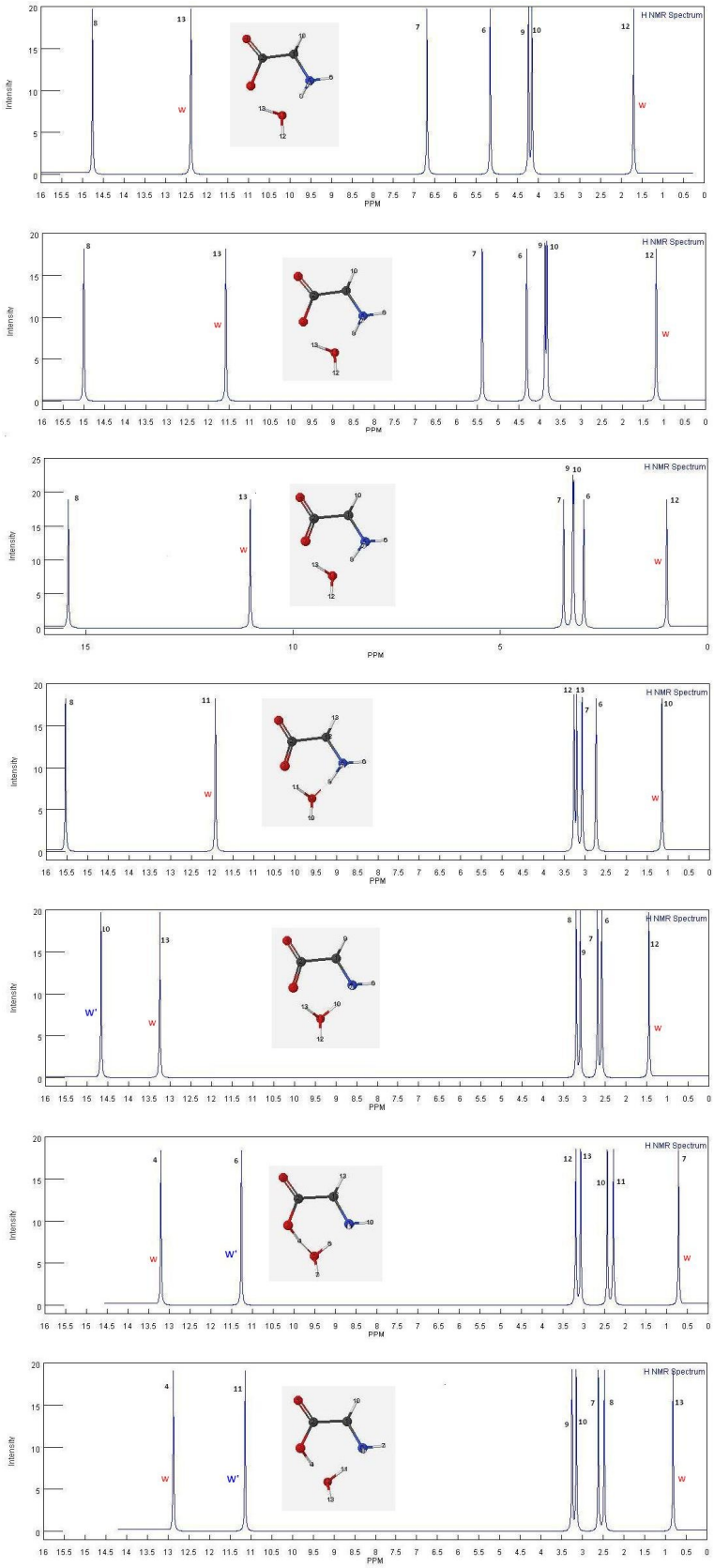


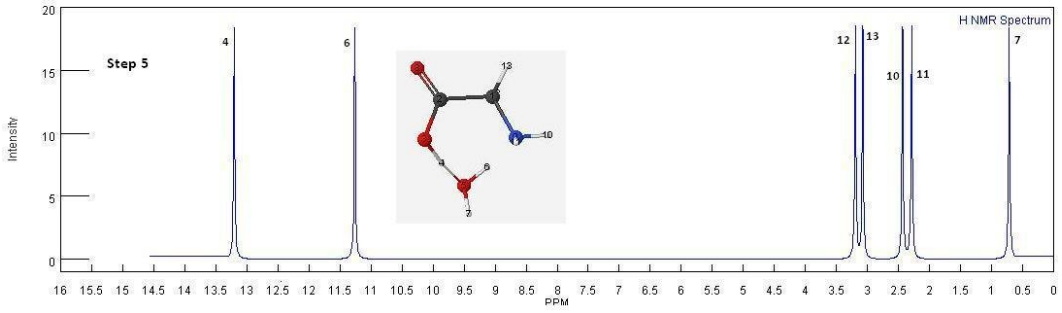
The successive iterative stages [steps ‘0’ to step’6’] during optimization; the corresponding calculated NMR Chemical shifts. ‘**W’-** marked peaks correspond to the water protons.

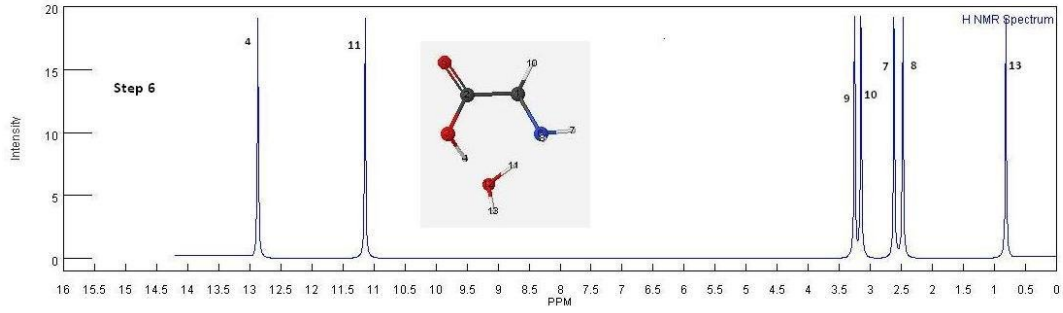
The optimization of Glycine molecule (Z.I.)and a water molecule in the neighborhood. The step ‘0’ is the input structure. Successsive six iterative steps are included in the diagram on the left.

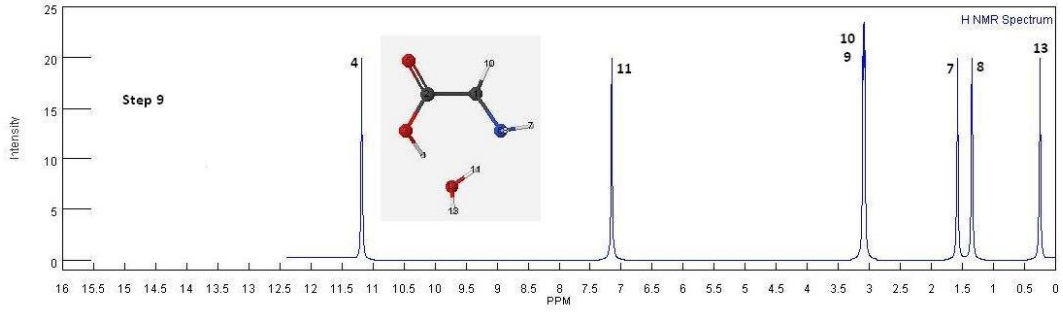
A Molecule of Glycine & a molecule of water; Possible dynamics by cluster optimization?

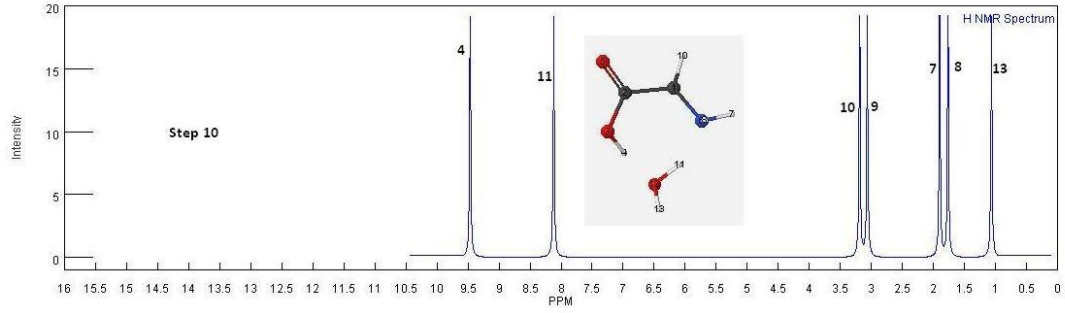
The proton-disposition around water molecule at this step seem to indicate that this could be average structure encountered during the optimization input to output. Can this correspond to the dynamic average when an equilibrium is envisaged between the input and output structure?

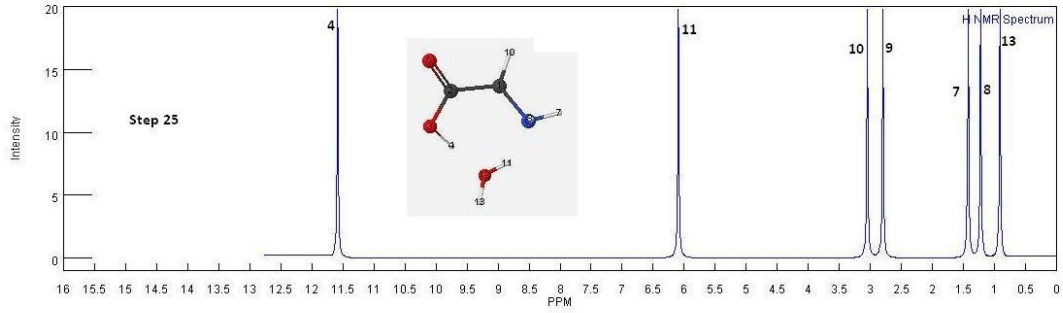
Further iteration steps are displayed in the next sheet


H NMR Spectrum
Step 5
Intensity
PPM
4
6
12
13
10
11
7


H NMR Spectrum
Step 6
Intensity
PPM
4
11
9
10
7
8
13


H NMR Spectrum
Step 9
Intensity
PPM
4
11
10
9
7
8
13


H NMR Spectrum
Step 10
Intensity
PPM
4
11
10
9
7
8
13


H NMR Spectrum
Step 25
Intensity
PPM
4
11
10
9
7
8
13