

Conformationally Constrained Nicotines: Polycyclic, Bridged and Spiroannulated Analogues as Novel Ligands for the Nicotinic Acetylcholine Receptor

Thomas Ullrich,^{*,†} Sylvia Krich,[†] Dieter Binder,[†] Kurt Mereiter,[‡] David J. Anderson,[§] Michael D. Meyer,[§] and Michael Pyerin[†]

[†]*Institute of Applied Synthetic Chemistry, Vienna University of Technology, Getreidemarkt 9/E163, A-1060 Vienna, Austria,*

[‡]*Institute of Chemical Technologies and Analytics, Vienna University of Technology, Getreidemarkt 9/E164, A-1060 Vienna, Austria,*

[§]*Neurological and Urological Diseases Research, Pharmaceutical Products Division, Abbott Laboratories, Dept. 47W, Bldg. AP-9A/311, 100 Abbott Park Rd., Abbott Park, IL 60064-6125, USA*

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Fig. S1 and Tables S1 to S5: Drawing, crystallographic data, atomic coordinates, hydrogen coordinates, anisotropic displacement parameters, bond lengths and bond angles of **16** = (2*R*,3*R*)-(-)-*O*,*O'*-di-*p*-toluoyltartrate of (*R*)-(-)-**4a** = (*R*)-(-)-1,3*a*-ethano-1,2,3,3*a*,4,8*b*-hexahydropyrrolo[3',2': 4,5]cyclopenta[1,2-*c*]-pyridine, salt with (2*R*,3*R*)-(-)-*O*,*O'*-di-*p*-toluoyltartaric acid.

Fig. S2 and Tables S6 to S10: Drawing, crystallographic data, atomic coordinates, hydrogen coordinates, anisotropic displacement parameters, bond lengths and bond angles of **17** = (2*S*,3*S*)-(+)-*O*,*O'*-di-*p*-toluoyltartrate of (4*aS*)-(+)-**4b** = [4*aS*-(4*α*,9*β*)]-(+)-2*H*-1,4*a*-ethano-3,4,5,9*b*-tetrahydro-1*H*-cyclopenta[2,1-*b*: 3,4-*c'*]dipyridine, salt with (2*S*,3*S*)-(+)-*O*,*O'*-di-*p*-toluoyltartaric acid.

Fig. S3 and Tables S11 to S15: Drawing, crystallographic data, atomic coordinates, hydrogen coordinates, anisotropic displacement parameters, bond lengths and bond angles of (*R*)-(-)-**5b**·2*HCl* = (*R*)-(-)-1,2,3,4,10,11-*h*-hexahydro-1-methylspiro[7*H*-2-pyridine-7,2'-2*H*-pyrrole]dihydrochloride.

Fig. S1. Chemical diagram and thermal ellipsoid plot (20% ellipsoids) of the asymmetric unit of the crystal structure of **16** = (2*R*,3*R*)-(-)-*O*,*O'*-di-*p*-toluoyltartrate of (*R*)-(-)-**4a**.

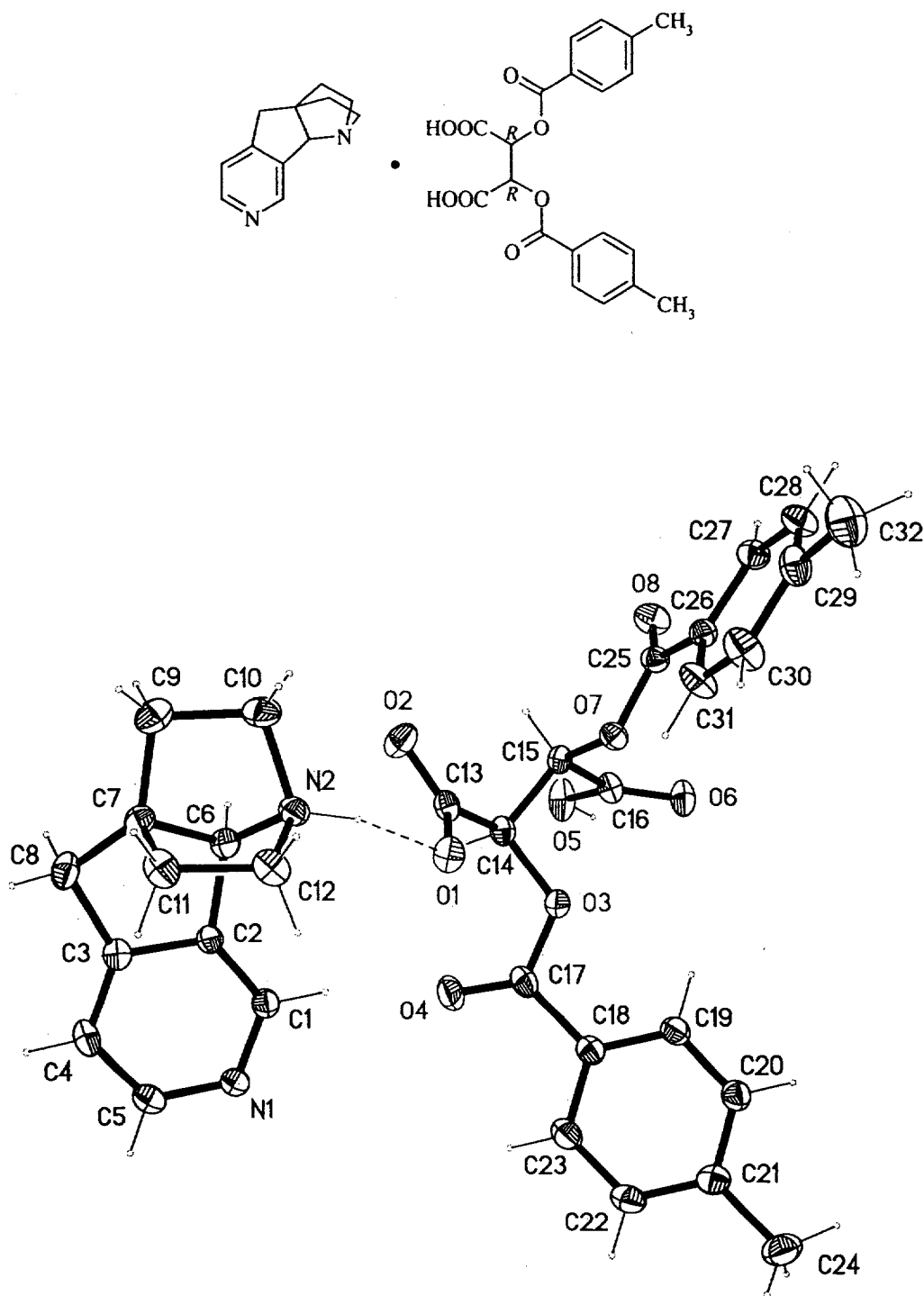


Table S1. Crystal data and structure refinement of **16** = (2*R*,3*R*)-(-)-*O*,*O'*-di-*p*-toluoyltartrate of (*R*)-(-)-**4a**.

Identification code	443j3fr
Empirical formula	C ₃₂ H ₃₂ N ₂ O ₈
Formula weight	572.60
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system, space group	orthorhombic, P2 ₁ 2 ₁ 2 ₁ (No. 19)
Unit cell dimensions §	a = 12.277(5) Å α = 90 deg. b = 15.126(5) Å β = 90 deg. c = 15.957(5) Å γ = 90 deg.
Volume	2963.2(18) Å ³
Z, Calculated density	4, 1.283 Mg/m ³
Absorption coefficient	0.093 mm ⁻¹
F(000)	1208
Crystal size	0.24 x 0.20 x 0.18 mm, colorless prism
Diffractometer	Siemens SMART 3-circle with CCD area detector (sealed X-ray tube, Mo Kα radiation, graphite monochromator, detector distance 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 20 sec. per frame, complete Ewald sphere, 4 x 606 frames
Theta range for data collection	1.9 to 25.0 deg.
Index ranges	-14 ≤ h ≤ 14, -17 ≤ k ≤ 17, -18 ≤ l ≤ 18
Reflections collected / unique	29164 / 5177 [R(int)=0.074, R(sigma)=0.044]
Completeness to theta = 24.99°	99.6%
Absorption correction	none
Structure solution	Direct methods (program SHELXS97)
Refinement method	Full-matrix least-squares on F ² (SHELXL97)
Data / restraints / parameters	5177 / 0 / 388
Goodness-of-fit on F ²	1.102
Final R indices [I>2sigma(I)]	R1 = 0.0562, wR2 = 0.0890 (4078 data)
R indices (all data)	R1 = 0.0797, wR2 = 0.0970 (5177 data)
Absolute structure parameter §§	0.9(12)
Extinction coefficient	0.0055(5)
Largest diff. peak and hole	0.127 and -0.131 e Å ⁻³

$$R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad wR2 = \left[\frac{\sum (w(F_o^2 - F_c^2)^2)}{\sum (w(F_o^2)^2)} \right]^{1/4}$$

§) Compounds 16 (Tables S1 – S5) and 17 (Tables S6 – S10) form an enantiomeric pair of almost identical structures, which differ only by one ring CH₂ group but not in the basic spatial arrangement, orientation, and mutual hydrogen bonding of their constituents.

§§) Absolute structure via known chirality of (2R,3R)-(-)-O,O'-di-p-toluoyltartaric acid

Table S2. Atomic coordinates and equivalent isotropic displacement parameters (Å² x 10³) of 16 = (2R,3R)-(-)-O,O'-di-p-toluoyltartrate of (R)-(-)-4a. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

x	y	z	U _{eq}
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Amine				
N(1)	0.2678(2)	0.5616(2)	0.6505(2)	52(1)
N(2)	0.4185(2)	0.3612(2)	0.4564(2)	49(1)
C(1)	0.3263(2)	0.5232(2)	0.5901(2)	48(1)
C(2)	0.3695(2)	0.4403(2)	0.5998(2)	41(1)
C(3)	0.3556(2)	0.3952(2)	0.6756(2)	46(1)
C(4)	0.2919(3)	0.4335(2)	0.7370(2)	56(1)
C(5)	0.2492(3)	0.5169(2)	0.7210(2)	57(1)
C(6)	0.4415(2)	0.3848(2)	0.5455(2)	44(1)
C(7)	0.4232(3)	0.2919(2)	0.5803(2)	49(1)
C(8)	0.4154(3)	0.3073(2)	0.6749(2)	62(1)
C(9)	0.5105(3)	0.2423(2)	0.5312(2)	70(1)
C(10)	0.5011(3)	0.2886(2)	0.4440(2)	61(1)
C(11)	0.3124(3)	0.2679(2)	0.5415(2)	61(1)
C(12)	0.3079(3)	0.3217(2)	0.4601(2)	58(1)
(2R,3R)-(-)-O,O'-di-p-toluoyltartaric acid				
O(1)	0.4252(2)	0.5136(1)	0.3759(1)	57(1)
O(2)	0.5990(2)	0.4865(2)	0.4035(2)	68(1)
O(3)	0.4640(2)	0.6880(1)	0.3448(1)	48(1)
O(4)	0.4016(2)	0.6979(2)	0.4763(1)	68(1)
O(5)	0.7114(2)	0.7745(2)	0.3628(2)	73(1)
O(6)	0.6450(2)	0.7849(1)	0.2330(1)	64(1)
O(7)	0.6007(2)	0.6069(1)	0.2306(1)	46(1)
O(8)	0.7685(2)	0.6144(2)	0.1754(1)	63(1)
C(13)	0.5230(3)	0.5357(2)	0.3838(2)	47(1)
C(14)	0.5530(2)	0.6339(2)	0.3720(2)	44(1)
C(15)	0.6408(2)	0.6462(2)	0.3062(2)	42(1)
C(16)	0.6662(3)	0.7432(2)	0.2949(2)	49(1)
C(17)	0.3954(3)	0.7182(2)	0.4037(2)	49(1)
C(18)	0.3133(2)	0.7784(2)	0.3667(2)	46(1)
C(19)	0.3306(3)	0.8204(2)	0.2908(2)	52(1)
C(20)	0.2524(3)	0.8750(2)	0.2576(2)	57(1)
C(21)	0.1540(3)	0.8881(2)	0.2987(2)	56(1)
C(22)	0.1381(3)	0.8472(2)	0.3748(2)	63(1)
C(23)	0.2176(3)	0.7939(2)	0.4092(2)	60(1)
C(24)	0.0671(3)	0.9445(3)	0.2599(3)	85(1)
C(25)	0.6754(3)	0.5909(2)	0.1703(2)	45(1)
C(26)	0.6278(2)	0.5406(2)	0.1000(2)	42(1)
C(27)	0.6914(3)	0.5211(2)	0.0317(2)	51(1)
C(28)	0.6519(3)	0.4700(2)	-0.0329(2)	63(1)
C(29)	0.5486(3)	0.4358(2)	-0.0305(2)	60(1)
C(30)	0.4844(3)	0.4566(3)	0.0369(2)	75(1)
C(31)	0.5230(3)	0.5082(2)	0.1016(2)	66(1)
C(32)	0.5090(4)	0.3751(3)	-0.0999(2)	91(1)

Table S3. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 16 = (2*R*,3*R*)-(-)-*O*,*O'*-di-*p*-toluoyltartrate of (*R*)-(-)-4a.

	x	y	z	U_{iso}
Amine				
H(2N)	0.4220 (20)	0.4110 (20)	0.4161 (19)	59
H(1)	0.3380	0.5534	0.5402	57
H(4)	0.2780	0.4046	0.7873	67
H(5)	0.2053	0.5429	0.7616	69
H(6)	0.5178	0.4023	0.5522	53
H(8A)	0.3739	0.2612	0.7026	74
H(8B)	0.4868	0.3119	0.7006	74
H(9A)	0.4944	0.1796	0.5275	84
H(9B)	0.5821	0.2503	0.5557	84
H(10A)	0.5708	0.3129	0.4270	73
H(10B)	0.4767	0.2472	0.4016	73
H(11A)	0.3081	0.2051	0.5300	73
H(11B)	0.2533	0.2842	0.5787	73
H(12A)	0.2943	0.2840	0.4120	70
H(12B)	0.2521	0.3670	0.4627	70
(2 <i>R</i> ,3 <i>R</i>)-(-)- <i>O</i> , <i>O'</i> -di- <i>p</i> -toluoyltartaric acid				
H(50)	0.7240 (30)	0.8340 (30)	0.3550 (20)	88
H(14)	0.5800	0.6570	0.4254	53
H(15)	0.7069	0.6151	0.3240	50
H(19)	0.3957	0.8116	0.2620	63
H(20)	0.2654	0.9036	0.2070	68
H(22)	0.0729	0.8556	0.4034	76
H(23)	0.2065	0.7683	0.4615	72
H(24A)	-0.0032	0.9215	0.2745	128
H(24B)	0.0753	0.9441	0.2001	128
H(24C)	0.0737	1.0039	0.2803	128
H(27)	0.7622	0.5429	0.0289	61
H(28)	0.6961	0.4583	-0.0789	75
H(30)	0.4133	0.4355	0.0390	89
H(31)	0.4778	0.5213	0.1467	79
H(32A)	0.4308	0.3740	-0.1002	137
H(32B)	0.5362	0.3164	-0.0904	137
H(32C)	0.5349	0.3964	-0.1529	137

Except H(2N) and H(50), which were refined in *x,y,z* without restraints, hydrogen atoms were inserted in idealized positions and were refined riding with the atoms to which they were bonded. All hydrogen atoms had $U_{iso} = U_{eq} \times 1.2$ ($\times 1.5$ for CH_3) of their carrier atoms.

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **16** = (2*R*,3*R*)-(-)-*O*,*O'*-di-*p*-toluoyltartrate of (*R*)-(-)-**4a**. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Amine						
N(1)	57(2)	55(2)	45(2)	-1(1)	6(1)	9(1)
N(2)	53(2)	47(2)	47(2)	-2(1)	7(1)	0(1)
C(1)	54(2)	45(2)	44(2)	3(2)	4(2)	2(2)
C(2)	43(2)	39(2)	40(2)	1(1)	0(1)	-4(1)
C(3)	52(2)	44(2)	43(2)	0(1)	-4(2)	-7(2)
C(4)	71(2)	56(2)	40(2)	5(2)	6(2)	-10(2)
C(5)	56(2)	64(2)	51(2)	-9(2)	9(2)	0(2)
C(6)	42(2)	40(2)	50(2)	0(1)	2(1)	-2(1)
C(7)	60(2)	35(2)	54(2)	-2(1)	2(2)	3(2)
C(8)	84(3)	45(2)	56(2)	11(2)	-6(2)	1(2)
C(9)	77(3)	51(2)	83(3)	-3(2)	-2(2)	13(2)
C(10)	63(2)	49(2)	70(2)	-14(2)	10(2)	7(2)
C(11)	71(2)	51(2)	62(2)	-6(2)	7(2)	-20(2)
C(12)	53(2)	66(2)	55(2)	-10(2)	-1(2)	-15(2)
(2 <i>R</i> ,3 <i>R</i>)-(-)- <i>O</i> , <i>O'</i> -di- <i>p</i> -toluoyltartaric acid						
O(1)	54(1)	56(1)	60(1)	5(1)	-8(1)	-12(1)
O(2)	57(2)	55(1)	92(2)	22(1)	-6(1)	2(1)
O(3)	56(1)	51(1)	39(1)	4(1)	0(1)	9(1)
O(4)	95(2)	69(2)	40(1)	4(1)	11(1)	10(1)
O(5)	105(2)	61(2)	54(1)	9(1)	-26(1)	-35(2)
O(6)	97(2)	51(1)	44(1)	7(1)	-6(1)	-8(1)
O(7)	48(1)	50(1)	40(1)	-5(1)	1(1)	-4(1)
O(8)	48(1)	70(2)	71(2)	-13(1)	7(1)	-12(1)
C(13)	53(2)	53(2)	34(2)	1(1)	-4(2)	-9(2)
C(14)	50(2)	46(2)	36(2)	-3(1)	-5(1)	-4(1)
C(15)	44(2)	44(2)	38(2)	2(1)	-7(1)	-1(1)
C(16)	55(2)	53(2)	40(2)	2(2)	1(2)	-10(2)
C(17)	62(2)	43(2)	43(2)	-1(2)	10(2)	-9(2)
C(18)	53(2)	40(2)	45(2)	-3(1)	5(2)	-2(2)
C(19)	52(2)	53(2)	52(2)	2(2)	12(2)	2(2)
C(20)	67(2)	51(2)	52(2)	4(2)	7(2)	4(2)
C(21)	59(2)	43(2)	66(2)	-9(2)	5(2)	0(2)
C(22)	61(2)	62(2)	67(2)	-10(2)	19(2)	7(2)
C(23)	73(2)	52(2)	54(2)	0(2)	19(2)	2(2)
C(24)	75(3)	83(3)	97(3)	-6(2)	-1(2)	27(2)
C(25)	45(2)	43(2)	49(2)	1(2)	6(2)	0(2)
C(26)	42(2)	42(2)	43(2)	2(1)	3(1)	-1(1)
C(27)	46(2)	51(2)	57(2)	-2(2)	9(2)	-2(2)
C(28)	68(2)	69(2)	52(2)	-17(2)	10(2)	3(2)
C(29)	76(3)	58(2)	47(2)	-1(2)	-4(2)	-12(2)
C(30)	61(2)	100(3)	63(2)	-9(2)	6(2)	-34(2)
C(31)	57(2)	93(3)	48(2)	-14(2)	14(2)	-18(2)
C(32)	117(4)	90(3)	67(2)	-16(2)	-14(2)	-26(3)

Table S5. Bond lengths [Å] and angles [deg] for 16 = (2R,3R)-(-)-O,O'-di-p-toluoyltartrate of (R)-(-)-4a.

Bond lengths		C(15)-C(16)	1.511(4)
		C(15)-H(15)	0.98
N(1)-C(5)	1.331(4)	C(17)-C(18)	1.481(4)
N(1)-C(1)	1.335(4)	C(18)-C(23)	1.376(4)
N(2)-C(12)	1.484(4)	C(18)-C(19)	1.385(4)
N(2)-C(6)	1.493(4)	C(19)-C(20)	1.373(4)
N(2)-C(10)	1.509(4)	C(19)-H(19)	0.93
N(2)-H(2N)	0.99(3)	C(20)-C(21)	1.388(4)
C(1)-C(2)	1.370(4)	C(20)-H(20)	0.93
C(1)-H(1)	0.93	C(21)-C(22)	1.376(4)
C(2)-C(3)	1.399(4)	C(21)-C(24)	1.500(5)
C(2)-C(6)	1.496(4)	C(22)-C(23)	1.380(5)
C(3)-C(4)	1.382(4)	C(22)-H(22)	0.93
C(3)-C(8)	1.518(4)	C(23)-H(23)	0.93
C(4)-C(5)	1.390(5)	C(24)-H(24A)	0.96
C(4)-H(4)	0.93	C(24)-H(24B)	0.96
C(5)-H(5)	0.93	C(24)-H(24C)	0.96
C(6)-C(7)	1.528(4)	C(25)-C(26)	1.476(4)
C(6)-H(6)	0.98	C(26)-C(27)	1.373(4)
C(7)-C(9)	1.525(4)	C(26)-C(31)	1.378(4)
C(7)-C(8)	1.531(4)	C(27)-C(28)	1.377(4)
C(7)-C(11)	1.537(5)	C(27)-H(27)	0.93
C(8)-H(8A)	0.97	C(28)-C(29)	1.370(5)
C(8)-H(8B)	0.97	C(28)-H(28)	0.93
C(9)-C(10)	1.563(5)	C(29)-C(30)	1.370(5)
C(9)-H(9A)	0.97	C(29)-C(32)	1.518(5)
C(9)-H(9B)	0.97	C(30)-C(31)	1.378(5)
C(10)-H(10A)	0.97	C(30)-H(30)	0.93
C(10)-H(10B)	0.97	C(31)-H(31)	0.93
C(11)-C(12)	1.535(4)	C(32)-H(32A)	0.96
C(11)-H(11A)	0.97	C(32)-H(32B)	0.96
C(11)-H(11B)	0.97	C(32)-H(32C)	0.96
C(12)-H(12A)	0.97		
C(12)-H(12B)	0.97		
		Bond angles	
O(1)-C(13)	1.252(3)	C(5)-N(1)-C(1)	118.7(3)
O(2)-C(13)	1.234(4)	C(12)-N(2)-C(6)	103.4(2)
O(3)-C(17)	1.342(3)	C(12)-N(2)-C(10)	109.1(3)
O(3)-C(14)	1.432(3)	C(6)-N(2)-C(10)	99.9(2)
O(4)-C(17)	1.201(3)	C(12)-N(2)-H(2N)	111.6(18)
O(5)-C(16)	1.306(4)	C(6)-N(2)-H(2N)	115.2(17)
O(5)-H(5O)	0.92(4)	C(10)-N(2)-H(2N)	116.3(18)
O(6)-C(16)	1.201(3)	N(1)-C(1)-C(2)	121.8(3)
O(7)-C(25)	1.351(3)	N(1)-C(1)-H(1)	119.1
O(7)-C(15)	1.433(3)	C(2)-C(1)-H(1)	119.1
O(8)-C(25)	1.199(3)	C(1)-C(2)-C(3)	119.7(3)
C(13)-C(14)	1.542(4)	C(1)-C(2)-C(6)	132.7(3)
C(14)-C(15)	1.516(4)	C(3)-C(2)-C(6)	107.4(3)
C(14)-H(14)	0.98		

C(4)-C(3)-C(2)	118.5(3)	C(16)-O(5)-H(50)	108(2)
C(4)-C(3)-C(8)	130.3(3)	C(25)-O(7)-C(15)	116.1(2)
C(2)-C(3)-C(8)	111.2(3)	O(2)-C(13)-O(1)	126.1(3)
C(3)-C(4)-C(5)	117.7(3)	O(2)-C(13)-C(14)	115.5(3)
C(3)-C(4)-H(4)	121.2	O(1)-C(13)-C(14)	118.3(3)
C(5)-C(4)-H(4)	121.2	O(3)-C(14)-C(15)	105.3(2)
N(1)-C(5)-C(4)	123.5(3)	O(3)-C(14)-C(13)	113.9(2)
N(1)-C(5)-H(5)	118.3	C(15)-C(14)-C(13)	111.9(2)
C(4)-C(5)-H(5)	118.3	O(3)-C(14)-H(14)	108.5
N(2)-C(6)-C(2)	125.0(2)	C(15)-C(14)-H(14)	108.5
N(2)-C(6)-C(7)	95.6(2)	C(13)-C(14)-H(14)	108.5
C(2)-C(6)-C(7)	102.6(2)	O(7)-C(15)-C(16)	111.9(2)
N(2)-C(6)-H(6)	110.5	O(7)-C(15)-C(14)	106.7(2)
C(2)-C(6)-H(6)	110.5	C(16)-C(15)-C(14)	110.4(2)
C(7)-C(6)-H(6)	110.5	O(7)-C(15)-H(15)	109.3
C(9)-C(7)-C(6)	99.4(2)	C(16)-C(15)-H(15)	109.3
C(9)-C(7)-C(8)	128.7(3)	C(14)-C(15)-H(15)	109.3
C(6)-C(7)-C(8)	103.1(2)	O(6)-C(16)-O(5)	125.8(3)
C(9)-C(7)-C(11)	107.4(3)	O(6)-C(16)-C(15)	124.3(3)
C(6)-C(7)-C(11)	101.6(2)	O(5)-C(16)-C(15)	109.9(3)
C(8)-C(7)-C(11)	112.2(3)	O(4)-C(17)-O(3)	123.2(3)
C(3)-C(8)-C(7)	99.8(2)	O(4)-C(17)-C(18)	125.8(3)
C(3)-C(8)-H(8A)	111.8	O(3)-C(17)-C(18)	111.0(3)
C(7)-C(8)-H(8A)	111.8	C(23)-C(18)-C(19)	118.9(3)
C(3)-C(8)-H(8B)	111.8	C(23)-C(18)-C(17)	119.3(3)
C(7)-C(8)-H(8B)	111.8	C(19)-C(18)-C(17)	121.7(3)
H(8A)-C(8)-H(8B)	109.5	C(20)-C(19)-C(18)	120.4(3)
C(7)-C(9)-C(10)	100.6(3)	C(20)-C(19)-H(19)	119.8
C(7)-C(9)-H(9A)	111.6	C(18)-C(19)-H(19)	119.8
C(10)-C(9)-H(9A)	111.6	C(19)-C(20)-C(21)	120.8(3)
C(7)-C(9)-H(9B)	111.6	C(19)-C(20)-H(20)	119.6
C(10)-C(9)-H(9B)	111.6	C(21)-C(20)-H(20)	119.6
H(9A)-C(9)-H(9B)	109.4	C(22)-C(21)-C(20)	118.5(3)
N(2)-C(10)-C(9)	105.0(2)	C(22)-C(21)-C(24)	121.3(3)
N(2)-C(10)-H(10A)	110.7	C(20)-C(21)-C(24)	120.3(3)
C(9)-C(10)-H(10A)	110.7	C(21)-C(22)-C(23)	120.8(3)
N(2)-C(10)-H(10B)	110.7	C(21)-C(22)-H(22)	119.6
C(9)-C(10)-H(10B)	110.7	C(23)-C(22)-H(22)	119.6
H(10A)-C(10)-H(10B)	108.8	C(18)-C(23)-C(22)	120.5(3)
C(12)-C(11)-C(7)	104.3(2)	C(18)-C(23)-H(23)	119.7
C(12)-C(11)-H(11A)	110.9	C(22)-C(23)-H(23)	119.7
C(7)-C(11)-H(11A)	110.9	C(21)-C(24)-H(24A)	109.5
C(12)-C(11)-H(11B)	110.9	C(21)-C(24)-H(24B)	109.5
C(7)-C(11)-H(11B)	110.9	H(24A)-C(24)-H(24B)	109.5
H(11A)-C(11)-H(11B)	108.9	C(21)-C(24)-H(24C)	109.5
N(2)-C(12)-C(11)	102.4(3)	H(24A)-C(24)-H(24C)	109.5
N(2)-C(12)-H(12A)	111.3	H(24B)-C(24)-H(24C)	109.5
C(11)-C(12)-H(12A)	111.3	O(8)-C(25)-O(7)	123.1(3)
N(2)-C(12)-H(12B)	111.3	O(8)-C(25)-C(26)	125.5(3)
C(11)-C(12)-H(12B)	111.3	O(7)-C(25)-C(26)	111.4(3)
H(12A)-C(12)-H(12B)	109.2	C(27)-C(26)-C(31)	118.0(3)
		C(27)-C(26)-C(25)	119.3(3)
C(17)-O(3)-C(14)	117.5(2)	C(31)-C(26)-C(25)	122.7(3)

C31-C26-C27-C28	-0.8(5)	C28-C29-C30-C31	-1.8(6)
C25-C26-C27-C28	176.2(3)	C32-C29-C30-C31	176.7(4)
C26-C27-C28-C29	-0.9(5)	C27-C26-C31-C30	1.2(5)
C27-C28-C29-C30	2.1(5)	C25-C26-C31-C30	-175.7(3)
C27-C28-C29-C32	-176.3(3)	C29-C30-C31-C26	0.1(6)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O5-H5O	0.920	1.672	169.63	2.582	N1 [x+1/2, -y+3/2, -z+1]
N2-H2N	0.994	1.676	162.17	2.640	O1
N2-H2N	0.994	2.464	116.08	3.036	O2

Fig. S2. Chemical diagram and thermal ellipsoid plot (20% ellipsoids) of the asymmetric unit of the crystal structure of **17** = (2*S*,3*S*)-(+)-*O,O'*-di-*p*-toluoyltartrate of (4*aS*)-(+)-**4b**.

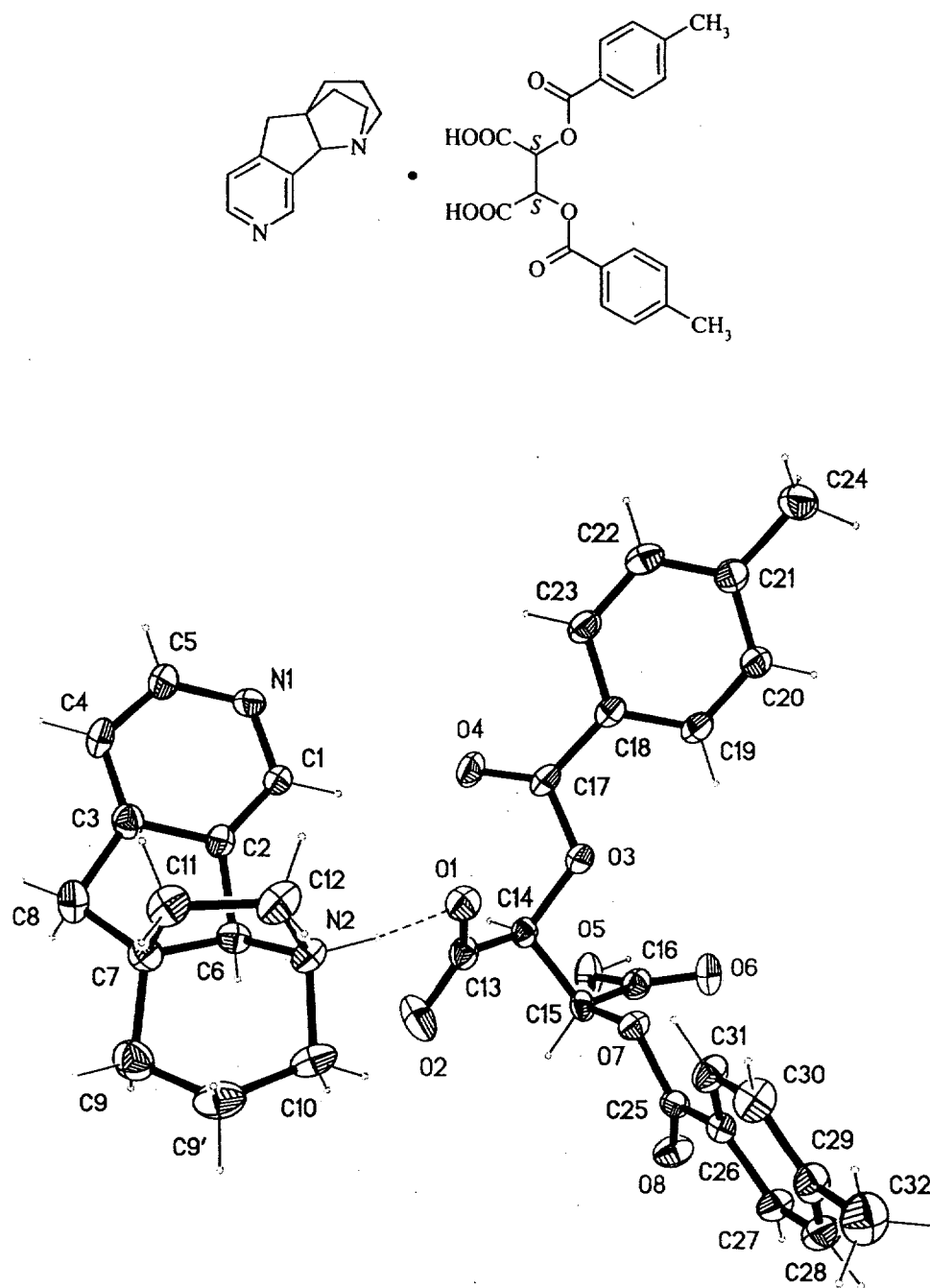


Table S6. Crystal data and structure refinement of 17 = (2*S*,3*S*)-(+)-*O*,*O'*-di-*p*-toluoyltartrate of (4*aS*)-(+)-4*b*.

Identification code	444j3fr
Empirical formula	C ₃₃ H ₃₄ N ₂ O ₈
Formula weight	586.62
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system, space group	orthorhombic, P2 ₁ 2 ₁ 2 ₁ (No. 19)
Unit cell dimensions §	a = 12.369(8) Å α = 90 deg. b = 15.446(8) Å β = 90 deg. c = 15.711(8) Å γ = 90 deg.
Volume	3002(3) Å ³
Z, Calculated density	4, 1.298 Mg/m ³
Absorption coefficient	0.093 mm ⁻¹
F(000)	1240
Crystal size	0.32 x 0.24 x 0.24 mm, colorless prism
Diffractionmeter	Siemens SMART 3-circle with CCD area detector (sealed X-ray tube, Mo Kα radiation, graphite monochromator, detector distance 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 20 sec. per frame, complete Ewald sphere, 4 x 606 frames
Theta range for data collection	2.1 to 22.5 deg.
Index ranges	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -16 ≤ l ≤ 16
Reflections collected / unique	23123 / 3871 [R(int)=0.122, R(sigma)=0.061]
Completeness to theta = 22.49	99.2%
Absorption correction	none
Structure solution	Direct methods (program SHELXS97)
Refinement method	Full-matrix least-squares on F ² (SHELXL97)
Data / restraints / parameters	3871 / 0 / 397
Goodness-of-fit on F ²	1.176
Final R indices [I>2sigma(I)]	R1 = 0.0685, wR2 = 0.1335 (3273 data)
R indices (all data)	R1 = 0.0848, wR2 = 0.1410 (3871 data)
Absolute structure parameter §§	3(2)
Extinction coefficient	0.0069(11)
Largest diff. peak and hole	0.156 and -0.142 e Å ⁻³

$$R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad wR2 = \left[\frac{\sum (w(F_o^2 - F_c^2)^2)}{\sum (w(F_o^2)^2)} \right]^{1/2}$$

§) Compounds 16 (Tables S1 – S5) and 17 (Tables S6 – S10) form an enantiomeric pair of almost identical structures, which differ only by one ring CH₂ group but not in the basic spatial arrangement, orientation, and mutual hydrogen bonding of their constituents.

§§) Absolute structure via known chirality of (2*S*,3*S*)-(+)-*O*,*O'*-di-*p*-toluoyltartaric acid

Table S7. Atomic coordinates and equivalent isotropic displacement parameters (Å² x 10³) of 17 = (2*S*,3*S*)-(+)-*O*,*O'*-di-*p*-toluoyltartrate of (4*aS*)-(+)-4*b*. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U _{eq}
Amine				
N(1)	0.7230(3)	0.4346(3)	0.3489(3)	61(1)
N(2)	0.5763(3)	0.6277(3)	0.5344(3)	59(1)
C(1)	0.6611(4)	0.4746(3)	0.4061(3)	51(1)
C(2)	0.6220(4)	0.5556(3)	0.3917(3)	50(1)
C(3)	0.6455(4)	0.5970(3)	0.3147(3)	59(1)
C(4)	0.7120(5)	0.5551(4)	0.2569(4)	68(2)
C(5)	0.7482(5)	0.4750(4)	0.2764(3)	66(2)
C(6)	0.5500(4)	0.6141(3)	0.4436(3)	54(1)
C(7)	0.5741(4)	0.7038(3)	0.4049(3)	58(1)
C(8)	0.5915(5)	0.6836(4)	0.3105(3)	72(2)
C(9)	0.4838(5)	0.7648(4)	0.4301(4)	82(2)
C(9') *	0.4817(5)	0.7709(4)	0.5276(5)	93(2)
C(10)	0.4900(4)	0.6835(4)	0.5732(4)	74(2)
C(11)	0.6800(5)	0.7275(4)	0.4492(4)	74(2)
C(12)	0.6834(4)	0.6739(4)	0.5318(4)	74(2)
(2 <i>S</i> ,3 <i>S</i>)-(+)- <i>O</i> , <i>O'</i> -di- <i>p</i> -toluoyltartaric acid				
O(1)	0.5762(3)	0.4761(2)	0.6135(2)	61(1)
O(2)	0.4055(3)	0.4969(3)	0.5791(3)	95(2)
O(3)	0.5387(3)	0.3064(2)	0.6531(2)	56(1)
O(4)	0.6089(3)	0.2972(3)	0.5225(2)	75(1)
O(5)	0.2869(3)	0.2244(3)	0.6328(2)	78(1)
O(6)	0.3483(3)	0.2188(2)	0.7654(2)	72(1)
O(7)	0.3995(2)	0.3905(2)	0.7611(2)	50(1)
O(8)	0.2324(3)	0.3906(3)	0.8139(3)	73(1)
C(13)	0.4809(4)	0.4524(4)	0.6035(3)	56(1)
C(14)	0.4506(4)	0.3577(3)	0.6211(3)	50(1)
C(15)	0.3616(4)	0.3498(3)	0.6861(3)	48(1)
C(16)	0.3312(4)	0.2564(4)	0.7019(4)	57(1)
C(17)	0.6118(4)	0.2780(3)	0.5968(3)	56(1)
C(18)	0.6915(4)	0.2204(3)	0.6361(3)	53(1)
C(19)	0.6735(5)	0.1795(4)	0.7134(3)	63(2)
C(20)	0.7485(4)	0.1257(4)	0.7482(4)	65(2)
C(21)	0.8466(5)	0.1122(4)	0.7084(4)	62(2)
C(22)	0.8642(5)	0.1520(4)	0.6311(4)	74(2)
C(23)	0.7876(4)	0.2045(4)	0.5951(4)	65(2)
C(24)	0.9301(5)	0.0549(5)	0.7482(4)	89(2)
C(25)	0.3264(4)	0.4113(3)	0.8198(3)	49(1)
C(26)	0.3717(4)	0.4624(3)	0.8903(3)	48(1)
C(27)	0.3095(4)	0.4817(4)	0.9592(4)	62(2)
C(28)	0.3483(5)	0.5306(4)	1.0237(4)	75(2)
C(29)	0.4514(5)	0.5656(4)	1.0210(4)	66(2)
C(30)	0.5137(5)	0.5449(4)	0.9519(4)	77(2)
C(31)	0.4756(4)	0.4941(4)	0.8865(3)	67(2)
C(32)	0.4913(6)	0.6224(5)	1.0910(4)	105(2)

* Atom designation C(9') used in order to have for all other atoms the same atom labels as for the pseudo-isostructural **16** = (2*R*,3*R*)-(-)-*O*,*O'*-di-*p*-toluoyltartrate of (*R*)-(-)-**4a**

Table S8. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 17 = (2*S*,3*S*)-(+)-*O*,*O'*-di-*p*-toluoyltartrate of (4*aS*)-(+)-4b.

	x	y	z	U_{iso}
Amine				
H(2N)	0.5730 (40)	0.5650 (40)	0.5710 (30)	71
H(1)	0.6444	0.4467	0.4569	62
H(4)	0.7314	0.5816	0.2059	81
H(5)	0.7926	0.4467	0.2376	79
H(6)	0.4737	0.5987	0.4363	64
H(8A)	0.5234	0.6805	0.2801	86
H(8B)	0.6376	0.7264	0.2836	86
H(9A)	0.4151	0.7431	0.4093	98
H(9B)	0.4961	0.8216	0.4056	98
H(9'A)	0.4151	0.7991	0.5448	112
H(9'B)	0.5413	0.8073	0.5459	112
H(10A)	0.5063	0.6930	0.6329	89
H(10B)	0.4210	0.6538	0.5698	89
H(11A)	0.6820	0.7889	0.4620	89
H(11B)	0.7412	0.7134	0.4132	89
H(12A)	0.7427	0.6327	0.5305	89
H(12B)	0.6919	0.7112	0.5810	89
(2 <i>S</i> ,3 <i>S</i>)-(+)- <i>O</i> , <i>O'</i> -di- <i>p</i> -toluoyltartaric acid				
H(5O)	0.2680 (50)	0.1560 (50)	0.6460 (40)	93
H(14)	0.4254	0.3317	0.5678	60
H(15)	0.2978	0.3810	0.6655	58
H(19)	0.6088	0.1891	0.7420	76
H(20)	0.7336	0.0978	0.7993	78
H(22)	0.9293	0.1431	0.6029	89
H(23)	0.8007	0.2296	0.5423	78
H(24A)	1.0006	0.0789	0.7387	134
H(24B)	0.9262	-0.0017	0.7232	134
H(24C)	0.9169	0.0508	0.8083	134
H(27)	0.2390	0.4608	0.9620	74
H(28)	0.3049	0.5410	1.0709	90
H(30)	0.5841	0.5658	0.9490	92
H(31)	0.5196	0.4814	0.8402	80
H(32A)	0.5657	0.6369	1.0810	158
H(32B)	0.4850	0.5925	1.1443	158
H(32C)	0.4489	0.6744	1.0928	158

Except H(2N) and H(5O), which were refined in *x,y,z* without restraints, hydrogen atoms were inserted in idealized positions and were refined riding with the atoms to which they were bonded. All hydrogen atoms had $U_{\text{iso}} = U_{\text{eq}} \times 1.2$ ($\times 1.5$ for CH_3) of their carrier atoms.

Table S9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 17 = (2*S*,3*S*)-(+)-*O*,*O'*-di-*p*-toluoyltartrate of (4*aS*)-(+)-4*b*. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a'^2 U_{11} + \dots + 2 h k a' b' U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Amine						
O(1)	53(2)	69(2)	61(2)	-4(2)	-1(2)	-7(2)
O(2)	65(3)	87(3)	132(4)	52(3)	-30(3)	-17(2)
O(3)	60(2)	69(2)	40(2)	-1(2)	4(2)	7(2)
O(4)	106(3)	80(3)	40(2)	4(2)	19(2)	14(2)
O(5)	105(3)	76(3)	52(2)	9(2)	-25(2)	-38(2)
O(6)	101(3)	68(3)	49(2)	13(2)	-15(2)	-10(2)
O(7)	44(2)	61(2)	45(2)	-9(2)	3(2)	-2(2)
O(8)	51(2)	87(3)	81(3)	-23(2)	5(2)	-9(2)
N(1)	61(3)	64(3)	57(3)	-1(3)	4(2)	16(2)
N(2)	55(3)	70(3)	52(3)	-5(2)	9(2)	-10(2)
C(1)	55(3)	55(3)	43(3)	3(3)	7(3)	2(3)
C(2)	52(3)	52(3)	47(3)	3(3)	1(3)	-7(3)
C(3)	66(3)	52(3)	58(4)	3(3)	1(3)	-1(3)
C(4)	86(4)	72(4)	45(3)	12(3)	11(3)	-10(3)
C(5)	76(4)	76(4)	45(3)	5(3)	6(3)	7(3)
C(6)	47(3)	58(3)	55(3)	-8(3)	-10(3)	-2(3)
C(7)	64(3)	46(3)	63(3)	-5(3)	2(3)	-3(3)
C(8)	89(4)	65(4)	61(4)	12(3)	-2(3)	-6(3)
C(9)	89(4)	59(4)	98(5)	1(4)	1(4)	3(3)
C(9')	78(4)	77(5)	124(6)	-29(5)	19(4)	-6(4)
C(10)	60(3)	76(4)	86(4)	-30(4)	25(3)	-7(3)
C(11)	71(4)	71(4)	79(4)	-12(3)	7(3)	-17(3)
(2 <i>S</i> ,3 <i>S</i>)-(+)- <i>O</i> , <i>O'</i> -di- <i>p</i> -toluoyltartaric acid						
C(12)	58(3)	101(5)	63(4)	-19(4)	0(3)	-28(3)
C(13)	50(3)	75(4)	43(3)	5(3)	-7(3)	-6(3)
C(14)	54(3)	63(3)	33(3)	0(2)	-8(2)	-1(3)
C(15)	47(3)	58(3)	39(3)	6(3)	-12(2)	-3(2)
C(16)	52(3)	71(4)	46(4)	-3(3)	0(3)	-4(3)
C(17)	68(3)	54(3)	45(3)	-6(3)	17(3)	-10(3)
C(18)	61(3)	47(3)	49(3)	-4(3)	12(3)	-7(3)
C(19)	62(3)	70(4)	57(4)	0(3)	18(3)	-2(3)
C(20)	74(4)	64(4)	58(3)	3(3)	12(3)	12(3)
C(21)	71(4)	58(4)	58(4)	-13(3)	3(3)	4(3)
C(22)	72(4)	77(4)	73(4)	-15(4)	20(3)	9(3)
C(23)	72(4)	67(4)	55(3)	-6(3)	18(3)	4(3)
C(24)	86(4)	98(5)	84(4)	-9(4)	-1(4)	23(4)
C(25)	46(3)	47(3)	55(3)	3(3)	2(3)	5(3)
C(26)	45(3)	49(3)	49(3)	1(2)	-1(2)	4(2)
C(27)	50(3)	74(4)	61(4)	-10(3)	10(3)	0(3)
C(28)	77(4)	83(4)	65(4)	-13(4)	8(3)	10(4)
C(29)	85(4)	60(4)	53(4)	-13(3)	-12(3)	0(3)
C(30)	70(4)	79(4)	81(4)	-8(4)	-3(4)	-26(3)
C(31)	54(3)	91(4)	55(3)	-6(3)	5(3)	-12(3)
C(32)	125(6)	97(5)	94(5)	-20(4)	-14(5)	-12(5)

Table S10. Bond lengths [Å] and angles [deg] for 17 = (2*S*,3*S*)-(+)-*O*,*O*'-di-*p*-toluoyltartrate of (4*aS*)-(+)-4*b*.

Bond lengths		C(13)-C(14)	1.535(7)
		C(14)-C(15)	1.507(6)
N(1)-C(1)	1.332(6)	C(14)-H(14)	0.98
N(1)-C(5)	1.336(7)	C(15)-C(16)	1.510(7)
N(2)-C(6)	1.478(6)	C(15)-H(15)	0.98
N(2)-C(10)	1.501(7)	C(17)-C(18)	1.466(7)
N(2)-C(12)	1.505(7)	C(18)-C(23)	1.374(7)
N(2)-H(2N)	1.13(6)	C(18)-C(19)	1.386(7)
C(1)-C(2)	1.360(7)	C(19)-C(20)	1.360(7)
C(1)-H(1)	0.93	C(19)-H(19)	0.93
C(2)-C(3)	1.398(7)	C(20)-C(21)	1.381(7)
C(2)-C(6)	1.508(7)	C(20)-H(20)	0.93
C(3)-C(4)	1.387(7)	C(21)-C(22)	1.378(8)
C(3)-C(8)	1.496(8)	C(21)-C(24)	1.497(8)
C(4)-C(5)	1.352(8)	C(22)-C(23)	1.369(8)
C(4)-H(4)	0.93	C(22)-H(22)	0.93
C(5)-H(5)	0.93	C(23)-H(23)	0.93
C(6)-C(7)	1.541(7)	C(24)-H(24A)	0.96
C(6)-H(6)	0.98	C(24)-H(24B)	0.96
C(7)-C(9)	1.514(8)	C(24)-H(24C)	0.96
C(7)-C(11)	1.527(8)	C(25)-C(26)	1.471(7)
C(7)-C(8)	1.531(8)	C(26)-C(27)	1.361(7)
C(8)-H(8A)	0.97	C(26)-C(31)	1.377(7)
C(8)-H(8B)	0.97	C(27)-C(28)	1.352(8)
C(9)-C(9')	1.534(9)	C(27)-H(27)	0.93
C(9)-H(9A)	0.97	C(28)-C(29)	1.386(8)
C(9)-H(9B)	0.97	C(28)-H(28)	0.93
C(9')-C(10)	1.534(9)	C(29)-C(30)	1.370(8)
C(9')-H(9'A)	0.97	C(29)-C(32)	1.491(8)
C(9')-H(9'B)	0.97	C(30)-C(31)	1.375(8)
C(10)-H(10A)	0.97	C(30)-H(30)	0.93
C(10)-H(10B)	0.97	C(31)-H(31)	0.93
C(11)-C(12)	1.540(8)	C(32)-H(32A)	0.96
C(11)-H(11A)	0.97	C(32)-H(32B)	0.96
C(11)-H(11B)	0.97	C(32)-H(32C)	0.96
C(12)-H(12A)	0.97		
C(12)-H(12B)	0.97		
		Bond angles	
O(1)-C(13)	1.244(6)	C(1)-N(1)-C(5)	119.5(5)
O(2)-C(13)	1.220(6)	C(6)-N(2)-C(10)	108.5(4)
O(3)-C(17)	1.339(6)	C(6)-N(2)-C(12)	103.6(4)
O(3)-C(14)	1.437(6)	C(10)-N(2)-C(12)	111.4(4)
O(4)-C(17)	1.205(6)	C(6)-N(2)-H(2N)	111(3)
O(5)-C(16)	1.313(6)	C(10)-N(2)-H(2N)	105(3)
O(5)-H(5O)	1.09(7)	C(12)-N(2)-H(2N)	117(3)
O(6)-C(16)	1.175(6)	N(1)-C(1)-C(2)	121.3(5)
O(7)-C(25)	1.331(6)	N(1)-C(1)-H(1)	119.4
O(7)-C(15)	1.416(5)	C(2)-C(1)-H(1)	119.4
O(8)-C(25)	1.209(6)		

C(1)-C(2)-C(3)	119.4(5)	H(11A)-C(11)-H(11B)	108.7
C(1)-C(2)-C(6)	132.1(5)	N(2)-C(12)-C(11)	104.7(4)
C(3)-C(2)-C(6)	108.4(4)	N(2)-C(12)-H(12A)	110.8
C(4)-C(3)-C(2)	118.5(5)	C(11)-C(12)-H(12A)	110.8
C(4)-C(3)-C(8)	130.8(5)	N(2)-C(12)-H(12B)	110.8
C(2)-C(3)-C(8)	110.8(5)	C(11)-C(12)-H(12B)	110.8
C(5)-C(4)-C(3)	118.4(5)	H(12A)-C(12)-H(12B)	108.9
C(5)-C(4)-H(4)	120.8		
C(3)-C(4)-H(4)	120.8	C(17)-O(3)-C(14)	117.5(4)
N(1)-C(5)-C(4)	122.9(5)	C(16)-O(5)-H(50)	107(3)
N(1)-C(5)-H(5)	118.5	C(25)-O(7)-C(15)	117.3(4)
C(4)-C(5)-H(5)	118.5	O(2)-C(13)-O(1)	126.7(5)
N(2)-C(6)-C(2)	118.5(4)	O(2)-C(13)-C(14)	114.0(4)
N(2)-C(6)-C(7)	102.1(4)	O(1)-C(13)-C(14)	119.2(5)
C(2)-C(6)-C(7)	102.2(4)	O(3)-C(14)-C(15)	105.8(4)
N(2)-C(6)-H(6)	111.1	O(3)-C(14)-C(13)	113.8(4)
C(2)-C(6)-H(6)	111.1	C(15)-C(14)-C(13)	112.2(4)
C(7)-C(6)-H(6)	111.1	O(3)-C(14)-H(14)	108.3
C(9)-C(7)-C(11)	111.4(5)	C(15)-C(14)-H(14)	108.3
C(9)-C(7)-C(8)	118.9(5)	C(13)-C(14)-H(14)	108.3
C(11)-C(7)-C(8)	111.7(5)	O(7)-C(15)-C(14)	106.6(4)
C(9)-C(7)-C(6)	108.3(4)	O(7)-C(15)-C(16)	111.7(4)
C(11)-C(7)-C(6)	101.6(4)	C(14)-C(15)-C(16)	111.7(4)
C(8)-C(7)-C(6)	103.1(4)	O(7)-C(15)-H(15)	108.9
C(3)-C(8)-C(7)	101.6(4)	C(14)-C(15)-H(15)	108.9
C(3)-C(8)-H(8A)	111.4	C(16)-C(15)-H(15)	108.9
C(7)-C(8)-H(8A)	111.4	O(6)-C(16)-O(5)	126.2(5)
C(3)-C(8)-H(8B)	111.4	O(6)-C(16)-C(15)	124.6(5)
C(7)-C(8)-H(8B)	111.4	O(5)-C(16)-C(15)	109.2(5)
H(8A)-C(8)-H(8B)	109.3	O(4)-C(17)-O(3)	122.6(5)
C(7)-C(9)-C(9')	108.2(5)	O(4)-C(17)-C(18)	125.4(5)
C(7)-C(9)-H(9A)	110.1	O(3)-C(17)-C(18)	112.0(4)
C(9')-C(9)-H(9A)	110.1	C(23)-C(18)-C(19)	118.0(5)
C(7)-C(9)-H(9B)	110.1	C(23)-C(18)-C(17)	119.5(5)
C(9')-C(9)-H(9B)	110.1	C(19)-C(18)-C(17)	122.5(5)
H(9A)-C(9)-H(9B)	108.4	C(20)-C(19)-C(18)	121.3(5)
C(9)-C(9')-C(10)	114.3(5)	C(20)-C(19)-H(19)	119.3
C(9)-C(9')-H(9'A)	108.7	C(18)-C(19)-H(19)	119.3
C(10)-C(9')-H(9'A)	108.7	C(19)-C(20)-C(21)	120.6(5)
C(9)-C(9')-H(9'B)	108.7	C(19)-C(20)-H(20)	119.7
C(10)-C(9')-H(9'B)	108.7	C(21)-C(20)-H(20)	119.7
H(9'A)-C(9')-H(9'B)	107.6	C(22)-C(21)-C(20)	118.0(6)
N(2)-C(10)-C(9')	111.3(5)	C(22)-C(21)-C(24)	121.6(5)
N(2)-C(10)-H(10A)	109.4	C(20)-C(21)-C(24)	120.4(6)
C(9')-C(10)-H(10A)	109.4	C(23)-C(22)-C(21)	121.3(5)
N(2)-C(10)-H(10B)	109.4	C(23)-C(22)-H(22)	119.3
C(9')-C(10)-H(10B)	109.4	C(21)-C(22)-H(22)	119.3
H(10A)-C(10)-H(10B)	108.0	C(22)-C(23)-C(18)	120.6(5)
C(7)-C(11)-C(12)	106.2(4)	C(22)-C(23)-H(23)	119.7
C(7)-C(11)-H(11A)	110.5	C(18)-C(23)-H(23)	119.7
C(12)-C(11)-H(11A)	110.5	C(21)-C(24)-H(24A)	109.5
C(7)-C(11)-H(11B)	110.5	C(21)-C(24)-H(24B)	109.5
C(12)-C(11)-H(11B)	110.5	H(24A)-C(24)-H(24B)	109.5

C(21)-C(24)-H(24C)	109.5	N2-C6-C7-C9	-74.8(5)
H(24A)-C(24)-H(24C)	109.5	C2-C6-C7-C9	162.2(4)
H(24B)-C(24)-H(24C)	109.5	N2-C6-C7-C11	42.6(5)
O(8)-C(25)-O(7)	122.4(5)	C2-C6-C7-C11	-80.4(5)
O(8)-C(25)-C(26)	124.5(5)	N2-C6-C7-C8	158.4(4)
O(7)-C(25)-C(26)	113.1(4)	C2-C6-C7-C8	35.4(5)
C(27)-C(26)-C(31)	119.0(5)	C4-C3-C8-C7	-156.8(6)
C(27)-C(26)-C(25)	120.1(4)	C2-C3-C8-C7	22.6(6)
C(31)-C(26)-C(25)	120.9(5)	C9-C7-C8-C3	-154.9(5)
C(28)-C(27)-C(26)	121.1(5)	C11-C7-C8-C3	73.2(6)
C(28)-C(27)-H(27)	119.4	C6-C7-C8-C3	-35.2(5)
C(26)-C(27)-H(27)	119.4	C11-C7-C9-C9'	-50.0(6)
C(27)-C(28)-C(29)	121.5(6)	C8-C7-C9-C9'	177.9(5)
C(27)-C(28)-H(28)	119.3	C6-C7-C9-C9'	60.9(6)
C(29)-C(28)-H(28)	119.3	C7-C9-C9'-C10	-45.8(7)
C(30)-C(29)-C(28)	116.8(5)	C6-N2-C10-C9'	-58.9(6)
C(30)-C(29)-C(32)	122.5(6)	C12-N2-C10-C9'	54.5(6)
C(28)-C(29)-C(32)	120.8(6)	C9-C9'-C10-N2	44.9(7)
C(29)-C(30)-C(31)	122.2(5)	C9-C7-C11-C12	92.1(6)
C(29)-C(30)-H(30)	118.9	C8-C7-C11-C12	-132.3(5)
C(31)-C(30)-H(30)	118.9	C6-C7-C11-C12	-23.0(5)
C(30)-C(31)-C(26)	119.4(5)	C6-N2-C12-C11	31.4(6)
C(30)-C(31)-H(31)	120.3	C10-N2-C12-C11	-85.0(6)
C(26)-C(31)-H(31)	120.3	C7-C11-C12-N2	-4.3(6)
C(29)-C(32)-H(32A)	109.5		
C(29)-C(32)-H(32B)	109.5	C17-O3-C14-C15	157.5(4)
H(32A)-C(32)-H(32B)	109.5	C17-O3-C14-C13	-78.8(5)
C(29)-C(32)-H(32C)	109.5	O2-C13-C14-O3	-177.6(5)
H(32A)-C(32)-H(32C)	109.5	O1-C13-C14-O3	3.5(7)
H(32B)-C(32)-H(32C)	109.5	O2-C13-C14-C15	-57.6(6)
		O1-C13-C14-C15	123.5(5)
		C25-O7-C15-C14	163.3(4)
		C25-O7-C15-C16	-74.4(5)
		O3-C14-C15-O7	66.0(5)
		C13-C14-C15-O7	-58.6(5)
		O3-C14-C15-C16	-56.3(5)
		C13-C14-C15-C16	179.1(4)
		O7-C15-C16-O6	-8.3(7)
		C14-C15-C16-O6	111.1(6)
		O7-C15-C16-O5	173.9(4)
		C14-C15-C16-O5	-66.8(5)
		C14-O3-C17-O4	3.7(7)
		C14-O3-C17-C18	-174.9(4)
		O4-C17-C18-C23	19.3(8)
		O3-C17-C18-C23	-162.1(4)
		O4-C17-C18-C19	-159.6(5)
		O3-C17-C18-C19	18.9(7)
		C23-C18-C19-C20	0.4(8)
		C17-C18-C19-C20	179.4(5)
		C18-C19-C20-C21	1.8(9)
		C19-C20-C21-C22	-2.4(9)
		C19-C20-C21-C24	178.2(5)
		C20-C21-C22-C23	0.8(9)
Torsion angles			
C5-N1-C1-C2	0.8(7)		
N1-C1-C2-C3	1.2(7)		
N1-C1-C2-C6	178.7(5)		
C1-C2-C3-C4	-2.7(8)		
C6-C2-C3-C4	179.3(5)		
C1-C2-C3-C8	177.8(5)		
C6-C2-C3-C8	-0.2(6)		
C2-C3-C4-C5	2.2(8)		
C8-C3-C4-C5	-178.4(6)		
C1-N1-C5-C4	-1.3(8)		
C3-C4-C5-N1	-0.3(9)		
C10-N2-C6-C2	-176.6(4)		
C12-N2-C6-C2	64.9(6)		
C10-N2-C6-C7	72.2(5)		
C12-N2-C6-C7	-46.3(5)		
C1-C2-C6-N2	48.9(7)		
C3-C2-C6-N2	-133.4(5)		
C1-C2-C6-C7	160.1(5)		
C3-C2-C6-C7	-22.3(5)		

C24-C21-C22-C23	-179.9(6)	C31-C26-C27-C28	-0.5(8)
C21-C22-C23-C18	1.4(8)	C25-C26-C27-C28	-178.1(5)
C19-C18-C23-C22	-2.1(8)	C26-C27-C28-C29	2.3(9)
C17-C18-C23-C22	178.9(5)	C27-C28-C29-C30	-3.0(9)
C15-O7-C25-O8	5.9(7)	C27-C28-C29-C32	177.5(6)
C15-O7-C25-C26	-173.1(4)	C28-C29-C30-C31	2.1(9)
O8-C25-C26-C27	7.2(8)	C32-C29-C30-C31	-178.4(6)
O7-C25-C26-C27	-173.8(4)	C29-C30-C31-C26	-0.4(9)
O8-C25-C26-C31	-170.3(5)	C27-C26-C31-C30	-0.4(8)
O7-C25-C26-C31	8.6(7)	C25-C26-C31-C30	177.1(5)

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O5-H5O	1.094	1.515	167.70	2.595	N1 [x-1/2, -y+1/2, -z+1]
N2-H2N	1.128	1.528	173.85	2.651	O1
N2-H2N	1.128	2.329	116.56	3.007	O2

Fig. S3. Chemical diagram and thermal ellipsoid plot (20% ellipsoids) of the asymmetric unit of the crystal structure of (R)-(-)-5b·2HCl.

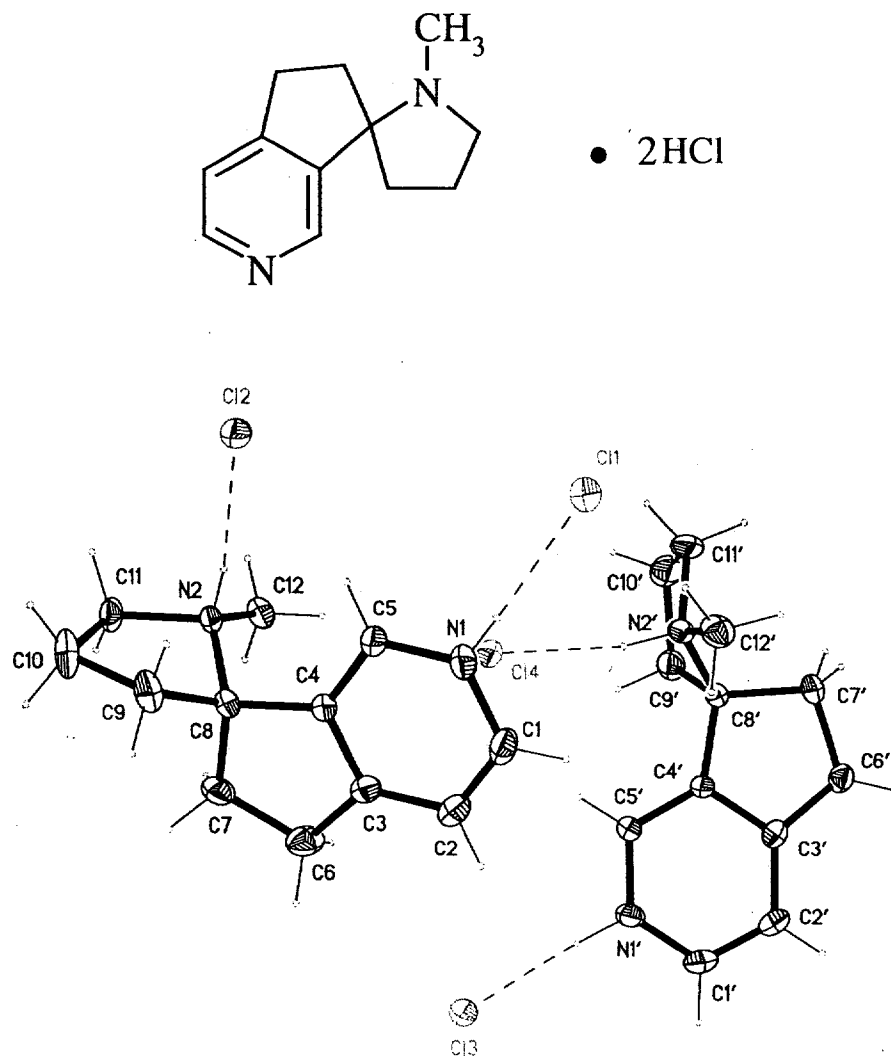


Table S11. Crystal data and structure refinement of (R)-(-)-5b·2HCl.

Identification code	446j3fr
Empirical formula	C ₁₂ H ₁₈ Cl ₂ N ₂
Formula weight	261.18
Temperature	295(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2 ₁ (No. 4)
Unit cell dimensions	a = 11.225(3) Å α = 90 deg.
(by 4-circle diffractometry	b = 10.221(4) Å β = 93.30(1) deg.
40 reflections, θ = 10 - 24°)	c = 11.617(4) Å γ = 90 deg.
Volume	1330.6(8) Å ³
Z, Calculated density	4, 1.304 Mg/m ³ (§)
Absorption coefficient	0.464 mm ⁻¹
F(000)	552
Crystal size	0.40 x 0.40 x 0.65 mm, colorless block
Diffractometer	Siemens SMART 3-circle with CCD area detector (sealed X-ray tube, Mo Kα radiation, graphite monochromator, detector distance 44.50 mm, 512x512 pixels)
Scan type / width / speed	ω-scan frames / Δω = 0.3° / 10 sec. per frame, complete Ewald sphere, 4 x 606 frames
Theta range for data collection	1.8 to 30.0 deg.
Index ranges	-15 ≤ h ≤ 15, -14 ≤ h ≤ 14, -16 ≤ h ≤ 16
Reflections collected / unique	19224 / 7549 [R(int)=0.019, R(sigma)=0.021]
Completeness to theta = 30.00°	99.0%
Absorption correction	Multi-scan (progr. SADABS; Sheldrick, 1996)
Transmission factors	0.78 - 0.86
Structure solution	Direct methods (program SHELXS97)
Refinement method	Full-matrix least-squares on F ² (SHELXL97)
Data / restraints / parameters	7549 / 1 / 302
Goodness-of-fit on F ²	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0365, wR2 = 0.0891 (6940 data)
R indices (all data)	R1 = 0.0413, wR2 = 0.0934 (7549 data)
Absolute structure parameter §§	-0.06(4)
Extinction coefficient	0.0059(11)
Largest diff. peak and hole	0.273 and -0.259 e Å ⁻³

$$R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}, \quad wR2 = \left[\frac{\sum (w(F_o^2 - F_c^2)^2)}{\sum (w(F_o^2)^2)} \right]^{1/4}$$

§) Z = 4, compound contains two independent di-protonated molecules of (R)-(-)-5b and four independent chloride ions in the asymmetric unit.

§§) Absolute structure via anomalous dispersion and Flack absolute structure parameter.

Table S12. Atomic coordinates and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) of (R)-(-)-5b·2HCl. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Cl(1) *	0.40632(6)	0.17218(5)	0.05019(5)	69(1)
Cl(2)	0.09976(4)	0.49953(5)	-0.17551(4)	50(1)
Cl(3)	0.39945(6)	0.82780(5)	0.54168(5)	67(1)
Cl(4)	0.11443(5)	0.46425(5)	0.30642(4)	53(1)
amine molecule 1				
N(1)	0.3789(2)	0.4498(2)	0.1312(2)	50(1)
N(2)	0.0978(1)	0.7210(1)	-0.0058(1)	40(1)
C(1)	0.4234(2)	0.4856(2)	0.2356(2)	55(1)
C(2)	0.4002(2)	0.6075(2)	0.2784(2)	57(1)
C(3)	0.3291(2)	0.6910(2)	0.2113(2)	46(1)
C(4)	0.2885(2)	0.6532(2)	0.1008(2)	40(1)
C(5)	0.3129(2)	0.5301(2)	0.0623(2)	48(1)
C(6)	0.2831(2)	0.8235(3)	0.2391(2)	67(1)
C(7)	0.2178(2)	0.8729(2)	0.1305(2)	65(1)
C(8)	0.2211(2)	0.7623(2)	0.0393(2)	45(1)
C(9)	0.2726(2)	0.8072(2)	-0.0738(2)	64(1)
C(10)	0.1690(3)	0.8773(3)	-0.1382(2)	76(1)
C(11)	0.0561(2)	0.8274(2)	-0.0875(2)	55(1)
C(12)	0.0106(2)	0.6858(2)	0.0790(2)	53(1)
amine molecule 2				
N(1')	0.3624(1)	0.5524(2)	0.6270(2)	47(1)
N(2')	0.1930(1)	0.2185(2)	0.4333(1)	45(1)
C(1')	0.4169(2)	0.5170(2)	0.7283(2)	54(1)
C(2')	0.3992(2)	0.3960(2)	0.7729(2)	53(1)
C(3')	0.3227(2)	0.3108(2)	0.7125(1)	42(1)
C(4')	0.2688(1)	0.3489(2)	0.6067(1)	36(1)
C(5')	0.2891(2)	0.4722(2)	0.5648(1)	41(1)
C(6')	0.2798(2)	0.1796(2)	0.7466(2)	53(1)
C(7')	0.2187(2)	0.1243(2)	0.6359(2)	54(1)
C(8')	0.1847(2)	0.2443(2)	0.5605(1)	39(1)
C(9')	0.0517(2)	0.2791(2)	0.5619(2)	55(1)
C(10')	-0.0102(2)	0.1893(3)	0.4718(2)	71(1)
C(11')	0.0870(2)	0.1339(2)	0.4022(2)	66(1)
C(12')	0.3078(2)	0.1690(2)	0.3934(2)	62(1)

*.asymmetric unit contains four independent Cl ions and two independent amine molecules.

Table S13. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (R)-(-)-5b·2HCl.

	x	y	z	U_{iso}
amine molecule 1				
H(1N)	0.3920 (20)	0.3690 (30)	0.1050 (20)	60
H(2N)	0.1076 (18)	0.6490 (20)	-0.0517 (18)	49
H(1)	0.4705	0.4274	0.2796	66
H(2)	0.4315	0.6331	0.3508	68
H(5)	0.2841	0.5026	-0.0104	57
H(6A)	0.3485	0.8816	0.2623	80
H(6B)	0.2293	0.8183	0.3014	80
H(7A)	0.2564	0.9509	0.1030	78
H(7B)	0.1360	0.8944	0.1453	78
H(9A)	0.3394	0.8661	-0.0587	77
H(9B)	0.2989	0.7329	-0.1176	77
H(10A)	0.1761	0.9712	-0.1279	91
H(10B)	0.1681	0.8578	-0.2200	91
H(11A)	0.0169	0.8967	-0.0470	66
H(11B)	0.0009	0.7932	-0.1475	66
H(12A)	0.0427	0.6174	0.1281	80
H(12B)	-0.0618	0.6562	0.0393	80
H(12C)	-0.0060	0.7611	0.1248	80
amine molecule 2				
H(1'N)	0.3690 (20)	0.6370 (30)	0.5990 (20)	57
H(2'N)	0.1779 (19)	0.3020 (20)	0.3978 (19)	54
H(1')	0.4671	0.5758	0.7682	65
H(2')	0.4376	0.3709	0.8425	64
H(5')	0.2528	0.4995	0.4949	49
H(6'A)	0.2239	0.1869	0.8069	64
H(6'B)	0.3460	0.1245	0.7738	64
H(7'A)	0.1481	0.0748	0.6529	65
H(7'B)	0.2726	0.0674	0.5969	65
H(9'A)	0.0222	0.2633	0.6375	65
H(9'B)	0.0385	0.3703	0.5418	65
H(10C)	-0.0524	0.1197	0.5089	85
H(10D)	-0.0669	0.2383	0.4227	85
H(11C)	0.1030	0.0433	0.4227	80
H(11D)	0.0652	0.1389	0.3203	80
H(12D)	0.3707	0.2285	0.4169	92
H(12E)	0.3025	0.1619	0.3108	92
H(12F)	0.3243	0.0844	0.4266	92

N-bonded hydrogen atoms were refined in x,y,z without restraints; C-bonded hydrogen atoms were inserted in idealized positions and were refined riding with the atoms to which they were bonded. All hydrogen atoms had $U_{iso} = U_{eq} \times 1.2$ ($\times 1.5$ for CH_3) of their carrier atoms.

Table S14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for (*R*)-(-)-5b·2HCl. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl(1)	91(1)	47(1)	66(1)	1(1)	-22(1)	7(1)
Cl(2)	58(1)	45(1)	46(1)	-6(1)	-2(1)	2(1)
Cl(3)	89(1)	41(1)	68(1)	-3(1)	-27(1)	1(1)
Cl(4)	65(1)	49(1)	43(1)	11(1)	-12(1)	-11(1)
amine molecule 1						
N(1)	54(1)	40(1)	56(1)	9(1)	-3(1)	7(1)
N(2)	53(1)	29(1)	39(1)	6(1)	-1(1)	4(1)
C(1)	46(1)	62(1)	55(1)	19(1)	-9(1)	2(1)
C(2)	52(1)	69(1)	47(1)	2(1)	-10(1)	-1(1)
C(3)	43(1)	52(1)	42(1)	-3(1)	-1(1)	-4(1)
C(4)	44(1)	35(1)	41(1)	4(1)	-4(1)	0(1)
C(5)	61(1)	37(1)	44(1)	3(1)	-9(1)	6(1)
C(6)	69(1)	64(1)	65(1)	-24(1)	-8(1)	8(1)
C(7)	79(2)	36(1)	78(2)	-11(1)	-12(1)	0(1)
C(8)	54(1)	30(1)	50(1)	5(1)	-4(1)	1(1)
C(9)	66(1)	53(1)	75(1)	24(1)	15(1)	2(1)
C(10)	94(2)	65(1)	71(2)	39(1)	18(1)	18(1)
C(11)	67(1)	45(1)	53(1)	17(1)	-5(1)	14(1)
C(12)	64(1)	40(1)	57(1)	5(1)	13(1)	2(1)
amine molecule 2						
N(1')	49(1)	38(1)	55(1)	-9(1)	-2(1)	-7(1)
N(2')	58(1)	35(1)	41(1)	-2(1)	-3(1)	-9(1)
C(1')	49(1)	61(1)	51(1)	-18(1)	-6(1)	-7(1)
C(2')	49(1)	70(1)	39(1)	-4(1)	-7(1)	-3(1)
C(3')	40(1)	49(1)	36(1)	2(1)	2(1)	3(1)
C(4')	38(1)	34(1)	35(1)	-3(1)	0(1)	0(1)
C(5')	46(1)	31(1)	44(1)	-2(1)	-6(1)	-2(1)
C(6')	54(1)	58(1)	47(1)	15(1)	-2(1)	-3(1)
C(7')	72(1)	37(1)	54(1)	11(1)	-5(1)	-3(1)
C(8')	47(1)	33(1)	37(1)	3(1)	-1(1)	-5(1)
C(9')	47(1)	51(1)	65(1)	6(1)	1(1)	-7(1)
C(10')	56(1)	77(2)	79(2)	10(1)	-12(1)	-24(1)
C(11')	80(2)	53(1)	64(1)	-3(1)	-17(1)	-29(1)
C(12')	73(1)	54(1)	59(1)	-11(1)	10(1)	4(1)

Table S15. Bond lengths [Å] and angles [deg] for (R)-(-)-5b·2HCl.

Bond lengths		C(6')-C(7')	1.531(3)
N(1)-C(1)	1.336(3)	C(6')-H(6'A)	0.97
N(1)-C(5)	1.339(2)	C(6')-H(6'B)	0.97
N(1)-H(1N)	0.89(3)	C(7')-C(8')	1.543(2)
N(2)-C(12)	1.473(2)	C(7')-H(7'A)	0.97
N(2)-C(11)	1.501(2)	C(7')-H(7'B)	0.97
N(2)-C(8)	1.511(2)	C(8')-C(9')	1.536(3)
N(2)-H(2N)	0.92(2)	C(9')-C(10')	1.529(3)
C(1)-C(2)	1.372(3)	C(9')-H(9'A)	0.97
C(1)-H(1)	0.93	C(9')-H(9'B)	0.97
C(2)-C(3)	1.379(3)	C(10')-C(11')	1.505(4)
C(2)-H(2)	0.93	C(10')-H(10C)	0.97
C(3)-C(4)	1.391(2)	C(10')-H(10D)	0.97
C(3)-C(6)	1.492(3)	C(11')-H(11C)	0.97
C(4)-C(5)	1.368(2)	C(11')-H(11D)	0.97
C(4)-C(8)	1.505(2)	C(12')-H(12D)	0.96
C(5)-H(5)	0.93	C(12')-H(12E)	0.96
C(6)-C(7)	1.509(3)	C(12')-H(12F)	0.96
C(6)-H(6A)	0.97		
C(6)-H(6B)	0.97	Bond angles	
C(7)-C(8)	1.551(3)	C(1)-N(1)-C(5)	122.63(19)
C(7)-H(7A)	0.97	C(1)-N(1)-H(1N)	119.8(16)
C(7)-H(7B)	0.97	C(5)-N(1)-H(1N)	117.6(16)
C(8)-C(9)	1.536(3)	C(12)-N(2)-C(11)	113.85(15)
C(9)-C(10)	1.524(3)	C(12)-N(2)-C(8)	117.82(15)
C(9)-H(9A)	0.97	C(11)-N(2)-C(8)	105.24(14)
C(9)-H(9B)	0.97	C(12)-N(2)-H(2N)	107.5(13)
C(10)-C(11)	1.516(3)	C(11)-N(2)-H(2N)	104.8(13)
C(10)-H(10A)	0.97	C(8)-N(2)-H(2N)	106.7(13)
C(10)-H(10B)	0.97	N(1)-C(1)-C(2)	120.62(18)
C(11)-H(11A)	0.97	N(1)-C(1)-H(1)	119.7
C(11)-H(11B)	0.97	C(2)-C(1)-H(1)	119.7
C(12)-H(12A)	0.96	C(1)-C(2)-C(3)	118.19(19)
C(12)-H(12B)	0.96	C(1)-C(2)-H(2)	120.9
C(12)-H(12C)	0.96	C(3)-C(2)-H(2)	120.9
N(1')-C(5')	1.343(2)	C(2)-C(3)-C(4)	119.86(19)
N(1')-C(1')	1.344(3)	C(2)-C(3)-C(6)	129.43(19)
N(1')-H(1'N)	0.93(3)	C(4)-C(3)-C(6)	110.70(17)
N(2')-C(12')	1.483(3)	C(5)-C(4)-C(3)	119.73(16)
N(2')-C(11')	1.499(2)	C(5)-C(4)-C(8)	129.11(16)
N(2')-C(8')	1.509(2)	C(3)-C(4)-C(8)	111.16(16)
N(2')-H(2'N)	0.96(2)	N(1)-C(5)-C(4)	118.84(18)
C(1')-C(2')	1.360(3)	N(1)-C(5)-H(5)	120.6
C(1')-H(1')	0.93	C(4)-C(5)-H(5)	120.6
C(2')-C(3')	1.385(3)	C(3)-C(6)-C(7)	106.20(18)
C(2')-H(2')	0.93	C(3)-C(6)-H(6A)	110.5
C(3')-C(4')	1.394(2)	C(7)-C(6)-H(6A)	110.5
C(3')-C(6')	1.486(3)	C(3)-C(6)-H(6B)	110.5
C(4')-C(5')	1.375(2)	C(7)-C(6)-H(6B)	110.5
C(4')-C(8')	1.504(2)	H(6A)-C(6)-H(6B)	108.7
C(5')-H(5')	0.93	C(6)-C(7)-C(8)	107.36(18)

C(6)-C(7)-H(7A)	110.2	C(3')-C(4')-C(8')	110.37(14)
C(8)-C(7)-H(7A)	110.2	N(1')-C(5')-C(4')	118.50(16)
C(6)-C(7)-H(7B)	110.2	N(1')-C(5')-H(5')	120.7
C(8)-C(7)-H(7B)	110.2	C(4')-C(5')-H(5')	120.7
H(7A)-C(7)-H(7B)	108.5	C(3')-C(6')-C(7')	104.23(15)
C(4)-C(8)-N(2)	112.52(14)	C(3')-C(6')-H(6'A)	110.9
C(4)-C(8)-C(9)	115.07(17)	C(7')-C(6')-H(6'A)	110.9
N(2)-C(8)-C(9)	99.73(15)	C(3')-C(6')-H(6'B)	110.9
C(4)-C(8)-C(7)	104.29(16)	C(7')-C(6')-H(6'B)	110.9
N(2)-C(8)-C(7)	112.58(17)	H(6'A)-C(6')-H(6'B)	108.9
C(9)-C(8)-C(7)	113.00(18)	C(6')-C(7')-C(8')	105.51(16)
C(10)-C(9)-C(8)	104.27(18)	C(6')-C(7')-H(7'A)	110.6
C(10)-C(9)-H(9A)	110.9	C(8')-C(7')-H(7'A)	110.6
C(8)-C(9)-H(9A)	110.9	C(6')-C(7')-H(7'B)	110.6
C(10)-C(9)-H(9B)	110.9	C(8')-C(7')-H(7'B)	110.6
C(8)-C(9)-H(9B)	110.9	H(7'A)-C(7')-H(7'B)	108.8
H(9A)-C(9)-H(9B)	108.9	C(4')-C(8')-N(2')	113.63(13)
C(11)-C(10)-C(9)	106.40(16)	C(4')-C(8')-C(9')	114.96(15)
C(11)-C(10)-H(10A)	110.4	N(2')-C(8')-C(9')	99.56(14)
C(9)-C(10)-H(10A)	110.4	C(4')-C(8')-C(7')	103.47(14)
C(11)-C(10)-H(10B)	110.4	N(2')-C(8')-C(7')	112.93(15)
C(9)-C(10)-H(10B)	110.4	C(9')-C(8')-C(7')	112.74(16)
H(10A)-C(10)-H(10B)	108.6	C(10')-C(9')-C(8')	104.91(18)
N(2)-C(11)-C(10)	104.58(16)	C(10')-C(9')-H(9'A)	110.8
N(2)-C(11)-H(11A)	110.8	C(8')-C(9')-H(9'A)	110.8
C(10)-C(11)-H(11A)	110.8	C(10')-C(9')-H(9'B)	110.8
N(2)-C(11)-H(11B)	110.8	C(8')-C(9')-H(9'B)	110.8
C(10)-C(11)-H(11B)	110.8	H(9'A)-C(9')-H(9'B)	108.8
H(11A)-C(11)-H(11B)	108.9	C(11')-C(10')-C(9')	106.22(17)
N(2)-C(12)-H(12A)	109.5	C(11')-C(10')-H(10C)	110.5
N(2)-C(12)-H(12B)	109.5	C(9')-C(10')-H(10C)	110.5
H(12A)-C(12)-H(12B)	109.5	C(11')-C(10')-H(10D)	110.5
N(2)-C(12)-H(12C)	109.5	C(9')-C(10')-H(10D)	110.5
H(12A)-C(12)-H(12C)	109.5	H(10C)-C(10')-H(10D)	108.7
H(12B)-C(12)-H(12C)	109.5	N(2')-C(11')-C(10')	104.06(18)
		N(2')-C(11')-H(11C)	110.9
C(5')-N(1')-C(1')	122.76(18)	C(10')-C(11')-H(11C)	110.9
C(5')-N(1')-H(1'N)	116.3(15)	N(2')-C(11')-H(11D)	110.9
C(1')-N(1')-H(1'N)	120.8(15)	C(10')-C(11')-H(11D)	110.9
C(12')-N(2')-C(11')	114.81(18)	H(11C)-C(11')-H(11D)	109.0
C(12')-N(2')-C(8')	117.99(15)	N(2')-C(12')-H(12D)	109.5
C(11')-N(2')-C(8')	104.12(15)	N(2')-C(12')-H(12E)	109.5
C(12')-N(2')-H(2'N)	107.8(13)	H(12D)-C(12')-H(12E)	109.5
C(11')-N(2')-H(2'N)	107.0(13)	N(2')-C(12')-H(12F)	109.5
C(8')-N(2')-H(2'N)	104.2(13)	H(12D)-C(12')-H(12F)	109.5
N(1')-C(1')-C(2')	120.65(18)	H(12E)-C(12')-H(12F)	109.5
N(1')-C(1')-H(1')	119.7		
C(2')-C(1')-H(1')	119.7	Torsion angles	
C(1')-C(2')-C(3')	118.54(18)	C5-N1-C1-C2	1.7(3)
C(1')-C(2')-H(2')	120.7	N1-C1-C2-C3	0.5(3)
C(3')-C(2')-H(2')	120.7	C1-C2-C3-C4	-3.4(3)
C(2')-C(3')-C(4')	119.78(17)	C1-C2-C3-C6	175.3(2)
C(2')-C(3')-C(6')	129.25(17)	C2-C3-C4-C5	4.2(3)
C(4')-C(3')-C(6')	110.85(16)	C6-C3-C4-C5	-174.7(2)
C(5')-C(4')-C(3')	119.74(15)		
C(5')-C(4')-C(8')	129.64(14)		

C2-C3-C4-C8	-175.44(18)	C11'-N2'-C8'-C7'	73.7(2)
C6-C3-C4-C8	5.6(2)	C6'-C7'-C8'-C4'	22.4(2)
C1-N1-C5-C4	-0.9(3)	C6'-C7'-C8'-N2'	145.70(16)
C3-C4-C5-N1	-2.1(3)	C6'-C7'-C8'-C9'	-102.40(19)
C8-C4-C5-N1	177.54(18)	C4'-C8'-C9'-C10'	158.18(16)
C2-C3-C6-C7	175.9(2)	N2'-C8'-C9'-C10'	36.39(19)
C4-C3-C6-C7	-5.3(3)	C7'-C8'-C9'-C10'	-83.5(2)
C3-C6-C7-C8	2.9(3)	C8'-C9'-C10'-C11'	-14.2(2)
C5-C4-C8-N2	54.5(3)	C12'-N2'-C11'-C10'	168.76(18)
C3-C4-C8-N2	-125.81(17)	C8'-N2'-C11'-C10'	38.3(2)
C5-C4-C8-C9	-58.8(3)	C9'-C10'-C11'-N2'	-14.3(2)
C3-C4-C8-C9	120.87(19)		
C5-C4-C8-C7	176.9(2)		
C3-C4-C8-C7	-3.5(2)		
C12-N2-C8-C4	65.3(2)		
C11-N2-C8-C4	-166.54(15)		
C12-N2-C8-C9	-172.23(16)		
C11-N2-C8-C9	-44.09(18)		
C12-N2-C8-C7	-52.2(2)		
C11-N2-C8-C7	75.95(19)		
C6-C7-C8-C4	0.1(3)		
C6-C7-C8-N2	122.4(2)		
C6-C7-C8-C9	-125.5(2)		
C4-C8-C9-C10	160.06(19)		
N2-C8-C9-C10	39.4(2)		
C7-C8-C9-C10	-80.3(2)		
C8-C9-C10-C11	-21.2(3)		
C12-N2-C11-C10	162.18(19)		
C8-N2-C11-C10	31.7(2)		
C9-C10-C11-N2	-6.0(3)		
C5'-N1'-C1'-C2'	-0.2(3)		
N1'-C1'-C2'-C3'	-0.8(3)		
C1'-C2'-C3'-C4'	1.9(3)		
C1'-C2'-C3'-C6'	-173.9(2)		
C2'-C3'-C4'-C5'	-2.0(3)		
C6'-C3'-C4'-C5'	174.50(16)		
C2'-C3'-C4'-C8'	-176.80(16)		
C6'-C3'-C4'-C8'	-0.3(2)		
C1'-N1'-C5'-C4'	0.2(3)		
C3'-C4'-C5'-N1'	0.9(2)		
C8'-C4'-C5'-N1'	174.64(16)		
C2'-C3'-C6'-C7'	-169.2(2)		
C4'-C3'-C6'-C7'	14.7(2)		
C3'-C6'-C7'-C8'	-22.7(2)		
C5'-C4'-C8'-N2'	49.0(2)		
C3'-C4'-C8'-N2'	-136.87(15)		
C5'-C4'-C8'-C9'	-64.8(2)		
C3'-C4'-C8'-C9'	109.32(17)		
C5'-C4'-C8'-C7'	171.80(18)		
C3'-C4'-C8'-C7'	-14.04(19)		
C12'-N2'-C8'-C4'	62.6(2)		
C11'-N2'-C8'-C4'	-168.81(16)		
C12'-N2'-C8'-C9'	-174.67(16)		
C11'-N2'-C8'-C9'	-46.07(19)		
C12'-N2'-C8'-C7'	-54.9(2)		

Hydrogen bonds with H..A < r(A) + 2.000 Angstroms and <DHA > 110 deg.

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
N1-H1N	0.894	2.119	174.42	3.011	C11
N2-H2N	0.917	2.098	168.49	3.002	C12
N1'-H1'N	0.926	2.097	175.22	3.021	C13
N2'-H2'N	0.959	2.073	168.29	3.018	C14
