

# KETI 의뢰 ESP 계산

부제목 : 아닐린, ABN, 니트로 아닐린 타겟

작성일자 : 2025 01 20

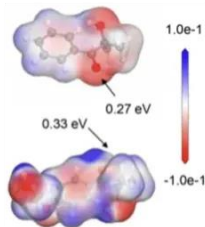
작성자 : 안용상

## 실험 개요

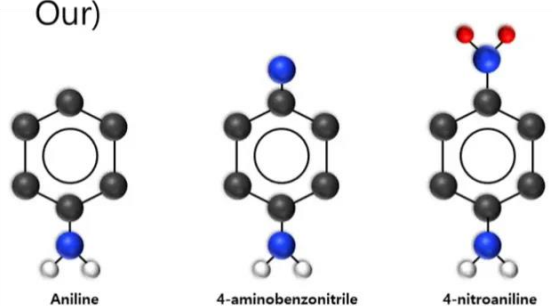
### 실험 배경

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.

```

- GENERATING ELECTROSTATIC POTENTIAL MAP FROM
"ORCA" OUTPUT FILE

1) run ALLPOP KEEPDENS keywords for optimized
geometry in ORCA

2) USE orca_plot tool on the gbw file


3) OPEN CUBE FILE WITH AVOGADRO

4) GENERATE SURFACE and SAVE MOL2 FILE

5) OPEN MOL2 WITH JMOL
  
```

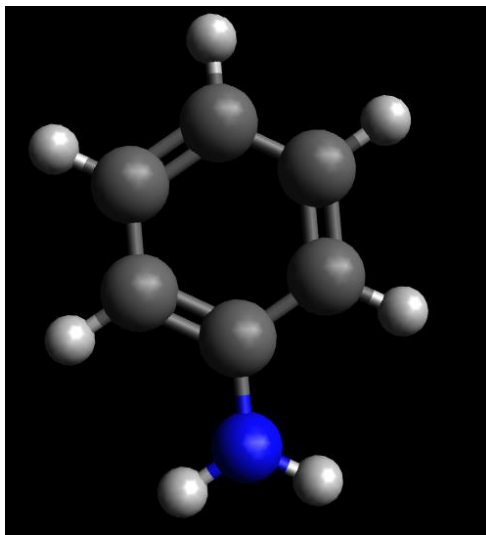
## 구조 파일 확보

## pubchem3d 데이터베이스 활용 .mol 구조파일 수집

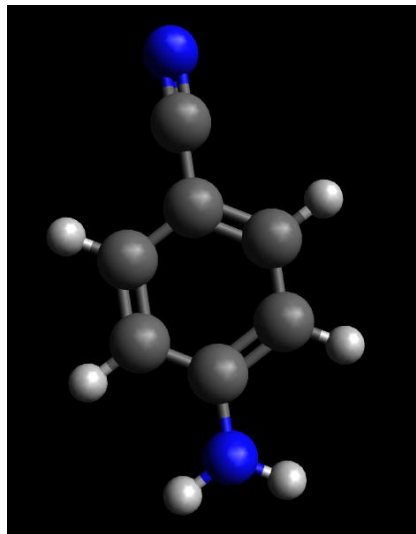
\* pubchem3d-> mol file Crop -> visualizing by  Avogadro



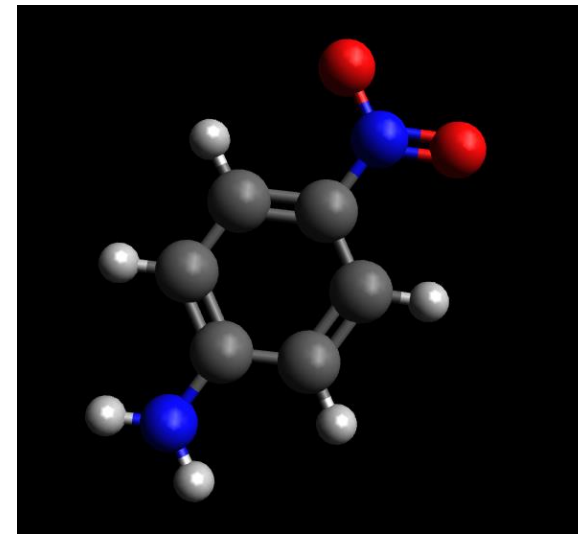
아닐린



ABN




4-니트로아닐린




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

## 구조 파일 확보






## |||.mol -&gt; .xyz 파일로 변환










\*  openbabel 소프트웨어 사용

```
[01]Data >  transform_mol_to_xyz.sh
```

```
1 obabel 4-nitro-aniline.mol -O 4-nitro-aniline.xyz
2 obabel 4-nitro-benzonitrile.mol -O 4-nitro-benzonitrile.xyz
3 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

## .inp 파일들 작성 예시

```

1  ! B3LYP def2-SVP OPT ALLPOP KEEPDENS
2
3  %pal
4  nprocs 10
5  end
6
7  * xyz 0 1
8  N      -2.40460      0.00000      0.00050
9  C      -0.99410     -0.00020     -0.00030
10 C      -0.29690      1.20790     -0.00030
11 C      -0.29650     -1.20800     -0.00030
12 C       1.09800      1.20800      0.00010
13 C       1.09840     -1.20780      0.00010
14 C       1.79570      0.00020      0.00030
15 H      -0.82890      2.15580     -0.00030
16 H      -0.82830     -2.15610     -0.00020
17 H       1.64110      2.14860      0.00020
18 H       1.64170     -2.14820      0.00020
19 H       2.88180      0.00040      0.00060
20 H      -2.91090     -0.87550     -0.00050
21 H      -2.91070      0.87560     -0.00060
22 *

```

빠른 계산을 위한 병렬 CPU코드 (openmpi 필요)

## 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 &

```

1  ! B3LYP def2-SVP OPT ALLPOP KEEPDENS
2
3  %pal
4  nprocs 10
5  end
6
7  * xyz 0 1
8  N      3.25020     -0.00010      0.00000
9  N     -3.54080      0.00010      0.00000
10 C      1.83980      0.00000      0.00000
11 C      1.14220     -1.20800      0.00000
12 C      1.14240      1.20810      0.00000
13 C     -0.94990     -0.00010      0.00000
14 C     -0.25260     -1.20800      0.00000
15 C     -0.25250      1.20800      0.00000
16 C     -2.37880      0.00000      0.00000
17 H      1.67430     -2.15590      0.00010
18 H      1.67460      2.15600      0.00000
19 H     -0.78210     -2.15780      0.00000
20 H     -0.78210      2.15780      0.00000
21 H      3.75640      0.87540     -0.00060
22 H      3.75630     -0.87570     -0.00060
23 *

```

```

! 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\_plot으로 .gpw file을 처리 > .cube파일 생성

다음 명령을 이용해 qbw파일을 처리한다

```
orca_plot aniline_opt.gbwh -i
```

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

```

Entering interactive generation of plots ...
GBW-file      : aniline_opt.gbw
-----
... the gbw file was successfully read
... the default volumetric output format is Cube
... the output filenames are aniline_opt.moxy.plt
-----
NOTE: x=no of the MO to plot:
      y='a' for op=0 (spin up or closed shell)
      y='b' for op=1 (spin-down)
-----
=====
====>>> Number of available orbitals : 133
====>>> Number of operators          : 1
=====
Current-settings:

PlotType      ... MO-PLOT
MO/Operator   ... 0 0
Output file   ... (null)
Format        ... Grid3d/Cube
Resolution    ... 40 40 40
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 or 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 A0(=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 1

```

```

Plot-Type is presently: 1
-----
Searching for Ground State Electron or Spin Densities:
-----
  1 - molecular orbitals
  2 - (scf) electron density ..... (scfp) ) => AVAILABLE
  3 - (scf) spin density ..... (scfr) ) - NOT AVAILABLE
  4 - natural orbitals
  5 - corresponding orbitals
  6 - atomic orbitals
  7 - mdc1 electron density ..... (mdc1p) ) - NOT AVAILABLE
  8 - mdc1 spin density ..... (mdc1r) ) - NOT AVAILABLE
  9 - 00-RI-MP2 density ..... (pmp2re) ) - NOT AVAILABLE
 10 - 00-RI-MP2 spin density ..... (pmp2ur) ) - NOT AVAILABLE
 11 - MP2 relaxed density ..... (pmp2re) ) - NOT AVAILABLE
 12 - MP2 unrelaxed density ..... (pmp2ur) ) - NOT AVAILABLE
 13 - MP2 relaxed spin density ..... (pmp2re) ) - NOT AVAILABLE
 14 - MP2 unrelaxed spin density ..... (pmp2ur) ) - NOT AVAILABLE
 15 - LED dispersion interaction density ..... (ded21) ) - NOT AVAILABLE
 16 - Atom pair density
 17 - Shielding Tensors
 18 - Polarizability Tensor
 19 - AutoCI relaxed density ..... (autoc1pr) ) - NOT AVAILABLE
 20 - AutoCI unrelaxed density ..... (autoc1ur) ) - NOT AVAILABLE
 21 - AutoCI relaxed spin density ..... (autoc1re) ) - NOT AVAILABLE
 22 - AutoCI unrelaxed spin density ..... (autoc1ur) ) - NOT AVAILABLE
-----
Searching for State or Transition State AO Electron Densities:
-----
 23 - CIS unrelaxed transition AO density ..... (Tdens-CIS) ) - NOT AVAILABLE
 24 - ROCIS unrelaxed transition AO density ..... (Tdens-ROCIS) ) - NOT AVAILABLE
 25 - CAS unrelaxed transition AO density ..... (Tdens-CAS) ) - NOT AVAILABLE
 26 - ICE unrelaxed transition AO density ..... (Tdens-ICE) ) - NOT AVAILABLE
 27 - MC1 unrelaxed transition AO density ..... (Tdens-MC1) ) - NOT AVAILABLE
 28 - LFT unrelaxed transition AO density ..... (Tdens-LFT) ) - NOT AVAILABLE
-----
Searching for State or Transition State MO Electron Densities:
-----
 29 - CIS unrelaxed transition MO density ..... (Tdens-CISMO) ) - NOT AVAILABLE
 30 - ROCIS unrelaxed transition MO density ..... (Tdens-ROCISMO) ) - NOT AVAILABLE
 31 - CAS unrelaxed transition MO density ..... (Tdens-CASMO) ) - NOT AVAILABLE
 32 - ICE unrelaxed transition MO density ..... (Tdens-ICEMO) ) - NOT AVAILABLE
 33 - MC1 unrelaxed transition MO density ..... (Tdens-MC1MO) ) - NOT AVAILABLE
 34 - LFT unrelaxed transition MO density ..... (Tdens-LFTMO) ) - NOT AVAILABLE
-----
Searching for State or Transition State QDPT AO Electron Densities:
-----
 35 - CAS QDPT unrelaxed transition AO density ..... (Tdens-CASQDSC) ) - NOT AVAILABLE
 36 - DDCAS QDPT unrelaxed transition AO density ..... (Tdens-CASQDQDSC) ) - NOT AVAILABLE
 37 - CAS CUSTOM QDPT unrelaxed transition AO density ..... (Tdens-CASCUSTOMQDSC) ) - NOT AVAILABLE
 38 - NEVP72 QDPT unrelaxed transition AO density ..... (Tdens-CASQPTQDSC) ) - NOT AVAILABLE
 39 - QDNEVP72 QDPT unrelaxed transition AO density ..... (Tdens-CASQDPTQDSC) ) - NOT AVAILABLE
 40 - MC1 QDPT unrelaxed transition AO density ..... (Tdens-MC1QDSC) ) - NOT AVAILABLE
 41 - ROCIS QDPT unrelaxed transition AO density ..... (Tdens-ROCISQDSC) ) - NOT AVAILABLE
 42 - LFT QDPT unrelaxed transition AO density ..... (Tdens-LFTQDSC) ) - NOT AVAILABLE
-----
Enter Type: 2

```

```
Current-settings:

PlotType      ... DENSITY-PLOT
ElDens File   ... aniline_opt.scfp
Output file    ... MyElDens
Format        ... Grid3d/Cube
Resolution    ... 40 40 40
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 A0(=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: 4
Enter NGRID: 80
```

## 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 A0(=1) vs M0(=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 A0(=1) vs M0(=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 A0(=1) vs M0(=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!

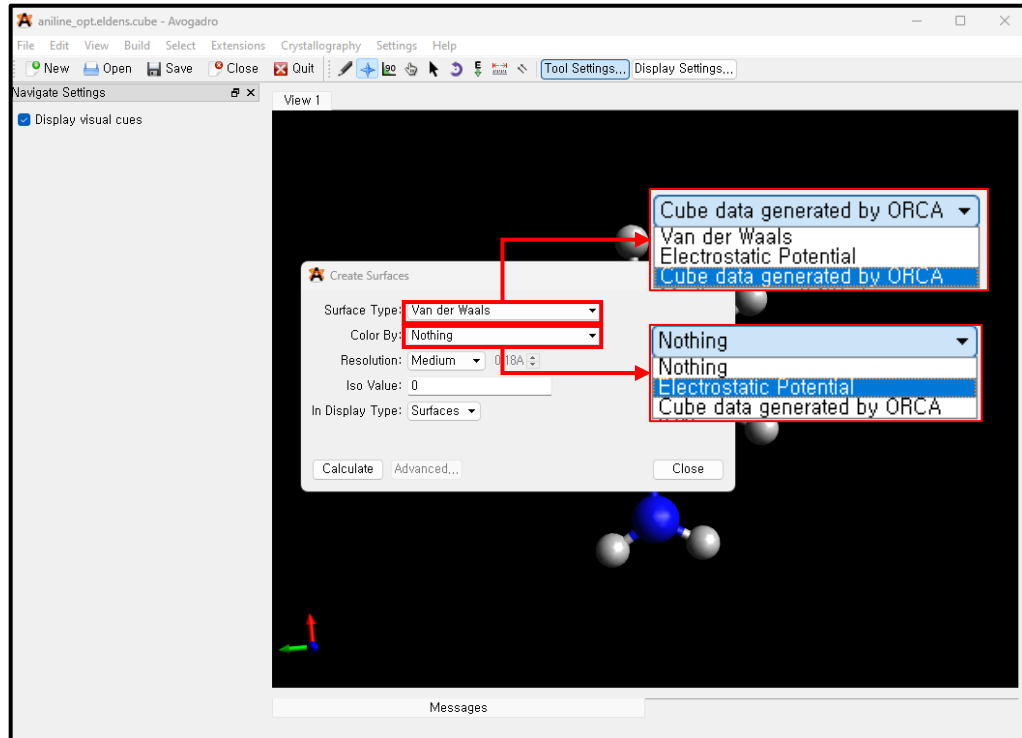
이름	수정한 날짜	유형
 4-nitro-aniline_opt.eldens.cube	2025-01-20 오전 11:38	CUBE 파일
 4-nitro-benzonitrile_opt.eldens.cube	2025-01-20 오전 11:38	CUBE 파일
 aniline_opt.eldens.cube	2025-01-20 오전 10:51	CUBE 파일



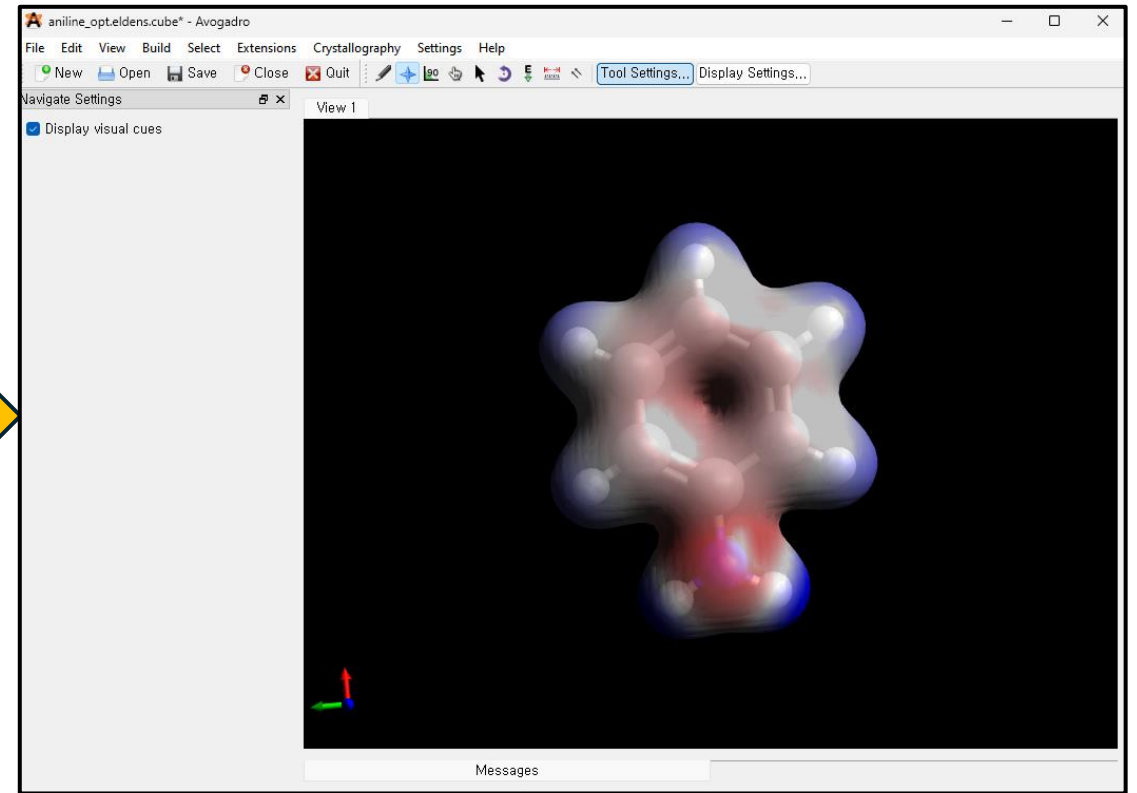
## .cube파일을 AVOGADRO를 통해 Open

### Avogadro를 통해 Open & Create Surfaces 진행

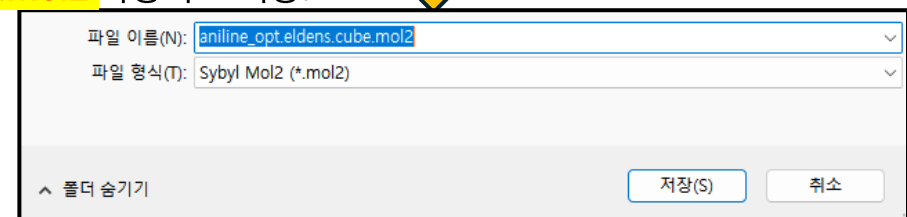
Avogadro로 .cube를 열고 상단리본 > Extensions > **Create Surfaces** 선택



위와 같은 화면이 나올것이다.



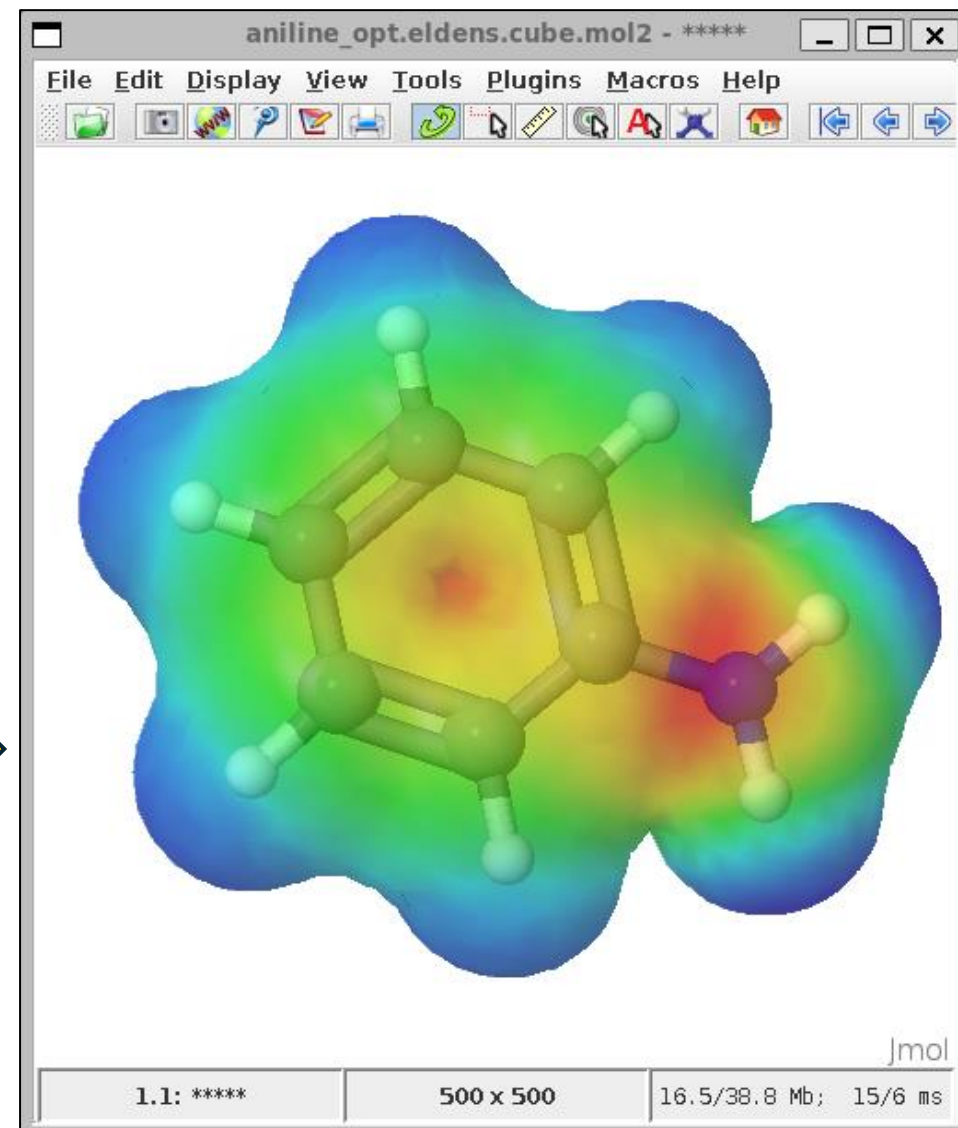
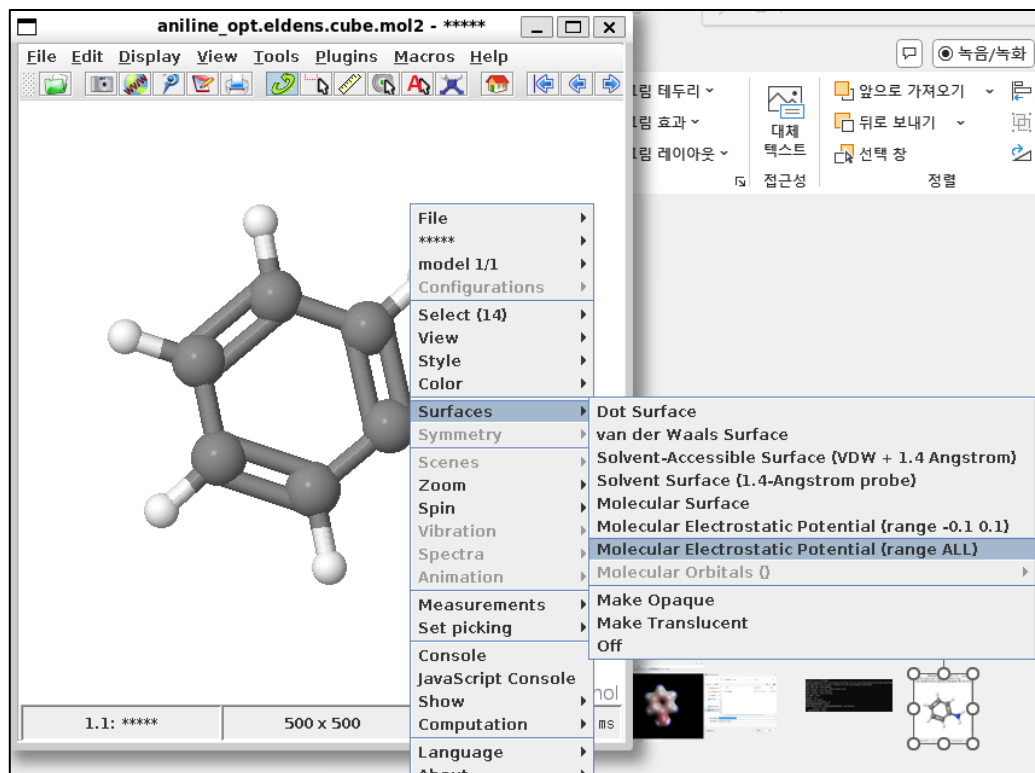
그리고 **.mol2** 확장자로 저장!



## jmol 소프트웨어에서 저장한 .mol2 File을 열고 ESP 확인

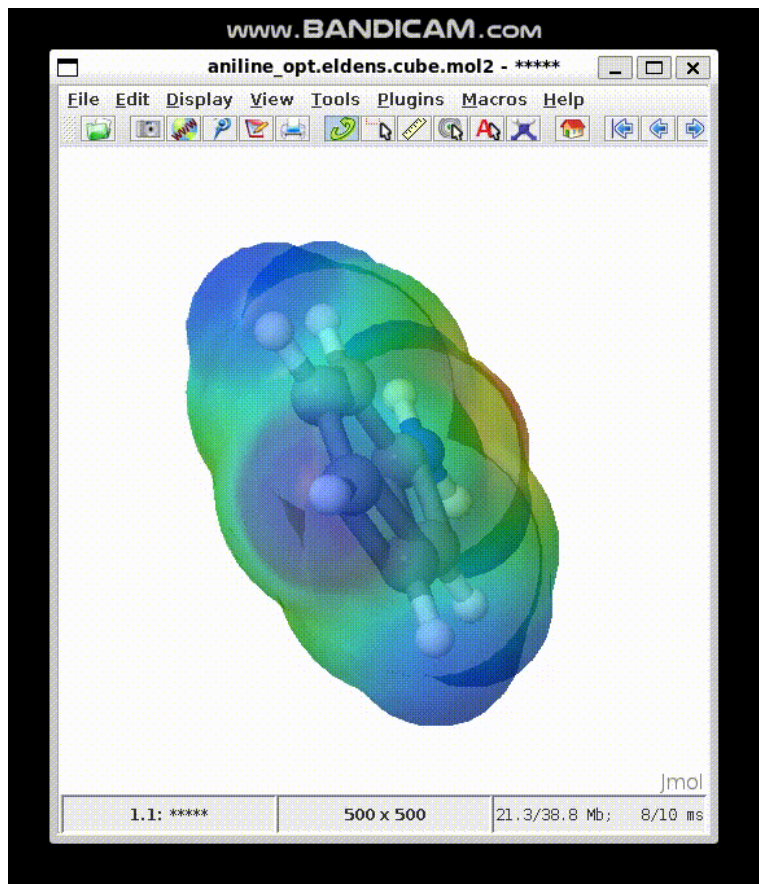
## jmol 소프트웨어로 ESP그리기

```
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
```

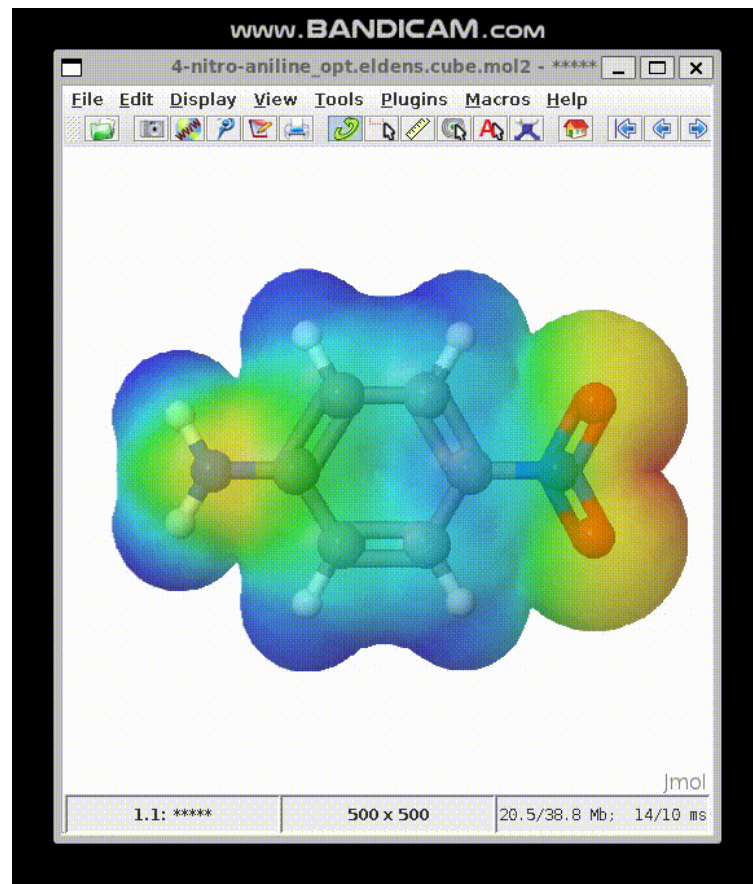


# 최종 결과물

Aniline



4-nitro-aniline



4-nitro-benzonitrile

