

VOLUME 288 (2013) PAGES 27059–27067

DOI 10.1074/jbc.A113.491530

Comparison of the inhibition mechanisms of Adalimumab and Infliximab in treating tumor necrosis factor α -associated diseases from a molecular view.

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The interactions between TNF α and the Adalimumab Fab listed in Table 2 and the references to these data in the text were incorrect. The corrected Table 2 and references to these data are provided.

PAGE 27062:

In the left column, the second sentence of the last paragraph should be as follows. “The Adalimumab epitope on TNF α is composed of a number of discontinuous segments, including residues ^{TNF}Pro-20, ^{TNF}Gln-21, ^{TNF}Glu-23, ^{TNF}Lys-65 to ^{TNF}Gln-67, ^{TNF}Glu-110 to ^{TNF}Pro-113, ^{TNF}Tyr-141, and ^{TNF}Ala-145, to ^{TNF}Glu-146 and ^{TNF}Thr-72, ^{TNF}His-73, ^{TNF}Thr-77, ^{TNF}Thr-79, ^{TNF}Ser-81, ^{TNF}Lys-90 to ^{TNF}Asn-92, and ^{TNF}Glu-135 to ^{TNF}Asn-137 of an adjacent TNF α protomer (Figs. 3 and 4).”

PAGE 27063:

In the right column, “^{TNF}Lys-72” in line four of the last paragraph should be “^{TNF}Thr-72.”

PAGE 27064:

In the left column, “^{TNF}Pro-21” in the first line of the last paragraph should be “^{TNF}Pro-20.”

These corrections do not affect the interpretation of the results or the conclusions of this work.

Authors are urged to introduce these corrections into any reprints they distribute. Secondary (abstract) services are urged to carry notice of these corrections as prominently as they carried the original abstracts.

TABLE 2
Complete list of interactions between TNF α and Adalimumab Fab (≤ 3.65 Å)

TNF α		Adalimumab Fab			Distance
Residue	Atom	Residue	Atom	CDR loop	
					Å
Pro-20	O	Arg-93 _L	N ^ε	L3	3.25
	O		C ^δ		3.58
Gln-21	N ^{ε2}	Asp-1 _L	O ^{δ1}		2.77
	N ^{ε2}		C ^{γ1}		3.41
	C ^δ		O ^{δ1}		3.33
	C ^δ		O ^{δ2}		3.35
	C ^δ		O ^{δ1}		3.33
	C ^γ		O ^{δ1}		3.59
Glu-23	O ^{ε1}	Arg-93 _L	N ^{θ1}	L3	3.20
	O ^{ε1}	Gln-27 _L	O ^{ε1}	L1	3.00
	O ^{ε1}	Asp-1 _L	O ^{δ2}	L1	3.26
	C ^δ	Gln-27 _L	O ^{ε1}	L1	3.29
	C ^δ	Arg-93 _L	N ^{θ1}	L3	3.18
	C ^γ	Arg-93 _L	N ^{θ1}	L3	3.18
	C ^γ	Gln-27 _L	O ^{ε1}	L1	3.26
Lys-65	O	Arg-30 _L	N ^{θ2}	L1	2.36
	O	Arg-30 _L	C ^ε	L1	3.47
	C	Arg-30 _L	N ^{θ2}	L1	3.35
	C ^γ	Tyr-32 _L	OH	L1	3.32
	C ^δ	Tyr-32 _L	OH	L1	3.74
	C ^ε	Asn-92 _L	O	L3	3.44
	N ^ε	Asn-92 _L	O	L3	2.64
Gly-66	N	Tyr-32 _L	OH	L1	3.27
	C ^α		OH	L1	3.22
	C		OH	L1	3.42
Gln-67	N ^{ε2}	Asn-31 _L	O ^{δ1}	L1	3.10
	N ^{ε2}		O	L1	2.87
	N ^{ε2}		C ^γ	L1	3.52
	N ^{ε2}		C	L1	3.37
	N ^{ε2}		C ^α	L2	3.60
	O		N ^δ	L1	3.23
Thr-72	C ^{γ2}	Tyr-101 _H	OH	H3	3.66
His-73	C ^β	Tyr-101 _H	C ^{ε1}	H3	3.65
Thr-77	C ^{γ2}	Trp-53 _H	N ^{ε1}	H2	3.53
	C ^{γ2}		C ^{ε2}	H2	3.66
Thr-79	O ^{γ1}	Asn-54 _H	N ^{δ2}	H2	3.11
Ser-81	O ^γ	Asn-54 _H	N ^{δ2}	H2	3.54
Lys-90	O	Ser-55 _H	O	H2	3.63
	C ^ε	Asn-54 _H	O	H2	3.01
	N ^ε	Asn-54 _H	O	H2	3.10
Val-91	C ^α	Gly-56 _H	O	H2	3.49
	C ^{γ1}		O	H2	3.64
Asn-92	N	Gly-56 _H	O	H2	3.02
	C ^γ	Gly-56 _H	C ^α	H2	3.64
	N ^{δ2}	Gly-56 _H	C ^α	H2	3.49
	O ^{δ1}	Asn-54 _H	N ^{δ2}	H2	3.47
	O ^{δ1}	Asn-54 _H	O ^{δ1}	H2	3.63
Glu-110	C ^α	Thr-53 _L	O ^{γ1}	L2	3.52
Ala-111	N	Thr-53 _L	O ^{γ1}	L2	2.97
Pro-113	C ^γ	Tyr-101 _H	C ^{δ2}	H3	3.57
Tyr-115	OH	Ser-103 _H	C ^β	H3	3.56
Glu-135	O ^{ε1}	Asn-54 _H	N ^{δ2}	H2	2.98
Ile-136	C	Trp-53 _H	C ^{θ2}	H2	3.41
	O		C ^{θ2}	H2	3.53
Asn-137	O	Asp-31 _H	O ^{δ1}	H1	3.41
	N	Trp-53 _H	C ^{θ2}	H2	3.58
Arg-138	C ^δ	Asp-31 _H	O ^{δ2}	H1	3.38
Asp-140	O	Arg-30 _L	C ^δ	L1	3.30
	O		N ^ε	L1	3.13
	O		C ^ε	L1	3.51
Tyr-141	C ^{ε2}	Arg-30 _L	N ^{θ1}	L1	3.61
	C ^{δ2}		N ^{θ1}	L1	3.45
	C ^γ		N ^{θ1}	L1	3.59
	C ^α		N ^{θ2}	L1	3.67
Ala-145	O	His-57 _H	N ^{ε2}	H2	3.00
	O	His-57 _H	C ^{δ2}	H2	3.60
	O	Asp-59 _H	O ^{δ2}	H2	3.13
	C ^β	Ala-105 _H	C ^β	H3	3.55
Glu-146	O ^{ε1}	Ser-103 _H	O ^γ	H3	2.59
	O ^{ε1}	Ser-103 _H	C ^β	H3	3.37
	O ^{ε1}	Ser-103 _H	C ^α	H3	3.50
	O ^{ε1}	Thr-104 _H	N	H3	3.51
	C ^γ	Thr-104 _H	O ^{γ1}	H2	3.64