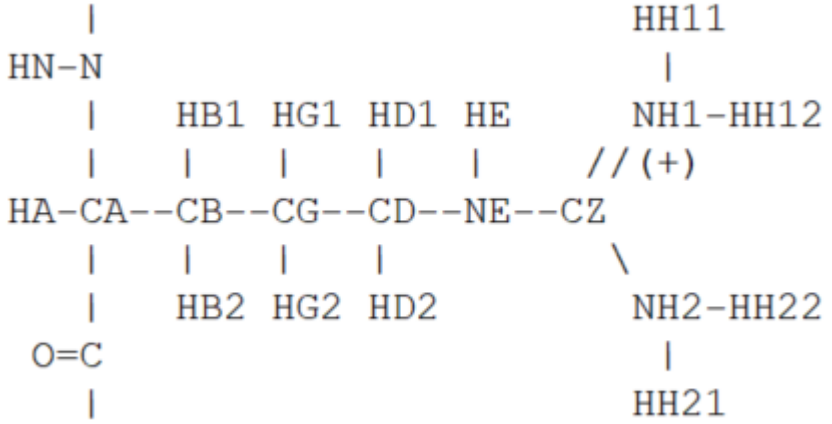
如何生成自己的topology

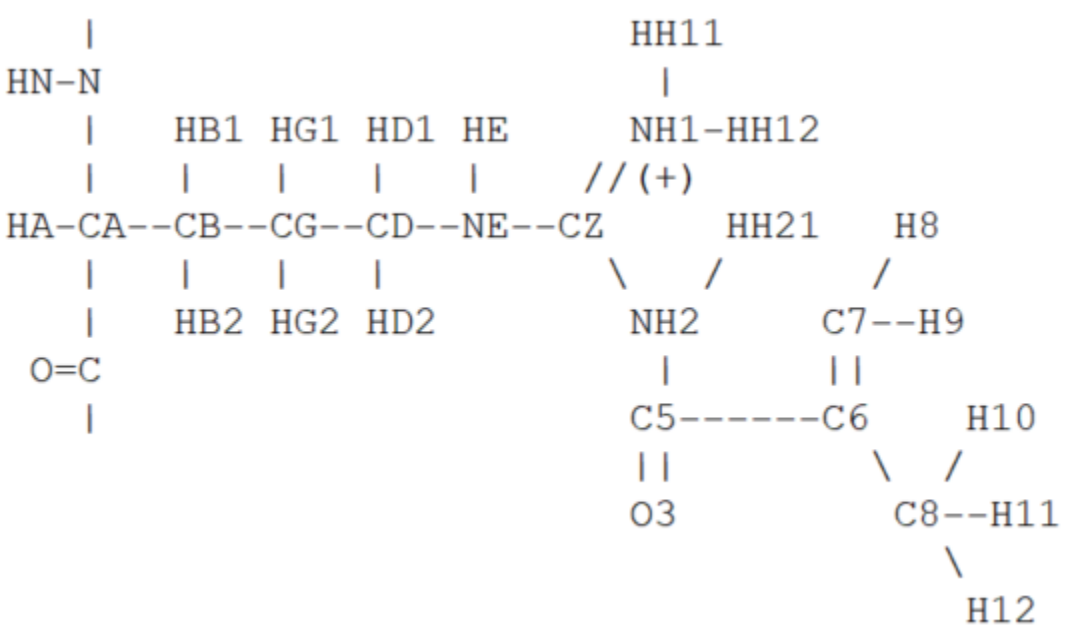
1_25 有成 澄葦

課題一：如何改質胺基酸的topo

原始ARG



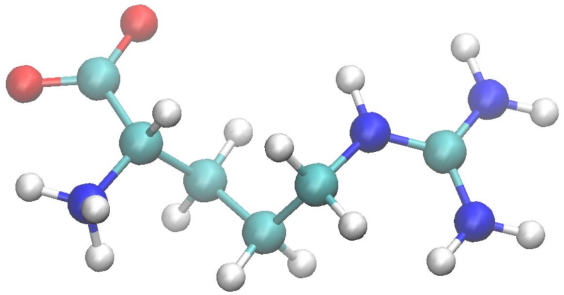
ARG_MA



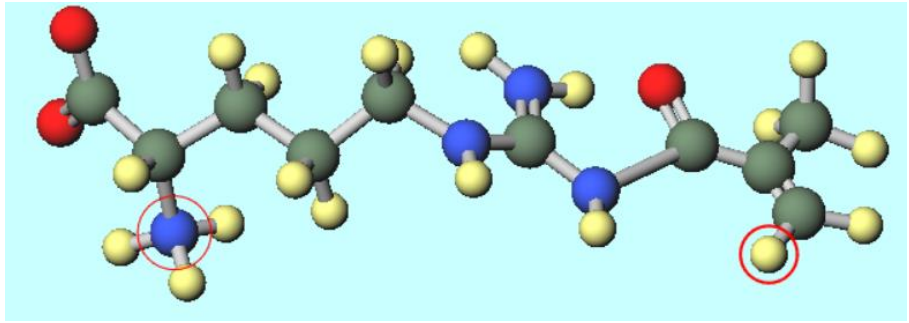
A. 原始top_all36_prot.rtf中的ARG

```
RESI ARG          1.00
GROUP
ATOM N     NH1    -0.47
ATOM HN    H       0.31
ATOM CA    CT1     0.07
ATOM HA    HB1     0.09
GROUP
ATOM CB    CT2    -0.18
ATOM HB1   HA2     0.09
ATOM HB2   HA2     0.09
GROUP
ATOM CG    CT2    -0.18
ATOM HG1   HA2     0.09
ATOM HG2   HA2     0.09
GROUP
ATOM CD    CT2     0.20
ATOM HD1   HA2     0.09
ATOM HD2   HA2     0.09
ATOM NE    NC2    -0.70
ATOM HE    HC      0.44
ATOM CZ    C       0.64
ATOM NH1   NC2    -0.80
ATOM HH11  HC      0.46
ATOM HH12  HC      0.46
ATOM NH2   NC2    -0.80
ATOM HH21  HC      0.46
ATOM HH22  HC      0.46
GROUP
ATOM C     C       0.51
ATOM O     O      -0.51
```

B. 原始ARG構型

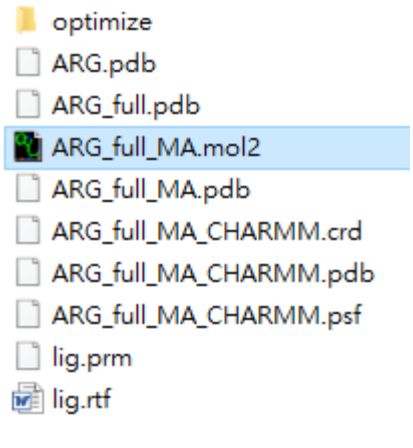


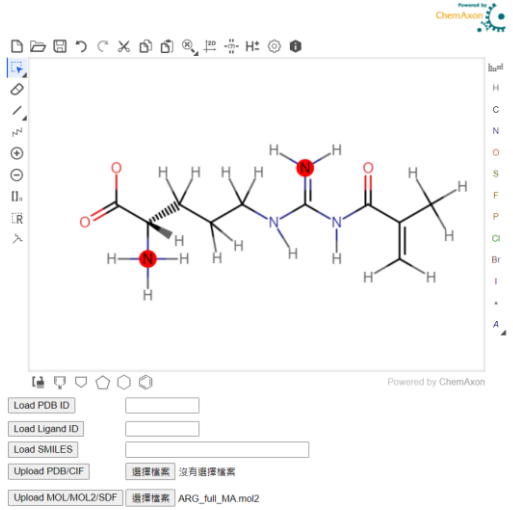
C. 更改ARG構型：在Winmostar繪製ARG_MA



D. 畫完匯出mol2檔
上傳至Charmm GUI: Ligand Reader

(https://charmm-gui.org/?doc=input/ligandrm)



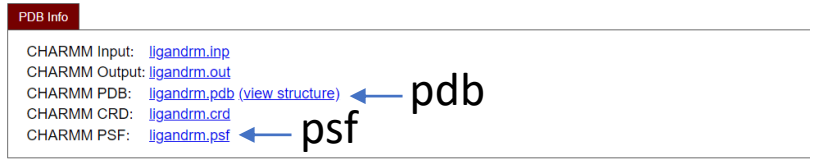


F. Charmm GUI: Ligand Reader

下載Cgenff下的：**.pdb .psf**

下載補充**topology**檔：**lig.rtf**

下載補充參數檔：**lig.prm**



Computed Energy:

Please beware of that the computed energy is CHARMM single-point energy and is displayed to make sure all the coordinates are defined.

	Eval#	ENERgy	Delta-E	GRMS		
ENER INTERN:		BONDs	ANGLes	UREY-b	DIHEdrals	IMPRopers
ENER EXTERN:		VDWaals	ELEC	HBONds	ASP	USER
ENER>	0	-119.44416	3.93222	1.79693		
ENER INTERN>		4.51106	15.34930	1.23020	12.78290	0.07422
ENER EXTERN>		18.00764	-171.39949	0.00000	0.00000	0.00000

Topology and Parameter Files:

Below is the topology and parameter files that are generated by automatic method.

LIG
Topology: lig.rtf ← **rtf，接下來會先檢視這個檔案**
Topology: lig_g.rtf
Parameter: lig.prm ← prm

G. 檢視下載的rtf，看一下penalty是否太多超過50的

1. **Penalty>50**，代表Cgenff近似的結果可能不會太好
   特別是**charge penalty**很高**(93.016)**，說明電荷分布的狀況不太理想

D:\Keratin\combine_data_file\ARG\lig.rtf - Notepad++

```
1  * Topologies generated by
2  * CHARMM General Force Field (CGenFF) program version 2.5.1
3  *
4  36 1
5
6  ! "penalty" is the highest penalty score of the associated parameters.
7  ! Penalties lower than 10 indicate the analogy is fair; penalties between 10
8  ! and 50 mean some basic validation is recommended; penalties higher than
9  ! 50 indicate poor analogy and mandate extensive validation/optimization.
10
11 RESI lig            1.000 ! param penalty=  74.000 ; charge penalty=  93.016
12 GROUP              ! CHARGE   CH_PENALTY
13 ATOM N1      NG321  -1.077 !    6.901
14 ATOM H1      HGPAM2  0.396 !    2.558
15 ATOM H2      HGPAM2  0.396 !    2.558
16 ATOM C1      CG311   0.326 !    6.441
17 ATOM H3      HGA1    0.090 !    0.000
18 ATOM C2      CG321  -0.289 !    2.514
19 ATOM H4      HGA2    0.090 !    0.300
```

3. 留意下半部構型資訊**(bond, improper)**，待會要補在**top_all36_prot.rtf**檔中

```
80  BOND C9    H16
81  BOND C10   H17
82  BOND C10   H18
83  BOND N3    C7
84  BOND N4    H19
85  IMPR C5      N2      N3      N4
86  IMPR C6      C1      O1      O2
87  IMPR C7      C8      N3      O3
88
89  END
90
```

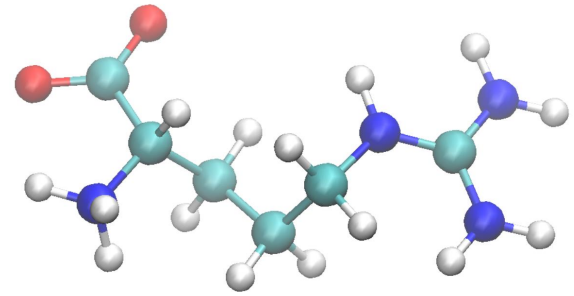
留意：**cgenff**中的**ARG_MA**只考慮**3**個**improper**結構

2. **Charge Penalty>50**的位置在改質的**N-C**與周圍位置，並非整個結構壞掉，決定用**GAMESS**做這個結構看看
(也要確認**.par**中**penalty**高的地方，這邊省略**)**

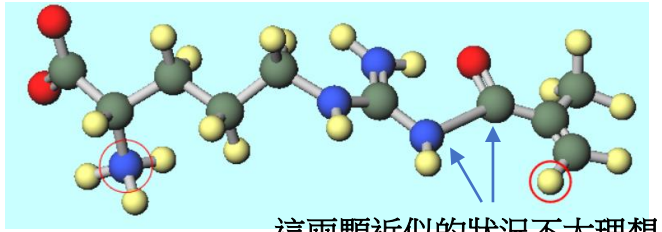
```
RESI lig            1.000 ! param penalty=  74.000 ; charge penalty=  93.016
GROUP              ! CHARGE   CH_PENALTY
ATOM N1      NG321  -1.077 !    6.901
ATOM H1      HGPAM2  0.396 !    2.558
ATOM H2      HGPAM2  0.396 !    2.558
ATOM C1      CG311   0.326 !    6.441
ATOM H3      HGA1    0.090 !    0.000
ATOM C2      CG321  -0.289 !    2.514
ATOM H4      HGA2    0.090 !    0.300
ATOM H5      HGA2    0.090 !    0.300
ATOM C3      CG321  -0.151 !    2.182
ATOM H6      HGA2    0.090 !    0.000
ATOM H7      HGA2    0.090 !    0.000
ATOM C4      CG324   0.204 !    0.000
ATOM H8      HGA2    0.090 !    0.000
ATOM H9      HGA2    0.090 !    0.000
ATOM N2      NG2P1  -0.672 !    2.500
ATOM H10     HGP2    0.440 !    0.000
ATOM C5      CG2N1   0.617 !   31.182
ATOM N3      NG2P1  -1.339 !   92.161
ATOM H11     HGP2    0.475 !    7.268
ATOM N4      NG2P1  -0.737 !    2.500
ATOM H12     HGP2    0.438 !    0.000
ATOM C6      CG2O2   0.779 !    6.226
ATOM O1      OG2D1  -0.548 !    2.558
ATOM O2      OG311  -0.553 !    3.286
ATOM H13     HGP1    0.290 !    0.000
ATOM C7      CG2O1   1.247 !   93.016
ATOM C8      CG2DC1  0.289 !   19.526
ATOM C9      CG331  -0.284 !    9.902
ATOM H14     HGA3    0.090 !    0.450
ATOM H15     HGA3    0.090 !    0.450
ATOM H16     HGA3    0.090 !    0.450
ATOM O3      OG2D1  -0.590 !   12.160
ATOM C10     CG2DC3 -0.415 !    9.042
ATOM H17     HGA5    0.210 !    0.100
ATOM H18     HGA5    0.210 !    0.100
```

這兩顆近似的狀況不太理想

原始ARG



ARG_MA

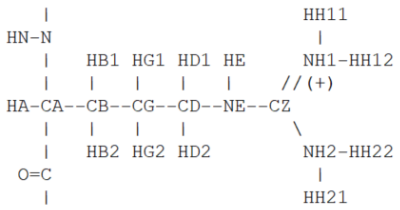


這兩顆近似的狀況不太理想

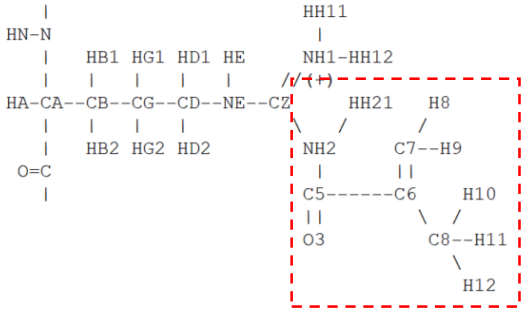
H. 根據下載的rtf檔案，手動改動top_all36_prot.rtf中的ARG：

1.構型改動(不影響結果，僅用來視覺化。注意：要定義好原子名稱，別重複)

原始ARG



ARG_MA



3. 根據下載的lig.rtf調整topology內bond、improper，並刪除不存在原子的資訊

原始ARG

```
BOND CB   CA   CG   CB   CD CG   NE CD   CZ NE
BOND NH2 CZ   N   HN   N   CA
BOND C    CA   C   +N   CA HA   CB HB1
BOND CB   HB2 CG   HG1 CG HG2 CD HD1 CD HD2
BOND NE   HE   NH1 HH11  NH1 HH12  NH2 HH21  NH2 HH22
DOUBLE O  C     CZ  NH1
IMPR N  -C  CA  HN   C CA +N O
IMPR CZ  NH1  NH2  NE
IMPR NH1 HH11 HH12 CZ
IMPR NH2 HH21 HH22 CZ
CMAP -C  N  CA  C   N  CA  C  +N
DONOR HN N
DONOR HE NE
DONOR HH11 NH1
DONOR HH12 NH1
DONOR HH21 NH2
DONOR HH22 NH2
```

ARG_MA

```
BOND CB   CA   CG   CB   CD CG   NE CD   CZ NE
BOND NH2 CZ   N   HN   N   CA
BOND C    CA   C   +N   CA HA   CB HB1
BOND CB   HB2 CG   HG1 CG HG2 CD HD1 CD HD2
BOND NE   HE   NH1 HH11  NH1 HH12  NH2 HH21  NH2 C5
BOND C5 C6 C6 C8
DOUBLE C5 O3 C6 C7
BOND C7 H8 C7 H9 C8 H10 C8 H11 C8 H12
DOUBLE O  C     CZ  NH1
IMPR N  -C  CA  HN   C CA +N O
IMPR CZ  NH1  NH2  NE
IMPR NH1 HH11 HH12 CZ
IMPR NH2 HH21 C5 CZ
IMPR C5 C6 NH2 O3
CMAP -C  N  CA  C   N  CA  C  +N
DONOR HN N
DONOR HE NE
DONOR HH11 NH1
DONOR HH12 NH1
DONOR HH21 NH2
```

留意：**CHARMM36+cgenff中的ARG_MA共考慮6個improper結構**

2 topology內原子改動：

補上原子，原子種類要留意需不需要變化

看一下電荷的差別會不會太大(本範例並沒有太大的電荷差異)

將多的電荷分配給鄰近原子，並確認電荷總和相同

原始ARG

```
RESI ARG          1.00
GROUP
ATOM N     NH1    -0.47
ATOM HN    H       0.31
ATOM CA    CT1     0.07
ATOM HA    HB1     0.09
GROUP
ATOM CB    CT2    -0.18
ATOM HB1   HA2     0.09
ATOM HB2   HA2     0.09
GROUP
ATOM CG    CT2    -0.18
ATOM HG1   HA2     0.09
ATOM HG2   HA2     0.09
GROUP
ATOM CD    CT2     0.20
ATOM HD1   HA2     0.09
ATOM HD2   HA2     0.09
ATOM NE    NC2    -0.70
ATOM HE    HC      0.44
ATOM CZ    C       0.64
ATOM NH1   NC2    -0.80
ATOM HH11  HC      0.46
ATOM HH12  HC      0.46
ATOM NH2   NC2    -0.80
ATOM HH21  HC      0.46
ATOM HH22  HC      0.46
GROUP
ATOM C     C       0.51
ATOM O     O      -0.51
```

ARG_MA

```
RESI ARG          1.00
GROUP
ATOM N     NH1    -0.47
ATOM HN    H       0.31
ATOM CA    CT1     0.07
ATOM HA    HB1     0.09
GROUP
ATOM CB    CT2    -0.18
ATOM HB1   HA2     0.09
ATOM HB2   HA2     0.09
GROUP
ATOM CG    CT2    -0.18
ATOM HG1   HA2     0.09
ATOM HG2   HA2     0.09
GROUP
ATOM CD    CT2     0.20
ATOM HD1   HA2     0.09
ATOM HD2   HA2     0.09
ATOM NE    NC2    -0.672
ATOM HE    HC      0.44
ATOM CZ    C       0.617
ATOM NH1   NC2    -0.737
ATOM HH11  HC      0.438
ATOM HH12  HC      0.438
ATOM NH2   NG2P1  -1.3275
ATOM HH21  HC      0.475
ATOM C5    CG2O1   1.2585
ATOM C6    CG2DC1  0.289
ATOM C8    CG331  -0.284
ATOM H10   HGA3    0.090
ATOM H11   HGA3    0.090
ATOM H12   HGA3    0.090
ATOM O3    OG2D1  -0.590
ATOM C7    CG2DC3 -0.415
ATOM H8    HGA5    0.210
ATOM H9    HGA5    0.210
GROUP
ATOM C     C       0.51
```

H. 根據下載的rtf檔案，手動改動top_all36_prot.rtf中的ARG：

2 topology內原子改動：

(1) 補上原子，原子種類要留意需不需要變化

(2) 看一下電荷的差別會不會太大**(本範例並沒有太大的電荷差異)**

(3) 將多的電荷分配給鄰近原子，並確認電荷總和相同

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47
ATOM HN   H       0.31
ATOM CA   CT1     0.07
ATOM HA   HB1     0.09
GROUP
ATOM CB   CT2    -0.18
ATOM HB1  HA2     0.09
ATOM HB2  HA2     0.09
GROUP
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
GROUP
ATOM CD   CT2     0.20
ATOM HD1  HA2     0.09
ATOM HD2  HA2     0.09
ATOM NE   NC2    -0.70
ATOM HE   HC      0.44
ATOM CZ   C       0.64
ATOM NH1  NC2    -0.80
ATOM HH11 HC      0.46
ATOM HH12 HC      0.46
ATOM NH2  NC2    -0.80
ATOM HH21 HC      0.46
ATOM HH22 HC      0.46
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
```

補上多的原子

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47
ATOM HN   H       0.31
ATOM CA   CT1     0.07
ATOM HA   HB1     0.09
GROUP
ATOM CB   CT2    -0.18
ATOM HB1  HA2     0.09
ATOM HB2  HA2     0.09
GROUP
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
GROUP
ATOM CD   CT2     0.20
ATOM HD1  HA2     0.09
ATOM HD2  HA2     0.09
ATOM NE   NC2    -0.672
ATOM HE   HC      0.44
ATOM CZ   C       0.617
ATOM NH1  NC2    -0.737
ATOM HH11 HC      0.438
ATOM HH12 HC      0.438
ATOM NH2  NG2P1  -1.3275
ATOM HH21 HC      0.475
ATOM C5   CG2O1   1.2585
ATOM C6   CG2DC1  0.289
ATOM C8   CG331  -0.284
ATOM H10  HGA3    0.090
ATOM H11  HGA3    0.090
ATOM H12  HGA3    0.090
ATOM O3   OG2D1  -0.590
ATOM C7   CG2DC3 -0.415
ATOM H8   HGA5    0.210
ATOM H9   HGA5    0.210
GROUP
ATOM C    C       0.51
```

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47
ATOM HN   H       0.31
ATOM CA   CT1     0.07
ATOM HA   HB1     0.09
GROUP
ATOM CB   CT2    -0.18
ATOM HB1  HA2     0.09
ATOM HB2  HA2     0.09
GROUP
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
GROUP
ATOM CD   CT2     0.20
ATOM HD1  HA2     0.09
ATOM HD2  HA2     0.09
ATOM NE   NC2    -0.70
ATOM HE   HC      0.44
ATOM CZ   C       0.64
ATOM NH1  NC2    -0.80
ATOM HH11 HC      0.46
ATOM HH12 HC      0.46
ATOM NH2  NC2    -0.80
ATOM HH21 HC      0.46
ATOM HH22 HC      0.46
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
```

原子種類從原本NC2(CHARMM36中NH2結構的N)
更改成NG2P1(Cgenff中的HN-C的N)

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47
ATOM HN   H       0.31
ATOM CA   CT1     0.07
ATOM HA   HB1     0.09
GROUP
ATOM CB   CT2    -0.18
ATOM HB1  HA2     0.09
ATOM HB2  HA2     0.09
GROUP
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
GROUP
ATOM CD   CT2     0.20
ATOM HD1  HA2     0.09
ATOM HD2  HA2     0.09
ATOM NE   NC2    -0.672
ATOM HE   HC      0.44
ATOM CZ   C       0.617
ATOM NH1  NC2    -0.737
ATOM HH11 HC      0.438
ATOM HH12 HC      0.438
ATOM NH2  NG2P1  -1.3275
ATOM HH21 HC      0.475
ATOM C5   CG2O1   1.2585
ATOM C6   CG2DC1  0.289
ATOM C8   CG331  -0.284
ATOM H10  HGA3    0.090
ATOM H11  HGA3    0.090
ATOM H12  HGA3    0.090
ATOM O3   OG2D1  -0.590
ATOM C7   CG2DC3 -0.415
ATOM H8   HGA5    0.210
ATOM H9   HGA5    0.210
GROUP
ATOM C    C       0.51
```

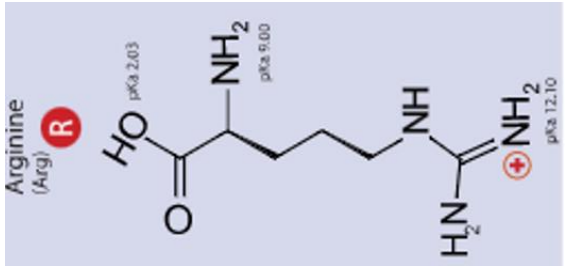
確保電荷總和不便

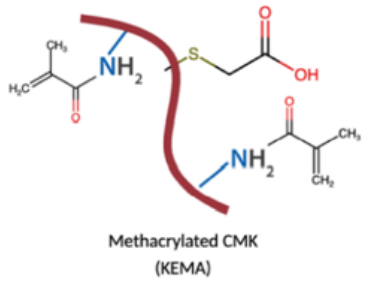
```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47
ATOM HN   H       0.31
ATOM CA   CT1     0.07
ATOM HA   HB1     0.09
GROUP
ATOM CB   CT2    -0.18
ATOM HB1  HA2     0.09
ATOM HB2  HA2     0.09
GROUP
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
GROUP
ATOM CD   CT2     0.20
ATOM HD1  HA2     0.09
ATOM HD2  HA2     0.09
ATOM NE   NC2    -0.70
ATOM HE   HC      0.44
ATOM CZ   C       0.64
ATOM NH1  NC2    -0.80
ATOM HH11 HC      0.46
ATOM HH12 HC      0.46
ATOM NH2  NC2    -0.80
ATOM HH21 HC      0.46
ATOM HH22 HC      0.46
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
```

鄰近原子的電荷分配

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47
ATOM HN   H       0.31
ATOM CA   CT1     0.07
ATOM HA   HB1     0.09
GROUP
ATOM CB   CT2    -0.18
ATOM HB1  HA2     0.09
ATOM HB2  HA2     0.09
GROUP
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
GROUP
ATOM CD   CT2     0.20
ATOM HD1  HA2     0.09
ATOM HD2  HA2     0.09
ATOM NE   NC2    -0.672
ATOM HE   HC      0.44
ATOM CZ   C       0.617
ATOM NH1  NC2    -0.737
ATOM HH11 HC      0.438
ATOM HH12 HC      0.438
ATOM NH2  NG2P1  -1.3275
ATOM HH21 HC      0.475
ATOM C5   CG2O1   1.2585
ATOM C6   CG2DC1  0.289
ATOM C8   CG331  -0.284
ATOM H10  HGA3    0.090
ATOM H11  HGA3    0.090
ATOM H12  HGA3    0.090
ATOM O3   OG2D1  -0.590
ATOM C7   CG2DC3 -0.415
ATOM H8   HGA5    0.210
ATOM H9   HGA5    0.210
GROUP
ATOM C    C       0.51
```

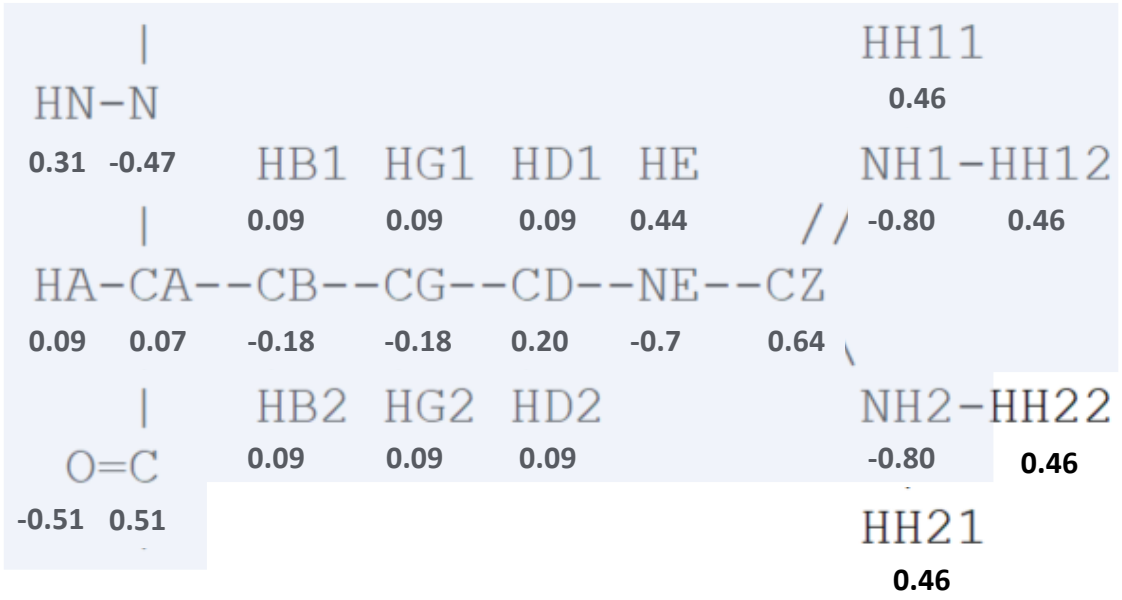
2 topology內原子改動：
補上原子
看一下電荷的差別會不會太大(本範例並沒有太大的電荷差異)
將多的電荷分配給鄰近原子，並確認電荷總和相同



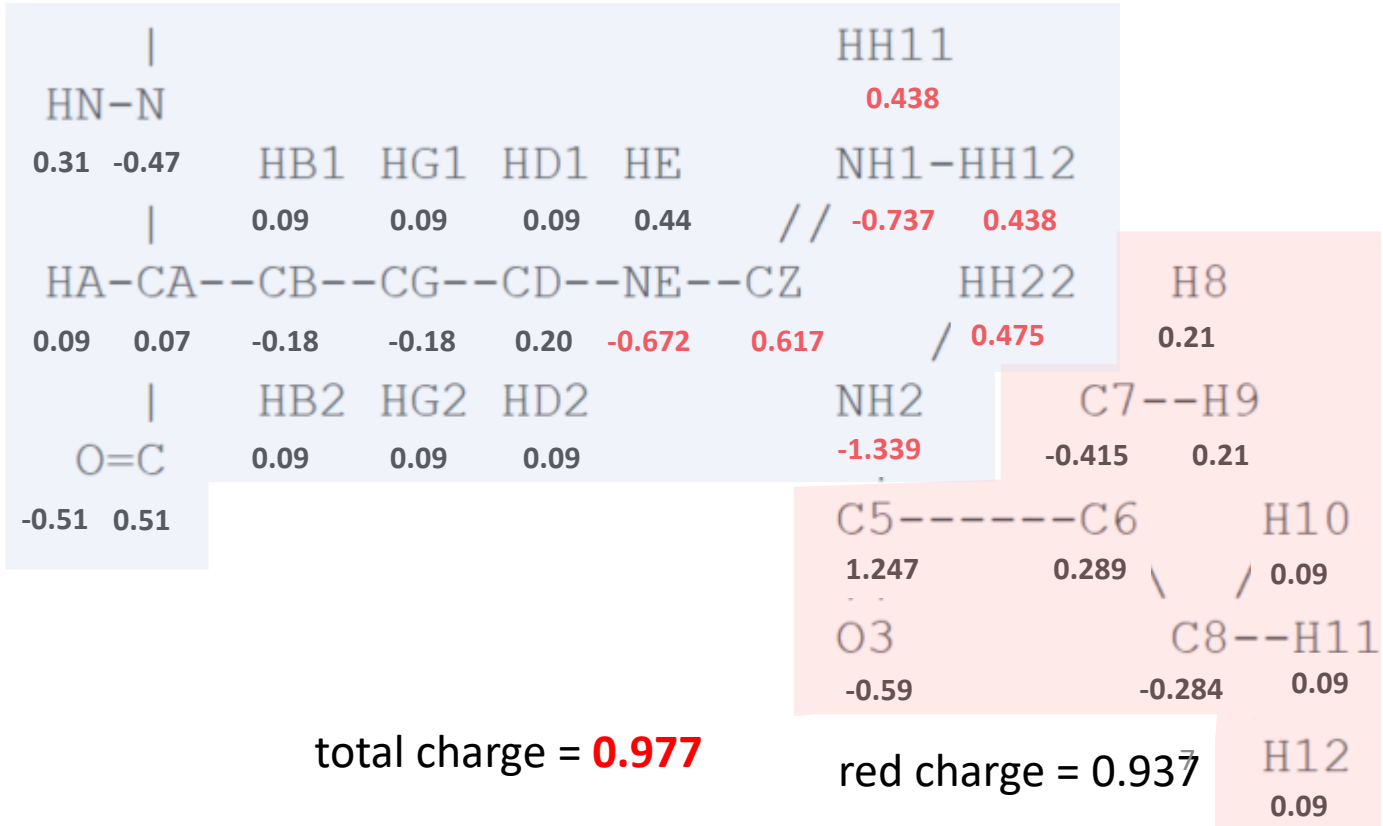


ARG and ARGMA

把多的電荷均分給NH2和C5
NH2電荷：**-1.339 + (1-0.977)/2 = -1.3275**
C5電荷：1.247+ **(1-0.977)/2 = 1.2585**



total charge = 1.00

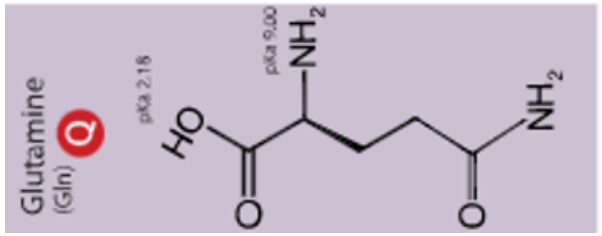


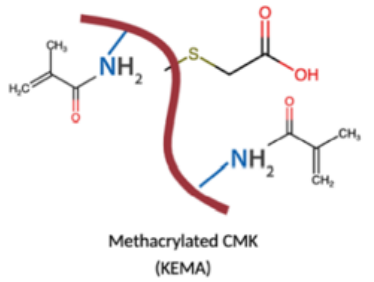
total charge = **0.977**

red charge = 0.937

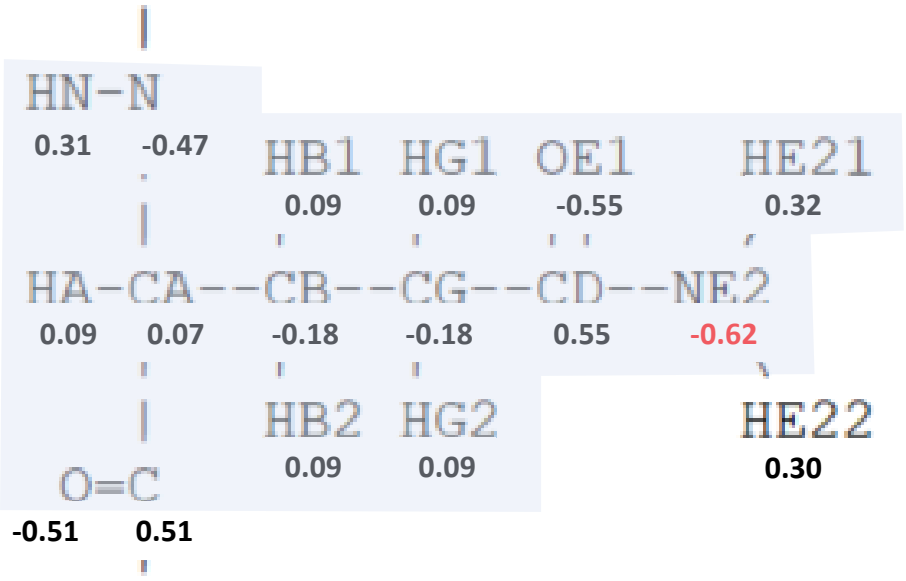
2 topology內原子改動：
補上原子
看一下電荷的差別會不會太大**(本範例並沒有太大的電荷差異)**
將多的電荷分配給鄰近原子，並確認電荷總和相同

GLN and GLNMA

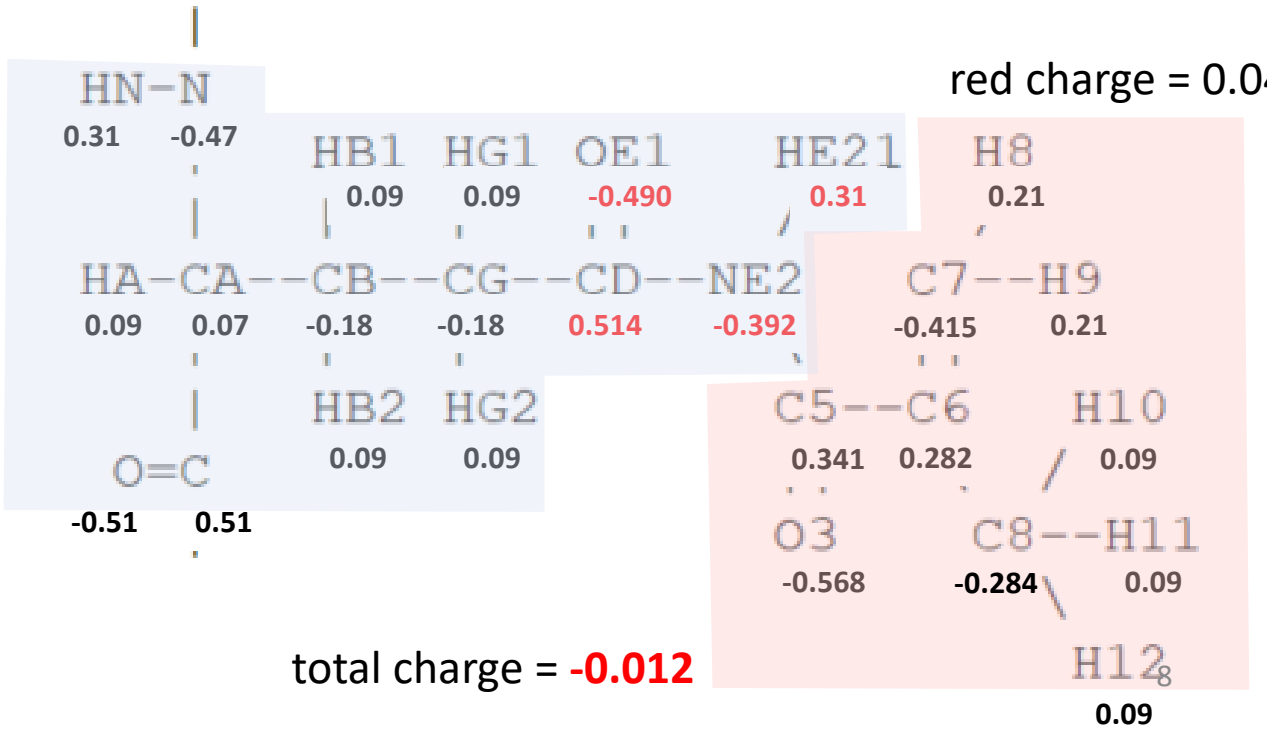




把多的電荷均分給NE2和C5
NE2電荷：**-0.392 + 0.012/2 = -0.386**
C5電荷：0.341 + **0.012/2 = 0.347**



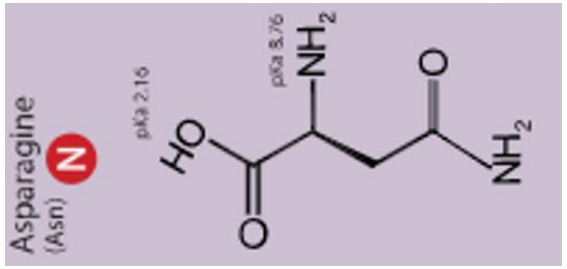
total charge = 0.00

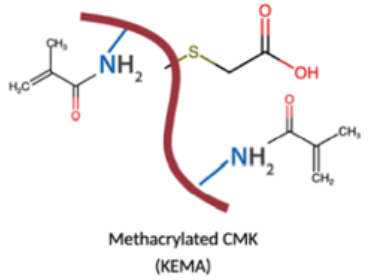


red charge = 0.046

total charge = **-0.012**

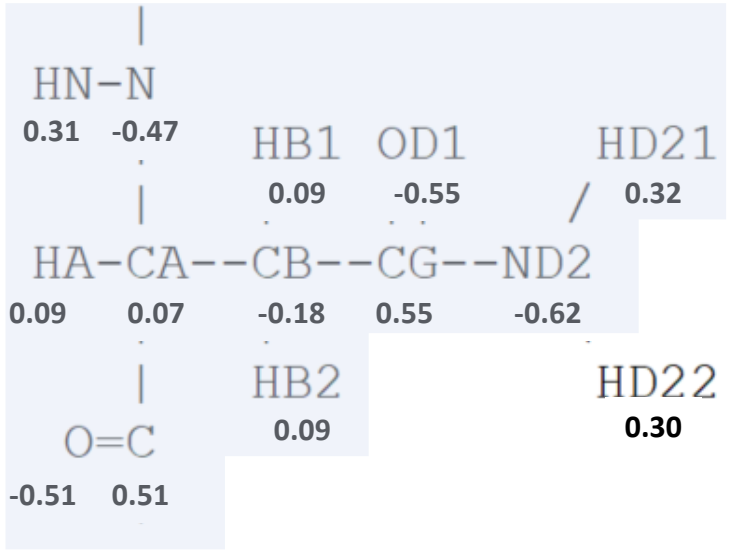
2 topology內原子改動：
補上原子
看一下電荷的差別會不會太大**(本範例並沒有太大的電荷差異)**
將多的電荷分配給鄰近原子，並確認電荷總和相同



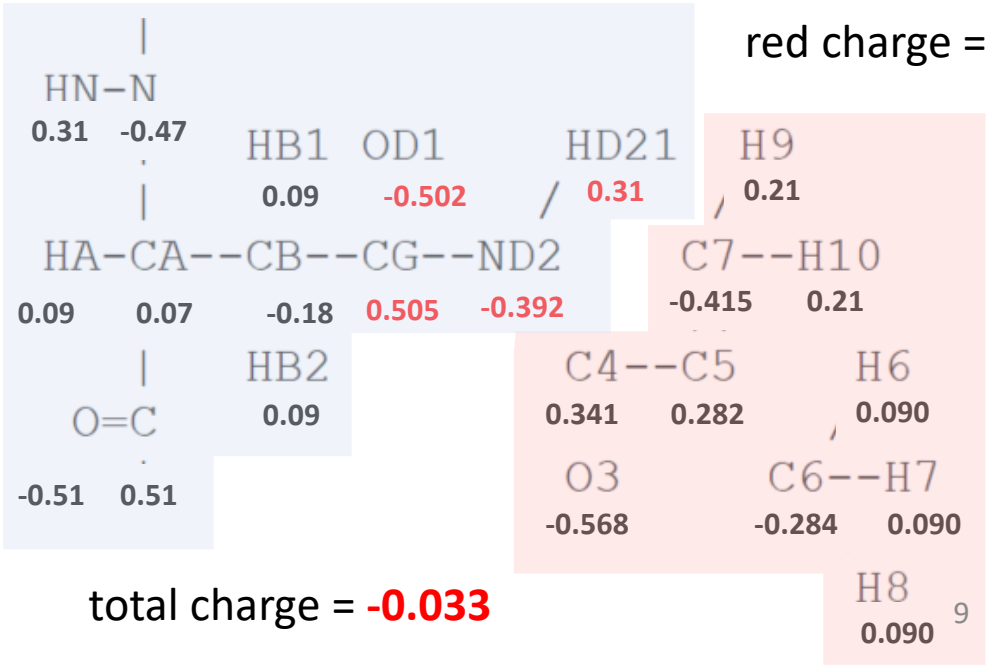


ASN and ASNMA

把多的電荷均分給ND2和C4
ND2電荷：**-0.392 + 0.033/2 = -0.3755**
C4電荷：0.341 + **0.033/2 = 0.3575**



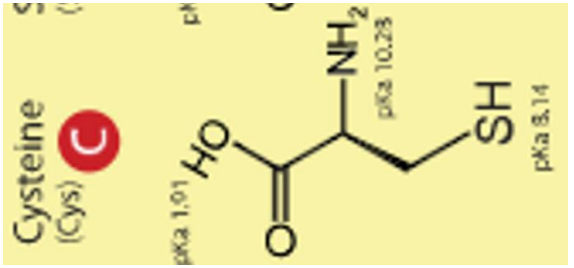
total charge = 0.00

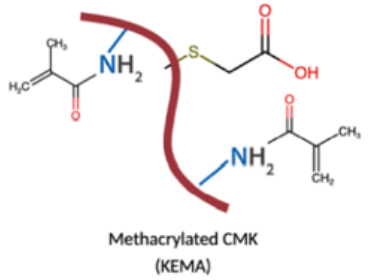


red charge = 0.046

total charge = **-0.033**

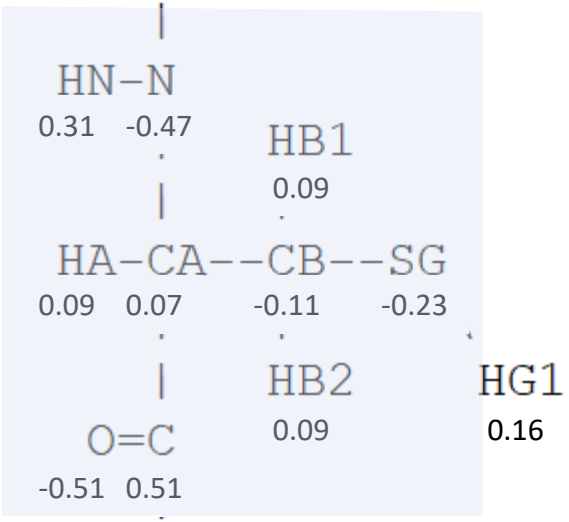
2 topology內原子改動：
補上原子
看一下電荷的差別會不會太大**(**本範例並沒有太大的電荷差異**)**
將多的電荷分配給鄰近原子，並確認電荷總和相同

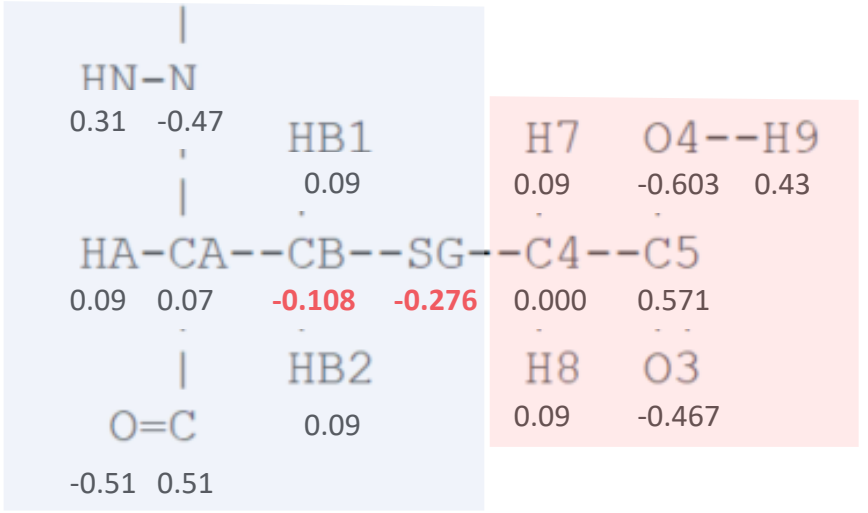




CYS and Acid-CYS

把多的電荷均分給SG和C4
SG電荷：**-0.276+ 0.093/2 = -0.2295**
C4電荷：0.000+ **0.093/2 = 0.0465**





total charge = 0.00

total charge = **-0.093**

H. 根據下載的rtf檔案，手動改動top_all36_prot.rtf中的ARG：

4. top_all36_prot.rtf補上新增原子種類：

註 原子的編號(如原始ARG中的-1)是CHARMM2LAMMPS讀取rtf檔時需要改動的，如果僅用VMD autopsf生成結構，就不需要管他

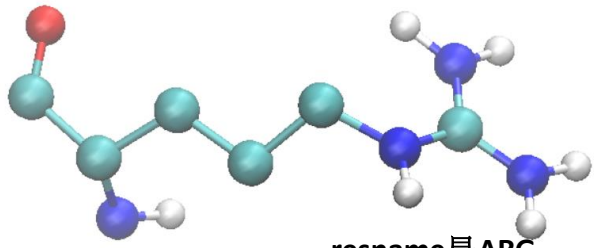
原始ARG

```
MASS  -1  NH1       14.00700 ! peptide nitrogen
MASS  -1  NH2       14.00700 ! amide nitrogen
MASS  -1  NH3       14.00700 ! ammonium nitrogen
MASS  -1  NC2       14.00700 ! guanidinium nitrogen
MASS  -1  NY        14.00700 ! TRP N in pyrrole ring
MASS  -1  NP        14.00700 ! Proline ring NH2+ (N-terminal)
MASS  -1  O         15.99940 ! carbonyl oxygen
MASS  -1  OB        15.99940 ! carbonyl oxygen in acetic acid
MASS  -1  OC        15.99940 ! carboxylate oxygen
MASS  -1  OH1       15.99940 ! hydroxyl oxygen
MASS  -1  OS        15.99940 ! ester oxygen
MASS  -1  S         32.06000 ! sulphur
MASS  -1  SM        32.06000 ! sulfur C-S-S-C type
MASS  -1  SS        32.06000 ! thiolate sulfur

DECL -CA
DECL -C
DECL -O
DECL +N
DECL +HN
DECL +CA
DEFA FIRS NTER LAST CTER
AUTO ANGLES DIHE PATCH

RESI ALA          0.00
GROUP
ATOM N    NH1    -0.47  !      |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !      |      HB1
ATOM HA   HB1     0.09  !      |    /
GROUP                   !  HA-CA--CB-HB2
ATOM CB   CT3    -0.27  !      |    \
ATOM HB1  HA3     0.09  !      |      HB3
ATOM HB2  HA3     0.09  !    O=C
ATOM HB3  HA3     0.09  !      |
```

ARG_MA

```
MASS  67  N         14.00700 ! proline N
MASS  68  NR1       14.00700 ! neutral his protonated ring nitrogen
MASS  69  NR2       14.00700 ! neutral his unprotonated ring nitrogen
MASS  70  NR3       14.00700 ! charged his ring nitrogen
MASS  71  NH1       14.00700 ! peptide nitrogen
MASS  72  NH2       14.00700 ! amide nitrogen
MASS  73  NH3       14.00700 ! ammonium nitrogen
MASS  74  NC2       14.00700 ! guanidinium nitrogen
MASS  75  NY        14.00700 ! TRP N in pyrrole ring
MASS  76  NP        14.00700 ! Proline ring NH2+ (N-terminal)
MASS  77  O         15.99940 ! carbonyl oxygen
MASS  78  OB        15.99940 ! carbonyl oxygen in acetic acid
MASS  79  OC        15.99940 ! carboxylate oxygen
MASS  80  OH1       15.99940 ! hydroxyl oxygen
MASS  81  OS        15.99940 ! ester oxygen
MASS  82  S         32.06000 ! sulphur
MASS  83  SM        32.06000 ! sulfur C-S-S-C type
MASS  84  SS        32.06000 ! thiolate sulfur
MASS  85  CG2O1     12.01100 !
MASS  86  CG2DC1    12.01100 !
MASS  87  CG2DC3    12.01100 !
MASS  88  CG331     12.01100 !
MASS  89  OG2D1     15.99940 !
MASS  90  HGA5       1.00800 !
MASS  91  HGA3       1.00800 !
MASS  92  CG2O2     12.01100 !
MASS  93  CG321     12.01100 !
MASS  94  HGP1       1.00800 !
MASS  95  HGA1       1.00800 !
MASS  96  HGA2       1.00800 !
MASS  97  HGPAM      1.00800 !
MASS  98  OG311     15.99940 !
MASS  99  NG2S1     14.00700 !
MASS  100 NG321     14.00700 !
MASS  101 NG2P1     14.00700 !
MASS  102 CG2DC3    12.01100 !
MASS  103 CG2O1     12.01100 !

DECL -CA
DECL -C
DECL -O
DECL +N
```

骨幹結構(不包含所有的H)



resname是ARG

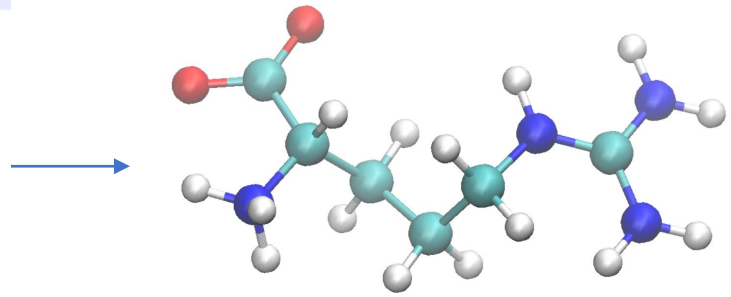
骨幹結構的pdb(不包含所有的H)

```
ATOM    4360   N    ARG
ATOM    4361   H    ARG
ATOM    4362   CA   ARG
ATOM    4363   CB   ARG
ATOM    4364   CG   ARG
ATOM    4365   CD   ARG
ATOM    4366   NE   ARG
ATOM    4367   HE   ARG
ATOM    4368   CZ   ARG
ATOM    4369   NH1  ARG
ATOM    4370  HH11  ARG
ATOM    4371  HH12  ARG
ATOM    4372   NH2  ARG
ATOM    4373  HH21  ARG
ATOM    4374  HH22  ARG
ATOM    4375   C    ARG
ATOM    4376   O    ARG
END
```

調整前

原始ARG

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47  !      |                      HH11
ATOM HN   H       0.31  !  HN-N                       |
ATOM CA   CT1     0.07  !      |   HB1 HG1 HD1 HE     NH1-HH12
ATOM HA   HB1     0.09  !      |   |   |   |   |    //(+)
GROUP                   !  HA-CA--CB--CG--CD--NE--CZ
ATOM CB   CT2    -0.18  !      |   |   |   |         \
ATOM HB1  HA2     0.09  !      |   HB2 HG2 HD2        NH2-HH22
ATOM HB2  HA2     0.09  !   O=C                       |
GROUP                   !      |                     HH21
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
```



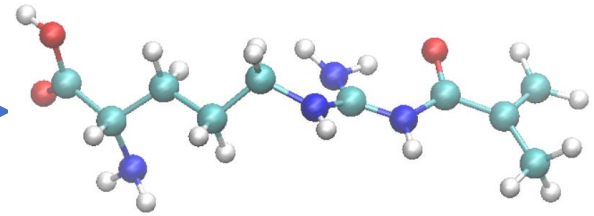
原始ARG

調整後

ARG_MA

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47  !      |                      HH11
ATOM HN   H       0.31  !  HN-N                       |
ATOM CA   CT1     0.07  !      |   HB1 HG1 HD1 HE     NH1-HH12
ATOM HA   HB1     0.09  !      |   |   |   |   |    //(+)
GROUP                   !  HA-CA--CB--CG--CD--NE--CZ     HH21   H8
ATOM CB   CT2    -0.18  !      |   |   |   |         \   /      /
ATOM HB1  HA2     0.09  !      |   HB2 HG2 HD2        NH2     C7--H9
ATOM HB2  HA2     0.09  !   O=C                        |      ||
GROUP                   !      |                     C5------C6    H10
ATOM CG   CT2    -0.18  !                            ||        \  /
ATOM HG1  HA2     0.09  !                            O3         C8--H11
ATOM HG2  HA2     0.09  !                                        \
GROUP                   !                                       H12
ATOM CD   CT2     0.20
```

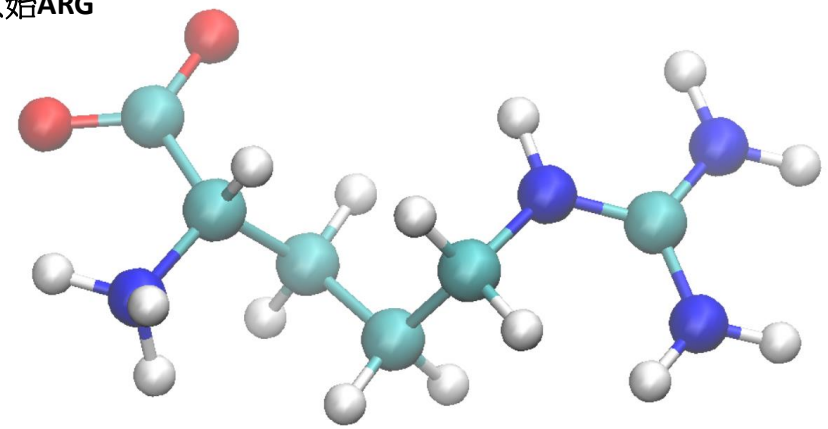
ARG_MA(有一顆H是多顯示的不用管他)



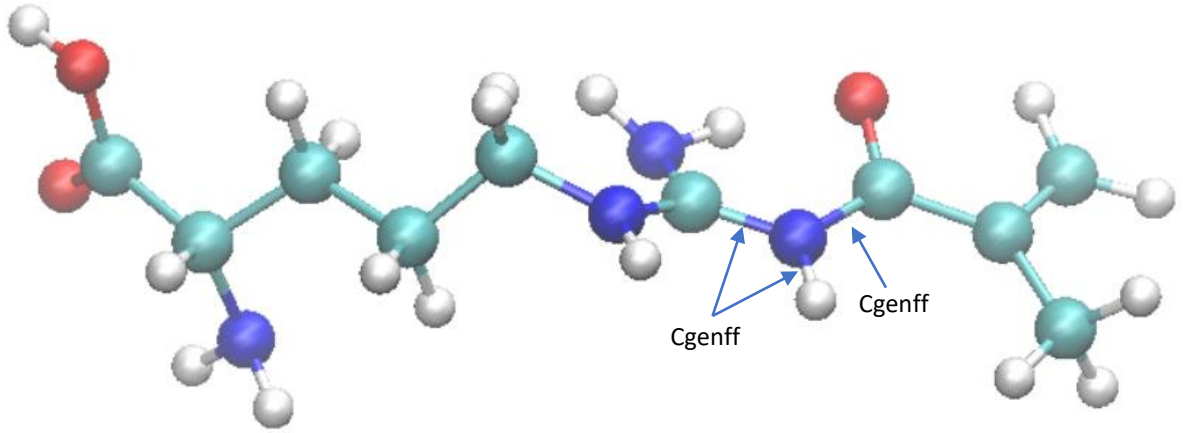
Comment

1. 把Cgenff得到的rtf檔(**lig.rtf**)與Charmm36(**top_all36_prot.rtf)**合併時，原子種類上會**優先尊重Cgenff**，因為Cgenff得到的參數才是改動後的原子種類的力場參數

原始ARG



ARG_MA(有一顆H是多顯示的不用管他)



Comment

2.因此合併**rtf後生成的結構**，和**Cgenff 得到的結構**相比：

- **必有相同的atom、bond與angle數量**
- **dihedral與improper數量可能會比較多(CHARMM36和Cgenff考慮到的構型數量會不一樣)**

這是因為我們保留Charmm36的結果，並補上Cgenff多生出來的結構

改質名稱	ARGMA		ASNMA		GLNMA		CYS_COOH	
比較項目	Cgenff*	Self Topo*	Cgenff	Self Topo	Cgenff	Self Topo	Cgenff	Self Topo
Atom	36	36	26	26	29	29	20	20
Bond	35	35	25	25	28	28	19	19
Angle	60	60	42	42	48	48	32	32
Dihedral	78	78	52	52	61	61	38	38
Improper	**3**	**5**	**3**	**4**	**3**	**4**	2	2
差異原因	**Cgenff未考慮以N為中心的NH2 improper(共2個)**		**Cgenff未考慮以N為中心的NH2 improper(共1個)**		**Cgenff未考慮以N為中心的NH2 improper(共1個)**		~	
備註	**parameter penalty = 74 charge penalty = 93 改質處 N-C 電荷、bond不穩定**		**parameter penalty =25.7 Charge penalty = 18.328 Structure accepted**		**parameter penalty =24.5 Charge penalty = 14.118 Structure accepted**		**parameter penalty =55 Charge penalty = 14.053 改質O-C-C-S dihedral不穩定**	

Cgenff = ARGMA -> Ligand Reader -> pdb, psf
Self Topo = ARG pdb -> VMD autopsf + revise topology -> pdb, psf

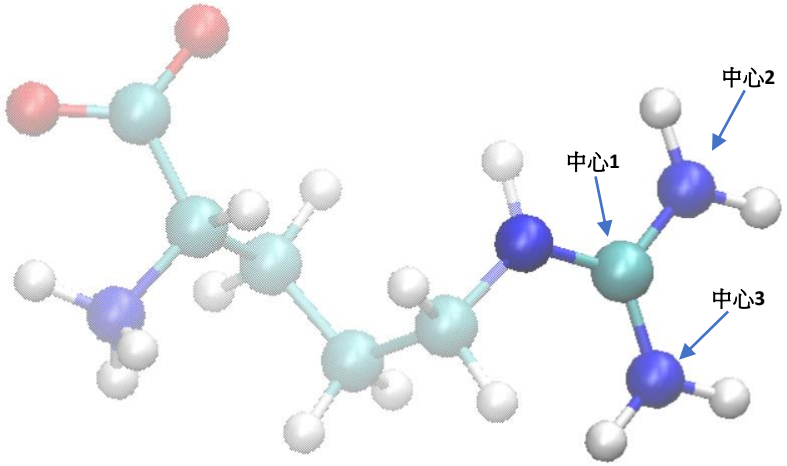
Comment

2.因此合併**rtf後生成的結構**，和**Cgenff 得到的結構**相比：

- **必有相同的atom、bond與angle數量**
- **dihedral與improper數量可能會比較多(CHARMM36和Cgenff考慮到的構型數量會不一樣)**

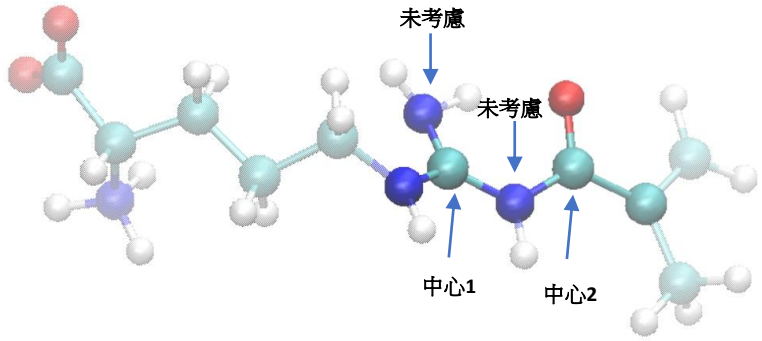
這是因為我們保留會Charmm36的結果，並補上Cgenff多生出來的結構

原始ARG有考慮的improper



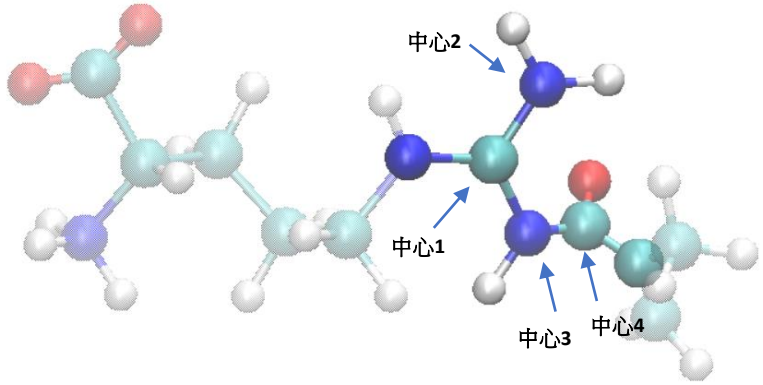
Charmm36中的ARG末端考慮了**3個**improper

Lig.rtf有考慮的improper



針對改質的ARG_MA結構，Cgenff只在末端抓到**2個**improper
而且相比Charmm36，還**漏考慮了2個**improper

合併ARG_MA有考慮的improper(有一顆H是多顯示的不用管他)



保留Charmm36的參數，並補上Cgenff新定義的improper，末端總共得到**4個**improper

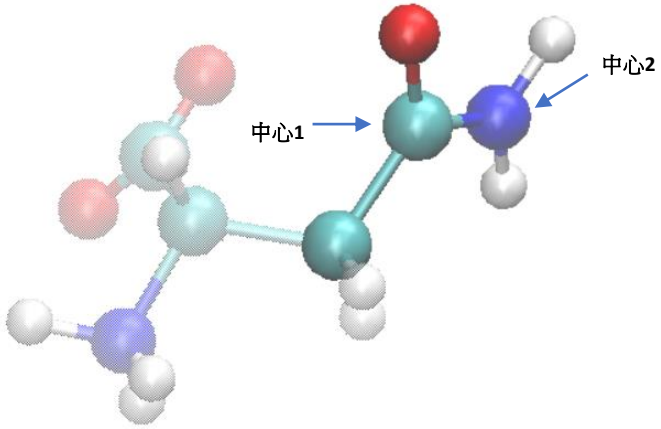
Comment

2.因此**合併rtf後生成的結構**，和**Cgenff 得到的結構**相比：

- **必有相同的atom、bond與angle數量**
- **dihedral與improper數量可能會比較多(CHARMM36和Cgenff考慮到的構型數量會不一樣)**

這是因為我們保留會Charmm36的結果，並補上Cgenff多生出來的結構

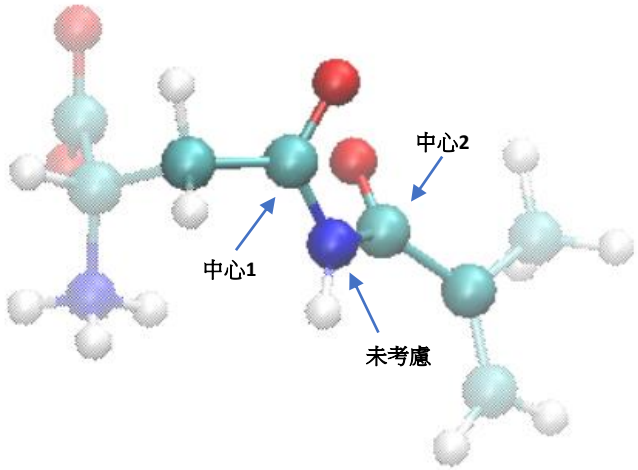
原始ASN有考慮的improper



Charmm36中的ASN末端考慮了**2個**improper

+

Lig.rtf有考慮的improper



針對改質的ASN_MA結構，Cgenff只在抓到**2個**improper
而且相比Charmm36，還**漏考慮了1個**improper

=

合併ASN_MA有考慮的improper

保留Charmm36的參數，並補上Cgenff新定義的improper，末端總共得到**3個**improper

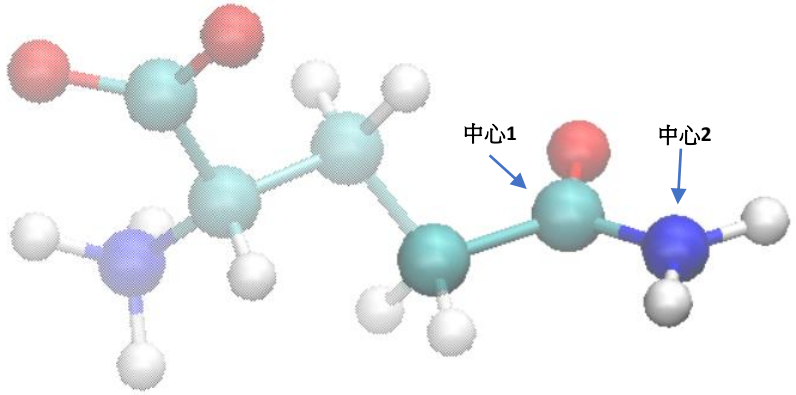
Comment

2.因此合併**rtf後生成的結構**，和**Cgenff 得到的結構**相比：

- **必有相同的atom、bond與angle數量**
- **dihedral與improper數量可能會比較多(CHARMM36和Cgenff考慮到的構型數量會不一樣)**

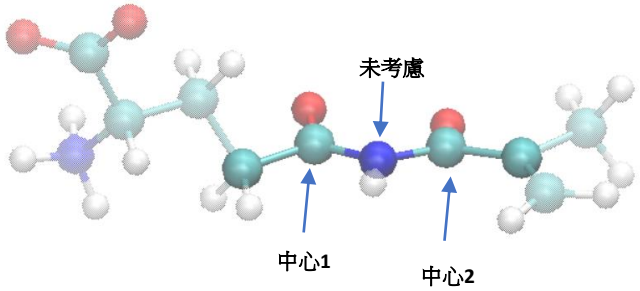
這是因為我們保留會Charmm36的結果，並補上Cgenff多生出來的結構

原始GLN有考慮的improper



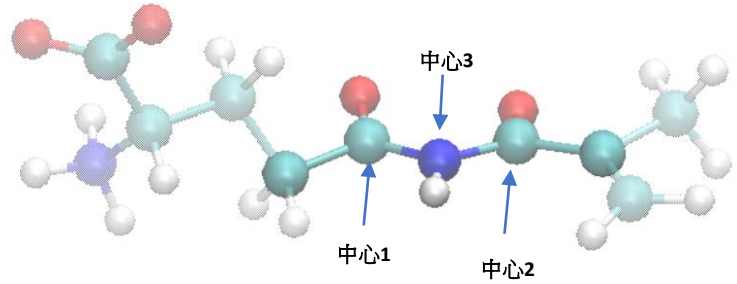
Charmm36中的GLN末端考慮了**2個**improper

Lig.rtf有考慮的improper



針對改質的GLN_MA結構，Cgenff只在末端抓到**2個**improper
而且相比Charmm36，還**漏考慮了1個**improper

合併GLN_MA有考慮的improper



保留Charmm36的參數，並補上Cgenff新定義的improper，末端總共得到**3個**improper

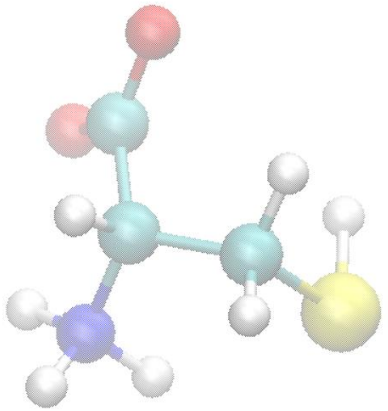
Comment

2.因此**合併rtf後生成的結構**，和**Cgenff 得到的結構**相比：

- **必有相同的atom、bond與angle數量**
- **dihedral與improper數量可能會比較多(CHARMM36和Cgenff考慮到的構型數量會不一樣)**

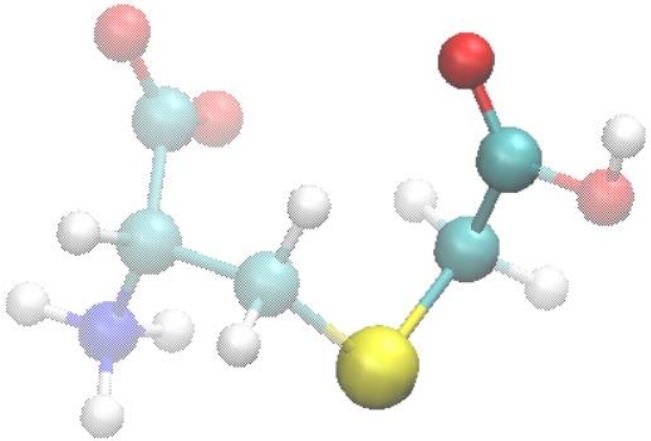
這是因為我們保留會Charmm36的結果，並補上Cgenff多生出來的結構

原始CYS有考慮的improper



Charmm36中的CYS<u>沒有</u>improper

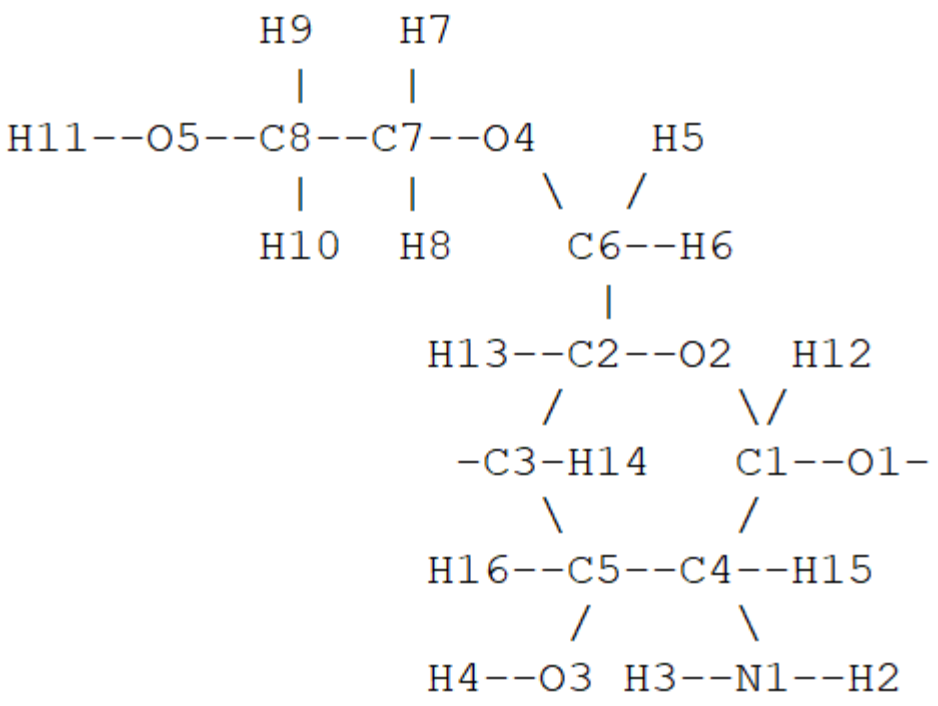
CYS_COOH



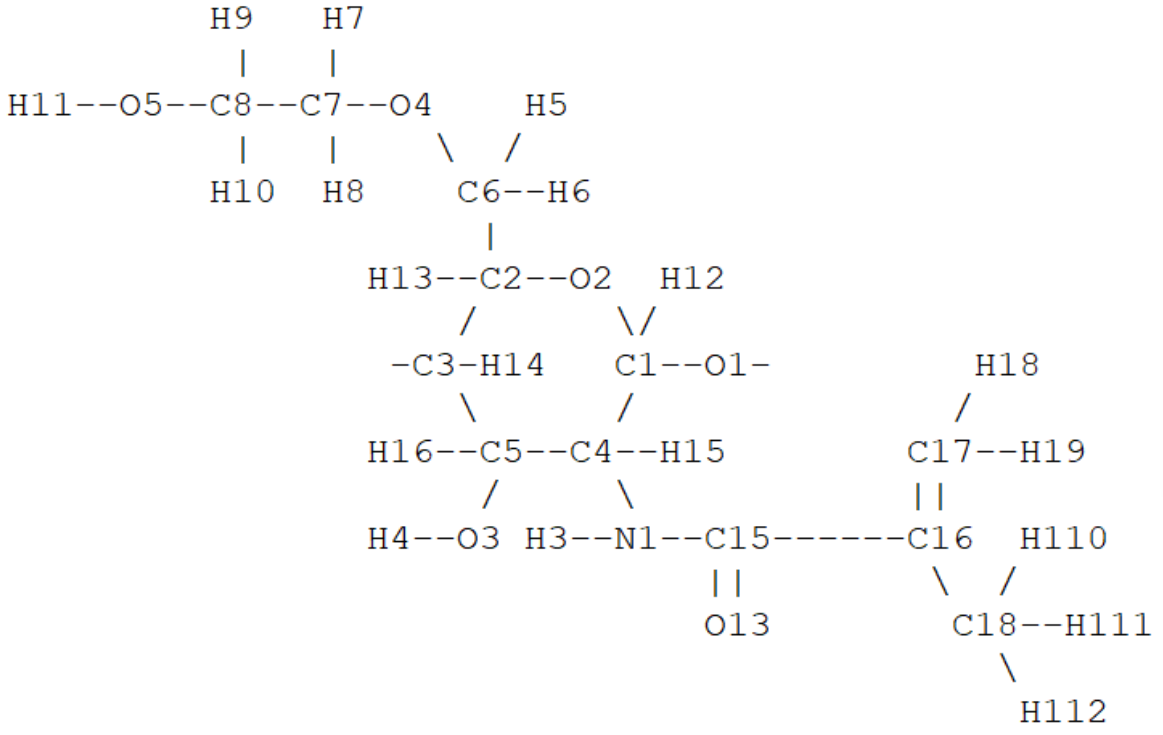
O-C-C-S dihedral有高penalty(55)

課題二：如何生成GC和改質GCMA的topo

Glycol Chitosan (GC)

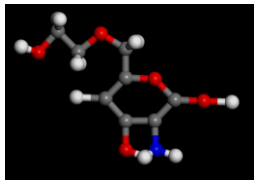


GCMA

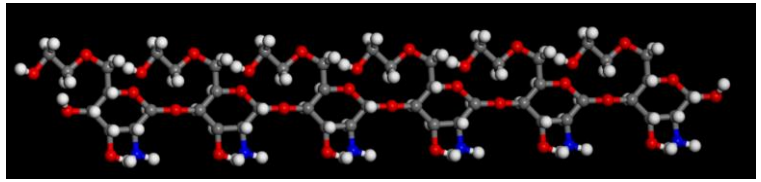


A. 在material studio繪製GC和GCMA結構(繪製6個聚合度，之後看電荷等資訊取中間段當標準)
完成後將6mer聚合物export成GC.mol2和GCMA.mol2

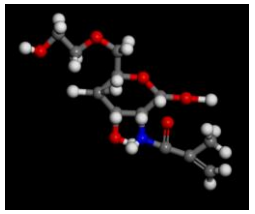
GC monomer



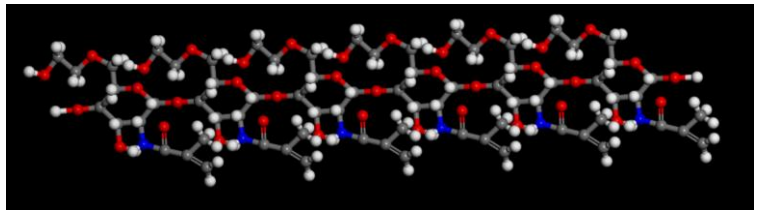
6-mer GC



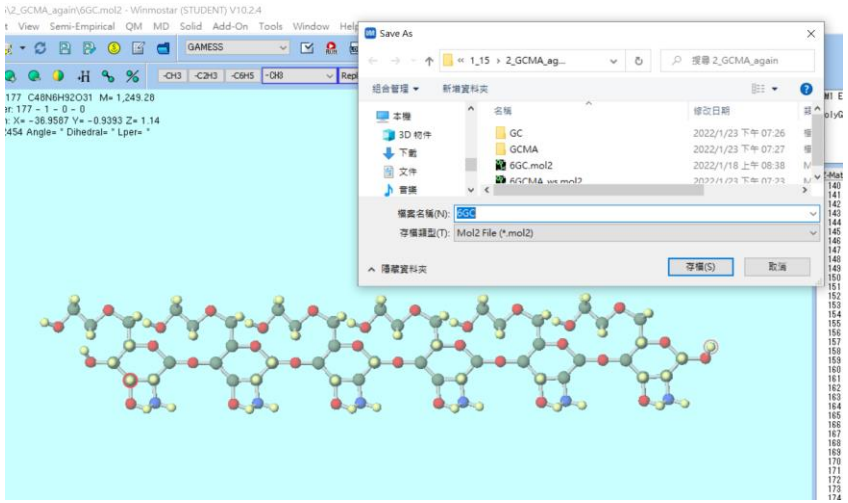
GCMA monomer



6-mer GCMA



B. 把GC.mol2和GCMA.mol2用winmostar打開，重新存成mol2檔



C. 把GC.mol2和GCMA.mol2上傳到Charmm GUI: Ligand Reader
下載Cgenff下的：.pdb .psf
下載補充topology檔：lig.rtf
下載補充參數檔：lig.prm

PDB Info

CHARMM Input: ligandrm.inp
CHARMM Output: ligandrm.out
CHARMM PDB: ligandrm.pdb (view structure) ← pdb
CHARMM CRD: ligandrm.crd
CHARMM PSF: ligandrm.psf ← psf

Computed Energy:

Please beware of that the computed energy is CHARMM single-point energy and is displayed to make sure all the coordinates are defined.

ENER ENR:	Eval#	ENERgy	Delta-E	GRMS		
ENER INTERN:		BONDs	ANGLes	UREY-b	DIHEdrals	IMPRopers
ENER EXTERN:		VDWaals	ELEC	HBONds	ASP	USER
ENER>	0	-119.44416	3.93222	1.79693		
ENER INTERN>		4.51106	15.34930	1.23020	12.78290	0.07422
ENER EXTERN>		18.00764	-171.39949	0.00000	0.00000	0.00000

Topology and Parameter Files:

Below is the topology and parameter files that are generated by automatic method.

LIG
Topology: lig.rtf ← **rtf**
Topology: lig_g.rtf
Parameter: lig.prm ← **prm**

D. 確認新結構rtf檔中的penalty落在可以接受的範圍內

6-mer GC

```
RESI lig          0.000 ! param penalty=  12.000 ; charge penalty=   9.166
```

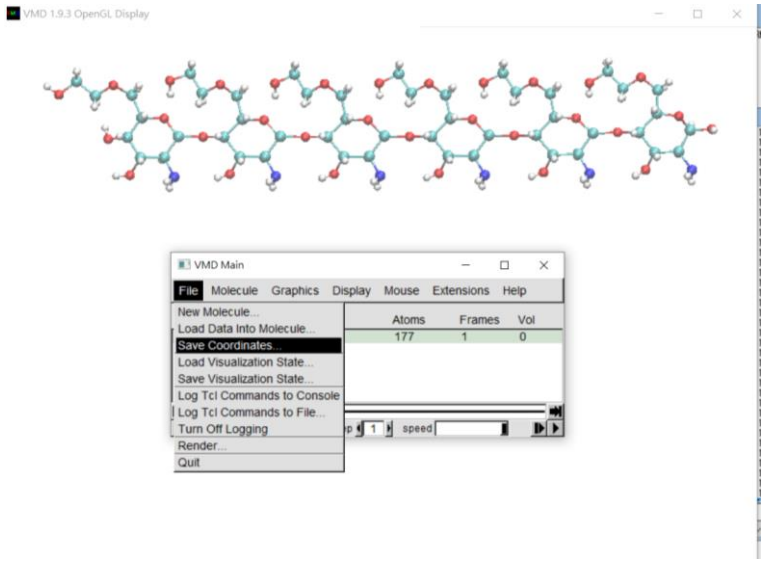
Penalty可以接受 (<50)

6-mer GCMA

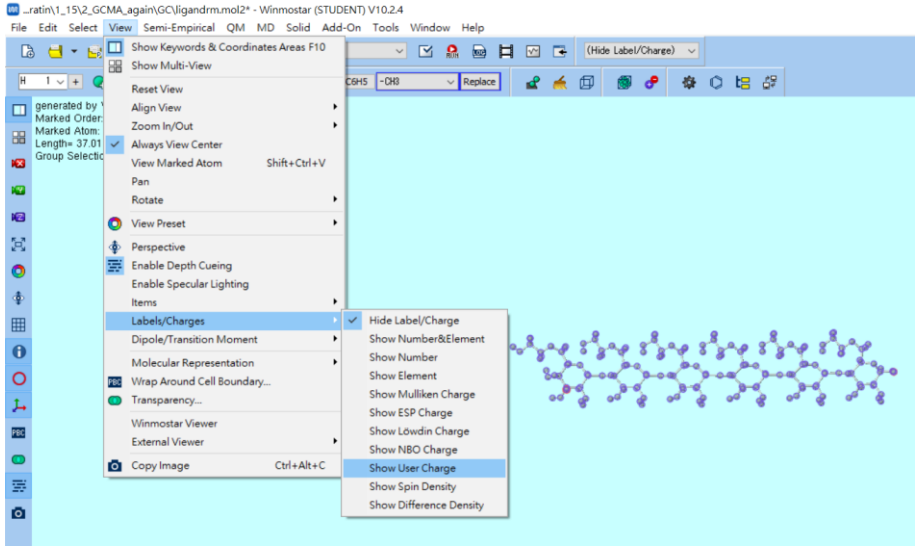
```
RESI lig          0.000 ! param penalty=  15.000 ; charge penalty=   9.499
```

Penalty可以接受 (<50)

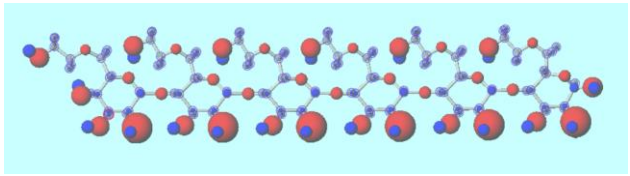
E. 將下載的**pdb, psf**讀入**VMD**，確認結構無誤後存出**mol2**檔



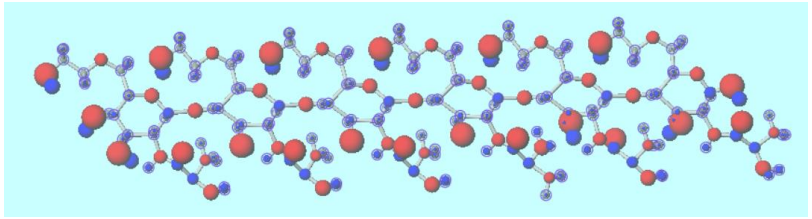
F. 新存出來的**mol2**用**winmostar**打開，從**View>Labels/Charges>Show User Charges**將電荷視覺化，取分布均勻段當作單體(本案例看起來都很均勻)



6-mer GC



6-mer GCMA



2 topology內原子改動：

補上原子

看一下電荷的差別會不會太大**(本範例並沒有太大的電荷差異)**

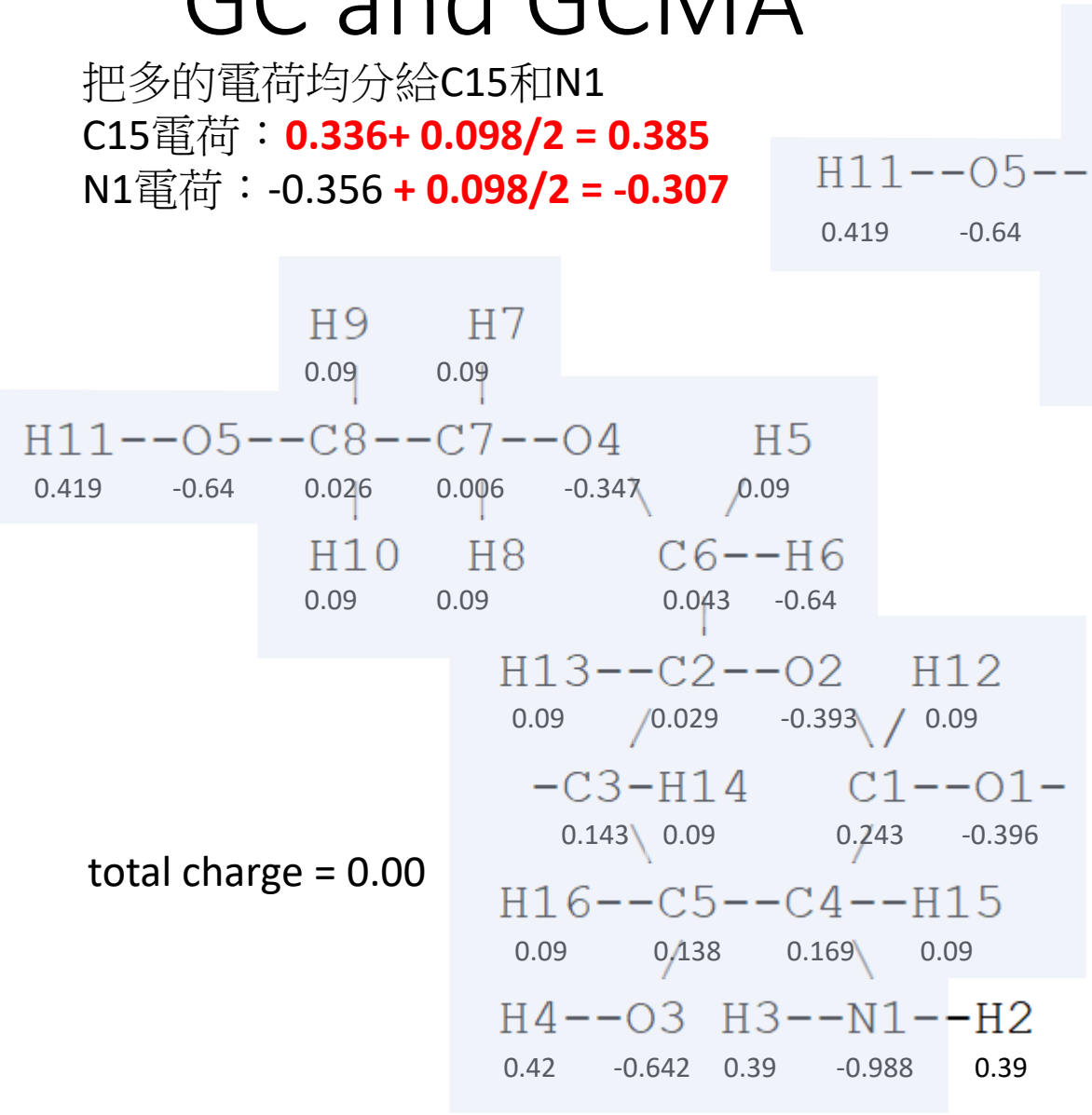
將多的電荷分配給鄰近原子，並確認電荷總和相同

GC and GCMA

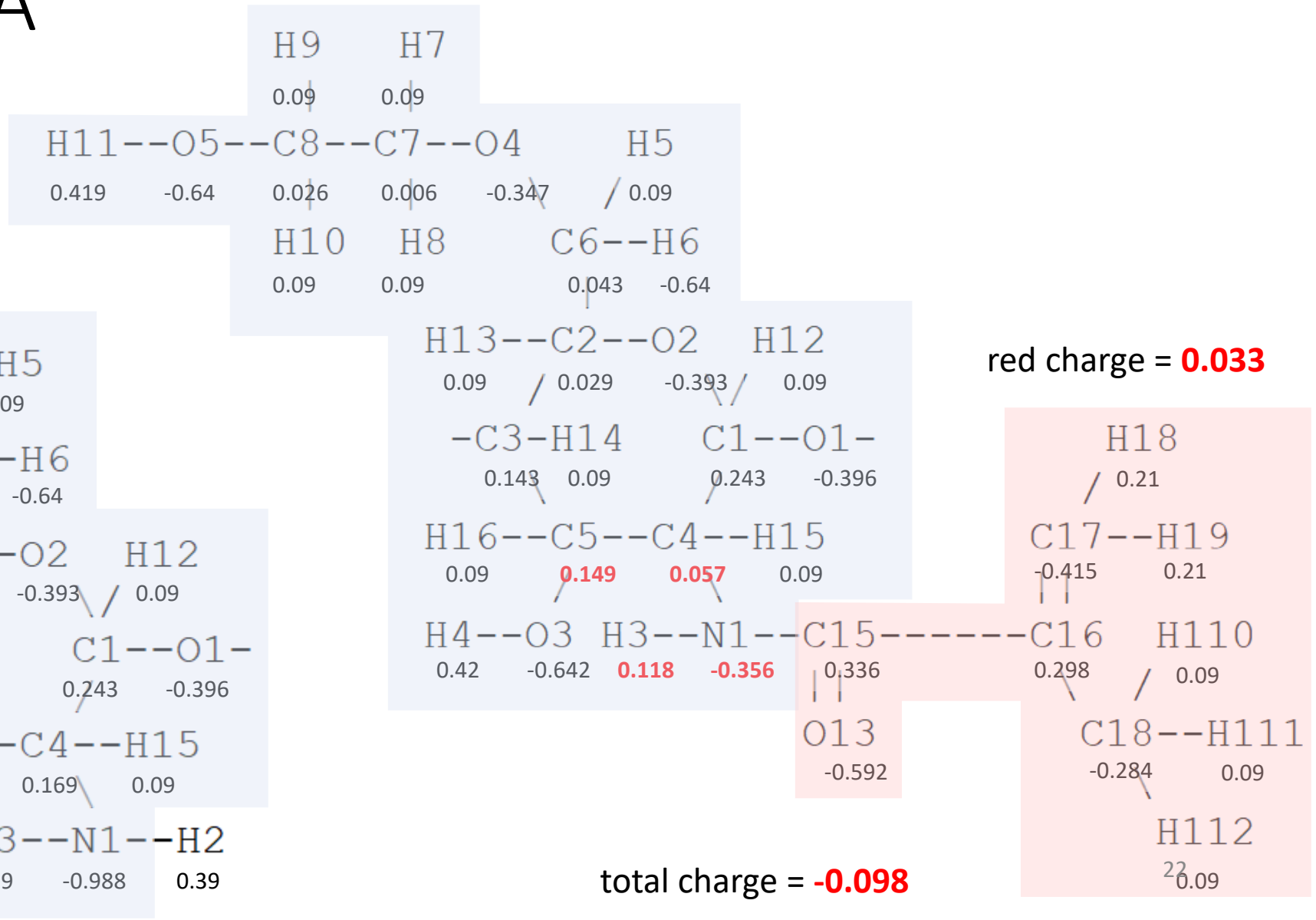
把多的電荷均分給C15和N1

C15電荷：**0.336+ 0.098/2 = 0.385**

N1電荷：-0.356 **+ 0.098/2 = -0.307**



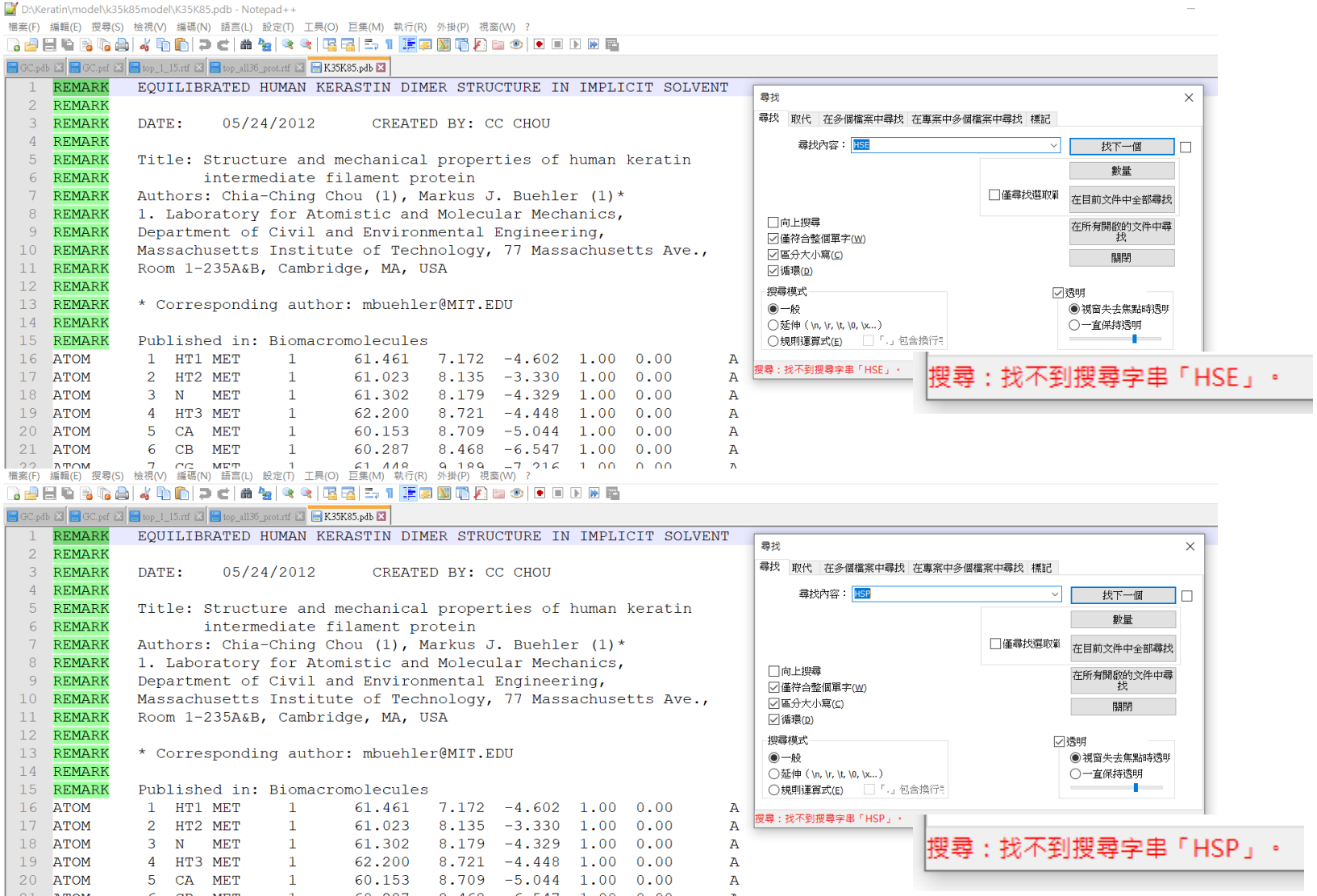
total charge = 0.00



red charge = **0.033**

total charge = **-0.098**

G. 找兩個原始PDB檔中用不到的胺基酸：這邊找到的是HSE和HSP(不同質子化狀態的HIS)



H. 將top_all36_prot.rtf中的HSE和HSP(不同質子化狀態的HIS)分別取代成GC和GCMA

HSE

```
RESI HSE          0.00  ! neutral His, proton on NE2
GROUP
ATOM N    NH1    -0.47  !     |                HE1
ATOM HN   H       0.31  !  HN-N                __ /
ATOM CA   CT1     0.07  !     |    HB1     ND1--CE1
ATOM HA   HB1     0.09  !     |    |     /       |
GROUP                   !  HA-CA--CB--CG        |
ATOM CB   CT2    -0.08  !     |    |     \\      |
ATOM HB1  HA2     0.09  !     |    HB2    CD2--NE2
ATOM HB2  HA2     0.09  !   O=C              |     \
ATOM ND1  NR2    -0.70  !     |              HD2    HE2
ATOM CG   CPH1    0.22
ATOM CE1  CPH2    0.25
ATOM HE1  HR1     0.13
GROUP
ATOM NE2  NR1    -0.36
ATOM HE2  H       0.32
ATOM CD2  CPH1   -0.05
ATOM HD2  HR3     0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB   CA    CG   CB    ND1 CG
BOND NE2 CD2    N    HN    N   CA
BOND C    CA    C    +N    NE2 CE1   CA  HA    CB HB1
BOND CB   HB2   NE2  HE2   CD2 HD2   CE1 HE1
```

變成GC的HSE(GC的rtf中沒有improper)

```
RESI HSE
GROUP             ! CHARGE  0
ATOM O1     OG301  -0.396 !
ATOM C1     CG311   0.243 !
ATOM O2     OG3C61 -0.393 !           H9   H7
ATOM C2     CG311   0.029 !           |    |
ATOM H16    HGA1    0.09  ! H11--O5--C8--C7--O4    H5
ATOM C4     CG311   0.169 !           |    |    \   /
ATOM C5     CG311   0.138 !          H10   H8    C6--H6
ATOM N1     NG321  -0.988 !                      |
ATOM H2     HGPAM2  0.39  !                 H13--C2--O2  H12
ATOM O3     OG311  -0.642 !                     /      \/
ATOM C6     CG321   0.043 !                  -C3-H14   C1--O1-
ATOM O4     OG301  -0.347 !                     \      /
ATOM C7     CG321   0.006 !                 H16--C5--C4--H15
ATOM C8     CG321   0.026 !                     /      \
ATOM O5     OG311  -0.64  !                 H4--O3 H3--N1--H2
ATOM H3     HGPAM2  0.39  !
ATOM H4     HGP1    0.42  !
ATOM H5     HGA2    0.09  !
ATOM H6     HGA2    0.09  !
ATOM H7     HGA2    0.09  !
ATOM H8     HGA2    0.09  !
ATOM H9     HGA2    0.09  !
```

HSP

```
RESI HSP          1.00  ! Protonated His
GROUP
ATOM N    NH1    -0.47  !     |          HD1    HE1
ATOM HN   H       0.31  !  HN-N           |     /
ATOM CA   CT1     0.07  !     |    HB1    ND1--CE1
ATOM HA   HB1     0.09  !     |    |     /      ||
GROUP                   !  HA-CA--CB--CG       ||
ATOM CB   CT2A   -0.05  !     |    |     \\     ||
ATOM HB1  HA2     0.09  !     |    HB2    CD2--NE2(+)
ATOM HB2  HA2     0.09  !   O=C            |     \
ATOM CD2  CPH1    0.19  !     |          HD2    HE2
ATOM HD2  HR1     0.13
ATOM CG   CPH1    0.19
GROUP
ATOM NE2  NR3    -0.51
ATOM HE2  H       0.44
ATOM ND1  NR3    -0.51
ATOM HD1  H       0.44
ATOM CE1  CPH2    0.32
ATOM HE1  HR2     0.18
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB   CA    CG   CB    ND1 CG   CE1 ND1
BOND NE2 CD2    N    HN    N   CA
BOND C    CA    C    +N    CA  HA   CB HB1
BOND CB   HB2   ND1  HD1   NE2 HE2  CD2 HD2 CE1 HE1
```

變成GCMA的HSP(GCMA的rtf中只有1個improper)

```
RESI HSP
GROUP             ! CHARGE
ATOM O1     OG301  -0.396 !
ATOM C1     CG311   0.243 !
ATOM O2     OG3C61 -0.393 !           H9   H7
ATOM C2     CG311   0.029 !           |    |
ATOM H16    HGA1    0.09  ! H11--O5--C8--C7--O4    H5
ATOM C4     CG311   0.106 !           |    |    \   /
ATOM C5     CG311   0.149 !          H10   H8    C6--H6
ATOM N1     NG2S1  -0.307 !                      |
ATOM O3     OG311  -0.642 !                 H13--C2--O2  H12
ATOM C6     CG321   0.043 !                     /      \/
ATOM O4     OG301  -0.347 !                  -C3-H14   C1--O1-         H18
ATOM C7     CG321   0.006 !                     \      /              /
ATOM C8     CG321   0.026 !                 H16--C5--C4--H15        C17--H19
ATOM O5     OG311  -0.64  !                     /      \            ||
ATOM H3     HGP1    0.118 !                 H4--O3 H3--N1--C15------C16  H110
ATOM H4     HGP1    0.42  !                              ||        \  /
ATOM H5     HGA2    0.09  !                             O13        C18--H111
ATOM H6     HGA2    0.09  !                                         \
ATOM H7     HGA2    0.09  !                                          H112
ATOM H8     HGA2    0.09  !
ATOM H9     HGA2    0.09  !
ATOM H10    HGA2    0.09  !
ATOM H11    HGP1    0.419 !
ATOM H12    HGA1    0.09  !
```

I. 挑選本案沒有用到的GLUP和LSN做為GC和GCMA的patch

Patching的目的是針對聚合物的頭尾進行修飾：中間斷重複的結構，電荷皆相同，但在末端OH處會有小改動，因此用Patching來修改。

將top_all36_prot.rtf中的PRES GLUP和PRES LSN修改成OH端

修改前的GLUP和LSN

```
PRES GLUP         0.00 ! patch for protonated glutamic acid, proton on oe2
                       ! via acetic acid, use in a patch statement and
                       ! follow with AUTOgenerate ANGLes DIHEdrals command
GROUP
ATOM CG   CT2    -0.21 !
ATOM HG1  HA2     0.09 ! HG1    OE1
ATOM HG2  HA2     0.09 !  |    //
ATOM CD   CD      0.75 ! -CG--CD
ATOM OE1  OB     -0.55 !  |     \
ATOM OE2  OH1    -0.61 ! HG2     OE2-HE2
ATOM HE2  H       0.44 !
BOND OE2 HE2
DONOR HE2 OE2
IC HE2  OE2  CD   OE1   0.0000  0.0000  0.0000  0.0000  0.0000

PRES LSN          0.00 ! patch for neutral lysine based on methylamine
                       ! use in a patch statement
                       ! follow with AUTOgenerate ANGLes DIHEdrals command
!delete atom and reassign charges
DELETE ATOM HZ3
GROUP
ATOM CE   CT2     0.13
ATOM HE1  HA2     0.075
ATOM HE2  HA2     0.075
ATOM NZ   NH2    -0.96
ATOM HZ1  HC      0.34
ATOM HZ2  HC      0.34
```

修改後的GLUP和LSN:，並以OH作為結尾

OH結尾修飾
針對末端的C電荷改動

```
PRES GLUP                ! standard N-terminus
GROUP                    ! use in generate statement
ATOM O1    OG311  -0.65  !
ATOM HT2   HGP1    0.403 ! --C1--O1--HT2
ATOM C1    CG311   0.294 !   |
ATOM H12   HGA1    0.09  !   H12
BOND HT2 O1
DONOR HT2 O1

PRES LSN                 ! standard N-terminus
GROUP                    ! use in generate statement
ATOM OC1   OG311  -0.643 !
ATOM HCT   HGP1    0.42  ! --C3--OC1--HCT
ATOM C3    CG311   0.166 !   |
ATOM H14   HGA1    0.09  !   H14
BOND OC1 C3
BOND HCT OC1
DONOR HCT OC1
IC C4   C5   C3    OC1   0.0000  0.0000  180.0000  0.0000  0.0000
```

J. 要注意：**top_all36_prot.rtf的default patching是CTER和NTER，所以要先宣告重複單體端的原子，並在RESI HSE和 RESI HSP最後一行加上 PATCHING FIRS GLUP LAST LSN**

預設重複單體端的原子

```
DECL -CA
DECL -C
DECL -O
DECL +N
DECL +HN
DECL +CA
DEFA FIRS NTER LAST CTER
AUTO ANGLES DIHE PATCH
```

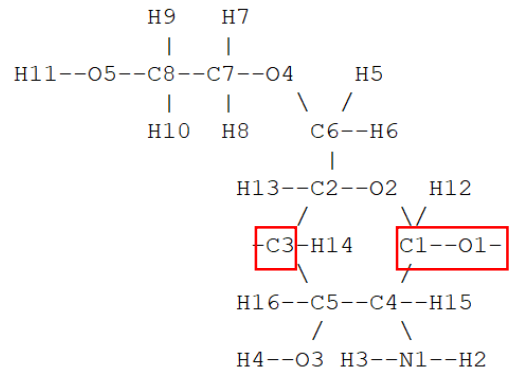
多宣告重複單體端的原子

```
DECL -CA
DECL -C
DECL -O
DECL +N
DECL +HN
DECL +CA
DECL -C3
DECL +O1
DECL +C1
DECL +H12
DEFA FIRS NTER LAST CTER
AUTO ANGLES DIHE PATCH
```

在RESI最後一行補上更改的Patching

```
BOND C7   H7
BOND C7   H8
BOND C8   O5
BOND C8   H9
BOND C8   H10
BOND O5   H11
BOND C1   H12
BOND C2   H13
BOND C3   H14
BOND C4   H15
BOND C5   H16
BOND C3   +O1
PATCHING FIRS GLUP LAST LSN
```

需要多宣告的原子示意圖



Comment

改質名稱	GC		GCMA	
比較項目	Cgenff*	Self Topo*	Cgenff	Self Topo
Atom	32	32	41	41
Bond	32	32	41	41
Angle	57	57	72	72
Dihedral	84	84	102	102
Improper	0	0	1	1
差異原因	~		~	
備註	**parameter penalty = 12 charge penalty = 9.166**		**parameter penalty =15 Charge penalty = 9.499**	

如何驗證自己的parameter

charmm2lammps結果驗證

parameter validation結果

改質名稱	ARGMA			ASNMA			GLNMA			CYS_COOH		
比較項目	Self Topo psf*	Cgenff*	Data*	Self Topo psf*	Cgenff	Data	Self Topo psf*	Cgenff	Data	Self Topo psf*	Cgenff	Data
Atom	36	36	36	26	26	26	29	29	29	20	20	20
Bond	35	35	35	25	25	25	28	28	28	19	19	19
Angle	60	60	60	42	42	42	48	48	48	32	32	32
Dihedral	**78**	**88**	**90**	**52**	**64**	**65**	**61**	**73**	**74**	**38**	**42**	**42**
Improper	**5**	**5**	**3**	**4**	**3**	**3**	**4**	**3**	**3**	2	2	2
差異原因	**Dihedral因為all36m和cgenff差異導致數量增加(下頁說明)**											
備註	**Improper有2個是0**			**Improper有1個是0**			**Improper有1個是0**			**~**		

Self Topo PSF= ARG pdb -> VMD autopsf + revise topology -> psf file
Cgenff = ARGMA -> Ligand Reader -> pdb, psf, rtf, prm -> Force Field Convertor -> Official LAMMPS input data file
Data = Self Topo pdb, psf -> CHARMM2LAMMPS + revise topology & parameter file -> LAMMPS input data file

1. **Cgenff和Data的dihedral數量 > psf的dihedral數量**：一個結構會有複數個parameter描述
2. **Data的dihedral數量 != Cgenff的dihedral數量**：all36m_prot描述的方式和Cgenff不同
3. **Data的improper數量 <= Cgenff的improper數量**：Charmm2lammps會把參數為0的improper省略

parameter validation結果

改質名稱	GC			GCMA		
比較項目	Self Topo psf*	Cgenff*	Data*	Self Topo psf*	Cgenff	Data
Atom	32	32	32	41	41	41
Bond	32	32	32	41	41	41
Angle	57	57	57	72	72	72
Dihedral	**84**	**125**	**125**	**102**	**146**	**146**
Improper	0	0	0	1	1	1
差異原因	**Dihedral因為all36m和cgenff差異導致數量增加(下頁說明)**					
備註	~			~		

Self Topo PSF= ARG pdb -> VMD autopsf + revise topology -> psf file
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1. Cgenff和Data的dihedral數量 > psf的dihedral數量：一個結構會有複數個parameter描述
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1. Charmm2lammps後bonding資訊為何增加(Cgenff和Data的dihedral數量 > psf的dihedral數量)

- 發現dihedral有<u>相同構型</u>對應到<u>不同的**dihedral type**</u>

```
14      37      4       1       5       6       # HB1   CT1   NH3   HC
15      18      5       7       10      13      # CT1   CT2   CT2   CT2
16      19      5       7       10      13      # CT1   CT2   CT2   CT2
17      20      5       7       10      13      # CT1   CT2   CT2   CT2
18      21      5       7       10      11      # CT1   CT2   CT2   HA2
```

- 上去對應後發現這些dihedral type有<u>完全不同的**parameter**</u>

```
7       0.1             3       0       1       # CC    CT1   NH3   HC
18      0.63            1       180     1       # CT1   CT2   CT2   CT2
19      0.01            2       0       0       # CT1   CT2   CT2   CT2
20      0.15            3       0       0       # CT1   CT2   CT2   CT2
21      0.19            3       0       1       # CT1   CT2   CT2   HA2
```

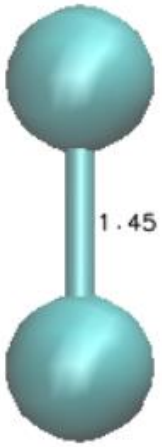
- 回到prm中發現確實有<u>給了不同參數的**dihedral定義**</u>：

```
! Fit dihedrals
! Variable cutoff based on QM and weighted in favor of alphaR and EXT (5:5:1)
! Shared dihedrals were fitted simultaneously

! Group-fitted for Lys/Arg/Gln/Met
C     CT1   CT2   CT2        0.3500  1    180.00
C     CT1   CT2   CT2        0.4200  2    180.00
C     CT1   CT2   CT2        1.9100  3    180.00
CT2   CT2   CT1   NH1        0.8800  1    180.00
CT2   CT2   CT1   NH1        0.0000  2    180.00
CT2   CT2   CT1   NH1        1.9000  3      0.00
CC    CT2   CT2   CT1        1.8400  1    180.00
CC    CT2   CT2   CT1        0.8400  2    180.00
CC    CT2   CT2   CT1        0.3900  3    180.00
CT1   CT2   CT2   CT2        0.6300  1    180.00
CT1   CT2   CT2   CT2        0.0100  2      0.00
CT1   CT2   CT2   CT2        0.1500  3      0.00
CT1   CT2   CT2   S          0.1400  1    180.00
CT1   CT2   CT2   S          0.5400  2      0.00
CT1   CT2   CT2   S          0.6900  3      0.00
```

Shared dihedrals were fitted simultaneously
說明這些是**疊加的dihedral potential**
這樣的結果在官方**Charmm GUI: Force Field Convertor**裡也會發現

1. Charmm2lammps後bonding資訊為何增加：確認lammps的potental確實會疊加，不可省略

C-C Model



C-C Model Data file

```
Bond Coeffs

     1   923.7     1.2

Bonds

       1      1         1         2
```

```
Bond Coeffs

     1   923.7     1.2

Bonds

       1      1         1         2
       2      1         1         2
```

Run 0 result:

Harmonic potential (1-2 IJ pair potential is ignored when bonded):

$$923.7 \times (1.2 - 1.45)^2 = 57.73$$

LAMMPS result:

```
Step Time Temp PotEng KinEng TotEng
      0            0            0    58.145936            0    58.145936
Loop time of 0 on 1 procs for 0 steps with 2 atoms
```

Harmonic potential (1-2 IJ pair potential is ignored when bonded):

$$2 \times 923.7 \times (1.2 - 1.45)^2 = 115.463$$

LAMMPS result:

```
Step Time Temp PotEng KinEng TotEng
      0            0            0    116.29187            0    116.29187
Loop time of 0 on 1 procs for 0 steps with 2 atoms
```

Duplicated bonding will lead to additional potential calculations in LAMMPS

2. all36m和cgenff差異導致數量增加(Data的dihedral數量 != Cgenff的dihedral數量)

all36m: ASN.pdb->pdb reader->psf, crd->force field convertor + all36m_prot(default)

```
17  atoms
16  bonds
27  angles
38  dihedrals
 5  impropers
 0  crossterms

11  atom types
11  bond types
19  angle types
16  dihedral types
 4  improper types
```

cgenff: ASN.pdb->ASN.mol2->Ligand reader->psf, crd, rtf, prm->force field convertor + cgenff + rtf, prm:

```
17  atoms
16  bonds
27  angles
34  dihedrals
 2  impropers
 0  crossterms

12  atom types
11  bond types
19  angle types
18  dihedral types
 2  improper types
```

鍵結數量的差異說明：

1. Cgenff並非完全重現all36m_prot的結果，而是為求泛用性做了一些改變
2. 這些改變不一定是簡化或劣化，因為改變後位能可能一模一樣，只知道參數上改變了表示方法
3. 這樣的簡化也導致同樣的氨基酸結構(ASN)在兩種力場得到不同的bonding parameter

3. Charmm2lammps後bonding資訊為何減少(Data的improper數量 <= Cgenff的improper數量)

- 因為charmm2lammps會自動忽略位能為0的參數：
  - In .prm we found an improper with **parameter 0**

```
C    HC     HC    NC2        0.0            0        0.0
                  ! mp2/6-311g** guan vibrational data, adm jr., 1/04
```

  - In .data we may also find the **improper coeff**:

```
Improper Coeffs # harmonic

       1              0              0  # C     CG2O1     HC    NG2P1
       2              0              0  # C     HC    HC    NC2
       3             45              0  # C     NC2   NG2P1     NC2
       4             96              0  # CC    CT1   OC    OC
       5            120              0  # CG2O1     CG2DC1    NG2P1     OG2D1
```

  - However, this structure will be **ignored** in **improper**

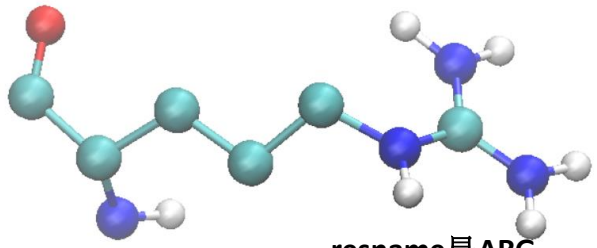
```
Impropers

       1        3        18       19       22       16   # C     NC2   NG2P1     NC2
       2        5        24       25       22       30   # CG2O1     CG2DC1    NG2P1     OG2D1
       3        4        34        5       36       35   # CC    CT1   OC    OC
```

no improper type 2

Conclusion

- 已驗證單個monomer的topology的正確性，因此確保整個結構的正確
  - 因為是把all36m_prot蛋白質末端改成cgenff的MA結構，沒有動到backbone的結構，所以聚合以後不用擔心出問題
  - 驗證方法是比較all36m_prot蛋白質末端改成cgenff的MA結構 與 全cgenff結構的psf檔結構數量
- 已驗證單個mononer的parameter的正確性，因此確保charmm2lammps執行正確
  - 驗證方法是去比較all36m_prot蛋白質末端改成cgenff的MA結構的data file和全cgenff結構的data file的結構數量

骨幹結構(不包含所有的H)



resname是ARG

骨幹結構的pdb(不包含所有的H)

```
ATOM    4360   N    ARG
ATOM    4361   H    ARG
ATOM    4362   CA   ARG
ATOM    4363   CB   ARG
ATOM    4364   CG   ARG
ATOM    4365   CD   ARG
ATOM    4366   NE   ARG
ATOM    4367   HE   ARG
ATOM    4368   CZ   ARG
ATOM    4369   NH1  ARG
ATOM    4370  HH11  ARG
ATOM    4371  HH12  ARG
ATOM    4372   NH2  ARG
ATOM    4373  HH21  ARG
ATOM    4374  HH22  ARG
ATOM    4375   C    ARG
ATOM    4376   O    ARG
END
```

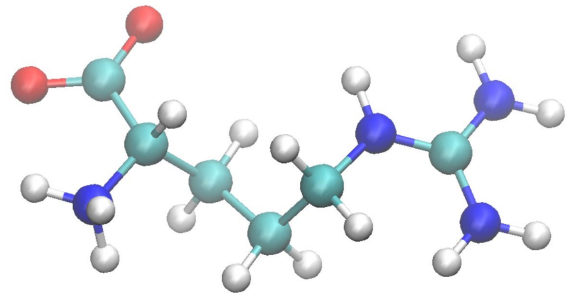
調整前

調整後

原始ARG

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47  !      |                      HH11
ATOM HN   H       0.31  !  HN-N                       |
ATOM CA   CT1     0.07  !      |   HB1 HG1 HD1 HE     NH1-HH12
ATOM HA   HB1     0.09  !      |   |   |   |   |    //(+)
GROUP                   !  HA-CA--CB--CG--CD--NE--CZ
ATOM CB   CT2    -0.18  !      |   |   |   |         \
ATOM HB1  HA2     0.09  !      |   HB2 HG2 HD2        NH2-HH22
ATOM HB2  HA2     0.09  !   O=C                       |
GROUP                   !      |                      HH21
ATOM CG   CT2    -0.18
ATOM HG1  HA2     0.09
ATOM HG2  HA2     0.09
```

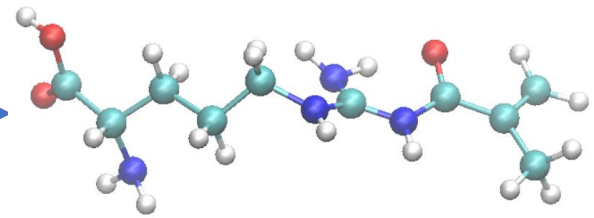
原始ARG



ARG_MA

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47  !      |                      HH11
ATOM HN   H       0.31  !  HN-N                       |
ATOM CA   CT1     0.07  !      |   HB1 HG1 HD1 HE     NH1-HH12
ATOM HA   HB1     0.09  !      |   |   |   |   |    //(+)
GROUP                   !  HA-CA--CB--CG--CD--NE--CZ     HH21   H8
ATOM CB   CT2    -0.18  !      |   |   |   |         \   /      /
ATOM HB1  HA2     0.09  !      |   HB2 HG2 HD2        NH2     C7--H9
ATOM HB2  HA2     0.09  !   O=C                       |       ||
GROUP                   !      |                     C5------C6    H10
ATOM CG   CT2    -0.18  !                            ||        \  /
ATOM HG1  HA2     0.09  !                            O3         C8--H11
ATOM HG2  HA2     0.09  !                                        \
GROUP                   !                                       H12
ATOM CD   CT2     0.20
```

ARG_MA(有一顆H是多顯示的不用管他)



ARGMA, ASNMA, GLNMA
GC, GCMA皆完成結構與參數上的驗證