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Understanding the effects of salinity and temperature variations on conformational changes in a thermohalostable lipase: Insights from molecular dynamics simulations

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Supplementary data

Suppl. Table 1 — The sequence of amino acid in lipase PLS 80

Sequence		Residue	Type of residue	Sequence		Residue	Type of residue
1	R	Arginine	Polar positive	56	N	Asparagine	Polar neutral
2	A	Alanine	Nonpolar	57	W	Tryptophan	Aromatic
3	N	Asparagine	Polar neutral	58	D	Aspartic acid	Polar negative
4	D	Aspartic acid	Polar negative	59	R	Arginine	Polar positive
5	S	Serine	Polar neutral	60	A	Alanine	Nonpolar
6	P	Proline	Nonpolar	61	C	Cystein	Polar neutral
7	I	Isoleucine	Nonpolar	62	E	Glutamic acid	Polar negative
8	V	Valine	Nonpolar	63	A	Alanine	Nonpolar
9	L	Leucine	Nonpolar	64	Y	Tyrosin	Aromatic
10	L	Leucine	Nonpolar	65	A	Alanine	Nonpolar
11	H	Histidine	Polar positive	66	Q	Glutamine	Polar neutral
12	G	Glycine	Nonpolar	67	L	Leucine	Nonpolar
13	F	Phenylalanine	Aromatic	68	V	Valine	Nonpolar
14	T	Threonine	Polar neutral	69	G	Glycine	Nonpolar
15	G	Glycine	Nonpolar	70	G	Glycine	Nonpolar
16	W	Tryptophan	Aromatic	71	T	Threonine	Polar neutral
17	G	Glycine	Nonpolar	72	V	Valine	Nonpolar
18	R	Arginine	Polar positive	73	D	Aspartic acid	Polar negative
19	E	Glutamic acid	Polar negative	74	Y	Tyrosin	Aromatic
20	E	Glutamic acid	Polar negative	75	G	Glycine	Nonpolar
21	M	Methionine	Nonpolar	76	A	Alanine	Nonpolar
22	F	Phenylalanine	Aromatic	77	A	Alanine	Nonpolar
23	G	Glycine	Nonpolar	78	H	Histidine	Polar positive
24	F	Phenylalanine	Aromatic	79	A	Alanine	Nonpolar
25	K	Lysine	Polar positive	80	A	Alanine	Nonpolar
26	Y	Tyrosin	Aromatic	81	K	Lysine	Polar positive
27	W	Tryptophan	Aromatic	82	H	Histidine	Polar positive
28	G	Glycine	Nonpolar	83	G	Glycine	Nonpolar
29	G	Glycine	Nonpolar	84	H	Histidine	Polar positive
30	V	Valine	Nonpolar	85	A	Alanine	Nonpolar
31	R	Arginine	Polar positive	86	R	Arginine	Polar positive
32	G	Glycine	Nonpolar	87	F	Phenylalanine	Aromatic
33	D	Aspartic acid	Polar negative	88	G	Glycine	Nonpolar
34	I	Isoleucine	Nonpolar	89	R	Arginine	Polar positive
35	E	Glutamic acid	Polar negative	90	T	Threonine	Polar neutral
36	Q	Glutamine	Polar neutral	91	Y	Tyrosin	Aromatic
37	W	Tryptophan	Aromatic	92	P	Proline	Nonpolar

38	L	Leucine	Nonpolar	93	G	Glycine	Nonpolar
39	N	Asparagine	Polar neutral	94	L	Leucine	Nonpolar
40	D	Aspartic acid	Polar negative	95	L	Leucine	Nonpolar
41	N	Asparagine	Polar neutral	96	P	Proline	Nonpolar
42	G	Glycine	Nonpolar	97	E	Glutamic acid	Polar negative
43	Y	Tyrosin	Aromatic	98	L	Leucine	Nonpolar
44	R	Arginine	Polar positive	99	K	Lysine	Polar positive
45	T	Threonine	Polar neutral	100	R	Arginine	Polar positive
46	Y	Tyrosin	Aromatic	101	G	Glycine	Nonpolar
47	T	Threonine	Polar neutral	102	G	Glycine	Nonpolar
48	L	Leucine	Nonpolar	103	R	Arginine	Polar positive
49	A	Alanine	Nonpolar	104	V	Valine	Nonpolar
50	V	Valine	Nonpolar	105	H	Histidine	Polar positive
51	G	Glycine	Nonpolar	106	I	Isoleucine	Nonpolar
52	P	Proline	Nonpolar	107	I	Isoleucine	Nonpolar
53	L	Leucine	Nonpolar	108	A	Alanine	Nonpolar
54	S	Serine	Polar neutral	109	H	Histidine	Polar positive
55	S	Serine	Polar neutral	110	S	Serine	Polar neutral
111	Q	Glutamine	Polar neutral	181	Q	Glutamine	Polar neutral
112	G	Glycine	Nonpolar	182	K	Lysine	Polar positive
113	K	Lysine	Polar positive	183	A	Alanine	Nonpolar
114	Q	Glutamine	Polar neutral	184	V	Valine	Nonpolar
115	T	Threonine	Polar neutral	185	L	Leucine	Nonpolar
116	A	Alanine	Nonpolar	186	E	Glutamic acid	Polar negative
117	R	Arginine	Polar positive	187	A	Alanine	Nonpolar
118	M	Methionine	Nonpolar	188	A	Alanine	Nonpolar
119	L	Leucine	Nonpolar	189	A	Alanine	Nonpolar
120	V	Valine	Nonpolar	190	V	Valine	Nonpolar
121	S	Serine	Polar neutral	191	A	Alanine	Nonpolar
122	L	Leucine	Nonpolar	192	S	Serine	Polar neutral
123	L	Leucine	Nonpolar	193	N	Asparagine	Polar neutral
124	E	Glutamic acid	Polar negative	194	V	Valine	Nonpolar
125	N	Asparagine	Polar neutral	195	P	Proline	Nonpolar
126	G	Glycine	Nonpolar	196	Y	Tyrosin	Aromatic
127	S	Serine	Polar neutral	197	T	Threonine	Polar neutral
128	Q	Glutamine	Polar neutral	198	S	Serine	Polar neutral
129	E	Glutamic acid	Polar negative	199	Q	Glutamine	Polar neutral
130	E	Glutamic acid	Polar negative	200	V	Valine	Nonpolar
131	R	Arginine	Polar positive	201	Y	Tyrosin	Aromatic
132	E	Glutamic acid	Polar negative	202	D	Aspartic acid	Polar negative
133	Y	Tyrosin	Aromatic	203	F	Phenylalanine	Aromatic
134	A	Alanine	Nonpolar	204	K	Lysine	Polar positive
135	K	Lysine	Polar positive	205	L	Leucine	Nonpolar
136	E	Glutamic acid	Polar negative	206	D	Aspartic acid	Polar negative
137	H	Histidine	Polar positive	207	Q	Glutamine	Polar neutral
138	N	Asparagine	Polar neutral	208	W	Tryptophan	Aromatic
139	V	Valine	Nonpolar	209	G	Glycine	Nonpolar
140	S	Serine	Polar neutral	210	L	Leucine	Nonpolar
141	L	Leucine	Nonpolar	211	R	Arginine	Polar positive
142	S	Serine	Polar neutral	212	R	Arginine	Polar positive
143	P	Proline	Nonpolar	213	Q	Glutamine	Polar neutral
144	L	Leucine	Nonpolar	214	P	Proline	Nonpolar
145	F	Phenylalanine	Aromatic	215	G	Glycine	Nonpolar
146	E	Glutamic acid	Polar negative	216	E	Glutamic acid	Polar negative
147	G	Glycine	Nonpolar	217	S	Serine	Polar neutral
148	G	Glycine	Nonpolar	218	F	Phenylalanine	Aromatic
149	H	Histidine	Polar positive	219	D	Aspartic acid	Polar negative
150	R	Arginine	Polar positive	220	H	Histidine	Polar positive
151	F	Phenylalanine	Aromatic	221	Y	Tyrosin	Aromatic
152	V	Valine	Nonpolar	222	F	Phenylalanine	Aromatic

153	L	Leucine	Nonpolar	223	E	Glutamic acid	Polar negative
154	S	Serine	Polar neutral	224	R	Arginine	Polar positive
155	V	Valine	Nonpolar	225	L	Leucine	Nonpolar
156	T	Threonine	Polar neutral	226	K	Lysine	Polar positive
157	T	Threonine	Polar neutral	227	R	Arginine	Polar positive
158	I	Isoleucine	Nonpolar	228	S	Serine	Polar neutral
159	A	Alanine	Nonpolar	229	P	Proline	Nonpolar
160	T	Threonine	Polar neutral	230	V	Valine	Nonpolar
161	P	Proline	Nonpolar	231	W	Tryptophan	Aromatic
162	H	Histidine	Polar positive	232	T	Threonine	Polar neutral
163	D	Aspartic acid	Polar negative	233	S	Serine	Polar neutral
164	G	Glycine	Nonpolar	234	T	Threonine	Polar neutral
165	T	Threonine	Polar neutral	235	D	Aspartic acid	Polar negative
166	T	Threonine	Polar neutral	236	T	Threonine	Polar neutral
167	L	Leucine	Nonpolar	237	A	Alanine	Nonpolar
168	V	Valine	Nonpolar	238	R	Arginine	Polar positive
169	N	Asparagine	Polar neutral	239	Y	Tyrosin	Aromatic
170	M	Methionine	Nonpolar	240	D	Aspartic acid	Polar negative
171	V	Valine	Nonpolar	241	L	Leucine	Nonpolar
172	D	Aspartic acid	Polar negative	242	S	Serine	Polar neutral
173	F	Phenylalanine	Aromatic	243	V	Valine	Nonpolar
174	T	Threonine	Polar neutral	244	S	Serine	Polar neutral
175	D	Aspartic acid	Polar negative	245	G	Glycine	Nonpolar
176	R	Arginine	Polar positive	246	A	Alanine	Nonpolar
177	F	Phenylalanine	Aromatic	247	E	Glutamic acid	Polar negative
178	F	Phenylalanine	Aromatic	248	K	Lysine	Polar positive
179	D	Aspartic acid	Polar negative	249	L	Leucine	Nonpolar
180	L	Leucine	Nonpolar	250	N	Asparagine	Polar neutral
251	Q	Glutamine	Polar neutral	321	S	Serine	Polar neutral
252	W	Tryptophan	Aromatic	322	M	Methionine	Polar neutral
253	V	Valine	Nonpolar	323	N	Asparagine	Polar neutral
254	Q	Glutamine	Polar neutral	324	G	Glycine	Nonpolar
255	A	Alanine	Nonpolar	325	P	Proline	Nonpolar
256	S	Serine	Polar neutral	326	K	Lysine	Polar positive
257	P	Proline	Nonpolar	327	R	Arginine	Polar positive
258	N	Asparagine	Polar neutral	328	G	Glycine	Nonpolar
259	T	Threonine	Polar neutral	329	S	Serine	Polar neutral
260	Y	Tyrosin	Aromatic	330	S	Serine	Polar neutral
261	Y	Tyrosin	Aromatic	331	D	Aspartic acid	Polar negative
262	L	Leucine	Nonpolar	332	R	Arginine	Polar positive
263	S	Serine	Polar neutral	333	I	Isoleucine	Nonpolar
264	F	Phenylalanine	Aromatic	334	V	Valine	Nonpolar
265	S	Serine	Polar neutral	335	P	Proline	Nonpolar
266	T	Threonine	Polar neutral	336	Y	Tyrosin	Aromatic
267	E	Glutamic acid	Polar negative	337	D	Aspartic acid	Polar negative
268	R	Arginine	Polar positive	338	G	Glycine	Nonpolar
269	T	Threonine	Polar neutral	339	A	Alanine	Nonpolar
270	Y	Tyrosin	Aromatic	340	L	Leucine	Nonpolar
271	R	Arginine	Polar positive	341	K	Lysine	Polar positive
272	G	Glycine	Nonpolar	342	K	Lysine	Polar positive
273	A	Alanine	Nonpolar	343	G	Glycine	Nonpolar
274	L	Leucine	Nonpolar	344	V	Valine	Nonpolar
275	T	Threonine	Polar neutral	345	W	Tryptophan	Aromatic
276	G	Glycine	Nonpolar	346	N	Asparagine	Polar neutral
277	N	Asparagine	Polar neutral	347	D	Aspartic acid	Polar negative
278	Y	Tyrosin	Aromatic	348	M	Methionine	Nonpolar
279	Y	Tyrosin	Aromatic	349	G	Glycine	Nonpolar
280	P	Proline	Nonpolar	350	T	Threonine	Polar neutral
281	E	Glutamic acid	Polar negative	351	Y	Tyrosin	Aromatic
282	L	Leucine	Nonpolar	352	N	Asparagine	Polar neutral
283	G	Glycine	Nonpolar	353	V	Valine	Nonpolar

284	M	Methionine	Nonpolar	354	D	Aspartic acid	Polar negative
285	N	Asparagine	Polar neutral	355	H	Histidine	Polar positive
286	A	Alanine	Nonpolar	356	L	Leucine	Nonpolar
287	F	Phenylalanine	Aromatic	357	E	Glutamic acid	Polar negative
288	S	Serine	Polar neutral	358	I	Isoleucine	Nonpolar
289	A	Alanine	Nonpolar	359	I	Isoleucine	Nonpolar
290	V	Valine	Nonpolar	360	G	Glycine	Nonpolar
291	V	Valine	Nonpolar	361	V	Valine	Nonpolar
292	C	Cystein	Polar neutral	362	D	Aspartic acid	Polar negative
293	A	Alanine	Nonpolar	363	P	Proline	Nonpolar
294	P	Proline	Nonpolar	364	N	Asparagine	Polar neutral
295	F	Phenylalanine	Aromatic	365	P	Proline	Nonpolar
296	L	Leucine	Nonpolar	366	S	Serine	Polar neutral
297	G	Glycine	Nonpolar	367	F	Phenylalanine	Aromatic
298	S	Serine	Polar neutral	368	D	Aspartic acid	Polar negative
299	Y	Tyrosin	Aromatic	369	I	Isoleucine	Nonpolar
300	R	Arginine	Polar positive	370	R	Arginine	Polar positive
301	N	Asparagine	Polar neutral	371	A	Alanine	Nonpolar
302	P	Proline	Nonpolar	372	F	Phenylalanine	Aromatic
303	T	Threonine	Polar neutral	373	Y	Tyrosin	Aromatic
304	L	Leucine	Nonpolar	374	L	Leucine	Nonpolar
305	G	Glycine	Nonpolar	375	R	Arginine	Polar positive
306	I	Isoleucine	Nonpolar	376	L	Leucine	Nonpolar
307	D	Aspartic acid	Polar negative	377	A	Alanine	Nonpolar
308	N	Asparagine	Polar neutral	378	E	Glutamic acid	Polar negative
309	R	Arginine	Polar positive	379	Q	Glutamine	Polar neutral
310	W	Tryptophan	Aromatic	380	L	Leucine	Nonpolar
311	L	Leucine	Nonpolar	381	A	Alanine	Nonpolar
312	E	Glutamic acid	Polar negative	382	S	Serine	Polar neutral
313	N	Asparagine	Polar neutral	383	C	Cystein	Polar neutral
314	D	Aspartic acid	Polar negative				
315	G	Glycine	Nonpolar				
316	I	Isoleucine	Nonpolar				
317	V	Valine	Nonpolar				
318	N	Asparagine	Polar neutral				
319	T	Threonine	Polar neutral				
320	V	Valine	Nonpolar				