

Allylmagnesium Halides Do Not React Chemoselectively Because Reaction Rates Approach the Diffusion Limit

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Supporting Information

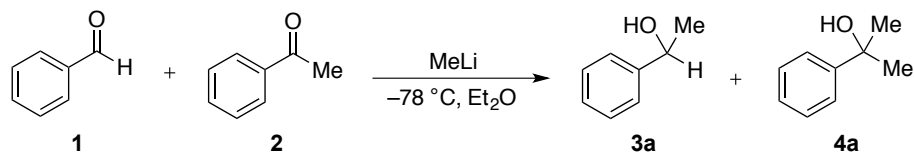
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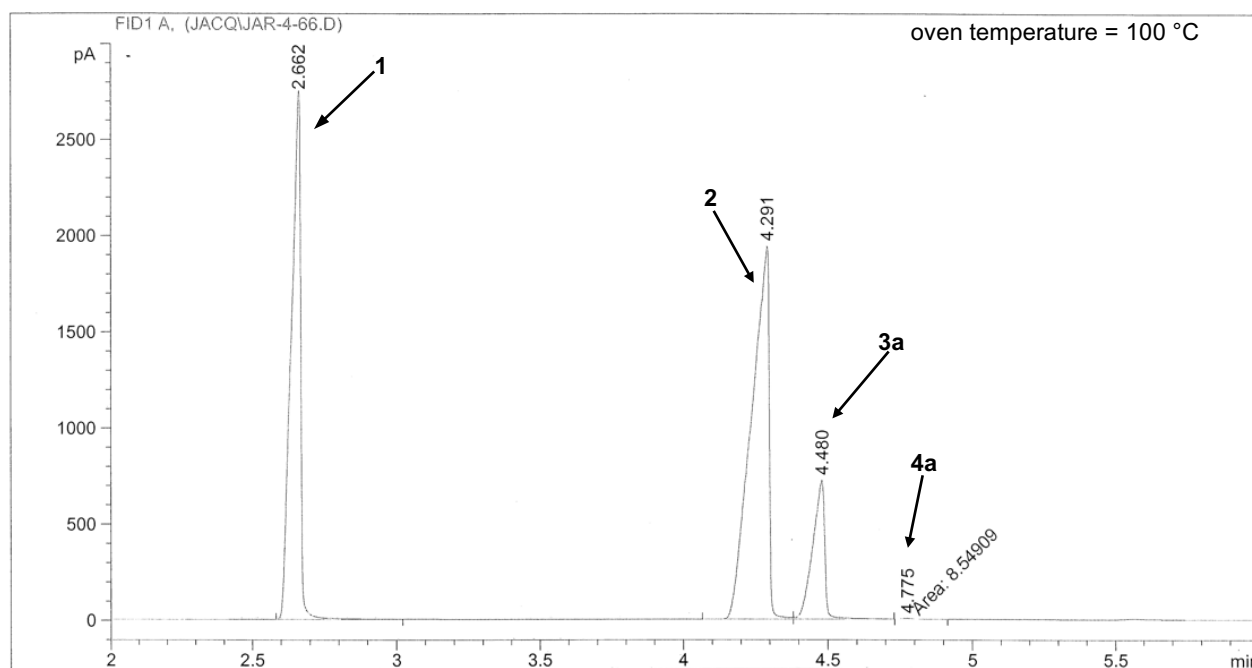
I. Analytical Data

A. Selected GC traces

The following pages contain GC traces used to calculate product ratios from the crude reaction mixtures of competition experiments.



244 : 1



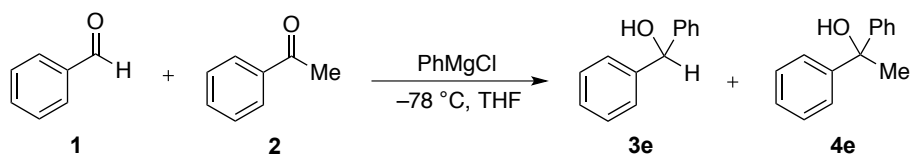
Area Percent Report

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Dilution : 1.0000

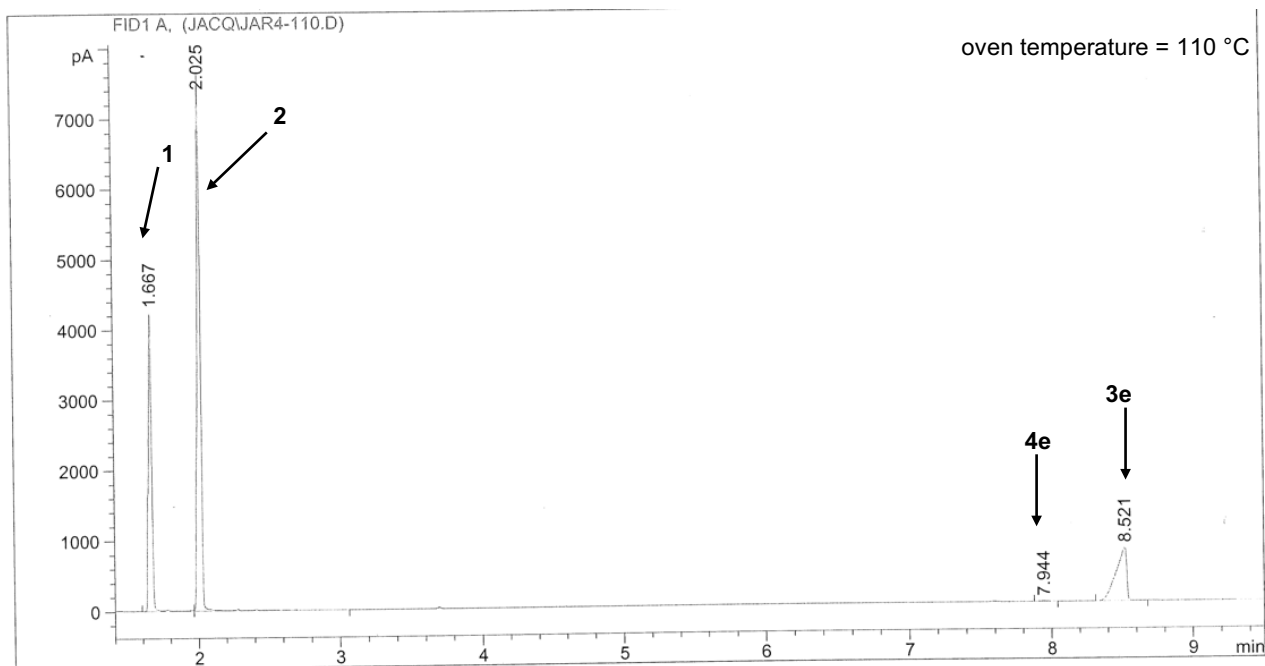
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	2.662	PB	0.0306	6160.96973	2750.35815	37.38766
2	4.291	VV	0.0532	8219.76074	1939.40625	49.88137
3	4.480	VV R	0.0402	2089.33911	723.15741	12.67909
4	4.775	MM T	0.0401	8.54909	3.55751	0.05188

Totals : 1.64786e4 5416.47932



206 : 1



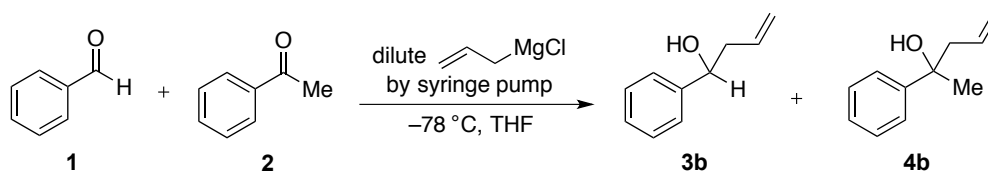
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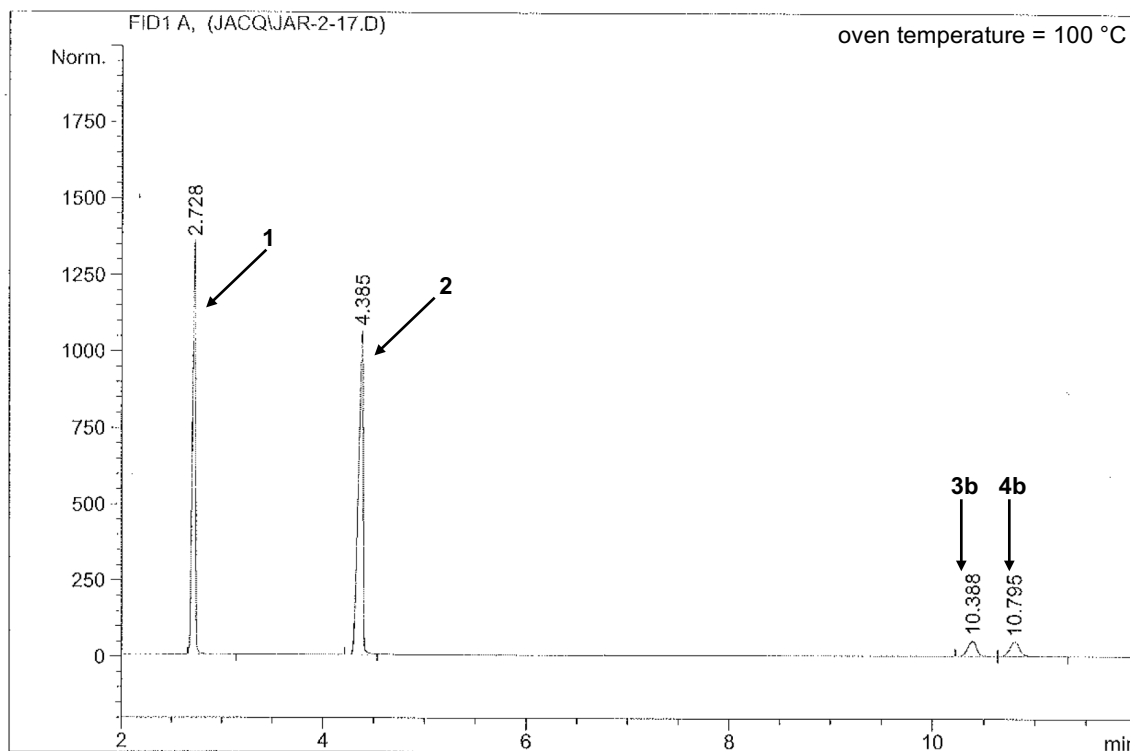
Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.667	VV S	0.0221	6763.63281	4240.90820	29.06086
2	2.025	VB S	0.0216	1.25933e4	7695.87939	54.10865
3	7.944	PB	0.0432	18.93830	5.86271	0.08137
4	8.521	PV	0.0653	3898.19556	754.03406	16.74912

Totals : 2.32740e4 1.26967e4



51 : 49



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 Area Percent Report
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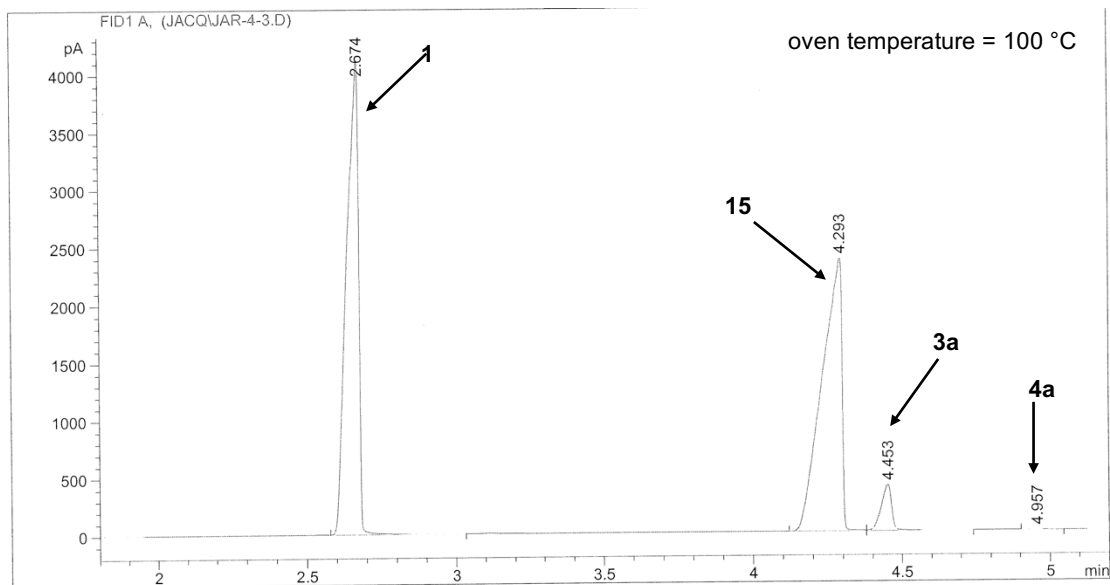
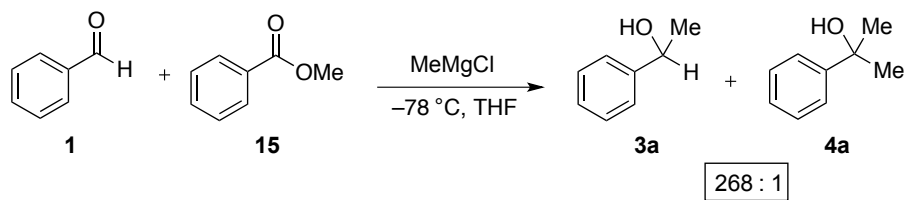
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Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	2.728	BV	0.0299	2882.10620	1350.51855	41.25205
2	4.385	VV	0.0442	3473.30981	1059.84131	49.71404
3	10.388	PV	0.0774	309.09039	51.23280	4.42406
4	10.795	VB	0.0873	322.07062	47.40386	4.60985

Totals : 6986.57703 2508.99652

The ratio of **3b**:**4b** obtained from GC analysis of the reaction mixture was 51:49. Correction for response factors by a GC to ¹H NMR calibration curve left the ratio unchanged.



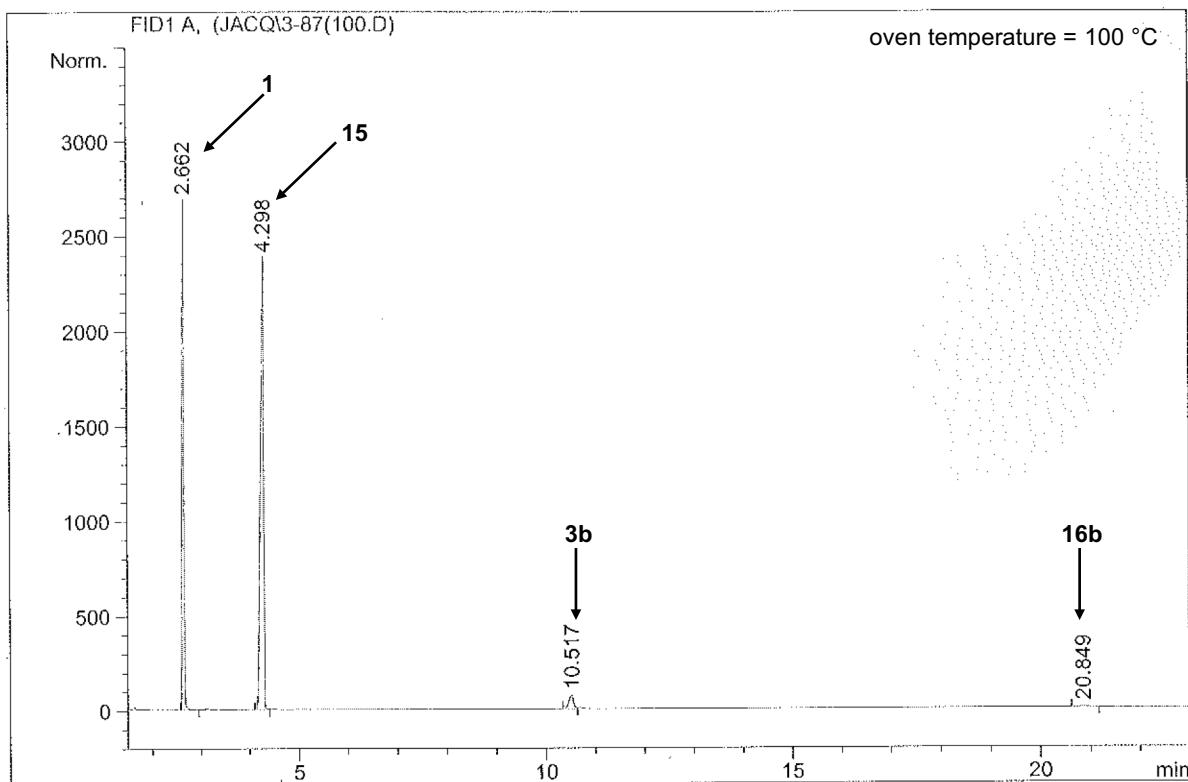
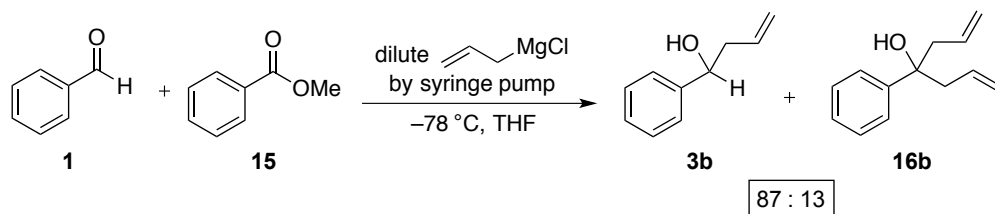
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 Area Percent Report
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Sorted By : Signal
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 Dilution : 1.0000

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	2.674	VB	0.0363	1.14887e4	4120.43457	49.06474
2	4.293	BV	0.0588	1.09384e4	2370.07666	46.71475
3	4.453	VB	0.0357	984.57367	399.63562	4.20481
4	4.957	PP	0.0406	3.67509	1.33585	0.01570

Totals : 2.34154e4 6891.48270



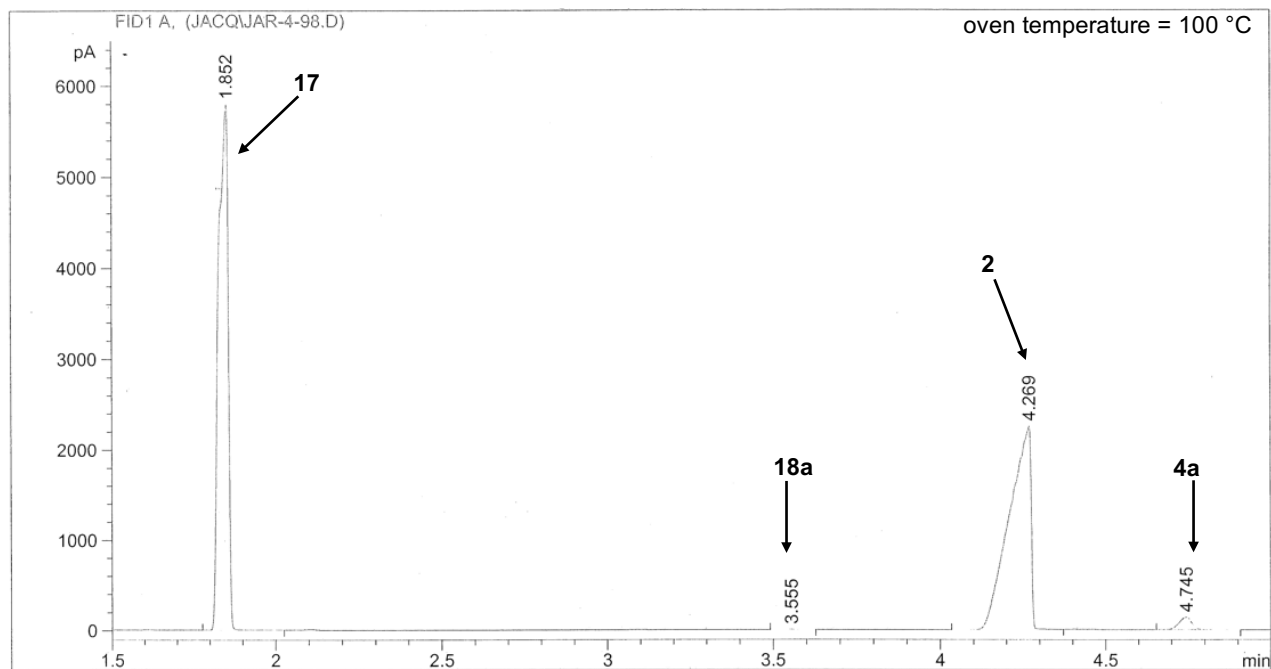
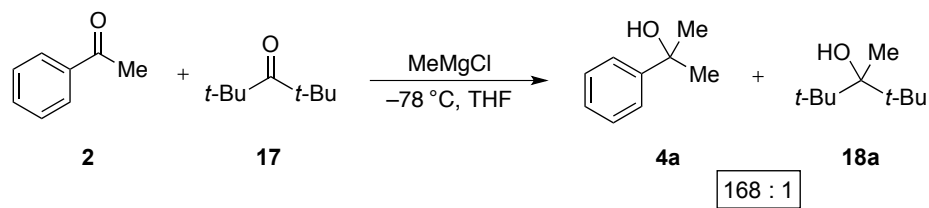
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 Area Percent Report
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Sorted By : Signal
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 Dilution : 1.0000

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	2.662	VB	0.0341	6691.66650	2682.20068	37.21246
2	4.298	BV	0.0568	1.07536e4	2377.73389	59.80098
3	10.517	BV	0.0860	468.11798	71.82910	2.60321
4	20.849	BB	0.1474	68.93552	5.62953	0.38335

Totals : 1.79823e4 5137.39320



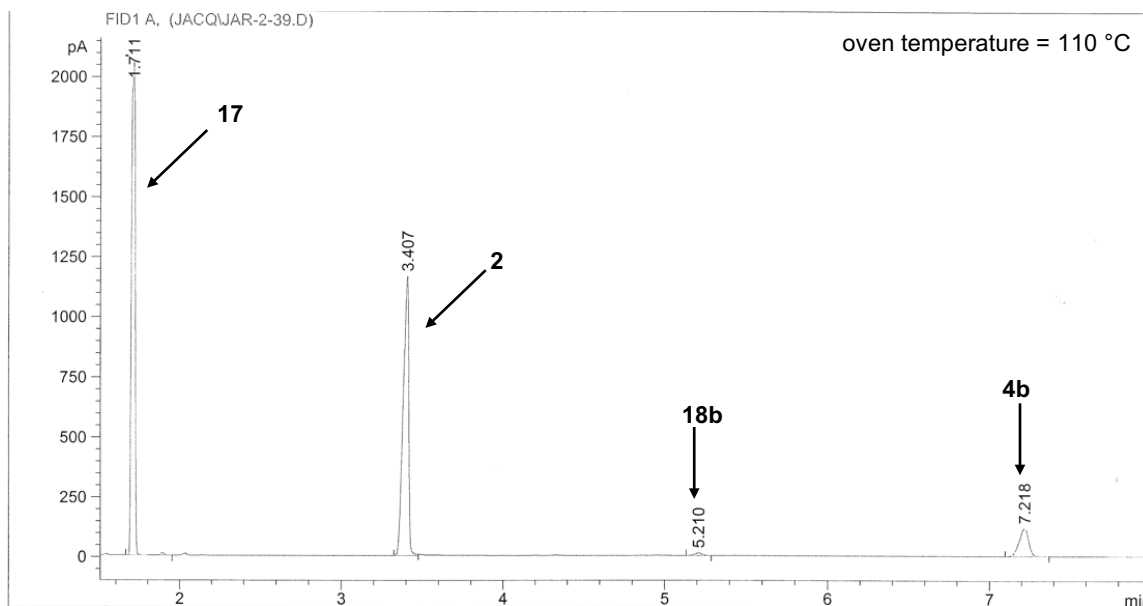
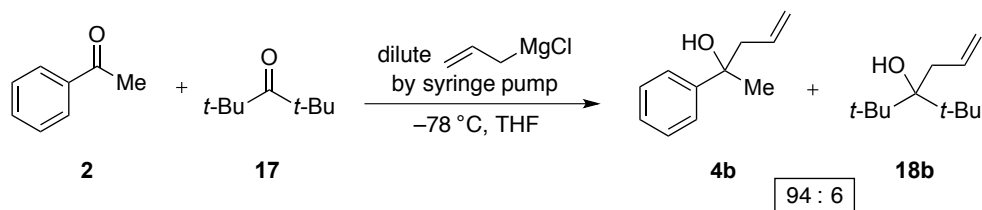
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 Area Percent Report
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Sorted By : Signal
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Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.852	VB S	0.0285	1.18974e4	5792.38086	52.74158
2	3.555	VP	0.0300	2.16854	8.89182e-1	0.00961
3	4.269	VV	0.0560	1.02949e4	2255.71777	45.63760
4	4.745	VP	0.0347	363.45599	139.05263	1.61121

Totals : 2.25579e4 8188.04044



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 Area Percent Report
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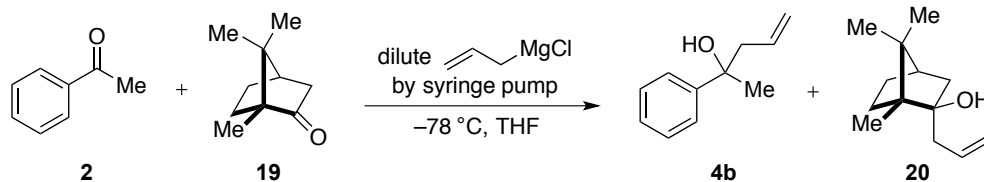
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Signal 1: FID1 A,

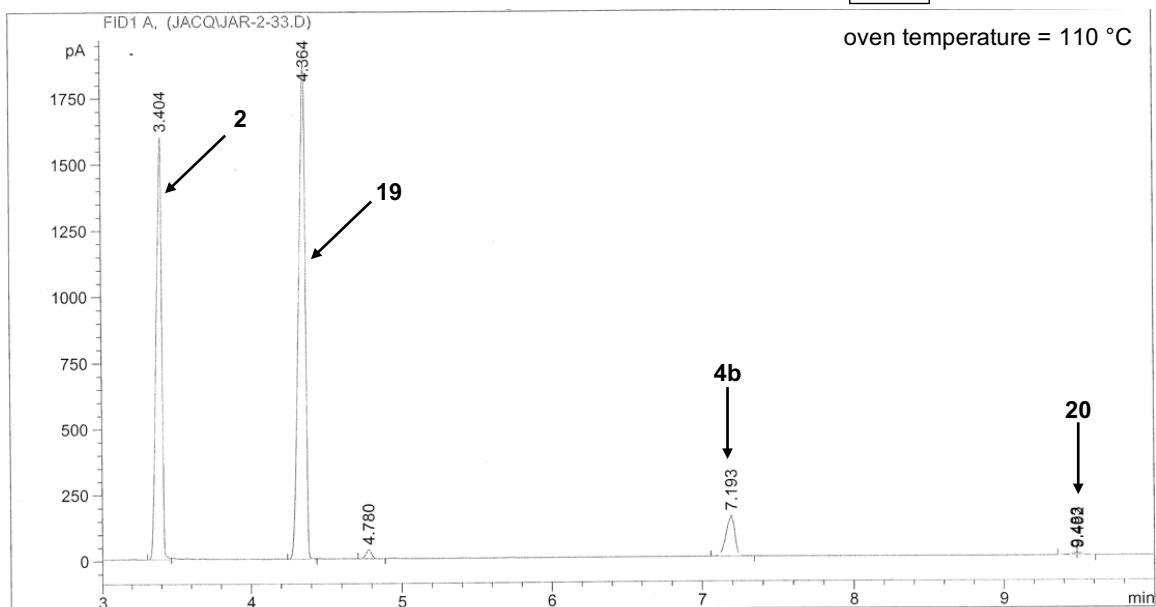
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	1.711	VB S	0.0227	3359.68677	2054.92969	50.73608
2	3.407	PV	0.0333	2751.12524	1165.32520	41.54593
3	5.210	BB	0.0382	32.05235	10.92461	0.48404
4	7.218	BB	0.0490	479.02402	118.35947	7.23395

Totals : 6621.88838 3349.53897

The ratio of **4b:18b** obtained from GC analysis of the reaction mixture was 94:6. Correction for response factors by a GC to ¹H NMR calibration curve left the ratio unchanged.



95 : 5



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 Area Percent Report
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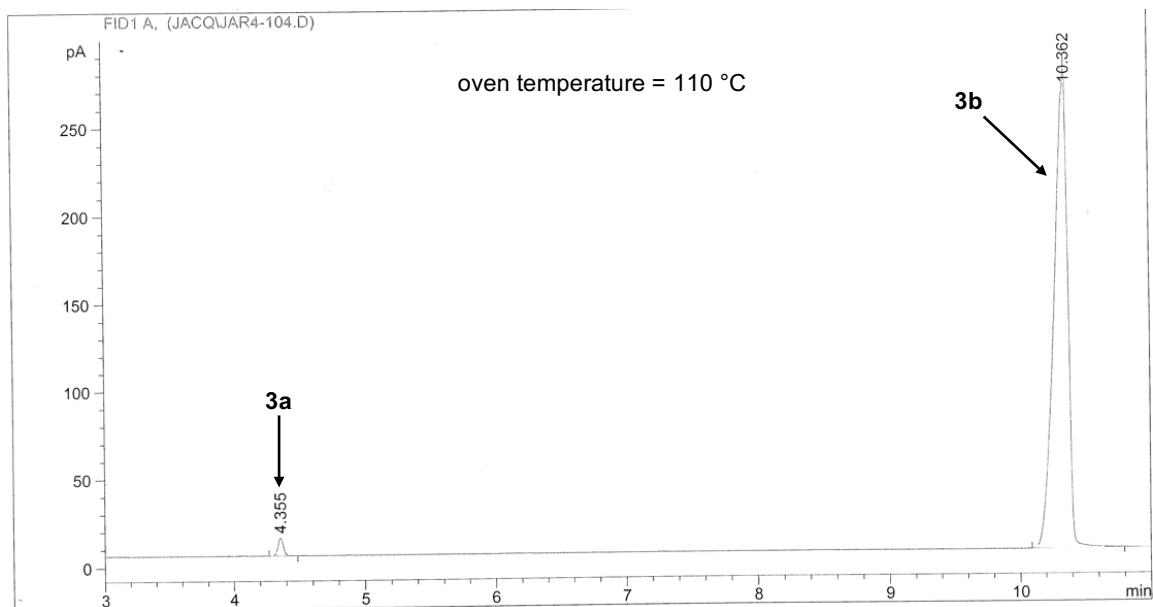
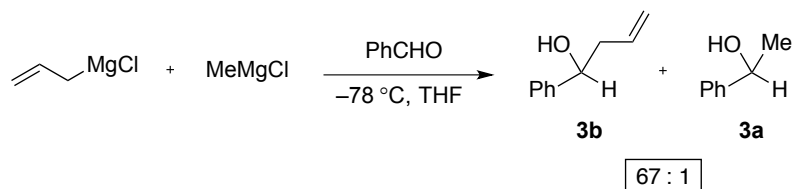
Sorted By : Signal
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 Dilution : 1.0000

Signal 1: FID1 A,

Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	3.404	VV	0.0336	4160.33643	1598.30359	38.92602
2	4.364	VV	0.0396	5796.92822	1871.03027	54.23872
3	4.780	VV	0.0366	90.46114	34.44381	0.84640
4	7.193	PB	0.0474	603.06775	155.07236	5.64258
5	9.483	BV	0.0330	18.97945	7.25847	0.17758
6	9.492	VB	0.0313	18.03049	7.18469	0.16870

Totals : 1.06878e4 3673.29318

The ratio of **4b**:**20** obtained from GC analysis of the reaction mixture was 94:6. This ratio was adjusted to correct for response factors using a GC to ¹H NMR calibration curve, which adjusted the final ratio to 95:5.



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 Area Percent Report
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Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000

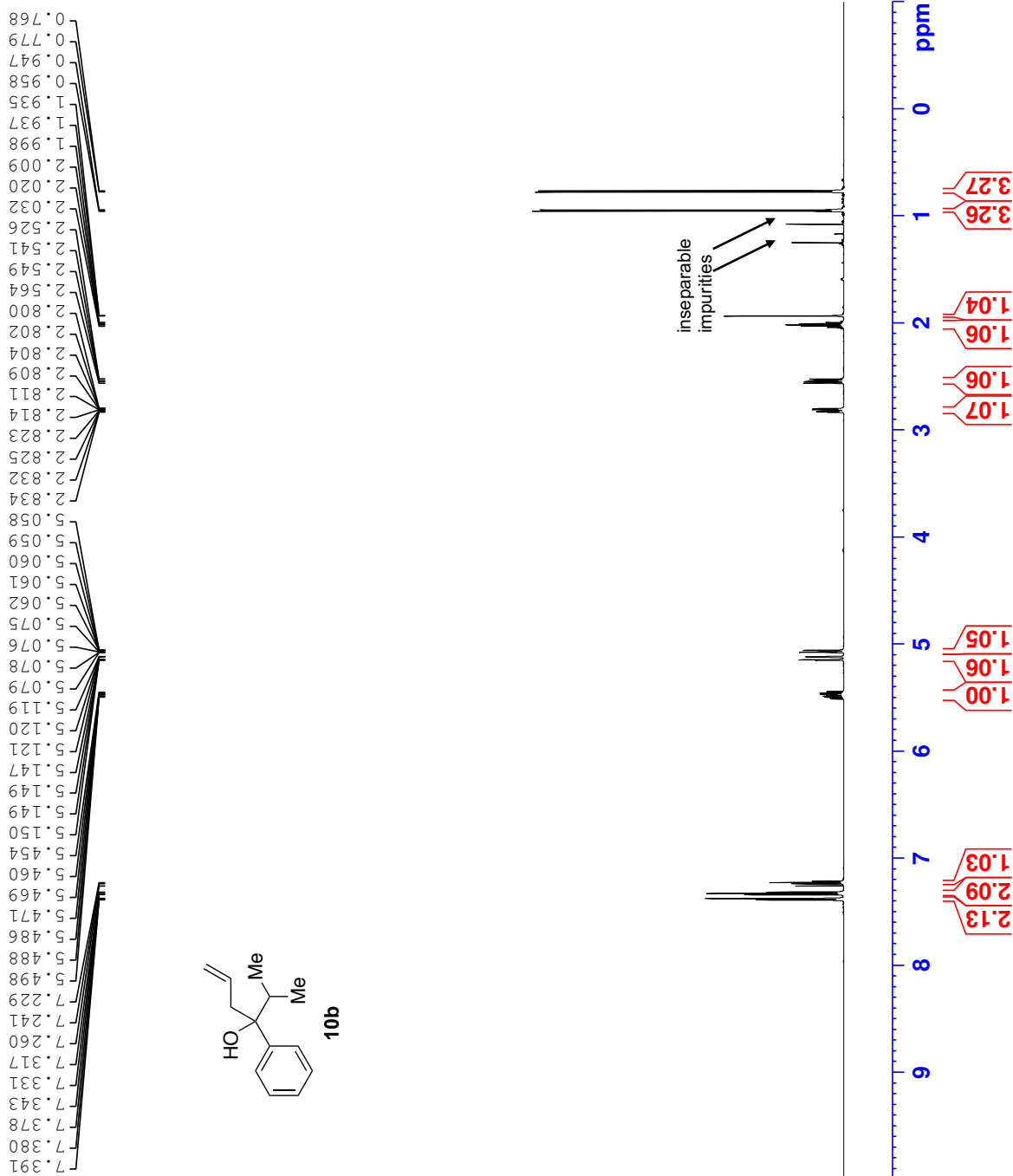
Signal 1: FID1 A,

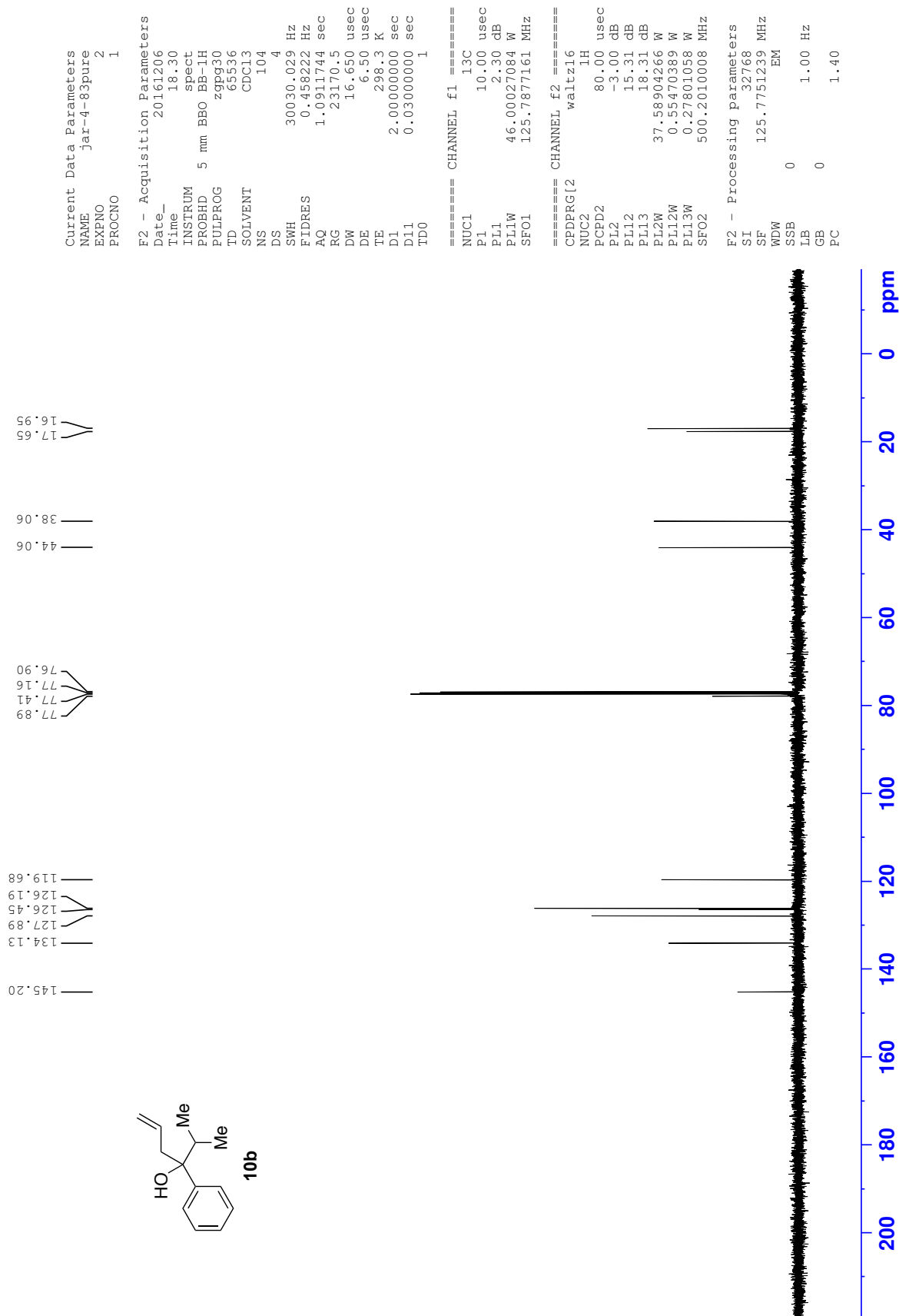
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.355	VV	0.0441	29.65533	10.15141	1.47148
2	10.362	PB	0.0915	1985.68457	279.25867	98.52852

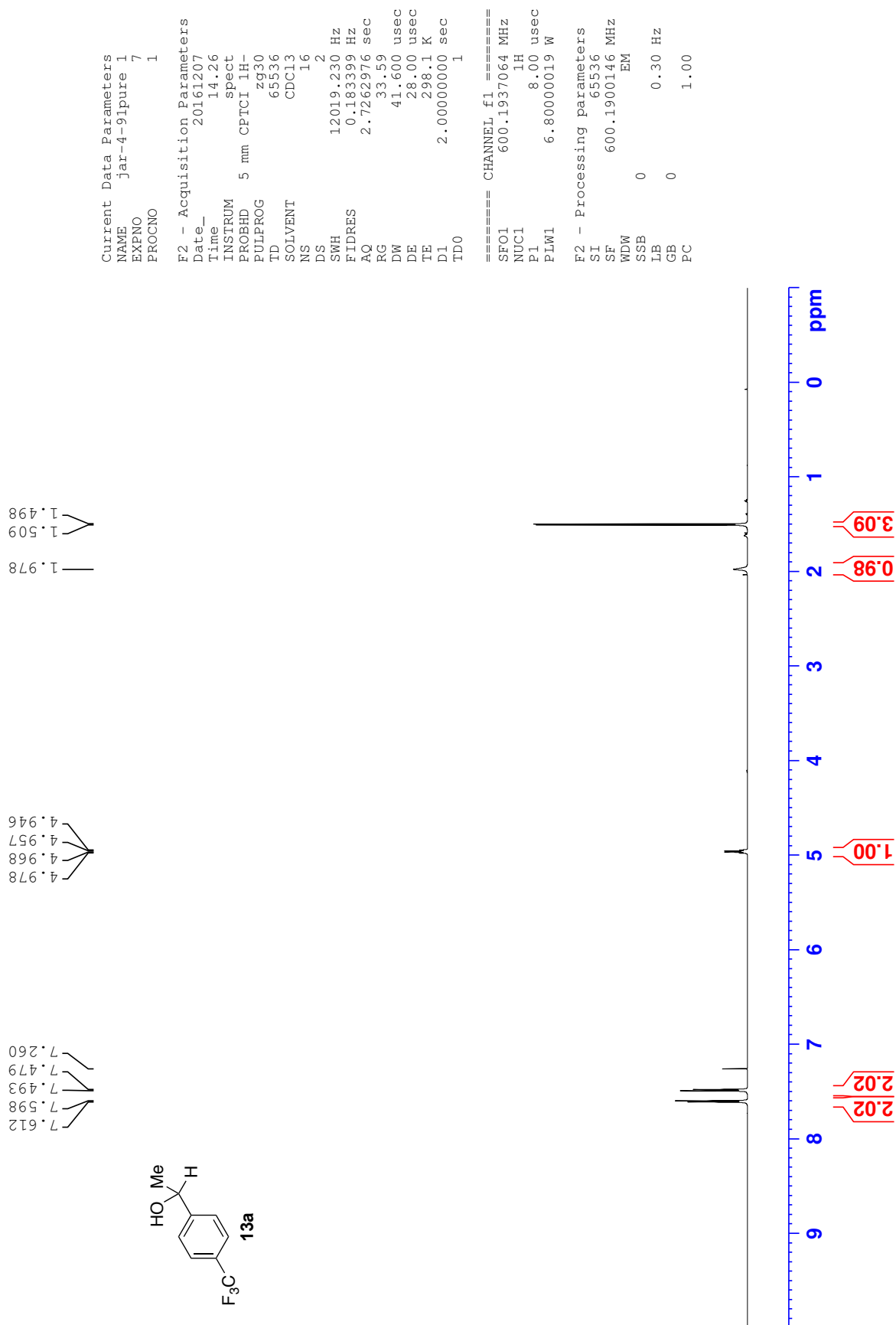
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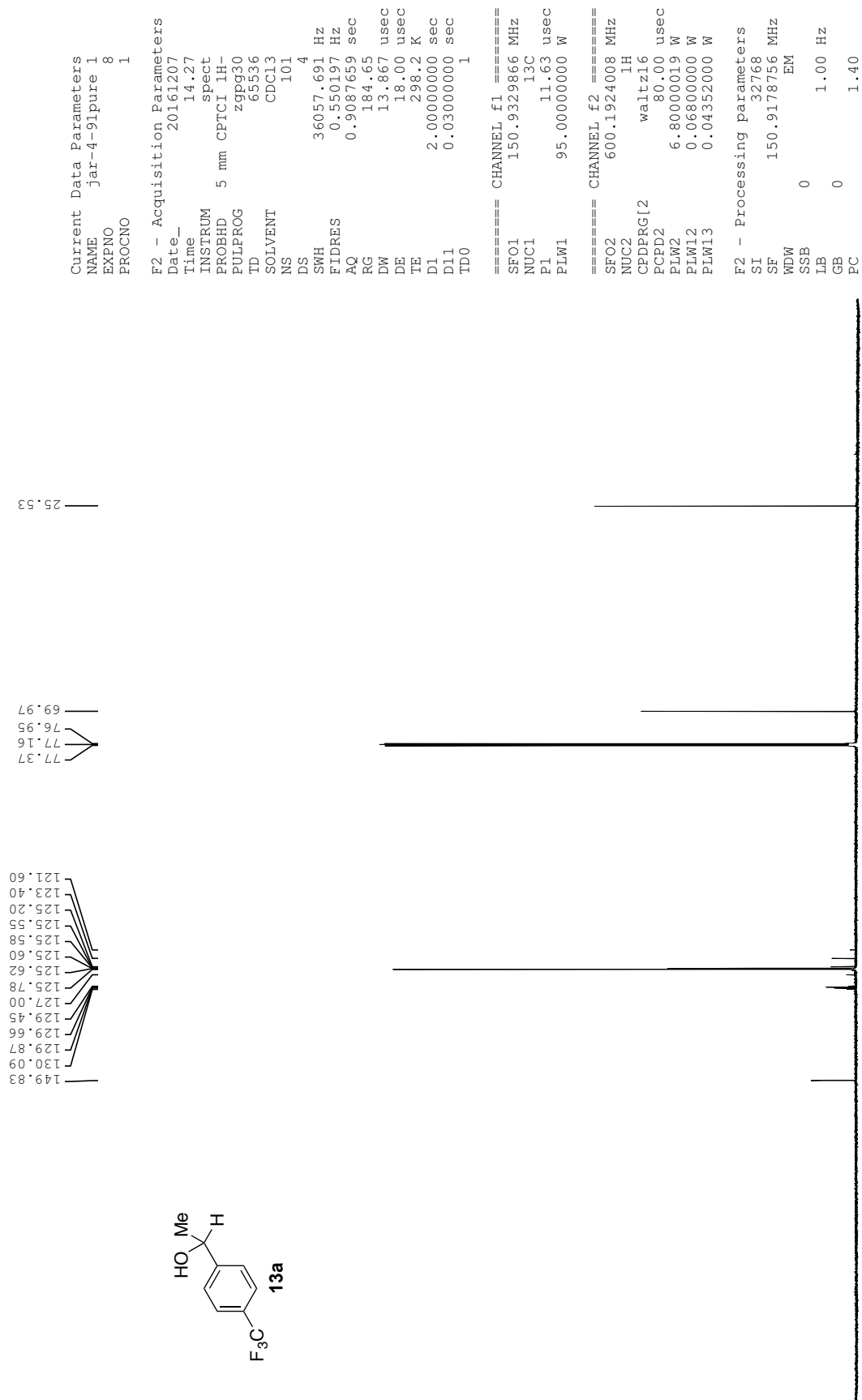
B. Selected ^1H and ^{13}C NMR spectra

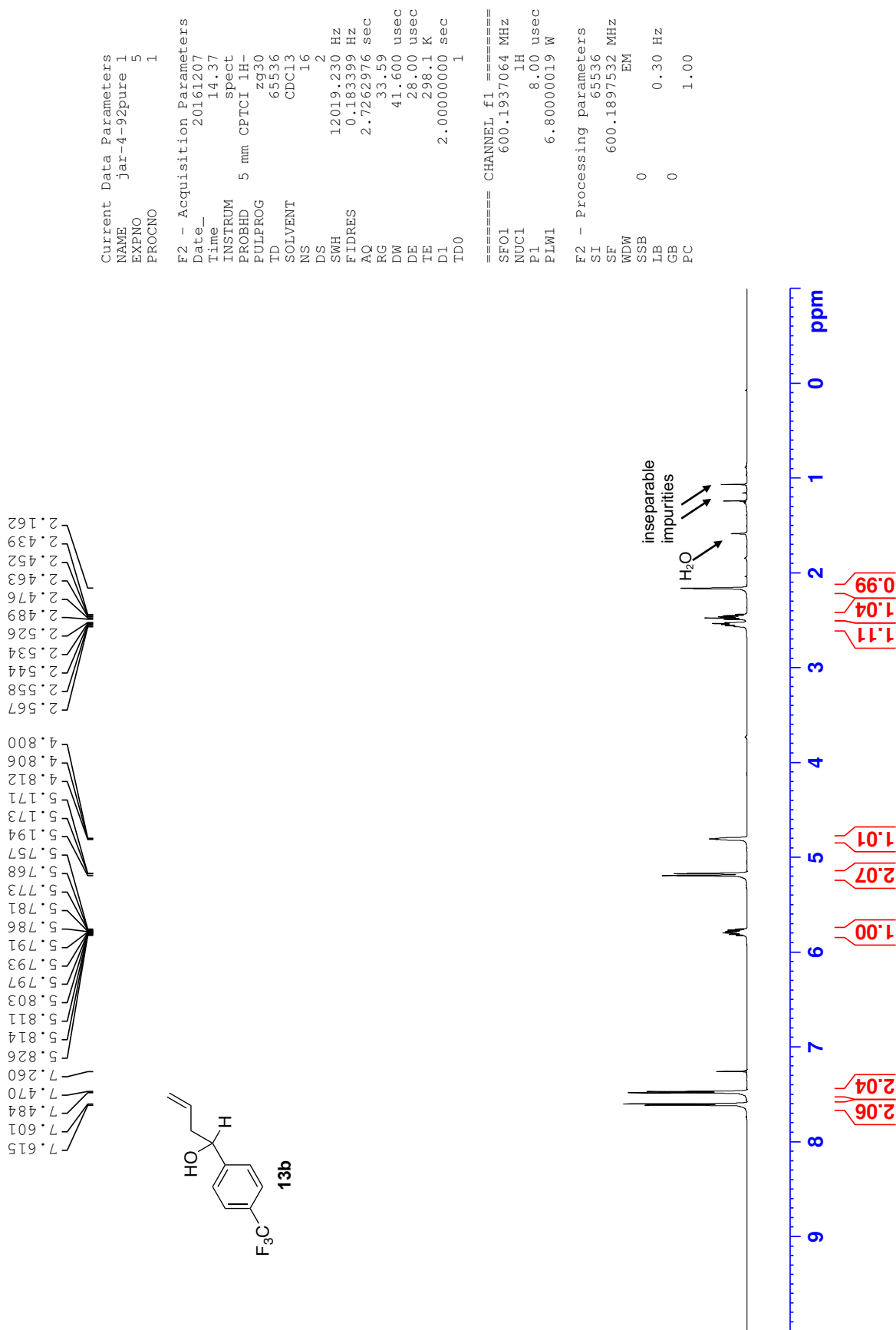
The following pages contain ^1H and ^{13}C NMR spectra for all known compounds made through new methods. A crude ^1H spectrum is also included, as it was used to calculate reaction conversion. There are no resonances with chemical shifts beyond the shown area of spectra.

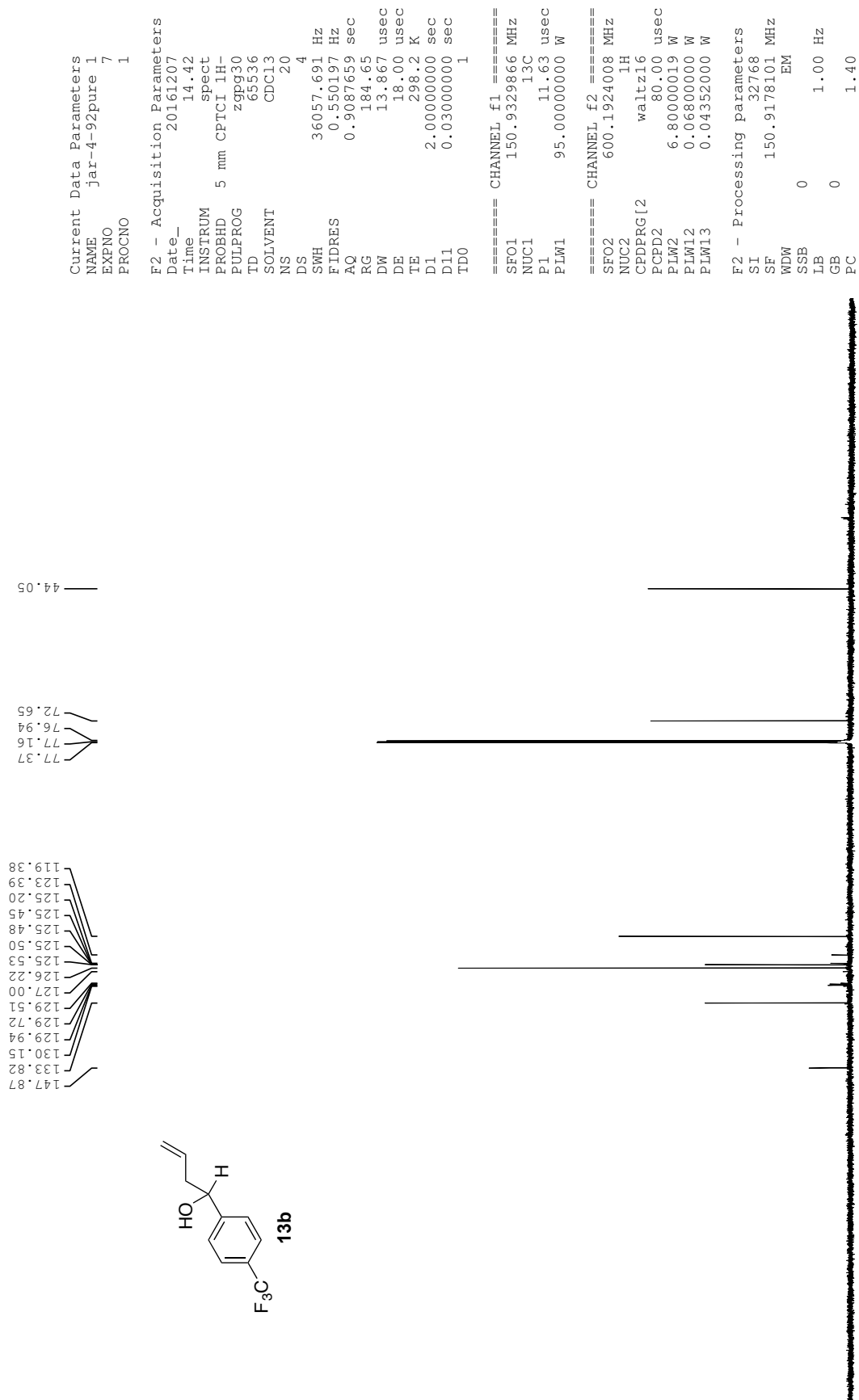


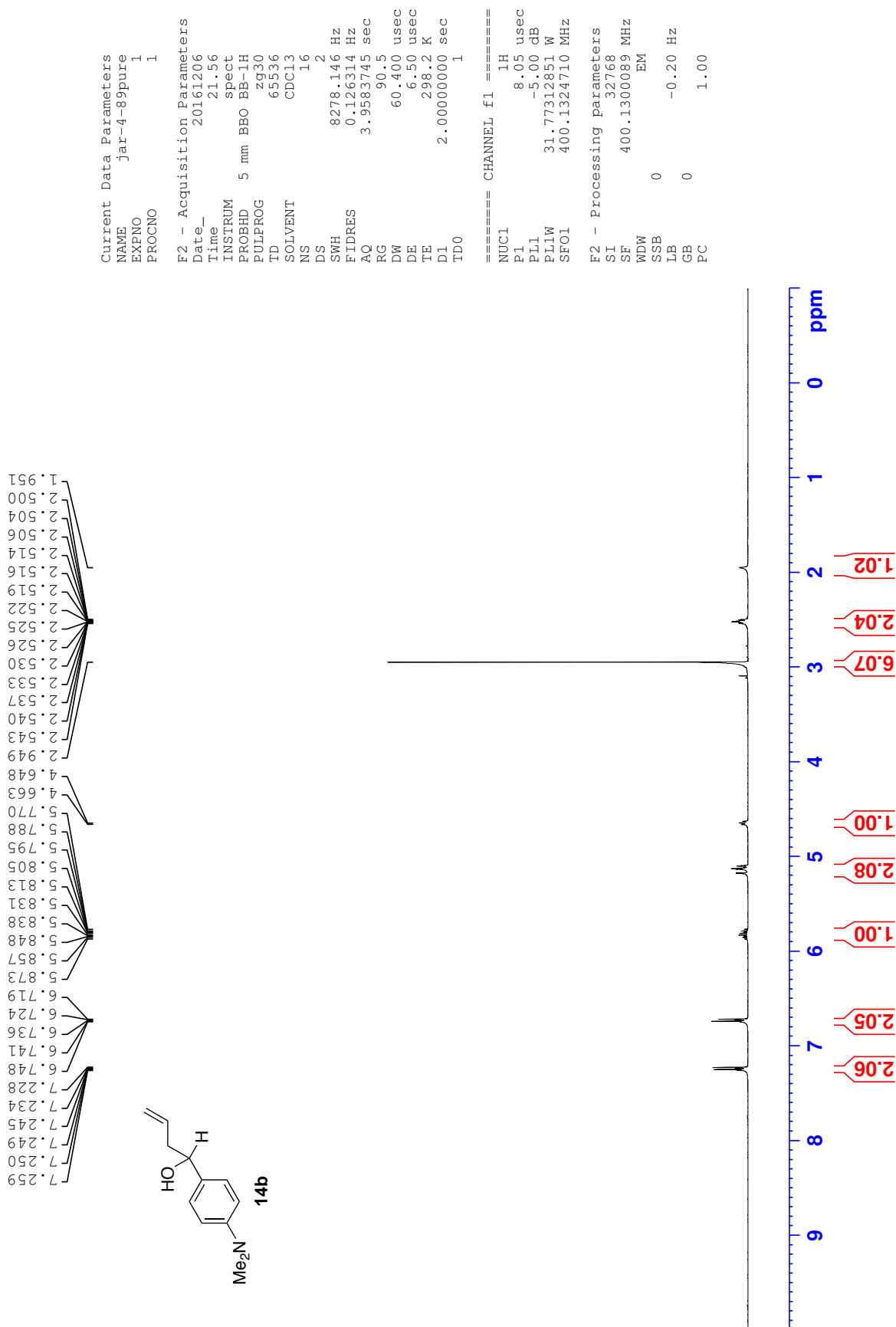












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EXPNO 2
PROCNO 1

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TD 65536
SOLVENT CDCl3
NS 111
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664256 sec
RG 20642.5
DW 20.850 usec
DE 6.50 usec
TE 298.2 K
D1 2.50000000 sec
D11 0.03000000 sec
TD0 1

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P1 7.75 usec
PL1 -2.70 dB
PL1W 18.70940590 W
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -5.00 dB
PL12 14.95 dB
PL13 16.84 dB
PL2W 31.77312851 W
PL12W 0.32141048 W
PL13W 0.20799839 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127591 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

