|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sr. No.** | **Mutations** | **DynaMut** | **iSTABLE** | **PremPS** |
| **ΔΔG kcal/mol** | **ΔΔG ENCoM kcal/mol** | **Δ Vibrational Entropy Energy (kcal/mol/K)** | **iMutant** | **Mupro** | **iSTABLE** | **ΔΔG kcal/mol** | **Location** |
| **Stability** | **ΔΔG kcal/mol** | **Stability** | **Conf. Score** | **Stability** | **Conf. Score** |
| 1 | A438T | -0.703 | 0.073 | -0.091 | Decrease | -0.81 | Decrease | -0.57202 | Decrease | 0.857809 | 1.41 | COR |
| 2 | A266V | 0.164 | 0.211 | -0.264 | Increase | 0 | Increase | 0.5893789 | Increase | 0.719844 | 0.3 | SUR |
| 3 | A435V | 0.411 | 0.327 | -0.408 | Decrease | -0.61 | Increase | 0.1668029 | Decrease | 0.530748 | 0.34 | COR |
| 4 | A438T | -0.703 | 0.073 | -0.091 | Decrease | -0.81 | Decrease | -0.57202 | Decrease | 0.857809 | 1.41 | COR |
| 5 | D160N | -0.068 | 0.119 | -0.148 | Decrease | null | Increase | 0.0705657 | Increase | 0.659769 | -0.13 | SUR |
| 6 | D202N | 0.118 | 0.098 | -0.123 | Decrease | -0.49 | Increase | 0.0890481 | Decrease | 0.547724 | 0.04 | SUR |
| 7 | D259V | 0.223 | -0.185 | 0.231 | Increase | 0.38 | Increase | 0.2114204 | Increase | 0.783784 | 0.01 | SUR |
| 8 | D279H | 0.241 | -0.05 | 0.063 | Decrease | -0.47 | Decrease | -0.585359 | Decrease | 0.725886 | -0.28 | SUR |
| 9 | D279N | 0.466 | -0.024 | 0.03 | Decrease | -0.65 | Decrease | -0.26929 | Decrease | 0.678655 | -0.56 | SUR |
| 10 | D279V | 0.364 | -0.059 | 0.074 | Decrease | 0.03 | Decrease | -0.647436 | Decrease | 0.727034 | -0.25 | SUR |
| 11 | D280N | 0.269 | -0.09 | 0.112 | Decrease | 0.03 | Decrease | -0.647436 | Decrease | 0.727034 | -0.56 | SUR |
| 12 | D380H | 0.346 | -0.06 | 0.075 | Decrease | -0.59 | Decrease | -0.630548 | Decrease | 0.792147 | -0.08 | SUR |
| 13 | E104K | 0.677 | -0.013 | 0.016 | Decrease | -0.23 | Increase | 0.1530343 | Decrease | 0.512288 | -0.02 | SUR |
| 14 | E142K | 0.611 | 0.363 | -0.454 | Decrease | -1.05 | Decrease | -0.729462 | Decrease | 0.854687 | 0.62 | COR |
| 15 | E164G | -0.391 | -0.012 | 0.015 | Decrease | -1.32 | Decrease | -0.812906 | Decrease | 0.852834 | 0.58 | SUR |
| 16 | E189K | -0.015 | 0.137 | -0.171 | Decrease | -1.34 | Decrease | -0.993354 | Decrease | 0.735389 | 0.07 | SUR |
| 17 | E236K | -0.326 | 0.081 | -0.102 | Decrease | -0.65 | Decrease | -0.190256 | Decrease | 0.849335 | 0.15 | SUR |
| 18 | E277G | -0.641 | -0.507 | 0.634 | Decrease | -1.63 | Decrease | -0.2033 | Decrease | 0.848988 | -0.09 | SUR |
| 19 | E287K | -0.985 | 0.13 | -0.162 | Decrease | -1.29 | Decrease | -0.335751 | Decrease | 0.841467 | 1.23 | COR |
| 20 | E329K | 0.49 | 0.315 | -0.394 | Decrease | -0.93 | Decrease | -0.416894 | Decrease | 0.796461 | 0.27 | SUR |
| 21 | E33G | -0.095 | -1.212 | 1.515 | Decrease | -1.42 | Decrease | -1 | Decrease | 0.887388 | 0.7 | COR |
| 22 | E343K | -0.143 | -0.049 | 0.061 | Decrease | -0.69 | Decrease | -0.228688 | Decrease | 0.891085 | 0.1 | SUR |
| 23 | E360D | -0.305 | -0.031 | 0.039 | Decrease | -0.04 | Increase | 0.2437461 | Decrease | 0.514238 | -0.13 | SUR |
| 24 | E364K | -0.224 | 0.009 | -0.012 | Decrease | -0.97 | Decrease | -0.312994 | Decrease | 0.784894 | -0.18 | SUR |
| 25 | E379K | -0.053 | -0.087 | 0.109 | Decrease | -1.11 | Decrease | -1 | Decrease | 0.803358 | -0.27 | SUR |
| 26 | E422K | 0.735 | -0.123 | 0.154 | Decrease | -0.68 | Decrease | -0.73734 | Decrease | 0.826613 | 0.21 | SUR |
| 27 | E441K | -0.505 | -0.068 | 0.085 | Decrease | -0.49 | Decrease | -1 | Decrease | 0.795435 | -0.18 | SUR |
| 28 | E45K | -0.644 | -0.554 | 0.692 | Decrease | -0.7 | Decrease | -0.729867 | Decrease | 0.81557 | 0.87 | COR |
| 29 | E65K | 0.744 | 0.315 | -0.394 | Decrease | -0.43 | Increase | 0.4665144 | Decrease | 0.538181 | 0.2 | COR |
| 30 | E66K | 0.592 | 0.219 | -0.273 | null | -0.43 | Decrease | -1 | Decrease | 0.809755 | -0.06 | SUR |
| 31 | E87D | -0.303 | -0.138 | 0.172 | Decrease | -0.37 | Decrease | -0.058508 | Decrease | 0.872645 | 0.5 | SUR |
| 32 | E90K | 0.103 | 0.216 | -0.27 | Decrease | -0.64 | Decrease | -0.348192 | Decrease | 0.804723 | 0.45 | SUR |
| 33 | F124I | -0.412 | -0.72 | 0.9 | Decrease | -0.83 | Decrease | -1 | Decrease | 0.765752 | 1.66 | COR |
| 34 | F195L | -0.001 | -0.455 | 0.568 | Decrease | -0.55 | Decrease | -1 | Decrease | 0.730661 | 0.97 | SUR |
| 35 | F219L | 0.102 | -0.986 | 1.232 | Decrease | -1.15 | Decrease | -0.209637 | Decrease | 0.668542 | 0.08 | SUR |
| 36 | F267L | -0.479 | -0.289 | 0.361 | Decrease | -0.71 | Decrease | -0.294853 | Decrease | 0.727071 | -0.09 | SUR |
| 37 | F430C | -0.756 | -0.629 | 0.786 | Decrease | -2.01 | Decrease | -0.94016 | Decrease | 0.851349 | 2.4 | COR |
| 38 | G137D | 0.702 | 0.344 | -0.431 | Decrease | -0.72 | Increase | 0.14931 | Increase | 0.507348 | 0.85 | SUR |
| 39 | G22R | -0.147 | -0.003 | 0.004 | Decrease | -0.43 | Decrease | -0.438191 | Decrease | 0.699248 | -0.1 | SUR |
| 40 | G401A | -1.127 | 0.049 | -0.061 | Decrease | -0.75 | Increase | 0.0714063 | Increase | 0.617953 | 0.13 | SUR |
| 41 | G52R | 2.558 | 0.859 | -1.073 | Decrease | -0.98 | Decrease | -0.102523 | Decrease | 0.802839 | 1.01 | SUR |
| 42 | H205R | -0.122 | -0.298 | 0.372 | Decrease | 0.15 | Decrease | -0.493013 | Decrease | 0.757935 | 0.87 | SUR |
| 43 | I275L | 0.233 | 0.003 | -0.004 | Decrease | -0.17 | Increase | 0.4304644 | Increase | 0.507031 | -0.47 | SUR |
| 44 | I288V | -1.416 | -0.284 | 0.354 | Decrease | -1.05 | Decrease | -0.973285 | Decrease | 0.894212 | 1.02 | COR |
| 45 | K123T | -0.203 | -0.382 | 0.477 | Decrease | -0.38 | Decrease | -0.51509 | Decrease | 0.726236 | 0.27 | SUR |
| 46 | K79M | 0.41 | -0.219 | 0.273 | Increase | -0.08 | Increase | 0.0013308 | Increase | 0.67761 | 0.54 | COR |
| 47 | L21P | -0.685 | -1.242 | 1.553 | Decrease | -1.36 | Decrease | -0.67207 | Decrease | 0.911386 | 1.88 | COR |
| 48 | L248F | 0.439 | 0.221 | -0.276 | Decrease | -0.17 | Increase | 0.4304644 | Increase | 0.507031 | -0.92 | SUR |
| 49 | L327F | 0.525 | 0.266 | -0.332 | Decrease | -0.7 | Decrease | -1 | Decrease | 0.839003 | -0.88 | COR |
| 50 | L331I | 0.113 | -0.019 | 0.023 | Decrease | -1.21 | Decrease | -0.84466 | Decrease | 0.783999 | 0.8 | COR |
| 51 | L344Q | -0.667 | -0.083 | 0.103 | Decrease | -2.03 | Decrease | -1 | Decrease | 0.882334 | 2.56 | COR |
| 52 | L59F | 1.061 | 0.537 | -0.671 | Decrease | -0.63 | Decrease | -0.572611 | Decrease | 0.852957 | 0.13 | SUR |
| 53 | M122I | -0.081 | -0.216 | 0.27 | Decrease | -0.64 | Decrease | -1 | Decrease | 0.77225 | 0.54 | SUR |
| 54 | M250I | 0.373 | 0 | 0 | Increase | -0.48 | Decrease | -0.495835 | Decrease | 0.561042 | 1.32 | COR |
| 55 | M258I | -0.044 | -0.25 | 0.313 | Increase | -0.75 | Decrease | -0.471965 | Decrease | 0.525856 | 0.86 | COR |
| 56 | M298I | -0.207 | -0.114 | 0.143 | Decrease | -1.15 | Decrease | -0.534325 | Decrease | 0.843696 | 0.88 | COR |
| 57 | M34V | -0.182 | -0.205 | 0.256 | Decrease | -1.29 | Decrease | -0.238979 | Decrease | 0.747749 | 0.8 | COR |
| 58 | N239I | 0.944 | 0.366 | -0.458 | Increase | 0.62 | Increase | 0.1677194 | Increase | 0.875654 | 0.2 | SUR |
| 59 | N427T | 0.404 | 0.196 | -0.245 | Increase | 0.24 | Decrease | -0.724318 | Decrease | 0.645298 | 0.33 | COR |
| 60 | P208L | 1.965 | 0.204 | -0.255 | Decrease | -0.29 | Decrease | -0.127473 | Decrease | 0.690688 | 0.13 | COR |
| 61 | P216T | 0.893 | 0.55 | -0.688 | Decrease | -0.99 | Decrease | -1 | Decrease | 0.822555 | 0.29 | COR |
| 62 | P221L | 2.633 | 0.541 | -0.676 | Decrease | -0.06 | Decrease | -0.327614 | Increase | 0.5 | 0.44 | SUR |
| 63 | P234L | 1.24 | 0.471 | -0.589 | Decrease | -0.25 | Increase | 0.140432 | Increase | 0.582478 | -0.45 | SUR |
| 64 | P234S | 0.846 | 0.227 | -0.283 | Decrease | -1.92 | Decrease | -0.961469 | Decrease | 0.812314 | -0.67 | SUR |
| 65 | P399S | 0.143 | 0.089 | -0.111 | Decrease | -1.47 | Decrease | -1 | Decrease | 0.885277 | 0.42 | SUR |
| 66 | P428H | 0.67 | -0.059 | 0.073 | Decrease | -1.65 | Decrease | -1 | Decrease | 0.793466 | 0.78 | SUR |
| 67 | Q119H | 0.63 | 0.178 | -0.223 | Decrease | -0.75 | Decrease | -0.600946 | Decrease | 0.86116 | 0.31 | SUR |
| 68 | Q255H | 0.91 | 0.334 | -0.417 | Decrease | -0.78 | Decrease | -0.837314 | Decrease | 0.775381 | 0.02 | SUR |
| 69 | Q256P | 0.226 | -0.146 | 0.183 | Decrease | -0.68 | Increase | 0.3964904 | Decrease | 0.53288 | 0.14 | SUR |
| 70 | Q440H | -0.052 | -0.294 | 0.367 | Decrease | -0.73 | Decrease | -0.166729 | Decrease | 0.795885 | 1.28 | COR |
| 71 | Q47K | 0.054 | -0.106 | 0.133 | Decrease | -0.61 | Decrease | -0.172535 | Decrease | 0.75541 | -0.45 | SUR |
| 72 | R127H | -0.171 | -0.122 | 0.152 | Decrease | -1.55 | Decrease | -1 | Decrease | 0.813657 | 0.9 | SUR |
| 73 | R138L | 0.042 | -0.335 | 0.419 | Decrease | -0.57 | Increase | 0.5803076 | Increase | 0.627947 | 0.6 | COR |
| 74 | R158C | 0.026 | 0.041 | -0.051 | Decrease | -1.29 | Decrease | -0.382551 | Decrease | 0.815774 | 0.35 | SUR |
| 75 | R167Q | 0.14 | -0.098 | 0.123 | Decrease | -0.93 | Decrease | -1 | Decrease | 0.710089 | -0.11 | SUR |
| 76 | R182H | -0.33 | 0.109 | -0.136 | Decrease | -1.87 | Decrease | -0.258606 | Decrease | 0.794243 | 0.6 | SUR |
| 77 | R198W | 1.216 | 0.48 | -0.601 | Decrease | -0.06 | Increase | 0.1937582 | Increase | 0.691732 | 0.41 | SUR |
| 78 | R214Q | -0.929 | -0.353 | 0.441 | Decrease | -0.69 | Decrease | -0.495164 | Decrease | 0.745084 | 0.54 | COR |
| 79 | R214W | 1.29 | 0.466 | -0.582 | Decrease | -0.24 | Decrease | -0.060978 | Decrease | 0.731628 | 1.25 | COR |
| 80 | R224H | 0.263 | 0.138 | -0.173 | Decrease | -1.66 | Decrease | -0.766824 | Decrease | 0.817205 | 0.9 | COR |
| 81 | R227H | -1.043 | -0.094 | 0.117 | Decrease | -1.71 | Decrease | -0.426636 | Decrease | 0.719087 | 1.59 | COR |
| 82 | R276Q | -0.517 | -0.472 | 0.59 | Decrease | -0.77 | Decrease | -0.843845 | Decrease | 0.795613 | -0.15 | COR |
| 83 | R282L | 1.102 | 0.693 | -0.866 | Decrease | -0.72 | Decrease | -0.560786 | Decrease | 0.81469 | 1.17 | COR |
| 84 | R282W | -1.11 | -0.309 | 0.386 | Decrease | -0.62 | Decrease | -0.882593 | Decrease | 0.786766 | 1.34 | COR |
| 85 | R286L | 0.029 | -0.298 | 0.372 | Decrease | -0.71 | Increase | 0.2679039 | Increase | 0.586793 | 0.59 | SUR |
| 86 | R297W | -0.132 | -0.109 | 0.137 | Decrease | -0.47 | Decrease | -1 | Decrease | 0.811831 | 0.42 | SUR |
| 87 | R324Q | -0.4 | -0.6 | 0.75 | Decrease | -0.77 | Decrease | -0.934796 | Decrease | 0.768929 | 0.99 | COR |
| 88 | R325L | 0.62 | 0.24 | -0.3 | Decrease | -0.65 | Increase | 0.5256466 | Increase | 0.567863 | -0.22 | SUR |
| 89 | R371W | 0.385 | 0.127 | -0.158 | Decrease | -0.23 | Increase | 0.0479765 | Increase | 0.760866 | 0.44 | SUR |
| 90 | R385W | -0.316 | -0.156 | 0.195 | Increase | 0.13 | Decrease | -0.615082 | Increase | 0.549013 | 0.28 | SUR |
| 91 | R443H | -0.696 | -0.088 | 0.11 | Decrease | -1.43 | Decrease | -0.852186 | Decrease | 0.864468 | 1.24 | SUR |
| 92 | R447W | 2.16 | 0.913 | -1.142 | Decrease | -0.33 | Increase | 0.3341114 | Increase | 0.52027 | 0.37 | COR |
| 93 | R67C | -0.159 | -0.007 | 0.009 | Increase | -0.41 | Decrease | -0.493641 | Decrease | 0.562108 | 0.43 | SUR |
| 94 | S148L | 0.476 | -0.182 | 0.228 | Increase | 0.54 | Increase | 0.4867282 | Increase | 0.689589 | 0.29 | SUR |
| 95 | S161F | 0.818 | 0.436 | -0.545 | Increase | 0.53 | Increase | 0.2081276 | Increase | 0.800171 | 0.25 | SUR |
| 96 | S17N | -0.016 | 0.048 | -0.06 | Increase | 0.3 | Decrease | -0.260624 | Increase | 0.546957 | 0.31 | SUR |
| 97 | S223F | 0.638 | 0.157 | -0.196 | Increase | 0.32 | Increase | 0.3745152 | Increase | 0.644418 | -0.26 | COR |
| 98 | S223Y | 0.298 | 0.104 | -0.13 | Increase | -0.08 | Increase | 0.5003893 | Increase | 0.724837 | 0.16 | COR |
| 99 | S330F | 1.967 | 0.962 | -1.202 | Increase | 0.67 | Decrease | -0.485454 | Decrease | 0.539142 | 0.41 | COR |
| 100 | S357F | 1.923 | 0.581 | -0.727 | Increase | 0.89 | Increase | 1 | Increase | 0.709665 | -0.34 | SUR |
| 101 | S400F | 1.314 | 0.503 | -0.629 | Increase | 0.27 | Increase | 0.7481912 | Increase | 0.738297 | 0.12 | SUR |
| 102 | T170M | 0.66 | -0.083 | 0.103 | Increase | 0.01 | Increase | 0.0961113 | Increase | 0.785641 | 0.22 | SUR |
| 103 | T203A | -0.525 | -0.45 | 0.563 | Decrease | -0.84 | Decrease | -1 | Decrease | 0.804289 | 0.06 | SUR |
| 104 | T63A | 0.511 | -0.166 | 0.207 | Decrease | -1.24 | Decrease | -0.77433 | Decrease | 0.81261 | 0.53 | SUR |
| 105 | V128I | 0.964 | 0.159 | -0.198 | Decrease | -0.75 | Decrease | -0.502486 | Decrease | 0.805797 | 0.36 | COR |
| 106 | V136L | 0.78 | 0.156 | -0.195 | Decrease | -1.5 | Increase | 0.0167572 | Increase | 0.5734 | 0.36 | SUR |
| 107 | V20F | -0.098 | 0.137 | -0.171 | Decrease | -1.85 | Decrease | -0.968481 | Decrease | 0.831371 | 0.41 | COR |
| 108 | V26I | 0.43 | -0.045 | 0.057 | Decrease | -0.08 | Increase | 0.222806 | Decrease | 0.512774 | 0.1 | SUR |
| 109 | V389A | -0.231 | -0.357 | 0.446 | Decrease | -2.19 | Decrease | -1 | Decrease | 0.864153 | 0.77 | SUR |
| 110 | V398I | 0.298 | 0.07 | -0.087 | Decrease | -0.59 | Decrease | -1 | Decrease | 0.753369 | 0.06 | SUR |
| 111 | V419D | -3.015 | -0.306 | 0.383 | Decrease | -1.52 | Decrease | -1 | Decrease | 0.803474 | 3.14 | COR |
| 112 | V50F | 0.212 | 0.041 | -0.052 | Decrease | -1.22 | Decrease | -0.384289 | Decrease | 0.849278 | 0.27 | SUR |
| 113 | V53L | 0.265 | -0.066 | 0.083 | Increase | -0.35 | Decrease | -0.753722 | Decrease | 0.585295 | 0.25 | SUR |
| 114 | W110C | -0.561 | -0.905 | 1.132 | Decrease | -1.22 | Decrease | -0.790016 | Decrease | 0.821447 | 2.15 | COR |
| 115 | W153C | -0.626 | -0.276 | 0.345 | Decrease | -1.96 | Decrease | -1 | Decrease | 0.712708 | 0.79 | SUR |
| 116 | W350L | -2.012 | -1.027 | 1.283 | Decrease | -1 | Decrease | -0.152737 | Decrease | 0.856693 | 0.39 | COR |
| 117 | Y442H | -0.583 | -0.25 | 0.313 | Decrease | -1.1 | Decrease | -0.840586 | Decrease | 0.802781 | 1.17 | COR |

**Supplementary Table 1**: Mutation induced changes in protein stability as predicted by DynaMut, iSTABLE, and PremPS .