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| **S.No** | **Codes** | **Structure** | **MMass** | | **SMILES** | **IC50+SD** |
| 1 | FI-3 |  | | 583 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(NN)=O)C(Br)=C3 | 17.44 ± 0.05 |
| 2 | FI-3-1 |  | | 717 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=CC(OC)=C4O)=O)C(Br)=C3 | 16.39 ± 0.79 |
| 3 | FI-3-2 |  | | 761 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC(OC)=C(OC)C(OC)=C4)=O)C(Br)=C3 | 51.32 ± 2.08 |
| 4 | FI-3-4 |  | | 738 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(Cl)C=C4Cl)=O)C(Br)=C3 | 52.45 ± 1.62 |
| 5 | FI-3-5 |  | | 703 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(O)C=C4O)=O)C(Br)=C3 | 31.85 ± 0.06 |
| 6 | FI-3-6 |  | | 731 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(OC)C=C4OC)=O)C(Br)=C3 | 76.07 ± 2.63 |
| 7 | FI-3-7 |  | | 717 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(OC)C(O)=C4)=O)C(Br)=C3 | 20.39 ± 0.30 |
| 8 | FI-3-8 |  | | 716 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=CC([N+]([O-])=O)=C4)=O)C(Br)=C3 | 34.04 ± 0.36 |
| 9 | FI-3-9 |  | | 842 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC(Br)=C(O)C(Br)=C4)=O)C(Br)=C3 | 10.93 ± 0.23 |
| 10 | FI-3-10 |  | | 687 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=CC(O)=C4)=O)C(Br)=C3 | 10.61 ± 0.21 |
| 11 | FI-3-11 |  | | 737 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=C(O)C=CC5=C4C=CC=C5)=O)C(Br)=C3 | 16.25 ± 0.24 |
| 12 | FI-3-12 |  | | 687 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(O)C=C4)=O)C(Br)=C3 | 14.1 ± 0.35 |
| 13 | FI-3-13 |  | | 766 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(Br)C=C4F)=O)C(Br)=C3 | 29.3 ± 1.34 |
| 14 | FI-3-14 |  | | 731 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(OC)C(OC)=C4)=O)C(Br)=C3 | 11.6 ± 0.61 |
| 15 | FI-3-15 |  | | 699 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(C([H])=O)C=C4)=O)C(Br)=C3 | 12.7 ± 0.74 |
| 16 | FI-3-16 |  | | 714 | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(N(C)C)C=C4)=O)C(Br)=C3 | 32.19 ± 0.91 |
|  |  | **SMILES of FI (1-16)** | |  | O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(NN)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=CC(OC)=C4O)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC(OC)=C(OC)C(OC)=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(Cl)C=C4Cl)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(O)C=C4O)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(OC)C=C4OC)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(OC)C(O)=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=CC([N+]([O-])=O)=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC(Br)=C(O)C(Br)=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=CC(O)=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=C(O)C=CC5=C4C=CC=C5)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(O)C=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(Br)C=C4F)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(OC)C(OC)=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(C([H])=O)C=C4)=O)C(Br)=C3  O=C(CC(C)(C)C1)C2=C1NC(C)=C(C(OCC)=O)C2C3=CC(Br)=C(OCC(N/N=C\C4=CC=C(N(C)C)C=C4)=O)C(Br)=C3 |  |

**All the compounds are soluble in Chloroform**