Supporting information

Ethionamide biomimetic activation and an unprecedented mechanism for its conversion into the active and non-active metabolites

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X-ray data for compound 2

Table :

a =	8.2425(11) Å	α =	90.149(11)°
b =	8.4394(10) Å	β =	100.435(12)°
c =	13.236(2) Å	γ =	104.134(11)°
Volume	877.0(2) $Å^3$	Crystal Class	triclinic
Space group	P -1	Z =	4
Formula	$C_8 H_{10} N_2 O_1 S_1$	M_r	182.25
Cell determined from	5724 reflections	Cell θ range =	5 - 71°
Temperature	180K		
Shape	planar		
Colour	yellow	Size	0.08 × 0.18 × 0.22 mm
D_x	1.38	F000	384.000
μ	2.894 mm^{-1}		
Absorption correction	multi-scan		
T_{min}	0.59	T_{max}	0.79

Data Collection

Diffractometer	multi-scan
Scan type	φ and ω scans
Reflections measured	12822
Independent reflections	3331
Rint	0.0397
θ_{max}	70.4663
h =	-10 → 10

k = -8 → 10
l = -16 → 16

Refinement

$\Delta\rho_{min}$ = -0.24 e Å^{-3}
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
Reflections used 2741
Cutoff: I > 3.00σ(I)
Parameters refined 217
S = 1.06
R-factor 0.034
weighted R-factor 0.042
Δ/σ_{max} 0.0012
Refinement on F
w = $w' \times [1 - (\Delta F_{obs} / 6 \times \Delta F_{est})^2]^2$
w′ = $[P_0T_0'(x) + P_1T_1'(x) + ...P_{n-1}T_{n-1}'(x)]^{-1}$, where P_i are the coefficients of a Chebychev series in $t_i(x)$, and x = $F_{calc}/F_{calcmax}$.
P_0 - P_{n-1} = 11.3 -0.914 9.69

Parameters

Label	*x*	*y*	*Z*	$U_{iso/equiv}$	Occupancy
N1	1.4056(2)	0.7216(2)	0.51910(12)	0.0471	1.0000
C2	1.5164(2)	0.6695(2)	0.59039(14)	0.0376	1.0000
C3	1.4666(2)	0.58143(19)	0.67309(13)	0.0328	1.0000
C4	1.2964(2)	0.54474(19)	0.68445(13)	0.0303	1.0000
C5	1.1824(2)	0.6015(2)	0.61100(15)	0.0396	1.0000
C6	1.2430(3)	0.6872(2)	0.53086(16)	0.0482	1.0000
C7	1.23884(19)	0.44741(18)	0.76964(13)	0.0285	1.0000
S8	1.03543(5)	0.33844(5)	0.75391(3)	0.0355	1.0000
O9	1.01814(15)	0.25476(15)	0.85495(10)	0.0398	1.0000
N10	1.34351(17)	0.44043(17)	0.85614(11)	0.0326	1.0000
C11	1.6996(3)	0.7124(3)	0.57608(17)	0.0501	1.0000
C12	1.7766(3)	0.8957(3)	0.58380(17)	0.0531	1.0000
N21	0.46902(16)	0.09063(17)	0.86163(11)	0.0316	1.0000
C22	0.35980(19)	-0.0284(2)	0.79415(13)	0.0305	1.0000
C23	0.18838(19)	0.05550(19)	0.80109(12)	0.0292	1.0000
C24	0.12645(18)	0.15023(18)	0.87833(12)	0.0263	1.0000
C25	0.2402(2)	0.21161(19)	0.94913(13)	0.0305	1.0000
C26	0.4086(2)	0.17789(19)	0.93652(14)	0.0323	1.0000
C27	0.05623(18)	0.18744(19)	0.88610(11)	0.0265	1.0000
S28	0.14470(4)	0.38218(4)	0.90636(3)	0.0304	1.0000
O29	0.32418(13)	0.38727(14)	0.92550(9)	0.0348	1.0000
N30	0.14107(16)	0.07281(16)	0.87777(11)	0.0306	1.0000
C31	0.4292(2)	0.0716(2)	0.71017(14)	0.0399	1.0000
H31	1.5472(2)	0.54525(19)	0.72113(13)	0.0409	1.0000
C32	0.5930(2)	0.1997(2)	0.74814(15)	0.0400	1.0000
H51	1.0671(2)	0.5838(2)	0.61803(15)	0.0489	1.0000
H61	1.1648(3)	0.7255(2)	0.48231(16)	0.0592	1.0000

H101	1.44776(17)	0.50137(17)	0.86933(11)	0.0407	1.0000
H102	1.30798(17)	0.38895(17)	0.91017(11)	0.0421	1.0000
H111	1.7657(3)	0.6622(3)	0.62784(17)	0.0624	1.0000
H112	1.7057(3)	0.6695(3)	0.50993(17)	0.0609	1.0000
H121	1.7783(3)	0.9407(3)	0.65110(17)	0.0811	1.0000
H122	1.7087(3)	0.9454(3)	0.53216(17)	0.0805	1.0000
H123	1.8907(3)	0.9175(3)	0.57112(17)	0.0794	1.0000
H231	0.11660(19)	0.00981(19)	0.75376(12)	0.0367	1.0000
H251	0.2067(2)	0.27066(19)	1.00359(13)	0.0374	1.0000
H261	0.4867(2)	0.22013(19)	0.98326(14)	0.0400	1.0000
H301	0.08923(16)	0.03026(16)	0.87257(11)	0.0395	1.0000
H302	0.25022(16)	0.09752(16)	0.87780(11)	0.0370	1.0000
H311	0.3457(2)	0.1267(2)	0.67587(14)	0.0498	1.0000
H312	0.4483(2)	-0.0024(2)	0.66281(14)	0.0499	1.0000
H321	0.6790(2)	0.1477(2)	0.77766(15)	0.0612	1.0000
H322	0.6252(2)	0.2629(2)	0.69097(15)	0.0601	1.0000
H323	0.5761(2)	0.2727(2)	0.79894(15)	0.0609	1.0000

Thermal Parameters

Label	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0546(10)	0.0388(8)	0.0400(8)	0.0095(7)	0.0059(7)	-0.0014(7)
C2	0.0419(9)	0.0299(8)	0.0397(9)	0.0021(7)	0.0133(7)	0.0022(7)
C3	0.0316(8)	0.0292(8)	0.0380(8)	0.0037(7)	0.0105(7)	0.0054(6)
C4	0.0296(8)	0.0246(7)	0.0350(8)	0.0003(6)	0.0063(6)	0.0033(6)
C5	0.0319(8)	0.0330(8)	0.0472(10)	0.0046(7)	-0.0004(7)	0.0014(7)
C6	0.0470(11)	0.0409(10)	0.0463(10)	0.0129(8)	-0.0051(8)	0.0011(8)
C7	0.0242(7)	0.0241(7)	0.0381(8)	0.0007(6)	0.0082(6)	0.0057(6)
S8	0.0221(2)	0.0344(2)	0.0451(2)	0.00457(17)	0.00550(16)	0.00145(15)
O9	0.0304(6)	0.0359(6)	0.0502(7)	0.0075(5)	0.0123(5)	-0.0005(5)
N10	0.0222(6)	0.0355(7)	0.0380(7)	0.0057(6)	0.0076(5)	0.0015(5)
C11	0.0507(12)	0.0481(11)	0.0548(11)	0.0090(9)	0.0288(9)	0.0047(9)
C12	0.0455(11)	0.0520(12)	0.0512(11)	0.0058(9)	0.0064(9)	-0.0062(9)
N21	0.0198(6)	0.0339(7)	0.0414(8)	0.0000(6)	0.0084(5)	0.0054(5)
C22	0.0220(7)	0.0345(8)	0.0339(8)	-0.0012(6)	0.0071(6)	0.0038(6)
C23	0.0207(7)	0.0331(8)	0.0333(8)	0.0033(6)	0.0057(6)	0.0055(6)
C24	0.0189(7)	0.0248(7)	0.0353(8)	0.0009(6)	0.0070(6)	0.0044(5)
C25	0.0244(7)	0.0295(8)	0.0391(8)	0.0061(6)	0.0091(6)	0.0071(6)
C26	0.0220(7)	0.0301(8)	0.0460(9)	0.0033(7)	0.0052(6)	0.0094(6)
C27	0.0196(7)	0.0299(7)	0.0299(7)	0.0043(6)	0.0064(5)	0.0047(6)
S28	0.0212(2)	0.0274(2)	0.0433(2)	0.00694(15)	0.01040(15)	0.00382(14)
O29	0.0192(5)	0.0401(6)	0.0437(6)	0.0089(5)	0.0094(4)	0.0021(4)
N30	0.0181(6)	0.0292(7)	0.0462(8)	0.0071(6)	0.0114(5)	0.0051(5)
C31	0.0246(8)	0.0572(11)	0.0368(9)	0.0062(8)	0.0108(7)	0.0045(7)
C32	0.0309(8)	0.0388(9)	0.0505(10)	0.0131(8)	0.0119(7)	0.0058(7)

Distances

N1	C2	1.343(3)Å		N1	C6	1.338(3)Å

C2	C3	1.392(2)Å		C2	C11	1.511(3)Å
C3	C4	1.397(2)Å		C3	H31	0.941Å
C4	C5	1.396(2)Å		C4	C7	1.476(2)Å
C5	C6	1.385(3)Å		C5	H51	0.946Å
C6	H61	0.941Å		C7	S8	1.6792(15)Å
C7	N10	1.314(2)Å		S8	O9	1.5272(13)Å
N10	H101	0.873Å		N10	H102	0.895Å
C11	C12	1.517(3)Å		C11	H111	0.962Å
C11	H112	0.961Å		C12	H121	0.964Å
C12	H122	0.966Å		C12	H123	0.959Å
N21	C22	1.351(2)Å		N21	C26	1.333(2)Å
C22	C23	1.395(2)Å		C22	C31	1.508(2)Å
C23	C24	1.392(2)Å		C23	H231	0.932Å
C24	C25	1.395(2)Å		C24	C27	1.4839(19)Å
C25	C26	1.389(2)Å		C25	H251	0.922Å
C26	H261	0.945Å		C27	S28	1.6711(15)Å
C27	N30	1.319(2)Å		S28	O29	1.5360(11)Å
N30	H301	0.879Å		N30	H302	0.873Å
C31	C32	1.511(2)Å		C31	H311	0.970Å
C31	H312	0.943Å		C32	H321	0.949Å
C32	H322	0.966Å		C32	H323	0.962Å

Angles

C2	N1	C6	117.31(16)°		N1	C2	C3	122.27(17)°
N1	C2	C11	116.14(17)°		C3	C2	C11	121.59(17)°
C2	C3	C4	120.14(16)°		C2	C3	H31	120.125°
C4	C3	H31	119.734°		C3	C4	C5	117.30(16)°
C3	C4	C7	121.34(15)°		C5	C4	C7	121.35(15)°
C4	C5	C6	118.61(17)°		C4	C5	H51	119.750°
C6	C5	H51	121.609°		N1	C6	C5	124.35(18)°
N1	C6	H61	118.053°		C5	C6	H61	117.581°
C4	C7	S8	118.94(12)°		C4	C7	N10	121.78(14)°
S8	C7	N10	119.25(12)°		C7	S8	O9	105.67(7)°
C7	N10	H101	121.990°		C7	N10	H102	122.362°
H101	N10	H102	114.575°		C2	C11	C12	112.24(18)°
C2	C11	H111	109.182°		C12	C11	H111	108.846°
C2	C11	H112	109.332°		C12	C11	H112	109.135°
H111	C11	H112	108.013°		C11	C12	H121	110.674°
C11	C12	H122	108.323°		H121	C12	H122	109.756°
C11	C12	H123	109.367°		H121	C12	H123	109.375°
H122	C12	H123	109.322°		C22	N21	C26	117.95(13)°
N21	C22	C23	121.55(15)°		N21	C22	C31	117.71(14)°
C23	C22	C31	120.74(15)°		C22	C23	C24	119.77(15)°
C22	C23	H231	119.437°		C24	C23	H231	120.792°
C23	C24	C25	118.55(14)°		C23	C24	C27	121.55(14)°
C25	C24	C27	119.89(14)°		C24	C25	C26	117.67(15)°
C24	C25	H251	121.938°		C26	C25	H251	120.372°

N21	C26	C25	124.47(15)°		N21	C26	H261	116.923°
C25	C26	H261	118.602°		C24	C27	S28	115.53(11)°
C24	C27	N30	121.49(13)°		S28	C27	N30	122.97(11)°
C27	S28	O29	106.34(7)°		C27	N30	H301	121.035°
C27	N30	H302	120.615°		H301	N30	H302	118.348°
C22	C31	C32	113.78(15)°		C22	C31	H311	109.607°
C32	C31	H311	107.949°		C22	C31	H312	106.825°
C32	C31	H312	109.339°		H311	C31	H312	109.285°
C31	C32	H321	109.351°		C31	C32	H322	108.825°
H321	C32	H322	111.021°		C31	C32	H323	109.895°
H321	C32	H323	109.507°		H322	C32	H323	108.225°