

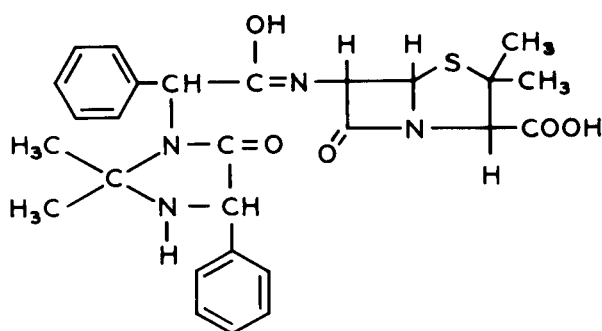
6-[2-(5-Oxo-4-phenyl-2,2-dimethyl-1-imidazolidinyl)-2-phenyl-1-hydroxyethylimino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic Acid.

Naseem Muhammad and David L. Mays

Control Division, Bristol Laboratories, Division of Bristol-Myers Company,  
Syracuse, New York 13201

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In connection with our analytical work with antibiotics of the penicillin family, we have prepared the compound of structure 1, which is structurally related to the antibiotic hetacillin (1). A limited MIC spectrum *vs.* a total of 18 gram positive and gram negative organisms indicates that the compound has little or no bioactivity.



EXPERIMENTAL

The melting point (uncorrected) was taken by capillary method using a Mettler FPI automatic melting point apparatus. The uv absorption spectrum was measured with a Cary Model 14 spectrophotometer and expressed as  $\lambda$  max (solvent) nm ( $\epsilon$ ). The ir spectrum was obtained by means of a Perkin Elmer 221 spectrophotometer. The nmr spectrum was obtained by means of a Varian HR-100 spectrometer with tetramethylsilane as the internal standard; s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet. The mass spectrum was obtained by means of the LKB9000 spectrometer.

6-[2-(5-Oxo-4-phenyl-2,2-dimethyl-1-imidazolidinyl)-2-phenyl-1-hydroxyethylimino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic Acid.

To a slurry of 0.5 g. (0.001 mole) of 6-[2-(2-amino-2-phenylacetamido)-2-phenylacetamido]penicillanic acid in 2.5 ml. of acetone was added 0.35 ml. of triethylamine. The mixture was stirred for 20 hours at room temperature. The clear light yellow solution was added slowly to 2.5 ml. of water maintained at 0-5° and at pH 2.5-3.0 by simultaneous addition of 0.1 N sulfuric acid. The slurry was stirred for 4 hours at pH 2.5-3.0. The solid crystalline compound was filtered, washed with cold acetone, dried at 40° to produce 1, 0.325 g. (60%), m.p. 173.6°; uv (95% ethanol + 0.2% TEA) 308 (341); ir (potassium bromide): 1770 ( $\beta$ -lactam), 1720 (COOH), 1680 ( $\gamma$ -lactam C=O), 695  $\text{cm}^{-1}$  ( $\text{C}_6\text{H}_5$ ); nmr (DMSO- $d_6$ ):  $\delta$  8.86 (1H, d, J = 4 Hz, imidazole-3-NH), 7.40 (10H, m, aromatic H), 5.40 (1H, d,  $\text{C}_6$ -H), 5.32 (1H, d, J = 4 Hz, imidazole-4-CH), 4.76 (1H, s,  $\text{C}_2$ -H), 4.70 (1H, s, -CH-C-), 4.58 (1H, d,  $\text{C}_5$ -H), 1.55 (3H, s, - $\text{CH}_3$ ), 1.52 (3H, s, - $\text{CH}_3$ ), 1.46 (6H, s, - $\text{CH}_3$ ) ppm; on addition of deuterium oxide to the sample solution in DMSO- $d_6$  the signal at  $\delta$  8.86 disappeared and the signal at  $\delta$  5.32 changed to singlet; mass spectrum: (70 ev) *m/e* (rel. intensity) 536 (0.25, parent ion), 534 (0.2), 460 (9), 445 (9), 306 (12), 247 (70), 230 (20), 173 (25), 146 (25), 118 (30), 115 (75), 114 (40), 106 (60), 100 (100).

*Anal.* Calcd. for  $\text{C}_{27}\text{H}_{30}\text{N}_4\text{O}_5\text{S}\cdot\text{H}_2\text{O}$ : C, 59.97; H, 5.97; N, 10.36. Found: C, 60.01; H, 6.09; N, 10.38.

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REFERENCES

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