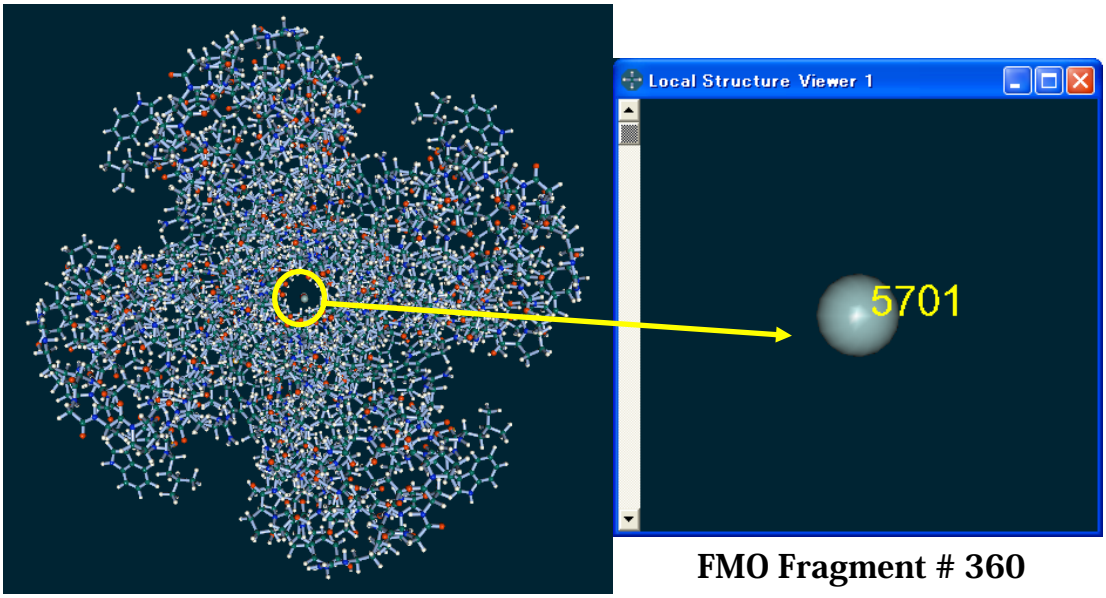
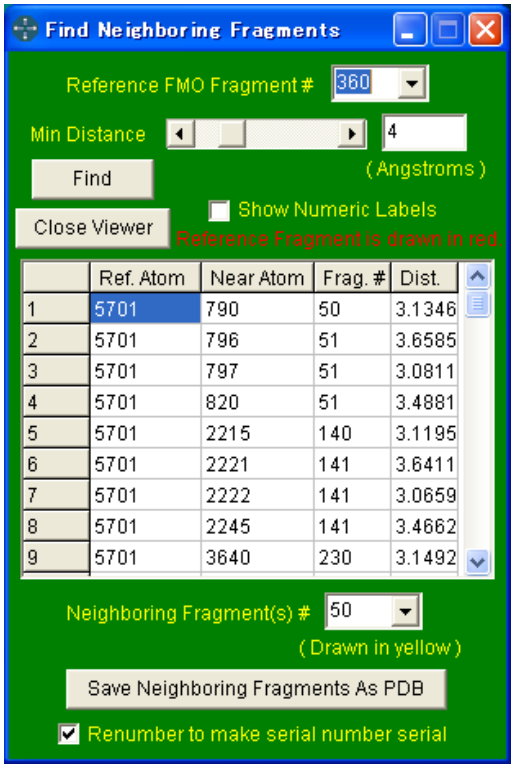
----- Ver.16.4.2 ----- March 30, 2013 Bug fixes and some modifications
----- Ver.16.4.1 ----- Aug 8, 2012 Bug fixes and some modifications
----- Ver.16.3.1 ----- Aug 4, 2012 Bug fixes and some modifications
----- Ver.16.2.1 ----- May 26, 2012 Bug fixes and some modifications
----- Ver.16.1.1 ----- March 30, 2012

(1) New function to find neighboring FMO fragments within specified distance and save them as PDB.



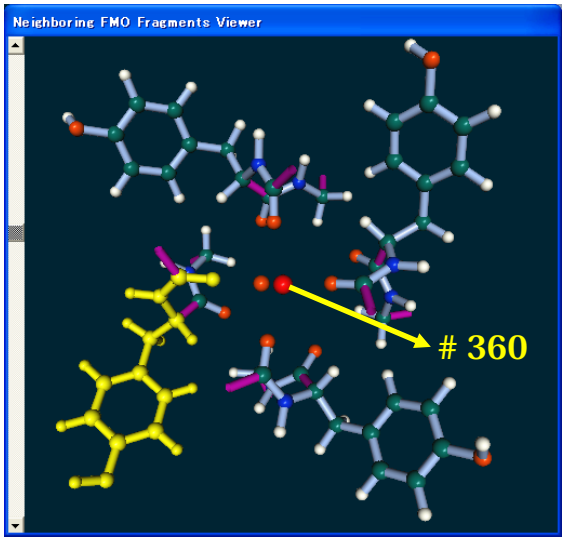
1BL8.pdb (Potassium channel)

FMO Fragment # 360
(K^+ ion)



	Ref. Atom	Near Atom	Frag. #	Dist.
1	5701	790	50	3.1346
2	5701	796	51	3.6585
3	5701	797	51	3.0811
4	5701	820	51	3.4881
5	5701	2215	140	3.1195
6	5701	2221	141	3.6411
7	5701	2222	141	3.0659
8	5701	2245	141	3.4662
9	5701	3640	230	3.1492

Finding neighboring FMO fragments within 4 Angstroms of # 360.



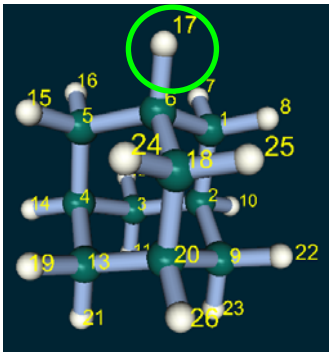
Neighboring fragments :
 # 50, 51, 140, 141, 230, 231, 320, 320, 321 and 363

Save as PDB

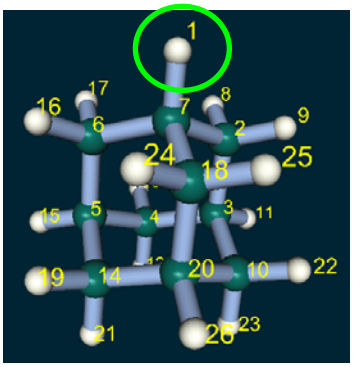
----- Ver.15.1.2 ----- January 22, 2012 Compatible with GAMESS VERSION = 11 AUG 2011 (R1)

----- Ver.15.1.1 ----- July 18, 2011

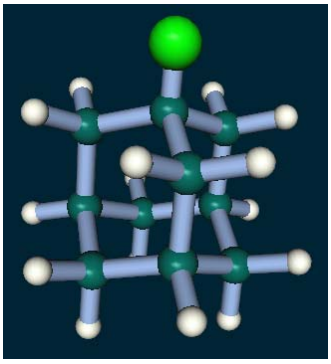
(1) User defined substituent



Example to make 1-adamantyl from adamantane



Change atom #17 to #1 with Utilities menu >> Reassign Atom Numbers.

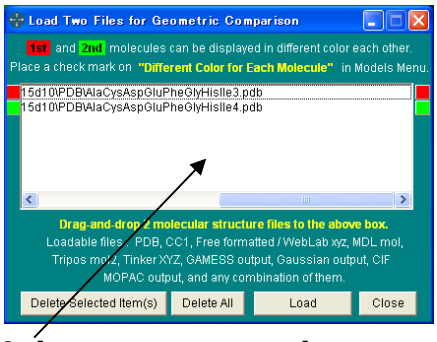


Save as User Defined Substituent from File menu

How to use : Place check mark on User Defined Substituent of "Replace H with" in Edit menu. Then click the hydrogen to be substituted. Substituent list will appear. Select substituent you want.

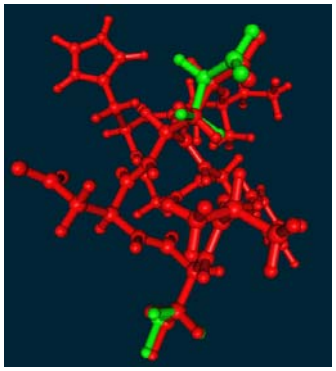
(2) RMS fit

Geometry Comparison >>
Load Two Molecules for Geometry Comparison in the Utilities menu



Drag & drop two structures to be compared.

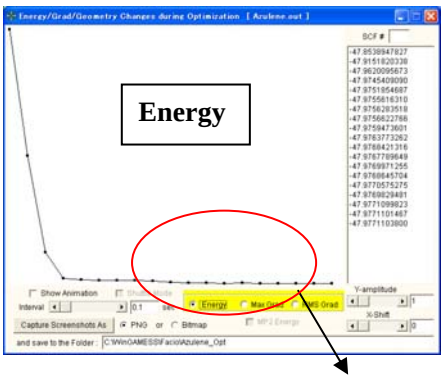
Geometry Comparison >> RMS Fit by Quaternion in the Utilities menu

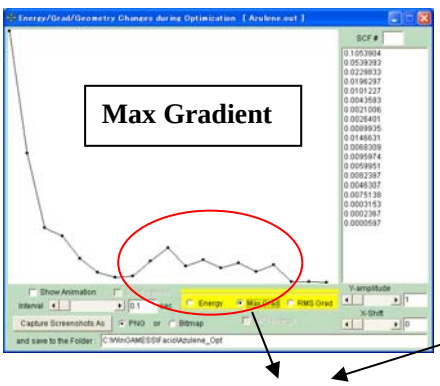


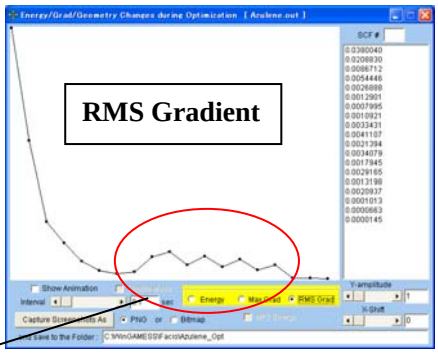
Different Colors for Two Molecules in the Models menu.

(3) Compatible with new FMO 4.0 features (gradient and optimization with PCM, and empirical dispersion correction)

(4) Max and RMS gradient changes during optimization are shown as a graph, such as below.







Energy seems to be converged...

But it's not yet.