



Supplementary Material

Studies on the Mitochondrial tRNA Gene Variants in Patients with Coronary Artery Disease and Pathogenicity Assessment by *in silico* Analysis

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Supplementary Fig. S1. Sequence alignment of normal and mutant mtRNA the mutant residues are highlighted in black (A). tRNA^{Pro} showing the variant U13C (B). tRNA^{Leu2} variant U20C (C). tRNA^{Leu2} variant A43G (D). tRNA^{Thr} variant G40A.

Supplementary Table SI. Comparison between the interaction of normal and mutant tRNA^{PRO} and prolyl-tRNA synthetase.

Index	Normal					Mutant				
	Residue	AA	Distance H-A	Donor Atom	Acceptor Atom	Residue	AA	Distance H-A	Donor Atom	Acceptor Atom
1	1034R	LYS	2.17	305 (N3+)	7862 (O3)	1034R	LYS	3.11	305 (N3+)	7909 (O3)
2	1036R	GLU	1.84	9525 (Npl)	337 (O.co2)	1050R	ARG	1.97	563 (Ng+)	9526 (Npl)
3	1050R	ARG	2.86	563 (Ng+)	9513 (O-)	1050R	ARG	3.04	560 (Ng+)	9526 (Npl)
4	1054R	TYR	2.36	8255 (Nam)	636 (O3)	1052R	TRP	2.77	591 (Nam)	9559 (Npl)
5	1058R	GLU	2.49	8225 (Nam)	706 (O.co2)	1054R	TYR	1.79	636 (O3)	9481 (O-)
6	1061R	LYS	1.56	751 (N3+)	8224 (O2)	1331R	ARG	2.23	4983 (Ng+)	9595 (O3)
7	1075R	ASN	2.01	981 (Nam)	8275 (O-)	1342R	ARG	2.7	5193 (Ng+)	9564 (O3)
8	1147R	TRP	1.7	2124 (Nam)	8274 (O2)	1345R	LEU	1.69	5230 (Nam)	9640 (O2)
9	1342R	ARG	3.3	5193 (Ng+)	9530 (O3)	1346R	ARG	2.92	5258 (Ng+)	7970 (Npl)
10	1342R	ARG	2.96	5194 (Ng+)	9521 (N2)	1346R	ARG	2.32	5249 (Nam)	9640 (O2)
11	1345R	LEU	3.04	5230 (Nam)	9609 (O2)	1349R	TYR	2.35	7937 (Npl)	5310 (O3)
12	1346R	ARG	2.95	5258 (Ng+)	9523 (N2)	1349R	TYR	1.93	5310 (O3)	9746 (Npl)
13	1346R	ARG	3.48	5259 (Ng+)	9523 (N2)	1350R	SER	1.59	5325 (O3)	7858 (O-)
14	1348R	ASN	1.62	5292 (Nam)	9673 (O-)	1353R	TRP	1.87	5360 (Nar)	7906 (N2)
15	1349R	TYR	2.96	9492 (Npl)	5310 (O3)	1353R	TRP	2.51	5352 (Nam)	7858 (O-)
16	1349R	TYR	2.69	7937 (Npl)	5310 (O3)	1356R	ASN	1.71	5425 (Nam)	7890 (O2)
17	1349R	TYR	1.72	5310 (O3)	9715 (O2)	1361R	LYS	3.02	5515 (N3+)	9557 (N2)
18	1350R	SER	1.71	5325 (O3)	7791 (O-)					
19	1352R	GLY	2.67	5345 (Nam)	7790 (O2)					
20	1353R	TRP	1.94	5360 (Nar)	7872 (N2)					
21	1356R	ASN	1.67	5425 (Nam)	7857 (O2)					
22	1361R	LYS	2.96	5515 (N3+)	9530 (O3)					

Supplementary Table SII. Comparison between the interaction of normal and mutant tRNA^{THR} and threonyl-tRNA synthetase.

Index	Normal			Mutant				
	Residue	AA	Distance H-A	Residue	AA	Distance H-A	Donor Atom	Acceptor Atom
1	354R	ARG	2.54	357T	ARG	3.3	65 (Ng+)	7760 (O3)
2	354R	ARG	3.05	357T	ARG	2.4	64 (Ng+)	7622 (N2)
3	354R	ARG	2.84	521T	SER	3.14	7053 (Npl)	2764 (O2)
4	354R	ARG	2.15	521T	SER	1.9	2766 (O3)	7012 (O3)
5	358R	LYS	3.68	526T	SER	1.93	2840 (O3)	7088 (N2)
6	526R	SER	2.59	582T	LYS	2.69	3733 (N3+)	7151 (N2)
7	526R	SER	2.38	526T	SE	3.08	3830 (O3)	7107 (O-)
8	582R	LYS	1.93	582T	LYS	1.69	5415 (O3)	6657 (O-)
9	582R	LYS	2.95	692T	ASN	1.79	5443 (Nam)	6657 (O-)
10	691R	LEU	2.55	696T	ARG	3.01	5529 (Ng+)	6581 (O3)
11	692R	ASN	1.95	726T	ASN	1.53	6018 (Nam)	6597 (O-)
12	692R	ASN	2.8	731T	GLU	1.94	6087 (Nam)	6800 (O2)
13	696R	ARG	3.31	696T	ARG	3.55	6109 (Ng+)	6830 (Npl)
14	696R	ARG	2.36	732T	ARG	1.62	6112 (Ng+)	6863 (O2)
15	722R	ARG	2.75	732T	ARG	2.38	6111 (Ng+)	6863 (O2)
16	726R	ASN	2.31	740T	ARG	2.11	6242 (Ng+)	6928 (N2)
17	728R	VAL	3.22	743T	GLN	1.71	6301 (Nam)	6947 (O-)
18	751R	GLN	3.06	749T	SER	2.92	6415 (O3)	6992 (Npl)
19	751R	GLN	3.27	750T	LYS	1.97	6429 (N3+)	7023 (O2)

Supplementary Table SIII. Comparison between the interaction of normal and mutant tRNA^{Leu2} variant U20C, tRNA^{Leu2} variant A43G and threonyl-tRNA synthetase.

In- dex	Normal			tRNA ^{Leu2} variant U20C					tRNA ^{Leu2} variant A43G				
	Resi- due	AA	Distance H-A	Resi- due	AA	Distance H-A	Donor Atom	Acceptor Atom	Resi- due	AA	Distance H-A	Donor Atom	Acceptor Atom
1	354R	ARG	2.54	357T	ARG	3.3	65 (Ng+)	7760 (O3)	262R	GLN	2.46	3625 (Nam)	17312 (O2)
2	354R	ARG	3.05	357T	ARG	2.4	64 (Ng+)	7622 (N2)	457R	ARG	2.35	6695 (Ng+)	17186 (O-)
3	354R	ARG	2.84	521T	SER	3.14	7053 (Npl)	2764 (O2)	473R	TYR	2	6978 (O3)	17377 (O2)
4	354R	ARG	2.15	521T	SER	1.9	2766 (O3)	7012 (O3)	512R	LYS	1.83	7602 (N3+)	17254 (N2)
5	358R	LYS	3.68	526T	SER	1.93	2840 (O3)	7088 (N2)	559R	ARG	1.56	8359 (Ng+)	17418 (O2)
6	526R	SER	2.59	582T	LYS	2.69	3733 (N3+)	7151 (N2)	559R	ARG	3.06	8360 (Ng+)	17418 (O2)
7	526R	SER	2.38	588T	TYR	3.08	3830 (O3)	7107 (O-)	907R	HIS	3.21	16722 (Npl)	13896 (Nar)
8	582R	LYS	1.93	690T	THR	1.69	5415 (O3)	6657 (O-)	907R	HIS	2.27	13893 (Nar)	16688 (O2)
9	582R	LYS	2.95	692T	ASN	1.79	5443 (Nam)	6657 (O-)	910R	ARG	2.49	13945 (Ng+)	16654 (N2)
10	691R	LEU	2.55	696T	ARG	3.01	5529 (Ng+)	6581 (O3)	914R	LYS	2.22	14029 (N3+)	16627 (N2)
11	692R	ASN	1.95	726T	ASN	1.53	6018 (Nam)	6597 (O-)	915R	ASN	1.96	16593 (Nam)	14046 (O2)
12	692R	ASN	2.8	731T	GLU	1.94	6087 (Nam)	6800 (O2)	966R	LEU	2.95	14614 (Nam)	17569 (O2)
13	696R	ARG	3.31	732T	ARG	3.55	6109 (Ng+)	6830 (Npl)	969R	ASN	1.7	14666 (Nam)	17637 (O3)
14	696R	ARG	2.36	732T	ARG	1.62	6112 (Ng+)	6863 (O2)	983R	LYS	2.02	18445 (Npl)	14871 (O2)
15	722R	ARG	2.75	732T	ARG	2.38	6111 (Ng+)	6863 (O2)	983R	LYS	1.63	14876 (N3+)	18025 (O2)
16	726R	ASN	2.31	740T	ARG	2.11	6242 (Ng+)	6928 (N2)	984R	LYS	1.67	14898 (N3+)	18061 (O3)
17	728R	VAL	3.22	743T	GLN	1.71	6301 (Nam)	6947 (O-)	987R	LYS	1.67	14958 (N3+)	18412 (O2)
18	751R	GLN	3.06	749T	SER	2.92	6415 (O3)	6992 (Npl)	1001R	GLU	3.46	17554 (O3)	15201(O.co2)
19	751R	GLN	3.27	750T	LYS	1.97	6429 (N3+)	7023 (O2)	1002R	LYS	2.36	15216 (N3+)	16818 (Nam)
20	965R	LYS	2.66	751R	GLN	1.99	6242 (Ng+)	6928 (N2)	100R	LYS2	2.40		