

Supporting Information

(JO034679b)

Synthesis of a New Stable Conformationally Constrained

2,7-Anhydrosialic Acid Derivative

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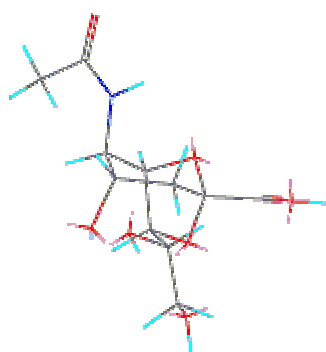
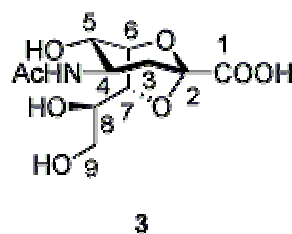
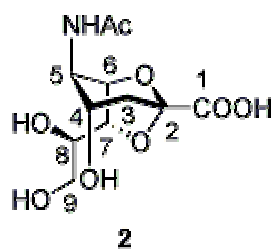
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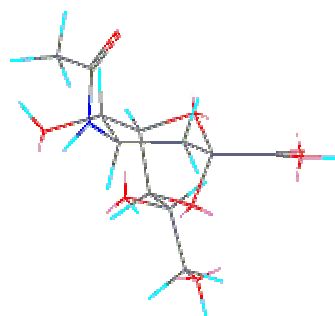
Experimental Section

General ^1H NMR was recorded a 300-MHz spectrometer in CDCl_3 or CD_3OD with TMS as internal standard. ^{13}C -NMR spectra were also recorded on a 300-MHz spectrometer. Elemental analyses were obtained from Vario EL spectrometer. IR spectra were recorded on Bio-Rad FTS-185 spectrometer. HRMS (EI and ESI) spectra were obtained on an APEXIII 7.0 Tesla FTMS mass spectrometer. Flash column chromatography was performed on silica gel (10-40 μm).

**Colored molecular presentations of 2 and 3 with lowest energy
calculated by MM2**



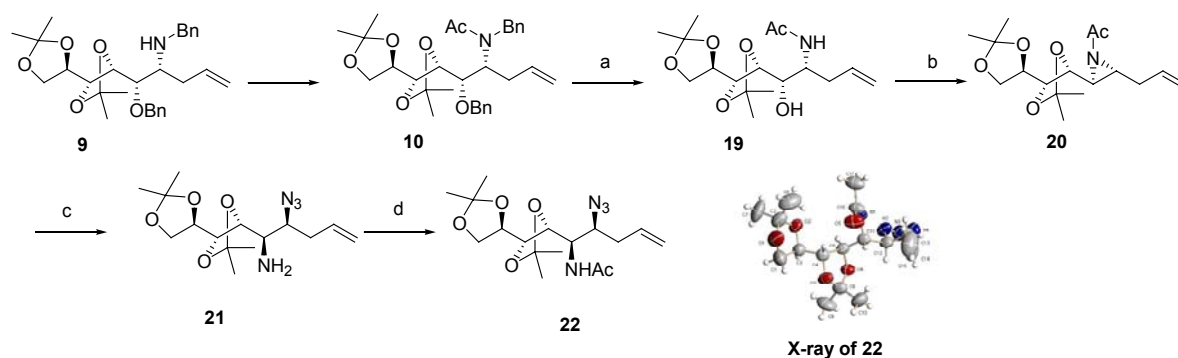
2
MM2 minimized energy
24.5348 kcal/mol



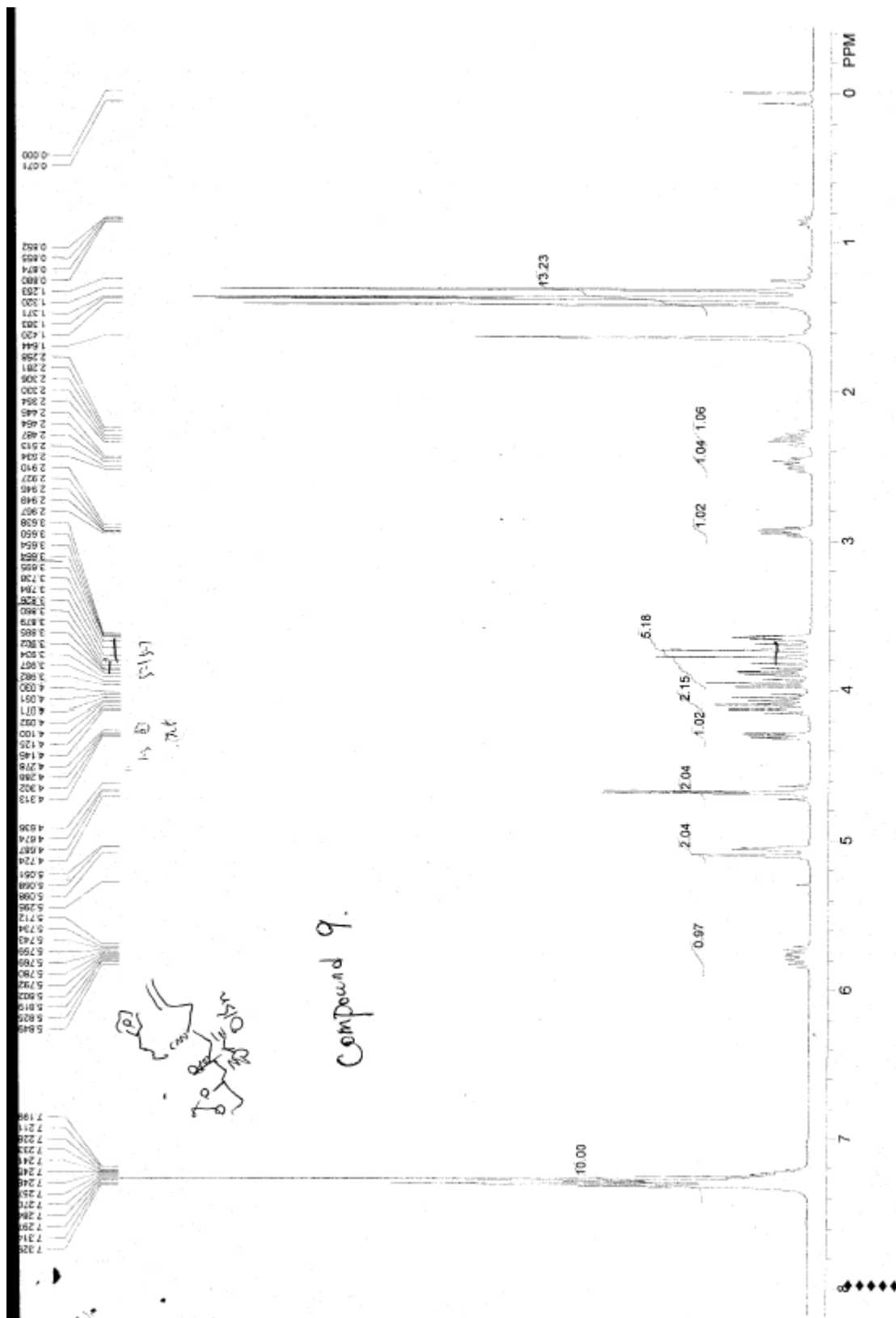
3
MM2 minimized energy
15.4993 kcal/mol

Indirect Configuration Confirmation of **9** by the X-ray

The configuration of **9** was finally confirmed by x-ray image of single crystal of **22** through 4 steps of chemical transformations from **10** (unpublished results, see the following scheme).

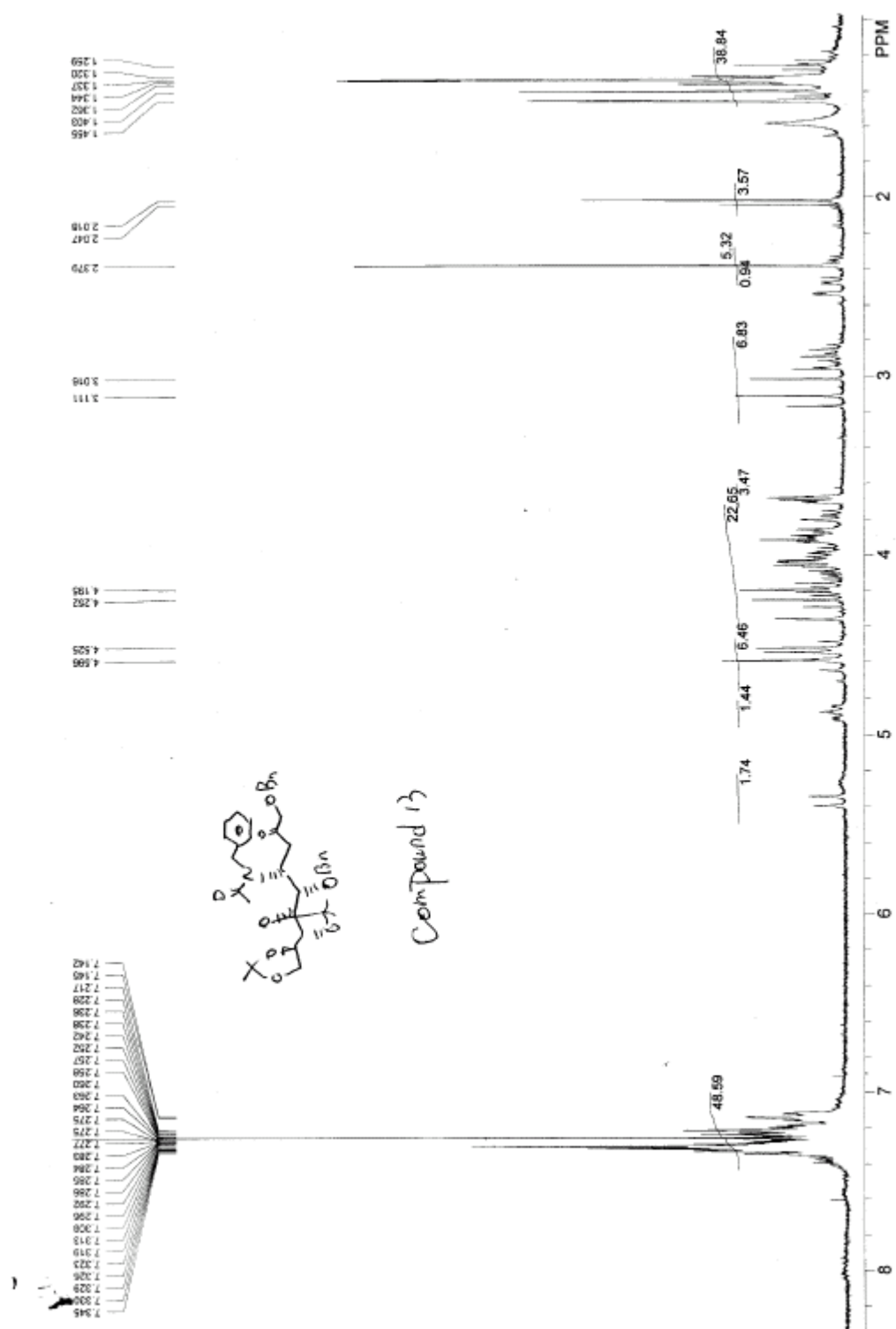


Reagents and conditions: a) Li-NH₃ (l), -78°C, 82%. b) 1. MsCl, TEA, 0°C to rt, 84%. 2. NaH, THF, 40°C, 87%. c) NaN₃, EtOH, aq. NH₄Cl, reflux, 68%. d) Ac₂O, TEA, DCM, rt, 99%.

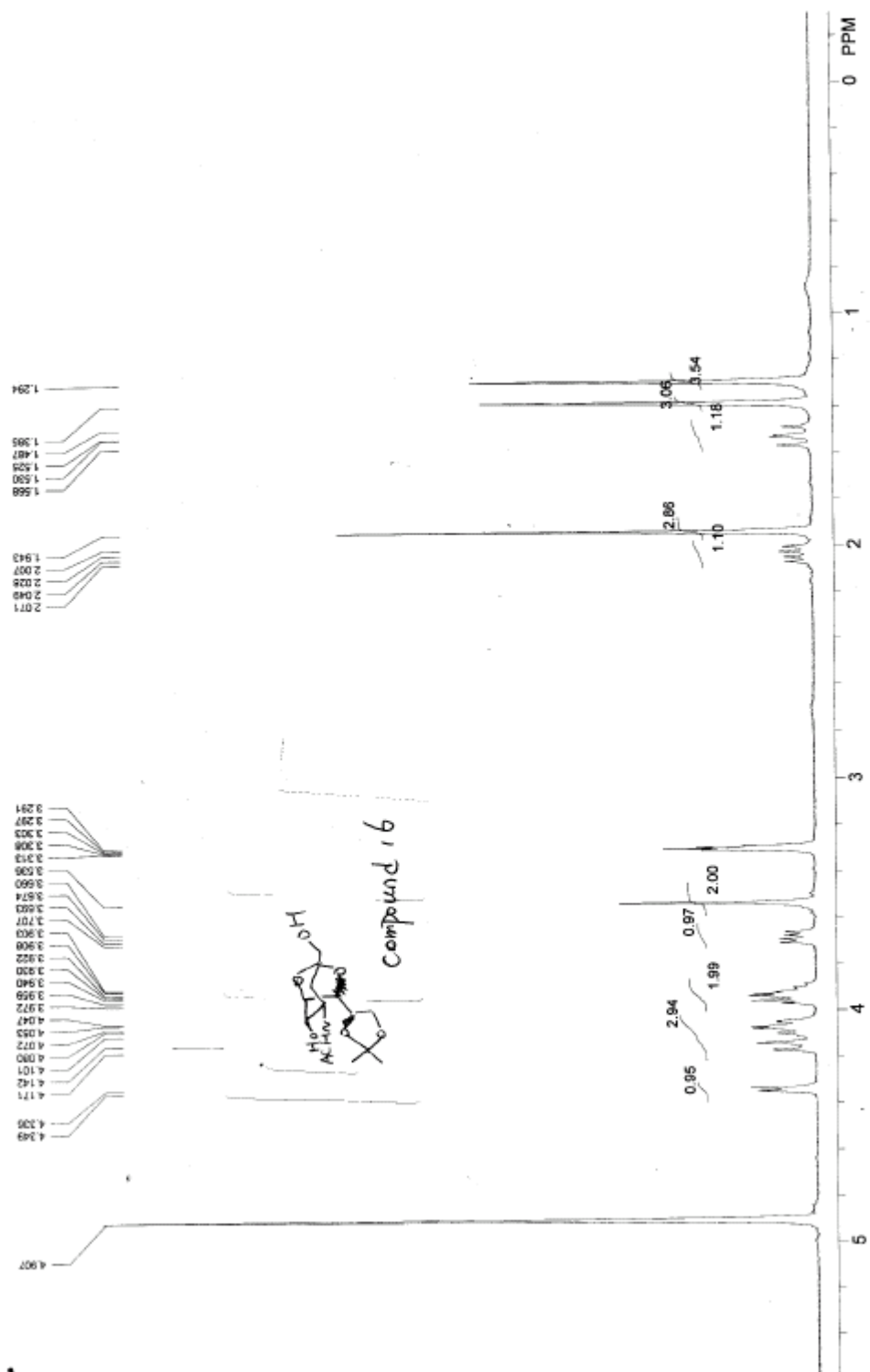






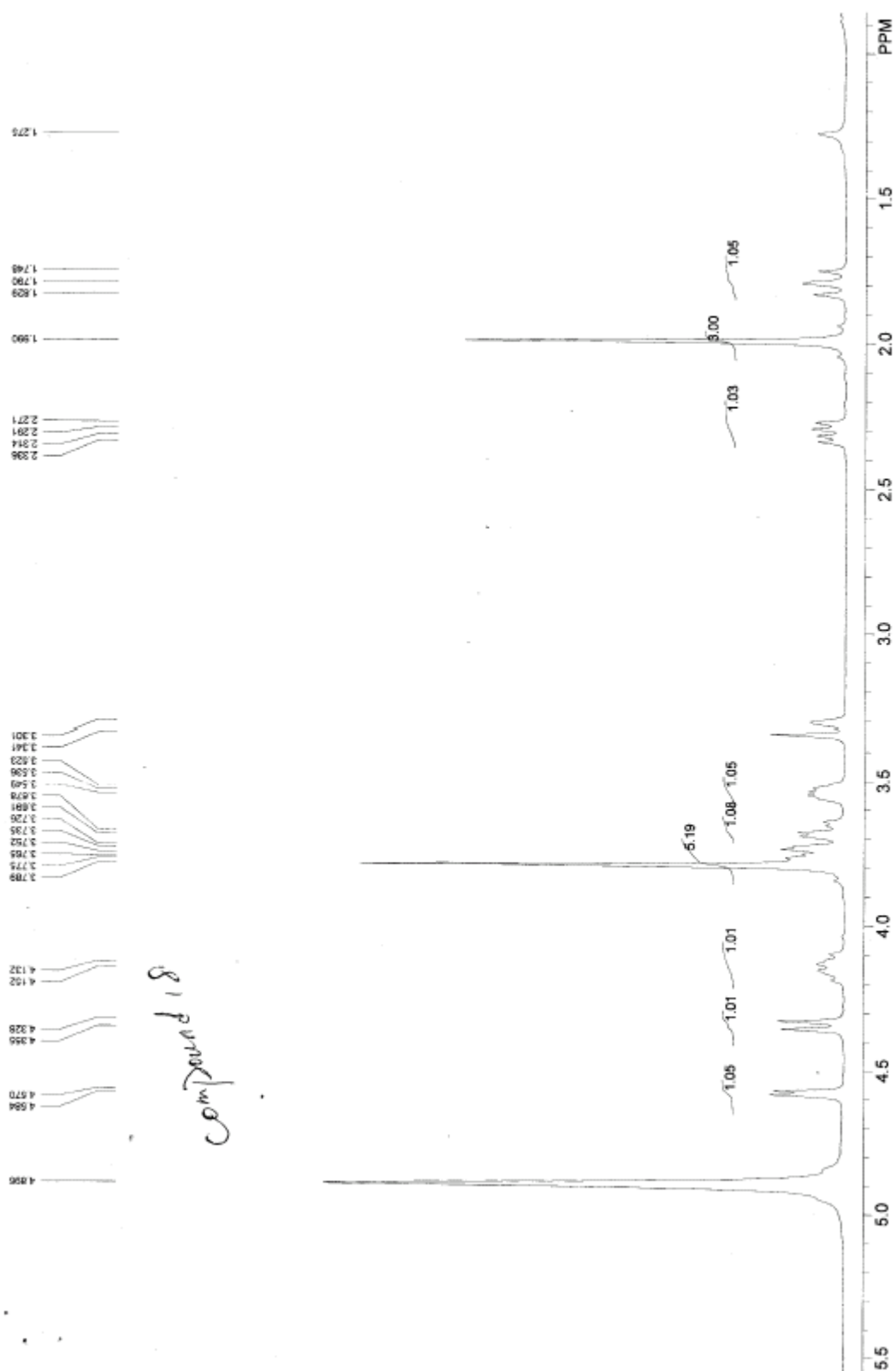




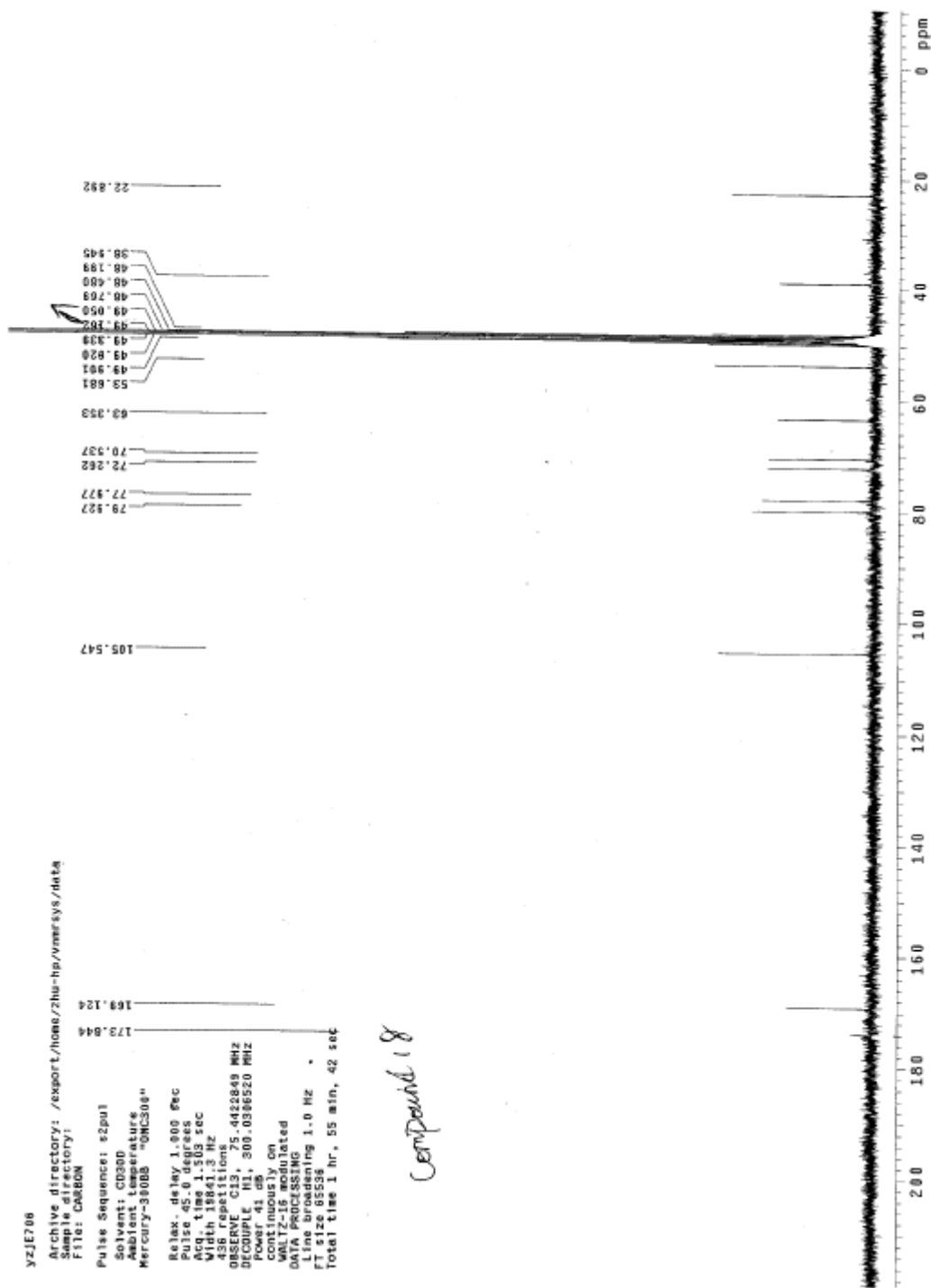




Compound 17



yzj2708
 Archive directory: /export/home/zhu-hp/vmr/sys/data
 Sample directory:
 File: CARBON
 Pulse Sequence: s2pul
 Solvent: CD3OD
 Ambient temperature
 Mercury-350BS "QNC30g"
 Relax delay 1.000 sec
 Pulse delay 0.000 sec
 Acq. time 1.513 sec
 Width 18841.3 Hz
 436 repetitions
 OBSERVE C13, 75.4422849 MHz
 DECOUPLE H1, 300.0366520 MHz
 Power 0.000000
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 85536
 Total time 1 hr, 55 min, 42 sec



Compound 18