

1.1

```
[ese-zhaoan@login01 ~]$ ln -s data_demo data_demo_link
[ese-zhaoan@login01 ~]$ ls
data_demo data_demo_link exam
[ese-zhaoan@login01 ~]$
```

1.2

```
[ese-zhaoan@login01 ~]$ echo *
data_demo data_demo_link exam
[ese-zhaoan@login01 ~]$
```

1.3

```
[ese-zhaoan@login01 molecules]$ touch test.pdb
[ese-zhaoan@login01 molecules]$ ls
cubane.pdb ethane.pdb methane.pdb octane.pdb pentane.pdb propane.pdb test.pdb
[ese-zhaoan@login01 molecules]$
```

1.4

```
./Cr.xml
./Rn.xml
./Ge.xml
./Co.xml
./Tc.xml
./Pm.xml
./Rb.xml
./C.xml
./Yb.xml
./Zn.xml
./Cs.xml
./Fm.xml
./Ni.xml
./Ar.xml
[ese-zhaoan@login01 elements]$ find . -type f -print | wc -l
103
```

1.5

```
[ese-zhaoan@login01 pdb]$ diff ethane.pdb ethanol.pdb
1,11c1,12
< COMPND      ETHANE
< AUTHOR      DAVE WOODCOCK  95 12 18
< ATOM        1  C          1      -0.752   0.001  -0.141  1.00  0.00
< ATOM        2  C          1       0.752  -0.001   0.141  1.00  0.00
< ATOM        3  H          1     -1.158   0.991   0.070  1.00  0.00
< ATOM        4  H          1     -1.240  -0.737   0.496  1.00  0.00
< ATOM        5  H          1     -0.924  -0.249  -1.188  1.00  0.00
< ATOM        6  H          1      1.158  -0.991  -0.070  1.00  0.00
< ATOM        7  H          1      0.924   0.249   1.188  1.00  0.00
< ATOM        8  H          1      1.240   0.737  -0.496  1.00  0.00
< TER         9          1
---
> COMPND      ETHANOL
> AUTHOR      DAVE WOODCOCK  96 01 03
> ATOM        1  C          1     -0.426  -0.115  -0.147  1.00  0.00
> ATOM        2  O          1     -0.599   1.244  -0.481  1.00  0.00
> ATOM        3  H          1     -0.750  -0.738  -0.981  1.00  0.00
> ATOM        4  H          1     -1.022  -0.351   0.735  1.00  0.00
> ATOM        5  H          1     -1.642   1.434  -0.689  1.00  0.00
> ATOM        6  C          1      1.047  -0.383   0.147  1.00  0.00
> ATOM        7  H          1      1.370   0.240   0.981  1.00  0.00
> ATOM        8  H          1      1.642  -0.147  -0.735  1.00  0.00
> ATOM        9  H          1      1.180  -1.434   0.405  1.00  0.00
> TER        10          1
[ese-zhaoan@login01 pdb]$
```

1.6

```
LittleWomen.txt:15
[ese-zhaoan@login01 data]$ grep -c 'But she' LittleWomen.txt
15
[ese-zhaoan@login01 data]$
```

1.7

```
[ese-zhaoan@login01 data]$ du -h
407K    ./pdb
52K     ./elements
1.0K    ./animal-counts
1.1M    .
```

1.8

```
[ese-zhaoan@login01 data_demo]$ cp -r writing writing_new
[ese-zhaoan@login01 data_demo]$ ls
creatures  data  draft.txt  molecules  north-pacific-gyre  notes  pizza.cfg  solar.pdf  thesis  writing  writing_new
[ese-zhaoan@login01 data_demo]$
```

```
[ese-zhaoan@login01 data_demo]$ zip writing_new.zip writing_new
adding: writing_new/ (stored 0%)
[ese-zhaoan@login01 data_demo]$
```

```
[ese-zhaoan@login01 data_demo]$ unzip writing_new.zip
Archive:  writing_new.zip
[ese-zhaoan@login01 data_demo]$
```

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1.9

```
[ese-zhaoan@login01 ~]$ chmod -rwxr-xr-x data_demo/writing_new/
[ese-zhaoan@login01 ~]$
```

1.10

```
[ese-zhaoan@login01 data_demo]$ history 10
170  exit
171  cd data_demo/writing/
172  cd ..
173  ls
174  zip test.zip test
175  zip writing_new.zip writing_new
176  ls
177  unzip writing_new.zip
178  history
179  history 10
[ese-zhaoan@login01 data_demo]$
```

2

```
(my_mpi) [ese-zhaoan@login02 pdb]$ for file in *.pdb
> do
> du -b $file
> done
1516   aldrin.pdb
306    ammonia.pdb
1444   ascorbic-acid.pdb
1030   benzaldehyde.pdb
1830   camphene.pdb
5049   cholesterol.pdb
1090   cinnamaldehyde.pdb
1694   citronellal.pdb
2452   codeine.pdb
1158   cubane.pdb
895    cyclobutane.pdb
1384   cyclohexanol.pdb
695    cyclopropane.pdb
622    ethane.pdb
690    ethanol.pdb
2396   ethylcyclohexane.pdb
765    glycol.pdb
4209   heme.pdb
1064   lactic-acid.pdb
2562   lactose.pdb
11193  lanoxin.pdb
3395   lsd.pdb
2562   maltose.pdb
2164   menthol.pdb
422    methane.pdb
490    methanol.pdb
1869   mint.pdb
2288   morphine.pdb
2123   mustard.pdb
1680   nerol.pdb
2729   norethindrone.pdb
1828   octane.pdb
1226   pentane.pdb
2287   piperine.pdb
```