Supplementary Information

Table S1. Identification of bioactive compounds in the ethanol extract of *S. flavescens* root by HR-LCMS (Positive ESI and Negative ESI).

SF-EXT OF *S. flavescens* root. +VE

S. No	Compound name	RT (min)	Mass	Formula	DB Diff (ppm)
1	5-MOT / 5-Methoxytryptamine	3.235	190.1104	$C_{11}H_{14}N_2O$	1.3
2	Cadiamine	4.042	282.193	$C_{15}H_{26}N_2O_3$	4.92
3	19-Noretiocholanolone	4.925	276.2055	$C_{18}H_{28}O_2$	12.24
4	(10Z,14E,16E)-10,14,16-Octadecatrien-12-ynoic acid	5.108	274.1902	$C_{18}H_{26}O_2$	11.34
5	Formononetin	6.134	269.0805	$C_{16}H_{12}O_4$	-2.20
6	Apiosylglucosyl 4-hydroxybenzoate	6.345	432.1241	$C_{18}H_{24}O_{12}$	6.09
7	ar-Artemisene	6.346	270.2319	$C_{20}H_{30}$	10.4
8	Kaur-16-en-18-ol	6.431	288.2422	$C_{20}H_{32}O$	10.93
9	Axisothiocyanate 3	6.451	263.1747	$C_{16}H_{25}NS$	-14.78
10	(+)-Mahanimbicine	6.498	331.1981	$C_{23}H_{25}NO$	-13.53
11	Retinol / Retinol skeleton	6.553	286.2259	$C_{20}H_{30}O$	13.24
12	3-Hydroxyropivacaine	6.593	290.1973	$C_{17}H_{26}N_2O_2$	7.42
13	Retinaldehyde	7.244	284.2116	$C_{20}H_{28}O$	8.42
14	7-Dehydrologanin tetraacetate	7.31	556.1787	$C_{25}H_{32}O_{14}$	0.86

15	Smyrindioloside	7.936	424.1372	$C_{20} H_{24} O_{10}$	-0.56
16	Neogrifolin	8.619	328.2373	$C_{22} H_{32} O_2$	8.83
17	Lippioside II	8.942	554.1637	$C_{25} H_{30} O_{14}$	-0.32
18	Oleuropein	9.051	540.1844	$C_{25} H_{32} O_{13}$	-0.25
19	Sakacin A	9.186	288.1835	$C_{12} H_{24} N_4 O_4$	-13.14
20	Azidopine	9.368	557.1873	$C_{27} H_{26} F_3 N_5 O_5$	2.34
21	Orientaloside	9.426	540.1841	$C_{25} H_{32} O_{13}$	0.35
22	Convalloside	9.823	712.3207	$C_{35} H_{52} O_{15}$	13.95
23	Prunetin	10.26	284.0676	$C_{16} H_{12} O_5$	3
24	Orientalone	10.682	260.0695	$C_{14} H_{12} O_5$	-4.03
25	Armillarilin	11.619	430.1993	$C_{24} H_{30} O_7$	-0.45
26	Clerodin	11.675	434.2304	$C_{24} H_{34} O_7$	0.09
27	Lagerstroemine	12.424	437.218	$C_{26} H_{31} N O_5$	5.12
28	3-O-Methylcoumestrol	12.638	282.052	$C_{16} H_{10} O_5$	2.87
29	9,10,13-trihydroxy-11-octadecenoic acid	12.981	330.2389	$C_{18} H_{34} O_5$	5.34
30	Gibberellin A45	13.055	332.1634	$C_{19} H_{24} O_5$	-3.13
31	Sulfolithocholylglycine	13.493	513.2728	$C_{26} H_{43} N O_7S$	6.35
32	Piscerythramine	13.791	451.1973	$C_{26} H_{29} N O_6$	4.95
33	Kurarinone	14.464	438.2033	$C_{26} H_{30} O_6$	2.2

34	4-O-Methylmelleolide	14.9	414.2036	$C_{24} H_{30} O_6$	1.45
35	Diasarone 2	14.793	416.2206	$C_{24} H_{32} O_6$	-1.61
36	1-Dehydro-9-fluoro-11-oxotestololactone	15.126	332.1451	$C_{19} H_{21} F O_4$	-8.3
37	Staurosporine	15.332	466.1987	$C_{28} H_{26} N_4 O_3$	3.87
38	Lucidone B	15.619	400.2257	$C_{24} H_{32} O_5$	-1.81
39	10-Hydroxymelleolide	15.879	416.1848	$C_{23} H_{28} O_7$	-3.03
40	Corrinoid	15.891	306.1844	$C_{19} H_{22} N_4$	0.2
41	Citreoviridin	16.034	402.2048	$C_{23} H_{30} O_6$	-1.47
42	Kanzonol K	16.303	436.1875	$C_{26} H_{28} O_6$	2.61
43	Osajin	16.401	404.1605	$C_{25} H_{24} O_5$	4.62
44	Cinegalline	16.721	430.2071	$C_{23} H_{30} N_2 O_6$	7.76
45	Fluocinolone acetonide	20.059	452.1988	$C_{24} H_{30} F_2 O_6$	4.91
46	Schizandrin	11.33	432.2139	$C_{24} H_{32} O_7$	1.98

SF-EXT OF *S. flavescens* root. _-VE. d

S. No	Compound name	RT (min)	Mass	Formula	DB Diff (ppm)
1	Brompheniramine	1.89	318.0724	$C_{16} H_{19} Br N_2$	2.42
2	(R)-(+)-2-Pyrrolidone-5-carboxylic acid	2.445	129.042	$C_5 H_7 N O_3$	4.61
3	Fukiic acid	4.131	272.0533	$C_{11} H_{12} O_8$	-0.35
4	Mollicellin D	4.268	404.0971	$C_{21} H_{21} Cl O_6$	13.77
5	D-Lombricine	4.397	270.0746	$C_6 H_{15} N_4 O_6 P$	-6.19
6	Sophocarpine	3.555	249.1956	$C_{15}H_{22}N_2O$	1.3
7	3-Phenoxypropionic acid	4.702	166.0626	$C_9 H_{10} O_3$	2.21
8	5-Hydroxyferulate	4.709	210.0527	$C_{10} H_{10} O_5$	0.64
9	(Z)-2-Methyl-2-butene-1,4-diol 4-O-β-D-glucopyranoside	5.183	264.1212	$C_{11} H_{20} O_7$	-0.98
10	7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone-7-glucoside	5.575	438.154	$C_{21} H_{26} O_{10}$	-3.26
11	Irigenin 7-O-glucoside	6.056	522.1396	$C_{24} H_{26} O_{13}$	-4.27
12	Monomethyl phthalate	6.128	180.0417	$C_9 H_8 O_4$	3.17
13	(1R,6R)-6-Hydroxy-2-succinyl-2,4-cyclohexadiene-1-carboxylate	6.403	240.0634	$C_{11} H_{12} O_6$	0.08
14	Gentisic acid	6.657	154.0262	$C_7 H_6 O_4$	2.33

15	Neocarthamin	6.738	450.1178	$C_{21} H_{22} O_{11}$	-3.45
16	Eriocitrin	6.803	596.1767	$C_{27} H_{32} O_{15}$	-4.41
17	Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	7.483	624.1726	$C_{28} H_{32} O_{16}$	-5.72
18	Norrubrofusarin 6-beta-gentiobioside	7.783	582.1614	$C_{26} H_{30} O_{15}$	-5.02
19	Piperenol C	8.401	448.1387	$C_{22} H_{24} O_{10}$	-4.01
20	Chamaemeloside	8.76	576.1512	$C_{27} H_{28} O_{14}$	-5.72
21	Ginkgetin	8.765	566.1204	$C_{32} H_{22} O_{10}$	1.53
22	7-Hydroxy-3-methoxy-1-primeverosyloxyxanthone	9.043	552.1412	$C_{25} H_{28} O_{14}$	12.21
23	Kaempferol 3-xylosylglucoside	9.044	580.1455	$C_{26} H_{28} O_{15}$	-4.66
24	Mulberroside F	9.4	566.1662	$C_{26} H_{30} O_{14}$	-4.71
25	Camellianin B	9.648	578.167	$C_{27} H_{30} O_{14}$	-5.99
26	1-Octen-3-yl primeveroside	9.714	422.2174	$C_{19} H_{34} O_{10}$	-5.26
27	Tricin 5-glucoside	10.243	492.1291	$C_{23} H_{24} O_{12}$	-4.64
28	7-Chloro-3,3',4',5,6,8-hexamethoxyflavone	10.247	436.0947	$C_{21} H_{21} Cl O_8$	-4.94
29	Deacetylnomilin	10.356	472.2117	$C_{26} H_{32} O_8$	-4.19
30	Wogonin	10.503	284.0691	$C_{16} H_{12} O_5$	-2.28

31	Butyrylmallotochromene	10.817	470.1961	$C_{26} H_{30} O_8$	-4.41
32	9-Hydroxyrisperidone	10.985	426.2063	$C_{23} H_{27} F N_4 O_3$	0.98
33	Austinol	11.042	458.1962	$C_{25} H_{30} O_8$	-4.68
34	Samidin	11.282	386.1381	$C_{21} H_{22} O_7$	-4.13
35	Tricoccin S3	11.388	454.2011	$C_{26} H_{30} O_7$	-4.25
36	Kurarinol	11.527	456.2149	$C_{26} H_{32} O_7$	-0.22
37	Baicalein	11.555	270.0531	$C_{15} H_{10} O_5$	-1.19
38	BisindolylmaleimideI	11.663	412.1904	$C_{25} H_{24} N_4 O_2$	-1.16
39	Phrymarolin I	11.823	488.1344	$C_{24} H_{24} O_{11}$	-5.29
40	Rheidin A	11.827	524.1092	$C_{30} H_{20} O_9$	2.93
41	Fragransol D	11.937	370.1427	$C_{21} H_{22} O_6$	-2.85
42	(9S,12S,13S)-Trihydroxy-10E-octadecenoic acid	12.083	330.2415	$C_{18} H_{34} O_5$	-2.65
43	9α-Fluoro-11β,16α,17α,21-tetrahydroxypregn-4-ene-3,20-dione	12.148	396.1948	$C_{21} H_{29} F O_6$	0.07
44	Cochliophilin A	12.577	282.0532	$C_{16} H_{10} O_5$	-1.23
45	Casegravol isovalerate	12.73	360.1581	$C_{20} H_{24} O_6$	-2.36
46	Dalbergin	12.792	268.0739	$C_{16} H_{12} O_4$	-1.42
47	Triamcinolone	12.815	394.1796	$C_{21} H_{27} F O_6$	-1.02
48	2,3-Dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(1proenyl)benzofuran	13.023	354.1476	$C_{21} H_{22} O_5$	-2.57

49	PIP(18:2(9Z,12Z)/18:0	13.412	942.5258	$C_{45} H_{84} O_{16} P_2$	-2.44
50	Cubebin	13.488	356.1269	$C_{20} H_{20} O_6$	-2.58
51	Mollicellin H	13.782	368.1265	$C_{21} H_{20} O_6$	-1.37
52	5,7Dihydroxychromone	13.905	178.0264	$C_9 H_6 O_4$	1.37
53	Kanzonol G	14.491	438.2062	$C_{26} H_{30} O_6$	-4.39
54	Sugeonyl acetate	14.495	276.173	$C_{17} H_{24} O_3$	-1.8
55	Sophoridine	2.454	249.1956	$C_{15}H_{24}N_2O$	-0.8
56	1,6-Dihydroxy-3,7-dimethoxy-2-(3-methyl-2-butenyl)-8-(2-hydroxy-3-methyl-3-butenyl)-xanthone	14.756	440.1862	$C_{25} H_{28} O_7$	-6.1
57	Desmethylxanthohumol	14.858	340.132	$C_{20} H_{20} O_5$	-2.77
58	Bakkenolide D	15.019	408.1603	$C_{21} H_{28} O_6 S$	0.93
59	Sesamin	15.117	354.1113	$C_{20} H_{18} O_6$	-2.59
60	Lipiferolide	15.17	306.1474	$C_{17} H_{22} O_5$	-2.11
61	Glyurallin B	15.547	422.1751	$C_{25} H_{26} O_6$	-5.14
62	Fludrocortisone acetate	15.625	422.2106	$C_{23} H_{31} F O_6$	-0.26
63	Artonin V	15.773	438.1694	$C_{25} H_{26} O_7$	-3.64
64	17β-Acetyl-1,2,3,4,6α,7α,10,12,13,14α,16,17-dodecahydro-3β-hydroxy-10β,13β-dimethyl-5β,8β-etheno-15H-	15.886	452.2188	$C_{27} H_{32} O_6$	2.39

	cyclopenta[a]phenanthrene-6,7-dicarboxylic anhydride acetate				
65	3''-Hydroxy-geranylhydroquinone	16.077	262.1571	$C_{16} H_{22} O_3$	-0.69
66	6alpha-Fluoroprednisolone	16.081	378.1847	$C_{21} H_{27} F O_5$	-1.17
67	2,3-Dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(prop-1-enyl)benzofuran"	17.239	354.1478	$C_{21} H_{22} O_5$	-3.08
68	3-Hydroxycoumarin	18.335	162.0312	$C_9 H_6 O_3$	2.79
69	PD 123319	18.808	508.2482	$C_{31} H_{32} N_4 O_3$	-1.54
70	17,21-Epoxy-9-fluoro-11-hydroxypregn-4-ene-3,20-dione	18.993	362.1892	$C_{21} H_{27} F O_4$	0.52
71	Prosolanapyrone II	19.532	304.1677	$C_{18} H_{24} O_4$	-0.78
72	Roxburghine B	20.307	492.2529	$C_{31} H_{32} N_4 O_2$	-0.69
73	16-Feruloyloxypalmitate	21.763	448.2837	$C_{26} H_{40} O_6$	-2.77
74	Ethyl 2E,4Z-hexadecadienoate	23.33	280.2405	$C_{18} H_{32} O_2$	-1.13

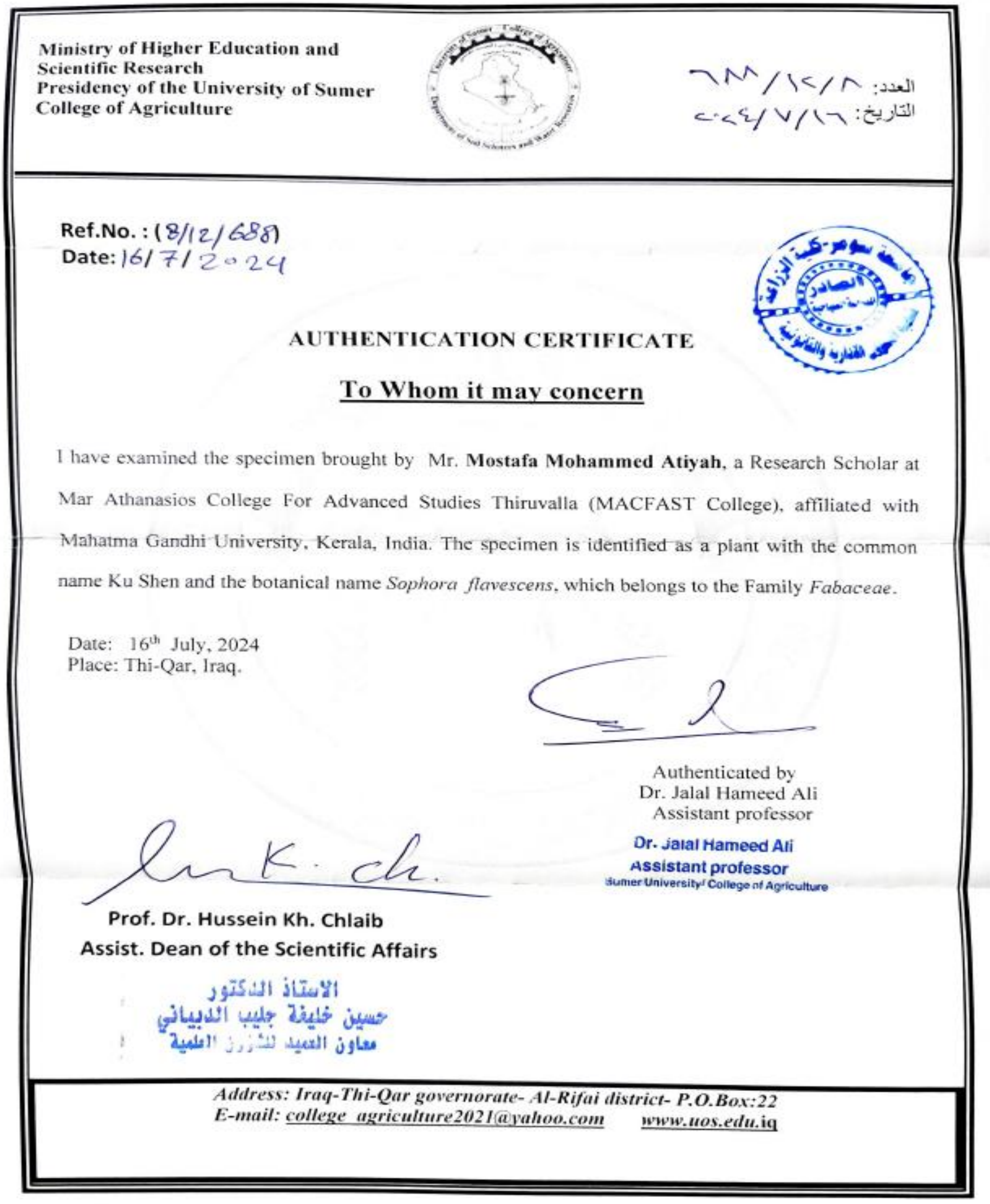
Table S2. Binding affinities (docking scores) of bioactive compounds from *S. flavescens* root against *C. albicans* CYP51 (PDB ID: 5V5Z).

S. No	Compounds	Binding Affinity (Kcal/mol)
1	(+)-Mahanimbicine	-10.1
2	(10Z,14E,16E)-10,14,16-Octadecatrien-12-ynoic acid	-6.4
3	1-Dehydro-9-fluoro-11-oxotestololactone	-9.7
4	3-Hydroxyropivacaine	-7.5
5	3-O-Methylcoumestrol	-8.3
6	4-O-Methylmelleolide	-9.7
7	7-Dehydrologanin tetraacetate	-7.0
8	9,10,13-trihydroxy-11-octadecenoic acid	-6.6
9	19-Noretiocholanolone	-8.0
10	ar-Artemisene	-8.3
11	Armillarilin	-9.5
12	Axisothiocyanate 3	-7.6
13	Azidopine	-8.0
14	Cadiamine	-7.2
15	Cinegalline	-8.0
16	Citreoviridin	-7.9
17	Clerodin	-7.4
18	Piscerythramine	-8.5
19	Convalloside	-8.5
20	Diasarone 2	-6.4
21	Fluocinolone acetonide	-9.4
22	Gibberellin A45	-8.5
23	Kanzonol K	-8.0
24	Kaur-16-en-18-ol	-8.5

25	Kurarinone	-8.6
26	Lagerstroemine	-7.5
27	Neogrifolin	-7.8
28	Oleuropein	-8.5
29	Orientalone	-7.7
30	Osajin	-8.3
31	Prunetin	-8.2
32	Retinaldehyde	-8.7
33	Retinol / Retinol skeleton	-7.1
34	Schizandrin	-6.6
35	Smyrindioloside	-8.9
36	Sulfolithocholylglycine	-9.2
37	Lucidone B	-9.2
38	10-Hydroxymelleolide	-7.9
39	(1R,6R)-6-Hydroxy-2-succinyl-2,4-cyclohexadiene-1-carboxylate	-6.3
40	(Z)-2-Methyl-2-butene-1,4-diol 4-O-β-D-glucopyranoside	-6.2
41	1,6-Dihydroxy-3,7-dimethoxy-2-(3-methyl-2-butenyl)-8-(2-hydroxy-3-methyl-3-butenyl)-xanthone	-8.5
42	2,3-Dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(prop-1-enyl)benzofuran	-9.1
43	3''-Hydroxy-geranylhydroquinone	-8.0
44	3-Hydroxycoumarin	-6.3
45	5,7 Dihydroxychromone	-8.6
46	5-Hydroxyferulate	-6.2
47	6alpha-Fluoroprednisolone	-8.5
48	7-Chloro-3,3',4',5,6,8-hexamethoxyflavone	-7.5
49	9α-Fluoro-11β,16α,17α,21-tetrahydroxypregn-4-ene-3,20-dione	-8.6
50	9-Hydroxyrisperidone	-10.0
51	9S,12S,13S-trihydroxy-10E-octadecenoic acid	-6.0

52	Artonin V	-8.8
53	Austinol	-10.5
54	Baicalein	-9.1
55	Bakkenolide D	-7.3
56	Brompheniramine	-6.9
57	Butyrylmallotochromene	-7.9
58	Camellianin B	-9.5
59	Casegravol isovalerate	-7.4
60	Chamaemeloside	-7.6
61	Cubebin	-10.4
62	Dalbergin	-7.6
63	Cochliophilin A	-9.0
64	Deacetylnomilin	-8.1
65	Desmethylxanthohumol	-8.0
66	Eriocitrin	-10.2
67	Fludrocortisone acetate	-9.0
68	Fragransol D	-7.7
69	Fukiic acid	-6.8
70	Ginkgetin	-11.0
71	Glyurallin B	-9.2
72	Irigenin 7-O-glucoside	-7.9
73	Kaempferol 3-xylosylglucoside	-9.3
74	Kanzonol G	-7.7
75	Kurarinol	-8.7
76	Lipiferolide	-8.0
77	Mollicellin D	-6.9
78	Mollicellin H	-9.4
79	Mulberroside F	-10.5

80	Neocarthamin	-8.1
81	PD 123319	-9.6
82	Phrymarolin I	-8.3
83	Piperenol C	-7.3
84	Prosolanapyrone II	-6.8
85	Rheidin A	-9.4
86	Roxburghine B	-10.7
87	Samidin	-7.5
88	Sophocarpine	-7.9
89	Sesamin	-9.8
90	Sophoridine	-7.3
91	Triamcinolone	-8.6
92	Tricin 5-glucoside	-7.4
93	Wogonin	-7.7
94	7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone7-glucoside	-6.6
95	Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]	-8.7
96	Norrubrofusarin 6- beta-gentiobioside	-9.5
97	1-Octen-3-yl primeveroside	-7.9
98	Tricoccin S3	-8.6
99	BisindolylmaleimideI	-8.2
100	PIP(18:2(9Z,12Z)/18:0)	-6.6
101	Control positive (Itraconazole)	-9.3



Ministry of Higher Education and
Scientific Research
Presidency of the University of Sumer
College of Agriculture

العدد: ٨/١٢/٦٨٨
التاريخ: ١٦/٧/٢٠٢٤

Ref.No. : (8/12/688)
Date: 16/7/2024

AUTHENTICATION CERTIFICATE

To Whom it may concern

I have examined the specimen brought by Mr. **Mostafa Mohammed Atiyah**, a Research Scholar at Mar Athanasios College For Advanced Studies Thiruvalla (MACFAST College), affiliated with Mahatma Gandhi University, Kerala, India. The specimen is identified as a plant with the common name Ku Shen and the botanical name *Sophora flavescens*, which belongs to the Family *Fabaceae*.

Date: 16th July, 2024
Place: Thi-Qar, Iraq.

Authenticated by
Dr. Jalal Hameed Ali
Assistant professor

Dr. Jalal Hameed Ali
Assistant professor
Sumer University/ College of Agriculture

Prof. Dr. Hussein Kh. Chlaib
Assist. Dean of the Scientific Affairs

الاستاذ الدكتور
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Figure S1. Authentication certificate of *S. flavescens*.

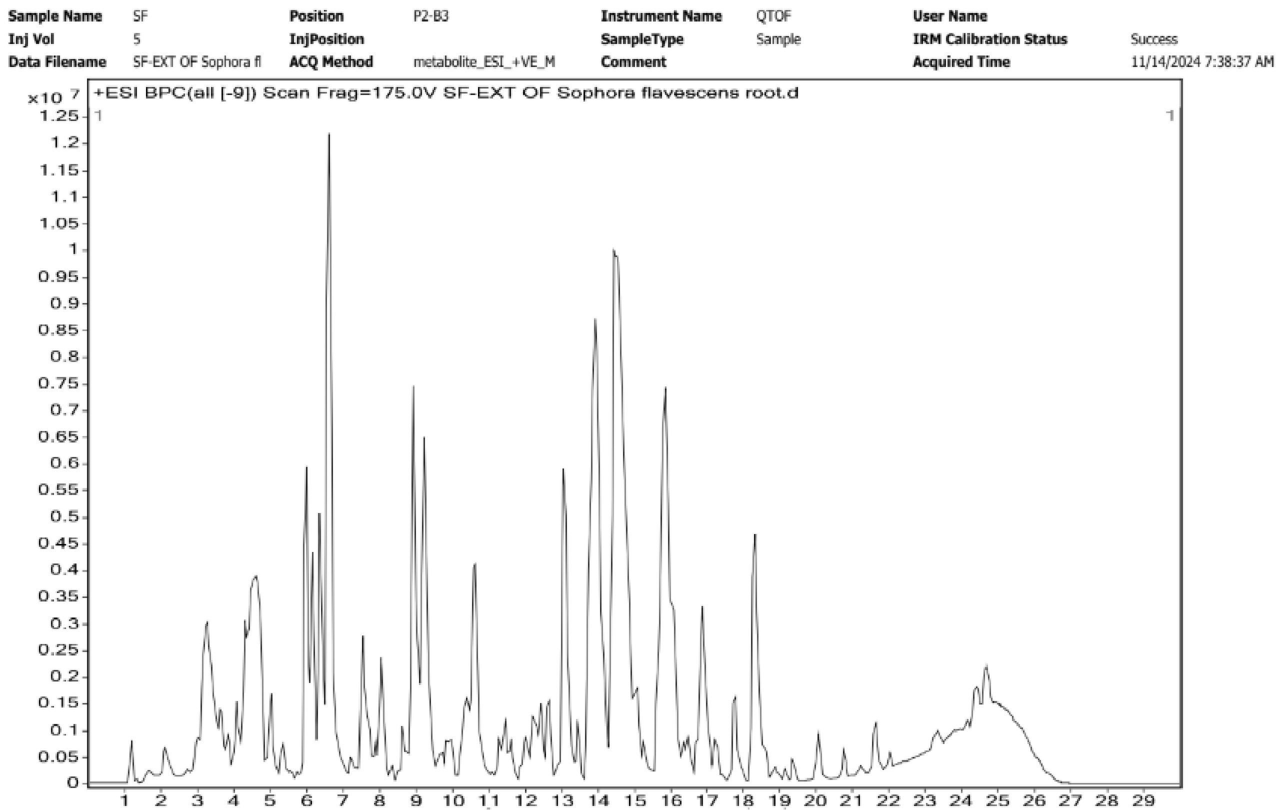


Figure S2. HR-LCMS Profile of *S. flavescens* root extract in Positive ESI Mode

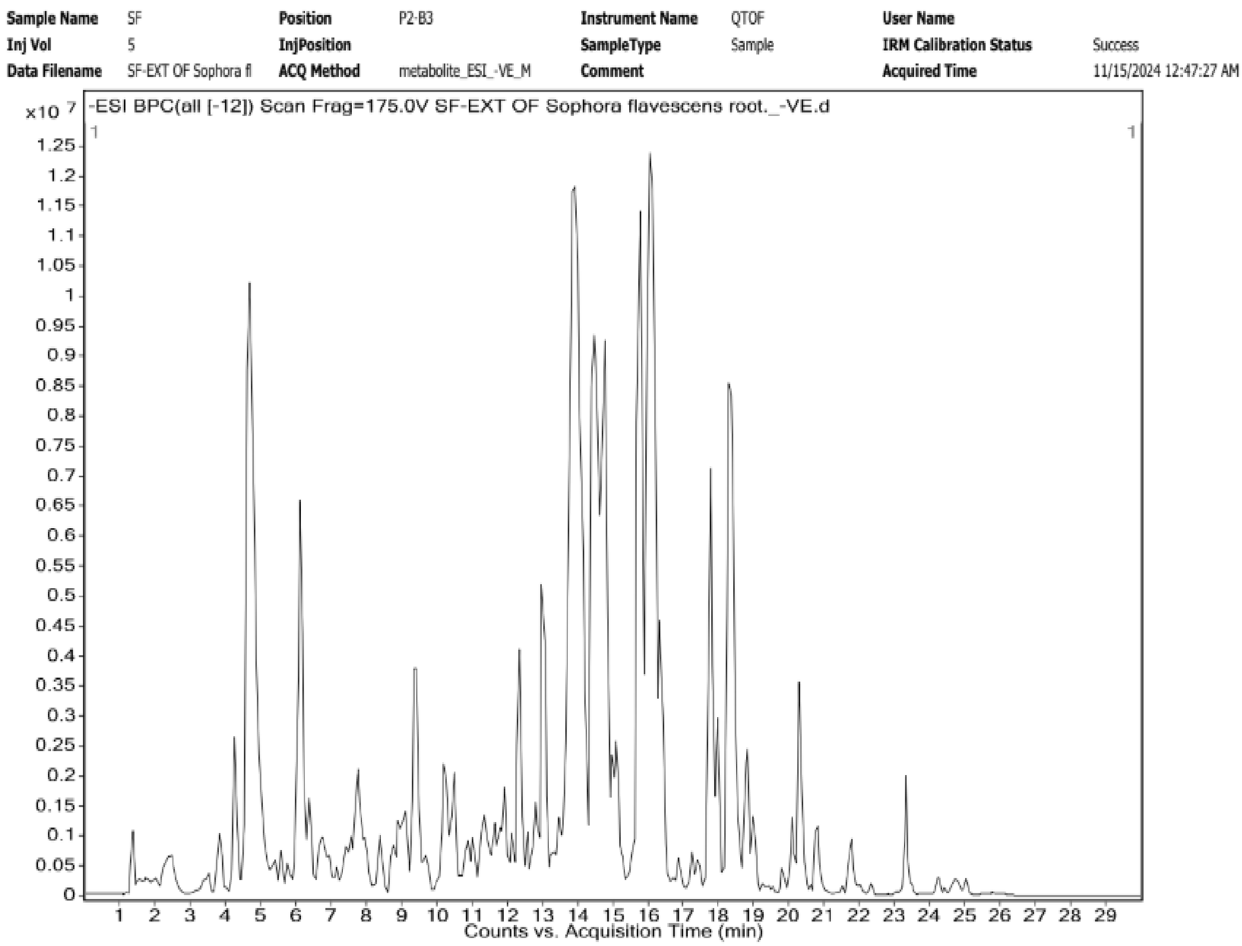


Figure S3. HR-LCMS Profile of *S. flavescens* root extract in Negative ESI Mode

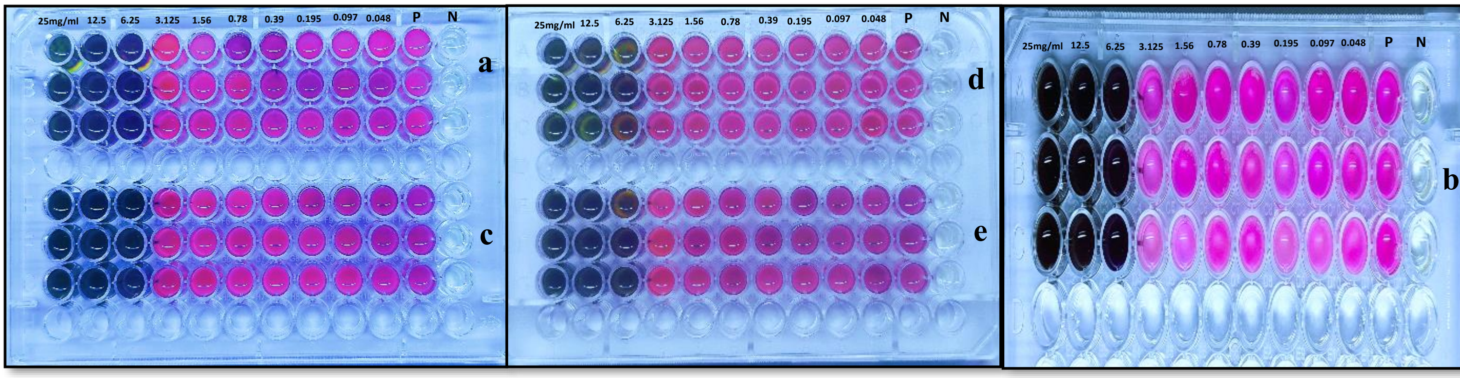


Figure S4: MIC determination using the microdilution assay for: (a) *C. auris*, (b) *C. krusei*, (c) *C. parapsilosis*, (d) *C. albicans*, and (e) *C. glabrata*.

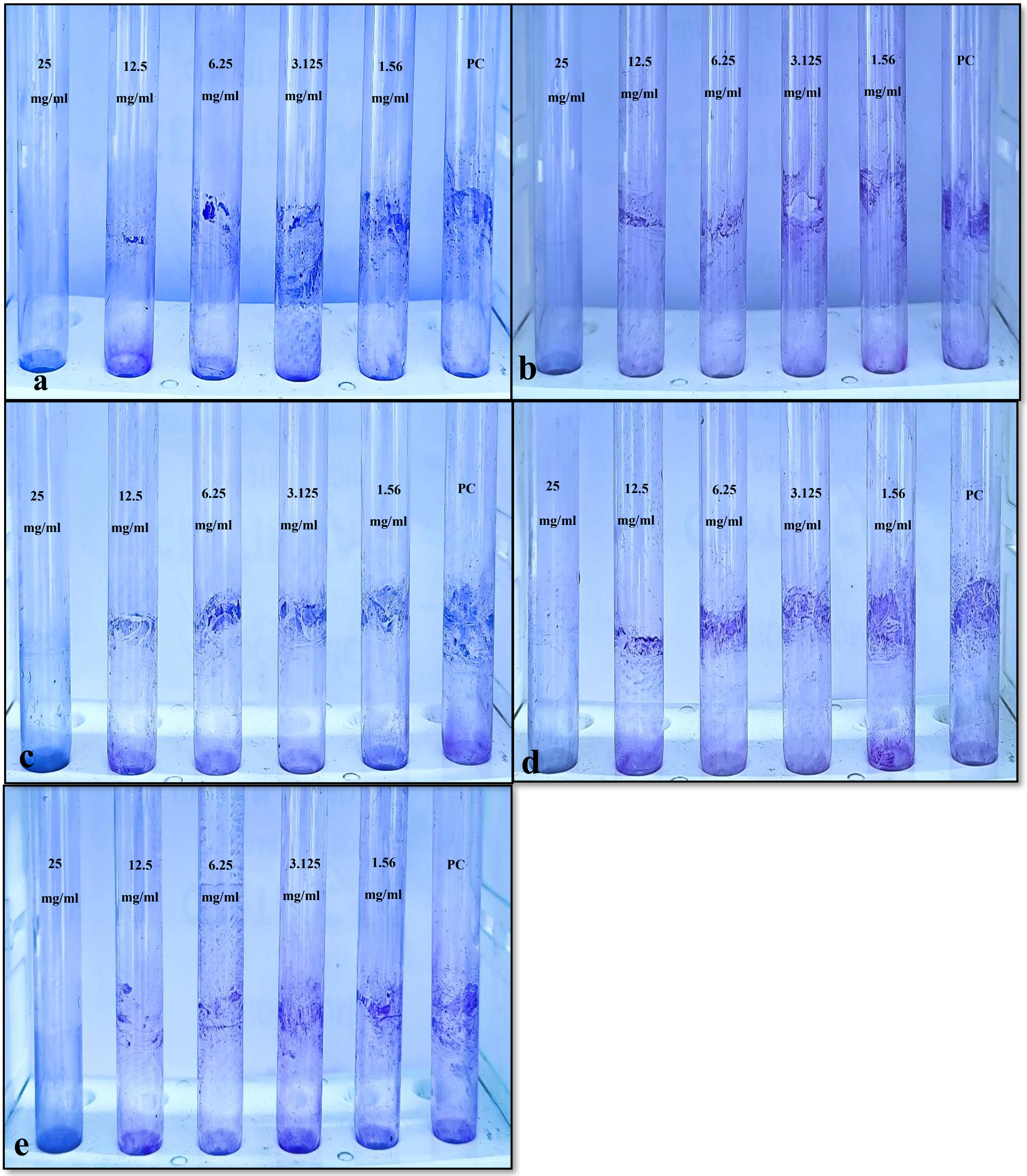
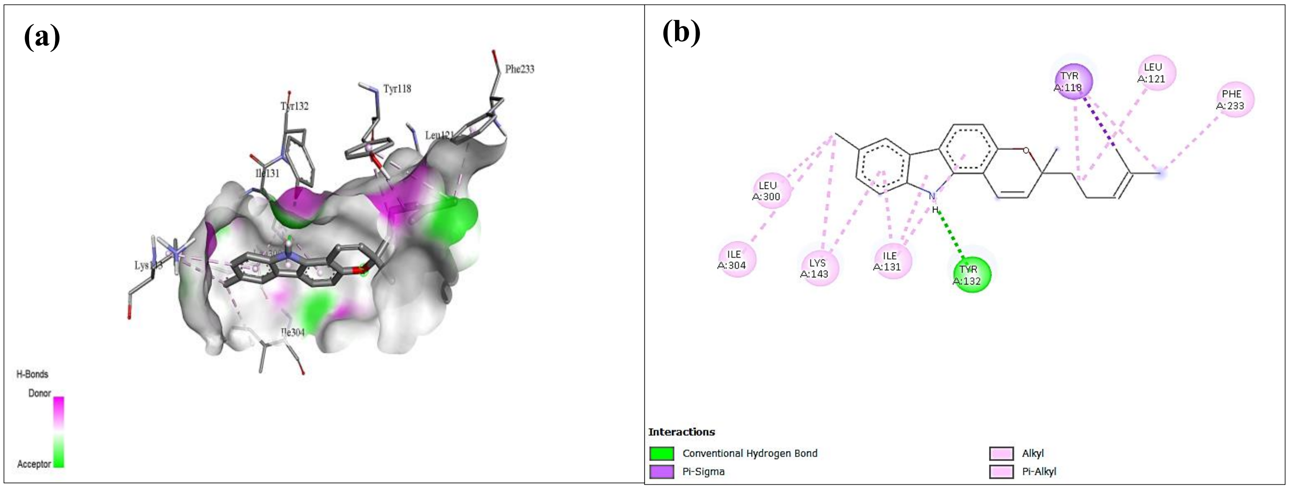
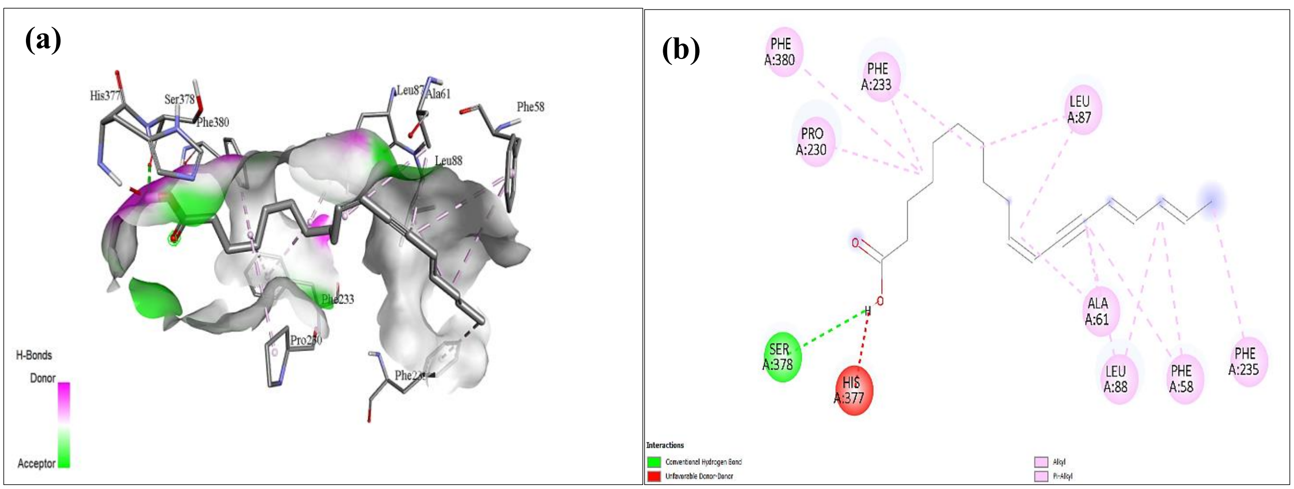


Figure S5: Biofilm formation on glass surfaces by *Candida* species isolates at inhibitory concentrations: (a) *C. auris*, (b) *C. krusei*, (c) *C. parapsilosis*, (d) *C. albicans*, and (e) *C. glabrata*. A positive control (PC) was included for comparison.

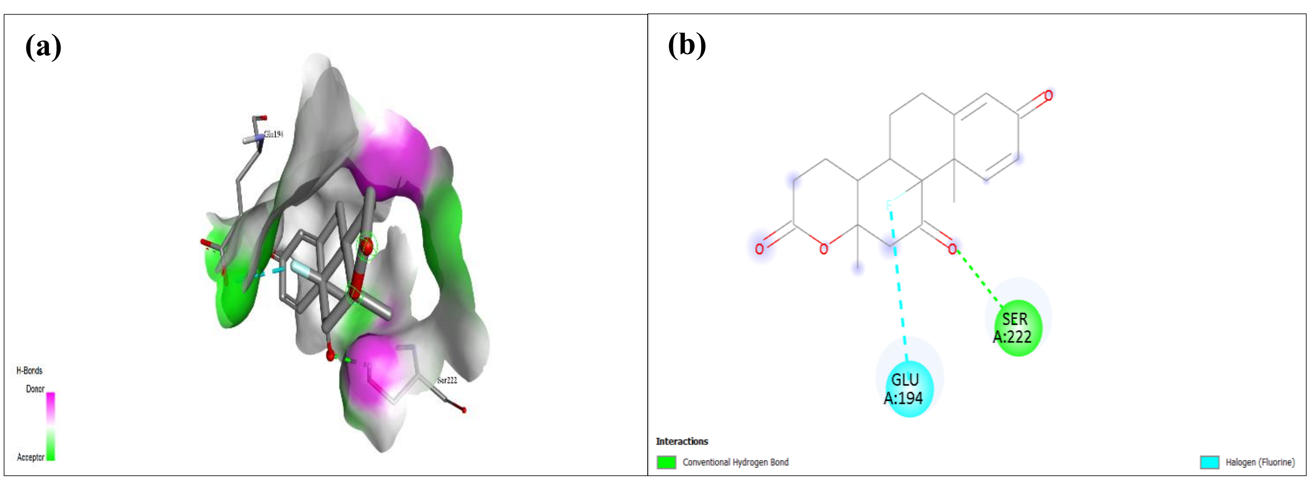


No. 1: Docked pose (+)-Mahanimbicine in the CYP51(5V5Z) active site.

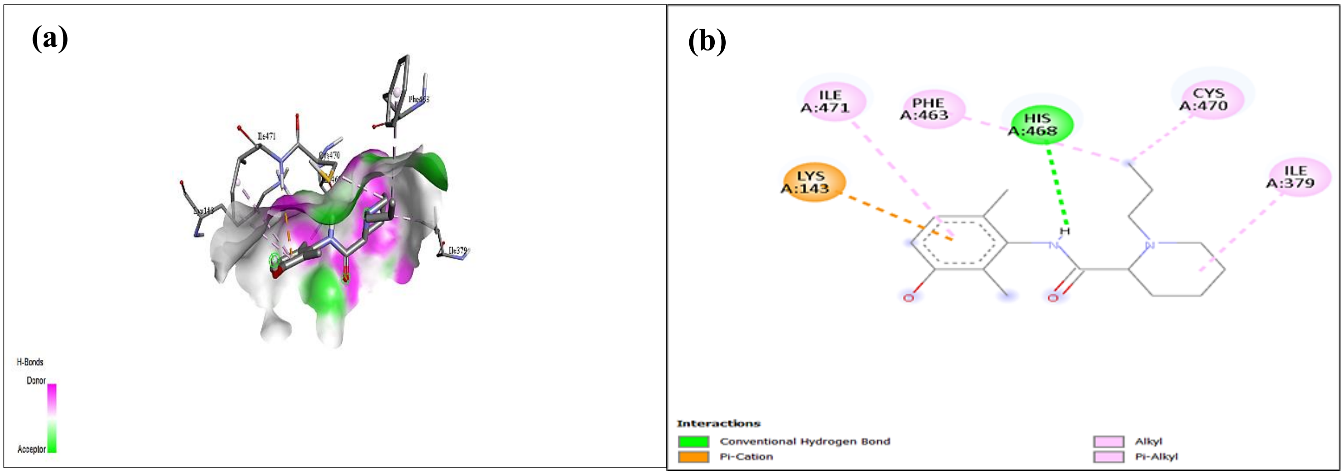


No. 2: Docked pose (10Z,14E,16E)-10,14,16-Octadecatrien-12-ynoic acid

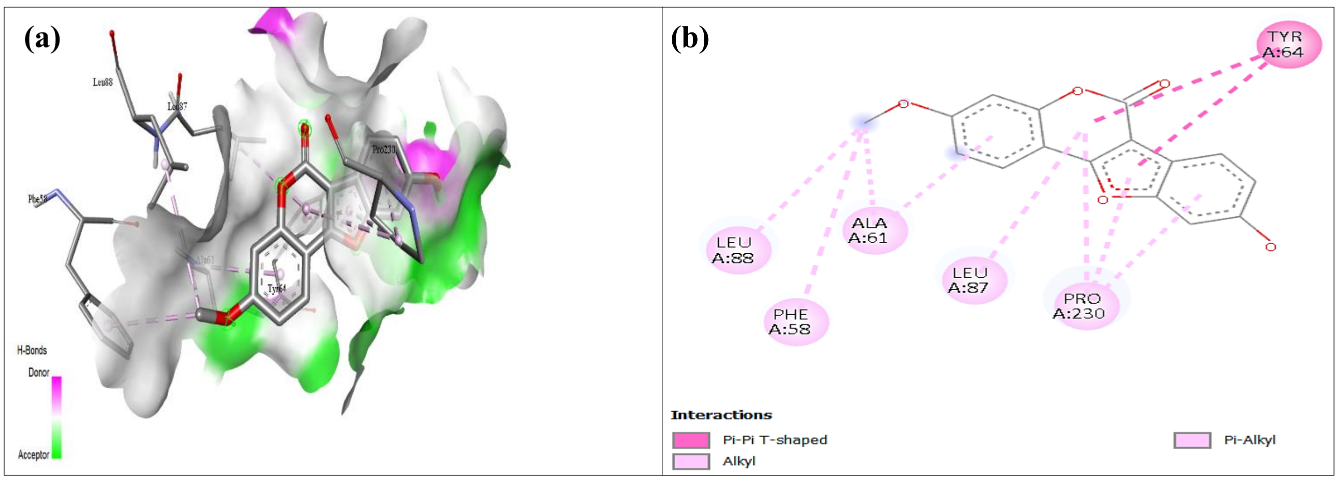
in the CYP51(5V5Z) active site.



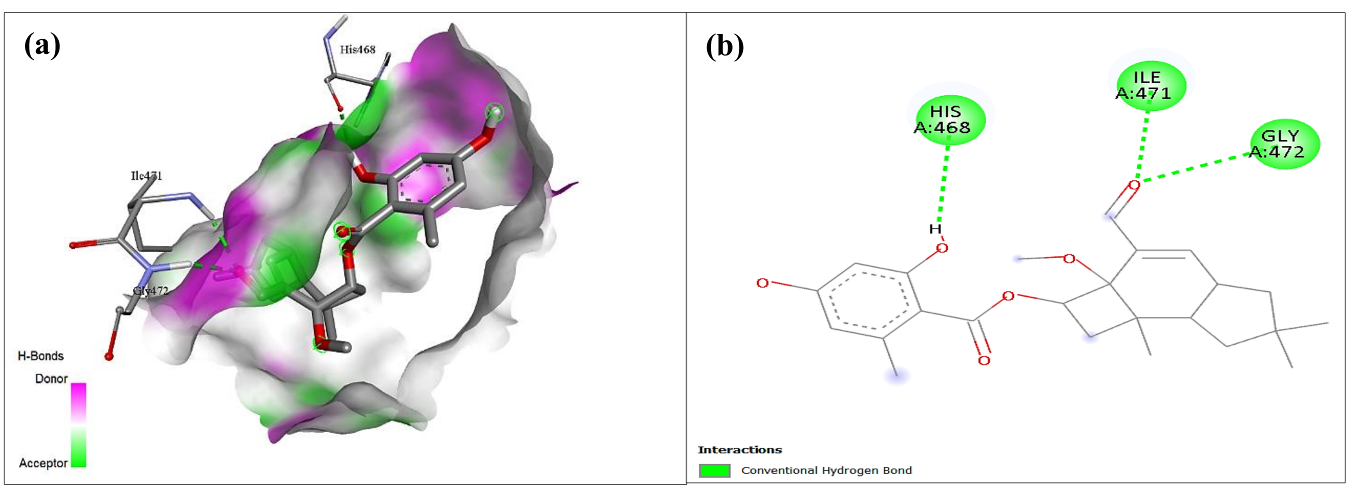
No. 3: Docked pose 1-Dehydro-9-fluoro-11-oxotestololactone in the CYP51(5V5Z) active site.



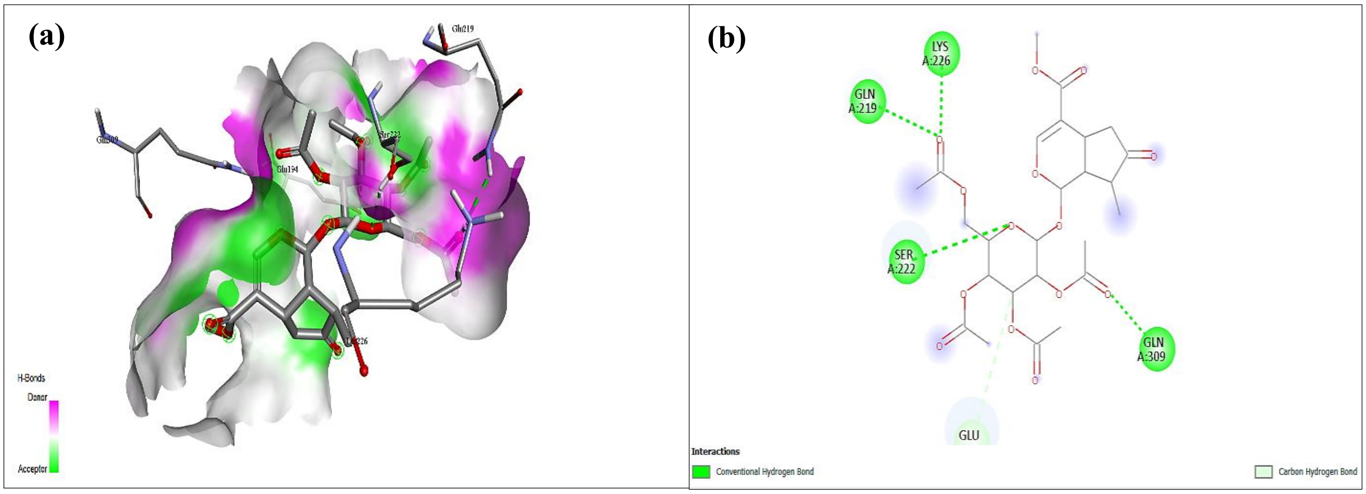
No. 4: Docked pose 3-Hydroxyropivacaine in the CYP51(5V5Z) active site.



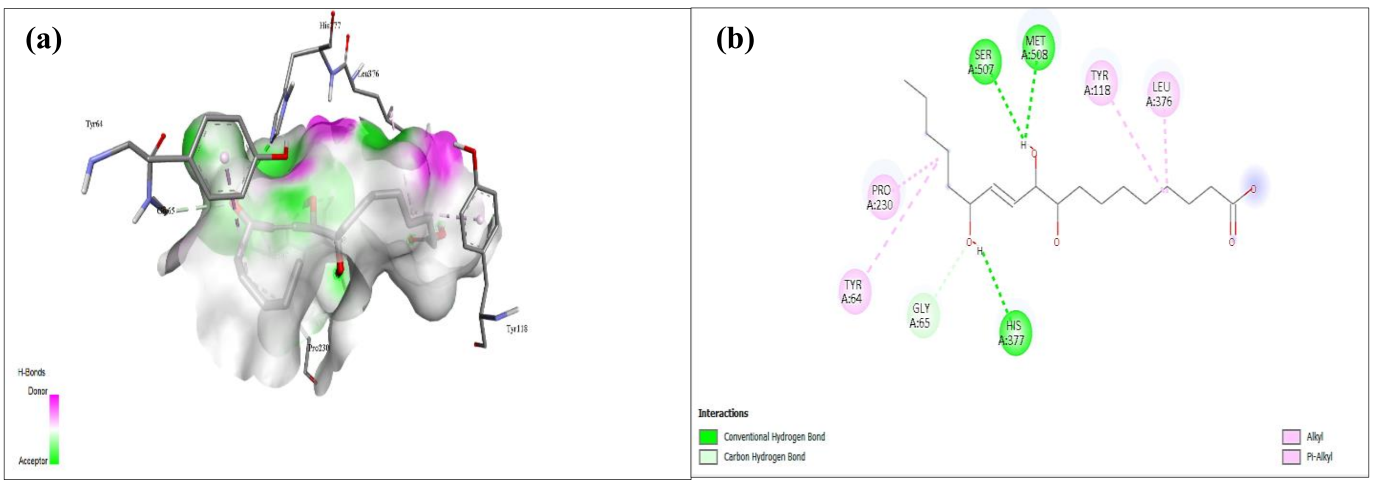
No. 5: Docked pose 3-O-Methylcoumestrol in the CYP51(5V5Z) active site.



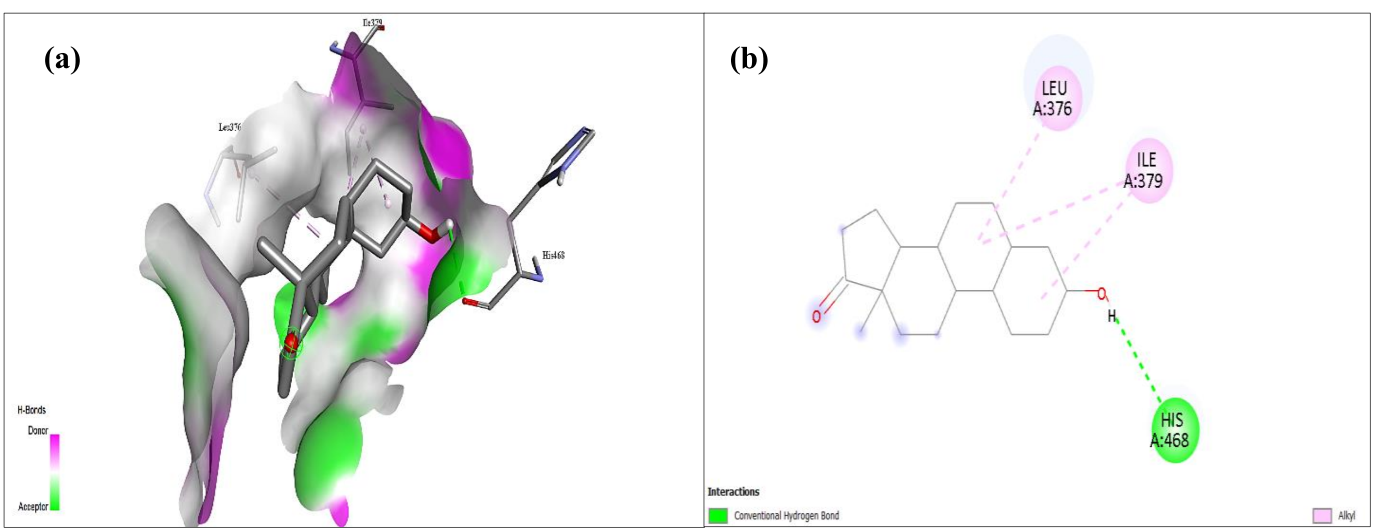
No. 6: Docked pose 4-O-Methylmelleolide in the CYP51(5V5Z) active site.



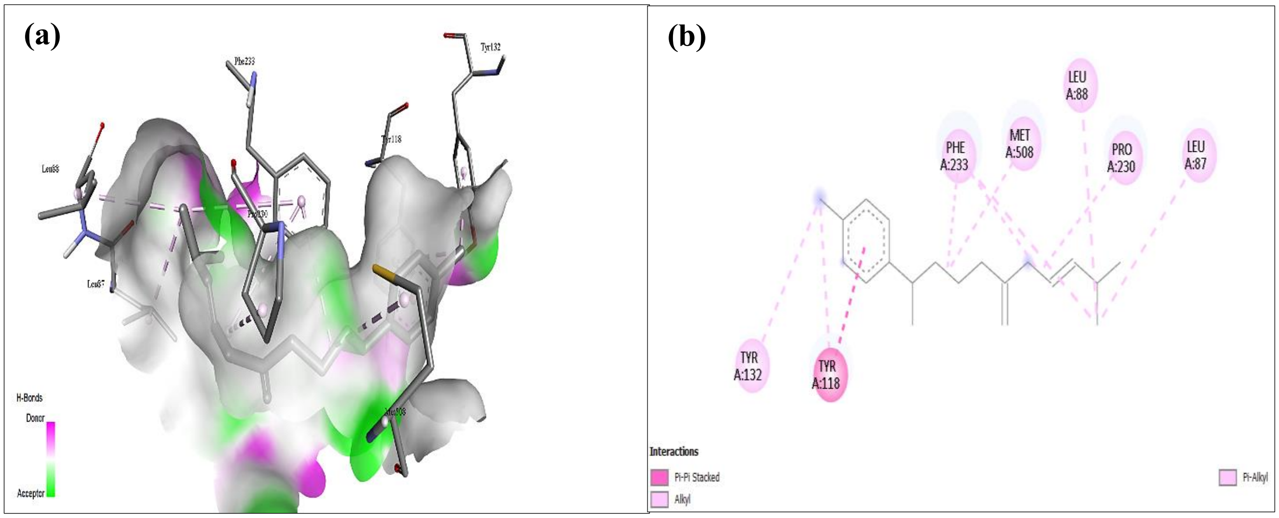
No. 7: Docked pose 7-Dehydrologanin tetraacetate in the CYP51(5V5Z) active site.



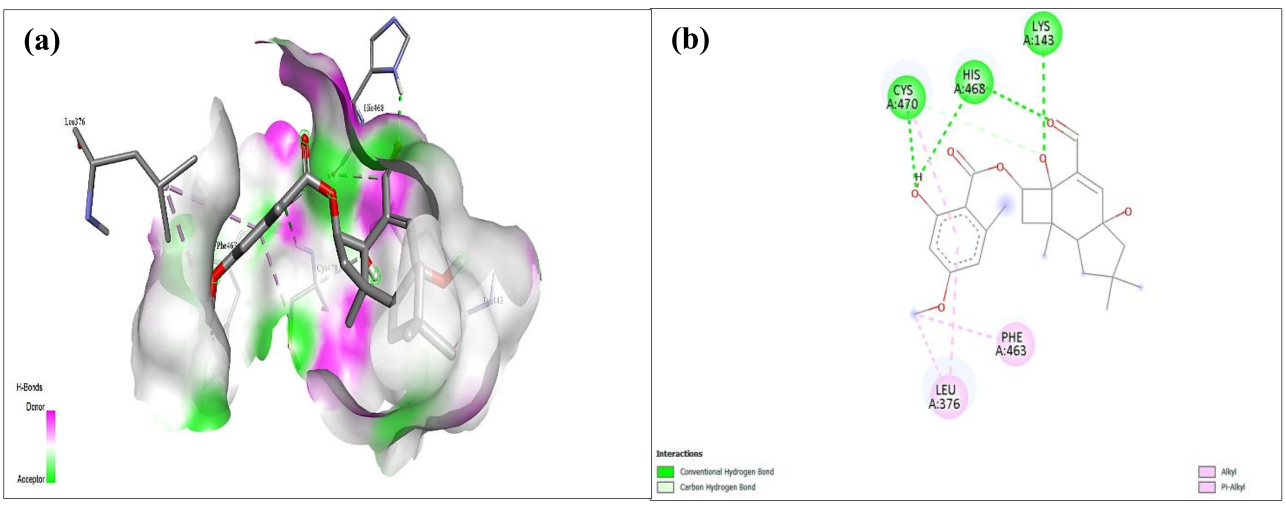
No. 8: Docked pose 9,10,13-trihydroxy-11- octadecenoic acid in the CYP51(5V5Z) active site.



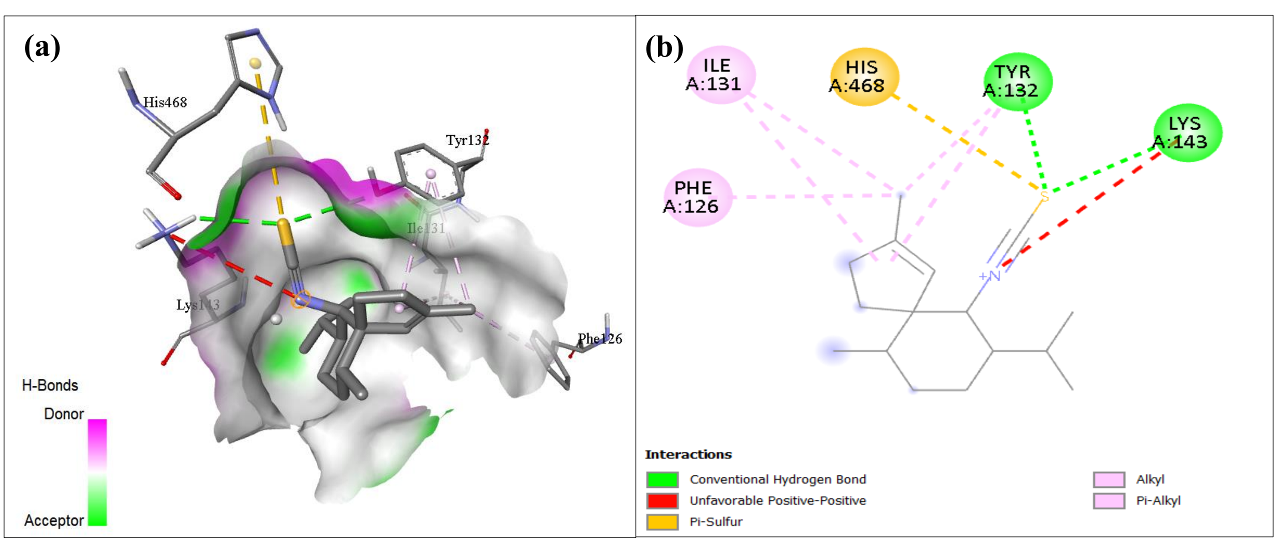
No. 9: Docked pose 19-Noretiocholanolone in the CYP51(5V5Z) active site.



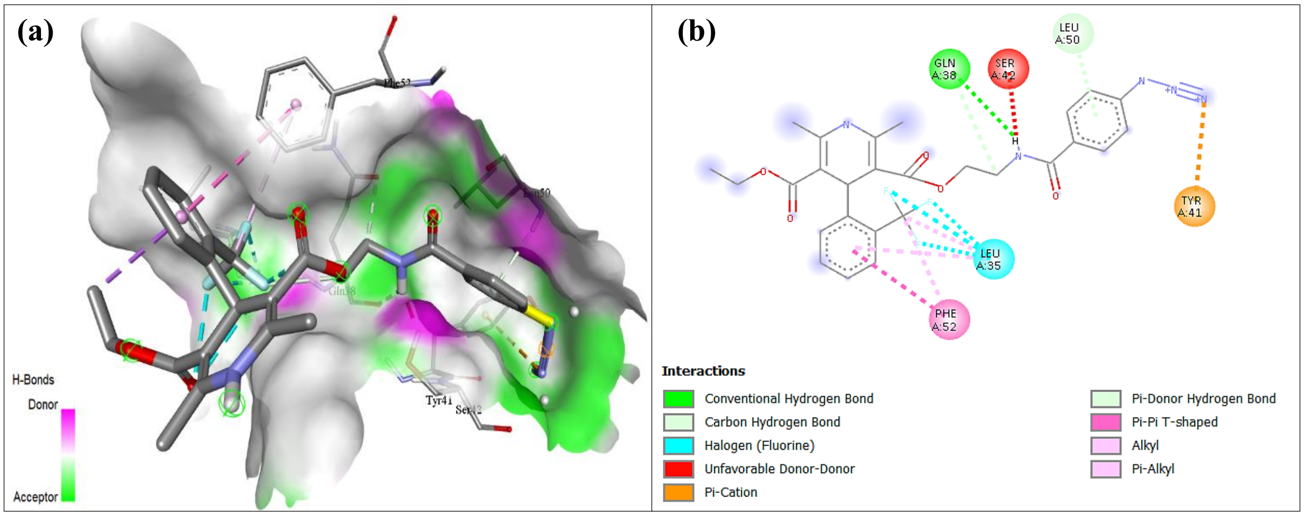
No. 10: Docked pose ar-Artemisene in the CYP51(5V5Z) active site.



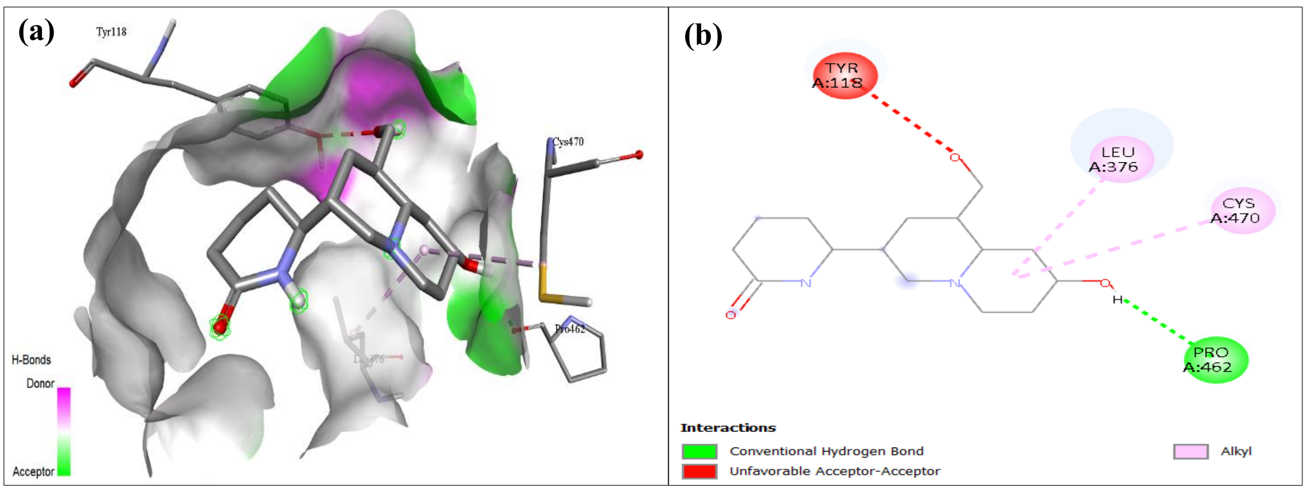
No. 11: Docked pose Armillarilin in the CYP51(5V5Z) active site.



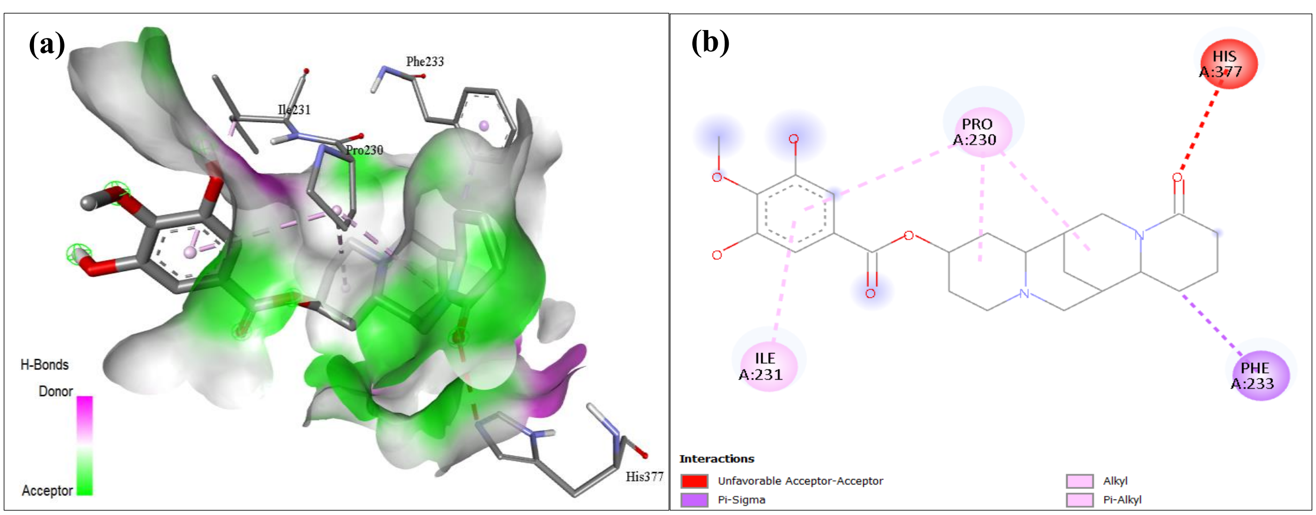
No. 12: Docked pose Axisothiocyanate 3 in the CYP51(5V5Z) active site.



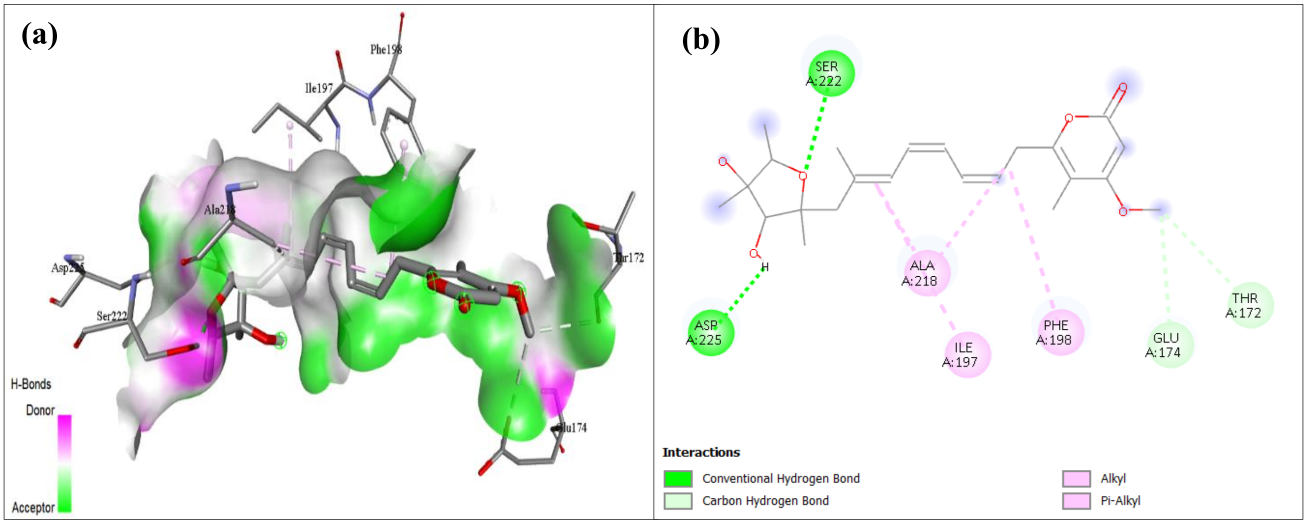
No. 13: Docked pose Azidopine in the CYP51(5V5Z) active site.



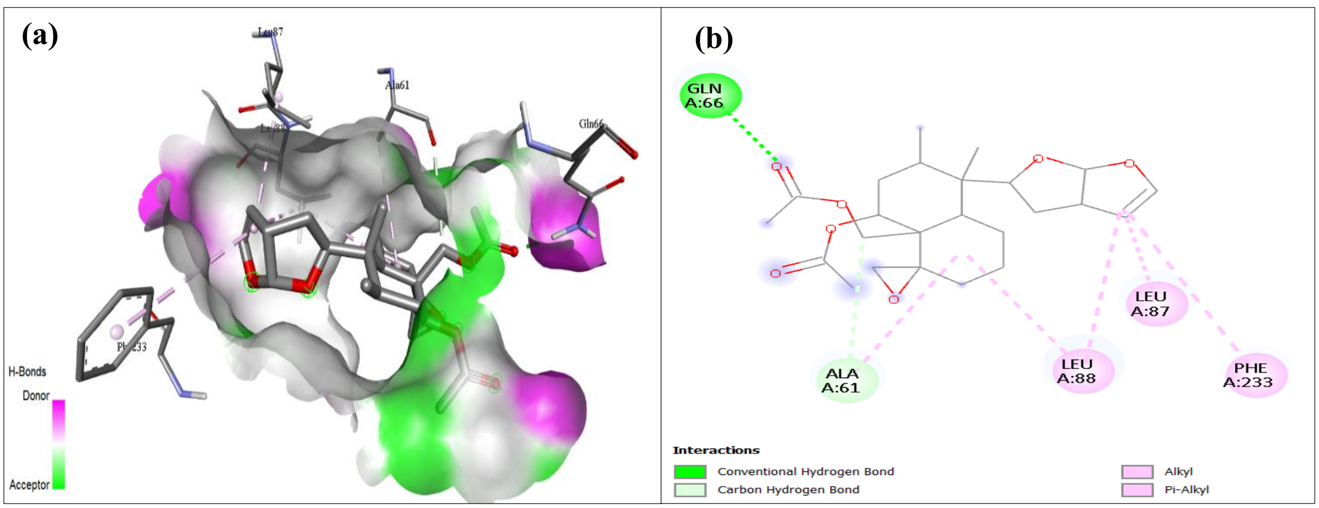
No. 14: Docked pose Cadiamine in the CYP51(5V5Z) active site.



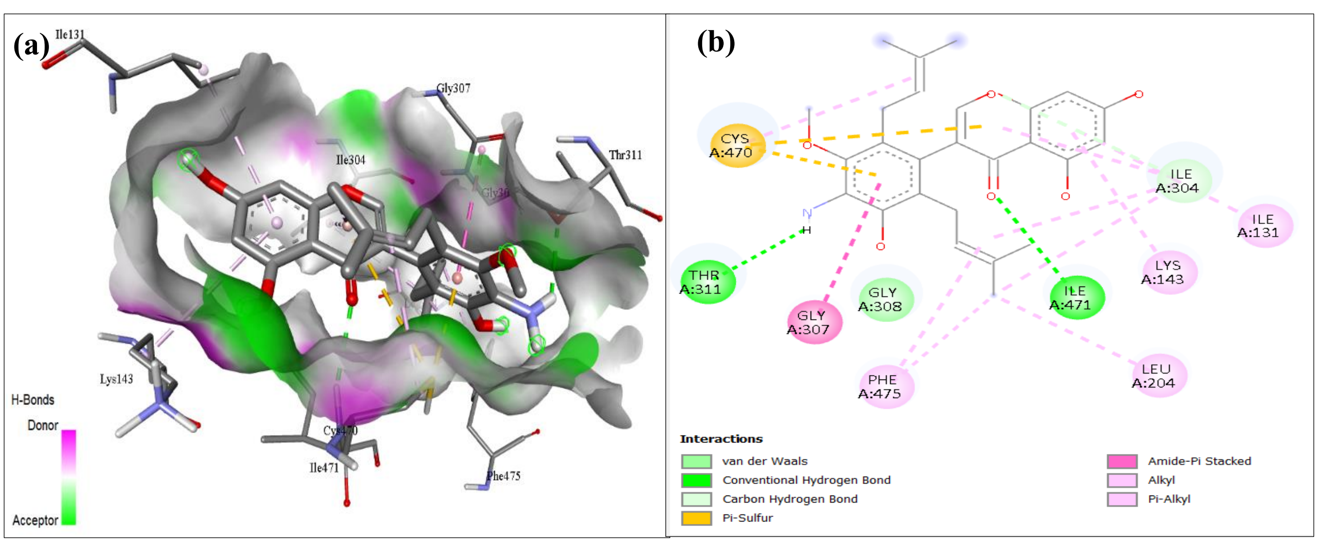
No. 15: Docked pose Cinegalline in the CYP51(5V5Z) active site.



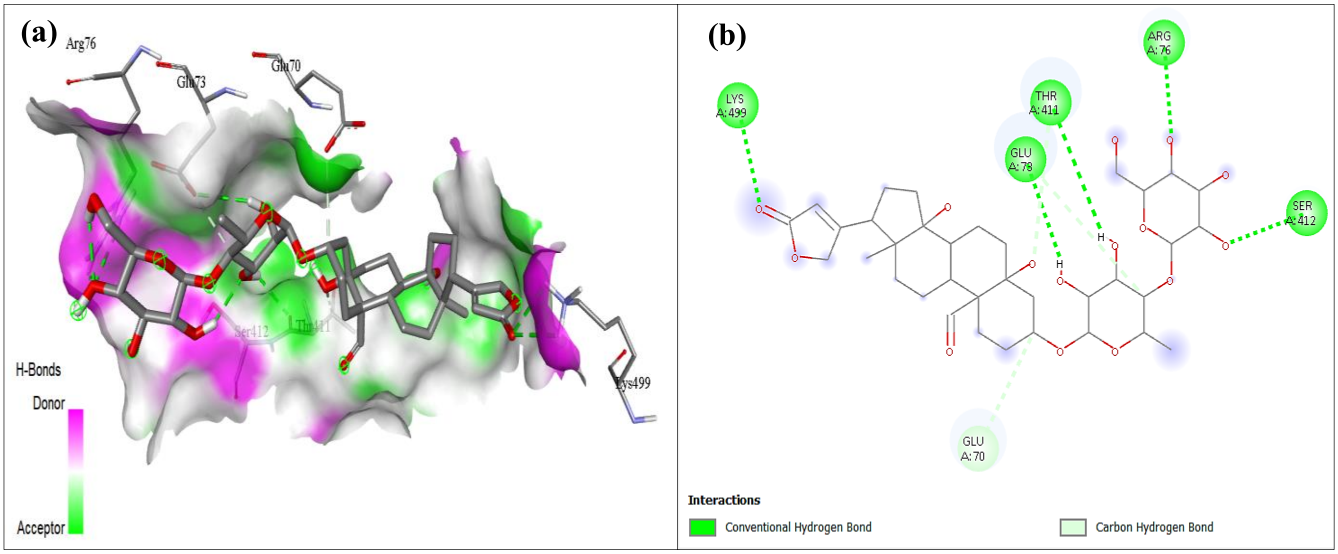
No.16: Docked pose Citreoviridin in the CYP51(5V5Z) active site.



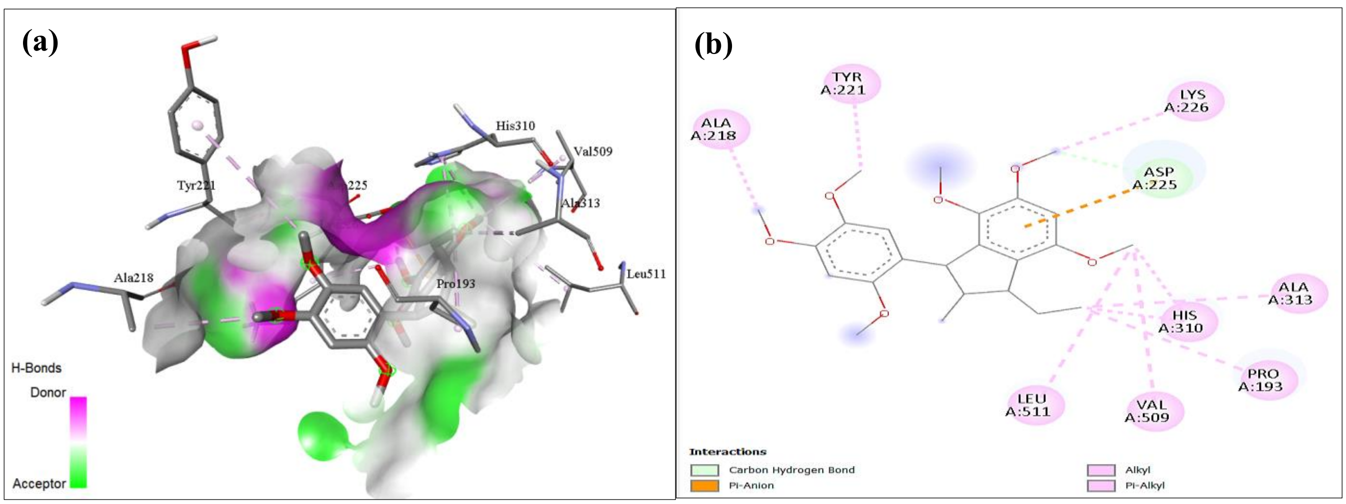
No. 17: Docked pose Clerodin in the CYP51(5V5Z) active site.



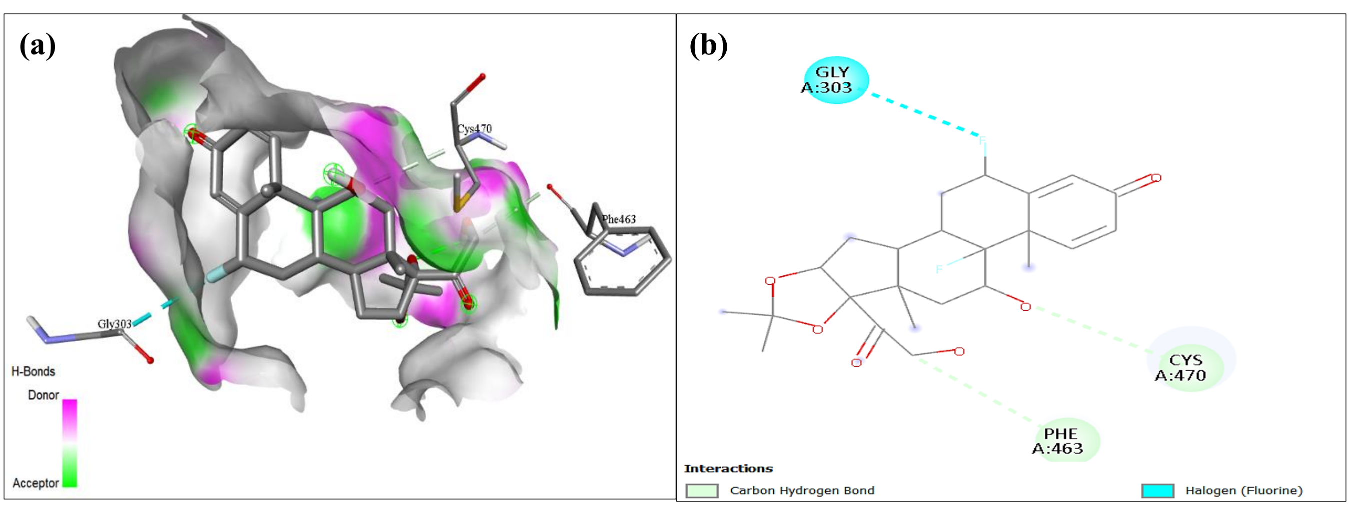
No. 18: Docked pose Piscerythramine in the CYP51(5V5Z) active site.



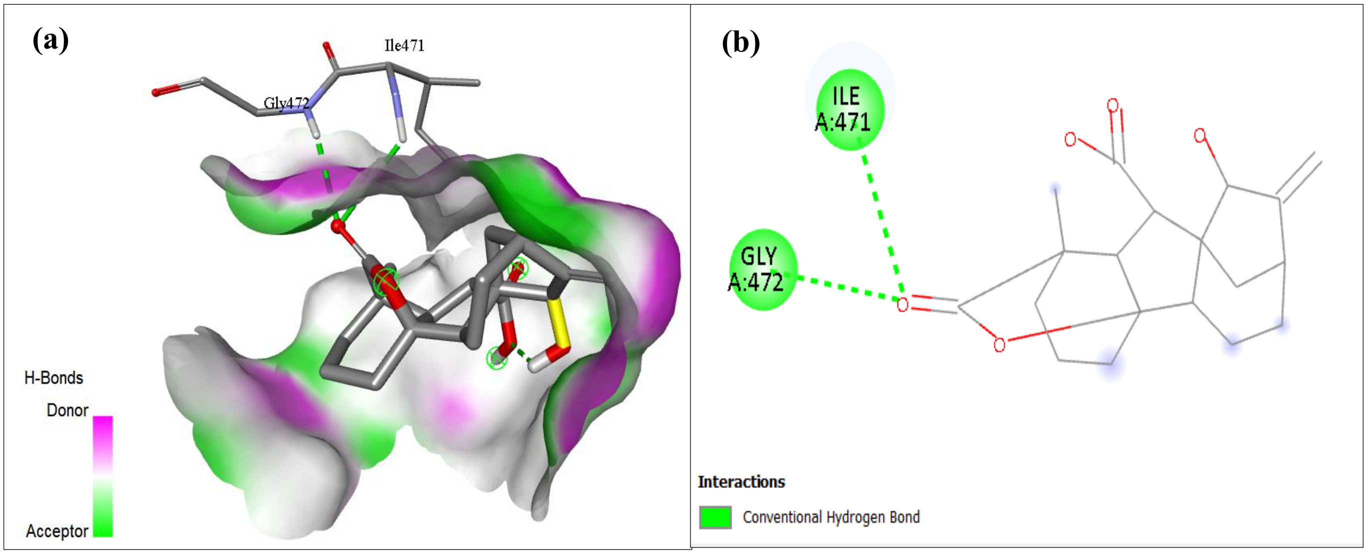
No. 19: Docked pose Convalloside in the CYP51(5V5Z) active site.



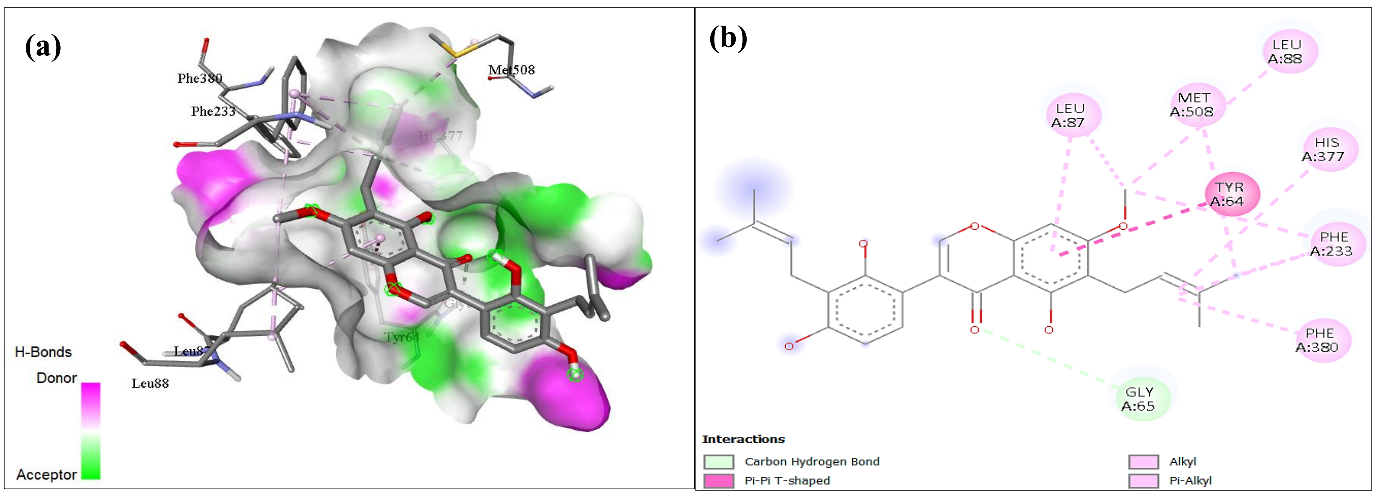
No. 20: Docked pose Diasarone 2 in the CYP51(5V5Z) active site.



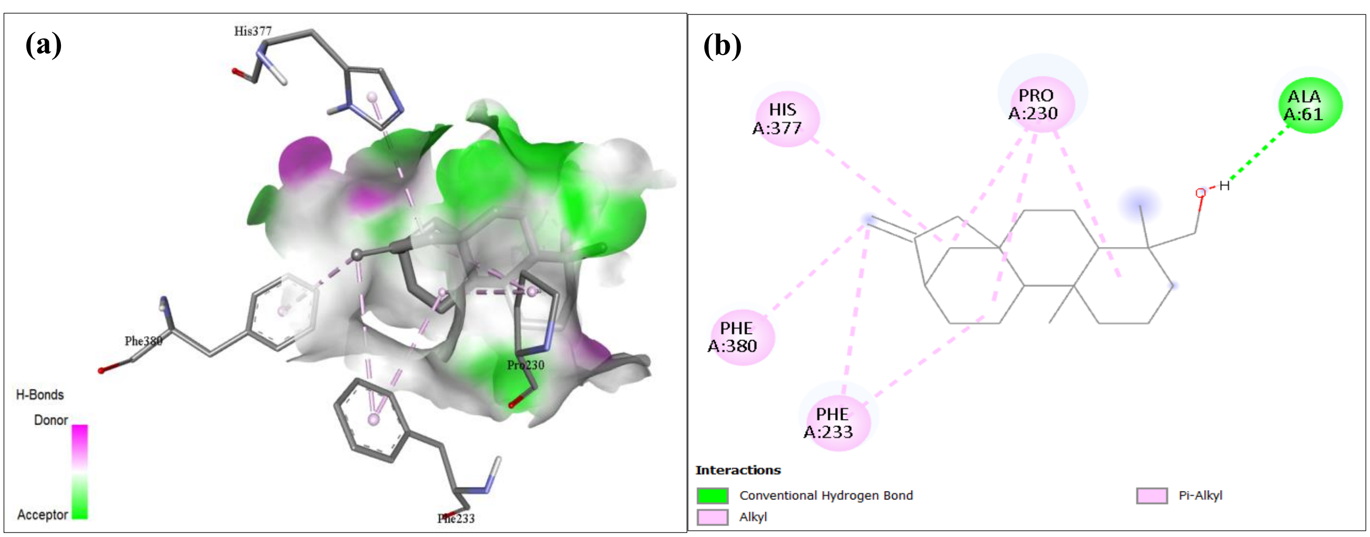
No.21: Docked pose Fluocinolone acetonide in the CYP51(5V5Z) active site.



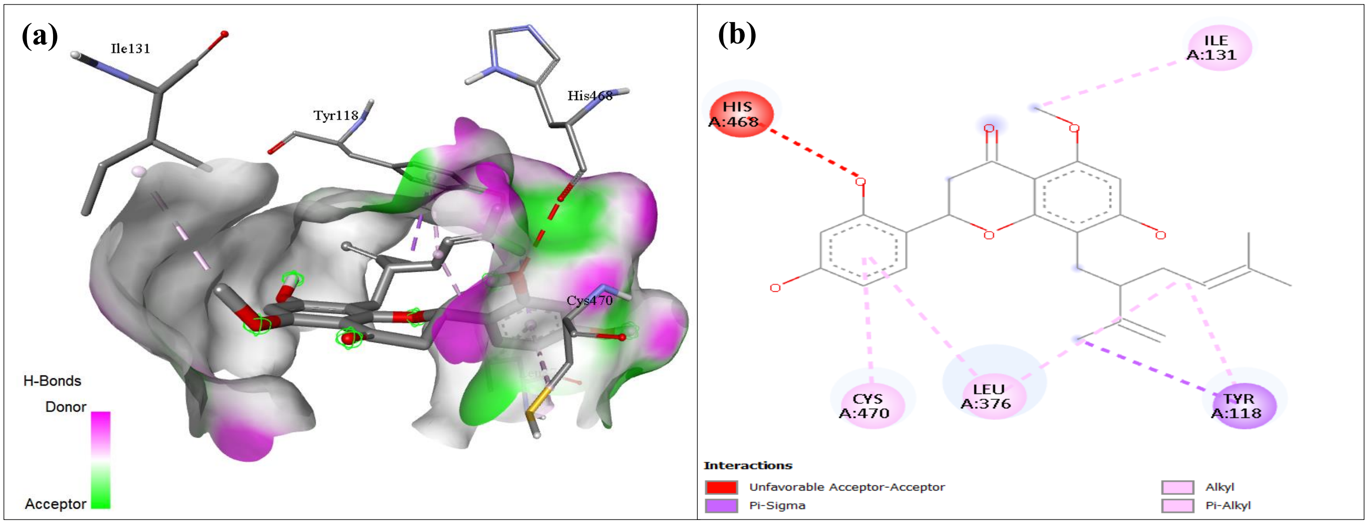
No 22: Docked pose Gibberellin A45 in the CYP51(5V5Z) active site.



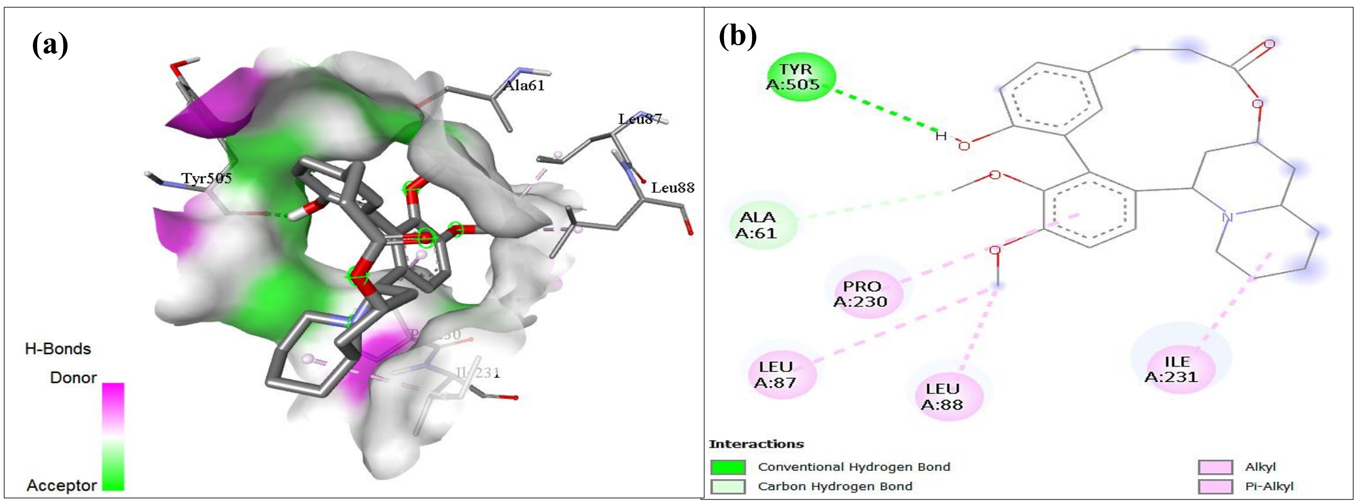
No. 23: Docked pose Kanzonol K in the CYP51(5V5Z) active site.



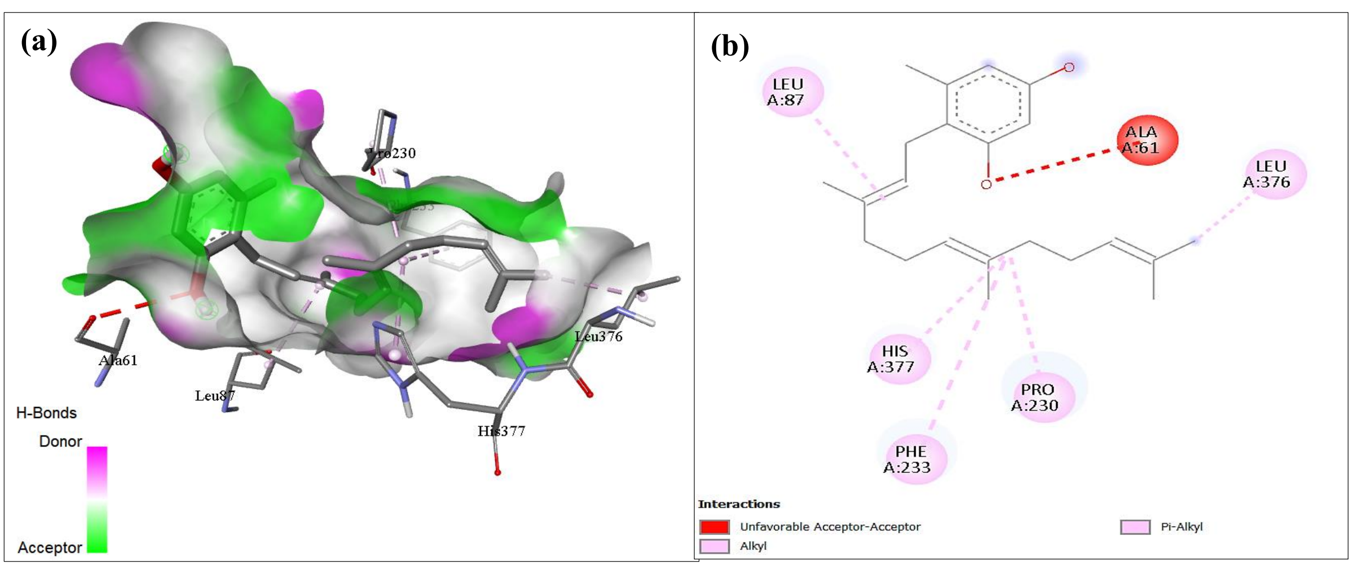
No. 24: Docked pose Kaur-16-en-18-ol in the CYP51(5V5Z) active site.



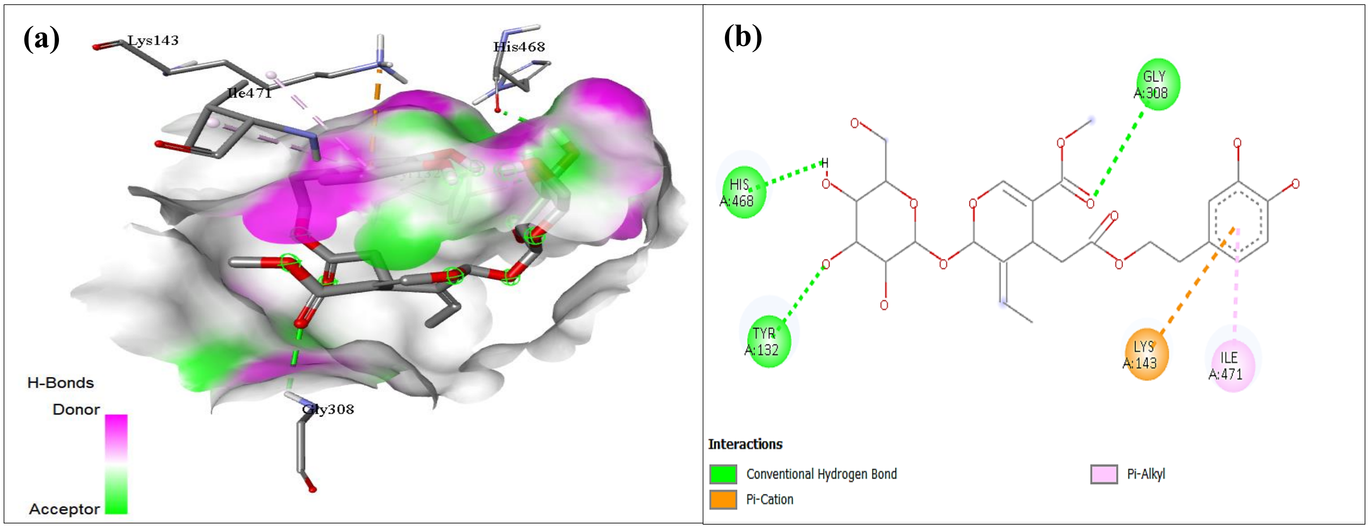
No. 25: Docked pose Kurarinone in the CYP51(5V5Z) active site.



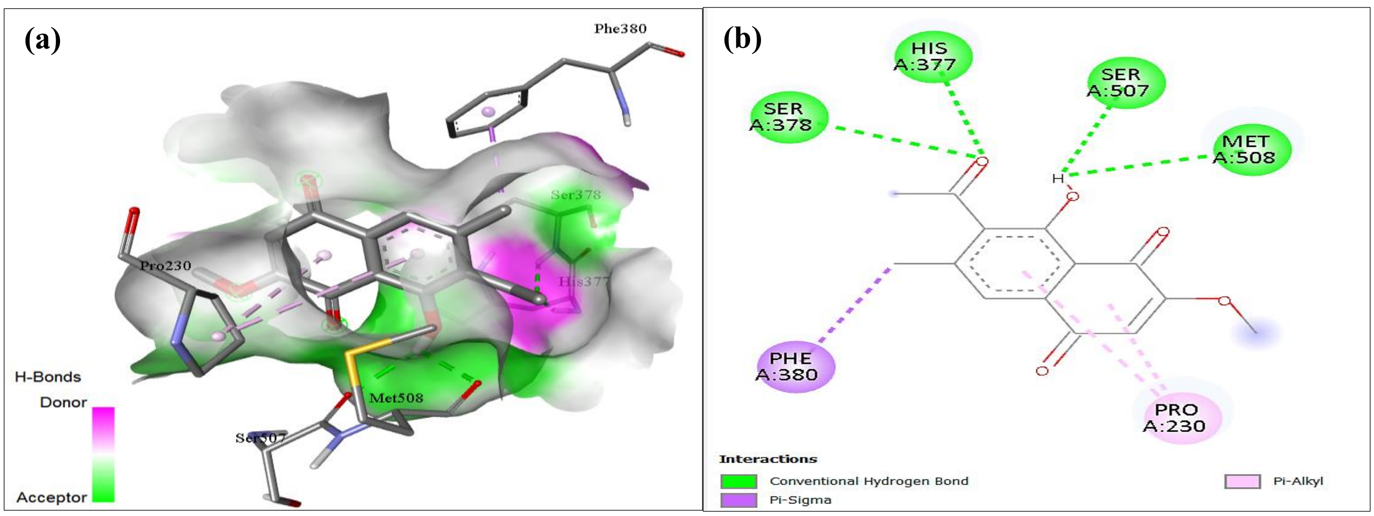
No. 26: Docked pose Lagerstroemine in the CYP51(5V5Z*)* active site.



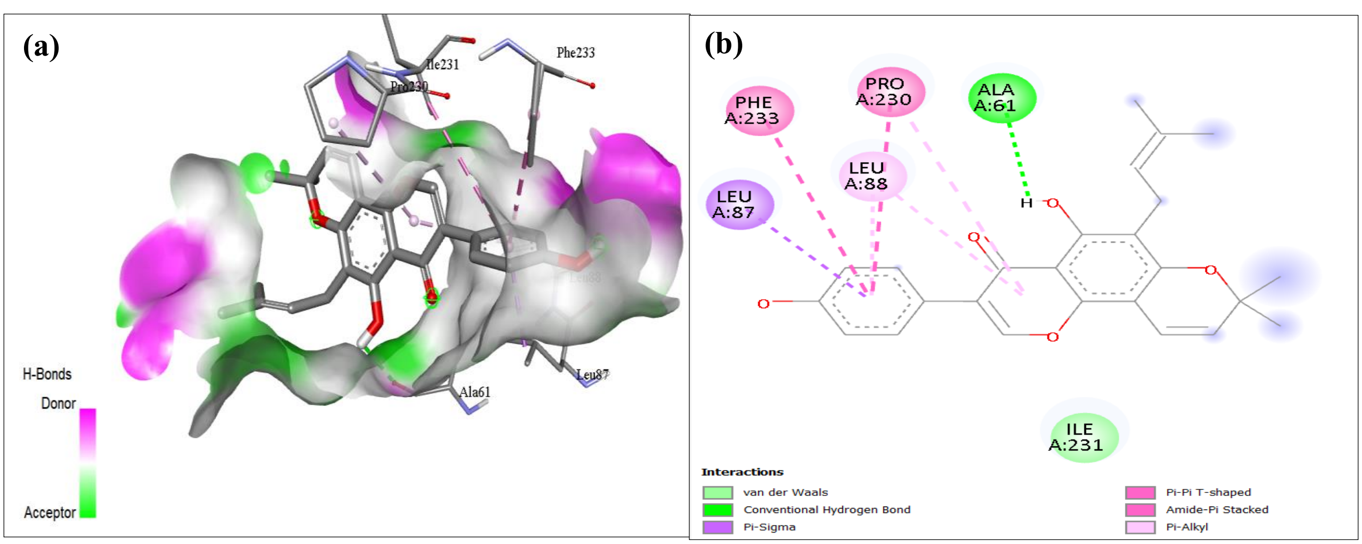
No. 27: Docked pose Neogrifolin in the CYP51(5V5Z) active site.



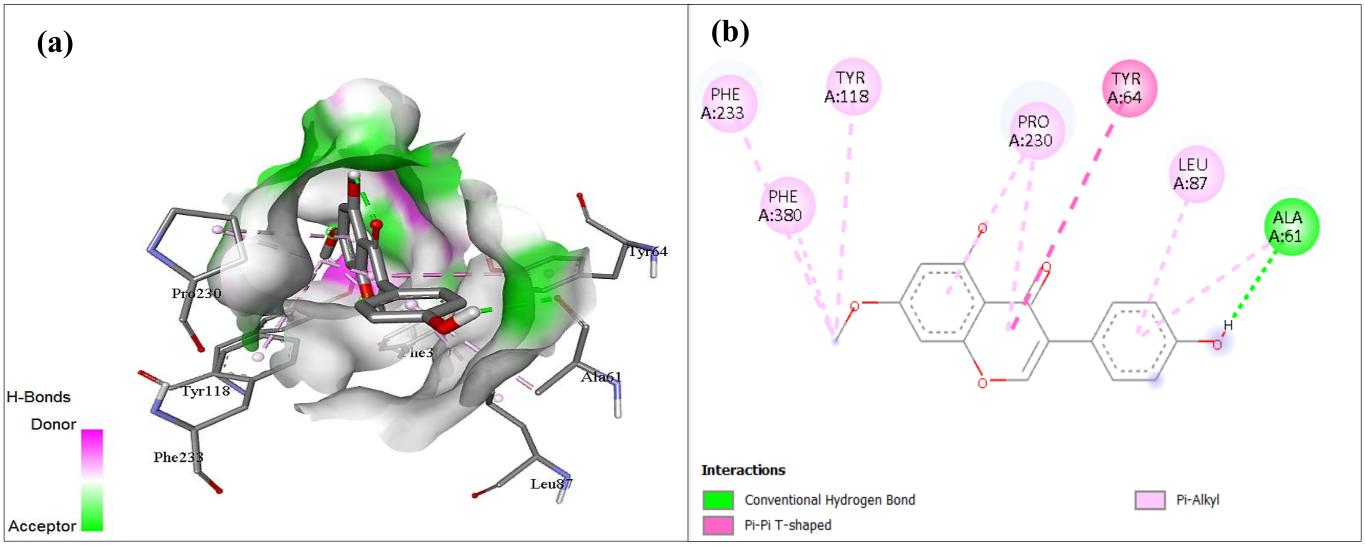
No. 28: Docked pose Oleuropein in the CYP51(5V5Z) active site.



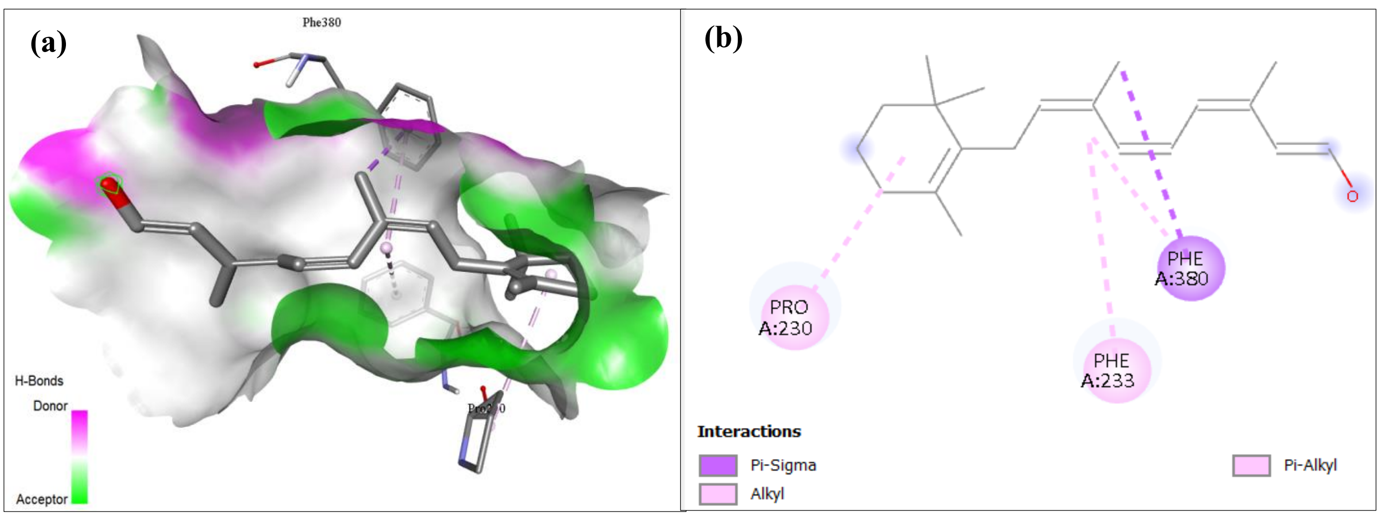
No. 29: Docked pose Orientalone in the CYP51(5V5Z) active site.



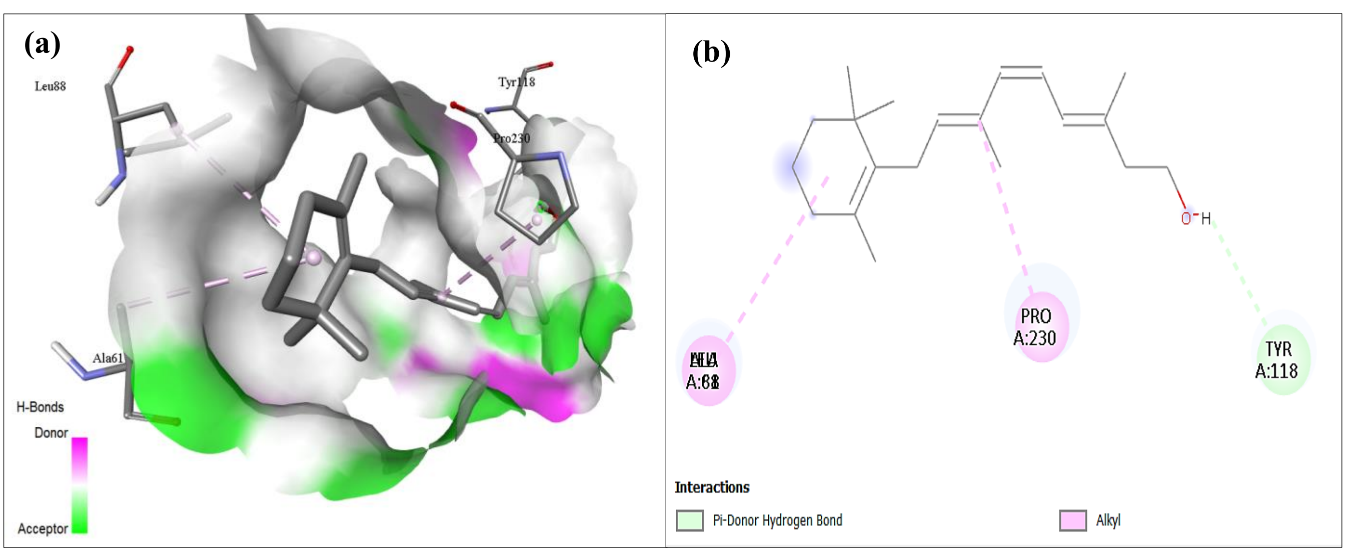
No. 30: Docked pose Osajin in the CYP51(5V5Z) active site.



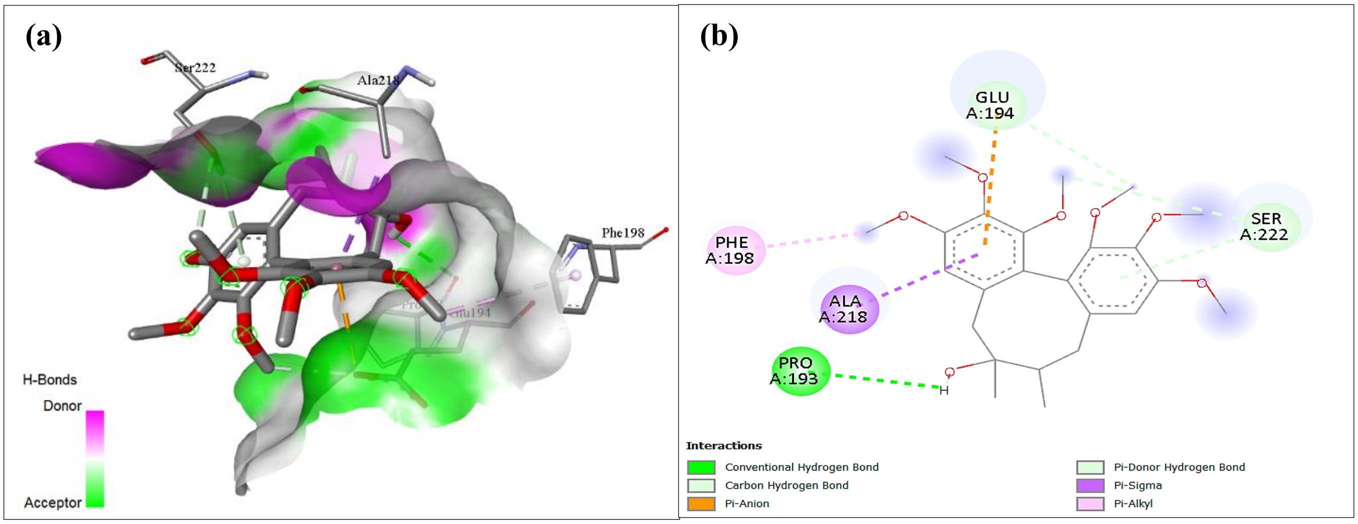
No. 31: Docked pose Prunetin in the CYP51(5V5Z) active site.



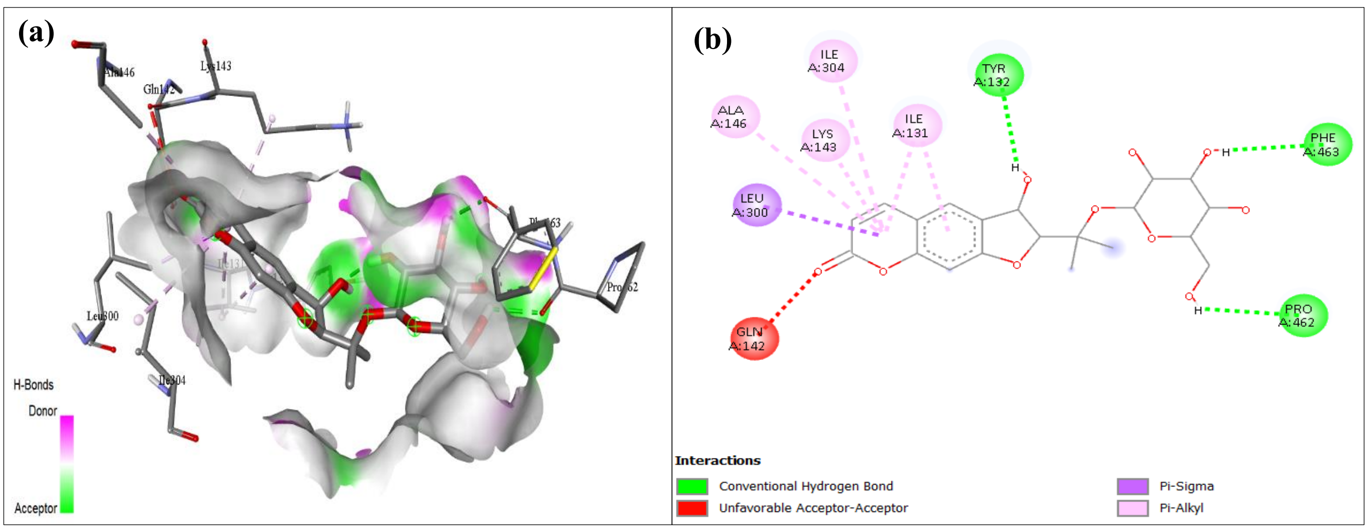
No. 32: Docked pose Retinaldehyde in the CYP51(5V5Z) active site.



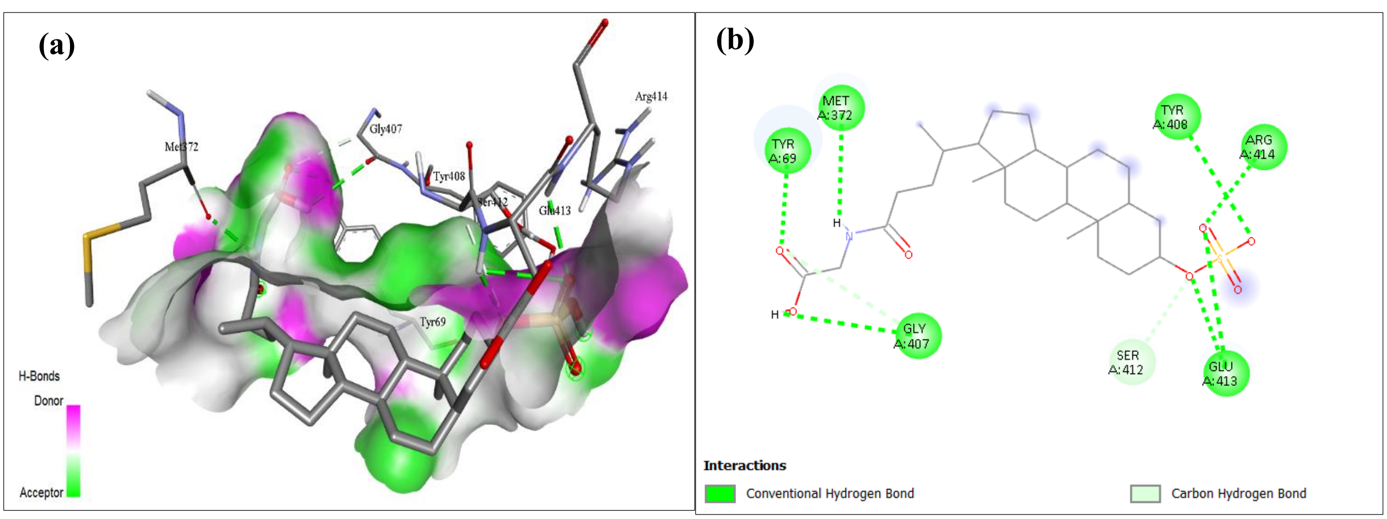
No. 33: Docked pose Retinol / Retinol skeleton in the CYP51(5V5Z) active site.



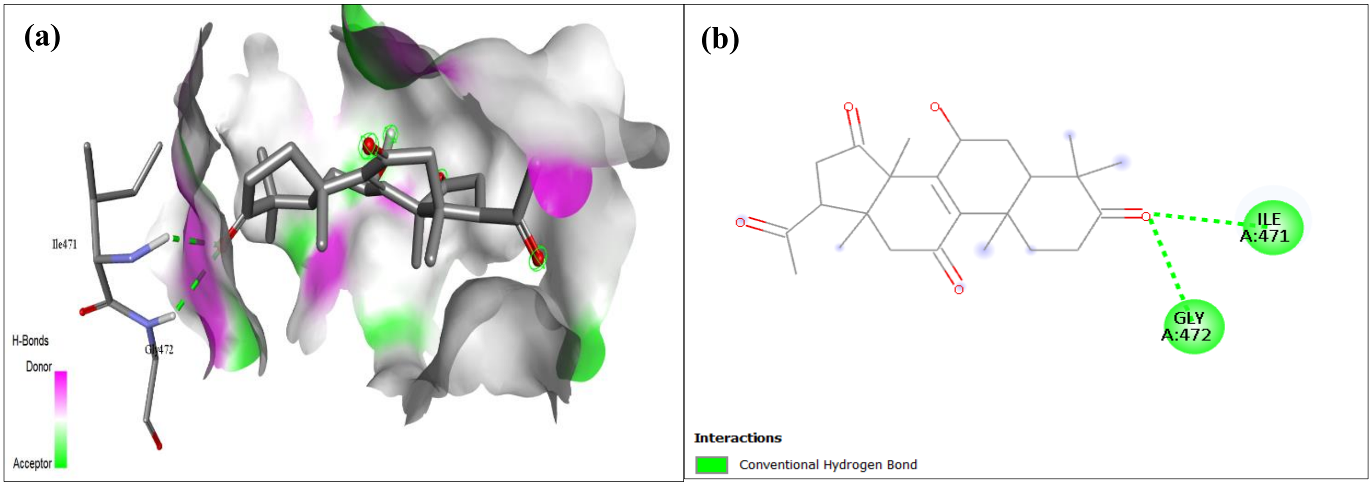
No. 34: Docked pose Schizandrin in the CYP51(5V5Z) active site.



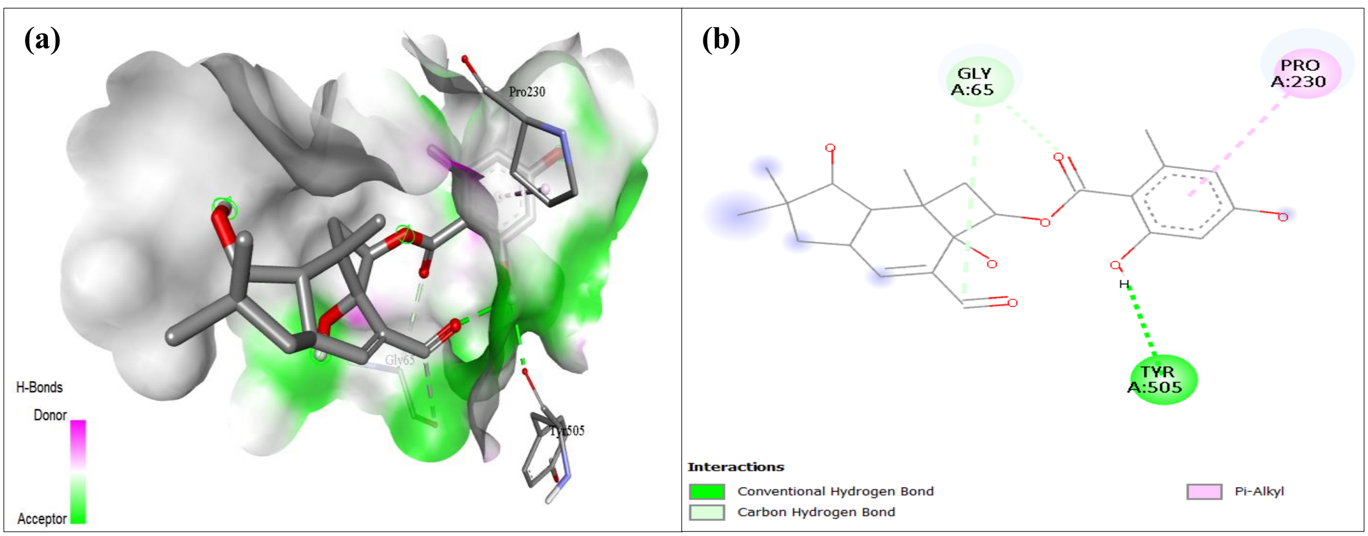
No. 35: Docked pose Smyrindioloside in the CYP51*(*5V5Z) active site.



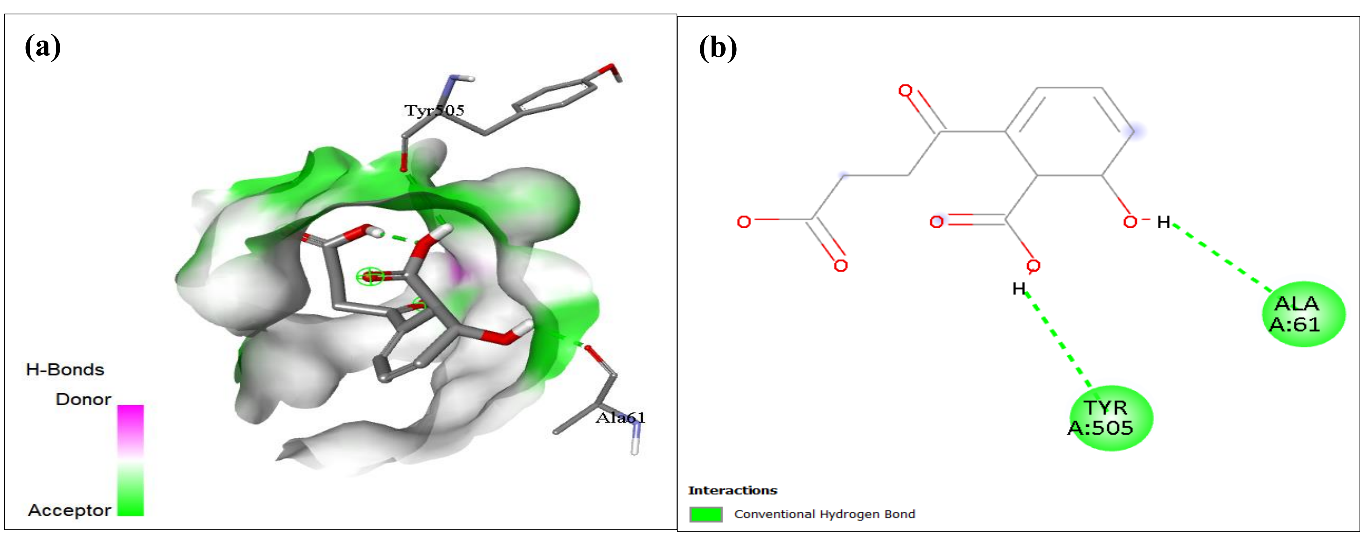
No. 36: Docked pose Sulfolithocholylglycine in the CYP51(5V5Z) active site.



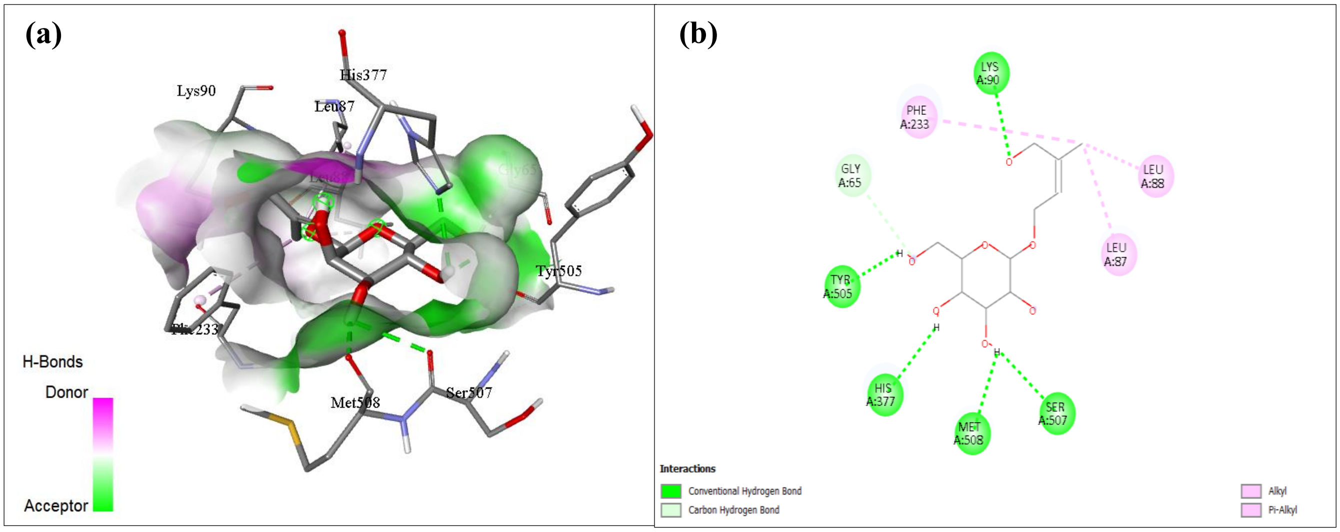
No. 37: Docked pose Lucidone B in the CYP51(5V5Z) active site.



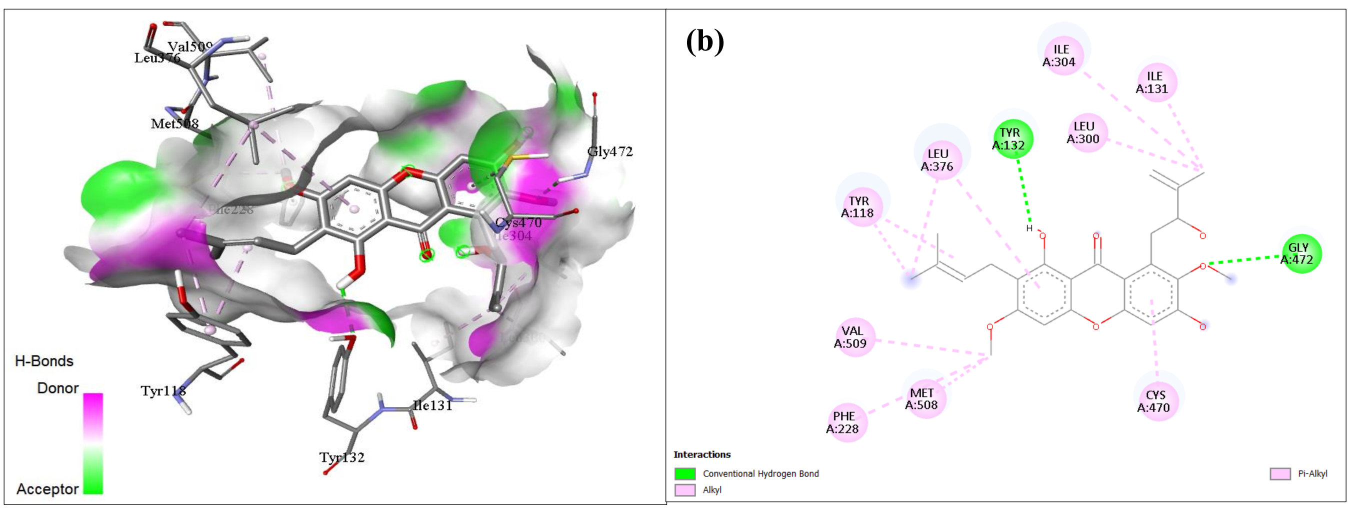
No. 38: Docked pose 10-Hydroxymelleolide in the CYP51(5V5Z) active site.



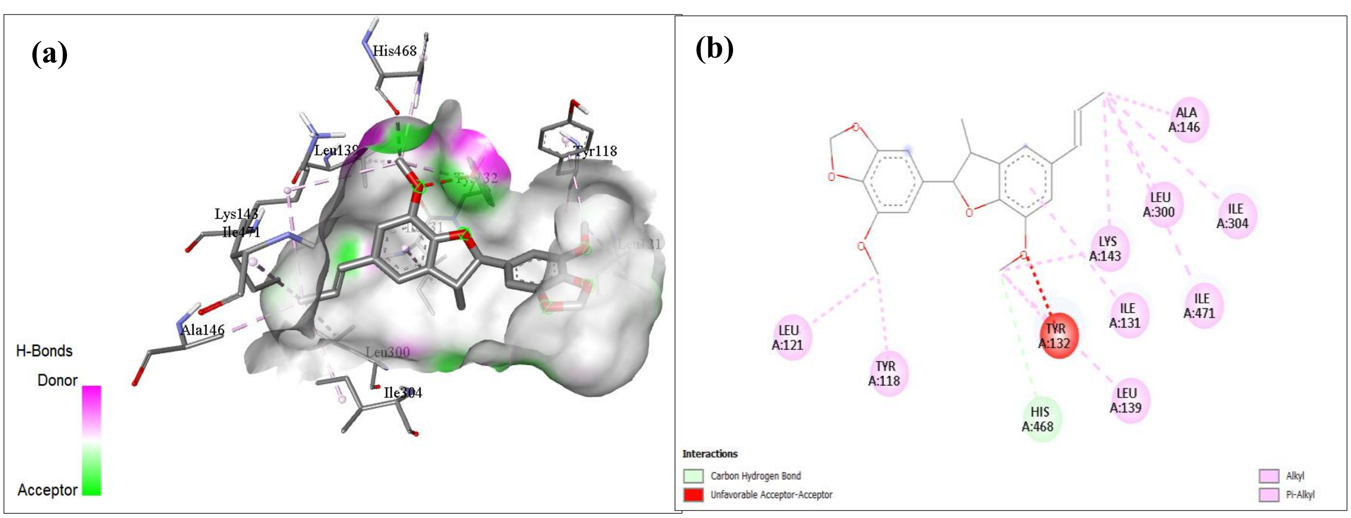
No. 39: Docked pose (1R,6R)-6-Hydroxy-2-succinylcyclohexa-2,4-diene-1-carboxylate in the CYP51(5V5Z) active site.



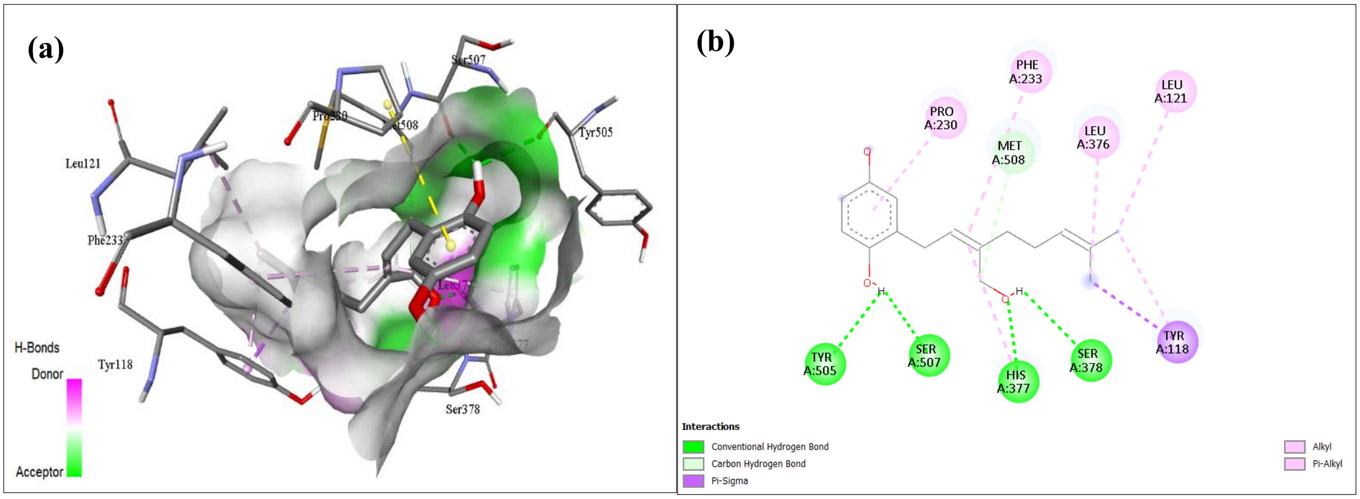
(a) **No.40**: Docked pose (Z)-2-Methyl-2-butene-1,4-diol 4-O-beta-D Glucopyranoside in the CYP51*(*5V5Z) active site.



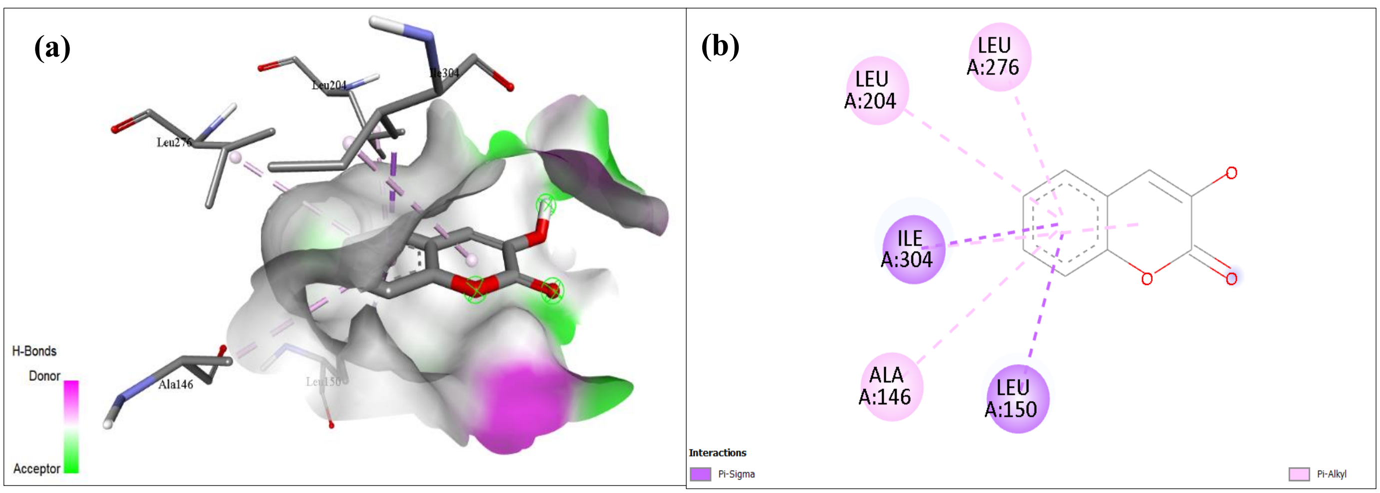
No. 41: Docked pose 1,6-Dihydroxy-3,7-dimethoxy-2-(3-methyl-2-butenyl)-8-(2-hydroxy-3-methyl-3-butenyl)-xanthone in the CYP51(5V5Z) active site.



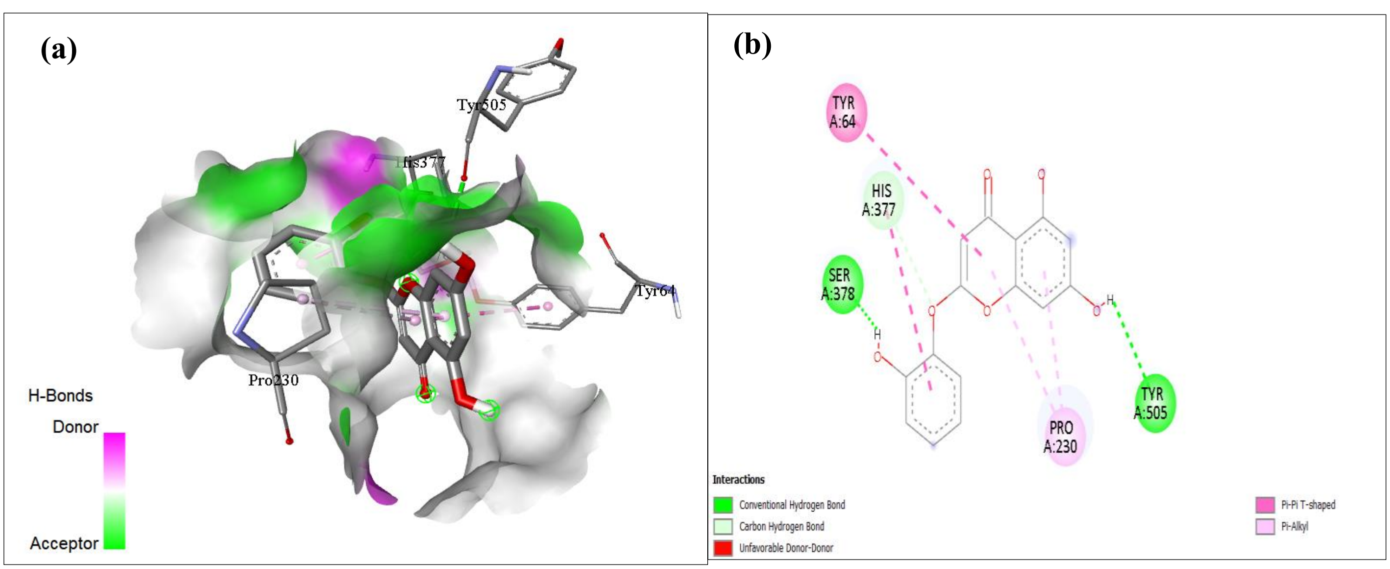
No. 42: Docked pose 2,3-Dihydro-7-methoxy-2-(3-methoxy-4,5-methylenedioxyphenyl)-3-methyl-5-(prop-1-enyl)benzofuran in the CYP51(5V5Z) active site.



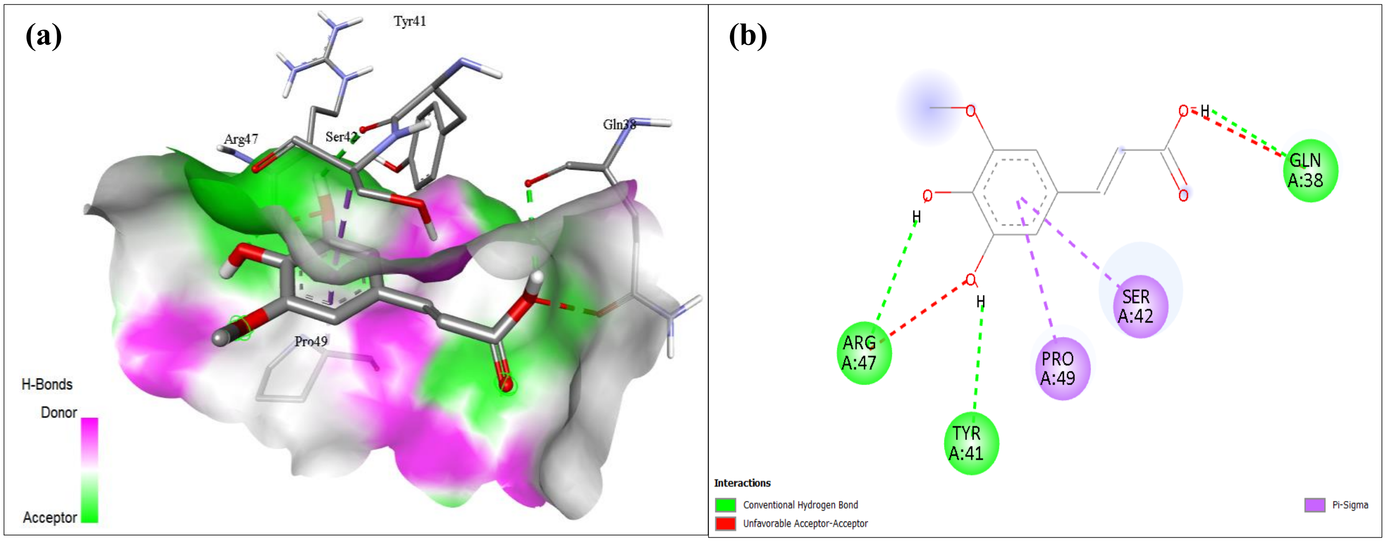
No. 43: Docked pose 3''-Hydroxy-geranylhydroquinone in the CYP51(5V5Z) active site.



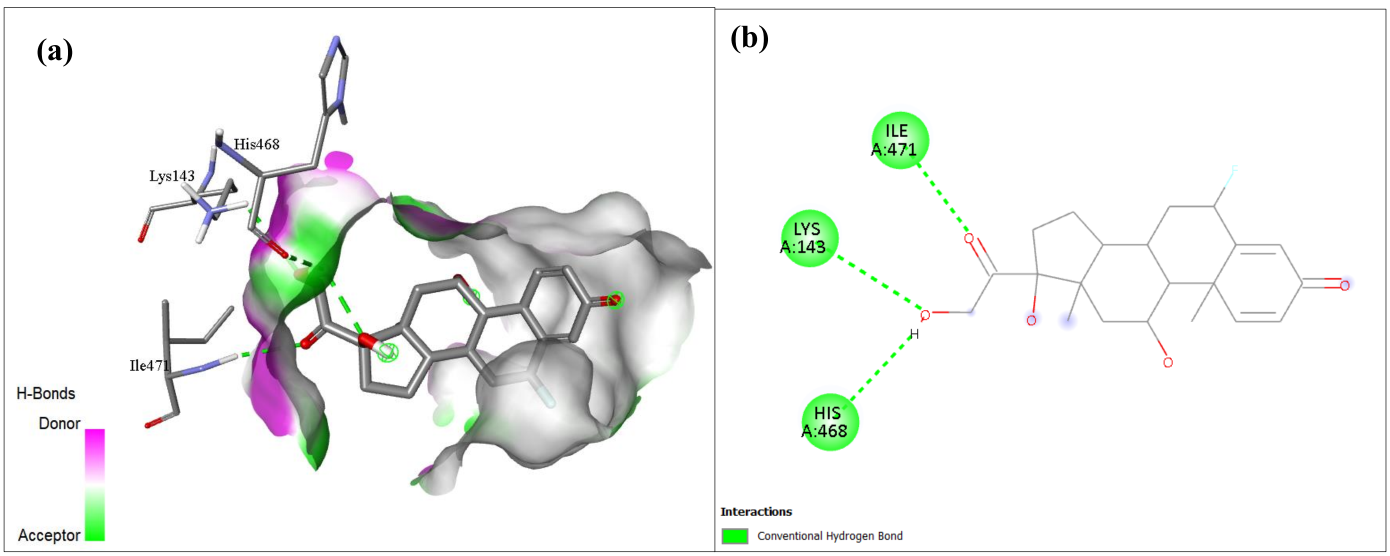
No. 44: Docked pose 3-Hydroxycoumarin in the CYP51(5V5Z) active site.



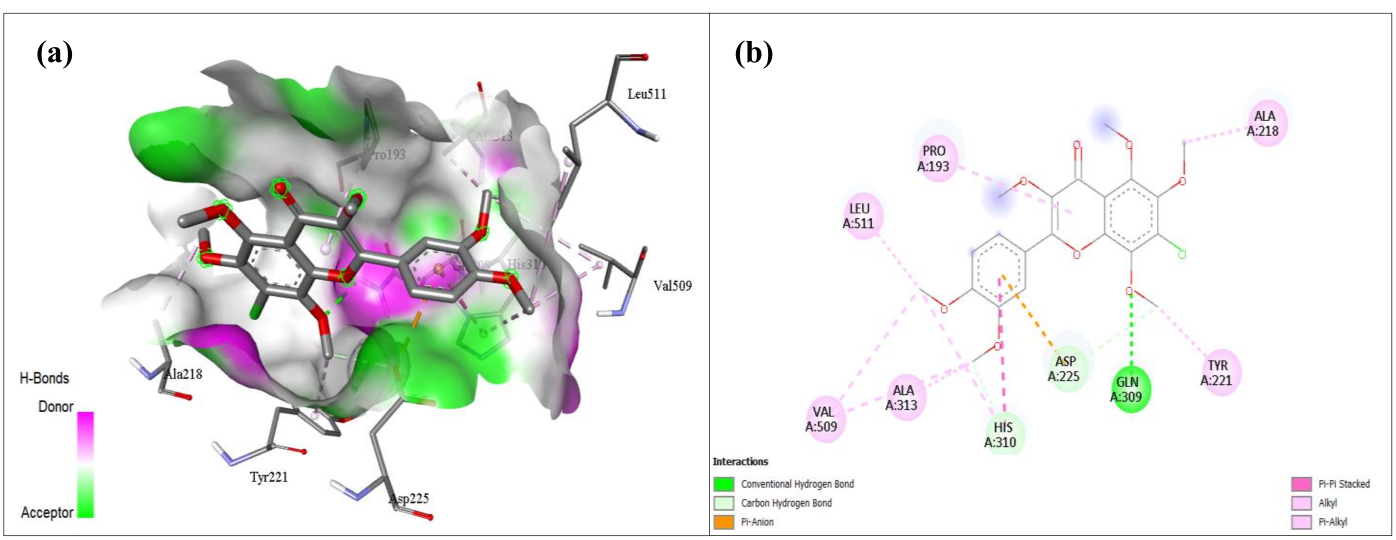
No. 45: Docked pose 5,7Dihydroxychromone in the CYP51(5V5Z) active site.



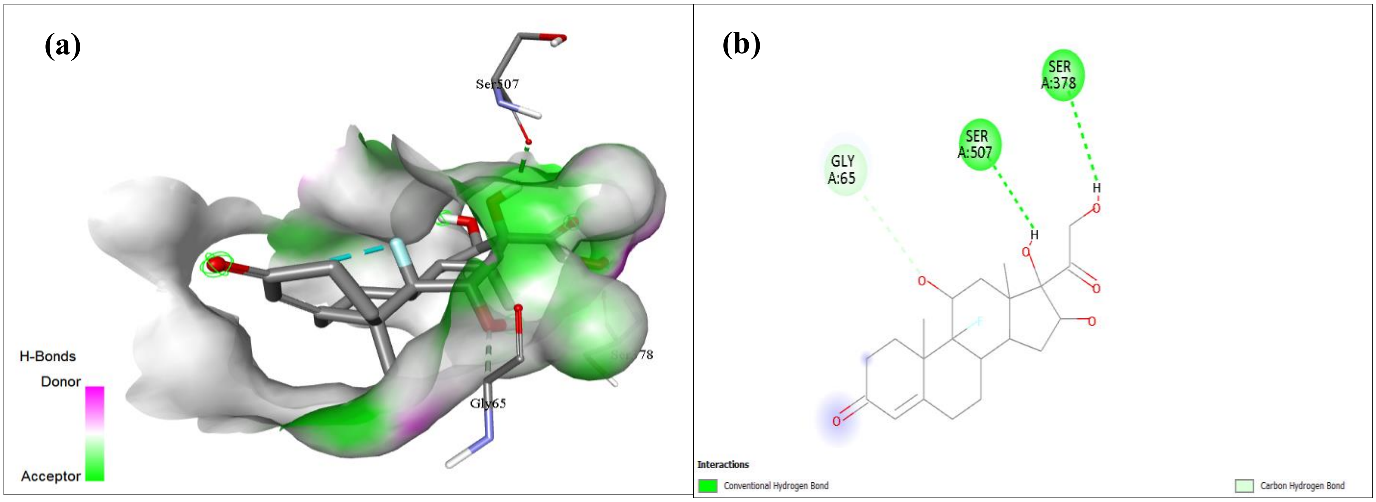
No. 46: Docked pose 5-Hydroxyferulate in the CYP51(5V5Z) active site.



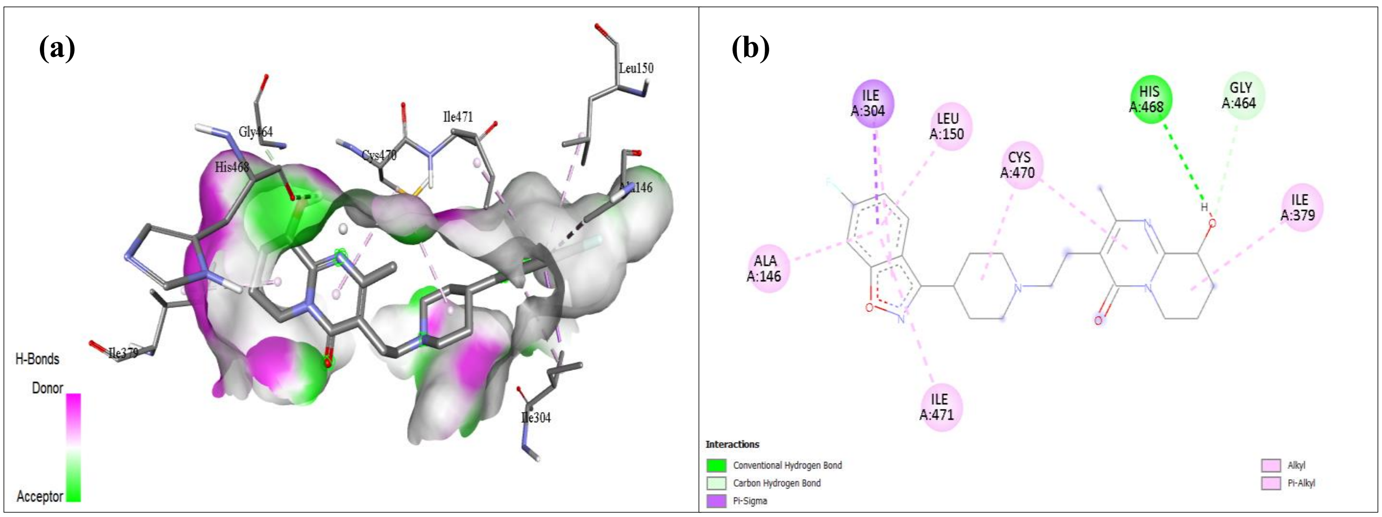
No. 47: Docked pose 6alpha-Fluoroprednisolone in the CYP51(5V5Z) active site.



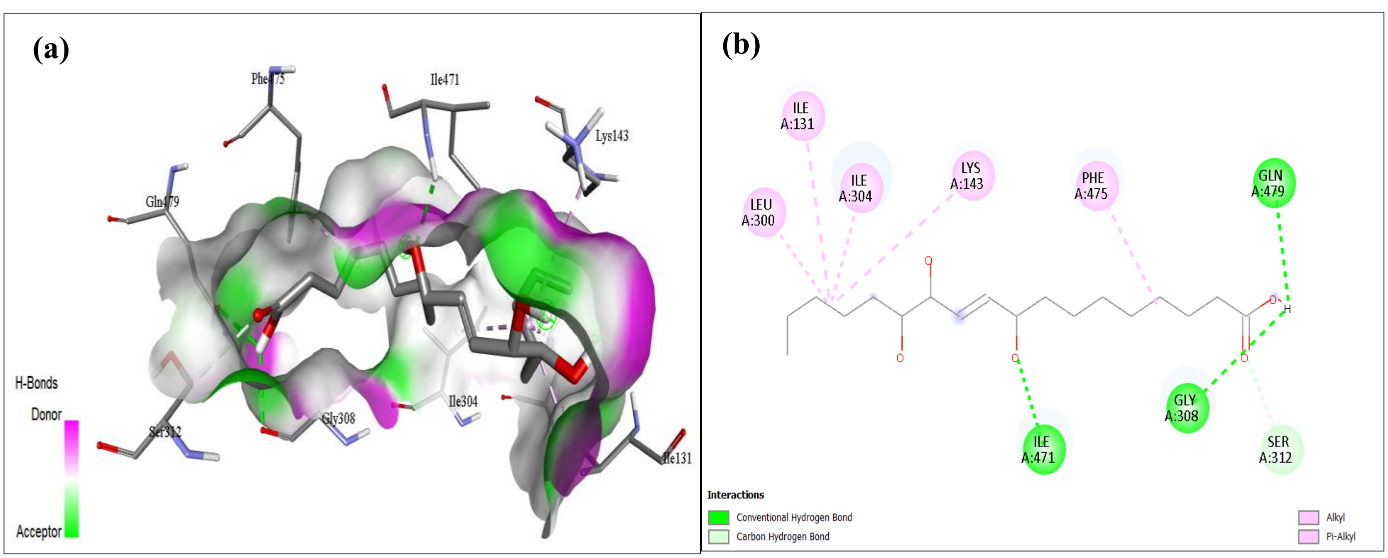
No. 48: Docked pose 7-Chloro-3,3',4',5,6,8-hexamethoxyflavone in the CYP51(5V5Z) active site.



No. 49: Docked pose 9alpha-Fluoro-11beta,16alpha,17alpha,21-tetrahydroxypregn-4-ene-3,20-dione in the CYP51(5V5Z) active site.



No. 50: Docked pose 9-Hydroxyrisperidone in the CYP51(5V5Z) active site.



No. 51: Docked pose 9S,12S,13S-trihydroxy-10E-octadecenoic acid-in the CYP51(5V5Z) active site.

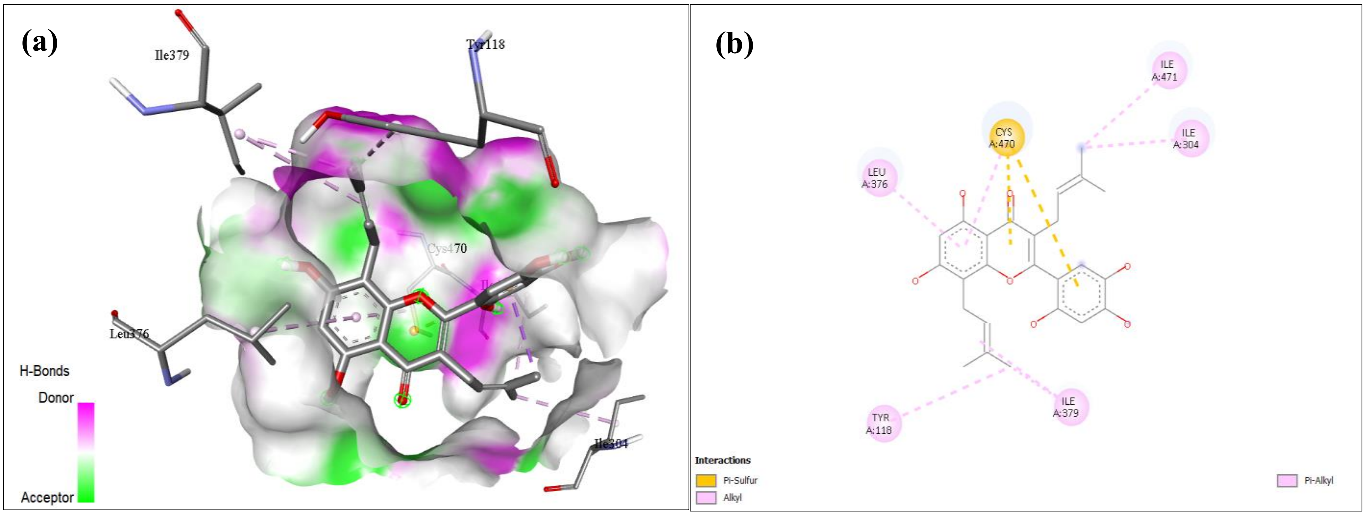
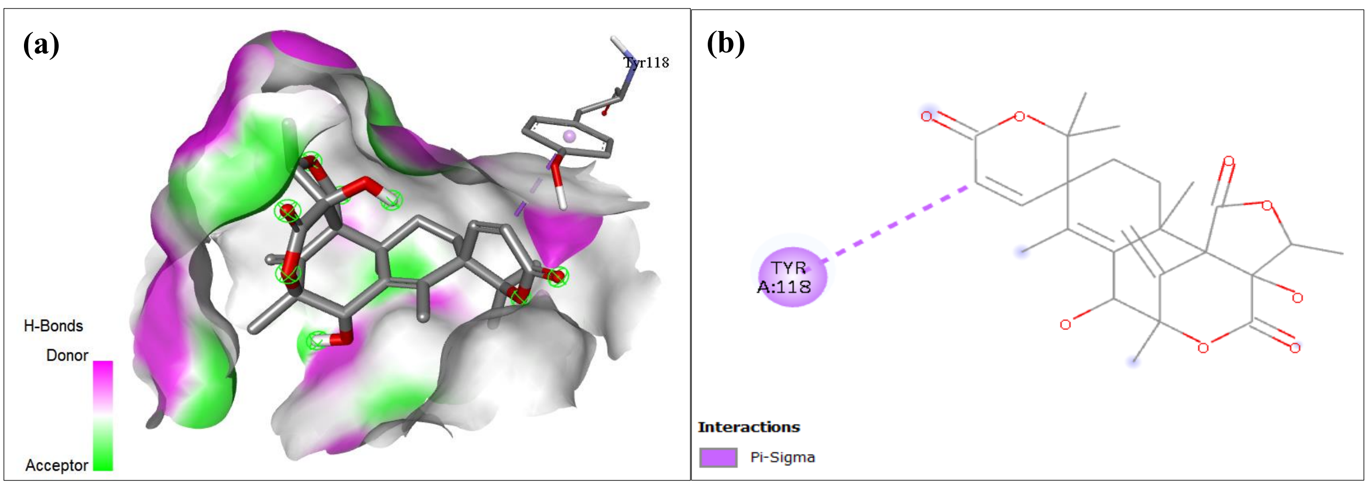
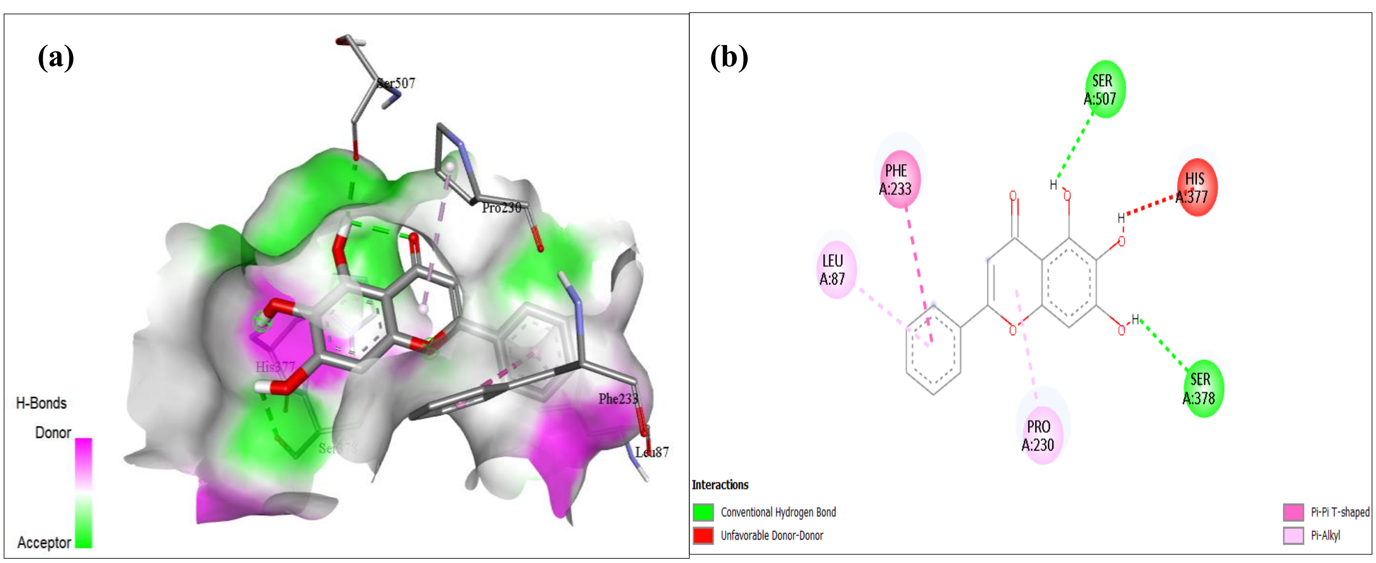


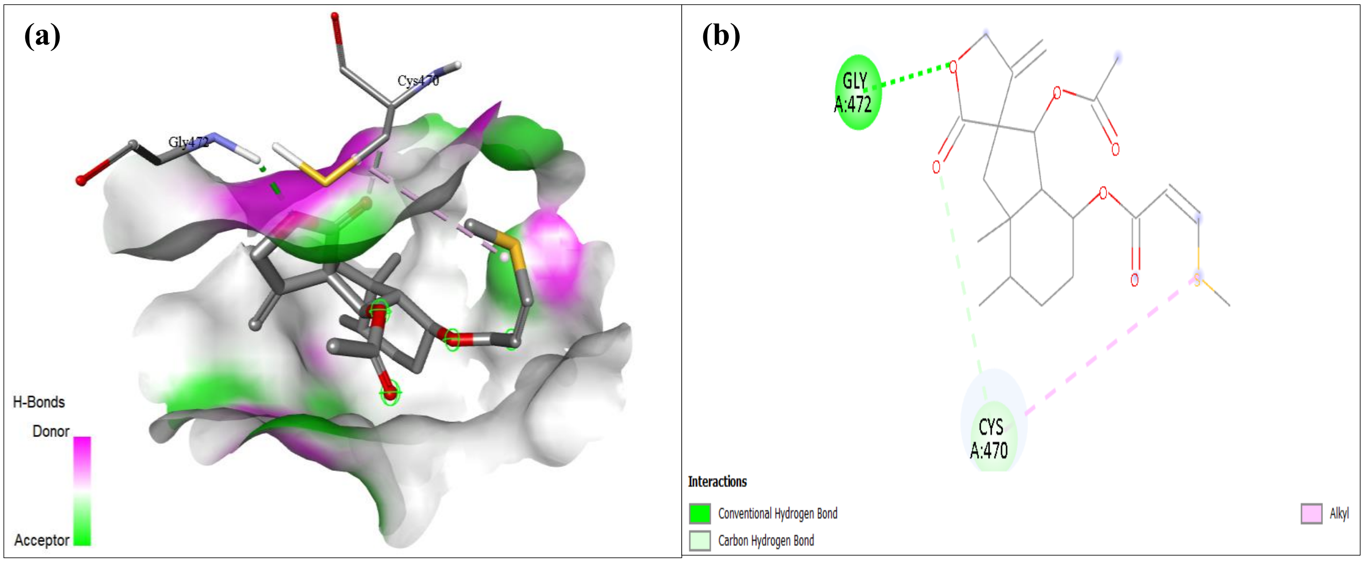
Figure 52: Docked pose Artonin V in the CYP51(5V5Z) active site.



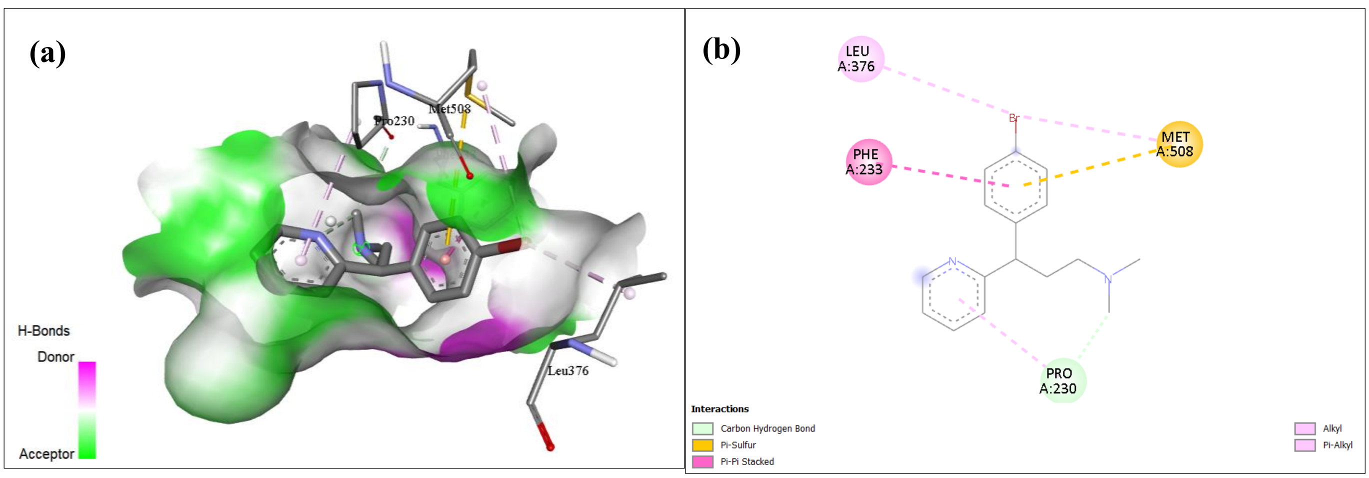
No. 53: Docked pose Austinol in the CYP51(5V5Z) active site.



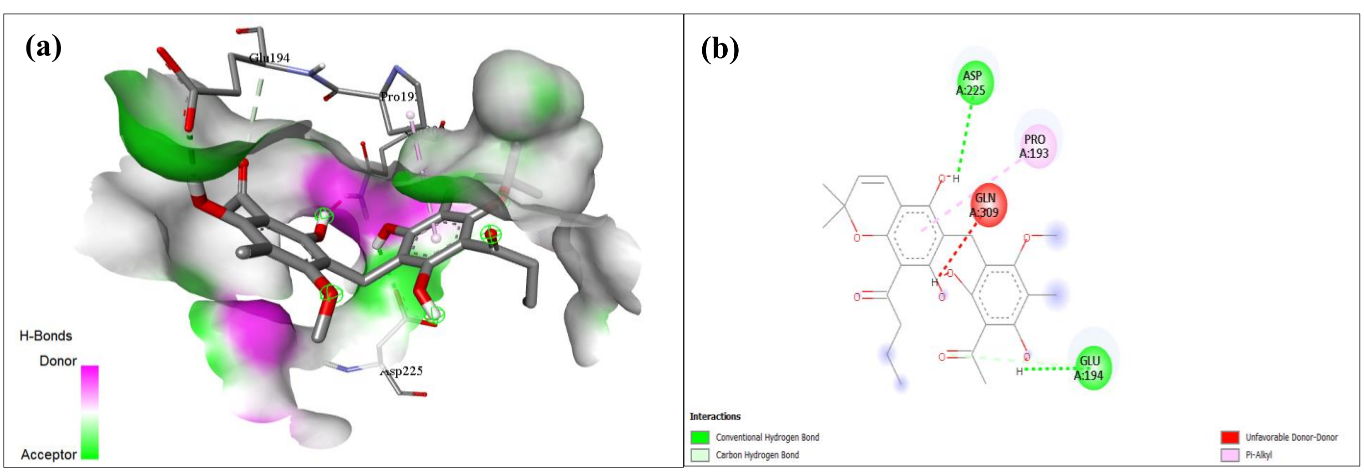
No. 54: Docked pose Baicalein in the CYP51(5V5Z) active site.



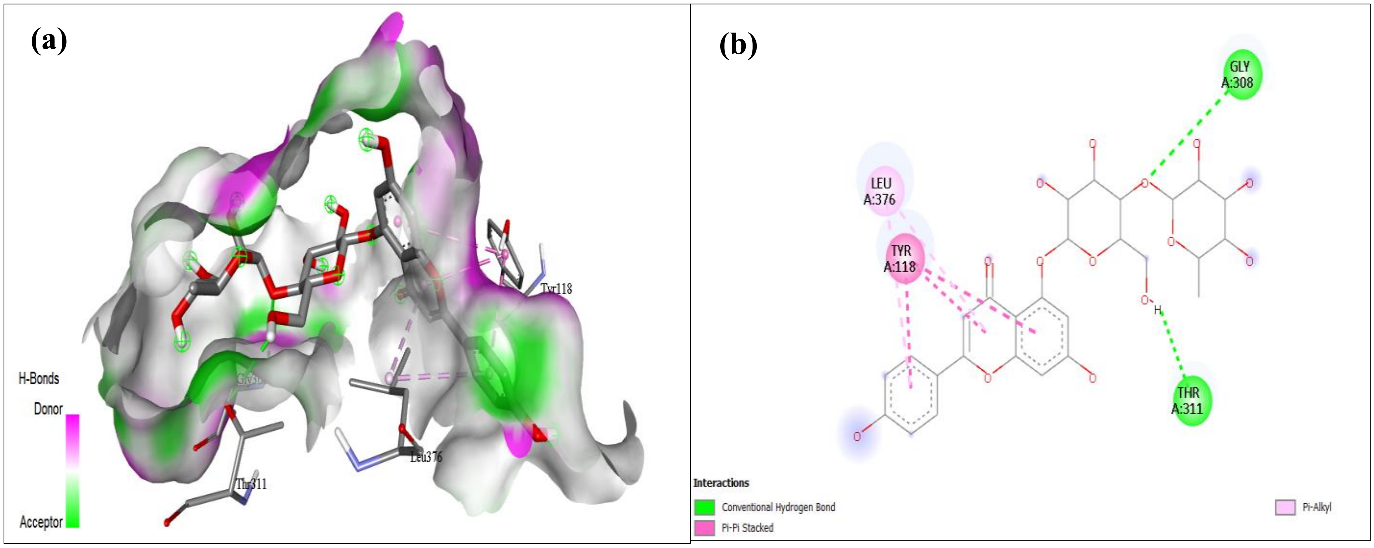
No. 55: Docked pose Bakkenolide D in the CYP51(5V5Z) active site.



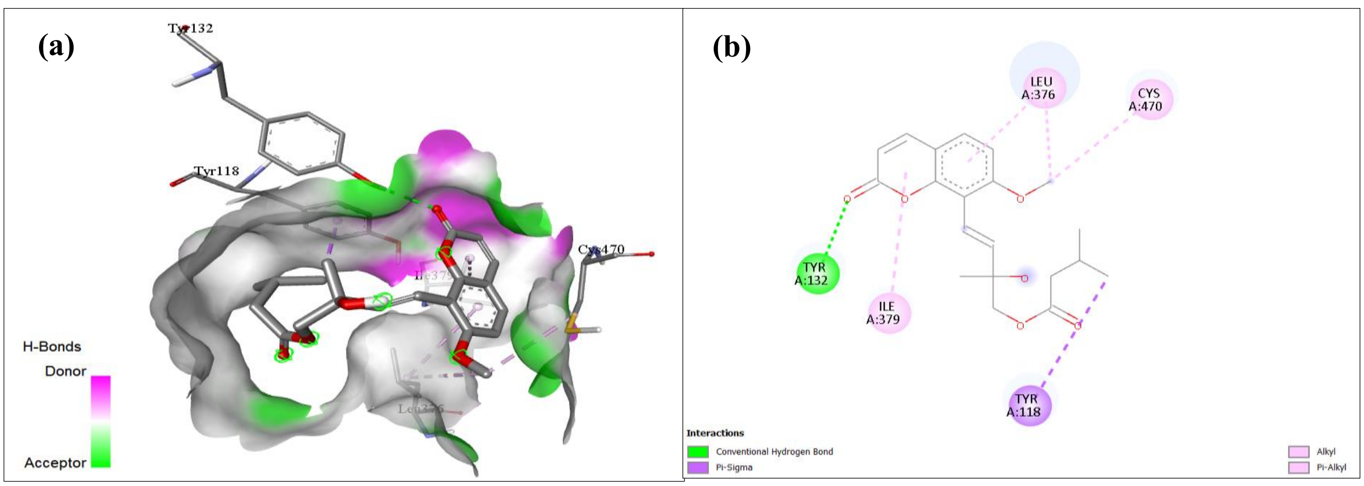
No.56: Docked pose Brompheniramine in the CYP51(5V5Z) active site.



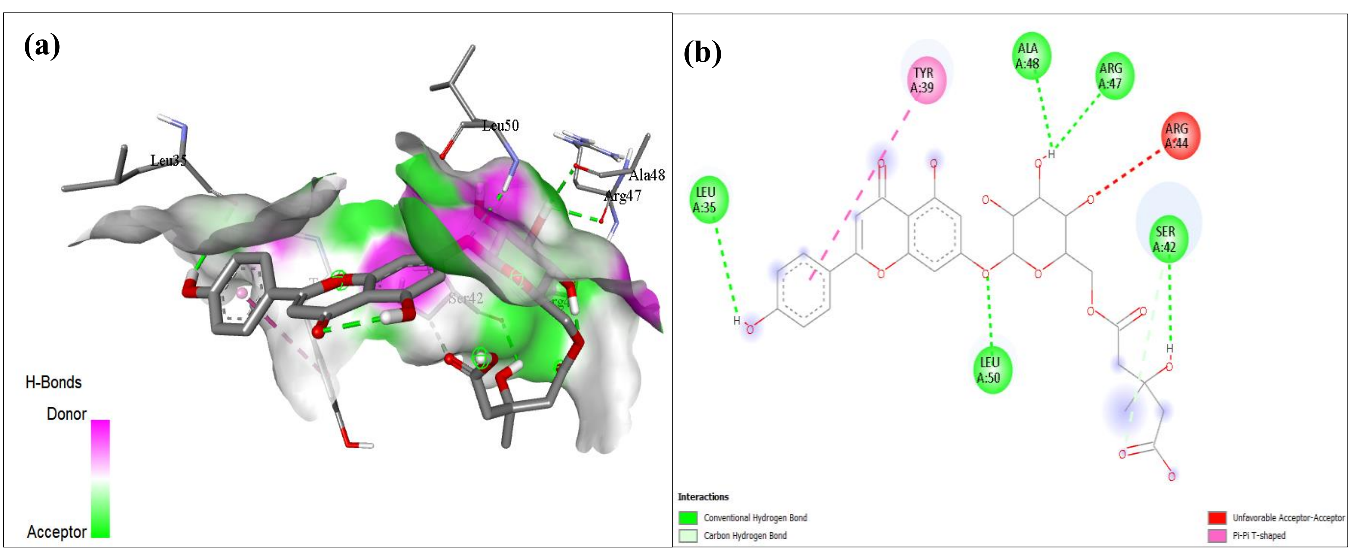
No. 57: Docked pose Butyrylmallotochromene in the CYP51(5V5Z) active site.



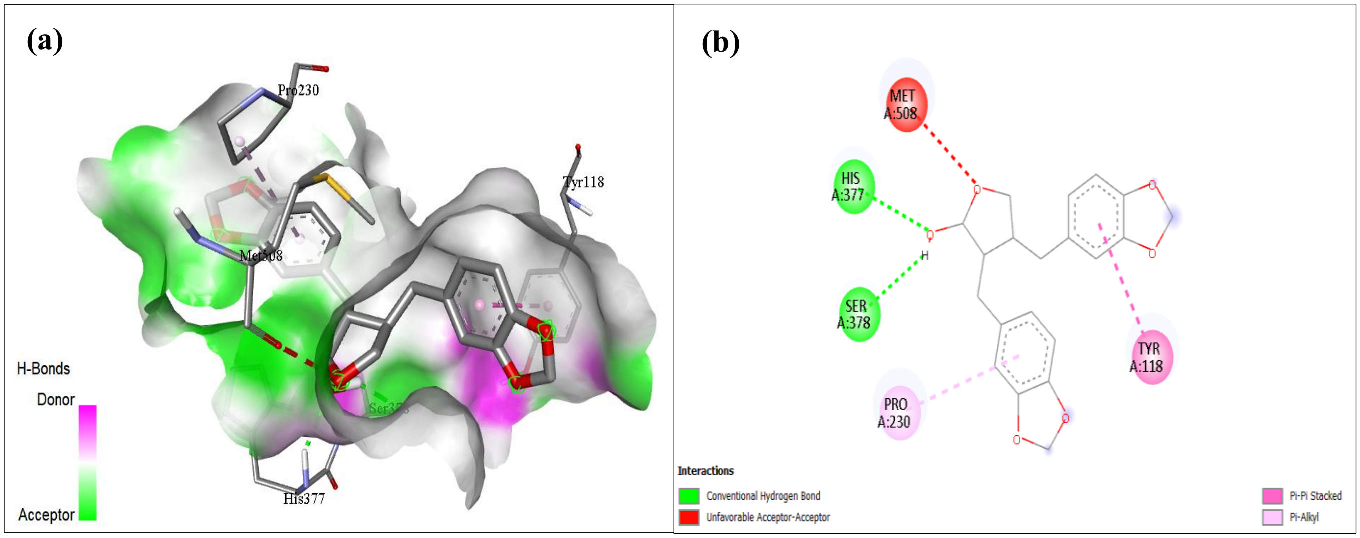
No. 58: Docked pose Camellianin B in the CYP51(5V5Z) active site.



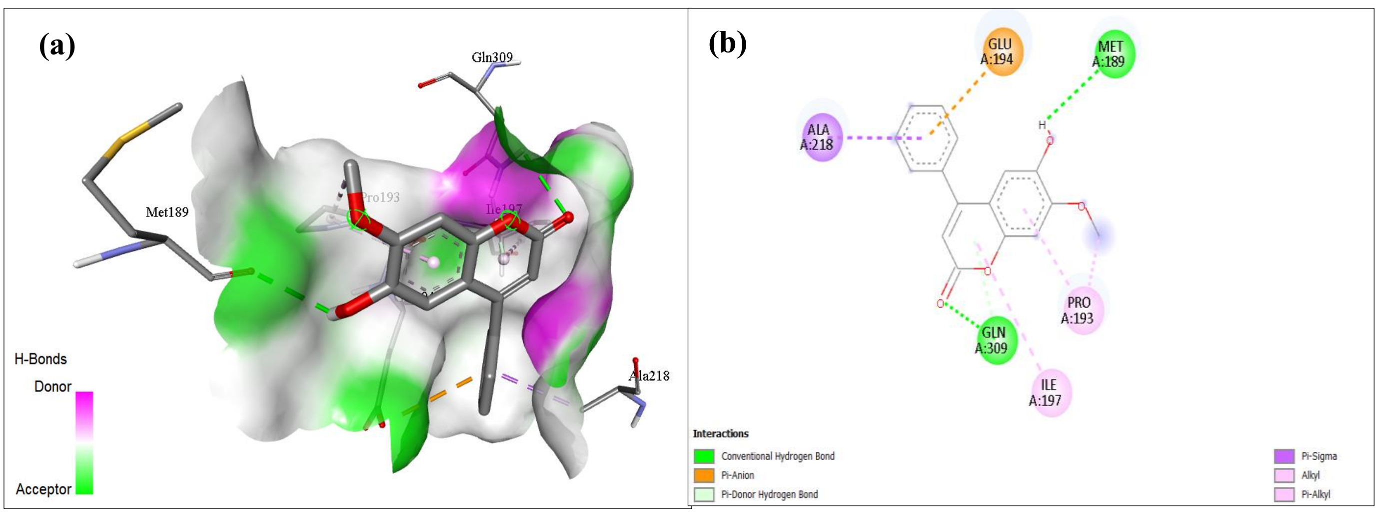
No.59: Docked pose Casegravol isovalerate in the CYP51(5V5Z) active site.



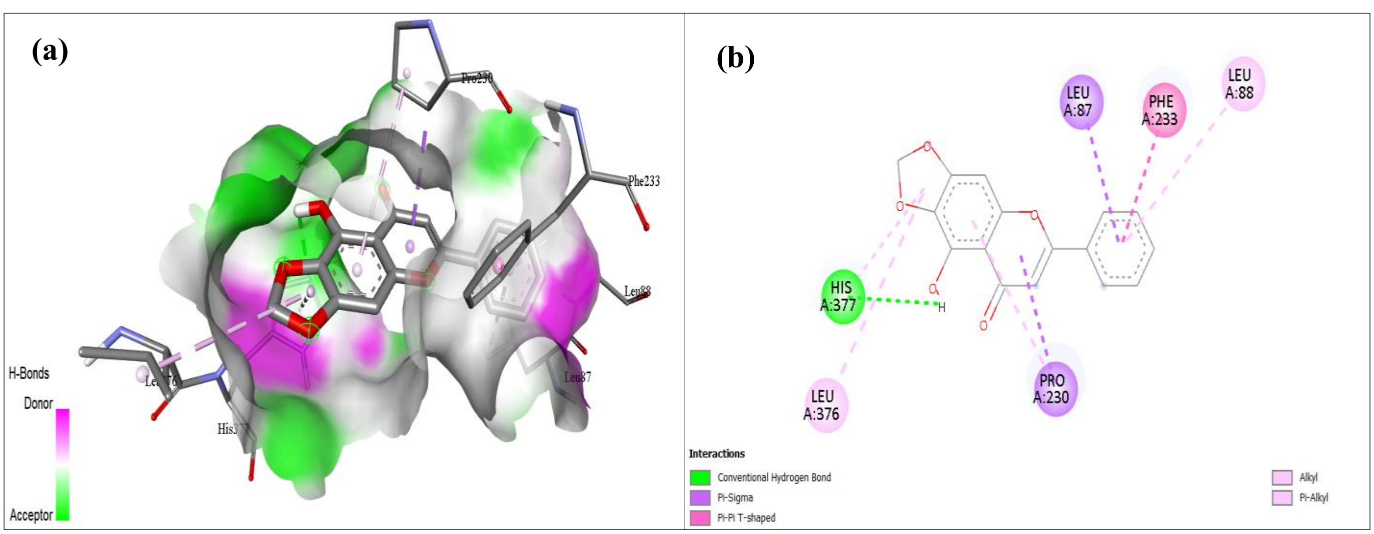
No. 60: Docked pose Chamaemeloside in the CYP51(5V5Z) active site.



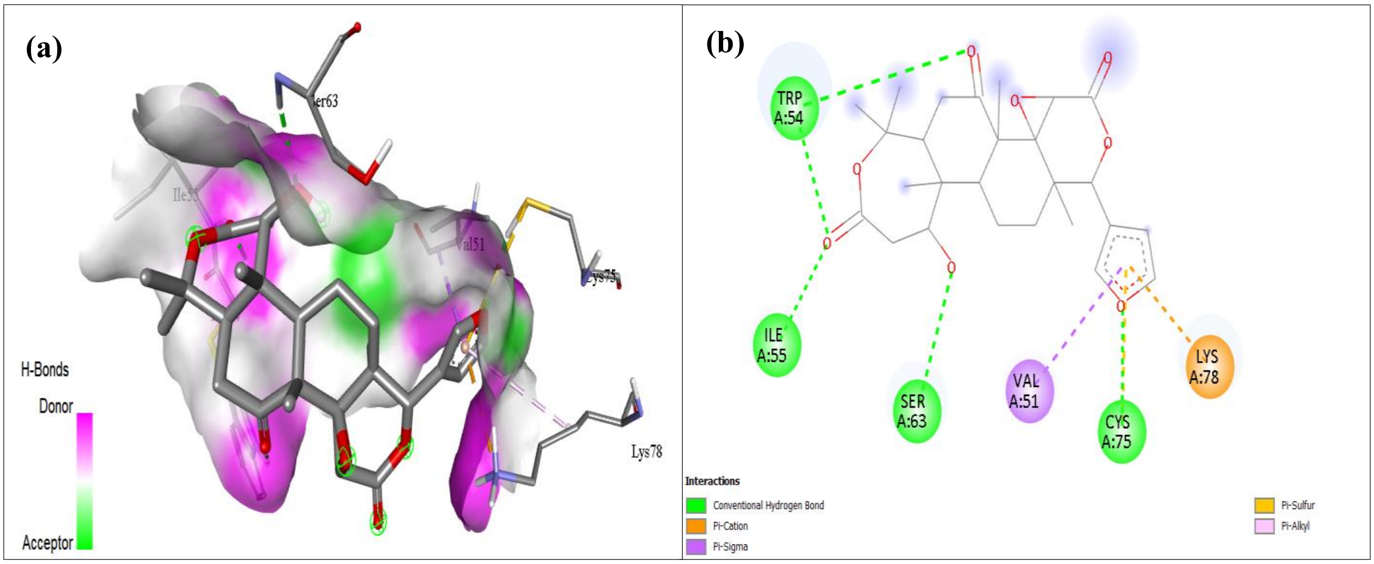
No. 61: Docked pose Cubebin in the CYP51(5V5Z) active site.



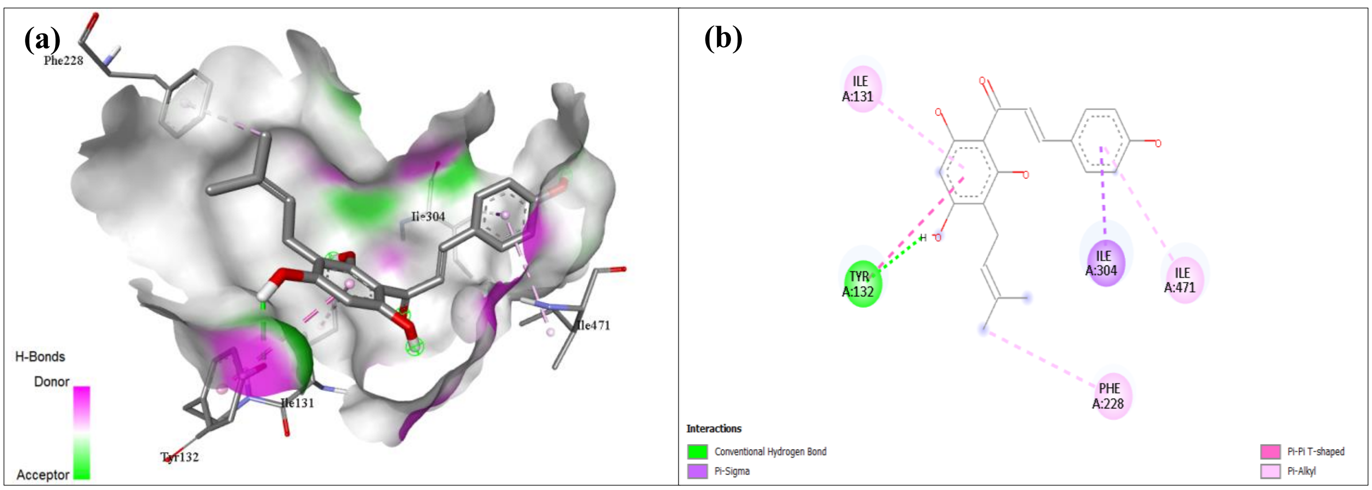
No. 62: Docked pose Dalbergin in the CYP51(5V5Z) active site.



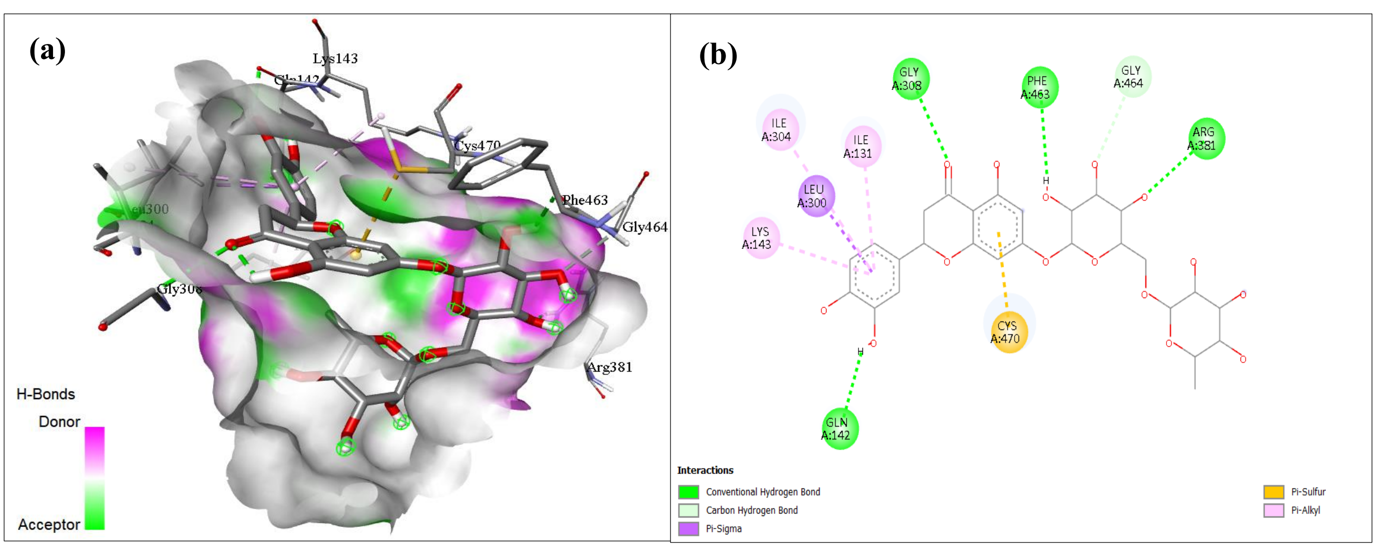
No. 63: Docked pose Cochliophilin A in the CYP51(5V5Z) active site.



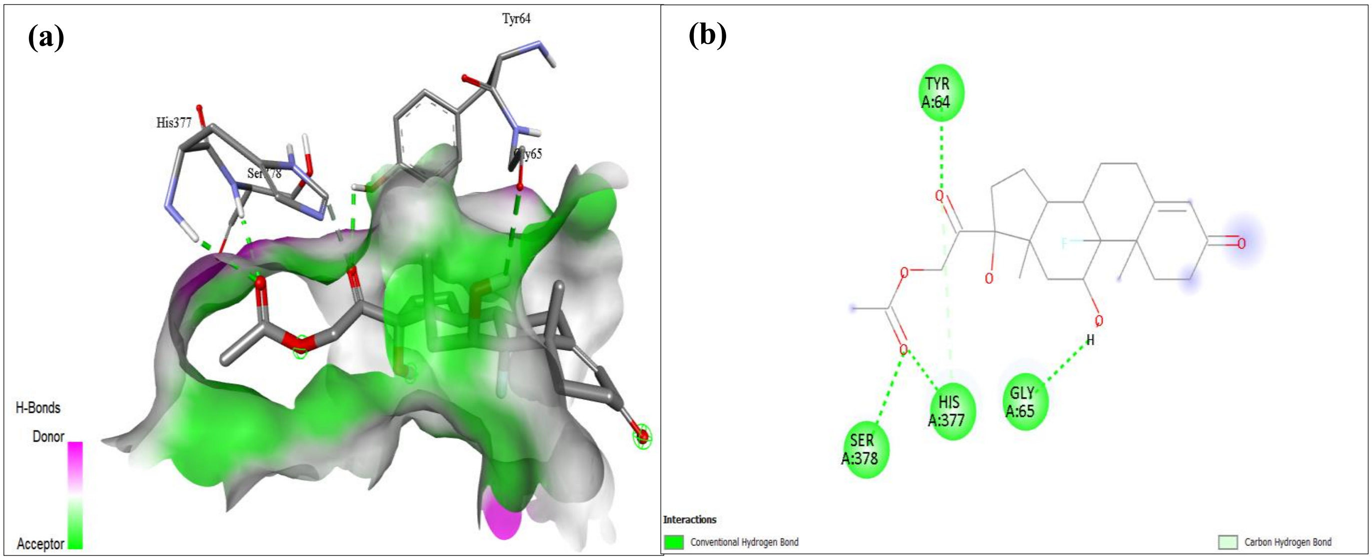
No. 64: Docked pose Deacetylnomilin in the CYP51(5V5Z) active site.



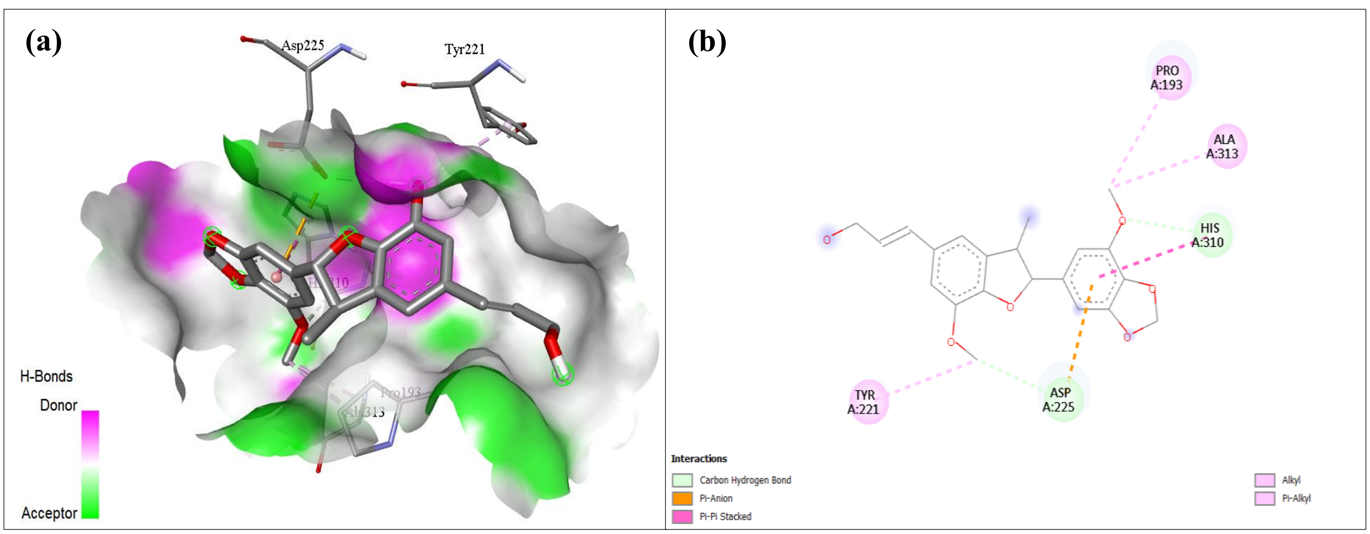
No. 65: Docked pose Desmethylxanthohumol in the CYP51(5V5Z) active site.



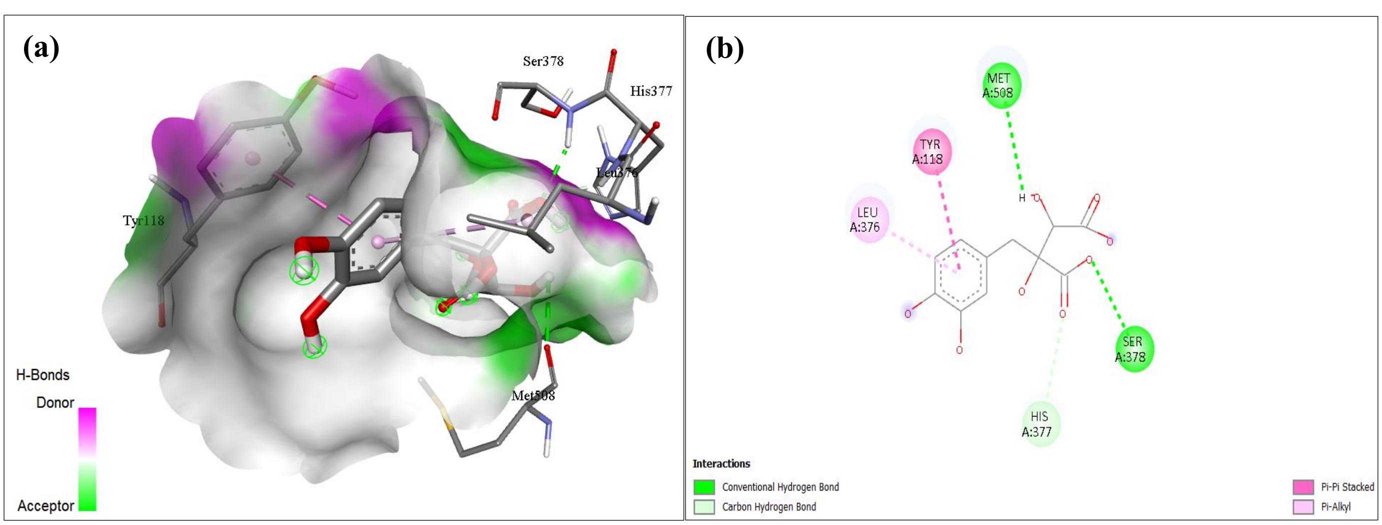
No. 66: Docked pose Eriocitrin in the CYP51(5V5Z) active site.



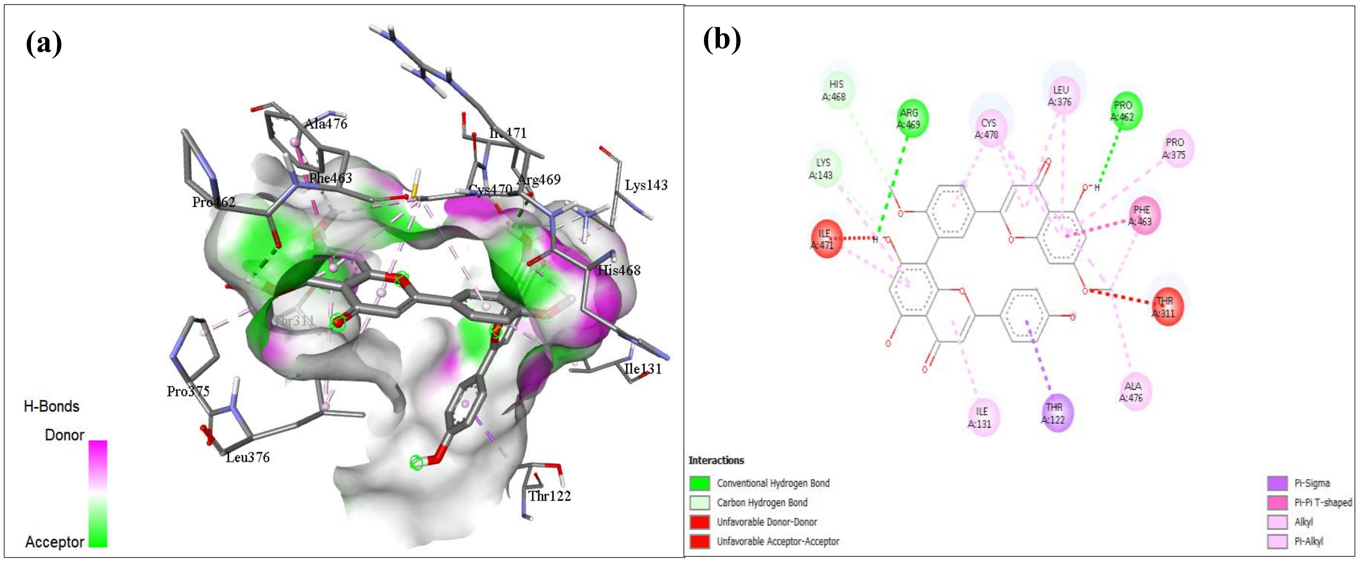
No.67: Docked pose Fludrocortisone acetate in the CYP51(5V5Z) active site.



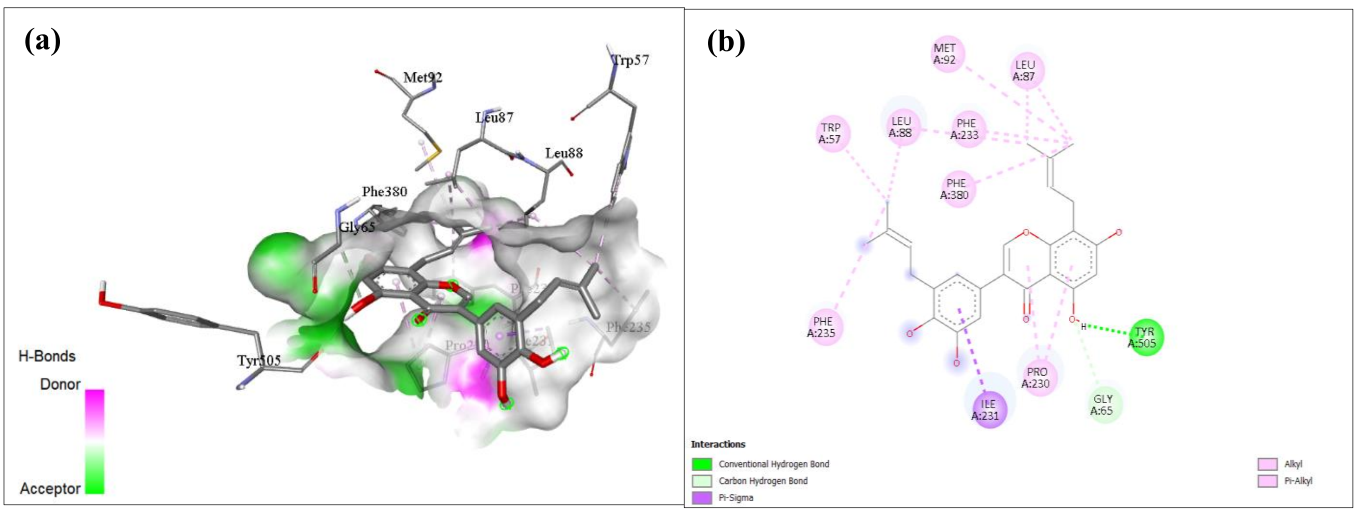
No. 68: Docked pose Fragransol D in the CYP51(5V5Z) active site.



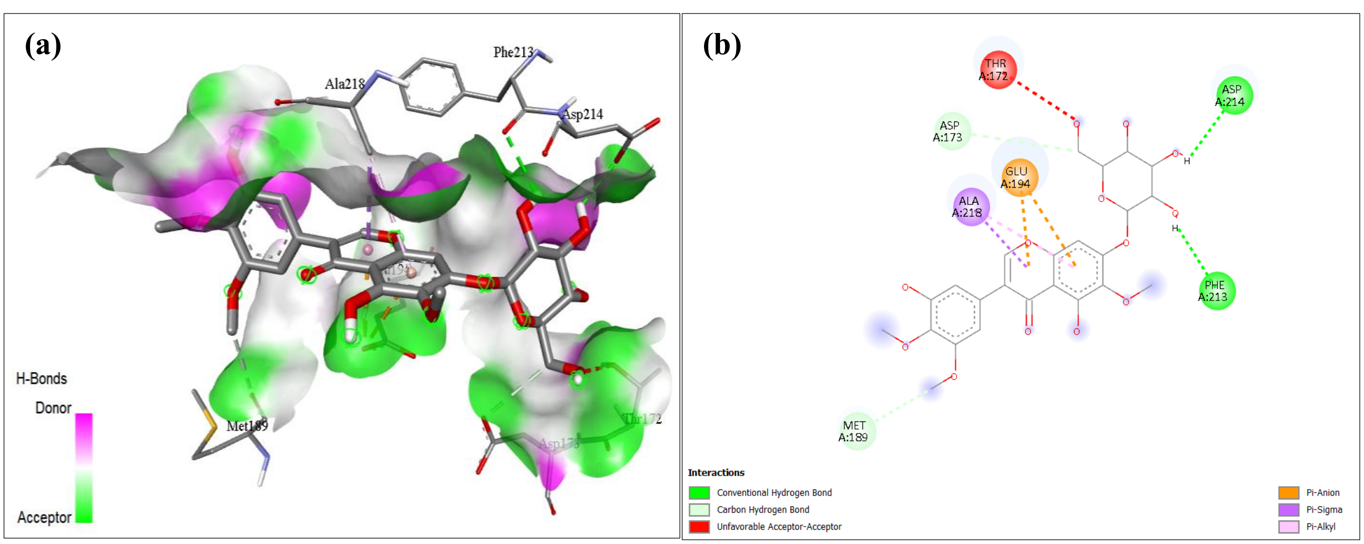
No. 69: Docked pose Fukiic acid in the CYP51(5V5Z) active site.



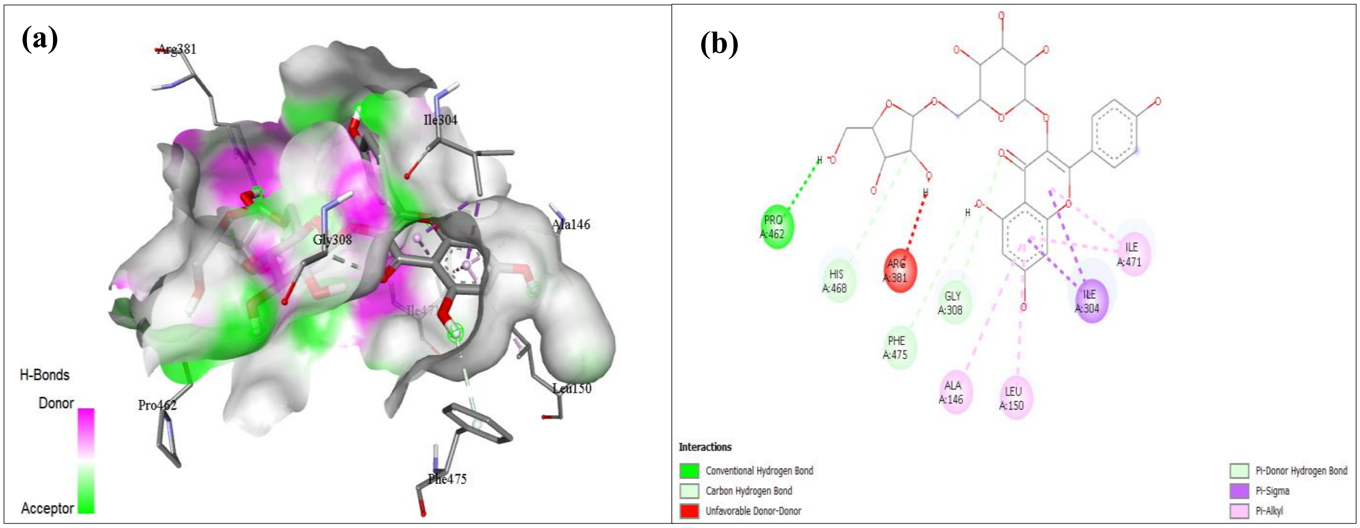
No.70: Docked pose Ginkgetin in the CYP51(5V5Z) active site.



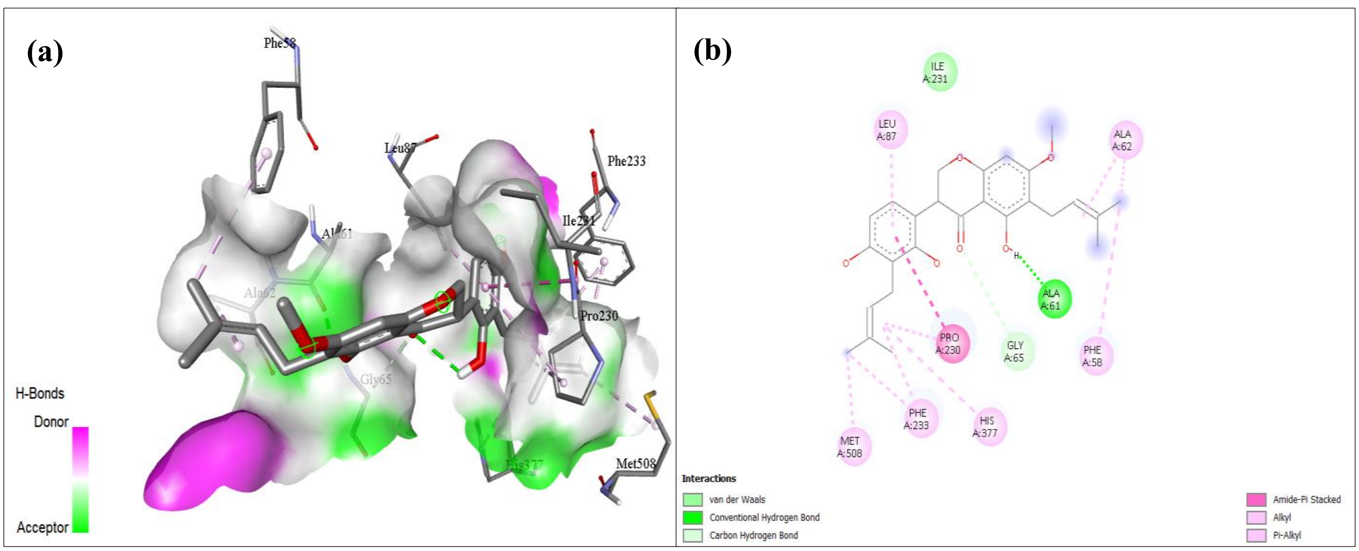
No.71: Docked pose Glyurallin B in the CYP51(5V5Z) active site.



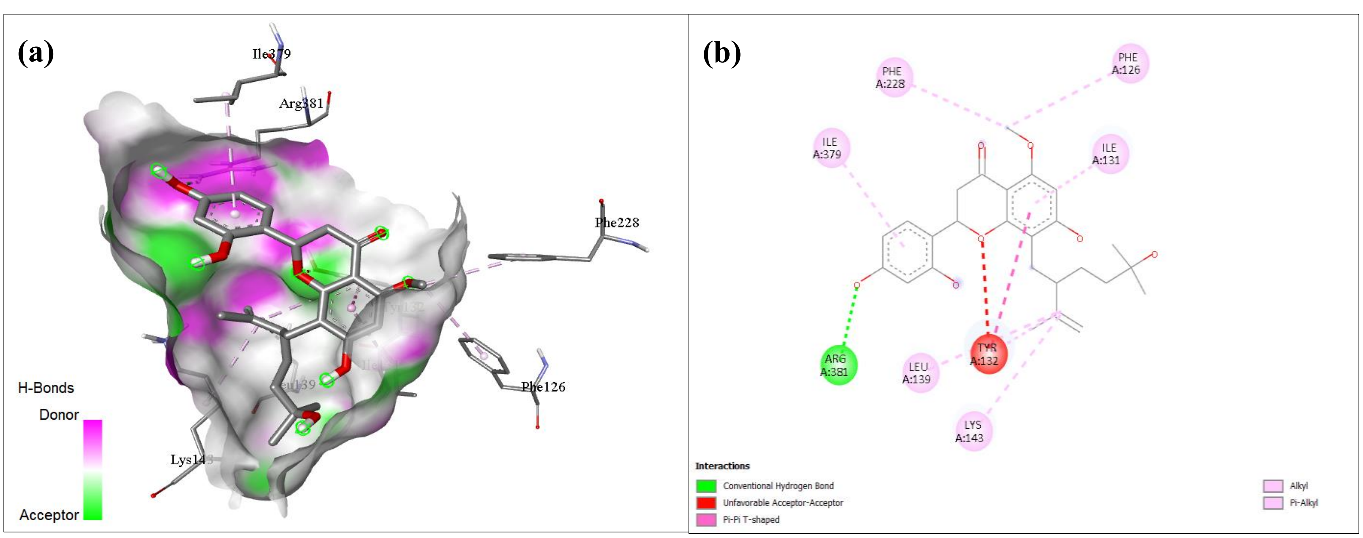
No. 72: Docked pose Irigenin 7-O-glucoside in the CYP51(5V5Z) active site.



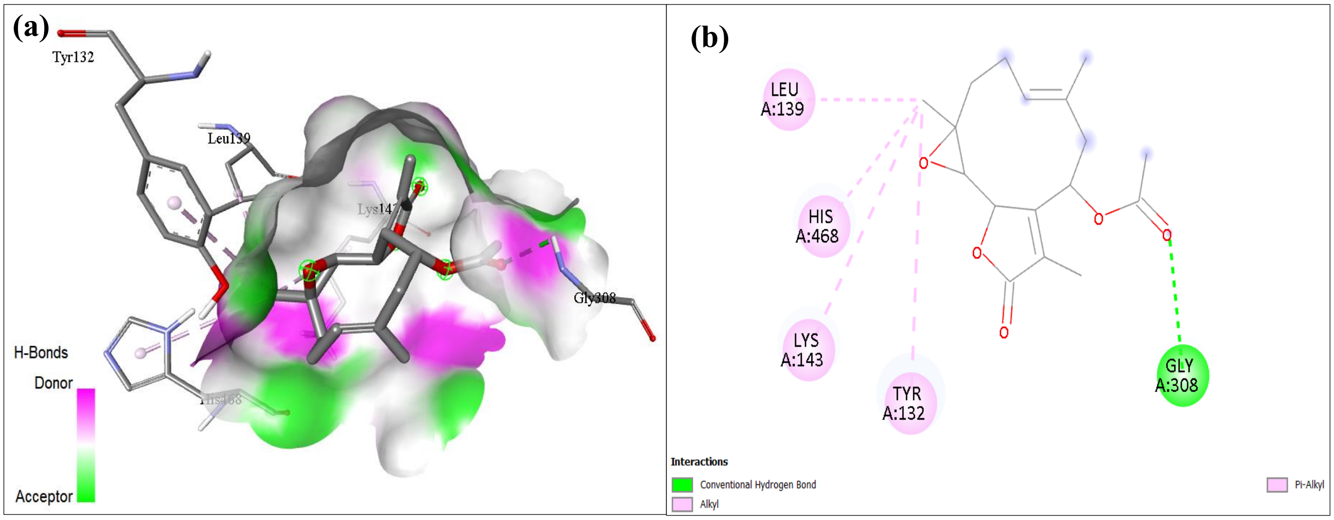
No.73: Docked pose Kaempferol 3-xylosylglucoside in the CYP51(5V5Z) active site.



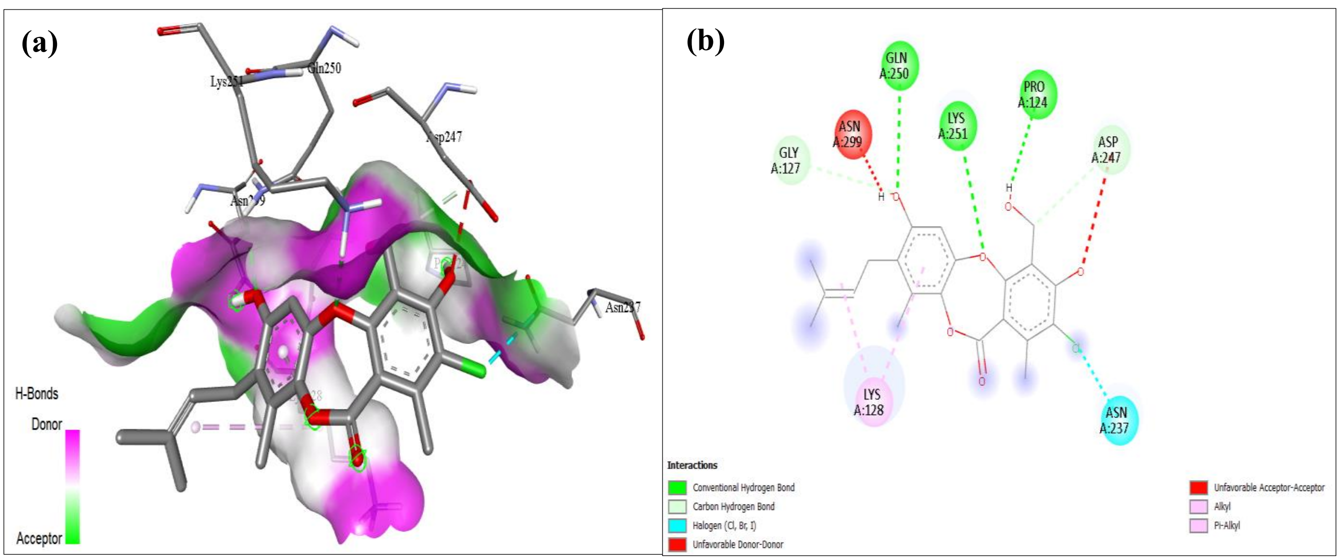
No.74: Docked pose Kanzonol G in the CYP51(5V5Z) active site.



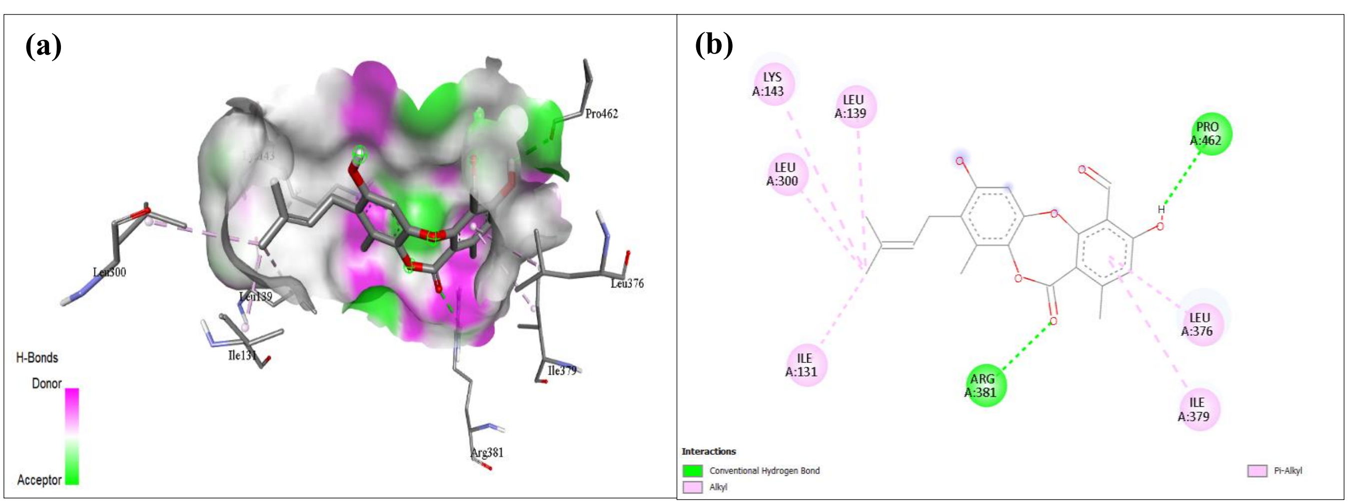
No.75: Docked pose Kurarinol in the CYP51(5V5Z) active site.



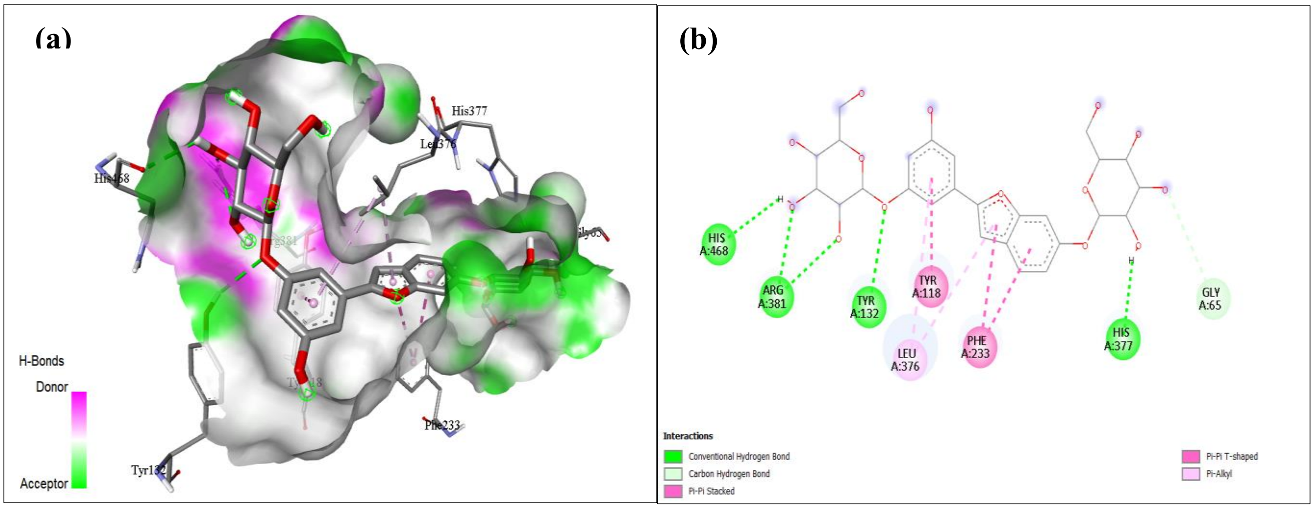
No. 76: Docked pose Lipiferolide in the CYP51(5V5Z) active site.



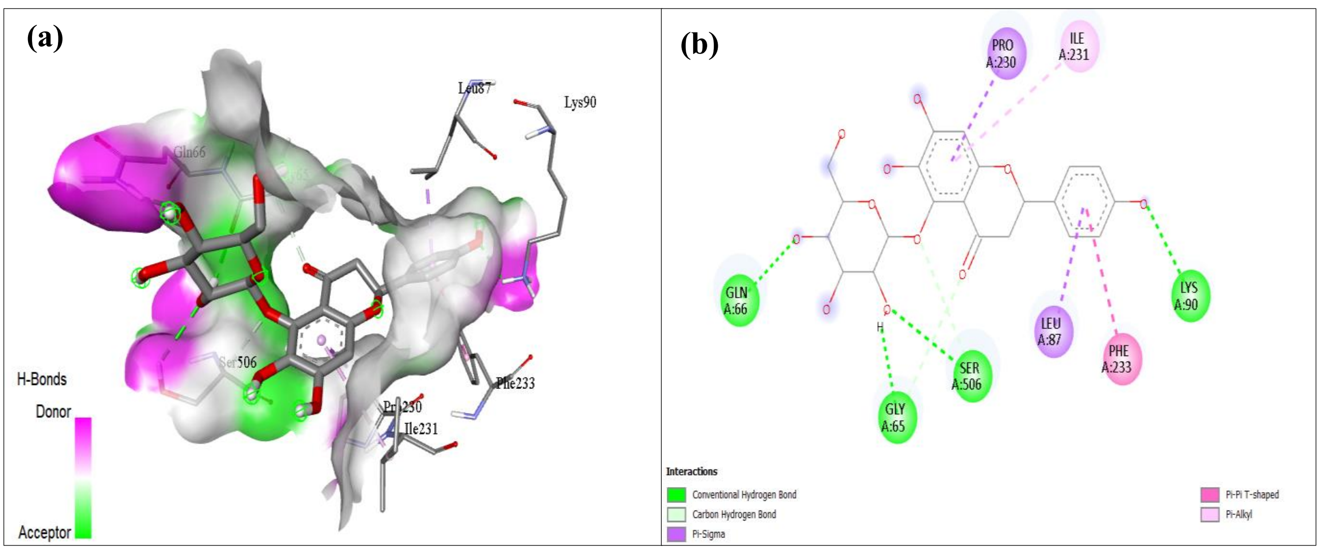
No. 77: Docked pose Mollicellin D in the CYP51(5V5Z) active site.



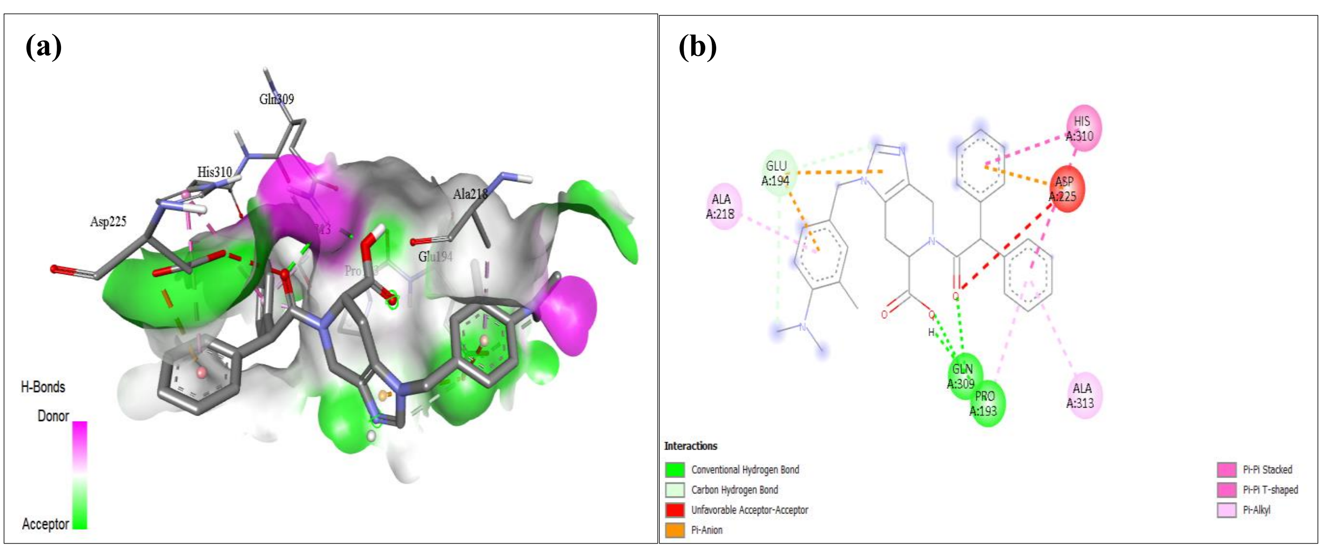
No. 78: Docked pose Mollicellin H in the CYP51(5V5Z) active site.



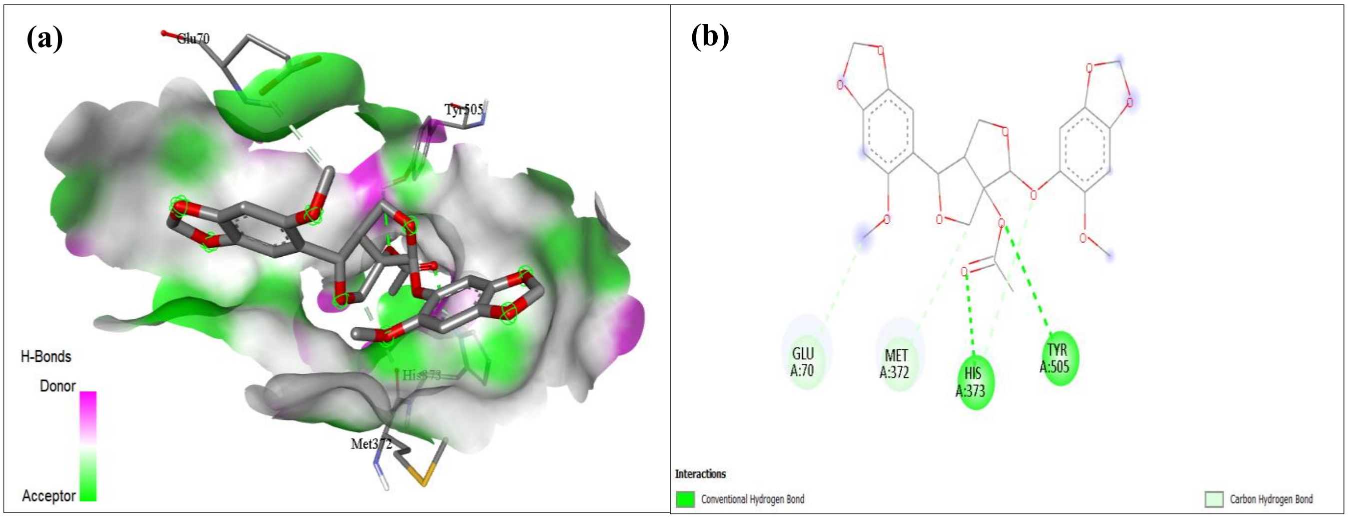
No. 79: Docked pose Mulberroside F in the CYP51(5V5Z) active site.



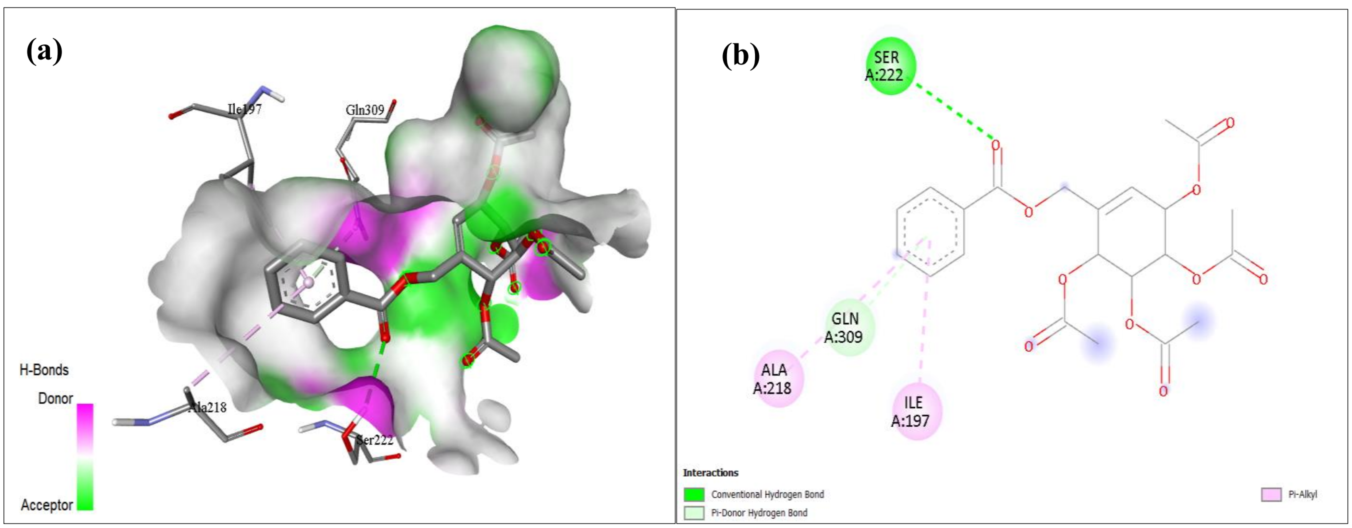
No. 80: Docked pose Neocarthamin in the CYP51(5V5Z) active site.



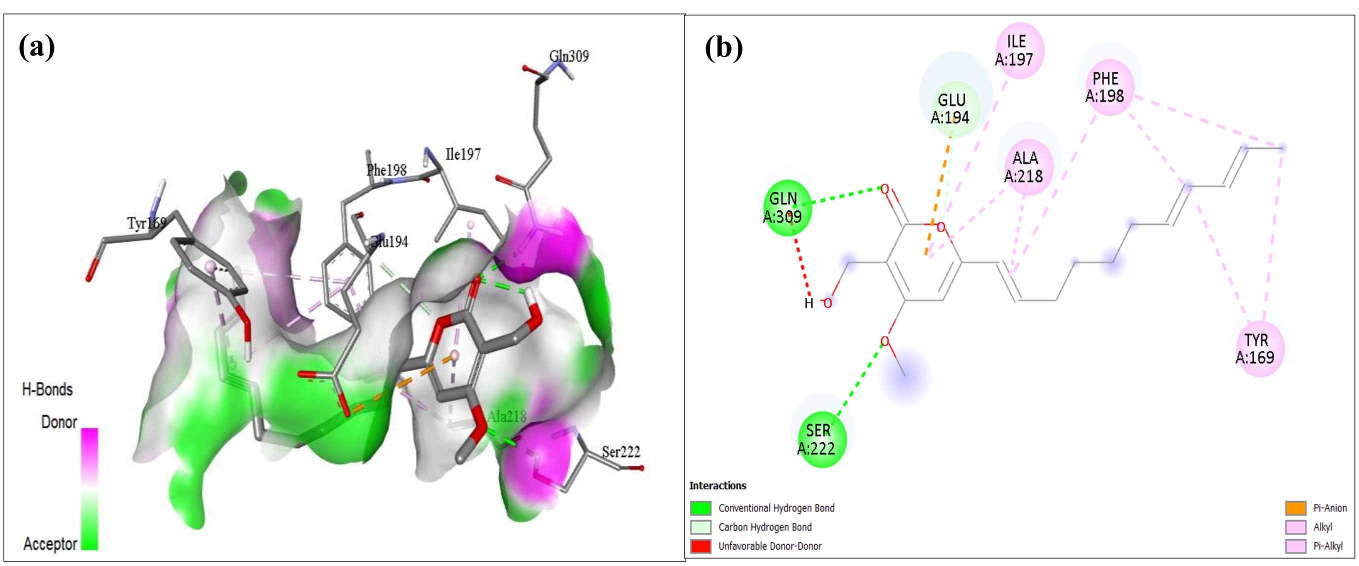
No. 81: Docked pose PD 123319 in the CYP51(5V5Z) active site.



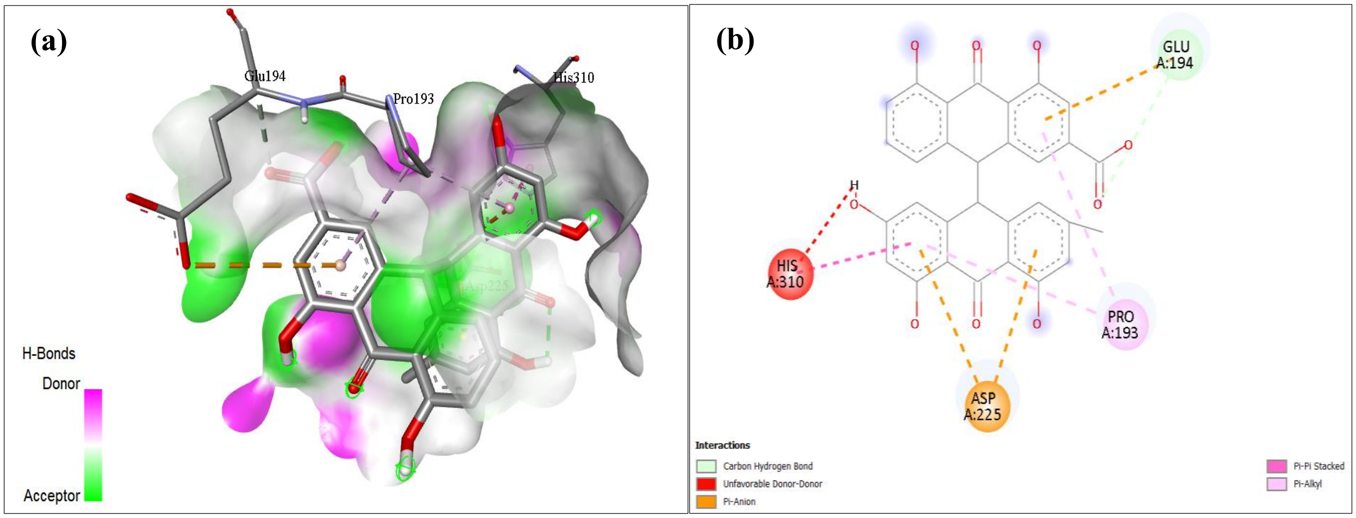
No. 82: Docked pose Phrymarolin I in the CYP51(5V5Z) active site.



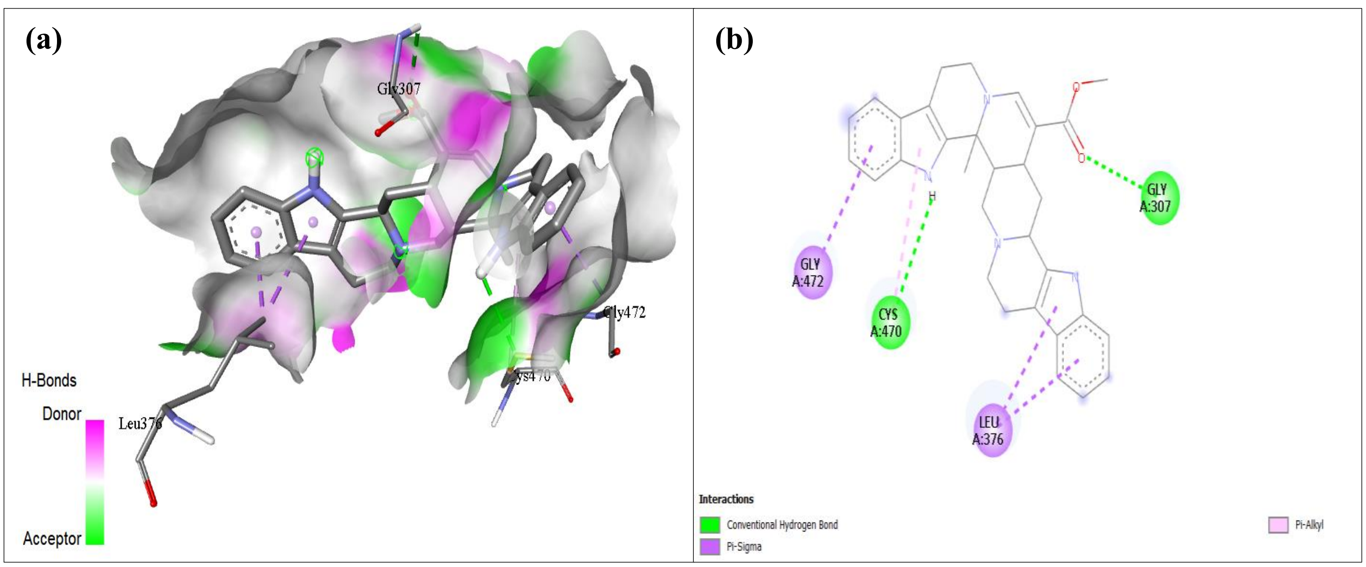
No. 83: Docked pose Piperenol C in the CYP51(5V5Z) active site.



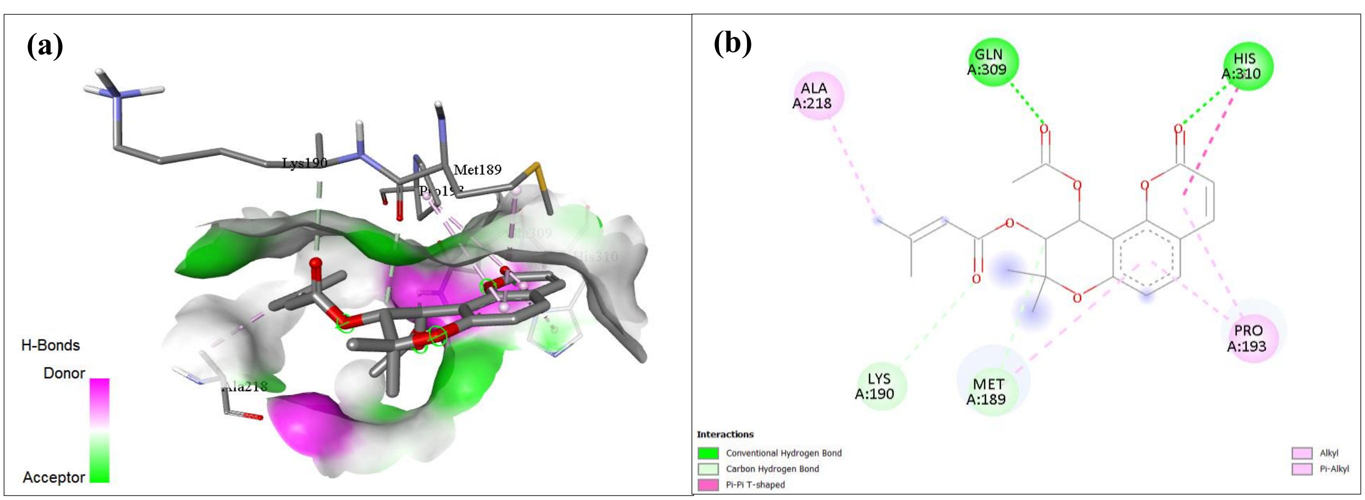
No. 84: Docked pose Prosolanapyrone II in the CYP51(5V5Z) active site.



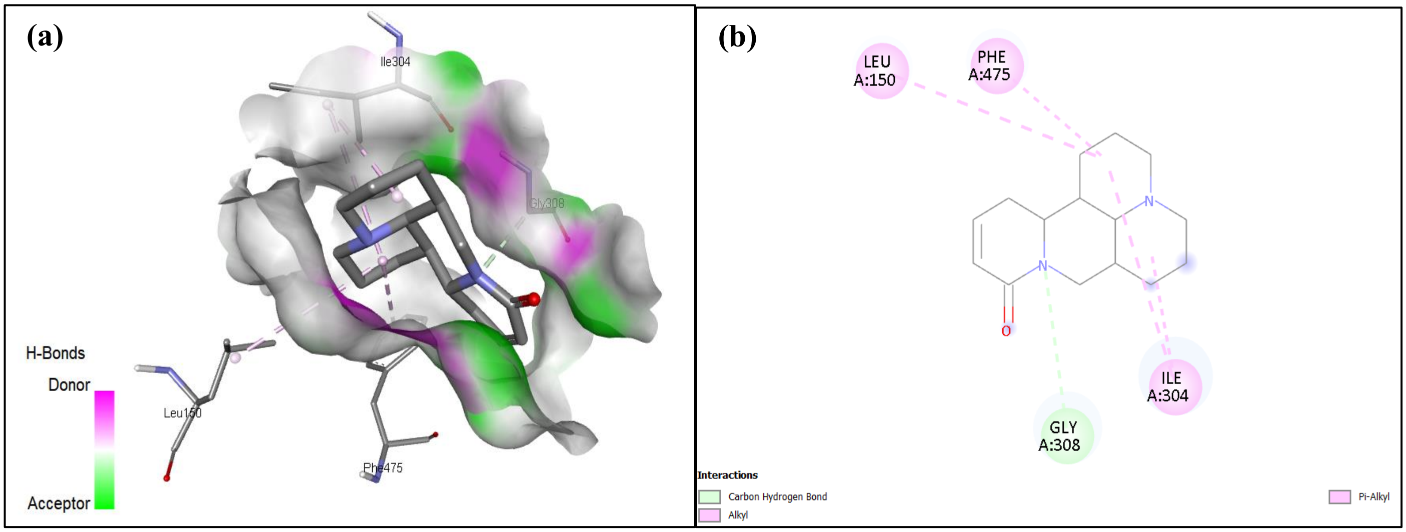
No. 85: Docked pose Rheidin A in the CYP51(5V5Z) active site.



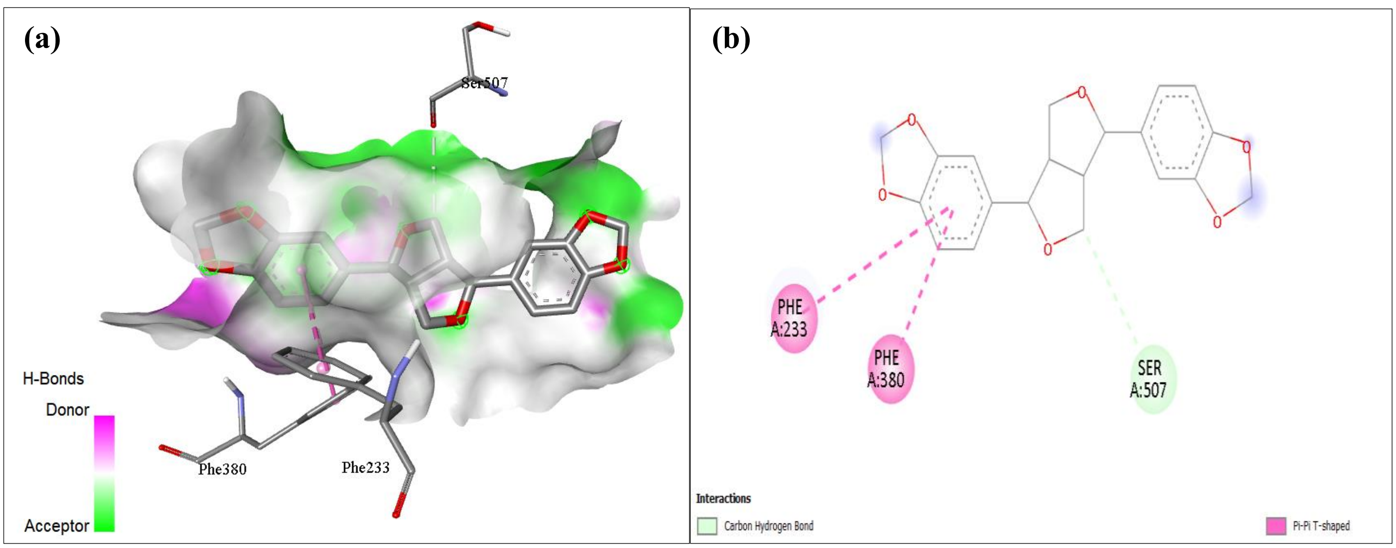
No. 86: Docked pose Roxburghine B in the CYP51(5V5Z) active site.



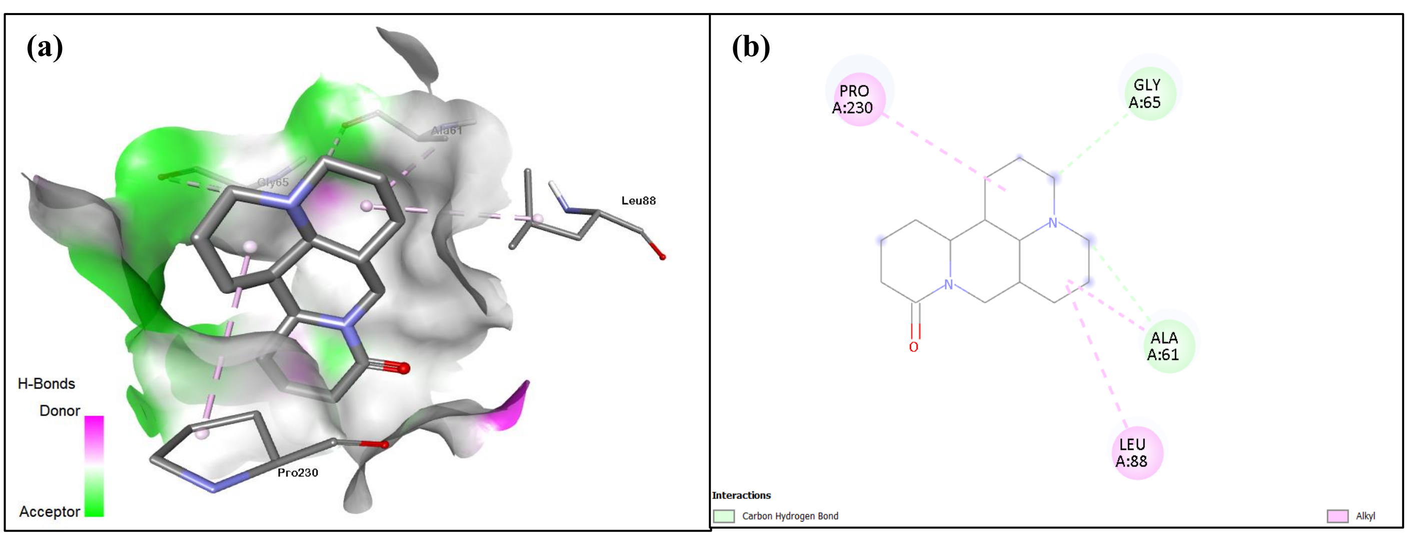
No. 87: Docked pose Samidin in the CYP51(5V5Z) active site.



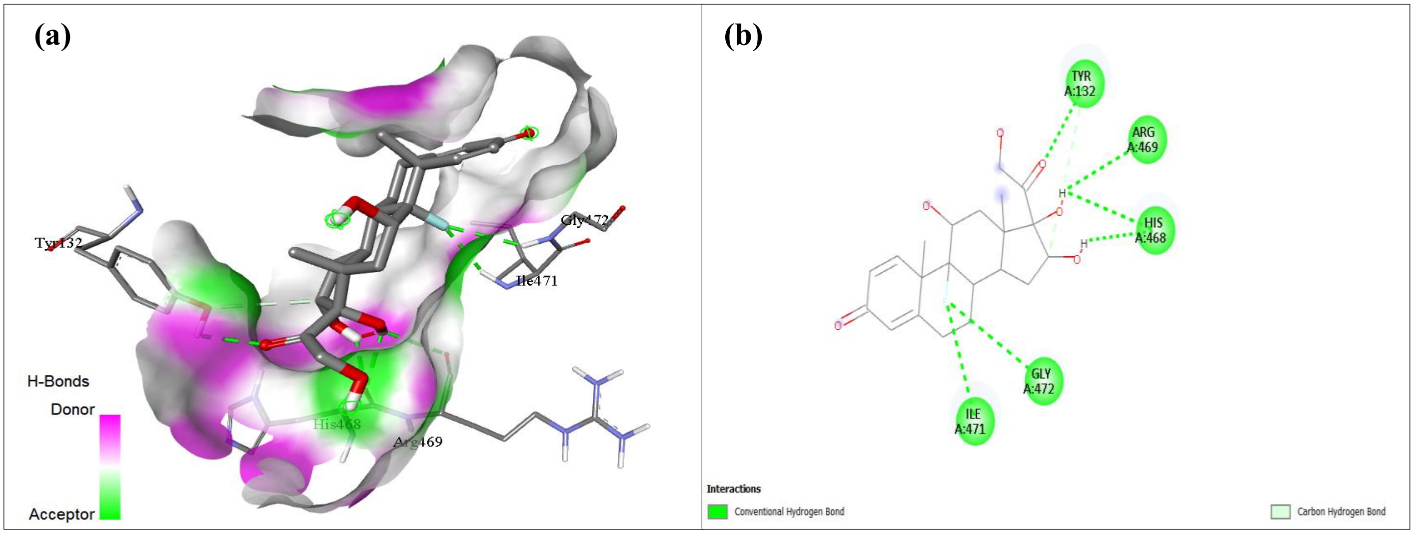
No. 88: Docked pose Sophocarpine in the CYP51(5V5Z) active site.



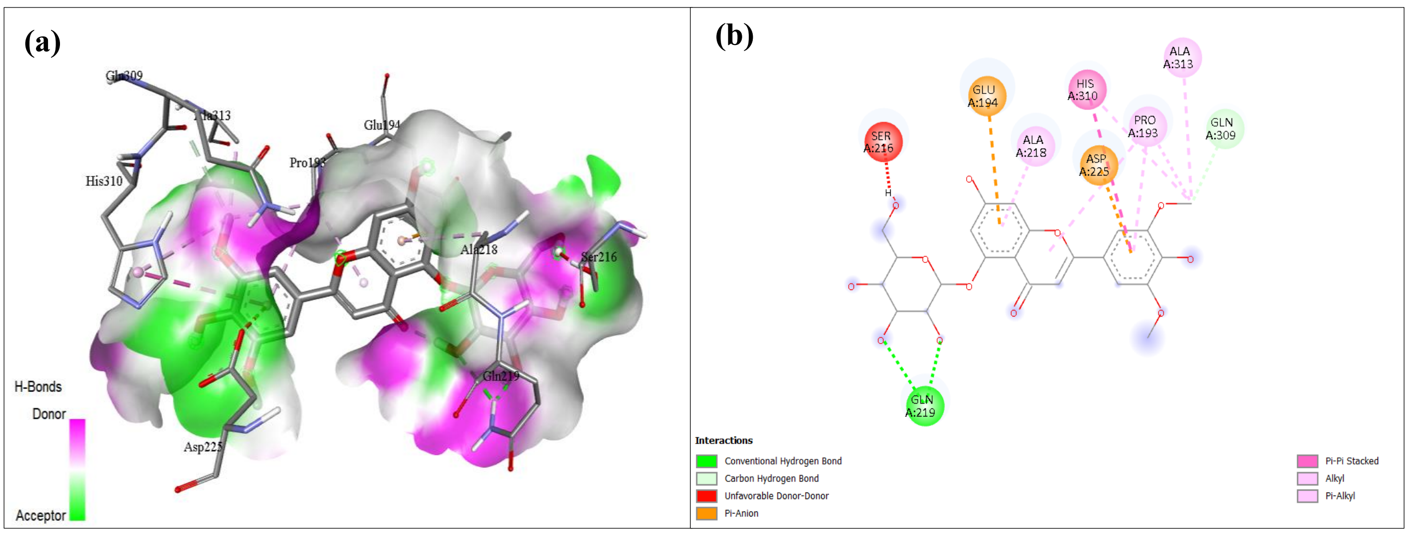
No. 89: Docked pose Sesamin in the CYP51(5V5Z) active site.



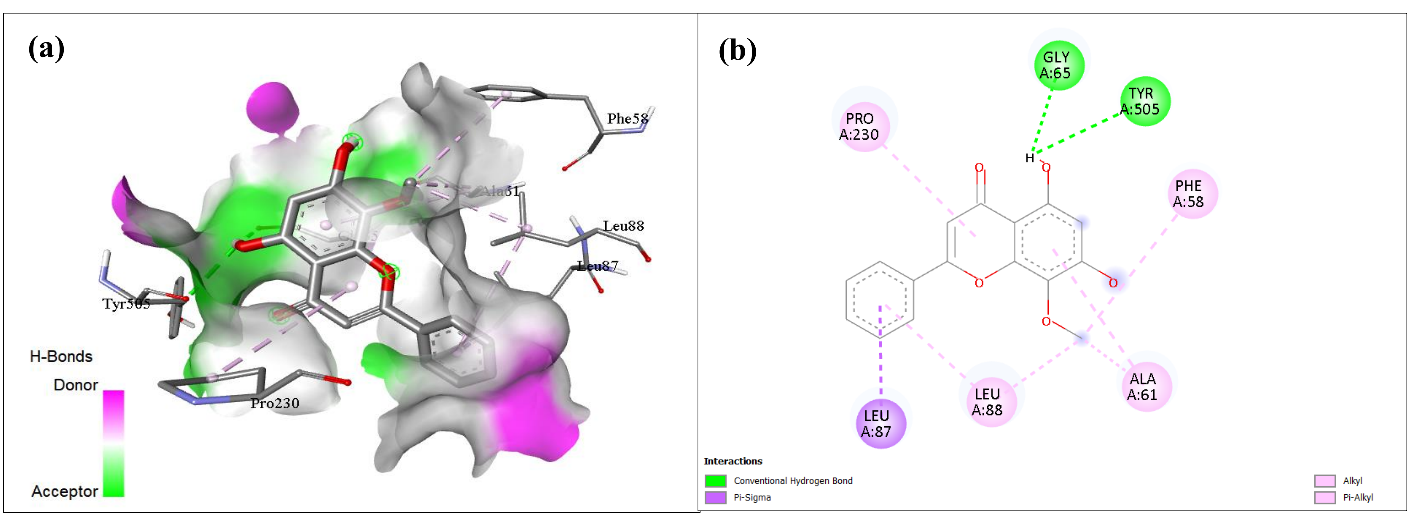
No. 90: Docked pose Sophoridine in the CYP51(5V5Z) active site.



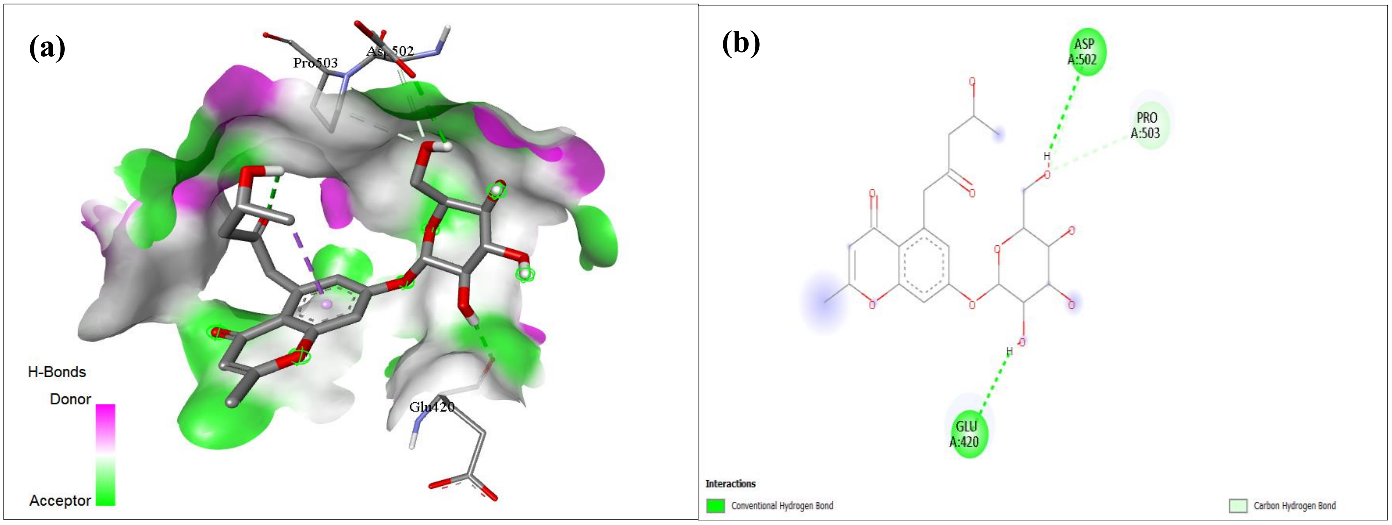
No. 91*:* Docked pose Triamcinolone in the CYP51(5V5Z) active site.



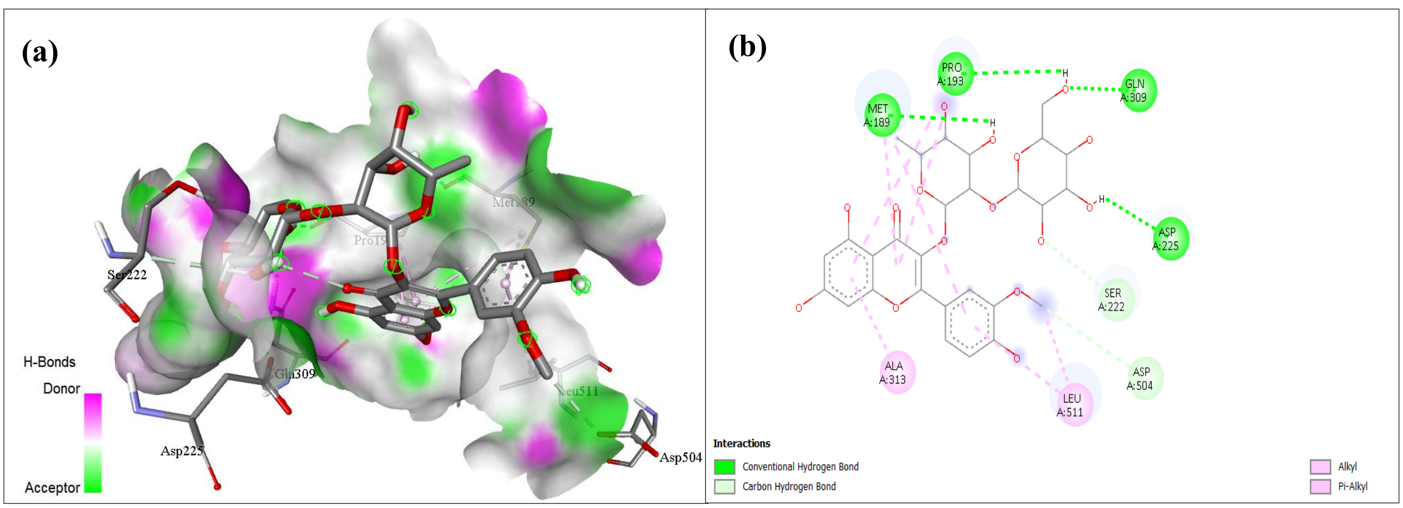
No. 92: Docked pose Tricin 5-glucoside in the CYP51(5V5Z) active site.



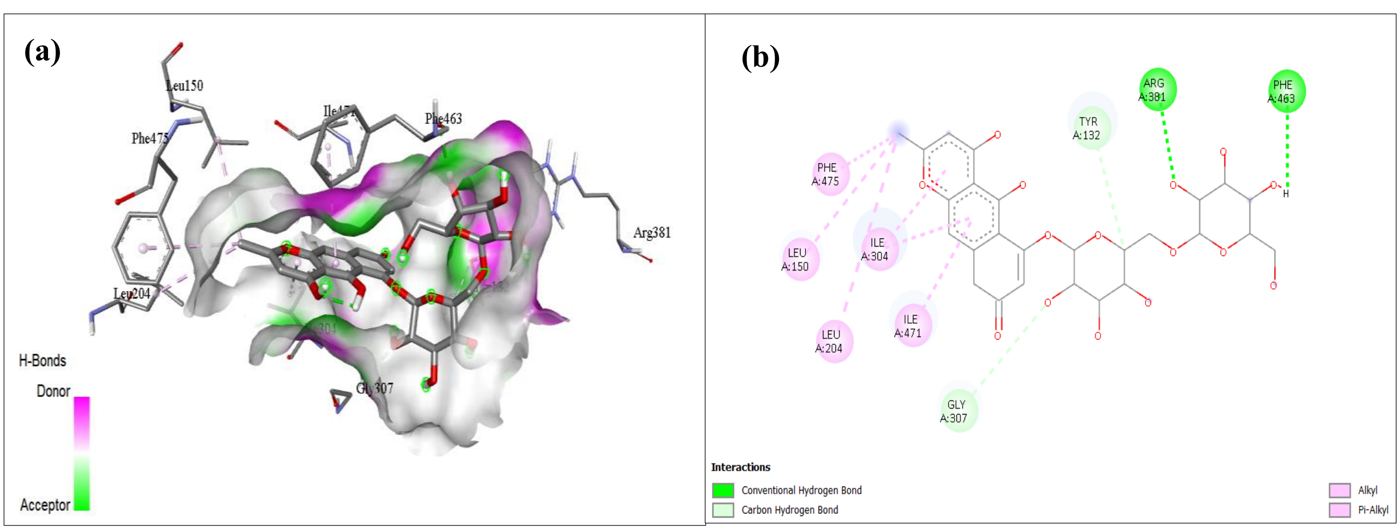
No.93: Docked pose Wogonin in the CYP51(5V5Z) active site.



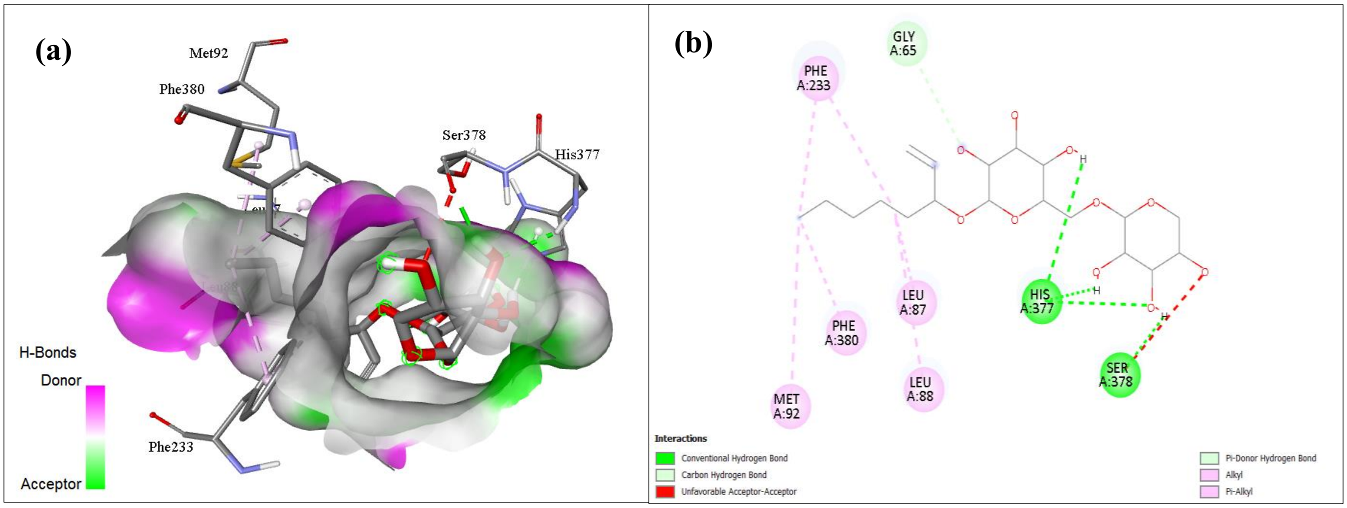
No. 94*:* Docked pose 7-Hydroxy-5-(4-hydroxy-2-oxopentyl)-2-methylchromone7-glucoside in the CYP51(5V5Z) active site



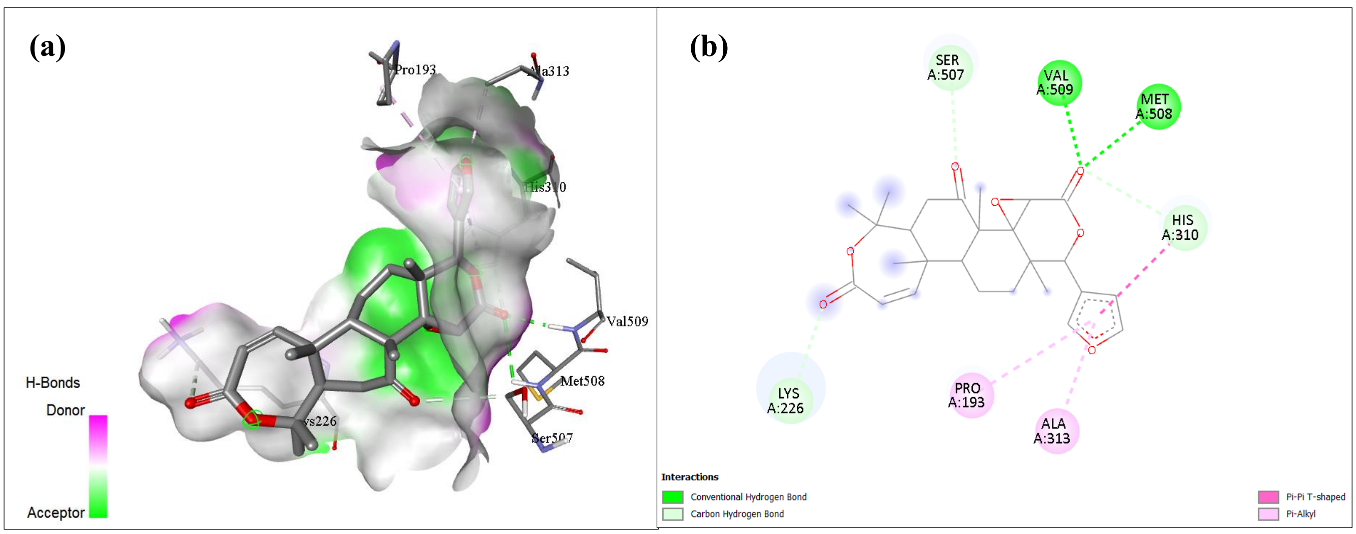
No. 95: Docked pose Isorhamnetin 3-O-[b-D-glucopyranosyl-(1->2)-a-L-rhamnopyranoside]in the CYP51(5V5Z) active site.



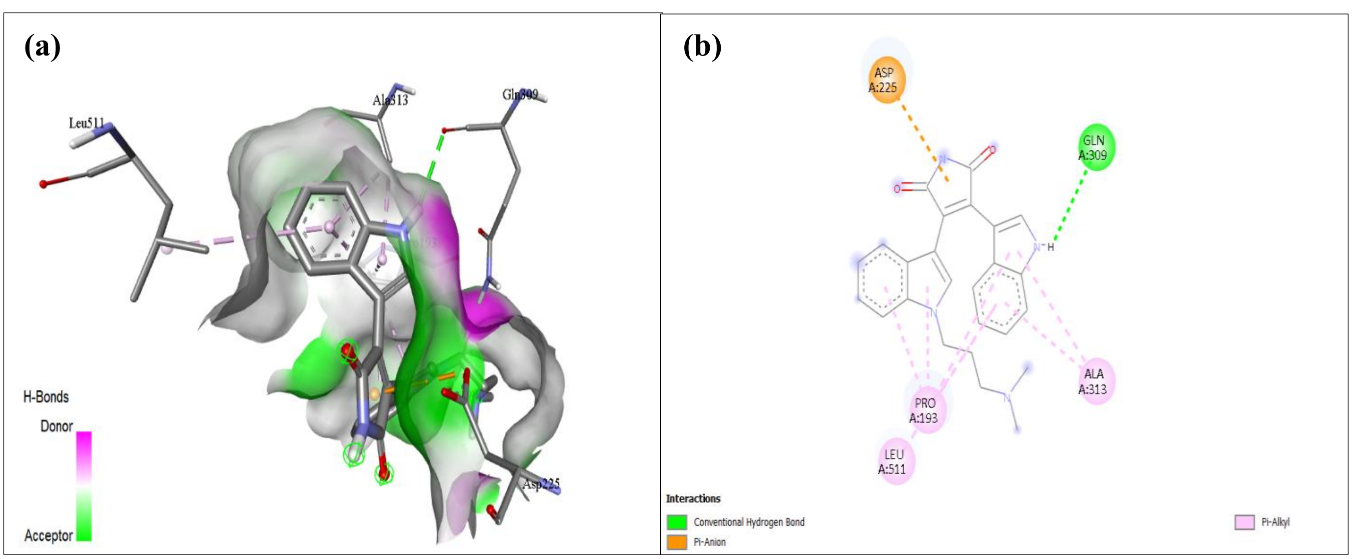
No. 96: Docked pose Norrubrofusarin 6-beta-gentiobioside in the CYP51(5V5Z) active site.



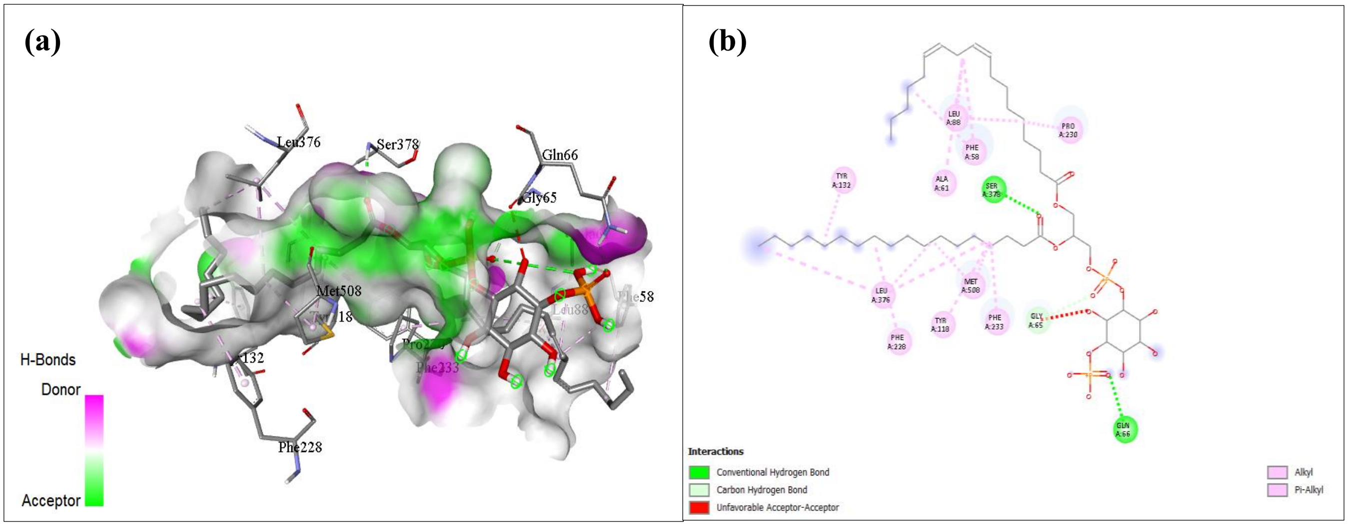
No. 97: Docked pose 1-Octen-3-yl primeveroside in the CYP51(5V5Z) active site.



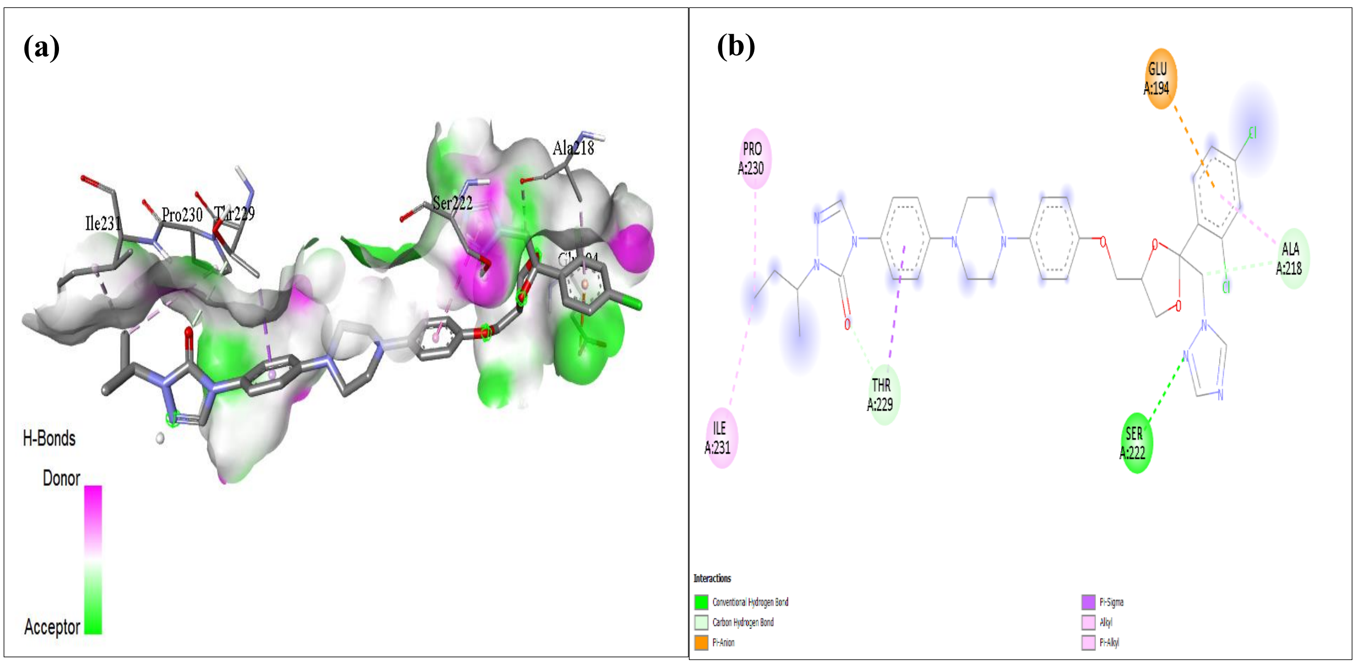
No. 98: Docked pose Tricoccin S3 in the CYP51(5V5Z) active site.



No. 99: Docked pose BisindolylmaleimideI in the CYP51(5V5Z) active site.



No 100: Docked pose PIP(18:2(9Z,12Z)/18:0) in the CYP51(5V5Z) active site.



No. 101: Docked pose Itraconazole in the CYP51(5V5Z) active site.

Figure S6: 3D and 2D binding interactions of bioactive compounds (1-100) from *S. flavescens* root and positive control (Itraconazole) (101) within the CYP51 active site.