

Supporting Information

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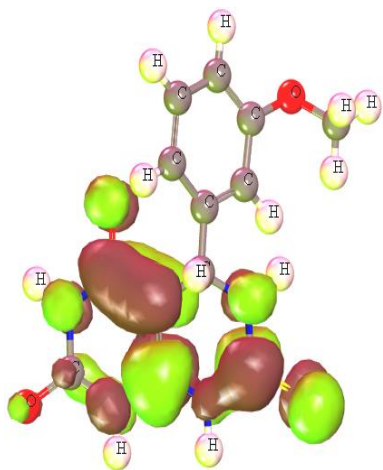
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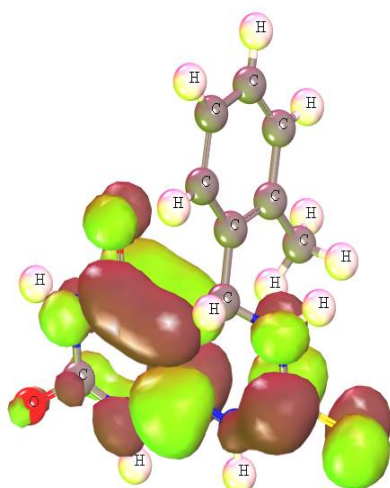
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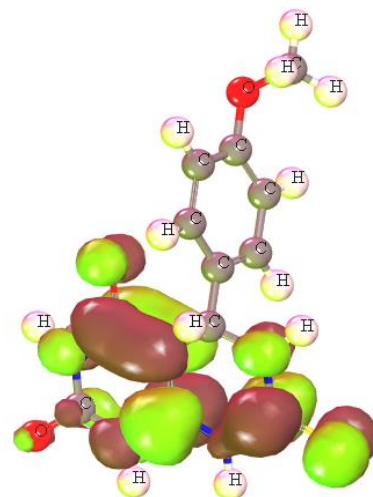
LUMO



PP4

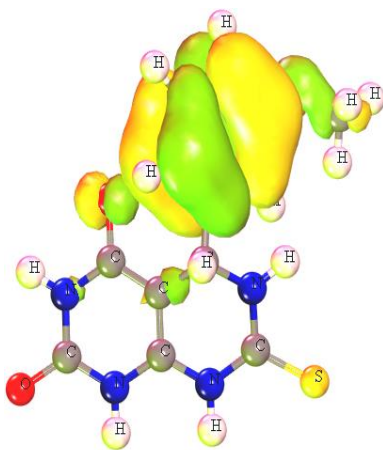


PP5

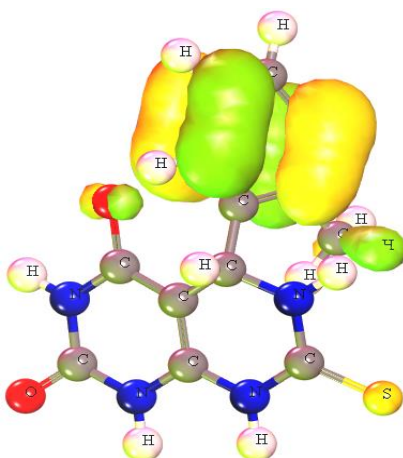


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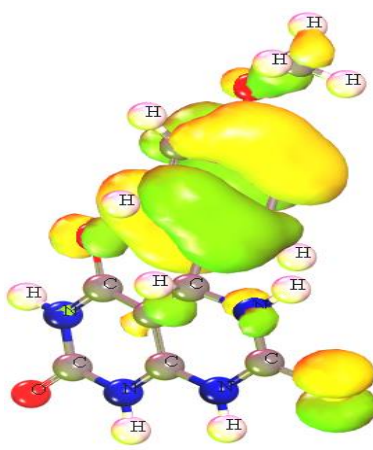
HOMO



PP4

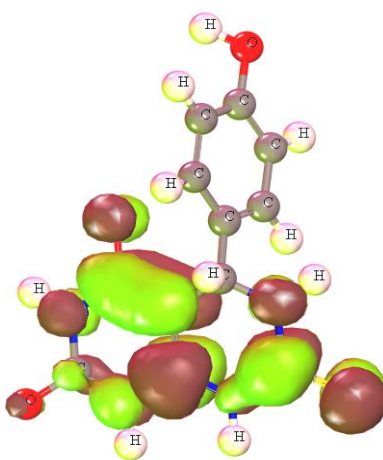


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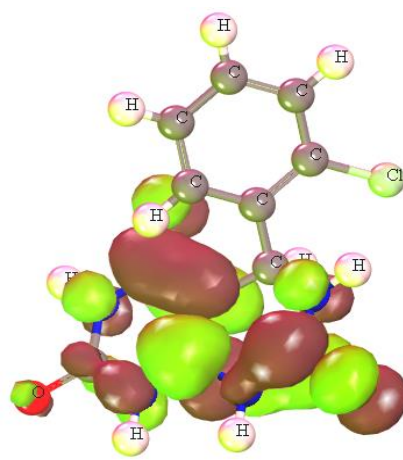


PP6

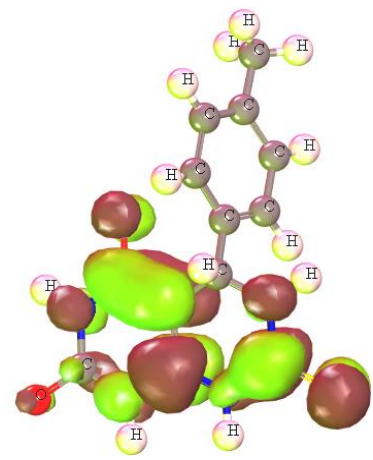
LUMO



PP7



PP8



PP9

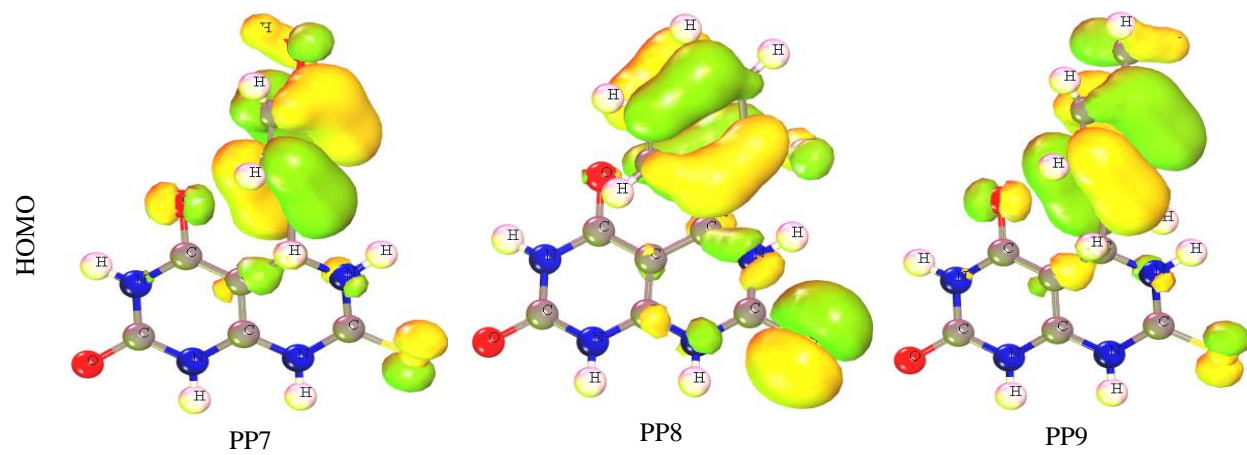


Figure S1: Frontier molecular orbital diagram for HOMO and LUMO

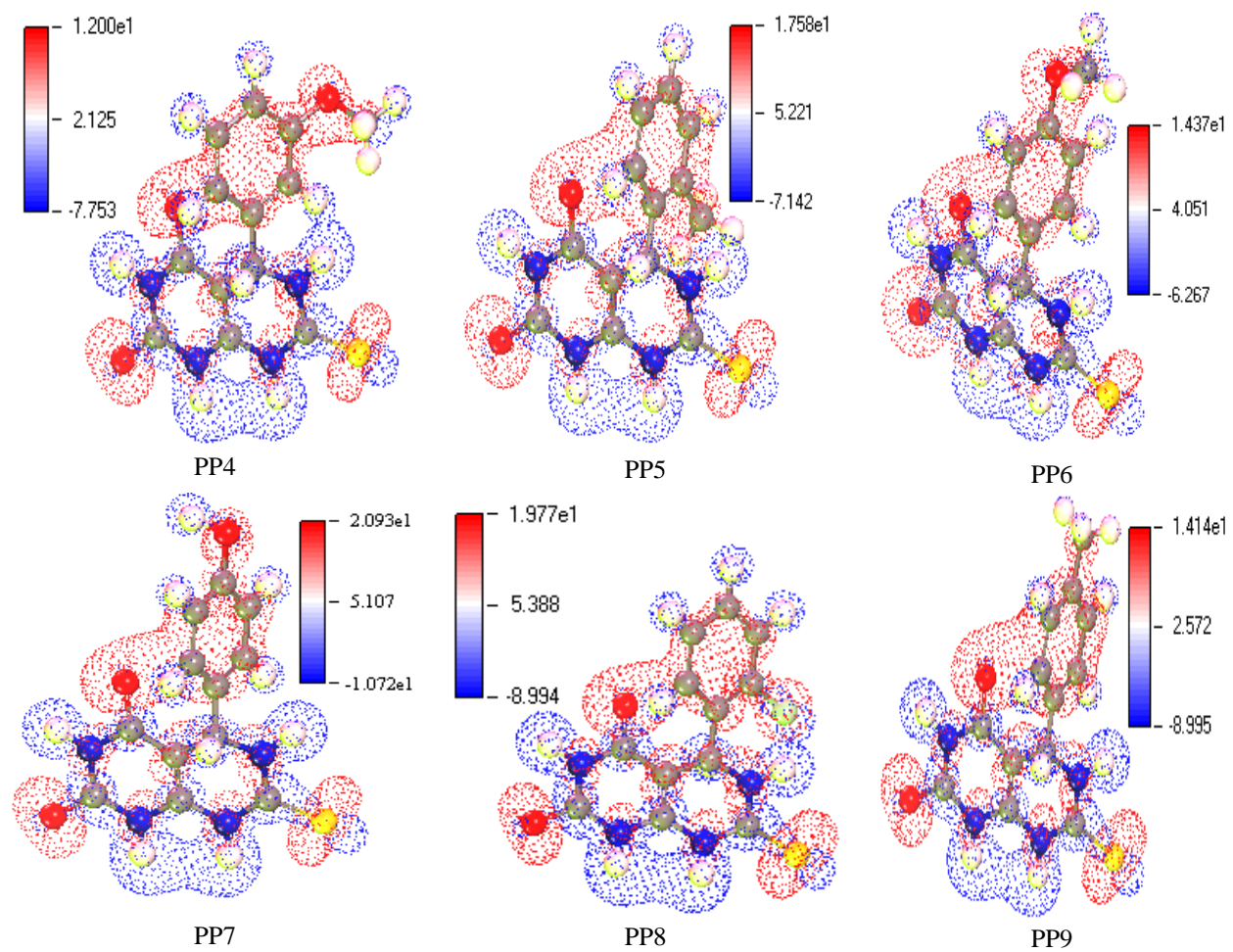


Figure S2: Map of molecular electrostatic potential (MEP) charge distribution of the reported compounds

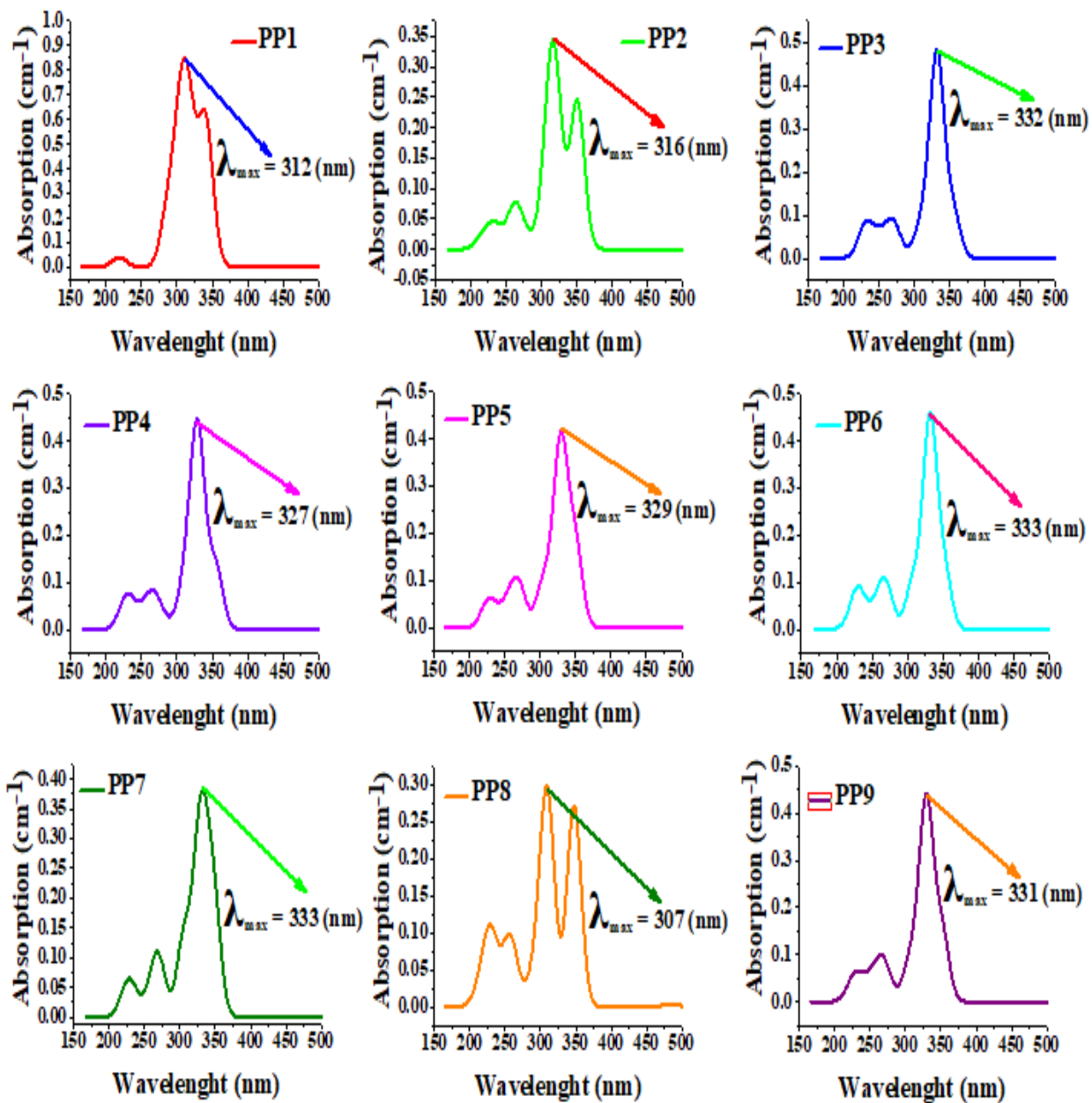


Figure S3: UV-visible Spectrum data of nine compounds

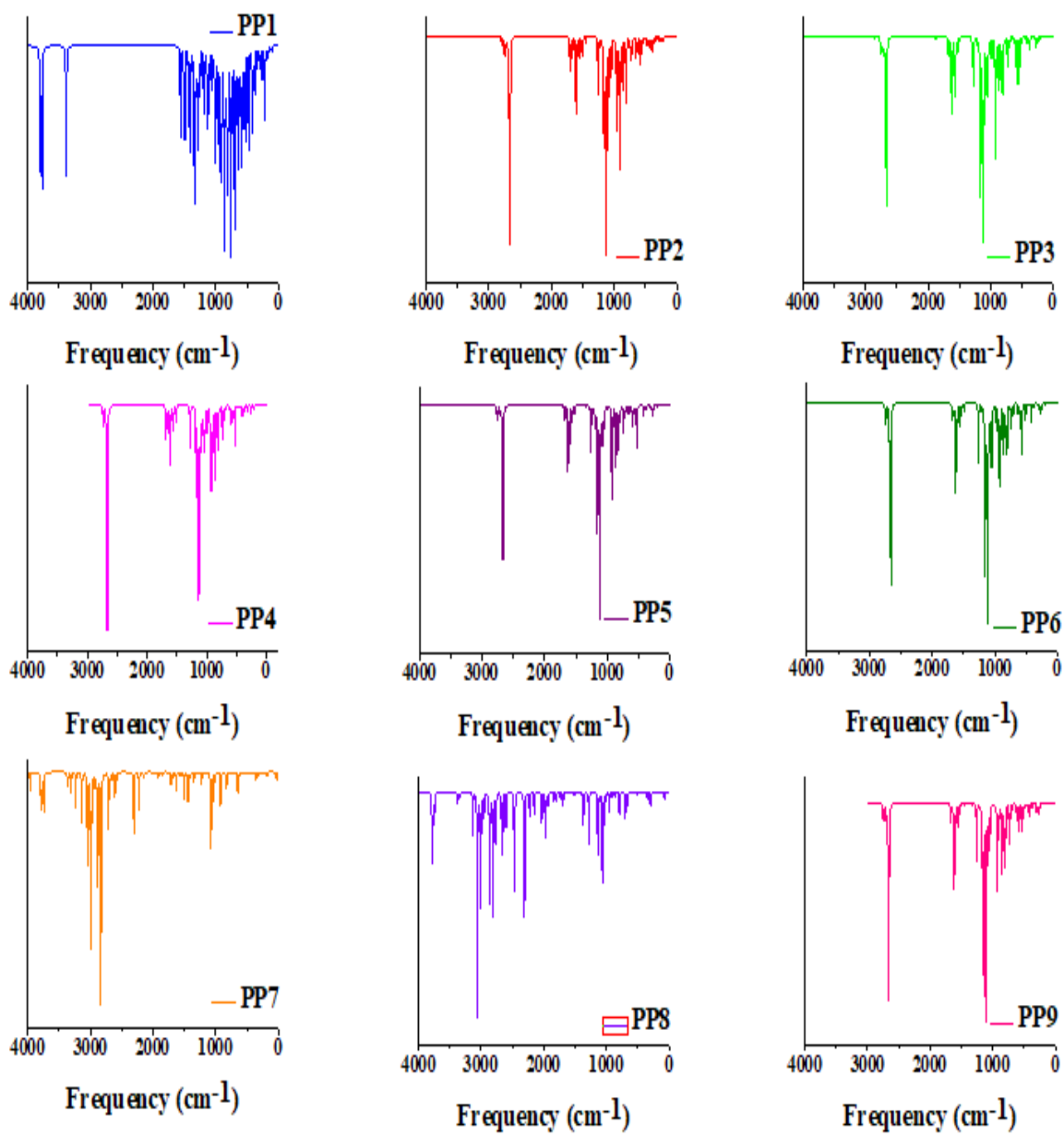


Figure S4: Calculated data of FTIR

Table S1: Protein ligand interaction of *Bacillus cereus*

L/N	Hydrogen Bond		Hydrophobic Bond		L/N	Hydrogen Bond		Hydrophobic Bond	
	Interacting Residue of amino Acid	Distance Å	Interacting Residue of amino Acid	Distance Å		Interacting Residue of amino Acid	Distance Å	Interacting Residue of amino Acid	Distance Å
PP1	ASN147	2.088	HIS142	4.995	PP6	TRP1	2.830	PHE66	4.156
	GLU4	2.807	GLU146	3.335		GLU146	2.635	TYR56	4.945
			PHE66	5.386		GLU146	2.534		
			PHE66	4.591					
			PHE66	4.116					
PP2	TYR79	2.667	GLU146	4.588	PP7	TRP1	2.834	HIS128	4.849
	THR65	2.337	PHE66	4.154		GLU146	2.607	PHE66	4.231
	TYR79	2.121	PHE66	5.183		GLU146	2.549		
	THR65	3.252	PHE66	4.380					
	TRP1	3.396	HIS128	4.312					
	ASP122	3.711							
PP3	TRP1	3.045	GLU146	3.313	PP8	TRP1	2.850	GLU146	3.841
	ASP55	2.366	HIS142	4.911		TRP1	2.325	ASP55	4.441
	SER143	3.721	LEU135	4.569		HIS128	2.877	PHE66	3.908
			TYR79	5.196		TRP1	2.302	PHE66	4.865
				ASP55	2.798				
				GLU146	2.876				
PP4	TYR79	2.734	GLU146	4.760	PP9	HIS69	2.499	HIS128	4.207
	THR65	2.137	PHE66	3.799		ASP55	2.874	HIS142	4.509
	TYR79	2.312	HIS142	5.746		GLU146	2.142	HIS142	5.354
	THR65	3.343						LEU1	5.058
	GLU146	3.667							
PP5	ASN147	2.002	GLU146	4.797					
	GLU4	2.439	GLU146	3.423					
			PHE66	3.736					
			PHE66	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	2.644	PHE374	4.709	PP6	Absent	Absent	GLU1014	3.758
	PHE371	2.826	PHE374	3.740		GLU1014	4.952		
			TYR366	5.364		ARG1011	4.014		
PP2	SER527	2.536	LYS526	3.860	PP7	ARG243	2.236	ARG243	4.105
	SER527	2.301				ASP140	2.043	LYS142	3.725
	PRO327	2.802				ASP250	2.342		
	ILE329	2.755				SER244	2.240		
	ILE329	2.885				LYS142	3.532		
PP3	TRP433	2.321	LYS437	4.153	PP8	ARG185	2.903	VAL124	3.825
	PHE339	2.737	ALA369	4.584		ARG185	2.611		
	LEU368	2.855	LEU438	5.445		ILE99	2.450		
						ARG100	2.427		
PP4	ARG243	3.049	VAL124	3.776	PP9	PHE371	2.860	PHE374	3.713
	ILE99	2.343	VAL124	5.179		PHE371	3.124	TYR362	4.278
	ARG100	2.336	PHE170	5.258				PHE374	4.384
	ASN119	3.162							
PP5	Absent	Absent	TRP102	5.311					
			PHE187	5.058					
			ILE117	5.075					
			VAL124	4.611					
			TRP102	4.788					
			VAL124	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	5.050	PP6	THR173	2.490	LYS171	4.653
			TYR30	4.723		TYR257	2.895	ARG176	4.180
			ARG105	4.699		GLU259	2.734	LYS171	5.122
			CYS103	4.4114		TYR257	2.410		
PP2	THR74	2.673	TYR30	5.036	PP7	TRP106	2.671	TYR30	4.947
	ARG105	2.177	ARG105	4.396		VAL73	2.680		
	TRP106	2.569	ARG128	4.478		HIS104	3.074		
	TRP106	2.259	TRP208	4.977		CYS103T	3.648		
	GLU126	3.633	TRP208	5.232		RP1	2.958		
	GLU126	3.571	ARG105	4.620					
			ARG128	5.152					
PP3	ILE177	2.613	PHE258	4.863	PP8	ILE177	2.126	HIS256	5.360
	TYR257	2.998	PHE258	4.409		ARG176	3.539	ARG176	4.048
	ASP175	2.901	ARG176	4.227		LEU170	3.587		
	GLU259	3.032							
	GLU259	3.001							
PP4	ILE177	1.933	PHE258	4.525	PP9	ASP175	3.01529	LEU17	3.801
	GLU259	2.342	PHE258	5.139		GLU2	2.73352	LEU170	4.648
	TYR257	2.516	ARG176	4.283				HIS256	5.167
	GLU259	2.599						ARG176	4.382
PP5	THR107	2.420	TYR30	4.745					
	TRP106	2.411	TYR30	5.348					
			ARG105	4.466					
			CYS103	4.681					