

Electronic Supplementary Information

**3-*O*-Carbamoyl-5,7,20-*O*-trimethylsilybins: Synthesis and preliminary antiproliferative evaluation**

Sitong Wu<sup>a</sup>, Guanglin Chen<sup>a</sup>, Qiang Zhang<sup>b,c</sup>, Guangdi Wang<sup>b,c</sup>, and Qiao-Hong Chen<sup>\*a</sup>

<sup>a</sup>Department of Chemistry and Biochemistry, California State University, Fresno, 2555 E. San Ramon Avenue, M/S SB70, Fresno, CA 93740, USA

<sup>b</sup>Department of Chemistry and <sup>c</sup>RCMI Cancer Research Center, Xavier University of Louisiana, 1 Drexel Drive, New Orleans, LA 70125, USA

**List of Contents:**

<b>Figure S1:</b> <sup>1</sup> H NMR spectrum of <b>5</b> in CDCl <sub>3</sub> .....	S3
<b>Figure S2:</b> <sup>13</sup> C NMR spectrum of <b>5</b> in CDCl <sub>3</sub> .....	S4
<b>Figure S3:</b> COSY spectrum of <b>5</b> in CDCl <sub>3</sub> .....	S5
<b>Figure S4:</b> HSQC spectrum of <b>5</b> in CDCl <sub>3</sub> .....	S6
<b>Figure S5:</b> HMBC spectrum of <b>5</b> in CDCl <sub>3</sub> .....	S7
<b>Figure S6:</b> High resolution mass spectrum of <b>5</b> .....	S8
<b>Figure S7:</b> HPLC chromatogram of <b>5</b> .....	S9
<b>Figure S8:</b> <sup>1</sup> H NMR spectrum of <b>4</b> in CDCl <sub>3</sub> .....	S10
<b>Figure S9:</b> <sup>13</sup> C NMR spectrum of <b>4</b> in CDCl <sub>3</sub> .....	S11
<b>Figure S10:</b> High resolution mass spectrum of <b>4</b> .....	S12
<b>Figure S11:</b> HPLC chromatogram of <b>4</b> .....	S13
<b>Figure S12:</b> <sup>1</sup> H NMR spectrum of <b>6</b> in CDCl <sub>3</sub> .....	S14
<b>Figure S13:</b> <sup>13</sup> C NMR spectrum of <b>6</b> in CDCl <sub>3</sub> .....	S15
<b>Figure S14:</b> High resolution mass spectrum of <b>6</b> .....	S16
<b>Figure S15:</b> HPLC chromatogram of <b>6</b> .....	S17
<b>Figure S16:</b> <sup>1</sup> H NMR spectrum of <b>7</b> in CDCl <sub>3</sub> .....	S18
<b>Figure S17:</b> <sup>13</sup> C NMR spectrum of <b>7</b> in CDCl <sub>3</sub> .....	S19
<b>Figure S18:</b> High resolution mass spectrum of <b>7</b> .....	S20
<b>Figure S19:</b> HPLC chromatogram of <b>7</b> .....	S21
<b>Figure S20:</b> <sup>1</sup> H NMR spectrum of <b>8</b> in CDCl <sub>3</sub> .....	S22
<b>Figure S21:</b> <sup>13</sup> C NMR spectrum of <b>8</b> in CDCl <sub>3</sub> .....	S23

<b>Figure S22:</b> High resolution mass spectrum of <b>8</b> .....	S24
<b>Figure S23:</b> HPLC chromatogram of <b>8</b> .....	S25
<b>Figure S24:</b> <sup>1</sup> H NMR spectrum of <b>9</b> in CDCl <sub>3</sub> .....	S26
<b>Figure S25:</b> <sup>13</sup> C NMR spectrum of <b>9</b> in CDCl <sub>3</sub> .....	S27
<b>Figure S26:</b> High resolution mass spectrum of <b>9</b> .....	S28
<b>Figure S27:</b> HPLC chromatogram of <b>9</b> .....	S29
<b>Figure S28:</b> <sup>1</sup> H NMR spectrum of <b>10</b> in CDCl <sub>3</sub> .....	S30
<b>Figure S29:</b> <sup>13</sup> C NMR spectrum of <b>10</b> in CDCl <sub>3</sub> .....	S31
<b>Figure S30:</b> High resolution mass spectrum of <b>10</b> .....	S32
<b>Figure S31:</b> <sup>1</sup> H NMR spectrum of <b>11</b> in CDCl <sub>3</sub> .....	S33
<b>Figure S32:</b> <sup>13</sup> C NMR spectrum of <b>11</b> in CDCl <sub>3</sub> .....	S34
<b>Figure S33:</b> High resolution mass spectrum of <b>11</b> .....	S35
<b>Figure S33:</b> HPLC chromatogram of <b>11</b> .....	S36
<b>Figure S34:</b> <sup>1</sup> H NMR spectrum of <b>12</b> in CDCl <sub>3</sub> .....	S37
<b>Figure S35:</b> <sup>13</sup> C NMR spectrum of <b>12</b> in CDCl <sub>3</sub> .....	S38
<b>Figure S36:</b> High resolution mass spectrum of <b>12</b> .....	S39
<b>Figure S37:</b> HPLC chromatogram of <b>12</b> .....	S40
<b>Figure S38:</b> <sup>1</sup> H NMR spectrum of <b>13</b> in CDCl <sub>3</sub> .....	S41
<b>Figure S39:</b> <sup>13</sup> C NMR spectrum of <b>13</b> in CDCl <sub>3</sub> .....	S42
<b>Figure S40:</b> High resolution mass spectrum of <b>13</b> .....	S43
<b>Figure S41:</b> HPLC chromatogram of <b>13</b> .....	S44
<b>Figure S42:</b> <sup>1</sup> H NMR spectrum of <b>14</b> in CDCl <sub>3</sub> .....	S45
<b>Figure S43:</b> <sup>13</sup> C NMR spectrum of <b>14</b> in CDCl <sub>3</sub> .....	S46
<b>Figure S44:</b> High resolution mass spectrum of <b>14</b> .....	S47
<b>Figure S45:</b> <sup>1</sup> H NMR spectrum of <b>15</b> in CDCl <sub>3</sub> .....	S48
<b>Figure S46:</b> <sup>13</sup> C NMR spectrum of <b>15</b> in CDCl <sub>3</sub> .....	S49
<b>Figure S47:</b> High resolution mass spectrum of <b>15</b> .....	S50
<b>Figure S48:</b> <sup>1</sup> H NMR spectrum of <b>16</b> in CDCl <sub>3</sub> .....	S51
<b>Figure S49:</b> <sup>13</sup> C NMR spectrum of <b>16</b> in CDCl <sub>3</sub> .....	S52
<b>Figure S50:</b> High resolution mass spectrum of <b>16</b> .....	S53
<b>Figure S51:</b> <sup>1</sup> H NMR spectrum of <b>17</b> in CDCl <sub>3</sub> .....	S54
<b>Figure S52:</b> <sup>13</sup> C NMR spectrum of <b>17</b> in CDCl <sub>3</sub> .....	S55
<b>Figure S53:</b> High resolution mass spectrum of <b>17</b> .....	S56
<b>Figure S54:</b> The concentration-effect curves .....	S57-S101



SW-66-24

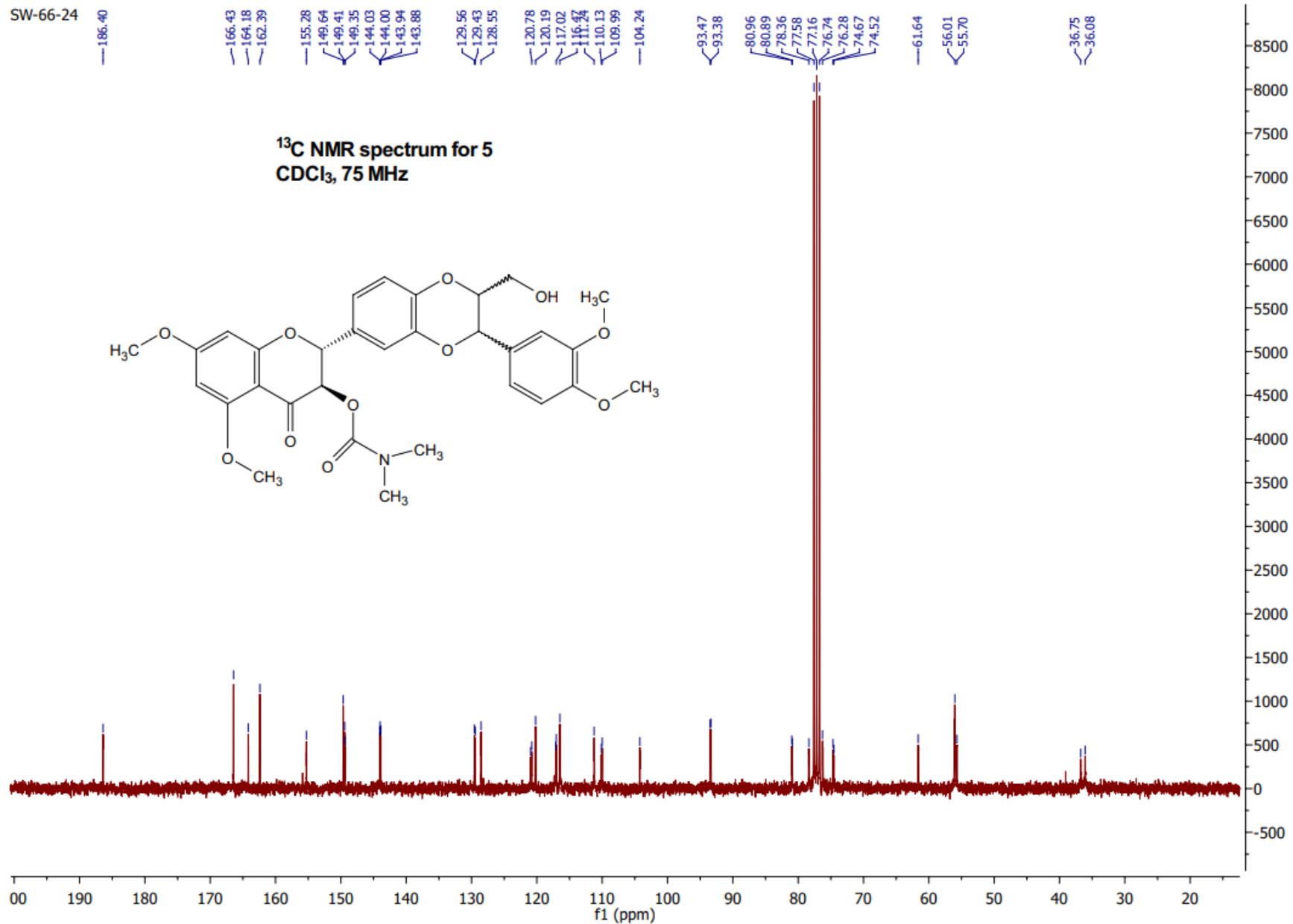


Figure S2:  $^{13}\text{C}$  NMR spectrum of 5 in  $\text{CDCl}_3$

COSY for compound 5

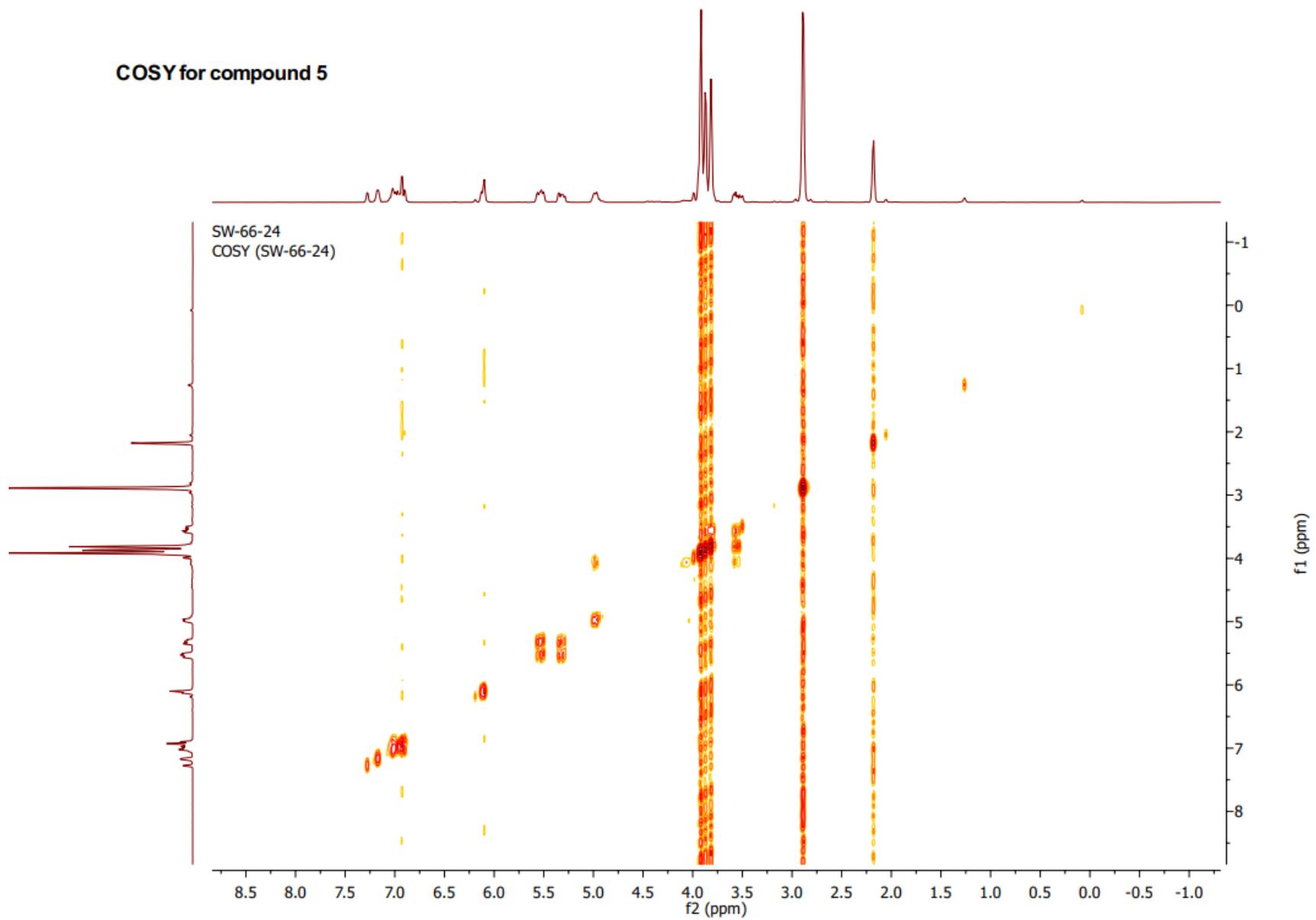


Figure S3: COSY spectrum of **5** in  $\text{CDCl}_3$

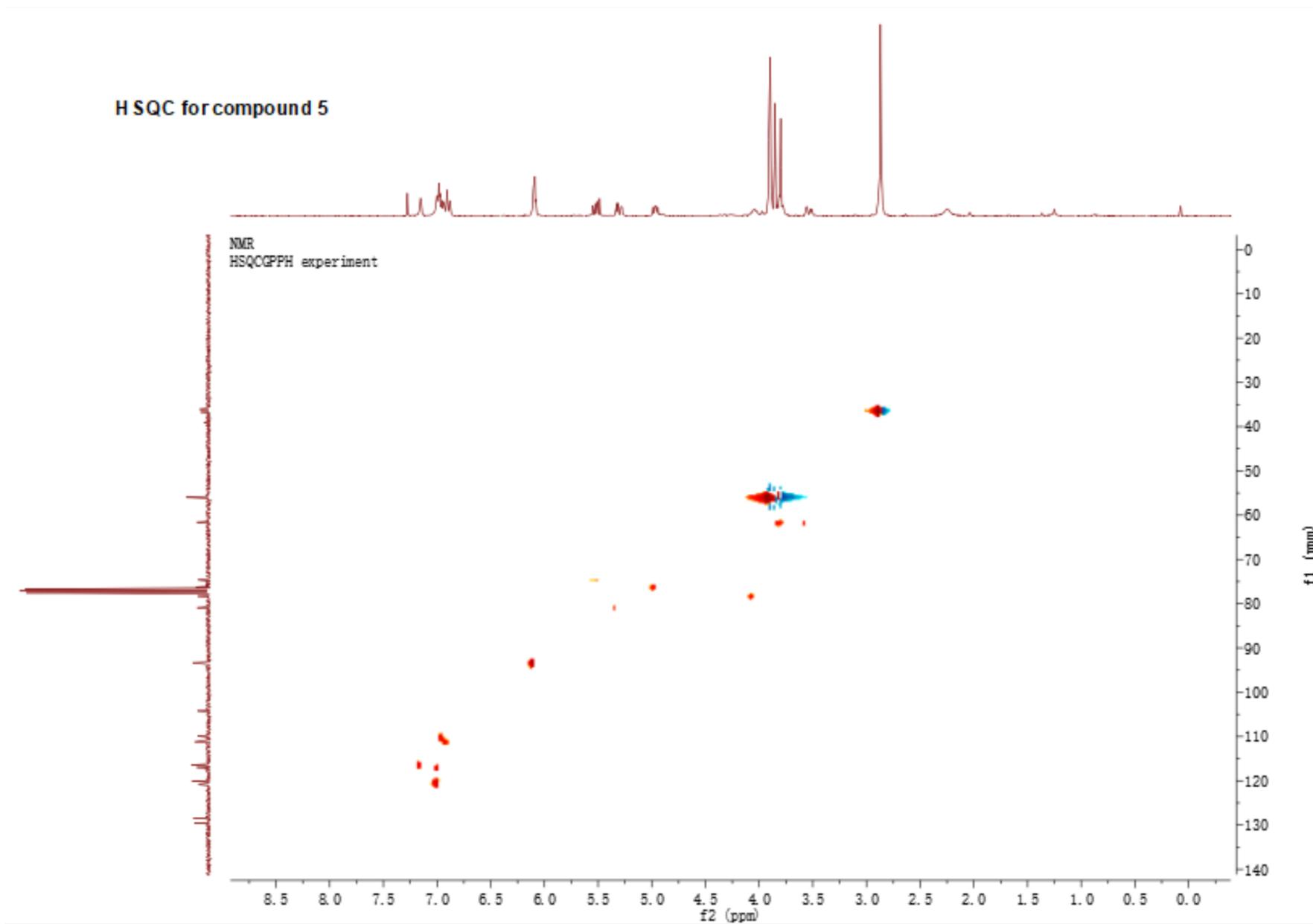


Figure S4: HSQC spectrum of **5** in  $\text{CDCl}_3$

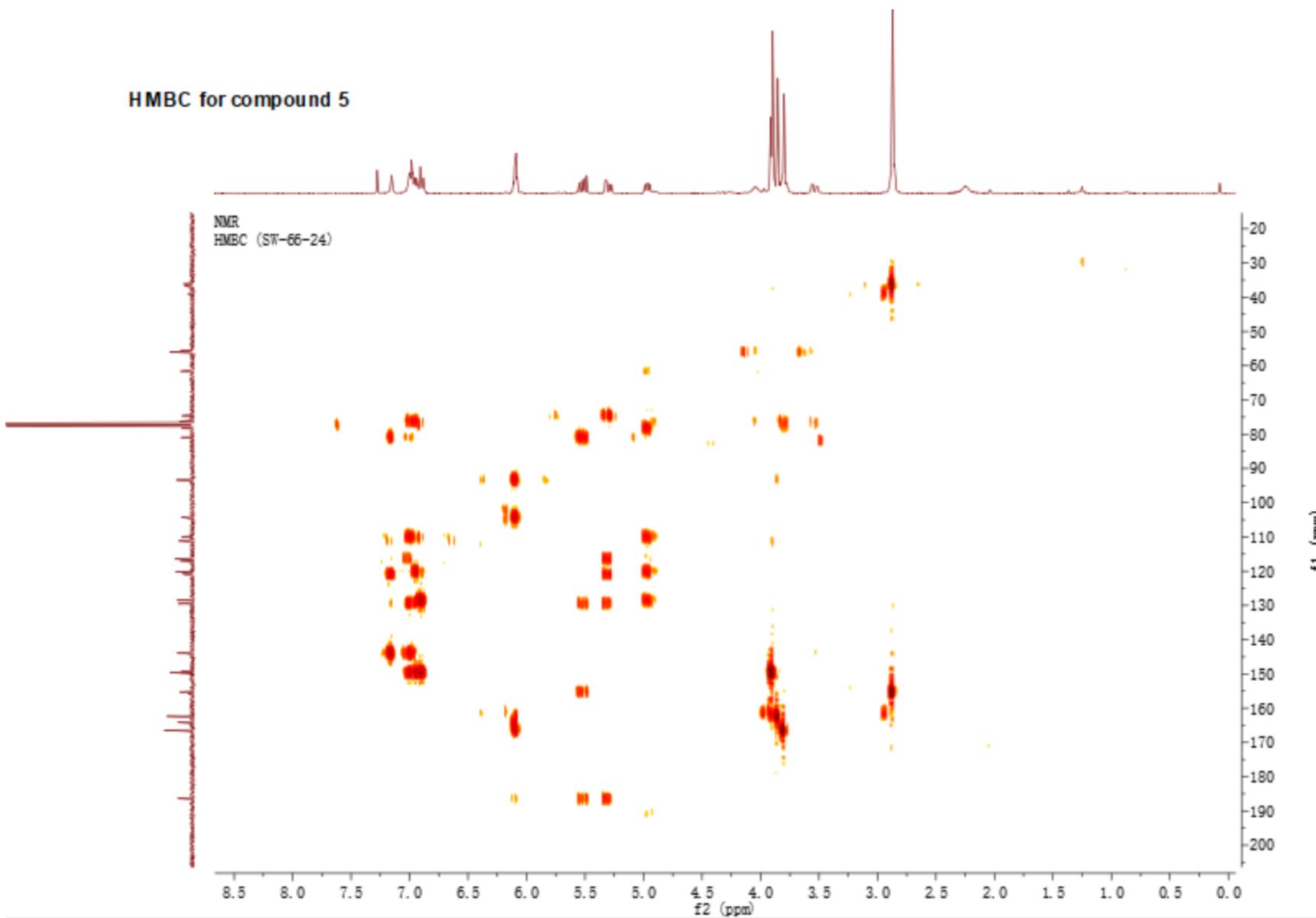


Figure S5: HMBC spectrum of **5** in  $\text{CDCl}_3$

comps	Mol. Formula	Exact Mass	M+H	Observed	delta	ppm
QGC-68-136	C31H33NO11	595.2054	596.2132	596.2128	-0.0004	-0.69

qgc-68-136 #2178-3544 RT: 12.82-19.90 AV: 1367 NL: 3.63E8  
T: FTMS + c NSI Full ms [150.0000-1000.0000]

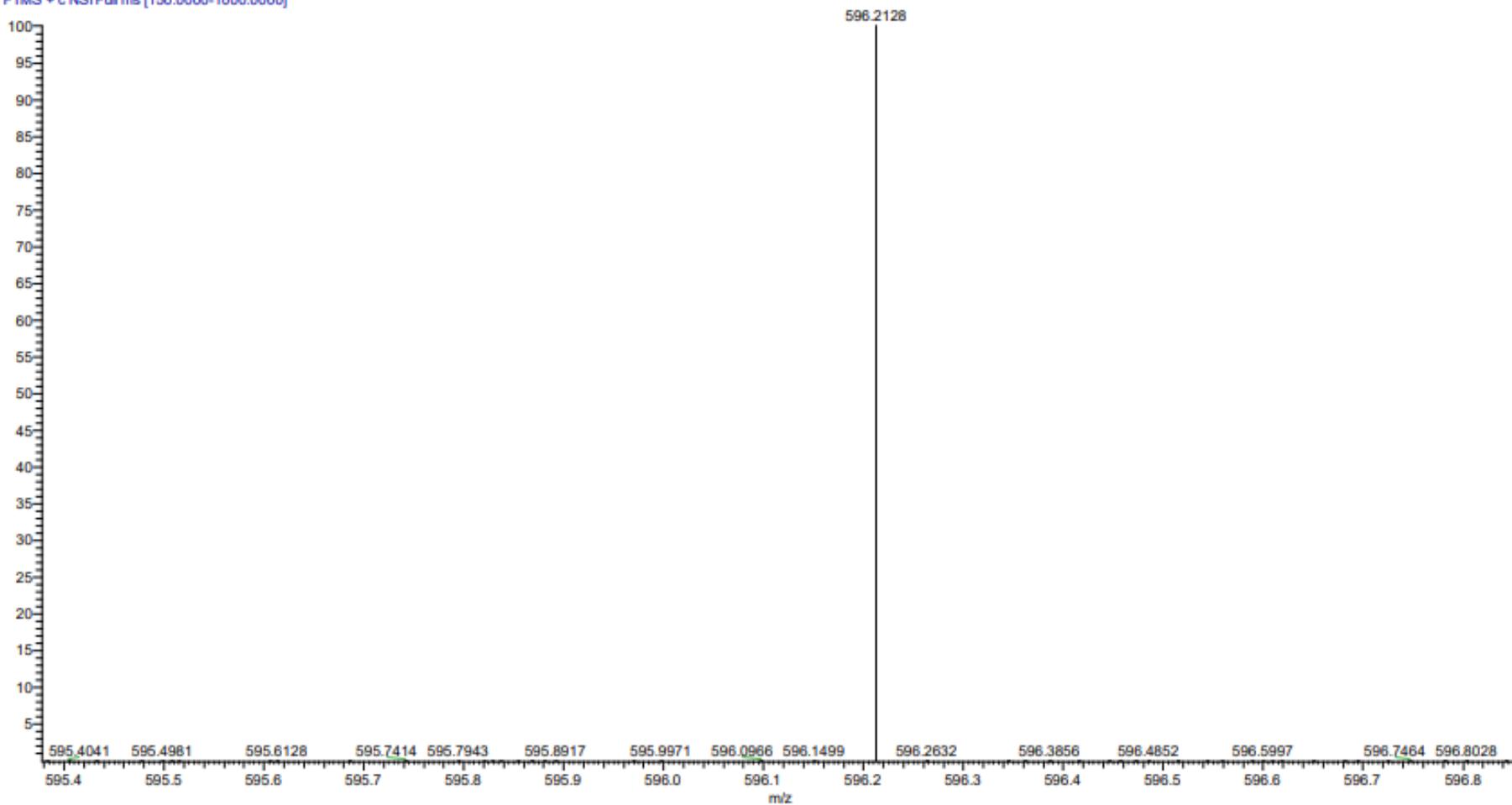
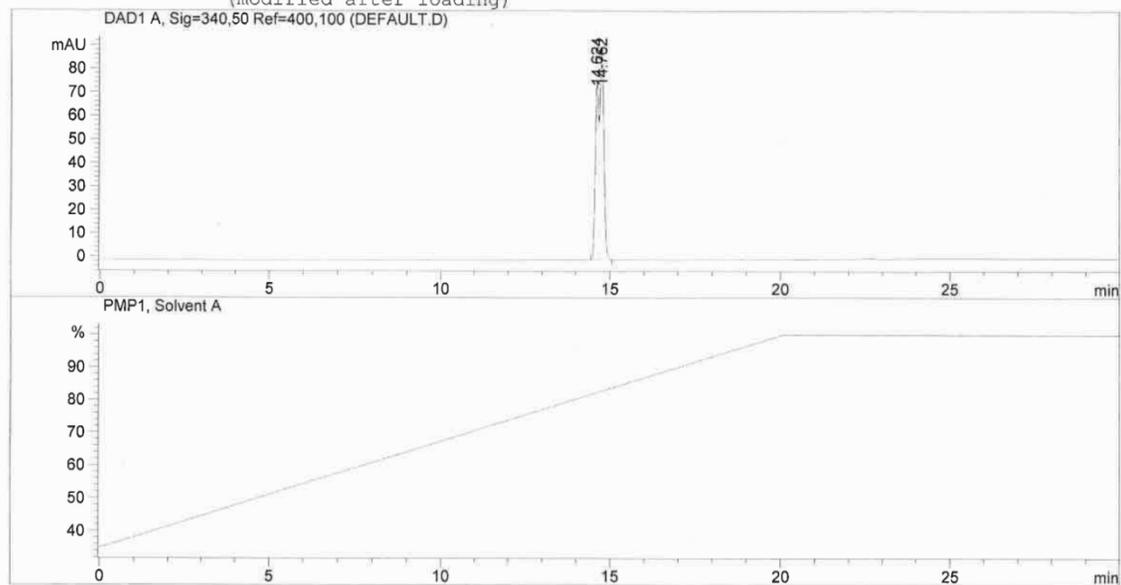


Figure S6: High resolution mass spectrum of 5

```

=====
Injection Date   : 9/17/2021 4:49:32 PM
Sample Name     : SW-66-24                Location  : Vial 1
Acq. Operator   :
Method          : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed    : 9/17/2021 4:42:01 PM
                  (modified after loading)
=====

```



```

=====
                          Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000

```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.624	BV	0.1086	539.64001	76.22746	42.6786
2	14.762	VB	0.1216	724.78864	90.29533	57.3214

```
Totals :                      1264.42865  166.52280
```

Results obtained with enhanced integrator!

```

=====
*** End of Report ***
=====

```

Figure S7: HPLC chromatogram of 5

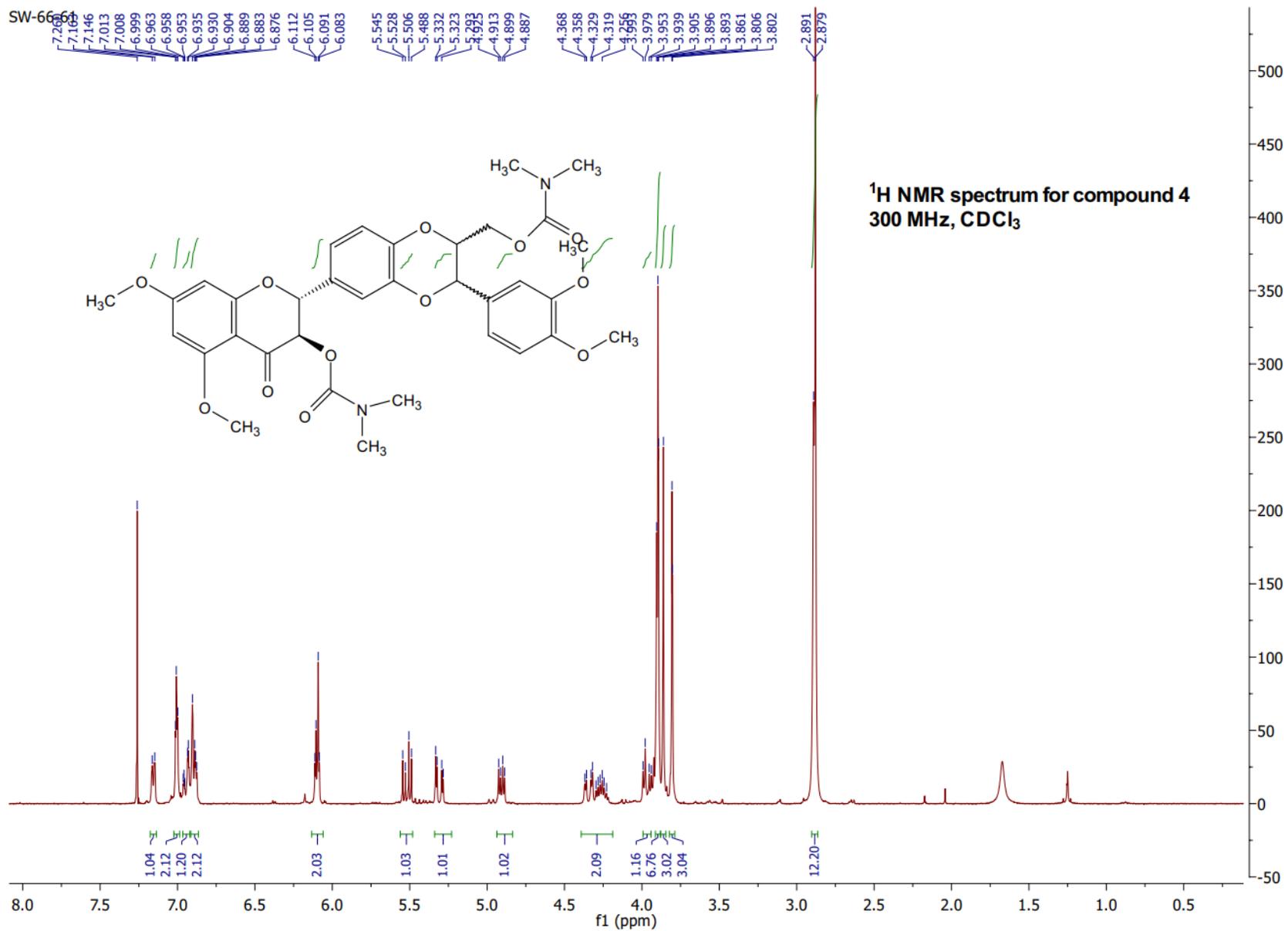


Figure S8: <sup>1</sup>H NMR spectrum of 4 in CDCl<sub>3</sub>

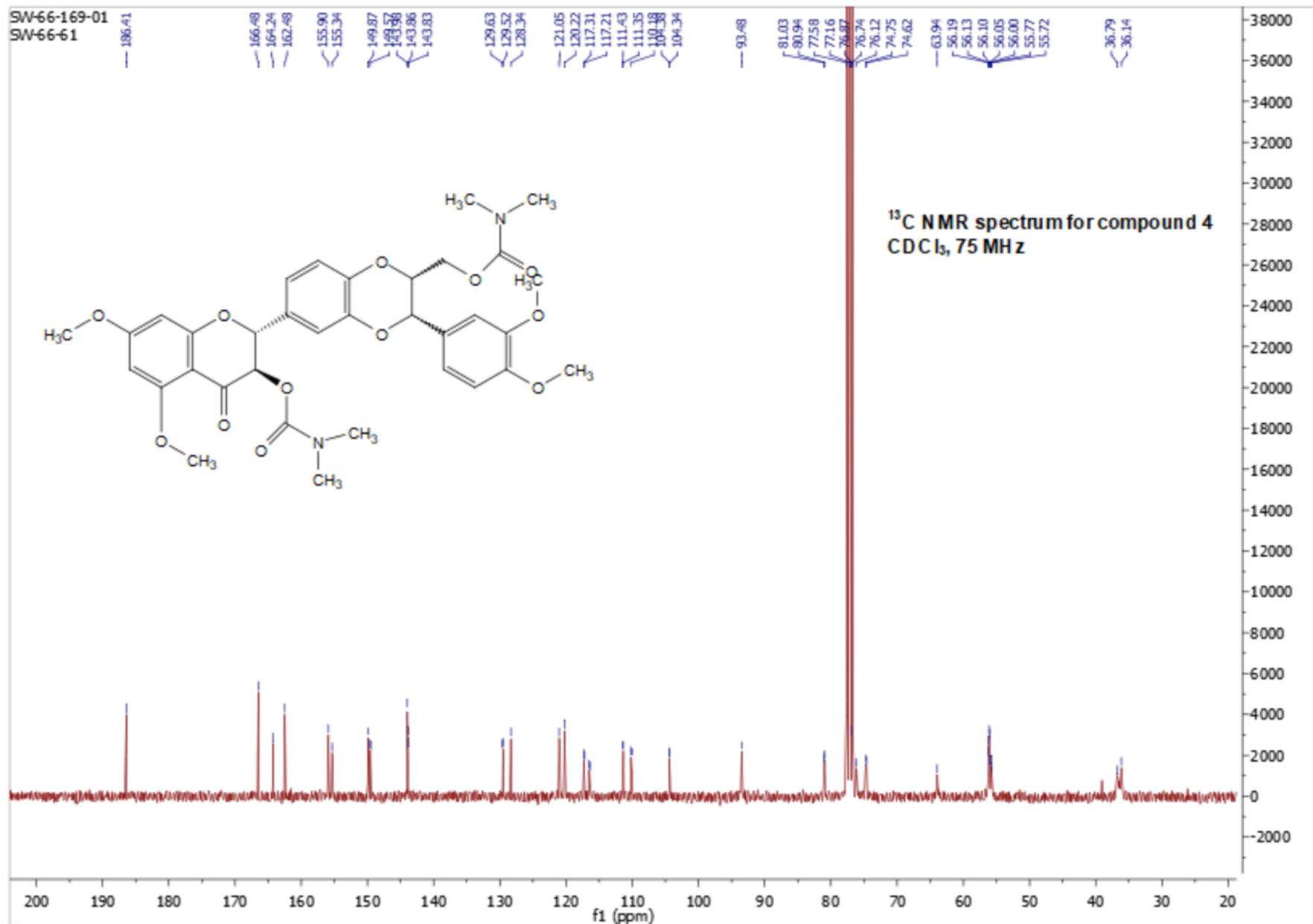
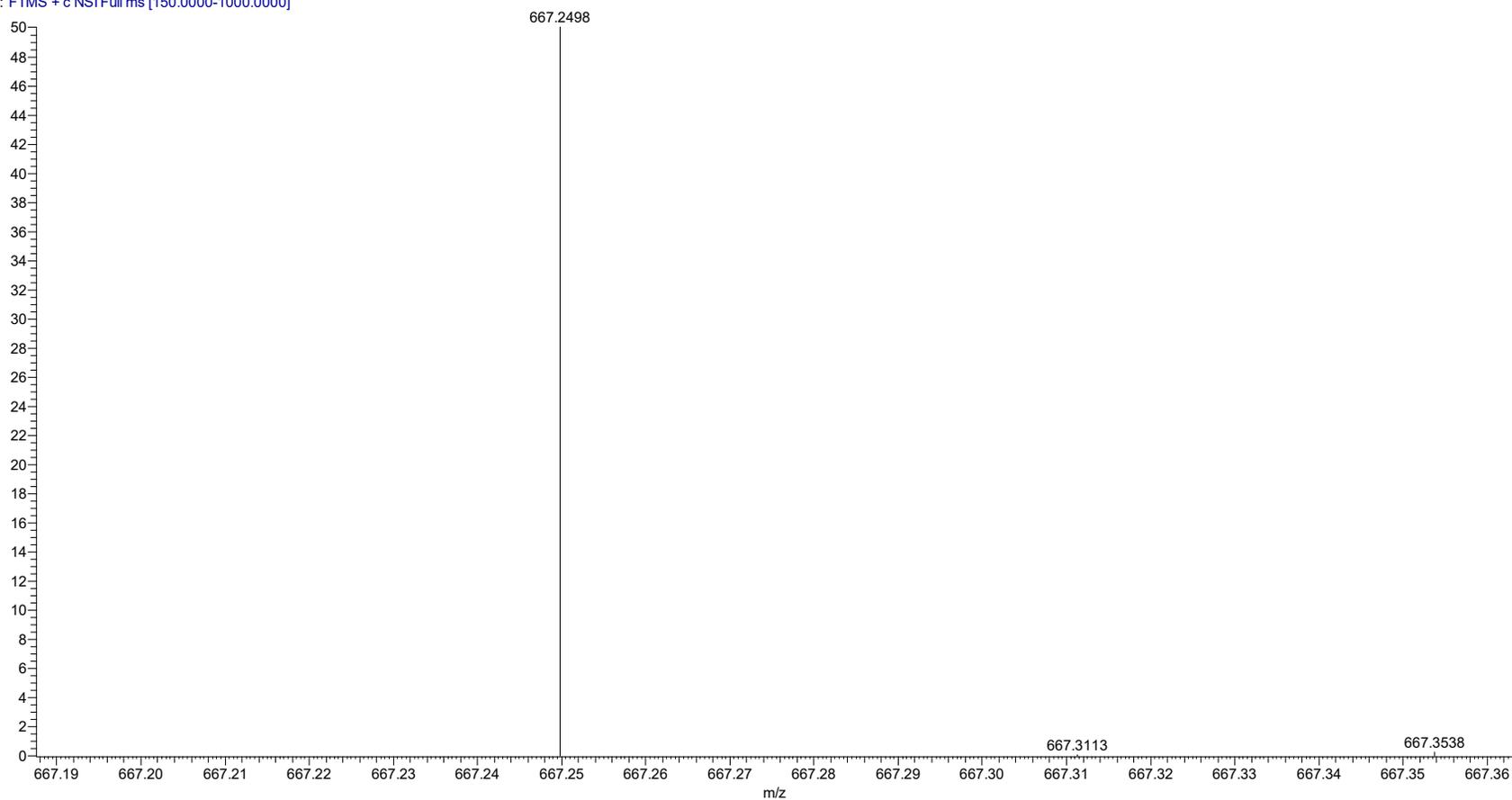


Figure S9: <sup>13</sup>C NMR spectrum of 4 in CDCl<sub>3</sub>

compds	Mol. Formula	Exact Mass	M+H	Observed	delta	ppm
SW-66-61	C <sub>34</sub> H <sub>38</sub> N <sub>2</sub> O <sub>12</sub>	666.2425	667.2503	<b>667.2498</b>	-0.0005	-0.81

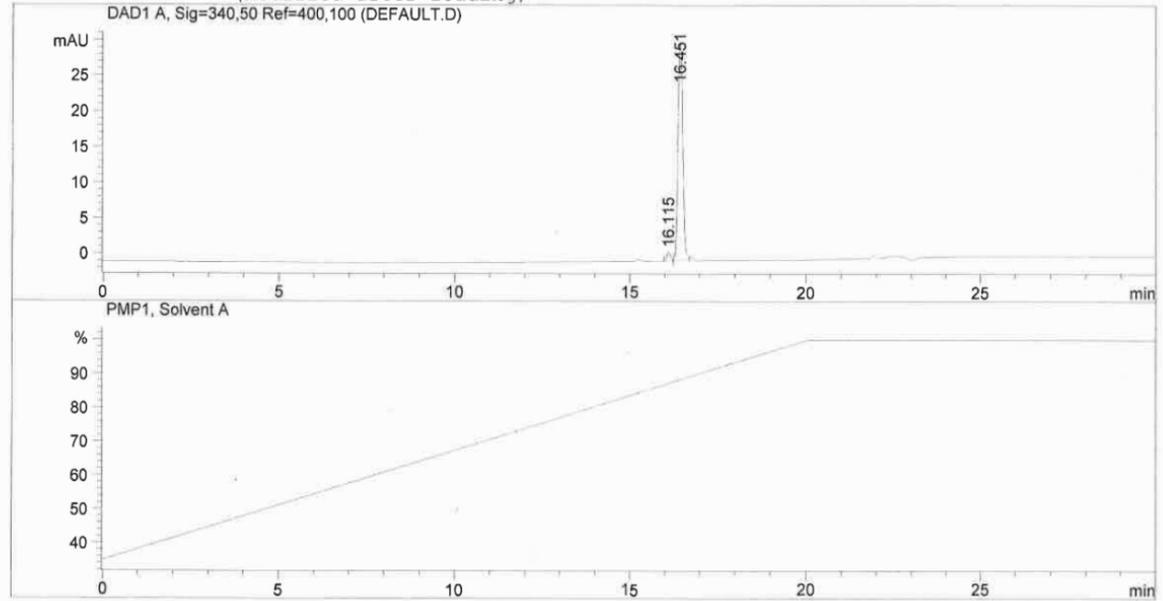
SW-66-61 #2203-2839 RT: 11.59-14.92 AV: 637 NL: 2.36E8  
T: FTMS + c NSI Full ms [150.0000-1000.0000]



**Figure S10:** High resolution mass spectrum of **4**

```

=====
Injection Date   : 9/16/2021 2:21:42 PM
Sample Name     : SW-66-61                Location  : Vial 1
Acq. Operator   :
Method          : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed    : 9/16/2021 2:14:33 PM
                  (modified after loading)
    
```



Area Percent Report

```

=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
    
```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.115	PV	0.1108	9.05094	1.27589	3.0535
2	16.451	VB	0.1501	287.36374	30.44066	96.9465

Totals :                    296.41468    31.71655

Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*

Figure S11: HPLC chromatogram of 4

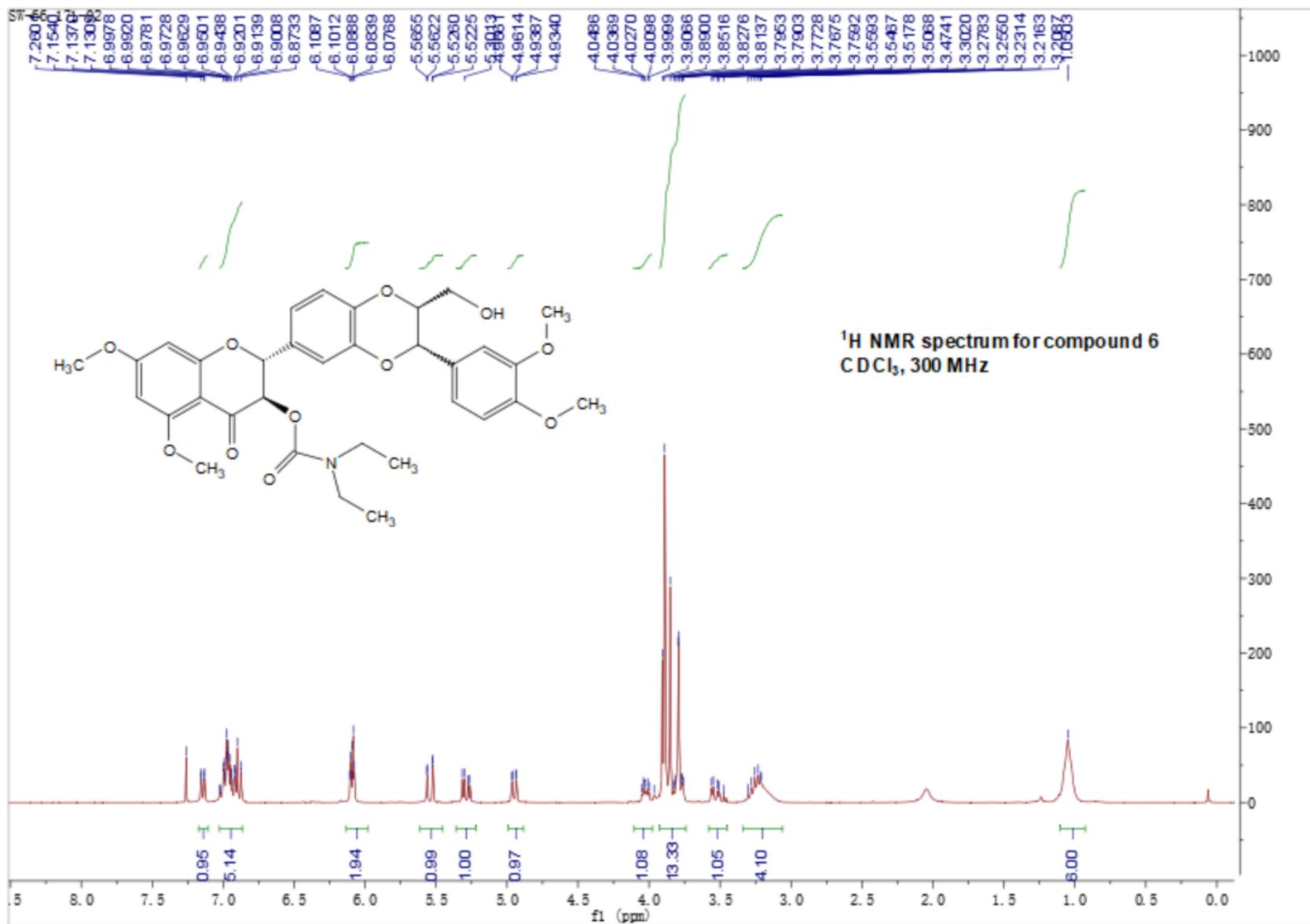


Figure S12: <sup>1</sup>H NMR spectrum of 6 in CDCl<sub>3</sub>

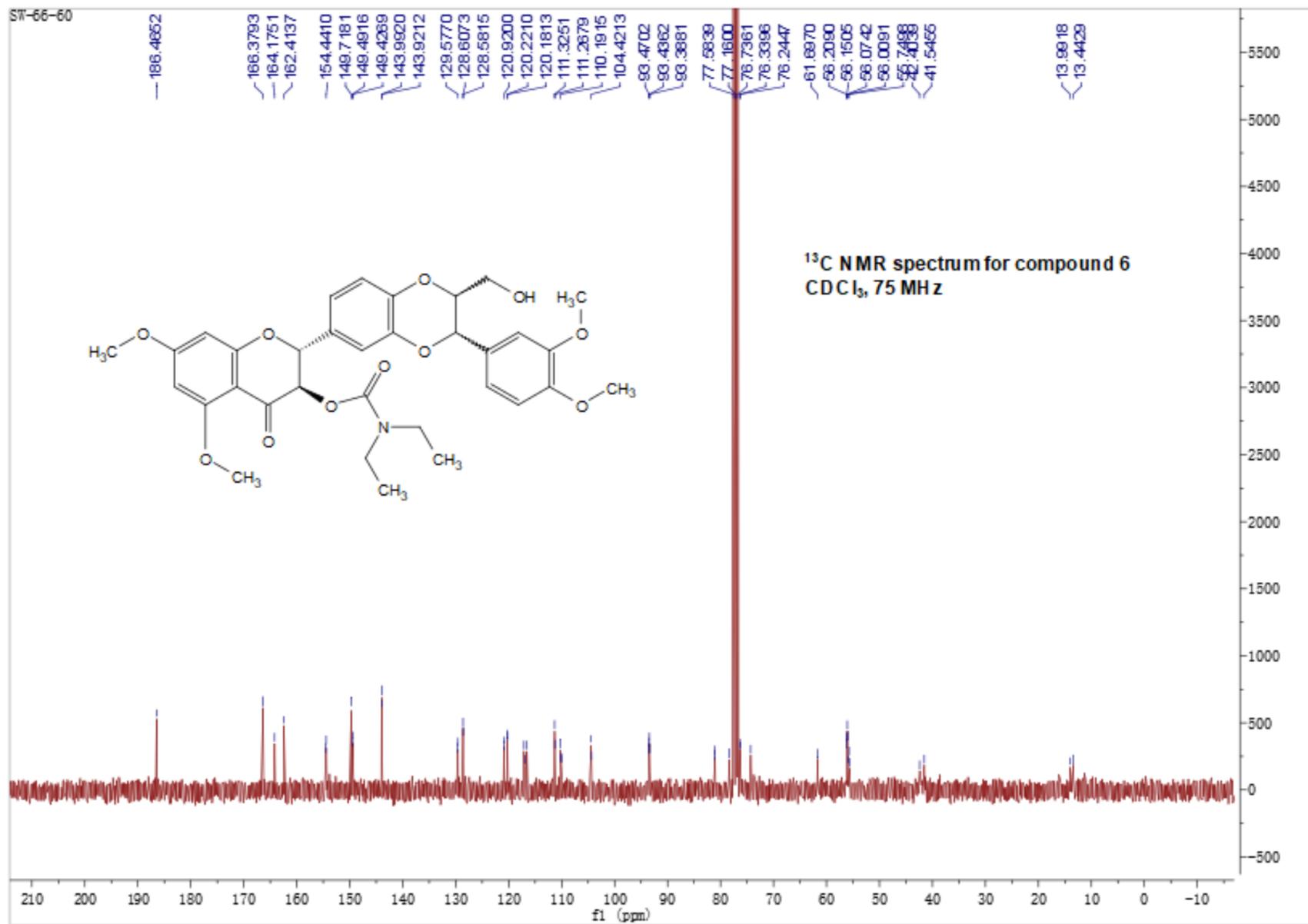
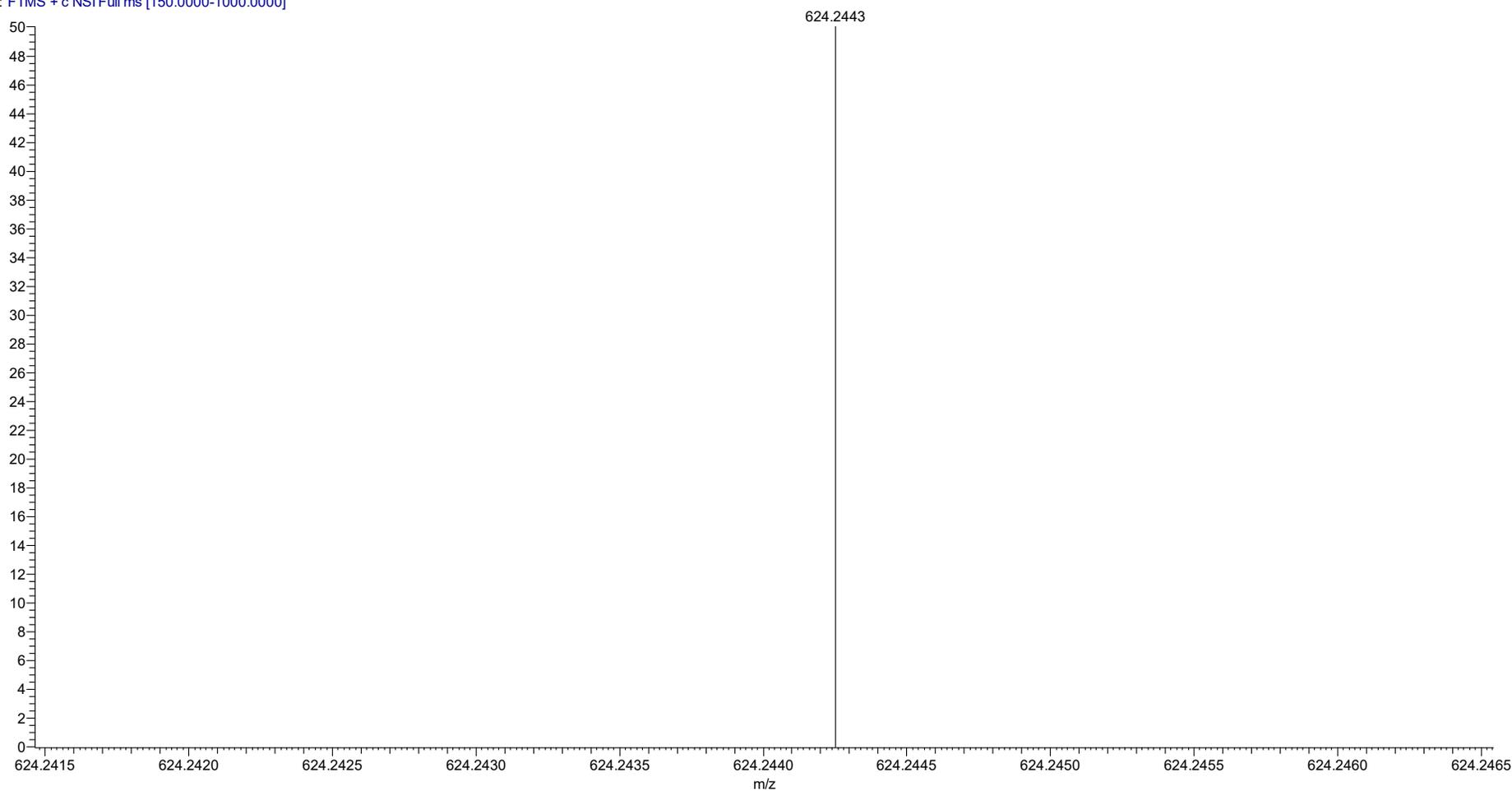


Figure S13: <sup>13</sup>C NMR spectrum of 6 in CDCl<sub>3</sub>

compds	Mol. Formula	Exact Mass	M+H	Observed	delta	ppm
SW-66-60	C33H37NO11	623.2367	624.2445	<b>624.2443</b>	-0.0002	-0.34

SW-66-60 #2101-2856 RT: 11.05-15.01 AV: 756 NL: 2.46E8  
T: FTMS + c NSI Full ms [150.0000-1000.0000]

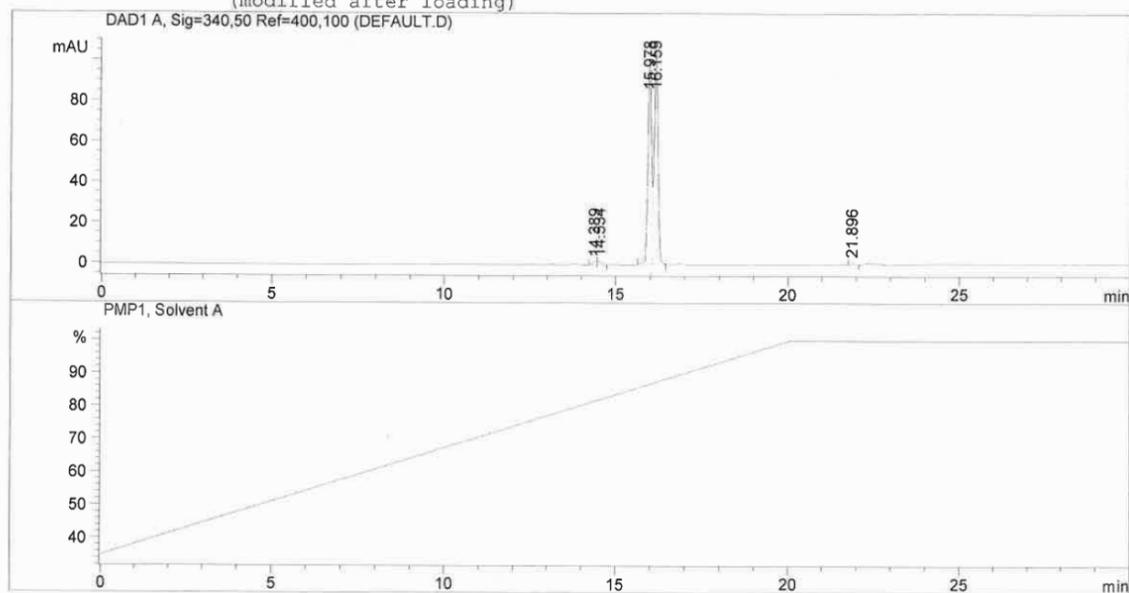


**Figure S14:** High resolution mass spectrum of **6**

```

=====
Injection Date   : 9/16/2021 3:34:17 PM
Sample Name     : SW-66-60
Acq. Operator   :                               Location : Vial 1
Method          : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed    : 9/16/2021 3:26:08 PM
                  (modified after loading)
=====

```



```

=====
Area Percent Report
=====

```

```

Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000

```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.389	PV	0.1156	12.35465	1.64579	0.7808
2	14.534	VB	0.1193	13.75756	1.72044	0.8695
3	15.978	BV	0.1128	744.94830	100.14996	47.0812
4	16.159	VB	0.1149	802.74286	105.38542	50.7339
5	21.896	BP	0.0996	8.45884	1.34011	0.5346

```
Totals :                1582.26220  210.24171
```

```
Results obtained with enhanced integrator!
```

```
*** End of Report ***
```

Figure S15: HPLC chromatogram of 6



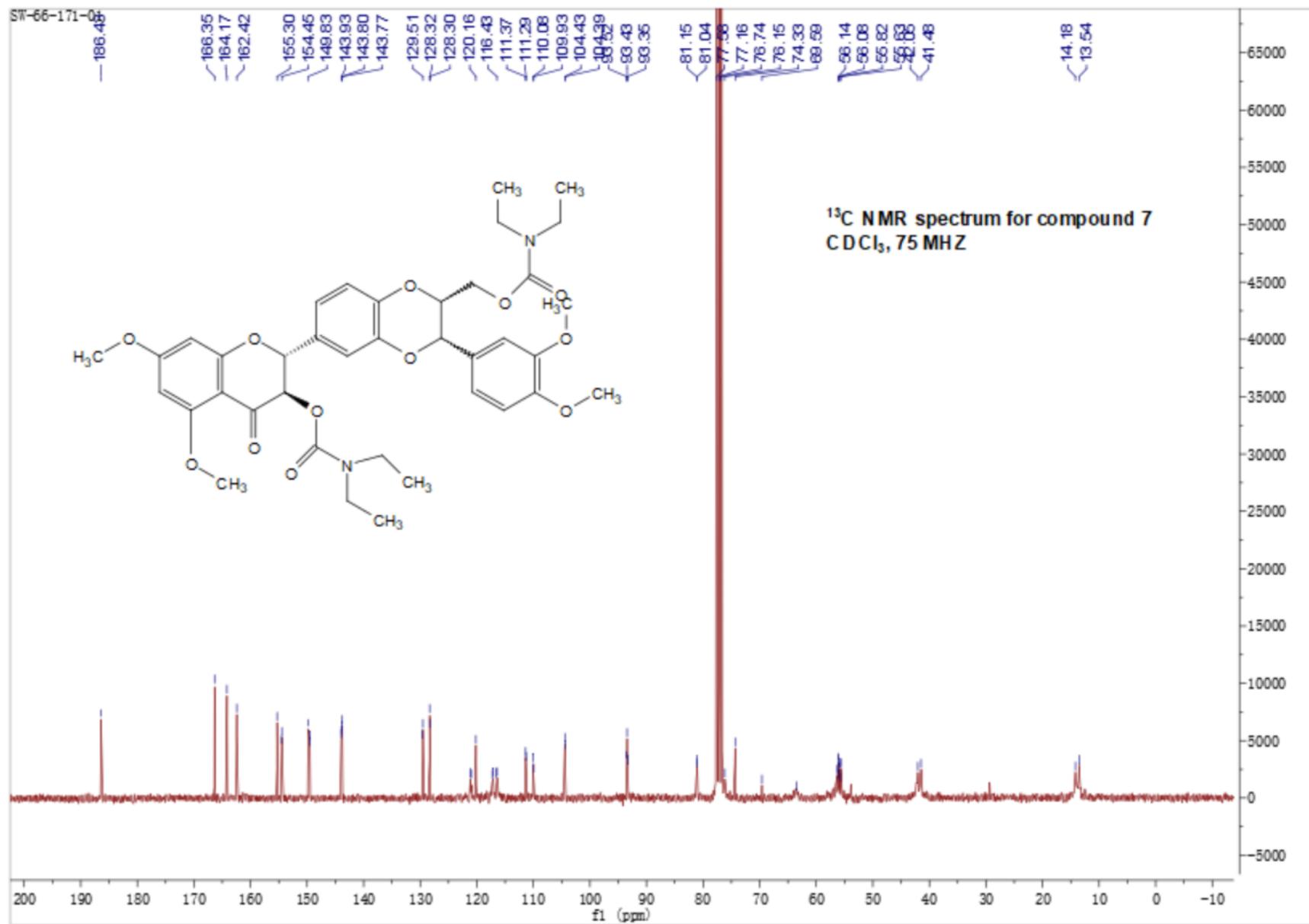


Figure S17: <sup>13</sup>C NMR spectrum of 7 in CDCl<sub>3</sub>

Sample Name	Mol Formula	MW	M+H	observed	delta	ppm
SW-66-171-01	C <sub>38</sub> H <sub>46</sub> N <sub>2</sub> O <sub>12</sub>	722.3051	723.3129	723.3129	0.0000	0.00

SW-66-171-01 #2474-2537 RT: 13.37-13.69 AV: 64 NL: 1.28E8  
T: FTMS + c NSI Full ms [300.0000-1000.0000]

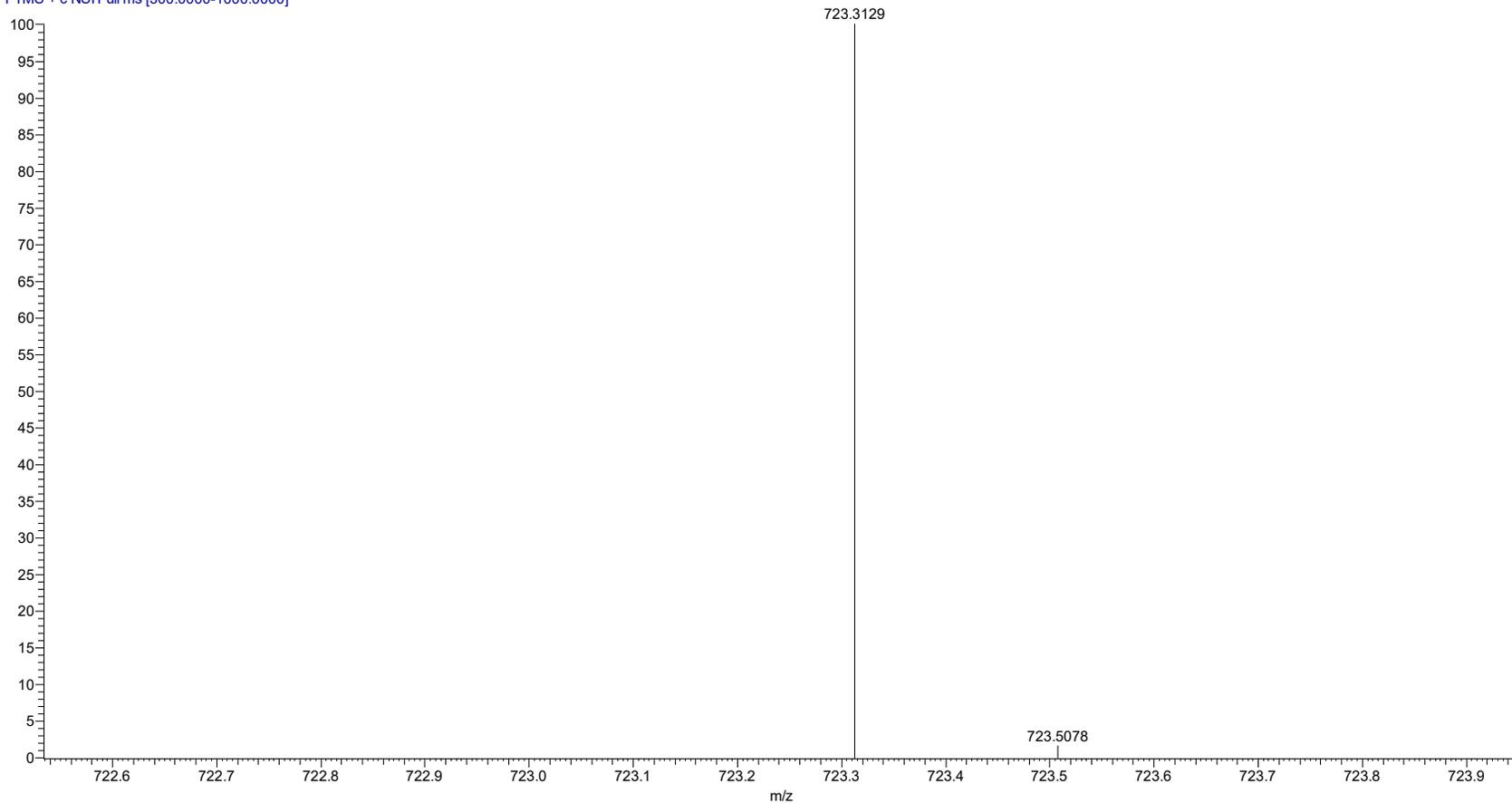
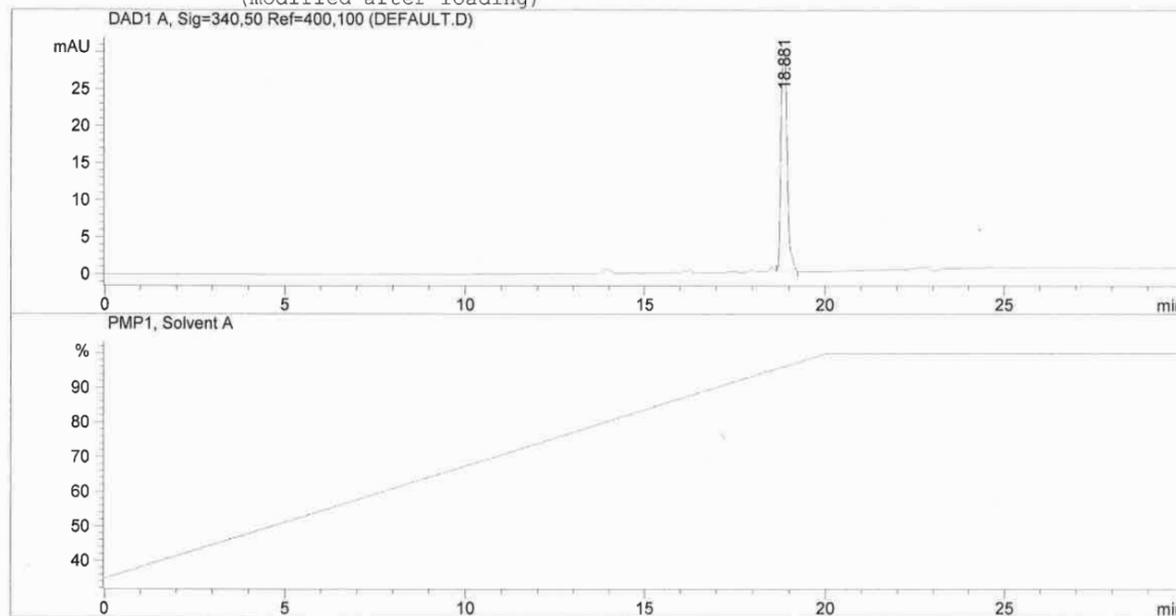


Figure S18: High resolution mass spectrum of 7

```

=====
Injection Date : 9/20/2021 2:44:39 PM
Sample Name   : SW-66-171                Location : Vial 1
Acq. Operator :
Method       : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed  : 9/20/2021 1:10:34 PM
                (modified after loading)
    
```



=====  
 Area Percent Report  
 =====

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
    
```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.881	VB	0.1887	352.03210	30.04979	100.0000

Totals :                                    352.03210    30.04979

Results obtained with enhanced integrator!

=====  
 \*\*\* End of Report \*\*\*

Figure S19: HPLC chromatogram of 7

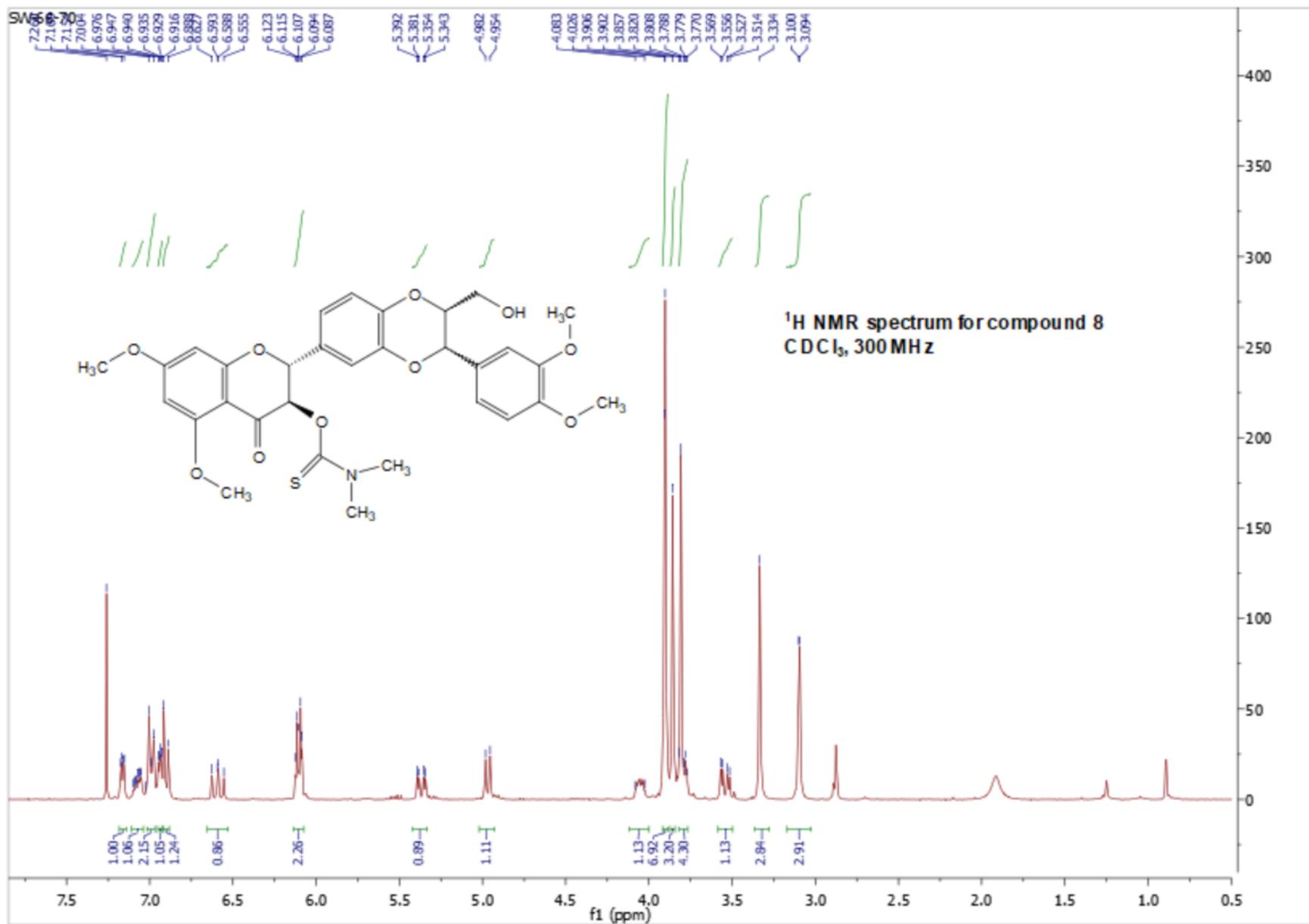


Figure S20: <sup>1</sup>H NMR spectrum of **8** in CDCl<sub>3</sub>

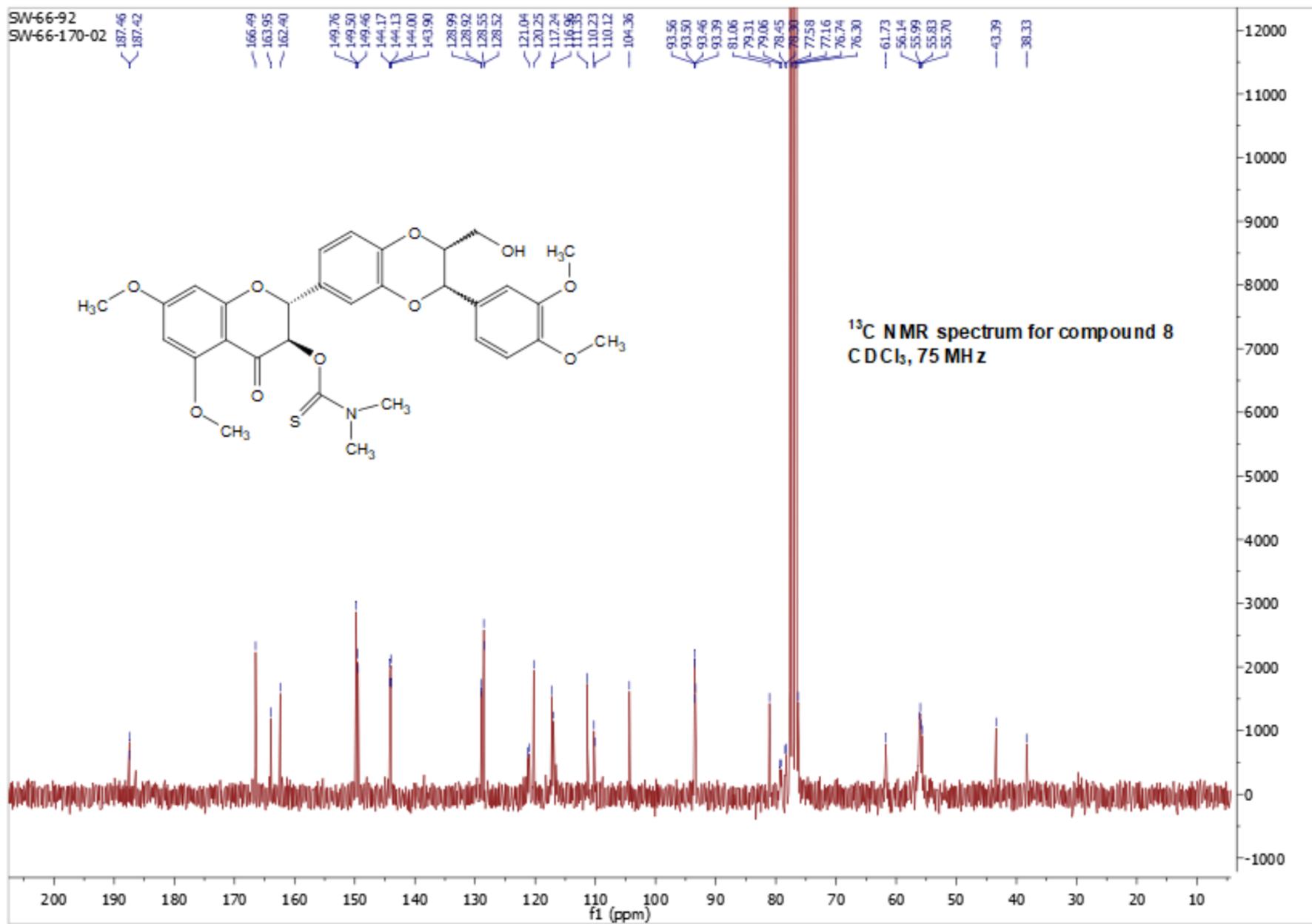


Figure S21: <sup>13</sup>C NMR spectrum of **8** in CDCl<sub>3</sub>

compds	Mol. Formula	Exact Mass	M+H	Observed	delta	ppm
SW-66-70	C31H33NO10S	611.1826	612.1904	<b>612.1920</b>	0.0016	2.68

SW-66-70 #4861-4923 RT: 26.28-26.61 AV: 63 NL: 3.26E8  
T: FTMS + c NSI Full ms [150.0000-1000.0000]

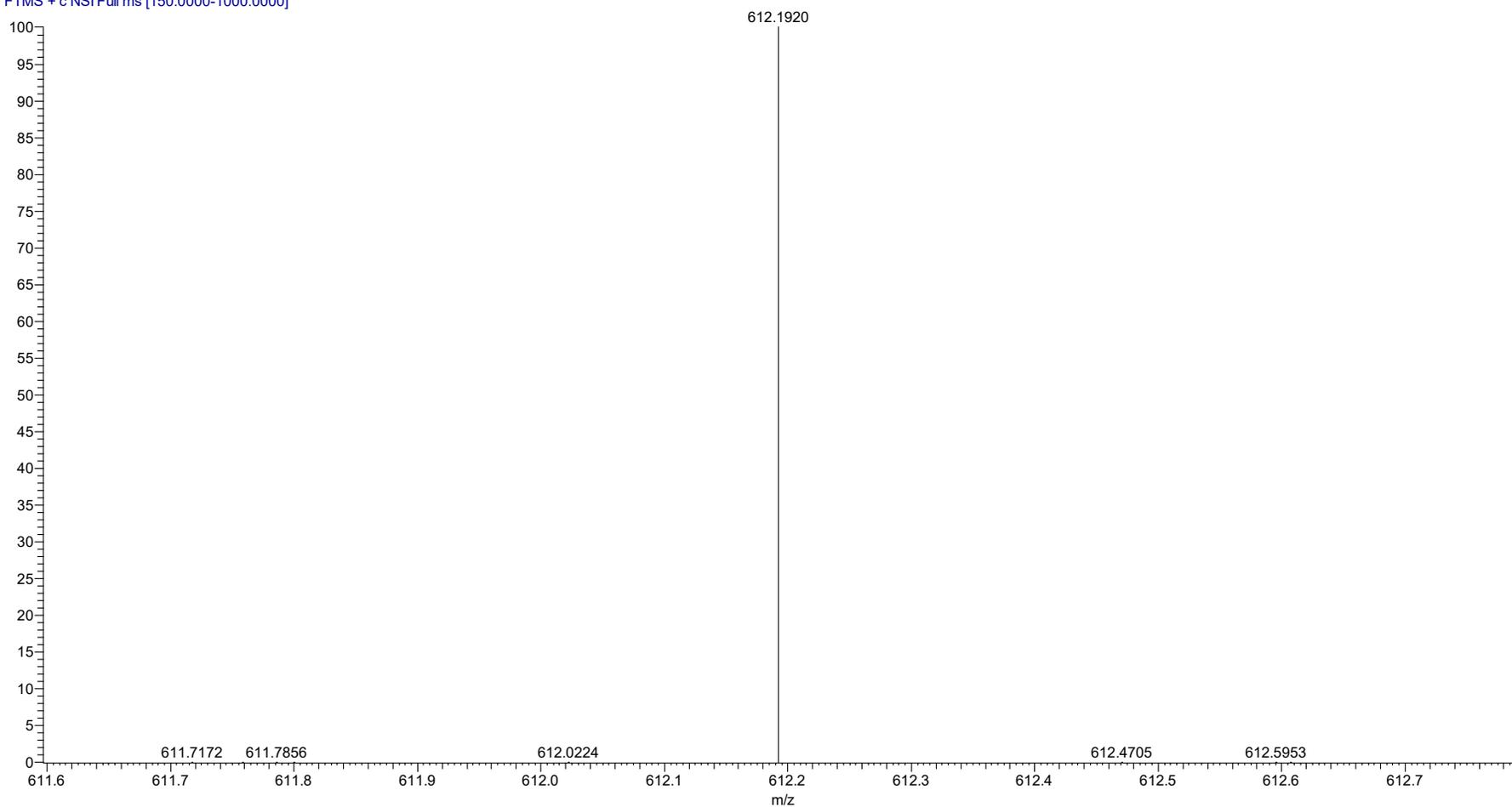
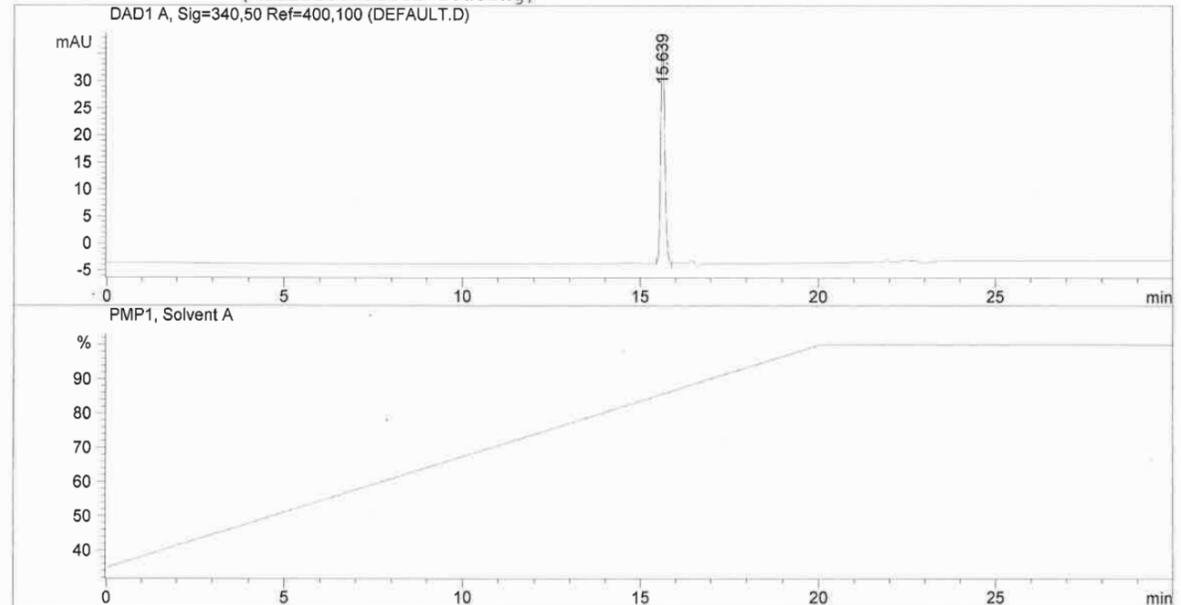


Figure S22: High resolution mass spectrum of **8**

```

=====
Injection Date   : 9/17/2021 10:18:16 AM
Sample Name     : SW-66-70                Location  : Vial 1
Acq. Operator   :
Method          : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed    : 9/17/2021 10:10:55 AM
                  (modified after loading)
=====
    
```



```

=====
                          Area Percent Report
=====
Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak RetTime Type Width Area Height Area
# [min] [min] [min] [mAU*s] [mAU] [%]
-----|-----|-----|-----|-----|-----|
1 15.639 BB 0.1241 326.80460 40.52058 100.0000

Totals :                      326.80460 40.52058

Results obtained with enhanced integrator!
=====
    
```

Figure S23: HPLC chromatogram of 8

\*\*\* End of Report \*\*\*

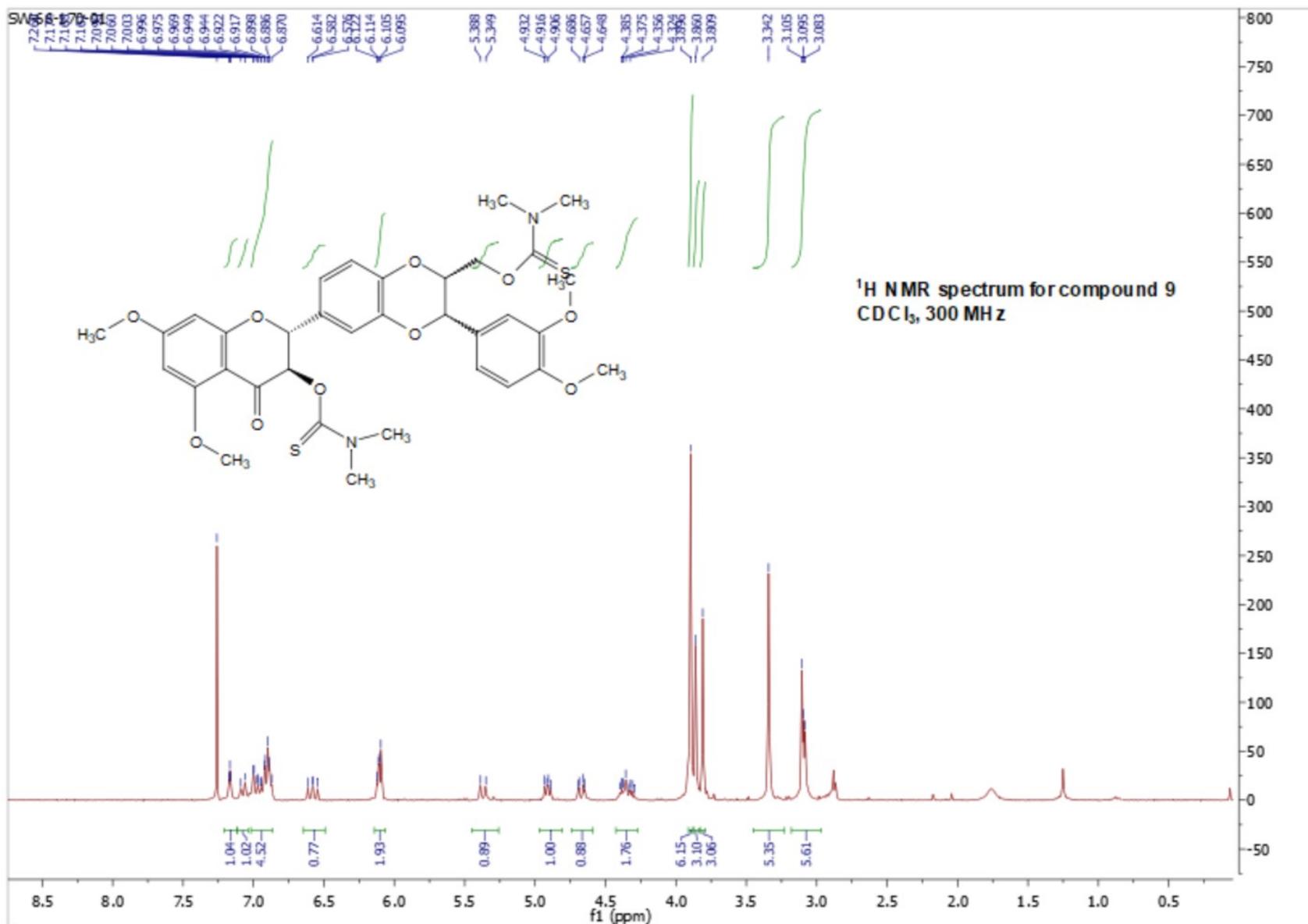


Figure S24: <sup>1</sup>H NMR spectrum of **9** in CDCl<sub>3</sub>

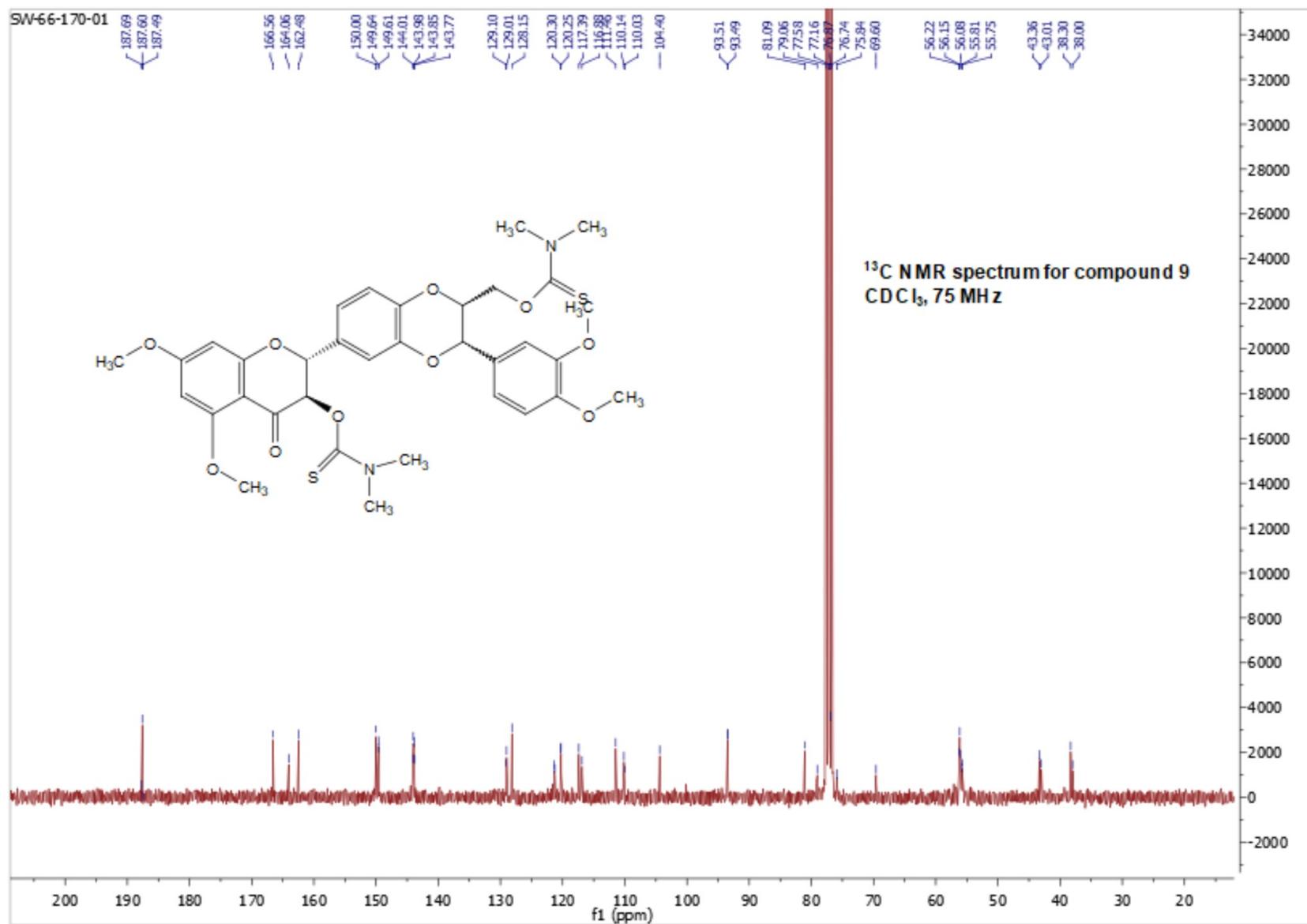


Figure S25: <sup>13</sup>C NMR spectrum of **9** in CDCl<sub>3</sub>

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
SW-66-170-01	C34H38N2O10S2	698.1968	699.2046	699.2050	0.0004	0.51

SW-66-170-01 #2436-2464 RT: 13.17-13.32 AV: 29 NL: 2.05E8  
T: FTMS + c NSI Full ms [300.0000-1000.0000]

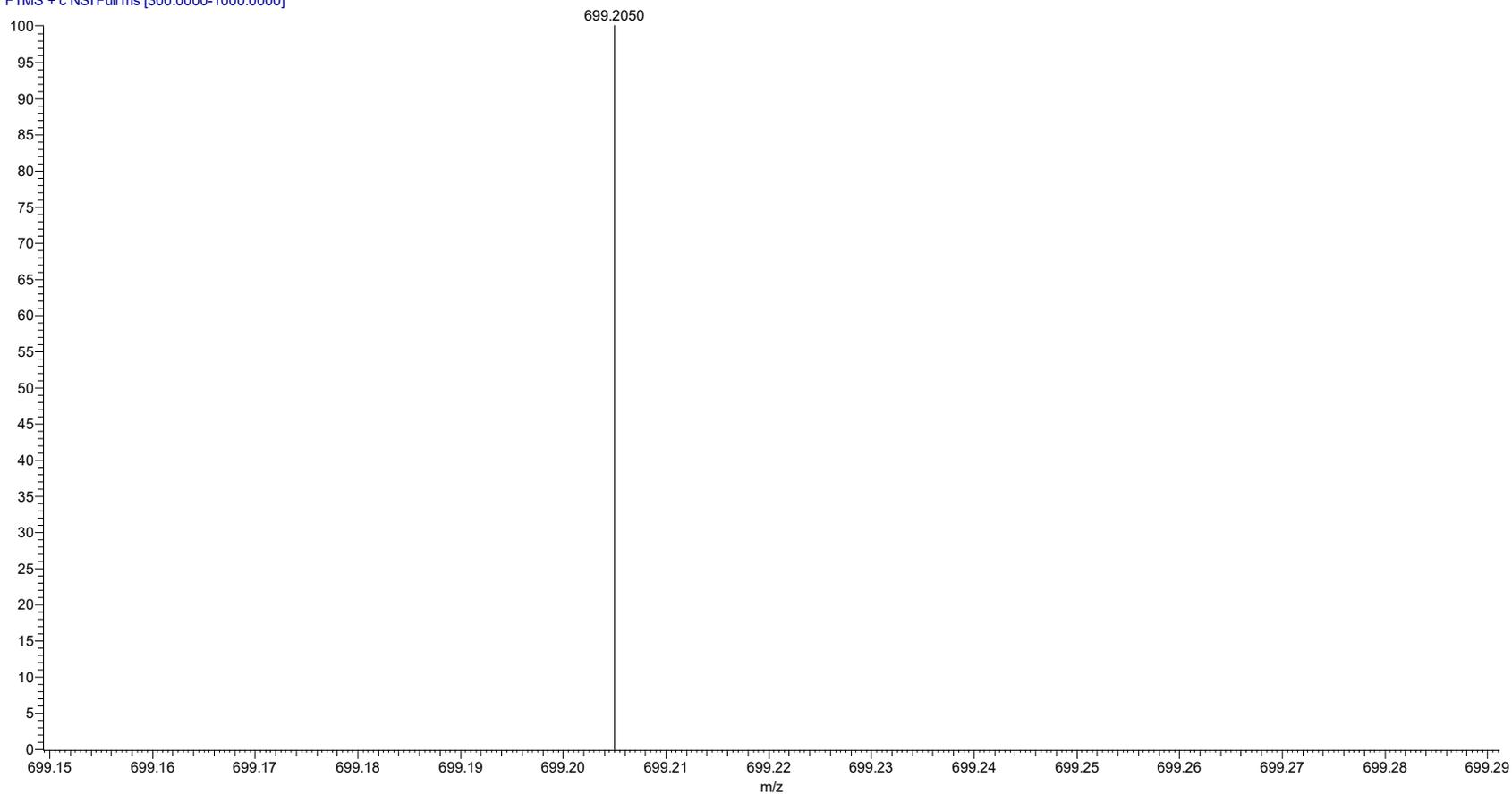
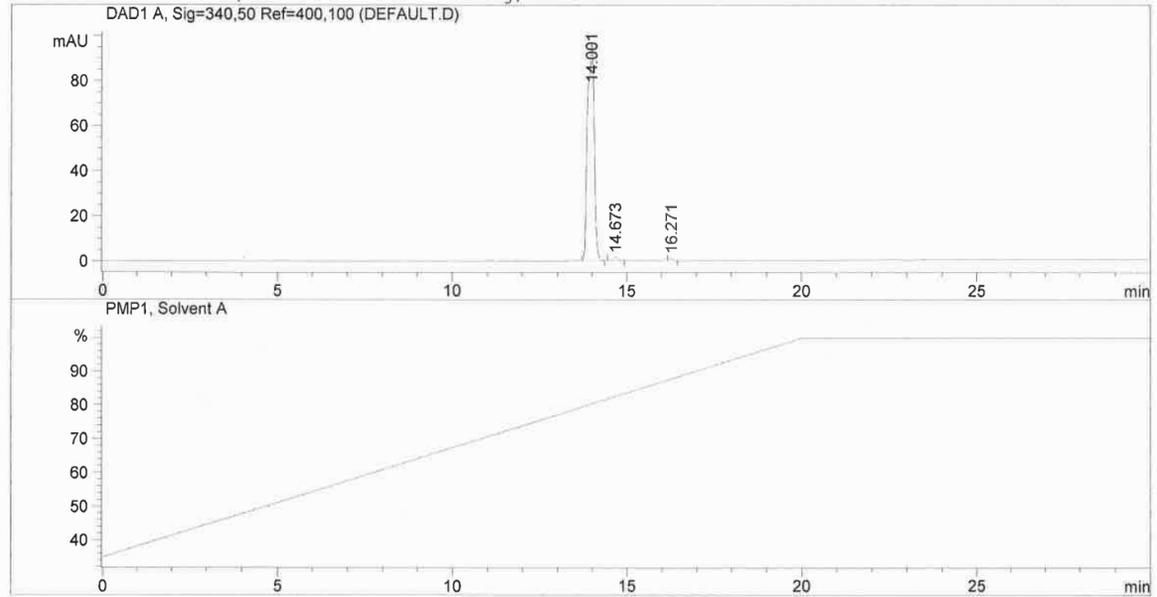


Figure S26: High resolution mass spectrum of 9

```

=====
Injection Date : 9/18/2021 11:40:15 AM
Sample Name    : SW-66-170                Location : Vial 1
Acq. Operator  :
Method         : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed   : 9/18/2021 9:26:55 AM
                (modified after loading)
    
```



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
    
```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.001	BB	0.1829	1281.49658	96.52377	97.8661
2	14.673	BP	0.1679	19.23740	1.67563	1.4691
3	16.271	VP	0.1173	8.70405	1.13770	0.6647

Totals : 1309.43803 99.33710

Results obtained with enhanced integrator!

\*\*\* End of Report \*\*\*

Figure S27: HPLC chromatogram of 9

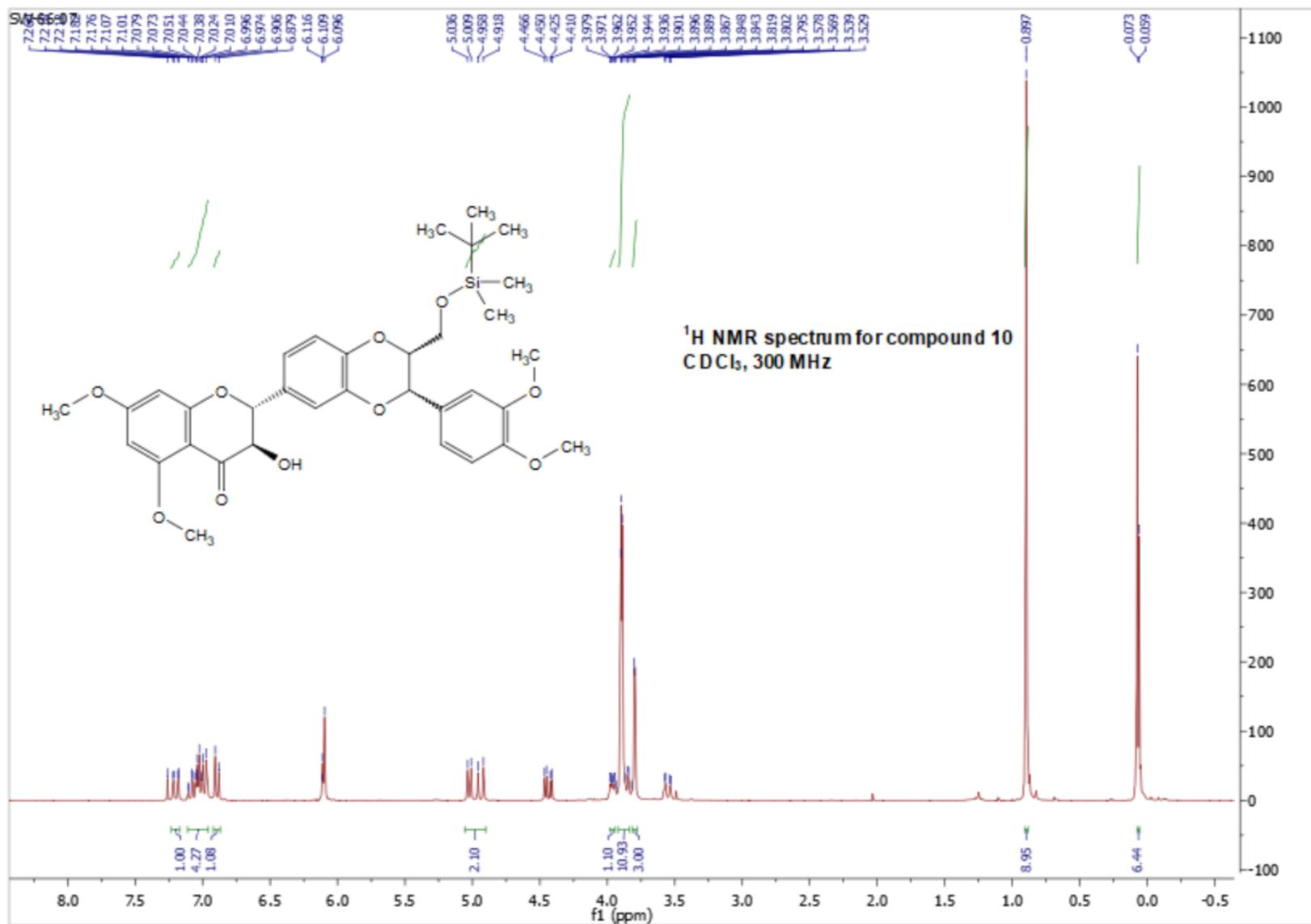


Figure S28: <sup>1</sup>H NMR spectrum of 10 in CDCl<sub>3</sub>

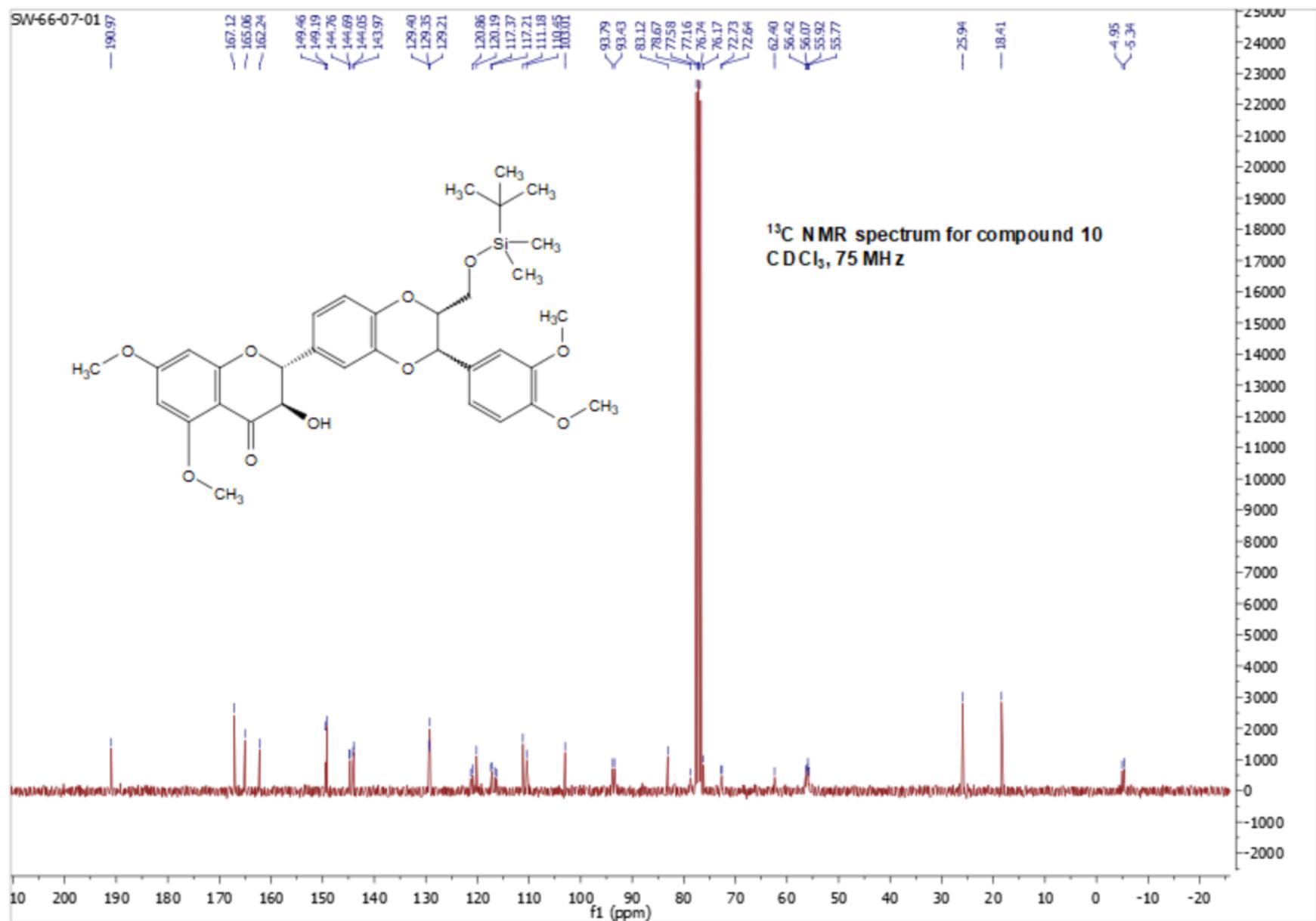
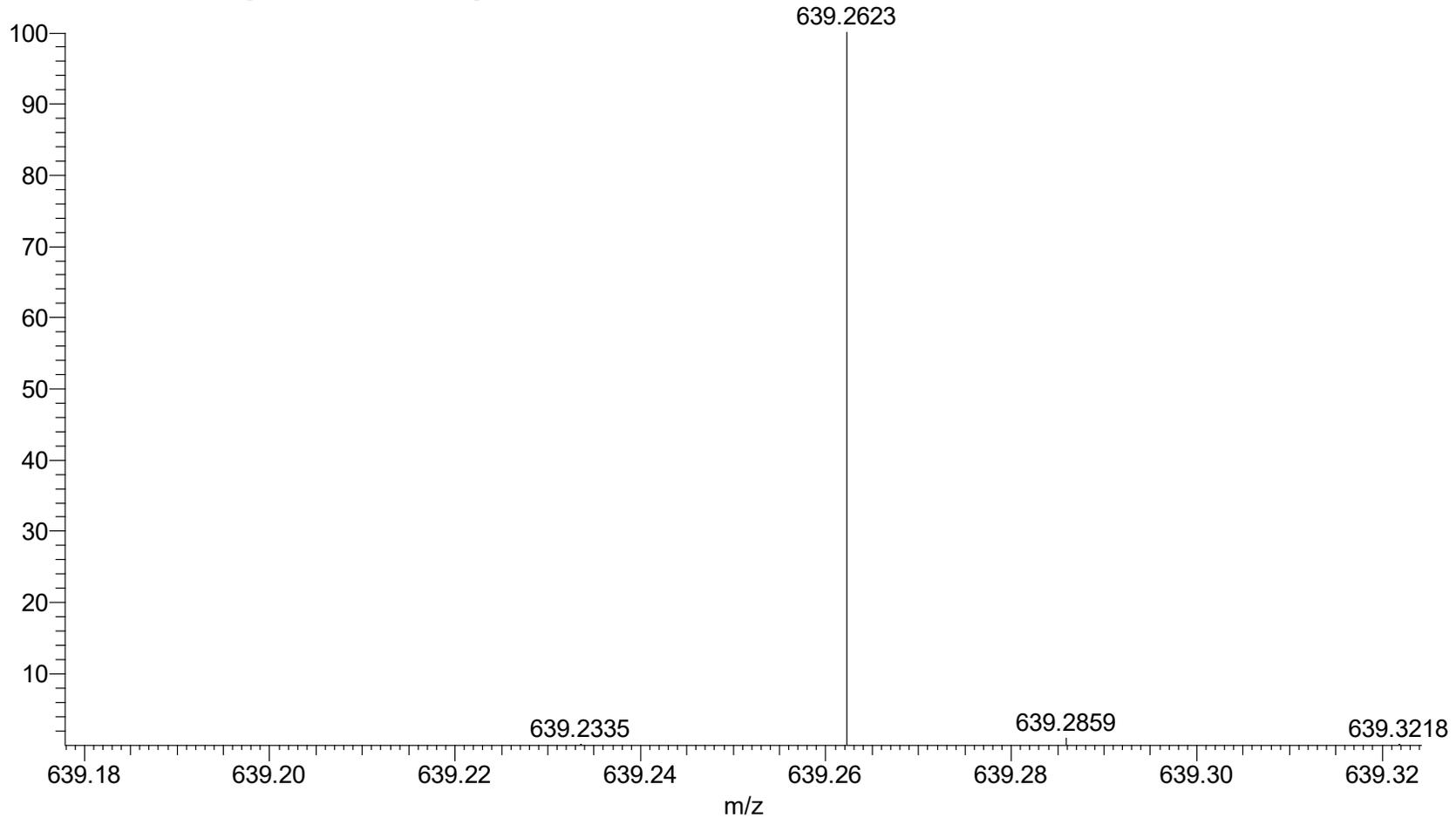


Figure S29: <sup>13</sup>C NMR spectrum of 10 in CDCl<sub>3</sub>

compds	Mol. Formula	Exact Mass	M+H	Observed	delta	ppm
SW-66-07	C <sub>24</sub> H <sub>42</sub> O <sub>10</sub> Si	638.2548	639.2626	<b>639.2623</b>	<b>-0.0003</b>	<b>-0.44</b>

SW-66-07 #3249-3816 RT: 17.93-20.88 AV: 568 NL: 9.92E6  
T: FTMS + c NSI Full ms [150.0000-1000.0000]



**Figure S30:** High resolution mass spectrum of **10**

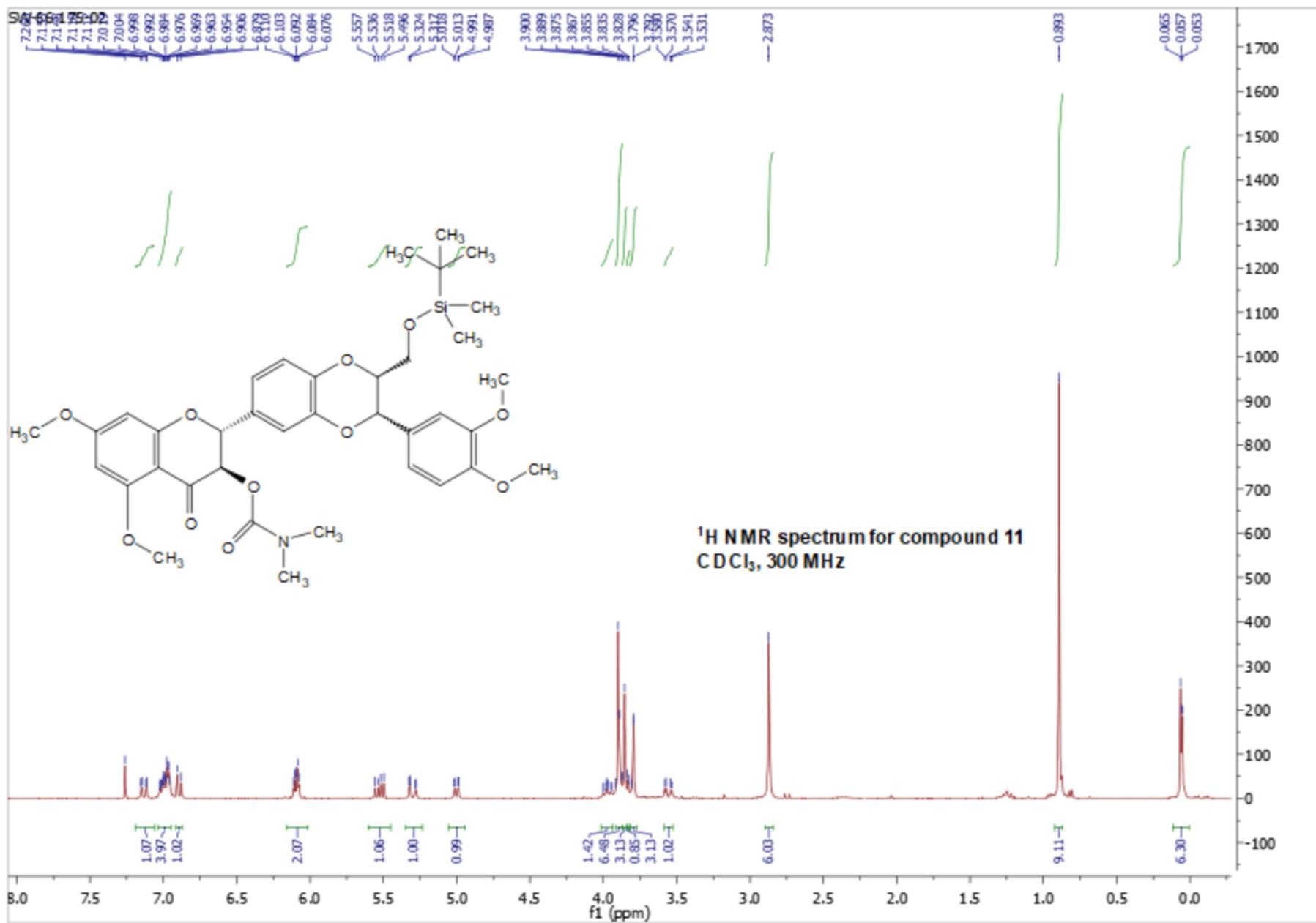


Figure S31: <sup>1</sup>H NMR spectrum of **11** in CDCl<sub>3</sub>

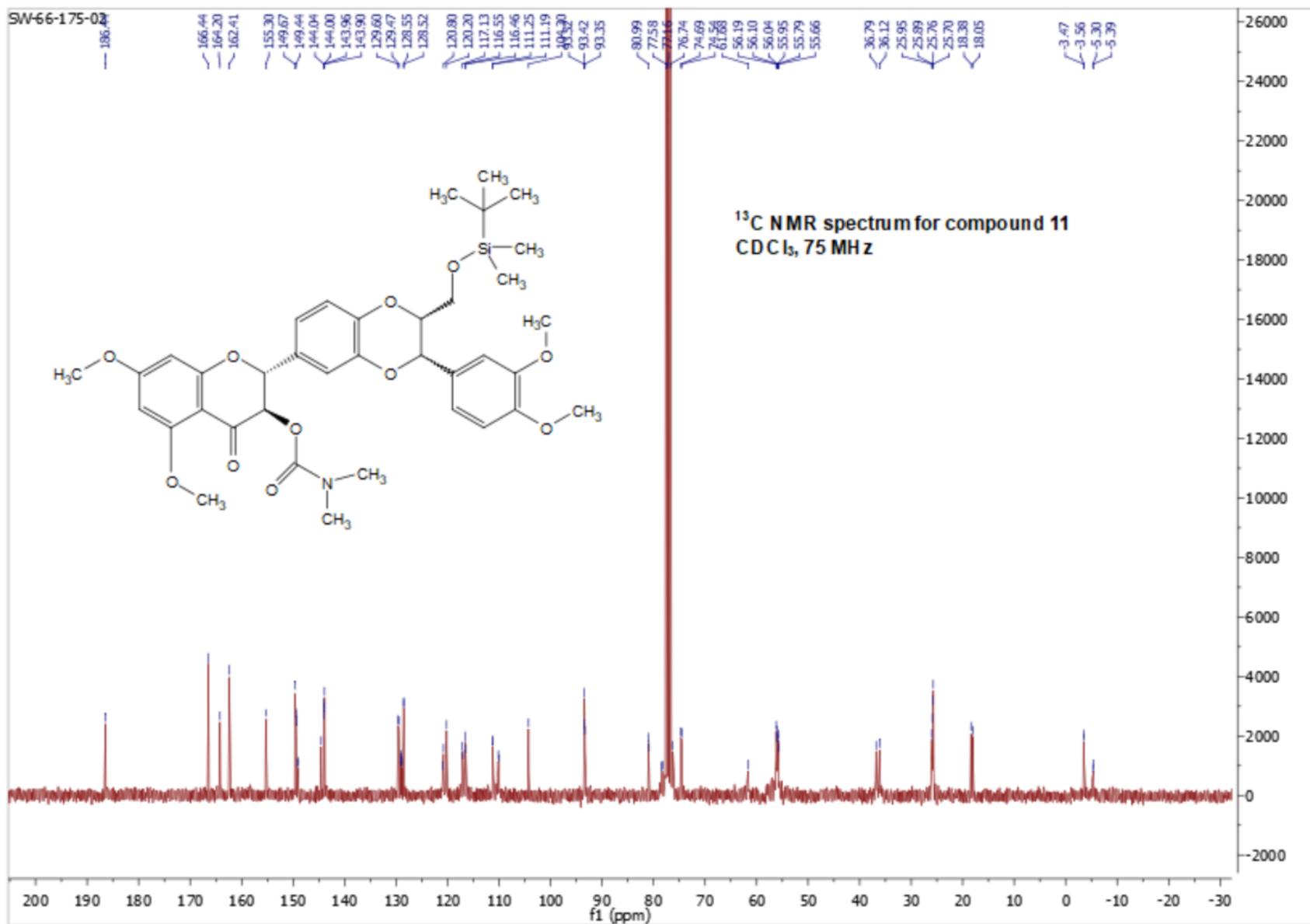


Figure S32: <sup>13</sup>C NMR spectrum of **11** in CDCl<sub>3</sub>

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
SW-66-175-02	C <sub>37</sub> H <sub>47</sub> NO <sub>11</sub> Si	709.2919	710.2997	710.3006	0.0009	1.27

SW-66-175-02 #3050-3236 RT: 16.38-17.39 AV: 187 NL: 1.96E7  
T: FTMS + c NSI Full ms [300.0000-1000.0000]

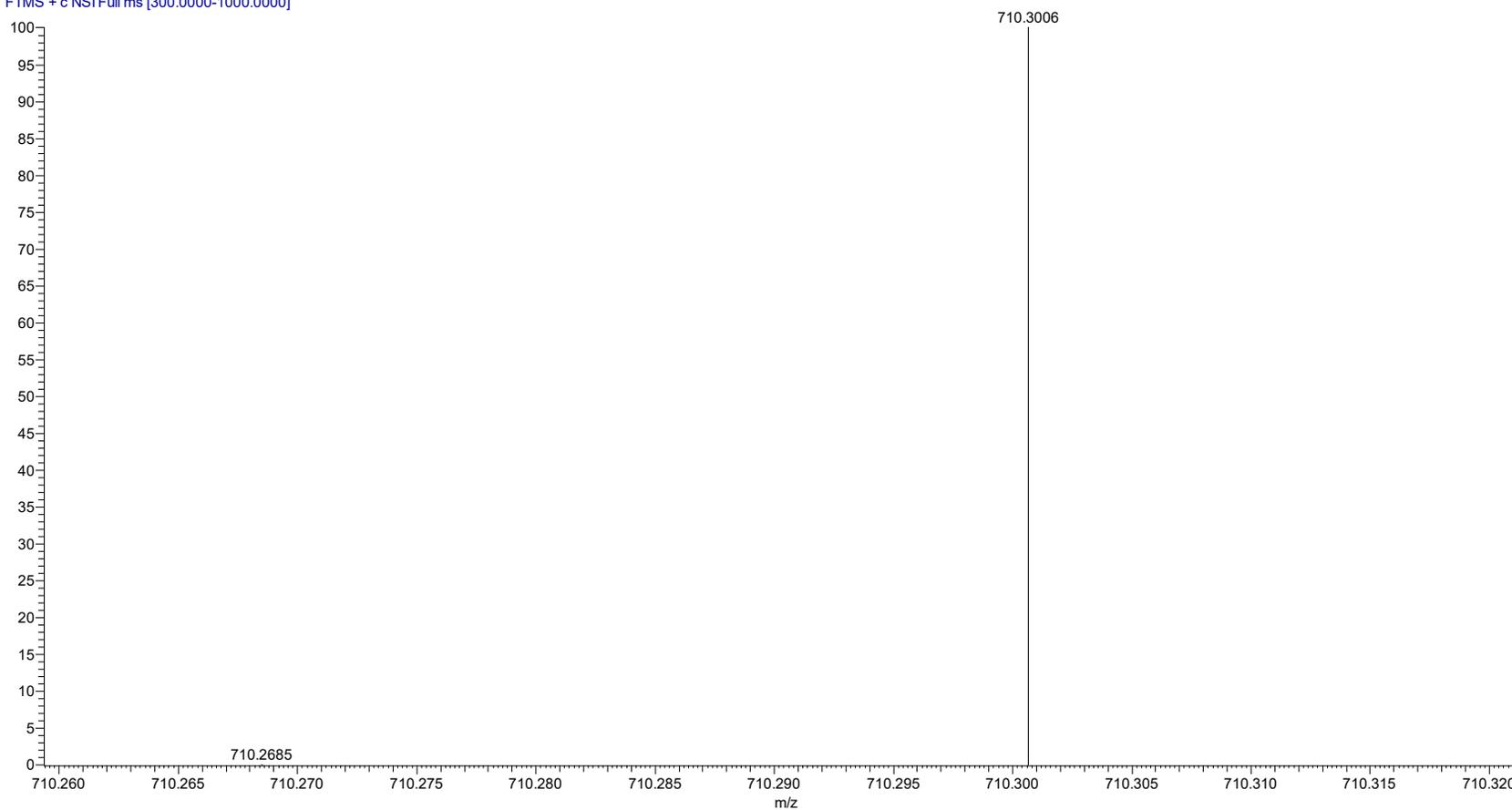
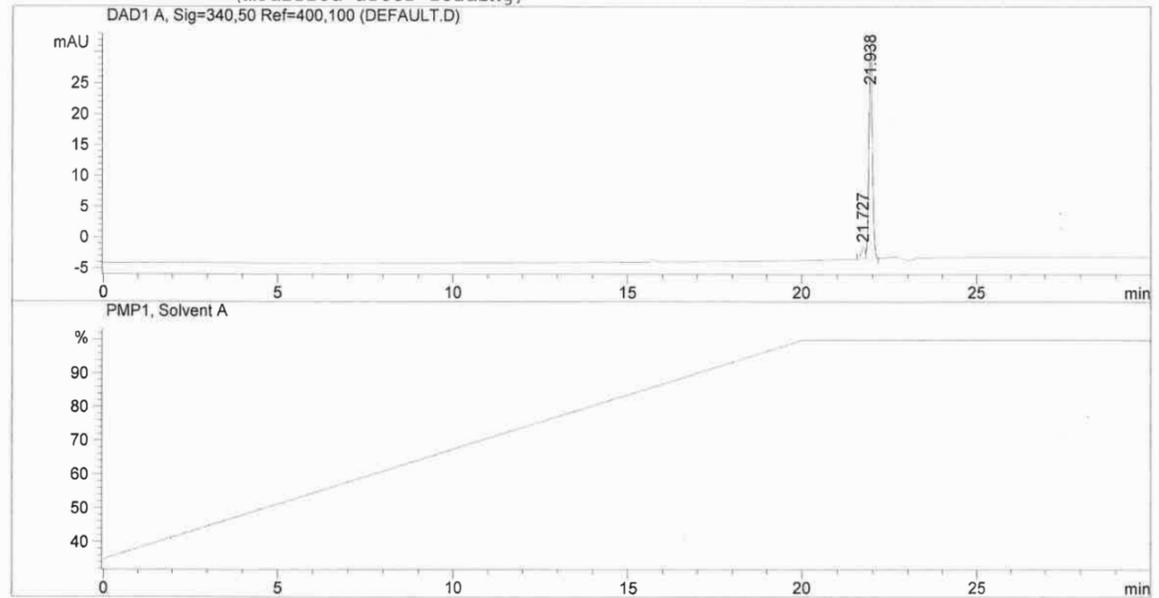


Figure S33: High resolution mass spectrum of 11

```

=====
Injection Date   : 9/17/2021 11:10:47 AM
Sample Name     : SW-66-175-02           Location  : Vial 1
Acq. Operator   :
Method          : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed    : 9/17/2021 10:10:55 AM
                  (modified after loading)
    
```



=====  
Area Percent Report  
=====

```

Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
    
```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.727	BV	0.1121	14.86666	1.96797	5.8414
2	21.938	VB	0.1067	239.63838	34.64161	94.1586

Totals : 254.50505 36.60958

Results obtained with enhanced integrator!

=====  
\*\*\* End of Report \*\*\*

Figure S33: HPLC chromatogram of 11

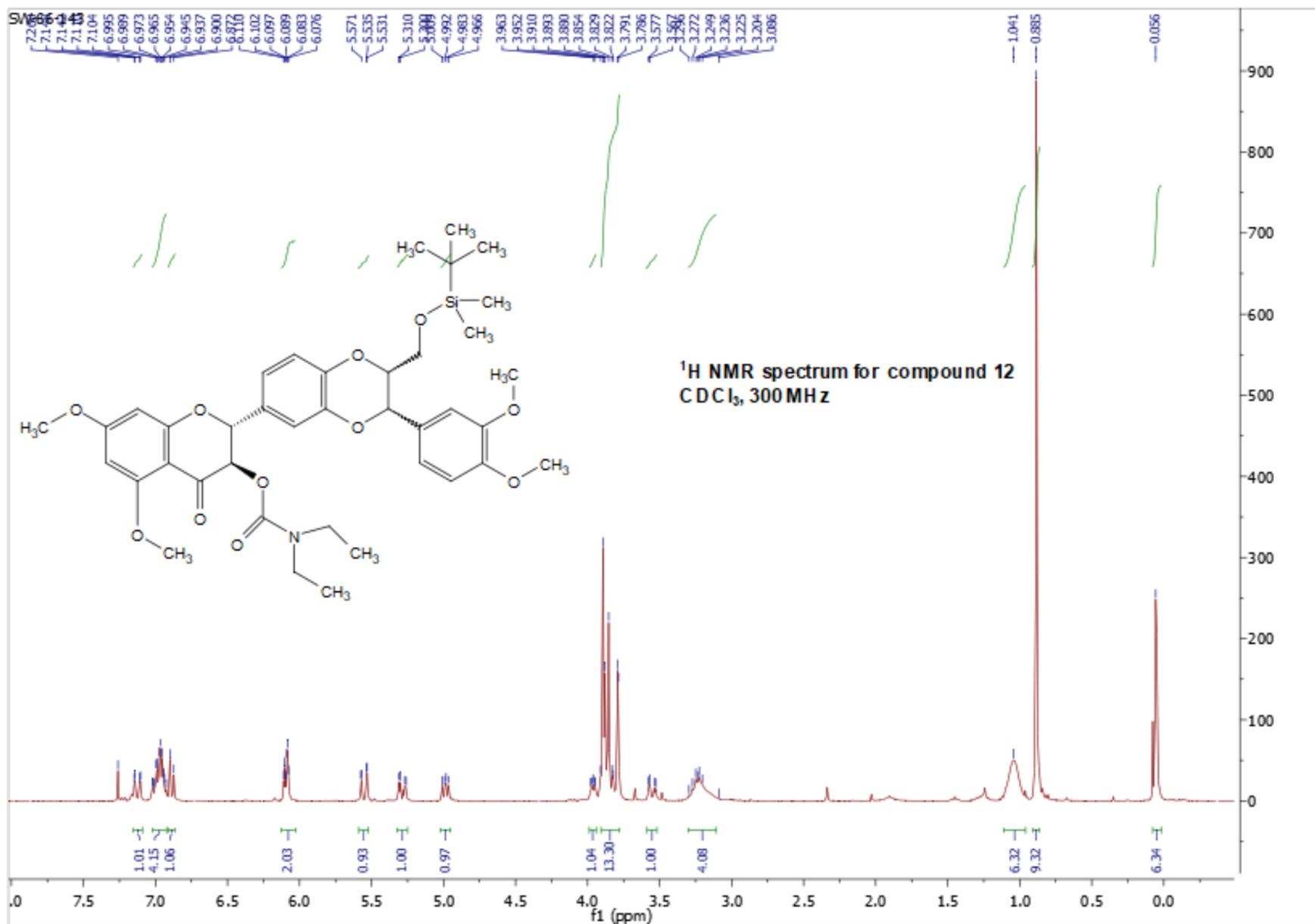


Figure S34: <sup>1</sup>H NMR spectrum of 12 in CDCl<sub>3</sub>

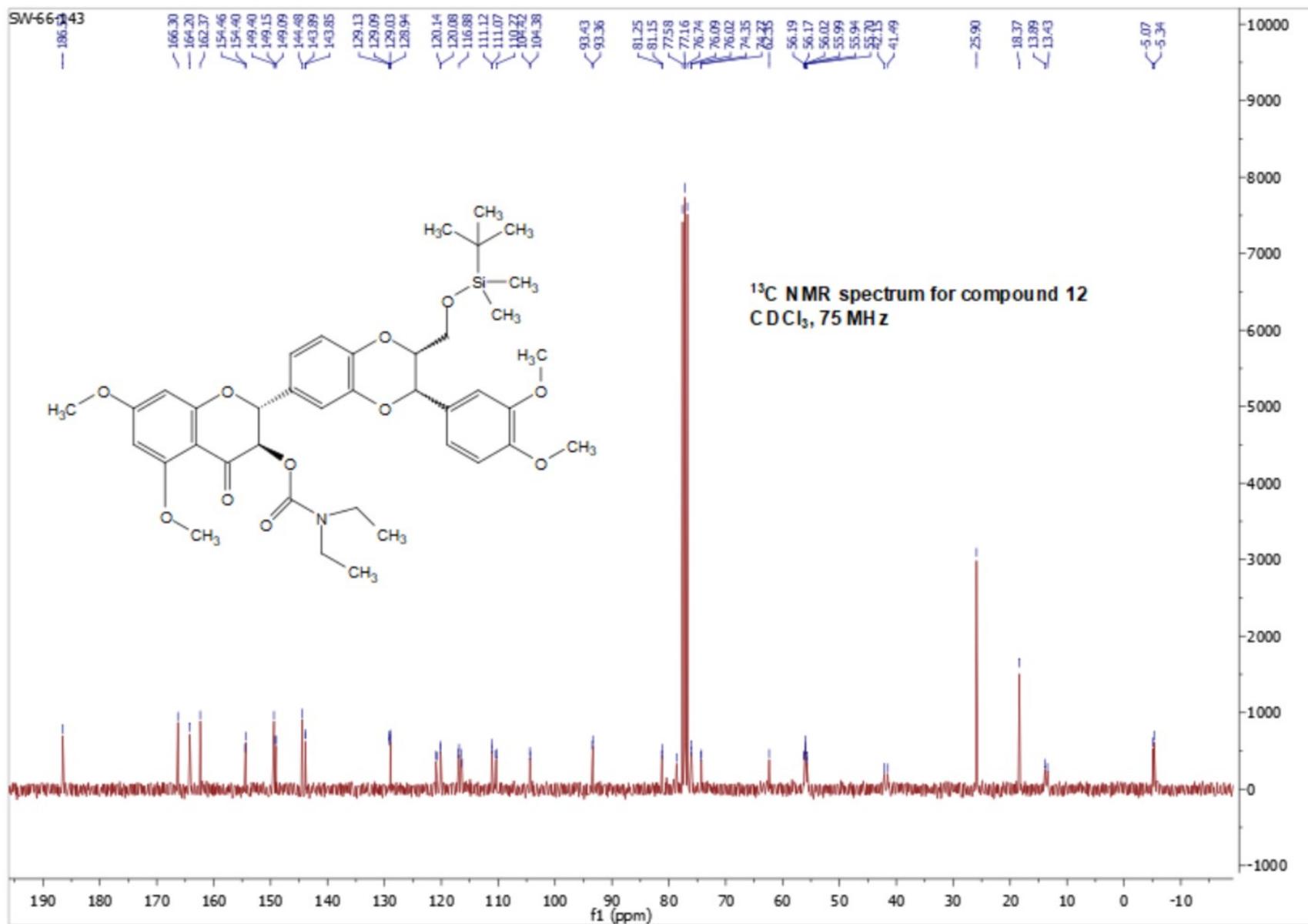
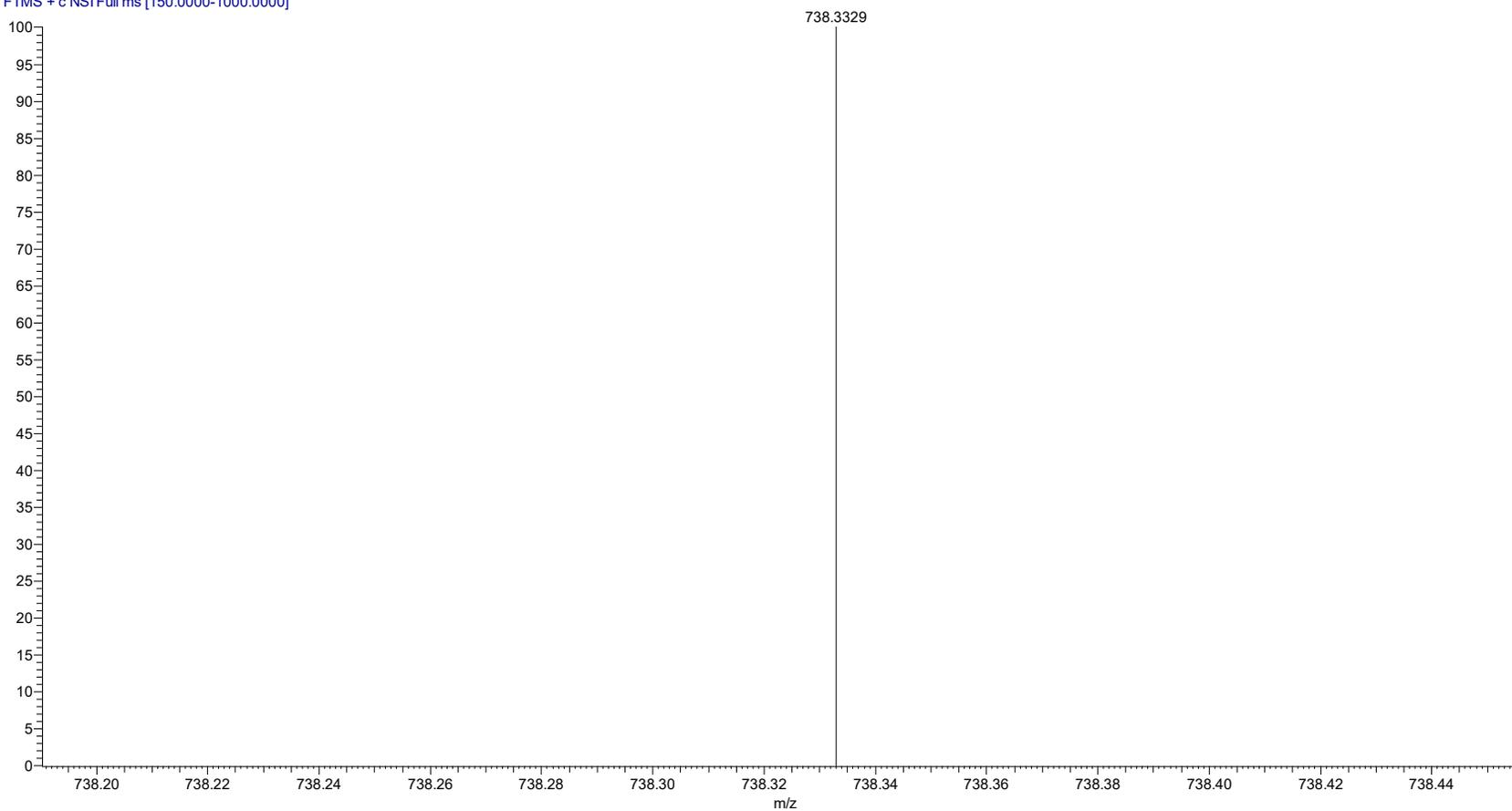


Figure S35: <sup>13</sup>C NMR spectrum of 12 in CDCl<sub>3</sub>

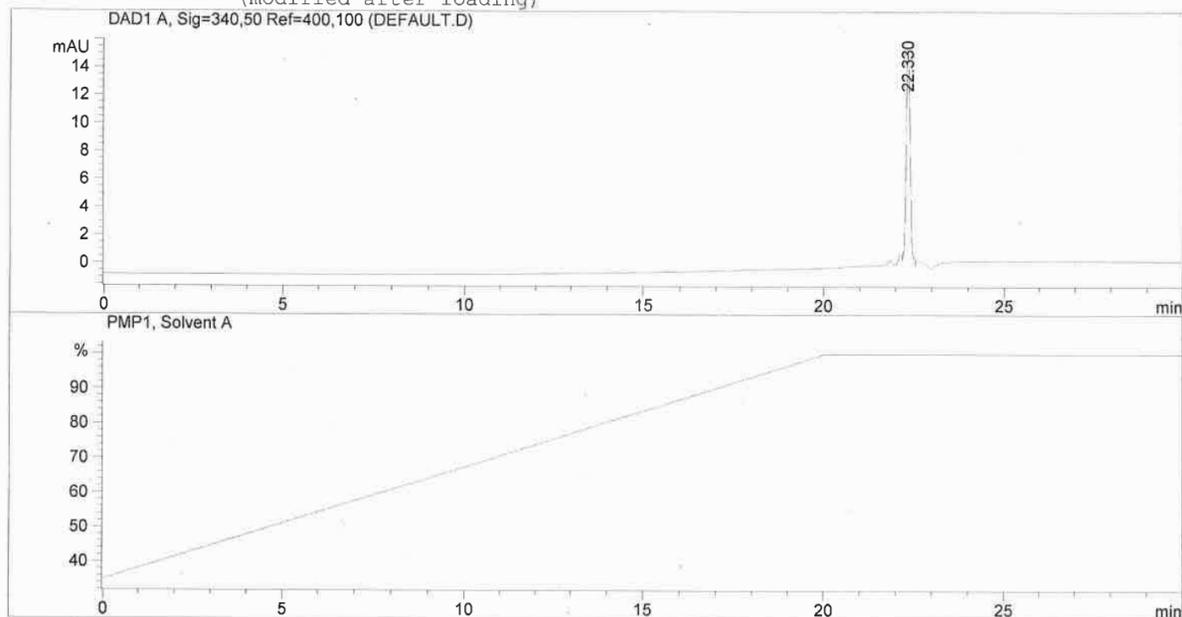
compds	Mol. Formula	Exact Mass	M+H	Observed	delta	ppm
SW-66-143	C <sub>39</sub> H <sub>51</sub> NO <sub>11</sub> Si	737.3232	738.3310	<b>738.3329</b>	0.0019	2.57

SW-66-143 #2970-3159 RT: 15.56-16.59 AV: 190 NL: 5.40E8  
T: FTMS + c NSI Full ms [150.0000-1000.0000]



**Figure S36:** High resolution mass spectrum of **12**

```
=====
Injection Date   : 9/13/2021 2:48:00 PM
Sample Name      : SW-66-95                Location : Vial 1
Acq. Operator    :
Method           : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed     : 9/13/2021 2:42:55 PM
                  (modified after loading)
=====
```



```
=====
Area Percent Report
=====
```

```
Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	22.330	VB	0.1206	115.30704	15.17783	100.0000

```
Totals :                115.30704    15.17783
```

Results obtained with enhanced integrator!

```
=====
*** End of Report ***
=====
```

Figure S37: HPLC chromatogram of 12

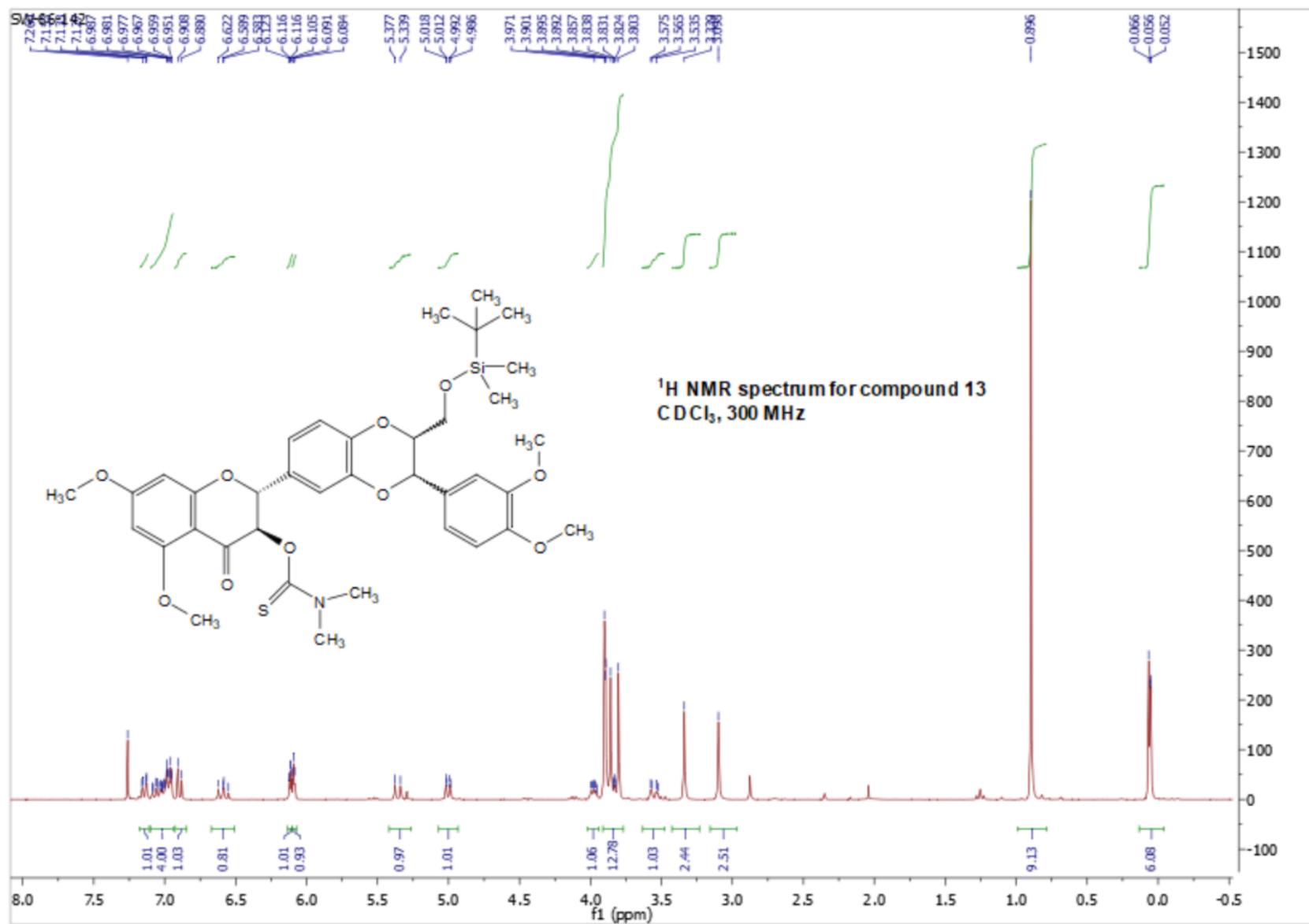


Figure S38: <sup>1</sup>H NMR spectrum of 13 in CDCl<sub>3</sub>

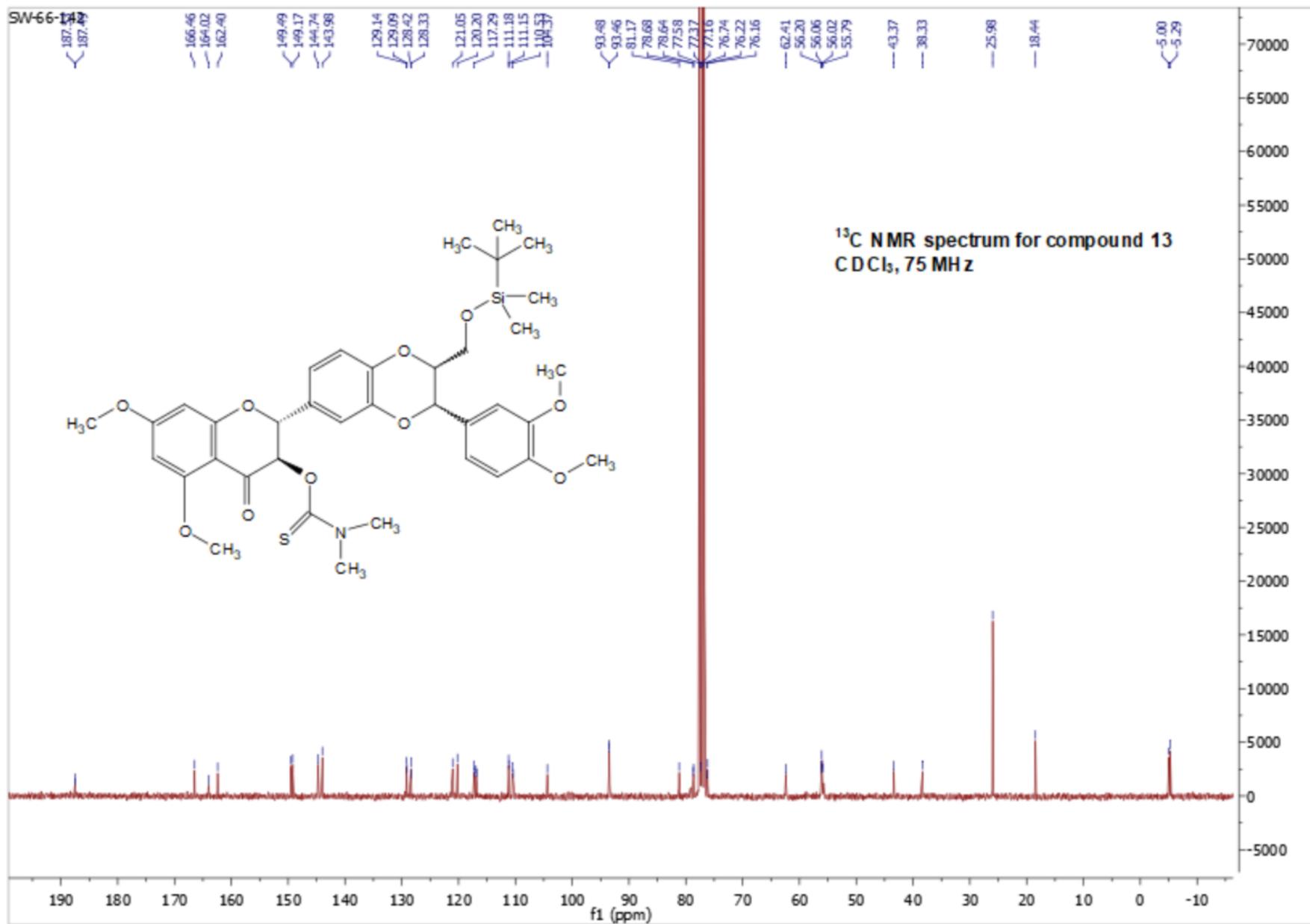


Figure S39: <sup>13</sup>C NMR spectrum of 13 in CDCl<sub>3</sub>

compds	Mol. Formula	Exact Mass	M+H	Observed	delta	ppm
SW-66-142	C37H47NO10Si	725.2691	726.2769	<b>726.2796</b>	0.0027	3.79

SW-66-142 #4940-5072 RT: 26.70-27.40 AV: 133 NL: 8.33E7  
T: FTMS + c NSI Full ms [150.0000-1000.0000]

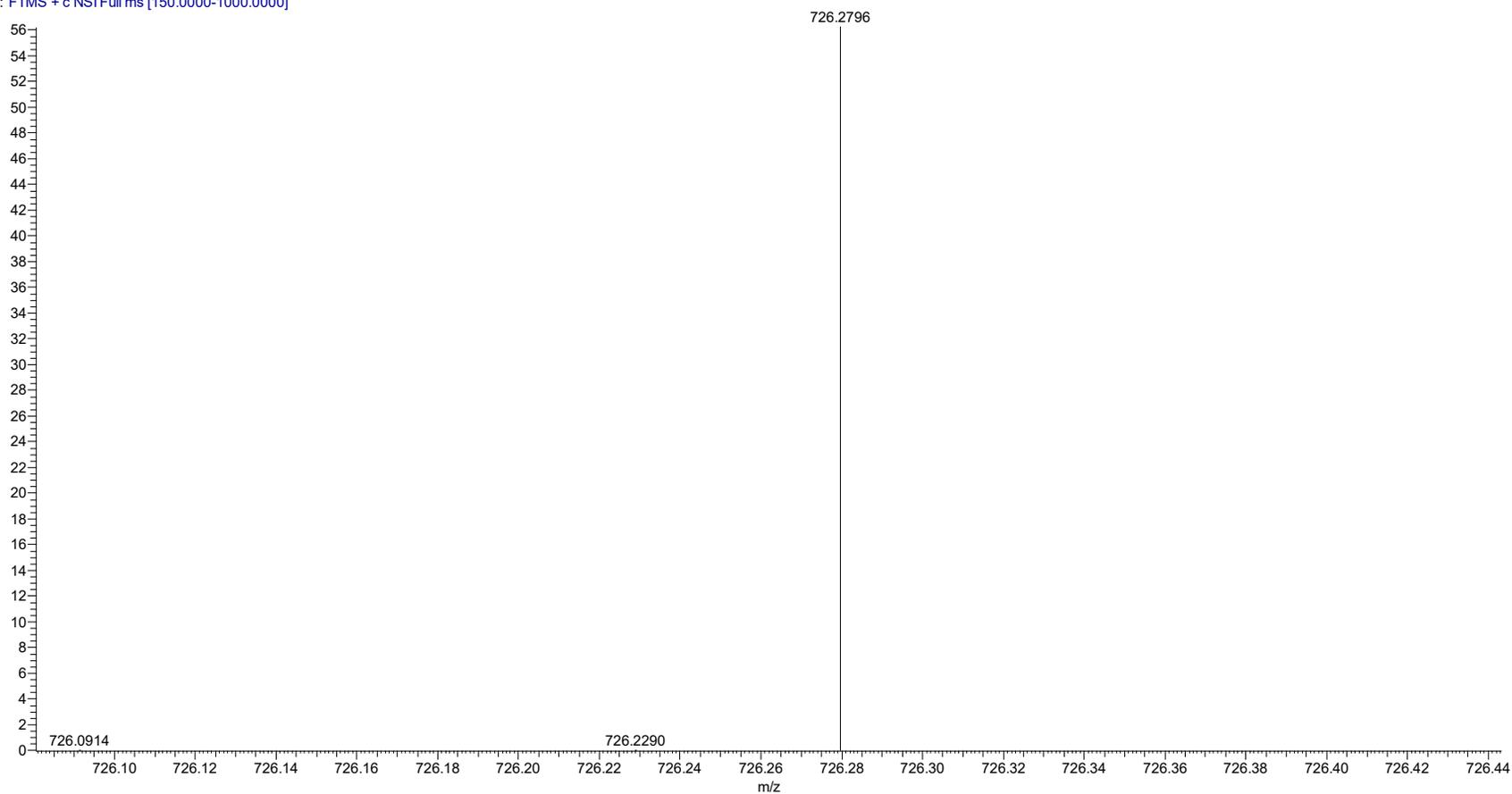
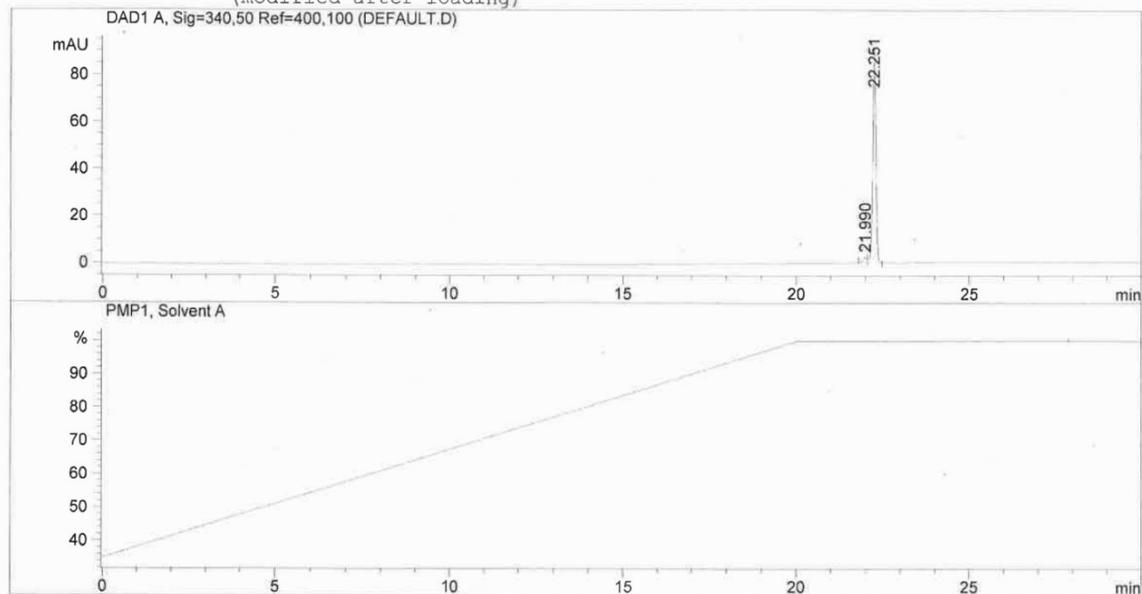


Figure S40: High resolution mass spectrum of 13

```

=====
Injection Date : 9/13/2021 11:55:21 AM
Sample Name    : SW-66-94                Location : Vial 1
Acq. Operator  :
Method        : C:\HPCHEM\1\METHODS\JNP2015.M
Last changed  : 9/13/2021 11:53:45 AM
                (modified after loading)
=====

```



```

=====
Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000

```

Signal 1: DAD1 A, Sig=340,50 Ref=400,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.990	BV	0.1080	19.44175	2.57780	3.3204
2	22.251	VB	0.0966	566.07684	91.02409	96.6796

```
Totals :                585.51859   93.60189
```

Results obtained with enhanced integrator!

```

=====
*** End of Report ***
=====

```

Figure S41: HPLC chromatogram of 13

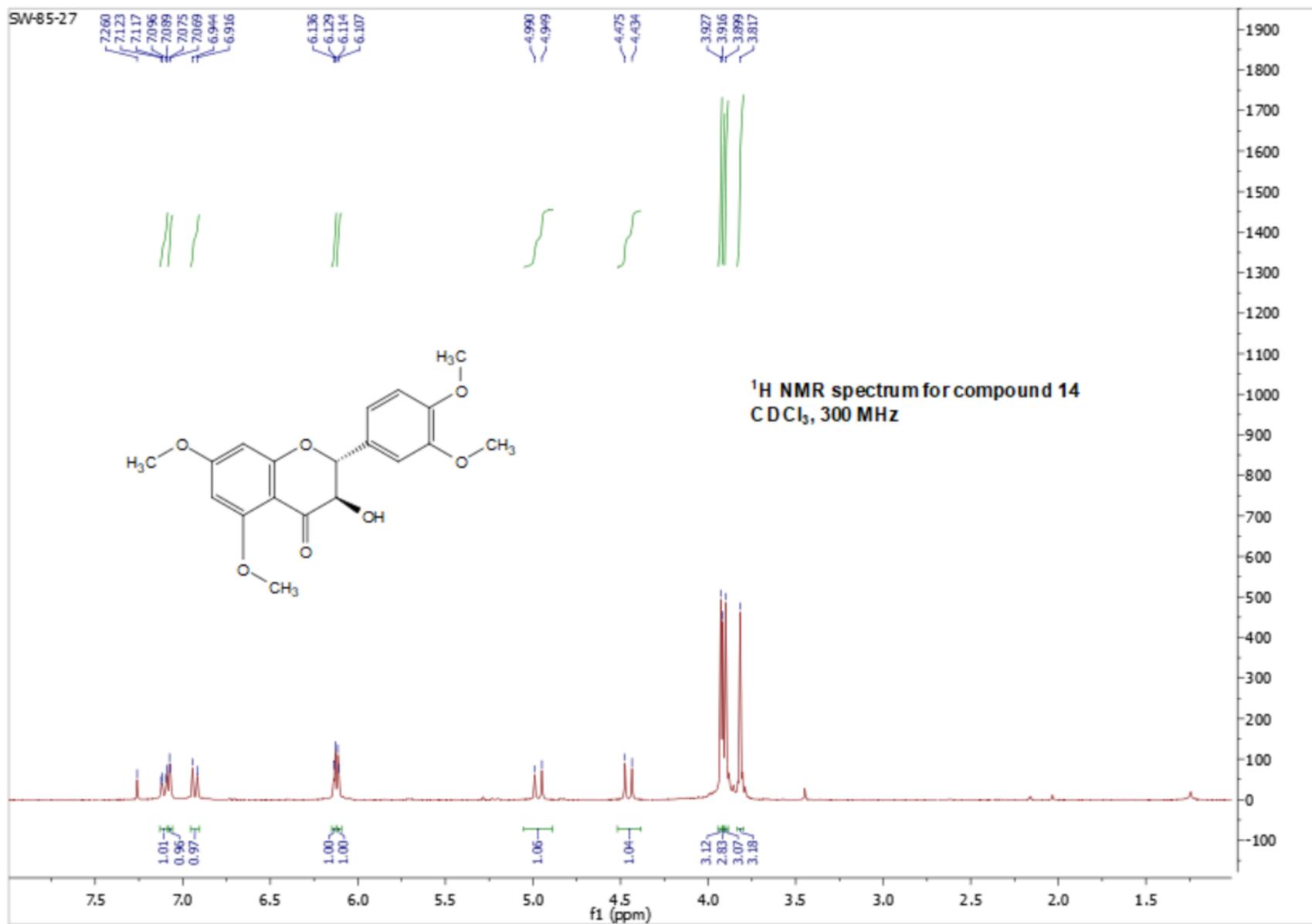


Figure S42: <sup>1</sup>H NMR spectrum of **14** in CDCl<sub>3</sub>

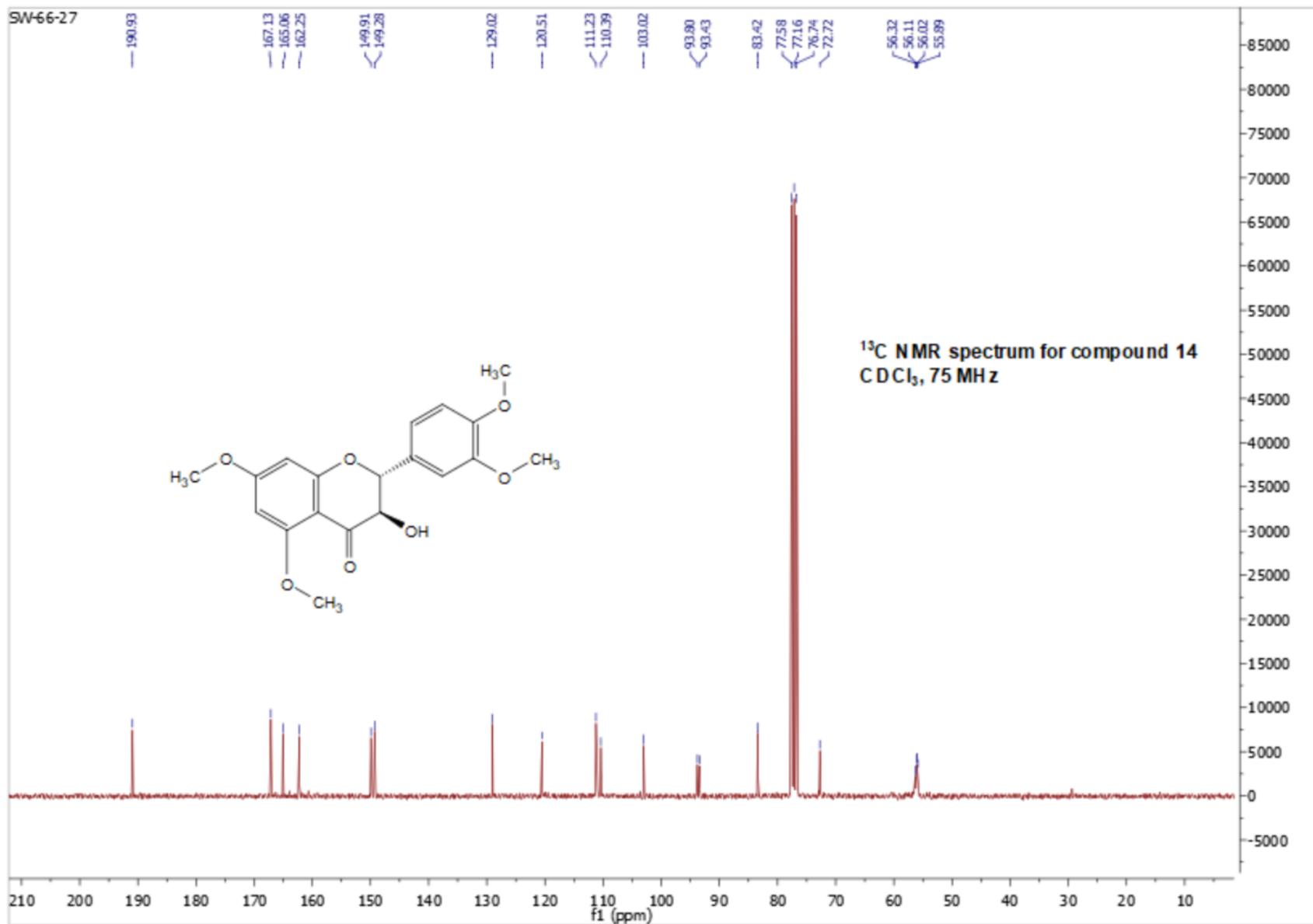


Figure S43: <sup>13</sup>C NMR spectrum of **14** in CDCl<sub>3</sub>

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
SW-85-27	C19H20O7	360.1209	361.1287	361.1281	-0.0006	-1.77

SW-85-27 #1554-1728 RT: 8.67-9.55 AV: 175 NL: 2.86E9  
T: FTMS + c NSI Full ms [300.0000-1000.0000]

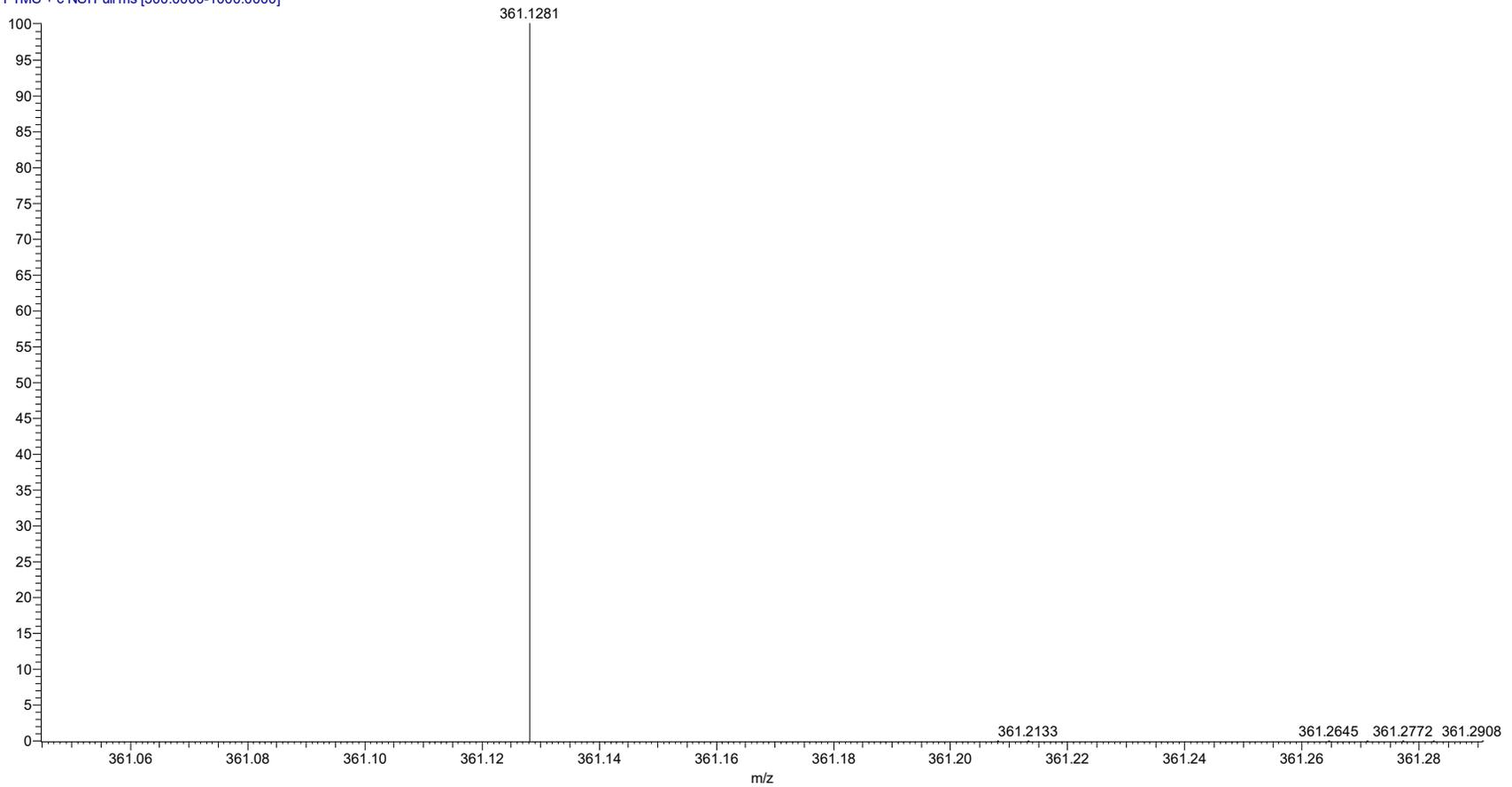


Figure S44: High resolution mass spectrum of 14

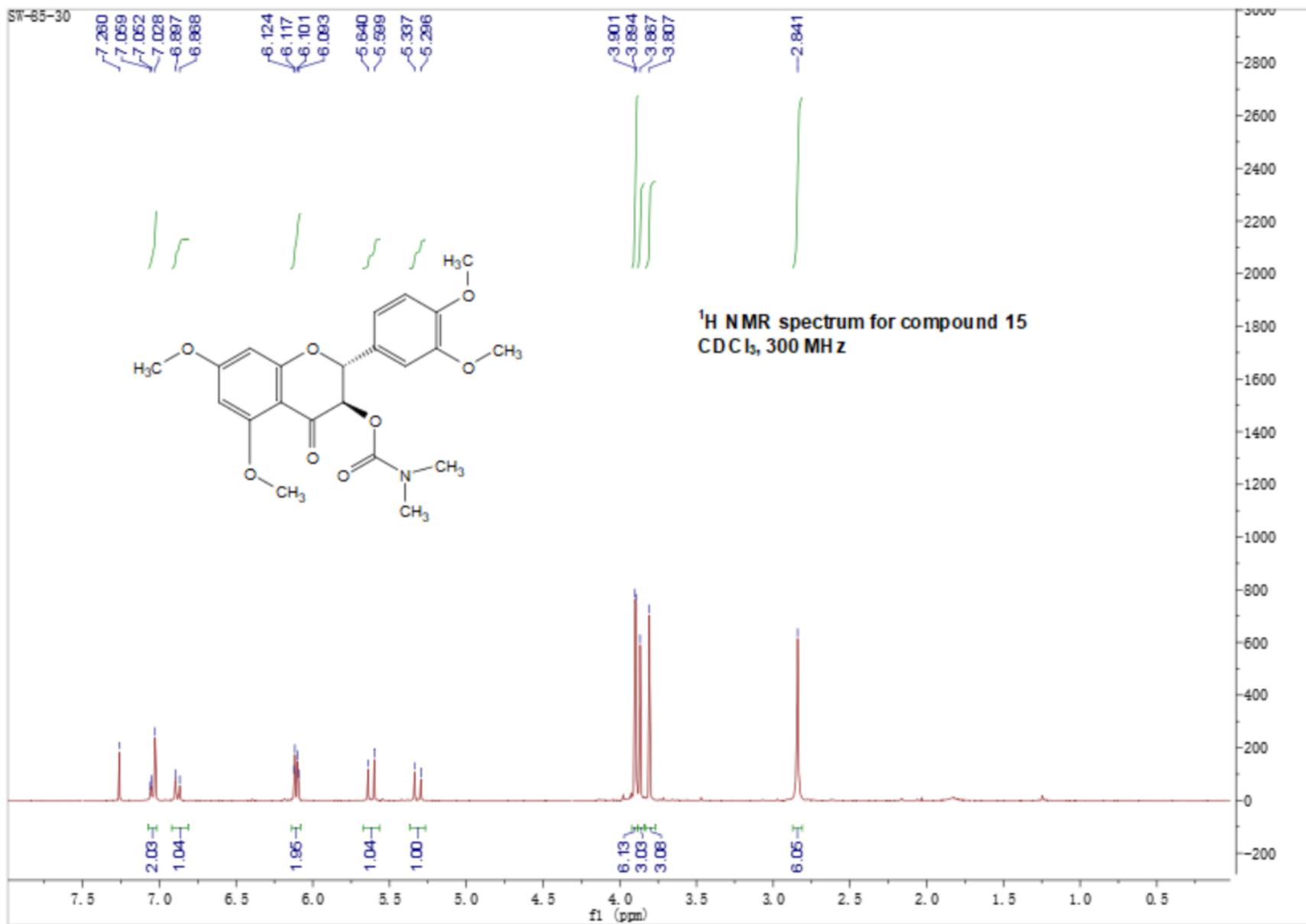


Figure S45: <sup>1</sup>H NMR spectrum of **15** in CDCl<sub>3</sub>

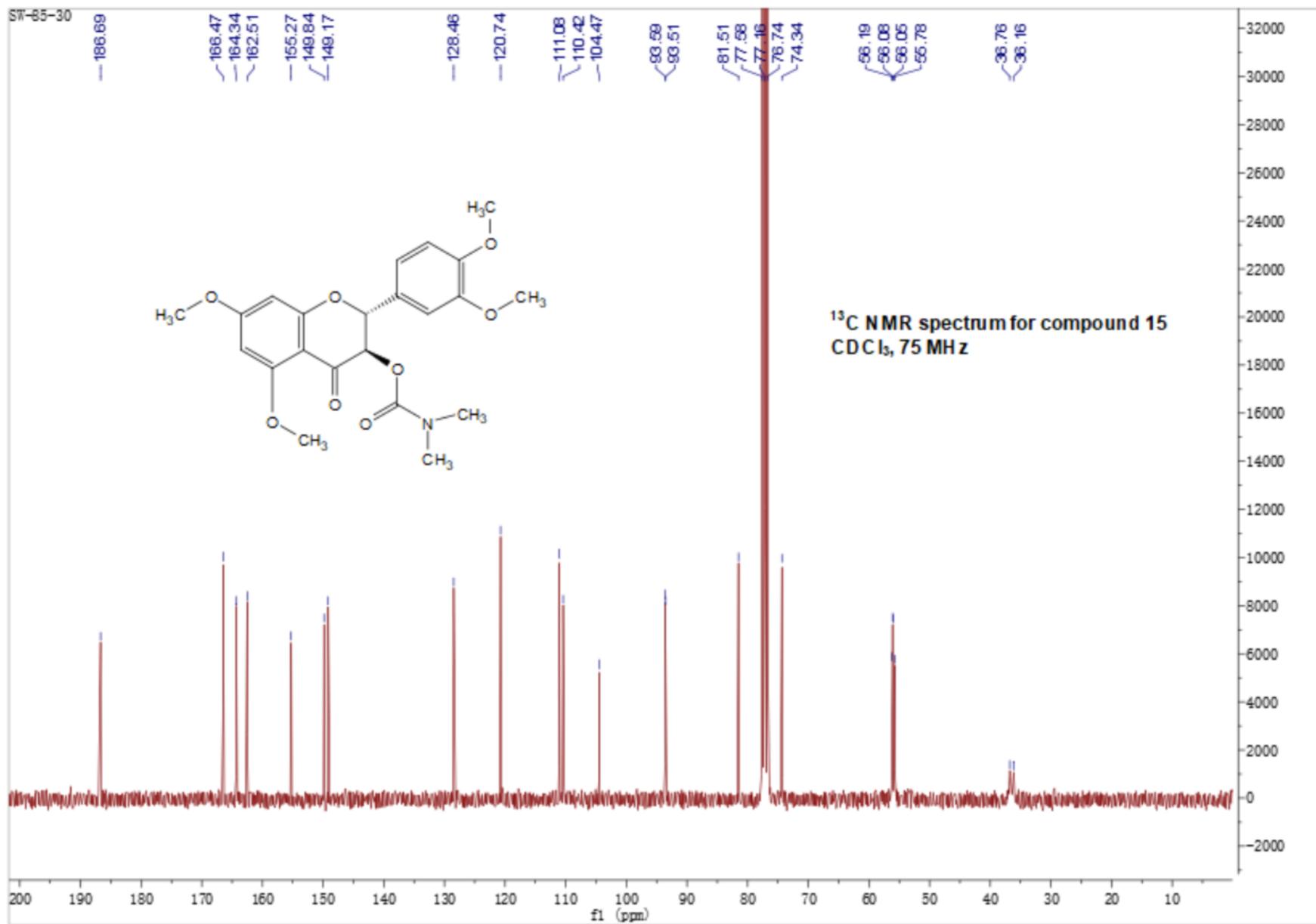


Figure S46:  $^{13}\text{C}$  NMR spectrum of **15** in CDCl<sub>3</sub>

Sample Name	Mol Formula	MW	M+H	observed	delta	ppm
SW-85-30	C22H25NO8	431.1581	432.1659	432.1657	-0.0002	-0.37

SW-85-30 #1788-1933 RT: 9.86-10.60 AV: 146 NL: 1.78E9  
T: FTMS + c NSI Full ms [300.0000-1000.0000]

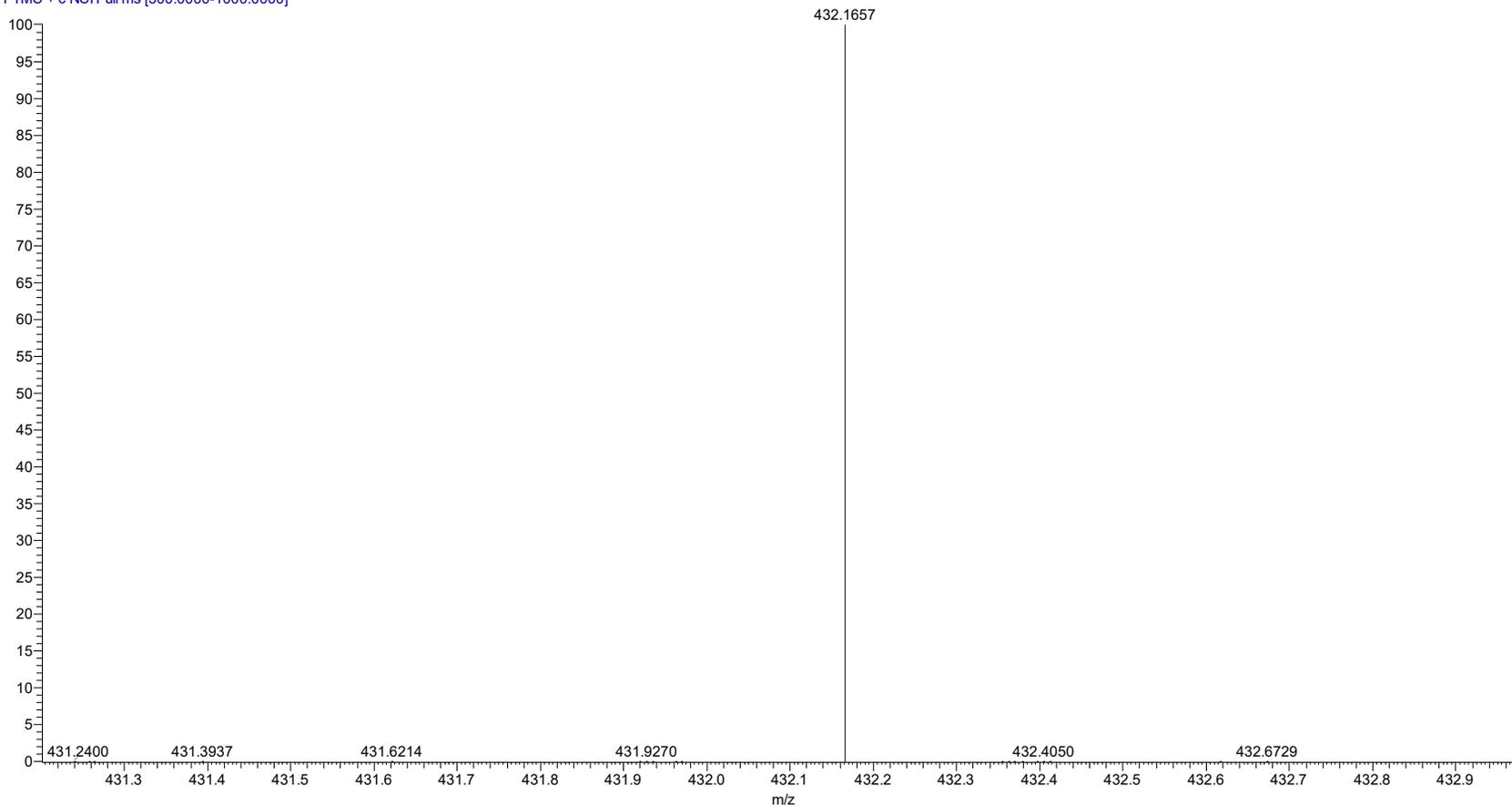


Figure S47: High resolution mass spectrum of 15

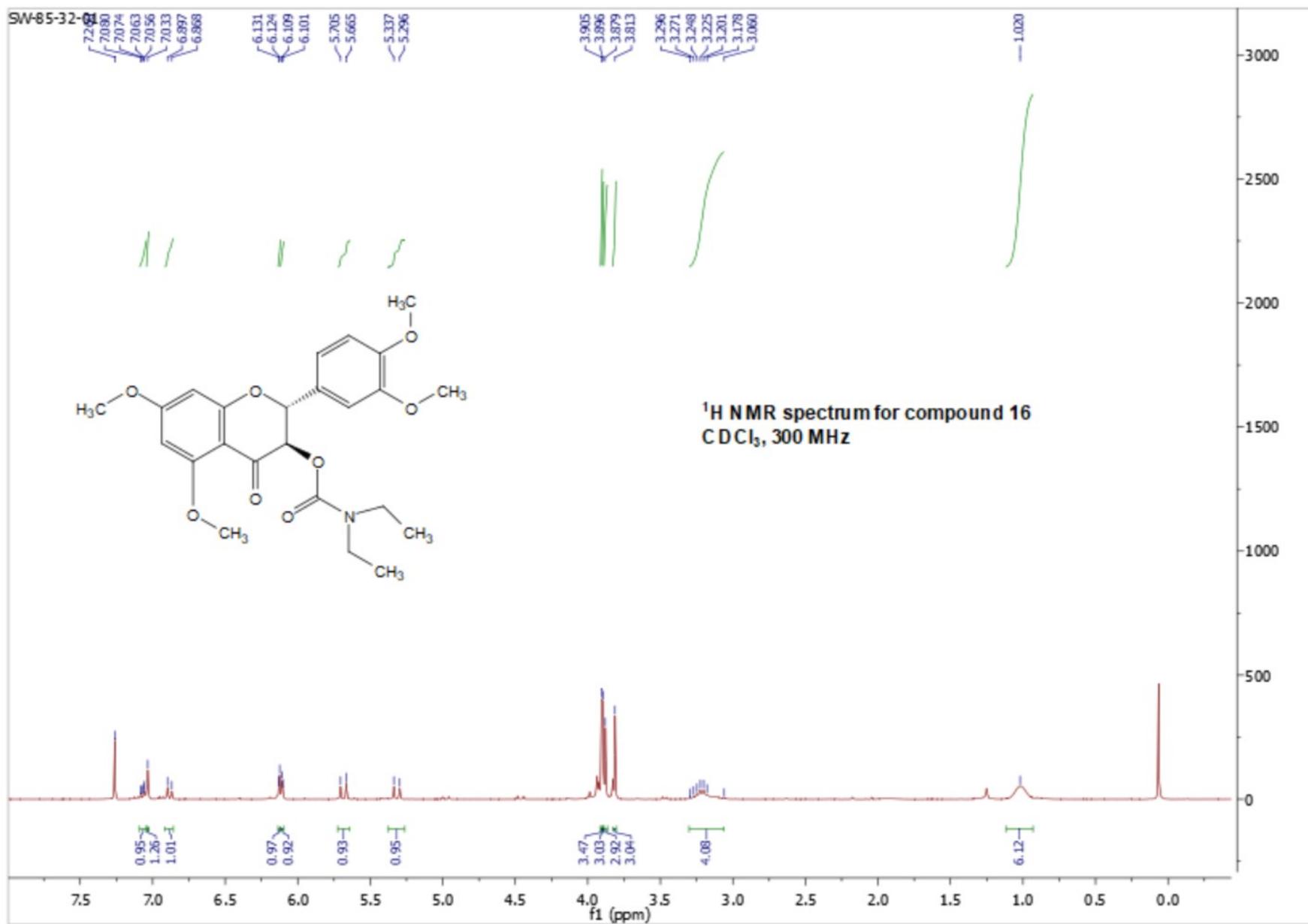


Figure S48: <sup>1</sup>H NMR spectrum of 16 in CDCl<sub>3</sub>

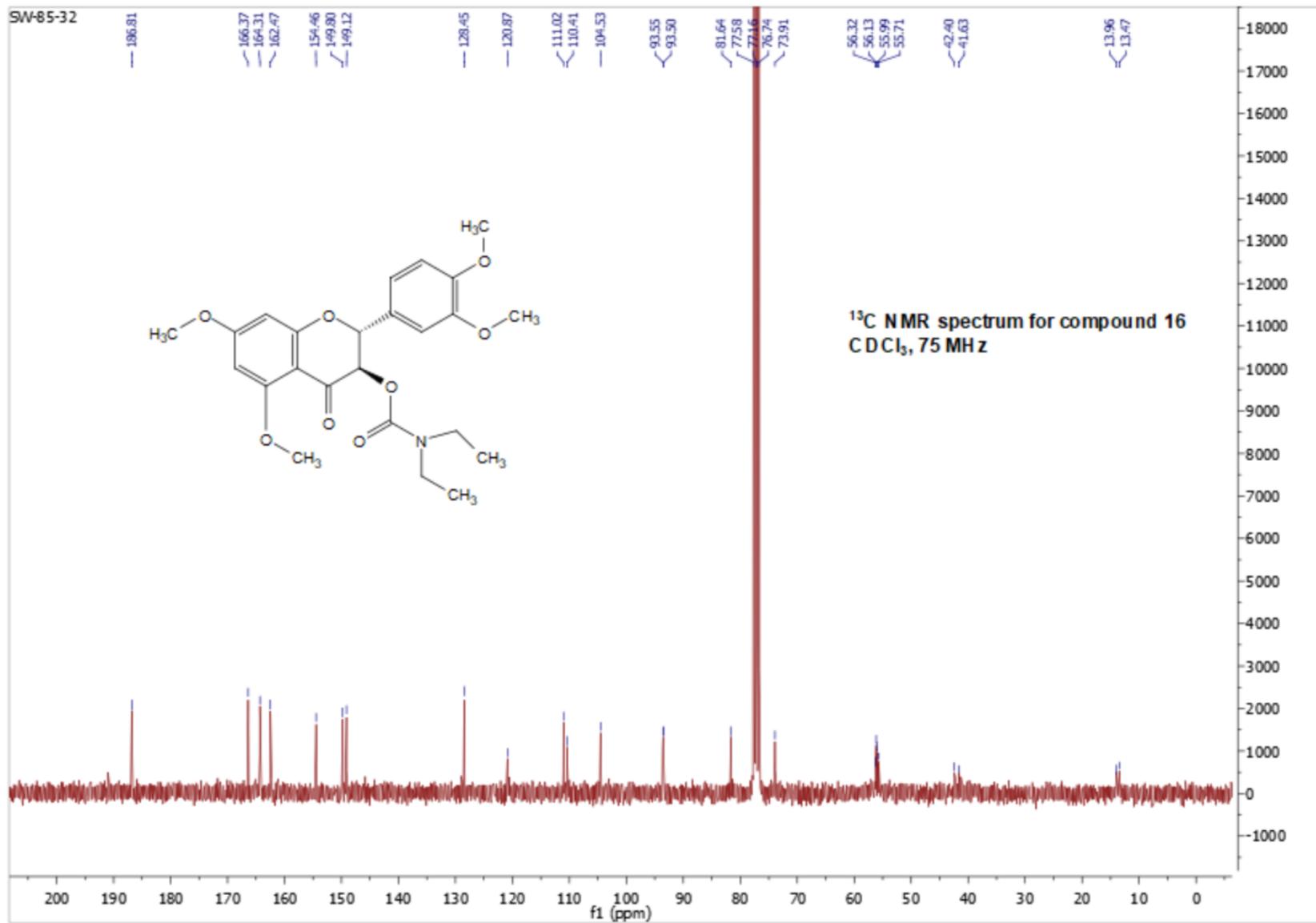


Figure S49: <sup>13</sup>C NMR spectrum of 16 in CDCl<sub>3</sub>

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
SW-85-32	C24H29NO8	459.1894	460.1972	460.1970	-0.0002	-0.35

SW-85-32 #1912-2071 RT: 10.49-11.30 AV: 160 NL: 9.20E8  
T: FTMS + c NSI Full ms [300.0000-1000.0000]

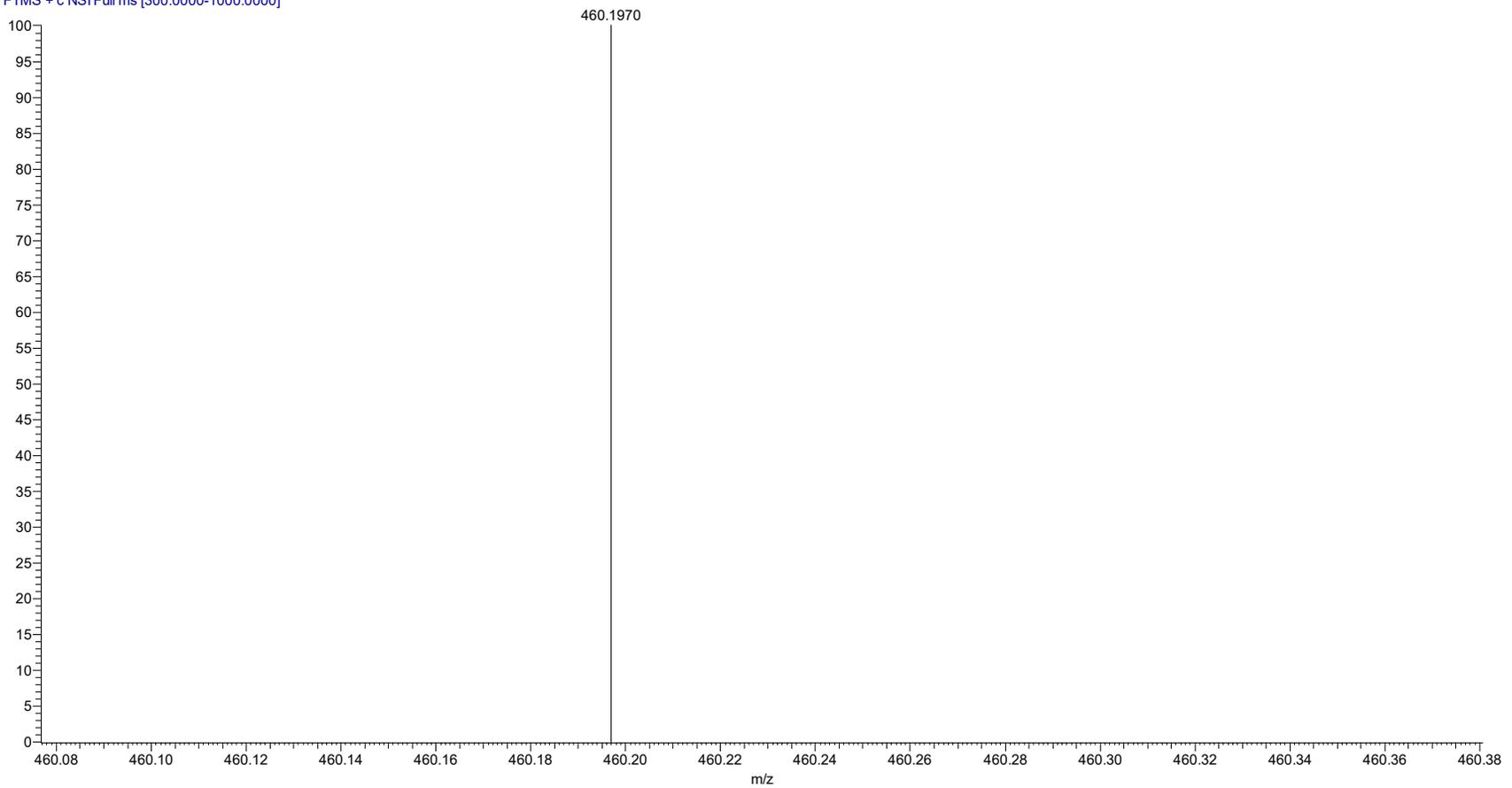
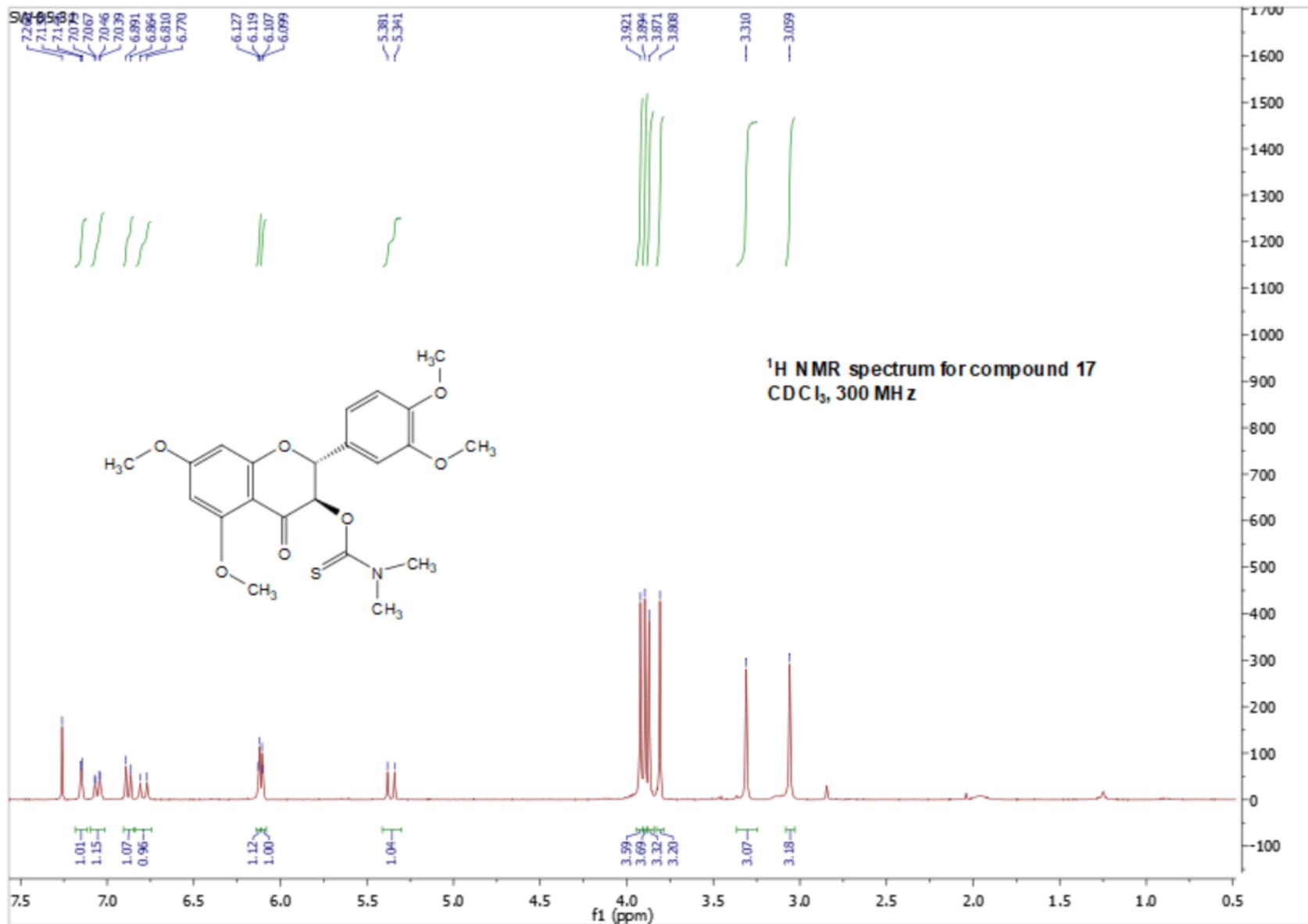


Figure S50: High resolution mass spectrum of 16



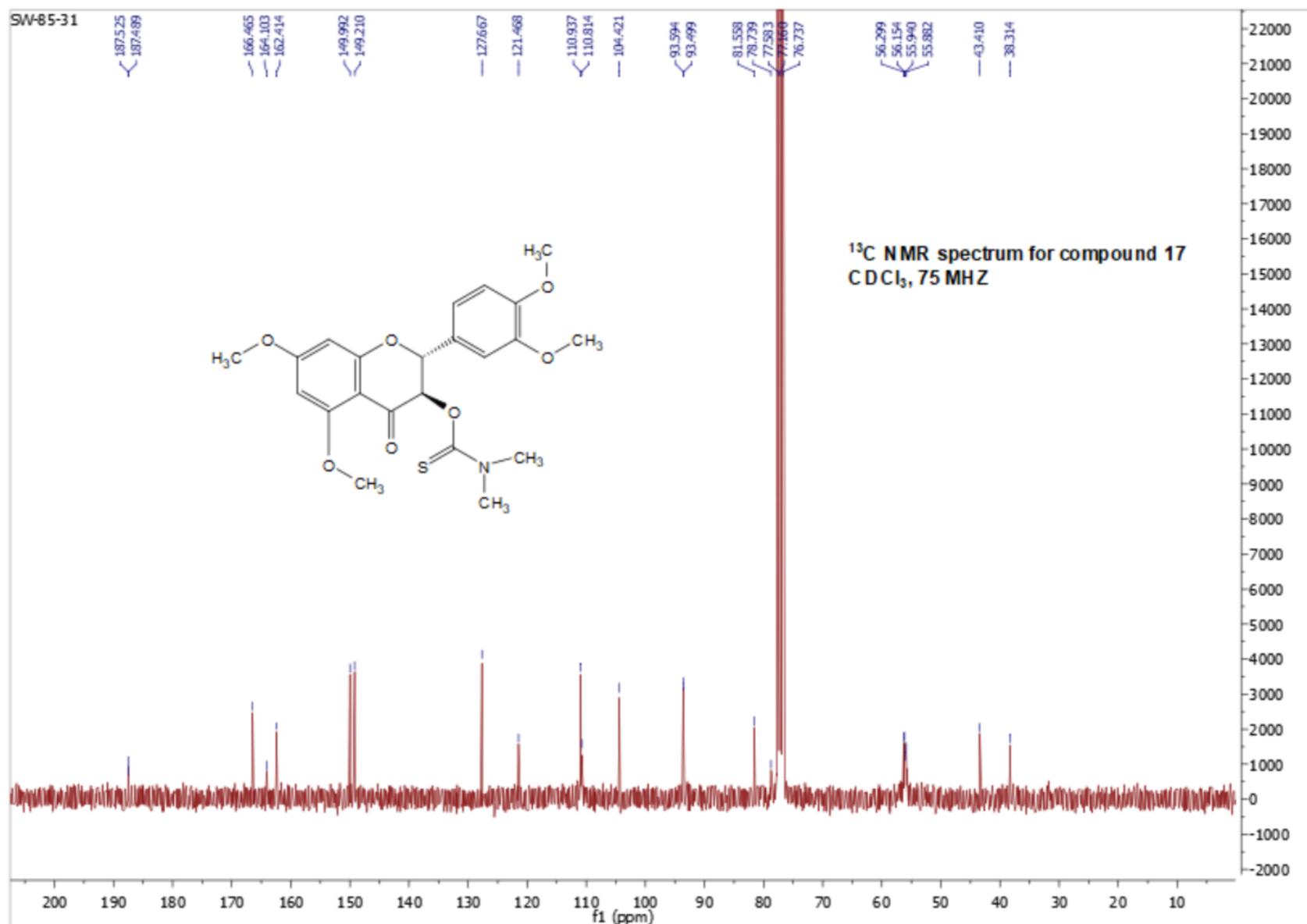


Figure S52: <sup>13</sup>C NMR spectrum of 17 in CDCl<sub>3</sub>

Sample Name	Mol Fomula	MW	M+H	observed	delta	ppm
SW-85-31	C22H25NO7S	447.1352	448.1430	448.1431	0.0001	0.20

SW-85-31 #1933-2007 RT: 10.60-10.98 AV: 75 NL: 1.55E9  
T: FTMS + c NSI Full ms [300.0000-1000.0000]

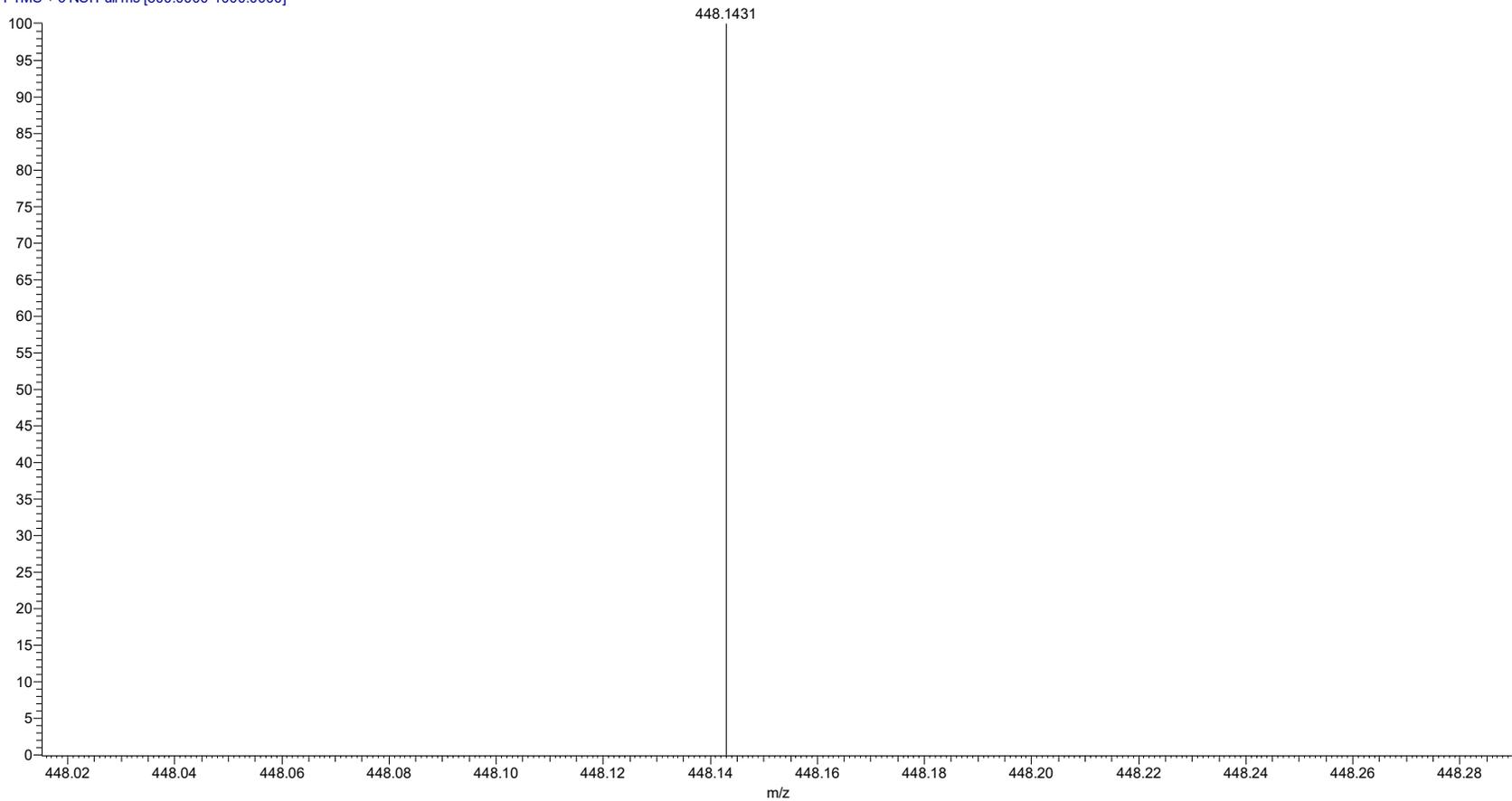
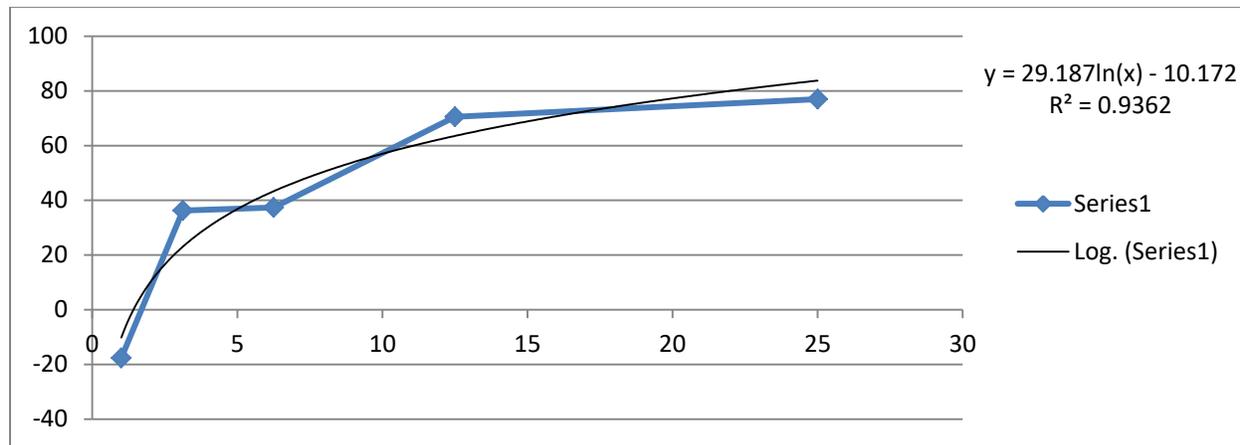


Figure S53: High resolution mass spectrum of 17

**Figure S54:** The concentration-effect curves that were used to calculate the IC<sub>50</sub> values from the WST-1 cell proliferation assay

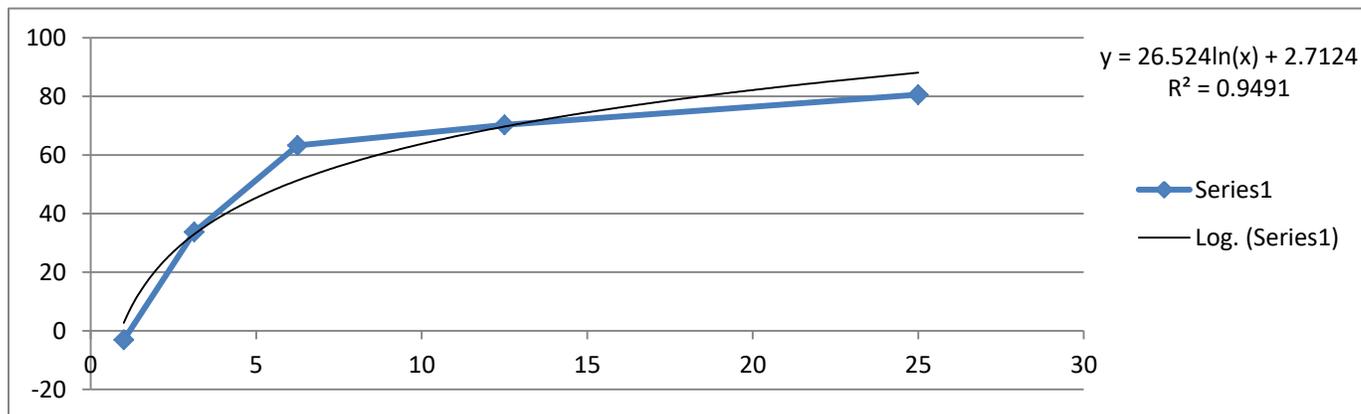
1. The curves that we used to calculate the IC<sub>50</sub> value for compound **3** against PC-3



X-axis = concentration (µM) of compound **3**

Y-axis = % Cell Proliferation Inhibition

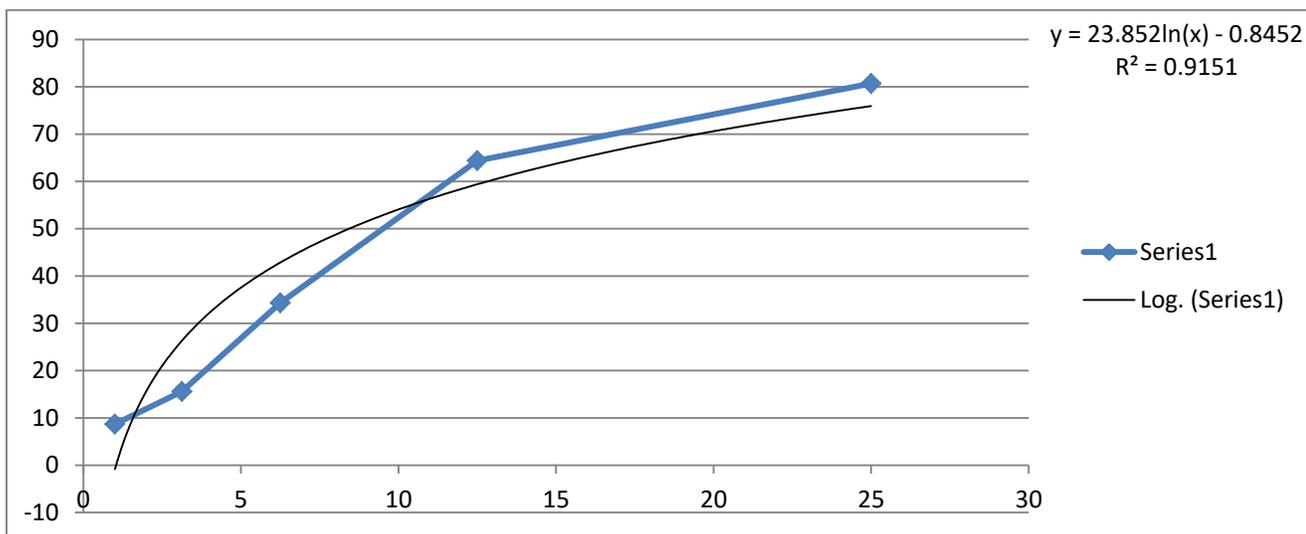
IC<sub>50</sub> = 7.858 µM



X-axis = concentration (µM) of compound **3**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 5.946 µM

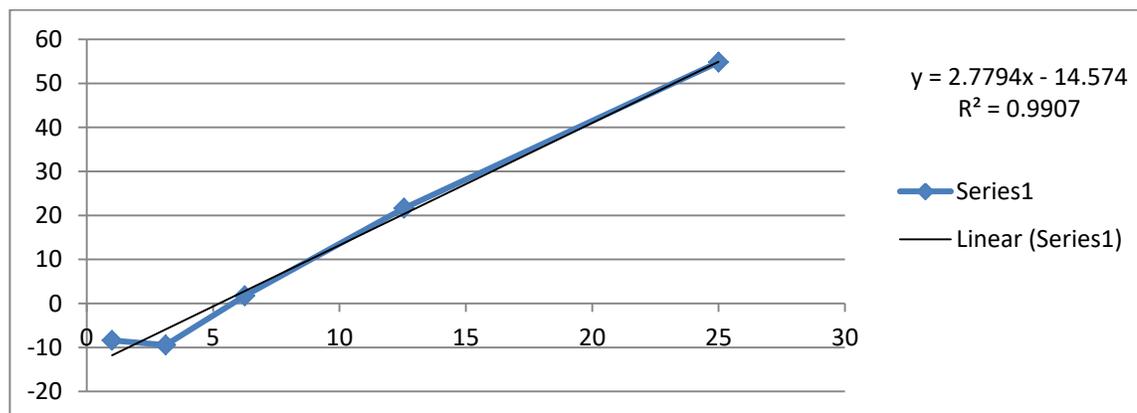


X-axis = concentration ( $\mu\text{M}$ ) of compound **3**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 8.429 \mu\text{M}$

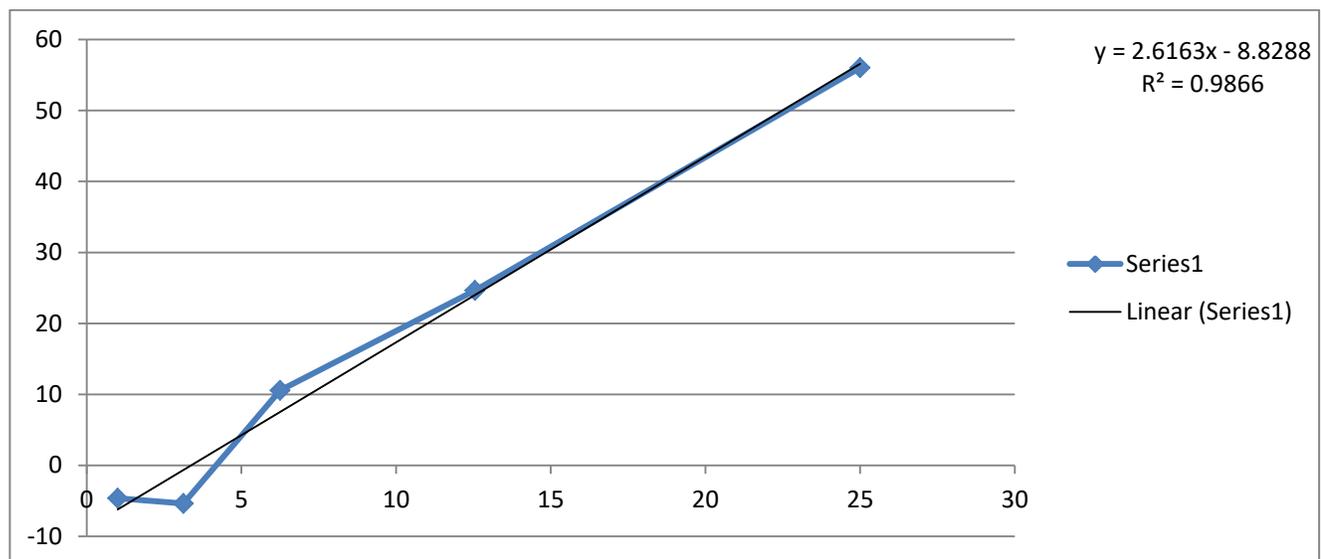
2. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **3** against DU145



X-axis = concentration ( $\mu\text{M}$ ) of compound **3**

Y-axis = % Cell Proliferation Inhibition

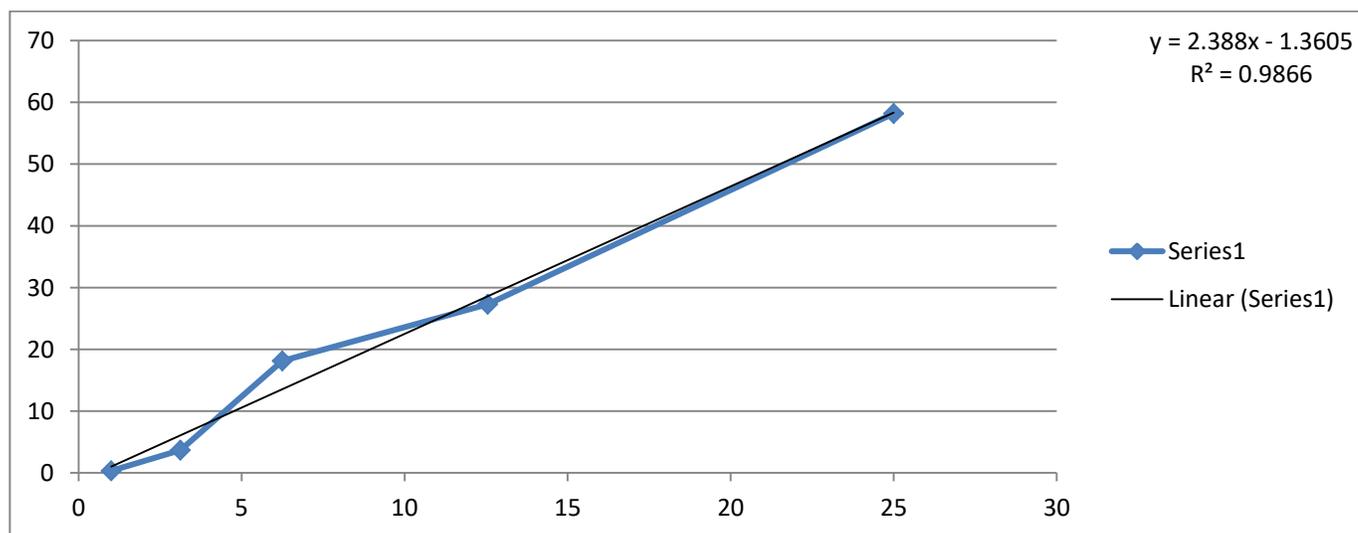
$\text{IC}_{50} = 23.233 \mu\text{M}$



X-axis = concentration (µM) of compound **3**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 22.485 µM

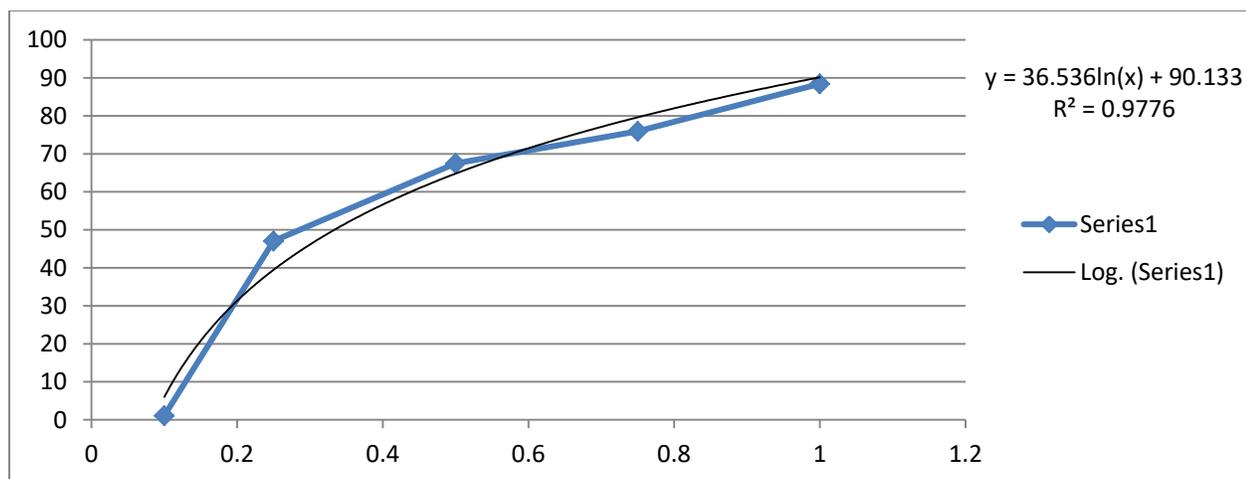


X-axis = concentration (µM) of compound **3**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 21.508 µM

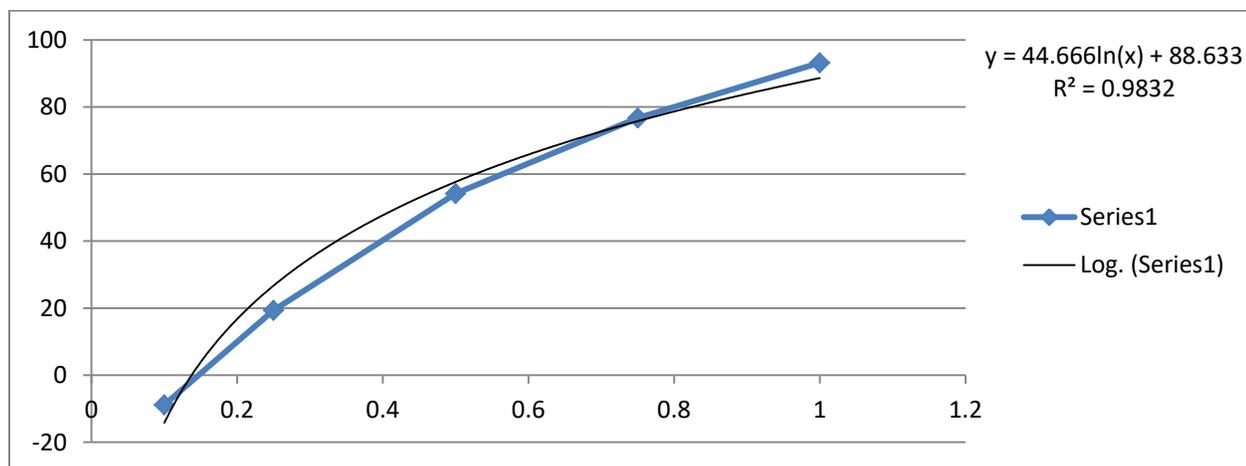
3. The curves that we used to calculate the IC<sub>50</sub> value for compound **3** against LNCaP



X-axis = concentration (µM) of compound **3**

Y-axis = % Cell Proliferation Inhibition

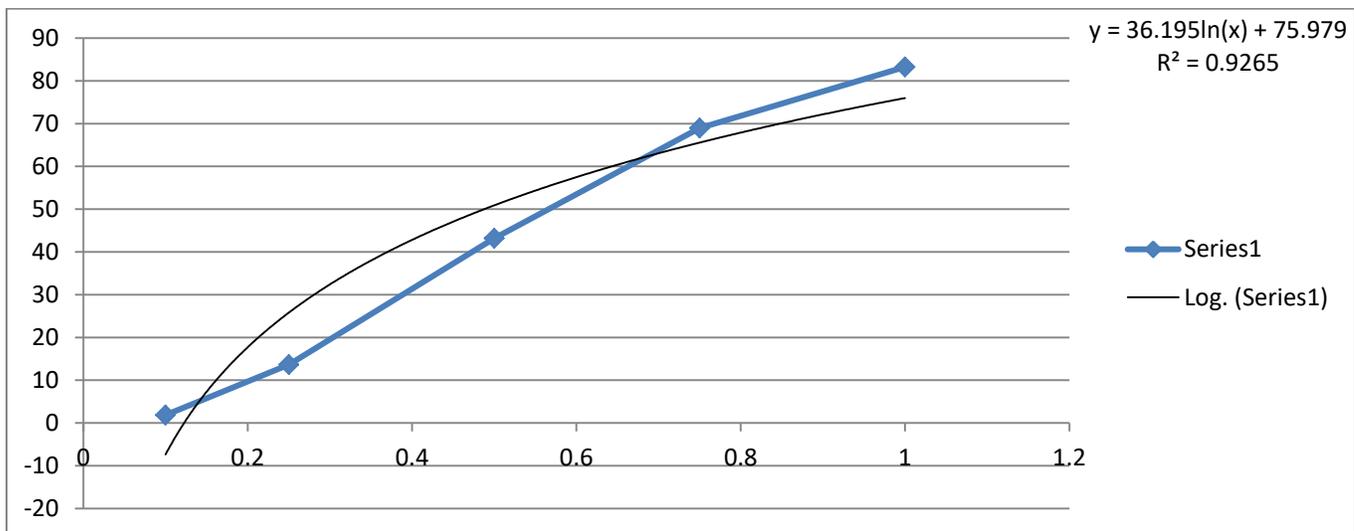
IC<sub>50</sub> = 0.333 µM



X-axis = concentration (µM) of compound **3**

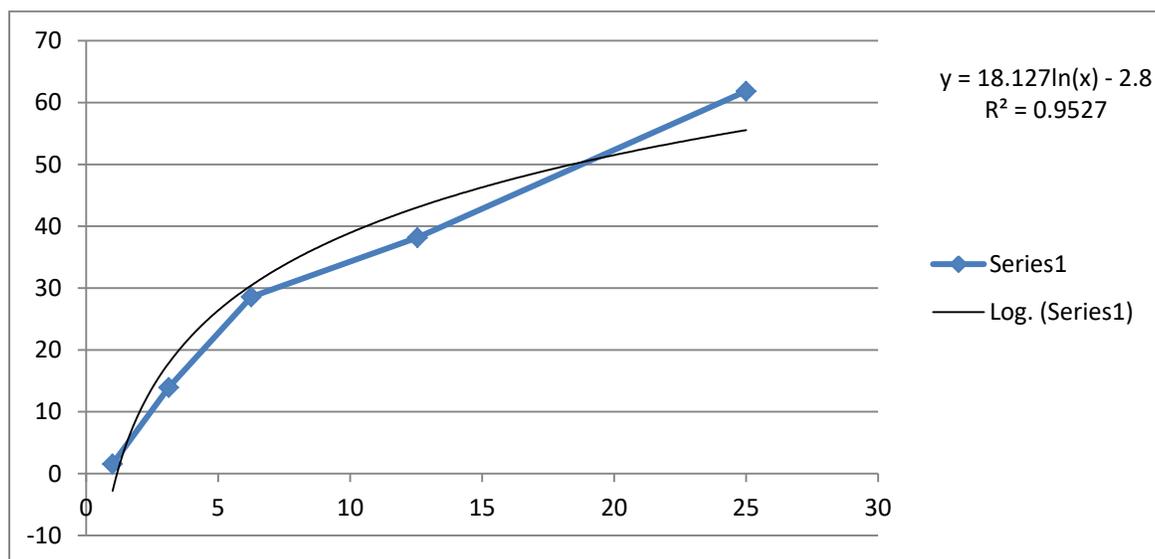
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 0.421 µM

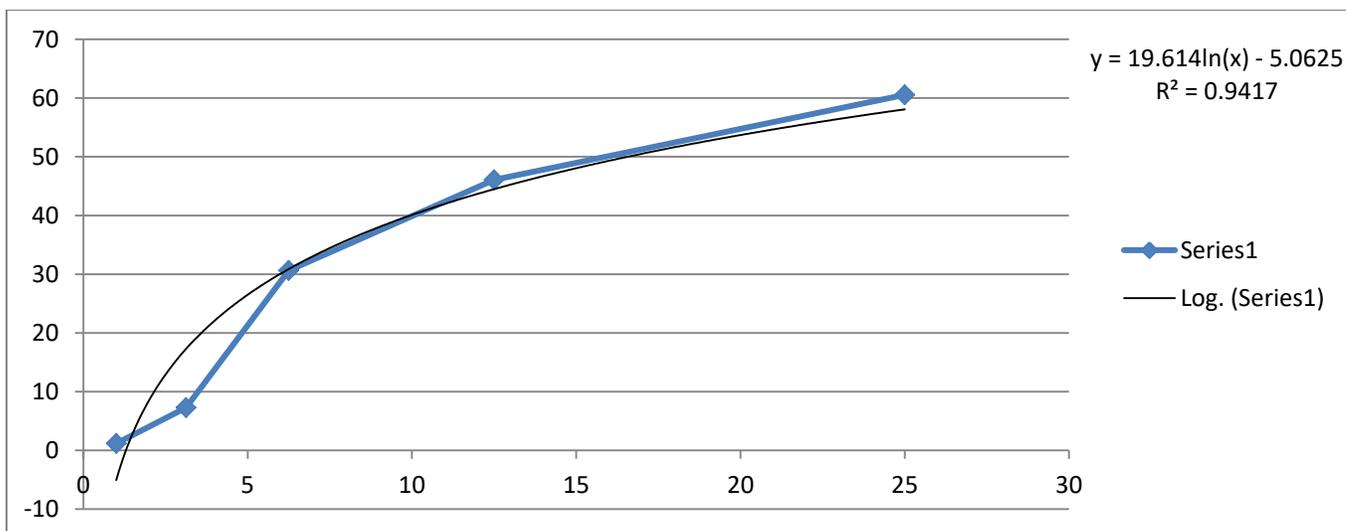


X-axis = concentration ( $\mu\text{M}$ ) of compound **3**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} = 0.488 \mu\text{M}$

4. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **4** against PC-3



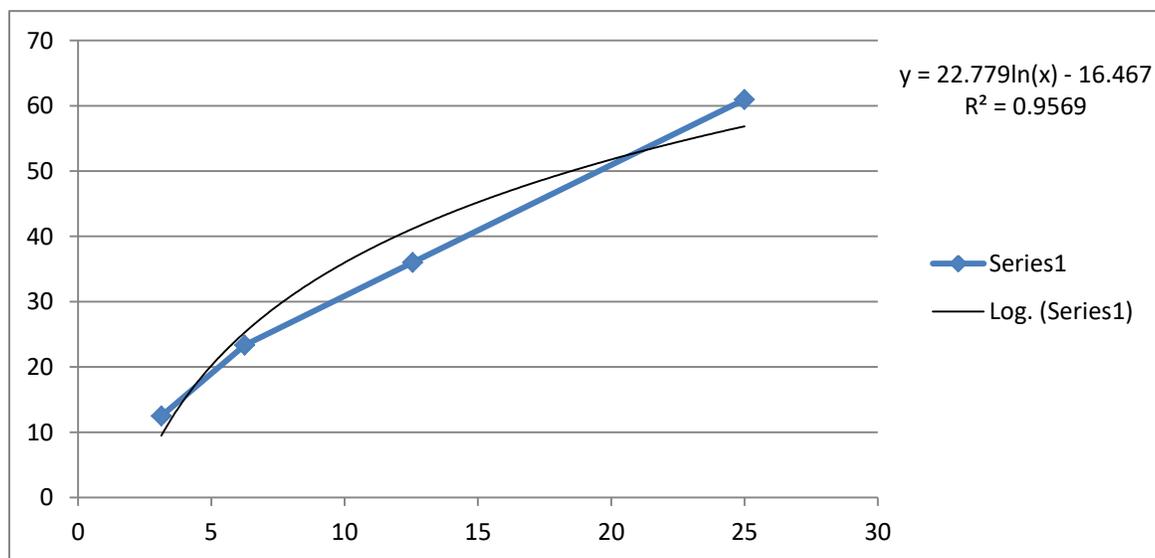
X-axis = concentration ( $\mu\text{M}$ ) of compound **4**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} = 18.408 \mu\text{M}$



X-axis = concentration ( $\mu\text{M}$ ) of compound 4

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 16.565 \mu\text{M}$

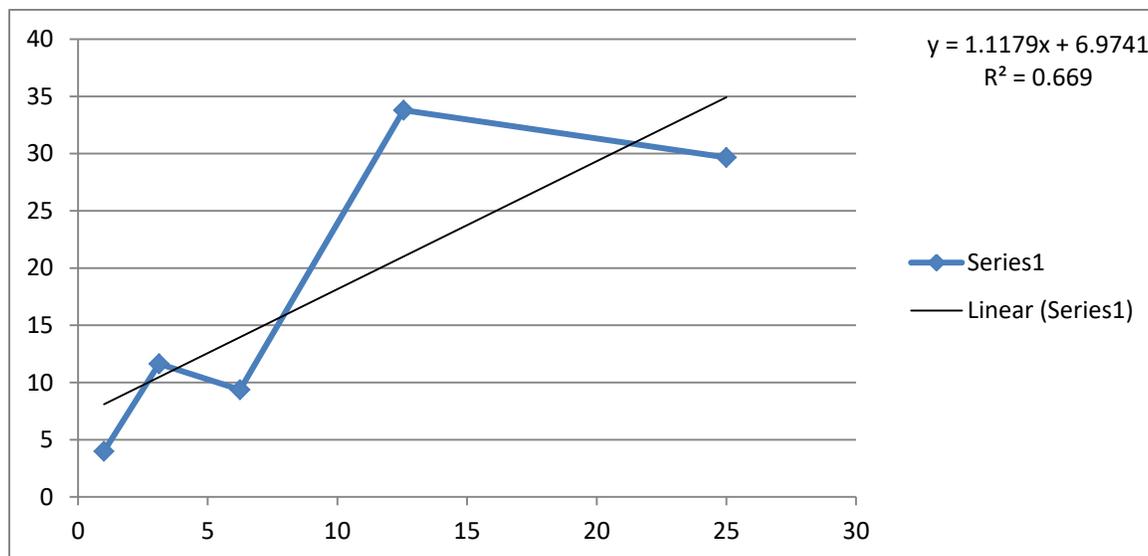


X-axis = concentration ( $\mu\text{M}$ ) of compound 4

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 18.5025 \mu\text{M}$

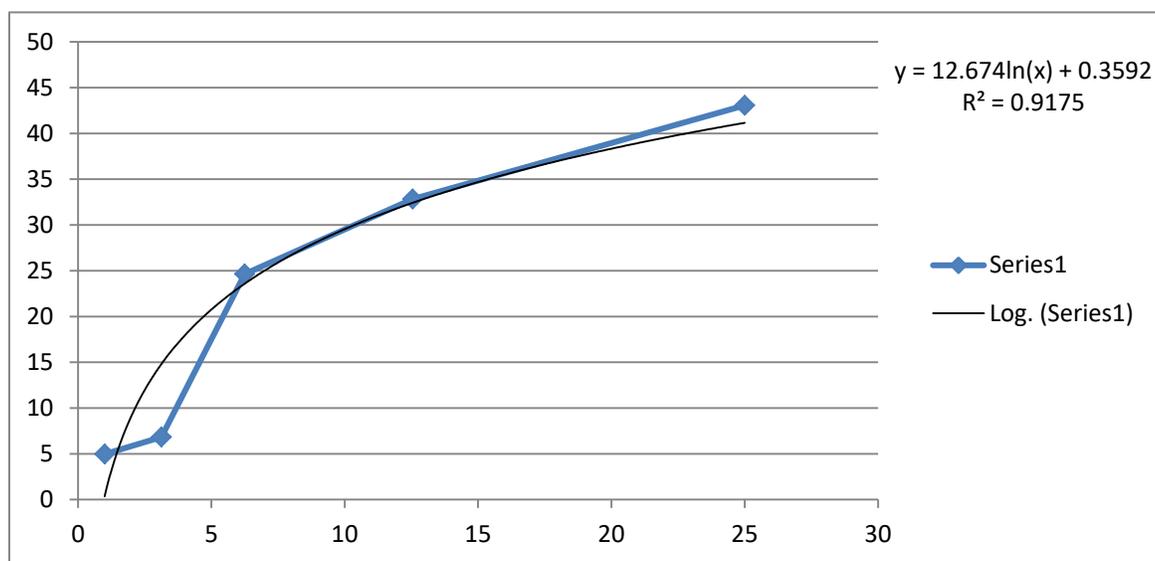
5. The curves that we used to calculate the IC<sub>50</sub> value for compound **4** against DU145



X-axis = concentration (µM) of compound **4**

Y-axis = % Cell Proliferation Inhibition

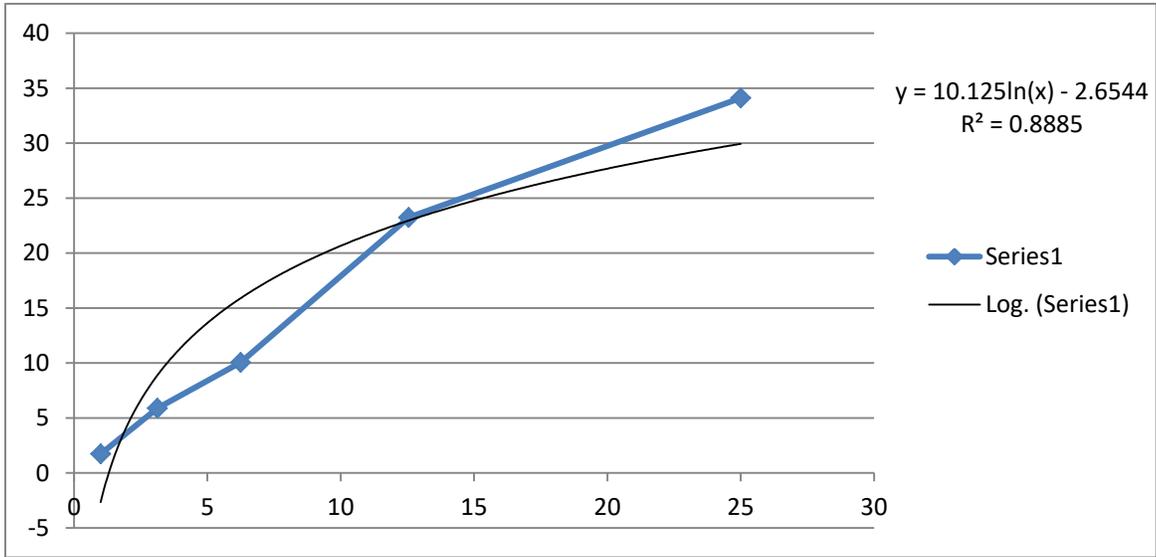
IC<sub>50</sub> > 25 µM



X-axis = concentration (µM) of compound **4**

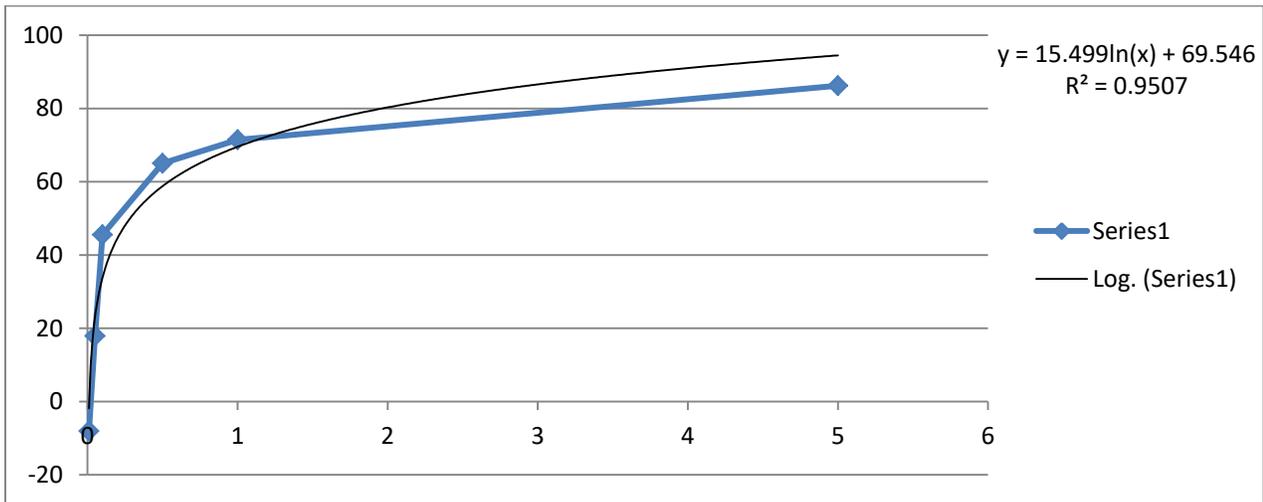
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

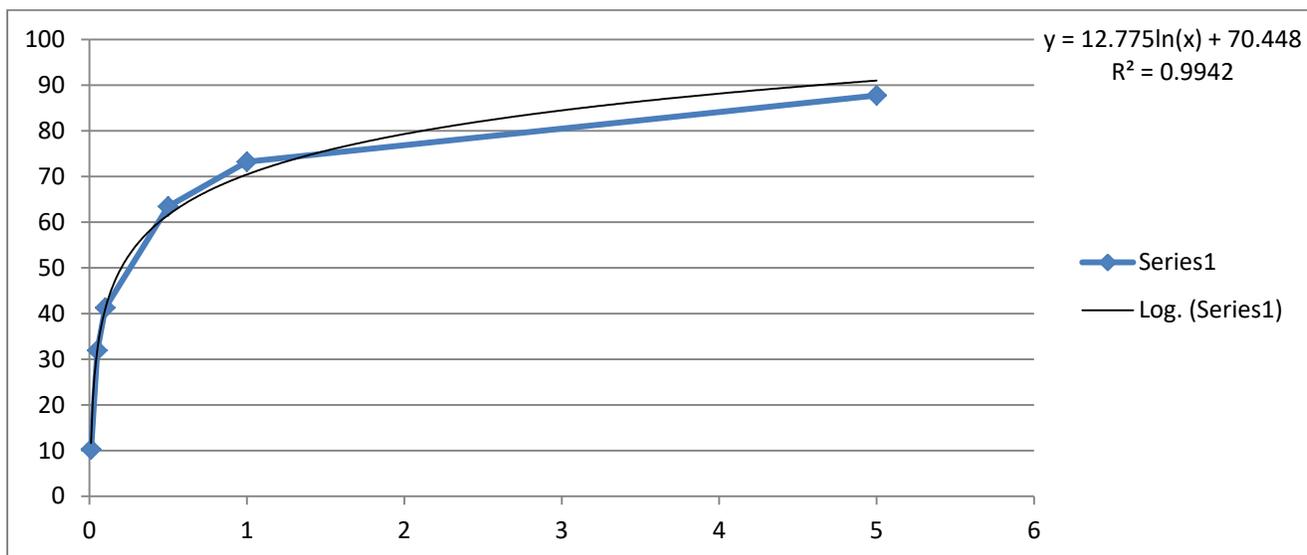


X-axis = concentration (μM) of compound **4**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$

6. The curves that we used to calculate the  $IC_{50}$  value for compound **4** against LNCaP



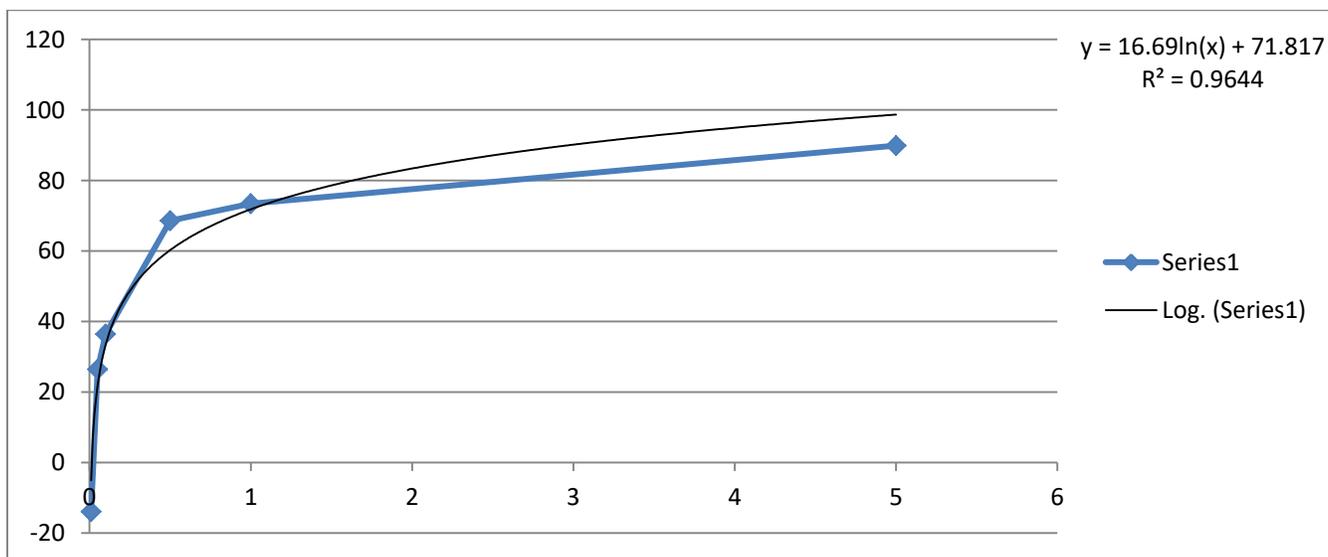
X-axis = concentration (μM) of compound **4**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} = 0.283 \mu M$



X-axis = concentration (µM) of compound 4

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 0.202 µM

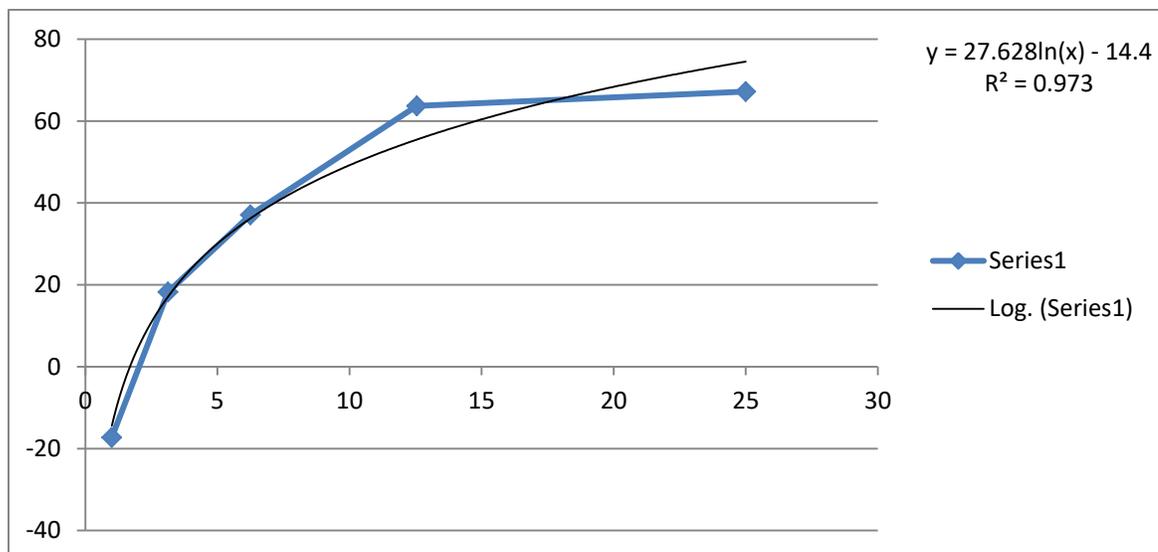


X-axis = concentration (µM) of compound 4

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 0.271 µM

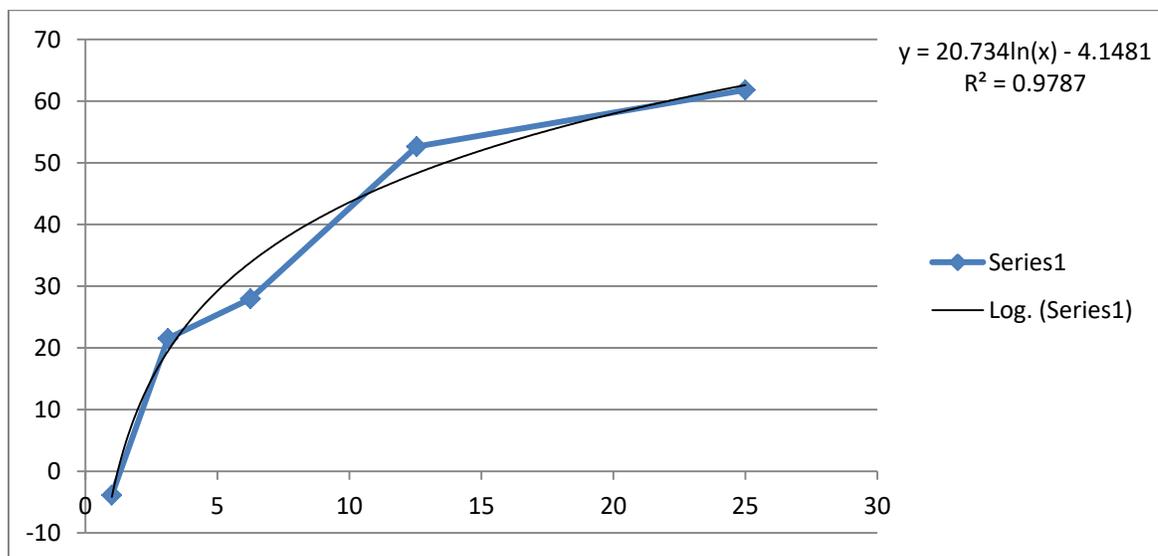
7. The curves that we used to calculate the IC<sub>50</sub> value for compound **5** against PC-3



X-axis = concentration (µM) of compound **5**

Y-axis = % Cell Proliferation Inhibition

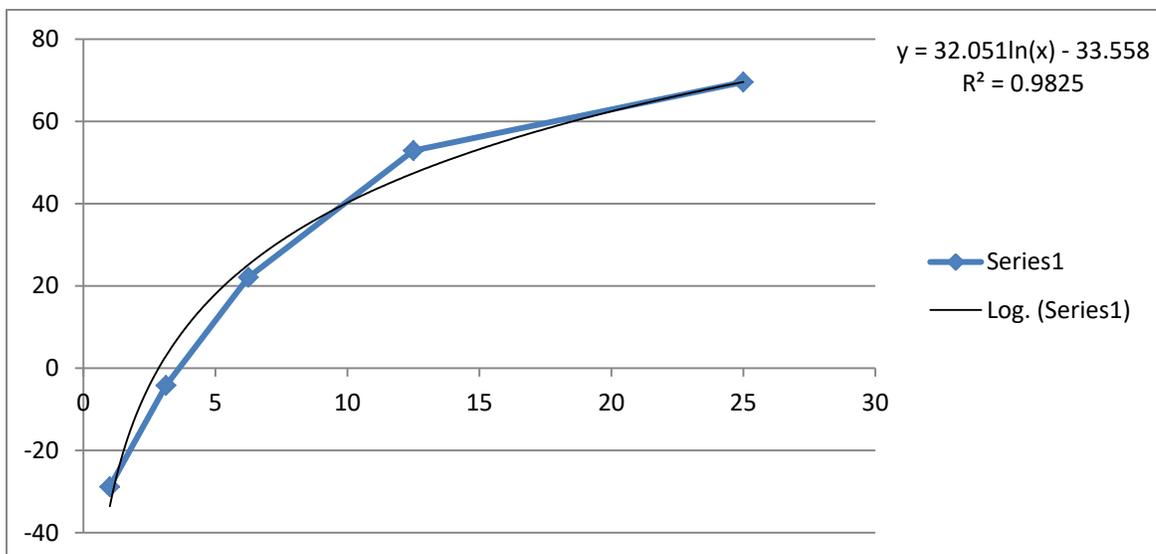
IC<sub>50</sub> = 10.288 µM



X-axis = concentration (µM) of compound **5**

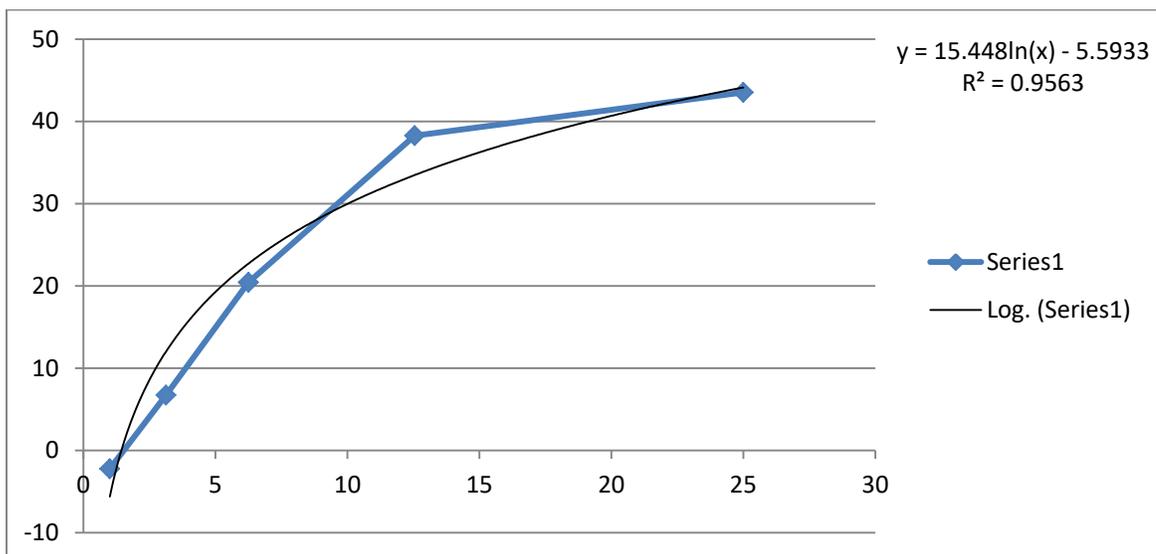
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 13.620 µM

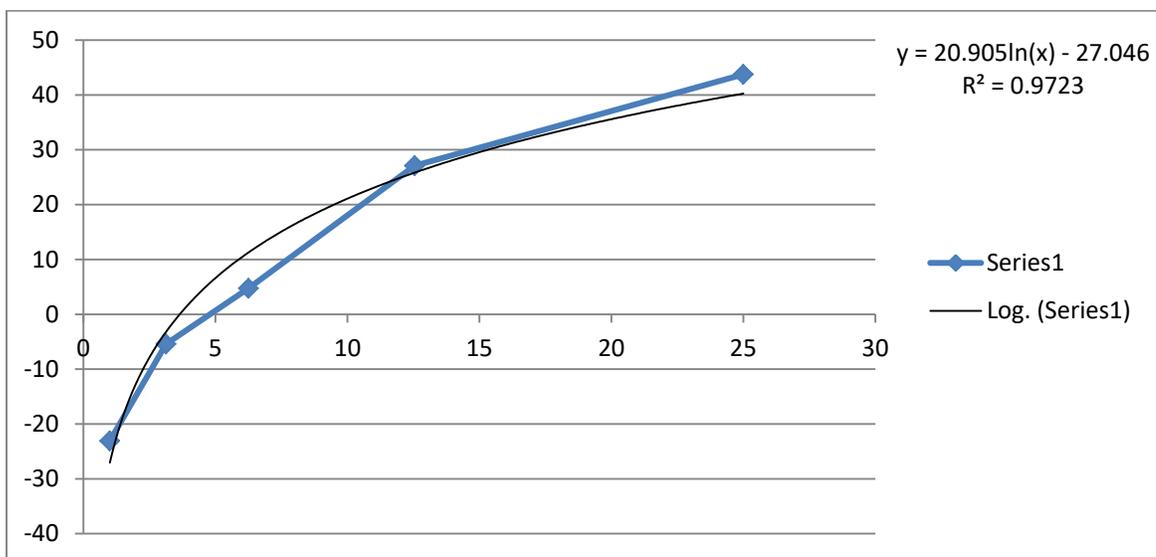


X-axis = concentration ( $\mu\text{M}$ ) of compound **5**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} = 13.575 \mu\text{M}$

8. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **5** against DU145



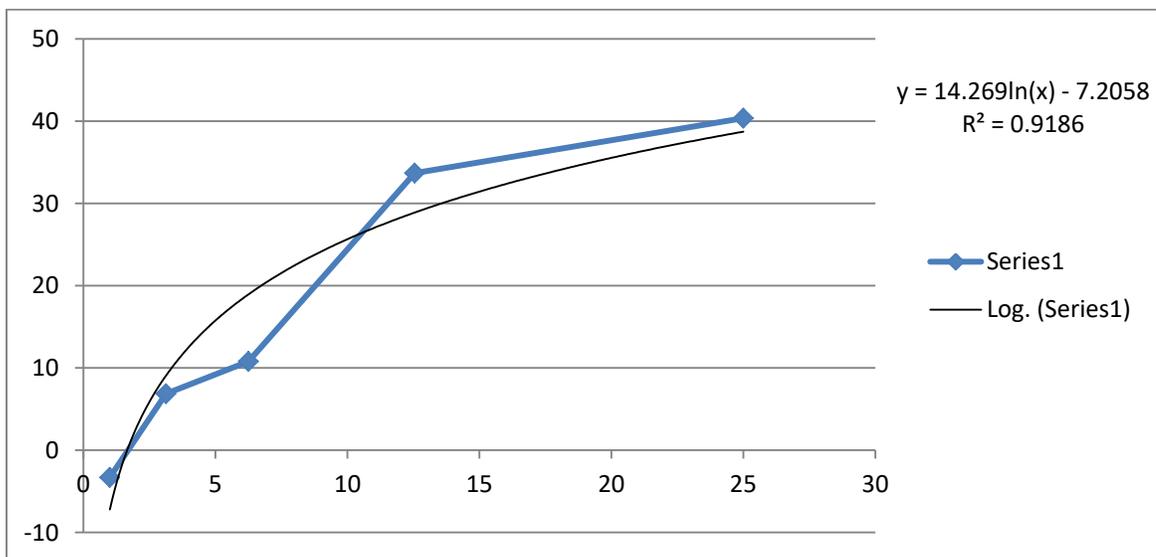
X-axis = concentration ( $\mu\text{M}$ ) of compound **5**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} > 25 \mu\text{M}$



X-axis = concentration (µM) of compound **5**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

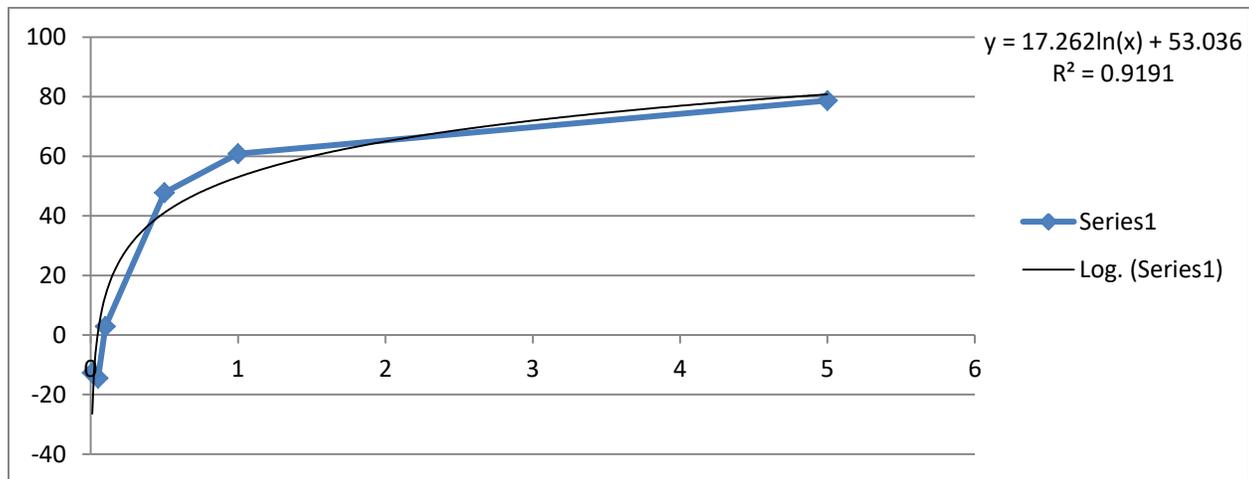


X-axis = concentration (µM) of compound **5**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

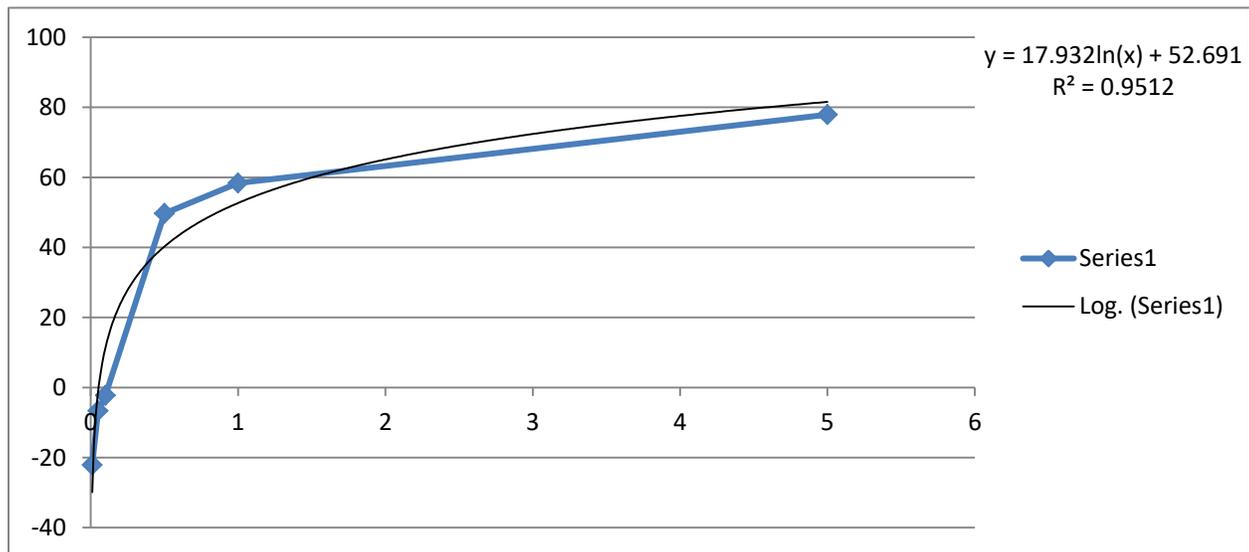
9. The curves that we used to calculate the IC<sub>50</sub> value for compound **5** against LNCaP



X-axis = concentration (µM) of compound **5**

Y-axis = % Cell Proliferation Inhibition

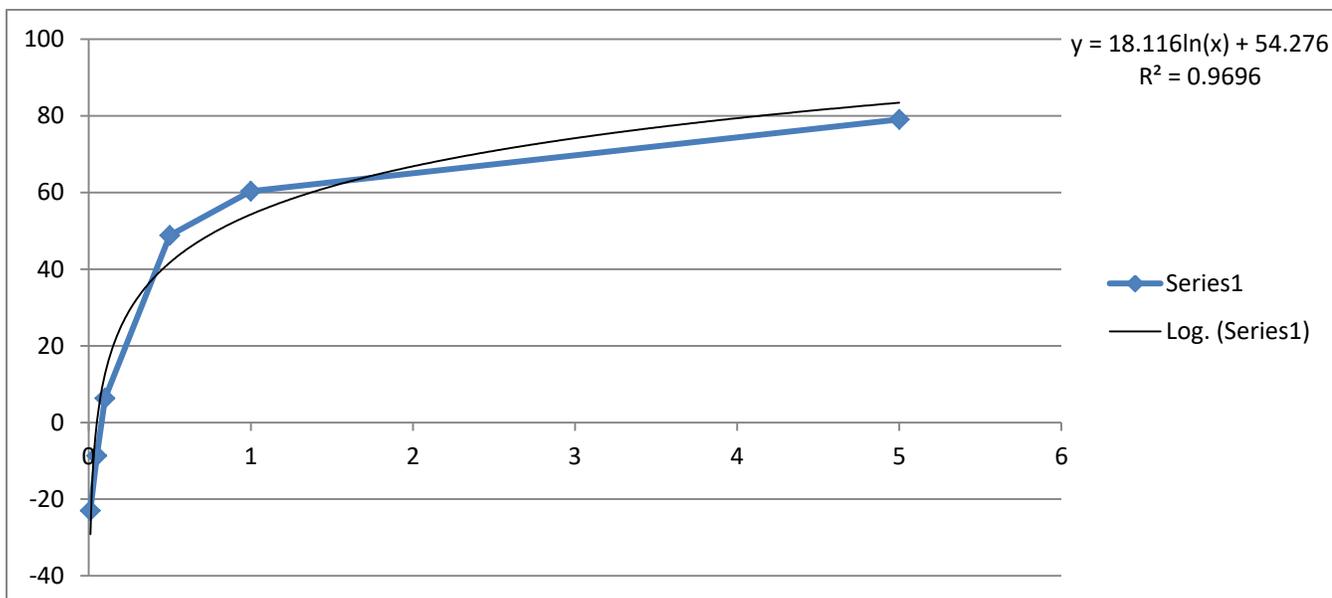
IC<sub>50</sub> = 0.839 µM



X-axis = concentration (µM) of compound **5**

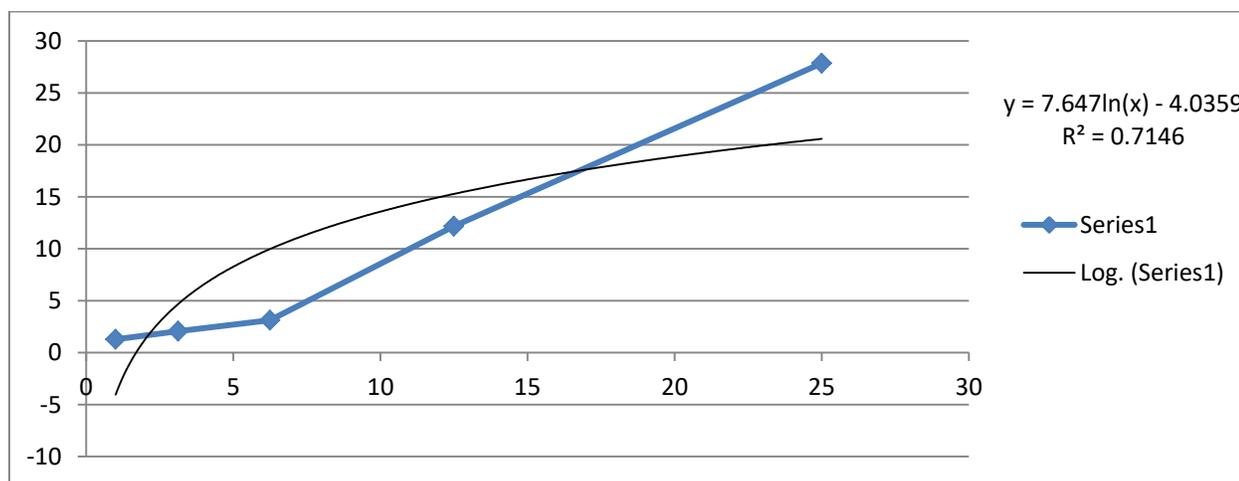
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 0.861 µM

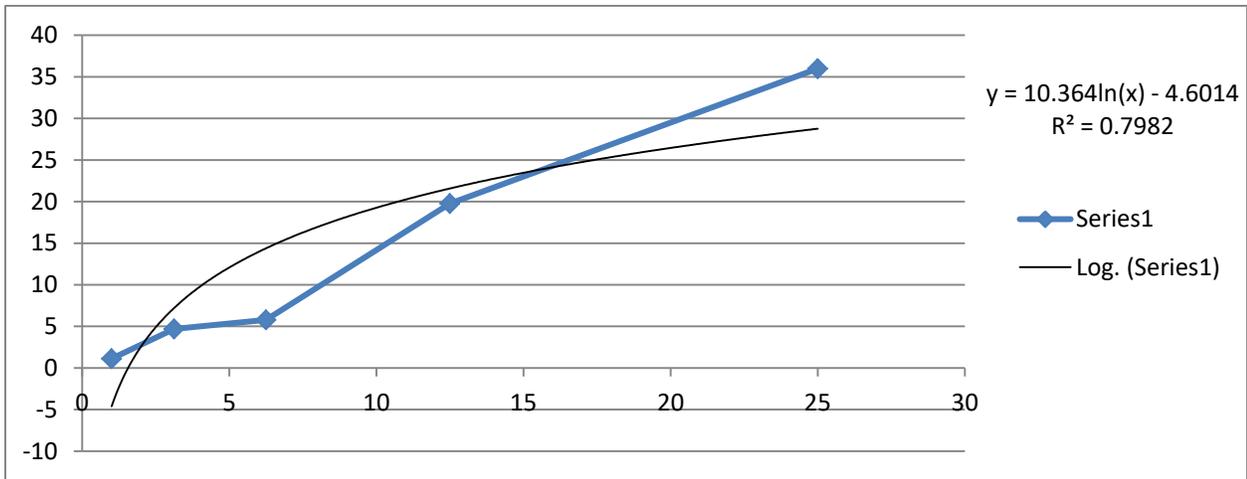


X-axis = concentration ( $\mu\text{M}$ ) of compound 5  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} = 0.790 \mu\text{M}$

10. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound 6 against PC-3



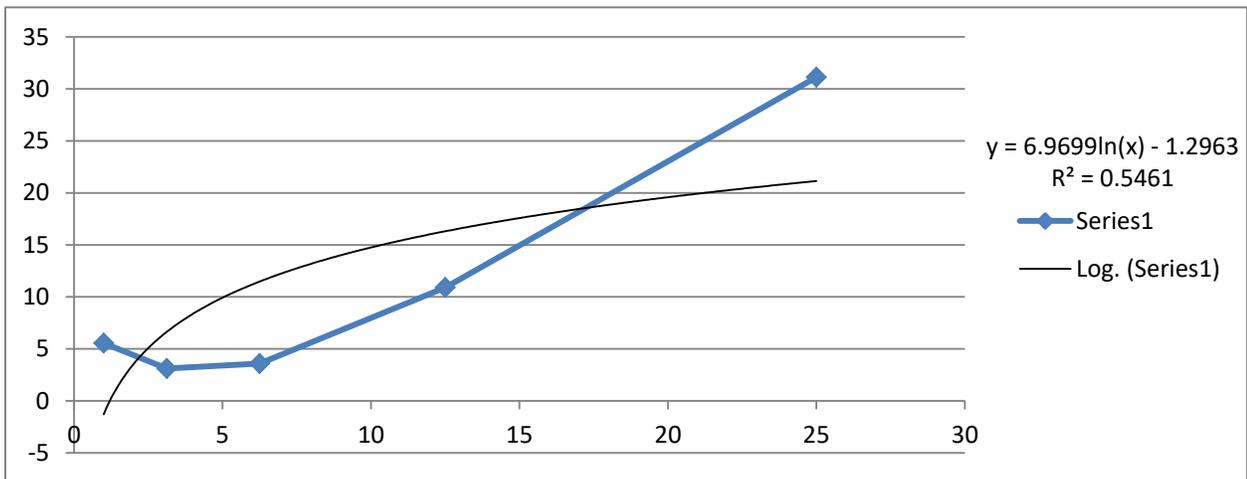
X-axis = concentration ( $\mu\text{M}$ ) of compound 6  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} > 25 \mu\text{M}$



X-axis = concentration (µM) of compound 6

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

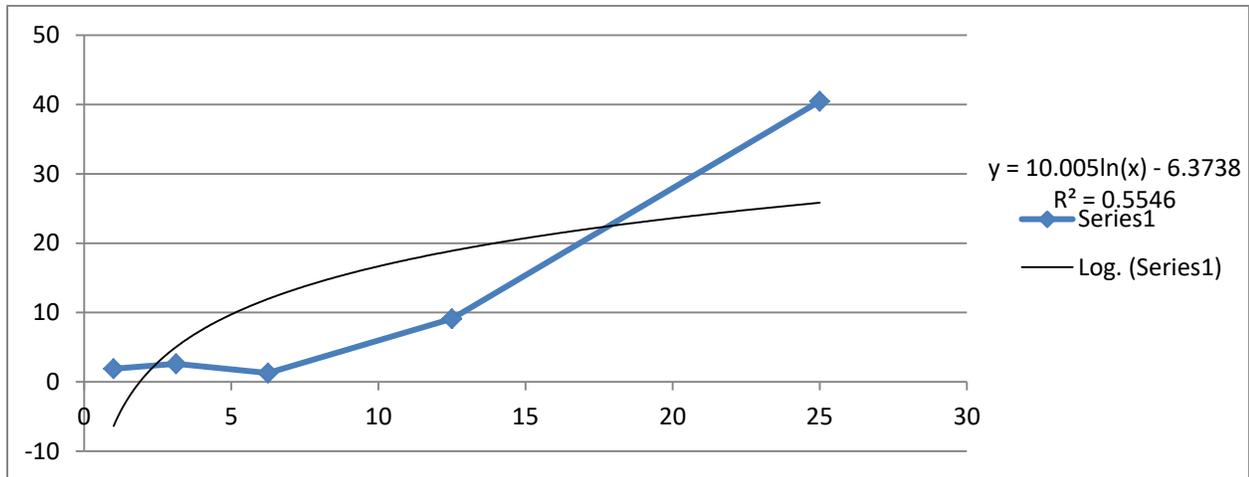


X-axis = concentration (µM) of compound 6

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

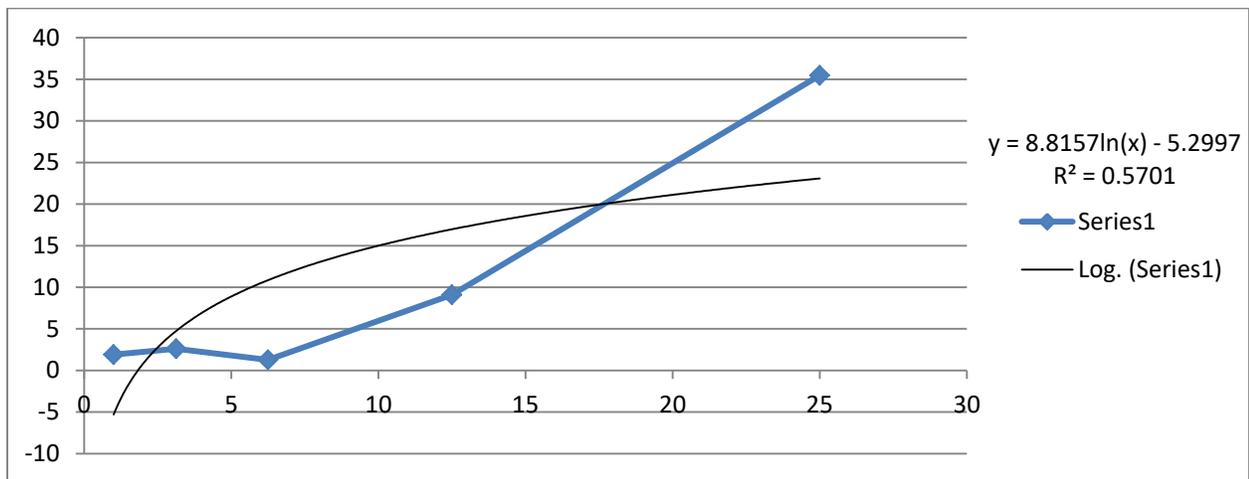
11. The curves that we used to calculate the IC<sub>50</sub> value for compound **6** against DU145



X-axis = concentration (µM) of compound **6**

Y-axis = % Cell Proliferation Inhibition

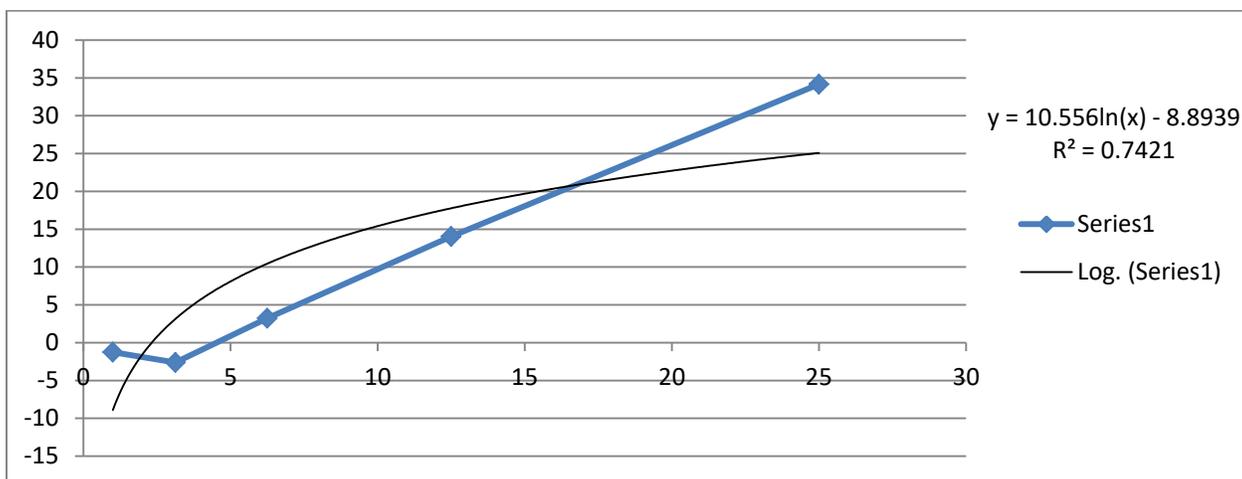
IC<sub>50</sub> > 25 µM



X-axis = concentration (µM) of compound **6**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

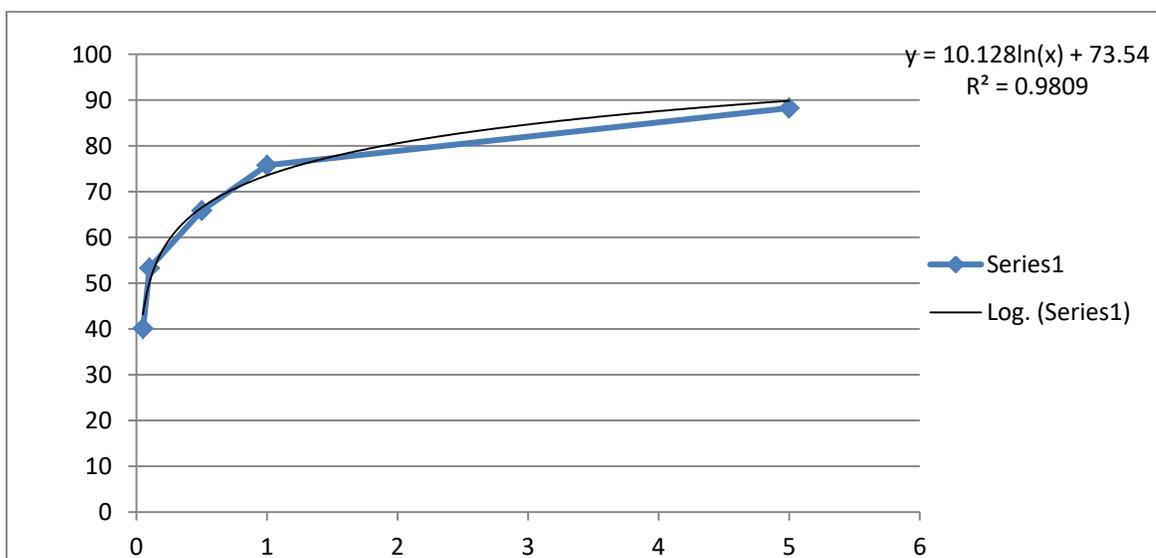


X-axis = concentration ( $\mu\text{M}$ ) of compound **6**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} > 25 \mu\text{M}$

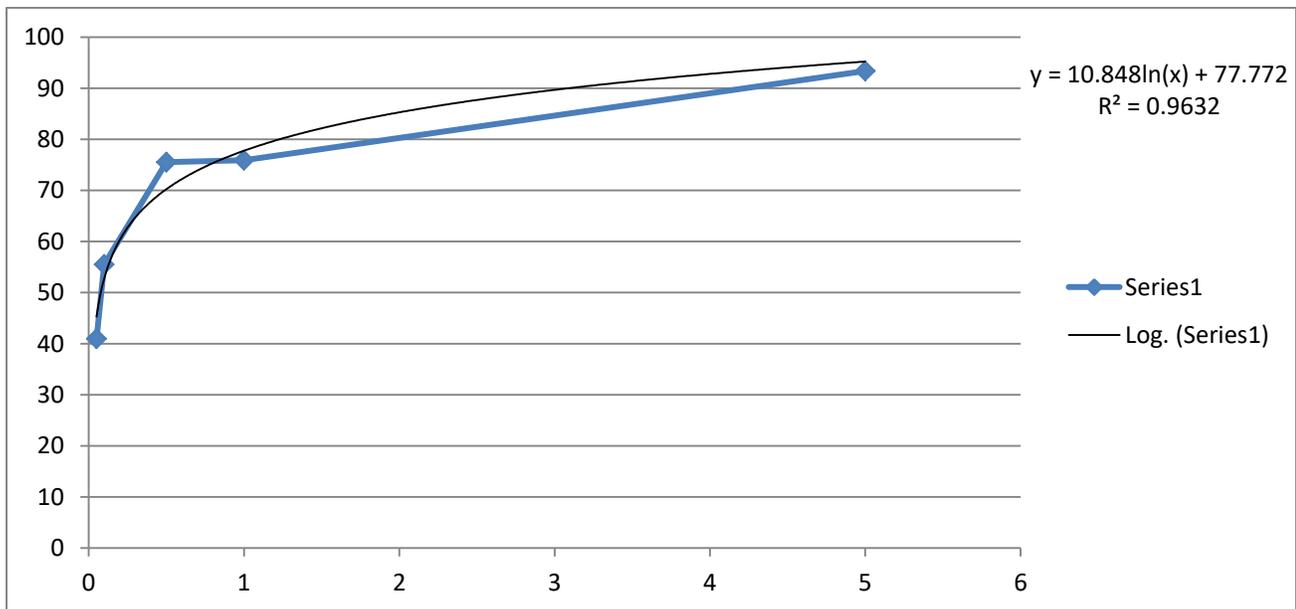
12. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **6** against LNCaP



X-axis = concentration ( $\mu\text{M}$ ) of compound **6**

Y-axis = % Cell Proliferation Inhibition

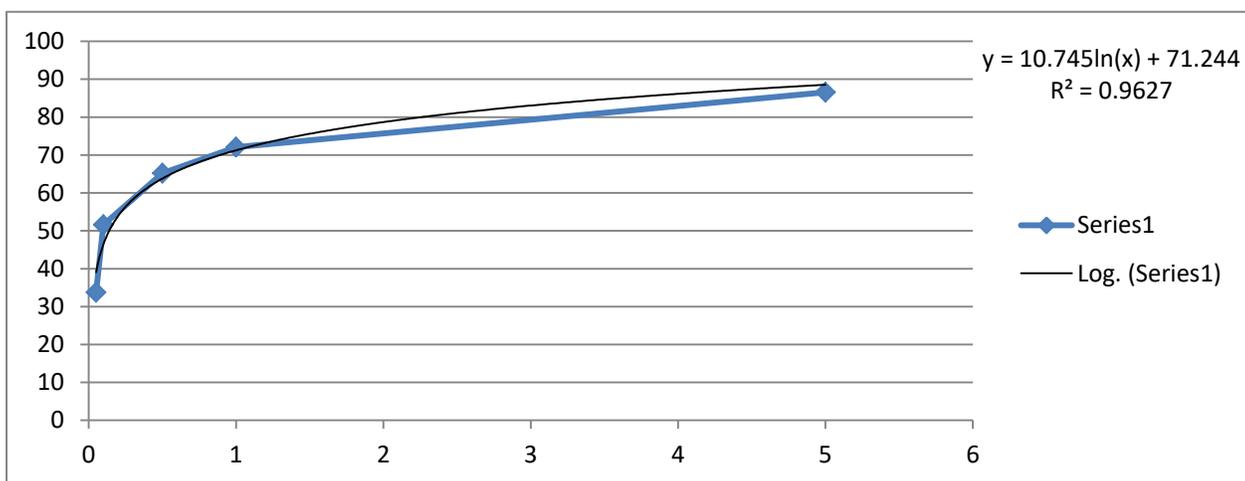
$\text{IC}_{50} = 0.0979 \mu\text{M}$



X-axis = concentration (µM) of compound **6**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 0.0773 µM

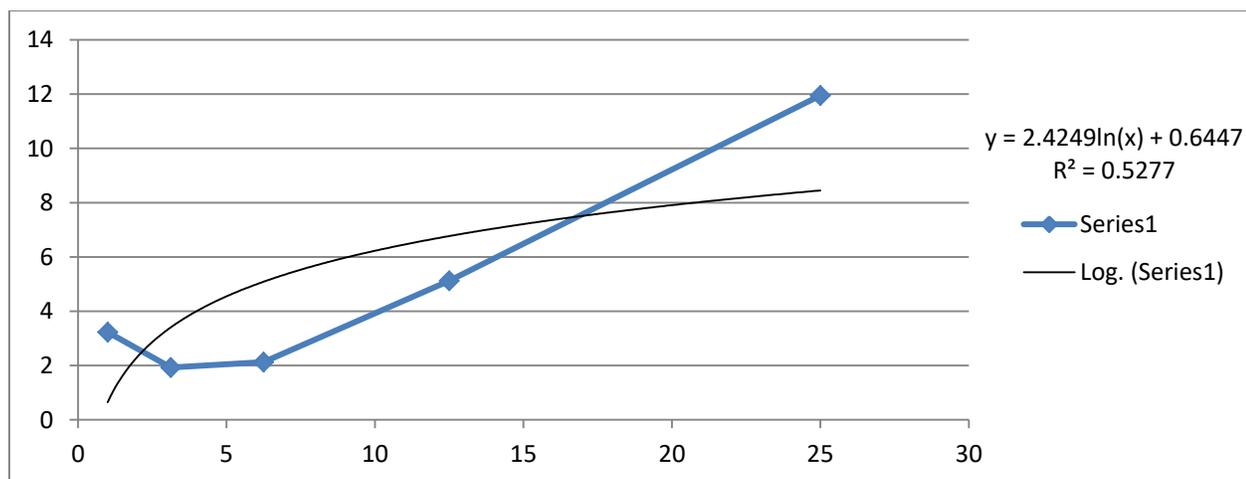


X-axis = concentration (µM) of compound **6**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 0.1385 µM

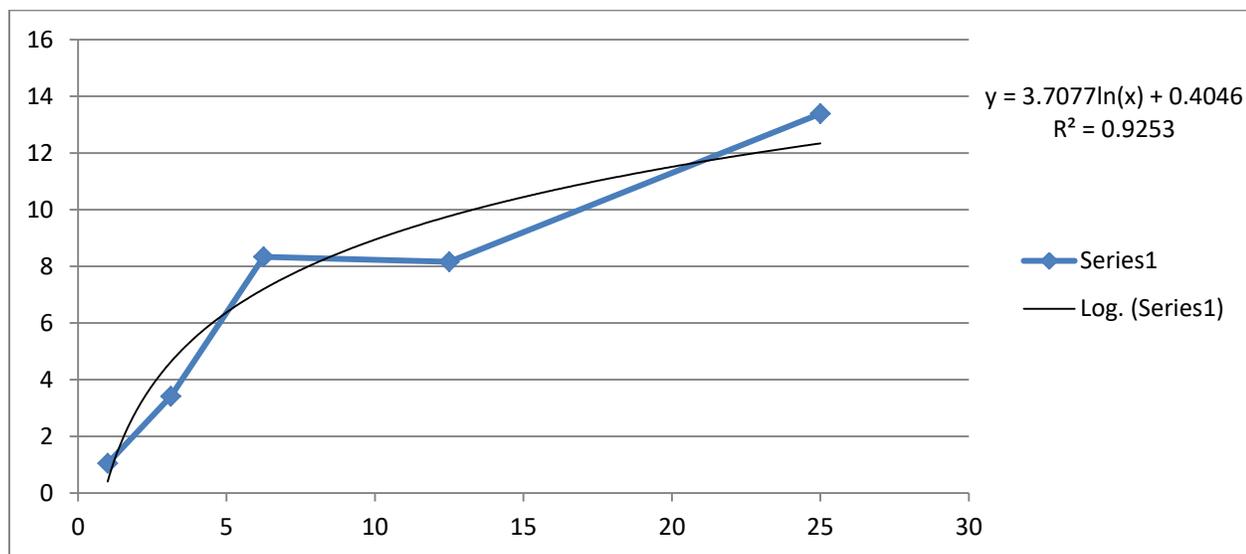
13. The curves that we used to calculate the IC<sub>50</sub> value for compound 7 against PC-3



X-axis = concentration (µM) of compound 7

Y-axis = % Cell Proliferation Inhibition

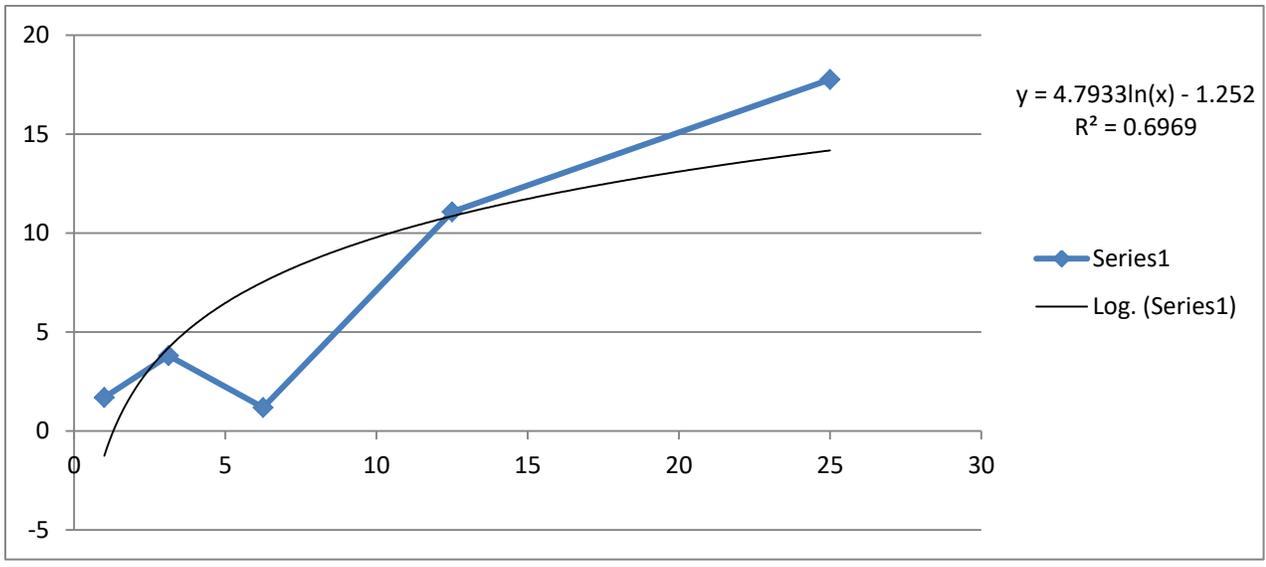
IC<sub>50</sub> > 25 µM



X-axis = concentration (µM) of compound 7

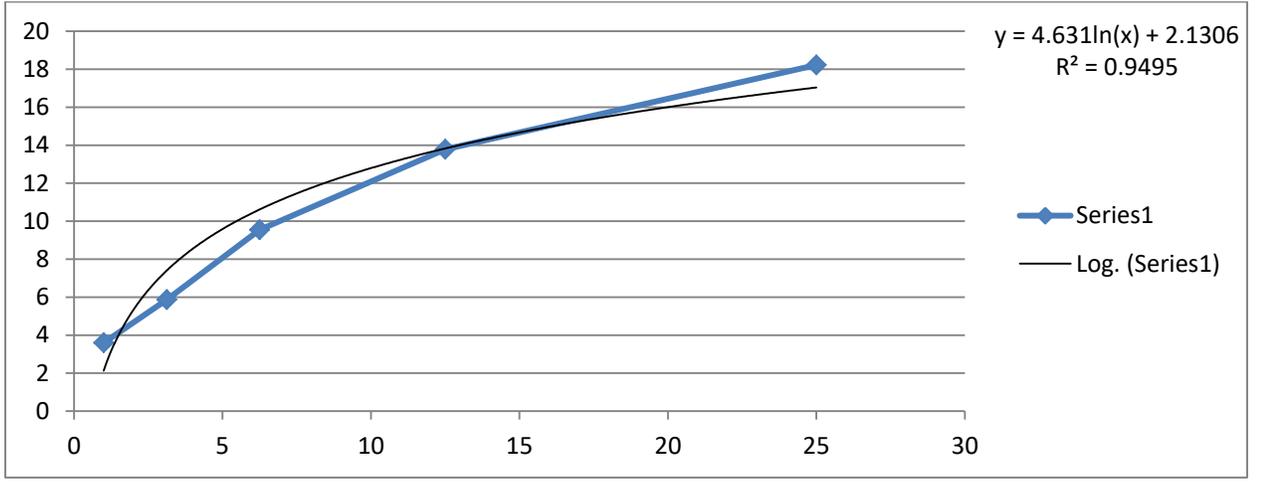
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

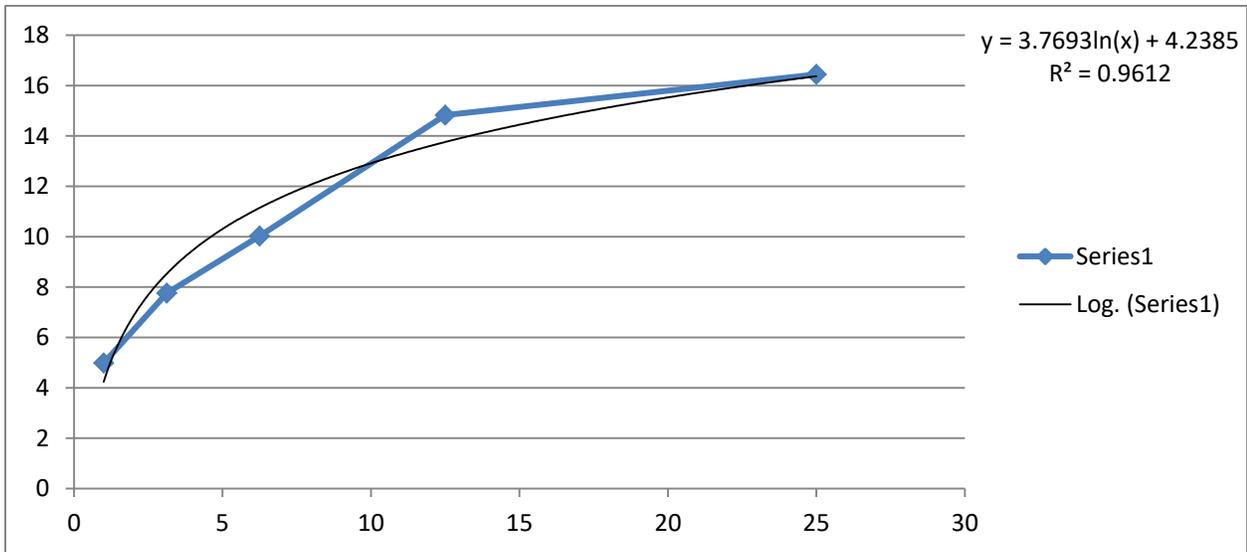


X-axis = concentration (µM) of compound 7  
 Y-axis = % Cell Proliferation Inhibition  
 IC<sub>50</sub> > 25 µM

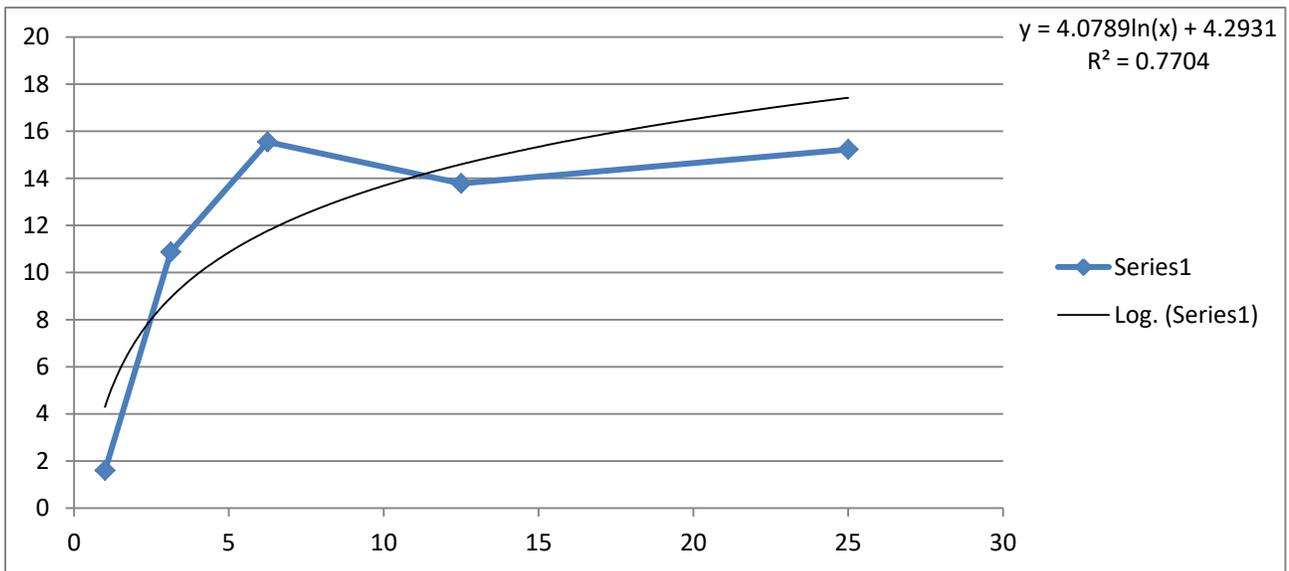
14. The curves that we used to calculate the IC<sub>50</sub> value for compound 7 against DU145



X-axis = concentration (µM) of compound 7  
 Y-axis = % Cell Proliferation Inhibition  
 IC<sub>50</sub> > 25 µM

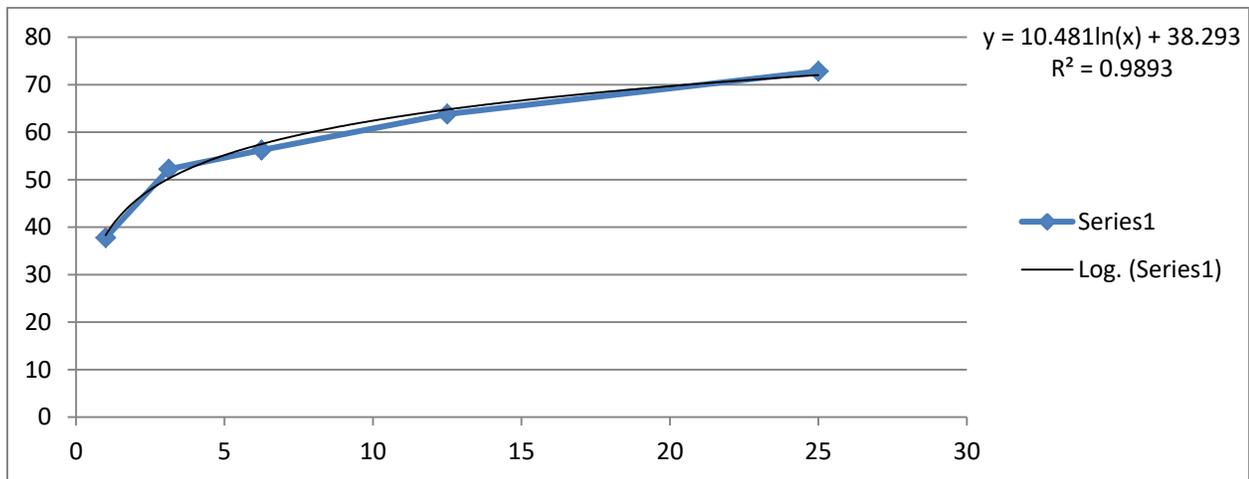


X-axis = concentration (µM) of compound 7  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$



X-axis = concentration (µM) of compound 7  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$

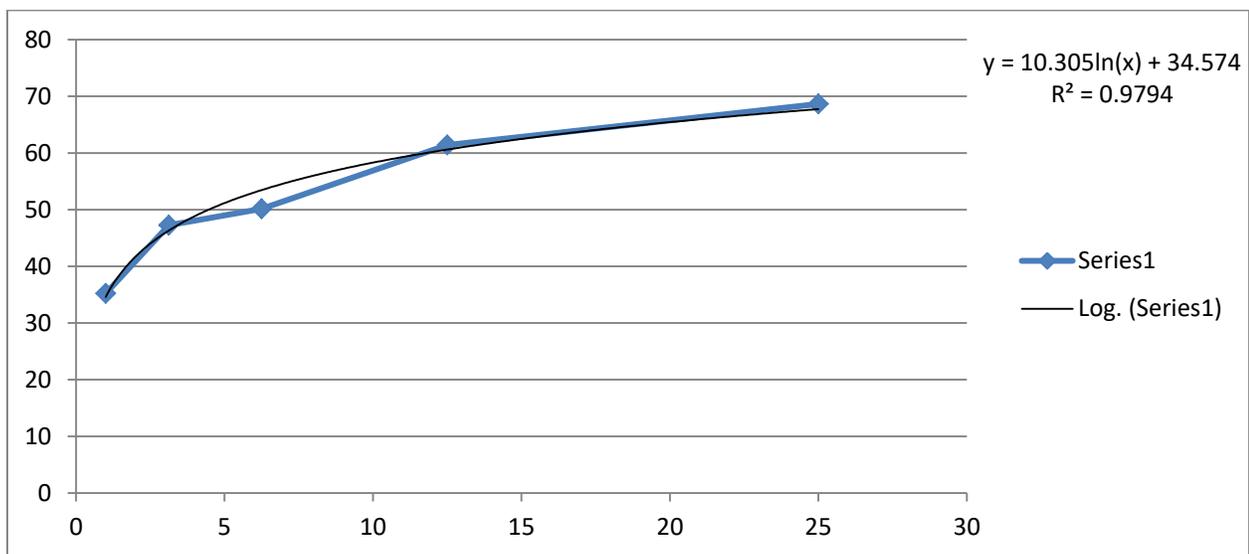
15. The curves that we used to calculate the IC<sub>50</sub> value for compound 7 against LNCaP



X-axis = concentration (µM) of compound 7

Y-axis = % Cell Proliferation Inhibition

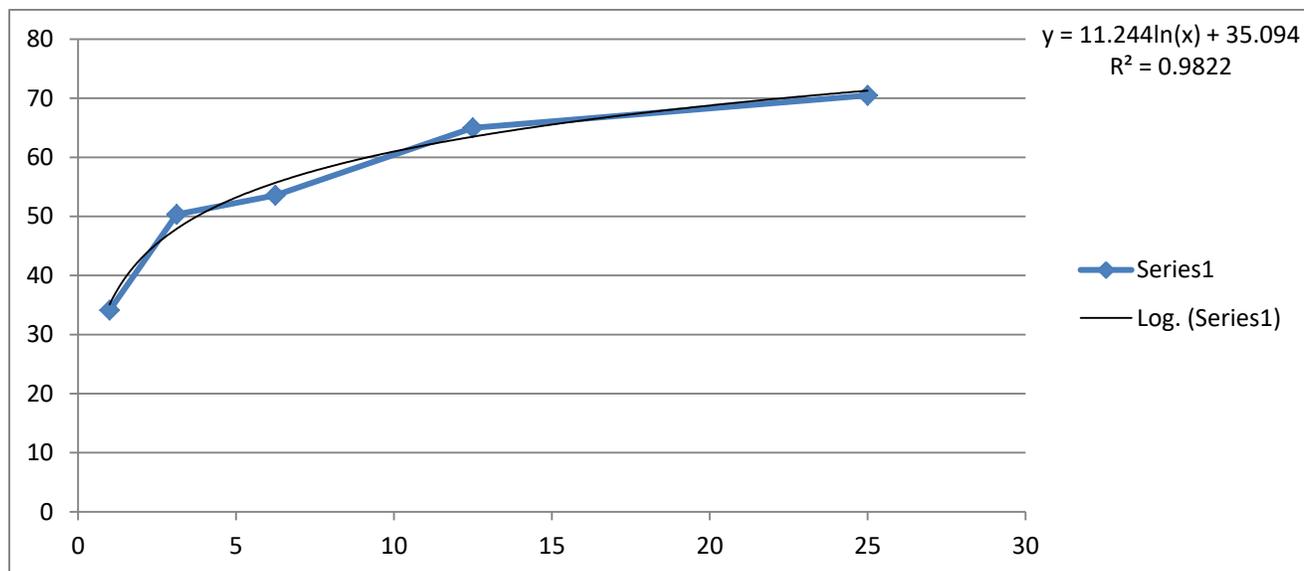
IC<sub>50</sub> = 3.055 µM



X-axis = concentration (µM) of compound 7

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 4.468 µM

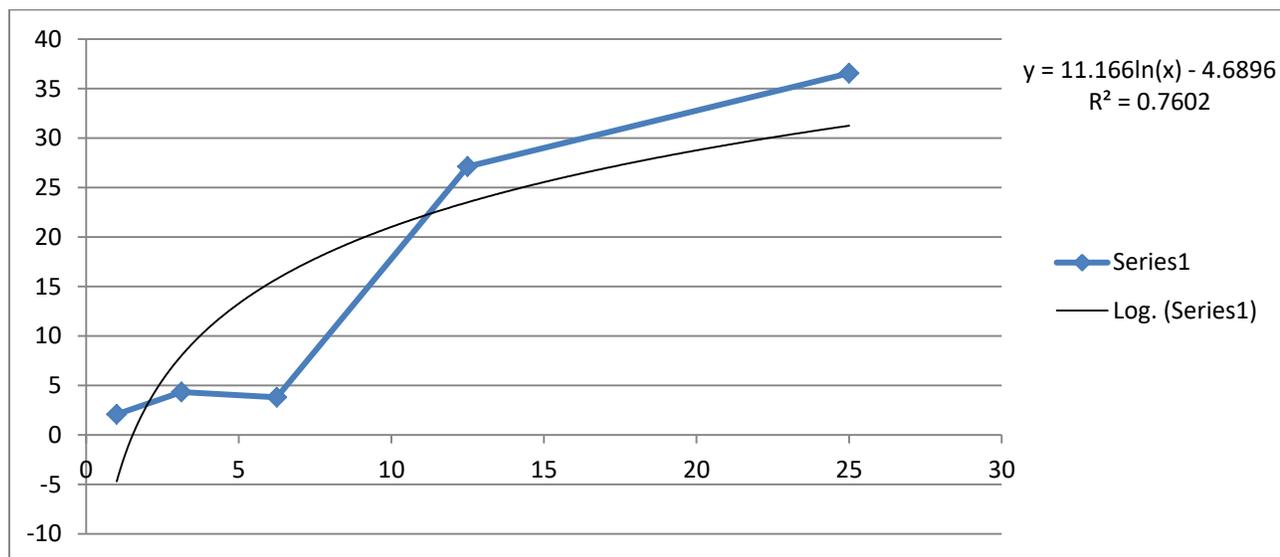


X-axis = concentration ( $\mu\text{M}$ ) of compound **7**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 3.765 \mu\text{M}$

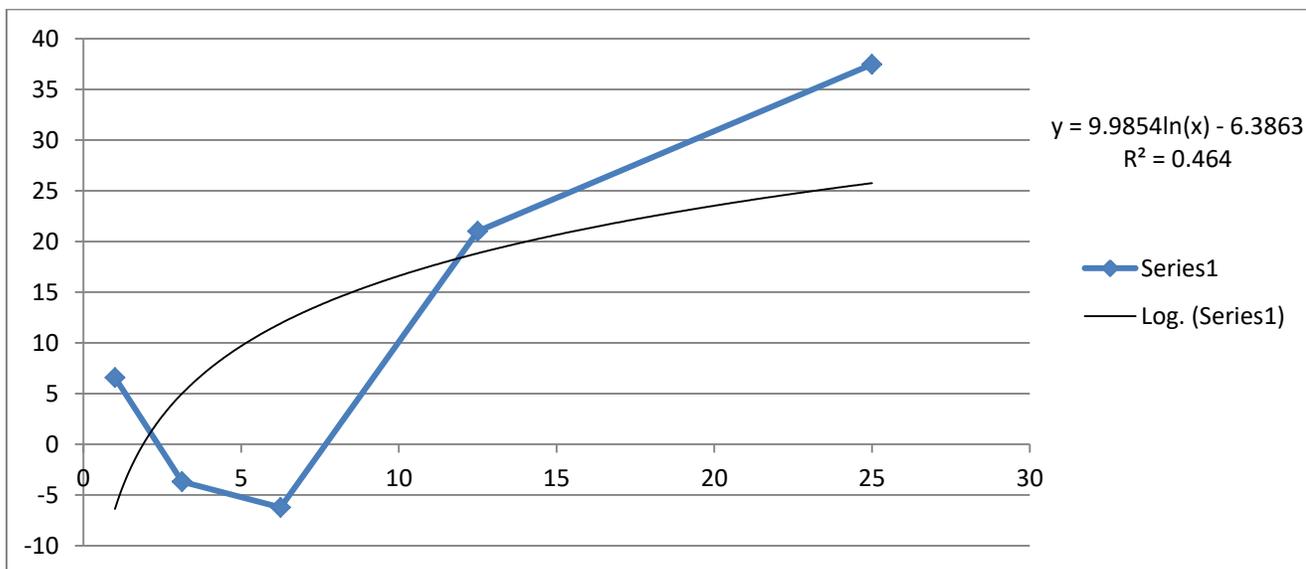
16. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **8** against PC-3



X-axis = concentration ( $\mu\text{M}$ ) of compound **8**

Y-axis = % Cell Proliferation Inhibition

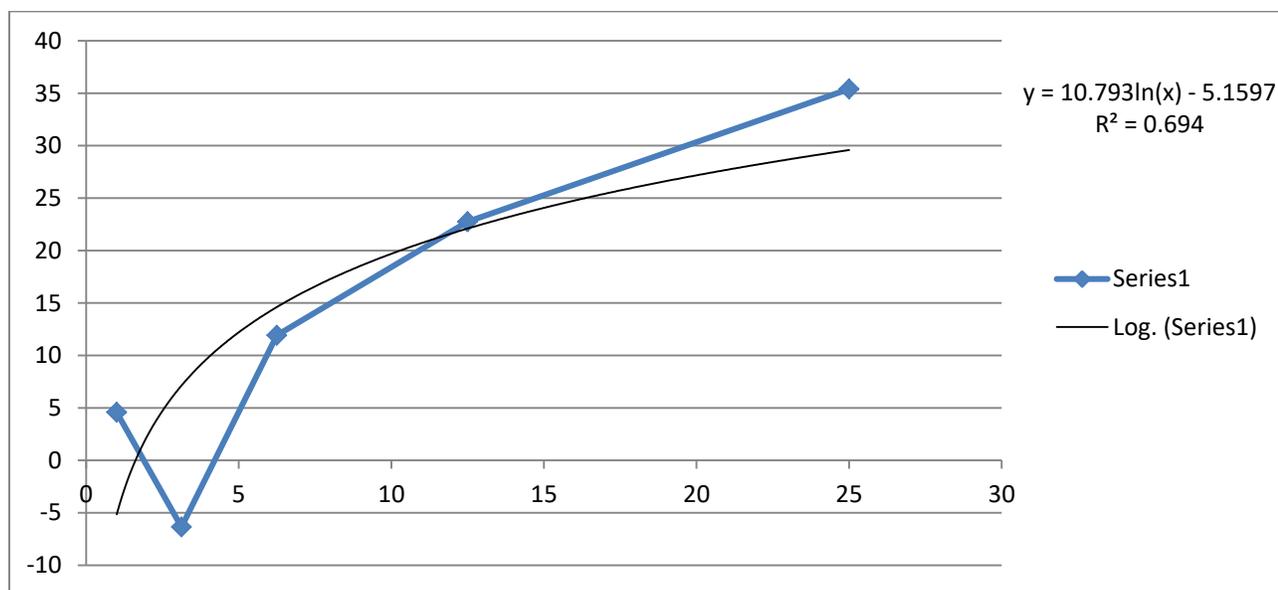
$\text{IC}_{50} > 25 \mu\text{M}$



X-axis = concentration (µM) of compound **8**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

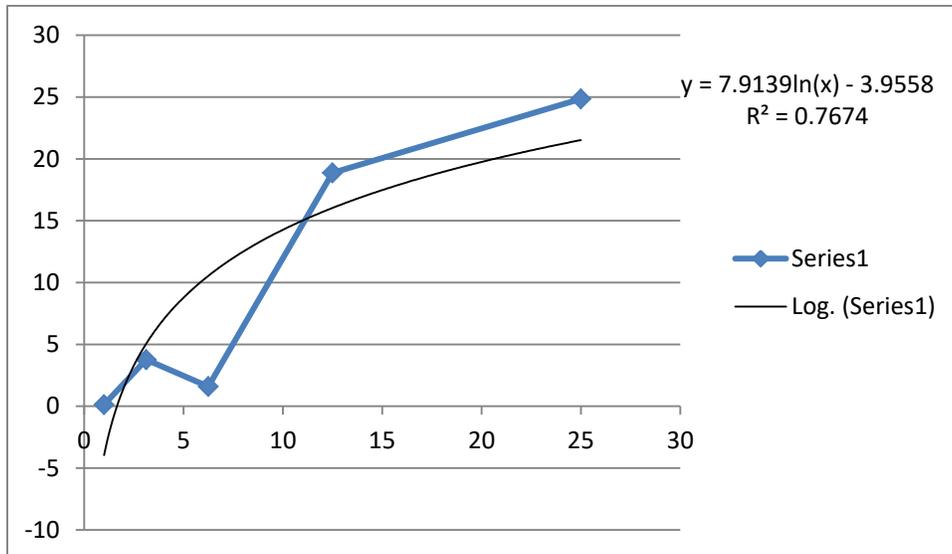


X-axis = concentration (µM) of compound **8**

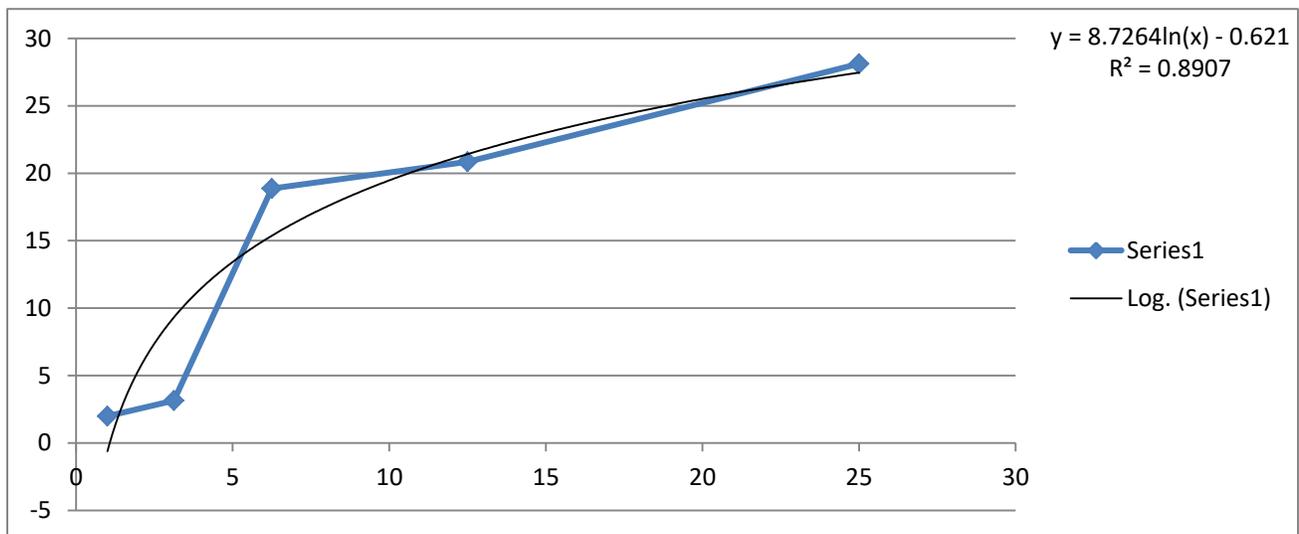
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

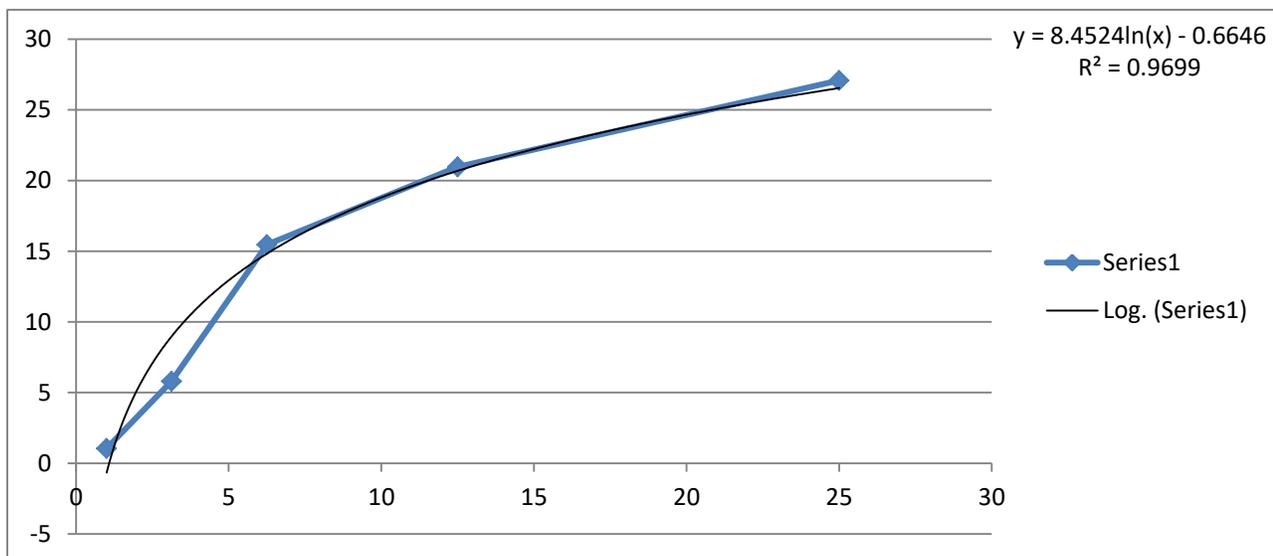
17. The curves that we used to calculate the IC<sub>50</sub> value for compound **8** against DU145



X-axis = concentration (µM) of compound **8**  
Y-axis = % Cell Proliferation Inhibition  
IC<sub>50</sub> > 25 µM

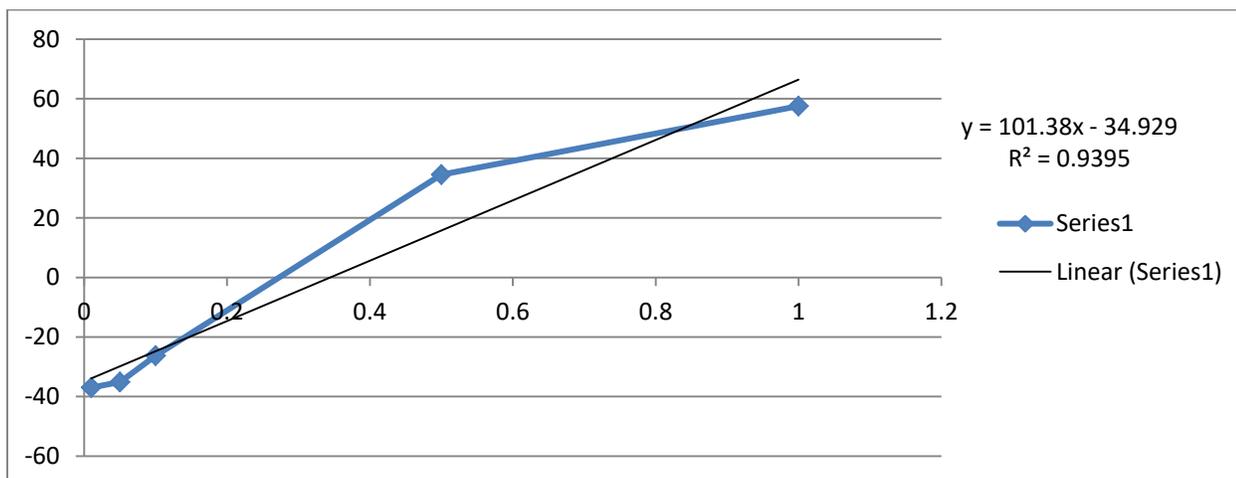


X-axis = concentration (µM) of compound **8**  
Y-axis = % Cell Proliferation Inhibition  
IC<sub>50</sub> > 25 µM

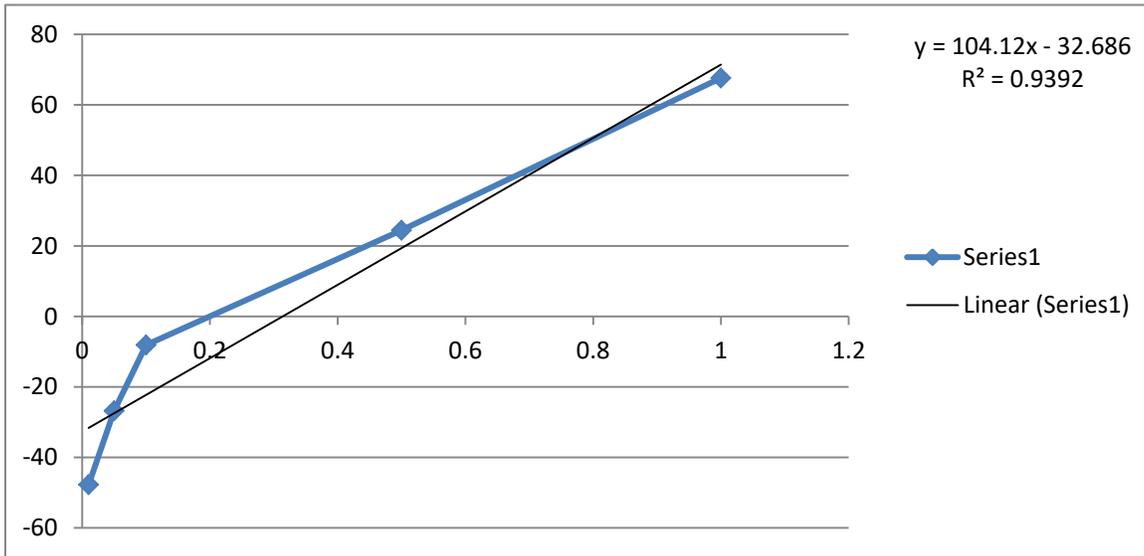


X-axis = concentration (μM) of compound **8**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$

18. The curves that we used to calculate the  $IC_{50}$  value for compound **8** against LNCaP



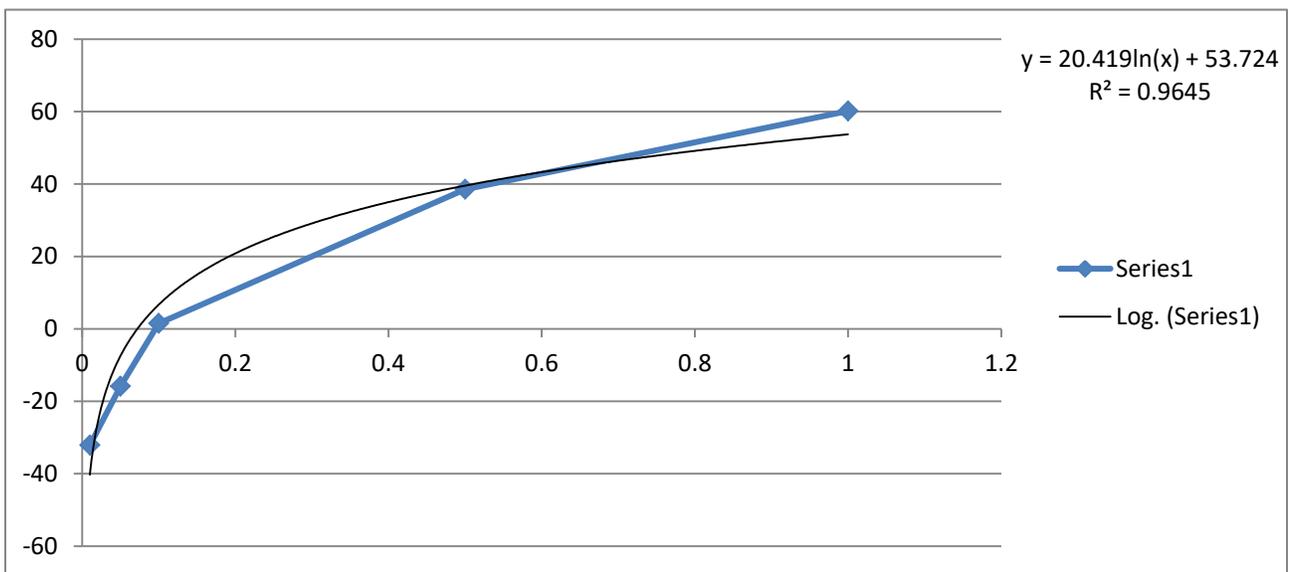
X-axis = concentration (μM) of compound **8**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} = 0.838 \mu M$



X-axis = concentration ( $\mu\text{M}$ ) of compound **8**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 0.794 \mu\text{M}$

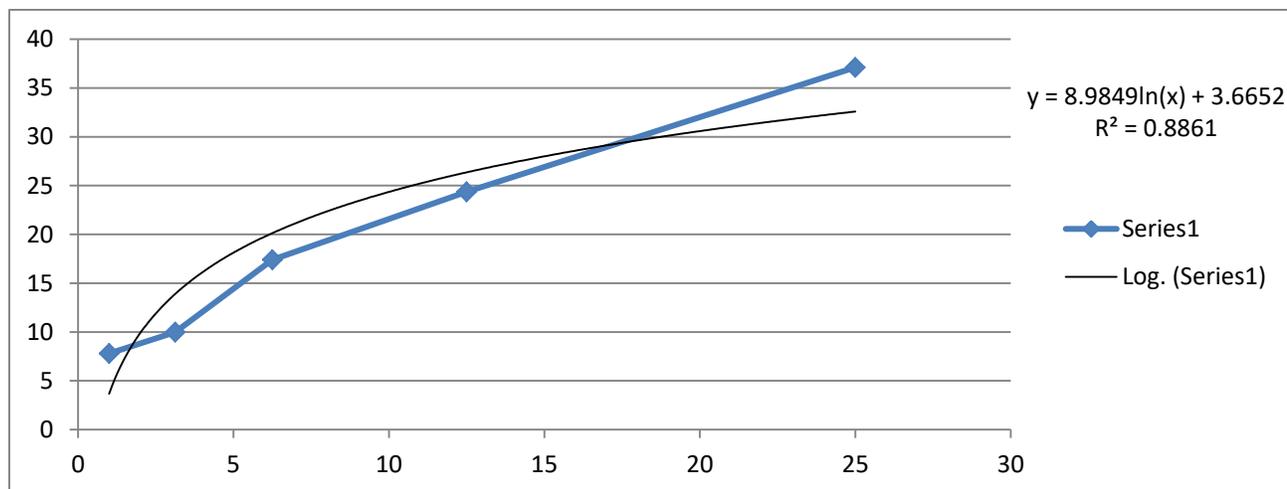


X-axis = concentration ( $\mu\text{M}$ ) of compound **8**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 0.833 \mu\text{M}$

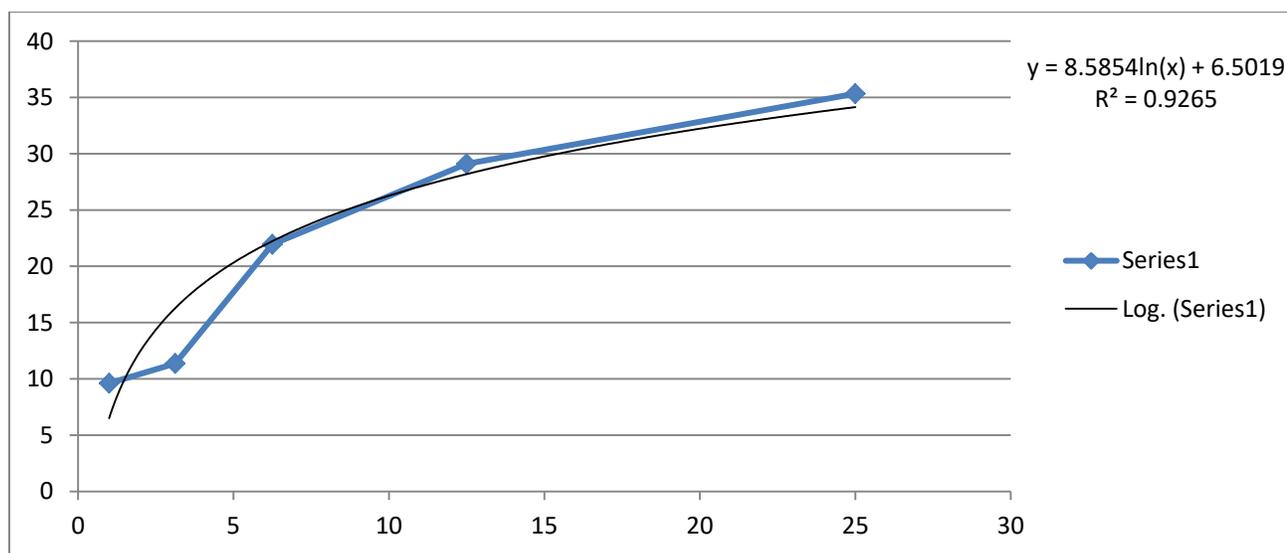
19. The curves that we used to calculate the IC<sub>50</sub> value for compound **9** against PC-3



X-axis = concentration (µM) of compound **9**

Y-axis = % Cell Proliferation Inhibition

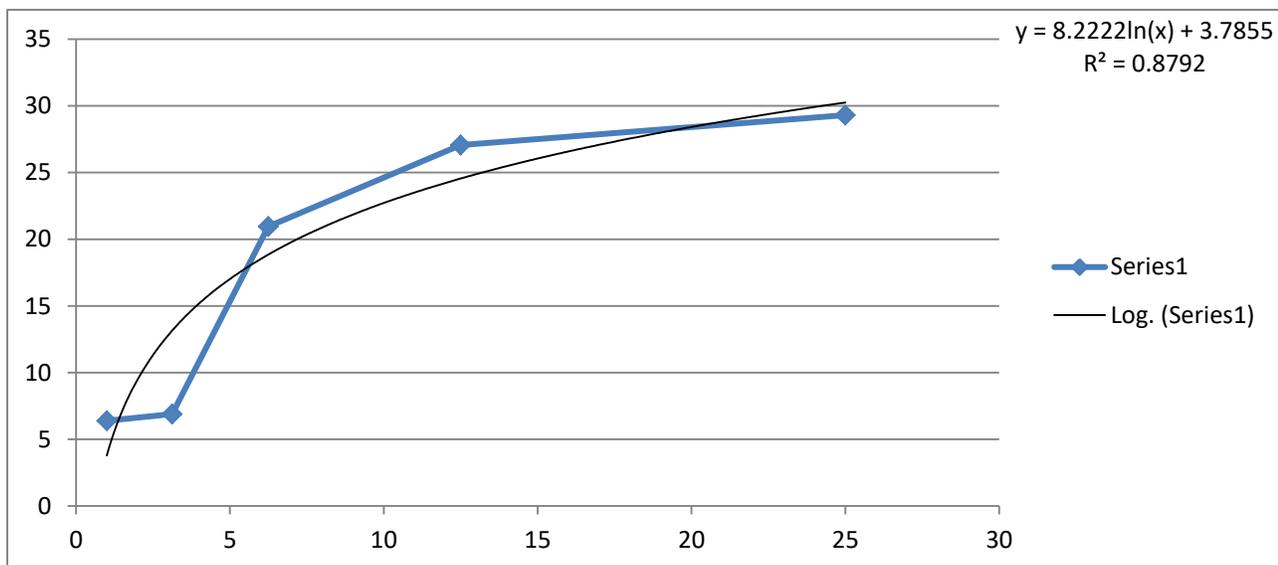
IC<sub>50</sub> > 25 µM



X-axis = concentration (µM) of compound **9**

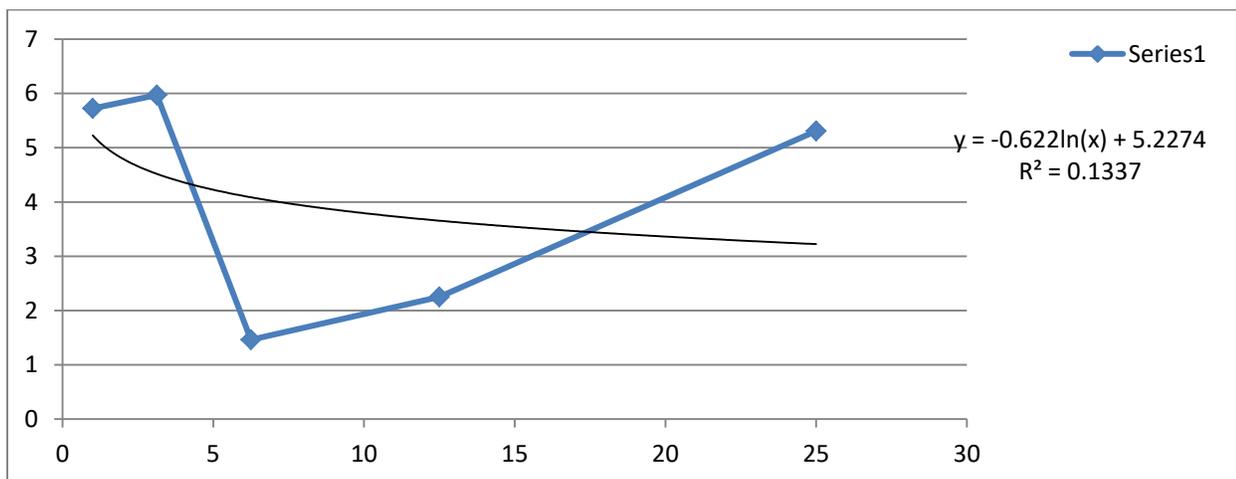
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

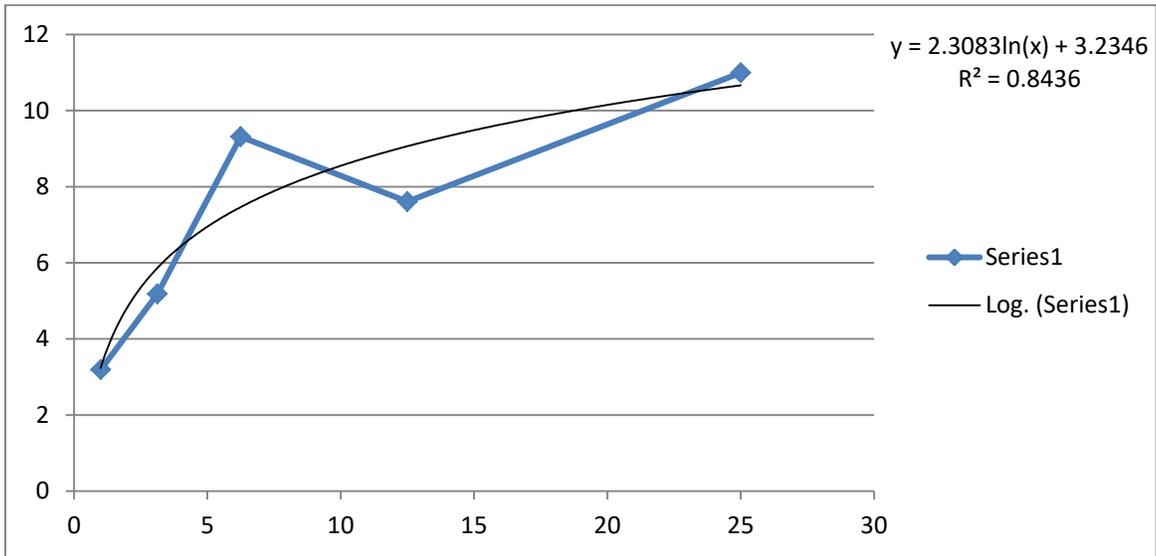


X-axis = concentration (µM) of compound **9**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$

20. The curves that we used to calculate the  $IC_{50}$  value for compound **9** against DU145



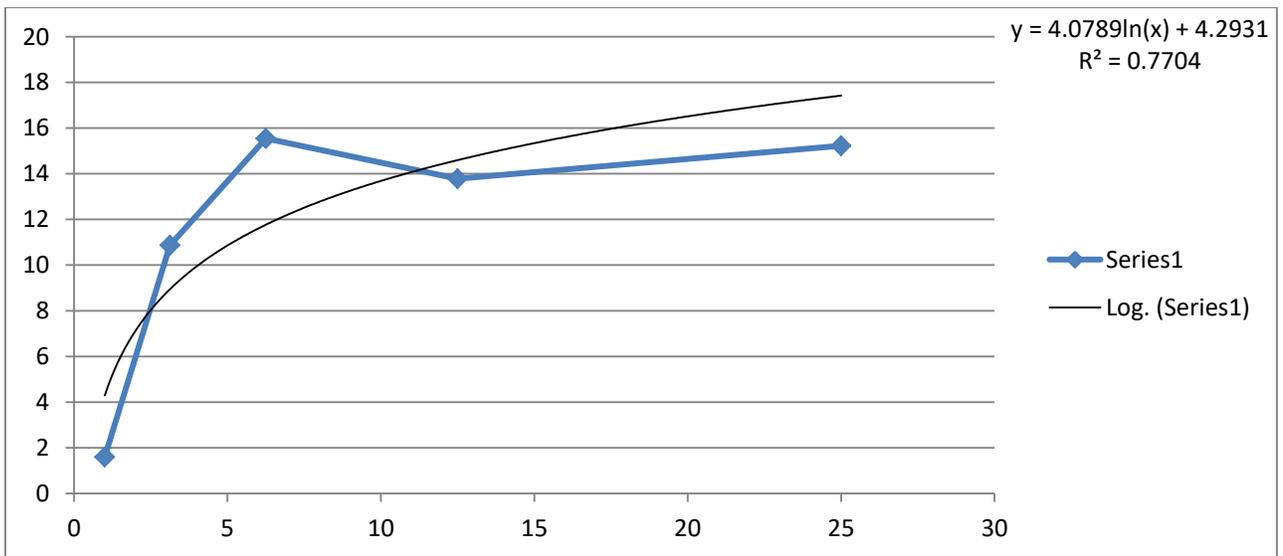
X-axis = concentration (µM) of compound **9**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$



X-axis = concentration (µM) of compound **9**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

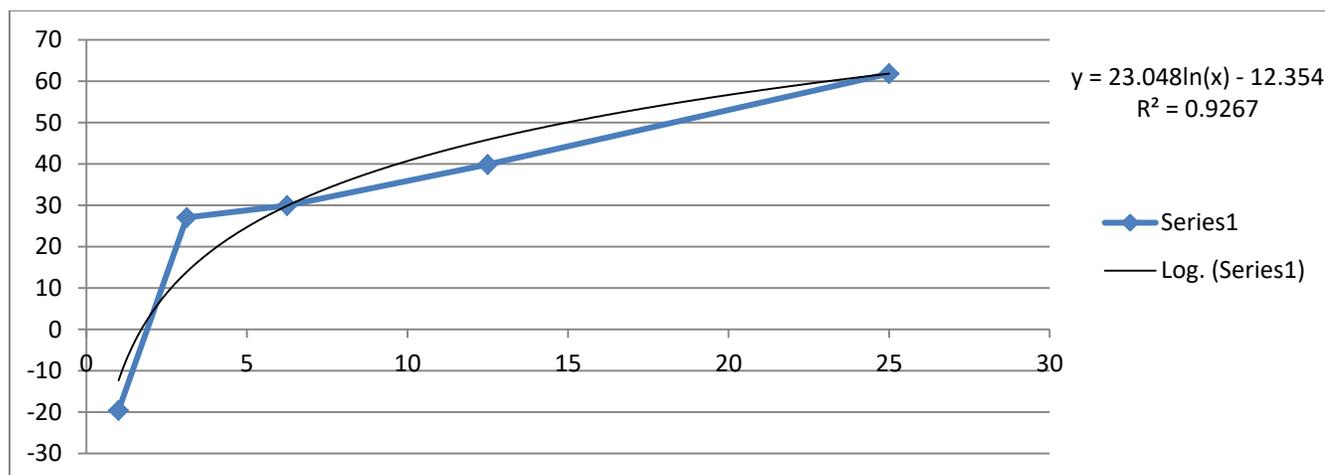


X-axis = concentration (µM) of compound **9**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

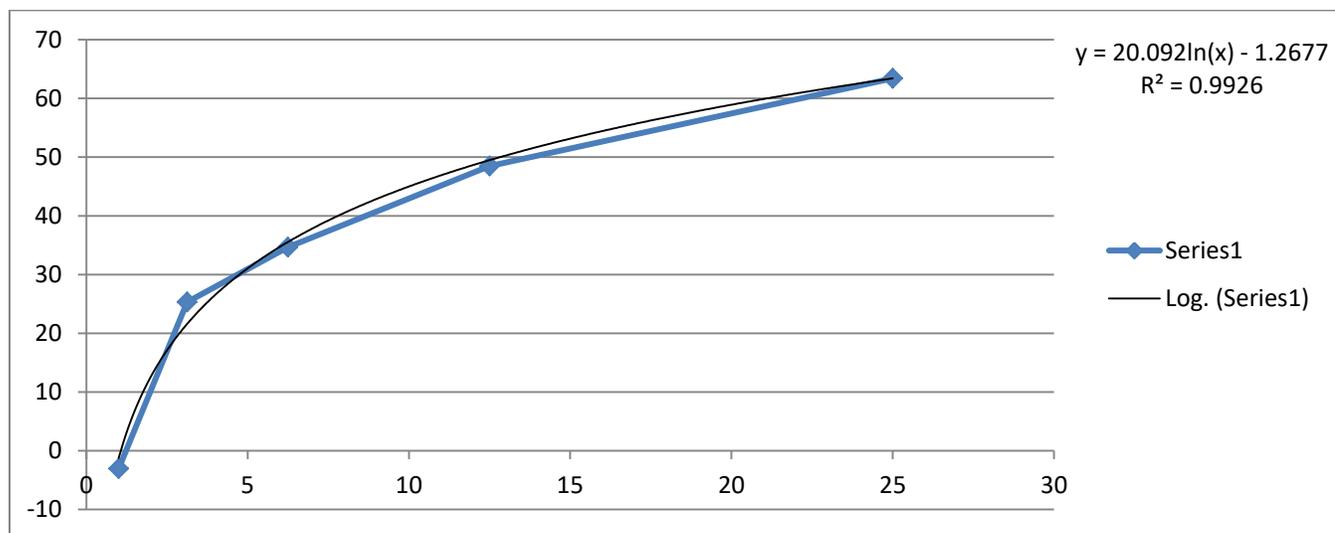
21. The curves that we used to calculate the IC<sub>50</sub> value for compound **9** against LNCaP



X-axis = concentration (µM) of compound **9**

Y-axis = % Cell Proliferation Inhibition

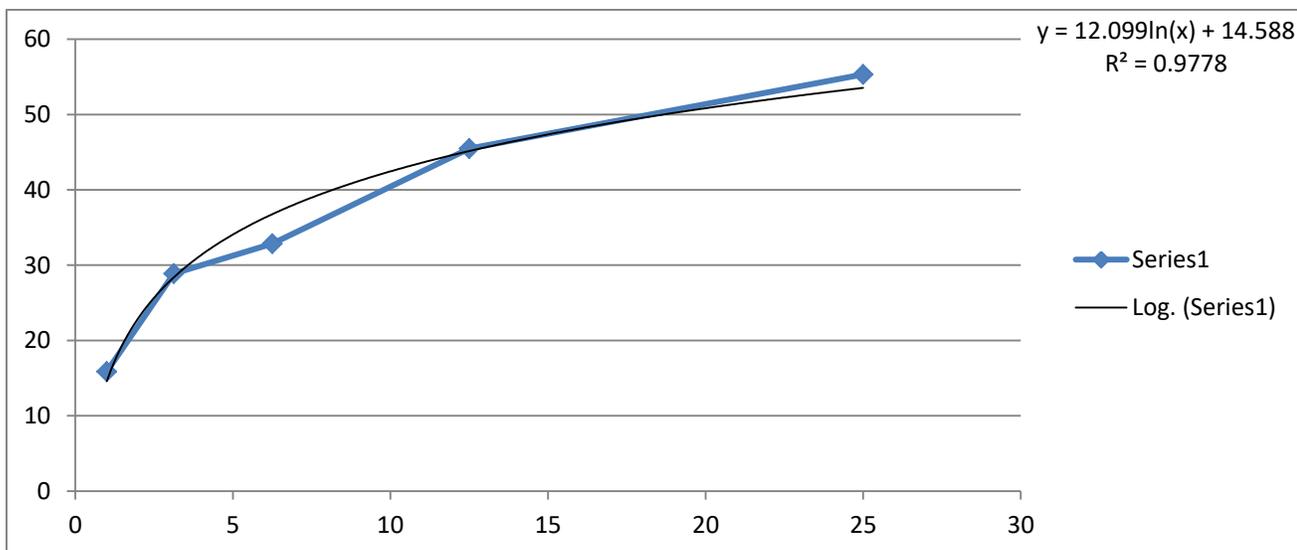
IC<sub>50</sub> = 14.960 µM



X-axis = concentration (µM) of compound **9**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 12.828 µM

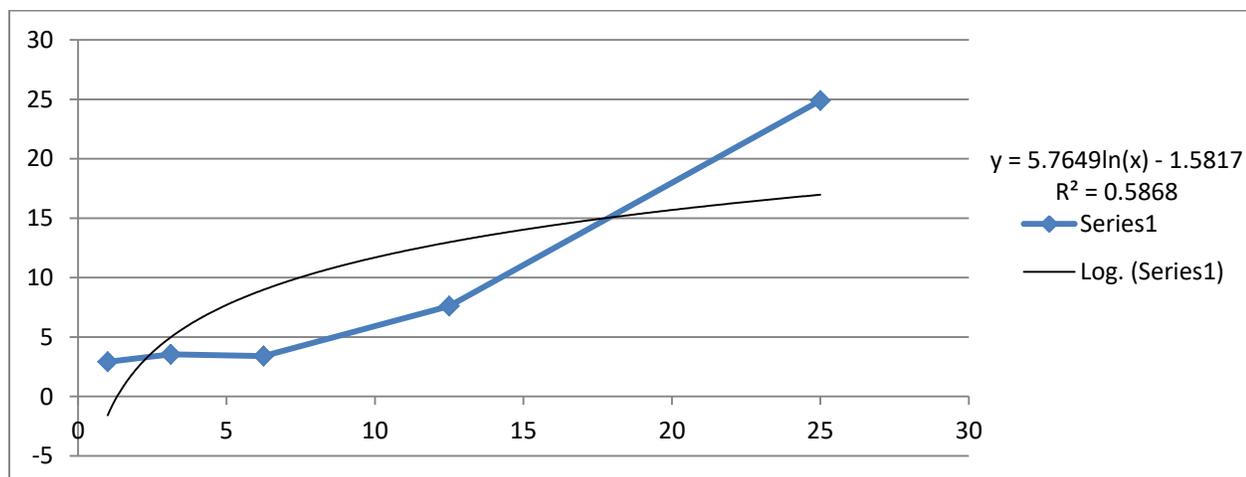


X-axis = concentration ( $\mu\text{M}$ ) of compound **9**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 18.669 \mu\text{M}$

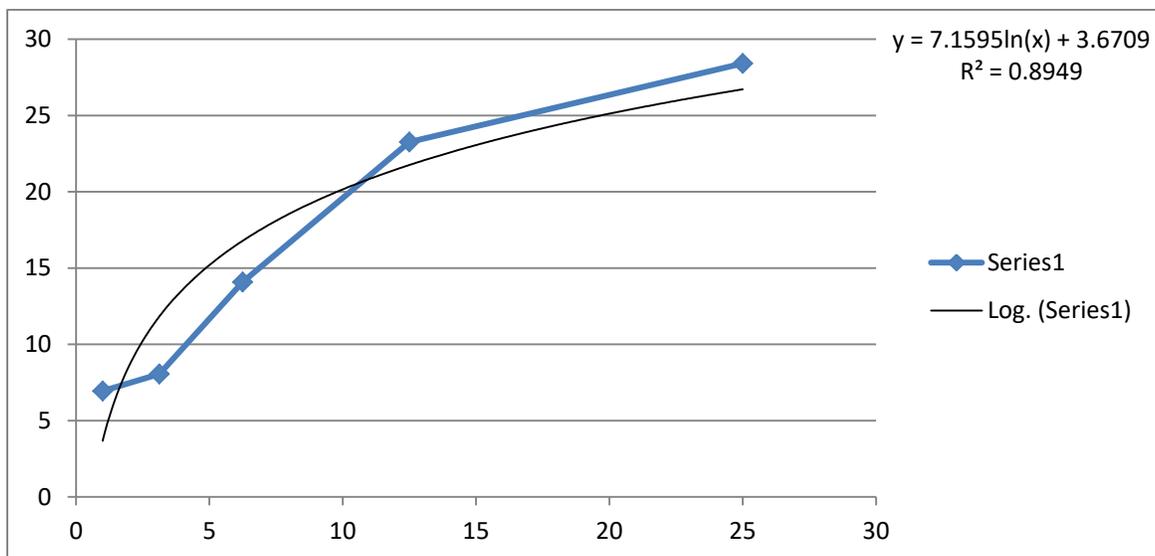
22. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **11** against PC-3



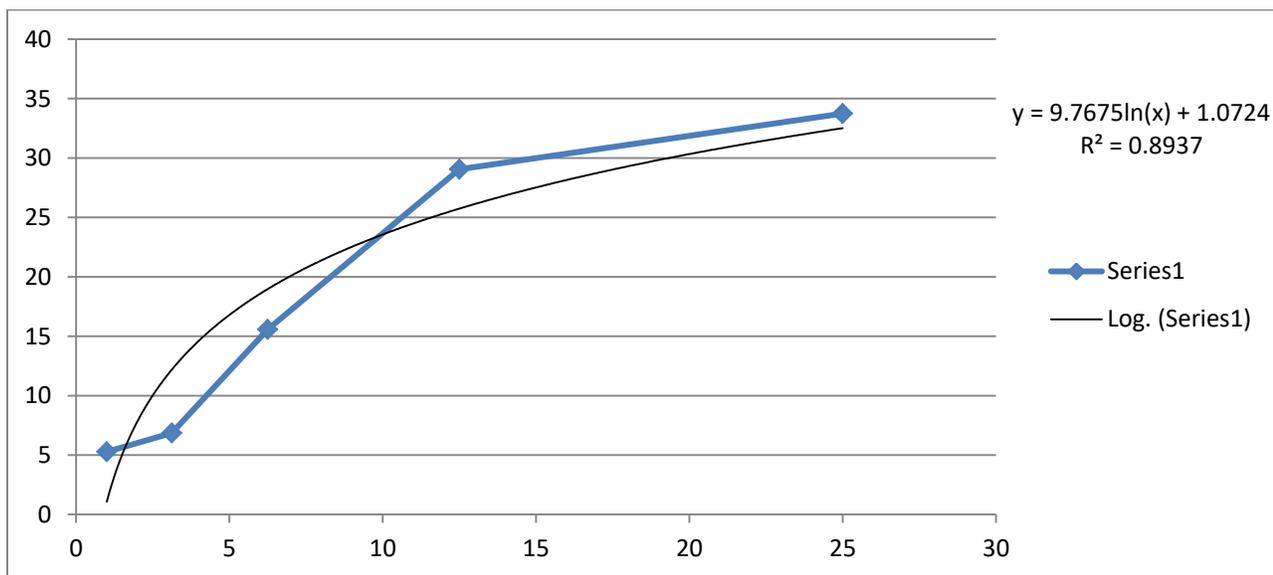
X-axis = concentration ( $\mu\text{M}$ ) of compound **11**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} > 25 \mu\text{M}$

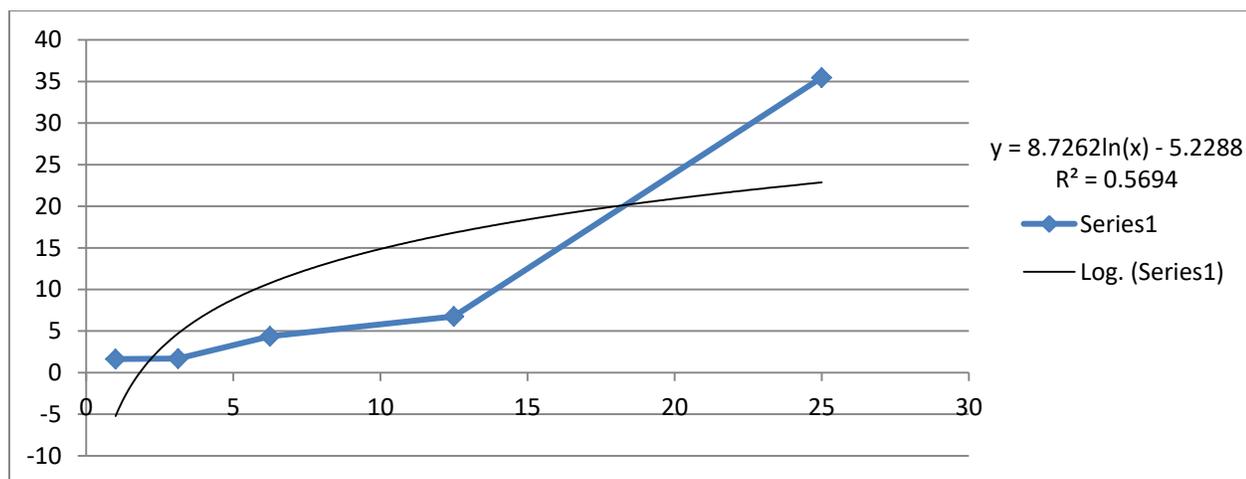


X-axis = concentration (µM) of compound **11**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu\text{M}$



X-axis = concentration (µM) of compound **11**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu\text{M}$

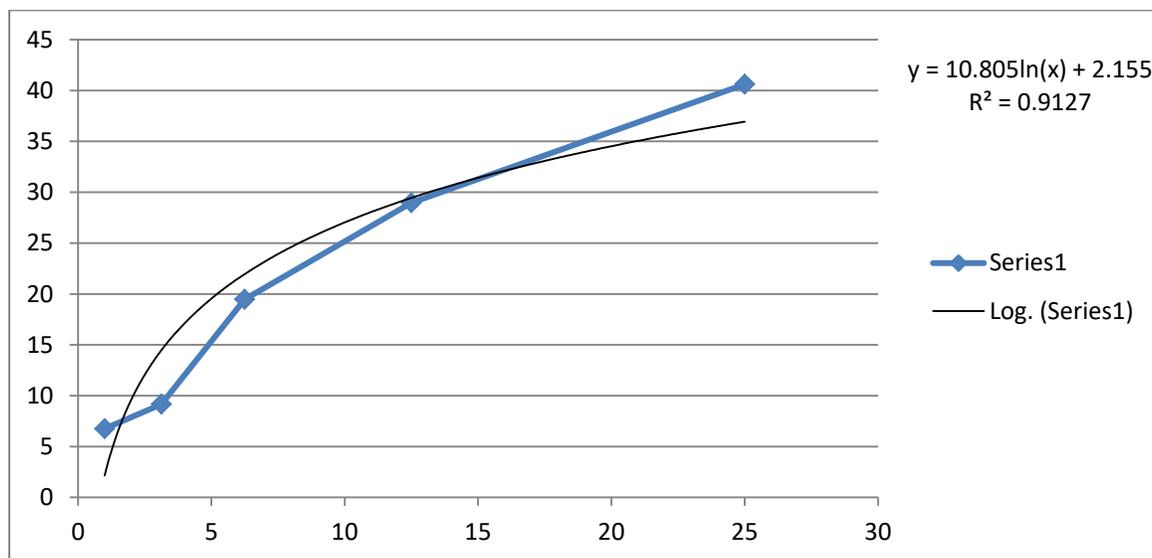
23. The curves that we used to calculate the IC<sub>50</sub> value for compound **11** against DU145



X-axis = concentration (µM) of compound **11**

Y-axis = % Cell Proliferation Inhibition

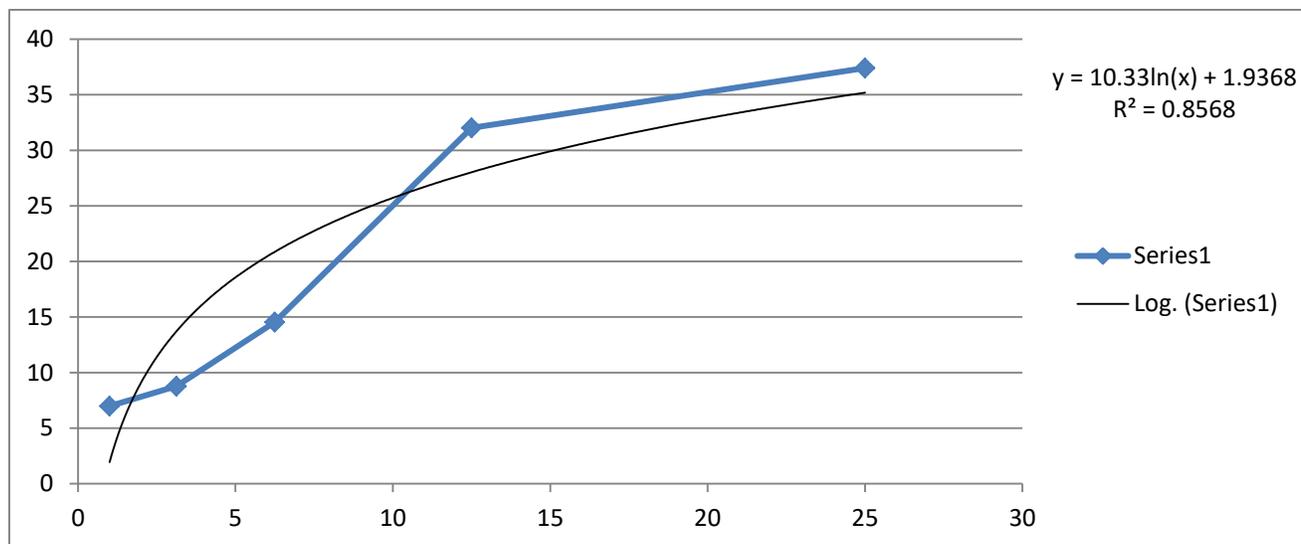
IC<sub>50</sub> > 25 µM



X-axis = concentration (µM) of compound **11**

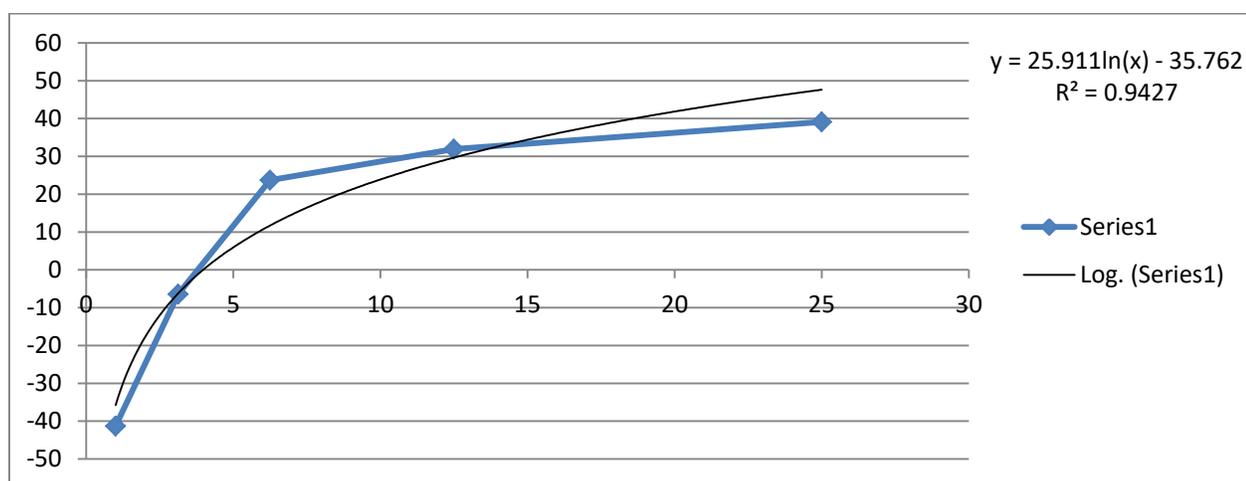
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

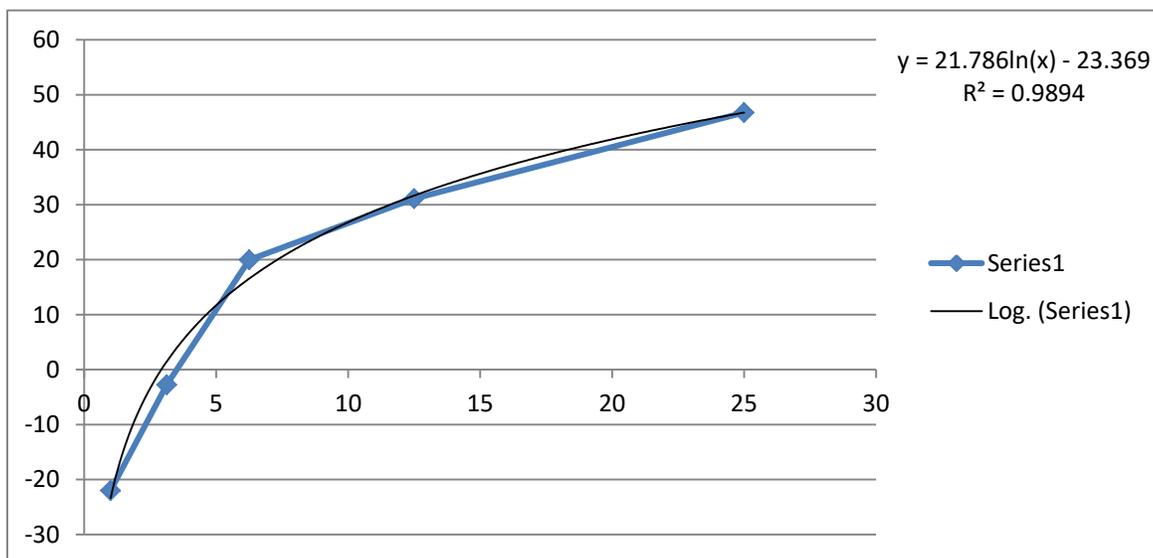


X-axis = concentration ( $\mu\text{M}$ ) of compound **11**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} > 25 \mu\text{M}$

24. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **11** against LNCaP



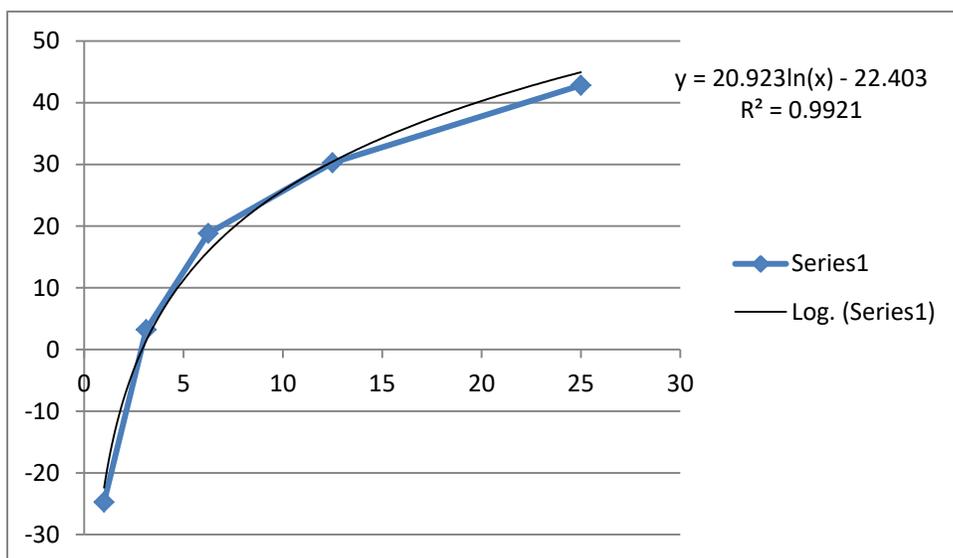
X-axis = concentration ( $\mu\text{M}$ ) of compound **11**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} = 27.381 \mu\text{M}$



X-axis = concentration (µM) of compound **11**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 29.012 µM

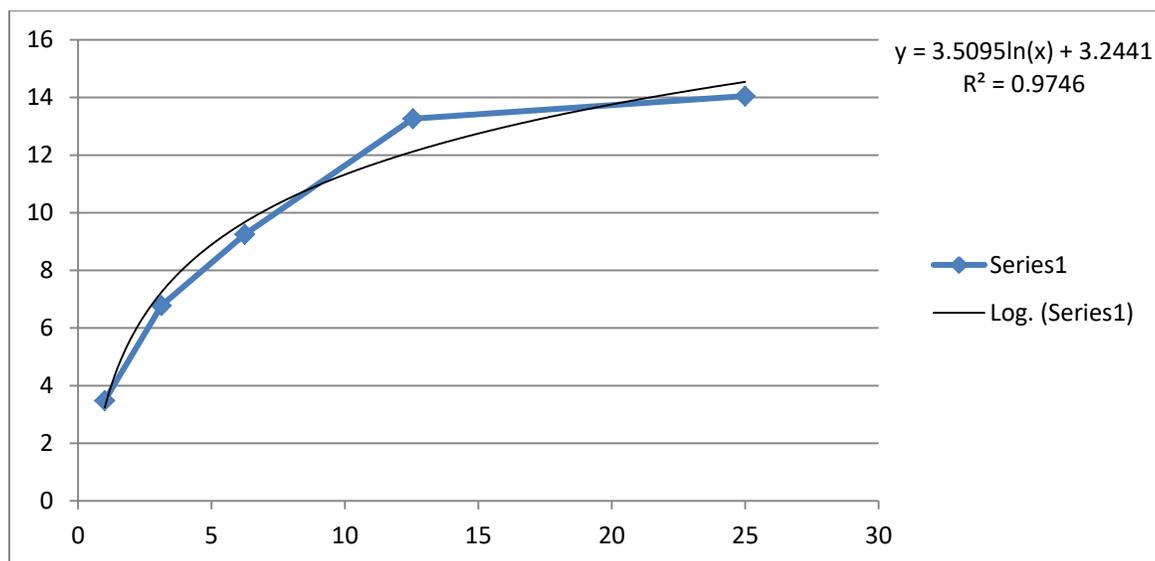


X-axis = concentration (µM) of compound **11**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 31.831 µM

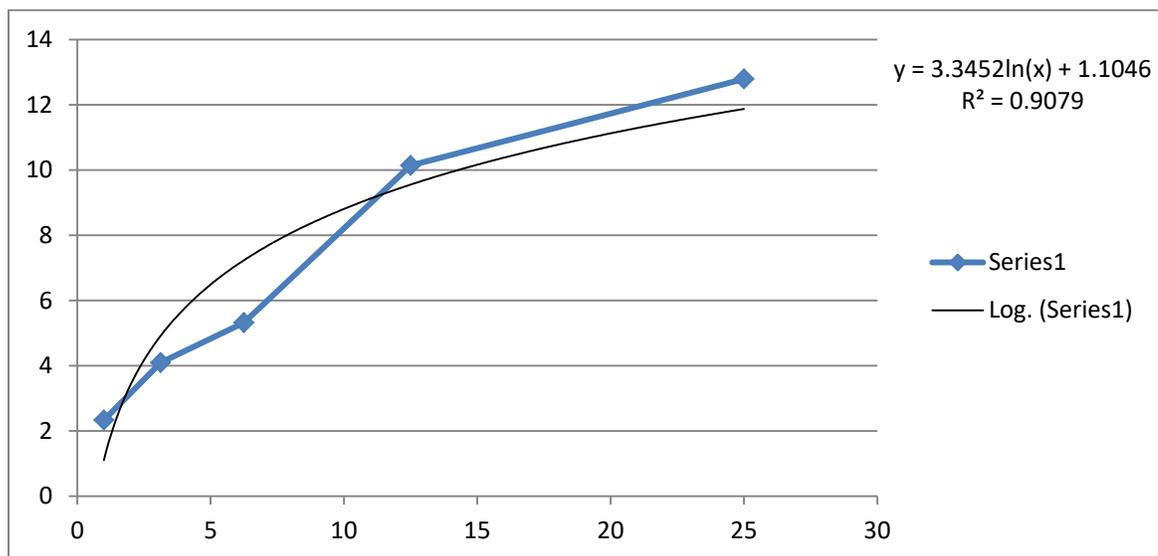
25. The curves that we used to calculate the IC<sub>50</sub> value for compound **12** against PC-3



X-axis = concentration (µM) of compound **12**

Y-axis = % Cell Proliferation Inhibition

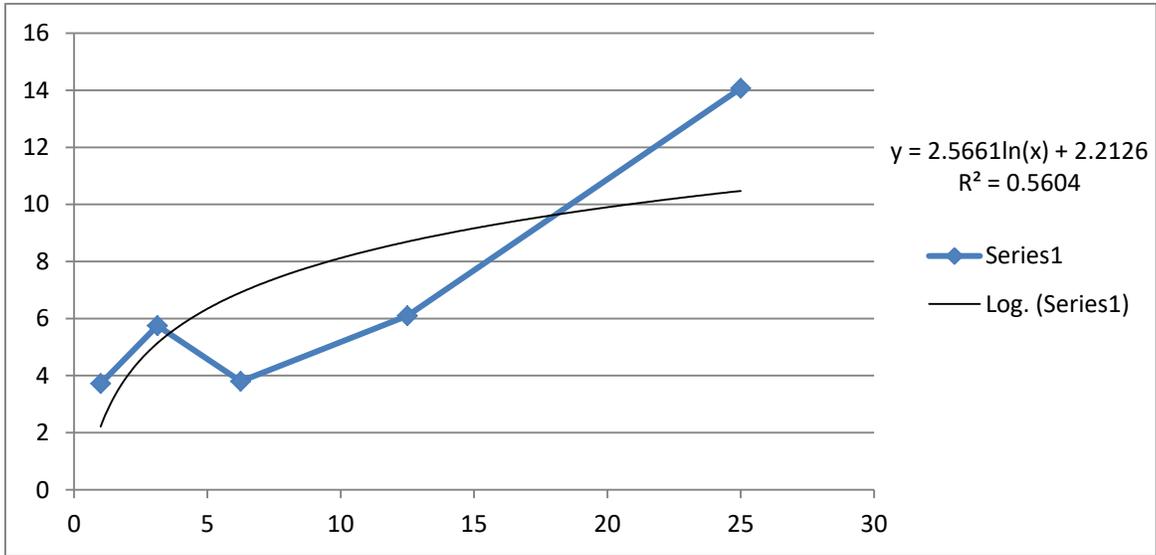
IC<sub>50</sub> > 25 µM



X-axis = concentration (µM) of compound **12**

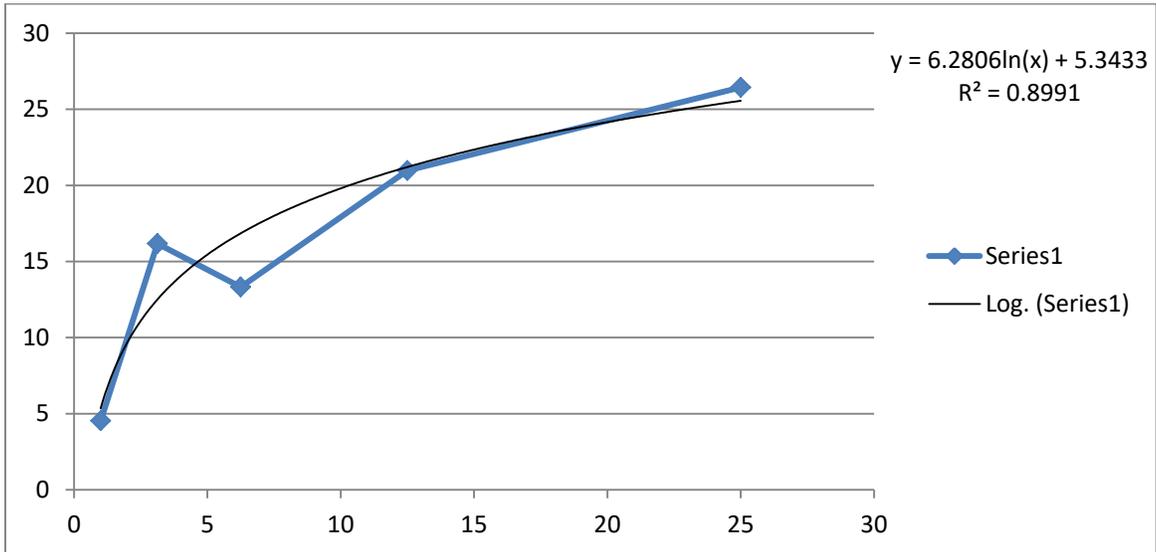
Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

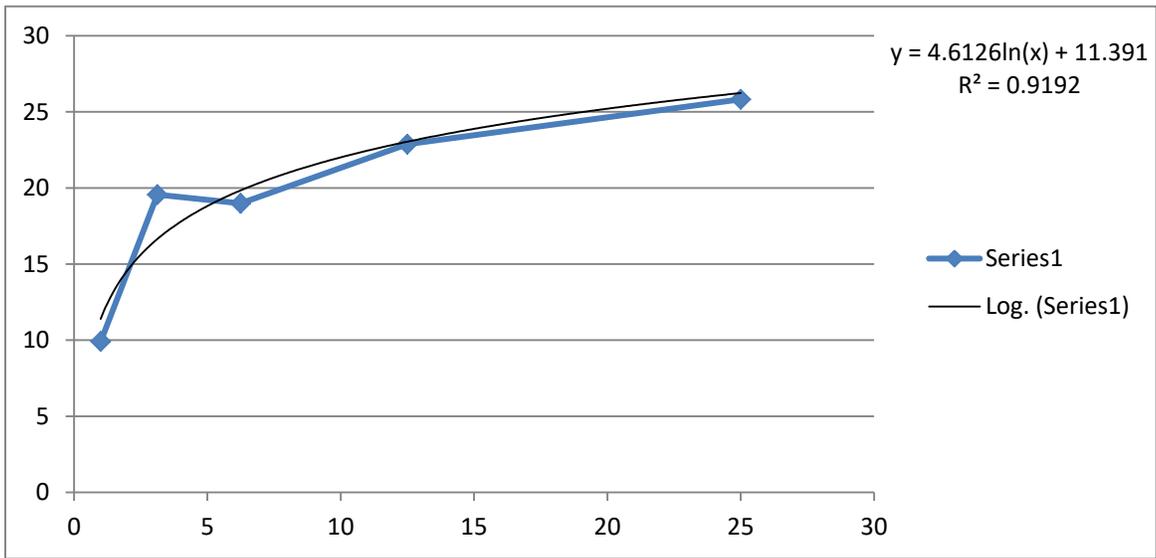


X-axis = concentration ( $\mu\text{M}$ ) of compound **12**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} > 25 \mu\text{M}$

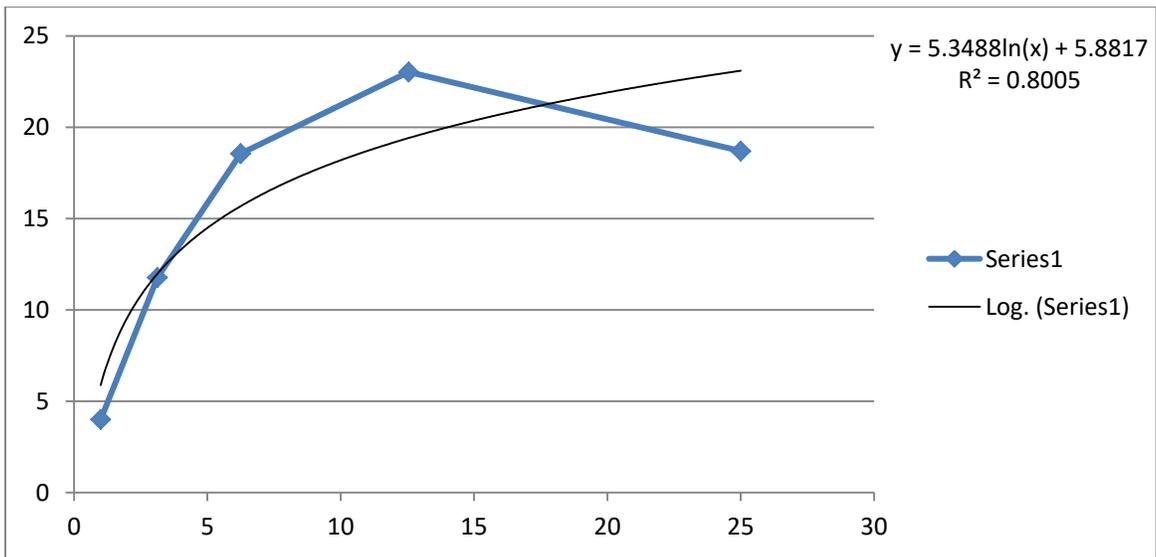
26. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **12** against DU145



X-axis = concentration ( $\mu\text{M}$ ) of compound **12**  
 Y-axis = % Cell Proliferation Inhibition  
 $\text{IC}_{50} > 25 \mu\text{M}$

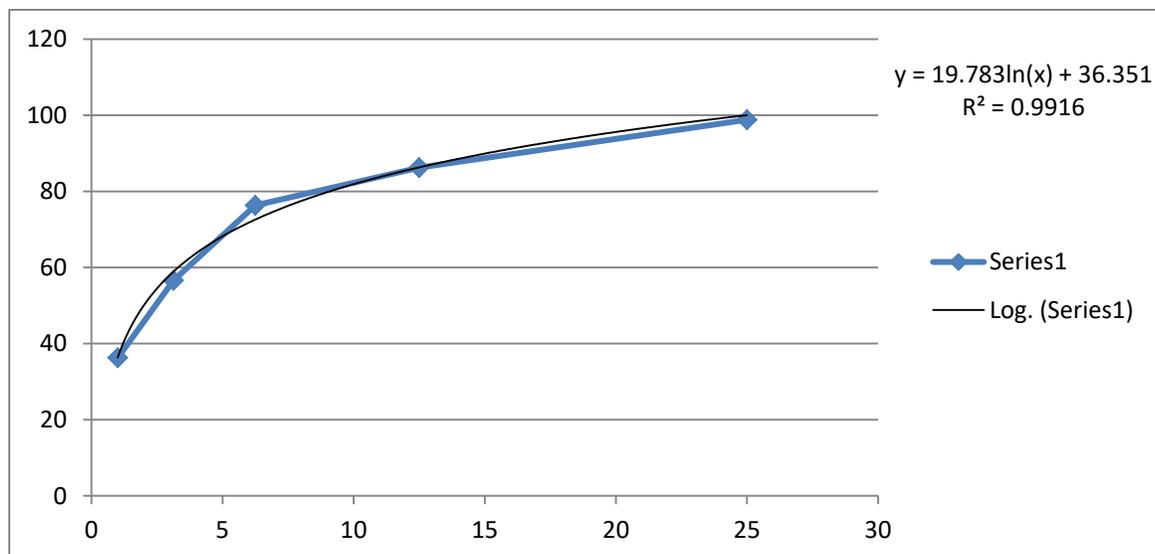


X-axis = concentration (µM) of compound **12**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$



X-axis = concentration (µM) of compound **12**  
 Y-axis = % Cell Proliferation Inhibition  
 $IC_{50} > 25 \mu M$

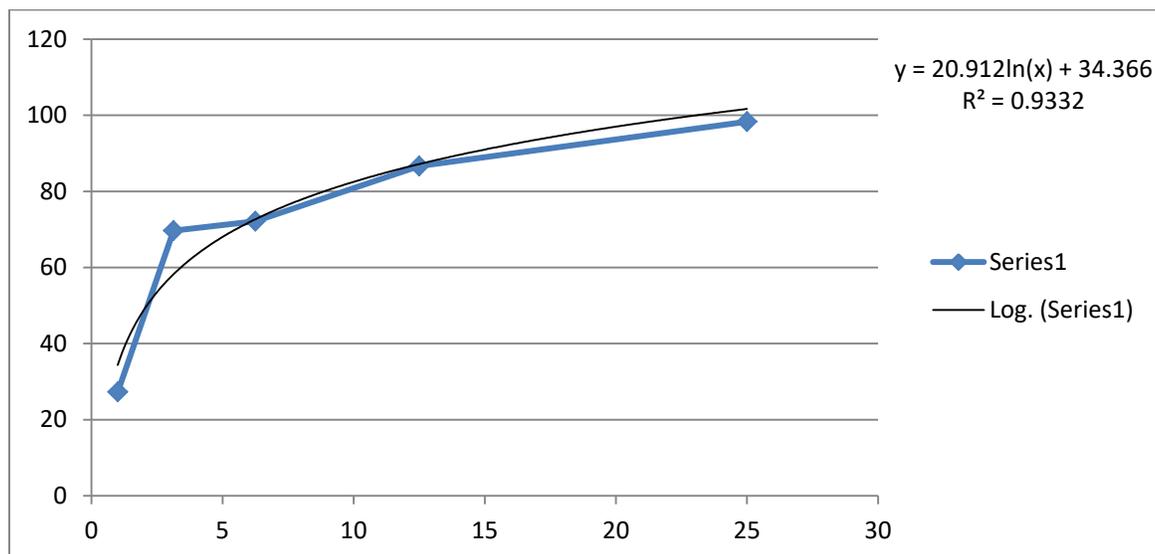
27. The curves that we used to calculate the IC<sub>50</sub> value for compound **12** against LNCaP



X-axis = concentration (µM) of compound **12**

Y-axis = % Cell Proliferation Inhibition

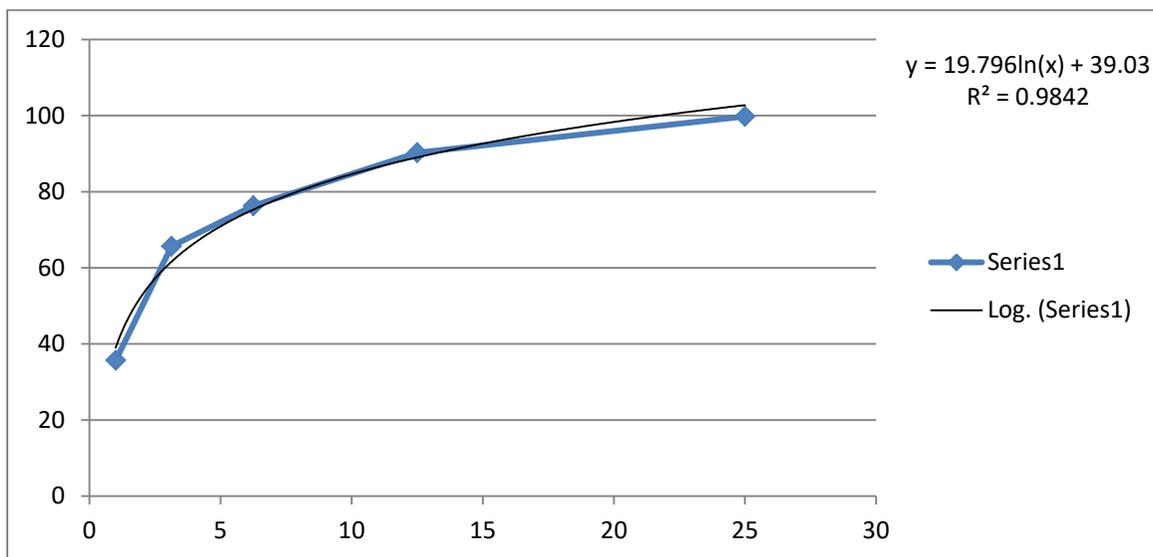
IC<sub>50</sub> = 1.994 µM



X-axis = concentration (µM) of compound **12**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 2.112 µM

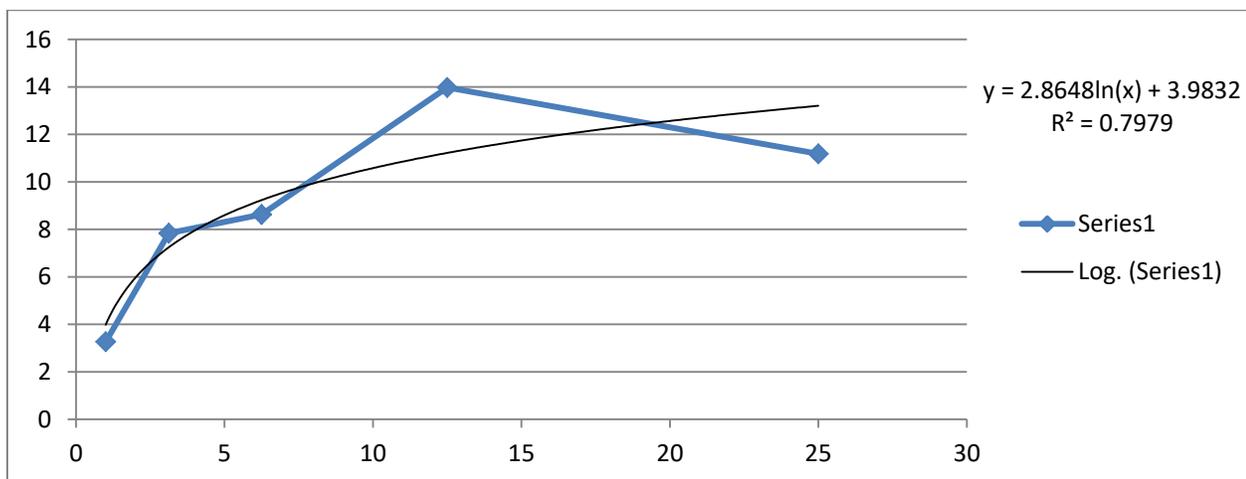


X-axis = concentration ( $\mu\text{M}$ ) of compound **12**

Y-axis = % Cell Proliferation Inhibition

$\text{IC}_{50} = 1.740 \mu\text{M}$

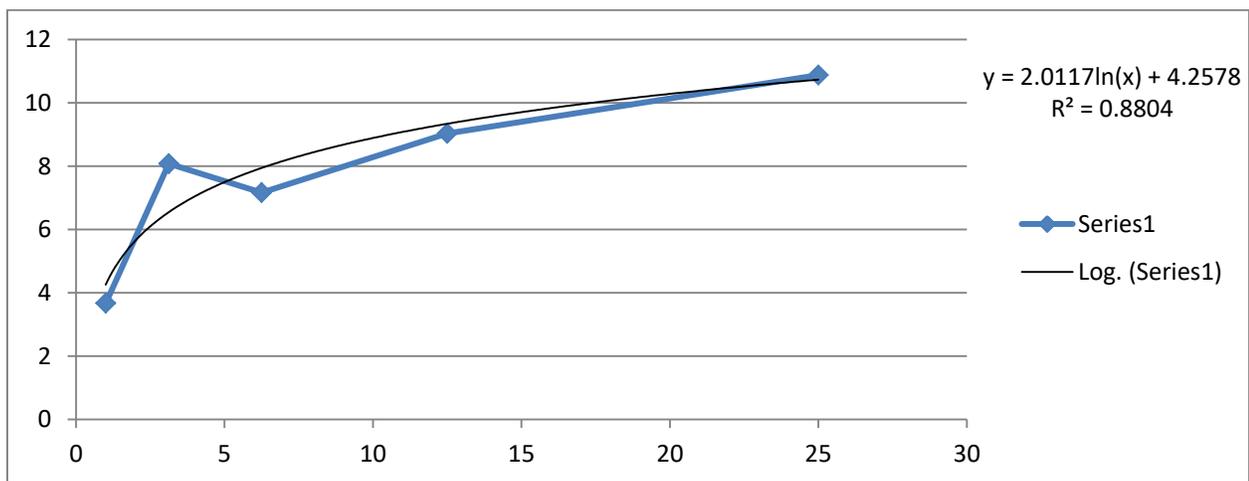
28. The curves that we used to calculate the  $\text{IC}_{50}$  value for compound **13** against PC-3



X-axis = concentration ( $\mu\text{M}$ ) of compound **13**

Y-axis = % Cell Proliferation Inhibition

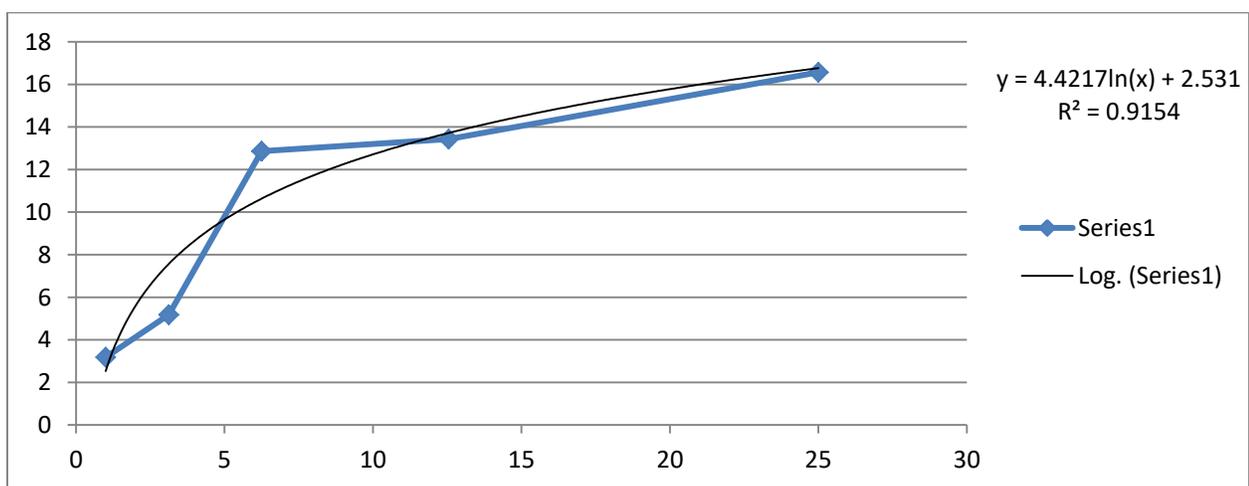
$\text{IC}_{50} > 25 \mu\text{M}$



X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

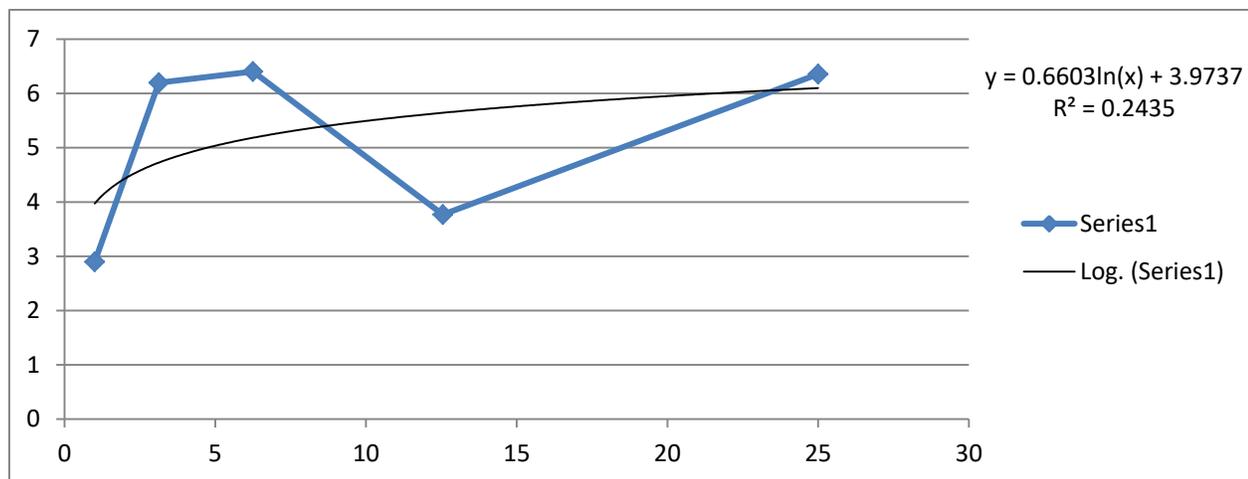


X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

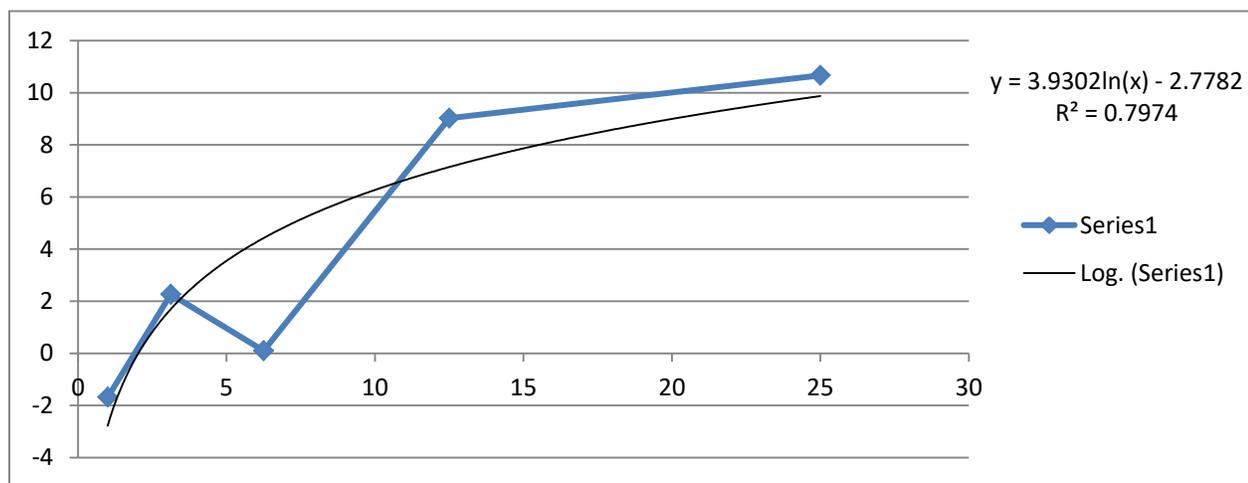
29. The curves that we used to calculate the IC<sub>50</sub> value for compound **13** against DU145



X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

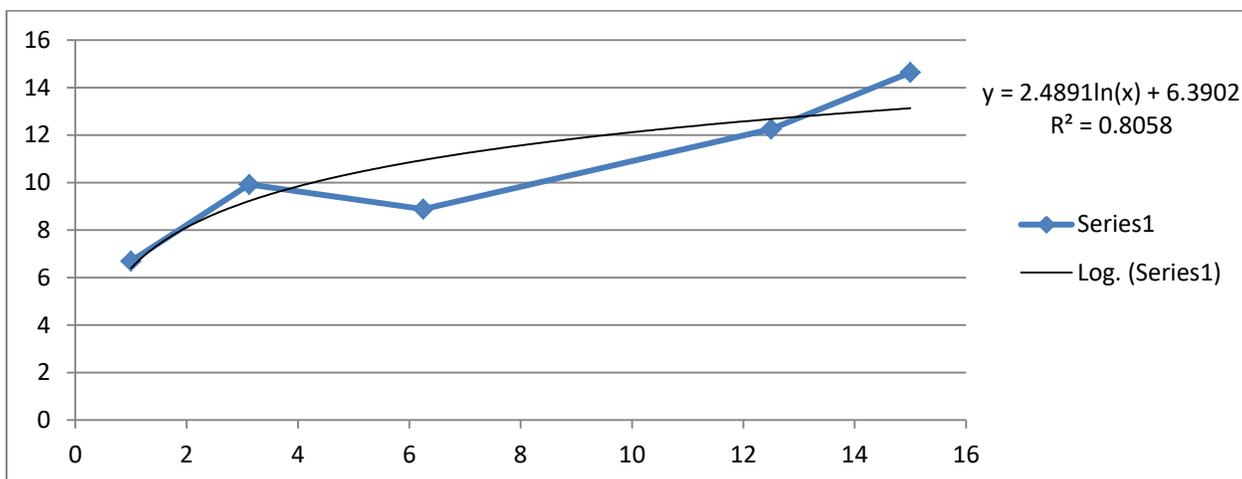
IC<sub>50</sub> > 25 µM



X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

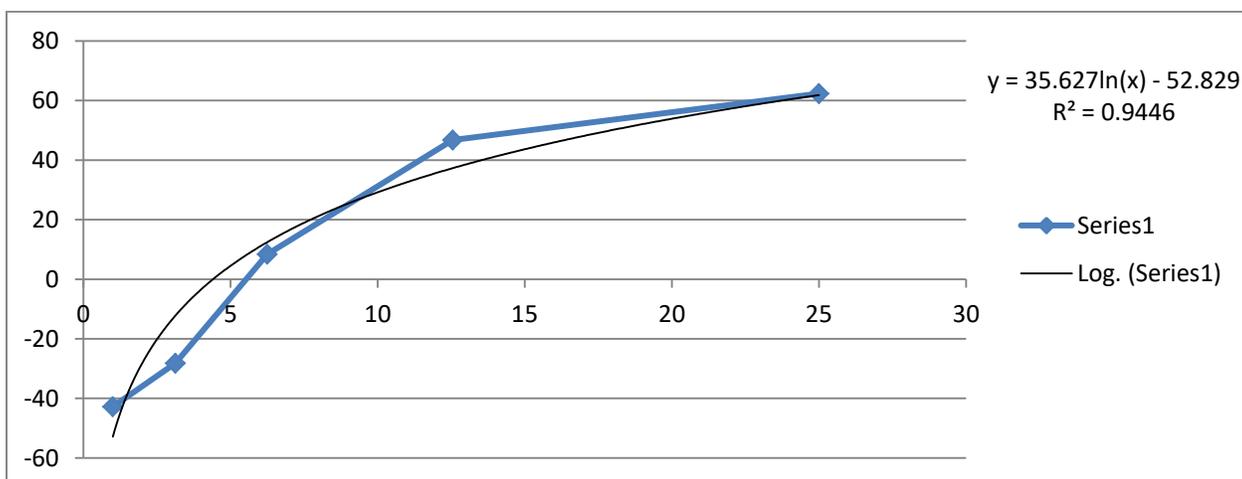


X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> > 25 µM

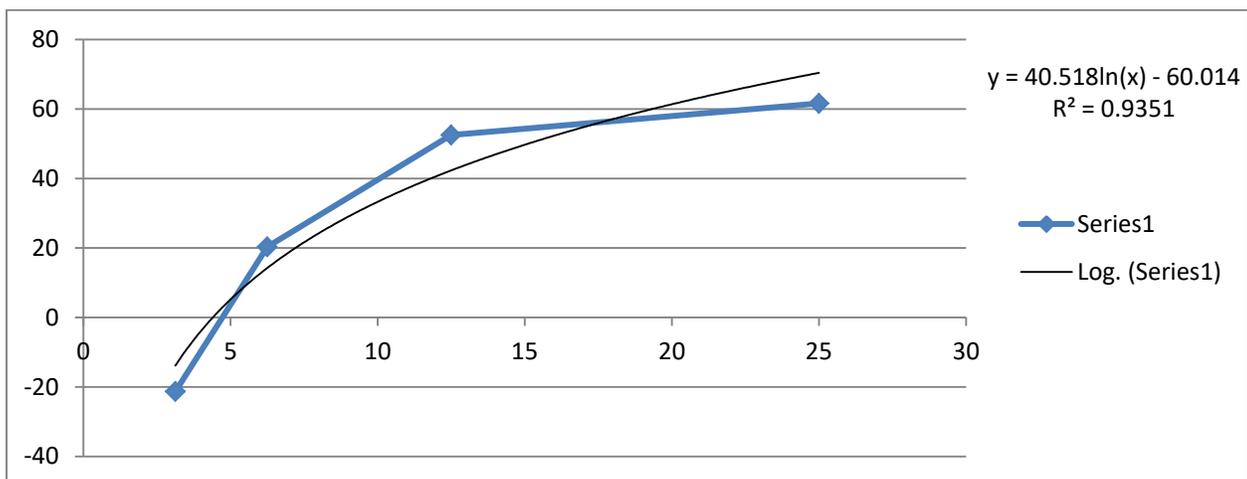
30. The curves that we used to calculate the IC<sub>50</sub> value for compound **13** against LNCaP



X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

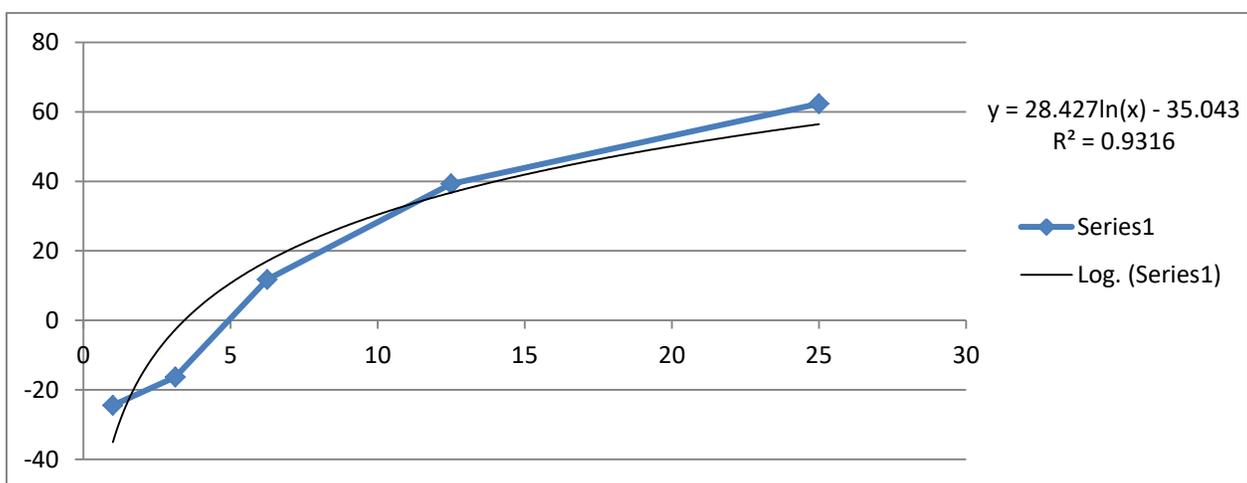
IC<sub>50</sub> = 17.926 µM



X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 15.123 µM



X-axis = concentration (µM) of compound **13**

Y-axis = % Cell Proliferation Inhibition

IC<sub>50</sub> = 19.918 µM