Supplementary Materials: Loxoscelism: Advances and Challenges in the Design of Antibody Fragments with Therapeutic Potential

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Table S1. Hydrogen Bonds between the amino acid residues of the antibodies and Lid1.

Antibody	Antibody Domain	Amino Acids		Described Hotspots of Relevance in Ag	Distances (Å)
		Antibody(Ab)	Antigen (Ag)		
LimAb7	H:CDR1	Ser31	Lys59	Felicori et al; 2006	2.68
	H:CDR2	Tyr52	Asn56	Murakami et al; 2005	2.87
	H:CDR2	Tyr52	Lys58	Felicori et al; 2006	2.84
	H:CDR2	Asp55	Lys58	Felicori et al; 2006	2.41
	H:CDR3	Tyr103	Gly18		2.73
	H:CDR3	Tyr103	Lys59		2.69
	H:CDR3	Tyr106	Arg55	Murakami et al; 2005	3.03
	H:CDR3	Tyr107	Gly54	Murakami et al; 2005	2.74
	L:CDR2	Val33	Lys234	De Moura et al; 2011	2.66
	L:CDR2	Asn34	Arg235	De Moura et al; 2011	3.29
	L:CDR2	Asn34	Asp233	De Moura et al; 2011	3.01
	L:CDR2	Glu35	Arg235		3.02
	L:CDR2	Glu35	Ser236		3.00
	L:CDR2	Asn36	Arg235		2.61
scFv$_{15}$hLi7	H:CDR1	Ser31	Lys59	Felicori et al; 2006	2.58
	H:CDR1	Asp55	Asn56	Murakami et al; 2005	3.08
	H:CDR2	Asp55	Lys58	Felicori et al; 2006	2.77
	H:CDR2	Tyr101	Arg55		2.84
	H:CDR2	Tyr103	Asp21		2.91
	H:CDR2	Lys105	Asp21	Felicori et al; 2009	2.72
	H:CDR2	Lys105	Asp25	Felicori et al; 2009	2.56
	H:CDR2	Tyr106	Glu22		2.91
	H:CDR2	Tyr106	Arg55	Murakami et al; 2005	2.79
	H:CDR3	Tyr107	Asp255		2.85
	H:CDR3	Tyr108	Asp255		2.81
	L:CDR2	Val33	Lys234	De Moura et al; 2011	2.74
	L:CDR2	Asn34	Arg235	De Moura et al; 2011	2.92
	L:CDR2	Glu35	Arg235		2.85
	L:CDR2	Glu35	Arg235		3.02
	L:CDR2	Glu35	Ser236		2.95
	L:CDR2	Asn36	Arg235		2.87
	L:CDR2	Asn36	Arg235		2.90
	L:CDR2	Asn36	Asp255		2.77
	L:CDR2	Asn37	Arg235		2.74

Table S2. In silico modelling data.

Antibodies	Template (PDB:chain)	% Identity	Resolution (Å)	RMSD (Å)
LimAb7	5YD3_A	59%	1.35	0.871
scFv$_{15}$hLi7	5YD3_A	61.5%	1.35	0.659