

2-Chloro-3-hydroxy-6-hydroxymethyl-pyridine. A solution of 2-chloro-3-pyridinol (**1**) (20.0 g, 0.154 mol) and NaHCO₃ (19.5 g, 0.232 mol) in 150 mL of H₂O was stirred at rt for several minutes and heated to 90° C. After 5 minutes at 90° C, the first of 6 unequal doses of 37% formaldehyde (40.5 mL, 0.541 mol, 3.5eq.) was added; 12 mL initially, 3 x 8 mL followed by 1 x 2.2 mL all at 90 minute intervals with the final 2.3 mL added after maintaining at 90° C overnight (15 h). The reaction mixture was heated for an additional 4 h after the last dosing. The mixture was cooled to 0° C and 100 mL of crushed ice was added followed by 39 mL of 6 N HCl (to pH 1). The precipitated slurry was stirred for 1.5 h at 0° C. The undesired precipitated side product was filtered off and washed once with 75 mL of ice water. The yellow filtrate was extracted seven times with EtOAc. The organic extracts were dried with anhydrous Na₂SO₄ and concentrated. Toluene was added and the mixture was reconcentrated to azeotrope any remaining water. The addition of CH₂Cl₂ to suspend the material followed by reconcentration afforded the title compound as a pale yellow solid (19.93 g, 81 %). Mp: 133.5-135.0°C; ¹H NMR (d₆ DMSO): δ 10.47 (brs, 1H), 7.38-7.19 (m, 2H), 5.33 (brs, 1H), 4.38 (s, 2H); ¹³C NMR (d₆ DMSO): δ 63.7, 121.2, 124.9, 137.0, 148.5, 152.5; UV (λ max, ethanol): 225 (7680), 288 (5930) nm; IR 1299, 1194, 2925, 2956, 3055, 1562, 3038, 1008, 2896, 1317, 2855, 1092, 1224, 847, 2872, 1489, 690, 2820, 2765, 2720, 1418, 1280, 2613, 1140, 633 cm⁻¹. MS: M/Z (relative intensity %): 159 (41), 158 (42), 132 (31), 130 (100), 94 (34); Anal: Calcd for C₆H₆ClNO₂: C, 45.16; H, 3.79; N, 8.78. Found: C, 44.88; H, 3.76; N, 8.57.

2-Chloro-3-hydroxy-6-hydroxymethyl-4-iodo-pyridine (2). A mixture of 2-chloro-3-hydroxy-6-hydroxymethyl-pyridine (11.6 g, 72.7 mmol) and NaHCO₃ (18.3 g, 218 mmol) in 200 mL of H₂O was stirred until homogeneous, cooled to 0°C, and was treated with I₂ (19.4 g, 76.3 mmol). The reaction was stirred over the weekend as the cooling bath expired. The pH of the mixture was adjusted to 3 with 2N NaHSO₃ and the mixture was extracted with 4 x 50 mL of EtOAc. The combined organics were dried over anhydrous MgSO₄ and were concentrated *in vacuo* to a yellow solid. The crude solid was washed with EtOAc to provide 12.9 g (62%) of **2** as an off-white solid. The filtrate was concentrated to a small volume and was chromatographed over 250 g of silica gel (230–400 mesh) eluting with EtOAc/CH₂Cl₂/hexane/HOAc 2.5:4.5:4:0.1 to afford an additional 2.4 g (12%) of pure **2**. Mp 147–149 °C; ¹H NMR (d₆DMSO): δ 4.38 (s, 2H), 7.73 (s, 1H), 10.35 (s, 1H); IR: 3156, 2925, 1541, 1455, 1361, 1248, 1239, 1015, 875 cm⁻¹; MS, [M/Z](Relative Intensity): [285](80). Anal: Calcd for C₆H₅ClINO₂: C, 25.25; H, 1.77; N, 4.91. Found: C, 25.06 H, 1.81; N, 4.92.

2-Chloro-3-hydroxy-6-hydroxymethyl-4-trimethylsilylethynyl-pyridine (3). A mixture of 2-chloro-3-hydroxy-6-hydroxymethyl-4-iodo-pyridine (**2**) (13.9 g, 48.6 mmol), trimethylsilylacetylene (9.6 mL, 68 mmol), bis(triphenylphosphine) palladium dichloride (1.02 g, 1.46 mmol) and CuI (139 mg, 0.73 mmol) in 80 mL of chloroform and 40 mL of THF under N₂ was treated with Et₃N (21 mL, 151 mmol) and was stirred for 3 h at rt. The reaction was diluted with 200 mL of CHCl₃ and was washed with 2 x 150 mL of 5% HCl. The combined aqueous layers were extracted with 2 x 50 mL of CHCl₃ and the combined

organics were washed with 100 mL of 50% saturated NaCl, dried over anhydrous MgSO_4 , and were concentrated *in vacuo* to an amber oil. The crude material was chromatographed over 350 g of silica gel (230-400 mesh), eluting with 35% EtOAc/hexane to afford 11.4 g (92%) of **3** as a golden solid. Mp: 97-98 °C; ^1H NMR (d_6 DMSO): δ 0.28 (s, 9H), 4.63 (s, 2H), 7.24 (s, 1H); ^{13}C NMR (d_6 DMSO): δ -0.4, 63.8, 96.1, 107.4, 119.7, 122.4, 137.4, 147.8, 150.8; IR: 3151, 2924, 1602, 1464, 1423, 1376, 1347, 1301, 1246, 1196, 962, 846 cm^{-1} ; MS: [M/Z](Relative Intensity): [255](25). Anal: Calcd for $\text{C}_{11}\text{H}_{14}\text{ClNO}_2\text{Si}$: C, 51.66; H, 5.52; N, 5.48. Found: C, 51.39; H, 5.41; N, 5.37.

7-Chloro-5-hydroxymethyl-furo[2,3-c]pyridine (4). A mixture of 2-chloro-3-hydroxy-6-hydroxymethyl-4-trimethylsilylethynyl-pyridine (**3**) (11.4 g, 44.6 mmol) was combined with CuI (424 mg, 2.23 mmol) in 60 mL of EtOH and 60 mL of Et_3N and warmed to 75°C for 3 h. The reaction mixture was treated with DARCO, diluted with 60 mL of MeOH and was refluxed for 20 min. The mixture was cooled and filtered through celite. The filtrate was treated with 25 mL of saturated NaHCO_3 and 25 mL of 2N NaOH (50 mmol) and stirred overnight at rt. The volatiles were removed *in vacuo* and the residue was partitioned between 250 mL of 50% saturated NaCl and 4 x 75 mL of CH_2Cl_2 . The combined organics were dried over anhydrous K_2CO_3 and were concentrated *in vacuo* to give a crude tan solid. The crude material was chromatographed over 300 g of silica gel (230-400 mesh) eluting with 40% EtOAc/hexane to afford 6.6 g (80%) of **4** as a white solid. Mp: 102-103 °C; ^1H NMR (CDCl_3): δ 3.37 (bs, 1H), 4.79 (s, 2H), 6.82 (d, $J = 2$ Hz, 1H), 7.51 (s, 1H), 7.79 (d, $J = 2$ Hz, 1H); ^{13}C NMR (CDCl_3): δ 64.6, 107.1, 112.5, 133.1, 136.8, 146.9, 149.3, 153.1; IR: 3312,

3099, 2924, 1611, 1572, 1444, 1365, 1304, 1206, 1143, 1062, 870 cm^{-1} ; MS: [M/Z](Relative Intensity): [183](53). Anal: Calcd for $\text{C}_8\text{H}_5\text{ClNO}_2$: C, 52.34; H, 3.29; N, 7.63. Found: C, 52.27; H, 3.23; N, 7.57.

7-Chloro-5-formyl-furo[2,3-c]pyridine (5). A solution of oxalyl chloride (831 μL , 9.5 mmol) in 30 mL of CH_2Cl_2 under N_2 at -60°C was treated with DMSO (1.34 mL, 18.9 mmol) in 5 mL of CH_2Cl_2 and stirred for 20 min. The solution was treated with **4** (1.5 g, 8.2 mmol) in 2 x 5 mL of CH_2Cl_2 at -60°C , was stirred for 20 min, and was treated with Et_3N (5.83 mL, 41.8 mmol). The reaction was diluted with 50 mL of CH_2Cl_2 and was washed with 100 mL of 1:1 saturated NaCl / 5% HCl. The organics were dried over anhydrous MgSO_4 and concentrated *in vacuo* to give 1.5 g of a crude off-white solid. The crude material was chromatographed over 60 g of silica gel (230-400 mesh), eluting with 25% EtOAc/hexane to provide 1.42 g (95%) of **5**. Mp: $140\text{--}142^\circ\text{C}$; ^1H NMR (CDCl_3): δ 7.03 (d, $J = 2$ Hz, 1H), 7.92 (d, $J = 2$ Hz, 1H), 8.23 (s, 1H), 10.09 (s, 1H); ^{13}C NMR (CDCl_3): δ 108.2, 115.2, 134.8, 136.2, 146.9, 150.0, 150.0, 191.3; IR: 2924, 1713, 14007, 1306, 1126, 1119, 1020, 869, 786 cm^{-1} ; MS: [M/Z](Relative Intensity): [181](47). Anal: Calcd for $\text{C}_8\text{H}_4\text{ClNO}_2$: C, 52.92; H, 2.22; N, 7.71. Found: C, 52.72; H, 2.37; N, 7.63.

7-Chloro-5-(1-hydroxyethyl)-furo[2,3-c]pyridine (6). A solution of **5** (6.47 g, 35.6 mmol) in 105 mL of THF and 155 mL of Et_2O under N_2 was treated dropwise with methyl magnesium bromide (18 mL, 53.4 mmol, 3M in Et_2O) at rt and was warmed to reflux for 2 h. The reaction was cooled to 0°C and was quenched with 150 mL of 5% HCl. The aqueous layer was washed with 2 x 50 mL of CH_2Cl_2 and the combined organics were dried over

anhydrous MgSO_4 . The organics were concentrated *in vacuo*. The yellow oil was chromatographed over 300 g of silica gel (230–400 mesh), eluting with 50% EtOAc/hexane, to afford 5.65 g (80%) of **6**. Mp: 71–73 °C; ^1H NMR (CDCl_3): δ 1.56 (d, J = 6.5 Hz, 3H), 4.96 (q, J = 6.5 Hz, 1H), 6.84 (d, J = 2 Hz, 1H), 7.51 (s, 1H), 7.81 (d, J = 2 Hz, 1H); ^{13}C NMR (CDCl_3): δ 24.4, 69.5, 107.2, 111.3, 132.8, 136.8, 146.8, 149.2, 157.3; IR: 3205, 2925, 1611, 1572, 1445, 1342, 1122, 1034, 985 cm^{-1} . MS: $[\text{M}/\text{Z}]$ (relative intensity): [197](3); Anal: Calcd for $\text{C}_9\text{H}_8\text{ClNO}_2$: C, 54.70; H, 4.08; N, 7.09. Found: C, 54.46; H, 4.01; N, 7.04.

5-(1-Hydroxyethyl)-furo[2,3-c]pyridine (7). A solution of **6** (3.95 g, 20 mmol) in 110 mL of MeOH containing 20% $\text{Pd}(\text{OH})_2$ on carbon (1 g) under N_2 was treated with cyclohexene (19.8 mL, 200 mmol) followed by 2N NaOH (15 mL, 30 mmol) and the reaction was refluxed for 3.5 h. The mixture was cooled, filtered through celite, and the filter cake was washed well with fresh MeOH. The filtrate was concentrated *in vacuo* to a yellow paste. The residue was partitioned between 50 mL of water and 4 x 25 mL of CH_2Cl_2 and the organics were dried over K_2CO_3 and were concentrated *in vacuo* to a pale oil (3.16 g). The crude material was chromatographed over 125 g of silica gel (230–400 mesh), eluting with 60% EtOAc/hexane to give 2.52 g (77%) of **7** as a pale oil. ^1H NMR (CDCl_3 , TMS): δ 1.55 (d, J = 6.5 Hz, 3H), 4.19 (bs, 1H), 5.01 (q, J = 6.5 Hz, 1H), 6.78 (d, J = 2 Hz, 1H), 7.56 (s, 1H), 7.76 (d, J = 2 Hz, 1H), 8.76 (s, 1H); ^{13}C NMR (CDCl_3): δ 24.7, 69.6, 106.1, 111.8, 132.0, 135.0, 148.8, 151.4, 156.5; IR: 3355, 2973, 1614, 1465, 1280, 1130, 1096, 1034, 880 cm^{-1} . HRMS: Calcd for $\text{C}_9\text{H}_9\text{NO}_2$: 163.0633. Found: 163.0646.

7-(1-Chloroethyl)-furo[2,3-c]pyridine (8). A solution of **7** (450 mg, 2.76 mmol) in 6 mL of CH₂Cl₂ under N₂ at 0 °C was treated with thionyl chloride (300 µl, 4.14 mmol) in 2 mL of CH₂Cl₂ and the reaction was stirred for 20 min at 0 °C and for 1 h at rt. The reaction was quenched with 10 mL of saturated NaHCO₃ and the aqueous layer was extracted with 3 x 10 mL of CH₂Cl₂. The combined organics were dried over K₂CO₃ and were concentrated *in vacuo* to give 478 mg (96%) of **8** as a colorless oil. ¹H-NMR (CDCl₃): δ 1.94 (d, *J* = 6.5 Hz, 3H), 5.30 (q, *J* = 6.5 Hz, 1H), 6.81 (d, *J* = 2 Hz, 1H), 7.73 (s, 1H), 7.78 (d, *J* = 2 Hz, 1H), 8.84 (s, 1H); ¹³C-NMR (CDCl₃): δ 25.4, 59.3, 106.3, 113.6, 133.0, 134.9, 148.8, 151.5, 153.8; IR: 2980, 1610, 1462, 1303, 1127, 1033, 760 cm⁻¹; MS: [M/Z](relative intensity): [181](4). Anal: Calcd for C₉H₈ClNO: C, 59.32; H, 4.46; N, 7.69 @ 0.34% water found. Found: C, 59.05; H, 4.39; N, 7.58.

4-Amino-6-chloro-2-(1-(furo[2,3-c]pyridin-5-yl)ethyl)thiopyrimidine (10). A solution of 4-amino-6-chloro-2-thiopyrimidine, mesylate salt (**9**) (602 mg, 2.3 mmol) in 4 mL of dry DMF under N₂ at 0 °C was treated with NaH (186 mg, 4.66 mmol, 60% in oil) and the mixture was stirred for 1 h at rt. A solution of **8** (424 mg, 2.3 mmol) in 2 x 1 mL of dry DMF was added to the reaction and the mixture was stirred overnight at rt. The mixture was diluted with 50 mL of Et₂O and the organic layer was washed with 4 x 25 mL of 50% saturated NaCl. The organics were dried over K₂CO₃ and were concentrated *in vacuo* to a yellow oil. The crude material was chromatographed over 30 g of silica gel (230-400 mesh), eluting with 50% EtOAc/hexane to afford a 509 mg of a pale foam. Crystallization from Et₂O provided 432 mg (60%) of **10** as a white solid. Mp: 187-188 °C; ¹H-NMR (d₆ DMSO):

δ 1.66 (d, J = 6.5 Hz, 3H), 5.08 (q, J = 6.5 Hz, 1H), 6.11 (s, 1H), 6.96 (d, J = 2 Hz, 1H), 7.29 (bs, 2H), 7.74 (s, 1H), 8.16 (d, J = 2 Hz, 1H), 8.84 (s, 1H); ^{13}C -NMR (d_6 DMSO): δ 21.9, 44.9, 98.6; 106.3, 114.2, 132.9, 134.3, 149.8, 150.7, 153.7, 157.4, 164.2, 170.4; UV (λ max, EtOH): 231 (26,000); 248 (18,900); 281 (10,200); 287 (10,300); 296 (6,340); IR: 3453, 2925, 1640, 1567, 1532, 1467, 1370, 1284, 821 cm^{-1} ; MS: $[\text{M}/\text{Z}]$ (relative intensity): [306](8). Anal: Calcd for $\text{C}_{13}\text{H}_{11}\text{ClN}_4\text{OS}$: C, 50.90; H, 3.61; N, 18.26. Found: C, 50.82; H, 3.66; N, 18.28.

Resolution of 4-Amino-6-chloro-2-(1-(furo[2,3-*c*]pyridin-5-yl)ethyl)thiopyrimidine (10).

A 200 mg sample of **10** was resolved over a Chiralcel OD-H column, eluting with 20% isopropanol/hexane at a flow rate of 0.5 mL/min. Two pools of material were isolated with retention times of 15.6 min (74 mg, 100% ee) and 26.1 min (97 mg, 98.6% ee) respectively. The column isolates were individually chromatographed over 10 g of silica gel (230-400 mesh), eluting with 45% EtOAc/hexane to afford yellow oils. Crystallization of each from hexane/Et₂O afforded 55 mg (pool A) and 59 mg (pool B) of the (-)- and (+)-enantiomers, respectively, as white solids. Pool A, (-)-enantiomer **PNU-142721**: Optical Rotation: $[\alpha]_{\text{D}} = -301.8^\circ$ (c = 0.55, CHCl_3); Mp: 144-145 $^\circ\text{C}$; ^1H NMR (d_6 DMSO): δ 1.70 (d, J = 7 Hz, 3H), 5.11 (q, J = 7 Hz, 1H), 6.15 (s, 1H), 7.00 (d, J = 1.5 Hz, 1H), 7.30 (bs, 2H), 7.79 (s, 1H), 8.20 (d, J = 2.0 Hz, 1H), 8.88 (s, 1H); IR: 3314, 3211, 2925, 1612, 1566, 1531, 1463, 1370, 1283, 1119, 828 cm^{-1} ; MS: Calcd for $\text{C}_{13}\text{H}_{11}\text{N}_4\text{OS}$: 306.0342. Found: 306.0342. Recrystallization from EtOAc provides an analytically pure sample: Calcd for $\text{C}_{13}\text{H}_{11}\text{N}_4\text{OS}$: C, 50.90; H, 3.61; N, 18.26. Found: C, 50.89; H, 3.72; N, 18.11. Pool B, (+)-enantiomer **11**: Optical Rotation:

$[\alpha]_D = +299.6^\circ$ ($c = 0.50$, CHCl_3); Mp: 144-145 $^\circ\text{C}$; ^1H NMR (d_6DMSO): δ 1.70 (d, $J = 7$ Hz, 3H), 5.11 (q, $J = 7$ Hz, 1H), 6.15 (s, 1H), 7.00 (m, 1H), 7.30 (bs, 2H), 7.78 (s, 1H), 8.20 (d, $J = 2$ Hz, 1H), 8.88 (s, 1H); IR: 3472, 3111, 2925, 1612, 1566, 1529, 1466, 1370, 1286, 826 cm^{-1} ; MS: Calcd for $\text{C}_{13}\text{H}_{11}\text{N}_4\text{OS}$: 306.0342. Found: 306.0338. Calcd for $\text{C}_{13}\text{H}_{11}\text{N}_4\text{OS}$: C, 50.90; H, 3.61; N, 18.26. Found: C, 50.66; H, 3.78; N, 17.73.

X-Ray Crystallographic Analysis of PNU-142721

Crystal Data

$C_{13}H_{11}N_4OSCl$	Cu $K\alpha$ radiation
$M_r=306.77$	$\lambda=1.54178 \text{ \AA}$
Orthorhombic	Cell parameters from 42 reflections
$P2_12_12_1$	$\theta = 13.2 - 27.2$
$a=8.698(1) \text{ \AA}$	$\mu= 3.748 \text{ mm}^{-1}$
$b=10.685(1) \text{ \AA}$	$T = 293(2) \text{ K}$
$c=15.366(1) \text{ \AA}$	Chunky block
$V=1428.1(2) \text{ \AA}^3$	$0.52 \times 0.31 \times 0.40 \text{ mm}$
$Z = 4$	Clear
$D_x=1.427 \text{ Mg m}^{-3}$	

Data Collection

Siemens P4 four-circle diffractometer	$R_{\text{int}} = 0.0374$
ω scans	$\theta_{\text{max}} = 55.66$
Absorption correction: none	$h = -1 \rightarrow 9$
1321 reflections measured	$k = -1 \rightarrow 11$
1174 Independent reflections	$l = -1 \rightarrow 16$
1130 reflections with $I > 2\sigma(I)$	3 standards reflections every 97 reflections
	intensity decay: none

Refinement

Refinement on F^2	$\Delta\rho_{\text{max}} = 0.320 \text{ e \AA}^{-3}$
$R[F^2 > 2\sigma(F^2)] = 0.0419$	$\Delta\rho_{\text{min}} = -0.253 \text{ e \AA}^{-3}$
$wR(F^2) = 0.110$	Extinction correction: <i>SHELX96</i>
$S = 1.029$	Extinction coefficient: $0.0077(11)$
1174 reflections	Scattering factors from <i>International Tables for Crystallography</i> (Vol. C)
182 parameters	
$(\Delta/\sigma)_{\text{max}} = 0.031$	
Absolute configuration: Flack (1983)	
Flack parameter = $-0.01(3)$	

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve and refine structure: *SHELX96* (Sheldrick, 1996). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1994).

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for PNU-142721.

$$U(\text{eq}) = (1/3)\sum_i\sum_j U^{ij} a_i^* a_j^* a_i a_j.$$

	x	y	z	U(eq)
C(1)	-1809(9)	6580(6)	-5416(4)	89(2)
C(2)	-850(8)	5933(6)	-4915(4)	79(2)
C(3)	-669(7)	4719(4)	-5319(3)	57(1)
C(4)	88(6)	3592(4)	-5166(2)	51(1)
C(5)	-70(5)	2652(4)	-5771(2)	43(1)
N(6)	-926(5)	2770(3)	-6493(2)	51(1)
C(7)	-1667(6)	3844(4)	-6633(3)	55(1)
C(8)	-1540(6)	4796(4)	-6056(3)	55(1)
O(9)	-2264(5)	5955(3)	-6119(2)	78(1)
C(10)	740(5)	1412(4)	-5663(2)	49(1)
C(11)	1783(6)	1137(6)	-6445(3)	70(2)
S(12)	-590(2)	114(1)	-5575(1)	53(1)
C(13)	-1132(6)	102(4)	-4473(2)	45(1)
N(14)	-583(4)	969(3)	-3936(2)	47(1)
C(15)	-1063(5)	840(4)	-3120(2)	53(1)
Cl(15)	-371(2)	1944(1)	-2391(1)	79(1)
C(16)	-2027(5)	-73(5)	-2838(3)	60(1)
C(17)	-2533(6)	-927(4)	-3460(2)	49(1)
N(18)	-3528(5)	-1841(4)	-3274(3)	71(1)
N(19)	-2095(4)	-829(3)	-4297(2)	47(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for PNU-142721.

C(1)-C(2)	1.329(8)
C(1)-O(9)	1.331(7)
C(2)-C(3)	1.447(7)
C(3)-C(8)	1.365(7)
C(3)-C(4)	1.392(6)
C(4)-C(5)	1.375(6)
C(5)-N(6)	1.343(5)
C(5)-C(10)	1.509(6)
N(6)-C(7)	1.334(5)
C(7)-C(8)	1.354(6)
C(8)-O(9)	1.392(6)
C(10)-C(11)	1.534(6)
C(10)-S(12)	1.812(4)
S(12)-C(13)	1.758(4)
C(13)-N(19)	1.329(5)
C(13)-N(14)	1.329(5)
N(14)-C(15)	1.328(5)
C(15)-C(16)	1.358(6)
C(15)-Cl(15)	1.734(4)
C(16)-C(17)	1.392(7)
C(17)-N(18)	1.336(6)

C(17)-N(19)	1.346(5)
C(2)-C(1)-O(9)	113.3(5)
C(1)-C(2)-C(3)	106.7(5)
C(8)-C(3)-C(4)	117.1(4)
C(8)-C(3)-C(2)	103.9(5)
C(4)-C(3)-C(2)	139.0(5)
C(5)-C(4)-C(3)	118.1(4)
N(6)-C(5)-C(4)	123.0(4)
N(6)-C(5)-C(10)	115.6(3)
C(4)-C(5)-C(10)	121.4(3)
C(7)-N(6)-C(5)	118.8(3)
N(6)-C(7)-C(8)	120.1(4)
C(3)-C(8)-C(7)	122.9(4)
C(3)-C(8)-O(9)	111.3(4)
C(7)-C(8)-O(9)	125.8(4)
C(1)-O(9)-C(8)	104.8(5)
C(5)-C(10)-C(11)	111.0(3)
C(5)-C(10)-S(12)	112.5(3)
C(11)-C(10)-S(12)	106.8(3)
C(13)-S(12)-C(10)	104.4(2)
N(19)-C(13)-N(14)	128.5(3)
N(19)-C(13)-S(12)	111.7(3)
N(14)-C(13)-S(12)	119.8(3)
C(15)-N(14)-C(13)	113.6(4)
N(14)-C(15)-C(16)	124.7(4)
N(14)-C(15)-Cl(15)	115.4(4)
C(16)-C(15)-Cl(15)	119.8(3)
C(15)-C(16)-C(17)	116.5(4)
N(18)-C(17)-N(19)	116.4(4)
N(18)-C(17)-C(16)	122.4(4)
N(19)-C(17)-C(16)	121.1(4)
C(13)-N(19)-C(17)	115.5(4)

References

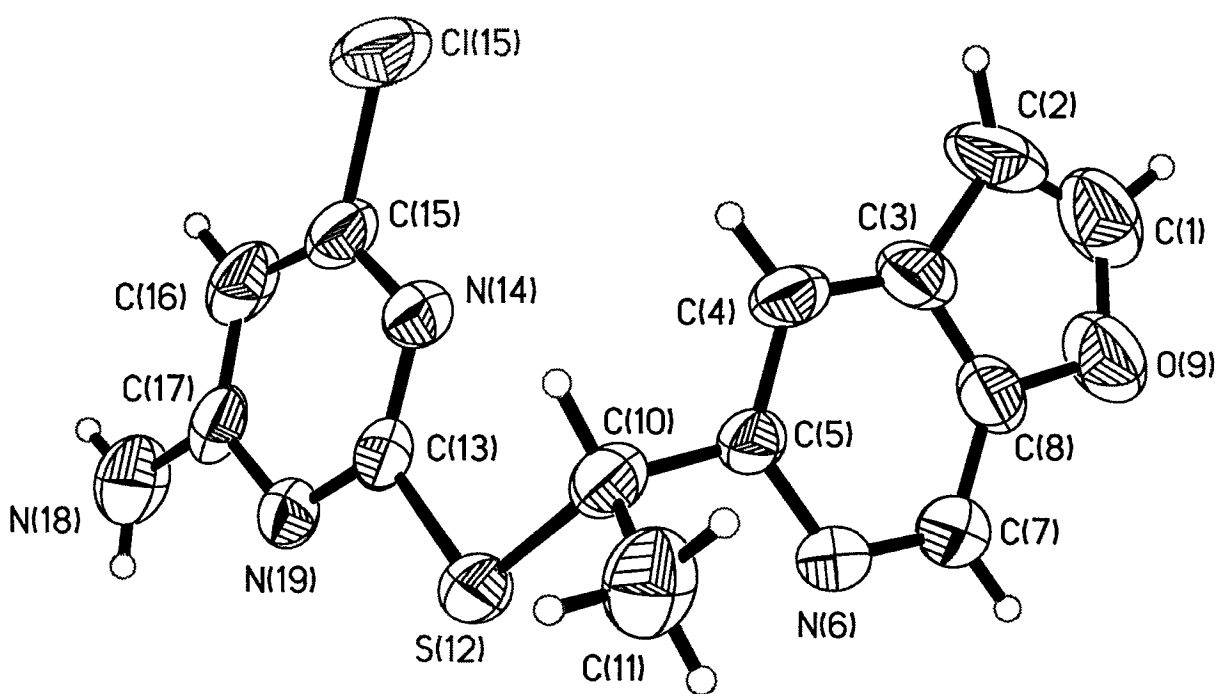
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876-881.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Sheldrick, G. M. (1994). *SHELXTL/PC*. Version 5.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1996). *SHELX96. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Siemens (1994). *XSCANS Users Manual*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.



ORTEP (Johnson, 1976) drawing of the molecule of PNU-142721 with ellipsoids at the 50% probability level and H atoms shown as small circles of arbitrary radii.