NON COVALENT INCLUSION OF NUCLEOSIDES AND NUCLEOTIDES IN WATER-SOLUBLE MOLECULAR CLIPS.

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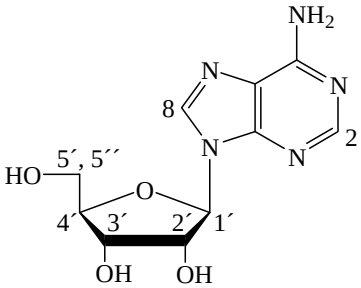
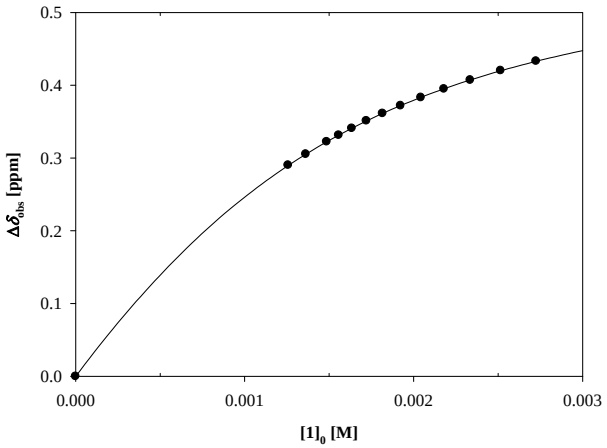
Supporting Information

^{1}H-NMR titration experiments with phosphate clip 1:

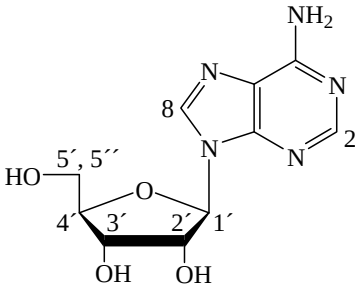
receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	267.10
T [°C]	25	m_R [mg]	1.02
substrate	adenosine (**A**)	m_S [mg]	0.83
	δ_0 (1´-H) [ppm] = 6.072	V_0 [mL]	2.5
	δ_0 (3´-H) [ppm] = 4.429	[S]$_0$ [mM]	1.23
	δ_0 (4´-H) [ppm] = 4.292		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.832, 3.910		
	δ_0 (2-H) [ppm] = 8.338		
	δ_0 (8-H) [ppm] = 8.253		

V [mL]	[1]$_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	2.72	5.639	0.433	0.433
0.65	2.52	5.652	0.420	0.420
0.70	2.34	5.665	0.407	0.407
0.75	2.18	5.677	0.395	0.395
0.80	2.04	5.689	0.383	0.383
0.85	1.92	5.700	0.372	0.372
0.90	1.82	5.711	0.361	0.361
0.95	1.72	5.721	0.351	0.351
1.00	1.63	5.731	0.341	0.341
1.05	1.56	5.740	0.331	0.332
1.10	1.49	5.749	0.322	0.322
1.20	1.36	5.767	0.305	0.305
1.30	1.26	5.782	0.290	0.290

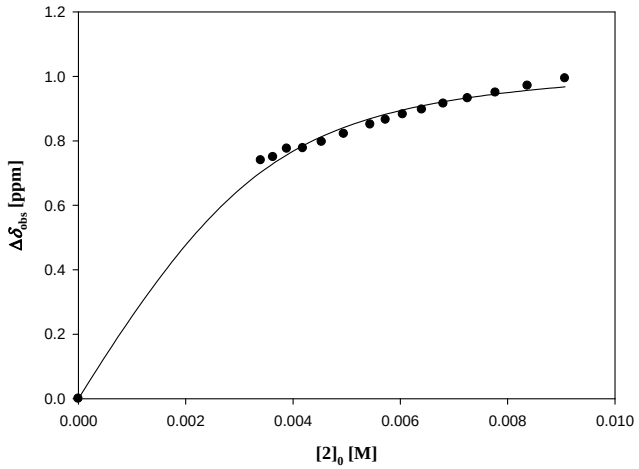


K_a [M^{-1}] = 1470 ± 300
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.60
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.06
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.11
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.08, - 0.13
$\Delta\delta_{max}$ (2-H) [ppm] = 2.20
$\Delta\delta_{max}$ (8-H) [ppm] = 2.15

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	267.10
T [°C]	25	m_R [mg]	1.02
substrate	adenosine (**A**)	m_S [mg]	0.83
	δ_0 (1´-H) [ppm] = 6.072	V_0 [mL]	2.5
	δ_0 (3´-H) [ppm] = 4.429	$[S]_0$ [mM]	1.23
	δ_0 (4´-H) [ppm] = 4.292		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.832, 3.910		
	δ_0 (2-H) [ppm] = 8.338		
	δ_0 (8-H) [ppm] = 8.253		

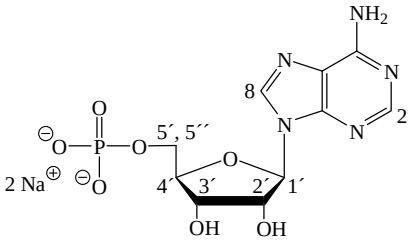
***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (2-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	8.84	7.344	0.993	0.967
0.65	8.16	7.367	0.971	0.957
0.70	7.58	7.388	0.949	0.945
0.75	7.07	7.406	0.932	0.933
0.80	6.63	7.422	0.915	0.921
0.85	6.24	7.441	0.897	0.909
0.90	5.89	7.455	0.882	0.896
0.95	5.58	7.472	0.865	0.882
1.00	5.31	7.487	0.850	0.869
1.10	4.82	7.516	0.822	0.841
1.20	4.42	7.541	0.797	0.813
1.30	4.08	7.560	0.777	0.785
1.40	3.79	7.562	0.775	0.757
1.50	3.54	7.588	0.749	0.729
1.60	3.32	7.598	0.740	0.703



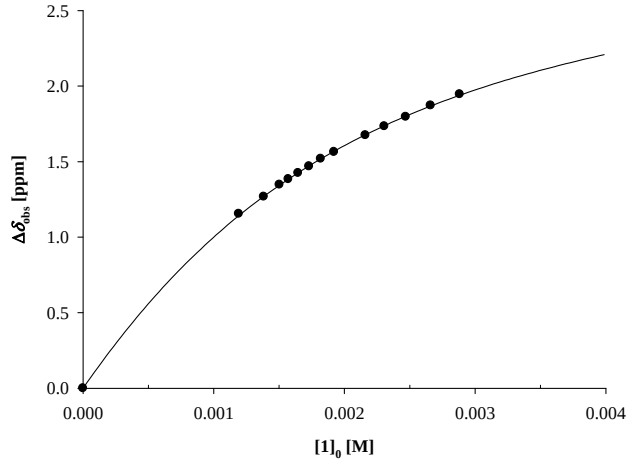
K_a [M^{-1}] = 1120 ± 150
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.44
$\Delta\delta_{max}$ (2-H) [ppm] = 1.13
$\Delta\delta_{max}$ (8-H) [ppm] = 1.59

^{1}H-NMR titration experiments with phosphate clip 1:

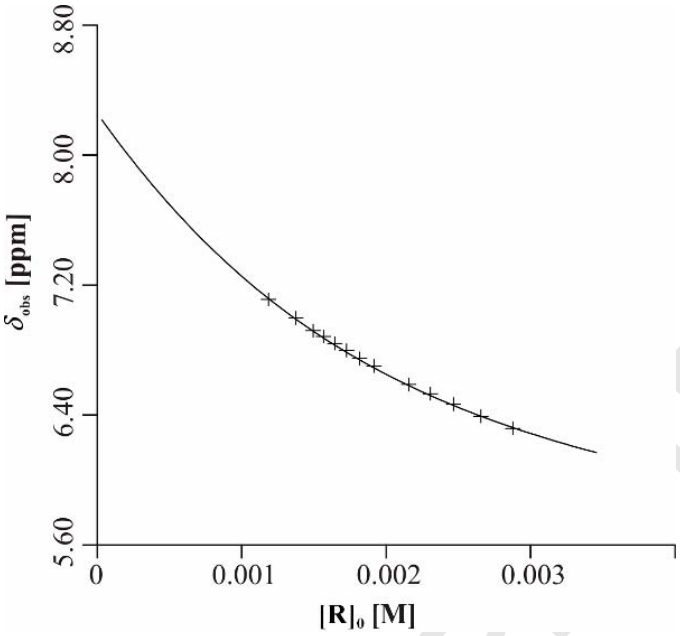
receptor	**Clip 1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	347.06
T [°C]	25	m_R [mg]	1.08
substrate	**AMP**	m_S [mg]	0.84
	δ_0 (1´-H) [ppm] = 6.134	V_0 [mL]	2
	δ_0 (3´-H) [ppm] = 4.505	$[S]_0$ [mM]	1.19
	δ_0 (4´-H) [ppm] = 4.364		
	δ_0 (5´-H, 5´´-H) [ppm] = 4.017		
	δ_0 (2-H) [ppm] = 8.589		
	δ_0 (8-H) [ppm] = 8.257		



***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (8-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	2.88	6.312	1.946	1.939
0.65	2.66	6.386	1.872	1.868
0.70	2.47	6.461	1.797	1.801
0.75	2.31	6.523	1.734	1.738
0.80	2.16	6.582	1.675	1.678
0.90	1.92	6.694	1.564	1.569
0.95	1.82	6.739	1.519	1.519
1.00	1.73	6.789	1.469	1.471
1.05	1.65	6.832	1.425	1.427
1.10	1.57	6.874	1.384	1.384
1.15	1.50	6.910	1.347	1.344
1.25	1.38	6.990	1.268	1.270
1.35	1.28	-	-	-
1.45	1.19	7.103	1.155	1.143



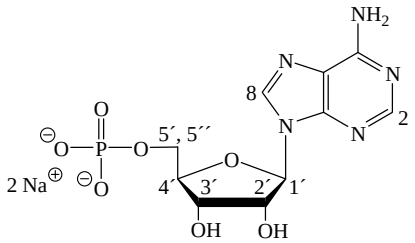
K_a [M^{-1}] = 683 ± 60
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.48
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.08
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.02
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.06, - 0.14
$\Delta\delta_{max}$ (2-H) [ppm] = 0.74
$\Delta\delta_{max}$ (8-H) [ppm] = 3.14



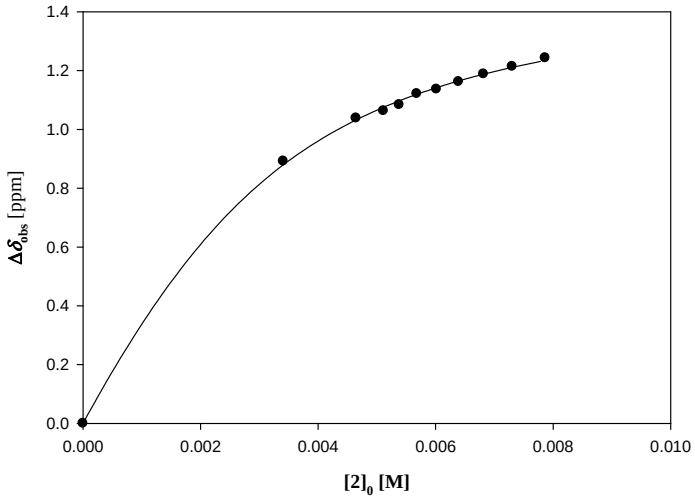
evaluation of the signals of the proton 8-H with the computer programme HOSTEST assuming a 1:1 complex stochoimetry
K_a [M^{-1}] = 776 ± 162*
$\Delta\delta_{max}$ (8-H) [ppm] = 3.10
* limit of the 95% confidence interval

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	347.06
T [°C]	25	m_R [mg]	3.10
substrate	**AMP**	m_S [mg]	3.00
	δ_0 (1´-H) [ppm] = 6.134	V_0 [mL]	3
	δ_0 (3´-H) [ppm] = 4.505	$[S]_0$ [mM]	2.88
	δ_0 (4´-H) [ppm] = 4.364		
	δ_0 (5´-H, 5´´-H) [ppm] = 4.017		
	δ_0 (2-H) [ppm] = 8.589		
	δ_0 (8-H) [ppm] = 8.257		



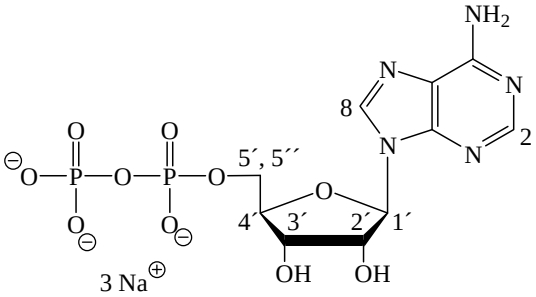
***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (8-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	8.50	7.032	1.226	1.234
0.65	7.90	7.014	1.243	1.234
0.70	7.30	7.043	1.214	1.211
0.75	6.80	7.069	1.188	1.187
0.80	6.40	7.095	1.162	1.164
0.85	6.00	7.121	1.137	1.142
0.90	5.70	7.136	1.121	1.119
0.95	5.40	7.174	1.084	1.097
1.00	5.10	7.194	1.063	1.075
1.10	4.60	-	-	-
1.20	4.30	-	-	-
1.30	3.90	-	-	-
1.40	3.70	-	-	-
1.50	3.40	7.365	0.892	1.032
1.60	3.20	7.366	0.892	0.879
1.80	2.80	-	-	-



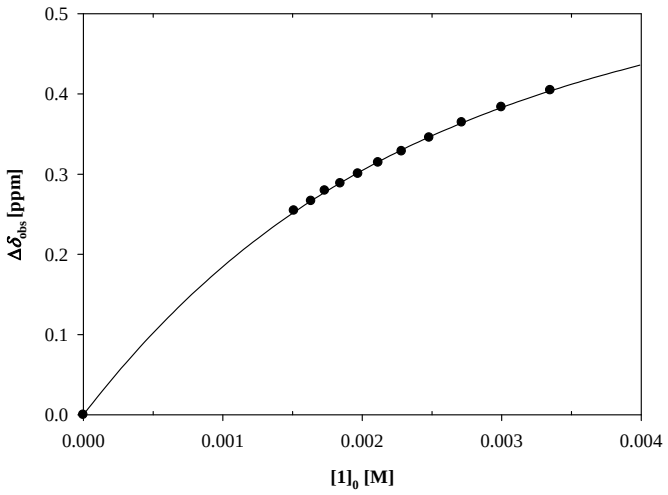
K_a [M^{-1}] = 910 ± 80
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.27
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.07
$\Delta\delta_{max}$ (2-H) [ppm] = 0.38
$\Delta\delta_{max}$ (8-H) [ppm] = 1.51

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	501.01
T [°C]	25	m_R [mg]	1.25
substrate	**ADP**	m_S [mg]	2.60
	δ_0 (1´-H) [ppm] = 6.136	V_0 [mL]	4
	δ_0 (3´-H) [ppm] = 4.590	[S]$_0$ [mM]	1.27
	δ_0 (4´-H) [ppm] = 4.370		
	δ_0 (2-H) [ppm] = 8.523		
	δ_0 (8-H) [ppm] = 8.254		



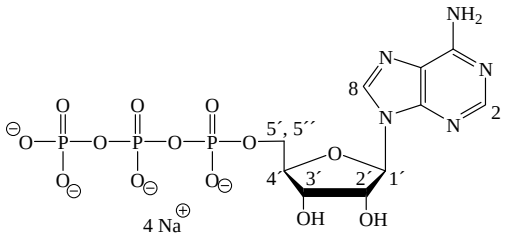
V [mL]	[1]$_0$ [mM]	δ_{obs} (2-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	3.35	8.118	0.405	0.404
0.67	3.00	8.139	0.384	0.383
0.74	2.71	8.158	0.365	0.364
0.81	2.48	8.177	0.346	0.346
0.88	2.28	8.194	0.329	0.330
0.95	2.11	8.208	0.315	0.315
1.02	1.97	8.222	0.301	0.302
1.09	1.84	8.234	0.289	0.289
1.16	1.73	8.243	0.280	0.277
1.23	1.63	8.256	0.267	0.267
1.33	1.51	8.268	0.255	0.252



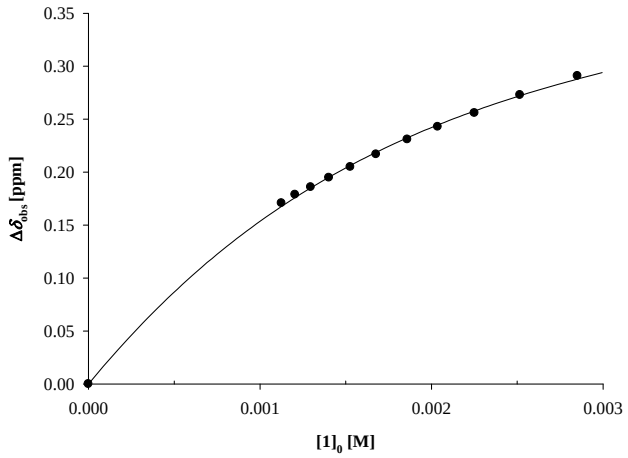
K_a [M^{-1}] = 630 ± 60
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.54
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.08
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.00
$\Delta\delta_{max}$ (2-H) [ppm] = 0.67
$\Delta\delta_{max}$ (8-H) [ppm] = 3.68

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	550.96
T [°C]	25	m_R [mg]	1.06
substrate	**ATP**	m_S [mg]	2.59
	δ_0 (1´-H) [ppm] = 6.135	V_0 [mL]	4
	δ_0 (3´-H) [ppm] = 4.602	$[S]_0$ [mM]	1.07
	δ_0 (4´-H) [ppm] = 4.389		
	δ_0 (5´-H, 5´´-H) [ppm] = 4.199, 4.278		
	δ_0 (2-H) [ppm] = 8.540		
	δ_0 (8-H) [ppm] = 8.256		



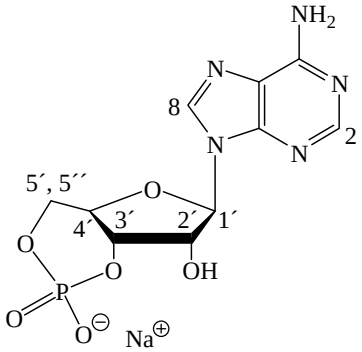
***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	2.85	5.844	0.291	0.288
0.68	2.52	5.862	0.273	0.272
0.76	2.25	5.879	0.256	0.258
0.84	2.04	5.892	0.243	0.245
0.92	1.86	5.904	0.231	0.232
1.02	1.68	5.918	0.217	0.219
1.12	1.53	5.930	0.205	0.206
1.22	1.40	5.940	0.195	0.195
1.32	1.30	5.949	0.186	0.185
1.42	1.20	5.956	0.179	0.176
1.52	1.13	5.964	0.171	0.168



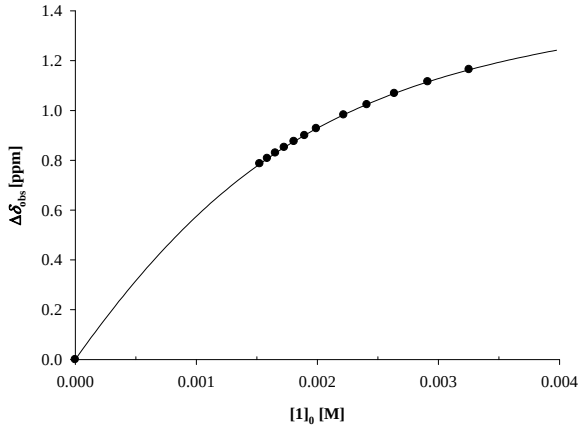
K_a [M^{-1}] = 810 ± 110
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.45
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.07
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.00
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.02, - 0.14
$\Delta\delta_{max}$ (2-H) [ppm] = 0.56
$\Delta\delta_{max}$ (8-H) [ppm] = 3.14

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	329.05
T [°C]	25	m_R [mg]	0.79
substrate	**cAMP**	m_S [mg]	2.05
	δ_0 (1´-H) [ppm] = 6.200	V_0 [mL]	4
	δ_0 (2-H) [ppm] = 8.247	$[S]_0$ [mM]	1.53
	δ_0 (8-H) [ppm] = 8.263		



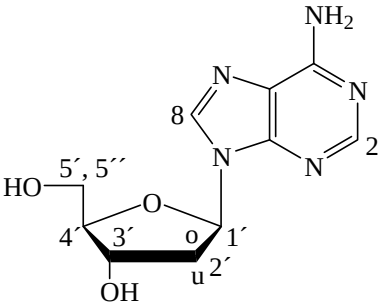
***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (2-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	3.25	7.083	1.164	1.163
0.67	2.91	7.132	1.115	1.115
0.74	2.64	7.179	1.068	1.069
0.81	2.41	7.224	1.023	1.025
0.88	2.22	7.265	0.982	0.983
0.93	2.10	-	-	-
0.98	1.99	7.320	0.927	0.927
1.03	1.89	7.348	0.899	0.901
1.08	1.81	7.372	0.875	0.876
1.13	1.73	7.396	0.851	0.851
1.18	1.65	7.418	0.829	0.828
1.23	1.59	7.440	0.807	0.806
1.28	1.52	7.461	0.786	0.785



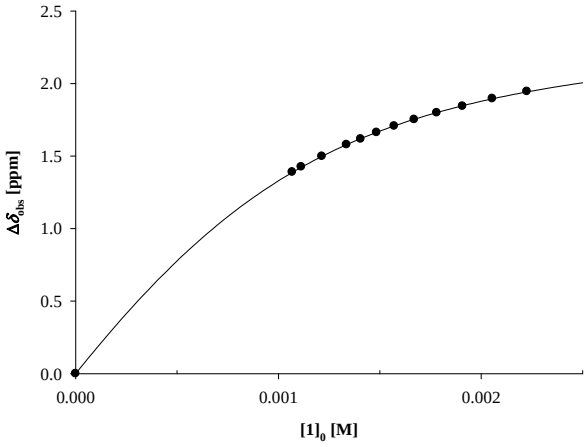
K_a [M^{-1}] = 1260 ± 10
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.76
$\Delta\delta_{max}$ (2-H) [ppm] = 1.60
$\Delta\delta_{max}$ (8-H) [ppm] = 3.11

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	**Clip 1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	349.08
T [°C]	25	m_R [mg]	0.82
substrate	**DA**	m_S [mg]	0.73
	δ_0 (1´-H) [ppm] = 6.484	V_0 [mL]	2
	δ_0 (3´-H) [ppm] = 4.650	$[S]_0$ [mM]	1.04
	δ_0 (4´-H) [ppm] = 4.186		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.777, 3.838		
	δ_0 (2-H) [ppm] = 8.323		
	δ_0 (8-H) [ppm] = 8.242		



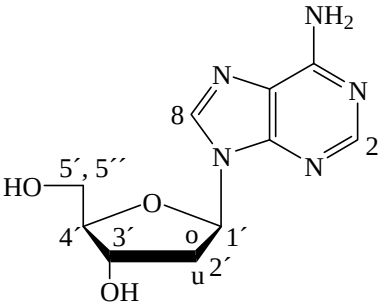
***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (2-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	2.23	6.377	1.946	1.942
0.65	2.05	6.426	1.897	1.895
0.70	1.91	6.478	1.844	1.847
0.75	1.78	6.524	1.798	1.800
0.80	1.67	6.571	1.751	1.754
0.85	1.57	6.616	1.707	1.708
0.90	1.48	6.660	1.663	1.664
0.95	1.41	6.705	1.617	1.620
1.00	1.34	6.744	1.579	1.578
1.10	1.21	6.824	1.498	1.498
1.20	1.11	6.897	1.426	1.423
1.25	1.07	6.933	1.390	1.387
1.30	1.03	-	-	-



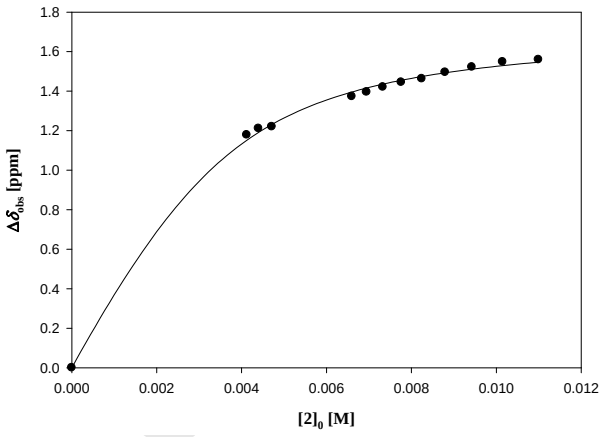
K_a [M^{-1}] = 3150 ± 540
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.98
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.14
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.13
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.01, - 0.03
$\Delta\delta_{max}$ (2-H) [ppm] = 2.46
$\Delta\delta_{max}$ (8-H) [ppm] = 2.15

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	349.08
T [°C]	25	m_R [mg]	2.70
substrate	**DA**	m_S [mg]	4.00
	δ_0 (1´-H) [ppm] = 6.484	V_0 [mL]	3
	δ_0 (3´-H) [ppm] = 4.650	[S]$_0$ [mM]	3.58
	δ_0 (4´-H) [ppm] = 4.186		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.777, 3.838		
	δ_0 (2-H) [ppm] = 8.323		
	δ_0 (8-H) [ppm] = 8.242		



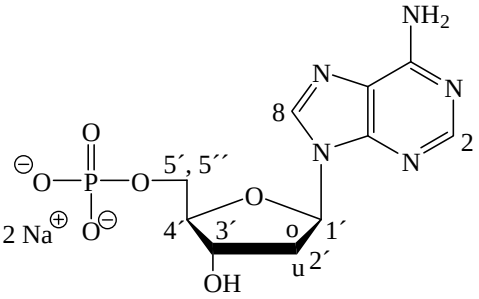
***V* [mL]**	**[2]$_0$ [mM]**	**δ_{obs} (8-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	11.00	6.683	1.559	1.546
0.65	10.10	6.694	1.548	1.529
0.70	9.40	6.720	1.522	1.511
0.75	8.80	6.747	1.496	1.493
0.80	8.80	6.780	1.463	1.474
0.85	7.80	6.798	1.445	1.455
0.90	7.30	6.822	1.420	1.435
0.95	6.90	6.847	1.396	1.416
1.00	6.60	6.869	1.373	1.396
1.10	6.00	-	-	-
1.20	6.00	-	-	-
1.30	5.10	-	-	-
1.40	4.70	7.022	1.231	1.231
1.50	4.40	7.031	1.191	1.151
1.60	4.10	7.064	1.151	1.151



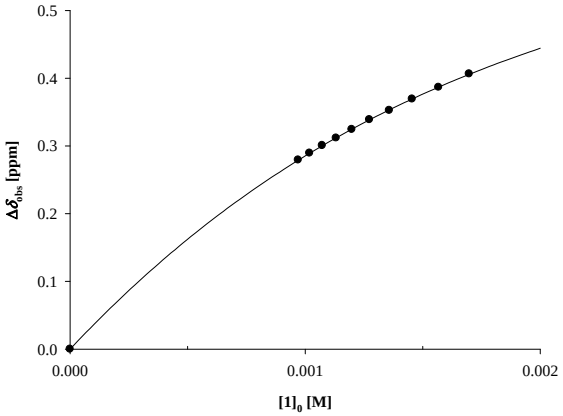
K_a [M^{-1}] = 840 ± 130
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.98
$\Delta\delta_{max}$ (2-H) [ppm] = 2.39
$\Delta\delta_{max}$ (8-H) [ppm] = 1.67

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	**Clip 1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	349.08
T [°C]	25	m_R [mg]	0.63
substrate	**DAMP**	m_S [mg]	0.75
	δ_0 (1´-H) [ppm] = 6.513	V_0 [mL]	2
	δ_0 (2´o-H) [ppm] = 2.835	$[S]_0$ [mM]	1.05
	δ_0 (2´u-H) [ppm] = 2.580		
	δ_0 (3´-H) [ppm] = 4.719		
	δ_0 (4´-H) [ppm] = 4.258		
	δ_0 (2-H) [ppm] = 8.533		
	δ_0 (8-H) [ppm] = 8.249		



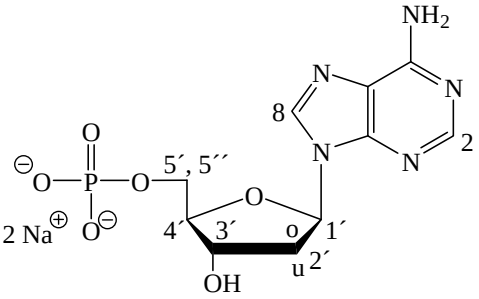
V [mL]	$[1]_0$ [mM]	δ_{obs} (2-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	1.70	8.126	0.406	0.406
0.65	1.57	8.146	0.387	0.387
0.70	1.46	8.163	0.369	0.369
0.75	1.36	8.180	0.353	0.353
0.80	1.27	8.194	0.339	0.339
0.85	1.20	8.208	0.324	0.325
0.90	1.13	8.221	0.312	0.312
0.95	1.07	8.232	0.301	0.300
1.00	1.02	8.243	0.289	0.289
1.05	0.97	8.253	0.279	0.279



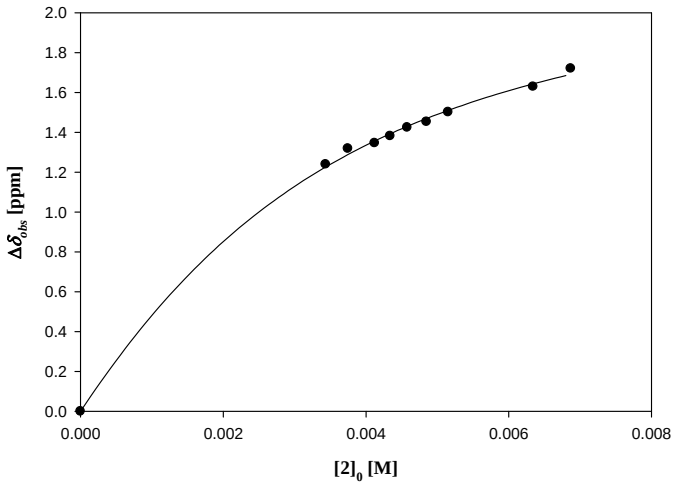
K_a [M^{-1}] = 920 ± 20
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.60
$\Delta\delta_{max}$ (2´o-H) [ppm] = 0.05
$\Delta\delta_{max}$ (2´u-H) [ppm] = 0.33
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.06
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.03
$\Delta\delta_{max}$ (2-H) [ppm] = 0.79
$\Delta\delta_{max}$ (8-H) [ppm] = 3.44

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	349.08
T [°C]	25	m_R [mg]	2.50
substrate	**DAMP**	m_S [mg]	2.28
	δ_0 (1´-H) [ppm] = 6.513	V_0 [mL]	3
	δ_0 (2´o-H) [ppm] = 2.835	$[S]_0$ [mM]	2.29
	δ_0 (2´u-H) [ppm] = 2.580		
	δ_0 (3´-H) [ppm] = 4.719		
	δ_0 (4´-H) [ppm] = 4.258		
	δ_0 (2-H) [ppm] = 8.533		
	δ_0 (8-H) [ppm] = 8.249		

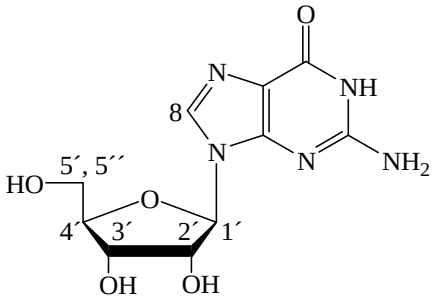


***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (8-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	6.90	6.530	1.719	1.691
0.65	6.30	6.621	1.629	1.643
0.70	5.90	-	-	-
0.75	5.50	-	-	-
0.80	5.20	6.748	1.501	1.511
0.85	4.90	6.797	1.453	1.470
0.90	4.60	6.825	1.424	1.431
0.95	4.30	6.868	1.381	1.431
1.00	4.10	6.903	1.346	1.357
1.10	3.70	6.931	1.319	1.289
1.05	3.40	7.010	1.239	1.226

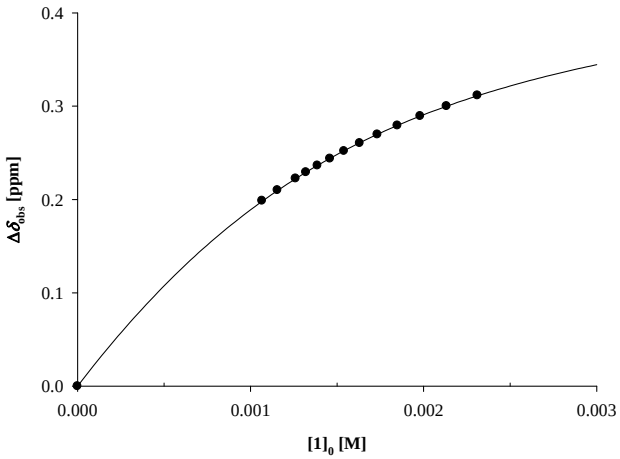


K_a [M^{-1}] = 650 ± 70
$\Delta\delta_{max}$ (1´-H) [ppm] = 1.00
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.28
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.24
$\Delta\delta_{max}$ (5´-H) [ppm] = 0.20
$\Delta\delta_{max}$ (5´´-H) [ppm] = 0.24
$\Delta\delta_{max}$ (2-H) [ppm] = 1.74
$\Delta\delta_{max}$ (8-H) [ppm] = 2.36

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	283.09
T [°C]	25	m_R [mg]	0.86
substrate	guanosine (**G**)	m_S [mg]	0.83
	δ_0 (1´-H) [ppm] = 5.908 δ_0 (2´-H) [ppm] = 4.729 δ_0 (3´-H) [ppm] = 4.403 δ_0 (4´-H) [ppm] = 4.229 δ_0 (5´-H, 5´´-H) [ppm] = 3.812, 3.881 δ_0 (8-H) [ppm] = 7.995	V_0 [mL] $[S]_0$ [mM]	2.5 1.15

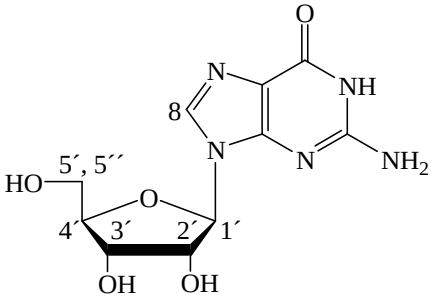
V [mL]	$[1]_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	2.31	5.596	0.312	0.311
0.65	2.13	5.608	0.300	0.300
0.70	1.98	5.618	0.289	0.289
0.75	1.85	5.629	0.279	0.279
0.80	1.73	5.638	0.270	0.270
0.85	1.63	5.647	0.260	0.261
0.90	1.54	5.656	0.252	0.252
0.95	1.46	5.664	0.244	0.244
1.00	1.39	5.671	0.236	0.236
1.05	1.32	5.679	0.229	0.229
1.10	1.26	5.685	0.223	0.222
1.20	1.16	5.698	0.210	0.210
1.30	1.07	5.709	0.199	0.198



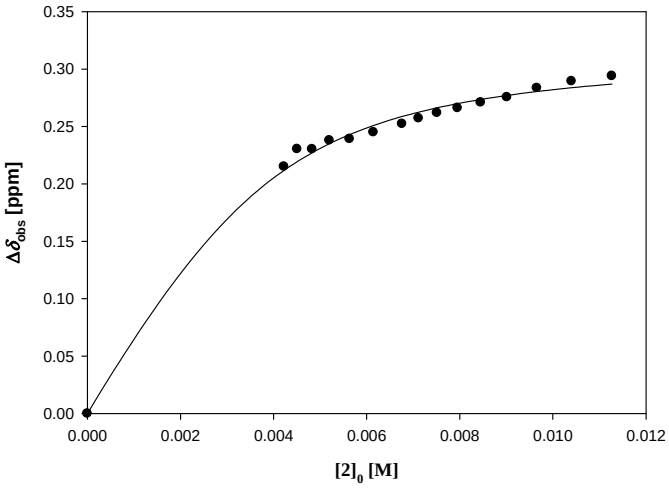
K_a [M^{-1}] = 1120 ± 110
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.48
$\Delta\delta_{max}$ (2´-H) [ppm] = 0.34
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.09
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.07
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.06, 0.03
$\Delta\delta_{max}$ (8-H) [ppm] = 0.82

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	283.09
T [°C]	25	m_R [mg]	4.10
substrate	guanosine (**G**)	m_S [mg]	3.30
	δ_0 (1´-H) [ppm] = 5.908	V_0 [mL]	3.0
	δ_0 (2´-H) [ppm] = 4.729	$[S]_0$ [mM]	3.88
	δ_0 (3´-H) [ppm] = 4.403		
	δ_0 (4´-H) [ppm] = 4.229		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.812, 3.881		
	δ_0 (8-H) [ppm] = 7.995		



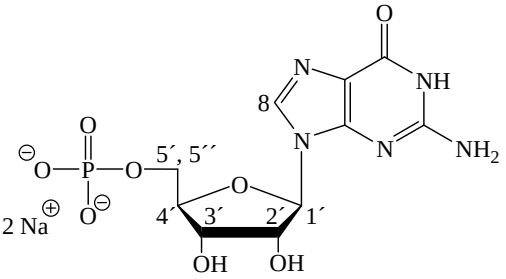
V [mL]	$[2]_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	1127	5.614	0.294	0.287
0.65	10.40	5.618	0.289	0.284
0.70	9.66	5.624	0.283	0.280
0.75	9.01	5.632	0.275	0.277
0.80	8.45	5.637	0.271	0.273
0.85	7.95	5.642	0.266	0.270
0.90	7.51	5.646	0.262	0.266
0.95	7.12	5.651	0.257	0.2625
1.00	6.76	5.655	0.252	0.259
1.10	6.15	5.663	0.245	0.251
1.20	5.63	5.669	0.239	0.243
1.30	5.20	5.670	0.238	0.235
1.40	4.83	5.678	0.230	0.227
1.50	4.51	5.677	0.230	0.219
1.60	4.23	5.693	0.215	0.212



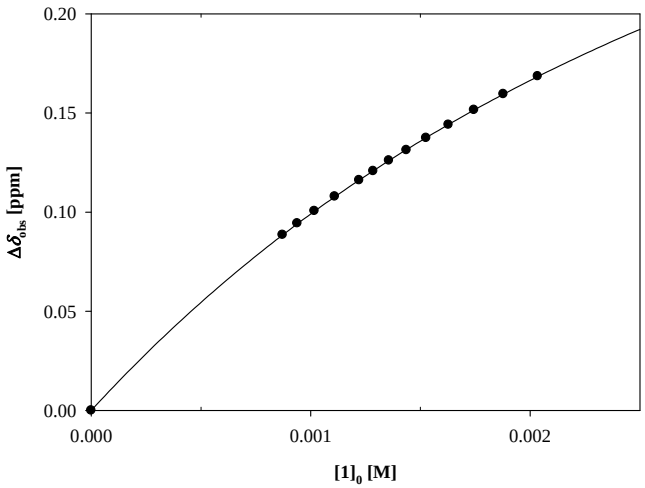
K_a [M^{-1}] = 750 ± 90
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.34
$\Delta\delta_{max}$ (2´-H) [ppm] = 0.27
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.12
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.07
$\Delta\delta_{max}$ (8-H) [ppm] = 0.47

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	407.02
T [°C]	25	m_R [mg]	0.76
substrate	**GMP**	m_S [mg]	0.67
	δ_0 (1´-H) = 5.932	V_0 [mL]	2
	δ_0 (3´-H) = 4.480	$[S]_0$ [mM]	0.82
	δ_0 (4´-H) = 4.317		
	δ_0 (8-H) = 8.192		



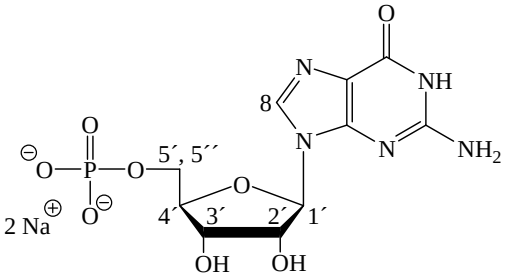
***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	2.03	5.764	0.169	0.168
0.65	1.88	5.773	0.160	0.160
0.70	1.74	5.781	0.152	0.151
0.75	1.63	5.788	0.144	0.144
0.80	1.53	5.795	0.137	0.138
0.85	1.44	5.801	0.131	0.132
0.90	1.36	5.806	0.126	0.126
0.95	1.29	5.811	0.121	0.121
1.00	1.22	5.816	0.116	0.116
1.10	1.11	5.824	0.108	0.108
1.20	1.02	5.832	0.101	0.100
1.30	0.94	5.838	0.094	0.094
1.40	0.87	5.844	0.089	0.088



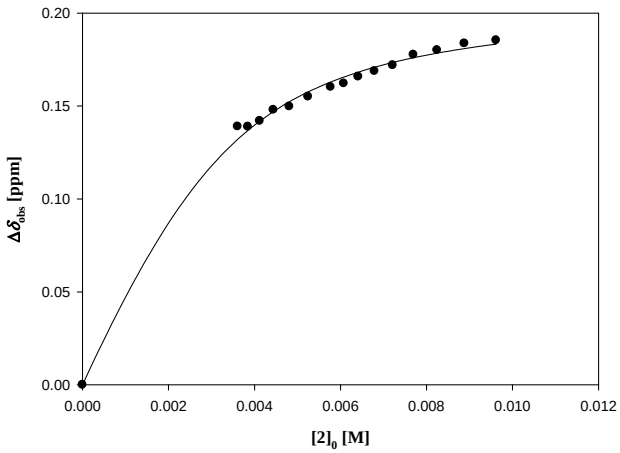
K_a [M^{-1}] = 350 ± 20
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.46
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.07
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.02
$\Delta\delta_{max}$ (8-H) [ppm] = 0.37

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	407.02
T [°C]	25	m_R [mg]	3.50
substrate	**GMP**	m_S [mg]	4.00
	δ_0 (1´-H) = 5.932	V_0 [mL]	3
	δ_0 (3´-H) = 4.480	$[S]_0$ [mM]	3.27
	δ_0 (4´-H) = 4.317		
	δ_0 (8-H) = 8.192		

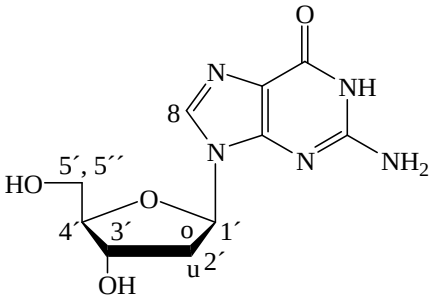


V [mL]	$[2]_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	9.62	5.747	0.185	0.183
0.65	8.88	5.748	0.184	0.181
0.70	8.25	5.752	0.180	0.178
0.75	7.70	5.754	0.178	0.176
0.80	7.21	5.760	0.172	0.173
0.85	6.79	5.763	0.169	0.171
0.90	6.41	5.766	0.166	0.168
0.95	6.08	5.770	0.162	0.166
1.00	5.77	5.772	0.160	0.163
1.10	5.25	5.777	0.155	0.158
1.20	4.81	5.782	0.150	0.152
1.30	4.44	5.784	0.148	0.147
1.40	4.12	5.790	0.142	0.142
1.50	3.85	5.793	0.139	0.137
1.60	3.61	5.793	0.139	0.132

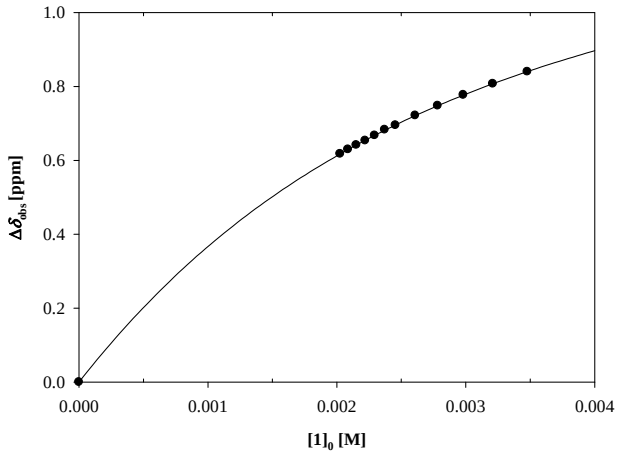


K_a [M^{-1}] = 1140 ± 130
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.21
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.06
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.04
$\Delta\delta_{max}$ (8-H) [ppm] = 0.17

^{1}H-NMR titration experiments with phosphate clip 1:

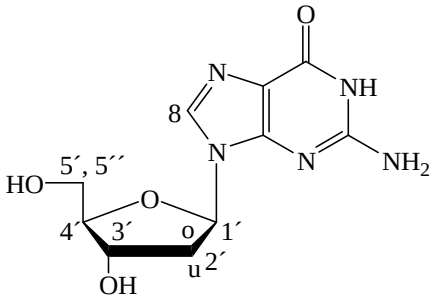
receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	267.10
T [°C]	25	m_R [mg]	1.41
substrate	**DG**	m_S [mg]	0.64
	δ_0 (1´-H) [ppm] = 6.301	V_0 [mL]	2
	δ_0 (2´o-H) [ppm] = 2.504	$[S]_0$ [mM]	1.21
	δ_0 (3´-H) [ppm] = 4.617		
	δ_0 (4´-H) [ppm] = 4.123		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.752, 3.812		
	δ_0 (8-H) [ppm] = 7.979		

***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (8-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	3.48	7.140	0.840	0.840
0.65	3.21	7.172	0.807	0.807
0.70	2.98	7.202	0.777	0.777
0.75	2.78	7.231	0.748	0.748
0.80	2.61	7.258	0.721	0.721
0.85	2.46	7.285	0.695	0.696
0.88	2.37	7.297	0.683	0.682
0.91	2.29	7.312	0.667	0.668
0.94	2.22	7.326	0.654	0.654
0.97	2.15	7.338	0.642	0.642
1.00	2.09	7.350	0.630	0.629
1.03	2.03	7.362	0.618	0.617

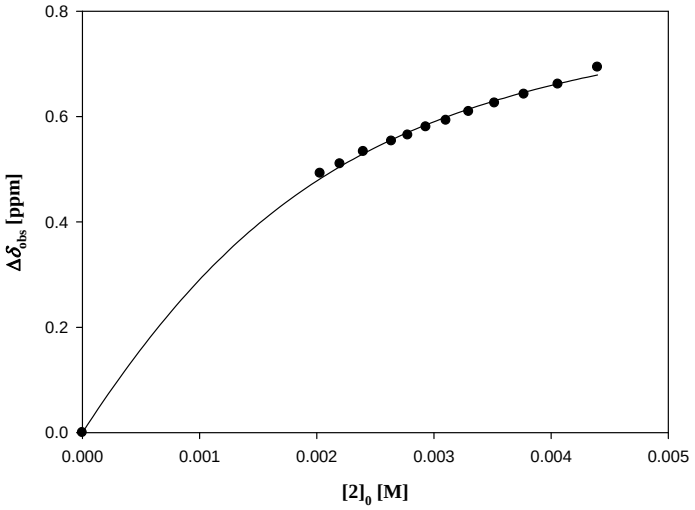


K_a [M^{-1}] = 490 ± 30
$\Delta\delta_{max}$ (1´-H) [ppm] = 1.03
$\Delta\delta_{max}$ (2´o-H) [ppm] = 0.36
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.21
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.19
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = 0.05, 0.09
$\Delta\delta_{max}$ (8-H) [ppm] = 1.48

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	267.10
T [°C]	25	m_R [mg]	1.60
substrate	**DG**	m_S [mg]	1.30
	δ_0 (1´-H) [ppm] = 6.301	V_0 [mL]	3
	δ_0 (2´o-H) [ppm] = 2.504	$[S]_0$ [mM]	1.52
	δ_0 (3´-H) [ppm] = 4.617		
	δ_0 (4´-H) [ppm] = 4.123		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.752, 3.812		
	δ_0 (8-H) [ppm] = 7.979		

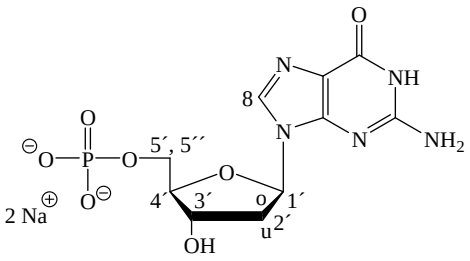
***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	4.40	5.607	0.693	0.679
0.65	4.10	5.639	0.661	0.662
0.70	3.80	5.658	0.642	0.646
0.75	3.50	5.675	0.626	0.630
0.80	3.30	5.691	0.609	0.614
0.85	3.10	5.708	0.593	0.599
0.90	2.90	5.720	0.580	0.584
0.95	2.80	5.736	0.564	0.570
1.00	2.60	5.747	0.553	0.556
1.10	2.40	5.767	0.533	0.530
1.20	2.20	5.790	0.510	0.505
1.30	2.00	5.808	0.492	0.483



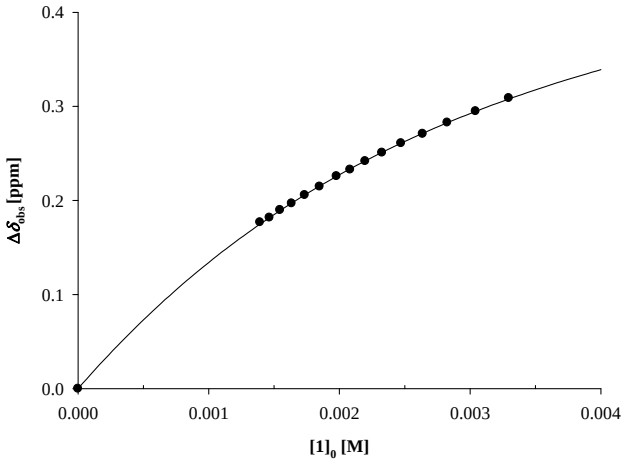
K_a [M^{-1}] = 740 ± 80
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.90
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.28
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.22
$\Delta\delta_{max}$ (8-H) [ppm] = 1.27

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	436.20
T [°C]	25	m_R [mg]	1.23
substrate	**DGMP**	m_S [mg]	2.13
	δ_0 (1´-H) [ppm] = 6.310	V_0 [mL]	3.5
	δ_0 (2´o-H) [ppm] = 2.490	$[S]_0$ [mM]	1.40
	δ_0 (2´u-H) [ppm] = 2.783		
	δ_0 (3´-H) [ppm] = 4.692		
	δ_0 (4´-H) [ppm] = 4.204		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.937		
	δ_0 (8-H) [ppm] = 8.142		



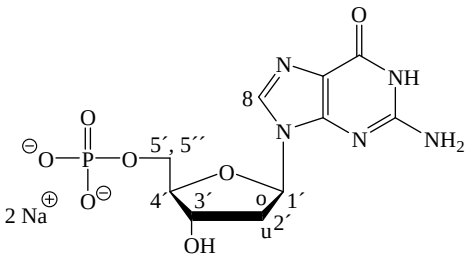
V [mL]	$[1]_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	3.30	6.001	0.309	0.308
0.65	3.04	6.015	0.295	0.295
0.70	2.83	6.027	0.283	0.283
0.75	2.64	6.039	0.271	0.271
0.80	2.47	6.049	0.261	0.261
0.85	2.33	6.059	0.251	0.251
0.90	2.20	6.068	0.242	0.242
0.95	2.08	6.077	0.233	0.234
1.00	1.98	6.084	0.226	0.226
1.07	1.85	6.095	0.215	0.215
1.14	1.74	6.104	0.206	0.206
1.21	1.63	6.113	0.197	0.197
1.28	1.55	6.120	0.190	0.189
1.35	1.47	6.128	0.182	0.182
1.42	1.39	6.133	0.177	0.175



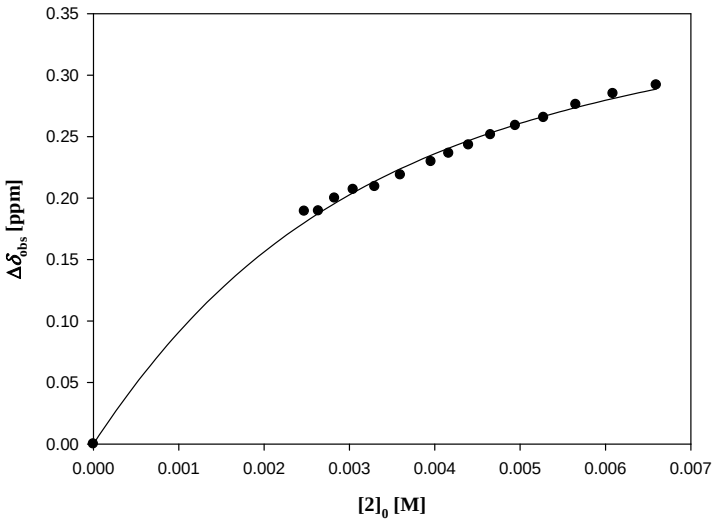
K_a [M^{-1}] = 470 ± 30
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.58
$\Delta\delta_{max}$ (2´o-H) [ppm] = 0.09
$\Delta\delta_{max}$ (2´u-H) [ppm] = 0.33
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.08
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.05
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.04
$\Delta\delta_{max}$ (8-H) [ppm] = 0.50

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	436.20
T [°C]	25	m_R [mg]	2.40
substrate	**DGMP**	m_S [mg]	2.20
	δ_0 (1´-H) [ppm] = 6.310	V_0 [mL]	3.0
	δ_0 (2´o-H) [ppm] = 2.490	$[S]_0$ [mM]	1.68
	δ_0 (2´u-H) [ppm] = 2.783		
	δ_0 (3´-H) [ppm] = 4.692		
	δ_0 (4´-H) [ppm] = 4.204		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.937		
	δ_0 (8-H) [ppm] = 8.142		

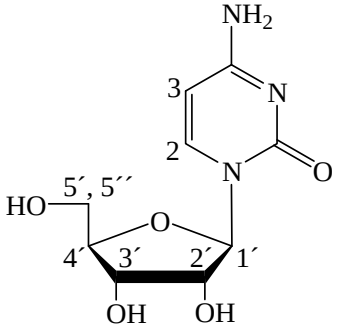


V [mL]	$[2]_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	6.60	6.018	0.292	0.289
0.65	6.09	6.025	0.285	0.281
0.70	5.65	6.034	0.276	0.274
0.75	5.28	6.044	0.265	0.266
0.80	4.95	6.051	0.259	0.260
0.85	4.66	6.058	0.251	0.247
0.90	4.40	6.067	0.243	0.241
0.95	4.17	6.073	0.236	0.235
1.00	3.96	6.080	0.230	0.224
1.10	3.60	6.091	0.219	0.214
1.20	3.30	6.100	0.209	0.204
1.30	3.04	6.103	0.207	0.196
1.40	2.83	6.110	0.200	0.188
1.50	2.64	6.120	0.190	0.182
1.60	2.47	6.121	0.189	0.180

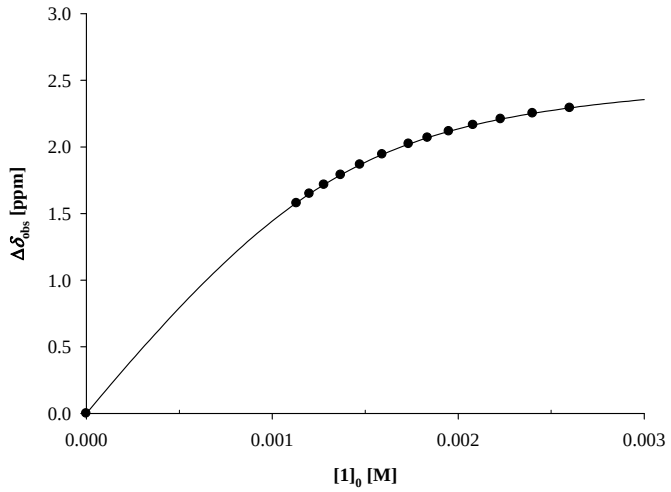


K_a [M^{-1}] = 460 ± 40
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.42
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.08
$\Delta\delta_{max}$ (8-H) [ppm] = 0.41

^{1}H-NMR titration experiments with phosphate clip 1:

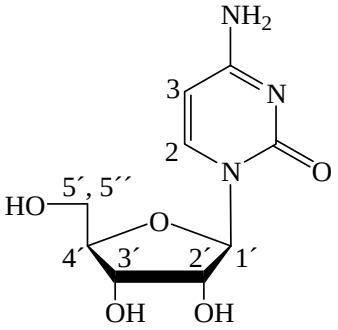
receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	243.22
T [°C]	25	m_R [mg]	0.97
substrate	cytidine (**C**)	m_S [mg]	0.67
	δ_0 (1´-H) [ppm] = 5.893 δ_0 (2´-H) [ppm] = 4.296 δ_0 (5´-H, 5´´-H) [ppm] = 3.797, 3.910 δ_0 (2-H) [ppm] = 7.829 δ_0 (3-H) [ppm] = 6.044	V_0 [mL] $[S]_0$ [mM]	2 1.36

***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (2-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	2.60	5.537	2.292	2.293
0.65	2.40	5.577	2.252	2.252
0.70	2.23	5.620	2.209	2.208
0.75	2.08	5.665	2.164	2.163
0.80	1.95	5.712	2.116	2.117
0.85	1.84	5.760	2.069	2.069
0.90	1.73	5.806	2.022	2.021
0.98	1.59	5.884	1.944	1.943
1.06	1.47	5.962	1.867	1.866
1.14	1.37	6.039	1.790	1.790
1.22	1.28	6.112	1.716	1.717
1.30	1.20	6.181	1.648	1.647
1.38	1.13	6.252	1.577	1.580

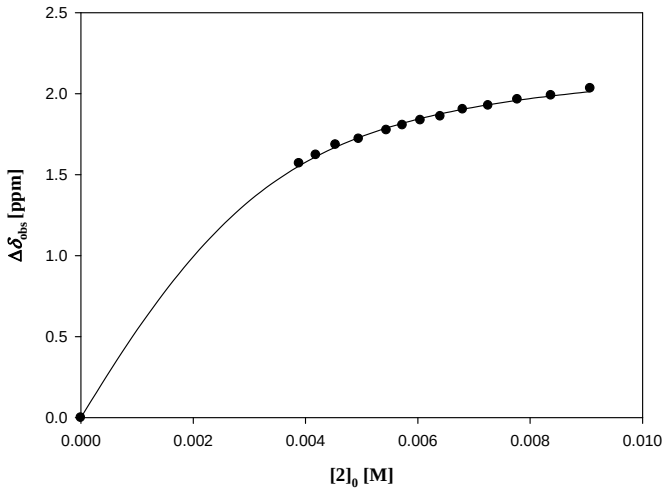


K_a [M^{-1}] = 5240 ± 420
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.76
$\Delta\delta_{max}$ (2´-H) [ppm] = 0.48
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.20, - 0.21
$\Delta\delta_{max}$ (2-H) [ppm] = 2.63
$\Delta\delta_{max}$ (3-H) [ppm] = 4.73

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	243.22
T [°C]	25	m_R [mg]	3.30
substrate	cytidine (**C**)	m_S [mg]	2.30
	δ_0 (1´-H) [ppm] = 5.893	V_0 [mL]	3
	δ_0 (2´-H) [ppm] = 4.296	$[S]_0$ [mM]	3.15
	δ_0 (5´-H, 5´´-H) [ppm] = 3.797, 3.910		
	δ_0 (2-H) [ppm] = 7.829		
	δ_0 (3-H) [ppm] = 6.044		

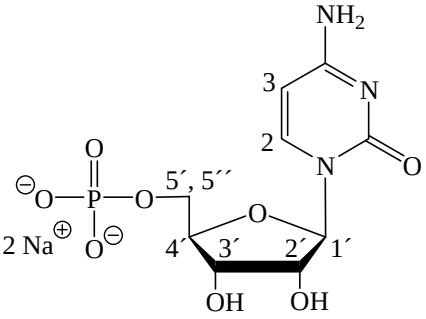
V [mL]	$[2]_0$ [mM]	δ_{obs} (2-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	9.07	5.796	2.033	2.012
0.65	8.37	5.840	1.989	1.986
0.70	7.77	5.864	1.964	1.959
0.75	7.26	5.902	1.927	1.932
0.80	6.80	5.926	1.903	1.904
0.85	6.40	5.969	1.860	1.875
0.90	6.05	5.993	1.836	1.846
0.95	5.73	6.023	1.806	1.817
1.00	5.44	6.054	1.775	1.788
1.10	4.95	6.108	1.720	1.729
1.20	4.53	6.144	1.685	1.670
1.30	4.19	6.208	1.621	1.611
1.40	3.89	6.259	1.569	1.554



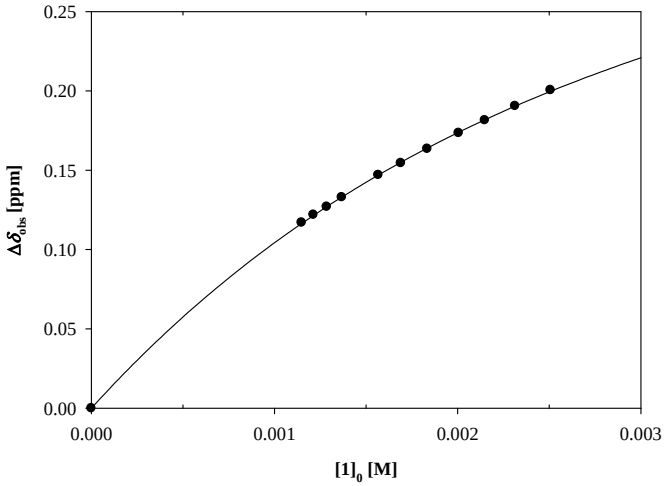
K_a [M^{-1}] = 1070 ± 50
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.75
$\Delta\delta_{max}$ (2-H) [ppm] = 2.39

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	323.05
T [°C]	25	m_R [mg]	0.94
substrate	**CMP**	m_S [mg]	1.49
	δ_0 (1´-H) [ppm] = 5.994	V_0 [mL]	4
	δ_0 (2´-H) [ppm] = 4.334	$[S]_0$ [mM]	1.10
	δ_0 (3´-H) [ppm] = 4.324		
	δ_0 (4´-H) [ppm] = 4.233		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.975, 4.054		
	δ_0 (2-H) [ppm] = 8.079		
	δ_0 (3-H) [ppm] = 6.122		



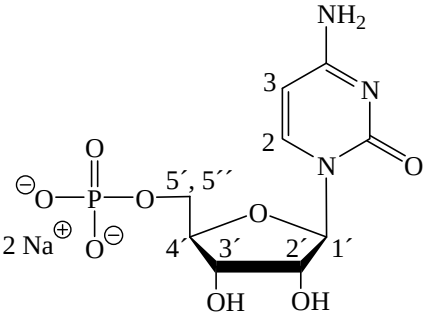
***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	2.51	5.793	0.201	0.200
0.65	2.31	5.803	0.190	0.190
0.70	2.15	5.812	0.182	0.182
0.75	2.01	5.820	0.173	0.174
0.82	1.83	5.830	0.163	0.164
0.89	1.69	5.839	0.154	0.155
0.96	1.57	5.847	0.147	0.147
1.10	1.37	5.861	0.133	0.133
1.17	1.29	5.867	0.127	0.127
1.24	1.21	5.872	0.122	0.121
1.31	1.15	5.877	0.117	0.116



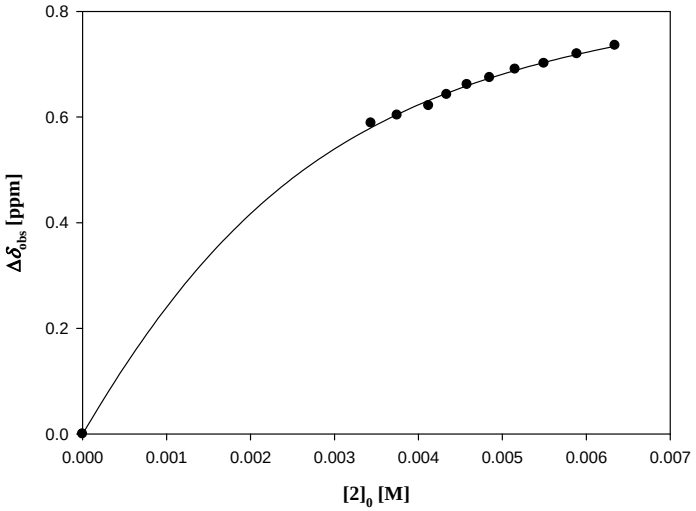
K_a [M^{-1}] = 440 ± 10
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.43
$\Delta\delta_{max}$ (2´-H) [ppm] = 0.14
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.18
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.05
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.14, - 0.17
$\Delta\delta_{max}$ (2-H) [ppm] = 1.74
$\Delta\delta_{max}$ (3-H) [ppm] = 2.72

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	323.05
T [°C]	25	m_R [mg]	2.50
substrate	**CMP**	m_S [mg]	2.10
	δ_0 (1´-H) [ppm] = 5.994	V_0 [mL]	3
	δ_0 (2´-H) [ppm] = 4.334	$[S]_0$ [mM]	2.16
	δ_0 (3´-H) [ppm] = 4.324		
	δ_0 (4´-H) [ppm] = 4.233		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.975, 4.054		
	δ_0 (2-H) [ppm] = 8.079		
	δ_0 (3-H) [ppm] = 6.122		



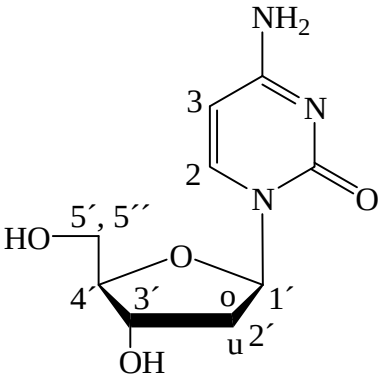
V [mL]	$[2]_0$ [mM]	δ_{obs} (2-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	6.90	-	-	-
0.65	6.30	7.587	0.735	0.727
0.70	5.90	7.603	0.719	0.715
0.75	5.50	7.621	0.701	0.704
0.80	5.20	7.632	0.690	0.692
0.85	4.90	7.648	0.674	0.680
0.90	4.60	7.661	0.651	0.657
0.95	4.30	7.680	0.642	0.645
1.00	4.10	7.701	0.621	0.622
1.10	3.70	7.719	0.603	0.600
1.20	3.40	7.734	0.588	0.579



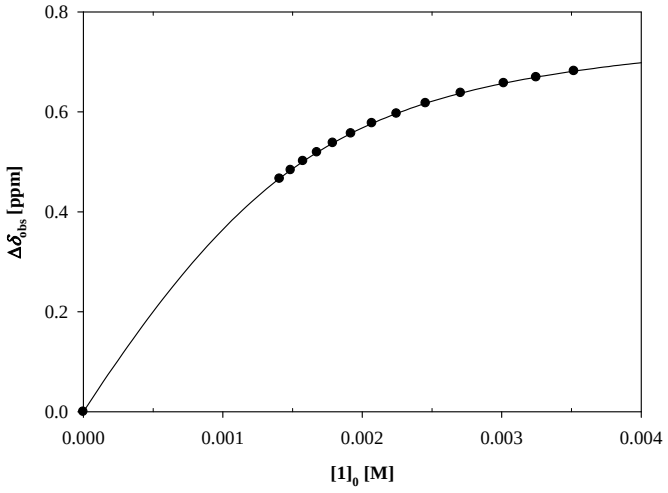
K_a [M^{-1}] = 320 ± 20
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.20
$\Delta\delta_{max}$ (2´-H) [ppm] = 0.14
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.11
$\Delta\delta_{max}$ (2-H) [ppm] = 0.86
$\Delta\delta_{max}$ (3-H) [ppm] = 1.16

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	245.10
T [°C]	25	m_R [mg]	1.42
substrate	**DC**	m_S [mg]	1.84
	δ_0 (1´-H) [ppm] = 6.260	V_0 [mL]	5
	δ_0 (2´u-H) [ppm] = 2.415	$[S]_0$ [mM]	1.49
	δ_0 (2´o-H) [ppm] = 2.289		
	δ_0 (3´-H) [ppm] = 4.421		
	δ_0 (5´-H v 5´´-H) [ppm] = 3.740		
	δ_0 (2-H) [ppm] = 7.815		



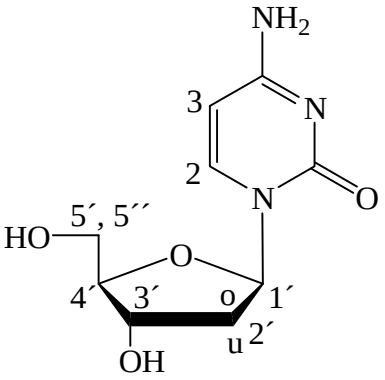
***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	3.52	5.578	0.682	0.682
0.65	3.25	5.591	0.669	0.670
0.70	3.02	5.603	0.658	0.657
0.78	2.71	5.622	0.638	0.637
0.86	2.45	5.643	0.617	0.617
0.94	2.25	5.664	0.596	0.597
1.02	2.07	5.683	0.577	0.577
1.10	1.92	5.703	0.557	0.557
1.18	1.79	5.722	0.538	0.538
1.26	1.68	5.741	0.519	0.519
1.34	1.58	5.759	0.501	0.501
1.42	1.49	5.777	0.483	0.483
1.50	1.41	5.794	0.466	0.467



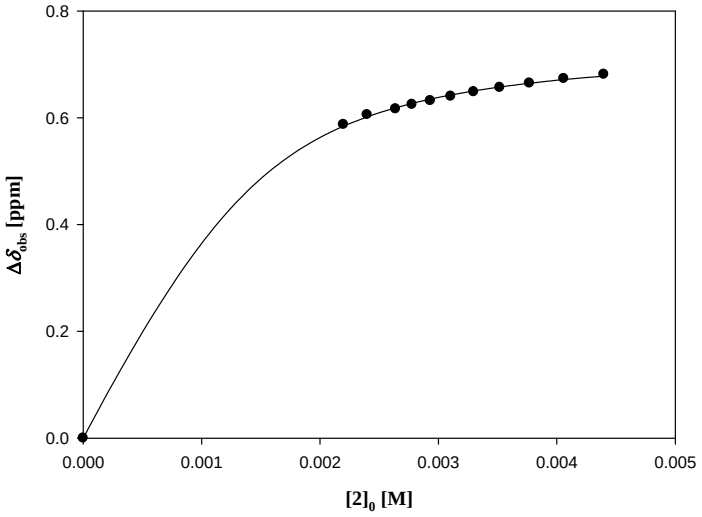
K_a [M^{-1}] = 2640 ± 40
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.80
$\Delta\delta_{max}$ (2´o-H) [ppm] = 0.49
$\Delta\delta_{max}$ (2´u-H) [ppm] = 0.19
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.11
$\Delta\delta_{max}$ (5´-H v 5´´-H) [ppm] = - 0.18
$\Delta\delta_{max}$ (2-H) [ppm] = 2.51

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	245.10
T [°C]	25	m_R [mg]	1.60
substrate	**DC**	m_S [mg]	1.10
	δ_0 (1´-H) [ppm] = 6.260	V_0 [mL]	3
	δ_0 (2´u-H) [ppm] = 2.415	$[S]_0$ [mM]	1.49
	δ_0 (2´o-H) [ppm] = 2.289		
	δ_0 (3´-H) [ppm] = 4.421		
	δ_0 (5´-H v 5´´-H) [ppm] = 3.740		
	δ_0 (2-H) [ppm] = 7.815		



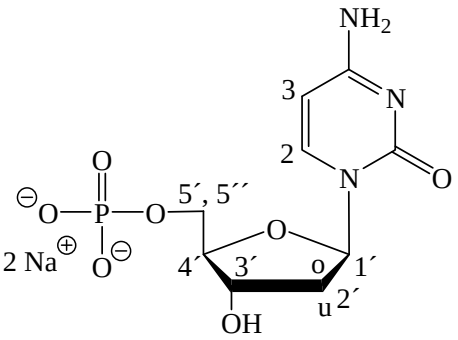
***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	4.40	5.579	0.681	0.678
0.65	4.10	5.587	0.673	0.671
0.70	3.80	5.595	0.665	0.665
0.75	3.50	5.603	0.657	0.658
0.80	3.30	5.611	0.649	0.650
0.85	3.10	5.620	0.640	0.643
0.90	2.90	5.628	0.632	0.635
0.95	2.80	5.635	0.625	0.627
1.00	2.60	5.644	0.616	0.619
1.10	2.40	5.654	0.606	0.602
1.20	2.20	5.673	0.587	0.584



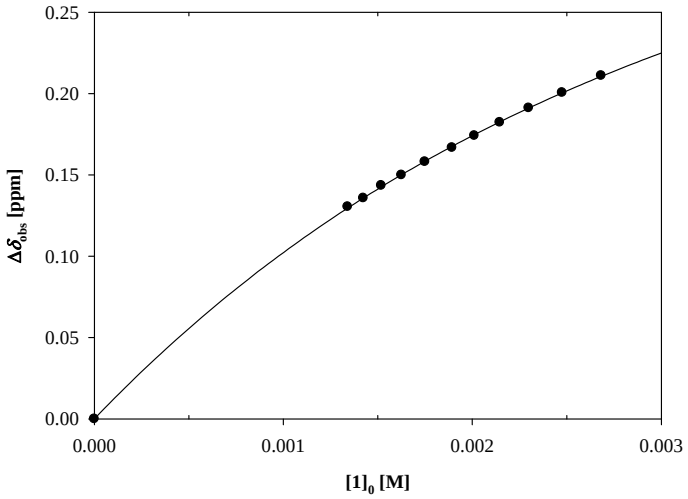
K_a [M^{-1}] = 3000 ± 190
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.74
$\Delta\delta_{max}$ (2´o-H) [ppm] = 0.55
$\Delta\delta_{max}$ (2´u-H) [ppm] = 0.20
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.17
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.08
$\Delta\delta_{max}$ (2-H) [ppm] = 2.33

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	291.06
T [°C]	25	m_R [mg]	1.00
substrate	**DCMP**	m_S [mg]	1.67
	δ_0 (1´-H) [ppm] = 6.325	V_0 [mL]	4
	δ_0 (2´u-H) [ppm] = 2.387	$[S]_0$ [mM]	1.38
	δ_0 (2´o-H) [ppm] = 2.311		
	δ_0 (3´-H) [ppm] = 4.548		
	δ_0 (4´-H) [ppm] = 4.151		
	δ_0 (2-H) [ppm] = 8.037		
	δ_0 (3-H) [ppm] = 6.108		



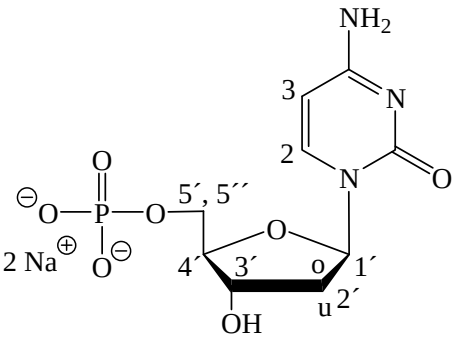
V [mL]	$[1]_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	2.68	6.114	0.211	0.211
0.65	2.48	6.124	0.201	0.200
0.70	2.30	6.133	0.191	0.191
0.75	2.15	6.142	0.182	0.183
0.80	2.01	6.150	0.174	0.175
0.85	1.89	6.158	0.167	0.168
0.92	1.75	6.167	0.158	0.158
0.99	1.63	6.175	0.150	0.150
1.06	1.52	6.181	0.144	0.143
1.13	1.42	6.189	0.136	0.136
1.20	1.34	6.194	0.130	0.130



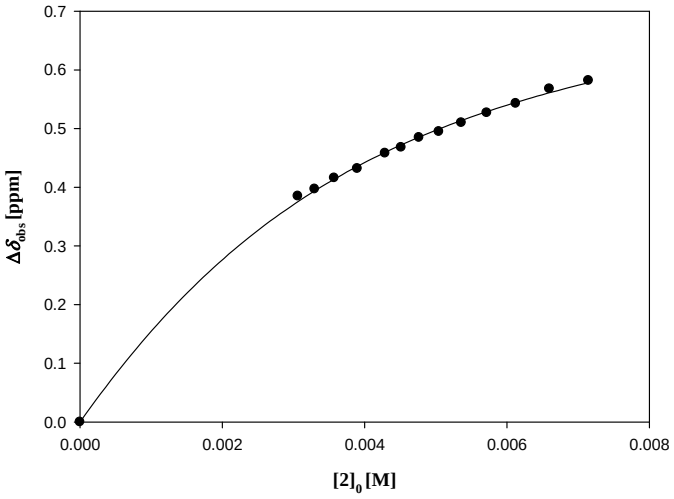
K_a [M^{-1}] = 430 ± 20
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.46
$\Delta\delta_{max}$ (2´o-H) [ppm] = 0.23
$\Delta\delta_{max}$ (2´u-H) [ppm] = 0.09
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.08
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.06
$\Delta\delta_{max}$ (2-H) [ppm] = 1.67
$\Delta\delta_{max}$ (3-H) [ppm] = 2.70

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	291.06
T [°C]	25	m_R [mg]	2.60
substrate	**DCMP**	m_S [mg]	2.20
	δ_0 (1´-H) [ppm] = 6.325	V_0 [mL]	3
	δ_0 (2´u-H) [ppm] = 2.387	$[S]_0$ [mM]	2.25
	δ_0 (2´o-H) [ppm] = 2.311		
	δ_0 (3´-H) [ppm] = 4.548		
	δ_0 (4´-H) [ppm] = 4.151		
	δ_0 (2-H) [ppm] = 8.037		
	δ_0 (3-H) [ppm] = 6.108		

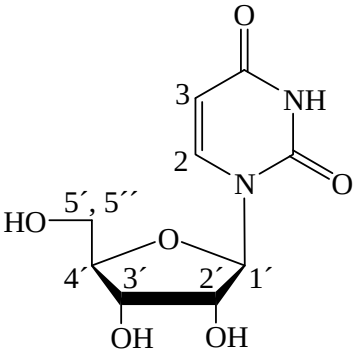


***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (2-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	7.10	7.455	0.582	0.578
0.65	6.60	7.469	0.568	0.561
0.70	6.10	7.494	0.543	0.545
0.75	5.70	7.510	0.527	0.529
0.80	5.40	7.527	0.510	0.514
0.85	5.00	7.542	0.495	0.499
0.90	4.80	7.552	0.485	0.485
0.95	4.50	7.569	0.468	0.472
1.00	4.30	7.579	0.458	0.459
1.10	3.90	7.605	0.432	0.436
1.20	3.60	7.621	0.416	0.414
1.30	3.30	7.640	0.397	0.394
1.40	3.10	7.652	0.385	0.376

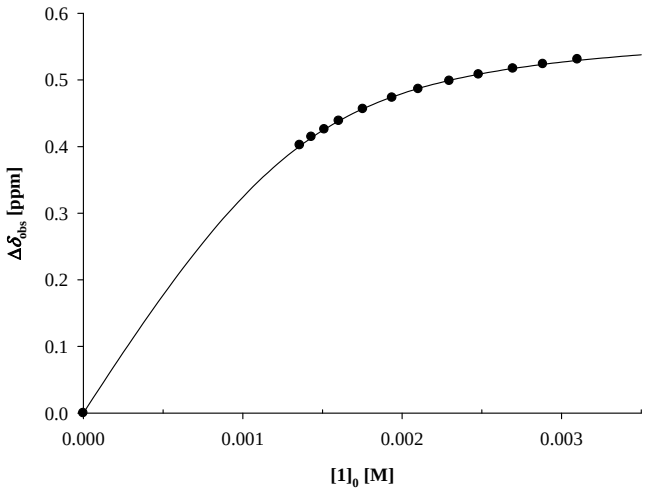


K_a [M^{-1}] = 370 ± 20
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.26
$\Delta\delta_{max}$ (2-H) [ppm] = 0.84
$\Delta\delta_{max}$ (3-H) [ppm] = 1.32

^{1}H-NMR titration experiments with phosphate clip 1:

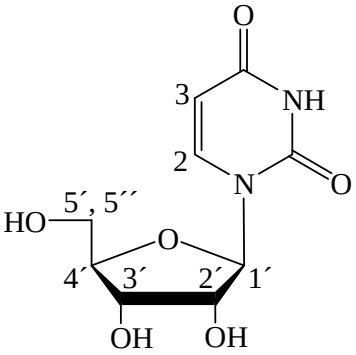
receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	244.07
T [°C]	25	m_R [mg]	1.16
substrate	uridine (**U**)	m_S [mg]	1.36
	δ_0 (1´-H) [ppm] = 5.903	V_0 [mL]	4
	δ_0 (2´-H) [ppm] = 4.341	[S]$_0$ [mM]	1.38
	δ_0 (3´-H) [ppm] = 4.215		
	δ_0 (5´-H v 5´´-H) [ppm] = 3.895		
	δ_0 (2-H) [ppm] = 7.861		
	δ_0 (3-H) [ppm] = 5.886		

V [mL]	[1]$_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	3.10	5.372	0.531	0.529
0.65	2.88	5.379	0.524	0.523
0.69	2.70	5.386	0.517	0.517
0.75	2.48	5.395	0.508	0.509
0.81	2.30	5.405	0.499	0.499
0.89	2.10	5.417	0.486	0.487
0.96	1.94	5.430	0.473	0.474
1.06	1.76	5.447	0.456	0.457
1.16	1.60	5.465	0.438	0.439
1.23	1.51	5.477	0.426	0.426
1.30	1.43	5.489	0.414	0.413
1.37	1.36	5.501	0.402	0.401

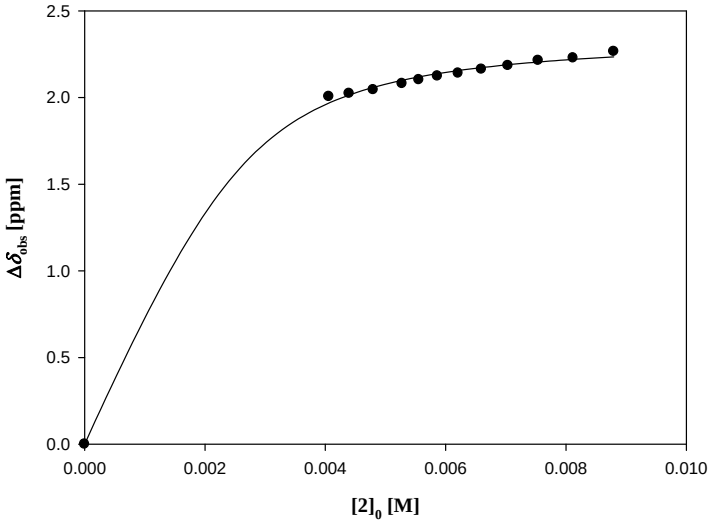


K_a [M^{-1}] = 5390 ± 200
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.58
$\Delta\delta_{max}$ (2´-H) [ppm] = 0.18
$\Delta\delta_{max}$ (3´-H) [ppm] = - 0.04
$\Delta\delta_{max}$ (5´-H v 5´´-H) [ppm] = - 0.25
$\Delta\delta_{max}$ (2-H) [ppm] = 2.74
$\Delta\delta_{max}$ (3-H) [ppm] = 4.80

^{1}H-NMR titration experiments with phosphonate clip 2:

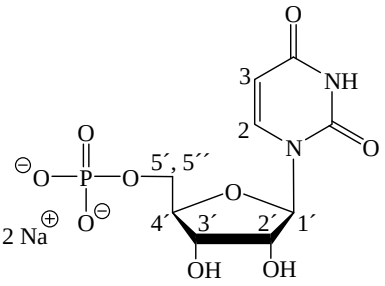
receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	244.07
T [°C]	25	m_R [mg]	3.20
substrate	uridine (**U**)	m_S [mg]	2.00
	δ_0 (1´-H) [ppm] = 5.903	V_0 [mL]	3
	δ_0 (2´-H) [ppm] = 4.341	$[S]_0$ [mM]	2.73
	δ_0 (3´-H) [ppm] = 4.215		
	δ_0 (5´-H v 5´´-H) [ppm] = 3.895		
	δ_0 (2-H) [ppm] = 7.861		
	δ_0 (3-H) [ppm] = 5.886		

V [mL]	$[2]_0$ [mM]	δ_{obs} (2-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	8.790	5.596	2.265	2.235
0.65	8.12	5.633	2.228	2.220
0.70	7.54	5.648	2.214	2.205
0.75	7.04	5.677	2.184	2.189
0.80	6.60	5.698	2.163	2.173
0.85	6.21	5.721	2.140	2.155
0.90	5.86	5.738	2.123	2.137
0.95	5.55	5.759	2.102	2.119
1.00	5.28	5.781	2.080	2.099
1.10	4.80	5.817	2.044	2.058
1.20	4.40	5.838	2.023	2.014
1.30	4.06	5.856	2.005	2.968

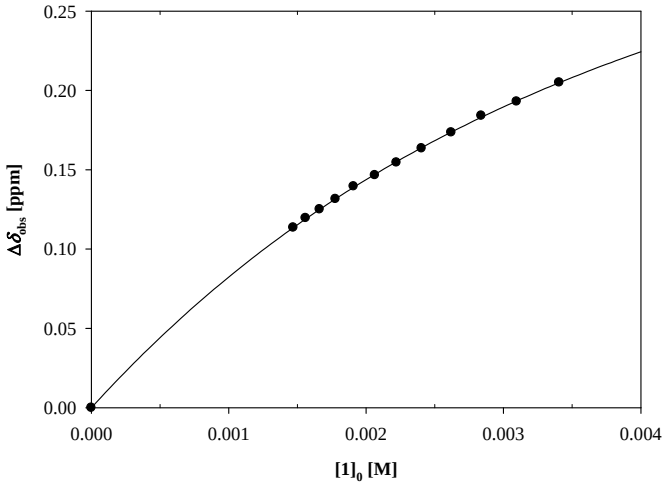


K_a [M^{-1}] = 2490 ± 240
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.59
$\Delta\delta_{max}$ (2-H) [ppm] = 2.36

^{1}H-NMR titration experiments with phosphate clip 1:

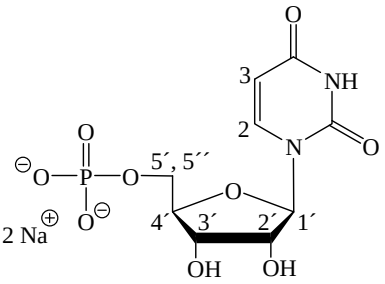
receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	368.00
T [°C]	25	m_R [mg]	1.27
substrate	**UMP**	m_S [mg]	2.45
	δ_0 (1´-H) [ppm] = 5.986	V_0 [mL]	4
	δ_0 (2´-H) [ppm] = 4.407	[S]$_0$ [mM]	1.65
	δ_0 (3´-H) [ppm] = 4.351		
	δ_0 (4´-H) [ppm] = 4.248		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.965, 4.025		
	δ_0 (2-H) [ppm] = 8.095		

V [mL]	[1]$_0$ [mM]	δ_{obs} (1´-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	3.41	5.781	0.205	0.205
0.66	3.10	5.793	0.193	0.193
0.72	2.84	5.802	0.184	0.183
0.78	2.62	5.812	0.174	0.174
0.85	2.40	5.822	0.164	0.164
0.92	2.22	5.831	0.155	0.155
0.99	2.06	5.839	0.147	0.147
1.07	1.91	5.846	0.140	0.139
1.15	1.78	5.854	0.132	0.132
1.23	1.66	5.861	0.125	0.125
1.31	1.56	5.866	0.120	0.119
1.39	1.47	5.872	0.114	0.114

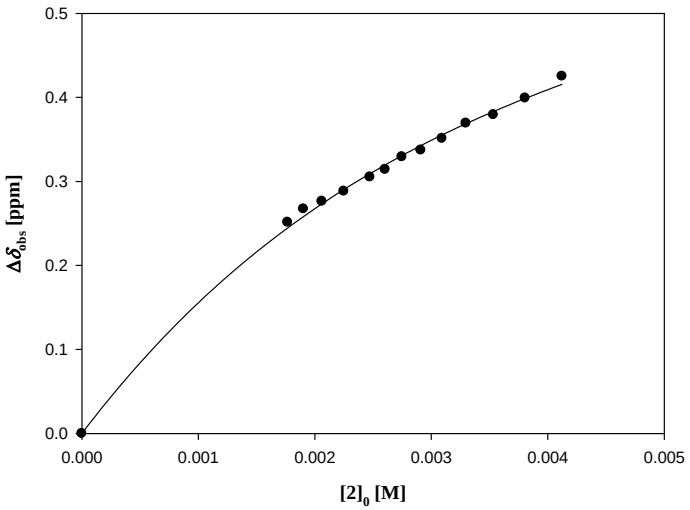


K_a [M^{-1}] = 340 ± 20
$\Delta\delta_{max}$ (1´-H) [ppm] = 0.43
$\Delta\delta_{max}$ (2´-H) [ppm] = 0.10
$\Delta\delta_{max}$ (3´-H) [ppm] = 0.05
$\Delta\delta_{max}$ (4´-H) [ppm] = 0.05
$\Delta\delta_{max}$ (5´-H, 5´´-H) [ppm] = - 0.20, - 0.23
$\Delta\delta_{max}$ (2-H) [ppm] = 2.01

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	368.00
T [°C]	25	m_R [mg]	1.50
substrate	**UMP**	m_S [mg]	1.60
	δ_0 (1´-H) [ppm] = 5.986	V_0 [mL]	3
	δ_0 (2´-H) [ppm] = 4.407	$[S]_0$ [mM]	1.45
	δ_0 (3´-H) [ppm] = 4.351		
	δ_0 (4´-H) [ppm] = 4.248		
	δ_0 (5´-H, 5´´-H) [ppm] = 3.965, 4.025		
	δ_0 (2-H) [ppm] = 8.095		

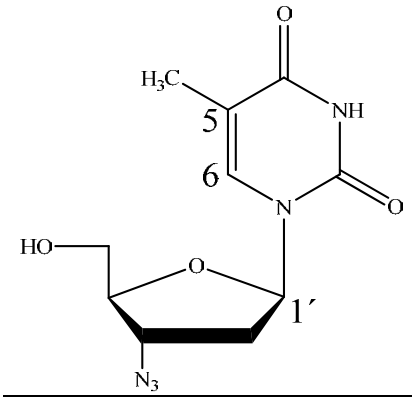
V [mL]	$[2]_0$ [mM]	δ_{obs} (2-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	4.10	7.660	0.435	0.425
0.65	3.80	7.686	0.409	0.409
0.70	3.50	7.706	0.389	0.393
0.75	3.30	7.716	0.379	0.379
0.80	3.10	7.734	0.361	0.365
0.85	2.90	7.748	0.347	0.353
0.90	2.70	7.756	0.339	0.341
0.95	2.60	7.771	0.324	0.330
1.00	2.50	7.780	0.315	0.320
1.10	2.20	7.797	0.298	0.300
1.20	2.10	7.809	0.286	0.283
1.30	1.90	7.818	0.277	0.268
1.40	1.80	7.834	0.261	0.254



K_a [M^{-1}] = 460 ± 50
$\Delta\delta_{max}$ (1´-H) [ppm] = 1.03
$\Delta\delta_{max}$ (2-H) [ppm] = 0.73
$\Delta\delta_{max}$ (3-H) [ppm] = 0.19

^{1}H-NMR titration experiments with phosphate clip 1:

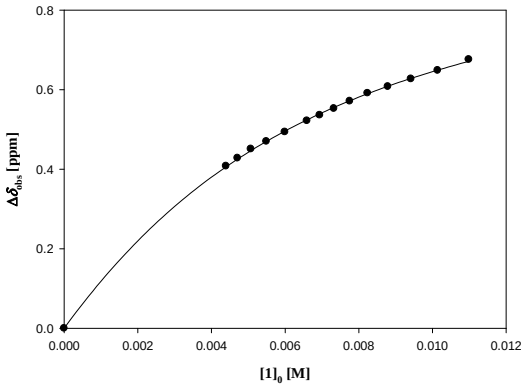
receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	267.25
T [°C]	25	m_R [mg]	4.10
substrate	**AZT**	m_S [mg]	2.70
	δ_0 (1´-H) [ppm] = 6.217	V_0 [mL]	3
	δ_0 (5-CH_3) [ppm] = 1.887	$[S]_0$ [mM]	3.37
	δ_0 (6-H) [ppm] = 7.638		



***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	10.99	5.541	0.676	0.671
0.65	10.14	5.568	0.649	0.649
0.70	9.42	5.589	0.627	0.628
0.75	9.01	5.609	0.608	0.609
0.80	8.79	5.625	0.591	0.590
0.85	8.24	5.645	0.571	0.572
0.90	7.32	5.664	0.553	0.555
0.95	6.94	5.681	0.536	0.539
1.00	6.59	5.695	0.522	0.524
1.10	5.99	5.723	0.494	0.496
1.20	5.49	5.747	0.470	0.470
1.30	5.07	5.766	0.451	0.447
1.40	4.71	5.789	0.428	0.425
1.50	4.39	5.809	0.408	0.406

***V* [mL]**	**$[1]_0$ [mM]**	**δ_{obs} (5-CH_3)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	10.99	0.726	1.161	1.154
0.65	10.14	0.772	1.115	1.115
0.70	9.42	0.810	1.077	1.078
0.75	9.01	0.846	1.042	1.043
0.80	8.79	0.876	1.012	1.010
0.85	8.24	0.910	0.977	0.979
0.90	7.32	0.943	0.945	0.949
0.95	6.94	0.971	0.917	0.921
1.00	6.59	0.997	0.891	0.894
1.10	5.99	1.046	0.842	0.845
1.20	5.49	1.087	0.800	0.801
1.30	5.07	1.121	0.767	0.760
1.40	4.71	1.161	0.727	0723
1.50	4.39	1.193	0.694	0.690

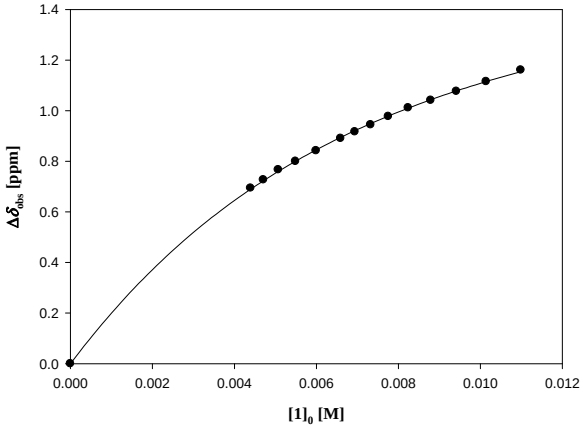
V [mL]	$[1]_0$ [mM]	δ_{obs} (6-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	10.99	5.821	1.817	1.807
0.65	10.14	5.891	1.747	1.749
0.70	9.42	5.947	1.691	1.694
0.75	9.01	5.997	1.641	1.641
0.80	8.79	6.044	1.594	1.591
0.85	8.24	6.097	1.541	1.544
0.90	7.32	6.145	1.493	1.499
0.95	6.94	6.189	1.449	1.456
1.00	6.59	6.226	1.412	1.416
1.10	5.99	6.305	1.333	1.340
1.20	5.49	6.567	1.271	1.271
1.30	5.07	6.420	1.218	1.209
1.40	4.71	6.481	1.157	1.152
1.50	4.39	6.532	1.106	1.099



Fitting for 1′-H

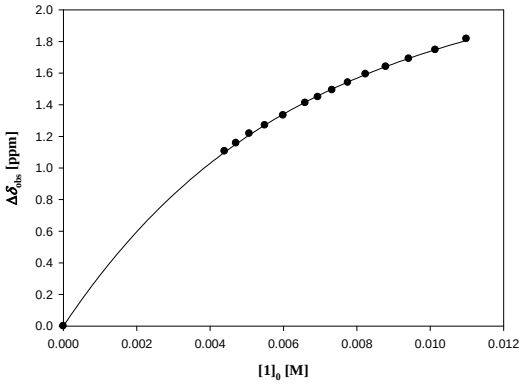
K_a [M^{-1}] = 210 ± 5

K_a [M^{-1}] = 208 ± 5
$\Delta\delta_{max}$ (1´-H) [ppm] = 1.03
$\Delta\delta_{max}$ (5-CH_3) [ppm] = 1.82
$\Delta\delta_{max}$ (6-H) [ppm] = 2.75



Fitting for 5-CH_3

K_a [M^{-1}] = 195 ± 5

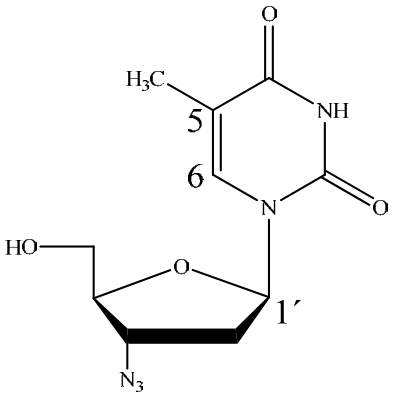


Fitting for 6-H

K_a [M^{-1}] = 219 ± 5

^{1}H-NMR titration experiments with phosphonate clip 2:

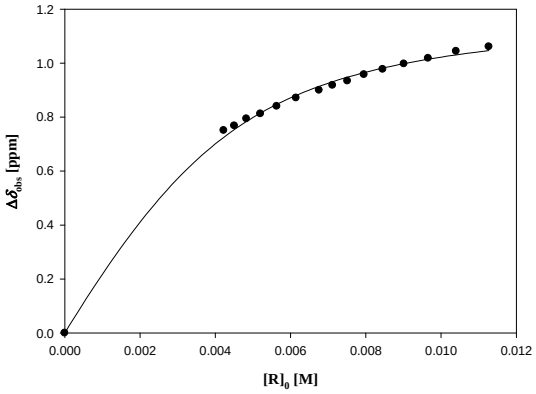
receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	267.25
T [°C]	25	m_R [mg]	4.10
substrate	**AZT**	m_S [mg]	2.90
	δ_0 (1´-H) [ppm] = 6.2166	V_0 [mL]	3
	δ_0 (5-CH_3) [ppm] = 1.8875	$[S]_0$ [mM]	3.62
	δ_0 (6-H) [ppm] = 7.6381		



***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (1´-H)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	11.27	5.156	1.060	1.046
0.65	10.40	5.173	1.044	1.030
0.70	9.66	5.199	1.018	1.014
0.75	9.01	5.220	0.997	0.998
0.80	8.45	5.240	0.977	0.981
0.85	7.95	5.259	0.957	0.965
0.90	7.51	5.283	0.934	0.948
0.95	7.12	5.299	0.918	0.931
1.00	6.76	5.317	0.899	0.914
1.10	6.15	5.345	0.871	0.880
1.20	5.63	5.377	0.840	0.847
1.30	5.20	5.405	0.812	0.815
1.40	4.83	5.423	0.794	0.784
1.50	4.51	5.449	0.768	0.754
1.60	4.23	5.466	0.750	0.725

***V* [mL]**	**$[2]_0$ [mM]**	**δ_{obs} (5-CH_3)**	**$\Delta\delta_{obs}$**	**$\Delta\delta_{calc}$**
0.60	11.27	0.692	1.196	1.183
0.65	10.40	0.711	1.176	1.165
0.70	9.66	0.737	1.150	1.145
0.75	9.01	0.761	1.127	1.127
0.80	8.45	0.783	1.104	1.108
0.85	7.95	0.806	1.082	1.089
0.90	7.51	0.830	1.058	1.070
0.95	7.12	0.849	1.038	1.051
1.00	6.76	0.869	1.019	1.032
1.10	6.15	0.901	0.986	0.996
1.20	5.63	0.936	0.951	0.960
1.30	5.20	0.967	0.920	0.925
1.40	4.83	0.986	0.901	0.891
1.50	4.51	1.016	0.872	0.859
1.60	4.23	1.036	0.852	0.829

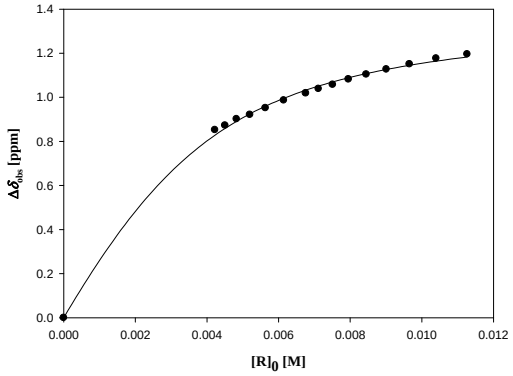
V [mL]	$[2]_0$ [mM]	δ_{obs} (6-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
0.60	11.27	5.114	2.524	1.786
0.65	10.40	5.155	2.483	1.850
0.70	9.66	5.199	2.439	1.917
0.75	9.01	5.246	2.392	1.986
0.80	8.45	5.290	2.348	2.058
0.85	7.95	5.332	2.306	2.130
0.90	7.51	5.382	2.256	2.204
0.95	7.12	5.428	2.210	2.242
1.00	6.76	5.460	2.178	2.279
1.10	6.15	5.528	2.110	2.316
1.20	5.63	5.597	2.041	2.353
1.30	5.20	5.661	1.977	2.390
1.40	4.83	5.701	1.937	2.427
1.50	4.51	5.764	1.874	2.463
1.60	4.23	5.805	1.833	2.498



Fitting for 1′-H

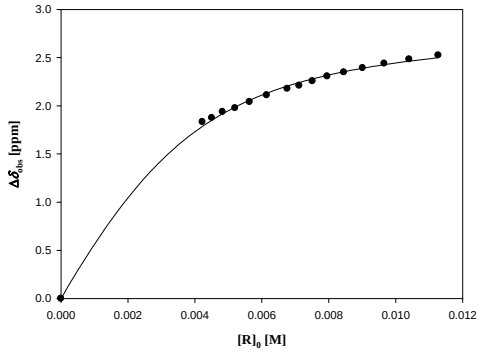
K_a [M^{-1}] = 810 ± 50

K_a [M^{-1}] = 811 ± 58
$\Delta\delta_{max}$ (1´-H) [ppm] = 1.20
$\Delta\delta_{max}$ (5-CH_3) [ppm] = 1.38
$\Delta\delta_{max}$ (6-H) [ppm] = 2.87



Fitting for CH_3

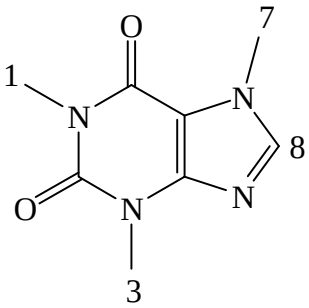
K_a [M^{-1}] = 729 ± 47



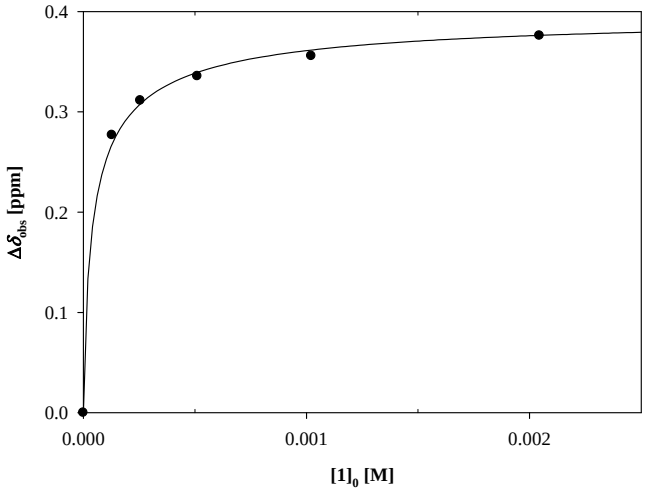
Fitting for 6-H

K_a [M^{-1}] = 833 ± 52

^{1}H-NMR titration experiments with phosphate clip 1:

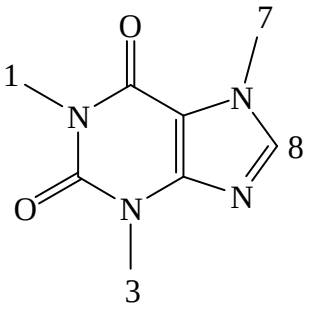
receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	194.08
T [°C]	25	m_R [mg]	4.24
substrate	caffeine (**CAF**)	m_S [mg]	1.19
	δ_0 (1-H) [ppm] = 3.526	V_0 [mL]	2
	δ_0 (3-H) [ppm] = 3.344	$[R]_0$ [mM]	4.08
	δ_0 (7-H) [ppm] = 3.946	$[S]_0$ [mM]	3.06

$[1]_0$ [mM]	$[CAF]_0$ [mM]	δ_{obs} (1-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
2.04	1.53	3.150	0.376	0.376
1.02	0.77	3.170	0.356	0.362
0.51	0.38	3.190	0.336	0.339
0.26	0.19	3.215	0.311	0.308
0.13	0.10	3.249	0.277	0.267

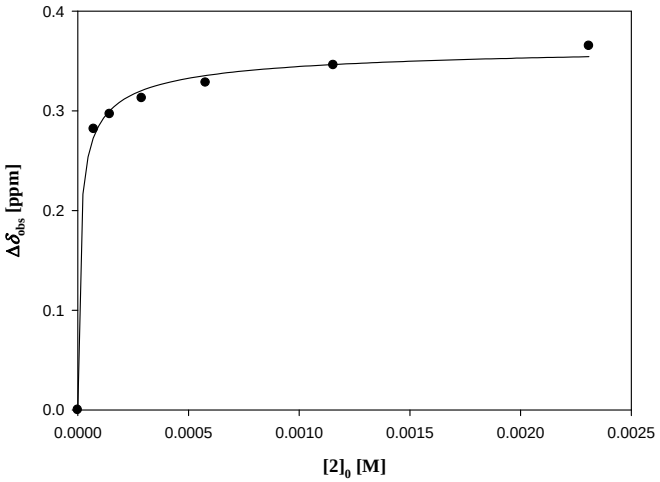


K_a [M^{-1}] = 31400 ± 2300
$\Delta\delta_{max}$ (1-H) [ppm] = 0.40
$\Delta\delta_{max}$ (3-H) [ppm] = 0.17
$\Delta\delta_{max}$ (7-H) [ppm] = 0.94

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	**Clip 2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	194.08
T [°C]	25	m_R [mg]	4.20
substrate	caffeine (**CAF**)	m_S [mg]	1.30
	δ_0 (1-H) [ppm] = 3.526	V_0 [mL]	3
	δ_0 (3-H) [ppm] = 3.344	$[R]_0$ [mM]	2.31
	δ_0 (7-H) [ppm] = 3.946	$[S]_0$ [mM]	2.23

$[2]_0$ [mM]	$[CAF]_0$ [mM]	δ_{obs} (1-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
2.31	2.23	3.161	0.365	0.354
1.15	1.11	3.180	0.346	0.346
0.58	0.56	3.198	0.328	0.335
0.29	0.28	3.213	0.313	0.320
0.14	0.14	3.229	0.297	0.300
0.07	0.07	3.244	0.282	0.274



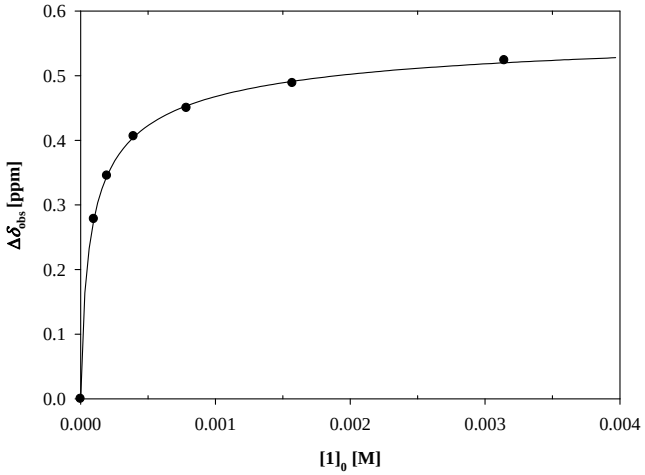
K_a [M^{-1}] = 9550 ± 1170
$\Delta\delta_{max}$ (1-H) [ppm] = 0.71
$\Delta\delta_{max}$ (3-H) [ppm] = 0.25
$\Delta\delta_{max}$ (7-H) [ppm] = 1.02

^{1}H-NMR titration experiments with phosphate clip 1:

receptor	Clip **1**	M_R [g/mol]	622.13
solvent	phosphate buffer	M_S [g/mol]	179.06
T [°C]	25	m_R [mg]	3.91
substrate	theophylline (**THE**)	m_S [mg]	1.06
O	δ_0 (1-H) [ppm] = 3.273	V_0 [mL]	2
1 ‖ H	δ_0 (3-H) [ppm] = 3.459	$[R]_0$ [mM]	3.14

$[S]_0$ [mM]	2.96

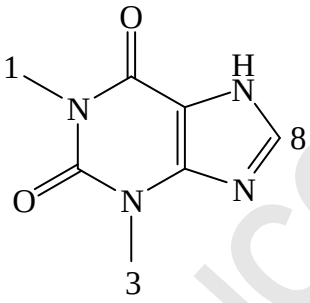
$[1]_0$ [mM]	$[THE]_0$ [mM]	δ_{obs} (3-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
3.14	2.96	2.936	0.524	0.520
1.57	1.48	2.971	0.489	0.491
0.79	0.74	3.009	0.450	0.453
0.39	0.37	3.053	0.406	0.405
0.20	0.18	3.114	0.345	0.345
0.10	0.09	3.181	0.278	0.278



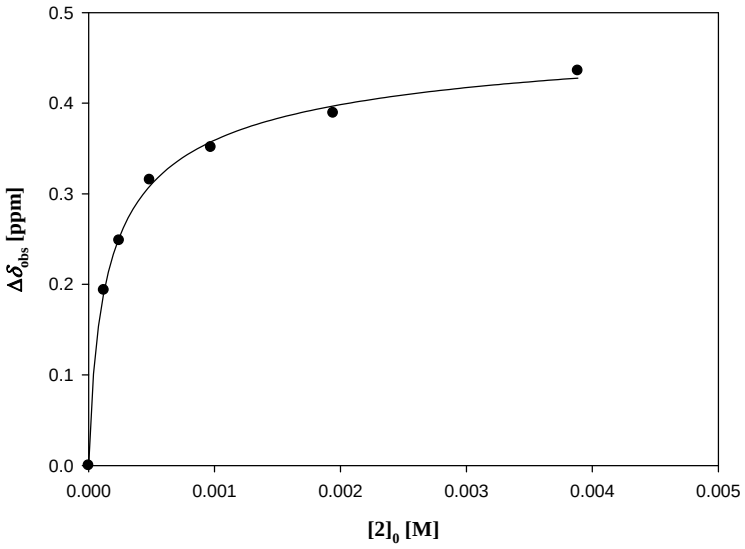
K_a [M^{-1}] = 16800 ± 1260
$\Delta\delta_{max}$ (1-H) [ppm] = 0.17
$\Delta\delta_{max}$ (3-H) [ppm] = 0.58

^{1}H-NMR titration experiments with phosphonate clip 2:

receptor	Clip **2**	M_R [g/mol]	606.41
solvent	phosphate buffer	M_S [g/mol]	179.06
T [°C]	25	m_R [mg]	4.60
substrate	theophylline (**THE**)	m_S [mg]	1.40
	δ_0 (1-H) [ppm] = 3.273	V_0 [mL]	2
	δ_0 (3-H) [ppm] = 3.459	$[R]_0$ [mM]	3.79
		$[S]_0$ [mM]	3.88



$[2]_0$ [mM]	$[THE]_0$ [mM]	δ_{obs} (3-H)	$\Delta\delta_{obs}$	$\Delta\delta_{calc}$
3.79	3.88	3.024	0.436	0.428
1.90	1.94	3.070	0.389	0.397
0.95	0.97	3.108	0.351	0.357
0.47	0.49	3.144	0.315	0.308
0.24	0.24	3.211	0.248	0.252
0.12	0.12	3.266	0.193	0.191



K_a [M^{-1}] = 8700 ± 640
$\Delta\delta_{max}$ (1-H) [ppm] = 0.17
$\Delta\delta_{max}$ (3-H) [ppm] = 0.50