MPER ₍₈₆₂₋₈₆₃₎ MPER ₍₈₆₂₋₈₆₃₎ SAH-MPER ₍₆₆₂₋₈₆₃₎ (A) SAH-MPER ₍₆₆₂₋₈₆₃₎ (B)	ELDKWASLWNWFNITNWLWYIK ELDKWASLWNWFNITNWLWYIK XLDKXASLWNWFNITNWLWYIK	Biotin-PEG2- FITC-βAla-	3,467 3,385	1,157
MPER ₍₆₂₋₆₈₃₎ SAH-MPER ₍₆₆₂₋₆₈₃₎ (A) SAH-MPER ₍₆₆₂₋₆₈₃₎ (B)	ELDKWASLWNWFNITNWLWYIK XLDKXASLWNWFNITNWLWYIK	FITC-βAla-	3,385	1 1 2 0
SAH-MPER ₍₆₆₂₋₆₈₃₎ (A) SAH-MPER ₍₆₆₂₋₆₈₃₎ (B)	XLDKXASLWNWENITNWLWYIK		,	1,129
SAH-MPER ₍₆₆₂₋₆₈₃₎ (B)		FITC-βAla-	3,320	1,108
(002 000) · ·	EXDKWXSLWNWFNITNWLWYIK	FITC-βAla-	3,451	1,151
SAH-MPER(662, 683) (C)	ELXKWAXLWNWFNITNWLWYIK	FITC-βAla-	3,433	1,145
SAH-MPER (con con) (D)	ELDXWASXWNWFNITNWLWYIK	- FITC-βAla-	3.394	1.132
SAH-MPER	ELDKXASLXNWENITNWLWYIK	FITC-BAla-	3.263	1.089
SAH-MPER (E)		FITC-BAla-	3 450	1 151
SAH-MPER (G)		FITC-BAla-	3 335	1 113
SAH-MPER (H)		FITC-BAla-	3 409	1 137
SAH-MDER (1)		FITC-BAla-	3 3/8	1 117
SAL MEED (1)		EITC BAID	3 358	1,117
SAH-MDER (K)		FITC PAIA-	3 3 3 6	1 113
SAH MDED (L)		FITC PAIA-	2,000	1,110
SAH MDED (M)		FITC-pAla-	2,07	1 1 2 7
			3,407	1,137
SAH-MPER ₍₆₆₂₋₆₈₃₎ (N)	ELDKWASLWNWFNXINXLWYIK	FITC-BAIa-	3,336	1,113
SAH-MPER ₍₆₆₂₋₆₈₃₎ (O)	ELDKWASLWNWFNIXNWXWYIK	FITC-BAla-	3,421	1,141
SAH-MPER _(662–683) (P)	ELDKWASLWNWFNITXWLXYIK	FΠC-βAla-	3,335	1,113
SAH-MPER _(662–683) (Q)	ELDKWASLWNWFNITNXLWXIK	FITC-βAla-	3,286	1,096
SAH-MPER _(662–683) (R)	ELDKWASLWNWFNITNWXWYXK	FITC-βAla-	3,409	1,137
SAH-MPER ₍₆₆₂₋₆₈₃₎ (S)	ELDKWASLWNWFNITNWLXYIX	FITC-βAla-	3,321	1,108
			0.000	740
MPER _(671-683KKK)	NWFNITNWLWYIKKKK	Ac-	2,222	742
SAH-MPER _(671-683KKK) (Q)	NWFNITNXLWXIKKKK	Ac-	2,123	709
SAH-MPER _(671–683KKK) (q)	NWFNITNZLWXIKKKK	Ac-	2,095	699
SAH-MPER _(671–683KKK) (q)	NWFNITNZLWXIKKKK	Ac-	2,095	699
SAH-MPER _(671-683KKK) (q)pSer	NWFNITNZLWXI*KKK	Ac-	2,291	765
SAH-MPER _(662–683) (q)	ELDKWASLWNWFNITNZLWXIK	FITC-βAla-	3,258	1,087
SAH-MPER _(662–683) (A,q)	XLDKXASLWNWFNITNZLWXIK	FITC-βAla-	3,194	1,066
SAH-MPER ₍₆₆₂₋₆₈₃₎ (B,q)	EXDKWXSLWNWFNITNZLWXIK	FITC-βAla-	3,325	1,109
SAH-MPER ₍₆₆₂₋₆₈₃₎ (C,q)	ELXKWAXLWNWFNITNZLWXIK	FITC-βAla-	3,307	1,103
SAH-MPER ₍₆₆₂₋₆₈₃₎ (D,q)	ELDXWASXWNWFNITNZLWXIK	FITC-βAla-	3,268	1,090
SAH-MPER(662-683)(E,q)	ELDKXASLXNWFNITNZLWXIK	FITC-βAla-	3,136	1,046
MPER (SE2 SE3/ KK)	ELDKWASLWNWFNITNWLWYIKKKK	Ac-	3,351	1,118
SAH-MPER	ELDKWASLWNWFNITNZLWXIKKKK	Ac-	3,224	1,076
SAH-MPER	XLDKXASLWNWFNITNZLWXIKKKK	Ac-	3,159	1.054
SAH-MPER (B.g)	EXDKWXSLWNWENITNZLWXIKKKK	Ac-	3.290	1.098
SAH-MPER (C.g)	ELXKWAXLWNWENITNZLWXIKKKK	Ac-	3.272	1.092
SAH-MPER (D.g.)	ELDXWASXWNWENTTNZI WXTKKKK	Ac-	3 233	1 079
SAH-MPER (E g)		Ac-	3 102	1.035
(662–683KKK) (E, 9)		710	0,102	1,000
MPER _{(BBB656-683BBB})	RRRNEQELLELDKWASLWNWFDITNWLWYIRRRR	Biotin-PEG2-	5,161	1,721
MPER ₍₆₆₂₋₆₈₃₎	ELDKWASLWNWFNITNWLWYIK	FITC-βAla-	3,385	1,129
SAH-MPER ₍₆₆₂₋₆₈₃₎ (q)	ELDKWASLWNWFNITNZLWXIK	FITC-βAla-	3,258	1,087
SAH-MPER(662 683) (A,q)	XLDKXASLWNWFNITNZLWXIK	FITC-βAla-	3,194	1,066
SAH-MPER	EXDKWXSLWNWFNITNZLWXIK	FITC-βAla-	3,325	1,109
SAH-MPER (622 (623) (C,q)	ELXKWAXLWNWFNITNZLWXIK	FITC-βAla-	3,307	1,103
SAH-MPER	ELDXWASXWNWFNITNZLWXIK	FITC-BAla-	3.268	1.090
SAH-MPER	ELDKXASLXNWENITNZI WXTK	FITC-BAla-	3 136	1.046
SAH-MPER (B a)		Ac-	3 290	1 054
SAH-MPER _(662–683KKK) (D,q)	NWFNITNZLWXIKKKK	Ac-	2,095	699
MPER _(662-683KKK)	NWFNITNWLWYIKKKK	Ac-	2,222	742
SAH-MPER _(662-683KKK) (q)	NWFNITNZLWXIKKKK	Ac-	2,095	699
SAH-MPER _(662–683KKK) (q)pSer(*683)	NWFNITNZLWXI*KKK	Ac-	2,291	765
SAH-MPER _(662–683K*K) (q)pSer(*685)	NWFNITNZLWXIKK*K	Ac-	2,291	765
SAH-MPER(662-683KKK) (q)	ELDKWASLWNWFNITNZLWXIKKKK	Ac-	3,224	1,076
SAH-MPER (662-683KKK) (D,q)	ELDXWASXWNWFNITNZLWXIKKKK	Ac-	3,233	1,079
SAH-MPER	EXDKWXSLWNWFNITNZLWXIKKKK	Ac-	3,290	1,054
	SAH-MPER ₍₆₂₂₋₆₃₃)(G) SAH-MPER ₍₆₂₂₋₆₃₃)(G) SAH-MPER ₍₆₂₂₋₆₃₃)(J) SAH-MPER ₍₆₂₂₋₆₃₃)(J) SAH-MPER ₍₆₂₂₋₆₃₃)(J) SAH-MPER ₍₆₂₂₋₆₃₃)(J) SAH-MPER ₍₆₂₂₋₆₃₃)(J) SAH-MPER ₍₆₂₂₋₆₃₃)(J) SAH-MPER ₍₆₂₂₋₆₃₃)(D) SAH-MPER ₍₆₂₂₋₆₃₃)(D) SAH-MPER ₍₆₂₂₋₆₃₃)(C) SAH-MPER ₍₆₂₂₋₆₃₃)(R) SAH-MPER ₍₆₂₂₋₆₃₃)(R) SAH-MP	SAH-MPER (G) ELDKWASLWNVFXITNKLWYIK SAH-MPER (G) ELDKWASLWNVFXITNKLWYIK SAH-MPER (G) ELDKWASLWNVFNITNKWLYIK SAH-MPER (G) ELDKWASLWNVFNITNKLWYIK SAH-MPER (G) ELDKWASLWNVFNITNKLWYIK SAH-MPER (G) ELDKWASLWNVFNITNKLWYIK SAH-MPER (G) WFNITNKLWYIK SAH-MPER (G) WFNITNKLWYIK SAH-MPER (G) WFNITNKLWYIK SAH-MPER (G) WFNITNKLWYIKKK SAH-MPER (G) WFNITNKLWYIKKK SAH-MPER (G) ELDKWASLWNVFNITNKLWYIKKKK SAH-MPER (G) WFNITNKLWYIKKKK SAH-MPER (G) WFNITNKLWYIKKKK SAH-MPER (G) WFNITNKLWYIKKKK SAH-MPER (G) WFNITNKLWYI	SAH-MPER_matrix FIC-BAIL SAH-MPER_matrix FITC-BAIL SAH-MPER_matrix FITC-BAIL	SAH-MEER_matrix (F) ELDKASLUMPERTINKLYTIK FTC-GAIa- FTC-GAIA- 3.409 3.335 SAH-MEER_matrix (I) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.409 3.409 SAH-MEER_matrix (I) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.58 3.54 SAH-MEER_matrix (I) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.58 3.54 SAH-MEER_matrix (I) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.34 3.34 SAH-MEER_matrix (I) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.34 3.34 SAH-MEER_matrix (II) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.34 3.34 SAH-MEER_matrix (III) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.34 3.34 SAH-MEER_matrix (IIII) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.34 3.34 SAH-MEER_matrix (IIIIIIIIII) ELDKASLUMPERTNEWYTIK FTC-GAIA- 3.34 3.34 SAH-MEER_matrix (IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII

Supplementary Table 1. MPER Peptide Compositions

		RMSD* (Å)					
gp41 Residue Range		Cα	All Atoms ⁺				
668	683	2.4	3.3				
669	683	1.6	2.7				
670	683	0.6	1.8				
671	683	0.6	1.0				
672	683	0.5	1.0				

*Comparison of atoms in native and stapled peptide chains P. *Excluding atoms unique to S5 and R3.

Supplementary Table 2. C α and all atom RMSDs comparing SAH-MPER_(662-683KKK)(B,q) and MPER_(RRR656-683RRR) peptides for residue ranges between 668-683.

Α			10E8-SAH	-MPER (662	_{2-683ККК)} (В,q)	М	IPER (RRR656	5-683RRR)	
7 (ASA [‡]	BSA§	%	ASA [‡]	BSA§	%	
	Chain chain	Residue	(A ²)	(A ²)	BSA ^{ss}	(A ²)	(A ²)	BSA ^{ss}	_
	gp4 i	P.JER000	127	1	I	03 131	34 39		
		P:TRP670	233	36	Ш	137	10		
		P:ASN671	73	31	iim	73	32	iIII	
		P:TRP672	178	129		179	139		
		P:PHE673	163	85		148	93		
		P:ASP674	85 74			67			
		P:THR676	54	53		40	49		
		P:ASN677	123	11	I	99	19	II	
		P:R3 (678)				144			
		P:LEU679	127	56		108	50		
		P:1RP080 P:S5 (681)	169	00	11111	101	00		
		P:ILE 682	160	11	I	119	15	Ш	
		P:LYS 683	155	74	iuu	183	108	iim	
	10E8	H:ASN 31				86	17		
	Heavy	H:TRP 33	30	26		33	31		
	Chain	H:ARG 50	20	3		14	5 5		
		H:PRO 52B	65	1		70	30		
		H:GLY 52C	73	53	innn	74	60	iiiiiiIII	
		H:GLU 53	80	55		79	58		
		H:SER 56	52	6		53	7		
		H:ASP 30	00 115	3	1	111	40		
		H:TYR 98	121	43	1111	118	40	1111	
		H:TYR 99	111	78	imm	111	82	iuuu	
		H:PHE100A	151	78	11111	155	87		
		H:TRP100B	225	45	II	225	29		
		H:SER100C	94	1		93	6		
			23	11		26	17		
		H·PRO100E	82	56		88	64		
		H:PRO100G	140	69	1111	133	65		
		H:GLY 100H	91	1	I				
		H:GLU 100I	65	3	Ì	98	1		
		H:GLU 100J	151	78		57	6		_
		All Interactions w ‡ASA, Accessible §BSA, Buried Sur §§Bars represent Data shown are fo MPER _(RRR855-663RRR)	Surface Area, Å Surface Area, Å ² . buried area pero r Chain H, L, ar structure.	centage (100 x d P of the 10E	//www.ebi.ac.uk/msc : BSA/ASA), one bar :8-SAH-MPER (B,q)	per 10%. structure and cha	in/piserver). ins B, D, and F	of the	
R			10E	8-SAH-MF	PER (662-683KKK) ((B,q)	MPER	(RRR656-683)	RRR)
	Chain	Residue	Δ .S.Δ	‡ (Ų)	вбА ³ % (Å ²) ВС	o A A§§ A	ASA⁺ I (Ų)	LSA ³ (Å ²)	% BS4
	gp41	P:TRP67	2 17	8	6 I	1	79 [·]	12	1
	51	P:PHE67	316	3	52	1	48 5	52	İIII
	10E8	L:ARG 9	1 87		10	8	34	16	
	Light Ci	All interactions w +All interactions w +ASA, Accessible §BSA, Buried Sur	oB 22 ere performed w Surface Area, Å ace Area, Å ² . B	4 /ith PISA (http: /². ars represent b	46 //www.ebi.ac.uk/msc puried area percenta	d-srv/prot_int/cgi-b ige, one bar per 10	26 : in/piserver). 0%.	55	
		Sobars represent Data shown are for MPER	r Chain H, L, ar structure.	Id P of the 10E	8-SAH-MPER (656-683)	(B,q) structure	and chains A, B	8, and C of the	