

Table S1A. Theoretical tryptic peptides of anti-CD11a mAb without reduction, including linked disulfides (lines), cysteine position (parentheses), and molecular weight.

Tryptic peptides in heavy chain			
T2	20-38	LSCAASGYSFTGHWMNWVR (Cys 22)	MW= 3430.5115
T11	88-98	AEDTAVYYCAR (Cys 96)	
T14	138-151	STSGGTAALGCLVK (Cys 148)	MW= 7916.9351
T15	152-214	DYFPEPVTVSWNSGALTSGVHTFPAVLQSSGLYSLSSVV TVPSSSLGTQTYICNVNHKPSNTK (Cys 204)	
T19	227-252	THTCPPCPAPELLGGPSVFLFPPKPK (Cys 230; Cys 233)	MW= 5454.8148
T19	227-252	THTCPPCPAPELLGGPSVFLFPPKPK (Cys 230; Cys 233)	
T21	260-278	TPEVTCVVVDVSHEDPEVK (Cys 265)	MW= 2328.1135
T27	325-326	CK (Cys 324)	
T35	365-374	NQVSLTGLVK (Cys 371)	MW= 3844.8393
T40	421-443	WQQGNVFSCSVMHEALHNHYTQK (Cys 428)	
Tryptic peptides in light chain			
T2	19-24	VTITCR (Cys 23)	MW= 5311.4548
		FSGSGSGTDFTLTISLQPEDFATYYCQQHNEYPLTFGQ	
T7	62-103	GTK (Cys 88)	
T10	127-142	SGTASVVCLLNNFYPR (Cys 134)	MW= 3555.7647
T17	191-207	VYACEVTHQGLSSPVTK (Cys 194)	
Tryptic peptide between heavy and light chain			
T18(H)	223-226	SCDK (Cys 224 from H chain)	MW= 912.3587
T19(L)	212-214	GEC (Cys 214 from L chain)	
Lys-C digested peptide between heavy and light chain			
T18(H)	223-226	SCDK (Cys 224 from H chain)	MW= 1260.5021
T18T19(L)	208-214	SFNRGEC (Cys 214 from L chain)	

Table S1B. The assignment of different chain combinations along with their corresponding disulfide linkages and major scrambled disulfides in the gel bands from the time point at 35 min of Figure 7A.

Band #	Chain combination ^a	Disulfides	Observed m/z (charge)	Highest intensity	Retention time (min)
A2	1L	T17 (L) with T18T19 (L) ^b	658.33 (4+)	6.63E+05	29.55
		T2 (L) with T17 (L)	628.42 (4+)	1.84E+05	32.54
A1d	1H	T11 (H) with T14 (H)	842.25 (3+)	2.06E+05	33.62
		Intra disulfide in T19 (H)	683.33 (4+)	2.95E+05	43.69
A1c	1 H with 1L	T18T19 (L) ^b with T18T19 (H) ^c	795.81 (5+)	1.01E+05	40.69
		Intra disulfide in T19 (H)	683.58 (4+)	2.75E+05	44.01
A1b	2H	T18T19 (H) ^c with T18T19 (H) ^c	791.97 (8+)	1.41E+05	41.04
A1a	2H with 1L	T11 (H) with T14 (H)	842.25 (3+)	3.43E+05	33.37
		T18T19 (L) ^b with T18T19 (H) ^c	795.81 (5+)	2.76E+04	32.46
		Intra disulfide in T19 (H)	683.58 (4+)	9.04E+04	43.35
A1	2H with 2L	T18 (H) with T18T19 (L) ^b	631.87 (2+)	4.43E+05	30.27
		T19 (H) with T19 (H)	781.29 (7+)	8.58E+04	43.34

a, b, and c: the same footnotes as in Table 3.

Table S2A. Theoretical tryptic peptides of CNTO736 mAb without reduction, including linked disulfides (lines), cysteine position (parentheses), and molecular weight.

Tryptic peptides in heavy chain			
T5	50-76	YGPPCPPCPAPEAAGGPSVFLFPPKPK (Cys 54; Cys 57)	MW= 5436.6991
T5	50-76	YGPPCPPCPAPEAAGGPSVFLFPPKPK (Cys 54; Cys 57)	
T7	84-116	PEVTCVVVDVSQEDPEVQFNWYVDGVEVHNAK(Cys 89)	MW= 3977.8609
T12	149-150	CK (Cys 149)	
T19	189-198	NQVSLTCLVK (Cys 195)	MW= 3845.8233
T24	245-267	WQEGNVFSCSVMHEALHNHYTQK(Cys 253)	

Table S2B. Assignment of major scrambled disulfides of CNTO 736 mAb in the gel band 2 from the time point at 35 min of Figure 7B.

	Observed m/z (charge)	Highest intensity	Retention Time (min)
T12 with T19	451.67 (3+)	4.20E+05	29.80
T12 with T24	599.83 (5+)	3.08E+04	35.13
T7 with T19	968.25 (5+)	1.02E+05	51.98
T5 with T24	912.42 (6+)	2.49E+05	45.56
Intra disulfide in T5	907.83 (3+)	6.01E+06	44.49