

SUPPLEMENTARY INFORMATION (PART 3)

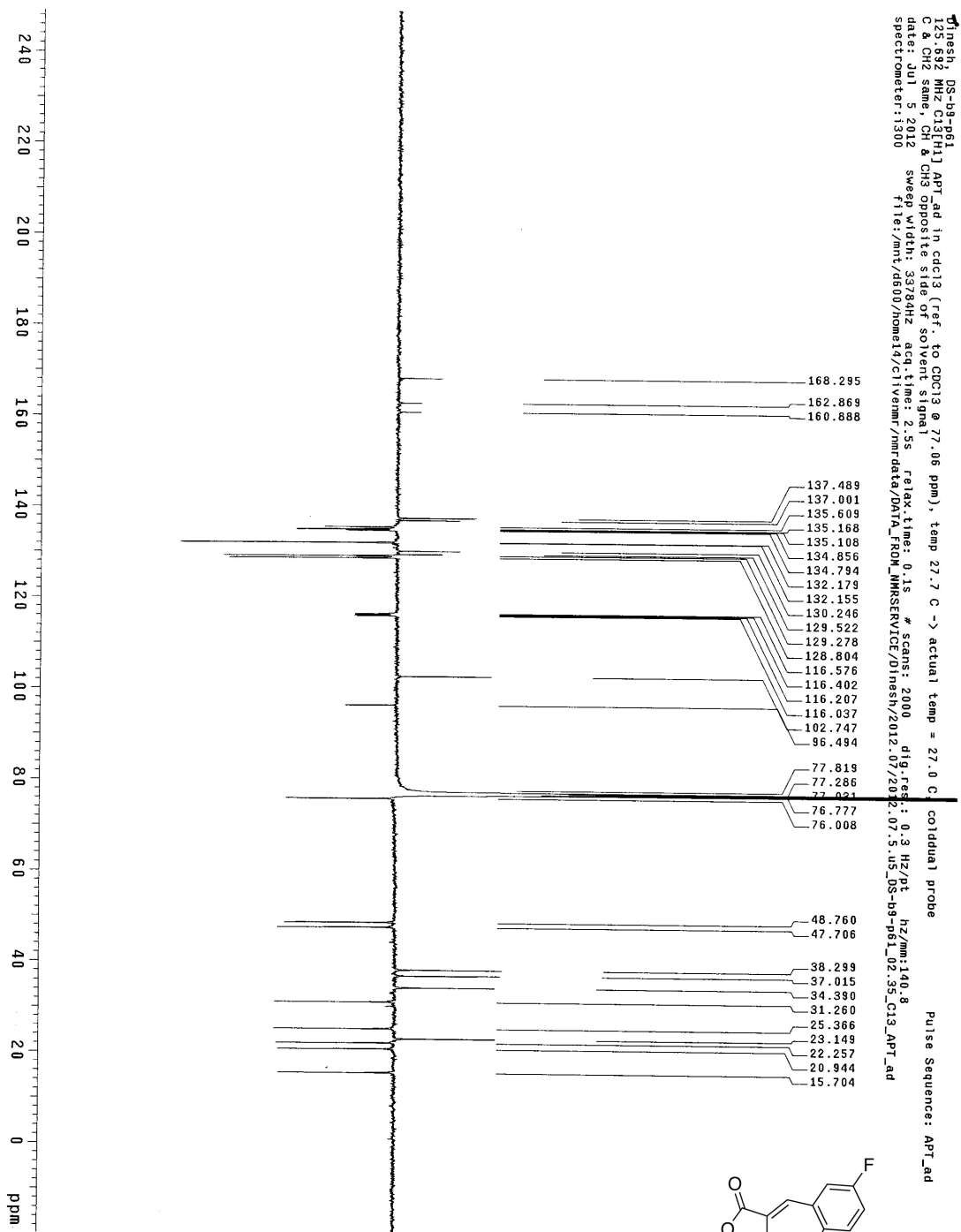
Asymmetric synthesis of carbocycles: use of intramolecular conjugate displacement

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Chemistry Department, University of Alberta, Edmonton, Alberta T6G 2G2, Canada

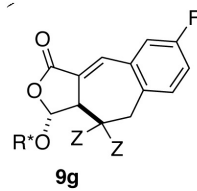
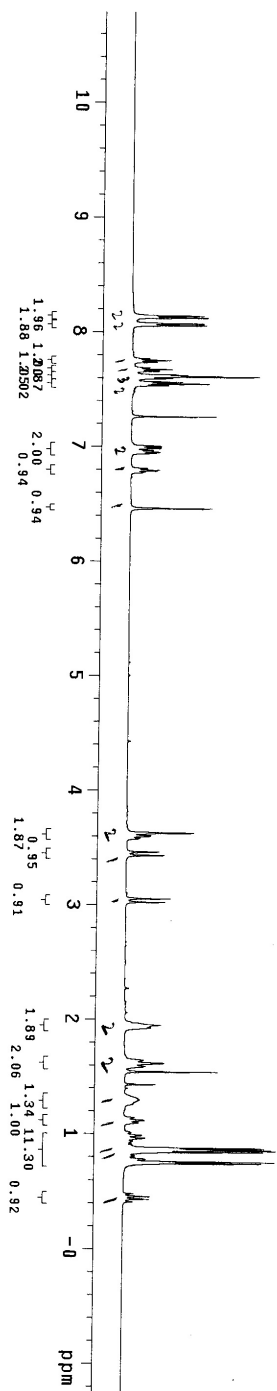
derrick.clive@ualberta.ca

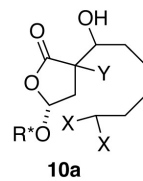
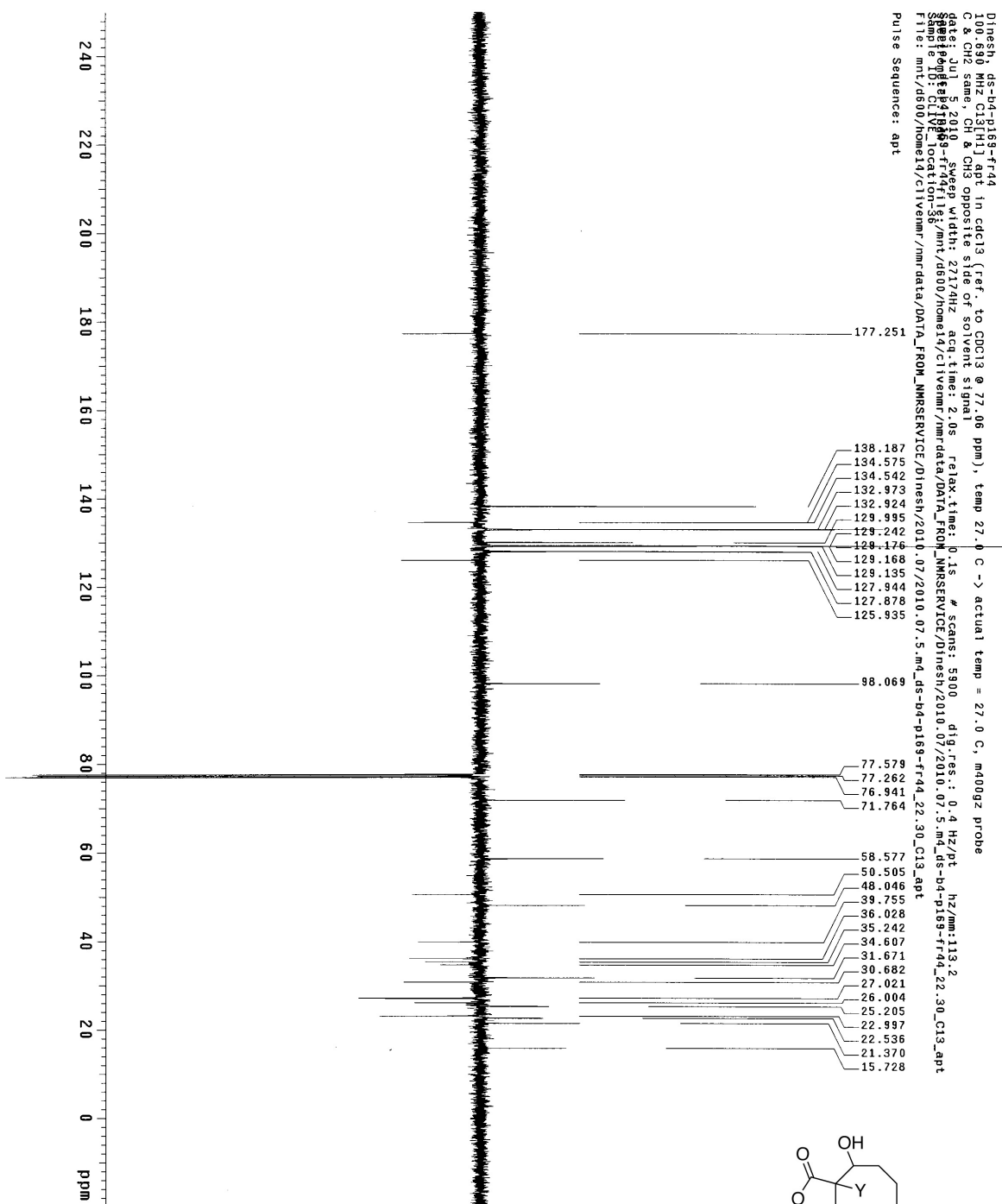
NMR spectra of compound 9g	S163
NMR spectra of compound 10a	S165
NMR spectra of compound 10a'	S167
NMR spectra of compound 10b	S169
NMR spectra of compound 10b'	S171
NMR spectra of compound 10c	S173
NMR spectra of compound 10c'	S175
NMR spectra of compound 11	S177
NMR spectra of compound 11a	S179
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NMR spectra of compound 11c	S183
NMR spectra of compound 12	S185
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NMR spectra of compound 12b	S189
NMR spectra of compound 13	S191
NMR spectra of compound 13b	S193
NMR spectra of compound 13b'	S195
NMR spectra of compound 14	S197
NMR spectra of compound 15 less polar isomer	S199
NMR spectra of compound 15 mixture of isomers	S201



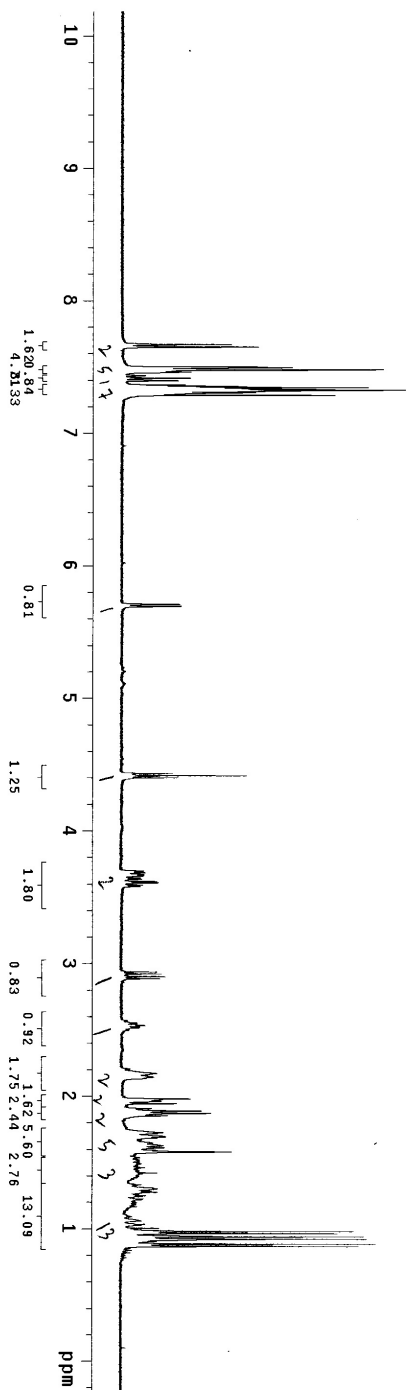
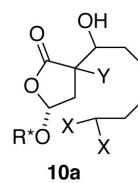
DS-49-P61
499.122 MHz H1 1D in cdCl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxtdb probe

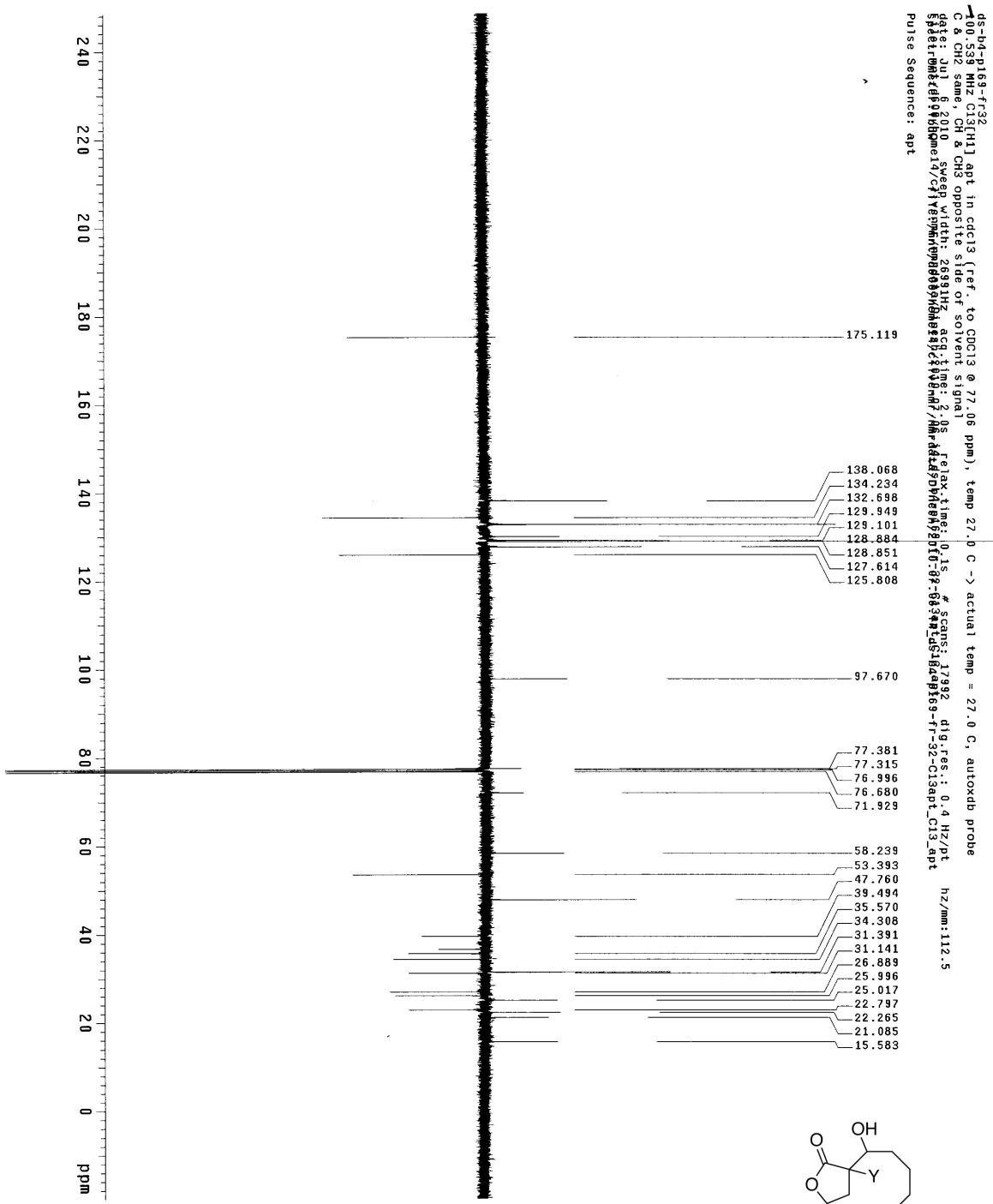
Pulse Sequence: szpu1



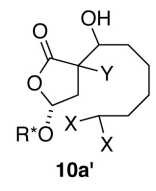


Dinesh; ds-b4-p169-fr44
400.393 MHz H1 ID in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.0 C -> actual temp = 27.0 C, m400gz probe
Sample: ds-b4-p169-fr44
Sample ID: CLIVE106411
File: mnt/d600/home14/clivenmr/nmrdata/DATA_FROM_NMRSERVICE/Dinesh/2010.07/2010.07.5.m4_ds-b4-p169-fr44_22.28_H1_ID
Pulse Sequence: szpu1

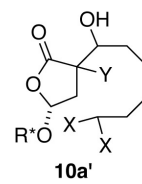
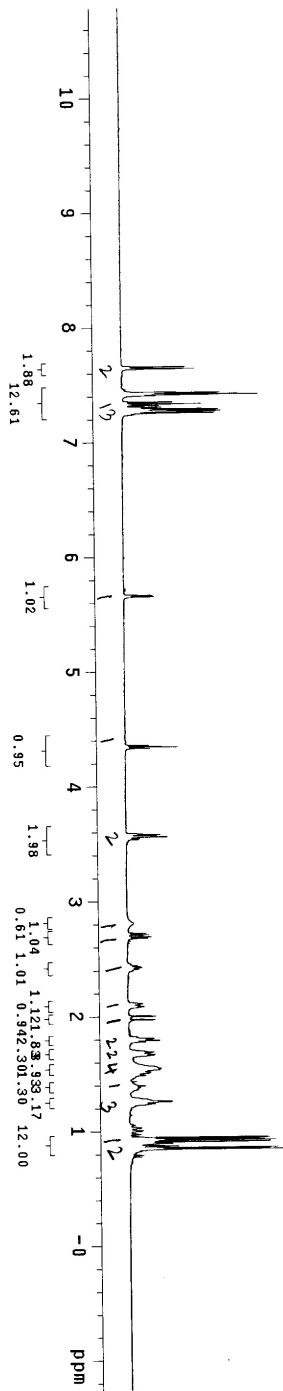


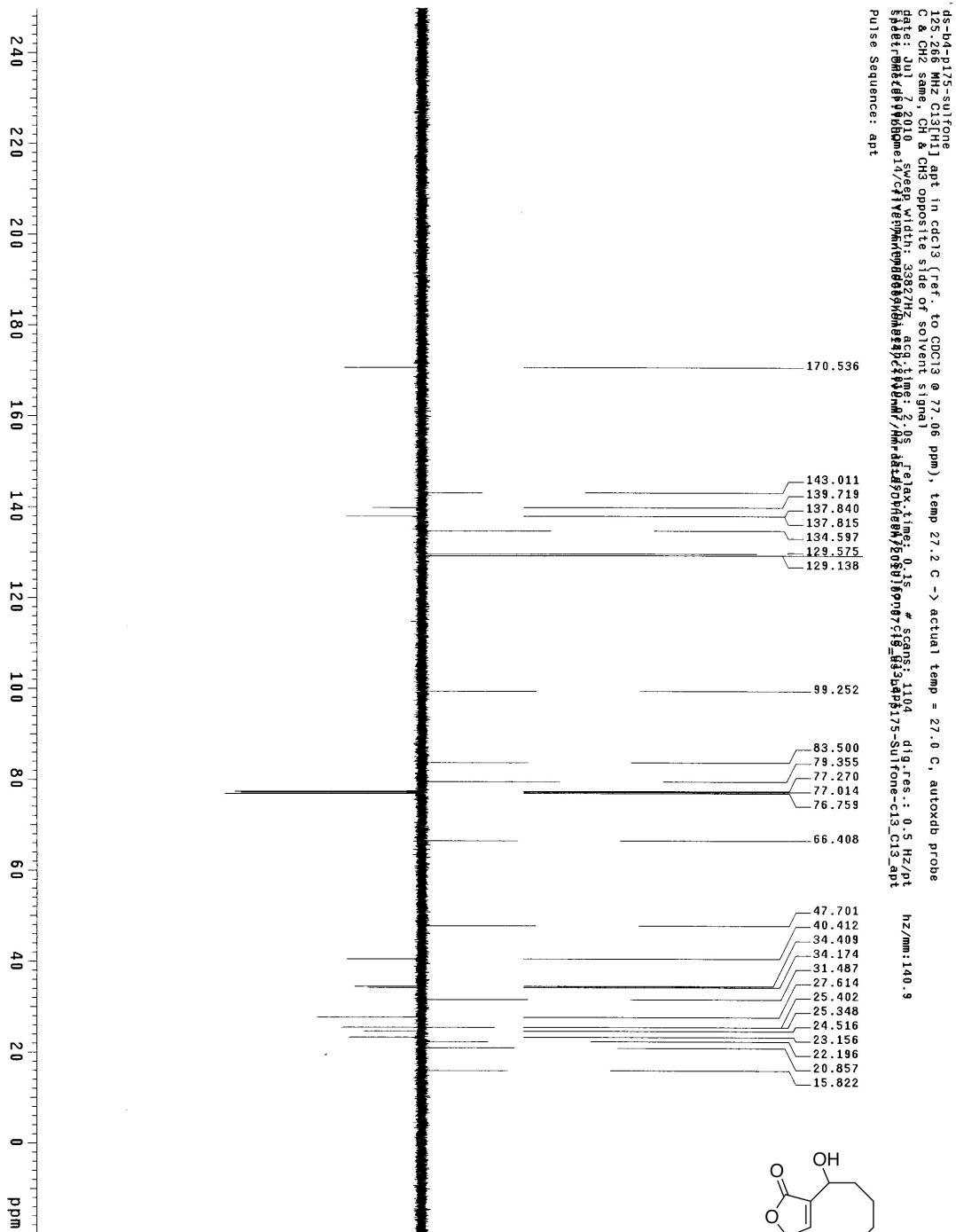


ds-b4-p169-fr32
100.539 MHz C13[H1] apt in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 27.0 C -> actual temp = 27.0 C, autotxnb probe
C & CH2 same, CH & CH3 opposite side of solvent signal
Date: Jul 6, 2010 Sweep width: 26931Hz acq. time: 2.08 refax time: 0.15 # scans: 1792 dig.res.: 0.4 Hz/pt
Spect: dmtdf9166me14/c1ve9mte00009166me14/c1ve9mte00009166me14/10-09-08-3M L4S-B4p169-fr-32-Cl3apt_C13_apt
Pulse Sequence: apt



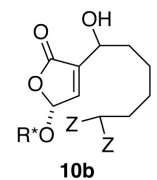
ds-b4-p169-fr32-8nm
498.122 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxidb probe
File: mt/d600/home14/ctivemr/nmrdata/01mesh/2010.07.06.15_ds-b4-p169-fr-32-H1_1D
Pulse Sequence: s2pul



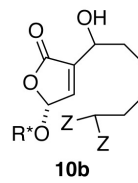
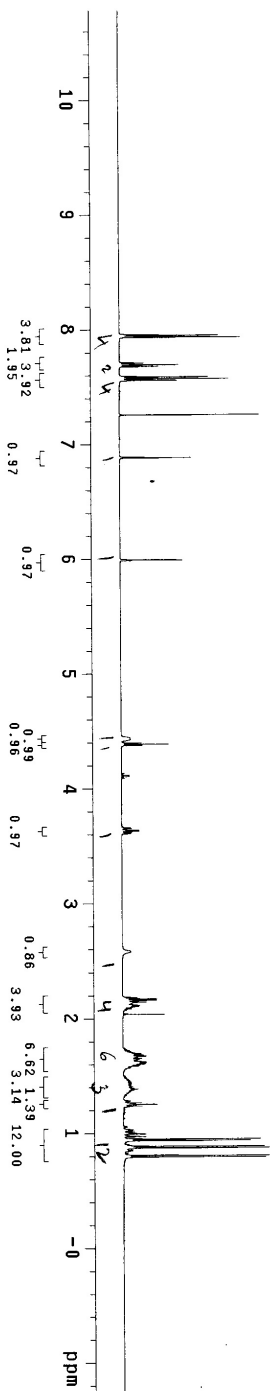


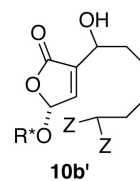
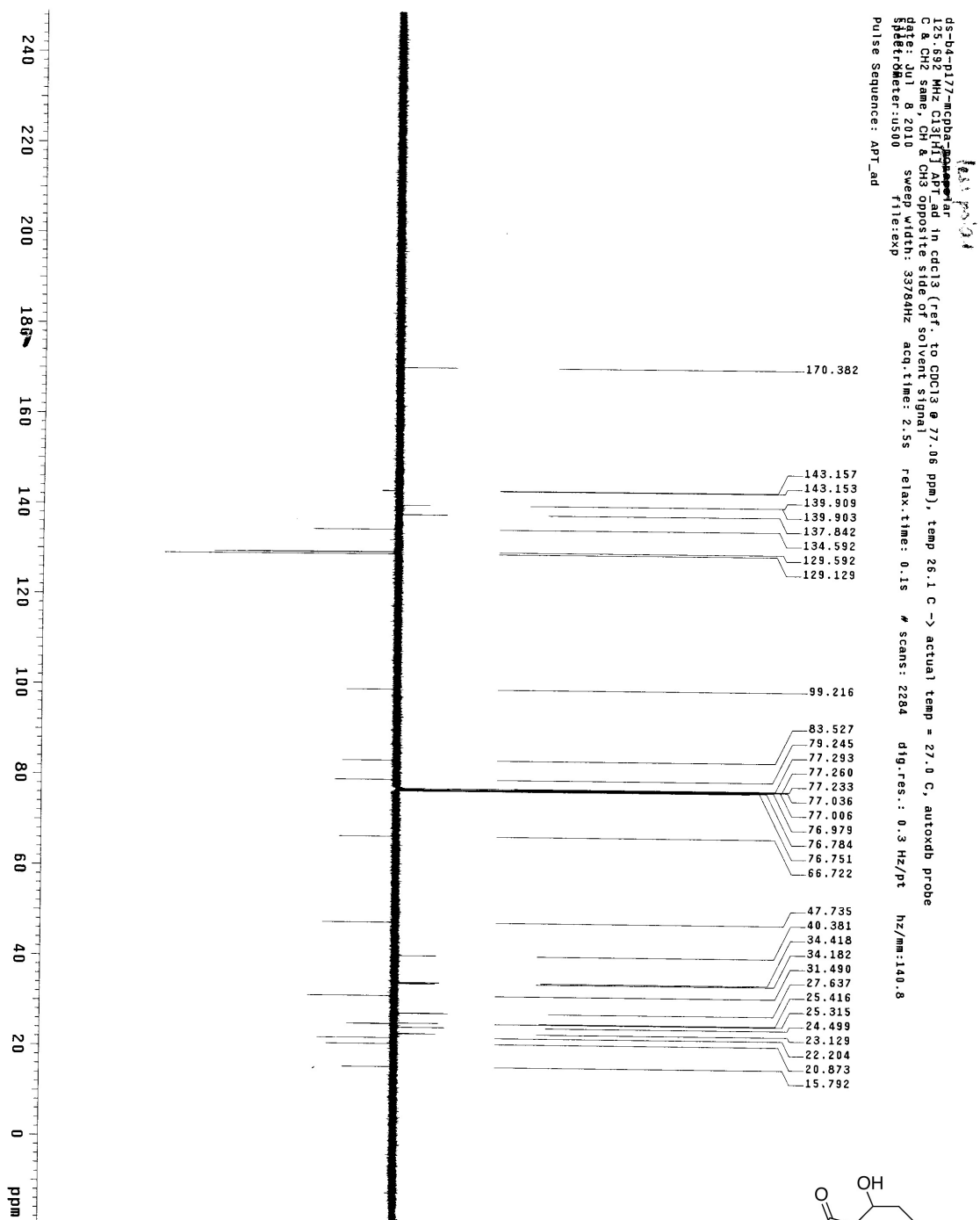
ds-b4-p175-sulfone
Date: Jul 7 2010
Pulse Sequence: apt

hz/mm:140.9



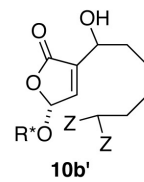
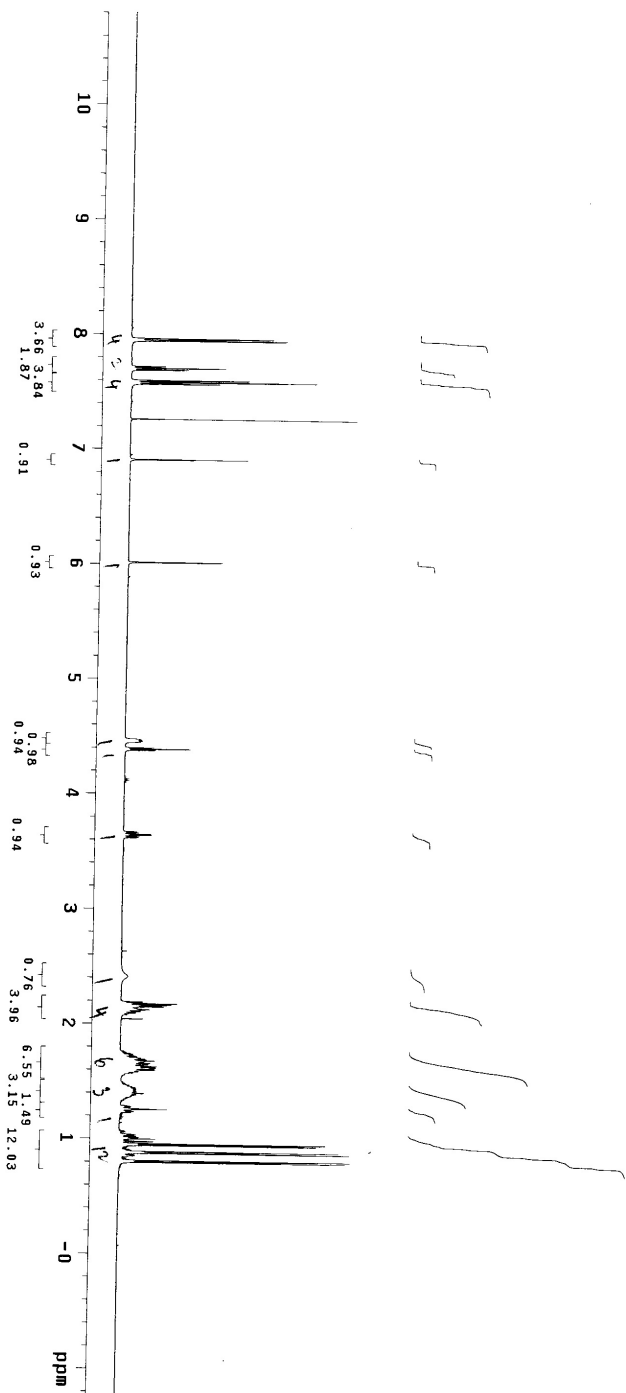
ds-b4-p175-sulfone
496.122 MHz H1 ID in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxadb probe
File: mnt/d800/home14/c11vnmr/mmrdata/D1nesh/2010.07.07.15_ds-b4-p175-Sulfone-H1_H1_ID
Pulse Sequence: s2pul1

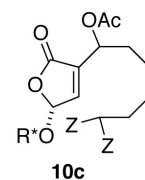
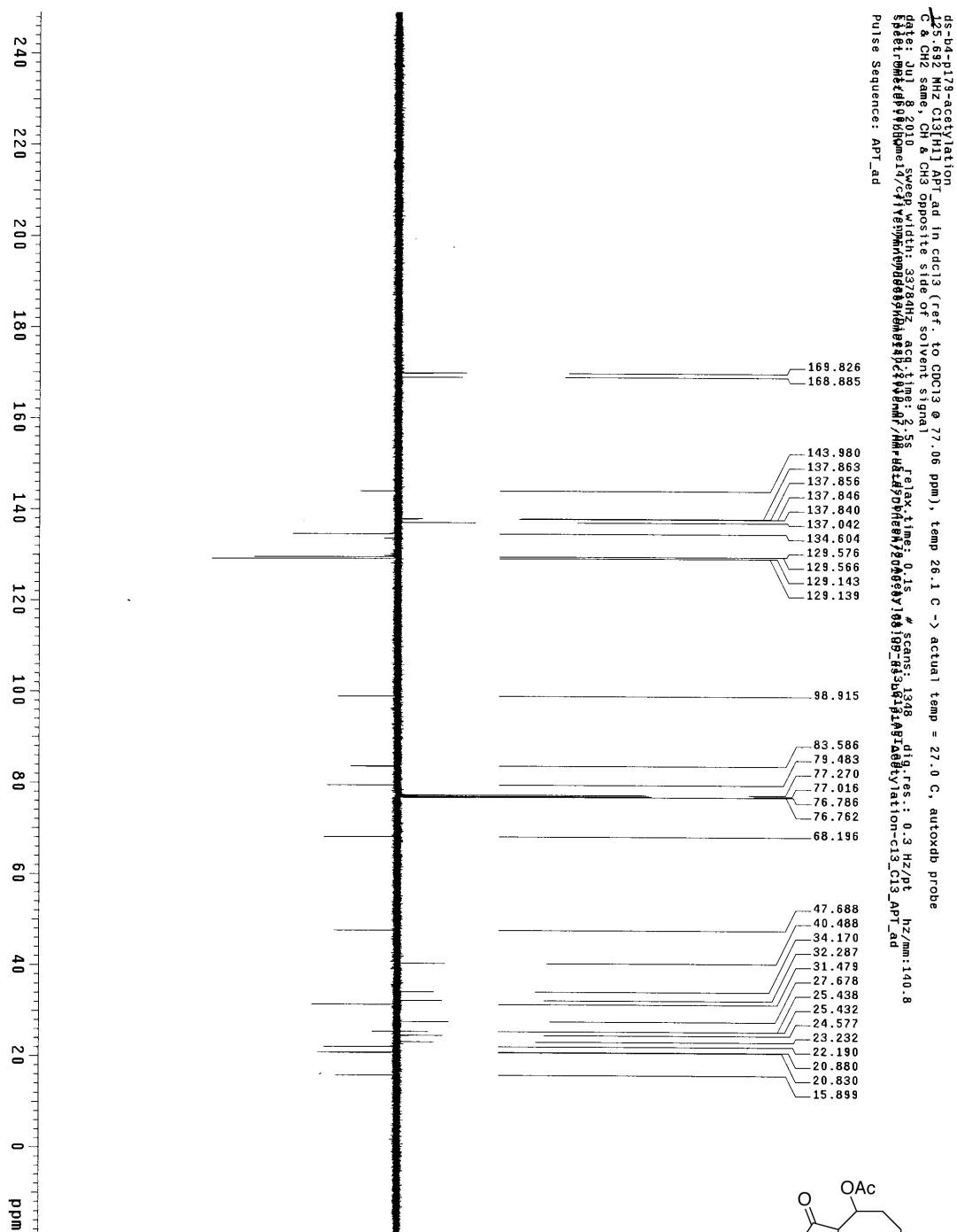




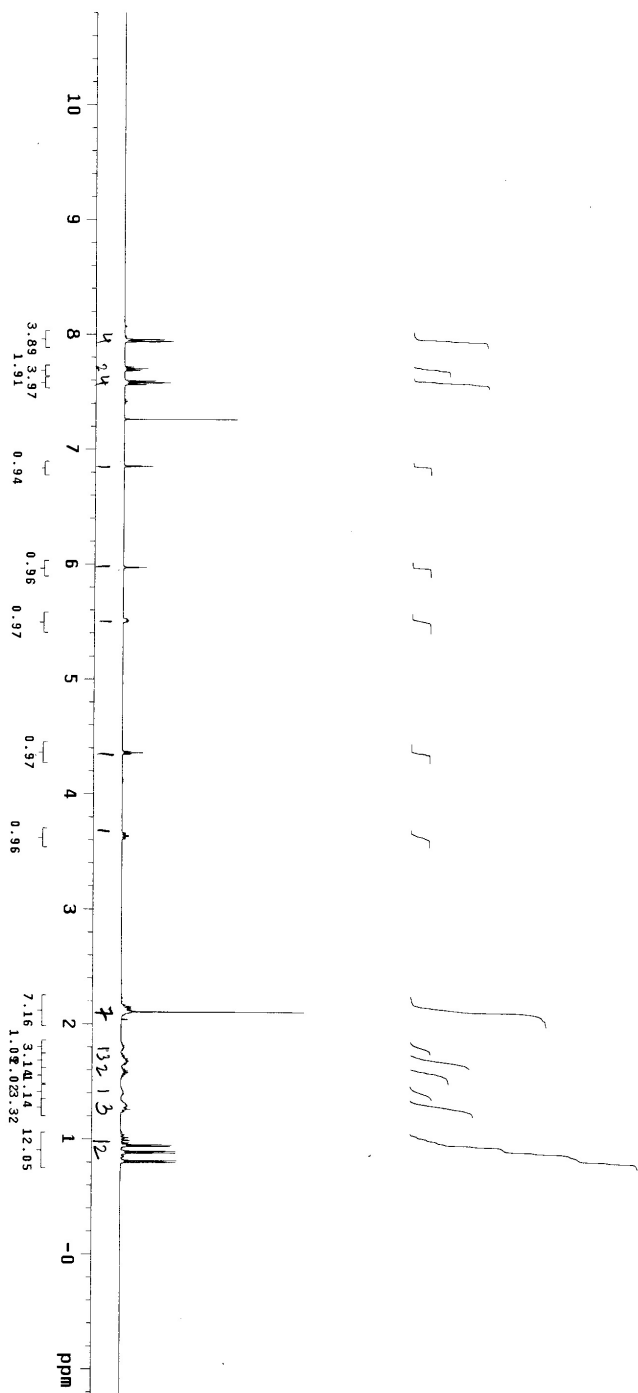
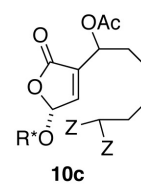
ds-b4-pl77-mcpba-~~proton~~ar
125.692 MHz C13 N13 APT-ad in cdcl3 (ref. to CDCl3 @ 77.06 ppm), temp 26.1 C -> actual temp = 27.0 C, autotxnb probe
C & CH2 same, CH & CH3 opposite side of solvent signal!
Date: Jul 8 2010 sweep width: 33784Hz acq.time: 2.5s relax.time: 0.1s # scans: 2284 dig.res.: 0.3 Hz/pt hz/mm:140.8
Spectrometer:us00 file:exp
Pulse Sequence: APT_ad

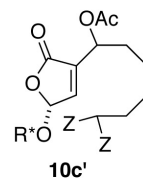
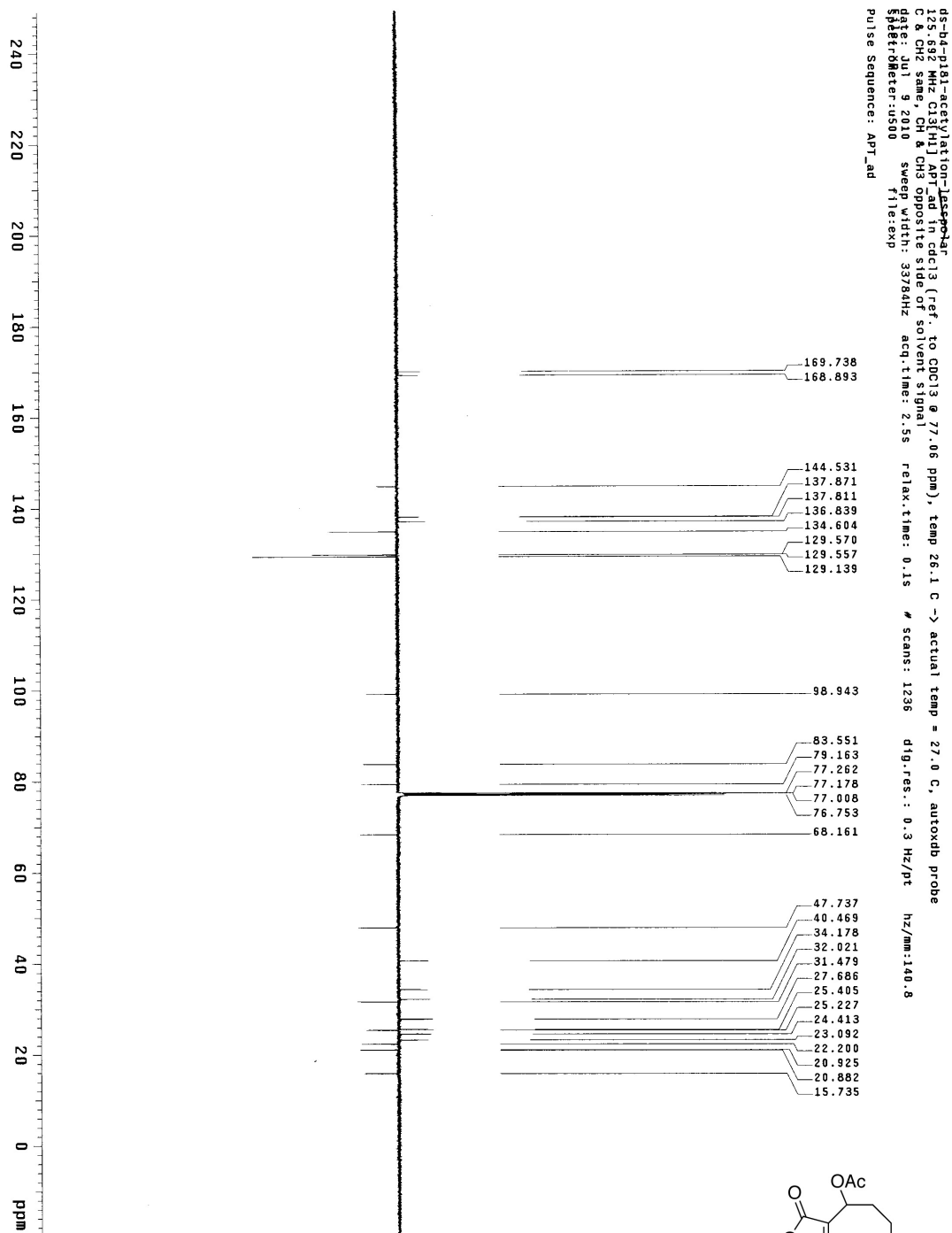
ds-b4-p177-mcpba-lesspoliar
439.815 MHz H1 10 in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 26.1 C -> actual temp = 27.0 C, autoxtdb probe
File: mnt/d600/home14/clivemr/mrdata/Dinesh/2010.07.08.us_ds-b4-p177-mcpba-lesspoliar-H1_10
Pulse Sequence: szpu)



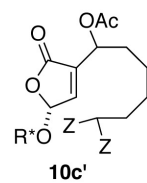
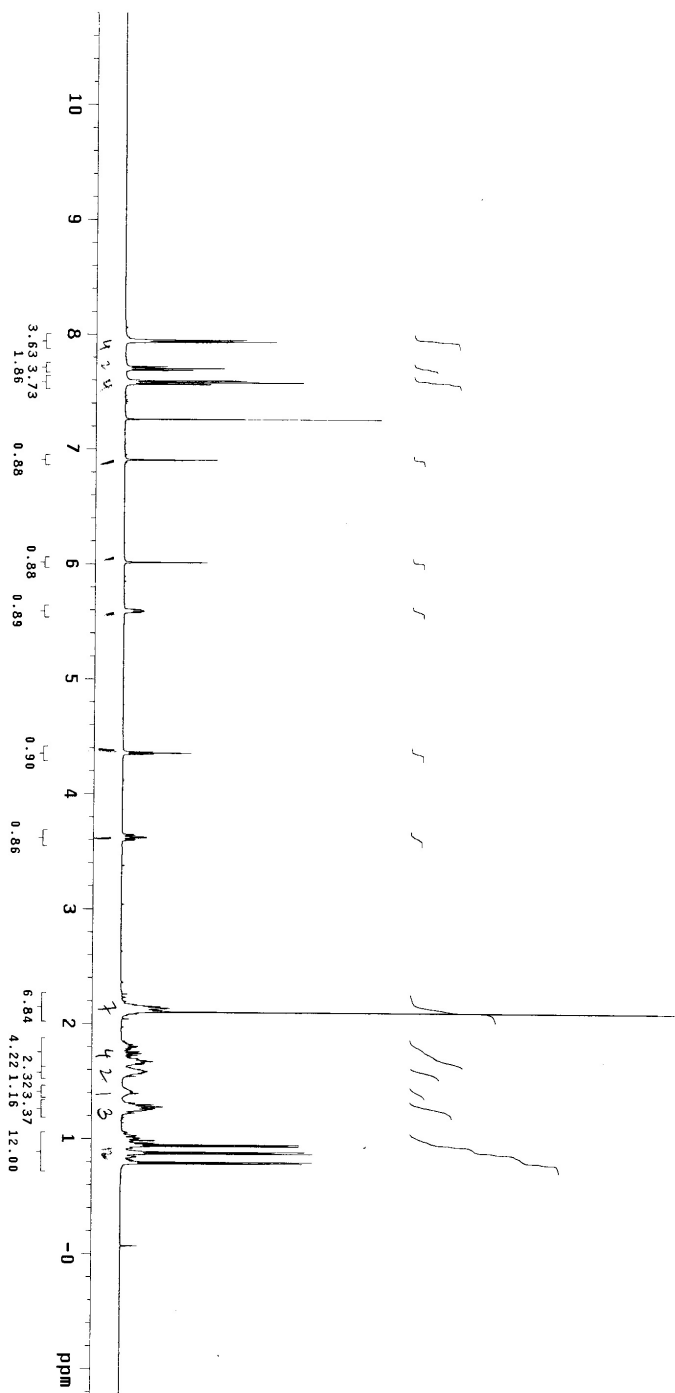


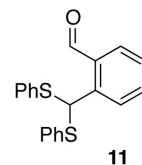
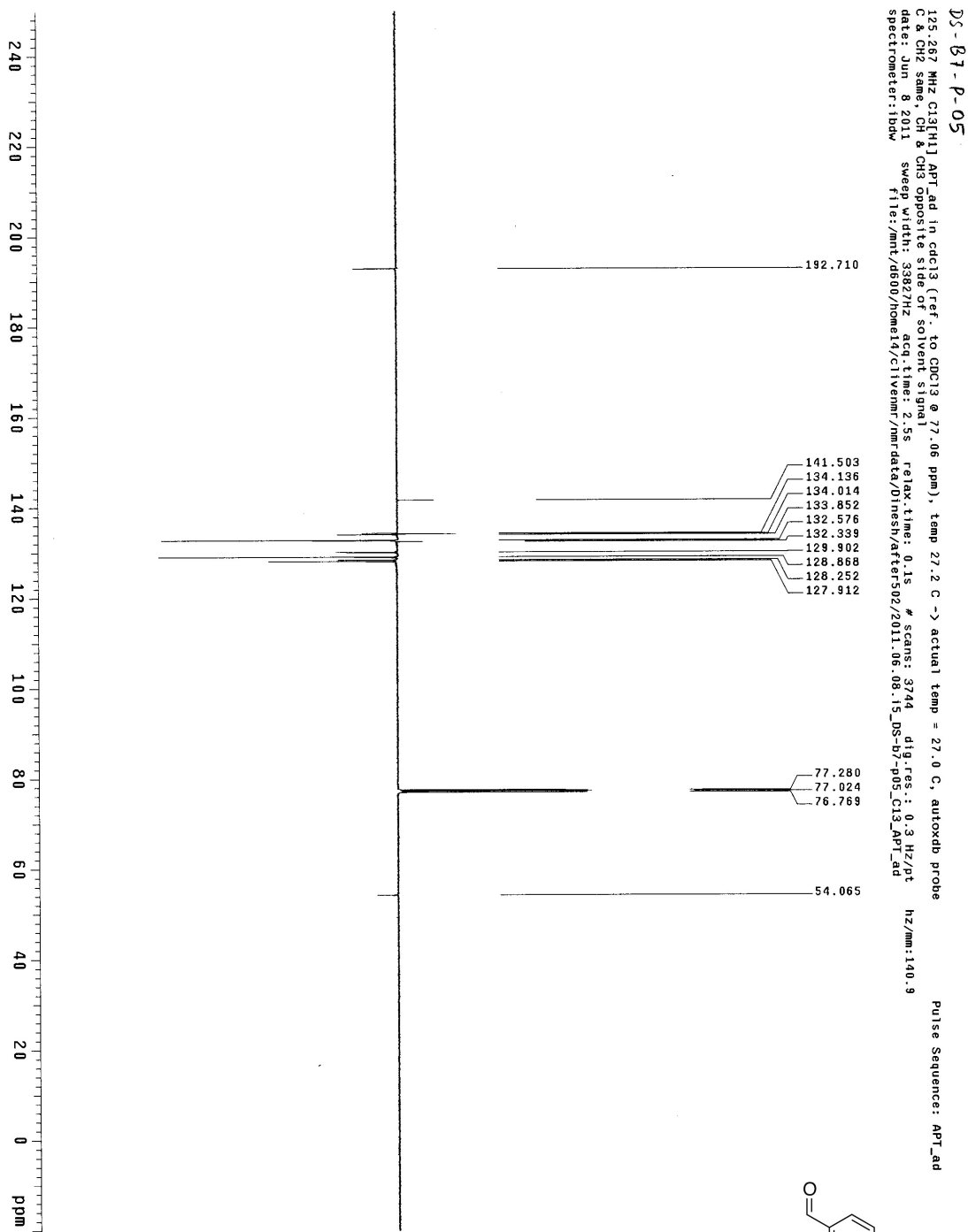
ds-b4-pl79-acetyl)ation
499.815 MHz H1_10 in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 26.1 C -> actual temp = 27.0 C, autotxdo probe
File: nnt/d60/home14/ctivenmr/nmrdata/Dinesh/2010.07.08.us_ds-b4-pl79-acetyl)ation-H1_10
Pulse Sequence: s2pu1





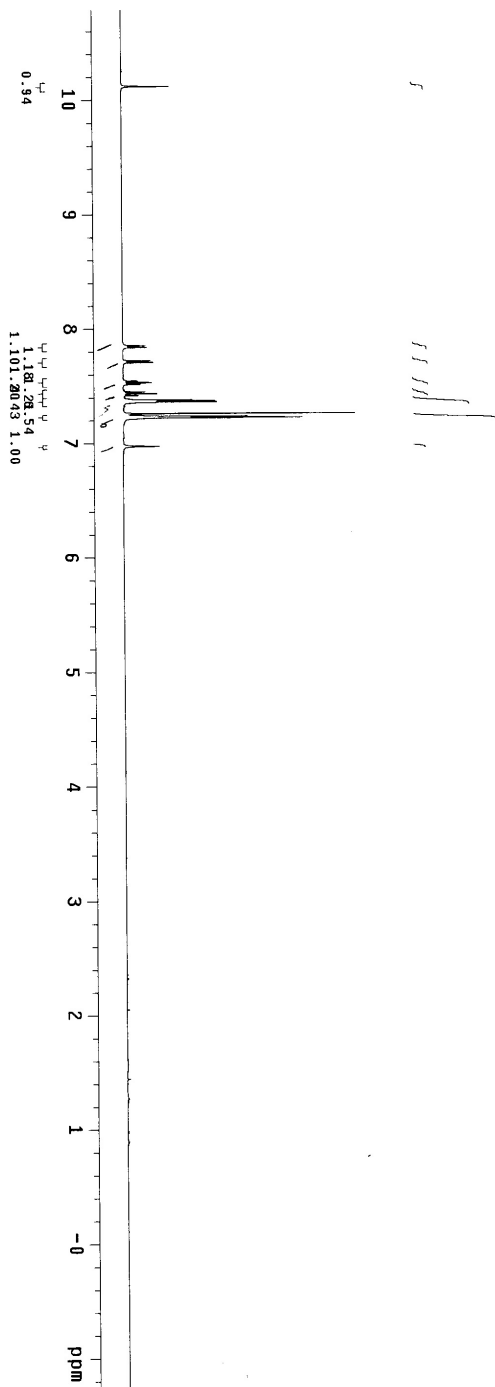
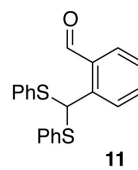
ds-bd-p181-Acetylation-lesspolar-H1
499.815 MHz H1 ID in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 26.1 C -> actual temp = 27.0 C, autotxdb probe
File: mnt/d600/home4/clivenmr/nmrdata/01nesh/2010_07_09_US_ds-bd-p181-acetylation-lesspolar-H1_H1_ID
Pulse Sequence: szpul

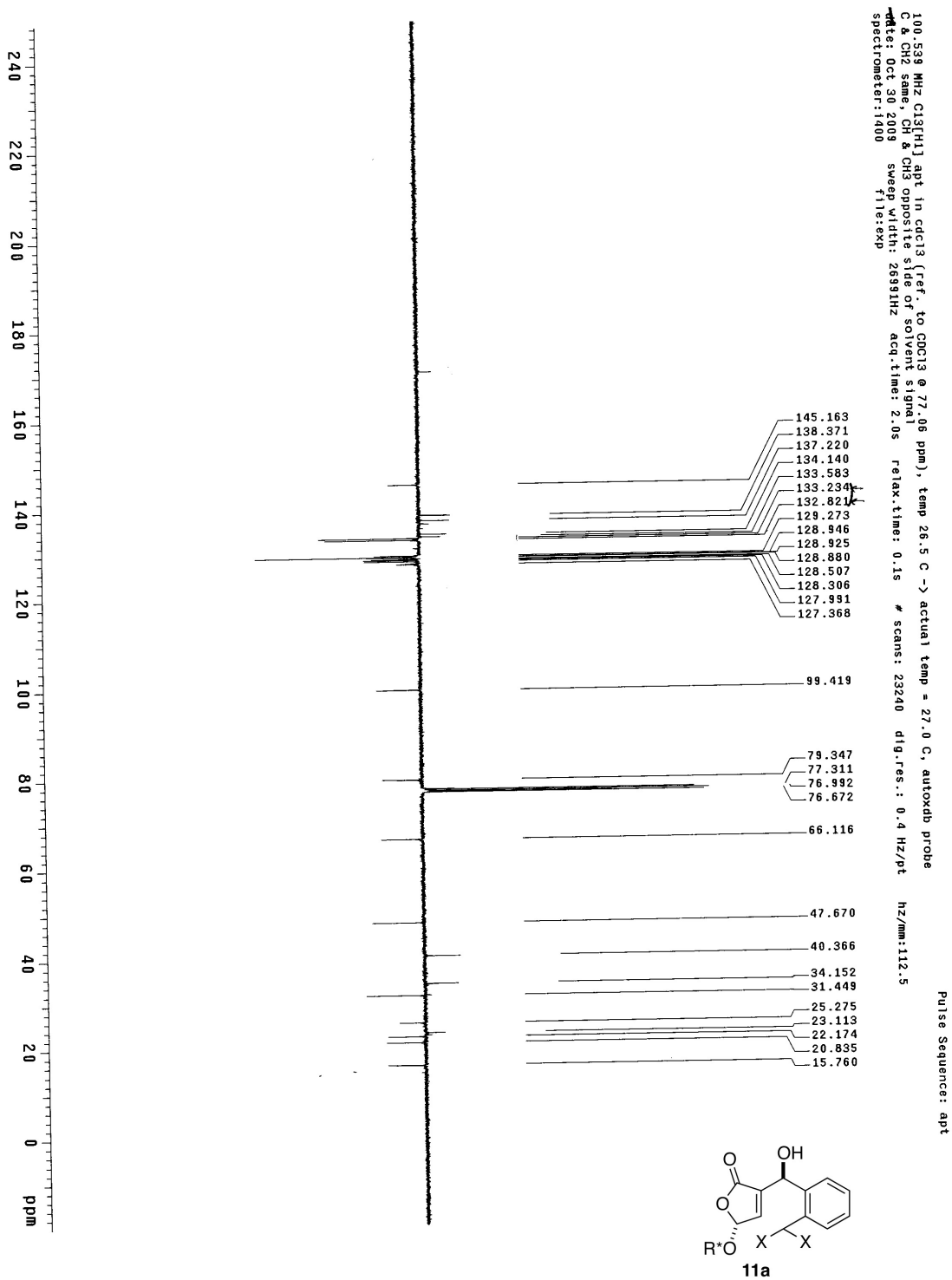




DS-b7-p05
498.122 MHz H1 1D In cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxdo probe

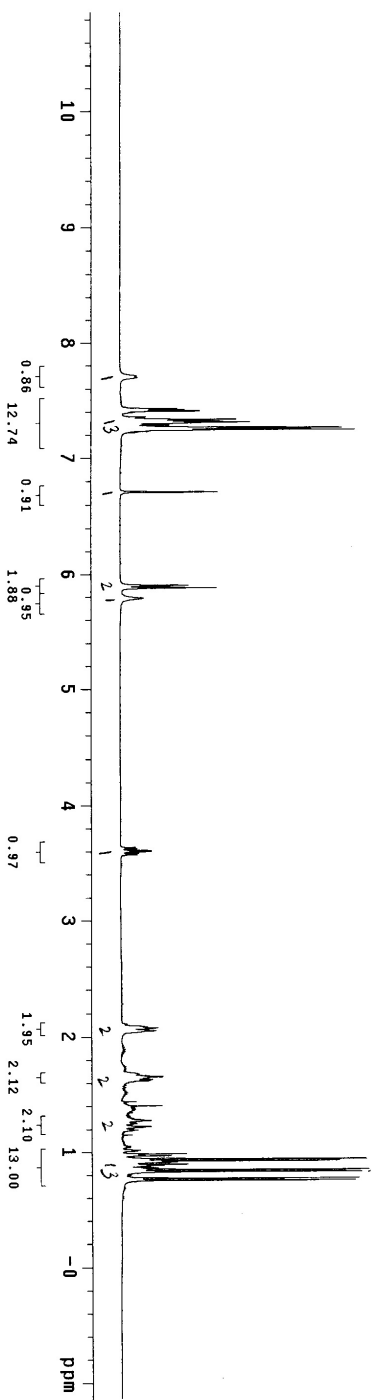
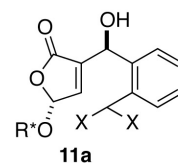
Pulse Sequence: s2pu1

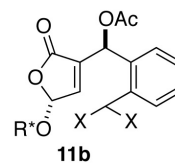
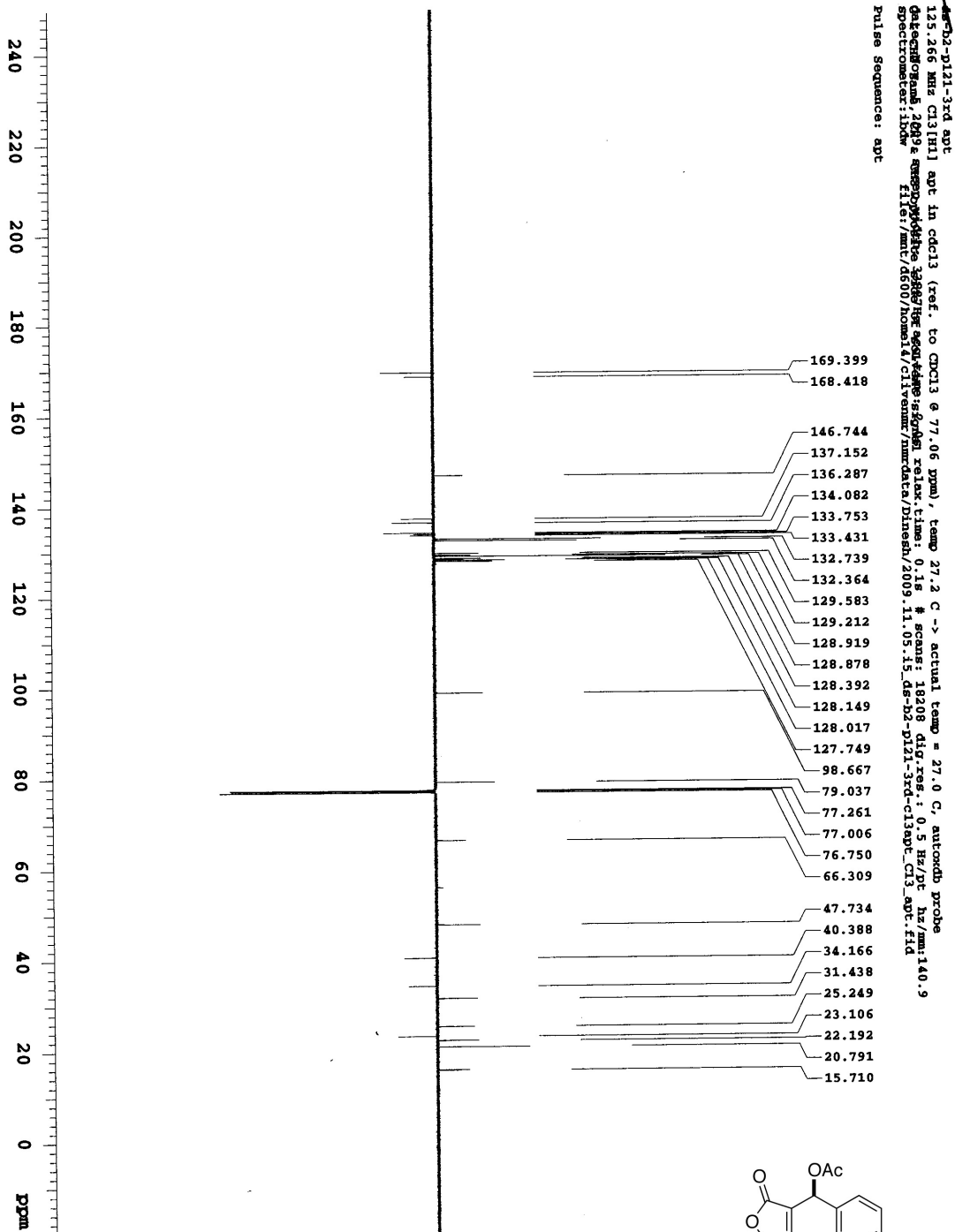




ds-b2-p113
399.794 MHz ¹H 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 26.5 C -> actual temp = 27.0 C, autotxdb probe

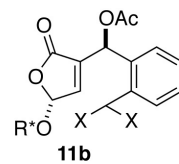
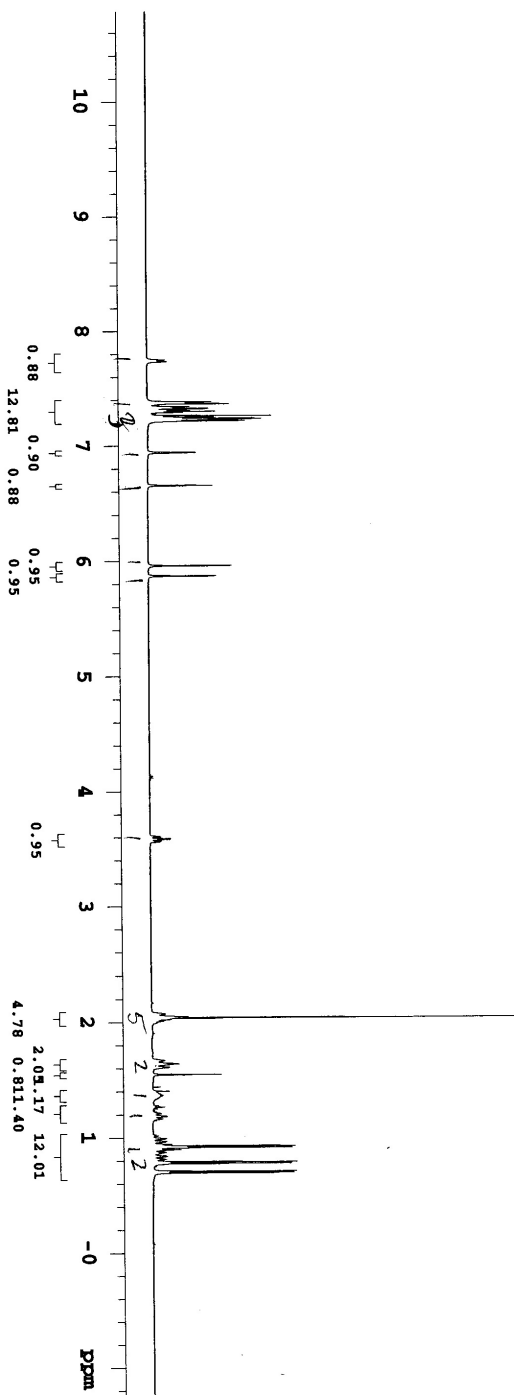
Pulse Sequence: szpu1

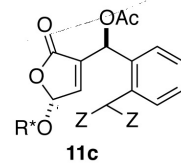
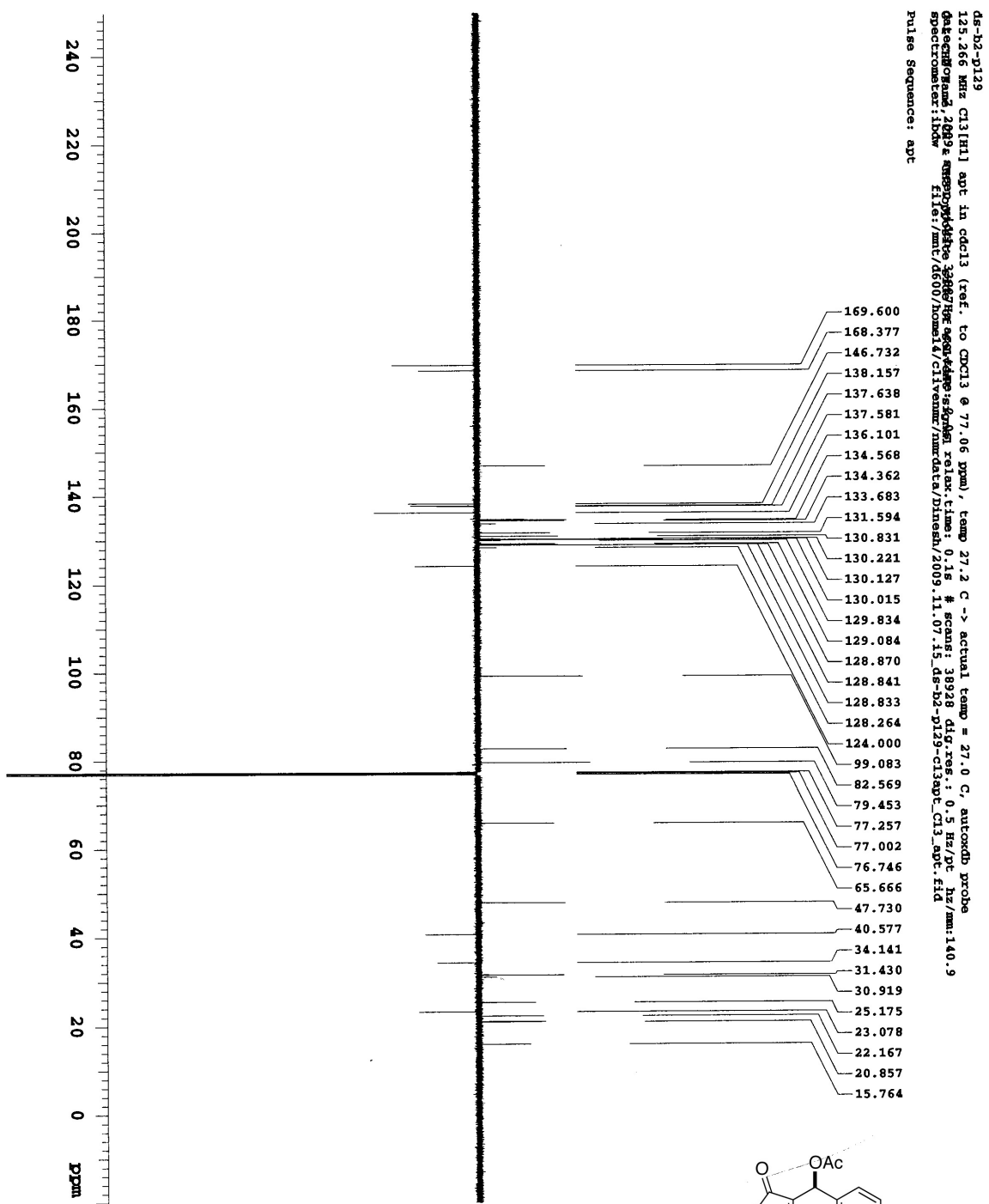




¹H NMR spectrum of 11b in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 27.2 °C -> actual temp = 27.0 °C, autoexdp probe

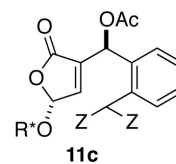
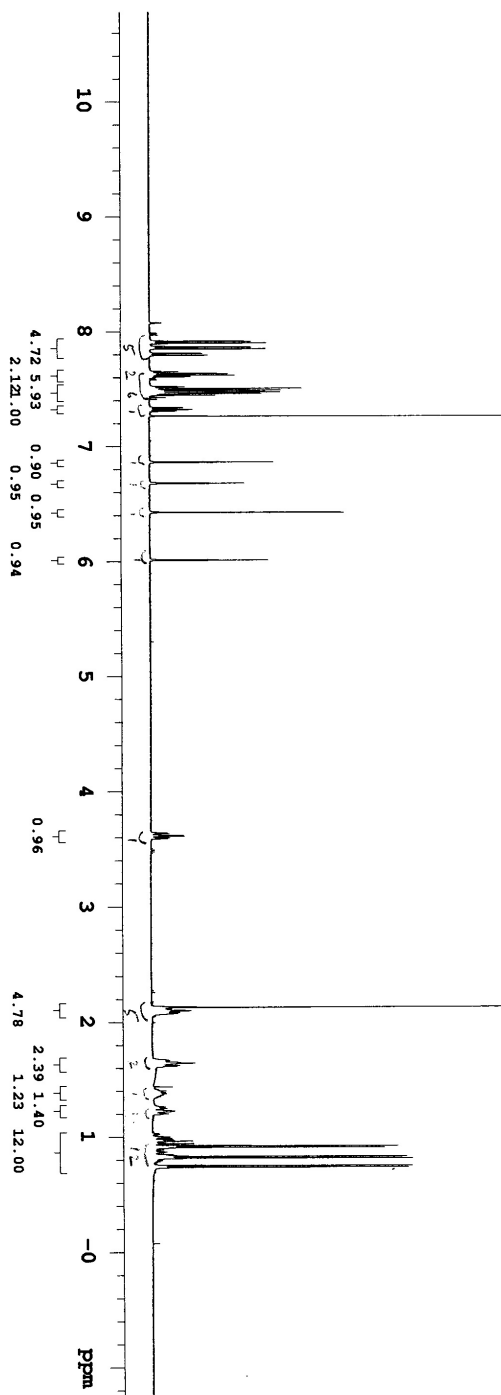
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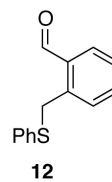
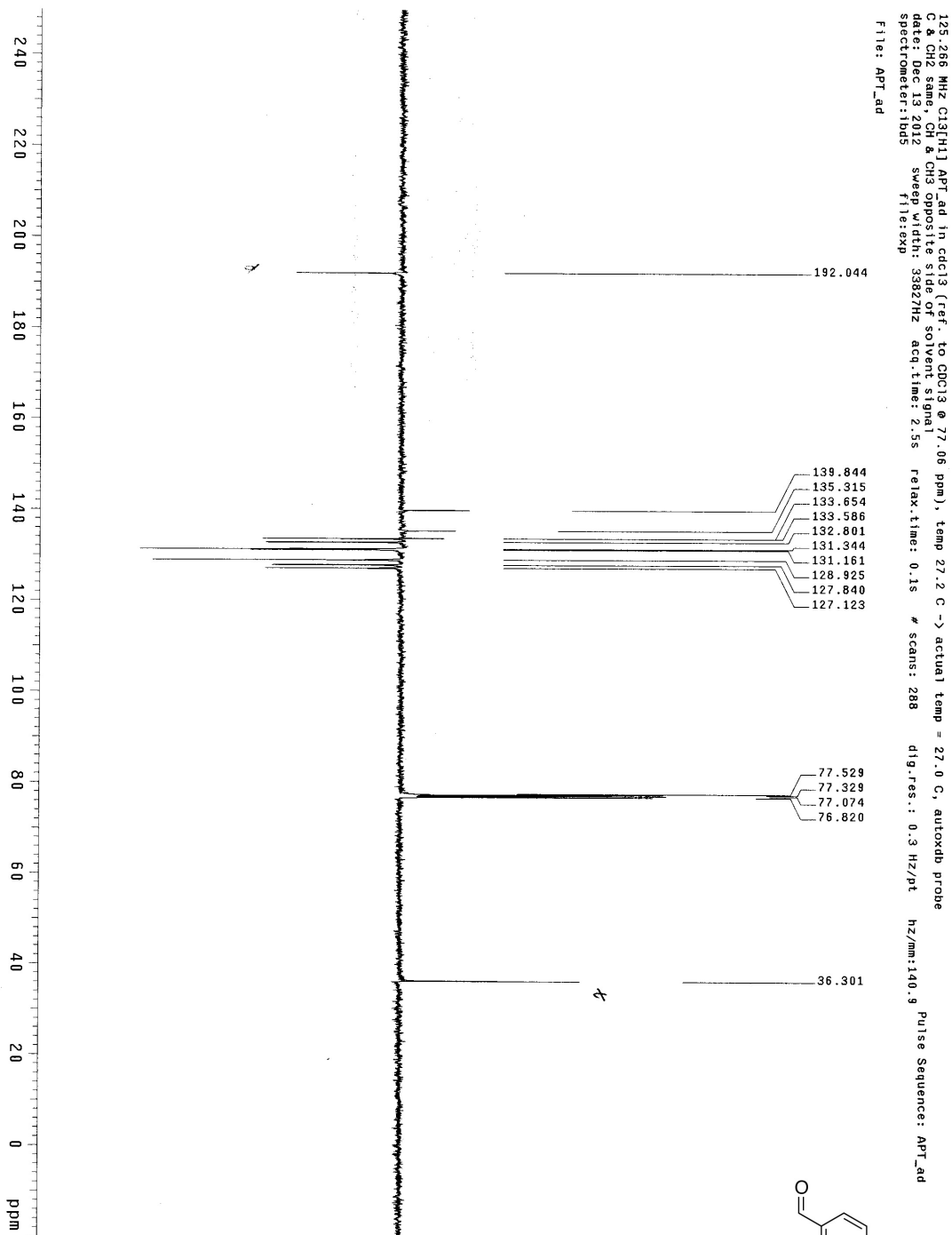




05-b2-129
498.122 MHz H1 D0 in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxorb probe

Pulse Sequence: s2pu1

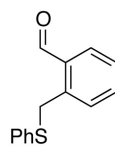




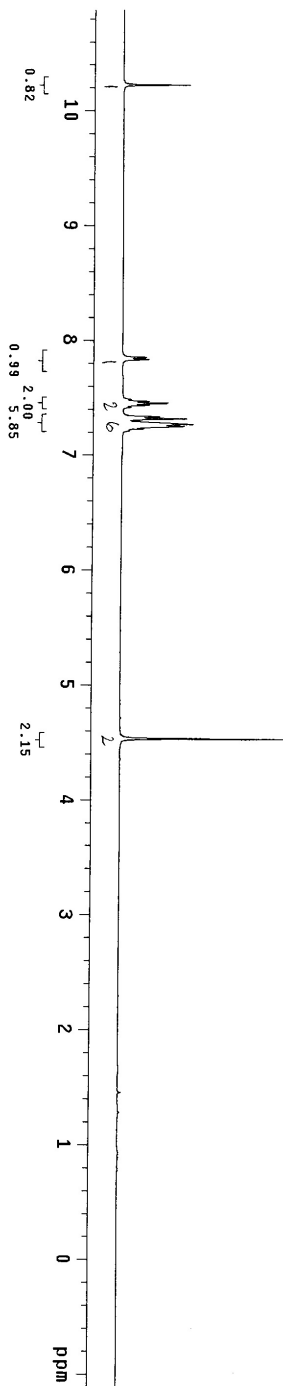
05-21

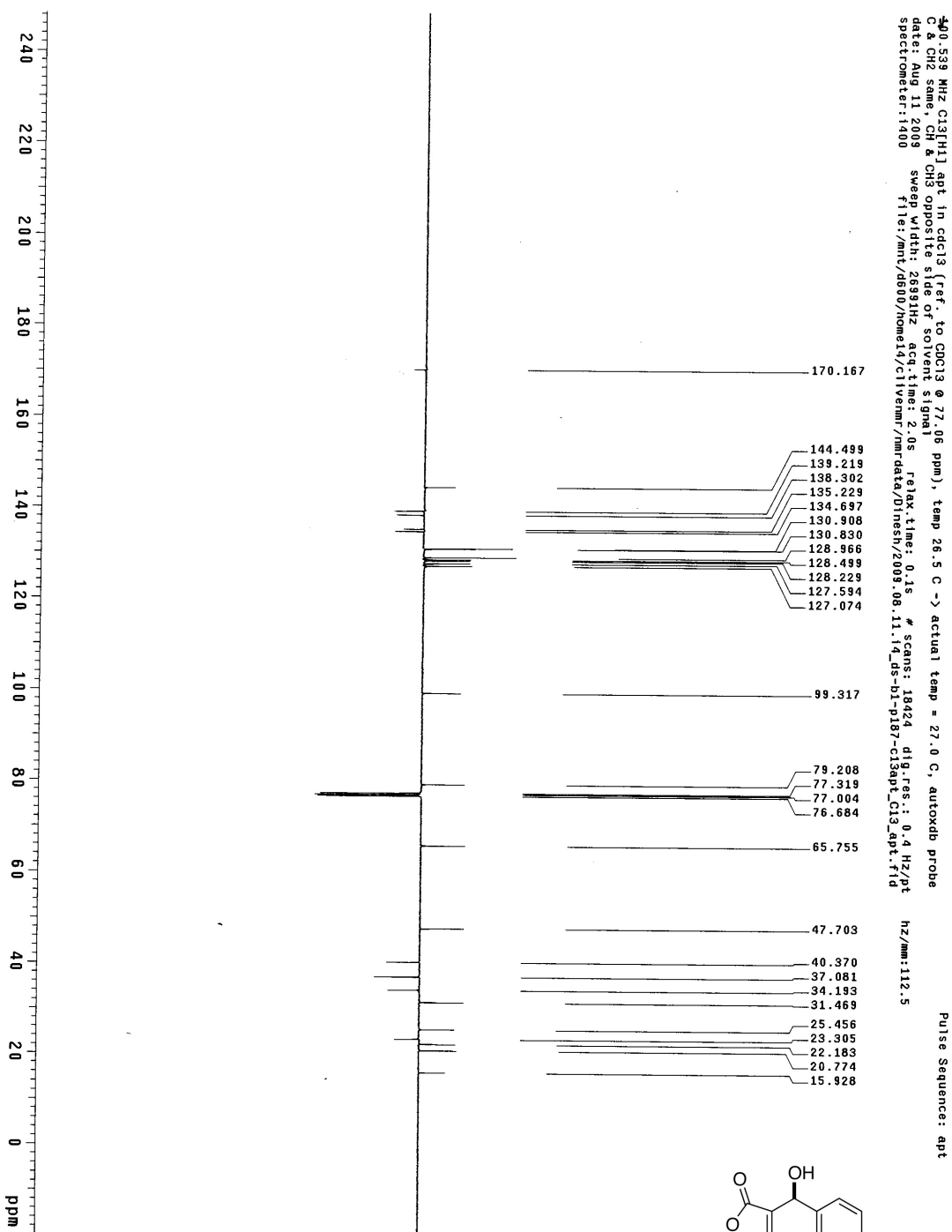
DS-B5-p121-a1d
399.794 MHz H1 1D 1h cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.0 C -> actual temp = 27.0 C, autotxdr probe
File: PROTON

Pulse Sequence: szpu1



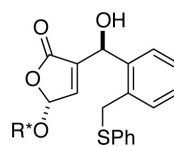
12



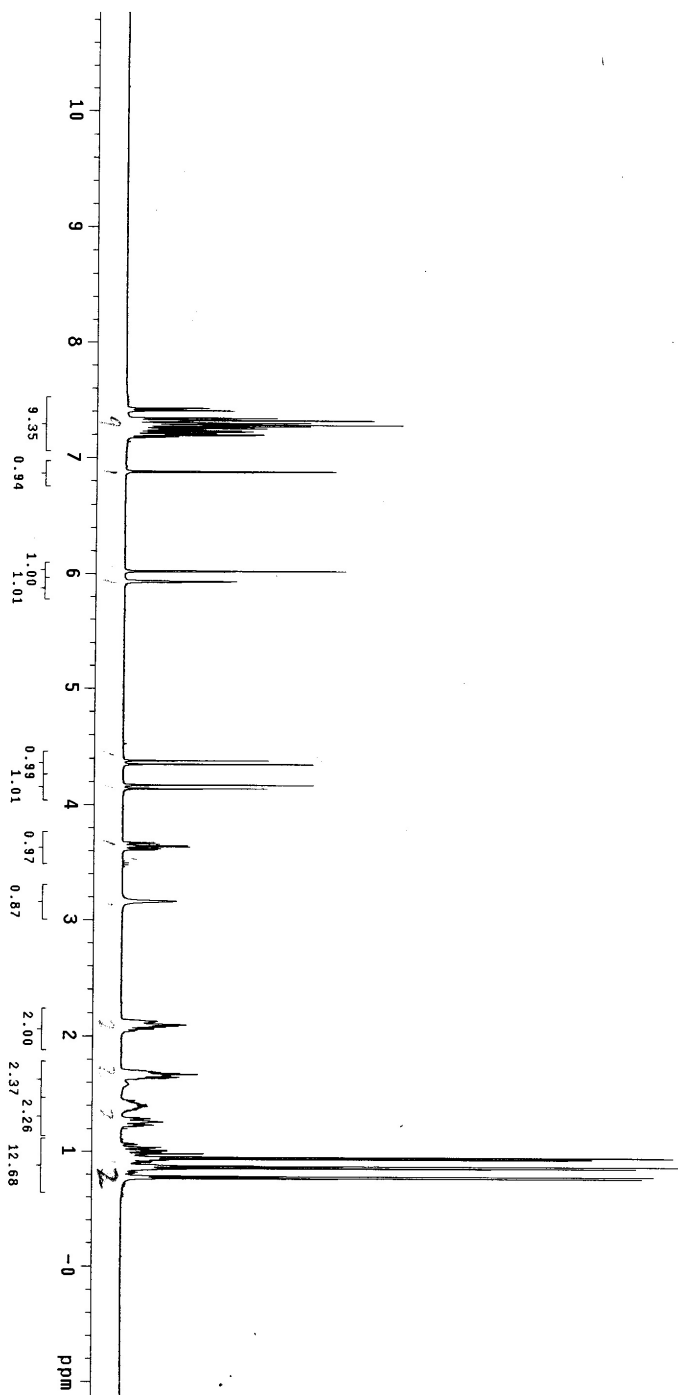


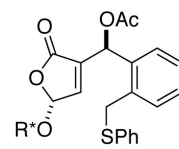
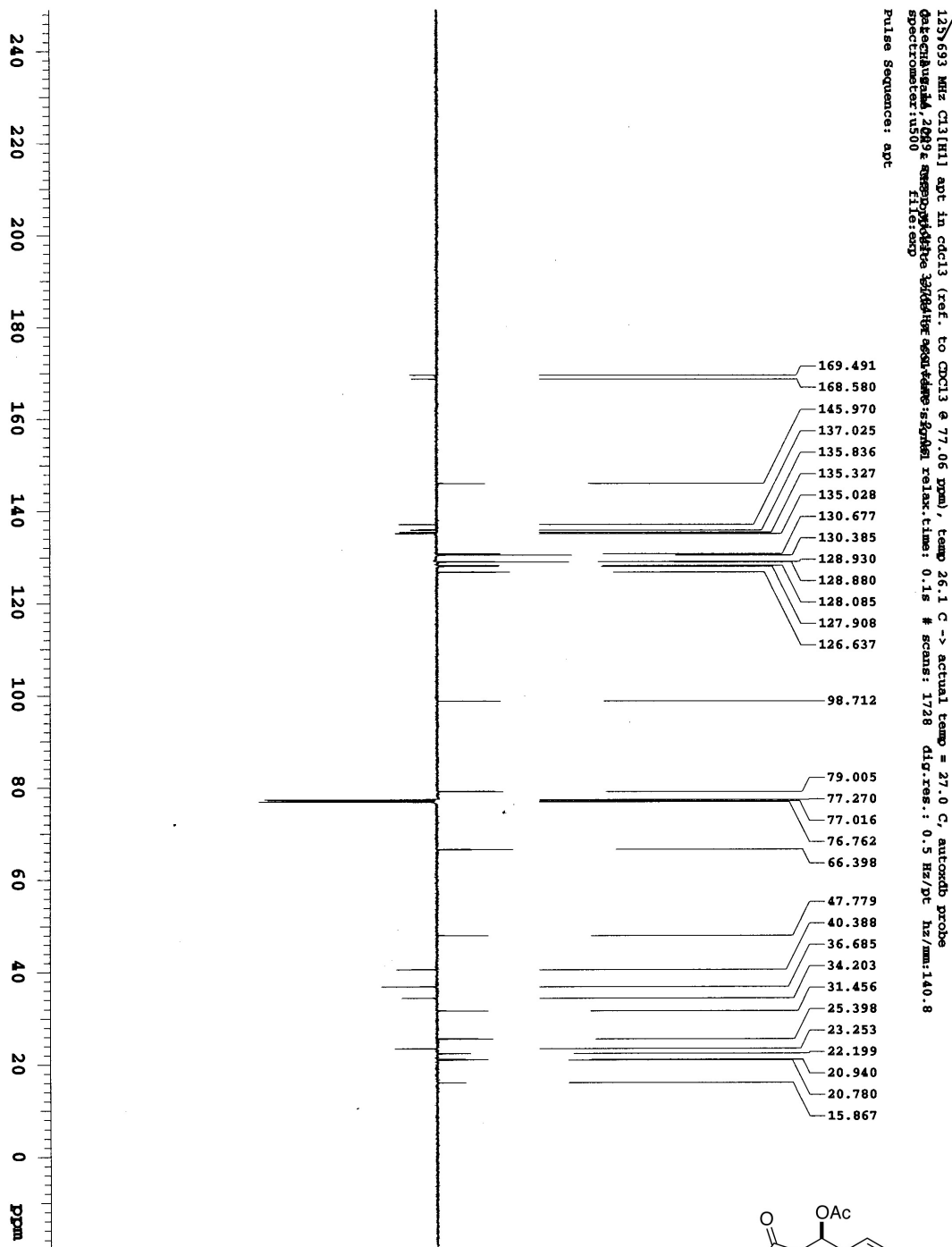
ds-b1-p187-f1-28
399.794 MHz H₁ 1D in cdcl3 (ref. to CDCl₃ @ 7.26 ppm), temp 26.5 C -> actual temp = 27.0 C, autokwd probe

Pulse Sequence: s2pu1



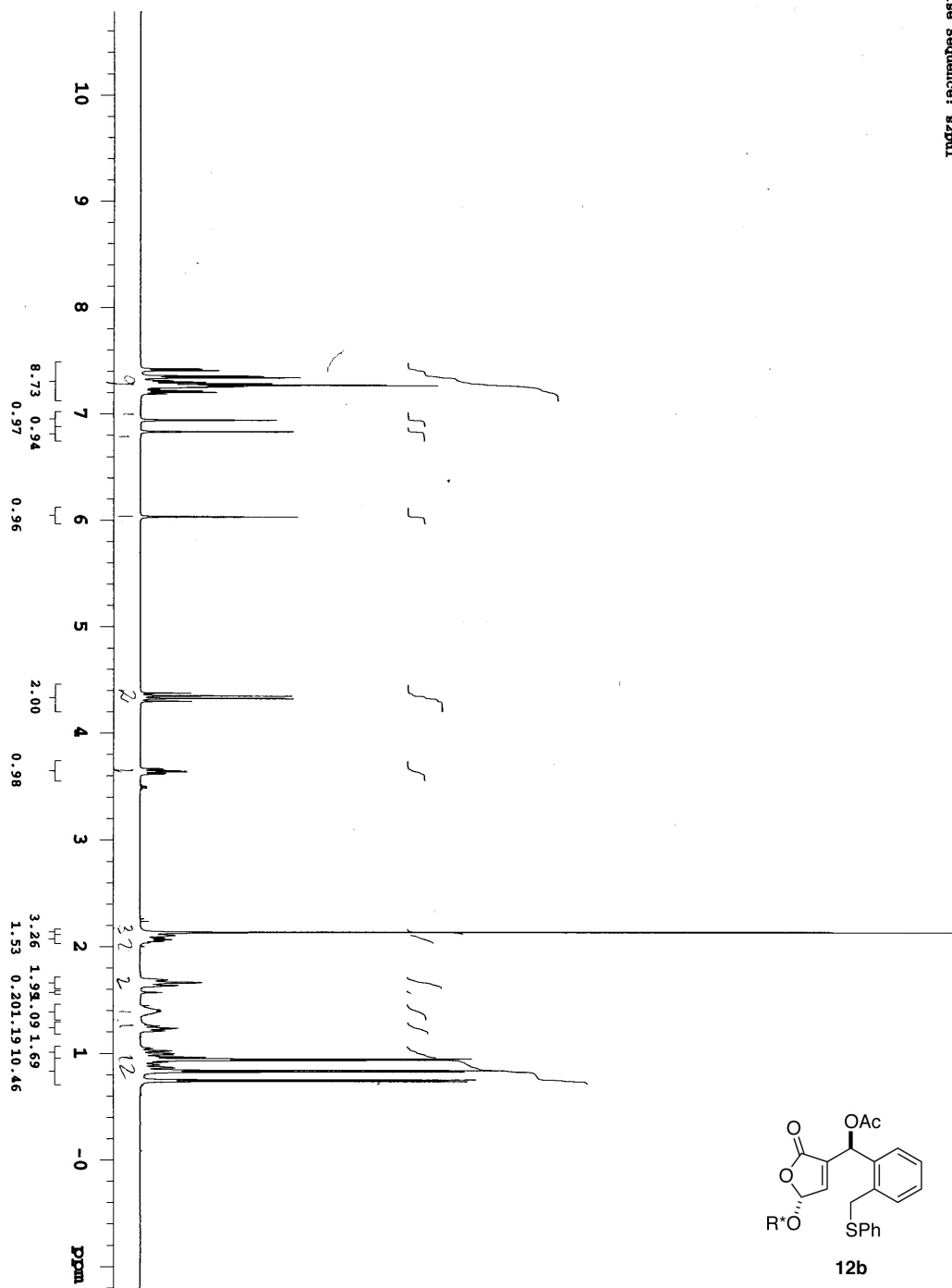
12a

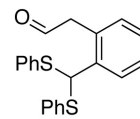
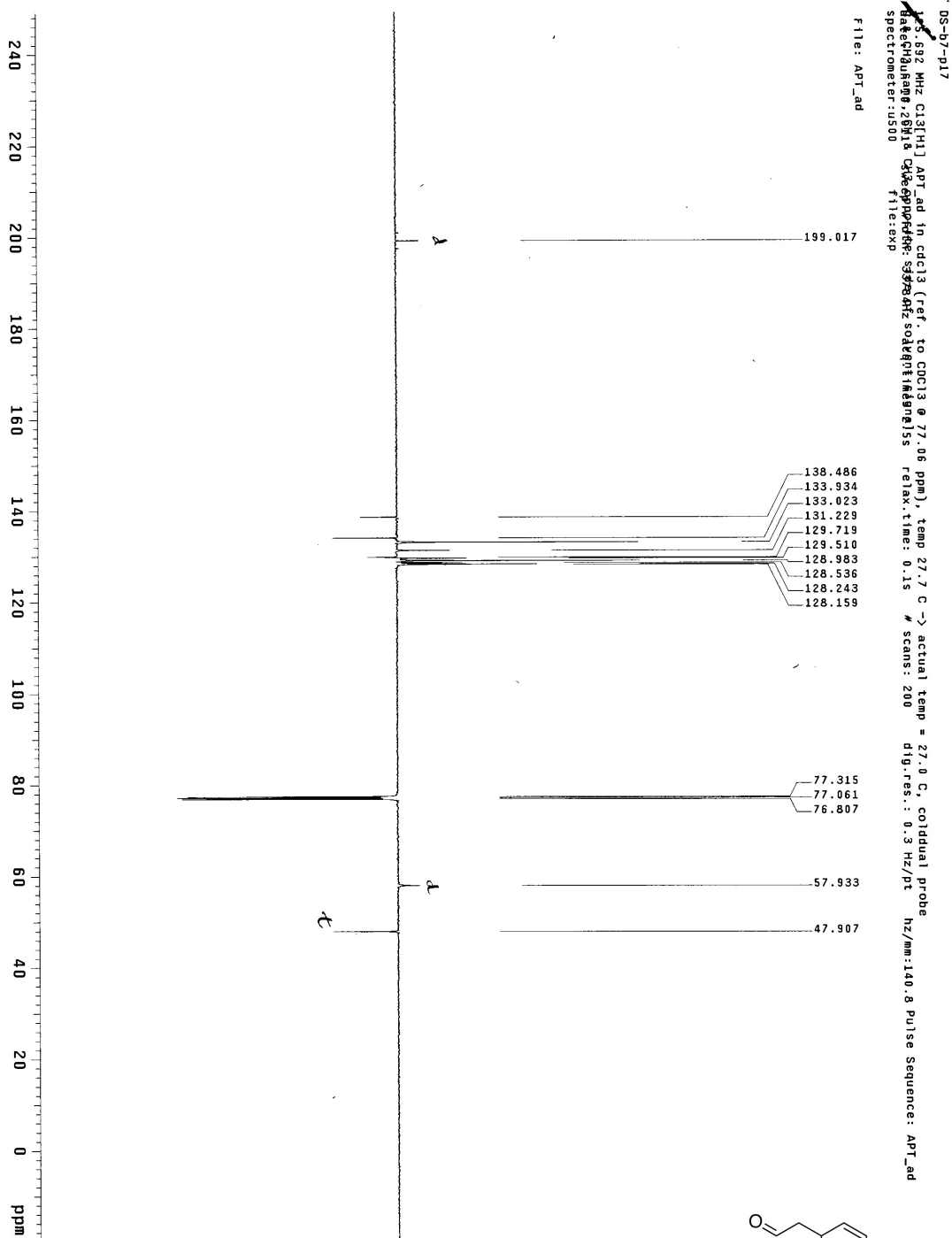


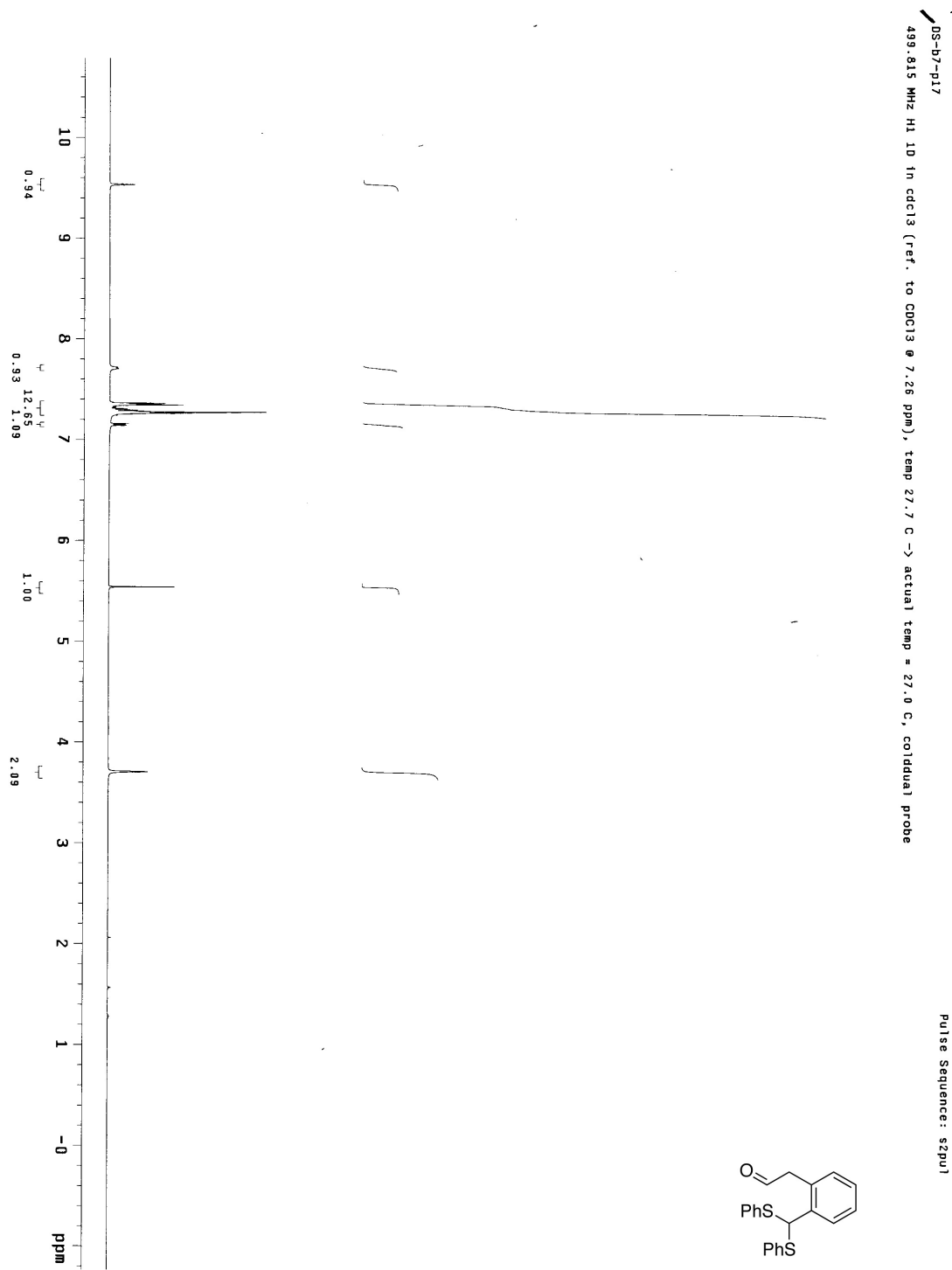


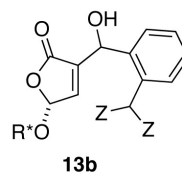
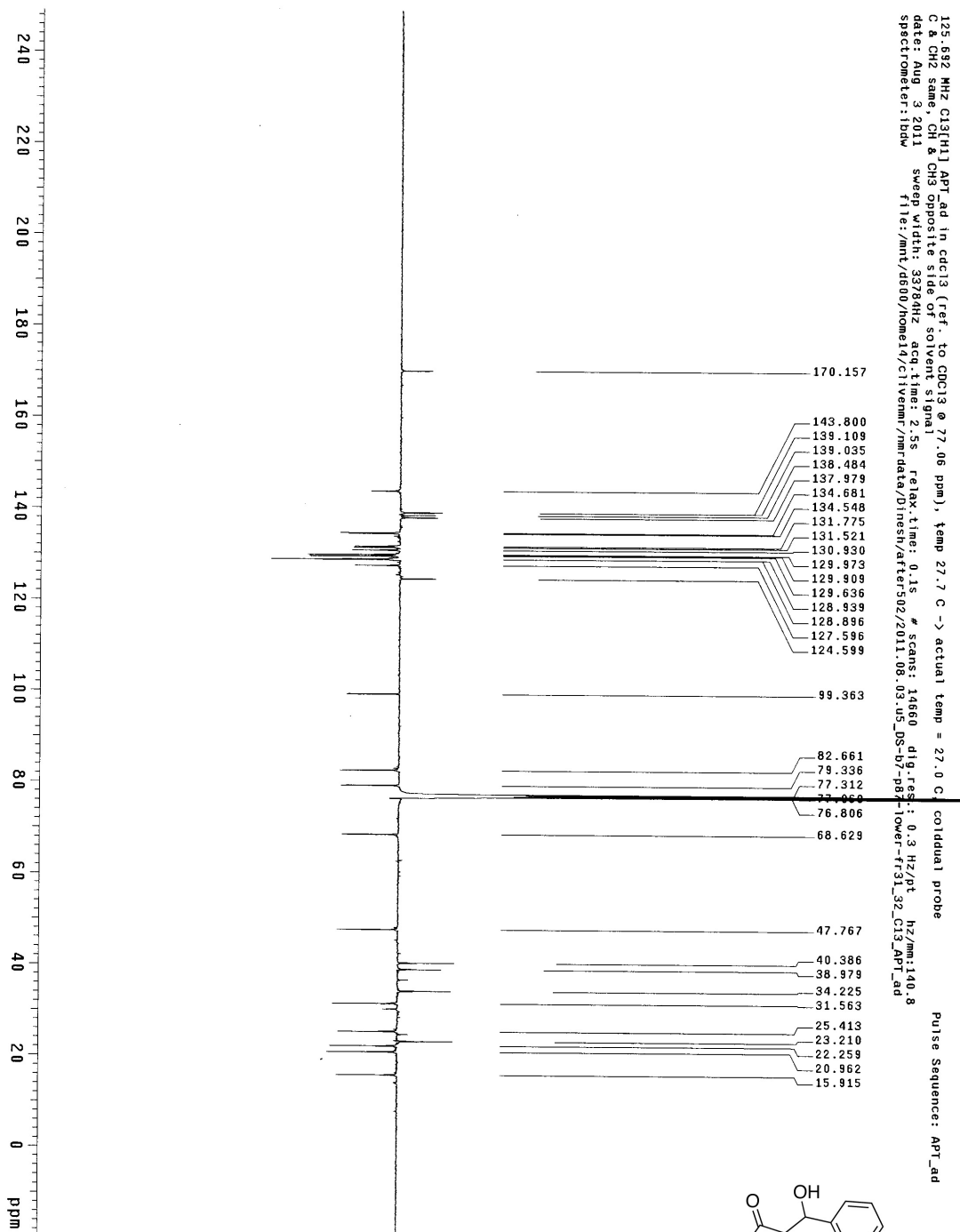
12b

4g-b1-p197-acylation
499.821 MHz H1 ID in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 26.1 C -> actual temp = 27.0 C, autoexdp probe
Pulse Sequence: s2pul



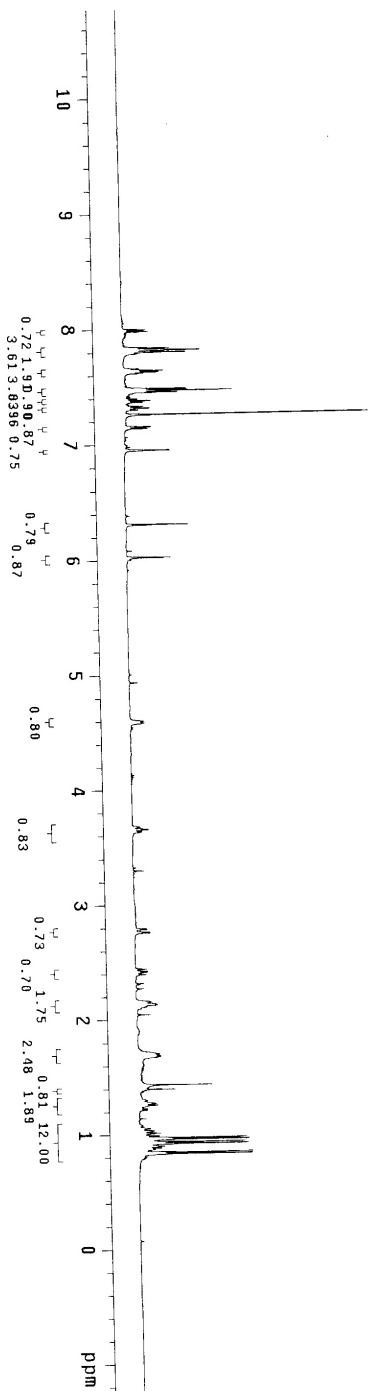
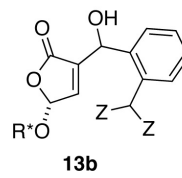


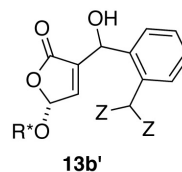
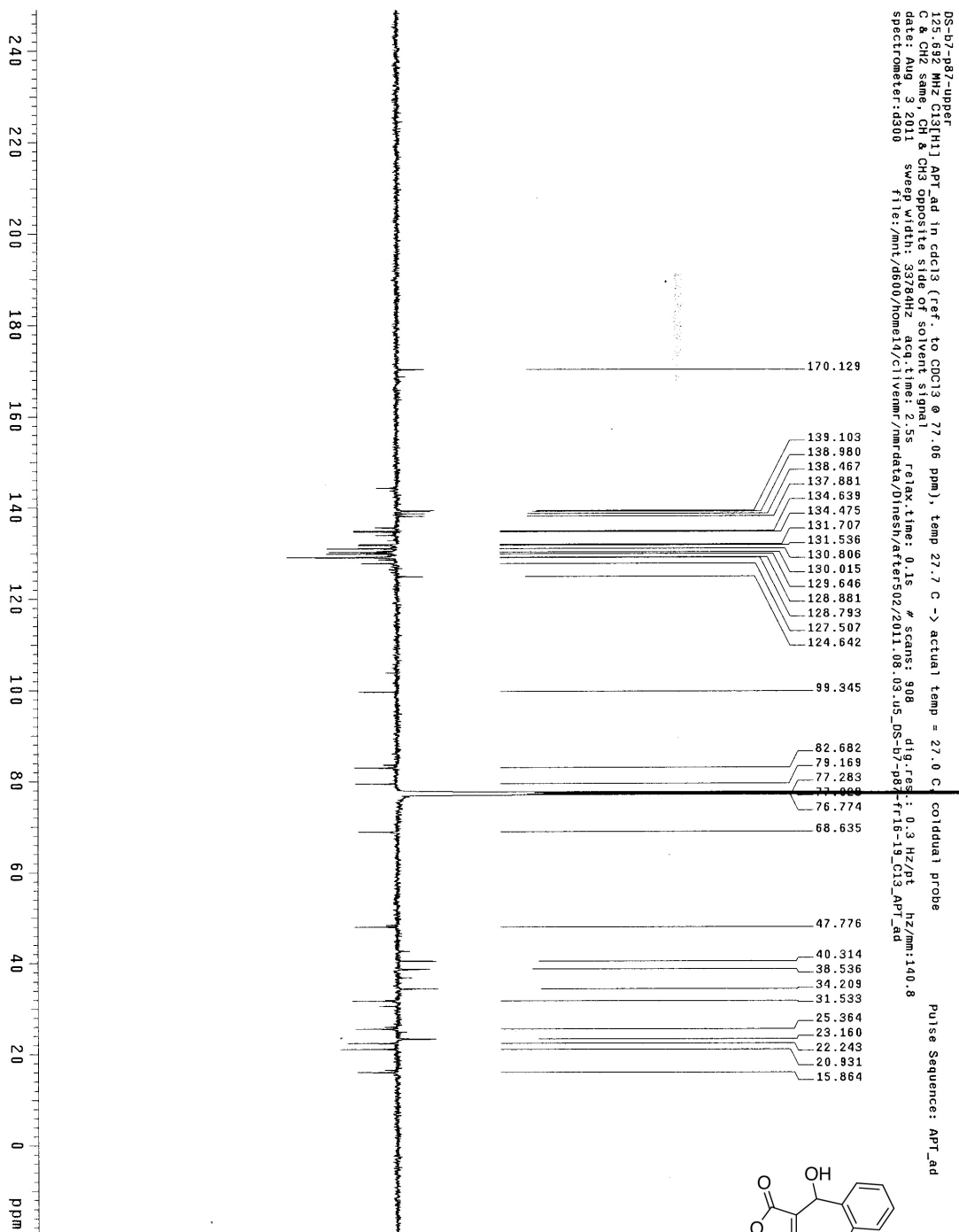




DS-b7-p87-fr29-32-10wvfr
499.815 MHz H1 1D In cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, coil(dua) probe

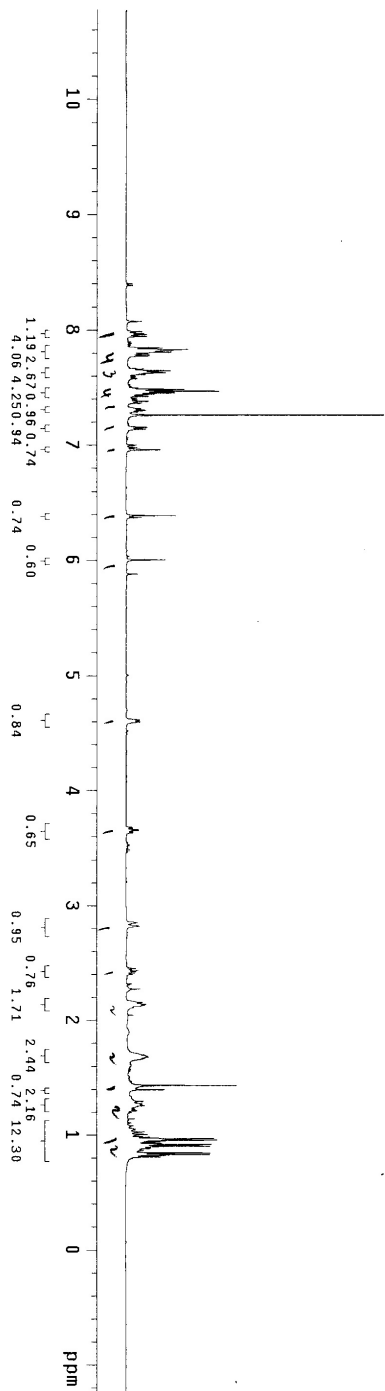
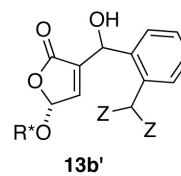
Pulse Sequence: szpu1

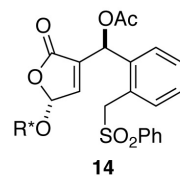
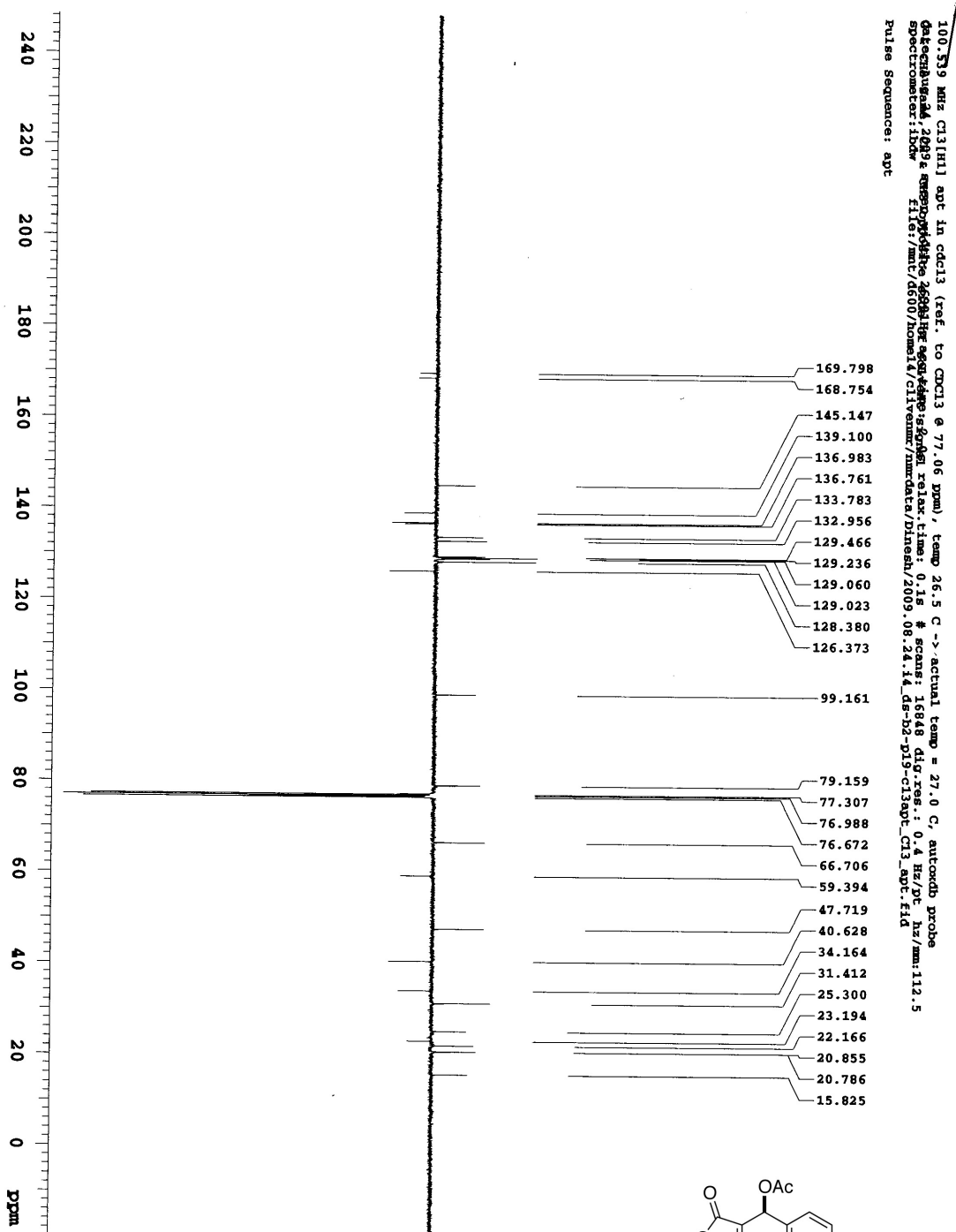




DS-h7-p87-upper-f16_19
499.815 MHz H1 1D 1h cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.7 C -> actual temp = 27.0 C, cotidual probe

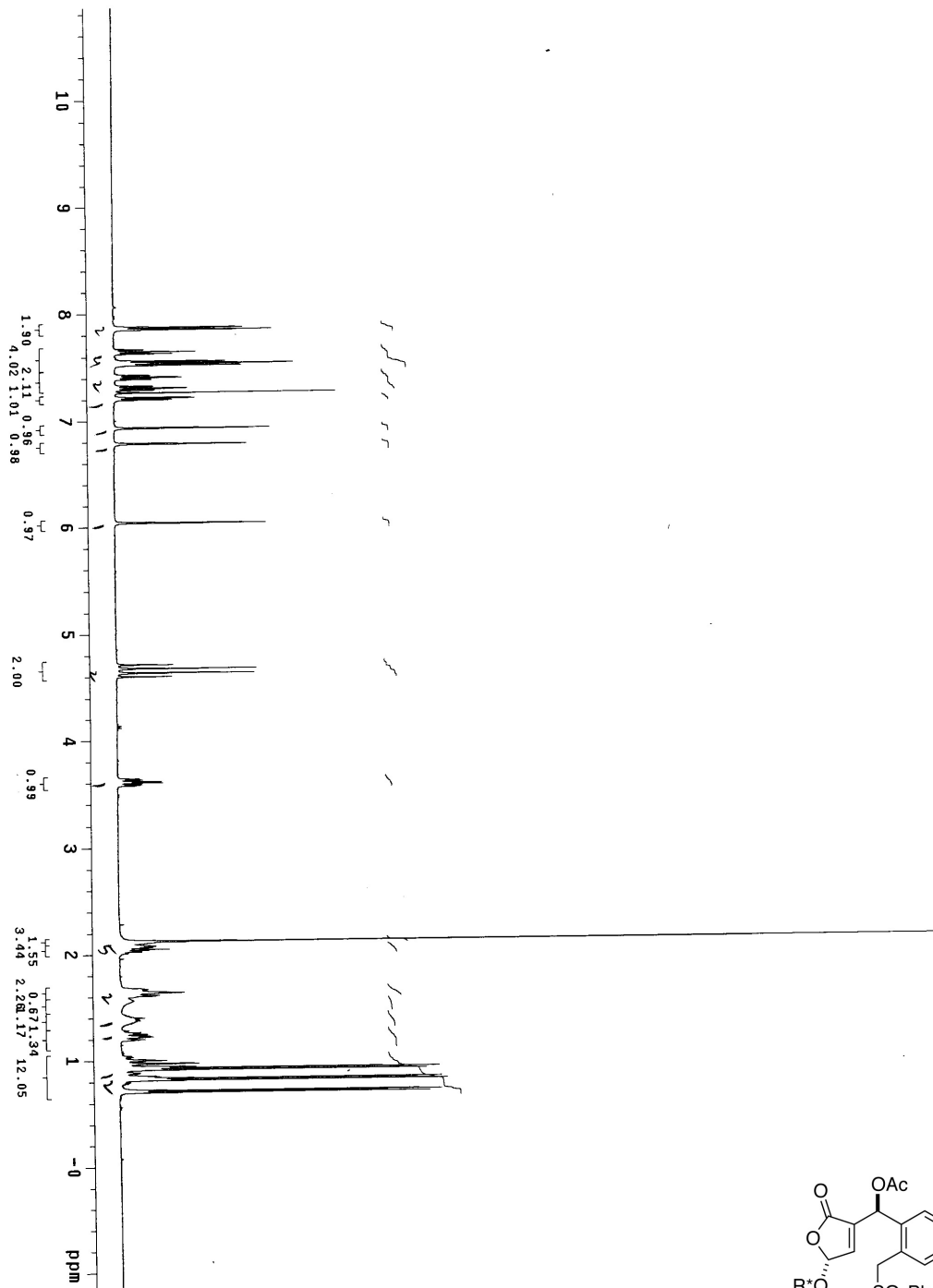
Pulse Sequence: s2pul

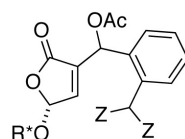
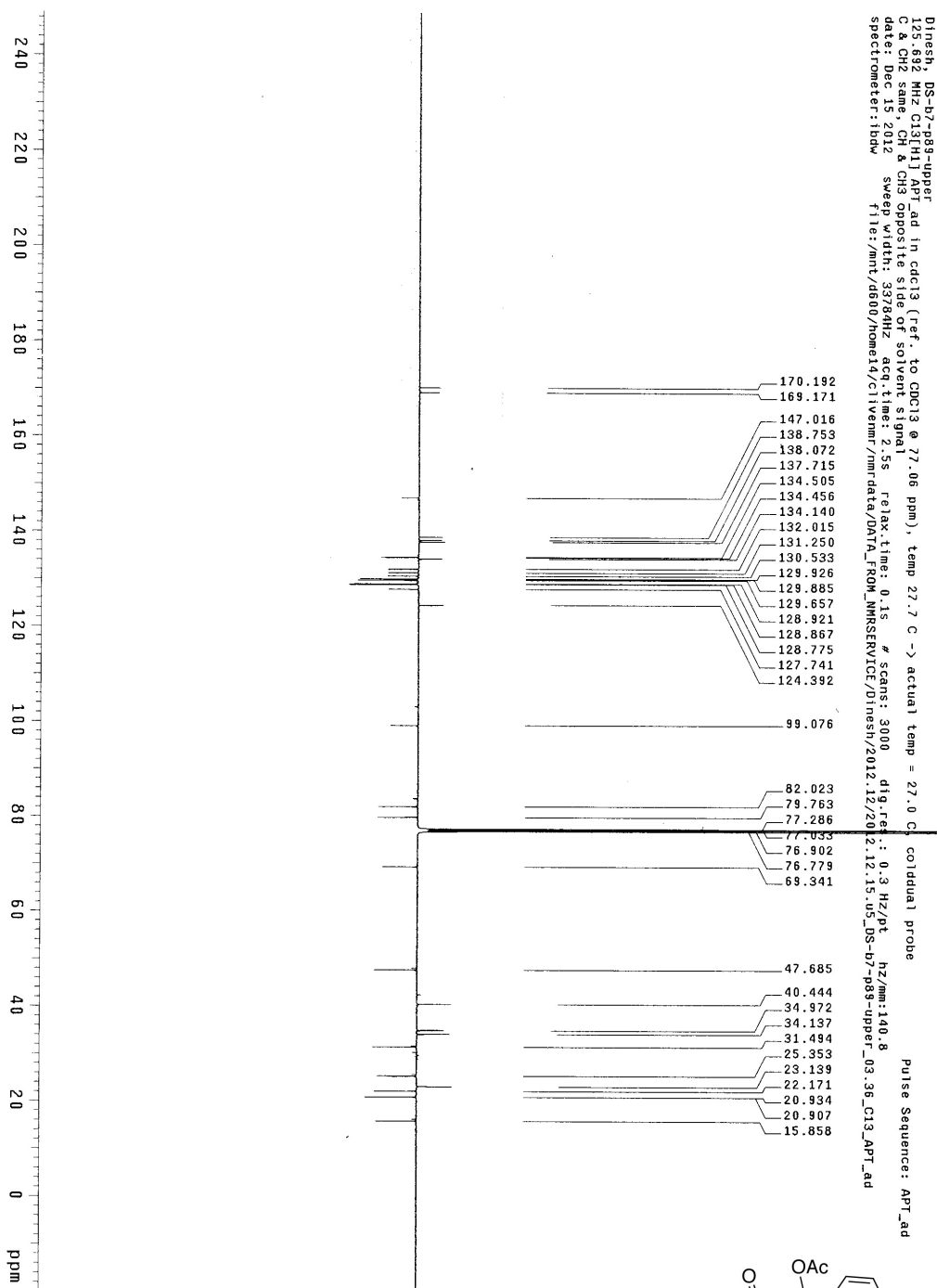




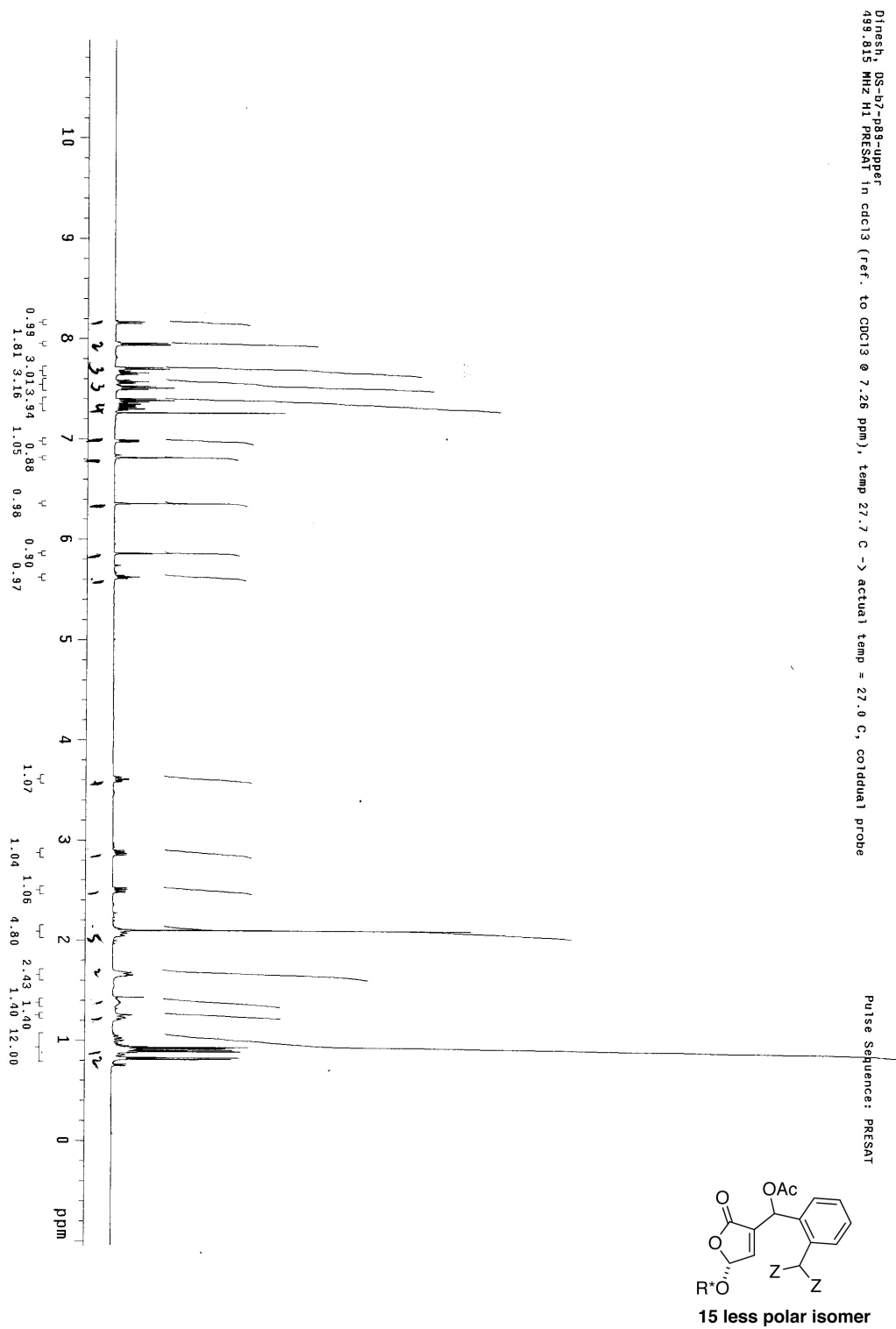
ds-12-119
-244.794 MHz ¹H 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 26.5 C -> actual temp = 27.0 C, autotxdr probe

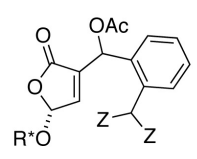
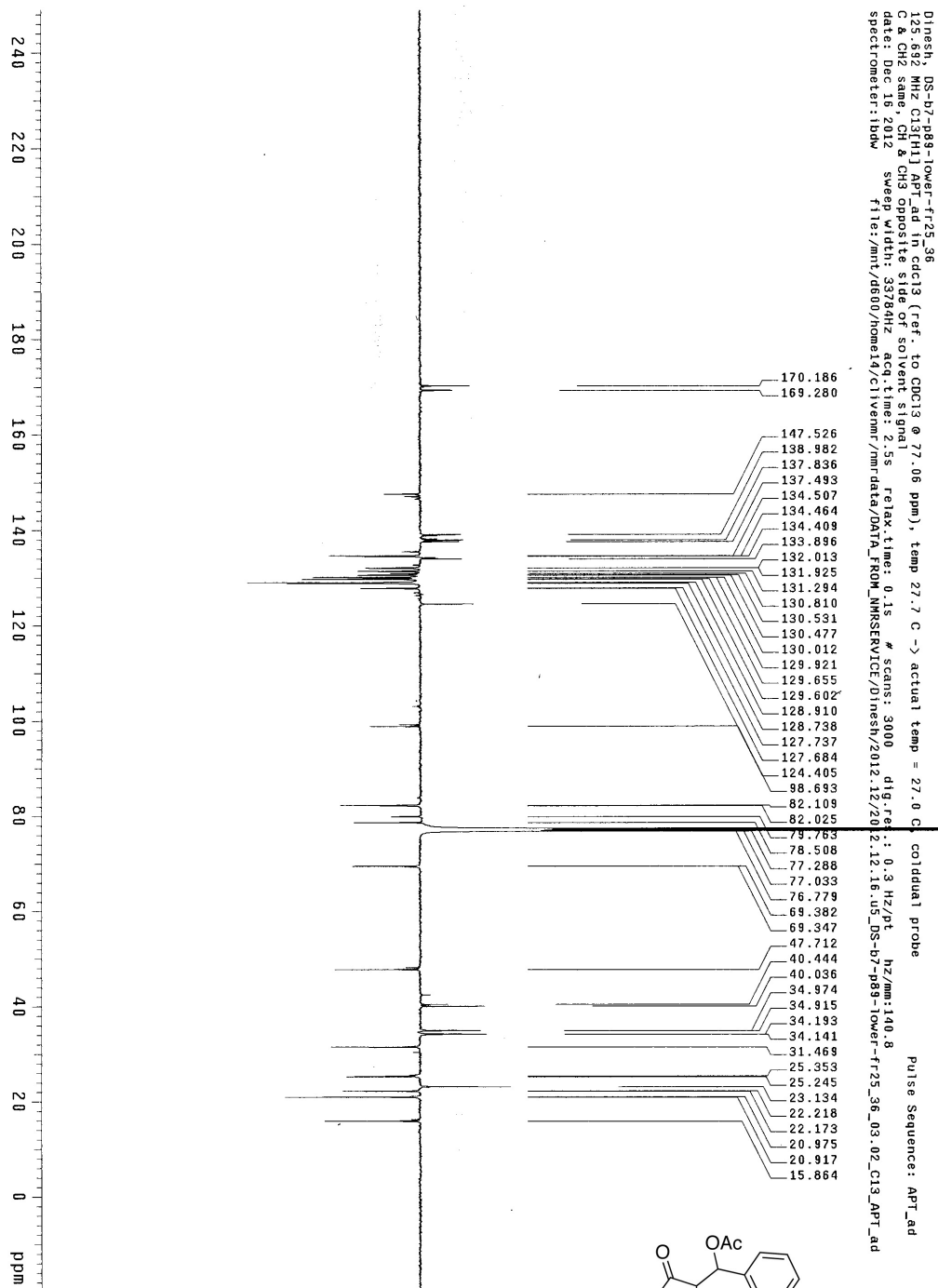
Pulse Sequence: s2pul1





15 less polar isomer



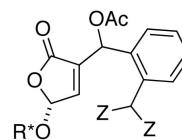
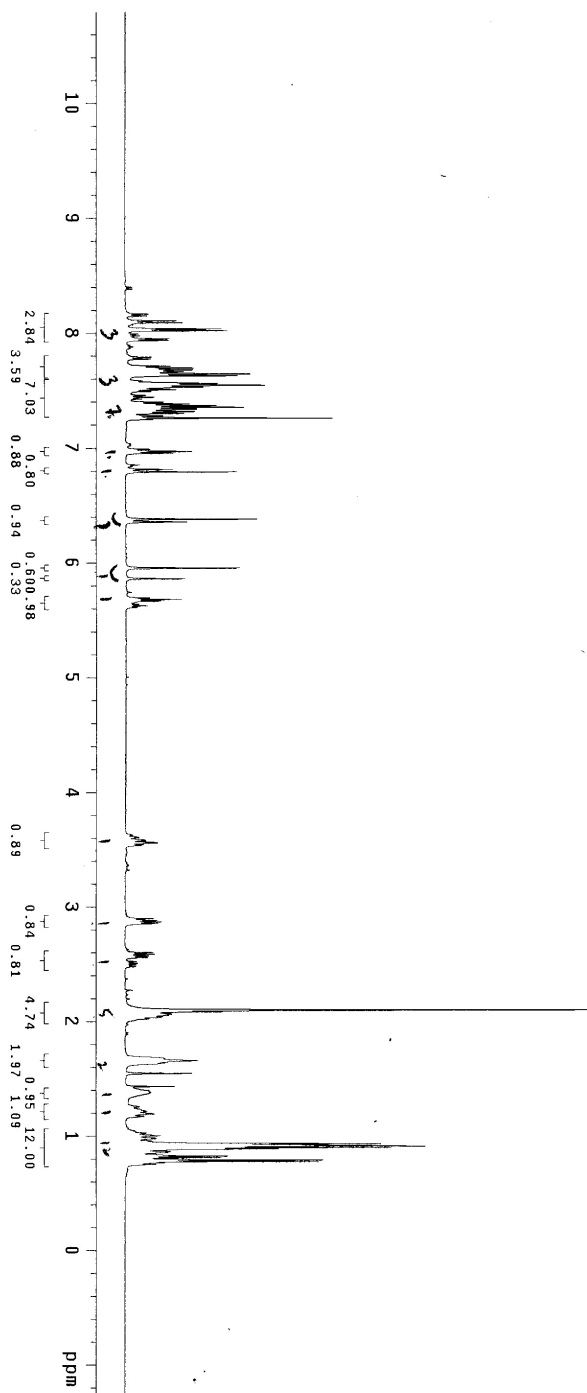


15 mixture of isomers

DS-b7-p89-lower-fr25-36
498.118 MHz T1 10 in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 27.2 C -> actual temp = 27.0 C, autoxddd probe

File: PROTON

Pulse Sequence: szpu1



15 mixture of isomers