MCCE Commands

MCCE commands explanation and examples.

MCCE Program Run and Debug

Commands and Tools

getpdb

Command line tool to download pdb file from PDB

Author: Yanjun Wang

Syntax:

`getpdb pdbID [file]`

This program gets a pdb file from Protein Data Bank, and saves to a file with its PDB name or a user named file.

Example:

```
getpdb 1akk
Download with url https://files.rcsb.org/download/1akk.pdb.
Download completed.
```

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vdw_bk.py

Calculate conformer to backbone vdw (Lennard-Jones potential).

Author: Junjun Mao

Syntax:

`vdw_bk.py [-h] [-c cutoff] confID`

Compute vdw1 breakdown at conformer level. The conformer ID can be found in head3.lst.

positional arguments:
  confID   Conformer ID as in head3.lst

optional arguments:
  -h, --help show this help message and exit
  -c cutoff   Cutoff value of displaying conf vdw pairwise

Example:

```
(base) jmao@Jupiter:~/projects/1akk$ vdw_bk.py GLU-1A0090_005 -c 0.1
LEUBKA0064_000  -0.104
METBKA0065_000  -0.499
LEUBKA0068_000  -0.825
GLUBKA0069_000  -0.758
ILEBKA0085_000  -0.571
LYSBKA0086_000  -0.990
LYSBKA0087_000  -1.005
LYSBKA0088_000  -1.011
THRBKA0089_000  -0.876
GLUBKA0090_000   1.424
ARGBKA0091_000   2.383
GLUBKA0092_000  -0.204
ASPBKA0093_000  -0.113
LEUBKA0094_000  -0.120
Total           -3.616
```

---

vdw_conf2conf.py

Calculate conformer to conformer pairwise vdw (Lennard-Jones potential).

Author: Junjun Mao

Syntax:

`vdw_conf2conf.py [-h] [-c cutoff] [-v] confID confID`

Compute detailed conformer to conformer vdw.

positional arguments:
  confID   Conformer ID as in head3.lst, two IDs required.

optional arguments:
  -h, --help show this help message and exit
  -c cutoff   Cutoff value of displaying atom to atom vdw
  -v   Turn on verbose mode, displaying more details

This program calculates Lennard-Jones potential between a conformer pair, which should be consistent with the number in opp file under energies directory. The pair could be self to self, which is vdw0 term in head3.lst. The programs reports atom to atom interaction and atom connectivity as well.

The conformer ID can be found in head3.lst.

Example:

```
(base) jmao@Jupiter:~/projects/1akk$ vdw_conf2conf.py GLU-1A0090_005 THR01A0089_002 -c 0.01 -v
       ATOM1            ATOM2            vdw     dist   cnct       r1     e1     r2     e2
R_sum  E_par
 CB GLU0090A005 ->  CB THR0089A002:   -0.024    5.446   none   1.9080 0.1094 1.9080 0.1094
3.8160 0.1094
 CB GLU0090A005 ->  OG1THR0089A002:   -0.010    6.361   none   1.9080 0.1094 1.7210 0.2104
3.6290 0.1517
 CG GLU0090A005 ->  CB THR0089A002:   -0.016    5.883   none   1.9080 0.1094 1.9080 0.1094
3.8160 0.1094
GLU-1A0090_005 - THR01A0089_002: -0.150
```

---

vdw_pw.py

Update Lennard-Jones potential of step 3 in files head3.lst and energies/.opp*

Author: Junjun Mao

Syntax:

`vdw_pw.py`

This program updates Lennard-Jones potential of step 3 in

- file head3.lst (vdw0 and vdw 1) and
- files energies/*.opp (vdw column).

A copy of head3.lst will be made as head3.lst_bak and the copy of energies directory will be made as energies_bak. It corrects the some parameter issues in mcce step 3 and offers a chance to rerun vdw calculation without running PB solver again. Also it checks the possible inconsistancy in parameter files and comes with two other tools: vdw_conf2conf.py and vdw_bk.py to inspect the vdw interaction clashes.

Example:

`vdw_pw.py`

MCCE Parameter Preparation

MCCE Data Analysis

MCCE data analysis tools

fitpka.py

Fit the titration curve of an ionizable residue.

Syntax:

```
fitpka.py [-h] RES [RES ...]
```

Fit a titration of charged residues

positional arguments:
  RES   Charged residue names to plot, as in sum_crg.out or pK.out

optional arguments:
  -h, --help show this help message and exit

Required input file

- sum_crg.out

Example:

Find the residue IDs:

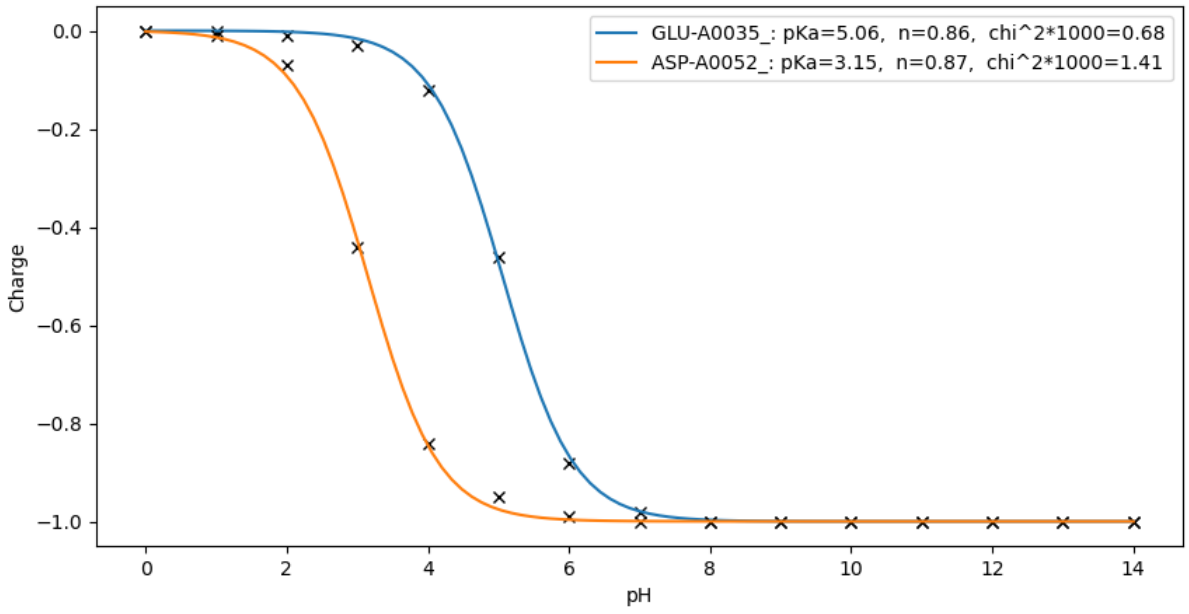
```
$ cat sum_crg.out
  pH           0     1     2     3     4     5     6     7     8     9    10    11    12
13    14
NTR+A0001_  1.00  1.00  1.00  1.00  0.99  0.96  0.70  0.20  0.03  0.00  0.00  0.00  0.00
0.00  0.00
LYS+A0001_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.97  0.78  0.27  0.04  0.00
0.00  0.00
ARG+A0005_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.97  0.80
0.38  0.08
GLU-A0007_ -0.00 -0.01 -0.07 -0.38 -0.84 -0.98 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
LYS+A0013_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.95  0.67  0.19
```

```
0.03  0.00
ARG+A0014_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.94
0.66  0.19
HIS+A0015_  1.00  1.00  1.00  1.00  1.00  0.98  0.83  0.36  0.06  0.01  0.00  0.00  0.00
0.00  0.00
ASP-A0018_ -0.01 -0.10 -0.49 -0.89 -0.99 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
TYR-A0020_ -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.03 -0.09 -0.32
-0.73
ARG+A0021_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.91
0.59  0.22
TYR-A0023_ -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01 -0.06 -0.32 -0.76 -0.96 -0.99
-1.00
LYS+A0033_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.97  0.78  0.27  0.05
0.01  0.00
GLU-A0035_ -0.00 -0.00 -0.01 -0.03 -0.12 -0.46 -0.88 -0.98 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
ARG+A0045_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.91
0.56  0.21
ASP-A0048_ -0.03 -0.21 -0.69 -0.95 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
ASP-A0052_ -0.00 -0.01 -0.07 -0.44 -0.84 -0.95 -0.99 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
TYR-A0053_ -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00
-0.00
ARG+A0061_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.98
0.90  0.57
ASP-A0066_ -0.03 -0.20 -0.68 -0.93 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
ARG+A0068_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.95
0.76  0.34
ARG+A0073_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.98  0.85
0.39  0.09
ASP-A0087_ -0.01 -0.08 -0.44 -0.88 -0.98 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
LYS+A0096_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.96  0.76  0.33  0.08
0.02  0.01
LYS+A0097_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.98  0.85  0.40  0.08
0.01  0.00
ASP-A0101_ -0.00 -0.00 -0.01 -0.09 -0.51 -0.91 -0.99 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
```

```
-1.00
ARG+A0112_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.98  0.87
0.43  0.09
ARG+A0114_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.94
0.63  0.17
LYS+A0116_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.97  0.75  0.27  0.05  0.01
0.00  0.00
ASP-A0119_ -0.00 -0.00 -0.03 -0.19 -0.71 -0.96 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
ARG+A0125_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.90
0.55  0.13
ARG+A0128_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.99  0.97
0.79  0.31
CTR-A0129_ -0.00 -0.04 -0.29 -0.75 -0.96 -0.99 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00 -1.00
-1.00
----------
Net_Charge 18.93 18.34 16.22 13.47 11.05  9.70  8.68  7.57  7.01  6.38  4.53  1.82 -0.64 -4.61
-9.32
Protons    18.93 18.34 16.22 13.47 11.05  9.70  8.68  7.57  7.01  6.38  4.53  1.82 -0.64 -4.61
-9.32
Electrons   0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00  0.00
0.00  0.00
```

Fit the titration curves of residue GLU-A0035_ and ASP-A0052_:

```
fitpka.py GLU-A0035_ ASP-A0052_
```



mfe.py

Analyze ionization free energy of a residue. It tells you why a residue has that pKa and what factors played a role.

Syntax

`mfe.py [-h] [-p pH/Eh] [-x TS_correction] [-c cutoff] residue`

- residue: residue ID as in pK.out
- pH/Eh: pH value at which ionization energy is calculated. Default is the pKa (midpoint) where dG = 0.
- cut_off: Report only pairwise interaction bigger than this value.
- TS_correction: "t" to include entropy in G, "f" not to include, "r" (default) will look for run.prm. If entropy correction was turned on in step 4, mfe should not include this term as entropy has been "removed".

Required files:

- run.prm
- head3.lst
- extra.tpl for scaling factors that are not equal to 1.
- energies/*.opp for pairwise interactions

Example:

Check titration result in pKa.out:

```
cat pK.out
...
ASP-A0052_        3.152
...
```

ASP-A0052_ is the residue_ID. Its calculated pKa is 3.152. At this point, the free energy of reaction from ASP neutral to ASP ionized should be close to 0.

Run

```
$ mfe.py ASP-A0052_ -c 0.1
Residue ASP-A0052_ pKa/Em=3.152
================================
Terms           pH     meV    Kcal
--------------------------------
vdw0        -0.01   -0.85   -0.02
```

```
vdw1          0.00     0.23     0.01
tors         -0.10    -5.86    -0.14
ebkb         -1.27   -73.44    -1.73
dsol          1.99   115.38     2.71
offset       -0.62   -36.17    -0.85
pH&pK0        1.60    92.75     2.18
Eh&Em0        0.00     0.00     0.00
-TS           0.00     0.00     0.00
residues     -1.36   -79.01    -1.86
**********************************
TOTAL         0.22    13.04     0.31  sum_crg
**********************************
ASNA0044_    -0.46   -26.92    -0.63     0.00
ARGA0045_    -0.11    -6.36    -0.15     1.00
ASNA0046_    -0.19   -11.09    -0.26     0.00
ASPA0048_     0.50    28.96     0.68    -0.96
SERA0050_     0.13     7.28     0.17     0.00
GLNA0057_     0.22    12.78     0.30     0.00
ASNA0059_    -0.99   -57.18    -1.34     0.00
ARGA0061_    -0.26   -15.37    -0.36     1.00
ASPA0066_     0.27    15.72     0.37    -0.94
ARGA0112_    -0.19   -11.11    -0.26     1.00
ARGA0114_    -0.10    -5.86    -0.14     1.00
==================================
```

You can do mfe calculation at pH other than mid-point.