

Supporting Information

Metal-free metathesis reaction between alkyl halides and *N*-haloimides

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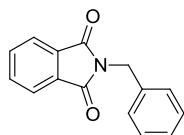
I. General

All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. The products were purified by column chromatography over silica gel. ^1H NMR and ^{13}C NMR spectra were recorded at 25 °C on a Varian 500 MHz and 125 MHz, respectively, and TMS as internal standard. Mass spectra were recorded on Agilent 1100 LCMsD mass spectrometer.

II. Synthesis and Analytical Data of 3, 4, 7 and 8

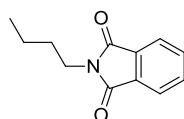
General procedure for the preparation of 3, 4, 7 and 8 (3a as an example): To a solution of NCP (1.2 mmol, 217.8 mg) and DBU (1.2 mmol, 182.4 mg) in dry DMSO (2.0 ml), benzyl chloride **1a** (1.0 mmol, 126.6 mg) was added. The reaction mixture was stirred at room temperature for 10 min. After the starting material **1a** was consumed as indicated by TLC, the reaction mixture was poured into water and then extracted with CH_2Cl_2 (3 $\times$ 5 mL). The combined organic phase was washed with water (3 $\times$ 10 mL), dried over anhydrous MgSO_4 , filtered and concentrated under reduced pressure. The crude product was purified by flash chromatography (silica gel, petroleum ether : ethyl acetate = 30 : 1) to give **3a** (215.8 mg, 91%) as a white solid.

2-Benzylisoindoline-1,3-dione (3a)



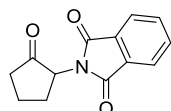
White solid. m.p. 115-116 °C. ^1H NMR (500 MHz, CDCl_3) δ 4.85 (s, 2H), 7.27 (d, J = 8.5 Hz, 1H), 7.32 (d, J = 7.5 Hz, 2H), 7.43 (d, J = 7.5 Hz, 2H), 7.70-7.71 (m, 2H), 7.84-7.85 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 41.5, 123.3, 127.8, 128.6, 128.6, 132.0, 133.9, 136.3, 168.0; HRMS (ESI) m/z calcd for $\text{C}_{15}\text{H}_{11}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 238.0868; found: 238.0860.

2-Butylisoindoline-1,3-dione (3b)



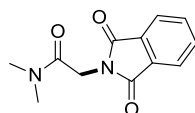
White solid. m.p. 32-33 °C. ^1H NMR (500 MHz, CDCl_3) δ 0.95 (t, J = 7.5 Hz, 3H), 1.37 (q, J = 7.5 Hz, 2H), 1.66 (t, J = 7.5 Hz, 2H), 3.69 (t, J = 7.5 Hz, 2H), 7.70-7.72 (m, 2H), 7.83-7.85 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 13.6, 20.0, 30.5, 37.7, 123.0, 132.1, 133.7, 168.4; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{13}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 204.1025; found: 204.1033.

2-(2-Oxocyclopentyl)isoindoline-1,3-dione (3c)



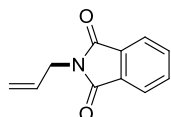
White solid. m.p. 167-168 °C. ^1H NMR (500 MHz, CDCl_3) δ 1.91 (m, 1H), 2.25 (m, 1H), 2.37 (m, 2H), 2.50 (m, 2H), 4.58 (t, J = 10.5 Hz, 1H), 7.72-7.74 (m, 2H), 7.83-7.85 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 19.0, 27.2, 36.1, 55.4, 123.4, 131.9, 134.1, 167.4, 212.2; HRMS (ESI) m/z calcd for $\text{C}_{13}\text{H}_{11}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 230.0817; found: 230.0811.

2-(1,3-Dioxoisindolin-2-yl)-*N,N*-dimethylacetamide (3d)



White solid. m.p. 177-178 °C. ^1H NMR (500 MHz, CDCl_3) δ 2.97 (s, 3H), 3.11 (s, 3H), 4.49 (s, 2H), 7.71-7.73 (m, 2H), 7.86-7.88 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 35.7, 36.1, 39.1, 123.4, 132.2, 133.9, 165.2, 168.0; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$: 233.0926; found: 233.0931.

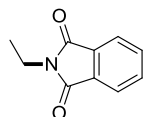
2-Allylisoindoline-1,3-dione (3e)



White solid. m.p. 58-59 °C. ^1H NMR (500 MHz, CDCl_3) δ 4.30 (d, J = 5.5 Hz, 2H), 5.20 (d, J = 10.5 Hz, 1H), 5.25 (d, J = 17 Hz, 1H), 5.86-5.93 (m, 1H), 7.72-7.75 (m, 2H), 7.85-7.87 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 39.8, 117.4, 123.0, 131.3,

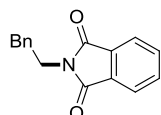
131.8, 133.7, 167.6; HRMS (ESI) m/z calcd for $C_{11}H_9NO_2$ $[M+H]^+$: 188.0712; found: 188.0716.

2-Ethylisoindoline-1,3-dione (3f)



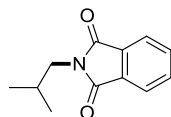
White solid. m.p. 76-77 °C. 1H NMR (500 MHz, $CDCl_3$) δ 1.28 (t, J = 7.5 Hz, 3H), 3.75 (q, J = 7.5 Hz, 2H), 7.70-7.72 (m, 2H), 7.83-7.85 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 13.9, 32.9, 123.1, 132.2, 133.8, 168.2; HRMS (ESI) m/z calcd for $C_{10}H_9NO_2$ $[M+H]^+$: 176.0712; found: 176.0718.

2-Phenethylisoindoline-1,3-dione (3g)



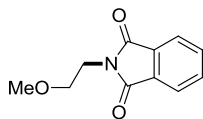
White solid. m.p. 104-105 °C. 1H NMR (500 MHz, $CDCl_3$) δ 2.99 (t, J = 8.0 Hz, 2H), 3.93 (t, J = 8.0 Hz, 2H), 7.20-7.25 (m, 1H), 7.26-7.39 (m, 4H), 7.70-7.71 (m, 2H), 7.81-7.84 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 34.6, 39.2, 123.2, 126.6, 128.5, 128.8, 132.0, 133.9, 137.9, 168.1; HRMS (ESI) m/z calcd for $C_{16}H_{13}NO_2$ $[M+H]^+$: 252.1025; found: 252.1020.

2-Isobutylisoindoline-1,3-dione (3h)



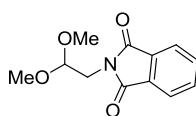
White solid. m.p. 90-91 °C. 1H NMR (500 MHz, $CDCl_3$) δ 0.95 (d, J = 7.0 Hz, 6H), 2.11-2.16 (m, 1H), 3.51 (d, J = 7.5 Hz, 2H), 7.70-7.74 (m, 2H), 7.83-7.87 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 20.1, 27.8, 45.2, 123.1, 132.0, 133.8, 168.6; HRMS (ESI) m/z calcd for $C_{12}H_{13}NO_2$ $[M+H]^+$: 204.1025; found: 204.1033.

2-(2-Methoxyethyl)isoindoline-1,3-dione (3i)



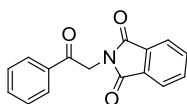
White solid. m.p. 145-146 °C. ^1H NMR (500 MHz, CDCl_3) δ 3.36 (s, 3H), 3.64 (t, J = 5.5 Hz, 2H), 3.91 (t, J = 5.5 Hz, 2H), 7.71-7.73 (m, 2H), 7.85-7.87 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 37.3, 58.6, 69.4, 123.3, 132.1, 133.9, 168.3; HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{11}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 206.0817; found: 206.0811.

2-(2,2-Dimethoxyethyl)isoindoline-1,3-dione (3j)



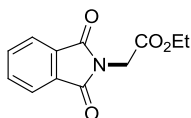
White solid. m.p. 104-105 °C. ^1H NMR (500 MHz, CDCl_3) δ 3.37 (s, 6H), 3.81 (d, J = 6.0 Hz, 2H), 4.75 (t, J = 6.0 Hz, 1H), 7.70-7.72 (m, 2H), 7.83-7.85 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 38.7, 53.1, 99.9, 123.3, 132.0, 134.0, 168.0; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{13}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 236.0923; found: 236.0916.

2-(2-Oxo-2-phenylethyl)isoindoline-1,3-dione (3k)



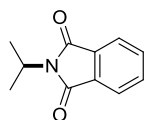
White solid. m.p. 162-163 °C. ^1H NMR (500 MHz, CDCl_3) δ 5.13 (s, 2H), 7.50 (t, J = 7.5 Hz, 2H), 7.62 (t, J = 7.5 Hz, 1H), 7.74 (d, J = 3.5 Hz, 2H), 7.88-7.89 (m, 2H), 7.99-8.00 (d, J = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 44.1, 123.4, 128.0, 128.8, 132.0, 133.9, 134.0, 134.2, 167.7, 190.9; HRMS (ESI) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{NO}_3$ $[\text{M}+\text{H}]^+$: 266.0817; found: 266.0810.

Ethyl 2-(1,3-dioxoisindolin-2-yl)acetate (3l)



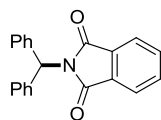
White solid. m.p. 110-111 °C. ^1H NMR (500 MHz, CDCl_3) δ 1.19 (t, J = 7.0 Hz, 3H), 4.13 (q, J = 7.0 Hz, 2H), 4.34 (s, 2H), 7.65 (s, 2H), 7.77 (d, J = 2.5 Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 13.9, 38.7, 61.7, 123.4, 131.8, 134.0, 167.1, 167.2; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{11}\text{NO}_4$ $[\text{M}+\text{H}]^+$: 234.0766; found: 234.0772.

2-Isopropylisoindoline-1,3-dione (3m)



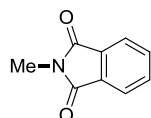
White solid. m.p. 78-79 °C. ^1H NMR (500 MHz, CDCl_3) δ 1.49 (d, J = 7.0 Hz, 6H), 4.54 (t, J = 7.0 Hz, 1H), 7.69-7.71 (m, 2H), 7.81-7.83 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 20.1, 42.9, 122.9, 132.1, 133.7, 168.4; HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{11}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 190.0868; found: 190.0874.

2-Benzhydrylisoindoline-1,3-dione (3n)



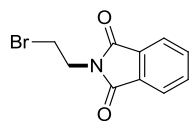
White solid. m.p. 141-142 °C. ^1H NMR (500 MHz, CDCl_3) δ 6.72 (s, 1H), 7.28-7.32 (m, 6H), 7.34-7.39 (m, 4H), 7.69-7.72 (m, 2H), 7.81-7.85 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 57.7, 123.4, 127.7, 128.4, 128.7, 131.8, 134.1, 138.1, 167.9; HRMS (ESI) m/z calcd for $\text{C}_{21}\text{H}_{15}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 314.1181; found: 314.1177.

2-Methylisoindoline-1,3-dione (3p)



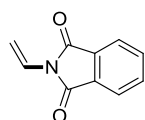
White solid. m.p. 128-129 °C. ^1H NMR (500 MHz, CDCl_3) δ 3.18 (s, 3H), 7.70-7.73 (m, 2H), 7.83-7.84 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 23.8, 123.0, 132.1, 133.7, 168.3; HRMS (ESI) m/z calcd for $\text{C}_9\text{H}_7\text{NO}_2$ $[\text{M}+\text{H}]^+$: 162.0555; found: 162.0549.

2-(2-Bromoethyl)isoindoline-1,3-dione (3q)



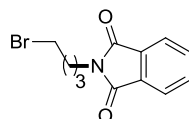
White solid. m.p. 83-84 °C. ^1H NMR (500 MHz, CDCl_3) δ 3.62 (t, J = 7.0 Hz, 2H), 4.11 (t, J = 7.0 Hz, 2H), 7.75 (m, 2H), 7.88 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 28.1, 39.2, 123.4, 131.7, 134.1, 167.7; HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_8\text{BrNO}_2$ $[\text{M}+\text{H}]^+$: 253.9817; found: 253.9810.

2-Vinylisoindoline-1,3-dione (4)



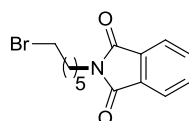
White solid. m.p. 86-87 °C. ^1H NMR (500 MHz, CDCl_3) δ 5.05 (d, J = 9.5 Hz, 1H), 6.09 (d, J = 16.5 Hz, 1H), 6.88 (dd, J = 9.5 Hz, 16.5 Hz, 1H), 7.74-7.77 (m, 2H), 7.86-7.89 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 104.4, 123.6, 123.8, 131.6, 134.4, 166.4; HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_7\text{NO}_2$ $[\text{M}+\text{H}]^+$: 174.0555; found: 174.0548.

2-(4-Bromobutyl)isoindoline-1,3-dione (3r)



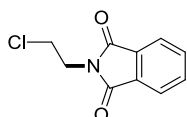
White solid. m.p. 75-76 °C. ^1H NMR (500 MHz, CDCl_3) δ 1.84-1.93 (m, 4H), 3.45 (t, J = 6.5 Hz, 2H), 3.73 (t, J = 6.5 Hz, 2H), 7.72-7.74 (m, 2H), 7.84-7.86 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 27.2, 29.8, 32.8, 36.9, 123.2, 132.0, 134.0, 168.3; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{12}\text{BrNO}_2$ $[\text{M}+\text{H}]^+$: 282.0130; found: 282.0125.

2-(6-Bromohexyl)isoindoline-1,3-dione (3s)



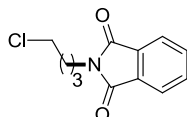
White solid. m.p. 53-54 °C. ^1H NMR (500 MHz, CDCl_3) δ 1.38-1.41 (m, 2H), 1.46-1.52 (m, 2H), 1.67-1.73 (m, 2H), 1.83-1.89 (m, 2H), 3.40 (t, $J = 7.0$ Hz, 2H), 3.69 (t, $J = 7.0$ Hz, 2H), 7.71-7.73 (m, 2H), 7.84-7.85 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 26.0, 27.6, 28.4, 32.5, 33.7, 37.8, 123.1, 132.1, 133.8, 168.4; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{16}\text{BrNO}_2$ $[\text{M}+\text{H}]^+$: 310.0443; found: 310.0449.

2-(2-Chloroethyl)isoindoline-1,3-dione (3t)



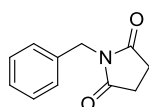
White solid. m.p. 82-83 °C. ^1H NMR (500 MHz, CDCl_3) δ 3.78 (t, $J = 6.5$ Hz, 2H), 4.06 (t, $J = 6.5$ Hz, 2H), 7.74-7.76 (m, 2H), 7.87-7.89 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 39.4, 40.8, 123.5, 131.8, 134.2, 167.9; HRMS (ESI) m/z calcd for $\text{C}_{10}\text{H}_8\text{ClNO}_2$ $[\text{M}+\text{H}]^+$: 210.0322; found: 210.0317.

2-(4-Chlorobutyl)isoindoline-1,3-dione (3u)



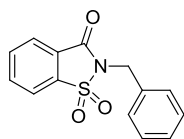
White solid. m.p. 68-69 °C. ^1H NMR (500 MHz, CDCl_3) δ 1.84-1.93 (m, 4H), 3.45 (t, $J = 6.5$ Hz, 2H), 3.73 (t, $J = 6.5$ Hz, 2H), 7.72-7.74 (m, 2H), 7.84-7.86 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 27.2, 29.8, 32.8, 36.9, 123.2, 132.0, 134.0, 168.3; HRMS (ESI) m/z calcd for $\text{C}_{12}\text{H}_{12}\text{ClNO}_2$ $[\text{M}+\text{H}]^+$: 238.0635; found: 238.0631.

1-Benzylpyrrolidine-2,5-dione (7)



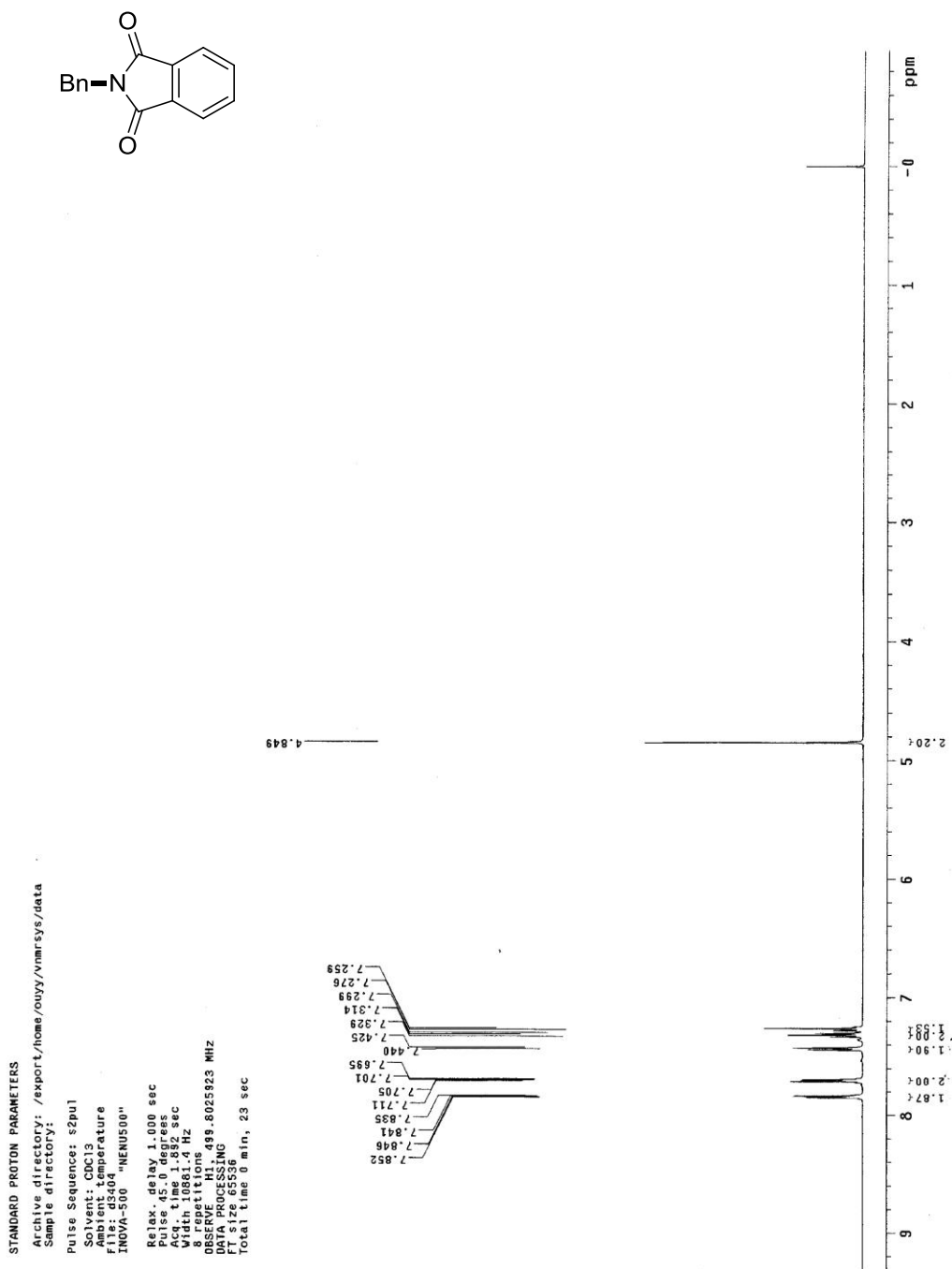
White solid. m.p. 98-99 °C. ^1H NMR (500 MHz, CDCl_3) δ 2.69 (s, 4H), 4.65 (s, 2H), 7.27-7.32 (m, 3H), 7.38-7.39 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 28.1, 42.3, 127.9, 128.5, 128.8, 135.7, 176.8; HRMS (ESI) m/z calcd for $\text{C}_{11}\text{H}_{11}\text{NO}_2$ $[\text{M}+\text{H}]^+$: 190.0868; found: 190.0872.

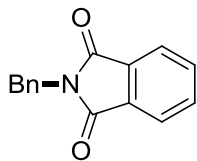
2-Benzylbenzo[d]isothiazol-3(2H)-one 1,1-dioxide (8)



White solid. m.p. 94-95 °C. ^1H NMR (500 MHz, CDCl_3) δ 4.91 (s, 2H), 7.30-7.36 (m, 3H), 7.50 (d, J = 6.5 Hz, 2H), 7.79-7.84 (m, 2H), 7.91 (d, J = 7.0 Hz, 1H), 8.03 (d, J = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 42.5, 120.9, 125.0, 125.1, 127.1, 128.2, 128.6, 128.6, 134.3, 134.4, 134.6, 134.7, 137.6, 158.8; HRMS (ESI) m/z calcd for $\text{C}_{14}\text{H}_{11}\text{NO}_3\text{S}$ $[\text{M}+\text{H}]^+$: 274.0538; found: 274.0545.

III. Copies of ^1H and ^{13}C NMR spectra for compounds 3, 4, 7 and 8





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrSYS/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: 1-14-87

File: d3724

INNOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

Observed F1 125.6754680 MHz

Observed C1 125.6754680 MHz

Decouple H1 439.8050805 MHz

Power 42 dB

Continuously on

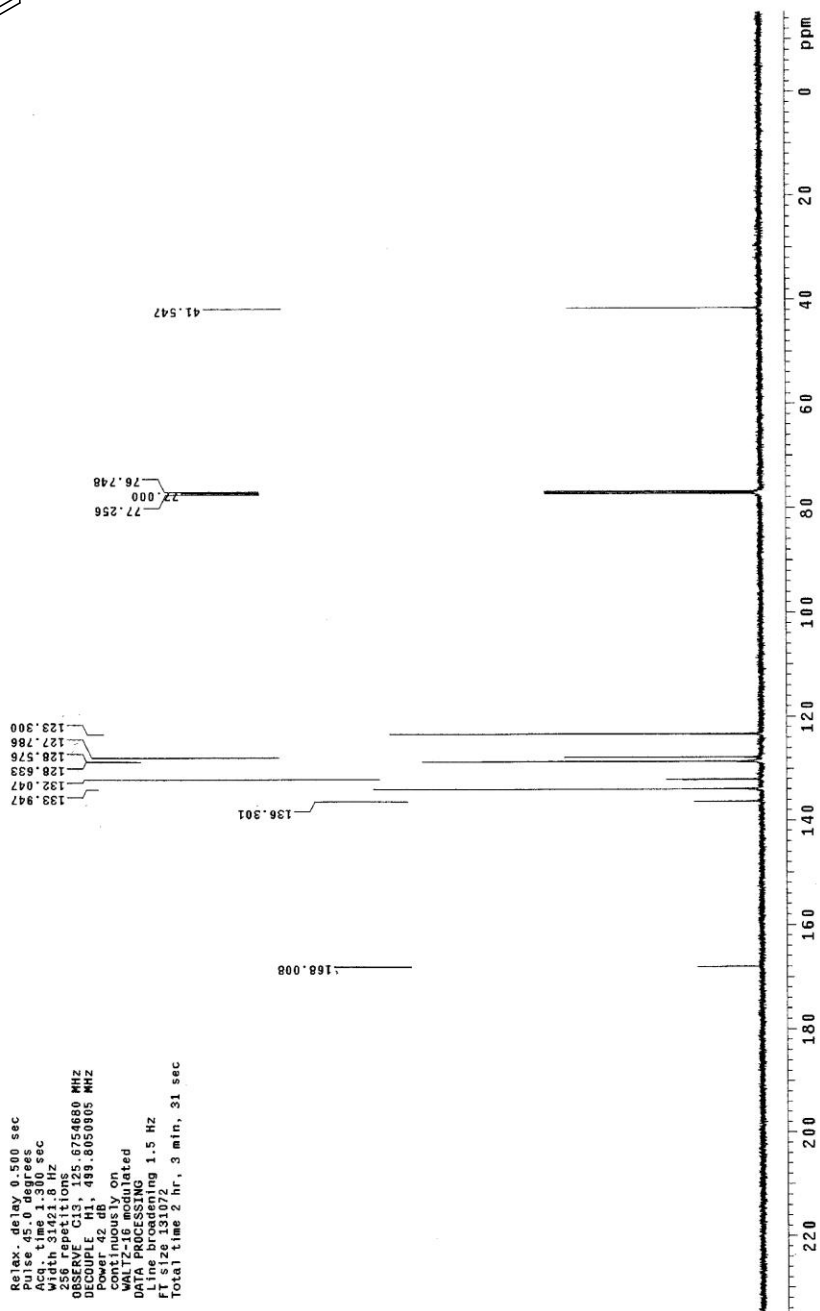
Watergate gated

DATA PROCESSING

Line broadening 1.5 Hz

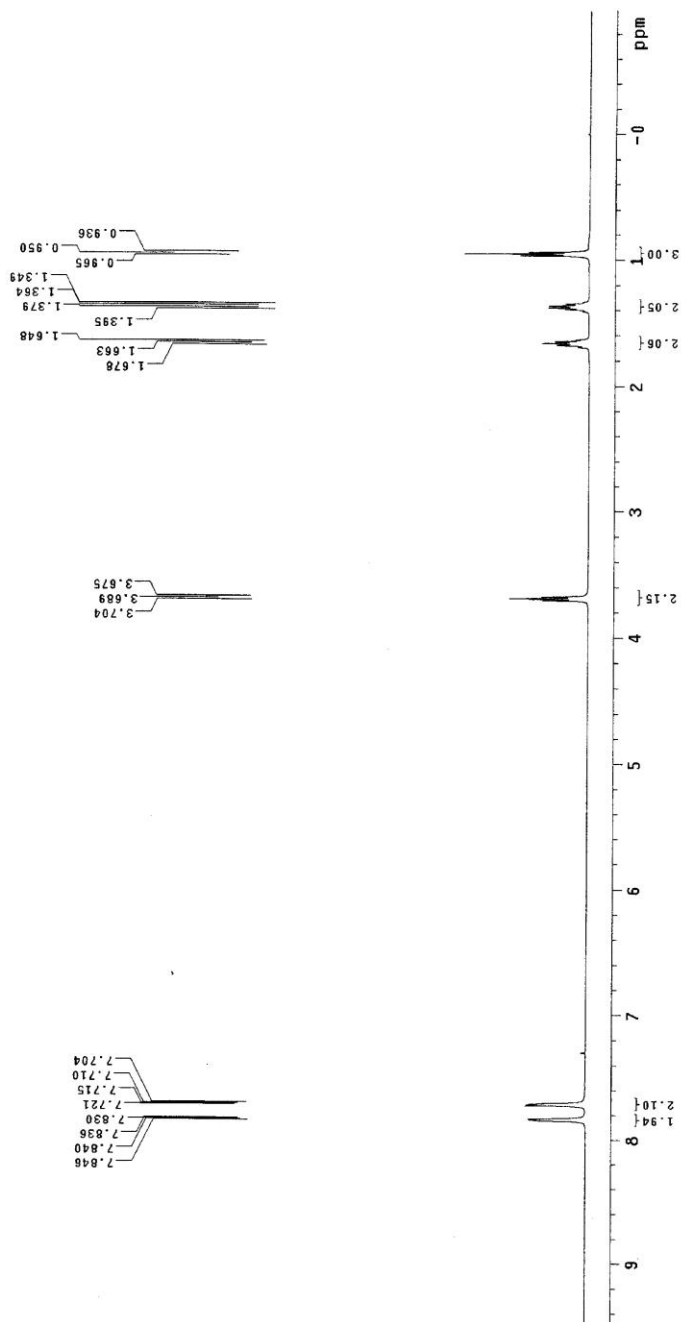
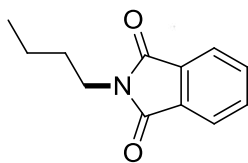
FT size 131072

Total time 2 hr, 3 min, 31 sec



STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouxy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pu1
Solvent: CDCl3
Ambient temperature
File: d4262 "NENU500"
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse delay 0.000 sec
Acq. time 1.892 sec
Width 10768.6 Hz
8 repetitions
Observed F2 99.8025712 MHz
Observed F1 500.136098 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec

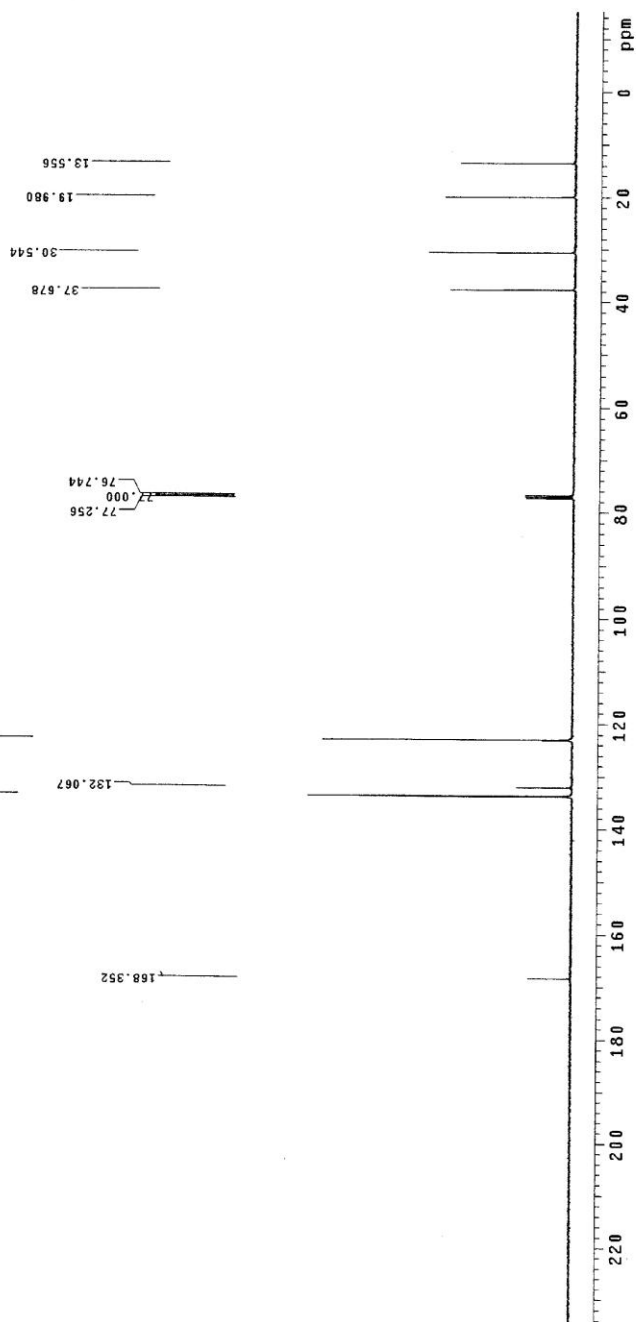
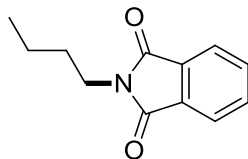


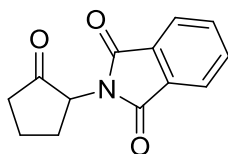
STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

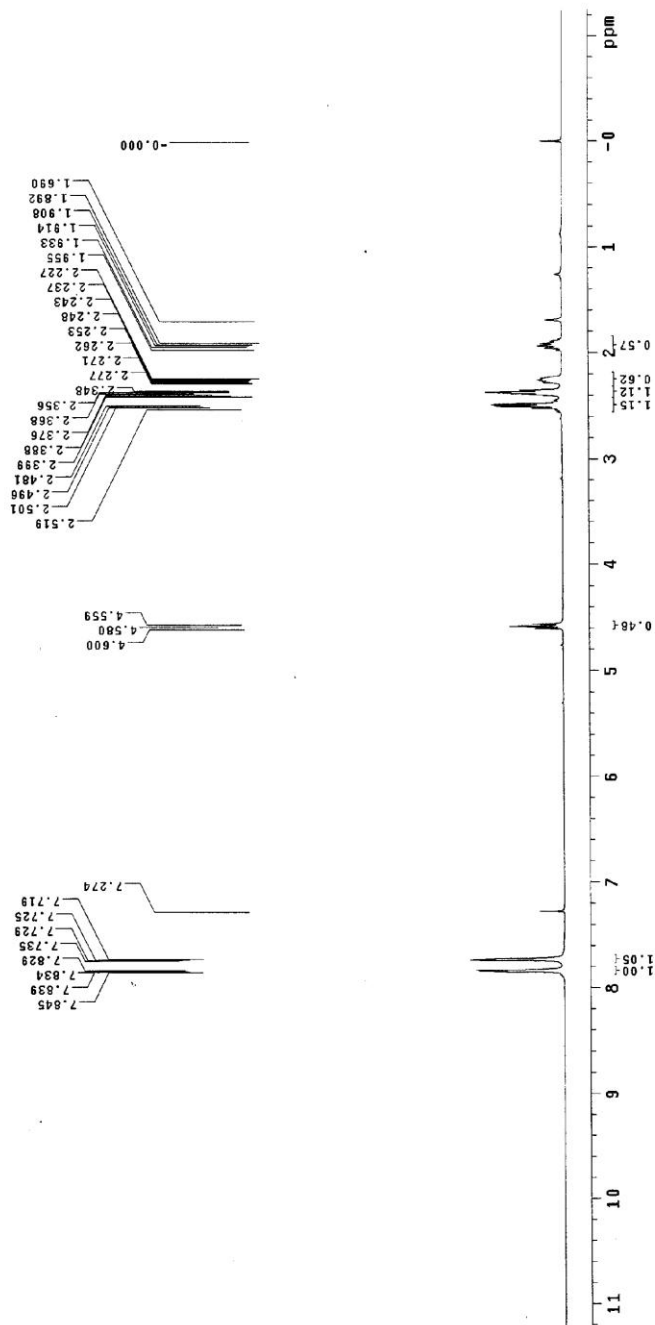
Pulse Sequence: szpul
Solvent: cdcl3
Ambient temperature
User: yyy-87
File: d4263
INOVA-500 "NENU500"

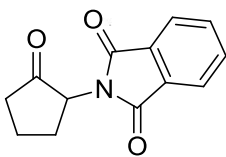
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
F1 125.754689 MHz
128 repetitions
OBSERVE C13, 125.754689 MHz
DECOUPLE H1, 499.8050905 MHz
Power H2/H1 on
Cont. INUSV on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
F2 size 131072
Total time 2 hr, 3 min, 31 sec





STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouy/vnmrSYS/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl₃
 Acquisition temperature: 300 K
 File: d4672
 INOVA-500 "HENU500"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.150 sec
 Width 10158.1 Hz
 4 repetitions
 OBSERVE H1 499.8025835 MHz
 DATA PROCESSING
 11 scans
 Total time 0 min, 11 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouvy/vmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: j4-87

File: d676"MENU500"

INOVA-500

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

NUC1 13C1013

NUC2 13C1013

4480.100000000000

OBSERVE C13, 125.6754656 MHZ

DECOUPLE H1, 499.8050805 MHZ

Power 42 dB

Contingency ON

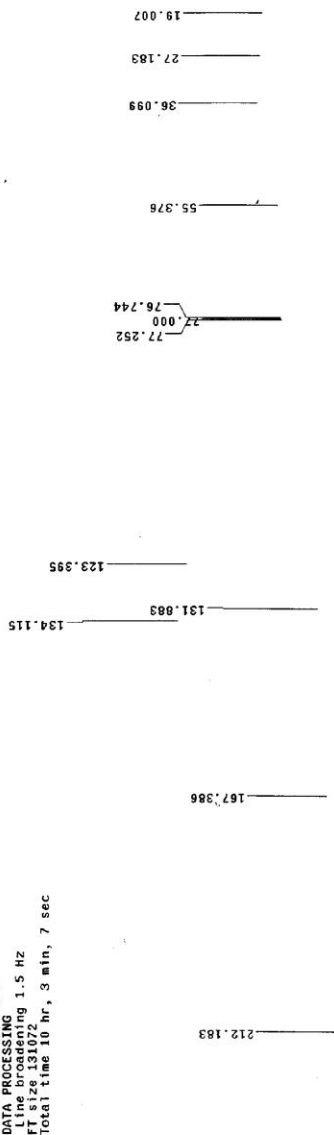
WALTZ-16 modulated

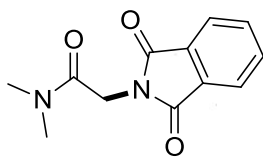
DATA PROCESSING

Line broadening 1.5 Hz

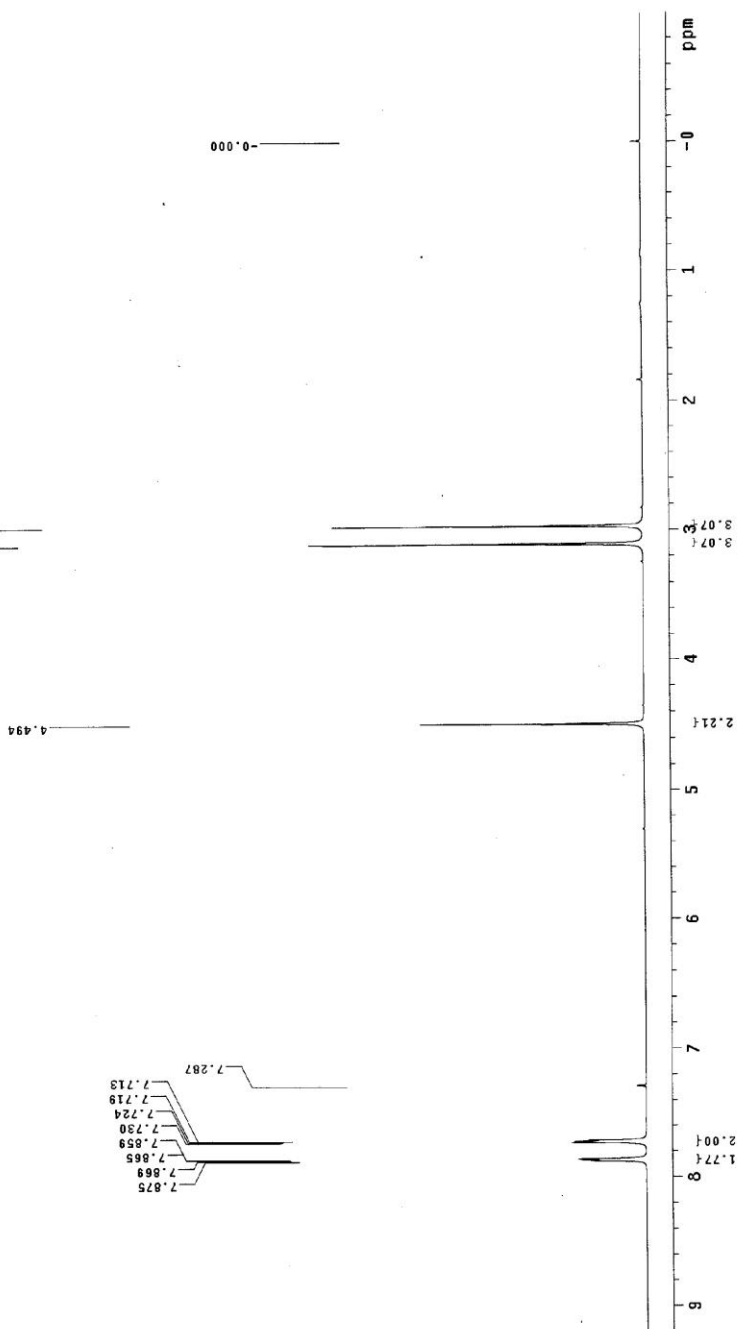
FT size 131072

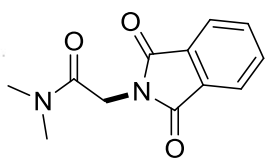
Total time 10 hr, 3 min, 7 sec



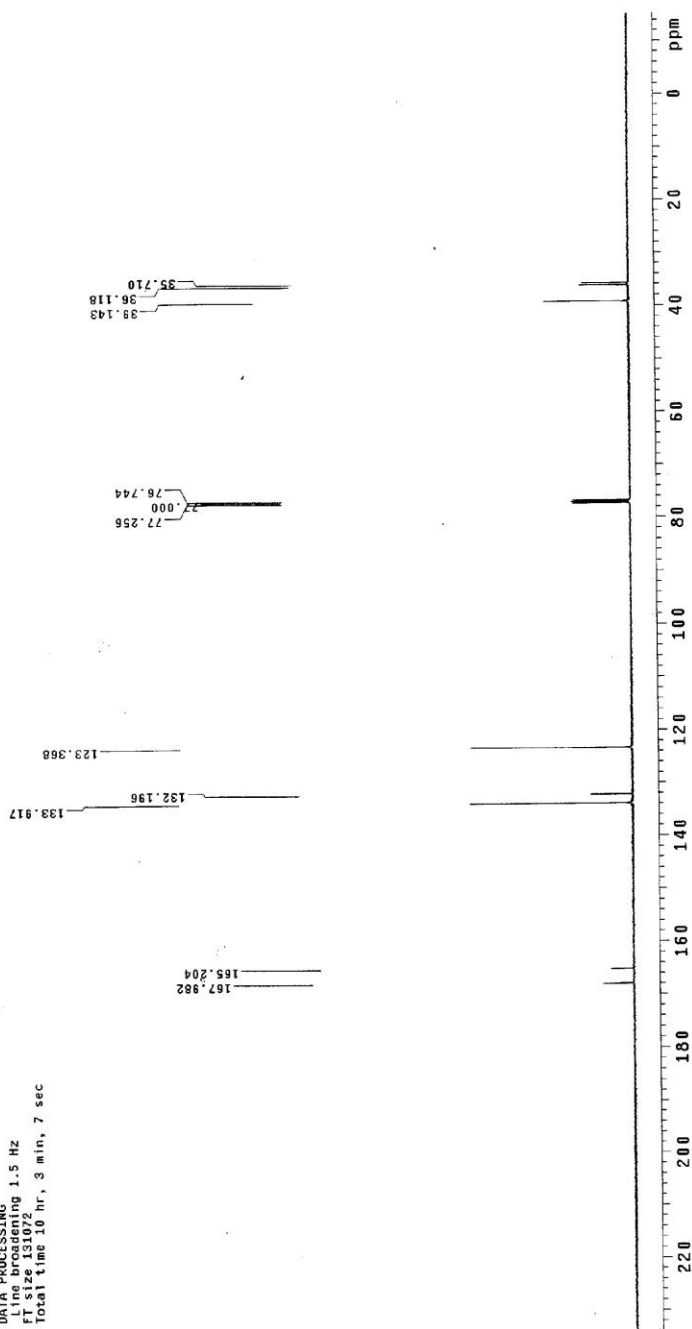


STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouyy/vnmrsws/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl₃
 Ambient temperature
 File: d4661
 INOVA-500 "HENU500"
 Relax. delay: 1.000 sec
 Pulse: 45.0 degrees
 Acq. time: 1.892 sec
 Width: 10138.1 Hz
 8 repetitions
 Observed: 499.8025770 MHz
 DATA PROCESSING
 FT size: 65536
 Total time: 0 min, 23 sec





STANDARD CARBON PARAMETERS
 Archive directory: /export/home/ouvy/vnmr/sys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: cdcl3
 Name: 1-14-B7
 Experiment: 1-14-B7
 File: d4662
 INOVA-500 "NMR500"
 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Width 1.300 sec
 Width 31421.8 Hz
 256 repetitions
 OBSERVE C13, 125.6754714 MHz
 DECOUPLE H1, 499.6058903 MHz
 Lock on continuously
 WALTZ-16 modulated
 DATA PROCESSING
 Time domain 1.5 Hz
 FT size 131072
 Total time 10 hr, 3 min, 7 sec



STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmr/sys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Acquisition temperature

File: d5c533

INNOVA-500 "NENU500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.00 sec

Width 10861.4 Hz

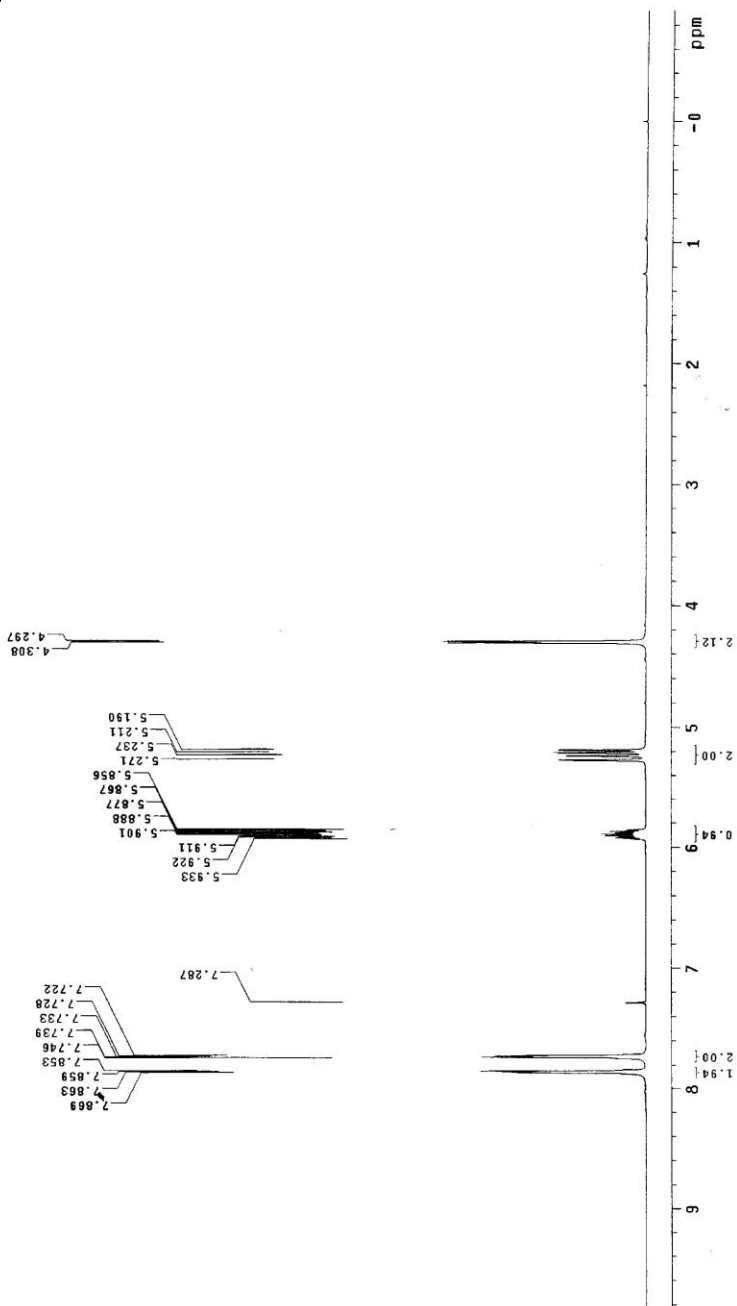
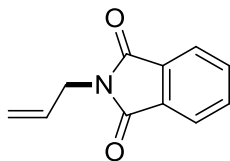
4 repetitions

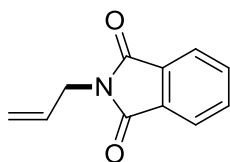
OBSERVE H1: 499.8025783 MHz

DATA PROCESSING

File: d5c533

Total time 0 min, 11 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrSYS/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: i-13-87

File: d3754 "NENU500"

INOVA-500

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

Observed C13 125.6754862 MHz

Decouple C13 125.6754862 MHz

Decouple H1 499.8050905 MHz

Power 42 dB

Continuous on

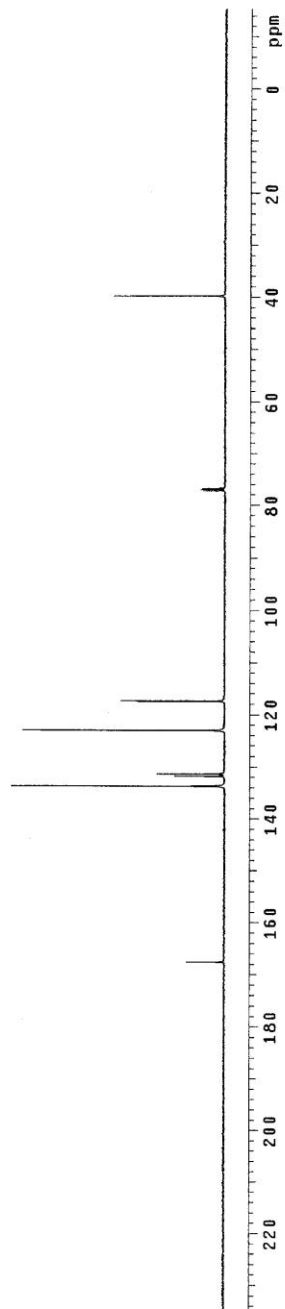
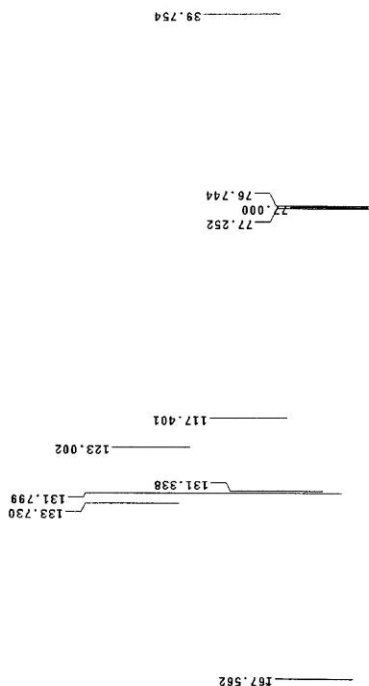
WALT160

DATA PROCESSING

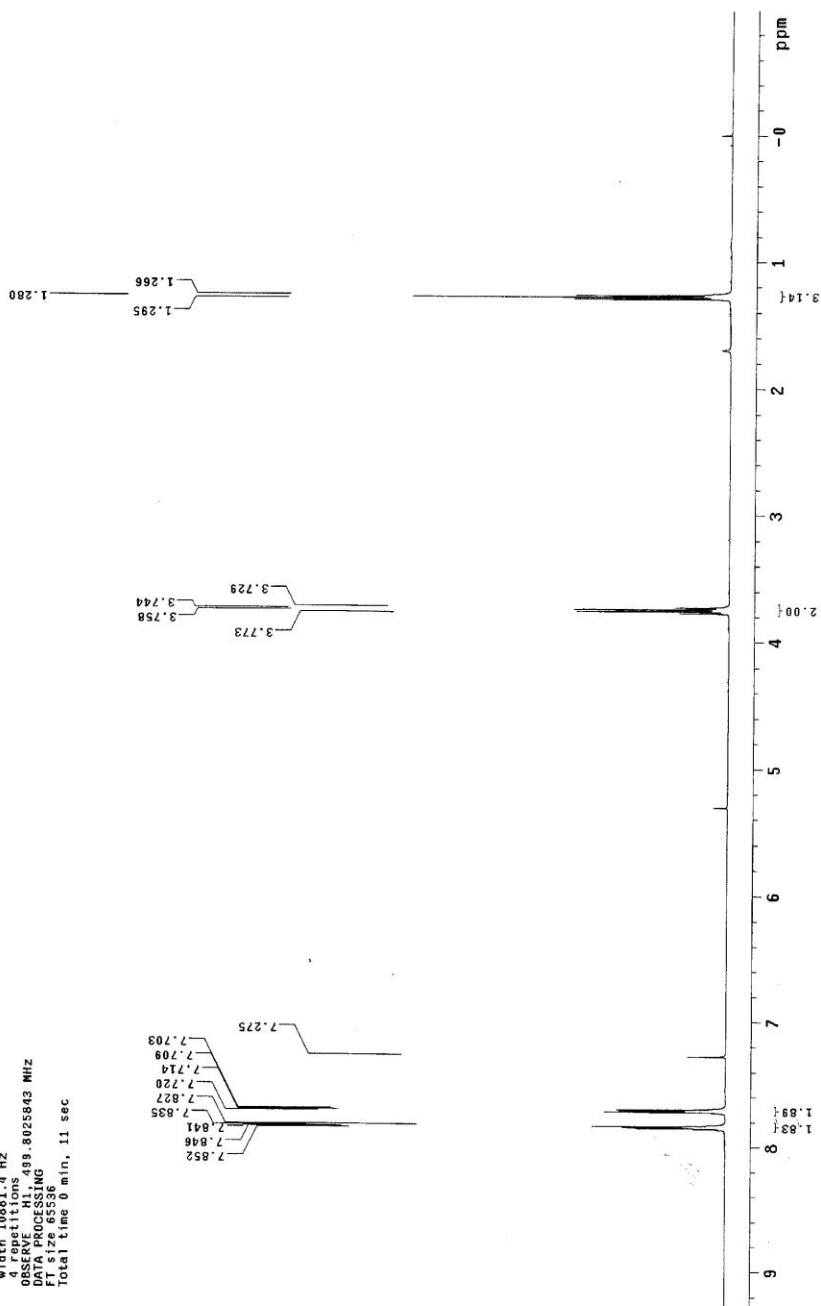
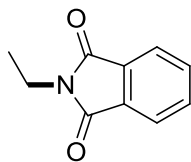
Line broadening 1.5 Hz

FT size 131072

Total time 3 hr, 56 sec



STANDARD PROTON PARAMETERS
 Archive directory: /export/home/duffy/vnmr-sys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Acquisition temperature
 File: d3721.nu
 INOVA-500 "NMR500"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.494 sec
 Width 10061 Hz
 4 repetitions
 OBSERVE H1, 499.8025843 MHz
 DATA PROCESSING
 F2 - F1
 Total time 0 min, 11 sec



STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouy/vmarsys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Acquisition temperature

User: l-14-87

File: d3723

INOVA-500 "MNU500"

Relax. delay 0.500 sec

Pulse delay 0.000 sec

Acq. time 1.300 sec

Width 31421.8 Hz

128/repetitions 6754651 MHZ

DECOUPLE H1 488.8050805 MHZ

Power 42 dB

continuously on

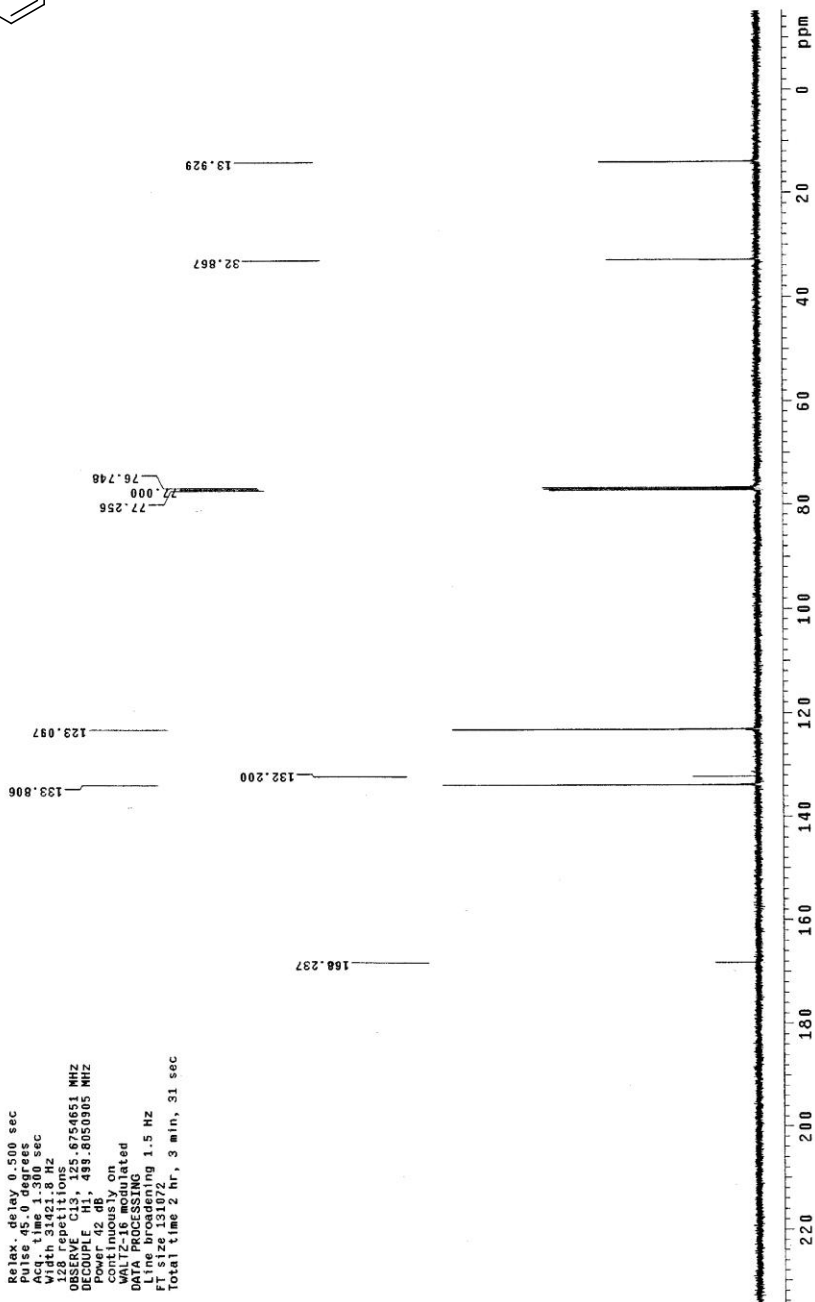
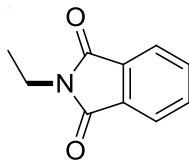
Waltz 16 modulated

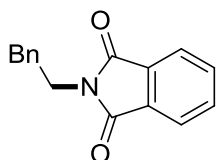
DATA PROCESSING

Line broadening 1.5 Hz

FT size 131072

Total time 2 hr, 3 min, 31 sec





STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouy/vmr/sys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Acquisition temperature

File: d34f51

INOVA-500 "MNU500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 11.00 sec

Width 10861.4 Hz

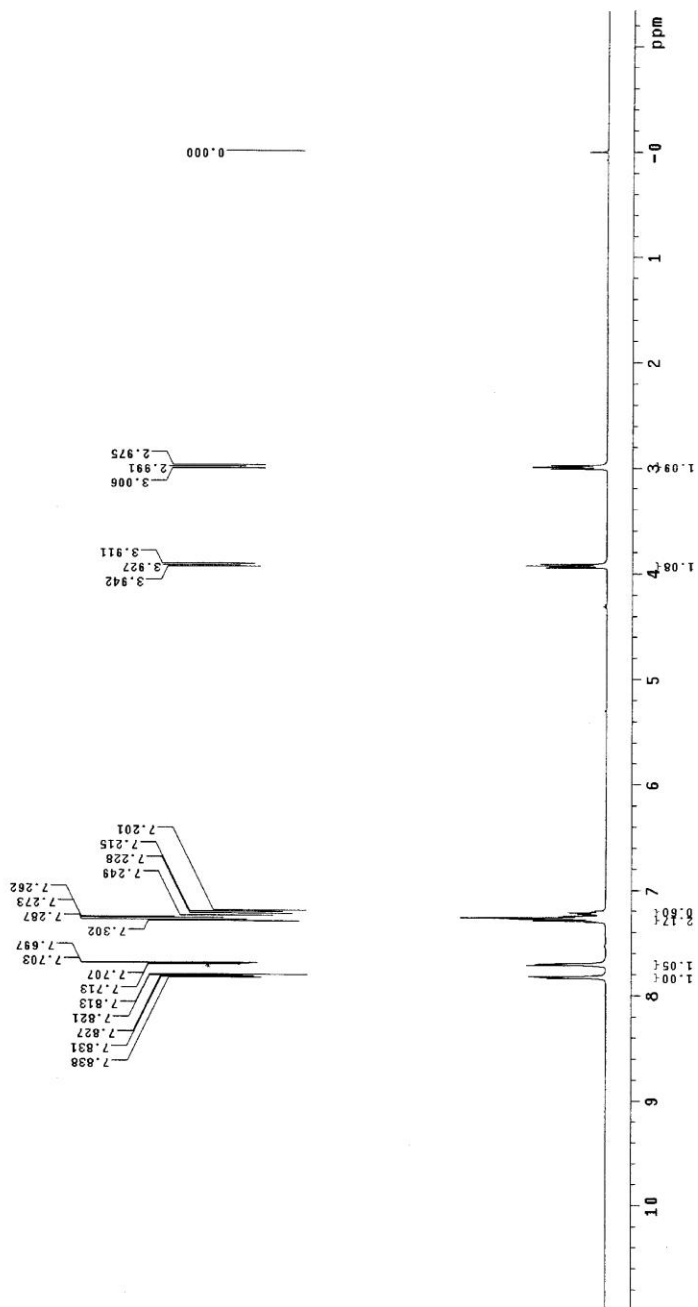
4 repetitions

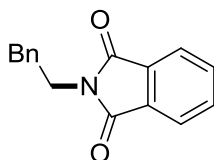
OBSERVE H1, 499.8025903 MHz

DATA PROCESSING

File: 65536

Total time 0 min, 11 sec





STANDARD CARBON PARAMETERS
 Archive directory: /export/home/ougy/vnmr/sys/data
 Sample directory:

Pulse Sequence: s2pul
 Solvent: cdcl3
 Ambient temperature
 File: d3758
 INOVA-500 "NENU500"

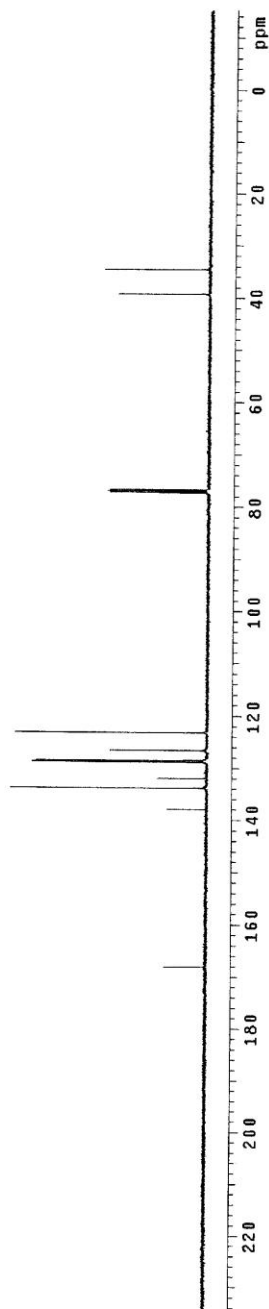
Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Width 31421.8 Hz
 128 repetitions
 OBSERVE C13, 125.675489 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power 42 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 F1 size 131072
 Total time 3 hr, 56 sec

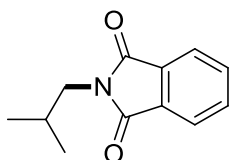
137.938
 133.852
 131.983
 128.797
 126.492
 126.580
 123.158

77.252
 77.000
 76.744

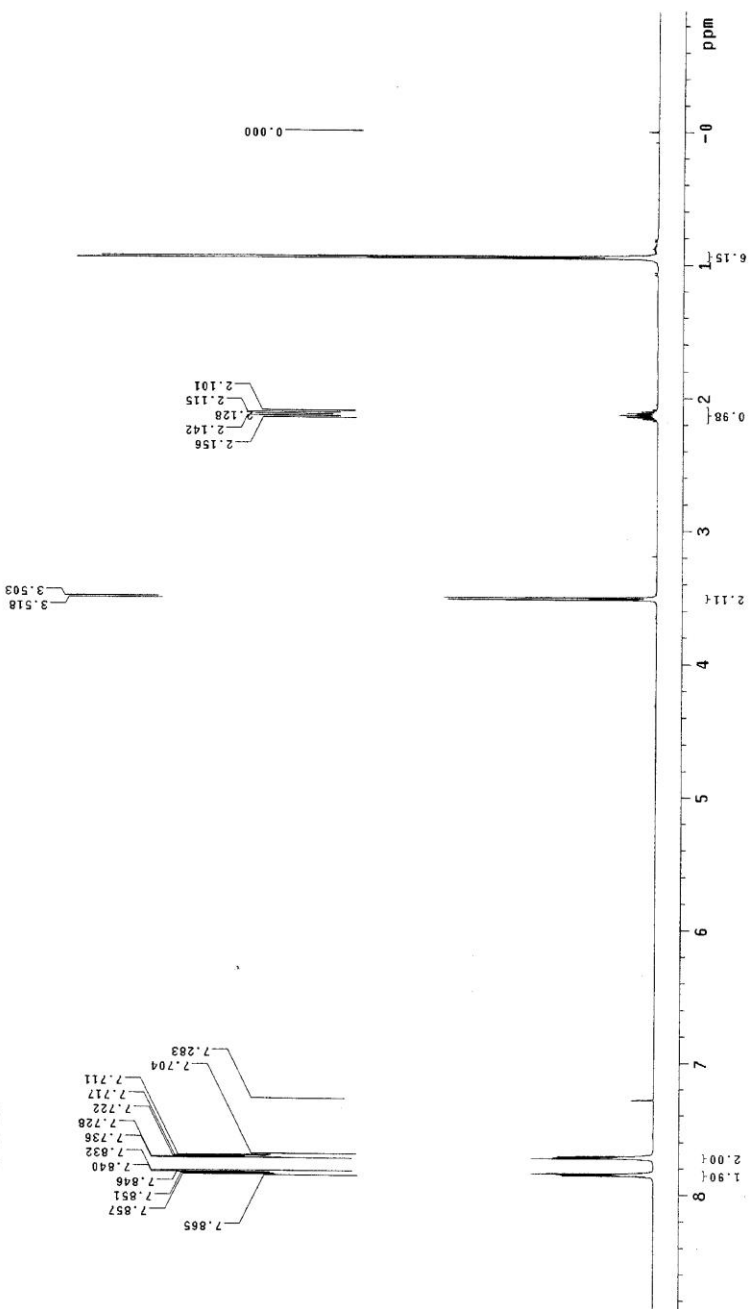
39.223
 34.561

166.111





STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouuy/vnmrsvs/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: CDCl3
 Sample temperature
 File: d3983
 INOVA-500 "NENU500"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.59 sec
 Width 10768.6 Hz
 8 repetitions
 OBSERVE H1: 499.8025807 MHz
 CHANNEL F2: 65536
 FT S1: 65536
 Total time 0 min, 23 sec





```
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
```

Pulse Sequence: s2pul

Solvent: cdcl_3

Ambient temperature 14.07

User: 1-14-87
File: d3984

File: d3984
INOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees
Acc. time 1.200 sec

Acq. time 1.300 sec
Width 31421.8 Hz

Width 31421.8 Hz
320 repetitions

DBSERVE C13, 125.6754

DECOUPLE H1, 499.8050
Power 42 dB

Power 42 dB
continuously on

WALTZ-16 modulated

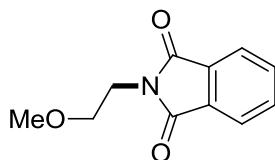
DATA PROCESSING

Line broadening 2.0 H:
FT size 131072

Particle size 131072
Total time 2 hr, 3 min

1930, 1931, 1932, 1933, 1934, 1935, 1936, 1937, 1938, 1939, 1940, 1941, 1942, 1943, 1944, 1945, 1946, 1947, 1948, 1949, 1950, 1951, 1952, 1953, 1954, 1955, 1956, 1957, 1958, 1959, 1960, 1961, 1962, 1963, 1964, 1965, 1966, 1967, 1968, 1969, 1970, 1971, 1972, 1973, 1974, 1975, 1976, 1977, 1978, 1979, 1980, 1981, 1982, 1983, 1984, 1985, 1986, 1987, 1988, 1989, 1990, 1991, 1992, 1993, 1994, 1995, 1996, 1997, 1998, 1999, 2000, 2001, 2002, 2003, 2004, 2005, 2006, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2020, 2021, 2022, 2023, 2024, 2025, 2026, 2027, 2028, 2029, 2030, 2031, 2032, 2033, 2034, 2035, 2036, 2037, 2038, 2039, 2040, 2041, 2042, 2043, 2044, 2045, 2046, 2047, 2048, 2049, 2050, 2051, 2052, 2053, 2054, 2055, 2056, 2057, 2058, 2059, 2060, 2061, 2062, 2063, 2064, 2065, 2066, 2067, 2068, 2069, 2070, 2071, 2072, 2073, 2074, 2075, 2076, 2077, 2078, 2079, 2080, 2081, 2082, 2083, 2084, 2085, 2086, 2087, 2088, 2089, 2090, 2091, 2092, 2093, 2094, 2095, 2096, 2097, 2098, 2099, 2100, 2101, 2102, 2103, 2104, 2105, 2106, 2107, 2108, 2109, 2110, 2111, 2112, 2113, 2114, 2115, 2116, 2117, 2118, 2119, 2120, 2121, 2122, 2123, 2124, 2125, 2126, 2127, 2128, 2129, 2130, 2131, 2132, 2133, 2134, 2135, 2136, 2137, 2138, 2139, 2140, 2141, 2142, 2143, 2144, 2145, 2146, 2147, 2148, 2149, 2150, 2151, 2152, 2153, 2154, 2155, 2156, 2157, 2158, 2159, 2160, 2161, 2162, 2163, 2164, 2165, 2166, 2167, 2168, 2169, 2170, 2171, 2172, 2173, 2174, 2175, 2176, 2177, 2178, 2179, 2180, 2181, 2182, 2183, 2184, 2185, 2186, 2187, 2188, 2189, 2190, 2191, 2192, 2193, 2194, 2195, 2196, 2197, 2198, 2199, 2200, 2201, 2202, 2203, 2204, 2205, 2206, 2207, 2208, 2209, 2210, 2211, 2212, 2213, 2214, 2215, 2216, 2217, 2218, 2219, 2220, 2221, 2222, 2223, 2224, 2225, 2226, 2227, 2228, 2229, 2230, 2231, 2232, 2233, 2234, 2235, 2236, 2237, 2238, 2239, 2240, 2241, 2242, 2243, 2244, 2245, 2246, 2247, 2248, 2249, 2250, 2251, 2252, 2253, 2254, 2255, 2256, 2257, 2258, 2259, 2260, 2261, 2262, 2263, 2264, 2265, 2266, 2267, 2268, 2269, 2270, 2271, 2272, 2273, 2274, 2275, 2276, 2277, 2278, 2279, 2280, 2281, 2282, 2283, 2284, 2285, 2286, 2287, 2288, 2289, 2290, 2291, 2292, 2293, 2294, 2295, 2296, 2297, 2298, 2299, 2300, 2301, 2302, 2303, 2304, 2305, 2306, 2307, 2308, 2309, 2310, 2311, 2312, 2313, 2314, 2315, 2316, 2317, 2318, 2319, 2320, 2321, 2322, 2323, 2324, 2325, 2326, 2327, 2328, 2329, 2330, 2331, 2332, 2333, 2334, 2335, 2336, 2337, 2338, 2339, 2340, 2341, 2342, 2343, 2344, 2345, 2346, 2347, 2348, 2349, 2350, 2351, 2352, 2353, 2354, 2355, 2356, 2357, 2358, 2359, 2360, 2361, 2362, 2363, 2364, 2365, 2366, 2367, 2368, 2369, 2370, 2371, 2372, 2373, 2374, 2375, 2376, 2377, 2378, 2379, 2380, 2381, 2382, 2383, 2384, 2385, 2386, 2387, 2388, 2389, 2390, 2391, 2392, 2393, 2394, 2395, 2396, 2397, 2398, 2399, 2400, 2401, 2402, 2403, 2404, 2405, 2406, 2407, 2408, 2409, 2410, 2411, 2412, 2413, 2414, 2415, 2416, 2417, 2418, 2419, 2420, 2421, 2422, 2423, 2424, 2425, 2426, 2427, 2428, 2429, 2430, 2431, 2432, 2433, 2434, 2435, 2436, 2437, 2438, 2439, 2440, 2441, 2442, 2443, 2444, 2445, 2446, 2447, 2448, 2449, 2450, 2451, 2452, 2453, 2454, 2455, 2456, 2457, 2458, 2459, 2460, 2461, 2462, 2463, 2464, 2465, 2466, 2467, 2468, 2469, 2470, 2471, 2472, 2473, 2474, 2475, 2476, 2477, 2478, 2479, 2480, 2481, 2482, 2483, 2484, 2485, 2486, 2487, 2488, 2489, 2490, 2491, 2492, 2493, 2494, 2495, 2496, 2497, 2498, 2499, 2500, 2501, 2502, 2503, 2504, 2505, 2506, 2507, 2508, 2509, 2510, 2511, 2512, 2513, 2514, 2515, 2516, 2517, 2518, 2519, 2520, 2521, 2522, 2523, 2524, 2525, 2526, 2527, 2528, 2529, 2530, 2531, 2532, 2533, 2534, 2535, 2536, 2537, 2538, 2539, 2540, 2541, 2542, 2543, 2544, 2545, 2546, 2547, 2548, 2549, 2550, 2551, 2552, 2553, 2554, 2555, 2556, 2557, 2558, 2559, 2560, 2561, 2562, 2563, 2564, 2565, 2566, 2567, 2568, 2569, 2570, 2571, 2572, 2573, 2574, 2575, 2576, 2577, 2578, 2579, 2580, 2581, 2582, 2583, 2584, 2585, 2586, 2587, 2588, 2589, 2590, 2591, 2592, 2593, 2594, 2595, 2596, 2597, 2598, 2599, 2600, 2601, 2602, 2603, 2604, 2605, 2606, 2607, 2608, 2609, 2610, 2611, 2612





STANDARD PROTON PARAMETERS

Archive directory: /export/home/ruyy/vnmr/sys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Temperature

File: d4013

INNOVA-500 "NENU500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.00 sec

Width 10768.6 Hz

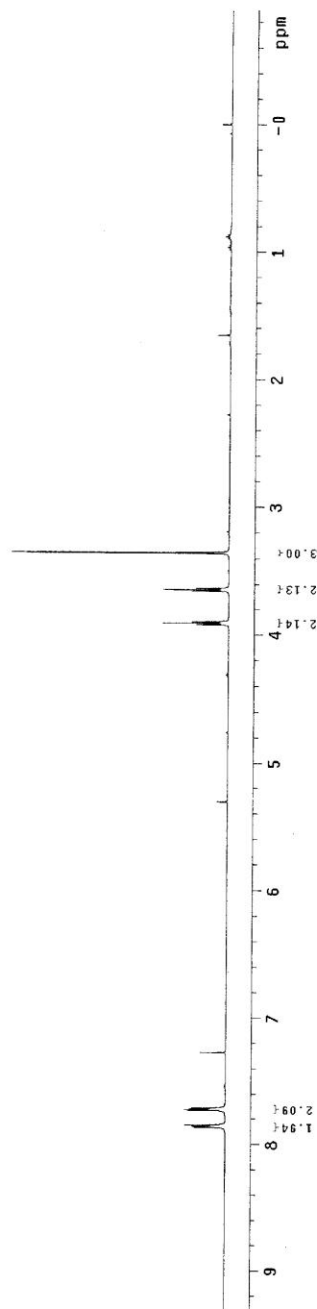
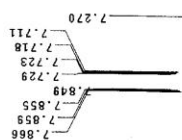
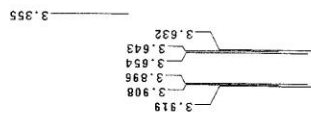
8 repetitions

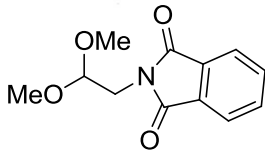
OBSERVE H1, 499.8025870 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 23 sec





STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouyy/vnmr/sys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 File: 58174 "MENU500"
 INOVA-500
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10766.6 Hz
 F2 (nu1) 500.136 MHz
 F1 (nu2) 125.761 MHz
 OBSERVE H1, 499.8025908 MHz
 DATA PROCESSING
 FT size 65536
 Total time 0 min, 23 sec

3.965

3.816
3.804

4.764
4.753
4.741

7.262
7.699
7.705
7.709
7.715
7.826
7.834
7.838
7.845

ppm

-0

1

2

3

4

5

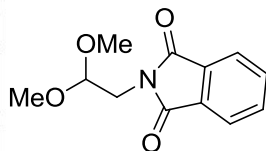
6

7

8

9

0.924
0.994



STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouvy/vmarsys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Temperature:

User: 1-14-87

File: d4184

INOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse delay 0.000 sec

Acq. time 1.300 sec

Width 31421.8 Hz

128 repetitions

DESSOLVE 13.554665 MHz

DECOUPLE H₁ 499.8050905 MHz

Power 42 dB

continuously on

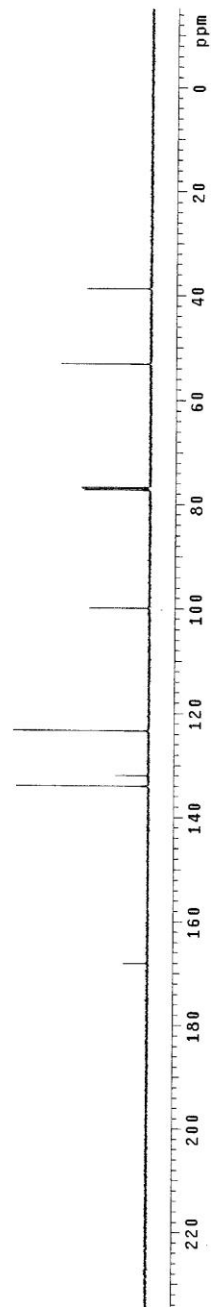
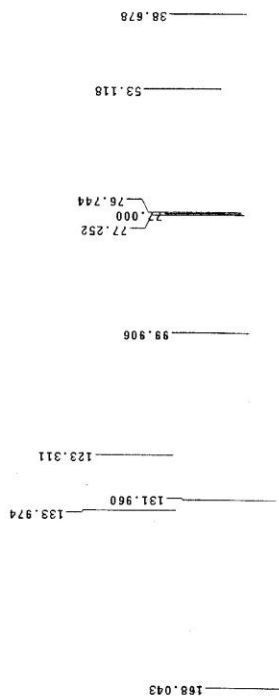
MTF 1500000

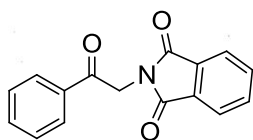
DATA PROCESSING

Line broadening 1.5 Hz

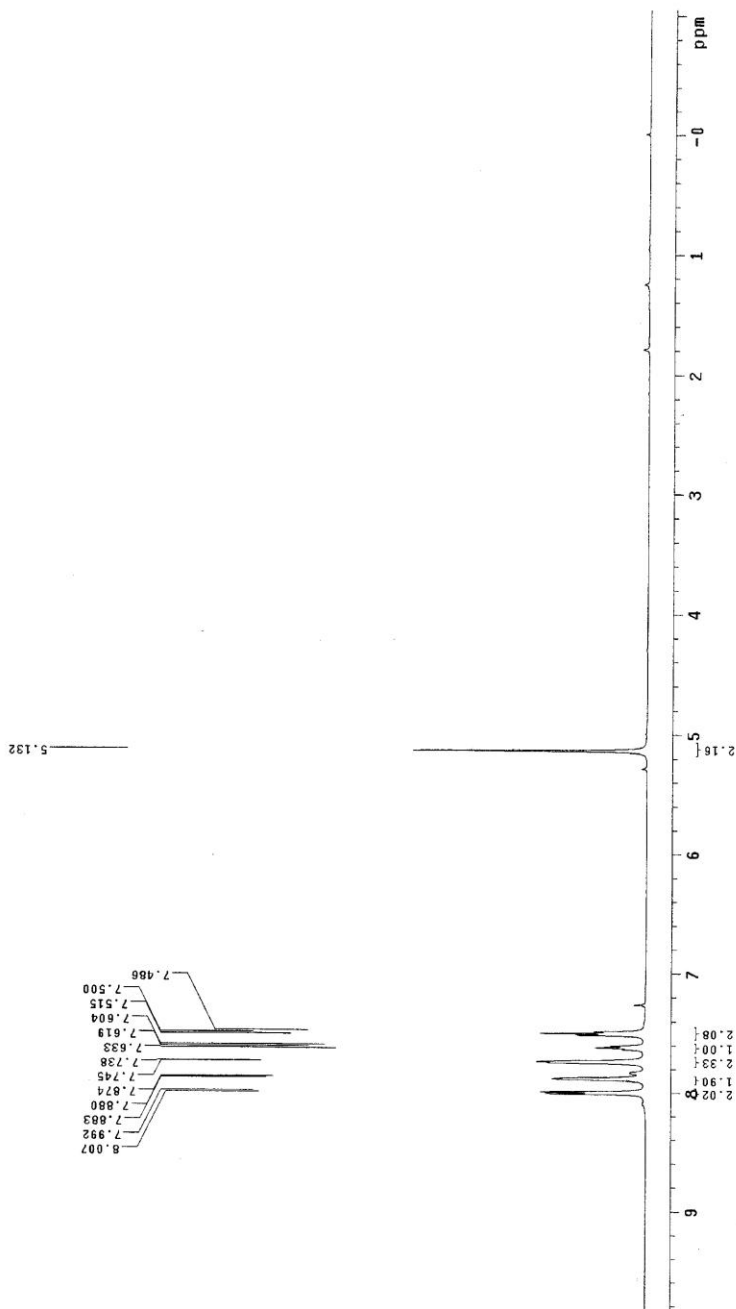
FT size 131072

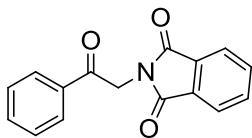
Total time 2 hr, 3 min, 31 sec



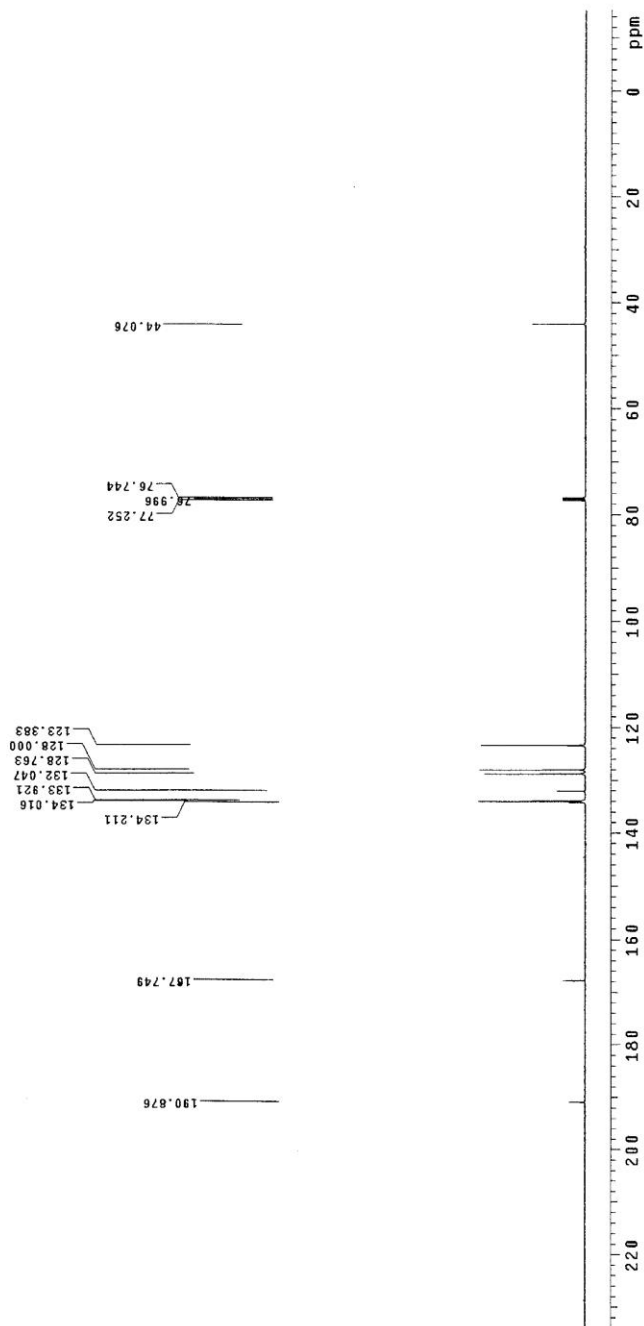


STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouyy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 File: 02241-NEW500
 INOVA-500
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10768.0 Hz
 SFO 499.8025909 MHz
 OBSERVE HL 499.8025909 MHz
 DATA PROCESSING
 FT size 65536
 Total time 0 min, 23 sec





STANDARD CARBON PARAMETERS
 Archive directory: /export/home/ouyy/vnmrSYS/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: cdcl3
 Ambient temperature
 User: jk-87
 File: d4303
 INOVA-500 "NMRUS00"
 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 0.00 sec
 Width 31421.8 Hz
 128 repetitions
 OBSERVE C13, 125.6754781 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power level 120.000
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 File: d4303
 Total time 2 hr, 3 min, 31 sec



STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouy/vnmr/sys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Temp: 300.2 K

File: d4384

INOVA-500 "NENUS00"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.55 sec

Width 10768.8 Hz

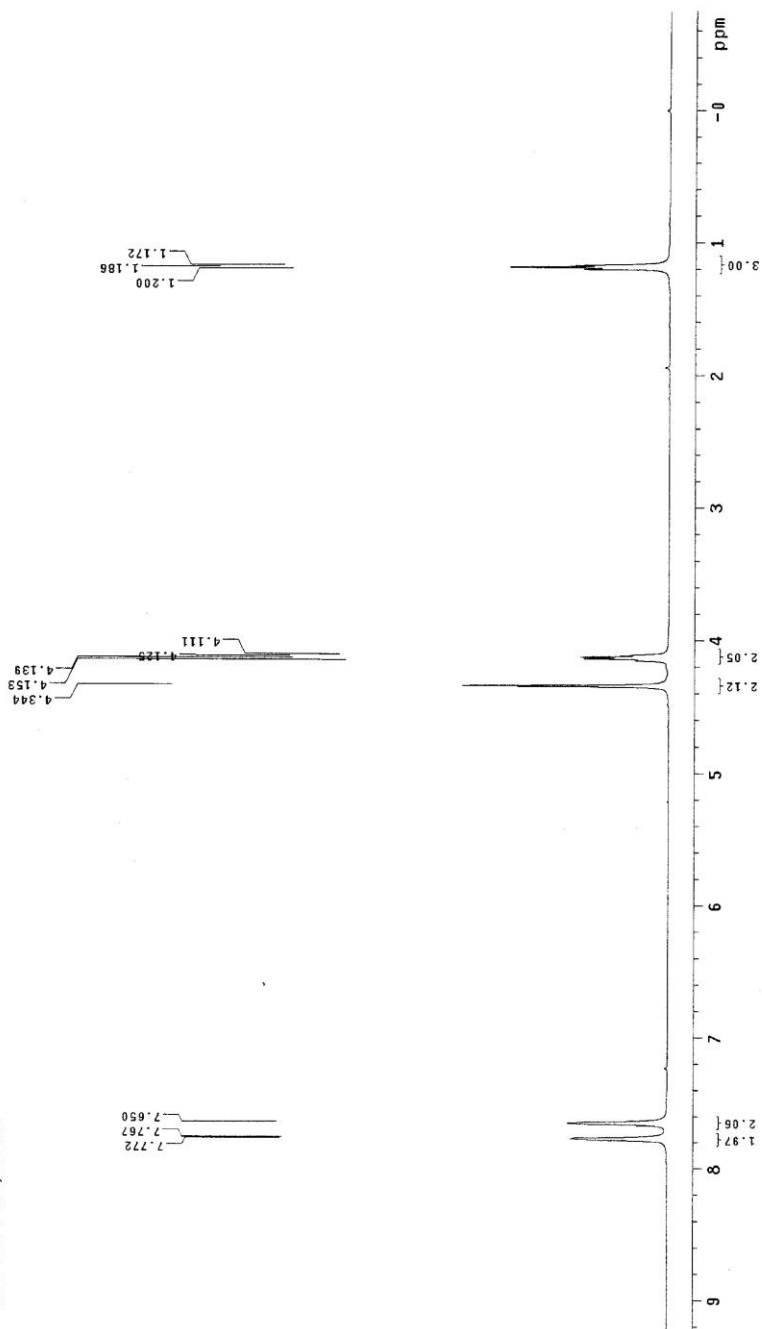
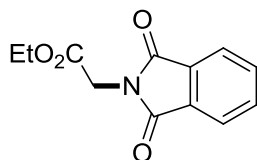
4 repetitions

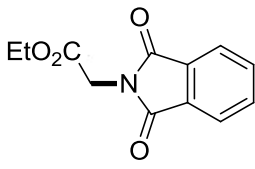
OBSERVE H1, 499.8026057 MHz

DATA PROCESSING

100.000 sec

Total time 0 min, 11 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouvy/vnmr/sys/data

Sample directory:

Pulse Sequence: s2pul1

Solvent: cdcl3

Acquisition temperature

User: 1-14-87

File: d4386

INNOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Pulse length 0.000 sec

Width 31421.8 Hz

64 repetitions

OBSERVE C13, 125.8754814 MHz

DECOUPLE H1, 499.8050895 MHz

Power 42 dB

continuously on

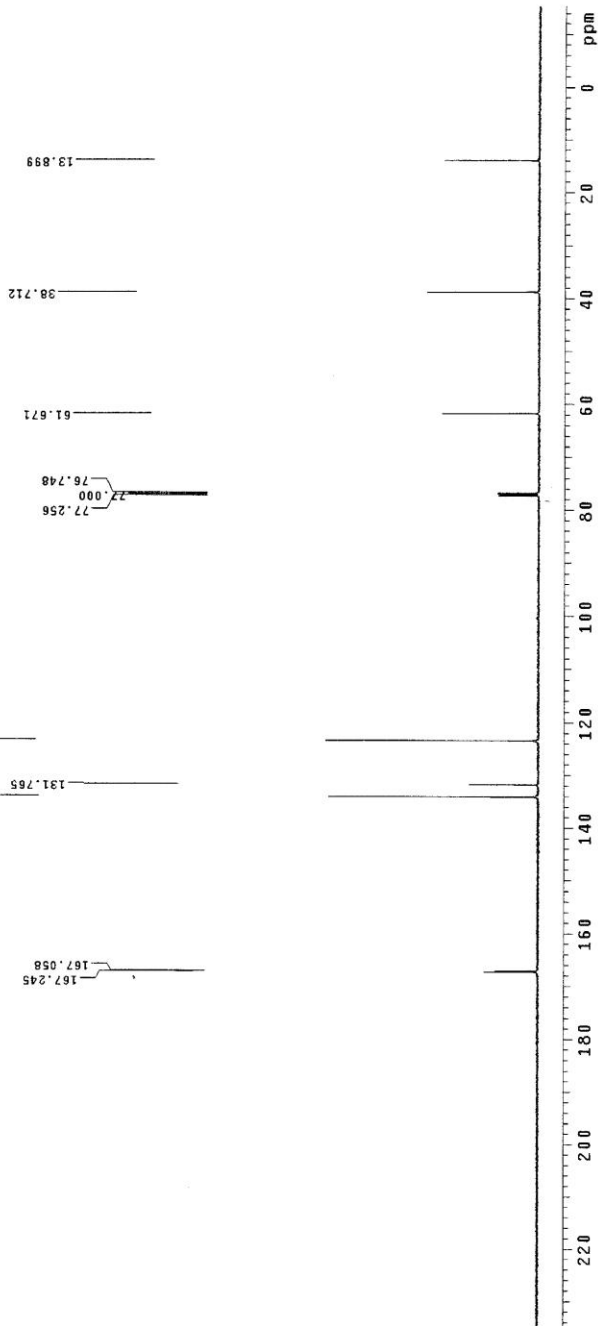
WALTZ-16 modulated

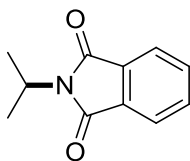
DATA PROCESSING

Time consuming 1.5 Hz

FT size 131072

Total time 7 hr, 32 min, 20 sec



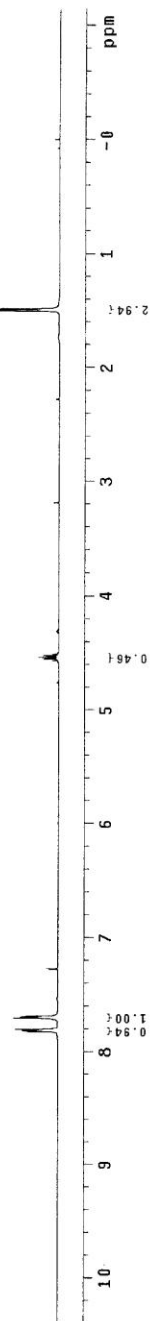


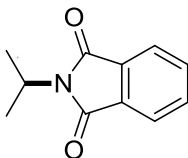
STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouyx/vnmr/sys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Acquisition temperature
 File: dd025
 INOVA-500 "NEU500"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acquisition time 1.000 sec
 Width 10768.6 Hz
 4 repetitions
 OBSERVE H1, 499.8025827 MHz
 DATA PROCESSING
 File: dd025
 Total time 0 min, 11 sec

1.509
1.489

4.555
4.541
4.527

7.825
7.819
7.814
7.807
7.809
7.792
7.698
7.692
7.278



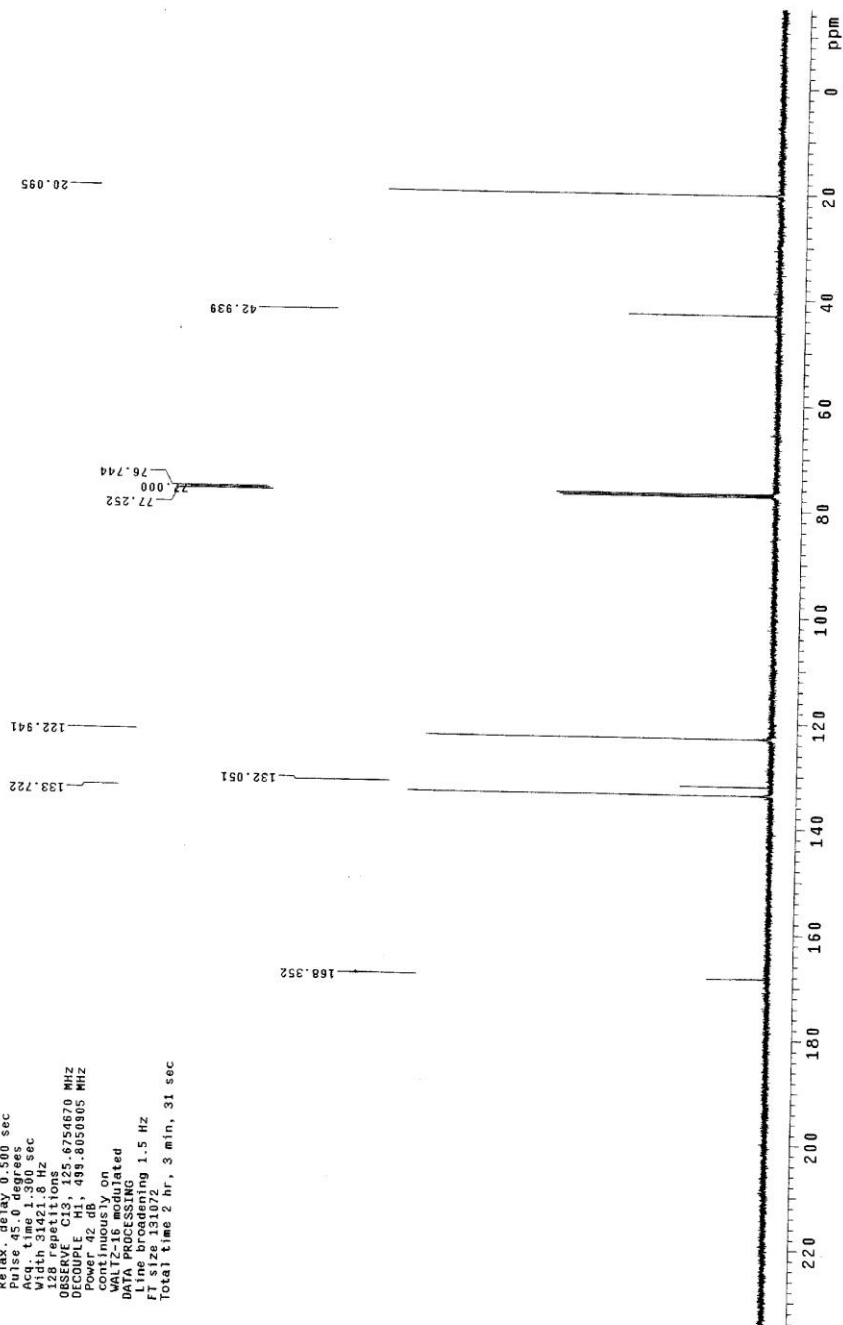


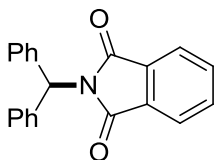
STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:

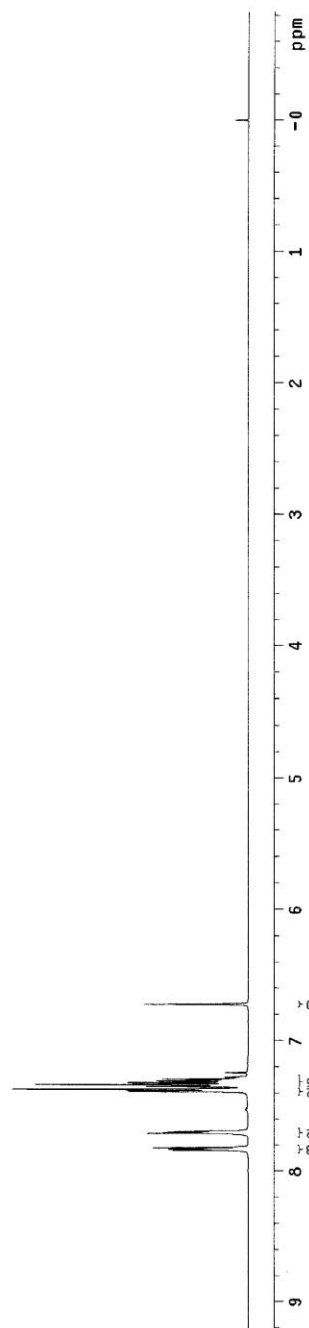
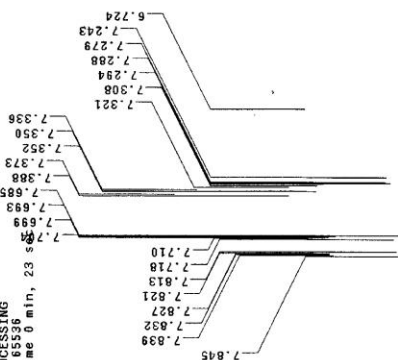
Pulse Sequence: szpul
Solvent: cdcl3
Ambient temperature
File: d4026
INOVA-500 "MNU500"

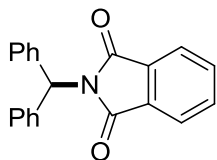
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.300 sec
Width 31421.300 Hz
128 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8050905 MHz
Pulse delay
cont/Inquity on
VALT2-15 modulated
DATA PROCESSING
Line broadening 1.5 Hz
F1 resolution 177.1
Total time 2 hr, 3 min, 31 sec



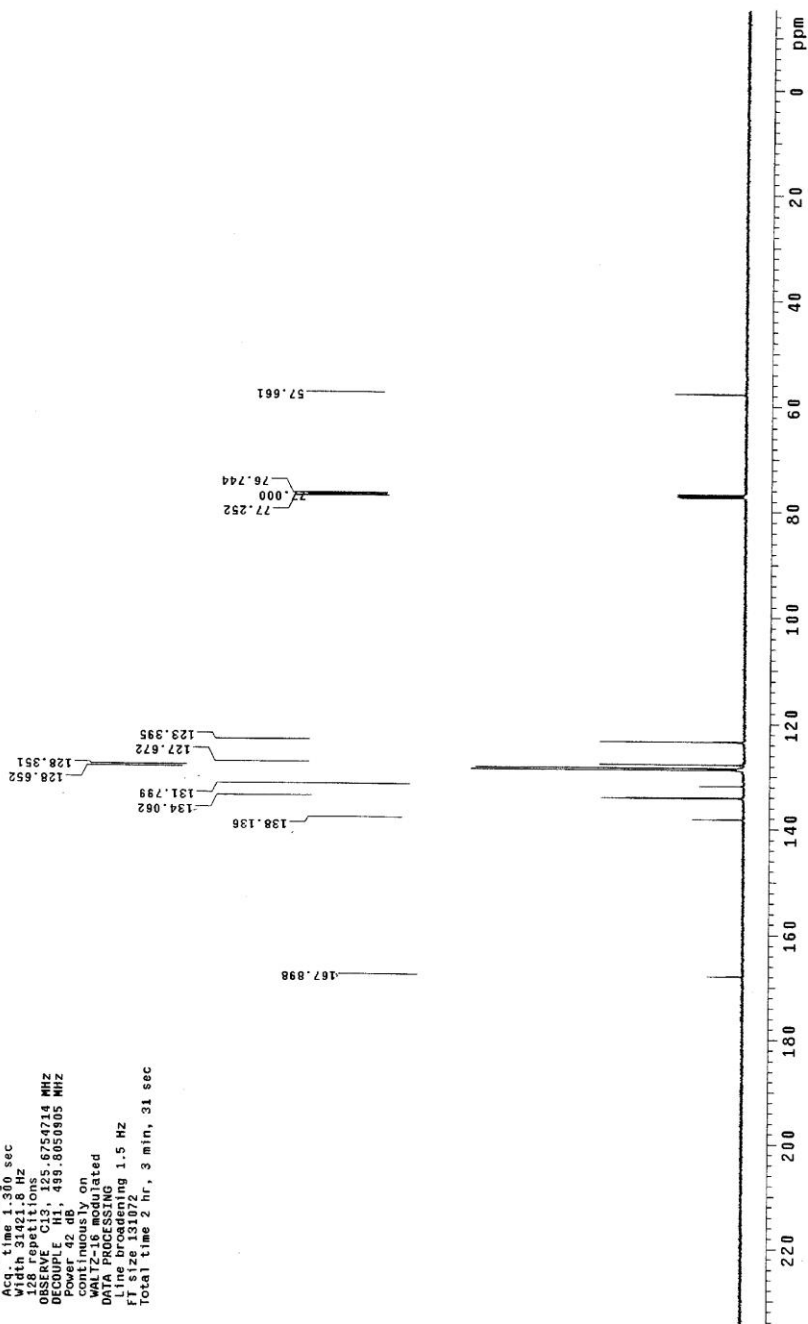


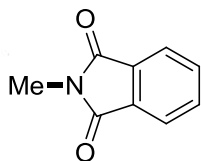
STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 File: d3553
 INOVA-500 "NMR500"
 Relax: delay 1.000 sec
 Pulse: 45.0 degrees
 Acq. time 1.892 sec
 Width 10081.4 Hz
 8 repetitions
 QSDNMR 400.146 MHz
 DATA PROCESSING
 FT size 65536
 Total time 0 min, 23 s



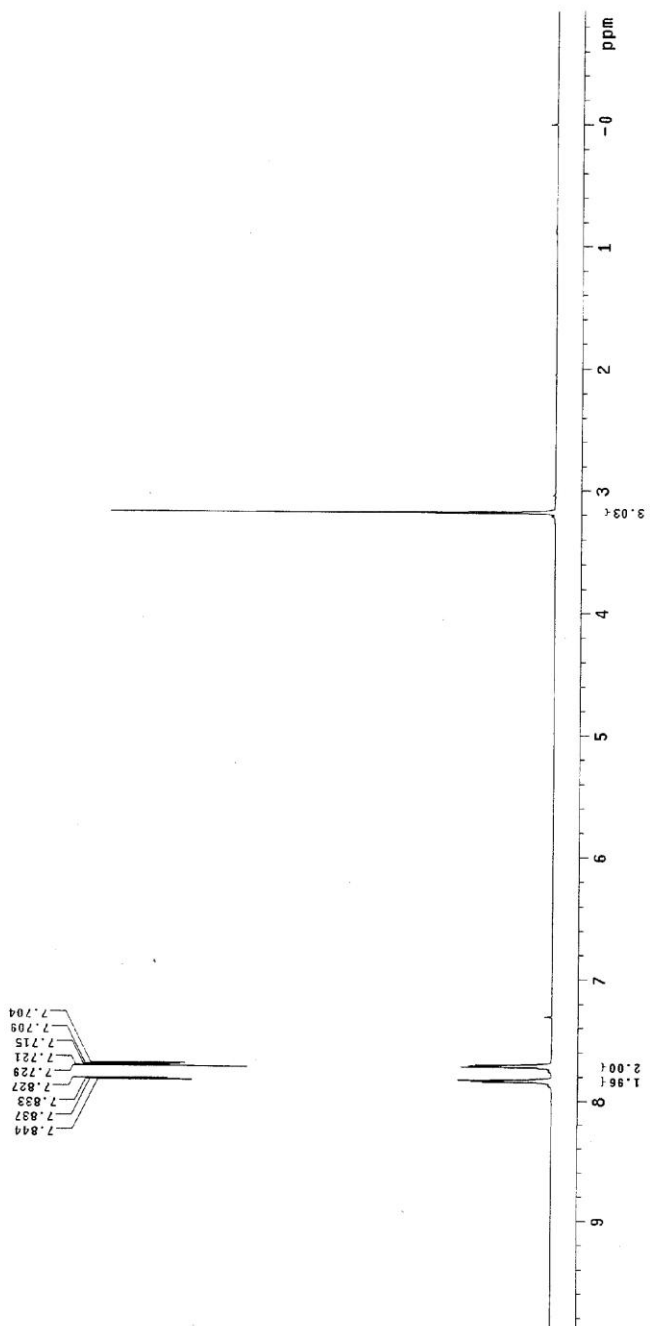


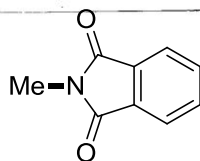
STANDARD CARBON PARAMETERS
 Archive directory: /export/home/oucy/vnmrsv/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: cdcl3
 Sample temperature: 125.0
 File: d3736
 INOVA-500 "NMRUS00"
 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acquisition time 0.500 sec
 Width 31421.8 Hz
 128 repetitions
 OBSERVE C13, 125.6754714 MHz
 DECOUPLE H1, 499.8050905 MHz
 Post-acquisition processing
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 F1 frequency 125.6754714 MHz
 F2 101.6261197 MHz
 Total time 2 hr, 3 min, 31 sec





STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouy/vmarsys/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 File: d4480
 INOVA-500 "MENU500"
 Relax delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Width 10768.6 Hz
 Repetitions
 OBSERVED F1 100.625669 MHz
 DATA PROCESSING
 FT size 65536
 Total time 0 min, 11 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouy/vnmrsvs/data
Sample directory:

Pulse Sequence: t2pu1

Solvent: cdcl3

Ambient temperature

User: 1-14-87

File: d4484

INDVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

128 repetitions

Observed C-13 45.6754718 MHz

DECOUPLE CH1 499.8050405 MHz

Power 42 dB

continuously on

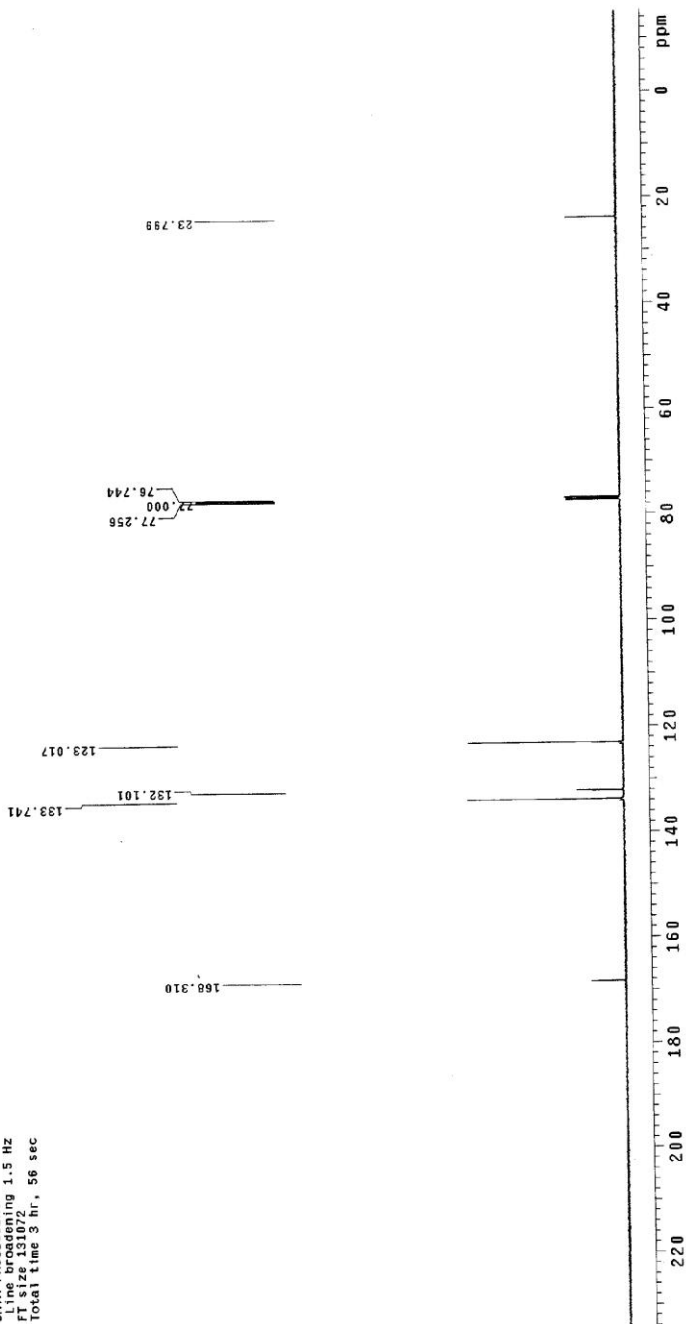
WALTZ-16 modulated

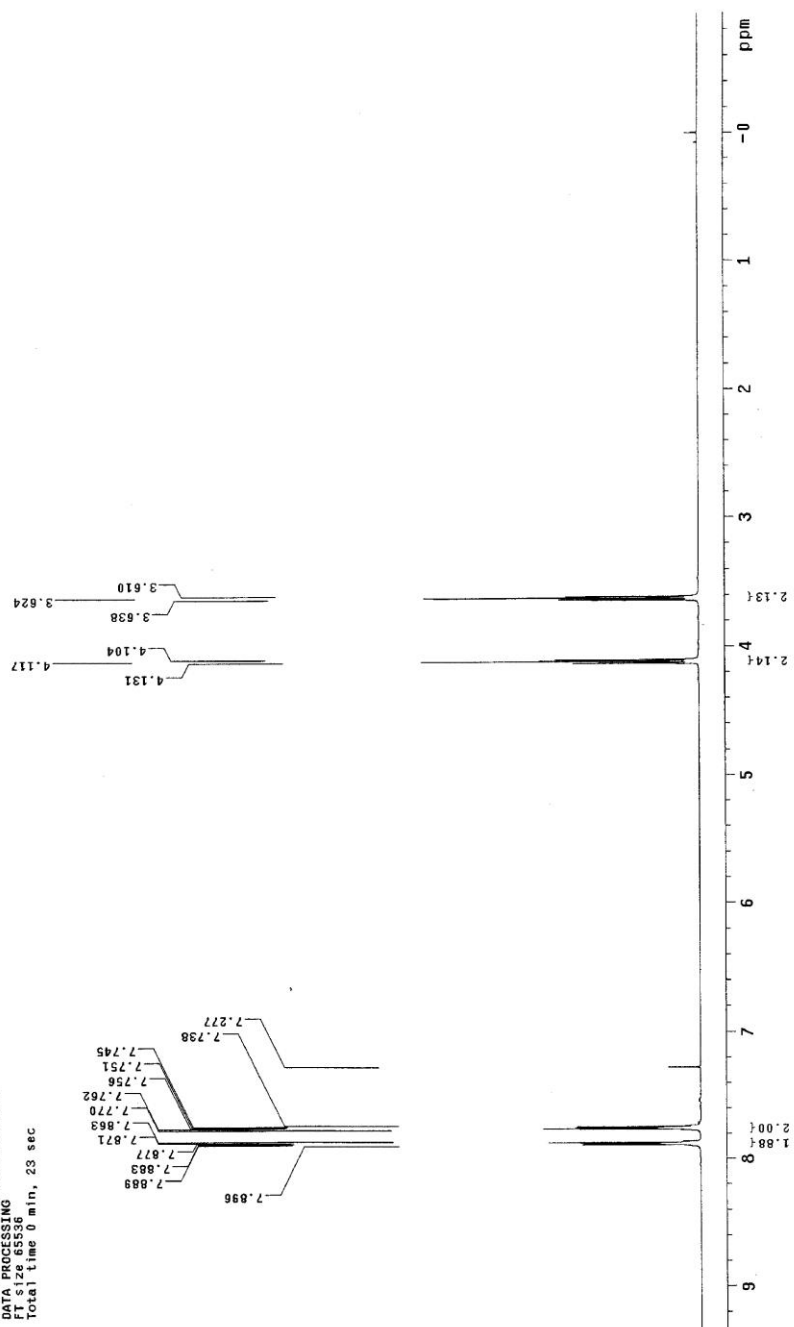
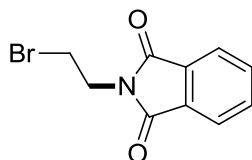
DATA PROCESSING

Line broadening 1.5 Hz

FT size 131072

Total time 3 hr, 56 sec





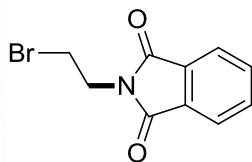
```

STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmr5s/data
Sample directory:

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature: 300.2 K
P1: 12.00
NUC1: 1H
NUC2: 13C
INVOA-500 "MNU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10891.4 Hz
F2 500.135 MHz
F1 125.761 MHz
F2 offset 499.825833 MHz
DATA PROCESSING
FF size 65536
Total time 0 min, 23 sec

```

STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouvy/vmr/sys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdc13

Ambient temperature

User: i-14-87

File: d3766

INNOVA-500 "NMRUS00"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.390 sec

Width 31421.8 Hz

128 repetitions

Observed 13C, 125.754747 MHz

DECOUPLE H1, 499.8050905 MHz

Power 42 dB

continuously on

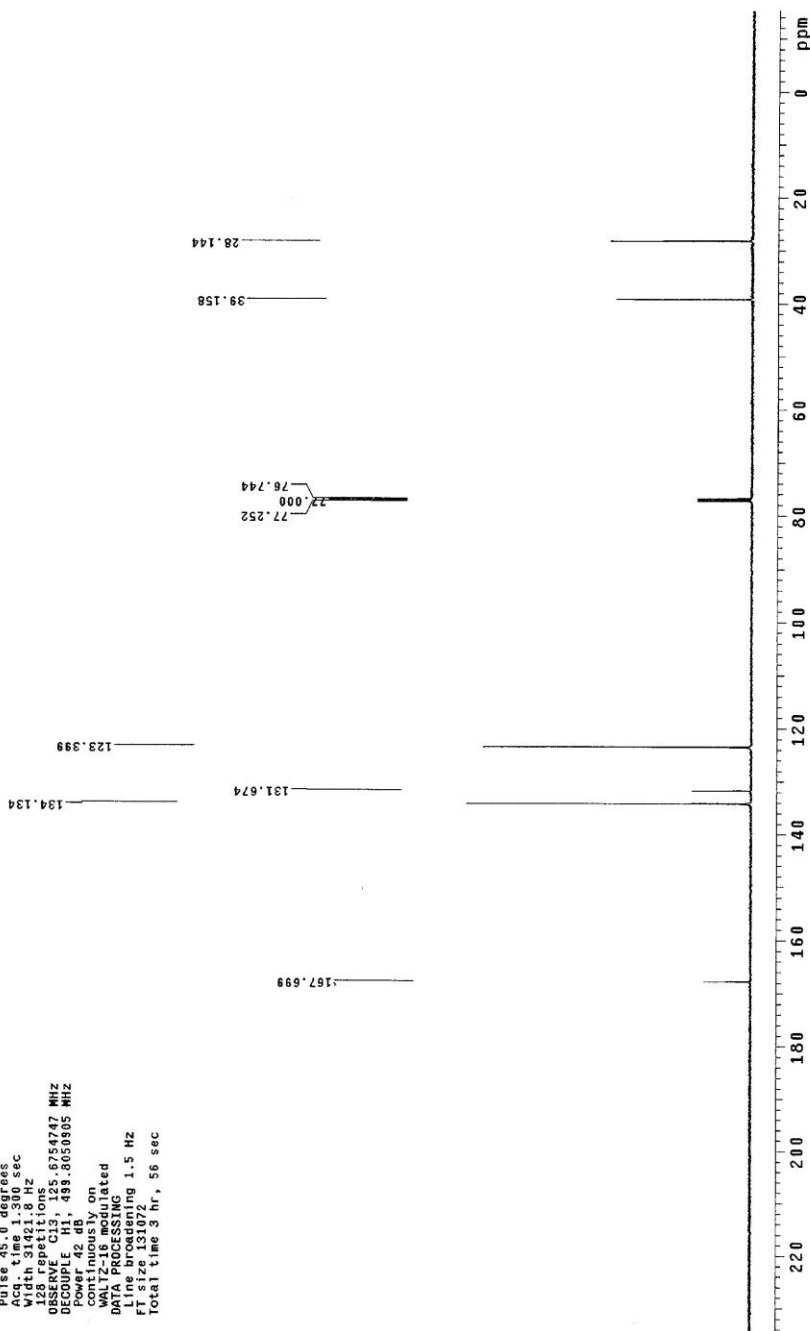
Waltz16 modulated

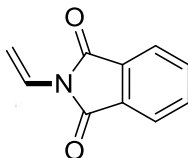
Digital resolution

Line broadening 1.5 Hz

FT size 131072

Total time 3 hr, 56 sec





STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmr/sys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: d4405

INDY-500 "NMRUS00"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Pulse time 0.15 sec

Width 10768.6 Hz

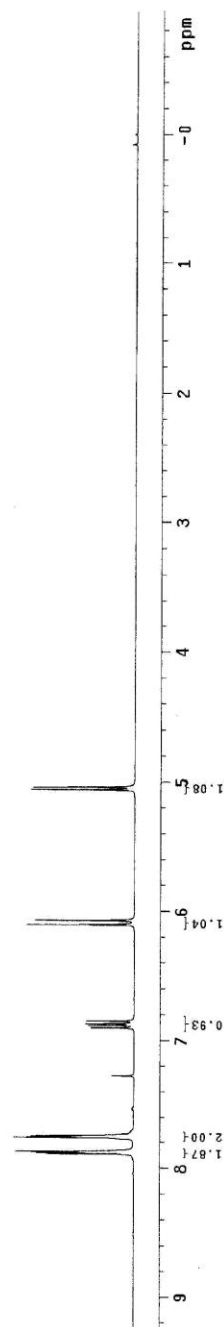
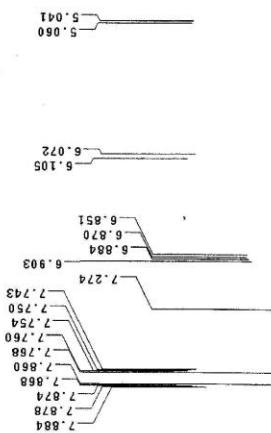
8 repetitions

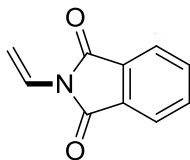
OBSERVE F1, 499.8025847 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 23 sec



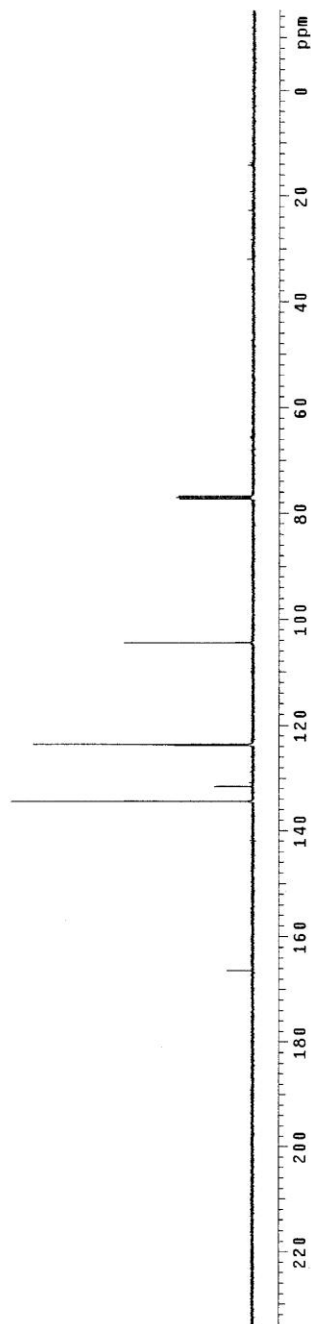
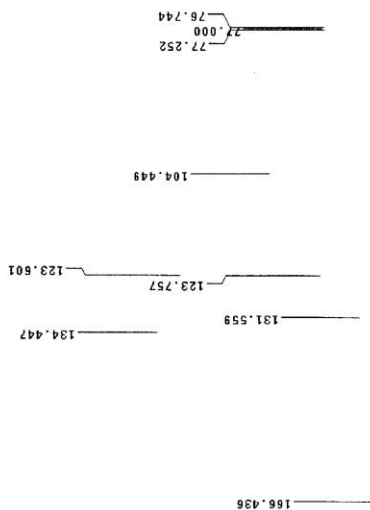


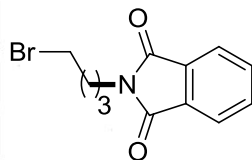
STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouvy/vnmrsvs/data
Sample directory:

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
User: j-ls-87
File: cdcl3-131072
INOVA-500 "NMRUS00"

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Wait 12.000 sec
192 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 42 dB
Lock mode: ON
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
F1 size 131072
Total time 2 hr, 3 min, 31 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouy/vnmr/sy/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: i-17-87

File: cdcl3

INOVA-500 "MNU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

Observed 192

OBSERVE C13, 125.6754651 MHz

DECOUPLE H1, 499.8050805 MHz

Power 42 dB

Continuously on

WALTZ-16 MODULATED

DATA PROCESSING

Line broadening 1.5 Hz

FT size 131072

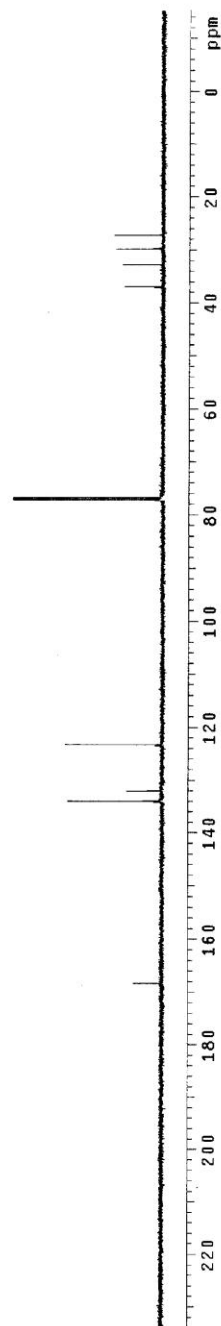
Total time 3 hr, 56 sec

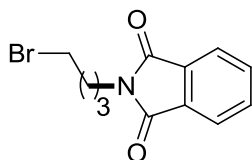
77.256
77.000
76.748

133.955
131.998
123.227

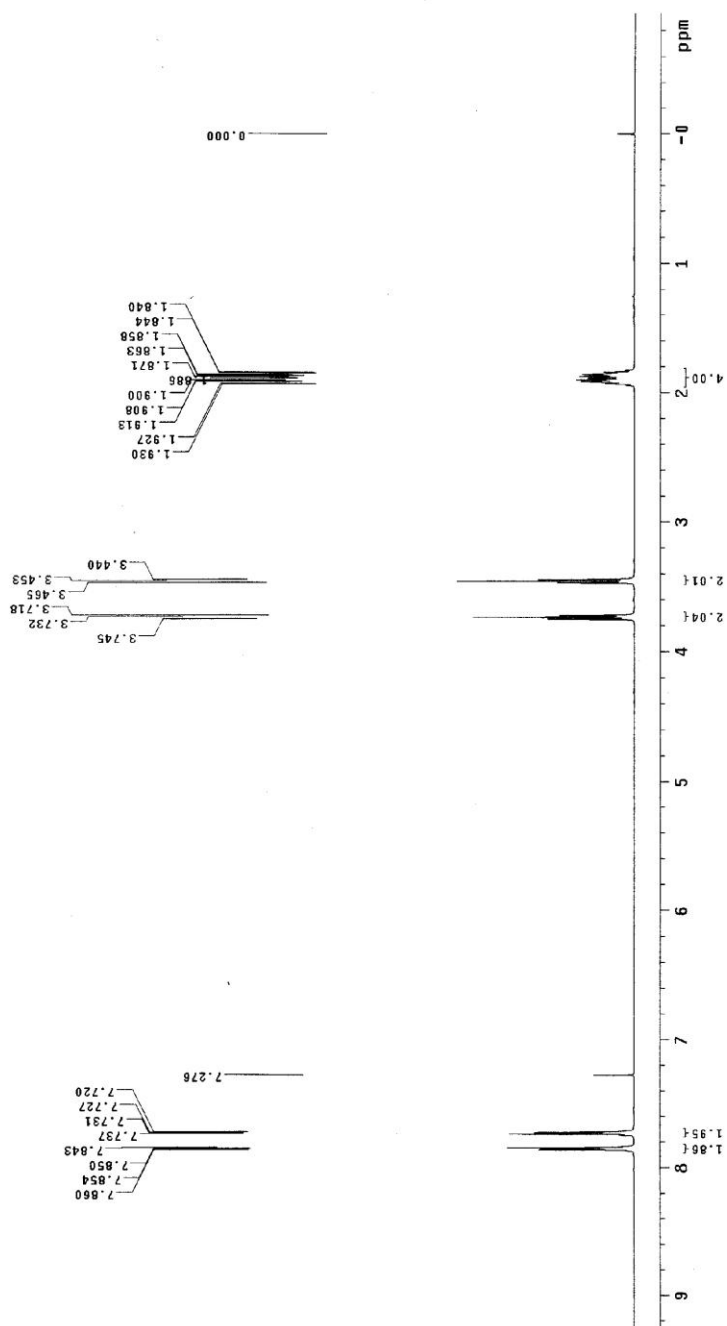
168.329

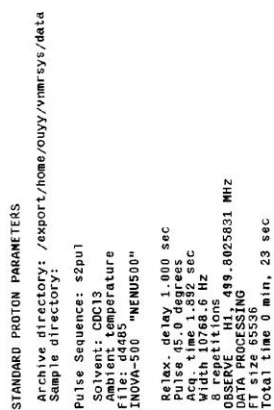
36.911
32.764
29.792
27.202





STANDARD PROTON PARAMETERS
 Archive directory: /export/home/ouy/vnmrsvs/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 F1: 500.13635 MHz
 INOVA-500 "NMR500"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.892 sec
 Frequency 500.13635 MHz
 4 repetitions
 OBSERVE H1, 499.8025837 MHz
 DATA PROCESSING
 F1 size 65536
 Total time 0 min, 11 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouy/vnmrsws/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: 1-14-87

File: d4514

INOVA-500 "NMR500"

Relax. delay 0.500 sec

Pulse 450 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

Q32 repetitions

Observed F1 158.5660 MHz

Observed F2 489.805905 MHz

DECOUPLE H1, 489.805905 MHz

Power 42 dB

continuously on

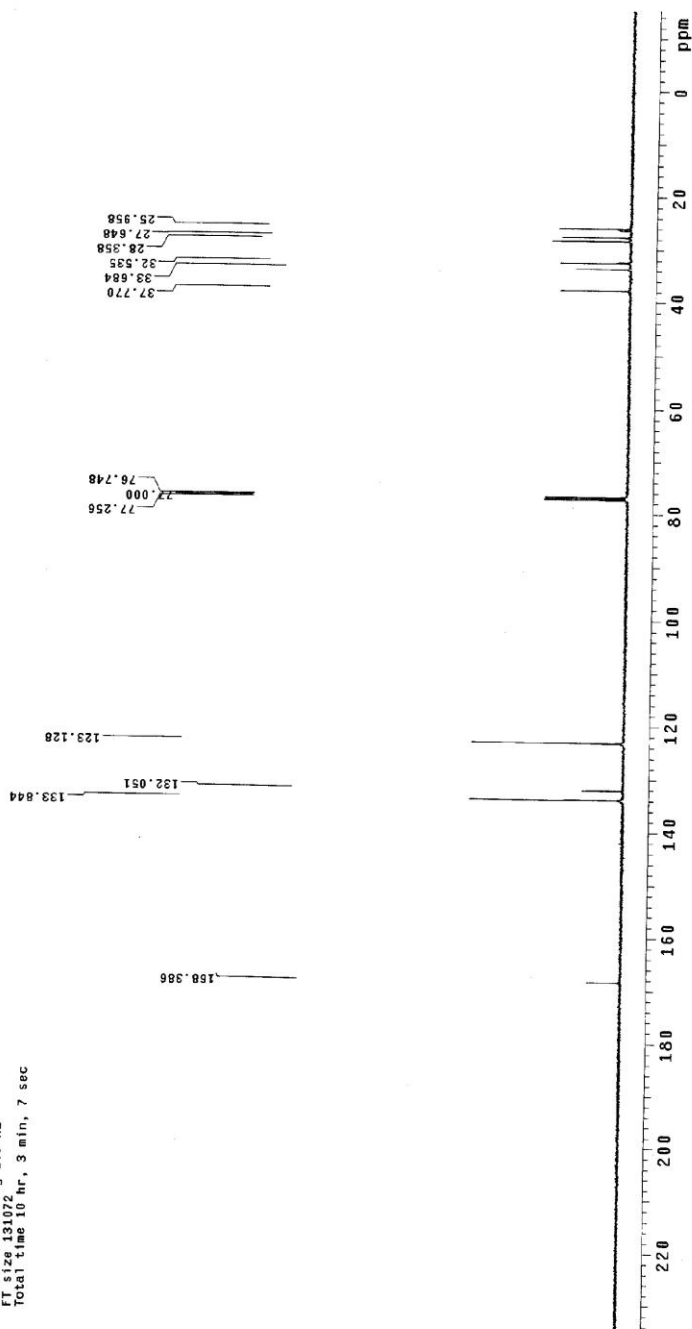
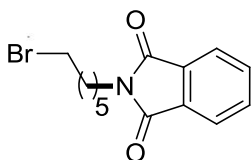
WALTZ16 modulated

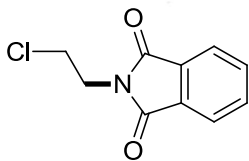
DATA F2 158.5660 MHz

Line broadening 1.5 Hz

FT size 131072

Total time 10 hr, 3 min, 7 sec





STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmr/sys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

File: d3447

INOVA-500 "NMRUS00"

Relax. delay 1.000 sec

Pulse width 12.000 sec

Acq. time 1.892 sec

Width 10081.4 Hz

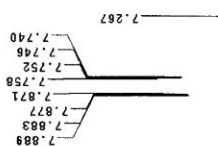
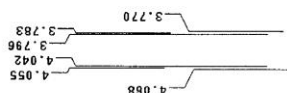
8 repetitions

QSSNRECIN 499.8025873 MHz

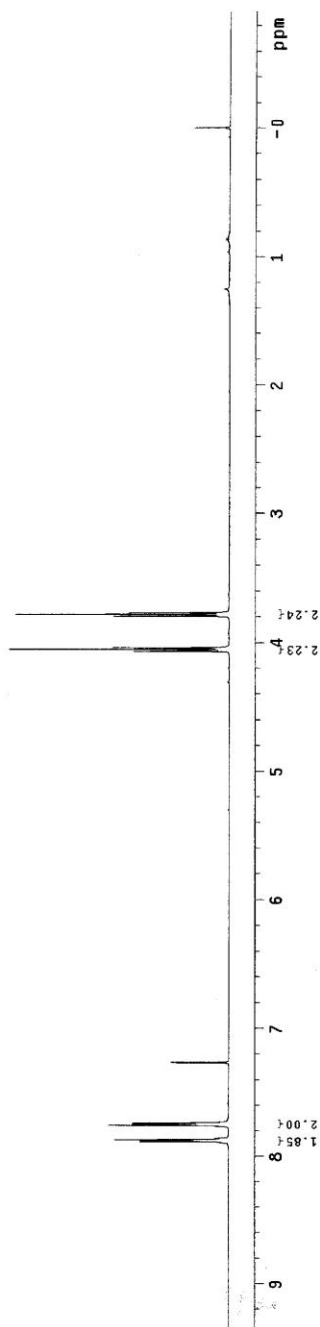
DATA PROCESSING

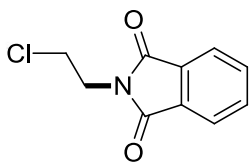
FT size 65536

Total time 0 min, 23 sec



-0.000





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouy/vnmrSYS/data
Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: 1-14-87

File: d3737

INOVA-500 "MENV500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

QZG repetitions

DECOUPLE H1, 489.8050805 MHz

Power 42 dB

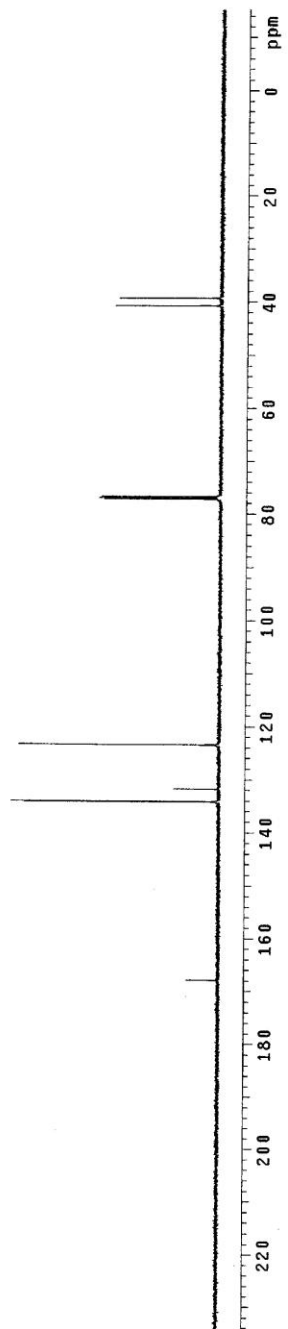
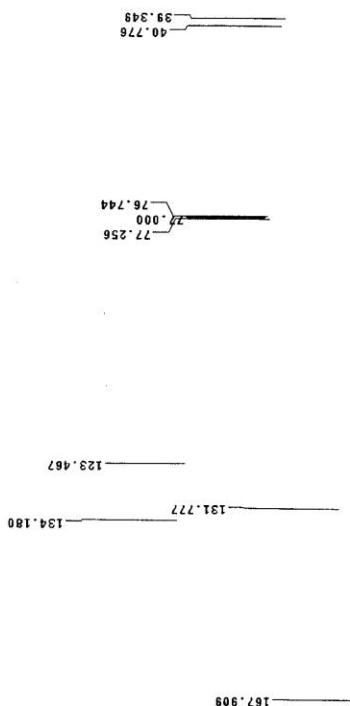
continuously on

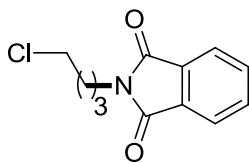
DATA F2 16.000000 MHz

Line broadening 1.5 Hz

FT size 131072

Total time 2 hr, 3 min, 31 sec





STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: d4655

INOVA-500 "NMR500"

Relax. delay 1.000 sec

Number of scans 64

Acq. time 1.892 sec

Width 10138.1 Hz

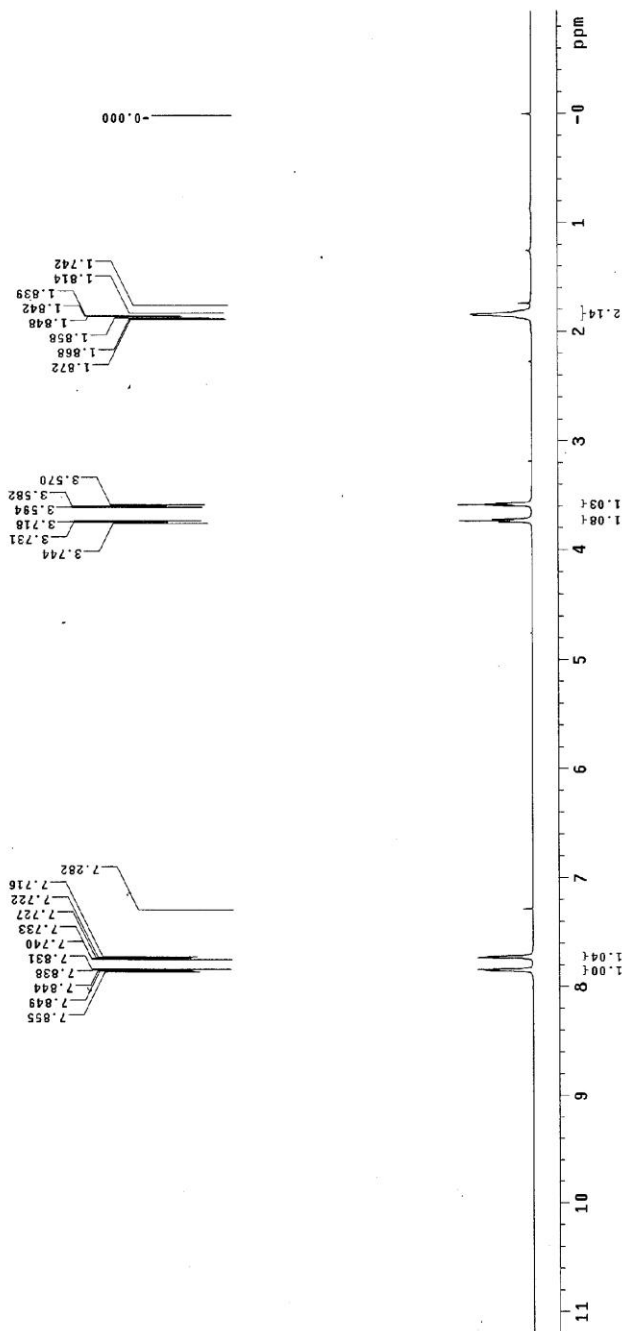
4 repetitions

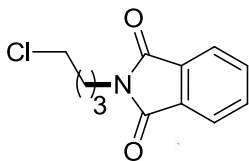
OBSERVED F1: 99.8025801 MHz

DATA PROCESSING

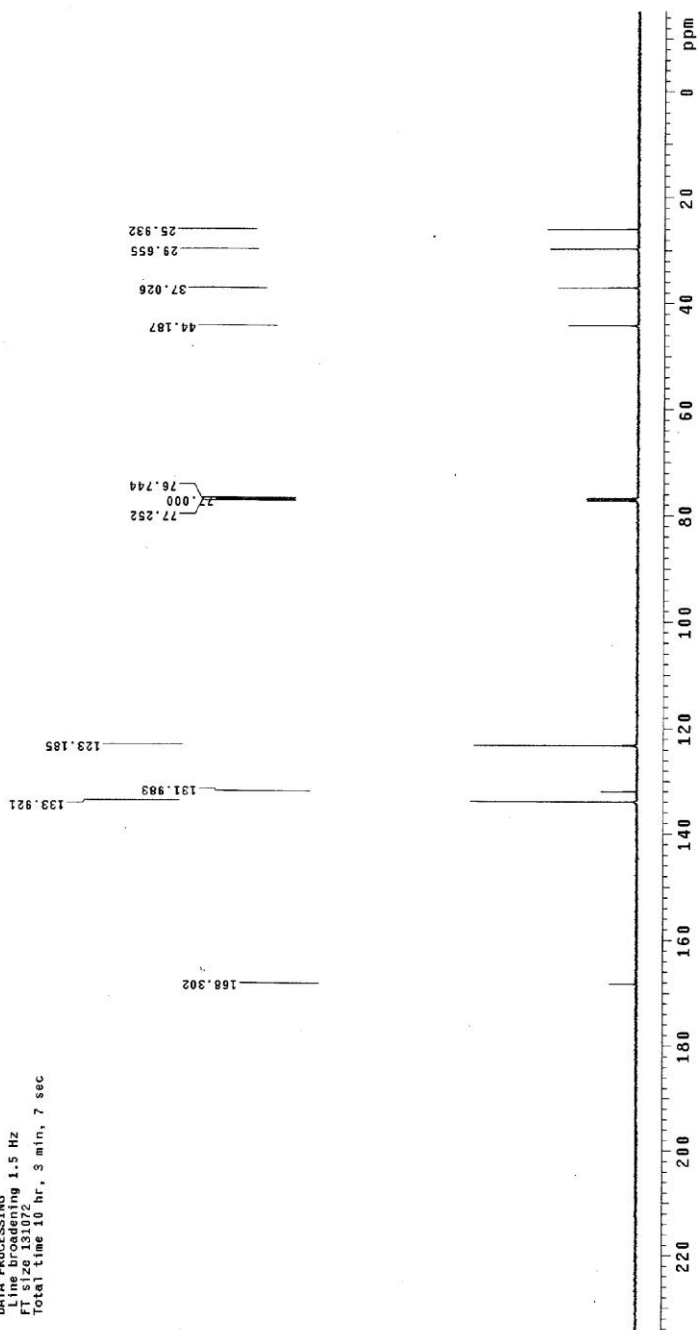
FT size 65536

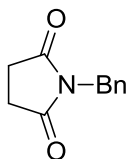
Total time 0 min, 11 sec





STANDARD CARBON PARAMETERS
 Archive directory: /export/home/ouyy/vnmrSYS/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: cdcl3
 Acquisition temperature
 User: 1-14-87
 File: d4656
 INOVA-500 "MENU500"
 Relax. delay 0.500 sec
 Pulse delay 0.050 sec
 Acq. time 1.300 sec
 Width 31421.6 Hz
 128 repetitions
 OBSERVE C13, 125.6754670 MHz
 DECOUPLER H1, 499.8603003 MHz
 Power 42 dB, continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 F2 size 131072
 FT size 131072
 Total time 10 hr, 3 min, 7 sec



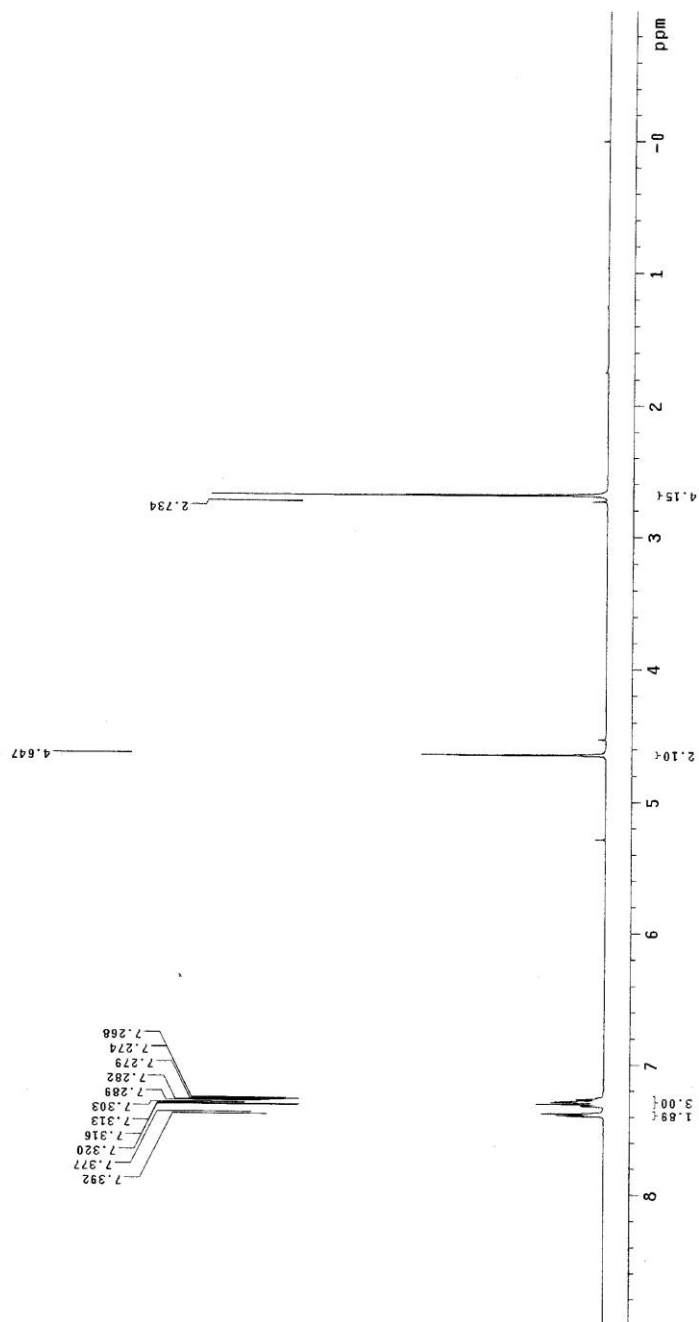


STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouvy/vnmrSYS/data
Sample directory:

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
F1: 600822.20 MHz
INQV-500 "NENU500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 10768.6 Hz
Spectral width 10768.6 Hz
OBSERVE H1 499.8025900 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec



STANDARD CARBON PARAMETERS
 Archive directory: /export/home/ouyy/vmarsys/data
 Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Acidant: none

User: 1-14-87

File: d4084

INOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. t 1.000 sec

Width 31421.8 Hz

132 repetitions

OBSERVE C13, 125.6754793 MHz

DECOUPLE H1, 499.8059395 MHz

Power 42 dB

continuously on

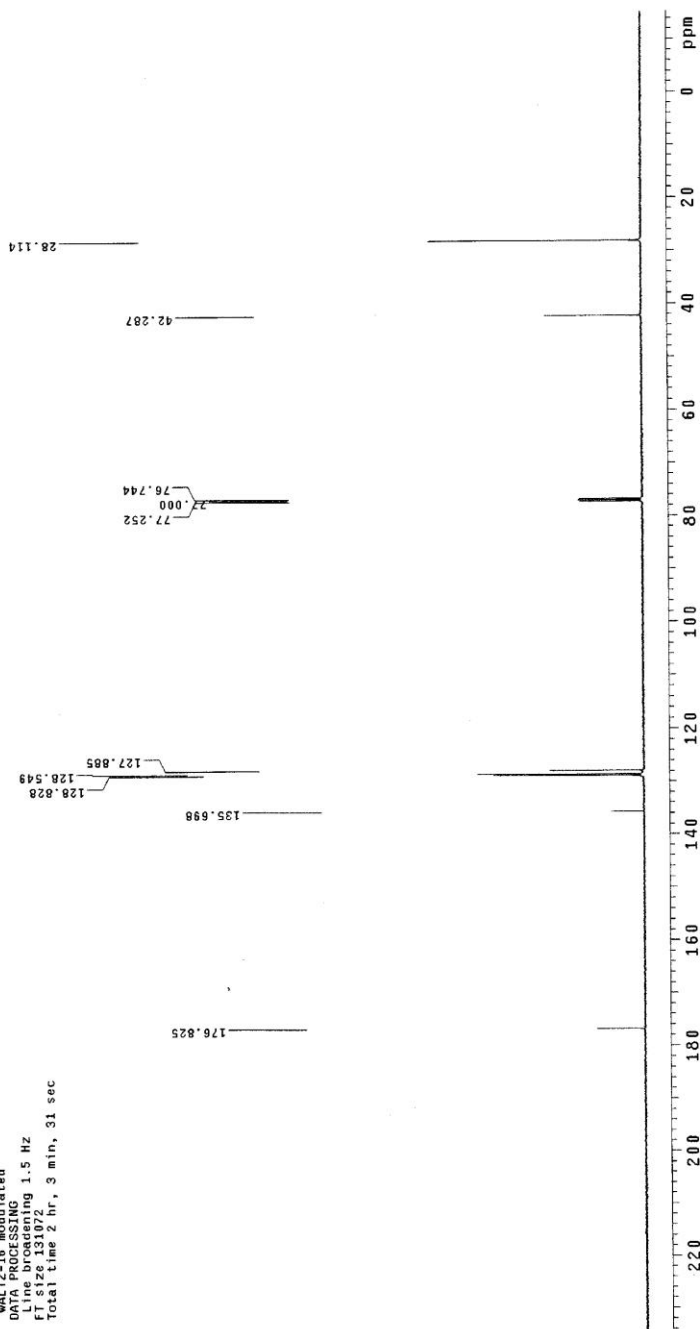
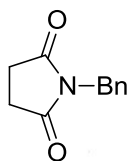
WALTZ-16 modulated

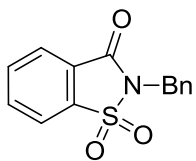
DATA PROCESSING

Time Domain 1.5 Hz

FT size 131072

Total time 2 hr, 3 min, 31 sec





STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmrsvs/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: d4312

INOVA-500 "HREUS00"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 10768.6 Hz

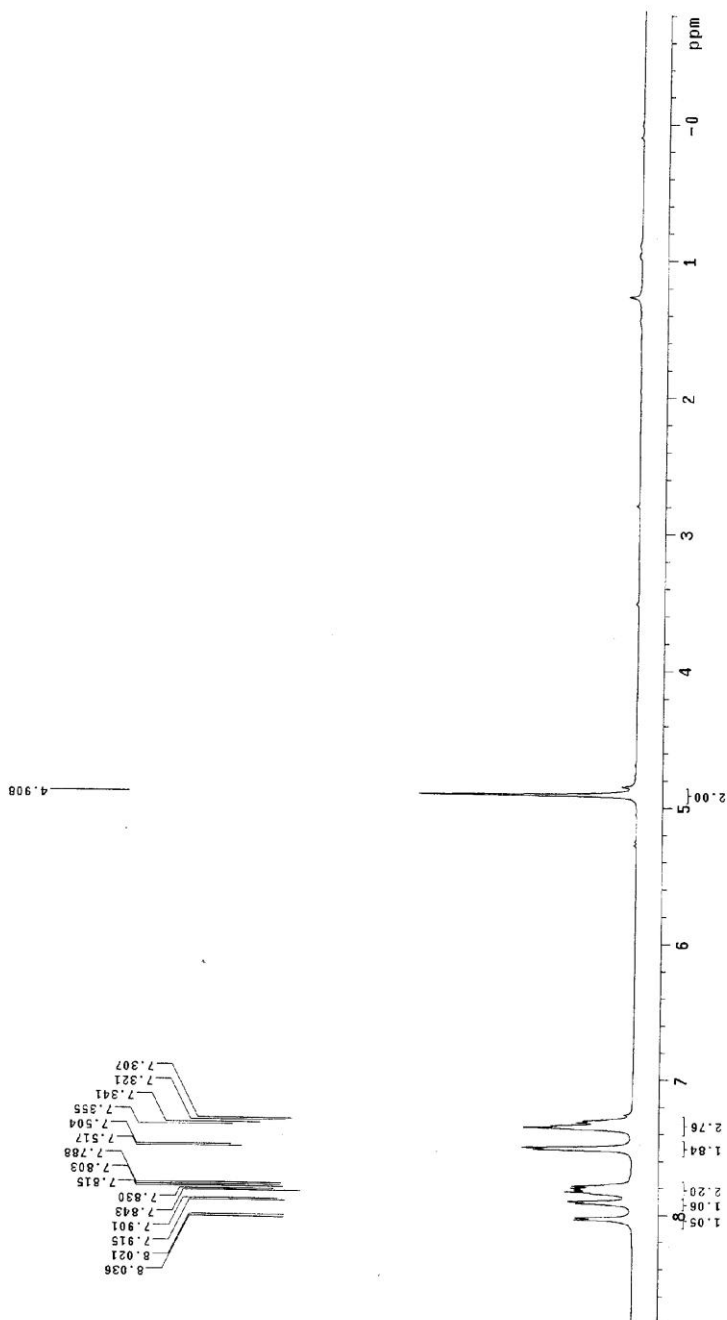
Repetitions

Observed 498.8025916 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 23 sec



STANDARD CARBON PARAMETERS
 Archive directory: /export/home/ovuy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: cdc13
 Ambient temperature
 User: 1-14-87
 File: 0002
 INOVA-500 "NMRUS00"
 Relax. delay 0.500 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31821.00 Hz
 256 channels
 OBSERVE C13, 125.6754762 MHz
 DECOUPLE H1, 499.5050905 MHz
 Power 42 dB
 Locking on
 WALTZ16
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 3 hr, 56 sec

