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File Name(s)

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MMT_1632399_1ndg-epi90-side.png
MMT_1632399_1FSK-LOorigCA.png
MMT_1632399_3BT2-botEigen.png
MMT_1632399_2R0L-sapNet-top.png
MMT_1632399_agg.png
MMT_1632399_agg_red.png
MMT_1632399_agg_blue.png

Brief Description

For each multimedia item, please include a brief non-technical description, which will be used for writing captions. Use a separate page for additional space.

Two multipanel figures, with the panels corresponding to the following files:

Figure 1:

A: MMT_1632399_1ndg-epi90-side.png
B: MMT_1632399_1FSK-LOorigCA.png
C: MMT_1632399_3BT2-botEigen.png
D: MMT_1632399_2R0L-sapNet-top.png

Illustrations of epitope predictions using SmrtMolEpitope. An epitope is the patch of residues on an antigens that bind an antibody. A: Epitopes residues of hen egg white lysozyme from PDB 1NDG. Red and green indicate core and peripheral epitope residues, respectively. B: Epitope propensity calculation captures the epitope in birch pollen allergen (pdb 1FSK). The actual epitope is shown in spheres, and residues with high and low epitope propensity are shown in red and blue, respectively. C: Network centrality captures the epitope in the urokinase-urokinase receptor-vitronectin complex (pdb 3BT2). The actual epitope is shown in spheres, and residues with high and low network centrality are shown in red and blue, respectively. This suggests that (low) network centrality captures residues on the ends of proteins that are more likely to be epitopes. D: Spatial aggregation propensity captures the epitope in hepatocyte growth factor activator (pdb 2R0L). The actual epitope is shown in spheres, and residues with high and low epitope propensity are shown in red and blue, respectively. This suggests that exposed hydrophobic residues are likely to be epitopes.

Figure 2:

A: MMT_1632399_agg.png
B: MMT_1632399_agg_red.png
C: MMT_1632399_agg_blue.png

Illustrations of aggregation predictions using SmrtMolAggregation. Aggregation propensity is an indicator of areas on a protein that are likely to aggregate, or bind to each other. Areas of high aggregation propensity are shown in red, low propensity in blue. A: Aggregation propensity of the antigen binding region of an antibody, indicating a high propensity for binding in a correct location. B/C: High aggregation propensity region is identified on the left-hand side of the antibody in a region with undesired binding (panel B). Using design algorithms, the aggregation propensity is reduce without affecting binding by a single mutation (panel C).

Keywords

Include any relevant keywords. Use a separate page for additional space.
antibody; aggregation; epitope mapping; developability;

Suggested Credit

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Does This Material Show NSF-Supported Research? Yes ☒ No ☐

If yes, please explain and, if possible, provide the NSF grant number.

This work was supported in part by a Phase II SBIR Grant for the development of automated antibody design tools.

Grant # 1632399

Date Of Material

Please narrow down the creation date as closely as possible, even if you can give only the decade.

April 28, 2017

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