# 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:

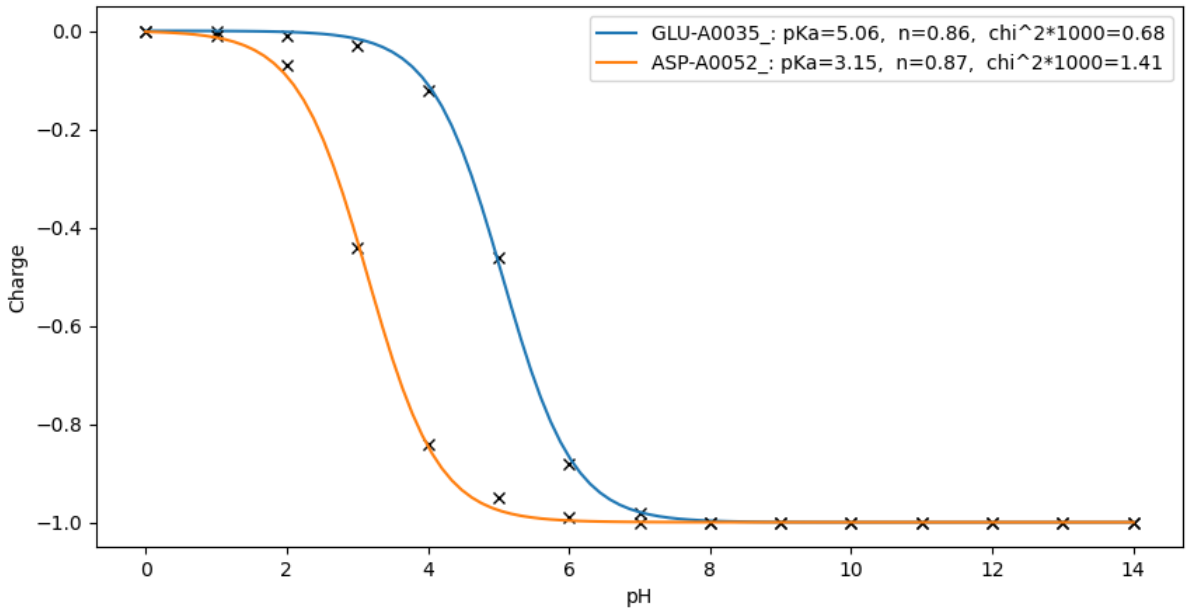
```
$ cat sum_crg.out
  pH           0     1     2     3     4     5     6     7     8     9    10    11    12
13    14
NTR+A0001_  1.00  1.00  1.00  1.00  0.99  0.96  0.70  0.20  0.03  0.00  0.00  0.00  0.00
0.00  0.00
LYS+A0001_  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  0.97  0.78  0.27  0.04  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 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 -0.00 -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 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 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
-1.00
ARG+A0045_ 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 0.99 0.91
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
-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
-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
-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 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
-1.00
ARG+A0068_ 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00 0.99 0.95
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 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
-1.00
LYS+A0096_ 1.00 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 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.

---

Revision #3
Created 5 March 2023 18:15:17 by Junjun Mao
Updated 15 March 2023 16:27:09 by Junjun Mao