Catalogue of validated GPCR Ligands

In the following table we list the available ligands, with information about their selectivity, the emission and excitation wavelengths, their affinity measured by a radioligand binding assay and the specific further assays in which they have been validated.

Receptor	Code	λexc/λem	Affinity[1]	Selectivity[1]	Validation
Dopamine Receptor					
D_2	CELT-174	589/616	1.06 nM	**Selective** K_i (D_3)=136.5 nM K_i (D_4)=152.7 nM	Fluorescence Microscopy in transfected cells Flow cytometry
	CELT-426	560/571	89.3 nM	**Partially Selective** K_i (D_3)=194.8 nM K_i (D_4)=263 nM	Fluorescence polarization Flow cytometry
	CELT-175	748/776	3.15 nM	**Selective** K_i (D_3)=294.6 nM K_i (D_4)=220.3 nM	Fluorescence Microscopy in transfected cells (ongoing)
D_3	CELT-429	589/616	75.4 nM	**Selective** % displ.1 µM (D_2)= 6% % displ.1 µM (D_4)= 3%	Fluorescence Microscopy in transfected cells (ongoing)
	CELT-419	560/571	65.6 nM	**Partially Selective** K_i (D_2)=151.4 nM	Fluorescence polarization
D_2/D_3	CELT-240	589/616	D_3 = 2.14 nM D_2 = 2.34 nM	**Selective against D_4** % displ.1 µM (D_4)= 1%	Flow cytometry
	CELT-241	646/662	D_3 = 4.77 nM D_2 = 5.22 nM	**Selective against D_4** K_i (D_4)=302.55 nM	Fluorescence Microscopy in transfected cells (ongoing)
Adenosine Receptor					
PAN-ADO	CELT-298	646/662	A_1 = 20.9 nM A_{2A} = 171 nM A_{2B} = 44.7 nM A_3 = 95.2 nM	**Non Selective**	Fluorescence Microscopy in transfected cells

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A_1	**CELT-448**	560/571	26.2 nM	**Selective** % displ.1 µM (A_{2A})= 11% % displ.1 µM (A_{2B})= 22% % displ.1 µM (A_3)= 24%	Fluorescence polarization (ongoing) Fluorescence Microscopy in transfected cells (ongoing)
	CELT-372 (A_1/A_{2B})	589/616	A_1 = 1.89 nM A_{2B} = 24.75 nM	**Partially Selective** K_i (A_{2A})=80.33 nM K_i (A_3)=967.8 nM	Fluorescence Microscopy in transfected cells
	CELT-360	646/662	8.6 nM	**Non Selective** K_i (A_{2A})=98.38 nM K_i (A_{2B})=72.24 nM K_i (A_3)=231.01 nM	Fluorescence Microscopy in transfected cells
A_{2A}	**CELT-316**	589/616	116.1 nM	**Selective** % displ.1 µM (A_1)= 18% % displ.1 µM (A_{2B})= 33% % displ.1 µM (A_3)= 31%	Fluorescence Microscopy in native cells
	CELT-300	646/662	8.35 nM	**Selective** % displ.1 µM (A_1)= 31% % displ.1 µM (A_{2B})= 18% % displ.1 µM (A_3)= 38%	Fluorescence Microscopy in transfected cells (ongoing)
A_{2B}/A_3	**CELT-327**	589/616	A_{2B} = 35.6 nM A_3 = 45.7 nM	**Selective** % displ.1 µM (A_1)=41% % displ.1 µM (A_{2A})=1%	Fluorescence Microscopy in native cells[10]
A_3	**CELT-228**	560/571	52.7 nM	**Selective** % displ.1 µM (A_1)= 2% % displ.1 µM (A_{2A})= 1% % displ.1 µM (A_{2B})= 5%	Fluorescence Microscopy in native cells[10] Fluorescence polarization[9]
	CELT-171	589/616	6.13 nM	**Selective** % displ.1 µM (A_1)=2.1% % displ.1 µM (A_{2B})= 1.9%	Fluorescence Microscopy in transfected and native cells
Serotonin Receptor					
$5HT_{2A}$/$5HT_{2C}$	**CELT-402**	589/616	$5HT_{2A}$=29.7nM $5HT_{2C}$= 14.6 nM	**Selective** K_i ($5HT_{2B}$)=222.9 nM	Fluorescence Microscopy in transfected cells (ongoing)
$5HT_{2B}$	**CELT-211**	589/616	56.32 nM	**Selective** % displ.1 µM ($5HT_{2A}$)=0.94% % displ.1 µM ($5HT_{2C}$)= 1.75%	Fluorescence Microscopy in transfected cells
Cannabinoid Receptor					

PAN-CB	**CELT-335**	646/662	CB_1 = 44.8 nM CB_2 = 7.4 nM	**Non Selective**	HTRF in adherent cells[3] High Content screening Fluorescence Microscopy in transfected cells
CB_2	**CELT-331**	646/662	75.9 nM	**Selective[2]** % displ.1 µM (CB_1)=20%	High Content screening Fluorescence Microscopy in transfected cells
Muscarinic Receptor					
M_1	**NIR-CELT 195**	748/776	57.77 nM	No data	Fluorescence Microscopy in transfected cells (ongoing)
GLP1 Receptor					
GLP1	**CELT-111 (LUXendin551)**	551/576	7.2	**Selective[4]**	Widefield/confocal/2-photon microscopy in live and fixed mammalian cells and tissue, as well as anaesthetized mice[4]
GLP1	**CELT-112 (LUXendin645)**	645/664	7.5	**Selective[5]**	Widefield/confocal/2-photon microscopy in live and fixed mammalian cells and tissue, as well as anaesthetized mice[5] TR-FRET[6,7,8]
GLP1	**CELT-113 (LUXendin762)**	762/784	7.0	**Selective[4]**	Widefield/confocal/2-photon microscopy in live and fixed mammalian cells and tissue, as well as anaesthetized mice[4]. Non-invasive fluorescence preclinical imaging

[1] K_i or % of displacement at 1 µM measured by radioligand binding assay. In the case of GLP1R ligands corresponds to pIC50
[2] Development of a CB_1 selective ligand is ongoing.
[3]Lu Raïch et al. "Similarities and differences upon binding of naturally occurring Δ9-tetrahydrocannabinol-derivatives to cannabinoid CB1 and CB2 receptors" Pharmacol. Res., 2021,174,105970.
[4]J. Ast, A. N. Novak, T. Podewin, N. H. F. Fine, B. Jones, A. Tomas, R. Birke, K. Roßmann, B. Mathes, J. Eichhorst, M. Lehmann, A. K. Linnemann, D. J. Hodson, J. Broichhagen, 2021, DOI 10.33774/chemrxiv- 2021-7rngq.
[5]J. Ast, A. Arvaniti, N. H. F. Fine, D. Nasteska, F. B. Ashford, Z. Stamataki, Z. Koszegi, A. Bacon, B. J. Jones, M. A. Lucey, S. Sasaki, D. I. Brierley, B. Hastoy, A. Tomas, G. D'Agostino, F. Reimann, F. C. Lynn, C. A. Reissaus, A. K. Linnemann, E. D'Este, D. Calebiro, S. Trapp, K. Johnsson, T. Podewin, J. Broichhagen, D. J. Hodson, Nat Commun 2020, 11, 467.
[6]A. Marzook, S. Chen, P. Pickford, M. Lucey, Y. Wang, I. R. Corrêa Jr, J. Broichhagen, D. J. Hodson, V. Salem, G. A. Rutter, T. M. Tan, S. R. Bloom, A. Tomas, B. Jones, Biochemical Pharmacology 2021, 190, 114656.
[7]M. Lucey, T. Ashik, A. Marzook, Y. Wang, J. Goulding, A. Oishi, J. Broichhagen, D. J. Hodson, J. Minnion, Y. Elani, R. Jockers, S. J. Briddon, S. R. Bloom, A. Tomas, B. Jones, Mol Pharmacol 2021, DOI 10.1124/molpharm.121.000270.
[8]Z. Fang, S. Chen, P. Pickford, J. Broichhagen, D. J. Hodson, J. Ivan R. Corrêa, S. Kumar, F. Görlitz, C. Dunsby, P. M. W. French, G. A. Rutter, T. Tan, S. R. Bloom, A. Tomas, B. Jones, ACS Pharmacology & Translational Science 2020, DOI 10.1021/acsptsci.0c00022.
[9]D. Miranda-Pastoriza, R. Bernárdez, J. Azhuaje, R. Prieto-Díaz, M. Majellaro, A. V. Tamhankar, L. Koenekoop, A. González, C. Gioe-Gallo, A. Mallo-Abreu, J. Brea, M. I. Loza, A. García-Rey, X. García-Mera, H. Gutiérrez de Terán and E. Sotelo. ACS Medicinal Chemistry Letters. DOI: 10.1021/acsmedchemlett.1c00598.
[10]J. Barbazán, M. Majellaro, A. L.Martínez, J. M. Brea, E. Sotelo and M. Abal Identification of A2BAR as a potential target in colorectal cancer using novel fluorescent GPCR ligands. Biomedicine & Pharmacotherapy 2022 https://doi.org/10.1016/j.biopha.2022.113408

In case you are interested by any of these ligands and they have not been validated yet for the kind of assay you want to test, please let us know: based on our experience we could advise you about which fluorophore works better for each assay, and eventually develop new versions -i.e. keeping the pharmacophore but changing the fluorophore- in a turnaround of 4-6 weeks.

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