**Computational Screening and Biochemical Analysis of *Pistacia Integerrima* and** ***Pandanus Odorifer* Plants To Find Effective Inhibitors Against Receptor-Binding Domain (RBD) of the Spike Protein of SARS-Cov-2**

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**Table S1:**DPPH scavenging activity of methanolic leaves and fruits extract of *P. integerrima* and *P. odorifer* with BHT as a standard.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Conc.  (μg/mL) | Standard | | *P. integerrima* plant extracts | | | | *P. odorifer* plant extracts | | | |
| BHT  Scavenging  (%) | IC50 (μg/mL) | Leaves  Scavenging (%) | IC50 (μg/mL) | Fruits Scavenging (%) | IC50 (μg/mL) | Leaves  Scavenging (%) | IC50 (μg/mL) | Fruits Scavenging (%) | IC50 (μg/mL) |
| 50 | 22.00±4.82 | 145.96 | 22.22±1.52 | 142.10 | 12.78±3.14 | 173.58 | 38.21±6.44 | 112.50 | 7.598±1.28 | 292.71 |
| 100 | 44.31±1.59 | 36.93±0.86 | 33.60±2.12 | 45.76±1.72 | 13.13±1.96 |
| 150 | 55.64±4.29 | 53.05±2.21 | 40.36±1.10 | 64.95±1.94 | 20.82±1.99 |
| 200 | 61.88±14.9 | 69.08±2.00 | 60.91±2.58 | 81.6±1.42 | 31.62±2.11 |
| 250 | 81.07±0.81 | 84.67±0.55 | 68.82±4.21 | 96.53±1.50 | 46.68±1.80 |

**Table S2:** Cytotoxic mortality percentage of leaves and fruits extracts of *P. integerrima* and *P. odorifer*, where different significant letters indicate significant differences between mean ± SD of replications (n=3) at a P ≤ 0.05 significant level.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Conc.  (μg/mL) | No. of Artemia taken | *P. integerrima* plant extracts | | | | *P. odorifer* plant extracts | | | |
| Leaves  Mortality (%) | LC50 (μg/mL) | Fruits Mortality (%) | LC50 (μg/mL) | Leaves  Mortality (%) | LC50 (μg/mL) | Fruits  Mortality (%) | LC50 (μg/mL) |
| 50 | 15 | 22.22±10.18**ab** | 95.54 | 31.11±7.70**bc** | 82.27 | 13.33±6.67**a** | 117.00 | 40.00±6.67**c** | 67.51 |
|  | 35.56±10.18**ab** | 46.67±6.68**bc** | 24.44±3.85**a** | 57.78±3.85**c** |
| 100 | 55.56±13.88**ab** | 64.44±10.18**ab** | 46.67±6.67**a** | 68.89±1.96**b** |
| 150 | 80.00±6.67**ab** | 88.89±3.85**bc** | 73.33±6.67**a** | 93.33±1.99**c** |
| 200 | 84.44±10.18**a** | 93.33±6.67**a** | 84.44±3.85**a** | 97.78±2.11**a** |
| 250 | 100.0±0.00**a** | 100.0±0.00**b** | 91.11±6.70**b** | 100.0±1.80**b** |

**Table S3:** Phytochemicals present in leaves extract of *P. integerrima.* Data were obtained from GC-MS analysis.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Peak**  **Name** | **IUPAC**  **Name** | **Canonical SMILES** | **CID** | **Molecular**  **Weight&**  **Formula** | **%**  **Area** | **Ret Time** |
| Phenol, 4-(methoxymethyl)- | acetic acid;4-(methoxymethyl)phenol | CC(=O)O.COCC1=CC=C(C=C1)O | 71360603 | 198.22 g/mol  [C10H14O4](https://pubchem.ncbi.nlm.nih.gov/#query=C10H14O4) | 0.22 | 3.787 |
| 3,3-Dimethoxy-2-butanone | 3,3-dimethoxybutan-2-one | CC(=O)C(C)(OC)OC | 140871 | 132.16 g/mol  [C6H12O3](https://pubchem.ncbi.nlm.nih.gov/#query=C6H12O3) | 0.14 | 3.968 |
| Benzyl alcohol, benzyldimethylsilyl ether | benzyl-dimethyl-phenylmethoxysilane | C[Si](C)(CC1=CC=CC=C1)OCC2=CC=CC=C2 | |  | | --- | | 91724157 | | 256.41 g/mol  [C16H20OSi](https://pubchem.ncbi.nlm.nih.gov/#query=C16H20OSi) | 0.13 | 4.15 |
| 8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, endo- | 8-methyl-8-azabicyclo[3.2.1]octan-3-ol | CN1C2CCC1CC(C2)O | 8424 | 141.21 g/mol  [C8H15NO](https://pubchem.ncbi.nlm.nih.gov/#query=C8H15NO) | 4.25 | 8.169 |
| Octanoic acid, 8-hydroxy-, methyl ester | methyl 8-hydroxyoctanoate | COC(=O)CCCCCCCO | 554055 | 174.24 g/mol  [C9H18O3](https://pubchem.ncbi.nlm.nih.gov/#query=C9H18O3) | 0.13 | 9.252 |
| 3,4-Dichloroatropine | (8-methyl-8-azabicyclo[3.2.1]octan-3-yl) 2-(3,4-dichlorophenyl)-3-hydroxypropanoate | CN1C2CCC1CC(C2)OC(=O)C(CO)C3=CC(=C(C=C3)Cl)Cl | 580026 | 358.3 g/mol  [C17H21Cl2NO3](https://pubchem.ncbi.nlm.nih.gov/#query=C17H21Cl2NO3) | 0.42 | 9.539 |
| 2,4-Di-tert-butylphenol | 2,4-di*tert*-butylphenol | CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C | 7311 | 206.32 g/mol  [C14H22O](https://pubchem.ncbi.nlm.nih.gov/#query=C14H22O) | 0.56 | 11.045 |
| Dodecanoic acid, methyl ester | methyl dodecanoate | CCCCCCCCCCCC(=O)OC | 8139 | |  | | --- | | 214.34 g/mol |   [C13H26O2](https://pubchem.ncbi.nlm.nih.gov/#query=C13H26O2) | 0.12 | 11.156 |
| 3,4-Dichloroatropine | (8-methyl-8-azabicyclo[3.2.1]octan-3-yl) 2-(3,4-dichlorophenyl)-3-hydroxypropanoate | CN1C2CCC1CC(C2)OC(=O)C(CO)C3=CC(=C(C=C3)Cl)Cl | 580026 | |  | | --- | | 358.3 g/mol |   [C17H21Cl2NO3](https://pubchem.ncbi.nlm.nih.gov/#query=C17H21Cl2NO3) | 0.24 | 11.329 |
| Isopropyl 5-hydroxy-3,7,11-trimethyl-11-methoxy-2-dodecenoate | propan-2-yl (*E*)-5-hydroxy-11-methoxy-3,7,11-trimethyldodec-2-enoate | CC(C)OC(=O)C=C(C)CC(CC(C)CCCC(C)(C)OC)O | |  | | --- | | 5366521 | | |  | | --- | | 328.5 g/mol |   [C19H36O4](https://pubchem.ncbi.nlm.nih.gov/#query=C19H36O4) | 0.2 | 11.924 |
| Methyl tetradecanoate | methyl tetradecanoate | CCCCCCCCCCCCCC(=O)OC | |  | | --- | | 31284 | | 242.4 g/mol  [C15H30O2](https://pubchem.ncbi.nlm.nih.gov/#query=C15H30O2) | 0.36 | 13.302 |
| 5,5,8a-Trimethyl-3,5,6,7,8,8a-hexahydro-2H-chromene | 5,5,8*a*-trimethyl-3,6,7,8-tetrahydro-2*H*-chromene | CC1(CCCC2(C1=CCCO2)C)C | 580068 | 180.29 g/mol  [C12H20O](https://pubchem.ncbi.nlm.nih.gov/#query=C12H20O) | 0.57 | 14.288 |
| Neophytadiene | 7,11,15-trimethyl-3-methylidenehexadec-1-ene | CC(C)CCCC(C)CCCC(C)CCCC(=C)C=C | 10446 | 278.5 g/mol  [C20H38](https://pubchem.ncbi.nlm.nih.gov/#query=C20H38) | 1.6 | 14.839 |
| 2-Pentadecanone, 6,10,14-trimethyl- | 6,10,14-trimethylpentadecan-2-one | CC(C)CCCC(C)CCCC(C)CCCC(=O)C | |  | | --- | | 10408 | | |  | | --- | | 268.5 g/mol | | [C18H36O](https://pubchem.ncbi.nlm.nih.gov/#query=C18H36O) | | 0.51 | 14.911 |
| 3,7,11,15-Tetramethyl-2-hexadecen-1-ol | (*E*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C | 5366244 | 296.5 g/mol  [C20H40O](https://pubchem.ncbi.nlm.nih.gov/#query=C20H40O) | 0.36 | 15.188 |
| 3,7,11,15-Tetramethyl-2-hexadecen-1-ol | (*E*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C | |  | | --- | | 5366244 | | 296.5 g/mol  [C20H40O](https://pubchem.ncbi.nlm.nih.gov/#query=C20H40O) | 0.56 | 15.47 |
| Hexadecanoic acid, methyl ester | methyl hexadecanoate | CCCCCCCCCCCCCCCC(=O)OC | 8181 | |  | | --- | | 270.5 g/mol |   [C17H34O2](https://pubchem.ncbi.nlm.nih.gov/#query=C17H34O2) | 5.72 | 16.118 |
| Tropacocaine | [(1*R*,5*S*)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl] benzoate | CN1C2CCC1CC(C2)OC(=O)C3=CC=CC=C3 | |  | | --- | | 637578 | | |  | | --- | | 245.32 g/mol |   [C15H19NO2](https://pubchem.ncbi.nlm.nih.gov/#query=C15H19NO2) | 1.65 | 17.022 |
| Methyl 10-trans,12-cis-octadecadienoate | methyl (10*E*,12*Z*)-octadeca-10,12-dienoate | CCCCCC=CC=CCCCCCCCCC(=O)OC | 5471014 | 294.5 g/mol  [C19H34O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H34O2) | 1.77 | 18.83 |
| 8,11,14-Docosatrienoic acid, methyl ester | methyl (8*E*,11*E*,14*E*)-docosa-8,11,14-trienoate | CCCCCCCC=CCC=CCC=CCCCCCCC(=O)OC | 5364473 | 348.6 g/mol  [C23H40O2](https://pubchem.ncbi.nlm.nih.gov/#query=C23H40O2) | 3.84 | 18.936 |
| Phytol | (*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C | 5280435 | |  | | --- | | 296.5 g/mol |   [C20H40O](https://pubchem.ncbi.nlm.nih.gov/#query=C20H40O) | 0.94 | 19.11 |
| Methyl stearate | methyl octadecanoate | CCCCCCCCCCCCCCCCCC(=O)OC | 8201 | 298.5 g/mol  [C19H38O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H38O2) | 1.22 | 19.36 |
| 9-Octadecenamide, (Z)- | (*Z*)-octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N | 5283387 | |  | | --- | | 281.5 g/mol  [C18H35NO](https://pubchem.ncbi.nlm.nih.gov/#query=C18H35NO) | | 0.38 | 19.883 |
| Octadecanamide | octadecanamide | CCCCCCCCCCCCCCCCCC(=O)N | |  | | --- | | 31292 | | |  | | --- | | 283.5 g/mol |   [C18H37NO](https://pubchem.ncbi.nlm.nih.gov/#query=C18H37NO) | 0.49 | 20.217 |
| 4,8,12,16-Tetramethylheptadecan-4-olide | 5-methyl-5-(4,8,12-trimethyltridecyl)oxolan-2-one | CC(C)CCCC(C)CCCC(C)CCCC1(CCC(=O)O1)C | 567149 | 324.5 g/mol   |  | | --- | | [C21H40O2](https://pubchem.ncbi.nlm.nih.gov/#query=C21H40O2) | | 0.27 | 23.083 |
| Cyclopropaneoctanoic acid, 2-[[2-[(2-ethylcyclopropyl)methyl]cyclopropyl]methyl]-, methyl ester | methyl 8-[2-[[2-[(2-ethylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]octanoate | CCC1CC1CC2CC2CC3CC3CCCCCCCC(=O)OC | 534619 | 334.5 g/mol  [C22H38O2](https://pubchem.ncbi.nlm.nih.gov/#query=C22H38O2) | 0.14 | 23.14 |
| 9-Octadecenamide, (Z)- | (*Z*)-octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N | 5283387 | |  | | --- | | 281.5 g/mol  [C18H35NO](https://pubchem.ncbi.nlm.nih.gov/#query=C18H35NO) | | 10.75 | 23.25 |
| 3-Hexenedioic acid, dimethyl ester, (Z)- | dimethyl (*Z*)-hex-3-enedioate | COC(=O)CC=CCC(=O)OC | 5365366 | 172.18 g/mol   |  | | --- | | [C8H12O4](https://pubchem.ncbi.nlm.nih.gov/#query=C8H12O4) | | 0.5 | 23.355 |
| Squalene | (6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene | CC(=CCCC(=CCCC(=CCCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C | 638072 | 410.7 g/mol  [C30H50](https://pubchem.ncbi.nlm.nih.gov/#query=C30H50) | 2.97 | 30.283 |
| .gamma.-Tocopherol | 2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol | CC1=C(C=C2CCC(OC2=C1C)(C)CCCC(C)CCCC(C)CCCC(C)C)O | |  | | --- | | 14986 | | 416.7 g/mol  [C28H48O2](https://pubchem.ncbi.nlm.nih.gov/#query=C28H48O2) | 1.4 | 33.609 |
| Vitamin E | (2*R*)-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-ol | CC1=C(C2=C(CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C)C(=C1O)C)C | |  | | --- | | 14985 | | |  | | --- | | 430.7 g/mol |   [C29H50O2](https://pubchem.ncbi.nlm.nih.gov/#query=C29H50O2) | 1.16 | 34.797 |
| .alpha.-Tocopheryl acetate | [(2*R*)-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-yl] acetate | CC1=C(C(=C(C2=C1OC(CC2)(C)CCCC(C)CCCC(C)CCCC(C)C)C)OC(=O)C)C | 86472 | 472.7 g/mol  [C31H52O3](https://pubchem.ncbi.nlm.nih.gov/#query=C31H52O3) | 0.9 | 34.905 |
| Cholest-5-ene, 3-methoxy-, (3.beta.)- | 3-methoxy-10,13-dimethyl-17-(6-methylheptan-2-yl)-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthrene | CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)OC)C)C | 79146 | |  | | --- | | 400.7 g/mol |   [C28H48O](https://pubchem.ncbi.nlm.nih.gov/#query=C28H48O) | 0.54 | 36.622 |
| Stigmasterol | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(*E*,2*R*,5*S*)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol | CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C | |  | | --- | | 5280794 | | |  | | --- | | 412.7 g/mol |   [C29H48O](https://pubchem.ncbi.nlm.nih.gov/#query=C29H48O) | 2.18 | 37.102 |
| .beta.-Sitosterol | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(2*R*,5*R*)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol | CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C | 222284 | 414.7 g/mol   |  | | --- | | [C29H50O](https://pubchem.ncbi.nlm.nih.gov/#query=C29H50O) | | 13.29 | 38.306 |
| 24-Noroleana-3,12-diene | (4*aS*,6*aR*,6*bS*,8*aR*,12*aR*,14*aR*,14*bS*)-4,6*a*,6*b*,8*a*,11,11,14*b*-heptamethyl-2,4*a*,5,6,7,8,9,10,12,12*a*,14,14*a*-dodecahydro-1*H*-picene | CC1=CCCC2(C1CCC3(C2CC=C4C3(CCC5(C4CC(CC5)(C)C)C)C)C)C | 15427754 | |  | | --- | | 394.7 g/mol |  |  | | --- | | [C29H46](https://pubchem.ncbi.nlm.nih.gov/#query=C29H46) | | 8.15 | 38.685 |
| Lup-20(29)-en-3-ol, acetate, (3.beta.)- | [(9*R*)-3*a*,5*a*,5*b*,8,8,11*a*-hexamethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7*a*,9,10,11,11*b*,12,13,13*a*,13*b*-hexadecahydrocyclopenta[a]chrysen-9-yl] acetate | CC(=C)C1CCC2(C1C3CCC4C5(CCC(C(C5CCC4(C3(CC2)C)C)(C)C)OC(=O)C)C)C | 6432150 | 468.8 g/mol   |  | | --- | | [C32H52O2](https://pubchem.ncbi.nlm.nih.gov/#query=C32H52O2) | | 15.24 | 38.953 |
| 24-Noroleana-3,12-diene | (4*aS*,6*aR*,6*bS*,8*aR*,12*aR*,14*aR*,14*bS*)-4,6*a*,6*b*,8*a*,11,11,14*b*-heptamethyl-2,4*a*,5,6,7,8,9,10,12,12*a*,14,14*a*-dodecahydro-1*H*-picene | CC1=CCCC2(C1CCC3(C2CC=C4C3(CCC5(C4CC(CC5)(C)C)C)C)C)C | 15427754 | 394.7 g/mol   |  | | --- | | [C29H46](https://pubchem.ncbi.nlm.nih.gov/#query=C29H46) | | 12.32 | 39.343 |
| Lup-20(29)-en-3-one | (1*R*,3*aR*,5*aR*,5*bR*,7*aR*,11*aR*,11*bR*,13*aR*,13*bR*)-3*a*,5*a*,5*b*,8,8,11*a*-hexamethyl-1-prop-1-en-2-yl-2,3,4,5,6,7,7*a*,10,11,11*b*,12,13,13*a*,13*b*-tetradecahydro-1*H*-cyclopenta[a]chrysen-9-one | CC(=C)C1CCC2(C1C3CCC4C5(CCC(=O)C(C5CCC4(C3(CC2)C)C)(C)C)C)C | |  | | --- | | 92158 | | |  | | --- | | 424.7 g/mol |   [C30H48O](https://pubchem.ncbi.nlm.nih.gov/#query=C30H48O) | 3.61 | 39.727 |

**Table S4:** Phytochemicals present in fruits extract of *P. integerrima.* Data were obtained from GC-MS analysis.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound  Name | IUPAC Name | Canonical SMILES | CID | Molecular Weight & Formula | %  Area | Ret Time |
| Spiro[androst-5-ene-17,1'-cyclobutan]-2'-one, 3-hydroxy-, (3.beta.,17.beta.)- | 3-hydroxy-10,13-dimethylspiro[1,2,3,4,7,8,9,11,12,14,15,16-dodecahydrocyclopenta[a]phenanthrene-17,2'-cyclobutane]-1'-one | CC12CCC(CC1=CCC3C2CCC4(C3CCC45CCC5=O)C)O | 534435 | 328.5 g/mol   |  | | --- | | [C22H32O2](https://pubchem.ncbi.nlm.nih.gov/#query=C22H32O2) | | 1.45 | 3.519 |
| Acetic acid, butyl ester | butyl acetate | CCCCOC(=O)C | 31272 | 116.16 g/mol  [C6H12O2](https://pubchem.ncbi.nlm.nih.gov/#query=C6H12O2) or CH3COO(CH2)3CH3 | 0.19 | 3.685 |
| Phenol, 4-(methoxymethyl)- | 4-(methoxymethyl)phenol | COCC1=CC=C(C=C1)O | 79310 | 138.16 g/mol   |  | | --- | | [C8H10O2](https://pubchem.ncbi.nlm.nih.gov/#query=C8H10O2) | | 0.41 | 3.793 |
| Oxime-, methoxy-phenyl-\_ | methyl (*Z*)-*N*-hydroxybenzenecarboximidate | COC(=NO)C1=CC=CC=C1 | 9602988 | 151.16 g/mol  [C8H9NO2](https://pubchem.ncbi.nlm.nih.gov/#query=C8H9NO2) | 0.23 | 4.39 |
| Glycerin | propane-1,2,3-triol | C(C(CO)O)O | |  | | --- | | 753 | | 92.09 g/mol  [C3H8O3](https://pubchem.ncbi.nlm.nih.gov/#query=C3H8O3) or CH2OH-CHOH-CH2OH | 0.45 | 5.286 |
| 8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, endo- | 8-methyl-8-azabicyclo[3.2.1]octan-3-ol | CN1C2CCC1CC(C2)O | 8424 | 141.21 g/mol  [C8H15NO](https://pubchem.ncbi.nlm.nih.gov/#query=C8H15NO) | 1.36 | 7.946 |
| 8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-, endo- | 8-methyl-8-azabicyclo[3.2.1]octan-3-ol | CN1C2CCC1CC(C2)O | 8424 | |  | | --- | | 141.21 g/mol |   [C8H15NO](https://pubchem.ncbi.nlm.nih.gov/#query=C8H15NO) | 3.72 | 8.166 |
| 2,4-Di-tert-butylphenol | 2,4-di*tert*-butylphenol | CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C | 7311 | 206.32 g/mol  [C14H22O](https://pubchem.ncbi.nlm.nih.gov/#query=C14H22O) | 0.55 | 11.042 |
| Octyl-.beta.-D-glucopyranoside | (2*R*,3*S*,4*S*,5*R*,6*R*)-2-(hydroxymethyl)-6-octoxyoxane-3,4,5-triol | CCCCCCCCOC1C(C(C(C(O1)CO)O)O)O | 62852 | 292.37 g/mol   |  | | --- | | [C14H28O6](https://pubchem.ncbi.nlm.nih.gov/#query=C14H28O6) | | 0.23 | 11.915 |
| 4-O-Methylmannose | 6-(hydroxymethyl)-5-methoxyoxane-2,3,4-triol | COC1C(OC(C(C1O)O)O)CO | 345716 | 194.18 g/mol   |  | | --- | | [C7H14O6](https://pubchem.ncbi.nlm.nih.gov/#query=C7H14O6) | | 79.26 | 13.534 |
| 13,13-Dimethyl-3,6,9-trioxa-13-silatetradecan-1-ol | 2-[2-[2-(3-trimethylsilylpropoxy)ethoxy]ethoxy]ethanol | C[Si](C)(C)CCCOCCOCCOCCO | 542367 | |  | | --- | | 264.43 g/mol |   [C12H28O4Si](https://pubchem.ncbi.nlm.nih.gov/#query=C12H28O4Si) | 0.22 | 13.8 |
| Silane, [(1,1-dimethyl-2-propenyl)oxy]dimethyl- | Silane, [(1,1-dimethyl-2-propenyl)oxy]dimethyl- | CC(C)(C=C)O[Si](C)C | 6329112 | 143.28 g/mol  [C7H15OSi](https://pubchem.ncbi.nlm.nih.gov/#query=C7H15OSi) | 1.62 | 14.871 |
| Hexadecanoic acid, methyl ester | methyl hexadecanoate | CCCCCCCCCCCCCCCC(=O)OC | 8181 | |  | | --- | | 270.5 g/mol  [C17H34O2](https://pubchem.ncbi.nlm.nih.gov/#query=C17H34O2) | | 1.04 | 16.11 |
| 9,12-Octadecadienoic acid, methyl ester | methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate | CCCCCC=CCC=CCCCCCCCC(=O)OC | 5284421 | |  | | --- | | 294.5 g/mol | | [C19H34O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H34O2) | | 0.57 | 18.824 |
| 6-Octadecenoic acid, methyl ester, (Z)- | methyl (*Z*)-octadec-6-enoate | CCCCCCCCCCCC=CCCCCC(=O)OC | 5362717 | 296.5 g/mol  [C19H36O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H36O2) | 0.8 | 18.929 |
| Methyl stearate | methyl octadecanoate | CCCCCCCCCCCCCCCCCC(=O)OC | 8201 | 298.5 g/mol  [C19H38O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H38O2) | 0.35 | 19.35 |
| Octadecanamide | octadecanamide | CCCCCCCCCCCCCCCCCC(=O)N | |  | | --- | | 31292 | | 283.5 g/mol   |  | | --- | | [C18H37NO](https://pubchem.ncbi.nlm.nih.gov/#query=C18H37NO) | | 0.23 | 20.213 |
| 9-Octadecenamide, (Z)- | (*Z*)-octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N | 5283387 | 281.5 g/mol   |  | | --- | | [C18H35NO](https://pubchem.ncbi.nlm.nih.gov/#query=C18H35NO) | | 6.78 | 23.24 |
| Dotriacontane | dotriacontane | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | |  | | --- | | 11008 | | 450.9 g/mol   |  | | --- | | [C32H66](https://pubchem.ncbi.nlm.nih.gov/#query=C32H66) | | 0.25 | 24.016 |
| Triacontane, 1-iodo- | 1-iodotriacontane | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCI | 12696145 | |  | | --- | | 548.7 g/mol  [C30H61I](https://pubchem.ncbi.nlm.nih.gov/#query=C30H61I) | | 0.29 | 25.619 |

**Table S5:** Phytochemicals present in leaves extract of *P. odorifer.* Data were obtained from GC-MS analysis.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound Name | IUPAC Name | Canonical SMILES | CID | Molecular Weight & Formula | %  Area | Ret Time |
| 3-trsns-(1,1-dimethylethyl)-4-trans-methoxycyclohexanol | 3-*tert*-butyl-4-methoxycyclohexan-1-ol | CC(C)(C)C1CC(CCC1OC)O | 545980 | 186.29 g/mol  C11H22O2 | 2.9 | 3.519 |
| Phenol, 4-(methoxymethyl)- | 4-(methoxymethyl)phenol | COCC1=CC=C(C=C1)O | 79310 | 138.16 g/mol  C8H10O2 | 1.12 | 3.772 |
| 3,3-Dimethoxy-2-butanone | 3,3-dimethoxybutan-2-one | CC(=O)C(C)(OC)OC | 140871 | 132.16 g/mol  C6H12O3 | 0.28 | 3.946 |
| Undecane | undecane | CCCCCCCCCCC | 14257 | 156.31 g/mol  C11H24 | 0.19 | 6.867 |
| 1-Heptanol, 6-methyl- | 6-methylheptan-1-ol | CC(C)CCCCCO | 15450 | 130.23 g/mol  C8H18O | 0.28 | 9.995 |
| 2,4-Di-tert-butylphenol | 2,4-di*tert*-butylphenol | CC(C)(C)C1=CC(=C(C=C1)O)C(C)(C)C | 7311 | 206.32 g/mol  C14H22O | 1.`13 | 11.04 |
| 3-O-Methyl-d-glucose | (2*R*,3*S*,4*R*,5*R*)-2,4,5,6-tetrahydroxy-3-methoxyhexanal | COC(C(C=O)O)C(C(CO)O)O | 8973 | 194.18 g/mol  C7H14O6 | 1.35 | 13.012 |
| 6-Hydroxy-4,4,7a-trimethyl-5,6,7,7a-tetrahydrobenzofuran-2(4H)-one | 6-hydroxy-4,4,7*a*-trimethyl-6,7-dihydro-5*H*-1-benzofuran-2-one | CC1(CC(CC2(C1=CC(=O)O2)C)O)C | 14334 | 196.24 g/mol  C11H16O3 | .039 | 13.733 |
| 2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin | (2,2,6-trimethyl-9,10-dioxatricyclo[6.2.2.01,6]dodecan-3-yl) acetate | CC(=O)OC1CCC2(CC3CCC2(C1(C)C)OO3)C | 538309 | 268.35 g/mol  C15H24O4 | 1.25 | 14.085 |
| 1-Cyclohexanone, 3-butyl-3-methyl- | 3-butyl-3-methylcyclohexan-1-one | CCCCC1(CCCC(=O)C1)C | 573884 | 168.28 g/mol  C11H20O | 0.29 | 14.145 |
| Methyl tetrahydroionol | 3-methyl-4-(2,2,6-trimethylcyclohexyl)butan-2-ol | CC1CCCC(C1CC(C)C(C)O)(C)C | 108425 | 212.37 g/mol  C14H28O | 0.41 | 14.226 |
| NEOPHYTADIENE | 7,11,15-trimethyl-3-methylidenehexadec-1-ene | CC(C)CCCC(C)CCCC(C)CCCC(=C)C=C | 10446 | 278.5 g/mol  C20H38 | 3.23 | 14.832 |
| [2-Pentadecanone, 6,10,14-trimethyl-](https://www.ncbi.nlm.nih.gov/pcsubstance/?term=" \t "https://pubchem.ncbi.nlm.nih.gov/compound/_self) | 6,10,14-trimethylpentadecan-2-one | CC(C)CCCC(C)CCCC(C)CCCC(=O)C | 10408 | 268.5 g/mol  C18H36O | O.5 | 14.904 |
| 3,7,11,15-TETRAMETHYL-2-HEXADECEN-1-OL | (*E*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C | 5366244 | 296.5 g/mol  C20H40O | 0.67 | 15.181 |
| NEOPHYTADIENE | 7,11,15-trimethyl-3-methylidenehexadec-1-ene | CC(C)CCCC(C)CCCC(C)CCCC(=C)C=C | 10446 | 278.5 g/mol  C20H38 | 0.98 | 15.461 |
| Hexadecanoic acid, methyl ester | methyl hexadecanoate | CCCCCCCCCCCCCCCC(=O)OC | 8181 | 270.5 g/mol  C17H34O2 | 8.53 | 16.109 |
| Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester | methyl 3-(3,5-di*tert*-butyl-4-hydroxyphenyl)propanoate | CC(C)(C)C1=CC(=CC(=C1O)C(C)(C)C)CCC(=O)OC | 62603 | 292.4 g/mol  C18H28O3 | 0.46 | 16.259 |
| [9,12-Octadecadienoic acid (Z,Z)-, methyl ester](https://www.ncbi.nlm.nih.gov/pcsubstance/?term=" \t "https://pubchem.ncbi.nlm.nih.gov/compound/_self) | methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate | CCCCCC=CCC=CCCCCCCCC(=O)OC | 5284421 | 294.5 g/mol  C19H34O2 | 5.23 | 18.822 |
| 8,11,14-Docosatrienoic acid, methyl ester | methyl (8*E*,11*E*,14*E*)-docosa-8,11,14-trienoate | CCCCCCCC=CCC=CCC=CCCCCCCC(=O)OC | 5364473 | 348.6 g/mol  C23H40O2 | 9.87 | 18.925 |
| Phytol | (*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | CC(C)CCCC(C)CCCC(C)CCCC(=CCO)C | 5280435 | 296.5 g/mol  C20H40O | 1.83 | 19.101 |
| METHYL STEARATE | methyl octadecanoate | CCCCCCCCCCCCCCCCCC(=O)OC | 8201 | 298.5 g/mol  C19H38O2 | 1.9 | 19.347 |
| [9-Octadecenamide, (Z)-](https://www.ncbi.nlm.nih.gov/pcsubstance/?term=" \t "https://pubchem.ncbi.nlm.nih.gov/compound/_self) | (*Z*)-octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N | 5283387 | 281.5 g/mol  C18H35NO | 0.58 | 19.874 |
| Tetradecanamide | tetradecanamide | CCCCCCCCCCCCCC(=O)N | 69492 | 227.39 g/mol  C14H29NO | 0.44 | 20.203 |
| [2-Cyclohexen-1-ol, 3-methyl-6-(1-methylethyl)-, trans-](https://www.ncbi.nlm.nih.gov/pcsubstance/?term=" \t "https://pubchem.ncbi.nlm.nih.gov/compound/_self) | (1*R*,6*R*)-3-methyl-6-propan-2-ylcyclohex-2-en-1-ol | CC1=CC(C(CC1)C(C)C)O | |  | | --- | | 85568 | | 154.25 g/mol  C10H18O | 1.06 | 20.976 |
| [12-Methyl-E,E-2,13-octadecadien-1-ol](https://www.ncbi.nlm.nih.gov/pcsubstance/?term=" \t "https://pubchem.ncbi.nlm.nih.gov/compound/_self) | (2*E*,13*E*)-12-methyloctadeca-2,13-dien-1-ol | CCCCC=CC(C)CCCCCCCCC=CCO | 90107969 | 280.5 g/mol  C19H36O | 0.34 | 22.278 |
| [9-Octadecenamide, (Z)-](https://www.ncbi.nlm.nih.gov/pcsubstance/?term=" \t "https://pubchem.ncbi.nlm.nih.gov/compound/_self) | (*Z*)-octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N | 5283387 | 281.5 g/mol  C18H35NO | 13.71 | 23.235 |
| Octatriacontyl pentafluoropropionate | octatriacontyl 2,2,3,3,3-pentafluoropropanoate | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(C(F)(F)F)(F)F | 91693082 | 697 g/mol  C41H77F5O2 | 0.33 | 23.847 |
| TETRACONTANE | tetracontane | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 20149 | 563.1 g/mol  C40H82 | 0.39 | 24.023 |
| hexadecanal | hexadecanal | CCCCCCCCCCCCCCCC=O | 984 | 240.42 g/mol   |  | | --- | | [C16H32O](https://pubchem.ncbi.nlm.nih.gov/#query=C16H32O) | | 0.32 | 24.394 |
| Bis(2-ethylhexyl) phthalate | bis(2-ethylhexyl) benzene-1,2-dicarboxylate | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | 8343 | |  | | --- | | 390.6 g/mol  [C24H38O4](https://pubchem.ncbi.nlm.nih.gov/#query=C24H38O4) or   C6H4(COOC8H17)2 | | 1.44 | 26.001 |
| Squalene | (6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene | CC(=CCCC(=CCCC(=CCCC=C(C)CCC=C(C)CCC=C(C)C)C)C)C | 638072 | 410.7 g/mol  C30H50 | 3.15 | 30.274 |
| dl-.alpha.-Tocopherol | 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol | CC1=C(C2=C(CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C)C(=C1O)C)C | 2116 | 430.7 g/mol   |  | | --- | | [C29H50O2](https://pubchem.ncbi.nlm.nih.gov/#query=C29H50O2) | | 4.64 | 32.375 |
| 15,17,19,21-Hexatriacontatetrayne | hexatriaconta-15,17,19,21-tetrayne | CCCCCCCCCCCCCCC#CC#CC#CC#CCCCCCCCCCCCCCC | |  | | --- | | 537054 | | 490.8 g/mol  C36H58 | 32.445 | 32.51 |
| (R)-6-Methoxy-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman | (2*R*)-6-methoxy-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromene | CC1=C(C(=C(C2=C1OC(CC2)(C)CCCC(C)CCCC(C)CCCC(C)C)C)OC)C | 182085 | 444.7 g/mol  C30H52O2 | 33.31 | 33.366 |
| |  | | --- | | DL-ALPHA-  TOCOPHEROL | | 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol | CC1=C(C2=C(CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C)C(=C1O)C)C | |  | | --- | | 2116 | | |  | | --- | | 430.7 g/mol  C29H50O2 | | 34.73 | 74.787 |
| VITAMIN E | (2*R*)-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-ol | CC1=C(C2=C(CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C)C(=C1O)C)C | |  | | --- | | 14985 | | 430.7 g/mol  C29H50O2 | 34.84 | 34.888 |
| STIGMASTEROL | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(*E*,2*R*,5*S*)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol | CCC(C=CC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C | 5280794 | 412.7 g/mol  C29H48O | 37.007 | 37.09 |
| GAMMA-SITOSTEROL | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(2*R*,5*S*)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol | CCC(CCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C)C(C)C | |  | | --- | | 457801 | | |  | | --- | | 414.7 g/mol  C29H50O | | 38.175 | 38.31 |
| 28-Demethyl-beta-amyrone | (4*aR*,6*aR*,6*bS*,8*aR*,12*aR*,14*aR*,14*bR*)-4,4,6*a*,6*b*,11,11,14*b*-heptamethyl-1,2,4*a*,5,6,7,8,8*a*,9,10,12,12*a*,14,14*a*-tetradecahydropicen-3-one | CC1(CCC2CCC3(C(=CCC4C3(CCC5C4(CCC(=O)C5(C)C)C)C)C2C1)C)C | 101616676 | 410.7 g/mol  C29H46O | 39.245 | 39.32 |

**Table S6:** Phytochemicals present in lfruits extract of *P. odorifer.* Data were obtained from GC-MS analysis.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Compound Name | IUPAC  Name | Canonical SMILES | CID | Molecular Weight & Formula | % Area | Ret Time |
| 2-Butanone, 4-hydroxy-3-methyl- | 4-hydroxy-3-methylbutan-2-one | CC(CO)C(=O)C | 18829 | 102.13 g/mol   |  | | --- | | [C5H10O2](https://pubchem.ncbi.nlm.nih.gov/#query=C5H10O2) | | 4.39 | 3.532 |
| Furazanamine, 4-nitro- | 4-nitro-1,2,5-oxadiazol-3-amine | C1(=NON=C1[N+](=O)[O-])N | 543119 | 130.06 g/mol   |  | | --- | | [C2H2N4O3](https://pubchem.ncbi.nlm.nih.gov/#query=C2H2N4O3) | | 1.93 | 3.595 |
| Cyclohexanecarboxamide, N-furfuryl- | *N*-(furan-2-ylmethyl)cyclohexanecarboxamide | C1CCC(CC1)C(=O)NCC2=CC=CO2 | 240161 | |  | | --- | | 207.27 g/mol |   [C12H17NO2](https://pubchem.ncbi.nlm.nih.gov/#query=C12H17NO2) | 1.57 | 3.635 |
| Acetic acid, butyl ester | butyl acetate | CCCCOC(=O)C | 31272 | |  | | --- | | 116.16 g/mol |   [C6H12O2](https://pubchem.ncbi.nlm.nih.gov/#query=C6H12O2) or CH3COO(CH2)3CH3 | 1.62 | 3.665 |
| Phenol, 4-(methoxymethyl)- | 4-(methoxymethyl)phenol | COCC1=CC=C(C=C1)O | 79310 | 138.16 g/mol   |  | | --- | | [C8H10O2](https://pubchem.ncbi.nlm.nih.gov/#query=C8H10O2) | | 6 | 3.776 |
| Methane, (methylsulfinyl)(methylthio)- | methylsulfanyl(methylsulfinyl)methane | CSCS(=O)C | 99129 | 124.23 g/mol   |  | | --- | | [C3H8OS2](https://pubchem.ncbi.nlm.nih.gov/#query=C3H8OS2) | | 2.08 | 3.826 |
| 2-Cyclopenten-1-one | cyclopent-2-en-1-one | C1CC(=O)C=C1 | 13588 | |  | | --- | | 82.1 g/mol |   [C5H6O](https://pubchem.ncbi.nlm.nih.gov/#query=C5H6O) | 1.26 | 3.88 |
| p-Dioxane-2,3-diol | 1,4-dioxane-2,3-diol | C1COC(C(O1)O)O | 96170 | 120.1 g/mol   |  | | --- | | [C4H8O4](https://pubchem.ncbi.nlm.nih.gov/#query=C4H8O4) | | 1.3 | 3.92 |
| 3,3-Dimethoxy-2-butanone | 3,3-dimethoxybutan-2-one | CC(=O)C(C)(OC)OC | 140871 | 132.16 g/mol  [C6H12O3](https://pubchem.ncbi.nlm.nih.gov/#query=C6H12O3) | 1.6 | 3.952 |
| 3-Methylbenzyl alcohol, TBDMS derivative | *tert*-butyl-dimethyl-[(3-methylphenyl)methoxy]silane | CC1=CC(=CC=C1)CO[Si](C)(C)C(C)(C)C | 22967275 | |  | | --- | | 236.42 g/mol  [C14H24OSi](https://pubchem.ncbi.nlm.nih.gov/#query=C14H24OSi) | | 0.96 | 3.99 |
| Ethanol, 2,2-diethoxy- | 2,2-diethoxyethanol | CCOC(CO)OCC | 12129 | |  | | --- | | 134.17 g/mol |   [C6H14O3](https://pubchem.ncbi.nlm.nih.gov/#query=C6H14O3) | 0.94 | 4.024 |
| Xylitol | (2*S*,4*R*)-pentane-1,2,3,4,5-pentol | C(C(C(C(CO)O)O)O)O | 6912 | 152.15 g/mol  [C5H12O5](https://pubchem.ncbi.nlm.nih.gov/#query=C5H12O5) | 0.73 | 4.445 |
| 1,2-Cyclopentanedione | cyclopentane-1,2-dione | C1CC(=O)C(=O)C1 | 566657 | 98.1 g/mol   |  | | --- | | [C5H6O2](https://pubchem.ncbi.nlm.nih.gov/#query=C5H6O2) | | 0.7 | 4.815 |
| Glycerin | propane-1,2,3-triol | C(C(CO)O)O | 753 | |  | | --- | | 92.09 g/mol |   [C3H8O3](https://pubchem.ncbi.nlm.nih.gov/#query=C3H8O3) or CH2OH-CHOH-CH2OH | 0.68 | 5.305 |
| Undecane | undecane | CCCCCCCCCCC | 14257 | 156.31 g/mol   |  | | --- | | [C11H24](https://pubchem.ncbi.nlm.nih.gov/#query=C11H24) | | 1.06 | 6.861 |
| Dehydromevalonic lactone | 4-methyl-2,3-dihydropyran-6-one | CC1=CC(=O)OCC1 | 557445 | 112.13 g/mol   |  | | --- | | [C6H8O2](https://pubchem.ncbi.nlm.nih.gov/#query=C6H8O2) | | 4.04 | 7.595 |
| 3,6-Undecandione | undecane-3,6-dione | CCCCCC(=O)CCC(=O)CC | 13264813 | 184.27 g/mol   |  | | --- | | [C11H20O2](https://pubchem.ncbi.nlm.nih.gov/#query=C11H20O2) | | 0.64 | 7.993 |
| Benzofuran, 2,3-dihydro- | 2,3-dihydro-1-benzofuran | C1COC2=CC=CC=C21 | 10329 | 120.15 g/mol  [C8H8O](https://pubchem.ncbi.nlm.nih.gov/#query=C8H8O) | 1.4 | 8.168 |
| .beta.-D-Ribopyranoside, methyl | (2*R*,3*R*,4*R*,5*R*)-2-methoxyoxane-3,4,5-triol | COC1C(C(C(CO1)O)O)O | 11579182 | 164.16 g/mol   |  | | --- | | [C6H12O5](https://pubchem.ncbi.nlm.nih.gov/#query=C6H12O5) | | 1.65 | 8.933 |
| Phenol, 3,5-bis(1,1-dimethylethyl)- | 3,5-di*tert*-butylphenol | CC(C)(C)C1=CC(=CC(=C1)O)C(C)(C)C | 70825 | 206.32 g/mol  [C14H22O](https://pubchem.ncbi.nlm.nih.gov/#query=C14H22O) | 1.58 | 11.041 |
| .alpha.-D-Galactopyranoside, methyl | (2*R*,3*R*,4*S*,5*R*,6*S*)-2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol | COC1C(C(C(C(O1)CO)O)O)O | 76935 | 194.18 g/mol   |  | | --- | | [C7H14O6](https://pubchem.ncbi.nlm.nih.gov/#query=C7H14O6) | | 0.83 | 11.528 |
| Sulfurous acid, decyl 2-propyl ester | decyl propan-2-yl sulfite | CCCCCCCCCCOS(=O)OC(C)C | 6420364 | 264.43 g/mol   |  | | --- | | [C13H28O3S](https://pubchem.ncbi.nlm.nih.gov/#query=C13H28O3S) | | 1.56 | 13.014 |
| Hexadecane, 1-iodo- | 1-iodohexadecane | CCCCCCCCCCCCCCCCI | 11007 | 352.34 g/mol  [C16H33I](https://pubchem.ncbi.nlm.nih.gov/#query=C16H33I) | 1.61 | 14.314 |
| N-Ethyl-hexahydro-1H-azepine | 1-ethylazepane | CCN1CCCCCC1 | 535585 | |  | | --- | | 127.23 g/mol |   [C8H17N](https://pubchem.ncbi.nlm.nih.gov/#query=C8H17N) | 1.85 | 15.327 |
| Hexadecanoic acid, methyl ester | methyl hexadecanoate | CCCCCCCCCCCCCCCC(=O)OC | 8181 | |  | | --- | | 270.5 g/mol  [C17H34O2](https://pubchem.ncbi.nlm.nih.gov/#query=C17H34O2) | | 3.51 | 16.111 |
| 9,12-Octadecadienoic acid (Z,Z)-, methyl ester | methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate | CCCCCC=CCC=CCCCCCCCC(=O)OC | 5284421 | 294.5 g/mol  [C19H34O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H34O2) | 4.96 | 18.8240 |
| 9-Octadecenoic acid, methyl ester, (E)- | methyl (*E*)-octadec-9-enoate | CCCCCCCCC=CCCCCCCCC(=O)OC | 5280590 | 296.5 g/mol  [C19H36O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H36O2) | 3.59 | 18.931 |
| Methyl stearate | methyl octadecanoate | CCCCCCCCCCCCCCCCCC(=O)OC | 8201 | 298.5 g/mol  [C19H38O2](https://pubchem.ncbi.nlm.nih.gov/#query=C19H38O2) | 2.19 | 19.352 |
| 9-Octadecenamide, (Z)- | (*Z*)-octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N | 5283387 | 281.5 g/mol  [C18H35NO](https://pubchem.ncbi.nlm.nih.gov/#query=C18H35NO) | 0.78 | 19.875 |
| Tetradecanamide | tetradecanamide | CCCCCCCCCCCCCC(=O)N | 69492 | 227.39 g/mol   |  | | --- | | [C14H29NO](https://pubchem.ncbi.nlm.nih.gov/#query=C14H29NO) | | 1.01 | 20.209 |
| Undecane, 2,4-dimethyl- | 2,4-dimethylundecane | CCCCCCCC(C)CC(C)C | 28476 | 184.36 g/mol  [C13H28](https://pubchem.ncbi.nlm.nih.gov/#query=C13H28) | 0.66 | 22.252 |
| Dodecane, 2,6,11-trimethyl- | 2,6,11-trimethyldodecane | CC(C)CCCCC(C)CCCC(C)C | 35768 | |  | | --- | | 212.41 g/mol |   [C15H32](https://pubchem.ncbi.nlm.nih.gov/#query=C15H32) | 0.94 | 22.393 |
| 9-Octadecenamide, (Z)- | (*Z*)-octadec-9-enamide | CCCCCCCCC=CCCCCCCCC(=O)N | 5283387 | 281.5 g/mol   |  | | --- | | [C18H35NO](https://pubchem.ncbi.nlm.nih.gov/#query=C18H35NO) | | 27.64 | 23.24 |
| 11-Methyltricosane | 11-methyltricosane | CCCCCCCCCCCCC(C)CCCCCCCCCC | 530326 | 338.7 g/mol   |  | | --- | | [C24H50](https://pubchem.ncbi.nlm.nih.gov/#query=C24H50) | | 0.89 | 24.012 |
| 1,1,3,6-tetramethyl-2-(3,6,10,13,14-pentamethyl-3-ethyl-pentadecyl)cyclohexane | 2-(3-ethyl-3,6,10,13,14-pentamethylpentadecyl)-1,1,3,6-tetramethylcyclohexane | CCC(C)(CCC1C(CCC(C1(C)C)C)C)CCC(C)CCCC(C)CCC(C)C(C)C | 91693134 | 448.8 g/mol   |  | | --- | | [C32H64](https://pubchem.ncbi.nlm.nih.gov/#query=C32H64) | | 0.76 | 24.47 |
| Pentadecane, 4-methyl- | 4-methylpentadecane | CCCCCCCCCCCC(C)CCC | 17751 | 226.44 g/mol  [C16H34](https://pubchem.ncbi.nlm.nih.gov/#query=C16H34) | 1.05 | 25.09 |
| 6-Tetradecanesulfonic acid, butyl ester | butyl tetradecane-6-sulfonate | CCCCCCCCC(CCCCC)S(=O)(=O)OCCCC | 551402 | 334.6 g/mol  [C18H38O3S](https://pubchem.ncbi.nlm.nih.gov/#query=C18H38O3S) | 0.64 | 25.375 |
| Bis-(3,4-dimethoxyphenyl)-hydroxyacetic acid, 1-methyl ester | (1-methylpiperidin-3-yl) 2,2-bis(3,4-dimethoxyphenyl)-2-hydroxyacetate | CN1CCCC(C1)OC(=O)C(C2=CC(=C(C=C2)OC)OC)(C3=CC(=C(C=C3)OC)OC)O | 566075 | 445.5 g/mol   |  | | --- | | [C24H31NO7](https://pubchem.ncbi.nlm.nih.gov/#query=C24H31NO7) | | 1.12 | 25.493 |
| Hexacontane | hexacontane | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC | 24318 | 843.6 g/mol   |  | | --- | | [C60H122](https://pubchem.ncbi.nlm.nih.gov/#query=C60H122) | | 1.32 | 25.61 |
| DEHP | bis(2-ethylhexyl) benzene-1,2-dicarboxylate | CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC | 8343 | 390.6 g/mol  [C24H38O4](https://pubchem.ncbi.nlm.nih.gov/#query=C24H38O4) or C6H4(COOC8H17)2 | 1.52 | 26.001 |
| Nonacos-1-ene | nonacos-1-ene | CCCCCCCCCCCCCCCCCCCCCCCCCCCC=C | 156989 | |  | | --- | | 406.8 g/mol  [C29H58](https://pubchem.ncbi.nlm.nih.gov/#query=C29H58) | | 0.76 | 26.773 |
| Fumaric acid, 2-decyl nonadecyl ester | 4-*O*-decan-2-yl 1-*O*-nonadecyl (*E*)-but-2-enedioate | CCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCCCCCC | 91692901 | |  | | --- | | 522.8 g/mol |   [C33H62O4](https://pubchem.ncbi.nlm.nih.gov/#query=C33H62O4) | 1.35 | 27.051 |
| 5-Methyl-Z-5-docosene | (*Z*)-5-methyldocos-5-ene | CCCCCCCCCCCCCCCCC=C(C)CCCC | 5365995 | 322.6 g/mol  [C23H46](https://pubchem.ncbi.nlm.nih.gov/#query=C23H46) | 1.28 | 27.159 |
| 3-Cyclohexenecarboxylic acid, 6,6-dimethyl-4-(4-morpholyl)-2-oxo-, methyl ester | methyl 6,6-dimethyl-4-morpholin-4-yl-2-oxocyclohex-3-ene-1-carboxylate | CC1(CC(=CC(=O)C1C(=O)OC)N2CCOCC2)C | 544174 | 267.32 g/mol   |  | | --- | | [C14H21NO4](https://pubchem.ncbi.nlm.nih.gov/#query=C14H21NO4) | | 1.24 | 27.649 |
| trans-Geranylgeraniol | (2*E*,6*E*,10*E*)-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraen-1-ol | CC(=CCCC(=CCCC(=CCCC(=CCO)C)C)C)C | 5281365 | 290.5 g/mol  [C20H34O](https://pubchem.ncbi.nlm.nih.gov/#query=C20H34O) | 0.81 | 30.27 |

**Table S7:** The pharmacological assessment of all molecules, where (+) indicates the positive result, (-) denotes negative, and WI indicates the weak inhibition.

**Table S7.1:** An ADMET properties of phytochemicals derived from *P. integerrima* leaves extract.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | acetic acid;4-(methoxymethyl)phenol | 3,3-dimethoxybutan-2-one | benzyl-dimethyl-phenylmethoxysilane | 8-methyl-8-azabicyclo[3.2.1]octan-3-o | methyl 8-hydroxyoctanoate |
| Molecular Weight | 198.22 | 132.16 | 256.42 | 141.21 | 174.24 |
| Log P | 1.6295 | 0.5844 | 4.1902 | 0.6039 | 1.4923 |
| Surface Area | 82.761 | 54.953 | 110.566 | 61.836 | 73.728 |
| Blood Brain Barrier | 0.9047(+) | 0.9953(+) | 0.9864(+) | 0.9827(+) | 0.9640(+) |
| Human Intestinal Absorption | 0.9802(+) | 0.9250(+) | 0.9774(+) | 0.9166(+) | 0.9207(+) |
| P-Glycoprotein Inhibition | 0.9893(-) | 0.9787(-) | 0.9301(-) | 0.9869(-) | 0.9795(-) |
| AMES Toxicity | 0.826(-) | 0.7679(-) | 0.8119(-) | 0.7551(-) | 0.9478(-) |
| HERG Inhibition | 0.7126(WI)) | 0.9961(WT) | 0.8959(WI) | 0.7328(WI) | 0.9455(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **Yes** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | (8-methyl-8-azabicyclo[3.2.1]octan-3-yl) 2-(3,4-dichlorophenyl)-3-hydroxypropanoate | 2,4-di*tert*-butylphenol | methyl dodecanoate | (8-methyl-8-azabicyclo[3.2.1]octan-3-yl) 2-(3,4-dichlorophenyl)-3-hydroxypropanoate | propan-2-yl (*E*)-5-hydroxy-11-methoxy-3,7,11-trimethyldodec-2-enoate |
| Molecular Weight | 358.26 | 206.329 | 214.349 | 358.265 | 328.493 |
| Log P | 3.24 | 3.9872 | 4.0803 | 3.2377 | 4.2568 |
| Surface Area | 145.870 | 93.145 | 94.394 | 145.870 | 141.801 |
| Blood Brain Barrier | 0.9672(+) | 0.9946(+) | 1.0000(+) | 0.9672(+) | 0.9301(+) |
| Human Intestinal Absorption | 0.9838(+) | 0.9928(+) | 0.9543(+) | 0.9838(+) | 0.9944(+) |
| P-Glycoprotein Inhibition | 0.8756(-) | 0.9682(-) | 0.9458(-) | 0.8756(-) | 0.8091(-) |
| AMES Toxicity | 0.7392(-) | 0.9494(-) | 0.9765(-) | 0.7392(-) | 0.8452(-) |
| HERG Inhibition | 0.7860(WI) | 0.9482(WI) | 0.9104(WI) | 0.7860(WI) | 0.9535(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| IUPAC Name | methyl tetradecanoate | 5,5,8*a*-trimethyl-3,6,7,8-tetrahydro-2*H*-chromene | 5,5,8*a*-trimethyl-3,6,7,8-tetrahydro-2*H*-chromene | 7,11,15-trimethyl-3-methylidenehexadec-1-ene | 6,10,14-trimethylpentadecan-2-one | (*E*)-3,7,11,15-tetramethylhexadec-2-en-1-ol |
| Molecular Weight | 242.403 | 180.291 | 180.291 | 278.524 | 268.485 | 296.539 |
| Log P | 4.8605 | 3.3019 | 3.3019 | 7.1677 | 6.0145 | 6.3641 |
| Surface Area | 107.124 | 81.166 | 81.166 | 128.294 | 121.105 | 133.778 |
| Blood Brain Barrier | 1.0000(+) | 0.9661(+) | 0.9661(+) | 0.9962(+) | 1.0000(+) | 0.9919(+) |
| Human Intestinal Absorption | 0.9543(+) | 0.9828(+) | 0.9828(+) | 0.9866(+) | 0.9822(+) | 0.9846(+) |
| P-Glycoprotein Inhibition | 0.9147(-) | 0.9747(-) | 0.9747(-) | 0.8692(-) | 0.8932(-) | 0.8620(-) |
| AMES Toxicity | 0.9765(-) | 0.9237 | 0.9237 | 0.9494(-) | 0.9413(-) | 0.9132(-) |
| HERG Inhibition | 0.9104(WI) | 0.7988(WI) | 0.7690(WI) | 0.8212(WI) | 0.8212(WI) | 0.7838(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |  |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | (*E*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | methyl hexadecanoate | [(1*R*,5*S*)-8-methyl-8-azabicyclo[3.2.1]octan-3-yl] benzoate | methyl (10*E*,12*Z*)-octadeca-10,12-dienoate | methyl (8*E*,11*E*,14*E*)-docosa-8,11,14-trienoate |
| Molecular Weight | 296.539 | 270.457 | 245.322 | 294.479 | 348.571 |
| Log P | 6.3641 | 5.6407 | 2.4686 | 5.9729 | 7.3093 |
| Surface Area | 133.778 | 119.853 | 107.739 | 131.204 | 155.974 |
| Blood Brain Barrier | 0.9919(+) | 1.0000(+) | 0.8952(+) | 0.9958(+) | 0.9958(+) |
| Human Intestinal Absorption | 0.9846(+) | 0.9543(+) | 0.9950(+) | 0.9795(+) | 0.9567(+) |
| P-Glycoprotein Inhibition | 0.8620(-) | 0.8550(-) | 0.9497(-) | 0.7120(-) | 0.6245(+) |
| AMES Toxicity | 0.9132(-) | 0.9765(-) | 0.7111(-) | 0.9321(-) | 0.9321(-) |
| HERG Inhibition | 0.7838(WI) | 0.9104(WI) | 0.8037(WI) | 0.8861(WI) | 0.8861(WI) |
| Hepatotoxicity | **No** | **No** | **Yes** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | (*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | methyl octadecanoate | (*Z*)-octadec-9-enamide | octadecanamid | 5-methyl-5-(4,8,12-trimethyltridecyl)oxolan-2-one |
| Molecular Weight | 296.539 | 298.511 | 281.484 | 283.5 | 324.549 |
| Log P | 6.3641 | 6.4209 | 5.5092 | 5.7332 | 6.5212 |
| Surface Area | 133.778 | 132.583 | 125.755 | 126.445 | 144.307 |
| Blood Brain Barrier | 0.9919(+) | 1.0000(+) | 0.9969(+) | 1.0000(+) | 0.9663(+) |
| Human Intestinal Absorption | 0.9846(+) | 0.9543(+) | 0.9186(+) | 0.8804(+) | 0.9695(+) |
| P-Glycoprotein Inhibition | 0.8620(-) | 0.8222(-) | 0.8555(-) | 0.8968(-) | 0.8478(-) |
| AMES Toxicity | 0.9132(-) | 0.9765(-) | 0.9131(-) | 0.9545(-) | 0.9290(-) |
| HERG Inhibition | 0.7838(WI) | 0.9104(WI) | 0.9685(WI) | 0.9758(WI) | 0.9278(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | methyl 8-[2-[[2-[(2-ethylcyclopropyl)methyl]cyclopropyl]methyl]cyclopropyl]octanoate | (*Z*)-octadec-9-enamide | dimethyl (*Z*)-hex-3-enedioate | (6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene | 2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol |
| Molecular Weight | 334.544 | 281.484 | 172.18 | 410.73 | 416.69 |
| Log P | 5.9886 | 5.5092 | 0.6688 | 10.605 | 8.53184 |
| Surface Area | 148.661 | 125.755 | 71.154 | 189.185 | 186.362 |
| Blood Brain Barrier | 0.9939(+) | 0.9969(+) | 0.9861(+) | 0.9962(+) | 0.9909(+) |
| Human Intestinal Absorption | 0.9838(+) | 0.9186(+) | 0.9205(+) | 0.9206(+) | 0.9962(+) |
| P-Glycoprotein Inhibition | 0.7080(-) | 0.8555(-) | 0.9757(-) | 0.6611(+) | 0.7993(-) |
| AMES Toxicity | 0.9163(-) | 0.9131(-) | 0.6971(-) | 0.9518(-) | 0.9132(-) |
| HERG Inhibition | 0.9007(WI) | 0.9685(WI) | 0.9582(WI) | 0.7689(WI) | 0.7192(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | (2*R*)-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-ol | [(2*R*)-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-yl] acetate | 3-methoxy-10,13-dimethyl-17-(6-methylheptan-2-yl)-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthrene | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(*E*,2*R*,5*S*)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(2*R*,5*R*)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol |
| Molecular Weight | 430.717 | 472.754 | 400.691 | 412.702 | 414.718 |
| Log P | 8.84026 | 9.05996 | 8.0428 | 7.8008 | 8.0248 |
| Surface Area | 192.727 | 209.938 | 180.993 | 186.349 | 187.039 |
| Blood Brain Barrier | 0.9909(+) | 0.9166(+) | 0.9580(+) | 0.9247(+) | 0.9247(+) |
| Human Intestainal Absorption | 0.9962(+) | 0.9949(+) | 0.9931(+) | 0.9914(+) | 0.9930(+) |
| P-Glycoprotein Inhibition | 0.9166(-) | 0.5061(-) | 0.4706(-) | 0.4322(-) | 0.5000(-) |
| AMES Toxicity | 0.9132(-) | 0.9275(-) | 0.9075(-) | 0.9132(-) | 0.9132(-) |
| HERG Inhibition | 0.7192(WI) | 0.8849(WI) | 0.6679(WI) | 0.8027(WI) | 0.8027(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| IUPAC Name | (4*aS*,6*aR*,6*bS*,8*aR*,12*aR*,14*aR*,14*bS*)-4,6*a*,6*b*,8*a*,11,11,14*b*-heptamethyl-2,4*a*,5,6,7,8,9,10,12,12*a*,14,14*a*-dodecahydro-1*H*-picene | [(9*R*)-3*a*,5*a*,5*b*,8,8,11*a*-hexamethyl-1-prop-1-en-2-yl-1,2,3,4,5,6,7,7*a*,9,10,11,11*b*,12,13,13*a*,13*b*-hexadecahydrocyclopenta[a]chrysen-9-yl] acetate | (4*aS*,6*aR*,6*bS*,8*aR*,12*aR*,14*aR*,14*bS*)-4,6*a*,6*b*,8*a*,11,11,14*b*-heptamethyl-2,4*a*,5,6,7,8,9,10,12,12*a*,14,14*a*-dodecahydro-1*H*-picene | (1*R*,3*aR*,5*aR*,5*bR*,7*aR*,11*aR*,11*bR*,13*aR*,13*bR*)-3*a*,5*a*,5*b*,8,8,11*a*-hexamethyl-1-prop-1-en-2-yl-2,3,4,5,6,7,7*a*,10,11,11*b*,12,13,13*a*,13*b*-tetradecahydro-1*H*-cyclopenta[a]chrysen-9-one |
| Molecular Weight | 394.687 | 468.766 | 394.687 | 424.713 |
| Log P | 8.7281 | 8.5956 | 8.7281 | 8.233 |
| Surface Area | 180.549 | 209.609 | 180.549 | 191.765 |
| Blood Brain Barrier | 0.9873(+) | 0.8324(+) | 0.9873(+) | 0.9767(+) |
| Human Intestinal Absorption | 0.9819(+) | 0.9906(+) | 0.9819(+) | 0.9914(+) |
| P-Glycoprotein Inhibition | 0.6221(-) | 0.5172(-) | 0.6221(-) | 0.6975(-) |
| AMES Toxicity | 0.8433(-) | 0.9560(-) | 0.8433(-) | 0.9620(-) |
| HERG Inhibition | 0.8724(WI) | 0.8983(WI) | 0.8724(WI) | 0.8295(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** |

**Table S7.2:** An ADMET properties of phytochemicals derived from *P. integerrima* fruits extract.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 3-hydroxy-10,13-dimethylspiro[1,2,3,4,7,8,9,11,12,14,15,16-dodecahydrocyclopenta[a]phenanthrene-17,2'-cyclobutane]-1'-one | butyl acetate | 4-(methoxymethyl)phenol | methyl (*Z*)-*N*-hydroxybenzenecarboximidate | propane-1,2,3-triol |
| Molecular Weight | 328.50 | 116.16 | 138.17 | 151.16 | 92.09 |
| LogP | 4.6594 | 1.3496 | 1.5386 | 1.4688 | -1.6681 |
| Surface Area | 145.640 | 49.839 | 1.5386 | 64.918 | -1.6681 |
| Blood Brain Barrier | 0.3250(-) | 1.0000(+) | 0.9644(+) | 0.9822(+) | 0.8929(-) |
| Human Intestinal Absorption | 0.9871(+) | 0.9543(+) | 0.9860(+) | 0.9960(+) | 0.8011(+) |
| P-Glycoprotein Inhibition | 0.8513(-) | 0.9871(-) | 0.9898(-) | 0.9838(-) | 0.9856(-) |
| AMES Toxicity | 0.9268(-) | 0.9363(-) | 0.9223(-) | 0.5000 | 0.8278(-) |
| HERG Inhibition | 0.9223(WI) | 0.9620(WI) | 0.7191(WI) | 0.9913(WI) | 0.9670(WI) |
| Hepatotoxicity | **Yes** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 8-methyl-8-azabicyclo[3.2.1]octan-3-ol | 8-methyl-8-azabicyclo[3.2.1]octan-3-ol | 2,4-di*tert*-butylphenol | (2*R*,3*S*,4*S*,5*R*,6*R*)-2-(hydroxymethyl)-6-octoxyoxane-3,4,5-triol | 6-(hydroxymethyl)-5-methoxyoxane-2,3,4-triol |
| Molecular Weight | 141.21 | 141.21 | 206.33 | 292.37 | 194.18 |
| LogP | 0.6039 | 0.6039 | 3.9872 | 0.1634 | -2.5673 |
| Surface Area | 0.6039 | 61.836 | 93.145 | 119.882 | 75.327 |
| Blood Brain Barrier | 0.9827(+) | 0.9827(+) | 0.9946(+) | 0.9084(+) | 0.8193(+) |
| Human Intestinal Absorption | 0.9166(+) | 0.9166(+) | 0.9928(+) | 0.9695(-) | 0.9252(-) |
| P Glycoprotein Inhibition | 0.9869(-) | 0.9869(-) | 0.9682(-) | 0.9311(-) | 0.9668(-) |
| AMES Toxicity | -0.755 (-) | 0.7551(-) | 0.9494(-) | 0.8908(-) | 0.6704(-) |
| HERG Inhibition | 0.7328(WI) | 0.7328(WI) | 0.9482(WI) | 0.8624(WI) | 0.9478(WI) |
| Hepatotoxicity | Yes | Yes | No | No | No |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 2-[2-[2-(3-trimethylsilylpropoxy)ethoxy]ethoxy]ethanol | Silane, [(1,1-dimethyl-2-propenyl)oxy]dimethyl- | methyl hexadecanoate | methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate | methyl (*Z*)-octadec-6-enoate |
| Molecular Weight | 264.44 | 143.28 | 270.46 | 294.48 | 296.50 |
| LogP | 1.7568 | 2.22 | 5.6407 | 5.9729 | 6.1969 |
| Surface Area | 106.269 | 1.368 | 119.853 | 131.204 | 131.894 |
| Blood Brain Barrier | 0.9725(+) | 0.9931(+) | 1.0000(+) | 0.9958(+) | 0.9958(+) |
| Human Intestinal Absorption | 0.9177(+) | 0.9777(+) | 0.9543(+) | 0.9567(+) | 0.9567(+) |
| P Glycoprotein Inhibition | 0.9347(-) | 0.9794(-) | 0.8550(-) | 0.7265(-) | 0.7542(-) |
| AMES Toxicity | 0.8236(-) | 0.8573(-) | 0.9765(-) | 0.9321(-) | 0.9321(-) |
| HERG Inhibition | 0.9582(WI) | 0.9255(WI) | 0.9104(WI) | 0.8861(WI) | 0.8861(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | methyl octadecanoate | octadecanamide | (*Z*)-octadec-9-enamide | dotriacontane | 1-iodotriacontane |
| Molecular Weight | 298.51 | 283.5 | 281.484 | 450.88 | 548.722 |
| LogP | 6.4209 | 5.7332 | 5.5092 | 12.73 | 12.3641 |
| Surface Area | 132.583 | 126.445 | 125.755 | 1.368 | 212.584 |
| Blood Brain Barrier | 1.0000(+) | 1.0000(+) | 0.9969(+) | 1.0000(+) | 1.0000(+) |
| Human Intestinal Absorption | 0.9543(+) | 0.8804(+) | 0.9186(+) | 0.8865(+) | 0.8662(+) |
| P Glycoprotein Inhibition | 0.8222(-) | 0.8968(-) | 0.8555(-) | 0.7551(-) | 0.8320(-) |
| AMES Toxicity | 0.9104(-) | 0.9545(-) | 0.9131(-) | 0.996 | 0.9550(-) |
| HERG Inhibition | 0.9104(WI) | 0.9758(WI) | 0.9685(WI) | 0.8620(WI) | 0.8538(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

**Table S7.3:** An ADMET properties of phytochemicals derived from *P. odorifer* leaves extract.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 3-*tert*-butyl-4-methoxycyclohexan-1-o | 4-(methoxymethyl)phenol | 3,3-dimethoxybutan-2-one | undecane | 6-methylheptan-1-ol |
| Molecular Weight | 186.29 | 138.17 | 132.16 | 156.31 | 130.23 |
| Log P | 2.21 | 1.54 | 0.58 | 4.54 | 2.20 |
| Surface Area | 81.291 | 1.368 | 54.953 | 72.389 | 58.088 |
| Blood Brain Barrier | 0.9511(+) | 0.9644(+) | 0.9953(+) | 1.0000(+) | 0.9973(+) |
| Human intestinal Absorption | 0.9861(+) | 0.9860(+) | 0.9250(+) | 0.8865(+) | 0.9801(+) |
| P-Glycoprotein Inhibition | 0.9503(-) | 0.9898(-) | 0.9787(-) | 0.9631(-) | 0.9814(-) |
| AMES Toxicity | 0.7018(-) | 0.9600(-) | 0.7500(-) | 1.0000(-) | 0.9400(-) |
| HERG Inhibition | 0.9104(WI) | 0.6938(WI) | 0.7933(WI) | 0.6573(WI) | 0.6547(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 2,4-di*tert*-butylpheno | (2*R*,3*S*,4*R*,5*R*)-2,4,5,6-tetrahydroxy-3-methoxyhexanal | 6-hydroxy-4,4,7*a*-trimethyl-6,7-dihydro-5*H*-1-benzofuran-2-one | (2,2,6-trimethyl-9,10-dioxatricyclo[6.2.2.01,6]dodecan-3-yl) acetate | 3-butyl-3-methylcyclohexan-1-one |
| Molecular Weight | 206.33 | 194.18 | 196.25 | 268.35 | 168.28 |
| LogP | 3.99 | -2.72 | 1.41 | 3.00 | 3.33 |
| Surface Area | 93.145 | 75.381 | 83.757 | 114.262 | 75.544 |
| Blood Brain Barrier | 0.9946(+) | 0.2656(-) | 0.9455(+) | 0.9367(+) | 0.9935(+) |
| Human Intestinal Absorption | 0.9928(+) | 0.7517(+) | 0.9864(+) | 0.9102(+) | 0.9652(+) |
| P-Glycoprotein Inhibitor | 0.9682(-) | 0.9629(-) | 0.9542(-) | 0.8378(-) | 0.9732(-) |
| AMES Toxicity | 0.8900(-) | 0.8100(-) | 0.6500(-) | 0.7479(-) | 0.8100(-) |
| HERG Inhibition | 0.7498(WI) | 0.6204(WI) | 0.8336(WI) | 0.5414(WI) | 0.6592(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 3-methyl-4-(2,2,6-trimethylcyclohexyl)butan-2-ol | 7,11,15-trimethyl-3-methylidenehexadec-1-ene | 6,10,14-trimethylpentadecan-2-one | (*E*)-3,7,11,15-tetramethylhexadec-2-en-1-ol | 7,11,15-trimethyl-3-methylidenehexadec-1-ene |
| Molecular Weight | 212.38 | 278.52 | 268.48 | 296.54 | 278.52 |
| Log P | 3.86 | 7.17 | 6.01 | 6.36 | 7.17 |
| Surface Area | 95.272 | 128.294 | 121.105 | 133.778 | 128.294 |
| Blood Brain Barrier | 1.0000(+) | 0.9962(+) | 1.0000(+) | 0.9919(+) | 0.9962(+) |
| Human Intestinal Absorption | 0.9849(+) | 0.9866(+) | 0.9822(+) | 0.9846(+) | 0.9866(+) |
| P-Glycoprotein Inhibitor | 0.9325(-) | 0.8692(-) | 0.8932(-) | 0.8620(-) | 0.8692(-) |
| AMES Toxicity | 0.8700(-) | 0.8400(-) | 0.9300(-) | 0.8400(-) | 0.8400(-) |
| HERG Inhibition | 0.7166(WI) | 0.5105(WI) | 0.5963(WI) | 0.4331(WI) | 0.5105(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | methyl hexadecanoate | methyl 3-(3,5-di*tert*-butyl-4-hydroxyphenyl)propanoate | methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate | methyl (8*E*,11*E*,14*E*)-docosa-8,11,14-trienoate | (*E*,7*R*,11*R*)-3,7,11,15-tetramethylhexadec-2-en-1-ol |
| Molecular Weight | 270.46 | 292.42 | 294.48 | 348.57 | 296.54 |
| Log P | 5.64 | 4.09 | 5.97 | 7.31 | 6.36 |
| Surface Area | 119.853 | 127.880 | 131.204 | 131.204 | 133.778 |
| Blood Brain Barrier | 1.0000(+) | 0.9102(+) | 0.9958(+) | 0.9958(+) | 0.9919(+) |
| Human Intestinal Absorption | 0.9543(+) | 0.9918(+) | 0.9567(+) | 0.9567(+) | 0.9846(+) |
| P-glycoprotein Inhibitor | 0.8550(-) | 0.9272(-) | 0.7265(-) | 0.6245(+) | 0.8620(-) |
| AMES Toxicity | 0.9900(-) | 0.9200(-) | 0.8200(-) | 0.8200(-) | 0.8400(-) |
| HERG Inhibition | 0.4084(WI) | 0.6593(WI) | 0.6775(WI) | 0.7877(WI) | 0.4331(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | methyl octadecanoate | (*Z*)-octadec-9-enamide | tetradecanamide | (1*R*,6*R*)-3-methyl-6-propan-2-ylcyclohex-2-en-1-ol | (2*E*,13*E*)-12-methyloctadeca-2,13-dien-1-ol |
| Molecular Weight | 298.51 | 281.48 | 227.39 | 154.25 | 280.50 |
| LogP | 6.42 | 5.51 | 4.17 | 2.36 | 6.04 |
| Surface Area | 132.583 | 125.755 | 100.985 | 69.123 | 126.723 |
| Blood Brain Barrier | 1.0000(+) | 0.9969(+) | 1.0000(+) | 0.9751(+) | 1.0000(+) |
| Human Intestinal Absorption | 0.9543(+) | 0.9186(+) | 0.8804(+) | 0.9859(+) | 0.9807(+) |
| P-Glycoprotein Inhibitor | 0.8222(-) | 0.8555(-) | 0.9491(-) | 0.9755(-) | 0.7970(-) |
| AMES Toxicity | 0.9900(-) | 0.8900(-) | 1.0000(-) | 0.8600(-) | 0.7900(-) |
| HERO Inhibition | 0.5865(WI) | 0.6754(WI) | 0.5000(WI) | 0.5673(WI) | 0.7006(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | (*Z*)-octadec-9-enamide | octatriacontyl 2,2,3,3,3-pentafluoropropanoate | tetracontane | hexadecanal | bis(2-ethylhexyl) benzene-1,2-dicarboxylate |
| Molecular Weight | 281.48 | 697.06 | 563.10 | 240.43 | 390.56 |
| LogP | 5.51 | 15.79 | 15.85 | 5.67 | 6.43 |
| Surface Area | 125.755 | 293.440 | 256.972 | 108.375 | 170.550 |
| Blood Brain Barrier | 0.9969(+) | 0.9938(+) | 1.0000(+) | 1.0000(+) | +0.9839(+) |
| Human Intestinal Absorption | 0.9186(+) | 0.9702(+) | 0.8865(+) | 0.9086(+) | 1.0000(+) |
| P-Glycoprotein Inhibitor | 0.8555(-) | 0.5866(+) | 0.7233(-) | 0.9272(-) | 0.7262(+) |
| AMES Toxicity | 0.8900(-) | 0.9100(-) | 1.0000(-) | 0.9900(-) | 1.0000(-) |
| HERG Inhibition | 0.6754(WI) | 0.3741(WI) | 0.7800(WI) | 0.3955(WI) | 0.8276((WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | (6*E*,10*E*,14*E*,18*E*)-2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene | 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol | hexatriaconta-15,17,19,21-tetrayne | (2*R*)-6-methoxy-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromene | 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-ol |
| Molecular Weight | 410.73 | 430.72 | 490.86 | 444.74 | 430.72 |
| LogP | 10.60 | 8.84 | 11.18 | 9.14 | 8.84 |
| Surface Area | 189.185 | 192.727 | 227.509 | 199.411 | 192.727 |
| Blood Brain Barrier | 0.9962(+) | 0.9909(+) | 1.0000(+) | 0.9783(+) | 0.9909(+) |
| Human Intestinal Absorption | 0.9206(+) | 0.9962(+) | 0.8637(+) | 0.9974(+) | 0.9962(+) |
| P-Glycoprotein Inhibitor | 0.6611(+) | 0.9166(-) | 0.5798(-) | 0.6900(-) | 0.9166(-) |
| AMES Toxicity | 0.9700(-) | 0.8600(-) | 0.9900(-) | 0.7500(-) | 0.8600(-) |
| HERG Inhibition | 0.6962(WI) | 0.6483(WI) | 0.7606(WI) | 0.7437(WI) | 0.6483(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| IUPAC Name | (2*R*)-2,5,7,8-tetramethyl-2-[(4*R*,8*R*)-4,8,12-trimethyltridecyl]-3,4-dihydrochromen-6-ol | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(*E*,2*R*,5*S*)-5-ethyl-6-methylhept-3-en-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-o | (3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-[(2*R*,5*S*)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1*H*-cyclopenta[a]phenanthren-3-ol | (4*aR*,6*aR*,6*bS*,8*aR*,12*aR*,14*aR*,14*bR*)-4,4,6*a*,6*b*,11,11,14*b*-heptamethyl-1,2,4*a*,5,6,7,8,8*a*,9,10,12,12*a*,14,14*a*-tetradecahydropicen-3-one |
| Molecular Weight | 430.72 | 412.70 | 414.72 | 410.69 |
| LogP | 8.84 | 7.80 | 8.02 | 7.99 |
| Surface Area | 192.727 | 186.349 | 187.039 | 185.400 |
| Blood Brain Barrier | 0.9909(+) | 0.9247(+) | 0.9247(+) | 0.9677(+) |
| Human Intestinal Absorption | 0.9962(+) | 0.9914(+) | 0.9930(+) | 0.9902(+) |
| P-Glycoprotein Inhibitor | 0.9166(-) | 0.4322(-) | 0.5000(-) | 0.6210(-) |
| AMES Toxicity | 0.8600(-) | 0.8300(-) | 0.8700(-) | 0.8000(-) |
| HERG Inhibition | 0.6483(WI) | 0.6568(WI) | 0.4632(WI) | 0.4327(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** |

**Supplementary Table-7.4:** An ADMET properties of phytochemicals derived from *P. odorifer* fruits extract.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 4-hydroxy-3-methylbutan-2-one | 4-nitro-1,2,5-oxadiazol-3-amine | *N*-(furan-2-ylmethyl)cyclohexanecarboxamide | butyl acetate | 4-(methoxymethyl)pheno |
| Molecular Weight | 102.13 | 130.06 | 207.27 | 116.16 | 138.17 |
| Log P | 0.20 | -0.44 | 6.1244 | 1.35 | 1.54 |
| Surface Area | 43.155 | 48.561 | 131.709 | 49.839 | 60.069 |
| Blood Brain Surface | 0.9967(+) | 0.9823(+) | 0.9947(+) | 1.0000 (+) | 0.9644(+) |
| Human Intestinal Absorption | 0.9779(+) | 0.9741(+) | 0.9021(+) | 0.9543(+) | 0.9860(+) |
| P-Glycoprotein Inhibitor | 0.9860(-) | 0.9708(-) | 0.9744(-) | 0.9871(-) | 0.9898(-) |
| AMES Toxicity | 0.8800(-) | 0.7500(+) | 0.8200(-) | 0.9700(-) | 0.9600 (-) |
| HERO Inhibition | 0.7976(WI) | 0.6769(WI) | 0.6655(WI) | 0.7401(WI) | 0.6938(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | methylsulfanyl(methylsulfinyl)methane | cyclopent-2-en-1-one | 1,4-dioxane-2,3-diol | 3,3-dimethoxybutan-2-one | *tert*-butyl-dimethyl-[(3-methylphenyl)methoxy]silane |
| Molecular Weight | 124.23 | 82.10 | 120.10 | 132.16 | 236.431 |
| Log P | 0.69 | 0.91 | -1.33 | 0.58 | 4.51682 |
| Surface Area | 44.966 | 36.665 | 46.644 | 54.953 | 100.969 |
| Blood Brain Barrier | 0.9812(+) | 0.9855(+) | 0.9268(+) | 0.9953(+) | 0.9924(+) |
| Human intestinal Absorption | 0.8843(+) | 0.9692(+) | 0.9126(+) | 0.9250(+) | 0.9899(+) |
| P - Glycoprotein Inhibition | 0.9785(-) | 0.9895(-) | 0.9779(-) | 0.9787(-) | 0.9429(-) |
| AMES Toxicity | 0.6700(-) | 0.8500(-) | 0.5800(+) | 0.7500(-) | 0.7800(-) |
| HERO Inhibition | 0.7688(WI) | 0.8326(WI) | 0.7187(WI) | 0.7933(WI) | 0.4561(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 2,2-diethoxyethanol | (2*S*,4*R*)-pentane-1,2,3,4,5-pentol | cyclopentane-1,2-dione | propane-1,2,3-triol | undecane |
| Molecular Weight | 134.175 | 152.15 | 98.10 | 92.09 | 156.31 |
| Log P | 0.3778 | -2.95 | 0.31 | -1.67 | 4.54 |
| Surface Area | 55.585 | 58.170 | 41.516 | 35.852 | 66.024 |
| Blood Brain Barrier | 0.9825(+) | 0.9930(-) | 0.9734(+) | 0.8929(-) | 1.0000(+) |
| Human intestinal Absorption | 0.8550(+) | 0.8011(+) | 0.9678(+) | 0.8011(+) | 0.8865(+) |
| P-Glycoprotein Inhibition | 0.9791(-) | 0.9823(-) | 0.9818(-) | 0.9856 | 0.9631(-) |
| AMES Toxicity | 0.8700(-) | 0.9600(-) | 0.5800(+) | 0.9000(-) | 1.0000(-) |
| HERO Inhibition | 0.7057(WI) | 0.5587(WI) | 0.7923(WI) | 0.6318(WI) | 0.6573(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 4-methyl-2,3-dihydropyran-6-one | undecane-3,6-dione | 2,3-dihydro-1-benzofuran | (2*R*,3*R*,4*R*,5*R*)-2-methoxyoxane-3,4,5-triol | 3,5-di*tert*-butylpheno |
| Molecular Weight | 112.13 | 184.279 | 120.15 | 164.16 | 206.33 |
| Log P | 0.88 | 2.8951 | 1.62 | -1.93 | 3.99 |
| Surface Area | 48.144 | 80.712 | 54.269 | 64.168 | 93.145 |
| Blood Brain Barrier | 0.9190(+) | 1.0000(+) | 0.9900(+) | 0.8304(+) | 0.9961(+) |
| Human Intestinal absorption | 0.9901(+) | 0.9508(+) | 0.9911(+) | 0.9569(-) | 0.9928(+) |
| 1. Glycoprotein Inhibition | 0.9893(-) | 0.9530(-) | 0.9920(-) | 0.9729(-) | 0.9405(-) |
| AMES Toxicity | 0.6300(-) | 0.9100(-) | 0.6400(-) | 0.6500(+) | 0.9100(-) |
| HERO Inhibition | 0.8104(WI) | 0.5981(WI) | 0.6335(WI) | 0.6859(WI) | 0.6908(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | (2*R*,3*R*,4*S*,5*R*,6*S*)-2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol | decyl propan-2-yl sulfite | 1-iodohexadecane | 1-ethylazepane | methyl hexadecanoate |
| Molecular Weight | 194.183 | 264.431 | 226.448 | 127.231 | 270.457 |
| Log P | -2.5673 | 4.1474 | 6.4876 | 1.8823 | 5.6407 |
| Surface area | 75.327 | 109.138 | 104.213 | 58.048 | 119.853 |
| Blood Brain Barrier | 0.8193(+) | 0.9808(+) | 1.0000(+) | 0.9960(+) | 1.0000(+) |
| Human intestinal Absorption | 0.9782(-) | 0.9538(+) | 0.8865(+) | 0.9634(+) | 0.9543(+) |
| P-Glycoprotein Inhibitor | 0.9612(-) | 0.9060(-) | 0.9287(-) | 0.9899(-) | 0.8550(-) |
| AMES Toxicity | 0.7500(-) | 0.9200(-) | 0.9300(-) | 0.6200(-) | 0.9900(-) |
| HERO Inhibition | 0.5371(WI) | 0.7186(WI) | 0.5618(WI) | 0.5865(WI) | 0.4084(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **Yes** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | methyl (9*Z*,12*Z*)-octadeca-9,12-dienoate | methyl (*E*)-octadec-9-enoate | methyl octadecanoate | (*Z*)-octadec-9-enamide | tetradecanamide |
| Molecular weight | 270.457 | 296.495 | 298.511 | 281.484 | 227.392 |
| Log P | 5.6407 | 6.1969 | 6.4209 | 5.5092 | 4.1728 |
| Surface Area | 119.853 | 131.894 | 132.583 | 125.755 | 100.985 |
| Blood Brain Barrier | 1.0000(+) | 0.9958(+) | 1.0000(+) | 0.9969(+) | 1.0000(+) |
| Human intestinal Absorption | 0.9543(+) | 0.9567(+) | 0.9543(+) | 0.9186(+) | 0.8804(+) |
| P-Glycoprotein Inhibitor | 0.8550(-) | 0.7372(-) | 0.8222(-) | 0.8555(-) | 0.9491(-) |
| AMES Toxicity | 0.8200(-) | 0.9500(-) | 0.9900(-) | 0.8900(-) | 1.0000(-) |
| HERO Inhibition | 0.6775(WI) | 0.6787(WI) | 0.5865(WI) | 0.6754(WI) | 0.5000(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 2,4-dimethylundecane | 2,6,11-trimethyldodecane | (*Z*)-octadec-9-enamide | 11-methyltricosane | 2-(3-ethyl-3,6,10,13,14-pentamethylpentadecyl)-1,1,3,6-tetramethylcyclohexane |
| Molecular Weight | 184.367 | 212.421 | 281.484 | 338.664 | 448.864 |
| Log P | 5.0291 | 5.6652 | 5.5092 | 9.4643 | 11.1863 |
| Surface Area | 85.119 | 97.848 | 125.755 | 155.133 | 205.047 |
| Blood Brain Barrier | 1.0000(+) | 1.0000(+) | 0.9969(+) | 1.0000(+) | 1.0000(+) |
| Human intestinal Absorption | 0.9588(+) | 0.9588(+) | 0.9186(+) | 0.9588(+) | 0.9692(+) |
| P-Glycoprotein Inhibition | 0.9342(-) | 0.9354(-) | 0.8555(-) | 0.7720(-) | 0.4934(-) |
| AMES Toxicity | 0.9800(-) | 0.9000(-) | 0.8900(-) | 1.0000(-) | 0.7800(-) |
| HERO Inhibition | 0.7073(WI) | 0.6567(WI) | 0.6754(WI) | 0.8160(WI) | 0.4136(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | nonacos-1-ene | 4-*O*-decan-2-yl 1-*O*-nonadecyl (*E*)-but-2-enedioate | (*Z*)-5-methyldocos-5-ene | methyl 6,6-dimethyl-4-morpholin-4-yl-2-oxocyclohex-3-ene-1-carboxylate | (2*E*,6*E*,10*E*)-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraen-1-ol |
| Molecular Weight | 406.783 | 522.855 | 322.621 | 267.325 | 290.49 |
| Log P | 11.334 | 10.4197 | 8.9943 | 0.9907 | 6.12 |
| Surface Area | 186.268 | 230.278 | 148.078 | 113.092 |  |
| Blood Brain Barrier | 1.0000(+) | 0.9928(+) | 0.9966(+) | 0.9532(+) | 0.9919(+) |
| Human intestinal Absorption | 0.9206(+) | 0.9928(+) | 0.9206(+) | 0.9685(+) | 0.9681(+) |
| P-Glycoprotein Inhibitor | 0.8309(-) | 0.6153(+) | 0.8043(-) | 0.8778(-) | 0.7547(-) |
| AMES Toxicity | 1.0000(-) | 0.9300(-) | 0.9600(-) | 0.6400(-) | 0.8700(-) |
| HERO Inhibitor | 0.5072(WI) | 0.6938(WI) | 0.4593(WI) | 0.4362(WI) | 0.7540(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | **No** |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC Name | 4-methylpentadecane | butyl tetradecane-6-sulfonate | (1-methylpiperidin-3-yl) 2,2-bis(3,4-dimethoxyphenyl)-2-hydroxyacetate | hexacontane | bis(2-ethylhexyl) benzene-1,2-dicarboxylate |
| Molecular Weight | 226.44 | 334.566 | 445.512 | 843.636 | 390.564 |
| Log p | 6.3435 | 5.8324 | 2.5943 | 23.652 | 6.433 |
| Surface Area | 104.213 | 138.891 | 188.145 | 384.271 | 170.550 |
| Blood Brain Barrier | 1.0000(+) | 0.9839(+) | 0.8611(+) | 1.0000(+) | 0.9839(+) |
| Human intestinal Absorption | 0.958(+) | 0.8718(+) | 0.9869(+) | 0.8865(+) | 1.0000(+) |
| P-Glycoprotein Inhibitor | 0.9143(-) | 0.8718(-) | 0.7144(+) | 0.7233(-) | 0.7262(+) |
| AMES Toxicity | 1.0000(-) | 0.8800(-) | 0.8000(-) | 1.0000(-) | 1.0000(-) |
| HERO Inhibitor | 0.5508(WI) | 0.5607(WI) | 0.6942(WI) | 0.7800(WI) | 0.8276(WI) |
| Hepatotoxicity | **No** | **No** | **No** | **No** | No |