Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Amphiphilic Allylation of Arylidene–1,3–oxazol–5(4*H*)–one Using Bis–π–allylpalladium Complexes: An Approach to Synthesis of Cyclohexyl and Cyclohexenyl α–Amino Acids

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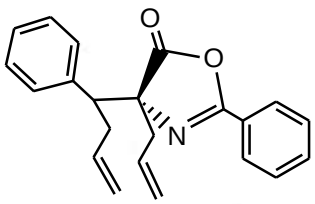
Contents of Supporting Information (50 Pages)

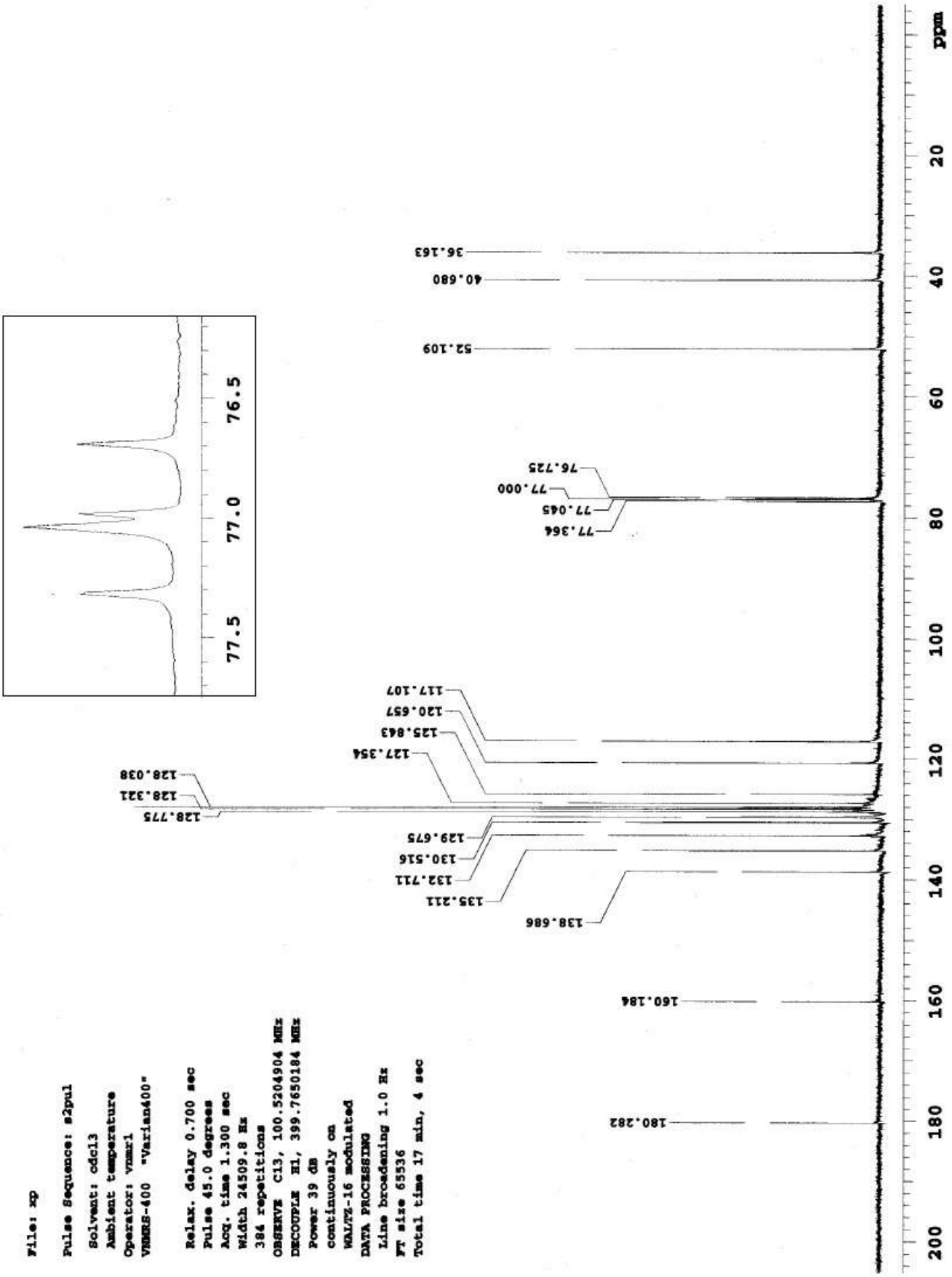
Allyl-2-phenyl-4-(1-phenyl-but-3-enyl)-4H-oxazol-5-one (3a)

^{1}H NMR (400 MHz, $CDCl_3$)



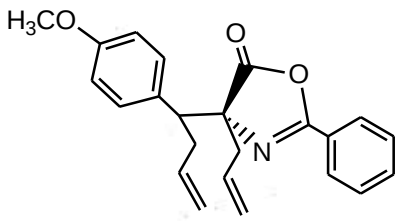
3a

^{13}C NMR (100 MHz, $CDCl_3$)



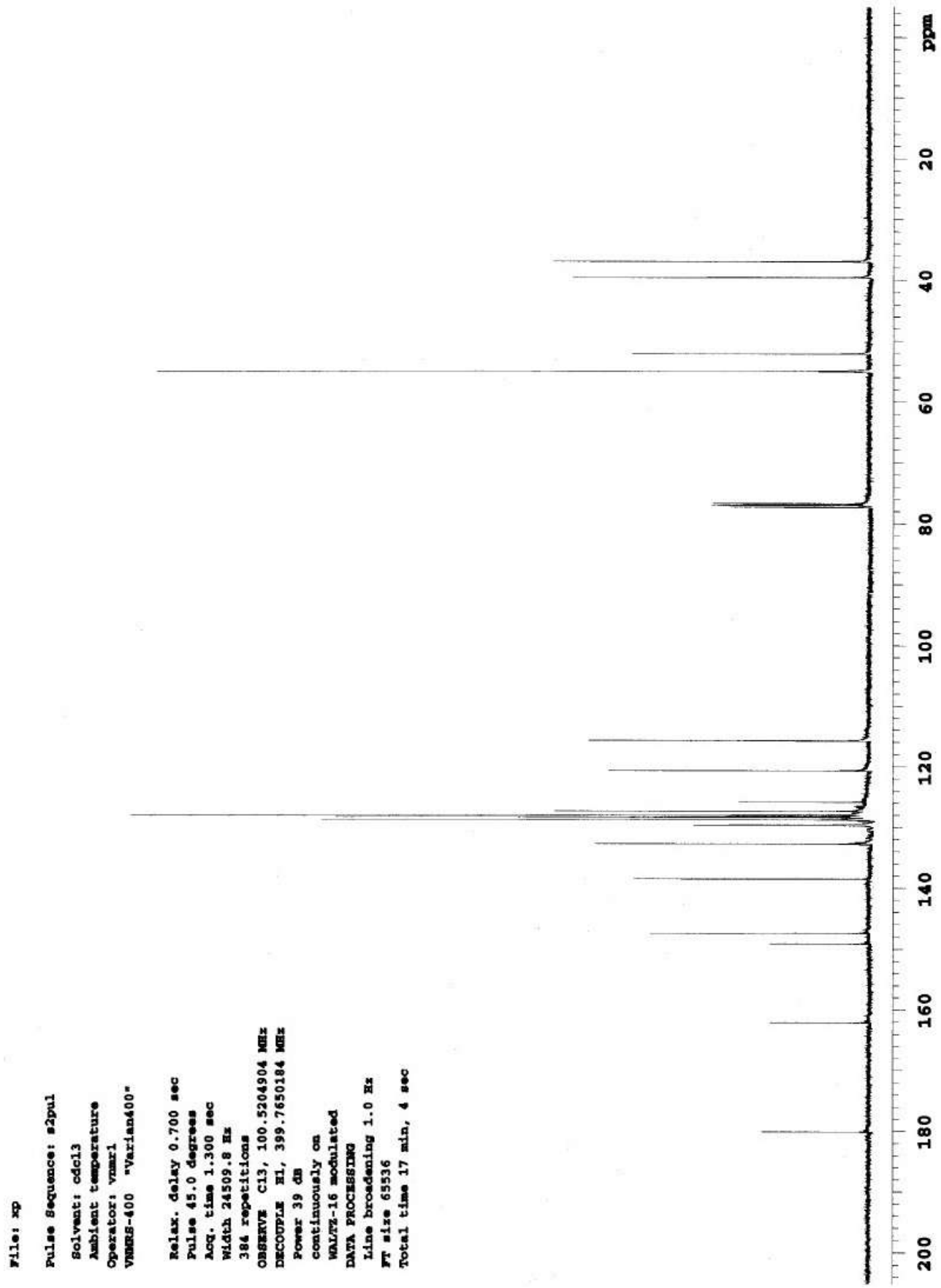
4-Allyl-4-[1-(4-methoxy-phenyl)-but-3-enyl]-2-phenyl-4H-oxazol-5-one (3b)

^{1}H NMR (400 MHz, $CDCl_3$)



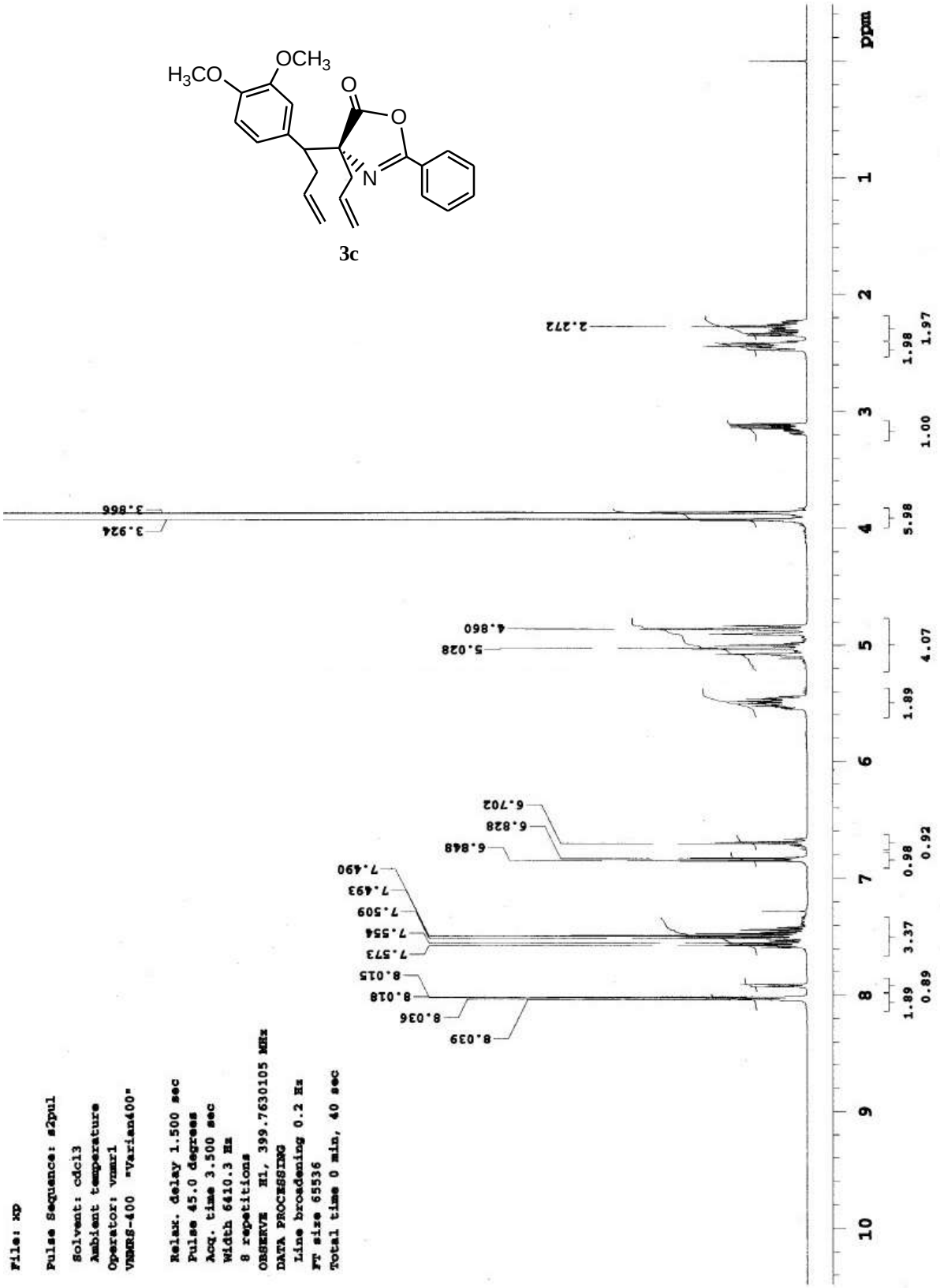
3b

^{13}C NMR (100 MHz, $CDCl_3$)

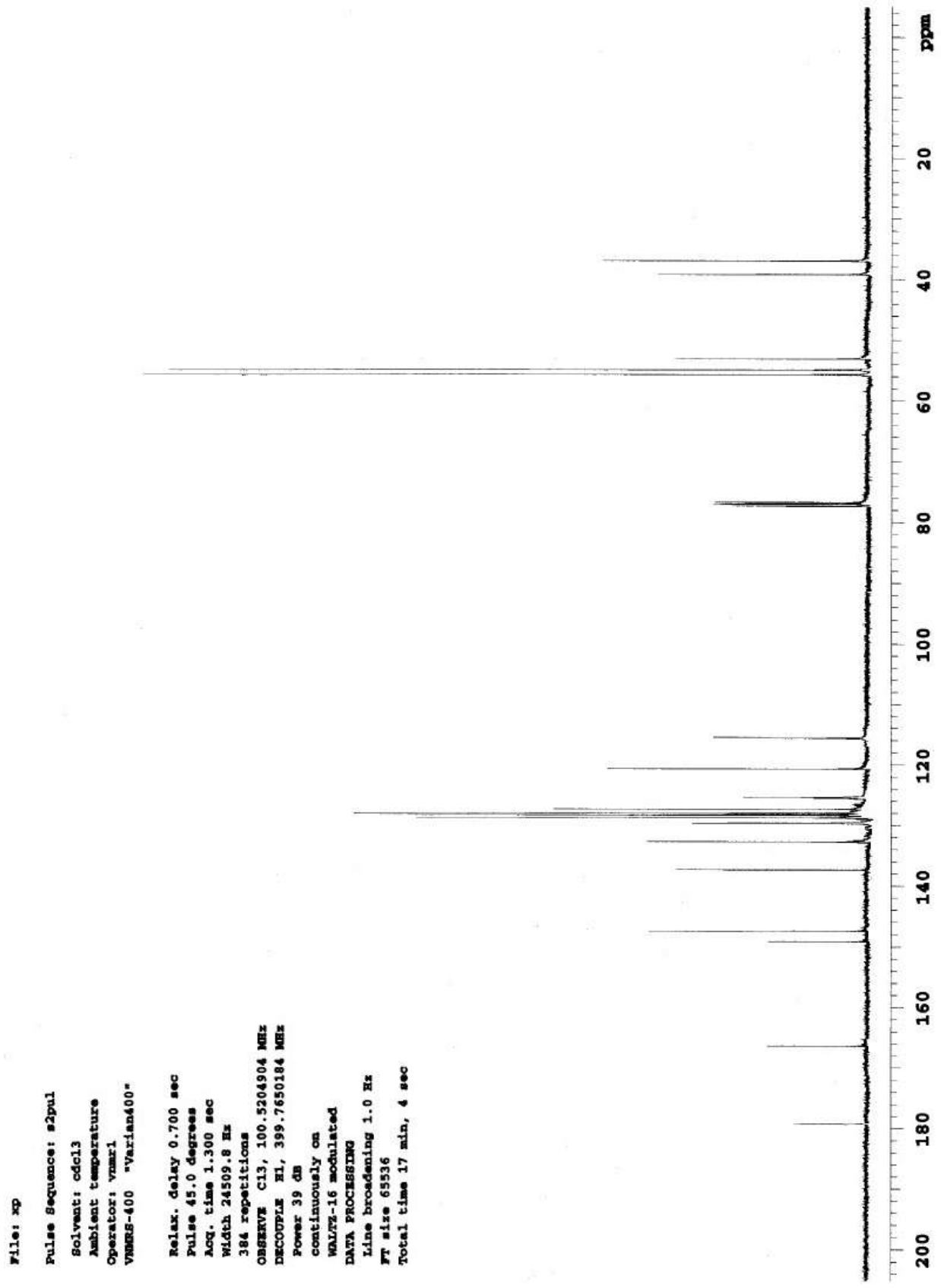


4-Allyl-4-[1-(3,4-dimethoxy-phenyl)-but-3-enyl]-2-phenyl-4H-oxazol-5-one (3c)

^{1}H NMR (400 MHz, $CDCl_3$)

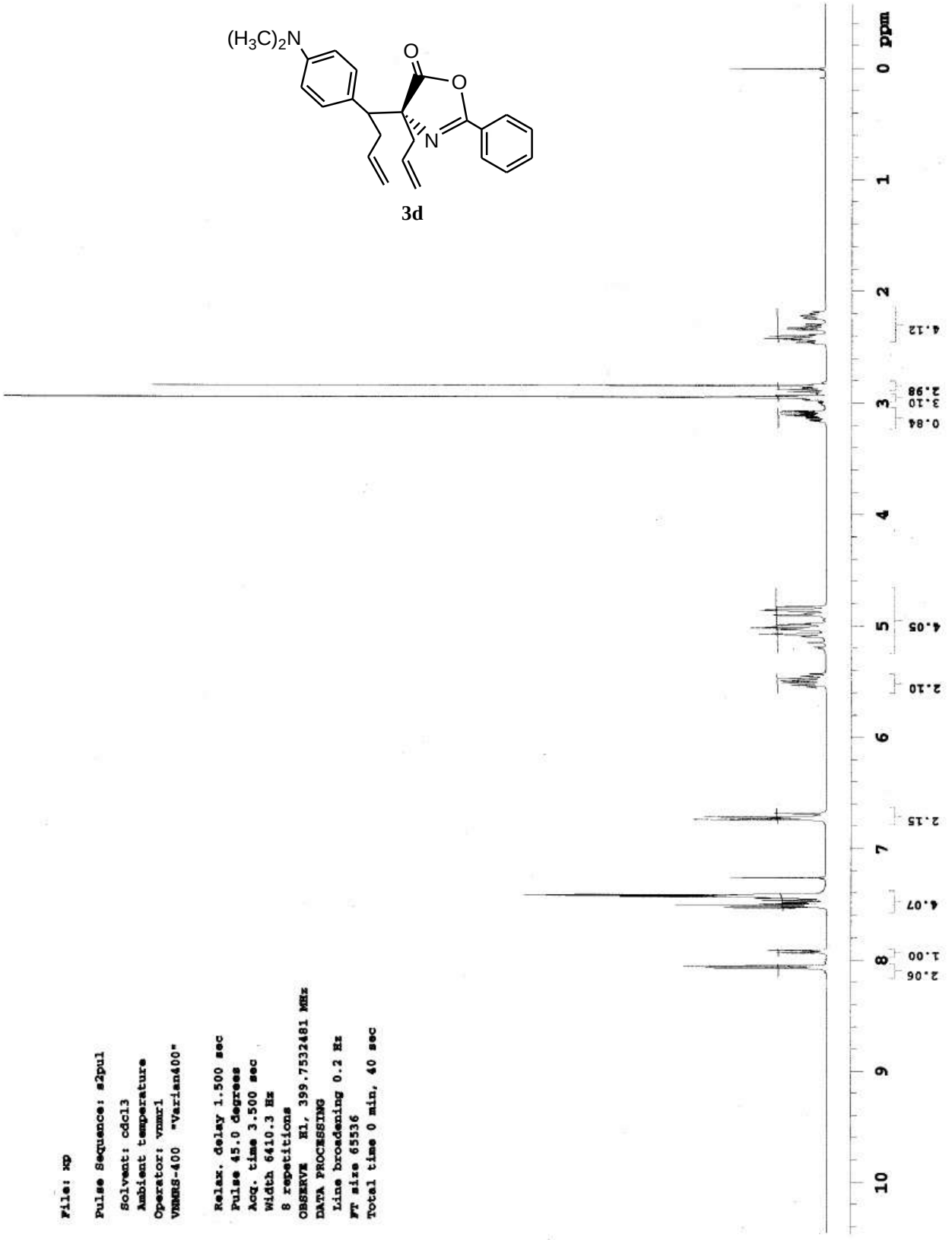


^{13}C NMR (100 MHz, $CDCl_3$)

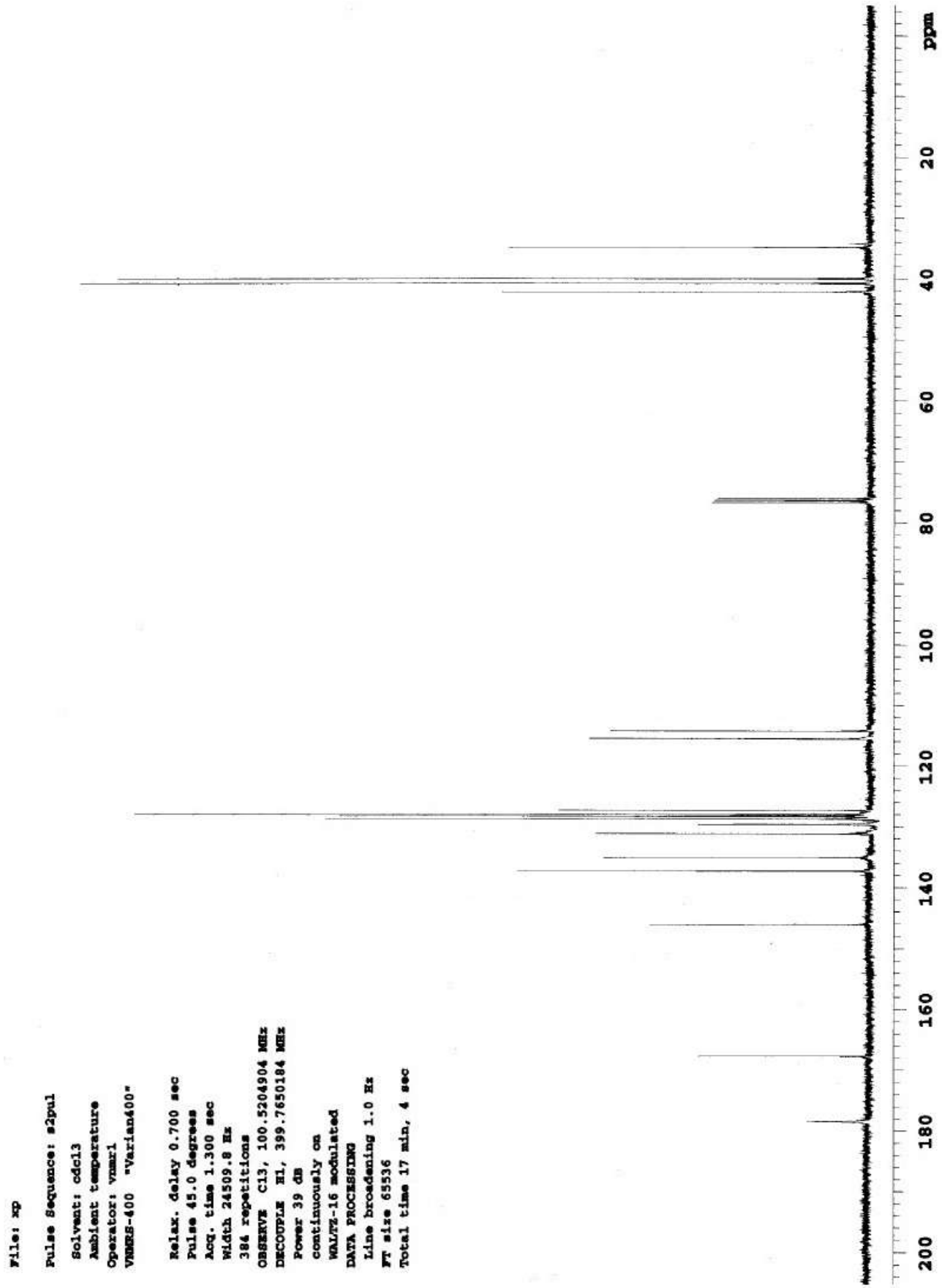


4-Allyl-4-[1-(4-dimethylamino-phenyl)-but-3-enyl]-2-phenyl-4H-oxazol-5-one (3d)

^{1}H NMR (400 MHz, $CDCl_3$)

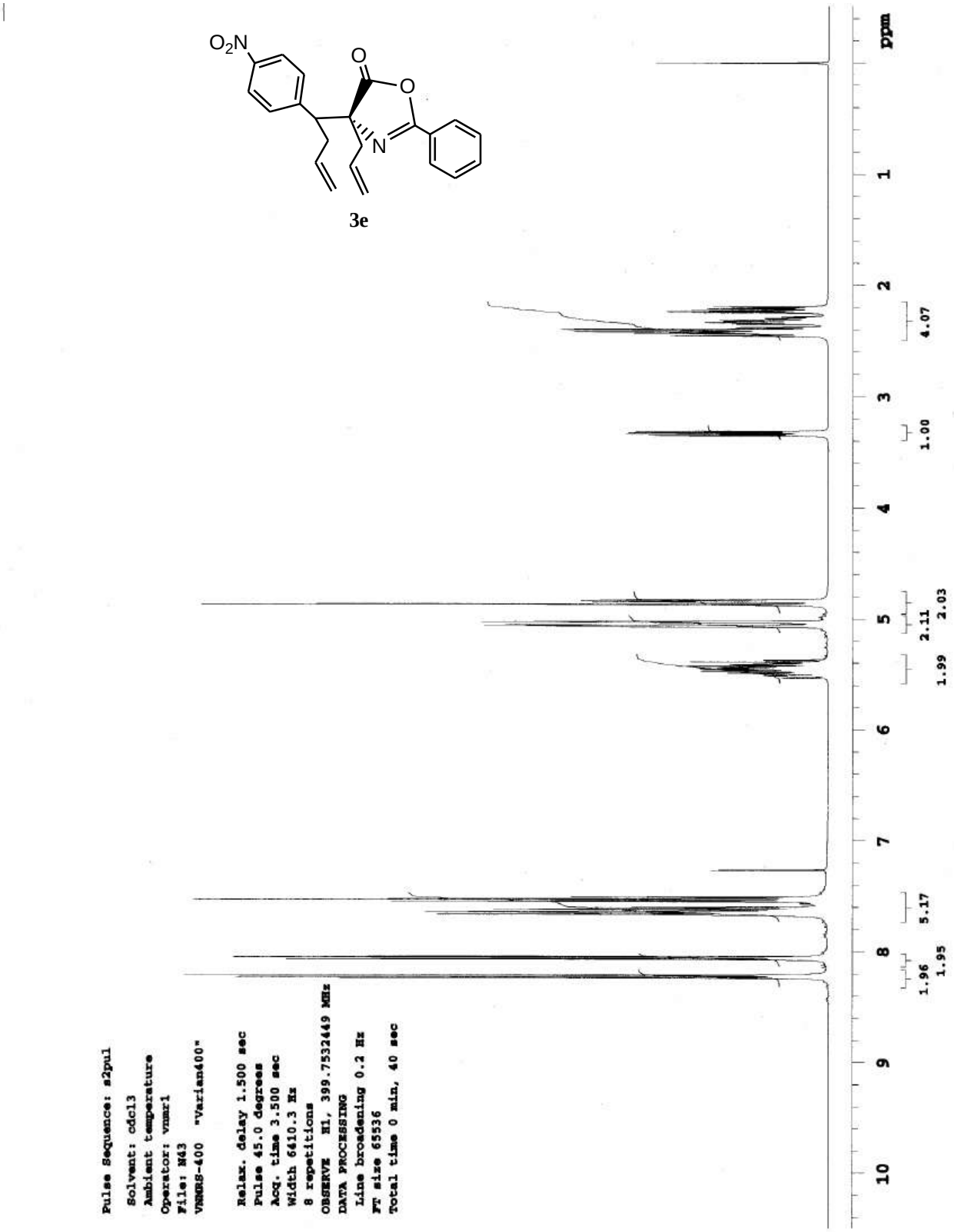


^{13}C NMR (100 MHz, $CDCl_3$)

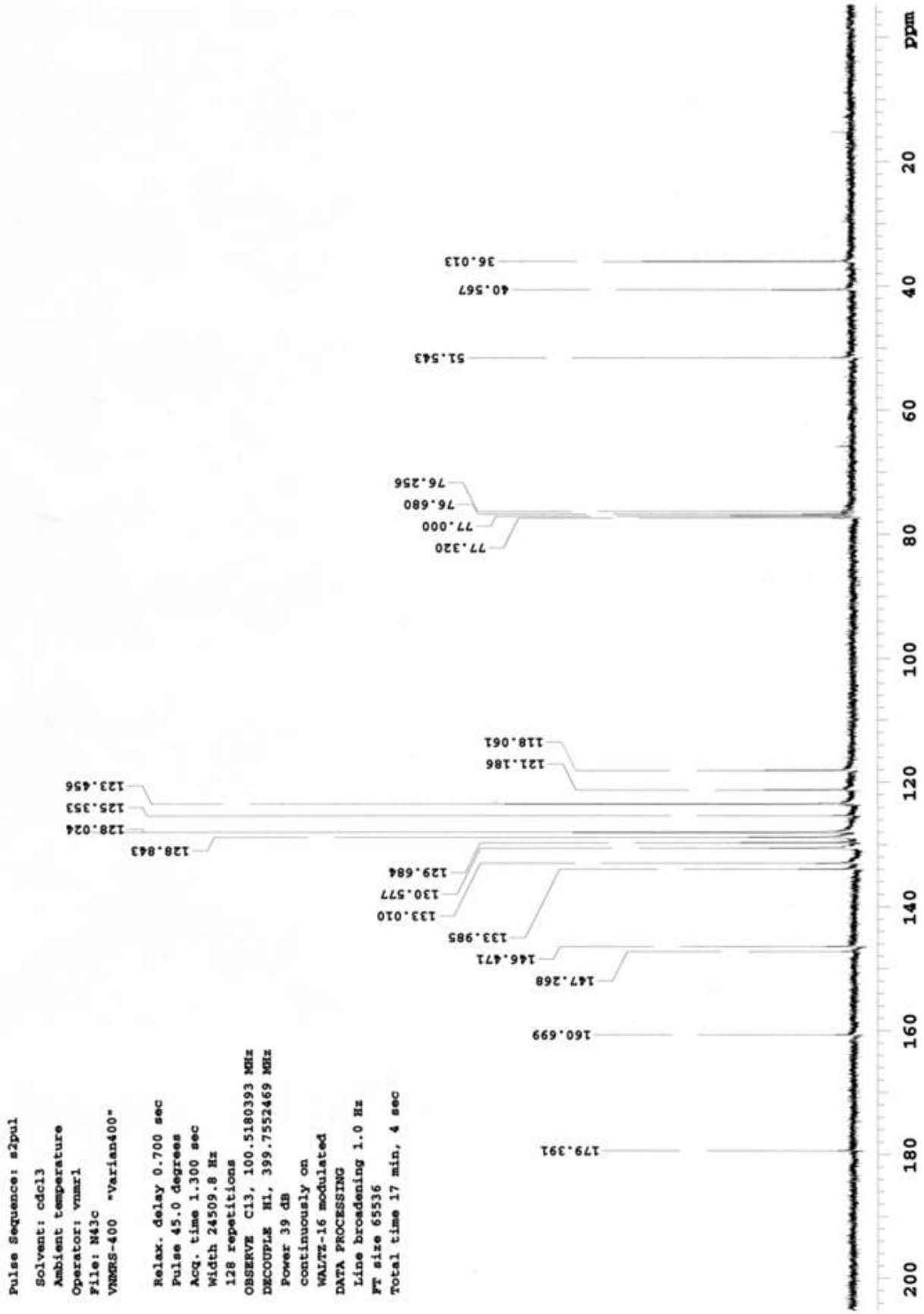


4-Allyl-4-[1-(4-nitro-phenyl)-but-3-enyl]-2-phenyl-4H-oxazol-5-one (3e)

^{1}H NMR (400 MHz, $CDCl_3$)

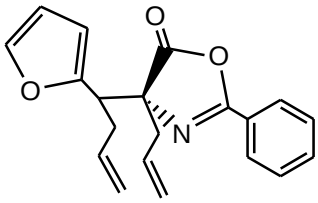


^{13}C NMR (100 MHz, $CDCl_3$)



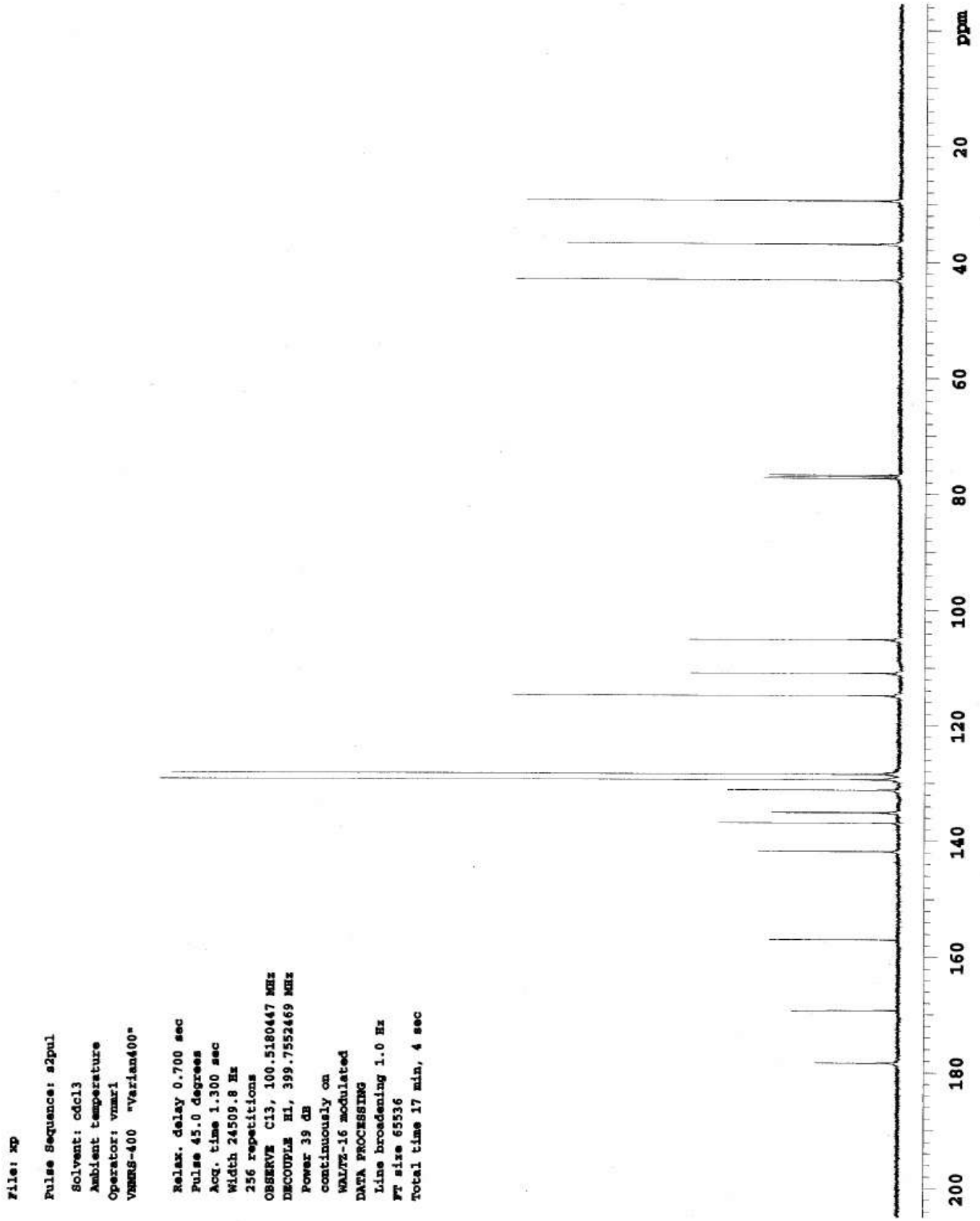
4-Allyl-4-(1-(furan-2-yl)but-3-enyl)-2-phenyloxazol-5(4H)-one (3f)

^{1}H NMR (400 MHz, $CDCl_3$)



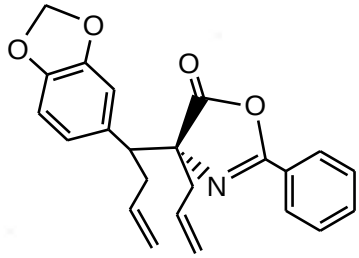
3f

^{13}C NMR (100 MHz, $CDCl_3$)



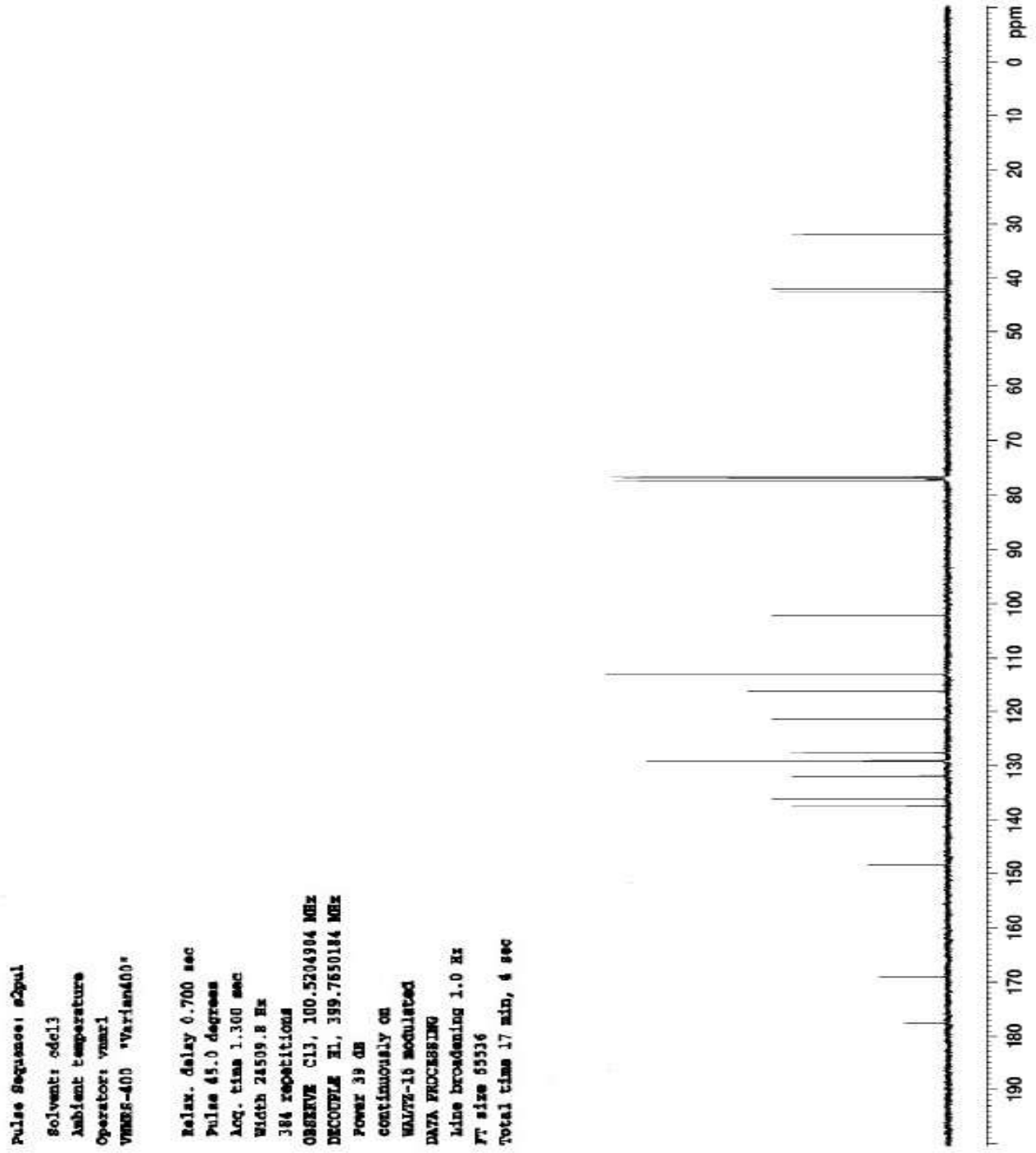
4-Allyl-4-(1-benzo[1,3]dioxol-5-yl-but-3-enyl)-2-phenyl-4H-oxazol-5-one (3g)

^{1}H NMR (400 MHz, $CDCl_3$)



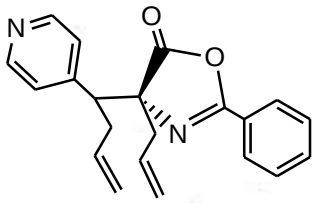
3g

^{13}C NMR (100 MHz, $CDCl_3$)



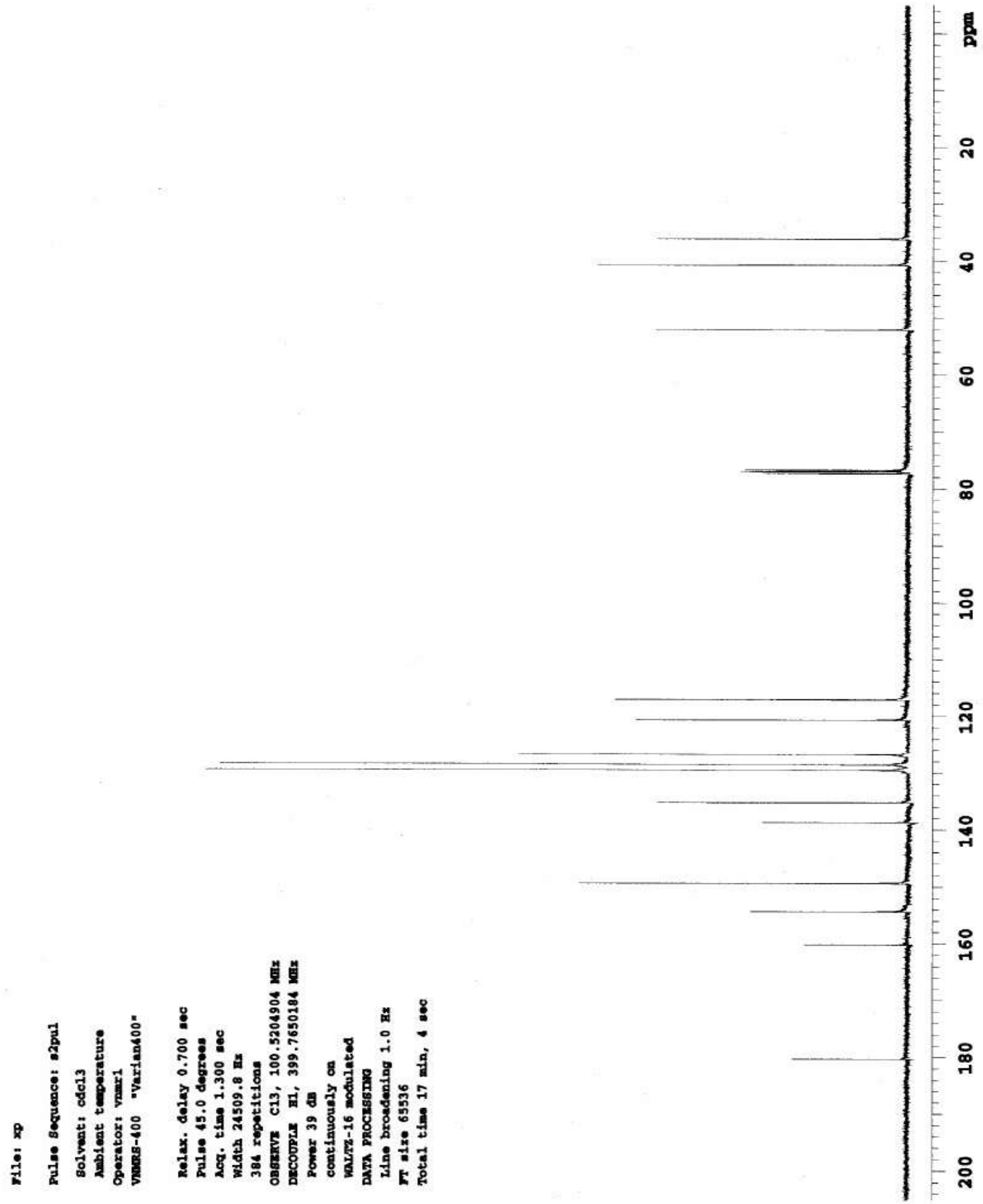
4-Allyl-2-phenyl-4-(1-(pyridin-4-yl)but-3-enyl)oxazol-5(4H)-one (3h)

^{1}H NMR (400 MHz, $CDCl_3$)



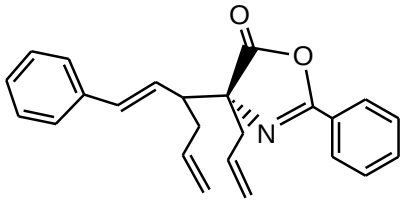
3h

^{13}C NMR (100 MHz, $CDCl_3$)



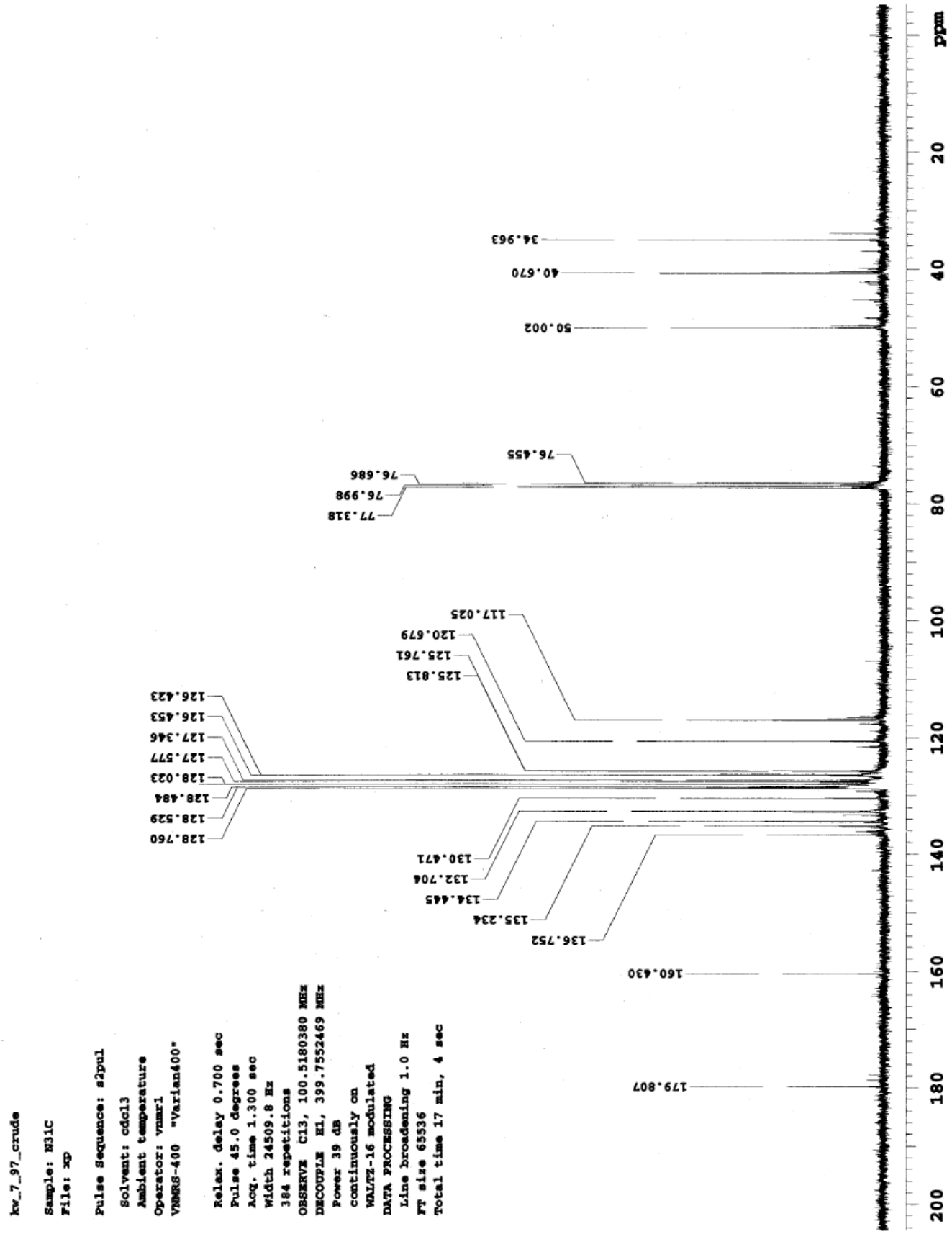
(*E*/*Z*)-4-allyl-2-phenyl-4-(1-phenylhexa-1,5-dien-3-yl)oxazol-5(4H)-one (3i)

^{1}H NMR (400 MHz, $CDCl_3$)



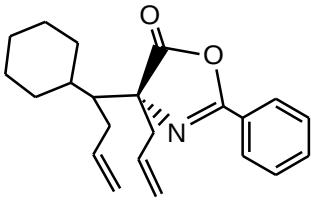
3i

^{13}C NMR (100 MHz, $CDCl_3$)



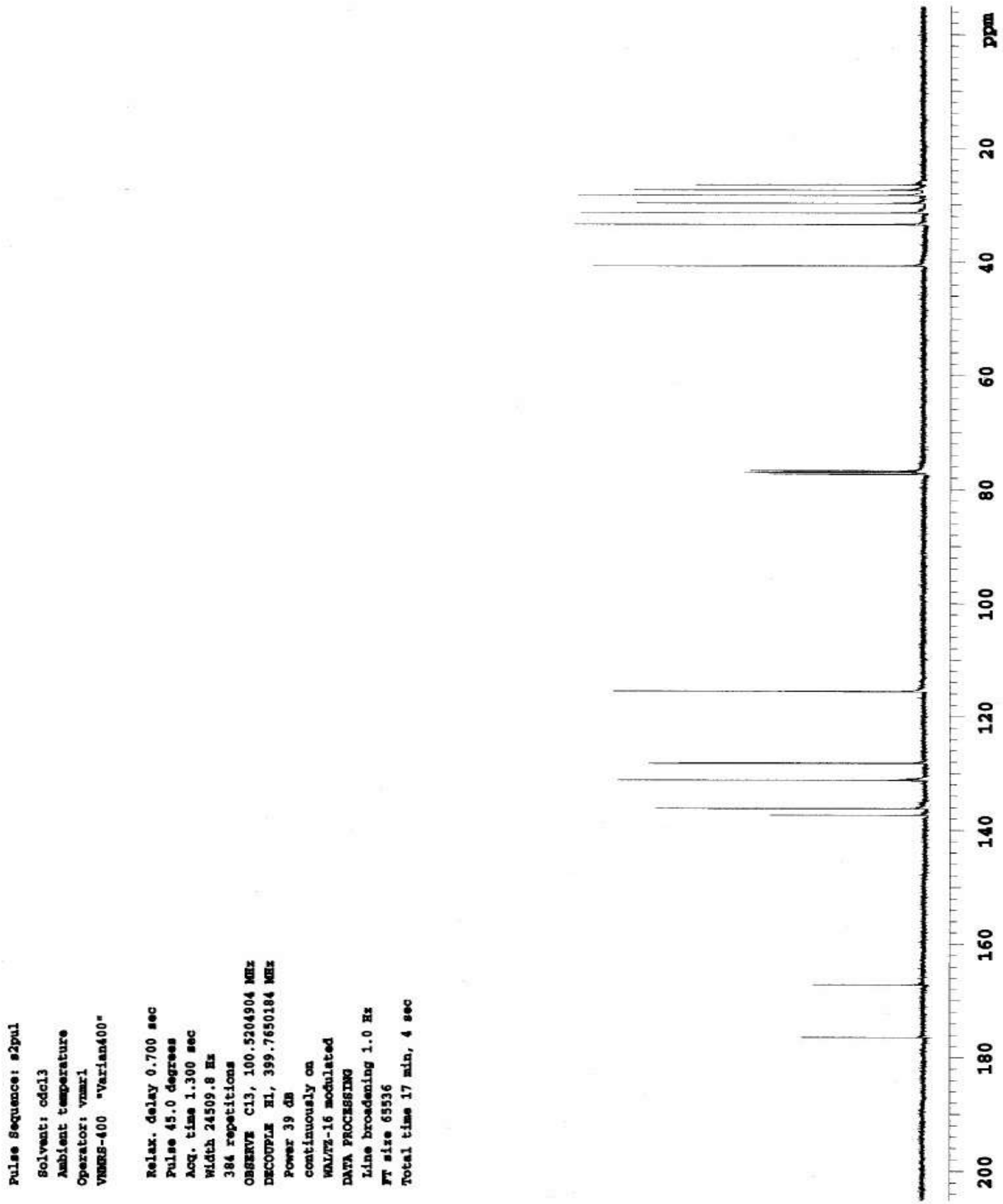
4-Allyl-4-(1-cyclohexylbut-3-enyl)-2-phenyloxazol-5(4H)-one (3j)

^{1}H NMR (400 MHz, $CDCl_3$)



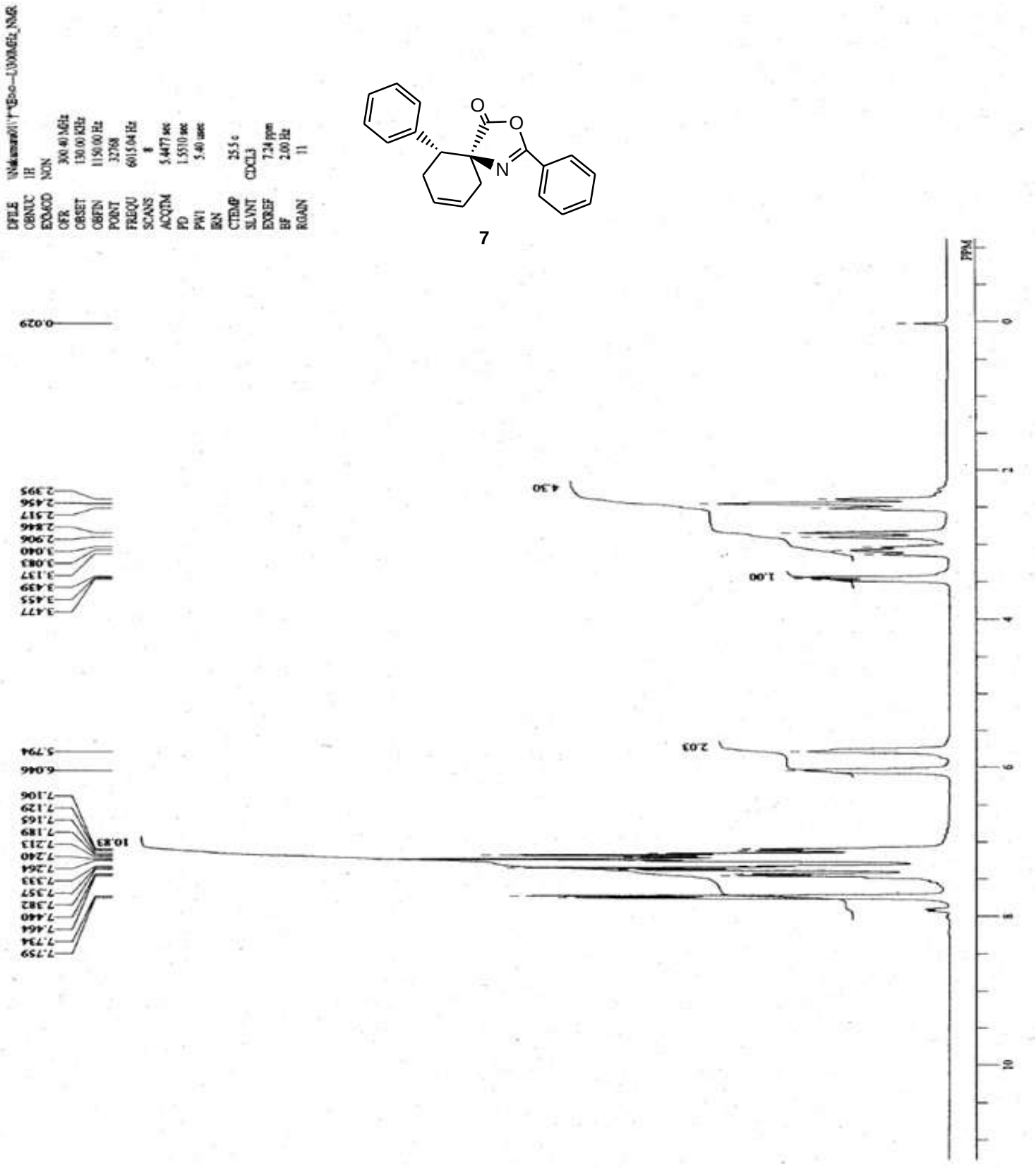
3j

^{13}C NMR (100 MHz, $CDCl_3$)

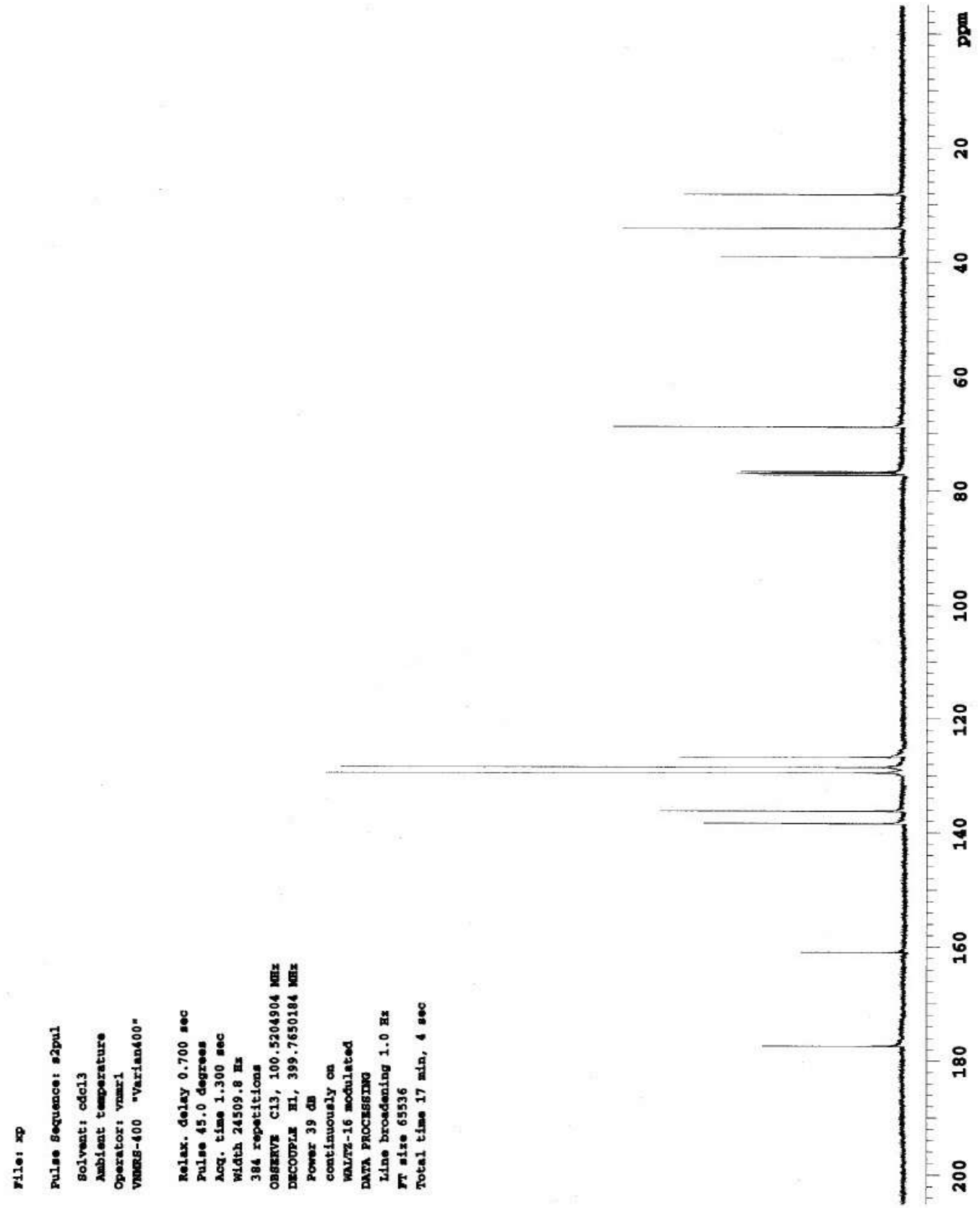


2,10-Diphenyl-3-oxa-1-aza-spiro[4.5]deca-1,7-dien-4-one (7)

^{1}H NMR (300 MHz, $CDCl_3$)

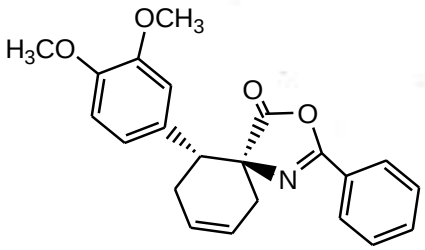


^{13}C NMR (100 MHz, $CDCl_3$)



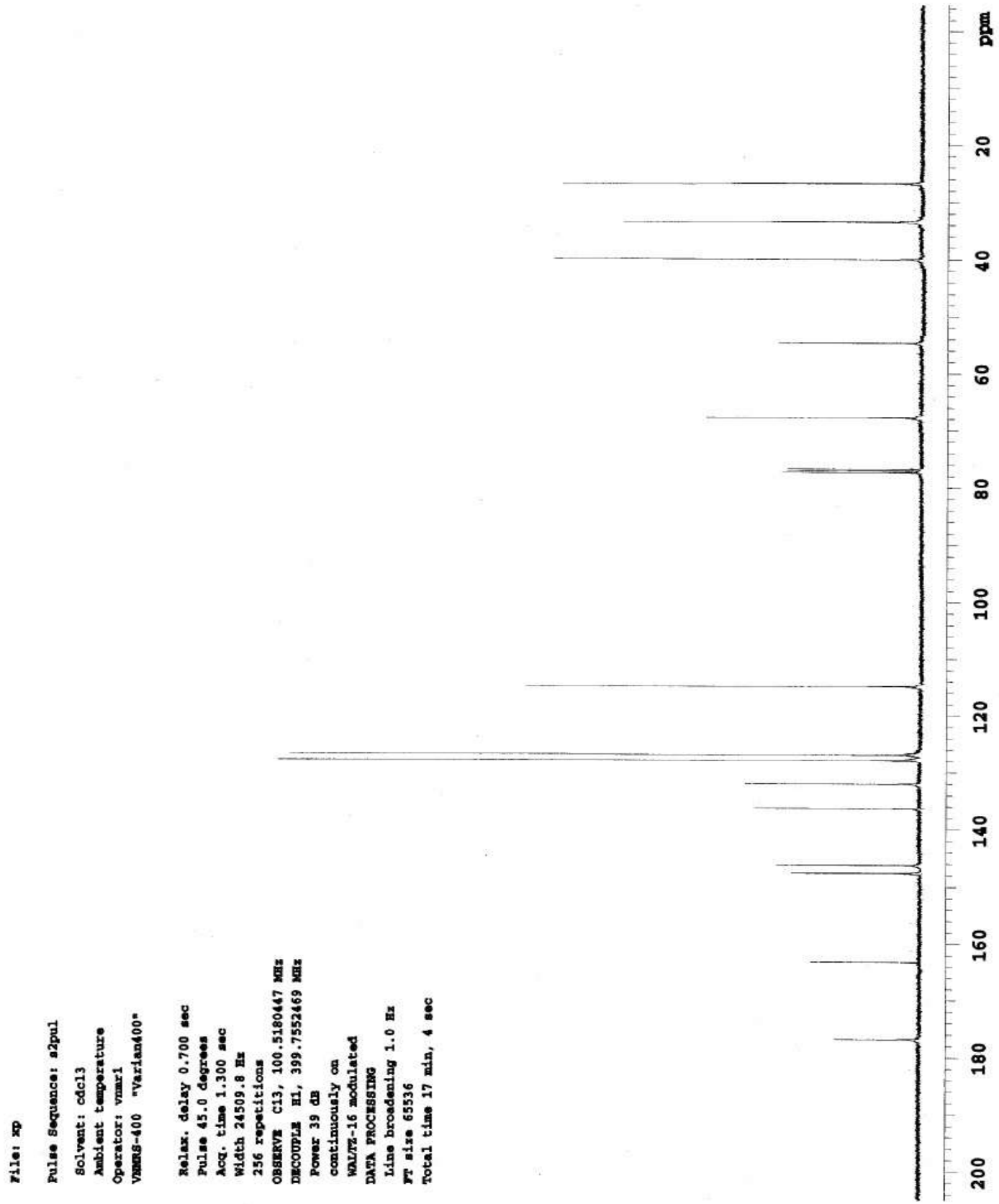
10-(3,4-Dimethoxy-phenyl)-2-phenyl-3-oxa-1-aza-spiro[4.5]deca-1,7-dien-4-one (8)

^{1}H NMR (400 MHz, $CDCl_3$)



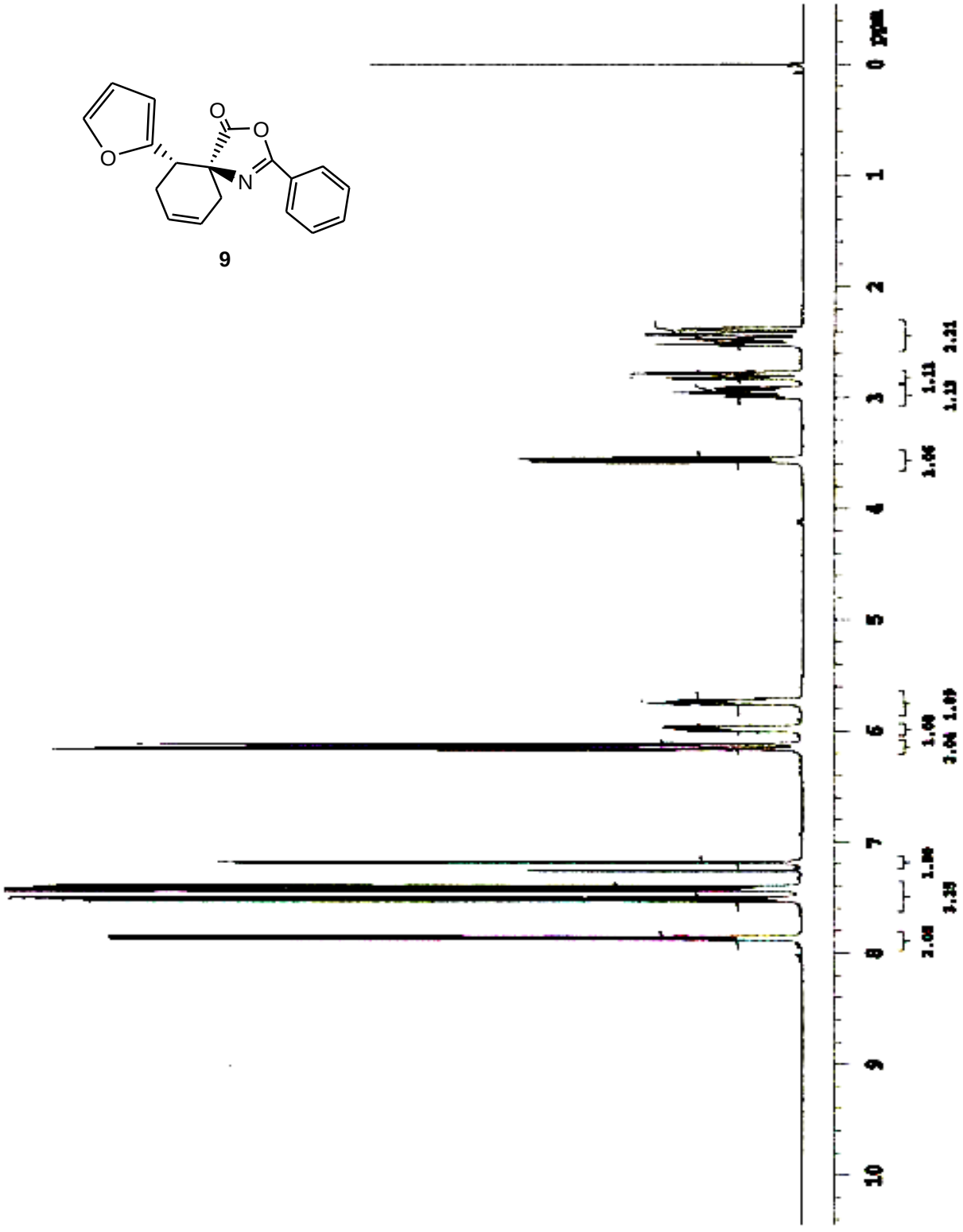
8

^{13}C NMR (100 MHz, $CDCl_3$)

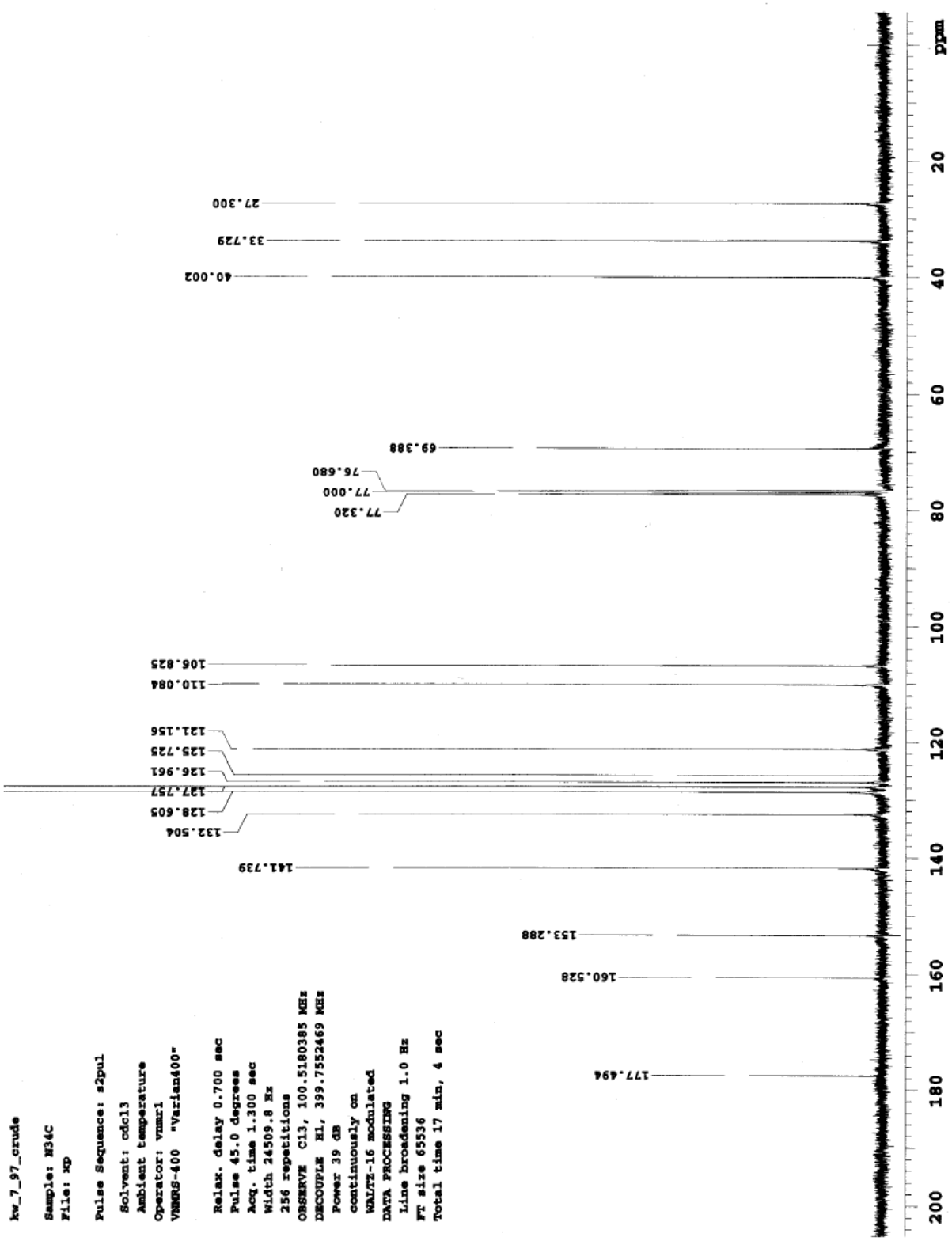


10-Furan-2-yl-2-phenyl-3-oxa-1-aza-spiro[4.5]deca-1,7-dien-4-one (9)

^{1}H NMR (400 MHz, $CDCl_3$)

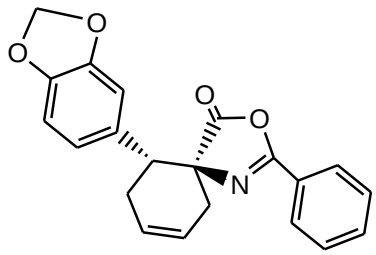


^{13}C NMR (100 MHz, $CDCl_3$)



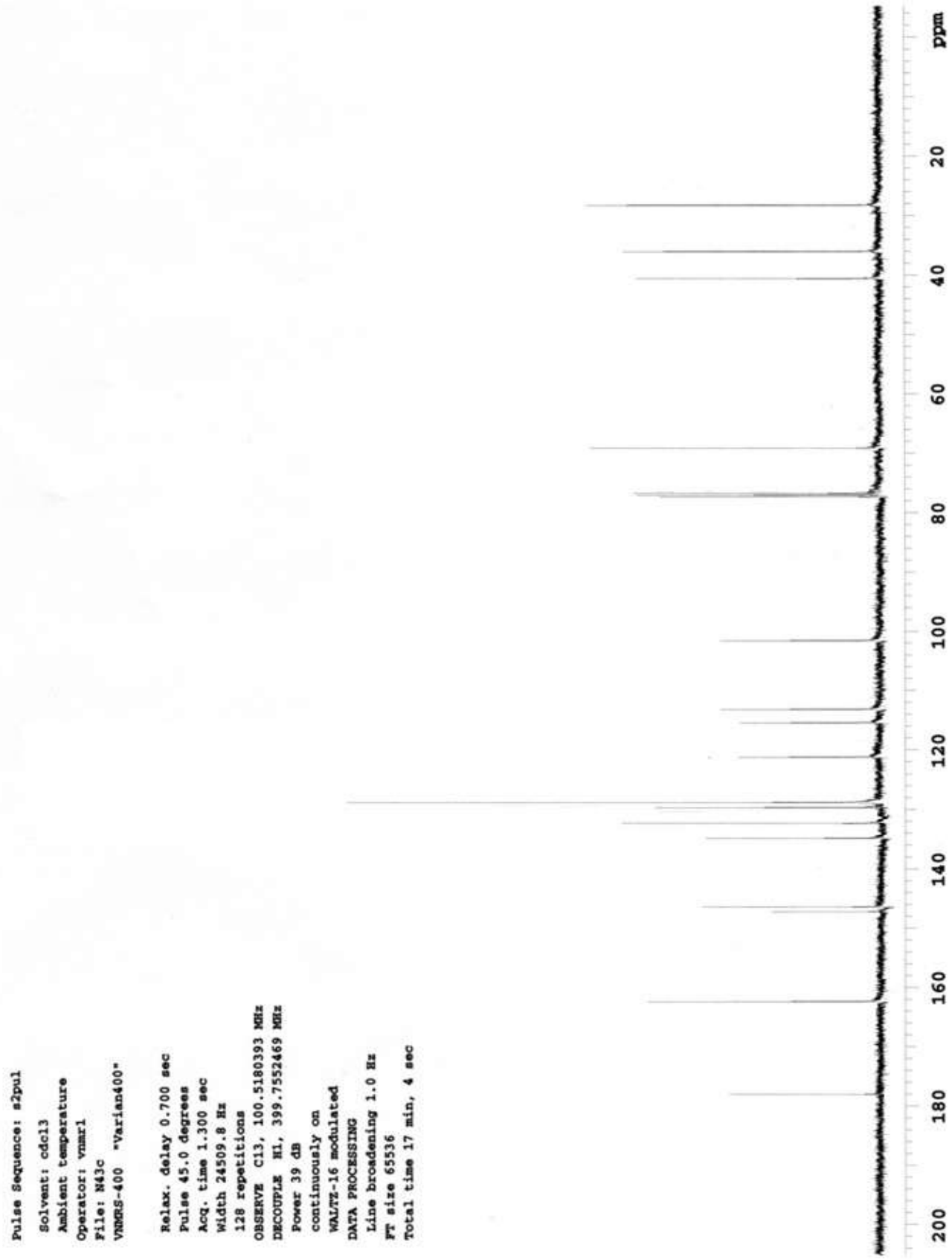
10-Benzo[1,3]dioxol-5-yl-2-phenyl-3-oxa-1-aza-spiro[4.5]deca-1,7-dien-4-one (10)

^{1}H NMR (400 MHz, $CDCl_3$)



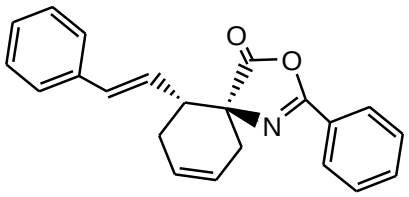
10

^{13}C NMR (100 MHz, $CDCl_3$)



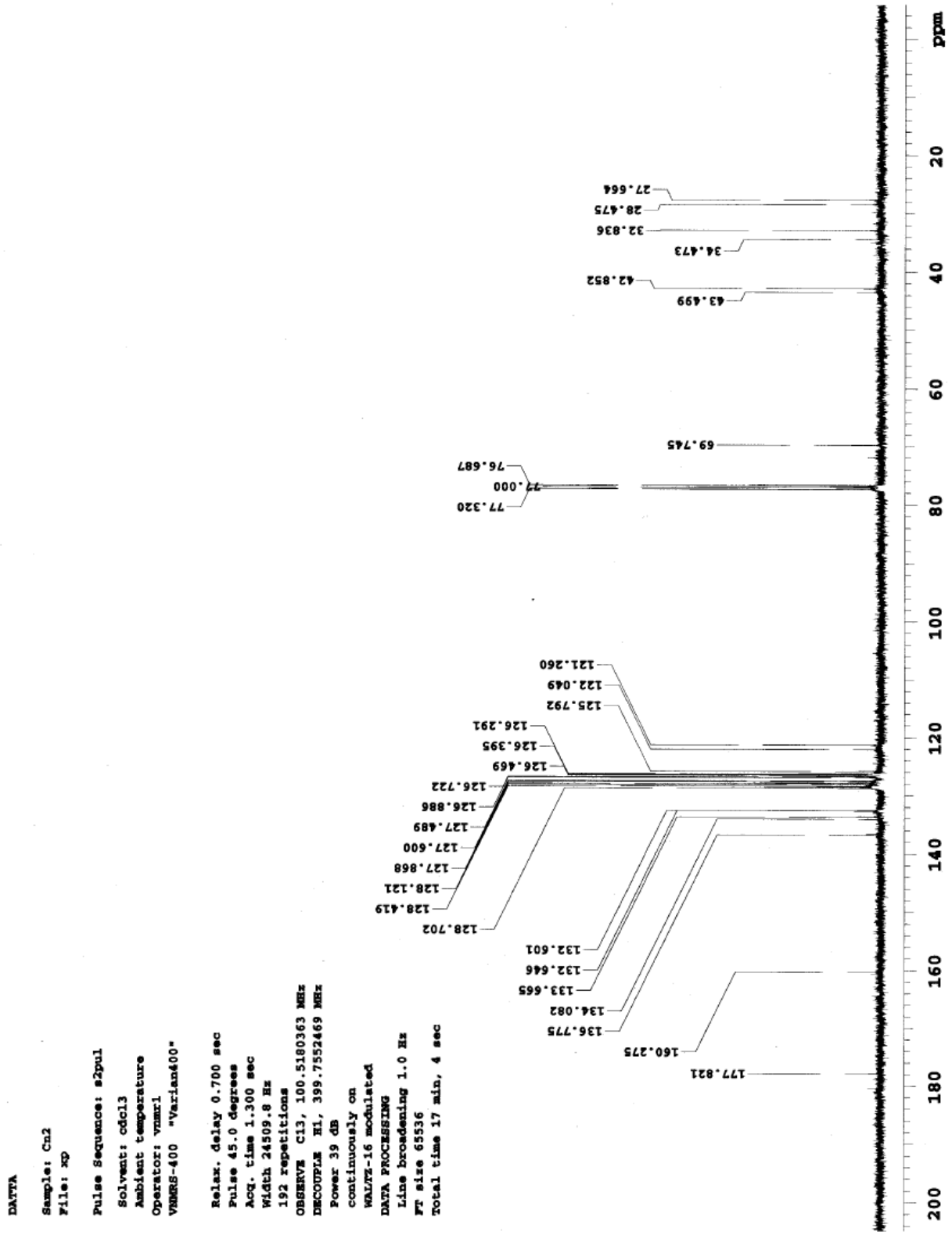
2-Phenyl-10-styryl-3-oxa-1-aza-spiro[4.5]deca-1,7-dien-4-one (11)

^{1}H NMR (400 MHz, $CDCl_3$)



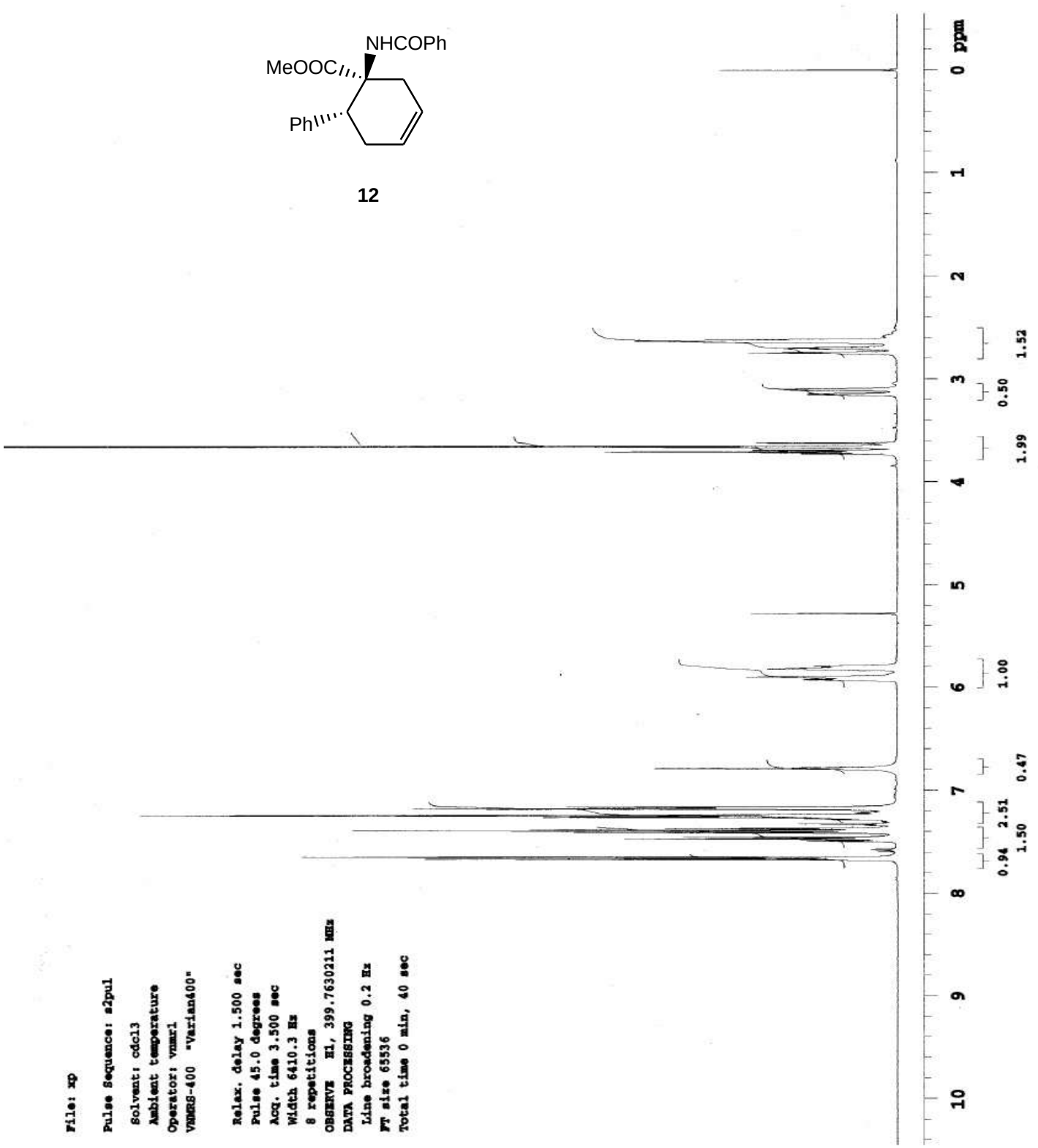
11

^{13}C NMR (100 MHz, $CDCl_3$)

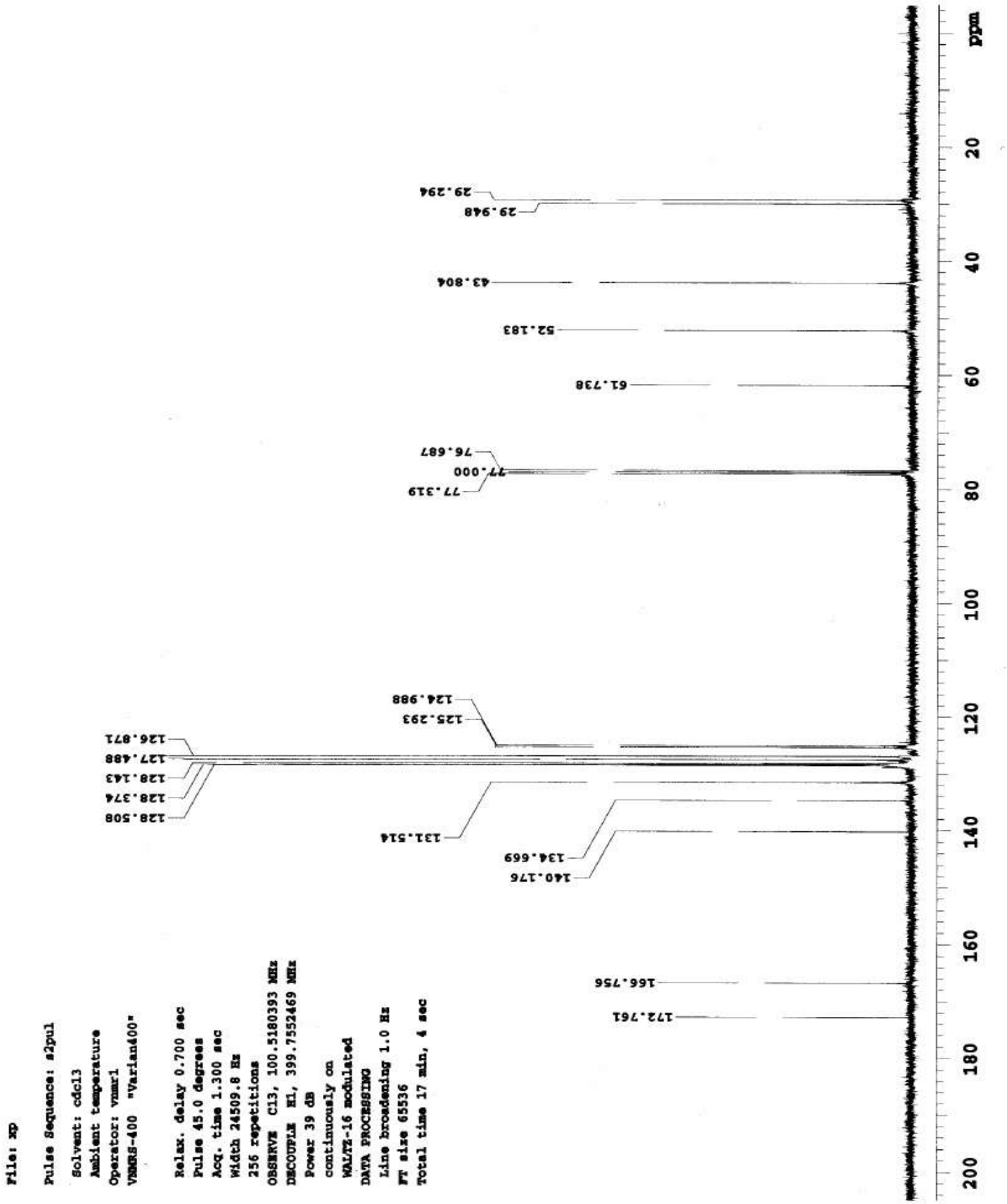


Methyl(1-Benzoylamino-6-phenyl-cyclohex-3-enecarboxylate) (12)

^{1}H NMR (400 MHz, $CDCl_3$)

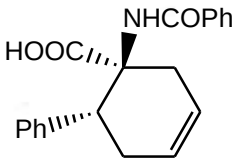


^{13}C NMR (100 MHz, $CDCl_3$)



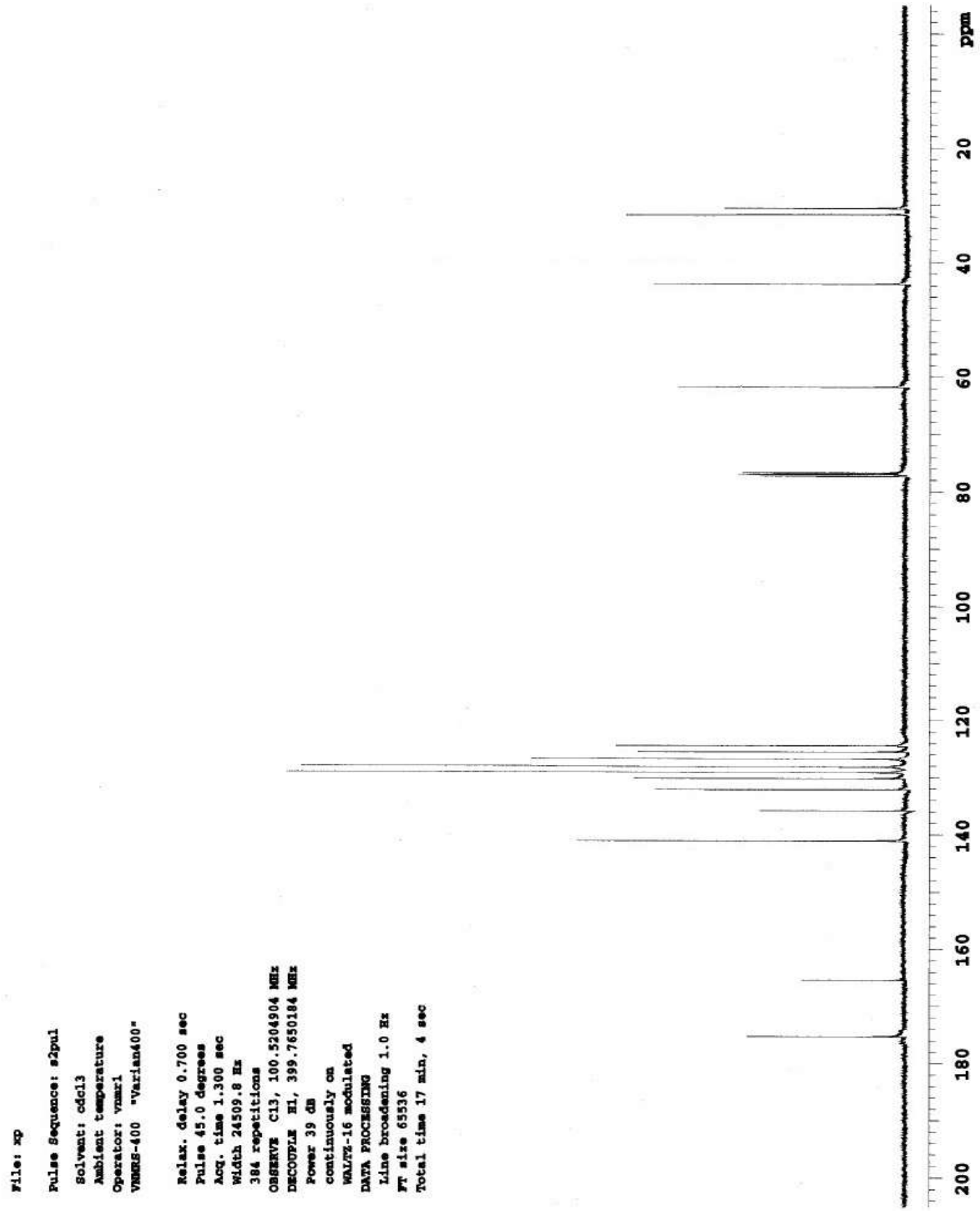
1-Benzoylamino-6-phenyl-cyclohex-3-enecarboxylic acid (13)

^{1}H NMR (400 MHz, $CDCl_3$)



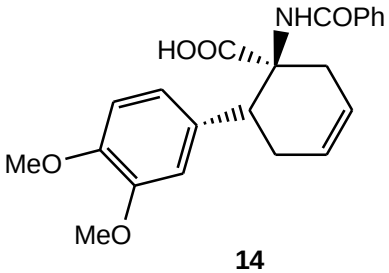
13

^{13}C NMR (100 MHz, $CDCl_3$)



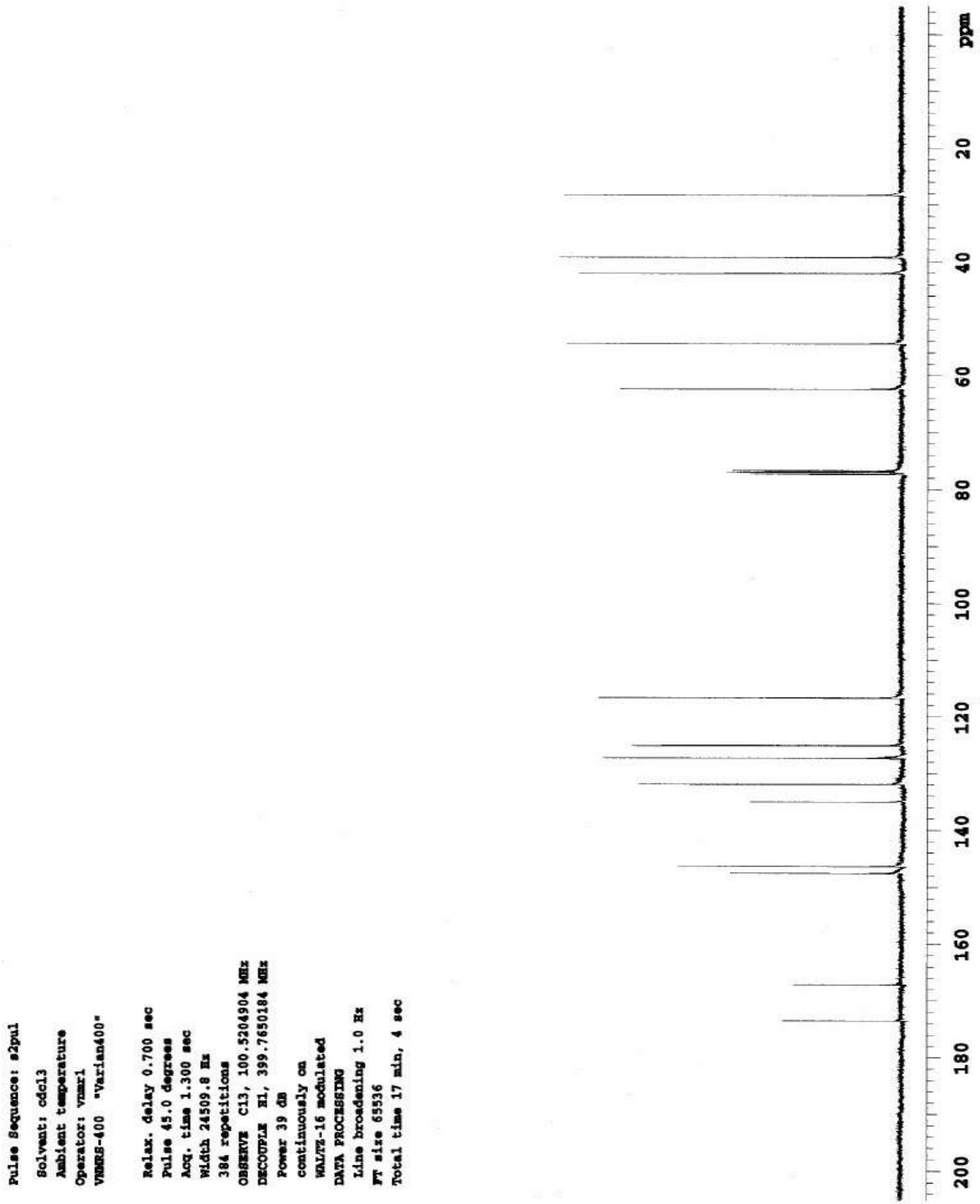
1-Benzoylamino-6-(3,4-dimethoxy-phenyl)-cyclohex-3-enecarboxylic acid (14)

^{1}H NMR (400 MHz, $CDCl_3$)



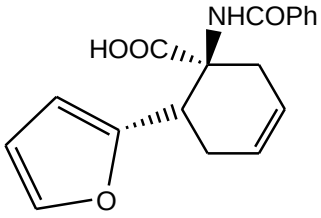
14

^{13}C NMR (100 MHz, $CDCl_3$)



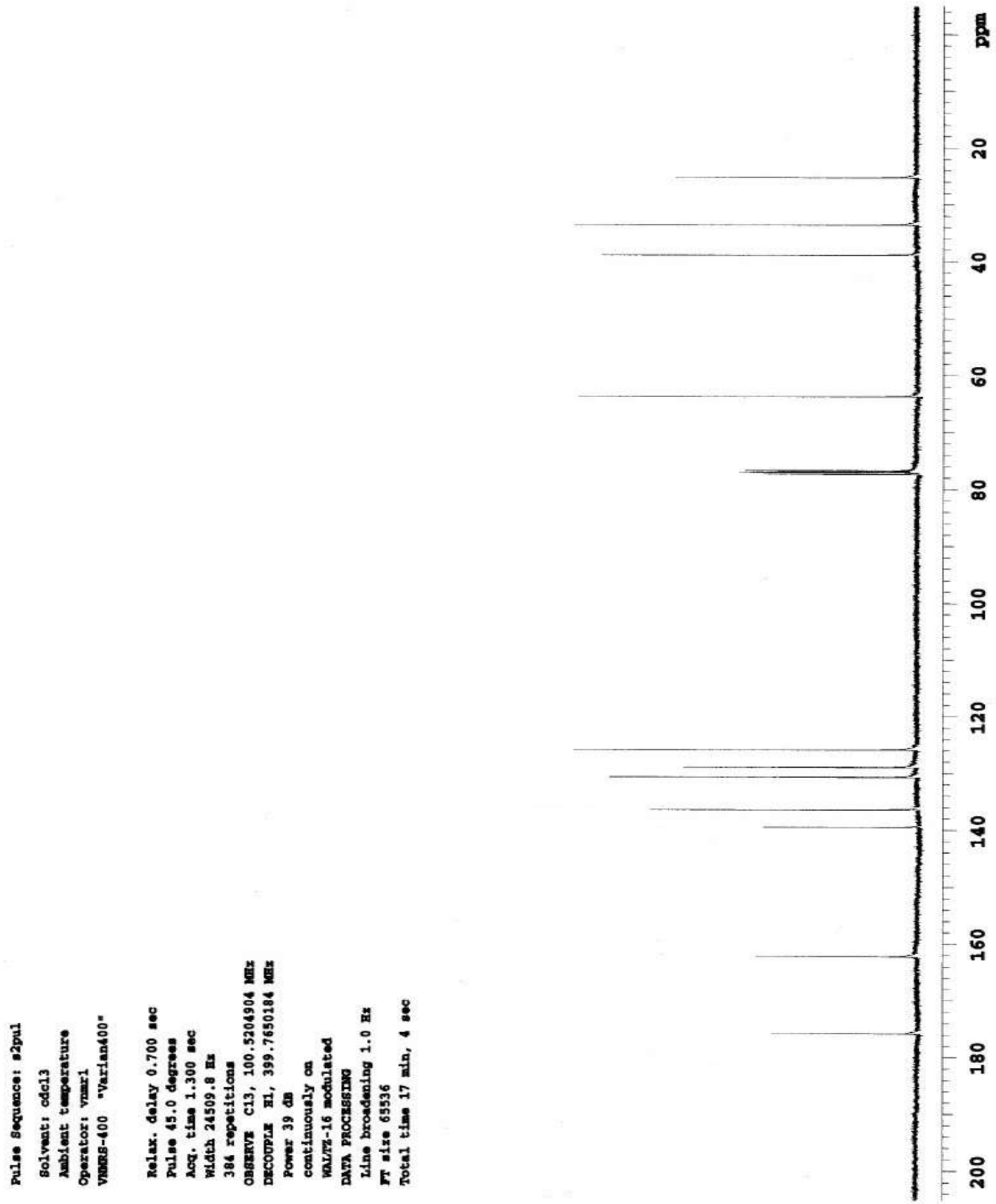
6-Benzo[1,3]dioxol-5-yl-1-benzoylamino-cyclohex-3-enecarboxylic acid (15)

^{1}H NMR (400 MHz, $CDCl_3$)



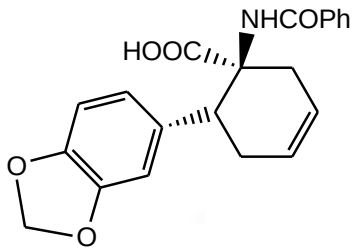
15

^{13}C NMR (100 MHz, $CDCl_3$)



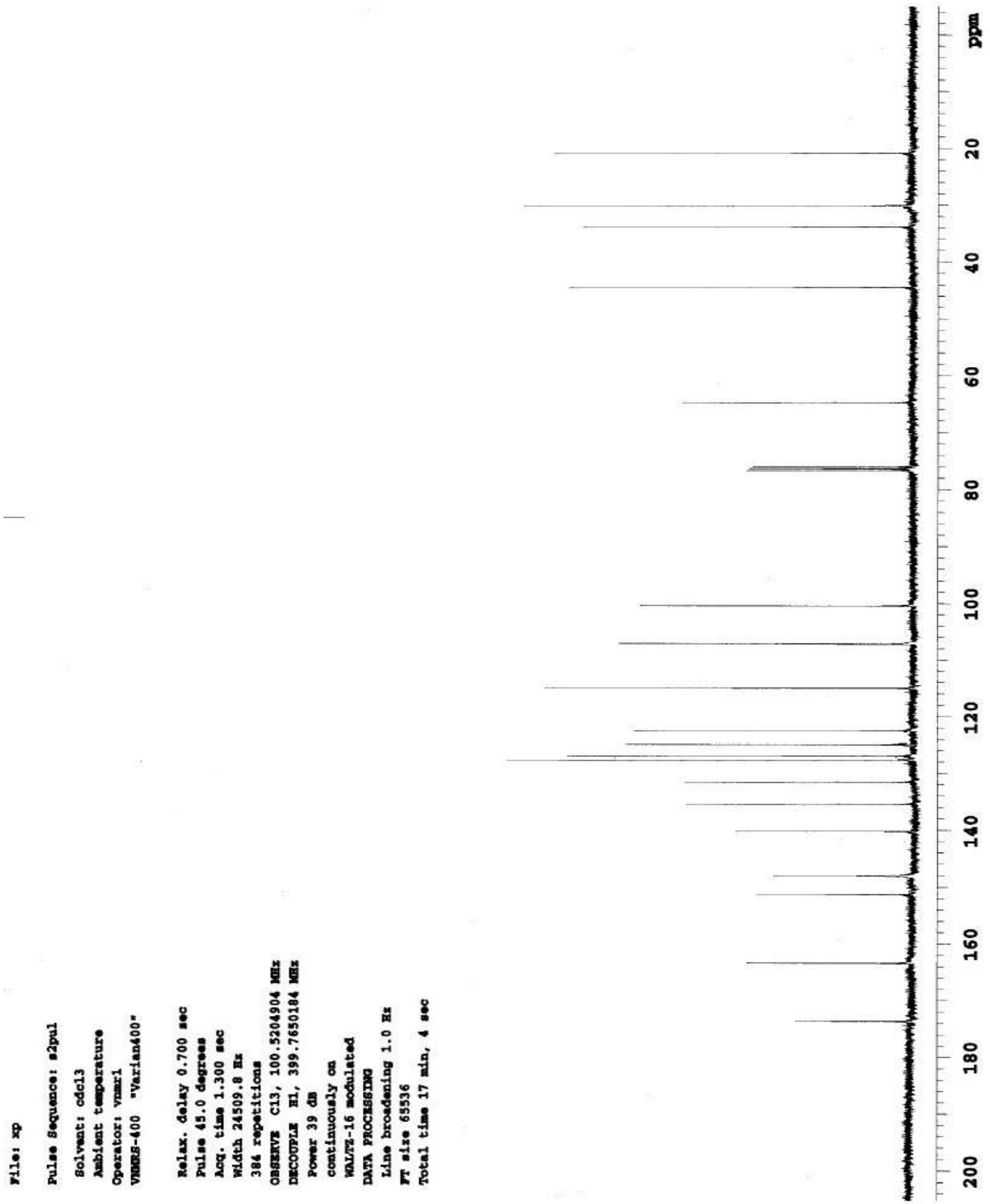
1-Benzoylamino-6-furan-2-yl-cyclohex-3-enecarboxylic acid (16)

^{1}H NMR (400 MHz, $CDCl_3$)



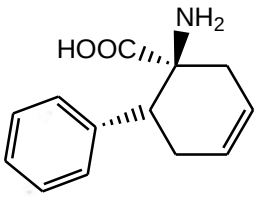
16

^{13}C NMR (100 MHz, $CDCl_3$)



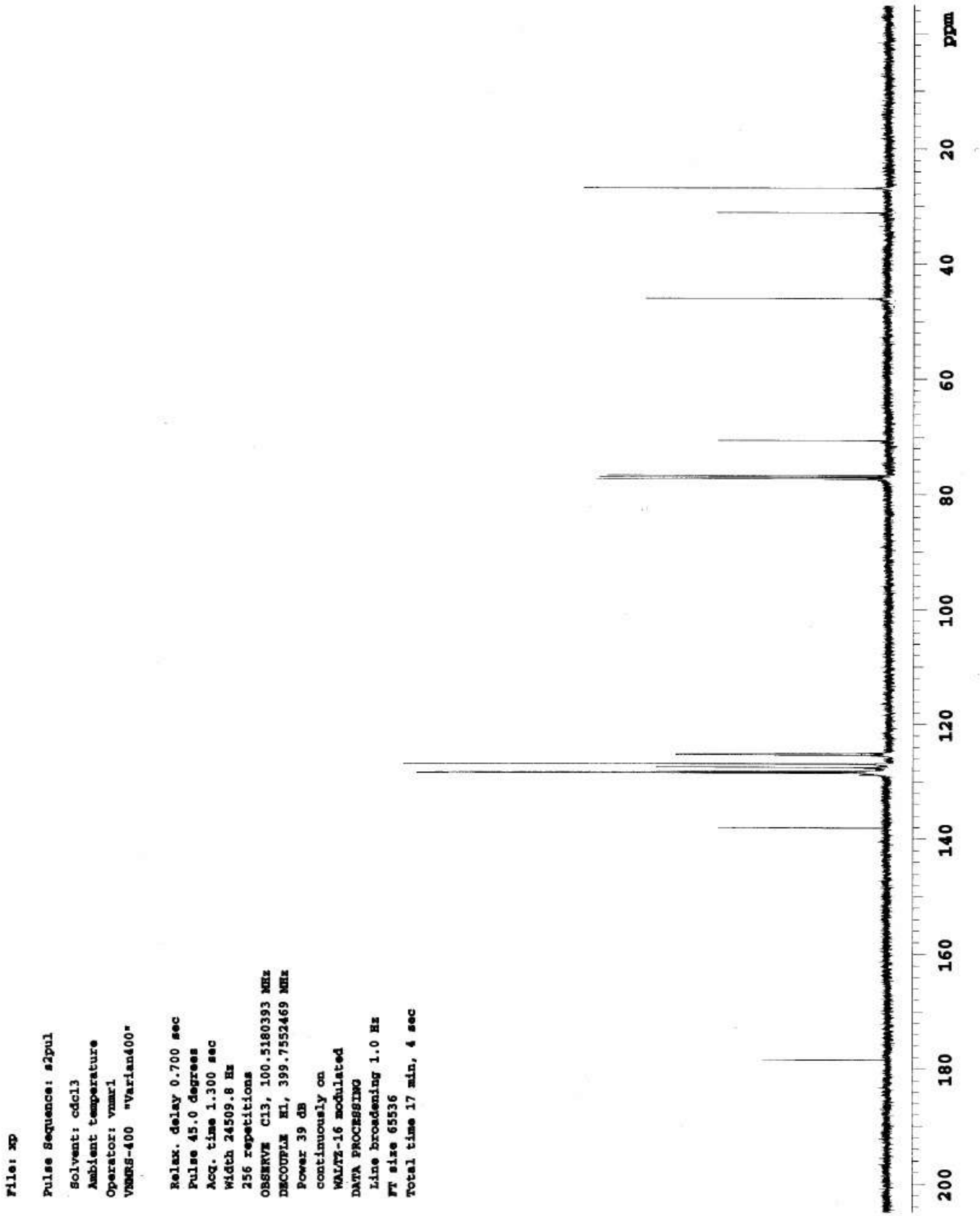
1-Amino-6-phenyl-cyclohex-3-enecarboxylic acid (17)

^{1}H NMR (400 MHz, $CDCl_3$)



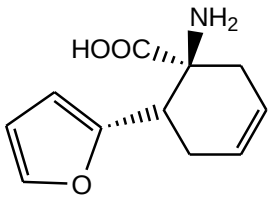
17

^{13}C NMR (100 MHz, $CDCl_3$)



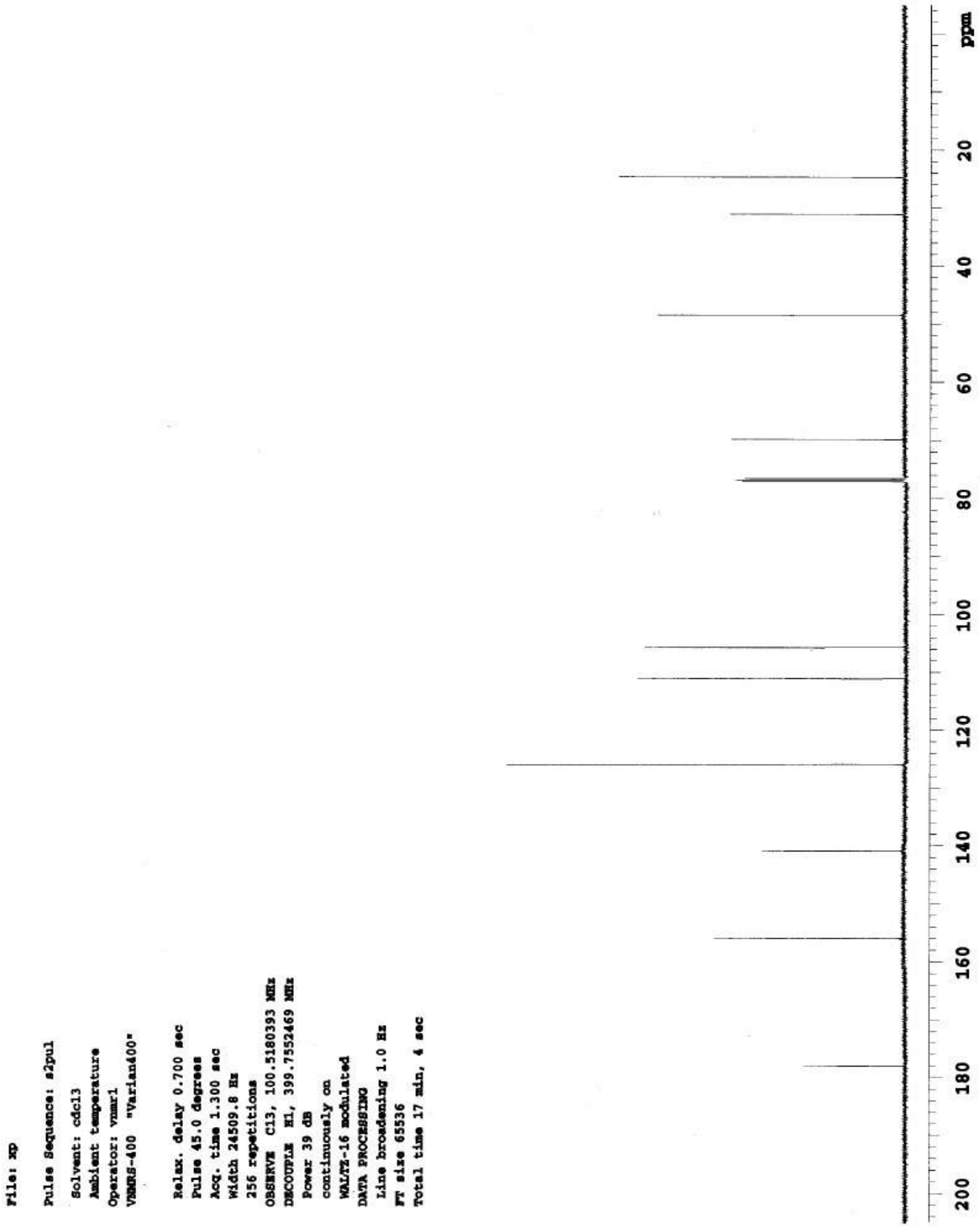
1-Amino-6-furan-2-yl-cyclohex-3-enecarboxylic acid (18)

^{1}H NMR (400 MHz, $CDCl_3$)



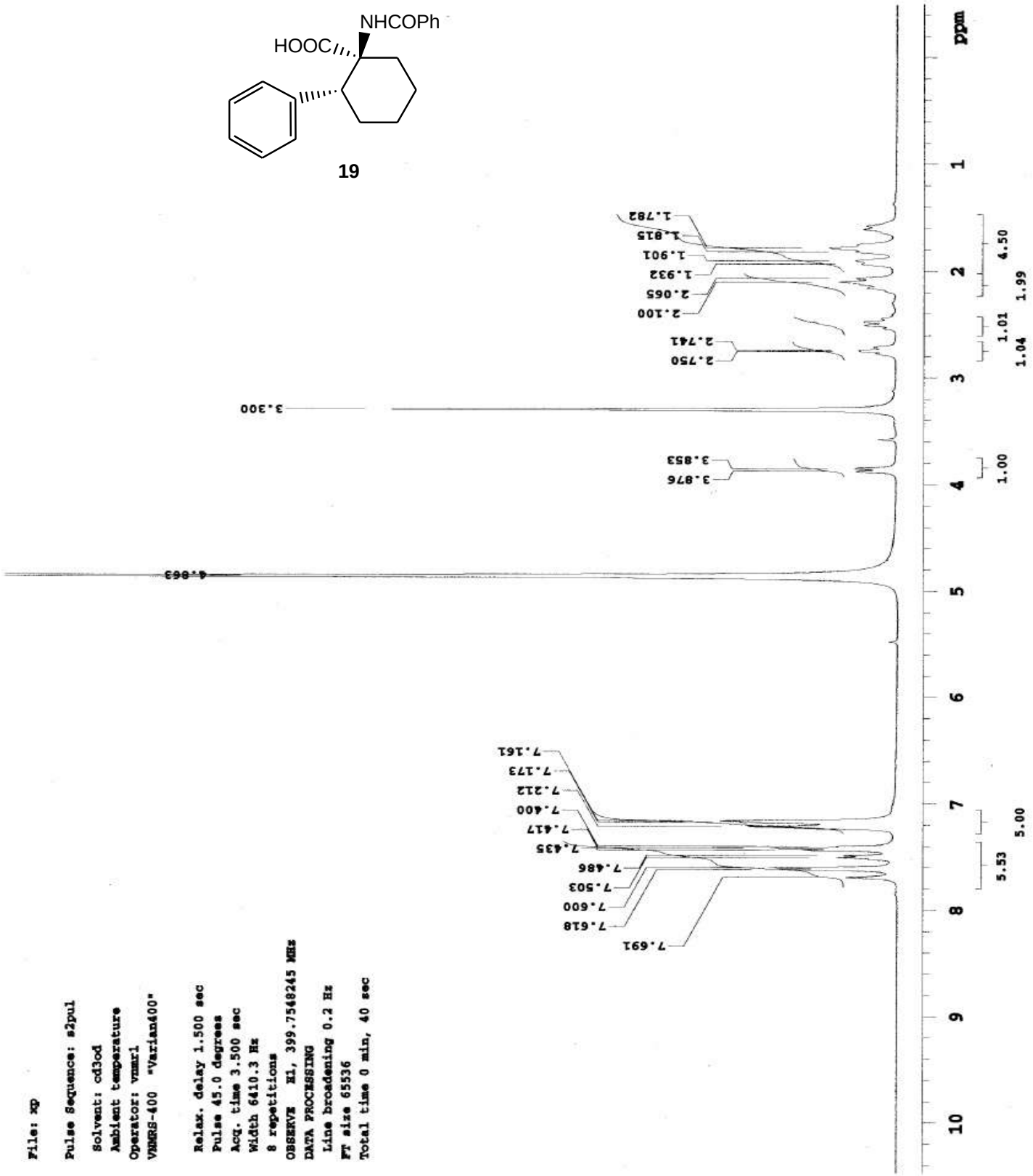
18

^{13}C NMR (100 MHz, $CDCl_3$)

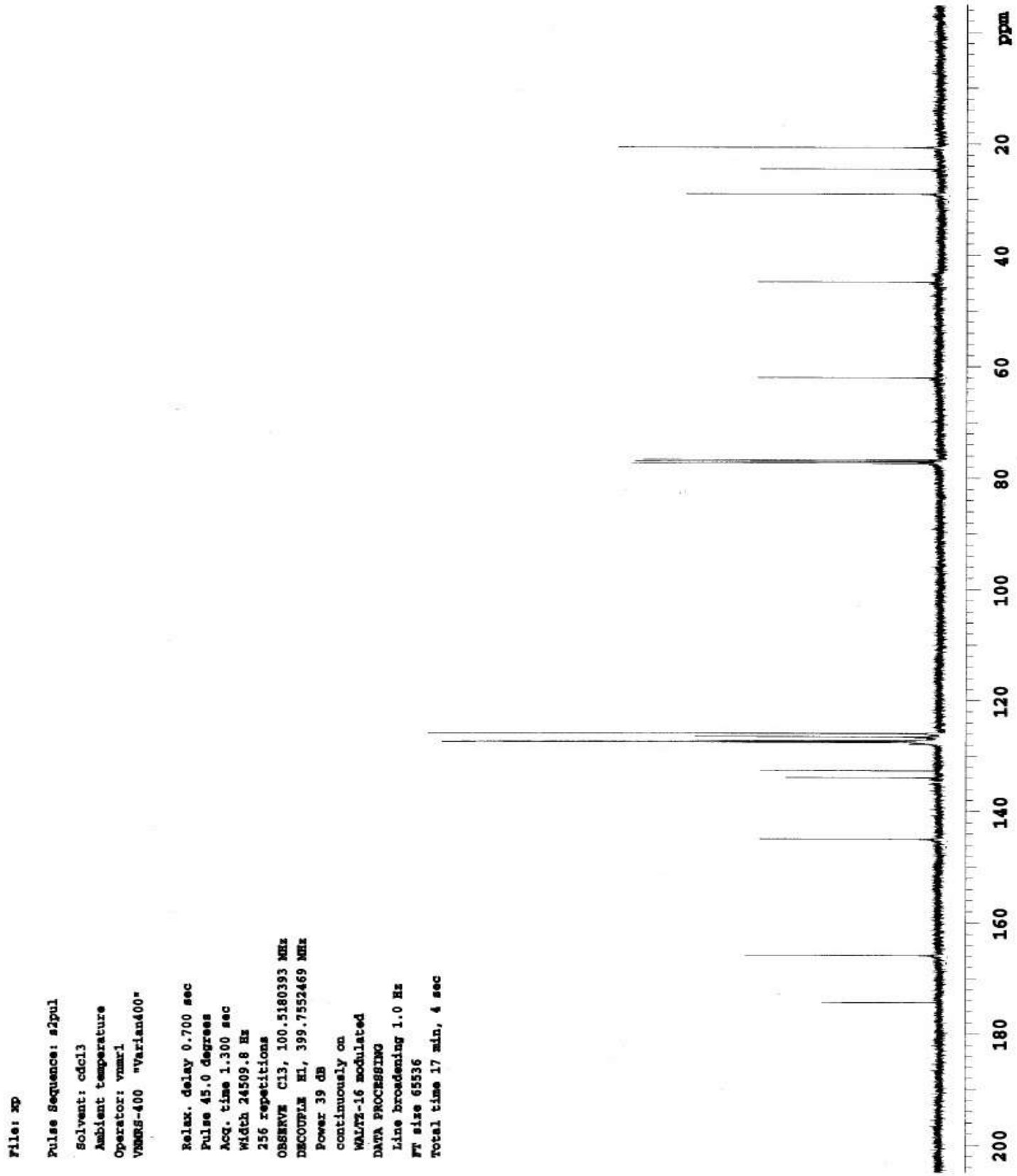


1-benzamido-2-phenylcyclohexanecarboxylic acid (19)

^{1}H NMR (400 MHz, $CDCl_3$)

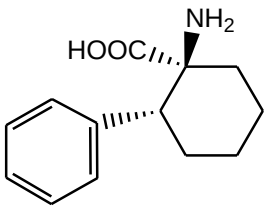


^{13}C NMR (100 MHz, $CDCl_3$)



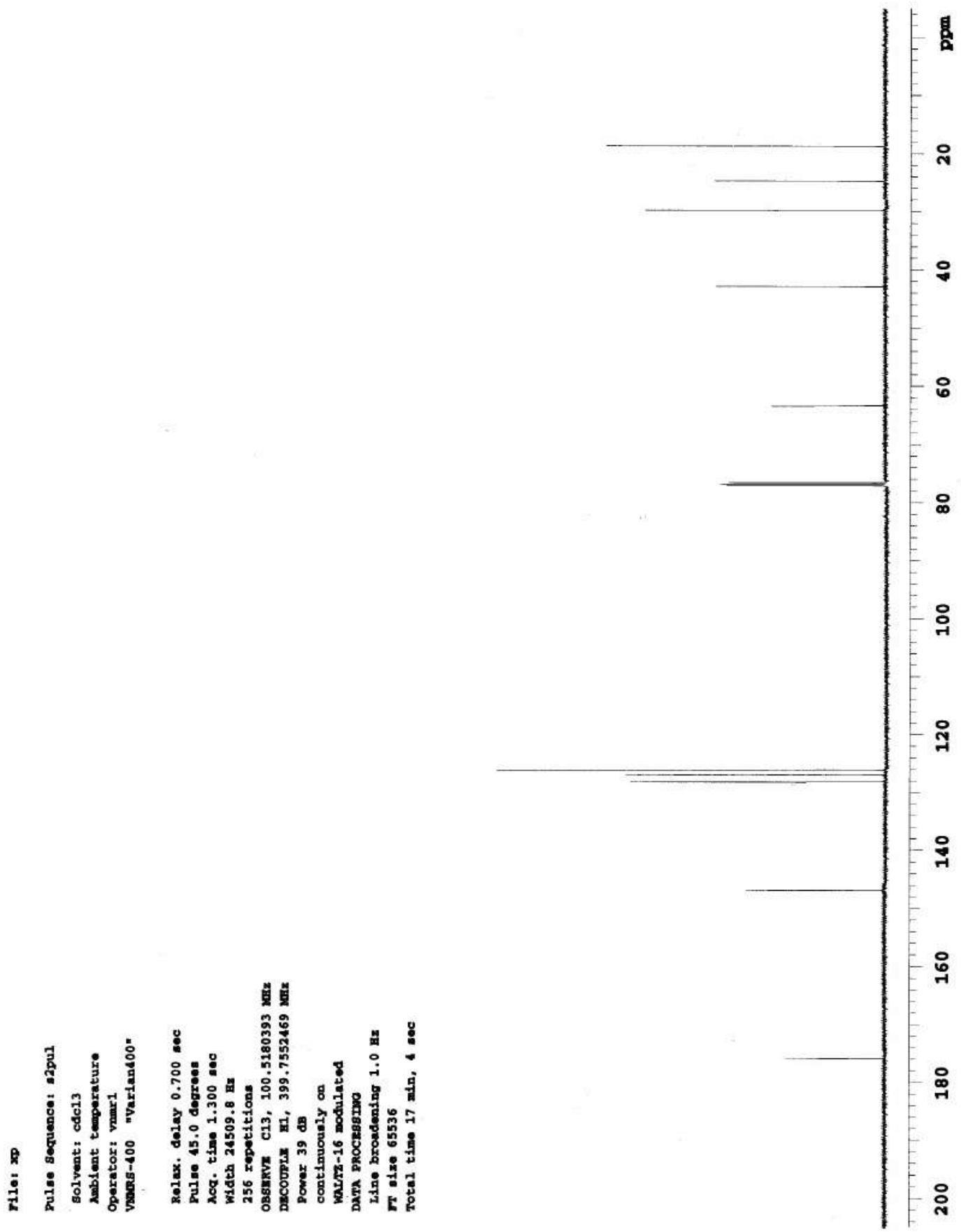
1-Amino-2-phenyl-cyclohexanecarboxylic acid (20)

^{1}H NMR (400 MHz, $CDCl_3$)



20

^{13}C NMR (100 MHz, $CDCl_3$)


File: xp
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Operator: vnmr1
VNMRS-400 "Varian400"
Relax. delay 0.700 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
256 repetitions
OBSERVE C13, 100.5180393 MHz
DECOUPLE H1, 399.7552469 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 17 min, 4 sec
200
180
160
140
120
100
80
60
40
20
ppm