SUPPORTING INFORMATION

Discovery of Novel Allosteric Inhibitors of Deoxyhypusine Synthase

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Table S1. Data collection and refinement statistics

X-Ray Structure	DHS-NAD-GC7 / PDB: 6P4V	DHS-**11g** / PDB: 6PGR
Data collection		
Resolution range (Å)	50-1.65 (1.68-1.65)	50-1.95(1.98-1.95)
Space group	$P3_22_1$	$P3_22_1$
Cell dimensions:		
***a, b, c* (Å)**	104.5, 104.5, 159.5	104.6, 104.6, 160.5
α, β, γ (°)	90.0, 90.0, 120.0	90.0, 90.0, 120.0
R_{sym}	10.1 (94.2)	9.1(91.9)
<I / σI>	12.0 (1.9)	20.3(2.6)
Completeness (%)	99.9 (100)	100(100)
Redundancy	5.6 (5.6)	7.3 (7.3)
Structure Refinement		
Resolution (Å)	43.7-1.65	49.8-1.95
No. reflections	113,578	70,577
No. reflections Rfree test set	6,006	3,744
Rwork / Rfree	16.1/17.4	16.8 /19.4
No. atoms:		
Protein	5,172	5,421
NAD	88	-
Inhibitor	24	44
MPD	8	-
Waters	328	359
Mean B Value (Å²):		
Protein B Value	29.0	31.5
NAD B Value	21.2	-
Inhibitor B Value	18.0	27.7
MPD B Value	36.3	-
Water B Value	34.5	35.6
RMS Bond lengths (Å)	0.007	0.008
RMS Bond angles (°)	1.317	1.28
Ramachandran statistics:		
Favored (%)	98.3	98.5
Outliers (%)	0	0

*Values in parentheses are for highest-resolution shell.

Figure S1. Closeup view highlighting the orientation of GC-7 (PDB IDs 6P4V and 1RQD). The 1.65 Å ternary complex of DHPS (yellow) is superposed with the previously published 3 Å structure containing the same ligands (cyan). For clarity, NAD and a part of protein are omitted. Presumably the well featured electron density map generated from our high resolution diffraction data allowed for a more accurate docking of **1**, this led to a disagreement between the final models where **1** appears rotated ~180° about its own short axis.

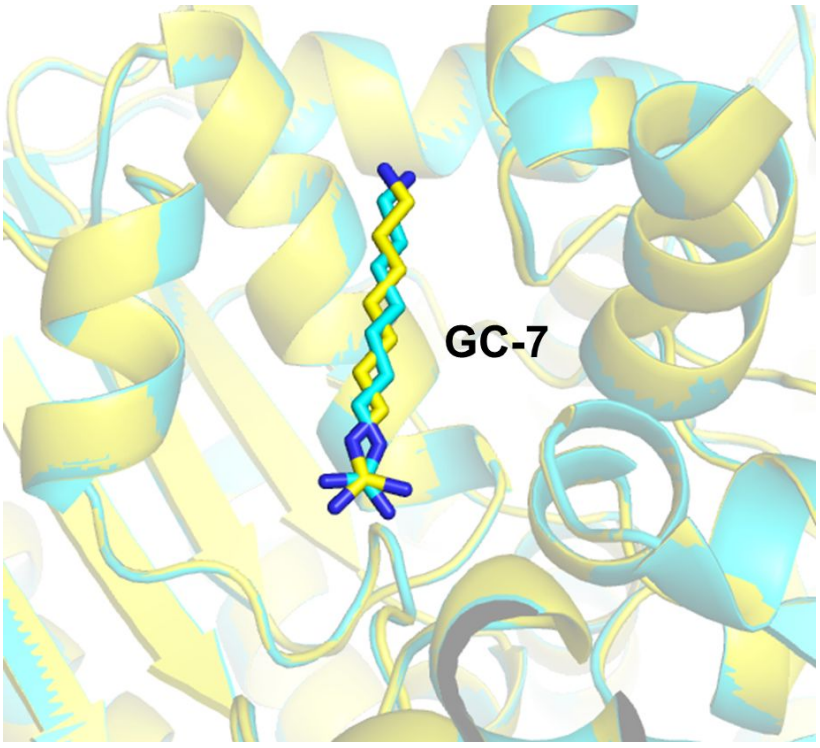

Figure S2. Omit electron density Fo-Fc map (rendered as mesh) corresponding to GC7 (displayed as green sticks). Map is contoured at ± 3.0 σ. Figure was created using Pymol.

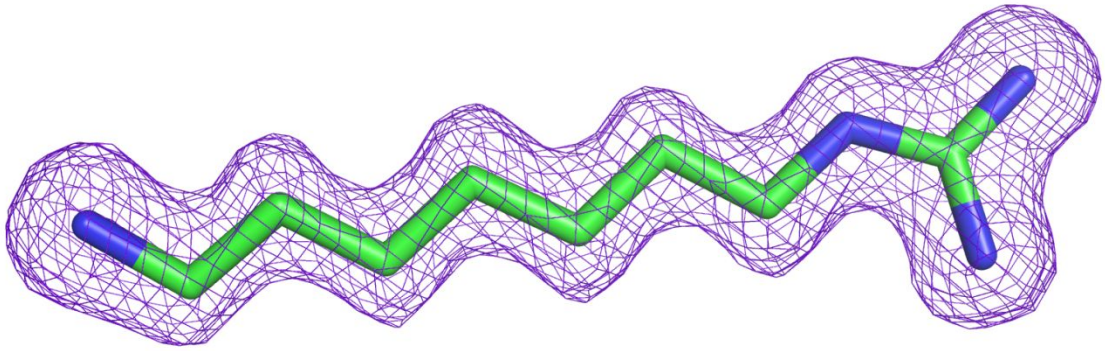

Figure S3. Omit electron density Fo-Fc map (rendered as mesh) corresponding to the compound **11g** (displayed as green sticks). Map is contoured at ± 3.0 σ. Figure was created using Pymol.