

Analysis of Coxsackievirus B5 Infections in the Central Nervous System in Brazil: Insights into Molecular Epidemiology and Genetic Diversity

Table S1. In silico Analysis of Virus Asymmetric Unit Mutations.

MUT	%(VOL)	1-hydrophathy	2-hydrophathy	Provean Result	Faulkner SASA%	Mutation SASA%
G4E	130.28	-0.4	-3.50	Neutral	NC	NC
A6S	0.45	1.8	-0.8	Neutral	NC	NC
I7V	-16.02	4.5	4.2	Neutral	NC	NC
R9Q	-17.07	-4.5	-3.5	Neutral	NC	NC
I18M	-2.28	4.5	1.9	Neutral	62.05	79.11
G19E	130.28	-0.4	-3.50	Neutral	53.36	63.01
G19S	48.09	-0.4	-0.8	Neutral	53.36	49.00
K54R	2.85	-3.9	-4.5	Neutral	36.45	56.61
H82Y	26.37	-3.2	-1.3	Neutral	51.26	45.98
T84A	-23.69	-0.7	1.8	Neutral	71.24	65.76
D87N	2.70	-3.50	-3.5	Neutral	55.96	58.80
A90G	-32.17	1.8	-0.4	Neutral	4.79	3.81
A90T	31.04	1.8	-0.7	Neutral	4.79	3.81
Q91Y	34.63	-3.5	-1.3	Neutral	44.26	54.42
N95S	-22.00	-3.5	-0.8	Neutral	6.77	8.01
S125T	30.45	-0.8	-0.7	Neutral	3.56	4.79
T130A	-23.69	-0.7	1.8	Deleterious	81.04	88.36
T130N	-1.72	-0.7	-3.5	Deleterious	81.04	75.59
K132Q	-14.71	-3.9	-3.5	Neutral	53.91	47.17
S136A	-0.45	-0.8	1.8	Neutral	21.45	35.62
V156I	19.07	4.2	4.5	Neutral	19.56	17.27
S158C	21.91	-0.8	2.5	Neutral	18.92	15.53
V169I	19.07	4.2	4.5	Neutral	3.50	23.15
M180I	2.33	1.9	4.5	Neutral	8.26	10.11
R200K	-2.77	-4.5	-3.90	Neutral	53.36	45.24
V235A	-36.71	4.2	1.8	Neutral	0.00	0.00
V235I	19.07	4.2	4.5	Neutral	0.00	0.00
V248I	19.07	4.2	4.5	Neutral	0.00	0.00
Q258E	-3.76	-3.5	-3.50	Neutral	28.50	33.14
N262S	21.30	-3.5	-3.50	Neutral	27.20	12.38
S268T	30.45	-0.8	-0.7	Neutral	29.04	26.75
G273S	48.09	-0.4	-0.8	Neutral	39.09	29.78
T275I	43.58	-0.7	4.5	Neutral	59.22	62.29
D276E	24.57	-3.50	-3.50	Neutral	32.07	40.53
T279A	-23.69	-0.7	1.8	Neutral	16.70	18.92

MUT, the position, and mutation in the amino acid one-letter code. %VOL, the percentual of volume change using the residue in the prototypic Faulkner strain. 1-Hydrophathy and 2-Hydrophathy, the hydrophathy parameter using the Kyte and Doolittle scale [29] for the prototypic residue and the mutation, respectively. The Provean result, the Provean algorithm classification for the mutation. Faulkner SASA% and Mutation SASA%, the percentual change in the solvent-accessible surface area (SASA) of amino acid residue in the asymmetric unit using as reference the SASA value for the

maximum surface exposure. Residues with a SASA value of less than 10% are colored in red, with the high-frequency mutations highlighted in yellow. NC, not calculated, The Faulkner SASA% and Mutation SASA% values were not calculated for residues G4, A6, I7, and R9 due to the location at the disordered N-terminal, which is not present in the structural models.