SUPPORTING INFORMATION

Predicting the Molecular Mechanism of CRIP1a–Cannabinoid 1 Receptor Interactions: Integration of Multiple Molecular Modeling Approaches

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Table S1. Algorithms used for detection of templates for CRIP1a with their generated results.

Algorithm	**Predicted template PDB ID (Chain ID)**									
pdbblast	3fcg (A)	2vl6 (A)	2p0o (A)	1x13 (A)	3nx6 (A)					
csblast	3fcg (A)	3nx6 (A)	1sif (A)	1o4y (A)	2drh (A)	2wp8 (A)	3lvf (O)	2j63 (A)	2r9q (A)	2cio (B)
coma	2hzp (A)									
hhblits	3g5w (A)	2k5l (A)	2k4y (A)	2h3j (A)	1ywu (A)	2l74 (A)	2v8f (A)	1qkl (A)	1yfm (A)	3hym (A)
prc	1oyw (A)	2axl (A)								
blastp	2vl6 (A)	2p0o (A)	3fcg (A)							
ffas	1qkl (A)	2pa2 (A)	3mep (A)	2qex (H)	3h0g (F)	2jhs (A)	2jht (A)	2jhw (A)	2bxw (A)	3kg6 (A)
hhsearch	2b39 (A)	2ec8 (A)	1l0q (A)	1aoh (A)	1jly (A)	1kmt (A)	1cyg (A)	3bws (A)	2eys (A)	2pn5 (A)
Sp3	1kbv (A)	1fso (A)	1j9q (A)	1iaz (A)	1eok (A)	1dss (G)	1acc (A)	1amp (A)	1qou (A)	1k8k (D)
phyre	2ha1 (A)	1m1x (A)	1wfj (A)	1hr0 (W)	1qg3 (B)	2yx2 (A)	2gcx (A)	2dmc (A)	1zru (A)	2e9j (A)
Pcons5	3g5w (A)	3g5w (A)	3fcg (A)	3pjl (A)	3fcg (A)	2jhw (A)	1qkl (A)	2jhs (A)	2bxw (A)	2jht (A)
jmbrank	3g5w (A)	3g5w (A)	3fcg (A)	3pjl (A)	3fcg (A)	2jhw (A)	1qkl (A)	2jhs (A)	2bxw (A)	2jht (A)
consens3d	2bxw (A)	2jhs (A)	2jhw (A)	2jht (A)	3g5w (A)	2qex (H)	2pa2 (A)	3kg6 (A)	1mpx (A)	3pjl (A)

Table S2. Generated Models arranged according to their calculated dope scores from lowest score to highest score (lower scores indicate better models).

Model	DOPE Score	Model	DOPE Score
Model_1DS6_A_1R17_A	-14212	LOMETS_model4	-7658.9
Model_1DS6_A	-13929	MUSTER_model1	-7658.9
Bhageerath_model1	-12264	Model_2gtq_A	-7649.2
I-Tasser_model5	-11508	Model_3bws_A	-7644.7
Robetta_Model3	-11449	Model_1jly_A	-7458.1
MUSTER_model8	-10908	RaptorX_model4	-7438.9
Robetta_Model1	-10768	Model_2ha1_A	-7397.7
Quark ab initio_model1	-10617	Model_2hlv_A	-7275.8
Quark ab initio_model7	-10517	Model_3mep_A	-7243.4
Model_2jhs_A	-10347	Quark ab initio_model4	-7131
Model_2bxw_A	-10300	Model_1iaz_A	-7124.7
Robetta_Model5	-10281	LOMETS_model9	-7109.5
Robetta_Model4	-10174	MUSTER_model2	-7056.5
Model_1eok_A	-10090	Model_1x13_A	-7034.3
Model_1kmt_A	-9837.2	Model_1l0q_A	-7032.9
I-Tasser_model4	-9804.4	Model_1aoh_A	-7026.5
LOMETS_model5	-9680	Model_3h0g_F	-6858.6
MUSTER_model3	-9666.6	Model_2hzp_A	-6848.2
Model_1fso_A	-9650.6	Model_2r9q_A	-6847.9
Model_2jht_A	-9590.3	MUSTER_model9	-6796.4
RaptorX_model6	-9535.8	LOMETS_model1	-6792.5

Quark ab initio_model5	-9421.8	MUSTER_model4	-6792.5
Quark ab initio_model2	-9419	LOMETS_model2	-6673.7
RaptorX_model8	-9407.7	Model_2qex_H	-6659.5
Robetta_Model2	-9378.8	Model_3ju4_A	-6633.8
I-Tasser_model1	-9373.8	Model_3pjl_A	-6594
Model_1cyg_A	-9336.9	Model_2gcx_A	-6591.2
Quark ab initio_model3	-9249	MUSTER_model7	-6559.3
Model_3kg6_A	-9191.6	Model_1qg3_B	-6542.1
Quark ab initio_model6	-9177.8	Model_1x9p_A	-6459.8
I-Tasser_model2	-9134.8	Model_2yx2_A	-6458
Model_2jhw_A	-9128.9	Model_3lvf_O	-6425.6
Quark ab initio_model10	-9045.5	Model_1qkl_A	-6329.2
Bhageerath_model5	-9016.9	Model_2k4y_A	-6274.4
RaptorX_model2	-8942.4	LOMETS_model3	-6246
Model_3g5w_A	-8779.1	Model_3fcg_A	-6234.3
Model_1amp_A	-8766.4	Model_2pn5_A	-6221.9
Quark ab initio_model9	-8732.1	Model_2h3j_A	-6204.1
LOMETS_model8	-8594.6	Model_2b39_A	-6089.5
RaptorX_model5	-8536.5	Model_2vl6_A	-6054.3
Model_4a1r_A	-8500.7	Model_3hym_A	-6046.9
Quark ab initio_model8	-8392.6	Model_1o4y_A	-5972.4
RaptorX_model9	-8260.9	Model_1ywu_A	-5954.5
Model_1j9q_A	-8252.6	Model_1oyw_A	-5939.6
Model_1acc_A	-8182.4	Model_1hr0_W	-5924.5
Model_1qou_A	-8160.8	Model_2axl_A	-5818.5

MUSTER_model6	-8159.5	Model_1sdd_A	-5739.3
Model_1wfj_A	-8140.2	Model_1yfm_A	-5700.4
Model_1kbv_A	-8088.8	Model_3nx6_A	-5661.3
Model_2ec8_A	-8070.9	Model_2l74_A	-5618.9
MUSTER_model5	-8070.2	Model_1sif_A	-5602.9
RaptorX_model10	-8052	Model_1mpx_A	-5585.4
Model_1dss_G	-8030.8	Model_3tp4_A	-5574.9
RaptorX_model3	-8001	Model_2k5l_A	-5465
MUSTER_model10	-7999.7	Model_2drh_A	-5338.7
Model_2dmc_A	-7993.5	Model_2v8f_A	-5306.6
RaptorX_model1	-7919.1	Model_2p0o_A	-5212.3
RaptorX_model7	-7874.5	Model_2e9j_A	-4805.4
Model_2pa2_A	-7727.3	Model_2j63_A	-4636.7
Model_1m1x_A	-7693.6	Model_2wp8_A	-3823.5
Model_1k8k_D	-7677.5	Model_1zru_A	-2695

Table S3. HINT table for the highest score CRIP1a-CB1R complex model.

Monomer Name	Atom Name	Monomer Name	Atom Name	Distance		Interaction	
				Angstroms	VDW	Score	Type
GLU60	O	THR4	OG1	4.991	166.36	24	Acid/Base
ASN61	O	THR4	OG1	2.925	97.51	238	Hydrogen Bond
ASN61	O	THR4	CG2	4.689	146.54	-26	Hydroph./Polar
ILE62	O	THR4	OG1	5.545	184.84	13	Acid/Base
ILE62	CD1	THR4	OG1	5.845	182.65	-12	Hydroph./Polar
ILE62	CD1	THR4	CG2	4.648	136.7	33	Hydrophobic
SER63	O	THR4	CG2	4.791	149.7	-21	Hydroph./Polar
SER63	CB	THR4	CG2	4.595	135.16	15	Hydrophobic
SER63	CB	SER5	CB	4.116	121.07	12	Hydrophobic
SER63	CB	SER5	OG	3.079	96.21	-27	Hydroph./Polar
SER63	OG	THR4	OG1	4.125	137.5	-17	Acid/Acid
SER63	OG	THR4	CG2	4.641	145.03	-16	Hydroph./Polar
SER63	OG	SER5	OG	4.119	137.29	-14	Acid/Acid
ILE64	O	SER5	CB	3.727	116.48	-23	Hydroph./Polar
ILE64	O	SER5	OG	2.721	90.69	128	Hydrogen Bond
ILE64	CG2	SER5	OG	5.28	164.99	-12	Hydroph./Polar
GLY65	CA	SER5	O	3.789	118.42	-25	Hydroph./Polar
GLY65	CA	SER5	CB	3.804	111.88	17	Hydrophobic
GLY65	CA	SER5	OG	3.66	114.37	-13	Hydroph./Polar
GLY65	O	SER5	O	4.545	151.49	-29	Base/Base
VAL67	CG1	ALA8	O	4.398	137.44	-32	Hydroph./Polar
VAL67	CG1	ALA8	CB	4.029	118.51	57	Hydrophobic
VAL67	CG1	LEU9	OXT	3.439	107.48	-103	Hydroph./Polar
VAL67	CG1	LEU9	OX2	4.333	135.41	-58	Hydroph./Polar
VAL67	CG2	SER5	O	3.914	122.32	-47	Hydroph./Polar
VAL67	CG2	ALA6	CB	5.298	155.81	16	Hydrophobic
VAL67	CG2	ALA8	O	5.196	162.36	-14	Hydroph./Polar
VAL67	CG2	ALA8	CB	4.204	123.66	47	Hydrophobic
VAL67	CG2	LEU9	OXT	5.774	180.44	-10	Hydroph./Polar
VAL67	CG2	LEU9	OX2	5.998	187.43	-12	Hydroph./Polar
LEU68	O	LEU9	OXT	4.989	166.31	-19	Base/Base
VAL69	CG2	LEU9	OXT	4.863	151.98	-25	Hydroph./Polar
VAL69	CG2	LEU9	CB	4.083	120.09	12	Hydrophobic
VAL69	CG2	LEU9	CD1	4.203	123.63	42	Hydrophobic
VAL69	CG2	LEU9	CD2	5.536	162.81	11	Hydrophobic
PRO70	CG	LEU9	OXT	4.956	154.89	-12	Hydroph./Polar

PRO70	CG	LEU9	CD1	4.686	137.82	14	Hydrophobic
PRO70	CG	LEU9	CD2	4.382	128.88	19	Hydrophobic
PRO70	CD	LEU9	OXT	3.806	118.94	-23	Hydroph./Polar
PRO70	CD	LEU9	CD1	4.477	131.68	12	Hydrophobic
PRO70	CD	LEU9	CD2	4.193	123.32	16	Hydrophobic
LEU71	O	LEU9	CD1	4.345	135.78	-29	Hydroph./Polar
LEU73	CD2	LEU9	CD1	4.724	138.93	27	Hydrophobic
LEU73	CD2	LEU9	CD2	4.317	126.96	39	Hydrophobic
LYS76	NZ	ALA8	O	5.468	179.27	16	Acid/Base
LYS76	NZ	LEU9	OXT	3.39	111.14	149	Hydrogen Bond
LYS76	NZ	LEU9	OX2	3.52	115.43	116	Hydrogen Bond
ASP81	CB	ALA6	CB	4.281	125.9	18	Hydrophobic
ASP81	OD1	ALA6	CB	3.642	113.81	-188	Hydroph./Polar
ASP81	OD2	SER5	CB	5.438	169.93	-13	Hydroph./Polar
ASP81	OD2	ALA6	CB	3.707	115.84	-176	Hydroph./Polar
ARG82	O	SER5	CB	3.223	100.71	-46	Hydroph./Polar
ARG82	O	SER5	OG	3.247	108.24	146	Hydrogen Bond
VAL83	O	SER5	OG	5.541	184.7	14	Acid/Base
VAL83	CG1	ASP3	CB	4.103	120.68	19	Hydrophobic
VAL83	CG1	ASP3	OD1	3.569	111.53	-167	Hydroph./Polar
VAL83	CG1	ASP3	OD2	4.787	149.58	-50	Hydroph./Polar
VAL83	CG1	SER5	CB	4.449	130.85	16	Hydrophobic
VAL83	CG1	SER5	OG	5.147	160.84	-13	Hydroph./Polar
VAL83	CG1	ALA6	CB	4.949	145.56	22	Hydrophobic
VAL83	CG2	ASP3	OD1	4.888	152.75	-45	Hydroph./Polar
VAL84	O	SER5	OG	4.46	148.67	35	Acid/Base
TYR85	CE1	ASP3	OD1	3.672	114.74	-35	Hydroph./Polar
TYR85	OH	ASP3	CB	3.965	123.9	-28	Hydroph./Polar
TYR85	OH	ASP3	OD1	3.06	102.01	451	Hydrogen Bond
TYR85	OH	ASP3	OD2	4.569	152.31	87	Acid/Base
GLN122	O	ALA8	CB	4.679	146.21	-27	Hydroph./Polar
GLN122	CB	ALA8	CB	3.963	116.54	17	Hydrophobic
GLN122	CG	ALA8	CB	4.611	135.62	12	Hydrophobic
GLN122	OE1	ALA8	O	5.749	191.63	-13	Base/Base
GLN122	OE1	ALA8	CB	3.606	112.69	-122	Hydroph./Polar
GLN122	OE1	LEU9	OXT	5.146	171.53	-29	Base/Base
GLN122	OE1	LEU9	CB	4.313	134.79	-10	Hydroph./Polar
GLN122	NE2	ALA8	CB	4.405	135.54	-22	Hydroph./Polar
LYS124	CD	GLU7	O	3.273	102.27	-10	Hydroph./Polar
LYS124	CD	ALA8	CB	4.219	124.09	10	Hydrophobic

LYS124	NZ	GLU7	O	2.834	92.92	166	Hydrogen Bond
LYS124	NZ	ALA8	CB	4.022	123.75	-56	Hydroph./Polar
TYR126	O	THR4	OG1	4.689	156.31	23	Acid/Base
TYR126	O	THR4	CG2	3.234	101.07	-97	Hydroph./Polar
TYR126	CB	THR4	CG2	4.5	132.34	11	Hydrophobic
ASN127	O	THR2	O	5.384	179.48	-12	Base/Base
ASN127	O	THR4	OG1	3.435	114.49	54	Hydrogen Bond
ASN127	O	THR4	CG2	3.85	120.3	-59	Hydroph./Polar
TYR128	O	SER1	O	5.34	178	-11	Base/Base
TYR128	O	THR2	O	3.441	114.69	-70	Base/Base
TYR128	CB	THR4	OG1	3.693	115.41	-11	Hydroph./Polar
TYR128	CE1	THR2	O	3.853	120.4	-11	Hydroph./Polar
TYR128	OH	THR2	OG1	4.938	164.61	-14	Acid/Acid
TYR128	OH	THR2	CG2	4.082	127.57	-46	Hydroph./Polar
LYS130	CG	GLU7	OE1	4.676	146.14	-10	Hydroph./Polar
LYS130	CD	GLU7	OE1	3.292	102.87	-37	Hydroph./Polar
LYS130	NZ	SER1	NI	4.704	151.75	-22	Acid/Acid
LYS130	NZ	SER1	O	2.652	86.95	223	Hydrogen Bond
LYS130	NZ	THR2	O	3.115	102.13	154	Hydrogen Bond
LYS130	NZ	ASP3	O	3.159	103.56	132	Hydrogen Bond
LYS130	NZ	THR4	O	4.391	143.96	38	Acid/Base
LYS130	NZ	THR4	CG2	5.285	162.62	-13	Hydroph./Polar
LYS130	NZ	ALA6	O	5.516	180.86	16	Acid/Base
LYS130	NZ	GLU7	OE1	3.158	103.54	302	Hydrogen Bond
LYS130	NZ	GLU7	OE2	5.31	174.1	36	Acid/Base
SER141	OG	ALA8	CB	5.601	175.03	-10	Hydroph./Polar

Total Interaction Constant 7.556328e+02

Contributions:

2.368696e+03 Hydrogen Bond

6.564771e+02 Acid/Base

9.198014e+02 Hydrophobic

-1.795490e+02 Acid/Acid

-5.790793e+02 Base/Base

-2.430713e+03 Hydroph./Polar