

Computational Analysis of Bioactive Phytocompounds from Methanolic Extract of *Pajanelia longifolia* (Willd.) K. Schum against EGFR and TGF- β Cancer Targets

Supplementary File

Table S1. Quantitative analysis of methanolic extract of *P. longifolia* Bark (PL-ME).

Total phenolic Content	
Plant Extract PL-ME	Concentration ($\mu\text{g/mL}$) 100.381
Total Flavonoid Content	
Plant Extract PL-ME	Concentration ($\mu\text{g/mL}$) 301.25
DPPH Free-Radical Scavenging Activity	
Plant Extract PL-ME	IC ₅₀ 348.105

Table S2. Compounds detected from the PL-ME extract of bark of *P. longifolia* through GC-MS analysis

S.N.	Methanol Compounds	Ret. Time
1	4-Vinylphenol	5.205
2	Paromomycin	5.766
3	2-Methoxy-4-vinylphenol	6.238
4	5-Aminovaleramide, <i>N</i> -methyl- <i>N</i> -[4-(1-pyrrolidinyl)-2-butynyl]-.....	6.732
5	Pyrrolizin-1,7-dione-6-carboxylic acid, methyl(ester)	6.970
6	Acetamide, <i>N</i> -methyl- <i>N</i> -[4-(3-hydroxypyrrolidinyl)-2-butynyl]-	7.344
7	Benzeneethanol, 4-hydroxy-	7.585
8	4-Vinylbenzene-1,2-diol	7.766
9	Benzofuran-2-carboxaldehyde	7.912
10	Melezitose	8.408
11	10-Heptadecen-8-ynoic acid, methyl ester	9.204
12	Acetic acid, 4a-methyl-octahydro-1-oxacyclopropa[<i>d</i>]naphthalen-7-yl ester	9.803
13	Dodecanoic acid, 3-hydroxy-.....	10.456
14	Desulphosinigrin	10.714
15	Ethanone, 1-(1-hydroxy-2,6,6-trimethyl-2,4-cyclohexadien-1-yl)-.....	11.255
16	(<i>E</i>)-4-(3-Hydroxyprop-1-en-1-yl)-2-methoxyphenol	11.371
17	1,3-Benzodioxole, 4-acetoxy-6-(2-propenyl)-.....	11.415
18	7-Methyl-Z-tetradecen-1-ol acetate	12.514
19	Caffeine	12.718
20	9-Hexadecenoic acid	13.058
21	Cyclopropanebutanoic acid, 2-[[2-[[2-(2-pentylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]methyl]-, methyl ester	13.493
22	<i>n</i> -Hexadecanoic acid	13.911
23	Ethyl iso-allocholate	14.456
24	Acetic acid, 2,6,6-trimethyl-3-methylene-7-(3-oxobutylidene)oxepan-2-yl ester	15.102
25	6,9,12,15-Docosatetraenoic acid, methyl ester	15.854
26	5,7,9(11)-Androstatriene	22.425
27	Spirost-8-en-11-one, 3-hydroxy-, (3b,5a,14b,20b,22b,25 <i>R</i>)-	32.689
28	9,11,18-Trihydroxy-6,18-epoxypimara-5,8(14),15-trien-7-one, 2Ac derivative	33.461
29	b-Sitosterol	35.111
30	4 <i>H</i> -Cyclopropa[5',6']benz[1',2':7,8]azuleno[5,6-b]oxiren-4-one, 8,8a-bis(acetyloxy)-2a-[(acetyloxy)methyl]-1,1a,1b,1c,2a,3,3a,6a,6b,7,8,8a-dodecahydro-3,3a,6b-trihydroxy-1,1,5,7-tetramethyl-	37.332

Table S3. (A): List of GC-MS reported methanolic extract compounds of *P. longifolia*. (B): List of LC-MS reported methanolic extract compounds of *P. longifolia*. List of LC-MS reported acetone extract compounds of *P. longifolia*.

(A)		
S.N.	Compound Name	References
1	<i>p</i> -Vinylguaiaicol	[60]
2	1,7-octadiene, 2,3,3-trimethyl-	
3	6-methyl-2-cyclohexenecarboxaldehyde	
4	2,4-Di-tert-butylphenol	
5	Megastigmatrienone 4	
6	Neophytadiene	
7	Phytol	
8	Hexadecanoic acid, ethyl ester	
9	<i>cis,cis,cis</i> -7,10,13-Hexadecatrienal	
10	Octadecanoic acid, ethyl ester	
11	Octadecanal	
12	(4,4-Dimethyl-2,4,5,6-tetrahydro-1 <i>H</i> -inden-2-yl)acetic acid	
13	9,12-Hexadecadienoic acid, methyl ester	
14	3,7,11,15-tetramethyl-2-hexadecen-1-ol	
15	9,12,15-Octadecatrienoic acid, ethyl ester	
(B)		
S.N.	Compound Name	References
1	Rescinnamine	[29]
2	Idarubicinol	
3	Cytochalasin E	
4	Salicin	
5	Gentiopicrin	
6	Nevirapine	
7	Acetylsalicylic acid	
8	Sildenafil	
9	Harpagoside	
10	Icariin	
(C)		
S.N.	Compound Name	References
1	D-Lombricine	[45]
2	Myoinositol 1-phosphate	
3	5-Hydroxy-3,3',7,8-tetramethoxy-4',5'-methylenedioxyflavone	
4	Tiracizine	
5	Ricinine	
6	1,5-Dibutyl methyl hydroxycitrate	
7	3,4,5-Trimethoxycinnamic acid	
8	2,4,6-Trihydroxytoluene	
9	Sulprostone	
10	(<i>R</i>)-Cryptone	
11	Funtumine	
12	Pivmecillinam	
13	Methylergonovine	
14	Puromycin	
15	Alfuzosin	
16	Istamycin C1	
17	Netilmicin	
18	3-Oxo-12,18-ursadien-28-oic acid	
19	Vernodalin	
20	16,17-Dihydro-16a,17-dihydroxygibberellin A4 17-glucoside	
21	Cubebin	
22	Methyl trans- <i>p</i> -methoxycinnamate	
23	N1,N5,N10-Tricoumaroyl spermidine	
24	Dihydrodeoxystreptomycin	
25	Manumycin A	
26	Neuraminic acid	
27	N-(1-Deoxy-1-fructosyl)serine	
28	Protorifamycin I	

29	Cortolone
30	Eugenol
31	Glycine, N-[(3a,5b,7a)-3-hydroxy-24-oxo-7-(sulfooxy)cholan-24-yl]-
32	1-(b-D-Ribofuranosyl)-1,4-dihydronicotinamide
33	Sulfadimidine
34	7-Hydroxyflavanone beta-D-glucopyranoside
35	Prunetin
36	5,6,7,8,3',4',5'-Heptamethoxyflavone
37	(9Z,11E,13E,15Z)-4-Oxo-9,11,13,15-octadecatetraenoic acid
38	Gingerenone C
39	Mitoxantrone
40	Butyl 2-aminobenzoate
41	Kanamycin
42	Cycloate
43	Medroxyprogesterone
44	Gingerglycolipid C
45	Irinotecan
46	Oxidized dinoflagellate luciferin
47	Pheophorbide a
48	Vanillylmandelic acid
49	Diethyl L-malate
50	MeIQ
51	8-D-Olivosyl-landomycin
52	Aspirin
53	Esculetin
54	Byakangelicin
55	Inumakilactone A glycoside
56	4',7-Di-O-methylcatechin
57	Phloroacetophenone 6'-[xylosyl-(1->6)-glucoside]
58	Silandrin
59	Isoacteoside
60	Lindleyin
61	(2S,2'R,3S,3'R,4S)-3,4',5,7-Tetrahydroxyflavan(2->7,4->8)- 3,3',5,5',7-pentahydroxyflavan
62	Glaucolide A
63	Guibourtinidol-(4alpha->6)-catechin
64	Aloesin
65	Artonol B
66	Ethofumesate
67	Methyl 3,4-dihydroxy-5-prenylbenzoate 3-glucoside
68	(2S,2''S,3S,3''R,4S)-3,4',5,7-Tetrahydroxyflavan(2->7,4->8)- 3,4',5,7-tetrahydroxyflavan
69	Salfredin
70	Mahuannin D
71	2-(3,4-Dihydroxyphenylethyl)-6-epi-elenaite
72	Vernolide
73	Morusignin B
74	Galactopinitol A
75	Elephantin
76	9Z-Octadecenedioic acid

Table S4. List of 308 target genes identified from metabolites of *P. longifolia* using the STRING database.

Gene list
CA9
TTR
APP
PIK3CB
CYP2C9
CYP3A4
CYP2C19
PIK3CA
PTPN22
CA2
LCK
SYK
RELA
CDK1
SI
VEGFA
CYP1A2
CYP1A1
CYP1B1
METAP2
TUBB3
ABCB1
MIF
AHR
TDO2
SRC
PTGS1
PARP1
NFE2L2
MAPT
DAO
CHRM3
CXCR4
ERBB2
EGFR
DRD1
CHEK1
PIM1
MAPKAPK2
CDK2
SLC6A2
MAPK14
MAPK1
JAK3
PTK2
JAK2
ROCK2
PRKCD
PRKCH
KDM1A
CDK4
KAT2B
GSK3B
MAP2K1
PTPRC
CDC25B
DUSP1
PPP1CA
ADAMTS5
AKR1B1
NAMPT
ESR2
IDO1
SLC6A3
HRH3

DPP7
PNP
TOP2A
MTAP
BCHE
AR
MAPK8
ILK
ADRB2
FLT1
KIT
KDR
P2RX7
NOS2
XIAP
BIRC2
NOS1
NOS3
HTR2C
ADRB3
DPP8
DPP9
ADRA1D
PLG
MAN1B1
KCNH2
PRKCI
ADRA2B
GBA
ROCK1
PRMT6
PDE1C
PRMT1
CCR3
HSP90AB1
MAPK11
SHBG
PTGS2
AKR1C3
ESR1
PTK2B
CSNK2A1
FLT3
CYP2A6
FGF1
FGF2
HSP90AA1
LGALS3
CYP2D6
ADRA1A
RORC
AMY2A
STAT3
HMGCR
PRF1
MDM2
PPP1CC
ADORA2B
ADRA1B
TNKS2
CTSC
CTSV
EPHX1
CCR2
PTPN1
PRKCA
ADORA3
MAPK10

CSNK1D
MMP9
CYP11B1
CYP11B2
FABP4
FABP5
PPARA
UGT2B7
PPARD
NR1H4
AKR1B10
G6PD
KDM2A
SERPINA6
CDC25A
PTGFR
CYP19A1
NPC1L1
MMP12
MMP13
MMP2
PHF8
KDM5C
VDR
IMPDH2
GSR
GABBR1
NR3C1
PIN1
GRK6
IMPDH1
MMP3
PDGFRB
FGFR1
CTSA
MME
ACE2
MCL1
KDM4A
CTNNB1
CREBBP
CDC45
ADAMTS4
CCR5
WEE1
TTK
AKT1
CCR1
CCR4
JAK1
TYK2
ALDH2
ALDH1A1
C1R
PDPK1
MKNK2
BRAF
CDC7
NOTUM
MET
CES1
TSPO
CD38
LRRK2
NPY1R
GAK
TLR4
STS

LIMK1
RAF1
ALPL
FABP1
MGMT
EP300
ALOX5
CYP17A1
HSD11B2
PGR
AKR1C1
MAOB
AURKB
BCL2
KIF11
TNKS
PREP
ALOX5AP
CXCR3
PDGFRA
RARG
BRD4
BRD2
BRD3
SNCA
CYP26A1
CASP3
CASP7
HMOX1
CTSB
PPARG
TERT
SCD
LTB4R
PDE4D
PTPN11
PLA2G1B
CD81
ACP1
PTGER1
MAPK3
SRD5A2
NR1I3
RORA
ENPP2
CPT1A
ACACA
ACACB
PTAFR
IGF1R
NR0B2
RXRA
CYP26B1
CACNA2D1
EPHX2
ABCC1
RORB
TTL
SIRT2
NR1I2
PDE3A
PDE3B
CDK8
MTOR
FASN
PIK3CD
PIK3CG
AURKA

PAM
CSNK2A2
PFKFB3
SLC5A1
SMO
PDE2A
MDM4
CYP24A1
OXTR
AXL
MERTK
MAP3K14
SLC6A9
FKBP1A
PPIA
LDHA
TYMS
PRKCG
RIPK1
F2
CDK9
FAP
MMP1
TGFBR1
PTK6
PRKACA
GLP1R
ADAM17
PABPC1
HIF1A
PER2
HSF1
EDNRA
KCNA3
SREBF2
DHCR7
SQLE