7.2.5 *Structural and Functional Analysis of NCoV 19 and SARS-CoV Using Human ACE2*

NCoV 19 spike protein with ACE2 human binding receptor generated by FRODOCK and SARS-CoV with human ACE2 binding receptor (PDB id 3D0G) [15] were downloaded from the Protein Data Bank. Then, binding patterns and affinity estimations for the interaction between the viral spike and ACE2 receptor were performed using Mol Star tools for web molecular graphics [16].

7.3 Results

Through bioinformatics analysis phylogenetic studies reveal that Novel CoV belongs to a group containing SARS-CoV family. The spike glycoprotein is approximately 97% similar to bat coronavirus, 90% to pangolin coronavirus and 80% closest to SARS CoV shown in Fig. 7.1.

The 3D structures of the COVID-19 spike protein (QHD43416.1.pdb) and SARS-CoV (3D0G) interacting with the receptor binding domain (RBD) site in human ACE2 were analyzed by Frodock web based protein-protein docking tool showing (−12.7 kcal/mol) and (−10.3 kcal/mol) respectively as shown in Tables 7.1 and Fig. 7.2a, b. The interaction pattern between the viral spike proteins is quite similar in COVID-19 as well as in SARS CoV. In the case of COVID-19 total 38 amino acid

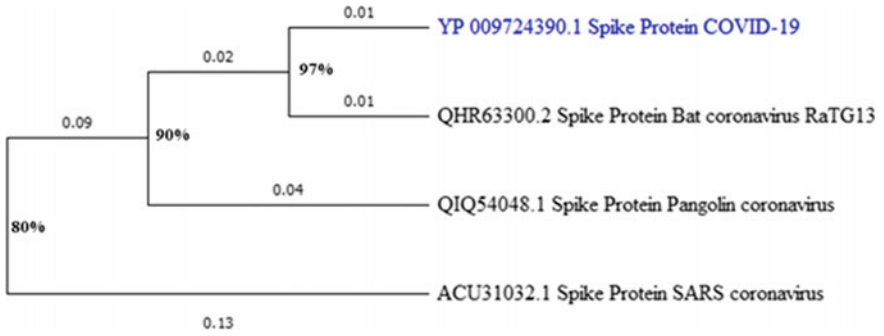

Fig. 7.1 Showing the Phylogenetic tree of Wuhan COVID-19 Spike glycoprotein sequences in context to nearest corona virus families drawn by MEGA 6.0

Table 7.1 Binding affinity (ΔG) and dissociation constant (Kd) predicted values for the interaction between viral spike and ACE2 receptor

Protein-protein complex (viral spike/ACE2)	ΔG (kcal/mol)
SARS-CoV-2	−12.7
SARS-CoV	−10.3