**The Preparation of 8-Amido 2-Dimethylamino-1,2,3,4-Tetrahydro-2-dibenzofurans
and Several Fluorinated Derivatives via [3,3]-Sigmatropic Rearrangement of *O*-
Aryloximes**

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Supporting Information

Page S2-S25: ¹H NMR spectra for **5, 6, 7, 8, 9, 11, 12, 13, 15a/16a, 15b/16b, 14c, 15c/16c, 15c, 17/18, 19, 20, 21, 22, 23b, 24, 25, 26, 27, 28**

S2

Current Data Parameters
 NAME AJS-A-8-28
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20010110
 Time 15.11
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 724.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.25 usec
 PL1 6.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 FIP 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07800 Hz/cm

Current Data Parameters
 NAME: RING-208
 EXPNO: 10
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20020308
 Time: 12.50
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zg30
 TO: 32768
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 4789.272 Hz
 FIDRES: 0.146157 Hz
 AQ: 3.4210291 sec
 RG: 1024
 DW: 104.400 usec
 DE: 6.00 usec
 TE: 300.0 K
 D1: 1.00000000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 9.50 usec
 PL1: 0.00 dB
 SFO1: 300.1319508 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1300056 MHz
 MON: no
 SSB: 0
 LB: 0.00 Hz
 GB: 0
 PC: 1.00

10 NMR plot parameters
 CX: 23.00 cm
 CY: 0.00 cm
 F1P: 10.000 ppm
 F2P: 300.130 Hz
 F2: -60.03 Hz
 PPMH: 0.44348 ppm/cm
 HZCM: 133.10114 Hz/cm

#	ADDRESS	F1 (Hz)	F2 (Hz)	INTENSITY
1	12817.8	2466.467	8.2180	9.06
2	12832.1	2464.375	8.2110	2.65
3	12866.3	2459.370	8.1944	2.12
4	12881.2	2457.195	8.1871	10.02
5	12903.0	2454.004	8.1765	0.86
6	12924.7	2187.763	7.2894	1.03
7	14747.0	2184.497	7.2785	10.28
8	14761.3	2182.402	7.2715	10.32
9	14775.6	2180.311	7.2645	15.11
10	14790.4	2177.398	7.2508	12.37
11	14810.4	2175.229	7.2416	9.86
12	22890.8	994.231	3.3127	1.25
13	22900.6	992.785	3.3079	1.18
14	22931.2	979.546	3.2637	1.33
15	23002.7	977.869	3.2582	1.34
16	24187.7	804.666	2.6811	1.06
17	24252.6	790.367	2.6354	1.35
18	24265.4	788.068	2.6285	1.15
19	24603.4	743.909	2.4786	1.15
20	24626.4	740.549	2.4674	2.22
21	24648.4	737.332	2.4567	1.25
22	24693.9	730.681	2.4345	1.27
23	24944.5	694.068	2.3126	74.72
24	24996.3	686.494	2.2873	1.89
25	25016.7	683.507	2.2774	1.37
26	25037.1	680.520	2.2674	1.38
27	25068.8	679.125	2.2627	1.92
28	25079.1	674.385	2.2470	2.02
29	25094.2	672.187	2.2397	1.47
30	25125.4	667.624	2.2244	2.44
31	25145.3	664.710	2.2147	1.38
32	25158.7	662.753	2.2082	1.66
33	25180.9	659.515	2.1974	1.37
34	25244.3	633.160	2.1763	1.15
35	25258.1	630.861	2.1665	1.15
36	25512.3	611.049	2.0360	0.93
37	25523.7	609.408	2.0305	1.51
38	25537.6	607.378	2.0237	1.40
39	25547.2	605.978	2.0191	1.81
40	25559.8	604.136	2.0139	1.76
41	25570.6	602.558	2.0077	1.31
42	25582.2	600.860	2.0020	1.27
43	25602.0	597.957	1.9923	0.94
44	25616.4	595.774	1.9826	0.98
45	25631.0	593.510	1.9635	0.98
46	25660.8	589.374	1.9637	1.03
47	25673.8	587.472	1.9574	1.04
48	26241.5	504.500	1.6809	0.93
49	26250.1	503.233	1.6767	1.03
50	26272.4	499.975	1.6659	1.68
51	26292.9	496.985	1.6559	1.05
52	26305.2	495.187	1.6499	1.12
53	26318.4	493.184	1.6412	1.16
54	26341.8	489.831	1.6321	1.59
55	26351.5	488.414	1.6273	1.68
56	26362.6	486.802	1.6220	1.64
57	26371.9	485.440	1.6174	1.60
58	26383.3	483.768	1.6119	1.13
59	26394.1	482.188	1.6066	0.95
60	26421.7	478.162	1.5932	0.92
61	26440.6	475.396	1.5840	1.15
62	26452.0	473.723	1.5784	1.15
63	26692.4	0.126	0.0004	26.17

Current Data Parameters
 NAME rnb-c-4-1
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020314
 Time 16.18
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 64
 DS 2
 SMH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 1024
 DW 104.400 usec
 DE 6.00 usec
 TE 300.0 K
 O1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.50 usec
 PL1 0.00 dB
 SF01 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300062 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 50.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.500 ppm
 F2 -150.06 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 157.56825 Hz/cm

F	ADDRESS	FREQUENCY (Hz)	INTENSITY
1	6277.9	2504.125	8.3435
2	6285.8	2501.808	4.131
3	6457.9	2451.488	8.1357
4	6466.0	2449.137	8.1681
5	6468.6	2442.519	8.1603
6	6496.7	2440.159	8.1382
7	7182.9	2239.554	8.1303
8	7213.7	2230.568	7.4619
9	7285.4	2181.111	7.4320
10	11395.6	881.270	2.6594
11	11804.7	888.559	2.9606
12	11814.7	895.629	2.9508
13	11876.6	867.532	2.8905
14	11884.2	865.311	2.8831
15	11916.7	855.801	2.8514
16	11934.3	850.666	2.8343
17	11957.9	840.254	2.7956
18	11975.8	835.586	2.7841
19	11985.9	831.742	2.7713
20	11999.0	829.165	2.7627
21	12007.9	827.131	2.7559
22	12014.8	824.751	2.7480
23	12023.0	804.641	2.6810
24	12031.8	802.482	2.6738
25	12099.1	791.080	2.6492
26	12113.3	791.187	2.6381
27	12137.7	788.021	2.6256
28	12148.6	780.118	2.5993
29	12175.6	785.729	2.5513
30	12224.9	746.069	2.4858
31	12282.1	725.833	2.4184
32	12361.4	706.093	2.3526
33	12428.9	678.219	2.2597
34	12524.2	673.937	2.2455
35	12538.9	665.533	2.2175
36	12549.0	663.440	2.2105
37	12567.6	663.440	2.2105
38	12574.8	663.440	2.2105
39	12574.8	663.440	2.2105
40	12574.8	663.440	2.2105
41	12845.9	584.203	1.9465
42	12866.9	578.042	1.9260
43	12881.7	573.722	1.9116
44	12889.6	571.422	1.9039
45	12903.5	565.384	1.8904
46	12917.9	563.145	1.8763
47	12925.4	560.949	1.8690
48	12935.4	556.849	1.9554
49	12939.4	554.733	1.8483
50	12946.7	554.142	1.8334
51	12962.0	544.142	1.8130
52	12982.9	490.593	1.6346
53	13166.1	376.422	1.4342
54	13266.7	376.422	1.4342
55	14456.5	20.261	0.0675
56	14775.1	3.122	0.0104
57	14833.7	0.001	0.0000
58	14844.4	-3.264	-0.0109
59	14855.6	-19.741	-0.0658
60	14911.9	-59.647	-0.1987
61	15048.5		0.15

F	ADDRESS	FREQUENCY (Hz)	INTENSITY (ppm)
1	7380.0	2116.8	1.60
2	7471.3	2155.827	7.1800
3	7500.3	2146.391	7.1515
4	7963.8	2010.966	6.7003
5	7971.5	2008.689	6.6927
6	8070.2	1979.855	6.5967
7	8078.2	1977.522	6.5889
8	8099.4	1971.306	6.5682
9	8107.5	1968.962	6.5604
10	8184.9	1948.715	3.101
11	11190.9	1087.698	3.5574
12	11691.9	1052.722	2.8745
13	11948.6	1046.147	2.8193
14	11969.2	1040.129	2.7992
15	11974.0	1038.720	2.7945
16	11985.4	1035.384	2.7834
17	11993.6	1033.001	2.7755
18	12009.1	1028.755	2.7613
19	12015.5	1026.590	2.7541
20	12022.8	1024.442	2.7478
21	12030.0	1022.312	2.7392
22	12047.0	1017.379	2.7234
23	12052.1	1015.092	2.7185
24	12060.7	1013.371	2.7101
25	12068.8	1011.015	2.7022
26	12208.4	970.192	2.5662
27	12217.8	967.437	2.5570
28	12223.9	965.675	2.5511
29	12246.5	959.062	2.5291
30	12258.5	956.144	2.5178
31	12263.2	954.181	2.5128
32	12269.9	952.231	2.5064
33	12280.5	949.132	2.4960
34	12302.2	942.766	2.4748
35	12308.2	941.027	2.4690
36	12312.8	939.682	2.4645
37	12378.3	920.534	2.4007
38	12570.5	864.357	2.2136
39	12580.5	861.889	2.2043
40	12586.3	859.716	2.1982
41	12594.5	857.338	2.1902
42	12605.1	854.235	2.1798
43	12613.8	851.685	2.1713
44	12621.6	849.428	2.1638
45	12629.3	847.156	2.1563
46	12637.9	844.641	2.1479
47	12935.1	557.780	1.8585
48	12956.6	551.307	1.8295
49	12970.0	548.212	1.8167
50	12978.0	545.232	1.8011
51	12994.0	540.558	1.7951
52	13000.1	538.771	1.7951
53	13010.1	535.851	1.7834
54	13015.4	534.295	1.7802
55	13031.2	529.669	1.7648
56	13037.5	527.848	1.7587
57	13051.6	523.668	1.7425
58	13074.7	516.980	1.7225
59	14832.2	3.213	0.0107
60	14843.2	-0.001	-0.0000
			22.30

Current Data Parameters
NAME ajs-b-190
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20020326
Time 14.31
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 456.1
DW 104.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 0.00 dB
SF01 300.1319508 MHz

F2 - Processing parameters

SI 16384
SF 300.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ID NMR plot parameters
CX 20.00 cm
CY 0.00 cm
F1P 10.000 ppm
F1 3001.30 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPHMC 0.52500 ppm/cm
HZCN 157.56825 Hz/cm

ALBANY MOLECULAR RESEARCH INC. ** 300 MHZ STANDARD PROTON NMR **

DMSO
 DATE 27-7-0
 SF 300.135
 SI 210.000
 SI 6200.000
 SI 16384
 TD 16384
 SM 7246.377
 HZ/PT 685
 PW 4.6
 RD 1.250
 AQ 1.130
 RG 20
 NS 32
 TE 297
 FM 8100
 O2 5050.000
 DP 63L P0
 LB 0.0
 GB 0.100
 CX 38.00
 CY 0.0
 F1 12.502P
 F2 -4.98P
 HZ/CM 102.680
 PPM/CM 342
 SR 4785.58

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#	CURSOR	FREQUENCY	PPM	INTENSITY
1	2894	2477.652	8.2551	3.873
2	2897	2475.261	8.2472	4.276
3	2906	2466.793	8.2190	3.315
4	2909	2464.410	8.2110	3.930
5	2927	2448.232	8.1571	3.941
6	2929	2446.659	8.1512	4.020
7	2933	2438.110	8.1234	4.509
8	3077	2315.615	7.7152	4.188
9	3087	2306.938	7.6853	7.000
10	3097	2298.219	7.5573	4.433
11	3541	1817.009	6.5540	5.524
12	4501	1056.329	3.5195	3.430
13	4529	1031.807	3.4378	2.089
14	4551	1011.830	3.3713	179.867
15	4574	991.713	3.3042	2.011
16	4598	974.026	3.1120	3.088
17	4656	919.207	3.0626	3.530
18	4825	783.510	2.5639	2.844
19	4843	754.060	2.5124	8.017
20	4859	739.144	2.4527	2.605
21	4870	729.671	2.4311	4.570
22	4878	722.900	2.4086	4.655
23	4883	718.063	2.3925	5.105
24	4898	713.844	2.3784	4.472
25	4895	707.567	2.3575	7.025
26	4900	703.246	2.3431	6.617
27	4907	697.043	2.3224	3.455
28	4911	693.205	2.3096	3.714
29	4927	679.130	2.2627	1.727
30	4950	659.013	2.1957	133.034
31	5044	575.447	1.9173	5.122
32	5053	562.572	1.8744	2.990
33	5133	496.734	1.5590	1.273
34	5139	492.211	1.5400	1.509
35	5143	482.584	1.5078	3.841
36	5161	472.190	1.5031	4.392
37	5176	458.683	1.5282	2.689
38	5188	448.647	1.4946	1.952
39	5193	444.135	1.4798	1.735
40	5694	46.767	1.0026	49.329

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Current Data Parameters
 NAME KTR-G-150
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020208
 Time 16.41
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 1024
 DW 104.400 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.50 usec
 PL1 0.00 dB
 SF01 300.1319508 MHz

F2 - Processing parameters
 SI 16384
 SF 300.1300061 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY -0.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.500 ppm
 F2 -150.06 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 157.56825 Hz/cm

S8

ALBANY MOLECULAR RESEARCH INC. ** 300 MHZ STANDARD PROTON NMR **

DMSO

DATE 29-8-0

SF 300.135

SI 210.0

SI 6200.000

SI 16384

SI 16384

SI 7246.377

SI 7246.377

SI 7246.377

SI 7246.377

SI 7246.377

SI 7246.377

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SI 7246.377

SI 7246.377

#	CURSOR	FREQUENCY	PPM	INTENSITY
1	1371	3289.207	10.9591	2.471
2	2131	3147.330	10.4854	10.632
3	2942	2423.875	8.0959	6.103
4	2948	2424.364	8.0776	7.689
5	2952	2421.269	8.0673	8.518
6	2958	2415.808	8.0491	7.377
7	2999	2379.774	7.9290	9.323
8	3106	2384.584	7.6119	4.754
9	3121	2271.295	7.5676	4.822
10	3171	2227.448	7.4215	6.501
11	3181	2218.667	7.3922	12.591
12	3191	2209.899	7.3630	6.517
13	4438	1106.455	3.6865	2.162
14	4552	1006.057	3.3520	73.226
15	4622	944.241	3.1461	2.029
16	4633	933.837	3.1114	2.798
17	4691	883.121	2.9424	6.846
18	4705	870.351	2.8999	5.348
19	4724	853.494	2.8437	35.592
20	4841	750.185	2.4995	12.564
21	5001	608.636	2.0279	2.138
22	5313	332.715	1.1086	.873
23	5321	325.700	1.0852	1.749
24	5625	56.903	.1896	.805
25	5691	-1.582	-.0056	219.519
26	5758	-61.162	-.2038	.980

Current Data Parameters
 NAME ajs-b-90
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011121
 Time 12.02
 INSTRUM spect
 PROBHD 5 mm BBI 1H-
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 406.4
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300059 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 100.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.500 ppm
 F2 -150.06 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 157.56827 Hz/cm

Current Data Parameters
 NAME ajs-b-89-1
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20011121
 Time 13.09
 INSTRUM spect
 PROBHD 5 mm BBI 1H-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 64
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 456.1
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 0.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300034 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 CY 150.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.500 ppm
 F2 -150.06 Hz
 PPMCM 0.52500 ppm/cm
 HZCM 157.56825 Hz/cm

Current Data Parameters
 NAME swt-c-20-2
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20001012
 Time 11.31
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 181
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
 P1 9.25 usec
 PL1 6.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300061 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 20.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.60000 ppm/cm
 HZCM 180.07800 Hz/cm

Current Data Parameters
NAME RUG-B-193
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020204
Time 14.17
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TO 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 114
DN 104.400 usec
DE 6.00 usec
TE 300.0 K
DT 1.0000000 sec
----- CHANNEL f1 -----
NUC1 1H
P1 9.50 usec
PL1 0.00 dB
SFO1 300.1319508 MHz
F2 - Processing parameters
SI 32768
SF 300.1300056 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 23.00 cm
CY 0.00 cm
FIP 10.000 ppm
F1 3001.30 Hz
F2 -0.200 ppm
F2 -60.03 Hz
PPMCH 0.44348 ppm/cm
HZCH 133.10114 Hz/cm

	ADDRESS	FREQUENCY (MHz)	INTENSITY
1	13498.5	235.181	4.68
2	13648.0	235.122	7.8026
3	13706.6	236.559	7.8137
4	14782.7	2179.286	7.7852
5	15326.3	2099.834	6.9864
6	15342.0	2097.534	6.9888
7	15413.8	2087.039	6.9538
8	15429.3	2084.772	6.9402
9	15481.5	2076.554	6.9188
10	15501.5	2074.326	6.9111
11	15541.8	2068.333	6.8915
12	15545.9	2067.735	6.8895
13	15561.7	2065.417	6.8817
14	15591.3	2060.055	3.2988
15	15621.1	2055.113	3.2930
16	15621.1	2055.113	3.2490
17	15621.1	2055.113	2.06
18	15621.1	2055.113	1.89
19	15621.1	2055.113	1.53
20	15621.1	2055.113	1.69
21	15621.1	2055.113	1.69
22	15621.1	2055.113	1.69
23	15621.1	2055.113	1.69
24	15621.1	2055.113	1.69
25	15621.1	2055.113	1.69
26	15621.1	2055.113	1.69
27	15621.1	2055.113	1.69
28	15621.1	2055.113	1.69
29	15621.1	2055.113	1.69
30	15621.1	2055.113	1.69
31	15621.1	2055.113	1.69
32	15621.1	2055.113	1.69
33	15621.1	2055.113	1.69
34	15621.1	2055.113	1.69
35	15621.1	2055.113	1.69
36	15621.1	2055.113	1.69
37	15621.1	2055.113	1.69
38	15621.1	2055.113	1.69
39	15621.1	2055.113	1.69
40	15621.1	2055.113	1.69
41	15621.1	2055.113	1.69
42	15621.1	2055.113	1.69
43	15621.1	2055.113	1.69
44	15621.1	2055.113	1.69
45	15621.1	2055.113	1.69
46	15621.1	2055.113	1.69
47	15621.1	2055.113	1.69
48	15621.1	2055.113	1.69
49	15621.1	2055.113	1.69
50	15621.1	2055.113	1.69
51	15621.1	2055.113	1.69
52	15621.1	2055.113	1.69
53	15621.1	2055.113	1.69
54	15621.1	2055.113	1.69
55	15621.1	2055.113	1.69
56	15621.1	2055.113	1.69
57	15621.1	2055.113	1.69
58	15621.1	2055.113	1.69
59	15621.1	2055.113	1.69
60	15621.1	2055.113	1.69
61	15621.1	2055.113	1.69
62	15621.1	2055.113	1.69
63	15621.1	2055.113	1.69
64	15621.1	2055.113	1.69

S13

ppm

CUC 1a Parameters
 NMR SMI-C-103-58
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20011026
 Time 12.25
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SFO1 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 128
 DN 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 ----- CHANNEL f1 -----
 NUC1 1H
 P1 9.50 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300601 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 23.00 cm
 CY 0.00 cm
 F1P 9.000 ppm
 F1 2701.17 Hz
 F2P -0.200 ppm
 F2 -50.03 Hz
 PPMH 0.40000 ppm/cm
 HZCM 120.05200 Hz/cm

ADDRESS	FREQUENCY (Hz)	INTENSITY
1	13691.4	7.8452
2	2354.584	4.85
3	13737.4	7.8163
4	13782.9	7.7878
5	14625.1	7.2592
6	15038.8	6.9995
7	15051.0	6.9918
8	15106.9	6.9568
9	15118.9	6.9493
10	15173.3	6.9114
11	15193.3	6.9127
12	15212.1	6.8907
13	15223.9	6.8833
14	20905.8	3.3170
15	20920.3	3.3079
16	20946.7	3.2914
17	20963.7	3.2681
18	20997.7	3.2581
19	21009.4	3.2535
20	21017.3	3.2520
21	21919.1	2.6810
22	21942.0	2.6667
23	21962.7	2.6536
24	21995.8	2.6329
25	22020.8	2.6172
26	22199.7	2.6064
27	22252.3	2.5049
28	22271.9	2.4719
29	22281.9	2.4386
30	22506.7	2.3122
31	22584.5	2.2859
32	22584.5	2.2634
33	22600.5	2.2533
34	22610.2	2.2473
35	22625.0	2.2380
36	22661.7	2.2149
37	22681.9	2.1749
38	22681.9	2.1648
39	22743.6	2.1577
40	22752.9	2.1477
41	22768.8	2.1477
42	22804.0	2.1256
43	22831.6	2.1083
44	22896.7	2.0674
45	22910.2	2.0590
46	22922.3	2.0511
47	22982.4	2.0086
48	23055.4	1.9678
49	23067.9	1.9600
50	23491.8	1.6939
51	23514.8	1.6795
52	23561.7	1.6500
53	23667.9	1.5833
54	23757.2	1.5773
55	23757.2	1.5773
56	24007.0	1.3705
57	24040.1	1.3497
58	24189.4	1.2561
59	26080.5	20.724
60	26173.4	3.220
61	26190.5	-0.000
62	26208.0	-0.0110
63	26235.7	-0.0660

S14

ppm

ALBANY MOLECULAR RESEARCH INC. ** 300 MHZ STANDARD PROTON NMR **

CD300
DATE 13-12-0
SF 300.135
SY 210.0
O1 6200.000
SI 16384
TD 16384
SW 6024.096
HZ/PT .735

PM 4.6
RD 1.250
AQ 1.360
RG 8
NS 59
TE 257

FM 7600
D2 5050.000
DP 63L P0
LB .500
GB 38.00
CX 0.0
CY 0.0
F1 12.500P
F2 /CH 102.500P
H2 /CH 102.500P
PDM/CM 342
SR 4550.58

#	CURSOR	FREQUENCY	PPM	INTENSITY
1	3301	2234.389	7.446	3.163
2	3310	2231.858	7.435	3.430
3	3323	2210.280	7.3643	2.868
4	3344	2202.350	7.3379	3.016
5	4320	1477.377	4.9224	32.412
6	4810	1124.983	3.7469	1.269
7	4986	994.759	3.3144	13.738
8	4988	994.758	3.3144	13.738
9	4991	991.300	3.2931	32.601
10	4993	989.887	3.2981	27.926
11	4995	988.504	3.2935	16.197
12	5031	952.046	3.2051	1.425
13	5057	942.753	3.1411	1.686
14	5116	876.839	2.7218	22.712
15	5116	877.339	2.7232	22.712
16	5329	721.312	2.1023	1.413
17	5452	652.576	2.1743	1.135
18	5465	642.884	2.1420	1.235
19	5474	635.933	2.1108	.907
20	6379	.001	.0000	45.572

S17

ALBANY MOLECULAR RESEARCH INC. ** 300. MHz STANDARD PROTON NMR **

 BRUKER

#	CURSOR	FREQUENCY	PPM	INTENSITY
1	3225	2419.768	8.0623	6.359
2	3231	2414.502	8.0447	8.571
3	3235	2411.265	8.0339	9.566
4	3241	2405.908	8.0161	7.879
5	3459	2213.000	7.3734	2.460
6	3469	2204.245	7.3442	6.713
7	3477	2197.231	7.3216	23.044
8	3485	2190.051	7.2959	10.938
9	3495	2181.344	7.2673	17.440
10	3503	2172.592	7.2307	18.695
11	4233	1475.685	4.8167	741.534
12	4328	1444.082	4.8115	5.263
13	4675	1137.789	3.7307	3.311
14	4836	994.137	3.3145	44.132
15	4838	993.616	3.3090	69.602
16	4840	945.301	3.1496	82.620
17	4852	933.704	3.1110	4.555
18	4853	903.948	3.0118	149.391
19	5141	725.705	2.4179	3.744
20	5215	659.804	2.1984	2.811
21	5226	649.974	2.1636	3.205
22	5234	642.930	2.1421	2.562
23	5525	385.819	1.2835	5.753
24	5561	.027	.0001	96.568

CD300
 DATE 1-9-0
 SF 300.135
 SY 210.0
 O1 6200.000
 SI 16384
 TD 16384
 SM 7246.377
 HZ/PT .885
 PW 4.6
 RD 0
 AO 1.130
 RB 40
 NS 64
 TE 287
 FW 9100
 O2 5050.000
 DP 63L P0
 LB .500
 BB .100
 CX .0
 F1 12.502P
 F2 12.505P
 HZ/CN 102.656
 PPM/CN
 SR 4550.28

ALBANY MOLECULAR RESEARCH INC. ** 300 MHZ STANDARD PROTON NMR **

 CD300
 DATE 1-9-0

 SF 300.135
 SY 210.0
 O1 6200.000
 SI 16384
 TD 16384
 SW 7246.377
 HZ/PT .885

PH	4.5	1	3226	2418.562	8.0583	2.805
DO	260	2	3232	2413.155	8.0402	3.203
AD	1.130	3	3242	2404.660	8.0119	2.621
RG	32	4	3303	2346.294	7.8175	2.722
NS	61	5	3316	2338.871	7.7927	2.973
IN	297	6	3446	2223.961	7.4099	3.073
TE		7	3457	2214.047	7.3768	3.215
FW	9100	8	3484	2189.802	7.2961	2.930
DO2	500.000	9	3494	2181.193	7.2674	5.273
DP	635L P0	10	3504	2172.481	7.2384	2.647
LB	500	11	4290	1476.324	1.3209	327.500
GB	500	12	4579	1132.529	1.1361	1.581
CV	36.00	13	4636	1090.125	1.0743	24.656
CV	0	14	4676	1040.770	1.0011	28.931
CF	12.502P	15	4876	958.906	1.1943	1.591
F2	102.656	16	4887	948.726	1.1610	1.816
PPM/CN	102.656	17	4938	903.655	1.0115	34.805
PPM/CN	342	18	5143	722.992	2.4089	1.331
SH	4551.17	19	5225	650.277	2.1666	1.075
		20	5225	384.941	1.2826	1.283
		21	5961	-847	-0.0028	23.981

NAME: USER-Chem1st, NAME-SUB-A-124-12, EXPNO=10, PROCNO=1
 F1=10.00000000 Hz, F2=0.30000000 Hz, M1=0.10000000 Hz, M2=0.10000000 Hz, PC=1.000

ADDRESS	F1 (Hz)	F2 (Hz)	INTENSITY
1	13843.7	2326.914	7.7530
2	13878.0	2320.286	7.7309
3	13891.2	2317.955	7.7232
4	13898.9	2316.501	7.7183
5	13926.3	2311.340	7.7011
6	13924.1	2309.881	7.6963
7	13924.1	2307.554	7.6895
8	13995.6	2307.554	7.6864
9	14624.9	2319.358	7.7084
10	15034.8	2102.529	6.9845
11	15068.1	2096.259	6.9725
12	15087.3	2092.642	6.9516
13	15120.5	2086.377	6.9396
14	15139.6	2082.781	6.9187
15	15173.0	2076.500	6.9187
16	15173.0	2076.500	6.9187
17	23716.8	476.053	1.5862
18	23726.6	465.185	1.5560
19	23774.2	456.200	1.5200
20	23851.5	441.628	1.4715
21	26195.9	-0.0000	-0.0000

Current Da
 NAME 124-12
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001128
 Time 10.14
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SFO1 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 128
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 DI 1.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 9.25 usec
 PL1 6.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 S1 32768
 SF 300.1300050 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID MR plot parameters
 CX 23.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.500 ppm
 F2 -150.07 Hz
 PH0H 0.45652 ppm/cm
 HZ0H 137.01587 Hz/cm

24

Current Data Parameters
 NAME RNB-A-120-g
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001129
 Time 11.45
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 161.3
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.25 usec
 PL1 6.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300047 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 9.000 ppm
 F1 2701.17 Hz
 F2P -0.500 ppm
 F2 -150.06 Hz
 PPMCM 0.47500 ppm/cm
 HZCM 142.56177 Hz/cm

ADDRESS	FREQUENCY [Hz]	INTENSITY	PPM
1	14074.8	2283.750	7.64
2	14110.2	2277.072	7.71
3	14135.9	2272.238	7.72
4	14171.2	2265.364	7.69
5	14553.2	2181.613	7.61
6	14597.9	2181.331	7.71
7	14616.4	2181.331	7.71
8	14625.0	2180.037	7.71
9	14652.4	2174.939	7.97
10	20868.6	1003.918	3.3449
11	20886.4	1000.565	3.3338
12	20903.6	999.220	3.3293
13	20920.8	995.980	3.3185
14	20938.0	990.470	3.3135
15	20940.0	989.068	3.3062
16	20947.5	989.579	3.2938
17	20966.0	984.362	3.2798
18	20975.5	981.021	3.2687
19	20990.2	806.842	2.6883
20	21931.8	802.493	2.6738
21	21937.9	798.597	2.6608
22	21958.6	797.093	2.6558
23	21981.8	792.353	2.6452
24	21991.7	787.940	2.6400
25	22015.1	784.310	2.6132
26	22034.4	782.867	2.6084
27	22042.1	745.792	2.4982
28	22217.6	746.446	2.4871
29	22235.4	743.238	2.4764
30	22252.4	738.901	2.4653
31	22267.7	733.370	2.4543
32	22304.9	728.766	2.4435
33	22322.6	728.766	2.4435
34	22339.9	692.650	2.2018
35	22521.0	683.320	2.2767
36	22570.5	680.442	2.2672
37	22585.8	678.699	2.2614
38	22600.2	675.886	2.2581
39	22615.1	673.123	2.2520
40	22630.0	669.125	2.2382
41	22645.9	667.942	2.2252
42	22662.8	664.514	2.2188
43	22679.7	662.760	2.2141
44	22713.8	656.331	2.1868
45	22741.4	651.123	2.1685
46	22878.5	625.304	2.0834
47	22901.5	619.841	2.0652
48	22934.6	617.981	2.0587
49	22962.9	612.043	2.0482
50	22977.2	609.397	2.0352
51	22993.2	606.708	2.0215
52	23004.5	601.695	2.0114
53	23020.0	598.648	2.0043
54	23034.8	595.852	1.9946
55	23050.0	590.226	1.9786
56	23063.3	587.362	1.9675
57	23079.9	585.339	1.9503
58	23470.5	513.786	1.7119
59	23493.7	509.417	1.6973
60	23522.9	498.275	1.6666
61	23562.9	496.377	1.6539
62	23600.1	490.842	1.6354
63	23615.3	486.511	1.6305
64	23623.5	484.960	1.6210
65	23682.6	473.819	1.5777
66	23746.9	461.715	1.5384
67	26197.9	-0.0001	-0.0000

S21

Current Data Parameters
 NAME RNB-B-5
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20010405
 Time 12.20
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084650 sec
 RG 812.7
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 JH
 P1 9.25 usec
 PL1 -3.00 dB
 SF01 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300049 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 180.07800 Hz/cm

26

Current Data Parameters
 NAME RNB-A-131-2
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20001205
 Time 11:41
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 65536
 SOLVENT MeOH
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 80.6
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.25 usec
 PL1 6.00 dB
 SF01 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300055 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.000 ppm
 F1 3301.43 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPWM 0.60000 ppm/cm
 HZCM 180.07800 Hz/cm

S23

Date_ 20010907
 File_ 13.26
 INSTRUM spect
 PULPROG 5 mm QNP 1H/13
 TO 2930
 SOLVENT H₂O
 NS 16
 DS 2
 SHH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084650 sec
 RG 456.1
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 O1 1.00000000 sec
 ***** CHANNEL f1 *****
 NUC1 1H
 P1 9.50 usec
 PL1 0.00 dB
 SF01 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300558 MHz
 MCW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 IO NMR plot parameters
 CX 23.00 cm
 F1P 10.000 ppm
 F1 3001.30 Hz
 F2P -0.500 ppm
 F2 -150.07 Hz
 PPHCH 0.45652 pps/cm
 HZCH 137.01587 Hz/cm

#	ADDRESS	FREQUENCY (Hz)	PPM	INTENSITY
1	15039.4	2100.910	7.0000	1.26
2	15071.9	2094.784	6.9796	1.32
3	15095.9	2090.264	6.9645	1.27
4	15128.4	2084.146	6.9441	1.18
5	18329.4	1481.143	4.9350	0.56
6	18434.1	1461.416	4.8693	45.51
7	18540.5	1441.365	4.8025	0.49
8	20122.7	1143.315	3.8094	0.60
9	20132.4	1141.484	3.8033	0.61
10	20172.9	1133.865	3.7779	0.41
11	20187.8	1131.056	3.7686	0.38
12	20203.5	1128.096	3.7587	0.40
13	20829.3	1010.211	3.3659	0.67
14	20862.9	1003.883	3.3448	0.77
15	20907.3	995.510	3.3169	6.06
16	20916.0	993.879	3.3115	9.86
17	20924.7	992.240	3.3060	12.72
18	20933.3	990.616	3.3006	9.10
19	20942.0	988.970	3.2951	5.23
20	21022.1	973.884	3.2449	0.26
21	21184.5	943.300	3.1430	0.68
22	21250.2	930.905	3.1017	0.74
23	21293.7	922.722	3.0744	0.74
24	21398.2	903.027	3.0088	25.90
25	21505.8	882.770	2.9413	0.44
26	21782.0	830.727	2.7679	0.13
27	22245.3	743.453	2.4771	0.54
28	22299.7	733.210	2.4430	0.69
29	22627.7	671.413	2.2371	0.27
30	22666.0	664.206	2.2131	0.35
31	22693.0	659.114	2.1961	0.56
32	22731.3	651.909	2.1721	0.54
33	22745.7	649.199	2.1631	0.62
34	22782.2	642.308	2.1401	0.46
35	22809.4	637.189	2.1230	0.28
36	22847.8	629.957	2.0989	0.19
37	24130.9	388.249	1.2936	0.16
38	24254.6	364.941	1.2159	0.10
39	26174.5	3.277	0.0109	0.63
40	26191.9	0.000	0.0000	8.86