CBP Tutorial

4th March 2024

NACCESS

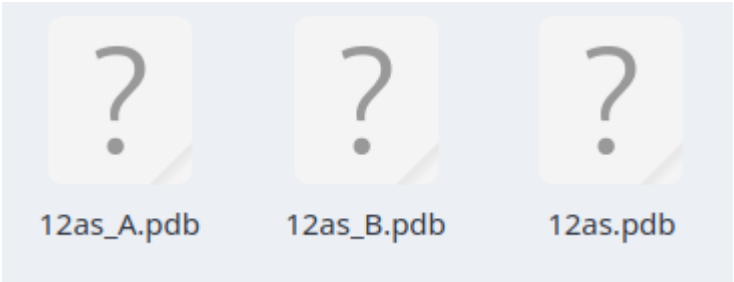
Download Link:

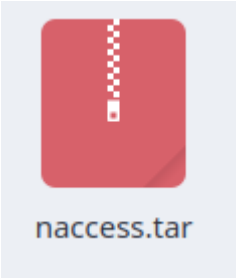
https://drive.google.com/file/d/1nzXI7qAmreq5XKXwtNHZi5wJj24fuwI6/view?usp=sharing

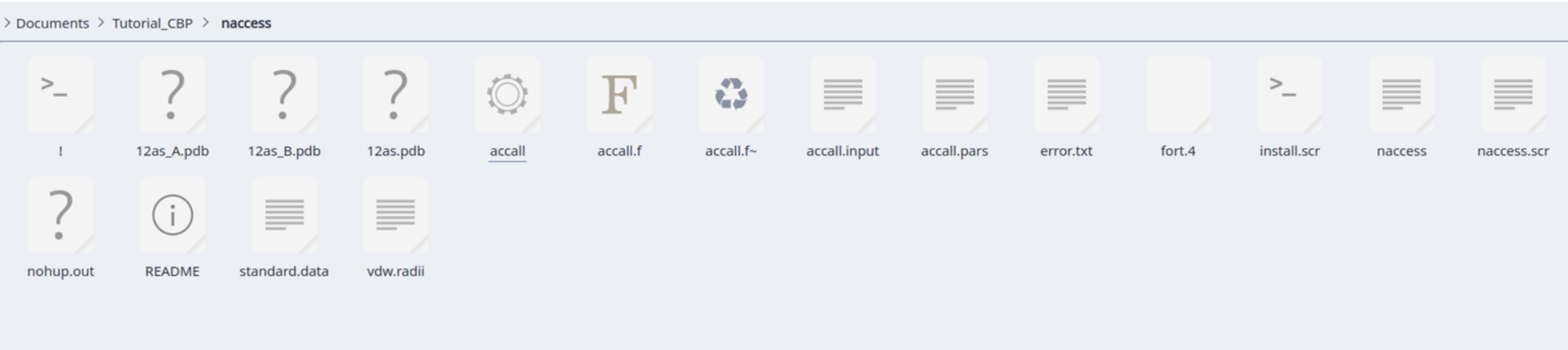
Original Link: http://www.bioinf.manchester.ac.uk/naccess/

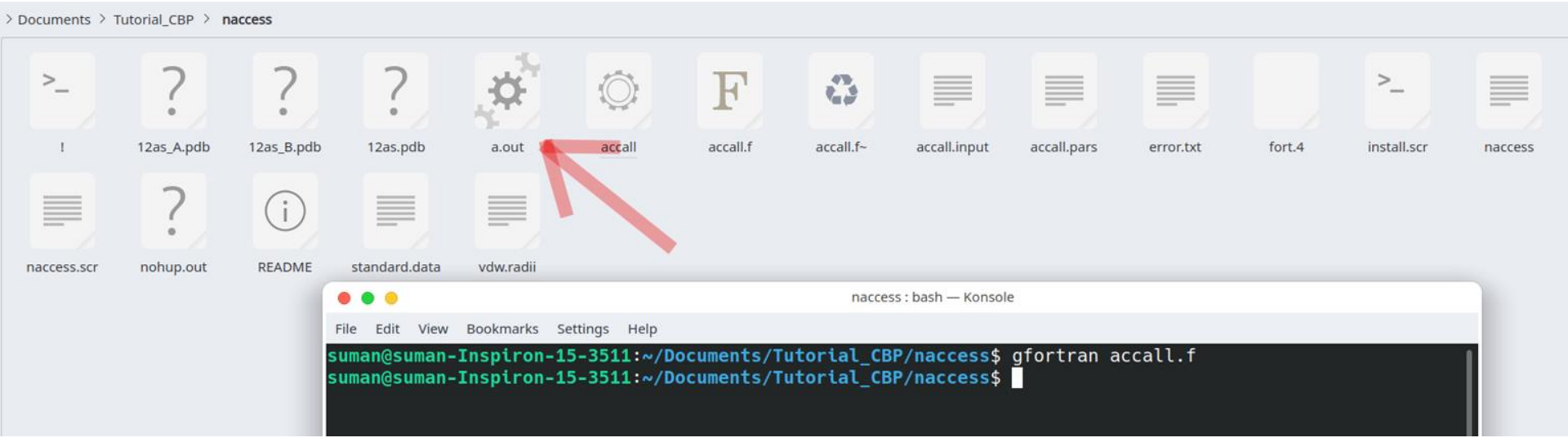
```
filename = '12as.pdb'

with open (filename, 'r') as f:
    lines = f.readlines()


atoms = [line for line in lines if line[0:4] == 'ATOM']

chains = set([atom[21:22].strip() for atom in atoms])
print(f'Chains in pdb {filename} are: {chains}')

for chain in chains:
    with open(filename.split('.')[0]+'_'+chain+'.pdb', 'w') as fc:
        for atom in atoms:
            if atom[21:22].strip() == chain:
                fc.write(atom)
```

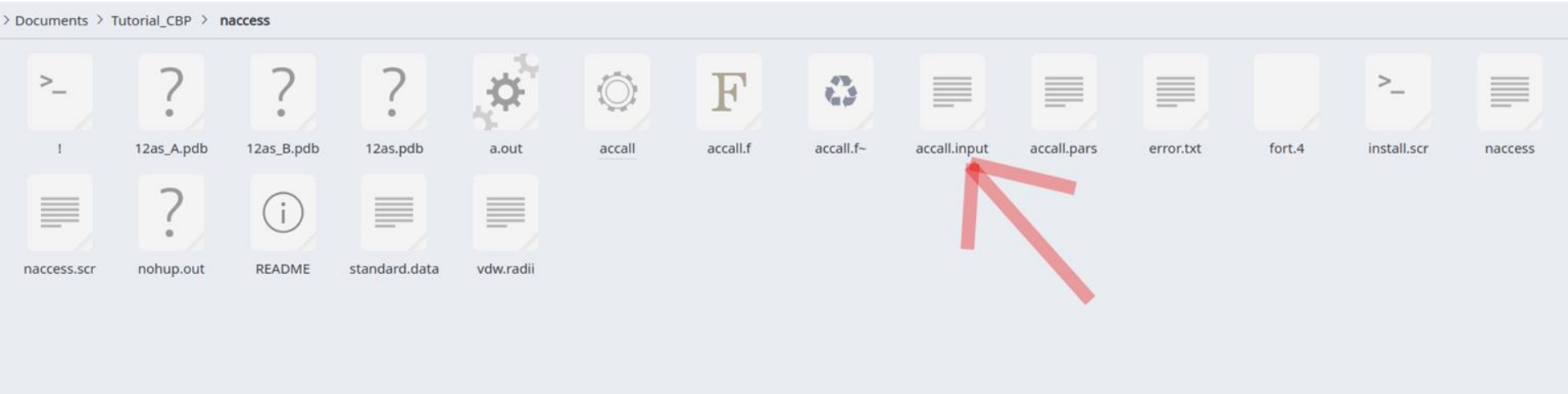
```
Chains in pdb 12as.pdb are: {'A', 'B'}
```

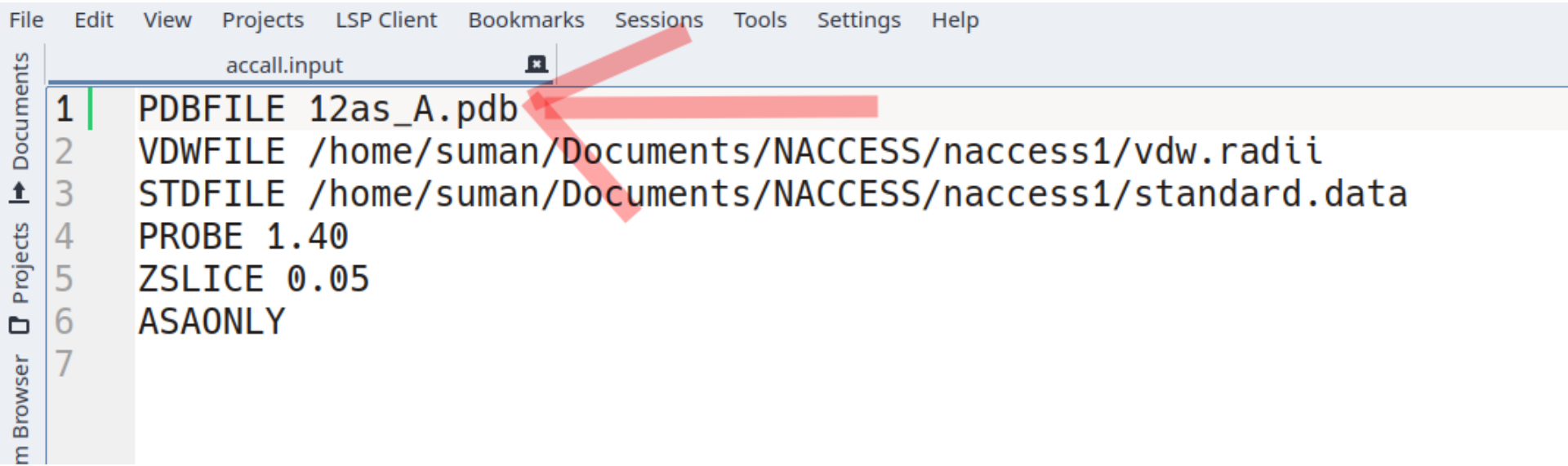


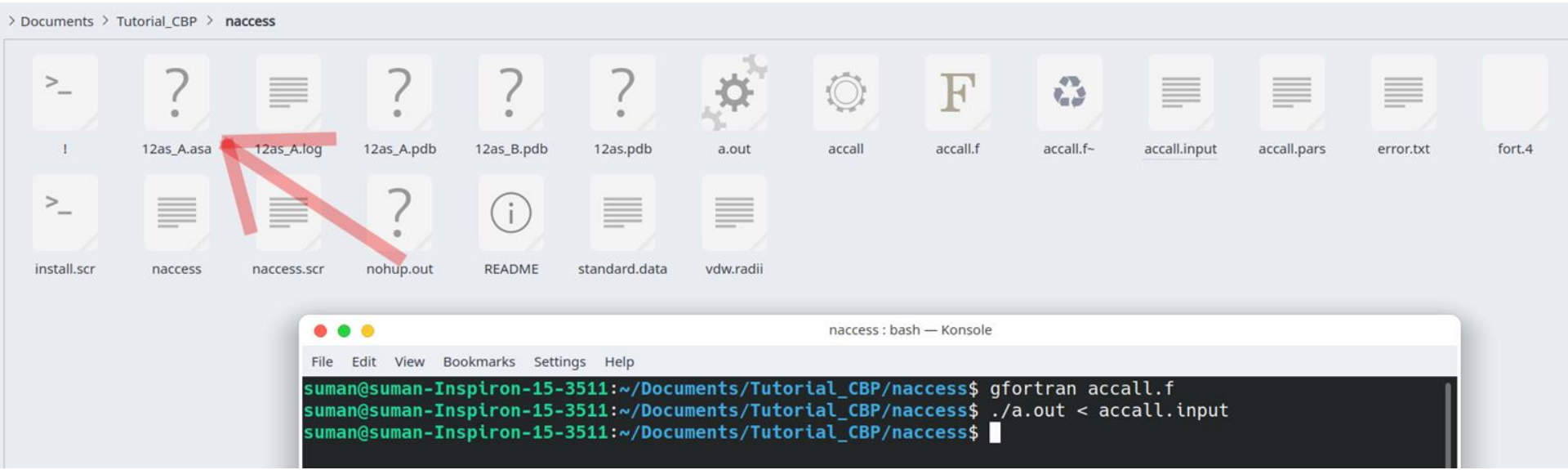

naccess.tar


Documents
Tutorial_CBP
naccess
!
12as_A.pdb
12as_B.pdb
12as.pdb
accall
accall.f
accall.f~
accall.input
accall.pars
error.txt
fort.4
install.scr
naccess
naccess.scr
nohup.out
README
standard.data
vdw.radii


Documents > Tutorial_CBP > naccess
!
12as_A.pdb
12as_B.pdb
12as.pdb
a.out
accall
accall.f
accall.f~
accall.input
accall.pars
error.txt
fort.4
install.scr
naccess
naccess.scr
nohup.out
README
standard.data
vdw.radii
naccess : bash — Konsole
File Edit View Bookmarks Settings Help
suman@suman-Inspiron-15-3511:~/Documents/Tutorial_CBP/naccess$ gfortran accall.f
suman@suman-Inspiron-15-3511:~/Documents/Tutorial_CBP/naccess$


Documents
Tutorial_CBP
naccess
!
12as_A.pdb
12as_B.pdb
12as.pdb
a.out
accall
accall.f
accall.f~
accall.input
accall.pars
error.txt
fort.4
install.scr
naccess
naccess.scr
nohup.out
README
standard.data
vdw.radii

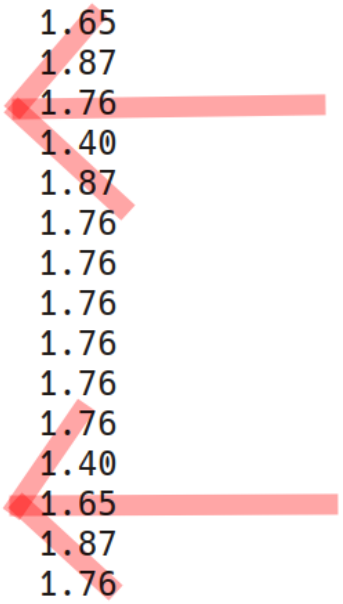

File Edit View Projects LSP Client Bookmarks Sessions Tools Settings Help
accall.input
Documents
Projects
m Browser
1 PDBFILE 12as_A.pdb
2 VDWFILE /home/suman/Documents/NACCESS/naccess1/vdw.radii
3 STDFILE /home/suman/Documents/NACCESS/naccess1/standard.data
4 PROBE 1.40
5 ZSLICE 0.05
6 ASAONLY
7

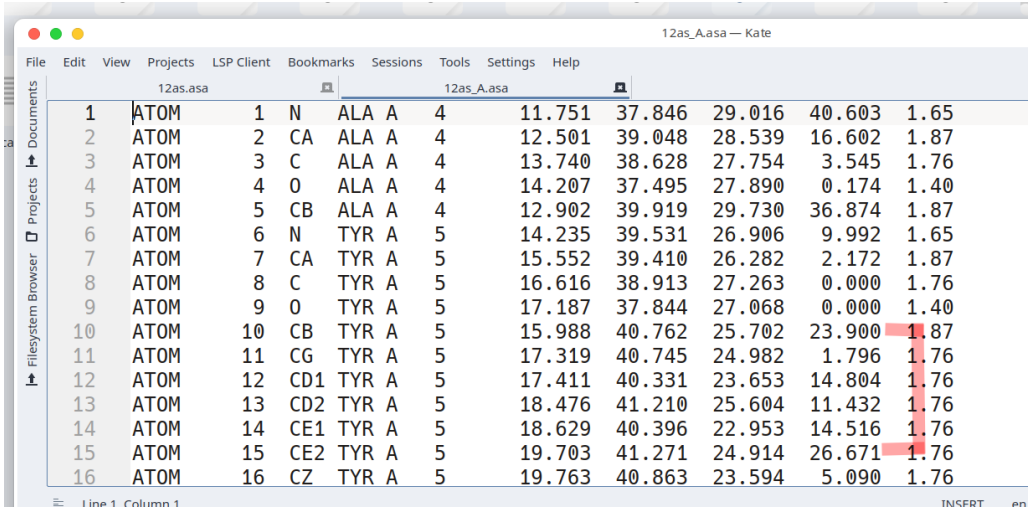

Documents
Tutorial_CBP
naccess
!
12as_A.asa
12as_A.log
12as_A.pdb
12as_B.pdb
12as.pdb
a.out
accall
accall.f
accall.f~
accall.input
accall.pars
error.txt
fort.4
install.scr
naccess
naccess.scr
nohup.out
README
standard.data
vdw.radii
naccess : bash — Konsole
File Edit View Bookmarks Settings Help
suman@suman-Inspiron-15-3511:~/Documents/Tutorial_CBP/naccess$ gfortran accall.f
suman@suman-Inspiron-15-3511:~/Documents/Tutorial_CBP/naccess$ ./a.out < accall.input
suman@suman-Inspiron-15-3511:~/Documents/Tutorial_CBP/naccess$

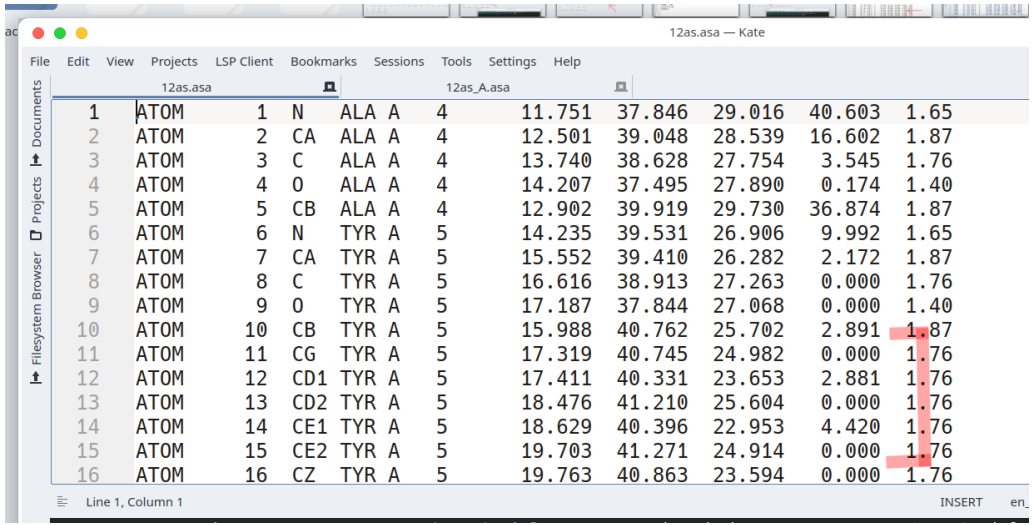
Edit View Projects LSP Client Bookmarks Sessions Tools Settings Help

12as_A.asa

1	ATOM	1	N	ALA	A	4	11.751	37.846	29.016	40.603	1.65
2	ATOM	2	CA	ALA	A	4	12.501	39.048	28.539	16.602	1.87
3	ATOM	3	C	ALA	A	4	13.740	38.628	27.754	3.545	1.76
4	ATOM	4	O	ALA	A	4	14.207	37.495	27.890	0.174	1.40
5	ATOM	5	CB	ALA	A	4	12.902	39.919	29.730	36.874	1.87
6	ATOM	6	N	TYR	A	5	14.235	39.531	26.906	9.992	1.65
7	ATOM	7	CA	TYR	A	5	15.552	39.410	26.282	2.172	1.87
8	ATOM	8	C	TYR	A	5	16.616	38.913	27.263	0.000	1.76
9	ATOM	9	O	TYR	A	5	17.187	37.844	27.068	0.000	1.40
10	ATOM	10	CB	TYR	A	5	15.988	40.762	25.702	23.900	1.87
11	ATOM	11	CG	TYR	A	5	17.319	40.745	24.982	1.796	1.76
12	ATOM	12	CD1	TYR	A	5	17.411	40.331	23.653	14.804	1.76
13	ATOM	13	CD2	TYR	A	5	18.476	41.210	25.604	11.432	1.76
14	ATOM	14	CE1	TYR	A	5	18.629	40.396	22.953	14.516	1.76
15	ATOM	15	CE2	TYR	A	5	19.703	41.271	24.914	26.671	1.76
16	ATOM	16	CZ	TYR	A	5	19.763	40.863	23.594	5.090	1.76
17	ATOM	17	OH	TYR	A	5	20.971	40.889	22.920	37.827	1.40
18	ATOM	18	N	ILE	A	6	16.789	39.630	28.369	0.000	1.65
19	ATOM	19	CA	ILE	A	6	17.791	39.281	29.375	1.348	1.87
20	ATOM	20	C	ILE	A	6	17.598	37.844	29.863	0.000	1.76
21	ATOM	21	O	ILE	A	6	18.538	37.050	29.854	0.000	1.40




12as_A.asa — Kate
File Edit View Projects LSP Client Bookmarks Sessions Tools Settings Help
12as.asa
12as_A.asa
Documents
Projects
Filesystem Browser
1 ATOM 1 N ALA A 4 11.751 37.846 29.016 40.603 1.65
2 ATOM 2 CA ALA A 4 12.501 39.048 28.539 16.602 1.87
3 ATOM 3 C ALA A 4 13.740 38.628 27.754 3.545 1.76
4 ATOM 4 O ALA A 4 14.207 37.495 27.890 0.174 1.40
5 ATOM 5 CB ALA A 4 12.902 39.919 29.730 36.874 1.87
6 ATOM 6 N TYR A 5 14.235 39.531 26.906 9.992 1.65
7 ATOM 7 CA TYR A 5 15.552 39.410 26.282 2.172 1.87
8 ATOM 8 C TYR A 5 16.616 38.913 27.263 0.000 1.76
9 ATOM 9 O TYR A 5 17.187 37.844 27.068 0.000 1.40
10 ATOM 10 CB TYR A 5 15.988 40.762 25.702 23.900 1.87
11 ATOM 11 CG TYR A 5 17.319 40.745 24.982 1.796 1.76
12 ATOM 12 CD1 TYR A 5 17.411 40.331 23.653 14.804 1.76
13 ATOM 13 CD2 TYR A 5 18.476 41.210 25.604 11.432 1.76
14 ATOM 14 CE1 TYR A 5 18.629 40.396 22.953 14.516 1.76
15 ATOM 15 CE2 TYR A 5 19.703 41.271 24.914 26.671 1.76
16 ATOM 16 CZ TYR A 5 19.763 40.863 23.594 5.090 1.76
Line 1, Column 1
INSERT


12as.asa — Kate
File Edit View Projects LSP Client Bookmarks Sessions Tools Settings Help
12as.asa
12as_A.asa
Documents
Projects
Filesystem Browser
1 ATOM 1 N ALA A 4 11.751 37.846 29.016 40.603 1.65
2 ATOM 2 CA ALA A 4 12.501 39.048 28.539 16.602 1.87
3 ATOM 3 C ALA A 4 13.740 38.628 27.754 3.545 1.76
4 ATOM 4 O ALA A 4 14.207 37.495 27.890 0.174 1.40
5 ATOM 5 CB ALA A 4 12.902 39.919 29.730 36.874 1.87
6 ATOM 6 N TYR A 5 14.235 39.531 26.906 9.992 1.65
7 ATOM 7 CA TYR A 5 15.552 39.410 26.282 2.172 1.87
8 ATOM 8 C TYR A 5 16.616 38.913 27.263 0.000 1.76
9 ATOM 9 O TYR A 5 17.187 37.844 27.068 0.000 1.40
10 ATOM 10 CB TYR A 5 15.988 40.762 25.702 2.891 1.87
11 ATOM 11 CG TYR A 5 17.319 40.745 24.982 0.000 1.76
12 ATOM 12 CD1 TYR A 5 17.411 40.331 23.653 2.881 1.76
13 ATOM 13 CD2 TYR A 5 18.476 41.210 25.604 0.000 1.76
14 ATOM 14 CE1 TYR A 5 18.629 40.396 22.953 4.420 1.76
15 ATOM 15 CE2 TYR A 5 19.703 41.271 24.914 0.000 1.76
16 ATOM 16 CZ TYR A 5 19.763 40.863 23.594 0.000 1.76
Line 1, Column 1
INSERT

```
import os

os.chdir('/home/suman/Documents/Tutorial_CBP/naccess')

original_asa = 0.0
chain_A_asa = 0.0
chain_B_asa = 0.0

with open(filename.split('.')[0]+'.asa', 'r') as foa:
    atoms = foa.readlines()
    for atom in atoms:
        original_asa += float(atom[55:63].strip())

original_asa
```

```
25299.946000000047
```

```
with open(filename.split('.')[0]+'_A'+'.asa', 'r') as foa_a:
    atoms = foa_a.readlines()
    for atom in atoms:
        chain_A_asa += float(atom[55:63].strip())

with open(filename.split('.')[0]+'_B'+'.asa', 'r') as foa_b:
    atoms = foa_b.readlines()
    for atom in atoms:
        chain_B_asa += float(atom[55:63].strip())
```

```
ia = ((chain_A_asa + chain_B_asa) - original_asa)/2.0
ia
```

```
1879.8349999999737
```

The complex set

PDB ID	IA ($Å^2$)
12AS	1879.8
1A05	2629.15
1A0F	1656.6
1A4I	1359.4
1A78	510.45
1ABR	1746.75
1AC6	594.45
1AD1	1476.55
1AFW	2400.35
1AJ8	4753.05
1AJS	3426.3
1ALV	2134.45
1AOG	3195.25
1AOR	1232.25
1AQK	1778.55
1AUI	2236
1B3A	746.15
1B5E	2578.55
1B5P	2907.45

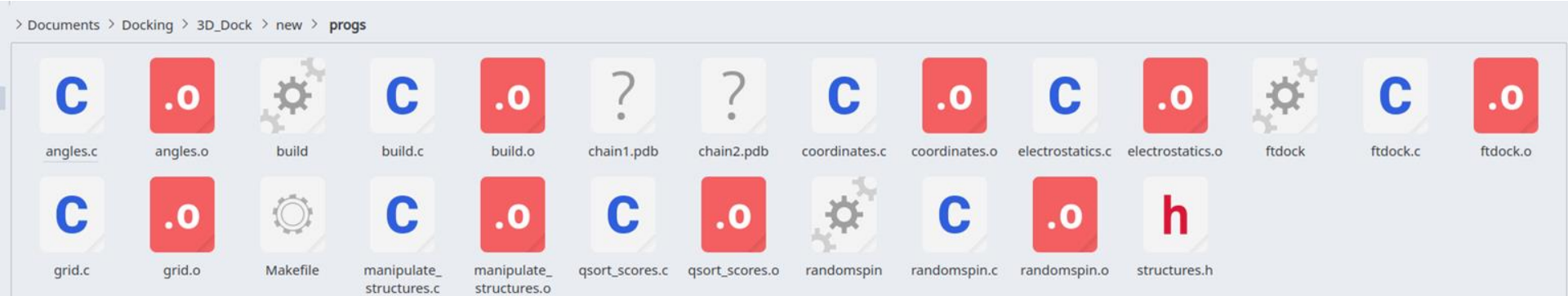
FTDock

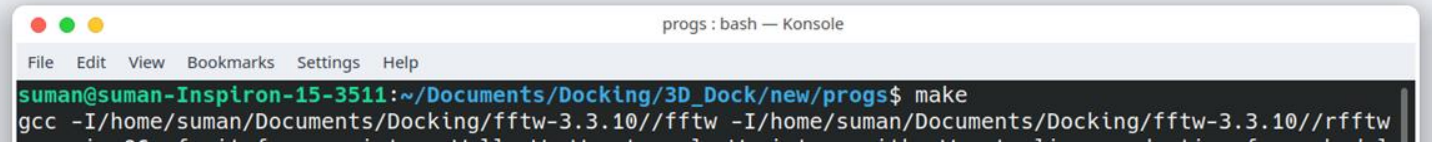
Download Link:
http://www.sbg.bio.ic.ac.uk/docking/ftdock.html

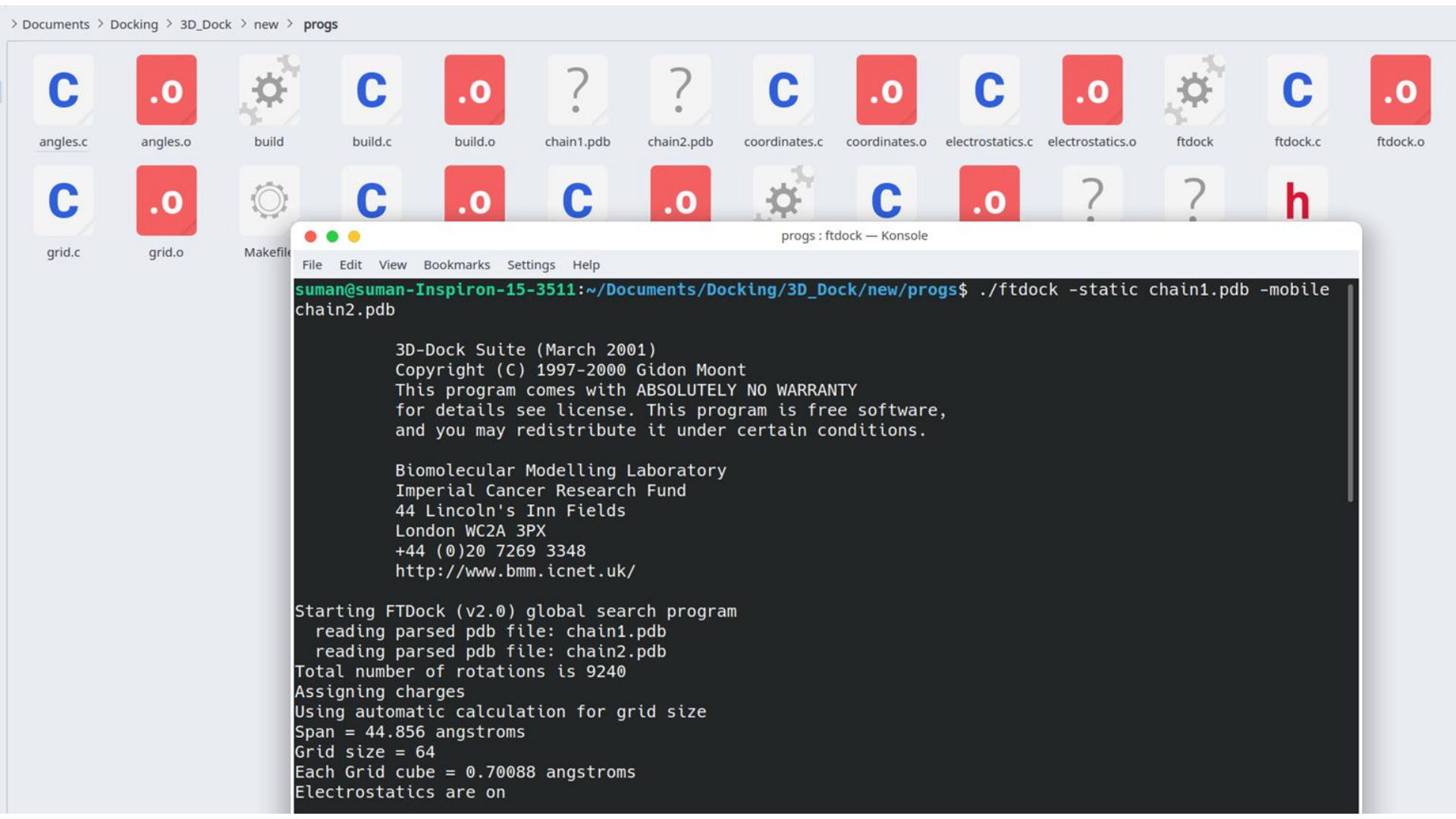
FFTW Installation Link:
https://www.youtube.com/watch?v=oWsjHU2xHWU&list=LL&index=32

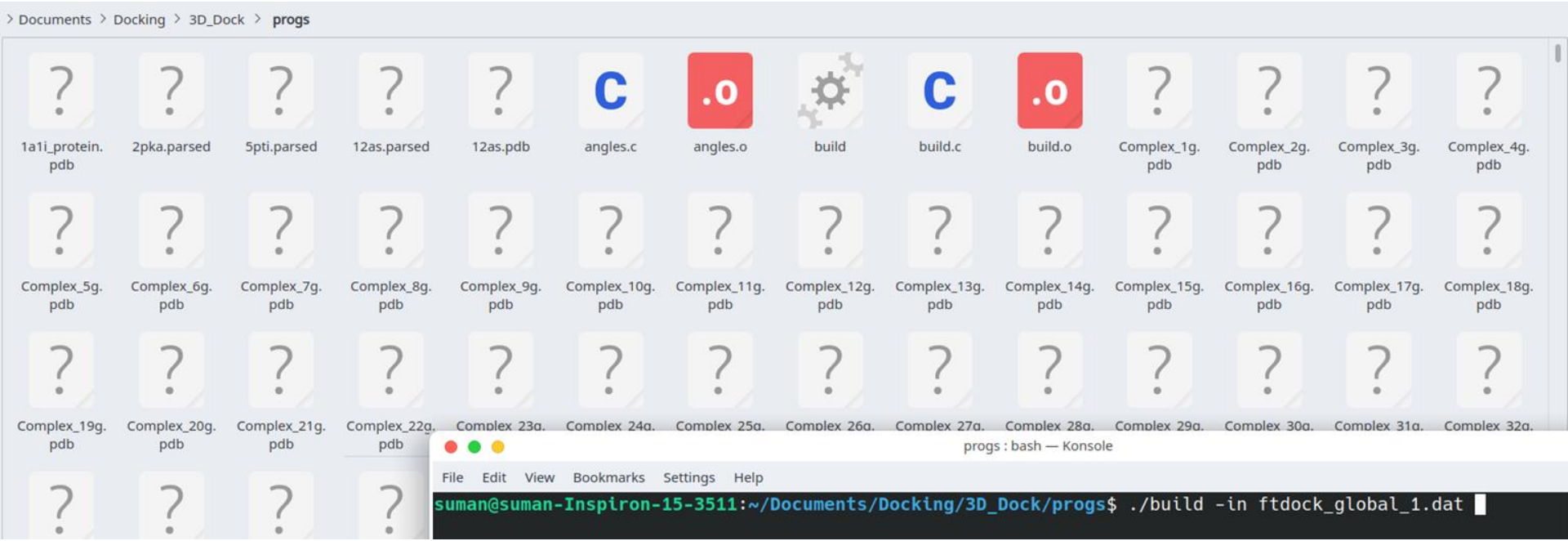
> Documents > Docking > 3D_Dock > new > **progs**

> Documents > Docking > 3D_Dock > new > **progs**






Documents > Docking > 3D_Dock > new > progs
angles.c
angles.o
build
build.c
build.o
chain1.pdb
chain2.pdb
coordinates.c
coordinates.o
electrostatics.c
electrostatics.o
ftdock
ftdock.c
ftdock.o
grid.c
grid.o
Makefile
progs : ftdock — Konsole
File Edit View Bookmarks Settings Help
suman@suman-Inspiron-15-3511:~/Documents/Docking/3D_Dock/new/progs$ ./ftdock -static chain1.pdb -mobile chain2.pdb
3D-Dock Suite (March 2001)
Copyright (C) 1997-2000 Gidon Moont
This program comes with ABSOLUTELY NO WARRANTY
for details see license. This program is free software,
and you may redistribute it under certain conditions.
Biomolecular Modelling Laboratory
Imperial Cancer Research Fund
44 Lincoln's Inn Fields
London WC2A 3PX
+44 (0)20 7269 3348
http://www.bmm.icnet.uk/
Starting FTDock (v2.0) global search program
reading parsed pdb file: chain1.pdb
reading parsed pdb file: chain2.pdb
Total number of rotations is 9240
Assigning charges
Using automatic calculation for grid size
Span = 44.856 angstroms
Grid size = 64
Each Grid cube = 0.70088 angstroms
Electrostatics are on


Documents > Docking > 3D_Dock > progs
1a1i_protein.pdb
2pka.parsed
5pti.parsed
12as.parsed
12as.pdb
angles.c
angles.o
build
build.c
build.o
Complex_1g.pdb
Complex_2g.pdb
Complex_3g.pdb
Complex_4g.pdb
Complex_5g.pdb
Complex_6g.pdb
Complex_7g.pdb
Complex_8g.pdb
Complex_9g.pdb
Complex_10g.pdb
Complex_11g.pdb
Complex_12g.pdb
Complex_13g.pdb
Complex_14g.pdb
Complex_15g.pdb
Complex_16g.pdb
Complex_17g.pdb
Complex_18g.pdb
Complex_19g.pdb
Complex_20g.pdb
Complex_21g.pdb
Complex_22g.pdb
Complex_23g.
Complex_24g.
Complex_25g.
Complex_26g.
Complex_27g.
Complex_28g.
Complex_29g.
Complex_30g.
Complex_31g.
Complex_32g.
progs : bash — Konsole
File Edit View Bookmarks Settings Help
suman@suman-Inspiron-15-3511:~/Documents/Docking/3D_Dock/progs$ ./build -in ftdock_global_1.dat