Table 3. Prediction of ligand toxicity

Ligand Name	herG		Carcinogenicity		Acute Oral Toxicity	
	Category	Score	Category	Score	Category	Score
2-Methoxy-4-vinylphenol	Weak Inhibitor	0.719	Non carcinogenic	0.630	III	0.860
2,6-bis(1,1-dimethylethyl)-4-methyl phenol	Weak Inhibitor	0.749	Carcinogenic	0.629	III	0.827
Hexadecanoic acid, methyl ester	Weak Inhibitor	0.408	Non carcinogenic	0.600	III	0.859
1,2-benzene-dicarboxylic acid, 2-butoxy-2-oxoethyl butyl ester	Strong Inhibitor	0.785	Non carcinogenic	0.729	IV	0.792
Hexanedioic acid, bis(2-ethylhexyl) ester	Weak Inhibitor	0.621	Non carcinogenic	0.671	IV	0.772
Oleic acid	Weak Inhibitor	0.394	Non carcinogenic	0.671	IV	0.829
Linoleic acid	Weak Inhibitor	0.461	Non carcinogenic	0.671	IV	0.829
Linolenic acid	Weak Inhibitor	0.360	Non carcinogenic	0.671	IV	0.639
Octadeca-8-10-dinoic acid	Weak Inhibitor	0.580	Non carcinogenic	0.671	IV	0.448
Octadeca-8-10-12-trinoate	Weak Inhibitor	0.689	Non carcinogenic	0.671	IV	0.448
Quercitrin	Weak Inhibitor	0.635	Non carcinogenic	0.986	III	0.518
Quercetin	Weak Inhibitor	0.841	Non carcinogenic	1.000	II	0.735
Aviculin	Strong Inhibitor	0.726	Non carcinogenic	0.971	III	0.618
(+)-Catechins	Weak Inhibitor	0.468	Non carcinogenic	0.929	IV	0.643
(-)-Epicatechin	Weak Inhibitor	0.468	Non carcinogenic	0.929	IV	0.643
(-)-Epicatechin-3-O-gallate	Strong Inhibitor	0.855	Non carcinogenic	0.986	IV	0.376
(-)Epigalocatechin-3-O-gallate	Strong Inhibitor	0.892	Non carcinogenic	0.986	IV	0.376

Description: Lipinski rules violation

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Description: Lipinski rules violation

Table 4. Molecular Docking Results					
Ligand Name	Energy Affinity (kcal/mol)	Amino Acid Residue	Number of Hydrophobic Bonds	Number of Hydrogen Bonds	Hydrogen Bond Length
Natural Ligand	-11.4	leu800; gly804; leu726; leu852; ala751; cys805; ser728; val734; lys753; thr862; phe864; leu796; met774; leu785; ser783; gly729; asp863; thr729; met801; gln799	18	2	Met801 3.03; Asp863 3.28
Cyclophosphamide (breast cancer therapy drug)	-5.4	met801; leu726; leu852; ala751; cys805; ser728; val734; thr862; gly729; gly727	10	0	
2-Methoxy-4-vinylphenol	-7.1	thr798; ser783; lys753; thr862; phe864; leu796; met774; leu785; asp863; ala 771	7	3	asp863 3.22; ser783 2.70; thr862 2.97
Hexadecanoic acid, methyl ester	-6.8	thr798; asp863; lys753; thr863; phe864; leu796; met774; leu785; ser783; arg784; ala771	8	3	asp863 3.24; thr863 2.93; ser783 2.71
Hexanedioic acid, bis(2-Ethylhexyl) ester	-7.6	leu726; leu852; ala751; cys805; ser728; val734; lys753; thr862; phe864; leu796; met774; leu785; ser783, asp863; thr798; met801; arg784; ile752; glu770; ala771	20	0	

Oleic acid	-7.2	leu800; leu726; leu852; ala751; val734; lys753; thr862; phe864; leu796; met774; leu785; ser783; asp863; thr798; met801; glu770; ala751	16	1	met801 2.79
Linoleic acid	-7.6	leu800; leu726; leu852; ala751; val734; lys753; thr862; phe864; leu796; met774; leu785; asp863; thr798; met801; glu770; ala751	15	2	met801 2.79 dan 3.04
Linolenic acid	-7.6	leu800; gly804; leu726; leu852; val734; lys753; thr862; phe864; leu796; met774; leu785; asp863; thr798; met801; ala771	14	2	met801 2.79 dan 2.92
Octadeca-8-10-dinoic acid	-7.5	leu800; leu726; leu852; ala751; val734; lys753; thr862; phe864; leu796; leu785; asp863; thr798; met801; ala771; glu770	14	2	met801 2.92 dan 2.97
Octadeca-8-10-12-trinoate	-7.5	met801; leu800; gly804; leu726; leu852; ala751; val734; lys753; thr862; phe864; leu796; met774; leu785; asp863; glu770; ala771	16	0	
Quercitrin	-8.1	leu800; gly804; leu852; ala751; cys805; leu726; ser728; val734; lys753; thr862;	13	3	met801 2.54; asp863 3.21; leu726 2.86

		leu796; asp863; gly729, thr798; met801; gly727			
(+)-Catechins	-9.3	thr798; ala751; leu852; cys805; val734; asn850; lys753; thr862; phe864; leu796; leu785; asp863; arg849; val797	11	4	asp863 3.22; asn850 2.54; arg849 2.92 dan 3.01
(-)-Epicatechin	-9.3	thr798; ala751; leu852; cys805; val734; asn850; lys753; thr862; phe864; leu796; leu785; asp863; arg849; val797	11	4	asp863 3.24;asn850 2.54; arg849 2.92 dan 3.01
Description: Amino acids on the binding site					

Table 5. Antioxidant activity test data (DPPH) sample of ethanol extract of parasite coffee stem

Concentration (ppm)	Absorbance		% Inhibition	
	1st Repetition	2nd Repetition	1st Repetition	2nd Repetition
0	0.873	0.873	0,000	0,000
15	0.770	0.797	11.798	8.740
30	0.632	0.676	27.629	22.520
45	0.578	0.559	33.837	35.956
60	0.396	0.455	54.685	47.846
75	0.333	0.300	61.856	65.601

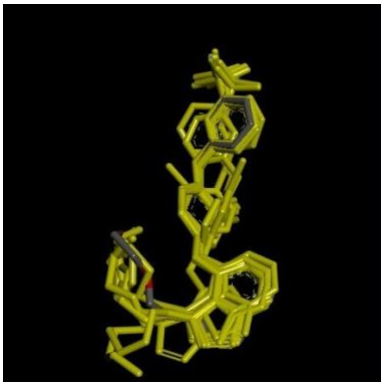
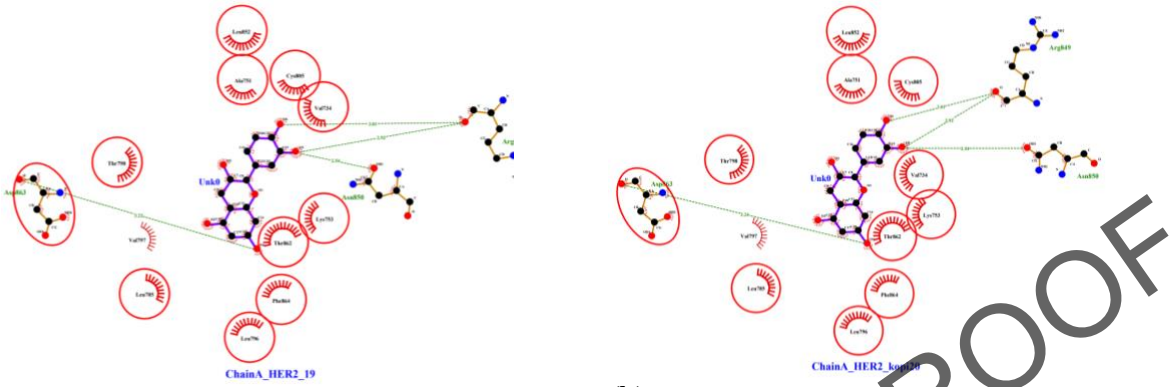


Figure 1. Molecular docking validation results. The average RMSD value is 1.17 Å



(a) (b)

Figure 2. 2D Visualization of (a) catechins and (b) epicatechins against receptors. The red circle indicates hydrophobic interactions between amino acids and ligands that interact on the same side of the receptor as the natural ligand. The dashed green line indicates hydrogen interactions between amino acids and ligands that interact on the same side of the receptor as the natural ligand

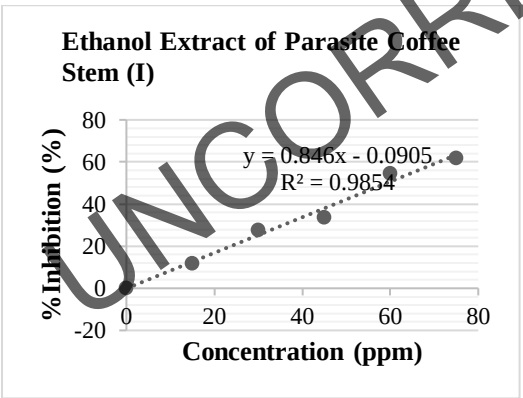
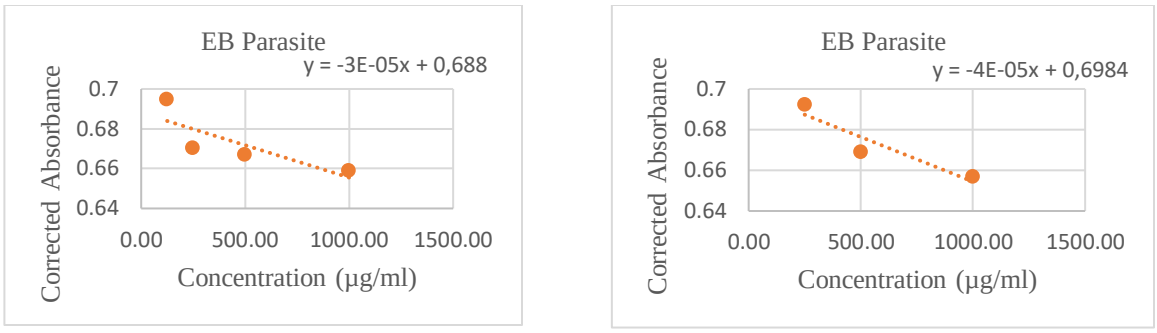


Figure 3. Diagram of antioxidant activity (DPPH) sample of ethanol extract of parasite coffee stem. The IC50 value is 59.736 ppm indicating strong antioxidant activity



(a) (b)

Figure 4. Parasite extract test results curve against (a) Hela cells and (b) MCF-7 cells. The IC50 value of this coffee parasite extract against cancer cells is weak or inactive.

(a) (b)

Figure 5. Documentation of Morphology of Parasite Extract Test Results (a) Hela cells (b) MCF-7 cells

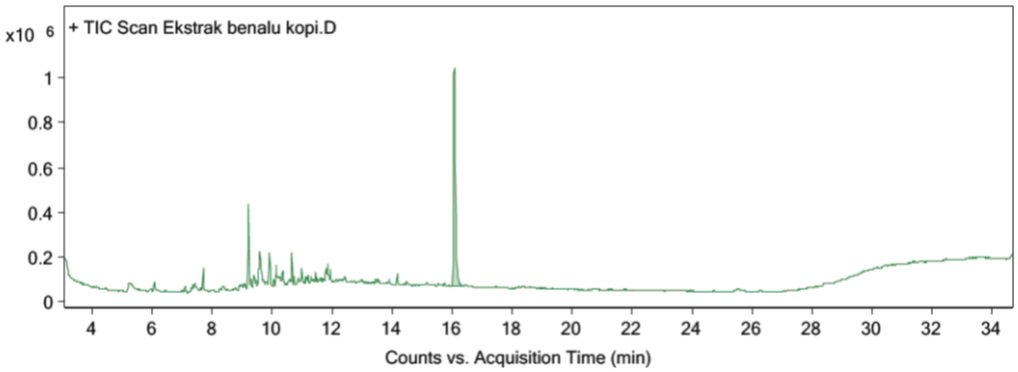


Figure 6. Spectrum of separation in GC-MS analysis showing retention time (RT) of 16.073 minutes indicating 100% of Bis (2- Ethylhexyl) phthalat

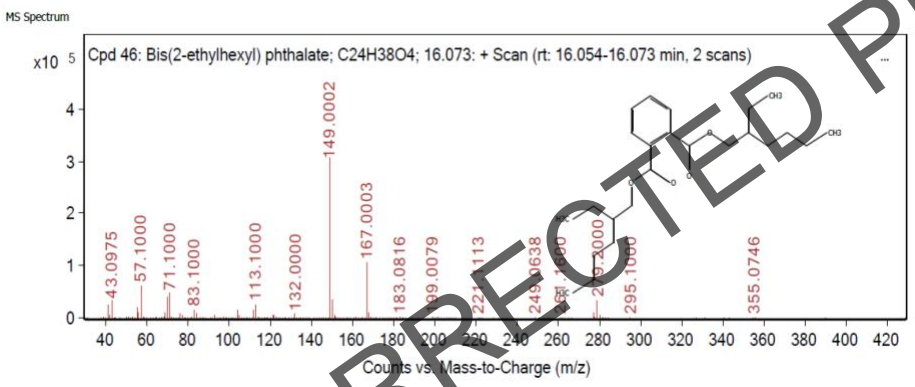


Figure 7. Peak fragmentation of compounds in GC-MS analysis showing the fragmentation of the bis (2-Ethylhexyl) phthalate

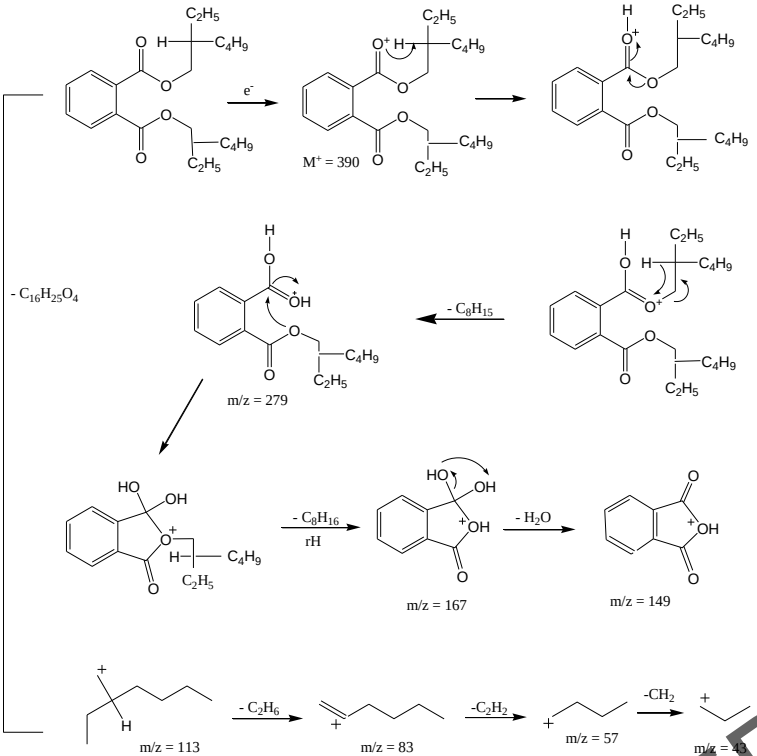


Figure 8. Fragmentation of bis(2-Ethylhexyl) phthalate compound