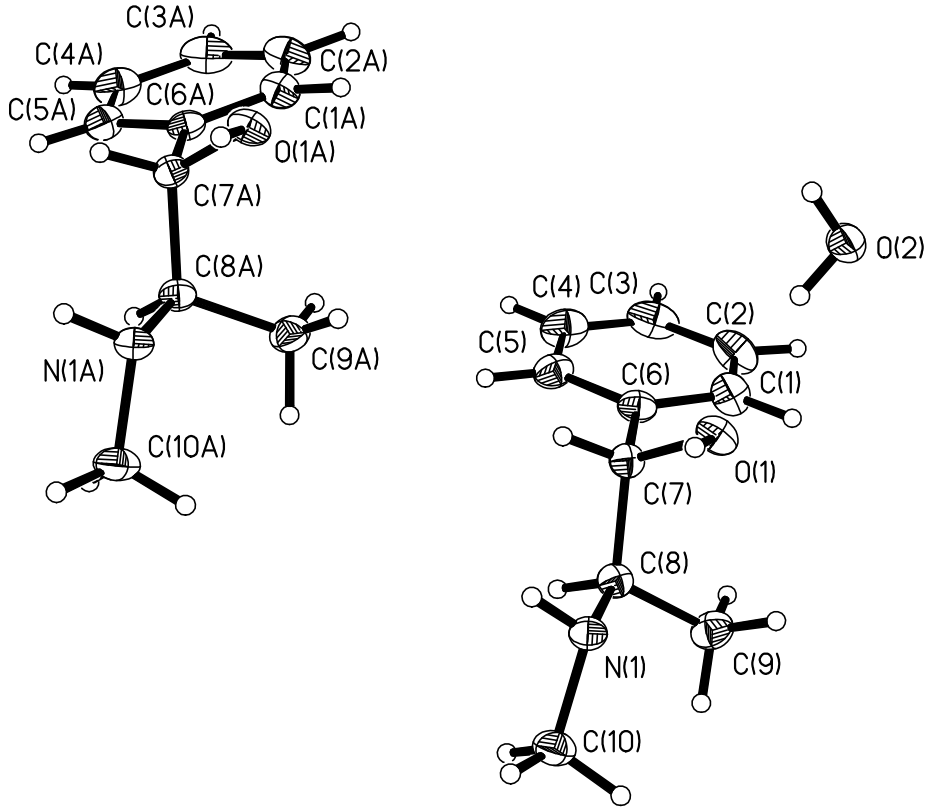
Supplementary data for the:

X-RAY study



ORTEP drawing of L-(-)ephedrine hemihydrate based on the single crystal X-ray data (50% ellipsoids).

Table 1. Crystal data and structure refinement for Xray.

Identification code	X-ray
Empirical formula	C20 H32 N2 O3
Formula weight	348.48
Temperature	120(2) K
Wavelength	0.71073 A
Crystal system	orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 7.3188(4) A alpha = 90 deg. b = 11.2018(6) A beta = 90 deg. c = 24.0156(14) A gamma = 90 deg.
Volume, Z	1968.89(19) A^3, 4
Density (calculated)	1.176 Mg/m^3
Absorption coefficient	0.079 mm^-1
F(000)	760
Crystal size	0.5 x 0.25 x 0.18 mm
Theta range for data collection	1.70 to 30.40 deg.
Limiting indices	-10<=h<=10, -15<=k<=15, -33<=l<=32
Reflections collected	25990
Independent reflections	5596 [R(int) = 0.0301]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5596 / 0 / 354
Goodness-of-fit on F^2	0.989
Final R indices [I>2sigma(I)]	R1 = 0.0335, wR2 = 0.0796
R indices (all data)	R1 = 0.0455, wR2 = 0.0843
Largest diff. peak and hole	0.231 and -0.199 e.A^-3

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

	x	y	z	U(eq)
N(1A)	4005(1)	1340(1)	1979(1)	20(1)
O(1A)	456(1)	2577(1)	2107(1)	22(1)
C(1A)	-980(2)	3171(1)	1057(1)	25(1)
C(2A)	-2002(2)	3376(1)	578(1)	32(1)
C(3A)	-2289(2)	2474(1)	199(1)	34(1)
C(4A)	-1563(2)	1359(1)	298(1)	33(1)
C(5A)	-538(2)	1148(1)	773(1)	25(1)
C(6A)	-235(1)	2055(1)	1158(1)	20(1)
C(7A)	924(1)	1800(1)	1664(1)	18(1)
C(8A)	2968(1)	1883(1)	1520(1)	19(1)
C(9A)	3589(2)	3159(1)	1423(1)	26(1)
C(10A)	5949(2)	1164(1)	1851(1)	27(1)
N(1)	8853(1)	6247(1)	1962(1)	20(1)
O(1)	5584(1)	7692(1)	2089(1)	23(1)
C(1)	4495(2)	8519(1)	1031(1)	29(1)
C(2)	3525(2)	8886(1)	568(1)	34(1)
C(3)	2754(2)	8053(1)	215(1)	35(1)
C(4)	2971(2)	6855(1)	325(1)	35(1)
C(5)	3976(2)	6485(1)	784(1)	26(1)
C(6)	4755(1)	7313(1)	1142(1)	22(1)
C(7)	5873(1)	6909(1)	1634(1)	19(1)
C(8)	7921(1)	6811(1)	1489(1)	20(1)
C(9)	8794(2)	8008(1)	1358(1)	28(1)
C(10)	10743(2)	5893(1)	1844(1)	26(1)
O(2)	2497(1)	8977(1)	2465(1)	29(1)

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

N(1A)-C(10A)	1.4687(14)
N(1A)-C(8A)	1.4695(13)
O(1A)-C(7A)	1.4161(12)
C(1A)-C(6A)	1.3853(16)
C(1A)-C(2A)	1.3924(16)
C(2A)-C(3A)	1.3770(19)
C(3A)-C(4A)	1.378(2)
C(4A)-C(5A)	1.3869(16)
C(5A)-C(6A)	1.3903(15)
C(6A)-C(7A)	1.5096(14)
C(7A)-C(8A)	1.5381(14)
C(8A)-C(9A)	1.5184(16)
N(1)-C(10)	1.4664(14)
N(1)-C(8)	1.4677(13)
O(1)-C(7)	1.4159(12)
C(1)-C(2)	1.3830(16)
C(1)-C(6)	1.3902(16)
C(2)-C(3)	1.381(2)
C(3)-C(4)	1.376(2)
C(4)-C(5)	1.3883(17)
C(5)-C(6)	1.3870(15)
C(6)-C(7)	1.5081(14)
C(7)-C(8)	1.5429(14)
C(8)-C(9)	1.5181(16)
C(10A)-N(1A)-C(8A)	113.50(9)
C(6A)-C(1A)-C(2A)	120.29(11)
C(3A)-C(2A)-C(1A)	120.51(12)
C(2A)-C(3A)-C(4A)	119.52(11)
C(3A)-C(4A)-C(5A)	120.33(12)
C(4A)-C(5A)-C(6A)	120.59(11)
C(1A)-C(6A)-C(5A)	118.76(10)
C(1A)-C(6A)-C(7A)	122.12(10)
C(5A)-C(6A)-C(7A)	119.11(10)
O(1A)-C(7A)-C(6A)	110.66(8)
O(1A)-C(7A)-C(8A)	111.51(8)
C(6A)-C(7A)-C(8A)	110.76(8)
N(1A)-C(8A)-C(9A)	110.51(9)
N(1A)-C(8A)-C(7A)	108.03(8)
C(9A)-C(8A)-C(7A)	112.50(9)
C(10)-N(1)-C(8)	113.88(8)
C(2)-C(1)-C(6)	120.82(12)
C(3)-C(2)-C(1)	120.20(13)
C(4)-C(3)-C(2)	119.57(11)
C(3)-C(4)-C(5)	120.32(12)
C(6)-C(5)-C(4)	120.65(12)
C(5)-C(6)-C(1)	118.41(10)
C(5)-C(6)-C(7)	120.59(10)
C(1)-C(6)-C(7)	121.00(10)
O(1)-C(7)-C(6)	109.77(8)
O(1)-C(7)-C(8)	111.34(8)
C(6)-C(7)-C(8)	111.78(8)
N(1)-C(8)-C(9)	110.23(9)
N(1)-C(8)-C(7)	107.89(8)
C(9)-C(8)-C(7)	113.11(10)

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

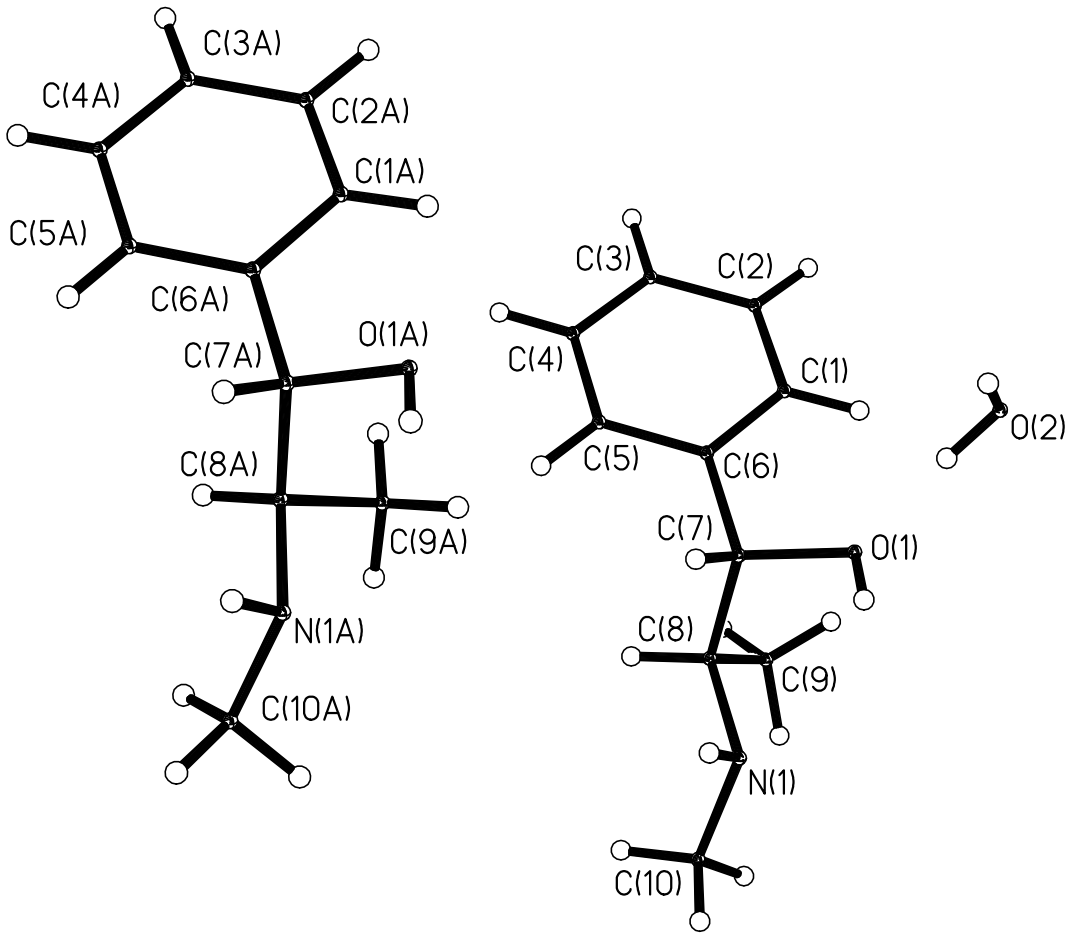
	U11	U22	U33	U23	U13	U12
N(1A)	16(1)	24(1)	20(1)	0(1)	2(1)	0(1)
O(1A)	22(1)	29(1)	16(1)	1(1)	3(1)	5(1)
C(1A)	26(1)	29(1)	20(1)	2(1)	1(1)	2(1)
C(2A)	29(1)	41(1)	24(1)	7(1)	0(1)	8(1)
C(3A)	26(1)	56(1)	21(1)	4(1)	-4(1)	2(1)
C(4A)	29(1)	45(1)	24(1)	-8(1)	-1(1)	-6(1)
C(5A)	24(1)	28(1)	24(1)	-1(1)	1(1)	-3(1)
C(6A)	17(1)	25(1)	17(1)	2(1)	2(1)	-3(1)
C(7A)	18(1)	20(1)	17(1)	1(1)	1(1)	-1(1)
C(8A)	18(1)	23(1)	16(1)	0(1)	1(1)	0(1)
C(9A)	23(1)	27(1)	29(1)	4(1)	3(1)	-4(1)
C(10A)	17(1)	35(1)	28(1)	-6(1)	1(1)	1(1)
N(1)	18(1)	23(1)	19(1)	1(1)	2(1)	0(1)
O(1)	25(1)	29(1)	15(1)	-1(1)	2(1)	5(1)
C(1)	34(1)	30(1)	23(1)	-1(1)	-4(1)	4(1)
C(2)	38(1)	38(1)	25(1)	5(1)	-1(1)	13(1)
C(3)	28(1)	57(1)	20(1)	1(1)	-4(1)	10(1)
C(4)	29(1)	51(1)	25(1)	-5(1)	-5(1)	-3(1)
C(5)	23(1)	32(1)	23(1)	-2(1)	0(1)	-4(1)
C(6)	19(1)	29(1)	17(1)	1(1)	2(1)	1(1)
C(7)	20(1)	22(1)	17(1)	-1(1)	0(1)	0(1)
C(8)	20(1)	24(1)	15(1)	-2(1)	2(1)	0(1)
C(9)	26(1)	29(1)	28(1)	6(1)	2(1)	-5(1)
C(10)	20(1)	31(1)	27(1)	-4(1)	2(1)	3(1)
O(2)	27(1)	22(1)	40(1)	1(1)	9(1)	1(1)

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

	x	y	z	U(eq)
H(1N)	8244(17)	5592(12)	2049(5)	22(3)
H(2N)	3548(19)	593(13)	2048(6)	30(4)
H(1O)	5870(20)	7261(13)	2387(6)	40(4)
H(1OA)	820(20)	2215(12)	2393(6)	36(4)
H(1W)	3320(20)	8523(14)	2337(7)	47(5)
H(2W)	1730(20)	8515(16)	2603(7)	55(5)
H(1)	5020(20)	9105(13)	1276(6)	42(4)
H(2)	3410(20)	9739(14)	486(6)	40(4)
H(3)	2050(20)	8312(13)	-108(6)	51(5)
H(4)	2410(20)	6270(13)	78(6)	41(4)
H(5)	4135(19)	5623(12)	863(6)	32(3)
H(7)	5477(17)	6127(11)	1740(5)	15(3)
H(8)	8012(17)	6295(11)	1159(5)	22(3)
H(1A)	-841(18)	3807(12)	1332(5)	29(3)
H(2A)	-2530(20)	4184(14)	515(6)	45(4)
H(3A)	-2980(20)	2595(13)	-128(6)	37(4)
H(4A)	-1770(20)	724(15)	52(6)	45(4)
H(5A)	-80(19)	385(14)	865(6)	38(4)
H(7A)	688(17)	1007(11)	1773(5)	18(3)
H(8A)	3178(16)	1440(11)	1162(5)	20(3)
H(91)	8143(19)	8402(13)	1027(6)	36(4)
H(92)	10060(20)	7897(12)	1280(5)	30(4)
H(93)	8670(20)	8566(13)	1671(6)	32(4)
H(91A)	4960(20)	3167(13)	1322(6)	38(4)
H(92A)	2890(20)	3526(13)	1116(6)	36(4)
H(93A)	3470(20)	3614(13)	1746(6)	36(4)
H(101)	10840(18)	5523(11)	1472(6)	27(3)
H(102)	11120(20)	5289(13)	2108(6)	35(4)
H(103)	11550(20)	6611(13)	1870(6)	36(4)
H(104)	6470(20)	507(15)	2096(7)	44(4)
H(105)	6645(19)	1888(13)	1902(6)	32(4)
H(106)	6140(20)	899(13)	1479(6)	35(4)

Supplementary data for the:

Neutron study



Labelling diagram of L-(-)ephedrine hemihydrate based on the powder neutron data.

Table 6. Crystal data and structure refinement for neutron.

Identification code	Neutron
Empirical formula	C20 H32 N2 O3
Formula weight	348.48
Temperature	6(1) K
Wavelength	1.5418 A
Crystal system	orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 7.3105(12) A alpha = 90 deg. b = 11.1878(18) A beta = 90 deg. c = 23.9795(42) A gamma = 90 deg.
Volume, Z	1961.24(98) A^3, 4
Density (calculated)	1.180 Mg/m^3
Crystal size	Powder
Theta range for data collection	5 to 70 deg.
Number of profile points	1348
Number of reflections	532
Refinement method	Rigid body Rietveld
R indices fit (R-P, R-WP)	0.00289, 0.00441
R indices model (R-P, R-WP)	0.0092, 0.0120

Table 7. Atomic coordinates (x 10^4) and the global isotropic displacement parameter (A^2 x 10^3) for neutron.

	x	y	z	U(eq)
N(1A)	4038	1318	1987	3
O(1A)	515	2594	2114	3
C(1A)	-975	3186	1075	3
C(2A)	-1991	3402	595	3
C(3A)	-2231	2517	203	3
C(4A)	-1463	1408	290	3
C(5A)	-444	1186	767	3
C(6A)	-189	2075	1164	3
C(7A)	965	1810	1671	3
C(8A)	3013	1871	1527	3
C(9A)	3666	3141	1428	3
C(10A)	5861	893	1824	3
N(1)	8893	6774	2027	3
O(1)	5590	8109	2100	3
C(1)	4097	8784	1101	3
C(2)	3128	9112	630	3
C(3)	2760	8281	219	3
C(4)	3379	7126	279	3
C(5)	4384	6800	746	3
C(6)	4761	7626	1162	3
C(7)	5880	7277	1664	3
C(8)	7930	7162	1521	3
C(9)	8756	8316	1303	3
C(10)	10794	6410	1929	3
O(2)	3091	9324	2469	3

Table 8. Bond lengths [A] and angles [deg] for neutron.

N(1A)-C(10A)	1.4687
N(1A)-C(8A)	1.4695
O(1A)-C(7A)	1.4161
C(1A)-C(6A)	1.3854
C(1A)-C(2A)	1.3925
C(2A)-C(3A)	1.3771
C(3A)-C(4A)	1.3778
C(4A)-C(5A)	1.3868
C(5A)-C(6A)	1.3904
C(6A)-C(7A)	1.5095
C(7A)-C(8A)	1.5381
C(8A)-C(9A)	1.5183
N(1)-C(10)	1.4663
N(1)-C(8)	1.4678
O(1)-C(7)	1.4158
C(1)-C(2)	1.3829
C(1)-C(6)	1.3902
C(2)-C(3)	1.3811
C(3)-C(4)	1.3765
C(4)-C(5)	1.3883
C(5)-C(6)	1.3870
C(6)-C(7)	1.5081
C(7)-C(8)	1.5429
C(8)-C(9)	1.5181
C(10A)-N(1A)-C(8A)	113.5
C(6A)-C(1A)-C(2A)	120.3
C(3A)-C(2A)-C(1A)	120.5
C(2A)-C(3A)-C(4A)	119.5
C(3A)-C(4A)-C(5A)	120.3
C(4A)-C(5A)-C(6A)	120.6
C(1A)-C(6A)-C(5A)	118.8
C(1A)-C(6A)-C(7A)	122.1
C(5A)-C(6A)-C(7A)	119.1
O(1A)-C(7A)-C(6A)	110.7
O(1A)-C(7A)-C(8A)	111.5
C(6A)-C(7A)-C(8A)	110.8
N(1A)-C(8A)-C(9A)	110.5
N(1A)-C(8A)-C(7A)	108.0
C(9A)-C(8A)-C(7A)	112.5
C(10)-N(1)-C(8)	113.9
C(2)-C(1)-C(6)	120.8
C(3)-C(2)-C(1)	120.2
C(4)-C(3)-C(2)	119.6
C(3)-C(4)-C(5)	120.3
C(6)-C(5)-C(4)	120.6
C(5)-C(6)-C(1)	118.4
C(5)-C(6)-C(7)	120.6
C(1)-C(6)-C(7)	121.0
O(1)-C(7)-C(6)	109.8
O(1)-C(7)-C(8)	111.3
C(6)-C(7)-C(8)	111.8
N(1)-C(8)-C(9)	110.2
N(1)-C(8)-C(7)	107.9
C(9)-C(8)-C(7)	113.1

Table 9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for neutron.

	x	y	z	U(eq)
H(1N)	8308	6147	2163	3
H(2N)	3419	653	2107	3
H(1O)	5876	7711	2409	3
H(1OA)	875	2229	2401	3
H(1W)	3914	8870	2341	3
H(2W)	2326	8862	2607	3
H(1)	4339	9366	1386	3
H(2)	2731	9942	586	3
H(3)	2055	8508	-109	3
H(4)	3102	6539	-9	3
H(5)	4833	5969	790	3
H(7)	5483	6506	1788	3
H(8)	8034	6545	1231	3
H(1A)	-870	3808	1358	3
H(2A)	-2551	4205	540	3
H(3A)	-2917	2646	-125	3
H(4A)	-1637	784	35	3
H(5A)	41	424	850	3
H(7A)	709	1019	1781	3
H(8A)	3212	1425	1168	3
H(92)	10112	8367	1410	3
H(93)	8094	8982	1449	3
H(91)	8715	8350	894	3
H(91A)	5049	3137	1340	3
H(92A)	3006	3507	1113	3
H(93A)	3521	3606	1748	3
H(101)	10883	5880	1601	3
H(102)	11222	5947	2244	3
H(103)	11570	7139	1877	3
H(105)	6832	1455	1977	3
H(106)	5983	835	1424	3
H(104)	6142	131	1978	3