**Supplementary Table: S2.** Lipinski Rule of Five (RO5) parameters of the *Ficus sp.* ligands retrieved from IMPPAT database.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sl No** | **Molecule ID** | **Ligands name** | **Total Mol weight** | **cLogP** | **cLogS** | **H-Acceptors** | **H-Donors** | **Rotatable Bonds** |
| **1** | 122130856 | Lupenone | 424.71 | 7.7906 | -6.854 | 1 | 0 | 1 |
| **2** | 101700567 | Glaucanol B acetate | 428.70 | 6.9869 | -6.72 | 2 | 0 | 2 |
| **3** | 76419085 | Bis(acetic acid); tannins | 1821.31 | 5.5312 | -7.599 | 46 | 25 | 31 |
| **4** | 71597391 | Triterpenoids | 472.66 | 3.9528 | -4.838 | 5 | 4 | 1 |
| **5** | 70699351 | Sitosterol glucoside | 576.86 | 6.0181 | -6.369 | 6 | 4 | 9 |
| **6** | 54685921 | Hispidin | 246.22 | 1.0298 | -2.374 | 5 | 3 | 2 |
| **7** | 24832108 | Vitamin P | 610.52 | -1.2573 | -2.398 | 16 | 10 | 6 |
| **8** | 16219576 | 3beta-Hydroxy-20(29)-lupene | 426.73 | 7.6469 | -6.803 | 1 | 1 | 1 |
| **9** | 13818995 | Methyloleanolate | 470.74 | 6.4922 | -6.256 | 3 | 1 | 2 |
| **10** | 12303662 | Phytosterols | 414.72 | 7.8552 | -6.669 | 1 | 1 | 6 |
| **11** | 11583623 | Dehydrotylophorine | 390.46 | 1.3055 | -5.722 | 5 | 0 | 4 |
| **12** | 10813969 | Isoquercitin | 464.38 | -0.3469 | -2.191 | 12 | 8 | 4 |
| **13** | 5742590 | Daucosterol | 576.86 | 6.0181 | -6.369 | 6 | 4 | 9 |
| **14** | 5460957 | Phenylalanine | 166.20 | -2.9932 | -1.541 | 3 | 2 | 3 |
| **15** | 5354133 | Methyl ricinoleate | 312.49 | 6.1252 | -4.28 | 3 | 1 | 16 |
| **16** | 5281697 | Scutellarein | 286.24 | 1.99 | -2.56 | 6 | 4 | 1 |
| **17** | 3286789 | Leucopelargonidin | 290.27 | 1.1284 | -1.512 | 6 | 5 | 1 |
| **18** | 3084839 | Triacontyl acetate | 480.86 | 13.258 | -8.447 | 2 | 0 | 30 |
| **19** | 3084390 | Sorbifolin | 300.27 | 2.2657 | -2.874 | 6 | 3 | 2 |
| **20** | 446611 | 2,4-Dihydroxycinnamic acid | 180.16 | 0.7825 | -1.407 | 4 | 3 | 2 |
| **21** | 440833 | Leucocyanidol | 306.27 | 0.7827 | -1.216 | 7 | 6 | 1 |
| **22** | 345510 | Beta-Amyrin acetate | 468.76 | 7.8252 | -7.063 | 2 | 0 | 2 |
| **23** | 293754 | Amyrin acetate | 468.76 | 7.763 | -7.046 | 2 | 0 | 2 |
| **24** | 244297 | Friedlein | 426.73 | 7.5888 | -6.968 | 1 | 0 | 0 |
| **25** | 240122 | Guaiol acetate | 264.41 | 4.1535 | -3.666 | 2 | 0 | 3 |
| **26** | 225689 | Beta.-amyrin | 426.73 | 7.3406 | -6.653 | 1 | 1 | 0 |
| **27** | 225688 | Alpha.-amyrin | 426.73 | 7.2784 | -6.636 | 1 | 1 | 0 |
| **28** | 189540 | Calotropenyl acetate | 468.76 | 7.8413 | -7.213 | 2 | 0 | 2 |
| **29** | 162506 | Hexadecyl docosanoate | 565.02 | 15.985 | -10.067 | 2 | 0 | 36 |
| **30** | 151467 | 4',5'-dihydropsoralen | 188.18 | 1.7232 | -2.737 | 3 | 0 | 0 |
| **31** | 147362 | 4,6-O-Benzylidene-D-glucose | 268.26 | -1.4439 | -1.282 | 6 | 3 | 4 |
| **32** | 115250 | Taraxasterol | 426.73 | 7.3567 | -6.803 | 1 | 1 | 0 |
| **33** | 101257 | Tirucallol | 426.73 | 8.4216 | -6.453 | 1 | 1 | 4 |
| **34** | 51283 | Dl-alanine-15n | 90.087 | -2.9911 | -0.406 | 3 | 2 | 1 |
| **35** | 26305 | Nodakenetin | 246.26 | 1.8611 | -3.095 | 4 | 1 | 1 |
| **36** | 12410 | Hentriacontane | 436.85 | 14.155 | -8.814 | 0 | 0 | 28 |
| **37** | 12209 | 2-methylbutyl acetate | 130.19 | 1.6622 | -1.587 | 2 | 0 | 4 |
| **38** | 10494 | Oleanolic acid | 456.71 | 6.0643 | -6.128 | 3 | 2 | 1 |
| **39** | 10212 | Imperatorin | 270.28 | 3.5483 | -4.283 | 4 | 0 | 3 |
| **40** | 7963 | 4-methylpyridine | 93.13 | 1.0026 | -1.165 | 1 | 0 | 0 |
| **41** | 6306 | L-isoleucine | 131.17 | -1.864 | -1.106 | 3 | 2 | 3 |
| **42** | 6212 | Chloroform | 119.38 | 1.6348 | -3.509 | 0 | 0 | 0 |
| **43** | 6199 | Psoralen | 186.17 | 1.949 | -3.529 | 3 | 0 | 0 |
| **44** | 4812 | Phylloquinone | 450.70 | 10.145 | -7.516 | 2 | 0 | 14 |
| **45** | 2356 | Vakerin | 328.27 | -1.626 | -0.949 | 9 | 5 | 2 |
| **46** | 2355 | Bergapten | 216.19 | 1.879 | -3.547 | 4 | 0 | 1 |