

1 **Supplementary material - Title page**

2 SERS detection of the biomarker hydrogen cyanide from *Pseudomonas aeruginosa* cultures  
3 isolated from cystic fibrosis patients

4

5 **Authors**

6 Rikke Kragh Lauridsen, Lea M. Sommer, Helle Krogh Johansen, Tomas Rindzevicius, Søren Molin,  
7 Lars Jelsbak, Søren Balling Engelsen, Anja Boisen

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## 10 **Supplementary material**

11

```
12 #!/bin/bash
```

```
13 ISO=$1 #Input: list of isolate names.
```

14

```
15 while read line
```

```
16 do
```

17

```
18     echo "$line is being aligned with BWA (v.0.7.12) aln paired end  
19 function (sampe) "
```

```
20     bwa aln lasR.fna $line.L*_1.fq.gz > "$line"_read1.sai
```

```
21     bwa aln lasR.fna $line.L*_2.fq.gz > "$line"_read2.sai
```

```
22     bwa sampe lasR.fna "$line"_read1.sai "$line"_read2.sai
```

```
23 $line.L*_1.fq.gz $line.L*_2.fq.gz > "$line"_aligned.sam
```

24

```
25     echo "$line is going through round one in SAMtools v.0.1.18"
```

```
26     samtools view -Shb -F4 "$line"_aligned.sam > "$line"_aligned.bam
```

```
27     samtools sort "$line"_aligned.bam "$line"_aligned_sort
```

```
28     samtools index "$line"_aligned_sort.bam
```

29

```
30     echo "$line read groups are added by Picard (v.1.140) "
```

```
31     java -Xmx2g -jar picard-tools-1.140/picard.jar AddOrReplaceReadGroups
```

```
32 INPUT="$line"_aligned_sort.bam OUTPUT="$line"_aligned.RG.bam RGID=CF
```

```
33 RGLB=CF_LIB1 RGPL=Illumina RGPU=CF_RG1_UNIT1 RGSM=$line
```

```
34 VALIDATION_STRINGENCY=LENIENT
```

35

```
36     echo "$line pileups and raw files are being produced by SAMtools  
37 v0.1.18"
```

```
38     samtools mpileup -q 20 -C50 -BDSsugf lasR.fna "$line"_aligned.RG.bam
```

```
39 | bcftools view -vg - > "$line"_raw.vcf
```

```
40 done<$ISO
```