Pattern of Amino Acid Substitutions in Transmembrane Domains of β-Barrel Membrane Proteins for Detecting Remote Homologs in Bacteria and Mitochondria

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Figure S3. The BBTM scoring matrices.

A. Scoring matrix bbTM$_{\text{all}}$. Scoring matrix at evolutionary time unit of 40 derived from Q_{all}. Note: The last line denotes the lowest score in all columns and rows to conform with format of BLOSUM and PAM for use in programs such as CLUSTALW.

```
# bbTMall
# Lowest score = -24 , Highest score = 24
    A   R   N   D   C   Q   E   G   H   I   L   K   M   F   P   S   T   W   Y   V   B   Z   X   *
A   6 -11  -7 -10 -19  -9 -10   1 -12  -2  -2  -9  -5  -5  -8  -1   0 -10 -10   0  -8  -4  -6 -24
R -11  10  -7 -11 -13  -4 -10 -12  -5 -12 -11  -1 -12 -11 -14  -6  -8 -14 -11 -12  -9 -11  -8 -24
N  -7  -7  10   0 -13  -4  -8  -7  -6 -12 -12  -5  -7 -12 -14   0  -2 -13 -10 -11   5  -7  -7 -24
D -10 -11   0  11 -13  -5  -2 -10 -10 -13 -11  -9 -12 -14 -14  -4  -8 -14 -14 -12   6  -6  -8 -24
C -16 -13 -14 -14  24 -11 -16 -16 -16 -15 -16 -14 -13 -14 -14 -12 -13 -16 -12 -15 -14 -16 -12 -24
Q  -9  -4  -4  -5 -11  10  -1 -11  -2  -9 -10  -4  -7 -13 -12  -4  -5 -13 -11  -9  -4  -6  -6 -24
E -10 -10  -8  -2 -24  -1  10 -11 -12 -14 -13 -10 -12 -15 -11  -8  -8 -14 -14 -12  -5  -0  -9 -24
G   1 -12  -7 -10 -24 -11 -11   7 -14  -8  -8 -12  -8 -10 -13  -2  -4 -13 -12  -6  -8  -2  -8 -24
H -12  -5  -6 -10 -24  -2 -12 -14  13 -13 -12 -11 -12 -11 -16  -9 -10 -10  -5 -13  -8 -13  -9 -24
I  -2 -12 -12 -13 -17  -9 -14  -8 -13   7   3 -12  -3  -2 -14  -9  -5  -8  -9   5 -12 -11  -7 -24
L  -2 -11 -12 -11 -18 -10 -13  -8 -12   3   6 -12   0   1 -13  -9  -6  -6  -6   3 -11 -10  -6 -24
K  -9  -1  -5  -9 -13  -4 -10 -12 -11 -12 -12  11 -11 -13 -14  -7  -6 -12 -14 -12  -7 -11  -8 -24
M  -5 -12  -7 -12 -13  -7 -12  -8 -12  -3   0 -11  12  -5 -15  -7  -2 -10 -10  -2  -9 -10  -7 -24
F  -5 -11 -12 -14 -13 -13 -15 -10 -11  -2   1 -13  -5   8 -11 -10  -9  -3   1  -1 -13 -12  -7 -24
P  -8 -14 -14 -14 -13 -12 -11 -13 -16 -15 -13 -14 -15 -11  14 -11 -12 -16 -16 -13 -14 -12 -11 -24
S  -1  -6   0  -4 -13  -4  -8  -2  -9  -9  -9  -7  -7 -10 -11   8   2 -15 -12  -7  -2  -5  -6 -24
T   0  -8  -2  -8 -13  -5  -8  -4 -10  -5  -6  -6  -2  -9 -12   2   8 -12 -10  -3  -5  -6  -5 -24
W -10 -14 -13 -14 -22 -13 -14 -13 -10  -8  -6 -12 -10  -3 -16 -15 -12  11  -1  -6 -13 -13 -10 -24
Y -10 -11 -10 -14 -13 -11 -14 -12  -5  -9  -6 -14 -10   1 -15 -12 -10  -1   7  -8 -12 -13  -8 -24
V   0 -12 -11 -12 -14  -9 -12  -6 -13   5   3 -12  -2  -1 -13  -7  -3  -6  -8   5 -11  -9  -6 -24
B  -8  -9   5   6 -14  -4  -5  -8  -8 -12 -11  -7  -9 -13 -14  -2  -5 -13 -12 -11  11  -4  -7 -24
Z  -4 -11  -7  -6 -16  -6  -0  -2 -13 -11 -10 -11 -10 -12 -12  -5  -6 -13 -13  -9  -4  10  -7 -24
X  -6  -8  -7  -8 -12  -6  -9  -8  -9  -7  -6  -8  -7  -7 -11  -6  -5 -10  -8  -6  -7  -7   1 -24
* -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24 -24   1
```

B. Scoring matrix bbTM$_{\text{out}}$. Scoring matrix at evolutionary time unit of 40 derived from Q_{out}.

```
# bbTMout
# Lowest score = -16 , Highest score = 25
    A   R   N   D   C   Q   E   G   H   I   L   K   M   F   P   S   T   W   Y   V   B   Z   X   *
A   6 -12 -11 -13 -12 -11 -10   1 -13  -1  -1 -13  -5  -3  -8  -3   0  -9  -8   0 -12  -4  -6 -16
R -12  14  -7  -9 -12  -5  -8 -10  -6 -12 -12  -4 -13 -13 -14 -11  -8 -12  -8 -12  -8  -9  -8 -16
N -11  -7  13  -1 -12  -3  -8  -9  -7 -13 -12  -7  -8 -12 -14  -3  -3 -14 -10 -12   6  -8  -7 -16
D -13  -9  -1  14 -12  -7  -5  -8 -12 -13 -11  -6 -12 -13 -14  -8 -11 -14 -11 -13   7  -6  -8 -16
C -14 -13 -11 -12  25 -11 -11 -14 -14 -14 -15 -14 -14 -14 -13 -14 -12 -14 -11 -13 -11 -12 -11 -16
Q -11  -5  -3  -7 -10  12  -4 -12  -2 -12 -12  -6  -9 -12 -10  -8  -4 -10  -8 -11  -5  -8  -7 -16
E -10  -8  -8  -5 -12  -4  17 -11 -12 -12 -12 -13 -14 -12 -16 -11  -8 -13 -13 -11  -6   3  -9 -16
G   1 -10  -9  -8 -12 -12 -11   8 -14  -6  -6 -13  -9  -7  -9  -4  -3 -11 -10  -5  -8  -1  -7 -16
H -13  -6  -7 -12 -12  -2 -12 -14  13 -12 -12 -10 -13 -11 -14  -9 -12  -9  -5 -13  -9 -13  -9 -16
I  -1 -12 -13 -13 -13 -12 -12  -6 -12   5   2 -14  -3  -1 -13  -9  -5  -6  -8   3 -13  -9  -7 -16
L  -1 -12 -12 -11 -15 -12 -12  -6 -12   2   4 -13  -2   1 -11  -9  -5  -5  -6   2 -11  -9  -6 -16
K -13  -4  -7  -6 -12  -6 -13 -13 -10 -14 -13  14 -12 -12 -12 -10  -9 -13 -12 -13  -6 -13  -9 -16
M  -5 -13  -8 -12 -12  -9 -14  -9 -13  -3  -2 -12  12  -3 -13 -10  -4  -9  -9  -3 -10 -11  -7 -16
F  -3 -13 -12 -13 -12 -12 -12  -7 -11  -1   1 -12  -3   6 -10 -10  -8  -3  -2   0 -12  -9  -6 -16
P  -8 -14 -14 -14 -12 -10 -16  -9 -14 -13 -11 -12 -14 -10  12  -8  -9 -13 -15 -12 -14 -12 -10 -16
S  -3 -11  -3  -8 -12  -8 -11  -4  -9  -9  -9 -10 -10 -10  -8  11  -1 -12 -11  -8  -5  -7  -7 -16
T   0  -8  -3 -11 -12  -4  -8  -3 -12  -5  -5  -9  -4  -8  -9  -1   9 -11  -8  -3  -7  -5  -5 -16
W  -9 -12 -14 -14 -12 -10 -13 -11  -9  -6  -5 -13  -9  -3 -13 -12 -11   9  -1  -5 -14 -12  -8 -16
Y  -8  -8 -10 -11 -12  -8 -13 -10  -5  -8  -6 -12  -9  -2 -15 -11  -8  -1   6  -7 -10 -11  -7 -16
V   0 -12 -12 -13 -13 -11 -11  -5 -13   3   2 -13  -3   0 -12  -8  -3  -5  -7   4 -12  -8  -6 -16
B -12  -8   6   7 -11  -5  -6  -8  -9 -13 -11  -6 -10 -12 -14  -5  -7 -14 -10 -12  14  -5  -8 -16
Z  -4  -9  -8  -6 -12  -8   3  -1 -13  -9  -9 -13 -11  -9 -12  -7  -5 -12 -11  -8  -5  15  -8 -16
X  -6  -8  -7  -8 -11  -7  -9  -7  -9  -7  -6  -9  -7  -6 -10  -7  -5  -8  -7  -6  -8  -8   1 -16
* -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16 -16   1
```

C. Scoring matrix bbTM$_{\text{in}}$. Scoring matrix at evolutionary time unit of 36 derived from Q_{in}.

```
#bbTMin
# Lowest score = -14 , Highest score = 23
    A   R   N   D   C   Q   E   G   H   I   L   K   M   F   P   S   T   W   Y   V   B   Z   X   *
A   7  -9  -4  -7 -14  -7  -6   1 -12  -6  -3  -8  -5 -10  -9   0   0 -12 -12  -2  -5  -2  -5 -14
R  -9   8  -8 -11 -12  -5 -11 -10  -6 -11  -9  -2 -12  -9 -14  -6  -7 -14 -11  -8  -9 -10  -8 -14
N  -4  -8   8  -1 -12  -4  -8  -6  -6 -10  -8  -5  -6 -11 -11   0  -2 -10  -9  -8   4  -7  -6 -14
D  -7 -11  -1   9 -14  -4   0  -6 -10 -12  -7 -10  -9 -10 -12  -5  -7 -11 -11  -8   4  -3  -7 -14
C -13 -12 -12 -14  23 -12 -11 -14 -14 -14 -14 -14 -14 -14 -14 -12 -13 -14 -11 -12 -13 -12 -11 -14
Q  -7  -5  -4  -4 -12   8   0 -10  -6  -6  -5  -3  -8 -11 -12  -4  -5 -11 -10  -6  -4  -5  -6 -14
E  -6 -11  -8   0 -11   0   8  -9 -12 -11 -10 -10  -8 -12 -11  -7  -7 -10 -11  -6  -4  -0  -7 -14
G   1 -10  -6  -6 -14 -10  -9   6 -13 -11  -9 -11  -9 -13 -13  -2  -5 -12 -13  -8  -6  -1  -8 -14
H -12  -6  -6 -10 -14  -6 -12 -13  14 -13 -10 -10 -14 -13 -14  -8  -9 -13  -9 -12  -8 -12  -9 -14
I  -6 -11 -10 -12 -14  -6 -11 -11 -13  12  -3 -10  -5  -8 -13  -8  -4 -13 -10   3 -11 -11  -7 -14
L  -3  -9  -8  -7 -14  -5 -10  -9 -10  -3  10  -9  -1  -6 -12  -8  -6 -12 -11  -1  -7  -9  -6 -14
K  -8  -2  -5 -10 -14  -3 -10 -11 -10 -10  -9   9 -12 -13 -12  -7  -6 -12 -14 -10  -7 -10  -8 -14
M  -5 -12  -6  -9 -14  -8  -8  -9 -14  -5  -1 -12  12  -5 -13  -4  -3 -12 -11  -6  -7  -8  -7 -14
F -10  -9 -11 -10 -14 -11 -12 -13 -13  -8  -6 -13  -5  11 -13  -9  -7 -11   2  -9 -10 -12  -8 -14
P  -9 -14 -11 -12 -14 -12 -11 -12 -14 -13 -12 -12 -13 -13  16 -10 -11 -11 -12 -12 -11 -11 -10 -14
S   0  -6   0  -5 -12  -4  -7  -2  -8  -8  -8  -7  -4  -9 -10   6   2 -10 -11  -5  -2  -4  -5 -14
T   0  -7  -2  -7 -14  -5  -7  -5  -9  -4  -6  -6  -3  -7 -11   2   7 -12  -7  -1  -4  -6  -5 -14
W -12 -14 -10 -11 -14 -11 -10 -12 -13 -13 -12 -12 -12 -11 -11 -10 -12  13  -7 -13 -10 -11 -10 -14
Y -12 -11  -9 -11 -11 -10 -11 -13  -9 -10 -11 -14 -11   2 -12 -11  -7  -7   9 -10 -10 -12  -8 -14
V  -2  -8  -8  -8 -12  -6  -6  -8 -12   3  -1 -10  -6  -9 -12  -5  -1 -13 -10  11  -8  -7  -6 -14
B  -5  -9   4   4 -13  -4  -4  -6  -8 -11  -7  -7  -7 -10 -11  -2  -4 -10 -10  -8   9  -4  -6 -14
Z  -2 -10  -7  -3 -12  -5  -0  -1 -12 -11  -9 -10  -8 -12 -11  -4  -6 -11 -12  -7  -4   8  -6 -14
X  -5  -8  -6  -7 -11  -6  -7  -8  -9  -7  -6  -8  -7  -8 -10  -5  -5 -10  -8  -6  -6  -6   1 -14
* -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14 -14   1
```