

SUPPLEMENTARY TABLE S3. EXOTIC BHB FREE ENERGY DONOR/ACCEPTOR RESIDUES OF VIRAL CAPSIDS

Human Adenovirus 2 (1X9P)

Chain A

90–94% 464/439 227/285 183/178 263/424 237/212 474/516
 95–98% 114/533 249/273 276/246 131/553 546/549 538/109 235/232 446/441 72/559 217/214 565/120 560/71 234/
 231 452/448 174/134
 99% 240/211 386/389 198/192 280/277 206/202
 100% 53/49 61/58 123/562 152/199 182/178 194/189 195/190 200/197 201/197 221/225 230/226 390/385 395/400
 460/456 471/468 485/481 549/545

Foot and Mouth Virus (1FOD)

Chain 1

90–94% 57/53 89/104 43/176 3:167/122 182/75 70/66
 95–98% 71/186 172/83 174/46 21/15 190/68 2:148/6 3:168/122
 99% 115/3:10 39/36 20/16 151/147
 100% 134/2:173 139/136 142/2:172

Chain 2

90–94% 170/101 217/3:138 105/206 77/183 189/118 154/149 20/22
 95–98% 23/19 121/185 148/1:6
 99% 11/8 194/189
 100% 13/6 30/13 139/135 1:134/173 1:142/172

Chain 3

90–94% 57/85 2:217/138 54/203 80/182 100/213 167/1:122 50/45 97/92 81/78 126/143
 95–98% 150/119 58/61 207/104 168/1:122 119/192 121/190
 99% 1:115/10 197/66
 100% 100/212 206/48 12/8

Chain 4

90–94%
 95–98%
 99%
 100% 70/65 70/66

Hepatitis A Virus (5WTE)

Chain A

90–94% 267/C96 184/179 126/270 75/72 245/148 250/93 77/26 96/247 71/43 151/242 230/109 137/258 107/173
 95–98% 143/250 136/259 136/258 52/48 B138/263 89/84 210/B166 C30/201
 99% 129/124 224/219
 100% C27/199

Chain B

90–94% 171/104 218/100 124/188
 95–98% 138/A263 C61/139 58/53 188/123
 99%
 100% 30/13 76/186 103/214 151/154 210/107

Chain C

90–94% A267/96 54/50 202/136 139/199 88/61 75/71 245/86 208/130 229/55
 95–98% 184/196 61/B139 91/95 30/A201
 99% 83/80 74/206 69/218
 100% 27/A199 47/43

Hepatitis E Virus (2ZTN)

Chain A Acceptors

90–94% 144/298 172/320 156/278 286/203 313/181 341/332 424/418 432/331 532/534 437/327 324/440 500/474 600/
 471 581/570 392/219 252/248 261/270 567/564 373/439 328/436 603/540 397/371 354/446
 95–98% 141/300 178/173 393/220 374/394 408/405 132/308 195/242 378/149 487/484 451/447 333/340 287/291 273/
 268 351/346 507/502 515/510
 99% 283/151 258/254 437/434 503/507 590/587 469/601 357/353
 100% 142/166 199/297 203/199 315/312 323/169 330/434 338/334 361/358 364/360 393/388 395/390 396/390 449/
 351 485/482 522/524 573/578

(continued)

SUPPLEMENTARY TABLE S3. (CONTINUED)

Polio Virus (5O5B)

Chain 1

90–94% 204/126 194/3:22 92/101 163/159 269/125

95–98% 276/2:183 717/2:267 125/268 130/263

99% 134/259

100% 3:25/193

Chain 2

90–94% 37/33

107/209 235/121 175/133

95–98% 3:125/116 17/23 1:276/183 123/197 1:217/267 178/157 144/171 226/82 103/218 55/259

99% 261/101

100% 86/81 101/260 182/176 184/179 203/198

Chain 3

90–94% 196/129 63/58 97/92 215/51 1:194/22

95–98% 178/110 56/67 125/2:116 197/129 22/4:38

99%

100% 25/1:193 53/2:187 57/67 109/223

Chain 4

90–94%

95–98% 3:22/38

99%

100%

Rhinovirus (4AYM)

Chain 1

90–94% 85/230 76/238 68/3:41 120/241 181/3:22 189/2:207 233/82 236/125 280/3:57 3:25/180 24/53 114/110

95–98% 254/2:176 115/246 3:85/282

99% 3:163/35 2:75/15

100% 75/3:15 241/71

Chain 2

90–94% 256/98 175/169 141/137 220/82 86/81 106/247 189/207 103/211 122/227 219/82 134/174 102/252 196/191

38/34 168/133 176/172

95–98% 144/164 60/56

99% 94/89 228/121 190/1:38

100% 29/12 177/172 178/172 3:53/180

Chain 3

90–94% 1:68/41 221/110 1:181/22 1:280/57 171/168 11/7 25/1:180

95–98% 108/222 216/47 65/61 85/1:282 152/133

99% 163/1:35 96/91 95/91 196/128

100% 53/2:180 57/67 1:75/15

Chain 4

90–94% 29/3 4/28

95–98%

99%

100%

Donor/acceptor residues of BHBs in order of non-decreasing Π -values, with 7.5, 8.5, 9.5, and 9.85, respectively, corresponding to percentiles 90, 95, 99, and 100.