

# Panel 331 Datasheet

Moleculomics offer *in silico* screening platforms to enable analysis of the predicted interaction between any compound and panels of selected target proteins. These quantitative simulation methods offer significant savings as the first step in the drug discovery process for identification of the most problematic off-target interactions.

## Panel 331: A panel of 229 protein targets, fully representative of the 331 enzymatic and receptor signaling assays featured in the ToxCast database (Sipes et al., 2013)<sup>1</sup>, including;

1. Profiling 976 ToxCast Chemicals across 331 Enzymatic and Receptor Signaling Assays - Sipes et al 2013, Chem. Res. Toxicol. 2013, 26, 878–895.

	<b>Protein</b>	<b>Organism</b>			
1	5HT1	Rattus norvegicus	35	AR	Homo sapiens
2	5HT2A	Homo sapiens	36	AR	Rattus norvegicus
3	5HT2C	Sus scrofa	37	AT1	Homo sapiens
4	5HT3	Homo sapiens	38	AT2	Bos taurus
5	5HT4	Cavia porcellus	39	AurA	Homo sapiens
6	5HT5A	Homo sapiens	40	BACE	Homo sapiens
7	5HT6	Homo sapiens	41	BK2	Caviaporcellus
8	5HT7	Homo sapiens	42	C5a	Homo sapiens
9	5HTNonSelective	Rattus norvegicus	43	CaBTZCH-L	Rattus norvegicus
10	AChE	Homo sapiens	44	CaCh-N	Rattus norvegicus
11	AChE	Rattus norvegicus	45	CaDHPRCh-L	Rattus norvegicus
12	ACP1	Homo sapiens	46	CAR	Homo sapiens
13	Adenylate Cyclase	Rattus norvegicus	47	CASP1	Homo sapiens
14	AdoRA Non Selective	Bos taurus	48	CASP10	Homo sapiens
15	AdoRA1	Homo sapiens	49	CASP2	Homo sapiens
16	AdoRA2a	Homo sapiens	50	CASP3	Homo sapiens
17	AdoT	Homo sapiens	51	CASP4	Homo sapiens
18	AdoT	Rattus norvegicus	52	CASP5	Homo sapiens
19	Adra1 Non Selective	Rattus norvegicus	53	CASP8	Homo sapiens
20	Adra1A	Rattus norvegicus	54	CCKAPeripheral	Mus musculus (Mouse)
21	Adra1B	Rattus norvegicus			
22	Adra2 Non Selective	Rattus norvegicus	55	CCKB	Rattus norvegicus
23	Adra2A	Homo sapiens	56	CDK2	Homo sapiens
24	Adra2B	Rattus norvegicus	57	CK1D	Homo sapiens
25	Adra2C	Homo sapiens	58	cNOS	Rattus norvegicus
26	Adrb Non Selective	Rattus norvegicus	59	COMT	Rattus norvegicus
27	ADRB1	Homo sapiens	60	COX1	Ovis aries
28	ADRB2	Homo sapiens	61	COX2	Ovis aries
29	ADRB3	Homo sapiens	62	CRF	Rattus norvegicus
30	AKT1	Homo sapiens	63	CSF1R	Homo sapiens
31	AKT2	Homo sapiens	64	CYP19A1	Homo sapiens
32	AMPA	Rattus norvegicus	65	CYP1A1	Homo sapiens
33	AMPKa1	Homo sapiens	66	CYP1A2	Homo sapiens
34	ANPA	Cavia porcellus	67	CYP2A6	Homo sapiens

	<b>Protein</b>	<b>Organism</b>			
68	CYP2B6	Homo sapiens	112	H3	Rattus norvegicus
69	CYP2C19	Homo sapiens	113	HDAC3	Homo sapiens
70	CYP2C9	Homo sapiens	114	HDAC6	Homo sapiens
71	CYP2D6	Homo sapiens	115	I2C	Oryctolagus cuniculus (Rabbit)
72	CYP3A4	Homo sapiens	116	IGF1R	Homo sapiens
73	CYP4F12	Homo sapiens	117	IKKa	Homo sapiens
74	DAT	Cavia porcellus	118	InsR	Homo sapiens
75	DAT	Homo sapiens	119	Jak2	Homo sapiens
76	DRD1	Homo sapiens	120	JNK2	Homo sapiens
77	DRD2s	Homo sapiens	121	KAR	Rattus norvegicus
78	DRD4.4	Homo sapiens	122	KATPCh	Rattus norvegicus
79	DR Non Selective	Bos taurus	123	KCaCh	Rattus norvegicus
80	DUSP3	Homo sapiens	124	KhERGCh	Homo sapiens
81	EGFR	Homo sapiens	125	LTB4	Cavia porcellus
82	Elastase	Homo sapiens	126	LTB4-BLT1	Homo sapiens
83	EphA1	Homo sapiens	127	LTD4	Cavia porcellus
84	EphA2	Homo sapiens	128	Lyn	Homo sapiens
85	EphB2	Homo sapiens	129	M1	Homo sapiens
86	ER	Bos taurus	130	M2	Homo sapiens
87	ER	Homo sapiens	131	M3	Homo sapiens
88	ERalpha	Mus musculus	132	M4	Homo sapiens
89	ES	Homo sapiens	133	M5	Homo sapiens
90	ETA	Homo sapiens	134	MAO-ACentral	Rattus norvegicus
91	ETB	Homo sapiens	135	MAO-APeripheral	Rattus norvegicus
92	FGFR1	Homo sapiens	136	MAO-BCentral	Rattus norvegicus
93	FKBP12	Homo sapiens	137	MAO-BPeripheral	Rattus norvegicus
94	FXR	Homo sapiens	138	MAPK1	Homo sapiens
95	Fyn	Homo sapiens	139	MAPK3	Homo sapiens
96	GABA Non Selective	Rattus norvegicus	140	MAPKAPK2	Homo sapiens
97	GABAA agonist	Bostaurus	141	Met	Homo sapiens
98	GABAA-a1	Bos taurus	142	mGluR1	Rattus norvegicus
99	GABAA-a5	Bos taurus	143	mGluR5	Rattus norvegicus
100	GABAA-a6	Rattus norvegicus	144	MMP1	Homo sapiens
101	GABBR	Rattus norvegicus	145	MMP13	Homo sapiens
102	GALN	Rattus norvegicus	146	MMP2	Homo sapiens
103	GHB	Rattus norvegicus	147	MMP3	Homo sapiens
104	GluNDMA agonist	Rattus norvegicus	148	MMP7	Homo sapiens
105	GluNMDA MK801 agonist	Rattus norvegicus	149	MMP9	Homo sapiens
106	GlyR Stry Sens	Rattus norvegicus	150	MNon-SelectivePeripheral	Cavia porcellus
107	GR	Homo sapiens	151	MR	Rattus norvegicus
108	GSK3b	Homo sapiens	152	Msk1	Homo sapiens
109	H1	Bos taurus	153	NaCh-site2	Rattus norvegicus
110	H1	Homo sapiens	154	NEK2	Homo sapiens
111	H2	Cavia porcellus	155	NET	Homo sapiens

	<b>Protein</b>	<b>Organism</b>			
156	NET	Rattus norvegicus	200	PTPN9	Homo sapiens
157	NK1	Rattus norvegicus	201	PTPRB	Homo sapiens
158	NK2	Homo sapiens	202	PTPRC	Homo sapiens
159	NK3	Rattus norvegicus	203	PTPRF	Homo sapiens
160	NNR-BungSens	Rattus norvegicus	204	PTPRM	Homo sapiens
161	NNR-NBungSens	Homo sapiens	205	PXR	Homo sapiens
162	NPY Non Selective	Bos taurus	206	RAF1	Homo sapiens
163	NPY1	Homo sapiens	207	RAR	Homo sapiens
164	NPY2	Homo sapiens	208	RARa	Homo sapiens
165	NTS	Homo sapiens	209	ROCK1	Homo sapiens
166	NTS	Rattus norvegicus	210	SERT	Homo sapiens
167	OplateD1	Homo sapiens	211	SERT	Rattus norvegicus
168	Oplate-K	Cavia porcellus	212	SIGMANon-Selective	Cavia porcellus
169	Oplate-mu	Homo sapiens	213	SIRT1	Homo sapiens
170	OplateNon-Selective	Rattus norvegicus	214	SIRT2	Homo sapiens
171	OplateNon-SelectiveNa+	Rattus norvegicus	215	SIRT3	Homo sapiens
172	ORL-1	Homo sapiens	216	SRC	Homo sapiens
173	OXT	Rattus norvegicus	217	SST	Rattus norvegicus
174	P2Y	Homo sapiens	218	Tie2	Homo sapiens
175	PAF	Oryctolagus cuniculus	219	TRa	Homo sapiens
176	PAK4	Homo sapiens	220	TRH	Rattus norvegicus
177	PBR	Homo sapiens	221	TrkA	Homo sapiens
178	PBR	Rattus norvegicus	222	TXA2	Homo sapiens
179	PDE10	Homo sapiens	223	V1	Rattus norvegicus
180	PDE4A1	Homo sapiens	224	V1A	Homo sapiens
181	PDE5	Homo sapiens	225	VEGFR1	Homo sapiens
182	PI3Ka	Homo sapiens	226	VEGFR2	Homo sapiens
183	PKA	Homo sapiens	227	VEGFR3	Homo sapiens
184	PPARa	Homo sapiens	228	VIPNon-Selective	Rattus norvegicus
185	PPARg	Homo sapiens	229	VMAT2	Rattus norvegicus
186	PPM1A	Homo sapiens			
187	PPP1CA	Homo sapiens			
188	PPP2CA	Homo sapiens			
189	PR	Bos taurus			
190	PR	Homo sapiens			
191	PTEN	Homo sapiens			
192	PTPN1	Homo sapiens			
193	PTPN11	Homo sapiens			
194	PTPN12	Homo sapiens			
195	PTPN13	Homo sapiens			
196	PTPN14	Homo sapiens			
197	PTPN2	Homo sapiens			
198	PTPN4	Homo sapiens			
199	PTPN6	Homo sapiens			