

Supplementary Table 2 MDDR unrelated orphans

Activity Class	Self E-value
Acetyl-CoA Thiolase Inhibitor	0
ATP Citrate Lyase Inhibitor	3.76×10^{-90}
Carbonic Anhydrase Inhibitor	5.98×10^{-318}
COMT Inhibitor	2.59×10^{-171}
CRF Antagonist	2.93×10^{-121}
GABA B Agonist	6.08×10^{-174}
GABA-B Receptor Antagonist	9.80×10^{-153}
Glucose-6-phosphate Translocase Inhibitor	4.56×10^{-237}
Glucuronidase (beta) Inhibitor	9.29×10^{-95}
Guanylate Cyclase Activator	0
Inosine Monophosphate Dehydrogenase Inhibitor	8.70×10^{-250}
mGlu1 Antagonist	1.22×10^{-129}
Muscarinic (M1) Agonist	1.70×10^{-151}
Nitric Oxide Synthase Inhibitor	4.64×10^{-105}
Phosphatidylinositol Kinase Inhibitor	1.31×10^{-251}
Poly(ADP-ribose)synthetase Inhibitor	3.44×10^{-111}
Thyroid Inhibitor	1.19×10^{-213}
Uridine Phosphorylase Inhibitor	3.31×10^{-199}

List of MDDR activity classes with best E-values > 1.0 to any other class.