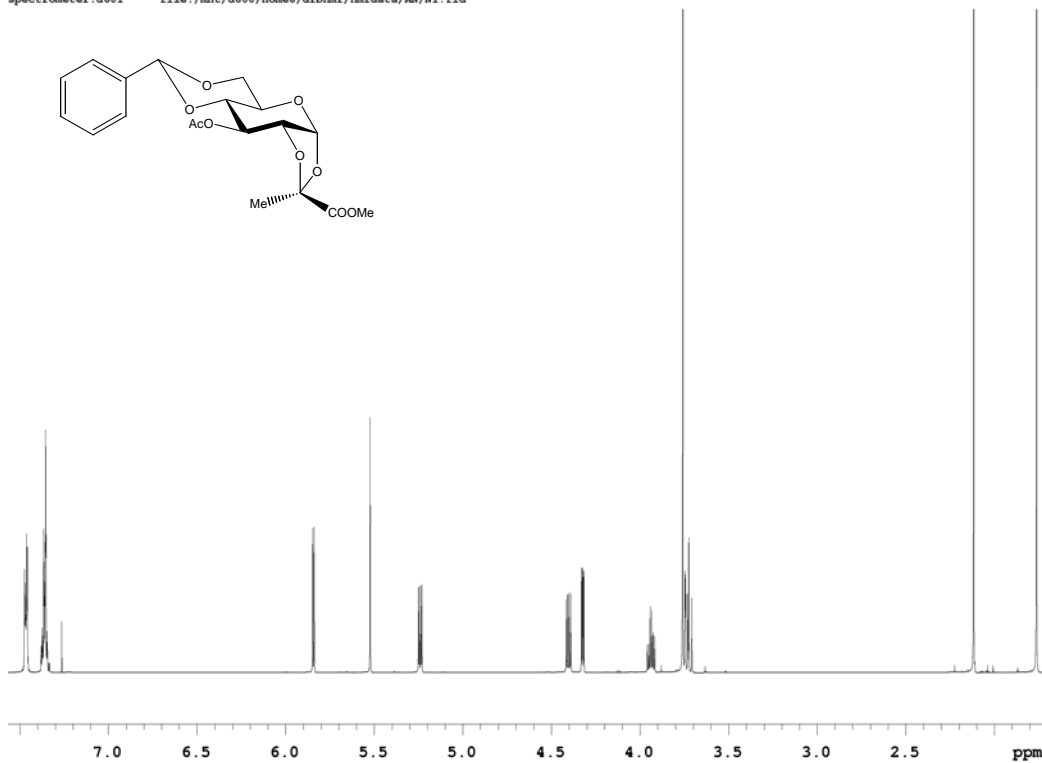


Appendix

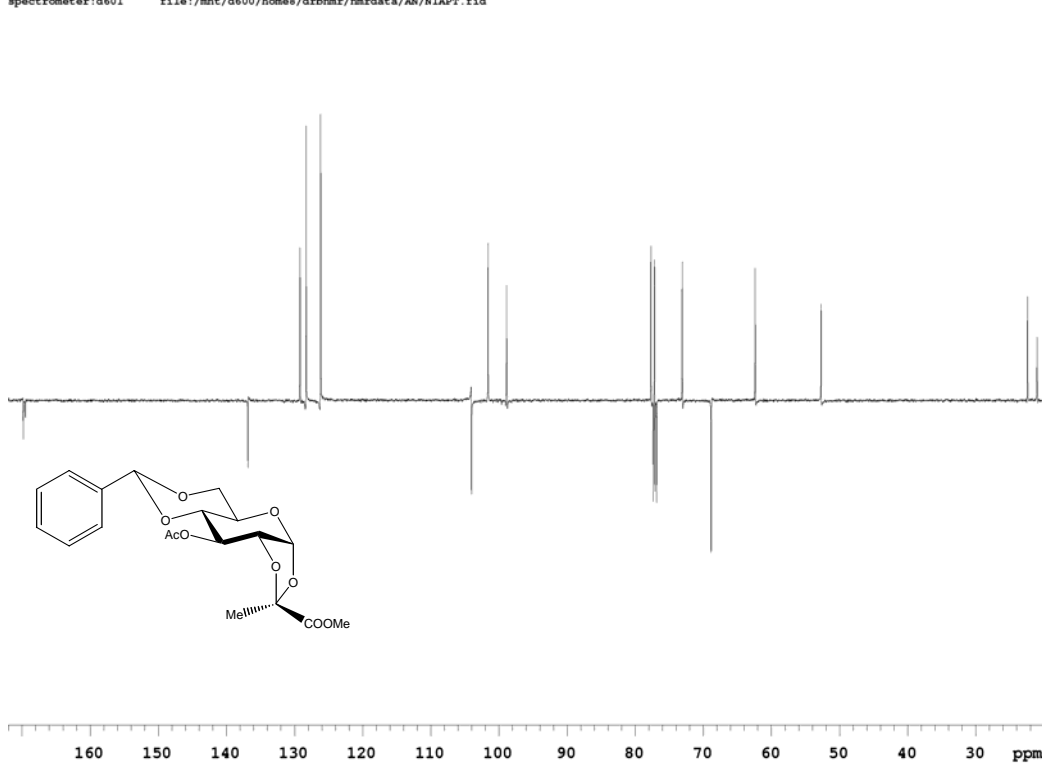
***In Vivo* Supramolecular Templating Enhances the Activity of Multivalent Ligands:
A potential therapeutic against the E. coli O157 AB₅ toxins**

Pavel I. Kitov,¹ George L. Mulvey,² Thomas P. Griener,² Tomasz Lipinski,¹ Dmitry Solomon,¹ Eugenia Paszkiewicz,¹ Jared M. Jacobson,¹ Joanna M. Sadowska,¹ Missao Suzuki,³ Ken-ichi Yamamura³, Glen D. Armstrong,² and David R. Bundle¹

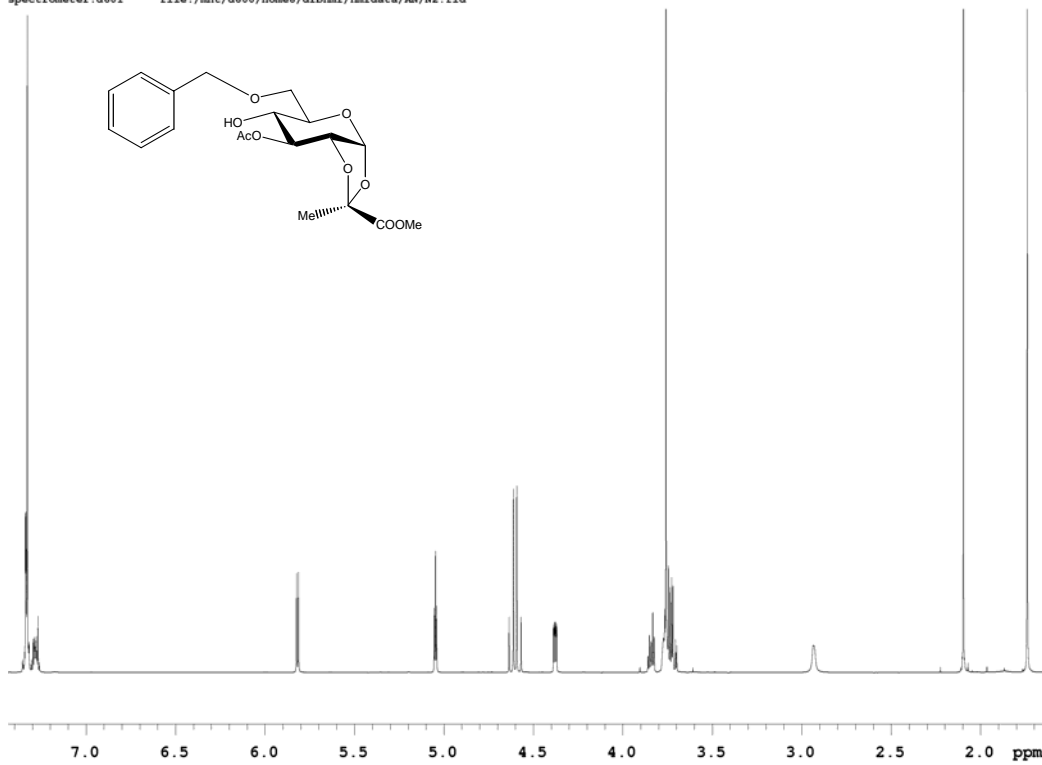
date: Oct 15 2007 sweep width: 7201Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:14.7
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N1.fid



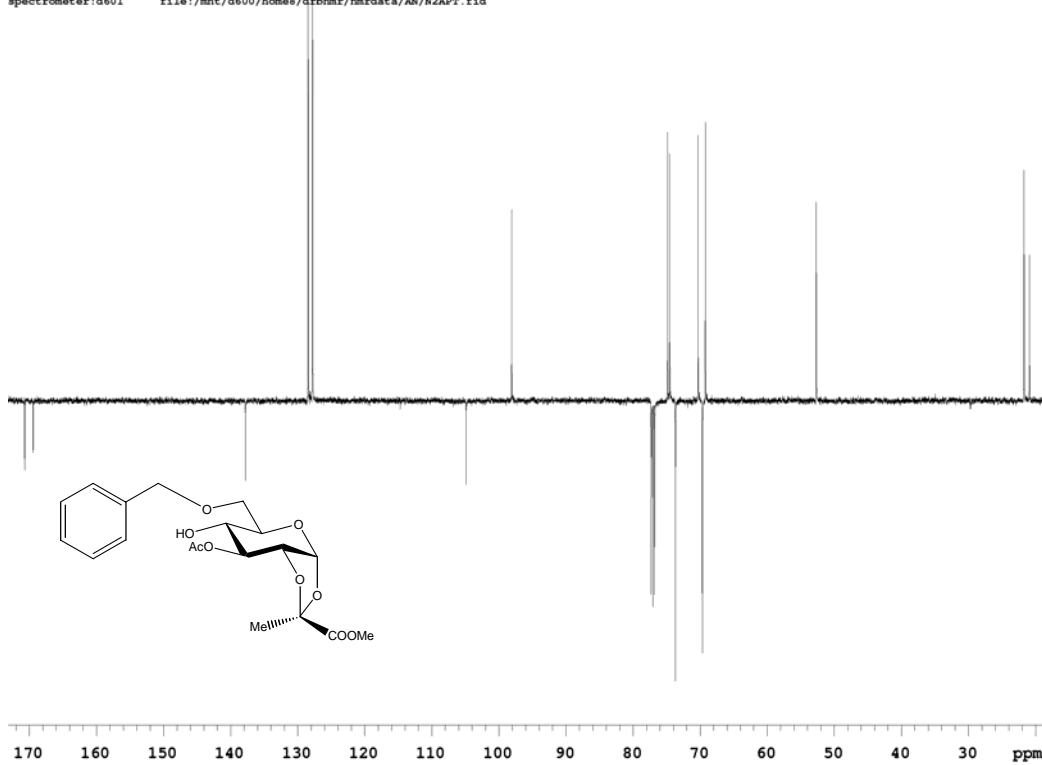
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Oct 12 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 1072 dig.res.: 0.5 Hz/pt hz/mm:80.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N1APT.fid



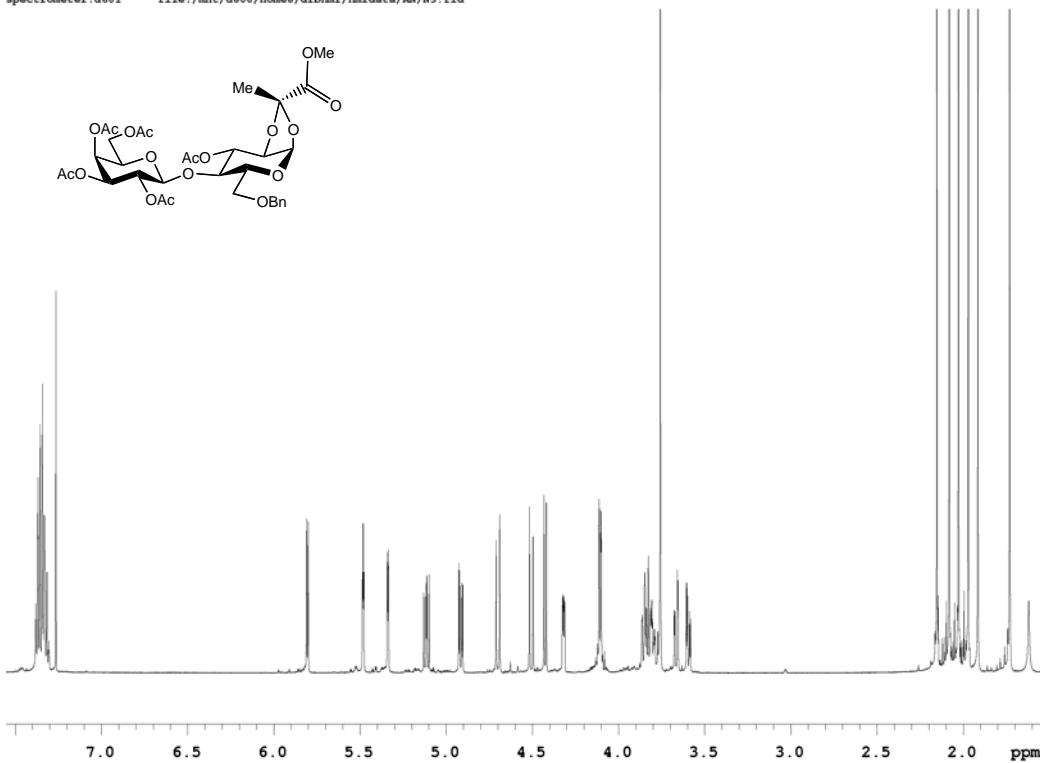
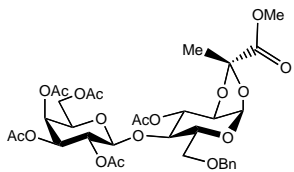
date: Oct 10 2007 sweep width: 6010Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:12.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N2.fid



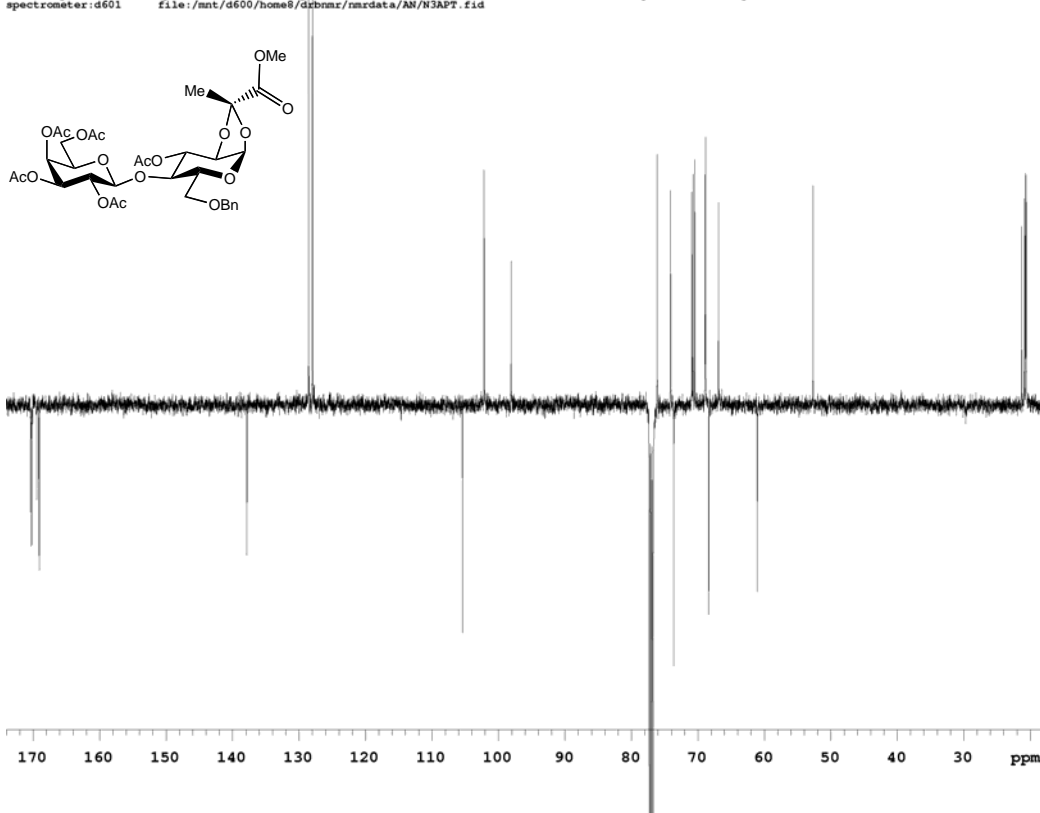
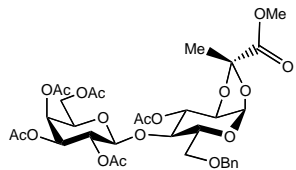
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Oct 17 2007 sweep width: 33827Hz acq.time: 2.0s relax.time: 0.1s # scans: 1160 dig.res.: 0.5 Hz/pt hz/mm:81.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N2APT.fid



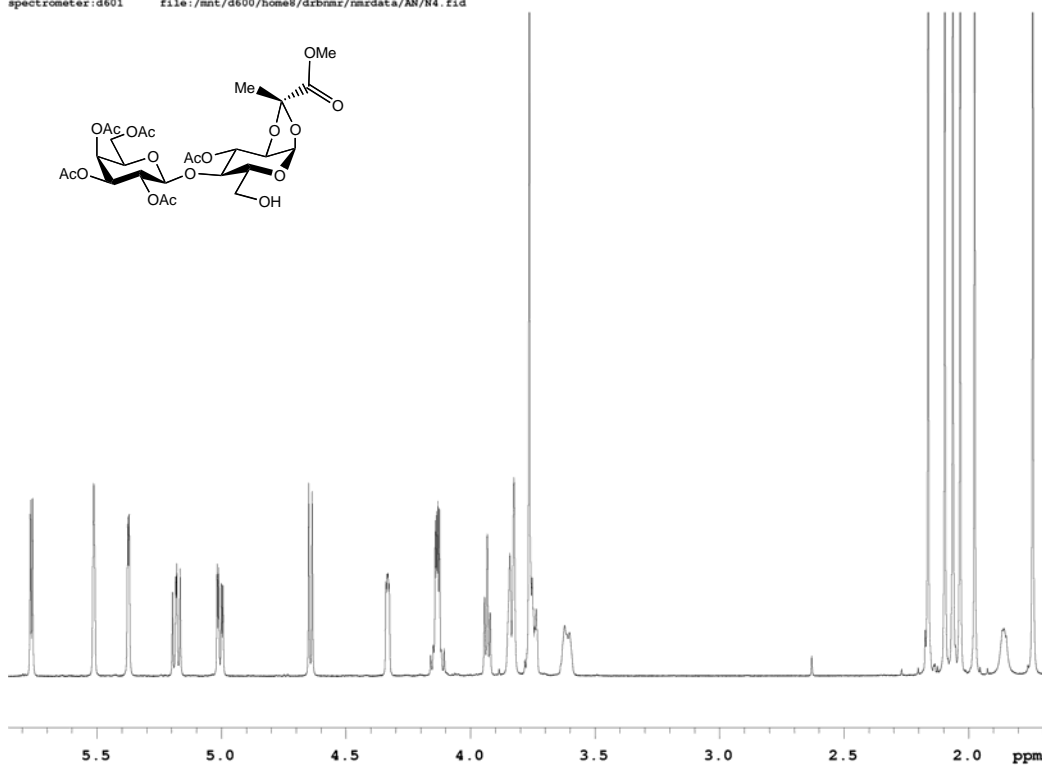
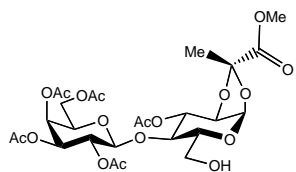
date: Oct 15 2007 sweep width: 7201Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:15.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N3.fid



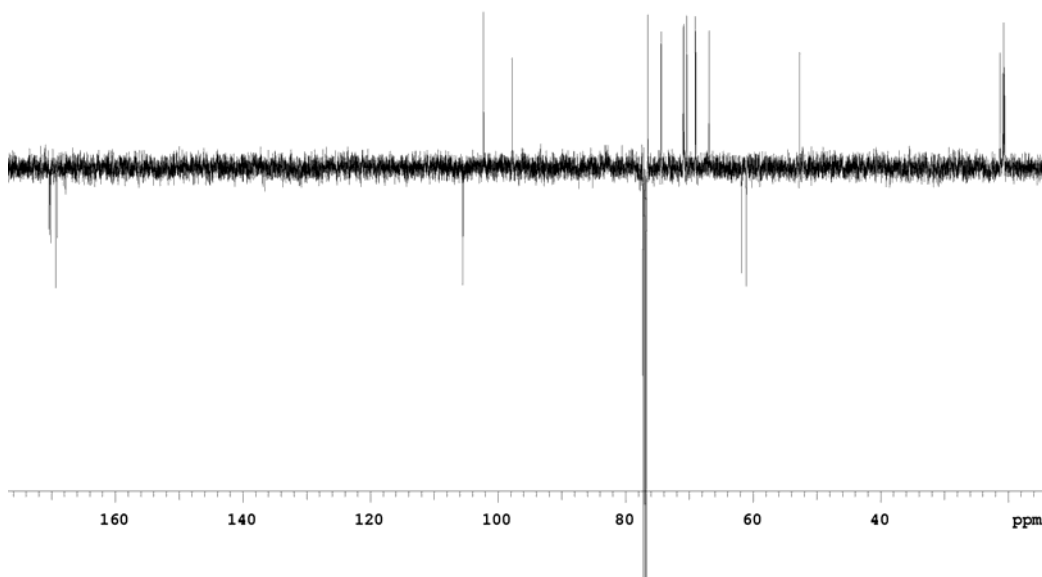
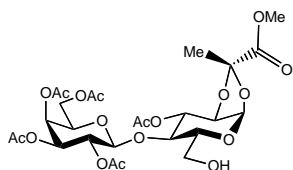
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Sep 18 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 27592 dig.res.: 0.5 Hz/pt hz/mm:82.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N3APT.fid



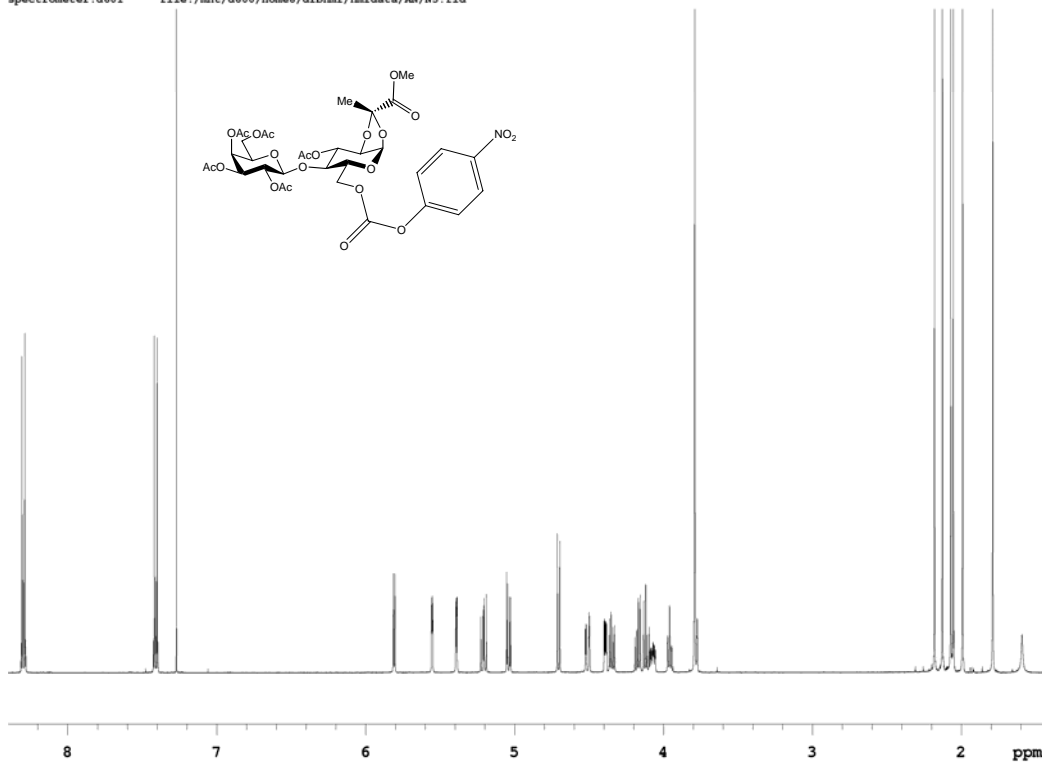
date: Oct 15 2007 sweep width: 7201Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:10.5
spectrometer:d601 file:/mnt/d600/home8/drbnmr/nmrdata/AN/N4.fid



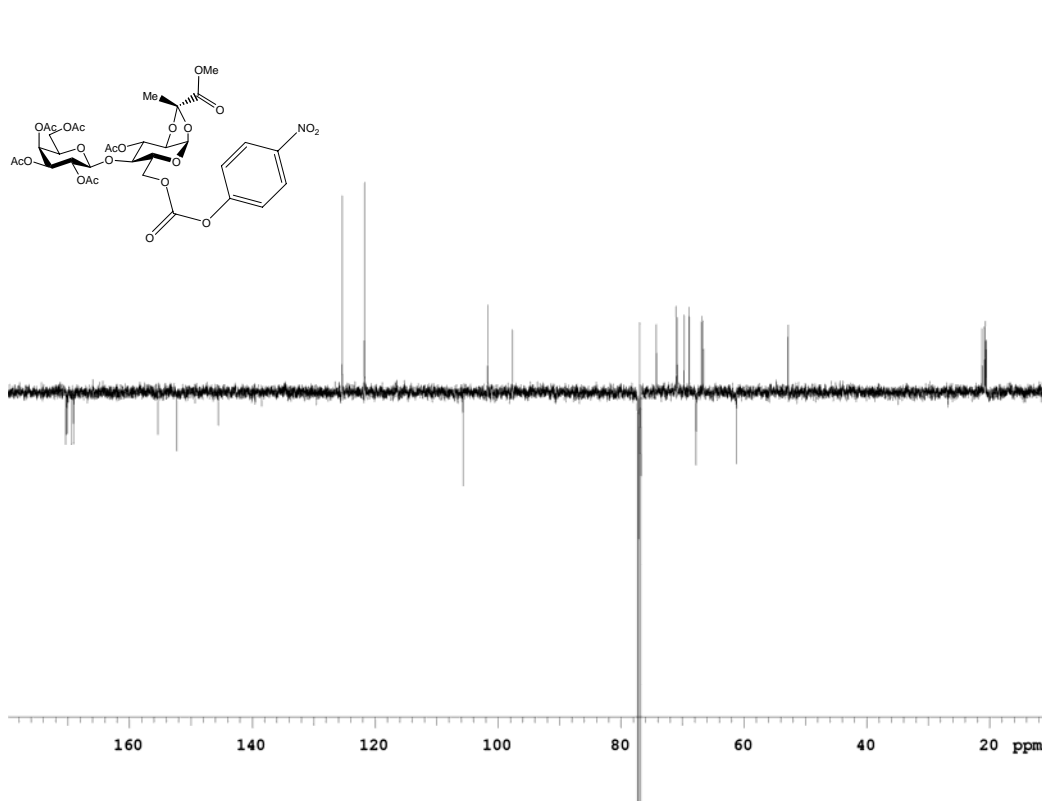
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Sep 16 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 608 dig.res.: 0.5 Hz/pt hz/mm:85.5
spectrometer:d601 file:/mnt/d600/home8/drbnmr/nmrdata/AN/N4APT.fid



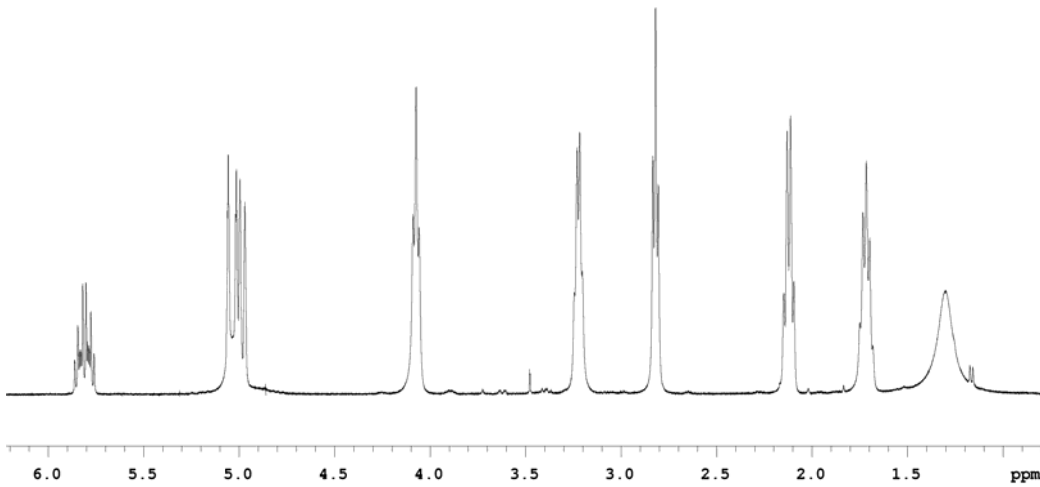
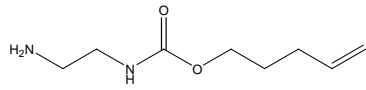
date: Sep 21 2007 sweep width: 6010Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:14.6
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N5.fid



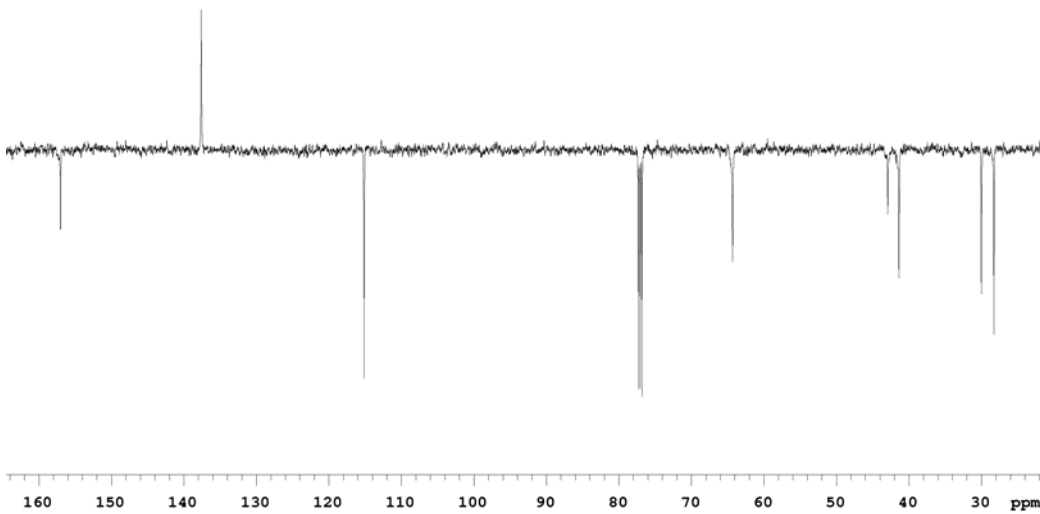
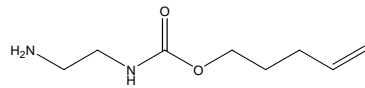
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Sep 21 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 200 dig.res.: 0.5 Hz/pt hz/mm:88.8
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N5APT.fid



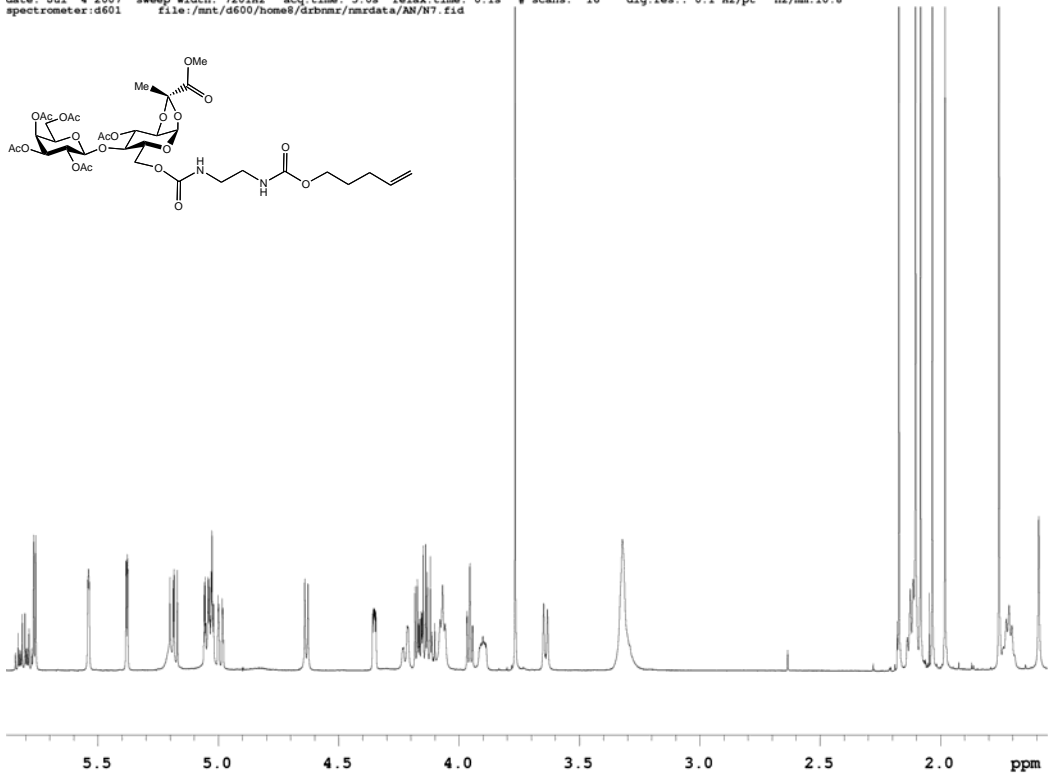
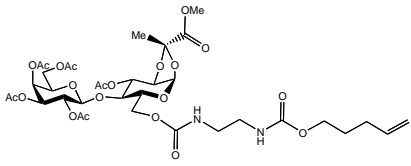
date: Aug 3 2007 sweep width: 4802Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:9.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N6.fid



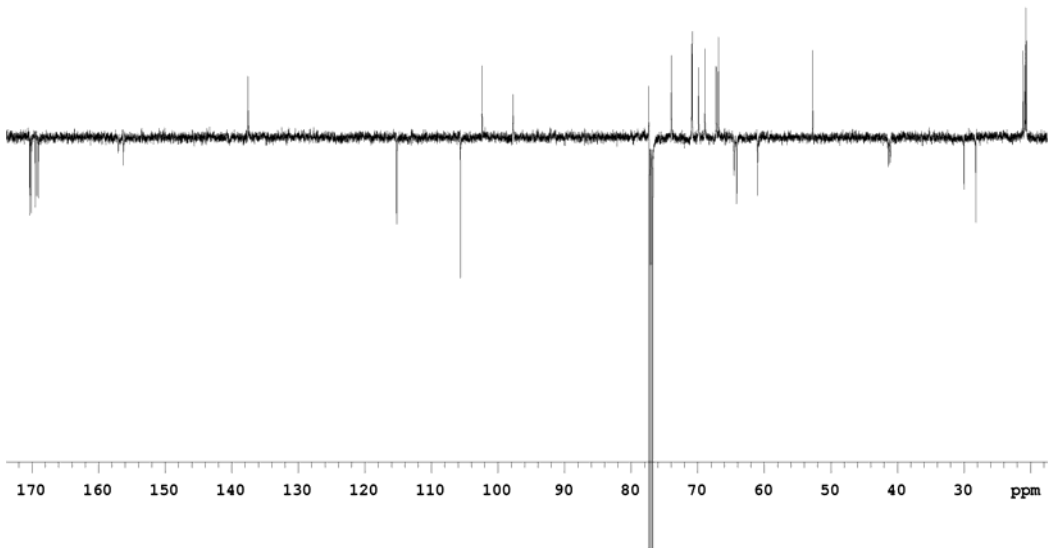
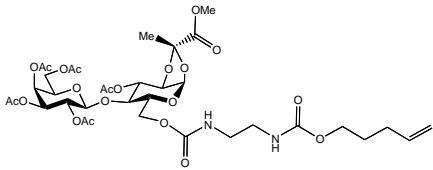
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Sep 27 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 240 dig.res.: 0.5 Hz/pt hz/mm:75.3
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N6APT.fid



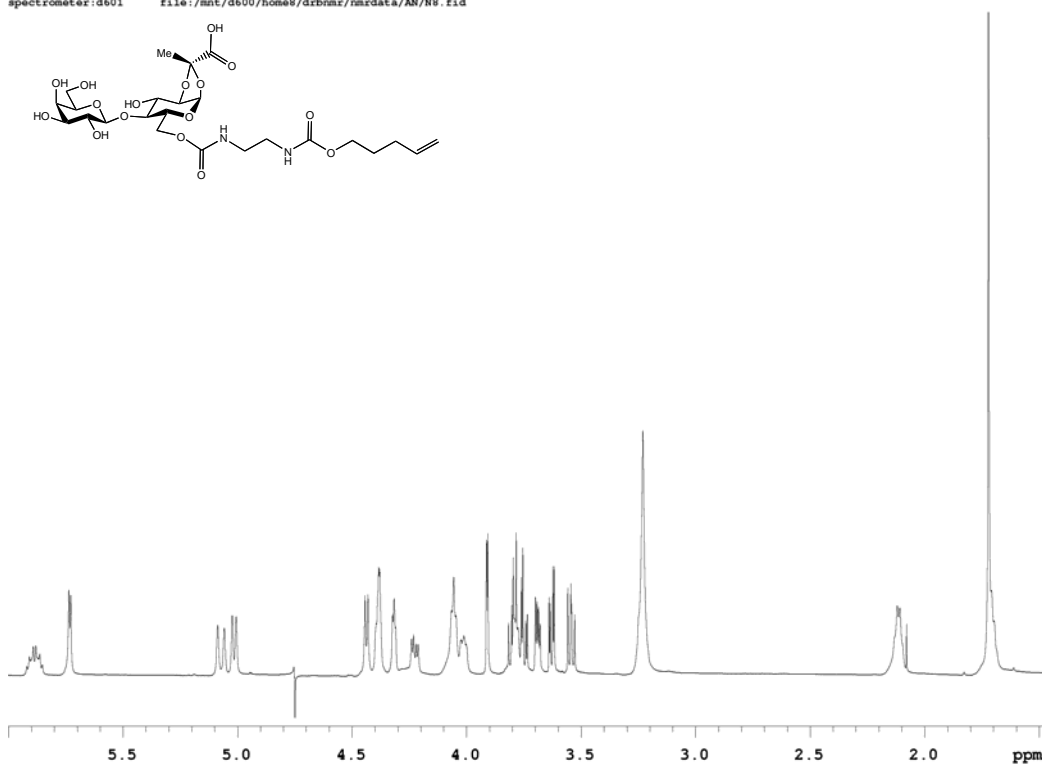
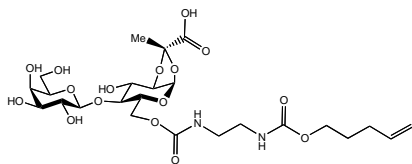
date: Jul 4 2007 sweep width: 7201Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:10.8
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N7.fid



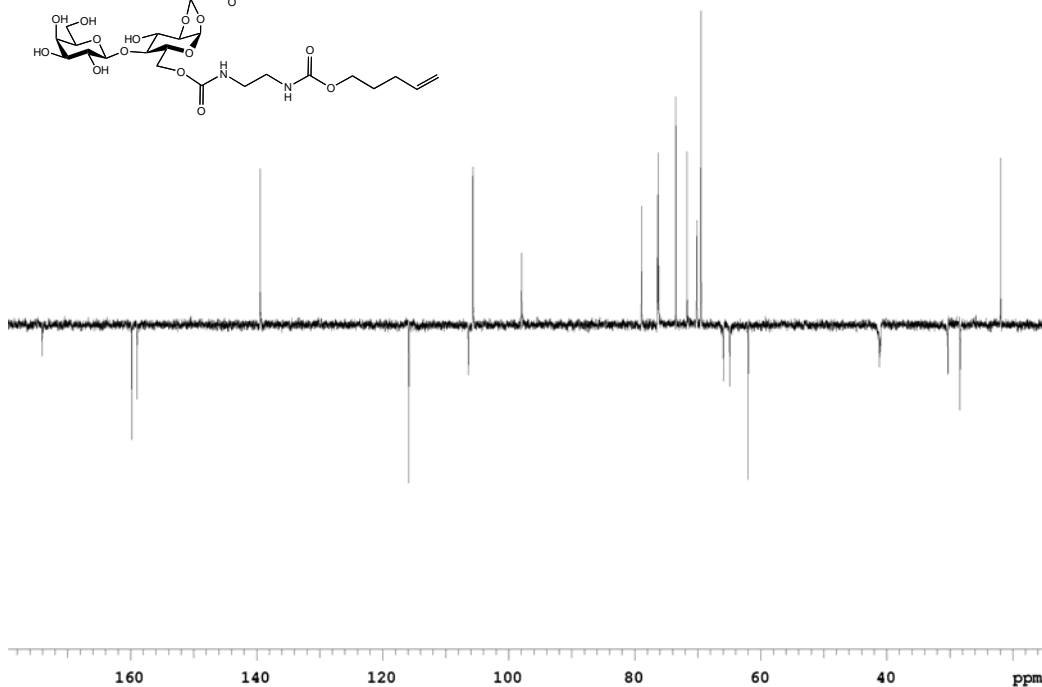
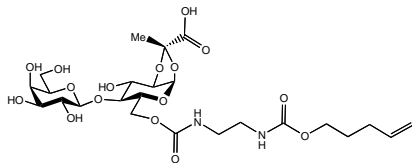
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Sep 21 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 2752 dig.res.: 0.5 Hz/pt hz/mm:82.0
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N7APT.fid



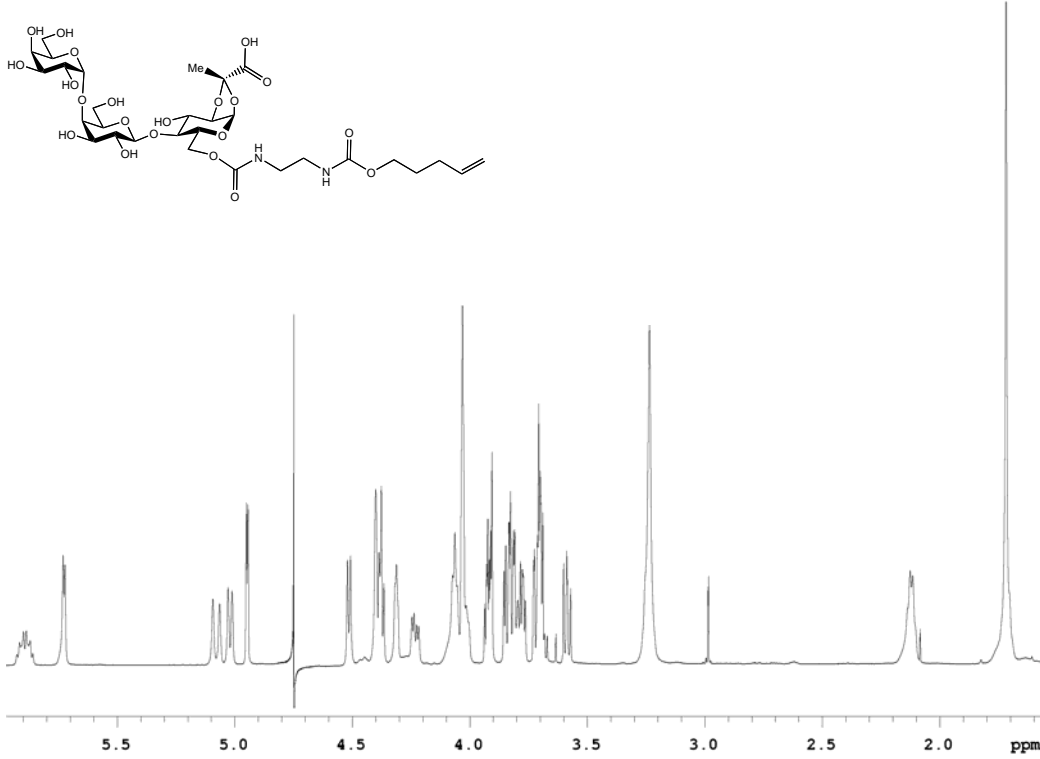
date: Oct 24 2007 sweep width: 7201Hz acq.time: 3.0s relax.time: 2.0s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:11.4
spectrometer:d601 file:/mnt/d600/home8/drbrmr/nmrdata/AN/N8.fid



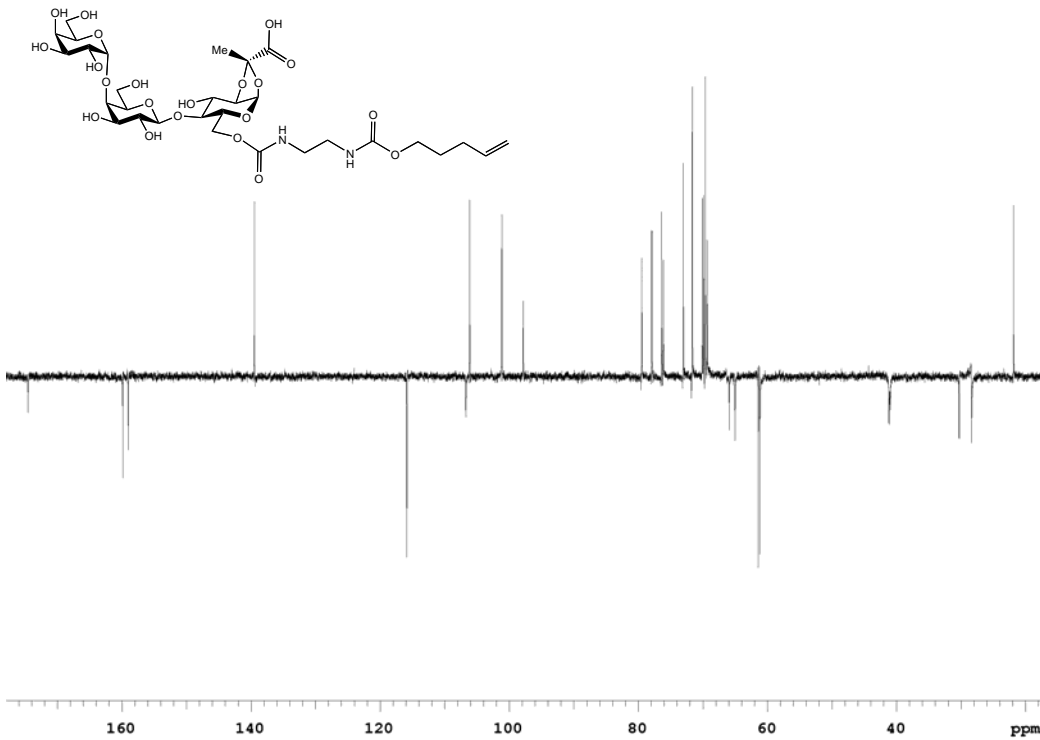
C & CH2 opposite side of CH & CH3
date: Oct 24 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 0 dig.res.: 0.5 Hz/pt hz/mm:86.6
spectrometer:d601 file:/mnt/d600/home8/drbrmr/nmrdata/AN/N8AcidicAPT.fid



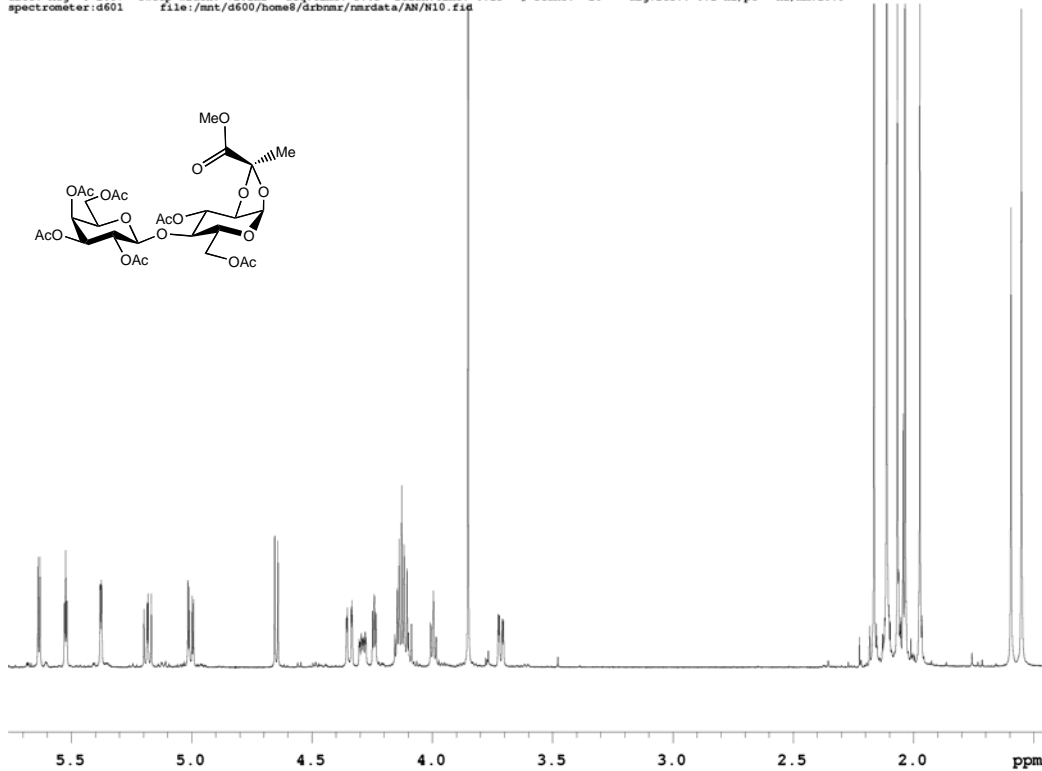
date: Sep 20 2007 sweep width: 7201Hz acq.time: 3.0s relax.time: 2.0s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:11.1
spectrometer:d601 file:/mnt/d600/home8/dzbrmr/rmrdata/AN/N9.fid



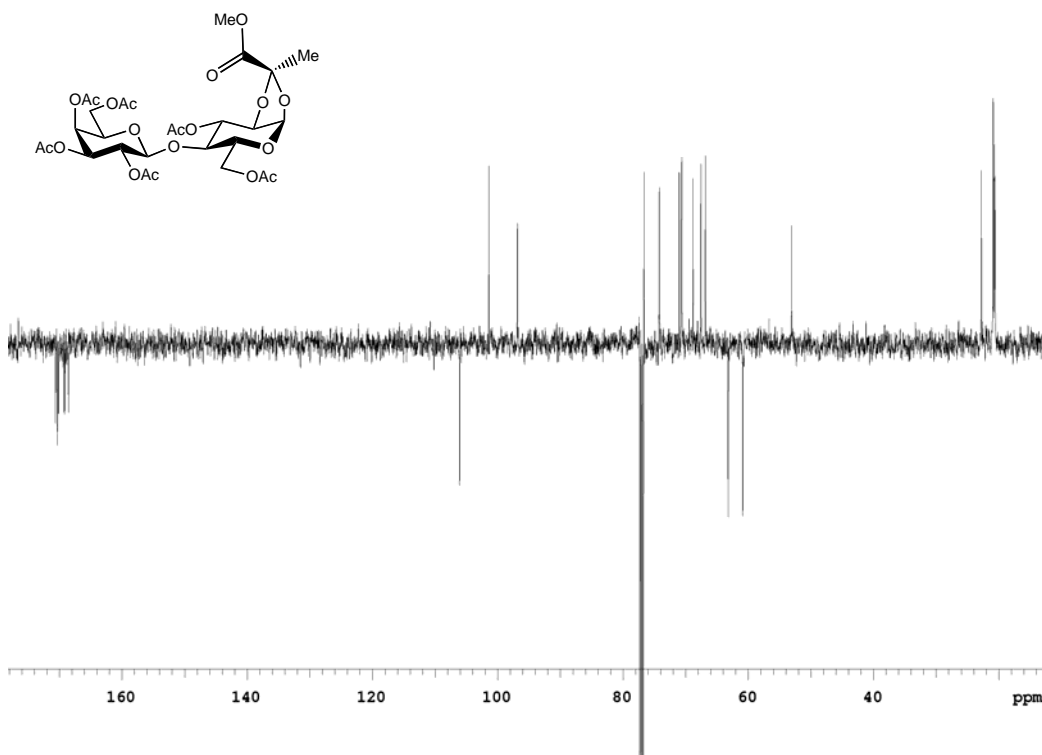
C 4 CH2 opposite side of CH 4 CH3
date: Sep 21 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 26104 dig.res.: 0.5 Hz/pt hz/mm:84.5
spectrometer:d601 file:/mnt/d600/home8/dzbrmr/rmrdata/AN/N9AP7.fid



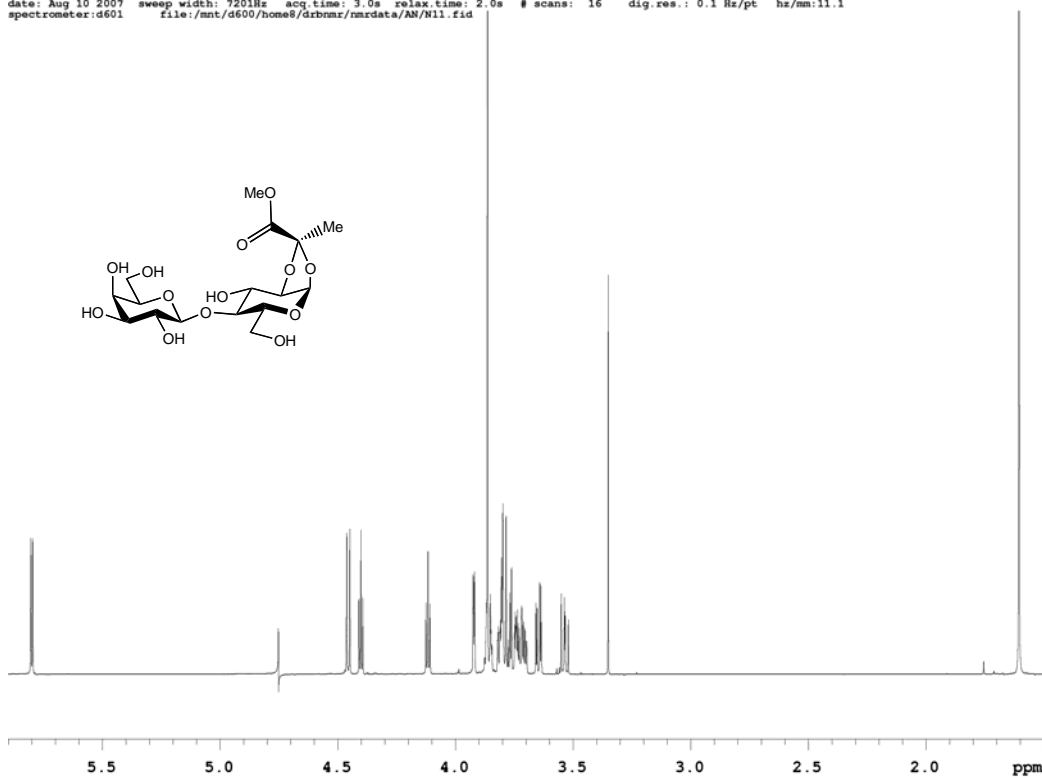
600 MHz 1D in CDCl3 (ref. to CDCl3 @ 7.26 ppm), temp 28.0 C -> actual temp = 27.0 C, id600 probe
date: Aug 8 2007 sweep width: 7201Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:10.8
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N10.fid



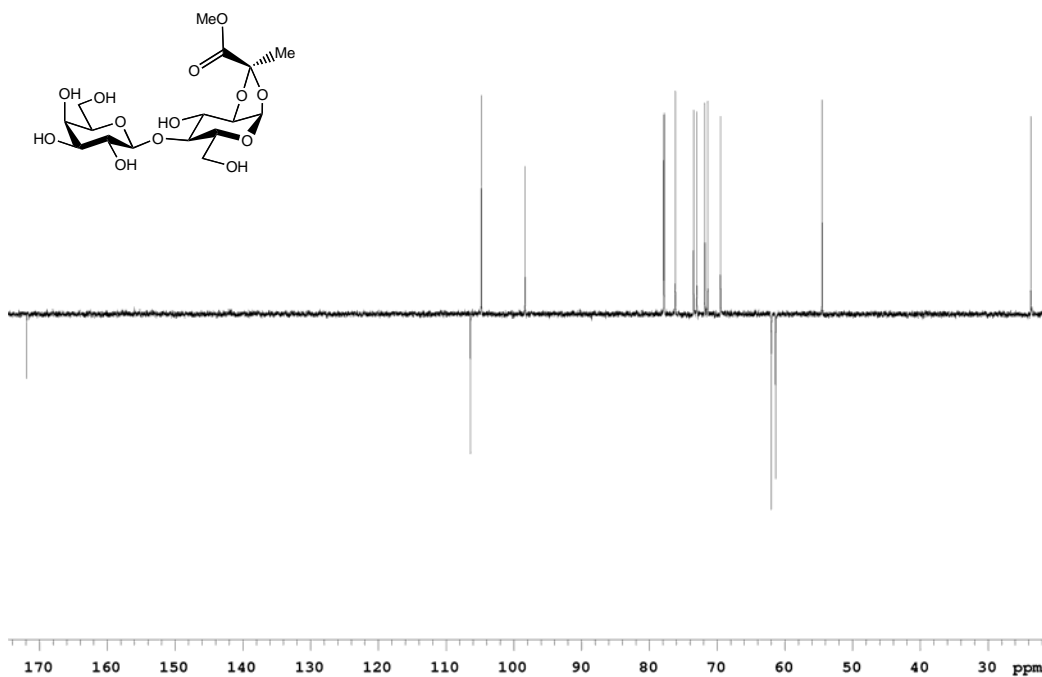
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Sep 7 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 1576 dig.res.: 0.5 Hz/pt hz/mm:87.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N10APT.fid



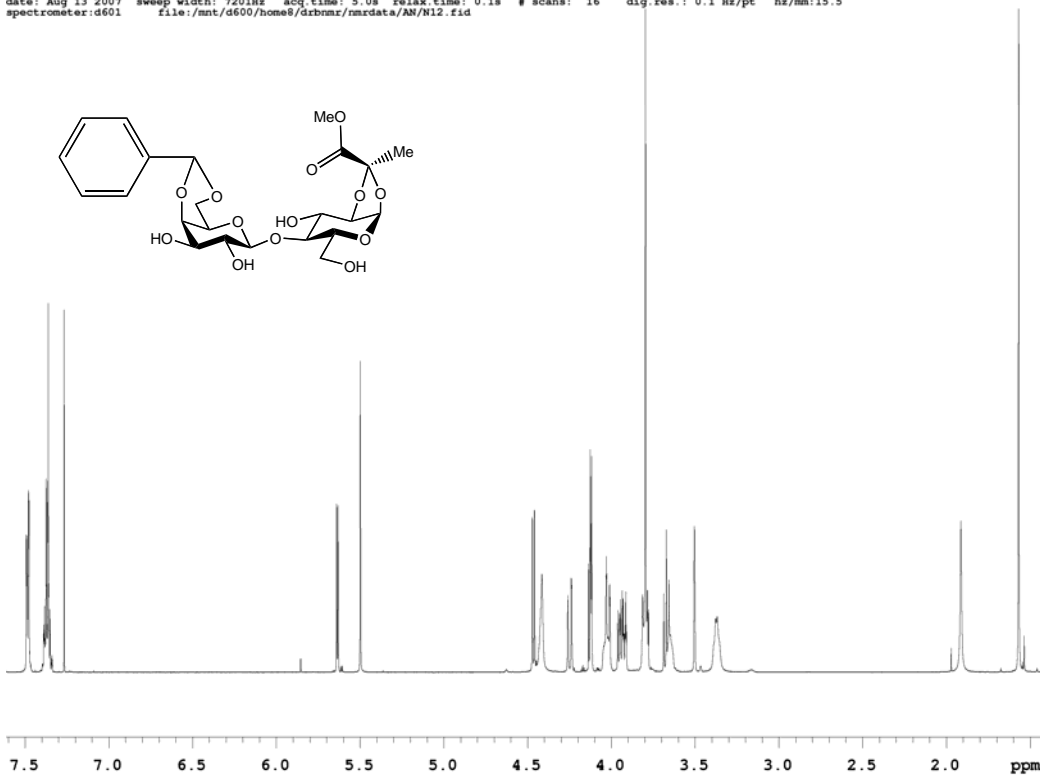
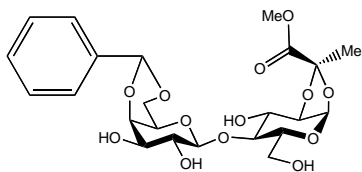
600 MHz 1D in D2O (ref. to 0.1 % ext. acetone @ 2.225 ppm), temp 28.0 C -> actual temp = 27.0 C, id600 probe
date: Aug 10 2007 sweep width: 7201Hz acq.time: 3.0s relax.time: 2.0s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:11.1
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N11.fid



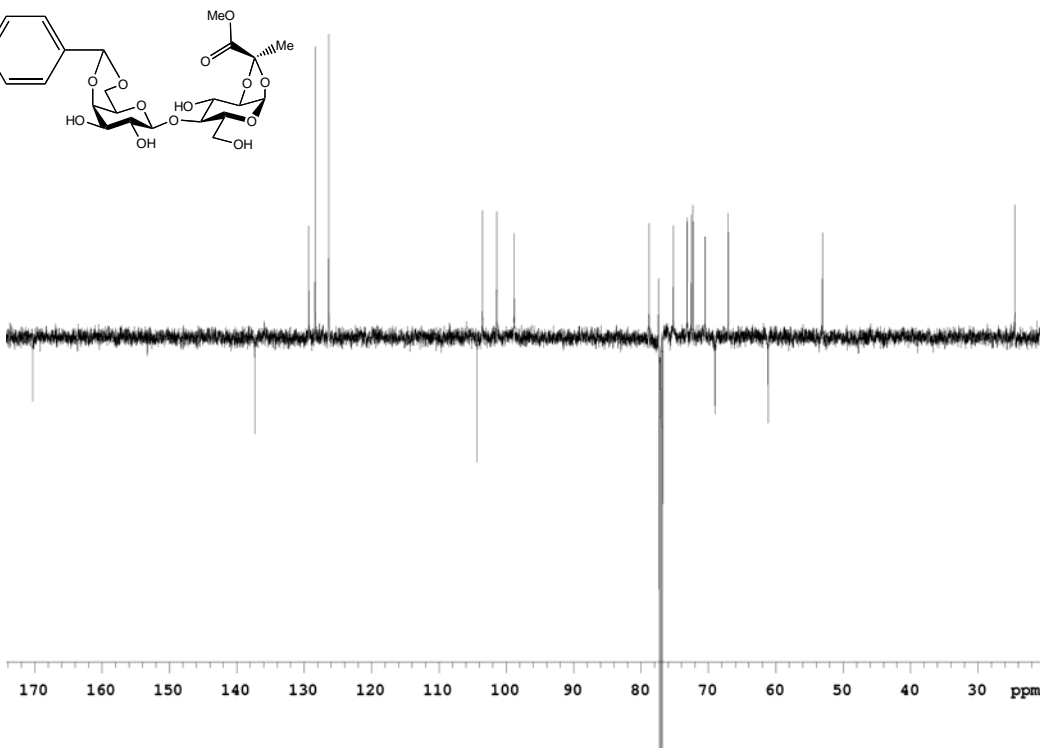
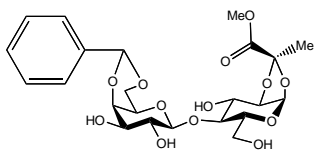
C & CH2 opposite side of CH & CH3
date: Oct 17 2007 sweep width: 33827Hz acq.time: 2.0s relax.time: 0.1s # scans: 2192 dig.res.: 0.5 Hz/pt hz/mm:80.2
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N11APT.fid



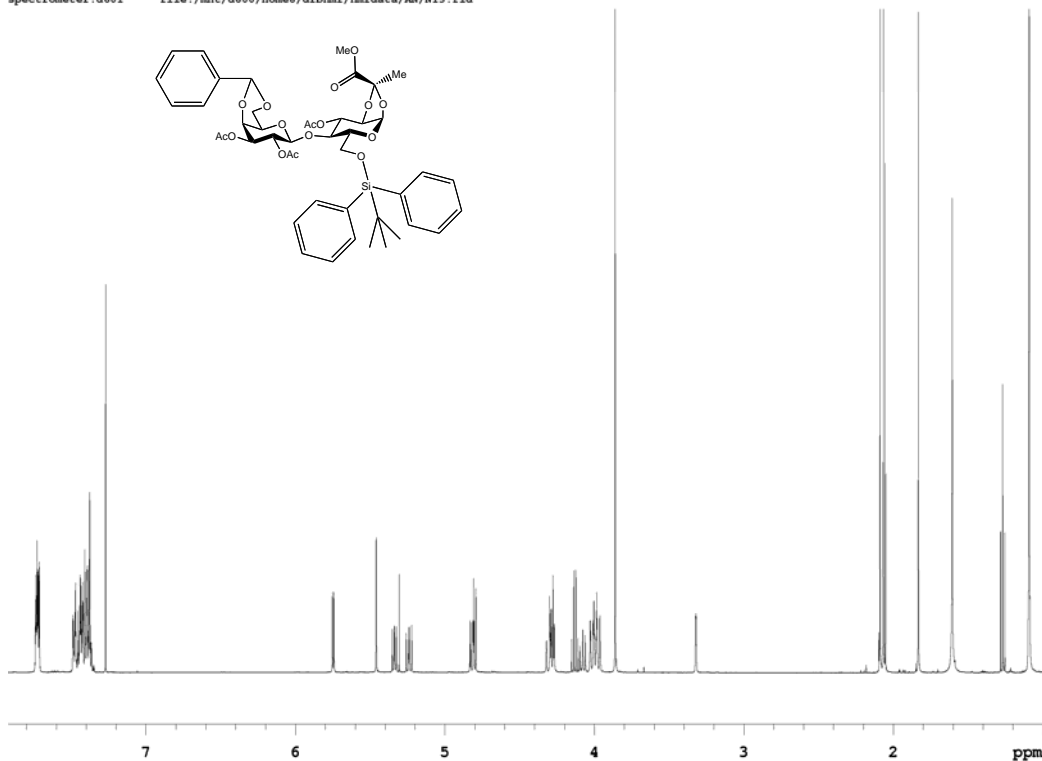
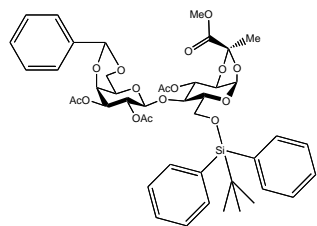
600 MHz 1D in CDCl3 (ref. to CDCl3 @ 7.26 ppm), temp 28.0 C -> actual temp = 27.0 C, id600 probe
date: Aug 13 2007 sweep width: 7201Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:15.5
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N12.fid



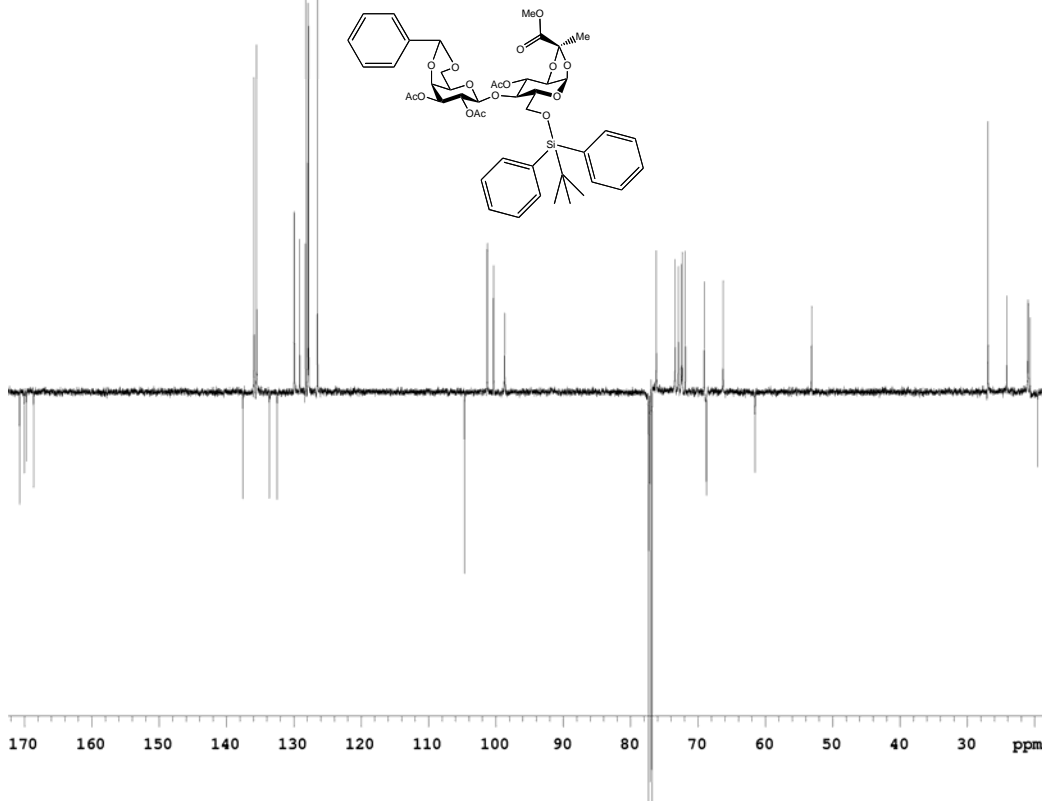
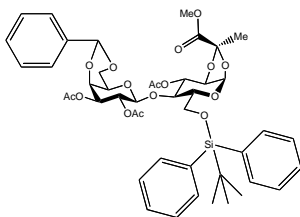
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Aug 13 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 888 dig.res.: 0.5 Hz/pt hz/mm:81.0
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N12APT.fid



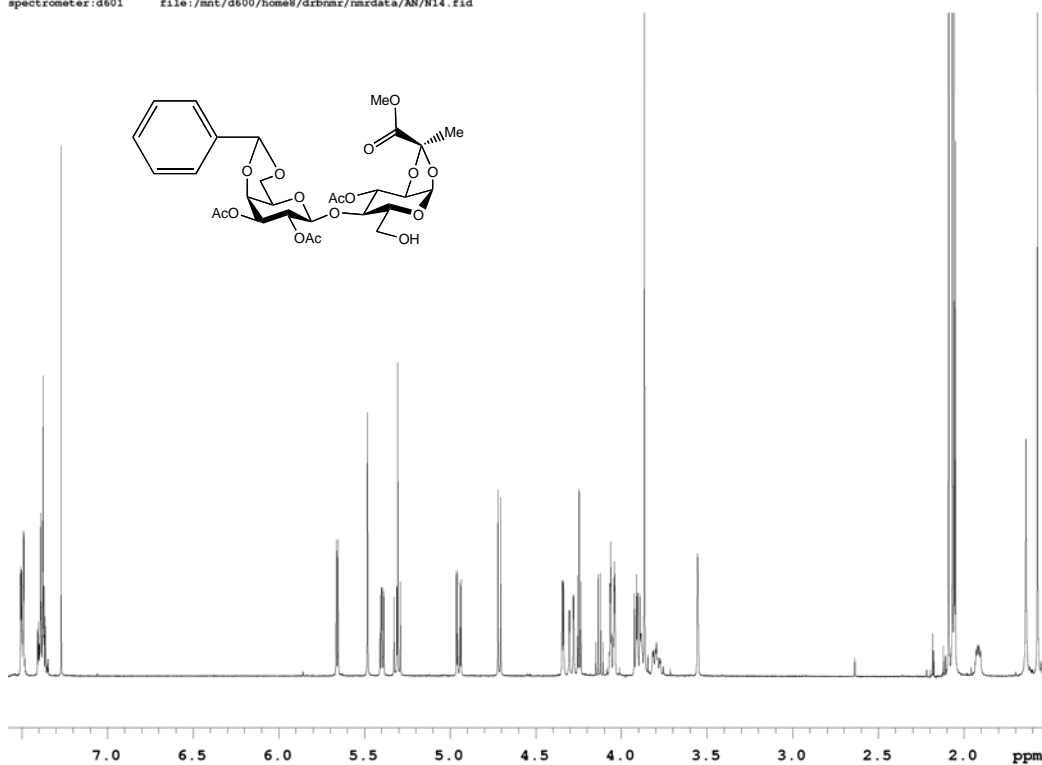
date: Aug 16 2007 sweep width: 6010Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:14.5
spectrometer:d601 file:/mnt/d600/home8/grbnmr/rmrdata/AN/N13.fid



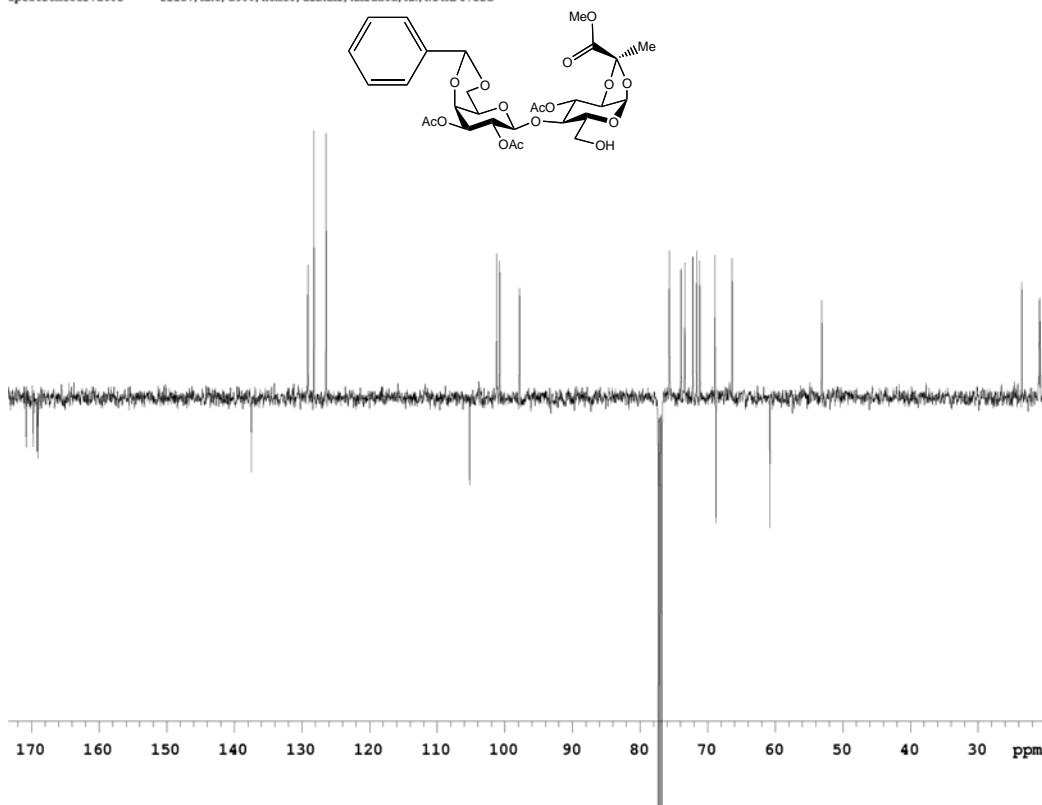
C 4 CH2 same, CH 4 CH3 opposite side of solvent signal
date: Dec 14 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 3360 dig.res.: 0.5 Hz/pt hz/mm:81.0
spectrometer:d601 file:/mnt/d600/home8/grbnmr/rmrdata/AN/2007.12.14.u5_N13-APT_C13_apt.fid



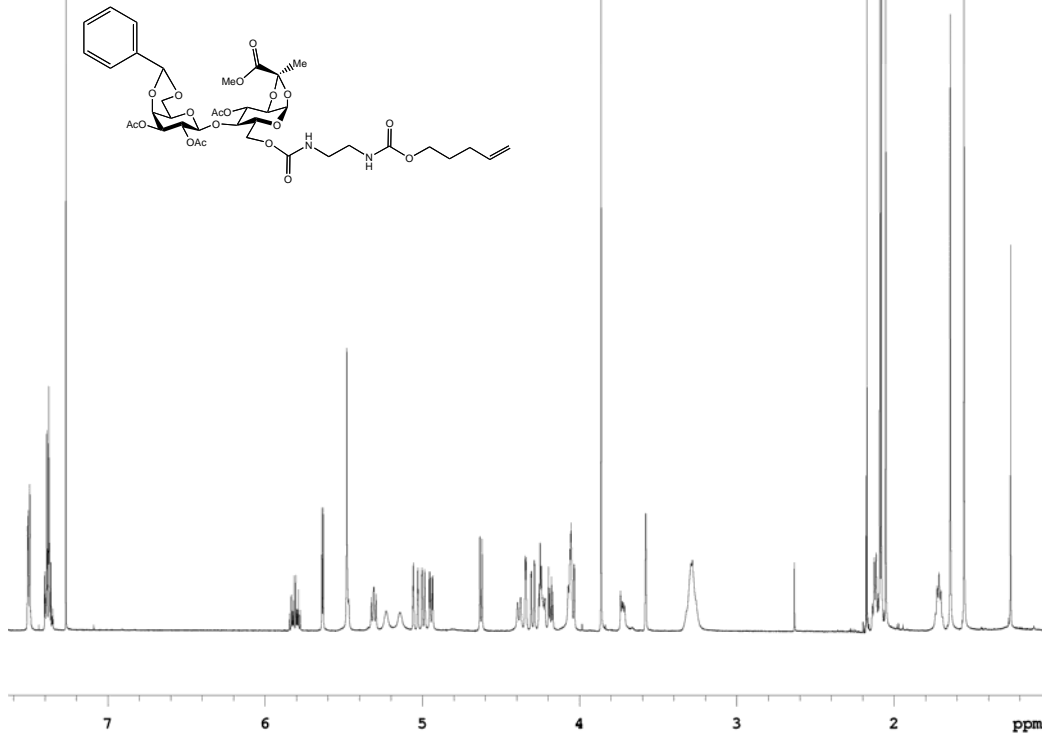
date: Aug 17 2007 sweep width: 6010Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:12.7
spectrometer:d601 file:/mnt/d600/home8/drbrnr/rmrdata/AN/N14.fid



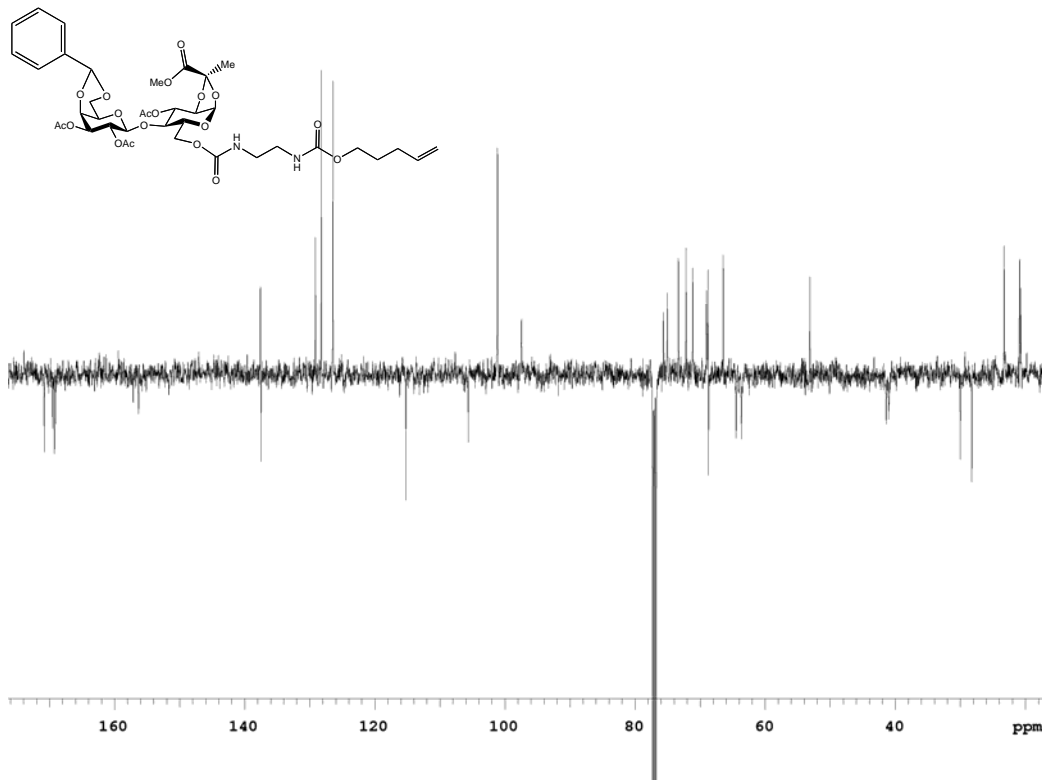
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Aug 17 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 1624 dig.res.: 0.5 Hz/pt hz/mm:80.7
spectrometer:d601 file:/mnt/d600/home8/drbrnr/rmrdata/AN/N14APT.fid



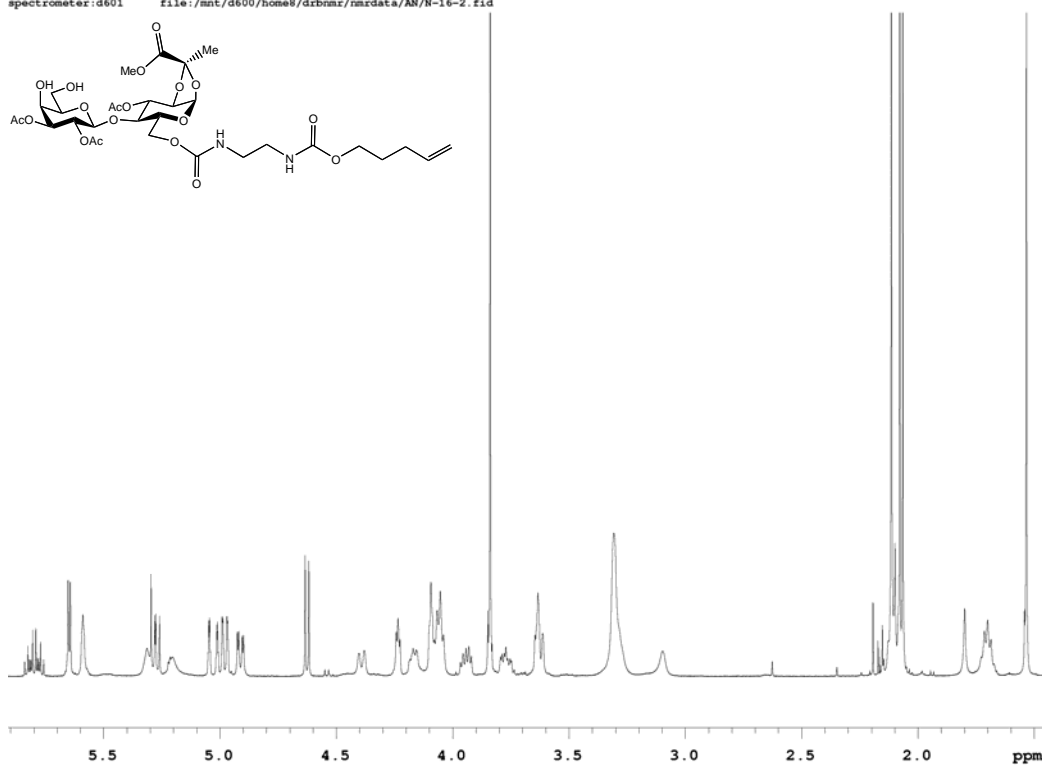
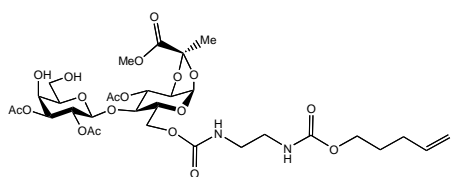
600 MHz 1D in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm), temp 28.0 C -> actual temp = 27.0 C, id600 probe
date: Aug 21 2007 sweep width: 72018Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:16.6
spectrometer:d601 file:/mnt/d600/home8/drbrnr/rmrdata/AN/N15.fid



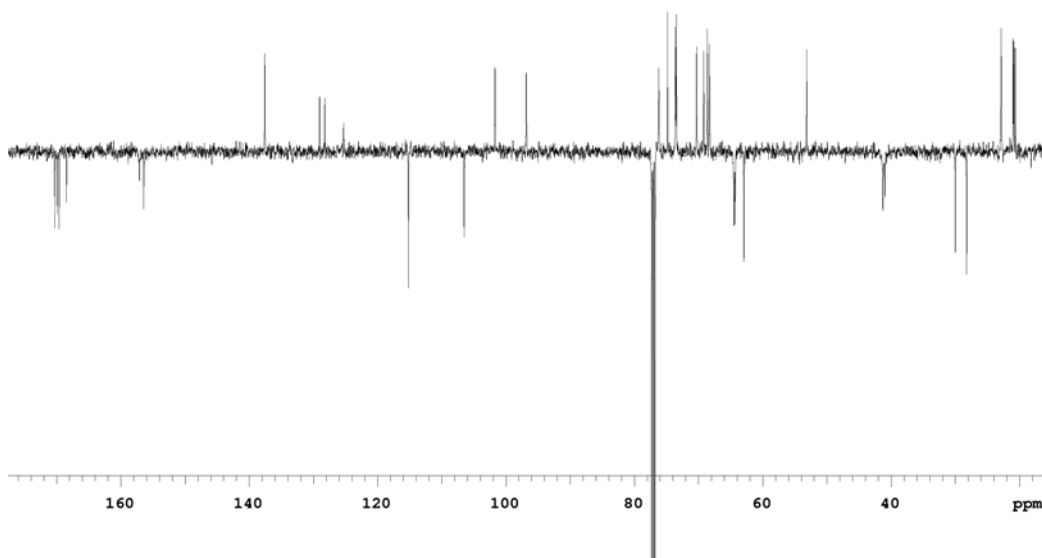
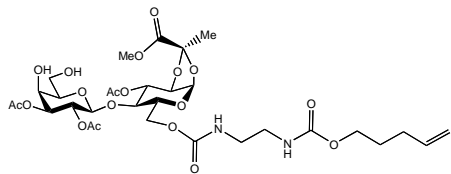
C 4 CH2 same, CH & CH3 opposite side of solvent signal
date: Aug 22 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 2024 dig.res.: 0.5 Hz/pt hz/mm:83.9
spectrometer:d601 file:/mnt/d600/home8/drbrnr/rmrdata/AN/N15APT-bad.fid



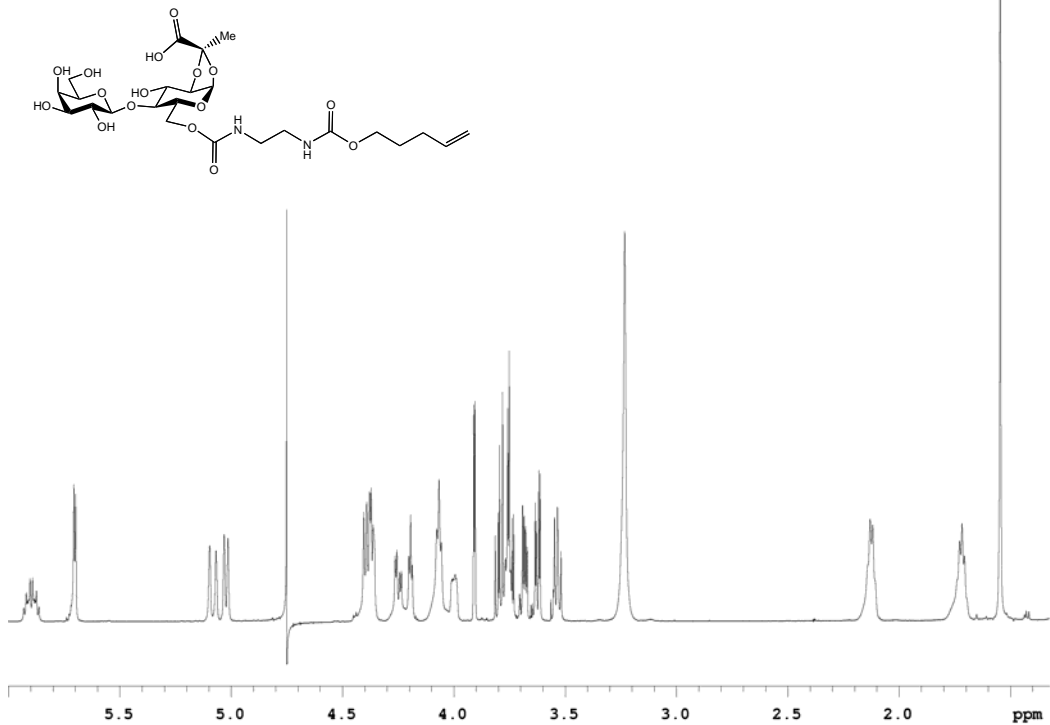
date: Oct 19 2007 sweep width: 6001Hz acq.time: 5.0s relax.time: 0.1s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm: 9.3
spectrometer: d601 file: /mnt/d600/home8/grbnmr/mrdata/AN/N-16-2.fid



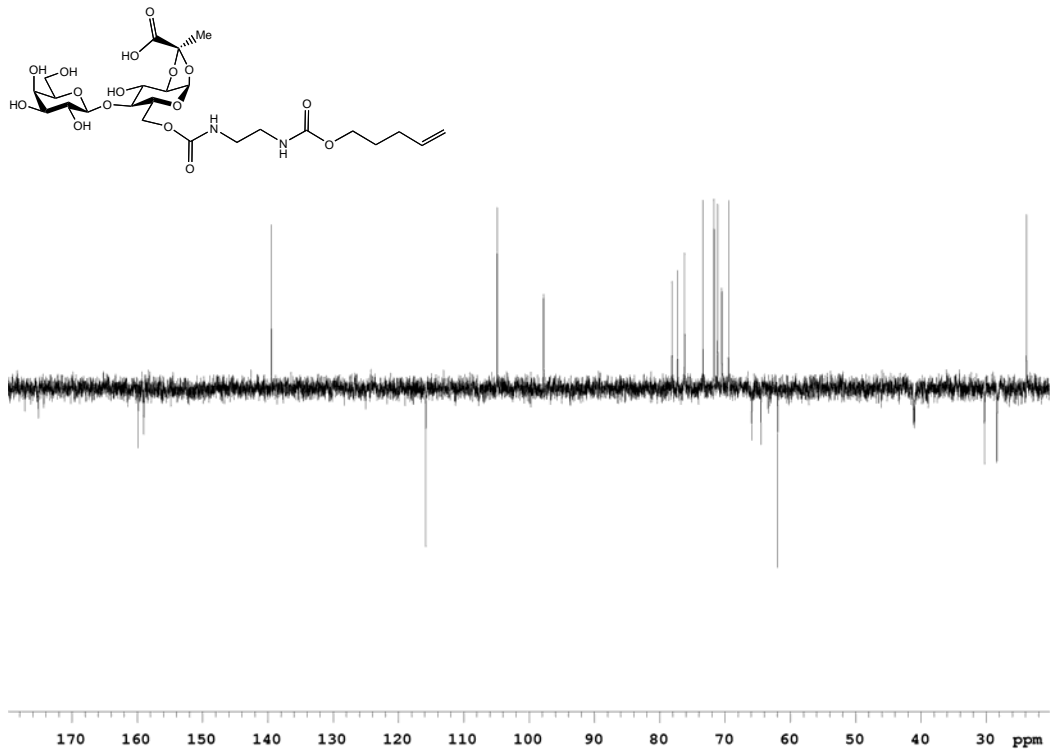
125 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 26.1 C -> actual temp = 27.0 C, autotx probe
date: Aug 22 2007 sweep width: 22384Hz acq.time: 1.0s relax.time: 0.1s # scans: 1536 dig.res.: 0.5 Hz/pt hz/mm: 85.0
spectrometer: d601 file: /mnt/d600/home8/grbnmr/mrdata/AN/N16APT.fid



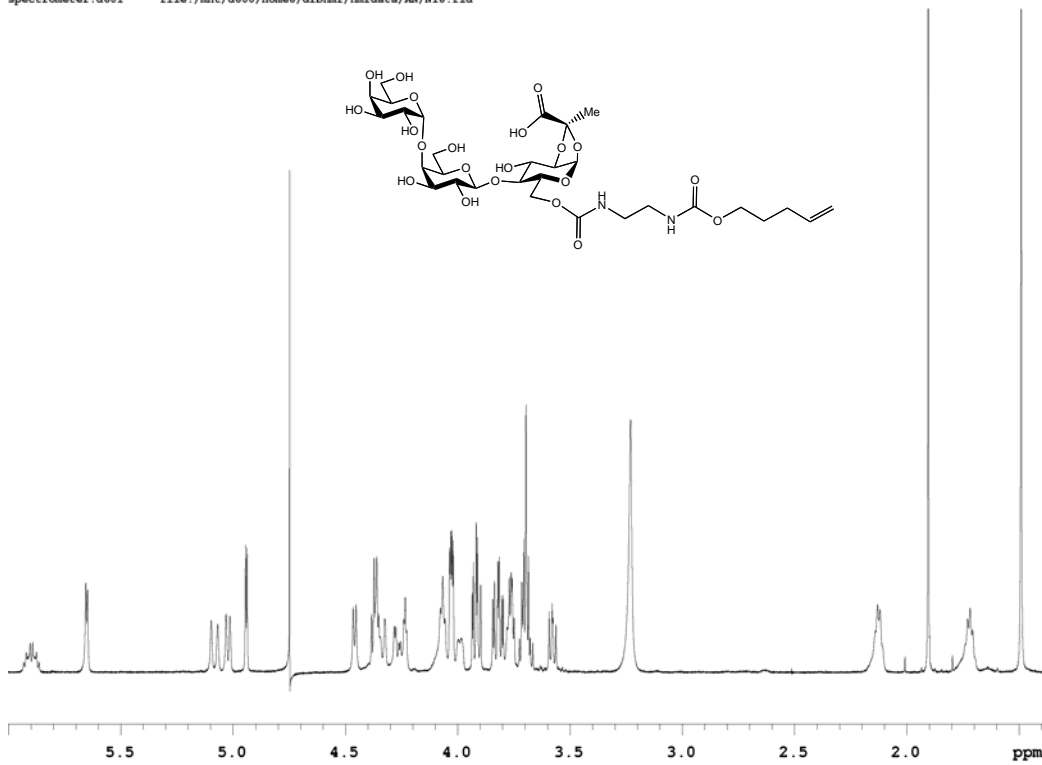
date: Aug 27 2007 sweep width: 7201Hz acq.time: 3.0s relax.time: 2.0s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:11.7
spectrometer:d601 file:/mnt/d600/home8/drbrnr/rmrdata/AN/N17.fid



C & CH2 opposite side of CH & CH3
date: Aug 27 2007 sweep width: 33827Hz acq.time: 2.0s relax.time: 0.1s # scans: 1360 dig.res.: 0.5 Hz/pt hz/mm:83.3
spectrometer:d601 file:/mnt/d600/home8/drbrnr/rmrdata/AN/N17APT.fid



date: Oct 17 2007 sweep width: 7201Hz acq.time: 3.0s relax.time: 2.0s # scans: 16 dig.res.: 0.1 Hz/pt hz/mm:11.6
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N18.fid



C & CH2 opposite side of CH & CH3
date: Sep 20 2007 sweep width: 33784Hz acq.time: 2.0s relax.time: 0.1s # scans: 2736 dig.res.: 0.5 Hz/pt hz/mm:85.5
spectrometer:d601 file:/mnt/d600/home8/drbrmr/rmrdata/AN/N18APT.fid

