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Three Dimensional Structure of Oligosaccharide Chain of GM1 Ganglioside Revealed by Distance
Mapping Procedure: a Rotating and Laboratory Frame Nuclear Overhauser Enhancement
Investigation of Native Glycolipid in Dimethyl Sulfoxide and in Water-Dodecylphosphocholine
Solutions

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Measured^a and Corrected^b Cross-Peak Volumes from 2D ROESY Spectra of GM1 and deac-GM1
in Me₂SO-*d*₆ Solution Recorded at Different Temperatures and Mixing Times^c

proton pair	GM1				deac-GM1			
	307K	493	293K	-	297K	293K	293K	-
IV1/IV5	390	493	nd ^d	-	nd		nd	-
IV1/III3	641	801	613	709	nd	nd	nd	-
IV1/III2	87	105	76	84	98	107	91	-
IV1/IIIAc	31	44	25	33	28	35	31	-
IV1/III4	64	73	nd	-	nd	-	nd	-
IV1/IIINH	35	36	45	48	34	35	47	48
I VOH2/IV1	150	172	nd	-	nd	-	nd	-
I VOH3/IV3,2	515	630	730	827	714	807	767	867
I VOH3/IV4	93	111	103	114	142	153	125	135
I VOH4/IV4	420	518	509	576	498	561	600	676
I VOH4/IV3,2	100	126	122	143	169	195	nd	-
I VOH2/IIIAc	25	37	31	43	37	49	40	53
I VOH2/I VOH3	nd	-	nd	-	46	49	31	33
I VOH3/I VOH4	nd	-	nd	-	100	104	137	142
III1/III2	84	87	nd	-	nd	-	nd	-
III1/III5	311	368	343	380	393	427	349	379
III1/III3	nd	-	nd	-	271	297	298	326
III1/II4	724	829	751	807	836	893	812	867
III1/N8	nd	-	nd	-	104	107	96	99
IIIAc/III2	27	39	22	29	29	38	24	31
IIIAc/II2	95	143	94	130	115	159	124	171
IIINH/III1	295	317	316	336	303	332	308	337
IIINH/III2	147	167	195	223	165	181	205	225
IIINH/III3	251	294	242	277	215	251	267	312
IIINH/IIIAc	257	399	243	352	211	314	218	324

IIIOH4/III2	175	211	197	223	215	236	200	219
IIIOH4/II4	510	623	550	616	591	655	610	676
IIIOH4/III3	nd	-	215	251	nd	-	215	241
III1/NOH8	288	309	296	305	312	315	324	327
III5/NOH8	47	55	51	57	60	65	57	72
III5/NOH9	63	76	68	75	67	73	56	61
IIIOH6/N9R	nd	-	nd	-	37	40	32	34
IIINH/II2	38	46	41	49	45	55	31	38
IIIAc/IIOH2	31	41	27	33	34	42	28	35
IIIOH6/IIOH6	79	91	112	123	107	111	175	181
IIIOH6/NOH9	nd	-	345	363	323	333	359	370
N3ax/N3eq	1250	3292	1373	3010	1620	3290	1590	3230
N3ax/N5	122	311	171	305	158	173	171	187
N3eq/N4	241	465	256	412	287	417	315	458
N4/N6	297	392	281	343	311	380	290	354
N7/N5	nd	-	nd	-	115	150	105	137
N7/N6	212	293	199	251	nd	-	nd	-
N7/N8	144	195	137	169	nd	-	nd	-
N7/N9S	38	50	41	49	nd	-	nd	-
N7/N9R	107	141	115	183	nd	-	nd	-
NAc/N7	47	137	54	125	41	84	32	66
NOH7/N5	671	830	615	701	211	249	215	255
NOH7/N7	720	901	810	928	nd	-	nd	-
NOH8/N6	431	518	427	490	443	486	461	506
NNH/N4	417	483	435	492	407	466	395	452
NNH/N5	154	180	185	216	126	161	137	175
NNH/N6	171	201	193	225	154	182	144	170
NNH/N7	79	95	68	80	81	99	90	110
NNH/NOH4	267	290	271	291	254	279	231	254
N3ax/II3	615	1163	794	1112	845	1402	784	1300
N3eq/IIOH2	139	227	147	186	156	190	140	170
N3ax/IIOH2	70	101	75	80	68	91	73	96
NOH7/II4	66	80	62	66	70	76	81	88
II1/II2	100	128	100	118	100	120	100	120
II1/II5	nd	-	381	436	403	466	396	458
II1/II3	nd	-	324	367	342	383	nd	-
II3/II5	367	474	nd	-	nd	-	nd	-
II4/II5	452	571	518	605	nd	-	561	649
II1/I4	nd	-	987	1155	nd	-	nd	-
II1/I6'	nd	-	107	120	94	106	84	95

IOH2/II2	974	1194	1023	1174	1076	1235	1005	1153
IOH2/II3	144	168	118	129	nd	-	nd	-
IOH2/II1	71	80	126	132	115	122	94	100
IOH6/II6,6'	632	780	710	799	681	860	710	896
IOH6/II5	nd	-	nd	-	247	277	nd	-
IOH6/II4	84	101	114	126	nd	-	148	166
IOH2/I6	41	48	42	46	63	57	74	80
IOH2/I6'	72	85	96	104	114	124	97	105
III1/IOH3	140	162	77	90	128	136	<20	<20
II6'/IOH3	nd	-	nd	-	54	60	115	128
II1/IOH6	nd	-	<20	<20	<20	<20	<20	<20
IOH2/IOH3	nd	-	54	56	89	92	88	91
IOH2/IOH6	nd	-	nd	-	<20	<20	<20	<20
I1/I2	104	135	97	117	115	137	97	115
I1/I5	390	487	nd	-	nd	-	nd	-
IOH2/I2	931	1154	988	1147	954	1095	984	1129
IOH2/I3	107	129	121	140	nd	-	nd	-
IOH2/I1	151	171	215	226	238	253	254	270
IOH3/I3,4	848	801	1048	1214	nd	-	nd	-
IOH3/I2	102	130	87	103	106	123	95	110
IOH2/IOH3	nd	-	72	75	115	118	148	152

^aLeft column for each temperature. ^bRight column for each temperature. The cross-peaks volumes were corrected according to the formula: $V_{\text{cor}} = V_{\text{m}} / (\sin\delta_i \sin\delta_j - 0.5 \cos\delta_i \cos\delta_j)$, where V_{cor} and V_{m} are corrected and measured cross-peak volumes respectively, and δ_i and δ_j are angles the spin lock axis of the spins i and j form with z axis. The peak volumes in all spectra were scaled to the III1/II2 cross peak volume. ^cThe spectra were recorded under the following conditions: GM1: 307 K, B_1 (frequency 2.65 KHz, offset 6.4 ppm), mixing time 155 ms; 293 K, B_1 (2.6 kHz, 5.8 ppm), mixing time 80 ms; deac-GM1: 297 K, B_1 (2.4 kHz, 5.5 ppm), mixing time 100 ms; 293 K, B_1 (2.4 kHz, 5.5 ppm), mixing time 150 ms. ^d not detected due to spectral overlap.