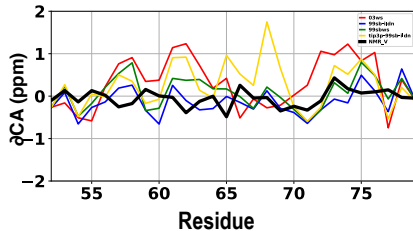


a)



RMSD

Amberff03ws : 0.73

Amber99SB-ILDN-Q TIP4P-D : 0.36ppm

Amber99sbws : 0.42ppm

Amber99SB-ILDN TIP3P : .65ppm

b)

