The procedures for the synthesis of the following compounds can be found in the experimental section of this paper.

1-Phenyl-2-(benzotriazol-1-yl)-3-(4-chlorophenyl)aziridine (3b): *cis* and *trans* mixture (*cis/trans* = 55/45), white solids, mp 56-68 °C; ^{1}H NMR δ_H (two isomers, ratio 1:1) 3.89 (d, 0.5H, J = 4.9 Hz), 4.72 (d, 0.5H, J = 1.9 Hz), 5.27 (d, 0.5H, J = 4.9 Hz), 5.41 (d, 0.5H, J = 1.9 Hz), 6.79-6.82 (m, 1H), 6.93-7.60 (m, 10H), 7.82-7.90 (m, 1H), 7.97-8.10 (m, 1H); ^{13}C NMR δ_C (two isomers) 44.7, 47.3, 56.5, 56.6, 109.7, 110.8, 119.6, 119.9, 120.4, 120.5, 123.6, 124.1, 124.3, 124.4, 127.9, 128.2, 128.5, 128.7, 128.8, 129.1, 129.8, 141.2, 151.5. Anal. Calcd for $C_{20}H_{15}ClN_4$: C, 68.26; H, 4.36; N, 15.15. Found: C, 68.43; H, 4.47; N, 15.18.

1-Isobutyl-2-(benzotriazol-2-yl)aziridine (8b): colorless oil; ^{1}H NMR δ_H 1.0 (d, 6H, J = 6.6 Hz), 1.96-2.02 (m, 2H), 2.38-2.50 (m, 2H), 3.02 (br s, 1H), 4.59-4.60 (m, 1H), 7.35-7.38 (m, 2H), 7.84-7.88 (m, 2H); ^{13}C NMR δ_C 20.7, 28.8, 34.5, 57.2, 67.3, 118.1, 126.5, 144.3. Anal. Calcd for $C_{12}H_{16}N_4$: C, 66.64; H, 7.46; N, 25.90. Found: C, 66.94; H, 7.25; N, 26.03.

1-Decyl-2-(benzotriazol-2-yl)aziridine (8c): colorless oil; ^{1}H NMR δ_H 0.89 (t, 3H, J = 6.0 Hz), 1.26-1.37 (m, 14H), 1.64-1.69 (m, 2H), 1.92 (d, 1H, J = 5.4 Hz), 2.41-2.50 (m, 1H), 2.62-2.70 (m, 1H), 2.98 (br s, 1H), 4.60-4.61 (m, 1H), 7.32-7.35 (m, 2H), 7.83-7.87 (m, 2H); ^{13}C NMR δ_C 13.7, 22.2, 26.7, 28.8, 28.9, 29.0, 31.5, 34.0, 56.6, 59.1, 117.7, 126.0, 143.9. Anal. Calcd for $C_{18}H_{28}N_4$: C, 71.96; H, 9.39; N, 18.65. Found: C, 71.57; H, 9.67; N, 18.71.

1-Butyl-2-(benzotriazol-2-yl)aziridine (8d): colorless oil; ^{1}H NMR δ_H 0.94 (t, 3H, J = 7.2 Hz), 1.39-1.46 (m, 2H), 1.65-1.74 (m, 2H), 1.97 (d, 1H, J = 5.4 Hz), 2.45-2.52 (m, 1H), 2.65-2.72 (m, 1H), 2.99 (br s, 1H), 4.61-4.63 (m, 1H), 7.36-7.39 (m, 2H), 7.85-7.88 (m, 2H); ^{13}C NMR δ_C

13.7, 20.0, 31.0, 34.2, 56.8, 58.9, 117.8, 126.3, 144.1. Anal. Calcd for $C_{12}H_{16}N_4$: C, 66.64; H, 7.46; N, 25.90. Found: C, 66.43; H, 7.81; N, 25.92.

1-Cyclohexyl-2-(benzotrazol-2-yl)aziridine (8e): colorless oil; ^{1}H NMR δ_H 1.15-1.30 (m, 3H), 1.45-1.79 (m, 4H), 1.80-1.86 (m, 3H), 2.00-2.13 (m, 2H), 2.96 (d, 1H, J = 1.6 Hz), 4.64 (d, 1H, J = 3.6 Hz), 7.36 (dd, 2H, J = 3.0, 6.6 Hz), 7.84 (dd, 2H, J = 3.0, 6.5 Hz); ^{13}C NMR δ_C 24.5, 24.6, 25.8, 31.6, 32.3, 33.2, 56.2, 67.6, 118.2, 126.5, 144.1. Anal. Calcd for $C_{14}H_{18}N_4$: C, 69.39; H, 7.49; N, 23.12. Found: C, 69.29, H, 7.70; N, 23.23.

1-Benzyl-2-(benzotriazol-2-yl)aziridine (8f): colorless oil; ^{1}H NMR δ_H 2.05 (d, 1H, J = 5.4 Hz), 3.04 (d, 1H, J = 2.1 Hz), 3.61 (d, 1H, J = 13.5 Hz), 3.93 (d, 1H, J = 13.5 Hz), 4.75-4.76 (m, 1H), 7.24-7.37 (m, 7H), 7.82-7.85 (m, 2H); ^{13}C NMR δ_C 33.9, 56.7, 61.9, 117.9, 126.4, 127.2, 127.9, 128.2, 137.0, 144.1.

1-Propyl-2-(benzotriazol-2-yl)aziridine (8g): colorless oil; ^{1}H NMR δ_H 0.98 (t, 3H, J = 7.5 Hz), 1.68-1.78 (m, 2H), 1.97 (d, 1H, J = 3.6 Hz), 2.41-2.48 (m, 1H), 2.56-2.66 (m, 1H), 2.99 (d, 1H, J = 1.7 Hz), 4.61 (d, 1H, J = 3.6 Hz), 7.36 (dd, 2H, J = 3.0, 6.6 Hz), 7.84 (dd, 2H, J = 3.0, 6.5 Hz); ^{13}C NMR δ_C 11.7, 22.6, 34.5, 57.0, 61.2, 118.1, 126.6, 141.4.

1-(1,2-Dibromoethyl)benzotriazole (10): Prepared as for 2-(1,2-dibromoethyl)benzotriazole (**5a**), starting from 1-vinylbenzotriazole, in 22% yield; colorless oil; ^{1}H NMR δ_H 4.33 (dd, 1H, J = 4.1, 11.0 Hz), 4.89 (t, 1H, J = 10.9 Hz), 6.95 (dd, 1H, J = 4.1, 11.0 Hz), 7.47 (t, 1H, J = 7.0 Hz), 7.61-7.65 (m, 2H), 8.13 (d, 1H, J = 8.4 Hz); ^{13}C NMR δ_C 31.4, 55.4, 109.7, 120.7, 125.1, 128.7, 131.2, 145.5.

1-(1-Bromovinyl)benzotriazole (11): Formed from the reaction of **10** and butylamine at rt for 12 h in almost quantitative yield; colorless oil; ^{1}H NMR δ_H 5.90 (d, 1H, J = 2.8 Hz), 6.20 (d, 1H, J = 2.8 Hz), 7.35 (t, 1H, J = 8.4 Hz), 7.50 (t, 1H, J = 8.4 Hz), 7.69 (d, 1H, J = 8.4 Hz), 7.99 (d, 1H, J = 8.4 Hz); ^{13}C NMR δ_C 111.1, 116.8, 117.9, 120.3, 124.8, 128.6, 132.0, 145.1.

Diethyl 1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (14a): colorless oil; ^{1}H NMR δ_H 1.21 (t, 3H, J = 7.2 Hz), 1.37 (t, 3H, J = 6.9 Hz), 4.24 (q, 2H, J = 7.2 Hz), 4.34 (q, 2H, J = 6.6 Hz), 7.05-7.32 (m, 10H), 7.51 (s, 1H); ^{13}C NMR δ_C 13.9, 14.3, 60.2, 60.9, 115.7, 117.1, 125.9, 127.7, 127.9, 128.1, 129.1, 129.9, 130.4, 135.1, 138.6, 163.6, 165.5; HRMS (FAB) Calcd for $C_{22}H_{21}NO_4$ + H 364.1549, found 364.1544.

1-Cyclohexyl-2-methyl-2-(benzotriazol-2-yl)aziridine (20): white solids, mp 90-91 °C; ^{1}H NMR δ_H 1.10-1.34 (m, 3H), 1.38-1.69 (m, 3H), 1.70-1.88 (m, 4H), 2.00-2.10 (m, 5H), 3.05 (s, 1H), 7.34-7.37 (m, 2H), 7.86-7.89 (m, 2H); ^{13}C NMR δ_C 24.5, 24.7, 25.7, 32.1, 33.4, 37.4, 61.7, 118.3, 126.3, 144.0. Anal. Calcd for $C_{15}H_{20}N_4$: C, 70.28; H, 7.86; N, 21.86. Found: C, 70.28; H, 8.19; N, 21.82.

Diethyl 1-isobutyl-1*H*-pyrrole-2,3-dicarboxylate (18b): colorless oil; ^{1}H NMR δ_H 0.88 (d, 6H, J = 6.9 Hz), 1.31-1.38 (m, 6H), 1.96-2.10 (m, 1H), 3.95 (d, 2H, J = 7.2 Hz), 4.25-4.37 (m, 4H), 6.47 (d, 1H, J = 2.7 Hz), 6.65 (d, 1H, J = 2.7 Hz); ^{13}C NMR δ_C 14.0, 14.2, 19.8, 30.2, 56.4, 60.3, 61.0, 109.7, 118.9, 120.9, 125.5, 161.9, 165.0. Anal. Calcd for $C_{14}H_{21}NO_4$: C, 62.90; H, 7.92; N, 5.24. Found: C, 62.77; H, 7.98; N, 5.85.

Diethyl 1-decyl-1*H*-pyrrole-2,3-dicarboxylate (18c): colorless oil; ^{1}H NMR δ_H 0.88 (t, 3H, J = 6.3 Hz), 1.26-1.39 (m, 20H), 1.71-1.76 (m, 2H), 4.13 (t, 2H, J = 7.2 Hz), 4.25-4.38 (m, 4H), 6.47 (d, 1H, J = 2.7 Hz), 6.69 (d, 1H, J = 2.7 Hz); ^{13}C NMR δ_C 14.1, 14.2, 14.3, 22.6, 26.6,

29.1, 29.3, 29.4, 31.5, 31.8, 49.2, 60.4, 61.0, 110.0, 120.7, 124.3, 124.8, 161.5, 164.8. $C_{20}H_{33}NO_4$: C, 68.34; H, 9.46, N, 3.99. Found: C, 68.26; H, 9.58; N, 4.39.

Diethyl 1-butyl-1*H*-pyrrole-2,3-dicarboxylate (18d): colorless oil; ^{1}H NMR δ_H 0.92 (t, 3H, J = 7.2 Hz), 1.27-1.38 (m, 8H), 1.67-1.72 (m, 2H), 4.14 (t, 2H, J = 7.5 Hz), 4.25-4.35 (m, 4H), 6.46 (d, 1H, J = 2.4 Hz), 6.68 (d, 1H, J = 2.4 Hz); ^{13}C NMR δ_C 13.5, 14.0, 14.2, 19.7, 33.5, 48.9, 60.3, 61.0, 109.9, 120.7, 124.2, 124.9, 161.5, 164.8. Anal. Calcd for $C_{14}H_{21}NO_4$: C, 62.90; H, 7.92; N, 5.24. Found: C, 62.70; H, 8.09; N, 5.85.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **14b**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	3721(1)	1268(1)	7884(2)	24(1)
C(2)	3758(2)	1631(1)	7745(2)	23(1)
C(3)	2648(1)	1757(1)	7830(2)	22(1)
C(4)	1923(2)	1464(1)	8040(2)	25(1)
C(5)	2618(2)	1170(1)	8063(2)	27(1)
C(11)	4688(2)	1026(1)	7905(2)	24(1)
C(12)	5243(2)	1016(1)	6585(2)	29(1)
C(13)	6183(2)	782(1)	6650(2)	33(1)
C(14)	6539(2)	557(1)	8002(2)	33(1)
C(15)	5964(2)	568(1)	9309(2)	32(1)
C(16)	5040(2)	804(1)	9275(2)	28(1)
C(21)	4843(1)	1830(1)	7647(2)	23(1)
C(22)	5949(2)	1766(1)	8753(2)	27(1)
C(23)	6938(2)	1973(1)	8729(2)	29(1)
C(24)	6808(2)	2248(1)	7602(2)	27(1)
Cl(1)	8032(1)	2520(1)	7617(1)	38(1)
C(25)	5729(2)	2316(1)	6469(2)	27(1)
C(26)	4746(2)	2104(1)	6492(2)	24(1)
C(31)	2318(1)	2134(1)	7775(2)	22(1)
O(31)	2874(1)	2357(1)	8672(2)	31(1)
O(32)	1329(1)	2200(1)	6575(2)	30(1)
C(32)	924(2)	2561(1)	6472(3)	34(1)
C(41)	741(2)	1473(1)	8414(2)	25(1)
O(41)	271(1)	1729(1)	8842(2)	34(1)
O(42)	234(1)	1151(1)	8251(2)	34(1)
C(42)	-927(2)	1130(1)	8632(3)	43(1)
N(1')	-346(1)	-1207(1)	6885(2)	23(1)
C(2')	-705(1)	-864(1)	7076(2)	22(1)
C(3')	-1852(1)	-878(1)	7342(2)	23(1)
C(4')	-2193(1)	-1241(1)	7301(2)	23(1)
C(5')	-1245(2)	-1431(1)	7029(2)	24(1)
C(11')	761(1)	-1324(1)	6531(2)	23(1)
C(12')	1859(2)	-1179(1)	7316(2)	27(1)
C(13')	2890(2)	-1296(1)	6881(2)	31(1)
C(14')	2823(2)	-1559(1)	5687(2)	33(1)
C(15')	1729(2)	-1709(1)	4958(2)	31(1)
C(16')	694(2)	-1594(1)	5372(2)	25(1)
C(21')	72(1)	-565(1)	6869(2)	22(1)
C(22')	454(2)	-526(1)	5386(2)	24(1)
C(23')	1276(2)	-269(1)	5236(2)	26(1)
C(24')	1726(2)	-53(1)	6603(2)	26(1)
Cl(1')	2810(1)	260(1)	6466(1)	37(1)
C(25')	1338(2)	-78(1)	8070(2)	27(1)
C(26')	507(2)	-334(1)	8198(2)	26(1)
C(31')	-2552(2)	-562(1)	7511(2)	24(1)
O(31')	-2134(1)	-288(1)	8131(2)	35(1)
O(32')	-3726(1)	-608(1)	6858(2)	30(1)

C(32')	-4479(2)	-313(1)	7024(3)	36(1)
C(41')	-3266(1)	-1411(1)	7647(2)	23(1)
O(41')	-4058(1)	-1271(1)	8141(2)	34(1)
O(42')	-3244(1)	-1757(1)	7353(2)	31(1)
C(42')	-4179(2)	-1963(1)	7799(2)	27(1)

Table 2. Bond lengths [A] and angles [deg] for **14b**.

N(1)-C(5)	1.360(2)
N(1)-C(2)	1.391(2)
N(1)-C(11)	1.438(2)
C(2)-C(3)	1.377(2)
C(2)-C(21)	1.474(2)
C(3)-C(4)	1.426(2)
C(3)-C(31)	1.483(2)
C(4)-C(5)	1.373(2)
C(4)-C(41)	1.460(2)
C(11)-C(12)	1.377(2)
C(11)-C(16)	1.386(2)
C(12)-C(13)	1.391(3)
C(13)-C(14)	1.382(3)
C(14)-C(15)	1.383(3)
C(15)-C(16)	1.384(2)
C(21)-C(22)	1.393(2)
C(21)-C(26)	1.397(2)
C(22)-C(23)	1.384(2)
C(23)-C(24)	1.381(3)
C(24)-C(25)	1.382(2)
C(24)-Cl(1)	1.741(2)
C(25)-C(26)	1.389(2)
C(31)-O(31)	1.204(2)
C(31)-O(32)	1.336(2)
O(32)-C(32)	1.449(2)
C(41)-O(41)	1.206(2)
C(41)-O(42)	1.350(2)
O(42)-C(42)	1.440(2)
N(1')-C(5')	1.365(2)
N(1')-C(2')	1.389(2)
N(1')-C(11')	1.439(2)
C(2')-C(3')	1.384(2)
C(2')-C(21')	1.480(2)
C(3')-C(4')	1.435(2)
C(3')-C(31')	1.471(2)
C(4')-C(5')	1.366(2)
C(4')-C(41')	1.476(2)
C(11')-C(12')	1.386(2)
C(11')-C(16')	1.387(2)
C(12')-C(13')	1.386(2)
C(13')-C(14')	1.388(3)
C(14')-C(15')	1.379(3)
C(15')-C(16')	1.382(2)
C(21')-C(22')	1.391(2)
C(21')-C(26')	1.396(2)
C(22')-C(23')	1.384(2)
C(23')-C(24')	1.386(2)
C(24')-C(25')	1.378(3)
C(24')-Cl(1')	1.745(2)
C(25')-C(26')	1.387(2)
C(31')-O(31')	1.209(2)

C(31')-O(32')	1.336(2)
O(32')-C(32')	1.441(2)
C(41')-O(41')	1.203(2)
C(41')-O(42')	1.341(2)
O(42')-C(42')	1.443(2)

C(5)-N(1)-C(2)	109.26(14)
C(5)-N(1)-C(11)	123.82(14)
C(2)-N(1)-C(11)	126.88(14)
C(3)-C(2)-N(1)	107.17(14)
C(3)-C(2)-C(21)	128.84(15)
N(1)-C(2)-C(21)	123.86(14)
C(2)-C(3)-C(4)	107.83(14)
C(2)-C(3)-C(31)	124.59(15)
C(4)-C(3)-C(31)	127.54(15)
C(5)-C(4)-C(3)	106.77(14)
C(5)-C(4)-C(41)	125.49(16)
C(3)-C(4)-C(41)	127.15(15)
N(1)-C(5)-C(4)	108.96(15)
C(12)-C(11)-C(16)	121.08(16)
C(12)-C(11)-N(1)	120.44(15)
C(16)-C(11)-N(1)	118.48(15)
C(11)-C(12)-C(13)	119.10(17)
C(14)-C(13)-C(12)	120.47(17)
C(13)-C(14)-C(15)	119.67(17)
C(14)-C(15)-C(16)	120.50(17)
C(15)-C(16)-C(11)	119.17(16)
C(22)-C(21)-C(26)	118.91(15)
C(22)-C(21)-C(2)	121.78(15)
C(26)-C(21)-C(2)	119.17(15)
C(23)-C(22)-C(21)	120.99(16)
C(24)-C(23)-C(22)	118.85(16)
C(23)-C(24)-C(25)	121.73(16)
C(23)-C(24)-Cl(1)	119.17(14)
C(25)-C(24)-Cl(1)	119.10(14)
C(24)-C(25)-C(26)	118.93(16)
C(25)-C(26)-C(21)	120.55(16)
O(31)-C(31)-O(32)	123.27(15)
O(31)-C(31)-C(3)	124.92(15)
O(32)-C(31)-C(3)	111.80(14)
C(31)-O(32)-C(32)	115.26(13)
O(41)-C(41)-O(42)	123.52(16)
O(41)-C(41)-C(4)	125.54(16)
O(42)-C(41)-C(4)	110.93(15)
C(41)-O(42)-C(42)	115.39(15)
C(5')-N(1')-C(2')	109.20(13)
C(5')-N(1')-C(11')	122.87(14)
C(2')-N(1')-C(11')	127.89(14)
C(3')-C(2')-N(1')	107.36(14)
C(3')-C(2')-C(21')	131.93(15)
N(1')-C(2')-C(21')	120.56(14)
C(2')-C(3')-C(4')	107.32(14)
C(2')-C(3')-C(31')	122.90(15)
C(4')-C(3')-C(31')	129.66(15)

C(5')-C(4')-C(3')	106.89(14)
C(5')-C(4')-C(41')	122.05(15)
C(3')-C(4')-C(41')	130.75(15)
N(1')-C(5')-C(4')	109.22(15)
C(12')-C(11')-C(16')	120.61(15)
C(12')-C(11')-N(1')	122.03(15)
C(16')-C(11')-N(1')	117.36(15)
C(13')-C(12')-C(11')	119.27(17)
C(12')-C(13')-C(14')	120.31(17)
C(15')-C(14')-C(13')	119.77(16)
C(14')-C(15')-C(16')	120.52(17)
C(15')-C(16')-C(11')	119.46(16)
C(22')-C(21')-C(26')	118.91(15)
C(22')-C(21')-C(2')	120.30(15)
C(26')-C(21')-C(2')	120.61(15)
C(23')-C(22')-C(21')	120.98(15)
C(22')-C(23')-C(24')	118.65(16)
C(25')-C(24')-C(23')	121.79(16)
C(25')-C(24')-Cl(1')	118.95(13)
C(23')-C(24')-Cl(1')	119.25(13)
C(24')-C(25')-C(26')	118.88(16)
C(25')-C(26')-C(21')	120.70(16)
O(31')-C(31')-O(32')	122.70(15)
O(31')-C(31')-C(3')	125.07(15)
O(32')-C(31')-C(3')	112.22(14)
C(31')-O(32')-C(32')	115.53(13)
O(41')-C(41')-O(42')	122.91(15)
O(41')-C(41')-C(4')	126.95(16)
O(42')-C(41')-C(4')	110.14(13)
C(41')-O(42')-C(42')	116.20(13)

Table 3. Anisotropic displacement parameters (A^2 x 10^3) for **14b**.
The anisotropic displacement factor exponent takes the form:
$-2P^2[h^2a^{*2}$ U11 + ... + 2hka*b*U12].

	U11	U22	U33	U23	U13	U12
N(1)	22(1)	18(1)	31(1)	0(1)	5(1)	1(1)
C(2)	25(1)	19(1)	23(1)	0(1)	3(1)	1(1)
C(3)	22(1)	21(1)	22(1)	-1(1)	2(1)	-1(1)
C(4)	23(1)	23(1)	26(1)	-1(1)	3(1)	-1(1)
C(5)	25(1)	21(1)	32(1)	-1(1)	4(1)	-4(1)
C(11)	23(1)	17(1)	32(1)	-4(1)	5(1)	-1(1)
C(12)	32(1)	25(1)	29(1)	0(1)	6(1)	0(1)
C(13)	33(1)	32(1)	37(1)	-7(1)	13(1)	-1(1)
C(14)	27(1)	24(1)	46(1)	-5(1)	8(1)	2(1)
C(15)	33(1)	23(1)	40(1)	3(1)	7(1)	3(1)
C(16)	31(1)	22(1)	32(1)	0(1)	10(1)	1(1)
C(21)	23(1)	21(1)	24(1)	-4(1)	6(1)	1(1)
C(22)	28(1)	23(1)	29(1)	1(1)	4(1)	2(1)
C(23)	24(1)	28(1)	32(1)	-5(1)	2(1)	1(1)
C(24)	27(1)	23(1)	34(1)	-9(1)	14(1)	-5(1)
Cl(1)	32(1)	35(1)	48(1)	-7(1)	14(1)	-12(1)
C(25)	30(1)	24(1)	28(1)	1(1)	12(1)	2(1)
C(26)	24(1)	24(1)	24(1)	-1(1)	7(1)	4(1)
C(31)	21(1)	22(1)	25(1)	1(1)	7(1)	0(1)
O(31)	33(1)	22(1)	33(1)	-3(1)	0(1)	0(1)
O(32)	25(1)	21(1)	38(1)	1(1)	-3(1)	3(1)
C(32)	29(1)	24(1)	46(1)	7(1)	4(1)	7(1)
C(41)	24(1)	25(1)	25(1)	3(1)	2(1)	-1(1)
O(41)	31(1)	35(1)	38(1)	-3(1)	11(1)	2(1)
O(42)	25(1)	30(1)	45(1)	5(1)	8(1)	-6(1)
C(42)	28(1)	49(1)	52(1)	15(1)	9(1)	-10(1)
N(1')	21(1)	20(1)	28(1)	-1(1)	8(1)	1(1)
C(2')	25(1)	20(1)	22(1)	-1(1)	5(1)	1(1)
C(3')	24(1)	21(1)	22(1)	-1(1)	5(1)	1(1)
C(4')	23(1)	21(1)	23(1)	-1(1)	5(1)	0(1)
C(5')	25(1)	20(1)	30(1)	0(1)	9(1)	-2(1)
C(11')	22(1)	20(1)	26(1)	4(1)	7(1)	4(1)
C(12')	27(1)	26(1)	27(1)	1(1)	5(1)	0(1)
C(13')	22(1)	35(1)	35(1)	7(1)	5(1)	1(1)
C(14')	28(1)	37(1)	36(1)	10(1)	13(1)	12(1)
C(15')	37(1)	27(1)	31(1)	2(1)	12(1)	8(1)
C(16')	27(1)	23(1)	25(1)	1(1)	5(1)	1(1)
C(21')	21(1)	18(1)	27(1)	0(1)	5(1)	2(1)
C(22')	28(1)	20(1)	24(1)	-3(1)	3(1)	2(1)
C(23')	29(1)	24(1)	28(1)	0(1)	9(1)	1(1)
C(24')	23(1)	19(1)	35(1)	3(1)	5(1)	0(1)
Cl(1')	36(1)	29(1)	49(1)	-3(1)	14(1)	-11(1)
C(25')	28(1)	23(1)	29(1)	-4(1)	4(1)	-1(1)
C(26')	28(1)	24(1)	24(1)	-1(1)	7(1)	1(1)
C(31')	25(1)	23(1)	23(1)	0(1)	6(1)	1(1)
O(31')	32(1)	26(1)	44(1)	-13(1)	6(1)	2(1)
O(32')	23(1)	21(1)	43(1)	-2(1)	5(1)	4(1)
C(32')	29(1)	27(1)	50(1)	2(1)	9(1)	9(1)

C(41')	23(1)	22(1)	22(1)	1(1)	3(1)	2(1)
O(41')	29(1)	26(1)	52(1)	-2(1)	19(1)	2(1)
O(42')	32(1)	20(1)	46(1)	-4(1)	19(1)	-5(1)
C(42')	26(1)	25(1)	30(1)	3(1)	9(1)	-4(1)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **14b**.

	x	y	z	U(eq)
H(5)	2368	935	8185	32
H(12)	4987	1167	5643	35
H(13)	6584	777	5757	40
H(14)	7176	396	8035	39
H(15)	6204	413	10236	39
H(16)	4652	813	10179	33
H(22)	6026	1578	9535	32
H(23)	7693	1926	9474	34
H(25)	5661	2503	5688	32
H(26)	4000	2147	5716	28
H(32A)	783	2633	7559	51
H(32B)	177	2583	5599	51
H(32C)	1539	2713	6189	51
H(42A)	-901	1248	9704	65
H(42B)	-1143	883	8718	65
H(42C)	-1527	1243	7735	65
H(5')	-1217	-1679	6952	29
H(12')	1905	-1001	8143	32
H(13')	3645	-1196	7404	37
H(14')	3528	-1634	5372	39
H(15')	1688	-1894	4165	37
H(16')	-58	-1698	4868	30
H(22')	145	-678	4463	29
H(23')	1527	-242	4217	32
H(25')	1634	79	8978	32
H(26')	231	-353	9202	31
H(32D)	-4303	-237	8202	53
H(32E)	-5324	-382	6664	53
H(32F)	-4321	-119	6318	53
H(42D)	-4124	-1940	9009	40
H(42E)	-4085	-2209	7520	40
H(42F)	-4964	-1878	7169	40

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **19**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	5286(4)	7934(3)	-1915(2)	41(1)
C(2)	6883(4)	8331(3)	-2141(3)	35(1)
C(3)	6703(4)	9259(3)	-3101(3)	33(1)
C(4)	4979(4)	9397(3)	-3428(3)	40(1)
C(5)	4156(5)	8580(3)	-2700(3)	45(1)
C(11)	4720(5)	7049(4)	-956(3)	56(1)
C(12)	4405(6)	7634(4)	-25(3)	67(1)
C(13)	2983(6)	8731(5)	-163(4)	80(2)
C(14)	2623(7)	9226(6)	820(4)	106(2)
C(21)	8394(5)	7768(4)	-1456(3)	44(1)
O(21)	8293(3)	6949(2)	-637(2)	60(1)
O(22)	9885(3)	8153(2)	-1761(2)	53(1)
C(31)	7996(5)	10012(3)	-3656(3)	41(1)
O(31)	7371(3)	10903(2)	-4474(2)	57(1)
O(32)	9528(3)	9871(2)	-3404(2)	57(1)
N(1')	2563(4)	3571(3)	3989(2)	41(1)
C(2')	1007(4)	3821(3)	3466(3)	35(1)
C(3')	1224(4)	4694(3)	2508(3)	36(1)
C(4')	2927(5)	4962(4)	2486(3)	52(1)
C(5')	3711(5)	4265(4)	3399(3)	53(1)
C(11')	3036(5)	2786(4)	5063(3)	48(1)
C(12')	2672(7)	3566(4)	5875(3)	77(2)
C(13')	3258(8)	2770(5)	7021(4)	92(2)
C(14')	1884(8)	2019(5)	7457(4)	101(2)
C(21')	-461(5)	3182(4)	3905(3)	45(1)
O(21')	-381(4)	2413(3)	4763(2)	75(1)
O(22')	-1919(3)	3474(2)	3364(2)	54(1)
C(31')	-10(5)	5222(3)	1632(3)	42(1)
O(31')	610(3)	6008(2)	829(2)	56(1)
O(32')	-1496(3)	4973(2)	1641(2)	52(1)

Table 6. Bond lengths [A] and angles [deg] for **19**.

N(1)-C(5)	1.363(4)
N(1)-C(2)	1.377(4)
N(1)-C(11)	1.481(4)
C(2)-C(3)	1.406(4)
C(2)-C(21)	1.469(5)
C(3)-C(4)	1.399(4)
C(3)-C(31)	1.460(5)
C(4)-C(5)	1.353(5)
C(11)-C(12)	1.511(5)
C(12)-C(13)	1.493(6)
C(13)-C(14)	1.517(6)
C(21)-O(21)	1.227(4)
C(21)-O(22)	1.308(4)
C(31)-O(32)	1.226(4)
C(31)-O(31)	1.314(4)
N(1')-C(5')	1.357(4)
N(1')-C(2')	1.373(4)
N(1')-C(11')	1.481(4)
C(2')-C(3')	1.398(4)
C(2')-C(21')	1.458(5)
C(3')-C(4')	1.400(5)
C(3')-C(31')	1.471(5)
C(4')-C(5')	1.360(5)
C(11')-C(12')	1.522(5)
C(12')-C(13')	1.582(6)
C(13')-C(14')	1.468(7)
C(21')-O(21')	1.225(4)
C(21')-O(22')	1.317(4)
C(31')-O(32')	1.230(4)
C(31')-O(31')	1.311(4)
C(5)-N(1)-C(2)	108.9(3)
C(5)-N(1)-C(11)	122.0(3)
C(2)-N(1)-C(11)	128.9(3)
N(1)-C(2)-C(3)	106.7(3)
N(1)-C(2)-C(21)	121.6(3)
C(3)-C(2)-C(21)	131.7(3)
C(4)-C(3)-C(2)	107.3(3)
C(4)-C(3)-C(31)	124.4(3)
C(2)-C(3)-C(31)	128.3(3)
C(5)-C(4)-C(3)	107.7(3)
C(4)-C(5)-N(1)	109.5(3)
N(1)-C(11)-C(12)	111.7(3)
C(13)-C(12)-C(11)	115.4(4)
C(12)-C(13)-C(14)	113.5(4)
O(21)-C(21)-O(22)	120.3(3)
O(21)-C(21)-C(2)	122.1(3)
O(22)-C(21)-C(2)	117.5(3)
O(32)-C(31)-O(31)	121.1(3)
O(32)-C(31)-C(3)	125.2(3)

O(31)-C(31)-C(3)	113.7(3)
C(5')-N(1')-C(2')	109.4(3)
C(5')-N(1')-C(11')	120.3(3)
C(2')-N(1')-C(11')	130.1(3)
N(1')-C(2')-C(3')	106.8(3)
N(1')-C(2')-C(21')	121.4(3)
C(3')-C(2')-C(21')	131.7(3)
C(2')-C(3')-C(4')	107.2(3)
C(2')-C(3')-C(31')	128.9(3)
C(4')-C(3')-C(31')	123.9(3)
C(5')-C(4')-C(3')	107.7(3)
N(1')-C(5')-C(4')	108.9(3)
N(1')-C(11')-C(12')	110.2(3)
C(11')-C(12')-C(13')	111.4(4)
C(14')-C(13')-C(12')	107.2(5)
O(21')-C(21')-O(22')	119.9(3)
O(21')-C(21')-C(2')	121.9(3)
O(22')-C(21')-C(2')	118.3(3)
O(32')-C(31')-O(31')	122.1(3)
O(32')-C(31')-C(3')	124.1(3)
O(31')-C(31')-C(3')	113.8(3)

Table 7. Anisotropic displacement parameters (A^2 x 10^3) for **19**.
The anisotropic displacement factor exponent takes the form:
$-2P^2[h^2a^{*2}$ U11 + ... + 2hka*b*U12].

	U11	U22	U33	U23	U13	U12
N(1)	49(2)	37(2)	31(2)	5(2)	0(2)	-11(2)
C(2)	36(2)	32(2)	32(2)	0(2)	-4(2)	-3(2)
C(3)	33(2)	34(2)	28(2)	0(2)	-3(2)	-1(2)
C(4)	37(2)	42(2)	35(2)	-2(2)	-7(2)	-1(2)
C(5)	33(2)	53(3)	46(2)	-7(2)	-4(2)	-11(2)
C(11)	72(3)	45(2)	47(3)	4(2)	8(2)	-25(2)
C(12)	76(3)	74(3)	44(3)	3(2)	17(2)	-29(3)
C(13)	71(3)	102(4)	80(4)	-41(3)	6(3)	-24(3)
C(14)	102(4)	142(5)	100(4)	-70(4)	29(4)	-38(4)
C(21)	50(3)	40(2)	35(2)	-2(2)	-10(2)	2(2)
O(21)	73(2)	55(2)	37(2)	15(2)	-15(1)	-1(2)
O(22)	38(2)	62(2)	49(2)	5(1)	-15(1)	0(1)
C(31)	37(2)	44(2)	35(2)	-1(2)	0(2)	-6(2)
O(31)	51(2)	61(2)	41(2)	23(2)	-4(1)	-14(1)
O(32)	39(2)	67(2)	53(2)	14(1)	-3(1)	-14(1)
N(1')	41(2)	39(2)	37(2)	-2(2)	-7(2)	-1(2)
C(2')	31(2)	32(2)	38(2)	-3(2)	-3(2)	-2(2)
C(3')	37(2)	31(2)	31(2)	9(2)	-8(2)	-5(2)
C(4')	48(2)	54(3)	42(3)	10(2)	-4(2)	-13(2)
C(5')	39(2)	63(3)	52(3)	0(2)	-6(2)	-14(2)
C(11')	56(2)	48(2)	30(2)	1(2)	-14(2)	9(2)
C(12')	119(4)	60(3)	46(3)	-10(2)	-13(3)	6(3)
C(13')	123(5)	97(4)	56(3)	-29(3)	5(3)	-6(4)
C(14')	127(5)	93(4)	76(4)	-18(3)	7(4)	-6(4)
C(21')	42(2)	48(3)	41(3)	-3(2)	1(2)	-7(2)
O(21')	73(2)	77(2)	56(2)	28(2)	-4(2)	-30(2)
O(22')	40(2)	60(2)	55(2)	1(1)	0(1)	-14(1)
C(31')	48(3)	36(2)	34(2)	4(2)	-4(2)	-4(2)
O(31')	65(2)	52(2)	40(2)	14(1)	-10(1)	-9(1)
O(32')	43(2)	57(2)	47(2)	4(1)	-15(1)	-4(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **19**.

	x	y	z	U(eq)
H(4A)	4478	9963	-4049	48
H(5A)	2973	8474	-2732	54
H(11A)	5627	6301	-771	67
H(11B)	3632	6775	-1109	67
H(12A)	4124	6987	607	80
H(12B)	5503	7901	121	80
H(13C)	1900	8487	-359	96
H(13D)	3304	9409	-756	96
H(14A)	1674	9937	680	159
H(14B)	3677	9497	1007	159
H(14C)	2285	8565	1410	159
H(22)	9680	8956	-2492	80
H(31)	8357	11465	-4848	85
H(4'A)	3442	5530	1933	62
H(5'A)	4874	4264	3591	64
H(11C)	4289	2428	5071	57
H(11D)	2351	2087	5248	57
H(12C)	1409	3888	5888	93
H(12D)	3307	4291	5664	93
H(13A)	4381	2219	6980	110
H(13B)	3409	3328	7478	110
H(14D)	2219	1495	8163	151
H(14E)	1727	1485	6989	151
H(14F)	787	2574	7512	151
H(22')	-1874	4053	2608	80
H(31')	-276	6473	192	85