

[Re] Local alignment statistics - Amino acid frequencies

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Amino acid frequencies (Robinson & Robinson 1991)

Amino acid frequencies from Robinson and Robinson (1991) “Distribution of glutamine and asparagine residues and their near neighbors in peptides and proteins” PNAS. (R & R 1991). These frequencies are used by Altschul and Gish (1996) for their simulated polypeptides.

Make a vector of all letters that represent amino acid

```
# 1 letter codes
aa1 <- c("A", "C", "D", "E", "F", "G", "H",
        "I", "K", "L", "M", "N", "P", "Q",
        "R", "S", "T", "V", "W", "Y")

aa3 <- c("Ala", "Cys", "Asp", "Glu", "Phe", "Gly", "His",
        "Ile", "Lys", "Leu", "Met", "Asn", "Pro", "Gln",
        "Arg", "Ser", "Thr", "Val", "Trp", "Tyr")
```

Number of each amino acid reported in (R & R 1991):

```
aa.count <- c(35155, 8669, 24161, 28354, 17367,
              33229, 9906, 23161, 25872, 40625,
              10101, 20212, 23435, 19208, 23105,
              32070, 26311, 29012, 5990, 14488)
```

Check frequency; should sum to 450431

```
aa.total <- sum(aa.count)
aa.total
```

```
## [1] 450431
```

Setting up amino acid relative frequencies

Create dataframe of amino acid frequencies (Note: stringsAsFactors = F prevents a default R behavior which is annoying)

```
robinson.aafreq <- data.frame(aa3,
                              aa1,
                              aa.count = aa.count,
                              stringsAsFactors = F)
```

Calculate **relative frequency** of each amino acid:

```
robinson.aafreq$aa.freq <- robinson.aafreq$aa.count/aa.total
```

Check that relative frequency sums to 1

```
sum(robinson.aafreq$aa.freq)
```

```
## [1] 1
```

Save

```
write.csv(robinson.aafreq, file = "robinson_aafreq.csv")
```