The demo data and results can be downloaded from the following link: https://drive.google.com/drive/folders/1yLNTHNciC9vllmzdA7vuPHmrxjjQ04ce?usp=sharing

1. Demo data: the ms1 format can be obtained by converting raw data by RawXtractor

```
chuwang_pkuhpc:/lustre1/chuwang_pkuhpc/jobs/guxiao/SESTAR_demo$ ls
20170527_mouse_liver_1.ms1
```

2. Convert MS1 spectra in the ms1 format to the csv format for R to read.

```
chuwang_pkuhpc:/lustre1/chuwang_pkuhpc/jobs/guxiao/SESTAR_demo$ python ~/jobs/guxiao/scripts/Read_ms1.py 20170527_mouse_liver_1.ms1 20170527_mouse_liver_1.ms1.csv
['/home/chuwang_pkuhpc/lustre1/jobs/guxiao/scripts/Read_ms1.py', '20170527_mouse_liver_1.ms1', '20170527_mouse_liver_1.ms1.csv']
```

The result is:

```
chuwang_pkuhpc:/lustre1/chuwang_pkuhpc/jobs/guxiao/SESTAR_demo$ ls
20170527_mouse_liver_1.ms1    20170527_mouse_liver_1.ms1.csv
```

3. Run the main program to extract all the selenium coded envelopes.

```
chuwang_pkuhpc:/lustre1/chuwang_pkuhpc/jobs/guxiao/SESTAR_demo$ R --vanilla --args Se 20170527_mouse_liver_1.ms1.csv < ~/jobs/guxiao/scripts/SESTAR.r > SESTAR.rout &
[1] 21069
```

This step will result four files:

```
20170527_mouse_liver_1.ms1_envelop.csv
20170527_mouse_liver_1.ms1_envelop_valid.csv
20170527_mouse_liver_1.ms1_PNG
SESTAR.rout
```

The "20170527_mouse_liver_1.ms1_envelop.csv" file is all the envelopes detected with a selenium pattern.

The "20170527_mouse_liver_1.ms1_envelop_valid.csv" file is the integrated result file containing detections with more than two matched ms1 spectra.

The "20170527_mouse_liver_1.ms1_PNG" folder contains the plots for all the observed envelopes (black lines), simulated selenium containing envelopes (red dots) and simulated proteogenic envelopes (green dots).

The "SESTAR.rout" contains the standard output and error for the running process.