

Article

# Characterizing Epitope Binding Regions of Entire Antibody Panels by Combining Experimental and Computational Analysis of Antibody: Antigen Binding Competition

Benjamin D. Brooks <sup>1,2,3,\*</sup>, Adam Closmore <sup>4</sup>, Juechen Yang <sup>5</sup>, Michael Holland <sup>5</sup>, Tina Cairns <sup>3</sup>, Gary H. Cohen <sup>3</sup> and Chris Bailey-Kellogg <sup>6</sup>

<sup>1</sup> Department of Biomedical Sciences, Rocky Vista University, Ivins, UT 84738, USA

<sup>2</sup> Inovon Inc., Fargo, ND 58102, USA

<sup>3</sup> Department of Microbiology, School of Dental Medicine, University of Pennsylvania, Philadelphia, PA 19104, USA; tmcairns@upenn.edu (T.C.); ghc@upenn.edu (G.H.C.)

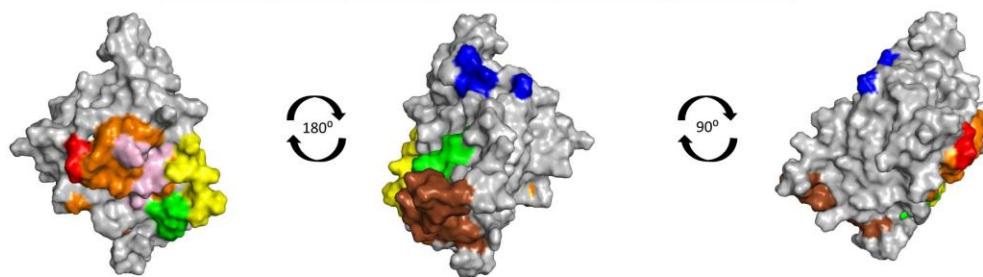
<sup>4</sup> Department of Pharmacy, North Dakota State University, Fargo, ND 58102, USA; Adam.Closmore@gmail.com

<sup>5</sup> Department of Biomedical Engineering, North Dakota State University, Fargo, ND 58102, USA; juechen.yang@gmail.com (J.Y.); mchollandred@gmail.com (M.H.)

<sup>6</sup> Computer Science Department, Dartmouth College, Hanover, NH 03755, USA; cbk@cs.dartmouth.edu

\* Correspondence: bbrooks@rvu.edu; Tel.: +1-435-222-1403

Community	gD mAb	Serotype	Neutralizing Activity	Fabs murine/recombinant	Epitope Residues (experimental)
	E317	Common	Yes	Commercial	38, 132, 139, 140, 215, 222, 235
	DL11	Common	Yes	+/+	38, 132, 140
	MC23	Common	Yes	+/+	213, 216
	MC2	Type-2	Yes	+/+	67, 243-246, 248
	MC5	Common	Yes	+/+	54, 75-77
	MC14	Common	No	+/+	262-272 <sup>*</sup>
	1D3	Common	Yes	+/+	1-29 <sup>*</sup>



**Figure S1.** Selected Abs and epitope residues with associated experimental data. Communities are colored on the structure of gD. Orange represents nectin binding region. Face #1 is the nectin binding face. Faces #2-4 are rotated by 90, 180, and 270 degrees around the y-axis. Face #5 is the view from above and Face #6 is the view from below.

**Table S1.** Agreement between epitope residues targeted by our control antibody, E317, according to the crystal structure vs. those identified from our dock binning based approach.

<b>Crystal Structure</b>	<b>Focused Docking</b>
Gln27	Gln27
Tyr38	Tyr38
Gln132	Gln132
Asp139	Asp139
Ser140	Ser140
Asp215	Asp215
Pro221	Pro221
Arg222	Arg222
Phe223	Phe223
Ile224	
Asn227	
Val231	
Ser235	
Ile238	Ile238