Supporting Information for

Novel Synthons from Mucochloric acid: The First Use of α,β -dichloro- γ -Butenolides
and γ -Butyrolactams for Direct Vinylogous Aldol Addition

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¹ H NMR assignment of the diastereomers	S2
¹ H and ¹³ C NMR data of the compounds	S3 – S53

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Acquisition Time (sec)	5.1298	Comment	86199X046	Date	Oct 10 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20051010\2601				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2413.9207
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.49	996.6	0.0607	19	6.40	2562.6	0.0914
2	2.50	998.5	0.1429	20	6.42	2568.2	0.0887
3	2.50	1000.3	0.2013	21	6.63	2653.6	0.0530
4	2.50	1002.2	0.1479	22	6.65	2658.9	0.0519
5	2.51	1004.0	0.0653	23	7.73	3092.4	0.0518
6	3.32	1328.2	1.0000	24	7.75	3100.6	0.0568
7	5.28	2114.0	0.0300	25	7.76	3105.9	0.1079
8	5.29	2115.9	0.0309	26	7.78	3114.3	0.1139
9	5.30	2119.8	0.0307	27	8.23	3292.2	0.0093
10	5.30	2121.8	0.0311	28	8.23	3294.6	0.0751
11	5.36	2146.0	0.0145	29	8.24	3296.7	0.0211
12	5.37	2148.9	0.0154	30	8.25	3301.6	0.0266
13	5.38	2151.0	0.0150	31	8.26	3303.2	0.1944
14	5.38	2154.2	0.0147	32	8.26	3305.1	0.0453
15	5.65	2262.0	0.0992	33	8.27	3310.0	0.0392
16	5.66	2263.7	0.0987	34	8.28	3311.9	0.1392
17	5.75	2299.2	0.0602	35	8.28	3314.5	0.0159
18	5.75	2302.1	0.0666				

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[5.27 .. 5.32]	1.016	1.78398e+9	1.016
2	[5.35 .. 5.39]	0.528	9.27223e+8	0.528
3	[5.64 .. 5.69]	1.012	1.77688e+9	1.012
4	[5.74 .. 5.77]	0.545	9.56251e+8	0.545
5	[6.39 .. 6.43]	1.000	1.75602e+9	1.000
6	[6.62 .. 6.66]	0.528	9.26777e+8	0.528
7	[7.72 .. 7.76]	1.048	1.84054e+9	1.048
8	[7.76 .. 7.80]	1.943	3.41259e+9	1.943
9	[8.22 .. 8.29]	2.899	5.09093e+9	2.899

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Acquisition Time (sec)	1.3566	Comment	86199X046	Date	May 8 2006
File Name	C:\Program Files\Common Files\SYSTEMMSAPI\1033\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060508\8302				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	8192
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	9991.7646
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	38.89	3912.8	0.1373	13	120.73	12147.6	0.0195
2	39.09	3933.4	0.4178	14	123.20	12396.0	0.1528
3	39.30	3954.8	0.8682	15	127.81	12859.7	0.1595
4	39.51	3975.4	1.0000	16	146.13	14703.3	0.0454
5	39.72	3996.8	0.8751	17	147.04	14794.7	0.0280
6	39.93	4017.4	0.4299	18	147.09	14799.9	0.0128
7	40.14	4038.8	0.1441	19	147.87	14878.0	0.0443
8	68.41	6883.5	0.0362	20	150.08	15100.7	0.0108
9	70.27	7070.8	0.0410	21	151.12	15205.3	0.0699
10	84.85	8537.7	0.0398	22	164.87	16589.0	0.0169
11	84.93	8545.8	0.0675	23	165.22	16623.6	0.0312
12	120.21	12095.3	0.0655

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Acquisition Time (sec)	5.1298	Comment	86199X136	Date	Apr 5 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\OTTO.CHEMISTRY.AA.WL.COM\SAMBA\20060405\1601				
Frequency (MHz)	399.80	Nucleus	1H	Number of Transients	8
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	42.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2417.3096	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.16	861.8	0.0164	14	7.38	2951.2	0.0418	27	7.45	2976.5	0.0444	1	[2.11 .. 2.18]	0.959	1.12098e+9	0.959
2	2.48	990.2	0.0100	15	7.39	2953.1	0.0210	28	7.45	2977.5	0.0353	2	[2.45 .. 2.50]	0.526	6.14382e+8	0.526
3	5.11	2044.3	0.0917	16	7.39	2955.6	0.0404	29	7.45	2979.4	0.0432	3	[5.10 .. 5.15]	1.996	2.33237e+9	1.996
4	5.12	2046.6	0.2156	17	7.40	2956.6	0.0315	30	7.46	2982.2	0.0211	4	[5.25 .. 5.28]	0.551	6.43592e+8	0.551
5	5.14	2053.3	0.0333	18	7.40	2959.4	0.0223	31	7.47	2984.5	0.0956	5	[5.32 .. 5.34]	0.484	5.65625e+8	0.484
6	5.27	2105.3	0.0189	19	7.41	2960.7	0.0463	32	7.47	2986.3	0.0925	6	[7.35 .. 7.50]	7.824	9.14442e+9	7.824
7	5.32	2128.5	0.1158	20	7.41	2963.1	0.0879	33	7.47	2987.4	0.0483					
8	5.33	2131.6	0.0908	21	7.41	2964.4	0.0805	34	7.48	2990.2	0.0206					
9	7.27	2906.5	1.0000	22	7.42	2967.7	0.0157	35	7.48	2991.5	0.0413					
10	7.27	2908.5	0.0191	23	7.43	2969.1	0.0415	36	7.48	2992.3	0.0389					
11	7.36	2942.2	0.0263	24	7.43	2970.9	0.1138	37	7.49	2994.2	0.0360					
12	7.37	2944.9	0.0370	25	7.44	2974.0	0.0162									
13	7.37	2948.4	0.2480	26	7.44	2975.1	0.0250

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Acquisition Time (sec)	1.3566	Comment	86199X136	Date	Mar 28 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060328\2602				
Frequency (MHz)	100.57	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10055.5254
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	72.01	7242.1	0.2674	11	128.79	12952.2	0.2228
2	73.63	7404.3	0.0644	12	129.04	12977.3	0.6318
3	76.90	7733.8	1.0000	13	129.23	12996.4	0.1027
4	77.23	7766.3	0.9355	14	129.29	13001.6	0.2668
5	77.54	7798.0	0.9803	15	135.83	13659.9	0.0502
6	84.62	8509.3	0.2194	16	138.04	13881.8	0.1432
7	84.86	8533.7	0.0791	17	150.02	15086.3	0.0556
8	122.41	12310.1	0.0696	18	165.19	16612.2	0.0258
9	126.70	12741.4	0.2812	19	165.51	16644.6	0.0409
10	126.93	12764.2	0.8402

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Acquisition Time (sec)	5.1298	Comment	86199X099	Date	Jan 5 2006
File Name	\\AACALVIN\ACDLabs\ACD80\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060105\1201				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	METHANOL-d4		
Spectrum Offset (Hz)	2409.1406	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	3.30	1321.1	0.2152	14	5.55	2219.4	0.2239
2	3.31	1322.6	0.4034	15	7.63	3052.9	0.1691
3	3.31	1324.4	0.5839	16	7.65	3061.1	0.2609
4	3.31	1325.9	0.4182	17	7.67	3069.5	0.3649
5	3.32	1327.5	0.2272	18	7.69	3077.7	0.6065
6	4.84	1938.4	1.0000	19	7.72	3089.0	0.2990
7	5.25	2101.2	0.2620	20	7.73	3091.0	0.0997
8	5.26	2103.0	0.2755	21	7.74	3095.8	0.0924
9	5.32	2128.9	0.1174	22	7.74	3097.8	0.2582
10	5.33	2131.6	0.1219	23	7.75	3099.5	0.7006
11	5.40	2160.1	0.5602	24	7.75	3101.7	0.1993
12	5.40	2162.0	0.5057	25	7.76	3106.4	0.1581
13	5.54	2216.4	0.2451	26	7.77	3108.1	0.3707

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[5.23 .. 5.27]	0.999	1.12455e+9	0.999
2	[5.31 .. 5.34]	0.466	5.24746e+8	0.466
3	[5.38 .. 5.42]	1.001	1.12574e+9	1.001
4	[5.53 .. 5.55]	0.466	5.24484e+8	0.466
5	[7.61 .. 7.80]	5.705	6.41920e+9	5.705

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Acquisition Time (sec)	1.3566	Comment	86199X099	Date	Jan 5 2006
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Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	8192
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	METHANOL-d4	Spectrum Offset (Hz)	10186.4443
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	48.51	4877.0	0.1065	16	119.63	12026.8	0.0055
2	48.72	4898.4	0.3816	17	119.73	12036.4	0.0188
3	48.94	4919.8	0.7555	18	122.78	12343.7	0.0089
4	49.15	4941.2	1.0000	19	123.33	12398.3	0.0038
5	49.36	4962.5	0.8553	20	128.88	12957.1	0.0910
6	49.43	4969.2	0.0042	21	129.01	12969.6	0.0281
7	49.58	4983.9	0.4564	22	133.22	13392.7	0.0459
8	49.65	4991.3	0.0083	23	133.35	13406.0	0.0608
9	49.79	5005.3	0.1511	24	144.89	14566.3	0.0088
10	71.00	7137.9	0.0432	25	146.92	14769.8	0.0241
11	72.98	7336.9	0.0140	26	151.04	15184.8	0.0064
12	86.49	8695.5	0.0420	27	152.00	15280.6	0.0164
13	86.59	8705.1	0.0146	28	166.65	16753.5	0.0069
14	112.98	11358.2	0.0208	29	167.03	16791.8	0.0135
15	113.19	11378.8	0.0088

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Acquisition Time (sec)	5.1298	Comment	86199X096	Date	Dec 16 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20051216\1701				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.0193	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.45	980.2	0.0682	16	7.40	2959.9	0.0709
2	2.46	986.1	0.0712	17	7.41	2965.1	0.1294
3	2.62	1049.0	0.4413	18	7.43	2973.1	0.1522
4	2.63	1052.9	1.0000	19	7.55	3021.7	0.0469
5	2.83	1131.9	0.0322	20	7.56	3023.4	0.0469
6	2.84	1137.0	0.0326	21	7.57	3029.5	0.0388
7	5.12	2047.5	0.2886	22	7.58	3031.4	0.0379
8	5.12	2049.9	0.3174	23	7.64	3056.4	0.1086
9	5.22	2087.7	0.0751	24	7.64	3058.1	0.1094
10	5.23	2090.6	0.0768	25	7.66	3064.2	0.0917
11	5.31	2123.2	0.1149	26	7.66	3066.1	0.0907
12	5.31	2126.3	0.1615	27	8.02	3208.4	0.0817
13	5.35	2139.0	0.0405	28	8.02	3210.2	0.0760
14	7.27	2908.8	0.6733	29	8.07	3227.9	0.1767
15	7.38	2951.9	0.0567	30	8.07	3229.7	0.1712

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.39 .. 2.51]	1.148	2.52672e+9	1.148
2	[2.61 .. 2.63]	1.403	3.08709e+9	1.403
3	[2.63 .. 2.65]	3.016	6.63687e+9	3.016
4	[2.79 .. 2.88]	0.547	1.20492e+9	0.547
5	[5.10 .. 5.14]	1.015	2.23442e+9	1.015
6	[5.20 .. 5.25]	1.080	2.37709e+9	1.080
7	[5.30 .. 5.32]	0.511	1.12380e+9	0.511
8	[5.33 .. 5.37]	0.509	1.12062e+9	0.509
9	[7.37 .. 7.40]	0.497	1.09272e+9	0.497
10	[7.40 .. 7.44]	1.075	2.36597e+9	1.075
11	[7.54 .. 7.59]	0.516	1.13634e+9	0.516
12	[7.63 .. 7.68]	1.107	2.43659e+9	1.107
13	[8.01 .. 8.03]	0.486	1.07037e+9	0.486
14	[8.05 .. 8.09]	1.002	2.20553e+9	1.002

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Acquisition Time (sec)	1.3566	Comment	86199X096	Date	Dec 16 2005
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Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10039.0166
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	20.26	2039.0	0.0976	14	130.80	13160.5	0.0498
2	21.93	2206.3	0.0300	15	131.17	13198.1	0.1170
3	70.52	7095.2	0.1075	16	133.22	13404.5	0.0464
4	72.08	7252.9	0.0449	17	133.45	13427.4	0.1067
5	76.68	7715.9	1.0000	18	134.42	13525.4	0.0351
6	77.00	7747.5	0.9790	19	135.44	13627.9	0.0277
7	77.32	7780.0	0.9460	20	137.30	13815.1	0.0441
8	83.98	8450.1	0.1032	21	141.45	14232.4	0.0249
9	84.23	8475.1	0.0386	22	142.89	14376.8	0.0197
10	121.95	12270.0	0.0290	23	149.08	15000.5	0.0392
11	122.72	12347.4	0.0361	24	149.19	15010.8	0.0219
12	122.77	12352.6	0.0448	25	166.27	16729.9	0.0224
13	122.89	12365.1	0.0990

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Acquisition Time (sec)	5.1298	Comment	86199X105	Date	Jan 11 2006
File Name	C:\Documents and Settings\dassak\Desktop\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060111\0801				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	56.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.2144	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.45	981.4	0.0541	17	7.27	2908.8	0.6756
2	2.47	986.9	0.0559	18	8.09	3236.5	0.0983
3	3.01	1205.8	0.0122	19	8.11	3244.7	0.1103
4	3.03	1211.0	0.0127	20	8.13	3253.3	0.0151
5	4.01	1603.5	1.0000	21	8.15	3261.5	0.0169
6	4.01	1605.0	0.1890	22	8.35	3340.4	0.0149
7	5.43	2171.3	0.1575	23	8.35	3342.2	0.0155
8	5.43	2172.9	0.1443	24	8.36	3346.3	0.0725
9	5.44	2174.6	0.0365	25	8.37	3348.0	0.0760
10	5.92	2367.6	0.0437	26	8.37	3350.0	0.0138
11	5.92	2368.4	0.0467	27	8.38	3354.5	0.0603
12	5.93	2372.9	0.0456	28	8.39	3356.2	0.0616
13	5.93	2373.5	0.0443	29	8.74	3497.0	0.1244
14	6.06	2425.9	0.0087	30	8.74	3498.7	0.1195
15	6.08	2430.8	0.0096	31	8.80	3520.5	0.0198
16	6.08	2434.3	0.0083	32	8.80	3522.1	0.0193

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.44 .. 2.48]	1.192	3.57264e+8	1.192
2	[3.00 .. 3.04]	0.331	9.90732e+7	0.331
3	[4.00 .. 4.03]	3.737	1.12001e+9	3.737
4	[5.42 .. 5.44]	1.222	3.66330e+8	1.222
5	[5.90 .. 5.94]	1.223	3.66613e+8	1.223
6	[6.06 .. 6.09]	0.268	8.02725e+7	0.268
7	[8.08 .. 8.12]	1.176	3.52553e+8	1.176
8	[8.13 .. 8.16]	0.296	8.85856e+7	0.296
9	[8.34 .. 8.36]	0.152	4.55920e+7	0.152
10	[8.36 .. 8.37]	0.627	1.87764e+8	0.627
11	[8.38 .. 8.39]	0.520	1.55878e+8	0.520
12	[8.73 .. 8.75]	1.001	2.99957e+8	1.001
13	[8.79 .. 8.81]	0.176	5.28322e+7	0.176

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Acquisition Time (sec)	1.3566	Comment	86199X105	Date	Jan 11 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060111\8302				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	8192
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10039.7539
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	52.95	5327.4	0.0896	12	126.38	12716.0	0.0111
2	66.20	6661.0	0.0797	13	130.80	13160.5	0.0305
3	68.96	6938.1	0.0115	14	131.87	13268.9	0.0175
4	76.68	7715.9	1.0000	15	134.20	13502.6	0.0092
5	77.00	7747.5	0.9106	16	134.53	13535.7	0.0700
6	77.21	7768.2	0.0342	17	136.83	13768.0	0.0082
7	77.32	7780.0	0.9835	18	138.64	13949.3	0.0526
8	83.08	8359.4	0.0760	19	147.11	14801.5	0.0141
9	83.11	8362.3	0.0172	20	149.16	15008.6	0.0173
10	122.59	12334.9	0.0337	21	164.49	16550.7	0.0458
11	125.91	12668.8	0.0680	22	165.14	16616.3	0.0302

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Acquisition Time (sec)	2.5649	Comment	86199X106	Date	Jan 11 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\AASUN702.RESEARCH.AA.WL.COM\NMR\HANN\NHFILES\2006\20060111\8401				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	256
Original Points Count	16384	Points Count	16384	Pulse Sequence	s2pul
Receiver Gain	56.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2411.1018
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.38	952.3	0.3206	12	5.84	2335.3	0.0034	1	[2.36 .. 2.42]	0.995	3.92381e+10	0.995
2	2.39	957.4	0.3250	13	7.27	2908.8	1.0000	2	[2.82 .. 2.86]	0.101	3.98268e+9	0.101
3	2.84	1135.5	0.0351	14	7.91	3164.2	0.0098	3	[4.99 .. 5.05]	1.000	3.94320e+10	1.000
4	2.85	1140.2	0.0328	15	7.93	3173.2	0.1296	4	[5.21 .. 5.24]	0.089	3.51979e+9	0.089
5	5.02	2006.6	0.3338	16	7.95	3181.3	0.1594	5	[5.61 .. 5.68]	1.160	4.57586e+10	1.160
6	5.02	2007.7	0.3093	17	7.96	3186.8	0.2666	6	[5.80 .. 5.85]	0.059	2.33834e+9	0.059
7	5.22	2089.2	0.0302	18	8.11	3245.7	0.1999	7	[7.90 .. 8.00]	2.156	8.49996e+10	2.156
8	5.23	2093.1	0.0303	19	8.13	3253.9	0.1641	8	[8.10 .. 8.15]	1.094	4.31267e+10	1.094
9	5.64	2257.3	0.1535	20	8.32	3328.7	0.0037	9	[8.30 .. 8.37]	0.072	2.83430e+9	0.072
10	5.65	2262.4	0.1478									
11	5.83	2331.4	0.0033	21	8.34	3336.9	0.0037

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Acquisition Time (sec)	1.9333	Comment	86199X106	Date	Jan 11 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060111\1502				
Frequency (MHz)	376.24	Nucleus	19F	Number of Transients	16
Original Points Count	131072	Points Count	131072	Pulse Sequence	s2pul
Receiver Gain	56.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	-41391.0781
Sweep Width (Hz)	67796.61	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	-63.51	-23895.8	1.0000
2	-58.67	-22075.6	0.7814

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Acquisition Time (sec)	1.3566	Comment	86199X106	Date	Jan 12 2006
File Name	C:\Program Files\Common Files\System\WAPI\1033\nt\AASUN702.RESEARCH.AA.WL.COM\NMR\HAHN\NHFILES\2006\20060111\8402				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	8192
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10039.7539
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	65.92	6633.0	0.0361	12	127.19	12797.8	0.0123
2	76.68	7715.9	0.9649	13	127.50	12828.8	0.0126
3	77.00	7747.5	1.0000	14	127.82	12860.5	0.0293
4	77.21	7768.2	0.0299	15	128.13	12892.2	0.0086
5	77.32	7779.2	0.8671	16	129.36	13016.0	0.0198
6	83.27	8378.6	0.0335	17	130.94	13175.3	0.1699
7	121.70	12245.0	0.0097	18	131.38	13218.8	0.0208
8	122.13	12288.5	0.0141	19	131.71	13252.7	0.0177
9	122.73	12348.9	0.0443	20	140.89	14176.3	0.0244
10	122.95	12371.0	0.0177	21	148.79	14971.0	0.0544
11	124.85	12562.0	0.0191	22	164.96	16597.9	0.0584

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Acquisition Time (sec)	5.1298	Comment	86199X117	Date	Mar 2 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060302\2201				
Frequency (MHz)	399.90	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	44.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2414.3774	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.30	921.6	0.0599	15	7.55	3017.6	0.2337	29	7.60	3039.5	0.0525	43	7.85	3139.5	0.0827	1	[2.22 .. 2.37]	1.300	5.61574e+8	1.300
2	2.70	1080.5	0.0320	16	7.55	3018.4	0.2323	30	7.60	3041.0	0.0823	44	7.85	3140.6	0.0616	2	[2.66 .. 2.73]	0.535	2.30967e+8	0.535
3	5.31	2122.8	0.6729	17	7.55	3020.6	0.1364	31	7.61	3042.8	0.1344	45	7.88	3151.8	0.0806	3	[5.28 .. 5.34]	0.997	4.30719e+8	0.997
4	5.31	2124.8	0.6747	18	7.56	3021.5	0.2062	32	7.61	3044.5	0.2345	46	7.89	3155.7	0.2046	4	[5.47 .. 5.49]	0.298	1.28718e+8	0.298
5	5.47	2188.5	0.1706	19	7.56	3022.7	0.2508	33	7.62	3045.9	0.1904	47	7.90	3159.4	0.0761	5	[5.93 .. 6.00]	0.994	4.29321e+8	0.994
6	5.48	2191.3	0.1718	20	7.56	3024.1	0.1384	34	7.62	3047.7	0.0535	48	7.91	3164.0	0.1875	6	[6.05 .. 6.08]	0.315	1.36220e+8	0.315
7	5.97	2386.0	0.1590	21	7.57	3025.6	0.2392	35	7.63	3049.4	0.0522	49	7.93	3172.0	0.2179	7	[7.49 .. 7.67]	3.482	1.50382e+9	3.482
8	6.06	2424.8	0.0561	22	7.57	3027.4	0.0862	36	7.63	3051.4	0.1210	50	7.94	3173.6	0.2396	8	[7.77 .. 7.82]	0.909	3.92500e+8	0.909
9	7.27	2907.3	1.0000	23	7.58	3029.5	0.2204	37	7.63	3052.9	0.1104	51	7.95	3180.2	0.2659	9	[7.83 .. 7.85]	0.289	1.24877e+8	0.289
10	7.51	3005.0	0.0678	24	7.58	3030.9	0.2000	38	7.79	3116.3	0.2164	52	7.96	3181.6	0.2126	10	[7.87 .. 8.07]	3.616	1.56135e+9	3.616
11	7.53	3010.2	0.1847	25	7.58	3032.4	0.0777	39	7.81	3123.5	0.1932	53	7.97	3188.0	0.0653					
12	7.53	3012.8	0.1175	26	7.59	3034.2	0.0781	40	7.83	3131.1	0.0550	54	8.00	3200.7	0.1791					
13	7.54	3014.7	0.1300	27	7.59	3036.0	0.1677	41	7.83	3132.3	0.0866	55	8.03	3209.3	0.1676					
14	7.54	3015.9	0.1236	28	7.60	3037.7	0.1971	42	7.83	3133.2	0.0676

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Acquisition Time (sec)	1.3566	Comment	86199X117	Date	Mar 2 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060302\2202				
Frequency (MHz)	100.57	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10034.2422
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	67.51	6788.9	0.1413	13	125.45	12616.2	0.2245
2	70.09	7049.1	0.0749	14	125.89	12660.4	0.0505
3	76.68	7711.8	0.9715	15	125.99	12670.0	0.2747
4	77.00	7743.5	1.0000	16	126.98	12770.2	0.2405
5	77.32	7775.2	0.8942	17	129.40	13013.5	0.1794
6	83.50	8397.4	0.2248	18	129.45	13017.9	0.1013
7	83.91	8438.7	0.0492	19	129.58	13031.2	0.2656
8	121.78	12246.8	0.2181	20	130.03	13076.9	0.0759
9	122.15	12283.7	0.0695	21	133.22	13396.8	0.1197
10	124.88	12558.7	0.1831	22	133.77	13452.1	0.1008
11	125.21	12591.8	0.0901	23	149.84	15068.7	0.0688
12	125.28	12599.2	0.0636	24	165.32	16625.6	0.0832

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Acquisition Time (sec)	5.1298	Comment	86199X116	Date	Mar 29 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060329\3301				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.4092	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.37	946.7	0.1014	17	7.53	3014.5	0.9163
2	2.70	1081.4	0.0344	18	7.54	3017.4	0.8326
3	5.19	2075.2	0.8463	19	7.55	3020.5	1.0000
4	5.19	2077.6	0.9768	20	7.55	3022.5	0.6042
5	5.28	2114.4	0.5779	21	7.56	3024.2	0.6117
6	5.29	2116.2	0.5677	22	7.58	3031.0	0.4649
7	5.38	2154.6	0.2515	23	7.58	3032.8	0.4893
8	5.39	2157.5	0.3866	24	7.85	3139.0	0.6365
9	5.42	2168.4	0.2332	25	7.85	3141.6	0.6424
10	5.43	2171.1	0.1770	26	7.86	3144.5	0.9173
11	7.27	2908.8	0.9666	27	7.87	3147.6	0.8135
12	7.45	2979.6	0.1455	28	7.87	3150.7	0.6493
13	7.45	2980.9	0.1503	29	7.88	3154.0	0.6796
14	7.47	2989.5	0.1738	30	7.89	3156.6	0.8000
15	7.51	3005.5	0.3198	31	7.91	3165.4	0.5972
16	7.53	3011.2	0.9692	32	7.93	3172.2	0.7622

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.29 .. 2.47]	1.110	4.04532e+9	1.110
2	[2.60 .. 2.80]	0.539	1.96576e+9	0.539
3	[5.16 .. 5.22]	1.099	4.00625e+9	1.099
4	[5.26 .. 5.31]	1.100	4.01052e+9	1.100
5	[5.35 .. 5.48]	0.907	3.30858e+9	0.907
6	[7.41 .. 7.64]	4.775	1.74098e+10	4.775
7	[7.78 .. 7.90]	4.481	1.63376e+10	4.481
8	[7.90 .. 7.92]	0.561	2.04406e+9	0.561
9	[7.92 .. 7.96]	1.134	4.13361e+9	1.134

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Acquisition Time (sec)	1.3566	Comment	86199X116	Date	Mar 29 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060329\3302				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10037.5420
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	71.96	7240.4	0.1536	14	126.65	12743.3	0.1935
2	73.53	7398.1	0.0517	15	126.72	12750.7	0.1786
3	76.68	7715.1	0.9768	16	127.75	12853.9	0.1807
4	77.00	7747.5	0.9779	17	128.15	12893.7	0.1816
5	77.32	7779.2	1.0000	18	128.81	12960.8	0.1538
6	84.42	8494.3	0.1984	19	133.03	13385.4	0.0511
7	84.63	8514.9	0.0405	20	133.49	13431.1	0.0763
8	122.30	12305.4	0.0472	21	135.20	13603.6	0.0931
9	123.63	12439.6	0.0622	22	149.03	14994.6	0.0325
10	124.03	12479.4	0.1321	23	149.72	15064.6	0.0503
11	126.09	12686.5	0.0603	24	164.89	16590.5	0.0321
12	126.13	12691.0	0.1716	25	165.25	16626.7	0.0487
13	126.58	12736.7	0.0718

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Acquisition Time (sec)	5.1298	Comment	86199X107	Date	Jan 12 2006
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060112\1001				
Frequency (MHz)	399.90	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	32.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2413.5977	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	3.80	1519.1	0.4882	16	6.92	2766.5	0.1933
2	3.82	1528.6	1.0000	17	6.93	2770.1	0.0944
3	5.09	2034.1	0.2111	18	7.00	2798.9	0.2689
4	5.09	2036.5	0.3910	19	7.00	2800.9	0.2427
5	5.10	2038.8	0.4191	20	7.02	2808.5	0.1361
6	5.10	2041.2	0.1292	21	7.24	2895.6	0.0268
7	5.22	2086.4	0.0953	22	7.25	2898.3	0.0413
8	5.29	2116.4	0.1001	23	7.27	2907.3	0.2963
9	5.30	2117.6	0.1221	24	7.30	2918.2	0.0879
10	5.30	2120.5	0.1208	25	7.32	2925.8	0.1381
11	6.86	2741.6	0.0539	26	7.34	2933.8	0.0697
12	6.89	2755.8	0.1239	27	7.36	2941.4	0.0128
13	6.89	2756.8	0.1234	28	7.37	2949.2	0.0157
14	6.90	2758.2	0.1280	29	7.39	2956.6	0.0093
15	6.91	2764.0	0.1537				

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.78 .. 3.80]	1.501	5.32223e+9	1.501
2	[3.81 .. 3.84]	3.055	1.08308e+10	3.055
3	[5.07 .. 5.12]	2.005	7.10752e+9	2.005
4	[5.20 .. 5.23]	0.504	1.78528e+9	0.504
5	[5.28 .. 5.31]	0.550	1.94955e+9	0.550
6	[6.82 .. 7.07]	4.801	1.70210e+10	4.801
7	[7.23 .. 7.41]	1.997	7.08232e+9	1.997

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Acquisition Time (sec)	1.3566	Comment	86199X107	Date	Jan 12 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060112\1002				
Frequency (MHz)	100.57	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10031.2939
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	55.32	5563.7	0.9297	14	118.66	11933.5	0.3012
2	55.43	5574.0	0.0778	15	118.78	11945.3	0.7986
3	71.63	7203.2	0.3759	16	122.15	12284.4	0.0774
4	73.18	7359.5	0.1208	17	122.59	12327.9	0.0397
5	76.68	7711.8	0.9492	18	129.60	13033.4	0.2363
6	77.00	7743.5	1.0000	19	129.87	13060.7	0.4969
7	77.32	7775.2	0.9756	20	137.27	13804.5	0.0681
8	84.40	8487.3	0.2429	21	139.42	14020.4	0.1700
9	84.65	8512.4	0.1225	22	149.14	14998.7	0.0377
10	111.99	11262.7	0.2677	23	149.79	15063.5	0.0895
11	112.32	11295.2	0.8460	24	159.86	16076.4	0.1515
12	114.45	11509.7	0.3781	25	165.04	16597.6	0.0386
13	114.61	11525.9	0.2075	26	165.30	16623.4	0.0528

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Acquisition Time (sec)	5.1298	Comment	86199X049	Date	Oct 13 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20051013\0501				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.2144	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	5.15	2062.4	0.1767	18	6.42	2569.0	0.3959	1	[5.14 .. 5.18]	1.082	8.02573e+8	1.082
2	5.28	2111.3	1.0000	19	6.43	2571.2	0.3726	2	[5.25 .. 5.30]	1.696	1.25805e+9	1.696
3	5.28	2113.6	0.9391	20	6.51	2606.5	0.3228	3	[5.37 .. 5.40]	0.707	5.24098e+8	0.707
4	5.38	2153.6	0.6747	21	6.52	2607.2	0.5575	4	[6.36 .. 6.39]	0.684	5.07399e+8	0.684
5	5.39	2156.7	0.4991	22	6.52	2608.0	0.3368	5	[6.39 .. 6.41]	0.664	4.92367e+8	0.664
6	6.37	2548.9	0.1749	23	6.52	2609.8	0.2750	6	[6.41 .. 6.43]	0.969	7.19097e+8	0.969
7	6.37	2550.7	0.1812	24	6.52	2610.5	0.4619	7	[6.51 .. 6.54]	0.975	7.23347e+8	0.975
8	6.38	2552.3	0.3781	25	6.53	2611.3	0.2648	8	[7.40 .. 7.42]	0.710	5.26803e+8	0.710
9	6.38	2554.0	0.4038	26	7.27	2908.8	0.7361	9	[7.44 .. 7.47]	1.008	7.47876e+8	1.008
10	6.39	2556.4	0.2937	27	7.40	2962.4	0.2920					
11	6.39	2557.1	0.4156	28	7.41	2963.4	0.3039					
12	6.39	2558.1	0.2674	29	7.41	2964.2	0.3016					
13	6.40	2559.7	0.1383	30	7.41	2965.1	0.3016					
14	6.40	2560.4	0.1792	31	7.45	2980.5	0.4412					
15	6.40	2561.4	0.1428	32	7.45	2981.3	0.4200					
16	6.41	2565.7	0.3153	33	7.45	2982.5	0.4476					
17	6.42	2567.5	0.3329	34	7.46	2983.3	0.4570

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5/5/2006 12:06 PM

Acquisition Time (sec)	1.4135	Comment	86199X049	Date	Oct 13 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20051013\0502				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10541.0342
Sweep Width (Hz)	23181.69	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	65.97	6637.6	0.2078	11	110.81	11149.8	0.1565
2	68.01	6843.4	0.0939	12	122.35	12310.8	0.0500
3	76.68	7715.0	0.9323	13	122.50	12325.6	0.0264
4	77.00	7747.6	1.0000	14	142.95	14383.7	0.1544
5	77.32	7779.4	0.9985	15	143.02	14390.0	0.1858
6	82.73	8324.2	0.2796	16	149.13	15005.5	0.0869
7	83.25	8376.5	0.1078	17	149.39	15031.7	0.0608
8	108.80	10947.5	0.1694	18	150.66	15159.0	0.1323
9	108.94	10961.6	0.1630	19	164.94	16595.9	0.0404
10	110.69	11137.1	0.2044	20	165.19	16620.7	0.0781

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7/3/2006 3:18 PM

Acquisition Time (sec)	5.1298	Comment	86199X147	Date	Jun 20 2006
File Name	C:\Program Files\Common Files\SYSTEMMSAPI\1033\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060620\1101				
Frequency (MHz)	399.90	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	32.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2412.8181	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.97	1187.7	0.0594	13	7.33	2932.6	0.6766	1	[2.81 .. 3.14]	1.430	1.00805e+10	1.430
2	5.09	2035.3	0.7158	14	7.36	2944.9	0.3253	2	[5.07 .. 5.10]	1.029	7.25833e+9	1.029
3	5.09	2037.1	0.9036	15	7.38	2950.6	1.0000	3	[5.13 .. 5.16]	1.050	7.40436e+9	1.050
4	5.10	2039.0	0.4701	16	7.38	2952.1	0.9322	4	[5.23 .. 5.31]	0.436	3.07167e+9	0.436
5	5.14	2056.4	0.7533	17	7.40	2958.4	0.8453	5	[7.32 .. 7.34]	0.843	5.94556e+9	0.843
6	5.15	2057.9	0.8035	18	7.41	2964.4	0.3523	6	[7.36 .. 7.46]	5.000	3.52558e+10	5.000
7	5.24	2097.3	0.0949	19	7.42	2966.2	0.3493					
8	5.25	2099.6	0.1264	20	7.42	2968.9	0.2562					
9	5.26	2102.4	0.0668	21	7.44	2975.5	0.9324					
10	5.29	2115.6	0.0987	22	7.46	2981.4	0.4559					
11	5.30	2118.7	0.1141	23	7.46	2983.1	0.4359					
12	5.31	2121.7	0.0496

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7/3/2006 3:19 PM

Acquisition Time (sec)	1.3566	Comment	86199X147	Date	Jun 20 2006
File Name	C:\Documents and Settings\DASSAK\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060620\1102				
Frequency (MHz)	100.57	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10055.5254
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	72.16	7256.9	0.0777	12	129.16	12989.1	0.0796
2	76.96	7739.0	0.1274	13	130.37	13110.7	0.0181
3	77.27	7770.7	0.1261	14	133.87	13462.3	0.0180
4	77.59	7803.1	0.1208	15	135.82	13659.1	0.0246
5	83.79	8426.0	0.0111	16	138.27	13905.4	0.0441
6	87.40	8789.4	0.0466	17	145.24	14606.4	0.0095
7	116.09	11674.7	0.0201	18	145.68	14649.9	0.0121
8	126.89	12760.5	0.0515	19	151.69	15254.4	0.0106
9	126.95	12767.2	1.0000	20	165.92	16685.9	0.0077
10	128.68	12940.4	0.0427	21	166.51	16744.9	0.0115
11	128.99	12972.1	0.2381

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Acquisition Time (sec)	5.1298	Comment	86199X141P1	Date	Apr 5 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060405\2401				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	40.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2390.7451
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	4.99	1996.3	0.4990	16	7.29	2914.9	0.6182
2	5.00	1998.8	0.5546	17	7.29	2916.2	0.8190
3	5.05	2019.7	0.4510	18	7.29	2918.6	0.4756
4	5.05	2022.2	0.4925	19	7.30	2920.3	0.5581
5	5.09	2034.9	0.7372	20	7.30	2921.9	0.6192
6	5.09	2037.2	0.6613	21	7.31	2924.2	0.8084
7	5.18	2073.3	0.6308	22	7.31	2925.8	0.8048
8	5.19	2076.0	0.6015	23	7.32	2930.6	0.3463
9	7.22	2888.0	0.2519	24	7.33	2932.2	0.4728
10	7.23	2892.8	0.1501	25	7.33	2933.6	0.3978
11	7.23	2894.6	0.2085	26	7.38	2954.6	0.6099
12	7.24	2896.1	0.1558	27	7.39	2956.4	0.6886
13	7.25	2901.0	0.5445	28	7.40	2962.8	0.5361
14	7.27	2908.8	1.0000	29	7.41	2964.2	0.4573
15	7.28	2913.1	0.3367				

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[4.97 .. 5.01]	1.217	1.52443e+9	1.217
2	[5.03 .. 5.07]	1.075	1.34640e+9	1.075
3	[5.07 .. 5.11]	1.149	1.43879e+9	1.149
4	[5.17 .. 5.20]	1.000	1.25245e+9	1.000
5	[7.21 .. 7.35]	8.661	1.08494e+10	8.661
6	[7.37 .. 7.42]	2.337	2.92756e+9	2.337

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Acquisition Time (sec)	1.3566	Comment	86199X141P1	Date	Apr 5 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060405\2402				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10031.6445
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	61.48	6185.5	0.3246	12	121.12	12186.7	0.0909
2	63.29	6368.3	0.1743	13	122.47	12322.4	0.0547
3	76.68	7715.1	0.4097	14	122.74	12349.7	0.0519
4	77.00	7747.5	0.4261	15	128.37	12915.8	1.0000
5	77.32	7779.2	0.4065	16	129.22	13001.3	0.3034
6	81.36	8186.2	0.0592	17	129.27	13006.5	0.3083
7	83.31	8382.2	0.2374	18	131.78	13259.3	0.6392
8	83.56	8407.3	0.2819	19	131.85	13266.7	0.7616
9	87.86	8840.0	0.0685	20	148.40	14931.9	0.0448
10	89.26	8981.6	0.0573	21	149.02	14993.9	0.0604
11	120.94	12169.0	0.0768	22	165.22	16623.7	0.0467

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Acquisition Time (sec)	5.1298	Comment	86199X118	Date	Mar 2 2006
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060302\1301				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	38.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.4092	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.76	704.0	0.3551	19	5.11	2046.4	0.0659	37	5.87	2347.2	0.0453	55	6.30	2521.1	0.0636	1	[1.64 .. 1.90]	4.566	1.05335e+10	4.566
2	1.78	711.0	1.0000	20	5.12	2049.1	0.0678	38	5.99	2395.9	0.0585	56	6.31	2525.9	0.0676	2	[2.06 .. 2.21]	0.999	2.30414e+9	0.999
3	1.79	718.0	0.6862	21	5.43	2171.1	0.0703	39	5.99	2396.9	0.0572	57	6.33	2534.3	0.1522	3	[2.52 .. 2.64]	0.528	1.21859e+9	0.528
4	2.10	841.6	0.0514	22	5.44	2178.2	0.0656	40	6.00	2400.0	0.0336	58	6.36	2544.5	0.1246	4	[4.52 .. 4.70]	1.452	3.34865e+9	1.452
5	2.12	847.7	0.0565	23	5.46	2186.3	0.0755	41	6.00	2400.8	0.0321	59	6.37	2549.3	0.1287	5	[4.88 .. 4.98]	1.002	2.31034e+9	1.002
6	2.16	865.0	0.0665	24	5.48	2193.6	0.0724	42	6.00	2402.5	0.0321	60	6.40	2559.9	0.1064	6	[5.07 .. 5.15]	0.514	1.18678e+9	0.514
7	2.18	870.5	0.0628	25	5.60	2241.5	0.0348	43	6.01	2406.4	0.0633	61	6.64	2657.3	0.0201	7	[5.40 .. 5.50]	0.544	1.25512e+9	0.544
8	2.54	1017.9	0.0275	26	5.63	2254.2	0.0369	44	6.02	2407.2	0.0639	62	6.69	2678.6	0.0357	8	[5.60 .. 5.73]	1.147	2.64562e+9	1.147
9	2.62	1048.5	0.0343	27	5.65	2260.0	0.1406	45	6.03	2413.5	0.1209	63	6.70	2679.7	0.0333	9	[5.73 .. 5.89]	1.428	3.29330e+9	1.428
10	4.55	1821.0	0.1191	28	5.67	2267.4	0.1326	46	6.06	2424.4	0.1287	64	6.72	2689.7	0.0366	10	[5.96 .. 6.13]	1.461	3.36975e+9	1.461
11	4.56	1826.1	0.0806	29	5.69	2275.4	0.1392	47	6.06	2425.3	0.1246	65	6.72	2690.7	0.0333	11	[6.27 .. 6.38]	1.089	2.51252e+9	1.089
12	4.66	1863.1	0.0556	30	5.71	2282.8	0.1326	48	6.07	2428.5	0.0710	66	6.73	2693.8	0.0336	12	[6.63 .. 6.78]	0.445	1.02695e+9	0.445
13	4.92	1969.4	0.6614	31	5.76	2304.7	0.0748	49	6.07	2429.2	0.0705	67	6.74	2695.0	0.0315					
14	4.93	1971.5	0.6605	32	5.78	2311.9	0.1035	50	6.07	2430.0	0.0705	68	6.76	2704.9	0.0339					
15	4.95	1979.5	0.1488	33	5.80	2319.1	0.1442	51	6.10	2439.6	0.0769	69	7.27	2908.8	0.2776					
16	4.95	1981.8	0.1458	34	5.81	2326.1	0.1519	52	6.10	2440.6	0.0817									
17	5.10	2039.9	0.2598	35	5.83	2333.3	0.1389	53	6.28	2510.7	0.0783									
18	5.11	2042.7	0.2356	36	5.85	2340.4	0.1181	54	6.28	2514.6	0.0364

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Acquisition Time (sec)	1.3566	Comment	86199X118	Date	Mar 2 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060302\1302				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10034.5938
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.48	1356.4	0.1559	13	127.67	12845.8	0.1778
2	18.14	1825.2	0.3593	14	129.62	13041.8	0.0953
3	70.36	7079.7	1.0000	15	129.88	13068.4	0.3607
4	72.07	7251.4	0.2617	16	129.92	13072.1	0.2335
5	76.68	7715.1	0.8795	17	132.74	13355.9	0.1592
6	77.00	7747.5	0.8115	18	132.88	13369.9	0.4009
7	77.32	7779.2	0.8771	19	135.16	13599.1	0.2958
8	84.25	8476.6	0.4757	20	135.30	13613.9	0.2037
9	84.56	8508.3	0.2442	21	149.28	15020.4	0.0451
10	121.82	12257.5	0.0618	22	149.83	15075.7	0.1245
11	122.82	12357.8	0.1916	23	165.28	16630.4	0.0659
12	125.37	12614.3	0.6206	24	165.52	16653.9	0.1185

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Acquisition Time (sec)	5.1298	Comment	86199X108	Date	Jan 13 2006
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060113\1401				
Frequency (MHz)	399.90	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	44.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2413.4026	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	4.74	1894.0	0.0497	17	6.78	2712.0	0.0549	33	7.35	2938.1	0.1642	1	[4.70 .. 4.77]	0.897	1.83810e+9	0.897
2	4.85	1939.8	0.0241	18	6.79	2715.3	0.1369	34	7.35	2939.5	0.2052	2	[4.82 .. 4.88]	0.487	9.97497e+8	0.487
3	5.02	2006.1	0.4192	19	6.83	2731.1	0.1127	35	7.36	2943.7	0.1369	3	[4.98 .. 5.05]	0.861	1.76434e+9	0.861
4	5.02	2008.2	0.3968	20	7.27	2907.3	1.0000	36	7.37	2945.5	0.4566	4	[5.16 .. 5.21]	0.462	9.45461e+8	0.462
5	5.18	2071.2	0.1789	21	7.28	2910.2	0.0495	37	7.38	2950.4	0.0699	5	[6.11 .. 6.19]	0.500	1.02431e+9	0.500
6	5.19	2074.1	0.1812	22	7.28	2912.2	0.0490	38	7.38	2952.5	0.1372	6	[6.33 .. 6.41]	0.917	1.87873e+9	0.917
7	6.12	2448.6	0.0752	23	7.30	2918.0	0.0602	39	7.39	2953.9	0.1451	7	[6.70 .. 6.87]	1.490	3.05156e+9	1.490
8	6.14	2455.4	0.0740	24	7.30	2920.5	0.0544	40	7.39	2956.0	0.0385	8	[7.27 .. 7.46]	5.871	1.20276e+10	5.871
9	6.16	2464.4	0.0840	25	7.31	2921.7	0.0585	41	7.41	2962.5	0.0401					
10	6.18	2471.2	0.0821	26	7.31	2925.2	0.1605	42	7.41	2964.8	0.2265					
11	6.34	2535.0	0.1585	27	7.32	2927.4	0.0758	43	7.42	2966.2	0.2329					
12	6.36	2542.4	0.1672	28	7.33	2929.3	0.0582	44	7.42	2967.3	0.1219					
13	6.38	2550.9	0.2046	29	7.33	2930.5	0.0972	45	7.43	2970.7	0.0544					
14	6.40	2558.3	0.1847	30	7.33	2932.2	0.1893	46	7.43	2972.8	0.1574					
15	6.74	2696.2	0.0585	31	7.34	2933.8	0.1275	47	7.44	2974.4	0.1198					
16	6.74	2697.3	0.0588	32	7.34	2935.8	0.0413

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Acquisition Time (sec)	1.3566	Comment	86199X108	Date	Jan 13 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20060113\1402				
Frequency (MHz)	100.57	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10034.2422
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	70.72	7111.8	0.1153	13	128.40	12912.5	0.0585
2	72.35	7276.2	0.0704	14	128.63	12935.3	0.0918
3	76.68	7711.8	0.9093	15	128.70	12942.7	0.2134
4	77.00	7743.5	1.0000	16	128.74	12947.1	0.1004
5	77.32	7775.2	0.9088	17	128.77	12949.4	0.5023
6	84.14	8461.5	0.1094	18	134.93	13569.3	0.0548
7	84.39	8486.6	0.0740	19	135.04	13580.4	0.0739
8	119.76	12044.1	0.0322	20	135.35	13611.3	0.0724
9	119.99	12067.0	0.0433	21	147.58	14841.6	0.0407
10	122.59	12328.7	0.0554	22	149.56	15040.7	0.0589
11	124.90	12560.1	0.0675	23	162.04	16296.1	0.0468
12	126.79	12750.3	0.2343	24	165.33	16626.3	0.0589

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Acquisition Time (sec)	5.1298	Comment	86199X119	Date	Mar 6 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060306\1501				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	38.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.6042	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.28	510.2	0.1100	17	4.36	1744.8	0.1751
2	1.29	517.2	0.2249	18	4.37	1746.7	0.1738
3	1.31	524.4	0.1184	19	4.37	1749.1	0.0269
4	1.32	529.9	0.4476	20	4.38	1752.0	0.1636
5	1.34	536.9	1.0000	21	4.38	1753.8	0.0629
6	1.36	544.1	0.4904	22	4.39	1755.5	0.0418
7	3.29	1318.1	0.0264	23	4.40	1759.0	0.0522
8	4.28	1712.4	0.0311	24	4.41	1762.7	0.0352
9	4.32	1728.8	0.0392	25	4.58	1831.2	0.1013
10	4.33	1731.3	0.0372	26	4.71	1885.7	0.0256
11	4.33	1732.3	0.0589	27	4.72	1887.7	0.0262
12	4.34	1736.0	0.0419	28	5.31	2123.0	0.3859
13	4.34	1737.6	0.0656	29	5.31	2124.7	0.3543
14	4.35	1739.5	0.1761	30	5.36	2146.4	0.0863
15	4.35	1742.1	0.0271	31	5.37	2148.5	0.0767
16	4.36	1743.0	0.0252	32	7.27	2908.8	0.0443

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.27 .. 1.32]	0.824	6.49903e+9	0.824
2	[1.32 .. 1.37]	3.228	2.54673e+10	3.228
3	[3.22 .. 3.36]	1.008	7.94829e+9	1.008
4	[3.39 .. 3.48]	0.248	1.95927e+9	0.248
5	[4.31 .. 4.41]	2.413	1.90323e+10	2.413
6	[4.56 .. 4.60]	1.043	8.23007e+9	1.043
7	[4.70 .. 4.73]	0.243	1.91599e+9	0.243
8	[5.30 .. 5.32]	1.006	7.93328e+9	1.006
9	[5.36 .. 5.38]	0.224	1.76524e+9	0.224

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Acquisition Time (sec)	1.3566	Comment	86199X119	Date	Mar 6 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060306\1502				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10032.3818
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.94	1402.8	0.2628	11	82.63	8313.7	0.2870
2	14.02	1410.9	1.0000	12	122.29	12304.7	0.2596
3	63.07	6345.5	0.1926	13	122.59	12334.9	0.0515
4	63.36	6375.0	0.9656	14	147.90	14881.8	0.0669
5	67.91	6832.7	0.9395	15	148.47	14938.6	0.3857
6	69.41	6983.8	0.2528	16	164.48	16549.3	0.0713
7	76.68	7715.1	0.8886	17	164.77	16578.7	0.3661
8	77.00	7747.5	0.8492	18	169.03	17007.8	0.0907
9	77.32	7779.2	0.8751	19	169.85	17089.6	0.6305
10	81.86	8236.3	0.7717

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5/8/2006 10:36 AM

Acquisition Time (sec)	5.1298	Comment	86199X128	Date	Mar 17 2006
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060317\2901				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	44.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.4092	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.31	524.3	0.2231	18	4.31	1726.1	0.0101
2	1.33	531.3	0.4185	19	4.32	1728.8	0.0740
3	1.35	538.5	0.4941	20	4.33	1730.6	0.0561
4	1.36	545.5	0.6493	21	4.33	1733.3	0.0111
5	1.38	552.7	0.3110	22	4.34	1735.8	0.0338
6	1.65	659.3	1.0000	23	4.34	1737.6	0.1648
7	1.68	673.2	0.7896	24	4.35	1741.7	0.0181
8	3.31	1325.3	0.0323	25	4.36	1744.0	0.1476
9	3.32	1327.6	0.0459	26	4.36	1744.8	0.1644
10	3.59	1437.0	0.0090	27	4.37	1748.9	0.0374
11	3.63	1451.4	0.0302	28	4.38	1751.2	0.0513
12	4.26	1703.7	0.0138	29	4.38	1752.0	0.0549
13	4.28	1710.9	0.0381	30	4.39	1755.9	0.0387
14	4.28	1714.4	0.0259	31	4.41	1763.1	0.0141
15	4.29	1718.1	0.0354	32	5.16	2066.1	0.3044
16	4.30	1721.6	0.0782	33	5.23	2094.3	0.4641
17	4.31	1725.1	0.0157	34	7.27	2908.8	0.1483

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.29 .. 1.41]	5.440	9.19742e+9	5.440
2	[1.63 .. 1.66]	3.121	5.27662e+9	3.121
3	[1.66 .. 1.71]	2.813	4.75595e+9	2.813
4	[3.29 .. 3.35]	1.011	1.70859e+9	1.011
5	[3.58 .. 3.65]	0.922	1.55945e+9	0.922
6	[4.24 .. 4.42]	3.962	6.69784e+9	3.962
7	[5.15 .. 5.19]	0.900	1.52162e+9	0.900
8	[5.22 .. 5.26]	1.002	1.69314e+9	1.002

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Acquisition Time (sec)	1.3566	Comment	86199X128	Date	Mar 17 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060317\2902				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10037.5420
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.01	1409.4	0.3190	12	84.23	8475.1	0.3113
2	14.04	1412.4	0.1751	13	84.58	8509.8	0.1523
3	22.34	2247.6	0.2495	14	122.94	12370.3	0.0754
4	23.64	2378.8	0.3265	15	123.31	12407.1	0.0619
5	63.24	6363.2	0.2335	16	148.10	14901.0	0.1163
6	63.42	6380.8	0.1551	17	148.26	14917.9	0.0426
7	74.08	7454.2	0.1541	18	164.39	16540.4	0.0637
8	74.61	7507.2	0.2047	19	164.47	16548.5	0.1145
9	76.68	7715.9	0.9121	20	172.51	17357.9	0.0860
10	77.00	7747.5	1.0000	21	172.65	17371.2	0.1497
11	77.32	7779.2	0.9457

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Acquisition Time (sec)	5.1298	Comment	86199X137	Date	Mar 28 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060328\5601				
Frequency (MHz)	400.11	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.4092	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.34	537.7	0.4836	13	4.38	1754.0	0.1853	1	[1.33 .. 1.40]	6.000	3.56334e+10	6.000
2	1.36	544.7	1.0000	14	4.39	1755.1	0.1499	2	[4.00 .. 4.06]	0.935	5.55443e+9	0.935
3	1.38	551.9	0.5006	15	4.40	1758.6	0.0426	3	[4.32 .. 4.45]	4.057	2.40921e+10	4.057
4	4.03	1611.5	0.2501	16	4.40	1761.2	0.2506	4	[5.90 .. 5.97]	0.907	5.38464e+9	0.907
5	4.03	1612.4	0.2593	17	4.41	1765.9	0.0404					
6	4.33	1730.8	0.0373	18	4.42	1768.2	0.1745					
7	4.33	1734.5	0.0461	19	4.44	1775.4	0.0428					
8	4.35	1741.5	0.1401	20	4.45	1778.9	0.0385					
9	4.36	1743.2	0.0456	21	5.93	2373.9	0.2869					
10	4.37	1747.9	0.1565	22	5.94	2374.9	0.2933					
11	4.37	1748.7	0.1686	23	7.27	2908.8	0.2277					
12	4.37	1750.5	0.0466

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Acquisition Time (sec)	1.3566	Comment	86199X137	Date	Mar 28 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060328\5602				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10038.2793
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	13.93	1402.1	0.4304
2	63.66	6405.2	0.3283
3	64.49	6488.5	0.3161
4	76.68	7715.8	0.9678
5	77.00	7747.5	1.0000
6	77.32	7779.2	0.9116
7	77.96	7844.1	0.2105
8	82.36	8287.2	0.3314
9	123.60	12435.9	0.0759
10	147.31	14822.1	0.1035
11	164.18	16519.8	0.1152
12	165.99	16701.1	0.1160
13	166.51	16754.2	0.2670

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Acquisition Time (sec)	5.1298	Comment	86199X121	Date	Mar 10 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060310\2101				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	38.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2400.8823	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.26	504.4	1.0000	18	6.96	2784.8	0.0484
2	1.48	592.1	0.8293	19	6.96	2785.8	0.0578
3	3.04	1216.9	0.0299	20	6.98	2791.8	0.1103
4	3.92	1567.6	0.1803	21	6.98	2793.2	0.1154
5	3.94	1576.8	0.3176	22	7.00	2799.1	0.1389
6	3.96	1585.5	0.2267	23	7.01	2805.5	0.0645
7	3.99	1595.3	0.0919	24	7.01	2806.5	0.0745
8	5.08	2033.3	0.3983	25	7.24	2898.5	0.0981
9	5.20	2081.5	0.3192	26	7.25	2901.6	0.1314
10	6.84	2736.5	0.1469	27	7.26	2903.5	0.0571
11	6.84	2737.3	0.1578	28	7.27	2908.8	0.2795
12	6.86	2745.1	0.1812	29	7.29	2916.2	0.2160
13	6.86	2746.2	0.1441	30	7.29	2917.6	0.2382
14	6.89	2755.6	0.1676	31	7.31	2922.8	0.0612
15	6.89	2756.6	0.1664	32	7.31	2925.0	0.1093
16	6.91	2764.4	0.1974	33	7.32	2927.3	0.0296
17	6.91	2765.3	0.1487				

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.25 .. 1.28]	2.999	2.89325e+9	2.999
2	[1.46 .. 1.50]	2.693	2.59777e+9	2.693
3	[2.97 .. 3.13]	2.577	2.48563e+9	2.577
4	[3.90 .. 4.00]	3.523	3.39859e+9	3.523
5	[5.07 .. 5.10]	0.998	9.62894e+8	0.998
6	[5.19 .. 5.22]	1.063	1.02583e+9	1.063
7	[6.83 .. 6.93]	4.255	4.10441e+9	4.255
8	[6.95 .. 7.03]	2.330	2.24734e+9	2.330
9	[7.23 .. 7.32]	4.232	4.08275e+9	4.232

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Acquisition Time (sec)	1.3566	Comment	86199X121	Date	Mar 10 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060310\2102				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10032.3818
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	18.78	1889.3	0.1735	12	114.39	11509.3	0.7495
2	21.95	2208.5	0.2889	13	114.58	11529.2	0.5746
3	70.65	7108.4	0.1239	14	121.83	12258.2	0.2870
4	71.90	7234.5	0.3878	15	121.87	12261.9	0.3290
5	73.48	7393.7	0.3590	16	122.27	12302.5	0.0974
6	74.03	7449.0	0.1740	17	129.60	13039.6	1.0000
7	76.68	7715.1	0.4089	18	150.69	15161.9	0.1523
8	77.00	7747.5	0.3921	19	150.96	15189.2	0.0970
9	77.32	7779.2	0.4150	20	157.44	15840.8	0.0948
10	83.04	8355.7	0.1809	21	157.58	15855.6	0.1314
11	84.22	8474.4	0.2225	22	164.87	16588.3	0.0464

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Acquisition Time (sec)	5.1298	Comment	86199X113	Date	Jan 23 2006
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060123\2201				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	44.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2409.6548	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.91	1163.7	0.1537	1	[2.89 .. 2.96]	2.000	1.04333e+10	2.000
2	2.93	1170.7	0.3076	2	[3.71 .. 3.77]	2.017	1.05237e+10	2.017
3	2.94	1177.9	0.1674	3	[3.77 .. 3.82]	1.975	1.03007e+10	1.975
4	3.72	1489.4	0.1613	4	[7.17 .. 7.36]	4.996	2.60612e+10	4.996
5	3.74	1496.6	0.3054					
6	3.76	1503.7	0.1516					
7	3.78	1513.0	1.0000					
8	7.19	2877.8	0.2061					
9	7.21	2885.2	0.2788					
10	7.23	2893.4	0.0402					
11	7.23	2894.6	0.0408					
12	7.25	2901.4	0.1182					
13	7.27	2908.8	0.2670					
14	7.30	2921.5	0.2158					
15	7.32	2928.5	0.2419					
16	7.34	2936.7	0.0873

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Acquisition Time (sec)	1.3566	Comment	86199X113	Date	Jan 23 2006
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060123\2202				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10035.3301
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	34.69	3490.4	0.4006
2	44.70	4497.4	0.3550
3	54.04	5437.3	0.3596
4	76.68	7715.9	0.4324
5	77.00	7747.5	0.4260
6	77.32	7780.0	0.4278
7	125.68	12646.0	0.0450
8	126.80	12758.0	0.4838
9	128.58	12937.2	1.0000
10	138.08	13893.3	0.2482
11	139.29	14014.9	0.0773
12	164.13	16513.9	0.0751

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Acquisition Time (sec)	5.1298	Comment	86199X052	Date	Oct 17 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20051017\3701				
Frequency (MHz)	399.77	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	44.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2408.0020
Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.06	424.7	0.0143	21	2.70	1081.3	0.0192	41	3.93	1570.6	0.0105	61	5.32	2128.4	0.0036	1	[1.05 .. 1.11]	0.332	7.26269e+8	0.332
2	1.08	432.0	0.0295	22	2.72	1086.6	0.0191	42	3.95	1577.8	0.0098	62	5.33	2130.3	0.0033	2	[1.14 .. 1.23]	2.913	6.37640e+9	2.913
3	1.10	439.0	0.0149	23	2.73	1093.0	0.0257	43	3.96	1585.0	0.0167	63	5.34	2133.2	0.0032	3	[2.57 .. 2.82]	2.355	5.15434e+9	2.355
4	1.17	465.9	0.1792	24	2.74	1094.6	0.0259	44	3.98	1593.0	0.0206	64	5.44	2172.8	0.0254	4	[3.56 .. 3.77]	1.484	3.24893e+9	1.484
5	1.18	473.1	0.3915	25	2.75	1100.8	0.0221	45	4.00	1599.5	0.0261	65	5.44	2175.1	0.0269	5	[3.89 .. 4.13]	3.349	7.33187e+9	3.349
6	1.20	480.1	0.1831	26	2.76	1102.9	0.0115	46	4.02	1607.3	0.0182	66	5.45	2177.5	0.0274	6	[4.87 .. 4.93]	0.942	2.06094e+9	0.942
7	2.49	995.7	0.0731	27	2.78	1109.4	0.0109	47	4.03	1612.3	0.0083	67	5.45	2180.0	0.0252	7	[4.94 .. 4.97]	0.122	2.67591e+8	0.122
8	2.50	997.7	0.1676	28	2.78	1110.7	0.0123	48	4.04	1613.9	0.0125	68	6.35	2537.9	0.0060	8	[5.30 .. 5.35]	0.153	3.33872e+8	0.153
9	2.50	999.4	0.2333	29	2.79	1117.2	0.0091	49	4.05	1619.4	0.0149	69	6.36	2543.6	0.0056	9	[5.39 .. 5.51]	1.062	2.32433e+9	1.062
10	2.50	1001.4	0.1690	30	3.32	1327.9	1.0000	50	4.06	1621.1	0.0497	70	6.43	2571.3	0.0618	10	[6.34 .. 6.38]	0.151	3.29764e+8	0.151
11	2.51	1003.1	0.0736	31	3.60	1437.7	0.0063	51	4.07	1626.6	0.0183	71	6.44	2576.1	0.0617	11	[6.40 .. 6.49]	1.000	2.18846e+9	1.000
12	2.59	1036.9	0.0070	32	3.61	1444.7	0.0104	52	4.07	1628.3	0.1581	72	7.66	3061.2	0.0129	12	[7.60 .. 7.72]	1.959	4.28752e+9	1.959
13	2.61	1043.9	0.0132	33	3.63	1451.5	0.0064	53	4.09	1635.3	0.1486	73	7.66	3063.5	0.0944	13	[7.72 .. 7.77]	0.248	5.42866e+8	0.248
14	2.63	1050.7	0.0136	34	3.67	1466.1	0.0128	54	4.11	1642.6	0.0473	74	7.68	3071.9	0.0971	14	[8.15 .. 8.19]	0.163	3.56769e+8	0.163
15	2.64	1057.1	0.0129	35	3.68	1472.4	0.0173	55	4.31	1723.7	0.0203	75	7.73	3092.2	0.0085	15	[8.19 .. 8.29]	2.022	4.42673e+9	2.022
16	2.65	1058.1	0.0121	36	3.69	1473.9	0.0148	56	4.90	1959.9	0.0716	76	7.76	3100.5	0.0089					
17	2.66	1065.1	0.0130	37	3.70	1480.4	0.0251	57	4.91	1962.3	0.0734	77	8.16	3261.2	0.0086					
18	2.67	1066.9	0.0219	38	3.72	1486.6	0.0195	58	4.95	1979.2	0.0066	78	8.18	3270.1	0.0104					
19	2.69	1073.5	0.0278	39	3.72	1488.2	0.0183	59	4.96	1981.8	0.0067	79	8.22	3285.7	0.1387					
20	2.69	1074.5	0.0282	40	3.74	1494.4	0.0135	60	5.32	2125.0	0.0033	80	8.24	3294.7	0.1268

7/3/2006 5:23 PM

Acquisition Time (sec)	1.4205	Comment	86199X052	Date	Oct 17 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20051017\3702				
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	DMSO-d ₆	Spectrum Offset (Hz)	10554.8516
Sweep Width (Hz)	23068.05	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.70	1477.8	0.0502
2	32.91	3308.2	0.0359
3	38.07	3827.1	0.0277
4	60.84	6116.5	0.0529
5	68.04	6840.2	0.0218
6	87.81	8827.6	0.0237
7	123.61	12427.1	0.0722
8	128.17	12885.5	0.0559
9	130.60	13129.7	0.0192
10	132.88	13359.2	0.0190
11	141.98	14273.7	0.0334
12	147.56	14834.8	0.0296
13	163.85	16472.3	0.0257
14	171.88	17279.1	0.0543

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7/5/2006 9:39 AM

Acquisition Time (sec)	5.1229	Comment	86199X114	Date	May 4 2006
File Name	C:\Documents and Settings\DASSAKIMy Documents\data\NMR\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20060504\001				
Frequency (MHz)	399.77	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	46.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	2407.5742
Sweep Width (Hz)	6396.42	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	2.49	995.9	0.3276	20	3.03	1212.0	0.0526	39	4.04	1615.9	0.0535	58	7.24	2895.5	0.3114	1	[2.82 .. 2.91]	1.598	2.70037e+8	1.598
2	2.50	997.7	0.6917	21	3.17	1266.7	0.0772	40	4.74	1895.2	0.3528	59	7.26	2902.7	0.1744	2	[2.95 .. 3.04]	1.262	2.13328e+8	1.262
3	2.50	999.4	0.9520	22	3.38	1349.2	1.0000	41	4.75	1897.6	0.3593	60	7.26	2904.1	0.1567	3	[3.59 .. 3.73]	1.893	3.19823e+8	1.893
4	2.50	1001.4	0.6805	23	3.60	1439.2	0.0633	42	4.90	1959.5	0.0593	61	7.28	2908.6	0.3129	4	[3.96 .. 4.05]	1.050	1.77461e+8	1.050
5	2.51	1003.1	0.3156	24	3.62	1446.9	0.0826	43	4.91	1961.8	0.0611	62	7.29	2915.2	0.6369	5	[4.72 .. 4.77]	1.000	1.69010e+8	1.000
6	2.83	1129.8	0.0668	25	3.64	1454.1	0.0641	44	5.33	2132.0	0.0415	63	7.30	2916.8	0.5160	6	[4.89 .. 4.92]	0.177	2.98724e+7	0.177
7	2.83	1132.8	0.0635	26	3.66	1462.3	0.0797	45	5.41	2161.7	0.2322	64	7.32	2924.4	0.5034	7	[5.31 .. 5.35]	0.182	3.08073e+7	0.182
8	2.85	1138.4	0.1088	27	3.67	1468.5	0.0902	46	6.47	2585.3	0.0503	65	7.33	2931.6	0.4376	8	[5.38 .. 5.44]	1.024	1.73077e+8	1.024
9	2.86	1141.7	0.0747	28	3.68	1471.3	0.0904	47	6.85	2738.4	0.0594	66	7.35	2938.8	0.1599	9	[6.36 .. 6.54]	0.960	1.62254e+8	0.960
10	2.87	1146.0	0.1154	29	3.69	1476.5	0.1289	48	6.87	2746.2	0.0595	67	7.58	3028.6	0.4735	10	[6.85 .. 6.87]	0.227	3.83274e+7	0.227
11	2.88	1152.5	0.0998	30	3.71	1482.2	0.0940	49	7.15	2857.8	0.0437	68	7.60	3037.2	0.5187	11	[7.17 .. 7.36]	7.433	1.25610e+9	7.433
12	2.89	1155.0	0.0979	31	3.71	1485.1	0.1011	50	7.16	2861.9	0.0628	69	7.77	3104.8	0.0789	12	[7.55 .. 7.62]	2.064	3.48851e+8	2.064
13	2.90	1161.1	0.0777	32	3.73	1491.2	0.0684	51	7.16	2863.9	0.1354	70	7.79	3113.4	0.0862	13	[7.75 .. 7.81]	0.401	6.76798e+7	0.401
14	2.96	1183.5	0.0707	33	3.97	1586.6	0.0694	52	7.18	2871.5	0.0945	71	8.19	3275.8	0.6105	14	[8.18 .. 8.24]	2.010	3.39623e+8	2.010
15	2.98	1189.8	0.0897	34	3.98	1592.9	0.0825	53	7.20	2877.3	0.0661	72	8.22	3284.7	0.5754	15	[8.24 .. 8.29]	0.426	7.19060e+7	0.426
16	2.98	1192.7	0.0999	35	3.99	1595.8	0.0839	54	7.20	2880.3	0.0558	73	8.25	3299.6	0.1092					
17	3.00	1198.5	0.0954	36	4.01	1601.5	0.0899	55	7.21	2883.0	0.0837	74	8.28	3308.4	0.0985					
18	3.01	1204.0	0.1032	37	4.02	1606.7	0.0674	56	7.23	2888.5	0.1466									
19	3.02	1206.0	0.0640	38	4.03	1609.7	0.0702	57	7.23	2890.2	0.1187

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Acquisition Time (sec)	1.3582	Comment	86199X114	Date	May 4 2006
File Name	C:\Documents and Settings\DASSAKMy Documents\data\NMR\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20060504\4002				
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	DMSO-d6	Spectrum Offset (Hz)	10052.2520
Sweep Width (Hz)	24125.45	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	34.32	3450.5	0.0354	13	126.15	12682.6	0.0215
2	39.59	3979.8	0.1427	14	127.11	12778.3	0.0464
3	39.79	4000.5	0.4345	15	128.19	12887.3	0.0688
4	40.01	4021.8	0.8681	16	129.20	12988.9	0.1077
5	40.21	4042.4	1.0000	17	129.28	12997.0	0.0349
6	40.42	4063.8	0.8691	18	129.40	13008.8	0.0839
7	40.63	4084.4	0.4185	19	139.46	14020.4	0.0368
8	40.84	4105.7	0.1395	20	141.61	14236.1	0.0285
9	43.67	4389.9	0.0280	21	147.56	14834.7	0.0215
10	67.92	6828.5	0.0283	22	147.66	14844.3	0.0298
11	70.43	7080.3	0.0265	23	163.68	16455.2	0.0212
12	123.57	12422.7	0.0692

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Acquisition Time (sec)	5.1298	Comment	111968X022	Date	May 31 2006
File Name	C:\Program Files\Common Files\SYSTEM5\MAP\1033\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060531\1201				
Frequency (MHz)	400.11	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	38.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.4092	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.22	488.2	0.4575	27	2.96	1185.3	0.0603	53	4.03	1610.5	0.0370	79	4.30	1722.0	0.1378	1	[1.19 .. 1.28]	3.067	9.06188e+9	3.067
2	1.24	495.4	1.0000	28	2.97	1187.5	0.0709	54	4.03	1614.0	0.0371	80	4.31	1725.3	0.0877	2	[1.29 .. 1.37]	2.213	6.53958e+9	2.213
3	1.26	502.6	0.4505	29	2.98	1192.3	0.0404	55	4.05	1619.8	0.0320	81	4.32	1727.3	0.0473	3	[2.74 .. 3.09]	5.091	1.50410e+10	5.091
4	1.31	523.7	0.3249	30	2.98	1194.1	0.0563	56	4.08	1631.7	0.0451	82	4.32	1729.0	0.0382	4	[3.37 .. 3.53]	1.892	5.58943e+9	1.892
5	1.33	530.7	0.7534	31	3.00	1199.1	0.0353	57	4.09	1637.6	0.0495	83	4.33	1732.5	0.0350	5	[3.96 .. 4.06]	0.861	2.54513e+9	0.861
6	1.34	537.9	0.3608	32	3.00	1200.7	0.0444	58	4.10	1640.7	0.0493	84	4.33	1734.5	0.1195	6	[4.07 .. 4.21]	1.960	5.78927e+9	1.960
7	2.73	1093.3	0.0219	33	3.02	1207.7	0.0340	59	4.11	1646.2	0.0793	85	4.34	1735.8	0.2007	7	[4.24 .. 4.37]	4.000	1.18177e+10	4.000
8	2.75	1098.9	0.0251	34	3.03	1212.6	0.1807	60	4.12	1650.4	0.0367	86	4.34	1737.6	0.2059	8	[4.52 .. 4.58]	0.800	2.36251e+9	0.800
9	2.75	1102.1	0.0274	35	3.04	1217.7	0.0424	61	4.13	1651.6	0.0505	87	4.35	1741.7	0.1057	9	[4.58 .. 4.64]	0.913	2.69736e+9	0.913
10	2.77	1106.9	0.0387	36	3.05	1221.2	0.0919	62	4.14	1654.9	0.0457	88	4.36	1745.2	0.0562	10	[7.11 .. 7.15]	0.597	1.76300e+9	0.597
11	2.78	1112.4	0.0351	37	3.06	1225.5	0.1470	63	4.14	1657.5	0.0823	89	4.37	1748.7	0.0353	11	[7.15 .. 7.18]	0.761	2.24937e+9	0.761
12	2.79	1115.5	0.0393	38	3.08	1232.1	0.0475	64	4.15	1661.0	0.0689	90	4.38	1752.4	0.0539	12	[7.18 .. 7.26]	3.781	1.11700e+10	3.781
13	2.80	1121.4	0.0365	39	3.09	1234.6	0.0487	65	4.16	1664.7	0.0800	91	4.56	1825.5	0.0795	13	[7.26 .. 7.36]	3.800	1.12258e+10	3.800
14	2.84	1137.7	0.0255	40	3.10	1241.1	0.0348	66	4.17	1668.2	0.1178	92	4.60	1840.7	0.1164					
15	2.86	1143.6	0.0315	41	3.40	1359.6	0.0402	67	4.18	1671.9	0.0295	93	7.14	2855.6	0.1316					
16	2.86	1146.1	0.0317	42	3.44	1375.4	0.0558	68	4.19	1675.4	0.1178	94	7.15	2860.1	0.0405					
17	2.88	1151.6	0.0661	43	3.45	1382.2	0.0599	69	4.21	1682.6	0.0401	95	7.15	2862.2	0.1802					
18	2.89	1157.2	0.0621	44	3.46	1383.8	0.0558	70	4.24	1697.4	0.0261	96	7.16	2863.8	0.1348					
19	2.90	1159.6	0.0837	45	3.47	1389.6	0.0677	71	4.25	1700.4	0.0477	97	7.20	2880.0	0.1702					
20	2.91	1162.7	0.0271	46	3.49	1396.4	0.0643	72	4.26	1704.1	0.0587	98	7.21	2886.6	0.2875					
21	2.91	1165.4	0.0930	47	3.49	1398.0	0.0626	73	4.27	1707.6	0.1638	99	7.22	2888.1	0.2292					
22	2.92	1168.5	0.0475	48	3.51	1404.8	0.0519	74	4.28	1711.1	0.3103	100	7.23	2893.0	0.1629					
23	2.93	1172.4	0.0342	49	3.97	1590.4	0.0356	75	4.28	1713.2	0.2694	...	...	...	...					
24	2.94	1174.8	0.0440	50	3.99	1596.3	0.0376	76	4.29	1714.8	0.2330									
25	2.95	1178.7	0.0731	51	4.00	1599.8	0.0395	77	4.29	1718.3	0.1037									
26	2.95	1181.8	0.0297	52	4.01	1605.0	0.0558	78	4.30	1719.8	0.0274

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Acquisition Time (sec)	1.3566	Comment	111968X022	Date	May 31 2006
File Name	C:\Documents and Settings\DASSAK\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060531\1202				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10033.1191
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.95	1403.5	0.3451	17	126.78	12756.6	0.3317
2	14.03	1411.6	0.2351	18	126.87	12765.4	0.0764
3	34.10	3431.5	0.2979	19	127.02	12780.9	0.1002
4	34.27	3447.7	0.4220	20	128.48	12926.8	0.7202
5	43.39	4366.2	0.2570	21	128.64	12943.1	0.9085
6	43.53	4380.2	0.2471	22	128.67	12946.0	1.0000
7	62.74	6312.3	0.2375	23	128.79	12958.5	0.0685
8	63.01	6339.6	0.2022	24	137.72	13857.1	0.2535
9	64.85	6525.3	0.2839	25	138.03	13888.1	0.1759
10	65.15	6554.8	0.2877	26	139.98	14084.9	0.1218
11	67.76	6818.0	0.2110	27	141.16	14202.9	0.0896
12	69.10	6952.9	0.2863	28	164.27	16528.6	0.1536
13	76.68	7715.8	0.7318	29	164.81	16582.4	0.1139
14	77.00	7747.5	0.8118	30	170.43	17147.8	0.2015
15	77.32	7779.2	0.7665	31	171.62	17268.0	0.1570
16	126.69	12747.7	0.3022

7/5/2006 11:12 AM

Acquisition Time (sec)	5.1298	Comment	111968X020	Date	May 26 2006
File Name	C:\Program Files\Common Files\SYSTEMMSAPI\1033\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060526\2101				
Frequency (MHz)	400.11	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	30.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2443.1853	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.34	535.0	0.3574	17	3.04	1214.7	0.0572	33	4.12	1647.5	0.0576	49	4.37	1748.9	0.2288	1	[1.29 .. 1.44]	6.000	3.16172e+10	6.000
2	1.34	535.9	0.3350	18	3.05	1220.2	0.0694	34	4.13	1652.0	0.0597	50	4.38	1751.2	0.4419	2	[2.77 .. 2.88]	1.062	5.59692e+9	1.062
3	1.36	542.2	1.0000	19	3.06	1225.1	0.0704	35	4.14	1657.5	0.0858	51	4.38	1752.2	0.3913	3	[3.02 .. 3.13]	1.069	5.63442e+9	1.069
4	1.36	543.2	0.8570	20	3.07	1227.4	0.0681	36	4.15	1661.2	0.0630	52	4.39	1755.9	0.1612	4	[3.32 .. 3.43]	1.049	5.52508e+9	1.049
5	1.37	548.0	0.7825	21	3.07	1230.3	0.0817	37	4.16	1666.0	0.0573	53	4.39	1758.4	0.1735	5	[4.09 .. 4.20]	1.088	5.73228e+9	1.088
6	1.37	548.8	0.9337	22	3.08	1232.7	0.0702	38	4.18	1672.1	0.0489	54	4.40	1762.0	0.1291	6	[4.28 .. 4.49]	4.998	2.63382e+10	4.998
7	1.39	555.1	0.3812	23	3.09	1238.1	0.0553	39	4.31	1726.1	0.0543	55	4.42	1769.2	0.0770	7	[5.00 .. 5.08]	1.006	5.29940e+9	1.006
8	1.39	556.0	0.3439	24	3.11	1243.8	0.0531	40	4.32	1726.9	0.0499	56	4.42	1770.1	0.0751	8	[7.23 .. 7.31]	2.963	1.56126e+10	2.963
9	2.78	1113.2	0.0488	25	3.34	1336.4	0.0725	41	4.33	1730.8	0.0746	57	5.04	2015.8	0.7652	9	[7.31 .. 7.38]	1.994	1.05072e+10	1.994
10	2.80	1118.8	0.0570	26	3.35	1341.8	0.0755	42	4.33	1733.1	0.0831	58	7.25	2901.2	0.3430					
11	2.81	1123.1	0.0631	27	3.36	1346.3	0.0741	43	4.33	1734.5	0.1040	59	7.27	2908.8	0.6053					
12	2.82	1126.4	0.0755	28	3.38	1351.4	0.1055	44	4.34	1736.8	0.2822	60	7.29	2915.0	0.1540					
13	2.82	1128.4	0.0761	29	3.39	1356.1	0.0816	45	4.34	1737.8	0.2706	61	7.32	2930.1	0.2887					
14	2.83	1131.9	0.0746	30	3.40	1360.4	0.0808	46	4.35	1741.7	0.2120	62	7.34	2937.9	0.2843					
15	2.84	1136.2	0.0761	31	3.41	1366.0	0.0664	47	4.36	1744.0	0.5299	63	7.35	2940.2	0.2152					
16	2.85	1142.0	0.0677	32	4.10	1641.9	0.0527	48	4.36	1745.0	0.4797	64	7.36	2945.5	0.1143

7/5/2006 11:17 AM

Acquisition Time (sec)	1.3566	Comment	111968X020	Date	May 26 2006
File Name	C:\Documents and Settings\DASSAK\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060526\2102				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10021.3242
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.63	1371.1	0.6602	11	126.45	12722.7	0.3791
2	34.00	3421.1	0.3746	12	128.16	12895.2	0.0838
3	44.65	4493.0	0.3016	13	128.39	12918.7	1.0000
4	63.27	6366.1	0.3786	14	128.52	12931.3	0.9337
5	63.56	6395.6	0.2465	15	137.81	13866.0	0.2820
6	65.21	6561.5	0.2669	16	140.09	14095.3	0.1249
7	76.68	7715.9	0.1181	17	164.79	16581.0	0.2189
8	77.00	7747.5	0.1215	18	167.16	16819.1	0.2282
9	77.32	7780.0	0.1187	19	167.40	16843.4	0.1487
10	78.94	7942.9	0.2679

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Acquisition Time (sec)	5.1298	Comment	111968X028	Date	Jun 9 2006
File Name	C:\Program Files\Common Files\SYSTEMMSAPI\1033\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060609\3201				
Frequency (MHz)	400.11	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	38.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2400.6646	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.09	435.9	0.2350	16	4.14	1658.4	0.0433	31	4.28	1711.8	0.0915	46	7.08	2832.8	0.1350
2	1.11	443.1	0.4833	17	4.15	1660.4	0.1342	32	4.29	1715.5	0.0568	47	7.10	2839.4	0.1521
3	1.13	450.2	0.2354	18	4.16	1663.9	0.0407	33	4.30	1718.7	0.4049	48	7.24	2898.1	0.2665
4	1.19	477.4	0.4660	19	4.16	1665.4	0.0506	34	4.36	1745.4	0.4130	49	7.25	2902.7	0.2127
5	1.21	484.7	1.0000	20	4.17	1667.4	0.1365	35	4.37	1747.3	0.4387	50	7.27	2909.4	0.5952
6	1.23	491.9	0.5123	21	4.18	1672.5	0.0833	36	4.42	1768.2	0.2228	51	7.28	2912.7	0.3066
7	3.90	1558.8	0.1350	22	4.19	1674.6	0.0578	37	4.42	1769.7	0.2404	52	7.28	2914.4	0.3299
8	3.94	1575.0	0.1434	23	4.19	1676.0	0.0378	38	4.54	1816.1	0.2063	53	7.29	2916.0	0.2649
9	4.01	1603.2	0.0468	24	4.20	1679.7	0.0781	39	4.54	1817.7	0.2001	54	7.29	2917.8	0.4203
10	4.03	1610.5	0.0528	25	4.21	1683.2	0.0609	40	4.64	1857.5	0.3570	55	7.30	2921.8	0.2876
11	4.03	1614.0	0.0629	26	4.22	1690.4	0.0607	41	4.65	1859.6	0.3535	56	7.31	2926.7	0.1497
12	4.05	1621.2	0.0623	27	4.23	1693.9	0.0488	42	5.14	2056.7	0.2201	57	7.32	2930.6	0.0808
13	4.12	1649.6	0.0905	28	4.25	1701.1	0.1392	43	5.18	2071.9	0.2045	58	7.33	2931.6	0.0825
14	4.13	1653.2	0.0498	29	4.26	1703.4	0.3367	44	5.23	2092.8	0.1024				
15	4.14	1656.7	0.0912	30	4.27	1708.1	0.1285	45	5.27	2108.7	0.0981

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Acquisition Time (sec)	1.3566	Comment	111968X028	Date	Jun 9 2006
File Name	C:\Documents and Settings\DASSAK\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060609\3202				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10033.1191
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.72	1380.7	0.2529	15	127.18	12796.4	0.6632
2	13.94	1402.8	0.4491	16	127.93	12871.6	0.2578
3	45.03	4530.6	0.2668	17	127.99	12878.2	0.5783
4	45.61	4589.5	0.3021	18	128.38	12917.3	0.9297
5	62.76	6314.5	0.1980	19	128.85	12964.4	1.0000
6	62.98	6336.6	0.1527	20	135.59	13642.6	0.2252
7	63.75	6414.0	0.1713	21	135.94	13678.0	0.4244
8	64.14	6453.8	0.2576	22	140.65	14152.0	0.0871
9	67.61	6802.5	0.2650	23	141.84	14271.4	0.0391
10	69.25	6967.6	0.3863	24	164.55	16556.6	0.1674
11	76.68	7715.1	0.4966	25	165.14	16616.3	0.0512
12	77.00	7747.5	0.5347	26	170.40	17144.9	0.1368
13	77.32	7779.2	0.5107	27	171.58	17263.6	0.1709
14	126.86	12764.7	0.0632

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Acquisition Time (sec)	5.1298	Comment	111968X027	Date	Jun 7 2006
File Name	\\AACALVIN\ACDLabs\ACD80\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060607\2901				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	38.00	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2411.4092	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	1.20	480.2	0.3889	16	4.33	1731.9	0.2527	1	[1.19 .. 1.24]	3.186	1.33642e+10	3.186
2	1.22	487.4	0.7871	17	4.37	1747.7	0.2689	2	[1.25 .. 1.30]	3.308	1.38742e+10	3.308
3	1.24	494.4	0.4051	18	4.99	1996.3	1.0000	3	[4.04 .. 4.12]	0.952	3.99292e+9	0.952
4	1.26	504.8	0.4652	19	5.09	2036.4	0.2540	4	[4.12 .. 4.18]	2.276	9.54691e+9	2.276
5	1.28	512.0	0.9659	20	5.13	2052.0	0.2311	5	[4.26 .. 4.32]	2.284	9.58060e+9	2.284
6	1.30	519.2	0.4860	21	7.21	2883.3	0.2867	6	[4.32 .. 4.38]	1.231	5.16251e+9	1.231
7	4.09	1637.2	0.0703	22	7.22	2890.1	0.3684	7	[5.08 .. 5.14]	1.132	4.75010e+9	1.132
8	4.13	1650.8	0.1565	23	7.26	2903.4	0.0479	8	[7.19 .. 7.24]	2.126	8.91761e+9	2.126
9	4.14	1658.0	0.4328	24	7.27	2907.1	0.0350	9	[7.25 .. 7.35]	3.457	1.44986e+10	3.457
10	4.16	1665.3	0.4195	25	7.27	2908.8	0.2507					
11	4.18	1672.3	0.1398	26	7.27	2910.6	0.1641					
12	4.26	1705.6	0.1564	27	7.29	2917.4	0.1793					
13	4.28	1712.6	0.4659	28	7.31	2923.8	0.3358					
14	4.30	1719.8	0.4616	29	7.33	2931.0	0.3311					
15	4.32	1727.1	0.1548	30	7.34	2937.9	0.1027

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Acquisition Time (sec)	1.3566	Comment	111968X027	Date	Jun 7 2006
File Name	C:\Documents and Settings\DASSAK\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20060607\2902				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Receiver Gain	50.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	10033.8564
Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	13.61	1369.6	0.3490	10	79.22	7970.9	0.3615
2	13.74	1382.2	0.4184	11	127.63	12841.3	0.9093
3	47.05	4734.0	0.2707	12	128.21	12900.3	0.0870
4	63.32	6371.3	0.3140	13	128.67	12946.8	1.0000
5	63.76	6415.5	0.2943	14	136.31	13715.6	0.2325
6	65.01	6540.8	0.3432	15	141.02	14188.9	0.1323
7	76.68	7715.1	0.3337	16	165.63	16665.7	0.2143
8	77.00	7747.5	0.3430	17	166.92	16795.5	0.1488
9	77.32	7779.2	0.3404	18	167.55	16858.9	0.1390