S1 Table. Known ligand library and decoys for each GPCR. Details about known ligand count, chiral center composition, as well as chemotype clusters names and counts. A chemical structure for the center of each chemotype cluster is represented, as well as each ligand from co-crystal X-ray structure.

		Chirality			Chemo	otype main clusters		
Library name	Known ligand count	% of compound s with at least one chiral center	avg. # of chiral center per compoun d	Name	Count	Center	Co-crystal ligand	Decoys #
AA2AR agonists	81	100.0	4.07	A 'CGS'	57	HO NH	CGS HO OH NH NH NH ₂	3198

				В	20	HO OH OH		
AA2AR inhibitors	361	14.40	0.26	А	32	Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z	ZM N N N N N N N N N N N N N	14078
				B 'ZM'	224			
				С	96	F NH ₂ N N N N N N N N N N N N N N N N N N N		

B1AR agonists	206	81.07	1.33	А	172	HO OH	DOB OH OH	8151
				В	14	OH NH		
				C 'DOB'	18	HO OH NH		
B1AR inhibitors	208	90.38	1.23	А		HO HN NH	CYP	8229

				B 'CYP'		NH OH		
				С		Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z Z		
B2AR agonists	204	81.28	1.35	А	125	HO OH OH	BI HO NH	8034
				B 'BI'	48	NH OH NH		
				С	21	HO OH		

B2AR inhibitors	192	90.63	1.22	А	20	HN N N N N N N N N N N N N N N N N N N	CAR	7955
				B 'CAR'	51	HN O O O O O O O O O O O O O O O O O O O		
				С	100	HO HN NH		
DOR agonists	357	45.35	1.52	А	165	NH NH		-

				В	39			
				С	42			
				D	78	N HO ON N		
DOR inhibitors	15	93.33	4.13	A 'NAL'	8	BHO N	NAL HOLD THE	624

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