

Table S3. Analysis of MHC-derived peptides from MoDCs.

AS1 [A2, 3; B8, 41; C7, 17] ^a												
Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 4.75%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance	RMSD (%) ^d	Abundance	RMSD (%)	n		
A2	98-108	MYGCDVGS DWR	673.27	673.27	2	2.00E+07	0.41%	1.42E+07	0.40%	7	9.09 ± 1.15	9.62 ± 0.83
A2	132-144	SWTAADMAAQ TTK	691.32	691.33	2	3.99E+07	0.68%	2.20E+07	0.35%	9	7.89 ± 2.07	
A2	316-341	KGGSYSQAASSDSAQGS DVS L TACKV	854.40	854.40	3	6.94E+06	0.29%	1.16E+07	0.17%	14	7.88 ± 2.08	
A iso	76-82	VDLG TLR	387.23	387.23	2	1.57E+08	0.61%	1.13E+08	1.55%	5	12.1 ± 0.85	
A iso	36-44	FSDAASQR	498.72	498.72	2	4.81E+06	0.43%	1.33E+06	0.48%	9	10.9 ± 2.41	
B41	36-44	FSDATSPR	498.23	498.23	2	2.09E+07	4.84%	6.05E+05	0.48%	10	10.6 ± 3.24	10.3 ± 0.86
B iso	49-62	APWIEQEGPEY WDR	888.41	888.40	2	6.19E+07	0.17%	4.88E+07	0.38%	15	12.8 ± 1.15	
B iso	220-239	DGEDQTQDEL VETRPAGDR	1116.50	1116.50	2	3.28E+06	0.37%	2.77E+06	0.76%	25	9.49 ± 1.61	
B iso	317-338	GGSYSQAACSDSAQGS DVS LTA	1059.95	1059.95	2	1.09E+07	0.46%	7.42E+06	0.27%	13	9.01 ± 1.24	

HD1 [A1, 2; B37, 49; Cw6, w7] ^a												
Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 4.93%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n		
A1	49-65	APWIEQEGPEY W DQETR	1067.48	1067.48	2	1.17E+07		2.25E+07	1.28%	20	5.78 ± 2.62	5.75 ± 1.00
A2	98-108	MYGCDVGS DWR	673.27	673.27	2	5.95E+06		1.82E+07	0.97%	5	6.17 ± 1.04	
A iso	22-35	FLAVGYVDDT QFVR	815.42	815.41	2	1.01E+08		1.42E+08	0.14%	7	5.23 ± 0.81	
B iso	49-62	APWIEQEGPEY WDR	888.41	888.40	2	9.29E+06		3.27E+07	0.94%	13	7.23 ± 2.06	
C iso	132-145	SWTAADTAAQITQR	760.38	760.38	2	2.25E+06		5.44E+06	1.10%	9	6.90 ± 2.43	

HD2 [A2, 32; B35, 60 (*40:01); Cw4, w10 (*03:04)] ^a												
Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 4.98%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n		
A2	132-144	SWTAADM[ox]AAQ TTK	699.32	699.33	2	2.49E+06		2.07E+06	0.92%	8	6.35 ± 1.11	6.37 ± 0.46
A32	49-65	APWIEQEGPEY W DQETR	1067.48	1067.48	2	4.68E+06		4.36E+06	0.58%	17	5.50 ± 0.84	
A32	112-131	GYQDAYDGDYIALNEDLR	783.03	783.04	3	2.16E+07		1.11E+07	0.45%	21	7.51 ± 0.11	
B35	98-108	MYGCDLGP DGR	620.76	620.76	2	9.54E+06		1.00E+07	0.41%	7	17.5 ± 1.12	
B60	132-145	SWTAADTAAQISQR	753.37	753.37	2	1.89E+07		5.10E+06	0.37%	11	11.1 ± 2.13	

HD3 [A2, 24; B27, 51; C14, 15] ^a												
Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 4.16%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n		
A iso	158-169	AYLEGT CVDGLR	677.33	677.33	2	7.75E+06		5.60E+06	0.69%	8	5.89 ± 2.21	5.89 ± 2.21
B iso	49-62	APWIEQEGPEY WDR	888.41	888.40	2	8.21E+06		1.62E+07	0.28%	15	6.24 ± 1.69	6.24 ± 1.69

HD4 [A3, 24; B7, 27; Cw2, w7] ^a												
Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 5.08%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n		
A3	316-341	KGGSYTQAASSDSAQGS DVS L TACKV	859.07	859.08	3	1.10E+07		2.53E+06	0.21%	10	8.47 ± 1.61	7.80 ± 0.65
A3	158-169	AYLDGTCV E WLR	741.86	741.86	2	4.11E+07		6.52E+06	0.48%	8	5.61 ± 0.86	
A3	132-144	SWTAADMAAQITK	697.34	697.34	2	2.96E+07		4.96E+06	0.32%	7	7.43 ± 1.49	
A3	132-144	SWTAADM[ox]AAQITK	705.34	705.34	2	2.36E+07		3.62E+06	0.74%	8	6.01 ± 1.85	
A3	115-131	QDAYDGDYIALNEDLR	666.99	666.99	3	6.15E+07		1.02E+07	0.30%	17	7.19 ± 1.00	
A3	49-65	APWIEQEGPEY W DQETR	1067.48	1067.48	2	1.30E+07		3.45E+06	0.28%	17	6.35 ± 1.18	
A24	158-169	AYLEGT CVDGLR	677.33	677.33	2	2.91E+07		6.56E+06	0.19%	7	12.3 ± 2.27	
A iso	22-35	FLAVGYVDDT QFVR	815.42	815.42	2	8.99E+07		3.76E+07	0.60%	7	11.1 ± 2.30	
B7	112-131	GHDQYAYDGDYIALNEDLR	786.03	786.03	3	3.42E+07		3.49E+06	0.49%	16	13.6 ± 2.82	

B iso	49-62	APWIEQEGPEYWDR	888.41	888.40	2	1.16E+08	4.09E+07	0.40%	13	11.2 ± 1.53	12.9 ± 1.53
-------	-------	----------------	--------	--------	---	----------	----------	-------	----	-------------	-------------

HD4 [A3, 24; B7, 27; Cw2, w7] ^a (LPS-stimulated)

Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 5.02%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n		
A3	316-341	KGGSYTQAASDSAQGSVDVSLTACKV	859.07	859.08	3	1.08E+07		6.07E+07	0.53%	10	4.41 ± 3.22	4.20 ± 0.99
A3	158-169	AYLDGTCVEWLR	741.86	741.86	2	4.11E+07		1.73E+08	0.58%	6	2.95 ± 3.53	
A3	132-144	SWTAADM[ox]AAQITK	705.34	705.34	2	2.34E+07		6.59E+07	0.74%	7	2.94 ± 4.67	
A3	115-131	QDAYDGKDYIALNEDLR	666.99	666.99	3	5.75E+07		1.89E+08	0.50%	15	4.55 ± 1.43	
A3	49-65	APWIEQEGPEYWDQETR	1067.48	1067.48	2	1.79E+07		1.31E+08	0.53%	16	3.91 ± 2.18	
A24	158-169	AYLEGTCDVGLR	677.33	677.33	2	2.90E+07		1.55E+08	0.30%	7	5.75 ± 7.69	
A24	316-341	KGGSYSQAASDSAQGSVDVSLTACKV	854.40	854.40	3	4.25E+06		4.93E+07	0.45%	11	6.02 ± 3.36	
A iso	22-35	FLAVGYVDDTQFVR	815.42	815.42	2	8.90E+07		6.20E+08	0.26%	6	4.45 ± 2.34	
B27	22-35	FLTVGYVDDTLFVR	822.94	822.93	2	7.40E+07		6.21E+08	0.08%	5	4.95 ± 4.83	4.91 ± 2.06
B iso	49-62	APWIEQEGPEYWDR	888.41	888.40	2	1.16E+08		1.04E+09	0.13%	12	4.86 ± 1.58	

HD5 [A2, 11; B27, 60 (*40:01); Cw1, w10 (*03:02)] ^a

Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 4.78%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n		
A2	49-65	APWIEQEGPEYWDQETR	688.31	688.31	3	8.29E+06		5.61E+06	0.43%	17	13.9 ± 1.68	9.51 ± 0.78
A2	244-256	WAARVVVPSGQEQQR	713.88	713.88	2	4.63E+07		9.79E+06	0.53%	6	9.39 ± 1.85	
A2	132-144	SWTAADMAAQTTK	699.32	699.32	2	4.61E+06		2.45E+06	0.40%	7	7.01 ± 1.30	
A11	49-65	APWIEQEGPEYWDQETR	1067.48	1067.48	2	1.12E+07		2.88E+06	0.53%	16	6.92 ± 0.61	
A11	115-131	QDAYDGKDYIALNEDLR	666.99	666.98	3	2.74E+07		7.15E+06	0.36%	18	9.62 ± 2.30	
A iso	220-243	DGEDQTQDTELVEVTRPAGDGTQK	879.74	879.74	3	8.02E+07		4.20E+07	0.21%	22	14.3 ± 2.59	12.1 ± 1.51
B40	132-145	SWTAADTAAQISQR (3+)	502.58	502.58	3	2.61E+07		4.77E+06	0.34%	10	10.3 ± 2.79	
B40	132-145	SWTAADTAAQISQR (2+)	753.37	753.37	2	4.99E+07		6.05E+06	0.26%	9	11.9 ± 2.90	
B iso	220-239	DGEDQTQDTELVEVTRPAGDR	744.67	744.67	3	1.49E+08		4.51E+07	0.32%	23	14.0 ± 1.99	
Cw1	112-131	GYDQYAYDGKDYIALNEDLR	794.70	794.73	3	6.15E+07		4.51E+06	0.55%	18	25.9 ± 7.26	23.7 ± 2.72
C iso	132-145	SWTAADTAAQITQR	760.38	760.38	2	2.15E+07		3.08E+06	0.59%	9	25.4 ± 4.98	
C iso	318-341	GGSCSQAASNSAQQSDESLIACK	791.34	791.34	3	4.87E+06		7.93E+05	0.40%	14	15.6 ± 4.71	
C iso	257-273	YTCHVQHGLPEPLTLR (3+)	684.01	684.01	3	8.83E+06		2.78E+06	0.84%	10	34.8 ± 5.85	
C iso	257-273	YTCHVQHGLPEPLTLR (4+)	513.26	513.26	4	4.50E+06		6.47E+06	0.35%	9	20.7 ± 6.35	

HD6 [A1, 24; B8, 27; Cw2, Cw7] ^a

Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 5.11%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n		
A1	115-131	QDAYDGKDYIALNEDLR	666.99	666.99	3	7.36E+07		4.98E+07	0.34%	20	7.23 ± 0.29	10.7 ± 1.26
A24	36-44	FSDAASQR	498.72	498.72	2	5.96E+07		1.32E+07	0.39%	10	10.9 ± 4.33	
A24	49-66	APWIEQEGPEYWDDEETGK	1082.48	1082.479	2	2.33E+07		1.42E+07	0.55%	21	14.4 ± 2.97	
A24	316-341	KGGSYSQAASDSAQGSVDVSLTACKV	854.40	854.40	3	8.91E+06		3.60E+07	0.60%	17	8.14 ± 2.98	
A iso	22-35	FLAVGYVDDTQFVR	815.42	815.42	2	1.91E+08		1.94E+08	0.23%	9	13.6 ± 4.12	
A iso	220-243	DGEDQTQDTELVEVTRPAGDGTQK	879.74	879.74	3	2.08E+08		2.49E+08	0.42%	26	12.6 ± 2.49	
B8	7-17	YFDTAM[ox]SRPGR	658.81	658.81	2	9.63E+06		4.20E+06	0.38%	12	9.79 ± 2.30	13.1 ± 1.26
B8	171-181	YLENGKDTLRLR	669.34	669.34	2	4.81E+07		6.29E+06	0.71%	9	20.2 ± 5.03	
B8	112-131	GHNQYAYDGKDYIALNEDLR	785.71	785.71	3	3.67E+07		3.92E+07	0.38%	16	10.7 ± 2.06	
B27	22-35	FLTVGYVDDTLFVR	822.94	822.94	2	1.72E+08		1.22E+08	0.43%	8	18.3 ± 6.48	
B iso	49-62	APWIEQEGPEYWDR	592.61	592.61	3	7.65E+06		7.26E+06	0.88%	15	9.46 ± 1.70	
B iso	220-239	DGEDQTQDTELVEVTRPAGDR	744.67	744.68	3	3.29E+08		2.40E+08	0.23%	25	14.1 ± 2.98	

HD7 [A24, 30; B13, 27; Cw2, w6] ^a

						Unlabeled	72 h labeled (p = 4.76%) ^e				
--	--	--	--	--	--	-----------	---------------------------------------	--	--	--	--

Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Abundance ^g	RMSD (%) ^d	Abundance	RMSD (%)	n	k (%/h) ^f	k _{iso} (%/h)
A iso	36-44	FSDSAASQR	498.72	498.73	2	6.29E+07		2.62E+06	0.59%	8	12.4 ± 3.02	14.4 ± 1.93
A iso	220-243	DGEDTQDTELVETRPAGDGTFOK	879.74	879.75	3	5.00E+07		1.70E+08	0.46%	23	16.4 ± 2.86	
B13	22-35	FITVGYVDDTQFVR	830.42	830.43	2	7.61E+07		1.28E+08	0.24%	7	11.9 ± 1.22	11.5 ± 1.32
B27	22-35	FITVGYVDDTLFVR	822.94	822.95	2	5.64E+07		6.79E+07	0.36%	7	12.4 ± 0.60	
B iso	49-62	APWIEQEGPEYWR	888.41	888.42	2	9.30E+07		2.66E+07	0.29%	13	13.3 ± 3.55	
B iso	220-239	DGEDTQDTELVETRPAGDR	1116.50	1116.52	2	2.92E+07		9.29E+06	0.57%	22	7.99 ± 2.69	

HD8 [A2, A2, B15, B35, C10 (*0302), C4] ^a												
Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 4.96%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance	RMSD (%) ^d	Abundance	RMSD (%)	n		
A2	317-340	GGSYSQAASSDSAQGSVDVSLTACK	1167.51	1167.52	2	2.46E+06	1.61%	4.37E+06	0.28%	14	9.00 ± 6.29	11.0 ± 1.80
A2	220-243	DGEDTQDTELVETRPAGDGTFOK	879.74	879.74	3	1.40E+08	0.06%	1.16E+09	0.63%	21	12.7 ± 2.82	
B15	152-157	EAEQWR	409.69	409.70	2	1.27E+07	1.82%	2.88E+08	0.50%	7	11.7 ± 4.02	14.3 ± 1.46
B iso	49-62	APWIEQEGPEYWR	888.41	888.41	2	1.98E+08	0.17%	3.25E+09	0.56%	12	14.3 ± 2.14	
B iso	317-338	GGSYSQAASSDSAQGSVDVSLTA	1023.45	1023.46	2	4.59E+07	4.20%	5.75E+08	0.55%	13	18.2 ± 1.30	
B iso	220-239	DGEDTQDTELVETRPAGDR	744.67	744.68	3	2.51E+08	0.16%	6.03E+09	0.83%	19	14.2 ± 2.61	
C10	18-35	GEPHFIAVGYVDDTQFVR	684.01	684.01	3	1.40E+07	1.39%	1.62E+08	0.14%	13	14.9 ± 5.31	15.9 ± 2.52
C iso	122-131	DYIALNEDLR	611.31	611.31	2	4.31E+06	2.11%	3.06E+07	0.31%	12	15.6 ± 5.43	
C iso	132-145	SWTAADTAAQITQR	760.38	760.38	2	1.44E+07	0.31%	1.72E+08	0.17%	13	15.2 ± 1.56	
C iso	256-273	YTCHVQHEGLPEPLTLR	684.01	684.01	3	5.19E+06	1.41%	8.48E+07	0.40%	12	18.8 ± 12.3	

HD8 [A2, A2, B15, B35, C10 (*0302), C4] ^a (LPS stimulated)												
Molecule	Residues	Sequence ^b	m/z (pred) ^c	m/z (obs)	z	Unlabeled		72 h labeled (p = 4.65%) ^e			k (%/h) ^f	k _{iso} (%/h)
						Abundance	RMSD (%) ^d	Abundance	RMSD (%)	n		
A2	49-65	APWIEQEGPEYWDGETR	1031.96	1031.97	2	1.92E+08	0.67%	6.55E+07	0.81%	9	6.87 ± 0.65	(5.18 ± 0.88)
A2	220-243	DGEDTQDTELVETRPAGDGTFOK	879.74	879.74	3	8.20E+08	0.11%	5.61E+07	0.50%	28	3.58 ± 0.60	(p = 0.031)
B15	152-157	EAEQWR	409.69	409.70	2	1.62E+08	0.75%	6.77E+06	0.39%	8	4.15 ± 0.69	4.49 ± 0.90
B35	98-108	MYGCDLGPDGR	620.76	620.76	2	5.16E+07	2.11%	1.01E+07	0.86%	6	4.54 ± 4.43	
B iso	49-62	APWIEQEGPEYWR	888.41	888.41	2	1.58E+09	0.08%	1.43E+08	0.41%	15	4.65 ± 0.83	
B iso	220-239	DGEDTQDTELVETRPAGDR	744.67	744.68	3	2.05E+09	0.18%	1.13E+08	0.78%	24	4.64 ± 0.75	
C10	18-35	GEPHFIAVGYVDDTQFVR	684.01	684.01	3	9.59E+07	1.54%	9.69E+06	1.00%	12	8.54 ± 1.09	9.06 ± 0.72
C iso	122-131	DYIALNEDLR	611.31	611.31	2	5.40E+07	1.05%	4.33E+06	0.88%	13	10.1 ± 1.65	
C iso	132-145	SWTAADTAAQITQR	760.38	760.38	2	1.13E+08	0.48%	9.41E+06	0.16%	15	8.58 ± 1.48	

- Notes:**
- ^a HLA types: given as serotypes (numerically equivalent to 2-digit genotypes except where noted in parentheses, in *italics*).
- By default, the 4-digit subtypes most prevalent in Caucasians were used for alignments (usually *xx:01). B27 was assumed to be B*27:05.
- ^b All peptides used for kinetic analysis are shown (single-letter code). Residue numbering is based on the mature protein sequence, with signal sequence cleavage as per the IMGT/HLA database.
- ^c m/z: mass to charge ratio, predicted from monoisotopic elemental masses or observed in Orbitrap mass spectra as indicated. Abundances were summed over all mass isotopomers used in the analysis.
- ^d RMSD, root mean square deviation of observed mass isotopomer distributions, as compared with MIDA models.
- ^e "p" represents measured 2H₂O enrichment in media. "n", number of labeling sites that yields best fit to MIDA models at this enrichment.
- ^f "k" represents fractional synthesis rates (% per hour, mean ± SE) based on single-exponential curve fit to data. "k_{iso}" represents pooled data for isotypes shown in Figs 5-8. Where k_{iso} values are shown in parentheses, the k values for individual peptides were significantly different (p value shown, F test).
- ^g Abundances in *italics* / RMSD blank: some unlabeled sample data acquired at 30,000 resolution, resulting in bias (R.B. et al., unpublished data). Where abundances are in plain font reported and RMSD values are given, mass spectra were acquired at 7,500 resolution. For consistency, fractional synthesis rates for all MoDC samples were calculated using the unlabeled MIDA model for baseline subtraction. (Where available, baseline subtraction using unlabeled data acquired at 7,500 resolution yielded similar results.)