**SUPPLEMENTARY FILE**



Figure S1. Schematic of the extract manufacturing process



Figure S2. Schematic of the *in silico* study

**Table S1**. Chemical compounds in *Phomopsis* ethyl acetate extract from LC-MS/MS analysis

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compounds | Anti-cancer potency | Formula | RT [min] | Area | Relative Abundance (%) | Class |
| 1. 7-Hydroxycoumarine
 | √ | C9H6O3 | 11.99 | 4.9E+10 | 53.18 | Phenolic |
| 1. Dimethyl phthalate
 | - | C10H10O4 | 11.99 | 1.4E+10 | 15.32 | Ester |
| 1. Sorbic acid
 | √ | C6H8O2 | 3.93 | 7.8E+09 | 8.54 | Carboxylic acid |
| 1. Diisobutylphthalate
 | - | C16H22O4 | 21.19 | 4.9E+09 | 5.31 | Ester |
| 1. Bis(2-ethylhexyl) phthalate
 | - | C24H38O4 | 29.25 | 1.9E+09 | 2.04 | Ester |
| 1. PPG n6
 | - | C18H38 O7 | 10.97 | 1.7E+09 | 1.91 | Alcohol |
| 1. PPG n8
 | - | C24H50O9 | 13.36 | 1.7E+09 | 1.84 | Alcohol |
| 1. PPG n5
 | - | C15H32O6 | 9.66 | 1.7E+09 | 1.82 | Alcohol |
| 1. PPG n7
 | - | C21H44O8 | 12.21 | 1.5E+09 | 1.68 | Alcohol |
| 1. Cyclo(phenylalanyl-prolyl)
 | √ | C14H16N2O2 | 8.22 | 1.3E+09 | 1.37 | Alcaloid |
| 1. NP-011220
 | - | C11H18N2O2 | 7.41 | 1.1E+09 | 1.18 | Phosphor |
| 1. (5E)-7-methylidene-10-oxo-4-(propan-2-yl)undec-5-enoic acid
 | - | C15H24O3 | 15.79 | 7.8E+08 | 0.86 | Fatty acid |
| 1. Phthaldialdehyde
 | - | C8H6O2  | 11.98 | 6.9E+08 | 0.76 | Benzaldehid |
| 1. Triphenyl phosphate
 | - | C18H15O4P | 19.42 | 6.2E+08 | 0.68 | Organophosphates |
| 1. 3-[(4-hydroxyphenyl)methyl]-octa hydropyrrolo[1,2-a]pyrazine-1,4-dione
 | √ | C14H16N2O3 | 5.29 | 5.3E+08 | 0.58 | Alcaloid |
| 1. Monobutyl phthalate
 | - | C12H14O4 | 21.19 | 3.2E+08 | 0.35 | Ester |
| 1. 1,3,7-Trihydroxy-6-methoxy-4,5-diisoprenylxanthone
 | √ | C24H26O6 | 23.07 | 2.6E+08 | 0.28 | Flavonoid |
| 1. 4-Methoxychalcone
 | √ | C16H14O2 | 17.04 | 2.1E+08 | 0.23 | Flavonoid |
| 1. Dibenzoylmethane
 | √ | C15H12O2 | 20.96 | 1.7E+08 | 0.19 | Flavonoid |
| 1. 4-Acetamidobutanoic acid
 | - | C6H11NO3 | 1.75 | 1.5E+08 | 0.17 | Acetamide |
| 1. 4-(hydroxymethyl)benzoic acid
 | √ | C8H8O3 | 7.07 | 1.4E+08 | 0.15 | Phenolic |
| 1. DL-Mandelic acid
 | - | C8H8O3 | 5.14 | 1.4E+08 | 0.15 | α-Hydroxy acids |
| 1. Ethyl palmitoleate
 | - | C18H34O2 | 21.75 | 1.4E+08 | 0.15 | Fatty acid |
| 1. 4-Hydroxybenzaldehyde
 | - | C7H6O2 | 6.43 | 1.3E+08 | 0.15 | Aromatic aldehyde |
| 1. N-Acetyl-L-leucine
 | - | C8H15NO3 | 7.02 | 1.1E+08 | 0.13 | Amino acid |
| 1. Terephthalic acid
 | - | C8H6O4 | 5.70 | 1E+08 | 0.11 | Dicarboxylic acid |
| 1. Monomethyl phthalate
 | - | C9H8O4 | 8.51 | 1E+08 | 0.11 | Ester |
| 1. Bis(3,5,5-trimethylhexyl) phthalate
 | - | C26H42O4 | 26.26 | 9.7E+07 | 0.11 | Ester |
| 1. Suberic acid
 | - | C8H14O4  | 7.76 | 6.7E+07 | 0.07 | Dicarboxylic acid |
| 1. Citral
 | √ | C10H16O | 14.83 | 5.7E+07 | 0.06 | Monoterpen |
| 1. Oxybenzone
 | - | C14H12O3 | 18.29 | 5.2E+07 | 0.06 | Aromatic ketones |
| 1. 9-Oxo-10(E),12(E)-octadecadienoic acid
 | √ | C18H30O3 | 20.92 | 4.7E+07 | 0.05 | Fatty acid |
| 1. Phenylglyoxylic acid
 | - | C8H6O3 | 6.81 | 4.2E+07 | 0.05 | Glyoxylic acid |
| 1. Pimelic acid
 | - | C7H12O4 | 5.94 | 4.1E+07 | 0.05 | Dicarboxylic acid |
| 1. 3-[(1-Carboxyvinyl)oxy]benzoic acid
 | √ | C10H8O5 | 8.82 | 3.6E+07 | 0.04 | Phenolic |
| 1. (+)-ar-Turmerone
 | √ | C15H20O | 20.52 | 3.3E+07 | 0.04 | Sesquiterpen |
| 1. 3-Allyl-2-hydroxybenzoic acid
 | √ | C10H10O3 | 11.28 | 3.2E+07 | 0.04 | Phenolic |
| 1. Ferulic acid
 | √ | C10H10O4 | 10.52 | 3.2E+07 | 0.03 | Phenolic |
| 1. 1,3-Diphenylacetone
 | - | C15H14O | 18.78 | 2.9E+07 | 0.03 | Ketones |
| 1. cis-12-Octadecenoic acid methyl ester
 | - | C19H36O2 | 25.77 | 2.6E+07 | 0.03 | Fatty acid |
| 1. 18-β-Glycyrrhetinic acid
 | - | C30H46O4 | 25.34 | 1.8E+07 | 0.02 | Triterpenoid |
| 1. Chalcone
 | √ | C15H12O | 20.46 | 1.9E+07 | 0.02 | Flavonoid |
| 1. 3,3-Dimethylglutaric acid
 | - | C7H12O4 | 6.98 | 1.7E+07 | 0.02 | Carboxylic acid |
| 1. Hydroxycinnamic acid
 | √ | C9H10O2  | 8.79 | 2E+07 | 0.02 | Phenolic |



Figure S3. Functions of the compounds contained in *Phomopsis* extract (base on literature)

**Table S2**. Detection of ethyl acetate in extract

