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Supporting information for article:

CRYSTAL STRUCTURE ANALYSIS OF EBASTINE (4-(4-BENZHYDRYLOXY-1-PIPERIDYL)-1-(4-TERT-BUTYLPHENYL) BUTAN-1-ONE): AN ORAL HISTAMINE ANTAGONIST

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Supplementary Data

Atom	U11	U22	U33	U23	U13	U12
C1	58(2)	87(2)	64(1)	9(1)	30(1)	12(1)
C2	57(2)	97(2)	66(2	-1(1)	32(1)	0(1)
C3	68(2)	79(2)	56(1)	-1(1)	23(1	-12(1)
C4	70(2)	67(2)	61(2)	7(1)	19(1)	4(1)
C5	58(2)	63(1)	66(1)	-2(1)	26(1)	4(1)
C6	52(1)	58(1)	56(1)	0(1)	24(1)	1(1)
C7	84(2)	112(2)	79(2)	34(2)	48(2)	35(2)
C8	110(3)	203(5)	96(3)	75(3)	62(3)	75(3)
C9	82(3)	319(9)	65(2)	31(4)	37(2)	37(4)
C10	91(3)	234(6)	82(3)	-44(3)	31(2)	-23(3)
C11	91(2)	124(3)	83(2)	-19(2)	31(2)	-5(2)
C12	67(2)	84(2)	57(1)	4(1)	36(1)	10(2)
C13	61(2)	59(1)	68(1)	4(1)	36(1)	11(1)
C14	59(2)	63(1)	65(1)	9(1)	34(1)	10(1)
C15	72(2)	76(2)	83(2)	-8(1)	47(1)	-6(1)
C16	65(2)	73(2)	69(2)	-8(1)	35(1)	-3(1)
C17	59(2)	79(2)	72(2)	-10(1)	28(1)	-3(1)
C18	67(2)	86(2)	61(1)	-3(1)	29(1)	9(1)
C19	63(2)	70(2)	79(2)	8(1)	38(1)	4(1)
C20	68(2)	79(2)	77(2)	10(1)	40(1)	2(1)
C21	57(1)	77(2)	62(1)	9(1)	28(1)	3(1)
C22	71(2)	64(2)	90(2)	11(1)	43(2)	4(1)
C23	54(1)	63(2)	65(1)	10(1)	28(1)	4(1)
C24	86(2)	65(2)	104(2)	-10(1)	56(2)	-13(1)
C25	77(2)	73(2)	95(2)	-14(1)	52(2)	-7(1)
C26	49(1)	66(2)	53(1)	8(1)	20(1)	3(1)
C27	72(2)	59(2)	86(2)	10(1)	43(2)	3(1)
C28	70(2)	65(2)	78(2)	9(1)	45(1)	9(1)
C29	60(2)	81(2)	68(2)	9(1)	33(1)	3(1)
C30	82(2)	99(2)	154(3)	10(2)	74(2)	9(2)
C31	101(2)	206(4)	65(2)	15(2)	38(2)	-21(2)
C32	84(2)	93(2)	116(2)	12(2)	56(2)	-12(2)
N1	50(1)	65(1)	62(1)	5(1)	26(1)	6(1)
O1	87(1)	66(1)	85(1)	15(1)	59(1)	20(1)
O2	153(2)	78(2)	206(3)	-7(2)	138(2)	-17(1)

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

Atom	X	Y	Z	U(eq)
C1	12891(2)	-1957(2)	4851(2)	68(1)
C2	12908(2)	-1583(2)	4071(2)	71(1)
C3	12304(2)	-753(2)	3562(2)	68(1)
C4	11687(2)	-297(2)	3830(2)	69(1)
C5	11667(2)	-676(2)	4609(2)	62(1)
C6	12270(1)	-1510(2)	5134(1)	55(1)
C7	13400(2)	-3380(3)	6963(2)	87(1)
C8	14220(3)	-3583(5)	7626(3)	130(2)
C9	14752(3)	-2632(7)	8015(3)	153(3)
C10	14484(3)	-1472(5)	7758(3)	137(2)
C11	13667(2)	-1264(3)	7095(2)	101(1)
C12	13120(2)	-2216(2)	6690(2)	66(1)
C13	12227(2)	-1987(2)	5968(1)	59(1)
C14	11353(2)	-1672(2)	6788(1)	59(1)
C15	11262(2)	-707(2)	7384(2)	72(1)
C16	10832(2)	-1223(2)	7958(2)	67(1)
C17	10046(2)	-2686(2)	6855(2)	70(1)
C18	10463(2)	-2218(2)	6261(2)	70(1)
C19	9546(2)	-2239(2)	7977(2)	67(1)
C20	9314(2)	-1317(2)	8514(2)	71(1)
C21	8746(2)	-1858(2)	8937(2)	64(1)
C22	8419(2)	-978(2)	9411(2)	72(1)
C23	7778(1)	-1366(2)	9774(1)	59(1)
C24	7451(2)	-520(2)	10178(2)	79(1)
C25	6864(2)	-854(2)	10528(2)	76(1)
C26	6575(1)	-2039(2)	10504(1)	56(1)
C27	6906(2)	-2877(2)	10097(2)	69(1)
C28	7493(2)	-2552(2)	9738(2)	66(1)
C29	5961(2)	-2388(2)	10946(2)	67(1)
C30	5223(2)	-1459(3)	10735(2)	103(1)
C31	6512(2)	-2454(4)	11927(2)	123(1)
C32	5523(2)	-3632(3)	10635(2)	93(1)
N1	9970(1)	-1738(2)	7433(1)	58(1)
O1	11741(1)	-1137(1)	6246(1)	71(1)
O2	8676(2)	78(2)	9505(2)	125(1)

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

C(1)-C(6)-C(13)-C(12)	39.0(3)
O(1)-C(14)-C(15)-C(16)	178.60(19)
C(18)-C(14)-C(15)-C(16)	55.8(3)
C(14)-C(15)-C(16)-N(1)	-57.9(3)
O(1)-C(14)-C(18)-C(17)	-175.63(18)
C(15)-C(14)-C(18)-C(17)	-55.0(3)
N(1)-C(17)-C(18)-C(14)	56.6(3)
N(1)-C(19)-C(20)-C(21)	170.28(19)
C(19)-C(20)-C(21)-C(22)	-174.5(2)
C(20)-C(21)-C(22)-O(2)	-6.5(4)
C(20)-C(21)-C(22)-C(23)	173.4(2)
O(2)-C(22)-C(23)-C(28)	-176.3(3)
C(21)-C(22)-C(23)-C(28)	3.8(4)
O(2)-C(22)-C(23)-C(24)	2.8(4)
C(21)-C(22)-C(23)-C(24)	-177.1(2)
C(28)-C(23)-C(24)-C(25)	-0.2(4)
C(22)-C(23)-C(24)-C(25)	-179.4(2)

Selected torsion angles (degrees)