(major [E] isomer; 400 MHz, DMSO- d_6) δ 8.09 (s, 1H), 7.94 (s, 1H), 7.18 (m, 3H), 4.96 (s, 2H), 3.75 (s, 2H), 3.31 (t, 2H, J = 6.2 Hz), 3.02 (m, 2H), 1.33 (s, 9H).

¹H NMR (minor [Z] isomer; 400 MHz, DMSO- d_6): δ 8.09 (s, 1H), 7.95 (s, 1H), 7.15 (m, 3H), 5.05 (s, 2H), 3.61 (s, 2H), 3.45 (m, 2H), 3.18 (m, 2H), 1.38 (s, 9H).

 ^{13}C NMR (starred peaks are due to the minor isomer; DMSO-d₆): δ 172.3*, 171.7, 167.3, 165.7*, 155.9, 155.7, 152.4, 149.9, 141.9, 118.1, 78.0*, 77.5, 56.0*, 52.6, 50.3*, 47.5, 43.8, 37.7, 28.3. Anal. Calcd for $C_{16}H_{22}N_{7}O_{5}Na\cdot H_{2}O$: C, 44.34; H, 5.58; N 22.63; Na, 5.30. Found: C, 44.31; H, 5.62; N 22.41; Na, 5.32.

1-(Boc-Aeg)cytosine, Sodium Salt (11). A mixture of 7 (7.66 g, 19 mmol) and 1 N NaOH (40 mL) was stirred at room temperature until all starting material was consumed (TLC: eluent EtOAc). The reaction mixture was washed with CH_2Cl_2 (30 mL). The aqueous layer was neutralized with 1 N HCl to pH 6 and concentrated to dryness. The residue was triturated with MeOH/EtOH and filtered. The filtrate was concentrated to a small volume on a rotary evaporator and left in a refrigerator overnight. The precipitated white solid was filtered, washed with EtOH and ether, and dried in a vacuum oven at 50 °C to afford 3.16 g (45%) of 11 as an off-white solid: mp 237 °C dec; R_f 0.3 (nBuOH/H₂O/AcOH 3:1:1); ¹H NMR (major [E] isomer; 400 MHz, DMSO- d_6) δ 7.33 (d, 1H, J = 7.2 Hz), 7.13 (m, 1H), 6.98 (bs, 2H), 5.64 (d, 1H, J = 7.2 Hz), 4.39 (s, 2H), 3.64 (s, 2H), 3.27 (t, 2H, J = 6.3 Hz), 3.00 (m, 2H), 1.34 (s, 9H).

¹H NMR (minor [Z] isomer; 400 MHz, DMSO- d_6): δ 7.35 (d, 1H, J = 7.2 Hz), 7.26 (m, 1H), 7.05 (bs, 2H), 5.66 (d, 1H, J = 7.2

Hz), 4.51 (s, 2H), 3.59 (s, 2H), 3.34 (t, 2H, J=6.3 Hz), 3.13 (m, 2H), 1.36 (s, 9H). Anal. Calcd for $C_{15}H_{22}N_5O_6Na\cdot0.75H_2O$: C, 44.49; H, 5.85; N 17.30; Na, 5.68. Found: C, 44.63; H, 5.81; N 17.23; Na, 5.51.

9-(Boc-Aeg)guanine (12). A mixture of **8** (2.35 g, 5.15 mmol) and 2.5 N NaOH (25 mL) was stirred at room temperature for 48 h. The yellow solution was neutralized with 4 N HCl and concentrated to dryness. The residue was purified by flash chromatography over Bakerbond Octadecyl (H₂O, 20% MeOH/H₂O) to afford 0.81 g (36%) of **12** as an off white solid: mp 280 °C dec; ¹H NMR (major [E] isomer; 400 MHz, DMSO- d_6): 11.25 (bs, 1H), 7.49 (s, 1H), 7.03 (m, 1H), 6.87 (s, 2H), 4.77 (s, 2H), 3.79 (s, 2H), 3.32 (t, 2H, d_6) = 6.4 Hz), 3.05 (m, 2H), 1.35 (s, 9H). ¹H NMR (minor [d_6] isomer; 400 MHz, DMSO- d_6): 11.25 (bs, 1H), 7.75 (s, 1H), 7.16 (m, 1H), 6.94 (s, 2H), 4.90 (s, 2H), 3.75 (s, 2H), 3.445 (m, 2H), 3.20 (m, 2H), 1.37 (s, 9H). Anal. Calcd for C₁₆H₂₂N₇O₆Na: C, 43.63; H, 5.26; N, 22.27; Na 5.22. Found: C, 43.60; H, 5.21; N, 22.23; Na 5.15.

Acknowledgment. The authors would like to thank Drs. Howard Sard and Michael Singer for discussions of the NMR work and Dr. Andrea Cochran for discussion of PNA synthesis. This work was funded under a contract to The Whitehead Institute (NIH P50-HG00098), Cambridge, Massachusetts.

JO9412488

Additions and Corrections

Vol. 59, 1994

Ranjit C. Desai,* Dennis J. Hlasta, George Monsour, and Manohar Saindane. An Efficient Large Scale Synthesis of 4-Isopropyl- and 4-Isopropyl-6-methoxybenzisothiazolones.

Page 7162, Scheme 2. Structure 5 should be drawn as follows:

JO944016H