Electronic Supplementary Information for Dynamics of Weak Interactions in the Ligand Layer of *meta*-Mercaptobenzoic Acid Protected Gold Nanoclusters Au_{68}(*m*-MBA)$_{32}$ and Au_{144}(*m*-MBA)$_{40}$

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Multimedia files showing the animation of the clusters during the molecular dynamics simulations at different temperatures are provided (in mpg format):

(i) Au_{68}(*m*-MBA)$_{32}$ at 300 K in 'Au68_300K.mpg',

(ii) Au_{144}(*m*-MBA)$_{40}$ at 300 K in 'Au144_300K.mpg', and

(iii) Au_{68}(*m*-MBA)$_{32}$ at 500 K in 'Au68_500K.mpg'.

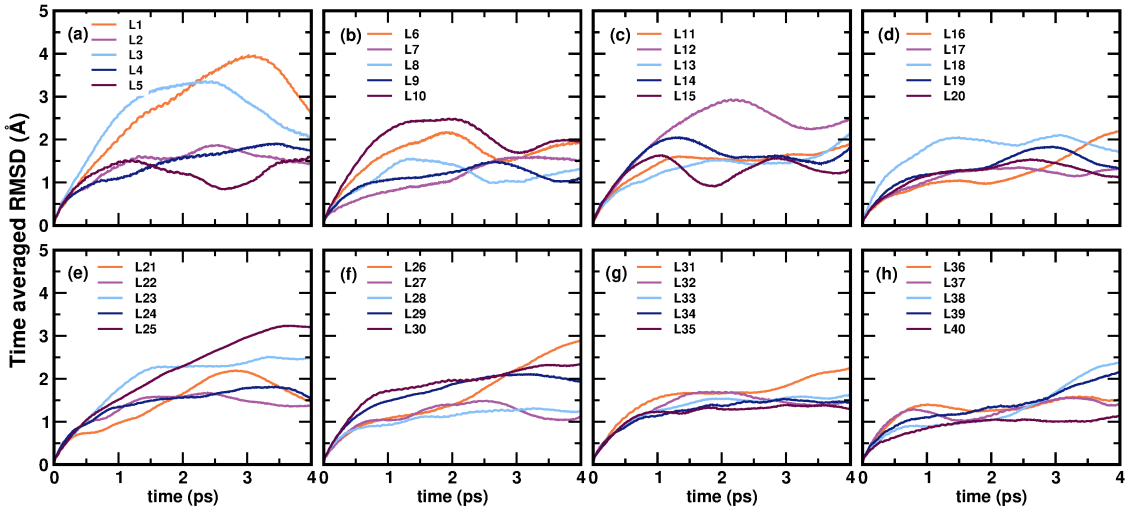


Figure S1: Time-averaged root-mean-square deviation (RMSD) of every individual ligand in the $Au_{144}(m\text{-MBA})_{40}$ cluster, after temperature equilibration, as a function of simulation time evaluated at 300 K.

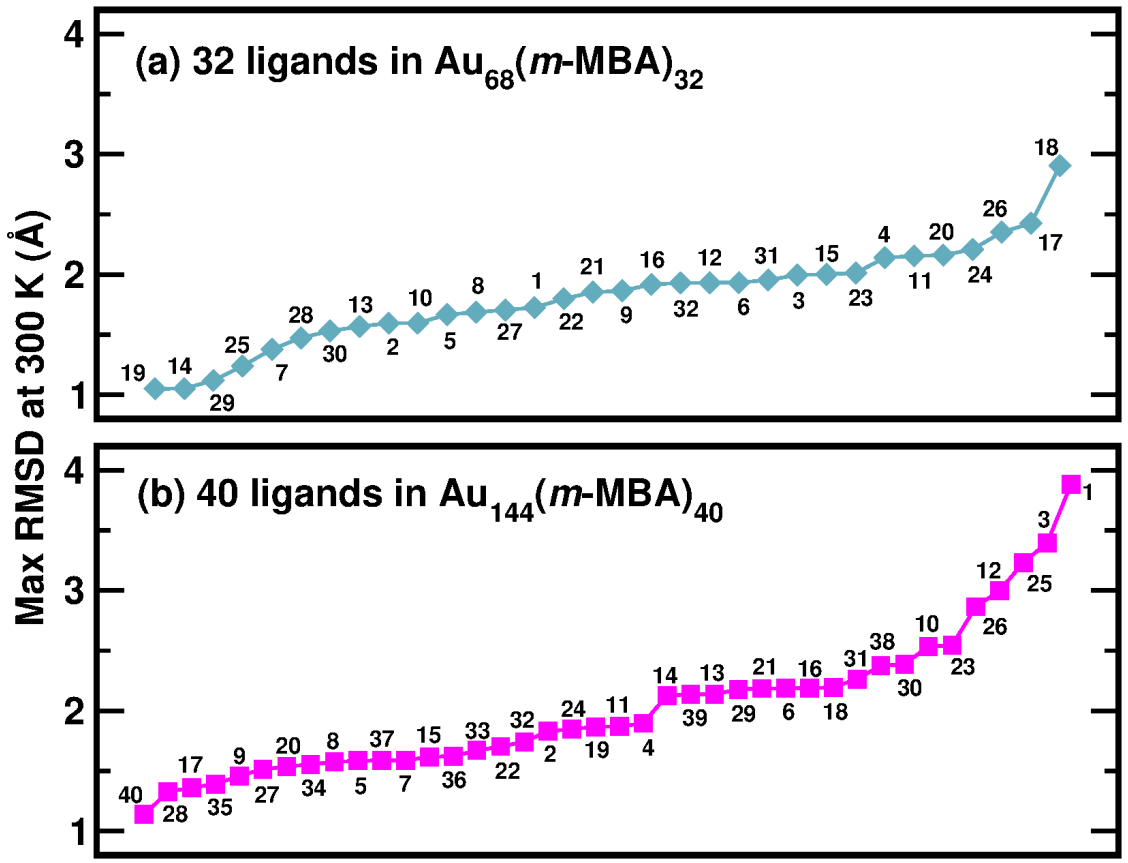
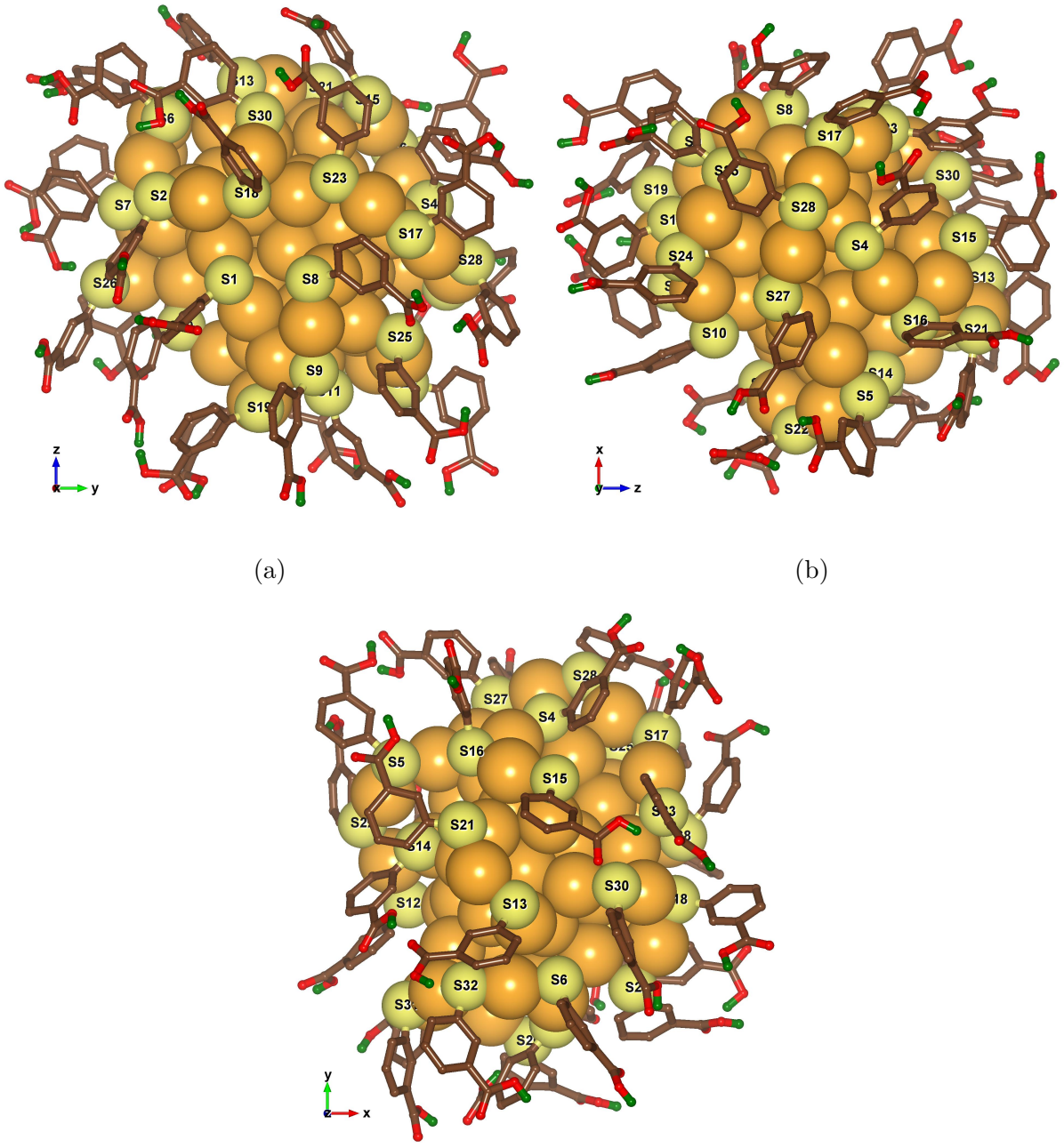


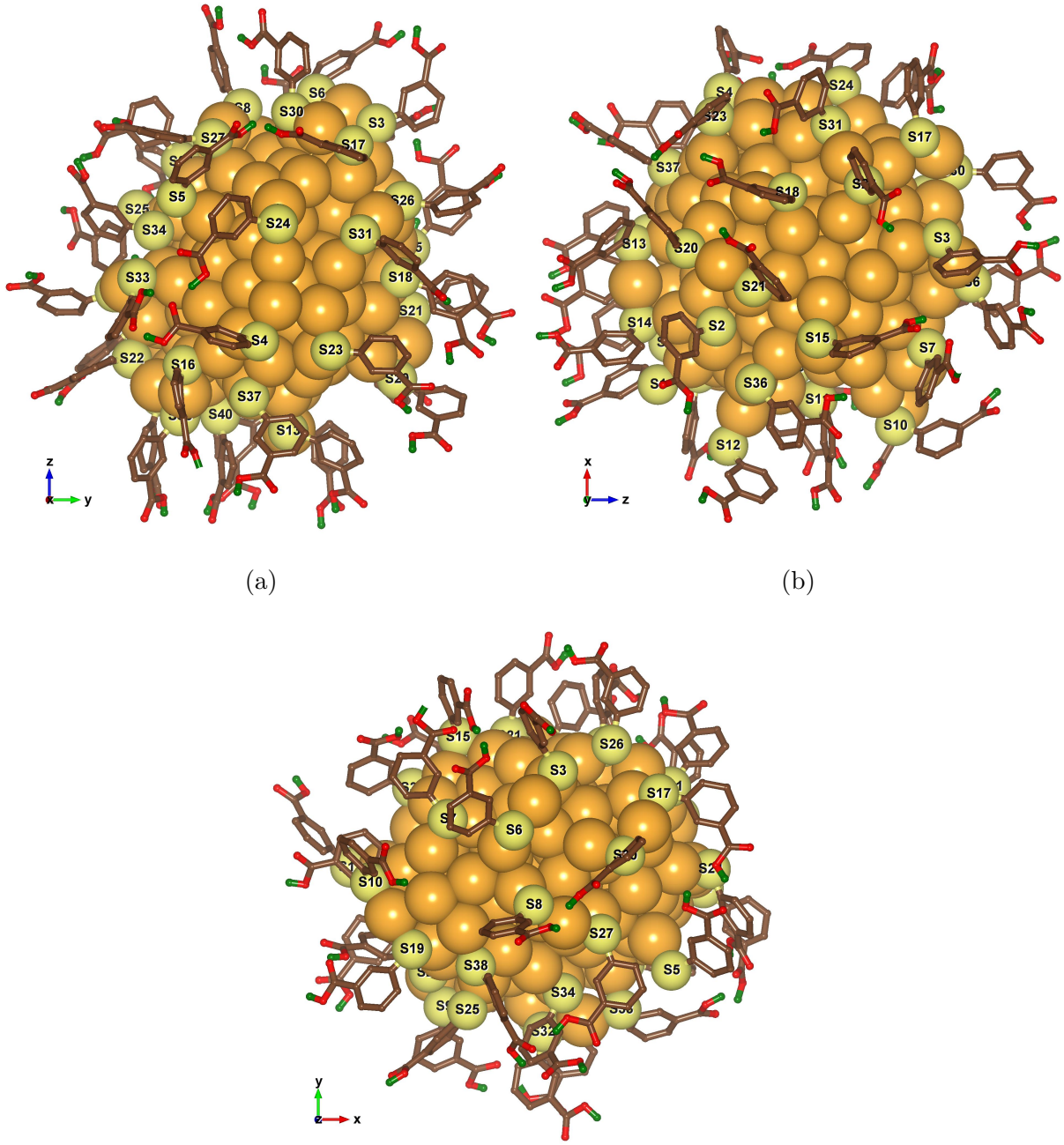
Figure S2: The maximum values of time-averaged RMSD of each ligand in the (a) 68-atom cluster and (b) 144-atom cluster, are plotted in ascending order. To see the labelled ligands in the respective clusters, see structures shown in Figs. S3 and S4.



(a) (b)

(c)

Figure S3: Structure of Au_{68}(*m*-MBA)$_{32}$ at 15 ps in three different orientations with every S atom labelled with the ligand number.



(a) (b)

(c)

Figure S4: Structure of Au_{144}(*m*-MBA)$_{40}$ at 8 ps in three different orientations with S atoms labelled with the ligand number.