)	-7(2)	0(2)
C(6A)	58(3)	36(2)	58(3)	-8(2)	-6(2)	1(2)
C(7A)	58(3)	40(2)	59(3)	-2(2)	-6(2)	11(2)
N(8A)	52(2)	46(2)	50(2)	-1(2)	-12(2)	12(2)
C(9A)	54(2)	40(2)	43(2)	0(2)	-8(2)	5(2)
C(10A)	68(3)	47(3)	79(3)	-15(2)	-16(3)	8(2)
C(11A)	88(4)	57(3)	182(7)	-36(4)	16(5)	-7(3)
C(12A)	88(4)	62(3)	138(5)	-38(3)	1(4)	-7(3)
N(1B)	73(3)	51(2)	72(3)	12(2)	-37(2)	-8(2)
N(2B)	71(2)	40(2)	66(2)	11(2)	-30(2)	-11(2)
C(3B)	42(2)	42(2)	46(2)	-4(2)	-6(2)	-1(2)
O(1B)	57(2)	38(2)	59(2)	6(1)	-21(2)	-3(1)
C(4B)	39(2)	37(2)	38(2)	-1(2)	-1(2)	1(2)
C(5B)	47(2)	48(2)	55(3)	0(2)	-9(2)	1(2)
C(6B)	60(3)	40(2)	76(3)	1(2)	-18(3)	-2(2)
C(7B)	65(3)	45(2)	60(3)	8(2)	-9(2)	6(2)
N(8B)	49(2)	46(2)	54(2)	4(2)	-16(2)	2(2)
C(9B)	47(2)	41(2)	47(2)	1(2)	-11(2)	2(2)
C(10B)	42(5)	53(4)	58(5)	6(4)	-2(4)	-9(4)
C(11B)	109(11)	52(5)	99(7)	-13(5)	38(8)	-7(7)
C(10C)	35(8)	44(8)	66(11)	-2(8)	-8(8)	-14(7)
C(11C)	51(9)	47(9)	104(16)	-9(9)	-14(10)	-6(9)
C(12B)	108(4)	50(3)	118(5)	-18(3)	-2(4)	-12(3)

Compound 16c

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	51(2)	80(3)	34(2)	5(2)	3(2)	0(2)
N(2)	41(2)	75(3)	38(2)	4(2)	1(2)	-1(2)
C(3)	51(2)	47(3)	33(2)	-3(2)	5(2)	-2(2)
O(1)	53(2)	89(2)	39(2)	7(2)	2(1)	8(2)
C(4)	48(2)	49(3)	35(2)	-4(2)	2(2)	0(2)
C(5)	58(3)	74(4)	47(2)	13(3)	7(2)	-3(3)
C(6)	48(3)	98(4)	57(3)	9(3)	7(2)	7(3)
C(7)	49(3)	85(4)	56(3)	5(3)	0(2)	10(3)
N(8)	47(2)	70(3)	49(2)	5(2)	-1(2)	10(2)
C(9)	46(2)	49(3)	39(2)	-4(2)	1(2)	0(2)
C(10)	51(2)	72(4)	48(2)	-6(3)	4(2)	-8(3)
C(11)	46(2)	69(4)	51(3)	-4(3)	3(2)	2(2)
C(12)	49(3)	82(4)	72(3)	7(3)	7(2)	0(3)
C(13)	61(3)	120(7)	96(5)	4(4)	29(3)	14(4)

Compound 30

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	31(1)	64(1)	55(1)	3(1)	3(1)	-3(1)
N(2)	34(1)	58(1)	53(1)	2(1)	3(1)	-3(1)
C(3)	35(1)	57(1)	46(1)	-3(1)	3(1)	-1(1)
O(1)	35(1)	71(1)	74(1)	17(1)	-5(1)	-6(1)
C(4)	42(1)	53(1)	42(1)	-6(1)	6(1)	1(1)
C(5)	53(1)	62(1)	49(1)	0(1)	6(1)	4(1)
C(6)	72(2)	61(1)	56(1)	8(1)	14(1)	1(1)
C(7)	67(1)	62(1)	62(1)	0(1)	23(1)	-10(1)
N(8)	48(1)	65(1)	60(1)	-3(1)	17(1)	-9(1)
C(9)	41(1)	54(1)	44(1)	-6(1)	11(1)	-2(1)
C(10)	35(1)	65(1)	70(1)	-2(1)	-2(1)	1(1)
C(11)	48(1)	99(2)	70(2)	14(1)	-10(1)	-3(1)
C(12)	82(2)	139(3)	83(2)	-31(2)	-10(1)	14(2)

Compound 32

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	73(1)	65(1)	62(1)	4(1)	29(1)	-5(1)
N(2)	68(1)	63(1)	61(1)	4(1)	27(1)	-4(1)
C(3)	65(1)	61(1)	62(1)	2(1)	22(1)	-4(1)
C(4)	61(1)	69(2)	56(1)	0(1)	16(1)	1(1)
C(5)	78(2)	82(2)	69(2)	-12(1)	22(1)	-1(1)
C(6)	87(2)	101(2)	68(2)	-13(2)	23(2)	13(2)
C(7)	78(2)	108(2)	59(2)	5(2)	26(1)	21(2)
N(8)	74(1)	94(2)	65(1)	12(1)	31(1)	9(1)
C(9)	59(1)	77(2)	51(1)	7(1)	17(1)	9(1)
O(1)	104(1)	66(1)	86(1)	-11(1)	50(1)	-20(1)
C(10)	128(3)	144(3)	91(2)	9(2)	66(2)	20(2)
C(11)	88(2)	62(2)	95(2)	11(1)	46(2)	1(1)
C(12A)	100(3)	61(2)	90(4)	-10(3)	45(3)	-17(2)
C(13A)	98(4)	107(4)	114(5)	0(4)	19(4)	13(3)
C(12B)	136(17)	96(11)	111(12)	-4(10)	31(11)	-28(11)
C(13B)	111(11)	107(10)	86(9)	21(8)	29(8)	12(8)
C(14)	104(3)	159(4)	205(5)	-18(4)	-9(3)	-19(3)

Compound 37b·H_2O

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	47(2)	55(2)	49(2)	-21(2)	-6(2)	-20(2)
N(2)	57(2)	54(2)	50(2)	-21(2)	-4(2)	-25(2)
C(3)	58(3)	65(3)	48(2)	-33(2)	5(2)	-30(2)
O(1)	80(2)	75(2)	74(2)	-33(2)	0(2)	-44(2)
C(4)	47(2)	73(3)	46(2)	-35(2)	5(2)	-27(2)
C(5)	50(3)	87(4)	58(3)	-41(3)	-2(2)	-27(2)
C(6)	47(3)	91(4)	65(3)	-42(3)	-11(2)	-15(3)
C(7)	49(3)	75(3)	47(2)	-30(2)	-3(2)	-10(2)
N(8)	51(2)	59(2)	49(2)	-23(2)	-3(2)	-18(2)
C(9)	44(2)	68(3)	40(2)	-29(2)	1(2)	-21(2)
C(10)	58(3)	50(2)	57(3)	-25(2)	-4(2)	-13(2)
C(11)	67(3)	76(4)	74(3)	-24(3)	-14(3)	-2(3)
C(12)	45(2)	61(3)	55(2)	-24(2)	-8(2)	-19(2)
C(13)	58(3)	72(3)	60(3)	-30(2)	0(2)	-30(2)
C(14)	56(3)	83(4)	76(3)	-36(3)	4(2)	-27(3)
C(15)	100(5)	155(7)	99(5)	-77(5)	34(4)	-60(5)
C(1')	48(2)	41(2)	47(2)	-15(2)	-11(2)	-9(2)
C(2')	66(3)	56(3)	52(2)	-15(2)	-11(2)	-28(2)
C(3')	74(3)	65(3)	63(3)	-27(2)	-17(3)	-24(3)
C(4')	58(3)	64(3)	51(3)	-27(2)	-18(2)	0(2)
Br	100(1)	115(1)	70(1)	-56(1)	-14(1)	-5(1)
C(5')	55(3)	68(3)	54(3)	-16(2)	-2(2)	-19(2)
C(6')	58(3)	52(2)	59(3)	-20(2)	-7(2)	-21(2)
OW	182(9)	249(12)	389(17)	-183(12)	-57(10)	-44(8)

Compound 41

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	12(1)	18(1)	10(1)	-2(1)	-1(1)	-4(1)
N(2)	13(1)	17(1)	14(1)	-5(1)	0(1)	-3(1)
C(3)	13(1)	20(1)	11(1)	0(1)	2(1)	-5(1)
O(1)	14(1)	29(1)	21(1)	-8(1)	-3(1)	-6(1)
C(4)	14(1)	16(1)	12(1)	-1(1)	1(1)	-4(1)
C(5)	13(1)	24(1)	18(1)	-1(1)	0(1)	-2(1)
C(6)	21(1)	18(1)	20(1)	-3(1)	2(1)	1(1)
C(7)	26(1)	16(1)	18(1)	-5(1)	-1(1)	-4(1)
N(8)	18(1)	18(1)	16(1)	-4(1)	-3(1)	-4(1)
C(9)	14(1)	17(1)	10(1)	0(1)	1(1)	-3(1)
C(10)	18(1)	15(1)	17(1)	-4(1)	2(1)	-5(1)
C(11)	16(1)	17(1)	14(1)	-5(1)	0(1)	0(1)
O(2)	29(1)	26(1)	23(1)	7(1)	-8(1)	-12(1)
C(1')	19(1)	13(1)	13(1)	-5(1)	1(1)	-6(1)
C(2')	15(1)	19(1)	19(1)	-4(1)	-1(1)	-1(1)
C(3')	21(1)	18(1)	14(1)	0(1)	-1(1)	-2(1)
C(4')	19(1)	16(1)	13(1)	-3(1)	2(1)	-7(1)
Br	25(1)	20(1)	16(1)	-1(1)	6(1)	-5(1)
C(5')	15(1)	19(1)	18(1)	-3(1)	-1(1)	-1(1)
C(6')	19(1)	17(1)	14(1)	-1(1)	-2(1)	-2(1)
O(3)	17(1)	30(1)	16(1)	2(1)	-7(1)	-8(1)
C(12)	28(1)	37(2)	18(1)	2(1)	-10(1)	-6(1)

Compound 44d

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	47(2)	51(2)	50(1)	-2(1)	4(1)	-6(1)
N(2)	45(1)	50(1)	54(1)	5(1)	2(1)	-8(1)
C(3)	39(1)	56(2)	63(2)	-10(1)	4(1)	-2(1)
O(1)	65(1)	87(2)	85(1)	-28(1)	9(1)	-28(1)
C(4)	41(1)	57(2)	50(2)	-1(1)	6(1)	4(1)
C(5)	64(2)	90(2)	51(2)	-4(2)	7(1)	-1(2)
C(6)	77(2)	92(2)	61(2)	16(2)	20(2)	1(2)
C(7)	70(2)	58(2)	78(2)	16(2)	25(2)	-1(2)
N(8)	60(1)	47(1)	65(2)	2(1)	18(1)	-3(1)
C(9)	40(1)	44(1)	52(1)	1(1)	8(1)	2(1)
C(10)	38(1)	57(2)	78(2)	11(2)	12(1)	-5(1)
C(11)	32(1)	48(2)	62(2)	7(1)	9(1)	-7(1)
C(12)	44(2)	73(2)	51(2)	-6(1)	0(1)	1(2)
C(13)	44(2)	66(2)	57(2)	-10(1)	3(1)	3(1)
C(14)	38(1)	46(1)	49(1)	2(1)	11(1)	-7(1)
C(15)	68(2)	61(2)	48(2)	0(1)	10(1)	5(2)
C(16)	63(2)	58(2)	63(2)	-1(1)	16(2)	12(2)
C(17)	44(1)	43(1)	41(1)	1(1)	11(1)	-5(1)
C(18)	52(2)	50(2)	65(2)	4(1)	9(1)	-16(1)
C(19)	74(2)	40(2)	63(2)	9(1)	15(2)	-11(2)
C(20)	64(2)	43(2)	49(2)	8(1)	8(1)	-1(1)
C(21)	49(1)	44(2)	43(1)	5(1)	4(1)	-6(1)
C(22)	44(1)	39(1)	34(1)	2(1)	8(1)	-3(1)
C(23)	37(1)	39(1)	35(1)	2(1)	5(1)	-2(1)
N(24)	41(1)	37(1)	41(1)	3(1)	4(1)	-5(1)
N(25)	34(1)	36(1)	36(1)	2(1)	5(1)	-2(1)
N(26)	53(1)	49(1)	55(1)	14(1)	-10(1)	-13(1)
N(27)	56(1)	48(1)	58(1)	18(1)	-10(1)	-13(1)
C(28)	38(1)	33(1)	37(1)	5(1)	8(1)	-1(1)
C(1A)	41(1)	43(1)	37(1)	3(1)	11(1)	3(1)
C(2A)	62(2)	102(2)	49(2)	11(2)	11(1)	-22(2)
C(3A)	68(2)	149(4)	49(2)	25(2)	17(2)	-9(2)
C(4A)	89(2)	117(3)	41(2)	-5(2)	10(2)	20(2)
C(5A)	117(3)	57(2)	54(2)	-5(2)	-19(2)	2(2)
C(6A)	84(2)	51(2)	47(2)	8(1)	0(1)	-12(2)
C(1B)	40(1)	37(1)	37(1)	6(1)	8(1)	-2(1)
C(2B)	47(2)	50(2)	68(2)	-4(1)	20(1)	-6(1)
C(3B)	43(2)	72(2)	80(2)	4(2)	20(1)	-5(2)
C(4B)	47(2)	63(2)	77(2)	5(2)	6(2)	-19(2)
C(5B)	57(2)	56(2)	75(2)	-13(2)	5(2)	-13(2)
C(6B)	42(1)	51(2)	58(2)	-5(1)	10(1)	-3(1)
C(1C)	37(1)	40(1)	45(1)	-7(1)	9(1)	-5(1)
C(2C)	54(2)	56(2)	49(1)	-12(1)	-2(1)	11(1)
C(3C)	54(2)	78(2)	83(2)	-36(2)	-12(2)	24(2)
C(4C)	51(2)	81(3)	133(3)	-53(2)	28(2)	0(2)
C(5C)	101(3)	79(2)	123(3)	-24(2)	78(2)	-17(2)
C(6C)	82(2)	53(2)	84(2)	2(2)	51(2)	6(2)

Compound 47

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	44(3)	40(3)	39(3)	1(3)	9(3)	1(3)
N(2)	42(3)	47(3)	29(3)	4(2)	7(2)	2(3)
C(3)	33(4)	52(4)	23(3)	2(3)	8(3)	-8(3)
O(1)	44(3)	57(2)	47(2)	2(2)	23(2)	2(2)
C(4)	27(4)	44(3)	25(2)	-1(3)	1(3)	1(3)
C(5)	47(5)	48(3)	36(3)	2(3)	8(3)	-7(3)
C(6)	57(5)	51(4)	55(4)	-1(3)	15(4)	6(4)
C(7)	46(4)	56(4)	44(3)	-5(3)	21(3)	8(4)
N(8)	37(3)	56(3)	35(3)	-4(2)	11(3)	-1(3)
C(9)	29(3)	49(3)	34(3)	-5(3)	5(3)	-4(3)
C(10)	34(4)	55(4)	38(4)	2(3)	3(3)	-11(4)
O(2)	51(3)	52(2)	56(3)	8(2)	18(2)	-5(2)
C(11)	52(4)	46(3)	42(3)	-1(3)	6(3)	11(3)
C(12)	68(5)	59(4)	69(4)	-7(3)	-1(4)	3(4)
C(13)	125(8)	47(4)	91(5)	-9(4)	-19(5)	10(5)
C(14)	214(16)	100(8)	156(10)	-60(7)	-55(11)	31(9)

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Analytical Data

compd	Formula	C Calcd Found	H	N
7a	$C_{23}H_{21}N_7O$	67.14	5.14	23.83
		67.22	5.11	23.78
7b	$C_{24}H_{23}N_7O \cdot 0.33\ H_2O$	66.80	5.53	22.72
		66.87	5.28	22.40
7c	$C_{24}H_{23}N_7O \cdot 0.33\ H_2O$	66.80	5.53	22.72
		66.72	5.42	23.04
7d	$C_{25}H_{25}N_7O \cdot 0.33\ H_2O$	67.40	5.81	22.01
		67.48	5.70	21.66
7e	$C_{25}H_{25}N_7O$	68.32	5.73	22.31
		68.06	5.77	21.97
7f	$C_{27}H_{21}N_7O$	70.57	4.61	21.34
		70.42	4.58	21.22
7g	$C_{23}H_{21}N_7O$	67.14	5.14	23.83
		67.32	5.05	23.53
7h	$C_{24}H_{23}N_7O \cdot H_2O$	65.00	5.68	22.11
		64.95	5.51	21.98
7i	$C_{25}H_{25}N_7O$	68.32	5.73	22.31
		68.48	5.79	22.17
7j	$C_{24}H_{22}ClN_7O \cdot 0.33\ H_2O$	61.87	4.90	21.04
		61.95	4.69	20.87
7k	$C_{24}H_{21}ClFN_7O$	60.31	4.43	20.52
		59.98	4.37	20.70
7l	$C_{24}H_{22}FN_7O \cdot 0.5\ H_2O$	63.71	5.12	21.67
		63.55	4.83	21.38
7m	$C_{24}H_{22}ClN_7O$	62.67	4.82	21.32
		62.46	4.58	21.65
7n	$C_{25}H_{25}N_7O_2 \cdot H_2O$	63.41	5.75	20.71
		63.59	5.56	20.47

7o	$C_{25}H_{26}N_8O \cdot H_2O$	63.54	5.97	23.71
		63.68	5.79	23.58
7p	$C_{28}H_{30}N_8O_2 \cdot 0.5\ H_2O$	64.72	6.01	21.57
		64.60	6.04	21.75
7q	$C_{24}H_{22}N_6O$	70.23	5.40	20.47
		70.37	5.48	20.38
8a	$C_{24}H_{23}N_7O \cdot 0.33\ H_2O$	66.80	5.53	22.72
		66.87	5.41	22.32
8b	$C_{25}H_{25}N_7O$	68.32	5.73	22.31
		68.21	5.67	22.25
8c	$C_{24}H_{22}ClN_7O$	62.67	4.82	21.32
		62.43	4.84	21.31
8d	$C_{21}H_{16}N_6O$	68.47	4.38	22.81
		68.19	4.26	22.63
8e	$C_{23}H_{20}N_6O$	69.68	5.08	21.20
		69.52	5.11	20.98
8f	$C_{24}H_{22}N_6O \cdot H_2O$	67.27	5.65	19.61
		66.89	5.49	19.37
8g	$C_{25}H_{24}N_6O$	70.73	5.70	19.80
		70.68	5.91	19.44
35a	$C_{23}H_{21}N_7O \cdot 0.33\ H_2O$	66.17	5.23	23.49
		66.25	5.13	23.31
35b	$C_{24}H_{23}N_7O$	67.75	5.45	23.04
		67.63	5.33	23.01
18	$C_{25}H_{24}N_6O \cdot 0.33\ H_2O$	69.75	5.78	19.52
		69.65	5.56	19.16
45	$C_{25}H_{23}N_7O_2$	66.21	5.11	21.62
		66.32	5.13	21.53