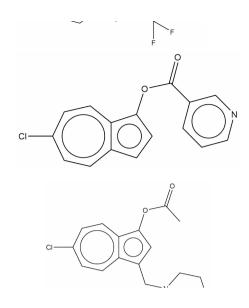
Summary_IC50_2

name.cmpd	synth.name	IC50	IC50.low	IC50.up
mPP-0076	IAT 39-II	1455.87124111046	5 1280.5097149860 <u>:</u>	L 1657.8799304739
mPP-0077	TL2-73	2490.11732544377	7 2154.64622169884	4 2854.57856485663
mPP-0078	AKIXVII103	2674.85052198937	' 1997.2402517319!	5 3653.95652725575
mPP-0077	TL2-73	2726.24499636303	3 2288.27181420616	3226.62898990925
mPP-0078	AKIXVII103	5239.72771868926	6 4428.4762661099	9 6153.45347465225
mPP-0031	MTI-73	6057.266900601	5553.5105903623	3 6580.82408146416
mPP-0224	NJ1-58	6937.60853356176	6 6186.6719951380¢	6 7784.17737260199
mPP-0084	AKI XVIII3	8293.52389262724	4323.31540529142	2 14725.2530329524

Summary_IC50_2

mPP-0082	TL4-63	9291.958261988	7999.9756077414	10701.3888474587
mPP-0083	TL4-58	9386.80463280459	8074.1512152215	10771.9283220089



O = c1c2c3c(c(C)c2NCCO)cc(C(C)C)Ccc3cc1C(F)(F)F

SMILES

O=Cc1c(c2C3C1)cC(C(C)C)CCC2CC(C(F)(F)F)(O)C3=O

O=C(NCc1cCc2c(sc(N)n2)c1)C3Nc4c(cccC4)c3

O = Cc1c(c2C3C1)cC(C(C)C)CCC2CC(C(F)(F)F)(O)C3 = O

 $\mathsf{CC}(\mathsf{C})(\mathsf{C})\mathsf{C1} = \mathsf{CC}(\mathsf{C}(\mathsf{C})(\mathsf{C})\mathsf{C}) = \mathsf{CC}(\mathsf{C2} = \mathsf{CC}(\mathsf{C}(\mathsf{O}) = \mathsf{O}) = \mathsf{NO2}) = \mathsf{C1}$

CC1=CC(C)=CC(C2=CC(C(OC3=C(Br)C=CC=C3)=O)=NO2)=C1

O = C(CCSc(c1c23)c(C)c2cc(C(C)C)ccc3cc(C(F)(F)F)c1 = O)O

Summary_IC50_2

O=C(Oc1c2ccc(Cl)ccc2cc1)c3cnccc3

Clc1ccc(c(OC(C)=O)cC2CN3CCOCC3)c2cc1