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Supplementary Table 1. Closure angles (°) of GluK1-LBC from 4-14 ns molecular dynamics simulations

Ligand	Chain ID	Average	Max	Min	Median	Standard deviation
apo	A	28	31.7	24.4	28.1	1.7
	B	29.3	32.7	25.1	29.4	1.9
(*S*)-glutamate	A	29.3	31.7	27	29.2	1.3
	B	30.4	33	27.5	30.5	1.4
neoDH	A	27.6	30.7	24	27.7	1.6
	B	28.5	31.9	24.8	28.6	1.6
9-F-8-epi-neoDH	A	29.7	32.8	25.2	30	1.9
	B	28.9	32.2	25.6	28.9	1.5
MSVIII-19	A	30.6	35.6	25.5	30.6	1.8
	B	28.9	34.3	26.6	28.6	1.6
8-deoxy-neoDH	A	29.1	31.9	26.4	29	1.4
	B	28	31.4	24.6	27.8	1.8
9-deoxy-neoDH	A	28.3	33.2	24.8	28.1	1.8
	B	26.6	31.6	20.9	26.2	3.1
8-epi-neoDH	A	29.8	32.7	26.8	29.9	1.3
	B	27.4	30.7	21.1	27.6	1.6
9-epi-neoDH	A	28.9	32.4	26.1	28.6	1.4
	B	29.8	33.5	26.3	29.7	1.7
8,9-epi-neoDH	A	29	32.6	24.6	28.9	1.6
	B	27.1	31.9	14.8	27.3	2.6

4-epi-neoDH	A	28.6	30.7	24.8	28.8	1.4
	B	27.8	31.4	23.9	27.5	1.6
2,4-epi-neoDH	A	25.5	29.7	15.8	26.4	3.1
	B	25.1	31.2	18.9	25.1	2.7