Supplementary information's

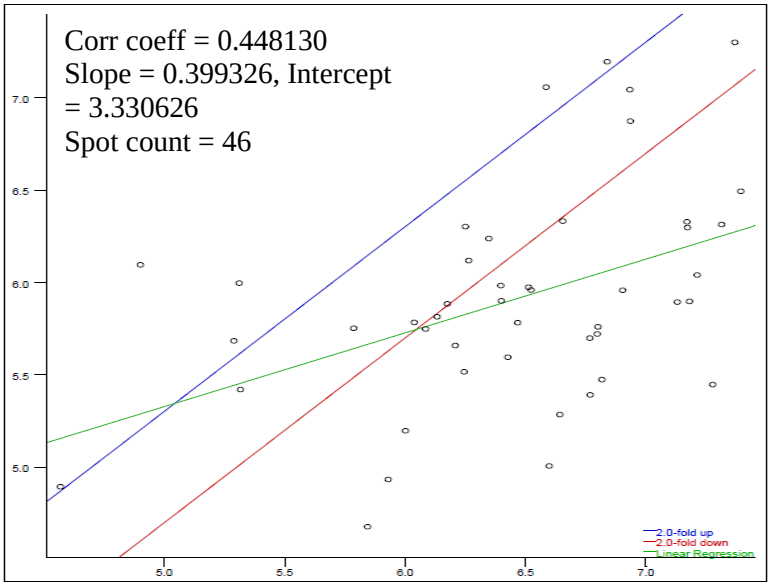

Figure 1. Correlation graph of spot matching. Analysis of protein spots in the homogenate of adult female parasites after the treatment of CA extract.

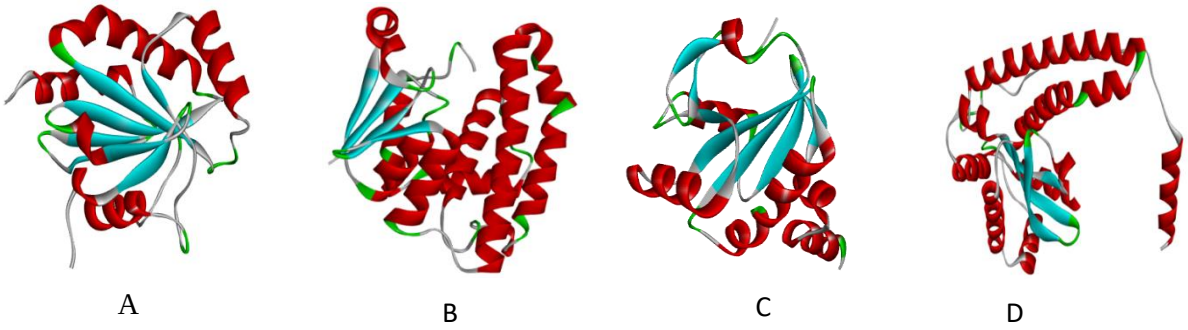

Figure 2. Three dimensional (3D) models of Anti-oxidant proteins (A) Glutathione peroxidase, (B) Glutathione-S-Transferase, (C) Thioredoxin transferase and (D) Superoxide dismutase.

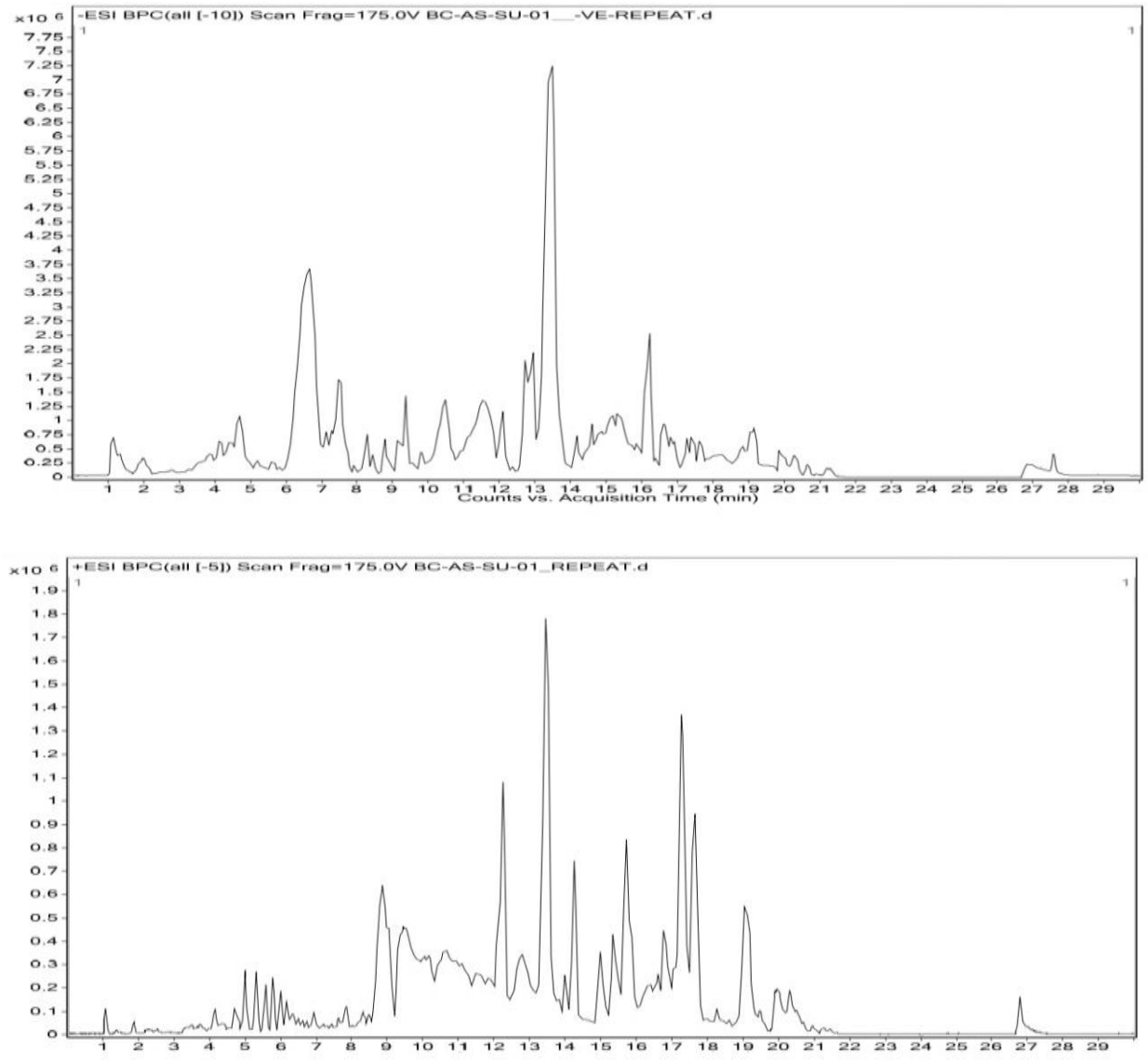

Figure 3. LC-MS of *Centratherum anthelminticum* ethanol seed extract, 30 minutes runs.

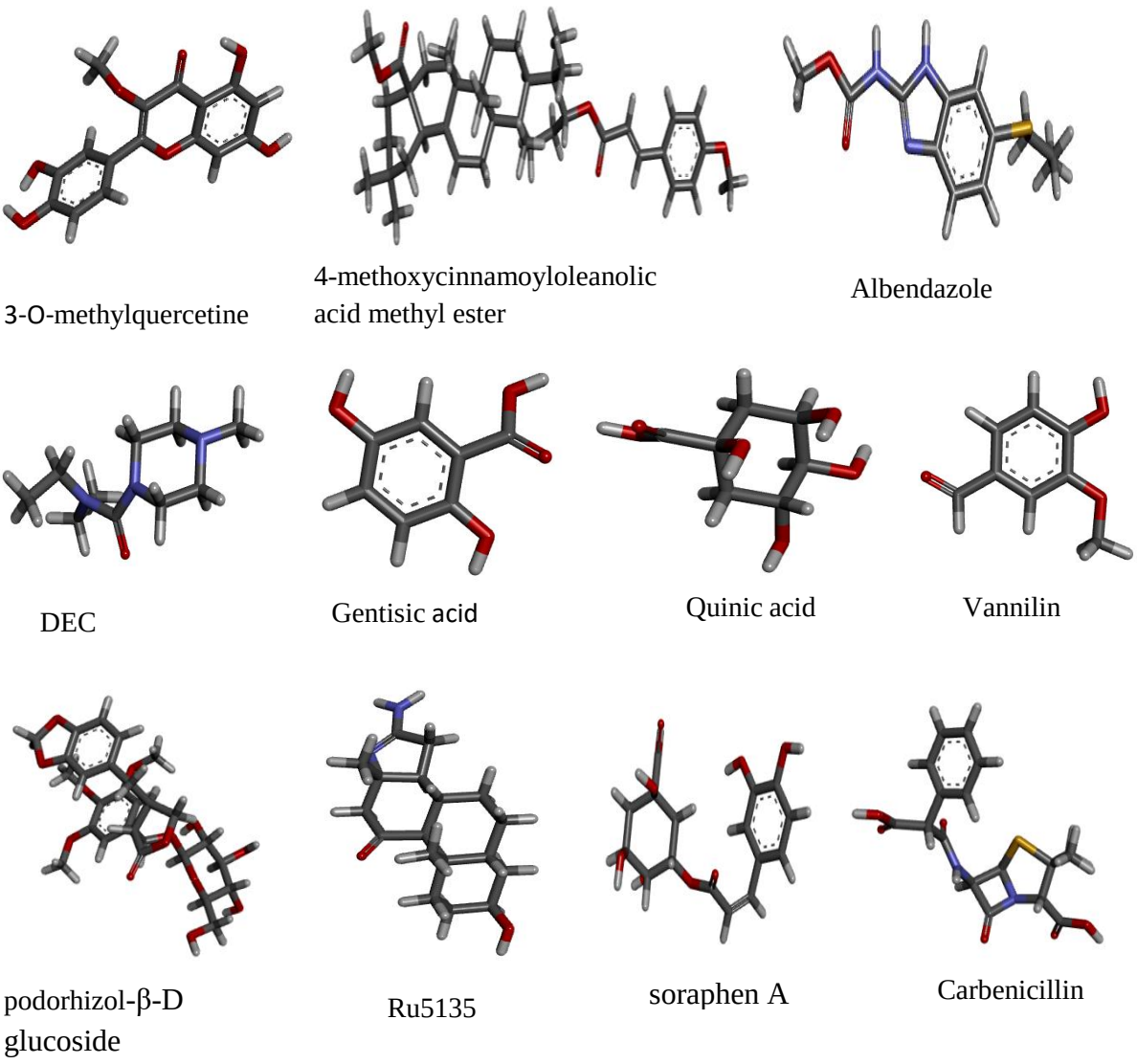

Figure 3. Three dimensional structures of CA bioactive compounds, i.e. selected for *in-silico* studies.

Table 1. Evaluating the accuracy of predicted protein structure of targeted filarial antioxidant proteins/enzymes models

Ramachandran plot analysis							
ProCheck server					**RAMPAGE server**		
Target protein	**Most favored regions**	**Additional allowed regions**	**Generously allowed regions**	**Disallowed regions**	**Number of residues in favored region**	**Number of residues in allowed region**	**Number of residues in outlier region**
GPx	134(93.1%)	10(6.9%)	0 (0.0%)	0 (0.0%)	153(93.0%)	10(7%)	0 (0.0%)

Hydrogen bond statistics

Mean H-bond distance		**Mean H-bond energy**		**Residue with H-bond**	
Target Protein	Observed	Expected	Observed	Expected	Observed	Expected
GPx	2.2 (sd=0.3)	2.2 (sd= 0.4)	-1.7 (sd=1.0)	-2.0 (sd=0.8)	348 (77%)	336 (75%)

Table 2A. Molecular Screening of negative LC-MS compounds by CA using PyRx (AutoDock Vina) and PatchDock server with Superoxide dismutase

S.N.	**Ligand**	**Binding Affinity**	**Score**	**Area**	**ACE**
1	2-Acetylthiophene	-3.7	2166	226.6	81.85
2	3-acetyl-6-methoxybenzaldehyde	-4.6	2978	335.5	-3.4
3	3-Methylindolepyruvate	-5.5	2818	326.4	9.33
4	3-O-Methylquercetin	-6.2	3352	415.4	-111.54
5	4-Dodecylbenzenesulfonic	-5.7	4658	502.5	-130.19
6	4-Methoxycinnamoyloleanolic acid methyl ester	-8.3	5480	629.9	-50.26
8	Annotemoyin 1	-4.5	5658	756.5	-256.21
9	Ascorbyl stearate	-4.9	5266	591.7	-72.7
10	Avocadene_2-acetate	-4.6	4758	522	-66.19
11	Beta-Obscurine	-6.7	2968	320.6	29.8
12	Carbenicillin	-6.2	3934	475.5	-212.64
13	3-Carboxyethenyl-3,5-cyclohexadiene-1,2-diol	-5.1	2686	291	5.38
14	Dibutyl decanedioate	-4.2	4650	533.6	-60.19
15	Flavine mononucleotide (FMN)	-6.4	4378	470	-121.8
16	Gentisic acid	-4.9	2282	252.3	6.44
17	PG(161(9Z)160)	-4.5	7084	907.5	-76.03

18	Podorhizol beta-D-glucoside	-6.0	4704	533.2	-79.67
19	Quinic acid	-5.7	2316	255.9	37.02
20	RU 5135	-6.5	3154	361.9	-100.79
21	Soraphen A	-5.8	3588	420.3	-82.71
22	DEC	-3.9	2936	342.3	-4.55
23	Vernodalin	-6.4	3766	437.6	-164.44
24	Ivermectin	-8.7	6912	891.7	-217.45
25	Albendazole	-5.0	3648	413.9	-109.75

Table- 2B Molecular Screening of negative LC-MS compounds by CA using PyRx (AutoDock Vina) and PatchDock server with Thioredoxin

S.N.	**Ligand**	**Binding Affinity**	**Score**	**Area**	**ACE**
1	2-Acetylthiophene	-3.9	2062	208.8	-120.34
2	3-acetyl-6-methoxybenzaldehyde	-5.3	2704	292.3	-113
3	3-Methylindolepyruvate	-6.3	2784	295.4	-104.09
4	4-Dodecylbenzenesulfonic acid	-5.4	3498	384.2	-184.9
5	3-O-Methylquercetin	-6.7	3920	423.6	-177.16
6	4-Methoxycinnamoyloleanolic acid methyl ester	-7.6	5324	587.3	2.92
8	Annotemoyin 1	-6.3	4392	520.6	-108.46
9	Ascorbyl stearate	-5.3	4582	586.4	-33.46
10	Avocadene 2-acetate	-4.9	4322	481.1	-52.61
13	Beta-Obscurine	-6.9	2994	331.7	-50.98
12	Carbenicillin	-6.9	3992	454.3	-163.83
13	3-Carboxyethenyl-3,5-cyclohexadiene-1,2-diol	-5.5	2582	270.1	-108.41
14	Dibutyl decanedioate	-5.2	4226	523.3	-56.34
15	Gentsic acid	-5.5	4290	493.8	-8.56
16	Flavine mononucleotide (FMN)	-7.5	2164	265.3	-12.96
17	PG(161(9Z)160)	-4.9	5960	754.3	-116.92
18	Podorhizol beta-D-glucoside	-6.7	4668	542.7	-138.9
19	Quinic acid	-5.3	2208	227	-80.32
20	RU 5135	-7.2	3432	377.5	-45.57
21	Soraphen A	-6.7	3520	383.7	-117.43
22	DEC	-4.6	3000	320.2	-95.42
23	Ivermectin	-7.5	3894	440.4	-32.07
24	Vernodalin	-6.6	6786	874.9	-143.65
25	Albendazole	-5.7	3374	363.3	-98.38

Table 2C. Molecular Screening of negative LC-MS compounds by CA using PyRx (AutoDock Vina) and PatchDock server with Glutathione-S-Transferase

S.N.	Ligand	Binding Affinity	Score	Area	ACE
1	2-Acetylthiophene	-4.6	2666	295	-123.3
2	3-acetyl-6-methoxybenzaldehyde	-5	3268	408.9	-105.3
3	3-Methylindolepyruvate	-6.2	3196	414	-144.16
4	3-O-Methylquercetin	-6.7	3746	450.5	-97.94
5	4-Dodecylbenzenesulfonic acid	-5.5	4614	505.2	-110.4
6	4-Methoxycinnamoyloleanolic acid methyl ester	-8.8	5830	848.9	-68.31
8	Annotemoyin 1	-6.4	5688	659.6	-89.5
9	Ascorbyl stearate	-4.6	5406	657.9	81.08
10	Avocadene 2-acetate	-4.8	4766	642.6	-67.44
11	beta-Obscurine	-6.9	3288	500.5	-176.07
12	Carbenicillin	-6.6	4260	493.5	-79.17
13	3-Carboxyethenyl-3,5-cyclohexadiene-1,2-diol	5.1	3054	373.1	-79.17
14	Dibutyl decanedioate	-4.4	4870	593.8	-96.45
15	Flavine mononucleotide (FMN)	-7.1	4710	506.7	-134.78
16	Gentisic acid	-5.5	2706	305.3	-86.24
17	PG(161(9Z)160)	-5.5	7192	884.6	-81.29
18	Podorhizol beta-D-glucoside	-7.5	4802	599.3	-138.33
19	Quinic acid	-5.1	2790	327.7	-84.51
20	RU 5135	-6.8	3488	492.5	-192.03
21	Soraphen A	-6.7	3730	486	-109.89
22	Ivermectin	-8.9	7318	935.7	-205.6
23	DEC	-4.3	3314	414.1	-151.1
24	Vernodalin	-6.8	3930	430.4	-138.6
25	Albendazole	-5.5	3540	466.6	-140.15

Table 2D. Molecular Screening of negative LC-MS compounds by CA using PyRx (AutoDock Vina) and PatchDock server with Glutathione Peroxidase

S.N.	Ligand	Binding Affinity	Score	Area	ACE
1	2-Acetylthiophene	-3.8	2808	292.70	-148.16
2	3-acetyl-6-methoxybenzaldehyde	-4.9	3084	378.00	-163.28
3	3-Methylindolepyruvate	-5.1	3556	417.10	-200.04
4	3-O-Methylquercetin	-5.9	3864	500.00	-243.56
5	4-Dodecylbenzenesulfonic acid	-5.3	4520	567.80	-306.45
6	4-Methoxycinnamoyloleanolic acid methyl ester	-7.6	5448	647.70	-174.14
8	Annotemoyin 1	-5.1	5624	733.10	-194.98
9	Ascorbyl stearate	-4.3	5490	807.30	-322.08

10	Avocadene 2-acetate	-4.5	4700	634.50	-240.66
11	beta-Obscurine	-5.9	4362	524.40	-208.93
12	Carbenicillin	-5.4	4542	590.10	-332.63
13	3-Carboxyethenyl-3,5-cyclohexadiene-1,2-diol	-4.9	3066	382.00	-138.69
14	Dibutyl decanedioate	-3.9	4732	648.20	-219.66
15	Flavine mononucleotide (FMN)	-5.4	5034	669.50	-272.01
16	Gentisic acid	-5.2	3010	310.50	-125.61
17	PG(161(9Z)160)	-3.6	6744	908.00	-227.14
18	Podorhizol beta-D-glucoside	-6.0	5060	748.80	-430.03
19	Quinic acid	-5.2	3066	322.40	-115.59
20	RU 5135	-6.1	3934	491.10	-254.34
21	Soraphen A	-5.6	4328	559.90	-226.38
22	Ivermectin	-7.6	7100	897.90	-278.94
23	DEC	-3.8	3708	454.50	-212.10
24	Vernodalin	-6.2	7100	897.90	-278.94
25	Albendazole	-4.9	3698	397.90	-165.80

Table 4. Drug likeness properties of CA bioactive compounds

Drug Name	PubChen CID	Molecular Weight g/mol	LogP value	H-bond Donor	H-bond Acceptor	Molar Refractivity
3-O-Methylquercetin	5280681	316.00	2.099299	4	7	78.430
4-Methoxycinnamoyloleanolic acid methyl ester	131751417	630.00	8.906134	0	5	175.970
Podorhizol beta-D-glucoside	443015	578.00	0.330600	4	13	137.899
RU 5135	656742	304.00	2.288500	3	4	85.427
Soraphen A	5281897	520.00	3.802699	2	8	138.595
Carbenicillin	20824	378.00	0.486500	3	8	92.477
Beta-Obscurine	5460546	272.0	2.456900	1	3	78.898
Gentisic acid	3469	154.0	0.796000	3	4	36.730
Quinic acid	6508	192.0	-2.321400	5	6	39.839
Vanillin	1183	152.0	1.213300	1	3	40.046
Albendazole	2082	265.00	3.243299	2	4	73.136
DEC	3052	199.00	0.695600	0	4	57.386

Table 5. Showing the interacting residue common in active site and ligand and protein complex involved in H-bonding

Receptor	S.N.	Drug Name (PubChem CID)	Interacting receptor residue	Ligand and Protein atom involved in H-bonding
GPx	1	3-O-Methylquercetin	THR^{15}, VAL^{16}, LYS^{17} ASP^{23}, SER^{102}, LYS^{103}, ILE^{104}, LYS^{105}, ASP^{110}, ALA^{111}, ASP^{112}	LYS^{17}:H - LIGAND:O4 LYS^{105}:H - LIGAND:O6
	2	4-Methoxycinnamoyloleanolic acid methyl ester	GLN^{74}, PHE^{75}, LYS^{105}, ASN^{107}, GLY^{108}, THR^{127}, ASN^{129}, ILE^{130}, LYS^{131}, TRP^{132}, PRO^{151}, THR^{152}	GLN^{74}:HE22 - LIGAND:O6
	3	Albendazole	SER^{7}, TRP^{8}, GLY^{108}, SER^{109}, LYS^{116}, PHE^{117}, LYS^{119}, SER^{120}, ASN^{128}, ASN^{129}	LYS^{119}:HZ1 - LIGAND:O2
	4	DEC	ASP^{18}, ILE^{19}, ASN^{20}, LYS^{87}, VAL^{90}, THR^{91}, VAL^{96}, GLN^{97}, PHE^{98}, ASP^{99}, MET^{100}	MET^{100}:H - LIGAND:O1
	5	Podorhizol beta-D-glucoside	LYS^{48}, ARG^{51}, GLN^{52}, GLN^{54}, GLU^{55}, THR^{58}, LYS^{93}, TYR^{94}, GLY^{95}, TYR^{156}	NA
	6	RU 5135	SER^{7}, TRP^{8}, LYS^{116}, PHE^{117}, SER^{120}, ARG^{121}	SER^{7}:HZ - LIGAND:O1 SER^{120}:HG - LIGAND:O2
	7	Soraphen A	ASP^{18}, ILE^{19}, ASN^{20}, LYS^{28}, LYS^{87}, THR^{91}, VAL A 96 GLN A 97 PHE^{98}, ASP^{99}, MET^{100}	ASN^{20}:HD21 - LIGAND:O7 LYS^{87}:HZ3- LIGAND:O7 LIGAND:H36 – GLN^{97}:O LIGAND:H42 – GLN^{97}:OE1
	8	Vanillin	HIS^{123}, GLY^{124}, THR^{125}, ILE^{130}, LYS^{131}, TRP^{132}, SER135 ARG^{148}, TYR^{149}, SER^{150}, PRO^{151}	ARG^{148}:HE- LIGAND:O3 ARG^{148}:HE21- LIGAND:O3
	9	Gentisic acid	HIS^{123} GLY^{124}, THR^{125}, LYS^{131}, ARG^{148}, SER^{150}, PRO^{151}	THR^{125}:H - LIGAND:O3 LYS^{131}:HZ3 - LIGAND:O3 ARG^{148}:HE- LIGAND:O4 ARG^{148}:HE21- LIGAND:O4 LIGAND:H17 – THR^{125}:OG1
	10	Quinic acid	GLY^{124}, THR^{125} ASN^{129}, ILE^{130}, LYS^{131}, TRP^{132}, SER^{135}, LYS^{136}, ARG^{148}, TYR^{149}, SER^{150}, PRO^{151}	THR^{125}:HG1 - LIGAND:O3 THR^{125}:HG1 - LIGAND:O4 LYS^{131}:H - LIGAND:O6 LYS^{131}:HZ2 - LIGAND:O1 ARG^{148}:HH21- LIGAND:O1 LIGAND:H23 – THR^{125}:OG1 LIGAND:H24 – THR^{125}:OG1 LIGAND:H25 – TYR^{149}:O
	11	Beta-Obscurine	HIS^{97}, GLN^{99}, ASP^{100}, ILE^{101}, ILE^{134}, PRO^{137}, GLY^{138}, LYS^{140}, ASP^{163}, ASP^{164}, VAL^{165}, PHE^{166}, HIS^{168}	LYS^{140}:HZ2 - LIGAND:O2 ASP^{164}:H- LIGAND:O1 ASP^{164}:H- LIGAND:O2 LIGAND:H22 – ASP^{164}:OD1
	12	Carbenicillin	PHE^{12}, SER^{13}, VAL^{15}, SER^{16}, ALA^{17}, VAL^{19}, TYR^{20}, PHE^{21}, LYS^{22}, GLU^{23}, GLU^{24}, ARG^{33}, TRP^{34}, ALA^{76}, LYS^{77}, PHE^{78}, GLU^{79}	LYS^{22}:H - LIGAND:O4 LYS^{77}:H - LIGAND:O4 LIGAND:H39 – GLU^{23}:OE1 LIGAND:H40 – LYS^{77}:O LIGAND:H41 – LYS^{12}:O
GST	1	3-O-Methylquercetin	ARG^{11}, ASP^{159}, GLN^{162}, ILE^{163}, HIS^{179}, GLU^{183}, ARG^{195}, ASN^{196}, LYS^{199}, ILE^{200}, GLN^{208},	HIS^{179}:HE2 - LIGAND:O7 GLN^{208}:HE21 - LIGAND:O3 LIGAND:H34 – ASP^{159}:OD1
	2	4-Methoxycinnamoyloleanolic acid methyl ester	TYR^{7}, PHE^{8}, PRO^{9}, ILE^{10}, LEU^{13}, ASN^{34}, ALA^{35}, TRP^{38}, GLN^{49}, LEU^{50}, HIS^{98}, THR^{102}, TYR^{106}, LYS^{199}, PRO^{201}, GLY^{204}, ASN^{205}	ALA^{35}:H - LIGAND:O4 GLN^{49}:HE21 - LIGAND:O3

	3	Albendazole	ARG[11], ASP[159], ILE[163], GLU[183], LYS[189], CYS[192], LYS[193], ARG[195], ASN[196]	ARG[195]:HH21- LIGAND:O3
	4	DEC	TYR[7], PHE[8], ILE[10], GLY[12], LEU[13], GLN[49], LEU[50], HIS[98], THR[102], TYR[106], VAL[202], ASN[203], GLY[204]	TYR[106]:HH - LIGAND:O1
	5	Podorhizol beta-D-glucoside	TYR[7], PHE[8], PRO[9], ILE[10], LEU[13], ALA[35], GLN[49], LEU[50], THR[102], LYS[103], TYR[106], GLY[204]	TYR[7]:HH - LIGAND:O2 LEU[50]:H - LIGAND:O5 TYR[106]:HH - LIGAND:O7 LIGAND:H60 – GLN[59:]OE1
	6	RU 5135	TYR[7], PHE[8], PRO[9], ILE[10], LEU[13], ALA[35], GLN[49], LEU[50], TYR[106], GLY[204]	NA
	7	Soraphen A	ARG[11], ASP[159], GLN[162], ILE[163], HIS[179], GLU[183], CYS[192], ARG[195], ASN[196], LYS[199], ILE[200], VAL[202], GLN[208]	ARG[11]:HH11 - LIGAND:O5 ARG[11]:HH12 - LIGAND:O8 ARG[195]:HH21 - LIGAND:O9 GLN[208]:HE43 - LIGAND:O6 LIGAND:H43 – CYS[192:]O
	8	Vanillin	ARG[11], ASP[159], ILE[163], CYS[192], ARG[195], ASN[196], LYS[199], ILE[200], GLN[208]	ILU[200]:H - LIGAND:O2 LIGAND:H19 – ARG[195]:O
	9	Gentisic acid	GLY[12], LEU[13], PRO[16], SER[63], GLY[64], LEU[67], CYS[91], VAL[94], ARG[95], HIS[98] VAL[153], GLU[156], GLU[157]	LIGAND:H15 – LUE[13]:O LIGAND:H16– GLU[157]:OE1
	10	Quinic acid	GLY[12], LEU[13], GLU[15], PRO[16], SER[63], LEU[67] CYS[91], VAL[94], ARG[95], HIS[98], VAL[153], GLU[156], GLU[157], ILE[160]	LIGAND:H24– GLU[157]:OE1
	11	Beta-Obscurine	ASN[9], GLY[10], PHE[11] ASN[34], ASP[35], PRO[36], PHE[37], ILE[38], MET[46], SER[83], LYS[84], ILE[89], THR[103], VAL[105], PHE[106]	LIGAND:H30 – ASN[34]:O
	12	Carbenicillin	ASN[9], GLY[10], PHE[11], GLY[12] ASN[34] ASP[35], PRO[36], PHE[37], ILE[38], SER[83], LYS[84], PRO[86], ILE[89], SER[102], THR[103], VAL[105], PHE[106]	LIGAND:H39 – SER[83]:O LIGAND:H33 – ILE[108]:O
SOD	1	3-O-Methylquercetin	ILE[108], SER[111], GLY[112], GLU[113], PRO[114], LEU[129], GLU[130], GLU[133], LYS[203], TRP[206], LYS[207], TRP[211]	LIGAND:H42 – ASP[35]:OD2
	2	4-Methoxycinnamoyloleanolic acid methyl ester	HIS[54], ALA[57], TYR[58], ALA[61], LYS[68], VAL[69], ALA[72], ALA[80], VAL[81], ALA[83], ALA[84] LYS[86], LEU[87], PHE[90], ASN[91], GLN[168], HIS[188]	NA
	3	Albendazole	ILE[108], SER[111], GLY[112], GLU[113], GLU[133], ASP[134], LYS[203], TRP[206], LYS[207], TRP[211]	LIGAND:H20 – GLU[133]:OE1 LIGAND:H30 – GLU[133]:OE2
	4	DEC	GLU[117], SER[120], ALA[121], LYS[124], ASP[125], TYR[153], LYS[158], ARG[159], LEU[160], TYR[218], LYS[222]	NA
	5	Beta-Obscurine	ILE[96], LEU[100], LYS[155], ILE[178], PRO[179], LEU[180], ARG[217], LYS[220], ALA[221]	NA
	6	RU 5135	LEU[100], GLU[103], LYS[155], GLN[172], ILE[178], PRO[179], LEU[180] ARG[217], LYS[220],	ARG[217]:HE - LIGAND:O2 LIGAND:H50 – LYS[220]:O

			ALA^{221}, GLY^{223}	
	7	Carbenicillin	ILE^{108}, SER^{111}, GLU^{133}, ASP^{134}, SER^{137}, LYS^{203}, TRP^{206}, LYS^{207}, ALA^{209} TRP^{211}	LIGAND:H38 – LYS^{207}:O
	8	Vanillin	LEU^{21}, ARG^{22}, GLN^{23}, LEU^{24}, GLU^{66}, VAL^{69}, LYS^{70}, LEU^{73}, MET^{88}	NA
	9	Gentisic acid	LEU^{21}, ARG^{22}, GLN^{23}, LEU^{24}, HIS^{26}, GLU^{66}, VAL^{69}, LYS^{70}, LEU^{73}	LUE^{24}:H - LIGAND:O4 LIGAND:H15 – ARG^{22}:O
	10	Quinic acid	ILE^{108}, LYS^{109}, SER^{111}, GLY^{112}, GLU^{113}, GLU^{133}, TRP^{206}, LYS^{207}, ALA^{209}, TRP^{211}	TYR^{211}:HE1 - LIGAND:O6 LIGAND:H21 – TRP^{206}:O LIGAND:H22 – GLY^{112}:O LIGAND:H23 – LYS^{207}:O
	11	Podorhizol beta-D-glucoside	GLY^{27}, PRO^{28}, PHE^{129}, ASP^{131}, VAL^{132}, SER^{133}, LEU^{137}, LEU^{162}, TYR^{165}, ILE^{166}, THR^{169}, ALA^{170}, VAL^{173}, LYS^{184}	NA
	12	Soraphen A	PRO^{28}, SER^{30}, GLY^{31}, LYS^{32}, GLY^{33}, THR^{34}, SER^{49}, GLY^{51}, ASP^{105}, TYR^{107}, ARG^{140}, ARG^{144}, THR^{147}, SER^{148},	GLY^{31}:H - LIGAND:O4 GLY^{33}:H - LIGAND:O2 ARG^{140}:HH11 - LIGAND:O3
TRx	1	3-O-Methylquercetin	LYS^{12}, LYS^{18}, ASP^{22}, ALA^{23}, LEU^{24}, ALA^{25}, LYS^{27}, TYR^{53}, ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61}, GLU^{62}, ASP^{85}, TRP^{86}, TYR^{87}	LYS^{12}:HZ3 - LIGAND:O4 LYS^{27}:HZ1 - LIGAND:O1 TYR^{87}:HH - LIGAND:O2 LIGAND:H29 – TYR^{53}:OH LIGAND:H34 – ASP^{58}:O LIGAND:H34 – ASP^{22}:O LIGAND:H34 – ALA^{23}:O
	2	4-Methoxycinnamoyloleanolic acid methyl ester	TRP^{38}, CYS^{39}, PRO^{40}, PRO^{41}, GLN^{44}, PHE^{45}, ILE^{48}, LEU^{68}, HIS^{70}, ALA^{106}, GLY^{107}, ILE^{108}, PRO^{109}, ARG^{126}, SER^{130}, LYS^{132}, PRO^{134}, PRO$_{135}$	NA
	3	Albendazole	LYS^{12}, LYS^{18}, ASP^{22}, ALA^{23}, ALA^{25} ,LYS^{27} TYR^{53}, GLU^{54}, ASP^{57}, ASP^{58}, ASP^{59}, GLU^{62}, ASP$_{85}$, TYR^{87}	LYS^{27}:HZ1 - LIGAND:O3 LYS^{27}:HZ1 - LIGAND:N5
	4	DEC	LYS^{27}, TYR^{53}, GLU^{54}, VAL^{56}, ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61}, ASP^{85}	NA
	5	Beta-Obscurine	LYS^{12}, LYS^{27}, TYR^{53}, GLU^{54}, ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61}, GLU^{62}, ASP^{85}, TYR^{87}	LYS^{12}:HZ3 - LIGAND:O1 LIGAND:H43 – GLU^{62}:OE2
	6	Carbenicillin	LYS^{12}, ASP^{22}, ALA^{23}, ALA^{25}, ASN^{26}, LYS^{27}, TYR^{53}, GLU^{54}, ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61}, GLU^{62}, ASP^{85}, TYR^{87}	LYS^{27}:HZ3 - LIGAND:O1 TYR^{87}:HH - LIGAND:O2 LIGAND:H43 – ASP^{58}:O
	7	RU 5135	LYS^{28}, VAL^{29}, ALA^{31}, PHE^{52}, VAL^{56}, ASP^{58}, GLN^{60}, PHE^{61}, LEU^{111}, VAL^{113}, ILE^{121}, VAL^{129}	NA
	8	Soraphen A	LYS^{12}, ALA^{23}, LYS^{27}, TYR^{53}, GLU^{54}, VAL^{56}, ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61}, GLU^{62}, ASP^{85}, TYR^{87}	LYS^{27}:HZ1 - LIGAND:O2 LYS^{27}:HZ1 - LIGAND:O4 TYR^{87}:HH - LIGAND:O5 LIGAND:HH33 – GLU^{62}:OE2 LIGAND:HH36 – TYR^{87}:OH LIGAND:HH43 – ASP^{51}:O LIGAND:HH33 – PHE^{61}:O
	9	Vanillin	LYS^{27}, TYR^{53}, GLU^{54}, VAL^{56}, ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61},	ASP^{58}:H - LIGAND:O1

		GLU^{62}	
10	Gentisic acid	LYS^{27}, TYR^{53}, GLU^{54}, VAL^{56} ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61}, GLU^{62}	ASP^{58}:H - LIGAND:O2 ASP^{58}:H - LIGAND:O2
11	Quinic acid	LYS^{27}, TYR^{53}, GLU^{54}, VAL^{56}, ASP^{57}, ASP^{58}, ASP^{59}, PHE^{61}, GLU^{62}, ASP^{85}	LYS^{27}:HZ3 - LIGAND:O5 ASP^{58}:H - LIGAND:O2 LIGAND:H25 – PHE^{61}:O
12	Podorhizol beta-D-glucoside	PRO^{28}, GLY^{29}, SER^{30}, GLY^{31}, LYS^{32}, GLY^{33}, THR^{34}, ASP^{37}, HIS^{47}, SER^{49}, GLY^{51}, ASP^{52}, ARG^{55}, ASP^{105}, TYR^{107}, ARG^{140}, HIS^{143}, ARG^{144}, SER^{148}, GLY^{149}, ARG^{150}, ARG^{161}	LYS^{32}:HZ1 - LIGAND:O8 ARG^{55}:HH12 - LIGAND:O10 ARG^{55}:HH22 - LIGAND:O10 TYR^{107}:HH - LIGAND:O8