

Supplementary Data.

Table S1. Parameters of docking sites for targets shared by calcitriol, depression and anxiety.

Gene Symbol	PDB ID	Ligand ID (Binding Site)	Gridbox (Center)			Gridbox (Size)		
VDR	1DB1	VDX	10	24	35	24	24	24
HRH3	7F61	1IB	-20	50	0	24	24	24
NR1H3	3IPQ	965	42	18	-5	24	24	24
CNR1	7WV9	9GF	136	102	93	24	24	24
PTCH1	6RTW	Y01	-15	7,5	-30	24	24	24
CNR2	6PT0	W15	100	110	125	24	24	24
HTR2A	6A93	8NU	15	0	60	24	24	24
CYP19A1	3ST9	ASD	87	55	45	24	24	24
HCRTR2	4S0V	SUV	50	9	55	24	24	24
TACR2	7XWO	α -helix	115	100	145	24	24	24
MTOR	4DRH	RAP	-5	20	-2	24	24	24
GHSR	7NA8	1KD	125	135	93	24	24	24
CCKBR	7XOW	gastrine	93	115	67	24	24	24
ESR1	1A52	EST	106	15	95	24	24	24
TACR1	6E59	L76	-15	55	55	24	24	24
HCRTR1	4ZJ8	SUV	-8	0	-55	24	24	24
PRKCA	3IW4	LW4	6	30	52	24	24	24
OPRL1	5DHG	DGV	-8	30	-2	24	24	24
ABL1	1OPL	P16	20	52	50	24	24	24
PDE5A	1T9S	5GP	40	46	1	24	24	24
TGFB1	1PY5	PY1	5	10	6	24	24	24
REN	1BIL	0IU	37	60	43	24	24	24
PRKCB	2I0E	PDS	40	55	35	24	24	24
CHUK	5EBZ	5TL	86	65	2	24	24	24
OPRD1	6PT2	KGCHM07 (peptide)	-20	40	-28	24	24	24
CCR1	7VL9	CLR	125	125	130	24	24	24
DRD3	8IRT	R5F	108	130	120	24	24	24
KDR	1Y6A	AAZ	0	30	18	24	24	24
INSR	1GAG	112	-22	28	9	24	24	24
CSK	1BYG	STU	26	45	13	24	24	24
CAMK1G	2JAM	J60	15	3	13	24	24	24
PDE3A	7KWE	X5M	-18	-20	43	24	24	24
OPRM1	8EF5	7V7	100	106	127	24	24	24
CNR2	6PT0	CLR	90	95	135	24	24	24
GSK3B	6B8J	65C	-2	42	19	24	24	24
PIK3CA	3ZIM	KKR	-23	12	28	24	24	24
OPRK1	4DJH	JDC	3	-23	60	24	24	24
EZH2	5HYN	SAH	80	-98	2	24	24	24
FGFR1	3DPK	8C5	5	27	8	24	24	24
AKT2	1GZK	α -helix	-20	120	-70	24	24	24
CNR1	7WV9	7IC	125	90	100	24	24	24
GC	1J78	VDY	-21	-60	47	24	24	24
PTAFR	AF-P25105*	α -helix	12	3	-12	24	24	24
MDM2	1RV1	IMZ	10	10	14	24	24	24
CSF1R	3BEA	IXH	5	30	8	24	24	24
KSR1	7JUY	ANP	-5	65	-3	24	24	24
MAPT	7NRS	center of protein	112	130	132	24	24	24
ALK	2XP2	VGH	29	45	9	24	24	24
IHH	3K7I	α -helix	-5	-25	3	24	24	24
AR	1T5Z	DHT	0	60	3	24	24	24
IKBKB	4KIK	KSA	48	30	-58	24	24	24
JAK1	4E4L	0NH	-12	28	0	24	24	24
AKT1	2UVM	GVF	15	11	15	24	24	24
PIK3R	1H9O	PTR	14	10	20	24	24	24
SHH	6PJV	GOL	-35	47	20	24	24	24
MAP3K14	4DN5	AGS	-10	30	-5	24	24	24
CHEK1	1ZLT	HYM	15	0	13	24	24	24
CA3	3UYQ	α -helix	60	12	30	24	24	24

* AlphaFold model

Table S2. Parameters of docking sites for targets shared by calcitriol and depression.

Gene Symbol	PDB ID	Ligand ID (Binding Site)	Gridbox (Center)	Gridbox (Size)
SMO	4QIM	ANTAXV(A8T)	14 -12 -23	24 24 24
HTR1D	7E32	SRO	100 121 112	24 24 24
EBP	6OHU	CTX	-15 10 26	24 24 24
GPBAR1	7CFM	P395 (FWX)	99 120 113	24 24 24
S1PR2	7T6B	S1P	112 145 138	24 24 24
S1PR1	7E04	BAF312 (J8C)	129 137 169	24 24 24
ADAMTS5	3B8Z	294	13 3 -5	24 24 24
GSK3A	7SXG	BIO8546(D1E)	-15 -15 17	24 24 24
ACAN	4MD4	α -helix	55 27 -6	24 24 24
ADAMTS4	2RJP	886	64 0 15	24 24 24
BRSK2	AF-Q8IWQ3*	α -helix	-20 10 0	24 24 24
S1PR3	7EW2	EFTY720(J89)	118 102 78	24 24 24
STAT6	4Y5W	α -helix	24 15 18	24 24 24
HTR1D	7E32	CLR	83 120 96	24 24 24
EPHB4	2VWU	7X1	12 9 12	24 24 24
JAK3	3ZC6	VFC	12 -2 44	24 24 24
TTK	2X9E	NMS-P715 (SVE)	-8 20 -1	24 24 24
EPHB3	5L6O	6P6	15 5 -5	24 24 24
WEE1	3BI6	PD352396 (396)	5 54 24	24 24 24
AKT3	2X18	EPE	24 66 -20	24 24 24
PRKD3	2D9Z	α -helix	-15 1 0	24 24 24
PTPN1	1BZC	TPI	-20 54 16	24 24 24

* AlphaFold model

Table S3. Parameters of docking sites for targets shared by calcitriol and anxiety.

Gene Symbol	PDB ID	Ligand ID (Binding Site)	Gridbox (Center)	Gridbox (Size)
AURKB	4AF3	VX6	22 -20 -10	24 24 24
HSP90B	3NMQ	EC44/7PP	30 10 8	24 24 24
AURKC	6GR9	VX6	30 8 7	24 24 24
INCENP	6GR8	α -helix	40 9 -18	24 24 24
BIRC5	2QFA	MES	45 6 42	24 24 24