

Supporting Information

Studies on the Chemistry and Reactivity of α -Substituted Ketones in Isonitrile-Based Multicomponent Reactions

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^1H -NMR and ^{13}C -NMR Spectra

LF-VI-17a

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature
INOVA-500 "inova500"

Relax. delay 2.000 sec

Pulse 61.4 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

8 repetitions

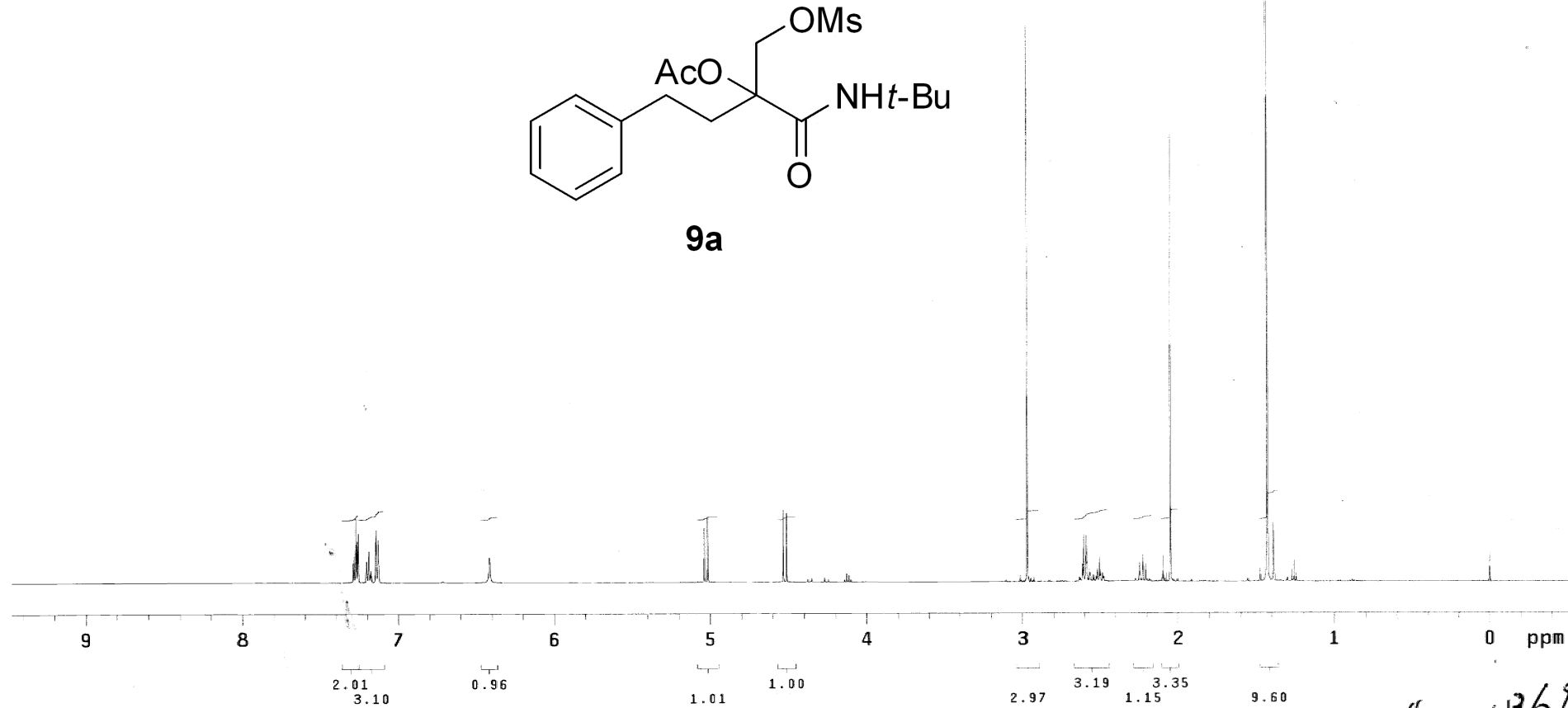
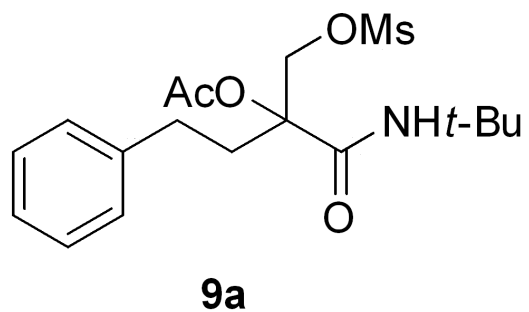
OBSERVE H1, 499.9172583 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 31 sec

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4 #B69
2.14 ppm
1.00

INDEX	FREQUENCY	PPM	HEIGHT
1	3636.230	7.274	10.2
2	3628.906	7.259	7.9
3	3572.266	7.146	7.3
4	3571.289	7.144	8.4
5	2517.578	5.036	8.7
6	2506.836	5.015	10.5
7	2265.625	4.532	11.6
8	2254.883	4.511	11.1
9	1483.398	2.967	88.3
10	1302.734	2.606	7.6
11	1293.945	2.588	7.5
12	1023.438	2.047	71.0
13	714.355	1.429	162.0
14	694.336	1.389	9.4

C13 LF-VI-17a

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec

Pulse 54.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

200 repetitions

OBSERVE C13, 125.7042385 MHz

DECOUPLE H1, 499.9197456 MHz

Power 38 dB

continuously on

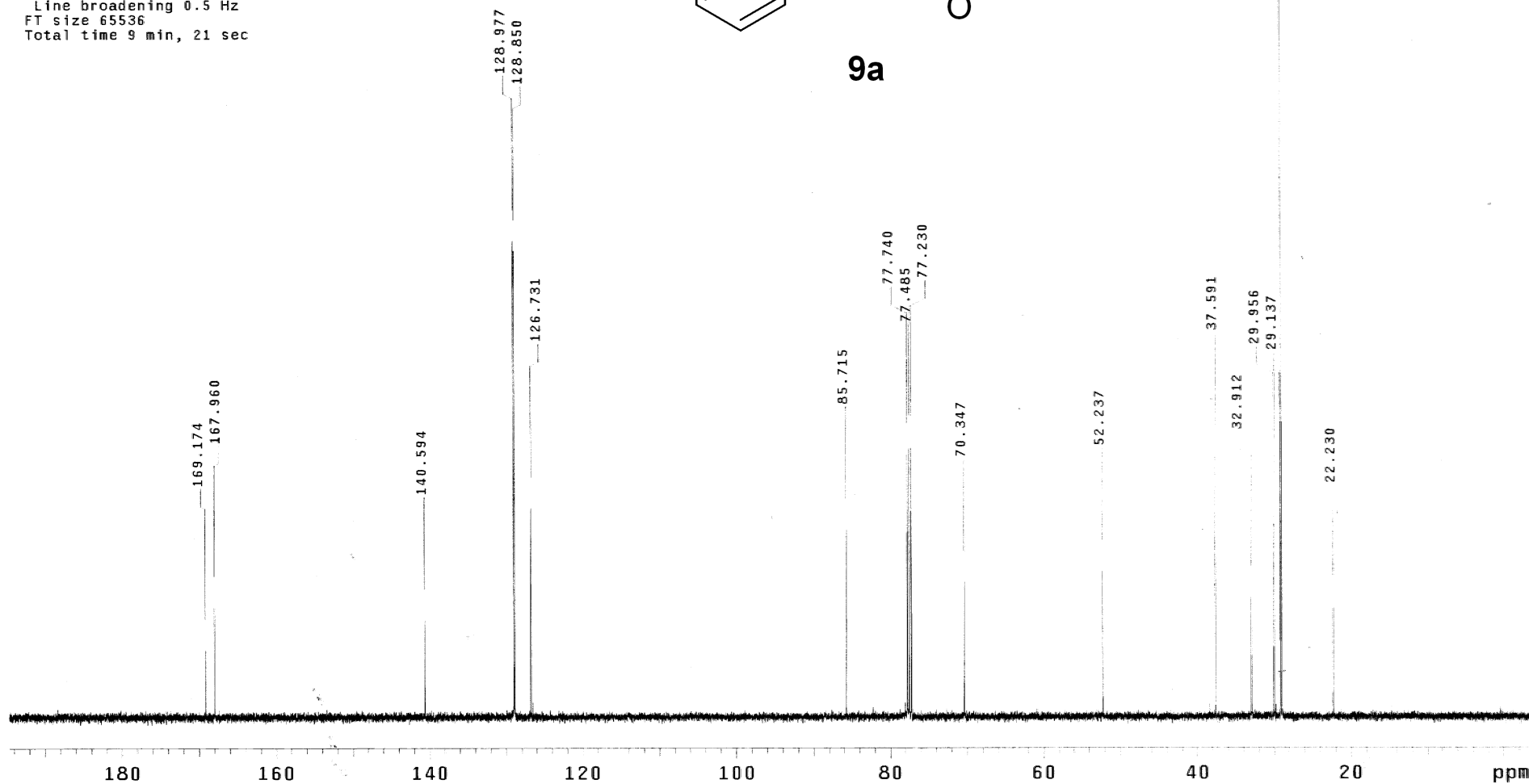
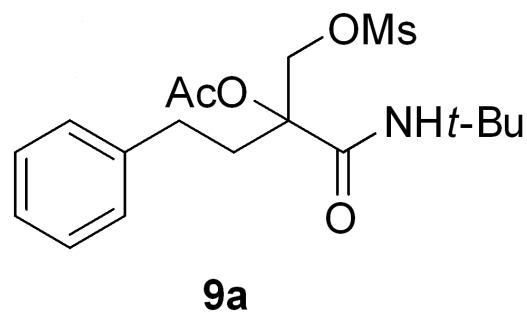
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 21 sec



LF-V-15a

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

INOVA-500 "inova500"

Relax. delay 2.000 sec

Pulse 61.4 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

8 repetitions

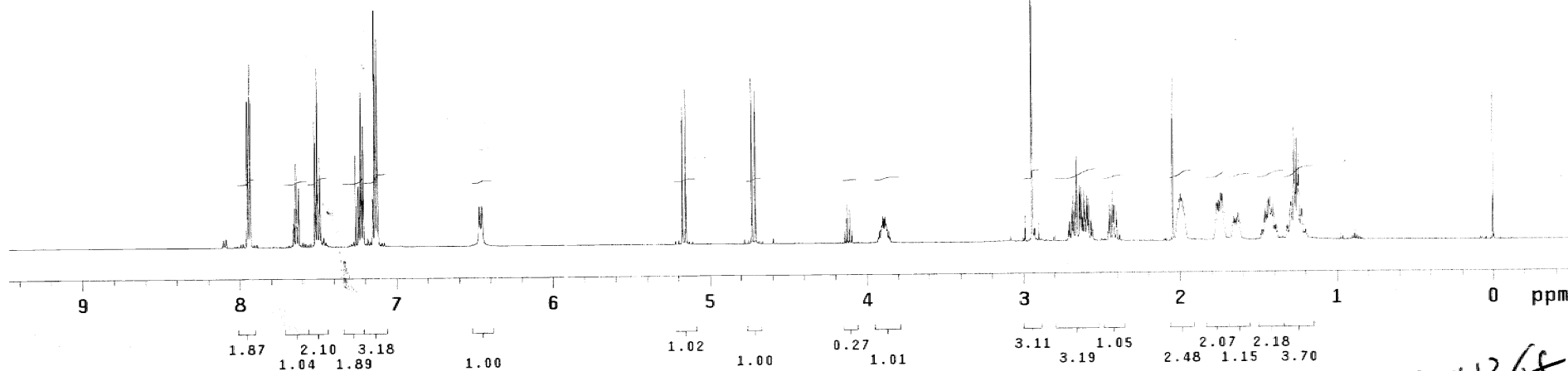
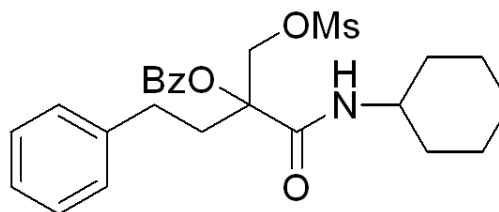
OBSERVE H1, 499.9172607 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 31 sec

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5 #1368
-2-14 ppm
CDCl3

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3975.098	7.952	23.0	40	621.094	1.242	13.7
2	3974.121	7.950	23.3	41	0.000	0.000	23.3
3	3968.750	7.939	7.3				
4	3966.797	7.935	29.2				
5	3965.332	7.932	22.8				
6	3819.824	7.641	13.3				
7	3812.012	7.625	9.4				
8	3759.766	7.521	20.1				
9	3751.953	7.505	28.5				
10	3744.141	7.490	14.4				
11	3629.395	7.260	14.6				
12	3620.605	7.242	9.6				
13	3612.793	7.227	24.7				
14	3607.422	7.216	7.3				
15	3605.469	7.212	19.3				
16	3575.195	7.152	8.1				
17	3573.730	7.149	7.6				
18	3567.871	7.137	37.5				
19	3560.059	7.121	33.0				
20	2585.449	5.172	21.9				
21	2574.707	5.150	24.7				
22	2364.746	4.730	26.4				
23	2354.004	4.709	24.4				
24	1471.191	2.943	162.0				
25	1338.867	2.678	7.3				
26	1329.102	2.659	13.7				
27	1319.336	2.639	8.9				
28	1314.453	2.629	8.7				
29	1304.688	2.610	8.3				
30	1296.387	2.593	7.3				
31	1212.891	2.426	8.8				
32	1020.996	2.042	26.0				
33	996.094	1.993	7.5				
34	868.164	1.737	7.7				
35	864.258	1.729	7.5				
36	714.844	1.430	7.2				
37	635.254	1.271	18.0				
38	627.930	1.256	16.3				
39	623.535	1.247	9.1				

C13 LF-VI-15a

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec

Pulse 54.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

200 repetitions

OBSERVE C13, 125.7042720 MHz

DECOUPLE H1, 499.9197456 MHz

Power 38 dB

continuously on

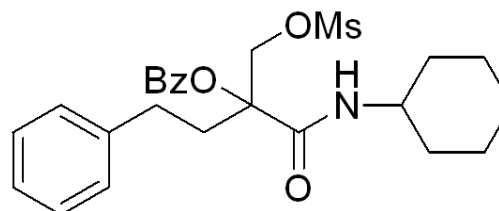
WALTZ-16 modulated

DATA PROCESSING

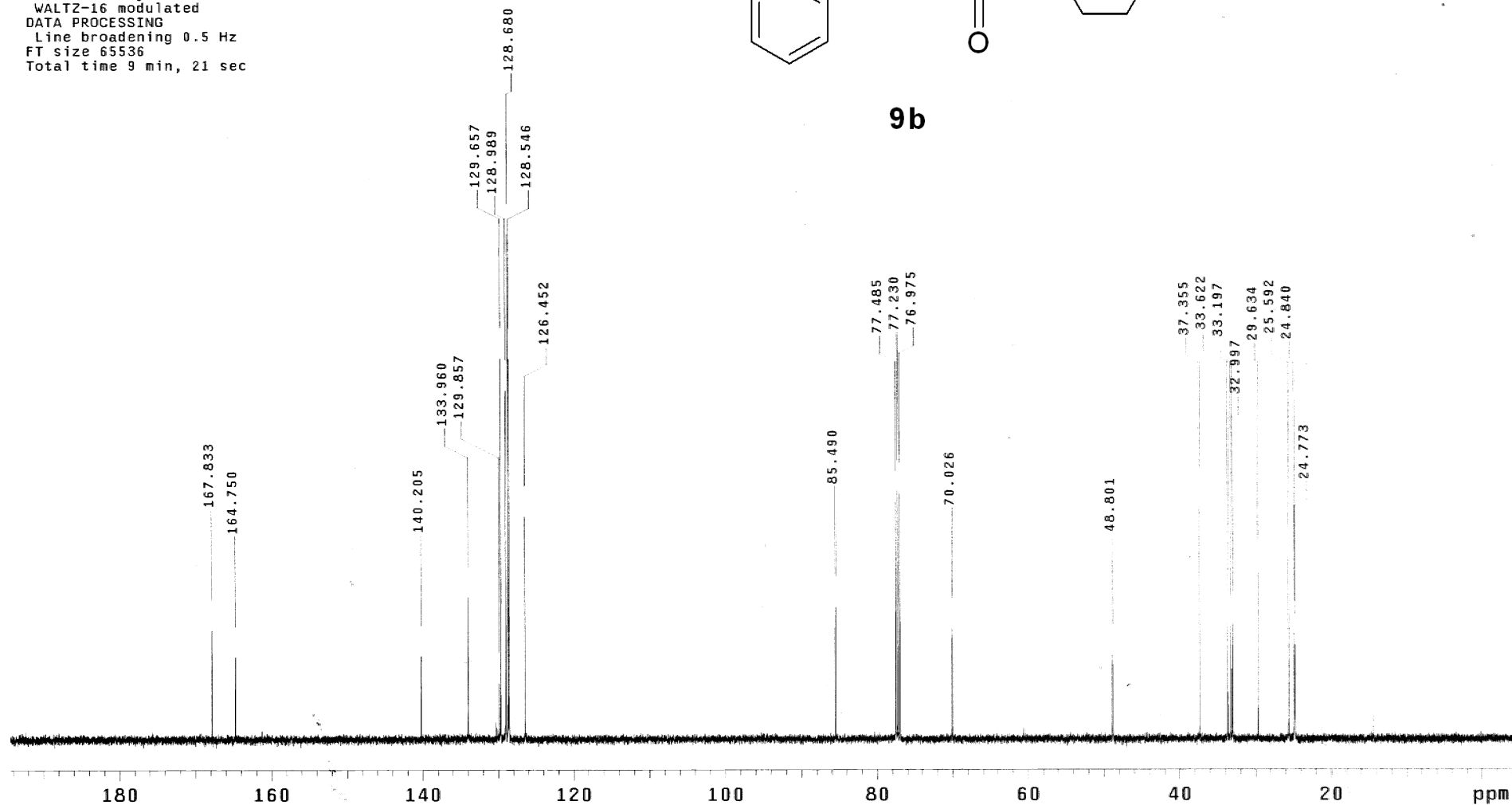
Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 21 sec



9b



LF-VI-79a

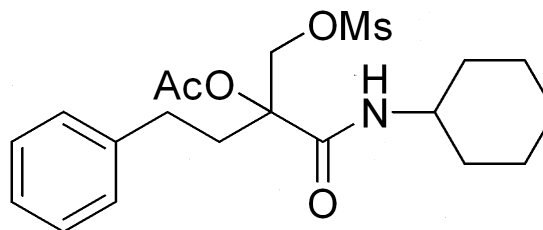
Sample directory:
File: PROTON

Pulse Sequence: s2pul

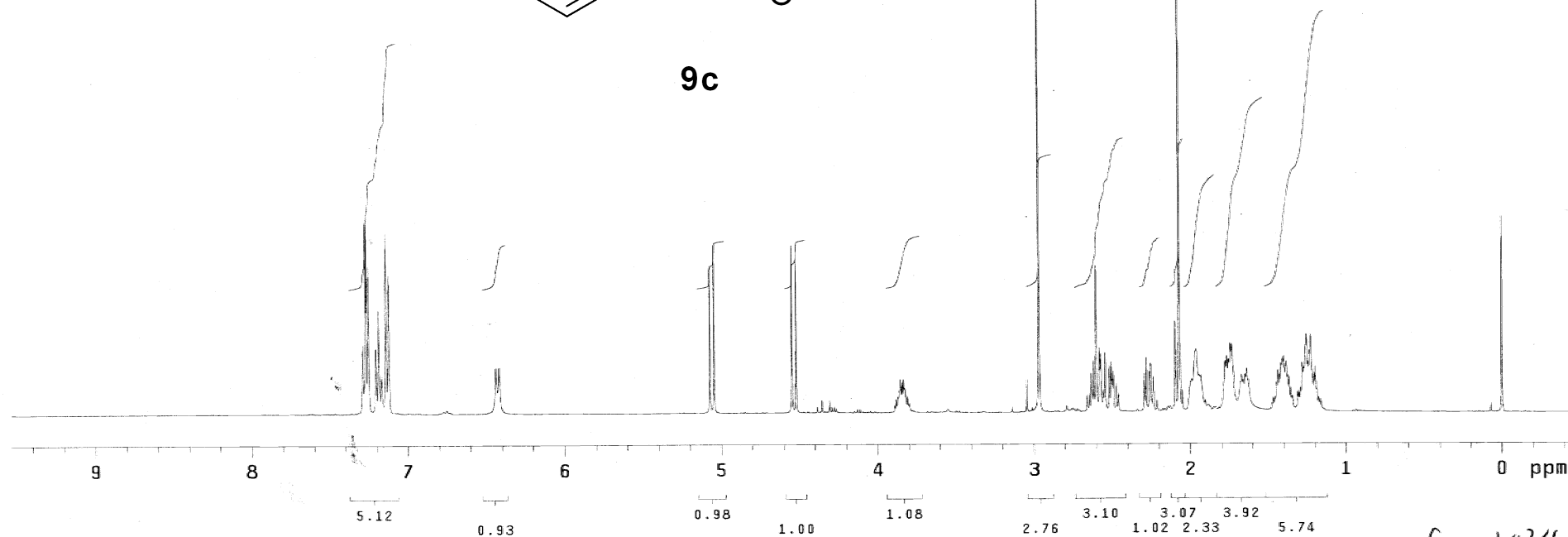
Solvent: CDCl3
Ambient temperature
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773431 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

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9c



6 #1434
-2-(477m
CO₂H

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2913.936	7.289	11.2	40	899.445	2.250	7.9	79	481.497	1.204	6.3
2	2906.919	7.271	30.6	41	892.817	2.233	5.8	80	477.989	1.196	7.4
3	2904.190	7.265	30.2	42	836.285	2.092	14.6	81	474.480	1.187	3.9
4	2899.121	7.252	23.6	43	826.538	2.067	151.9	82	-0.000	-0.000	31.1
5	2880.797	7.206	10.6	44	818.741	2.048	3.7				
6	2873.389	7.187	16.7	45	797.687	1.995	5.0				
7	2865.982	7.169	6.3	46	794.178	1.987	5.4				
8	2854.675	7.141	28.9	47	783.652	1.960	10.1				
9	2847.268	7.122	22.2	48	776.244	1.942	6.1				
10	2573.574	6.438	7.5	49	771.955	1.931	6.1				
11	2565.387	6.417	7.6	50	709.575	1.775	8.4				
12	2027.357	5.071	23.6	51	705.676	1.765	9.1				
13	2016.831	5.045	26.8	52	700.998	1.753	8.5				
14	1817.604	4.547	26.7	53	696.319	1.742	11.1				
15	1807.077	4.520	25.4	54	692.810	1.733	11.0				
16	1540.792	3.854	5.4	55	667.079	1.669	6.1				
17	1536.503	3.843	5.1	56	663.180	1.659	5.3				
18	1532.604	3.834	5.5	57	658.111	1.646	6.2				
19	1530.265	3.828	4.1	58	654.213	1.636	7.0				
20	1216.414	3.043	5.4	59	650.704	1.628	5.3				
21	1185.614	2.966	162.2	60	577.797	1.445	4.8				
22	1056.565	2.643	3.2	61	573.898	1.436	6.9				
23	1051.887	2.631	6.4	62	570.389	1.427	6.3				
24	1046.038	2.617	8.4	63	566.101	1.416	7.9				
25	1039.411	2.600	23.4	64	562.202	1.406	8.6				
26	1031.223	2.579	10.4	65	559.473	1.399	9.1				
27	1027.324	2.570	9.5	66	553.625	1.385	8.2				
28	1021.476	2.555	3.8	67	548.946	1.373	6.1				
29	1016.798	2.543	9.6	68	545.437	1.364	5.7				
30	1005.491	2.515	7.6	69	541.538	1.355	4.0				
31	1000.813	2.503	8.2	70	523.214	1.309	3.3				
32	998.474	2.498	5.4	71	520.095	1.301	3.5				
33	995.355	2.490	6.7	72	516.196	1.291	4.0				
34	987.947	2.471	4.7	73	511.908	1.280	8.0				
35	982.489	2.458	3.2	74	508.009	1.271	7.2				
36	915.820	2.291	6.3	75	500.991	1.253	12.6				
37	911.141	2.279	8.8	76	496.703	1.242	8.2				
38	903.344	2.260	6.6	77	493.584	1.235	9.9				
39	901.004	2.254	7.9	78	490.075	1.226	12.5				

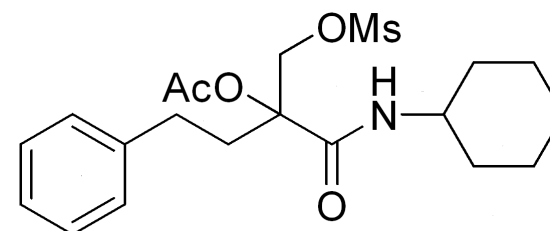
C13LF-VI-79a

Pulse Sequence: s2pul

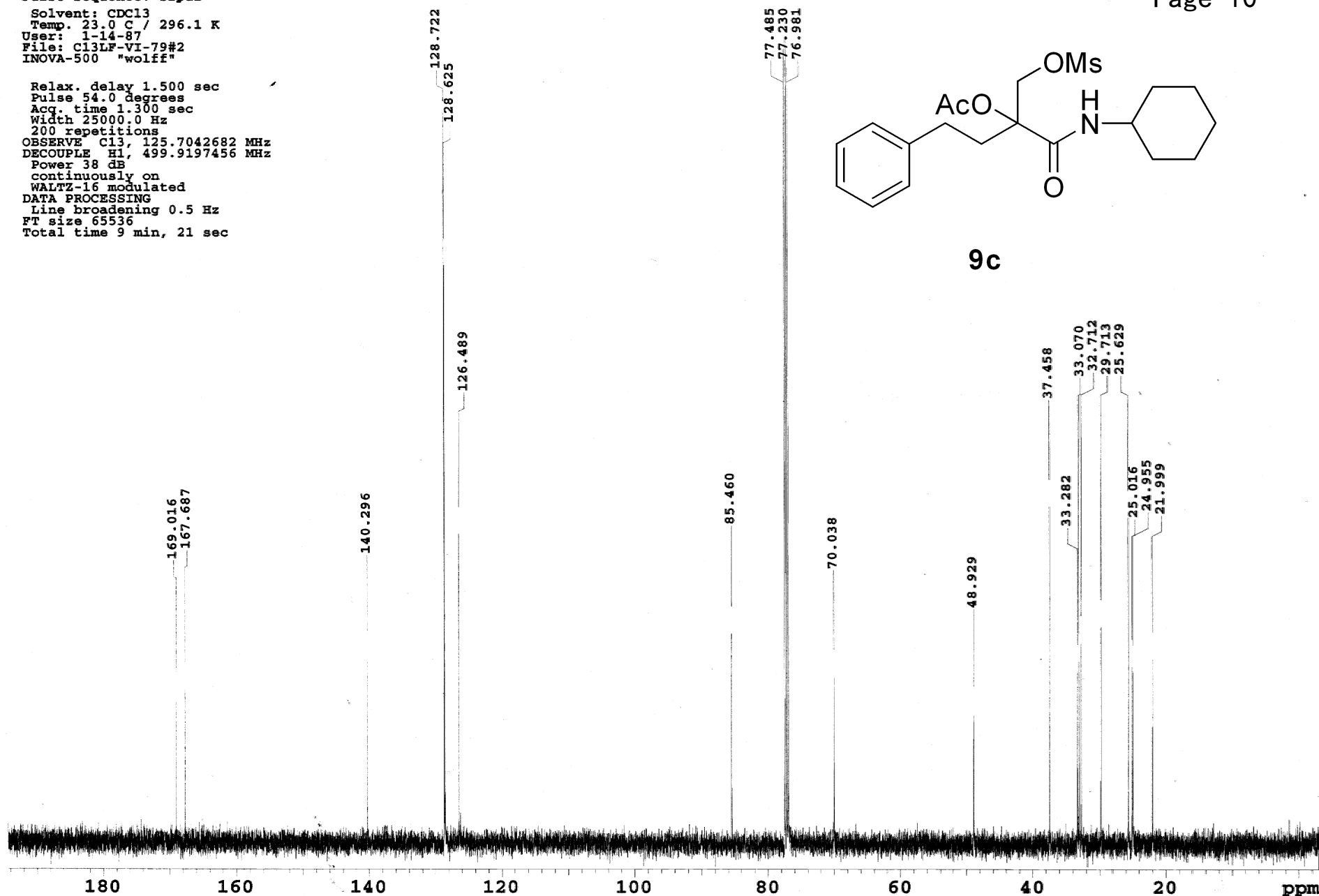
Solvent: CDCl3
Temp. 23.0 C / 296.1 K
User: 1-14-87
File: C13LF-VI-79#2
INNOVA-500 "wolff"

Relax. delay 1.500 sec
Pulse 54.0 degrees
Acq. time 1.300 sec
Width 25000.0 Hz
200 repetitions
OBSERVE C13, 125.7042682 MHz
DECOUPLE H1, 499.9197456 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 21 sec

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9c



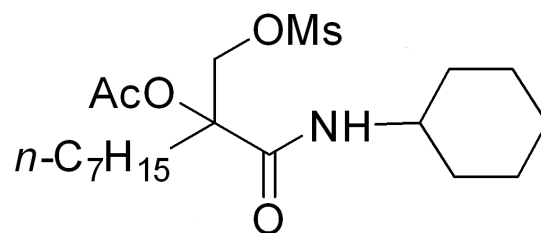
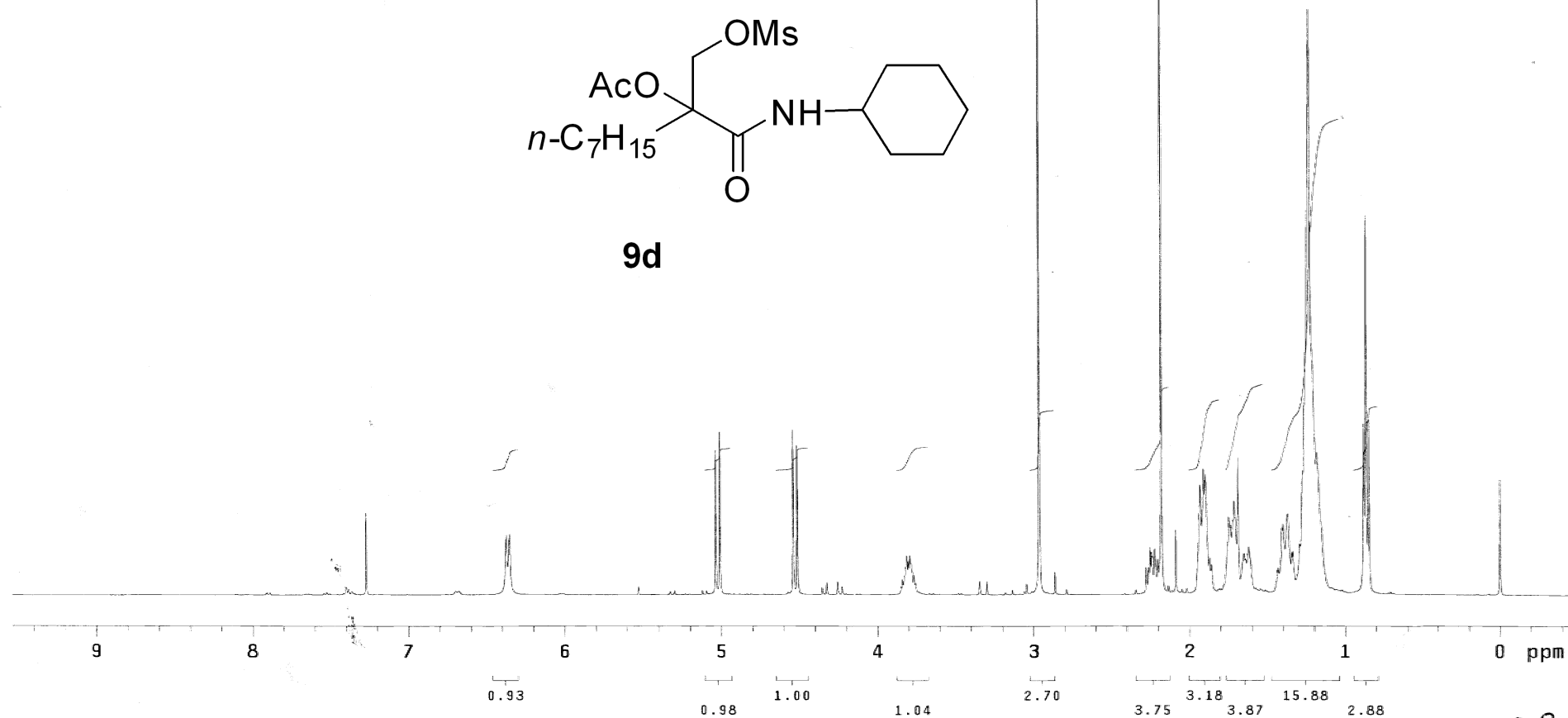
#157

Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773411 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

**9d**

#BPS
-214ppm

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2907.698	7.273	13.2	40	562.592	1.407	10.8
2	2548.622	6.375	9.7	41	559.863	1.400	11.4
3	2540.435	6.355	9.8	42	548.556	1.372	13.1
4	2013.322	5.036	23.1	43	537.640	1.345	7.0
5	2002.795	5.010	26.0	44	534.910	1.338	7.1
6	1815.265	4.541	26.3	45	516.976	1.293	8.3
7	1804.738	4.514	23.9	46	509.179	1.274	19.9
8	1524.027	3.812	6.4	47	492.804	1.233	93.1
9	1520.128	3.802	5.8	48	472.530	1.182	22.8
10	1515.840	3.792	6.4	49	352.058	0.881	27.3
11	1509.602	3.776	3.7	50	345.820	0.865	60.3
12	1505.313	3.765	3.3	51	338.803	0.847	28.0
13	1185.224	2.965	162.3	52	-0.000	-0.000	18.5
14	1144.677	2.863	3.7				
15	909.972	2.276	4.5				
16	903.734	2.261	4.4				
17	899.835	2.251	7.7				
18	895.936	2.241	7.0				
19	893.987	2.236	6.2				
20	888.139	2.222	7.4				
21	879.951	2.201	5.8				
22	872.543	2.183	153.1				
23	834.725	2.088	10.5				
24	772.735	1.933	17.7				
25	763.768	1.910	20.2				
26	759.089	1.899	19.3				
27	748.563	1.872	6.0				
28	743.104	1.859	4.9				
29	699.048	1.749	12.6				
30	695.540	1.740	11.2				
31	689.302	1.724	12.0				
32	685.793	1.715	15.1				
33	675.656	1.690	22.0				
34	660.451	1.652	6.7				
35	656.162	1.641	5.9				
36	651.094	1.629	6.7				
37	647.195	1.619	7.8				
38	574.678	1.437	4.1				
39	571.559	1.430	4.4				

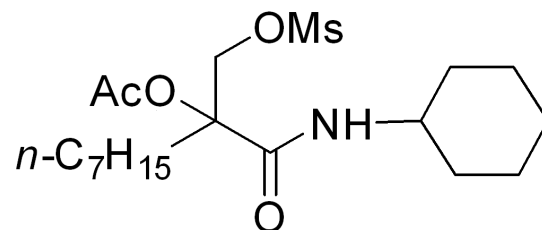
C13LF-VI-39b

Sample directory:
File: CARBON

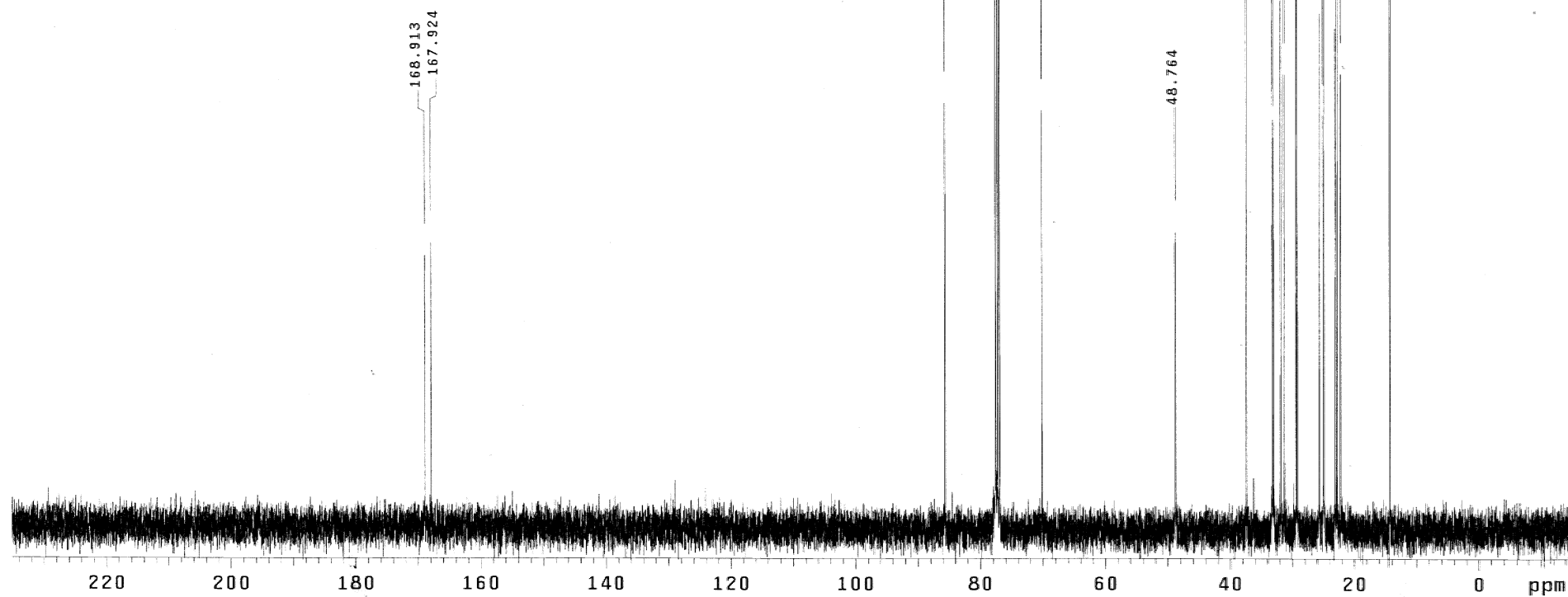
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
600 repetitions
OBSERVE C13, 100.5240733 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 23 min, 6 sec



9d



LF-VI-33pc

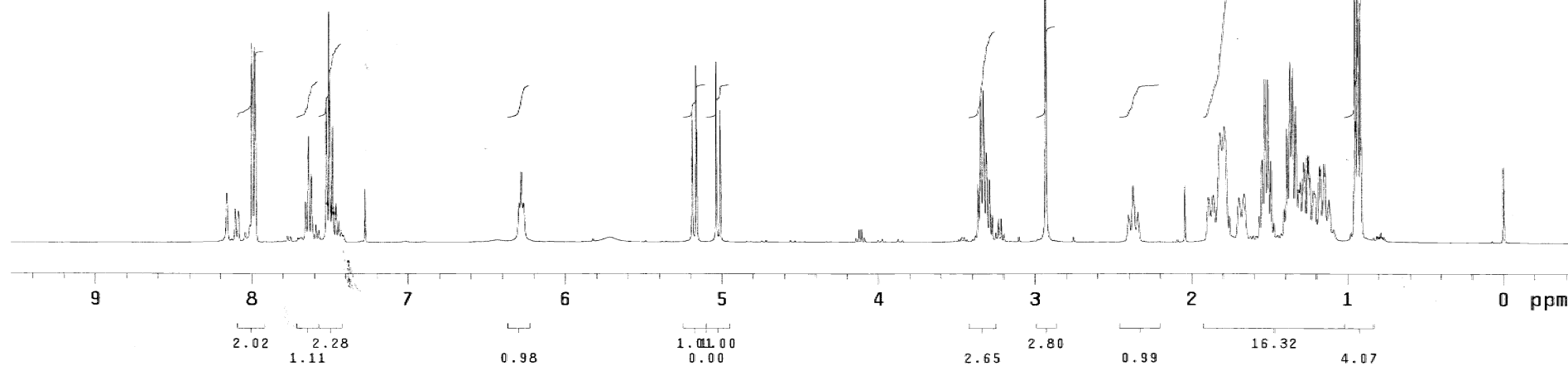
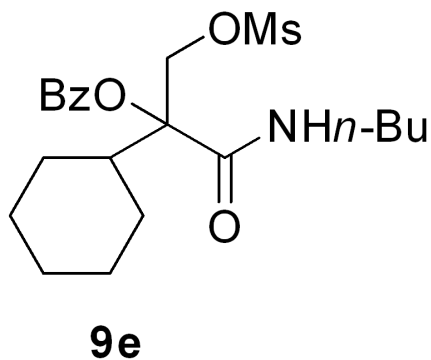
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Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773407 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec



9 #1390
2-14ppm
2/1/17

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3261.316	8.158	7.9	40	756.750	1.893	7.3				
2	3239.873	8.104	5.5	41	744.664	1.863	7.6				
3	3232.076	8.085	5.1	42	727.120	1.819	17.6				
4	3196.987	7.997	31.8	43	715.813	1.791	18.6				
5	3189.579	7.978	30.3	44	702.947	1.758	4.3				
6	3188.799	7.976	31.0	45	677.995	1.696	7.2				
7	3060.530	7.656	6.6	46	665.519	1.665	7.9				
8	3059.750	7.654	6.5	47	625.752	1.565	4.3				
9	3053.122	7.637	17.1	48	618.734	1.548	13.4				
10	3045.715	7.619	11.0	49	611.326	1.529	26.0				
11	3044.935	7.617	10.6	50	603.919	1.511	25.9				
12	3034.018	7.589	3.0	51	596.901	1.493	13.2				
13	3006.727	7.521	23.2	52	588.713	1.473	3.3				
14	2999.319	7.502	36.7	53	562.202	1.406	5.5				
15	2991.132	7.482	18.7	54	555.184	1.389	18.3				
16	2982.945	7.462	6.4	55	547.387	1.369	28.7				
17	2975.147	7.442	3.5	56	540.369	1.352	27.8				
18	2908.088	7.274	8.6	57	532.571	1.332	21.8				
19	2515.093	6.291	6.4	58	525.164	1.314	8.5				
20	2509.635	6.278	11.3	59	520.875	1.303	9.9				
21	2503.786	6.263	6.4	60	511.908	1.280	12.9				
22	2074.143	5.188	20.8	61	510.348	1.277	11.9				
23	2063.616	5.162	28.2	62	502.161	1.256	14.1				
24	2012.932	5.035	28.7	63	499.432	1.249	14.0				
25	2002.795	5.010	21.1	64	495.923	1.240	10.4				
26	1342.734	3.359	9.4	65	486.566	1.217	8.4				
27	1336.107	3.342	23.1	66	483.447	1.209	7.9				
28	1329.479	3.326	24.2	67	471.750	1.180	12.4				
29	1321.681	3.306	14.5	68	469.021	1.173	11.9				
30	1314.273	3.288	10.1	69	459.664	1.150	12.7				
31	1307.256	3.270	4.5	70	456.935	1.143	11.2				
32	1291.661	3.231	3.9	71	447.188	1.119	7.0				
33	1284.643	3.213	3.9	72	381.299	0.954	41.2				
34	1171.189	2.930	162.3	73	378.960	0.948	19.4				
35	959.876	2.401	4.5	74	373.892	0.935	76.3				
36	957.537	2.395	3.7	75	371.552	0.929	33.6				
37	948.179	2.372	9.2	76	366.484	0.917	35.6				
38	936.483	2.343	4.9	77	364.534	0.912	15.6				
39	816.791	2.043	9.1	78	-0.000	-0.000	12.1				

C13LF-VI-33c

Pulse Sequence: s2pu1

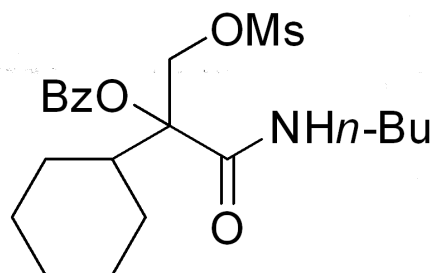
Solvent: CDCl3

Ambient temperature

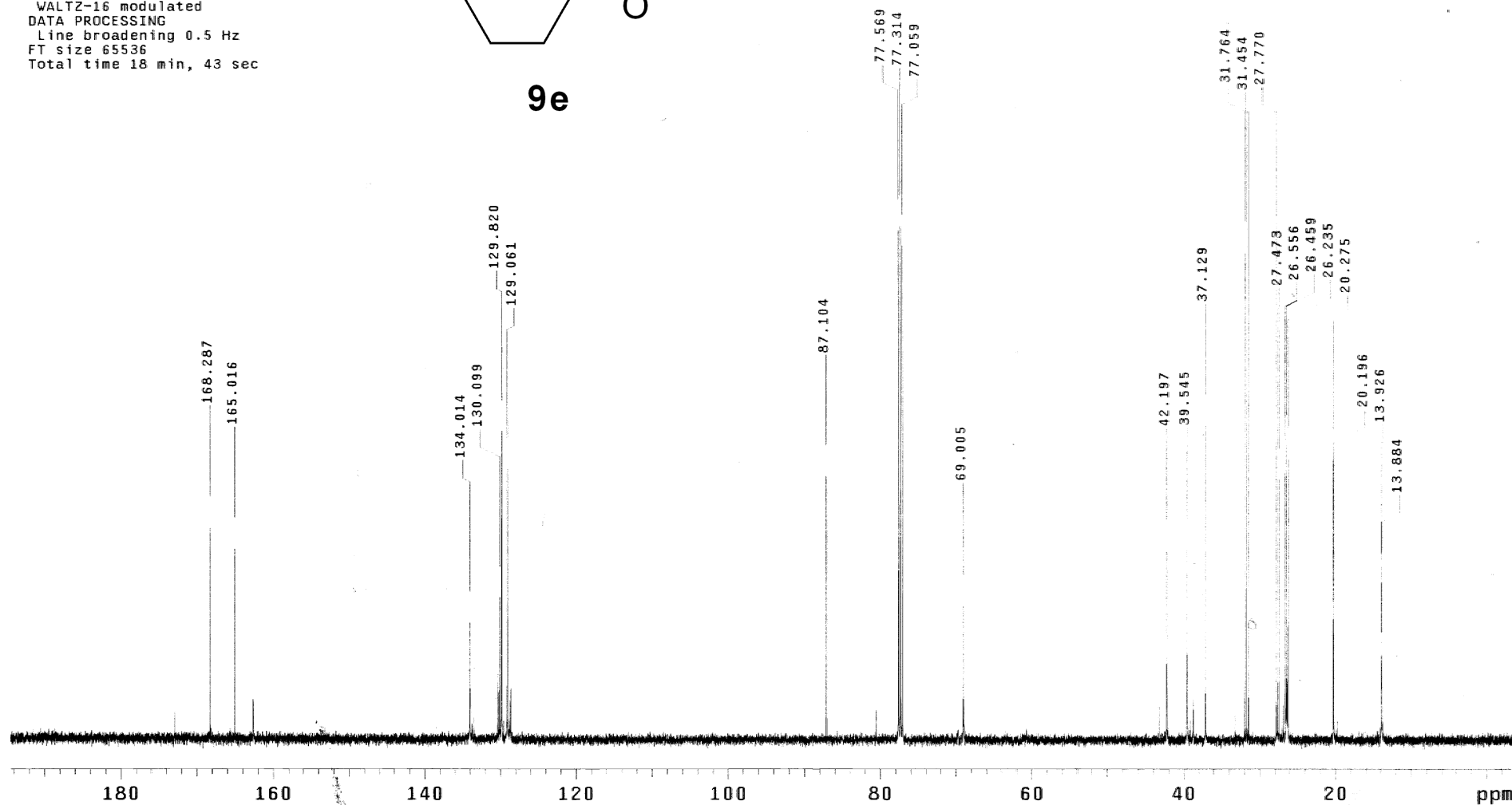
User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec
Pulse 54.0 degrees
Acq. time 1.300 sec
Width 25000.0 Hz
400 repetitions
OBSERVE C13, 125.7042615 MHz
DECOUPLE H1, 499.9197456 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 18 min, 43 sec



9e

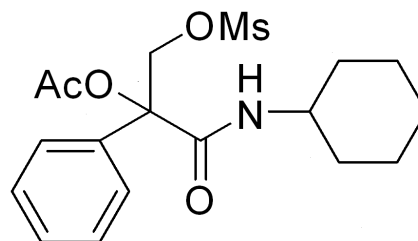


Sample directory:
File: PROTON

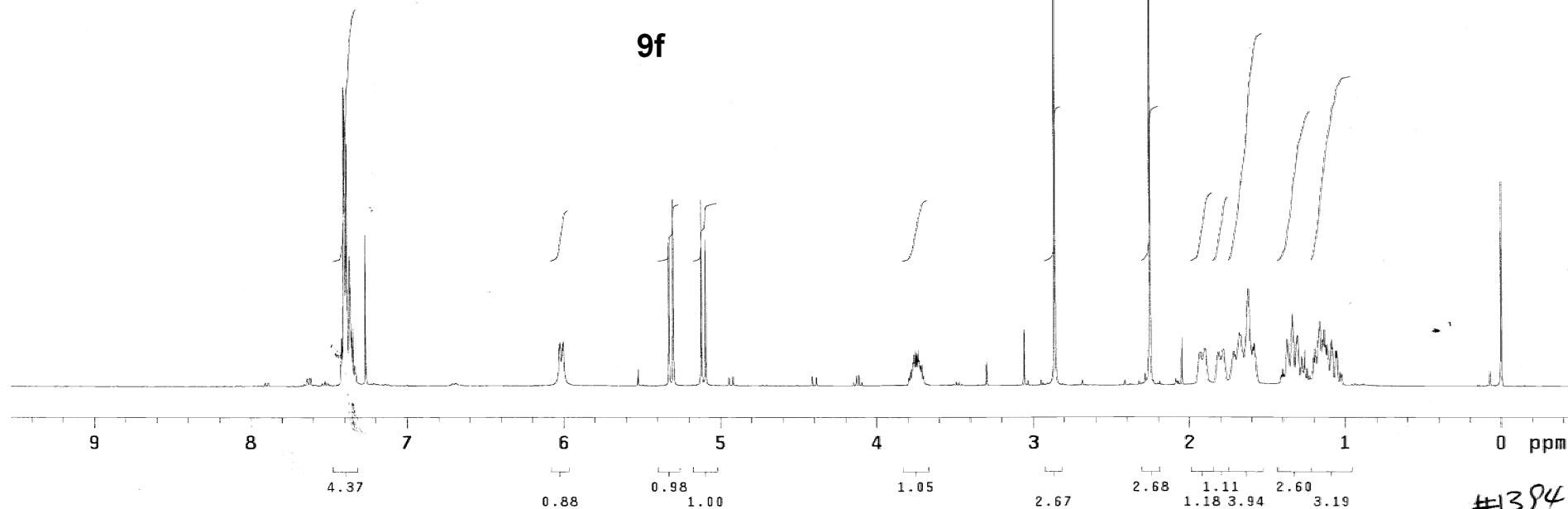
Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773438 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec



9f



#1384
-2- (KPP)
(DL)

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2967.350	7.423	3.6	40	667.858	1.671	8.3
2	2965.010	7.417	7.8	41	648.754	1.623	15.6
3	2958.382	7.400	47.4	42	636.668	1.593	6.3
4	2957.213	7.397	46.2	43	632.769	1.583	6.9
5	2954.484	7.390	15.1	44	548.556	1.372	7.6
6	2952.534	7.385	38.5	45	534.910	1.338	11.6
7	2944.737	7.366	20.8	46	521.655	1.305	8.2
8	2942.787	7.361	16.2	47	513.077	1.283	3.1
9	2940.058	7.354	9.0	48	510.348	1.277	4.8
10	2936.159	7.344	9.4	49	503.720	1.260	5.8
11	2931.871	7.334	3.4	50	479.938	1.201	4.7
12	2904.579	7.265	24.2	51	476.429	1.192	6.1
13	2408.657	6.025	7.1	52	474.090	1.186	4.8
14	2400.469	6.005	7.2	53	467.852	1.170	8.0
15	2208.650	5.525	3.0	54	464.733	1.162	10.5
16	2129.505	5.327	22.9	55	457.325	1.144	7.6
17	2118.978	5.300	29.8	56	453.426	1.134	9.0
18	2047.631	5.122	29.6	57	449.917	1.125	6.6
19	2036.715	5.095	23.4	58	446.019	1.116	6.8
20	1504.143	3.762	3.9	59	434.712	1.087	7.5
21	1501.804	3.757	5.7	60	431.593	1.080	6.2
22	1497.515	3.746	5.4	61	423.406	1.059	5.7
23	1493.227	3.735	5.8	62	420.287	1.051	5.7
24	1490.887	3.729	4.2	63	-0.000	-0.000	32.5
25	1486.989	3.720	3.4				
26	1482.700	3.709	3.5				
27	1317.392	3.295	4.0				
28	1221.873	3.056	9.0				
29	1143.508	2.860	162.2				
30	900.225	2.252	154.0				
31	818.351	2.047	7.8				
32	770.396	1.927	5.5				
33	761.039	1.904	6.0				
34	724.001	1.811	5.6				
35	715.033	1.789	5.7				
36	713.084	1.784	5.9				
37	685.793	1.715	5.6				
38	681.504	1.705	5.1				
39	671.367	1.679	8.6				

C13LF-VI-35b#2

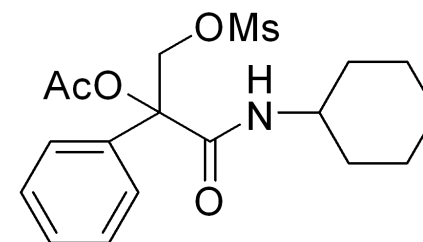
Sample directory:
File: CARBON

Pulse Sequence: s2pul

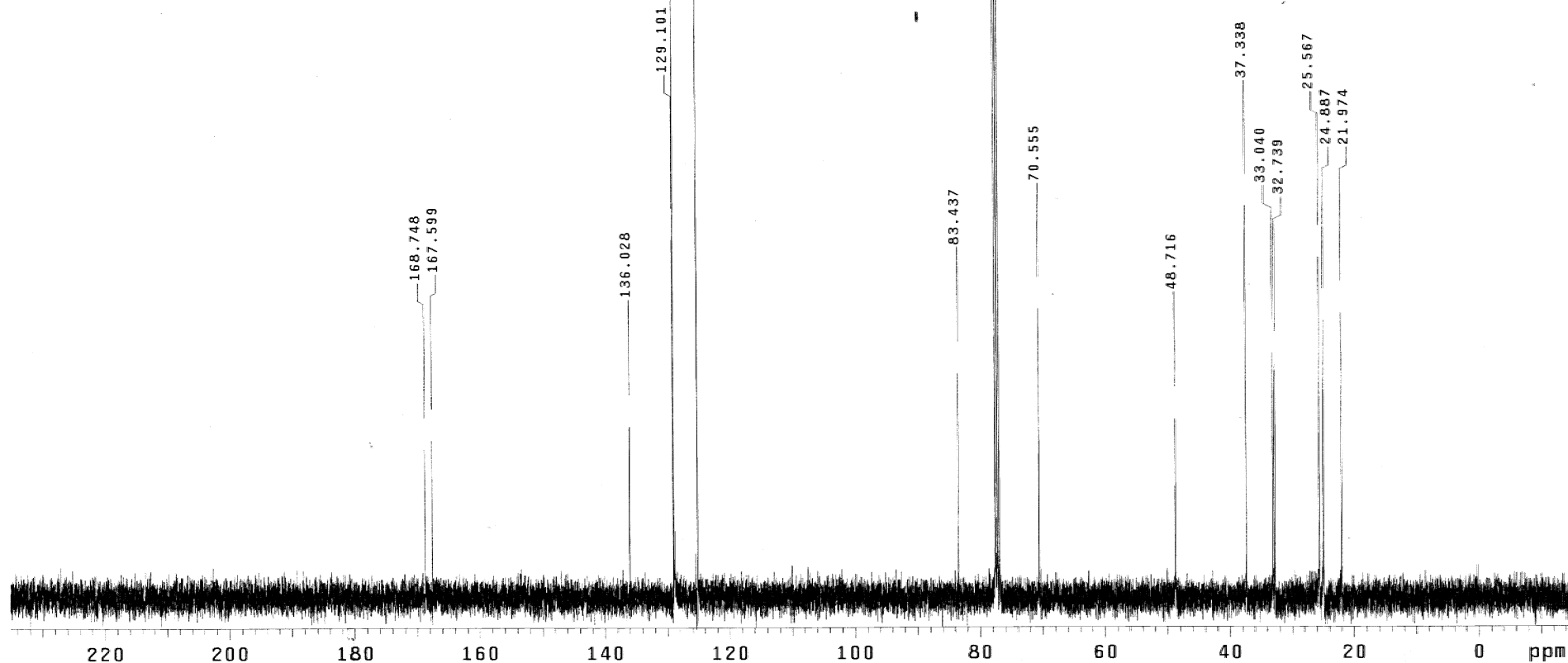
Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
600 repetitions
OBSERVE C13, 100.5240733 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 23 min, 6 sec

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#143
CDCl₃

LF-VI-51C#2

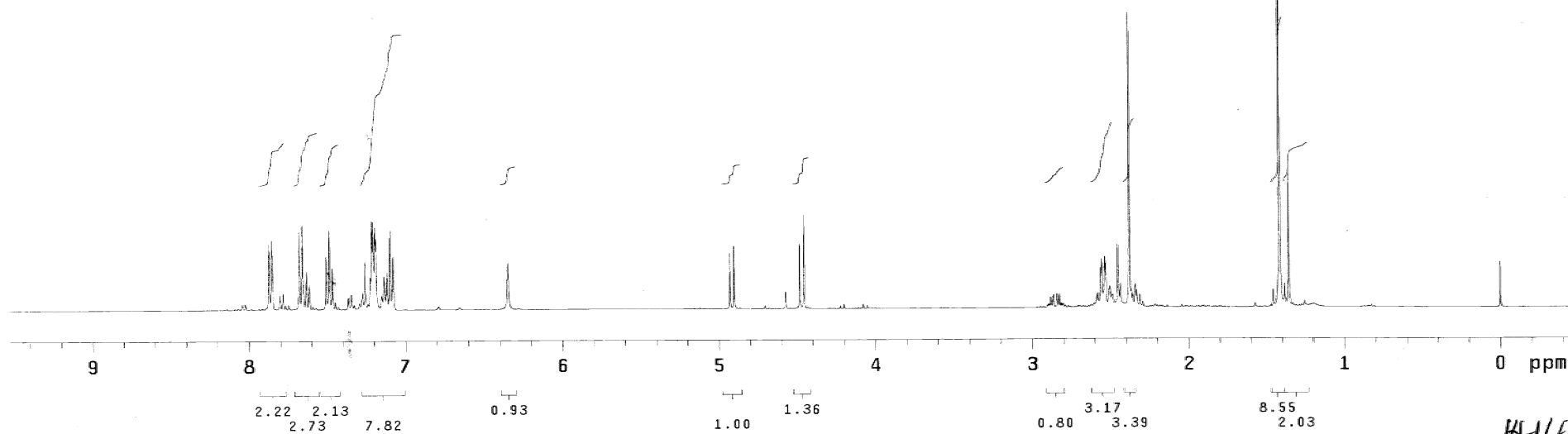
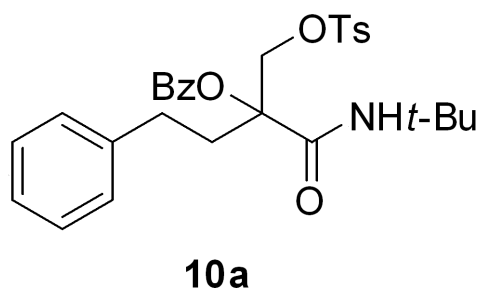
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773454 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

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#14
-2.14 ppm
1.0/1.0

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3146.303	7.870	10.7	40	553.235	1.384	3.9
2	3139.285	7.853	11.2	41	542.708	1.358	22.8
3	3137.726	7.849	9.6	42	-0.000	-0.000	7.3
4	3069.497	7.678	12.7				
5	3060.920	7.657	13.7				
6	3058.581	7.651	4.1				
7	3050.783	7.631	6.2				
8	3043.375	7.613	4.1				
9	3000.099	7.504	8.6				
10	2992.302	7.485	12.8				
11	2984.504	7.465	6.8				
12	2901.071	7.257	7.8				
13	2887.425	7.223	5.3				
14	2883.136	7.212	14.3				
15	2880.407	7.205	14.1				
16	2875.339	7.192	13.3				
17	2872.610	7.186	11.5				
18	2852.336	7.135	5.4				
19	2851.166	7.132	5.0				
20	2844.928	7.116	6.1				
21	2837.521	7.098	11.6				
22	2836.351	7.095	12.8				
23	2829.333	7.077	8.7				
24	2537.706	6.348	7.5				
25	1970.436	4.929	8.9				
26	1959.909	4.903	10.1				
27	1792.652	4.484	10.4				
28	1781.735	4.457	15.0				
29	1024.205	2.562	6.4				
30	1021.476	2.555	7.9				
31	1014.069	2.537	8.2				
32	1011.339	2.530	7.4				
33	1000.423	2.502	3.5				
34	979.759	2.451	10.1				
35	974.301	2.437	3.9				
36	950.519	2.378	46.8				
37	945.450	2.365	3.0				
38	935.314	2.340	3.8				
39	566.490	1.417	162.1				

C13LF-Vi-51c

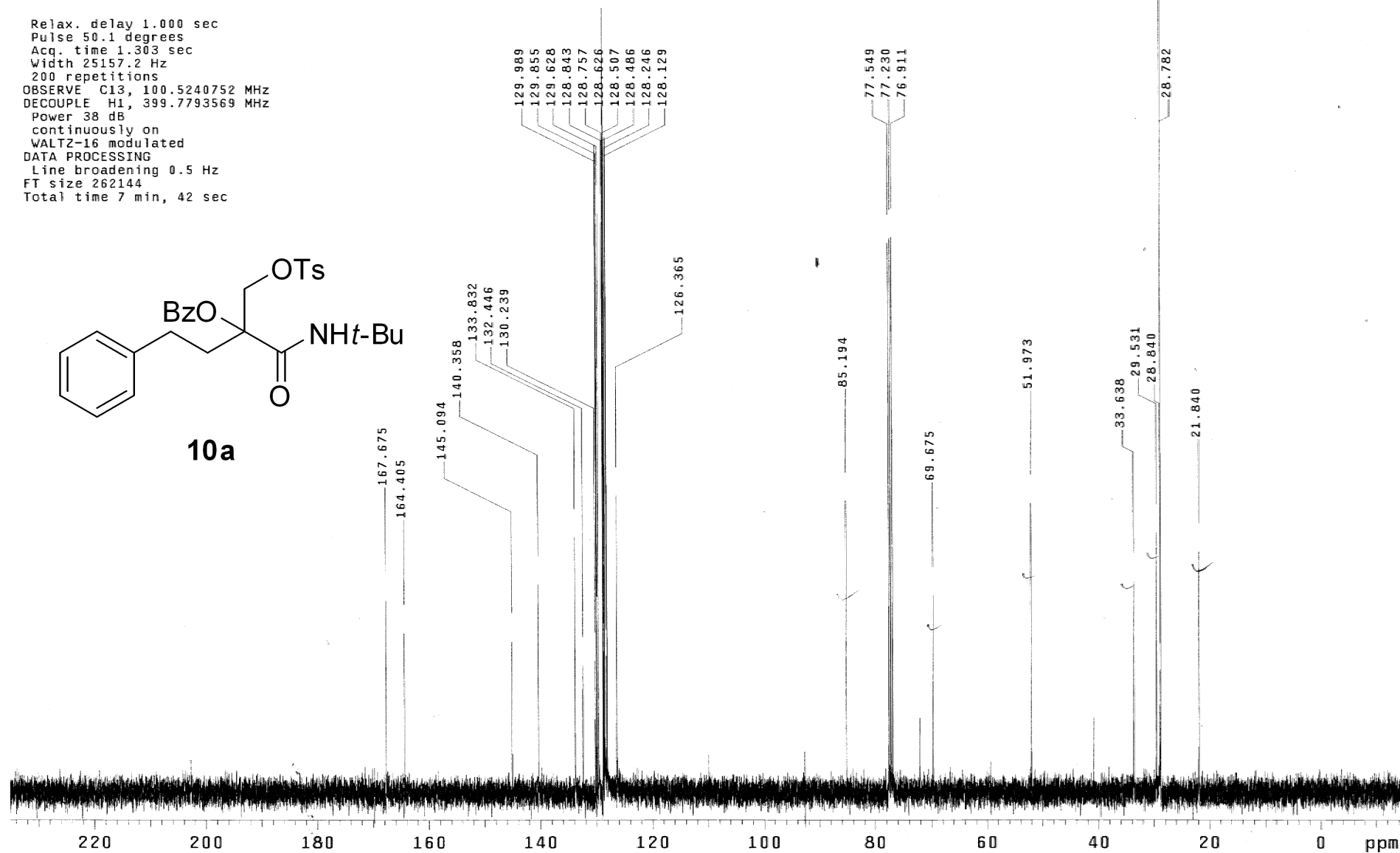
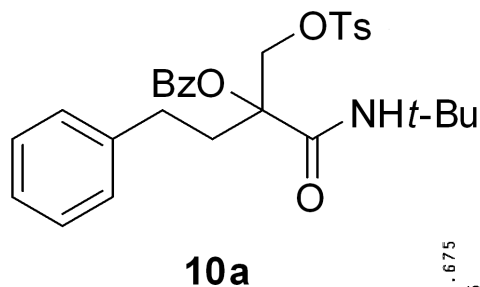
Sample directory:
File: CARBON

Pulse Sequence: s2pul

Solvent: CDC13
Temp. 20.0 C / 293.1 K
INNOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
200 repetitions
OBSERVE C13, 100.5240752 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 7 min, 42 sec

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LF-VI-53a

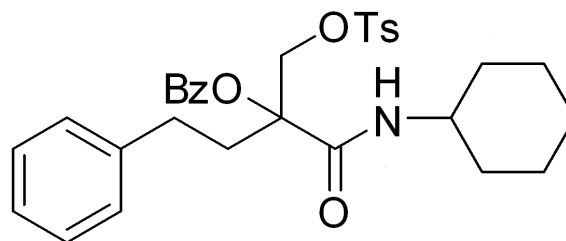
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

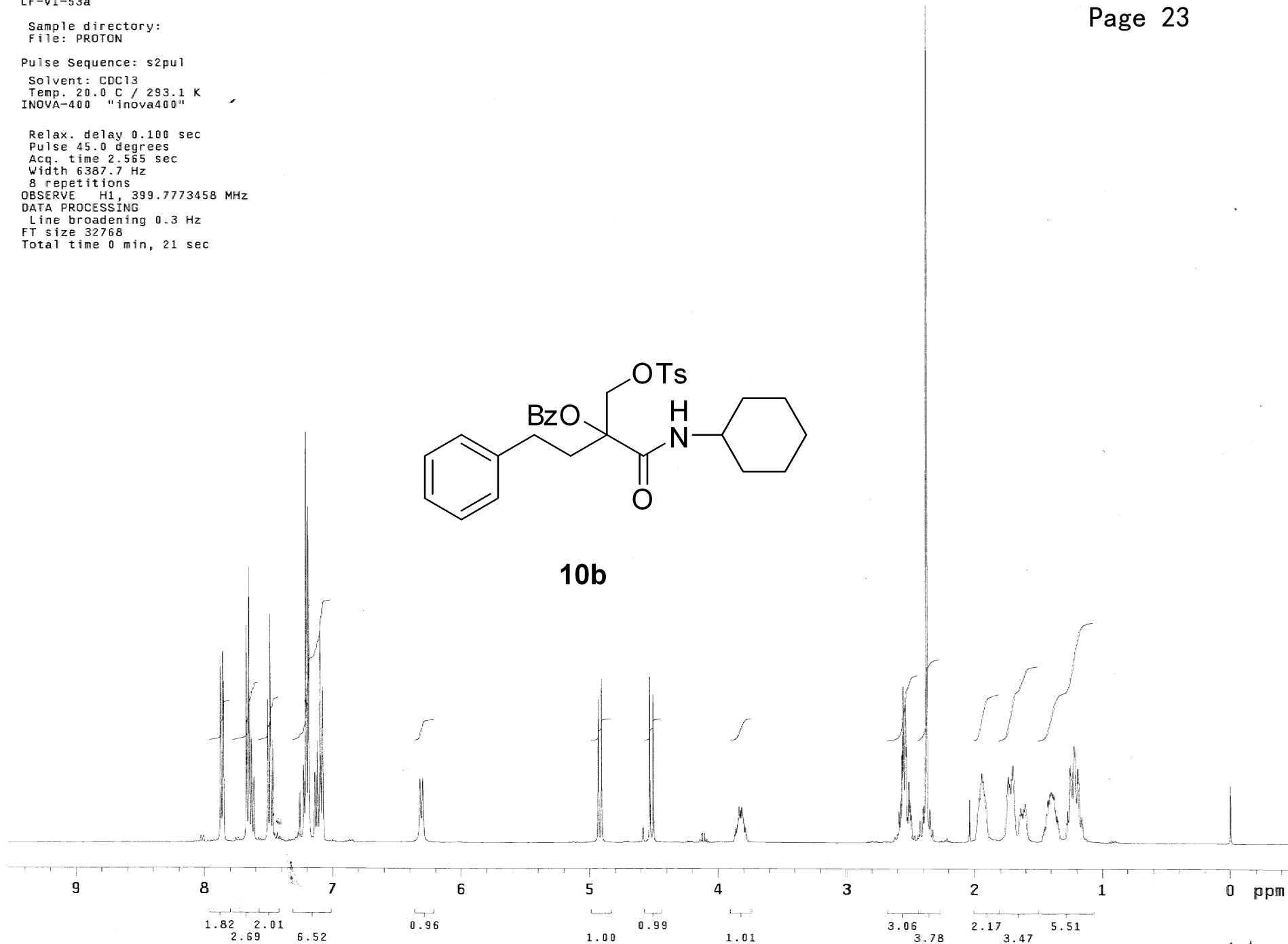
Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773458 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

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10b



12 #411
-2-14ppm
(CDCl₃)

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3147.083	7.872	36.0	40	996.914	2.494	5.6	79	494.363	1.237	11.6
2	3139.675	7.854	37.0	41	968.843	2.423	4.6	80	488.125	1.221	19.1
3	3066.768	7.671	42.0	42	959.096	2.399	7.1	81	476.819	1.193	14.6
4	3058.581	7.651	53.2	43	955.197	2.389	7.5	82	473.310	1.184	12.0
5	3051.563	7.633	20.4	44	948.959	2.374	162.3	83	465.123	1.163	5.3
6	3044.155	7.615	12.8	45	938.043	2.346	6.7	84	461.614	1.155	3.9
7	3000.489	7.505	28.0	46	815.232	2.039	8.6	85	-0.000	-0.000	11.4
8	2992.692	7.486	44.1	47	784.431	1.962	9.0				
9	2984.894	7.466	19.8	48	776.244	1.942	13.8				
10	2901.071	7.257	10.2	49	772.345	1.932	12.3				
11	2888.205	7.225	15.1	50	767.667	1.920	9.7				
12	2880.797	7.206	79.4	51	693.590	1.735	13.1				
13	2872.999	7.186	64.9	52	689.302	1.724	11.8				
14	2853.896	7.139	13.7	53	684.233	1.712	12.7				
15	2846.488	7.120	19.8	54	680.334	1.702	15.3				
16	2836.741	7.096	40.9	55	658.111	1.646	5.7				
17	2829.333	7.077	30.2	56	654.603	1.637	7.0				
18	2526.789	6.320	12.5	57	650.314	1.627	6.0				
19	2518.602	6.300	12.6	58	645.635	1.615	6.8				
20	1971.605	4.932	27.9	59	641.737	1.605	7.8				
21	1961.078	4.905	31.8	60	638.228	1.596	5.6				
22	1832.029	4.583	3.3	61	582.086	1.456	3.0				
23	1811.366	4.531	32.2	62	578.577	1.447	3.4				
24	1800.839	4.505	28.8	63	573.898	1.436	5.8				
25	1542.741	3.859	3.1	64	570.389	1.427	8.4				
26	1532.604	3.834	7.1	65	567.270	1.419	8.7				
27	1528.316	3.823	6.6	66	563.761	1.410	9.8				
28	1524.027	3.812	7.0	67	559.863	1.400	10.1				
29	1518.179	3.798	3.9	68	556.744	1.393	9.9				
30	1513.890	3.787	3.2	69	553.625	1.385	9.6				
31	1034.342	2.587	6.3	70	550.116	1.376	9.1				
32	1029.274	2.575	8.4	71	545.827	1.365	6.7				
33	1024.985	2.564	18.1	72	542.318	1.357	5.4				
34	1021.866	2.556	30.4	73	539.199	1.349	4.8				
35	1015.238	2.540	27.6	74	535.690	1.340	3.0				
36	1012.119	2.532	18.9	75	510.738	1.278	4.1				
37	1007.831	2.521	5.2	76	507.619	1.270	6.4				
38	1003.542	2.510	12.0	77	500.601	1.252	15.4				
39	999.643	2.500	8.1	78	499.432	1.249	13.5				

LF-VI-53a

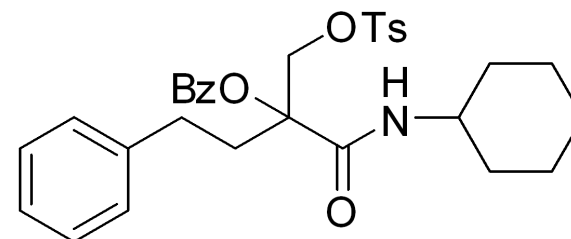
Sample directory:
File: CARBON

Pulse Sequence: s2pu1

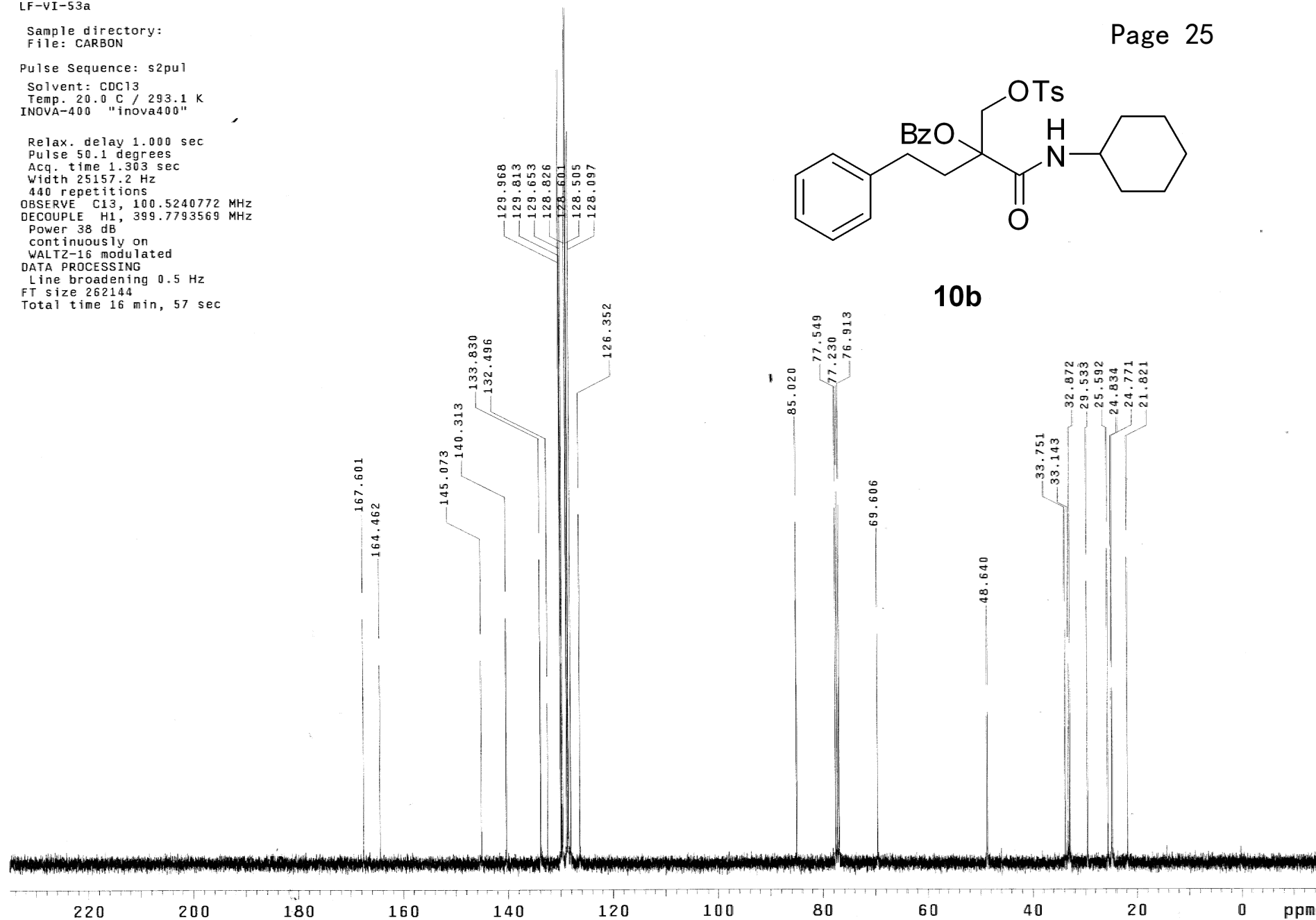
Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
440 repetitions
OBSERVE C13, 100.5240772 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 16 min, 57 sec

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LF-VI-55a

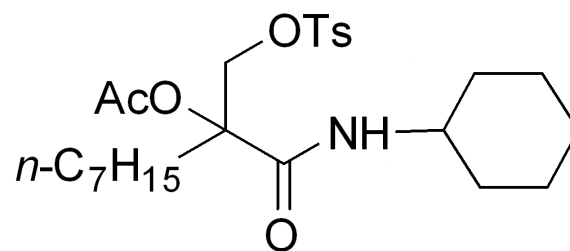
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

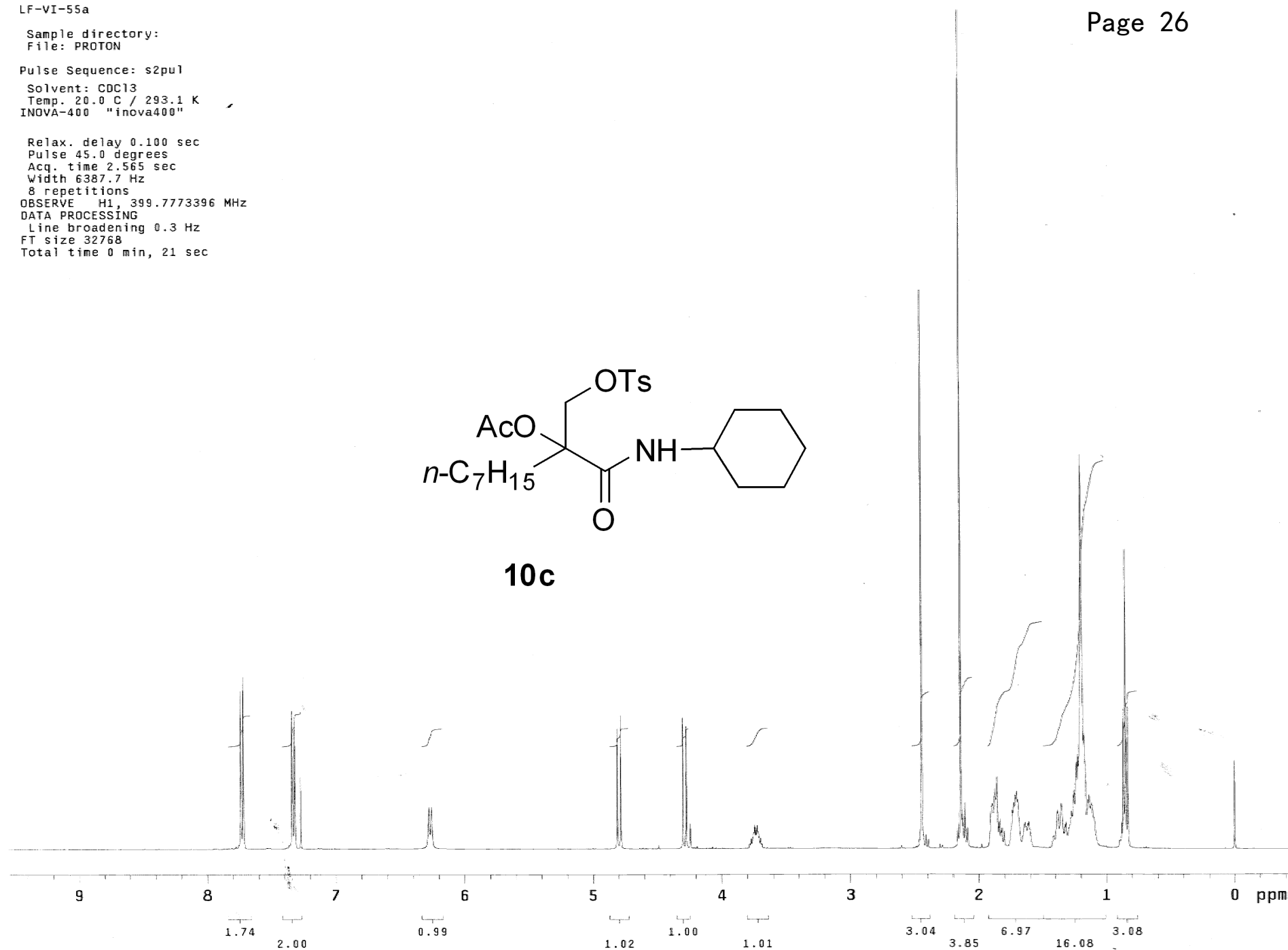
Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773396 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

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10c



13 #1405
-274ppm
-1.

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3094.059	7.739	30.6	40	677.215	1.694	9.7
2	3085.872	7.719	33.4	41	658.501	1.647	4.1
3	2934.600	7.341	26.8	42	654.992	1.638	5.2
4	2926.023	7.319	23.8	43	651.094	1.629	4.3
5	2907.309	7.272	14.1	44	646.025	1.616	5.0
6	2510.025	6.279	8.2	45	642.126	1.606	5.3
7	2501.837	6.258	8.3	46	638.618	1.597	3.8
8	1922.871	4.810	23.4	47	554.404	1.387	7.4
9	1912.344	4.784	25.9	48	552.065	1.381	7.6
10	1718.965	4.300	25.5	49	540.759	1.353	8.9
11	1708.439	4.273	23.9	50	532.571	1.332	3.3
12	1696.352	4.243	5.0	51	529.452	1.324	4.9
13	1500.634	3.754	3.1	52	526.723	1.318	5.3
14	1499.075	3.750	3.2	53	523.604	1.310	3.1
15	1497.126	3.745	4.7	54	517.756	1.295	4.1
16	1492.837	3.734	4.3	55	508.789	1.273	7.3
17	1488.548	3.723	4.7	56	501.771	1.255	11.5
18	1486.599	3.719	3.4	57	493.194	1.234	17.0
19	976.640	2.443	107.8	58	489.295	1.224	18.4
20	863.966	2.161	4.1	59	479.548	1.200	76.2
21	855.389	2.140	162.2	60	469.801	1.175	22.2
22	849.931	2.126	6.8	61	466.682	1.167	17.1
23	847.591	2.120	5.1	62	457.715	1.145	9.7
24	841.743	2.106	9.0	63	454.206	1.136	10.5
25	833.946	2.086	4.2	64	447.188	1.119	8.9
26	759.869	1.901	8.3	65	352.058	0.881	5.4
27	757.140	1.894	8.9	66	346.600	0.867	27.1
28	749.732	1.875	11.7	67	339.972	0.850	57.8
29	744.664	1.863	10.2	68	332.565	0.832	27.6
30	741.935	1.856	14.0	69	-0.000	-0.000	17.2
31	736.087	1.841	5.3				
32	733.747	1.835	5.9				
33	729.459	1.825	3.7				
34	726.730	1.818	4.1				
35	720.102	1.801	3.5				
36	693.980	1.736	7.6				
37	690.081	1.726	9.1				
38	685.403	1.714	10.5				
39	681.114	1.704	11.3				

LF-VI-55a

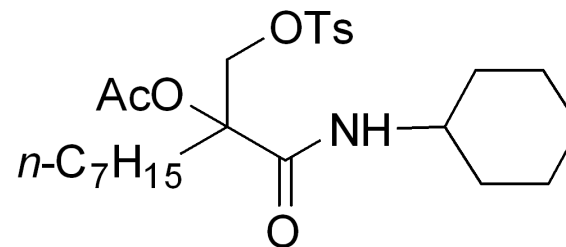
Sample directory:
File: CARBON

Pulse Sequence: s2pul

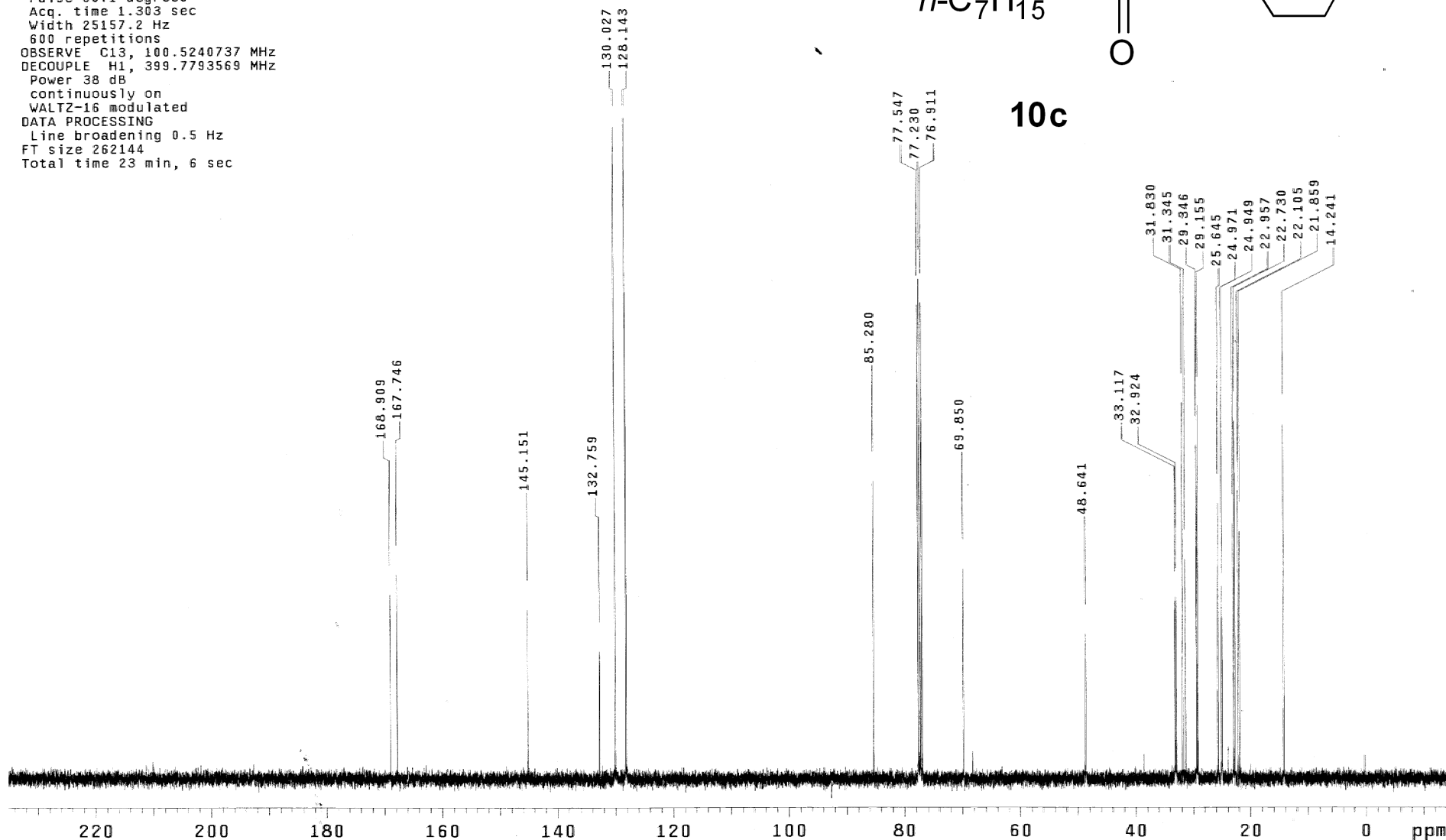
Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INNOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
600 repetitions
OBSERVE C13, 100.5240737 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 23 min, 6 sec

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10c



#178
2/19/20

LF-VI-35#2

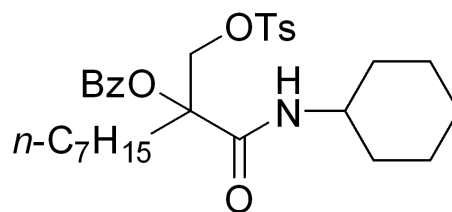
Sample directory:
File: PROTON

Pulse Sequence: s2pul

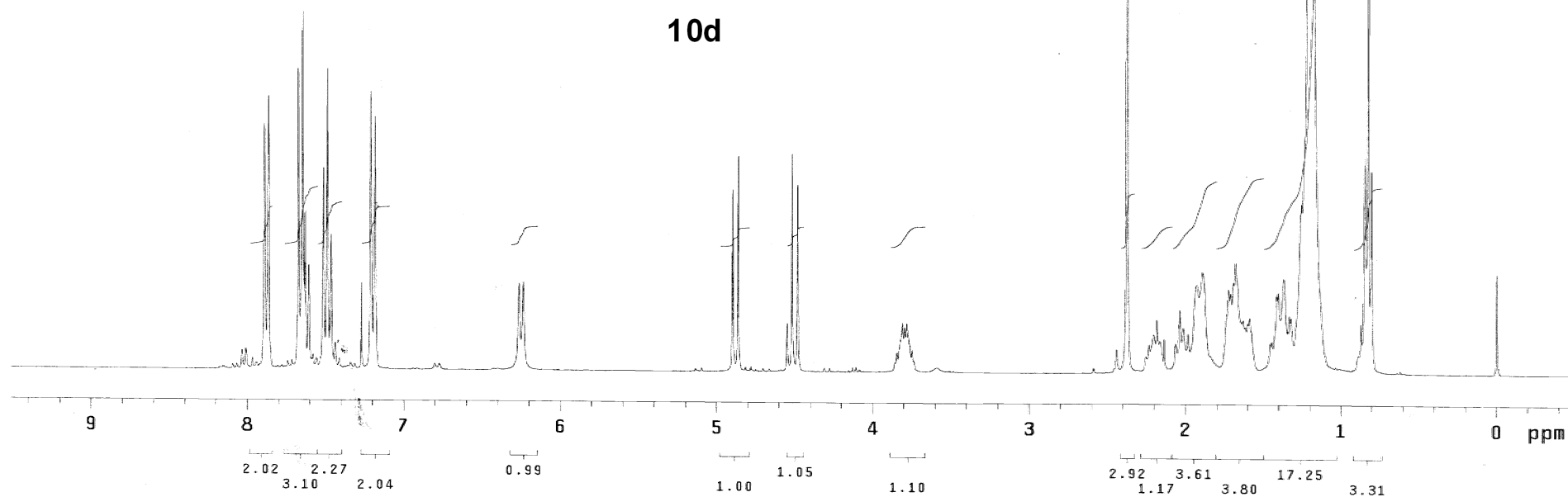
Solvent: CDCl₃
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611639 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 0 sec

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10d



#1413
14 274ppm

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2408.594	8.035	3.1	40	611.978	2.042	7.8
2	2401.433	8.011	3.3	41	609.932	2.035	10.1
3	2399.971	8.006	2.9	42	602.916	2.011	7.3
4	2365.915	7.893	39.0	43	594.292	1.983	6.3
5	2358.753	7.869	43.4	44	577.630	1.927	14.2
6	2357.438	7.864	37.9	45	566.960	1.891	16.2
7	2300.873	7.676	47.7	46	551.613	1.840	2.9
8	2292.542	7.648	56.7	47	516.827	1.724	13.5
9	2288.011	7.633	25.3	48	512.734	1.710	12.9
10	2280.557	7.608	16.7	49	507.619	1.693	14.6
11	2272.372	7.581	2.4	50	503.672	1.680	17.7
12	2252.932	7.516	32.0	51	489.202	1.632	8.5
13	2245.040	7.489	47.7	52	485.110	1.618	7.5
14	2237.439	7.464	21.6	53	479.994	1.601	8.0
15	2229.401	7.437	4.3	54	476.486	1.590	8.9
16	2179.413	7.270	13.9	55	435.561	1.453	5.1
17	2161.582	7.211	44.2	56	432.492	1.443	5.2
18	2153.104	7.183	40.2	57	424.161	1.415	12.5
19	1877.882	6.265	13.9	58	421.237	1.405	13.1
20	1869.697	6.237	14.1	59	410.421	1.369	15.3
21	1468.338	4.898	29.0	60	402.821	1.344	6.9
22	1457.814	4.863	34.2	61	399.605	1.333	9.3
23	1363.394	4.548	7.8	62	396.828	1.324	8.9
24	1353.893	4.517	34.7	63	376.512	1.256	27.0
25	1343.370	4.481	29.7	64	359.849	1.200	101.1
26	1152.629	3.845	3.2	65	356.049	1.188	99.3
27	1142.398	3.811	7.9	66	260.752	0.870	8.0
28	1138.159	3.797	7.2	67	254.321	0.848	34.4
29	1134.067	3.783	7.9	68	247.890	0.827	79.1
30	1123.689	3.749	3.6	69	240.874	0.804	32.4
31	730.953	2.438	3.8	70	-0.000	-0.000	16.2
32	712.245	2.376	162.4				
33	674.827	2.251	2.7				
34	669.273	2.233	4.6				
35	660.796	2.204	6.2				
36	653.926	2.181	8.6				
37	648.080	2.162	5.1				
38	639.602	2.134	5.5				
39	618.117	2.062	4.8				

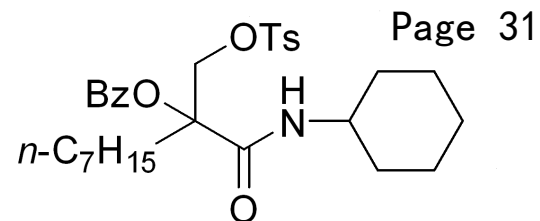
LF-VI-57a

Sample directory:
File: CARBON

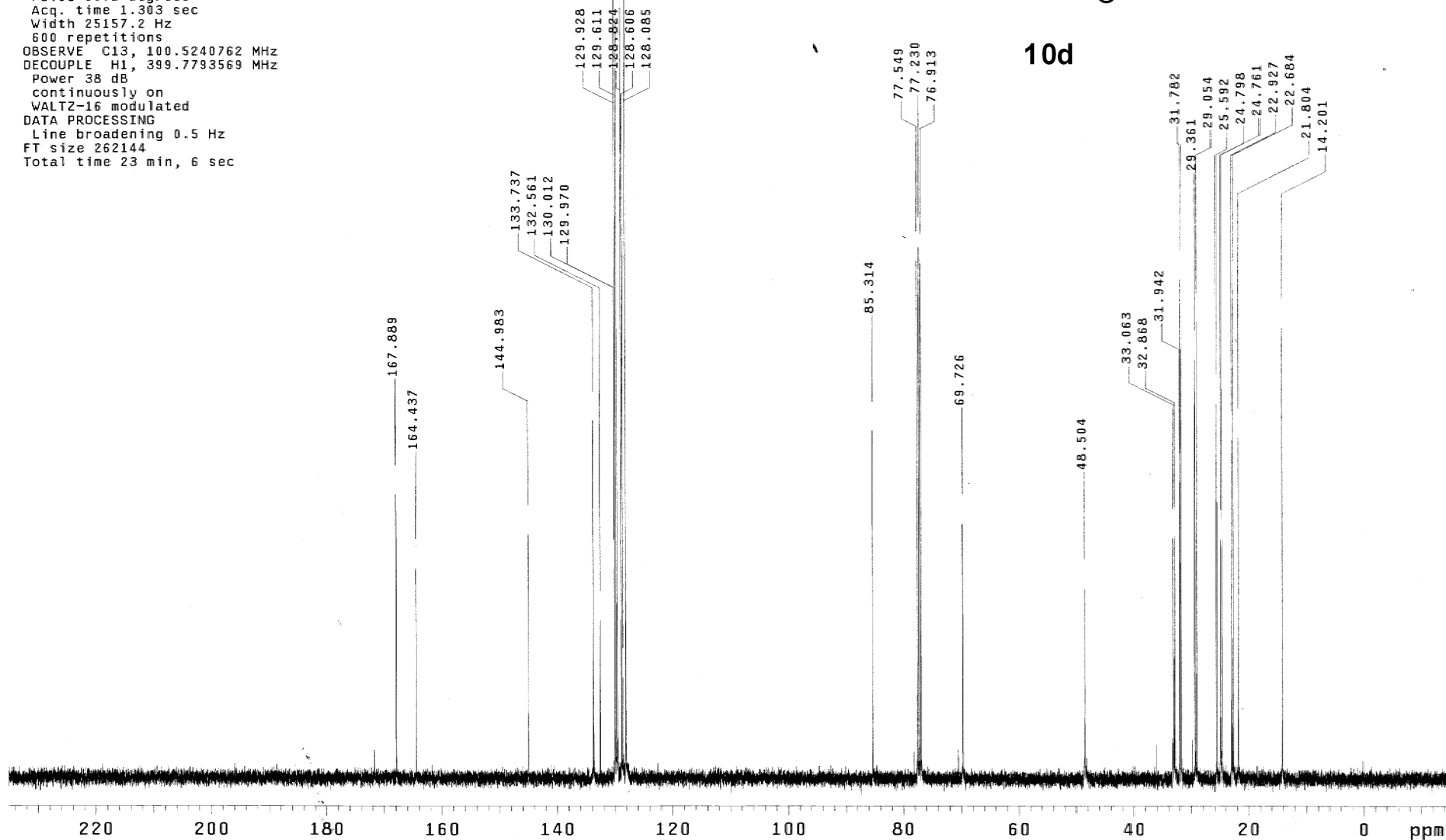
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
600 repetitions
OBSERVE C13, 100.5240762 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 23 min, 6 sec



10d



LF-VI-63a

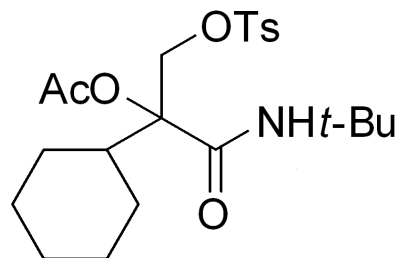
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

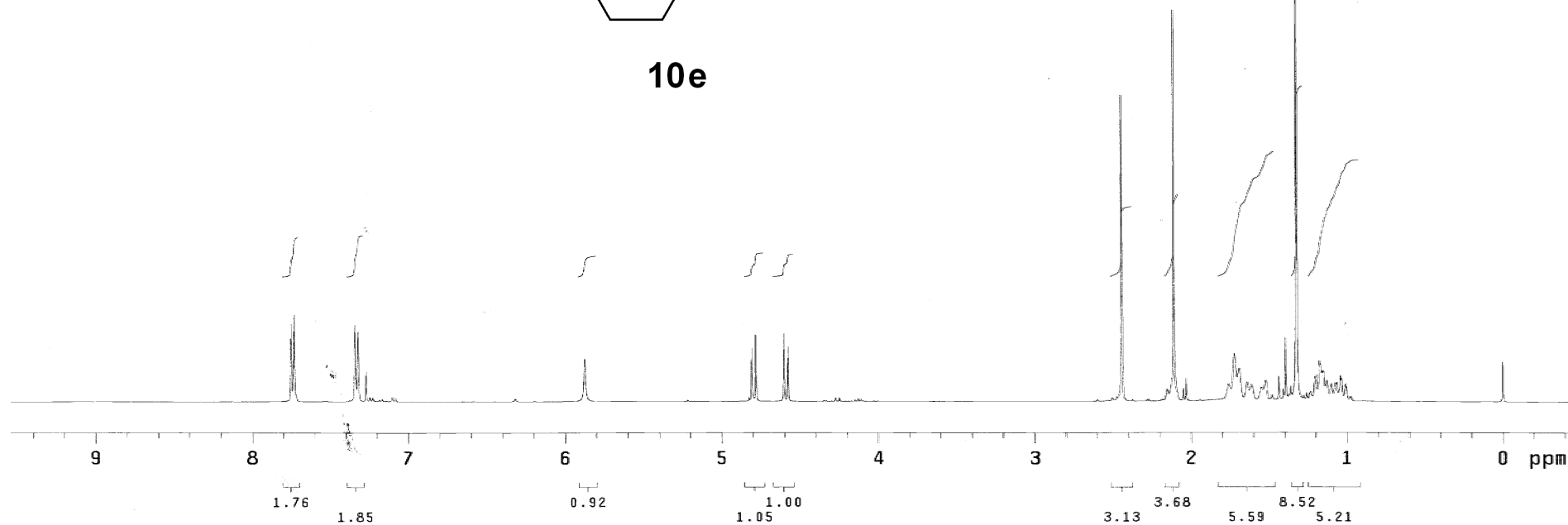
Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INNOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773396 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

Page 32



10e



15 #1418
-2-149pm

INDEX	FREQUENCY	PPM	HEIGHT
1	3099.128	7.752	12.5
2	3090.551	7.731	14.0
3	2935.380	7.343	12.3
4	2927.192	7.322	11.3
5	2906.919	7.271	4.9
6	2348.226	5.874	7.0
7	1922.091	4.808	8.5
8	1911.564	4.782	10.7
9	1840.217	4.603	10.9
10	1830.080	4.578	8.9
11	975.861	2.441	48.6
12	847.981	2.121	3.8
13	842.523	2.107	62.1
14	811.723	2.030	3.8
15	688.132	1.721	7.8
16	675.656	1.690	5.4
17	656.162	1.641	3.1
18	653.823	1.635	3.1
19	608.207	1.521	3.4
20	574.288	1.437	4.1
21	557.133	1.394	10.3
22	529.062	1.323	162.1
23	479.938	1.201	4.3
24	470.191	1.176	6.5
25	467.852	1.170	6.0
26	464.733	1.162	4.7
27	462.393	1.157	5.0
28	460.054	1.151	4.8
29	450.697	1.127	3.5
30	428.864	1.073	3.0
31	425.745	1.065	3.1
32	415.998	1.041	4.2
33	413.269	1.034	3.7
34	403.912	1.010	3.0
35	-0.000	-0.000	6.4

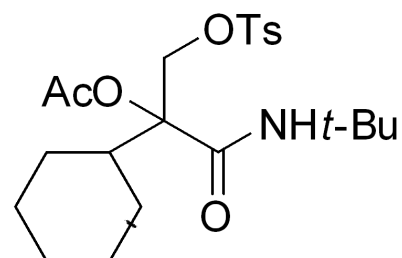
Lf-VI-63a

Sample directory:
File: CARBON

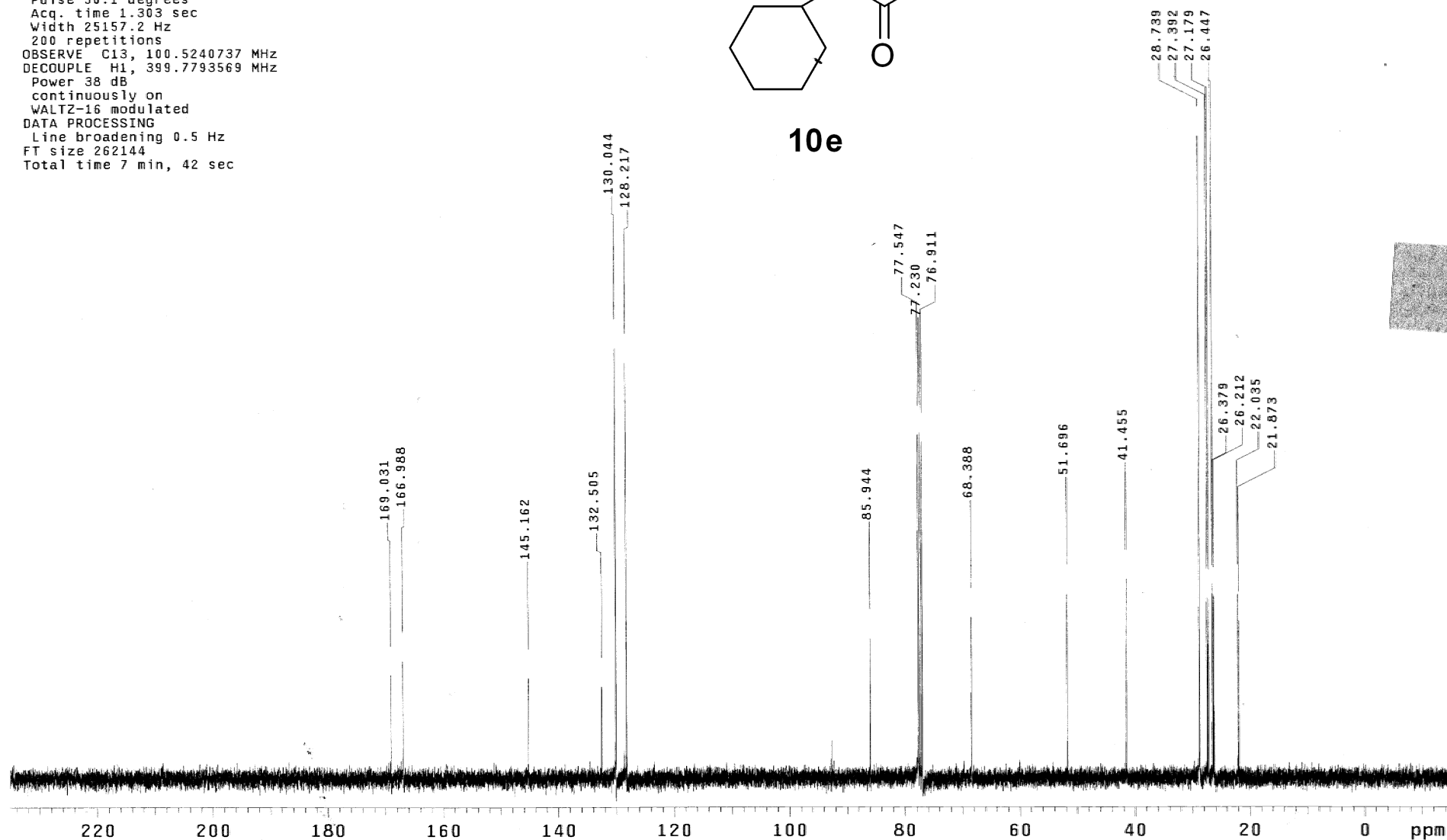
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
200 repetitions
OBSERVE C13, 100.5240737 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 7 min, 42 sec



10e



LF-VI-67c#2

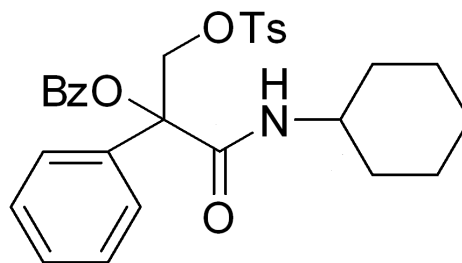
Page 35

Sample directory:
File: PROTON

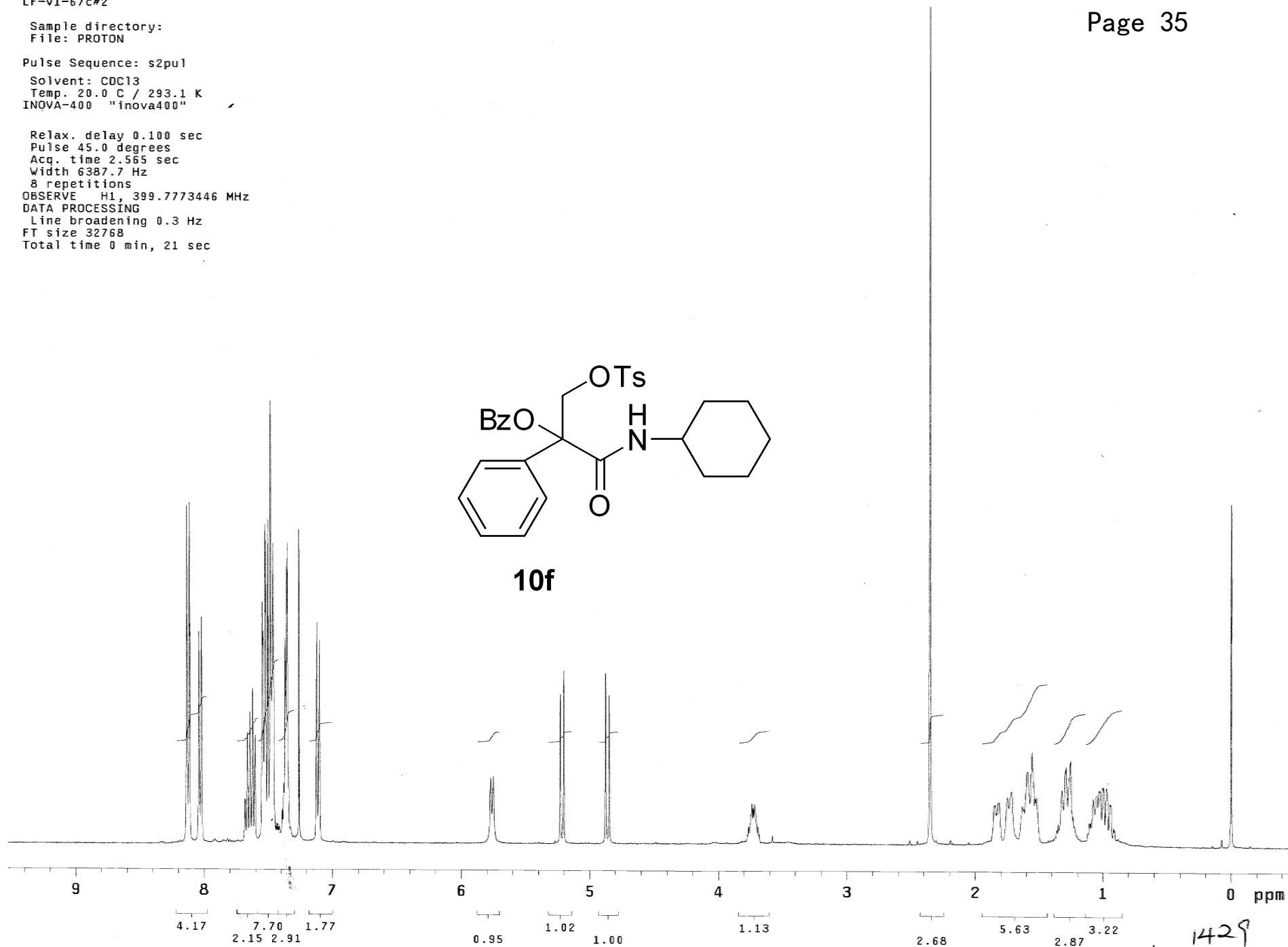
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INQVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773446 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec



10f



1429
16 -214ppm
CDCl₃

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3252.349	8.135	65.4	40	1504.533	3.763	3.8				
2	3244.162	8.115	65.9	41	1494.007	3.737	8.2				
3	3214.921	8.042	41.0	42	1490.108	3.727	7.4				
4	3206.734	8.021	43.8	43	1485.819	3.717	8.1				
5	3071.447	7.683	8.8	44	1475.292	3.690	3.8				
6	3070.667	7.681	8.7	45	940.382	2.352	162.4				
7	3063.649	7.663	21.7	46	737.646	1.845	8.1				
8	3056.631	7.646	19.7	47	724.780	1.813	8.6				
9	3055.462	7.643	25.6	48	699.048	1.749	9.6				
10	3054.292	7.640	18.4	49	686.962	1.718	10.7				
11	3047.664	7.623	30.1	50	651.873	1.631	7.9				
12	3040.646	7.606	21.2	51	647.585	1.620	7.3				
13	3039.477	7.603	20.4	52	635.499	1.590	14.7				
14	3017.254	7.547	46.8	53	621.853	1.555	18.4				
15	3015.304	7.542	41.2	54	612.106	1.531	9.4				
16	3008.676	7.526	61.9	55	608.207	1.521	9.7				
17	3007.507	7.523	58.6	56	543.878	1.360	3.3				
18	3000.099	7.504	62.7	57	539.979	1.351	4.5				
19	2992.302	7.485	85.7	58	527.893	1.320	11.1				
20	2984.114	7.464	58.1	59	518.146	1.296	15.0				
21	2969.689	7.428	4.0	60	515.417	1.289	15.6				
22	2963.841	7.414	3.5	61	501.381	1.254	16.9				
23	2954.874	7.391	6.6	62	493.584	1.235	6.0				
24	2950.195	7.380	12.0	63	489.295	1.224	4.0				
25	2946.296	7.370	39.8	64	442.120	1.106	4.7				
26	2943.957	7.364	29.2	65	438.611	1.097	4.8				
27	2940.838	7.356	53.4	66	430.034	1.076	9.4				
28	2939.668	7.353	58.2	67	420.287	1.051	10.0				
29	2929.142	7.327	3.4	68	411.710	1.030	11.0				
30	2903.020	7.262	60.7	69	408.980	1.023	11.0				
31	2902.240	7.260	56.8	70	400.793	1.003	11.7				
32	2847.657	7.123	42.8	71	398.454	0.997	11.5				
33	2839.470	7.103	39.4	72	389.097	0.973	11.5				
34	2307.679	5.772	13.0	73	378.570	0.947	8.4				
35	2299.491	5.752	13.3	74	375.841	0.940	8.4				
36	2091.687	5.232	29.2	75	367.264	0.919	3.7				
37	2080.771	5.205	33.7	76	363.755	0.910	3.3				
38	1949.772	4.877	33.3	77	0.000	0.000	66.3				
39	1939.245	4.851	29.1	78	-0.780	-0.002	64.8				

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 20.0 C / 293.1 K

File: C13LF-VI-67c

INNOVA-500 "wolff"

Relax. delay 1.000 sec

Pulse 50.1 degrees

Acq. time 1.303 sec

Width 25157.2 Hz

600 repetitions

OBSERVE C13, 100.5240724 MHz

DECOUPLE H1, 399.7793569 MHz

Power 38 dB

continuously on

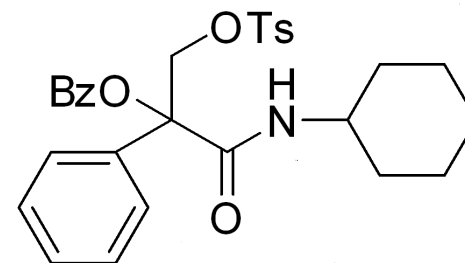
WALTZ-16 modulated

DATA PROCESSING

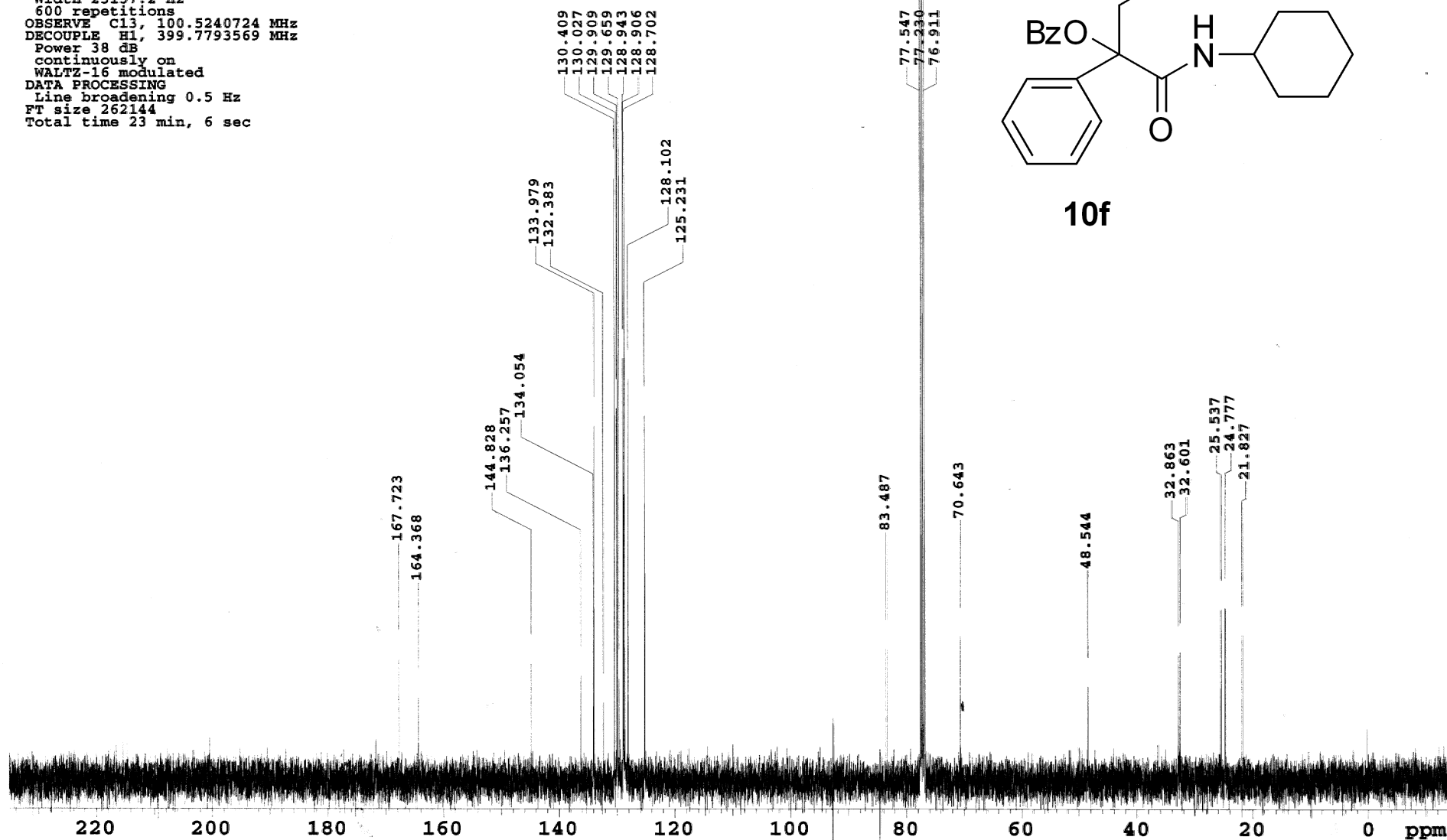
Line broadening 0.5 Hz

FT size 262144

Total time 23 min, 6 sec



10f

#151
-CDCl₃

Sample directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

File: LF-I-229a

Mercury-300BB "mercury300",

Relax. delay 1.000 sec

Pulse 49.2 degrees

Acq. time 3.000 sec

Width 4789.3 Hz

16 repetitions

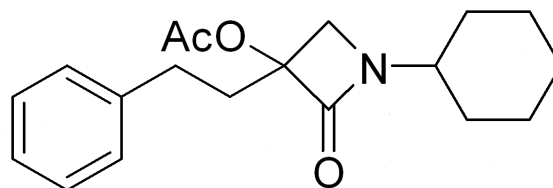
OBSERVE H1, 299.7611614 MHz

DATA PROCESSING

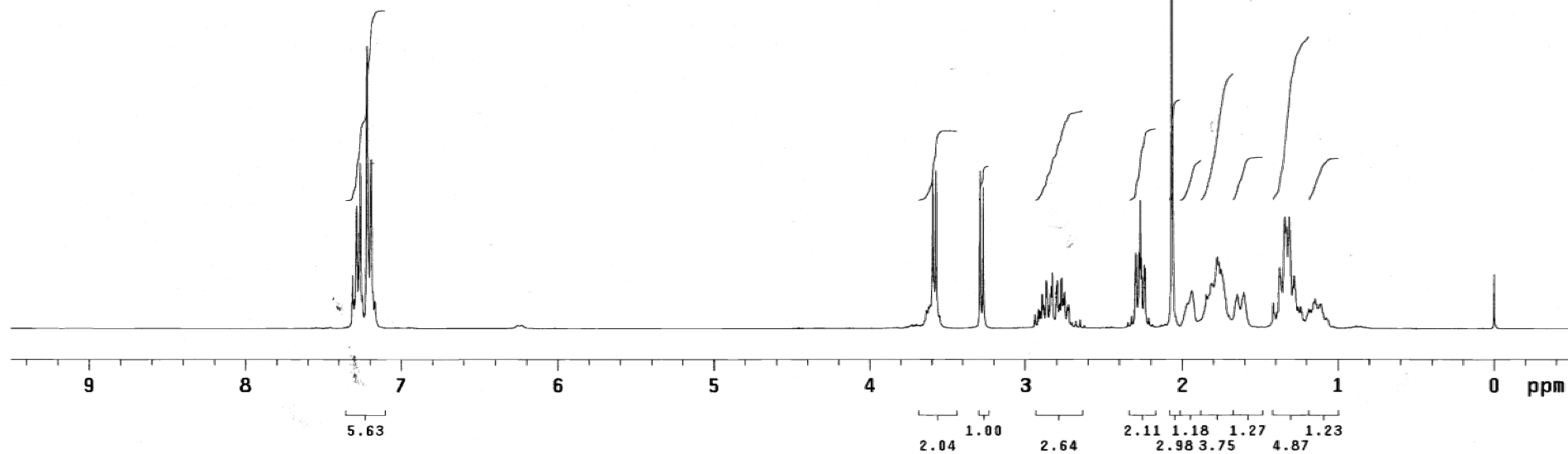
Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 18 sec



11a



17 #97

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2191.399	7.310	8.2	40	687.397	2.293	11.4	79	332.371	1.109	3.7
2	2189.791	7.305	4.0	41	681.989	2.275	11.7	80	-0.000	-0.000	8.3
3	2188.037	7.299	4.5	42	679.797	2.268	20.0				
4	2184.090	7.286	19.1	43	677.312	2.260	10.9				
5	2183.213	7.283	18.0	44	672.343	2.243	9.8				
6	2179.559	7.271	9.7	45	670.589	2.237	9.3				
7	2177.952	7.266	17.2	46	619.286	2.066	162.0				
8	2177.075	7.263	25.8	47	590.054	1.968	3.8				
9	2172.836	7.249	5.0	48	588.300	1.963	3.7				
10	2163.482	7.217	44.3	49	580.992	1.938	5.8				
11	2156.320	7.193	26.3	50	553.660	1.847	5.2				
12	2152.666	7.181	5.8	51	550.444	1.836	4.7				
13	2150.035	7.172	3.4	52	543.721	1.814	6.9				
14	2148.573	7.168	4.2	53	532.174	1.775	11.1				
15	2147.112	7.163	2.4	54	529.543	1.767	10.3				
16	1089.195	3.634	2.7	55	525.304	1.752	9.1				
17	1084.956	3.619	3.3	56	494.172	1.649	5.2				
18	1082.325	3.611	3.5	57	481.602	1.607	5.5				
19	1076.771	3.592	23.3	58	424.453	1.416	3.9				
20	1070.779	3.572	24.6	59	421.676	1.407	2.3				
21	985.274	3.287	24.6	60	417.145	1.392	2.4				
22	979.282	3.267	22.0	61	412.321	1.375	9.5				
23	873.461	2.914	2.9	62	410.567	1.370	8.1				
24	870.391	2.904	2.6	63	401.944	1.341	17.4				
25	866.299	2.890	5.2	64	399.021	1.331	15.8				
26	863.668	2.881	3.5	65	393.905	1.314	17.3				
27	858.698	2.865	7.4	66	386.159	1.288	6.4				
28	852.560	2.844	3.6	67	384.258	1.282	8.1				
29	849.783	2.835	6.5	68	381.481	1.273	6.0				
30	847.444	2.827	8.6	69	376.658	1.257	3.2				
31	839.259	2.800	6.6	70	371.689	1.240	3.3				
32	837.651	2.794	7.4	71	369.496	1.233	2.4				
33	833.413	2.780	3.7	72	355.903	1.187	2.9				
34	829.759	2.768	7.8	73	352.980	1.178	2.8				
35	826.543	2.757	4.6	74	346.549	1.156	4.0				
36	823.912	2.749	5.6	75	343.626	1.146	4.5				
37	818.504	2.731	3.2	76	340.848	1.137	3.7				
38	816.312	2.723	3.6	77	337.925	1.127	3.1				
39	688.859	2.298	11.7	78	334.417	1.116	3.7				

C13LF-I-229a

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: 13CLF-I-229a

INOVA-500 "wolff"

Relax. delay 1.000 sec

Pulse 45.3 degrees

Acq. time 0.996 sec

Width 18867.9 Hz

256 repetitions

OBSERVE C13, 75.3749925 MHz

DECOUPLE H1, 299.7627007 MHz

Power 36 dB

continuously on

WALTZ-16 modulated

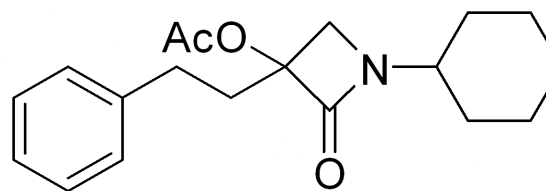
DATA PROCESSING

Line broadening 1.0 Hz

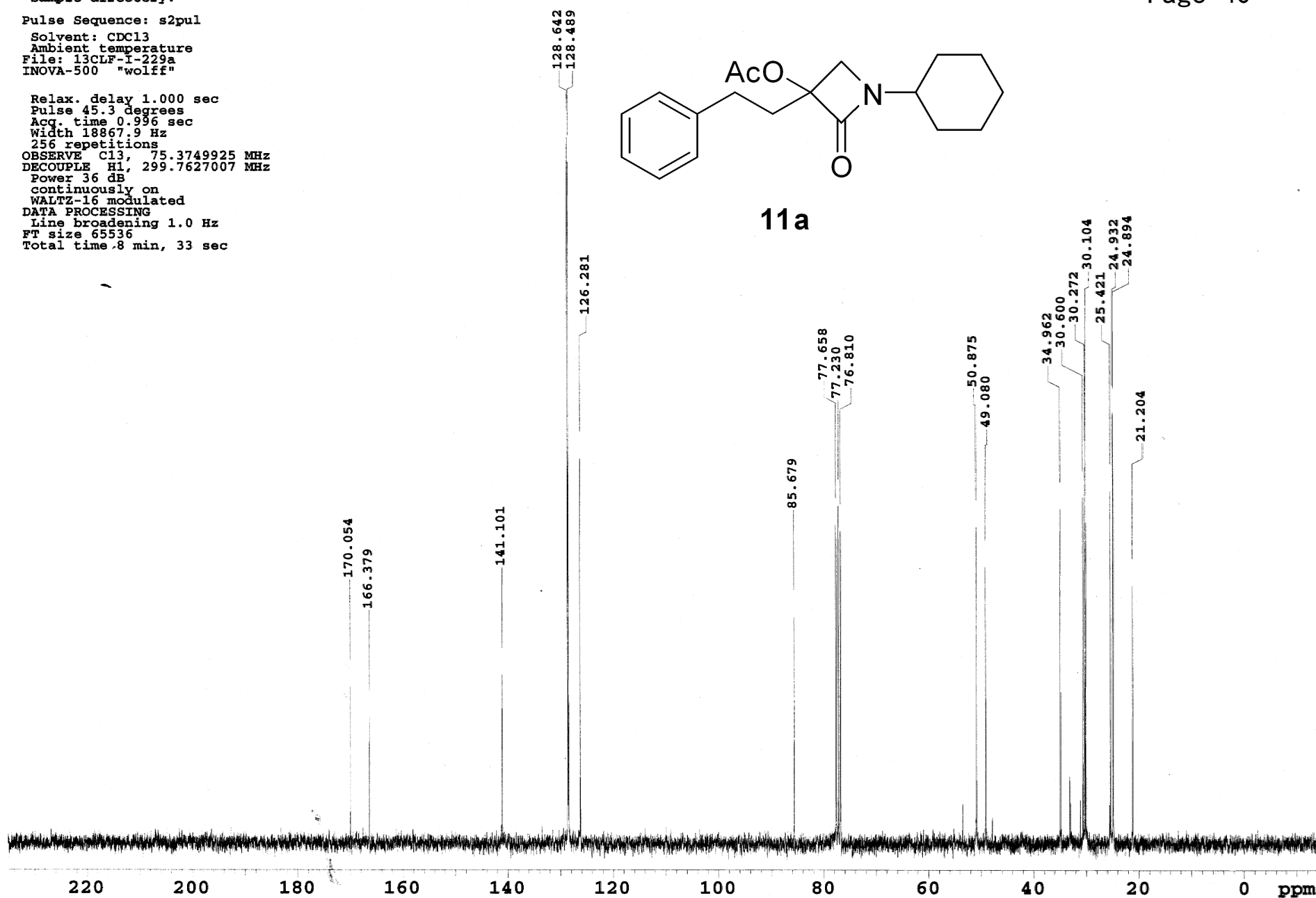
FT size 65536

Total time 8 min, 33 sec

Page 40



11a



#17
CDCl₃

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: LF-I-171

INOVA-500 "wittig"

Relax. delay 1.000 sec

Pulse 49.2 degrees

Acq. time 3.000 sec

Width 4789.3 Hz

16 repetitions

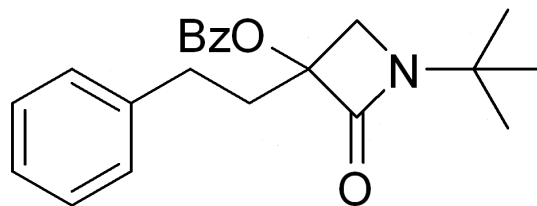
OBSERVE H1, 299.7611704 MHz

DATA PROCESSING

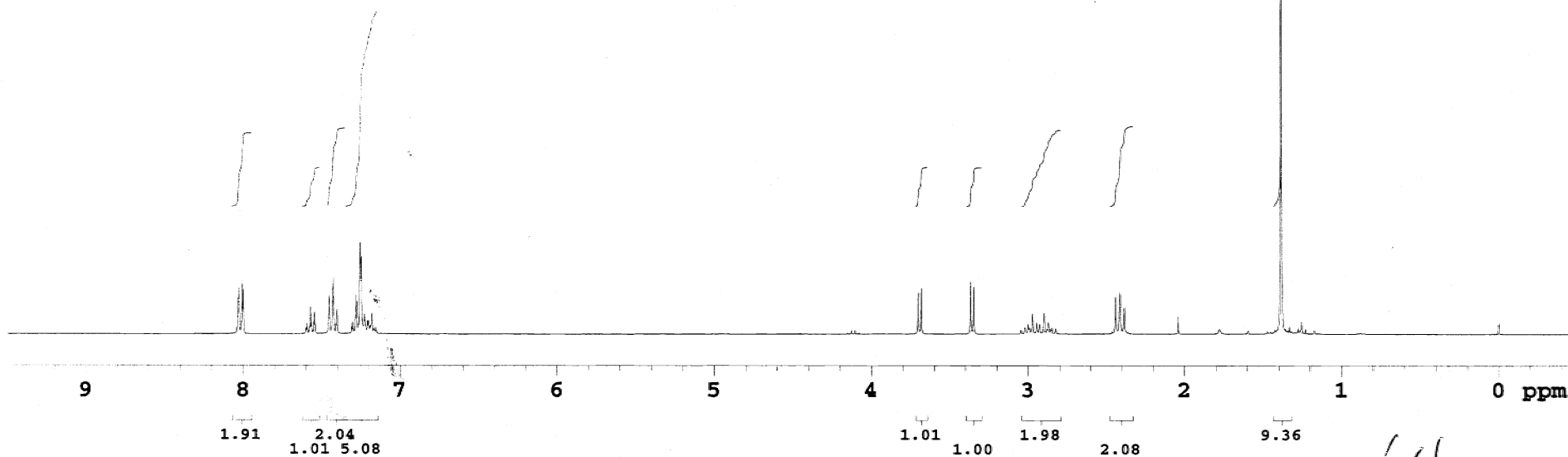
Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec



11b



18 # 64

INDEX	FREQUENCY	PPM	HEIGHT
1	2407.206	8.030	5.6
2	2406.767	8.029	5.6
3	2406.036	8.027	7.3
4	2400.921	8.009	2.1
5	2399.021	8.003	8.5
6	2397.559	7.998	6.8
7	2269.526	7.571	4.4
8	2262.072	7.546	3.4
9	2234.302	7.454	6.0
10	2232.840	7.449	2.5
11	2227.579	7.431	5.1
12	2226.555	7.428	8.8
13	2219.248	7.403	3.9
14	2183.878	7.285	2.9
15	2182.416	7.281	6.1
16	2181.393	7.277	5.1
17	2175.108	7.256	14.4
18	2172.624	7.248	12.2
19	2166.193	7.226	3.1
20	2160.931	7.209	2.2
21	2159.177	7.203	2.1
22	2152.308	7.180	3.2
23	1109.770	3.702	6.5
24	1103.924	3.683	7.2
25	1009.360	3.367	8.2
26	1003.368	3.347	7.5
27	890.827	2.972	3.2
28	868.757	2.898	3.3
29	731.516	2.440	5.8
30	723.331	2.413	6.5
31	714.854	2.385	4.2
32	611.082	2.039	2.8
33	415.232	1.385	162.0

C13LF-I-171

Sample directory:

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

File: 13CLF-I-171

INOVA-500 "wolff"

Relax. delay 1.000 sec

Pulse 45.3 degrees

Acq. time 0.996 sec

Width 18867.9 Hz

256 repetitions

OBSERVE C13, 75.3749942 MHz

DECOUPLE H1, 299.7627007 MHz

Power 36 dB

continuously on

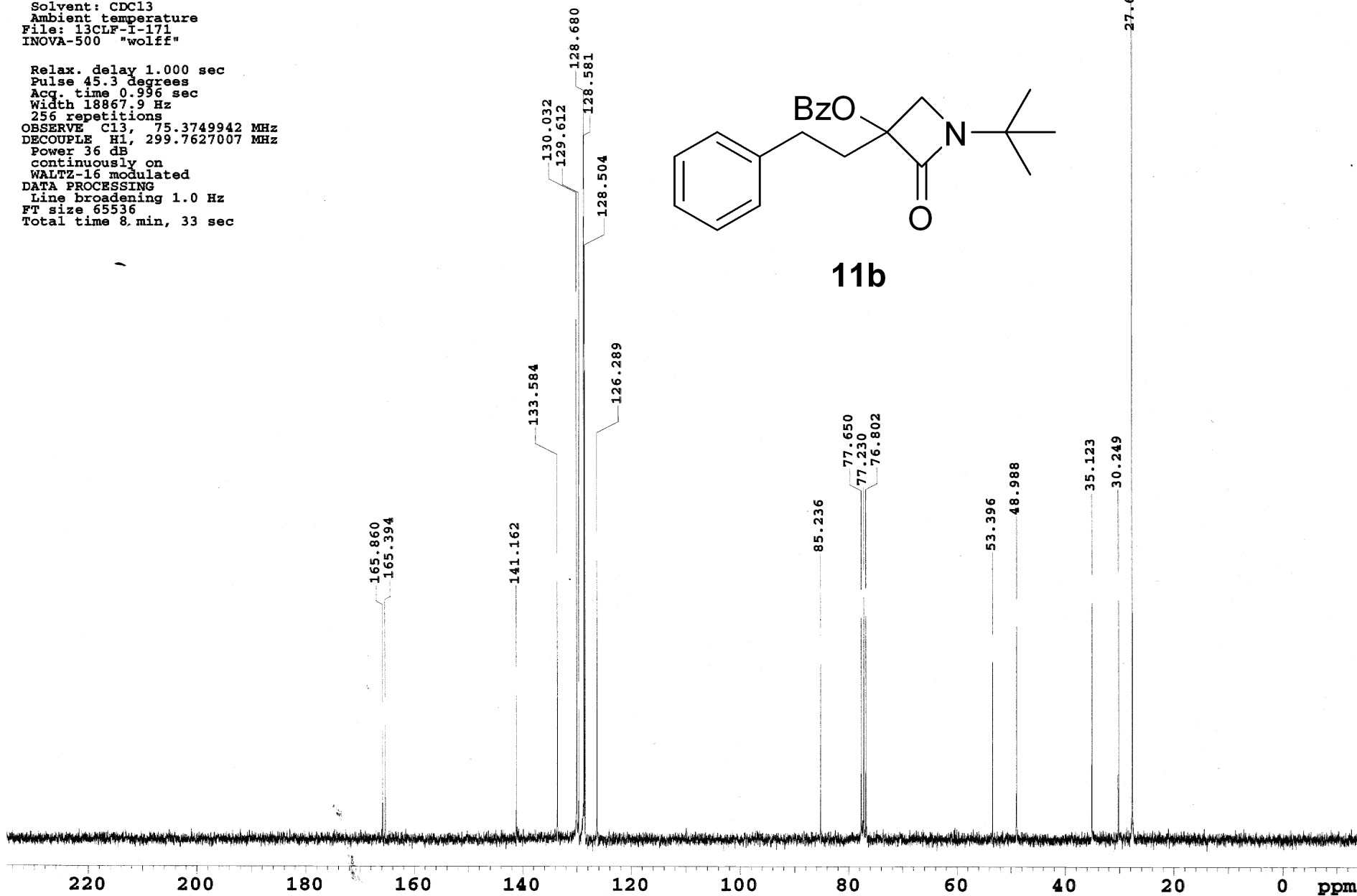
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

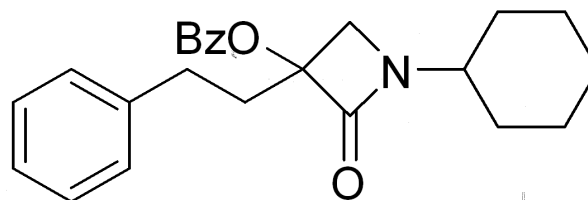
FT size 65536

Total time 8. min, 33 sec

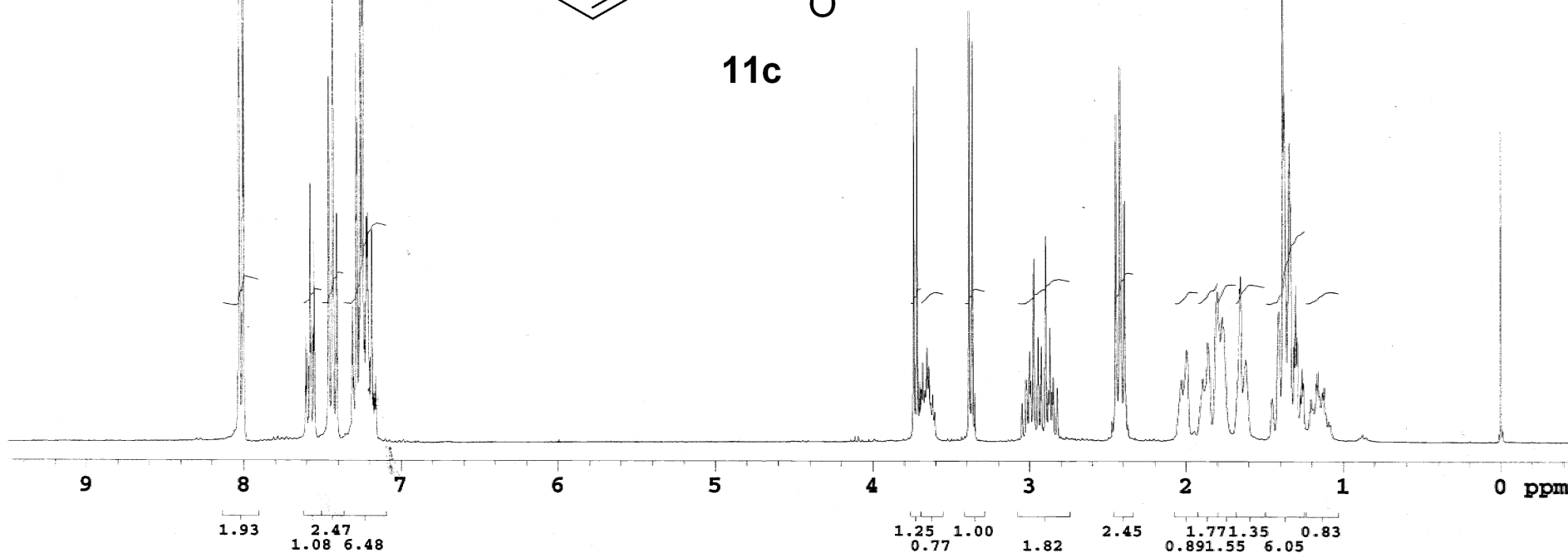


Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: LF-I-173
INOVA-500 "wittig"

Relax. delay 1.000 sec
Pulse 49.2 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611687 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 12 sec



11c



#65 19

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2409.398	8.038	8.3	40	2149.385	7.170	4.9	79	856.041	2.856	6.0	118	342.738	1.134	3.9
2	2407.644	8.032	54.5	41	2147.485	7.164	8.4	80	853.703	2.848	8.3	119	339.815	1.122	6.1
3	2406.475	8.028	69.1	42	2145.877	7.159	3.6	81	846.541	2.824	6.6	120	336.307	1.111	6.8
4	2401.359	8.011	18.5	43	2124.538	7.087	-2.1	82	734.439	2.450	49.6	121	333.092	-0.000	2.6
5	2399.459	8.005	80.4	44	2114.161	7.053	-2.1	83	731.808	2.441	10.4	122	-0.000	-0.000	47.0
6	2397.998	8.000	63.4	45	2106.122	7.026	-2.2	84	726.400	2.423	57.2				
7	2280.780	7.609	6.8	46	2099.107	7.003	-2.2	85	717.777	2.394	36.1				
8	2279.610	7.605	14.7	47	2090.629	6.974	-2.2	86	608.013	2.028	8.0				
9	2278.295	7.600	9.0	48	2078.937	6.935	-2.2	87	598.513	1.997	12.7				
10	2274.203	7.587	10.0	49	2071.921	6.912	-2.2	88	567.820	1.894	8.1				
11	2272.156	7.580	39.0	50	2068.560	6.901	-2.1	89	565.189	1.885	6.4				
12	2270.256	7.574	13.6	51	2059.206	6.869	-2.2	90	558.027	1.862	13.8				
13	2266.018	7.559	16.0	52	1994.312	6.653	-2.2	91	539.758	1.801	21.8				
14	2264.702	7.555	29.7	53	1796.269	5.992	-2.2	92	530.550	1.770	17.9				
15	2263.387	7.551	16.4	54	1793.785	5.984	-2.1	93	528.211	1.762	16.3				
16	2236.494	7.461	55.6	55	1120.878	3.739	54.0	94	498.249	1.662	22.4				
17	2235.179	7.457	25.3	56	1114.885	3.719	60.0	95	497.226	1.659	22.3				
18	2228.748	7.435	83.1	57	1110.208	3.704	7.6	96	495.911	1.654	24.3				
19	2222.902	7.416	12.5	58	1106.993	3.693	6.4	97	486.118	1.622	11.2				
20	2221.294	7.410	34.1	59	1104.216	3.684	10.8	98	437.156	1.458	4.3				
21	2191.916	7.312	11.9	60	1099.831	3.669	6.3	99	435.694	1.453	5.1				
22	2190.601	7.308	19.5	61	1095.885	3.656	13.2	100	423.563	1.413	18.8				
23	2189.139	7.303	8.3	62	1092.085	3.643	10.1	101	415.670	1.387	162.0				
24	2184.608	7.288	33.6	63	1089.016	3.633	4.3	102	412.893	1.377	53.0				
25	2183.439	7.284	59.2	64	1084.923	3.619	5.6	103	405.732	1.354	20.4				
26	2182.270	7.280	48.0	65	1081.123	3.607	2.8	104	402.955	1.344	45.2				
27	2178.908	7.269	19.3	66	1015.060	3.386	65.9	105	400.616	1.336	35.6				
28	2175.985	7.259	134.0	67	1009.068	3.366	61.2	106	393.893	1.314	13.2				
29	2172.770	7.248	69.0	68	1004.098	3.350	5.8	107	390.970	1.304	22.8				
30	2171.016	7.242	98.3	69	913.481	3.047	4.2	108	388.047	1.295	14.7				
31	2168.239	7.233	14.1	70	905.881	3.022	7.9	109	381.177	1.272	5.5				
32	2166.046	7.226	20.3	71	899.596	3.001	12.4	110	378.547	1.263	9.8				
33	2164.439	7.221	33.5	72	896.965	2.992	7.8	111	376.062	1.255	7.4				
34	2162.831	7.215	34.2	73	891.411	2.974	27.0	112	363.785	1.214	3.0				
35	2161.516	7.211	22.5	74	883.080	2.946	14.7	113	360.862	1.204	4.9				
36	2159.177	7.203	10.7	75	877.088	2.926	13.2	114	357.500	1.193	3.4				
37	2156.839	7.195	11.4	76	868.611	2.898	30.5	115	351.654	1.173	7.4				
38	2154.354	7.187	31.5	77	863.203	2.880	6.3	116	348.438	1.162	9.4				
39	2151.431	7.177	5.7	78	860.280	2.870	16.1	117	345.515	1.153	5.4				

C13 LF-I-173

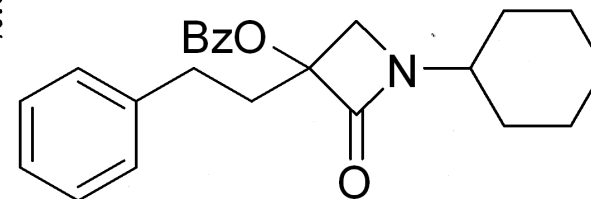
Sample directory:

Pulse Sequence: s2pul

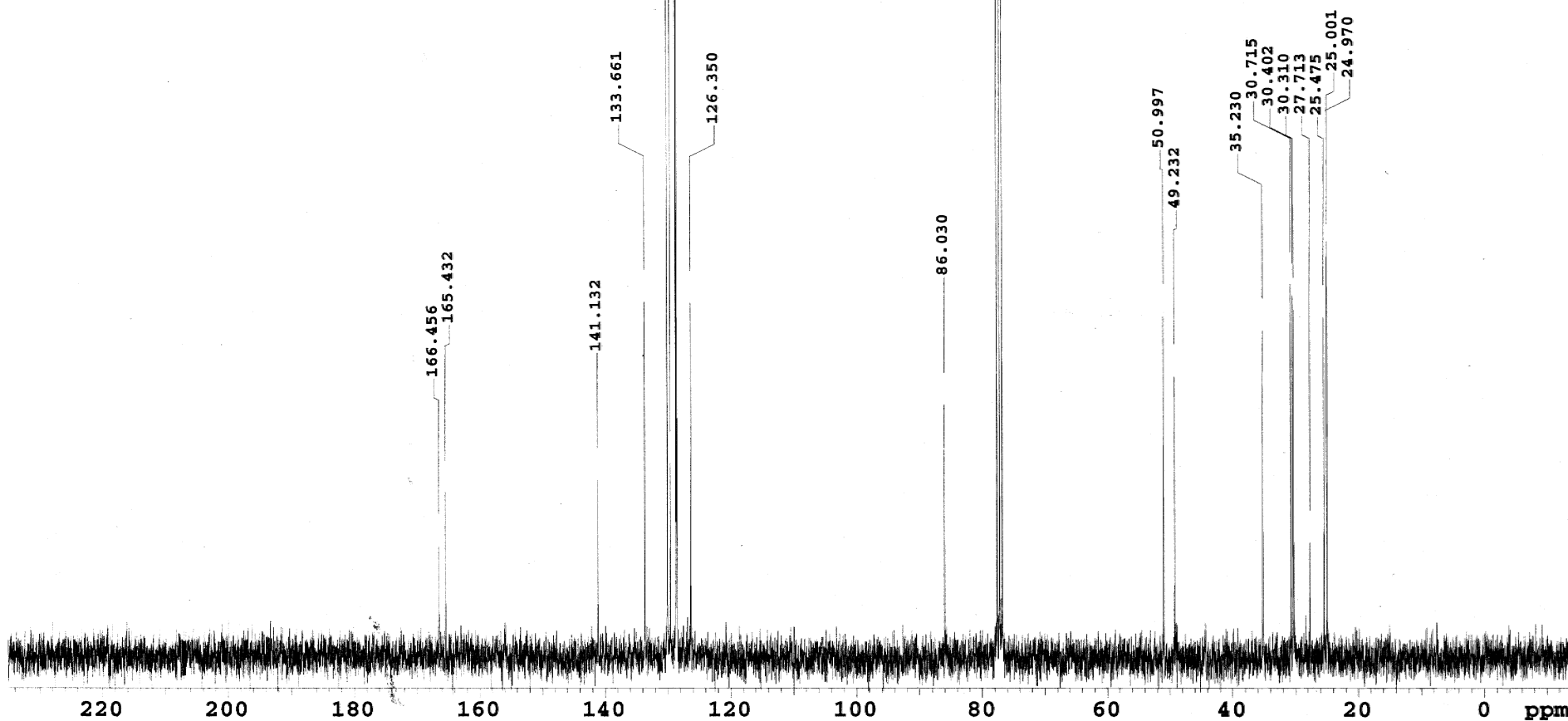
Solvent: CDCl₃
Ambient temperature
File: 13CLF-I-173
INOVA-500 "wolff"

Relax. delay 1.000 sec
Pulse 45.3 degrees
Acq. time 0.996 sec
Width 18867.9 Hz
256 repetitions
OBSERVE C13, 75.3749913 MHz
DECOUPLE H1, 299.7627007 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 8 min, 33 sec

Page 46



11c



#8

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: LF-I-242a

INOVA-500 "wittig"

Relax. delay 1.000 sec

Pulse 49.2 degrees

Acq. time 3.000 sec

Width 4789.3 Hz

16 repetitions

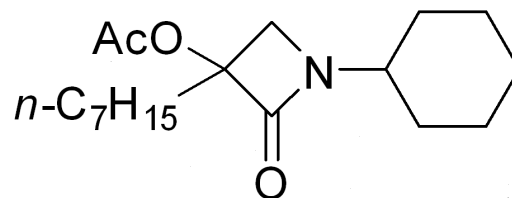
OBSERVE H1, 299.7611672 MHz

DATA PROCESSING

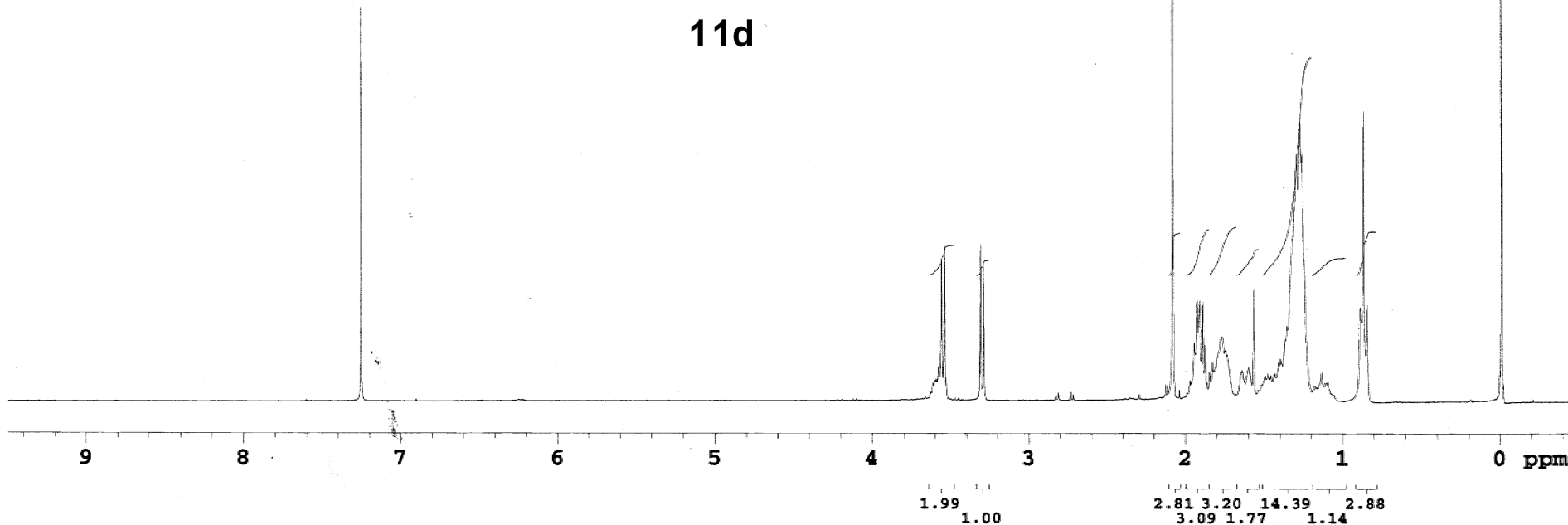
Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec



11d



106 v

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2174.184	7.253	61.7	40	381.569	1.273	44.1
2	1083.561	3.615	3.0	41	377.769	1.260	38.9
3	1079.322	3.601	3.3	42	352.484	1.176	2.6
4	1076.692	3.592	3.6	43	349.122	1.165	2.3
5	1072.599	3.578	5.6	44	346.784	1.157	2.3
6	1066.753	3.559	22.6	45	339.914	1.134	4.7
7	1060.907	3.539	24.6	46	332.752	1.110	3.0
8	992.067	3.310	24.9	47	328.075	1.094	3.1
9	986.220	3.290	21.4	48	266.397	0.889	15.0
10	636.321	2.123	2.7	49	259.820	0.867	45.7
11	623.313	2.079	163.0	50	252.951	0.844	15.3
12	590.573	1.970	3.4	51	-0.047	-0.000	4.9
13	582.535	1.943	9.4	52	-3.262	-0.011	106.3
14	576.981	1.925	16.0	53	-6.624	-0.022	3.0
15	572.596	1.910	16.1				
16	566.311	1.889	15.9				
17	561.196	1.872	9.0				
18	557.834	1.861	3.0				
19	552.719	1.844	4.6				
20	547.165	1.825	6.2				
21	532.111	1.775	9.9				
22	529.480	1.766	10.3				
23	522.903	1.744	8.2				
24	520.857	1.738	7.5				
25	491.187	1.639	5.0				
26	478.617	1.597	5.4				
27	468.825	1.564	17.8				
28	447.486	1.493	4.1				
29	441.639	1.473	4.5				
30	436.670	1.457	4.2				
31	430.824	1.437	4.3				
32	428.339	1.429	4.5				
33	421.762	1.407	6.4				
34	417.962	1.394	6.8				
35	409.193	1.365	9.8				
36	405.831	1.354	12.0				
37	393.115	1.311	30.8				
38	390.923	1.304	32.1				
39	387.123	1.291	38.9				

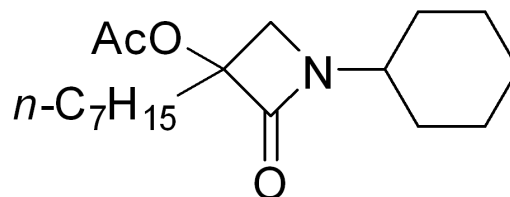
C13LF-I-242a#3

Sample directory:
File: CARBON

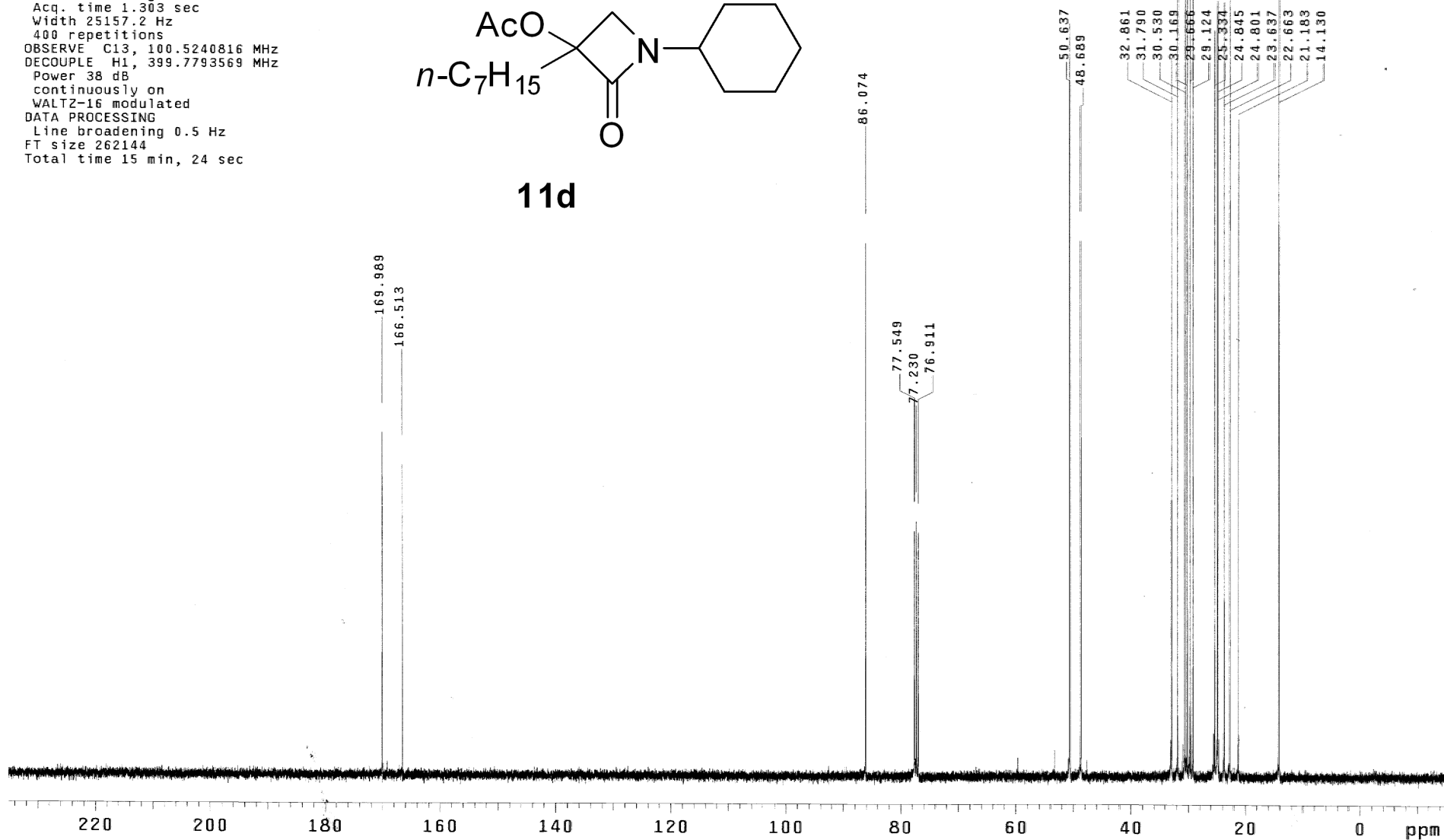
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
400 repetitions
OBSERVE C13, 100.5240816 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 15 min, 24 sec



11d



LF-I-165a

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

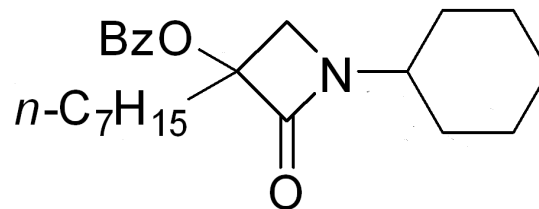
Ambient temperature

File: LF-I-165a

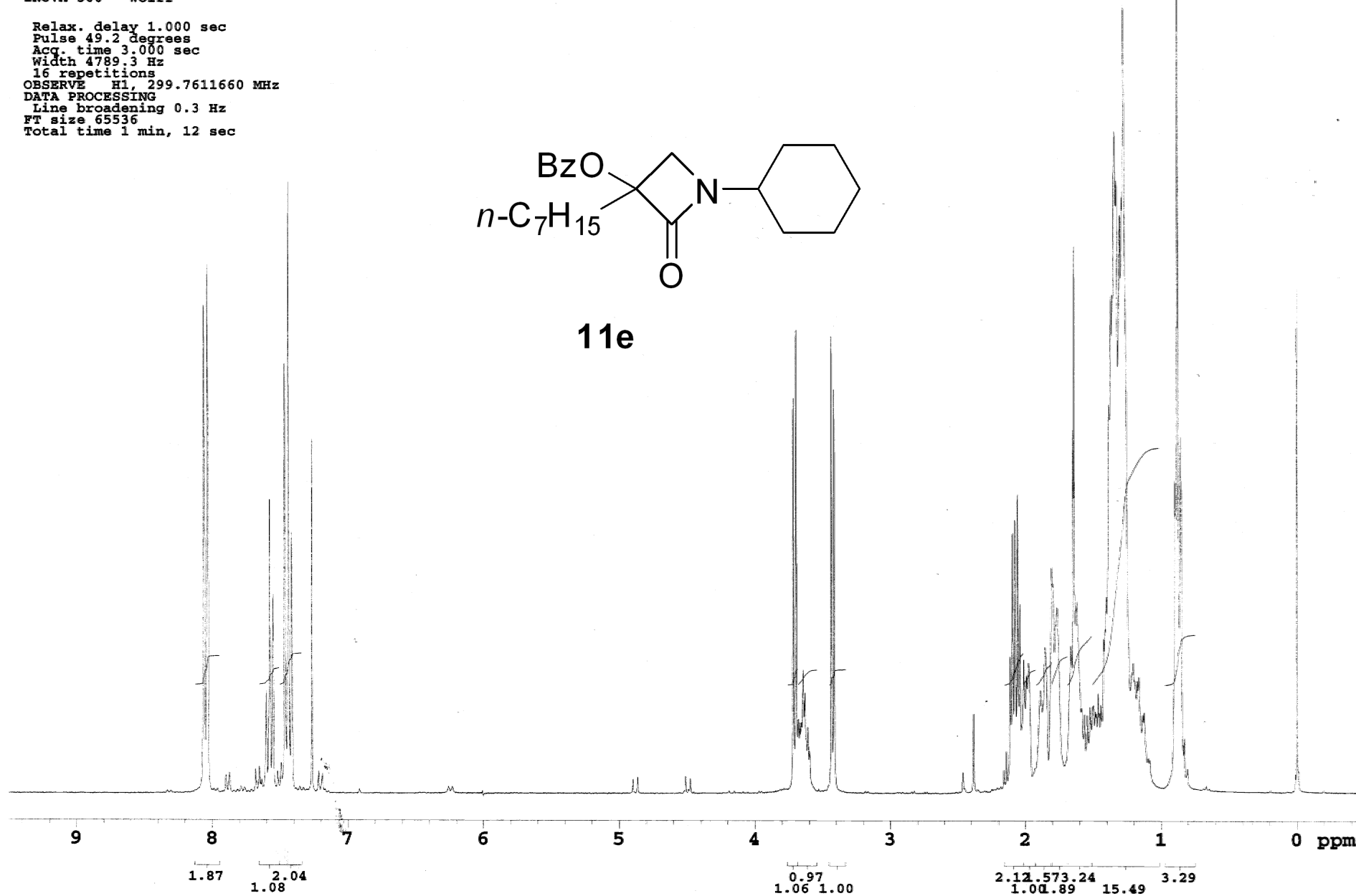
INOVA-500 "wolff"

Relax. delay 1.000 sec
Pulse 49.2 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611660 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 12 sec

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11e



#60 21

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2415.975	8.060	89.1	40	627.598	2.094	47.5	79	352.238	1.175	20.9
2	2408.521	8.035	96.3	41	622.483	2.077	50.0	80	349.169	1.165	21.6
3	2407.059	8.030	73.6	42	616.782	2.058	54.6	81	340.400	1.136	14.6
4	2367.451	7.898	3.3	43	611.521	2.040	34.7	82	336.892	1.124	15.0
5	2360.143	7.873	3.8	44	603.190	2.012	24.7	83	328.561	1.096	6.6
6	2302.265	7.680	4.4	45	597.344	1.993	21.8	84	324.761	1.083	6.2
7	2293.934	7.653	5.0	46	592.520	1.977	24.0	85	269.367	0.899	57.2
8	2288.965	7.636	2.5	47	566.504	1.890	19.0	86	262.790	0.877	166.6
9	2278.734	7.602	18.9	48	555.981	1.855	26.9	87	255.921	0.854	65.2
10	2271.572	7.578	53.6	49	541.512	1.806	41.4	88	248.467	0.829	10.3
11	2263.972	7.553	36.4	50	538.881	1.798	38.5	89	241.451	0.805	4.6
12	2254.033	7.519	4.0	51	529.673	1.767	34.2	90	3.215	0.011	3.6
13	2246.141	7.493	5.6	52	498.980	1.665	27.2	91	0.000	0.000	92.0
14	2238.102	7.466	78.5	53	494.157	1.649	66.4				
15	2230.209	7.440	111.4	54	491.964	1.641	99.8				
16	2222.609	7.415	47.6	55	486.264	1.622	35.2				
17	2178.178	7.266	64.6	56	475.303	1.586	15.8				
18	2163.416	7.217	4.0	57	469.310	1.566	14.6				
19	2155.231	7.190	3.6	58	463.025	1.545	14.4				
20	1468.147	4.898	2.6	59	456.302	1.522	16.0				
21	1457.624	4.863	3.1	60	449.579	1.500	16.3				
22	1351.514	4.509	3.1	61	445.340	1.486	15.2				
23	1341.136	4.474	2.7	62	442.710	1.477	14.7				
24	1114.447	3.718	72.3	63	438.909	1.464	18.6				
25	1108.455	3.698	84.6	64	436.279	1.455	14.9				
26	1103.924	3.683	13.7	65	432.917	1.444	16.4				
27	1099.831	3.669	13.0	66	426.632	1.423	28.5				
28	1096.908	3.659	13.1	67	423.709	1.413	30.2				
29	1092.962	3.646	22.7	68	420.932	1.404	36.1				
30	1089.162	3.633	18.6	69	414.647	1.383	71.1				
31	1082.146	3.610	12.2	70	409.970	1.368	91.0				
32	1078.200	3.597	7.8	71	406.609	1.356	91.0				
33	1029.822	3.435	83.5	72	401.786	1.340	120.7				
34	1023.976	3.416	73.8	73	398.278	1.329	111.7				
35	738.093	2.462	3.9	74	390.824	1.304	105.5				
36	714.415	2.383	14.7	75	386.439	1.289	108.7				
37	646.891	2.158	4.3	76	382.931	1.277	144.2				
38	641.191	2.139	7.8	77	363.931	1.214	22.4				
39	633.006	2.112	25.2	78	361.300	1.205	24.1				

LF-I-165a

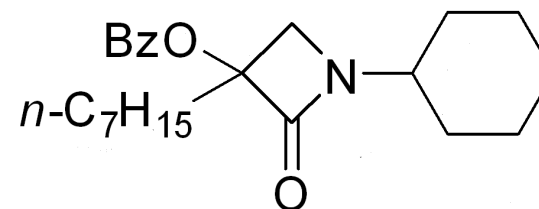
Sample directory:

Pulse Sequence: s2pul

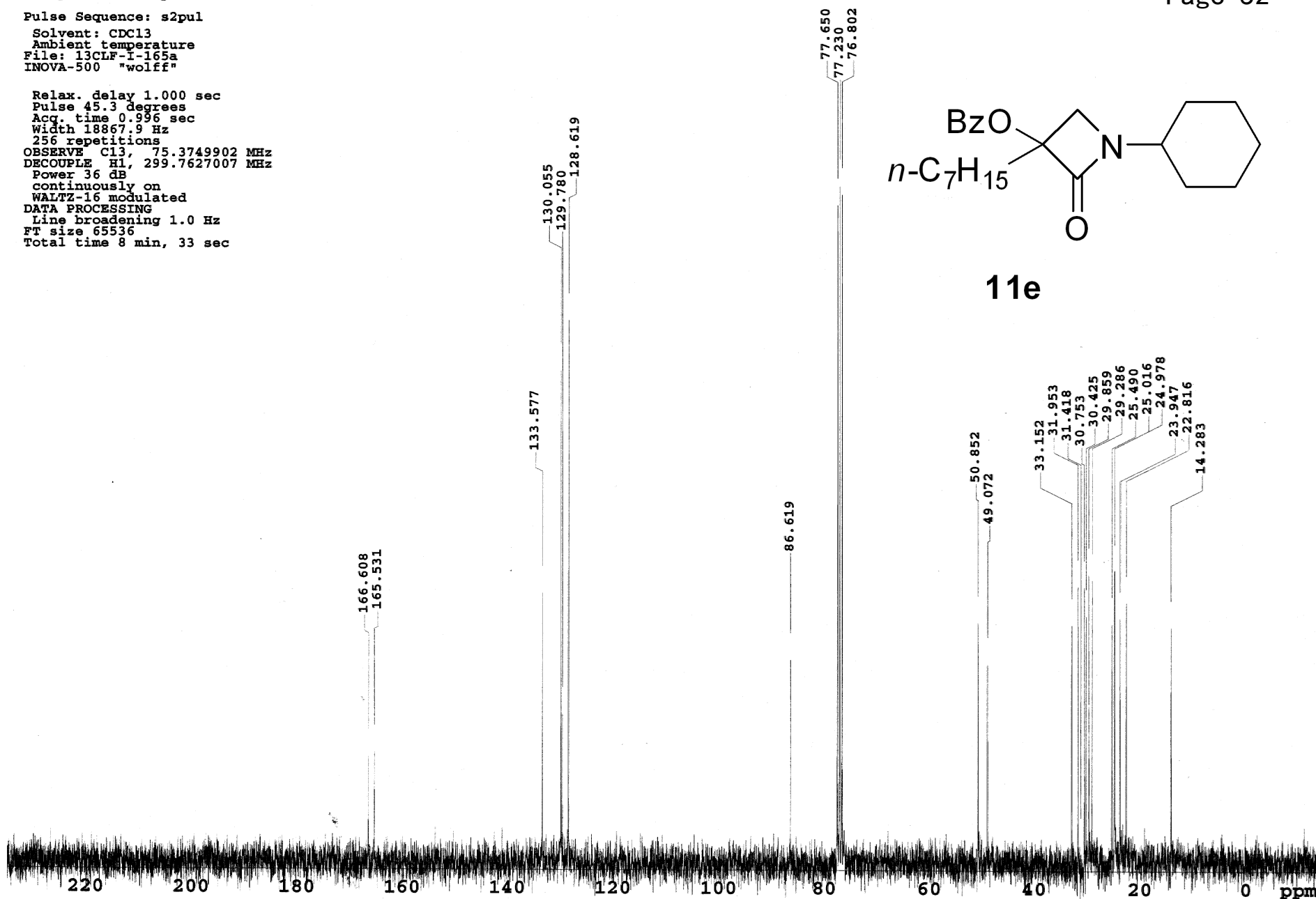
Solvent: CDCl₃
Ambient temperature
File: 13CLF-I-165a
INOVA-500 "wolff"

Relax. delay 1.000 sec
Pulse 45.3 degrees
Acq. time 0.996 sec
Width 18867.9 Hz
256 repetitions
OBSERVE C13, 75.3749902 MHz
DECOUPLE H1, 299.7627007 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 8 min, 33 sec

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11e



LF-III-116b

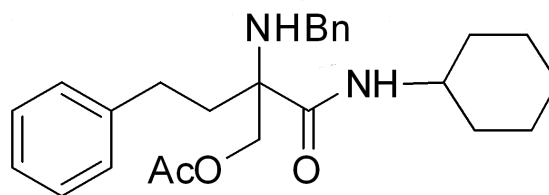
Sample directory:
File: PROTON

Pulse Sequence: s2pul

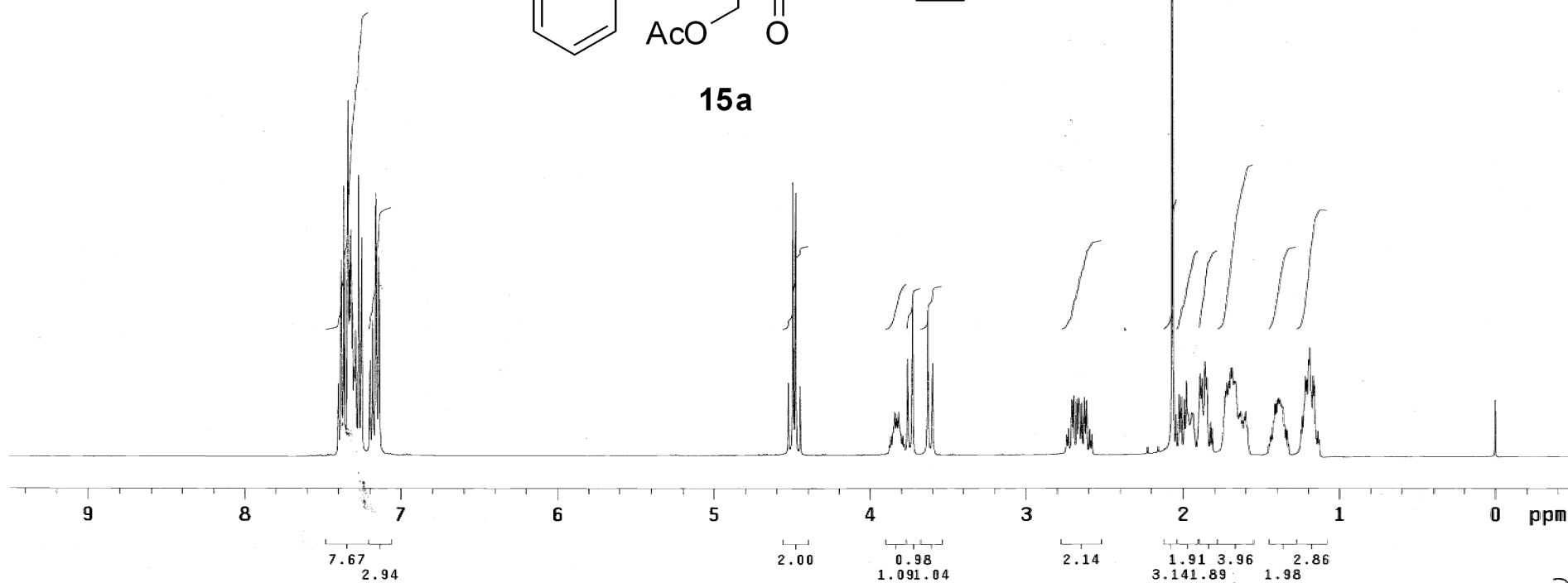
Solvent: CDCl3
Ambient temperature
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773501 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 32 sec

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15a



2~14ppm 22
4.15h

T-1

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2957.798	7.399	11.5	40	1077.424	2.695	9.6	79	569.025	1.423	5.6
2	2950.585	7.381	31.0	41	1069.626	2.676	9.0	80	565.516	1.415	8.3
3	2945.906	7.369	11.5	42	1064.558	2.663	9.2	81	562.397	1.407	8.3
4	2943.567	7.363	42.6	43	1062.608	2.658	8.3	82	558.888	1.398	9.1
5	2939.668	7.353	4.7	44	1056.955	2.644	8.4	83	557.328	1.394	8.4
6	2933.625	7.338	56.1	45	1049.937	2.626	9.3	84	555.379	1.389	9.2
7	2930.701	7.331	29.5	46	1044.479	2.613	8.9	85	553.819	1.385	8.8
8	2926.802	7.321	35.7	47	1036.487	2.593	4.3	86	552.065	1.381	8.9
9	2922.709	7.311	24.2	48	1031.028	2.579	3.5	87	548.751	1.373	8.3
10	2919.395	7.303	14.3	49	825.368	2.065	212.0	88	547.387	1.369	8.0
11	2917.835	7.299	13.6	50	816.791	2.043	6.6	89	545.632	1.365	7.9
12	2913.936	7.289	19.9	51	808.604	2.023	9.7	90	544.073	1.361	6.9
13	2906.724	7.271	44.3	52	802.951	2.008	9.4	91	540.564	1.352	5.1
14	2899.121	7.252	34.4	53	796.128	1.991	9.0	92	537.250	1.344	4.4
15	2897.172	7.247	14.2	54	790.474	1.977	11.9	93	533.936	1.336	4.1
16	2878.068	7.199	15.1	55	781.312	1.954	5.2	94	498.457	1.247	4.2
17	2870.855	7.181	21.4	56	777.024	1.944	6.9	95	494.753	1.238	6.3
18	2868.516	7.175	7.1	57	773.905	1.936	6.7	96	486.566	1.217	12.6
19	2862.668	7.161	40.0	58	756.555	1.892	13.0	97	483.057	1.208	12.2
20	2861.498	7.158	41.4	59	751.682	1.880	12.3	98	478.963	1.198	15.2
21	2854.480	7.140	31.4	60	744.079	1.861	15.0	99	475.649	1.190	17.1
22	1808.832	4.525	11.6	61	739.401	1.850	12.4	100	467.072	1.168	12.7
23	1797.330	4.496	43.1	62	730.239	1.827	5.5	101	463.758	1.160	11.2
24	1790.313	4.478	41.4	63	725.560	1.815	4.4	102	455.376	1.139	4.0
25	1778.616	4.449	11.0	64	691.836	1.731	10.3	103	-0.000	-0.000	8.9
26	1545.470	3.866	3.2	65	687.742	1.720	11.6				
27	1538.647	3.849	4.7	66	682.869	1.708	11.9				
28	1534.944	3.839	7.0	67	678.385	1.697	14.0				
29	1530.655	3.829	6.1	68	674.291	1.687	13.9				
30	1526.171	3.818	7.0	69	670.003	1.676	11.9				
31	1522.467	3.808	4.5	70	666.299	1.667	11.8				
32	1515.840	3.792	3.4	71	656.552	1.642	6.8				
33	1502.389	3.758	15.4	72	652.848	1.633	7.1				
34	1490.303	3.728	23.5	73	648.754	1.623	5.6				
35	1450.535	3.628	22.8	74	643.686	1.610	6.3				
36	1438.449	3.598	14.7	75	639.982	1.601	7.1				
37	1095.553	2.740	3.4	76	636.473	1.592	4.8				
38	1090.679	2.728	4.4	77	577.212	1.444	3.2				
39	1082.102	2.707	9.0	78	574.093	1.436	3.4				

LF-III-116b

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: C13LF-III-116b

INOVA-500 "wolff"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 25157.2 Hz

256 repetitions

OBSERVE C13, 100.5240800 MHz

DECOUPLE H1, 399.7793569 MHz

Power 38 dB

continuously on

WALTZ-16 modulated

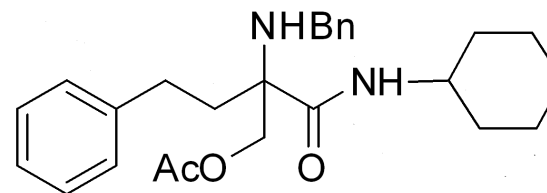
DATA PROCESSING

Line broadening 0.5 Hz

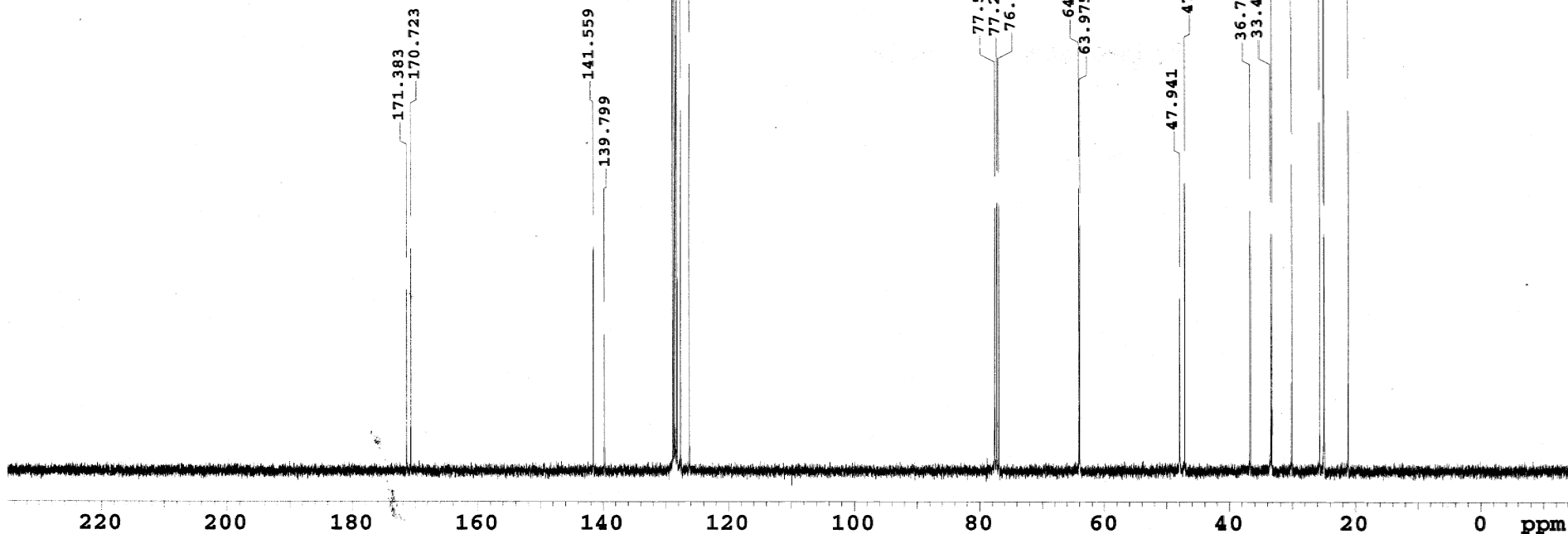
FT size 131072

Total time 12 min, 50 sec

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15a



#45

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: LF-III-193a#2

INOVA-500 "inova500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6387.7 Hz

8 repetitions

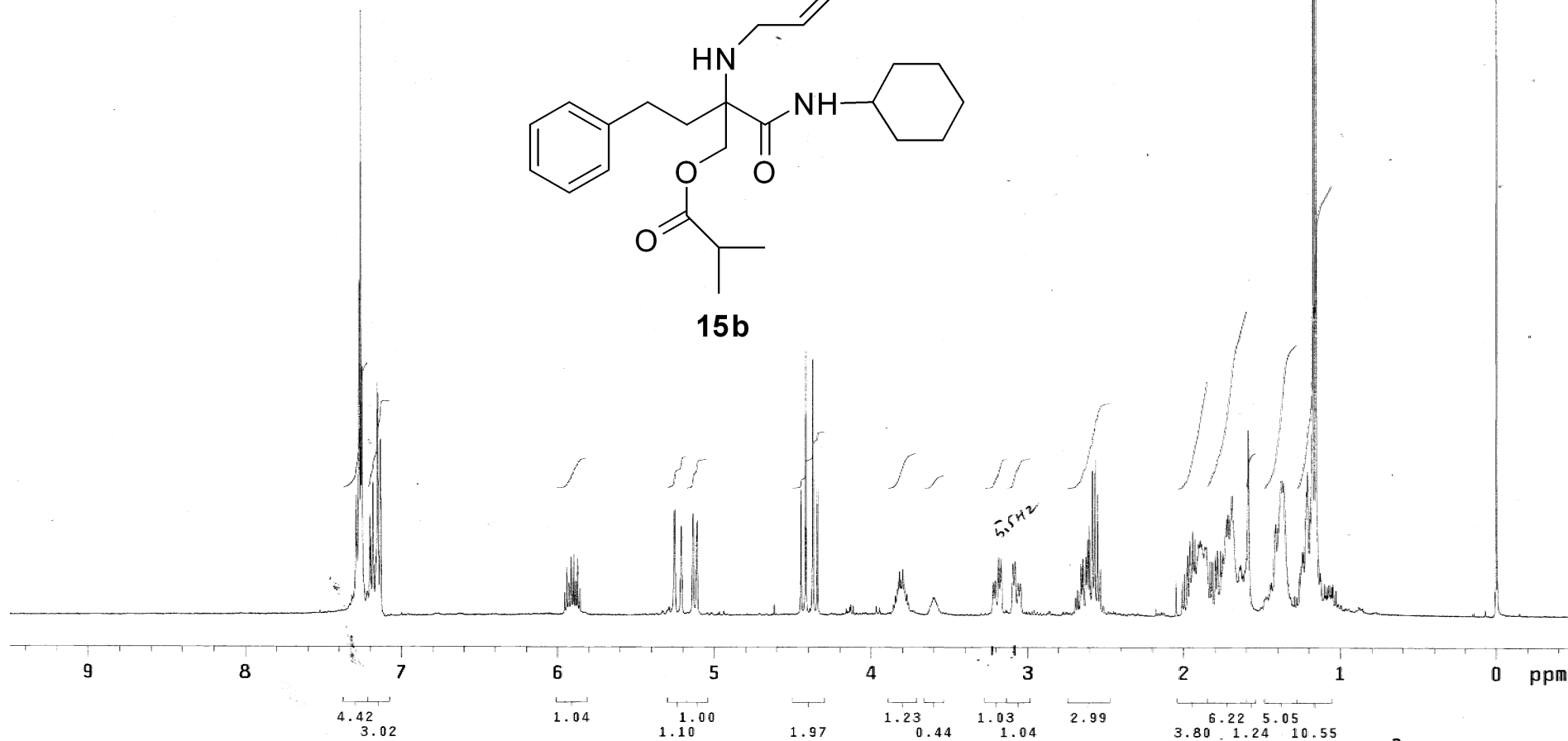
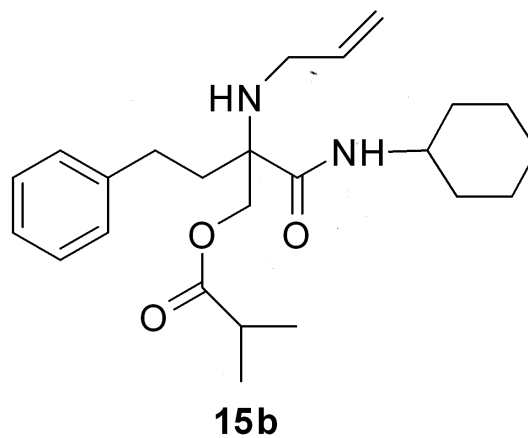
OBSERVE H1, 399.7773429 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 0 min, 32 sec



23 #530

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2925.243	7.317	3.1	40	1522.662	3.809	5.6	79	714.059	1.786	10.3	118	436.442	1.082	3.3
2	2914.716	7.291	18.8	41	1518.374	3.798	7.3	80	705.481	1.765	10.2	119	432.763	1.083	4.6
3	2913.157	7.287	11.5	42	1514.475	3.788	4.4	81	700.218	1.752	9.9	120	428.084	1.071	4.9
4	2907.698	7.273	52.8	43	1507.847	3.772	3.4	82	690.276	1.727	15.3	121	425.160	1.063	3.4
5	2903.410	7.263	95.3	44	1286.202	3.217	5.3	83	686.183	1.716	15.9	122	421.067	1.053	4.6
6	2900.096	7.254	40.1	45	1280.549	3.203	5.6	84	677.020	1.693	18.9	123	417.753	1.045	5.1
7	2887.035	7.222	3.7	46	1272.557	3.183	9.2	85	656.942	1.643	7.7	124	410.930	1.028	4.0
8	2879.043	7.202	16.0	47	1266.903	3.169	9.0	86	653.823	1.635	8.0	125	3.119	0.008	3.9
9	2877.873	7.199	12.2	48	1236.103	3.092	8.3	87	649.144	1.624	6.3	126	0.000	0.000	126.4
10	2871.635	7.183	20.9	49	1230.450	3.078	8.6	88	644.466	1.612	7.2	127	-3.314	-0.008	5.6
11	2869.491	7.178	7.8	50	1222.458	3.058	5.2	89	640.177	1.601	9.2				
12	2864.227	7.165	9.1	51	1216.804	3.044	5.1	90	634.914	1.588	29.3				
13	2860.913	7.156	32.4	52	1069.626	2.676	4.0	91	588.713	1.473	3.1				
14	2859.549	7.153	36.6	53	1061.244	2.655	8.1	92	581.696	1.455	3.4				
15	2852.726	7.136	27.7	54	1056.370	2.642	9.0	93	578.577	1.447	5.0				
16	2380.001	5.953	3.5	55	1048.963	2.624	9.3	94	575.847	1.440	5.3				
17	2374.348	5.939	7.5	56	1044.284	2.612	12.1	95	565.321	1.414	14.5				
18	2369.669	5.927	5.1	57	1039.606	2.600	14.1	96	558.888	1.398	13.9				
19	2364.016	5.913	9.1	58	1032.783	2.583	22.8	97	550.895	1.378	21.3				
20	2357.193	5.896	9.5	59	1025.765	2.566	24.5	98	549.726	1.375	21.3				
21	2352.514	5.885	5.4	60	1018.747	2.548	19.1	99	545.242	1.364	21.0				
22	2346.861	5.870	8.9	61	1011.729	2.531	7.4	100	526.528	1.317	3.0				
23	2341.208	5.856	4.2	62	818.546	2.048	5.6	101	516.976	1.293	3.2				
24	2100.654	5.255	16.5	63	802.561	2.008	5.4	102	511.128	1.279	3.0				
25	2099.095	5.251	16.6	64	797.297	1.994	6.6	103	503.915	1.260	6.2				
26	2097.535	5.247	6.8	65	788.915	1.973	9.6	104	501.381	1.254	6.8				
27	2083.695	5.212	13.8	66	784.626	1.963	8.3	105	496.508	1.242	10.1				
28	2081.940	5.208	14.1	67	783.262	1.959	11.8	106	493.973	1.236	9.7				
29	2053.869	5.138	16.0	68	776.634	1.943	13.5	107	492.609	1.232	7.8				
30	2052.505	5.134	15.3	69	770.981	1.929	12.0	108	486.761	1.218	19.5				
31	2043.537	5.112	14.9	70	761.429	1.905	11.3	109	483.642	1.210	22.7				
32	2042.173	5.108	14.5	71	757.725	1.895	11.9	110	476.819	1.193	16.3				
33	1777.642	4.447	19.8	72	754.216	1.887	11.3	111	470.191	1.176	148.8				
34	1765.945	4.417	41.8	73	745.054	1.864	10.9	112	469.411	1.174	149.9				
35	1747.816	4.372	40.4	74	741.935	1.856	10.8	113	463.173	1.159	141.0				
36	1736.315	4.343	19.8	75	731.408	1.830	8.6	114	462.393	1.157	145.1				
37	1537.478	3.846	3.1	76	726.340	1.817	8.6	115	450.892	1.128	6.8				
38	1531.045	3.830	4.2	77	719.322	1.799	9.7	116	448.943	1.123	5.9				
39	1527.146	3.820	7.0	78	717.763	1.795	8.0	117	439.586	1.100	5.1				

LF-III-193a

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec

Pulse 55.1 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 125.7042652 MHz

DECOUPLE H1, 499.9197456 MHz

Power 34 dB

continuously on

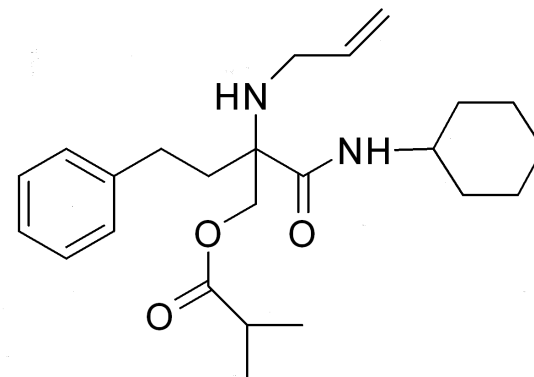
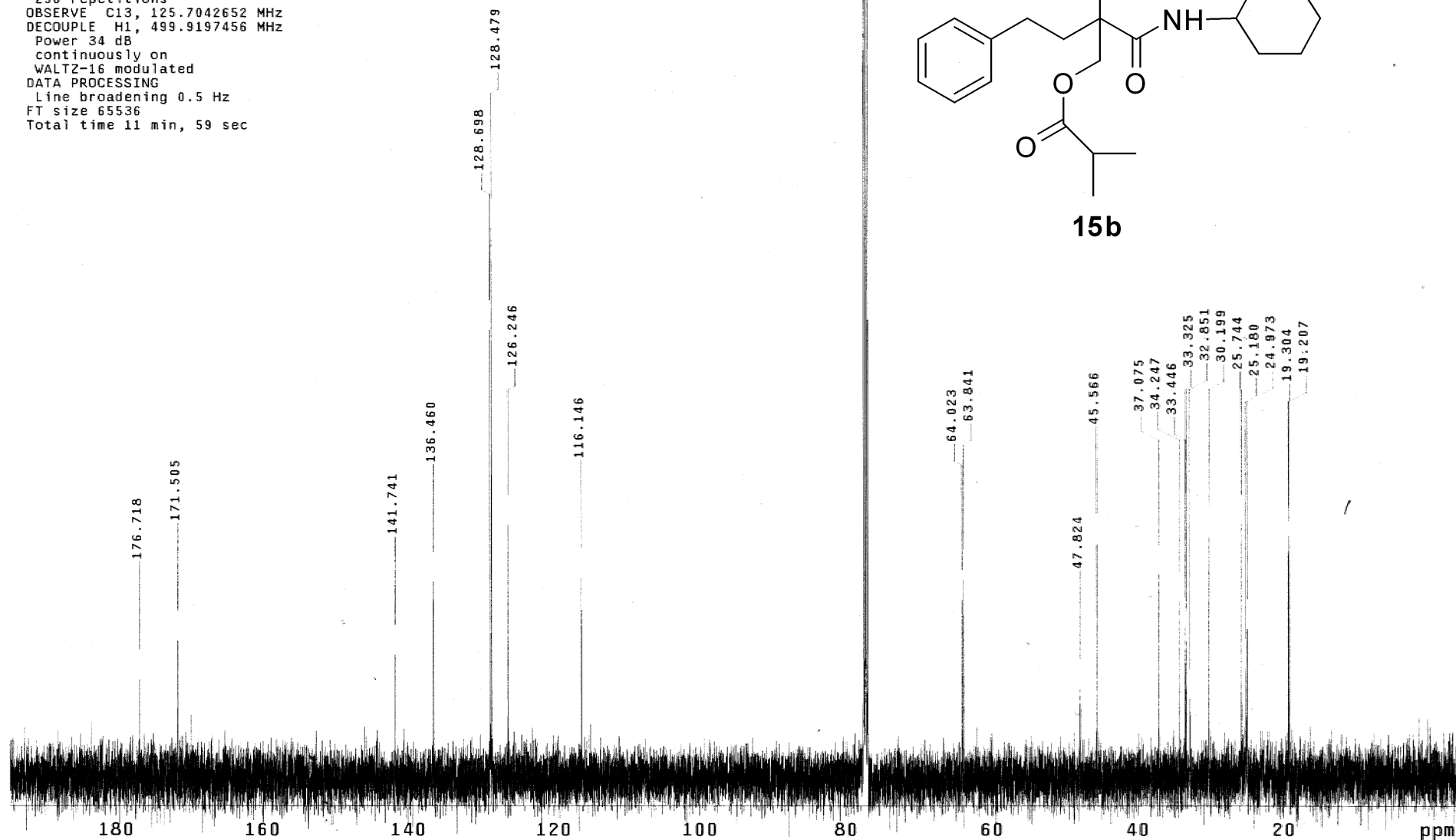
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 11 min, 59 sec



15b

LF-III-185a

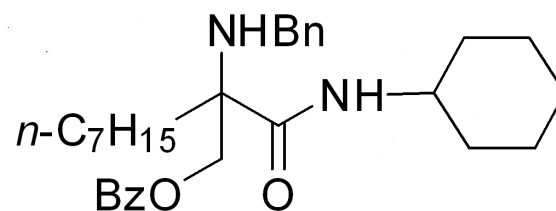
Sample directory:
File: PROTON

Pulse Sequence: s2pul

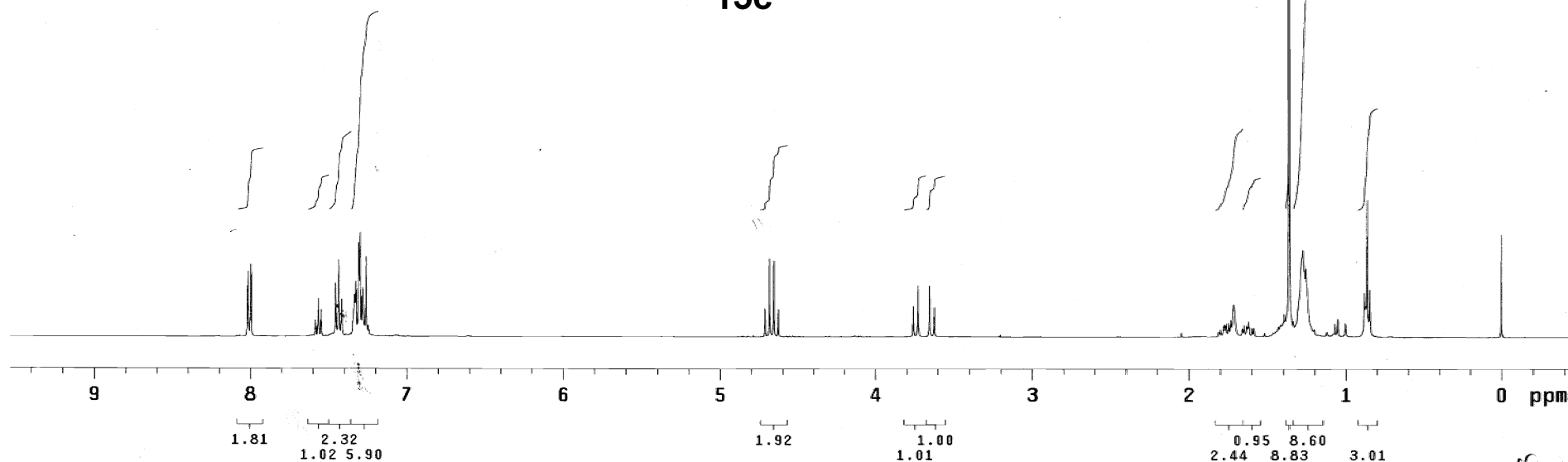
Solvent: CDCl₃
Ambient temperature
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773442 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 32 sec

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15c



24
#512

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3206.149	8.020	8.0	40	338.803	0.847	7.5
2	3205.759	8.019	7.7	41	0.000	0.000	16.1
3	3204.979	8.017	10.2				
4	3197.961	7.999	11.3				
5	3196.597	7.996	9.7				
6	3025.051	7.567	5.9				
7	3017.449	7.548	4.3				
8	2980.605	7.456	8.4				
9	2979.046	7.452	3.7				
10	2972.613	7.436	12.0				
11	2965.205	7.417	5.9				
12	2935.965	7.344	3.9				
13	2932.456	7.335	6.6				
14	2930.311	7.330	6.8				
15	2928.947	7.326	8.7				
16	2927.582	7.323	7.3				
17	2922.124	7.309	14.8				
18	2918.225	7.300	16.5				
19	2915.106	7.292	3.0				
20	2912.767	7.286	6.4				
21	2911.597	7.283	7.7				
22	2904.385	7.265	5.1				
23	2902.630	7.261	12.6				
24	1884.468	4.714	4.5				
25	1872.966	4.685	12.3				
26	1862.245	4.658	12.0				
27	1850.743	4.629	4.4				
28	1502.389	3.758	4.8				
29	<u>1450.108</u>	3.727	8.1				
30	1460.672	3.654	8.0				
31	1448.391	3.623	4.6				
32	685.793	1.715	5.1				
33	557.718	1.395	3.6				
34	544.852	1.363	162.1				
35	512.493	1.282	12.5				
36	510.153	1.276	13.7				
37	502.941	1.258	10.7				
38	352.643	0.882	6.9				
39	346.015	0.866	21.6				

LF-III-185a

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec

Pulse 55.1 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 125.7042293 MHz

DECOUPLE H1, 499.9197456 MHz

Power 34 dB

continuously on

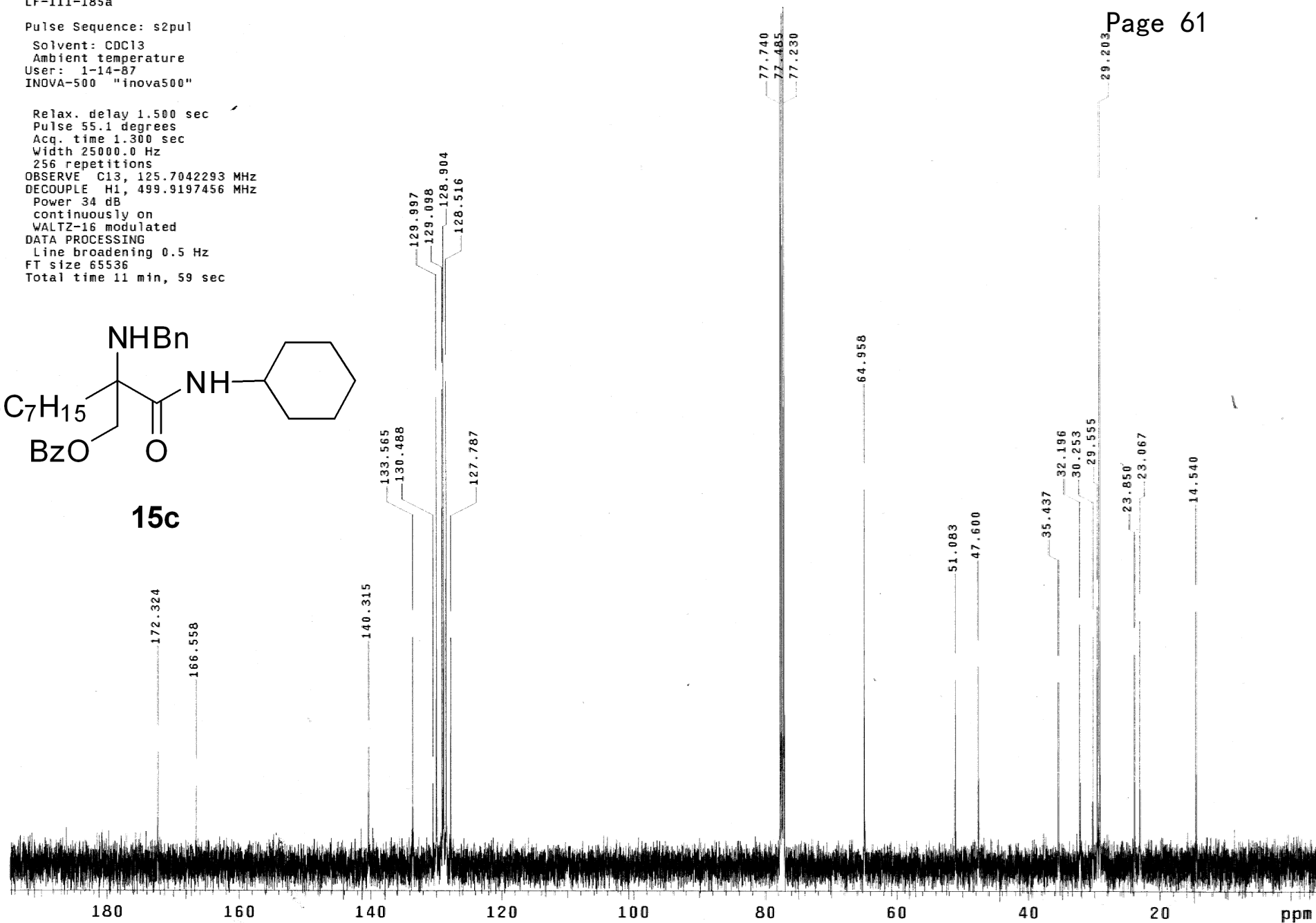
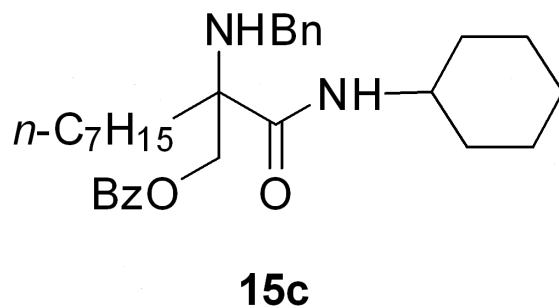
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 11 min, 59 sec



LF-III-195a

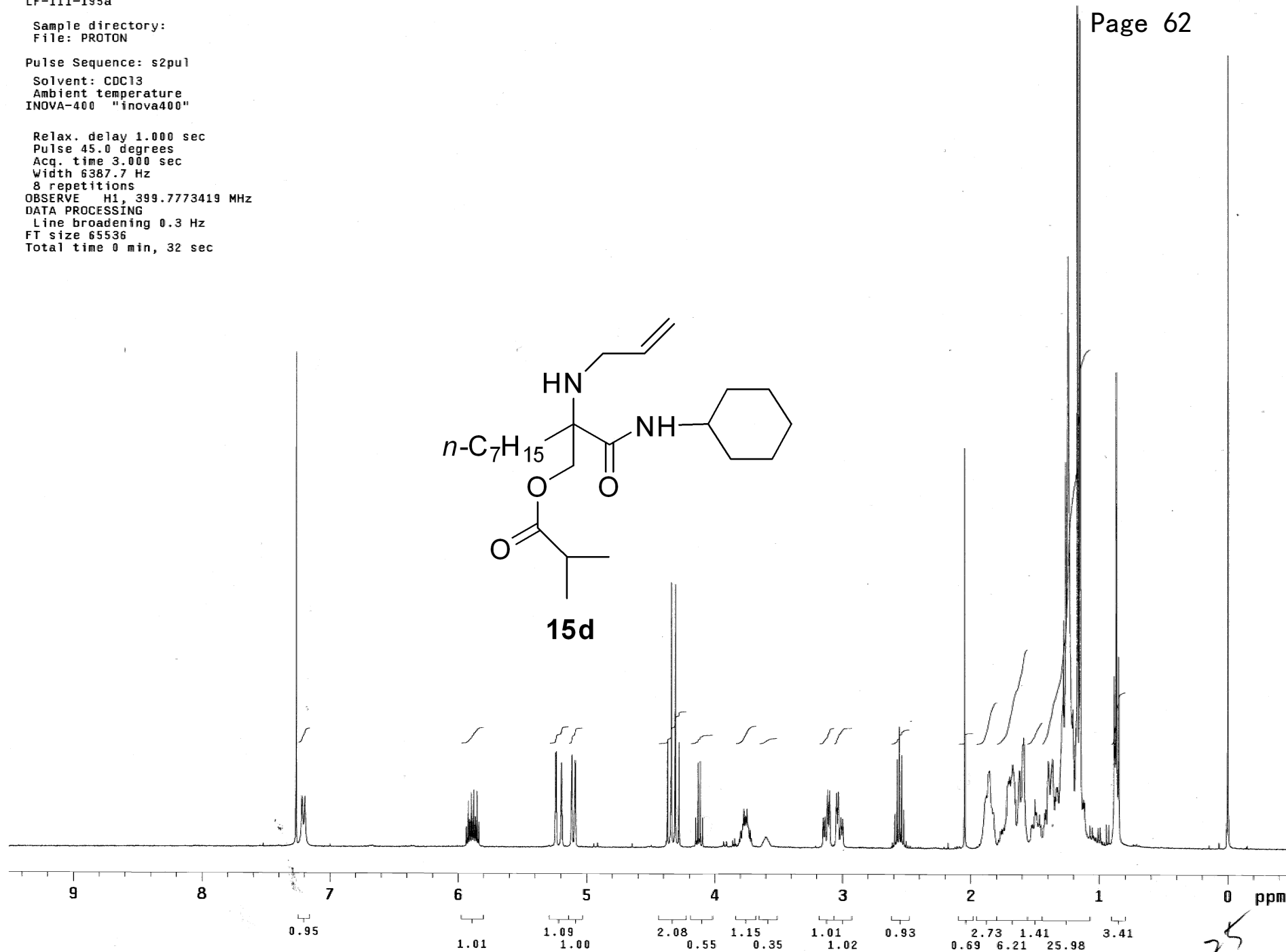
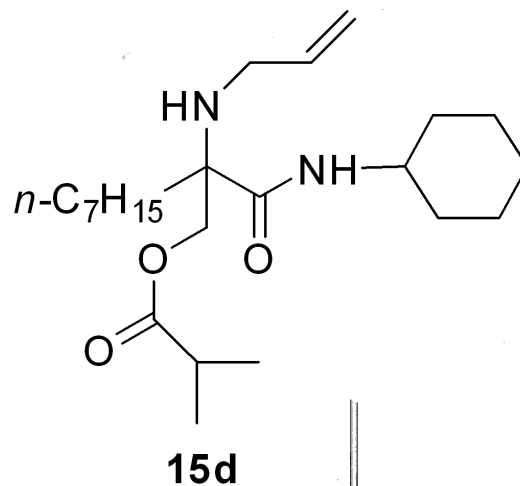
Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773419 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 32 sec

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#C11

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2904.190	7.265	95.4	40	1494.981	3.740	4.6	79	546.802	1.368	16.2
2	2886.060	7.219	9.8	41	1488.548	3.723	3.4	80	545.047	1.363	17.2
3	2877.288	7.197	9.7	42	1258.716	3.149	5.9	81	536.665	1.342	9.9
4	2372.983	5.936	4.0	43	1253.063	3.134	6.0	82	532.376	1.332	11.8
5	2367.330	5.922	8.9	44	1245.070	3.114	11.2	83	529.257	1.324	11.8
6	2362.846	5.910	5.4	45	1239.417	3.100	11.1	84	511.323	1.279	43.8
7	2361.677	5.907	5.1	46	1217.584	3.046	10.6	85	504.110	1.261	74.4
8	2357.193	5.896	10.5	47	1211.931	3.032	10.8	86	497.092	1.243	114.0
9	2356.023	5.893	6.3	48	1203.938	3.012	5.9	87	482.277	1.206	26.8
10	2350.175	5.879	11.0	49	1198.285	2.997	5.6	88	473.505	1.184	23.1
11	2345.692	5.867	5.9	50	1035.707	2.591	6.6	89	467.852	1.170	162.3
12	2344.717	5.865	5.8	51	1028.689	2.573	17.1	90	466.097	1.166	160.7
13	2340.038	5.853	10.8	52	1021.671	2.556	23.3	91	460.834	1.153	159.7
14	2334.385	5.839	4.8	53	1014.848	2.539	17.9	92	459.080	1.148	159.3
15	2096.366	5.244	7.0	54	1007.831	2.521	7.4	93	452.257	1.131	9.7
16	2094.806	5.240	18.2	55	818.741	2.048	77.0	94	449.333	1.124	8.7
17	2093.052	5.236	18.4	56	751.487	1.880	10.1	95	447.383	1.119	9.4
18	2091.492	5.232	7.1	57	742.130	1.856	14.9	96	445.434	1.114	8.8
19	2079.211	5.201	6.2	58	729.849	1.826	7.0	97	428.279	1.071	4.5
20	2077.652	5.197	16.3	59	706.651	1.768	3.4	98	421.261	1.054	4.1
21	2076.092	5.193	16.1	60	703.142	1.759	3.8	99	402.937	1.008	3.9
22	2074.533	5.189	6.1	61	697.099	1.744	4.0	100	396.114	0.991	4.1
23	2045.877	5.118	17.8	62	683.064	1.709	12.9	101	377.011	0.943	4.7
24	2044.512	5.114	17.3	63	678.775	1.698	13.8	102	370.188	0.926	4.6
25	2035.740	5.092	16.8	64	669.418	1.674	16.1	103	353.618	0.885	33.1
26	2034.180	5.088	16.2	65	660.256	1.652	9.4	104	346.990	0.868	91.7
27	1747.036	4.370	20.3	66	647.975	1.621	15.0	105	339.972	0.850	36.8
28	1735.535	4.341	51.0	67	635.109	1.589	21.2	106	3.314	0.008	5.0
29	1723.059	4.310	50.6	68	610.936	1.528	4.5	107	0.000	0.000	152.7
30	1711.363	4.281	20.2	69	607.427	1.519	4.7	108	-3.314	-0.008	5.6
31	1658.924	4.150	5.8	70	600.020	1.501	9.4				
32	1651.712	4.132	16.3	71	595.536	1.490	7.1				
33	1644.694	4.114	16.6	72	586.179	1.466	6.5				
34	1637.481	4.096	5.7	73	581.891	1.456	4.7				
35	1517.984	3.797	3.4	74	572.339	1.432	4.5				
36	1511.356	3.780	4.6	75	568.635	1.422	6.8				
37	1507.652	3.771	7.5	76	565.906	1.416	7.5				
38	1503.169	3.760	6.2	77	558.303	1.397	16.8				
39	1498.685	3.749	7.5	78	548.751	1.373	15.2				

LF-III-195b

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

File: C13LF-III-195b

INOVA-500 "wolff"

Relax. delay 1.500 sec

Pulse 55.1 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

256 repetitions

OBSERVE C13, 125.7042667 MHz

DECOUPLE H1, 499.9197456 MHz

Power 34 dB

continuously on

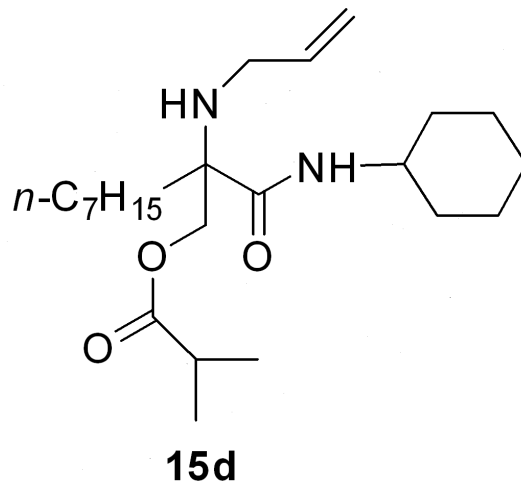
WALTZ-16 modulated

DATA PROCESSING

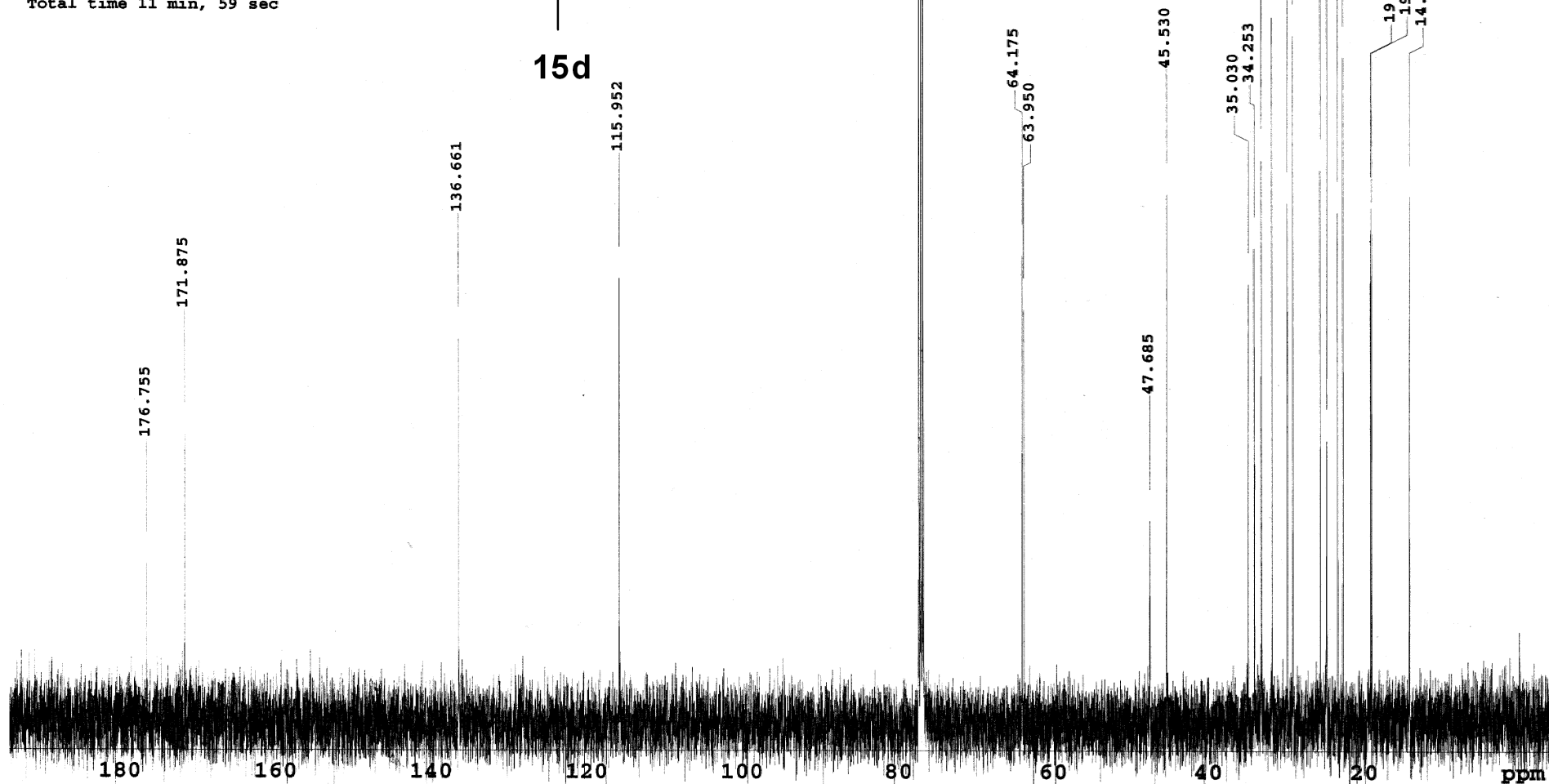
Line broadening 0.5 Hz

FT size 65536

Total time 11 min, 59 sec



15d



LF-VI-74b

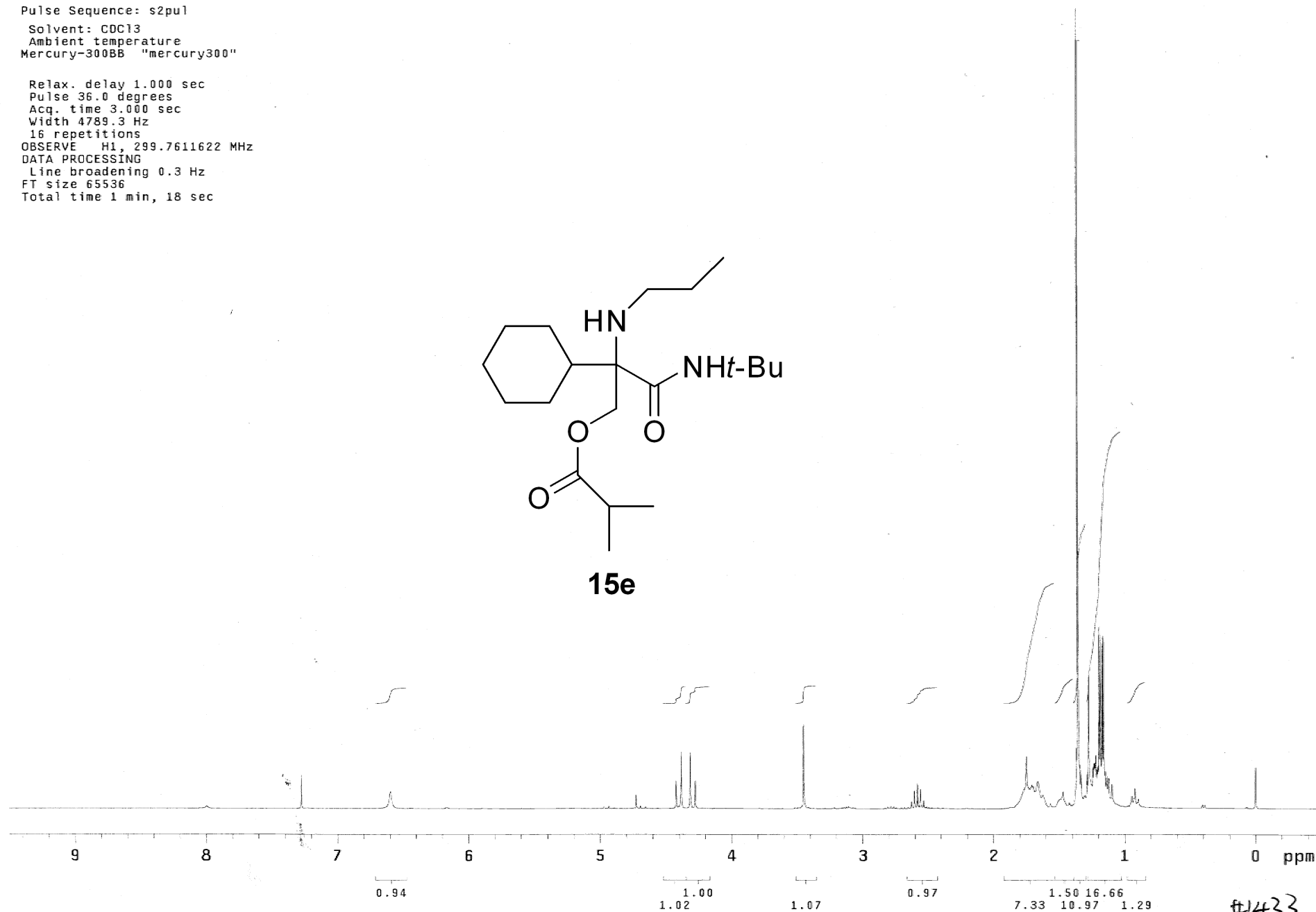
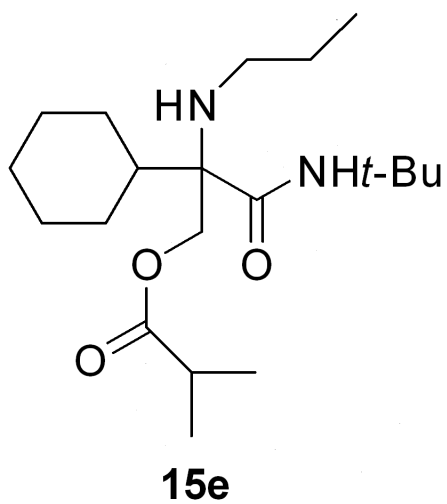
Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611622 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 18 sec

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#1433

26

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2180.875	7.275	6.3	40	336.317	1.122	5.8
2	1977.710	6.598	3.3	41	335.441	1.119	5.7
3	1416.158	4.724	2.6	42	328.571	1.096	4.7
4	1324.953	4.420	5.3	43	282.676	0.943	2.4
5	1313.553	4.382	10.7	44	275.368	0.919	3.9
6	1293.090	4.314	10.7	45	0.000	0.000	7.8
7	1281.544	4.275	5.3				
8	1033.800	3.449	16.0				
9	780.356	2.603	3.5				
10	773.340	2.580	4.8				
11	766.471	2.557	3.7				
12	530.420	1.769	3.6				
13	525.012	1.751	9.9				
14	512.296	1.709	4.5				
15	509.373	1.699	4.2				
16	498.557	1.663	5.2				
17	487.302	1.626	2.6				
18	442.723	1.477	2.2				
19	440.384	1.469	3.2				
20	409.983	1.368	11.5				
21	406.621	1.356	151.2				
22	402.236	1.342	8.3				
23	399.605	1.333	7.3				
24	390.982	1.304	2.5				
25	385.428	1.286	6.5				
26	381.774	1.274	24.9				
27	375.050	1.251	4.5				
28	372.419	1.242	8.0				
29	369.935	1.234	8.6				
30	367.596	1.226	8.7				
31	365.550	1.219	10.2				
32	362.773	1.210	7.4				
33	360.580	1.203	8.1				
34	357.657	1.193	34.3				
35	354.734	1.183	32.8				
36	350.641	1.170	32.5				
37	347.718	1.160	32.6				
38	343.626	1.146	7.2				
39	339.825	1.134	6.2				

C13LF-VI-74b

Pulse Sequence: s2pul

Solvent: CDC13

Temp. 23.0 C / 296.1 K

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec

Pulse 54.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

200 repetitions

OBSERVE C13, 125.7042682 MHz

DECOUPLE H1, 499.9197456 MHz

Power 38 dB

continuously on

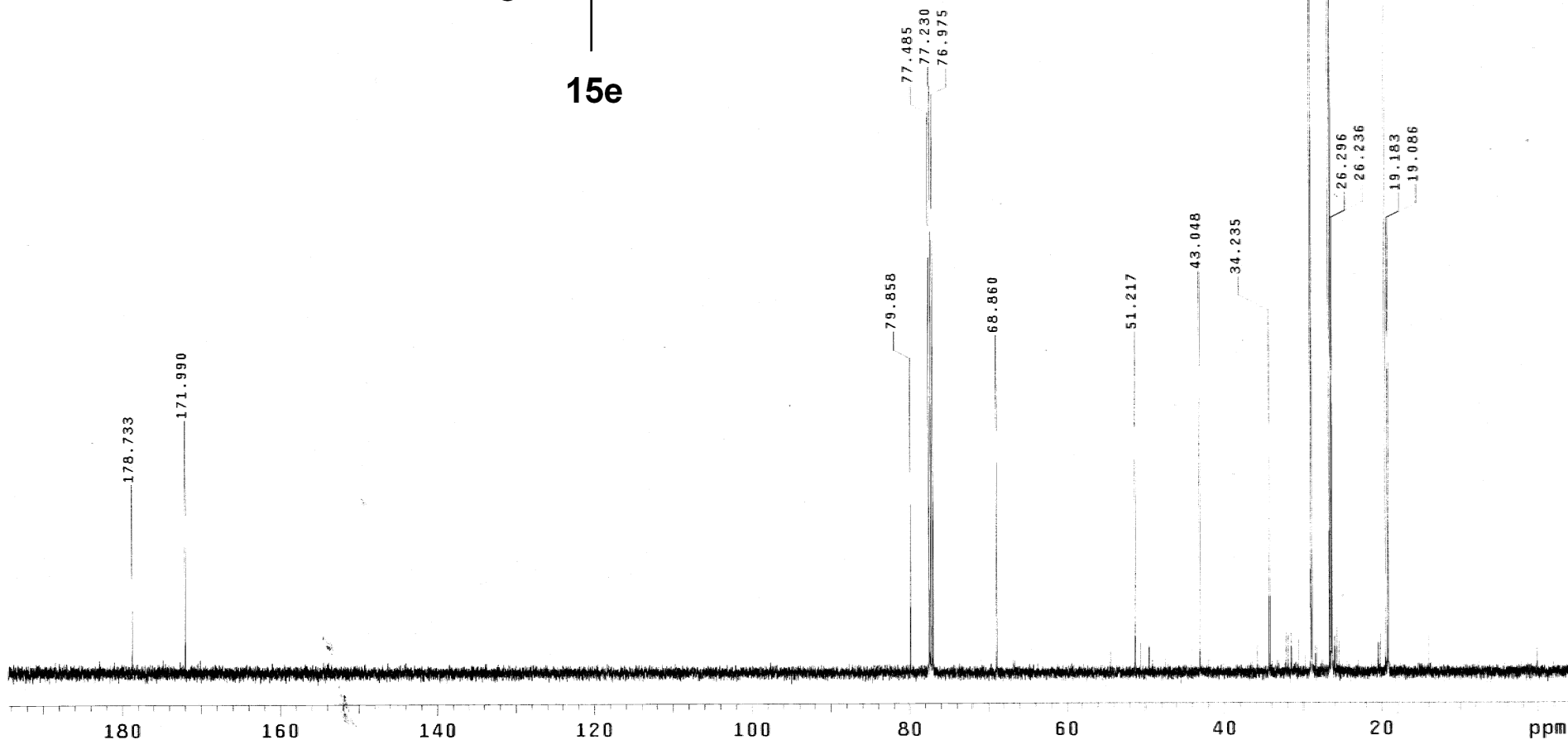
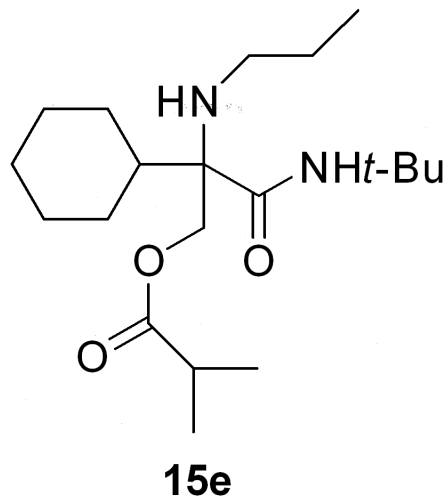
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min, 21 sec



LF-III-267c

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 22.0 C / 295.1 K

File: LF-III-267c

INOVA-500 "wittig"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 6387.7 Hz

8 repetitions

OBSERVE H1, 399.7773450 MHz

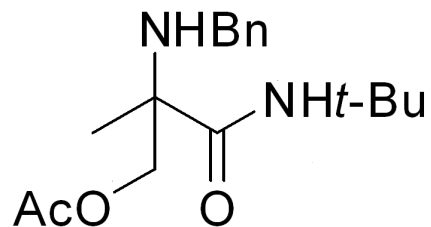
DATA PROCESSING

Line broadening 0.3 Hz

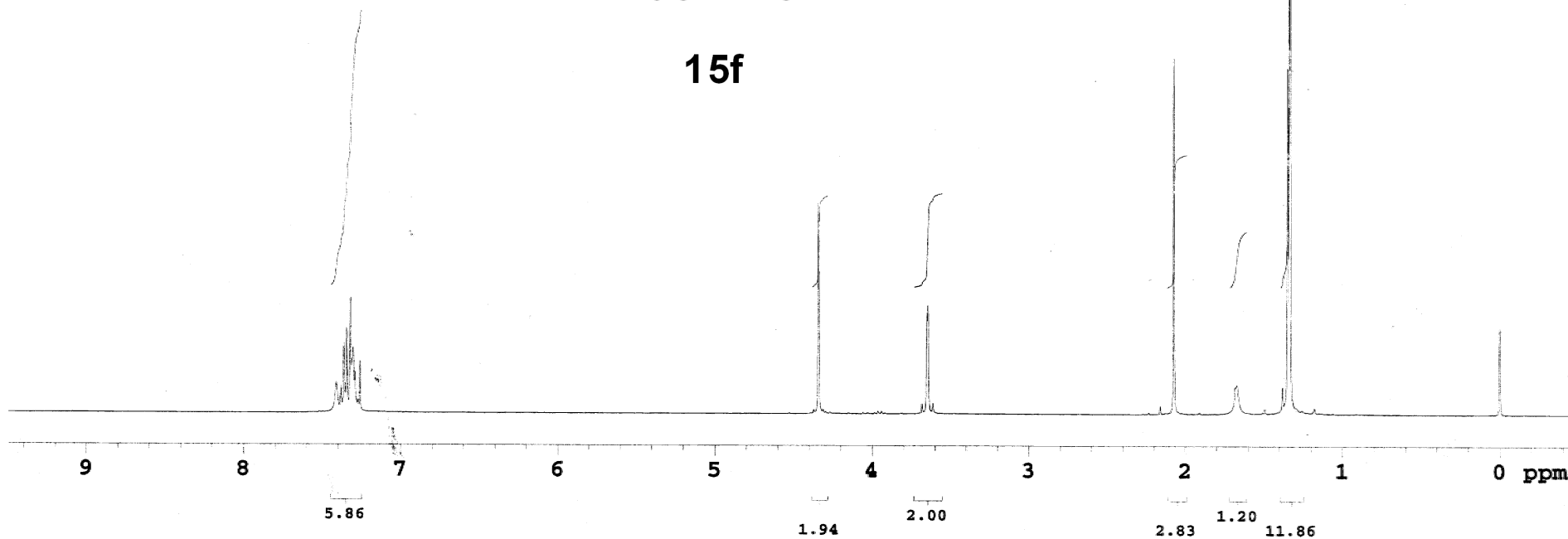
FT size 65536

Total time 0 min, 32 sec

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15f



-2~14ppm
27

LF-III-267C

INDEX	FREQUENCY	PPM	HEIGHT
1	2962.866	7.411	4.9
2	2951.365	7.383	4.2
3	2943.957	7.364	10.4
4	2943.177	7.362	11.0
5	2936.159	7.344	13.4
6	2926.997	7.322	18.2
7	2922.709	7.311	8.5
8	2920.175	7.305	10.3
9	2915.301	7.292	6.6
10	2903.410	7.263	8.1
11	2902.435	7.260	8.2
12	1735.340	4.341	33.2
13	1459.697	3.651	15.9
14	1457.358	3.645	17.1
15	829.072	2.074	56.3
16	828.487	2.072	54.9
17	672.147	1.681	4.4
18	669.028	1.674	4.7
19	552.650	1.382	4.4
20	539.589	1.350	54.5
21	535.105	1.339	162.1
22	-0.000	-0.000	13.6
23	-0.780	-0.002	13.3

C13LF-III-267c

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 22.0 C / 295.1 K

File: C13LF-III-267c

INOVA-500 "wolff"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 25157.2 Hz

256 repetitions

OBSERVE C13, 100.5240712 MHz

DECOUPLE H1, 399.7793569 MHz

Power 38 dB

continuously on

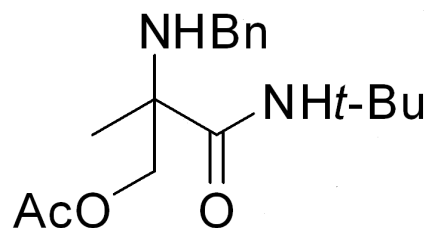
WALTZ-16 modulated

DATA PROCESSING

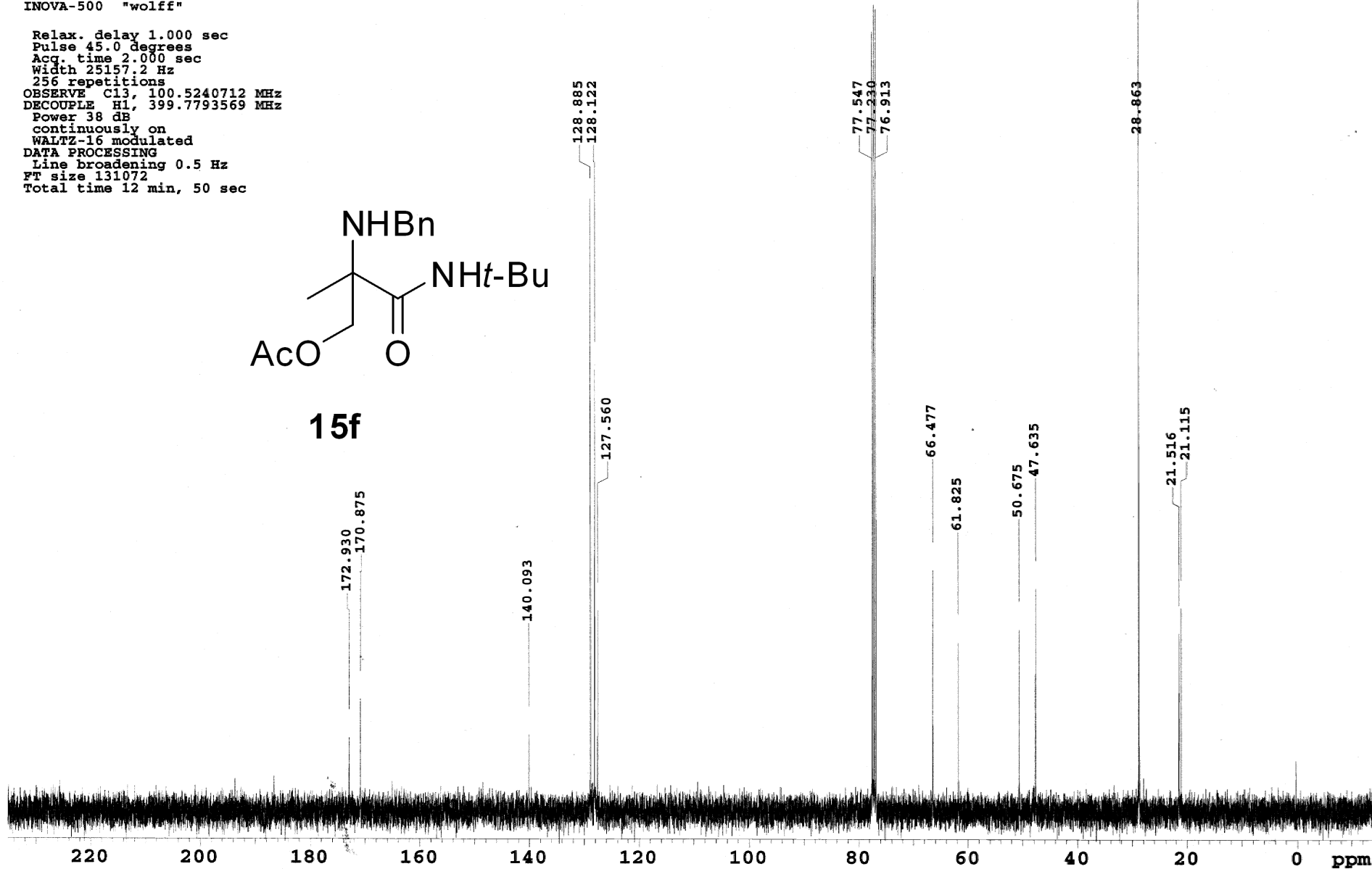
Line broadening 0.5 Hz

FT size 131072

Total time 12 min, 50 sec



15f



LF-VI-81c#3

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 20.0 C / 293.1 K

INNOVA-500 "inova500"

Relax. delay 2.000 sec

Pulse 61.4 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

8 repetitions

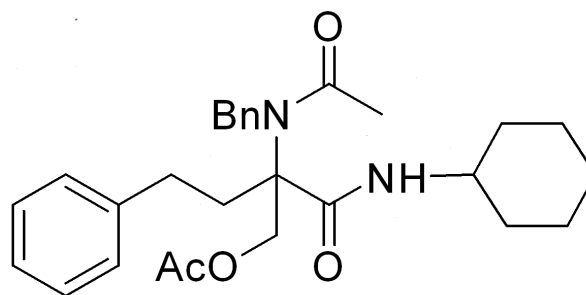
OBSERVE H1, 499.9172568 MHz

DATA PROCESSING

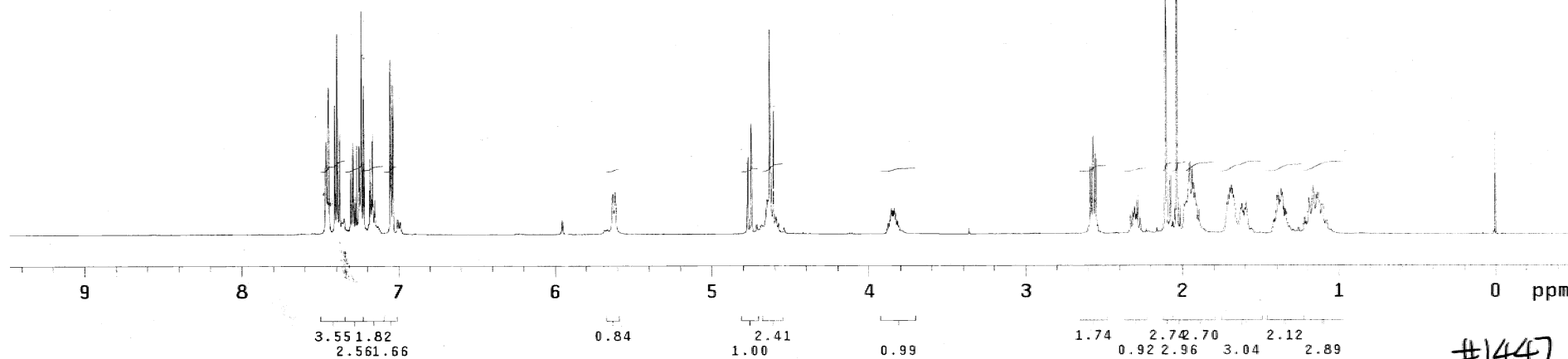
FT size 32768

Total time 0 min, 31 sec

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17a



#1447
26

INDEX	FREQUENCY	PPM	HEIGHT
1	3731.934	7.465	14.8
2	3724.121	7.449	23.3
3	3703.613	7.408	20.5
4	3696.289	7.394	31.7
5	3688.477	7.378	15.9
6	3652.344	7.306	9.8
7	3645.020	7.291	14.7
8	3633.301	7.268	14.2
9	3625.488	7.252	14.1
10	3624.023	7.249	7.4
11	3618.652	7.239	35.3
12	3610.840	7.223	23.7
13	3590.332	7.182	12.1
14	3589.355	7.180	8.4
15	3583.008	7.167	16.0
16	3526.855	7.055	22.1
17	3525.391	7.052	27.6
18	3518.555	7.038	23.7
19	2385.254	4.771	12.3
20	2374.023	4.749	17.6
21	2314.941	4.631	32.3
22	2303.711	4.608	19.7
23	1291.992	2.584	10.7
24	1283.691	2.568	15.7
25	1274.902	2.550	13.1
26	1050.781	2.102	113.5
27	1036.621	2.074	9.3
28	1015.625	2.032	162.0
29	975.586	1.951	11.6
30	967.285	1.935	10.6
31	963.379	1.927	8.2
32	847.656	1.696	7.4
33	843.750	1.688	7.9
34	839.355	1.679	7.3
35	683.594	1.367	7.3
36	583.008	1.166	7.8
37	-0.000	-0.000	16.2

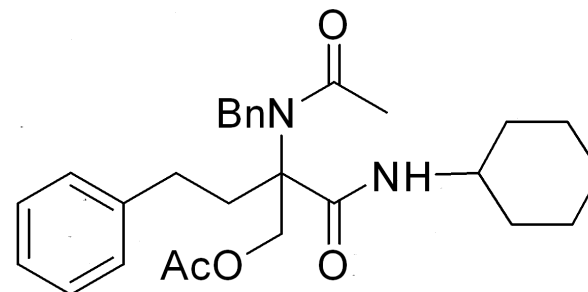
LF-VI-83c

Pulse Sequence: s2pu1

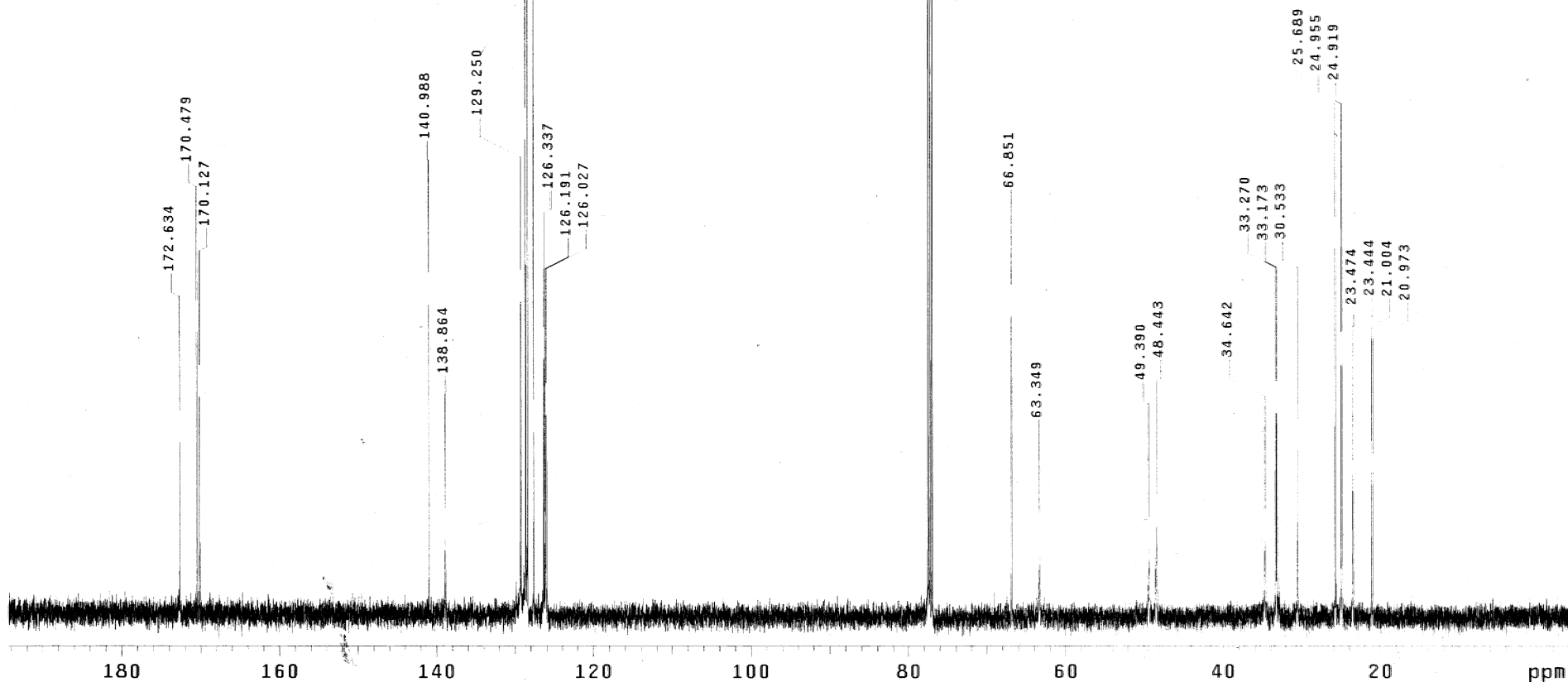
Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
User: 1-14-87
INOVA-500 "inova500"

Relax. delay 1.500 sec
Pulse 54.0 degrees
Acq. time 1.300 sec
Width 25000.0 Hz
200 repetitions
OBSERVE C13, 125.7042789 MHz
DECOUPLE H1, 499.9197456 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 21 sec

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17a



#158

LF-VI-85d#3

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 25.0 C / 298.1 K

INOVA-500 "inova500"

Relax. delay 2.000 sec

Pulse 68.4 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

8 repetitions

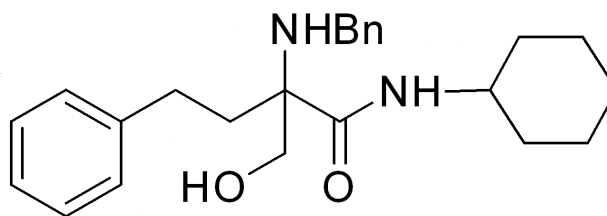
OBSERVE H1, 499.9172627 MHz

DATA PROCESSING

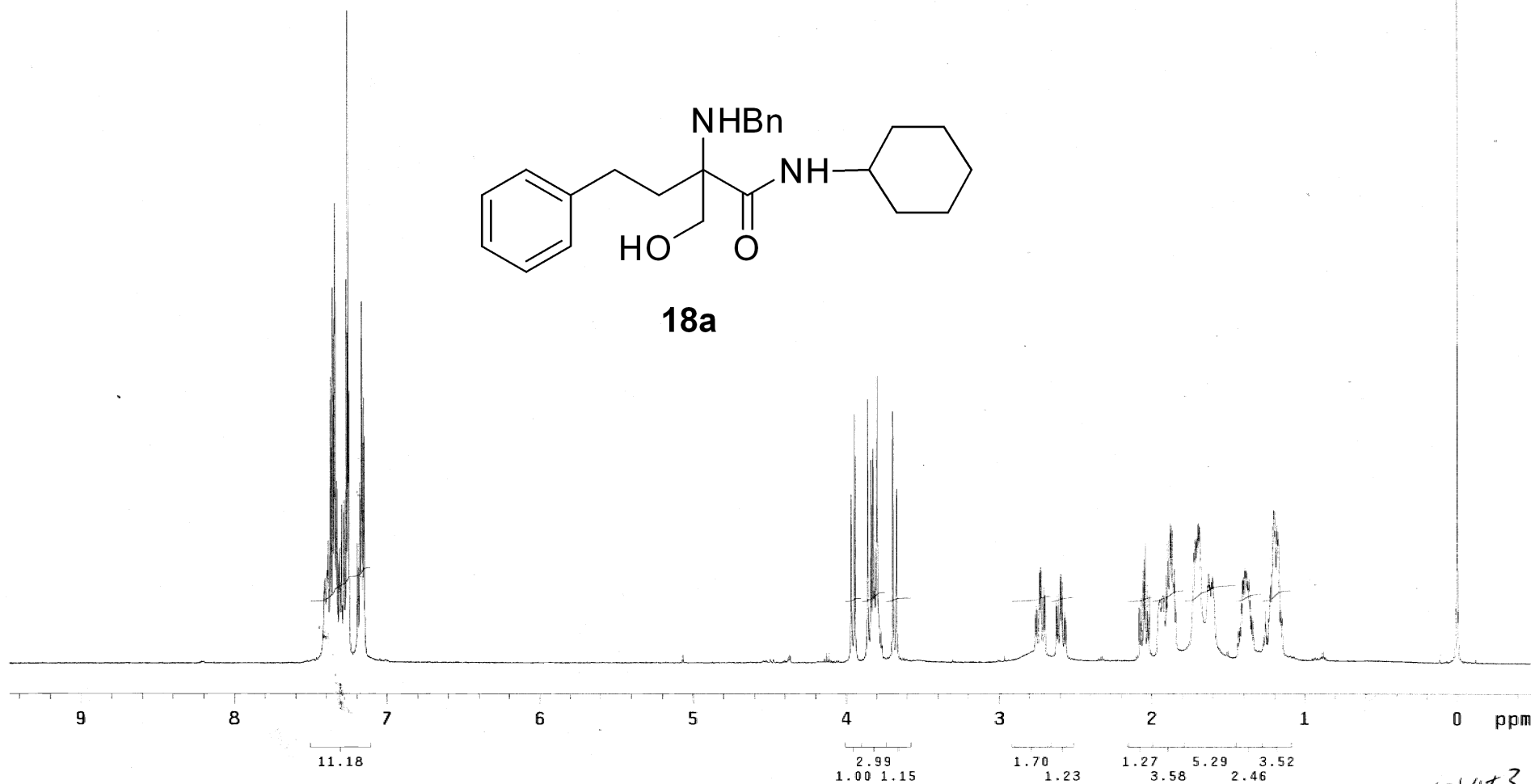
FT size 32768

Total time 0 min, 31 sec

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18a



#1453
-264ppm
CDCl₃

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3705.078	7.411	13.8	40	1305.664	2.612	11.2	79	689.941	1.380	14.7
2	3695.801	7.393	15.1	41	1298.340	2.597	14.5	80	687.988	1.376	13.0
3	3691.895	7.385	19.9	42	1292.969	2.586	14.5	81	686.035	1.372	13.4
4	3684.570	7.370	46.3	43	1285.156	2.571	8.4	82	684.570	1.369	12.6
5	3679.687	7.361	19.1	44	1279.785	2.560	7.5	83	682.617	1.365	13.7
6	3677.734	7.357	60.7	45	1039.551	2.079	9.1	84	678.223	1.357	10.1
7	3671.387	7.344	74.2	46	1034.180	2.069	10.7	85	674.316	1.349	7.8
8	3665.039	7.331	29.5	47	1026.855	2.054	12.3	86	670.898	1.342	7.5
9	3658.203	7.318	16.1	48	1025.391	2.051	15.0	87	628.906	1.258	8.4
10	3656.738	7.315	18.5	49	1021.484	2.043	19.4	88	617.187	1.235	7.2
11	3654.785	7.311	12.6	50	1020.020	2.040	15.4	89	611.816	1.224	12.7
12	3649.902	7.301	25.6	51	1012.695	2.026	12.8	90	601.562	1.203	24.5
13	3646.973	7.295	9.2	52	1007.324	2.015	11.1	91	600.098	1.200	24.8
14	3644.531	7.290	9.1	53	973.145	1.947	10.3	92	596.191	1.193	21.4
15	3640.625	7.282	26.4	54	960.937	1.922	11.0	93	589.844	1.180	22.3
16	3633.301	7.268	62.0	55	952.148	1.905	14.3	94	586.426	1.173	20.3
17	3628.418	7.258	105.4	56	947.266	1.895	19.8	95	578.613	1.157	8.7
18	3625.977	7.253	44.0	57	939.453	1.879	22.8	96	574.707	1.150	7.3
19	3596.680	7.195	19.4	58	937.988	1.876	20.9	97	2.930	0.006	8.9
20	3589.355	7.180	29.2	59	935.059	1.870	22.2	98	-0.000	-0.000	162.0
21	3587.402	7.176	15.9	60	933.105	1.867	21.4	99	-3.418	-0.007	8.4
22	3583.008	7.167	58.4	61	925.781	1.852	15.3				
23	3576.172	7.154	42.9	62	920.898	1.842	10.4				
24	1982.910	3.966	27.3	63	861.328	1.723	17.9				
25	1971.680	3.944	40.2	64	857.422	1.715	20.1				
26	1929.199	3.859	42.7	65	852.539	1.705	20.3				
27	1917.969	3.837	32.9	66	848.145	1.697	22.9				
28	1912.109	3.825	34.7	67	843.750	1.688	22.2				
29	1906.250	3.813	12.4	68	816.895	1.634	12.6				
30	1899.414	3.799	46.5	69	812.988	1.626	14.6				
31	1847.168	3.695	40.8	70	809.082	1.618	12.6				
32	1834.961	3.671	28.2	71	804.199	1.609	13.2				
33	1379.395	2.759	8.0	72	800.293	1.601	14.2				
34	1375.000	2.750	9.3	73	707.031	1.414	9.8				
35	1366.211	2.733	15.2	74	703.613	1.407	13.8				
36	1361.816	2.724	15.5	75	701.172	1.403	12.9				
37	1353.516	2.707	12.3	76	699.707	1.400	14.0				
38	1349.121	2.699	11.2	77	695.801	1.392	16.3				
39	1311.035	2.623	9.9	78	691.895	1.384	15.1				

LF-VI-85c

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 20.0 C / 293.1 K

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec

Pulse 54.0 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

600 repetitions

OBSERVE C13, 125.7042362 MHz

DECOUPLE H1, 499.9197456 MHz

Power 38 dB

continuously on

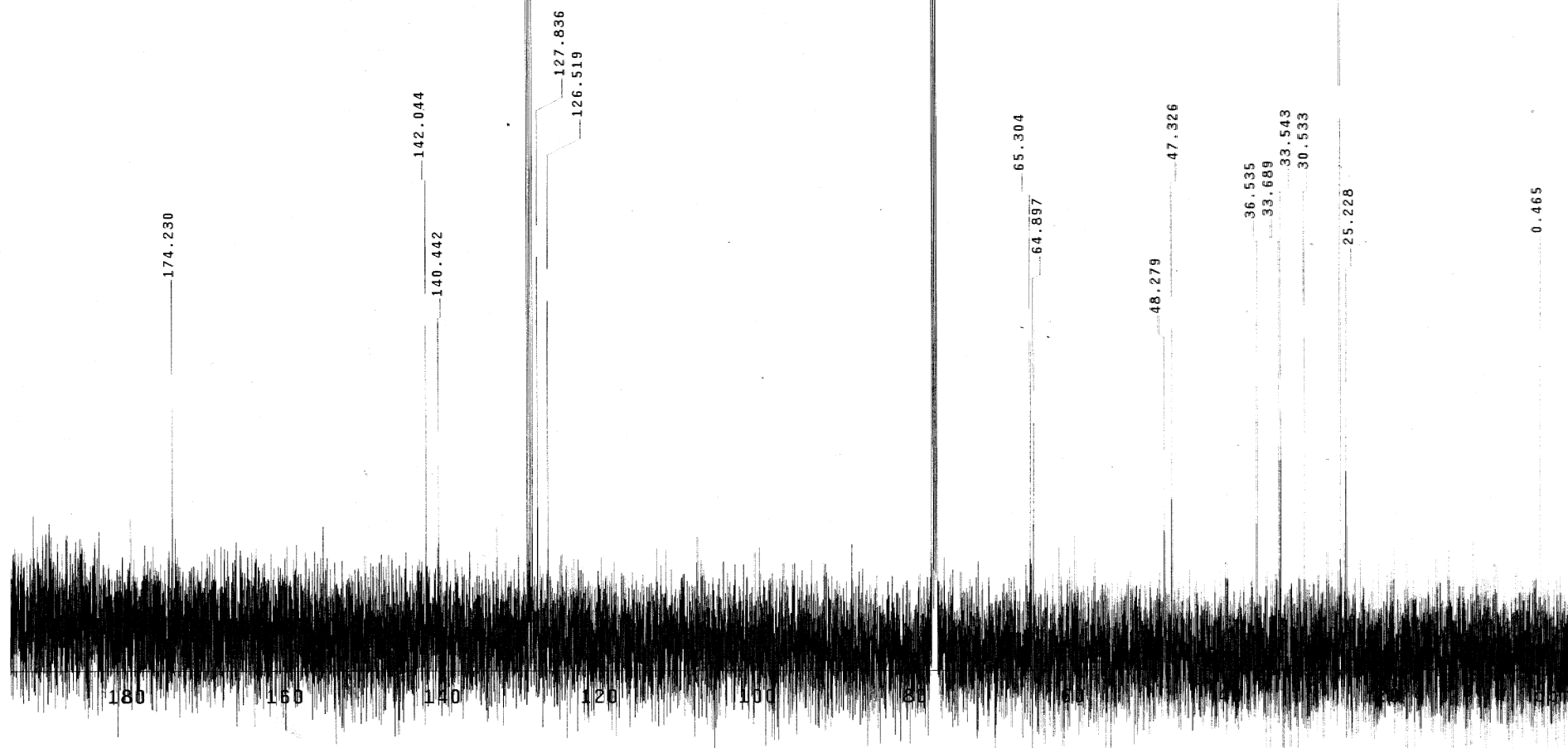
WALTZ-16 modulated

DATA PROCESSING

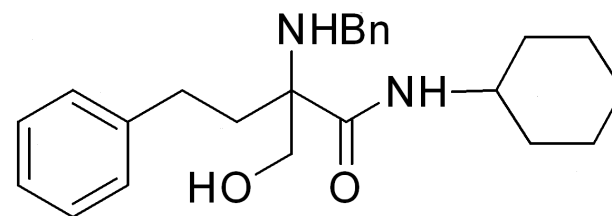
Line broadening 0.5 Hz

FT size 65536

Total time 28 min, 5 sec



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18a

LF-VI-61a

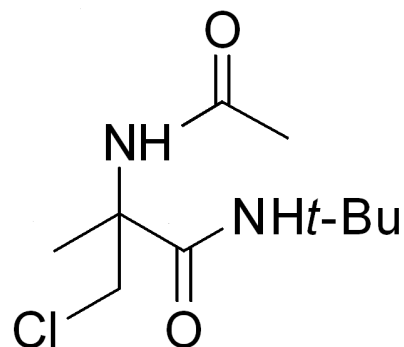
Sample directory:
File: PROTON

Pulse Sequence: s2pul

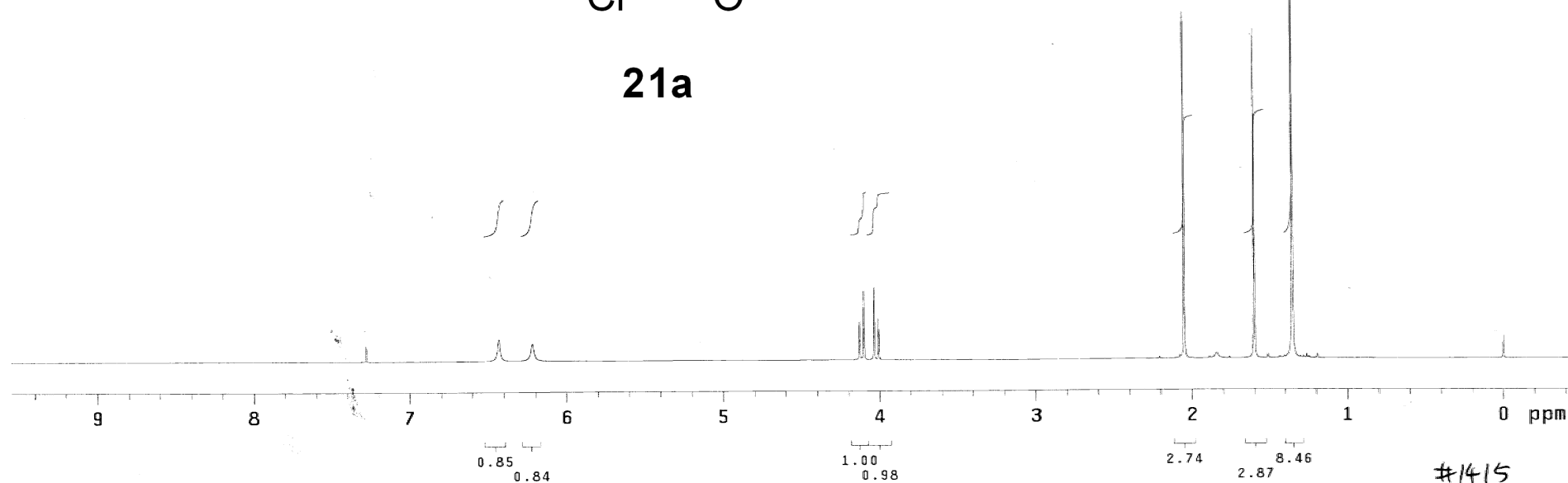
Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773364 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

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21a



#1415
30 -2-14ppm
CDCl₃

INDEX	FREQUENCY	PPM	HEIGHT
1	2570.845	6.431	3.5
2	1649.957	4.127	6.2
3	1638.651	4.099	11.1
4	1612.529	4.034	11.7
5	1601.223	4.005	6.6
6	818.741	2.048	55.0
7	639.397	1.599	52.3
8	541.148	1.354	162.0
9	-0.000	-0.000	3.6

~~13C OBSERVE~~

C¹³ LF-VI-61a

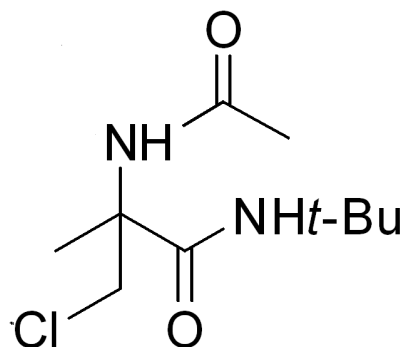
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Sample directory:
File: CARBON

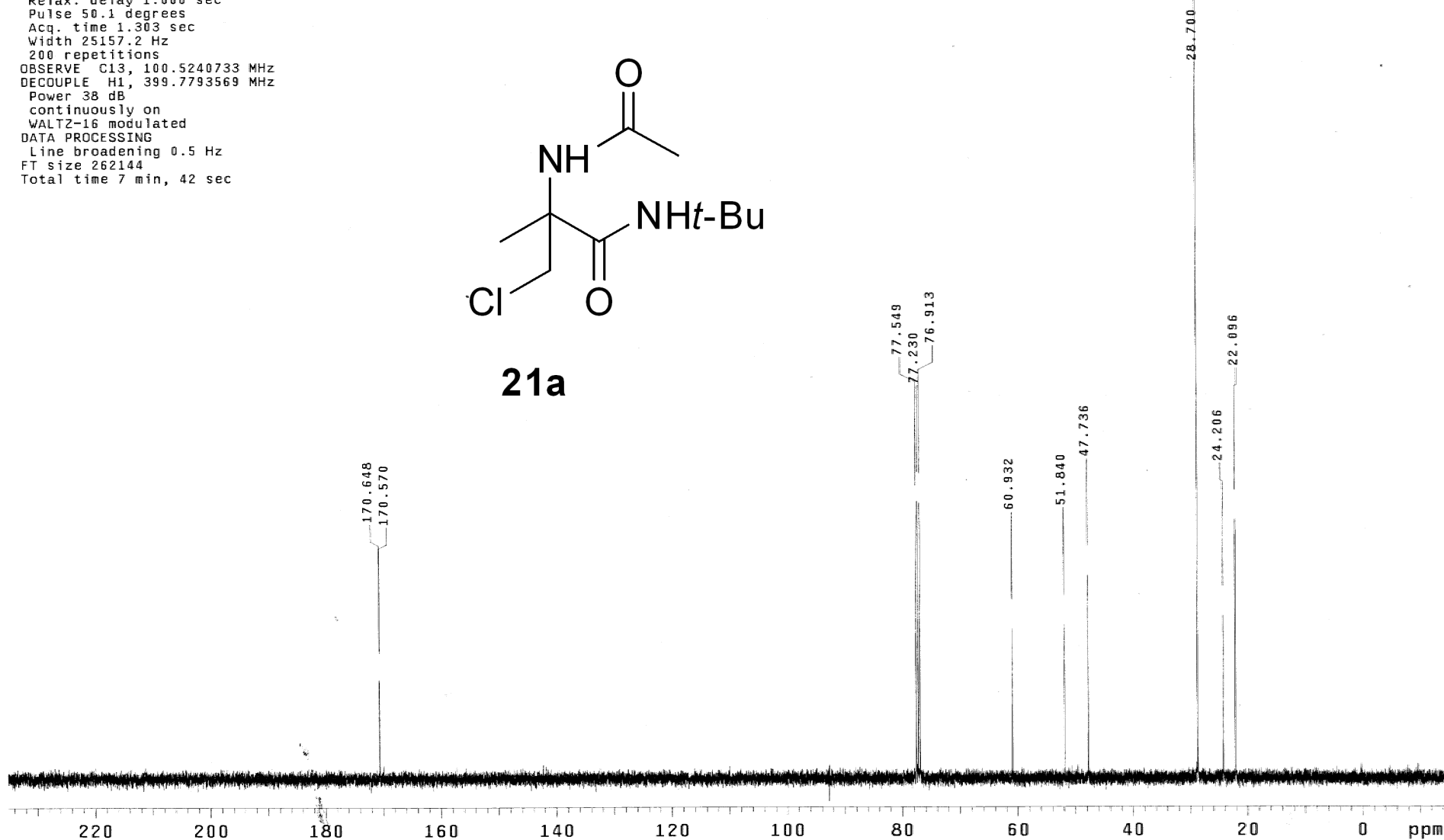
Pulse Sequence: s2pu1

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
200 repetitions
OBSERVE C13, 100.5240733 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 7 min, 42 sec



21a



LF-III-241b

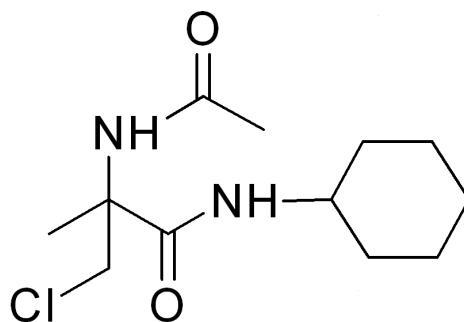
Sample directory:
File: PROTON

Pulse Sequence: s2pu1

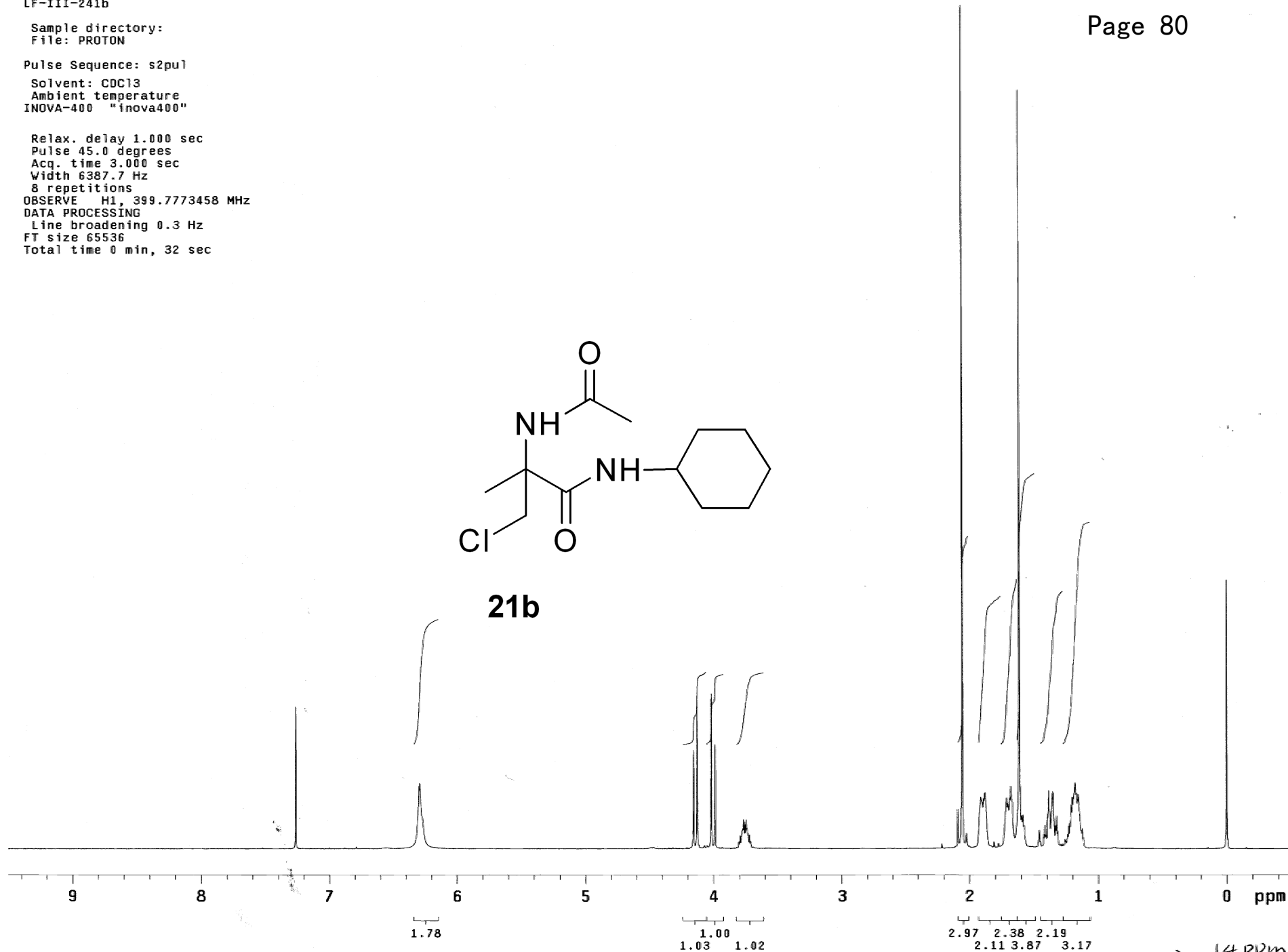
Solvent: CDCl₃
Ambient temperature
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773458 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 32 sec

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21b



-2~14 ppm

31 #571

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2905.164	7.267	27.2	40	465.123	1.163	9.4
2	2516.457	6.295	12.5	41	462.393	1.157	10.4
3	1661.848	4.157	18.9	42	450.697	1.127	3.9
4	1650.347	4.128	28.1	43	-0.000	-0.000	51.5
5	1606.291	4.018	29.7				
6	1594.790	3.989	20.0				
7	1509.212	3.775	3.8				
8	1506.872	3.769	5.6				
9	1502.779	3.759	5.2				
10	1498.685	3.749	5.6				
11	1496.346	3.743	4.0				
12	1492.447	3.733	3.0				
13	835.505	2.090	7.5				
14	822.054	2.056	162.2				
15	764.743	1.913	9.9				
16	756.750	1.893	9.6				
17	752.267	1.882	10.7				
18	685.598	1.715	9.7				
19	681.699	1.705	8.6				
20	676.046	1.691	9.7				
21	672.342	1.682	11.9				
22	646.025	1.616	145.9				
23	638.813	1.598	6.3				
24	634.719	1.588	6.4				
25	631.015	1.578	4.4				
26	583.840	1.460	3.6				
27	566.490	1.417	4.4				
28	558.498	1.397	6.7				
29	555.184	1.389	11.1				
30	541.928	1.356	10.9				
31	533.546	1.335	4.4				
32	530.232	1.326	6.3				
33	526.918	1.318	3.4				
34	492.609	1.232	4.3				
35	488.905	1.223	5.4				
36	485.006	1.213	8.4				
37	481.108	1.203	9.9				
38	472.920	1.183	12.6				
39	469.021	1.173	10.7				

Sample directory:

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

File: C13LF-III-241b

Mercury-300BB "mercury300",

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 25157.2 Hz

200 repetitions

OBSERVE C13, 100.5240726 MHz

DECOUPLE H1, 399.7793569 MHz

Power 38 dB

continuously on

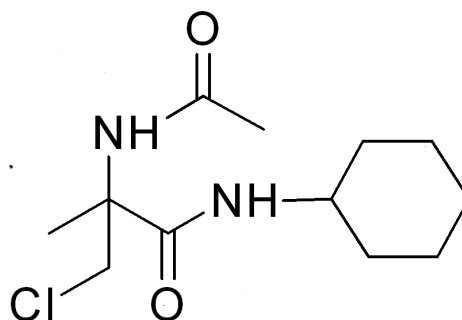
WALTZ-16 modulated

DATA PROCESSING

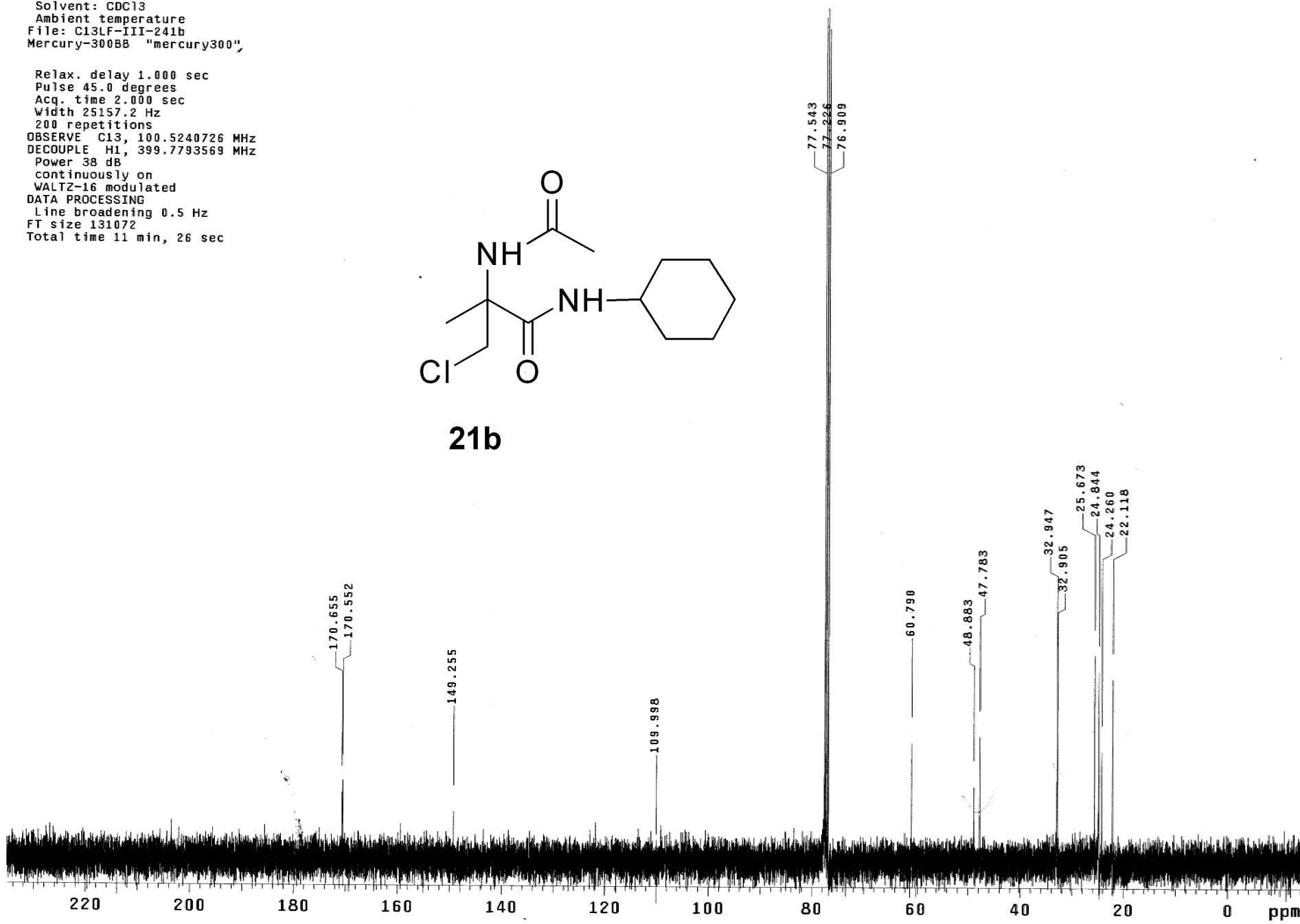
Line broadening 0.5 Hz

FT size 131072

Total time 11 min, 26 sec



21b

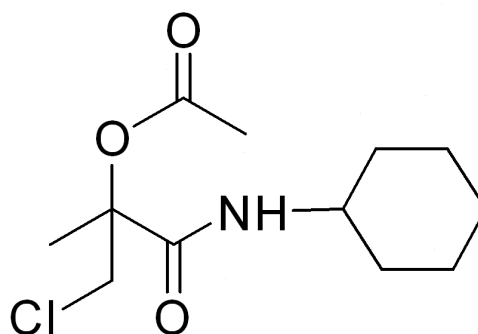
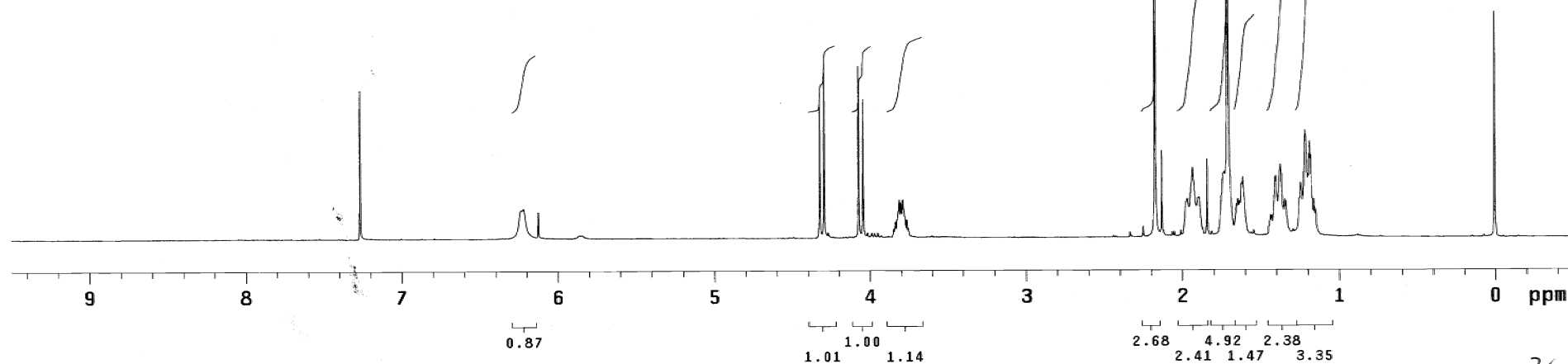


Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773458 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 32 sec

**22**

#570³²
1400m

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2906.139	7.269	23.5	40	460.639	1.152	4.6
2	2493.455	6.237	4.6	41	0.975	0.002	35.5
3	2487.607	6.222	4.8				
4	2449.594	6.127	4.3				
5	1729.687	4.327	21.1				
6	1718.185	4.298	26.9				
7	1628.904	4.075	27.2				
8	1617.402	4.046	22.0				
9	1523.637	3.811	6.1				
10	1519.543	3.801	5.7				
11	1515.255	3.790	6.2				
12	1504.728	3.764	3.0				
13	869.230	2.174	149.0				
14	852.465	2.132	13.8				
15	786.966	1.969	6.3				
16	773.710	1.935	11.1				
17	757.530	1.895	6.4				
18	736.866	1.843	12.4				
19	693.590	1.735	10.4				
20	683.648	1.710	151.2				
21	661.815	1.655	5.4				
22	658.306	1.647	6.2				
23	653.433	1.634	5.8				
24	648.559	1.622	8.6				
25	645.440	1.614	9.6				
26	575.653	1.440	3.7				
27	572.923	1.433	3.6				
28	563.761	1.410	9.6				
29	561.227	1.404	9.9				
30	549.921	1.376	11.6				
31	542.318	1.357	5.0				
32	539.004	1.348	6.2				
33	536.275	1.341	5.8				
34	498.652	1.247	8.7				
35	486.761	1.218	17.0				
36	479.353	1.199	10.0				
37	475.649	1.190	15.3				
38	472.530	1.182	13.1				
39	463.953	1.161	6.1				

Sample directory:

Pulse Sequence: s2pu1

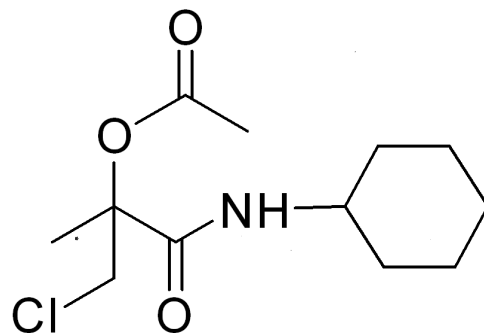
Solvent: CDCl3

Ambient temperature

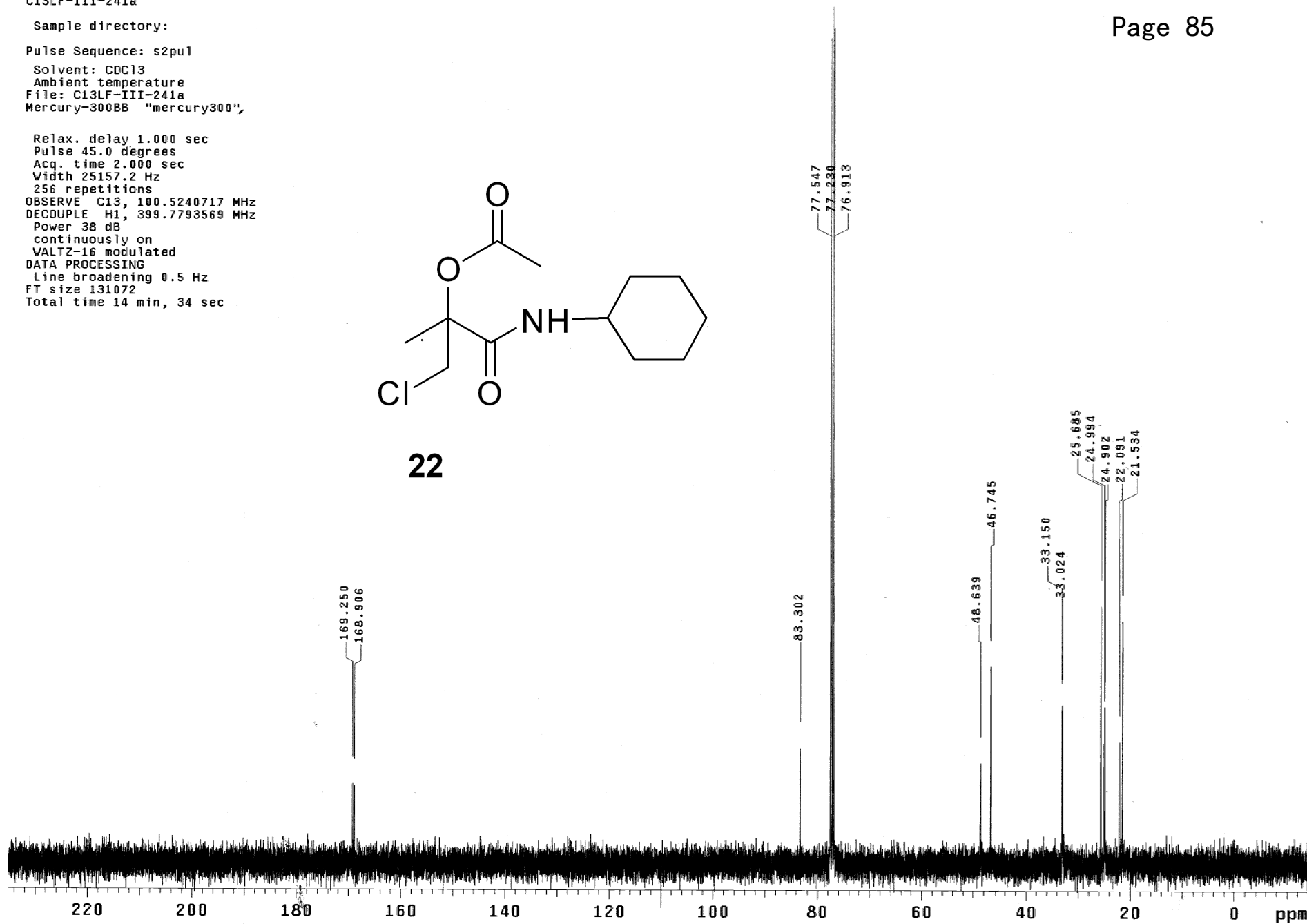
File: C13LF-III-241a

Mercury-300BB "mercury300",

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.000 sec
Width 25157.2 Hz
256 repetitions
OBSERVE C13, 100.5240717 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 14 min, 34 sec



22



LF-VI-83e#3

Pulse Sequence: s2pu1

Solvent: CDCl3

Temp. 23.0 C / 296.1 K

INOVA-500 "inova500"

Relax. delay 2.000 sec

Pulse 61.4 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

8 repetitions

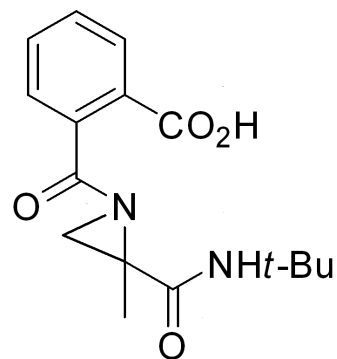
OBSERVE H1, 499.9172583 MHz

DATA PROCESSING

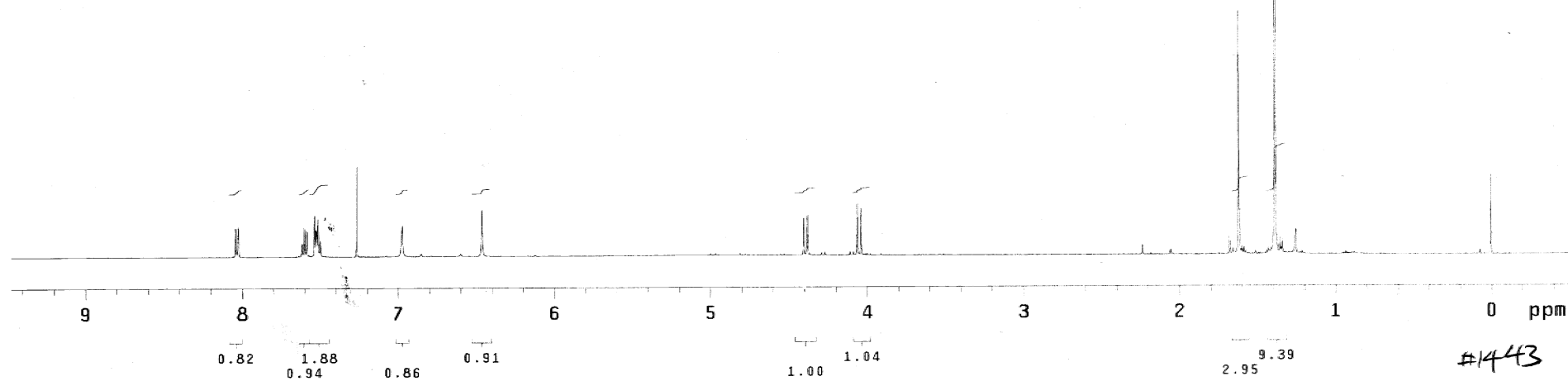
FT size 32768

Total time 0 min, 31 sec

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28



#1443

33

2-14ppm
CDCl₃

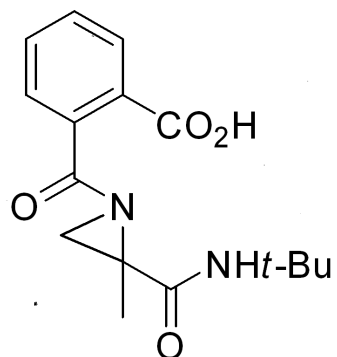
INDEX	FREQUENCY	PPM	HEIGHT
1	3631.836	7.265	14.4
2	3230.957	6.463	7.4
3	2030.762	4.062	8.3
4	2019.043	4.039	7.5
5	809.082	1.618	38.6
6	696.289	1.393	18.1
7	692.871	1.386	162.0
8	0.000	0.000	12.7

C13LF-VI-83e

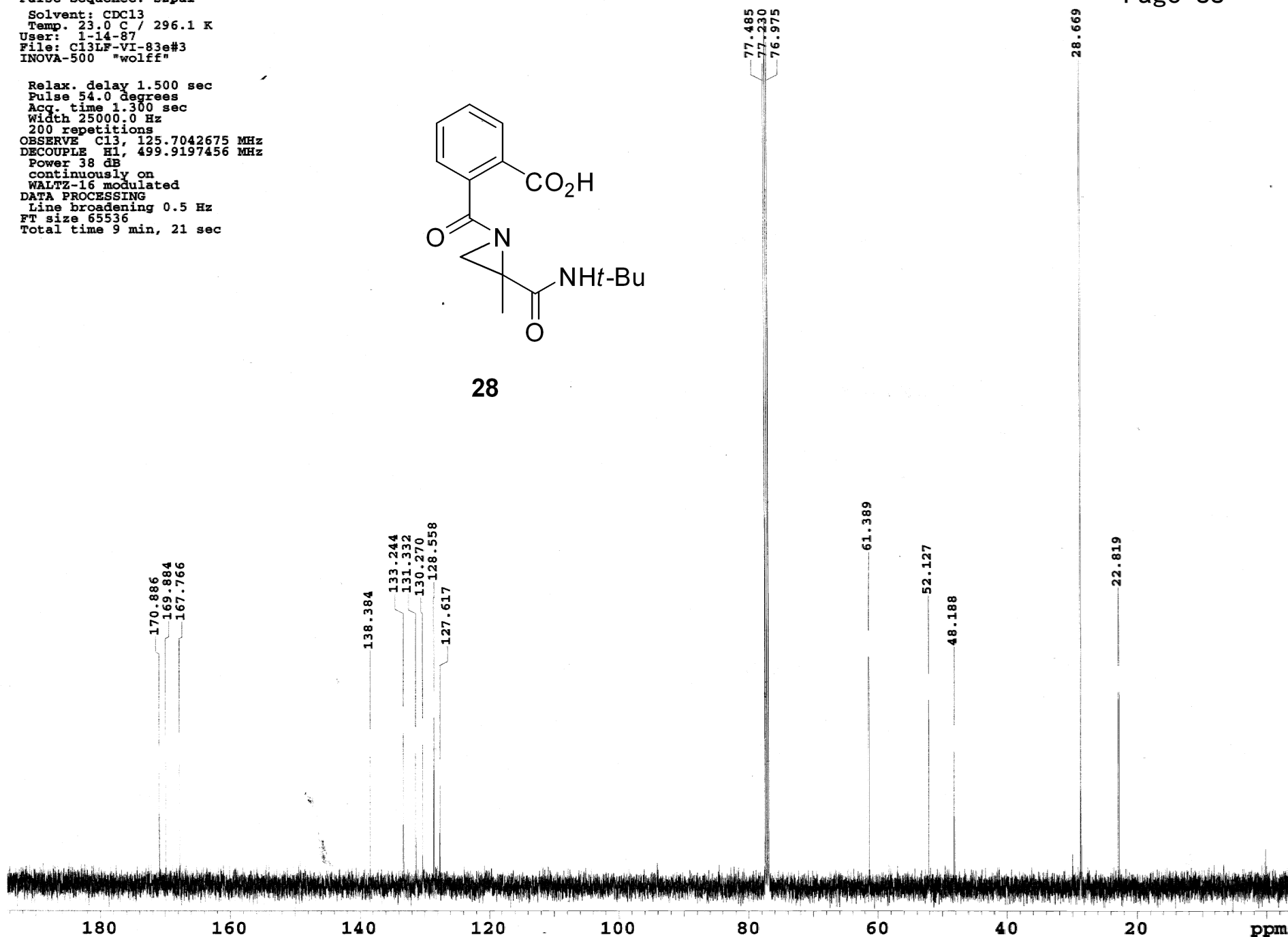
Pulse Sequence: s2pul

Solvent: CDCl₃
Temp. 23.0 C / 296.1 K
User: 1-14-87
File: C13LF-VI-83e#3
INNOVA-500 "wolff"

Relax. delay 1.500 sec
Pulse 54.0 degrees
Acq. time 1.300 sec
Width 25000.0 Hz
200 repetitions
OBSERVE C13, 125.7042675 MHz
DECOUPLE H1, 499.9197456 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 21 sec



28

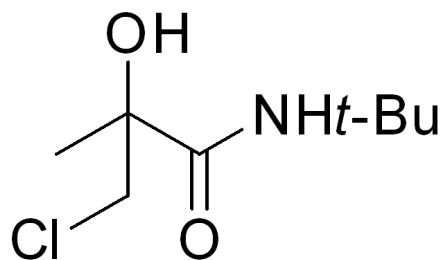
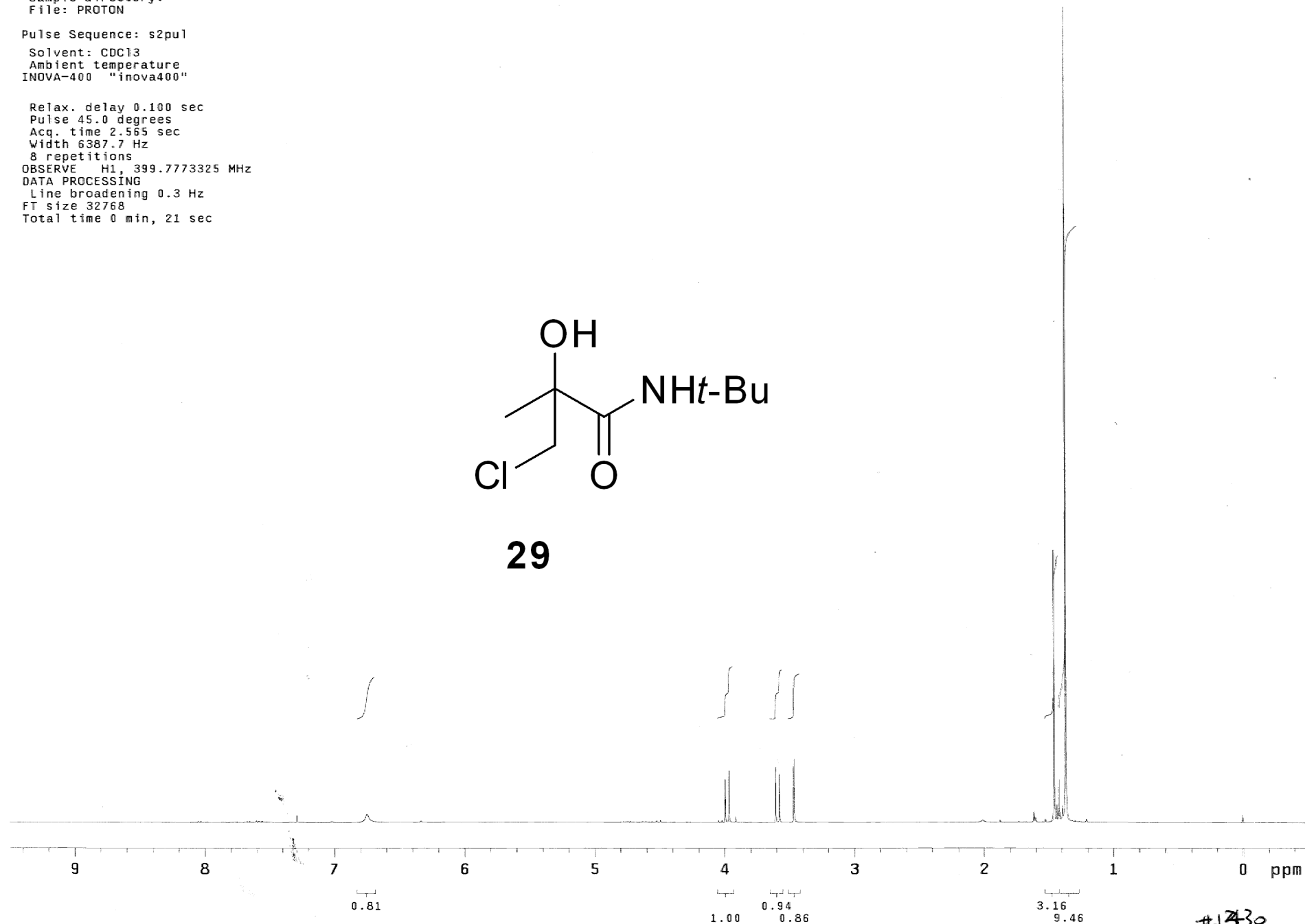


Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
INOVA-400 "inova400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773325 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

**29**

#1430
-214ppm
1.00

INDEX	FREQUENCY	PPM	HEIGHT
1	1596.934	3.995	8.4
2	1585.628	3.966	10.0
3	1441.373	3.605	10.7
4	1430.457	3.578	9.3
5	1385.231	3.465	12.2
6	583.645	1.460	52.0
7	575.458	1.439	3.6
8	569.220	1.424	8.2
9	557.523	1.395	3.3
10	548.166	1.371	156.1

Lf-VI-73a

Sample directory:

Pulse Sequence: s2pul

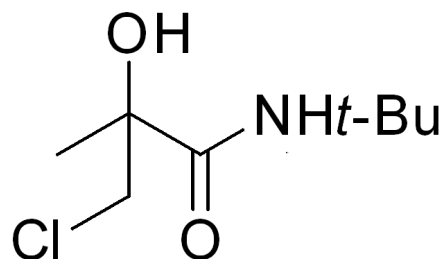
Solvent: CDCl₃

Ambient temperature

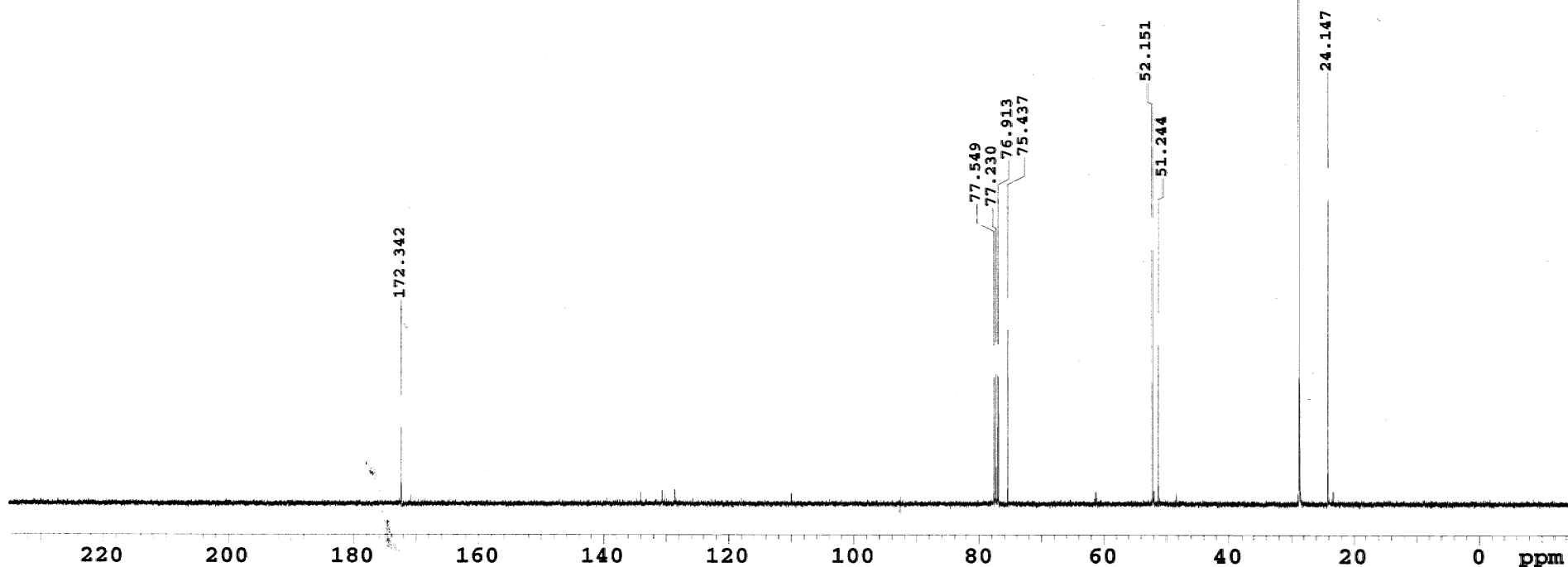
File: C13LF-VI-73a

INNOVA-500 "wolff"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
300 repetitions
OBSERVE C13, 100.5240745 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 11 min, 33 sec



29



LF-V-267aa

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

INOVA-500 "inova500"

Relax. delay 2.000 sec

Pulse 61.4 degrees

Acq. time 1.892 sec

Width 8000.0 Hz

8 repetitions

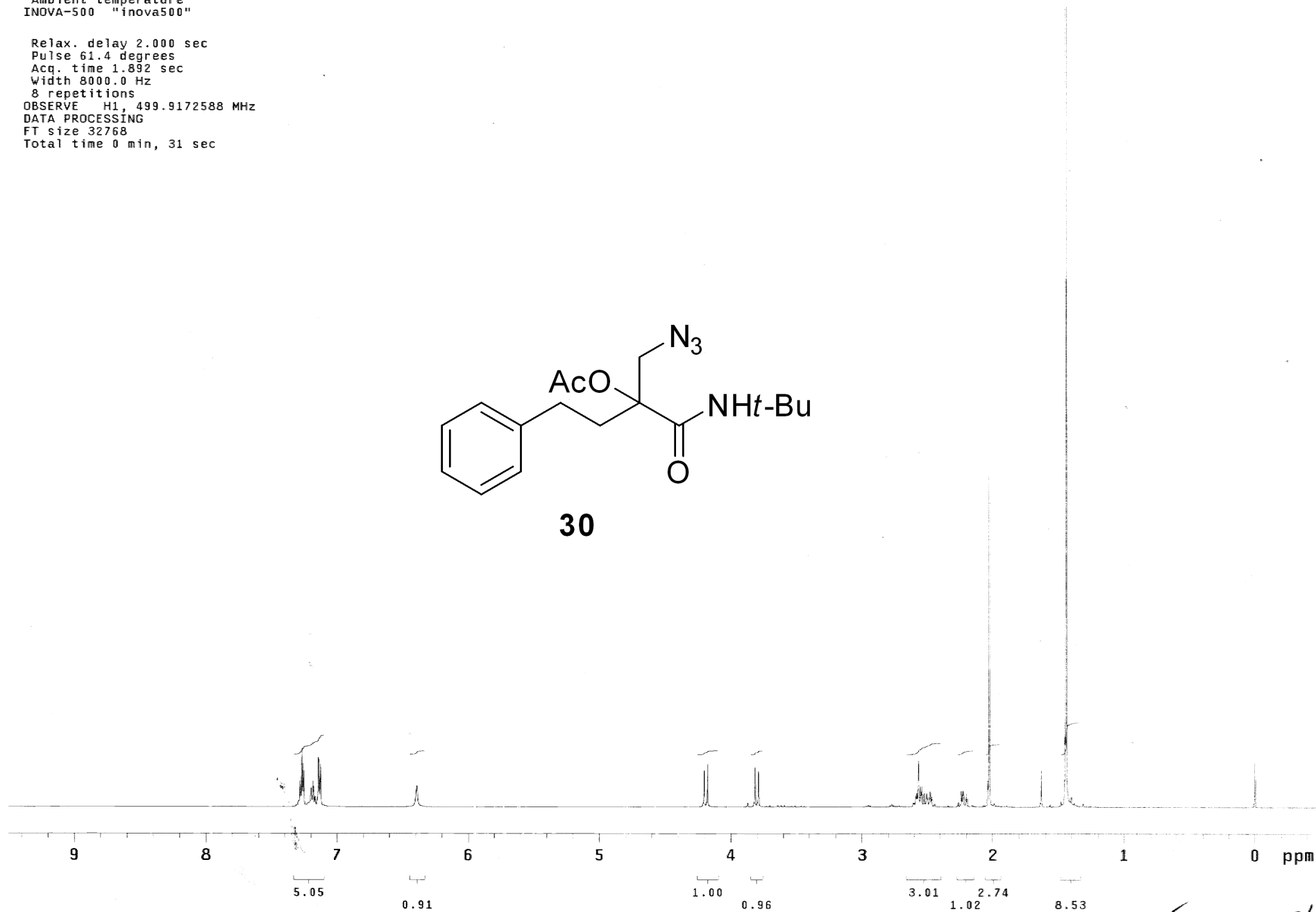
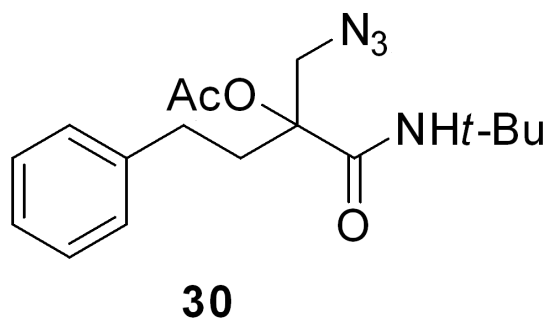
OBSERVE H1, 499.9172588 MHz

DATA PROCESSING

FT size 32768

Total time 0 min, 31 sec

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35

4386
-2-14974
in 1.

INDEX	FREQUENCY	PPM	HEIGHT
1	3633.789	7.269	11.2
2	3629.394	7.260	8.3
3	3570.800	7.143	9.4
4	3569.336	7.140	9.1
5	3562.500	7.126	8.1
6	2087.890	4.176	8.2
7	1907.226	3.815	7.5
8	1282.714	2.566	8.9
9	1013.183	2.027	62.6
10	725.586	1.451	13.4
11	720.214	1.441	151.2
12	-0.977	-0.002	8.6

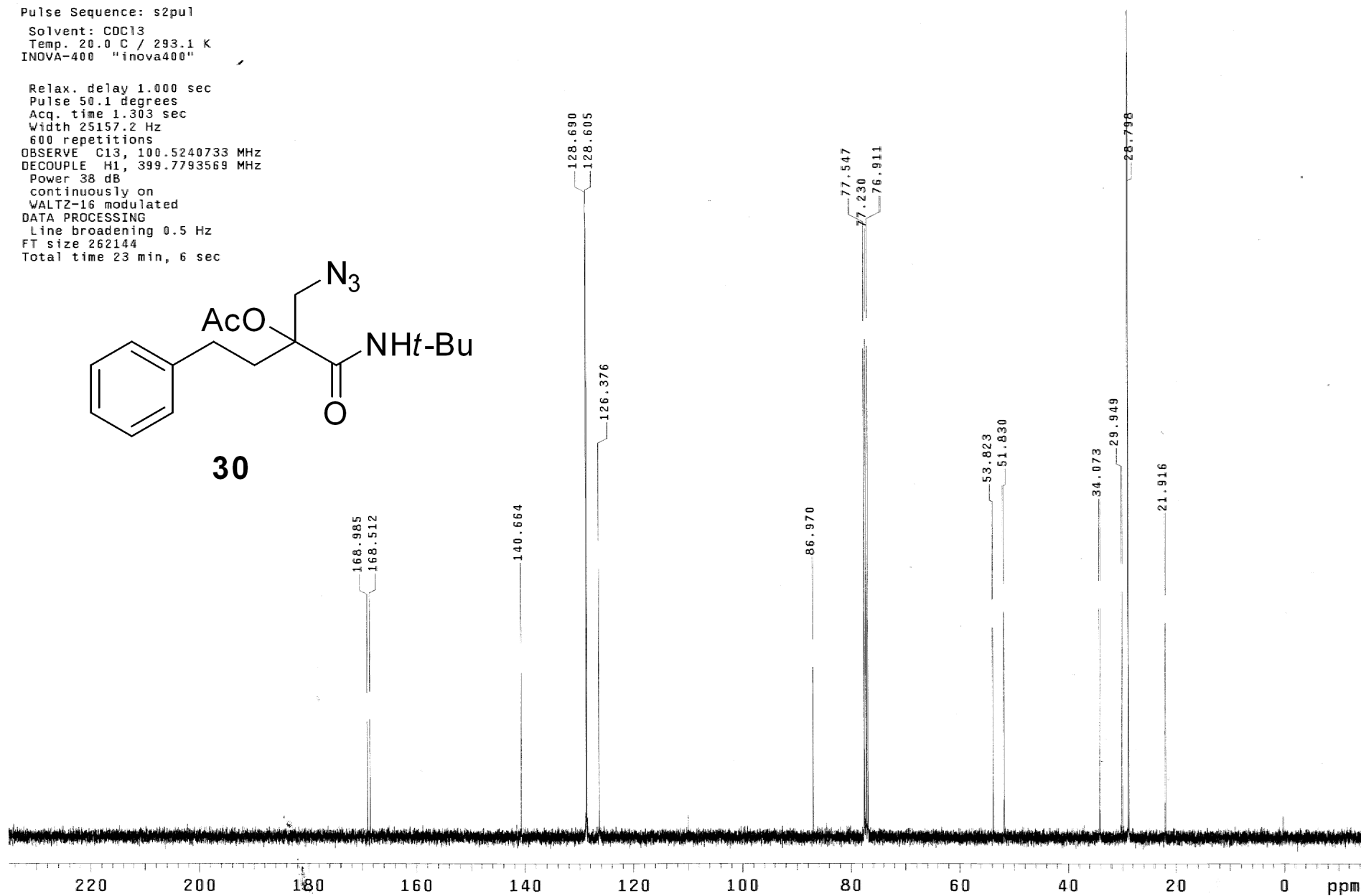
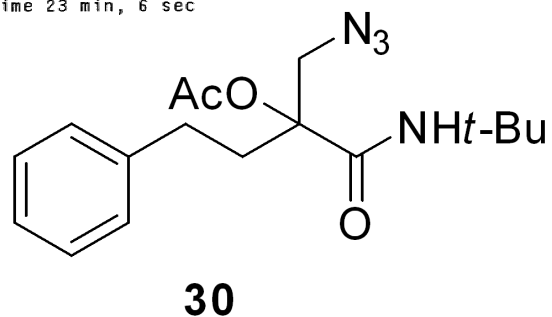
C13LF-VI-267

Sample directory:
File: CARBON

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Pulse Sequence: s2pul
Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
600 repetitions
OBSERVE C13, 100.5240733 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 23 min, 6 sec



#142
CDCl₃

LF-IV-109b

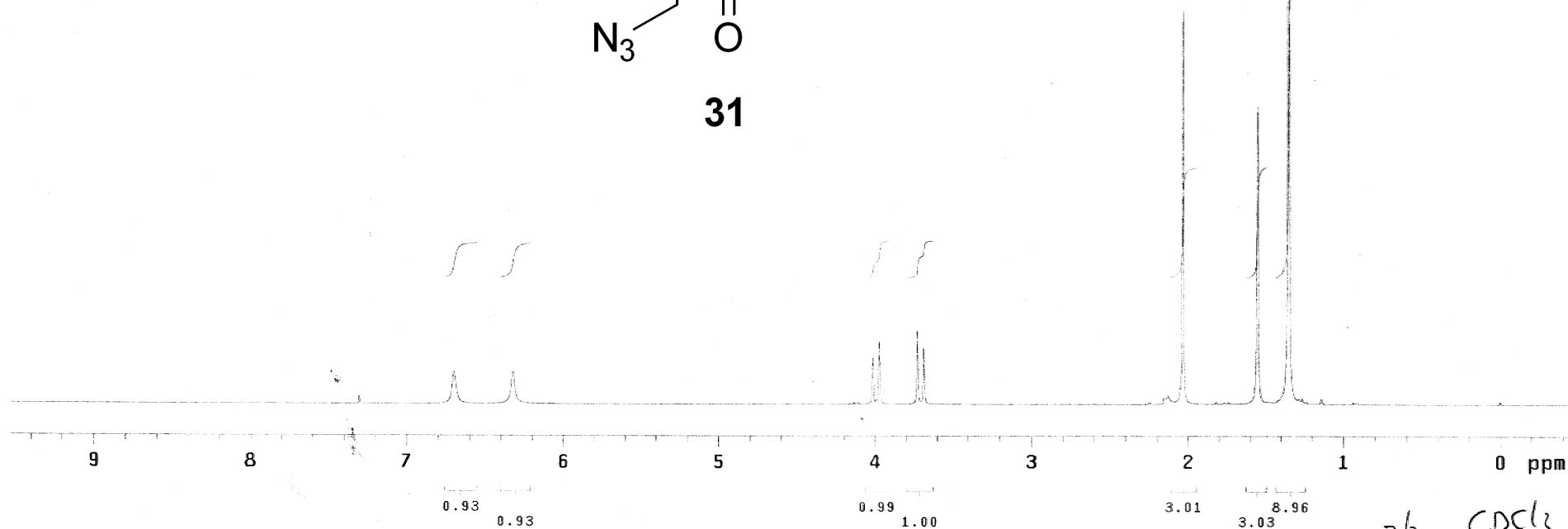
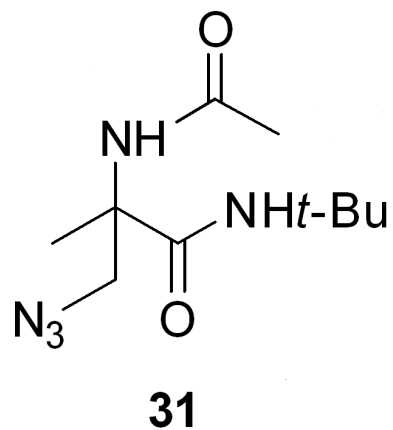
Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 43.8 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611557 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 0 sec

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36 CDCl₃
#741

INDEX	FREQUENCY	PPM	HEIGHT
1	2008.843	6.701	5.0
2	1896.006	6.325	5.1
3	1203.639	4.015	7.4
4	1191.070	3.973	9.9
5	1117.843	3.729	11.6
6	1105.419	3.688	8.8
7	614.609	2.050	2.6
8	609.493	2.033	62.4
9	465.670	1.553	46.9
10	464.647	1.550	46.1
11	405.598	1.353	162.2

LF-IV-109c

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: 1-14-87

INOVA-500 "inova500"

Relax. delay 1.500 sec

Pulse 55.1 degrees

Acq. time 1.300 sec

Width 25000.0 Hz

240 repetitions

OBSERVE C13, 125.7042690 MHz

DECOUPLE H1, 499.9197456 MHz

Power 34 dB

continuously on

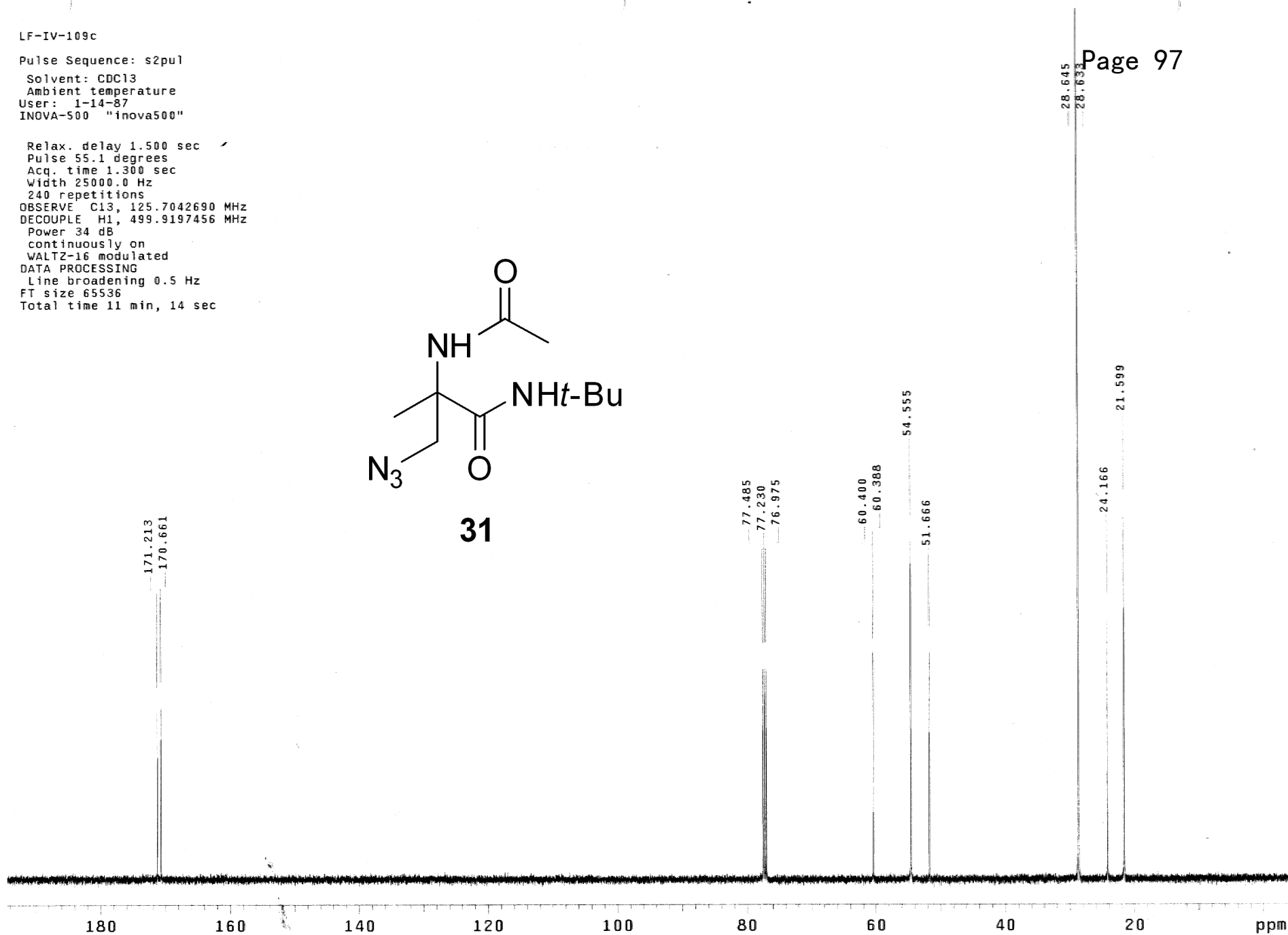
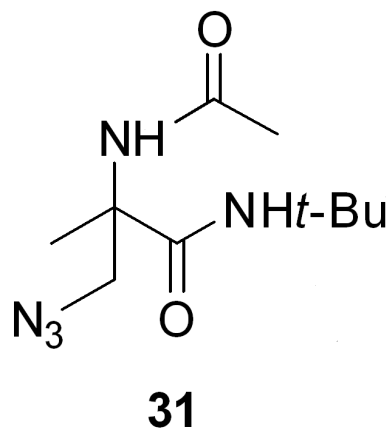
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 11 min, 14 sec

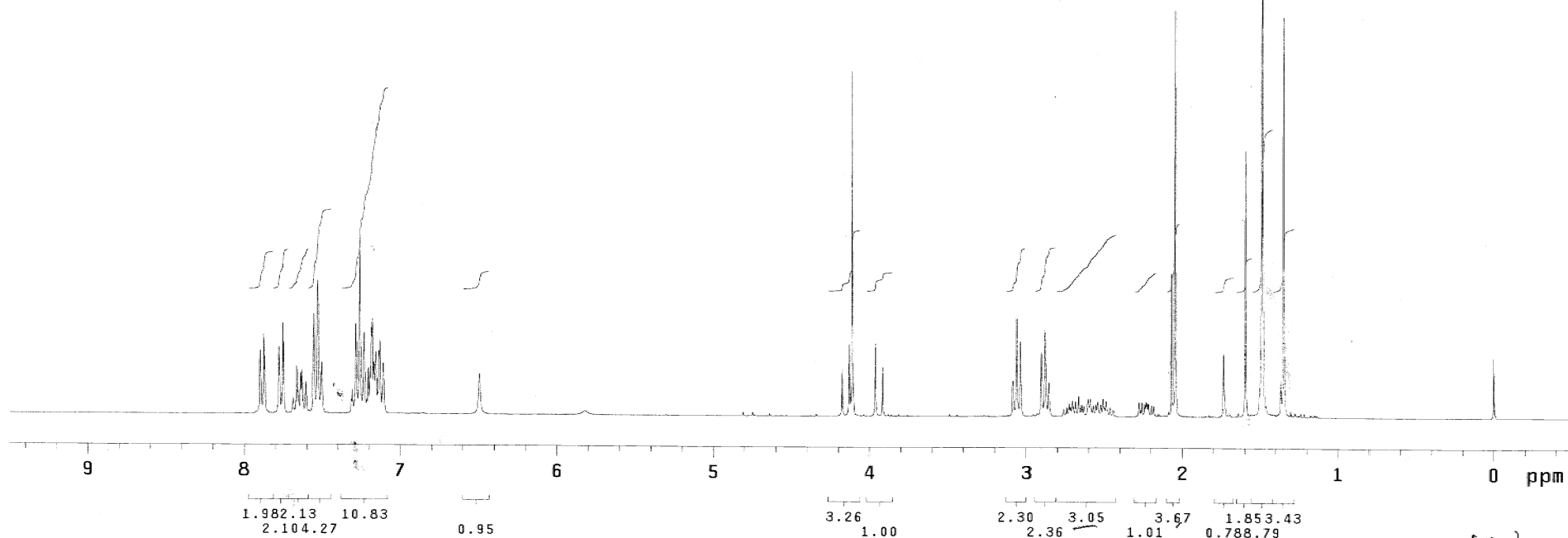
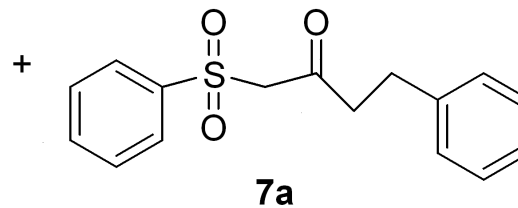
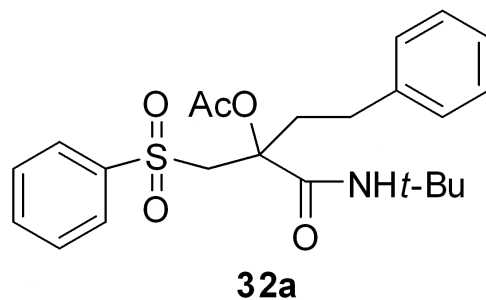


Sample directory:
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl₃
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611662 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 0 min, 0 sec



#403
-224PB

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2367.523	7.898	10.1	40	2141.850	7.145	3.5
2	2366.061	7.893	5.6	41	2139.657	7.138	10.2
3	2362.261	7.880	3.1	42	2138.050	7.133	11.9
4	2360.361	7.874	12.8	43	2131.180	7.110	8.2
5	2358.753	7.869	9.2	44	1947.163	6.496	6.5
6	2331.567	7.778	10.7	45	1252.019	4.177	7.6
7	2326.306	7.761	3.4	46	1238.134	4.130	11.5
8	2324.259	7.754	14.6	47	1232.579	4.112	54.6
9	2322.798	7.749	11.5	48	1188.146	3.964	11.6
10	2304.820	7.689	2.7	49	1174.261	3.917	7.9
11	2299.412	7.671	2.1	50	924.033	3.083	5.7
12	2297.366	7.664	7.7	51	917.017	3.059	15.7
13	2295.173	7.657	3.7	52	910.001	3.036	12.1
14	2291.081	7.643	3.8	53	870.538	2.904	10.3
15	2289.911	7.639	6.7	54	863.376	2.880	13.8
16	2287.427	7.631	7.1	55	855.921	2.855	5.4
17	2285.234	7.624	2.3	56	817.335	2.727	2.1
18	2281.288	7.610	3.2	57	811.196	2.706	2.6
19	2279.972	7.606	5.1	58	804.473	2.684	2.5
20	2278.803	7.602	2.9	59	798.626	2.664	3.3
21	2264.918	7.556	16.0	60	780.648	2.604	2.8
22	2257.610	7.531	21.3	61	776.117	2.589	2.9
23	2252.202	7.513	2.9	62	761.940	2.542	2.5
24	2250.594	7.508	6.9	63	751.854	2.508	2.9
25	2249.278	7.504	8.3	64	745.862	2.488	2.5
26	2192.422	7.314	2.4	65	682.282	2.276	2.3
27	2190.960	7.309	4.1	66	677.166	2.259	2.4
28	2189.352	7.304	2.1	67	669.127	2.232	2.4
29	2184.237	7.287	14.4	68	667.081	2.225	2.2
30	2182.775	7.282	11.5	69	620.309	2.069	22.9
31	2176.782	7.262	26.0	70	613.586	2.047	64.4
32	2168.451	7.234	13.0	71	520.335	1.736	10.1
33	2162.751	7.215	2.4	72	478.533	1.596	42.2
34	2160.266	7.207	7.4	73	450.908	1.504	4.7
35	2156.466	7.194	6.7	74	446.377	1.489	162.0
36	2154.274	7.187	13.9	75	410.421	1.369	5.9
37	2152.520	7.181	15.4	76	405.160	1.352	63.4
38	2149.450	7.171	8.3	77	-0.000	-0.000	9.7
39	2145.942	7.159	10.0				

LF-V-283ab

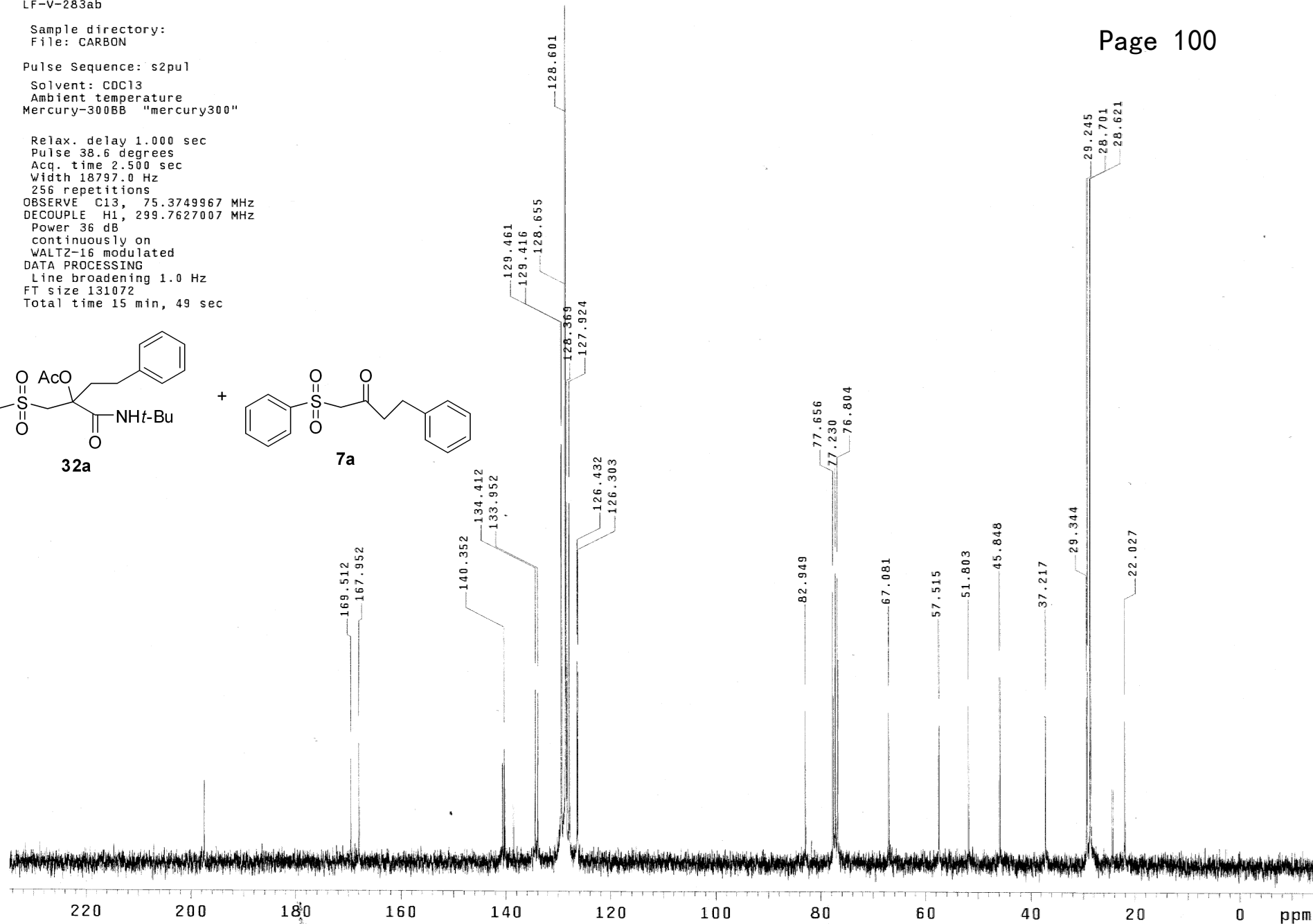
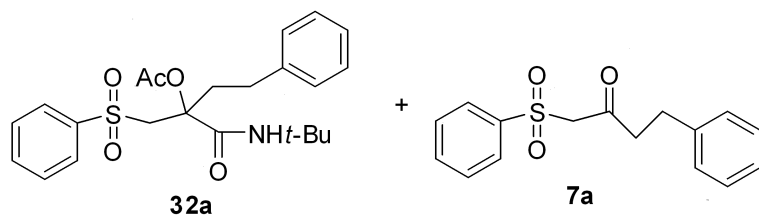
Sample directory:
File: CARBON

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 38.6 degrees
Acq. time 2.500 sec
Width 18797.0 Hz
256 repetitions
OBSERVE C13, 75.3749967 MHz
DECOUPLE H1, 299.7627007 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 15 min, 49 sec

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Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: JGP-II-33A

INOVA-500 "woodward"

Relax. delay 1.000 sec

Pulse 36.0 degrees

Acq. time 3.000 sec

Width 4789.3 Hz

16 repetitions

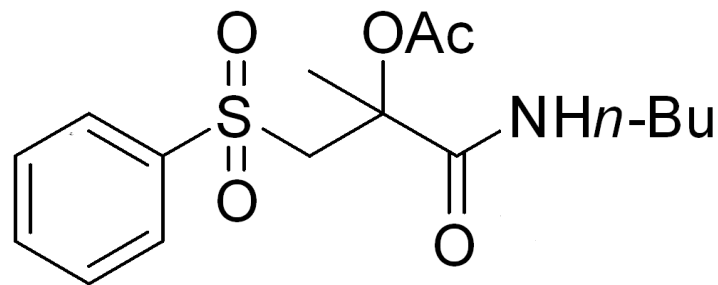
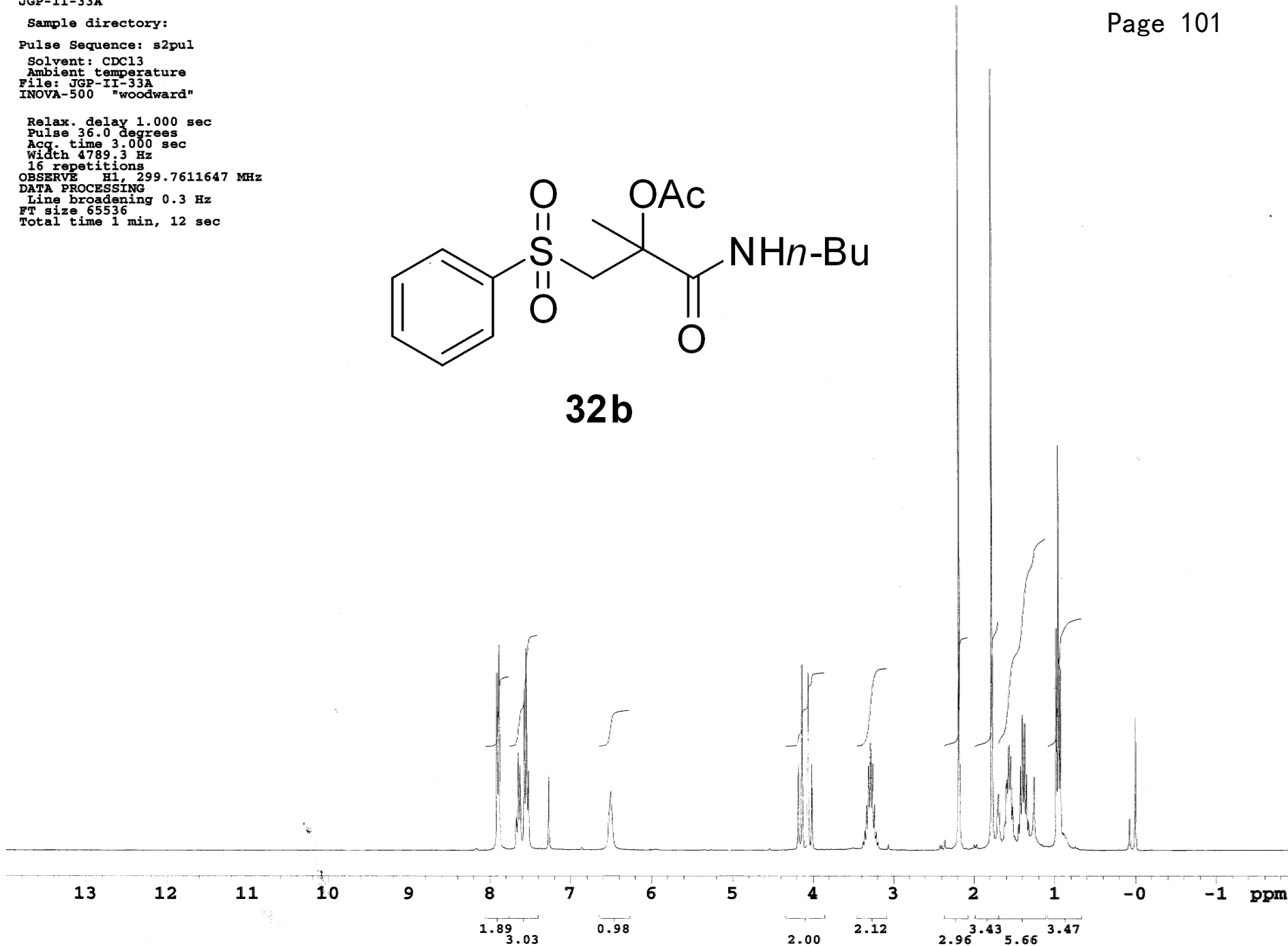
OBSERVE H1, 299.7611647 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec

**32b**# 93
JGP-II-33A

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	2370.666	7.909	34.1	40	286.175	0.955	77.6
2	2363.212	7.884	39.4	41	278.868	0.930	35.3
3	2299.634	7.672	6.4	42	268.929	0.897	3.5
4	2292.326	7.647	18.9	43	264.544	0.883	3.2
5	2285.018	7.623	16.3	44	257.090	0.858	2.5
6	2269.526	7.571	29.5	45	21.631	0.072	6.1
7	2261.779	7.545	38.7	46	-0.000	-0.000	25.5
8	2254.471	7.521	15.3				
9	2179.493	7.271	14.5				
10	1950.319	6.506	11.4				
11	1253.588	4.182	16.6				
12	1239.557	4.135	35.6				
13	1217.049	4.060	35.8				
14	1203.018	4.013	16.7				
15	1005.706	3.355	3.8				
16	999.421	3.334	8.8				
17	992.260	3.310	16.4				
18	984.660	3.285	20.8				
19	977.790	3.262	16.8				
20	970.482	3.238	8.8				
21	963.759	3.215	3.5				
22	654.345	2.183	162.0				
23	532.596	1.777	149.6				
24	508.919	1.698	10.9				
25	483.341	1.612	5.6				
26	478.664	1.597	13.0				
27	476.033	1.588	13.7				
28	469.164	1.565	20.3				
29	462.441	1.543	18.2				
30	455.864	1.521	8.4				
31	448.994	1.498	2.8				
32	433.940	1.448	5.2				
33	426.778	1.424	16.2				
34	419.471	1.399	26.1				
35	411.870	1.374	24.6				
36	404.563	1.350	14.7				
37	397.255	1.325	5.7				
38	376.354	1.256	14.4				
39	293.483	0.979	42.6				

¹³C OBSERVE

JGPII-33A

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: JGP-II-33A-C13

INNOVA-500 "wolff"

Relax. delay 1.000 sec

Pulse 38.6 degrees

Acq. time 2.500 sec

Width 18797.0 Hz

256 repetitions

OBSERVE C13, 75.3749875 MHz

DECOUPLE H1, 299.7627007 MHz

Power 36 dB

continuously on

WALTZ-16 modulated

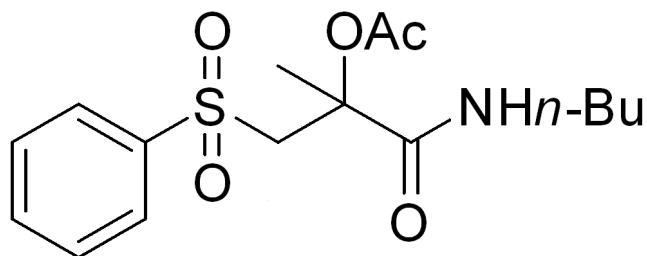
DATA PROCESSING

Line broadening 1.0 Hz

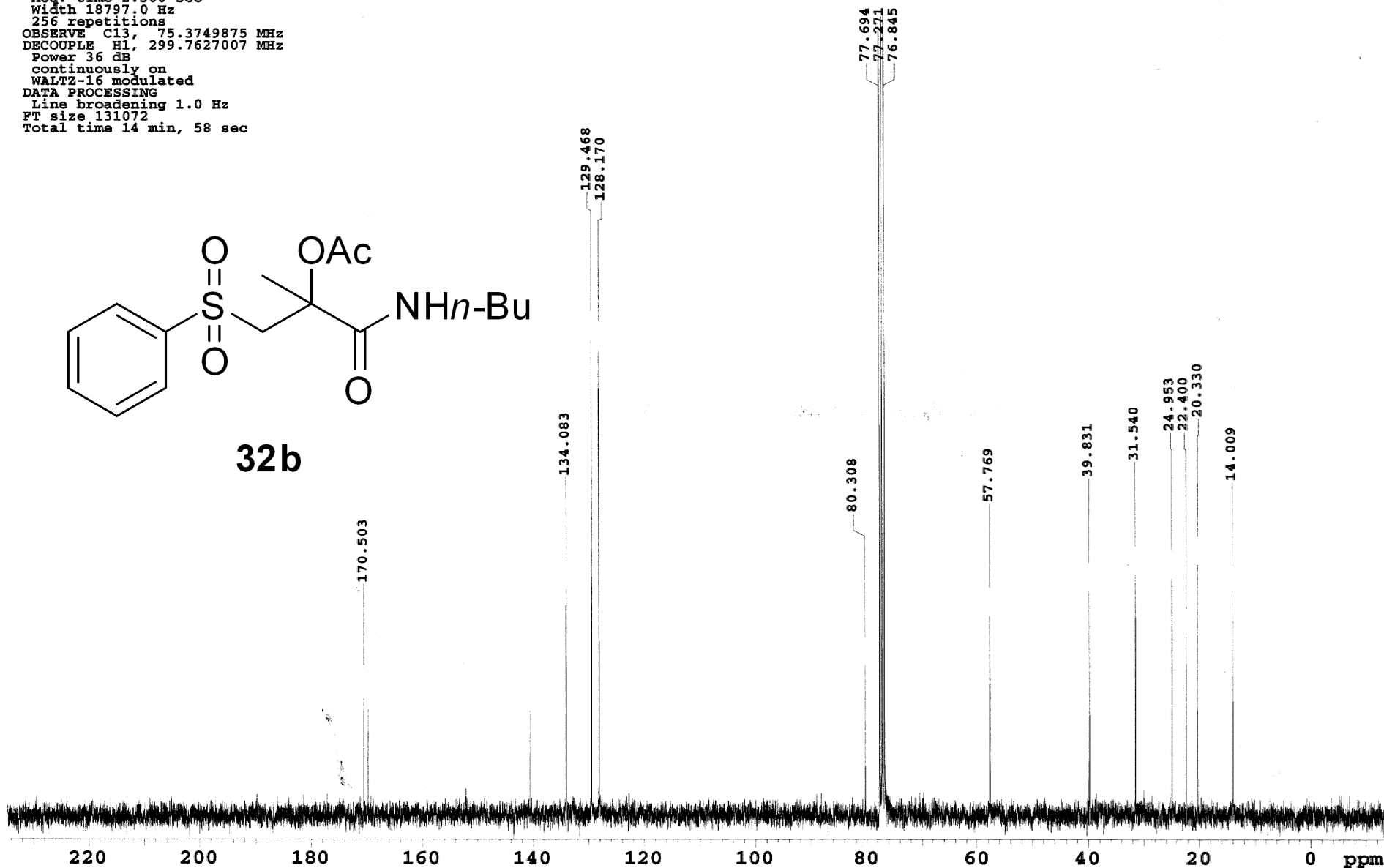
FT size 131072

Total time 14 min, 58 sec

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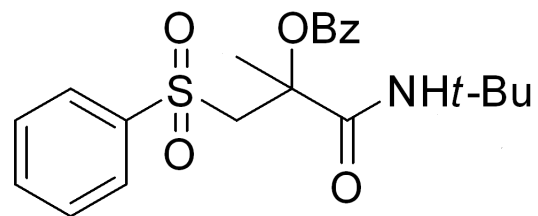
32b



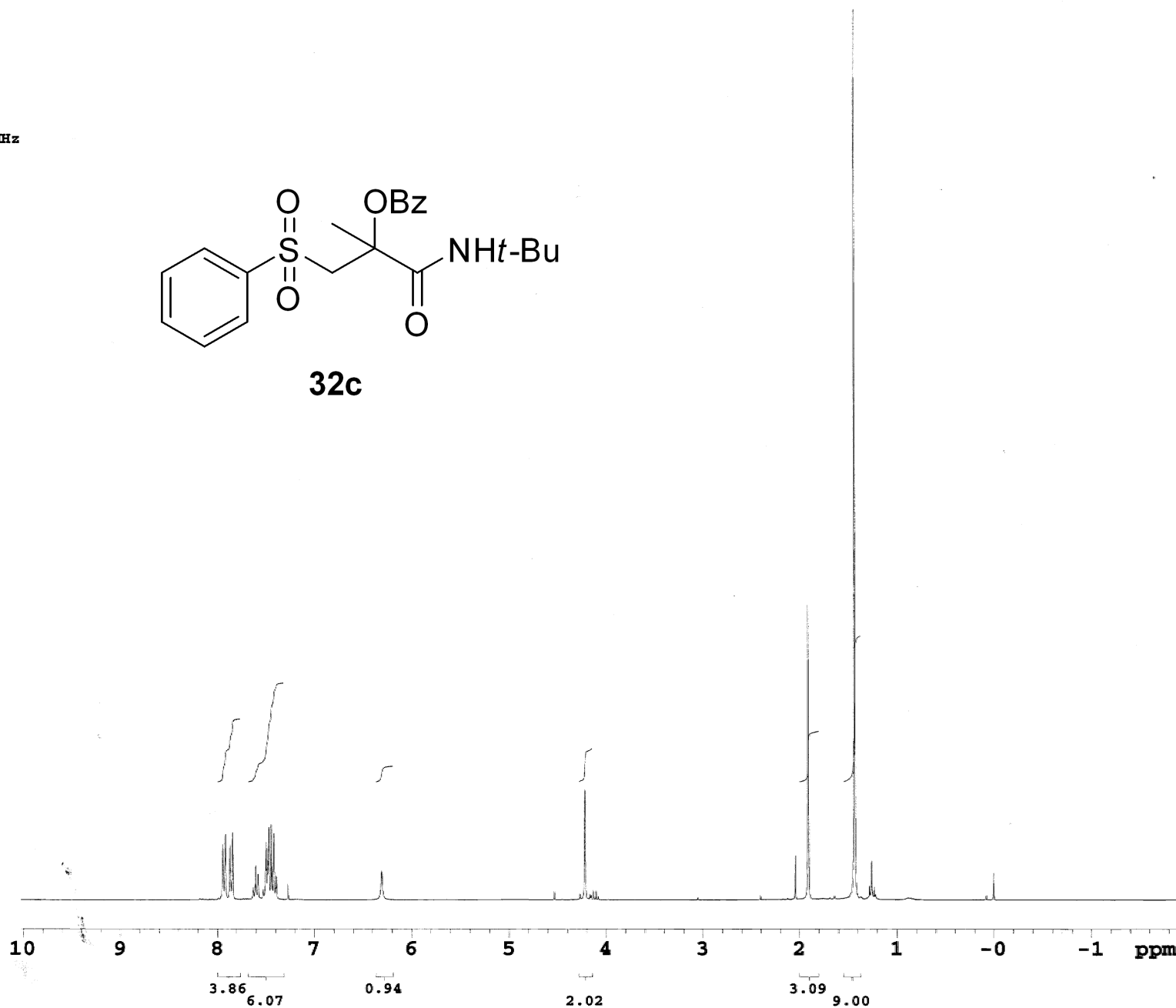
JGPII-33A, AX

Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: JGP-II-35B
INOVA-500 "wolff"

Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611634 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 12 sec



32c



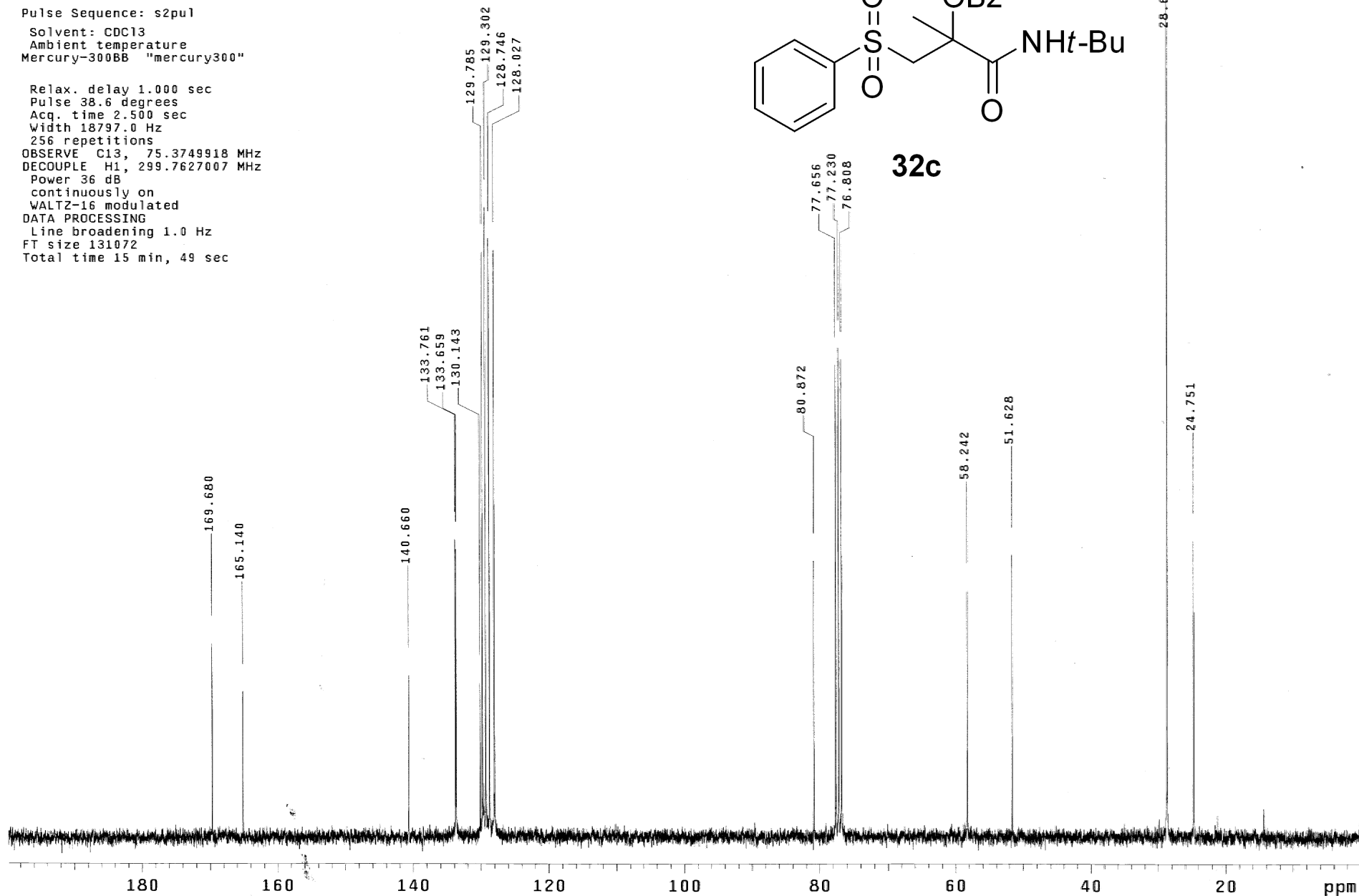
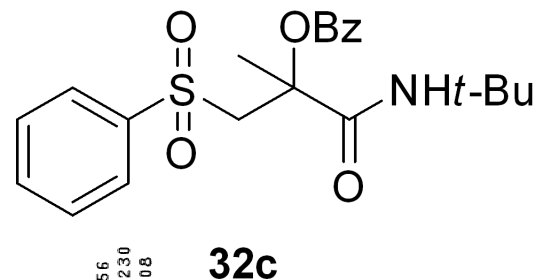
INDEX	FREQUENCY	PPM	HEIGHT
1	2380.605	7.942	9.5
2	2373.443	7.918	11.1
3	2371.982	7.913	8.8
4	2358.681	7.869	9.4
5	2353.420	7.851	3.3
6	2351.520	7.845	11.5
7	2350.058	7.840	8.2
8	2286.918	7.629	2.1
9	2281.511	7.611	2.2
10	2279.464	7.604	5.9
11	2273.326	7.584	3.0
12	2272.010	7.579	4.4
13	2248.771	7.502	7.0
14	2246.433	7.494	9.8
15	2242.779	7.482	4.5
16	2241.463	7.477	6.6
17	2238.687	7.468	12.3
18	2230.940	7.442	12.9
19	2224.363	7.420	6.5
20	2222.902	7.416	11.3
21	2215.886	7.392	4.2
22	2214.571	7.388	2.7
23	2179.201	7.270	2.7
24	1890.541	6.307	4.9
25	1265.281	4.221	18.7
26	1263.819	4.216	18.5
27	612.398	2.043	7.5
28	572.205	1.909	50.0
29	429.117	1.432	151.2
30	383.808	1.280	2.4
31	376.647	1.256	6.6
32	369.485	1.233	2.2
33	0.000	0.000	4.6

Sample directory:
File: CARBON

Pulse Sequence: s2pu1

Solvent: CDCl₃
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 38.6 degrees
Acq. time 2.500 sec
Width 18797.0 Hz
256 repetitions
OBSERVE C13, 75.3749918 MHz
DECOUPLE H1, 299.7627007 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 15 min, 49 sec



JGP-II-46A

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

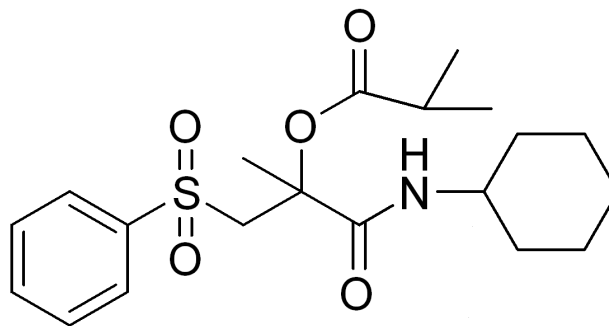
Temp. 20.0 C / 293.1 K

File: JGP-II-46A

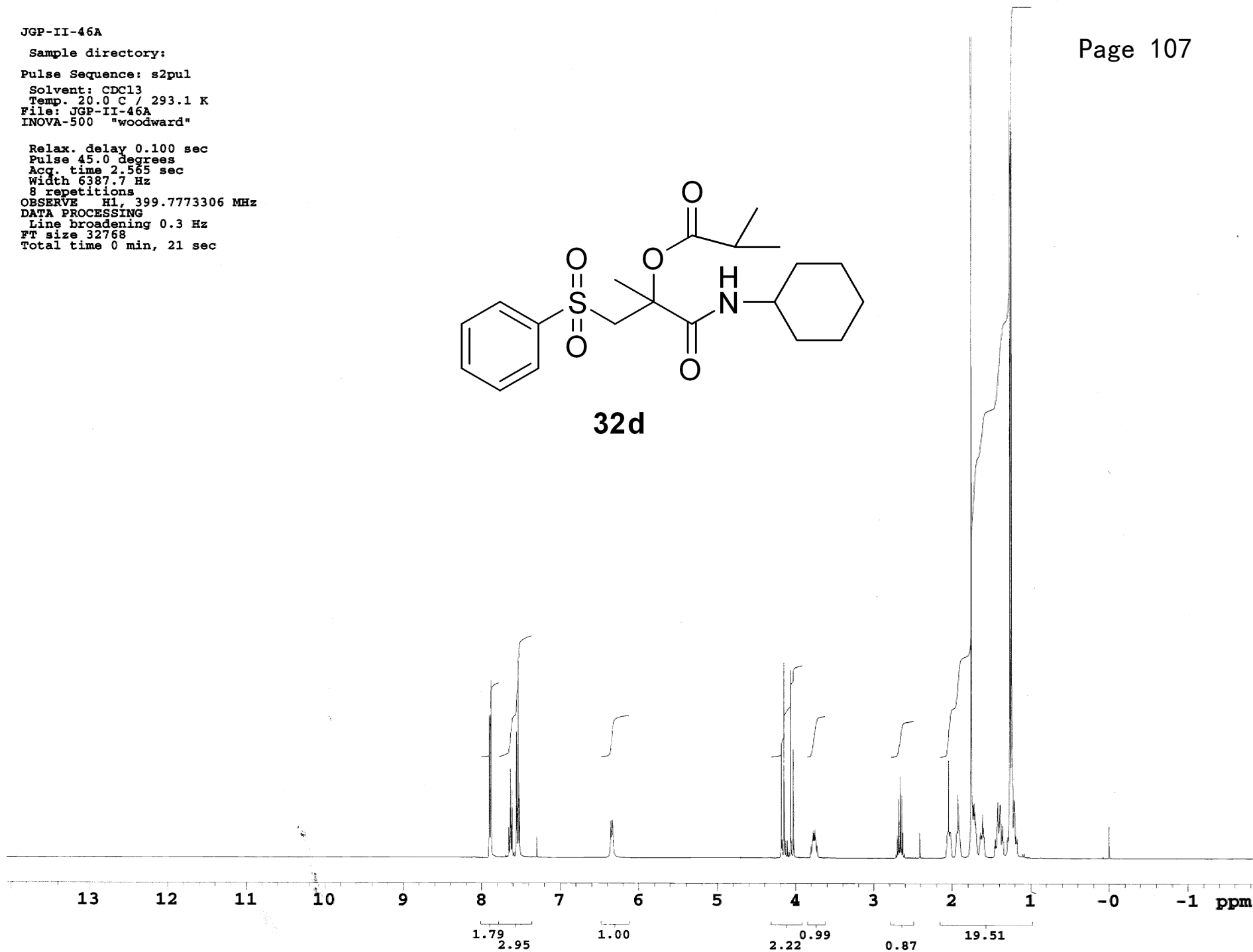
INOVA-500 "woodward"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773306 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec

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32d



H # 154

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3161.118	7.907	4.0	40	1065.532	2.665	16.2	79	481.887	1.205	9.9
2	3157.999	7.899	28.1	41	1058.515	2.648	12.5	80	475.649	1.190	4.6
3	3152.931	7.887	9.3	42	1051.497	2.630	5.2	81	473.700	1.185	3.6
4	3150.981	7.882	35.0	43	963.775	2.411	5.1	82	470.191	1.176	3.2
5	3149.422	7.878	26.2	44	819.910	2.051	5.4	83	468.631	1.172	3.9
6	3060.530	7.656	3.3	45	817.181	2.044	19.3	84	-0.000	-0.000	6.4
7	3059.360	7.653	6.2	46	811.333	2.029	5.3				
8	3058.191	7.650	4.1	47	808.214	2.022	5.2				
9	3053.902	7.639	4.6	48	773.515	1.935	5.5				
10	3051.953	7.634	17.7	49	768.836	1.923	12.7				
11	3050.003	7.629	6.4	50	761.819	1.906	5.6				
12	3045.715	7.619	7.9	51	702.167	1.756	162.0				
13	3044.545	7.616	13.6	52	692.421	1.732	10.6				
14	3043.375	7.613	8.1	53	688.132	1.721	10.9				
15	3020.763	7.556	24.8	54	683.843	1.711	9.2				
16	3012.965	7.537	35.5	55	679.555	1.700	7.4				
17	3007.117	7.522	6.7	56	657.332	1.644	4.0				
18	3005.557	7.518	14.9	57	653.823	1.635	5.2				
19	2915.886	7.294	4.2	58	649.924	1.626	4.6				
20	2539.265	6.352	7.5	59	645.246	1.614	8.8				
21	2531.468	6.332	7.7	60	640.957	1.603	6.1				
22	1672.960	4.185	22.5	61	637.058	1.594	4.4				
23	1668.281	4.173	3.8	62	582.865	1.458	2.4				
24	1658.924	4.150	38.6	63	579.356	1.449	3.9				
25	1649.957	4.127	3.6	64	575.847	1.440	2.5				
26	1642.939	4.110	3.6	65	571.169	1.429	6.4				
27	1625.395	4.066	37.0	66	568.050	1.421	11.2				
28	1611.359	4.031	21.5	67	563.371	1.409	6.7				
29	1519.738	3.801	2.4	68	556.354	1.392	10.6				
30	1515.450	3.791	2.8	69	554.794	1.388	10.7				
31	1513.110	3.785	3.6	70	546.607	1.367	4.4				
32	1509.212	3.775	5.6	71	543.098	1.359	6.5				
33	1505.313	3.765	5.2	72	539.979	1.351	3.6				
34	1501.024	3.755	5.7	73	518.926	1.298	3.8				
35	1497.126	3.745	3.7	74	515.807	1.290	4.3				
36	1495.176	3.740	3.1	75	505.280	1.264	147.3				
37	1490.887	3.729	2.6	76	502.551	1.257	28.9				
38	1079.568	2.700	4.6	77	498.262	1.246	149.9				
39	1072.550	2.683	11.7	78	484.616	1.212	11.6				

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp. 20.0 C / 293.1 K

File: JGP-II-46A-C13

INOVA-500 "woodward"

Relax. delay 1.000 sec

Pulse 50.1 degrees

Acq. time 1.303 sec

Width 25157.2 Hz

256 repetitions

OBSERVE C13, 100.5240783 MHz

DECOUPLE H1, 399.7793569 MHz

Power 38 dB

continuously on

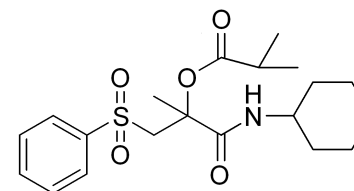
WALTZ-16 modulated

DATA PROCESSING

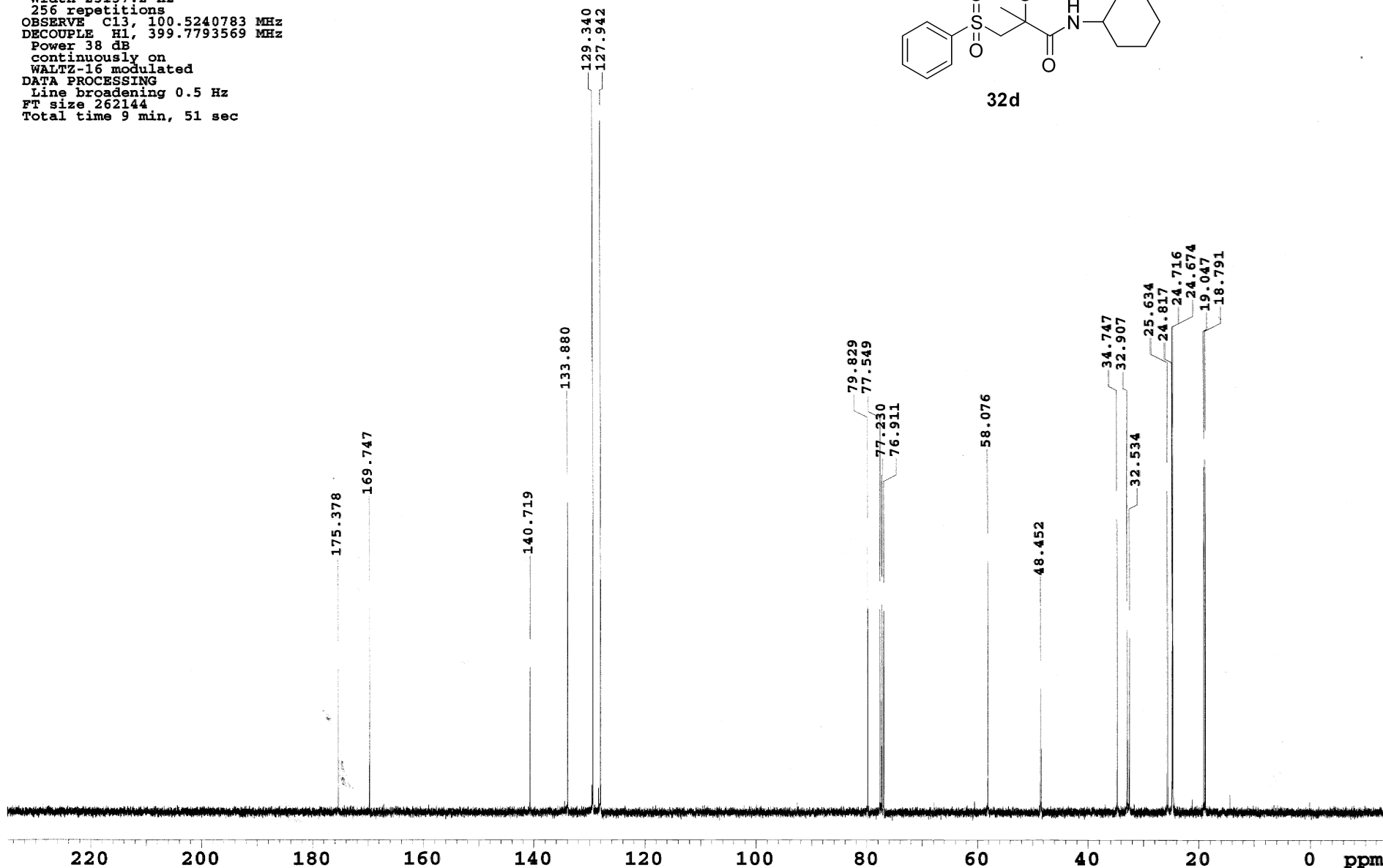
Line broadening 0.5 Hz

FT size 262144

Total time 9 min, 51 sec



32d

¹³C #10

Sample directory:

Pulse Sequence: s2pul

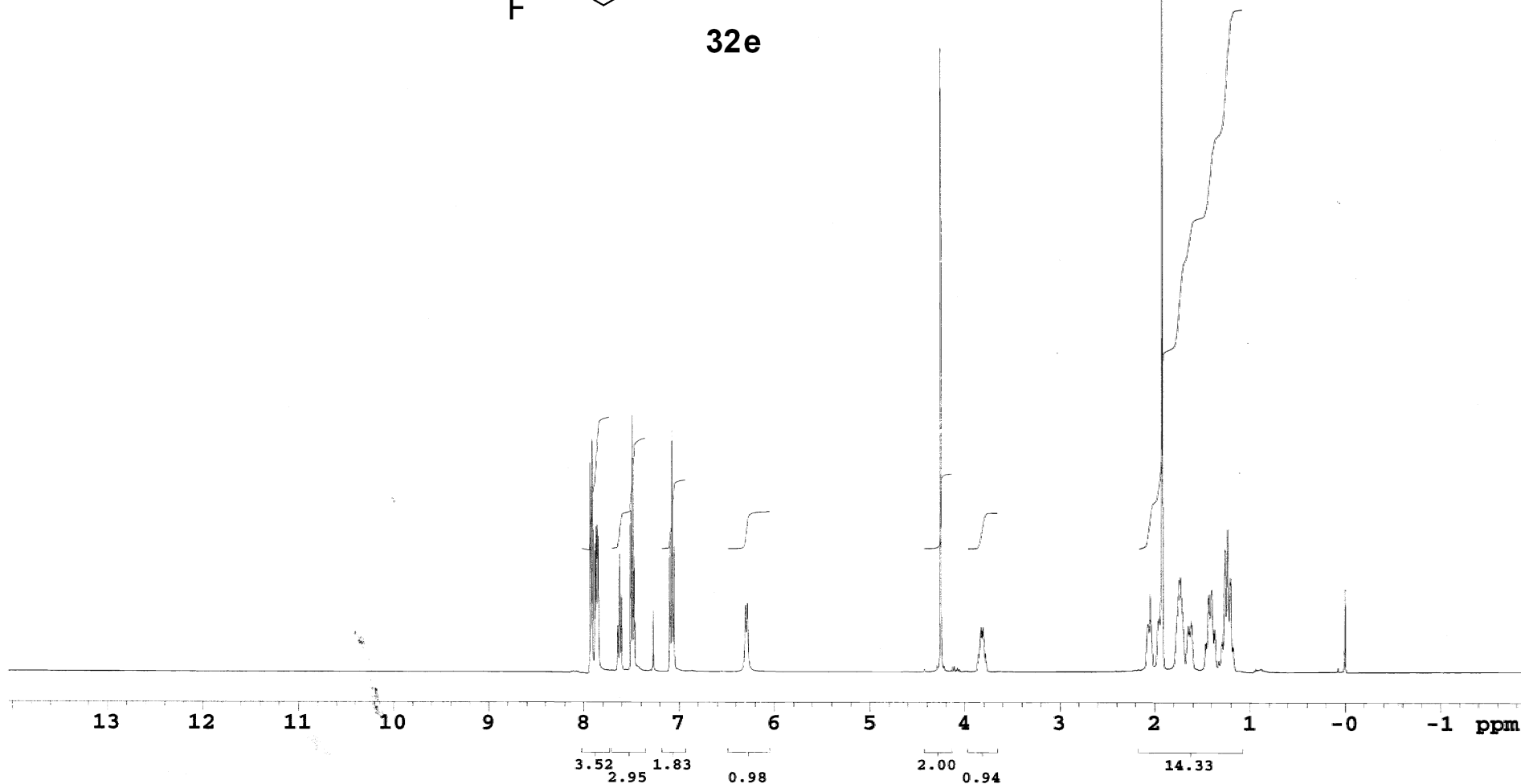
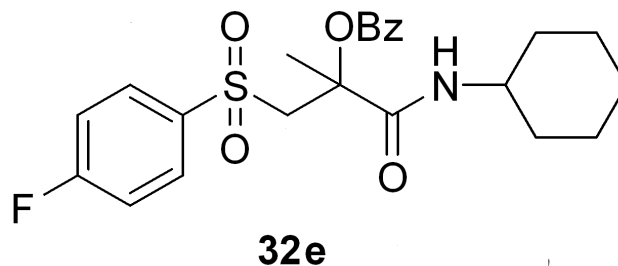
Solvent: CDCl₃

Ambient temperature

File: JGP-II-138C

INOVA-500 "woodward"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.7773345 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 0 min, 21 sec



JGP-II-138C

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3169.695	7.929	34.4	40	574.678	1.437	12.1
2	3161.898	7.909	37.9	41	571.169	1.429	12.7
3	3150.202	7.880	20.8	42	566.880	1.418	9.0
4	3145.133	7.867	23.6	43	560.642	1.402	13.5
5	3141.624	7.858	23.9	44	549.726	1.375	7.1
6	3136.556	7.846	22.0	45	546.217	1.366	6.3
7	3055.072	7.642	7.5	46	518.536	1.297	4.6
8	3048.054	7.624	19.2	47	515.417	1.289	5.0
9	3040.256	7.605	12.8	48	503.720	1.260	20.1
10	3000.879	7.506	26.1	49	493.194	1.234	23.3
11	2993.081	7.487	41.8	50	483.837	1.210	14.7
12	2985.284	7.467	18.8	51	481.108	1.203	15.4
13	2906.529	7.270	9.9	52	472.920	1.183	4.1
14	2837.131	7.097	21.1	53	469.411	1.174	4.1
15	2828.554	7.075	39.9	54	-0.000	-0.000	13.4
16	2819.976	7.054	20.4				
17	2519.382	6.302	10.8				
18	2511.194	6.281	11.1				
19	1701.031	4.255	101.4				
20	1541.571	3.856	3.0				
21	1531.045	3.830	7.3				
22	1527.146	3.820	6.7				
23	1522.857	3.809	7.3				
24	1512.721	3.784	3.1				
25	826.148	2.067	7.9				
26	817.571	2.045	12.7				
27	782.092	1.956	8.7				
28	767.277	1.919	161.9				
29	704.897	1.763	9.3				
30	700.608	1.752	12.3				
31	695.929	1.741	15.0				
32	692.031	1.731	15.5				
33	682.674	1.708	9.8				
34	658.111	1.646	7.5				
35	654.213	1.636	6.5				
36	649.144	1.624	7.5				
37	645.246	1.614	8.4				
38	586.374	1.467	4.6				
39	582.475	1.457	4.9				

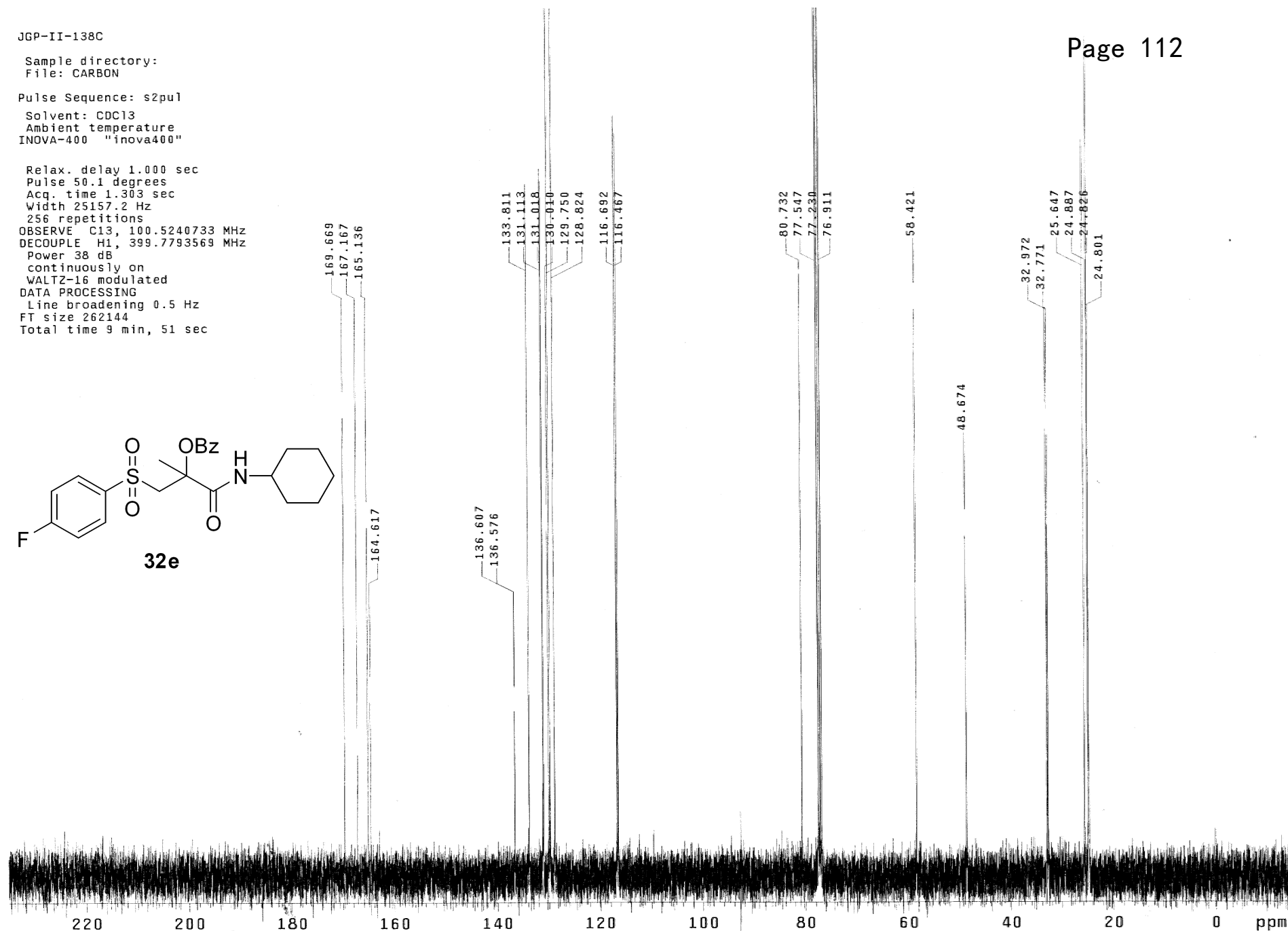
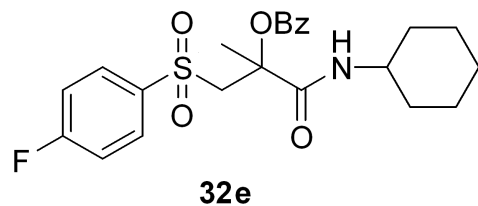
JGP-II-138C

Sample directory:
File: CARBON

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
INOVA-400 "inova400"

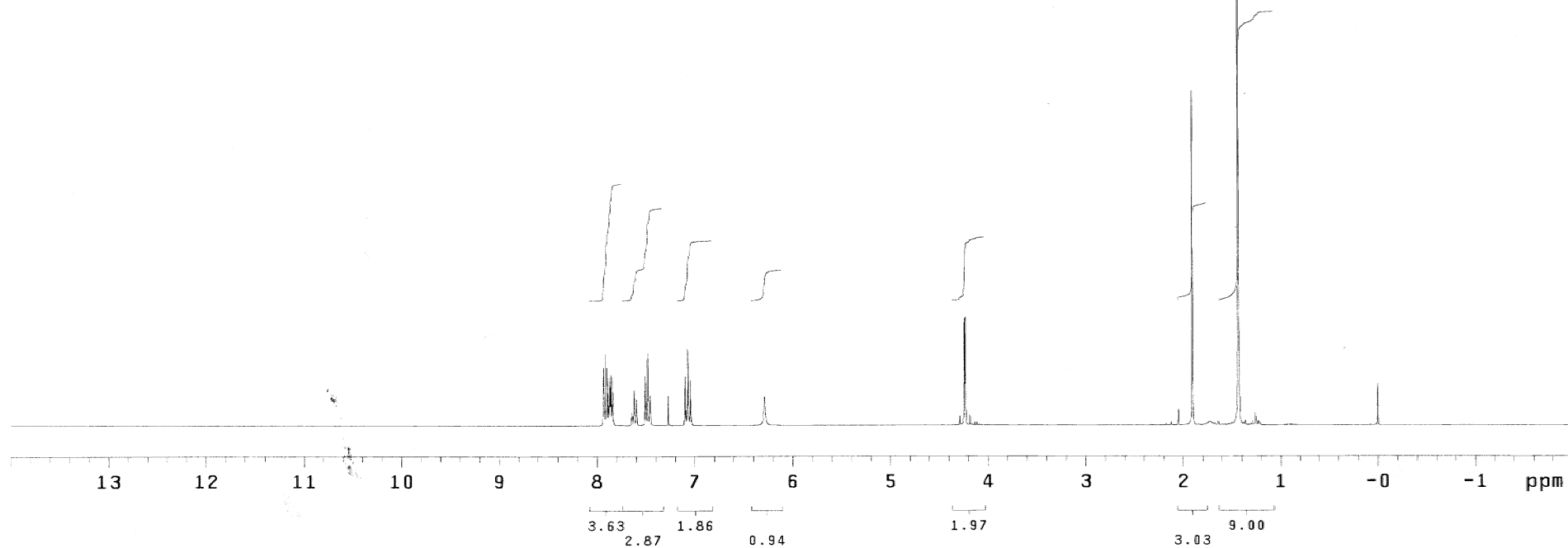
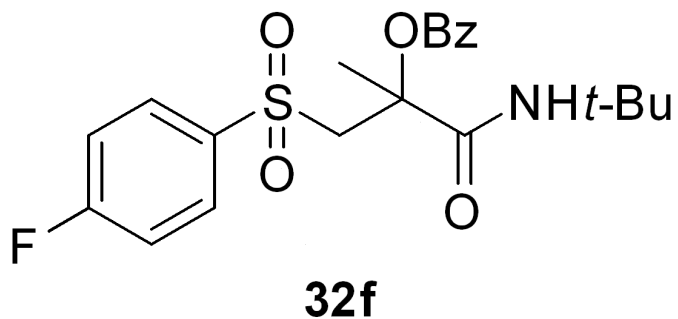
Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
256 repetitions
OBSERVE C13, 100.5240733 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 9 min, 51 sec



Sample directory:
File: PROTON

Pulse Sequence: s2pul
Solvent: CDCl₃
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 36.0 degrees
Acq. time 3.000 sec
Width 4789.3 Hz
16 repetitions
OBSERVE H1, 299.7611641 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 min, 18 sec



JGP-II-122B

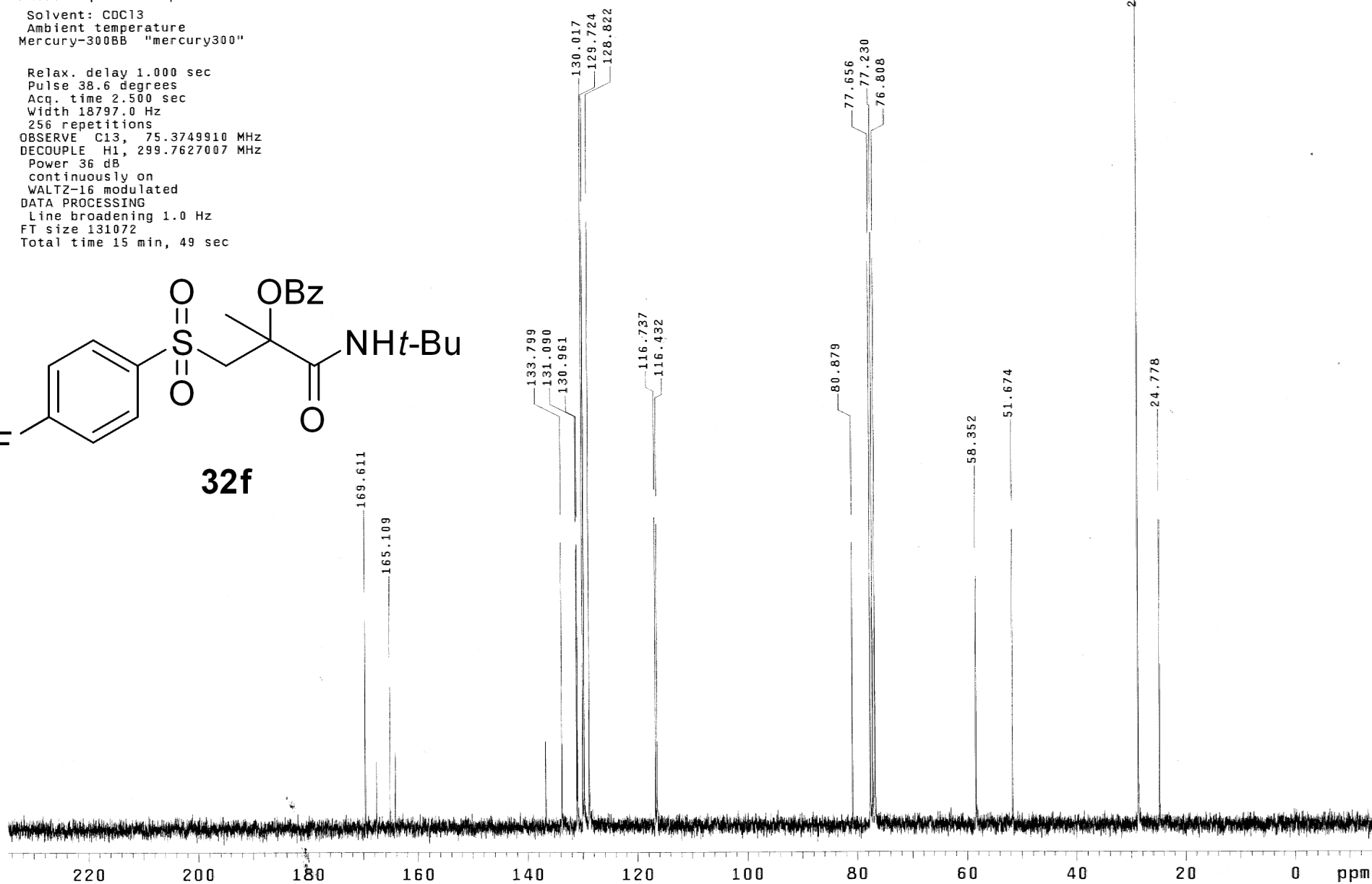
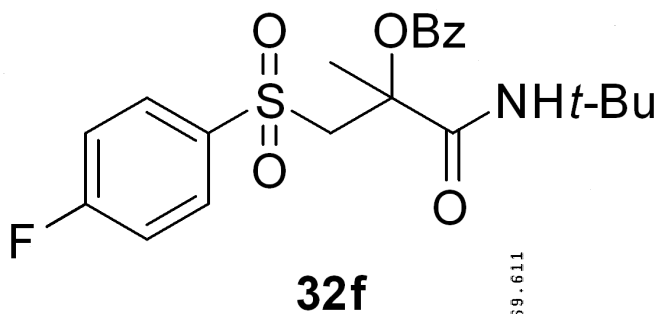
INDEX	FREQUENCY	PPM	HEIGHT
1	2376.147	7.927	9.4
2	2371.031	7.910	3.0
3	2369.131	7.903	11.5
4	2367.669	7.899	9.3
5	2363.577	7.885	7.6
6	2361.530	7.878	3.2
7	2358.607	7.868	7.8
8	2356.561	7.861	4.5
9	2354.661	7.855	8.2
10	2351.738	7.845	3.3
11	2349.691	7.839	7.7
12	2291.373	7.644	2.1
13	2283.919	7.619	5.8
14	2277.780	7.599	2.6
15	2276.464	7.594	4.2
16	2275.149	7.590	2.3
17	2249.717	7.505	8.0
18	2241.970	7.479	11.6
19	2236.124	7.460	2.2
20	2234.516	7.454	4.9
21	2179.121	7.270	4.8
22	2127.526	7.097	7.9
23	2125.334	7.090	2.5
24	2119.049	7.069	12.3
25	2112.325	7.047	2.4
26	2110.279	7.040	7.3
27	1883.729	6.284	4.6
28	1269.997	4.237	17.0
29	1267.512	4.228	17.3
30	613.001	2.045	2.6
31	570.468	1.903	53.1
32	428.692	1.430	162.1
33	-0.000	-0.000	6.7

Sample directory:
File: CARBON

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 38.6 degrees
Acq. time 2.500 sec
Width 18797.0 Hz
256 repetitions
OBSERVE C13, 75.3749910 MHz
DECOUPLE H1, 299.7627007 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 15 min, 49 sec



STANDARD 1H OBSERVE

JGP-II-131B

Sample directory:

Pulse Sequence: s2pul

Solvent: CDC13

Temp. 20.0 C / 293.1 K

File: JGP-II-131B

INOVA-500 "woodward"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.565 sec

Width 6387.7 Hz

8 repetitions

OBSERVE H1, 399.7773286 MHz

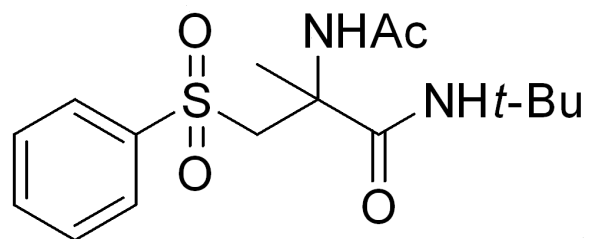
DATA PROCESSING

Line broadening 0.3 Hz

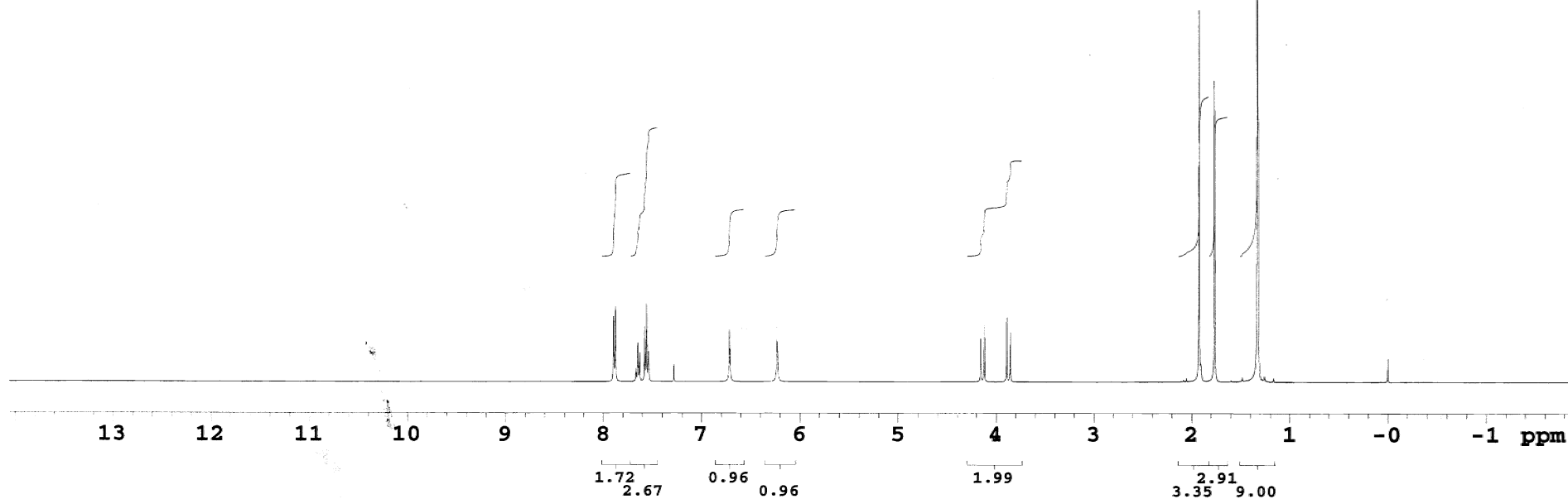
FT size 32768

Total time 0 min, 21 sec

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H #188

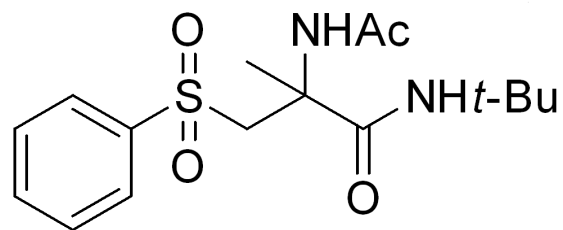
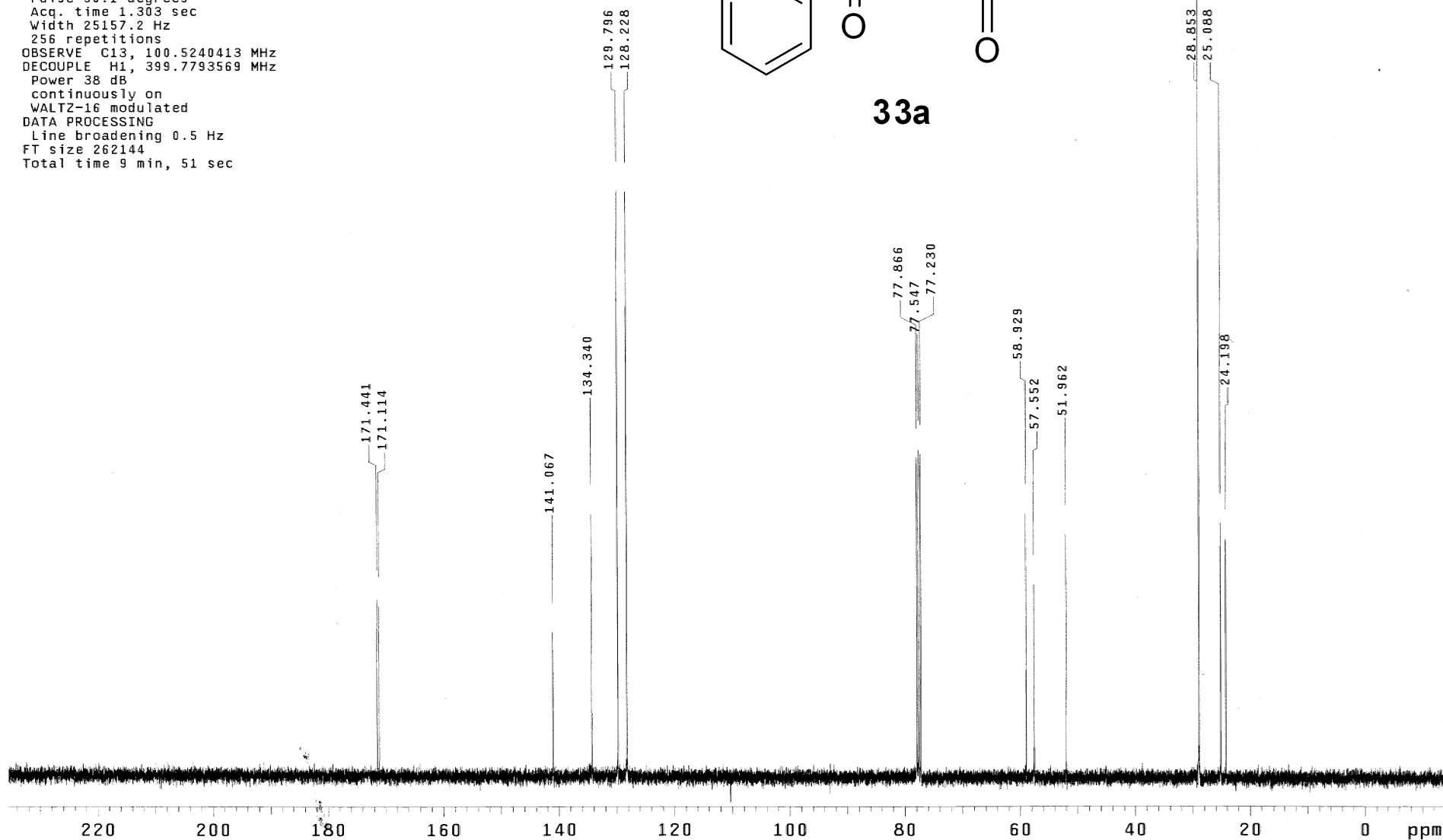
INDEX	FREQUENCY	PPM	HEIGHT
1	3155.660	7.894	10.4
2	3148.642	7.876	12.1
3	3147.083	7.872	9.3
4	3064.819	7.666	2.2
5	3057.411	7.648	6.3
6	3050.003	7.629	4.7
7	3028.950	7.577	8.9
8	3021.153	7.557	12.5
9	3013.745	7.539	4.9
10	2910.817	7.281	2.8
11	2683.909	6.714	8.4
12	2490.141	6.229	6.8
13	1661.263	4.155	7.0
14	1646.838	4.119	9.1
15	1555.217	3.890	10.3
16	1540.402	3.853	7.9
17	768.057	1.921	58.9
18	761.429	1.905	3.0
19	704.897	1.763	47.7
20	530.232	1.326	162.0
21	-0.000	-0.000	3.8

Sample directory:
File: CARBON

Pulse Sequence: s2pu1

Solvent: CDCl₃
Temp. 20.0 C / 293.1 K
INNOVA-400 "inova400"

Relax. delay 1.000 sec
Pulse 50.1 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
256 repetitions
OBSERVE C13, 100.5240413 MHz
DECOUPLE H1, 399.7793569 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 262144
Total time 9 min, 51 sec

**33a**

JGP-II-147C

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: JGP-II-147C

INOVA-500 "woodward"

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 2.565 sec

Width 6387.7 Hz

8 repetitions

OBSERVE H1, 399.7773310 MHz

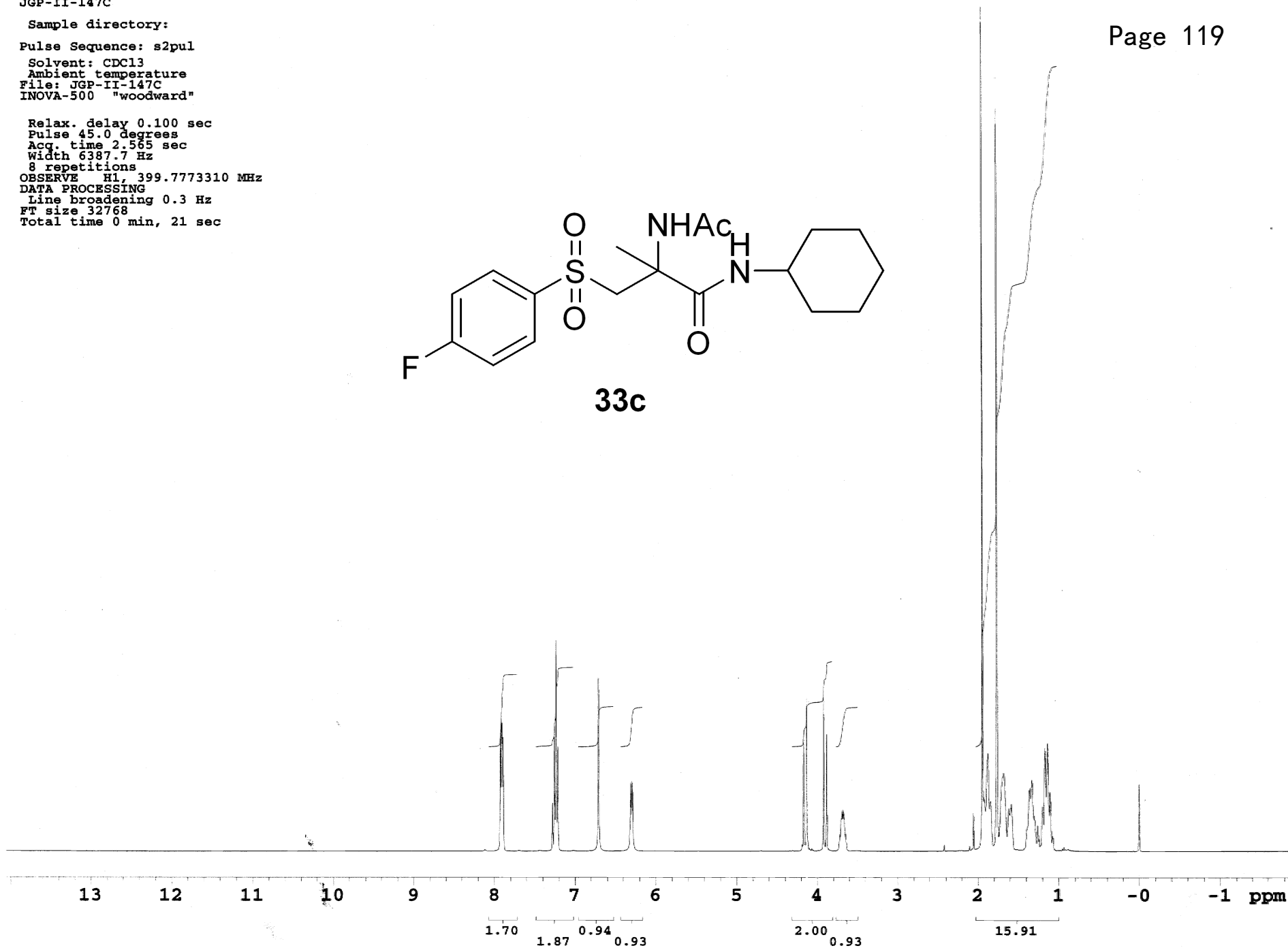
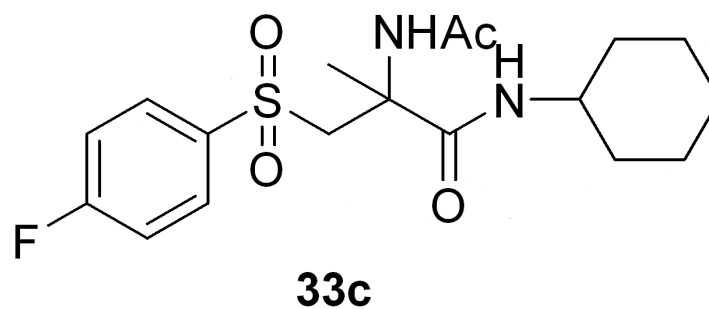
DATA PROCESSING

Line broadening 0.3 Hz

FT size 32768

Total time 0 min, 21 sec

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INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3167.746	7.924	21.5	40	521.655	1.305	6.8
2	3162.288	7.910	24.5	41	517.756	1.295	6.0
3	3159.169	7.902	24.6	42	512.298	1.281	3.7
4	3154.100	7.890	21.8	43	504.500	1.262	4.9
5	2910.038	7.279	9.2	44	497.872	1.245	2.4
6	2899.901	7.254	22.0	45	478.768	1.198	8.6
7	2891.714	7.233	40.6	46	467.072	1.168	19.7
8	2883.136	7.212	20.0	47	454.596	1.137	20.7
9	2681.960	6.709	33.3	48	442.510	1.107	11.3
10	2522.111	6.309	13.3	49	430.424	1.077	2.9
11	2514.313	6.289	13.4	50	426.915	1.068	2.6
12	1666.332	4.168	21.5	51	-0.000	-0.000	12.8
13	1651.517	4.131	29.4				
14	1566.913	3.919	29.2				
15	1552.098	3.882	22.4				
16	1486.209	3.718	3.2				
17	1476.072	3.692	7.9				
18	1471.784	3.682	7.2				
19	1467.885	3.672	7.9				
20	1457.358	3.645	3.3				
21	820.690	2.053	7.4				
22	777.024	1.944	162.0				
23	769.616	1.925	10.3				
24	749.732	1.875	18.8				
25	736.087	1.841	9.5				
26	705.286	1.764	142.5				
27	676.825	1.693	14.2				
28	672.927	1.683	15.0				
29	669.808	1.675	14.5				
30	646.025	1.616	8.2				
31	641.737	1.605	7.1				
32	636.668	1.593	8.3				
33	633.159	1.584	9.1				
34	557.913	1.396	4.3				
35	553.625	1.385	4.7				
36	545.827	1.365	11.7				
37	542.318	1.357	12.0				
38	538.419	1.347	10.6				
39	533.351	1.334	13.7				

Sample directory:
File: CARBON

Pulse Sequence: s2pul

Solvent: CDCl₃
Ambient temperature
Mercury-300BB "mercury300"

Relax. delay 1.000 sec
Pulse 38.6 degrees
Acq. time 2.500 sec
Width 18797.0 Hz
256 repetitions
OBSERVE C13, 75.3749915 MHz
DECOUPLE H1, 299.7627007 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 15 min, 49 sec

