

How To Run SNAP

(Uppercase indicates variable names.)

1. Make multiple mutations file:

```
makemuts → perl makeMuts.pl FULLPATH/NAME.fasta all
```

2. Split in to individual mutations files:

```
split -d -a 3 -l 19 NAME.muts NAME_Mut
```

(-d = Use numbers for output, -a = Length of numbers in output file names, -l = How many lines per file – default of 19)

3. Get files:

→ File 1

```
loop=1
```

```
last=N
```

```
while [ $loop -lt $last ] ; do pwd >> Column_1 | ((loop=$loop+1)) ; done
```

→ File 2

```
ls INDIVIDUAL_MUTATIONS_FOLDER >> Column_2
```

→ Final List File

```
paste -d'/' Column_1 Column_2 >> List.muts
```

(Do the same for fasta files, if necessary.)

4. Run:

```
#!/bin/sh
```

```
#$ -t 1-HOWMANYRESIDUES:1
```

```
#$ -o /tmp/
```

```
#$ -e /tmp/
```

```
#$ -m as
```

```
#$ -M USER@roslab.org
```

```
#$ -N NAMEFORRUN
```

```
~rost_db/src/fetchAll4Snap.pl
```

```
n=1
```

```
fasta=PATH/NAME.fasta
```

```
cat PATH/List.muts | while read mutation; do snapfun -i $fasta OPTIONS* -m $mutation -o PATH/SNAP/"$n"_NAME.snap | ((n=$n+1)); done
```

*Options include:

```
--quiet
```

```
--db_swiss=/var/tmp/rost_db/data/swissprot/dbswiss
```

```
--pfamdata=/var/tmp/rost_db/data/pfam_legacy/Pfam_ls
```

```
--swiss_dat=/var/tmp/rost_db/data/swissprot/uniprot_sprot.dat
```

```
--uniref=/var/tmp/rost_db/data/big/big --uniref90=/var/tmp/rost_db/data/big/big_80
```

```
--swiss=/var/tmp/rost_db/data/swissprot/uniprot_sprot
```