

Production of anticancer polyenes through precursor-directed biosynthesis

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Supporting Information:

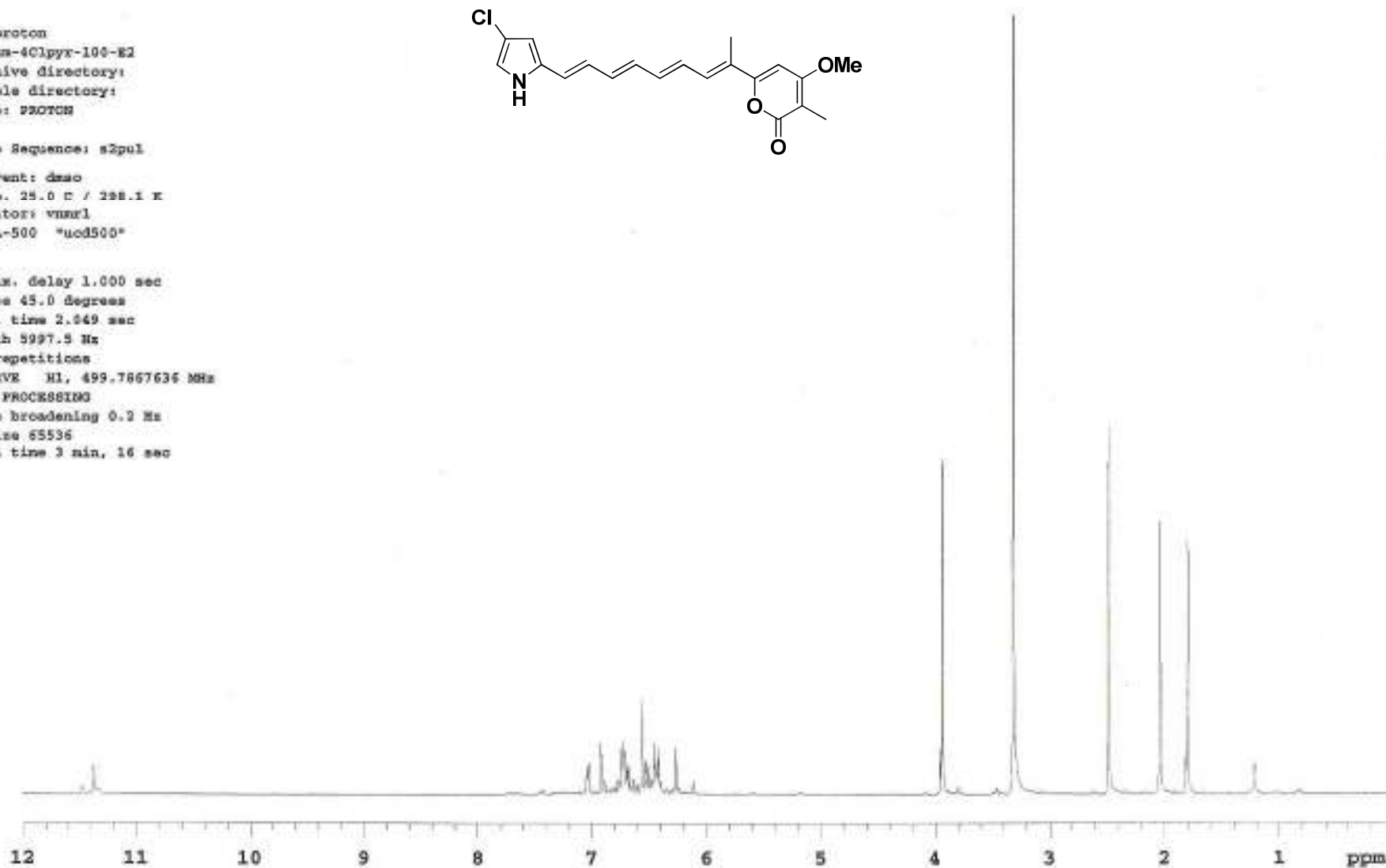
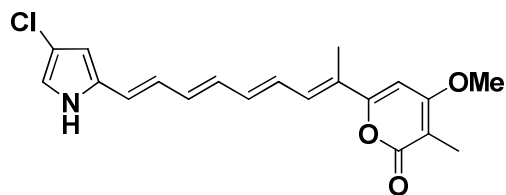
¹ H NMR Spectrum for 3-chloroisorumbrin (3)	S2
¹³ C NMR Spectrum for 3-chloroisorumbrin (3)	S3
¹ H NMR Spectrum for 3-bromoisorumbrin (4)	S4
¹³ C NMR Spectrum for 3-bromoisorumbrin (4)	S5
¹ H NMR Spectrum for 3-fluoroisorumbrin (5)	S6
¹³ C NMR Spectrum for 3-fluoroisorumbrin (5)	S7

Std proton
SC-Aum-4Clpyr-100-E2
Archive directory:
Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: dmsc
Temp. 29.0 C / 298.1 K
Operator: vmsrl
INOVA-500 "ucd500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 5997.5 Hz
64 repetitions
OBSERVE H1, 499.7867635 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 3 min, 16 sec



¹H NMR (*d*₆-DMSO, 500 MHz) Spectrum of 3-chloroisorumbrin (**3**)

BC-Aum-4Clpyr-100-E2

Archive directory:

Sample directory:

File: CARBON

Pulse Sequence: s2pul

Solvent: dmsc

Temp. 25.0 C / 298.1 K

Operator: vmmr1

INOVA-500 "ucd500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30165.9 Hz

15536 repetitions

OBSERVE C13, 125.6714817 MHz

DECOUPLE H1, 499.7892625 MHz

Power 40 dB

continuously on

WALTZ-16 modulated

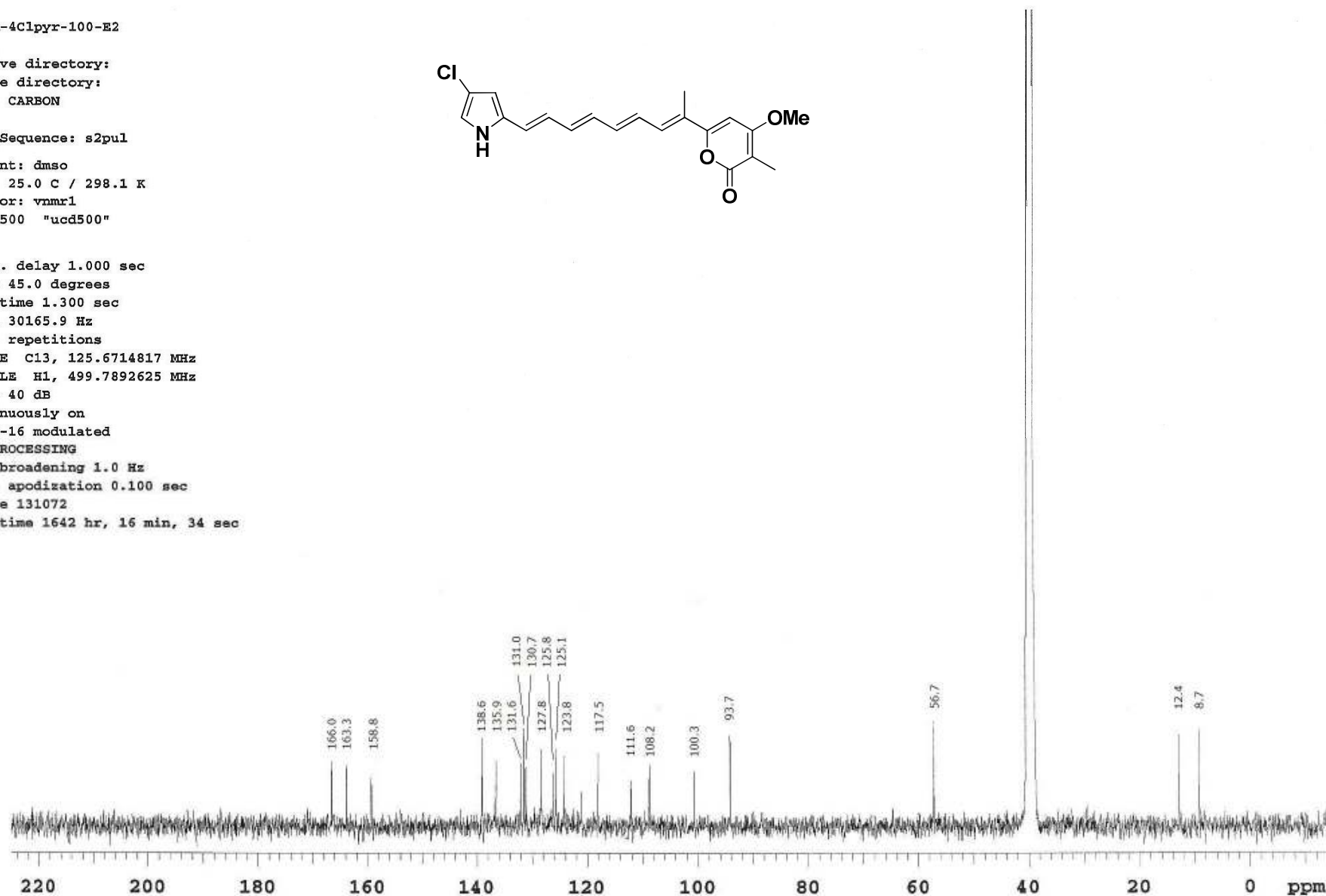
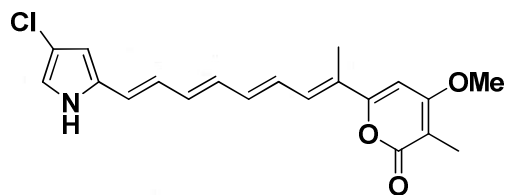
DATA PROCESSING

Line broadening 1.0 Hz

Gauss apodization 0.100 sec

FT size 131072

Total time 1642 hr, 16 min, 34 sec



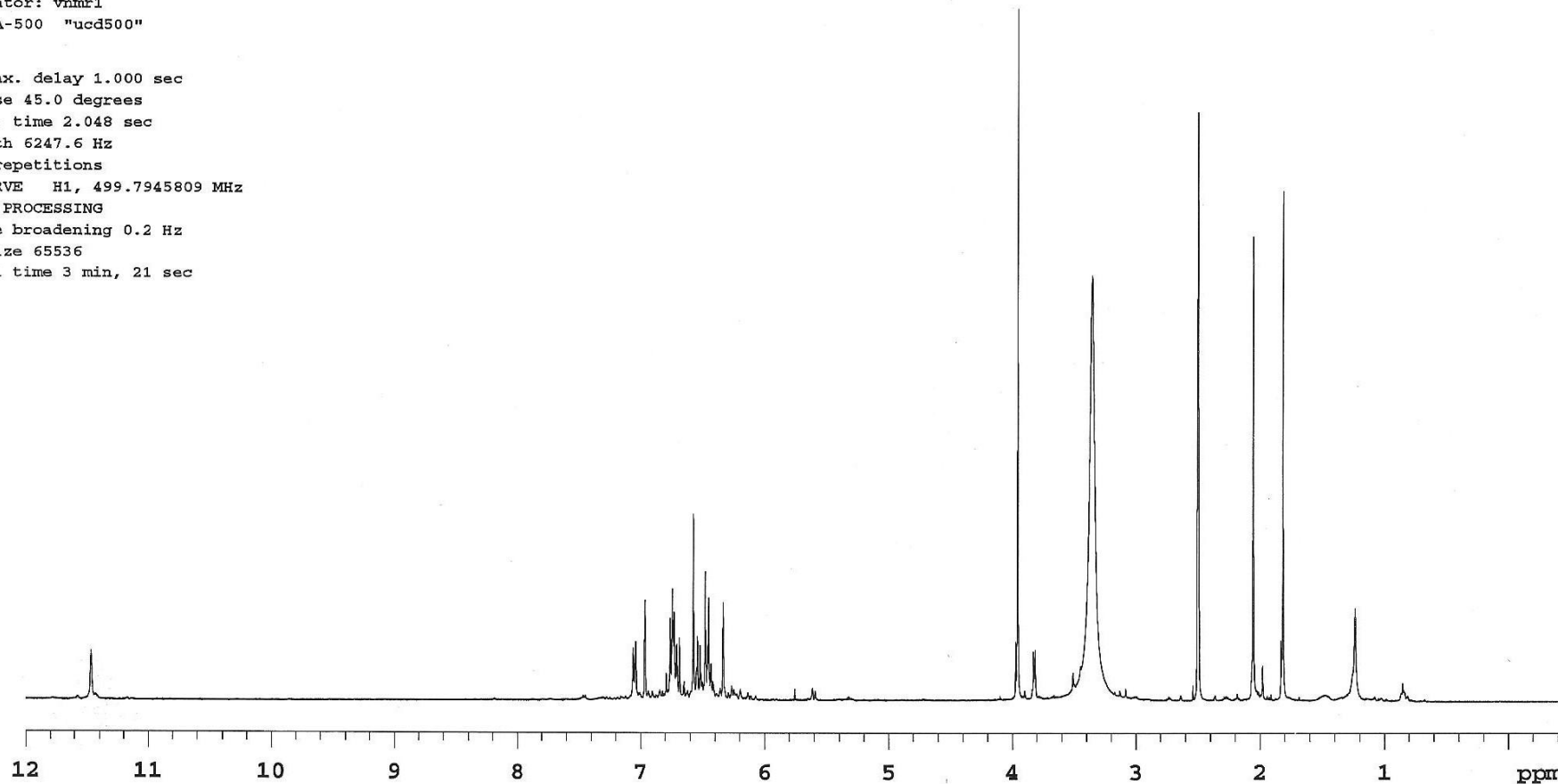
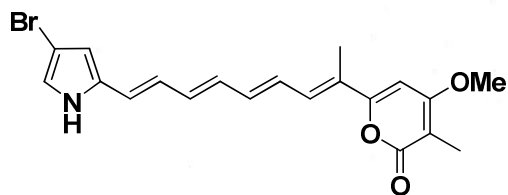
^{13}C NMR (d_6 -DMSO, 125 MHz) Spectrum of 3-chloroisorumbrin (**3**)

Std proton
BC-Aum-Bipyr-90-F
Archive directory:
Sample directory:
File: PROTON

Pulse Sequence: s2pul

Solvent: dmsc
Temp. 30.0 C / 303.1 K
Operator: vnmr1
INNOVA-500 "ucd500"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 6247.6 Hz
64 repetitions
OBSERVE H1, 499.7945809 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 3 min, 21 sec



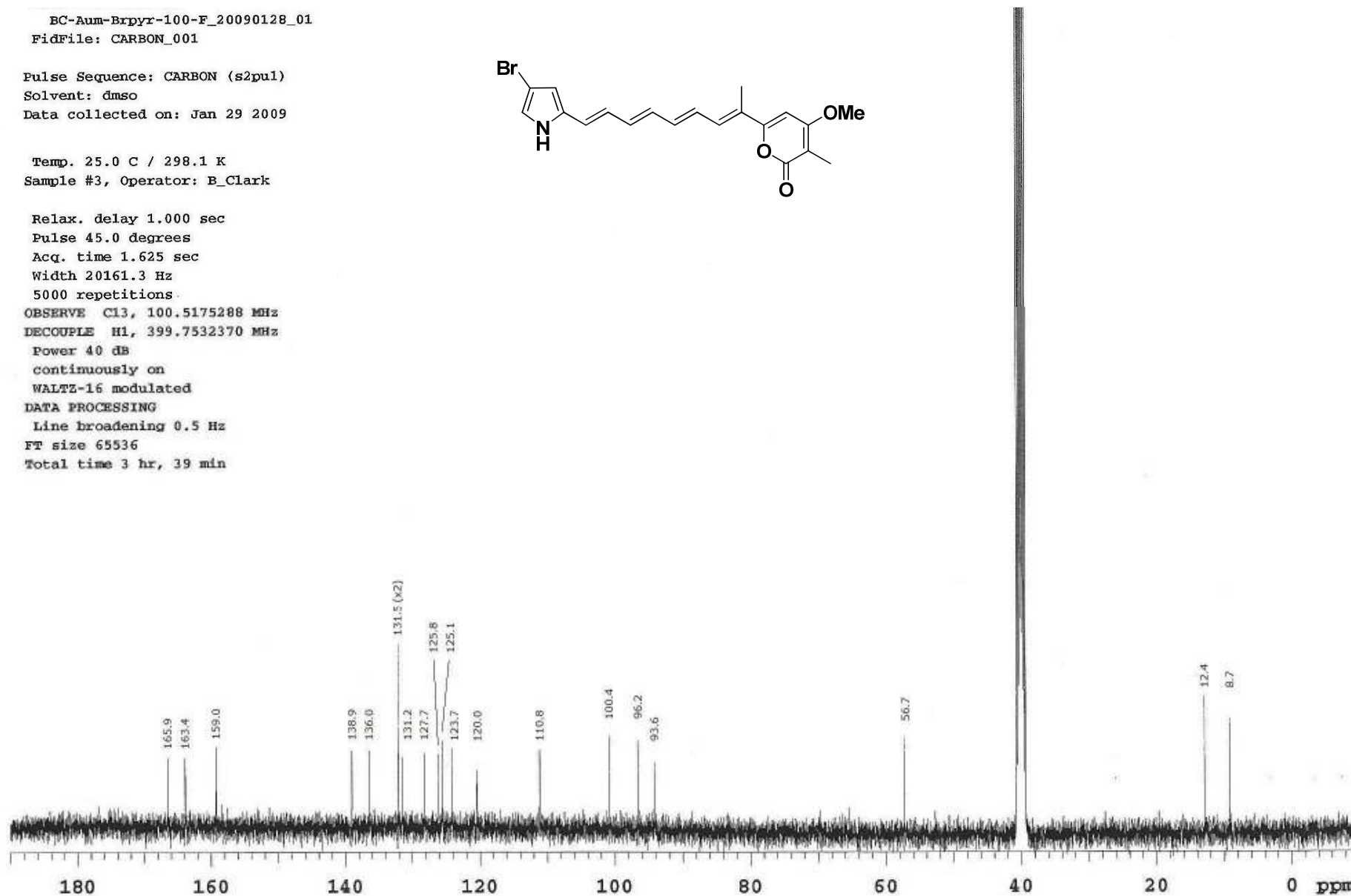
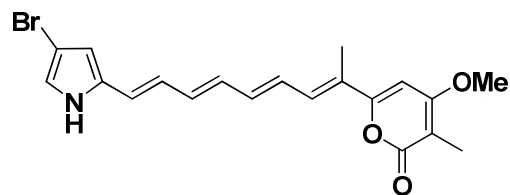
^1H NMR (d_6 -DMSO, 500 MHz) Spectrum of 3-bromoisorumbrin (**4**)

BC-Aum-Brpyr-100-F_20090128_01
FidFile: CARBON_001

Pulse Sequence: CARBON (s2pul)
Solvent: dmsc
Data collected on: Jan 29 2009

Temp. 25.0 C / 298.1 K
Sample #3, Operator: B_Clark

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.625 sec
Width 20161.3 Hz
5000 repetitions
OBSERVE C13, 100.5175288 MHz
DECOUPLE H1, 399.7532370 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 hr, 39 min

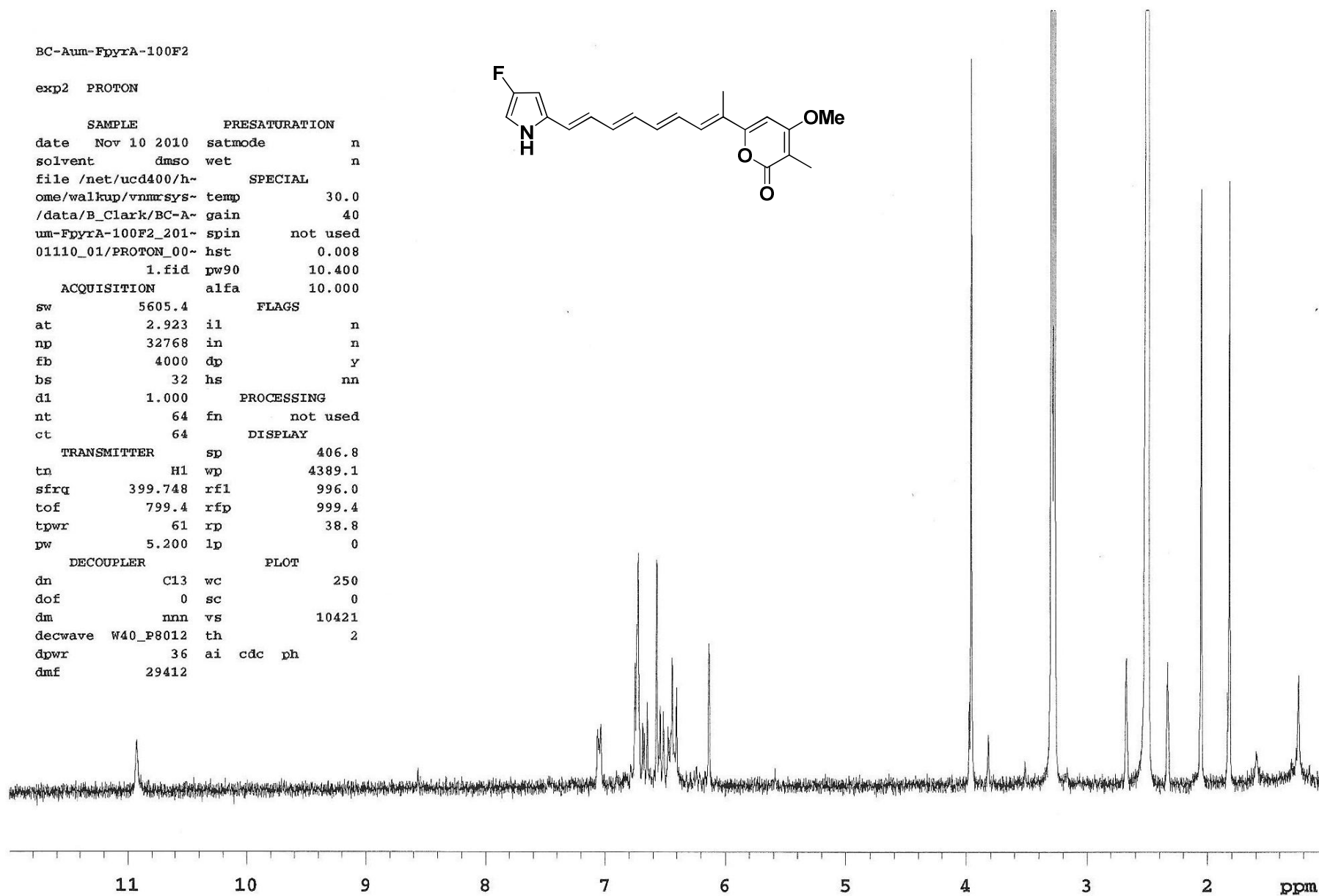
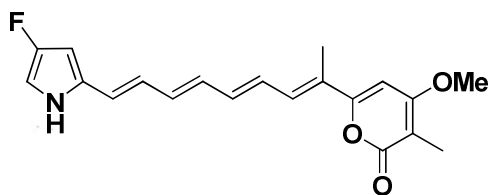


^{13}C NMR (d_6 -DMSO, 100 MHz) Spectrum of 3-bromisorumbrin (4)

BC-Aum-FpyrA-100F2

exp2 PROTON

SAMPLE		PRESATURATION	
date	Nov 10 2010	satmode	n
solvent	dms	wet	n
file	/net/ucd400/h-	SPECIAL	
ome/walkup/vnmrsys-	temp		30.0
/data/B_Clark/BC-A-	gain		40
um-FpyrA-100F2_201-	spin		not used
01110_01/PROTON_00-	hst		0.008
	1.fid	pw90	10.400
ACQUISITION		alfa	
sw	5605.4	FLAGS	
at	2.923	il	n
np	32768	in	n
fb	4000	dp	y
bs	32	hs	nn
d1	1.000	PROCESSING	
nt	64	fn	not used
ct	64	DISLAY	
TRANSMITTER		sp	
tn	H1	wp	4389.1
sfrq	399.748	rf1	996.0
tof	799.4	rfp	999.4
tpwr	61	rp	38.8
pw	5.200	lp	0
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nnn	vs	10421
decwave	W40_P8012	th	2
dpwr	36	ai	cdc
dmf	29412	ph	



¹H NMR (*d*₆-DMSO, 500 MHz) Spectrum of 3-fluoroisorumbrin (5)

STANDARD PROTON PARAMETERS
BC-Aum-FRYR-F2C

Archive directory:
Sample directory:

Pulse Sequence: s2pul

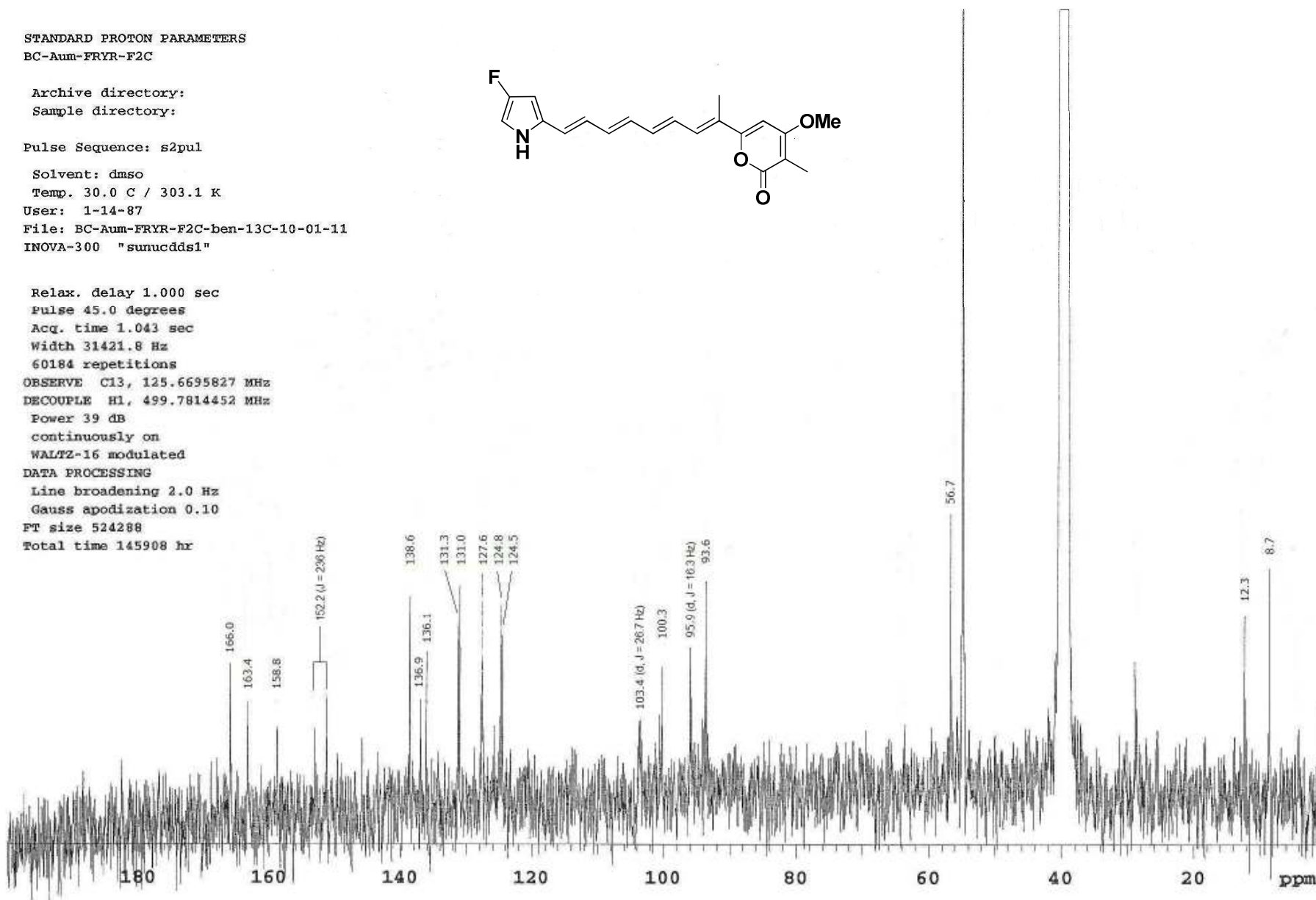
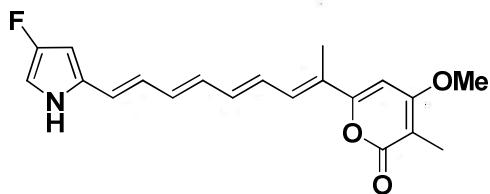
Solvent: dms

Temp. 30.0 C / 303.1 K

User: 1-14-87

File: BC-Aum-FRYR-F2C-ben-13C-10-01-11

INOVA-300 "sunucdd1"



^{13}C NMR (d_6 -DMSO, 125 MHz) Spectrum of 3-fluoroisorumbrin (5)