**Supplementary File**

**Table 1** Thirty (30) test compounds of propolis *Tetragonula sapiens* from South Sulawesi

| **Code** | **Name** | **Chemical Formula** | **Molecular Weight (g/mol)** | **SMILES\*** |
| --- | --- | --- | --- | --- |
| PS01 | L-(+)-Valinol | C5H13NO | 103.16 | CC(C)[C@H](N)CO |
| PS02 | 1,2,2-Trimethyl-3-[(4-methylphenyl) carbamoyl] cyclopentanecarboxylic acid | C17H23NO3 | 289.37 | CC1=CC=C(NC(=O)C2CCC(C)(C(O)=O)C2(C)C)C=C1 |
| PS03 | Linalyl anthranilate | C17H23NO2 | 273.37 | CC(C)=CCCC(C)(OC(=O)C1=C(N)C=CC=C1)C=C |
| PS04 | Yucalexin B7 | C20H28O2 | 300.44 | CC12CC3(CCC4C(C)(C)CC(=O)CC4(C)C3CC1=O)C=C2 |
| PS05 | Robustaol A | C25H30O9 | 474.50 | COC1=C(C)C(O)=C(CC2=C(O)C(C(=O)CC(C)C)=C(O)C(C=O)=C2O)C(O)=C1C(=O)C(C)C |
| PS06 | 1,5-Dimethyl-4-[[(2-methyl-6-phenylthieno[2,3-d]pyrimidin-4-yl)hydrazinylidene]methyl]pyrrole-2-carbonitrile | C21H18N6S | 386.47 | CN1C(C)=C(C=NNC2=C3C=C(SC3=NC(C)=N2)C2=CC=CC=C2)C=C1C#N |
| PS07 | Kadsurin | C25H30O8 | 458.50 | COC1=C(OC)C(OC)=C2C(C[C@@H](C)[C@@H](C)[C@@H](OC(C)=O)C3=CC4=C(OCO4)C(OC)=C23)=C1 |
| PS08 | 5-Hydroxymethyl tolterodine | C22H31NO2 | 341.49 | CC(C)N(CC[C@H](C1=CC=CC=C1)C1=C(O)C=CC(CO)=C1)C(C)C |
| PS09 | Dulxanthone C | C25H28O6 | 424.49 | COC1=CC(CC=C(C)C)=C2C(=O)C3=C(O)C=C(OC)C(CC=C(C)C)=C3OC2=C1O |
| PS10 | 9'-Carboxy-alpha-tocotrienol | C24H34O4 | 386.52 | C\C(CC\C=C(/C)C(O)=O)=C/CC[C@]1(C)CCC2=C(C)C(O)=C(C)C(C)=C2O1 |
| PS11 | Enokipodin D | C15H18O4 | 262.3 | CC1=CC(=O)C(=CC1=O)[C@@]1(C)[C@H](O)CC(=O)C1(C)C |
| PS12 | Mollicellin H | C21H20O6 | 101 | CC(C)=CCC1=C(C)C2=C(OC3=C(C(C)=CC(O)=C3C=O)C(=O)O2)C=C1O |
| PS13 | Glyurallin B | C25H26O6 | 422.47 | CC(C)=CCC1=CC(=CC(O)=C1O)C1=COC2=C(C(O)=CC(O)=C2CC=C(C)C)C1=O |
| PS14 | ([8]-Paridyl acetate) | C21H32O4 | 348.48 | CCCCCCCCCC(=O)CCC1=CC(OC)=C(OC(C)=O)C=C1 |
| PS15 | Macarangin | C25H26O6 | 422.47 | CC(C)=CCC\C(C)=C\CC1=C(O)C=C2OC(=C(O)C(=O)C2=C1O)C1=CC=C(O)C=C1 |
| PS16 | 3,4-Bis(octyloxy)benzaldehyde | C21H38O3 | 362.55 | CCCCCCCCOC1=C(OCCCCCCCC)C=C(C=O)C=C1 |
| PS17 | Oleandrigenin | C25H36O6 | 432.55 | CC(=O)O[C@H]1C[C@]2(O)[C@@H]3CC[C@@H]4C[C@@H](O)CC[C@]4(C)[C@H]3CC[C@]2(C)[C@H]1C1=CC(=O)OC1 |
| PK01 | Sulabiroin A | C22H22O7 | 398.41 | [H]C12COC[C@]1([H])[C@@H](C1=CC(OC)=C3OCOC3=C1)C1=C(OC)C3=C(OCO3)C=C1C2 |
| PK02 | Sulabiroin B | C23H26O7 | 414.45 | [H]C12COC[C@]1([H])[C@@H](C1=CC(OC)=C3OCOC3=C1)C1=C(OC)C(OC)=C(OC)C=C1C2 |
| PK03 | 2',3'-dihydro-3'-hydroxypapuanic acid | C25H38O7 | 450.57 | CCCCCC(CC(O)=O)C1=C(O)C2=C(O[C@H](C)[C@@H](C)C2=O)C(CCC(C)(C)O)=C1OC |
| PK04 | (–)-papuanic acid | C25H36O6 | 432.55 | CCCCCC(CC(O)=O)C1=C(O)C2=C(O[C@H](C)[C@@H](C)C2=O)C(CC=C(C)C)=C1OC |
| PK05 | (–)-isocalolongic acid | C23H32O6 | 404.50 | CCCC(CC(O)=O)C1=C(O)C2=C(O[C@H](C)[C@@H](C)C2=O)C(CC=C(C)C)=C1OC |
| PK06 | isopapuanic acid | C25H36O6 | 432.55 | CCCCCC(CC(O)=O)C1=C(O)C2=C(O[C@@H](C)[C@@H](C)C2=O)C(CC=C(C)C)=C1OC |
| PK07 | isocalopolyanic acid | C24H32O6 | 416.51 | CCCCCC(CC(O)=O)C1=C(O)C2=C(O[C@H](C)[C@@H](C)C2=O)C2=C1OC(C)(C)C=C2 |
| PK08 | glyasperin A | C25H26O7 | 422.47 | CC(C)=CCC1=CC(=CC=C1O)C1=C(O)C(=O)C2=C(O)C(CC=C(C)C)=C(O)C=C2O1 |
| PK09 | broussoflavonol F | C25H26O7 | 422.47 | CC(C)=CCC1=CC(=CC=C1O)C1=C(O)C(=O)C2=C(O)C=C(O)C(CC=C(C)C)=C2O1 |
| PK10 | (2S)-5,7-dihydroxy-4'-methoxy-8-prenylflavanone | C20H20O5 | 354.40 | COC1=CC=C(C=C1)[C@@H]1CC(=O)C2=C(O)C=C(O)C(CC=C(C)C)=C2O1 |
| PK11 | isorhamnetin | C16H12O7 | 316.26 | COC1=CC(=CC=C1O)C1=C(O)C(=O)C2=C(O)C=C(O)C=C2O1 |
| PK12 | (1'S)-2-trans,4-trans-abscisic acid | C15H20O4 | 264.32 | C\C(\C=C\[C@@]1(O)C(C)=CC(=O)CC1(C)C)=C\C(O)=O |
| PK13 | (1'S)-2-cis,4-trans-abscisic acid | C15H20O4 | 264.32 | C\C(\C=C\[C@@]1(O)C(C)=CC(=O)CC1(C)C)=C/C(O)=O |

Note: PS code = propolis compounds resulted from LC-MS; PK code = propolis compounds identified by Miyata et al. (Miyata et al., 2019, 2020)

\*SMILES: The Simplified Molecular Input Line Entry System (SMILES) is a specification in the form of a line notation for describing the structure of chemical species.

**Table 2** The Assessment of Drug likeness of a Compound Utilizing Lipinski Rule of Five (RO5)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound Code** | **Lipinski RO5 Parameter** | | | | **Meet Lipinski RO5**  **Criteria** |
| **MW (g/mol)** | **LogP** | **H Donor** | **H Acceptor** |
| PS01 | 103.16 | 0.00 | 2 | 2 | Yes |
| PS02 | 289.37 | 3.00 | 2 | 3 | Yes |
| PS03 | 273.37 | 4.83 | 1 | 2 | Yes |
| PS04 | 300.44 | 3.76 | 0 | 2 | Yes |
| PS05 | 474.50 | 5.19 | 5 | 9 | Yes |
| PS06 | 386.47 | 4.76 | 1 | 6 | Yes |
| PS07 | 458.50 | 4.59 | 0 | 8 | Yes |
| PS08 | 341.49 | 4.39 | 2 | 3 | Yes |
| PS09 | 424.49 | 6.6 | 2 | 6 | Yes |
| PS10 | 386.52 | 6.14 | 2 | 4 | Yes |
| PS11 | 262.30 | 0.78 | 1 | 4 | Yes |
| PS12 | 101.00 | 4.9 0 | 2 | 6 | Yes |
| PS13 | 422.47 | 6.16 | 4 | 6 | Yes |
| PS14 | 348.48 | 5.64 | 0 | 4 | Yes |
| PS15 | 422.47 | 6.30 | 4 | 6 | Yes |
| PS16 | 362.55 | 8.10 | 0 | 3 | Yes |
| PS17 | 432.55 | 1.93 | 2 | 6 | Yes |
| PK01 | 398.41 | 3.38 | 0 | 7 | Yes |
| PK02 | 414.45 | 3.51 | 0 | 7 | Yes |
| PK03 | 450.57 | 5.35 | 3 | 7 | Yes |
| PK04 | 432.55 | 6.73 | 2 | 6 | Yes |
| PK05 | 404.50 | 5.64 | 2 | 6 | Yes |
| PK06 | 432.55 | 6.73 | 2 | 6 | Yes |
| PK07 | 416.51 | 5.31 | 2 | 6 | Yes |
| PK08 | 422.47 | 5.75 | 4 | 6 | Yes |
| PK09 | 422.47 | 6.37 | 4 | 6 | Yes |
| PK10 | 354.40 | 4.64 | 2 | 5 | Yes |
| PK11 | 316.26 | 1.87 | 4 | 7 | Yes |
| PK12 | 264.32 | 1.61 | 2 | 4 | Yes |
| PK13 | 264.32 | 1.61 | 2 | 4 | Yes |