Supporting Information

X-ray Analysis of (+)-23.HCl

Intensity data ($2<\theta<24°$) were measured on a Siemens SMART CCD diffractometer. 4141 recorded reflections were merged yielding 1830 unique reflections and of these 1342 reflections with $I>2\sigma(I)$ were considered observed. Intensities were corrected for Lorentz, polarization, extinction and absorption effects and for crystal decay. The structure was solved by direct methods using the program SHELXS-86 (Sheldrick, 1990). The structure was refined by the full-matrix least-squares method using the program SHELXL-97 (Sheldrick, 1997). Convergence was reached at R=0.0700 and wR^2=0.2040 for observed reflections. At this stage a difference map showed a maximum and minimum electron density of 0.48 and –0.33 e Å^{-3}, respectively.

Crystal data: $C_{12}H_{16}ClNO_2S$, M=273.77, monoclinic, space group $P2_1$, Z=2, a=7.6773(4), b=7.4775(4), c=11.5310(6) Å, β=93.946(2)°, V=660.39(6) Å^3, D_x=1.377 g cm^{-3}, λ(Mo Kα)=0.71073 Å.

Table 1. Atomic coordinates and equivalent U values for the non-hydrogen atoms. Estimated standard deviations are given in parentheses.

Atom	x	y	z	Ueq
Cl1	0.2965(3)	0.6550(4)	0.5501(2)	0.0904(9)
O1	0.8305(7)	0.6317(10)	0.2242(6)	0.0869(19)
C2	0.9136(11)	0.6042(13)	0.3324(11)	0.105(4)
C3	0.7920(13)	0.6565(17)	0.4290(9)	0.097(3)
N4	0.6190(8)	0.5541(10)	0.4122(6)	0.0727(19)
C4A	0.5434(9)	0.5788(10)	0.2884(6)	0.0560(19)
C5	0.3809(8)	0.4699(10)	0.2696(6)	0.058(2)
S6	0.2702(2)	0.5267(4)	0.13265(19)	0.0789(7)
C6A	0.4432(10)	0.5262(12)	0.0424(7)	0.0675(19)
C7	0.3951(19)	0.5226(16)	-0.0748(9)	0.106(3)
C8	0.501(3)	0.534(2)	-0.1566(14)	0.140(5)
C9	0.675(3)	0.5351(17)	-0.1251(10)	0.136(6)
O9	0.798(2)	0.5414(14)	-0.2237(7)	0.178(5)
C9A	0.9424(15)	0.554(2)	-0.1707(11)	0.121(4)
C10	0.7429(14)	0.5365(14)	-0.0067(10)	0.096(3)
C10A	0.6189(11)	0.5339(12)	0.0805(7)	0.074(2)
C10B	0.6810(8)	0.5227(11)	0.2061(7)	0.062(2)

Table 2. Atomic coordinates and isotropic U values for the hydrogen atoms. The isotropic temperature factors were set to 1.2 times the Ueq value of the corresponding parent atom.

Atom	x	y	z	Uiso
H2A	1.0193	0.6755	0.3403	0.126
H2B	0.9463	0.4793	0.3409	0.126
H3A	0.7695	0.7841	0.4259	0.116
H3B	0.8486	0.6286	0.5046	0.116
H4A	0.6373	0.4371	0.4268	0.087
H4B	0.5434	0.5953	0.4622	0.087
H4A1	0.5148	0.7053	0.2755	0.067
H5A	0.3049	0.4925	0.3317	0.070
H5B	0.4103	0.3438	0.2706	0.070
H7	0.2768	0.5112	-0.0967	0.128
H8	0.4595	0.5405	-0.2342	0.167
H9A1	0.9478	0.6619	-0.1259	0.146
H9A2	1.0315	0.5553	-0.2251	0.146
H9A3	0.9603	0.4528	-0.1197	0.146
H10	0.8624	0.5391	0.0129	0.115
H10B	0.7147	0.3987	0.2237	0.074

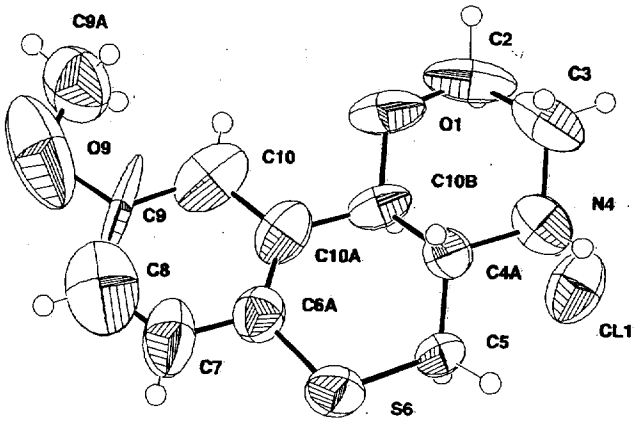

Fig 1. Molecular structure of (+)-23.HCl

Table 3. Anisotropic temperature factors for the non-hydrogen atoms. Estimated standard deviations are given in parentheses.

Atom	U11	U22	U33	U12	U13	U23
Cl1	0.1204(19)	0.0661(13)	0.0884(15)	-0.0138(13)	0.0336(14)	-0.0093(15)
O1	0.040(3)	0.086(4)	0.135(5)	0.020(4)	0.007(3)	-0.010(3)
C2	0.038(4)	0.077(7)	0.198(13)	-0.016(7)	-0.012(7)	-0.005(4)
C3	0.097(7)	0.068(5)	0.117(7)	-0.002(8)	-0.048(6)	-0.009(7)
N4	0.071(4)	0.062(4)	0.082(4)	0.001(4)	-0.016(3)	0.017(4)
C4A	0.053(4)	0.058(4)	0.056(4)	0.008(3)	-0.004(3)	0.007(3)
C5	0.042(4)	0.074(6)	0.060(4)	0.001(4)	0.012(3)	-0.006(3)
S6	0.0502(10)	0.1026(17)	0.0828(14)	0.0100(14)	-0.0034(9)	-0.0038(13)
C6A	0.079(5)	0.061(5)	0.063(5)	-0.002(5)	0.012(4)	-0.003(5)
C7	0.171(11)	0.085(7)	0.065(6)	0.012(6)	0.018(7)	-0.006(8)
C8	0.218(16)	0.075(8)	0.124(12)	0.003(8)	0.001(12)	0.022(12)
C9	0.300(19)	0.064(6)	0.059(6)	0.023(6)	0.118(10)	0.044(12)
O9	0.315(15)	0.106(6)	0.101(6)	-0.003(6)	-0.073(8)	0.041(10)
C9A	0.127(9)	0.129(10)	0.104(8)	0.020(8)	-0.023(8)	0.009(9)
C10	0.101(6)	0.061(6)	0.131(9)	0.022(6)	0.044(6)	0.024(6)
C10A	0.087(6)	0.059(5)	0.080(6)	0.017(5)	0.027(5)	0.015(6)
C10B	0.043(3)	0.050(4)	0.095(6)	0.009(5)	0.020(4)	0.002(4)

Table 4. Bond distances (Å). Estimated standard deviations are given in parentheses.

O1	C2	1.378(12)
O1	C10B	1.412(9)
C2	C3	1.552(14)
C3	N4	1.534(12)
N4	C4A	1.515(9)
C4A	C5	1.493(10)
C4A	C10B	1.526(10)
C5	S6	1.792(7)
S6	C6A	1.743(8)
C6A	C10A	1.390(11)
C6A	C7	1.377(12)
C7	C8	1.288(18)
C8	C9	1.37(2)
C9	C10	1.426(19)
C9	O9	1.527(16)
O9	C9A	1.229(13)
C10	C10A	1.432(12)
C10A	C10B	1.496(11)

Table 5. Bond angles (deg). Estimated standard deviations are given in parentheses.

C2	O1	C10B	111.7(7)
O1	C2	C3	110.4(7)
C2	C3	N4	110.0(8)
C4A	N4	C3	109.3(6)
C5	C4A	N4	109.4(6)
C5	C4A	C10B	111.5(6)
N4	C4A	C10B	108.4(5)
C4A	C5	S6	109.9(5)
C6A	S6	C5	101.0(4)
C10A	C6A	C7	120.0(9)
C10A	C6A	S6	125.0(6)
C7	C6A	S6	115.0(8)
C8	C7	C6A	125.3(14)
C9	C8	C7	117.5(14)
C8	C9	C10	122.7(11)
C8	C9	O9	116.6(14)
C10	C9	O9	120.6(16)
C9A	O9	C9	102.3(11)
C9	C10	C10A	117.2(11)
C6A	C10A	C10	117.1(9)
C6A	C10A	C10B	122.8(7)
C10	C10A	C10B	119.9(8)
O1	C10B	C10A	108.2(7)
O1	C10B	C4A	109.9(7)
C10A	C10B	C4A	113.5(6)

Elemental Analyses

(HRMS = High Resolution Mass Spectroscopy)

Compound	Formula	Calculated	Observed
13	$C_{10}H_{12}O_3S \cdot ¼H_2O$	% C 55.43	% C 55.75
		% H 5.77	% H 5.59
14	$C_{10}H_{10}O_2S$	HRMS: 194.0401	HRMS: 194.0400
15	$C_{10}H_{11}NO_2S$	% C 57.40	% C 57.39
		% H 5.26	% H 5.28
		% N 6.69	% N 6.64
16	$C_{10}H_{11}NO_2S$	HRMS: 209.0510	HRMS: 209.0512
17 and 18	$C_{10}H_{13}NO_2S$	HRMS: 211.0667	HRMS: 211.0687
19	$C_{12}H_{14}NO_3SCl$	% C 50.09	% C 50.15
		% H 4.90	% H 4.95
		% N 4.87	% N 4.74
20	$C_{12}H_{14}NO_3SCl$	HRMS: 287.0383	HRMS: 287.0409
21	$C_{12}H_{13}NO_3S$	% C 57.35	% C 57.00
		% H 5.21	% H 5.16
		% N 5.57	% N 5.53

22	$C_{12}H_{13}NO_3S$	% C 57.35	% C 57.10
		% H 5.21	% H 5.00
		% N 5.57	% N 5.43
23	$C_{12}H_{15}NO_2S \cdot \frac{1}{4}H_2O$	% C 59.63	% C 59.72
		% H 6.42	% H 6.32
		% N 5.80	% N 5.75
24	$C_{12}H_{15}NO_2S$	HRMS: 237.0823	HRMS: 237.0829
25	$C_{21}H_{23}NO_4S$	% C 65.45	% C 65.28
		% H 5.97	% H 6.06
		% N 3.64	% N 3.58
26	$C_{21}H_{23}NO_4S$	HRMS: 385.1348	HRMS: 385.1349
(+)-23	$C_{12}H_{15}NO_2S \cdot HCl$	% C 52.65	% C 52.51
		% H 5.89	% H 6.08
		% N 5.12	% N 5.08
(–)-23	$C_{12}H_{15}NO_2S \cdot HCl$	% C 52.65	% C 52.63
		% H 5.89	% H 5.86
		% N 5.12	% N 5.12
27	$C_{15}H_{21}NO_2S$	HRMS: 279.1293	HRMS: 279.1286
(–)-27	$C_{15}H_{21}NO_2S \cdot HCl$	% C 57.04	% C 56.84
		% H 7.02	% H 6.88
		% N 4.43	% N 4.36

(+)-27	$C_{15}H_{21}NO_2S \cdot HCl$	% C 57.04	% C 56.91
		% H 7.02	% H 7.10
		% N 4.43	% N 4.36
28	$C_{15}H_{21}NO_2S$	HRMS: 279.1293	HRMS: 279.1282
9	$C_{14}H_{19}NO_2S \cdot HCl$	% C 55.71	% C 55.52
		% H 6.68	% H 6.64
		% N 4.64	% N 4.38
(–)-9	$C_{14}H_{19}NO_2S \cdot HCl$	% C 55.71	% C 55.61
		% H 6.68	% H 6.66
		% N 4.64	% N 4.59
(+)-9	$C_{14}H_{19}NO_2S \cdot HCl$	% C 55.71	% C 55.58
		% H 6.68	% H 6.65
		% N 4.64	% N 4.64
10	$C_{14}H_{19}NO_2S \cdot HCl \cdot$	% C 53.28	% C 53.55
	$¾H_2O$	% H 6.82	% H 7.05
		% N 4.44	% N 4.24
11	$C_{14}H_{19}NO_3S$	HRMS: 281.1086	HRMS: 281.1100