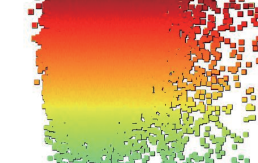


Site 1



A scatter plot showing the relationship between Molecular Weight (Mol Weight) on the x-axis and glide gscore on the y-axis. The x-axis ranges from 0 to 2000, and the y-axis ranges from -4 to -10. The data points are colored based on their glide gscore, with a color bar on the right indicating values from -5.0 (red) to -9.0 (dark blue). The plot shows a dense cluster of points at low molecular weight and high glide gscore, with a few outliers at higher molecular weight and lower glide gscore.

[illegible]

Compound library T001
n = 26836

Keep the top 50%
of compounds in
the docking score
n = 13418

Keep compounds
of the score < -7
kcal/mol
n = 262

PLIF
analysis and
clustering
n = 167

Visual
structural
inspection
n = 9

The figure displays two bar charts illustrating the distribution of amino acid mutations in the SARS-CoV-2 spike protein. The top chart shows mutations in the N-terminal domain (residues 1-319), and the bottom chart shows mutations in the C-terminal domain (residues 320-681). The x-axis for both charts lists the amino acid types and their corresponding residue numbers. The y-axis represents the frequency of mutations, with a scale break between 193 and 262.

Top Chart (N-terminal domain, residues 1-319):

- AAs: Asp 231, Glu 233, Glu 234, His 385, Lys 387, Phe 589, Arg 590, His 591, Ser 596, His 635, Thr 638, Ala 639, Gly 640, Tyr 644, Tyr 676.
- Frequency: The highest frequency is observed for Glu 233, with a value of approximately 262.

Bottom Chart (C-terminal domain, residues 320-681):

- AAs: Asp 231, Glu 233, Glu 234, His 385, Lys 387, Phe 589, Arg 590, His 591, Ser 596, His 635, Thr 638, Ala 639, Gly 640, Tyr 644, Tyr 676.
- Frequency: The highest frequency is observed for Glu 233, with a value of approximately 262.

AS1517499

Concentration (lg nM)	AS1517499 Inhibition (%)	1,2,3,4-tetrahydroquinoline Inhibition (%)	1,2,3,4-tetrahydroquinoline-2-carboxylic acid Inhibition (%)
-0.5	2	0	0
0	3	1	0
0.5	5	2	0
1	10	3	0
1.5	20	4	0
2	25	5	0
2.5	40	6	0
3	60	7	0
3.5	75	8	0
4	85	9	0