Indian Journal of Biochemistry & Biophysics
Vol. 61, July 2024, pp. 443-446
DOI: 10.56042/ijbb.v61i7.953

In silico study of 4-amino substituted-7-chloroquinoline derivatives as *Plasmodium falciparum* lactate dehydrogenase inhibitors

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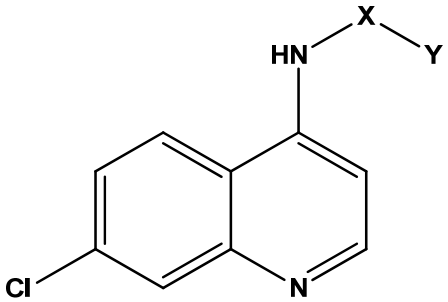
Received 28 April 2023; revised 25 April 2024

Supplementary Data

Table 1 — Amino acids residues interacting with 4-amino substituted-7-chloroquinoline

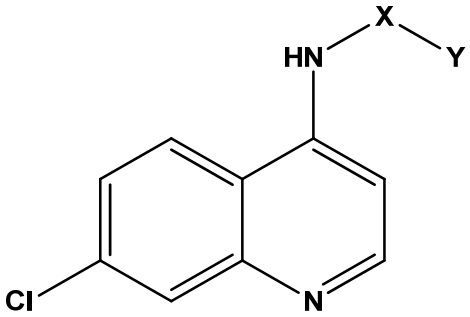


Compounds 1-25

Comp. No	X	Y	Amino acids residues interacting with 4-amino substituted-7-chloroquinoline
1	$-CH_2-CO-$	Phenyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Ile119 Glu122 Ile123
2	$-(CH_2)_2-CO-$	Phenyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Pro114 Ile119 Glu122 Ile123
3	$-(CH_2)_3-CO-$	Phenyl	Val26 Gly27 Ser28 Phe52 Asp53 Ile54 Lys56 Tyr85 Ala98 Gly99Ile119 Glu122 Ile123
4	$-(CH_2)_4-CO-$	Phenyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Ile119 Glu122 Ile123 His126
5	$-(CH_2)_5-CO-$	Phenyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Lys 118 Ile119 Glu122 Ile123
6	$-(CH_2)_6-CO-$	Phenyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Pro114 Leu115Asn117 Lys118 Ile119 Glu122 Ile123
7	$-CH_2-CO-$	2-Furyl	Gly27 Ser28 Gly29 Met30 Ile31 Gly32 Asp53 Thr97 Ala98 Gly99 Thr101 Val138 Thr139 Asn140 Ser245 Pro246 Tyr247
8	$-(CH_2)_2-CO-$	2-Furyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Lys118Ile119 Glu122 Ile123
9	$-(CH_2)_3-CO-$	2-Furyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Lys118Ile119 Glu122 Ile123
10	$-(CH_2)_4-CO-$	2-Furyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Lys118Ile119 Glu122 Ile123
11	$-(CH_2)_5-CO-$	2-Furyl	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Lys118Ile119 Glu122 Ile123
12	$-(CH_2)_6-CO-$	2-Furyl	Val26 Gly27 Ser28 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Pro114 Leu115Asn117 Lys118 Ile119 Glu122 Ile123

(*Contd.*)

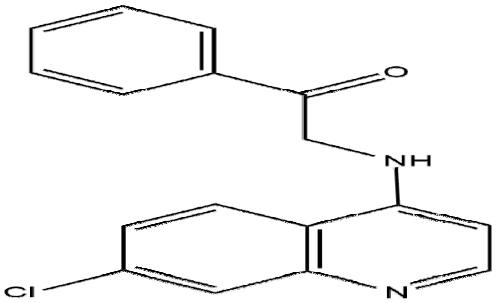
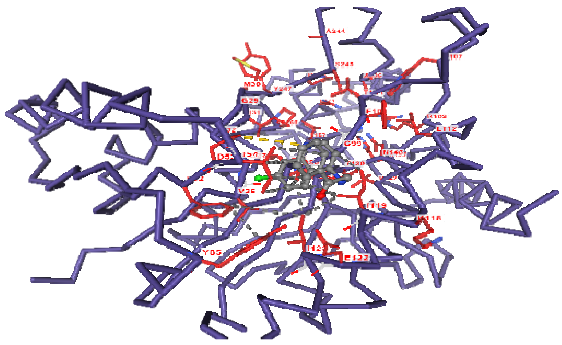
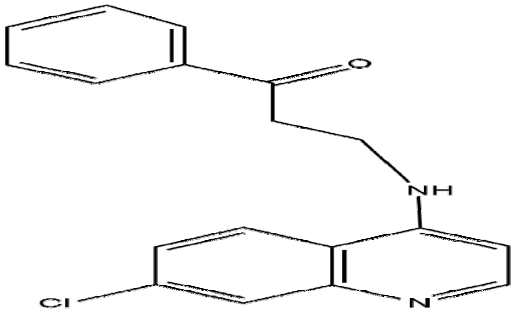
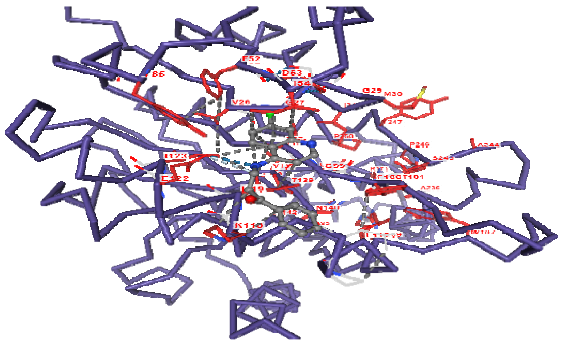
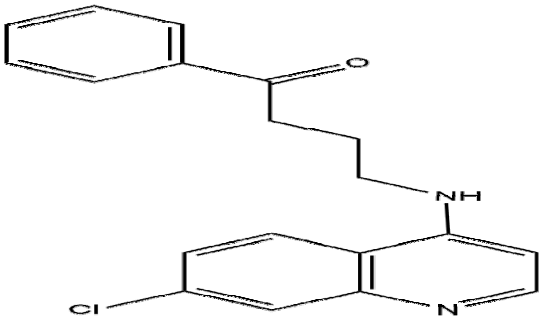
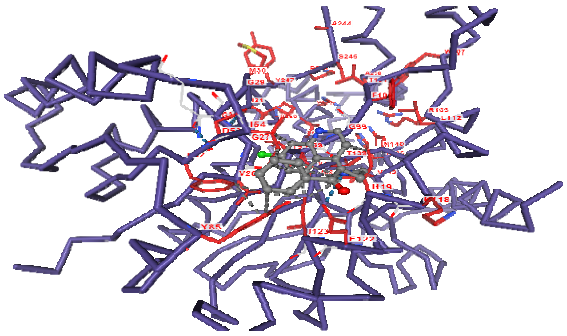
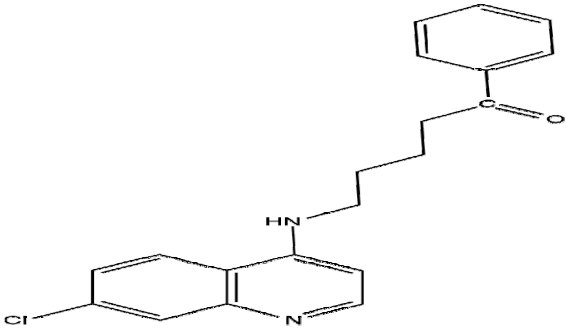
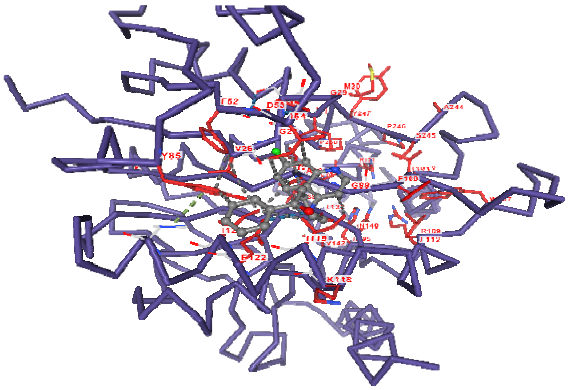
Table 1 — Amino acids residues interacting with 4-amino substituted-7-chloroquinoline (*Contd.*)



Compounds 1-25

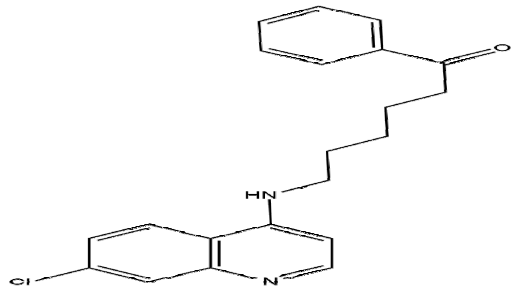
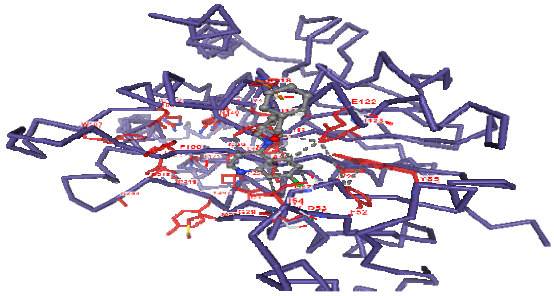
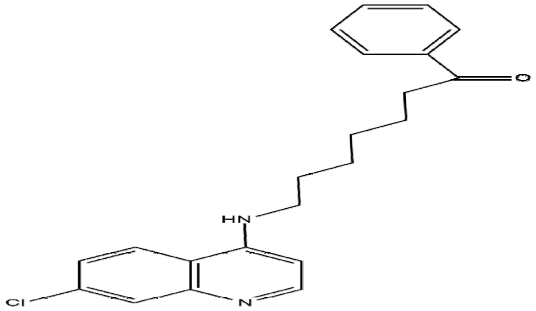
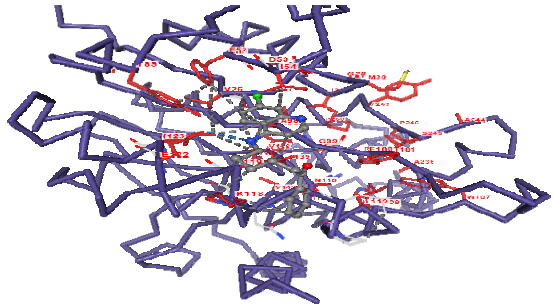
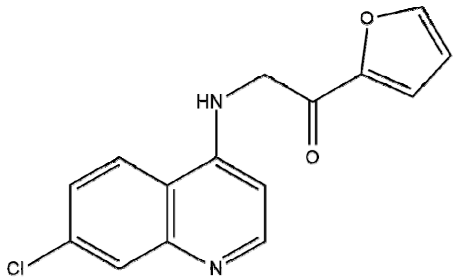
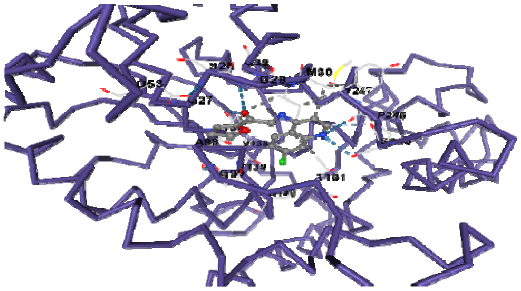
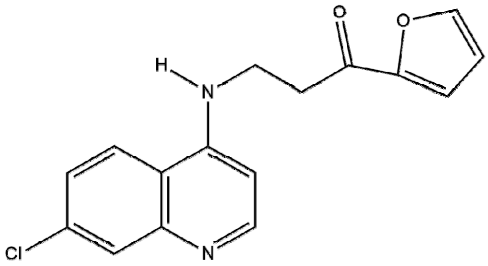
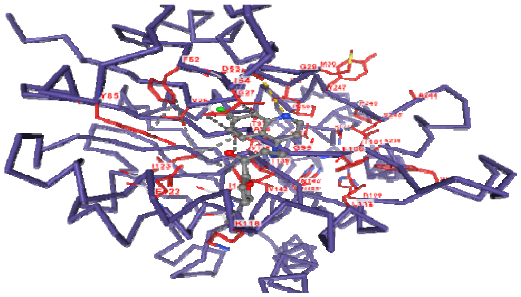
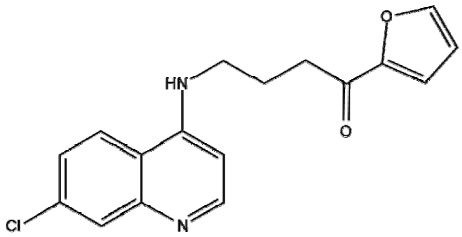
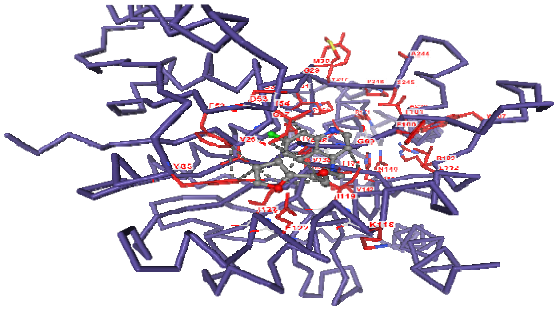
Comp. No	X	Y	Amino acids residues interacting with 4-amino substituted-7-chloroquinoline
13	$-CH_2-CO-$	2-Thiophene	Val26 Gly27 Ser28 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Thr101 Pro114 Leu115Asn117 Lys118 Ile119 Glu122 Ile123
14	$-(CH_2)_2-CO-$	2-Thiophene	Val26 Gly27 Ser28 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Leu115Asn117 Lys118 Ile119 Glu122 Ile123
15	$-(CH_2)_3-CO-$	2-Thiophene	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Leu115Asn117 Lys118 Ile119 Glu122 Ile123
16	$-(CH_2)_4-CO-$	2-Thiophene	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Leu115Asn117 Lys118 Ile119 Glu122 Ile123
17	$-(CH_2)_5-CO-$	2-Thiophene	Val26 Gly27 Ser28 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Leu115Asn117 Lys118 Ile119 Glu122 Ile123
18	$-(CH_2)_6-CO-$	2-Thiophene	Val26 Gly27 Ser28 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Leu115Asn117 Lys118 Ile119 Glu122 Ile123
19	$-CH_2-CO-$	2-Azole	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Leu115Lys118 Ile119 Glu122 Ile123
20	$-(CH_2)_2-CO-$	2-Azole	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Ile119 Glu122Ile123
21	$-(CH_2)_3-CO-$	2-Azole	Val26 Gly27 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Leu115Lys118 Ile119 Glu122 Ile123
22	$-(CH_2)_4-CO-$	2-Azole	Val26 Gly27Ser28 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Leu115Lys118 Ile119 Glu122 Ile123
23	$-(CH_2)_5-CO-$	2-Azole	Val26 Gly27 Ser28Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Leu115Lys118 Ile119 Glu122 Ile123
24	$-(CH_2)_6-CO-$	2-Azole	Val26 Gly27 Ser28Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Leu115Lys118 Ile119 Glu122 Ile123
25	$-(CH)-CH_3-$	3-NH_2Phenyl	Val26 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Ile119 Glu122Ile123
26	Chloroquine		Val26 Phe52 Asp53 Ile54 Tyr85 Ala98 Gly99 Phe100 Ile119 Glu122Ile123

Table 2 — Docking images of designed 4-aminosubstituted-7-chloroquinoline derivatives

Sr. No.	Structure	Docking images
1		
2		
3		
4		

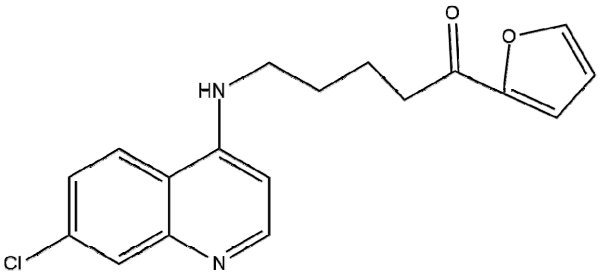
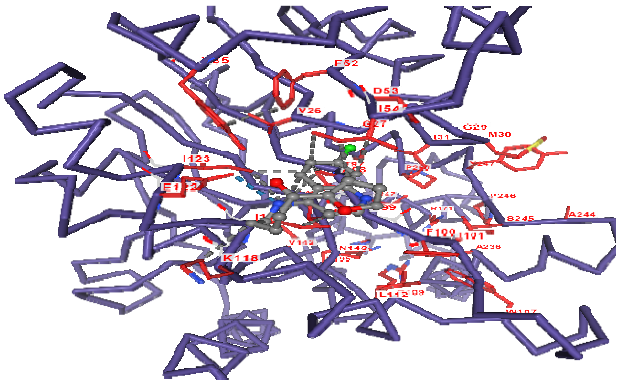
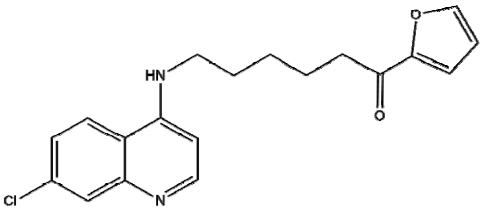
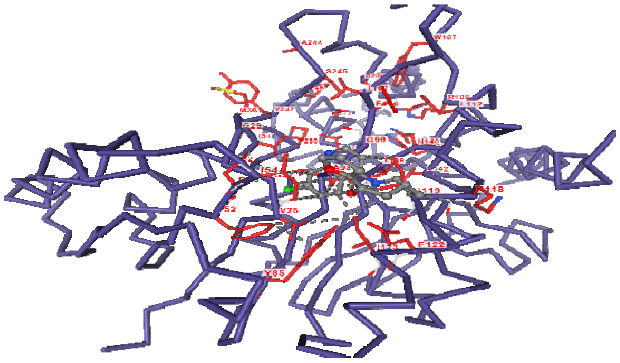
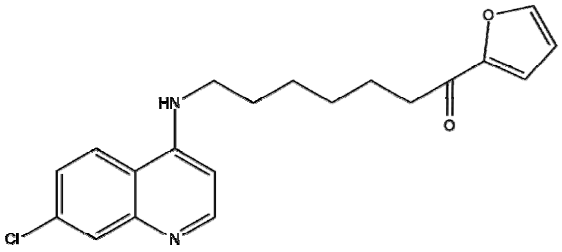
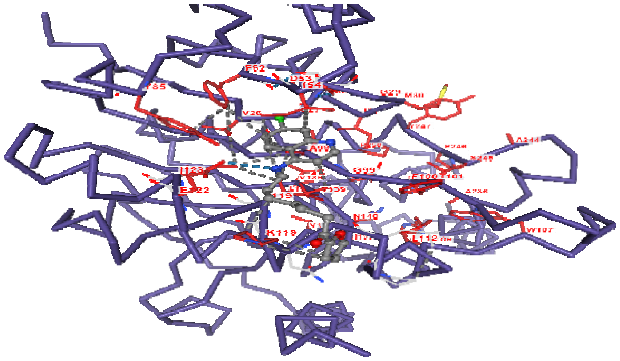
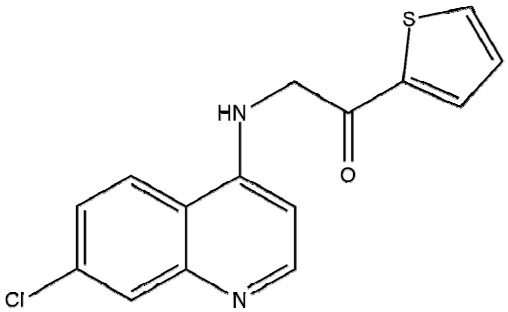
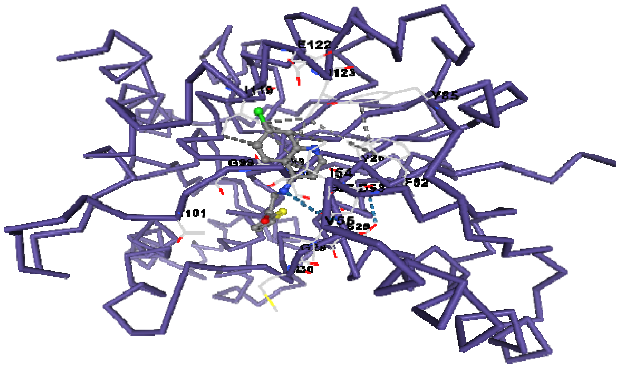
(*Contd.*)

Table 2 — Docking images of designed 4-aminosubstituted-7-chloroquinoline derivatives (*Contd.*)

Sr. No.	Structure	Docking images
5		
6		
7		
8		
9		

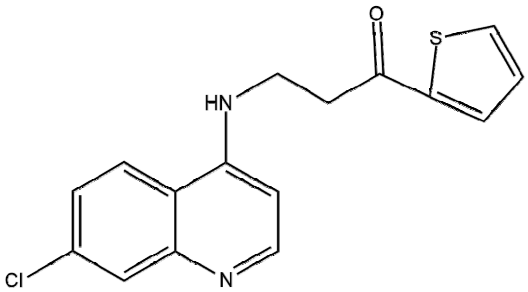
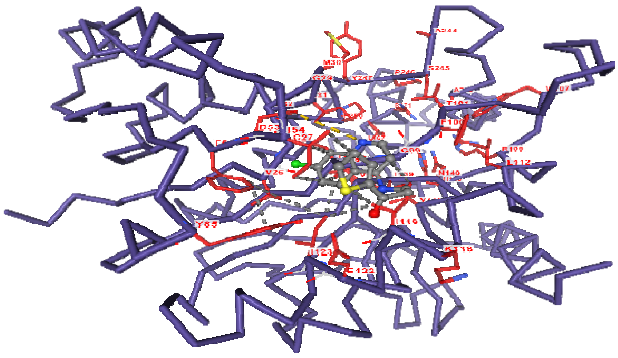
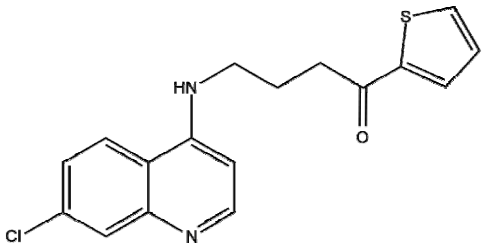
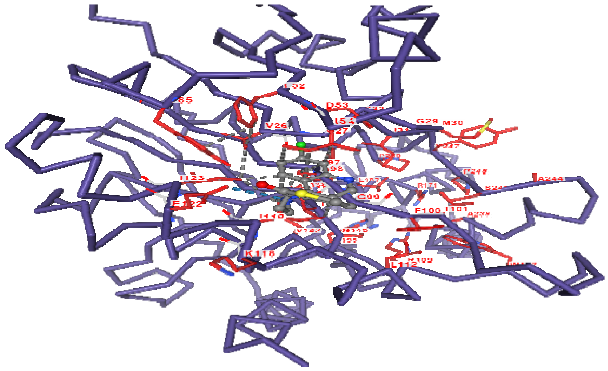
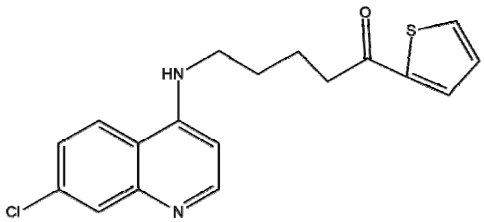
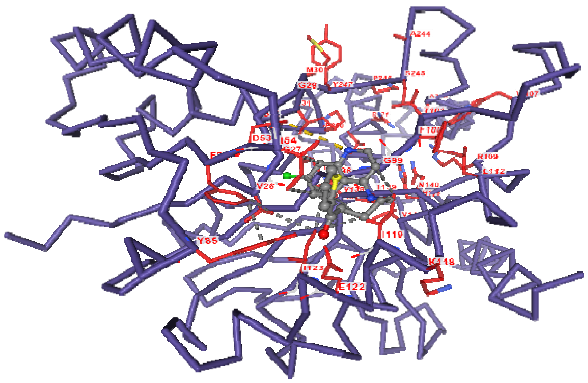
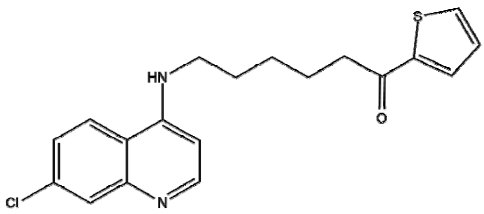
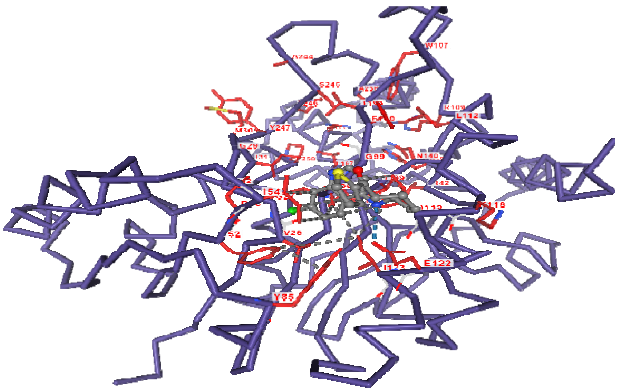
(*Contd.*)

Table 2 — Docking images of designed 4-aminosubstituted-7-chloroquinoline derivatives (*Contd.*)

Sr. No.	Structure	Docking images
10		
11		
12		
13		

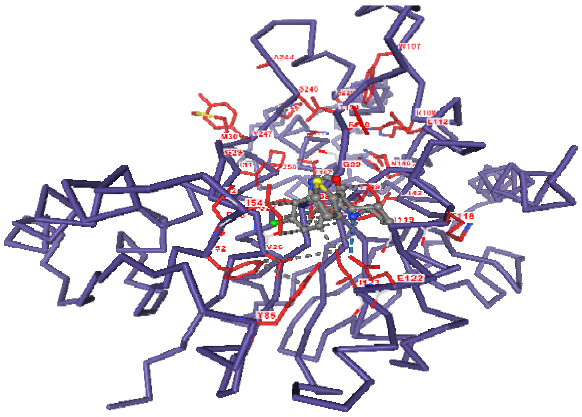
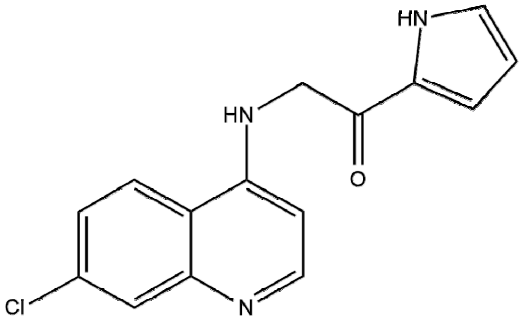
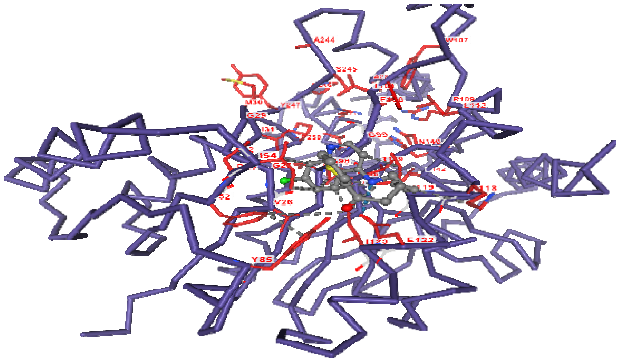
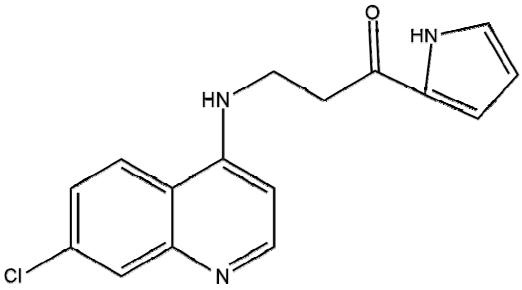
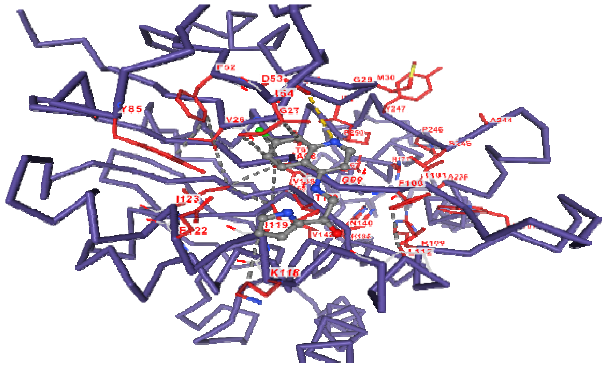
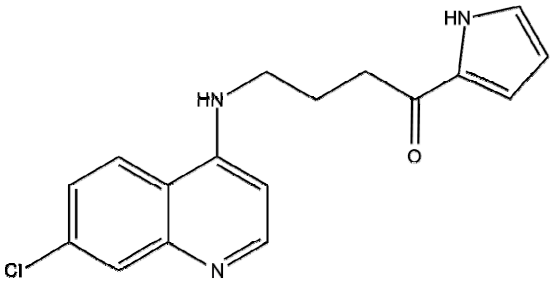
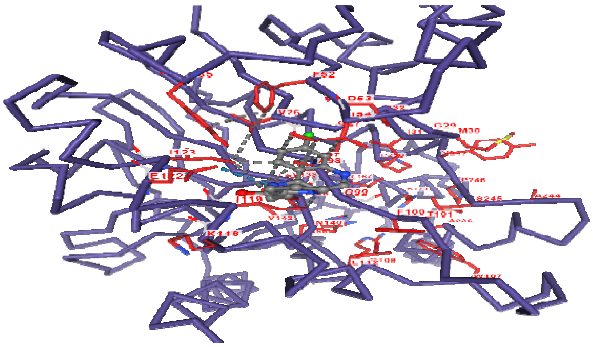
(*Contd.*)

Table 2 — Docking images of designed 4-aminosubstituted-7-chloroquinoline derivatives (*Contd.*)

Sr. No.	Structure	Docking images
14		
15		
16		
17		

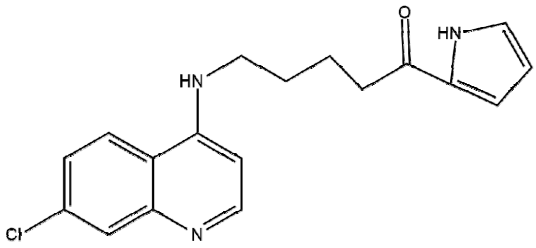
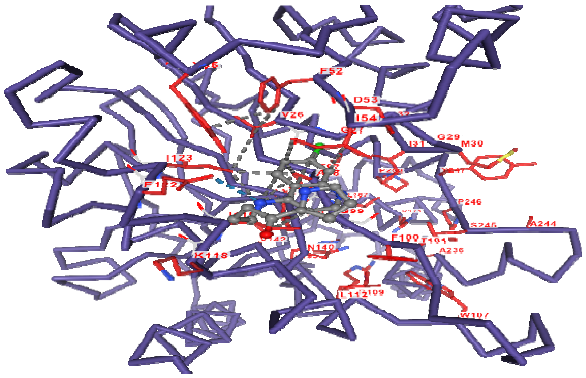
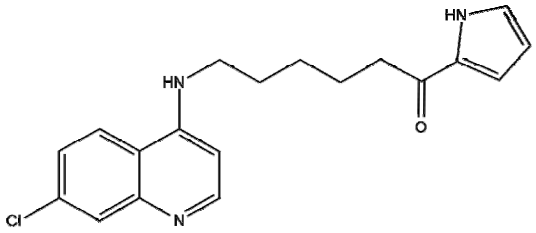
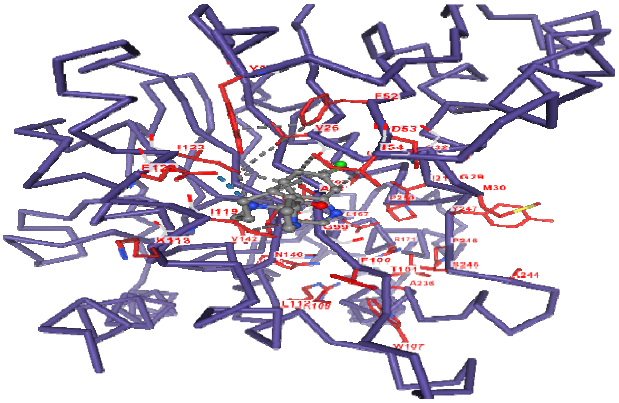
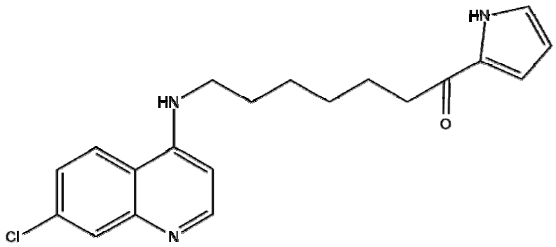
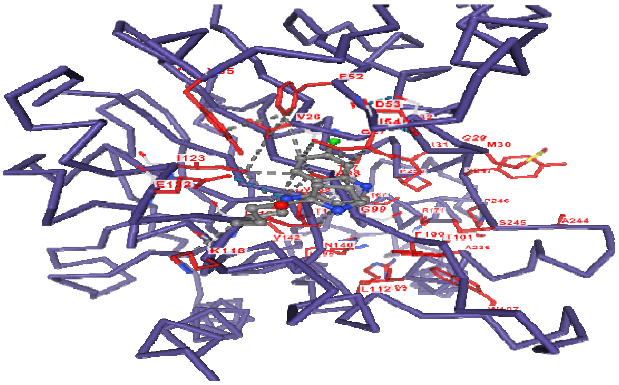
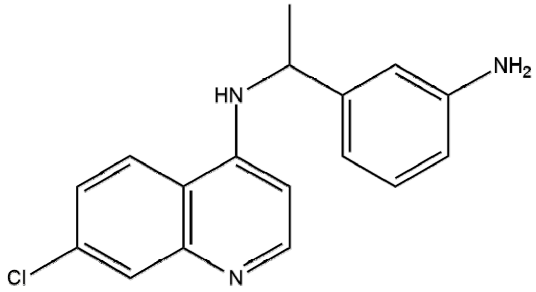
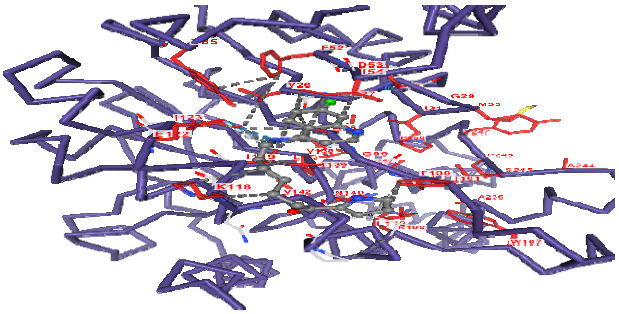
(*Contd.*)

Table 2 — Docking images of designed 4-aminosubstituted-7-chloroquinoline derivatives (*Contd.*)

Sr. No.	Structure	Docking images
18		
19		
20		
21		

(*Contd.*)

Table 2 — Docking images of designed 4-aminosubstituted-7-chloroquinoline derivatives (*Contd.*)

Sr. No.	Structure	Docking images
22		
23		
24		
25		

(*Contd.*)

Table 2 — Docking images of designed 4-aminosubstituted-7-chloroquinoline derivatives (*Contd*.)

Sr. No.	Structure	Docking images
26	Chloroquine