

Supplementary Materials

Structural and Mechanistic Basis for the Inactivation of Human Ornithine Aminotransferase by (S)-3-Amino-(S)-4-fluorocyclopentenecarboxylic Acid

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20190304_pt6471_nESI_OAT_m202_02#104 RT: 0.21 AV: 1 NL: 6.49E7
F: FTMS -p ESI d Full ms2 125.0234@ncd35.00 [50.0000-145.0000]

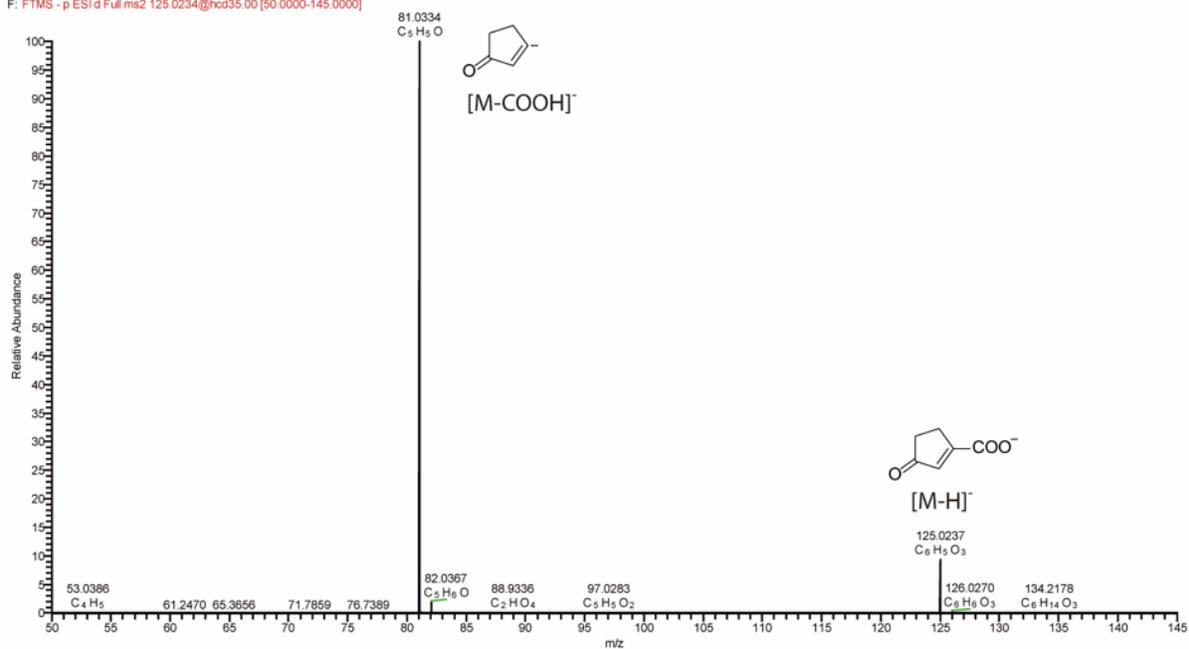


Figure S1. Primary metabolite Met II of 5 in *hOAT* (see Scheme 7)

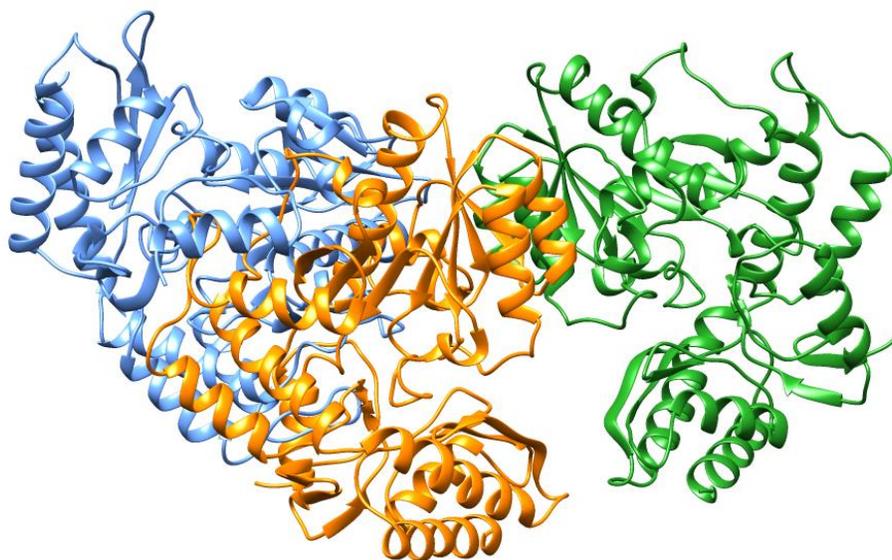


Figure S2. The asymmetric unit of the co-crystal structure of *hOAT* inactivated by **5**. The model contains three protein monomers, each monomer is shown in a different color.

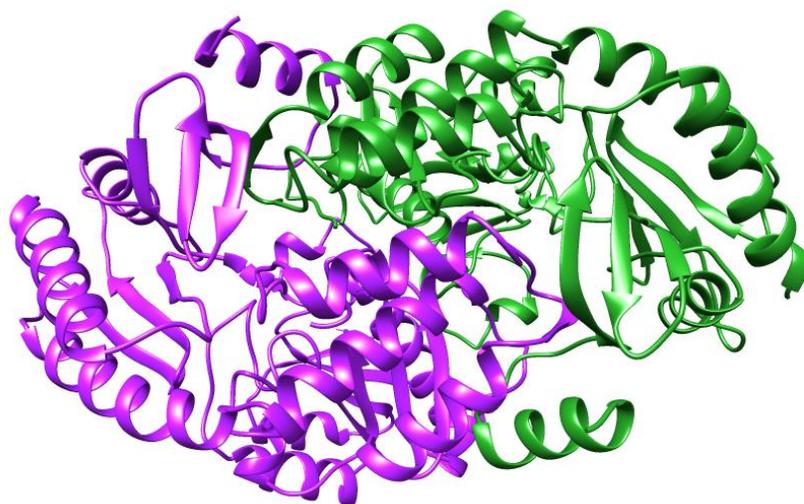


Figure S3. The biological assembly of *hOAT* represents a homodimer.

Table S1. Statistics of the crystal structures of *hOAT* inactivated by **5**

PDB code	8EZ1
Space group	C121
Cell dimension	
α, β, γ (deg)	90, 103.7, 90
a, b, c (Å)	202.2, 110.3, 57.1
Processed Resolution (Å)	1.91
Rmerge ^b (%)	18.5 (121.4)
Rpim ^d (%)	9.9 (67.3)
I/ σ (I)	6.1 (1.1)
CC _{1/2} ^e (%)	99.2 (46.4)
Completeness (%)	98.0 (95.5)
Multiplicity	4.2 (4.1)
No. Reflections	391615
No. Unique Reflections	92197
Refinement	
Rwork ^f / Rfree ^g (%)	18.85/23.66
No. of Atoms	
protein	9425
ligand	81
water	707
B factors (Å ²)	
protein	37.00
Ligand (copy A)	25.48
Ligand (copy B)	29.94
Ligand (copy C)	41.72
RMSD ^h	
bond lengths (Å)	0.012
bond angles (deg)	1.12
Ramachandran plot (%)	

avored	95.07
allowed	4.59
outliers	0.33
<p>^aProvided Resolution at $l/\sigma = 2$ for conventional assessment of data quality</p> <p>^b$R_{\text{merge}} = \Sigma I_{\text{obs}} - I_{\text{avg}} / \Sigma I_{\text{avg}}$</p> <p>^cThe values for the highest-resolution bin are in parentheses</p> <p>^dPrecision-indicating merging R</p> <p>^ePearson correlation coefficient of two “half” data sets</p> <p>^f$R_{\text{work}} = \Sigma F_{\text{obs}} - F_{\text{calc}} / \Sigma F_{\text{obs}}$</p> <p>^gFive percent of the reflection data were selected at random as a test set, and only these data were used to calculate R_{free}</p> <p>^hRoot-mean square deviation</p>	