SUPPLEMENTARY DATA

Molecular interactions of Bcl-2 and Bcl-xL with mortalin: identification and functional characterization

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Table S1 Predicted amino acid residues of proteins that participate in docking

Mortalin	Bcl-2	Bcl-xL
320–400	12–29, 87-103, 113–119, 215–last	8–21, 135–149, 145–170, 216–last

Table S2 List of functional residues at the interface of mortalin, Bcl-2 and Bcl-xL proteins

Protein	Residues
Mortalin	Val-373, Gly-376, Asp-377, Asp-380, Val-381, Leu-382, Leu-383, Leu-384, Val-386, Thr-387
Bcl-2	Ser-116, Cys-229, Val-92, Leu-95, Gln-118, Val-226, Ala-113
Bcl-xL	Tyr-15, Ser-18, Gln-19, Gly-21, Trp-213, Phe-214, Thr-216, Leu-226, Leu-229, Phe-230

Table S3 Interfacial residues in docked protein–protein complexes before MD simulations

Mortalin–Bcl-2 Complex		Mortalin–Bcl-xL Complex	
Mortalin	Bcl-2	Mortalin	Bcl-xL
Asp-145, Arg-148, Glu-182, Asp-318, Glu-320, Pro-411, Thr-412, Lys-413, Lys-481, Lys-483, Gly-486, Glu-488	Arg-109, Arg-110, Ala-113, Glu-114, Ser-117, Gln-118, His-120, Arg-164, Pro-208, Phe-212, Leu-215, Ser-216, Thr-219, Leu-220, Ala-224, Leu-225, Val-226, Gly-227, Ala-228, Cys-229, Gly-233, Ala-234, Tyr-235, Leu-236, His-238, Lys-239	Thr-379, Asp-380, Val-381, Leu-382, Leu-383, Leu-384, Asp-385, Gln-463, Glu-465, Asp-469, Asp-471, Ala-472, Asn-473	Trp-181, Asn-185, Gly-186, Asp-189, Thr-190, Glu-193, Leu-194, Tyr-195

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Table S4 Interfacial residues in docked protein–protein complexes after MD simulations

Mortalin-Bcl-2 complex		Mortalin-Bcl-xL complex	
Mortalin	Bcl-2	Mortalin	Bcl-xL
Arg-148, Lys-152, Glu-202, Gln-204, Lys-205, Gly-206, Val-207, Phe-208, Glu-209, Val-210, Lys-211, Val-378, Thr-379, Asp-380, Val-381, Leu-382, Leu-383, Leu-384, Asp-385	Arg-110, Glu-114, Ser-117, Gln-118, His-120, Arg-164, Glu-165, Leu-223, Val-226, Gly-237, His-238, His-239	Gln-204, Lys-205, Gly-206, Val-207, Phe-208, Glu-209, Leu-403, Ile-404, Asn-405, Arg-406, Asn-407, Thr-408, Pro-411, Thr-412, Lys-413, Lys-414, Ser-415, Gln-416, Val-417, Phe-418, Asp-471, Ala-472, Asn-473	Trp-181, Glu-184, Asn-185, Gly-186, Asp-189, Thr-190, Glu-193, Leu-194, Tyr-195

Table S5 H-bond occupancy of mortalin–Bcl-2 complex during MD simulation Stable H-bonds with high occupancy are shown in bold letters.

Mortalin	Bcl-2	Occupancy
Gln-204-side	**Ser-117-side**	**42.28%**
Val-381-main	Val-226-main	1.15%
Asp-380-side	**Arg-110-side**	**100.00%**
Glu-202-side	**Ser-117**-side	**69.08%**
Glu-320-side	**Arg-164-side**	**37.97%**
Val-210-main	Gln-118-side	11.60%
Asp-385-side	**Lys-239-side**	**34.47%**
Lys-205-main	Glu-114-side	6.62%
Gly-206-main	**Glu-114-side**	**25.60%**
Glu-182-side	Arg-109-side	1.25%
Lys-413-side	Leu-215-main	5.94%
Glu-209-side	Tyr-235-main	0.72%
Asp-380-side	Ala-228-main	2.83%
Glu-320-side	His-120-side	1.34%
Glu-209-side	Gln-118-side	8.15%
Glu-209-side	**Ala-234-main**	**32.89%**
Asp-380-main	Hie-238-side	0.10%
Val-207-main	Glu-114-side	7.19%
Lys-413-side	Thr-219-side	0.05%
Asp-380-side	Cys-229-side	0.05%
Thr-379-side	Arg-110-side	0.38%
Lys-481-side	Asp-211-side	1.01%
Thr-379-side	Arg-110-side	0.14%
Val-210-main	Tyr-235-side	2.25%

Table S6 H-bond occupancy of mortalin–Bcl-xL complex during MD simulation Stable H-bonds with high occupancy are shown in bold letters.

Mortalin	Bcl-xL	Occupancy
Lys-481-side	**Glu-202-side**	**34.52%**
Lys-483-side	Glu-193-side	0.96%
Glu-488-side	**Arg-204-side**	**100.00%**
Asp-471-side	**Arg-212-side**	**100.00%**
Lys-483-side	Glu-193-main	0.62%
Asn-405-side	Asp-133-side	5.32%
Asp-380-side	Arg-212-side	0.62%
Asp-380-side	Trp-213-main	8.44%
Ser-415-main	Asn-136-side	3.79%
Asp-385-side	Ser-231-side	2.73%
Gln-463-side	Thr-190-side	1.25%
Lys-414-side	Asn-136-side	0.14%
Val-417-main	Asn-185-side	8.34%
Asp-385-side	**Gly-227-main**	**20.13%**
Lys-414-side	**Asp-133-side**	**25.60%**
Gln-463-side	Thr-190-side	5.80%
Asn-405-side	Lys-233-side	0.24%
Asn-473-side	Arg-212-side	2.73%
Asp-385-side	Ser-231-main	4.46%
Asn-407-side	Lys-233-side	1.34%
Arg-406-main	Lys-233-side	6.57%
Gln-463-side	Asn-185-main	1.73%
Gln-416-side	Trp-181-side	0.14%
Arg-209-side	Asp-179-main	0.05%
Gln-463-side	Asp-189-side	0.91%
Asn-407-side	Ser-231-side	0.05%
Lys-483-side	Thr-190-side	3.88%
Arg-209-side	**Glu-182-side**	**67.02%**
Lys-481-side	Glu-193-side	18.98%
Lys-483-side	Thr-190-main	0.14%
Gln-416-side	Glu-184-side	0.10%
Arg-209-side	Lys-180-main	0.43%
Gln-463-side	Glu-184-main	0.10%
Gln-463-side	Glu-184-side	0.05%
Glu-465-side	Asn-185-side	0.14%
Lys-483-side	Asn-185-main	0.91%
Lys-413-side	Thr-219-side	0.34%
His-536-side	**Glu-184-side**	**33.27%**
Glu-543-side	Gln-183-side	0.24%
Lys-413-side	Phe-214-main	0.14%