psm Journals

International Journal of
Molecular Microbiology

Research Article **2025 | Volume 8 | Issue 1 | 52-69**

Open Access

Article Information

Received: October 10, 2025

Accepted: October 30, 2025

Published: November 7, 2025

Keywords
Apoptozole,
Cystic fibrosis,
Drug discovery,
Molecular docking,
Structural modeling.

Authors' Contribution
AN and AW conceived and designed the study; KR, NS, and AI performed the experiments and analyzed the results; ZA, HUT, and MP wrote and revised the manuscript.

How to cite
Noman, A., Sardar, N., Islam, A., Ramzan, K., Ali, M.Z., Tahir, H.U., Waheed, A., Parveen, M., 2025. Integrative Computational Analysis of CFTR Mutations Linked to Cystic Fibrosis. Int. J. Mol. Microbiol., 8(1): 52-69.

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Integrative Computational Analysis of CFTR Mutations Linked to Cystic Fibrosis

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Supplementary Files:

Table S1. Functional predictions of CFTR nsSNPs using SNAP2, PROVEAN, PolyPhen-2, CONDEL, and CADD tools.

Table S2. Disease association analysis of CFTR nsSNPs using P-Mut, PhD-SNP, SNPs & GO, and Meta-SNP tools.

Table S3. Protein stability analysis of CFTR variants using MuPro, I-Mutant, and iStable tools.

Table S4. Structural validation of wild-type and mutant protein models using SAVES v6.1 and TM-align.

Table S5. Interacting residues obtained from docking. CFTR and G1249R, I105N, and K273Q mutant protein structures with ligands show interaction residues and hydrophobic associations.

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Supplementary Materials

The following tables are included as supplementary materials in the manuscript.

Table S1. Functional predictions of CFTR nsSNPs using SNAP2, PROVEAN, PolyPhen-2, CONDEL, and CADD tools.

Variation ID	A.A	SNAP2		PROVEAN		Polyphen-2		CONDEL		CADD
		Effect	Sc	Effect	Sc	Effect	Sc	Sc 0.522	Label	Score
rs1031657153	P99A	Effect	75	Deleterious	-6.326	Probably damaging	1	0.689962767	Deleterious	26.5
rs397508467	P99L	Effect	89	Deleterious	-7.86	Probably damaging	1	0.690461493	Deleterious	26.3
rs397508490	L102P	Effect	76	Deleterious	-5.675	Probably damaging	1	0.653429886	Deleterious	27.5
rs397508509	I105N	Effect	96	Deleterious	-4.741	Probably damaging	1	0.639361713	Deleterious	28.5
rs397508522	Y109N	Effect	94	Deleterious	-4.14	Probably damaging	1	0.623628807	Deleterious	26.7
rs121909031	Y109C	Effect	28	Deleterious	-4.045	Probably damaging	1	0.623935753	Deleterious	25.9
rs113993958	D110Y	Effect	95	Neutral	-2.419	Probably damaging	1	0.6461576	Deleterious	26.4
rs140502196	P111L	Neutral	-9	Deleterious	-2.888	Probably damaging	0.997	0.626352695	Deleterious	23.7
rs397508551	N113I	Neutral	-55	Neutral	-2.479	Probably damaging	0.992	0.604836303	Deleterious	24.4
rs761370893	E116G	Neutral	-22	Neutral	-2.237	Probably damaging	1	0.631819172	Deleterious	32
rs201958172	A120P	Effect	90	Neutral	-0.594	Probably damaging	0.999	0.573850662	Deleterious	24.7
rs397508592	Y122H	Effect	5	Neutral	-2.374	Probably damaging	1	0.533685761	Deleterious	26
rs377295859	Y122C	Neutral	-4	Deleterious	-3.155	Probably damaging	1	0.533868225	Deleterious	25.3
rs397508609	G126D	Effect	45	Deleterious	-3.059	Probably damaging	1	0.612333936	Deleterious	27.1
rs1162745955	L129H	Effect	42	Deleterious	-3.805	Probably damaging	1	0.598494635	Deleterious	28
rs397508674	L137H	Effect	74	Deleterious	-4.032	Probably damaging	1	0.584131047	Deleterious	28.4
rs1800078	L138P	Effect	39	Deleterious	-5.019	Probably damaging	1	0.544893044	Deleterious	27.3
rs397508718	G149R	Effect	55	Deleterious	-6.594	Probably damaging	1	0.614160066	Deleterious	38
rs397508719	G149E	Effect	99	Deleterious	-6.559	Probably damaging	1	0.613969807	Deleterious	31
rs397508723	A155P	Effect	69	Deleterious	-3.221	Probably damaging	1	0.622122435	Deleterious	27.4
rs397508724	S158C	Neutral	-14	Deleterious	-3.24	Probably damaging	1	0.54546275	Deleterious	27.6
rs397508727	L159S	Effect	9	Neutral	-1.388	Probably damaging	1	0.590006845	Deleterious	40
rs397508729	Y161D	Effect	93	Deleterious	-8.82	Probably damaging	1	0.625738666	Deleterious	28.3
rs397508730	Y161S	Effect	86	Deleterious	-7.937	Probably damaging	1	0.625908003	Deleterious	29.4
rs397508736	L165S	Effect	70	Deleterious	-5.076	Probably damaging	1	0.624026793	Deleterious	37
rs80282562	G178R	Effect	39	Deleterious	-6.597	Probably damaging	1	0.623460666	Deleterious	39
rs397508748	G178E	Effect	96	Deleterious	-6.484	Probably damaging	1	0.623444642	Deleterious	28.9
rs397508751	L183I	Effect	13	Neutral	-1.298	Probably damaging	1	0.597193052	Deleterious	25.6
rs766640075	L188P	Effect	79	Deleterious	-2.737	Probably damaging	1	0.572304299	Deleterious	29.9
rs397508756	D192N	Effect	94	Neutral	-1.17	Probably damaging	1	0.628164312	Deleterious	32
rs397508758	D192G	Effect	94	Neutral	-2.456	Probably damaging	1	0.59406821	Deleterious	31
rs755405930	E193G	Effect	96	Deleterious	-3.525	Probably damaging	1	0.541998905	Deleterious	34
rs376008630	G194R	Effect	76	Neutral	-0.823	Probably damaging	1	0.536433678	Deleterious	45
rs397508765	H199Q	Effect	21	Deleterious	-3.161	Probably damaging	1	0.630271618	Deleterious	23.7
rs1457675231	F200S	Effect	64	Deleterious	-2.767	Probably damaging	1	0.598710441	Deleterious	31
rs121908803	P205S	Neutral	-9	Deleterious	-6.506	Probably damaging	1	0.62711446	Deleterious	24.7
rs397508769	P205R	Effect	98	Deleterious	-7.354	Probably damaging	1	0.626471433	Deleterious	25.3
rs121908752	L206W	Effect	42	Deleterious	-3.158	Probably damaging	1	0.602951749	Deleterious	38
rs1227994401	Q207H	Effect	71	Deleterious	-4.163	Probably damaging	1	0.589974325	Deleterious	23.3

rs759719664	L180F	Effect	30	Neutral	-2.338	Probably damaging	1	0.54889768	Deleterious	24
rs397508776	W216C	Effect	14	Deleterious	-7.936	Probably damaging	1	0.587346356	Deleterious	39
rs770891254	G226E	Effect	74	Deleterious	-6.071	Probably damaging	1	0.604404997	Deleterious	25.9
rs397508785	Q237H	Effect	55	Neutral	-2.07	Probably damaging	1	0.629183694	Deleterious	23.4
rs397508789	G241W	Effect	92	Deleterious	-3.354	Probably damaging	1	0.588153323	Deleterious	28.6
rs377514639	R258I	Effect	96	Deleterious	-4.712	Probably damaging	1	0.632108701	Deleterious	29.5
rs1296578005	K273Q	Effect	77	Deleterious	-3.396	Probably damaging	1	0.624575021	Deleterious	41
rs756036343	K273M	Effect	82	Deleterious	-5.094	Probably damaging	1	0.62411619	Deleterious	28
rs397508800	W277R	Effect	82	Deleterious	-11.885	Probably damaging	1	0.634257459	Deleterious	29.3
rs151073129	I285F	Neutral	-65	Deleterious	-2.77	Probably damaging	1	0.609117124	Deleterious	27.8
rs1204521684	V317G	Effect	51	Deleterious	-3.084	Probably damaging	1	0.543605135	Deleterious	27.7
rs121909011	R334W	Effect	96	Deleterious	-3.421	Probably damaging	1	0.540073147	Deleterious	24.7
rs397508146	L346P	Effect	55	Deleterious	-4.152	Probably damaging	1	0.611034144	Deleterious	29.1
rs77932196	R347P	Effect	58	Neutral	-0.718	Probably damaging	1	0.618903437	Deleterious	30
rs397508188	L441P	Effect	86	Deleterious	-5.288	Probably damaging	1	0.682955987	Deleterious	28.6
rs121908805	S466L	Effect	89	Deleterious	-5.025	Probably damaging	1	0.585878446	Deleterious	38
rs1800089	L467F	Effect	21	Deleterious	-2.687	Probably damaging	1	0.564902727	Deleterious	24.6
rs139573311	L467P	Effect	97	Deleterious	-5.874	Probably damaging	1	0.761524877	Deleterious	28.2
rs397508202	L468P	Effect	75	Deleterious	-5.83	Probably damaging	1	0.734640484	Deleterious	28.5
rs79282516	G480S	Effect	95	Deleterious	-5.046	Probably damaging	1	0.734211973	Deleterious	28.5
rs397508208	G480D	Effect	98	Deleterious	-5.978	Probably damaging	1	0.744839813	Deleterious	26.7
rs200626971	W496C	Effect	25	Deleterious	-11.907	Probably damaging	1	0.667176959	Deleterious	40
rs774945680	G500D	Effect	86	Deleterious	-3.722	Probably damaging	1	0.548933512	Deleterious	26.9
rs397508222	I502N	Effect	81	Deleterious	-5.352	Probably damaging	1	0.678737274	Deleterious	28.2
rs397508224	I506S	Effect	97	Deleterious	-5.235	Probably damaging	1	0.740253168	Deleterious	28
rs1800092	I506M	Effect	35	Deleterious	-2.654	Probably damaging	1	0.651641453	Deleterious	23.6
rs74571530	F508C	Effect	59	Deleterious	-6.794	Probably damaging	1	0.641843246	Deleterious	29.5
rs758745885	D513Y	Effect	90	Deleterious	-6.423	Probably damaging	1	0.597220422	Deleterious	28.6
rs368516826	C524R	Effect	87	Deleterious	-10.22	Probably damaging	1	0.569687905	Deleterious	28.3
rs1387755887	G545V	Effect	83	Deleterious	-8.502	Probably damaging	1	0.621163058	Deleterious	28.6
rs1469024267	L548P	Effect	94	Deleterious	-6.609	Probably damaging	1	0.777140505	Deleterious	28.1
rs121908757	S519R	Neutral	-81	Neutral	-1.239	Probably damaging	0.996	0.462454118	Deleterious	28
rs121908755	S519I	Neutral	-16	Deleterious	-3.24	Probably damaging	0.995	0.540770248	Neutral	27.4
rs121909005	S519R	Neutral	-81	Neutral	-1.239	Probably damaging	0.996	0.462454118	Neutral	25.2
rs75527207	G551D	Effect	40	Deleterious	-6.574	Probably damaging	1	0.75222989	Neutral	26.8
rs397508255	R555G	Effect	86	Deleterious	-6.602	Probably damaging	1	0.799480436	Neutral	38
rs75549581	A559S	Effect	89	Deleterious	-2.832	Probably damaging	0.999	0.691602273	Deleterious	27.6
rs397508259	A559E	Effect	97	Deleterious	-4.721	Probably damaging	1	0.757384078	Deleterious	31
rs397508260	R560G	Effect	98	Deleterious	-6.472	Probably damaging	1	0.689609802	Deleterious	49
rs121909006	Y563N	Effect	51	Deleterious	-8.199	Probably damaging	1	0.642969748	Deleterious	29.3
rs397508276	Y569D	Effect	30	Deleterious	-7.558	Probably damaging	1	0.669390533	Deleterious	29.7
rs397508277	Y569C	Effect	2	Deleterious	-6.446	Probably damaging	1	0.669521668	Deleterious	28.7
rs397508282	D572N	Effect	7	Deleterious	-4.655	Probably damaging	0.993	0.727034918	Deleterious	32
rs748393295	D572E	Effect	96	Deleterious	-3.744	Probably damaging	0.993	0.75866299	Deleterious	23.3
rs121908758	P574H	Effect	2	Deleterious	-6.571	Probably damaging	1	0.687942281	Deleterious	31
rs1800100	R668C	Effect	80	Deleterious	-2.577	Probably damaging	1	0.624800084	Deleterious	25.5

rs186089140	S737F	Neutral	-24	Deleterious	-3.438	Probably damaging	1	0.622634051	Deleterious	25.1
rs397508363	R766M	Effect	39	Deleterious	-2.56	Probably damaging	1	0.623460666	Deleterious	27.6
rs1386366130	Q767H	Neutral	-13	Neutral	-1.739	Probably damaging	1	0.62043366	Deleterious	24.7
rs1299482973	S707F	Effect	55	Neutral	-1.796	Probably damaging	0.744	0.585902379	Deleterious	25.8
rs397508375	D806G	Effect	34	Deleterious	-3.365	Probably damaging	1	0.621937441	Deleterious	29.5
rs757165481	Y849H	Effect	64	Deleterious	-3.629	Probably damaging	1	0.618107758	Deleterious	27.9
rs775570582	L165S	Effect	70	Deleterious	-5.076	Probably damaging	1	0.624026793	Deleterious	41
rs1402844924	L165F	Effect	51	Deleterious	-3.384	Probably damaging	1	0.624599327	Deleterious	23.1
rs121909035	H949Y	Effect	9	Deleterious	-5.061	Probably damaging	1	0.72050739	Deleterious	25.7
rs397508444	H949R	Effect	91	Deleterious	-6.732	Probably damaging	1	0.734552388	Deleterious	26.5
rs1191342069	G1241D	Effect	65	Deleterious	-5.962	Probably damaging	1	0.765063796	Deleterious	26
rs397508599	G1244R	Effect	99	Deleterious	-6.814	Probably damaging	1	0.796001161	Deleterious	43
rs267606723	G1244E	Effect	35	Deleterious	-6.815	Probably damaging	1	0.796001161	Deleterious	30
rs397508602	G1249R	Effect	99	Deleterious	-6.813	Probably damaging	1	0.796353604	Deleterious	29.3
rs121909040	G1249E	Effect	30	Deleterious	-6.813	Probably damaging	1	0.796353604	Deleterious	26.9
rs117400534	L1253F	Neutral	-15	Deleterious	-3.256	Probably damaging	1	0.568546906	Deleterious	23.8
rs11971167	D1270Y	Effect	93	Deleterious	-7.661	Probably damaging	1	0.679934439	Deleterious	28.9
rs765549490	D1270G	Effect	91	Deleterious	-5.959	Probably damaging	1	0.542053343	Deleterious	26.5
rs753920616	F508V	Effect	95	Deleterious	-5.778	Probably damaging	1	0.611318672	Deleterious	27.8
rs77010898	W1282C	Effect	76	Deleterious	-2.735	Probably damaging	1	0.537853353	Deleterious	46
rs77902683	R1283M	Effect	30	Deleterious	-5.11	Probably damaging	1	0.712796773	Deleterious	27.7
rs904990724	G1298R	Effect	93	Deleterious	-6.796	Probably damaging	1	0.560994579	Deleterious	48
rs193922522	G1298A	Effect	73	Deleterious	-5.081	Probably damaging	1	0.549625067	Deleterious	33
rs121909042	N1303H	Neutral	-60	Deleterious	-4.262	Probably damaging	1	0.691446673	Deleterious	26.5
rs121909042	N1303Y	Effect	97	Deleterious	-6.819	Probably damaging	1	0.679870663	Deleterious	26.5
rs397508636	N1303I	Effect	97	Deleterious	-7.672	Probably damaging	1	0.657683723	Deleterious	26.6
rs80034486	N1303K	Effect	98	Deleterious	-5.114	Probably damaging	1	0.72911327	Deleterious	23.5
rs201503139	P1306S	Effect	7	Deleterious	-6.819	Probably damaging	1	0.645146816	Deleterious	24.9
rs397508646	D1312G	Effect	43	Deleterious	-5.891	Probably damaging	1	0.61691217	Deleterious	28.2
rs397508653	L1324P	Effect	50	Deleterious	-5.598	Probably damaging	1	0.783795583	Deleterious	29.8
rs755917129	I1267M	Neutral	-80	Neutral	-2.426	Probably damaging	0.31	0.652946028	Deleterious	23.5
rs145545286	L1335F	Effect	61	Deleterious	-3.394	Probably damaging	1	0.615695152	Deleterious	29
rs397508660	L1339F	Effect	7	Neutral	-2.351	Probably damaging	1	0.584324218	Deleterious	26.3
rs544710550	L1339P	Effect	54	Deleterious	-4.351	Probably damaging	1	0.658029142	Deleterious	29.7
rs747324955	G1343S	Effect	57	Deleterious	-5.057	Probably damaging	1	0.558955073	Deleterious	29.6
rs773458471	G1343V	Effect	68	Deleterious	-7.455	Probably damaging	1	0.584477736	Deleterious	27.7
rs1313341594	L1346Q	Effect	84	Deleterious	-4.627	Probably damaging	1	0.764805862	Deleterious	29.5
rs201686600	G1349S	Effect	98	Deleterious	-4.991	Probably damaging	1	0.710090846	Deleterious	31
rs113857788	Q1352H	Effect	73	Deleterious	-4.19	Probably damaging	1	0.694902061	Deleterious	23.7
rs1252048837	L1356S	Effect	34	Deleterious	-4.705	Probably damaging	1	0.6901479	Deleterious	44
rs748223886	R1358T	Effect	83	Deleterious	-4.924	Probably damaging	1	0.702333972	Deleterious	29.9
rs397508670	A1364V	Neutral	-53	Deleterious	-2.678	Probably damaging	1	0.550771818	Deleterious	27.2
rs770345073	I1366F	Effect	49	Deleterious	-3.352	Probably damaging	0.999	0.599990147	Deleterious	28.2
rs200955612	I1366N	Effect	77	Deleterious	-5.759	Probably damaging	1	0.743459658	Deleterious	29.5
rs761271867	I1366M	Effect	39	Neutral	-2.459	Probably damaging	1	0.648275557	Deleterious	23.8
rs767002769	L1369F	Neutral	-19	Deleterious	-3.091	Probably damaging	1	0.554032643	Deleterious	26.5

rs760336091	D1370H	Effect	90	Deleterious	-5.681	Probably damaging	1	0.78358418	Deleterious	30

Table S2. Disease association analysis of CFTR nsSNPs using P-Mut, PhD-SNP, SNPs & GO, and Meta-SNP tools.

		P-Mut		**PhD-SNP**		**SNP &GO**		**Meta SNP**	
Variation ID	**Mutation**	**Prediction**	**Sc 0.79**	**Prediction**	**Sc ≥ 6**	**Prediction**	**Sc**	**Prediction**	**Sc**
rs1031657153	P99A	TRUE	0.7721	Disease	4	Disease	10	Disease	1
rs397508467	P99L	TRUE	0.9279	Disease	6	Disease	10	Disease	5
rs397508490	L102P	TRUE	0.9279	Disease	7	Disease	10	Disease	6
rs397508509	I105N	TRUE	0.9173	Disease	8	Disease	10	Disease	6
rs397508522	Y109N	TRUE	0.7118	Disease	1	Disease	10	Disease	6
rs121909031	Y109C	TRUE	0.7118	Disease	1	Disease	10	Disease	6
rs113993958	D110Y	TRUE	0.5124	Disease	3	Disease	10	Disease	6
rs140502196	P111L	TRUE	0.7213	neutral	3	Disease	10	neutral	0
rs397508551	N113I	TRUE	0.5655	neutral	3	Disease	10	neutral	0
rs761370893	E116G	FALSE	0.4718	neutral	7	Disease	10	neutral	2
rs201958172	A120P	TRUE	0.5839	neutral	6	Disease	10	Disease	3
rs397508592	Y122H	TRUE	0.7219	neutral	4	Disease	10	Disease	3
rs377295859	Y122C	TRUE	0.6933	neutral	4	Disease	10	Disease	5
rs397508609	G126D	TRUE	0.8055	Disease	6	Disease	10	Disease	6
rs1162745955	L129H	TRUE	0.9279	Disease	2	Disease	10	Disease	6
rs397508674	L137H	TRUE	0.8931	Disease	4	Disease	10	Disease	6
rs1800078	L138P	TRUE	0.9279	Disease	3	Disease	10	Disease	6
rs397508718	G149R	TRUE	0.7567	Disease	6	Disease	10	Disease	9
rs397508719	G149E	TRUE	0.8259	Disease	7	Disease	10	Disease	7
rs397508723	A155P	TRUE	0.9239	Disease	7	Disease	10	Disease	8
rs397508724	S158C	TRUE	0.5644	neutral	4	Disease	10	Disease	2
rs397508727	L159S	TRUE	0.5754	neutral	6	Disease	10	Disease	1
rs397508729	Y161D	TRUE	0.9279	Disease	6	Disease	10	Disease	7
rs397508730	Y161S	TRUE	0.9279	Disease	4	Disease	10	Disease	5
rs397508736	L165S	TRUE	0.7567	neutral	1	Disease	10	Disease	3
rs80282562	G178R	TRUE	0.9214	Disease	5	Disease	10	Disease	7
rs397508748	G178E	TRUE	0.9279	Disease	6	Disease	10	Disease	5
rs397508751	L183I	TRUE	0.6737	neutral	5	Disease	10	neutral	0
rs766640075	L188P	TRUE	0.6091	Disease	8	Disease	10	Disease	6
rs397508756	D192N	TRUE	0.5102	neutral	4	Disease	10	Disease	1
rs397508758	D192G	FALSE	0.4395	neutral	6	Disease	10	Disease	2
rs755405930	E193G	TRUE	0.609	neutral	2	Disease	10	Disease	4
rs376008630	G194R	TRUE	0.7822	neutral	6	Disease	10	Disease	6
rs397508765	H199Q	TRUE	0.6365	neutral	5	Disease	10	Disease	3
rs1457675231	F200S	TRUE	0.5613	neutral	6	Disease	10	Disease	1
rs121908803	P205S	TRUE	0.746	neutral	1	Disease	10	Disease	2
rs397508769	P205R	TRUE	0.9279	Disease	5	Disease	10	Disease	7
rs121908752	L206W	TRUE	0.7686	Disease	5	Disease	10	Disease	6
rs1227994401	Q207H	TRUE	0.7654	Disease	7	Disease	10	Disease	5
rs759719664	L180F	TRUE	0.581	neutral	4	Disease	10	Disease	5

rs397508776	W216C	TRUE	0.6975	neutral	4	Disease	10	Disease	6
rs770891254	G226E	TRUE	0.9279	Disease	5	Disease	10	Disease	6
rs397508785	Q237H	TRUE	0.724	Disease	3	Disease	10	Disease	6
rs397508789	G241W	TRUE	0.7215	neutral	0	Disease	10	Disease	6
rs377514639	R258I	TRUE	0.9279	Disease	6	Disease	10	Disease	7
rs1296578005	K273Q	TRUE	0.9279	Disease	6	Disease	10	Disease	4
rs756036343	K273M	TRUE	0.9279	Disease	1	Disease	10	Disease	5
rs397508800	W277R	TRUE	0.9279	Disease	6	Disease	10	Disease	7
rs151073129	I285F	TRUE	0.9239	neutral	3	Disease	10	Disease	0
rs1204521684	V317G	TRUE	0.7371	Disease	0	Disease	10	Disease	5
rs121909011	R334W	TRUE	0.77	Disease	4	Disease	10	Disease	5
rs397508146	L346P	TRUE	0.9279	Disease	7	Disease	10	Disease	6
rs77932196	R347P	TRUE	0.9279	Disease	3	Disease	10	Disease	6
rs397508188	L441P	TRUE	0.9279	Disease	7	Disease	10	Disease	4
rs121908805	S466L	TRUE	0.6073	neutral	3	Disease	10	Disease	2
rs1800089	L467F	FALSE	0.4722	neutral	5	Disease	10	Disease	2
rs139573311	L467P	TRUE	0.9279	Disease	7	Disease	10	Disease	5
rs397508202	L468P	TRUE	0.9279	Disease	6	Disease	10	Disease	5
rs79282516	G480S	TRUE	0.8104	Disease	6	Disease	10	Disease	3
rs397508208	G480D	TRUE	0.8661	Disease	6	Disease	10	Disease	3
rs200626971	W496C	TRUE	0.9279	Disease	7	Disease	10	Disease	6
rs774945680	G500D	TRUE	0.5927	neutral	5	Disease	10	Disease	3
rs397508222	I502N	TRUE	0.9279	Disease	5	Disease	10	Disease	5
rs397508224	I506S	TRUE	0.9279	Disease	7	Disease	10	Disease	5
rs1800092	I506M	TRUE	0.9239	Disease	2	Disease	10	Disease	5
rs74571530	F508C	TRUE	0.7808	Disease	5	Disease	10	Disease	5
rs758745885	D513Y	TRUE	0.8259	Disease	5	Disease	10	Disease	5
rs368516826	C524R	TRUE	0.9279	Disease	8	Disease	10	Disease	6
rs1387755887	G545V	TRUE	0.9279	Disease	8	Disease	10	Disease	9
rs1469024267	L548P	TRUE	0.9279	Disease	6	Disease	10	Disease	5
rs121908757	S519R	FALSE	0.4215	neutral	7	Disease	10	neutral	6
rs121908755	S519I	TRUE	0.514	neutral	5	Disease	10	neutral	4
rs121909005	S519R	TRUE	0.9279	neutral	7	Disease	10	neutral	6
rs75527207	G551D	TRUE	0.9279	Disease	6	Disease	10	Disease	7
rs397508255	R555G	TRUE	0.9279	Disease	6	Disease	10	Disease	7
rs75549581	A559S	TRUE	0.9174	Disease	6	Disease	10	Disease	5
rs397508259	A559E	TRUE	0.9279	Disease	7	Disease	10	Disease	7
rs397508260	R560G	TRUE	0.9279	Disease	6	Disease	10	Disease	7
rs121909006	Y563N	TRUE	0.9279	Disease	6	Disease	10	Disease	3
rs397508276	Y569D	TRUE	0.9279	Disease	7	Disease	10	Disease	5
rs397508277	Y569C	TRUE	0.8259	Disease	6	Disease	10	Disease	5
rs397508282	D572N	TRUE	0.9239	Disease	5	Disease	10	Disease	7
rs748393295	D572E	TRUE	0.9239	Disease	3	Disease	10	Disease	6
rs121908758	P574H	TRUE	0.9279	Disease	7	Disease	10	Disease	5
rs1800100	R668C	TRUE	0.529	Disease	5	Disease	10	Disease	4
rs186089140	S737F	TRUE	0.5851	neutral	4	Disease	10	neutral	3

rs397508363	R766M	TRUE	0.6808	neutral	5	Disease	10	Disease	5
rs1386366130	Q767H	FALSE	0.4504	Disease	2	Disease	10	neutral	4
rs1299482973	S707F	FALSE	0.4427	Disease	1	Disease	10	Disease	1
rs397508375	D806G	TRUE	0.5329	Disease	5	Disease	10	Disease	1
rs757165481	Y849H	TRUE	0.8113	Disease	5	Disease	10	Disease	5
rs775570582	L165S	TRUE	0.7567	neutral	1	Disease	10	Disease	3
rs1402844924	L165F	TRUE	0.6231	neutral	3	Disease	10	Disease	0
rs121909035	H949Y	TRUE	0.6803	neutral	1	Disease	10	Disease	3
rs397508444	H949R	TRUE	0.9239	neutral	1	Disease	10	Disease	6
rs1191342069	G1241D	TRUE	0.9279	Disease	7	Disease	10	Disease	4
rs397508599	G1244R	TRUE	0.9279	Disease	3	Disease	10	Disease	10
rs267606723	G1244E	TRUE	0.9279	Disease	4	Disease	10	Disease	10
rs397508602	G1249R	TRUE	0.9279	Disease	7	Disease	10	Disease	10
rs121909040	G1249E	TRUE	0.9279	Disease	8	Disease	10	Disease	10
rs117400534	L1253F	TRUE	0.6158	Disease	4	Disease	10	neutral	1
rs11971167	D1270Y	TRUE	0.9279	Disease	8	Disease	10	Disease	7
rs765549490	D1270G	TRUE	0.8661	Disease	5	Disease	10	Disease	4
rs753920616	F508V	TRUE	0.8132	Disease	7	Disease	10	Disease	5
rs77010898	W1282C	TRUE	0.7382	Disease	8	Disease	10	Disease	5
rs77902683	R1283M	TRUE	0.9279	Disease	4	Disease	10	Disease	9
rs904990724	G1298R	TRUE	0.9214	Disease	8	Disease	10	Disease	7
rs193922522	G1298A	TRUE	0.7953	neutral	6	Disease	10	neutral	1
rs121909042	N1303H	TRUE	0.9279	Disease	5	Disease	10	Disease	10
rs121909042	N1303Y	TRUE	0.7724	Disease	6	Disease	10	Disease	10
rs397508636	N1303I	TRUE	0.9279	Disease	7	Disease	10	Disease	10
rs80034486	N1303K	TRUE	0.9279	Disease	5	Disease	10	Disease	8
rs201503139	P1306S	TRUE	0.9239	neutral	1	Disease	10	Disease	2
rs397508646	D1312G	TRUE	0.9279	Disease	5	Disease	10	Disease	2
rs397508653	L1324P	TRUE	0.9279	Disease	7	Disease	10	Disease	4
rs755917129	I1267M	TRUE	0.6997	neutral	1	Disease	10	neutral	1
rs145545286	L1335F	TRUE	0.8347	Disease	6	Disease	10	Disease	2
rs397508660	L1339F	TRUE	0.5875	neutral	2	Disease	10	Disease	3
rs544710550	L1339P	TRUE	0.817	Disease	6	Disease	10	Disease	4
rs747324955	G1343S	TRUE	0.8335	Disease	1	Disease	10	Disease	4
rs773458471	G1343V	TRUE	0.9279	Disease	6	Disease	10	Disease	5
rs1313341594	L1346Q	TRUE	0.9279	Disease	4	Disease	10	Disease	5
rs201686600	G1349S	TRUE	0.9239	Disease	4	Disease	10	Disease	8
rs113857788	Q1352H	TRUE	0.9239	Disease	6	Disease	10	Disease	5
rs1252048837	L1356S	TRUE	0.9279	Disease	1	Disease	10	Disease	2
rs748223886	R1358T	TRUE	0.9279	Disease	3	Disease	10	Disease	10
rs397508670	A1364V	TRUE	0.7081	neutral	1	Disease	10	Disease	0
rs770345073	I1366F	TRUE	0.7909	Disease	3	Disease	10	Disease	1
rs200955612	I1366N	TRUE	0.9279	Disease	5	Disease	10	Disease	3
rs761271867	I1366M	TRUE	0.9174	neutral	6	Disease	10	Disease	3
rs767002769	L1369F	TRUE	0.7029	neutral	4	Disease	10	Disease	2
rs760336091	D1370H	TRUE	0.9279	neutral	2	Disease	10	Disease	10

Table S3. Protein stability analysis of CFTR variants using MuPro, I-Mutant, and iStable tools.

		Mu Pro		i-mutant		i-Stable	
Variation ID	**Mutation**	**Prediction**	**detal delta ≥ 0.5**	**stability**	**RI**	**Prediction**	**Score ≥ 0.6**
rs1031657153	P99A	DECREASE stability	-0.5557076	Decrease	9	Decrease	0.800281
rs397508467	P99L	INCREASE stability	0.6099566	Decrease	6	Decrease	0.798063
rs397508490	L102P	DECREASE stability	-1.5990922	Decrease	6	Decrease	0.801118
rs397508509	I105N	DECREASE stability	-1.9706942	Decrease	8	Decrease	0.830344
rs397508522	Y109N	DECREASE stability	-1.5829391	Decrease	8	Decrease	0.651673
rs121909031	Y109C	DECREASE stability	-1.4308958	Decrease	4	Decrease	0.701401
rs113993958	D110Y	DECREASE stability	-0.6992614	Decrease	0	Decrease	0.788
rs140502196	P111L	DECREASE stability	-0.7306786	Decrease	2	Decrease	0.746703
rs397508551	N113I	DECREASE stability	-0.648336	Increase	5	Increase	0.505217
rs761370893	E116G	DECREASE stability	-1.6066962	Decrease	6	Decrease	0.914007
rs201958172	A120P	DECREASE stability	-1.1242569	Increase	5	Increase	0.79477
rs397508592	Y122H	DECREASE stability	-1.7476217	Decrease	7	Decrease	0.801822
rs377295859	Y122C	DECREASE stability	-1.4771859	Decrease	5	Decrease	0.788527
rs397508609	G126D	DECREASE stability	-0.3152133	Decrease	6	Increase	0.656059
rs1162745955	L129H	DECREASE stability	-1.7093343	Decrease	8	Decrease	0.830763
rs397508674	L137H	DECREASE stability	-1.7937677	Decrease	8	Decrease	0.788962
rs1800078	L138P	DECREASE stability	-1.7996118	Decrease	3	Decrease	0.828728
rs397508718	G149R	DECREASE stability	-0.7848849	Decrease	0	Decrease	0.70064
rs397508719	G149E	DECREASE stability	-0.6846736	Decrease	1	Decrease	0.720955
rs397508723	A155P	DECREASE stability	-1.4022757	Increase	2	Increase	0.745779
rs397508724	S158C	DECREASE stability	-0.5678241	Decrease	2	Decrease	0.768076
rs397508727	L159S	DECREASE stability	-1.7831079	Decrease	9	Decrease	0.826367
rs397508729	Y161D	DECREASE stability	-1.6065272	Increase	2	Decrease	0.681074
rs397508730	Y161S	DECREASE stability	-2.0958528	Decrease	4	Decrease	0.88616
rs397508736	L165S	DECREASE stability	-2.5088231	Decrease	8	Decrease	0.896556
rs80282562	G178R	DECREASE stability	-1.1880191	Decrease	4	Increase	0.554817
rs397508748	G178E	DECREASE stability	-1.1226603	Increase	0	Increase	0.786076
rs397508751	L183I	DECREASE stability	-0.78709659	Decrease	7	Decrease	0.62128
rs766640075	L188P	DECREASE stability	-2.6840999	Decrease	3	Decrease	0.826112
rs397508756	D192N	DECREASE stability	-0.548786	Decrease	7	Decrease	0.777595
rs397508758	D192G	DECREASE stability	-1.2490357	Decrease	7	Decrease	0.851055
rs755405930	E193G	DECREASE stability	-1.2823724	Decrease	7	Decrease	0.530562
rs376008630	G194R	DECREASE stability	-0.41320231	Decrease	4	Decrease	0.719897
rs397508765	H199Q	DECREASE stability	-0.9776213	Decrease	4	Decrease	0.676365
rs1457675231	F200S	DECREASE stability	-1.5427317	Decrease	9	Decrease	0.807525
rs121908803	P205S	DECREASE stability	-1.2797582	Decrease	8	Decrease	0.770298
rs397508769	P205R	DECREASE stability	-1.1320674	Decrease	5	Decrease	0.742026
rs121908752	L206W	DECREASE stability	-1.0927885	Decrease	5	Decrease	0.871222
rs1227994401	Q207H	DECREASE stability	-0.814767	Decrease	8	Decrease	0.768691
rs759719664	L180F	DECREASE stability	-0.7117823	Decrease	4	Decrease	0.819394
rs397508776	W216C	DECREASE stability	-0.6594687	Decrease	7	Decrease	0.822703
rs770891254	G226E	DECREASE stability	-0.2546524	increase	4	Decrease	0.515619
rs397508785	Q237H	DECREASE stability	-0.63513713	Decrease	9	Decrease	0.598594

rs397508789	G241W	DECREASE stability	-0.3556606	increase	2	Increase	0.796031
rs377514639	R258I	DECREASE stability	-0.6400463	Decrease	4	Decrease	0.793303
rs1296578005	K273Q	DECREASE stability	-0.3246713	Decrease	6	Decrease	0.756817
rs756036343	K273M	INCREASE stability	0.1555522	Decrease	2	Increase	0.639595
rs397508800	W277R	DECREASE stability	-0.4583815	Decrease	7	Increase	0.679151
rs151073129	I285F	DECREASE stability	-0.82942098	Decrease	3	Decrease	0.872513
rs1204521684	V317G	DECREASE stability	-2.0775997	Decrease	10	Decrease	0.827884
rs121909011	R334W	DECREASE stability	-1.1541102	Decrease	2	Decrease	0.757645
rs397508146	L346P	DECREASE stability	-1.6409523	Decrease	6	Decrease	0.893797
rs77932196	R347P	DECREASE stability	-1.2978301	Decrease	3	Decrease	0.750586
rs397508188	L441P	DECREASE stability	-1.9945794	Decrease	8	Decrease	0.82827
rs121908805	S466L	INCREASE stability	0.3877408	Increase	3	Increase	0.753838
rs1800089	L467F	DECREASE stability	-1.2328324	Decrease	6	Decrease	0.86033
rs139573311	L467P	DECREASE stability	-1.9143963	Decrease	5	Decrease	0.851713
rs397508202	L468P	DECREASE stability	-2.1603347	Decrease	5	Decrease	0.833299
rs79282516	G480S	DECREASE stability	-1.1809141	Decrease	5	Decrease	0.810659
rs397508208	G480D	DECREASE stability	-0.9116127	Decrease	5	Decrease	0.792936
rs200626971	W496C	DECREASE stability	-0.9124014	Decrease	8	Decrease	0.812659
rs774945680	G500D	DECREASE stability	-0.3619342	Decrease	7	Increase	0.603067
rs397508222	I502N	DECREASE stability	-1.2472223	Decrease	7	Decrease	0.555645
rs397508224	I506S	DECREASE stability	-1.9224014	Decrease	9	Decrease	0.878466
rs1800092	I506M	DECREASE stability	-1.1512498	Decrease	9	Decrease	0.853986
rs74571530	F508C	DECREASE stability	-1.4364461	Decrease	7	Decrease	0.824526
rs758745885	D513Y	DECREASE stability	-0.2967828	Decrease	3	Increase	0.615206
rs368516826	C524R	DECREASE stability	-1.3820722	Decrease	3	Decrease	0.782475
rs1387755887	G545V	INCREASE stability	0.3815065	Decrease	5	Decrease	0.777367
rs1469024267	L548P	DECREASE stability	-2.1186779	Decrease	4	Decrease	0.835041
rs121908757	S519R	DECREASE stability	-1.3823772	Increase	1	Increase	0.703129
rs121908755	S519I	DECREASE stability	-0.9041675	Decrease	0	Increase	0.755216
rs121909005	S519R	DECREASE stability	-1.3823772	Increase	1	Increase	0.703129
rs75527207	G551D	DECREASE stability	-0.6971572	Decrease	2	Decrease	0.7189
rs397508255	R555G	DECREASE stability	-1.8597025	Decrease	7	Decrease	0.816327
rs75549581	A559S	DECREASE stability	-1.0994891	Decrease	9	Decrease	0.864647
rs397508259	A559E	DECREASE stability	-0.8854481	Decrease	7	Decrease	0.511478
rs397508260	R560G	DECREASE stability	-1.8293962	Decrease	7	Decrease	0.829416
rs121909006	Y563N	DECREASE stability	-1.2866212	Decrease	5	Decrease	0.788303
rs397508276	Y569D	DECREASE stability	-1.6791017	Decrease	6	Decrease	0.761464
rs397508277	Y569C	DECREASE stability	-1.4916056	Decrease	6	Decrease	0.777235
rs397508282	D572N	DECREASE stability	-0.7668229	Decrease	7	Decrease	0.577362
rs748393295	D572E	DECREASE stability	-0.41672522	Decrease	1	Increase	0.641062
rs121908758	P574H	DECREASE stability	-1.707245	Decrease	8	Decrease	0.807257
rs1800100	R668C	DECREASE stability	-0.743323	Decrease	3	Decrease	0.794376
rs186089140	S737F	DECREASE stability	-0.6939322	increase	6	Decrease	0.508201
rs397508363	R766M	DECREASE stability	-0.4649359	Decrease	5	Increase	0.595122
rs1386366130	Q767H	DECREASE stability	-1.1677499	Decrease	7	Decrease	0.736198
rs1299482973	S707F	INCREASE stability	0.3493291	increase	1	Increase	0.809512

rs397508375	D806G	DECREASE stability	-1.4655821	Decrease	2	Decrease	0.797931
rs757165481	Y849H	DECREASE stability	-1.4566337	Decrease	2	Decrease	0.84272
rs775570582	L165S	DECREASE stability	-2.5088231	Decrease	8	Decrease	0.896556
rs1402844924	L165F	DECREASE stability	-1.5734354	Decrease	3	Decrease	0.892523
rs121909035	H949Y	DECREASE stability	-0.680929	increase	7	Increase	0.523866
rs397508444	H949R	DECREASE stability	-0.7707563	Decrease	1	Decrease	0.756359
rs1191342069	G1241D	DECREASE stability	-0.8034987	increase	1	Increase	0.729624
rs397508599	G1244R	DECREASE stability	-0.6867931	increase	0	Decrease	0.57188
rs267606723	G1244E	DECREASE stability	-0.5285789	increase	7	Decrease	0.558142
rs397508602	G1249R	DECREASE stability	-0.6374709	Decrease	0	Increase	0.739014
rs121909040	G1249E	DECREASE stability	-0.4102457	increase	7	Increase	0.754535
rs117400534	L1253F	DECREASE stability	-1.0673433	Decrease	7	Decrease	0.867705
rs11971167	D1270Y	DECREASE stability	-0.9460165	increase	4	Decrease	0.513168
rs765549490	D1270G	DECREASE stability	-1.7353752	Decrease	1	Decrease	0.803916
rs753920616	F508V	DECREASE stability	-1.360253	Decrease	8	Decrease	0.842255
rs77010898	W1282C	DECREASE stability	-0.6226598	Decrease	8	Decrease	0.879048
rs77902683	R1283M	DECREASE stability	-0.3487679	Decrease	6	Increase	0.588298
rs904990724	G1298R	DECREASE stability	-0.3476638	Decrease	7	Increase	0.623493
rs193922522	G1298A	DECREASE stability	-0.59709621	Decrease	8	Decrease	0.77595
rs121909042	N1303H	DECREASE stability	-1.0868868	Decrease	9	Decrease	0.767533
rs121909042	N1303Y	DECREASE stability	-0.50017672	Decrease	1	Decrease	0.73393
rs397508636	N1303I	DECREASE stability	-0.19755439	increase	4	Increase	0.559203
rs80034486	N1303K	DECREASE stability	-1.0937566	Decrease	6	Decrease	0.750646
rs201503139	P1306S	DECREASE stability	-0.9820391	Decrease	8	Decrease	0.820418
rs397508646	D1312G	DECREASE stability	-1.404051	increase	6	Decrease	0.513825
rs397508653	L1324P	DECREASE stability	-1.9579279	Decrease	7	Decrease	0.876623
rs755917129	I1267M	DECREASE stability	-1.0247056	Decrease	8	Increase	0.607692
rs145545286	L1335F	DECREASE stability	-1.2160428	Decrease	6	Decrease	0.887374
rs397508660	L1339F	DECREASE stability	-1.1785594	Decrease	4	Decrease	0.849935
rs544710550	L1339P	DECREASE stability	-2.1528361	Decrease	5	Decrease	0.853875
rs747324955	G1343S	DECREASE stability	-0.9196335	Decrease	6	Decrease	0.676292
rs773458471	G1343V	DECREASE stability	-0.3173998	Decrease	4	Decrease	0.628187
rs1313341594	L1346Q	DECREASE stability	-1.334338	Decrease	7	Decrease	0.85213
rs201686600	G1349S	DECREASE stability	-1.1678918	Decrease	5	Decrease	0.863195
rs113857788	Q1352H	DECREASE stability	-0.478542	Decrease	7	Decrease	0.86203
rs1252048837	L1356S	DECREASE stability	-1.9304028	Decrease	8	Decrease	0.832741
rs748223886	R1358T	DECREASE stability	-1.2758966	Decrease	4	Decrease	0.812788
rs397508670	A1364V	DECREASE stability	-1.1830918	increase	5	Decrease	0.620044
rs770345073	I1366F	DECREASE stability	-1.1200946	Decrease	6	Decrease	0.892195
rs200955612	I1366N	DECREASE stability	-1.6891954	Decrease	4	Decrease	0.869505
rs761271867	I1366M	DECREASE stability	-0.93357778	Decrease	7	Decrease	0.875433
rs767002769	L1369F	DECREASE stability	-1.2780019	Decrease	3	Decrease	0.807223
rs760336091	D1370H	DECREASE stability	-1.2839117	Decrease	5	Decrease	0.695465

Table S4. Structural validation of wild-type and mutant protein models using SAVES v6.1 and TM-align.

	ERRAT	ProCheck				Verify 3D	TM Align	
rs ID	**Score**	**Core**	**Allow**	**Generously**	**Disallowed**	**Score**	**RMSD**	**TM score**
Q2IBA1.1.A	97.524	88.10%	8.10%	1.50%	1.80%	52.39%		
A559E	81.0252	88.50%	9.50%	1.00%	1.00%	8.37%	0.89	0.99467
A559S	79.495	88.90%	8.90%	1.20%	1.00%	8.87%	0.85	0.99562
C524R	79.6507	89.20%	8.30%	1.60%	0.90%	9.01%	0.82	0.99553
G480D	82.7454	88.30%	9.30%	1.30%	1.10%	9.30%	0.79	0.99576
G480S	79.7864	88.70%	9.00%	1.60%	0.60%	9.16%	0.69	0.99682
G545V	80.6279	88.40%	8.80%	1.70%	1.10%	8.51%	0.89	0.99544
G1249R	80.6748	88.50%	9.20%	1.30%	1.10%	8.44%	0.93	0.99497
K273Q	83.8258	88.10%	9.50%	1.60%	0.80%	8.37%	0.93	0.99491
L102P	81	89.40%	8.10%	1.60%	0.90%	9.08%	0.85	0.99262
P99L	82.479	88.50%	9.40%	1.10%	0.90%	9.37%	0.76	0.9961
P205R	79.3025	88.90%	8.60%	1.60%	0.90%	10.59%	0.92	0.99488
W496C	82.1705	88.50%	9.30%	1.20%	1.00%	9.23%	0.67	0.99698
Y161D	81.5159	88.50%	9.80%	1.10%	0.60%	9.08%	0.69	0.99672
Y161S	81.8462	89.10%	8.20%	1.60%	1.00%	8.66%	0.62	0.99736
P574H	82.7586	88.20%	9.70%	1.20%	0.90%	8.94%	0.72	0.99652
R258I	81.6031	89.30%	8.60%	1.30%	0.80%	8.51%	0.79	0.99595
W277R	82.5348	88.80%	8.80%	1.40%	1.00%	8.80%	0.71	0.99658
R560G	82.1705	88.50%	9.40%	1.20%	0.90%	9.51%	0.67	0.99695
L1324P	82.1835	88.40%	9.30%	1.10%	1.20%	9.23%	0.76	0.99612
N1303Y	81.0146	88.50%	9.10%	1.00%	1.30%	9.59%	0.74	0.99637
R555G	80.784	88.40%	9.30%	1.40%	0.90%	8.80%	0.8	0.99605
L468P	76.9406	87.80%	9.90%	1.40%	0.90%	9.66%	0.63	0.99733
L548P	80.8623	88.40%	9.80%	1.10%	0.70%	9.44%	0.61	0.99746
I105N	81.4043	88.40%	9.20%	1.60%	0.90%	10.09%	0.98	0.99449
I506S	82.2119	87.90%	10.20%	1.10%	0.80%	8.44%	0.84	0.99486
G149E	80.1836	89.10%	8.80%	1.00%	1.10%	8.80%	0.65	0.9971
L441P	81.6577	89.20%	8.60%	1.10%	1.10%	9.44%	0.9	0.99489
L467P	82.2941	89.00%	8.70%	1.20%	1.10%	8.94%	0.7	0.99672
D1370H	80.9451	88.80%	9.00%	1.20%	1.00%	9.44%	0.73	0.99647
F508V	82.7957	88.90%	9.00%	1.30%	0.90%	9.01%	0.63	0.99732

Table S5. Interacting residues obtained from docking. CFTR and G1249R, I105N, and K273Q mutant protein structures with ligands show interaction residues and hydrophobic associations.

Receptor-Ligands	Hydrophilic bonded interactions	Hydrophobic bonded interactions
CFTR+ Apoptozole	GLN376, LEU375, GLU379, GLN378, LYS381, LYS166, TRP57, GLU54	LYS377, GLN376, LEU61, PRO67, LEU159, LYS162
CFTR+ Chromophore	ASN1262, SER962, LEU1260, ASP1275, ILE1277, TRP1274, ASN1274, ASN1184, LYS1177, THR1278, GLU1280, GLN258, GLU1221, MET961	LEU1279, ARG1259
CFTR+ Congo Red	ARG1259, LEU1260, LEU1279, TRP1274, SER1276, ASN1184, THR1278, ILE`177, LYS1177, SER962, GLU1221, ASN1262, LEU1261, MET961, GLN1186	LEU1187, PRO96
CFTR+ Cpd-β	SER1188, THR1278, THR1263, ASN1184, SER1276, ILE1222, TRP1224, LEU1260, SER962, LEU1961	LEU1229, ARG1259, MET961, PRO960, ASN1262, LEU1229

CFTR+ cAMP	GLN378, LYS181, TYR380, SER168, GLU474, ARG170, LEU475, TRP401, SER478, PRO477	GLU476, GLU403
CFTR+ Melanin	TYR1073, GLU504, PRO499, THR1053, HIS1054, THR1057, PHE1074	LEU1077
G1249R + Apoptozole	LEU1279, ARG1259, THR1278, LEU1187, ALA959, SER955, THR1176, GLU279, GLN1280	ILE1277, GLN1186, GLY1185, GLN958, PRO1175, PRO960, GLU278, LEU957
G1249R + Chromophore	GLU278, ARG1283, LEU1261, MET961, ARG1259, LEU1260, PRO960, TRP1274, LYS1177, ILE1277, THR1278, ASN1184, PRO1175, ASP1275, ALA595, THR1176, GLN958	LYS273, LEU1279
G1249R + Congo Red	VAL171, GLN179, SER182, ASN186, ASN187, ILE371, PHE374, ARG170, LYS370, GLN378	LYS174, LYS377, LEU183, ILE175, LYS370
G1249R + Melanin	SER422, ASN423, GLU424, PHE409, LYS411, ALA412, LYS413, GLU410, GLN414, ASN418	THR421, ALA412
G1249R + NAD	GLN958, LEU1260, MET961, ARG1259, PRO960, LEU1261, THR1263, ASN1262, SER962,THR1220, GLU1221, LYS1174, THR1776, GLU278, ALA959, LEU957	ARG1283, LYS273
G1249R + Nelfinavir	SER962, THR1278, ARG1283, LYS273, LEU957, GLU279, PRO1175, PRO960, MET961, LEU1261, ASN1262, SER962	LEU1279, ARG1259, GLU278
I105N + Apoptozole	GLU402, SER431, GLY437, ASP173, PHE430, SER176, LEU428	ARG170, LEU436, PHE405, SER431, TRP401, LYS174
I105N + Chromophore	ARG1283, GLU1221, ASN1262, THR1220, SER962, LEU1261, TRP1274, THR1278, ILE1277, ALA959, PRO1175, THR1176, LYS273, GLN958, PRO960	ARG1259, LEU1279
I105N + cAMP	ASN1262, MET961, ALA959, ARG1283, LYS273, GLN958, PRO1175, PRO960, LEU1260, LEU1261, THR1263, ASN126	ARG1259
I105N + Congo Red	GLN958, HIS954, ASN1184, LYS1183, SER1276, ASP1275,ILE1277, GLN1280, LYS273, GLU282, GLU279	SER1188, LYS1177, GLU278, LEU957, THR1278
I105N + NAD	ARG1283, LEU1260, LEU1261, LEU1279, ASN1262, TRP1274, LYS1177, GLN1186, ASN1184, ALA959, GLN958, GLY1185, SER1188, SER1276, THR1278, MET961, PRO960, PRO1175	ILE1277, ARG1259
I105N + Cpd-β	CYS276, HIS954, GLU282, GLN958, LYS273, GLN1280, GLN1309, TYR1307	GLU279, LEU957, GLU278
K273Q + Apoptozole	GLN1280, ASP1275, THR1278, GLU278, GLN158, ALA959, THR1176, PRO960, ASN1262, LEU1261, LYS1177, ARG1259,MET96	TRP1274, ILE1277,PRO1175
K273Q + Chromophore	PHE430, GLN179, ASP373, LYS370, LEU183, LYS377, PHE374,VAL1171, ARG170, LEU428	LYS174, ILE175, PHE429
K273Q + Melanin	ILE175, PHE374, LYS377, LEU183, GLN179, SER182	ASP373, LYS370
K273Q + Congo Red	SER1178, LYS1180, GLY1185, PRO1175, ARG1259, LYS1177, GLN258, GLN273, ALA259, ARG1283, LEU1260	PRO960, THR1176, LEU1279, ASN1184, LYS1183
I105N + NAD	LEU957, PRO1175, GLN273, ARG1283, LEU1279, THR1278, SER118, PRO960, ARG1283, LEU1187, GLN273, ASN1184, LYS1177	TRP1274, ARG1259
K273Q + Nelfinavir	GLU278, GLU273, ARG1283, GLN958, MET961, SER1188, THR1278, LYS1177, GLN1280, TRP1274, ILE1277, ASN1275, SER1276, SER1188	PRO960, ILE1279