

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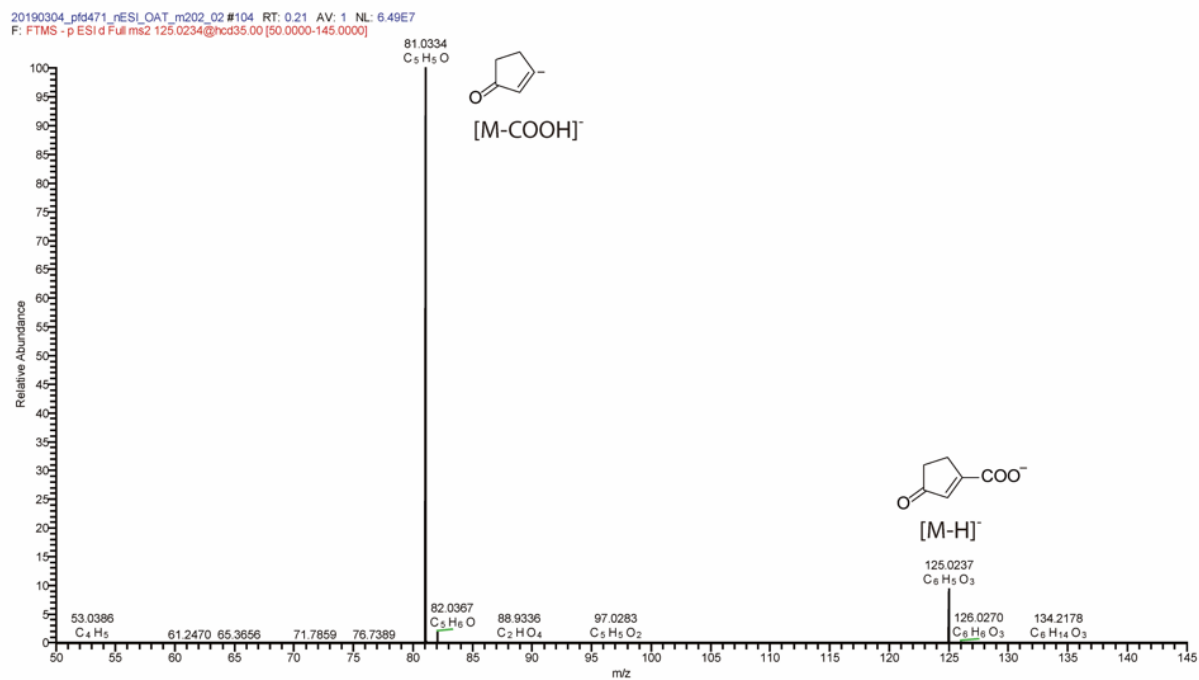
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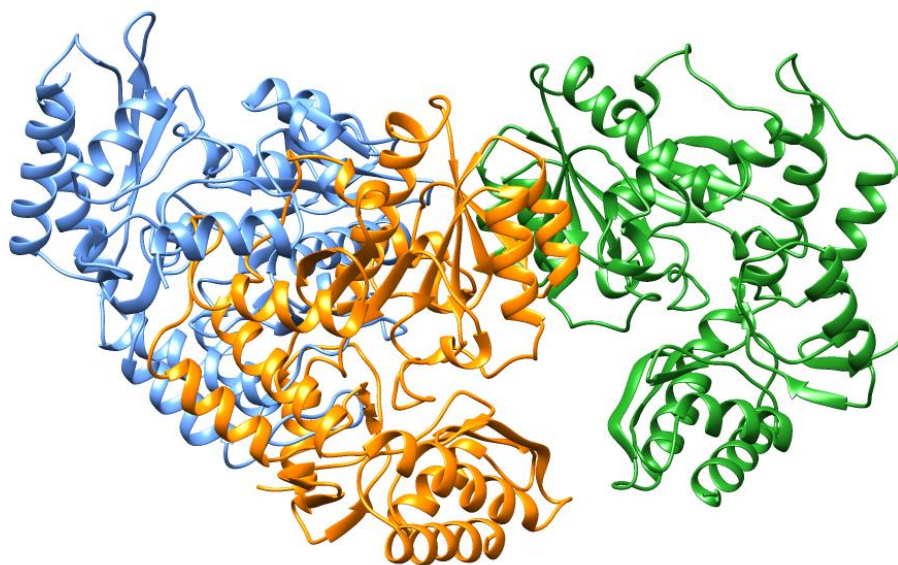
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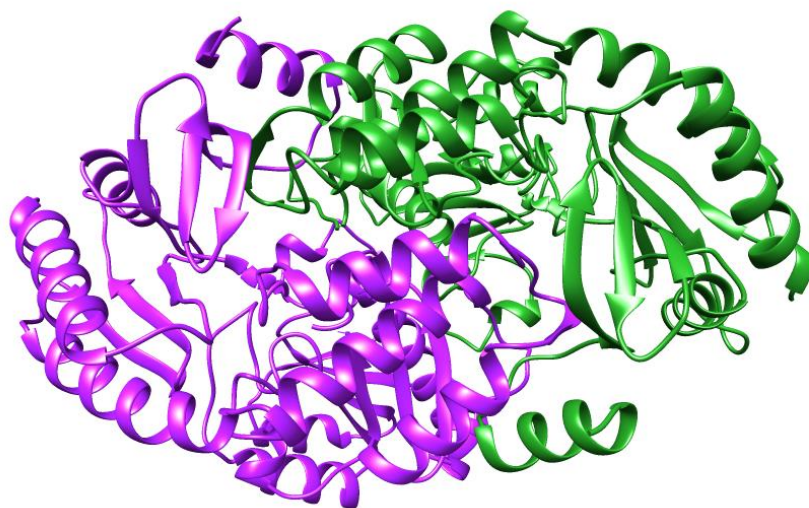
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**Figure S1.** Primary metabolite **Met II** of **5** in *h*OAT (see Scheme 7)



**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 *h*OAT inactivated by **5**

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

avored	95.07
allowed	4.59
outliers	0.33
<sup>a</sup> Provided Resolution at $I/\sigma = 2$ for conventional assessment of data quality <sup>b</sup> $R_{\text{merge}} = \Sigma  I_{\text{obs}} - I_{\text{avg}}  / \Sigma I_{\text{avg}}$ <sup>c</sup> The values for the highest-resolution bin are in parentheses <sup>d</sup> Precision-indicating merging R <sup>e</sup> Pearson correlation coefficient of two “half” data sets <sup>f</sup> $R_{\text{work}} = \Sigma  F_{\text{obs}} - F_{\text{calc}}  / \Sigma F_{\text{obs}}$ <sup>g</sup> Five percent of the reflection data were selected at random as a test set, and only these data were used to calculate $R_{\text{free}}$ <sup>h</sup> Root-mean square deviation	