Supporting Information:

Recent extensions of Morita-Baylis-Hillman reaction

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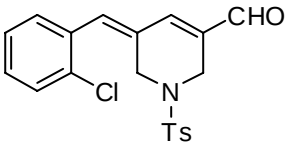
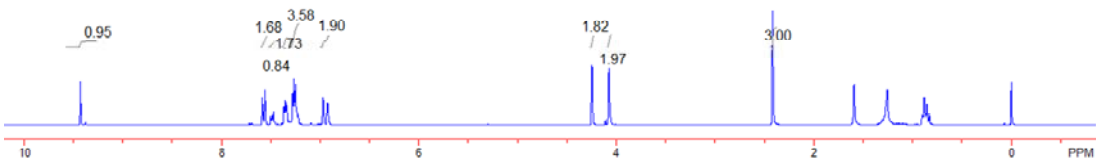
(*Z*)-5-(2-chlorobenzylidene)-1-tosyl-1,2,5,6-tetrahydropyridine-3-carbaldehyde (*Z*-71a):

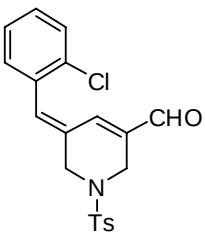


***Z*-71a**

Yield: 26 %; mp. 112-113 ^{o}C; IR (CH_2Cl_2, film) ν 2925, 2854, 1774, 1725, 1606, 1479, 1385, 1363, 1113, 1088, 725 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.43 (s, 1H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.51-7.47 (m, 1H), 7.37-7.33 (m, 2H), 7.28-7.20 (m, 3H), 6.97 (s, 1H), 6.93 (s, 1H), 4.24 (s, 2H), 4.07 (s, 2H), 2.43 (s, 3H); ESI-MS *m/z* (relative intensity %): 388.1 (100) [M^{+}+1]; HRMS (EI) Anal. Calcd. for $C_{20}H_{19}NO_3SCl$ [M^{+}+1]: 388.0774, Found: 388.0755.

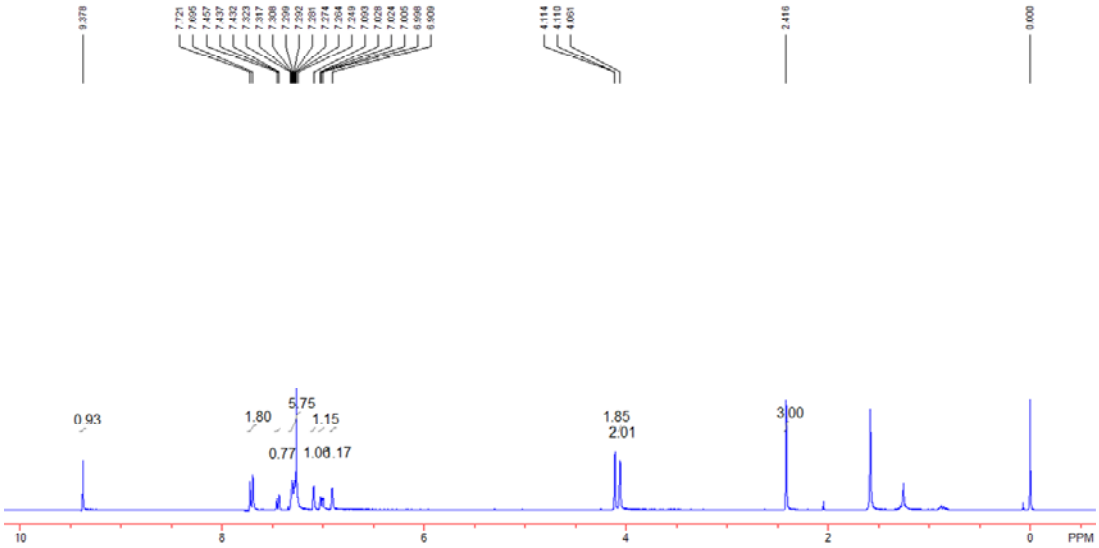


(*E*)-5-(2-chlorobenzylidene)-1-tosyl-1,2,5,6-tetrahydropyridine-3-carbaldehyde (*E*-71a):

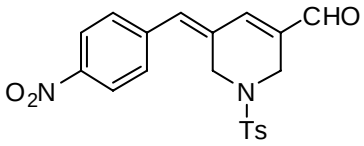


E-71a

Yield: 10 %; mp. 174-175 ^{o}C; IR (CH_2Cl_2, film) ν 2925, 2756, 1789, 1724, 1608, 1472, 1343, 1357, 1121, 1076, 719 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.38 (s, 1H), 7.71 (d, *J* = 7.8 Hz, 2H), 7.44 (dd, *J* = 1.5 Hz, 7.5 Hz, 1H), 7.32-7.23 (m, 4H), 7.09 (s, 1H), 7.01 (dd, *J* = 1.5 Hz, 7.5 Hz, 1H), 6.91 (s, 1H), 4.11 (s, 2H), 4.06 (s, 2H), 2.42 (s, 3H); ESI-MS *m/z* (relative intensity %): 388.1 (100) [M^{+}+1]; HRMS (EI) Anal. Calcd. for $C_{20}H_{19}NO_3SCl$ [M^{+}+1]: 388.0774, Found: 388.0759.

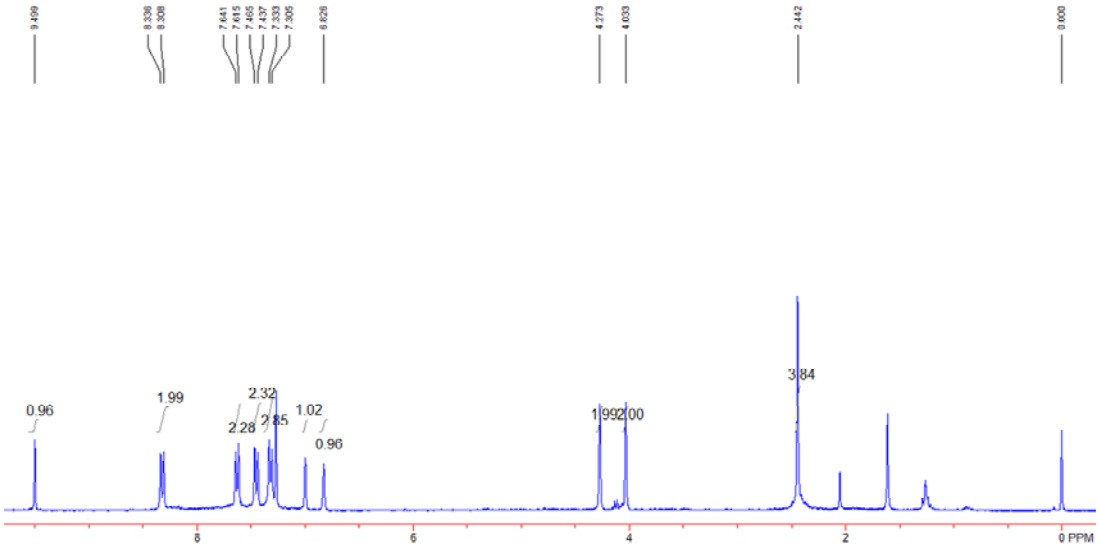


(*Z*)-5-(4-nitrobenzylidene)-1-tosyl-1,2,5,6-tetrahydropyridine-3-carbaldehyde (*Z*-71b)

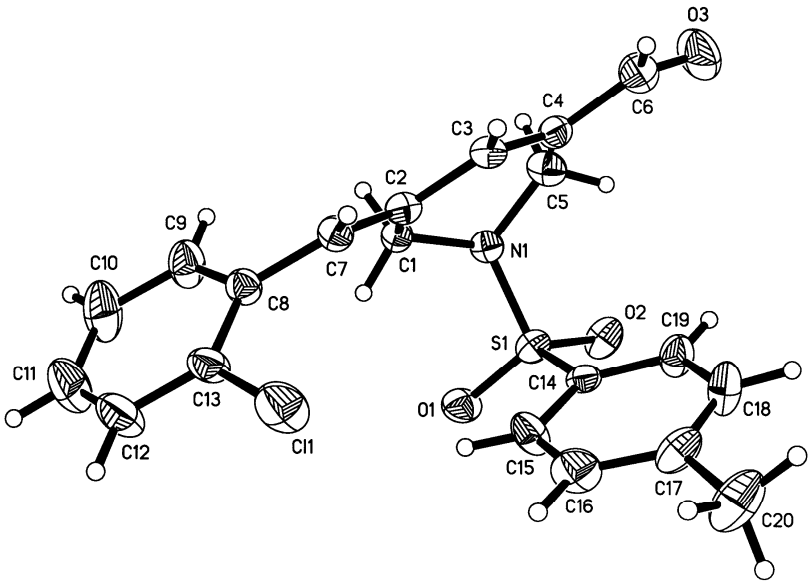


***Z*-71b**

Yield: 20 %; mp. 135-136 ^{o}C; IR (CH_2Cl_2, film) ν 3054, 2633, 1741, 1601, 1509, 1280, 1217, 1089, 818, 745, 694 cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.50 (s, 1H), 8.32 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 2H), 7.00 (s, 1H), 6.83 (s, 1H), 4.27 (s, 2H), 4.03 (s, 2H), 2.44 (s, 3H); ESI-MS *m/z* (relative intensity %): 399.1 (100) [M^{+}+1]; HRMS (EI) Anal. Calcd. for $C_{20}H_{19}NO_3SCl$ [M^{+}+1]: 399.1015, Found: 399.1023.



X-ray data of ***Z*-71a**:



The crystal data of Z-**71a** have been deposited in CCDC with number 710496. Temperature: 293K; Empirical Formula: $C_{20}H_{18}ClNO_3S$; Formula Weight: 387.86; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.475 x 0.366 x 0.157 mm; Crystal System: Monoclinic; Lattice Type: Primitive; Lattice Parameters: a = 24.333(5)Å, b = 8.0254(15)Å, c = 21.292(4)Å, $\alpha = 90^o$, $\beta = 113.925(4)^o$, $\gamma = 90^o$, V = 1973.1(11)Å^3; Space group: P2(1)/c; Z = 8; D_{calc} = 1.356 g/cm^3; F_{000} = 1616; Number of reflection: 7054; Number of independent reflections: 4265; R_{int} = 0.1307; Diffractometer: Rigaku AFC7R; Residuals: R; Rw: 0.1032, 0.2926. It should be noted that only one of the two independent molecules of the asymmetric unit is shown.

Table 1. Crystal data and structure refinement for cd28526.

Identification code	cd28526
Empirical formula	C20 H18 Cl N O3 S
Formula weight	387.86
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 24.333(5) A alpha = 90 deg. b = 8.0254(15) A beta = 113.925(4) deg. c = 21.292(4) A gamma = 90 deg.
Volume	3800.8(12) A^3
Z, Calculated density	8, 1.356 Mg/m^3
Absorption coefficient	0.330 mm^-1
F(000)	1616
Crystal size	0.475 x 0.366 x 0.157 mm
Theta range for data collection	1.91 to 25.50 deg.
Limiting indices	-29<=h<=24, -9<=k<=9, -25<=l<=25
Reflections collected / unique	19188 / 7054 [R(int) = 0.1307]
Completeness to theta = 25.50	99.6 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.7787
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7054 / 0 / 472
Goodness-of-fit on F^2	1.088
Final R indices [I>2sigma(I)]	R1 = 0.1032, wR2 = 0.2926
R indices (all data)	R1 = 0.1412, wR2 = 0.3099
Extinction coefficient	0.0020(9)
Largest diff. peak and hole	0.627 and -0.462 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cd28526.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	4320(1)	-477(2)	1297(1)	41(1)
S(2)	665(1)	-782(2)	1924(1)	45(1)
Cl(1)	5718(1)	3920(3)	150(1)	76(1)
Cl(2)	-787(1)	4071(3)	-562(1)	76(1)
N(1)	4565(2)	915(6)	1910(3)	39(1)
N(2)	392(2)	622(7)	2276(3)	41(1)
O(1)	4835(2)	-1414(6)	1347(2)	56(1)
O(2)	3841(2)	-1321(6)	1383(2)	55(1)
O(3)	3092(3)	4061(8)	1684(4)	85(2)
O(4)	159(2)	-1720(6)	1468(3)	57(1)
O(5)	1128(2)	-1629(6)	2473(3)	63(2)
O(6)	1824(3)	3918(9)	3433(4)	95(2)
C(1)	5133(3)	1794(8)	2025(3)	39(2)
C(2)	5028(3)	3391(8)	1624(3)	40(2)
C(3)	4466(3)	4226(8)	1486(3)	37(1)
C(4)	4049(3)	3606(8)	1679(3)	41(2)
C(5)	4124(3)	1955(9)	2031(4)	48(2)
C(6)	3499(3)	4544(10)	1538(4)	61(2)
C(7)	5420(3)	4021(8)	1388(3)	41(2)
C(8)	6014(3)	3360(8)	1505(3)	42(2)
C(9)	6425(3)	2847(11)	2136(4)	61(2)
C(10)	6995(4)	2273(14)	2244(5)	86(3)
C(11)	7155(4)	2231(13)	1697(5)	83(3)
C(12)	6765(4)	2743(12)	1063(4)	71(2)
C(13)	6205(3)	3304(9)	965(3)	50(2)
C(14)	4011(3)	512(8)	493(3)	38(1)
C(15)	4368(3)	806(10)	140(4)	54(2)
C(16)	4108(4)	1477(11)	-510(4)	64(2)
C(17)	3506(4)	1902(9)	-822(3)	55(2)
C(18)	3178(3)	1646(11)	-437(4)	63(2)
C(19)	3419(3)	953(10)	209(3)	53(2)
C(20)	3234(4)	2521(12)	-1545(4)	82(3)
C(21)	-177(3)	1470(8)	1846(3)	41(2)
C(22)	-71(3)	3075(8)	1542(3)	36(1)
C(23)	482(3)	3919(8)	1933(3)	41(2)
C(24)	896(3)	3329(8)	2517(3)	42(2)
C(25)	819(3)	1689(9)	2806(3)	48(2)
C(26)	1439(3)	4309(10)	2888(4)	61(2)
C(27)	-467(3)	3754(9)	953(3)	43(2)
C(28)	-1054(3)	3135(8)	506(3)	39(2)
C(29)	-1460(3)	2449(11)	747(4)	56(2)
C(30)	-2027(3)	1958(11)	310(5)	65(2)
C(31)	-2206(3)	2138(11)	-385(5)	66(2)
C(32)	-1825(4)	2786(10)	-643(4)	65(2)
C(33)	-1254(3)	3277(9)	-210(4)	49(2)
C(34)	1002(3)	214(8)	1439(3)	43(2)
C(35)	663(3)	599(10)	766(4)	56(2)
C(36)	921(4)	1371(10)	369(4)	58(2)
C(37)	1524(4)	1754(9)	644(4)	57(2)
C(38)	1849(4)	1408(11)	1314(5)	66(2)
C(39)	1608(3)	628(10)	1730(4)	57(2)
C(40)	1809(5)	2546(12)	205(5)	82(3)

Table 3. Bond lengths [A] and angles [deg] for cd28526.

S(1)-O(2)	1.423(5)
S(1)-O(1)	1.426(5)
S(1)-N(1)	1.636(5)
S(1)-C(14)	1.755(6)
S(2)-O(5)	1.426(5)
S(2)-O(4)	1.434(5)
S(2)-N(2)	1.635(5)
S(2)-C(34)	1.752(6)
Cl(1)-C(13)	1.729(7)
Cl(2)-C(33)	1.719(7)
N(1)-C(5)	1.462(8)
N(1)-C(1)	1.481(8)
N(2)-C(25)	1.462(9)
N(2)-C(21)	1.479(8)
O(3)-C(6)	1.215(9)
O(6)-C(26)	1.200(9)
C(1)-C(2)	1.503(9)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(7)	1.343(9)
C(2)-C(3)	1.442(9)
C(3)-C(4)	1.337(8)
C(3)-H(3)	0.9300
C(4)-C(6)	1.456(10)
C(4)-C(5)	1.496(9)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-H(6)	0.9300
C(7)-C(8)	1.464(9)
C(7)-H(7)	0.9300
C(8)-C(9)	1.372(10)
C(8)-C(13)	1.405(9)
C(9)-C(10)	1.389(12)
C(9)-H(9)	0.9300
C(10)-C(11)	1.370(13)
C(10)-H(10)	0.9300
C(11)-C(12)	1.362(12)
C(11)-H(11)	0.9300
C(12)-C(13)	1.369(11)
C(12)-H(12)	0.9300
C(14)-C(19)	1.363(9)
C(14)-C(15)	1.380(9)
C(15)-C(16)	1.377(10)
C(15)-H(15)	0.9300
C(16)-C(17)	1.385(11)
C(16)-H(16)	0.9300
C(17)-C(18)	1.373(10)
C(17)-C(20)	1.493(10)
C(18)-C(19)	1.374(10)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-C(22)	1.509(9)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(27)	1.349(9)
C(22)-C(23)	1.433(9)
C(23)-C(24)	1.330(9)
C(23)-H(23)	0.9300
C(24)-C(26)	1.463(10)
C(24)-C(25)	1.496(9)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-H(26)	0.9300
C(27)-C(28)	1.446(9)
C(27)-H(27)	0.9300

C(28)-C(29)	1.398(9)
C(28)-C(33)	1.404(9)
C(29)-C(30)	1.372(10)
C(29)-H(29)	0.9300
C(30)-C(31)	1.370(11)
C(30)-H(30)	0.9300
C(31)-C(32)	1.357(12)
C(31)-H(31)	0.9300
C(32)-C(33)	1.377(11)
C(32)-H(32)	0.9300
C(34)-C(35)	1.367(9)
C(34)-C(39)	1.387(9)
C(35)-C(36)	1.387(10)
C(35)-H(35)	0.9300
C(36)-C(37)	1.376(11)
C(36)-H(36)	0.9300
C(37)-C(38)	1.349(11)
C(37)-C(40)	1.512(10)
C(38)-C(39)	1.393(11)
C(38)-H(38)	0.9300
C(39)-H(39)	0.9300
C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600

O(2)-S(1)-O(1)	118.6(3)
O(2)-S(1)-N(1)	105.9(3)
O(1)-S(1)-N(1)	106.0(3)
O(2)-S(1)-C(14)	106.9(3)
O(1)-S(1)-C(14)	109.2(3)
N(1)-S(1)-C(14)	110.0(3)
O(5)-S(2)-O(4)	118.8(3)
O(5)-S(2)-N(2)	106.7(3)
O(4)-S(2)-N(2)	106.0(3)
O(5)-S(2)-C(34)	107.2(3)
O(4)-S(2)-C(34)	108.7(3)
N(2)-S(2)-C(34)	109.3(3)
C(5)-N(1)-C(1)	113.6(5)
C(5)-N(1)-S(1)	118.3(4)
C(1)-N(1)-S(1)	118.1(4)
C(25)-N(2)-C(21)	113.7(5)
C(25)-N(2)-S(2)	117.6(4)
C(21)-N(2)-S(2)	119.0(4)
N(1)-C(1)-C(2)	112.4(5)
N(1)-C(1)-H(1A)	109.1
C(2)-C(1)-H(1A)	109.1
N(1)-C(1)-H(1B)	109.1
C(2)-C(1)-H(1B)	109.1
H(1A)-C(1)-H(1B)	107.9
C(7)-C(2)-C(3)	120.5(6)
C(7)-C(2)-C(1)	123.4(6)
C(3)-C(2)-C(1)	116.1(6)
C(4)-C(3)-C(2)	122.8(6)
C(4)-C(3)-H(3)	118.6
C(2)-C(3)-H(3)	118.6
C(3)-C(4)-C(6)	119.6(6)
C(3)-C(4)-C(5)	121.9(6)
C(6)-C(4)-C(5)	118.5(6)
N(1)-C(5)-C(4)	111.5(5)
N(1)-C(5)-H(5A)	109.3
C(4)-C(5)-H(5A)	109.3
N(1)-C(5)-H(5B)	109.3
C(4)-C(5)-H(5B)	109.3
H(5A)-C(5)-H(5B)	108.0
O(3)-C(6)-C(4)	123.9(8)
O(3)-C(6)-H(6)	118.1
C(4)-C(6)-H(6)	118.1
C(2)-C(7)-C(8)	126.9(6)
C(2)-C(7)-H(7)	116.5
C(8)-C(7)-H(7)	116.5
C(9)-C(8)-C(13)	116.1(6)
C(9)-C(8)-C(7)	123.6(6)

C(13)-C(8)-C(7)	120.2(6)
C(8)-C(9)-C(10)	123.0(8)
C(8)-C(9)-H(9)	118.5
C(10)-C(9)-H(9)	118.5
C(11)-C(10)-C(9)	118.4(8)
C(11)-C(10)-H(10)	120.8
C(9)-C(10)-H(10)	120.8
C(12)-C(11)-C(10)	120.8(8)
C(12)-C(11)-H(11)	119.6
C(10)-C(11)-H(11)	119.6
C(11)-C(12)-C(13)	120.1(8)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(12)-C(13)-C(8)	121.7(7)
C(12)-C(13)-Cl(1)	118.8(6)
C(8)-C(13)-Cl(1)	119.5(5)
C(19)-C(14)-C(15)	119.9(6)
C(19)-C(14)-S(1)	120.6(5)
C(15)-C(14)-S(1)	119.5(5)
C(16)-C(15)-C(14)	118.8(7)
C(16)-C(15)-H(15)	120.6
C(14)-C(15)-H(15)	120.6
C(15)-C(16)-C(17)	122.9(7)
C(15)-C(16)-H(16)	118.6
C(17)-C(16)-H(16)	118.6
C(18)-C(17)-C(16)	115.8(7)
C(18)-C(17)-C(20)	123.0(8)
C(16)-C(17)-C(20)	121.1(8)
C(17)-C(18)-C(19)	122.8(7)
C(17)-C(18)-H(18)	118.6
C(19)-C(18)-H(18)	118.6
C(14)-C(19)-C(18)	119.8(7)
C(14)-C(19)-H(19)	120.1
C(18)-C(19)-H(19)	120.1
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(2)-C(21)-C(22)	112.3(5)
N(2)-C(21)-H(21A)	109.2
C(22)-C(21)-H(21A)	109.2
N(2)-C(21)-H(21B)	109.2
C(22)-C(21)-H(21B)	109.2
H(21A)-C(21)-H(21B)	107.9
C(27)-C(22)-C(23)	119.8(6)
C(27)-C(22)-C(21)	124.2(6)
C(23)-C(22)-C(21)	116.0(6)
C(24)-C(23)-C(22)	123.5(6)
C(24)-C(23)-H(23)	118.3
C(22)-C(23)-H(23)	118.3
C(23)-C(24)-C(26)	119.3(7)
C(23)-C(24)-C(25)	121.6(6)
C(26)-C(24)-C(25)	119.1(6)
N(2)-C(25)-C(24)	111.5(5)
N(2)-C(25)-H(25A)	109.3
C(24)-C(25)-H(25A)	109.3
N(2)-C(25)-H(25B)	109.3
C(24)-C(25)-H(25B)	109.3
H(25A)-C(25)-H(25B)	108.0
O(6)-C(26)-C(24)	124.2(8)
O(6)-C(26)-H(26)	117.9
C(24)-C(26)-H(26)	117.9
C(22)-C(27)-C(28)	128.0(6)
C(22)-C(27)-H(27)	116.0
C(28)-C(27)-H(27)	116.0
C(29)-C(28)-C(33)	116.4(6)
C(29)-C(28)-C(27)	123.4(6)
C(33)-C(28)-C(27)	120.1(6)
C(30)-C(29)-C(28)	122.0(7)
C(30)-C(29)-H(29)	119.0

C(28)-C(29)-H(29)	119.0
C(31)-C(30)-C(29)	119.6(8)
C(31)-C(30)-H(30)	120.2
C(29)-C(30)-H(30)	120.2
C(32)-C(31)-C(30)	120.5(7)
C(32)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7
C(31)-C(32)-C(33)	120.5(8)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(32)-C(33)-C(28)	121.0(7)
C(32)-C(33)-Cl(2)	118.7(6)
C(28)-C(33)-Cl(2)	120.3(6)
C(35)-C(34)-C(39)	119.6(7)
C(35)-C(34)-S(2)	119.5(5)
C(39)-C(34)-S(2)	120.9(6)
C(34)-C(35)-C(36)	120.7(7)
C(34)-C(35)-H(35)	119.6
C(36)-C(35)-H(35)	119.6
C(37)-C(36)-C(35)	120.5(8)
C(37)-C(36)-H(36)	119.8
C(35)-C(36)-H(36)	119.8
C(38)-C(37)-C(36)	118.1(7)
C(38)-C(37)-C(40)	121.4(8)
C(36)-C(37)-C(40)	120.5(8)
C(37)-C(38)-C(39)	123.2(7)
C(37)-C(38)-H(38)	118.4
C(39)-C(38)-H(38)	118.4
C(34)-C(39)-C(38)	117.9(7)
C(34)-C(39)-H(39)	121.0
C(38)-C(39)-H(39)	121.0
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd28526.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	48(1)	36(1)	40(1)	2(1)	17(1)	-5(1)
S(2)	51(1)	39(1)	56(1)	4(1)	33(1)	2(1)
Cl(1)	73(1)	115(2)	44(1)	10(1)	26(1)	23(1)
Cl(2)	89(2)	96(2)	56(1)	2(1)	43(1)	-19(1)
N(1)	43(3)	39(3)	37(3)	3(2)	20(2)	-2(2)
N(2)	44(3)	45(3)	40(3)	7(2)	24(3)	10(3)
O(1)	61(3)	47(3)	52(3)	-1(2)	16(2)	18(2)
O(2)	61(3)	47(3)	54(3)	6(2)	20(2)	-22(2)
O(3)	59(4)	96(5)	121(5)	-8(4)	56(4)	-6(3)
O(4)	65(3)	54(3)	68(3)	-12(3)	43(3)	-19(3)
O(5)	77(4)	52(3)	72(4)	22(3)	42(3)	21(3)
O(6)	51(4)	104(5)	89(5)	-8(4)	-14(3)	-14(4)
C(1)	37(3)	47(4)	34(3)	0(3)	16(3)	-3(3)
C(2)	45(4)	36(3)	35(3)	-1(3)	15(3)	2(3)
C(3)	44(4)	32(3)	36(3)	1(3)	18(3)	0(3)
C(4)	40(4)	46(4)	39(3)	-7(3)	18(3)	-6(3)
C(5)	58(4)	52(4)	47(4)	5(3)	35(4)	-3(3)
C(6)	53(5)	51(5)	80(6)	-9(4)	27(4)	-4(4)
C(7)	41(4)	47(4)	38(3)	0(3)	20(3)	-3(3)
C(8)	42(4)	47(4)	40(4)	1(3)	18(3)	1(3)
C(9)	43(4)	94(6)	43(4)	9(4)	12(3)	1(4)
C(10)	45(5)	122(8)	77(6)	31(6)	11(5)	8(5)
C(11)	54(5)	108(8)	91(7)	16(6)	32(5)	25(5)
C(12)	64(5)	101(7)	61(5)	0(5)	38(5)	20(5)
C(13)	54(4)	60(4)	43(4)	-3(3)	27(3)	7(4)
C(14)	44(4)	39(3)	35(3)	-9(3)	21(3)	-7(3)
C(15)	46(4)	69(5)	57(4)	11(4)	31(4)	11(4)
C(16)	78(6)	78(6)	46(4)	8(4)	36(4)	1(5)
C(17)	67(5)	52(4)	34(4)	2(3)	10(4)	-16(4)
C(18)	37(4)	85(6)	57(5)	10(4)	8(4)	-8(4)
C(19)	41(4)	81(5)	37(4)	3(4)	14(3)	-7(4)
C(20)	95(7)	93(7)	38(4)	15(4)	7(4)	-27(6)
C(21)	39(4)	47(4)	47(4)	0(3)	28(3)	-1(3)
C(22)	32(3)	44(4)	42(4)	-2(3)	25(3)	4(3)
C(23)	41(4)	43(4)	42(4)	-3(3)	21(3)	0(3)
C(24)	35(3)	48(4)	41(4)	-5(3)	14(3)	5(3)
C(25)	52(4)	58(4)	38(4)	3(3)	24(3)	10(4)
C(26)	41(4)	60(5)	75(6)	-11(4)	14(4)	1(4)
C(27)	45(4)	49(4)	44(4)	-1(3)	27(3)	2(3)
C(28)	30(3)	47(4)	41(3)	2(3)	17(3)	7(3)
C(29)	35(4)	90(6)	49(4)	2(4)	24(3)	0(4)
C(30)	37(4)	80(6)	76(6)	1(5)	20(4)	-2(4)
C(31)	36(4)	74(6)	72(6)	-5(5)	6(4)	-10(4)
C(32)	61(5)	68(5)	49(4)	-1(4)	5(4)	-2(4)
C(33)	59(5)	45(4)	43(4)	3(3)	23(4)	0(3)
C(34)	47(4)	45(4)	47(4)	-2(3)	29(3)	3(3)
C(35)	53(4)	67(5)	49(4)	2(4)	23(4)	-10(4)
C(36)	61(5)	66(5)	52(4)	8(4)	28(4)	-4(4)
C(37)	67(5)	52(4)	74(5)	1(4)	49(5)	1(4)
C(38)	44(4)	75(6)	88(6)	3(5)	37(5)	-2(4)
C(39)	38(4)	74(5)	59(5)	-1(4)	19(4)	-2(4)
C(40)	96(7)	80(6)	106(7)	13(6)	78(6)	-3(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cd28526.

	x	y	z	U(eq)
H(1A)	5387	1069	1892	46
H(1B)	5344	2038	2510	46
H(3)	4391	5237	1254	44
H(5A)	4254	2129	2521	57
H(5B)	3740	1382	1863	57
H(6)	3457	5575	1323	73
H(7)	5300	4980	1121	49
H(9)	6318	2886	2508	74
H(10)	7262	1925	2677	103
H(11)	7535	1848	1759	100
H(12)	6879	2712	695	86
H(15)	4776	555	338	65
H(16)	4349	1653	-750	76
H(18)	2774	1955	-620	76
H(19)	3180	787	451	64
H(20A)	3112	1591	-1855	123
H(20B)	3525	3172	-1635	123
H(20C)	2890	3200	-1610	123
H(21A)	-400	1707	2123	49
H(21B)	-419	731	1477	49
H(23)	555	4933	1770	49
H(25A)	1205	1130	3009	57
H(25B)	678	1877	3165	57
H(26)	1489	5297	2689	74
H(27)	-348	4743	817	52
H(29)	-1343	2321	1218	67
H(30)	-2288	1507	484	78
H(31)	-2591	1814	-682	79
H(32)	-1951	2899	-1115	78
H(35)	256	341	573	67
H(36)	684	1631	-88	70
H(38)	2253	1706	1507	79
H(39)	1846	391	2188	69
H(40A)	2141	3228	488	123
H(40B)	1517	3223	-143	123
H(40C)	1950	1691	-8	123

Table 6. Torsion angles [deg] for cd28526.

O(2)-S(1)-N(1)-C(5)	-46.8(5)
O(1)-S(1)-N(1)-C(5)	-173.7(4)
C(14)-S(1)-N(1)-C(5)	68.4(5)
O(2)-S(1)-N(1)-C(1)	169.7(4)
O(1)-S(1)-N(1)-C(1)	42.8(5)
C(14)-S(1)-N(1)-C(1)	-75.1(5)
O(5)-S(2)-N(2)-C(25)	48.2(5)
O(4)-S(2)-N(2)-C(25)	175.7(4)
C(34)-S(2)-N(2)-C(25)	-67.3(5)
O(5)-S(2)-N(2)-C(21)	-167.7(4)
O(4)-S(2)-N(2)-C(21)	-40.3(5)
C(34)-S(2)-N(2)-C(21)	76.7(5)
C(5)-N(1)-C(1)-C(2)	-53.2(7)
S(1)-N(1)-C(1)-C(2)	91.9(6)
N(1)-C(1)-C(2)-C(7)	-149.3(6)
N(1)-C(1)-C(2)-C(3)	29.3(7)
C(7)-C(2)-C(3)-C(4)	176.5(6)
C(1)-C(2)-C(3)-C(4)	-2.2(9)
C(2)-C(3)-C(4)-C(6)	178.3(6)
C(2)-C(3)-C(4)-C(5)	-2.4(10)
C(1)-N(1)-C(5)-C(4)	48.0(7)
S(1)-N(1)-C(5)-C(4)	-97.0(6)
C(3)-C(4)-C(5)-N(1)	-20.5(9)
C(6)-C(4)-C(5)-N(1)	158.8(6)
C(3)-C(4)-C(6)-O(3)	178.6(7)
C(5)-C(4)-C(6)-O(3)	-0.6(11)
C(3)-C(2)-C(7)-C(8)	177.5(6)
C(1)-C(2)-C(7)-C(8)	-3.9(10)
C(2)-C(7)-C(8)-C(9)	-45.6(11)
C(2)-C(7)-C(8)-C(13)	137.8(7)
C(13)-C(8)-C(9)-C(10)	-1.2(12)
C(7)-C(8)-C(9)-C(10)	-177.8(8)
C(8)-C(9)-C(10)-C(11)	0.6(15)
C(9)-C(10)-C(11)-C(12)	0.1(16)
C(10)-C(11)-C(12)-C(13)	-0.2(16)
C(11)-C(12)-C(13)-C(8)	-0.4(14)
C(11)-C(12)-C(13)-Cl(1)	-179.2(8)
C(9)-C(8)-C(13)-C(12)	1.1(11)
C(7)-C(8)-C(13)-C(12)	177.9(8)
C(9)-C(8)-C(13)-Cl(1)	179.8(6)
C(7)-C(8)-C(13)-Cl(1)	-3.4(9)
O(2)-S(1)-C(14)-C(19)	26.0(6)
O(1)-S(1)-C(14)-C(19)	155.5(6)
N(1)-S(1)-C(14)-C(19)	-88.6(6)
O(2)-S(1)-C(14)-C(15)	-152.4(6)
O(1)-S(1)-C(14)-C(15)	-22.9(6)
N(1)-S(1)-C(14)-C(15)	93.0(6)
C(19)-C(14)-C(15)-C(16)	-2.9(11)
S(1)-C(14)-C(15)-C(16)	175.5(6)
C(14)-C(15)-C(16)-C(17)	1.3(12)
C(15)-C(16)-C(17)-C(18)	1.3(12)
C(15)-C(16)-C(17)-C(20)	-175.9(8)
C(16)-C(17)-C(18)-C(19)	-2.4(12)
C(20)-C(17)-C(18)-C(19)	174.8(8)
C(15)-C(14)-C(19)-C(18)	1.8(11)
S(1)-C(14)-C(19)-C(18)	-176.5(6)
C(17)-C(18)-C(19)-C(14)	0.9(13)
C(25)-N(2)-C(21)-C(22)	52.7(7)
S(2)-N(2)-C(21)-C(22)	-92.6(6)
N(2)-C(21)-C(22)-C(27)	153.4(6)
N(2)-C(21)-C(22)-C(23)	-28.7(7)
C(27)-C(22)-C(23)-C(24)	-179.7(6)
C(21)-C(22)-C(23)-C(24)	2.3(9)
C(22)-C(23)-C(24)-C(26)	-178.3(6)
C(22)-C(23)-C(24)-C(25)	1.5(10)
C(21)-N(2)-C(25)-C(24)	-48.4(7)
S(2)-N(2)-C(25)-C(24)	97.4(6)
C(23)-C(24)-C(25)-N(2)	21.6(8)

C(26)-C(24)-C(25)-N(2)	-158.7(6)
C(23)-C(24)-C(26)-O(6)	176.5(8)
C(25)-C(24)-C(26)-O(6)	-3.2(12)
C(23)-C(22)-C(27)-C(28)	-177.2(6)
C(21)-C(22)-C(27)-C(28)	0.6(10)
C(22)-C(27)-C(28)-C(29)	41.2(10)
C(22)-C(27)-C(28)-C(33)	-141.9(7)
C(33)-C(28)-C(29)-C(30)	-0.8(11)
C(27)-C(28)-C(29)-C(30)	176.2(7)
C(28)-C(29)-C(30)-C(31)	0.1(13)
C(29)-C(30)-C(31)-C(32)	0.4(13)
C(30)-C(31)-C(32)-C(33)	-0.2(13)
C(31)-C(32)-C(33)-C(28)	-0.5(12)
C(31)-C(32)-C(33)-Cl(2)	179.4(7)
C(29)-C(28)-C(33)-C(32)	1.0(10)
C(27)-C(28)-C(33)-C(32)	-176.1(7)
C(29)-C(28)-C(33)-Cl(2)	-178.9(6)
C(27)-C(28)-C(33)-Cl(2)	4.0(9)
O(5)-S(2)-C(34)-C(35)	156.4(6)
O(4)-S(2)-C(34)-C(35)	26.8(7)
N(2)-S(2)-C(34)-C(35)	-88.4(6)
O(5)-S(2)-C(34)-C(39)	-24.1(7)
O(4)-S(2)-C(34)-C(39)	-153.6(6)
N(2)-S(2)-C(34)-C(39)	91.1(6)
C(39)-C(34)-C(35)-C(36)	1.2(12)
S(2)-C(34)-C(35)-C(36)	-179.3(6)
C(34)-C(35)-C(36)-C(37)	0.4(12)
C(35)-C(36)-C(37)-C(38)	-2.2(12)
C(35)-C(36)-C(37)-C(40)	178.1(8)
C(36)-C(37)-C(38)-C(39)	2.6(13)
C(40)-C(37)-C(38)-C(39)	-177.7(8)
C(35)-C(34)-C(39)-C(38)	-0.9(11)
S(2)-C(34)-C(39)-C(38)	179.6(6)
C(37)-C(38)-C(39)-C(34)	-1.1(13)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd28526 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(18)-H(18)...O(6)#1	0.93	2.47	3.227(10)	138.1

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z-1/2