Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Table 1: Description of the GluR2 residues interacting with FW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 2.0 to 10.0 Å

Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)	Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)
T480	**i**(C9)O91; **i**(N8)H	1.84; 1.96	2.0	-11.21(-20.06)	G733	**i**(N8)H	6.80	7.0	-0.48(-0.49)
R485	**i**(C9)O91; **i**(C9)O92	1.75; 1.88	2.0	-24.29(-32.79)	S403	**ii**(C5)F	7.17	7.5	-0.62(-0.65)
T655	**ii**(C2)O2; **ii**(N3)H	1.95, 2.38; 1.90	2.0	-8.80(-19.94)	D651	**ii**(N3)H	7.46	7.5	-0.62(-0.62)
E705	**i**(N8)H; **ii**(C4)O4	1.95; 1.99	2.0	-51.21(-63.95)	V683	**ii**(C4)O4	7.38	7.5	0.08(-0.02)
P478	**i**(N8)H	2.01	2.5	-13.97(-17.61)	A687	**ii**(C5)F	7.47	7.5	0.44(0.45)
S654	**i**(C9)O92	2.01	2.5	-19.53(-28.77)	F495	**i**(N8)H	7.72	8.0	0.02(-0.01)
L704	**ii**(C4)O4	2.34	2.5	-4.95(-7.45)	G499	**ii**(C4)O4	7.54	8.0	-0.65(-0.68)
Y732	**i**(N8)H	2.37	2.5	-1.31(-4.22)	M503	**ii**(C4)O4	7.87	8.0	-4.38(-2.03)
Y450	**i**(N8)H	2.82, 4.33	3.0	-15.60(-28.08)	G648	**ii**(C4)O4	7.89	8.0	-1.16(-1.19)
L479	**i**(C9)O91	2.71	3.0	-10.28(-14.07)	G689	**ii**(C4)O4	7.68	8.0	0.01(0.01)
L650	**ii**(C5); **ii**(C4)O4	2.95; 4.09	3.0	-10.36(-19.55)	V690	**ii**(C5)F	7.89	8.0	0.05(0.06)
G653	**i**(C7)H	2.60	3.0	-12.83(-15.53)	L401	**ii**(C6)H	8.41	8.5	0.03(0.01)
T686	**ii**(C5)F	2.71	3.0	-0.98(-1.71)	P404	**ii**(C5)F	8.44	8.5	0.06(0.04)
M708	**ii**(C6)H; **ii**(C5)F	2.53; 2.86	3.0	-5.96(-7.52)	G448	**i**(C7)H	8.02	8.5	-0.30(-0.33)
E402	**ii**(C6)H	3.88	4.0	-7.33(-7.73)	W460	**i**(C9)O92	8.34	8.5	-0.26(-0.31)
K656	**ii**(C2)O2	3.91; 4.14	4.0	-6.07(-8.78)	G462	**i**(C9)O92	8.34	8.5	0.04(-0.01)
S652	**i**(C7)H	4.03	4.5	-3.63(-3.79)	I489	**i**(C9)O91	8.30	8.5	0.12(0.15)
L703	**ii**(C4)O4	4.46	4.5	-1.39(-1.48)	R684	**ii**(C6)H	8.44	8.5	3.98(3.76)
I500	**ii**(N3)H	4.69	5.0	-0.56(-0.76)	I712	**ii**(C5)F	8.07	8.5	-0.08(-0.09)
T649	**ii**(N3)H	4.59	5.0	-2.38(-2.43)	V445	**i**(C7)H	8.98	9.0	-0.93(-0.97)
Y702	**ii**(C4)O4	4.61	5.0	1.76(-0.44)	N461	**i**(C9)O92	8.75	9.0	0.14(0.06)
I400	**i**(C7)H	5.23	5.5	-1.17(-1.31)	A475	**i**(C9)O91	8.97	9.0	0.32(0.33)
G451	**i**(C9)O92	5.32	5.5	1.91(1.88)	V484	**i**(C9)O92	8.52	9.0	-0.88(-0.89)
T482	**i**(C9)O91	5.37	5.5	-0.82(-0.71)	M496	**i**(N8)H	8.50	9.0	-4.82(-2.47)
L498	**i**(N8)H	5.15	5.5	0.10(-0.03)	I502	**ii**(C4)O4	8.95	9.0	-0.18(-0.21)
K730	**i**(C7)H	5.26	5.5	2.87(2.57)	F682	**ii**(N3)H	8.56	9.0	-0.20(-0.24)
Y405	**ii**(C5)F	5.55	6.0	0.42(0.30)	Y711	**ii**(C5)F	8.55	9.0	0.0003(-0.05)
M463	**i**(C9)O91	5.54	6.0	-4.93(-2.72)	D728	**ii**(N3)H	8.83	9.0	-0.93(-0.93)
I481	**i**(C9)O91	5.87	6.0	-1.26(-1.37)	A735	**i**(C9)O91	8.88	9.0	-0.41(-0.43)
E657	**ii**(C2)O2	5.70	6.0	3.82(3.64)	W767	**ii**(C5)F	8.59	9.0	-0.02(-0.02)
V464	**i**(C9)O91	6.45	6.5	-1.68(-1.75)	C425	**i**(N8)H	9.41	9.5	-5.00(-2.80)
A477	**i**(N8)H	6.17	6.5	1.04(1.07)	M674	**ii**(N3)H	9.46	9.5	-0.04(-0.05)
F491	**i**(C9)O91	6.23	6.5	0.10(0.06)	**E688**	**ii**(C5)F	9.27	9.5	1.47(1.35)
S501	**ii**(C4)O4	6.37	6.5	-0.16(-0.18)	E710	**ii**(C5)F	9.03	9.5	-3.93(-3.97)
S706	**ii**(C4)O4	6.37	6.5	-0.27(-0.35)	L727	**ii**(N3)H	9.17	9.5	0.13(0.12)
T707	**i**(N8)H	6.30	6.5	-0.52(-0.73)	T399	**i**(N8)H	9.53	10.0	-0.30(-0.30)
N709	**ii**(C4)O4	6.46	6.5	-2.67(-2.91)	V406	**ii**(C6)H	9.98	10.0	0.06(0.06)
G731	**i**(N8)H	6.14	6.5	0.71(0.69)	R453	**i**(C9)O92	9.57	10.0	-0.69(-0.64)
K449	**i**(C7)H	6.94	7.0	0.03(0.02)	I476	**i**(N8)H	9.54	10.0	0.78(0.81)
A452	**i**(C9)O92	6.74	7.0	-1.30(-1.46)	S497	**i**(N8)H	9.61	10.0	-0.52(-0.50)
F658	**ii**(C2)O2	6.63	7.0	-0.75(-0.83)	R660	**ii**(C2)O2	9.94	10.0	-3.17(-3.04)
F659	**ii**(N3)H	6.78	7.0	-0.20(-0.22)	Y700	**ii**(C4)O4	10.0	10.0	-0.14(-0.17)
T685	**ii**(C5)F	6.90	7.0	0.25(0.22)					

Table 2: Description of the GluR2 residues interacting with FW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 10.5 to 12.0 Å

Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)	Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)
G465	**i**(C9)O91	10.38	10.5	-0.71(-0.77)	S729	**i**(N8)H	10.68	11.0	0.31(0.31)
L467	**i**(C9)O91	10.23	10.5	-0.74(-0.75)	Y424	**i**(N8)H	11.19	11.5	-0.85(-0.89)
L483	**i**(C9)O91	10.26	10.5	-1.82(-1.81)	D447	**i**(C7)H	11.22	11.5	0.87(0.75)
E486	**i**(C9)O91	10.29	10.5	-6.16(-6.18)	R661	**i**(C9)O92	11.32	11.5	-2.68(-2.68)
P494	**i**(N8)H	10.07	10.5	0.47(0.47)	M670	**ii**(N3)H	11.28	11.5	-0.06(-0.04)
W671	**ii**(N3)H	10.43	10.5	-0.19(-0.15)	A691	**ii**(C4)O4	11.41	11.5	0.30(0.30)
V693	**ii**(C4)O4	10.42	10.5	-0.06(-0.10)	E713	**ii**(C5)F	11.44	11.5	-1.37(-1.48)
I734	**i**(C9)O91	10.12	10.5	-0.11(-0.11)	M407	**ii**(C5)F	11.87	12.0	-0.09(-0.10)
T398	**i**(C9)O91	10.75	11.0	-0.04(-0.04)	L428	**i**(N8)H	11.77	12.0	0.78(0.85)
V681	**ii**(C4)O4	10.9	11.0	-0.05(-0.08)	V488	**i**(C9)O91	11.74	12.0	0.25(0.28)
A701	**ii**(C4)O4	10.84	11.0	-0.80(-0.86)	Y647	**ii**(C4)O4	11.54	12.0	-0.88(-0.86)
K722	**ii**(C4)O4	10.51	11.0	2.54(2.48)	R692	**ii**(C4)O4	11.82	12.0	-1.52(-1.58)
N726	**ii**(N3)H	10.92	11.0	0.27(0.26)	K763	**ii**(C5)F	11.83	12.0	1.30(1.30)

Table 3: Description of the GluR2 residues interacting with HW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 2.0 to 10.0 Å

Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)	Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)
T480	**i**(C9)O91; **i**(N8)H	1.90; 2.15	2.0	-10.73(-18.67)	G733	**i**(N8)H	6.69	7.0	-0.81(-0.83)
R485	**i**(C9)O91; **i**(C9)O92	1.81; 1.84	2.0	-28.34(-36.44)	S403	**ii**(C5)H	7.50	7.5	-0.57(-0.61)
T655	**ii**(C2)O2; **ii**(N3)H	2.03, 2.43; 1.87	2.0	-10.37(-20.78)	D651	**ii**(C2)O2	7.43	7.5	0.92(0.96)
E705	**i**(N8)H; **ii**(C4)O4	1.96; 1.97	2.0	-47.77(-60.84)	T685	**ii**(C5)H	7.10	7.5	0.41(0.37)
P478	**i**(N8)H	2.02	2.5	-14.51(-17.97)	F495	**i**(N8)H	7.69	8.0	-0.002(-0.03)
S654	**i**(C9)O92	2.06	2.5	-20.74(-28.10)	G499	**ii**(C4)O4	7.56	8.0	-0.76(-0.80)
L704	**ii**(C4)O4	2.25	2.5	-4.70(-7.57)	M503	**ii**(C4)O4	7.94	8.0	-4.60(-2.32)
M708	**i**(C7)H; **ii**(C5)H	2.53; 2.38	2.5	-6.09(-8.93)	V683	**ii**(C4)O4	7.69	8.0	-1.29(-1.26)
L650	**i**(C7); **ii**(C4)O4	2.15; 4.15	2.5	-10.64(-19.76)	A687	**ii**(C5)H	7.66	8.0	0.72(0.77)
Y450	**i**(N8)H	2.89, 4.40	3.0	-14.00(-25.71)	G689	**ii**(C4)O4	7.82	8.0	0.30(0.32)
L479	**i**(C9)O91	2.64	3.0	-9.45(-13.25)	L401	**ii**(C6)H	8.39	8.5	-0.23(-0.24)
G653	**i**(C7)H	2.69	3.0	-15.36(-18.08)	G448	**i**(C7)H	8.22	8.5	-0.20(-0.22)
T686	**ii**(C5)H	2.93	3.0	-0.19(-0.84)	W460	**i**(C9)O92	8.24	8.5	-0.32(-0.34)
Y732	**i**(N8)H	2.52	3.0	-1.94(-4.51)	G462	**i**(C9)O92	8.33	8.5	-0.18(-0.24)
E402	**ii**(C6)H	3.76	4.0	-8.55(-9.08)	I489	**i**(C9)O91	8.29	8.5	0.19(0.23)
S652	**i**(C7)H	3.93	4.0	-6.00(-6.36)	G648	**ii**(C4)O4	8.02	8.5	-1.78(-1.84)
K656	**ii**(C2)O2	4.00	4.0	-1.07(-2.44)	V690	**ii**(C4)O4	8.05	8.5	0.23(0.22)
L498	**i**(N8)H	4.75	5.0	-0.03(-0.18)	I712	**ii**(C5)H	8.36	8.5	-0.07(-0.01)
I500	**ii**(N3)H	4.7	5.0	-0.64(-0.84)	P404	**ii**(C5)H	8.69	9.0	0.02(-0.01)
T649	**ii**(N3)H	4.67	5.0	-2.66(-2.72)	N461	**i**(C9)O92	8.91	9.0	1.34(1.34)
Y702	**ii**(C4)O4	4.56	5.0	-1.70(-0.59)	V484	**i**(C9)O92	8.67	9.0	-0.91(-0.93)
L703	**ii**(C4)O4	4.52	5.0	-1.30(-1.36)	M496	**i**(N8)H	8.58	9.0	-5.02(-2.75)
I400	**i**(C7)H	5.31	5.5	-1.56(-1.69)	I502	**ii**(C4)O4	8.97	9.0	-0.17(-0.19)
G451	**i**(C9)O92	5.3	5.5	2.28(2.30)	F682	**ii**(N3)H	8.67	9.0	-0.41(-0.44)
T482	**i**(C9)O91	5.41	5.5	0.07(0.24)	R684	**i**(C7)H	8.51	9.0	6.75(6.67)
K730	**i**(C7)H	5.45	5.5	1.94(1.63)	Y711	**ii**(C5)H	8.80	9.0	0.30(0.37)
Y405	**ii**(C5)H	5.76	6.0	0.48(0.37)	D728	**ii**(N3)H	8.91	9.0	-0.81(-0.81)
M463	**i**(C9)O91	5.58	6.0	-5.48(-3.35)	A735	**i**(C9)O91	8.94	9.0	-0.52(-0.53)
I481	**i**(N8)H	5.92	6.0	-1.25(-1.34)	W767	**ii**(C5)H	8.78	9.0	-0.01(-0.02)
E657	**ii**(C2)O2	5.8	6.0	5.17(5.07)	V445	**i**(C7)H	9.07	9.5	-0.14(-0.13)
T707	**i**(N8)H	5.75	6.0	1.12(1.03)	A475	**i**(C9)O91	9.00	9.5	0.29(0.28)
V464	**i**(C9)O91	6.44	6.5	-2.32(-2.36)	**E688**	**ii**(C5)H	9.46	9.5	1.53(1.49)
A477	**i**(N8)H	6.19	6.5	1.26(1.32)	E710	**ii**(C4)O4	9.09	9.5	-4.14(-4.14)
F491	**i**(C9)O91	6.33	6.5	0.20(0.17)	L727	**ii**(N3)H	9.27	9.5	0.07(0.06)
S501	**ii**(C4)O4	6.32	6.5	-0.06(-0.08)	T399	**i**(N8)H	9.57	10.0	-0.76(-0.77)
S706	**ii**(C4)O4	6.37	6.5	-0.10(-0.15)	V406	**ii**(C6)H	9.96	10.0	-0.04(-0.05)
N709	**ii**(C4)O4	6.36	6.5	-1.95(-2.07)	C425	**i**(N8)H	9.51	10.0	-5.14(-2.97)
G731	**i**(N8)H	6.29	6.5	0.36(0.34)	R453	**i**(C9)O92	9.65	10.0	-1.67(-1.69)
K449	**i**(C7)H	6.99	7.0	-0.04(-0.08)	I476	**i**(N8)H	9.64	10.0	0.57(0.58)
A452	**i**(C9)O92	6.81	7.0	-2.67(-2.84)	S497	**i**(N8)H	9.93	10.0	-0.41(-0.39)
F658	**ii**(C2)O2	6.71	7.0	-0.58(-0.65)	M674	**ii**(N3)H	9.86	10.0	-0.01(-0.02)
F659	**ii**(N3)H	6.83	7.0	-0.21(-0.23)					

Table 4: Description of the GluR2 residues interacting with HW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 10.5 to 12.0 $\mathrm{\AA}$

Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)	Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)
G465	**i**(C9)O91	10.43	10.5	-0.17(-0.18)	D447	**i**(C7)H	11.34	11.5	1.80(1.62)
L467	**i**(C9)O91	10.34	10.5	-0.69(-0.74)	M670	**ii**(N3)H	11.37	11.5	-0.04(-0.04)
L483	**i**(C9)O91	10.39	10.5	-2.12(-2.12)	V681	**ii**(C4)O4	11.07	11.5	-0.03(-0.03)
E486	**i**(C9)O91	10.42	10.5	-6.92(-6.99)	N726	**ii**(N3)H	11.07	11.5	0.37(0.35)
P494	**i**(N8)H	10.03	10.5	0.41(0.42)	S729	**i**(N8)H	11	11.5	0.32(0.32)
R660	**ii**(C2)O2	10.15	10.5	-4.60(-4.55)	R661	**i**(C9)O92	11.52	12	-3.21(-3.19)
V693	**ii**(C4)O4	10.47	10.5	0.10(0.06)	L428	**i**(N8)H	11.83	12	0.64(0.68)
Y700	**ii**(C4)O4	10.12	10.5	-0.11(-0.12)	V488	**i**(C9)O91	11.87	12	0.29(0.33)
K722	**ii**(C4)O4	10.47	10.5	2.52(2.44)	S492	**i**(N8)H	11.97	12	-0.17(-0.19)
I734	**i**(C9)O91	10.2	10.5	-0.15(-0.16)	Y647	**ii**(C4)O4	11.64	12	-1.42(-1.44)
T398	**i**(C9)O91	10.85	11	0.05(0.05)	A691	**ii**(C4)O4	11.53	12	0.28(0.28)
W671	**ii**(N3)H	10.72	11	-0.01(-0.001)	E713	**ii**(C5)H	11.67	12	-1.76(-1.76)
A701	**ii**(C4)O4	10.93	11	-0.57(-0.60)	K763	**ii**(C5)H	11.99	12	1.63(1.61)
Y424	**i**(N8)H	11.16	11.5	-0.61(-0.63)					

Table 5: Description of the GluR2 residues interacting with BrW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 2.0 to 10.0 Å

Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)	Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)
T480	**i**(C9)O91; **i**(N8)H	1.88; 2.11	2.0	-10.03(-17.21)	G733	**i**(N8)H	6.54	7.0	-0.87(-0.16)
R485	**i**(C9)O91; **i**(C9)O92	1.68; 1.74	2.0	-25.91(-32.97)	P404	**ii**(C5)Br	7.50	7.5	0.11(0.09)
T655	**ii**(C2)O2; **ii**(N3)H	2.03, 2.39; 1.91	2.0	-10.92(-19.82)	K449	**i**(C7)H	7.03	7.5	-1.31(0.30)
E705	**i**(N8)H; **ii**(C4)O4	1.84; 2.00	2.0	-51.24(-65.84)	D651	**ii**(C2)O2	7.33	7.5	-3.37(-2.15)
P478	**i**(N8)H	2.09	2.5	-13.47(-15.47)	R661	**ii**(C2)O2	7.43	7.5	-5.77(-3.85)
S654	**i**(C9)O92	2.04	2.5	-18.36(-23.79)	F495	**i**(N8)H	7.64	8.0	0.01(-0.02)
L704	**ii**(C4)O4	2.27	2.5	-8.55(-12.80)	G499	**ii**(C4)O4	7.53	8.0	-0.61(-0.64)
Y732	**i**(N8)H	2.27; 2.90	2.5	-4.12(-5.44)	M503	**ii**(C4)O4	7.77	8.0	23.09(10.16)
Y450	**i**(N8)H	3.00; 4.56	3.0	-16.13(-24.32)	G648	**ii**(N3)H	7.99	8.0	-3.55(-2.90)
L479	**i**(C9)O91	2.63	3.0	-19.16(-18.65)	V683	**ii**(C4)O4	7.65	8.0	-0.57(0.78)
G653	**i**(C9)O92	2.66	3.0	-22.78(-26.35)	T685	**ii**(C5)Br	7.52	8.0	-0.42(0.86)
T686	**ii**(C5)Br	2.93	3.0	-3.99(-3.69)	A687	**ii**(C5)Br	7.78	8.0	-0.59(0.48)
L650	**i**(C7); **ii**(C4)O4	3.05; 4.27	3.5	-13.13(-19.85)	G689	**ii**(C4)O4	7.80	8.0	-0.55(0.20)
M708	**ii**(C5)Br	3.09	3.5	25.80(8.45)	V690	**ii**(C5)Br	7.90	8.0	-1.04(0.28)
S652	**i**(C7)H	3.99	4.0	-6.55(-4.61)	Y711	**ii**(C5)Br	7.81	8.0	-0.24(-0.27)
K656	**ii**(C2)O2	3.99	4.0	-7.23(-9.24)	W767	**ii**(C5)Br	7.82	8.0	-3.70(-0.71)
E402	**ii**(C6)H	4.07	4.5	-7.45(-8.08)	I712	**ii**(C5)Br	7.91	8.5	-0.17(-0.17)
Y405	**ii**(C5)Br	4.85	5.0	-6.55(-0.92)	G448	**i**(C7)H	8.19	8.5	-0.95(-0.19)
L498	**i**(N8)H	4.55	5.0	-0.12(-0.28)	W460	**i**(C9)O92	8.45	8.5	-1.17(-1.26)
I500	**ii**(N3)H	4.87	5.0	-0.60(-0.78)	G462	**i**(C9)O92	8.25	8.5	-0.73(-0.79)
T649	**ii**(N3)H	4.54	5.0	-4.11(-3.07)	I489	**i**(C9)O91	8.27	8.5	-1.32(0.26)
Y702	**ii**(C4)O4	4.63	5.0	-1.51(-1.37)	L401	**ii**(C6)H	8.80	9.0	-2.66(-1.04)
L703	**ii**(C4)O4	4.57	5.0	-1.16(-1.27)	V445	**i**(C7)H	8.99	9.0	-1.90(-0.53)
I400	**i**(C7)H	5.36	5.5	-3.29(-1.85)	N461	**i**(C9)O92	8.73	9.0	1.50(1.53)
G451	**i**(C9)O92	5.28	5.5	1.15(1.88)	A475	**i**(C9)O91	8.96	9.0	-0.93(-0.08)
T482	**i**(C9)O91	5.21	5.5	-0.72(0.66)	V484	**i**(C9)O92	8.59	9.0	-1.36(0.09)
K730	**i**(N8)H	5.77	6.0	1.77(3.17)	M496	**i**(N8)H	8.56	9.0	25.66(11.44)
M463	**i**(C9)O91	5.73	6.0	27.20(12.58)	F682	**ii**(N3)H	8.62	9.0	-3.63(-1.21)
I481	**i**(N8)H	5.78	6.0	-3.75(-2.21)	R684	**i**(C7)H	8.53	9.0	3.62(5.56)
E657	**ii**(C2)O2	5.77	6.0	1.12(2.64)	E710	**ii**(C5)Br	8.64	9.0	-3.91(-3.94)
V464	**i**(C9)O91	6.44	6.5	-2.92(-3.00)	D728	**i**(C8)H	9.00	9.0	-3.11(-1.75)
A477	**i**(N8)H	6.25	6.5	-0.51(0.42)	A735	**i**(C9)O91	8.82	9.0	-1.48(-0.56)
F491	**i**(C9)O91	6.07	6.5	-0.09(-0.15)	C425	**i**(N8)H	9.43	9.5	27.20(12.13)
S501	**ii**(C4)O4	6.37	6.5	-0.13(-0.15)	I502	**ii**(C4)O4	9.38	9.5	-0.12(-0.14)
S706	**ii**(C4)O4	6.33	6.5	0.31(0.27)	L727	**ii**(N3)H	9.29	9.5	-1.79(-0.15)
T707	**ii**(C5)Br	6.20	6.5	-0.42(-0.83)	T399	**i**(N8)H	9.86	10.0	-2.12(-0.87)
N709	**ii**(C5)Br	6.48	6.5	-0.91(-1.00)	V406	**ii**(C5)Br	9.79	10.0	-0.06(-0.06)
G731	**i**(N8)H	6.19	6.5	0.53(1.26)	R453	**i**(C9)O92	9.61	10.0	-2.86(-0.84)
S403	**ii**(C5)Br	6.65	7.0	-0.88(-0.93)	I476	**i**(N8)H	9.68	10.0	-1.19(0.36)
A452	**i**(C9)O92	6.66	7.0	-1.83(-0.93)	S497	**i**(N8)H	9.82	10.0	-0.36(-0.37)
F658	**ii**(C2)O2	6.67	7.0	-2.96(-0.48)	R660	**ii**(C2)O2	9.99	10.0	-5.08(-3.07)
F659	**ii**(N3)H	6.83	7.0	-3.07(-0.72)	**E688**	**ii**(C5)Br	9.79	10.0	-1.02(0.67)

Table 6: Description of the GluR2 residues interacting with BrW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 10.5 to 12.0 Å

Residue	Atomic Group	d(Å)	r(Å)	$E_{GGA(LDA)}$	Residue	Atomic Group	d(Å)	r(Å)	$E_{GGA(LDA)}$
G465	**i**(C9)O92	10.25	10.5	-1.26(-1.34)	S729	**i**(N8)H	10.84	11.0	-1.36(-0.25)
L467	**i**(C9)O91	10.31	10.5	-1.01(-1.07)	M407	**ii**(C5)Br	11.46	11.5	-0.08(-0.08)
L483	**i**(C9)O91	10.18	10.5	-4.32(-2.67)	M670	**ii**(N3)H	11.27	11.5	-0.01(-0.01)
E486	**i**(C9)O91	10.32	10.5	-10.29(-8.67)	A691	**ii**(C4)O4	11.44	11.5	-0.27(0.76)
P494	**i**(N8)H	10.09	10.5	0.17(0.14)	E713	**ii**(C5)Br	11.07	11.5	-1.71(-1.83)
W671	**ii**(N3)H	10.49	10.5	0.02(0.02)	N726	**ii**(C4)O4	11.06	11.5	0.16(0.16)
M674	**ii**(N3)H	10.03	10.5	0.04(0.04)	K763	**ii**(C5)Br	11.28	11.5	0.44(2.18)
V693	**ii**(C4)O4	10.31	10.5	-1.12(0.30)	L428	**i**(N8)H	11.66	12.0	0.32(0.39)
Y700	**ii**(C4)O4	10.12	10.5	-3.03(-0.54)	D447	**i**(C9)O92	11.29	12.0	-1.00(0.36)
K722	**ii**(C4)O4	10.19	10.5	2.02(1.93)	V488	**i**(C9)O91	11.67	12.0	-1.21(0.25)
I734	**i**(C9)O91	10.17	10.5	-1.98(-0.42)	S492	**i**(N8)H	11.91	12.0	-0.44(-0.48)
T398	**i**(C9)O91	10.89	11.0	-1.76(-0.52)	Y647	**ii**(N3)H	11.64	12.0	-4.51(-2.02)
Y424	**i**(N8)H	10.95	11.0	-0.92(-0.95)	R692	**ii**(C4)O4	11.98	12.0	-2.53(-0.56)
V681	**ii**(C4)O4	10.93	11.0	-1.38(-0.09)	R715	**ii**(C5)Br	11.76	12.0	3.68(3.66)
A701	**ii**(C4)O4	10.91	11.0	-1.67(-0.79)					

Table 7: Description of the GluR2 residues interacting with IW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 2.0 to 10.0 Å

Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)	Residue	Atomic Group	d(Å)	r(Å)	EGGA(LDA)
T480	**i**(C9)O91; **i**(N8)H	1.87; 2.17	2.0	-7.38(-14.93)	N709	**ii**(C4)O4	6.51	7.0	-2.33(-3.36)
R485	**i**(C9)O91; **i**(C9)O92	1.71; 1.78	2.0	-23.47(-31.72)	G733	**i**(N8)H	6.61	7.0	-1.22(-0.98)
E705	**i**(N8)H; **ii**(C4)O4	1.78; 2.15	2.0	-53.80(-68.47)	F659	**ii**(N3)H	7.38	7.5	-2.42(-1.37)
P478	**i**(N8)H	2.00	2.5	-16.29(-20.02)	W767	**ii**(C5)I	7.46	7.5	-1.48(-0.001)
S654	**i**(C9)O92	2.02	2.5	-15.37(-22.46)	G448	**i**(C7)H	7.82	8.0	-0.46(-0.16)
T655	**ii**(C2)O2; **ii**(N3)H	2.03; 2.14	2.5	-9.88(-16.82)	F495	**i**(N8)H	7.55	8.0	0.82(-0.64)
L704	**ii**(C4)O4	2.42	2.5	-4.53(-7.20)	G499	**ii**(C4)O4	7.77	8.0	0.02(-0.50)
Y732	**i**(N8)H	2.18	2.5	-4.24(-7.85)	M503	**ii**(C4)O4	7.66	8.0	21.37(7.85)
Y450	**i**(N8)H	3.00, 4.55	3.0	-16.05(-26.76)	D651	**ii**(C2)O2	7.85	8.0	-2.41(-1.96)
L479	**i**(C9)O91	2.69	3.0	-27.27(-28.73)	V683	**ii**(C4)O4	7.72	8.0	0.68(1.35)
G653	**i**(C7)H	2.57	3.0	-7.59(-8.73)	T685	**ii**(C4)O4; **ii**(C5)	7.74; 7.74	8.0	-0.27(0.38)
M708	**ii**(C5)I	2.76	3.0	24.82(6.28)	A687	**ii**(C5)I	7.89	8.0	-0.35(0.26)
L650	**ii**(C4); **ii**(C4)O4	3.34; 5.75	3.5	-7.29(-10.69)	V690	**ii**(C4)O4	7.91	8.0	-0.91(-0.19)
T686	**ii**(C5)I	3.36	3.5	-3.95(-4.14)	Y711	**ii**(C5)I	7.53	8.0	0.43(-1.01)
E402	**ii**(C6)H	4.00	4.0	-7.32(-9.35)	I712	**ii**(C5)I	7.61	8.0	-0.21(-1.12)
K656	**ii**(C2)O2	3.99	4.0	-4.39(-3.79)	W460	**i**(C9)O92	8.24	8.5	0.79(-0.90)
Y702	**ii**(C4)O4	3.97	4.0	0.45(-1.56)	G462	**i**(C9)O92	8.18	8.5	-0.65(-1.18)
Y405	**ii**(C5)I	4.12	4.5	-0.09(-1.61)	I489	**i**(C9)O91	8.36	8.5	-0.62(0.15)
S652	**i**(C7)H	4.29	4.5	-2.06(-1.69)	M496	**i**(N8)H	8.50	8.5	25.65(10.57)
L498	**i**(N8)H	4.57	5.0	0.83(-0.13)	G648	**ii**(N3)H	8.34	8.5	-1.71(-1.54)
G451	**i**(C9)O92	5.22	5.5	4.04(4.64)	G689	**ii**(C4)O4	8.12	8.5	-0.25(0.15)
T482	**i**(C9)O91	5.26	5.5	-0.62(0.20)	L401	**ii**(C5)I	8.53	9.0	-1.93(-1.03)
I500	**ii**(N3)H	5.27	5.5	-0.05(-1.11)	C425	**i**(N8)H	8.75	9.0	26.07(10.55)
T649	**ii**(N3)H	5.06	5.5	-3.00(-2.46)	V445	**i**(C7)H	8.86	9.0	-0.58(0.15)
L703	**ii**(N3)H	5.02	5.5	-0.38(-1.37)	N461	**i**(C9)O92	8.78	9.0	1.62(0.83)
T707	**ii**(C5)I	5.38	5.5	-2.29(-3.88)	A475	**i**(C9)O91	8.99	9.0	-0.55(-0.26)
K730	**i**(C7)H	5.39	5.5	3.63(3.70)	V484	**i**(C9)O92	8.88	9.0	0.45(1.52)
I400	**i**(C7)H	5.61	6.0	-3.00(-2.43)	R684	**i**(C7)H	9.00	9.0	5.49(6.12)
M463	**i**(C9)O91	5.72	6.0	25.09(9.83)	E710	**ii**(C4)O4	8.77	9.0	-4.93(-5.86)
I481	**i**(C9)O91; **i**(N8)H	5.81; 5.81	6.0	-3.80(-3.20)	D728	**i**(C8)H	8.83	9.0	-2.86(-2.19)
E657	**ii**(C2)O2	5.98	6.0	1.00(1.72)	T399	**i**(N8)H	9.50	9.5	-1.49(-1.03)
S403	**ii**(C5)I	6.21	6.5	0.28(-0.24)	V406	**ii**(C5)I	9.01	9.5	0.53(-0.10)
A452	**i**(C9)O92	6.48	6.5	-0.06(0.33)	I502	**ii**(C4)O4	9.47	9.5	0.26(-0.62)
A477	**i**(N8)H	6.15	6.5	-0.02(0.43)	F682	**ii**(N3)H	9.11	9.5	-2.85(-1.92)
F491	**i**(C9)O91	6.29	6.5	1.70(0.35)	A735	**i**(C9)O91	9.03	9.5	-0.67(-0.29)
S706	**ii**(C4)O4	6.27	6.5	-0.69(-1.44)	R453	**i**(C9)O92	9.72	10.0	-1.06(-0.28)
G731	**i**(N8)H	6.36	6.5	-0.28(0.001)	I476	**i**(N8)H	9.61	10.0	-1.03(-0.26)
P404	**ii**(C5)I	6.94	7.0	0.55(-0.26)	P494	**i**(N8)H	9.99	10.0	0.67(-0.17)
K449	**i**(C9)O92; **i**(C7)H	6.85; 6.85	7.0	-0.68(0.17)	S497	**i**(N8)H	9.71	10.0	0.16(-0.31)
V464	**i**(C9)O91	6.68	7.0	-0.88(-1.58)	L727	**ii**(N3)H	9.57	10.0	-1.67(-0.98)
S501	**ii**(C4)O4	6.89	7.0	0.40(-0.22)	**E688**	**ii**(C4)O4	10.0	10.0	-1.15(-0.27)
F658	**ii**(C2)O2	6.75	7.0	-2.37(-1.37)					

Table 8: Description of the GluR2 residues interacting with IW. We show the functional groups and distances of the ligand to each amino acid in the binding pocket radius ranging from 10.5 to 12.0 $\mathrm{\AA}$

Residue	Atomic Group	d(Å)	r(Å)	$E_{GGA(LDA)}$	Residue	Atomic Group	d(Å)	r(Å)	$E_{GGA(LDA)}$
Y424	**ii**(C5)I	10.28	10.5	-0.75(-2.33)	Y700	**ii**(C4)O4	10.58	11.0	-1.91(-0.87)
G465	**i**(C9)O92	10.34	10.5	0.50(0.19)	N726	**ii**(N3)H	10.85	11.0	0.47(-0.30)
L467	**i**(C9)O91	10.21	10.5	-0.39(-1.15)	R661	**i**(C9)O92	11.08	11.5	-4.11(-3.23)
L483	**i**(C9)O91	10.31	10.5	-3.59(-2.81)	V681	**ii**(N3)H	11.46	11.5	-1.15(-0.54)
E486	**i**(C9)O91	10.30	10.5	-9.88(-9.08)	A701	**ii**(C4)O4	11.43	11.5	-1.13(-1.32)
R660	**ii**(C2)O2	10.03	10.5	-4.63(-3.65)	E713	**ii**(C5)I	11.25	11.5	-2.50(-3.50)
W671	**ii**(C2)O2	10.49	10.5	1.28(-0.39)	S729	**i**(N8)H	11.03	11.5	-1.73(-1.19)
K722	**ii**(C4)O4	10.17	10.5	2.90(2.05)	K770	**ii**(C5)I	11.02	11.5	5.64(4.94)
I734	**i**(C9)O91	10.27	10.5	-1.80(-1.09)	L428	**i**(N8)H	11.59	12.0	1.29(0.73)
K763	**ii**(C5)I	10.49	10.5	1.52(2.47)	V488	**i**(C9)O91	11.71	12.0	-0.53(0.35)
T398	**i**(C9)O91	10.78	11.0	-1.05(-0.57)	S492	**i**(N8)H	11.99	12.0	0.34(-0.30)
M407	**ii**(C5)I	10.62	11.0	0.13(-0.46)	M670	**ii**(N3)H	11.81	12.0	-0.08(-0.64)
D447	**i**(C9)O92	10.88	11.0	-0.87(-0.24)	A691	**ii**(C4)O4	11.60	12.0	-0.13(0.40)
M674	**ii**(N3)H	10.62	11.0	-0.17(-0.68)	R715	**ii**(C5)I	11.54	12.0	7.00(6.03)
V693	**ii**(C4)O4	10.70	11.0	-0.87(-0.13)					