

Blind docking of 4-Amino-7-Chloroquinoline analogs as potential dengue virus protease inhibitor using CB Dock a web server

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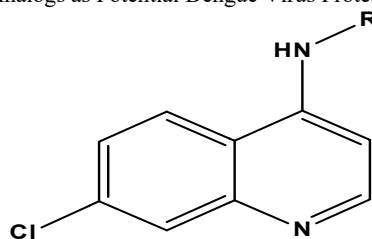
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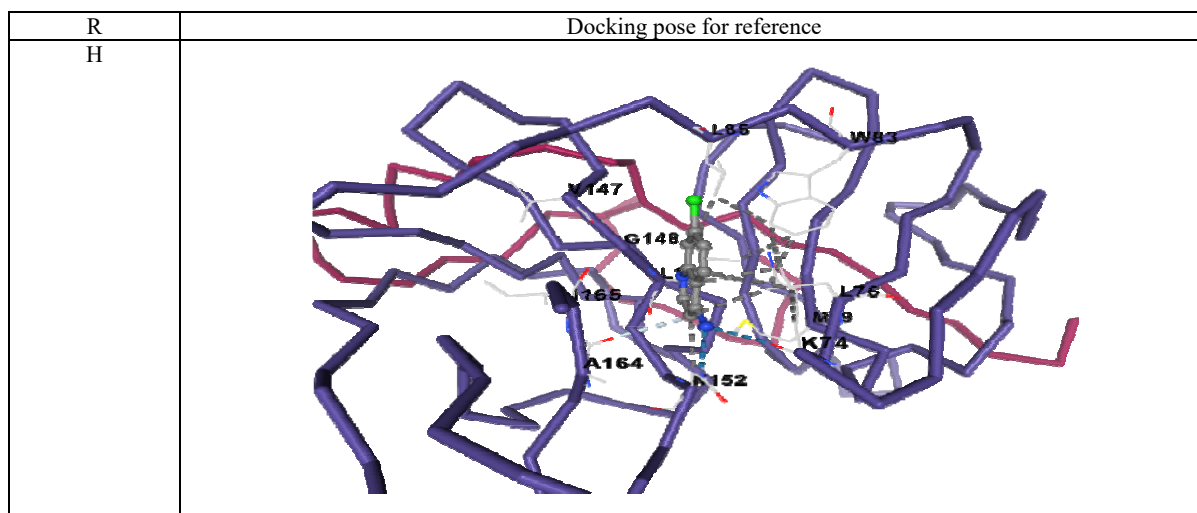
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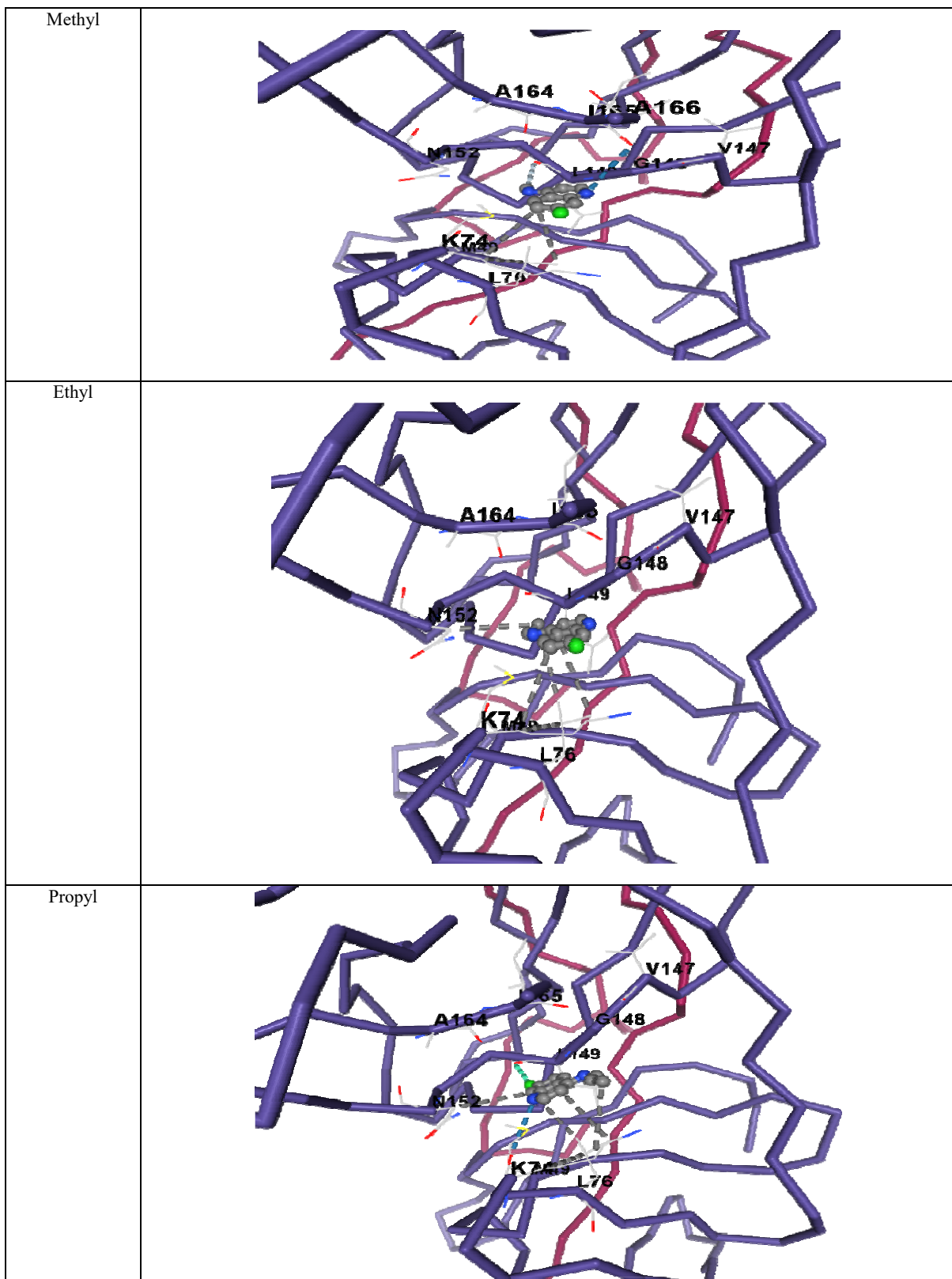
Supplementary data

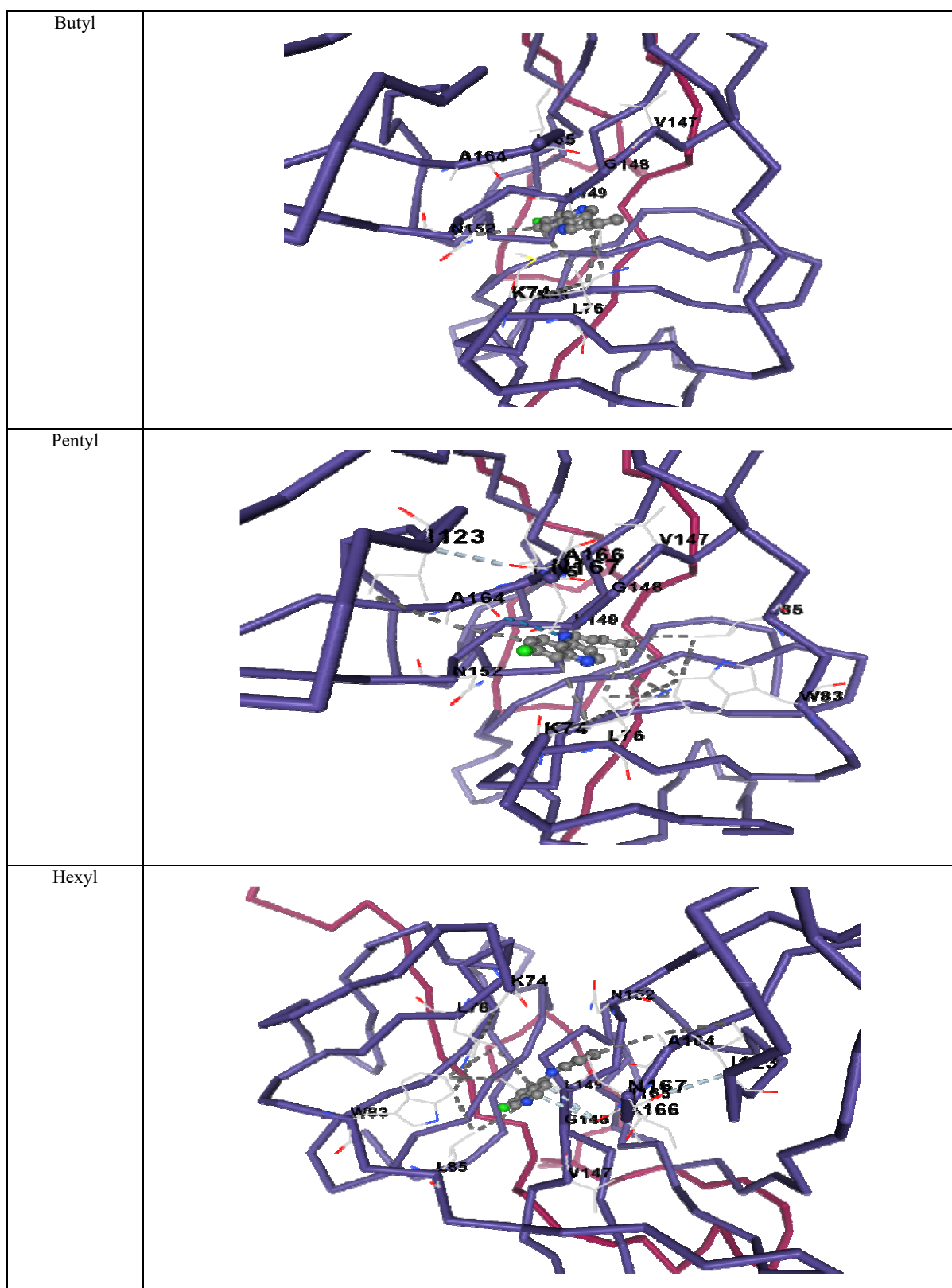
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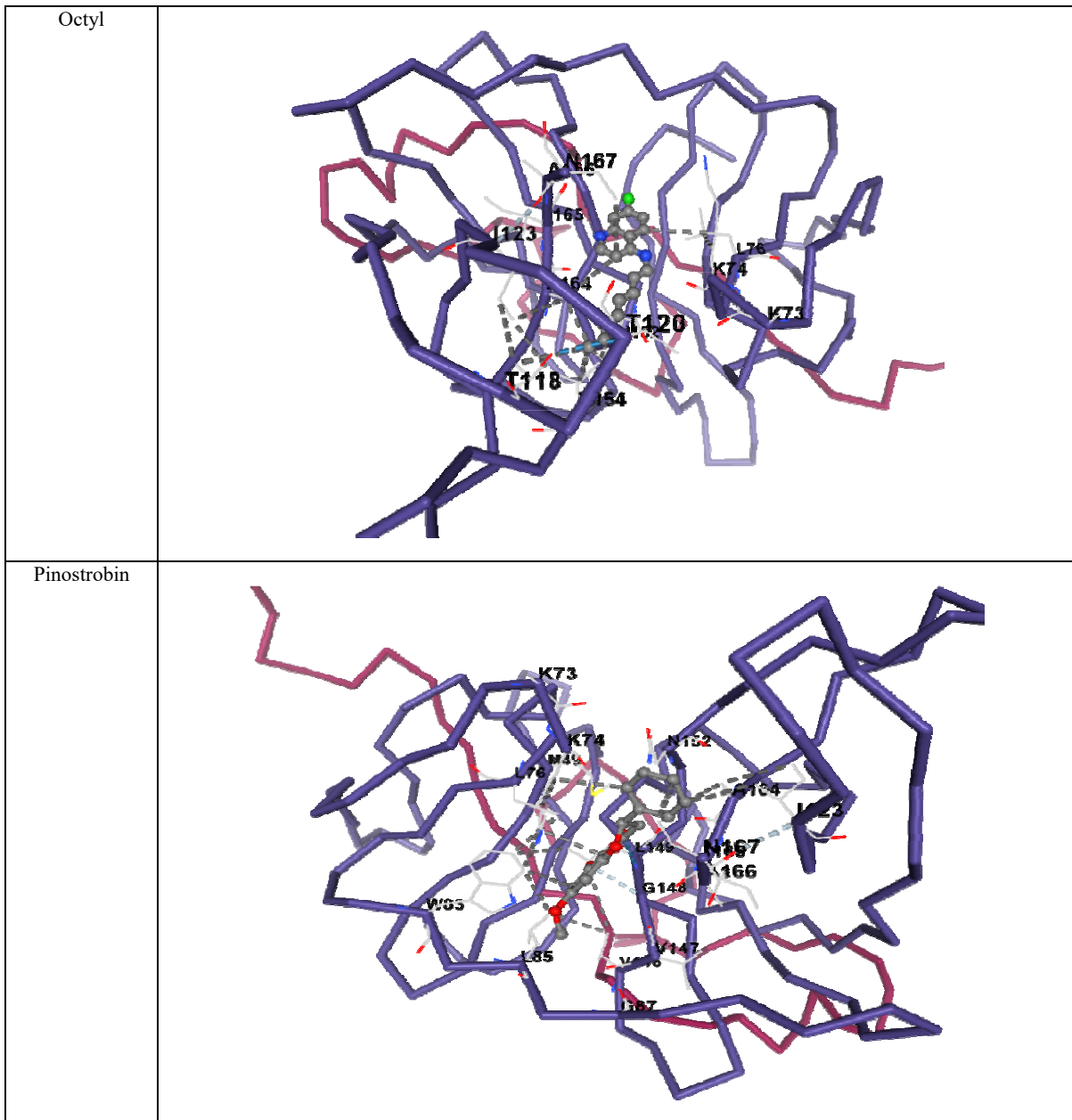


General Structure Compound









Table

Sr No	Compound	R chain	Amino acid residues or Contacting amino acid residues from CP dock.
1	Compound 1	H	MET49 LYS74 LEU76 TRP83 LEU85 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165
2	Compound 2	Methyl	MET49 LYS74 LEU76 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165 ALA166
3	Compound 3	Ethyl	MET49 LYS74 LEU76 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165
4	Compound 4	n-Propyl	MET49 LYS74 LEU76 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165
5	Compound 5	n-Butyl	MET49 LYS74 LEU76 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165
6	Compound 6	n-Pentyl	LYS74 LEU76 TRP83 LEU85 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165 ALA166 ASN167
7	Compound 7	n-Hexyl	LYS74 LEU76 TRP83 LEU85 ILE123 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165 ALA166 ASN167
8	Compound 8	n-Octyl	LYS73 LYS74 LEU76 THR118 THR120 ILE123 ASN152 VAL154 ALA164 ILE165 ALA166 ASN167
9	Pinostrobin	-	MET49 LYS73 LYS74 LEU76 TRP83 LEU85 GLY87 ILE123 VAL146 VAL147 GLY148 LEU149 ASN152 ALA164 ILE165 ALA166 ASN167

Graphical Abstract

