

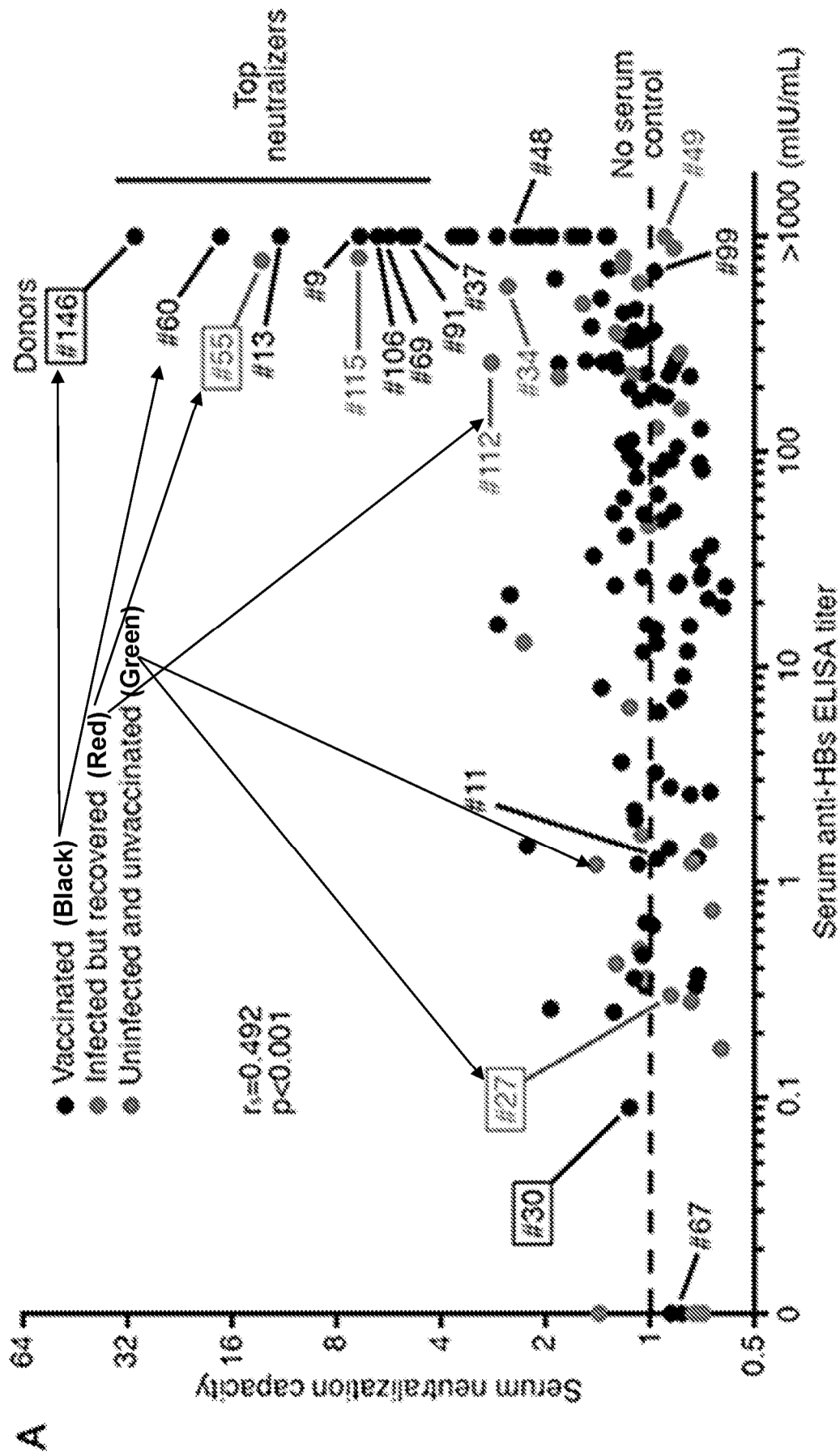


Fig. 1

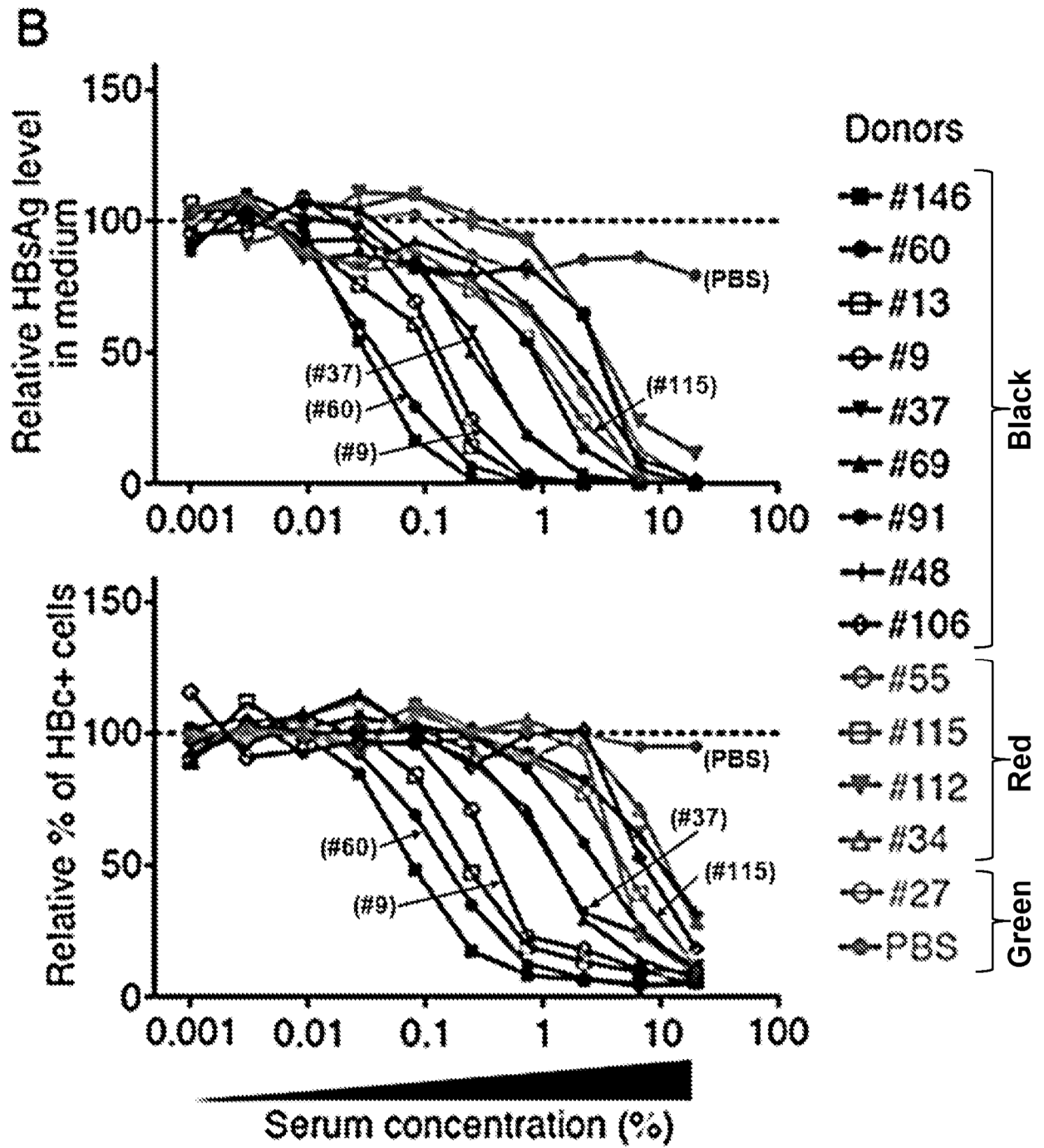


Fig. 1 (continued)

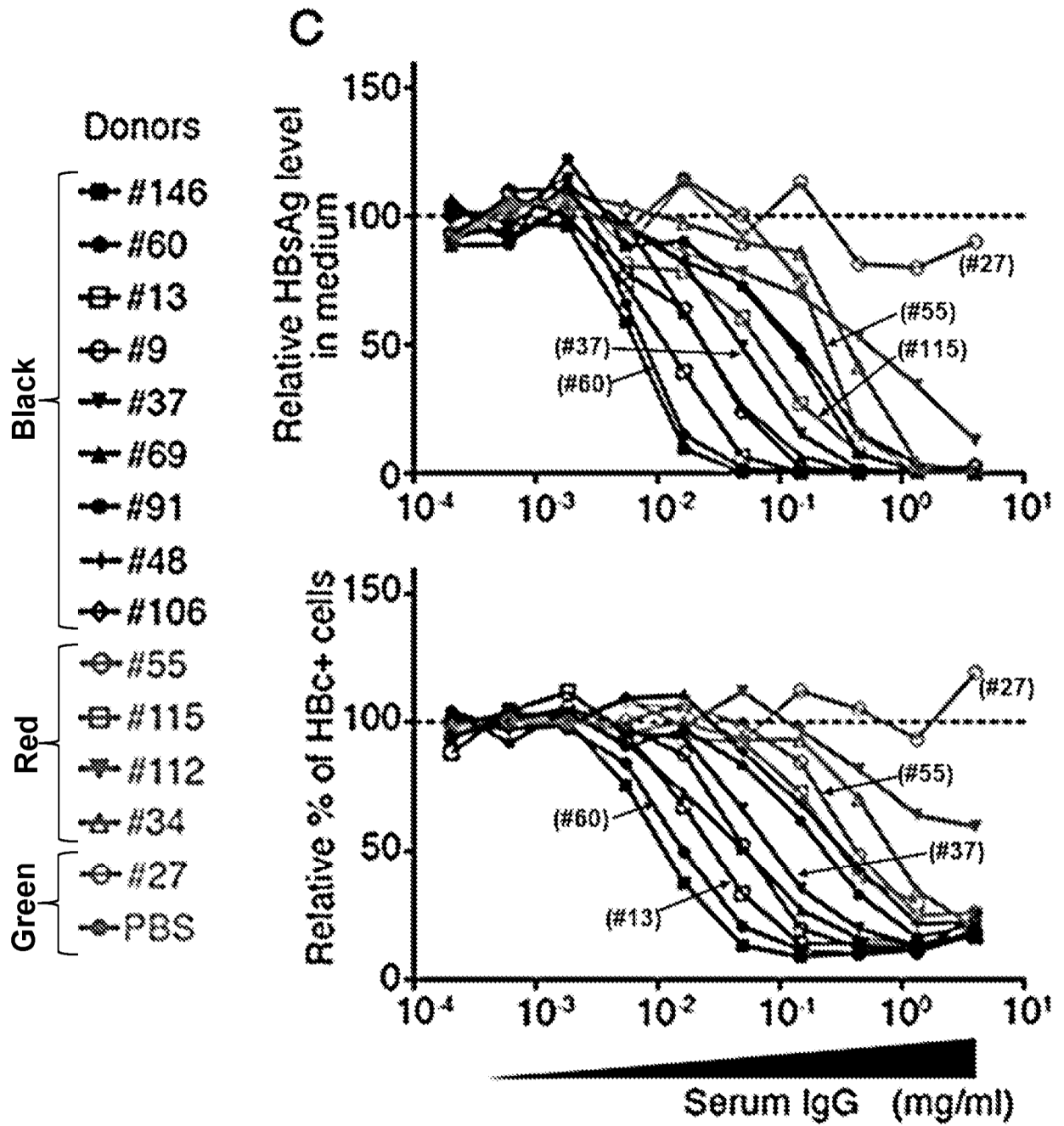


Fig. 1 (continued)

D

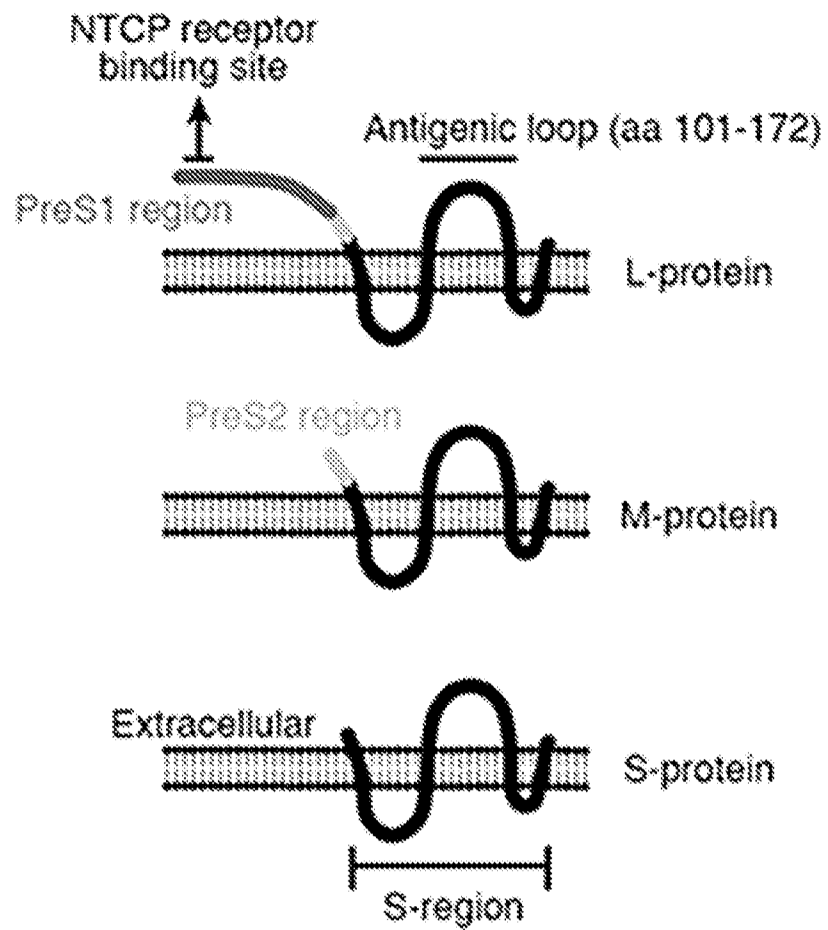


Fig. 1 (continued)

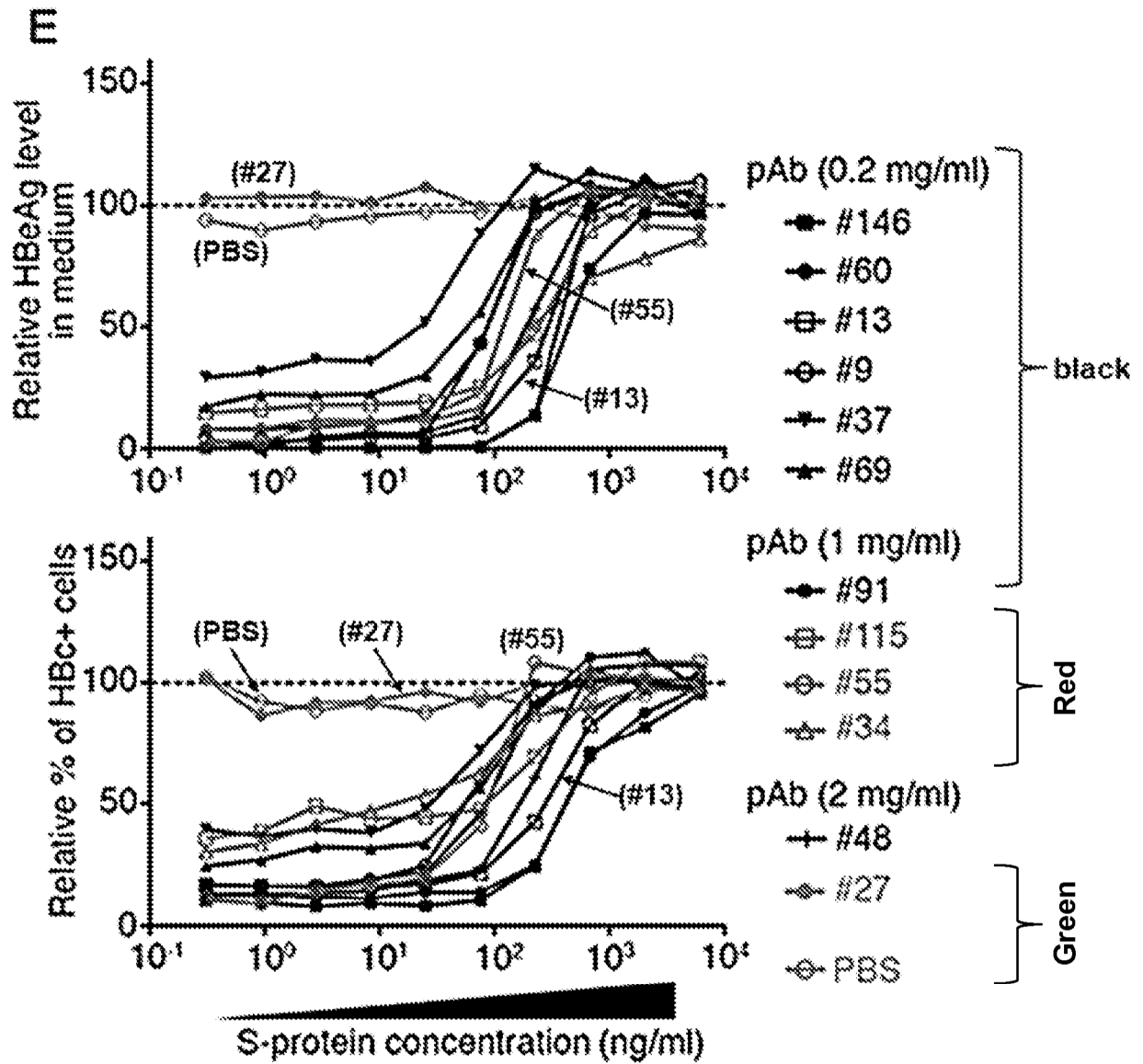


Fig. 1 (continued)

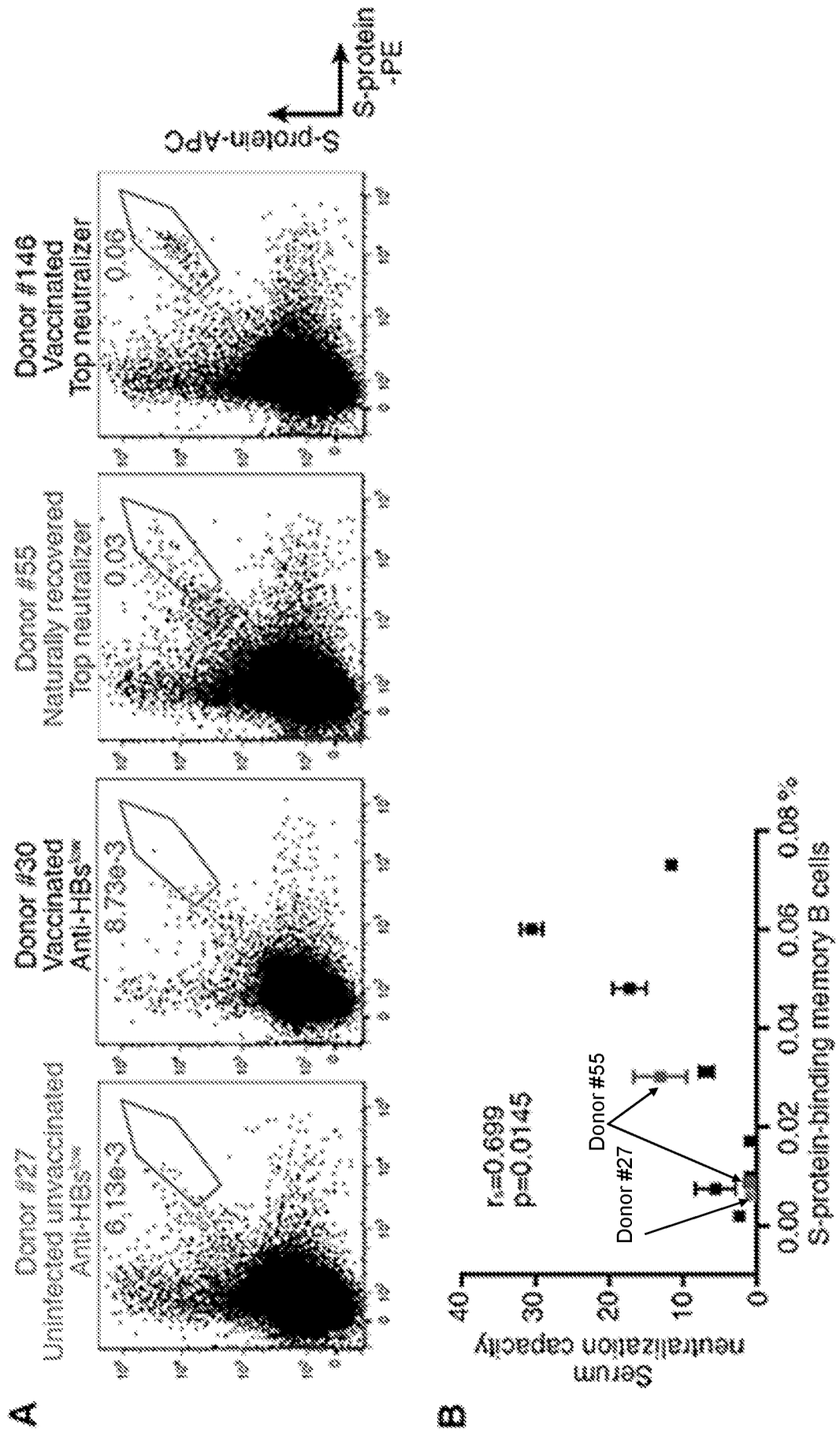


Fig. 2

C

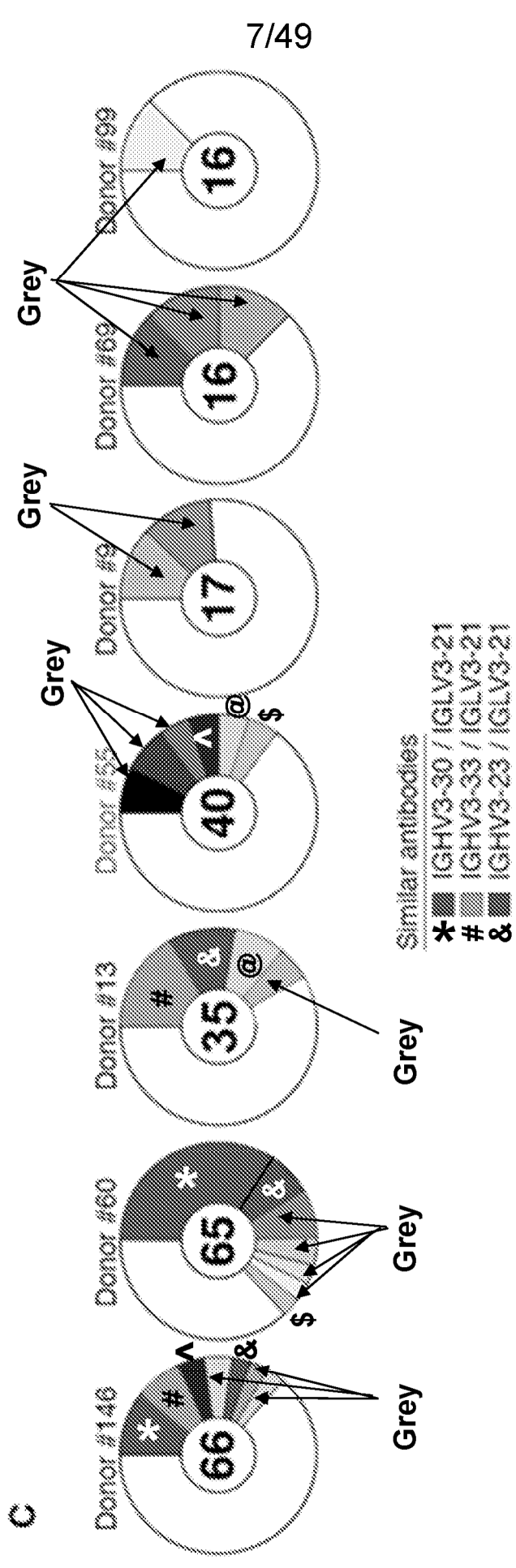


Fig. 2 (continued)

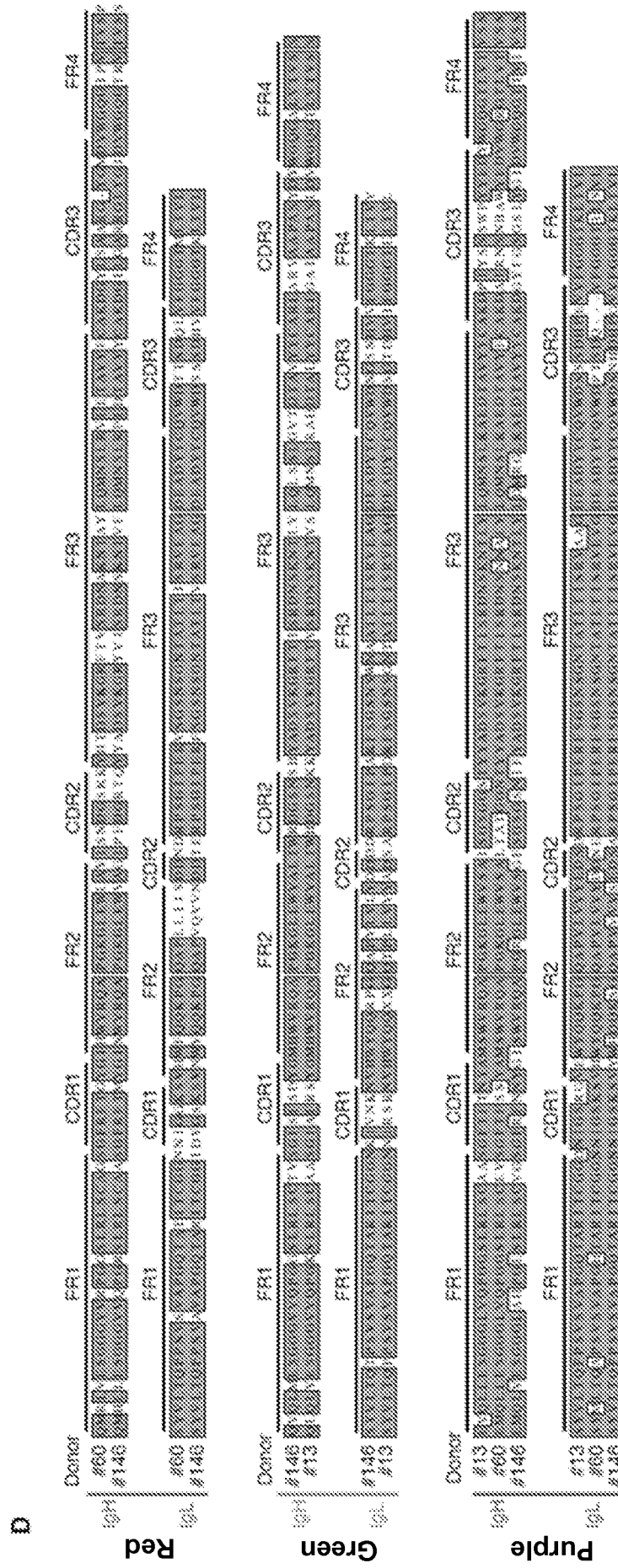


Fig. 2 (continued)

A

Antibody	Donor ID	Heavy chain V gene	Light chain V gene	adr CHO cell
H001	146	IGHV1-3*01	IGKV1-39*01	27.1
H002	146	IGHV2-70D*04	IGLV3-21*02	30.78
H003	60	IGHV3-23*01	IGLV3-21*02	33.76
H004	146	IGHV3-23*04	IGLV3-21*02	24.65
H005	60	IGHV3-30*18	IGLV3-21*02	69.82
H006	60	IGHV3-30*18	IGLV3-21*02	49.56
H007	146	IGHV3-30*18	IGKV3-20*01	46.77
H008	146	IGHV3-30*18	IGLV3-21*02	48.27
H009	60	IGHV3-30*18	IGLV3-21*02	38.02
H010	60	IGHV3-30*18	IGLV3-21*03	35.17
H011	13	IGHV3-33*01	IGKV3-11*01	18.66
H012	13	IGHV3-33*01	IGLV3-21*02	170.9
H013	146	IGHV3-33*01	IGLV3-21*02	351.2
H014	146	IGHV3-33*01	IGLV3-21*02	111.1
H015	60	IGHV3-33*01	IGKV1-39*01	74.87
H016	69	IGHV3-48*02	IGKV3-15*01	33.58
H017	55	IGHV3-74*01	IGLV2-14*01	40.87
H018	60	IGHV3-9*01	IGLV1-51*01	b.d.
H019	69	IGHV4-30-4*01	IGKV1-39*01	34.9
H020	55	IGHV4-59*08	IGKV1-12*01	29.58
libivirumab	(positive control)			105
10-1074	(negative control)			not binding

Red

Orange

Red

Yellow

White

Fig. 3

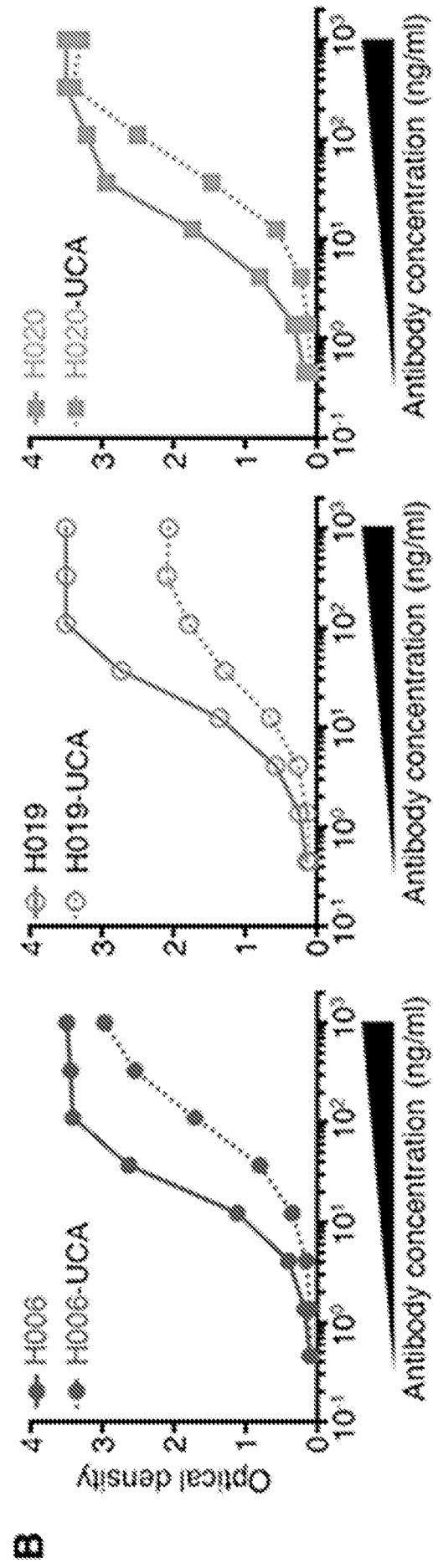


Fig. 3 (continued)

C

adr Yeast	adw Yeast	ad Human blood	ayw Yeast	ay Human blood
26.89	30.36	42.84	18.76	63.09
24.01	40.77	53.6	b.d.	167.4
21.99	25.27	40.17	159.5	42.75
16.07	23	25.51	27.75	13.39
25	27.83	40.43	17.38	130.6
50.61	40.2	28.98	17.57	115.5
47.33	40.63	43.26	16.57	197.1
46.62	36.83	49.28	18.1	115.3
40.41	41.26	25.49	20.82	40.49
44.93	42.59	22.69	232	38.76
21.95	19.41	609.4	29.52	b.d.
111.5	45.47	82.29	57.74	78.01
133.1	82.14	52.14	72.54	120.2
167.2	50	61.45	70.64	b.d.
23.07	b.d.	103.6	34.08	129.4
25.68	68.46	46.89	23.83	102.6
28.61	74.08	66.17	25.15	207.1
b.d.	b.d.	135.1	b.d.	b.d.
33.31	37.55	36.77	35.85	38.18
35.14	40.37	30.72	34.95	34.66
116.8	123.2	112.6	40.34	119.5
not binding	not binding	not binding	not binding	not binding

Red

Orange

Yellow

White

Fig. 3 (continued)

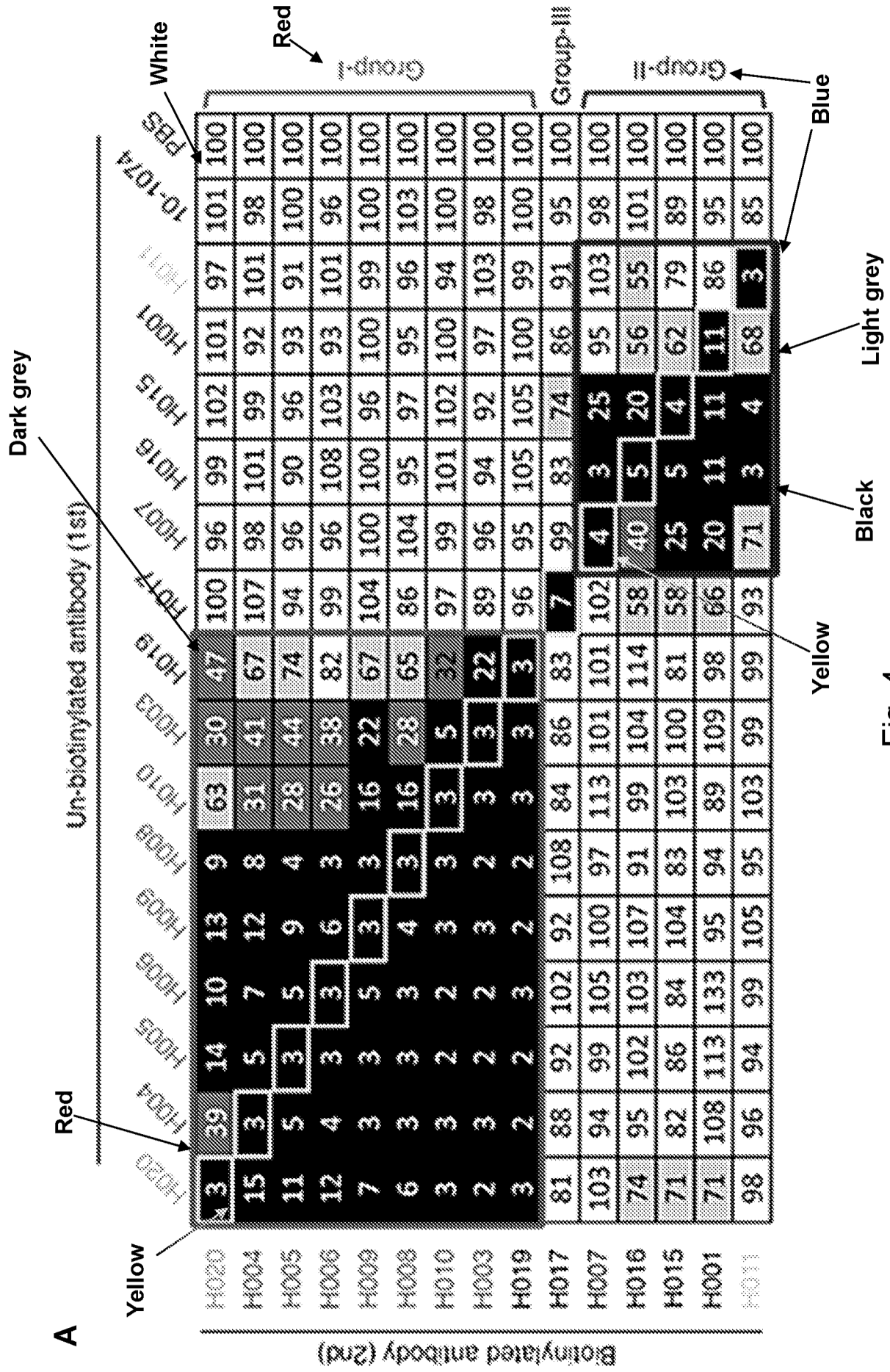


Fig. 4

B

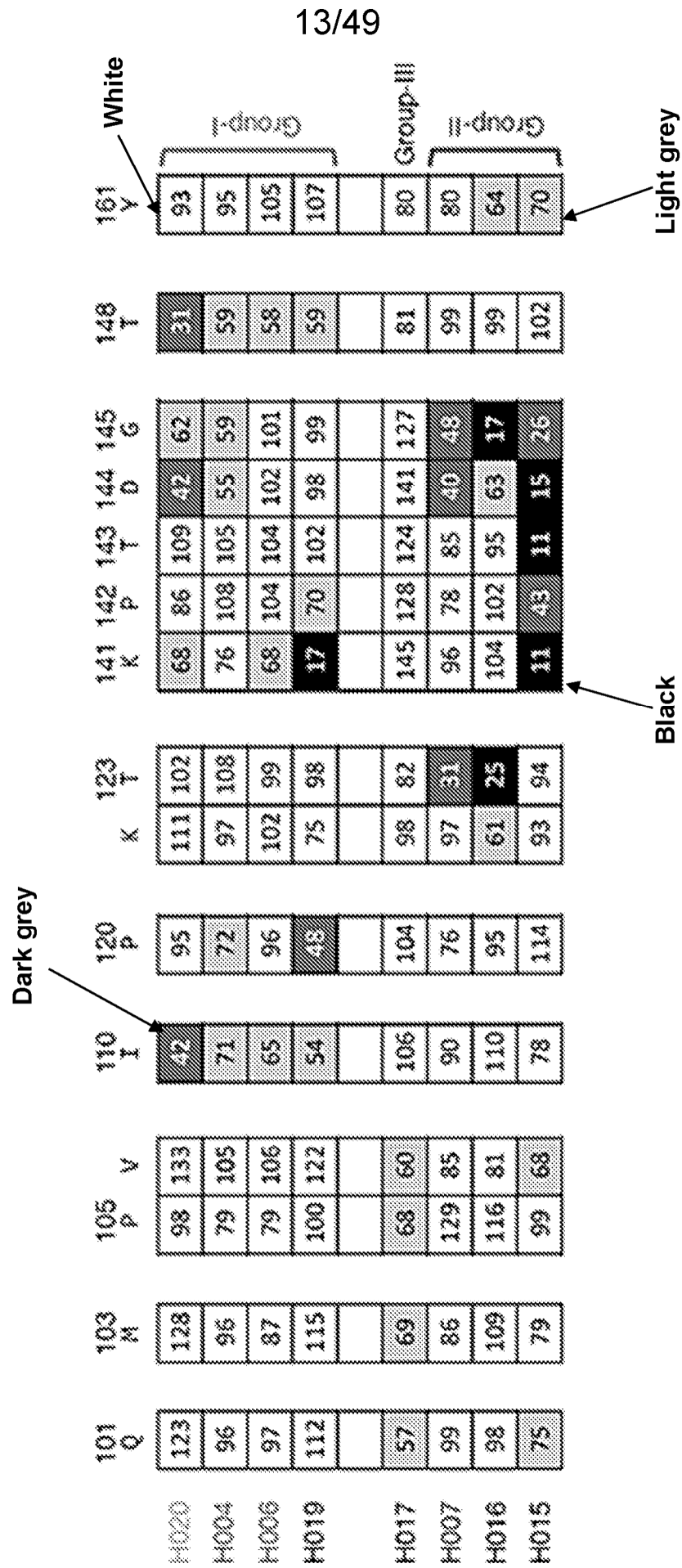


Fig. 4 (continued)

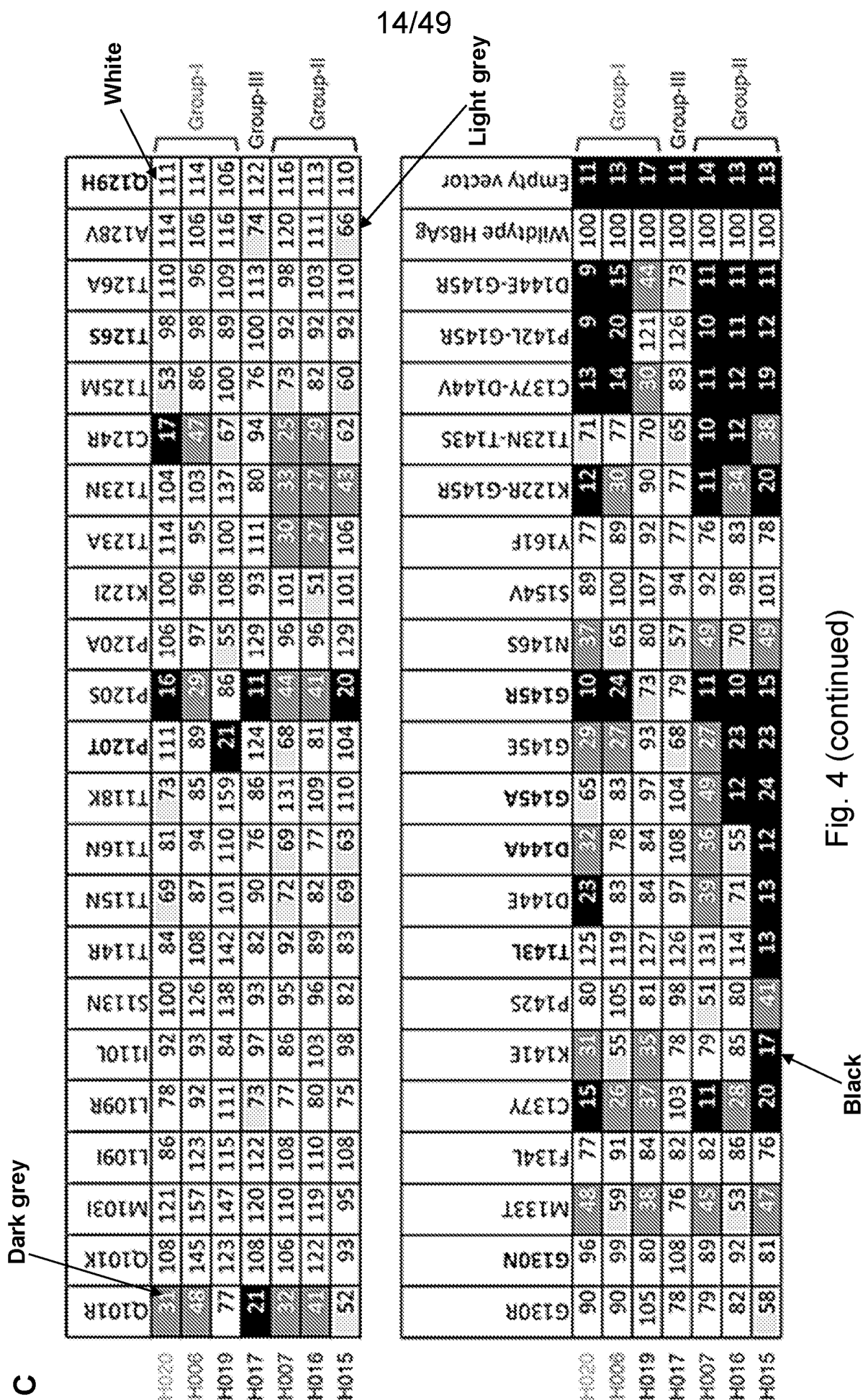


Fig. 4 (continued)

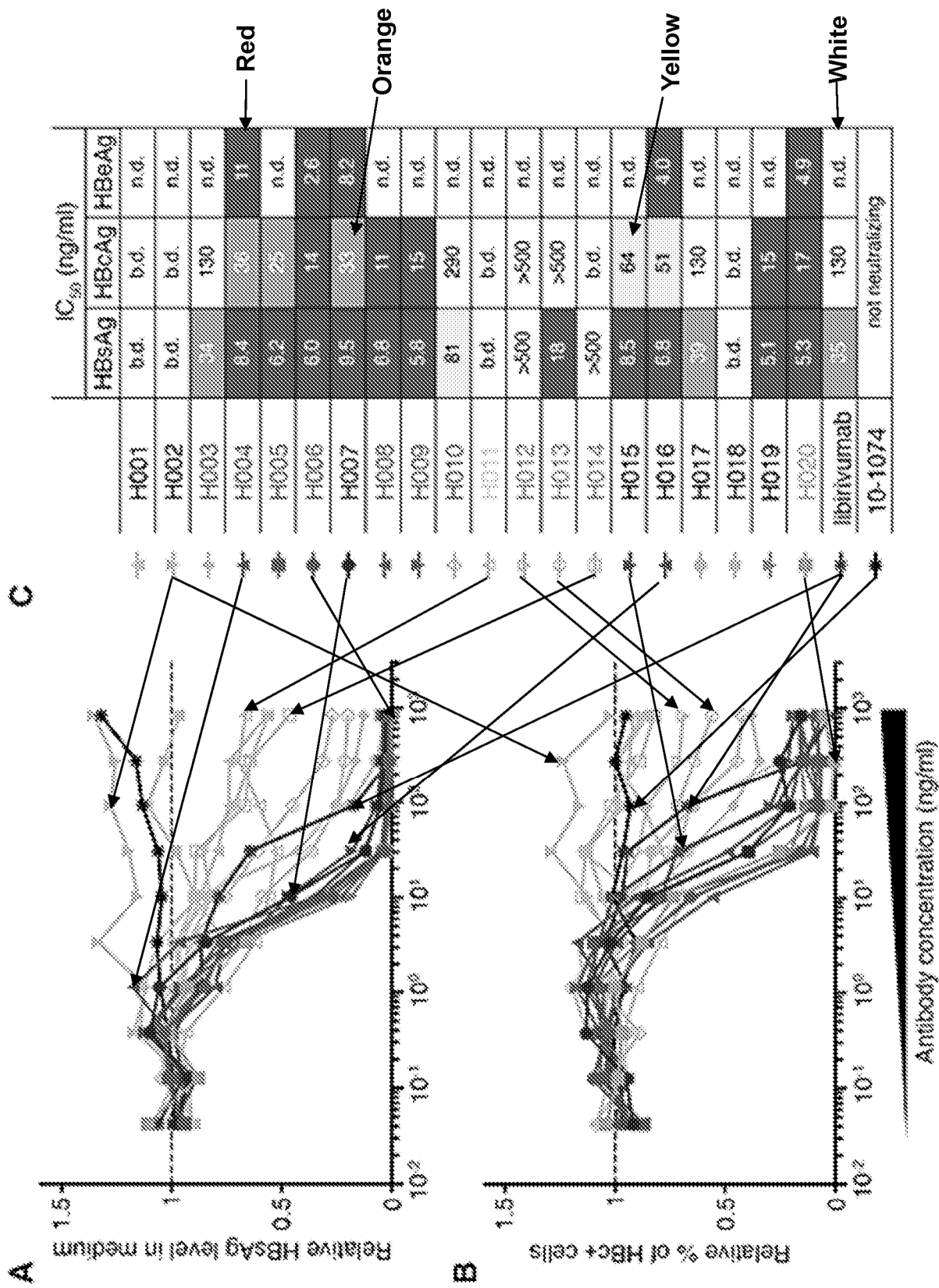


Fig. 5

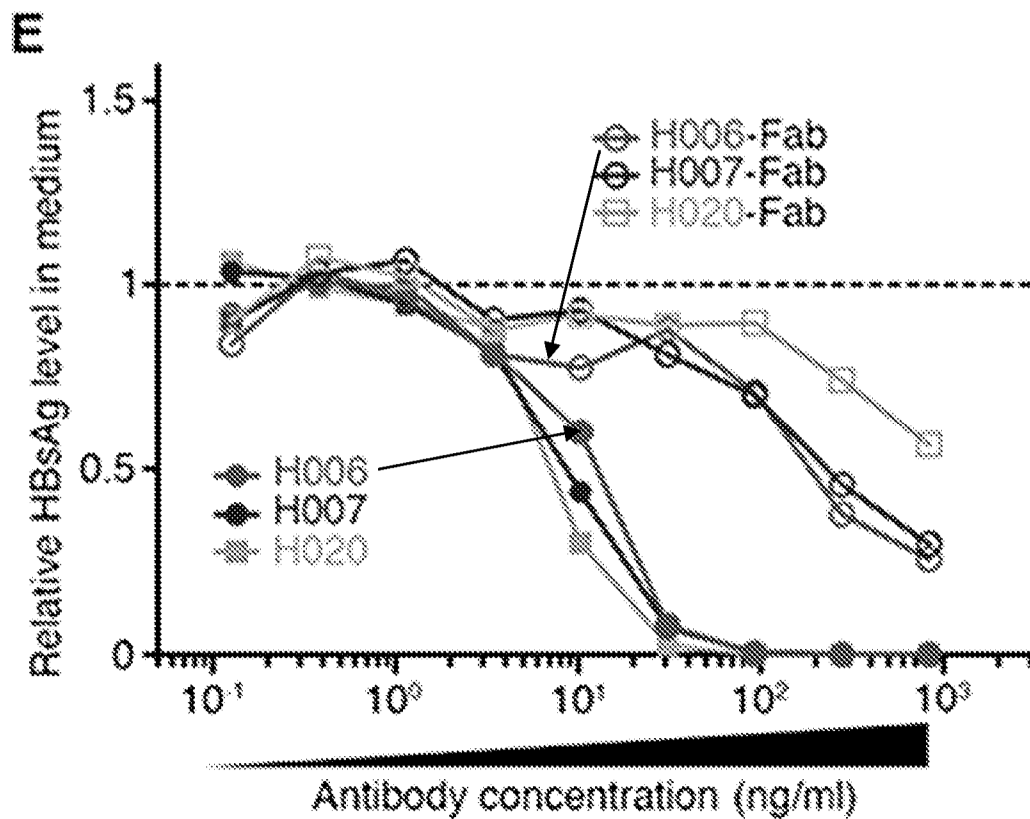
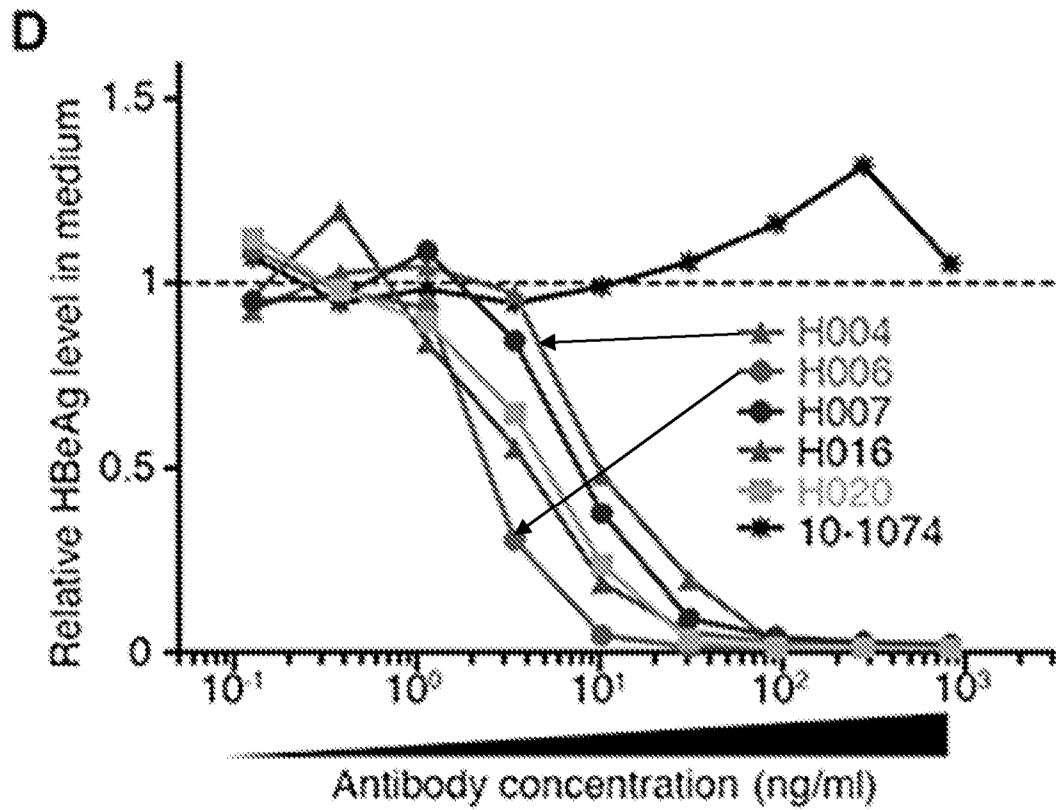


Fig. 5 (continued)

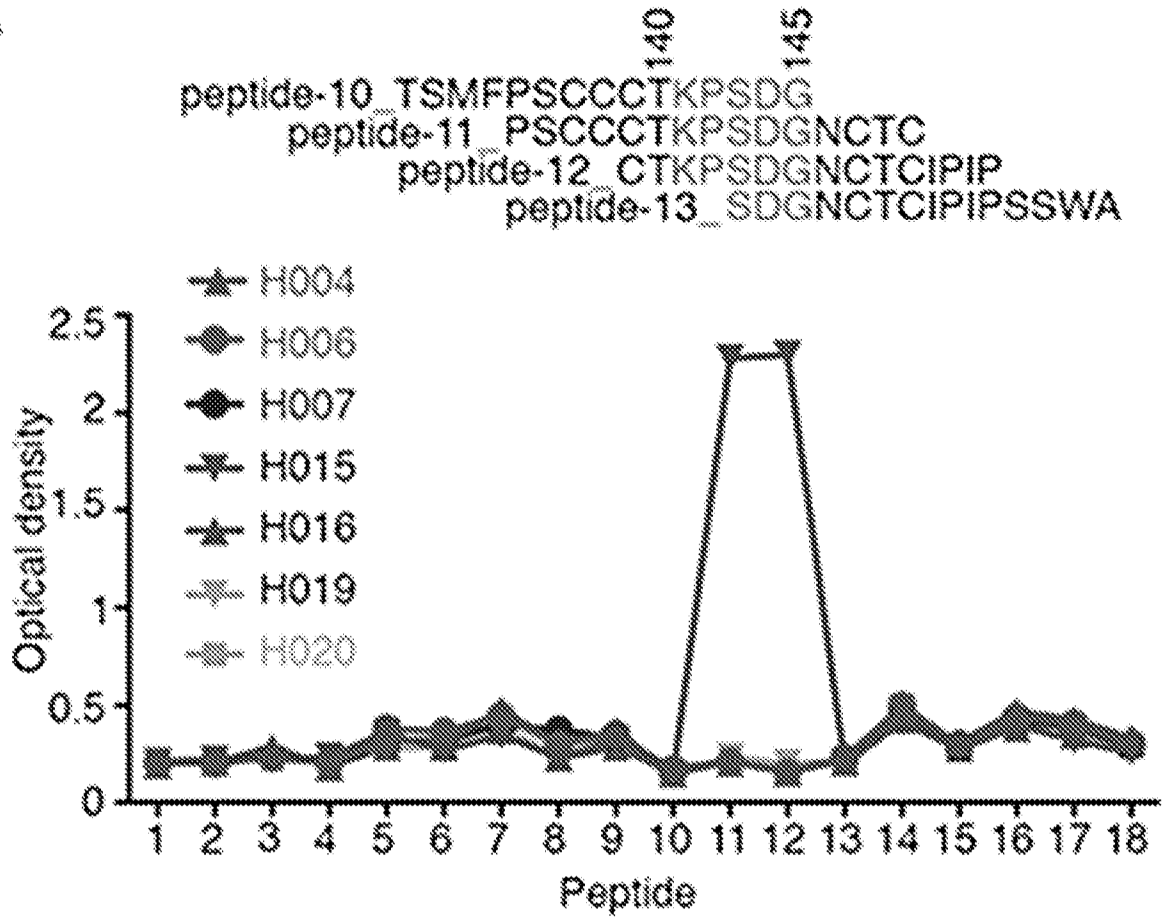
A

Fig. 6

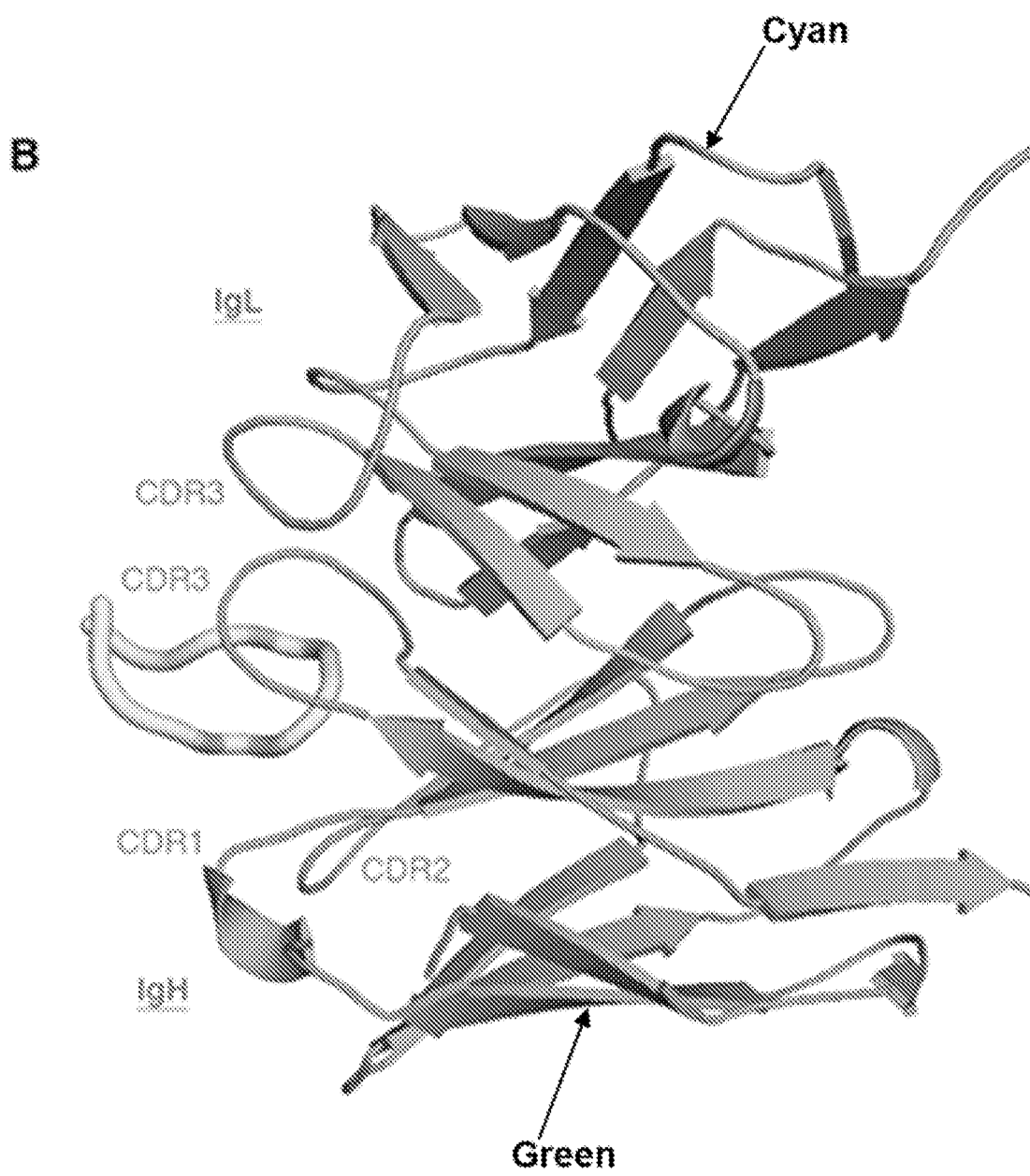


Fig. 6 (continued)

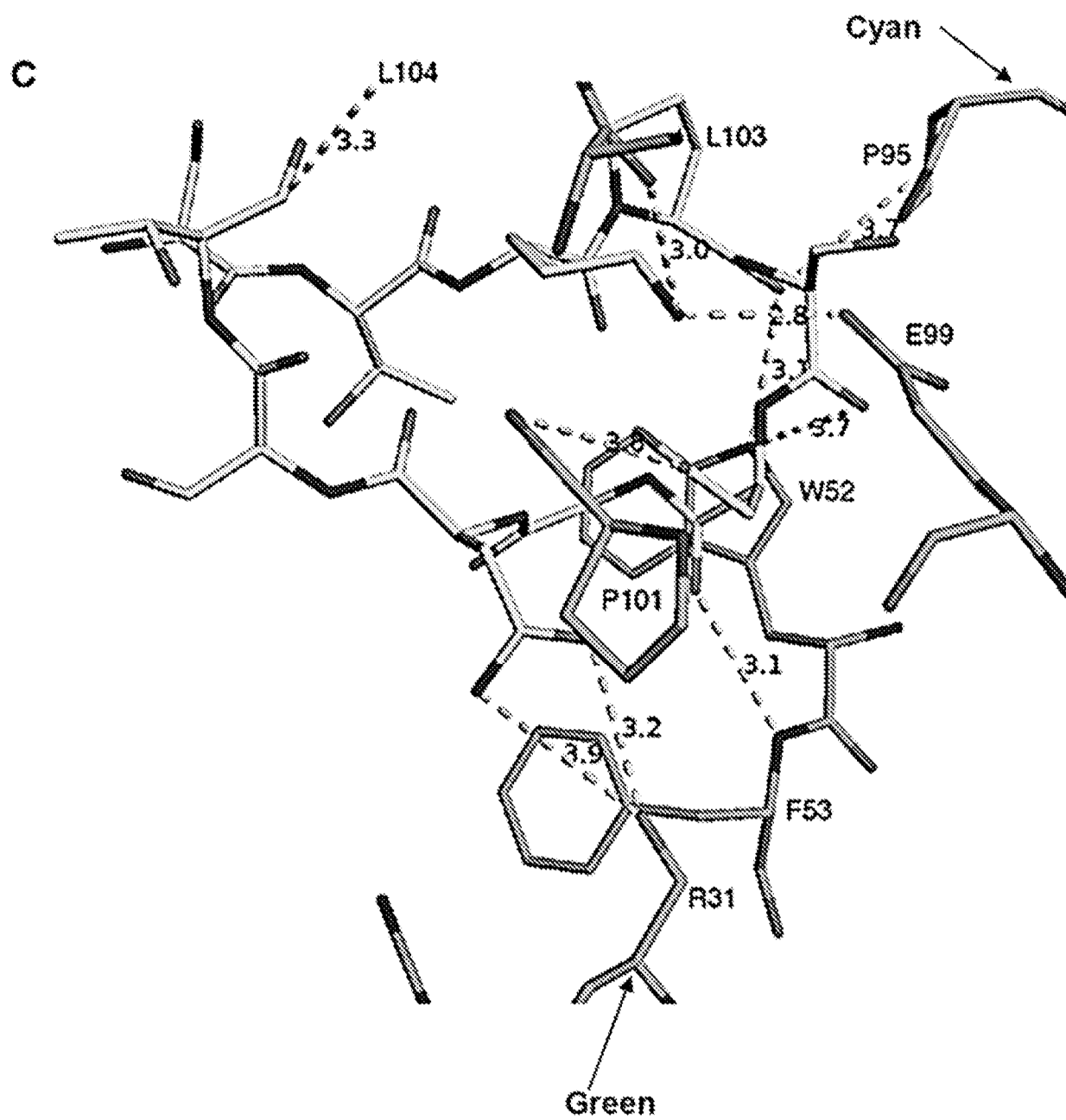


Fig. 6 (continued)

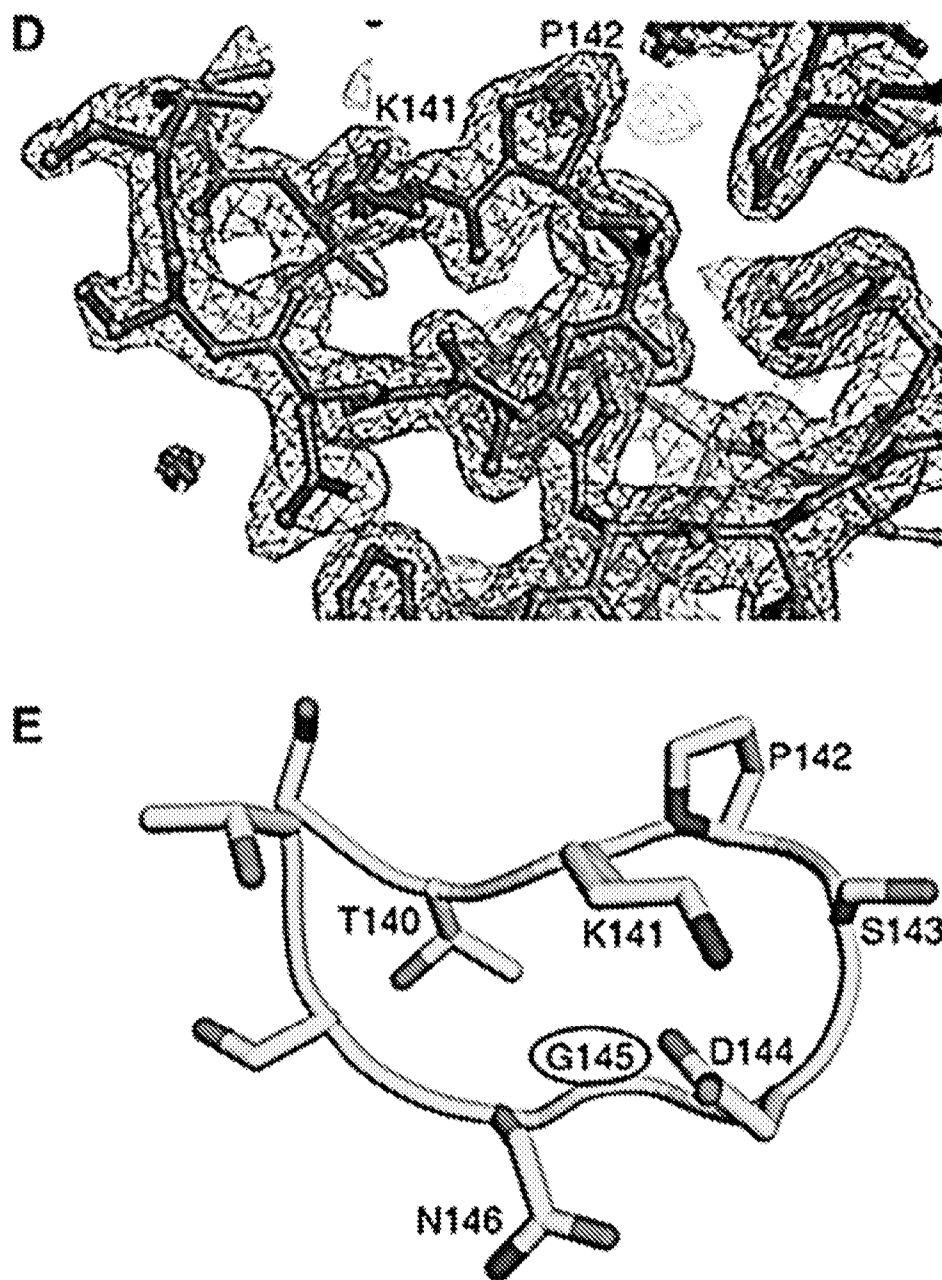


Fig. 6 (continued)

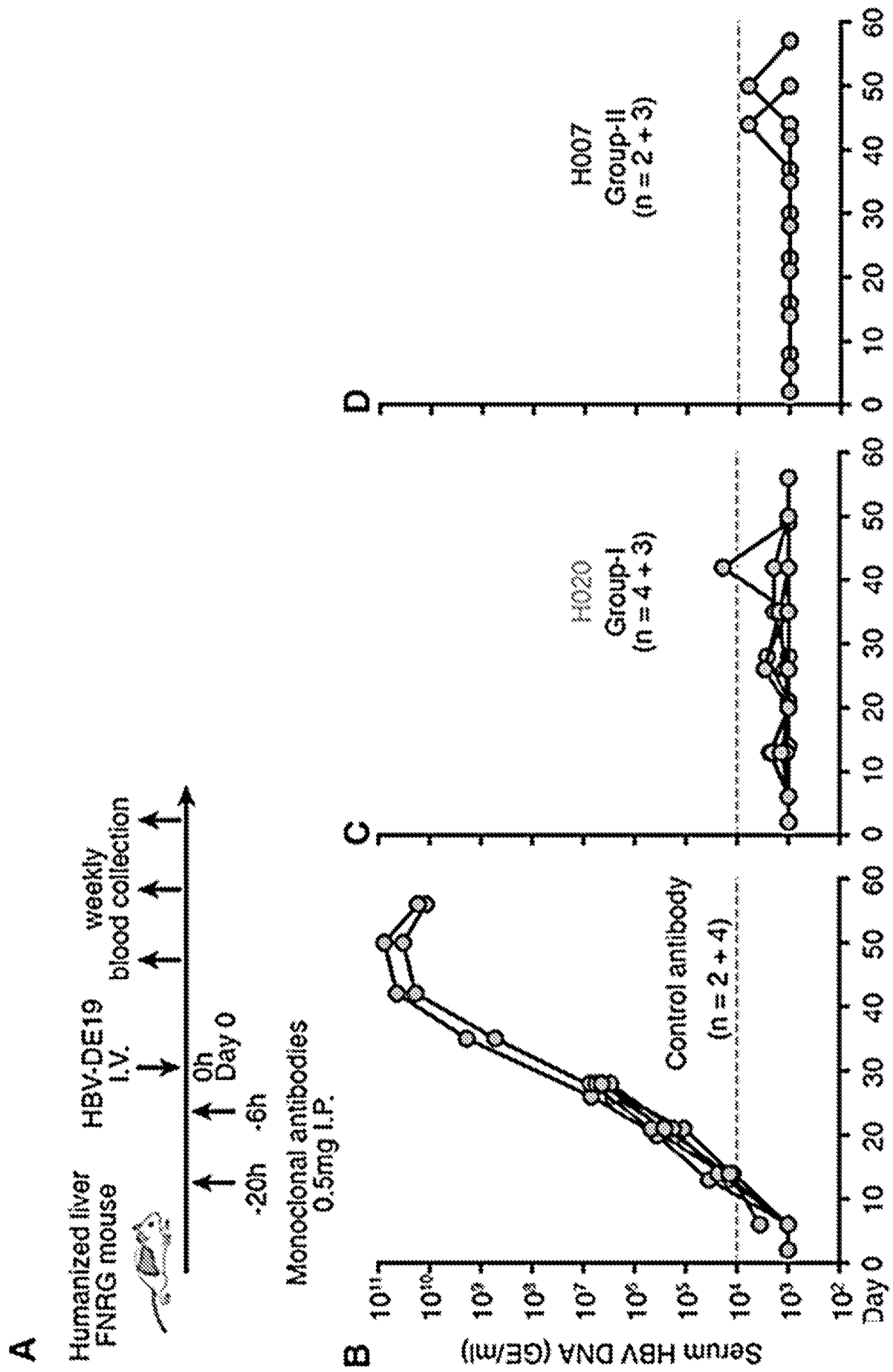


Fig. 7

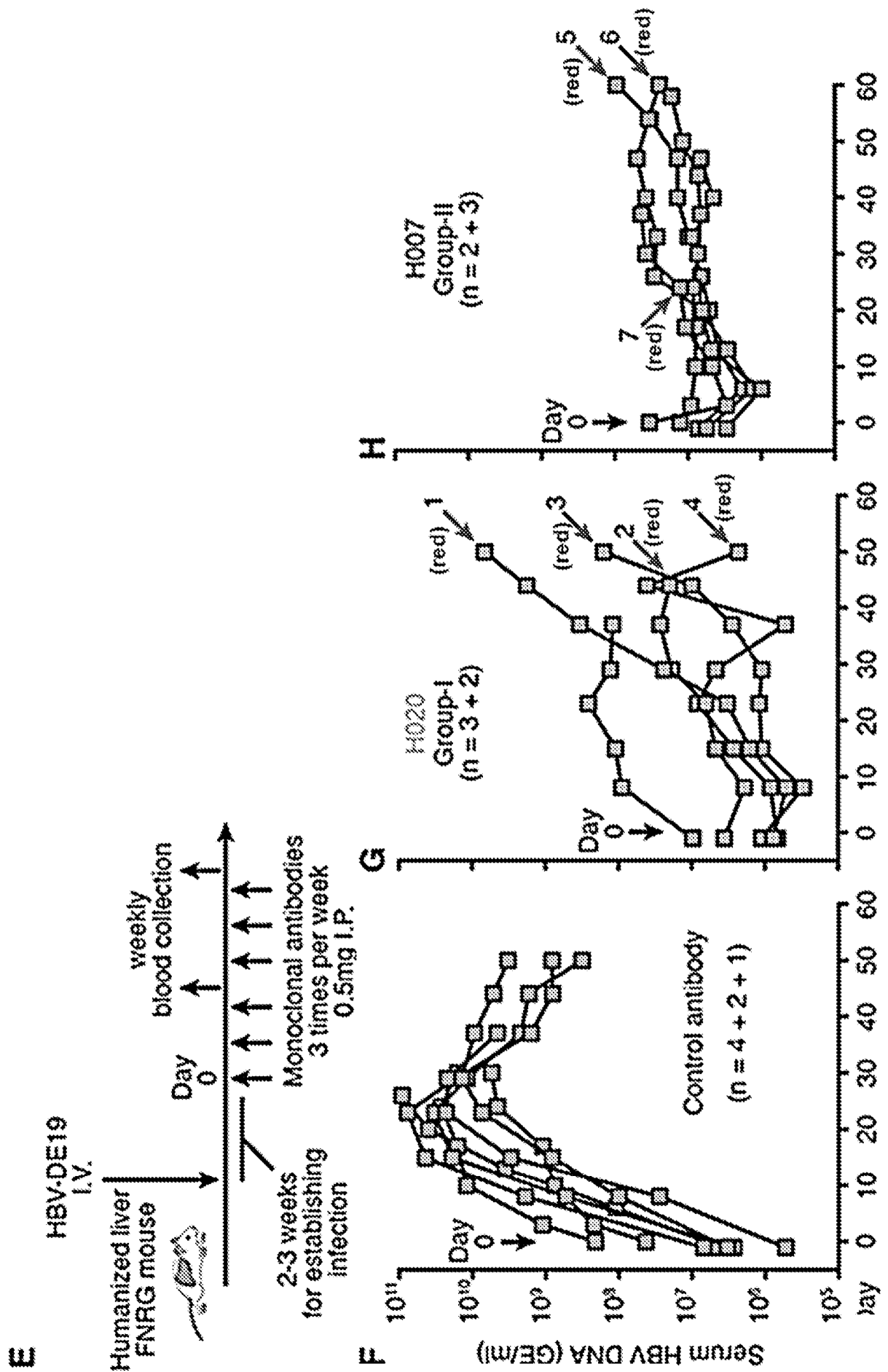


Fig. 7 (continued)

I	Red arrow	Escape mutation
	1	G145R
	2	G145R
	3	G145R
	4	G145E
	5	G145R
	6	G145R
	7	G145R
	8	K122R / G145R
	9	C137Y
	10	C137Y / D144V

Fig. 7 (continued)

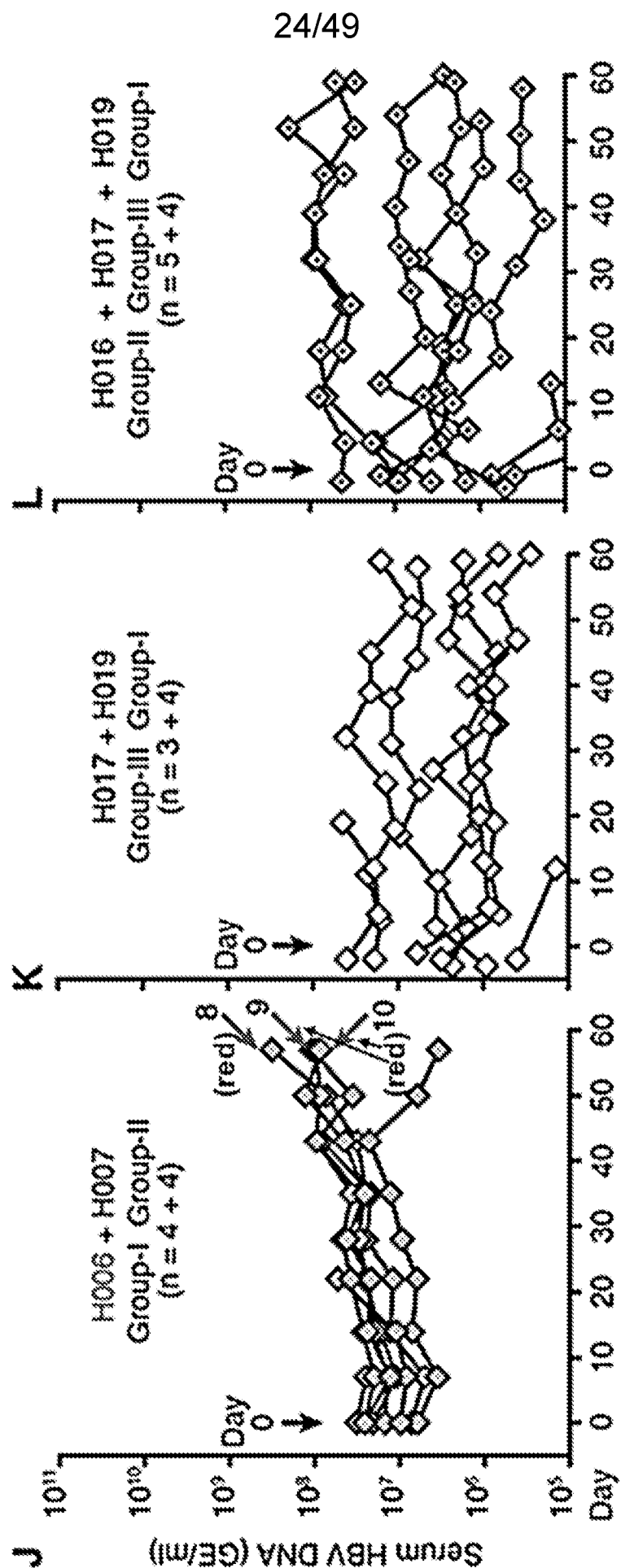


Fig. 7 (continued)

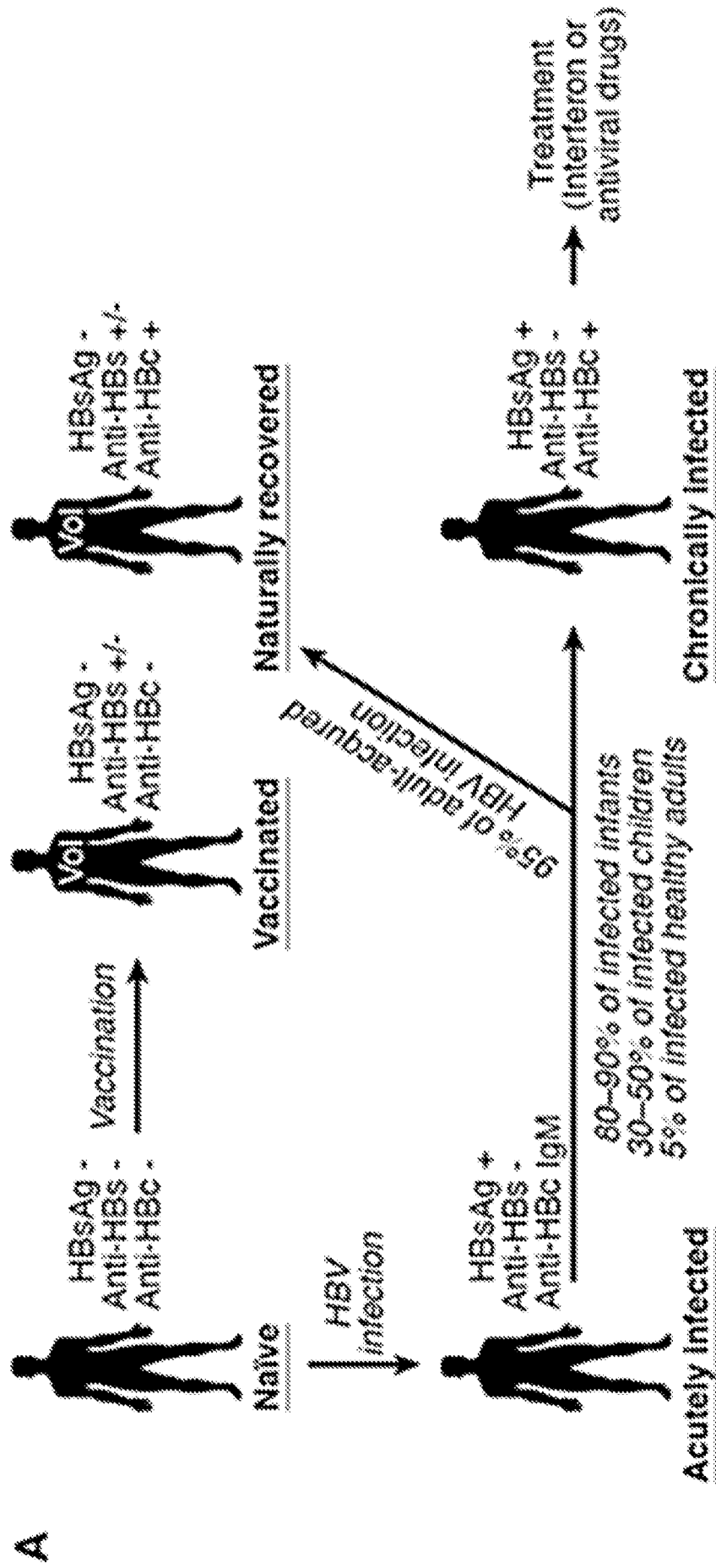


Fig. 8

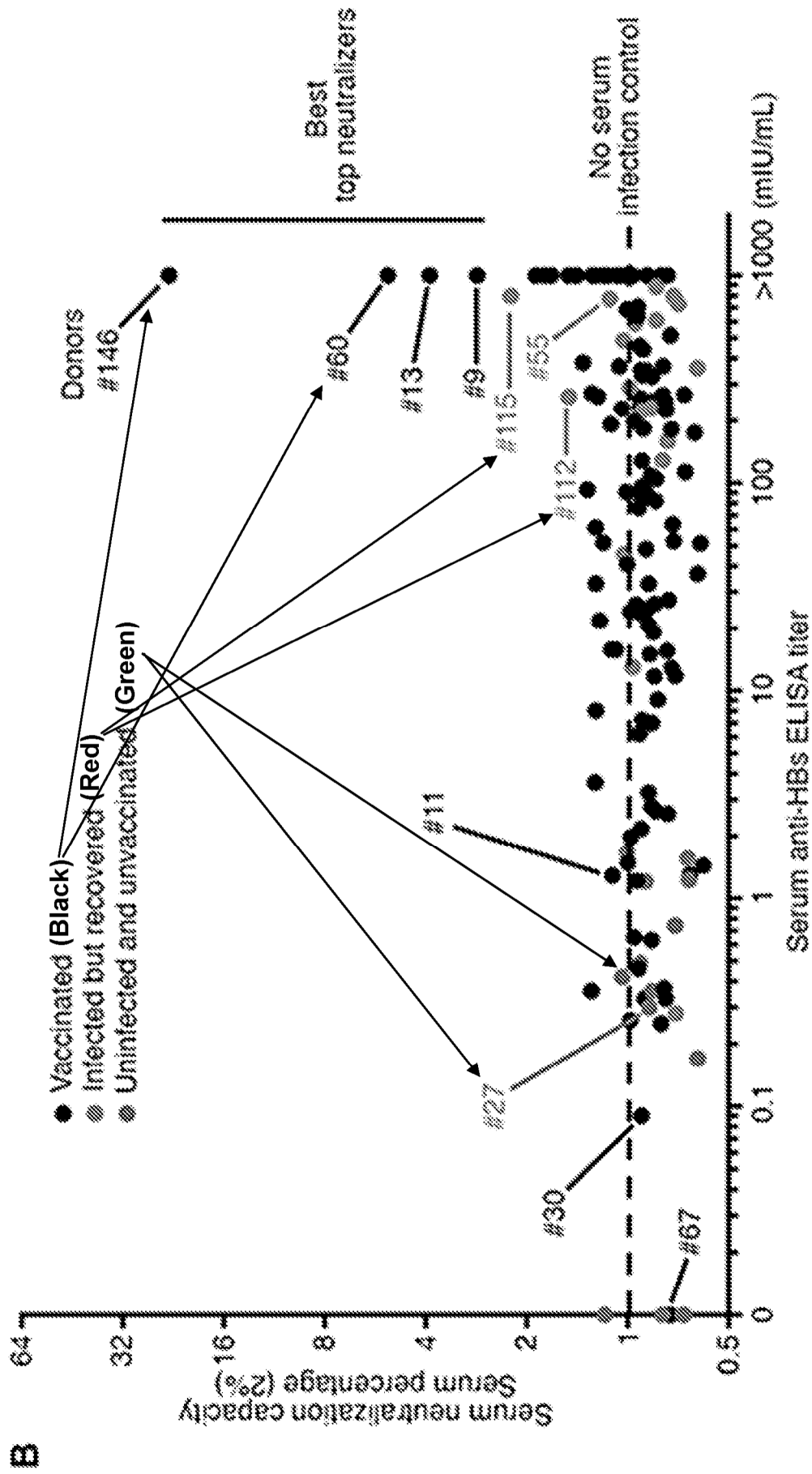


Fig. 8 (continued)

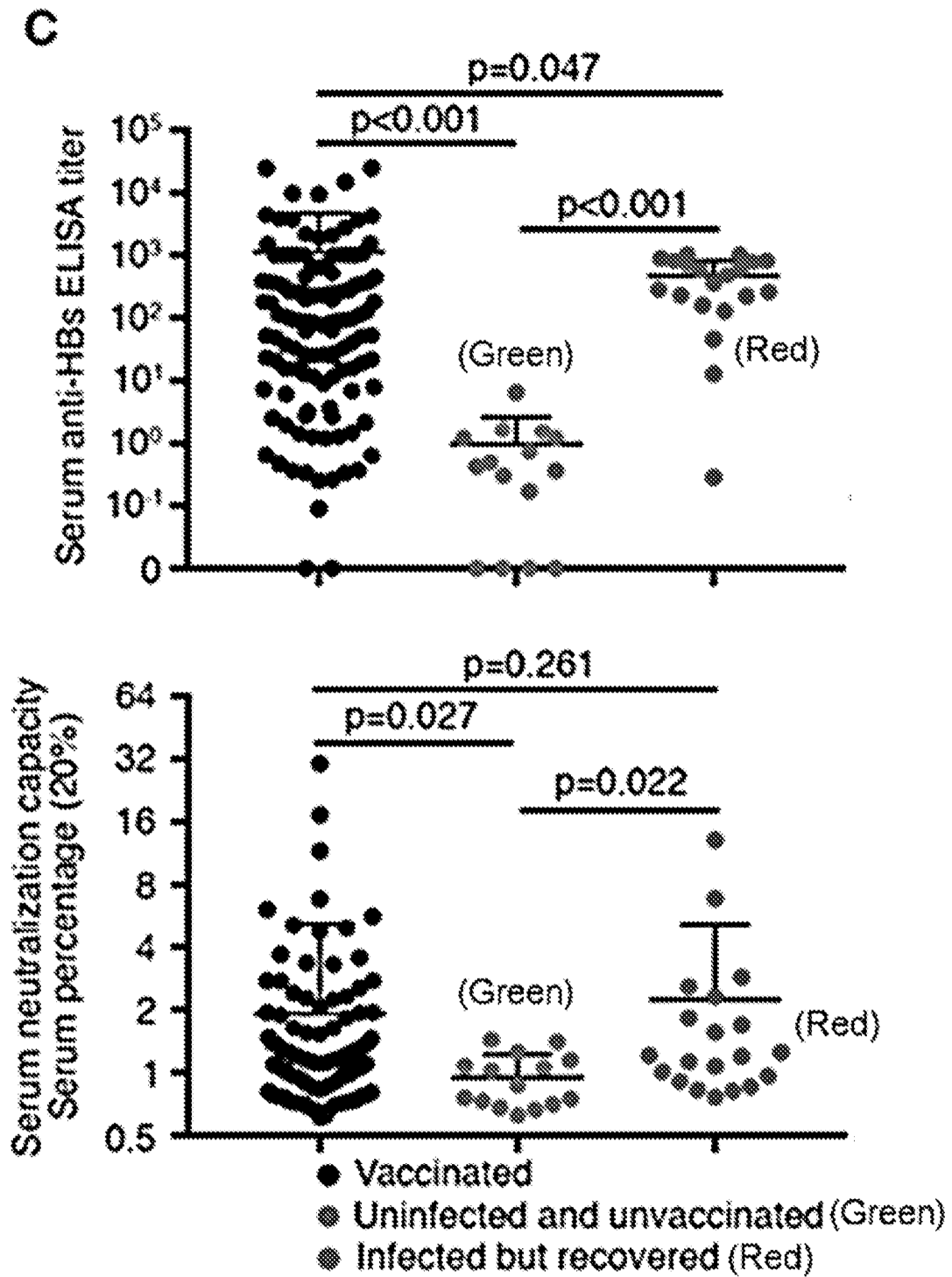


Fig. 8 (continued)

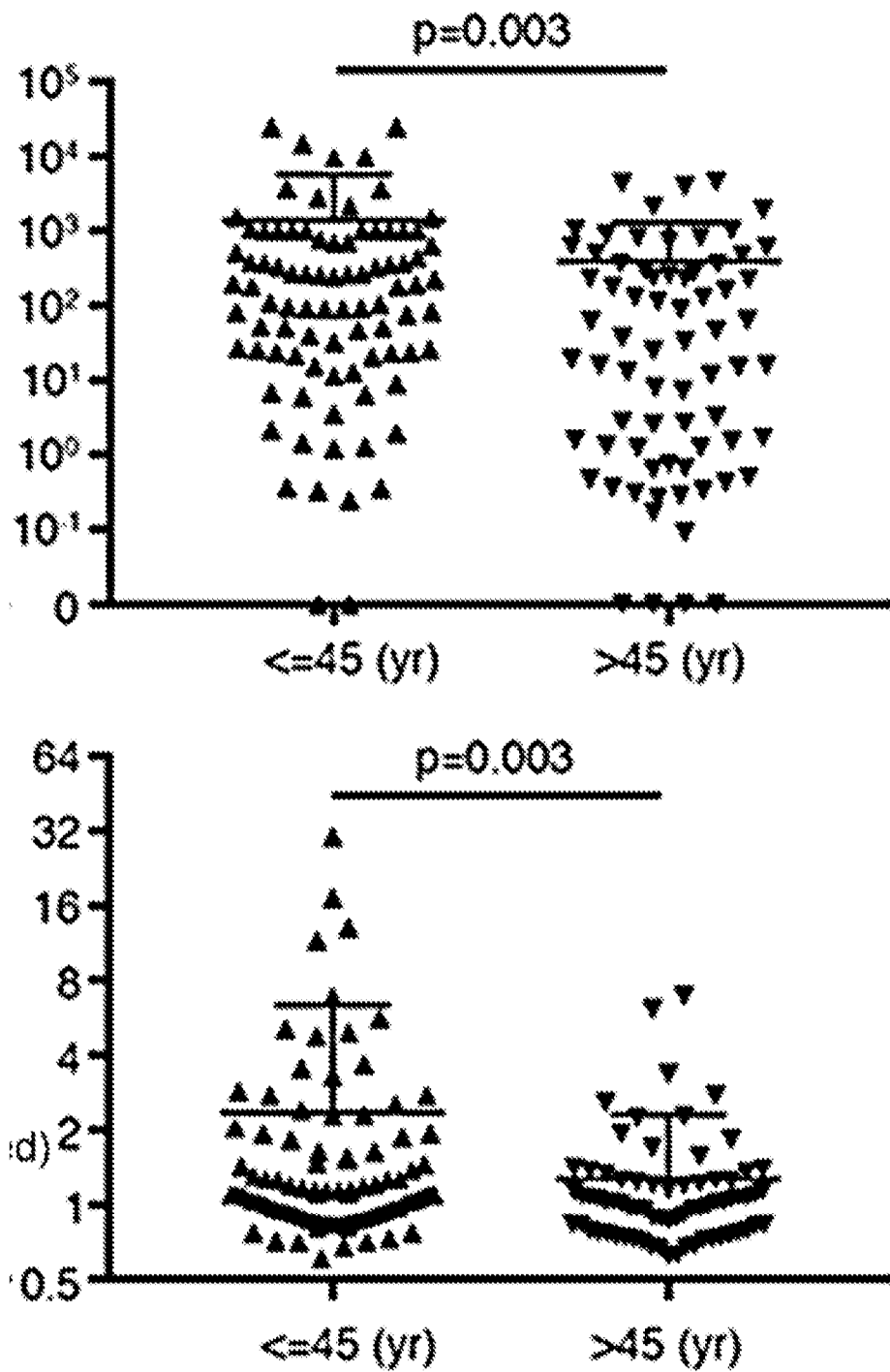
D

Fig. 8 (continued)

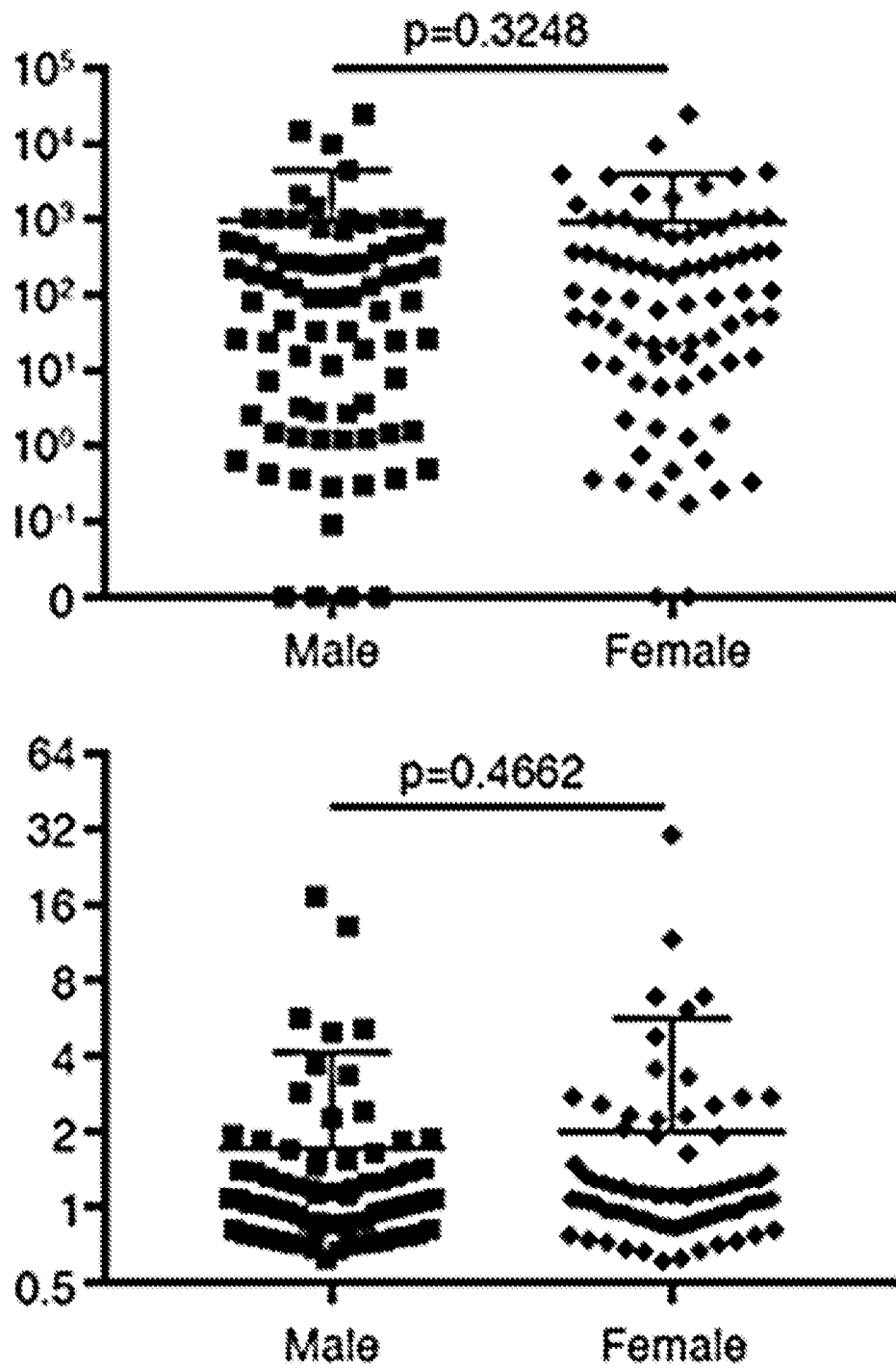
E

Fig. 8 (continued)

A

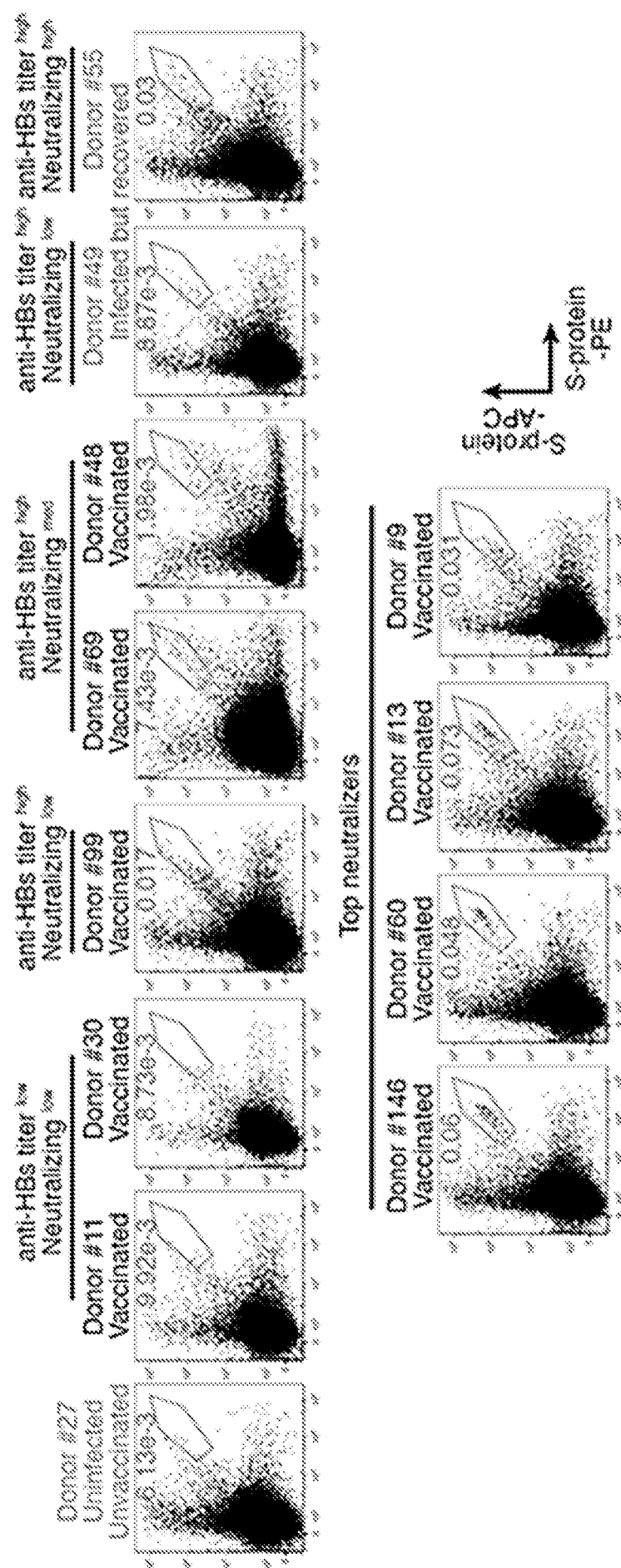


Fig. 9

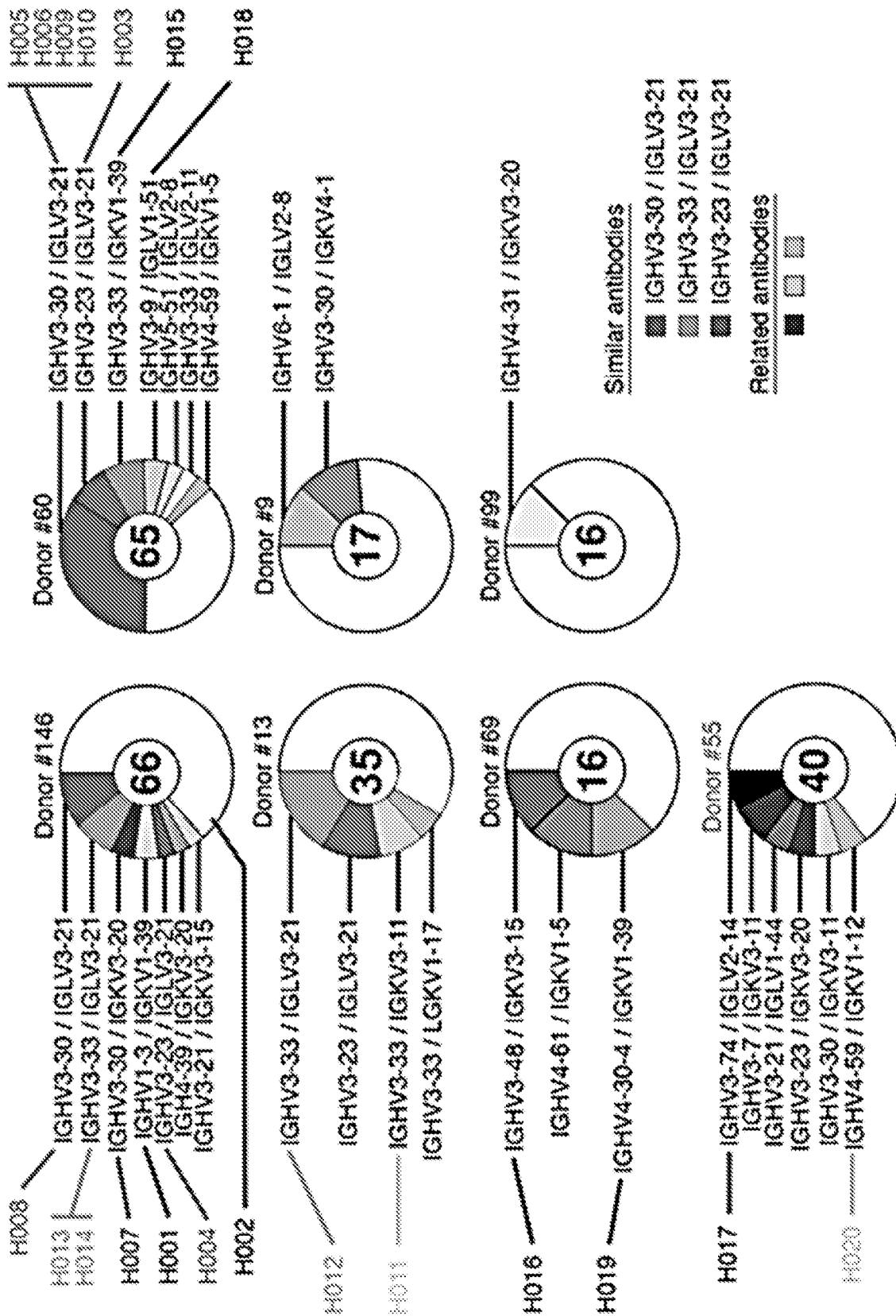


Fig. 9 (continued)

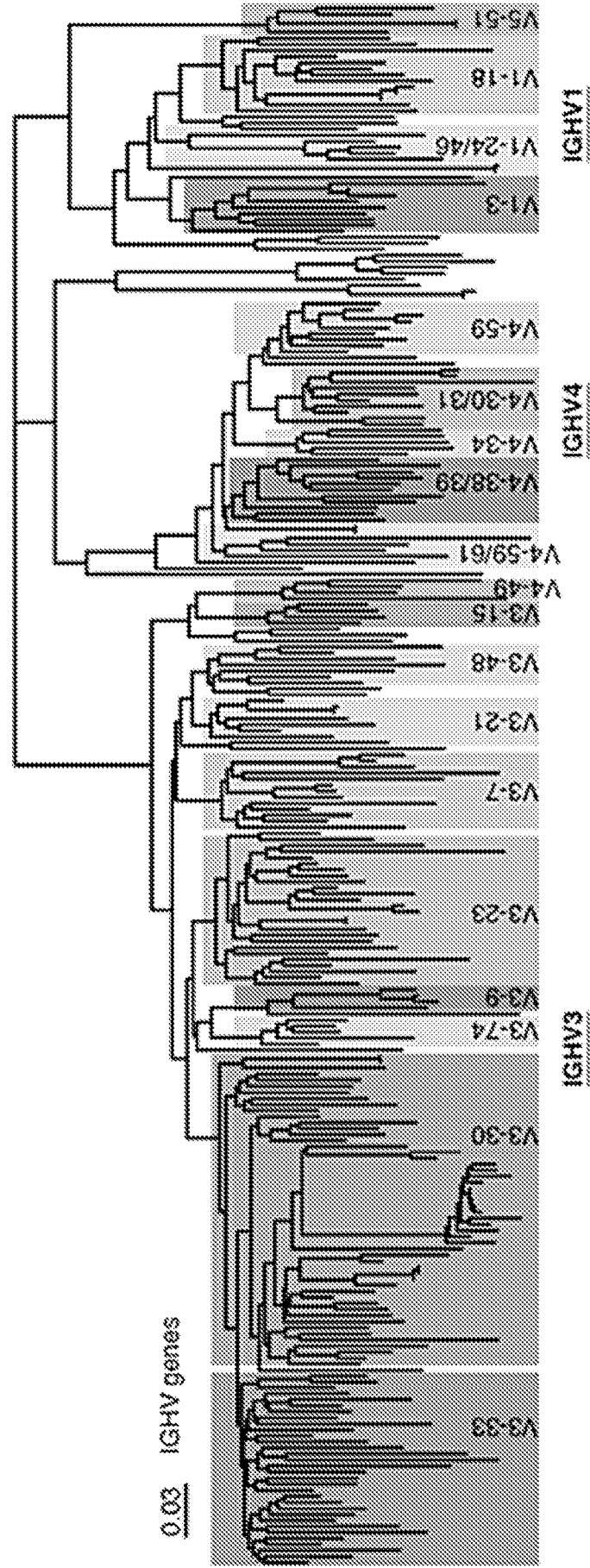


Fig. 9 (continued)

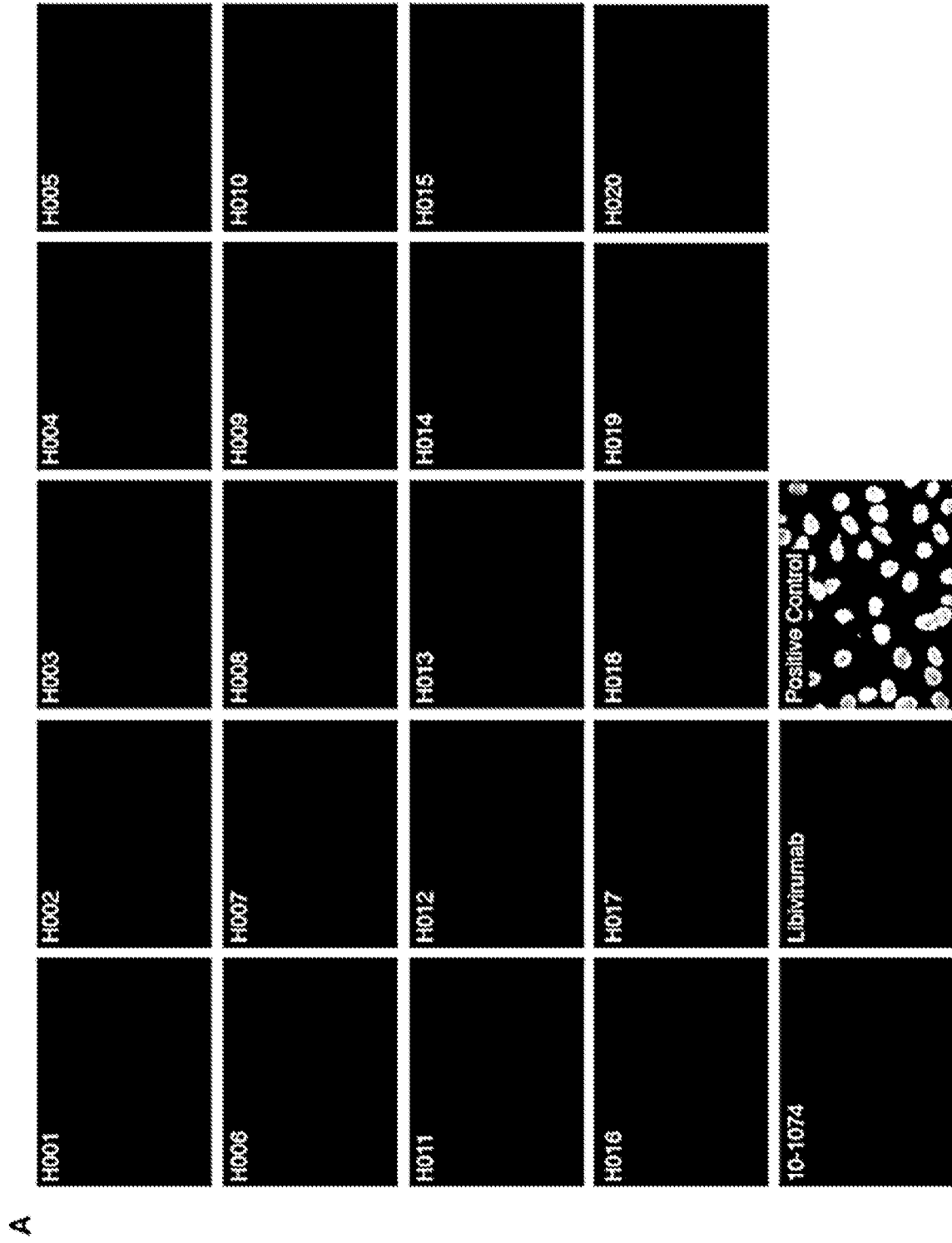


Fig. 10

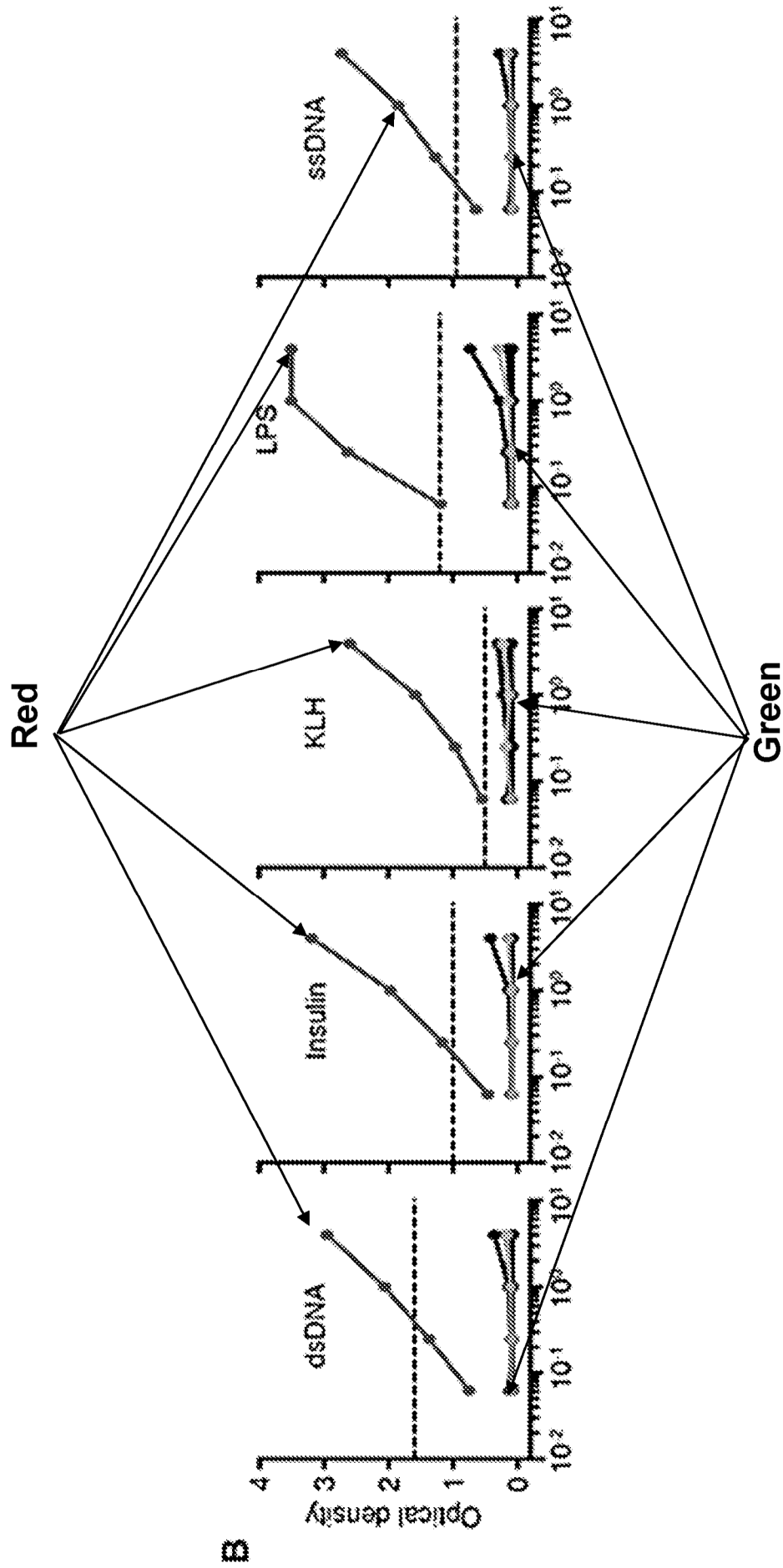


Fig. 10 (continued)

A

	Q	G	M	L	P	V	C	P	L	I	P	G	S	T	T	T	S	T	G	P	C	K	T	C	T
	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125
H020	123	128		98	133		121	107	95	110	108	106	98	105	102	93	93	93	93	95		111	102		103
H004	96	96		79	105		100	96	71	113	101	103	101	100	100	101	92	92	92	72		97	108		112
H006	97	87		79	106		92	110	65	114	102	97	98	96	98	95	92	92	96		102	99		103	
H019	112	115		100	122		105	106	54	112	99	92	92	99	91	95	114	75	75		75	98		83	
H017	57	69		68	60		87	85	106	100	80	91	90	91	88	89	84	104				98	82		78
H007	99	86		129	85		108	85	90	99	105	103	104	107	105	99	107	102	76			97	31		97
H016	98	109		116	81		94	96	110	86	97	103	102	104	103	106	109	113	95			61	25		95
H015	75	79		99	68		80	100	78	80	85	94	95	94	100	96	100	94	114			93	94		108

White

Dark grey

Black

Light grey

Group-I

Group-II

Group-III

Fig. 11

A (continued)

	T	P	A	Q	G	N	S	M	F	P	S	C	C	C	T	K	P	T	D	G	N	C	T	C	I	
H020	96	94		96	106	89	91	95	97	94	101				102	68	86	109	132	62	93			31		95
H004	110	107		101	102	95	99	102	108	101	100				109	76	108	105	55	59	92			59		112
H006	101	108		100	101	93	97	101	103	101	98				100	68	104	104	102	101	92			58		108
H019	102	91		94	88	81	91	89	84	89	103				101	17	70	102	98	99	102			59		86
H017	99	101		92	102	103	94	99	95	108	120				133	145	128	124	141	127	105			81		91
H007	98	104		103	102	111	104	107	105	104	98				97	96	78	85	40	45	106			99		99
H016	95	97		102	100	120	110	99	95	109	98				86	104	102	95	63	17	108			99		106
H015	97	99		105	101	111	108	106	109	103	101				105	11	33	11	15	26	107			102		94

White

Light grey

Dark grey

Black

Group-I

Group-II

Group-III

Fig. 11 (continued)

A (continued)

37/49

Dark grey

White

Light grey

Black

Group-I

Group-II

Group-III

A (continued)

	151				161				171				Emp WT												
	P	I	P	S	S	W	A	F	A	K	Y	L	W	E	W	A	S	V	R	F	S	W			
H020	103		104	98	115			99		99	93	110	107	100	99		104	105		96	93	100		19	100
H004	103		108	97	108			103		99	95	102	96	91	99		97	96		94	100	99		27	100
H006	100		108	102	111			109		106	105	102	94	93	99		98	102		106	101	105		17	100
H019	98		100	93	101			99		94	107	110	100	105	104		99	96		99	103	89		23	100
H017	109		145	113	117			117		106	80	94	101	99	92		110	104		106	102	96		16	100
H007	99		100	108	93			98		107	80	97	101	102	101		99	100		100	99	101		21	100
H016	98		90	99	85			95		97	64	94	102	104	103		104	101		107	106	105		20	100
H015	99		91	103	87			97		97	70	85	100	105	95		99	99		97	97	100		17	100

Fig. 11 (continued)

B

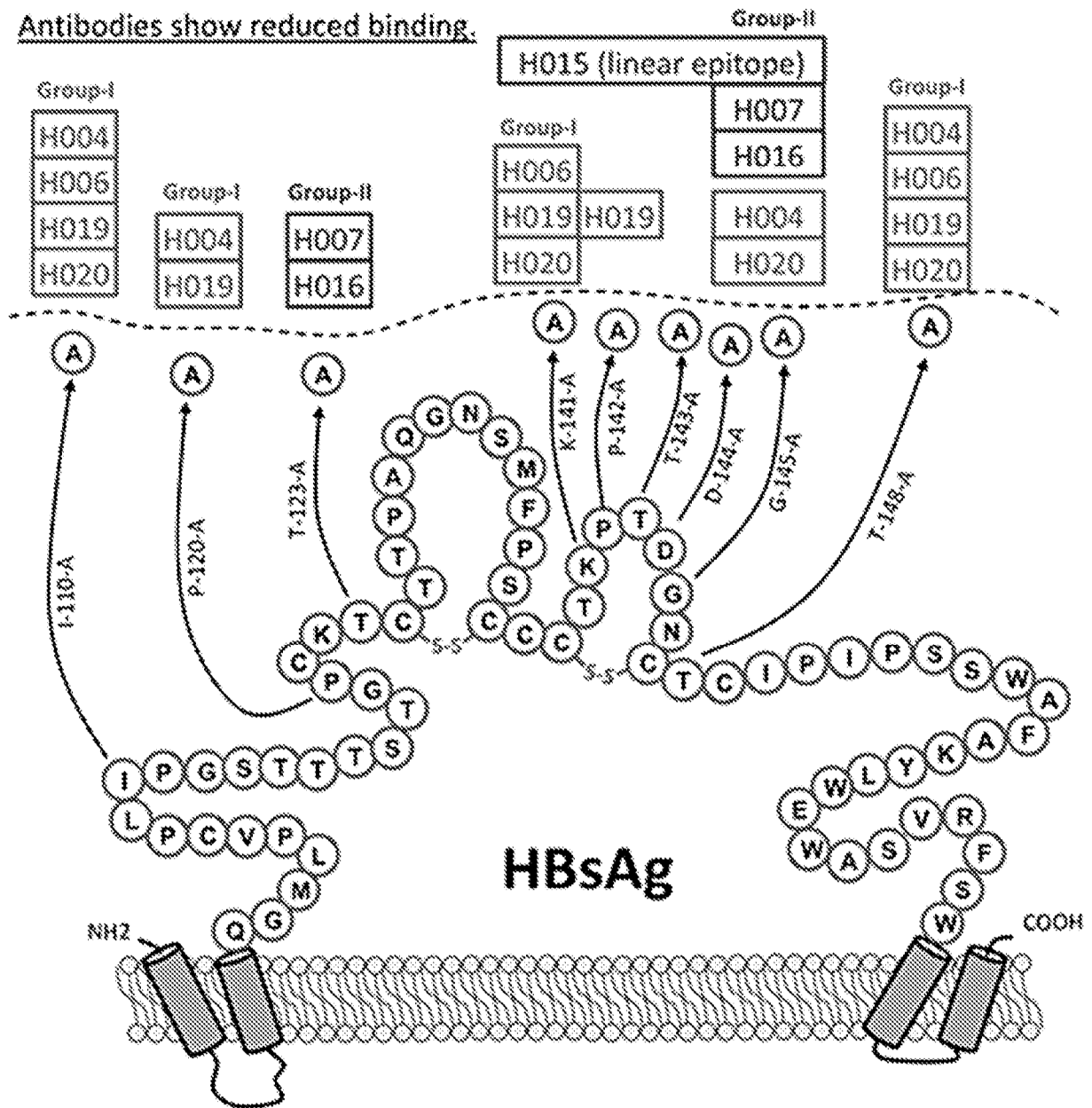
Antibodies show reduced binding.

Fig. 11 (continued)

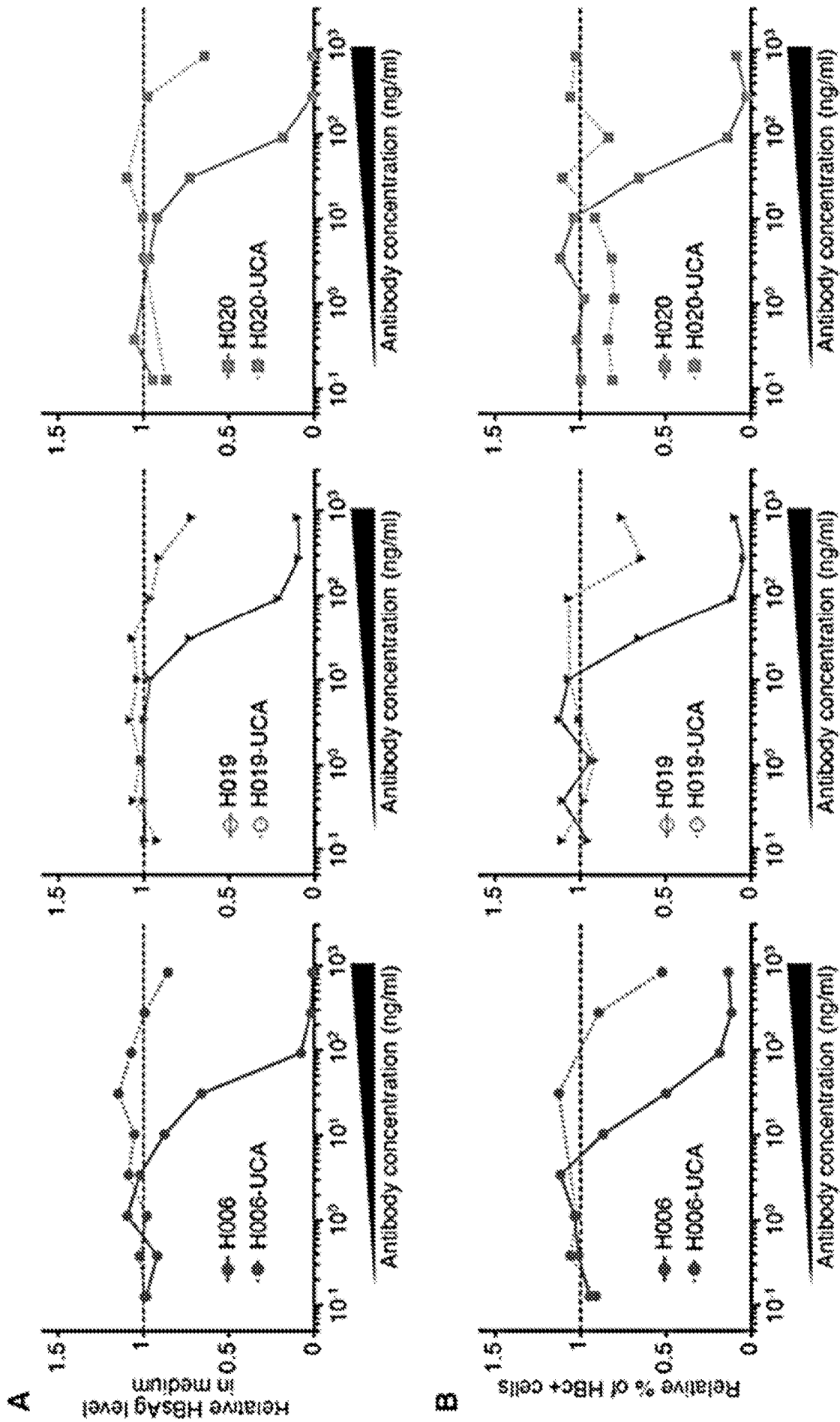


Fig. 12

C

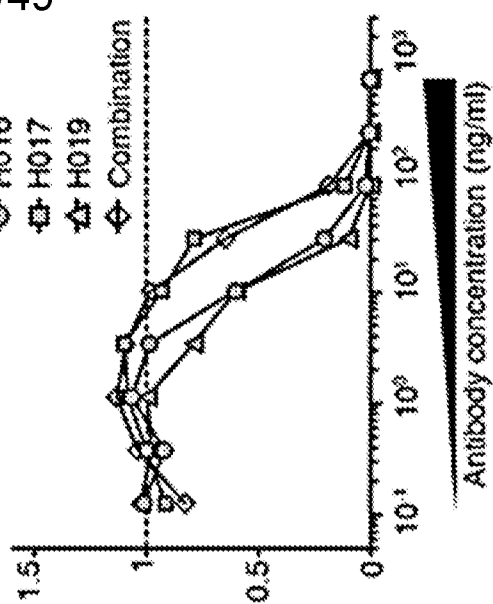
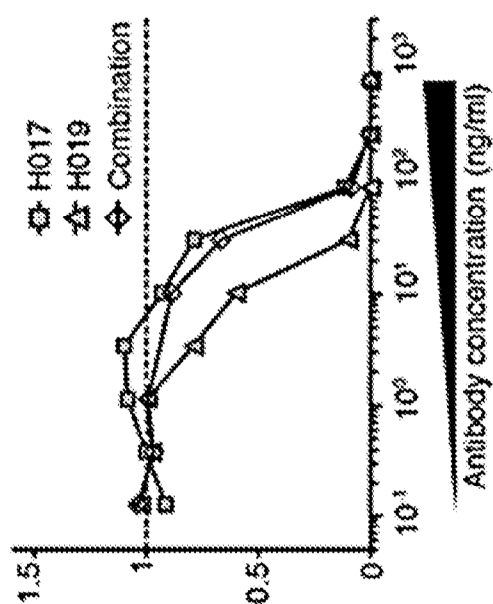
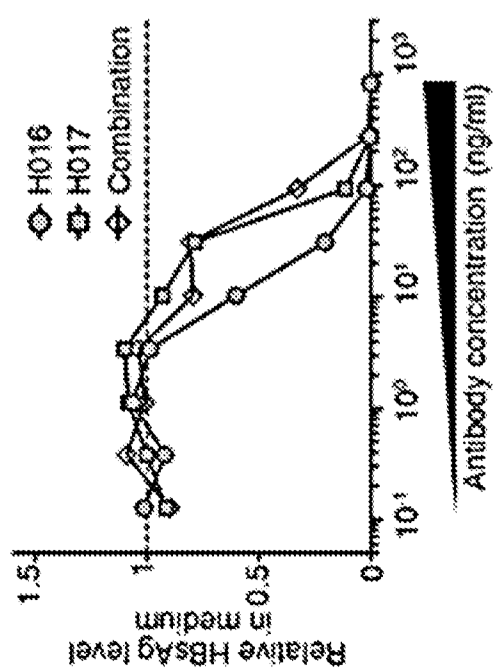
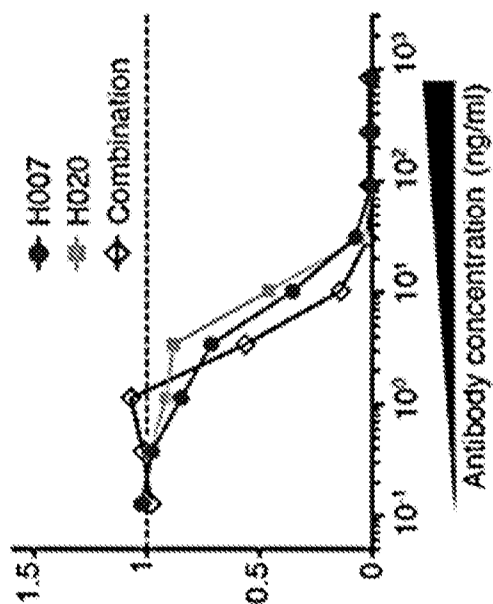
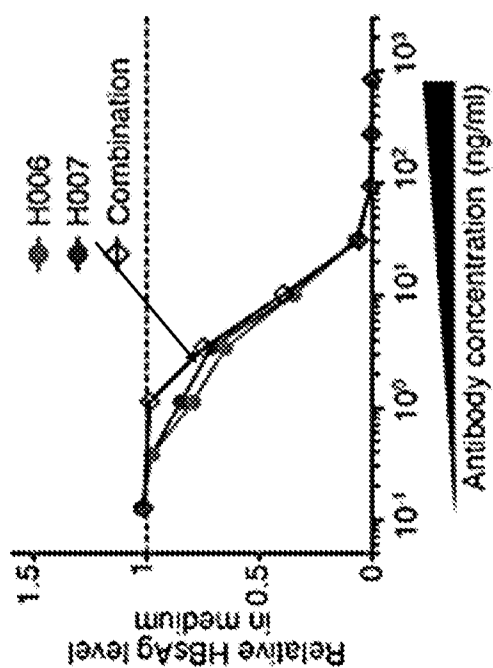


Fig. 12 (continued)

B

Wavelength (Å)	0.979		
Resolution range	67.35-1.78 (1.82-1.78)		
Space group	P2 ₁ 2 ₁ 2 ₁		
Unit cell	49.9 71.2 134.7		
Total reflections	615,285 (56,022)		
Unique reflections	46,432 (4,386)		
Multiplicity	12.9 (12.1)		
Completeness (%)	99.5 (91.0)		
Mean I/sigma (I)	17.2 (1.26)		
Wilson B-factor	33		
Anisotropy	0.449		
R-merge	0.084 (1.26)		
R-meas	0.090 (1.309)		
R-pim	0.034 (0.505)		
CC _{1/2}	0.999 (0.793)		
Reflections used in refinement	46432 (4380)		
Reflections used for R-free	1999 (188)		
R-work	0.182 (0.276)		
R-free	0.227 (0.293)		
Number of non-hydrogen atoms	3752		
Macromolecules	3391		
Solvent	361		
Protein residues	451		
RMSZ (bonds)	0.37		
RMSZ (angles)	0.55		
Ramachandran favored (%)	98		
Ramachandran allowed (%)	2		
Ramachandran outliers (%)	0.00		
Rotamer outliers (%)	0.00		
Clashscore	1.00		
Average B-factor	39		
Average B of H/L	39		
Average B of the peptide	49		
Macromolecules	38		
Solvent	43		
Fo,Fc correlation	0.97		
Bulk solvent k _{iso} (e/Å ³), B _{iso} (Å ²)	0.32, 42.8		

Fig. 13 (continued)

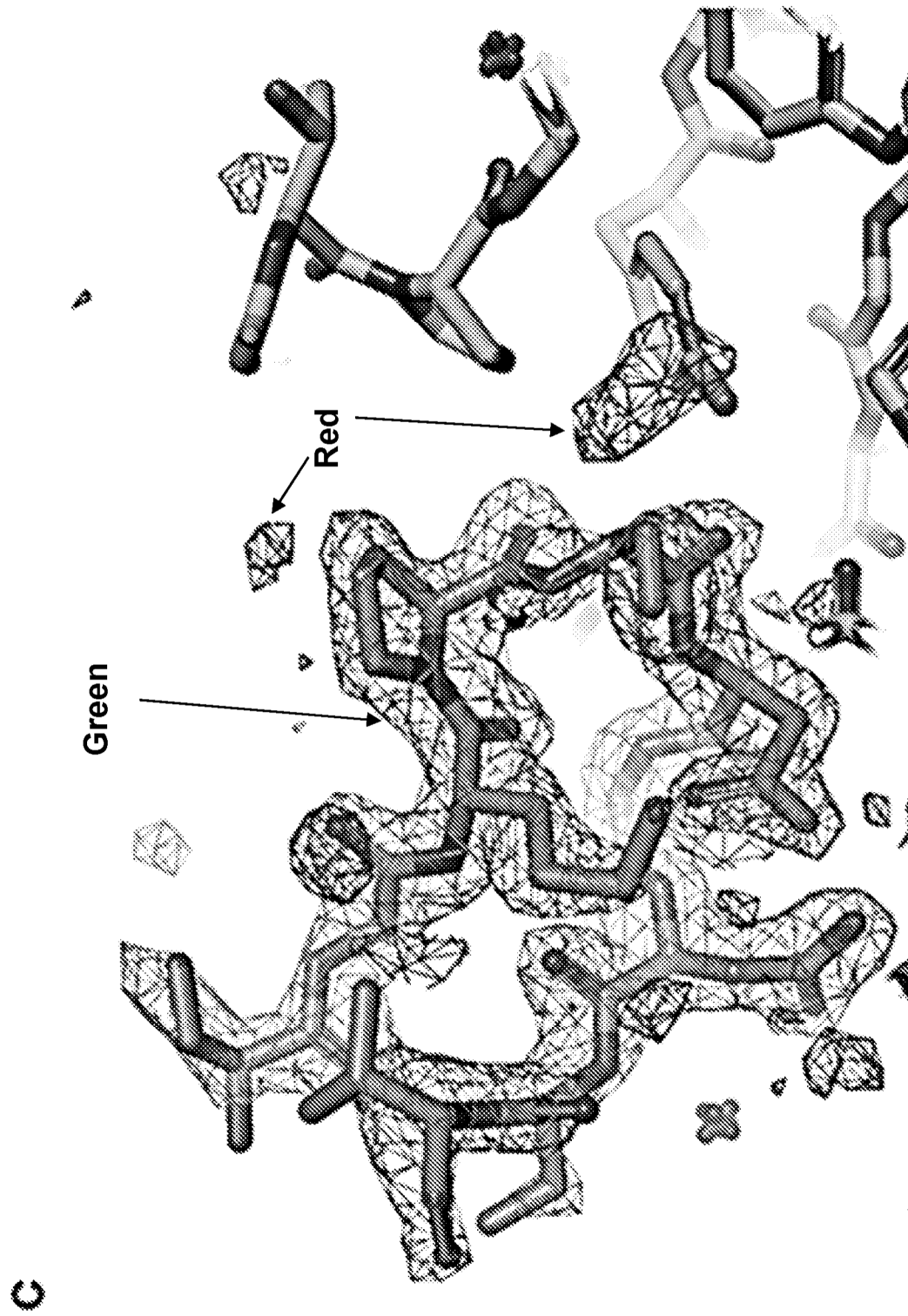


Fig. 13 (continued)

D

H-bonds within the peptide
Ser139(O) – Thr 148(N, OG1)
Lys141(N) – ASN146(O)
Lys141(O) – Gly145(N)
Asp144(OD2) – Asp146(N, ND2)
Asp144(OD1) – Asp146(N)
Salt bridge within the peptide
Lys141(NZ) – Asp144(OD2)
H-bonds between Fab and peptide
Lys141(NZ) – Asp H100(O)
Lys141(NZ) – Leu103(O)
Pro142(O) – Trp H52(NE1)
Ser143(O) – Tyr H59(OH)
Ser143(OG) – Glu H99(OE2)
Asp144(O) – Phe H53(N)
Salt Bridge between Fab and peptide
Lys141(NZ) – Glu H99(OE2)
Hydrophobic between Fab and peptide
Pro142 – Leu L29
Gly145 – Trp H52

Fig. 13 (continued)

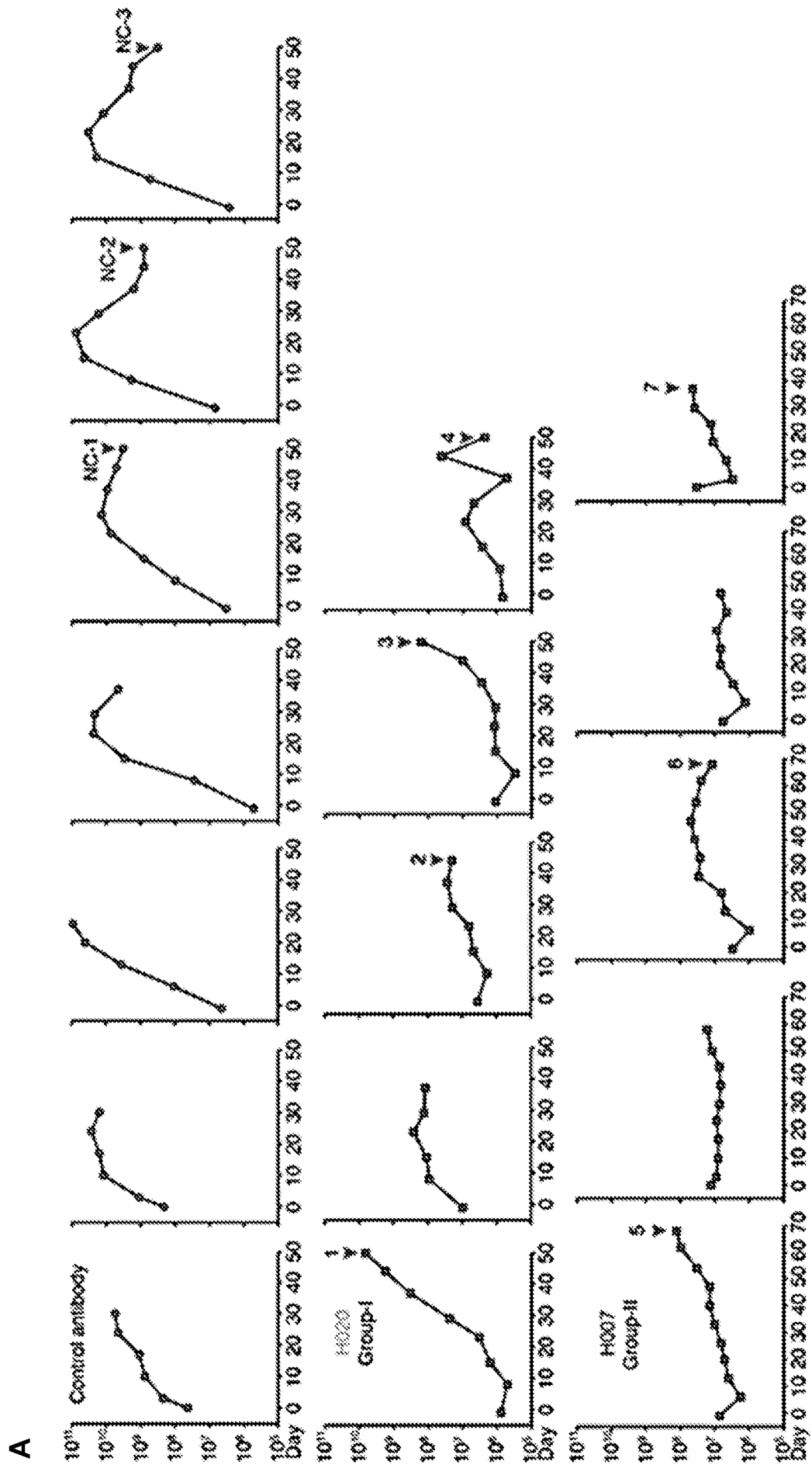


Fig. 14

A (continued)

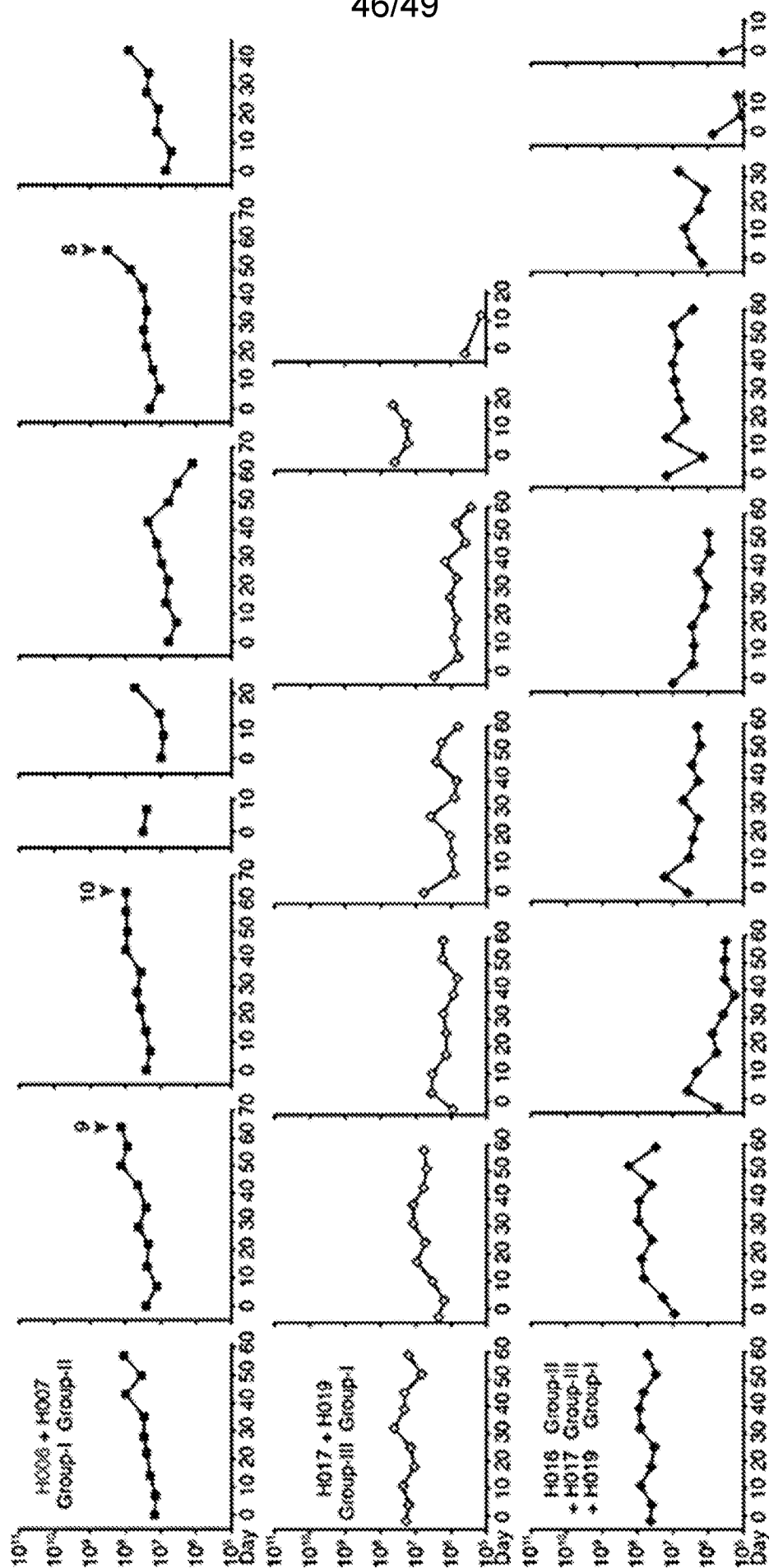


Fig. 14 (continued)

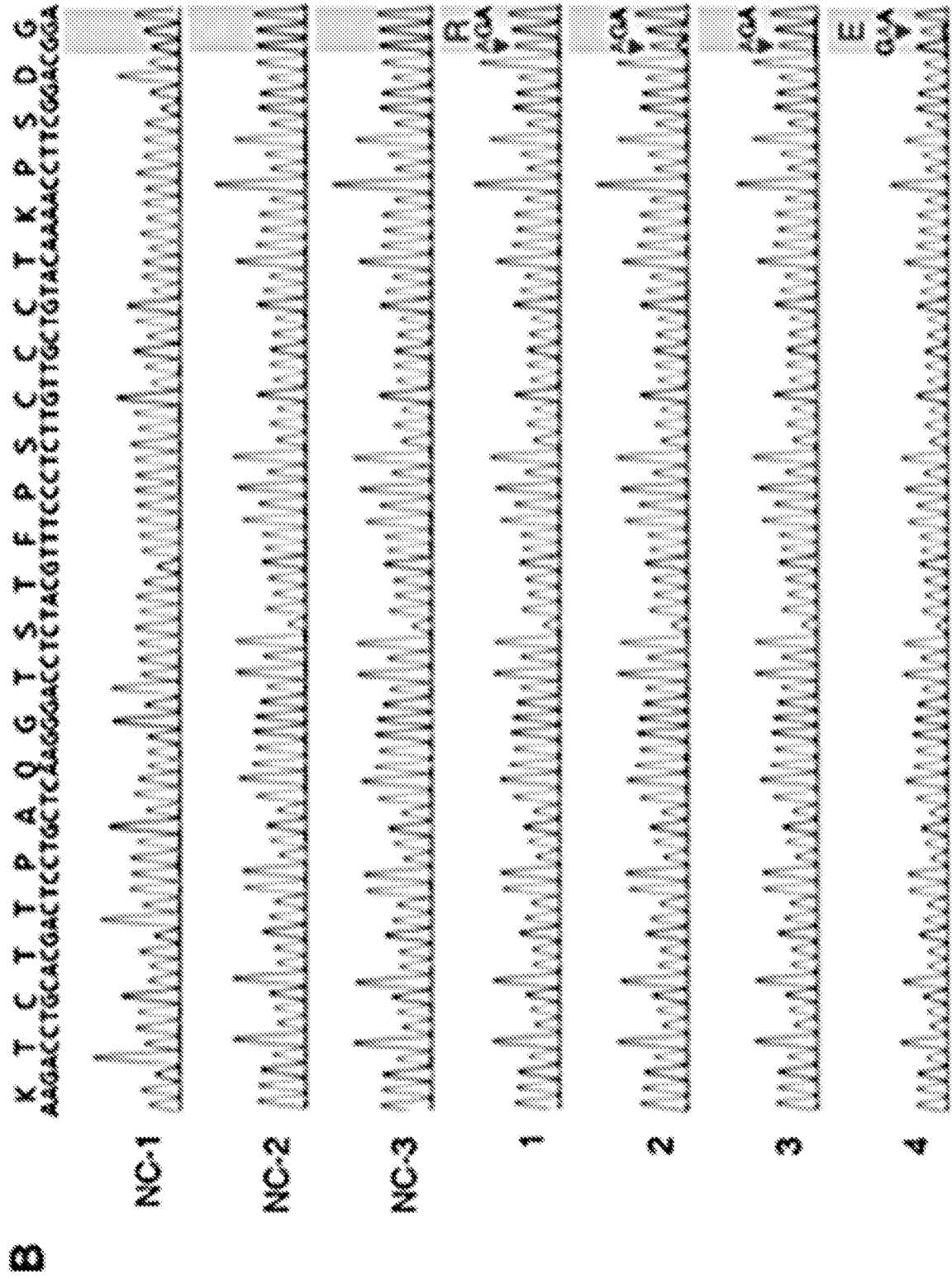


Fig. 14 (continued)

B (continued)

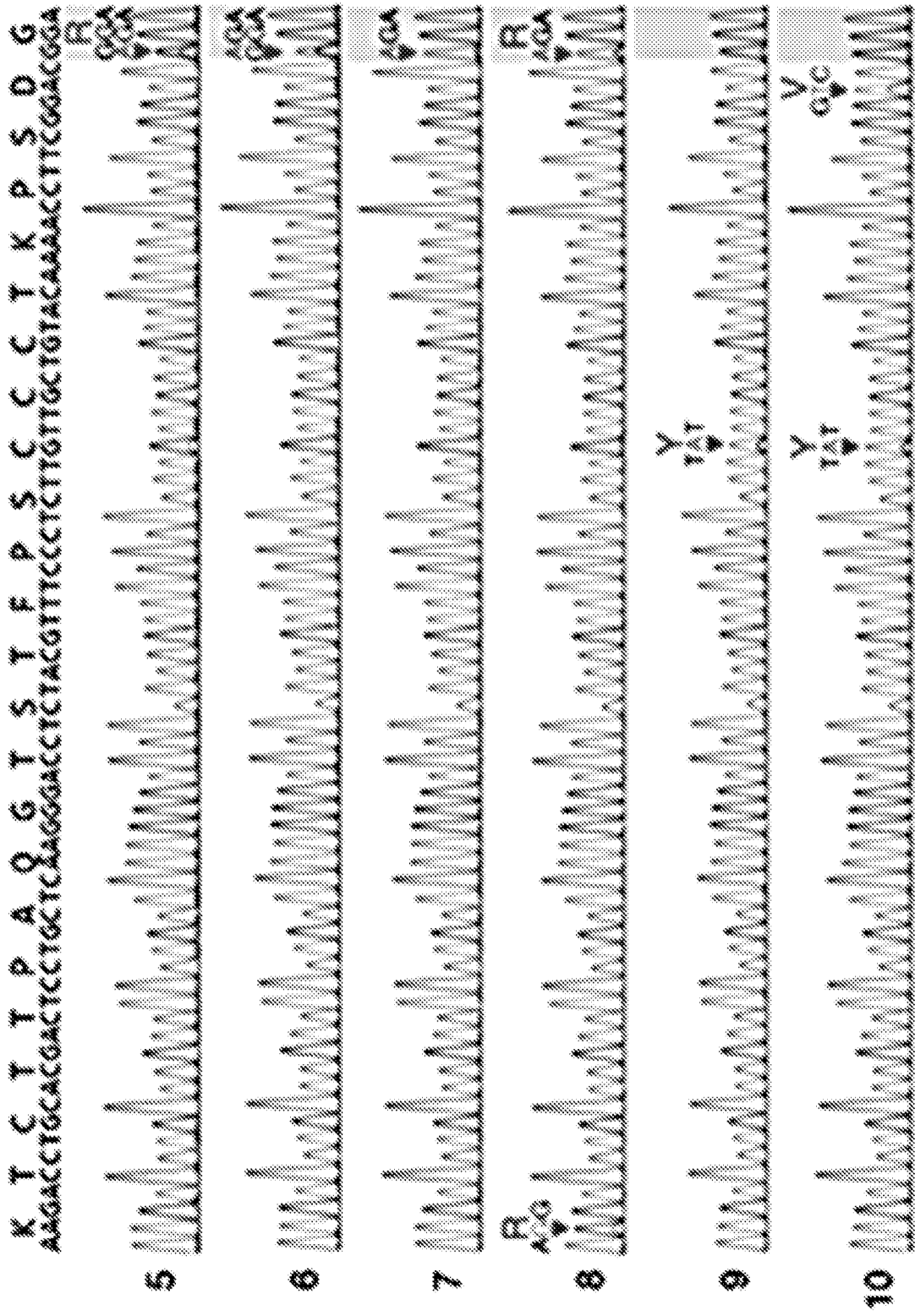


Fig. 14 (continued)

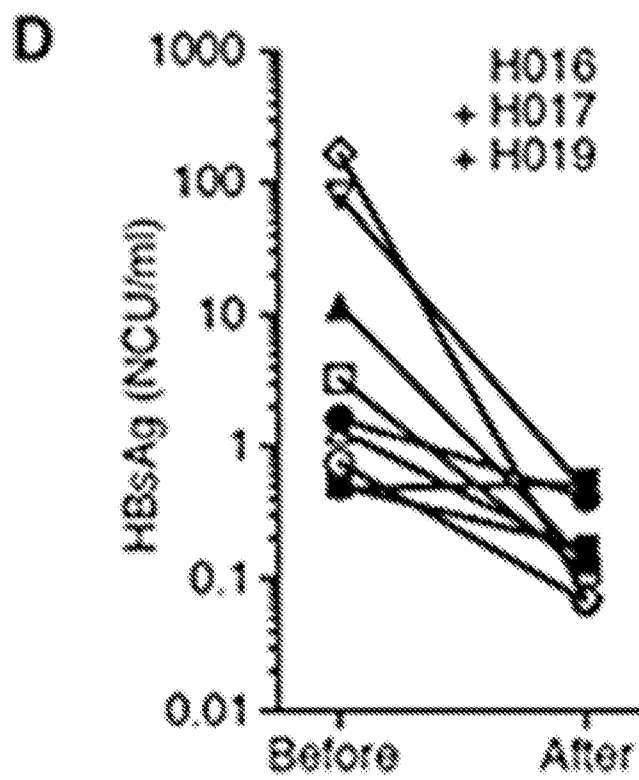
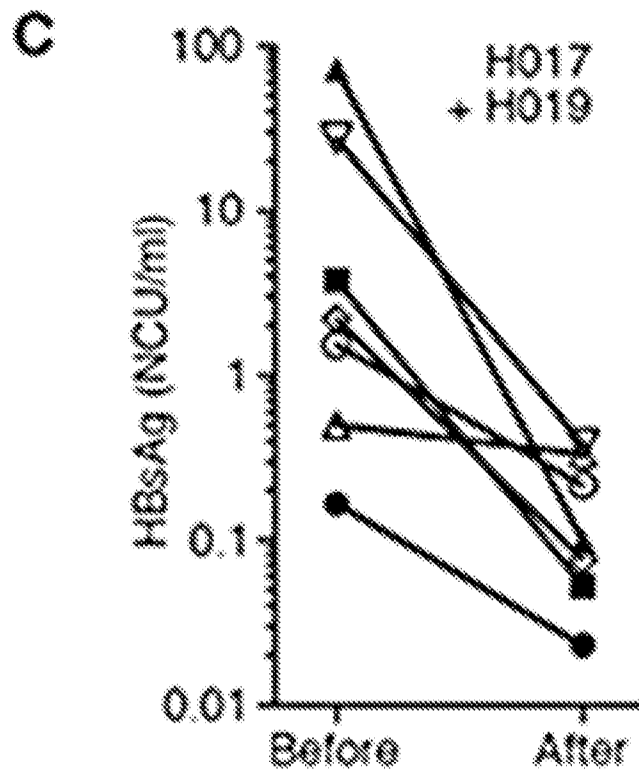


Fig. 14 (continued)