

Table of chemical shifts of the ASL^{Gly} molecules.

ASL(GCC)

#		C2/C5	H2/H5	C6/C8	H6/H8	C1'	H1'	C2'	H2'	C3'	H3'	C4'	H4'	C5'	H5'	H5"	NH	N(H)	NH2	N(H2)	A N3	C/U C2	A N3	A N1
G 1	27			140.13	8.05	-	5.75	-	4.86	-	4.37	-	4.62	-	4.01	3.92	12.72	147.69						
G 2	28			137.08	7.63	92.33	5.9	75.72	4.56	73.45	4.59	-	4.63	66.43	4.47	4.26	13.36	147.92						
G 3	29			136.75	7.31	93.25	5.79	75.17	4.63	72.95	4.38	-	4.66	66.02	4.47	4.11	11.46	145.01						
C 4	30	97.32	5.38	140.69	7.69	93.69	5.5	75.27	4.31	72.29	4.42	-	-	64.76	4.48	4.04			8.08, 6.65	98.03				
C 5	31	97.88	5.51	141.23	7.71	94.46	5.48	75.57	4.34	71.89	4.45	-	4.38	63.96	4.48	4.05			7.91, 6.65	97.37				
U 6	32	104.3	5.6	142.14	7.8	93.54	5.57	75.37	4.32	72.54	4.49	-	4.35	64.41	4.52	4.04	13.68/13.16	160.84						
U 7	33	103.3	5.37	142.14	7.79	92.23	5.72	76.02	4.35	74.41	4.51	-	4.37	65.57	4.39	4.07	12.94	161.16						
G 8	34			138.86	7.75	91.28	5.5	75.42	4.59	71.94	4.38	-	4.36	66.99	4.22	4.01	10.56	n.a.						
C 9	35	98.23	5.56	142.75	7.49	90.62	5.66	76.43	4.39	71.12	4.08	84.85	4.03	67.18	4.04	3.92			6.72, 6.24	92.71				
C 10	36	99.04	5.84	143.22	7.6	91.23	5.7	76.23	4.23	71.23	4.34	84.16	4.31	67.54	3.91	3.91			6.74, 6.21	93.76				
A 11	37	153.35	7.28	141.3	8.29	89.01	5.82	74.82	4.85	71.38	4.52	-	4.66	68.5	4.21	4.16					213.6		213.6	222.11
A 12	38	153.53	7.54	140.13	7.91	92.39	5.84	75.42	4.64	73.96	4.49	-	4.54	67.9	4.42	4.37					212.07		212.07	220.67
G 13	39			135.76	7.13	92.43	5.57	75.37	4.51	72.9	4.4	-	4.41	65.93	4.4	4.08	12.88	146.72						
G 14	40			135.76	7.13	92.93	5.69	76.38	4.53	72.49	4.34	-	4.4	65.37	4.53	4.31	12.91	147.56						
U 15	41	103.9	5.38	140.59	7.74	93.65	5.5	75.62	4.14	72.09	4.51	-	-	-	-	-	12.27	158.53						
C 16	42	97.44	5.66	142.61	7.95	93.85	5.64	75.57	4.2	72.19	4.46	-	4.45	64.56	4.51	4.03			7.96, 6.68	98.85				
C 17	43	98.18	5.53	141.91	7.64	92.74	5.71	77.63	3.95	70.27	4.11	83.21	4.12	65.11	4.45	3.99			7.89, 6.74	96.56				

ASL (UCC)

#		H2/H5	C2/C5	H8/H6	C8/C6	H1'	C1'	H2'	C2'	H3'	C3'	H4'	C4'	H5'	H5"	C5'	NH	N(H)	NH2	N(H2)	C/U C2	C/U C4	A N3	A N1
G 1	27			8.03	138.84	5.76	-	4.48	-	4.3	-	4.48	-	4.01	3.88	-	12.6	-						
G 2	28			7.41	137.43	5.87	93.07	4.75	75.33	4.52	72.68	4.52	-	4.14	4.5	65.38	10.73	142.55						
G 3	29			7.3	136.36	5.71	92.97	4.57	75.49	4.54	71.93	4.63	-	4.07	4.45	64.72	12.36	146.16						
A 4	30	7.74	153.73	7.99	139.41	6	93.06	4.61	75.55	4.53	72.26	4.56	-	4.54	4.07	64.88							212.32	222.45
C 5	31	5.13	97.31	7.21	140.22	5.32	94.04	4.44	74.83	4.15	72.26	4.36	81.95	3.98	4.42	64.8			8.26, 7.00	98.08	157.96	167.87		
C 6	32	5.6	97.63	7.83	141.33	5.73	93.98	4.06	75.5	4.52	72.84	4.36	82.29	3.93	4.49	64.22			7.10, 6.38	94.42	158.38	168.5		
U 7	33	5.74	104.81	7.79	142.63	5.74	91.77	4.18	75.74	4.53	72.59	4.3	82.37	4.08	4.12	66.46					n.o.	n.o.		
U 8	34	5.66	104.49	7.84	141.42	5.69	91.32	4.33	74.67	4.5	71.43	4.32	84.32	-	-	-					153.08	168.39		
C 9	35	5.63	98.29	7.77	143.05	5.62	92.55	3.96	75.4	4.18	74.2	4.08	83.45	3.98	4.46	65.3			6.84, 6.22	93.58	158.38	167.75		
C 10	36	5.67	98.44	7.76	141.86	5.61	92.41	4	77.57	4.09	70.19	4.28	84.1	-	-	-			6.43, 5.77	92.5	158.1	167.6		
A 11	37	7.74	154.14	8.25	140.56	5.9	91.83	4.82	75	4.54	72.68	4.65	-	4.24	4.33	67.29							214.88	222.24
A 12	38	8.02	149.91	7.75	139.61	5.53	92.86	4.23	-	4.41	71.85	4.66	-	-	-	-							214.03	n.o.
G 13	39			7.15	136.02	5.3	93.07	4.39	74.92	4.4	72.1	4.14	83.66	4.02	4.39	65.13	13.18	147.76						
U 14	40	5.05	102.37	7.91	143.77	5.58	93.53	4.5	75.16	4.18	-	4.55	-	-	-	-	14.33	162.25				152.09	168.58	
U 15	41	5.75	98.44	7.88	141.75	5.59	91.66	4.41	75.25	4.19	70.44	4.32	-	-	-	-			8.22, 7.04	97.5	157.96	168.4		
U 16	42	5.6	105.08	7.89	142.32	5.56	94.58	4.2	75.33	4.4	72.43	4.49	-	4.03	4.3	66.29	11.92	157.63			154.06	167		
C 17	43	5.75	97.76	7.88	142.97	5.75	92.76	3.89	77.41	4.23	-	4.3	-	4.01	4.45	-			8.52, 6.90	97.18	159.55	168.6		

np- ASL (UCC)

#		H2/H5	C2/C5	H8/H6	C8/C6	H1'	C1'	H2'	C2'	H3'	C3'	H4'	C4'	H5'	H5"	C5'	NH	N(H)	NH2	N(H2)	C/U C2	C/U C4
G	1	27		7.82		5.52	-	-	-	-	-	-	-	-	-	-	12.66					
G	2	28		7.31	137.72	5.82	92.92	4.68	75.22	4.57	72.24	4.46	81.89	4.09	4.51	69.9	10.8	142.57				
G	3	29		7.27	136.94	5.67	92.72	4.45	75.35	4.61	72.18	4.45	81.82	4.1	4.48	69.63	12.54	146.88				
A	4	30	7.78	151.98	7.84	139.50	5.961	92.71	4.46	75.54	4.5	72.37	4.46	81.82	4.1	4.56	69.74					
C	5	31	5.18	97.03	7.4	140.55	5.346	93.64	4.16	75.61	4.28	72.11	4.36	81.62	4	4.44	69.79		8.43, 7.02	98.12	157.87	168
C	6	32	5.33	97.92	7.53	141.06	5.54	93.64	4.37	75.61	4.29	72.16	-	-	4.01	4.47	69.63		8.44, 6.79	97.64	158.31	168.5
U	7	33	5.61	104.59	7.71	141.38	5.64	92.48	4.18	76.27	4.42	73.63	4.29	82.94	4.06	4.31	70.23				152.14	168.2
U	8	34	5.75	104.65	7.76	143.08	5.62	92.28	4.28	-	4.42	-	-	-	-	-					153.06	168.45
C	9	35	5.73	-	7.72	142.57	5.62	92.95	4.25	74.41	4.33	73.94	-	-	-	-			6.99, 6.34	93.32	158.56	167.84
C	10	36	5.62	98.16	7.7	141.60	5.59	93.23	4.4	-	4.48	71.96	-	-	-	-			7.03, 6.25	93.86	158.27	167.65
C	11	37	5.51	-	7.7	141.21	5.6	93.22	4.58	75.79	4.35	73.01	4.44	82.07	4.58	4.07	64.36		6.68, 6.07	93.73	158.31	167.45
G	12	38			7.8	138.45	5.55	94.03	4.56	75.26	4.31	72.16	-	-	4.58	4.74	69.69	12.74	147.81			
G	13	39			7.456	137.48	5.87	93.25	4.44	75.42	4.55	72.44	4.48	82.15	4.08	4.56	69.69	13.26	148.52			
U	14	40	5.07	102.27	7.87	141.99	5.58	93.23	4.74	75.06	4.48	74.4	-	-	-	-	14.33	162.89			152.14	168.41
C	15	41	5.6	98.28	7.81	141.45	5.56	93.63	4.53	78.57	4.46	73.54	4.48	82.33	-	-	-		8.37, 7.07	98.05	158.13	168.33
U	16	42	5.66	104.59	7.95	141.41	5.54	94.24	4.07	75.48	4.52	72.05	4.33	82.02	4.07	4.52	64.17	12.01	157.72		154.11	167.04
C	17	43	5.7	98.16	7.82	142.37	5.75	92.72	3.96	77.46	4.16	69.4	4.1	82.88	4	4.49	70.23		8.47, 6.90	96.02	158.78	168.7

The non-exchangeable ¹H chemical shifts were measured at 25 °C and pH 6.3 and are referenced with DSS set to 0.00 ppm. Exchangeable proton chemical shifts were measured at 12 °C. The uncertainties in the chemical shift values are ≈0.02 ppm. The 5' and 5" protons are not stereospecifically assigned. The ¹³C and ¹⁵N frequencies corresponding to 0.00 ppm were set according to the 0.00 ppm ¹H (DSS) frequency at 25 °C using the ratio γC/γH and γN/γH. The chemical shifts have uncertainties of ¹³C=0.05 ppm and ¹⁵N=0.10 ppm. Values listed as, (-), could not be unambiguously identified due to cross peak overlap or signal loss caused by relaxation.