

## Supporting Information

### **Halonium-initiated double oxa-cyclization cascade as a synthetic strategy for halogenated furo[3,2-*c*]pyran-4-ones**

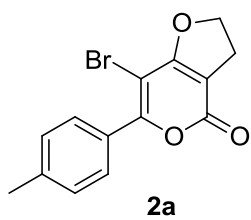
Enxiang Wei,<sup>a</sup> Bing Liu,<sup>a</sup> Shaoxia Lin,<sup>a</sup> Baozhong Zhao<sup>\*,a</sup> and Fushun Liang<sup>\*,a,b</sup>

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*E-mail: liangfs112@nenu.edu.cn*

**Copies of <sup>1</sup>H and <sup>13</sup>C NMR spectra for compounds 2-7**

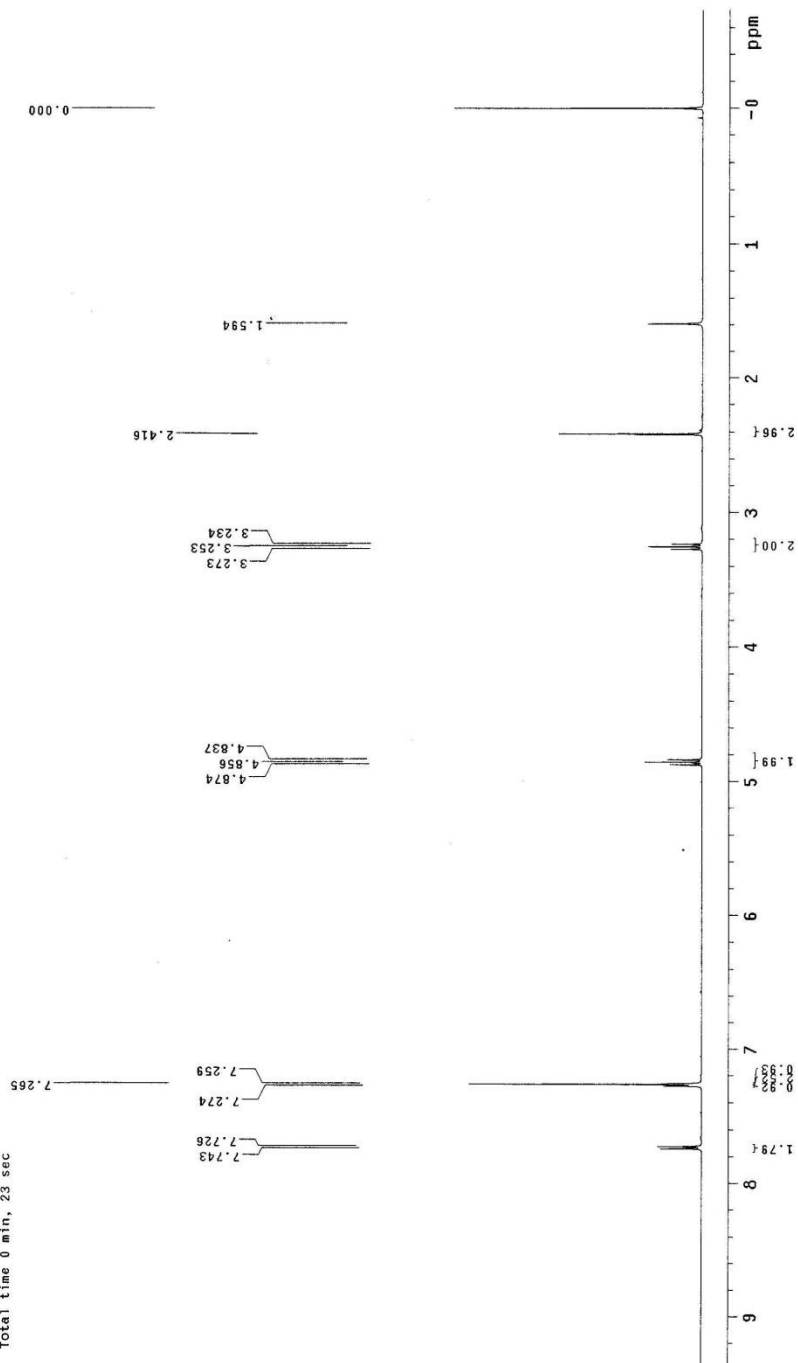


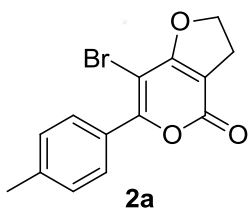
STANDARD PROTON PARAMETERS

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

Pulse Sequence: s2pul  
Solvent: CDCl3  
Ambient temperature  
File: d1406  
INOVA-500 "MNU500"

Relax. delay: 1.000 sec  
Acq. time: 1.897 sec  
Acq. time: 1.897 sec  
Width: 9329.4 Hz  
8 repetitions  
OBSERVE: H1, 499.8025894 MHz  
P1: 12.00000000  
P1 DELTA: 0.5536  
Total time: 0 min, 23 sec





STANDARD CARBON PARAMETERS

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

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

F1ser: 144-87

F2ser: d1413

INOVA-500 "NEU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Cr1 time 1.000 sec

Width 31421.8 Hz

6000 repetitions

OBSERVE C13, 125.6754685 MHz

DECOUPLE H1, 499.8050905 MHz

continuously on

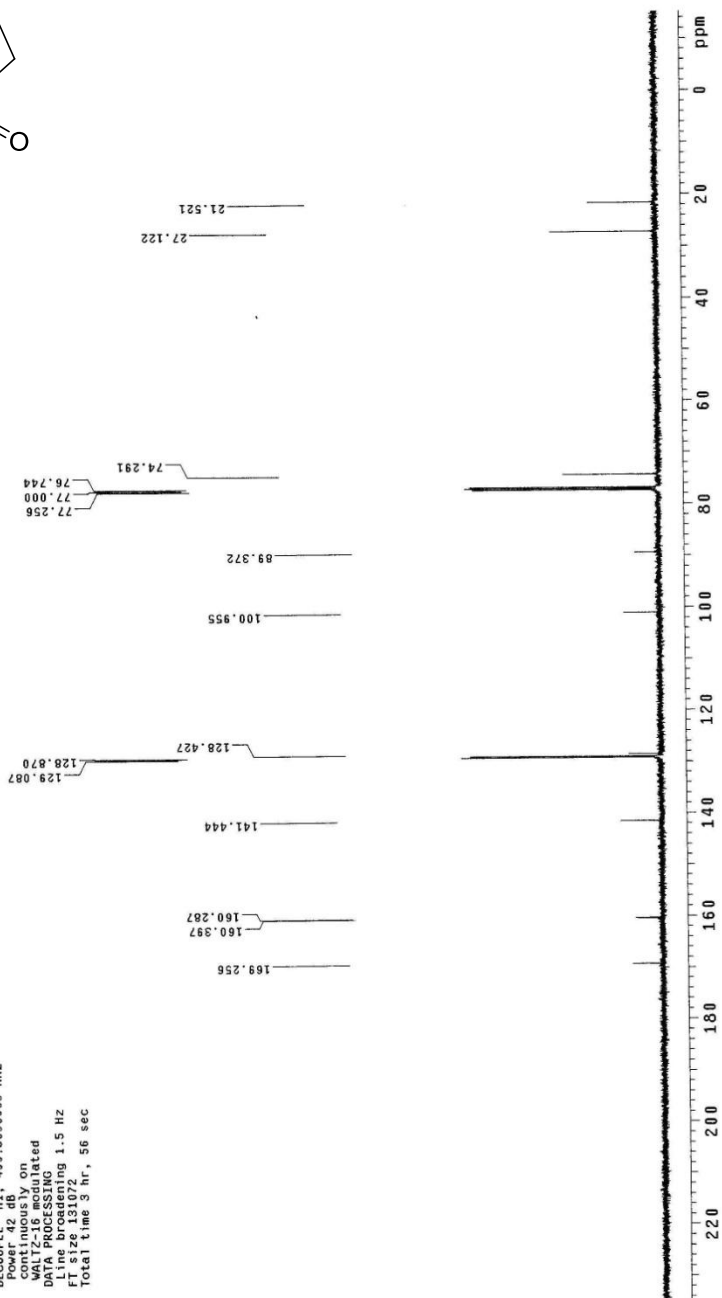
WALTZ-16 modulated

DATA PROCESSING

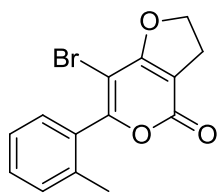
16 scans/pointing 1.5 Hz

FT size 131072

Total time 3 hr, 56 sec







2b

STANDARD CARBON PARAMETERS

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

Pulse Sequence: szpul1

Solvent: cdcl3

Acquire Date: 1-14-87

User: dl551

File: dl551

INOVA-500 "NENU500"

Relax. delay: 0.500 sec

Pulse: 45.0 degrees

Acq. time: 1.360 sec

Width: 31421.8 Hz

Observed F1: 125.631 MHz

Observed F2: 675.4656 MHz

DECOUPLE: H1, 489.8658905 MHz

Power: 42 dB

Continuously on

Cont. Frequency: 489.8658905 MHz

DATA PROCESSING

Line broadening: 1.0 Hz

FT size: 131072

Total time: 3 hr, 56 sec

77.252  
77.000  
76.744

19.448  
27.164

74.429

91.951

101.986

125.631  
129.812  
130.479  
130.529  
131.972

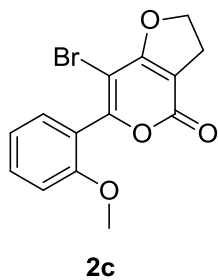
136.938

160.405

162.144

168.672





2c

STANDARD PROTON PARAMETERS

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

Sample directory:

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

F1: 400 MHz

INOVA-500 "HENU500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.294 sec

Waltz16 1000 MHz

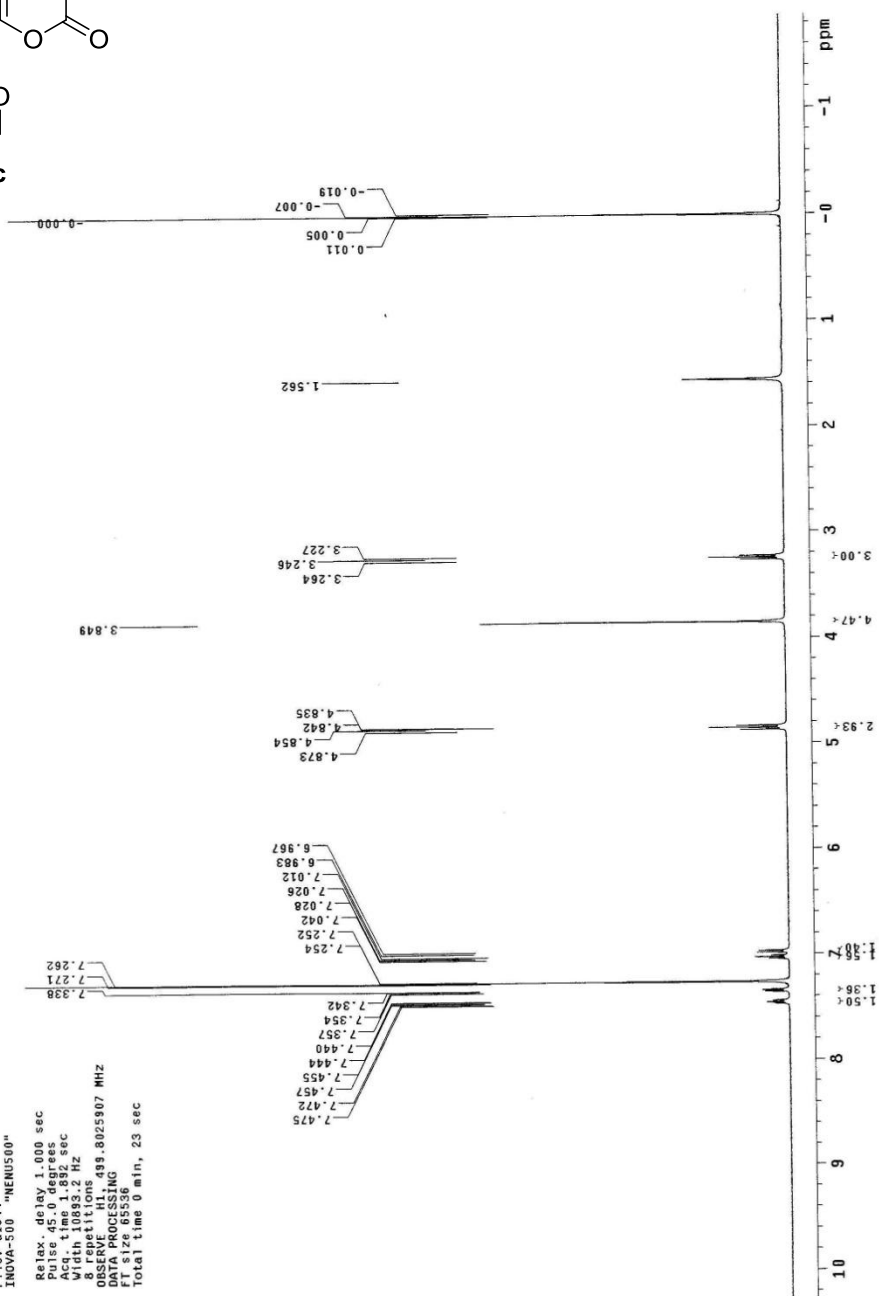
8 repetitions

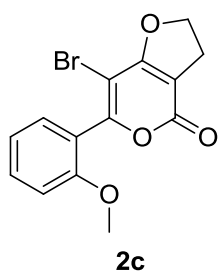
OBSERVE H1, 499.8025907 MHz

DATA PROCESSING

File: 13011301

Total time 0 min, 23 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouyy/vmmr/sys/data  
Sample directory:

Pulse Sequence: sZpul

Solvent: cdcl3

Ambient temperature

F1sr: 48-87

INNOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq time 0.00 sec

Width 31421.8 Hz

256 repetitions

OBSERVE C13, 125.6754661 MHz

DECOUPLE d1, 499.8050905 MHz

continuously on

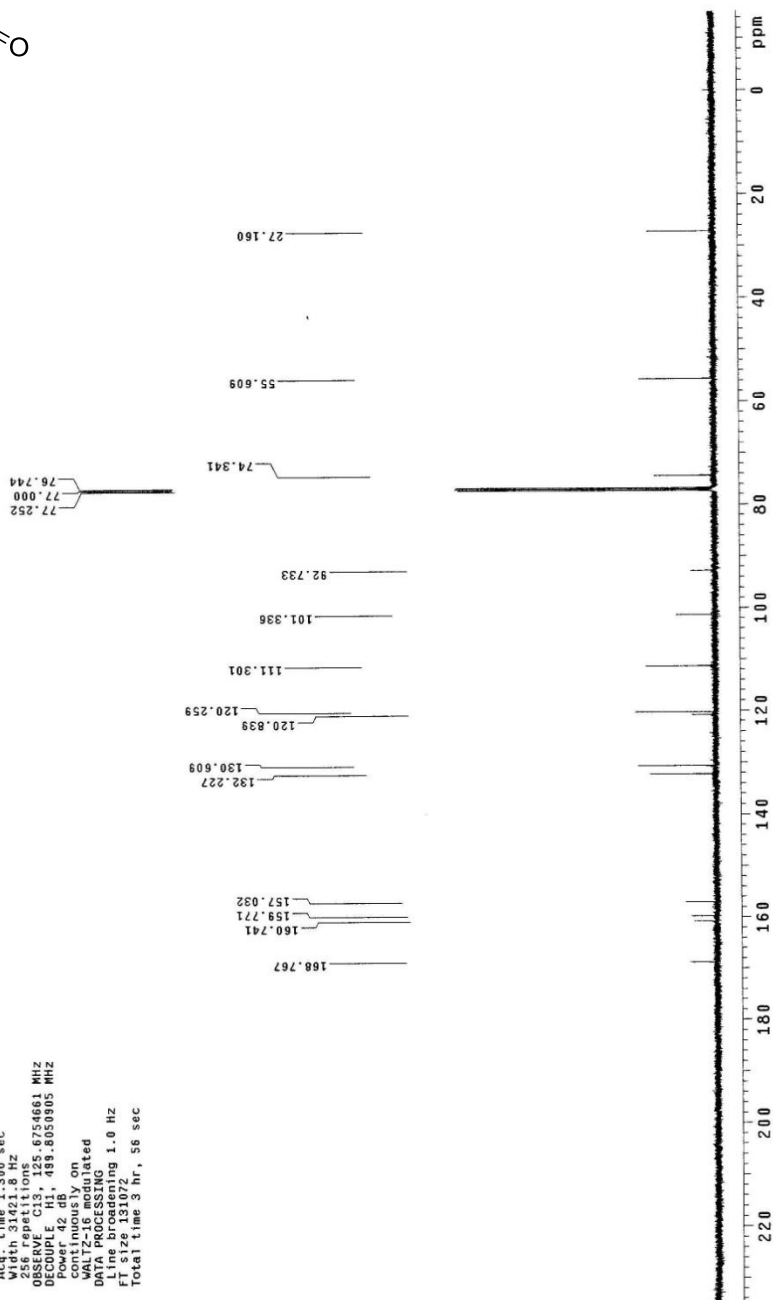
WALTZ-16 modulated

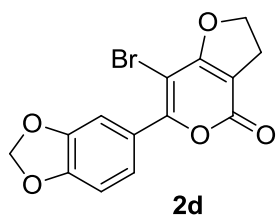
DATA PROCESSING

Frequency 1.0 Hz

FT size 131072

Total time 3 hr, 56 sec





STANDARD PROTON PARAMETERS

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

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

F1 freq: 500.13616 MHz

INOVA-500 "NMR0500"

Relax. delay: 1.000 sec

Pulse: 45.0 degrees

Acq. time: 1.892 sec

Dec. time: 1.0000 sec

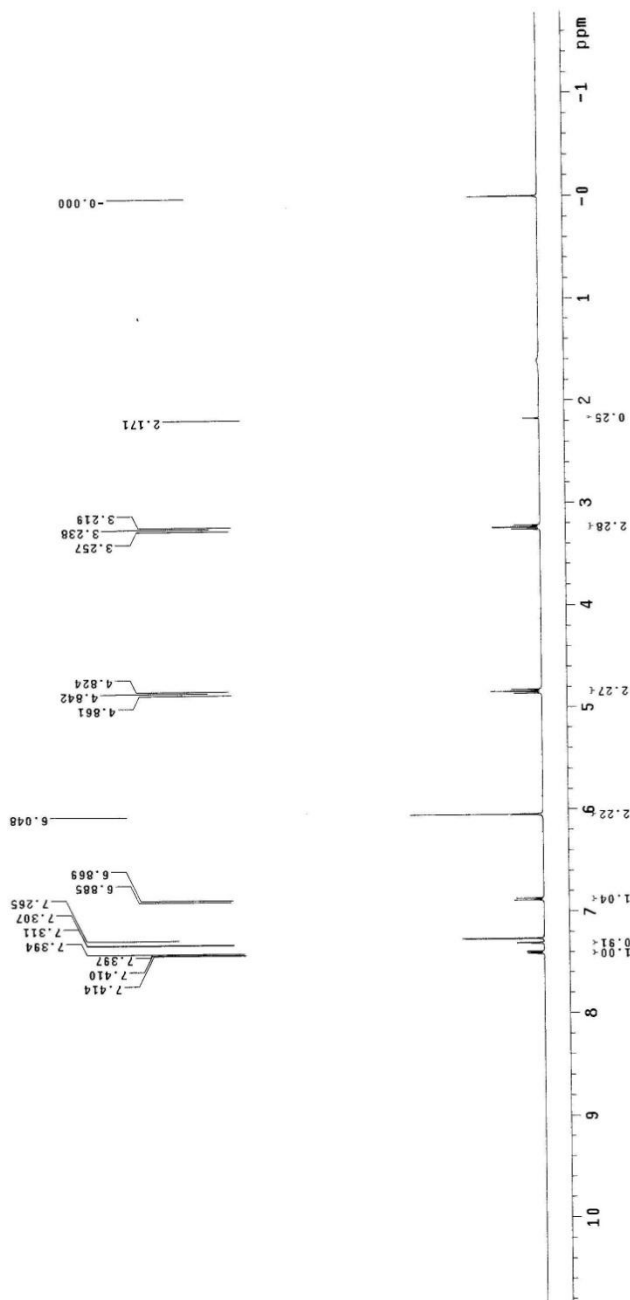
Obs. freq: 500.13616 MHz

OBSERVE: H1, 489.8025890 MHz

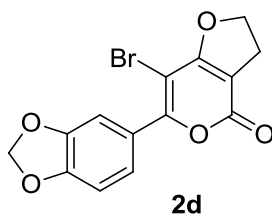
DATA PROCESSING

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

Temperature: 300

File: d1627

INOVA-500 "HENU500"

Relax. delay 0.500 sec

Acq. time 0 degrees

Acq. time 0.000 sec

Width 31421.8 Hz

256 repetitions

DECODE C13, 125.8754646 MHZ

Power 42 dB, 493.0050305 MHZ

continuously on

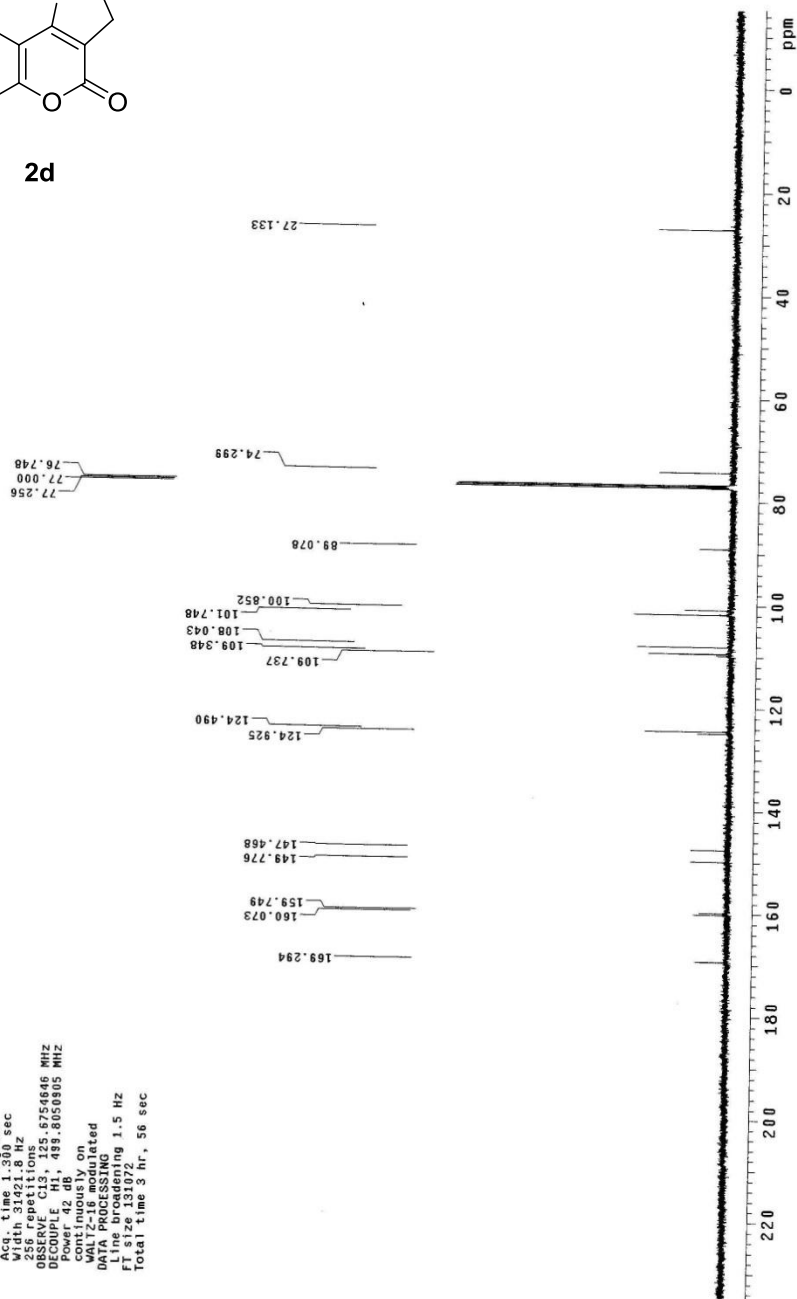
Walz-16 modulated

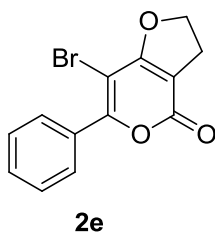
0.100 sec

Line broadening 1.5 Hz

FT size 131072

Total time 3 hr, 56 sec





STANDARD PROTON PARAMETERS

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

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

F1: 1378 "NMR500"

INOV-500 "NMR500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 3284.4 Hz

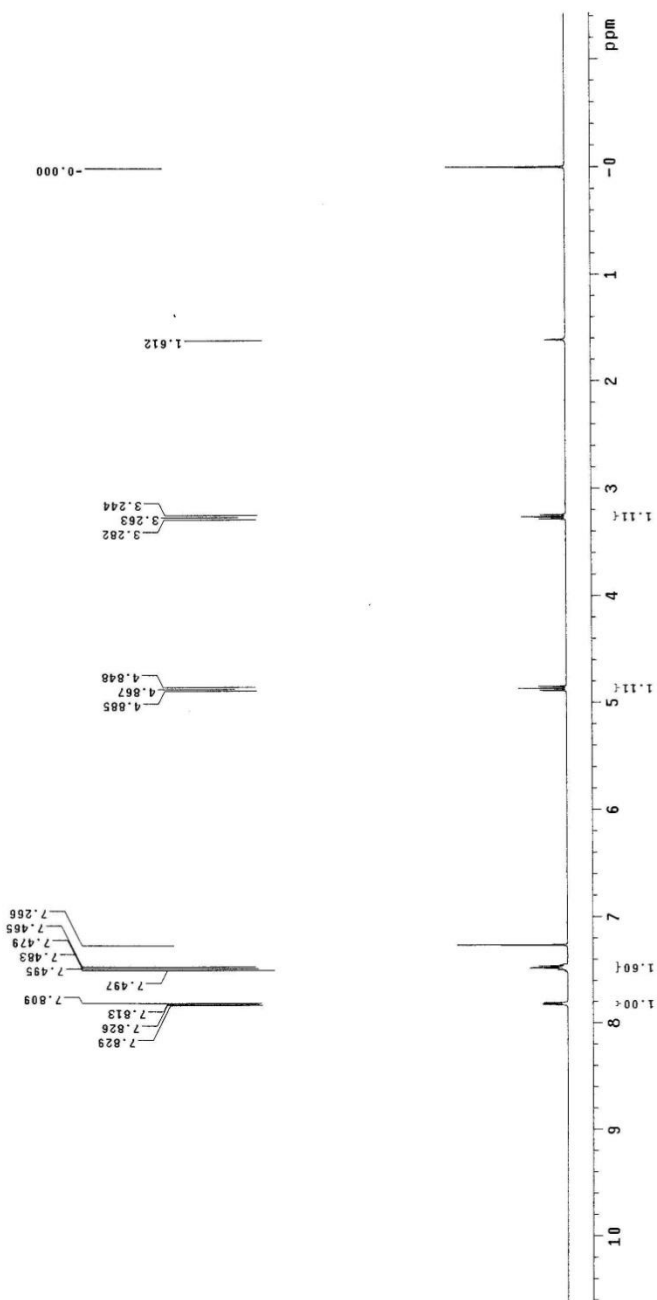
Offset 11.18 Hz

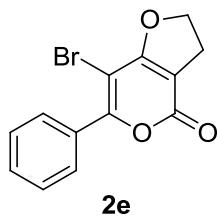
OBSERVE H1, 499.8025885 MHz

DATA PROCESSING

TT size 65536

Total time 0 min, 23 sec





2e

STANDARD CARBON PARAMETERS

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

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: d-14-87

File: 14899

INOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Obs. freq. 125.760 MHz

64 repetitions

OBSERVE C13, 125.6754670 MHz

DECOUPLE H1, 499.8050905 MHz

Power level continuously on

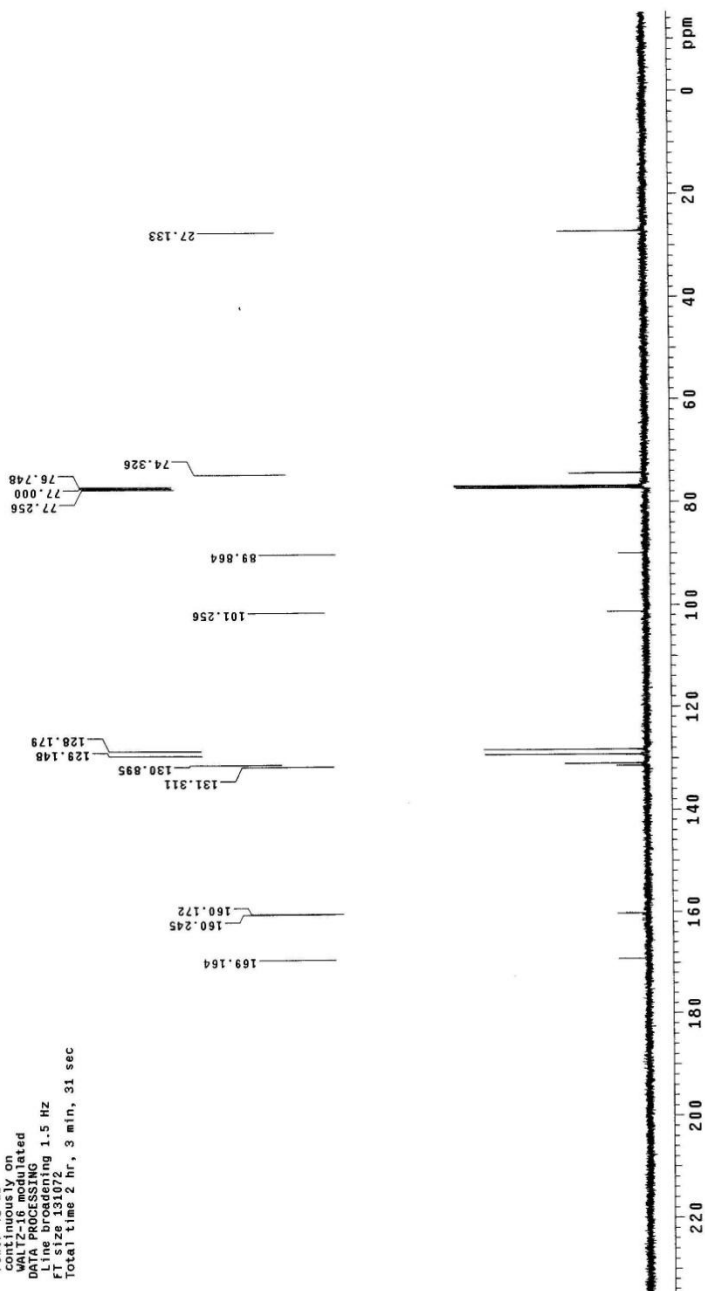
WALTZ-16 modulated

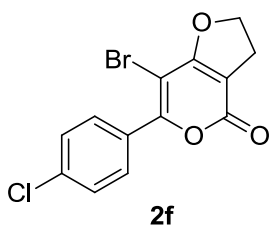
DATA PROCESSING

Line broadening 1.5 Hz

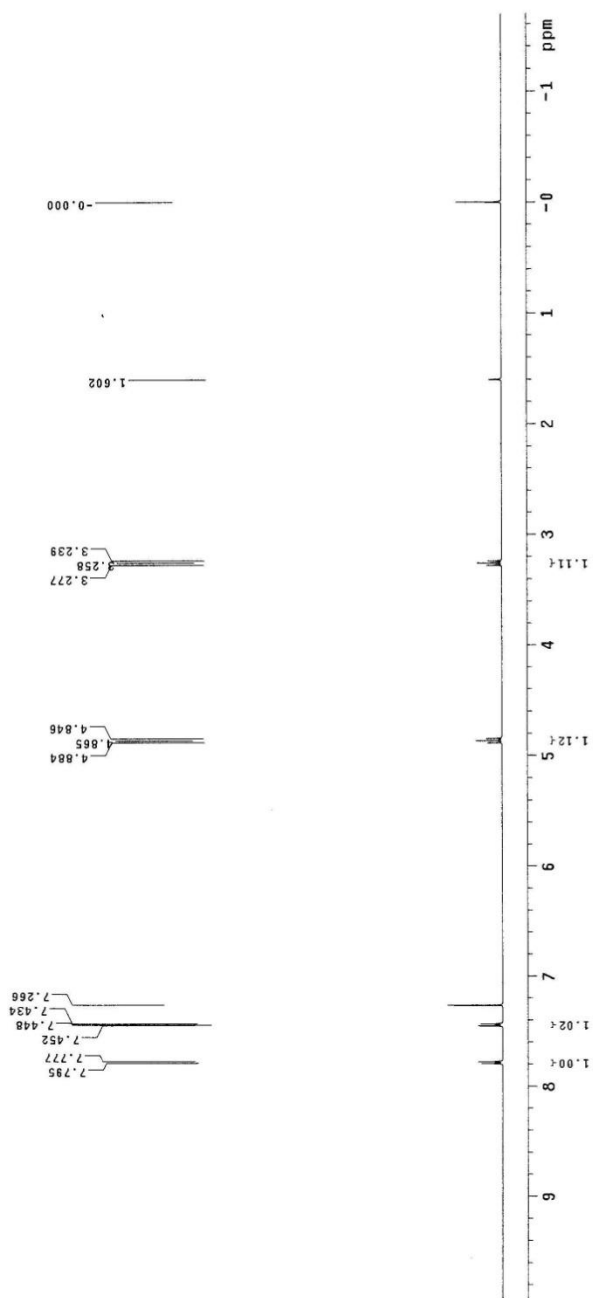
Resolution 0.3 Hz

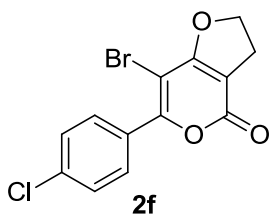
Total time 2 hr, 3 min, 31 sec





STANDARD PROTON PARAMETERS  
Archive directory: /export/home/ouxy/vnmrSYS/data  
Sample directory:  
Pulse Sequence: s2pul  
Solvent: CDCl3  
Ambient temperature  
File: d1348  
INOVA-500 "NMR500"  
Relax. delay: 1.000 sec  
Acq. delay: 0.000 sec  
Acq. time: 1.882 sec  
Width: 9525.4 Hz  
8 Repetitions  
Observed F1: 99.8025885 MHz  
DATA PROCESSING  
FT size: 65536  
Total time: 0 min, 23 sec





STANDARD CARBON PARAMETERS

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

Sample directory:

Pulse Sequence: s2pu1

Solvent: cdcl3

Ambient temperature

File: d1583

INOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 0.00 sec

Width 31421.8 Hz

192 repetitions

OBSERVE C13, 125.6754642 MHz

Decouple H1, 499.8050905 MHz

Power 42 db,

continuously on

WALTZ-16 modulated

DATA PROCESSING

Resolution 1.5 Hz

FT size 131072

Total time 2 hr, 3 min, 31 sec

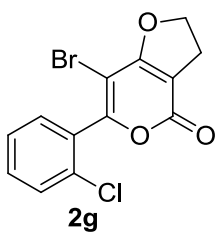
77.256  
77.000  
76.748

169.031  
159.886  
156.983  
137.129  
130.525  
129.694  
128.572

101.542  
90.135  
74.394  
27.172







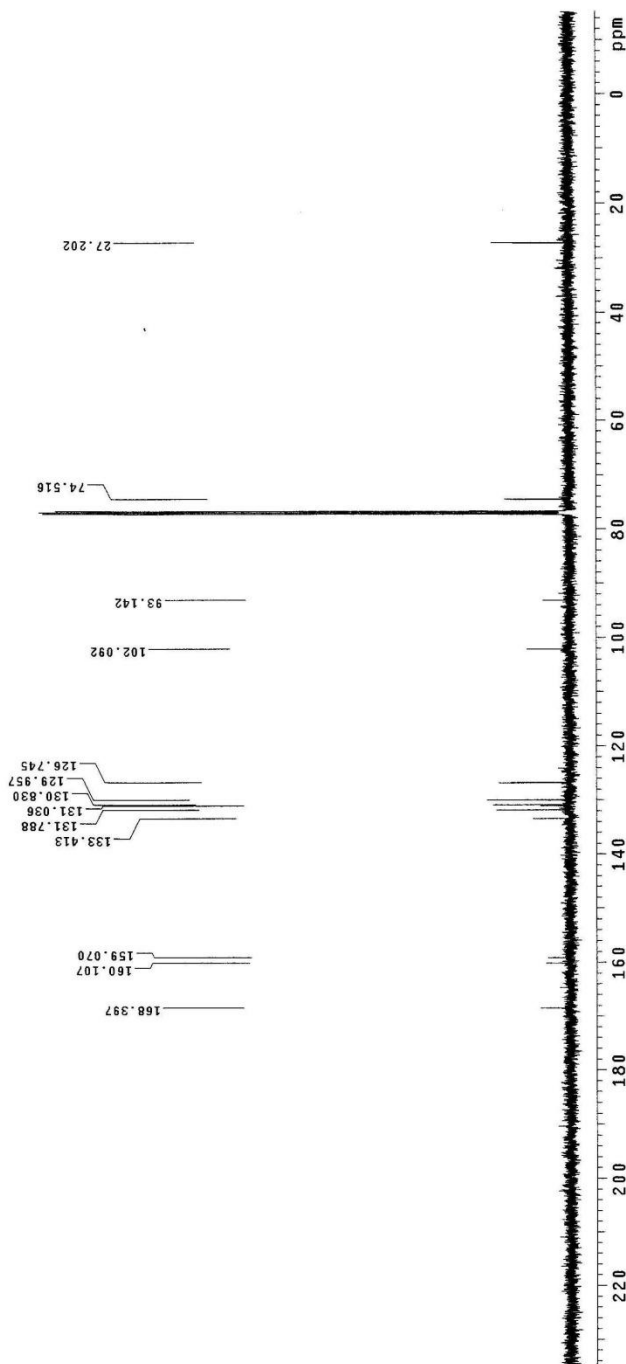
STANDARD CARBON PARAMETERS

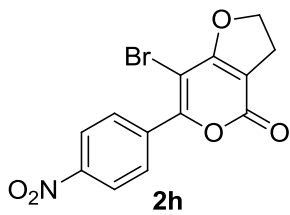
Archive directory: /export/home/ouyy/vnmrsys/data  
Sample directory:

Pulse Sequence: s2pul  
Solvent: cdcl3  
Ambient temperature  
User: 1-14-87  
File: d1549  
INOVA-500 "NENU500"

Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 31421.8 Hz  
192 repetitions  
PULSE PROG. zgpg30  
DECUPLE H1 433.8058905 MHz  
Power 42 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Solving 1.5 Hz  
FT size 131072  
Total time 3 hr, 56 sec

77.256  
77.000  
76.748





STANDARD PROTON PARAMETERS

Archive directory: /export/home/ouyy/vnmr/5/data

Sample directory:

Pulse Sequence: s2pul1

Solvent: CDCl3

Ambient temperature

File: d1817

INOVA-500 "NMR500"

Relax. delay: 1.000 sec

Acq. time: 0.882 sec

Acq. time: 1.882 sec

Width: 10893.2 Hz

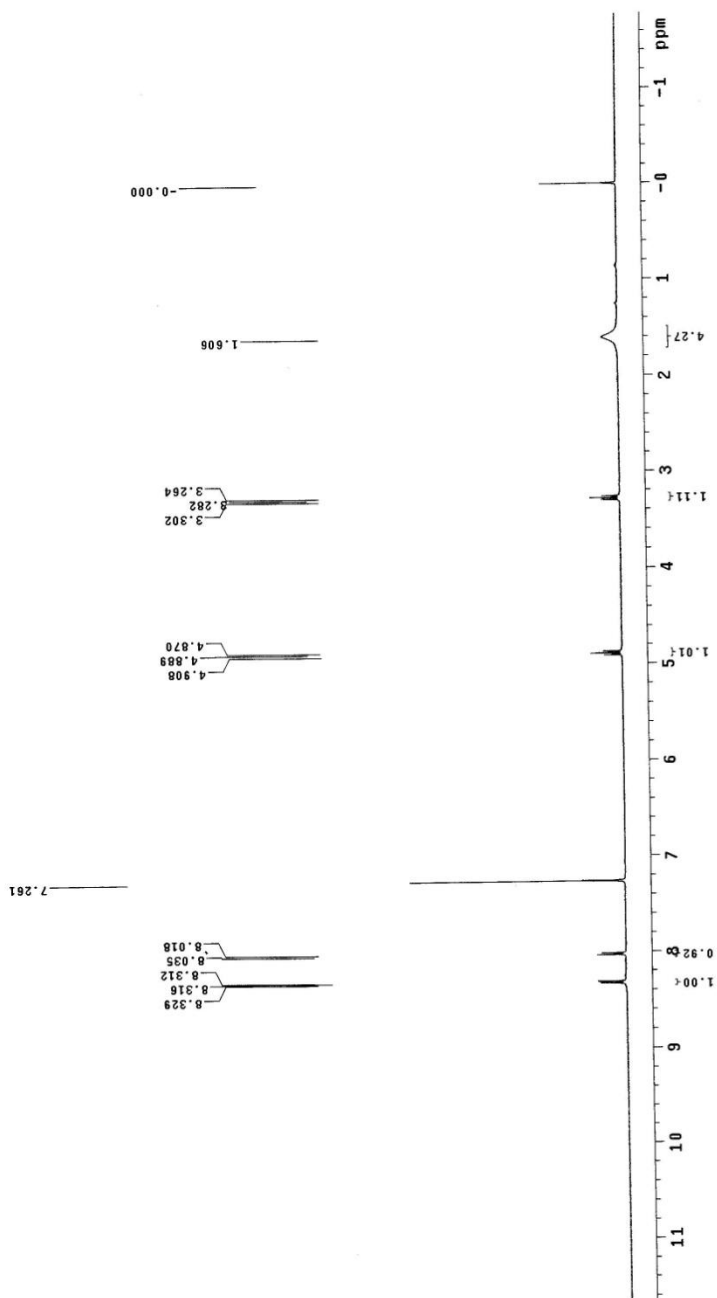
4 repetitions

OSPREY

DATA PROCESSING

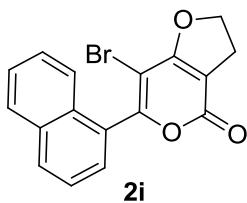
FT size: 65536

Total time: 0 min, 11 sec









STANDARD CARBON PARAMETERS  
Archive directory: /export/home/ouyy/vmarnys/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Temperature: 300

User: l-14-87

File: d1628

INOVA-500 "NMR500"

Relax. delay 0.500 sec

Acq. time 1.300 sec

Width 31421.8 Hz

128 repetitions

DECUPLE H1, 489.8058905 MHz

Power 42 dB

continuously on

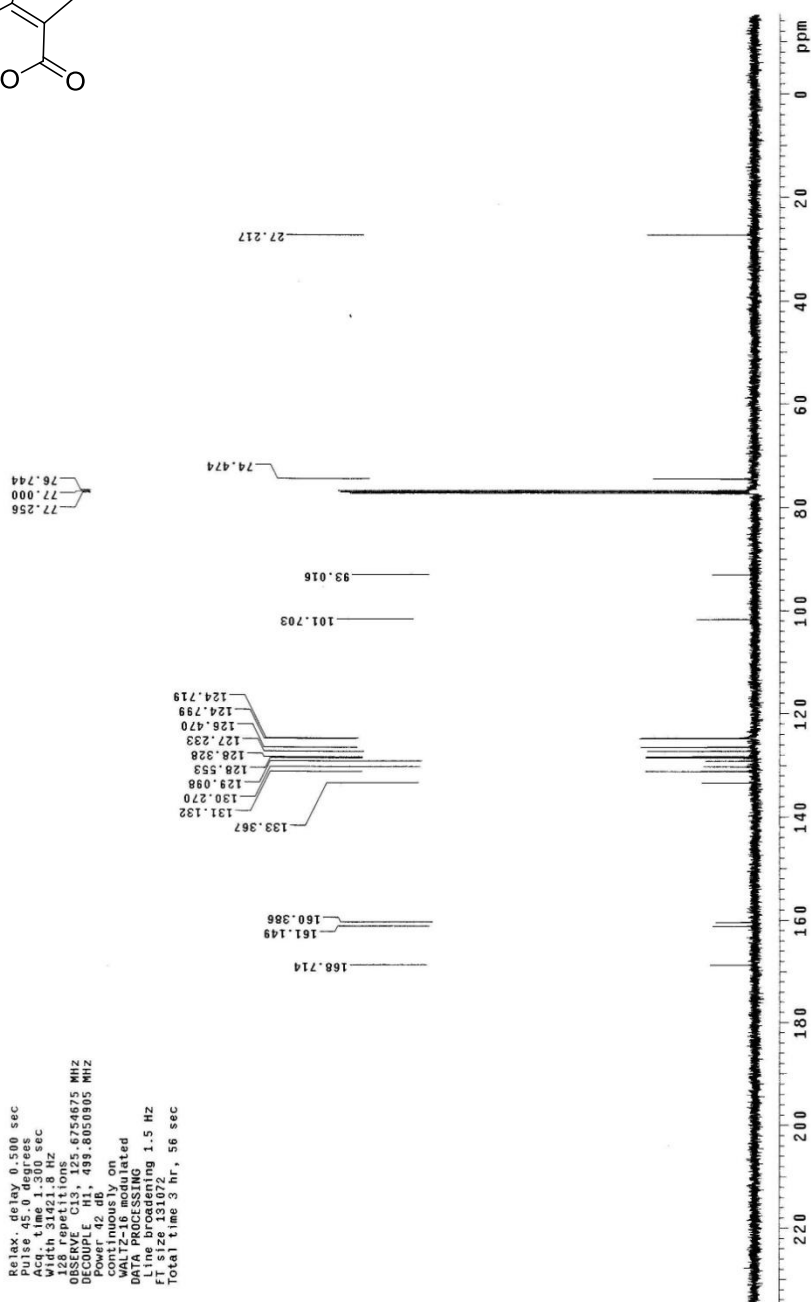
not pre-irradiated

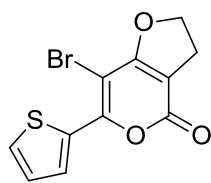
DATA PROCESSING

Line broadening 1.5 Hz

FT size 131072

Total time 3 hr, 56 sec





2j

STANDARD PROTON PARAMETERS

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

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

INOVA-500 "MHNUS00"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.882 sec

File size 1.33 MB

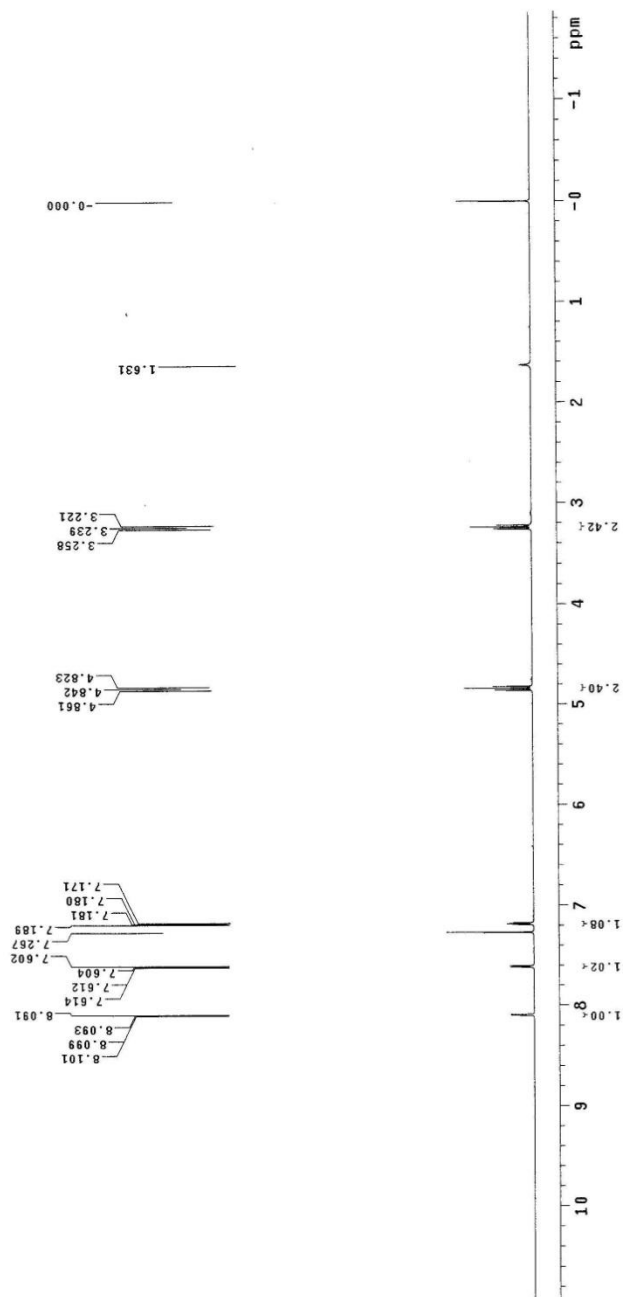
8 F2 acquisitions

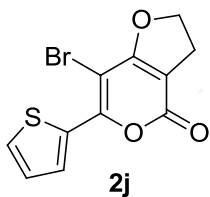
OBSERVE H1, 499.8025897 MHZ

DATA PROCESSING

File size 65556

Total time 0 min, 23 sec



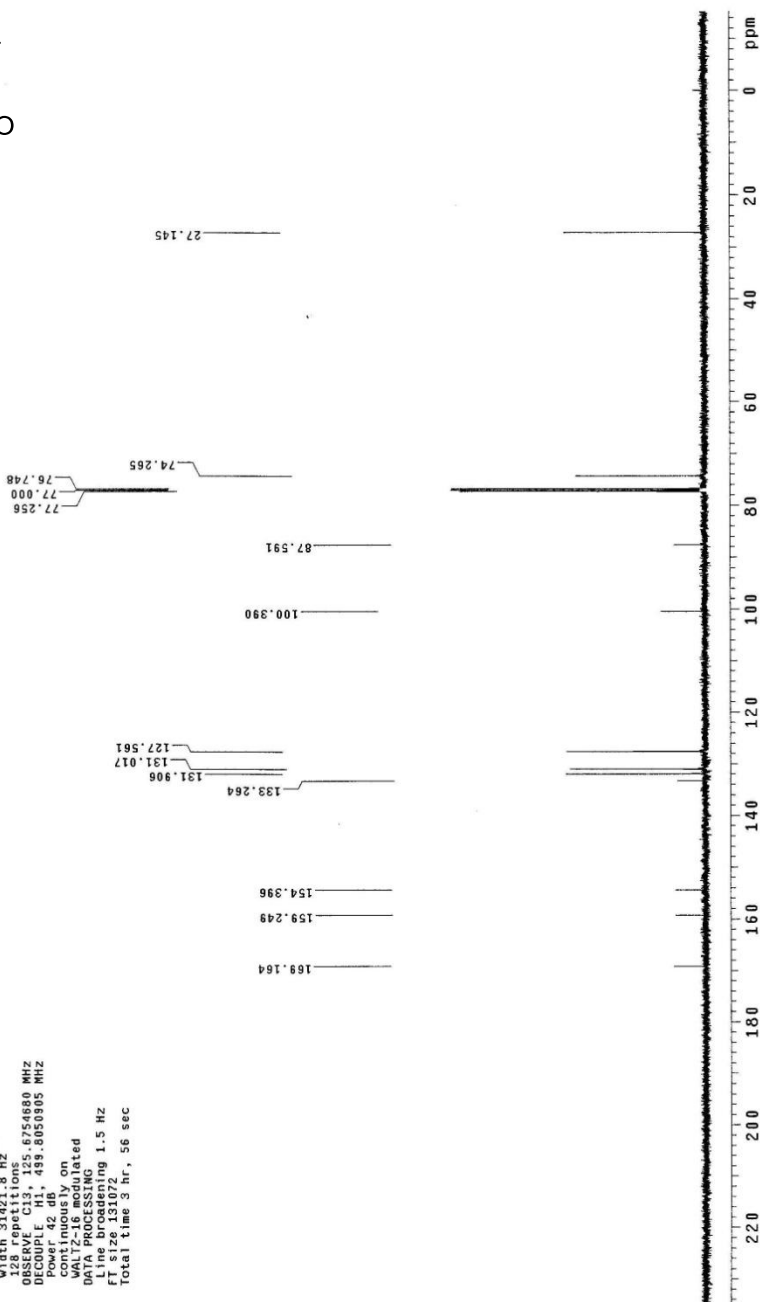


STANDARD CARBON PARAMETERS

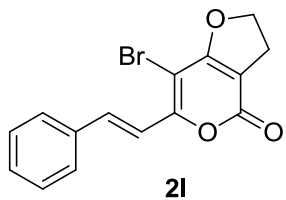
Archive directory: /export/home/ouyy/vmrsys/data  
Sample directory:

Pulse Sequence: s2pul  
Solvent: cdcl3  
Ambient temperature  
User: 1-14-87  
File: d1435 "MENU500"

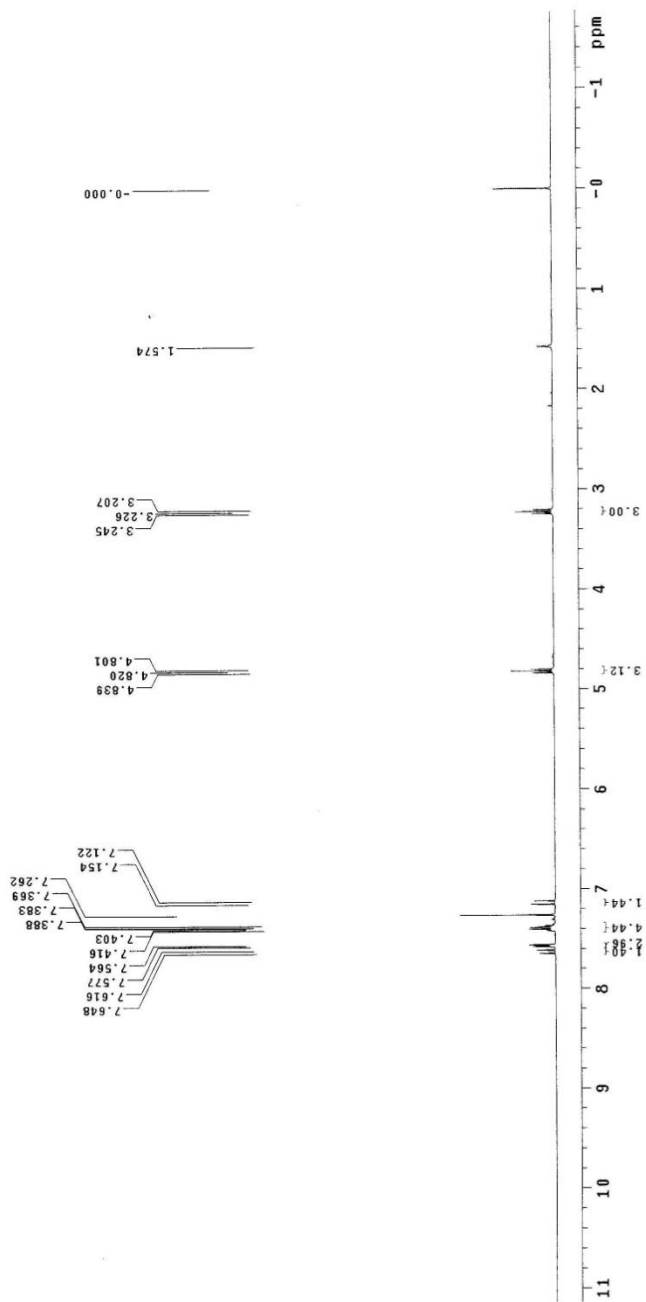
INVA-300 "MENU500"  
Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 1.300 sec  
Width 31421.8 Hz  
Y-axis gain 1.011  
OBSERVE C13 125.6754880 MHZ  
DECOUPLE H1 499.8050805 MHZ  
Power 42 db  
SOLVENT CDCL3  
WALTZ16 modulated  
DATA PROCESSING  
Line broadening 1.5 Hz  
F1 size 131072  
Total time 5 hr, 56 sec

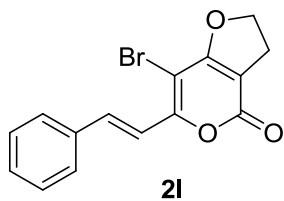




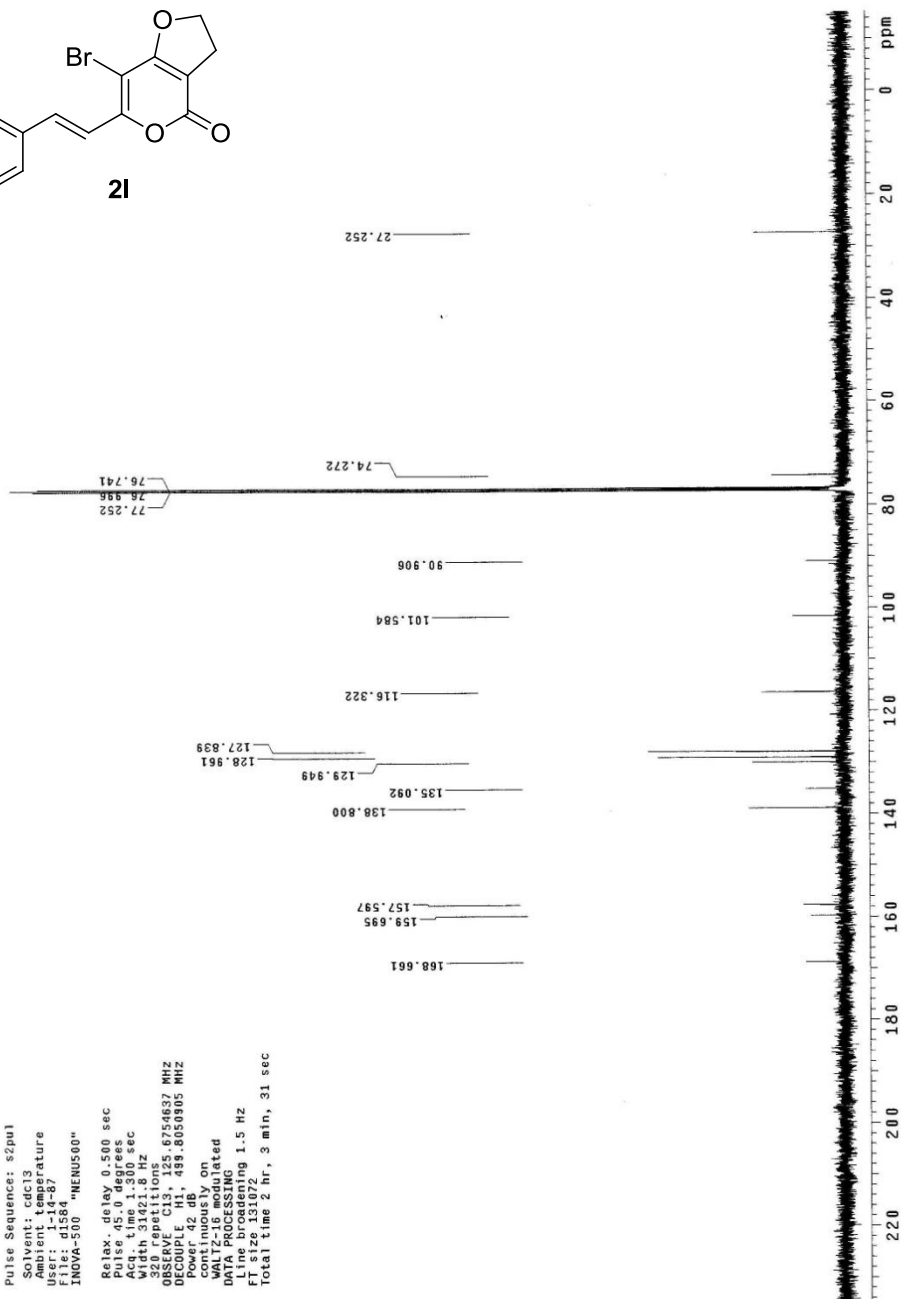


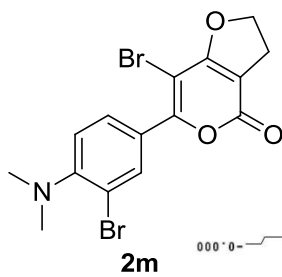
STANDARD PROTON PARAMETERS  
Archive directory: /export/home/ouby/vmrsys/data  
Sample directory:  
Pulse Sequence: s2pu1  
Solvent: CDCl3  
File: d158  
Temperature  
INOVAS-500 "HMENU500"  
Relax. delay 1.000 sec  
Pulse 45.0 degree  
Acq. time 0.23 sec  
Width 10843.2 Hz  
8 repetitions  
OBSERVE H1  
PULPROG zgpg30  
FT size 65536  
Total time 0 min, 23 sec





STANDARD CARBON PARAMETERS  
Archive directory: /export/home/ouyy/vmrsys/data  
Sample directory:  
Pulse Sequence: s2pul  
Solvent: cdcl3  
Ambient temperature  
User: 1-14-87  
File: d1584  
INOVA-500 "MENSU60"  
Relax. delay 0.500 sec  
Pulse 45.0 degrees  
Acq. time 1.500 sec  
Width 31421.8 Hz  
Spectral width 31421.8 Hz  
OBSERVE C13 125.6754637 MHz  
DECOUPLE H1 499.8050905 MHz  
Power 42 dB  
Continuously on  
Waltz16 1.5 Hz  
Waltz16 1.5 Hz  
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/vnmrsgs/data

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Sample temperature

File: d1668

INOVA-500 "NENU500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

CPD 0.000 sec

Width 10893.2 Hz

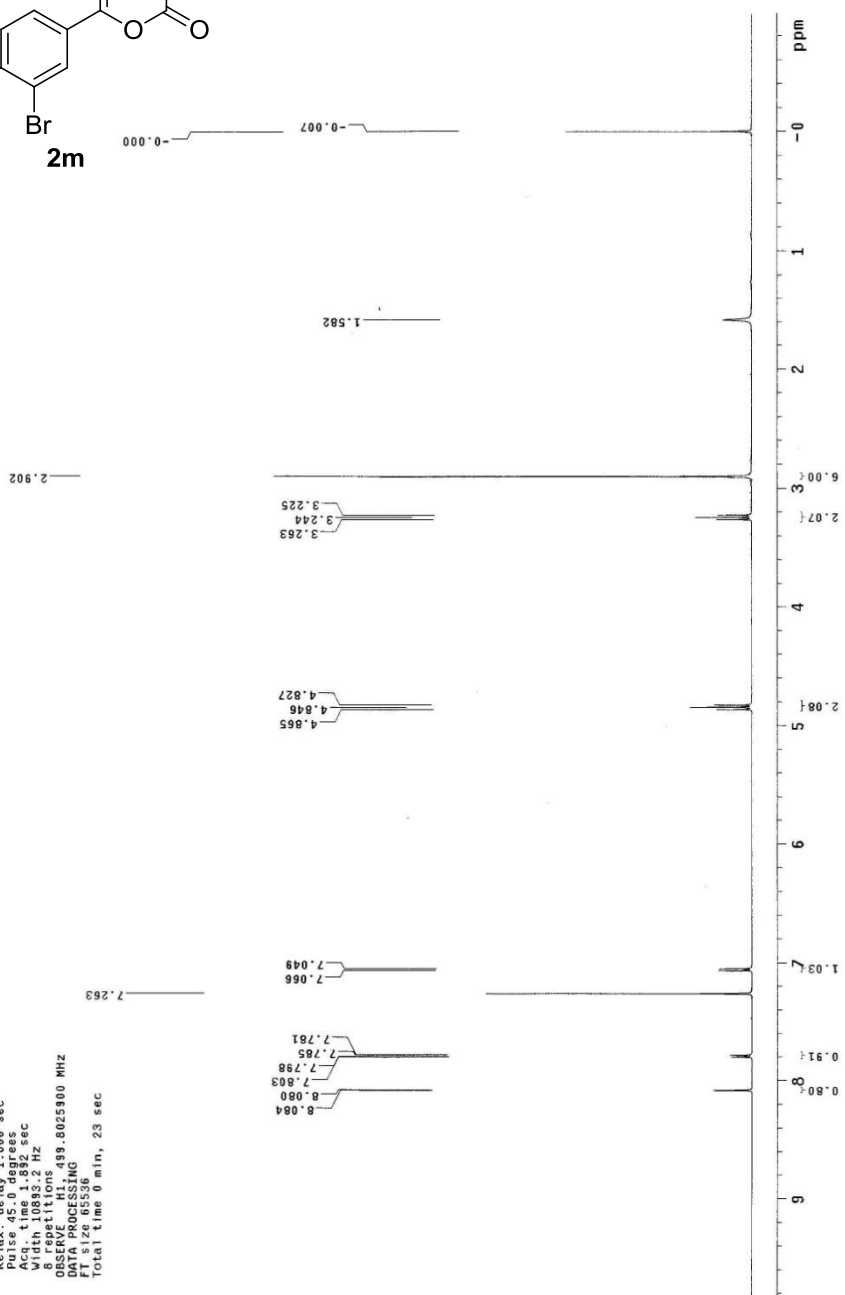
8 repetitions

OBSERVE H1: 499.8025900 MHz

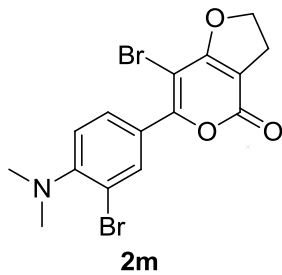
PROBHD 1H/13C/31P

PT 124.65536

Total time 0 min, 23 sec







STANDARD NMR PARAMETERS

Sample directory: /export/home/ouxy/vnmr/500/data

Sample directory:

Pulse Sequence: s2pu1

Solvent: cdcl3

Ambient temperature

Exp: 48-87

File: d1670

INOVA-500 "NENU500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 0.00 sec

Width 31421.8 Hz

704 repetitions

OBSERVE C13, 125.6754632 MHz

DCOUPL 42 db, 499.8050905 MHz

continuously on

WALTZ-16 modulated

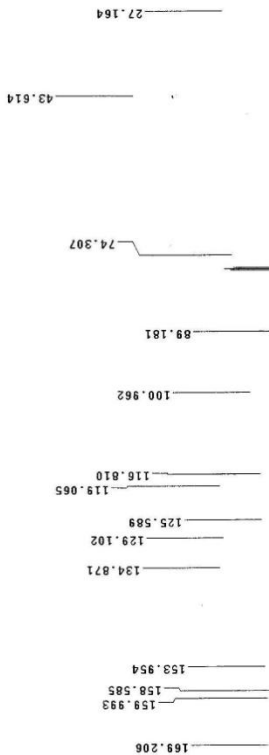
DATA PROCESSING

ftscanning 1.5 Hz

FT size 131072

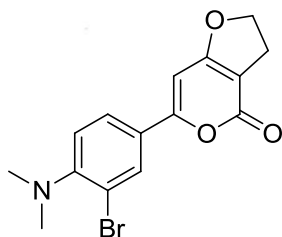
Total time 3 hr, 56 sec

77.256  
77.000  
76.744



220 200 180 160 140 120 100 80 60 40 20 0 ppm





3

STANDARD CARBON-13 PARAMETERS

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

Sample directory:

Pulse Sequence: s2pu1

Solvent: cdcl3

Temperature: 300

User: 1-14-87

File: dl665

PROVA-500 "MNM500"

Relax: delay 0.500 sec

Pulse: 45.0 degree

Acq. time 1.390 sec

Width 31421.8 Hz

Reference: TMS

OBSERVE: C13, 489.8058805 MHz

DECOUPLE: H1, 499.8058805 MHz

Power 42 dB

Continuously on

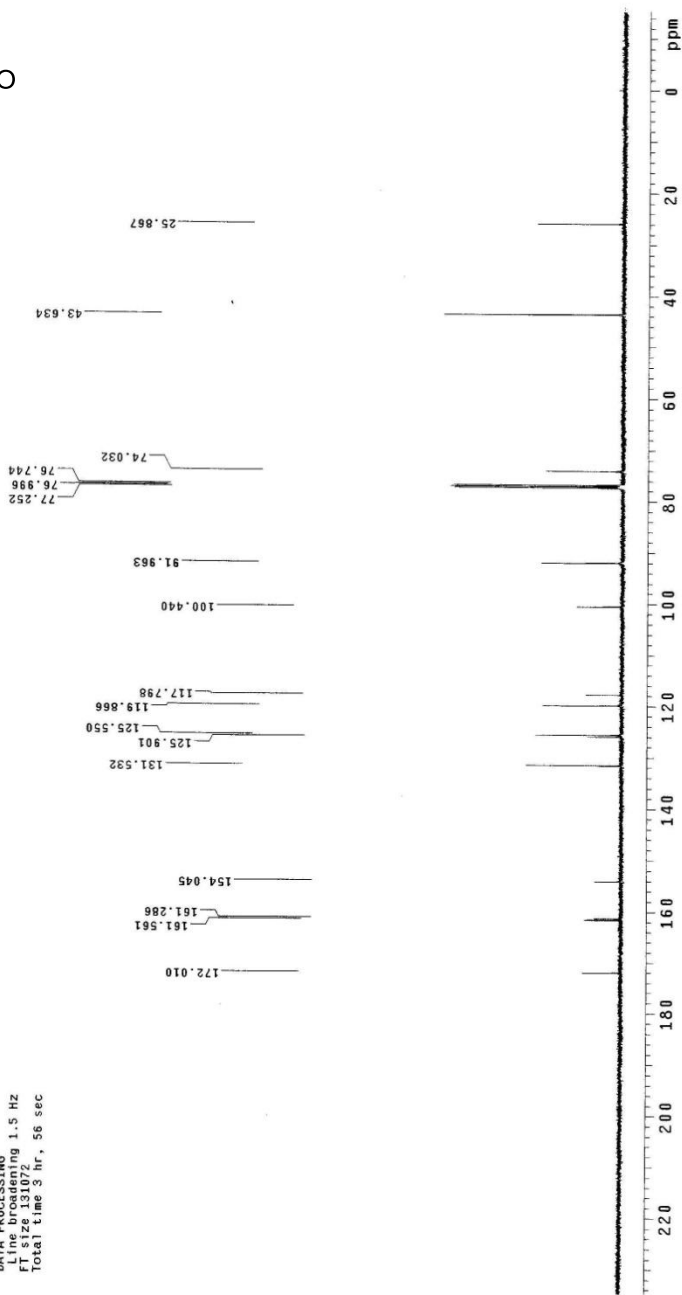
off for 1.000 sec

DATA PROCESSING

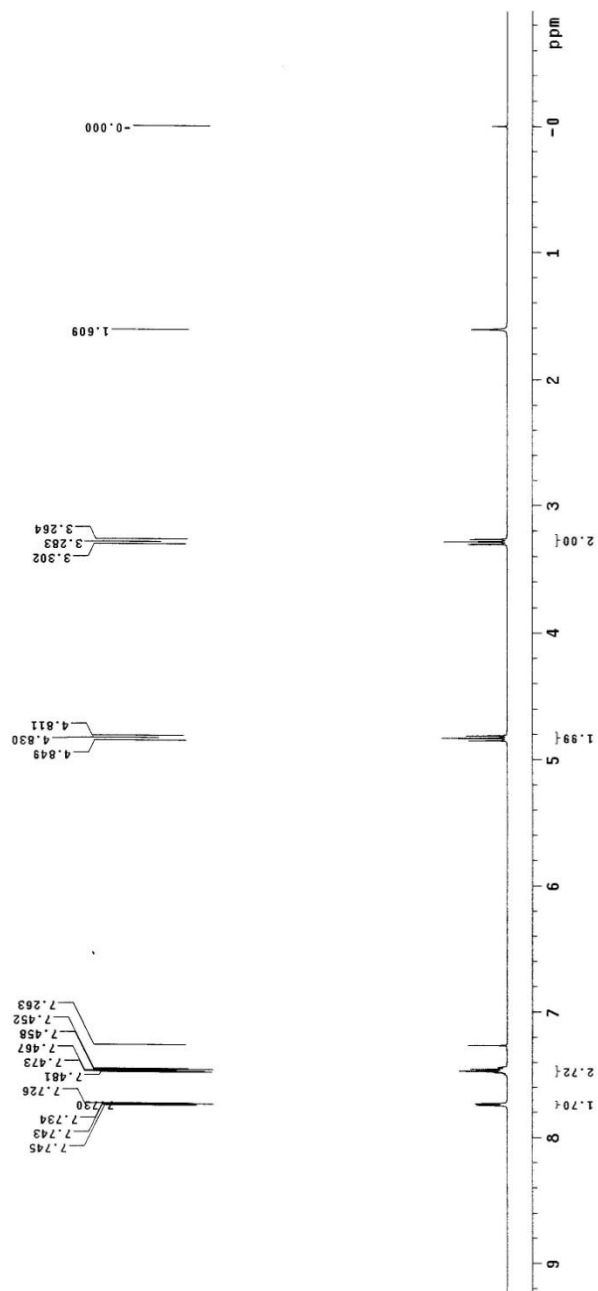
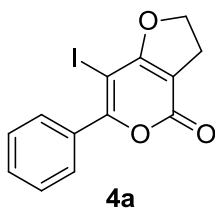
Line broadening 1.5 Hz

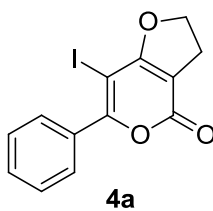
FT size 131072

Total time 3 hr, 56 sec



STANDARD PROTON PARAMETERS  
Archive directory: /export/home/ouyy/vmmsys/data  
Sample directory:  
Pulse Sequence: s2pu1  
Solvent: CDCl3  
Ambient temperature  
INOVA-500 "NENU500"  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.32 sec  
F1 frequency 500.136 MHz  
8 repetitions  
OBSERVE\_H1 499.8025904 MHZ  
DATA PROCESSING  
Total time 0 min, 23 sec





STANDARD CARBON PARAMETERS  
Archive directory: /export/home/ouyy/vnmr/5ys/data

Sample directory:

Pulse Sequence: szpu1

Solvent: cdcl3

Temperature: 300

User: 1-14-87

File: d1802

INOVA-500 "NMR500"

Relax. delay: 0.500 sec

Acq. delay: 0.000 sec

Acq. time: 1.300 sec

Width: 31421.8 Hz

320 repetitions

DECUPLE: H1, 499.8050905 MHz

Power: 42 dB

continuously on

off during relaxation

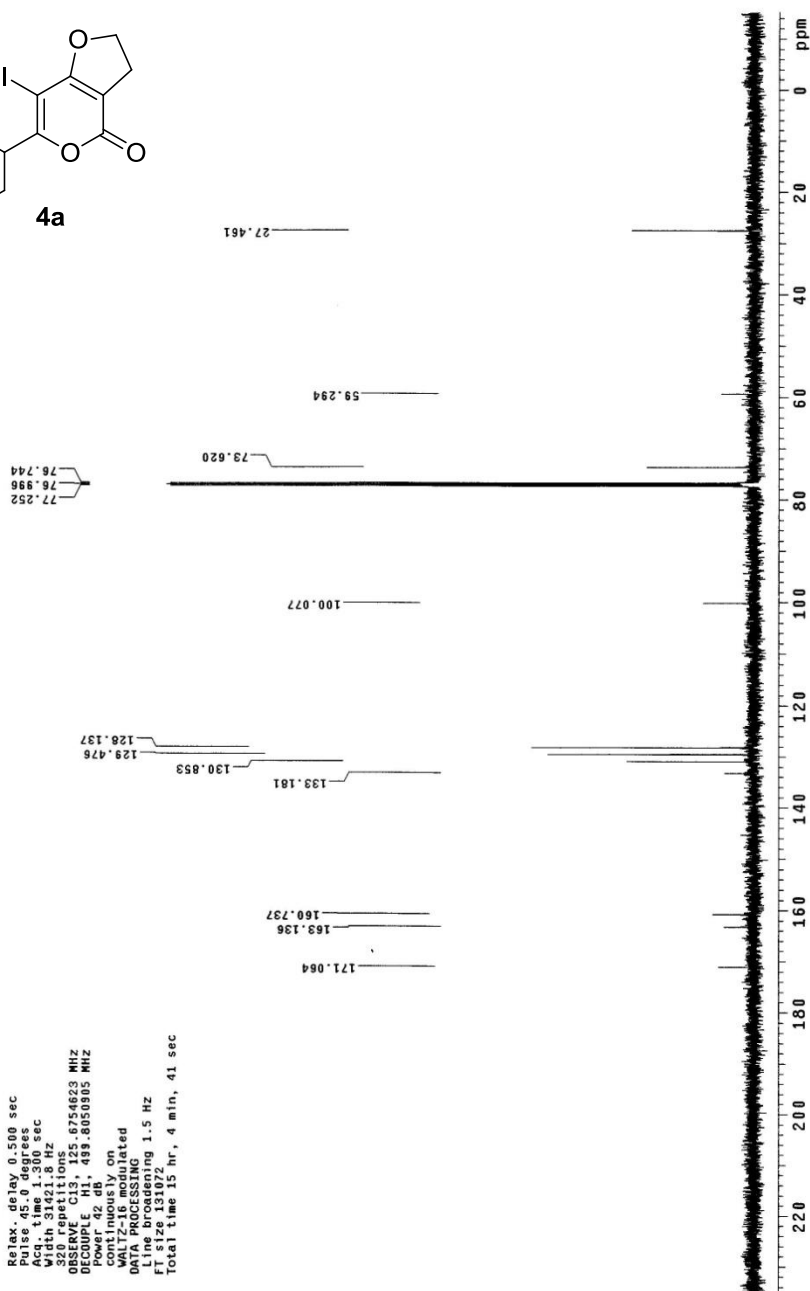
DATA ACQUISITION

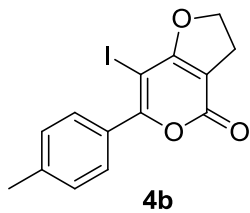
DATA PROCESSING

Line broadening: 1.5 Hz

FT size: 131072

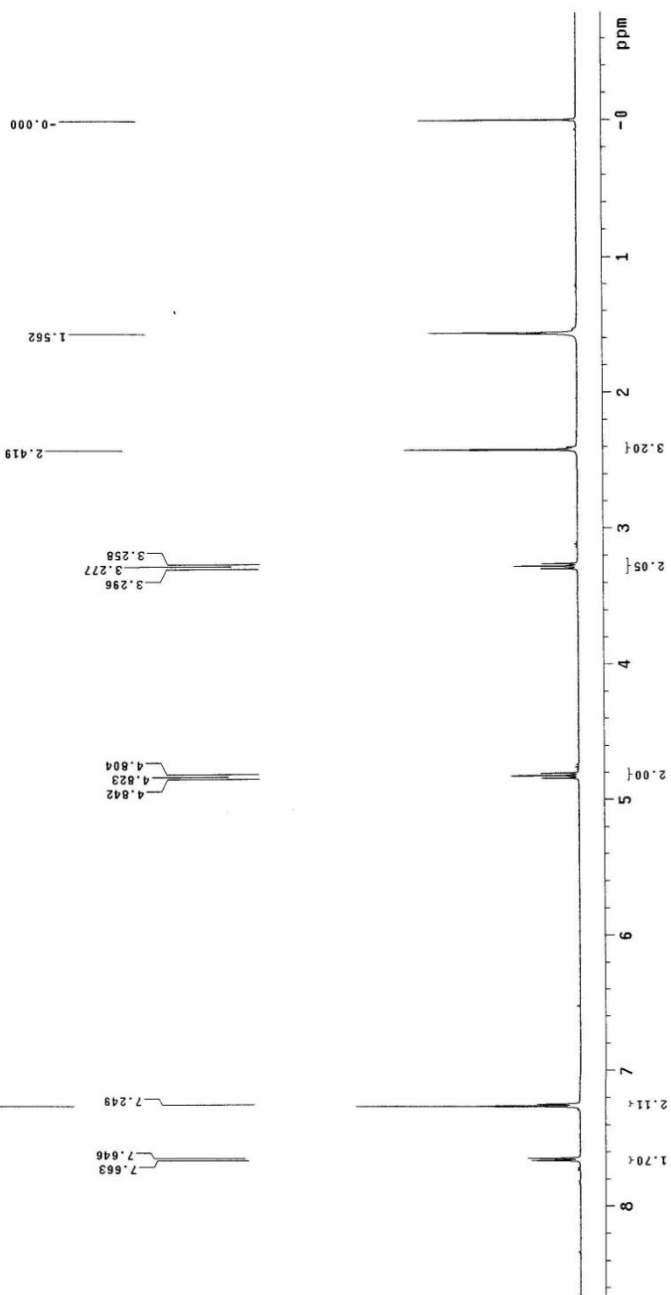
Total time: 15 hr, 4 min, 41 sec

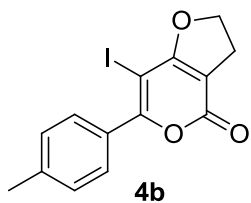




4b

STANDARD PROTON PARAMETERS  
Archive directory: /export/home/ouyy/vmmf/sys.  
Sample directory:  
Pulse Sequence: s2pu1  
Solvent: CDCl3  
Ambient temperature  
53.5 °C  
INOVA-500 "MNMU500"  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.892 sec  
F1 500.136 MHz  
8 repetitions  
OBSERVE H1, 499.8025914 MHz  
DATA PROCESSING  
F2 500.136 MHz  
Total time 0 min, 23 sec





STANDARD CARBON PARAMETERS

Archive directory: /export/home/ouuy/vmr/sy/data

Sample directory:

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

User: i-14-87

INSTR: 500 "NMR500"

Relax. delay 0.500 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Waltz16 1000000 Hz

384 repetitions

OBSERVE C13, 125.6754632 MHZ

DECOUPLE H1, 499.8050905 MHZ

Power 1200000

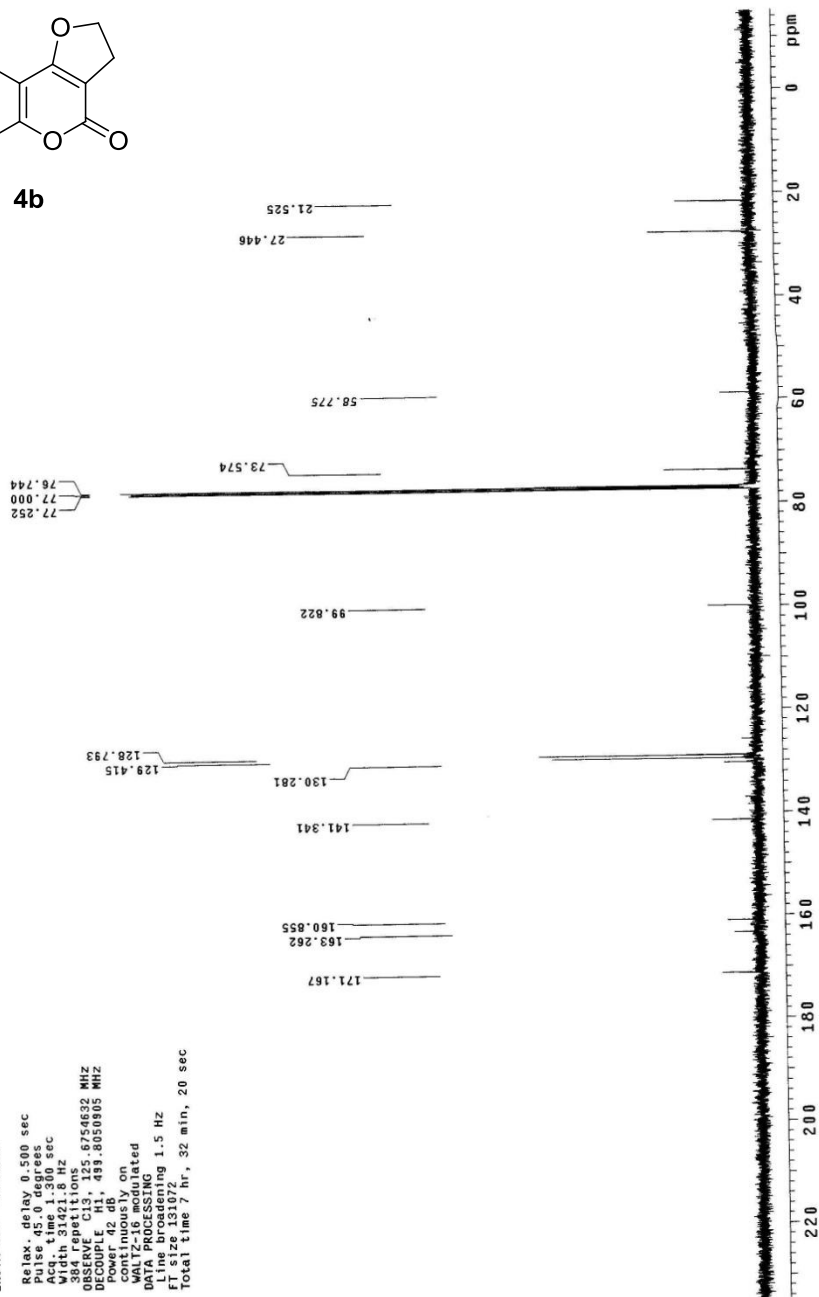
WALTZ-16 modulated

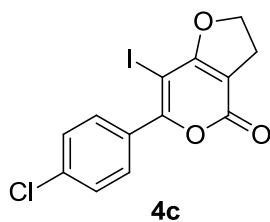
DATA PROCESSING

Line broadening 1.5 Hz

Frequency 500.136300 MHz

Total time 7 hr, 32 min, 20 sec





STANDARD PROTON PARAMETERS

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

Sample directory:

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: d1748 "NENU500"

IROVA-500 "NENU500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.892 sec

Width 10893.2 Hz

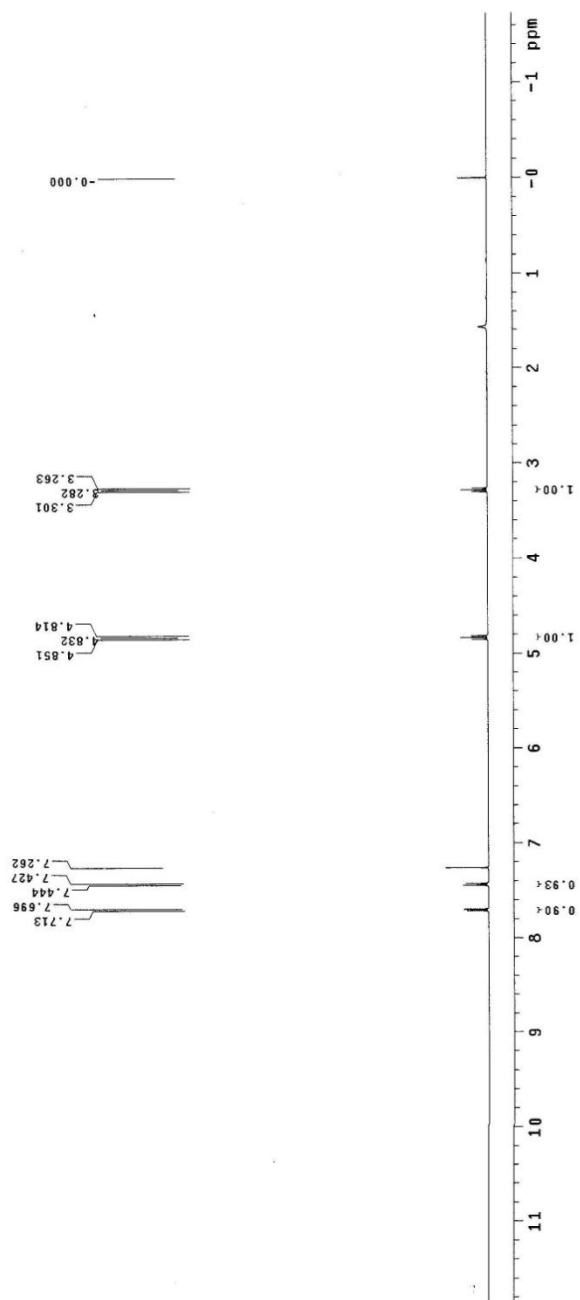
Observed F1 489.8025914 MHz

OBSERVE H1 489.8025914 MHz

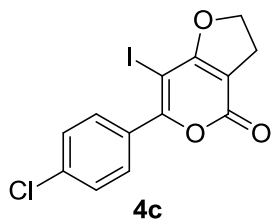
DATA PROCESSING

FT size 65536

Total time 0 min, 23 sec







STANDARD CARBON PARAMETERS

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

Pulse Sequence: s2pul

Solvent: cdc13

Ambient Temperature

40.00

File: d1754

INOVA-500 "MNU500"

Relax. delay 0.500 sec

Pulse 45.00 deg/sec

Width 31421.8 Hz

832 repetitions

OBSERVE C13, 125.675618 MHz

Power 42 db, 493.6558805 MHz

continuously on

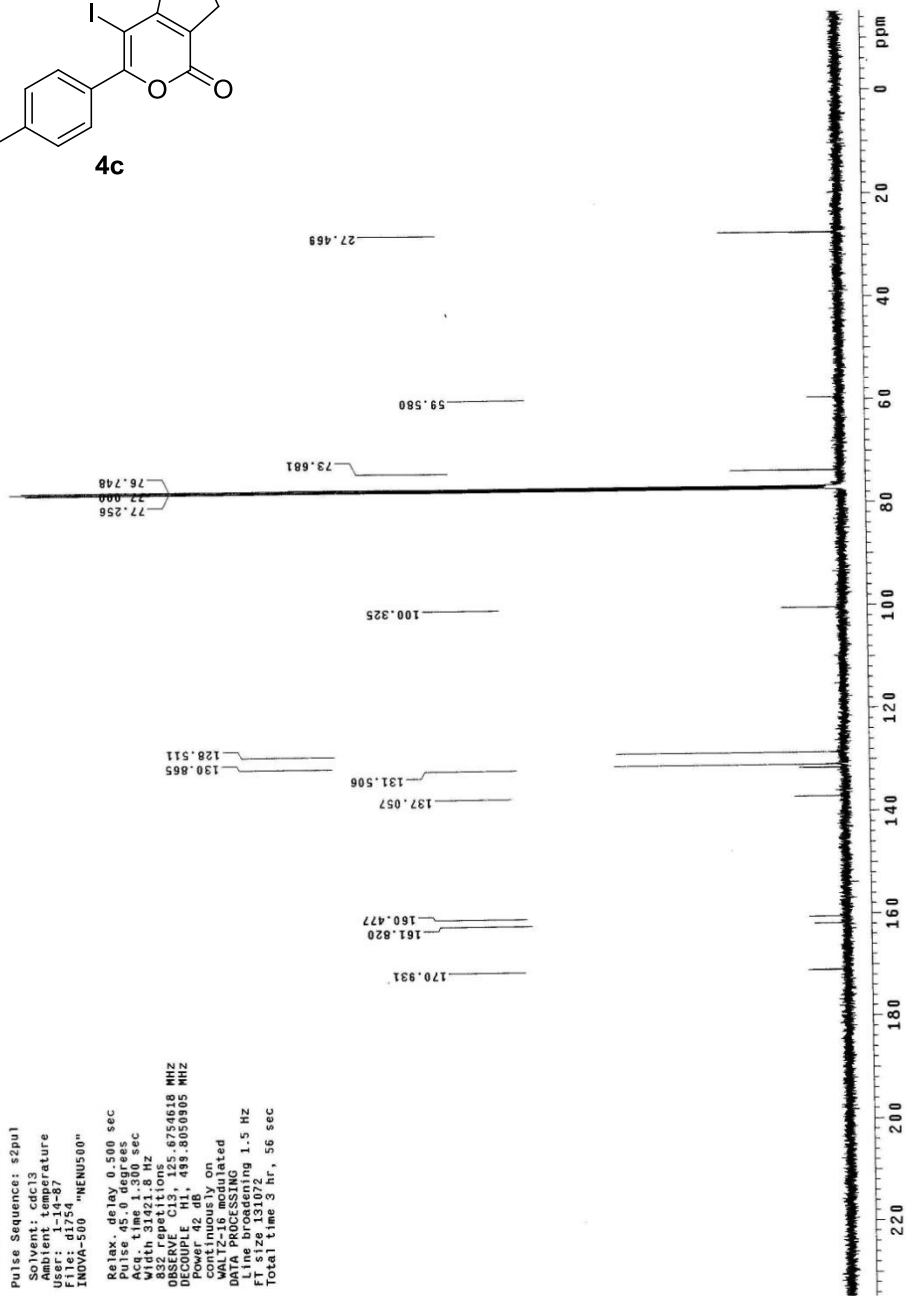
WALTZ-16 modulated

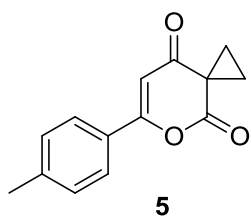
D1 1.00000000 sec

Line broadening 1.5 Hz

FT size 131072

Total time 3 hr, 56 sec





STANDARD PROTON PARAMETERS  
Archive directory: /export/home/ouss/vmrsys/data  
Sample directory:

Pulse Sequence: s2pu)

Solvent: CDCl3

Sample temperature

File: d125

INOVA-500 "MNU500"

Relax. delay 1.000 sec

Pulse 45.0 degree

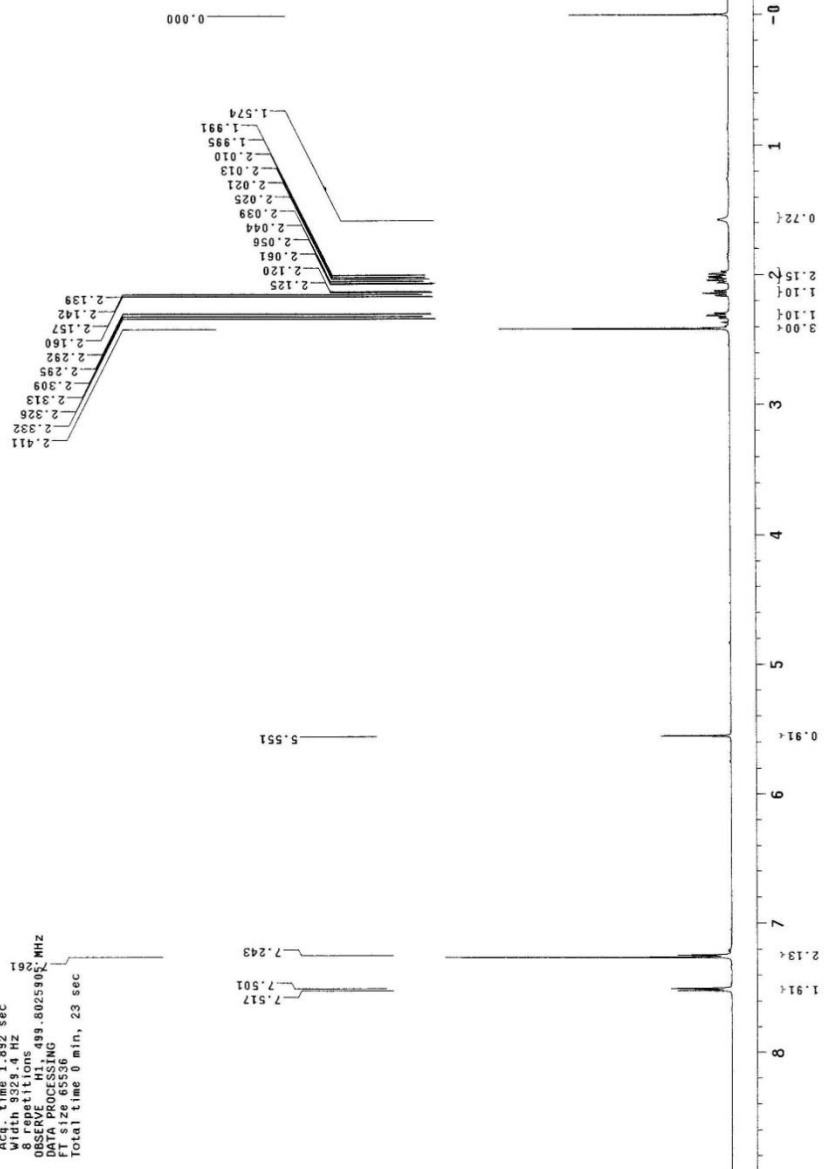
Width 928.4 Hz

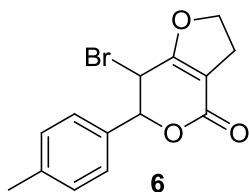
8 repetitions

OBSERVE H1, 493.8025905 MHz

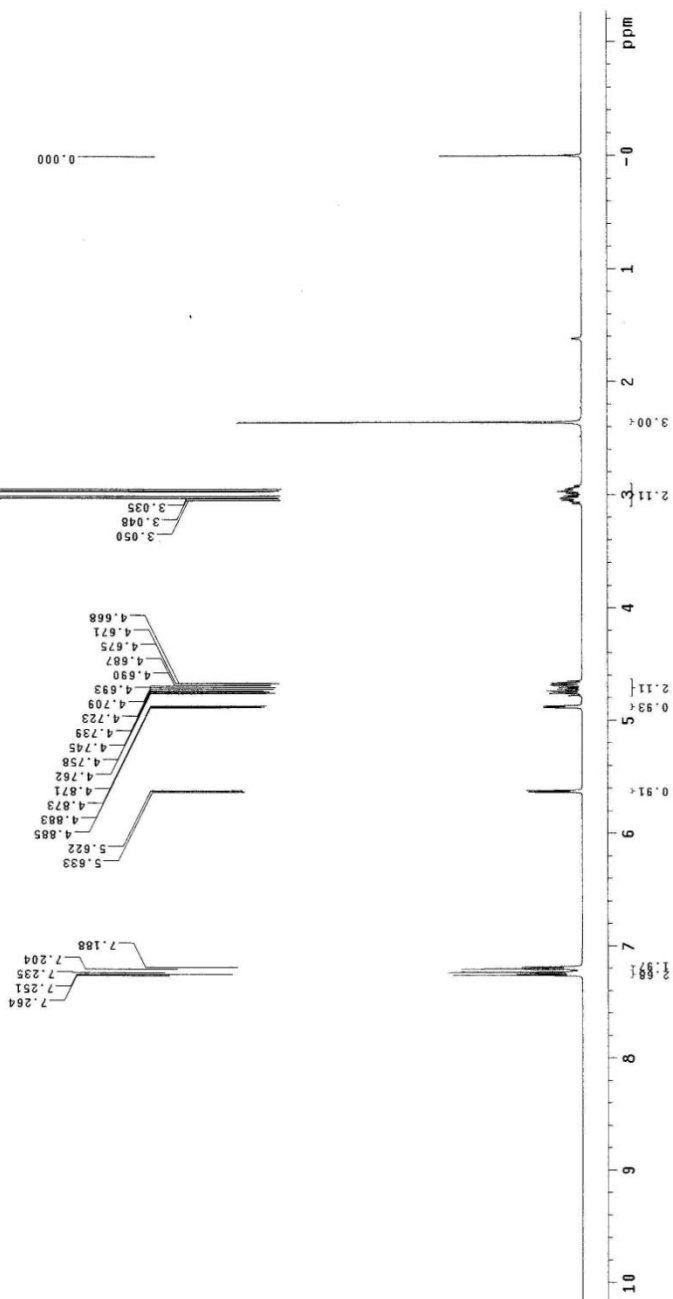
PROBHD 5MM QNP 1H/13

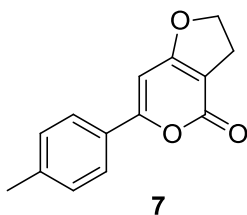
Total time 0 min, 23 sec





STANDARD PROTON PARAMETERS  
Archive directory: /export/home/ouxy/vnmrsys/data  
Sample directory:  
Pulse Sequence: szpu1  
Solvent: CDCl3  
Ambient temperature  
100 MHz  
INDVA=500 "HNU500"  
Relax . delay 1.000 sec  
Pulse 45.0 degrees  
Acq time 1.382 sec  
Sweep 32750 Hz  
8 repetitions  
OBSERVE H1, 499.8025908 MHz  
DATA PROCESSING  
F1: 12.00506  
Total time 0 min, 23 sec





STANDARD PROTON PARAMETERS  
Archive directory: /export/home/ouby/vnmrsys/data  
Sample directory:  
Pulse Sequence: s2pu1  
Solvent: CDCl3  
Pulse program: zgpg30  
Temperature  
File: d1218  
INOVA-500 "MNU500"  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Pulse width 12.000 sec  
Sweep width 9329.4 Hz  
AQ 0.191 sec  
RG 327.5  
Number of scans 8 repetitions  
OBSERVED F1 498.8025648 MHz  
PULPROG zgpg30  
PC 1.00000000  
FT size 65536  
Total time 0 min, 23 sec

