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Supplementary Information

IN SILICO ANALYSIS OF ENERGY INTERACTIONS BETWEEN NOCICEPTIN/ORFANIN FQ RECEPTOR AND TWO ANTAGONISTS WITH POTENTIAL ANTIDEPRESSIVE ACTION

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TABLE S1. Energy values of NOPR receptor amino acids residues interacting with the ligand C-35, distance radius and functional binding region of the residue.

Amino Acid	*Atomic group*	*Radius (Å)*	*Distance (Å)*	*ε=10*	*ε=40*
ASP130	ii(N)H	2	1.85	-24.31	-14.67
GLN107	iii(N)H	2.5	2.12	-9.85	-8.81
ASP110	iii(CB)H	2.5	2.33	-15.25	-7.79
TRP116	iii(CG)H	2.5	2.14	-2.61	-2.33
VAL126	iii(CAG)H	2.5	2.25	-2.88	-2.16
TYR131	iii(CAD)H	2.5	2.55	-4.91	-4.84
CYS200	iii(CD)H	2.5	2.16	-0.19	-0.14
ILE219	i(CBF)H	2.5	2.35	-1.86	-1.85
SER223	i(CBF)H	2.5	2.44	-1.73	-1.57
TRP276	ii(CAV)H	2.5	2.92	-3.09	-2.61
VAL279	ii(CAV)H	2.5	2.41	-1.68	-1.75
TYR309	ii(N)H	2.5	2.33	-3.13	-2.92
ILE127	iii(CAD)H	3	2.51	-5.38	-5.10
MET134	i(CAW)H	3	2.68	-0.86	-0.94
PHE135	i(CBE)H	3	2.56	-1.04	-1.11
LEU201	iii(CAD)H	3	2.94	0.01	0.29
VAL202	iii(CAD)H	3	2.90	-1.69	-1.54
GLN280	i(CBB)H	3	2.44	-3.49	-3.24
VAL283	ii(CAX)H	3	2.73	-1.83	-2.02
THR305	iii(CAR)H	3	2.56	-1.99	-1.74
PHE220	i(CBF)H	3.5	3.37	-1.78	-0.65
ILE111	iii(CB)H	4	3.94	-0.29	-0.44
GLU199	iii(CD)H	4	3.81	-8.30	-2.70
CYS123	iii(CD)H	4.5	4.41	-1.52	-1.01
PHE224	i(CBF)H	4.5	4.02	-0.52	-0.48
ARG302	iii(C)O	4.5	4.40	5.54	0.88
TYR58	iii(CAP)H	5	4.68	0.08	-0.17
THR103	iii(CG)H	5	4.53	-0.40	-0.34
PHE106	iii(CG)H	5	4.60	0.24	-0.04
VAL185	iii(CAA)H	5	4.55	-0.27	-0.28
LEU284	i(CBB)H	5	4.89	-0.25	-0.20
PHE118	iii(CG)H	5.5	5.32	0.21	-0.04
ASN133	ii(CAW)H	5.5	5.30	-0.53	-0.06
GLY108	iii(CG)H	6	5.87	-0.40	-0.24
ALA128	iii(CAB)H	6.5	5.89	-0.44	-0.23
TYR132	i(CBD)CLBC	6.5	5.90	0.11	-0.07
VAL281	i(CBA)CLAY	6.5	5.57	-0.19	-0.15
PHE282	i(CBA)CLAY	6.5	5.77	0.15	-0.14
LEU301	iii(CAR)H	6.5	5.73	-0.41	-0.25
GLY308	ii(CAV)H	6.5	5.54	0.52	0.12
VAL100	iii(CAO)H	7	6.02	-0.42	-0.23
LEU104	iii(N)H	7	6.76	-0.61	-0.26
THR109	iii(CG)H	7	6.13	0.47	0.14
PHE115	iii(CG)H	7	6.08	0.01	-0.05
PRO117	iii(CG)H	7	6.52	0.13	0.00
LEU122	iii(CD)H	7	6.13	-0.35	-0.15
LYS124	iii(CAG)H	7	6.84	3.94	0.83
ILE129	iii(CAB)H	7	6.49	0.53	0.20
THR138	i(CBE)H	7	6.93	0.18	0.00
VAL181	i(CBE)H	7	6.11	-0.14	-0.12
GLY189	iii(CAA)H	7	6.33	0.24	0.03
SER190	iii(CAD)H	7	6.70	-0.35	-0.14
ALA191	iii(CAD)H	7	6.58	-0.01	-0.04
GLU203	iii(CAD)H	7	6.94	-4.36	-1.14
ALA216	i(CBF)H	7	6.18	-0.35	-0.15

CYS218	i(CBF)H	7	6.56	0.15	0.01
LEU221	i(CBF)H	7	6.33	-0.07	-0.05
PHE222	i(CBF)H	7	6.83	0.27	0.07
ILE225	i(CBF)H	7	6.67	-0.01	-0.04
THR277	i(CBA)CLAY	7	6.77	-0.32	-0.15
PRO278	i(CBA)CLAY	7	6.45	0.12	0.00
CYS304	i(CAV)H	7	6.97	0.29	0.03
ALA306	iii(CAR)H	7	6.94	-0.33	-0.14
THR125	iii(CAC)H	7.5	7.16	0.06	-0.01
ILE204	iii(CAD)H	7.5	7.36	-0.13	-0.06
PHE215	i(CBF)H	7.5	7.10	-0.08	-0.07
GLN286	iii(CAR)H	7.5	7.48	-0.30	-0.16
PRO105	iii(CG)H	8	7.73	-0.13	-0.06
LEU112	iii(CB)H	8	7.50	0.06	0.00
GLY114	iii(CB)H	8	7.71	0.29	0.06
GLY119	iii(CD)H	8	7.68	-0.36	-0.11
GLY182	i(CBD)CLBC	8	7.77	-0.34	-0.11
MET188	iii(CAA)H	8	7.79	0.25	0.03
ILE198	iii(CD)H	8	7.74	0.25	0.08
ILE217	i(CBF)H	8	7.55	-0.19	-0.07
PHE272	ii(CAW)H	8	7.87	-0.28	-0.13
CYS275	ii(CAW)H	8	7.88	0.04	-0.01
ALA285	i(CBB)H	8	7.65	0.17	0.02
ILE54	iii(CAP)H	8.5	8.40	0.00	-0.03
VAL55	iii(CB)H	8.5	8.44	-0.17	-0.06
LEU113	iii(CG)H	8.5	8.17	0.28	0.05
THR136	i(CBE)H	8.5	8.06	0.21	0.03
SER137	ii(CAW)H	8.5	8.36	0.25	0.04
ALA186	iii(CAB)H	8.5	8.26	-0.25	-0.09
PRO227	i(CBF)H	8.5	8.00	0.19	0.03
GLY287	i(CBB)H	8.5	8.44	0.05	0.00
LEU307	ii(CAV)H	8.5	8.40	0.15	0.01
SER312	ii(CAV)H	8.5	8.43	0.09	0.01
ASN120	iii(CD)H	9	8.55	-0.71	-0.20
ALA178	i(CBE)H	9	8.79	-0.18	-0.06
GLN192	iii(CD)H	9	8.66	-0.23	-0.07
VAL226	i(CBF)H	9	8.82	0.13	0.03
VAL310	ii(CAV)H	9	8.88	0.03	-0.02
ASN311	ii(CAV)H	9	8.87	0.16	0.03
LYS51	iii(CB)H	9.5	9.25	4.13	1.02
LEU102	iii(CG)H	9.5	9.46	0.13	0.02
ALA121	iii(CD)H	9.5	9.36	-0.20	-0.06
PHE139	i(CBE)H	9.5	9.20	0.10	0.01
VAL228	i(CBF)H	9.5	9.30	0.10	0.02
PHE303	iii(CAP)H	9.5	9.45	-0.18	-0.07
VAL298	iii(C)O	10	9.65	-0.30	-0.09

TABLE S2. Energy values of NOPR receptor amino acids residues interacting with the ligand SB, distance radius and functional binding region of the residue.

Amino Acid	*Atomic group*	*Radius (Å)*	*Distance (Å)*	*ε=10*	*ε=40*
ASP130	ii(N)H	2	1.87	-20.56	-14.09
ARG302	iii(CAA)H	2	1.95	3.69	1.35
GLN107	iii(CAA)H	2.5	2.19	-5.02	-4.55
CYS200	iii(CAF)H	2.5	2.36	-2.24	-2.16
ILE219	i(CAE)H	2.5	2.48	-1.88	-1.85
SER223	i(CAE)H	2.5	2.27	-1.40	-1.22
GLN280	i(CAH)H	2.5	2.38	-2.93	-2.64
THR305	iii(CAR)H	2.5	2.43	-2.01	-0.54
TYR309	ii(CAO)H	2.5	2.36	-3.96	-3.79
ASP110	iii(CAA)H	3	2.7	-4.79	-2.32
ILE111	iii(CA)H	3	2.95	-0.60	-0.53
TRP116	iii(CAG)H	3	2.59	-1.99	-1.96
ILE127	iii(O)H	3	2.51	-2.30	-2.00
TYR131	i(CAU)CL	3	2.8	-3.29	-3.16
MET134	ii(CAO)H	3	2.61	-2.56	-2.26
PHE135	i(CAI)H	3	2.72	-0.68	-0.65
TRP276	ii(CAO)H	3	2.92	-2.74	-2.44
VAL279	i(CAT)CLAC	3	2.97	-1.90	-1.84
VAL283	ii(CBA)H	3	2.66	-1.34	-1.21
VAL126	iii(CAF)H	3.5	3.38	-1.64	-1.52
TYR58	iii(CAA)H	4	3.83	-0.09	-0.03
PHE220	i(CAE)H	4	3.73	-0.63	-0.56
PHE106	iii(CAG)H	4.5	4.39	0.06	-0.04
GLY108	iii(CA)H	4.5	4.31	-0.39	-0.32
LEU201	iii(CAY)O	4.5	4.17	0.08	-0.02
PHE224	i(CAE)H	4.5	4.3	-0.39	-0.36
CYS123	iii(CAF)H	5	4.75	-0.91	-0.75
GLU199	iii(CAF)H	5	4.98	-2.87	-0.98
VAL202	iii(O)H	5.5	5.22	-0.28	-0.24
LEU284	i(CAH)H	5.5	5.31	-0.19	-0.16
VAL100	ii(CAO)H	6	5.63	-0.21	-0.17
LEU104	iii(CAA)H	6	5.85	-0.93	-0.22
ASN133	ii(CAM)H	6	5.6	0.60	0.12
VAL181	i(CAI)H	6	5.74	-0.03	-0.02
VAL281	i(CAT)CLAC	6	5.72	-0.19	-0.16
PHE282	i(CAT)CLAC	6	5.89	0.08	-0.14
GLN286	ii(CAP)H	6	5.9	-0.34	-0.15
THR103	iii(CAA)H	6.5	6.06	-0.20	-0.19
THR109	iii(CAA)H	6.5	6.32	0.13	0.04
PHE115	iii(CAG)H	6.5	6.47	-0.09	-0.07
TYR132	i(CAU)CLAD	6.5	6.08	0.00	0.00
VAL185	i(CAU)CLAD	6.5	6.34	-0.05	-0.01
ALA216	i(CAE)H	6.5	6.33	-0.27	-0.12
LEU221	i(CAE)H	6.5	6.47	-0.07	-0.04
PRO278	i(CAT)CLAC	6.5	6.28	0.07	-0.01
LEU301	ii(CAP)H	6.5	6.19	-0.37	-0.25
GLY308	ii(CAM)H	6.5	6.24	0.32	0.06
VAL55	iii(CAA)H	7	6.96	-0.09	-0.05
LEU112	iii(CAA)H	7	6.9	0.04	0.03
PRO117	iii(CAG)H	7	6.51	0.03	-0.02
PHE118	iii(CAG)H	7	6.71	0.03	-0.03
LEU122	iii(CAF)H	7	6.7	-0.16	-0.09
ALA128	iii(O)H	7	6.58	-0.31	-0.15
THR138	i(CAE)H	7	6.95	0.08	-0.02
SER190	iii(CAJ)H	7	6.99	-0.15	-0.07
CYS218	i(CAE)H	7	6.72	0.09	0.00
PHE222	i(CAE)H	7	6.83	0.18	0.05
ILE225	i(CAE)H	7	6.88	0.04	0.01
THR277	i(CAT)CLAC	7	6.71	-0.23	-0.12
ALA306	iii(CAL)H	7	6.72	-0.99	-0.11

ILE54	iii(CAA)H	7.5	7.14	0.00	0.00
PRO105	iii(CAA)H	7.5	7.13	-0.07	-0.05
LYS124	iii(CAJ)H	7.5	7.33	1.67	0.35
ILE129	ii(CAM)H	7.5	7.12	0.24	0.08
GLY189	iii(CAY)O	7.5	7.37	0.10	0.00
ALA191	iii(CAF)H	7.5	7.1	0.03	-0.03
PHE215	i(CAE)H	7.5	7.2	-0.10	-0.07
CYS304	ii(CAO)H	7.5	7.18	0.25	0.04
GLY114	iii(CAG)H	8	7.94	0.03	0.01
GLY119	iii(CAF)H	8	7.72	-0.10	-0.04
THR125	iii(O)H	8	7.98	-0.09	-0.06
THR136	i(CAI)H	8	7.78	0.14	0.02
GLY182	i(CAU)CLAD	8	7.98	-0.14	-0.05
ILE198	iii(CAF)H	8	7.8	0.00	0.00
ILE217	i(CAE)H	8	7.88	-0.14	-0.06
PRO227	i(CAE)H	8	7.76	0.11	0.01
PHE272	ii(CM)H	8	7.86	-0.19	-0.10
LEU113	iii(CAG)H	8.5	8.43	0.07	0.00
SER137	i(CAI)H	8.5	8.44	0.17	0.02
CYS275	i(CAT)CLAC	8.5	8.13	-0.03	-0.02
ALA285	i(CAT)CLAC	8.5	8.33	0.11	0.01
SER312	ii(CAO)H	8.5	8.18	0.02	0.01
LEU46	iii(CAA)H	9	8.64	-0.04	-0.02
LYS51	iii(CAA)H	9	8.9	1.84	0.44
ASN120	iii(CAF)H	9	8.85	-0.11	-0.04
ALA178	i(CAI)H	9	8.9	-0.13	-0.04
ALA186	iii(O)H	9	8.95	-0.06	-0.03
GLN192	iii(CAF)H	9	8.54	-0.14	-0.05
GLY287	ii(CAM)H	9	8.54	0.06	0.00
VAL298	iii(CAK)H	9	8.56	-0.22	-0.08
PHE303	iii(CAL)H	9	8.67	-0.09	-0.05
LEU307	ii(CAO)H	9	8.81	0.13	0.01
PHE139	i(CAI)H	9.5	9.35	0.04	-0.01
GLU203	iii(CAY)O	9.5	9.47	-1.88	-0.48
VAL226	i(CAE)H	9.5	9.12	0.08	0.01
VAL228	i(CAE)H	9.5	9.29	0.06	0.01
ASN311	ii(CAM)H	9.5	9.23	0.26	0.05
LEU102	iii(CAA)H	10	9.83	0.06	0.00
ALA121	iii(CAF)H	10	9.83	-0.10	-0.03
ILE204	ii(CAN)H	10	9.84	-0.02	-0.02
VAL273	i(CAT)CLAC	10	9.71	-0.18	-0.06
VAL310	ii(CAO)H	10	9.52	2.41	-0.02