

## Supporting Information

### Design and Evaluation of Novel Glutaminase Inhibitors

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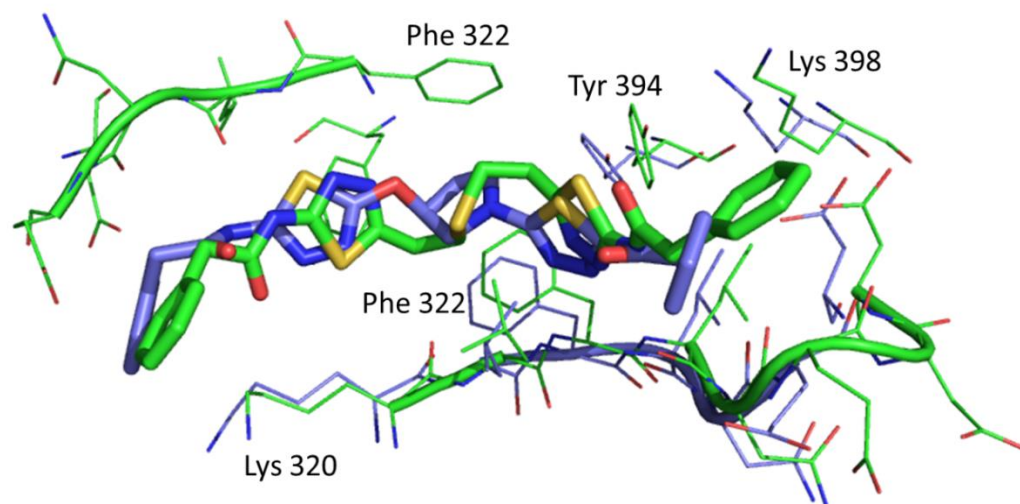
Refinement characteristics and data collection information for X-ray structures of compounds **7d**, **7e**, **14b** and **14d** in complex with GAC

Rendering of X-ray structure of **14b** in complex with GAC

Supplementary Table1. Data collection and structure refinement statistics

	<b>GAC/7d</b>	<b>GAC/7e</b>	<b>GAC/14b</b>	<b>GAC/14d</b>
<b>Data collection</b>				
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	P2 <sub>1</sub>
Cell dimensions				
a (Å)	98.05	50.69	99.17	49.44
b (Å)	138.62	139.03	138.83	137.79
c (Å)	176.32	176.78	176.65	175.76
β (°)	90	95.56	90	94.68
Resolution (Å)	50-2.3 (2.34-2.30)	50-2.5 (2.56-2.50)	50-2.3 (2.34-2.30)	50-2.98 (3.05-2.98)
No. unique observations	107128 (5310)	80375 (3641)	107585 (4899)	47296 (2396)
Redundancy	7.1 (6.8)	3.6 (3.3)	7.1 (5.9)	3.6 (3.6)
Completeness (%)	99.9 (100.0)	98.6 (89.4)	98.8 (90.6)	99.9 (100.0)
Average I/σI	14.9 (2.2)	11.2 (1.4)	14.1 (1.4)	11.6 (2.7)
R <sub>merge</sub>	0.125	0.102	0.099	0.243
<b>Structure refinement</b>				
Resolution (Å)	50-2.5	50-2.52	50-2.5	50-2.98
R <sub>work</sub> / R <sub>free</sub>	0.2247/0.2654	0.2091/0.2526	0.2176/0.2669	0.1730/0.2307
RMS deviations				
Bonds(Å)	0.010	0.010	0.084	0.010
Angles(°)	1.227	1.099	1.037	1.286
Ramachandran plot				
Most favored (%)	95.10	95.04	94.0	92.16
Allowed (%)	4.17	4.60	4.60	6.62
<b>PDB code</b>	5FI2	5FI6	5FI7	5I94

\* Values in parentheses are for the highest-resolution shell.



Supplementary Figure 1. X-ray structure of GAC in complex with compound **14b**