

## Supporting Information

# **OSCILLATOXIN E AND ITS C7 EPIMER SHOW DISTINCT GROWTH INHIBITION PROFILES AGAINST SEVERAL CANCER CELL LINES**

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### Contents

1. NMR spectra
2. Growth inhibition of **1** and **2** against 39 human cancer cell lines

----- PROCESSING PARAMETERS -----  
sweep( 0.2[Hz], 0.0[s] )  
expand(0[0%], 0[1%], 80[1%], 100[1%] )  
zeroFill( 1, TRUE )  
fft( 1, TRUE, 32KHz )  
machRephase  
ppm

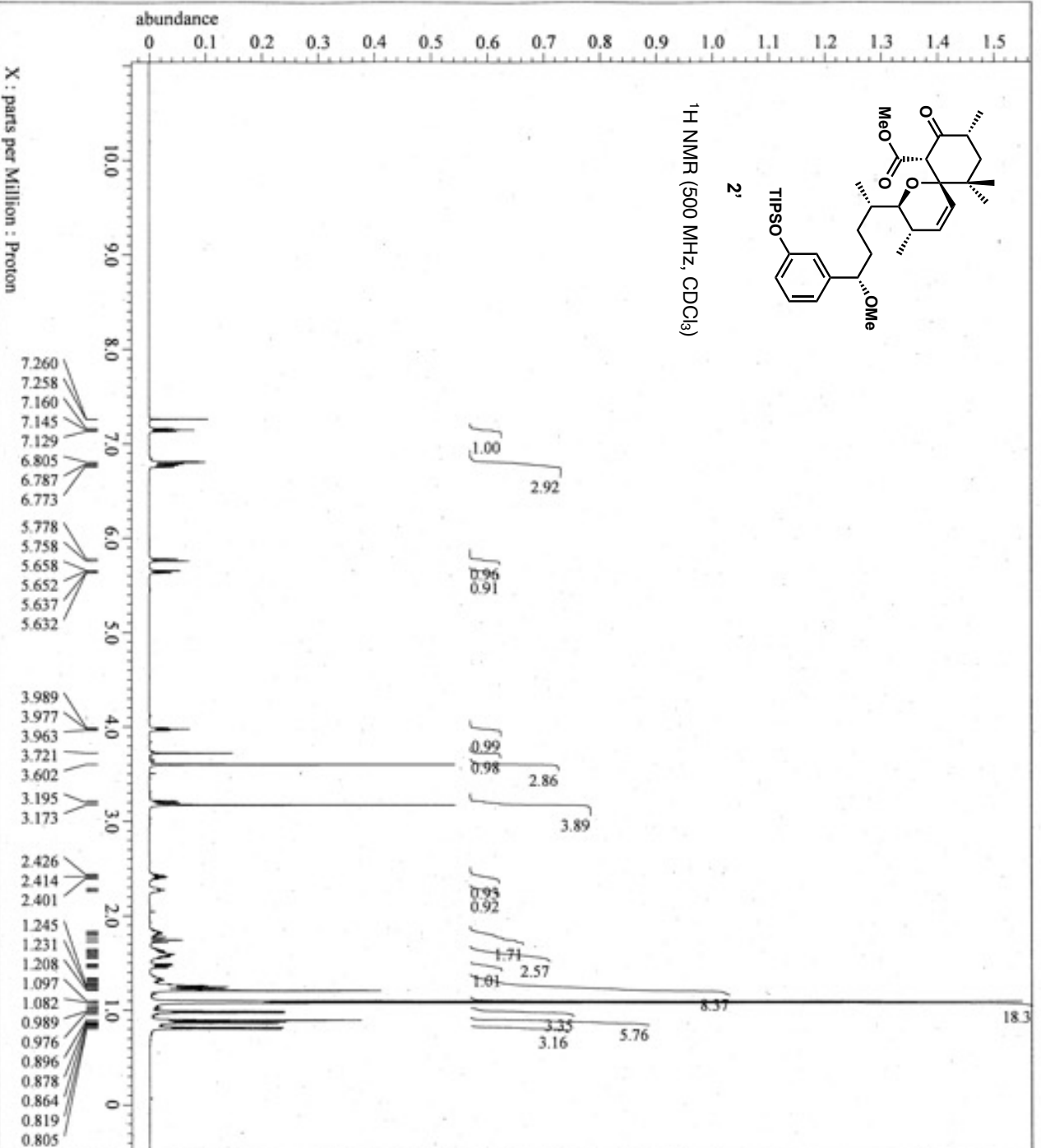
谱文件名: NGY1-151\*2\_proton-1-1-jdf

Filename NGY1-151\*2\_proton-1-2  
Author = daita  
Experiment = proton\_autc\_jsp  
Sample Id NGY1-151\*2  
CHLOROCFORM-D  
Actual Start Time = 26-APR-2021 09:00:05  
Revision Time = 26-APR-2021 08:48:40

Comment = single\_pulse  
Data Format = ID COMPTXK  
Dim Size = 13107  
X Domain = proton  
Dim File = proton  
Dim Units = [ppm]  
Dimensions = X  
Spectrometer = DELTAQ\_90K

Field Strength = 11.74735791[GHz] (500[MHz])  
Acq Duration = 1.74587904[s]  
X Domain = proton  
X Freq = 500.15991521[MHz]  
X Offset = 5.0[ppm]  
X Polarity = 16384  
X Prescans = 1  
X Resolution = 0.57277371[Hz]  
X Sweep = 9.38438438[KHz]  
X Sweep\_Clipped = 7.50750751[KHz]  
X Domain = proton  
X Freq = 500.15991521[MHz]  
X Offset = 5.0[ppm]  
X Domain = proton  
X Freq = 500.15991521[MHz]  
Tri\_Offset = 5.0[ppm]  
Tri\_Domain = proton  
Tri\_Freq = 500.15991521[MHz]  
Tri\_Offset = 5.0[ppm]  
Blacking = 2[us]  
Blinking = FALSE  
SOLAR = 16  
Total Scans = 16

Relaxation\_Delay = 5.1[s]  
Recor Gain = 36  
Temp\_Cor = 21.4[deg]  
X 90\_Width = 6.9[us]  
X Acq Time = 1.74587904[s]  
X Angle = 45[deg]  
X Alt = 9[deg]  
X Pulse = 1.45[us]  
X Mode = Off  
Tri\_Mode = Off





PROCESSING PARAMETERS  
segy( 2.0[Hz], 0.0[Hz] )  
tropicald( 0[Hz], 0[Hz], 80[Hz], 100[Hz] )  
refofill( 1, TRUE )  
f1( 1, TRUE, TRUE )  
machlinephase  
ppm

Platform: NORT-151\*2\_Carbon-  
Acetone: delta  
Experiment: carbon-auto.jpg  
Sample\_id: NORT-151\*2  
Solvent: C6H12O6(080)-D  
Actual\_Start\_Time: 26-APR-2021 09:02  
Revision\_Time: 13-JUL-2021 09:35

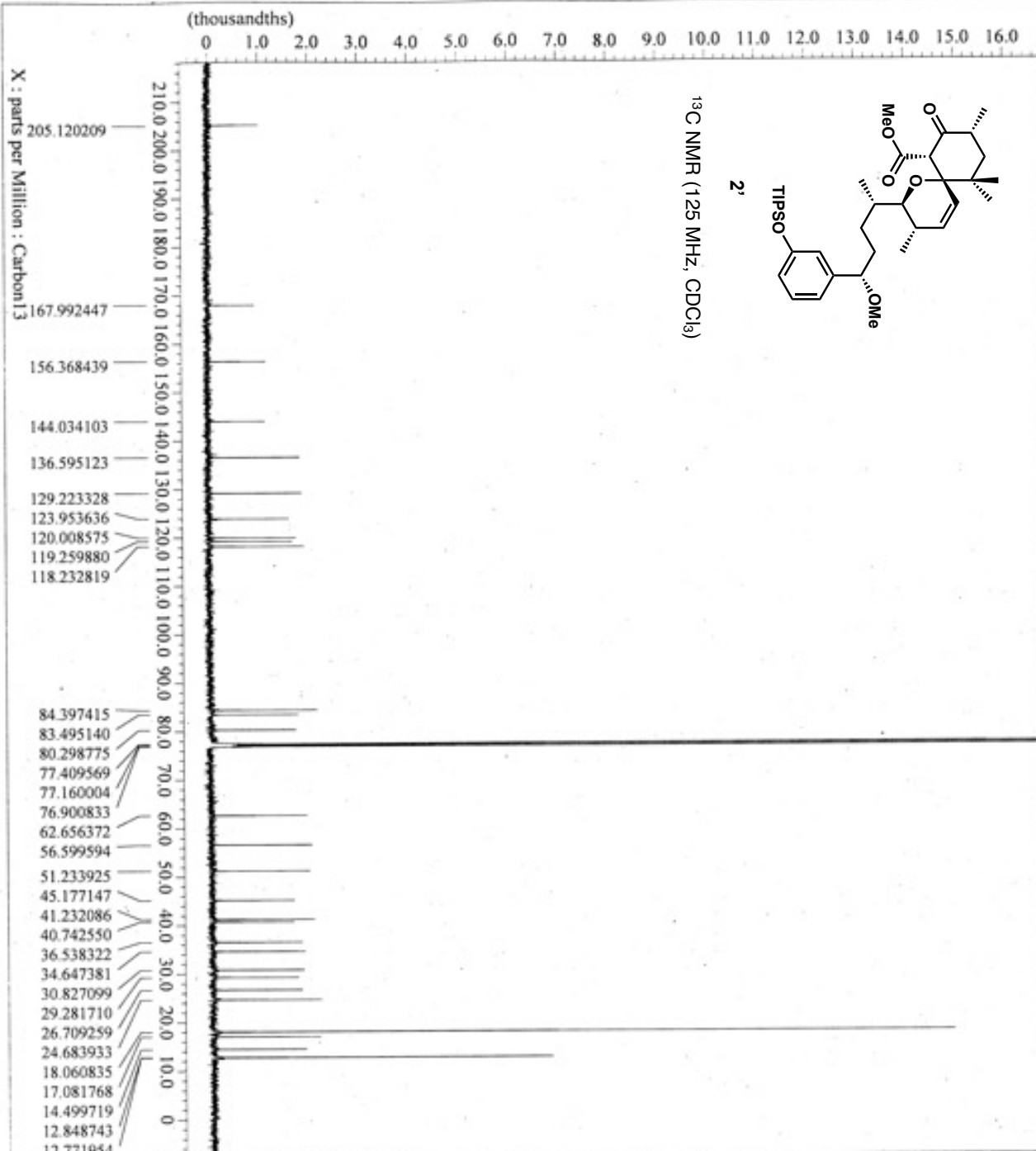
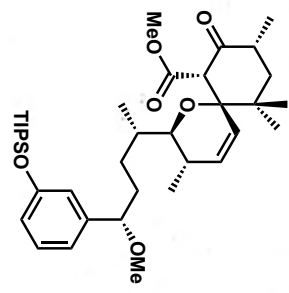
Comment: single pulse decou  
Data\_Format: 1D\_CGPR2EX  
Dim\_Size: 26214  
X\_Domain: Carbon13  
Dim\_Title: Carbon13  
Dim\_Units: [ppm]  
Dimensions: X : 14  
Spectrometer: DRUMAC\_Spec

Field\_Strength: 11.74735791[T] (1500  
X\_Acq\_Duration: 0.62837504[hr]  
X\_Domain: Carbon13  
X\_Freq: 125.76529768 [MHz]  
X\_Offset: 1001[ppm]  
X\_Points: 32768  
X\_Protocals: 4  
X\_Resolution: 1.20718264[Hz]  
X\_Sweep: 39.56694201[kHz]  
X\_Sweep\_Clippped: 31.64554642[kHz]  
Irr\_Domain: Proton  
Irr\_Freq: 500.15991521 [MHz]  
Irr\_Offset: 5.0 [ppm]  
Blacking: 2 [ua]  
Clipped: TRUE  
Sca: 1000  
Total\_Scans: 1000

Relaxation\_Delay: 21[s]  
Receiver\_Gain: 50  
Temp\_Gain: 20.6 [dB]  
X\_90\_Rf\_Phd: 11.4 [ua]  
X\_Acq\_Time: 0.62837504[hr]  
X\_Angle: 30 [deg]  
X\_Anu: 11.8 [deg]  
X\_Pulse: 3.8 [ua]  
Irr\_Alt\_Dec\_Calc: 31.4991 [dB]  
Irr\_Alt\_Dec\_Calc: 31.4991 [dB]  
Irr\_Alt\_Dec\_Default\_Calc: 31.4991 [dB]  
Irr\_Alt\_Non: 31.4991 [dB]  
Irr\_Dec\_Bandwidth\_Hz: 5.97896087 [kHz]

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)

2'

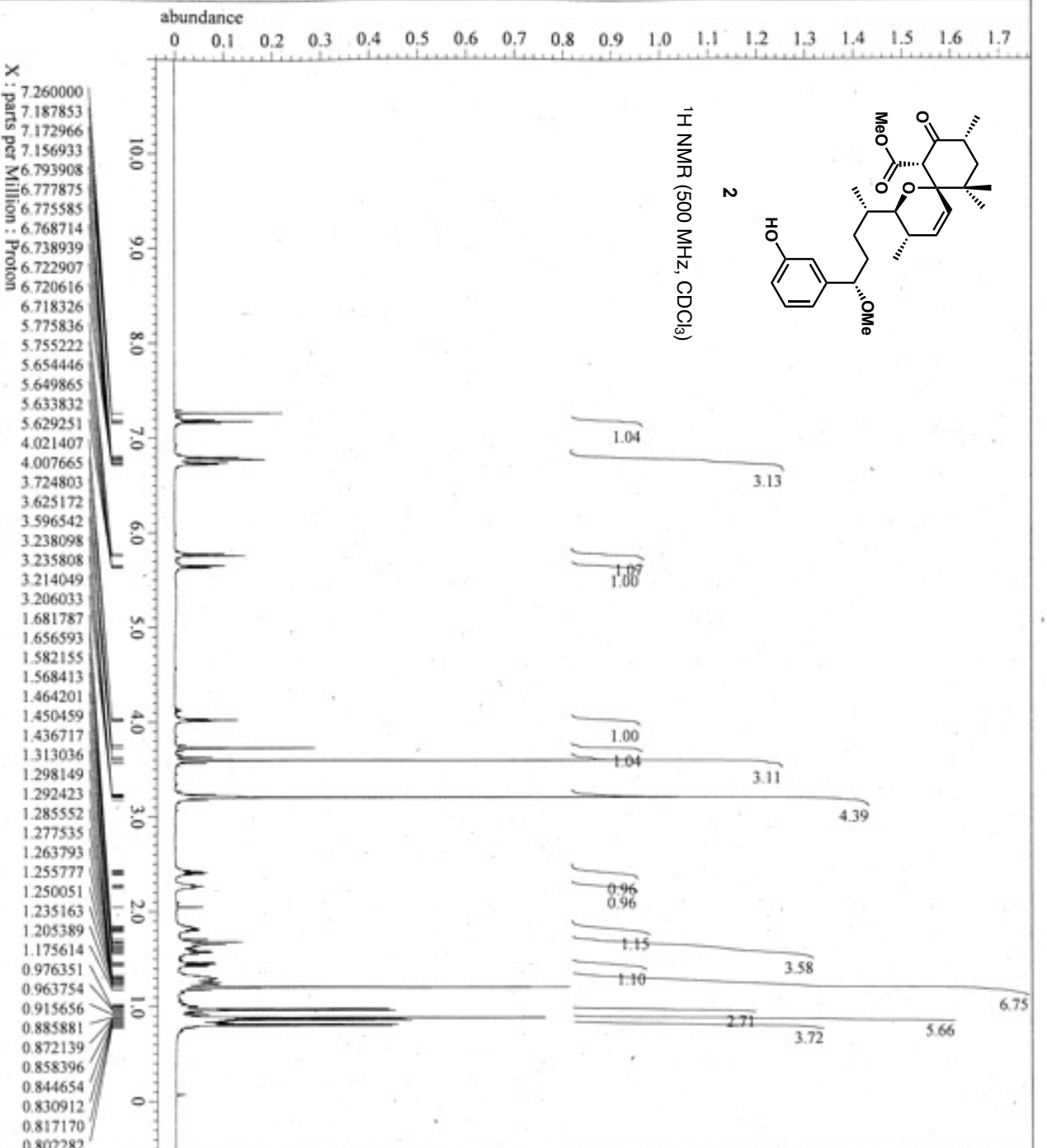
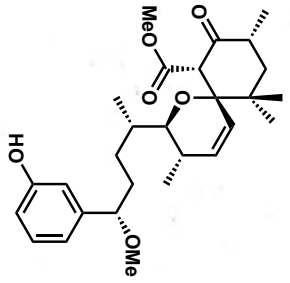


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----- PROCESSING PARAMETERS -----
smpf ( 0.21Hz, 0.01s )
tspresoldd ( 0%, 01%, 801%, 1001% )
zerofill ( 1, TRMR )
fft ( 1, TRMR, TRMR )
machinphase
ppe
  
```

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)

2



```

=====
Name: 1-053-1_Proton-1-3_1d
Author:
Experiment:
Sample Id: 1-053-1
Solvent: CHLOROFORM-D
Actual_Start_Time: 26-NOV-2021 15:28:25
Acquisition_Time: 2-DEC-2021 09:40:10
Comment:
Data Format:
Data Size: 13107
X_Domain:
D1a_Title:
D1a_Unita:
D1a_Dimensions:
Spectrometer:
Field Strength: 11.7473579 [T] (500 [MHz])
X_Acq Duration: 1.74587904 [s]
X_Domain:
X_P1:
X_P2:
X_P3:
X_P4:
X_P5:
X_P6:
X_P7:
X_P8:
X_P9:
X_P10:
X_P11:
X_P12:
X_P13:
X_P14:
X_P15:
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X_P96:
X_P97:
X_P98:
X_P99:
X_P100:
=====
  
```

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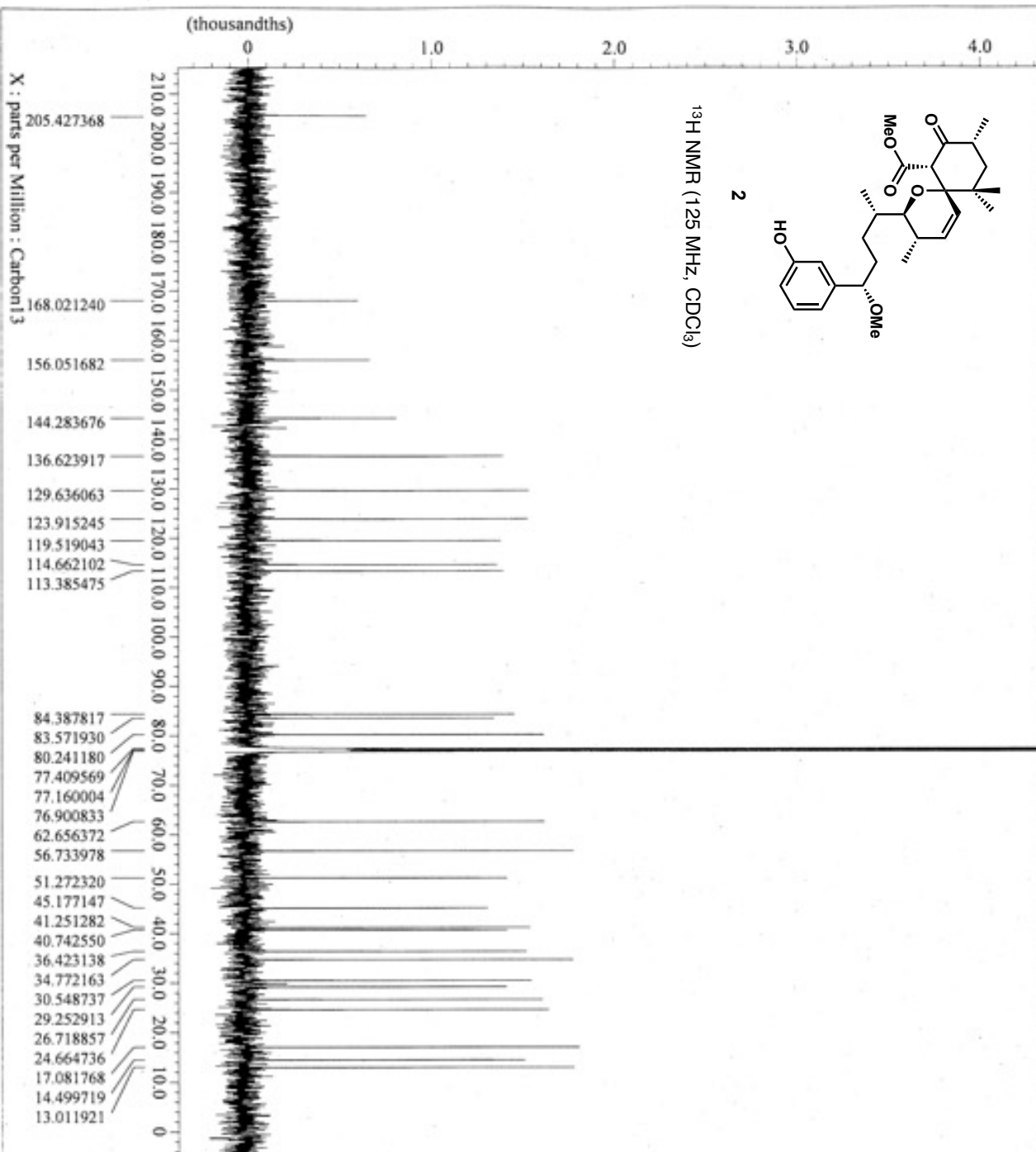
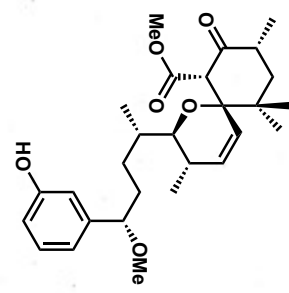
=====
Name: 1-053-1_Proton-1-3_1d
Author:
Experiment:
Sample Id: 1-053-1
Solvent: CHLOROFORM-D
Actual_Start_Time: 26-NOV-2021 15:28:25
Acquisition_Time: 2-DEC-2021 09:40:10
Comment:
Data Format:
Data Size: 13107
X_Domain:
D1a_Title:
D1a_Unita:
D1a_Dimensions:
Spectrometer:
Field Strength: 11.7473579 [T] (500 [MHz])
X_Acq Duration: 1.74587904 [s]
X_Domain:
X_P1:
X_P2:
X_P3:
X_P4:
X_P5:
X_P6:
X_P7:
X_P8:
X_P9:
X_P10:
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X_P92:
X_P93:
X_P94:
X_P95:
X_P96:
X_P97:
X_P98:
X_P99:
X_P100:
=====
  
```



----- PROCESSING PARAMETERS -----  
name: 2.0181, 0.0181 )  
temp: 300.0 (K), 0.0 (s), 90 (s), 100 (s) )  
ref: 1. TRICE, TRICE )  
f2: 1. TRICE, TRICE )  
magn: phase  
ppm

<sup>13</sup>H NMR (125 MHz, CDCl<sub>3</sub>)

2



Filename: 1-052-1-Carbon-1-3  
Author: delta  
Experiment: carbon auto\_jmp  
Sample Id: 1-052-1  
Solvent: CHLOROFORM-D  
Actual\_Start\_Time: 26-SEP-2021 15:30  
Revision\_Time: 13-SEP-2021 08:37  
Comment: Single pulse decou  
Data Format: 1D CQXPFLX  
Dir Size: 26316  
X\_Domain: Carbon13  
Dir Title: Carbon13  
Dim Units: [ppm]  
Dimensions: X  
Spectrometer: DELTA2\_NMR  
Field Strength: 11.74737917 (1000  
X Acq Duration: 0.82837504(s)  
X Domain: Carbon13  
X Freq: 125.76529768 (MHz)  
X Offset: 100 (ppm)  
X Points: 32768  
X Prescans: 4  
X Resolution: 1.20718268 (Hz)  
X Sweep Clipped: X  
X\_Sweep: 39.55662031 (kHz)  
X\_Domain: 31.64559962 (kHz)  
X\_Freq: 500.13991521 (MHz)  
X\_Offset: 5.0 (ppm)  
X\_Pulse: 2 (us)  
X\_Scans: 577  
Total Scans: 577  
Relaxation\_Delay: 2 (s)  
Receiver Gain: 80  
Temp: 300.0 (C)  
X Acq Width: 20.8 (us)  
X Acq Time: 11.4 (us)  
X Angle: 0.82837504 (s)  
X Ann: 30 (deg)  
X\_Pulse: 11.2 (us)  
X\_Ann\_Deco: 31.499 (us)  
X\_Ann\_Deco\_Calc: 31.499 (us)  
X\_Ann\_Deco\_Default\_Calc: 31.499 (us)  
X\_Ann\_Deco: 31.499 (us)  
X\_Ann\_Deco\_Bandwidth\_Hz: 5.97826087 (kHz)

## Growth inhibition of 1 and 2 against 39 human cancer cell lines

Cancer cell lines		OTX-E (1) <sup>a</sup>	7- <i>epi</i> -OTX-E (2)
<b>Breast</b>	HBC-4	-4.79	-4.75
	BSY-1	-4.79	-4.86
	HBC-5	-4.76	-4.76
	MCF-7	-4.87	-4.78
	MDA-MB-231	-4.81	-4.77
<b>CNS</b>	U251	-4.77	-4.76
	SF-268	-4.73	-4.75
	SF-295	-4.77	-4.77
	SF-539	-4.73	-4.73
	SNB-75	-4.81	-4.75
	SNS-78	-4.73	-4.73
<b>Colon</b>	HCC2998	-4.80	-4.76
	KM-12	-4.79	-4.74
	HT-29	-4.74	-4.74
	HCT-15	-4.79	-4.81
	HCT-116	-4.80	-4.84
<b>Lung</b>	NCI-H23	-4.75	-4.71
	NCI-H226	-4.74	-4.68
	NCI-H522	-4.90	-4.82
	NCI-H460	-4.81	-4.74
	A549	-4.82	-4.76
	DMS273	-4.82	-4.78
	DMS114	-4.92	-4.94
<b>Melanoma</b>	LOX-IMVI	-4.72	-4.71
<b>Ovarian</b>	OVCAR-3	-4.80	-4.84
	OVCAR-4	-4.78	-4.83
	OVCAR-5	-4.78	-4.73
	OVCAR-8	-4.74	-4.78
	SK-OV-3	-4.74	-4.78
<b>Renal</b>	RXF-631L	-4.77	-4.77
	ACHN	-4.72	-4.75
<b>Stomach</b>	St-4	-4.74	-4.77
	MKN1	-4.82	-4.77
	MKN-B	-5.01	-4.80
	MKN-A	-4.87	-4.78
	MKN45	-4.80	-4.75
	MKN74	-4.99	-4.81
<b>Prostate</b>	DU-145	-4.72	-4.71
	PC-3	-4.82	-4.83
<b>MG-MID<sup>b</sup></b>		-4.80	-4.77

<sup>a</sup> Y. Araki *et al. Biosci. Biotechnol. Biochem.* 2021, **85**, 1371.

<sup>b</sup> MG-MID: average of the log GI<sub>50</sub> values of each 39 human cancer cell line