Supporting Information

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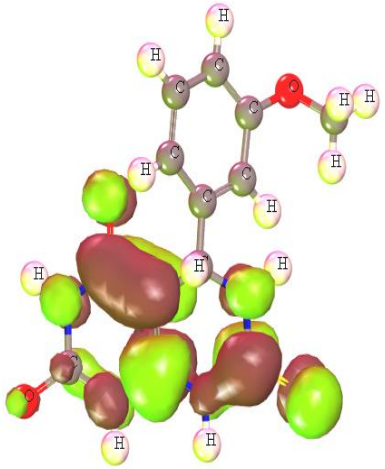
LUMO



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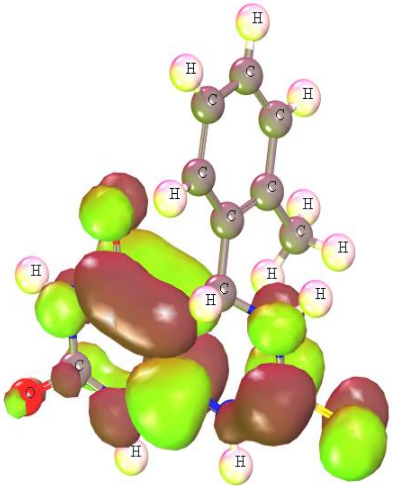

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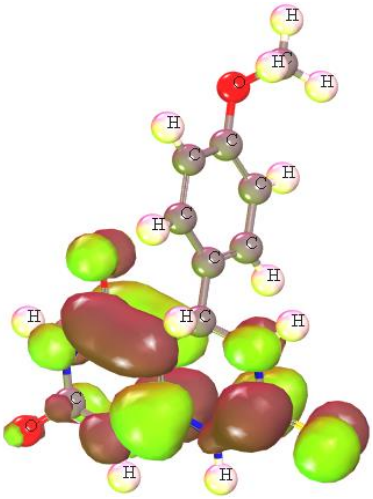

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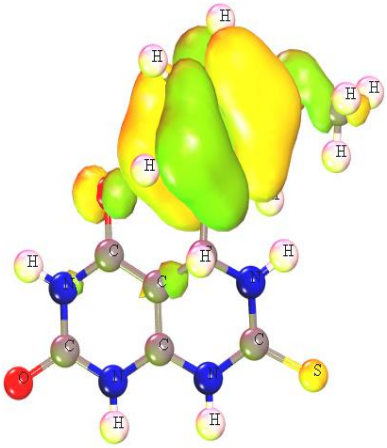

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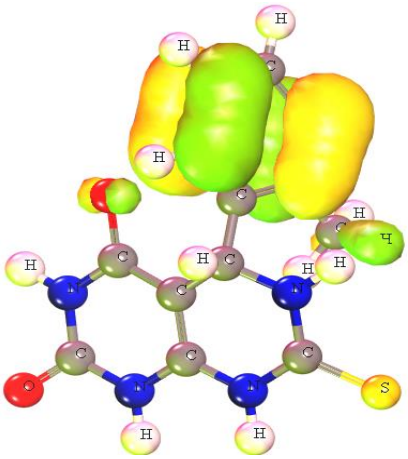

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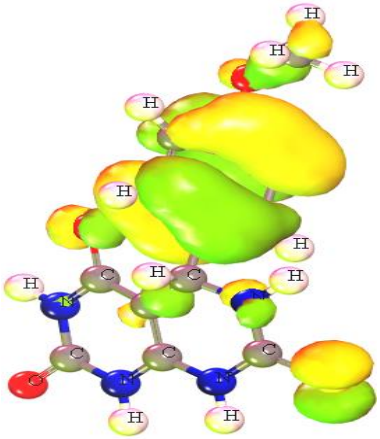

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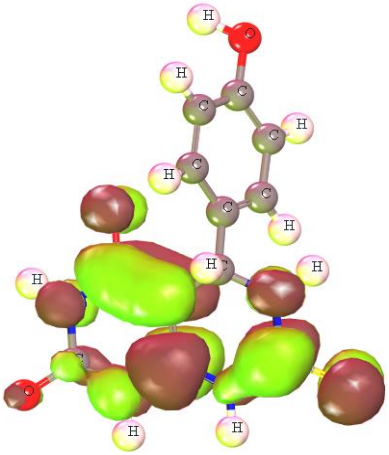

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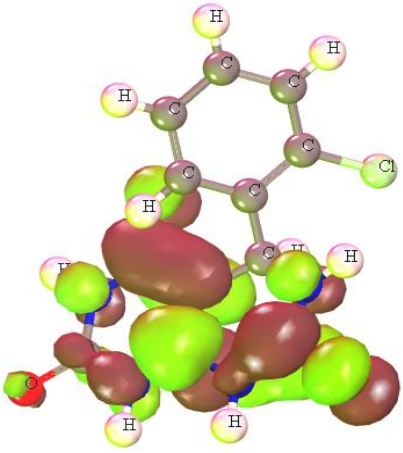

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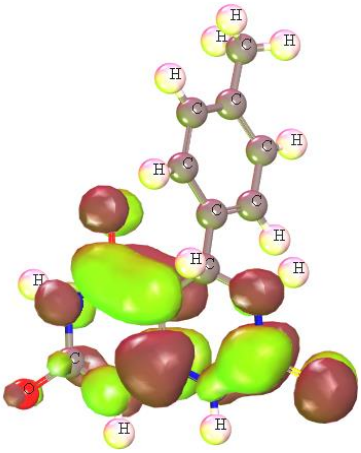

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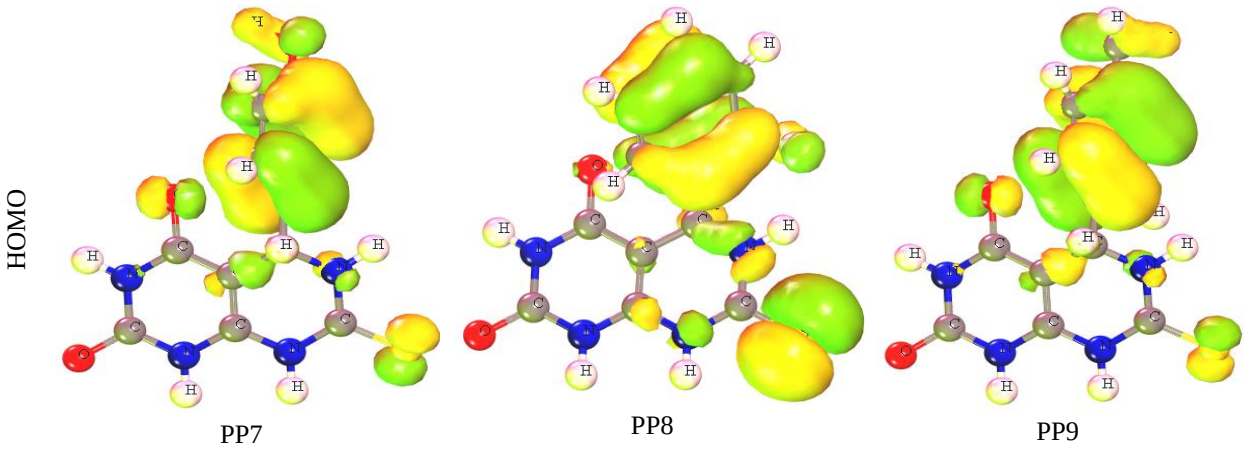

Figure S1: Frontier molecular orbital diagram for HOMO and LUMO

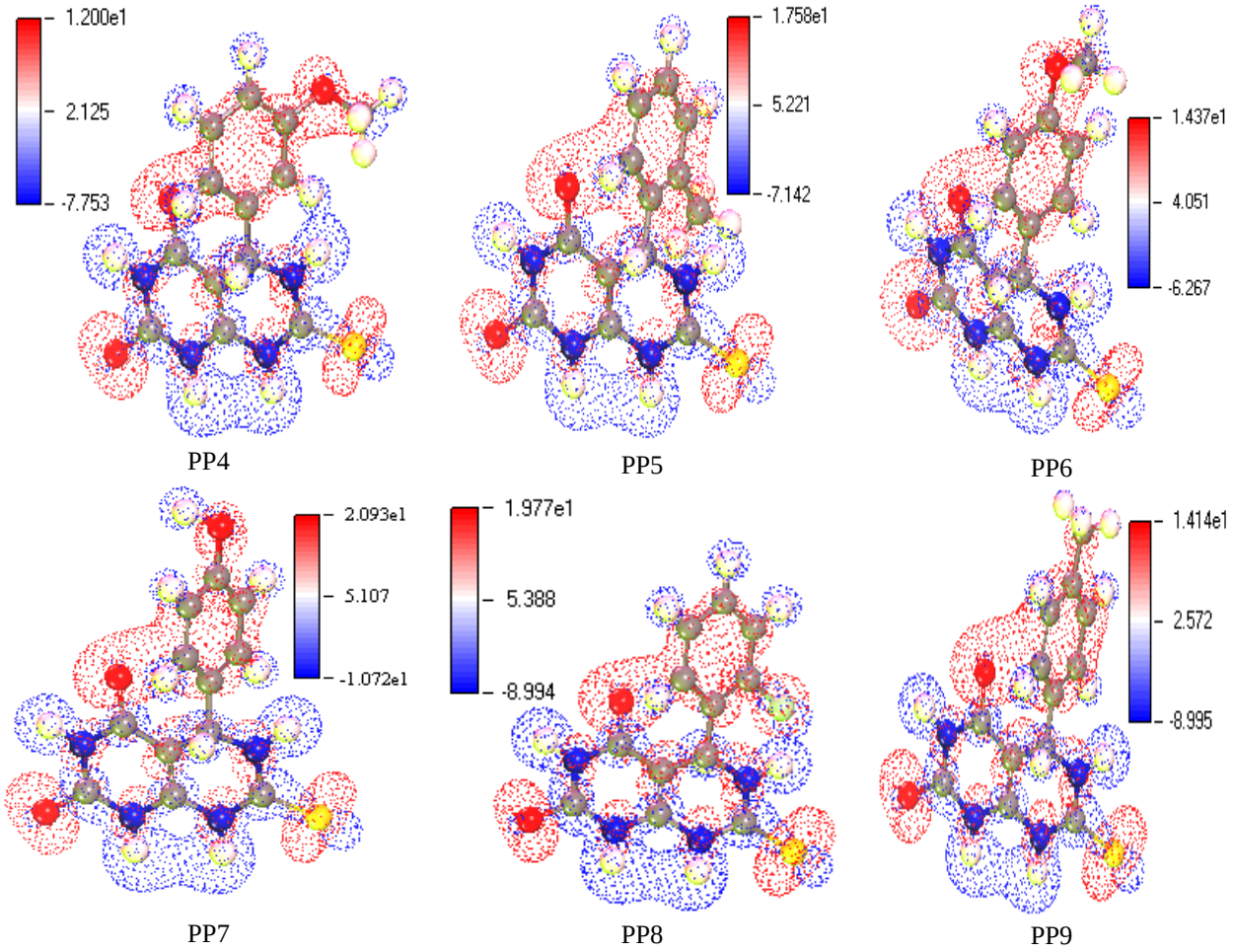

Figure S2: Map of molecular electrostatic potential (MEP) charge distribution of the reported compounds

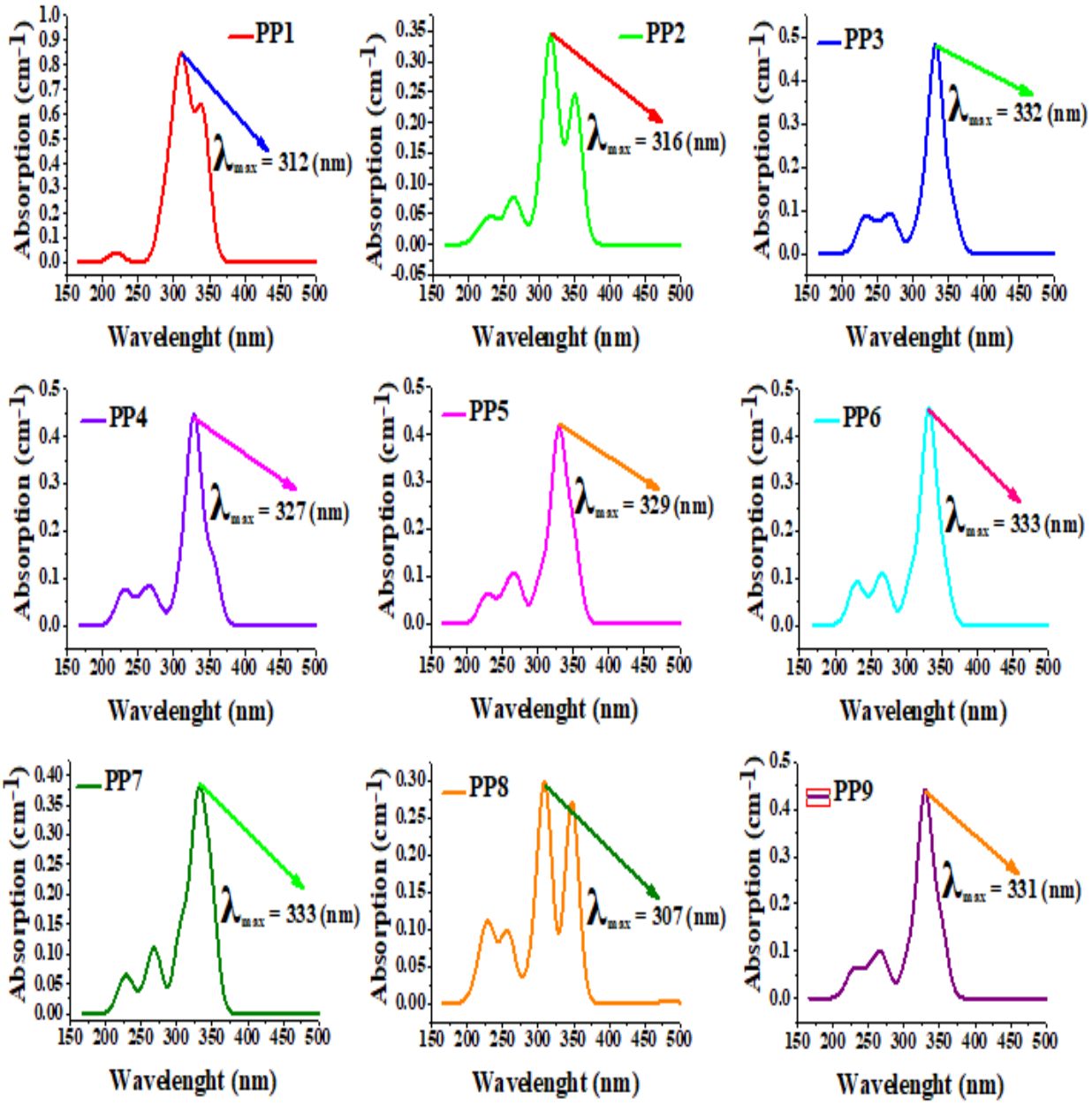

Figure S3: UV-visible Spectrum data of nine compounds

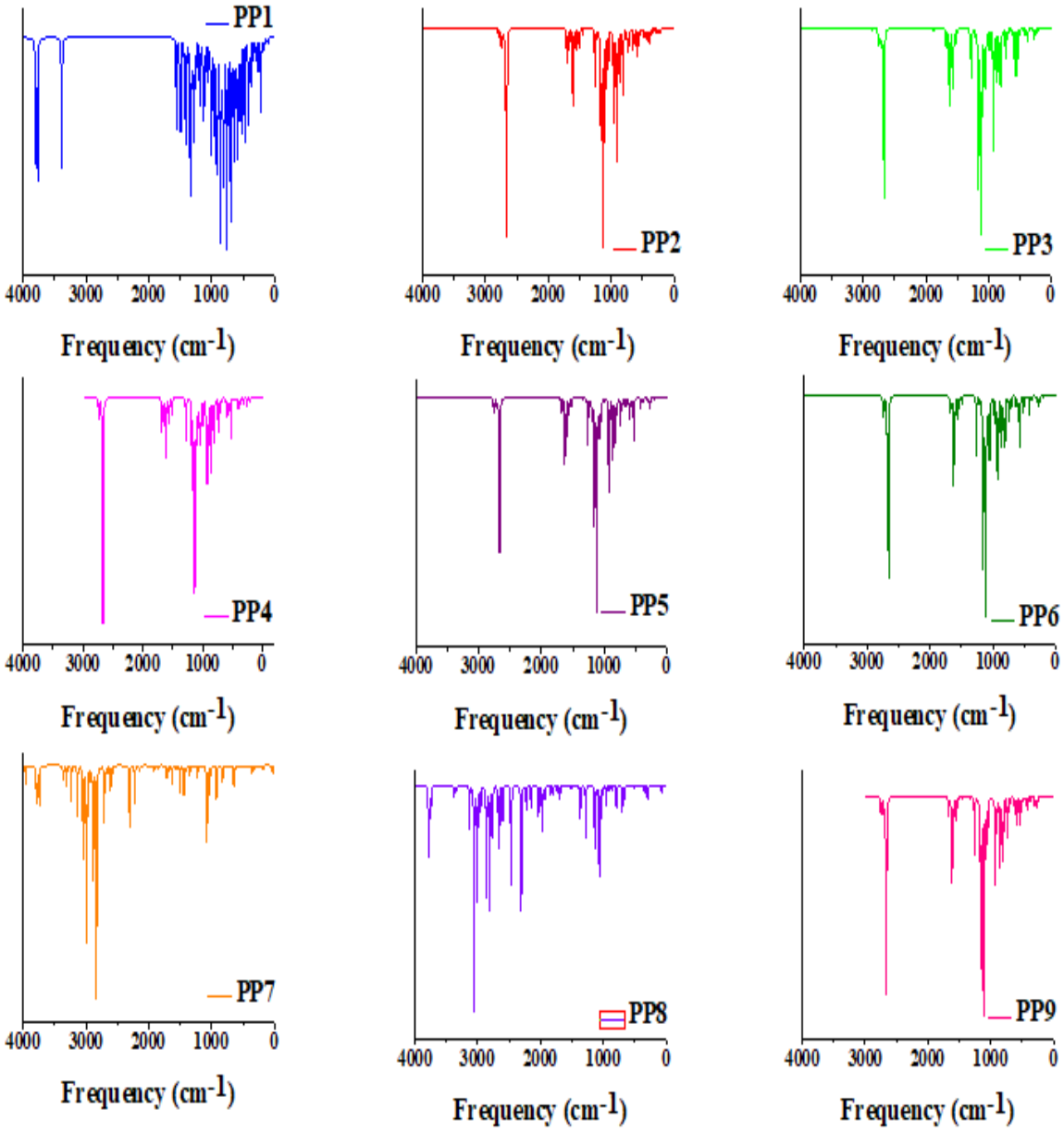

Figure S4: Calculated data of FTIR

Table S1: Protein ligand interaction of *Bacillus cereus*

	Hydrogen Bond		Hydrophobic Bond			Hydrogen Bond		Hydrophobic Bond	
L/N	**Interacting Residue of amino Acid**	**Distance A°**	**Interacting Residue of amino Acid**	**Distance A°**	**L/N**	**Interacting Residue of amino Acid**	**Distance A°**	**Interacting Residue of amino Acid**	**Distance A°**
PP1	ASN147 GLU4	2.088 2.807	HIS142 GLU146 PHE66 PHE66 PHE66	4.995 3.335 5.386 4.591 4.116	PP6	TRP1 GLU146 GLU146	2.830 2.635 2.534	PHE66 TYR56	4.156 4.945
PP2	TYR79 THR65 TYR79 THR65 TRP1 ASP122	2.667 2.337 2.121 3.252 3.396 3.711	GLU146 PHE66 PHE66 PHE66 HIS128	4.588 4.154 5.183 4.380 4.312	PP7	TRP1 GLU146 GLU146	2.834 2.607 2.549	HIS128 PHE66	4.849 4.231
PP3	TRP1 ASP55 SER143	3.045 2.366 3.721	GLU146 HIS142 LEU135 TYR79	3.313 4.911 4.569 5.196	PP8	TRP1 TRP1 HIS128 TRP1 ASP55 GLU146	2.850 2.325 2.877 2.302 2.798 2.876	GLU146 ASP55 PHE66 PHE66	3.841 4.441 3.908 4.865
PP4	TYR79 THR65 TYR79 THR65 GLU146	2.734 2.137 2.312 3.343 3.667	GLU146 PHE66 HIS142	4.760 3.799 5.746	PP9	HIS69 ASP55 GLU146	2.499 2.874 2.142	HIS128 HIS142 HIS142 LEU1	4.207 4.509 5.354 5.058
PP5	ASN147 GLU4	2.002 2.439	GLU146 GLU146 PHE66 PHE66	4.797 3.423 3.736 4.373					

Table S2: Protein ligand interaction of Omicron (7T9L)

	Hydrogen Bond		Hydrophobic Bond			Hydrogen Bond		Hydrophobic Bond	
L/N	**Interacting Residue of amino Acid**	**Distance A°**	**Interacting Residue of amino Acid**	**Distance A°**	**L/N**	**Interacting Residue of amino Acid**	**Distance A°**	**Interacting Residue of amino Acid**	**Distance A°**
PP1	ALA369 PHE371	2.644 2.826	PHE374 PHE374 TYR366	4.709 3.740 5.364	PP6	Absent	Absent	GLU1014 GLU1014 ARG1011 PRO725 LYS944	3.758 4.952 4.014 4.289 5.339
PP2	SER527 SER527 PRO327 ILE329 ILE329	2.536 2.301 2.802 2.755 2.885	LYS526	3.860	PP7	ARG243 ASP140 ASP250 SER244 LYS142 ARG243	2.236 2.043 2.342 2.240 3.532 3.521	ARG243 LYS142	4.105 3.725
PP3	TRP433 PHE339 LEU368	2.321 2.737 2.855	LYS437 ALA369 LEU438	4.153 4.584 5.445	PP8	ARG185 ARG185 ILE99 ARG100 ASN119	2.903 2.611 2.450 2.427 3.290	VAL124	3.825
PP4	ARG243 ILE99 ARG100 ASN119	3.049 2.343 2.336 3.162	VAL124 VAL124 PHE170	3.776 5.179 5.258	PP9	PHE371 PHE371	2.860 3.124	PHE374 TYR362 PHE374	3.713 4.278 4.384
PP5	Absent	Absent	TRP102 PHE187 ILE117 VAL124 TRP102 VAL124	5.311 5.058 5.075 4.611 4.788 4.674					

Table S3: Protein ligand interaction of *Aspergillus flavus*

	Hydrogen Bond		Hydrophobic Bond			Hydrogen Bond		Hydrophobic Bond	
L/N	**Interacting Residue of amino Acid**	**Distance A°**	**Interacting Residue of amino Acid**	**Distance A°**	**L/N**	**Interacting Residue of amino Acid**	**Distance A°**	**Interacting Residue of amino Acid**	**Distance A°**
PP1	VAL29	2.906	TYR30 TYR30 ARG105 CYS103	5.050 4.723 4.699 4.4114	PP6	THR173 TYR257 GLU259 TYR257	2.490 2.895 2.734 2.410	LYS171 ARG176 LYS171	4.653 4.180 5.122
PP2	THR74 ARG105 TRP106 TRP106 GLU126 GLU126	2.673 2.177 2.569 2.259 3.633 3.571	TYR30 ARG105 ARG128 TRP208 TRP208 ARG105 ARG128	5.036 4.396 4.478 4.977 5.232 4.620 5.152	PP7	TRP106 VAL73 HIS104 CYS103T RP1	2.671 2.680 3.074 3.648 2.958	TYR30	4.947
PP3	ILE177 TYR257 ASP175 GLU259 GLU259	2.613 2.998 2.901 3.032 3.001	PHE258 PHE258 ARG176	4.863 4.409 4.227	PP8	ILE177 ARG176 LEU170	2.126 3.539 3.587	HIS256 ARG176	5.360 4.048
PP4	ILE177 GLU259 TYR257 GLU259	1.933 2.342 2.516 2.599	PHE258 PHE258 ARG176	4.525 5.139 4.283	PP9	ASP175 GLU2	3.01529 2.73352	LEU17 LEU170 HIS256 ARG176	3.801 4.648 5.167 4.382
PP5	THR107 TRP106	2.420 2.411	TYR30 TYR30 ARG105 CYS103	4.745 5.348 4.466 4.681					