

Supplementary Information

Ligand-directed functional selectivity at the mu opioid receptor revealed by label-free integrative pharmacology on-target

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Supplementary Table 1 Opioid ligands, their binding affinity, and references

Table S1 Opioid ligands, their binding affinity, and references

Compound	Pharmacology	Ki (nM)	Kd (nM)	EC50 (nM)	IC50 (nM)	Ref
Naloxonazine	Opioid antagonist	0.054				1
CTOP	Mu Antagonist		0.18			1
Syndyphalin SD-25	Mu agonist				0.29	2
DAMME	Mu agonist				0.33	3
Dermorphin	Mu agonist		0.33			4
beta-Funaltrexamine	Mu antagonist	0.33				1
Endomorphin-2	Mu agonist		0.43			5
TAPP	Mu ligand		0.47			6
Endomorphin-1	Mu agonist	0.67				5
Naltrexone	Opioid antagonist	0.77				7
DAMGO	Mu agonist		1.1			9
DALDA	Mu agonist		1.69			9
Levallorphan	Opioid antagonist	1.7				7
nor-Binaltorphimine	Kappa antagonist	2.2				1
Naloxone HCl	Opioid antagonist	2.4				10
(Met5)-Enkephalin	Mu agonist	3				11
Deltorphin II	Delta agonist		3.3			4
(Leu5)-Enkephalin	Mu agonist		7.4			11
Nalbuphine	Mu antagonist/kappa agonist	11				1
N-Benzylnaltrindole	Delta antagonist				11.2	12
Dynorphin B	Kappa agonist	13				13
BNTX	Delta antagonist	18				4
Morphiceptin	Opioid agonist				19.8	14
Dynorphin A (1-8)	Kappa agonist	22.3				13
Naloxone methiodide	Opioid antagonist	28.9				15
Dynorphin A (1-13)	Kappa agonist		31			16
Naltrindole	Opioid antagonist	64				4
Naltriben	Delta antagonist.		80.8			1
DSLET	Delta agonist		120			17
NNC 63-0532	ORL1 agonist	140				10
DADLE	Opioid agonist		150			16
U-62066	Kappa agonist	252				18
(-)-Norcodeine	Opioid agonist		266.9			19
Nociceptin (1-13)	ORL1 agonist	270				20
DPDPE	Delta Agonist		600			8
(-)-U-50488	Kappa partial agonist		830			16
BRL52537	Kappa agonist	1560				21
U-69593	Kappa agonist	1600				10
Salvinorin A	Kappa agonist			1728		22
DIPPA	Kappa antagonist				1799	23
SKF10047	Opioid agonist/antagonist	1900			16	
Tramadol	Mu agonist	2400				24
ICI 199,441	Kappa agonist		4500			25

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