SUPPLEMENTARY MATERIAL

Exploring the Therapeutic Potential of *Antiaris africana*: Targeting Cyclin-Dependent Kinases 8 and 13 for Cancer Treatment through Molecular Docking Studies

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Supplementary Data

Table S1. Binding affinity between the *Antiaris africana* compounds and CDK8

S.No	Ligands	Binding Affinity
1.	Campesterol	-9.4
2.	Cortistatin A **Reference**	-9.1
3.	Bis(2-ethylhexyl) phthalate	-7.4
4.	1(2H)-Isoquinolinone, 3,4-dihydro-7-hydroxy-6-methoxy-2-methyl-	-7.4
5.	Dibutyl phthalate	-7.0
6.	2,6,10,15,19,23-Hexamethyl-tetracosa-2,10,14,18,22-pentaene-6,7-diol	-6.7
7.	Methyl stearate	-6.7
8.	N-(4-Aminobutyl)-2-ethylpiperidine	-6.5
9.	Methyl tetradecanoate	-6.5
10.	3-12-Formyl-digoxigenin	-6.4

11.	1-Pyrrolidinebutanoic acid, 2-[(1,1-dimethylethoxy)carbonyl]-.alpha.-nitro-, 2,6-bis(1,1-dimethylethyl)-4-methoxyphenyl ester	-6.4
12.	Megastigmatrienone	-6.2
13.	1,2-Benzenedicarboxylic acid, butyl methyl ester	-6.0
14.	N,N-Dimethyltryptamine	-6.0
15.	Dimethylmalonic acid, ethyl 2-ethylhexyl ester	-6.0
16.	2-Methoxy-4-vinylphenol	-6.0
17.	9-Octadecenoic acid, methyl ester, (E)-	-6.0
18.	2-Undecenoic acid	-5.9
19.	Hexadecanoic acid, methyl ester	-5.9
20.	Dodecanoic acid	-5.8
21.	n-Nonadecanol-1	-5.8
22.	Ethanone, 1-(2,5-dihydroxyphenyl)-	-5.8
23.	Ethanone, 1-(1-cyclohexen-1-yl)-	-5.7
24.	9,12-Octadecadienoic acid, methyl ester, (E,E)-	-5.7
25.	1,2-Benzenediol, 3-methoxy-	-5.7
26.	5-Acetoxymethyl-2-furaldehyde	-5.6
27.	Cyclohexanecarboxylic acid	-5.6
28.	Phenol, 2-methoxy-	-5.5
29.	9-Octadecenoic acid (Z)-, methyl ester	-5.5
30.	Phenol, 2,6-dimethoxy-	-5.3
31.	5-Hydroxymethylfurfural	-5.0
32.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	-5.0
33.	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	-4.9
34.	Hexahydrobenzo[1,3]dioxin-4-one	-4.8
35.	Hexanoic acid, 6-bromo-	-4.8
36.	Methyl 18-methylnonadecanoate	-4.7
37.	2-Furanmethanol	-4.4

Table S2. Binding affinity between the *Antiaris africana* compounds and CDK13

S.No.	Ligand	Binding Affinity
1.	THZ531R – **Reference**	-10.1
2.	Bis(2-ethylhexyl) phthalate	-8.4
3.	Dibutyl phthalate	-7.2
4.	3-12-Formyl-digoxigenin	-6.6
5.	9-Octadecenoic acid (Z)-, methyl ester	-6.5
6.	9,12-Octadecadienoic acid, methyl ester, (E,E)-	-6.4
7.	Dimethylmalonic acid, ethyl 2-ethylhexyl ester	-6.3
8.	Phenol, 2-methoxy-	-6.2
9.	Tetracosapentaene, 2,6,10,15,19,23-hexamethyl-	-6.2

10.	1-Pyrrolidinebutanoic acid, 2-[(1,1-dimethylethoxy)carbonyl]-.alpha.-nitro-, 2,6-bis(1,1-dimethylethyl)-4-methoxyphenyl ester	-6.1
11.	1(2H)-Isoquinolinone, 3,4-dihydro-7-hydroxy-6-methoxy-2-methyl-	-6.1
12.	Megastigmatrienone	-6.0
13.	Campesterol	-6.0
14.	N,N-Dimethyltryptamine	
15.	2-Methoxy-4-vinylphenol	-5.9
16.	Hexahydrobenzo[1,3]dioxin-4-one	-5.9
17.	1,2-Benzenedicarboxylic acid, butyl methyl ester	-5.8
18.	N-(4-Aminobutyl)-2-ethylpiperidine	-5.6
19.	Hexadecanoic acid, methyl ester	-5.6
20.	Ethanone, 1-(2,5-dihydroxyphenyl)-	-5.6
21.	Ethanone, 1-(1-cyclohexen-1-yl)-	-5.6
22.	Dodecanoic acid	-5.6
23.	Methyl 18-methylnonadecanoate	-5.5
24.	Methyl stearate	-5.5
25.	Methyl tetradecanoate	-5.4
26.	Cyclohexanecarboxylic acid	-5.3
27.	9-Octadecenoic acid, methyl ester, (E)-	-5.3
28.	1,2-Benzenediol, 3-methoxy-	-5.2
29.	2-Undecenoic acid	-5.2
30.	5-Acetoxymethyl-2-furaldehyde	-5.1
31.	n-Nonadecanol-1	-5.0
32.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	-5.0
33.	2,5-Dimethyl-4-hydroxy-3(2H)-furanone	-4.9
34.	Phenol, 2,6-dimethoxy-	-4.9
35.	Hexanoic acid, 6-bromo-	-4.9
36.	5-Hydroxymethylfurfural	-4.8
37.	2-Furanmethanol	-4.6
38.		-4.2