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Supplementary information

The ClusPro AbEMap web server for the prediction of antibody epitopes

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The ClusPro AbeMap web server for the prediction of antibody epitopes

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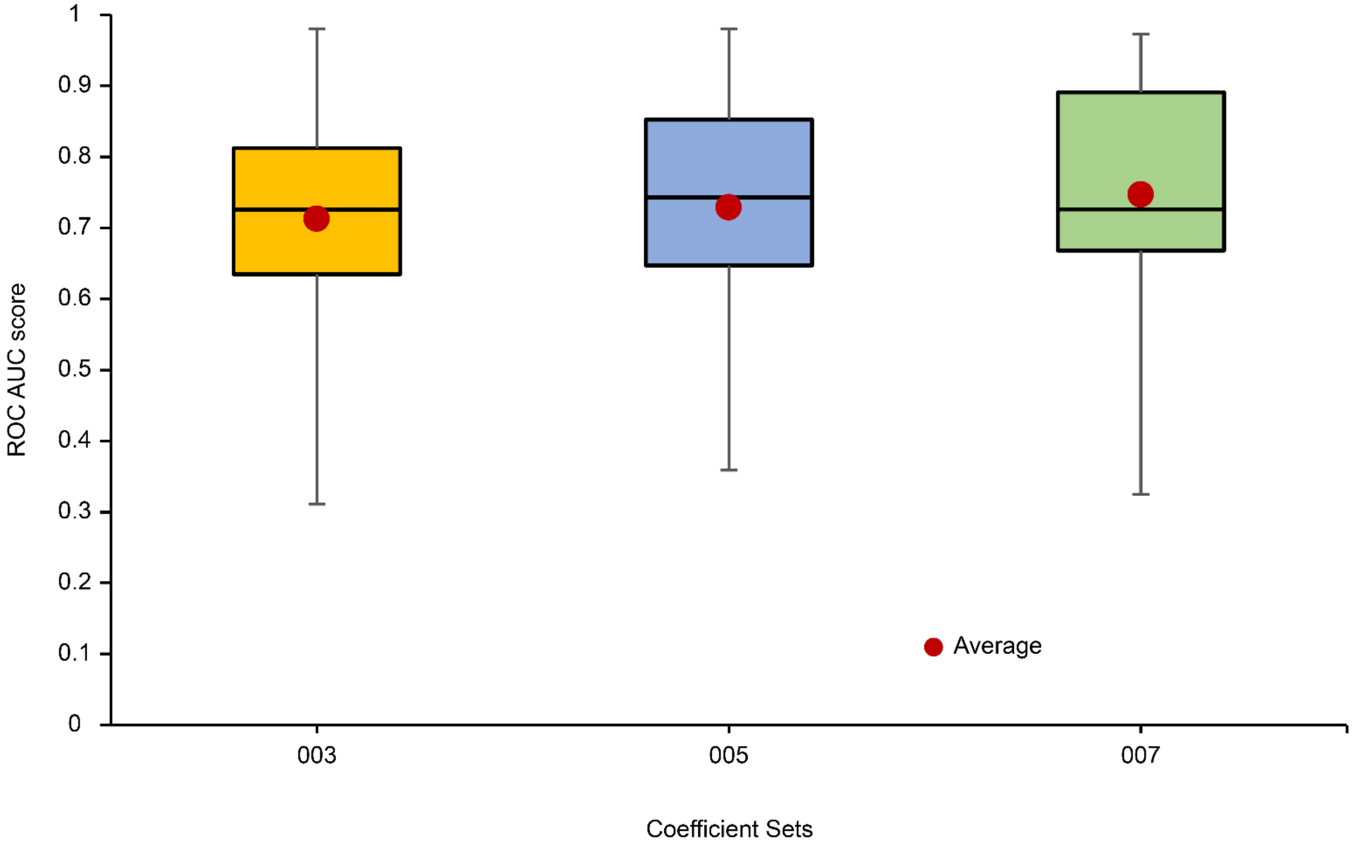
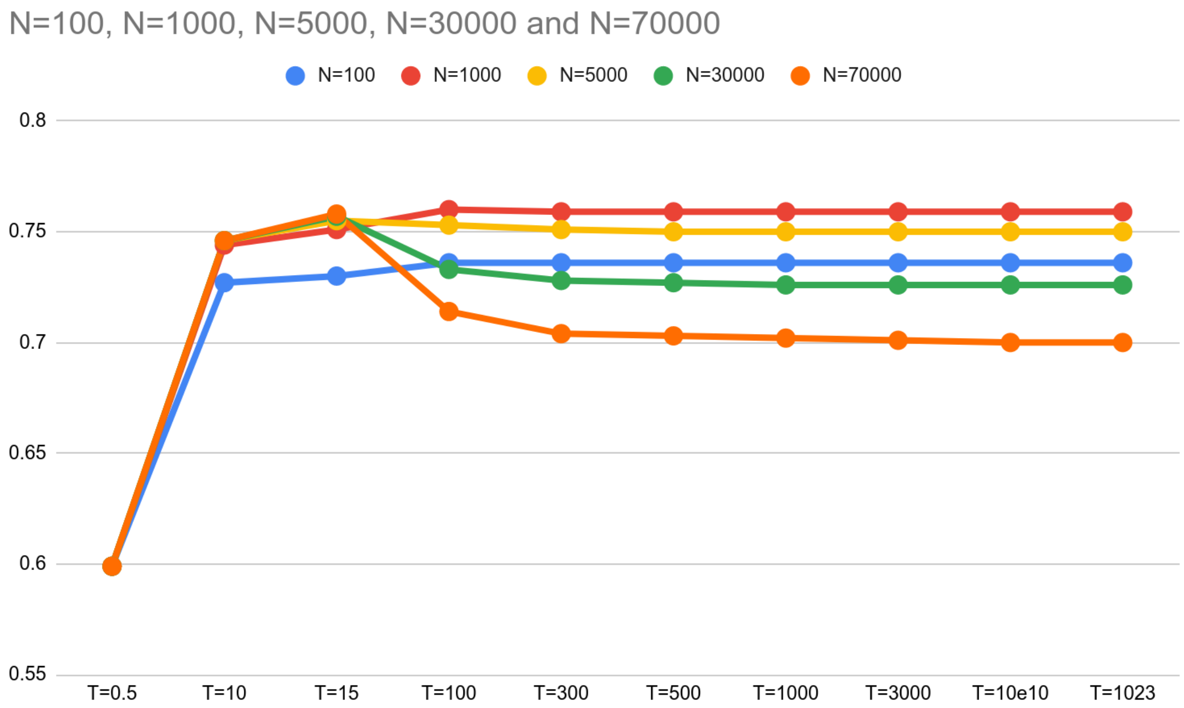


Supplementary Figure 1 | Impact of loosening the penalty on shape complementarity on the ROC AUC score for the 40 antibody-antigen complexes in the benchmark set BM5. With the hypothesis that reducing the shape complementarity requirements during docking will increase epitope prediction accuracy when dealing with less accurate antibody models, the Van der Waal's potential's contribution in ranking docking models was reduced. Coefficient 003 is the normal antibody-antigen coefficient set; coefficient 005 has its attractive Van der Waals potential halved from that of C003; coefficient 007 has weights of zero for both attractive and repulsive Van der Waals potentials. The general trend shows that reducing or removing Van der Waal's components improves the results to varying degrees when using homology-modelled antibodies. While several combinations were tested, two coefficient sets that improved from the normal antibody coefficient set (C003) were a) reduced attractive VdW (C005), and b) No VdW (C007). For the former set, the attractive Van der Waal's potential was halved from the normal antibody coefficient set used for crystal structure inputs. The latter coefficient had coefficients for both attractive and repulsive Van der Waals' potentials that were zero.



Supplementary Figure 2 | Impact of the temperature factor T and the number of decoys on the ROC AUC score for the 40 antibody-antigen complexes in the benchmark set BM5.

Supplementary Table 1 | True positives (TP) from the top 10 up to the top 50 ranked residues when using unbound antigens and the crystal structure (internal AbEMap homology models) of the unbound antibody with results for homology models shown in parentheses.

			Number of true positive epitope residues in the				
Complex	**Antibody**	**Antigen**	**Top 10**	**Top 20**	**Top 30**	**Top 40**	**Top 50**
1AHW_AB:C	1FGN_LH	1TFH_A	8 (10)	12 (16)	16 (19)	19 (23)	22 (24)
1BGX_HL:T	1AY1_HL	1TAQ_A	0 (0)	0 (1)	0 (2)	0 (2)	0 (4)
1BVK_DE:F	1BVL_BA	3LZT	2 (4)	4 (5)	8 (8)	10 (11)	10 (13)
1DQJ_AB:C	1DQQ_CD	3LZT	1 (1)	5 (5)	6 (7)	9 (8)	13 (14)
1E6J_HL:P	1E6O_HL	1A43	6 (4)	10 (7)	12 (10)	13 (12)	14 (14)
1JPS_HL:T	1JPT_HL	1TFH_B	9 (9)	16 (16)	21 (20)	23 (24)	24 (24)
1MLC_AB:E	1MLB_AB	3LZT	0 (0)	2 (0)	5 (0)	6 (0)	6 (2)
1VFB_AB:C	1VFA_AB	8LYZ_	6 (1)	11 (5)	14 (9)	15 (10)	17 (13)
1WEJ_HL:F	1QBL_HL	1HRC_	1 (0)	6 (1)	8 (3)	10 (5)	11 (8)
2FD6_HL:U	2FAT_HL	1YWH_A	0 (0)	0 (0)	1 (0)	3 (0)	3 (0)
2I25_N:L	2I24_N	3LZT	5 (0)	10 (2)	13 (7)	16 (11)	18 (14)
2VIS_AB:C	1GIG_LH	2VIU_ACE	0 (0)	1 (1)	3 (1)	3 (1)	3 (1)
2VXT_HL:I	2VXU_HL	1J0S_A(6)	6 (7)	9 (13)	14 (17)	15 (19)	16 (20)
2W9E_HL:A	2W9D_HL	1QM1_A	6 (9)	10 (14)	15 (18)	17 (18)	18 (18)
3EO1_AB:CF	3EO0_AB	1TGJ_AB	3 (3)	9 (8)	9 (11)	12 (12)	12 (12)
3EOA_LH:I	3EO9_LH	3F74_A	2 (3)	3 (5)	3 (6)	4 (6)	5 (7)
3G6D_LH:A	3G6A_LH	1IK0_A(10)	8 (9)	12 (12)	15 (16)	17 (19)	19 (19)
3HI6_XY:B	3HI5_HL	1MJN_A	2 (0)	3 (3)	4 (3)	4 (4)	6 (6)
3HMX_LH:AB	3HMW_LH	1F45_AB	0 (2)	2 (4)	5 (8)	6 (11)	10 (14)
3L5W_LH:I	3L7E_LH	1IK0_A(11)	7 (8)	8 (9)	8 (11)	9 (11)	10 (11)
3MXW_LH:A	3MXV_LH	3M1N_A	6 (4)	14 (9)	19 (15)	21 (18)	22 (20)
3RVW_CD:A	3RVT_CD	3F5V_A	5 (0)	7 (0)	10 (0)	10 (0)	13 (0)
3V6Z_AB:F	3V6F_AB	3KXS_F	0 (0)	2 (2)	3 (3)	3 (5)	4 (7)
4DN4_LH:M	4DN3_LH	1DOL_A	7 (8)	11 (12)	14 (14)	14 (14)	14 (14)
4FQI_HL:ABEFCD	4FQH_HL	2FK0_ABCDEF	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)
4G6J_HL:A	4G5Z_HL	4I1B_A	0 (0)	1 (0)	3 (0)	6 (3)	8 (5)
4G6M_HL:A	4G6K_HL	4I1B_A	5 (3)	9 (9)	13 (13)	16 (16)	19 (18)
4GXU_MN:ABEFCD	4GXV_HL	1RUZ_HIJKLM	0 (0)	0 (0)	0 (0)	0 (0)	0 (0)

Supplementary Table 2 | True Positives when considering the top 20 ranking residues for the 40 cases in BM5

Complex_Chain	Antibody	Antigen	Case Type[a]	AbEMap	SEPPA	BEpro	EpiPred
1AHW_AB:C	1FGN_LH	1TFH_A	a	12	7	3	7
1BGX_HL:T	1AY1_HL	1TAQ_A	a	0	6	3	0
1BJ1_HL:VW	1BJ1_HL	2VPF_GH	ab	2	10	6	0
1BVK_DE:F	1BVL_BA	3LZT	a	4	6	4	0
1DQJ_AB:C	1DQQ_CD	3LZT	a	5	15	7	5
1E6J_HL:P	1E6O_HL	1A43	a	10	11	0	0
1FSK_BC:A	1FSK_BC	1BV1	ab	15	14	5	0
1I9R_HL:ABC	1I9R_HL	1ALY_ABC	ab	1	3	1	4
1IQD_AB:C	1IQD_AB	1D7P_M	ab	7	10	8	0
1JPS_HL:T	1JPT_HL	1TFH_B	a	16	7	3	6
1K4C_AB:C	1K4C_AB	1JVM_ABCD	ab	0	5	3	1
1KXQ_H:A	1KXQ_H	1PPI	ab	9	4	11	7
1MLC_AB:E	1MLB_AB	3LZT	a	2	0	10	5
1NCA_HL:N	1NCA_HL	7NN9	ab	1	9	11	14
1NSN_HL:S	1NSN_HL	1KDC	ab	7	5	1	2
1QFW_HL:AB	1QFW_HL	1HRP_AB	ab	8	7	3	0
1VFB_AB:C	1VFA_AB	8LYZ_	a	11	4	5	7
1WEJ_HL:F	1QBL_HL	1HRC_	a	6	2	1	0
2FD6_HL:U	2FAT_HL	1YWH_A	a	0	5	2	0
2HMI_CD:AB	2HMI_CD	1S6P_AB	ab	6	0	7	0
2I25_N:L	2I24_N	3LZT	a	10	7	8	N/A
2JEL_HL:P	2JEL_HL	1POH	ab	12	6	7	1
2VIS_AB:C	1GIG_LH	2VIU_ACE	a	1	7	0	1
2VXT_HL:I	2VXU_HL	1J0S_A(6)	a	9	13	4	9
2W9E_HL:A	2W9D_HL	1QM1_A	a	10	11	12	0
3EO1_AB:CF	3EO0_AB	1TGJ_AB	a	9	6	5	2
3EOA_LH:I	3EO9_LH	3F74_A	a	3	7	4	0
3G6D_LH:A	3G6A_LH	1IK0_A(10)	a	12	7	6	3
3HI6_XY:B	3HI5_HL	1MJN_A	a	3	5	5	8
3HMX_LH:AB	3HMW_LH	1F45_AB	a	2	1	2	0
3L5W_LH:I	3L7E_LH	1IK0_A(11)	a	8	6	3	2
3MXW_LH:A	3MXV_LH	3M1N_A	a	14	8	2	2
3RVW_CD:A	3RVT_CD	3F5V_A	a	7	4	6	0
3V6Z_AB:F	3V6F_AB	3KXS_F	a	2	0	4	0
4DN4_LH:M	4DN3_LH	1DOL_A	a	11	1	2	6
4FQI_HL:ABEFCD	4FQH_HL	2FK0_ABCDEF	a	0	3	0	0
4G6J_HL:A	4G5Z_HL	4I1B_A	a	1	8	5	8
4G6M_HL:A	4G6K_HL	4I1B_A	a	9	0	4	0
4GXU_MN:ABEFCD	4GXV_HL	1RUZ_HIJKLM	a	0	2	3	0
1QFW_IM:AB	1QFW_IM	1HRP_AB	ab	4	1	5	5
Average				**6.23**	**5.83**	**4.53**	**2.69**

[a] a – unbound-unbound, ab – unbound-bound

Supplementary Table 3 | ROC AUC comparison of AbEMap with SEPPA and BEpro

Complex	**Antibody**	**Antigen**	**Case Type**	**AbEMap**	**SEPPA**	**BEpro**
1AHW_AB:C	1FGN_LH	1TFH_A	a	0.92	0.842	0.633
1BGX_HL:T	1AY1_HL	1TAQ_A	a	0.271	0.58	0.632
1BJ1_HL:VW	1BJ1_HL	2VPF_GH	ab	0.584	0.891	0.801
1BVK_DE:F	1BVL_BA	3LZT	a	0.636	0.691	0.603
1DQJ_AB:C	1DQQ_CD	3LZT	a	0.644	0.941	0.701
1E6J_HL:P	1E6O_HL	1A43	a	0.863	0.86	0.272
1FSK_BC:A	1FSK_BC	1BV1	ab	0.918	0.958	0.87
1I9R_HL:ABC	1I9R_HL	1ALY_ABC	ab	0.766	0.694	0.622
1IQD_AB:C	1IQD_AB	1D7P_M	ab	0.849	0.932	0.801
1JPS_HL:T	1JPT_HL	1TFH_B	a	0.973	0.839	0.663
1K4C_AB:C	1K4C_AB	1JVM_ABCD	ab	0.738	0.899	0.85
1KXQ_H:A	1KXQ_H	1PPI	ab	0.939	0.652	0.712
1MLC_AB:E	1MLB_AB	3LZT	a	0.477	0.492	0.823
1NCA_HL:N	1NCA_HL	7NN9	ab	0.847	0.863	0.907
1NSN_HL:S	1NSN_HL	1KDC	ab	0.752	0.636	0.512
1QFW_HL:AB	1QFW_HL	1HRP_AB	ab	0.916	0.66	0.769
1VFB_AB:C	1VFA_AB	8LYZ_	a	0.858	0.612	0.659
1WEJ_HL:F	1QBL_HL	1HRC_	a	0.73	0.456	0.455
2FD6_HL:U	2FAT_HL	1YWH_A	a	0.658	0.522	0.698
2HMI_CD:AB	2HMI_CD	1S6P_AB	ab	0.947	0.8	0.95
2I25_N:L	2I24_N	3LZT	a	0.802	0.718	0.675
2JEL_HL:P	2JEL_HL	1POH	ab	0.893	0.725	0.687
2VIS_AB:C	1GIG_LH	2VIU_ACE	a	0.684	0.946	0.618
2VXT_HL:I	2VXU_HL	1J0S_A(6)	a	0.796	0.86	0.654
2W9E_HL:A	2W9D_HL	1QM1_A	a	0.881	0.908	0.908
3EO1_AB:CF	3EO0_AB	1TGJ_AB	a	0.841	0.81	0.748
3EOA_LH:I	3EO9_LH	3F74_A	a	0.566	0.878	0.697
3G6D_LH:A	3G6A_LH	1IK0_A(10)	a	0.919	0.633	0.735
3HI6_XY:B	3HI5_HL	1MJN_A	a	0.501	0.799	0.667
3HMX_LH:AB	3HMW_LH	1F45_AB	a	0.851	0.577	0.726
3L5W_LH:I	3L7E_LH	1IK0_A(11)	a	0.883	0.783	0.735
3MXW_LH:A	3MXV_LH	3M1N_A	a	0.935	0.776	0.578
3RVW_CD:A	3RVT_CD	3F5V_A	a	0.848	0.662	0.782
3V6Z_AB:F	3V6F_AB	3KXS_F	a	0.434	0.399	0.587
4DN4_LH:M	4DN3_LH	1DOL_A	a	0.925	0.371	0.504
4FQI_HL:ABEFCD	4FQH_HL	2FK0_ABCDEF	a	0.599	0.771	0.631
4G6J_HL:A	4G5Z_HL	4I1B_A	a	0.557	0.774	0.617
4G6M_HL:A	4G6K_HL	4I1B_A	a	0.881	0.347	0.651
4GXU_MN:ABEFCD	4GXV_HL	1RUZ_HIJKLM	a	0.739	0.832	0.746
1QFW_IM:AB	1QFW_IM	1HRP_AB	ab	0.718	0.765	0.758
Average				**0.763**	**0.728**	**0.690**