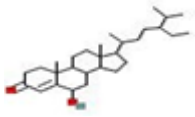
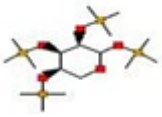
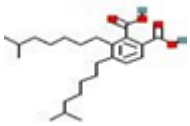
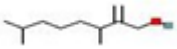
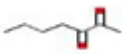
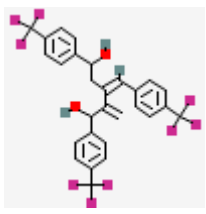
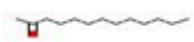
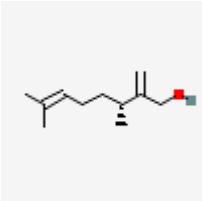
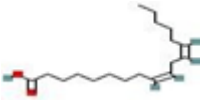
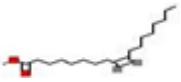
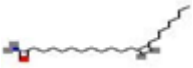
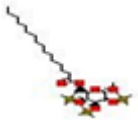
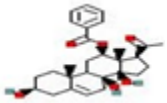
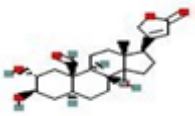
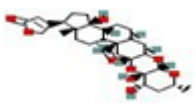
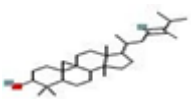
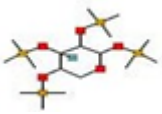
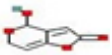
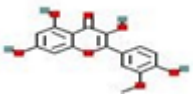
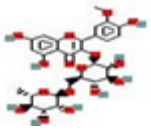
Table 1. Drugs used in the treatment of Lymphatic filariasis, their mechanism of action and side effects

Drug	Mechanism of Action	Side Effects
Diethylcarbamazine	Microfilaria to phagocytosis, Arachidonic acid metabolic pathway, cyclooxygenase pathway	Dizziness, nausea, fever, headache, and joint pain
Albendazole	Binds to the colchicine-sensitive site of tubulin, thus inhibiting its polymerization or assembly into microtubules. It also causes degenerative alterations in the intestinal cells of the worm by diminishing its energy production, ultimately leading to immobilization and death of the parasite.	Temporary hair loss, vomiting, spinning sensations, neck stiffness, and seizures
Ivermectin	Binds to the glutamate-gated chloride ion channels in invertebrate muscle and nerve cells of the microfilaria which results in hyperpolarization of the cell, leading to paralysis and death of the parasite.	Eye pain, puffy eyes, skin rash, itching, painful neck and armpits, diarrhea, rapid heartbeat
Doxycycline	Inhibits translation by binding to the 16S rRNA portion of the ribosome, preventing binding of tRNA to the RNA-30S bacterial ribosomal subunit which results in the replication of bacteria and produces a bacteriostatic effect.	Nausea, vomiting, stomach cramps, sore throat, unusual weight loss

Table 2. The list of 49 phytocompounds identified for screening based on H-bond interaction and S-score

Sl. No	Ligand	PubChem ID	2D Structure	H-Bond Interactions	S Score
1	(6beta,24R)-6-Hydroxystigmast-4-en-3-one	14769504		Trp38	82.3678
2	1,2,3,4-Tetrakis-O-(trimethylsilyl)pentopyranose	22211827		Tyr 106	98.0417
3	1,2-Benzenedicarboxylic acid, diisooctyl ester	33934		Gln49, Gln62, Arg95	63.6925
4	1,2-Benzenedicarboxylic acid, diisooctyl	18972250		Gln49, Gln62, Tyr106	92.9765
5	1-heptadecanol	15076		Gly12, Pro201	86.474
6	1-iododecane	16314		His98	55.668
7	1-Octanol, 3,7-dimethyl	3023988		Tyr7, Thr102, Asn203	105.201
8	1-Octanol	957		Gly12, Asp159	65.2532
9	2,3-heptanedione	60983		His98, Tyr116	64.2096
10	2-Dodecanol, 1,1-dichloro	13656289		Gln62, Ser63	63.8474
11	2-Hydroxyhexadecyl butanoate	551233		Gln49, Ser63, Arg95	93.0643
12	1,5-Bis[4-(trifluoromethyl)phenyl]-3-[(Z)-4-(trifluoromethyl)benzylidene]-2-methylene-1,5-pentanediol	101356327		Trp38, Lys42	78.2681
13	2-tridecanone	11622		Gln49, Gln62	72.3555

14	6-Octen-1-ol, 3,7-dimethyl acetate	6999975		Gln42, Lys91, Phe152	74.4469
15	6-Octen-1-ol, 3,7-dimethyl-2-methylene-, (R)- (R)-(-)-3,7-dimethyl-2-methylene-6-octen-1-ol	10877531		Gln62, Ser63, Gly64	55.0872
16	9,12-Octadecadienoic acid (Z,Z)-	5280450		Gln62, Ser63	102.942
17	9-Decenoate	5460709		Gln49, Gln62	69.9742
18	9-octadecenamide	5353370		Tyr7, Tyr106, Asn203	83.1727
19	9-Octadecenoic acid (Z)- methyl ester	5364509		Gln49, Gln62, Ser63	113.446
20	13-docosenamide	5365371		Gln62, Ser63, Arg95	83.3398
21	Acetogenins	393472		Tyr7, Tyr106, Gln49, Arg95	106.044
22	Alpha-D-glucopyranoside,methyl 2,3,4- Tris-O-(trimethylsilyl)-, hexadecanoate	91733360		Thr99, Thr102	130.647
23	Benzoylisolineolone	53068714		Tyr106	99.2344
24	Bis-(3,5,5-trimethylhexyl) ether	57048725		Tyr7	82.7279
25	Calotropagenin	212348		Tyr7, Tyr106, leu50, Asn203	68.4408
26	Calotropin	16142		Tyr7	84.6194

27	Cyclosadol	12312851		Thr102	81.8948
28	Digitoxin	441207		Gln49, Leu50, Gln62, Arg95	95.482
29	D-xylopyranose, 1,2,3,4-tetrakis-o-(trimethylsilyl)	523971		Thr102, Tyr106	81.2236
30	Gigantin	4696		Tyr7	62.3747
31	Hexadecanoic acid, ethyl ester	12366		Gln49, Gln62, Ser63	96.5709
32	Hexadecanoic acid, methyl ester	8181		Gln49, Gln62	95.9651
33	Isorhamnetin	5281654		Tyr7, Gly12, Gln49	56.1301
34	Isorhamnetin-3-O-rutinoside	5481663		Tyr7, Leu13, Leu50, Ser63, Arg95, Thr102	100.679
35	Methyl 9-octadecenoate	280590		Gln49,Gln62	102.933
36	Methyl behenate	13584		Gln49,Gln62	99.3199
37	N-Heptadecanoate	4113470		Ser63, Gly64, Arg95	64.2551
38	N-Hexadecanoate	504166		Trp38, Lys42, Leu50	87.2003
39	N-Octanoate	119389		Trp 38, L ys 42, Gln49	54.3566
40	Nonanoic acid, 7-methyl methyl ester	521322		Tyr7, Tyr106	65.5374
41	N-Pentadecanoate	13849		Tyr7, Tyr106	74.832
42	N-Tridecanoate	12530		Gln49, Pro51, Gln62, Ser63	98.5676

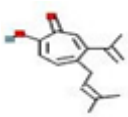
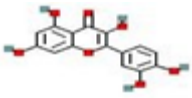
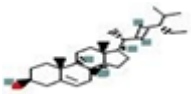
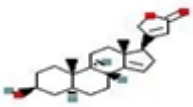
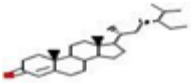
43	Procerin	594578		Gln62, Ser63	49.169
44	Quercetin	5280343		Tyr7, Leu50, Thr102, Pro201, Asn203	99.2158
45	Stigmasterol	5280794		His98, Lue97, Tyr116	59.035
46	Undecanoic acid	8180		Tyr7, Tyr106, Asn203	71.533
47	β-anhydroepidigitoxigenin	10784500		Gln49	68.2219
48	B-sitostenone	60123241		Trp38	91.0018
49	β sitosterol	222284		Asp159	87.6304

Table 3. List of ligands selected following the screening under Lipinski's rule of 5 and toxicity

Sl. No	Ligand	Mol. Wt.	ALogP	H-Donor	H-Acceptor	Toxicity
1	1-Octanol, 3,7-dimethyl	4.717	370.525	1	3	Non-Mutagen
2	1-Octanol	2.795	130.228	1	1	Non-Mutagen
3	2,3-heptanedione	1.351	128.169	0	2	Non-Mutagen
4	2-tridecanone	4.668	198.345	0	1	Non-Mutagen
5	6-Octen-1-ol, 3,7-dimethyl	3.239	168.276	1	1	Non-Mutagen
6	9-Decenoate	1.791	169.241	0	2	Non-Mutagen
7	Acetogenins	4.221	470.639	4	7	Non-Mutagen
8	Benzoylisolineol one	2.606	468.582	3	6	Non-Mutagen
9	Calotropagenin	1.577	404.497	2	4	Non-Mutagen
10	Gigantin	- 0.269	154.12	1	4	Non-Mutagen
11	N-Hexadecanoate	4.919	255.416	3	4	Non-Mutagen
12	N-Octanoate	1.269	143.203	0	2	Non-Mutagen
13	Nonanoic acid, 7-methyl methyl ester	3.676	186.291	1	3	Non-Mutagen
14	Procerin	3.517	230.302	1	2	Non-Mutagen
15	Undecanoic acid	4.111	186.291	2	3	Non-Mutagen
16	β - anhydroepidigitoxigenin	4.142	356.498	1	3	Non-Mutagen

Table 4. Ligand with desirable interaction and druggable features

Ligand	Interacting Residues	H-Bond Interaction	S- Score	Binding Affinity
N-Octanoate	Tyr 7, Phe 8, Ile 10, Trp 38, Lys 42, Gly 48, Gln 49, Leu 50, Tyr 106, Gly 204	Trp 38, Lys 42, Gln 49,	-3.1201	-4.9 kcal/mol