SUPPLEMENTARY MATERIALS

Towards Probing Conformational States of Y2 Receptor Using Hyperpolarized ^{129}Xe NMR

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SUPPLEMENTARY MATERIALS CONTENT

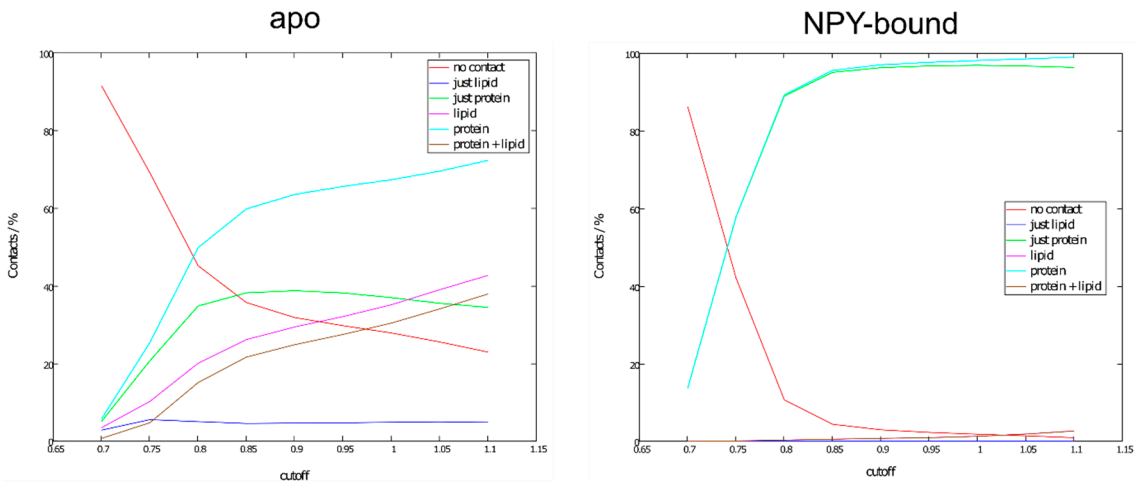

Figure S1. Plot of the different contact probabilities vs. the choice of cutoff in nm. From this figure we concluded that 0.85 nm is a good choice for the cutoff, where we have good separation of the different types of contact. A larger cutoff would lead to having contact to many different types of simulation constituents at the same time and a smaller cutoff would lead to very few contacts at all. In particular from the line “no contact” in the NPY-bound case it is clear that a cutoff of 0.85 nm is sufficient to capture almost all contacts.

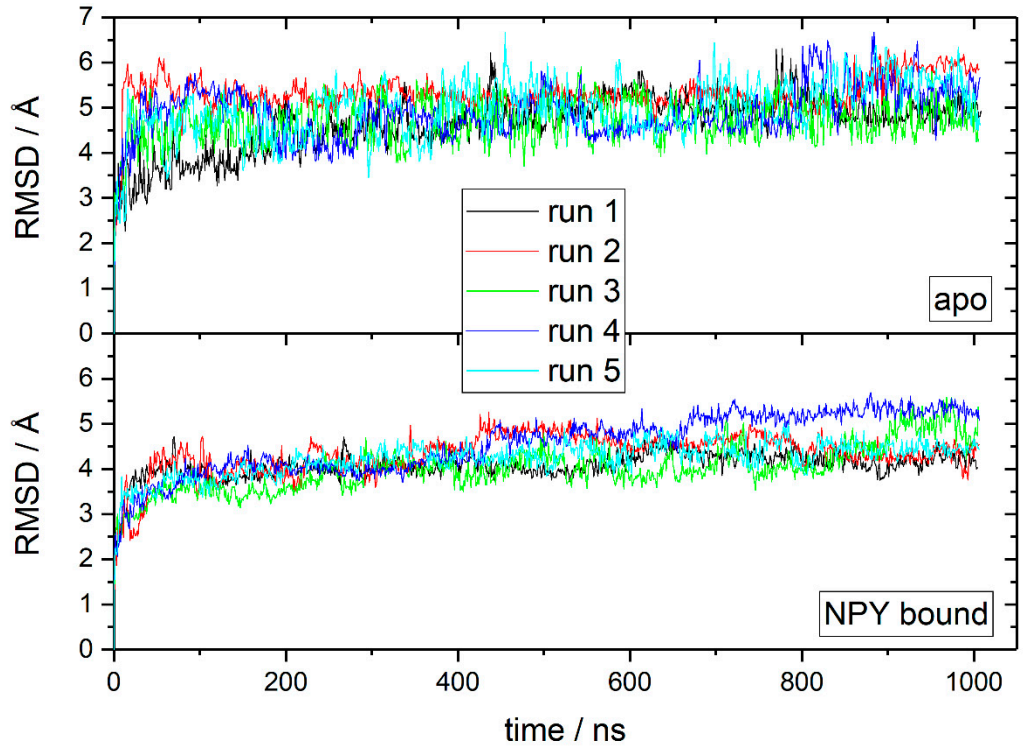

Figure S2. Plot of RMSD values over simulation time for run 1 through 5 (out of 30) for both systems in presence of the cage. For both systems RMSD values are below 7 Angstroem the whole time. Values are slightly higher for the apo system in general. This is to be expected since this system was started from a Y2R structure where NPY (and the G-proteins) were present and have been removed. This resulted in an empty ligand binding pocket, that was open and therefore easily accessible to the solvent and to the cage as well. This was intentional to check if the cage with the Xenon atom inside was able to penetrate the ligand binding pocket in the apo state. Therefore, this structure is slowly approaching the deactivated state, which is the reason for the slightly higher RMSD values.

Table S1. List of the contact probabilities with Xenon for each individual amino acid of Y2R in the apo state and in the NPY-bound state.

Y2R amino acid	40	41	42	43	44	45	46
apo Y2R	0.1760	0.1448	0.0365	0.0280	0.0463	0.0919	0.0595
NPY-bound Y2R	0.1949	0.0670	0.0262	0.0251	0.0114	0.0017	0.0004

47	48	49	50	51	52	53	54	55
0.0918	0.0131	0.0024	0.0133	0.0333	0.0000	0.0000	0.0021	0.0003
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

56	57	58	59	60	61	62	63	64
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

65	66	67	68	69	70	71	72	73
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

74	75	76	77	78	79	80	81	82
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

83	84	85	86	87	88	89	90	91
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

92	93	94	95	96	97	98	99	100
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

101	102	103	104	105	106	107	108	109
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

110	111	112	113	114	115	116	117	118
0.0000	0.0010	0.0571	0.0620	0.0102	0.0035	0.0000	0.0010	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

119	120	121	122	123	124	125	126	127

0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

128	129	130	131	132	133	134	135	136
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

137	138	139	140	141	142	143	144	145
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

146	147	148	149	150	151	152	153	154
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

155	156	157	158	159	160	161	162	163
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

164	165	166	167	168	169	170	171	172
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

173	174	175	176	177	178	179	180	181
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

182	183	184	185	186	187	188	189	190
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008	0.0038	0.0083
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

191	192	193	194	195	196	197	198	199
0.0356	0.0204	0.0047	0.0119	0.1224	0.0747	0.0111	0.0821	0.0368
0.0000	0.0002	0.0010	0.0050	0.2029	0.1493	0.0123	0.0109	0.0001

200	201	202	203	204	205	206	207	208
0.0028	0.0269	0.0000	0.0000	0.0101	0.0000	0.0198	0.0279	0.0239
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

209	210	211	212	213	214	215	216	217
0.0209	0.0111	0.0114	0.0026	0.0001	0.0011	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

218	219	220	221	222	223	224	225	226
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

227	228	229	230	231	232	233	234	235
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

236	237	238	239	240	241	242	243	244
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

245	246	247	248	249	250	251	252	253
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

254	255	256	257	258	259	260	261	262
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

263	264	265	266	267	268	269	270	271
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

272	273	274	275	276	277	278	279	280
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

281	282	283	284	285	286	287	288	289
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

290	291	292	293	294	295	296	297	298
0.0000	0.0000	0.0000	0.0002	0.0001	0.0011	0.0291	0.0032	0.0004
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

299	300	301	302	303	304	305	306	307
0.0207	0.0626	0.0050	0.0032	0.0000	0.0004	0.0000	0.0000	0.0000
0.0000	0.0186	0.0036	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000

308	309	310	311	312	313	314	315	316

0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

317	318	319	320	321	322	323	324	325
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

326	327	328	329	330	331	332	333	334
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

335	336	337	338	339	340	341	342	343
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S2. List of the contact probabilities with Xenon for each individual amino acid of NPY in the MD simulation of the NPY-bound state of Y2R.

NPY amino acid	1	2	3	4	5	6	7
NPY-bound Y2R	0.0001	0.0000	0.0001	0.0042	0.0003	0.0018	0.2453

8	9	10	11	12	13	14	15	16
0.2504	0.2527	0.3517	0.0989	0.2847	0.0253	0.3891	0.0205	0.0000

17	18	19	20	21	22	23	24	25
0.6526	0.2651	0.0053	0.1848	0.4804	0.0040	0.0000	0.0002	0.0142

26	27	28	29	30	31	32	33	34
0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

35	36
0.0000	0.0000