This folder contains the following files:

1. Three text files, employed by the program, containing information on three kinds of ASA basis sets:

3-21g.txt

6-311.txt

Huzin.txt

The third is organized in a different manner as the two previous, and the program takes care of this. Also it encompasses from H up to Xe.

1. A source fortran 95 program to compute molecular QSS measures:

Bounded Molecular Selfsimilarity.f95

This program needs an additional text file:

1. Molecule.txt

Containing information on the molecule to be computed and the file is organized as follows:

a) Title (30 characteres)

b) nix: (ASA file)

**1** (3-21G) **2** (6-311G) **3** (Huzinaga) and Parrot: /=0 verbose output =0 normal output

c) Moleculesp (Number of atoms) and ltoau: (transform coordinates to au (1) or not (0))

d) For each atom: Atomic Number, Coordinates X,Y,Z

e) Nxar: /=0 reads atom populations; =0 uses atomic number

f) when Nxar/=0: atom populations in a column (same order than coordinates) otherwise nothing.