Supporting Information

To test the dependence of the accuracy of the calculated backbone atom chemical shifts on the size of the basis sets, B3LYP calculations are performed using two different basis sets (6-31G** and a locally dense basis set of 6-311++G**/4-31G*) for $^{13}C_{\alpha}$, $^{13}C'$ and ^{15}N atoms of GB3. The results are compared with experimental values.

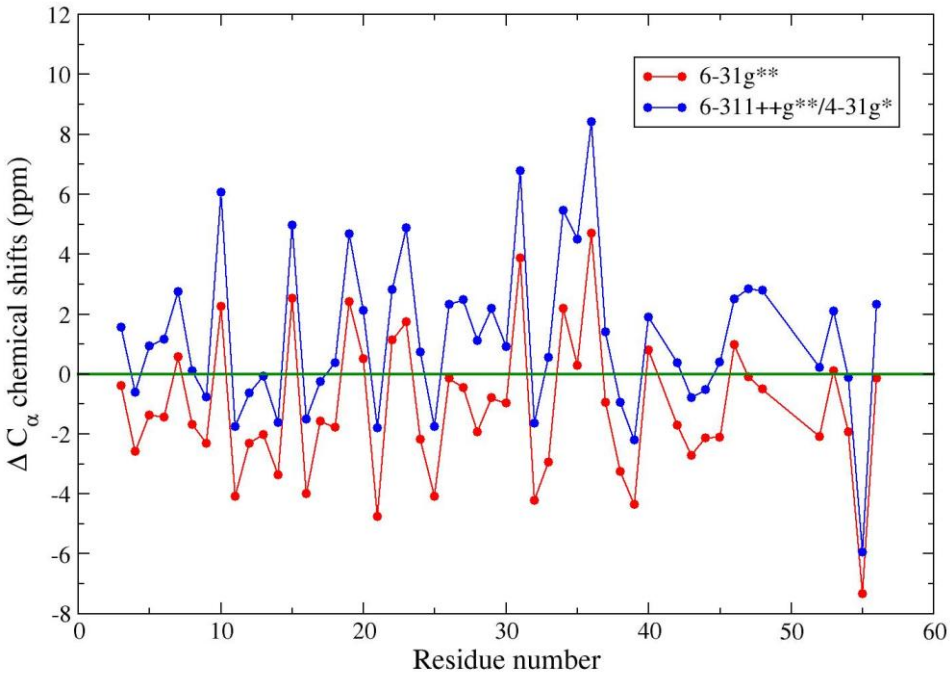

Figure S1. Difference between experimental and calculated $^{13}C_{\alpha}$ chemical shifts at the B3LYP/6-31G** and B3LYP/(6-311++G**/4-31G*) level.

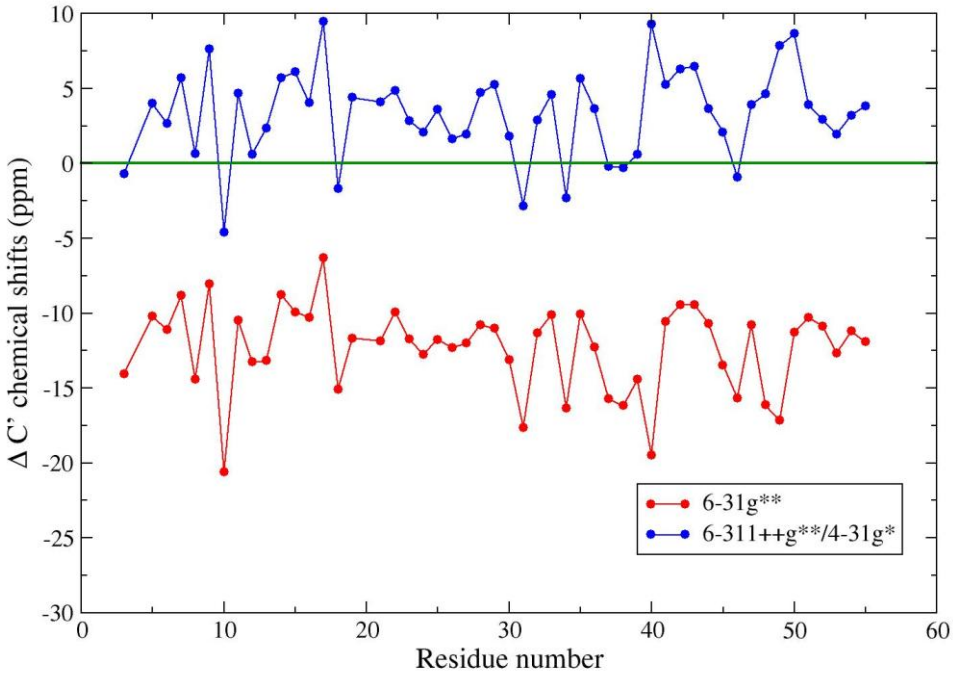

Figure S2. Difference between experimental and calculated ^{13}C'(carbonyl carbons) chemical shifts at the B3LYP/6-31G** and B3LYP/(6-311++G**/4-31G*) level.

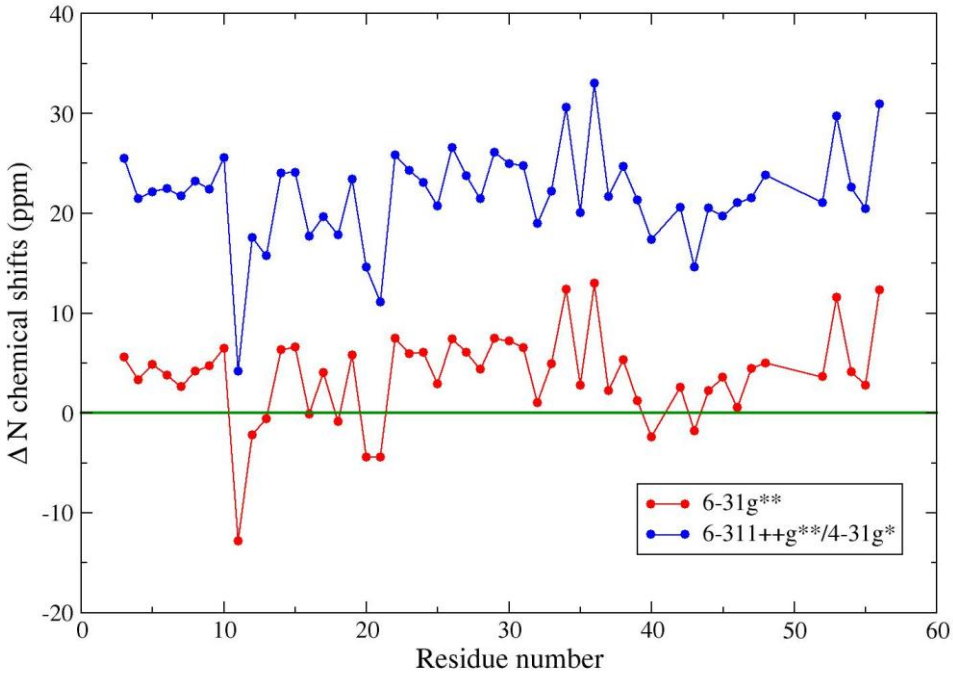

Figure S3. Difference between experimental and calculated ^{15}N chemical shifts at the B3LYP/6-31G** and B3LYP/(6-311++G**/4-31G*) level.