| Hit Compound | PubChem CID | CAS Number | RTECS Number | Route | $LD_{50}$ (mg/kg) | References |
|---|---|---|---|---|---|---|
| **Niclosamide** | 4477 | 50-65-7 | VN8400000 | Oral | 1000 | *[1], [2]* |
| | | | | IP | 7.5 | *[1], [3]* |
| **Pyrimethamine** | 4993 | 58-14-0 | UV8140000 | Oral | 92 | *[4], [5]* |
| | | | | IP | 74 | *[4], [6]* |
| **Vandetanib** | 3081361 | 443913-73-3 | VA0918650 | Oral | >1000 | *[7]* |

**Table S2. Acute toxicity of computationally identified, FDA-approved hit compounds.** Toxicity for hits identified in the SWEETLEAD database as having chemical similarity to query molecules as reported in the PubChem database. Data for oral and intraperitoneal administration are reported, where available. $LD_{50}$ values represent acute toxicity, for a single dose by the relevant delivery route.

References


1. *National Center for Biotechnology Information. PubChem Database. Niclosamide, CID=4477, https://pubchem.ncbi.nlm.nih.gov/compound/Niclosamide#section=Acute-Effects (accessed on June 23, 2020)*
2. *Wirksubstanzen der Pflanzenschutz und Schadlingsbekampfungsmittel, Perkow, W., Berlin, Verlag Paul Parey, 1971-1976.*
3. *Arzneimittel-Forschung. Drug Research., 10(884), 1960 [PMID:13712649].*
4. *National Center for Biotechnology Information. PubChem Database. Pyrimethamine, CID=4993, https://pubchem.ncbi.nlm.nih.gov/compound/Pyrimethamine#section=Acute-Effects (accessed on June 23, 2020)*
5. *British Journal of Pharmacology and Chemotherapy., 6(185), 1951 [PMID:14848451]*
6. *European Journal of Medicinal Chemistry--Chimie Therapeutique., 9(658), 1974*
7. *National Center for Biotechnology Information. PubChem Database. Vandetanib, CID=3081361, https://pubchem.ncbi.nlm.nih.gov/compound/Vandetanib#section=Toxicity-Summary (accessed on June 23, 2020)*