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SUPPORTING DATA

X-Ray Crystallographic Data for Compound **5**

Experimental

Colorless crystals of **5**•3HCl were obtained from methanol. The crystal used for data collection was a needle measuring 0.32 mm x 0.12 mm x 0.06 mm. All measurements were made on a Rigaku AFC6S diffractometer with graphite monochromated CuK_α (λ = 1.5418 Å) radiation using the ω - 2θ scan mode. The crystal temperature was maintained at 173 K by using a Molecular Structure Corporation low-temperature device. Cell determination (from 25 reflections in the range $23.0° < 2\theta < 48.3°$) and data collection were accomplished using MSC/AFC Diffractometer Control Software (Ref. 1). Crystal data: a = 12.370(4), b = 33.204(4), c = 10.894(4) Å; V = 4475(2) Å^3; space group $P2_12_12_1$; Z = 4; D_{calc} = 1.440 g cm^{-3} for formula $C_{42}H_{67}N_6O_{13}Cl_3$, formula weight = 970.4. Data were collected to a $2\theta_{max}$ of 140.3°. Intensities were corrected for a 20% decline (in spite of the low temperature) and for Lorentz and polarization effects. Absorption effects were corrected using the psi-scan method (trans. factors 0.87-1.00) (Ref. 2). A total of 7189 reflections were measured, of which 6481 were unique; 2287 reflections were classified as observed ($I > 3\sigma(I)$). Equivalent reflections were merged (R_{int} = 0.087). The structure was solved using the program *SHELXS* 86 (Ref. 3) and was refined and finished using the *TEXSAN* software package (Ref. 4). Hydrogen atoms bonded to carbon atoms were placed in calculated positions (C-H bond length = 0.95 Å). Attempts to locate hydrogen atoms bonded to N or O in difference maps were unsuccessful, so these hydrogens were omitted from the refinement model. Because of the low data-to-parameter ratio, only the chloride atoms were refined anisotropically; other non-hydrogen atoms were refined isotropically. Positional refinement of water molecules O1W, O2W, O5W, and O6W was done with site occupancy of 0.5, because a full occupancy model led to physically unreasonable isotropic displacement parameters. The final cycle of full-matrix least-squares refinement produced agreement factors R = 0.092, wR = 0.102. The maximum and minimum in the final difference map were 0.69 e$^-$/Å^3 and -0.42 e$^-$/Å^3.

References

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M1822-3 3

Positional parameters and B(eq)

atom	x	y	z	B(eq)
Cl(1)	0.2120(6)	-0.0384(2)	0.6299(5)	5.4(4)
Cl(2)	-0.1068(6)	0.1962(2)	0.0331(5)	4.5(3)
Cl(3)	-0.2032(7)	0.0924(2)	0.2771(6)	7.1(5)
O(1)	-0.141(1)	0.2052(4)	0.360(1)	2.2(3)
O(1W)*	-0.271(2)	0.3408(9)	0.108(2)	3.1(6)
O(2W)*	-0.439(3)	0.118(1)	0.207(3)	4.7(8)
O(2)	-0.170(1)	0.2702(4)	0.179(1)	3.1(3)
O(3)	0.058(1)	0.1786(4)	0.711(1)	2.7(3)
O(3W)	-0.644(3)	0.1299(8)	0.315(2)	14(1)
O(4W)	0.024(1)	-0.0815(5)	0.958(1)	5.2(4)
O(4)	-0.108(1)	0.0539(4)	0.552(1)	2.7(3)
O(5)	-0.297(1)	0.1099(4)	0.517(1)	4.6(4)
O(5W)*	-0.531(5)	0.109(2)	0.049(5)	13(2)
O(6W)*	-0.211(5)	0.344(2)	0.040(5)	11(1)
O(6)	0.122(1)	0.0068(4)	0.852(1)	3.2(3)
O(7W)	0.165(1)	0.1259(5)	0.116(1)	4.9(4)
N(1)	0.187(2)	0.0335(6)	0.423(2)	4.2(5)
N(2)	0.114(2)	0.0956(5)	0.382(1)	3.3(4)
N(3)	0.032(1)	0.1141(5)	0.569(1)	2.9(4)
N(4)	-0.008(1)	0.1509(5)	0.261(1)	2.2(4)
N(5)	-0.008(2)	0.2472(5)	0.796(2)	3.8(4)
N(6)	-0.051(2)	0.0011(5)	0.986(2)	3.7(4)
C(1)	0.022(2)	0.1636(6)	0.394(2)	2.8(5)
C(2)	-0.081(2)	0.1818(6)	0.452(2)	2.0(4)
C(3)	-0.051(2)	0.2143(6)	0.559(2)	2.3(4)
C(4)	0.055(2)	0.2089(6)	0.625(2)	1.9(4)
C(5)	0.150(2)	0.2038(7)	0.525(2)	4.4(6)

M1822-4

4

atom	x	y	z	B(eq)
C(6)	0.121(2)	0.1904(6)	0.395(2)	2.5(4)
C(7)	0.075(2)	0.2484(6)	0.694(2)	2.6(4)
C(8)	0.072(2)	0.2875(7)	0.623(2)	4.0(5)
C(9)	-0.001(2)	0.2874(7)	0.515(2)	3.5(5)
C(10)	-0.052(2)	0.2491(6)	0.482(2)	1.9(4)
C(11)	-0.106(2)	0.2447(6)	0.377(2)	2.2(4)
C(12)	-0.120(2)	0.2754(6)	0.292(2)	2.7(4)
C(13)	-0.073(2)	0.3114(7)	0.324(2)	3.7(5)
C(14)	-0.017(2)	0.3164(7)	0.436(2)	4.5(6)
C(15)	-0.144(2)	0.2123(6)	0.654(2)	2.9(5)
C(16)	-0.125(2)	0.2481(6)	0.741(2)	2.6(4)
C(17)	0.006(2)	0.2828(8)	0.894(2)	5.1(6)
C(18)	0.115(2)	0.2827(7)	0.947(2)	4.6(6)
C(19)	0.121(3)	0.288(1)	1.078(3)	6.7(7)
C(20)	0.145(2)	0.2445(7)	1.028(2)	4.4(6)
C(21)	0.081(2)	0.0724(6)	0.578(2)	2.4(5)
C(22)	-0.002(2)	0.0410(6)	0.609(2)	2.9(5)
C(23)	-0.032(2)	0.0364(6)	0.741(2)	2.5(5)
C(24)	0.054(2)	0.0426(6)	0.842(2)	2.8(5)
C(25)	0.119(2)	0.0781(6)	0.813(2)	2.9(5)
C(26)	0.170(2)	0.0738(7)	0.683(2)	4.0(5)
C(27)	-0.003(2)	0.0430(7)	0.965(2)	4.2(6)
C(28)	-0.083(2)	0.0807(7)	0.973(2)	4.5(6)
C(29)	-0.157(2)	0.0863(7)	0.860(2)	3.5(5)
C(30)	-0.120(2)	0.0683(6)	0.755(2)	2.2(4)
C(31)	-0.160(2)	0.0742(6)	0.648(2)	2.9(5)
C(32)	-0.245(2)	0.1004(7)	0.627(2)	3.8(5)
C(33)	-0.283(2)	0.1199(6)	0.738(2)	3.1(5)
C(34)	-0.236(2)	0.1127(6)	0.853(2)	2.5(5)

M1822-S 5

atom	x	y	z	B(eq)
C(35)	-0.091(2)	-0.0077(7)	0.762(2)	4.4(6)
C(36)	-0.135(2)	-0.0101(7)	0.895(2)	4.5(6)
C(37)	-0.112(2)	-0.0021(7)	1.111(2)	4.4(5)
C(38)	-0.033(2)	0.0009(7)	1.213(2)	4.3(6)
C(39)	-0.054(2)	-0.026(1)	1.323(3)	6.7(7)
C(40)	0.044(2)	-0.0350(8)	1.240(2)	6.0(7)
C(41)	0.056(2)	0.1225(6)	0.453(2)	2.3(4)
C(42)	0.133(2)	0.0661(6)	0.456(2)	2.6(4)
H(2)	-0.1259	0.1611	0.4847	2.4
H(5)	0.1853	0.2292	0.5181	5.3
H(5A)	0.1997	0.1846	0.5568	5.3
H(6)	0.1802	0.1760	0.3614	3.0
H(6A)	0.1067	0.2136	0.3468	3.0
H(7)	0.1441	0.2465	0.7319	3.1
H(8)	0.1431	0.2931	0.5946	4.7
H(8A)	0.0489	0.3083	0.6764	4.7
H(13)	-0.0778	0.3335	0.2688	4.4
H(14)	0.0101	0.3424	0.4547	5.5
H(15)	-0.2121	0.2148	0.6143	3.5
H(15A)	-0.1417	0.1876	0.6981	3.5
H(16)	-0.1760	0.2468	0.8065	3.1
H(16A)	-0.1349	0.2725	0.6970	3.1
H(17)	-0.0456	0.2794	0.9577	6.1
H(17A)	-0.0059	0.3079	0.8542	6.1
H(18)	0.1707	0.2943	0.8995	5.6
H(19)	0.1785	0.3035	1.1116	8.0
H(19A)	0.0570	0.2926	1.1236	8.0
H(20)	0.2167	0.2340	1.0276	5.3
H(20A)	0.0951	0.2231	1.0396	5.3

m1822-6 6

atom	x	y	z	B(eq)
H(22)	0.0200	0.0157	0.5763	3.5
H(25)	0.0742	0.1013	0.8155	3.5
H(25A)	0.1751	0.0807	0.8723	3.5
H(27)	0.0510	0.0468	1.0263	5.1
H(28)	-0.0400	0.1044	0.9821	5.3
H(28A)	-0.1272	0.0775	1.0435	5.3
H(30)	0.2106	0.0497	0.6802	4.8
H(31)	0.2157	0.0962	0.6686	4.8
H(33)	-0.3412	0.1383	0.7325	3.7
H(34)	-0.2601	0.1265	0.9242	3.0
H(35)	-0.0406	-0.0286	0.7483	5.3
H(35A)	-0.1496	-0.0104	0.7054	5.3
H(36)	-0.1582	-0.0369	0.9112	5.3
H(36A)	-0.1948	0.0077	0.9034	5.3
H(37)	-0.1485	-0.0273	1.1155	5.2
H(37A)	-0.1632	0.0191	1.1175	5.2
H(38)	-0.0058	0.0271	1.2300	5.2
H(39)	-0.0427	-0.0165	1.4037	8.1
H(39A)	-0.1135	-0.0443	1.3225	8.1
H(40)	0.1155	-0.0301	1.2692	7.2
H(40A)	0.0446	-0.0580	1.1880	7.2

*O1W, O2W, O5W, and O6W were refined with occupancy = 0.5

MB22-7 7

X-Ray Crystallographic Data for Compound **7**

Experimental

Crystals of **7** were grown from EtOAc/MeOH. Crystal was a rectangular plate 0.05 x 0.15 x 0.55 mm. Cell constants were determined by least-squares refinement of 25 reflections in the interval $40.75° < 2\Theta > 58.82°$. Crystal data: a = 16.723(2), b = 9.122(1), c = 14.261(2), $\alpha = \gamma = 90°$, $\beta = 105.00(1)$; V = 2101.2 Å^3; Space Group = $P2_1$, Z = 2 for asymmetric unit $(C_{21}N_3O_4H_{27})_2 \cdot C_4H_8O_2$; formula weight of asymmetric unit, 879.0; molecular weight of **7**, 395.5; D_c = 1.358 g/cc. Data were collected at 165K on a Siemens P3 computer-controlled diffractometer using Ni-filtered Cu K_α radiation (λ = 1.54184 A) and Θ-2Θ scans. The data extended to $(\sin\Theta)/\lambda = 0.65$, 3786 reflections were measured, merging to 3081 unique reflections, $R_{sym} = 0.015$ [$R_{sym} = \Sigma_i(Y_i - Y_{ave})/\Sigma Y_i$ ($Y = F^2$)]. Data processing was done with the DREAM suite of programs (ref 1). The structure was solved using MULTAN78 (ref 2) and QTAN incorporating NQEST (ref 3). Full-matrix least-squares refinement with anisotropic thermal parameters for C, N, and O atoms and isotropic refinement of H atoms led to conventional R = 0.035, S (goodness of fit) = 2.21; no correction for absorption or extinction (μ = 7.46 cm^{-1}). Final difference map had maximum and minimum of .29 and -.30 e/Å^3, respectively. The quality of the data and refinement is seen in the agreement in bond distances and angles between the two independent molecules in the asymmetric unit; most comparable values (except in isopropyl ring) differ by less than 2σ. Atomic coordinates are given in the tables.

M1822-B 8

References

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M 1822-9 9

Atomic coordinates and equivalent isotropic thermal parameters (Biso) for compound **7**, 6α-amino-6β-carboxamide naltrexone.

	X	Y	Z	BISO
Molecule A				
C 1	0.31152	0.63441	0.47927	1.81
C 2	0.28379	0.57844	0.38634	1.78
C 3	0.26802	0.66855	0.30407	1.82
C 4	0.28414	0.81609	0.32061	1.58
C 5	0.26851	1.06445	0.30709	1.69
C 6	0.17563	1.10507	0.30116	1.74
C 7	0.16736	1.17709	0.39609	1.79
C 8	0.21270	1.09456	0.48718	1.76
C 9	0.36137	1.02657	0.58692	1.90
C 10	0.34783	0.85957	0.59334	2.07
C 11	0.32681	0.78409	0.49584	1.61
C 12	0.31396	0.86948	0.41341	1.66
C 13	0.32563	1.03230	0.40835	1.65
C 14	0.30524	1.10291	0.49672	1.62
C 15	0.41659	1.06560	0.41052	2.18
C 16	0.47383	1.01444	0.50633	2.44
C 17	0.14912	1.22154	0.22172	1.85
C 18	0.50948	1.05173	0.68107	2.85
C 19	0.48981	1.13225	0.76453	2.63
C 20	0.55524	1.22650	0.82772	3.21
C 21	0.48189	1.29336	0.76042	3.37
N 1	0.44658	1.07450	0.58856	2.12
N 6	0.11794	0.98153	0.27891	2.01
N 17	0.07773	1.19996	0.15699	2.57
O 3	0.23694	0.61933	0.21138	2.25

	X	Y	Z	BISO
O 4	0.26926	0.92738	0.25167	1.81
O 14	0.32523	1.25602	0.50410	2.10
O 17B	0.19329	1.33110	0.22151	2.42
Molecule B				
C 1'	0.67166	0.34875	0.14100	1.99
C 2'	0.72027	0.46273	0.18876	1.82
C 3'	0.80302	0.44356	0.24046	1.57
C 4'	0.83526	0.30434	0.23825	1.50
C 5'	0.90856	0.09695	0.28940	1.56
C 6'	0.89508	0.05448	0.39009	1.37
C 7'	0.84100	-0.08336	0.38364	1.70
C 8'	0.76278	-0.07717	0.30150	1.66
C 9'	0.71018	-0.06935	0.11393	1.58
C 10'	0.65709	0.07103	0.10362	1.89
C 11'	0.70432	0.20846	0.14152	1.58
C 12'	0.78749	0.19287	0.18934	1.48
C 13'	0.83883	0.05814	0.19850	1.45
C 14'	0.78452	-0.07458	0.20507	1.44
C 15'	0.87206	0.04166	0.10782	1.68
C 16'	0.80197	0.01590	0.01621	1.99
C 17'	0.98109	0.01348	0.45748	1.58
C 18'	0.68658	-0.14562	-0.05900	2.23
C 19'	0.64228	-0.28533	-0.04915	2.61
C 20'	0.55933	-0.28571	-0.02782	3.95
C 21'	0.56689	-0.32599	-0.12681	4.35
N 1'	0.74686	-0.10286	0.03183	1.74
N 6'	0.85229	0.17325	0.42560	1.76

m1822-11

11

	X	Y	Z	BISO
N 17'	1.00896	0.09035	0.53767	2.16
O 3'	0.84929	0.55045	0.29587	2.10
O 4'	0.91425	0.25868	0.28576	1.51
O 14'	0.82834	-0.20778	0.19822	1.76
O 17B'	1.02023	-0.09215	0.43523	1.82
Ethyl Acetate				
C 24	0.16727	0.95662	0.01664	5.39
C 25	0.08037	0.98331	-0.02919	4.43
C 26	-0.01704	1.14321	-0.13360	5.33
C 27	-0.03142	1.10959	-0.23607	5.15
O 25	0.02619	0.90611	-0.01882	5.11
O 26	0.06577	1.10751	-0.08456	5.64

M1822-12 17

6α-Amino,6β-carboxamide-naltrexone (7). Fractional atomic coordinates (x104) and anisotropic thermal vibration parameters (x104 E2) T = exp(-2p2(U11h2a*2 + ... + 2U12hka*b* + ...))

Molecule A

atom	x/a(σ)	y/b(σ)	z/c(σ)	U11(σ)	U22(σ)	U33(σ)	U12(σ)	U23(σ)	U13(σ)
C(1)	3115(2)	6344(5)	4793(2)	203(17)	232(20)	267(18)	43(15)	37(16)	84(14)
C(2)	2838(2)	5784(5)	3863(2)	216(17)	192(20)	287(19)	9(15)	19(16)	101(14)
C(3)	2680(2)	6686(5)	3041(2)	213(17)	258(21)	223(17)	-11(16)	-59(16)	62(14)
C(4)	2841(2)	8161(5)	3206(2)	181(16)	196(20)	237(17)	5(15)	15(15)	80(13)
C(5)	2685(2)	10644(5)	3071(2)	265(18)	183(19)	217(17)	-32(16)	-33(15)	102(14)
C(6)	1756(2)	11051(5)	3012(2)	245(17)	182(18)	243(17)	-18(16)	-25(15)	79(14)
C(7)	1674(2)	11771(5)	3961(2)	218(16)	229(19)	234(17)	9(16)	-31(16)	57(13)
C(8)	2127(2)	10946(-)	4872(2)	231(16)	233(20)	216(16)	21(16)	-31(15)	79(13)
C(9)	3614(2)	10266(5)	5869(2)	224(17)	268(21)	230(17)	-28(17)	-70(16)	57(14)
C(10)	3478(2)	8596(5)	5933(2)	239(17)	317(21)	220(17)	3(17)	-5(16)	44(14)
C(11)	3268(2)	7841(5)	4958(2)	126(16)	247(21)	232(18)	46(15)	9(16)	32(13)
C(12)	3140(2)	8695(5)	4134(2)	164(16)	219(19)	257(18)	12(15)	-14(16)	72(14)
C(13)	3256(2)	10323(5)	4083(2)	189(16)	198(19)	244(17)	13(15)	8(15)	64(13)
C(14)	3052(2)	11029(5)	4967(2)	221(17)	169(19)	239(17)	-24(16)	-9(15)	82(14)
C(15)	4166(2)	10656(5)	4105(2)	204(16)	333(22)	307(18)	-33(17)	-46(17)	95(14)
C(16)	4738(2)	10144(5)	5063(2)	185(17)	361(23)	373(19)	-10(17)	-70(18)	60(15)
C(17)	1491(2)	12215(5)	2217(2)	247(17)	240(21)	242(17)	1(17)	-29(16)	108(14)
C(18)	5095(2)	10517(6)	6811(2)	253(18)	420(24)	348(19)	10(19)	-59(19)	-35(15)
C(19)	4898(2)	11323(6)	7645(2)	298(19)	390(24)	287(19)	-108(18)	25(18)	30(15)
C(20)	5552(2)	12265(6)	8277(2)	308(19)	597(30)	295(19)	-101(21)	-79(20)	45(16)
C(21)	4819(2)	12934(6)	7604(3)	461(23)	459(27)	355(21)	-4(22)	-64(20)	98(18)
N(1)	4466(1)	10745(5)	5886(2)	182(13)	349(18)	263(14)	-26(14)	-53(14)	34(11)
N(6)	1179(2)	9815(5)	2789(2)	258(14)	239(17)	276(14)	-39(13)	-42(13)	82(12)
N(17)	777(2)	12000(5)	1570(2)	278(15)	352(19)	309(15)	-11(15)	104(15)	11(13)
O(3)	2369(1)	6193(4)	2114(1)	376(13)	210(13)	257(12)	-66(12)	-62(11)	60(10)
O(4)	2693(1)	9274(4)	2517(1)	278(12)	194(12)	225(11)	11(11)	-26(11)	83(9)
O(14)	3252(1)	12560(4)	5041(2)	252(12)	211(13)	330(13)	-31(10)	-58(11)	63(10)
O(17B)	1933(1)	13311(4)	2215(2)	380(14)	227(15)	312(13)	-41(12)	22(11)	93(11)

M1822-13 19

Molecule B

atom	x/a(σ)	y/b(σ)	z/c(σ)	U11(σ)	U22(σ)	U33(σ)	U12(σ)	U23(σ)	U13(σ)
C(1')	6717(2)	3488(5)	1410(2)	207(17)	285(23)	248(17)	54(16)	35(16)	30(14)
C(2')	7203(2)	4627(5)	1888(2)	276(18)	159(20)	250(17)	19(16)	6(15)	53(14)
C(3')	8030(2)	4436(5)	2405(2)	257(17)	166(18)	162(16)	-27(16)	-16(15)	37(13)
C(4')	8353(2)	3043(5)	2383(2)	184(16)	187(19)	186(16)	-14(15)	28(15)	27(13)
C(5')	9086(2)	970(5)	2894(2)	200(16)	141(18)	256(17)	-11(15)	9(15)	67(13)
C(6')	8951(2)	545(5)	3901(2)	182(15)	161(17)	174(15)	5(15)	12(14)	41(12)
C(7')	8410(2)	-834(5)	3836(2)	265(17)	195(19)	188(16)	-13(16)	29(15)	62(13)
C(8')	7628(2)	-772(5)	3015(2)	213(16)	171(18)	232(16)	-69(16)	11(15)	30(13)
C(9')	7102(2)	-694(5)	1139(2)	221(17)	183(18)	195(16)	-38(16)	-2(15)	48(13)
C(10')	6571(2)	710(5)	1036(2)	195(16)	245(20)	251(18)	-8(16)	-2(16)	7(13)
C(11')	7043(2)	2085(5)	1415(2)	187(17)	215(20)	194(16)	-23(16)	30(15)	40(13)
C(12')	7875(2)	1929(5)	1893(2)	197(16)	171(18)	194(16)	22(16)	30(15)	47(13)
C(13')	8388(2)	581(5)	1985(2)	157(16)	164(18)	212(17)	15(15)	9(14)	13(13)
C(14')	7845(2)	-746(5)	2051(2)	190(16)	121(17)	240(17)	-5(15)	-3(15)	65(13)
C(15')	8721(2)	417(5)	1078(2)	193(15)	232(19)	217(16)	-6(15)	42(15)	62(13)
C(16')	8020(2)	159(5)	162(2)	266(17)	298(22)	190(16)	-68(17)	22(16)	58(14)
C(17')	9811(2)	135(5)	4575(2)	196(17)	190(20)	228(18)	-41(16)	44(15)	77(14)
C(18')	6866(2)	-1456(5)	-590(2)	309(18)	308(22)	199(16)	-13(17)	-32(16)	12(14)
C(19')	6423(2)	-2853(5)	-492(2)	358(19)	315(23)	280(18)	-68(19)	-43(17)	10(15)
C(20')	5593(2)	-2857(6)	-278(3)	334(20)	688(33)	453(22)	-137(24)	-44(24)	56(17)
C(21')	5669(3)	-3260(6)	-1268(3)	553(25)	619(31)	423(23)	-269(25)	-116(24)	24(19)
N(1')	7469(1)	-1029(4)	318(2)	251(14)	237(16)	160(13)	-36(13)	-12(12)	29(11)
N(6')	8523(1)	1732(5)	4256(2)	250(14)	193(15)	237(14)	11(13)	-9(13)	86(11)
N(17')	10090(2)	904(5)	5377(2)	258(15)	278(18)	225(15)	66(14)	-64(13)	-40(12)
O(3')	8493(1)	5505(4)	2959(1)	347(13)	149(12)	252(12)	-12(11)	39(10)	-17(10)
O(4')	9142(1)	2587(4)	2858(1)	164(11)	148(12)	238(11)	-8(9)	43(10)	7(9)
O(14')	8283(1)	-2078(4)	1982(1)	320(13)	165(13)	190(11)	40(11)	11(10)	74(10)
O(17B')	10202(1)	-922(4)	4352(1)	223(11)	208(14)	251(11)	33(11)	17(10)	41(9)
C(24)	1673(3)	9566(7)	166(3)	646(29)	999(44)	364(23)	214(32)	11(27)	60(21)
C(25)	804(3)	9833(7)	-292(3)	673(31)	632(35)	411(25)	-93(28)	-111(25)	198(23)

M 1822-14 14

atom	x/a(σ)	y/b(σ)	z/c(σ)	U11(σ)	U22(σ)	U33(σ)	U12(σ)	U23(σ)	U13(σ)
C(26)	-170(3)	11432(7)	-1336(3)	551(28)	771(39)	731(31)	260(28)	141(30)	214(24)
C(27)	-314(2)	11096(7)	-2361(3)	480(25)	879(40)	610(28)	66(28)	137(30)	165(21)
O(25)	262(2)	9061(5)	-188(2)	714(21)	546(22)	674(20)	-267(19)	-20(17)	169(16)
O(26)	658(2)	11075(5)	-846(2)	700(21)	827(26)	620(19)	-114(21)	148(21)	179(16)

M 182015 15

Atomic coordinates and isotropic thermal parameters (Biso) for hydrogen atoms of **7**, 6α-amino-6β-carboxamide-naltrexone.

	X	Y	Z	BISO
Molecule A				
H 1	0.31899	0.56332	0.53170	2.81
H 2	0.28316	0.46991	0.37870	2.78
H 3O	0.22020	0.54052	0.20405	3.25
H 5	0.29056	1.14359	0.27576	2.69
H 6N	0.10557	0.94105	0.33242	3.01
H 6NB	0.12993	0.92394	0.25257	3.01
H 7A	0.18882	1.28367	0.39989	2.79
H 7B	0.10633	1.17814	0.39455	2.79
H 8A	0.20219	1.13975	0.53908	2.76
H 8B	0.19977	0.99406	0.48034	2.76
H 9	0.35236	1.06871	0.64352	2.90
H 10A	0.39630	0.81384	0.64014	3.07
H 10B	0.30717	0.84314	0.61935	3.07
H 14O	0.37310	1.26228	0.53110	3.10
H 15A	0.42255	1.16755	0.40040	3.18
H 15B	0.43105	1.00635	0.35642	3.18
H 16A	0.53064	1.04944	0.51365	3.44
H 16B	0.47864	0.91403	0.50865	3.44
H 17A	0.05668	1.27069	0.10189	3.57
H 17B	0.04320	1.10834	0.15892	3.57
H 18A	0.51983	0.94071	0.69797	3.85
H 18B	0.56695	1.07912	0.67373	3.85
H 19	0.45183	1.07074	0.79490	3.63
H 20A	0.60598	1.22591	0.81026	4.21
H 20B	0.55630	1.23026	0.89175	4.21

m 1622-16 16

	X	Y	Z	BISO
H 21A	0.44292	1.33085	0.79368	4.37
H 21B	0.49202	1.33632	0.71080	4.37
Molecule B				
H 1'	0.61323	0.35668	0.11097	2.99
H 2'	0.70157	0.55753	0.18943	2.82
H 3'O	0.84588	0.61895	0.26765	3.10
H 5'	0.95852	0.06271	0.28276	2.56
H 6'N	0.83859	0.14656	0.47726	2.76
H 6'NB	0.88233	0.25143	0.43724	2.76
H 7'A	0.86909	-0.16264	0.37482	2.70
H 7'B	0.82605	-0.08764	0.44751	2.70
H 8'A	0.73163	-0.15315	0.30107	2.66
H 8'B	0.73101	0.01150	0.30602	2.66
H 9'	0.67238	-0.16212	0.11472	2.58
H 10'A	0.62889	0.07800	0.03400	2.89
H 10'B	0.60996	0.05412	0.13494	2.89
H 14'O	0.82383	-0.22132	0.14907	2.76
H 15'A	0.91128	-0.04009	0.12480	2.68
H 15'B	0.90022	0.12643	0.09790	2.68
H 16'A	0.82365	-0.01300	-0.04104	2.99
H 16'B	0.77045	0.11616	-0.00436	2.99
H 17A'	1.06335	0.06526	0.58543	3.16
H 17B'	0.97522	0.17327	0.55476	3.16
H 18'A	0.64367	-0.06847	-0.08043	3.23
H 18'B	0.71962	-0.15832	-0.10963	3.23
H 19'	0.67853	-0.36498	-0.01869	3.61
H 20'A	0.53197	-0.19107	-0.02678	4.95
H 20'B	0.54017	-0.36105	0.01681	4.95

	X	Y	Z	BISO
H 21'A	0.55106	-0.42429	-0.14528	5.35
H 21'B	0.55936	-0.26197	-0.16666	5.35
Ethyl Acetate				
H 24A	0.19437	1.06546	0.05775	6.39
H 24B	0.17595	0.86006	0.06217	6.39
H 24C	0.19597	0.96200	-0.04224	6.39
H 26A	-0.02624	1.23098	-0.11908	6.33
H 26B	-0.05393	1.10214	-0.10092	6.33
H 27A	-0.03175	0.99692	-0.23919	6.15
H 27B	-0.09166	1.14255	-0.28164	6.15
H 27C	0.00418	1.14227	-0.26894	6.15