NOTE: There are lots of steps in this tutorial, if you want to draw a map with similar effect but in a much simpler way, see Section 4.A.13 of Multiwfn manual

Plotting electrostatic potential colored molecular surface map with ESP surface extrema via Multiwfn and VMD

2014-Aug-7

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In this tutorial, I will describe how to plot electrostatic potential (ESP) colored molecular surface map with ESP surface extrema via VMD based on the data outputted by Multiwfn. A very simple molecule furan will be used as example.

Before reading this tutorial, please make sure that you have read Section 4.12.1 of Multiwfn manual. For more details about this topic you can consult my article http://sobereva.com/196 (in Chinese).

The version of Multiwfn and VMD used here are 3.3.5 and 1.9.1, respectively, they are freely available at http://sobereva.com/multiwfn and http://www.ks.uiuc.edu/Research/vmd/, respectively.

1 Performing quantitative molecular surface analysis of ESP

Boot up Multiwfn and input following commands

furan.wfn // Obtained at B3LYP/6-31G** level. If you don't know how to generate the wavefunction file, please consult the beginning of Chapter 4 of Multiwfn manual.

12 // Quantitative molecular surface analysis module

0 // Start calculation. The default mapped function is ESP, and the default molecular surface is defined as the isosurface of ρ=0.001

2 // Export surface extrema as *surfanalysis.pdb* in current folder

5 // Export molecule geometry as pdb file in current folder

furan.pdb // The name of the pdb file

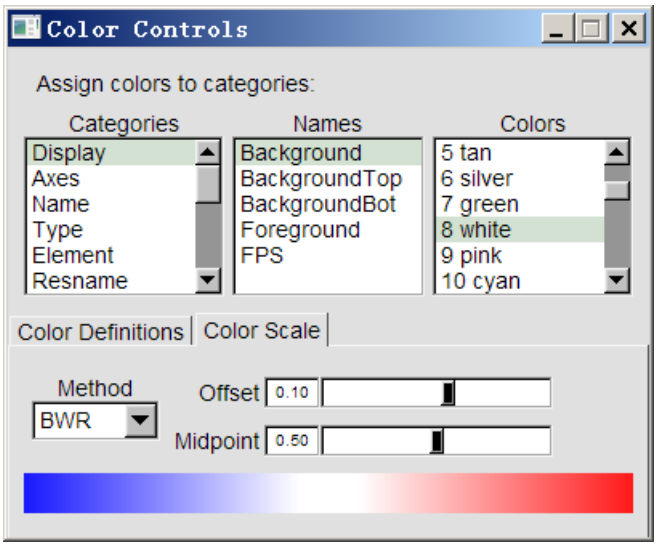
6 // Export all surface vertices as *vtx.pdb* in current folder

The resulting *surfanalysis.pdb* records the position of surface extrema of ESP, the carbons and oxygens correspond to local maxima and minimua, respectively. ESP values (kcal/mol) are recorded in B-factor field of the pdb file.

The *vtx.pdb* records the position of surface vertices, and the B-factor field corresponds to the ESP value at these points in kcal/mol

2 Plotting molecular surface and surface extrema in VMD

Boot up VMD, choose "Graphics"-"Colors" and select "Display"-"Background"-"white" to set background as white. (Alternatively, you can directly run the command *color Display Background white* in the command-line window of VMD) Then choose "Color scale" tab, set "Method" to "BWR". Now the window should look like below.

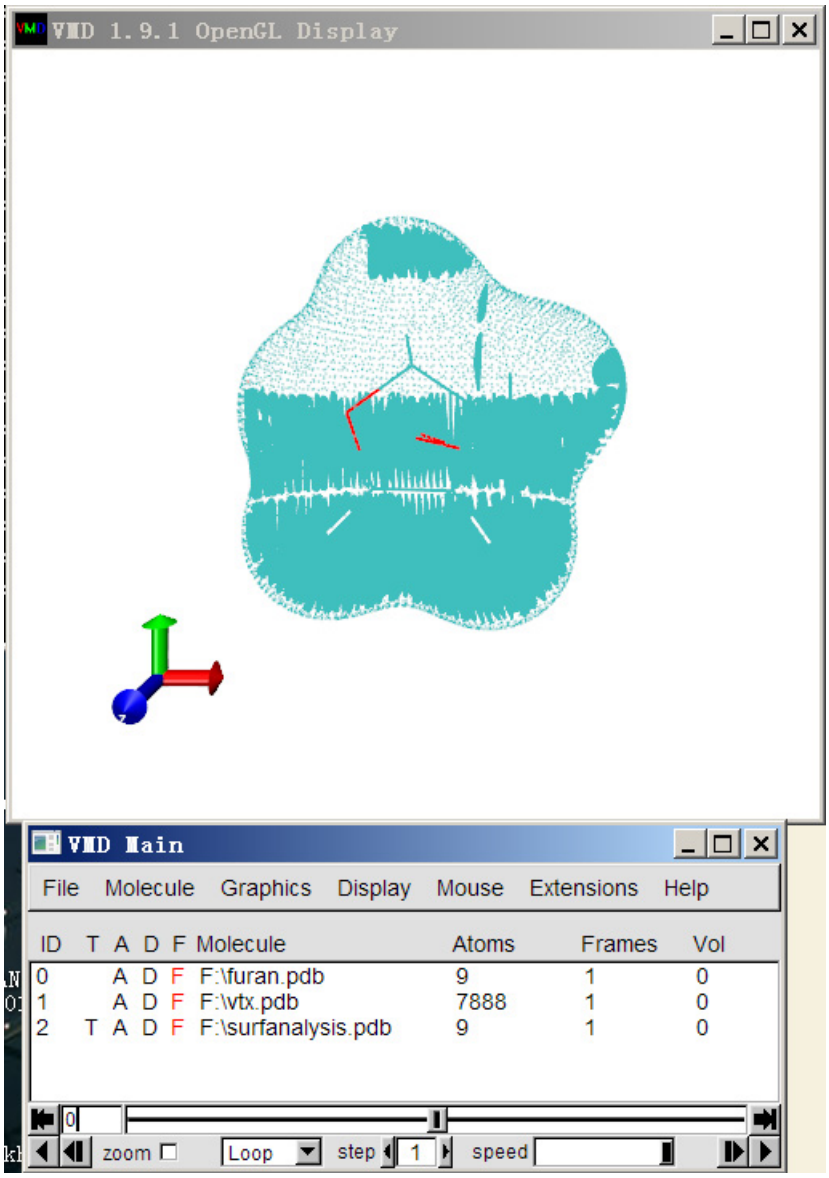


Choose "Display"-"Depth Cueing" in VMD main window to deselect it, this will make the graph more vivid.

Choose "Display"-"Axes"-"Off".

Make sure that the option in "Display"-"Rendermode" has been set to "Normal".

Drag *furan.pdb*, *vtx.pdb* and *surfanalysis.pdb* into VMD main window in turn, you will see



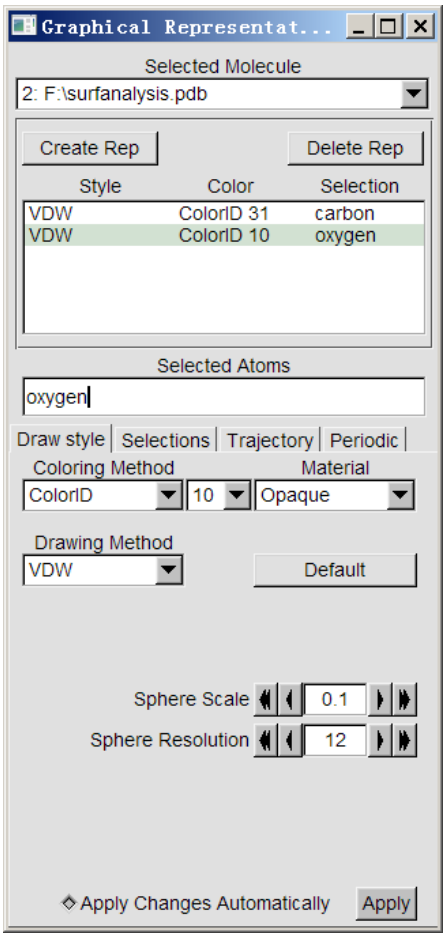
As you can see, each system has an ID, starting from 0.

Select "Graphics"-"Representations...". Choose the first term (ID=0) in "Selected molecule", change "Drawing method" as "Licorice", set "Bond Radius" as 0.1.

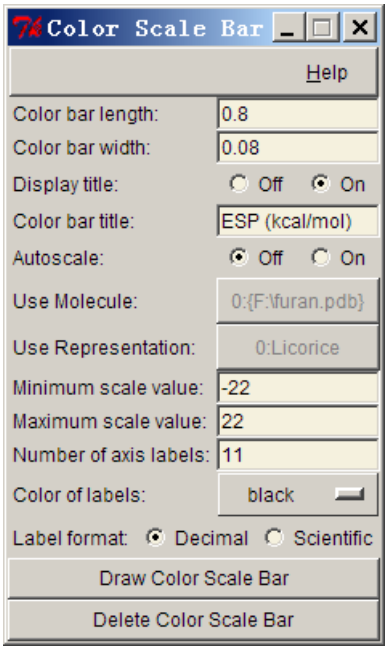
Choose the second term (ID=1) in "Selected molecule", set "Coloring method" to "Beta" (because Beta field in the pdb file corresponds to ESP value), set "Drawing method" to "Points", set "Size" to about 20. The choice of this value in fact depends on the size of VMD graphic window, if you enlarge the window size, you need to set the point size to a larger value to just make all interstices between surface points disappeared. Go to "Trajectory" tab, input -22 and 22 in "Color Scale Data Range" box and then click "Set" button.

Input *mol modstyle 0 2 VDW 0.06* in VMD command-line window. In VMD, each system can have multiple representations, this command set the first representation (index is 0) of the system with ID=2 as VDW style, and the radius is 0.06. Choose the third term (ID=2) in "Selected molecule", write *carbon* in the "Selected atoms" box and press ENTER button, choose "Coloring Method"-"ColorID", and then choose "31 Orange 2". Click "Create Rep" to create a new

representation, write *oxygen* in the "Selected atoms" box, choose "ColorID" in "Coloring Method" and choose "10 Cyan". Now the window should be



In VMD main window, select "Extensions"-"Visualization"-"Color Scale Bar", set the options as follows



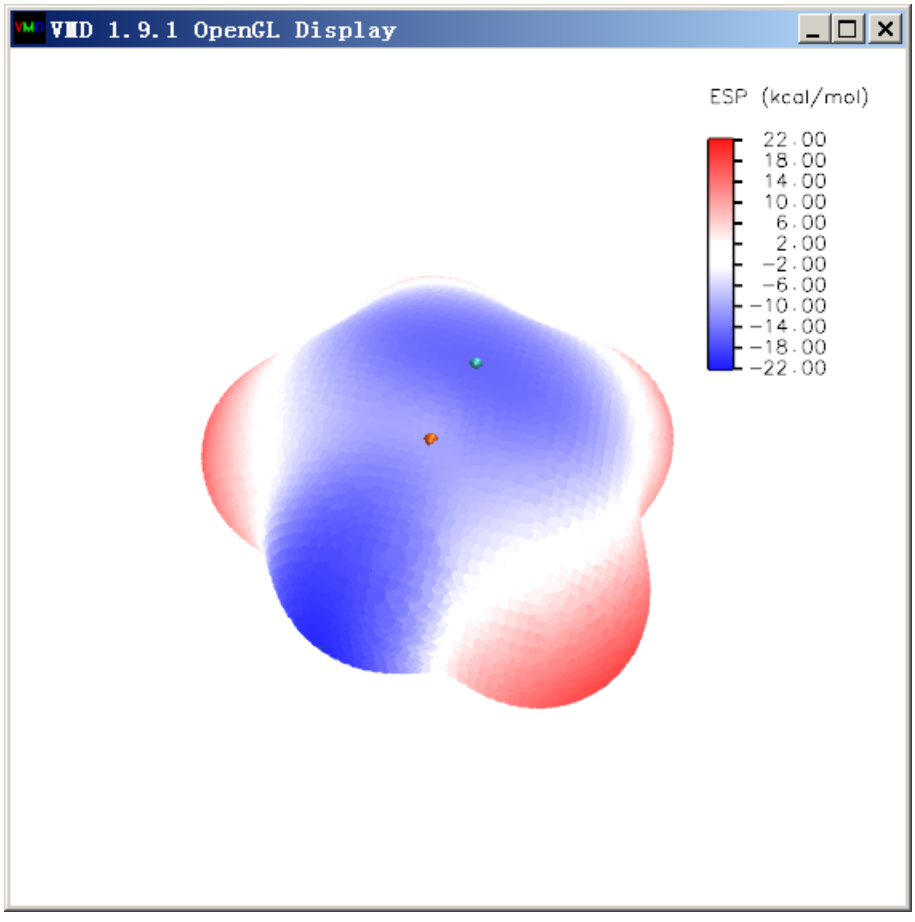
Then click "Draw Color Scale Bar", you will see the color bar appears on the graphic window, but its position needs to be adjusted.

Properly rotate and zoom the system to find a good view, then double click "F" label of ID=3 to cancel the freeze state of color bar, and double click others to make them freeze, see below

ID	T	A	D	F	Molecule
0		A	D	F	F:\furan.pdb
1		A	D	F	F:\vtx.pdb
2	T	A	D	F	F:\surfanalysis.pdb
3		A	D	F	Color Scale Bar

Choose "Mouse"-"Translate mode", drag your mouse on the VMD graphic window to move the color bar to a proper position, then double click "F" label to make it freeze again.

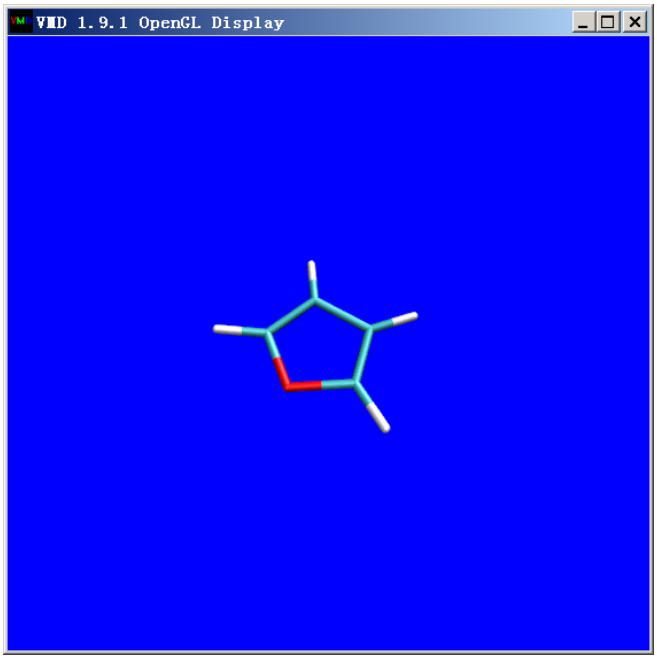
The current VMD graphical window should look like below. Blue, white and red correspond to ESP varying from -22 value to 22. Cyan and orange spheres correspond to ESP surface minima and maxima, respectively. Unfortunately, many surface extrema and molecular structure are invisible in current graph. In next section, we will use Photoshop to solve these issues.



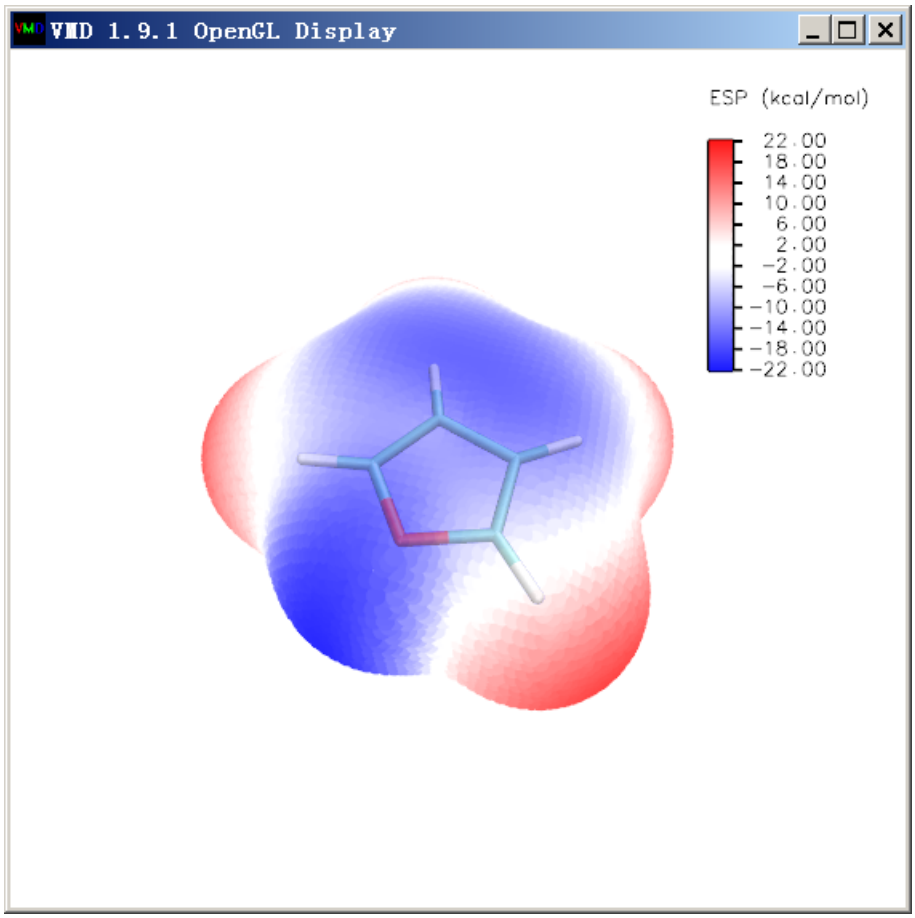
3 Use Photoshop to improve the graph

Make "D" label of ID=1 become red by double clicking it, now the surface extrema are not shown. Activate the VMD graphic window, press "ALT"+"Print screen" button to get screenshot of the window. Then boot up Photoshop, press "Ctrl"+"N" buttons to create a new image, and press "Ctrl"+"V" to paste the screenshot into it.

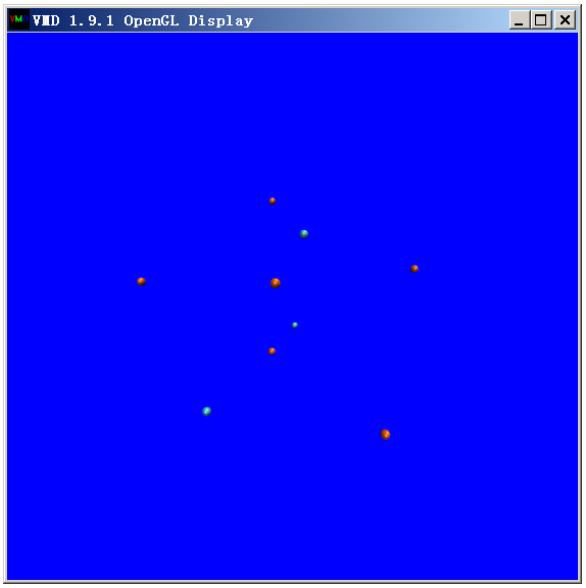
Set the background color of VMD window as blue. Then only make the molecular structure displayed by activating/deactivating "D" labels of corresponding systems. Now the VMD graphic window is



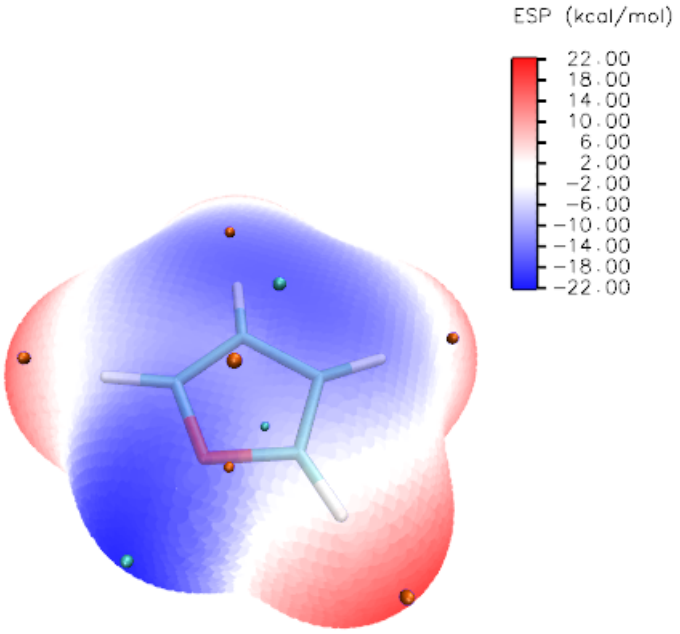
Get screenshot and paste it into the Photoshop window as a new layer. Select magic wand tool and set "Tolerance" to zero, then click the blue regions to select them, and then press "Delete" button to remove the blue background, then set the transparency of present layer to 40%, now the image in the Photoshop should be



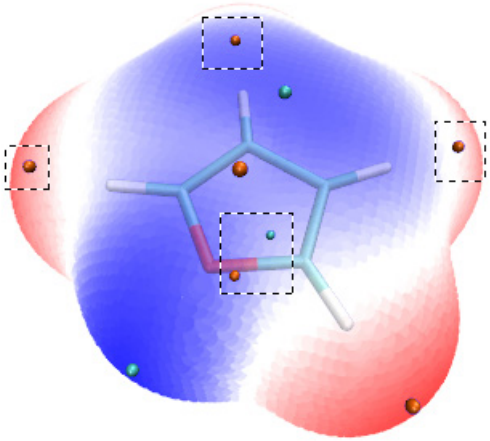
Next, only make surface extrema displayed in the VMD graphic window, i.e.



Get screenshot and paste it into the Photoshop window as a new layer and remove the blue background. Then use rectangle selection tool to select the interesting regions, and press "Ctrl"+"Q" buttons to discard other regions, new the graph in the Photoshop window should be

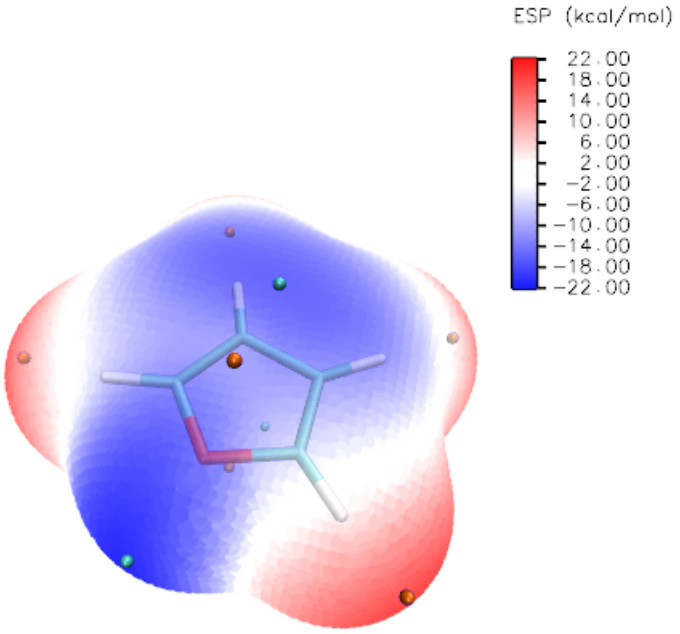


Evidently, some surface extrema in above graph are in the back of the molecule, it is better to make them displayed as transparent style. We select these extrema by holding "Shift" button and using reactangle selection tool many times, as below



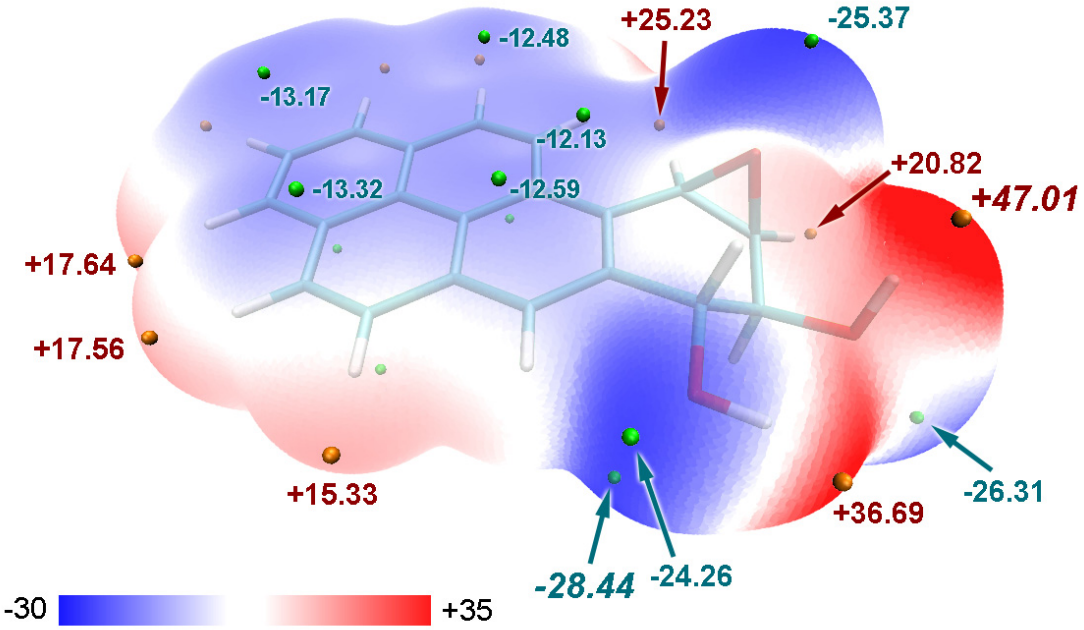
Click right mouse button on the graph and select "Layer via Cut" to transplant these extrema from current layer to a new layer. Set the transparency of the new layer to 40%.

The final graph of this tutorial is



You can then further mark the ESP value of interesting extrema on the graph. If you do not know how to obtain these values, please read Section 4.12.1 of Multiwfn manual carefully.

Below graph was created by similar manner and presented in my work *Struct. Chem.*, **25**, 1521 (2014) (DOI: 10.1007/s11224-014-0430-6).



By the way, via the same method, you can also use Multiwfn+VMD to plot color-filled molecular surface map with surface extrema for other kinds of real space functions, such as average local ionization energy, Fukui function and so on.