

Target Class	Assay Name	Assay Target	Mode	% Response Replicate 1	% Response Replicate 2	% Response Average
GPCR	Calcium Flux	ADORA2A	Agonist	-10.3	-4.2	-7.3
GPCR	Calcium Flux	ADORA2A	Antagonist	-4.8	-34.5	-19.7
GPCR	Calcium Flux	ADRA1A	Agonist	-0.4	-1.1	-0.7
GPCR	Calcium Flux	ADRA1A	Antagonist	3.6	-2.7	0.5
GPCR	cAMP	ADRA2A	Agonist	11.8	4.5	8.2
GPCR	cAMP	ADRA2A	Antagonist	-0.5	4.5	2.0
GPCR	cAMP	ADRB1	Agonist	-0.1	-0.7	-0.4
GPCR	cAMP	ADRB1	Antagonist	-42.0	-32.6	-37.3
GPCR	cAMP	ADRB2	Agonist	-0.7	2.0	0.7
GPCR	cAMP	ADRB2	Antagonist	-13.6	14.3	0.4
GPCR	Calcium Flux	AVPR1A	Agonist	-2.2	-2.7	-2.5
GPCR	Calcium Flux	AVPR1A	Antagonist	18.9	8.2	13.6
GPCR	Calcium Flux	CCKAR	Agonist	0.1	0.3	0.2
GPCR	Calcium Flux	CCKAR	Antagonist	6.3	4.8	5.6
GPCR	Calcium Flux	CHRM1	Agonist	-2.7	-0.9	-1.8
GPCR	Calcium Flux	CHRM1	Antagonist	29.9	20.1	25.0
GPCR	cAMP	CHRM2	Agonist	23.9	6.3	15.1
GPCR	cAMP	CHRM2	Antagonist	-21.1	-17.6	-19.4
GPCR	Calcium Flux	CHRM3	Agonist	-2.7	-1.0	-1.9
GPCR	Calcium Flux	CHRM3	Antagonist	4.2	8.6	6.4
GPCR	cAMP	CNR1	Agonist	5.0	8.1	6.6
GPCR	cAMP	CNR1	Antagonist	13.0	15.4	14.2
GPCR	cAMP	CNR2	Agonist	-40.7	-68.7	-54.7
GPCR	cAMP	CNR2	Antagonist	-1.1	-2.7	-1.9
GPCR	cAMP	DRD1	Agonist	1.2	0.2	0.7
GPCR	cAMP	DRD1	Antagonist	-14.2	-6.9	-10.6
GPCR	cAMP	DRD2S	Agonist	4.1	20.5	12.3
GPCR	cAMP	DRD2S	Antagonist	-0.4	0.4	0.0
GPCR	Calcium Flux	EDNRA	Agonist	2.2	-0.5	0.8
GPCR	Calcium Flux	EDNRA	Antagonist	8.2	1.2	4.7
GPCR	Calcium Flux	HRH1	Agonist	1.5	1.7	1.6
GPCR	Calcium Flux	HRH1	Antagonist	36.0	27.8	31.9
GPCR	cAMP	HRH2	Agonist	0.6	0.1	0.4
GPCR	cAMP	HRH2	Antagonist	6.4	16.0	11.2
GPCR	cAMP	HTR1A	Agonist	9.1	-9.8	-0.4
GPCR	cAMP	HTR1A	Antagonist	2.6	11.9	7.3
GPCR	cAMP	HTR1B	Agonist	5.5	1.5	3.5
GPCR	cAMP	HTR1B	Antagonist	-3.3	-2.5	-2.9
GPCR	Calcium Flux	HTR2A	Agonist	-3.1	-2.7	-2.9
GPCR	Calcium Flux	HTR2A	Antagonist	31.5	22.6	27.1
GPCR	Calcium Flux	HTR2B	Agonist	0.7	1.4	1.1
GPCR	Calcium Flux	HTR2B	Antagonist	53.6	50.3	52.0
GPCR	cAMP	OPRD1	Agonist	6.2	6.8	6.5
GPCR	cAMP	OPRD1	Antagonist	10.5	10.7	10.6
GPCR	cAMP	OPRK1	Agonist	60.8	53.6	57.2
GPCR	cAMP	OPRK1	Antagonist	-2.9	-3.1	-3.0
GPCR	cAMP	OPRM1	Agonist	2.9	-9.3	-3.2
GPCR	cAMP	OPRM1	Antagonist	-3.6	-3.6	-3.6
NHR	NHR Nuclear Translocation	AR	Agonist	-0.8	-0.6	-0.7
NHR	NHR Nuclear Translocation	AR	Antagonist	-4.3	-13.2	-8.8
NHR	NHR Protein Interaction	GR	Agonist	0.1	-0.3	-0.1
NHR	NHR Protein Interaction	GR	Antagonist	-84.9	-64.9	-74.9
Transporter	Transporter	DAT	Blocker	66.0	64.6	65.3
Transporter	Transporter	NET	Blocker	95.6	77.8	86.7
Transporter	Transporter	SERT	Blocker	8.4	7.3	7.9
Ion Channel	Ion Channel	CAV1.2	Blocker	4.1	3.3	3.7
Ion Channel	Ion Channel	GABAA	Opener	-6.1	-6.7	-6.4
Ion Channel	Ion Channel	GABAA	Blocker	-7.8	6.9	-0.4
Ion Channel	Ion Channel	hERG	Blocker	8.8	21.5	15.2
Ion Channel	Ion Channel	HTR3A	Opener	-1.1	-1.6	-1.3
Ion Channel	Ion Channel	HTR3A	Blocker	5.2	10.9	8.0
Ion Channel	Ion Channel	KvLQT1/minK	Opener	4.9	-2.0	1.4
Ion Channel	Ion Channel	KvLQT1/minK	Blocker	10.5	14.1	12.3
Ion Channel	Ion Channel	nAChR(a4/b2)	Opener	-10.3	-5.9	-8.1
Ion Channel	Ion Channel	nAChR(a4/b2)	Blocker	24.1	7.2	15.7
Ion Channel	Ion Channel	NAV1.5	Blocker	9.2	26.1	17.6
Ion Channel	Ion Channel	NMDAR (1A/2B)	Opener	0.0	-1.3	-0.6
Ion Channel	Ion Channel	NMDAR (1A/2B)	Blocker	14.4	12.6	13.5
Ion-Kinase Enzyme	Enzymatic	AChE	Inhibitor	11.6	6.3	9.0
Ion-Kinase Enzyme	Enzymatic	COX1	Inhibitor	-56.3	-68.6	-62.4
Ion-Kinase Enzyme	Enzymatic	COX2	Inhibitor	36.6	36.1	36.3
Ion-Kinase Enzyme	Enzymatic	MAOA	Inhibitor	-11.7	4.3	-3.7
Ion-Kinase Enzyme	Enzymatic	PDE3A	Inhibitor	8.8	-7.4	0.7
Ion-Kinase Enzyme	Enzymatic	PDE4D2	Inhibitor	-0.5	-5.4	-3.0
Kinases	Binding	INSR	Inhibitor	29.3	22.0	25.7
Kinases	Binding	LCK	Inhibitor	12.2	-3.6	4.3
Kinases	Binding	ROCK1	Inhibitor	16.2	4.8	10.5
Kinases	Binding	VEGFR2	Inhibitor	17.6	14.7	16.1

**Table S1.** Raw data from pharmacological profile screening for DJ101. Data was generated by DiscoverX via the Safety47™ panel of functional assays with all human targets for safety screening. Response values within ±70% are considered insignificant according to the vendor.

% Response Legend	
$x > 95\%$	
$95\% \leq x < 90\%$	
$90\% \leq x < 85\%$	
$85\% \leq x < 70\%$	
$x < 70\%$	