

1 The AEMD analysis report for enzyme 106 ---- Activity  
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3 1. ##### The conservative residues are listed below.  
4 L12 V17 F21 G22 V24 G25 H46 E47 F48 A50 A54 R59 G62 Q65 A66 T70 G72 P73 G74 N77 T80  
G81 S85 P91 Q111 D114 P121 K124 A142 A146 G152 P209 G214 P236 G245 G264 D279 G285  
G401 G424 G429 A438 P443 G452 D453 G454 D462 T465 D508 A513 G517  
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6 2. ##### The recommended mutation sites according to conservation  
degree are listed after the arrow (sorted by feasibility).  
7 The sites within 5A distance  
8 24 V(0.0281) -----> P(0.9418)  
9 428 F(0.0221) -----> M(0.8576) L(0.1194)  
10 400 I(0.0461) -----> V(0.8054) N(0.0652)  
11 405 H(0.0201) -----> M(0.6740) I(0.1946)  
12 403 F(0.0642) -----> H(0.6630) N(0.1264)  
13 427 S(0.1916) -----> T(0.7061)  
14 483 N(0.0181) -----> Y(0.4704) L(0.4504)  
15 291 D(0.0211) -----> R(0.4443) Y(0.3350)  
16 404 R(0.0201) -----> Q(0.4393) K(0.3972)  
17 402 F(0.0171) -----> Q(0.4303) A(0.2718)  
18 26 R(0.0201) -----> G(0.4283) E(0.3651)  
19 489 Y(0.0221) -----> W(0.4193) K(0.3300)  
20 426 S(0.0762) -----> G(0.4453) A(0.3159)  
21 241 Y(0.0782) -----> F(0.3942) L(0.3942)  
22 485 L(0.3390) -----> M(0.6329)  
23 23 V(0.1394) -----> Y(0.3591) I(0.3420)  
24 478 V(0.0652) -----> W(0.2808) L(0.2698)  
25 486 I(0.3972) -----> V(0.5797)  
26 71 L(0.4102) -----> S(0.5787)  
27 The sites not in 5A distance  
28 85 S(0.0261) -----> A(0.9629)  
29 66 A(0.0241) -----> V(0.9539)  
30 65 Q(0.0211) -----> G(0.9488) A(0.0271)  
31 48 F(0.0211) -----> Q(0.9218) T(0.0251)  
32 123 S(0.0241) -----> T(0.8907) V(0.0712)  
33 406 Y(0.0271) -----> W(0.8887)  
34 75 M(0.0181) -----> A(0.8776) V(0.0491)  
35 327 T(0.0140) -----> G(0.8586) A(0.0913)  
36 408 V(0.0211) -----> A(0.8636) S(0.0612)  
37 462 D(0.0772) -----> E(0.9007)  
38 143 V(0.0331) -----> F(0.8516) Y(0.0802)  
39 458 S(0.0221) -----> M(0.8365) F(0.1184)  
40 34 D(0.0171) -----> L(0.8305) I(0.0863)  
41 447 T(0.0191) -----> V(0.8265) I(0.1113)  
42 151 V(0.0171) -----> P(0.7854) K(0.0662)  
43 307 R(0.0191) -----> H(0.7813) Q(0.0853)  
44 216 A(0.0421) -----> G(0.8014) R(0.0933)  
45 313 N(0.0221) -----> A(0.7803) S(0.0642)  
46 374 V(0.0451) -----> P(0.7834) G(0.0692)  
47 536 G(0.0702) -----> A(0.8054)  
48 314 P(0.0181) -----> E(0.7382) D(0.0772)  
49 309 S(0.0341) -----> D(0.7402) N(0.0732)  
50 57 L(0.0291) -----> Y(0.7342) I(0.0812)  
51 333 V(0.0863) -----> L(0.7904) I(0.0883)  
52 99 S(0.0201) -----> V(0.7141) A(0.1113)  
53 242 I(0.0110) -----> M(0.6911) Q(0.1434)  
54 97 A(0.1274) -----> G(0.7994)  
55 461 S(0.0150) -----> Q(0.6750) N(0.1194)  
56 466 I(0.0843) -----> A(0.7372)  
57 305 T(0.0140) -----> I(0.6610) V(0.2598)  
58 336 F(0.0221) -----> L(0.6389) I(0.2427)  
59 520 A(0.1795) -----> G(0.7884)  
60 425 C(0.0211) -----> L(0.6148) F(0.1886)  
61 550 N(0.0431) -----> D(0.6289) E(0.1254)  
62 51 G(0.0752) -----> A(0.6570) S(0.1133)  
63 511 A(0.0702) -----> K(0.6510) Q(0.0913)  
64 312 V(0.0181) -----> P(0.5918) A(0.1304)  
65 93 I(0.1434) -----> V(0.7091)  
66 150 P(0.0311) -----> R(0.5958) K(0.3250)  
67 122 M(0.0140) -----> I(0.5757) V(0.2839)  
68 49 T(0.0251) -----> G(0.5848) A(0.1665)  
69 96 A(0.1184) -----> T(0.6780)  
70 282 L(0.1555) -----> I(0.7091)

71 95 L(0.1886) -----> I(0.7282)  
 72 140 D(0.0231) -----> R(0.5617) K(0.1605)  
 73 411 A(0.0251) -----> Y(0.5637) F(0.3009)  
 74 154 S(0.1133) -----> V(0.6510) T(0.1153)  
 75 272 Q(0.0080) -----> N(0.5386) D(0.1525)  
 76 500 P(0.0211) -----> S(0.5426) A(0.1515)  
 77 375 H(0.0291) -----> Q(0.5496) L(0.1264)  
 78 418 G(0.0261) -----> T(0.5426) H(0.1093)  
 79 212 V(0.0321) -----> L(0.5446) Y(0.1916)  
 80 68 W(0.0140) -----> L(0.5256) I(0.1755)  
 81 226 I(0.1505) -----> L(0.6620) V(0.1585)  
 82 203 L(0.2217) -----> I(0.7262)  
 83 498 H(0.0973) -----> R(0.6018)  
 84 29 A(0.0401) -----> L(0.5426) I(0.1775)

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 86 3. ##### The residues located within 5A distance from substrate and  
 cofactors are listed below. Saturated mutation recommended.  
 87 V23 V24 G25 R26 E47 T70 L71 P73 G74 N77 T80 H110 Q111 Y241 Y261 D291 I400 G401 F402  
 F403 R404 H405 S426 S427 F428 G452 D453 G454 G455 F456 V478 N480 T482 N483 G484 L485  
 I486 Y489 F504 Y551

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 89 4. ##### The residues located within 3A distance from tunnels are  
 listed below. Saturated mutation recommended.  
 90 Null sites

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 92 5. ##### The residues which located on the surface of protein are  
 listed below.  
 93 K1 P2 R13 R26 A28 A29 L32 D34 E37 R45 R63 E100 H102 D103 F105 P106 N107 D108 H110  
 D114 A117 A120 P121 Y125 Q130 R131 H133 E134 D137 S141 N144 D161 G164 S165 S166 E167  
 G168 D170 T172 V173 P174 P176 P177 N179 A182 V187 D190 Q193 K194 D197 Q198 A201 A204  
 E205 K207 P224 R227 A228 E231 R232 E252 N267 F268 P269 Q272 A276 G300 I301 E302 K304  
 V312 R317 R320 E334 H335 T338 A341 S342 F343 G344 A345 Q347 D350 E352 P353 A356 A359  
 E360 A363 P365 E366 T367 E369 D370 R373 E386 E387 E390 P391 E393 D444 H457 R468 N470  
 G493 H494 H495 R496 S497 H498 D499 P500 G505 G506 D508 V510 A511 E514 A515 G517 D519  
 T521 R522 N525 E527 E528 A531 R534 K535 E538 G540 R541

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 95 The sites from AEMD are only for reference. Any problems, please contact:  
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