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.

2) A source fortran 95 program to compute molecular QSS measures:

   Bounded Molecular Selfsimilarity.f95

   This program needs an additional text file:

3) 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.