KETI 의뢰 ESP 계산

부제목 : 아닐린, ABN, 니트로 아닐린 타겟

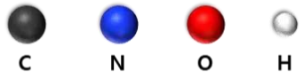
작성일자 : 2025 01 20

작성자 : 안용상

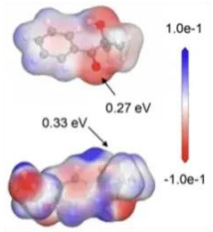
실험 개요

실험 배경

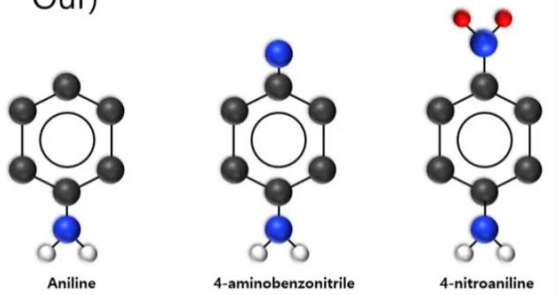
Electrostatic potential (ESP)



Reference)



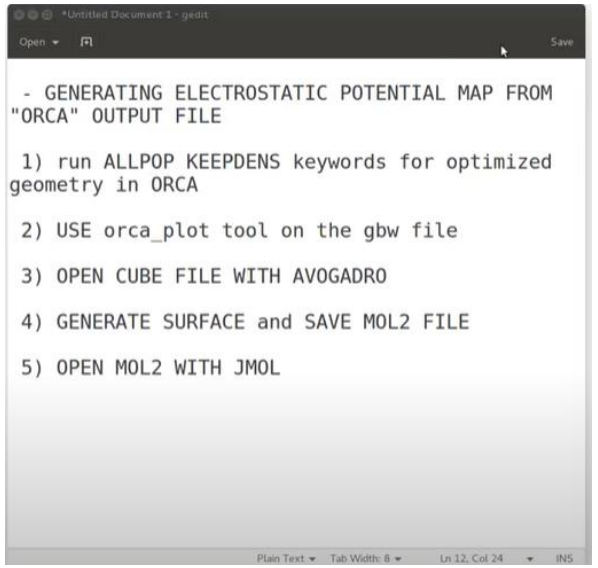
Our)



실험 과정 계획

1. Aniline, ABN, 4-nitroaniline 에 대한 구조 파일을 만들거나 구한다.
2. orca 이용; 각 분자 구조최적화
3. orca_plot사용; cube파일 제작
4. Avogadro로 Generate Surface
5. Jmol 소프트웨어에서 ESP확인

위 일련의 과정을 거쳐 ESP를 볼 수 있는 .jmol2파일들을 얻는 것이 목표이다.

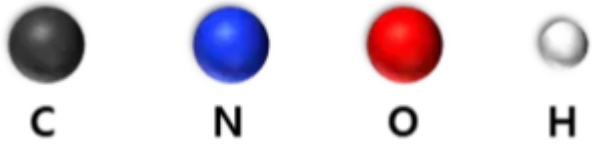


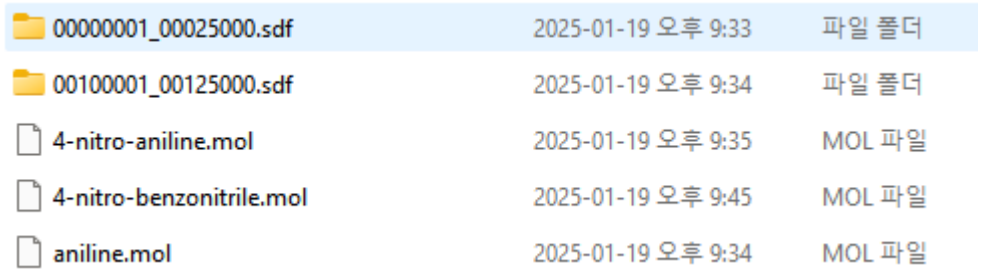
https://www.youtube.com/watch?v=jEpUQZiVOUw

구조 파일 확보

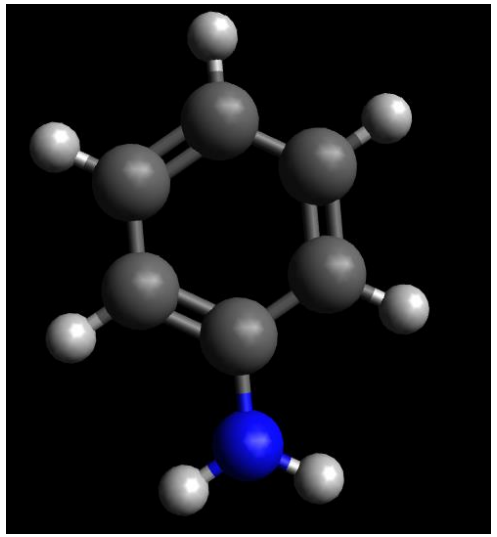
pubchem3d 데이터베이스 활용 .mol 구조파일 수집

* pubchem3d-> mol file Crop -> visualizing by Avogadro

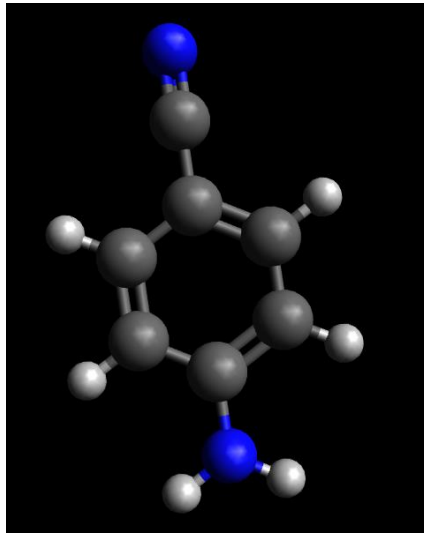




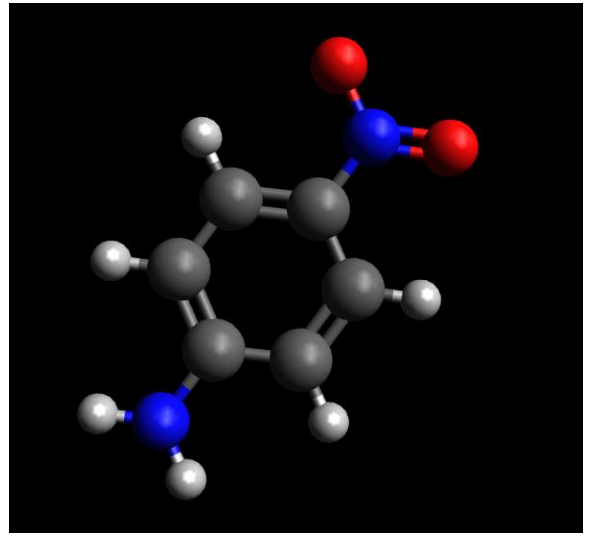
아닐린



ABN



4-니트로아닐린



구조 파일 확보

.mol -> .xyz 파일로 변환

*  openbabel 소프트웨어 사용

[01]Data > transform_mol_to_xyz.sh

```
obabel 4-nitro-aniline.mol -O 4-nitro-aniline.xyz
obabel 4-nitro-benzonitrile.mol -O 4-nitro-benzonitrile.xyz
obabel aniline.mol -O aniline.xyz
```

```
lsp32@celinux2:~/Desktop/[00]Pro
a$ sh transform_mol_to_xyz.sh
1 molecule converted
1 molecule converted
1 molecule converted
```

00000001_00025000.sdf	2025-01-19 오후 9:33	파일 폴더
00100001_00125000.sdf	2025-01-19 오후 9:34	파일 폴더
4-nitro-aniline.mol	2025-01-19 오후 9:35	MOL 파일
4-nitro-benzonitrile.mol	2025-01-19 오후 9:45	MOL 파일
aniline.mol	2025-01-19 오후 9:34	MOL 파일

이름	수정한 날짜	유형	크기
00000001_00025000.sdf	2025-01-19 오후 9:33	파일 폴더	
00100001_00125000.sdf	2025-01-19 오후 9:34	파일 폴더	
4-nitro-aniline.mol	2025-01-19 오후 9:35	MOL 파일	
4-nitro-benzonitrile.mol	2025-01-19 오후 9:45	MOL 파일	
aniline.mol	2025-01-19 오후 9:34	MOL 파일	
transform_mol_to_xyz.sh	2025-01-19 오후 9:53	SH 원본 파일	
4-nitro-aniline.xyz	2025-01-19 오후 9:53	XYZ 파일	
4-nitro-benzonitrile.xyz	2025-01-19 오후 9:53	XYZ 파일	
aniline.xyz	2025-01-19 오후 9:53	XYZ 파일	

ORCA를 이용한 구조 최적화

구조 최적화를 위한 .inp 파일 제작

4-nitro-aniline_opt.inp	2025-01-20 오전 11:24	INP 파일
4-nitro-benzonitrile_opt.inp	2025-01-20 오전 11:24	INP 파일
aniline_opt.inp	2025-01-20 오전 11:24	INP 파일

orca 명령어로 구조 최적화 진행

nohup /home/<사용자>/orca경로/orca <inputfile.inp> > <outputfile.inp>

예시) nohup /home/yongsang/orca_6_0_1_linux_x86-64_shared_openmpi416/orca \
4-nitro-benzonitrile_opt.inp > \
4-nitro-benzonitrile_opt.out &

.inp 파일들 작성 예시

```
! B3LYP def2-SVP OPT ALLPOP KEEPDENS

%pal
nprocs 10
end

* xyz 0 1
N          -2.40460        0.00000        0.00050
C          -0.99410       -0.00020       -0.00030
C          -0.29690        1.20790       -0.00030
C          -0.29650       -1.20800       -0.00030
C           1.09800        1.20800        0.00010
C           1.09840       -1.20780        0.00010
C           1.79570        0.00020        0.00030
H          -0.82890        2.15580       -0.00030
H          -0.82830       -2.15610       -0.00020
H           1.64110        2.14860        0.00020
H           1.64170       -2.14820        0.00020
H           2.88180        0.00040        0.00060
H          -2.91090       -0.87550       -0.00050
H          -2.91070        0.87560       -0.00060
*
```

빠른 계산을 위한 병렬 CPU코드 (openmpi 필요)

```
! B3LYP def2-SVP OPT ALLPOP KEEPDENS

%pal
nprocs 10
end

* xyz 0 1
N           3.25020       -0.00010        0.00000
N          -3.54080        0.00010        0.00000
C           1.83980        0.00000        0.00000
C           1.14220       -1.20800        0.00000
C           1.14240        1.20810        0.00000
C          -0.94990       -0.00010        0.00000
C          -0.25260       -1.20800        0.00000
C          -0.25250        1.20800        0.00000
C          -2.37880        0.00000        0.00000
H           1.67430       -2.15590        0.00010
H           1.67460        2.15600        0.00000
H          -0.78210       -2.15780        0.00000
H          -0.78210        2.15780        0.00000
H           3.75640        0.87540       -0.00060
H           3.75630       -0.87570       -0.00060
*
```

```
! B3LYP def2-SVP OPT ALLPOP KEEPDENS

%pal
nprocs 10
end

* xyz 0 1
O           2.73740        1.09760       -0.00070
O           2.73730       -1.09760        0.00030
N           2.12920        0.00000       -0.00010
N          -3.49080       -0.00010        0.00010
C           0.70930        0.00000        0.00050
C          -2.08040        0.00000       -0.00050
C           0.01200        1.20800        0.00050
C           0.01190       -1.20800        0.00010
C          -1.38290        1.20800        0.00000
C          -1.38300       -1.20790       -0.00040
H           0.52190        2.16800        0.00080
H           0.52180       -2.16800        0.00000
H          -1.91540        2.15580        0.00030
H          -1.91540       -2.15570       -0.00060
H          -3.99700        0.87550       -0.00160
H          -3.99700       -0.87560       -0.00190
*
```

orca_plot 명령으로 생성된 .gpw file을 처리

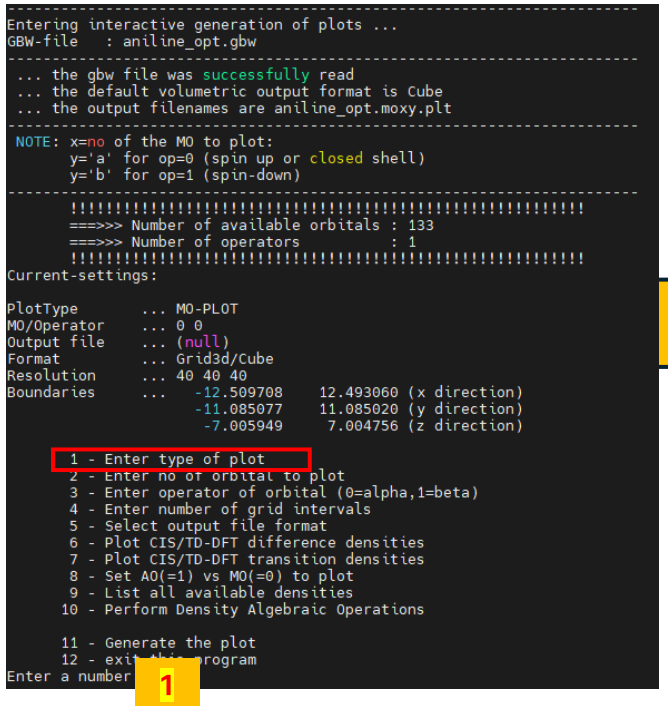
orca_plot으로 .gpw file을 처리 > .cube파일 생성

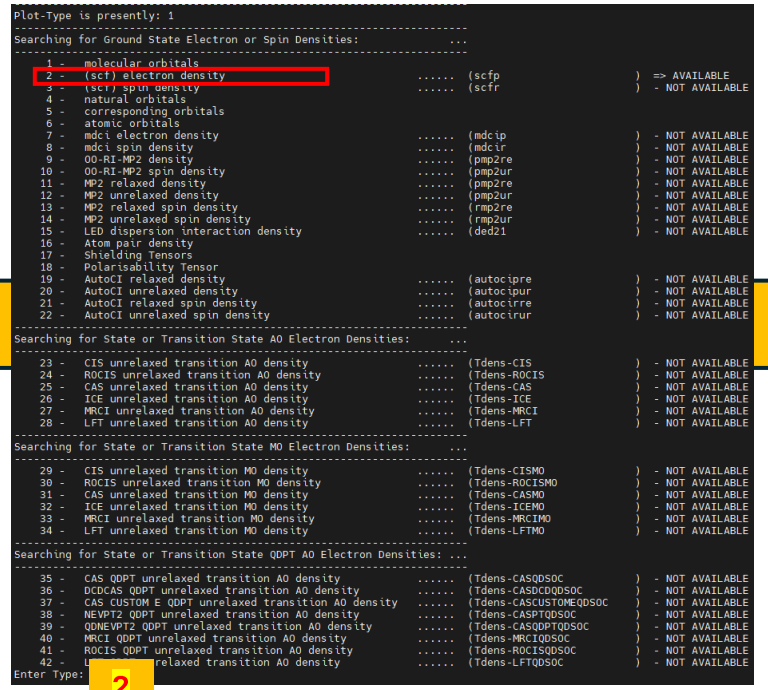
1) orca_plot 명령을 이용한 .cube 파일 생성

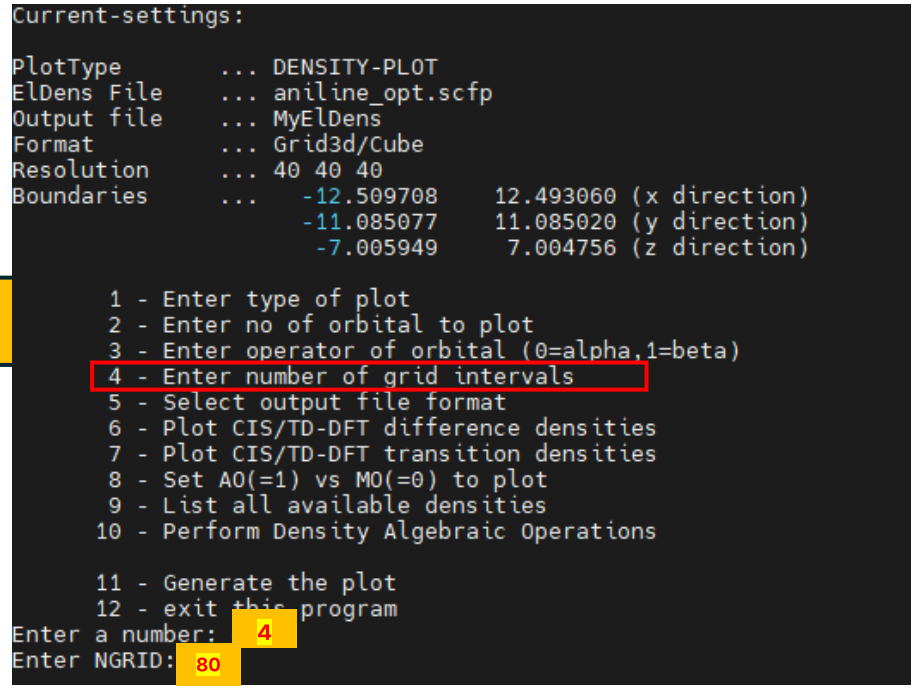
다음 명령을 이용해 gbw파일을 처리한다

```
orca_plot aniline_opt.gbw -i
```

아래와 같은 command line UI가 나오며 필요한 번호를 입력해 설정을 바꾼다.
ESP를 위한 설정은 다음 사진들을 따라오면 된다.







orca_plot 명령으로 생성된 .gpw file을 처리

orca_plot으로 gpwfile을 처리 > .cube파일 생성

...이어서

```
Current-settings:

PlotType        ... DENSITY-PLOT
ElDens File     ... aniline_opt.scfp
Output file     ... MyElDens
Format          ... Grid3d/Cube
Resolution      ... 80 80 80
Boundaries      ...    -12.509708    12.493060 (x direction)
                       -11.085077    11.085020 (y direction)
                        -7.005949     7.004756 (z direction)

       1 - Enter type of plot
       2 - Enter no of orbital to plot
       3 - Enter operator of orbital (0=alpha,1=beta)
       4 - Enter number of grid intervals
       5 - Select output file format
       6 - Plot CIS/TD-DFT difference densities
       7 - Plot CIS/TD-DFT transition densities
       8 - Set AO(=1) vs MO(=0) to plot
       9 - List all available densities
      10 - Perform Density Algebraic Operations

      11 - Generate the plot
      12 - exit this program
Enter a number: 5
```

```
Enter a number: 5
File-Format is presently: 7
     1 -  2D   Origin format
     2 -  2D   HPGL format
     3 -  2D   Gnuplot binary format
     4 -  2D   Gnuplot ascii format
     5 -  3D   Grid data binary (Fortran number format!)
     6 -  3D   Grid data ASCII
     7 -  3D   Gaussian cube
     8 -  3D   simple format
Enter Format: 7
```

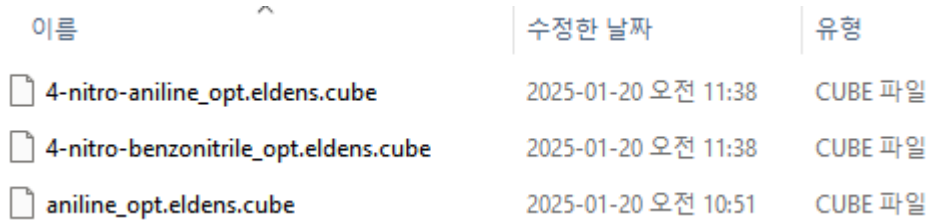
```
Current-settings:

PlotType        ... DENSITY-PLOT
ElDens File     ... aniline_opt.scfp
Output file     ... MyElDens
Format          ... Grid3d/Cube
Resolution      ... 80 80 80
Boundaries      ...    -12.509708    12.493060 (x direction)
                       -11.085077    11.085020 (y direction)
                        -7.005949     7.004756 (z direction)

       1 - Enter type of plot
       2 - Enter no of orbital to plot
       3 - Enter operator of orbital (0=alpha,1=beta)
       4 - Enter number of grid intervals
       5 - Select output file format
       6 - Plot CIS/TD-DFT difference densities
       7 - Plot CIS/TD-DFT transition densities
       8 - Set AO(=1) vs MO(=0) to plot
       9 - List all available densities
      10 - Perform Density Algebraic Operations

      11 - Generate the plot
      12 - exit this program
Enter a number: 11
```

```
Calling PlotGrid3d with ATOM-A,B=0,0
Entering PlotGrid3d with Plottype =2
                  *** PLOTTING FINISHED ***
 Output file: aniline_opt.eldens.cube
--------------------------------------------------------------------------------
Current-settings:

PlotType        ... DENSITY-PLOT
ElDens File     ... aniline_opt.scfp
Output file     ... aniline_opt.eldens.cube
Format          ... Grid3d/Cube
Resolution      ... 80 80 80
Boundaries      ...    -12.509708    12.493060 (x direction)
                       -11.085077    11.085020 (y direction)
                        -7.005949     7.004756 (z direction)

       1 - Enter type of plot
       2 - Enter no of orbital to plot
       3 - Enter operator of orbital (0=alpha,1=beta)
       4 - Enter number of grid intervals
       5 - Select output file format
       6 - Plot CIS/TD-DFT difference densities
       7 - Plot CIS/TD-DFT transition densities
       8 - Set AO(=1) vs MO(=0) to plot
       9 - List all available densities
      10 - Perform Density Algebraic Operations

      11 - Generate the plot
      12 - exit this program
Enter a number 12
```

orca_plot 명령으로 생성된 .gpw file을 처리

orca_plot으로 gpwfile을 처리 > .cube파일 생성

다음과 같이 .cube파일을 얻는데 까지 성공했다!

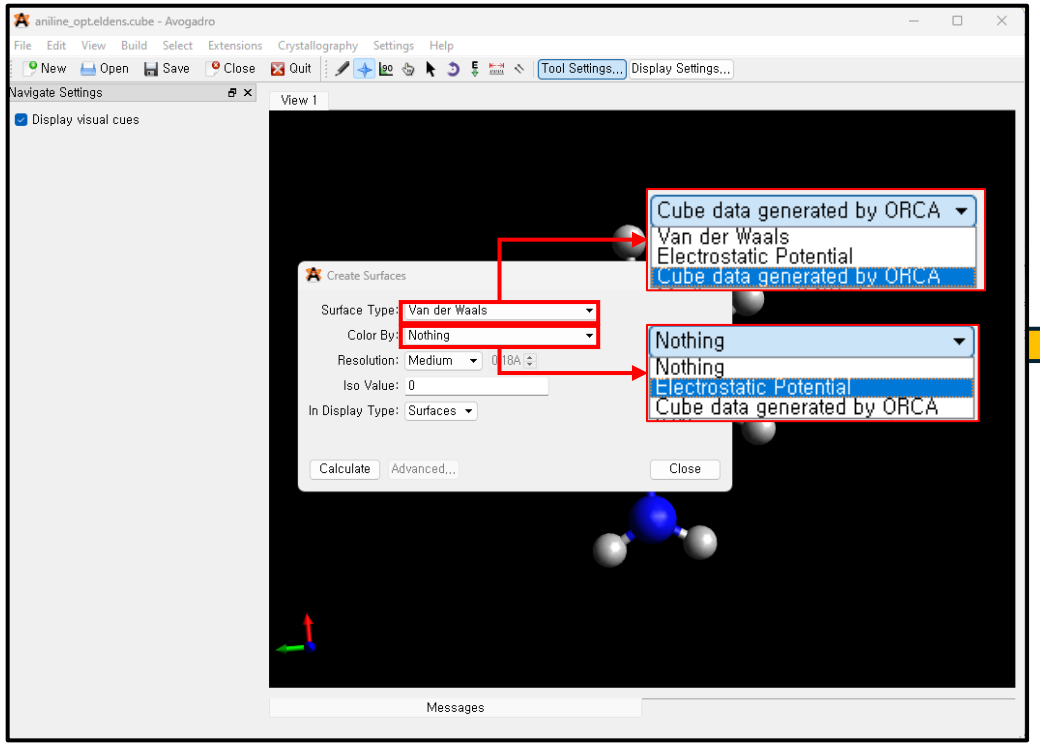


이름	수정한 날짜	유형
4-nitro-aniline_opt.eldens.cube	2025-01-20 오전 11:38	CUBE 파일
4-nitro-benzonitrile_opt.eldens.cube	2025-01-20 오전 11:38	CUBE 파일
aniline_opt.eldens.cube	2025-01-20 오전 10:51	CUBE 파일

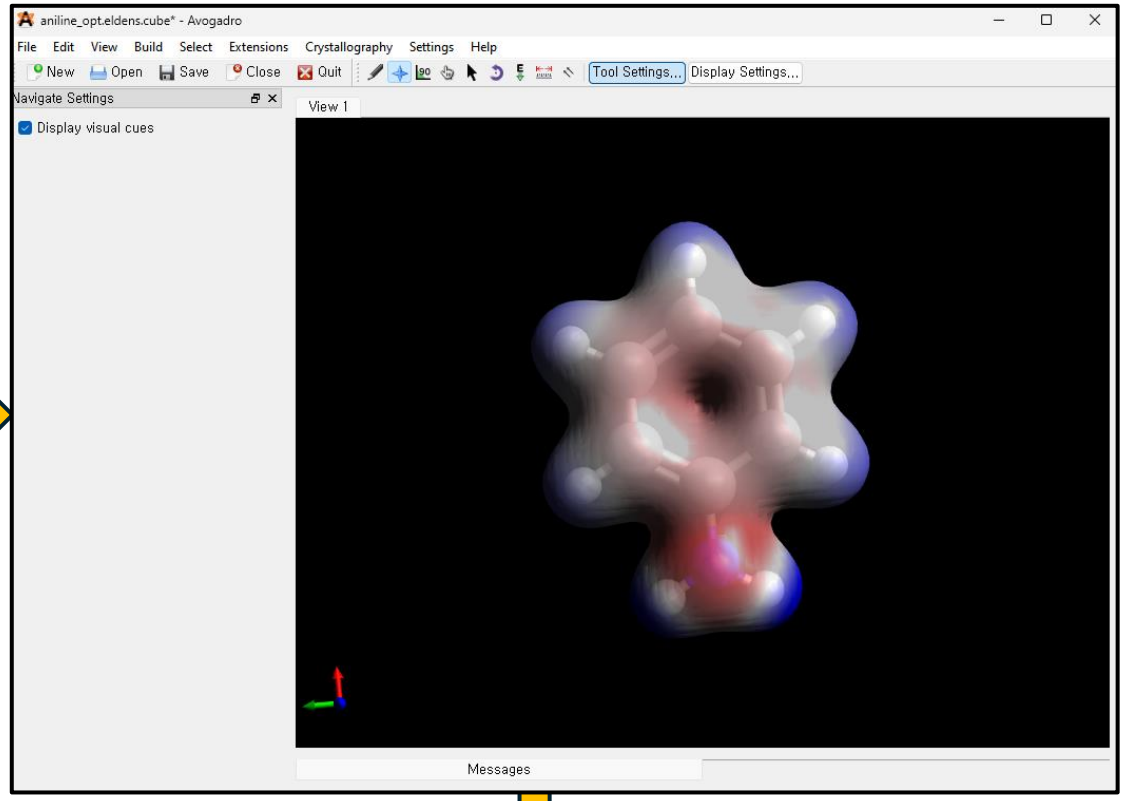
.cube파일을 AVOGADRO를 통해 Open

Avogadro를 통해 Open & Create Surfaces 진행

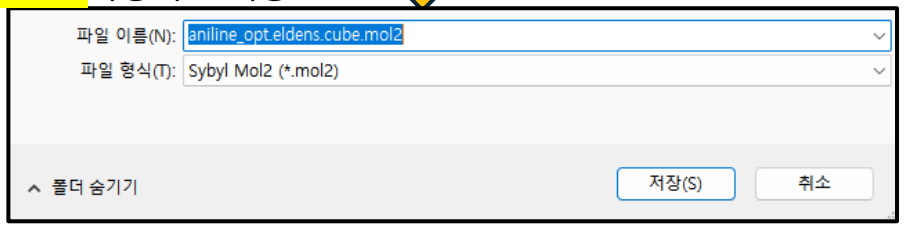
Avogadro로 .cube를 열고 상단리본 > Extensions > Create Surfaces 선택



위와 같은 화면이 나올것이다.



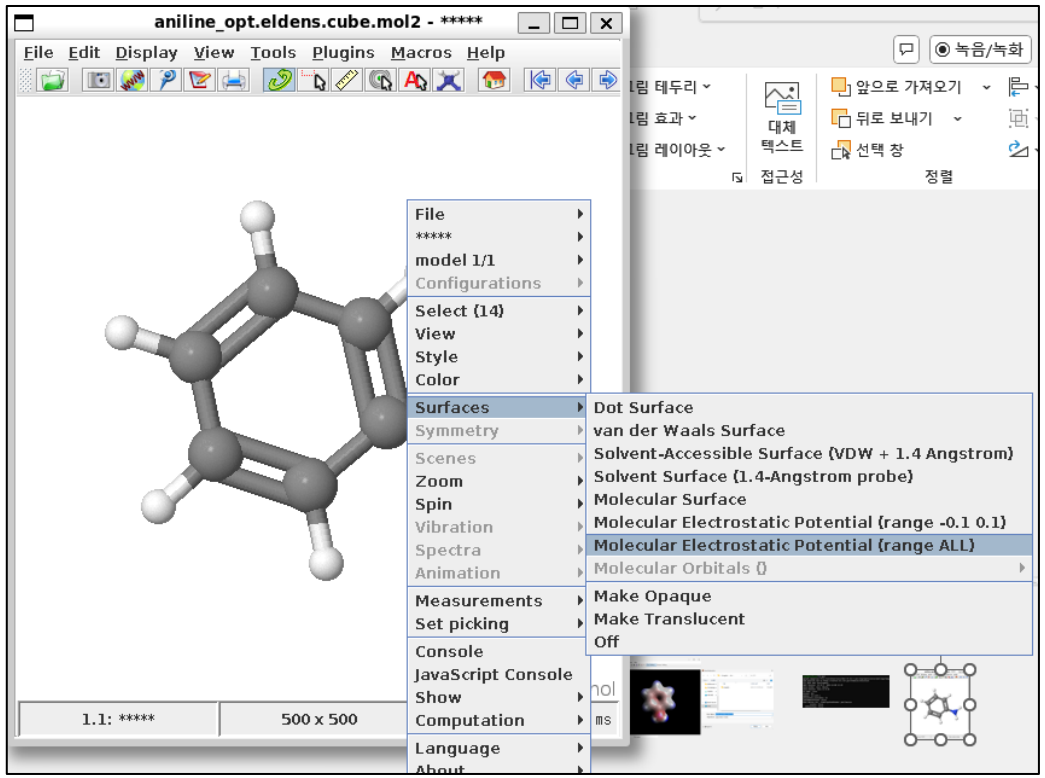
그리고 .mol2 확장자로 저장!

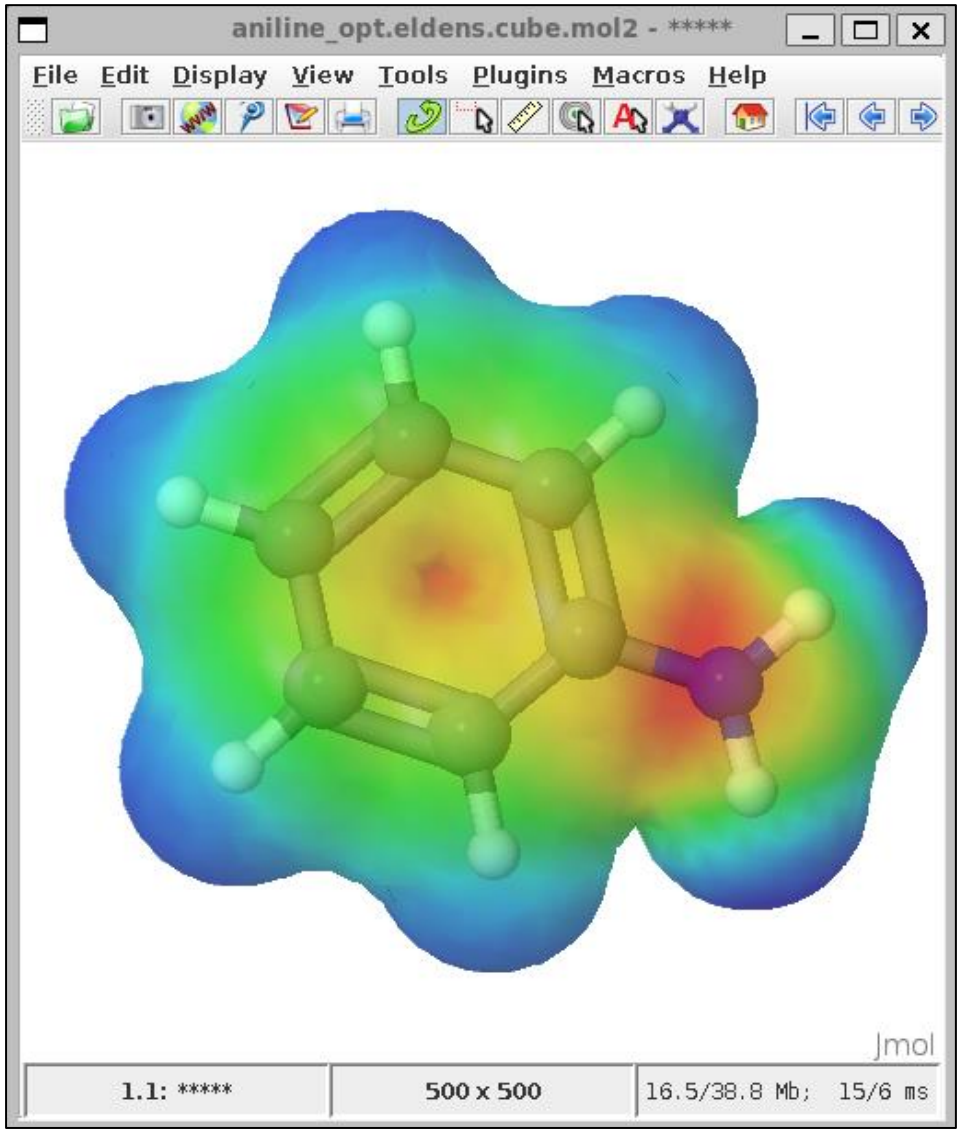


jmol 소프트웨어에서 저장한 .mol2 File을 열고 ESP 확인

jmol 소프트웨어로 ESP그리기

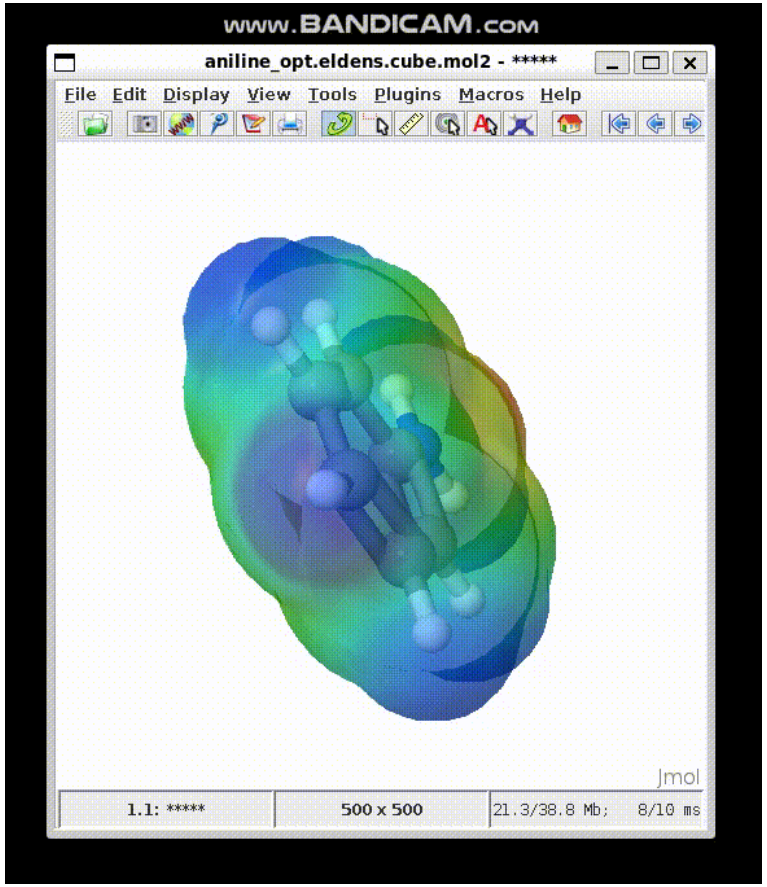
```
lsp32@celinux2:~$ jmol
splash_image=jar:file:/usr/share/java/Jmol-14.32.3.jar!/org/openscience/jmol/app/imag
CIR resolver set to https://cactus.nci.nih.gov/chemical/structure
(C) 2015 Jmol Development
Jmol Version: 14.32.3  2021-12-08 13:29
java.vendor: Java: Ubuntu
java.version: Java 11.0.25
os.name: Linux
Access: ALL
memory: 23.3/67.1
processors available: 12
useCommandThread: false
User macros dir: /home/dydtkddhkdwk/.jmol/macros
       exists: false
  isDirectory: false
```



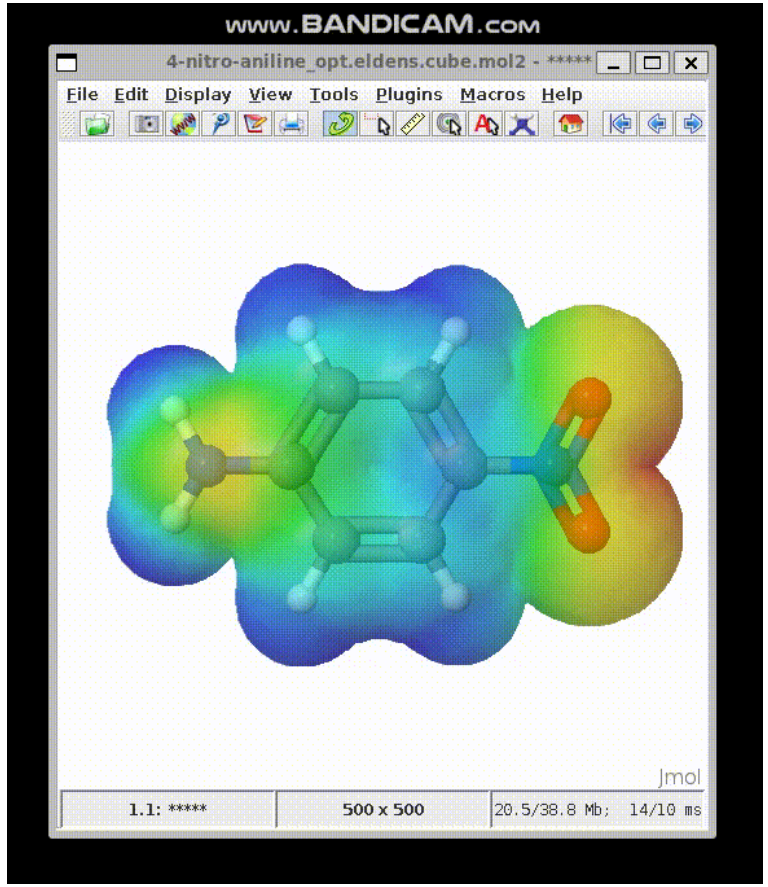


최종 결과물

Aniline



4-nitro-aniline



4-nitro-benzonitrile