Supporting Information for

Efficient Synthesis of Novel γ -substituted γ -butenolides by Lewis Acid Catalyzed Addition Metal Enolates of Active Methylene Compounds to Mucohalic Acids

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^1H and ^{13}C NMR data of the compounds	S2 – S39
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Acquisition Time (sec)	5.1188	Comment	86198X105	Date	Jan 21 2005
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20050121\3701				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	1.21	484.0	0.3650	17	2.01	802.9	0.0532	33	4.23	1691.0	0.1044	1	[1.18 .. 1.32]	6.947	2.65242e+9
2	1.22	486.2	0.2157	18	3.92	1567.7	0.2359	34	4.23	1693.5	0.2153	2	[3.90 .. 3.95]	1.017	3.88272e+8
3	1.23	491.1	1.0000	19	3.92	1568.7	0.2455	35	4.24	1694.7	0.1005	3	[4.14 .. 4.31]	4.509	1.72141e+9
4	1.23	492.2	0.3139	20	3.93	1572.2	0.2419	36	4.24	1695.7	0.1070	4	[5.52 .. 5.60]	1.000	3.81803e+8
5	1.23	493.2	0.4882	21	3.93	1573.2	0.2414	37	4.24	1697.8	0.1775				
6	1.24	496.7	0.0869	22	4.17	1669.7	0.0564	38	4.25	1699.0	0.0805				
7	1.25	498.3	0.4349	23	4.18	1671.1	0.0866	39	4.25	1700.6	0.2083				
8	1.25	500.1	0.5996	24	4.18	1672.6	0.0611	40	4.26	1702.7	0.0986				
9	1.26	502.2	0.2491	25	4.19	1676.7	0.1858	41	4.26	1705.1	0.1528				
10	1.26	504.0	0.0464	26	4.19	1678.1	0.2319	42	4.27	1707.0	0.0943				
11	1.27	507.3	0.9308	27	4.20	1680.5	0.1132	43	4.27	1707.8	0.0943				
12	1.27	509.2	0.4688	28	4.21	1682.6	0.0452	44	4.28	1712.1	0.0515				
13	1.29	514.3	0.4267	29	4.21	1684.0	0.1811	45	5.55	2221.6	0.2901				
14	1.29	515.5	0.1612	30	4.21	1685.3	0.2485	46	5.56	2222.8	0.2545				
15	1.29	516.5	0.2458	31	4.21	1686.3	0.1931	47	5.56	2226.1	0.2651				
16	2.00	800.5	0.1059	32	4.22	1687.7	0.1228	48	5.57	2227.3	0.2580				

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Acquisition Time (sec)	1.3570	Comment	86198X105	Date	Jan 21 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20050121\3702				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.13	1421.7	0.8497
2	52.85	5317.9	0.5646
3	62.89	6328.2	0.6777
4	78.98	7947.3	1.0000
5	122.87	12363.0	0.1161
6	149.66	15058.8	0.1867
7	164.24	16525.3	0.3544
8	164.96	16597.5	0.3585

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	1.18	470.9	0.4550	18	3.99	1596.7	0.8501	35	5.25	2098.3	0.3822	1	[1.16 .. 1.33]	3.537	1.53439e+10
2	1.20	477.9	0.9815	19	4.03	1611.9	0.1893	36	5.57	2224.8	0.3853	2	[3.93 .. 3.96]	0.162	7.03761e+8
3	1.21	485.1	0.8691	20	4.04	1616.4	0.1974	37	5.57	2228.3	0.4964	3	[3.96 .. 4.01]	0.715	3.10023e+9
4	1.23	491.9	1.0000	21	4.18	1672.7	0.2002	38	5.58	2229.3	0.4748	4	[4.01 .. 4.06]	0.198	8.60333e+8
5	1.24	496.6	0.1968	22	4.19	1674.3	0.2070	39	5.59	2232.8	0.4416	5	[4.14 .. 4.32]	2.151	9.33011e+9
6	1.25	499.1	0.4836	23	4.20	1679.7	0.2024	40	7.25	2900.1	0.9890	6	[5.13 .. 5.27]	2.117	9.18147e+9
7	1.25	499.9	0.4875	24	4.21	1681.9	0.2343	41	7.32	2925.6	0.2049	7	[5.54 .. 5.60]	1.000	4.33752e+9
8	1.26	503.8	0.4341	25	4.23	1689.1	0.2828	42	7.33	2928.5	0.3816	8	[7.27 .. 7.42]	4.716	2.04549e+10
9	1.27	506.9	0.1807	26	4.23	1692.0	0.1956	43	7.33	2931.1	0.3231				
10	1.28	511.0	0.1883	27	4.24	1696.1	0.2426	44	7.33	2932.2	0.3464				
11	1.28	512.4	0.1896	28	4.25	1699.2	0.1904	45	7.34	2933.8	0.3625				
12	1.30	519.6	0.4202	29	5.16	2061.8	0.3125	46	7.34	2935.3	0.3109				
13	1.32	526.8	0.1897	30	5.19	2075.3	0.3847	47	7.35	2939.8	0.8736				
14	2.03	813.4	0.5224	31	5.20	2077.0	0.3976	48	7.36	2941.8	0.7141				
15	3.94	1574.6	0.1804	32	5.20	2079.2	0.2548	49	7.37	2945.5	0.2133				
16	3.95	1579.1	0.1744	33	5.20	2080.3	0.2262								
17	3.98	1592.2	0.8397	34	5.23	2091.6	0.3796								

Acquisition Time (sec)	1.3570	Comment	86198X77	Date	Dec 16 2004
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20041216\3503				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.06	1414.3	0.2357	13	122.97	12373.4	0.0621
2	52.78	5310.5	0.4995	14	128.73	12952.6	0.4486
3	52.92	5324.5	0.3358	15	128.83	12962.9	0.7624
4	62.89	6327.5	0.1975	16	128.91	12970.3	0.8972
5	62.98	6337.1	0.1534	17	128.98	12977.7	0.5015
6	68.42	6884.6	0.3365	18	134.68	13551.7	0.1040
7	68.50	6892.7	0.3948	19	149.57	15049.2	0.1364
8	76.93	7740.2	0.9442	20	164.06	16507.6	0.1377
9	77.25	7772.7	1.0000	21	164.18	16519.4	0.1687
10	77.56	7804.3	0.9622	22	164.39	16540.8	0.1055
11	78.89	7937.7	0.1303	23	164.79	16580.6	0.1817
12	78.94	7942.9	0.3242	24	164.87	16588.7	0.1413

Acquisition Time (sec)	5.1298	Comment	86198X38	Date	Nov 19 2004
File Name	C:\Documents and Settings\dassak\Desktop\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041119\3101				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	6387.74
Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	4.03	1610.8	0.4097	15	7.27	2910.5	0.1762	1	[4.01 .. 4.06]	1.000	3.91940e+9
2	4.04	1615.3	0.4139	16	7.28	2914.4	0.2121	2	[5.12 .. 5.18]	2.206	8.64681e+9
3	4.69	1874.6	0.1281	17	7.29	2915.4	0.1908	3	[5.18 .. 5.22]	2.002	7.84743e+9
4	5.15	2060.8	1.0000	18	7.29	2918.3	0.2878	4	[5.53 .. 5.59]	1.006	3.94481e+9
5	5.19	2077.9	0.5919	19	7.30	2922.0	0.0797	5	[7.22 .. 7.31]	4.212	1.65076e+10
6	5.20	2079.7	0.5913	20	7.31	2925.6	0.0970	6	[7.31 .. 7.38]	6.531	2.55980e+10
7	5.56	2223.0	0.4533	21	7.32	2927.9	0.2864				
8	5.57	2227.5	0.4315	22	7.32	2929.5	0.6761				
9	7.24	2898.3	0.2820	23	7.33	2931.4	0.8853				
10	7.25	2901.0	0.1589	24	7.33	2934.1	0.6961				
11	7.25	2902.5	0.1784	25	7.34	2936.1	0.6210				
12	7.26	2903.9	0.2049	26	7.34	2938.0	0.4307				
13	7.26	2906.4	0.2549	27	7.35	2940.2	0.1929				
14	7.27	2908.2	0.1737	28	7.36	2944.7	0.1229				

Acquisition Time (sec)	1.3566	Comment	86198X38	Date	Nov 19 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041119\3102				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	52.79	5311.5	0.4302
2	68.54	6896.4	0.2961
3	68.61	6903.1	0.4472
4	76.94	7741.2	0.2420
5	77.25	7772.9	0.2457
6	77.57	7805.4	0.2401
7	78.89	7938.1	0.5958
8	123.03	12379.5	0.0699
9	128.74	12953.7	0.7933
10	128.82	12961.8	1.0000
11	128.92	12971.4	0.7313
12	128.98	12978.0	0.3835
13	134.47	13530.2	0.1405
14	134.57	13540.5	0.0891
15	149.37	15029.5	0.0792
16	164.26	16527.5	0.0690
17	164.71	16573.2	0.2520

Acquisition Time (sec)	5.1212	Comment	86198X90	Date	Jan 7 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20050107\1101				
Frequency (MHz)	399.90	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6398.46	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	1.24	494.6	0.3159
2	1.25	498.3	0.3459
3	1.25	501.8	0.7707
4	1.26	505.5	0.7289
5	1.27	509.0	0.3204
6	1.28	512.5	0.3313
7	1.43	573.3	1.0000
8	4.19	1677.3	0.1059
9	4.21	1684.6	0.3476
10	4.23	1691.6	0.3051
11	4.24	1694.9	0.1304
12	4.25	1697.6	0.1421
13	4.25	1698.8	0.1122
14	4.26	1701.9	0.1384
15	5.74	2294.0	0.4624
16	7.23	2893.3	0.2114

No.	(ppm)	Value	Absolute Value
1	[1.20 .. 1.31]	6.137	2.19224e+9
2	[1.41 .. 1.46]	3.000	1.07161e+9
3	[4.14 .. 4.31]	4.112	1.46896e+9
4	[5.70 .. 5.77]	0.883	3.15393e+8

Acquisition Time (sec)	1.3578	Comment	86198X90	Date	Jan 7 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20050107\1102				
Frequency (MHz)	100.57	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24132.73	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.06	1413.6	0.5616
2	14.09	1417.3	0.3298
3	15.40	1548.4	0.6474
4	56.73	5705.2	0.4275
5	62.76	6311.3	0.4698
6	62.96	6331.9	0.3538
7	76.89	7732.8	0.8396
8	77.21	7765.2	0.9549
9	77.53	7796.8	0.9142
10	82.96	8343.3	1.0000
11	123.36	12405.8	0.1717
12	150.10	15094.8	0.2229
13	164.39	16532.4	0.2333
14	167.21	16816.0	0.1931

Acquisition Time (sec)	5.1188	Comment	86198X78	Date	Dec 15 2004
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20041215\2601				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	1.27	506.7	0.0991
2	1.30	521.2	0.4389
3	1.32	528.4	0.9451
4	1.32	529.9	0.1513
5	1.34	534.6	1.0000
6	1.35	541.7	0.4582
7	1.54	614.9	0.3248
8	4.33	1733.8	0.1018
9	4.34	1736.3	0.2418
10	4.34	1737.3	0.2432

No.	(ppm)	(Hz)	Height
11	4.35	1738.9	0.2449
12	4.35	1741.2	0.2165
13	4.36	1743.4	0.2335
14	4.36	1744.3	0.2388
15	4.36	1745.9	0.2502
16	4.37	1748.4	0.2077
17	4.38	1751.6	0.0910
18	6.02	2407.2	0.5260
19	7.24	2898.7	0.4131

No.	(ppm)	Value	Absolute Value
1	[1.27 .. 1.39]	7.882	2.68254e+9
2	[4.28 .. 4.42]	5.179	1.76277e+9
3	[5.98 .. 6.08]	1.000	3.40354e+8

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Acquisition Time (sec)	1.3570	Comment	86198X78	Date	Dec 15 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20041215\2602				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.00	1408.4	0.1480
2	14.05	1413.6	0.1605
3	64.67	6506.6	0.1716
4	64.81	6521.3	0.1190
5	70.80	7124.1	0.0979
6	76.90	7737.3	0.9202
7	77.22	7769.7	0.9933
8	77.53	7801.4	1.0000
9	82.39	8290.0	0.3858
10	125.06	12583.4	0.0640
11	147.81	14872.3	0.0824
12	162.90	16391.2	0.0683
13	163.65	16466.3	0.0734

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Acquisition Time (sec)	5.1298	Comment	86198X33	Date	Nov 11 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041111\2401				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	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
1	0.99	396.7	0.0409	19	2.17	869.7	0.1387	37	4.19	1677.3	0.1004	1	[0.97 .. 1.08]	2.882	1.36686e+10
2	1.01	403.0	0.3251	20	2.19	877.5	0.1399	38	4.20	1679.9	0.0823	2	[1.16 .. 1.32]	6.000	2.84550e+10
3	1.03	410.6	0.7820	21	2.21	885.1	0.1228	39	4.20	1681.0	0.0680	3	[2.08 .. 2.29]	1.935	9.17729e+9
4	1.04	418.0	0.3482	22	2.23	891.9	0.0566	40	4.21	1683.4	0.0679	4	[4.05 .. 4.34]	4.036	1.91389e+10
5	1.19	477.4	0.4328	23	2.25	899.5	0.0441	41	4.21	1684.5	0.0880	5	[5.50 .. 5.56]	0.848	4.02312e+9
6	1.21	484.5	1.0000	24	4.08	1633.7	0.0356	42	4.22	1687.1	0.0746				
7	1.22	488.9	0.0494	25	4.10	1640.9	0.0377	43	4.22	1688.2	0.1720				
8	1.23	491.7	0.5095	26	4.12	1648.5	0.0615	44	4.24	1695.3	0.1598				
9	1.24	496.2	0.0850	27	4.13	1652.2	0.0580	45	4.24	1696.8	0.0722				
10	1.25	499.3	0.0684	28	4.14	1655.7	0.0642	46	4.25	1702.5	0.0579				
11	1.25	501.0	0.4769	29	4.15	1659.4	0.1782	47	4.26	1704.0	0.1702				
12	1.26	503.2	0.0848	30	4.15	1661.9	0.0735	48	4.28	1711.2	0.1487				
13	1.27	508.2	0.9861	31	4.16	1666.4	0.1768	49	4.29	1714.8	0.0759				
14	1.29	515.3	0.4448	32	4.17	1669.1	0.1919	50	4.29	1718.3	0.0515				
15	2.01	806.1	0.1735	33	4.18	1671.5	0.0382	51	4.30	1722.0	0.0740				
16	2.12	847.8	0.0460	34	4.18	1672.5	0.0480	52	5.53	2212.1	0.4917				
17	2.14	855.2	0.0665	35	4.18	1673.6	0.0704								
18	2.16	862.3	0.1277	36	4.19	1676.2	0.1719								

Acquisition Time (sec)	1.3570	Comment	86198X93	Date	Jan 8 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20050108\0102				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	9.40	945.6	0.3136
2	14.17	1426.1	0.4327
3	26.82	2698.1	0.4707
4	53.78	5410.8	0.1738
5	61.23	6161.0	0.4283
6	62.50	6288.5	0.4199
7	82.53	8304.0	0.8436
8	122.56	12332.1	0.1723
9	151.47	15240.8	0.2144
10	166.78	16781.0	0.3014
11	167.64	16868.0	0.1617
12	169.66	17071.4	0.1470

21 Feb 2005

Acquisition Time (sec)	5.1188	Comment	86198X97-1	Date	Jan 19 2005
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20050119\1601				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	DMSO-D6	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	3.62	1447.4	1.0000	1	[3.57 .. 3.66]	2.330	7.20722e+8
2	7.11	2844.2	0.7022	2	[7.02 .. 7.23]	1.000	3.09288e+8
3	12.89	5156.8	0.0094	3	[12.65 .. 13.19]	1.218	3.76710e+8

21 Feb 2005

Acquisition Time (sec)	1.3025	Comment	86198X28-1	Date	Nov 5 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20041105\2902				
Frequency (MHz)	100.53	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	DMSO-D6	Sweep Width (Hz)	25157.23	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	39.59	3979.8	0.1386
2	39.79	4000.5	0.4315
3	40.00	4021.3	0.8613
4	40.21	4042.8	1.0000
5	40.42	4063.5	0.8705
6	40.63	4084.2	0.4237
7	40.84	4105.7	0.1381
8	41.66	4187.9	0.5573
9	92.73	9322.7	0.6966
10	123.98	12464.3	0.1690
11	147.92	14871.3	0.1605
12	165.85	16674.0	0.1455
13	167.60	16849.8	0.1418

Acquisition Time (sec)	5.1298	Comment	86198X39	Date	Nov 16 2004
File Name	C:\Program Files\Common Files\System\WAPI\1033\int\BARTON.CHEMISTRY-AA.WL.COMSAMBA\20041116\3401				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	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
1	0.84	337.3	0.2923	17	1.37	548.6	0.0688	33	4.18	1671.1	0.0792	1	[0.81 .. 0.90]	3.000	1.59325e+10
2	0.86	344.3	0.7494	18	1.66	665.2	0.0672	34	4.25	1700.5	0.0870	2	[1.18 .. 1.42]	10.930	5.80455e+10
3	0.88	350.9	0.2503	19	1.67	669.1	0.0751	35	4.25	1701.9	0.1669	3	[1.60 .. 1.76]	2.114	1.12276e+10
4	1.21	485.8	0.3013	20	1.68	673.2	0.0831	36	4.26	1703.8	0.0673	4	[2.00 .. 2.05]	1.004	5.33409e+9
5	1.23	493.0	0.6767	21	1.69	675.9	0.1421	37	4.26	1705.4	0.0948	5	[4.05 .. 4.13]	0.738	3.91799e+9
6	1.25	500.3	0.6478	22	1.70	680.0	0.0851	38	4.27	1707.2	0.1049	6	[4.14 .. 4.19]	0.710	3.76855e+9
7	1.25	501.4	0.4490	23	1.71	683.9	0.1414	39	4.27	1708.7	0.0676	7	[4.22 .. 4.28]	0.794	4.21456e+9
8	1.26	502.8	0.4572	24	1.73	690.7	0.1037	40	4.28	1714.2	0.1985	8	[4.28 .. 4.34]	1.258	6.67888e+9
9	1.26	506.1	0.4251	25	2.02	806.7	1.0000	41	4.30	1721.0	0.3241	9	[5.52 .. 5.55]	0.281	1.49094e+9
10	1.27	508.6	0.4246	26	3.43	1371.3	0.2057	42	4.32	1727.8	0.1544	10	[5.55 .. 5.58]	0.540	2.86575e+9
11	1.28	513.3	0.3398	27	4.07	1626.8	0.0753	43	5.53	2212.3	0.1484				
12	1.30	519.9	0.2333	28	4.08	1634.0	0.2125	44	5.54	2215.8	0.1474				
13	1.34	535.3	0.1312	29	4.10	1641.1	0.2106	45	5.56	2224.3	0.3031				
14	1.35	540.4	0.1106	30	4.12	1648.3	0.0731	46	5.57	2226.9	0.3089				
15	1.36	543.7	0.1062	31	4.15	1662.1	0.1721								
16	1.36	544.9	0.1053	32	4.16	1664.5	0.1952								

Acquisition Time (sec)	1.3566	Comment	86198X39	Date	Nov 16 2004
File Name	C:\WINNT\system32\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041116\3402				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	24154.59
Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.26	1434.8	0.9970	12	76.92	7739.8	0.4546
2	22.80	2294.3	0.5657	13	77.24	7771.5	0.4494
3	25.78	2593.6	0.6355	14	77.55	7803.1	0.4041
4	28.39	2856.8	0.3715	15	78.31	7879.1	0.4302
5	28.44	2862.0	0.4410	16	110.48	11116.0	0.0774
6	29.22	2940.1	0.3993	17	124.57	12534.3	0.0474
7	29.26	2944.5	1.0000	18	147.39	14829.8	0.0457
8	31.91	3210.6	0.8998	19	161.29	16228.9	0.1595
9	40.63	4088.6	0.3205	20	161.91	16290.8	0.0663
10	40.72	4096.7	0.5315	21	163.21	16421.3	0.0318
11	68.85	6927.4	0.3658	22	171.33	17238.8	0.0562

Acquisition Time (sec)	5.1188	Comment	86198X31	Date	Nov 10 2004
File Name	C:\Documents and Settings\dassak\Desktop\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041110\2501				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D			Sweep Width (Hz)	6401.54
Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	1.28	511.4	0.4908	12	3.86	1543.3	0.0476	1	[1.24 .. 1.35]	3.328	3.30006e+9
2	1.30	518.6	1.0000	13	3.87	1550.3	0.1417	2	[3.73 .. 3.97]	2.218	2.19971e+9
3	1.31	525.6	0.5122	14	3.88	1552.5	0.0692	3	[5.76 .. 5.83]	1.000	9.91586e+8
4	3.75	1500.3	0.0288	15	3.89	1557.4	0.1410				
5	3.77	1507.4	0.0847	16	3.90	1559.7	0.1288				
6	3.77	1509.3	0.0619	17	3.91	1564.4	0.0482				
7	3.78	1514.4	0.0863	18	3.92	1566.7	0.1023				
8	3.79	1516.5	0.1413	19	3.93	1573.8	0.0296				
9	3.80	1521.4	0.0332	20	5.79	2317.1	0.6524				
10	3.81	1523.8	0.1313	21	7.24	2898.2	0.0816				
11	3.83	1530.8	0.0432								

Acquisition Time (sec)	1.3025	Comment	86198X31	Date	Nov 10 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041110\2502				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	25157.23	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	15.09	1517.9	1.0000
2	66.32	6673.4	0.4064
3	76.91	7738.3	0.2790
4	76.95	7742.9	0.1154
5	77.23	7770.5	0.2715
6	77.27	7775.1	0.1038
7	77.54	7802.0	0.2610
8	77.59	7806.6	0.0961
9	101.03	10165.2	0.4705
10	123.66	12442.4	0.0314
11	124.46	12523.0	0.0549
12	147.67	14858.5	0.0611
13	163.44	16445.5	0.1674

Acquisition Time (sec)	5.1188	Comment	86198X75	Date	Dec 14 2004
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20041214\3101				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.22	486.8	0.4684	16	4.22	1686.5	0.1940
2	1.23	493.8	0.9807	17	4.23	1690.8	0.0693
3	1.25	501.0	0.4905	18	4.23	1693.5	0.0646
4	1.27	507.7	0.4592	19	4.24	1695.5	0.0678
5	1.29	514.9	1.0000	20	4.24	1697.8	0.0727
6	1.30	522.1	0.4602	21	4.26	1702.5	0.1992
7	1.31	526.0	0.0653	22	4.26	1705.1	0.2051
8	1.35	541.1	0.0604	23	4.27	1709.8	0.1934
9	3.95	1580.4	0.3580	24	4.28	1712.3	0.1979
10	3.96	1584.7	0.3549	25	4.29	1716.8	0.0682
11	4.17	1669.5	0.0643	26	4.30	1719.3	0.0617
12	4.18	1672.0	0.0663	27	5.55	2219.9	0.4346
13	4.19	1676.7	0.1904	28	5.56	2224.2	0.4015
14	4.20	1679.3	0.2007	29	7.24	2898.6	0.1796
15	4.21	1683.8	0.2009				

Acquisition Time (sec)	1.3570	Comment	86198X75	Date	Dec 14 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20041214\3102				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.15	1423.9	0.5433
2	53.09	5342.2	0.6143
3	62.70	6308.4	0.4646
4	62.93	6331.9	0.3527
5	76.91	7738.8	0.8794
6	77.23	7771.2	1.0000
7	77.55	7802.9	0.9471
8	81.72	8222.2	0.4984
9	116.95	11767.6	0.2396
10	144.54	14543.7	0.1695
11	164.24	16525.3	0.4500
12	165.07	16609.3	0.1638
13	165.40	16641.7	0.1194

Acquisition Time (sec)	5.1188	Comment	86198X32	Date	Nov 10 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041110\2601				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	1.20	481.1	0.6591	12	4.10	1640.0	0.0501	1	[1.19 .. 1.28]	12.885	1.95998e+9
2	1.21	485.4	0.7152	13	5.02	2010.4	0.0534	2	[3.85 .. 3.93]	0.988	1.50320e+8
3	1.22	487.4	0.7766	14	5.04	2016.7	0.1235	3	[4.99 .. 5.16]	2.185	3.32415e+8
4	1.22	489.3	0.2068	15	5.06	2022.9	0.1584	4	[5.51 .. 5.60]	1.000	1.52119e+8
5	1.23	491.7	0.7983	16	5.07	2029.2	0.1207				
6	1.24	495.6	0.1636	17	5.09	2034.6	0.1340				
7	1.25	499.1	1.0000	18	5.10	2040.9	0.1526				
8	1.26	505.3	0.9741	19	5.12	2047.2	0.1096				
9	2.01	805.4	0.2409	20	5.54	2217.9	0.3832				
10	3.88	1552.7	0.3221	21	5.55	2222.0	0.3488				
11	3.89	1557.0	0.3723	22	7.24	2898.2	0.1384				

Acquisition Time (sec)	1.3025	Comment	86198X32	Date	Nov 10 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\BARTON.CHEMISTRY.AA.WL.COM\SAMBA\20041110\2602				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	25157.23	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	21.24	2136.7	0.0548
2	21.69	2182.8	1.0000
3	21.75	2188.9	0.8717
4	21.85	2198.1	0.0645
5	21.88	2202.0	0.0892
6	53.24	5356.7	0.9399
7	70.76	7120.2	0.3367
8	70.88	7131.7	0.5019
9	76.91	7739.0	0.4379
10	77.24	7771.3	0.4241
11	77.55	7802.8	0.4315
12	78.56	7904.1	0.0410
13	79.08	7957.1	0.5938
14	122.84	12360.2	0.1193
15	149.81	15073.5	0.1112
16	163.81	16482.3	0.5636
17	164.53	16554.5	0.5380

Acquisition Time (sec)	5.1188	Comment	86198X83	Date	Dec 22 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20041222\2801				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	1.18	472.9	0.7887	13	2.00	801.1	0.4308	1	[1.15 .. 1.22]	6.918	2.06233e+9
2	1.19	477.8	0.8392	14	3.90	1560.3	0.4169	2	[1.23 .. 1.29]	6.996	2.08561e+9
3	1.20	479.1	0.8972	15	3.91	1564.2	0.4254	3	[3.87 .. 3.95]	1.013	3.01875e+8
4	1.21	484.0	0.8116	16	5.01	2005.9	0.1283	4	[4.97 .. 5.15]	2.112	6.29643e+8
5	1.22	487.4	0.2622	17	5.03	2012.4	0.1743	5	[5.49 .. 5.58]	1.000	2.98131e+8
6	1.24	494.4	0.1529	18	5.05	2018.6	0.1307				
7	1.24	497.9	0.9871	19	5.08	2032.9	0.1307				
8	1.26	504.2	1.0000	20	5.10	2039.1	0.1767				
9	1.27	507.1	0.1639	21	5.11	2045.4	0.1324				
10	1.28	513.3	0.1177	22	5.52	2209.7	0.4325				
11	1.31	525.3	0.0998	23	5.53	2213.6	0.4302				
12	1.33	531.5	0.1016								

Acquisition Time (sec)	1.3570	Comment	86198X83	Date	Dec 22 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20041222\2802				
Frequency (MHz)	100.62	Nucleus	13C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	21.67	2180.8	0.6844
2	21.72	2185.2	0.5180
3	21.78	2191.1	0.4610
4	53.39	5372.4	0.9483
5	70.60	7103.5	0.5365
6	70.88	7132.2	0.5034
7	76.94	7741.7	0.4706
8	77.26	7773.4	0.4514
9	77.58	7805.8	0.4296
10	81.80	8231.0	1.0000
11	116.88	11760.2	0.3610
12	144.76	14565.8	0.3898
13	163.80	16481.1	0.3266
14	164.66	16567.3	0.2774
15	165.48	16650.6	0.2927

Acquisition Time (sec)	5.1298	Comment	86198X88	Date	Jan 5 2005
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20050105\3401				
Frequency (MHz)	399.77	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	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
1	1.16	464.2	0.2011	16	4.02	1606.0	0.7727	31	4.24	1695.5	0.1708	1	[1.11 .. 1.35]	4.135	1.54278e+10
2	1.18	471.5	0.4024	17	4.06	1621.2	0.1222	32	4.26	1702.9	0.0901	2	[3.96 .. 3.98]	0.139	5.17722e+8
3	1.20	478.7	0.2100	18	4.07	1625.5	0.1273	33	5.14	2053.2	0.1458	3	[3.99 .. 4.03]	0.727	2.71243e+9
4	1.20	479.4	0.1997	19	4.09	1636.0	0.1147	34	5.17	2067.1	0.3909	4	[4.04 .. 4.07]	0.135	5.05067e+8
5	1.21	482.4	0.2306	20	4.09	1637.0	0.1043	35	5.20	2078.8	0.1813	5	[4.07 .. 4.37]	2.804	1.04630e+10
6	1.23	489.8	0.5602	21	4.11	1643.3	0.1143	36	5.23	2091.4	0.2325	6	[5.09 .. 5.27]	2.119	7.90534e+9
7	1.24	496.8	0.5498	22	4.11	1644.2	0.1054	37	5.24	2094.6	0.2989	7	[5.50 .. 5.61]	1.000	3.73110e+9
8	1.26	503.0	0.2244	23	4.16	1662.4	0.1046	38	5.55	2216.8	0.1676	8	[7.27 .. 7.44]	4.868	1.81621e+10
9	1.28	509.9	0.0914	24	4.16	1664.3	0.1516	39	5.56	2220.9	0.3613				
10	1.29	517.1	0.1532	25	4.18	1669.6	0.1217	40	5.56	2224.6	0.2056				
11	2.02	808.7	0.4475	26	4.18	1671.5	0.1668	41	7.25	2900.1	0.2704				
12	2.03	809.7	0.3852	27	4.19	1677.0	0.0874	42	7.30	2916.8	0.1550				
13	3.96	1584.6	0.1110	28	4.20	1679.5	0.1182	43	7.32	2924.6	0.3628				
14	3.97	1588.7	0.1131	29	4.20	1680.7	0.1146	44	7.32	2926.6	0.3694				
15	4.01	1601.9	0.7806	30	4.22	1688.3	0.1835	45	7.35	2937.5	1.0000				

Acquisition Time (sec)	1.4205	Comment	86198X88	Date	Jan 5 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20050105\3402				
Frequency (MHz)	100.53	Nucleus	13C	Number of Transients	512
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	23068.05	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.10	1417.9	0.4507	13	68.44	6880.3	0.0579	25	129.10	12979.1	0.0908
2	14.18	1425.7	0.0926	14	68.48	6884.5	0.2150	26	134.64	13535.9	0.1577
3	14.43	1450.3	0.0932	15	68.56	6893.0	0.0532	27	134.74	13545.8	0.0840
4	21.26	2137.4	0.0757	16	76.99	7739.9	0.0943	28	144.57	14534.2	0.0390
5	52.92	5320.2	0.1815	17	81.63	8206.6	0.1361	29	164.07	16494.1	0.2973
6	53.11	5339.2	0.1800	18	81.67	8210.1	0.6302	30	164.19	16506.1	0.0455
7	60.59	6091.1	0.0725	19	81.73	8216.5	0.1462	31	164.26	16513.2	0.0821
8	62.69	6302.3	0.0695	20	116.98	11760.4	0.0519	32	164.92	16580.0	0.1281
9	62.78	6311.5	0.1865	21	128.72	12940.3	0.3874	33	165.00	16587.8	0.2150
10	62.93	6326.2	0.0828	22	128.82	12950.2	0.0613	34	165.09	16596.9	0.0591
11	62.98	6331.9	0.2640	23	128.89	12957.9	1.0000	35	165.28	16615.9	0.0574
12	68.33	6869.0	0.2097	24	128.96	12965.0	0.4588	36	165.35	16623.0	0.1286

Acquisition Time (sec)	5.1188	Comment	86198X82	Date	Dec 22 2004
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20041222\2701				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	1.26	502.4	0.4899
2	1.27	509.6	0.9978
3	1.29	516.7	0.5123
4	1.43	571.0	1.0000
5	4.23	1691.6	0.2044
6	4.25	1698.6	0.2696
7	5.77	2310.1	0.4289
8	7.24	2898.4	0.5073

No.	(ppm)	Value	Absolute Value
1	[1.22 .. 1.33]	6.552	1.61915e+9
2	[1.39 .. 1.47]	3.300	8.15505e+8
3	[4.16 .. 4.31]	4.369	1.07982e+9
4	[5.72 .. 5.81]	1.000	2.47136e+8

Acquisition Time (sec)	1.3570	Comment	86198X82	Date	Dec 22 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20041222\2702				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.12	1420.2	0.1519
2	15.26	1535.2	0.1533
3	56.95	5730.6	0.1091
4	62.96	6334.9	0.1737
5	85.52	8604.7	0.3019
6	116.81	11753.6	0.0635
7	144.73	14562.1	0.0714
8	165.33	16635.1	0.0680
9	167.31	16834.1	0.0533
10	167.60	16863.5	0.1100

Acquisition Time (sec)	5.1188	Comment	86198X84	Date	Dec 24 2004
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20041224\1201				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	DMSO-D6	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	2.47	988.1	0.1614
2	2.47	989.8	0.1204
3	3.21	1285.4	0.1991
4	3.60	1442.3	1.0000
5	7.08	2834.1	0.7175
6	12.95	5181.8	0.0096

No.	(ppm)	Value	Absolute Value
1	[3.54 .. 3.67]	2.463	1.72261e+9
2	[7.05 .. 7.13]	1.000	6.99282e+8
3	[12.75 .. 13.21]	1.089	7.61611e+8

Acquisition Time (sec)	1.3570	Comment	86198X84	Date	Dec 24 2004
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20041224\1202				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	DMSO-D6	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	39.57	3981.8	0.1608
2	39.78	4002.5	0.4264
3	39.98	4023.1	0.8549
4	40.20	4044.5	1.0000
5	40.40	4065.1	0.8237
6	40.61	4086.5	0.4296
7	40.83	4107.9	0.1311
8	41.67	4192.6	0.1595
9	94.96	9554.6	0.2181
10	118.51	11923.8	0.1030
11	144.43	14531.9	0.0934
12	165.87	16689.6	0.1941
13	167.65	16868.7	0.2029

Acquisition Time (sec)	5.1188	Comment	86198X140-1	Date	Feb 22 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20050222\1601				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	1.52	607.7	0.9657
2	1.54	615.1	1.0000
3	3.59	1437.8	0.0599
4	3.60	1441.7	0.0498
5	3.61	1445.0	0.2166
6	3.62	1448.9	0.1883
7	3.63	1452.5	0.2015
8	3.64	1456.2	0.1720
9	3.65	1459.7	0.0549
10	3.66	1463.6	0.0468
11	6.92	2769.8	0.5366
12	6.93	2772.2	0.7504
13	7.24	2898.7	0.3590
14	10.41	4163.3	0.0040

No.	(ppm)	Value	Absolute Value
1	[1.51 .. 1.58]	3.374	5.96758e+7
2	[3.58 .. 3.66]	1.000	1.76892e+7
3	[6.79 .. 7.04]	0.984	1.74067e+7
4	[9.83 .. 11.09]	0.864	1.52813e+7

Acquisition Time (sec)	1.3570	Comment	86198X140-1	Date	Feb 22 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY_AA.WL.COM\SAMBA\20050222\1602				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	13.45	1353.2	0.2413
2	45.80	4608.2	0.1948
3	91.82	9239.2	0.3941
4	124.97	12574.5	0.0637
5	146.89	14779.5	0.0831
6	167.51	16854.7	0.1310
7	174.57	17565.1	0.0608

Acquisition Time (sec)	5.1188	Comment	86198X98-1	Date	Jan 12 2005
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20050112\2701				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	0.85	339.1	0.4123	17	1.37	546.2	0.1500	33	4.24	1698.0	0.1152	1	[0.83 .. 0.89]	3.713	1.36594e+8
2	0.87	346.1	1.0000	18	1.67	667.7	0.0719	34	4.25	1699.6	0.1491	2	[1.21 .. 1.40]	12.034	4.42716e+8
3	0.88	352.6	0.3546	19	1.68	670.6	0.0848	35	4.25	1701.4	0.1831	3	[1.65 .. 1.75]	2.186	8.04312e+7
4	1.22	487.4	0.1439	20	1.69	677.4	0.1955	36	4.26	1705.7	0.0913	4	[4.17 .. 4.21]	0.738	2.71653e+7
5	1.22	488.3	0.1355	21	1.71	685.1	0.2176	37	4.27	1706.8	0.0849	5	[4.22 .. 4.33]	2.490	9.16140e+7
6	1.24	494.6	0.3471	22	1.73	692.1	0.1449	38	4.29	1714.6	0.2295	6	[5.51 .. 5.54]	0.306	1.12630e+7
7	1.24	495.4	0.3385	23	2.02	808.3	0.3353	39	4.30	1721.5	0.4425	7	[5.54 .. 5.56]	0.700	2.57523e+7
8	1.25	501.8	0.6207	24	2.02	809.3	0.2732	40	4.32	1728.3	0.2109				
9	1.26	502.6	0.6326	25	4.09	1635.5	0.0712	41	5.52	2208.7	0.2753				
10	1.26	504.5	0.6285	26	4.09	1636.5	0.0581	42	5.53	2212.0	0.2839				
11	1.27	508.5	0.5879	27	4.11	1642.7	0.0701	43	5.54	2217.3	0.6859				
12	1.28	510.2	0.5977	28	4.11	1643.7	0.0595	44	5.55	2219.9	0.7149				
13	1.29	514.9	0.4734	29	4.18	1671.1	0.1921	45	7.23	2893.9	0.0676				
14	1.30	521.7	0.3072	30	4.18	1673.4	0.2650	46	7.24	2898.2	0.4320				
15	1.34	537.4	0.1718	31	4.19	1675.0	0.2230								
16	1.36	542.6	0.1554	32	4.24	1696.3	0.1190								

Acquisition Time (sec)	1.3570	Comment	86198X98-1	Date	Jan 12 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20050112\2702				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.28	1437.2	0.7123	15	68.60	6902.3	0.2180
2	14.33	1441.6	0.1497	16	68.80	6923.0	0.4967
3	22.82	2295.7	0.8786	17	76.93	7741.0	0.8848
4	22.86	2300.1	0.1430	18	77.25	7772.7	0.8752
5	25.79	2594.9	0.6967	19	77.56	7804.3	0.8696
6	25.85	2600.8	0.2993	20	80.98	8148.5	0.2387
7	28.40	2858.0	0.3020	21	81.10	8160.3	0.5861
8	28.46	2863.2	0.6192	22	110.54	11122.0	0.0916
9	29.28	2945.7	1.0000	23	118.41	11914.3	0.0794
10	31.79	3198.5	0.1153	24	142.60	14347.6	0.0814
11	31.93	3212.5	0.8160	25	161.40	16240.1	0.1096
12	40.90	4115.2	0.2182	26	161.97	16297.6	0.2568
13	41.19	4144.0	0.6567	27	164.18	16519.4	0.0770
14	60.60	6097.6	0.0608				

Acquisition Time (sec)	5.1188	Comment	86198X62	Date	Mar 27 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY-AA.WL.COM\SAMBA\20050327\0301				
Frequency (MHz)	400.11	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6401.54	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value
1	1.20	479.5	0.4826	18	4.22	1689.0	0.1472	1	[1.16 .. 1.26]	1.700	3.74832e+8
2	1.22	486.8	1.0000	19	4.24	1696.1	0.1660	2	[1.26 .. 1.36]	1.144	2.52193e+8
3	1.23	493.8	0.4989	20	4.25	1699.8	0.1153	3	[3.76 .. 3.84]	0.603	1.32897e+8
4	1.29	514.5	0.2983	21	4.26	1703.3	0.0765	4	[3.84 .. 3.92]	0.413	9.09771e+7
5	1.30	521.7	0.6468	22	4.27	1707.0	0.1730	5	[4.07 .. 4.36]	2.019	4.45171e+8
6	1.32	529.0	0.3070	23	4.27	1710.1	0.0445	6	[5.64 .. 5.71]	0.415	9.14582e+7
7	3.80	1519.5	0.2726	24	4.28	1714.2	0.1260	7	[5.71 .. 5.78]	0.600	1.32318e+8
8	3.81	1522.6	0.2733	25	4.29	1717.4	0.1074				
9	3.87	1546.6	0.1663	26	4.30	1721.5	0.0421				
10	3.88	1550.5	0.1707	27	4.31	1724.4	0.1026				
11	4.12	1646.8	0.0882	28	4.32	1728.1	0.0403				
12	4.13	1650.6	0.0486	29	4.34	1735.3	0.0380				
13	4.13	1654.1	0.0888	30	5.67	2267.1	0.2103				
14	4.14	1657.8	0.1367	31	5.68	2271.0	0.2114				
15	4.16	1664.8	0.1393	32	5.74	2295.3	0.3233				
16	4.18	1672.0	0.0481	33	5.74	2298.2	0.3121				
17	4.20	1681.8	0.0503	34	7.24	2898.7	0.6649				

Acquisition Time (sec)	1.3570	Comment	86197X27-1	Date	Mar 17 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\HAHN.CHEMISTRY.AA.WL.COM\SAMBA\20050317\3102				
Frequency (MHz)	100.62	Nucleus	¹³ C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24147.30	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	14.04	1412.9	0.1173	10	79.77	8026.2	0.0858
2	14.14	1423.2	0.0808	11	79.96	8045.3	0.1292
3	51.81	5212.5	0.1112	12	122.33	12308.5	0.0217
4	52.59	5291.4	0.0712	13	150.55	15147.9	0.0407
5	63.03	6342.3	0.0958	14	150.89	15181.8	0.0474
6	63.30	6369.5	0.0796	15	164.84	16585.7	0.0376
7	76.90	7738.0	1.0000	16	166.10	16712.5	0.0648
8	77.23	7770.4	0.9607	17	166.50	16753.0	0.0549
9	77.54	7802.1	0.9760	18	167.30	16833.3	0.0477

Acquisition Time (sec)	5.1298	Comment	86197X17-1	Date	Mar 13 2005
File Name	C:\Program Files\Common Files\System\MAPI\1033\nt\FREEMAN.CHEMISTRY.AA.WL.COM\SAMBA\20050313\0301				
Frequency (MHz)	399.77	Nucleus	1H	Number of Transients	16
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	6387.74	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	1.29	516.7	0.1800
2	1.31	523.9	0.3548
3	1.32	527.2	0.0521
4	1.32	529.0	0.0543
5	1.33	530.9	0.1881
6	1.34	534.2	0.0805
7	1.34	535.8	0.0452
8	1.34	537.3	0.1156
9	1.35	539.9	0.0743
10	1.35	541.4	0.0547
11	1.36	544.6	0.2121
12	1.37	546.9	0.0495
13	1.38	551.6	0.1086
14	1.40	560.5	0.0607
15	1.41	564.0	0.0720

No.	(ppm)	(Hz)	Height
16	1.42	567.8	0.1118
17	1.43	571.1	0.1294
18	1.44	575.0	0.0696
19	1.45	578.3	0.0766
20	4.33	1730.0	0.0426
21	4.33	1731.4	0.0418
22	4.35	1737.0	0.0861
23	4.35	1738.6	0.0905
24	4.36	1744.2	0.0888
25	4.37	1745.8	0.0873
26	4.38	1751.5	0.0411
27	4.39	1753.4	0.0561
28	4.40	1760.6	0.1047
29	4.42	1767.8	0.1006
30	4.44	1775.0	0.0491

No.	(ppm)	(Hz)	Height
31	4.45	1780.3	0.0417
32	4.46	1783.6	0.0497
33	4.46	1784.6	0.0531
34	4.47	1787.1	0.0471
35	4.48	1790.6	0.0487
36	4.48	1791.8	0.0502
37	5.54	2214.8	0.0635
38	5.55	2219.1	0.0671
39	5.66	2261.0	0.0907
40	5.66	2263.8	0.1159
41	5.70	2279.6	0.0557
42	5.71	2283.7	0.0638
43	5.75	2297.5	0.1113
44	5.75	2300.2	0.1033
45	7.25	2899.9	1.0000

No.	(ppm)	Value	Absolute Value
1	[1.29 .. 1.47]	3.222	7.26707e+9
2	[4.33 .. 4.50]	2.000	4.51022e+9
3	[5.53 .. 5.68]	0.741	1.67126e+9
4	[5.68 .. 5.79]	0.730	1.64669e+9

Acquisition Time (sec)	1.3578	Comment	86198X100-2	Date	Jan 18 2005
File Name	C:\Documents and Settings\dassak\My Documents\data\NMR\SPIN.CHEMISTRY.AA.WL.COM\SAMBA\20050118\0302				
Frequency (MHz)	100.57	Nucleus	13C	Number of Transients	256
Original Points Count	32768	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24132.73	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	14.00	1407.7	0.2147
2	64.77	6513.9	0.1733
3	84.94	8542.2	0.1192
4	101.05	10162.5	0.0893
5	123.88	12458.1	0.0390
6	151.86	15271.5	0.0331
7	159.74	16064.0	0.0692
8	163.50	16442.6	0.0388