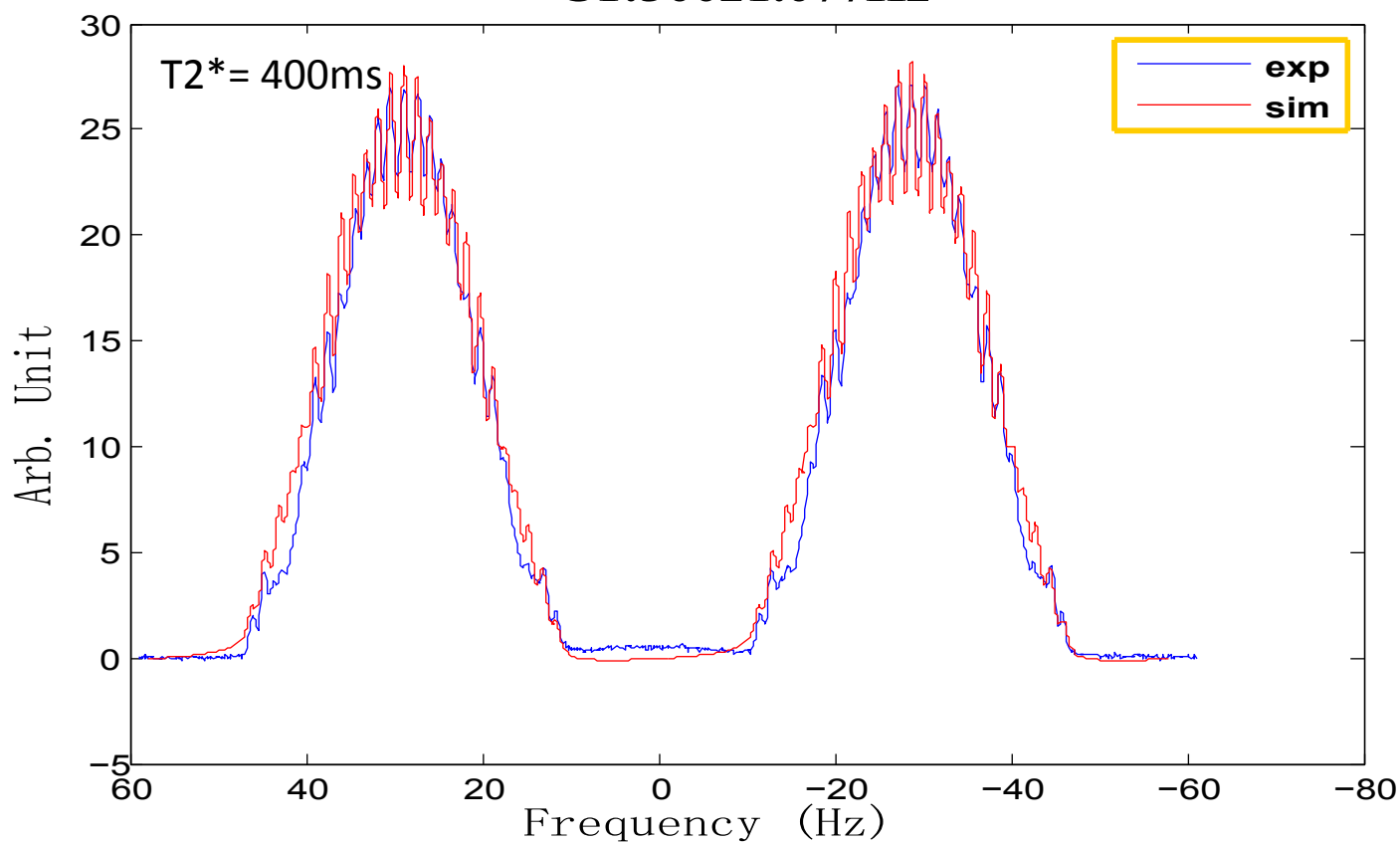


Use Gradient Algorithm to optimize the values of hetero-nuclear couplings
(takes about several minutes)

C1:30021.077Hz



J-couplings Before Optimization:

(From J_C1H1 to J_C1H5)

0, 4.41, 1.81, -13.19, 7.87

J-couplings After Optimization:

(From J_C1H1 to J_C1H5)

0, 4.067, 1.867, -10.095, 7.129

