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In silico screening of Chromeno-pyrano-oxazole derivatives as dengue virus protease inhibitors using CB-dock

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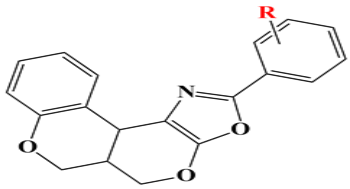
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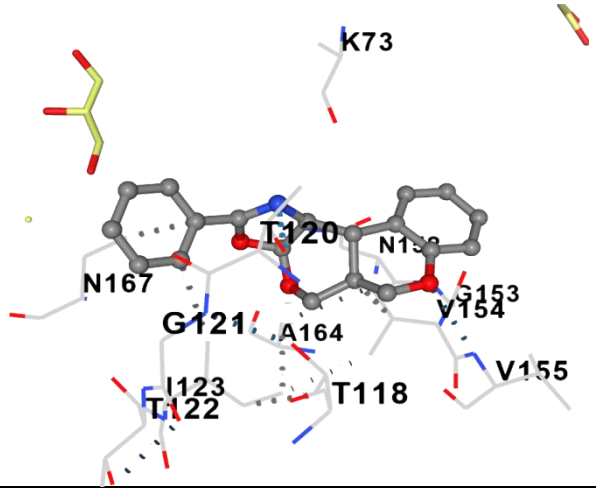
Supplementary data

Suppl. Table 1 — Dock Score, Docking poses and interacting amino acid residues

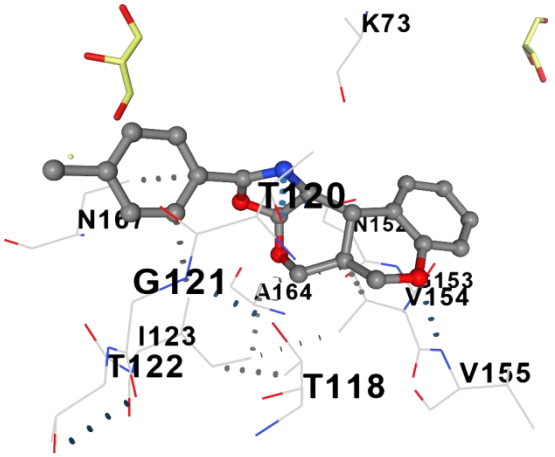


2-Phenyl-5,5a,6,11b-Tetrahydrochromeno[4',3':4,5]Pyrano[3,2-D]Oxazole Derivatives

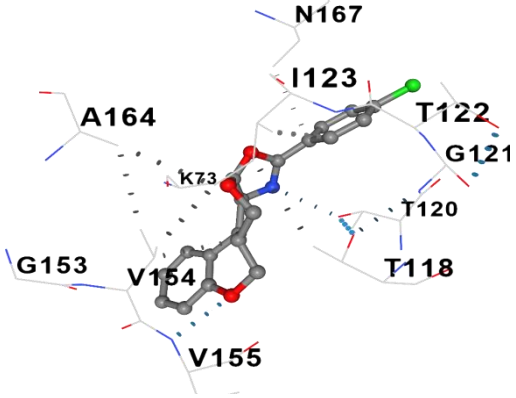
Sr No	R		Dock Score
1	H	Asp71 Lys73 Lys74 Leu76 Trp83 Leu85 Glu86 Gly87 Glu88 Trp89 Lys90 Glu91 Leu115 Thr118 Asn119 Thr120 Gly121 Thr122 Ile123 Gly124 Val146 Val147 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167	-6.3



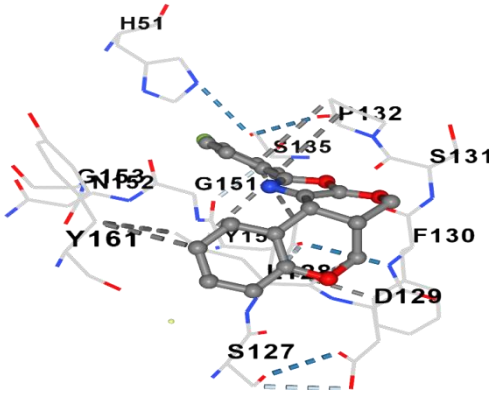
2	4-Methyl	Met49 Lys73 Lys74 Leu76 Trp83 Leu85 Gly87 Glu88 Trp89 Lys90 Glu91 Leu115 Thr118-6.5 Asn119 Thr120 Gly121 Thr122 Ile123 Val147 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



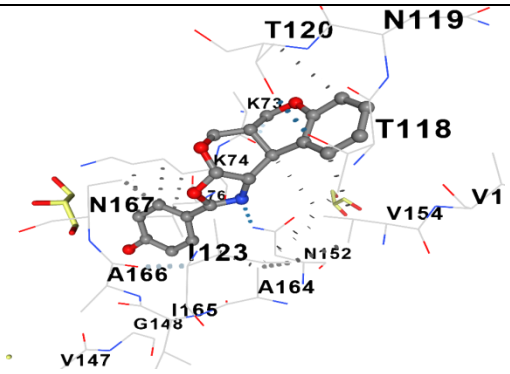
3	4-chloro	Trp50 His51 Arg54 Asp71 Val72 Lys73 Lys74 Asp75 Thr118 Asn119 Thr120 Gly121 Thr122-7.7 Ile123 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



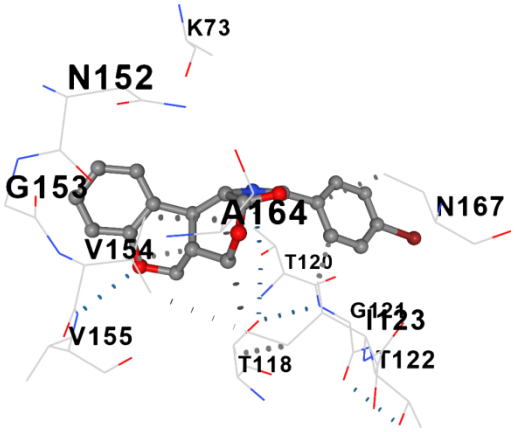
4	4-Fluoro	Trp50 His51 Arg54 Asp71 Val72 Lys73 Lys74 Asp75 Gly87 Glu88 Trp89 Lys90 Glu91 Leu115-6.7 Lys117 Thr118 Thr120 Gly121 Thr122 Ile123 Val147 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166, Asn167



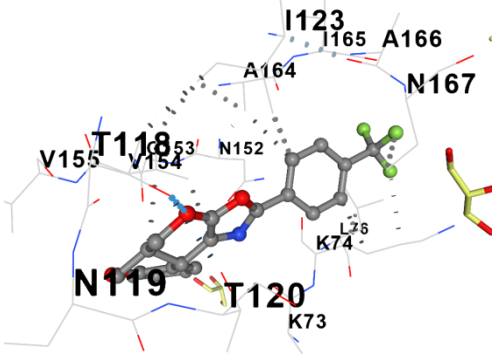
5	4-Hydroxy	Trp50 His51 Arg54 Val72 Lys73 Lys74 Asp75 Leu76 Gly87 Glu88 Trp89 Lys90 Glu91 Leu115-6.9 Thr118 Asn119 Thr120 Gly121 Thr122 Ile123 Val147 Gly148 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



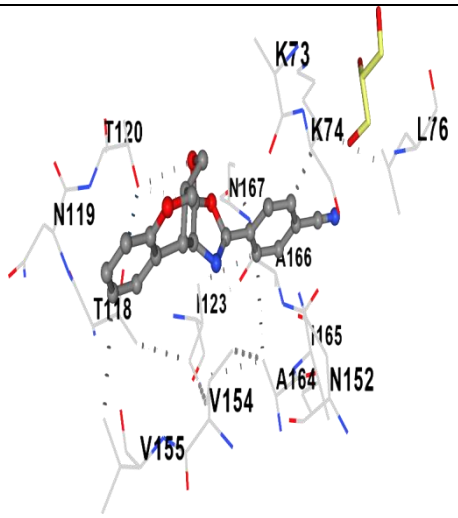
6	4-Bromo	Met49 Asp71 Lys73 Lys74 Leu76 Gly87 Glu88 Trp89 Lys90 Glu91 Leu115 Lys117 Thr118-6.4 Asn119 Thr120 Gly121 Thr122 Ile123 Val147 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



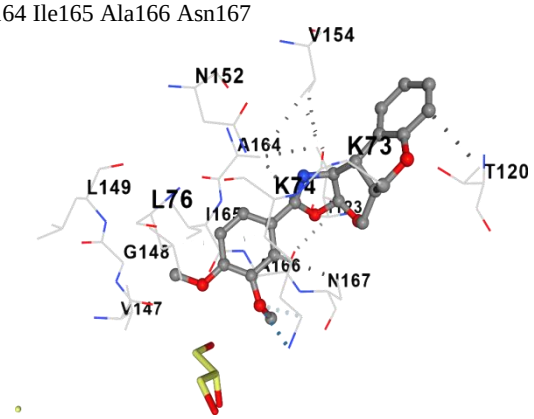
7	4-CF3	Asp71 Lys73 Lys74 Leu76 Trp83 Thr118 Asn119 Thr120 Gly121 Thr122 Ile123 Val147-6.9 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



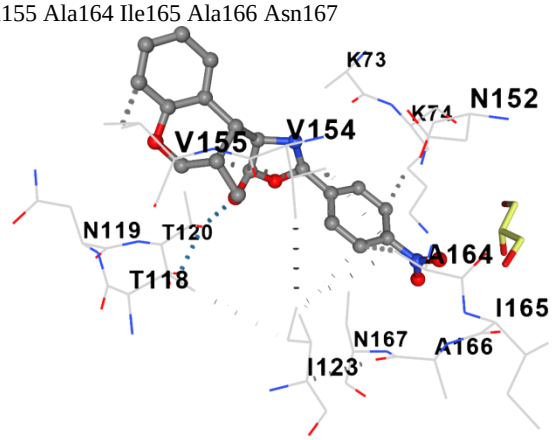
8	4-Cyano	Trp50 His51 Arg54 Val72 Lys73 Lys74 Asp75 Leu76 Thr118 Asn119 Thr120 Gly121 Thr122-7.0 Ile123 Asn152 Gly153 Val154 Val155 Tyr161 Ala164 Ile165 Ala166 Asn167



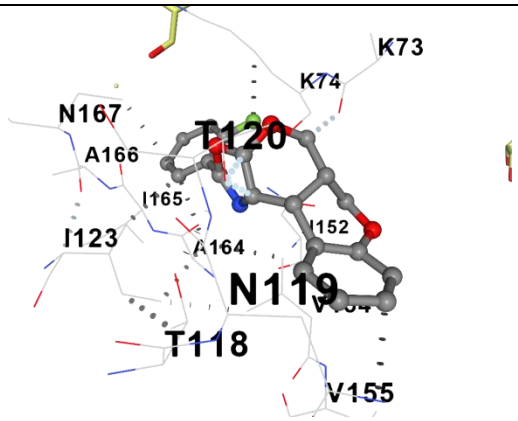
9	3,4-Dimethoxy	Met49 Val72 Lys73 Lys74 Asp75 Leu76 Leu85 Gly87 Glu88 Trp89 Lys90 Glu91 Leu115-6.6 Thr118 Asn119 Thr120 Gly121 Thr122 Ile123 Gly124 Val147 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



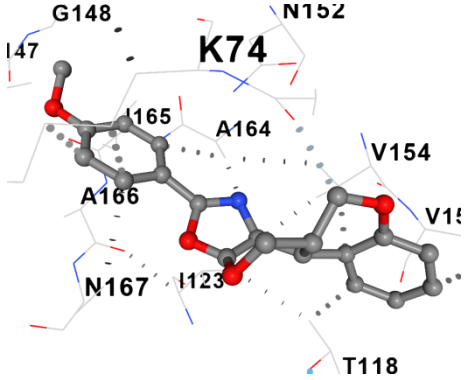
10	4-Nitro	Trp50 His51 Arg54 Val72 Lys73 Lys74 Asp75 Leu76 Trp83 Leu85 Glu86 Gly87 Glu88 Trp89-6.9 Lys90 Glu91 Leu115 Thr118 Asn119 Thr120 Gly121 Ile123 Val147 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



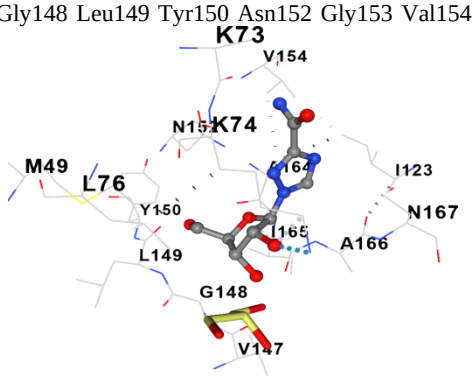
11	2-fluoro	Trp50 His51 Val72 Lys73 Lys74 Asp75 Thr118 Asn119 Thr120 Gly121 Thr122 Ile123 Asn152-6.4 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



12	4- Methoxy	Met49 Trp50 His51 Arg54 Asp71 Val72 Lys73 Lys74 Asp75 Leu76 Gly87 Glu88 Thr118-6.5 Asn119 Thr120 Gly121 Thr122 Ile123 Val147 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167

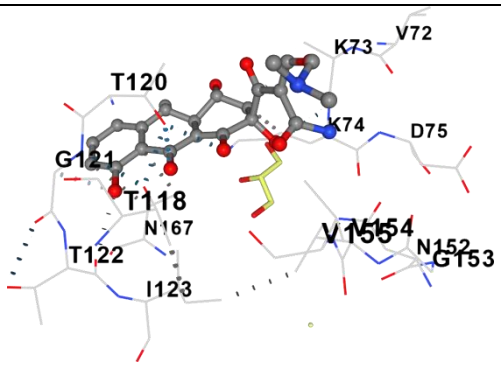


13	Ribavirin	Met49 Asp71 Lys73 Lys74 Asp75 Leu76 Gly87 Glu88 Thr118 Asn119 Thr120 Gly121 Thr122-6.5 Ile123 Val147 Gly148 Leu149 Tyr150 Asn152 Gly153 Val154 Val155 Thr156 Ala164 Ile165

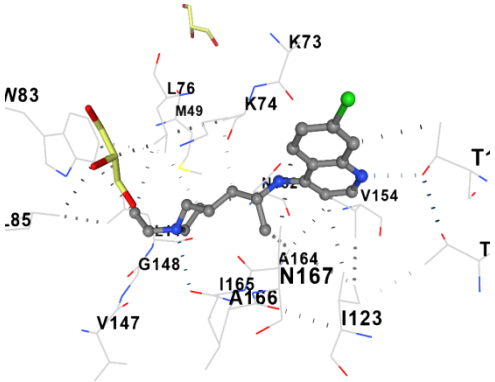


Ala166 Asn167

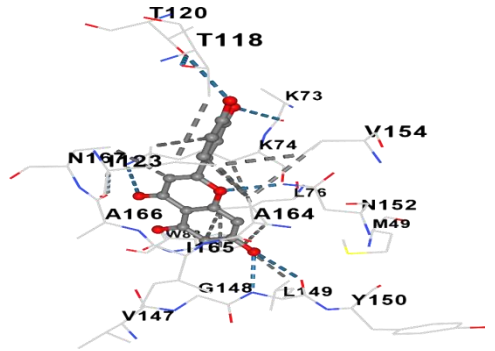
14	Doxycycline	His51 Asp71 Val72 Lys73 Lys74 Asp75 Leu76 Trp83 Leu85 Glu86 Gly87 Glu88 Trp89 Lys90-6.8 Glu91 Leu115 Thr118 Asn119 Thr120 Gly121 Thr122 Ile123 Gly124 Val146 Val147 Gly148 Gly151 Asn152 Gly153 Val154 Val155 Ala164 Ile165 Ala166 Asn167



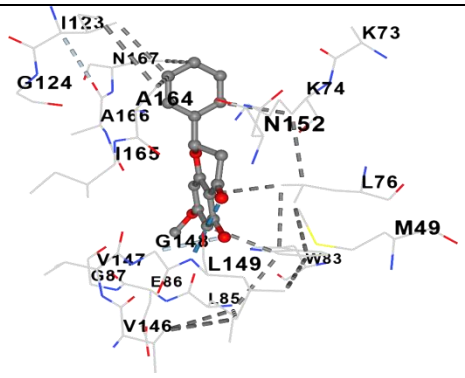
15	Chloroquine	Met49 Trp50 His51 Asp71 Val72 Lys73 Lys74 Asp75 Leu76 Trp83 Leu85 Thr118 Asn119 Thr120 Gly121 Thr122 Ile123 Val147 Gly148 Leu149 Gly151 Asn152 Gly153 Val154 Val155-5.8 Ala164 Ile165 Ala166 Asn167



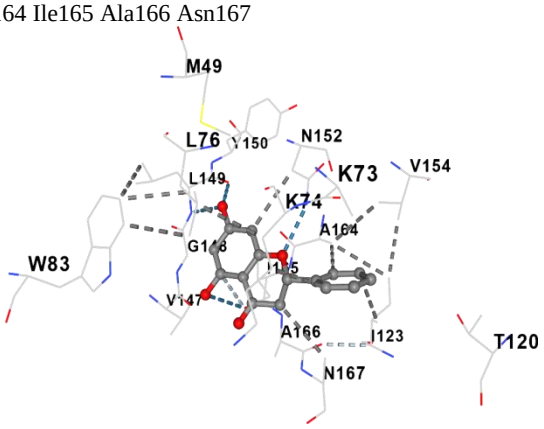
16	Luteolin	Met49 Trp69 Lys73 Lys74 Asp75 Leu76 Trp83 Lys84 Leu85 Glu86 Gly87 Glu88 Thr118-7.3 Thr120 Ile123 Val146 Val147 Gly148 Leu149 Tyr150 Asn152 Val154 Ala164 Ile165 Ala166 Asn167



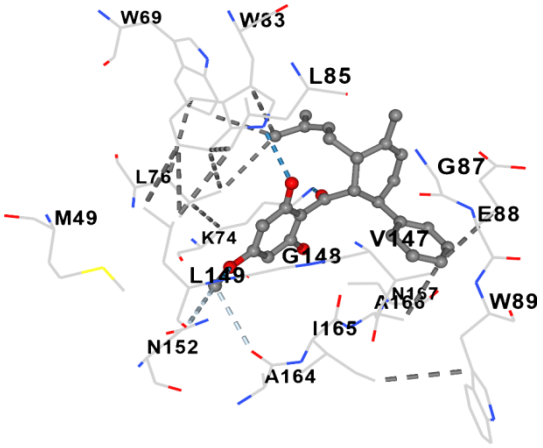
17	pinostrobin	Met49 Trp69 Lys73 Lys74 Leu76 Trp83 Leu85 Glu86 Gly87 Glu88 Trp89 Thr118 Asn119-7.2 Thr120 Gly121 Ile123 Gly124 Val146 Val147 Gly148 Leu149 Tyr150 Asn152 Val154 Val155 Ala164 Ile165 Ala166 Asn167



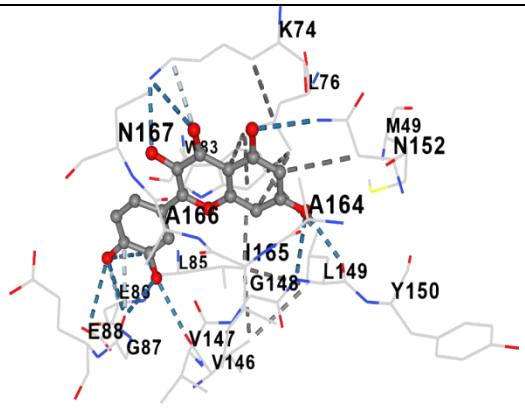
18	Pinocembrin	Met49 Lys73 Lys74 Leu76 Trp83 Leu85 Glu86 Gly87 Glu88 Trp89 Lys90 Thr118 Asn119-7.0 Thr120 Gly121 Ile123 Gly124 Val146 Val147 Gly148 Leu149 Tyr150 Asn152 Gly153 Val154 Val155 Thr156 Ala164 Ile165 Ala166 Asn167



19	Panduratin	Met49 Trp50 His51 Trp69 Val72 Lys73 Lys74 Asp75 Leu76 Trp83 Leu85 Glu86 Gly87 Glu88-7.3 Trp89 Thr118 Asn119 Thr120 Ile123 Val146 Val147 Gly148 Leu149 Asn152 Gly153 Val154 Val155 Tyr161 Ala164 Ile165 Ala166 Asn167



20	Quercetin	Met49 Trp50 His51 Trp69 Val72 Lys73 Lys74 Asp75 Leu76 Trp83 Leu85 Glu86 Gly87 Glu88-7.4 Thr118 Asn119 Thr120 Ile123 Gly124 Val146 Val147 Gly148 Leu149 Tyr150 Gly151 Asn152 Gly153 Val154 Val155 Thr156 Ala164 Ile165 Ala166 Asn167



Suppl. Table 2 — ADME Profile Data

Compound	H-bond acceptors	H-bond donors	GI absorption	BBB permeant	log Kp (cm/s)	Lipinski violations	Consensus Log P
Compound 1	4	0	High	Yes	-5.44	0	3.52
Compound 2	4	0	High	Yes	-5.27	0	3.86
Compound 3	4	0	High	Yes	-5.21	0	4.06
Compound 4	5	0	High	Yes	-5.48	0	3.83
Compound 5	5	1	High	Yes	-5.8	0	3.11
Compound 6	4	0	High	Yes	-5.43	0	4.14
Compound 7	7	0	High	No	-5.23	0	4.55
Compound 8	5	0	High	Yes	-5.79	0	3.29
Compound 9	6	0	High	Yes	-5.85	0	3.48
Compound 10	6	0	High	No	-5.84	0	2.94
Compound 11	5	0	High	Yes	-5.48	0	3.81
Compound 12	5	0	High	Yes	-5.65	0	3.51
Ribavirin	7	4	Low	No	-9.1	0	-2.94
Chloroquine	2	1	High	Yes	-4.96	0	4.19
Doxycycline	9	6	Low	No	-9.03	1	-0.86
Luteolin	6	4	High	No	-6.97	0	1.1
Pinostrobin	4	1	High	Yes	-5.68	0	2.64
Pinocembrin	4	2	High	Yes	-5.82	0	2.3
Panduratin	4	2	High	No	-4.55	0	5.19
Quercetin	7	5	High	No	-7.01	0	0.79