

SI Table 1 Hydrogen bonding monitor between SAM and the SAM-I riboswitch (SAM_TRAJ)

Donor	Acceptor	Occupancy (%) ^a	Distance(Å)		Angle(°)		Lifetime (ns) ^b		Maximum occupancy ^c
			Mean	STD	Mean	STD	Mean	STD	
G11:N2	SAM:OX T	99.99	2.808	0.10	21.28	9.19	66.66	75.45	17254
G58:N2	SAM:OX T	99.88	2.886	0.14	19.28	8.74	8.32	9.27	4100
G11:N1	SAM:O	99.69	3.126	0.20	23.88	8.77	3.32	5.15	2432
G11:N1	SAM:OX T	98.87	3.101	0.20	39.41	7.88	0.94	1.91	1298
SAM:N(HT 2)	G58:N3	51.74	2.997	0.14	20.89	11.98	0.35	0.89	704
SAM:N(HT 1)	G58:N3	33.79	2.99	0.16	20.23	11.38	0.26	0.76	715
SAM:N	G58:N3	12.2	3.013	0.16	23.19	12.44	0.16	0.54	551
SAM:N(HT 3)	G58:O2'	11.77	2.904	0.15	45.33	12.05	0.02	0.02	26
SAM:N(HT 2)	G58:O2'	11.52	2.906	0.15	44	12.49	0.02	0.03	54
SAM:N(HT 1)	G58:O2'	5.29	2.875	0.14	42.63	12.43	0.02	0.03	19
A45:O2'	SAM:N1	1.2	3.139	0.28	29.54	14.86	0.03	0.05	37
SAM:N6	A45:N3	1	3.175	0.25	45.27	10.29	0.02	0.03	23

- Occupancy indicates the percentage of the time that this hydrogen bond is formed.
- The average time that this hydrogen bond is formed.
- The maximum number of consecutive frames (10 ps/frame) that this hydrogen bond is formed in the trajectory.