## Supplementary Information

## SAR-based approach to explore in silico ferrocene analogues as the potential inhibitors of major viral proteins of SARS-CoV-2 virus and human Ca<sup>2+</sup>-channel blocker

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Table S1: Grid Dimensions used in molecular docking of major viral proteins of SARS- CoV-2.											
Protein	Grid dimensions				Grid center						
	X	Y	Ζ	Spacing	X	Y	Z				
Spike protein	126	126	100	0.375	287.854	252.491	345.512				
RdRp protein	126	80	100	0.375	103.434	97.322	112.476				
M <sub>pro</sub> protein	126	126	126	0.375	11.554	-0.133	5.627				
N protein	126	126	126	0.675	12.76	-12.033	-24.877				
Ca channel protein	80	84	126	0.375	176.642	168.446	188.42				



Fig. S1 - The best dock pose exhibiting non-covalent interactions between ferroquine and the  $M_{pro}$  protein of SARS-CoV-2. (b) Schematic representation of showing the all the non-covalent interactions with GLN127, LYS5, ASP289, GLN288 residues.



(b)

(a)

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Fig. S9 - The best dock pose exhibiting non-covalent interactions between compound 1 and the N protein of SARS-CoV-2. (b) Schematic representation of showing the all the non-covalent interactions with GLN164, LYS170, GLN164, LEU160, LEU162, LEU168 and PRO163 residues.



Fig. S10 - The best dock pose exhibiting non-covalent interactions between compound 2 and the spike protein of SARS-CoV-2. (b) Schematic representation of showing the all the non-covalent interactions with ASP405, ALA386, GLY354, ARG393, TYR505, ILE548, PRO620 and ALA386 residues.



Fig. S11 - The best dock pose exhibiting non-covalent interactions between compound 2 and the RdRp protein of SARS-CoV-2. (b) Schematic representation of showing the all the non-covalent interactions with LYS545, ASP623, ARG553 and ARG555 residues.



Fig. S12 - The best dock pose exhibiting non-covalent interactions between compound 2 and the N protein of SARS-CoV-2. (b) Schematic representation of showing the all the non-covalent interactions with LEU162, THR166, GLU137 and GLN161 residues.



Fig. S13 - The best dock pose exhibiting non-covalent interactions between compound 3 and the RdRp protein of SARS-CoV-2. (b) Schematic representation of showing the all the non-covalent interactions with THR801, GLU802, HIS810 and TRP800 residues.



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(a)

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Fig. S17 - The best dock pose exhibiting non-covalent interactions between compound 4 and the RdRp protein of SARS-CoV-2. (b) Schematic representation of showing the all the noncovalent interactions with LEU473, SER4, PHE440, PHE843, CYS8, LYS438, LYS7, LEU437 and SER1 residues.

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Fig. S18 - The best dock pose exhibiting non-covalent interactions between compound 4 and the  $M_{pro}$  protein of SARS-CoV-2. (b) Schematic representation of showing the all the non-covalent interactions with LYS173, GLN71 and LEU5 residues.



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