Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.


# Supporting Information

## Total synthesis and structural revision of an isopanepoxydone analog isolated from *Lentinus strigellus*

***Yi Man,[a] Shaomin Fu,*[a] Juan Chen,[b] and Bo Liu*[a]***

[a]Key Laboratory of Green Chemistry &Technology of the Ministry of Education, College of Chemistry, Sichuan University, Chengdu, Sichuan 610064, China

[b] Analytical & Testing Center, Sichuan University, Chengdu, Sichuan 610064, China

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Table S1. Comparison of $^{1}$H NMR data for natural product with synthetic compound **1**

| Position | Natural (400 MHz, $CDCl_3$) | Synthetic (400 MHz, $CDCl_3$) | $\Delta\delta^{*}$ (ppm) |
|---|---|---|---|
| 1 | 3.49 d, (2.1,3.9) | 3.44 s | -0.05 |
| 2 | -- | -- | -- |
| 3 | 5.77 m, (2.1) | 5.81 s, | 0.04 |
| 4 | -- | -- | -- |
| 5 | 4.52 dd, (3.2,9.1) | 4.54 d, ( 8.7 ), | 0.02 |
| 6 | 3.86 dd, (3.2,3.9) | 3.79 d, (3.5 ) | -0.07 |
| 7 | 3.03 br d, (2.9,7.2) | 3.04 qd, (17.0, 7.3), | 0.01 |
| 8 | 5.13 dd,(2.9,7.2) | 5.14 t, (6.9) | 0.01 |
| 9 | -- | -- | -- |
| 10 | 1.62 s | 1.64 s | 0.02 |
| 11 | 1.74 s | 1.76 s | 0.02 |
| 5-OH | 2.21 d, (9.1) | 2.24 d, (8.8) | 0.03 |

*The chemical shift of synthetic product minus the chemical shift of Natural product.

Table S2. Comparison of $^{13}C$ NMR data for natural product with synthetic compound **1**

| Position | Natural (100 MHz, $CDCl_3$) | Synthetic (100 MHz, $CDCl_3$) | $\Delta\delta^*$ (ppm) |
|---|---|---|---|
| 1 | 66.8 | 65.9 | -0.9 |
| 2 | 192.8 | 193.9 | 1.1 |
| 3 | 122.1 | 123.0 | 0.9 |
| 4 | 159.6 | 159.1 | -0.5 |
| 5 | 54.7 | 52.6 | -2.1 |
| 6 | 55.6 | 56.9 | 1.3 |
| 7 | 32.4 | 33.5 | 1.1 |
| 8 | 118.6 | 118.2 | -0.4 |
| 9 | 136.5 | 137.0 | 0.5 |
| 10 | 25.87 | 25.9 | 0 |
| 11 | 17.8 | 18.0 | 0.2 |

*The chemical shift of synthetic product minus the chemical shift of Natural product.

Table S3. Comparison of $^{1}$H NMR data for natural product with synthetic compound **2**

| Position | Natural (400 MHz, $CDCl_3$) | Synthetic (400 MHz, $CDCl_3$) | $\Delta\delta^{*}$(ppm) |
|---|---|---|---|
| 1 | 3.49 d, (2.1,3.9) | 3.49 dd, (3.7, 2.1) | 0.00 |
| 2 | -- | -- | -- |
| 3 | 5.77 m, (2.1) | 5.78 s | 0.01 |
| 4 | -- | -- | -- |
| 5 | 4.52 dd, (3.2,9.1) | 4.53 d, (10.2 ) | 0.01 |
| 6 | 3.86 dd, (3.2,3.9) | 3.87 d, (3.2 ) | 0.01 |
| 7 | 3.03 br d, (2.9,7.2) | 3.03 d, (7.3) | 0.00 |
| 8 | 5.13 dd, (2.9,7.2) | 5.13 t, (7.3) | 0 |
| 9 | -- | -- | -- |
| 10 | 1.62 s | 1.63 s | 0.01 |
| 11 | 1.74 s | 1.74 s | 0.00 |
| 5-OH | 2.21 d, (9.1) | 2.19 d, (10.7) | -0.02 |

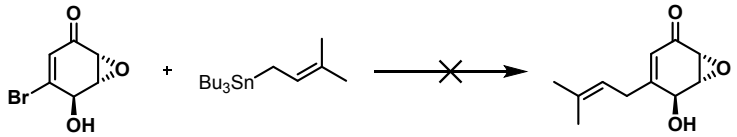
*The chemical shift of synthetic product minus the chemical shift of Natural product.

Table S4. Comparison of $^{13}C$ NMR data for natural product with synthetic compound **2**

| Position | Natural (100 MHz, $CDCl_3$) | Synthetic (100 MHz, $CDCl_3$) | $\Delta\delta^*$(ppm) |
|---|---|---|---|
| 1 | 66.8 | 66.7 | -0.1 |
| 2 | 192.8 | 192.9 | 0.1 |
| 3 | 122.1 | 122.0 | -0.1 |
| 4 | 159.6 | 159.7 | 0.1 |
| 5 | 54.7 | 54.6 | -0.1 |
| 6 | 55.6 | 55.6 | 0.0 |
| 7 | 32.4 | 32.3 | -0.1 |
| 8 | 118.6 | 118.4 | -0.2 |
| 9 | 136.5 | 136.5 | 0.0 |
| 10 | 25.87 | 25.8 | -0.1 |
| 11 | 17.8 | 17.8 | 0.0 |

*The chemical shift of synthetic product minus the chemical shift of Natural product.

Table S5 Synthesis of compound **1** via Stille coupling reaction between compound **12** and tributy (3-methyl-2-buten-1-yl) stannan



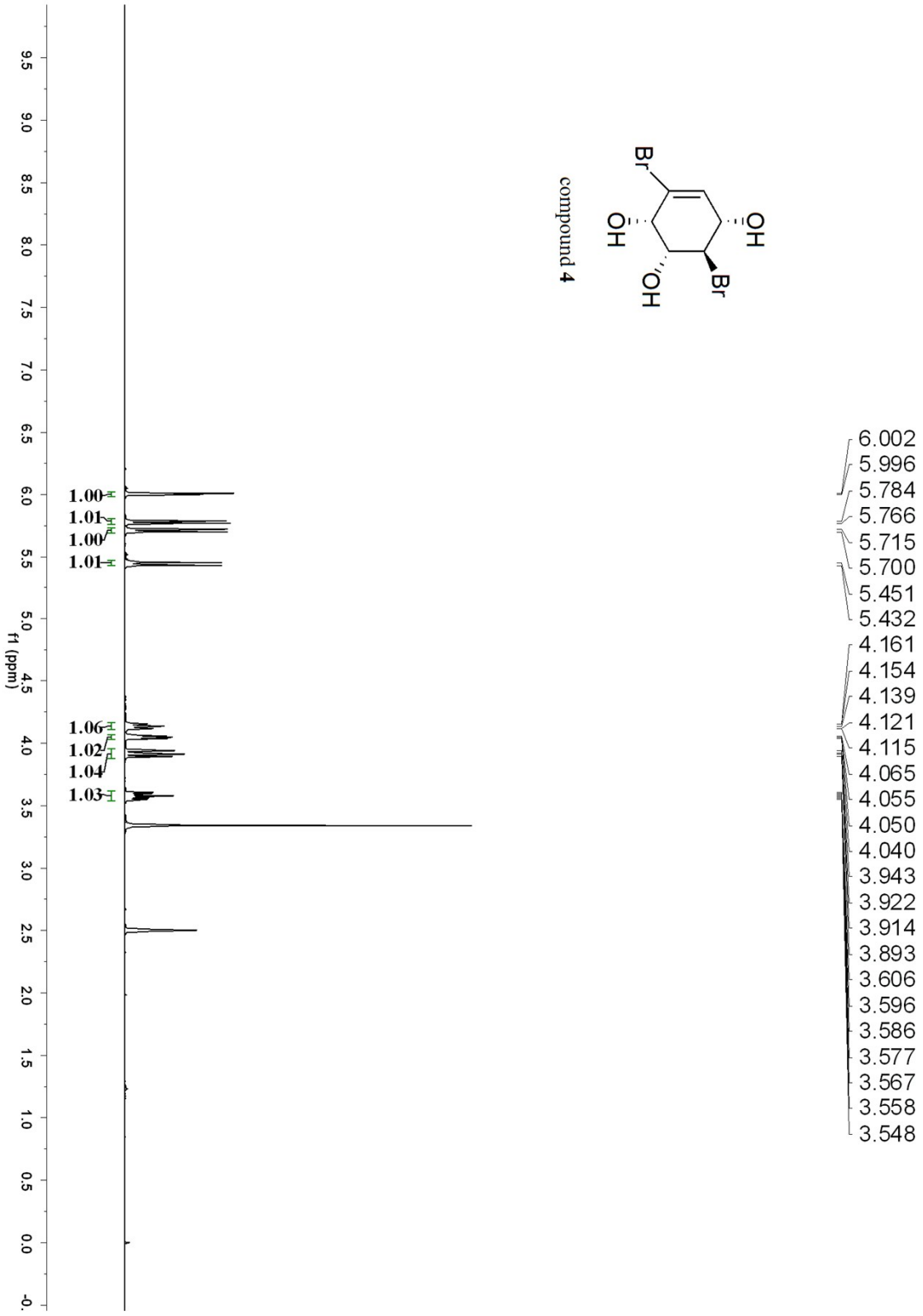

**12** **1**

| entry | condition | solvent | temperature(℃) | results |
|---|---|---|---|---|
| 1 | $Pd(CH_3CN)_2Cl_2$ | THF | 70 | **12**: degradation |
| 2 | $Pd(CH_3CN)_2Cl_2$ | DMF | 70 | **12**: degradation |
| 3 | $Pd(CH_3CN)_2Cl_2$, CuCl | THF | 70 | **12**: degradation |
| 4 | $Pd(CH_3CN)_2Cl_2$, $AsPh_3$ | toluene | 70 | **12**: degradation |
| 5 | $Pd(PPh_3)_4$, $PPh_3$ | THF | 70 | **12**: degradation |
| 6 | $Pd(dppf)Cl_2$ | DMF | 80 | **12**: degradation |
| 7 | $Pd_2(dba)_3$, $PPh_3$, CuCl | toluene | 80 | **12**: degradation |

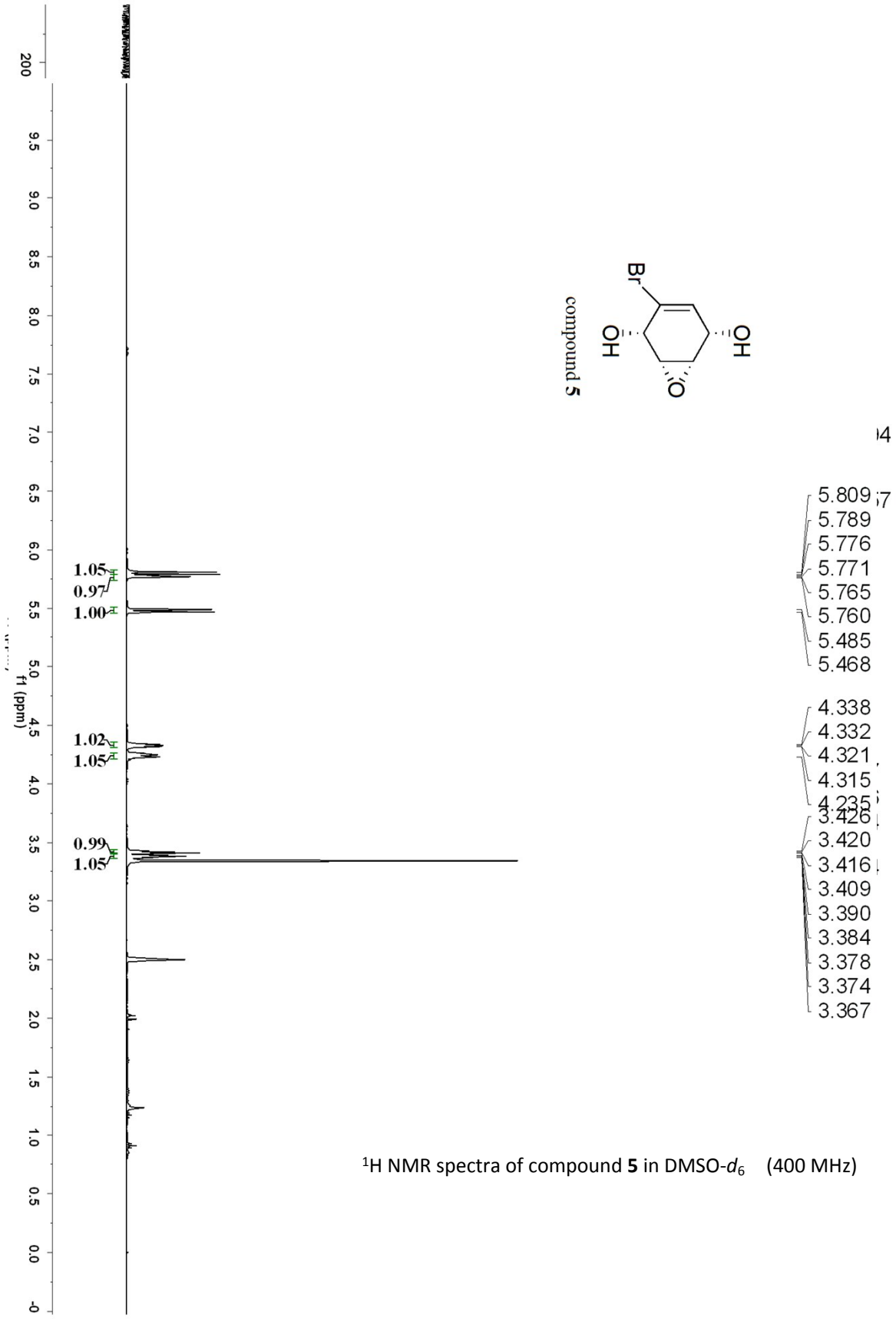
Note: The examined conditions all resulted in degradation of **12**.

Spectra for Compounds

$^1$H NMR spectra of compound **4** in DMSO-$d_6$ (400 MHz)

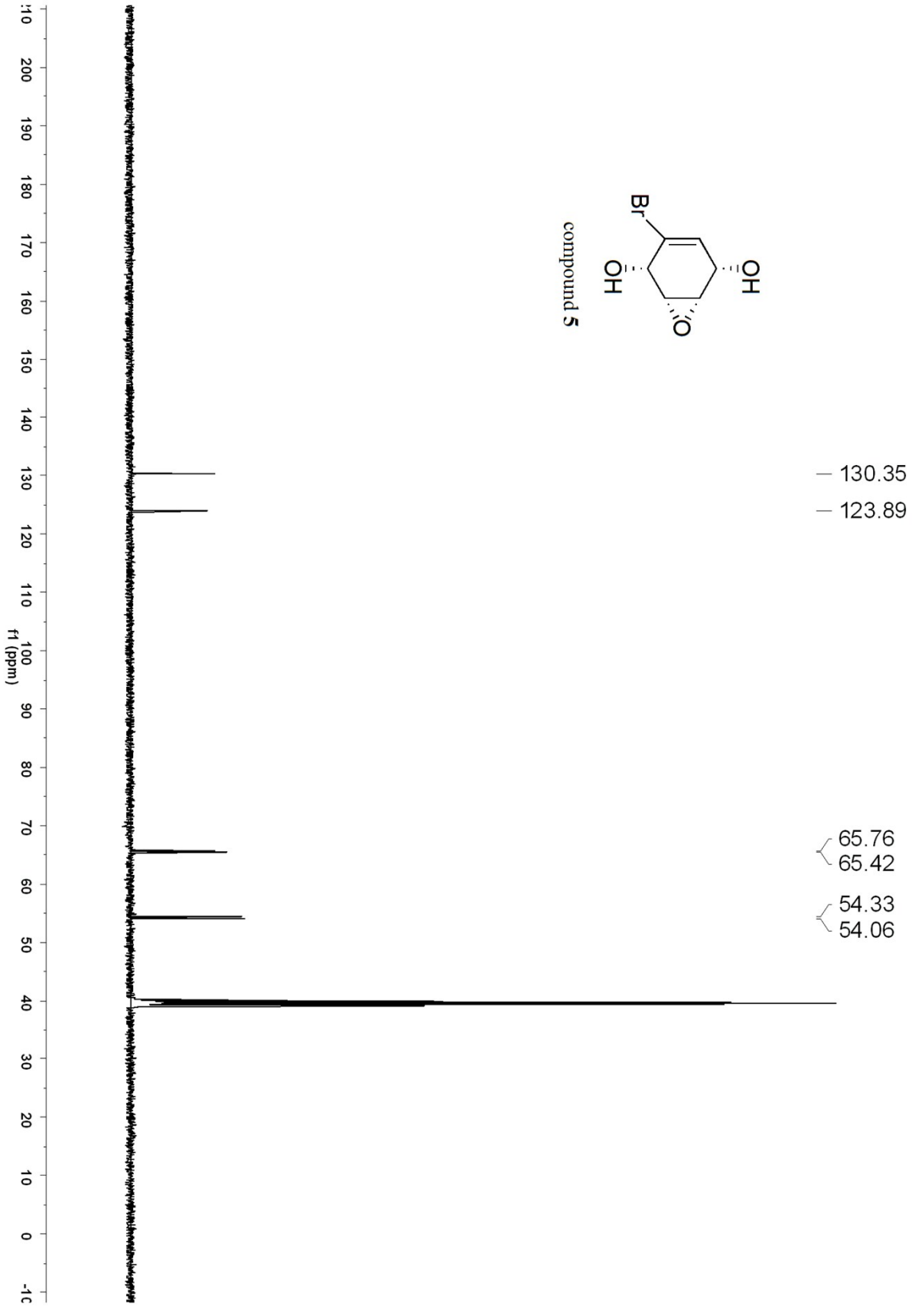


$^{13}$C NMR spectra of compound **4** in DMSO-$d_6$ (100 MHz)

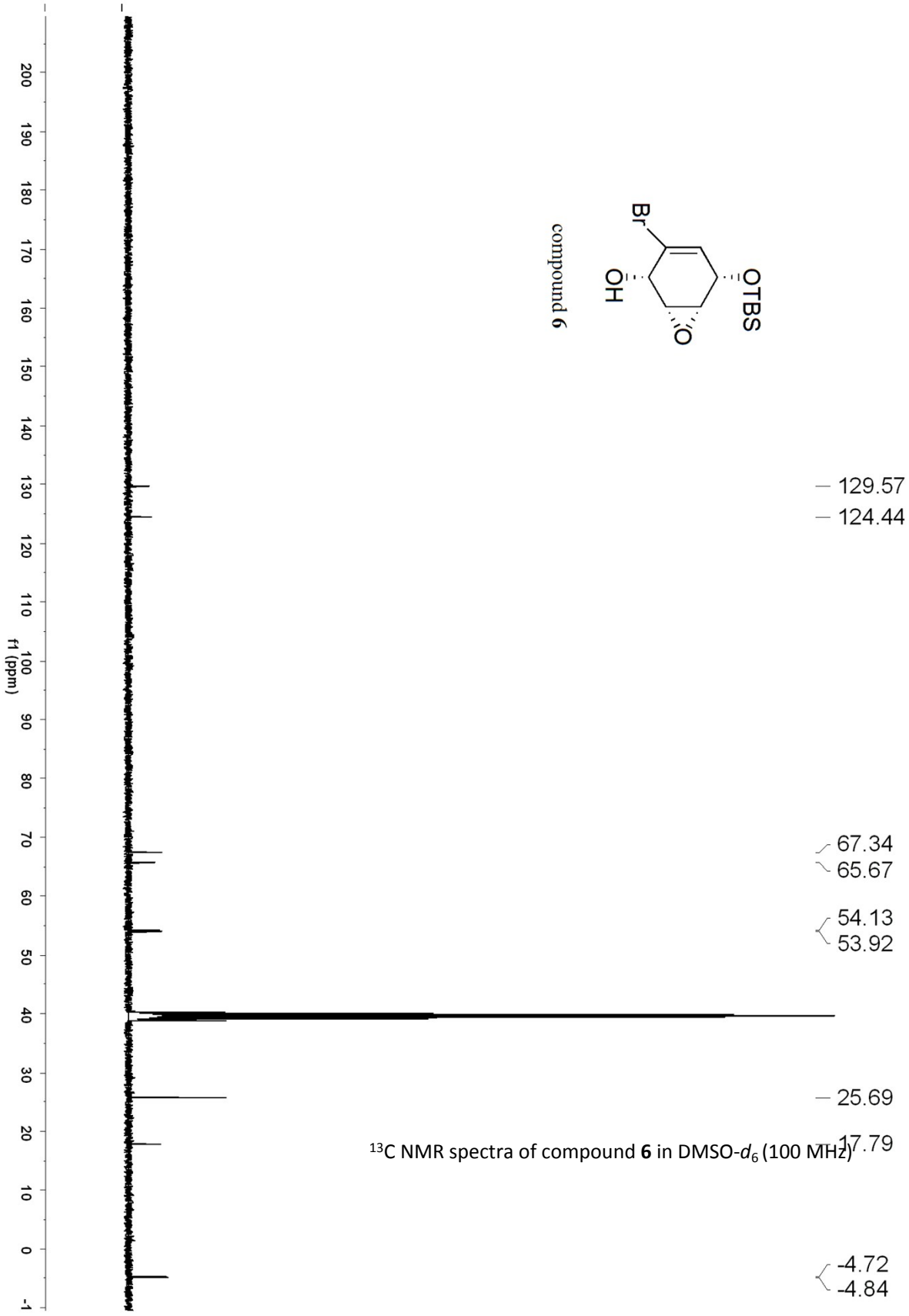



$^{1}$H NMR spectra of compound **5** in DMSO-$d_6$ (400 MHz)

$^{13}$C NMR spectra of compound **5** in DMSO-$d_6$ (100 MHz)

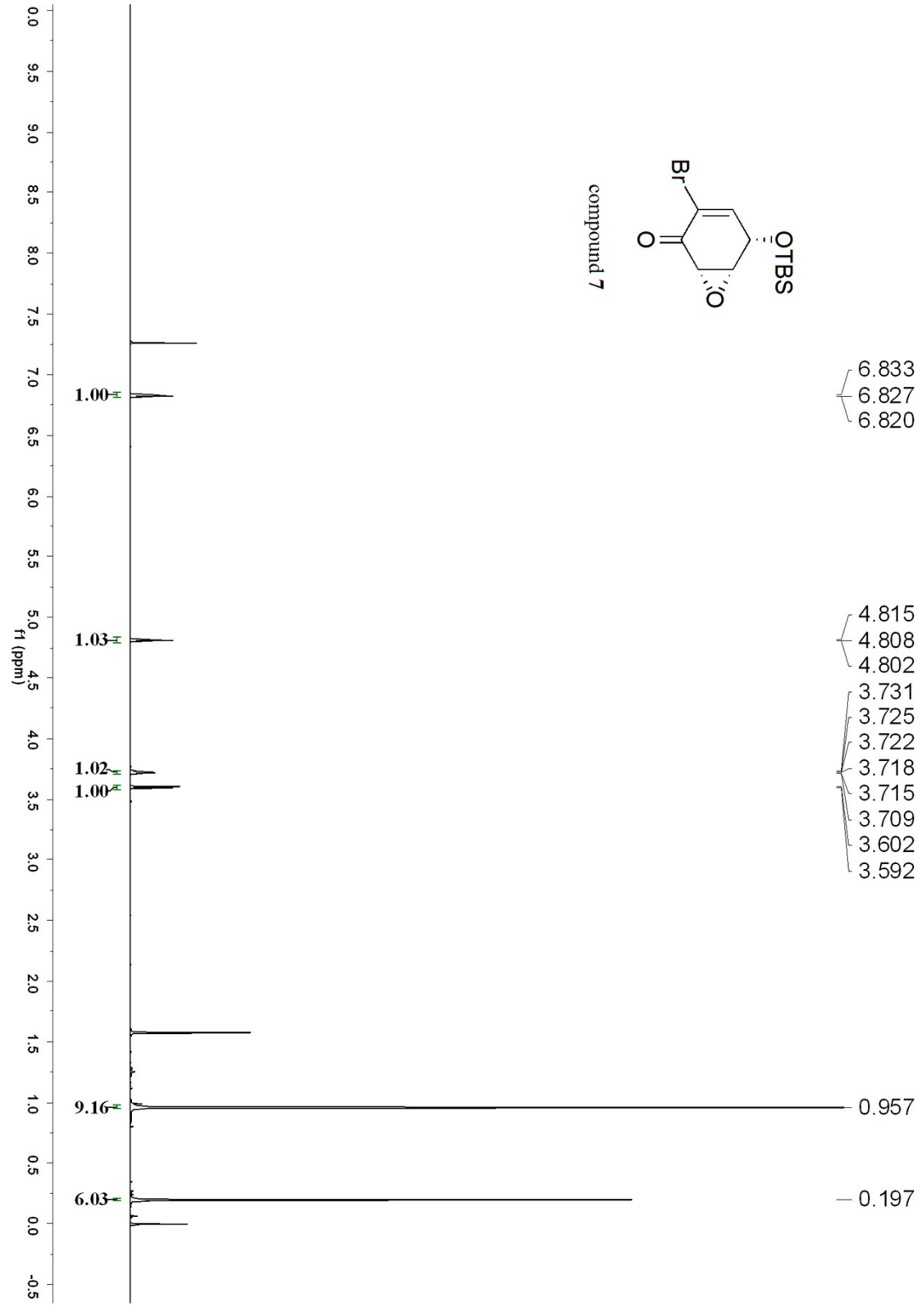


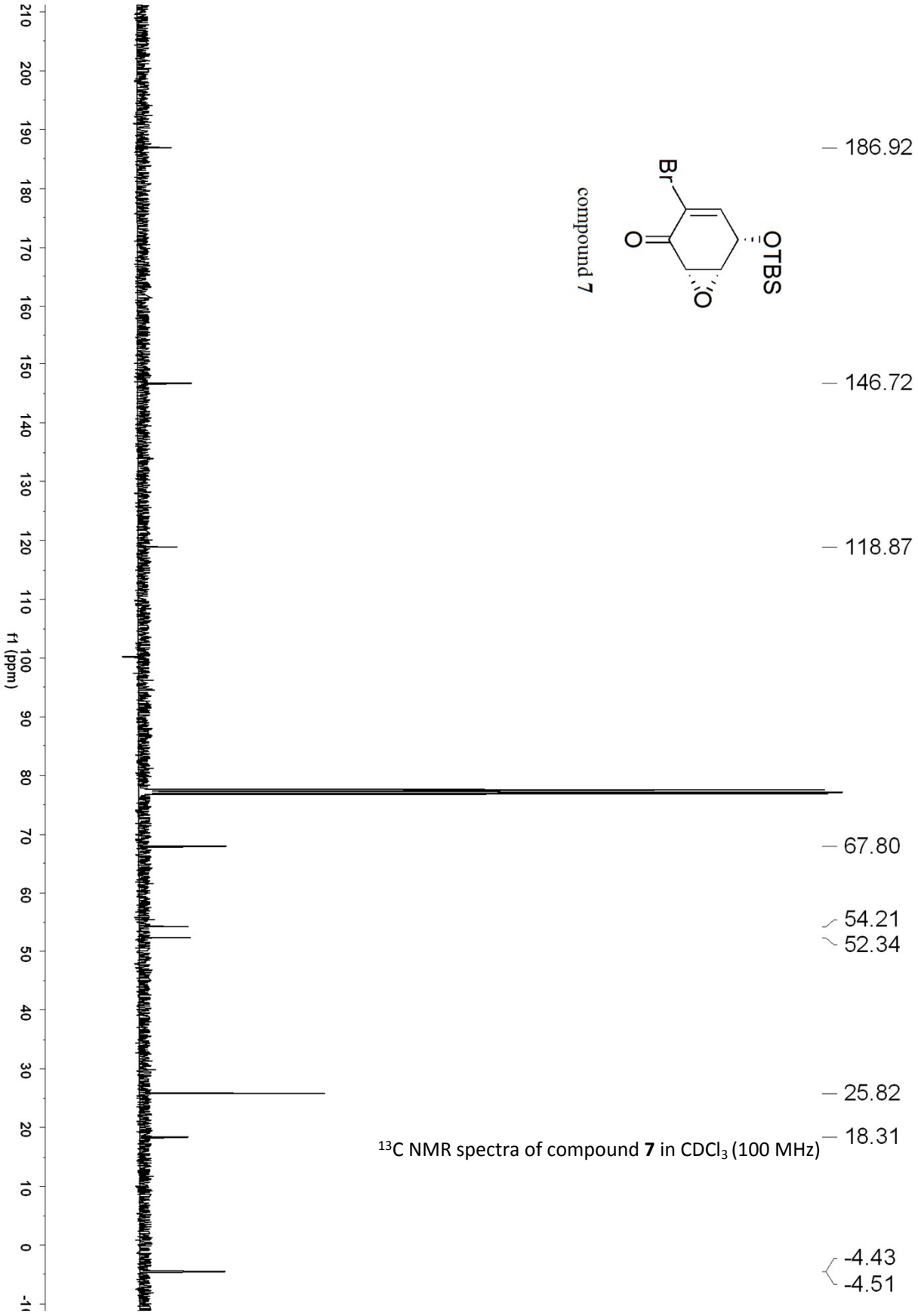
$^{1}$H NMR spectra of compound **6** in $CDCl_3$ (400 MHz)




$^{13}$C NMR spectra of compound **6** in DMSO-$d_6$ (100 MHz)

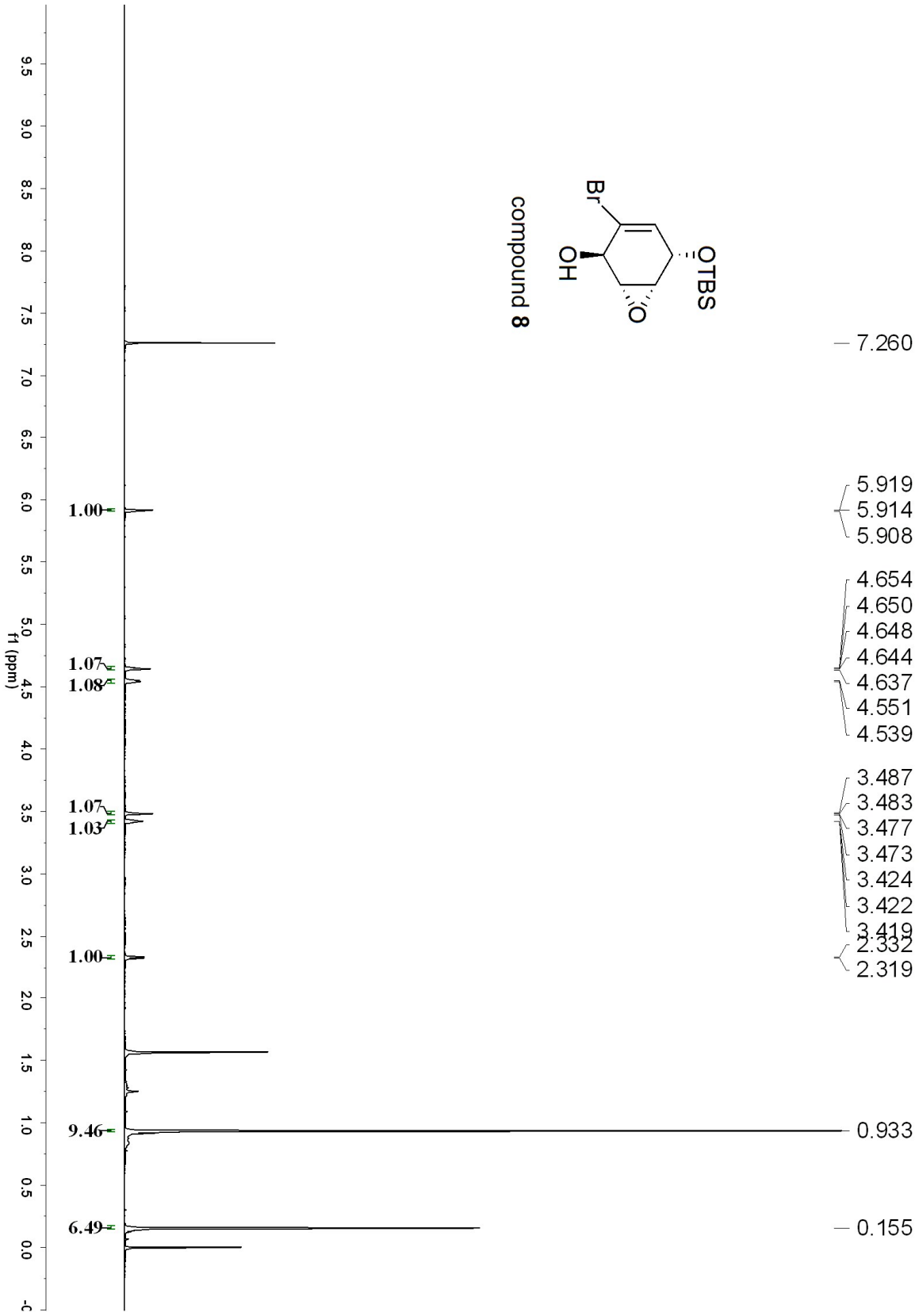
$^{1}$H NMR spectra of compound **7** in $CDCl_3$ (400 MHz)



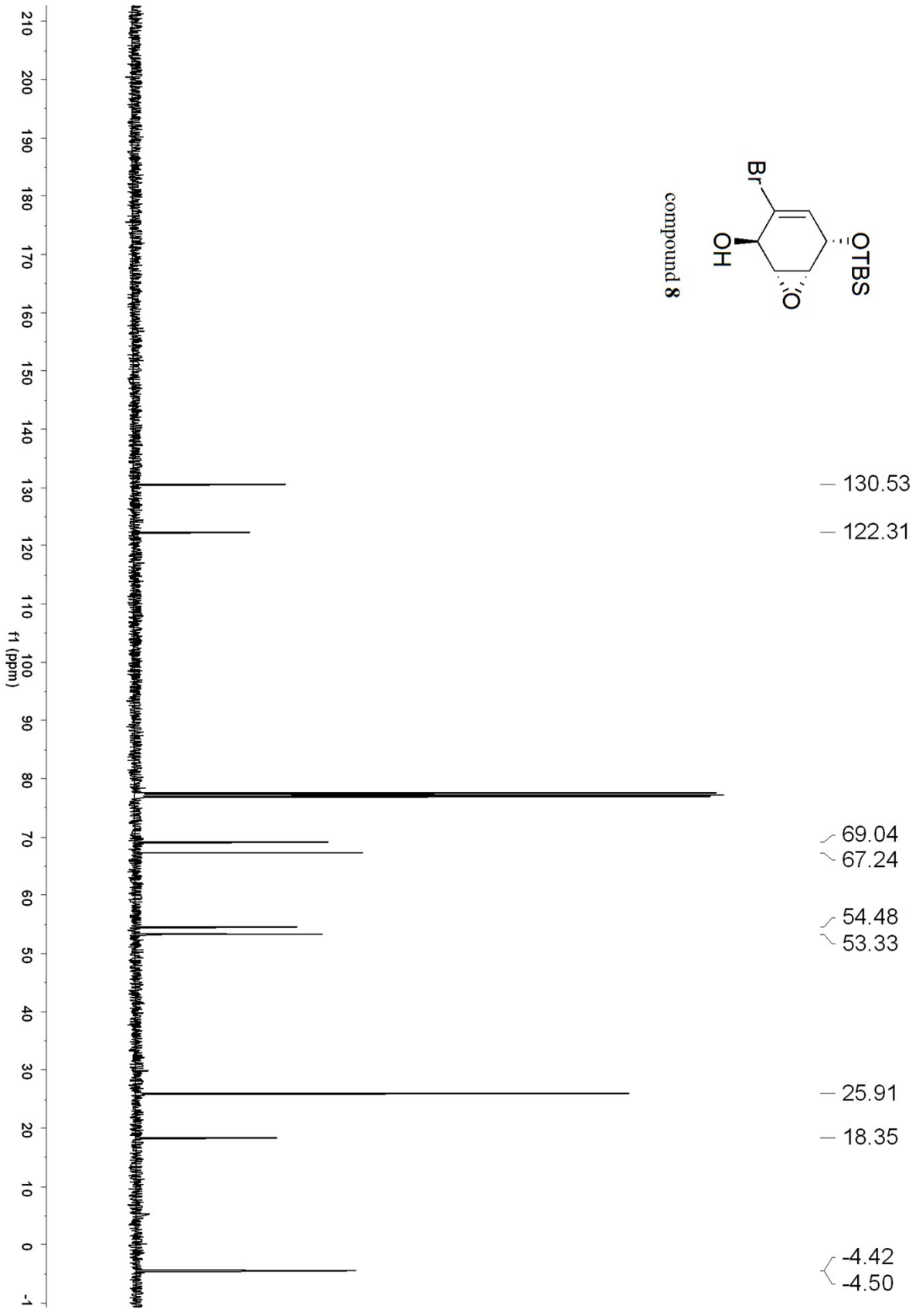



$^{13}C$ NMR spectra of compound **7** in $CDCl_3$ (100 MHz)

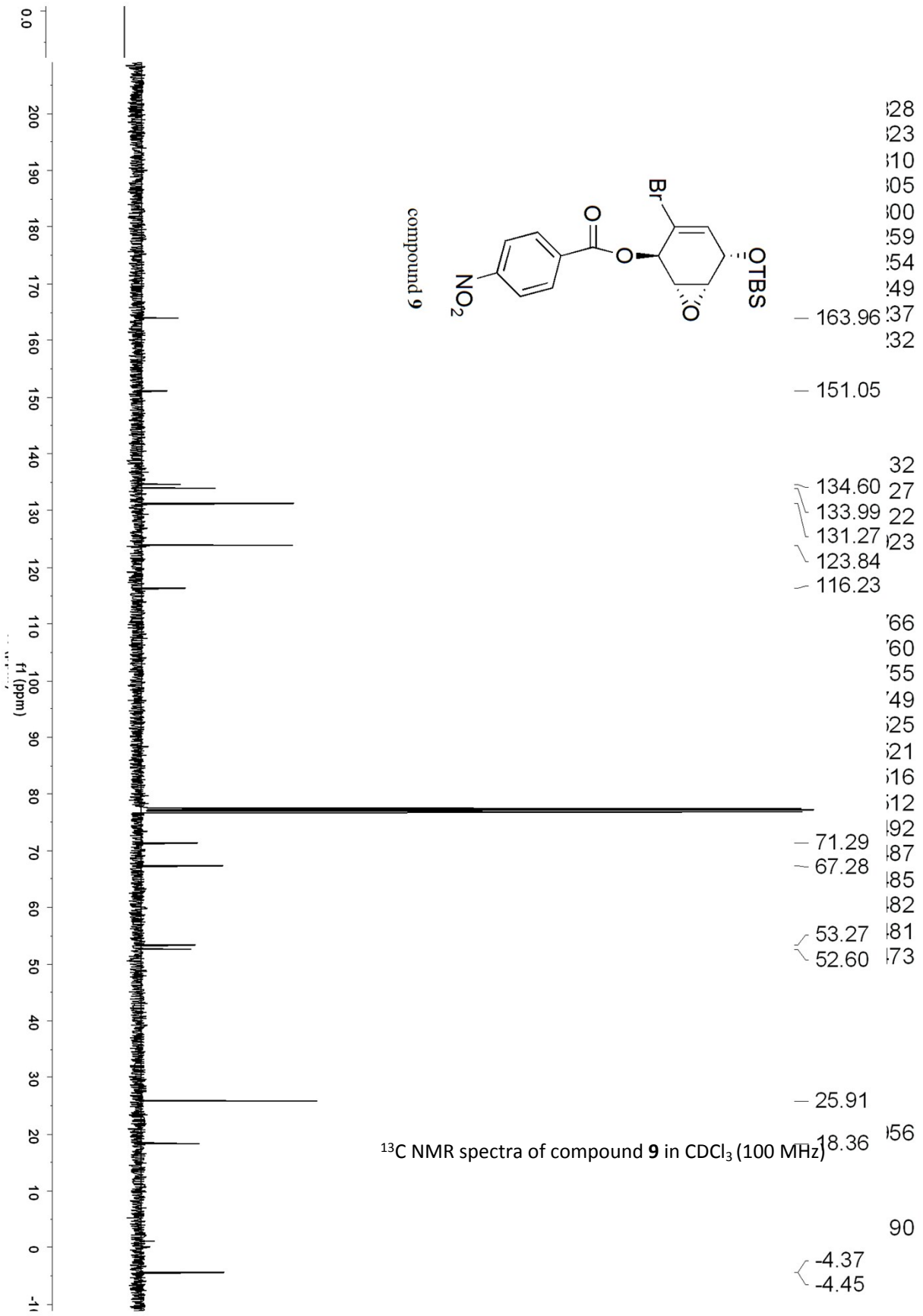
$^{1}$H NMR spectra of compound **8** in $CDCl_3$ (400 MHz)



$^{13}C$ NMR spectra of compound **8** in $CDCl_3$ (100 MHz)

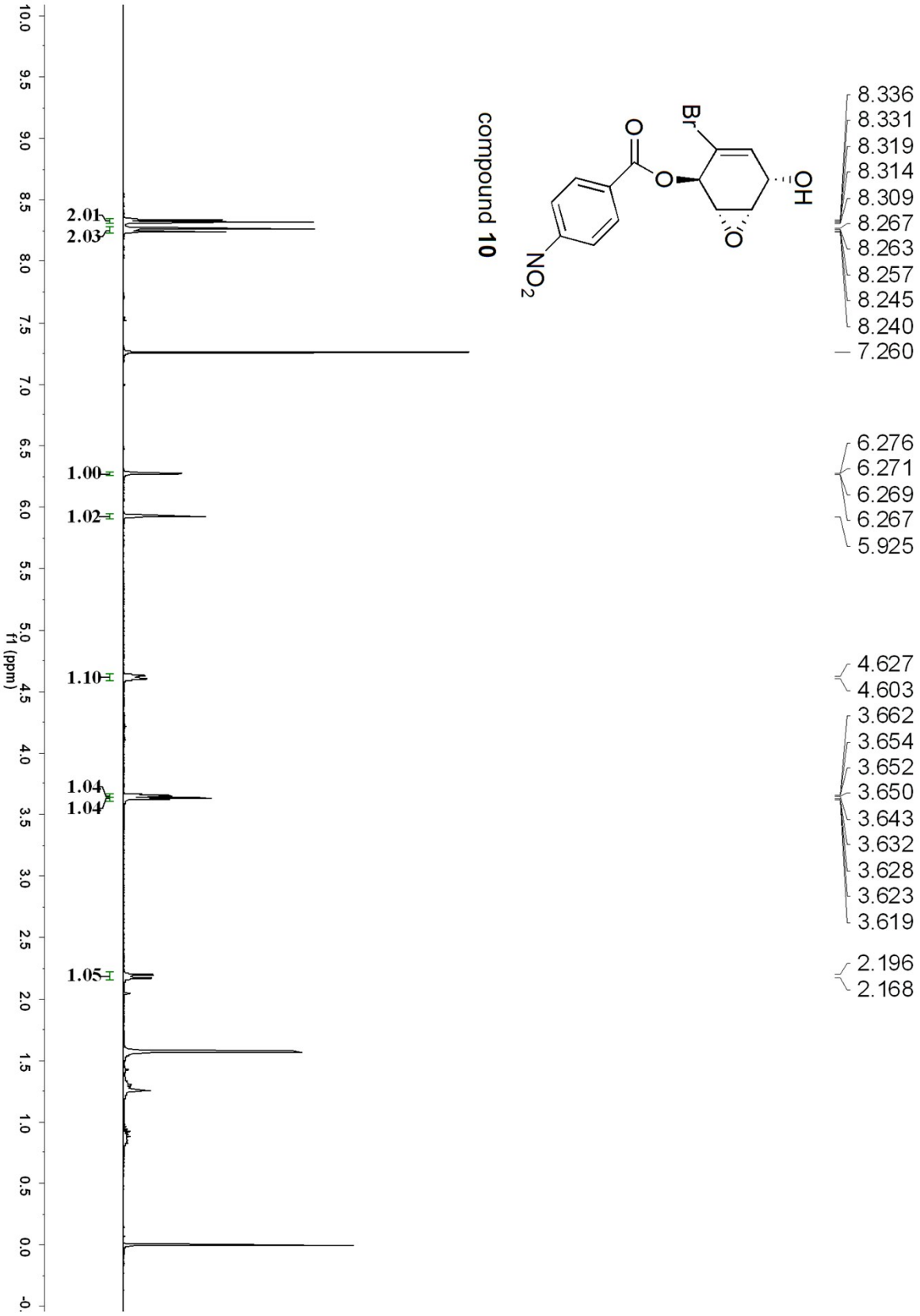


$^{1}$H NMR spectra of compound **9** in $CDCl_3$ (400 MHz

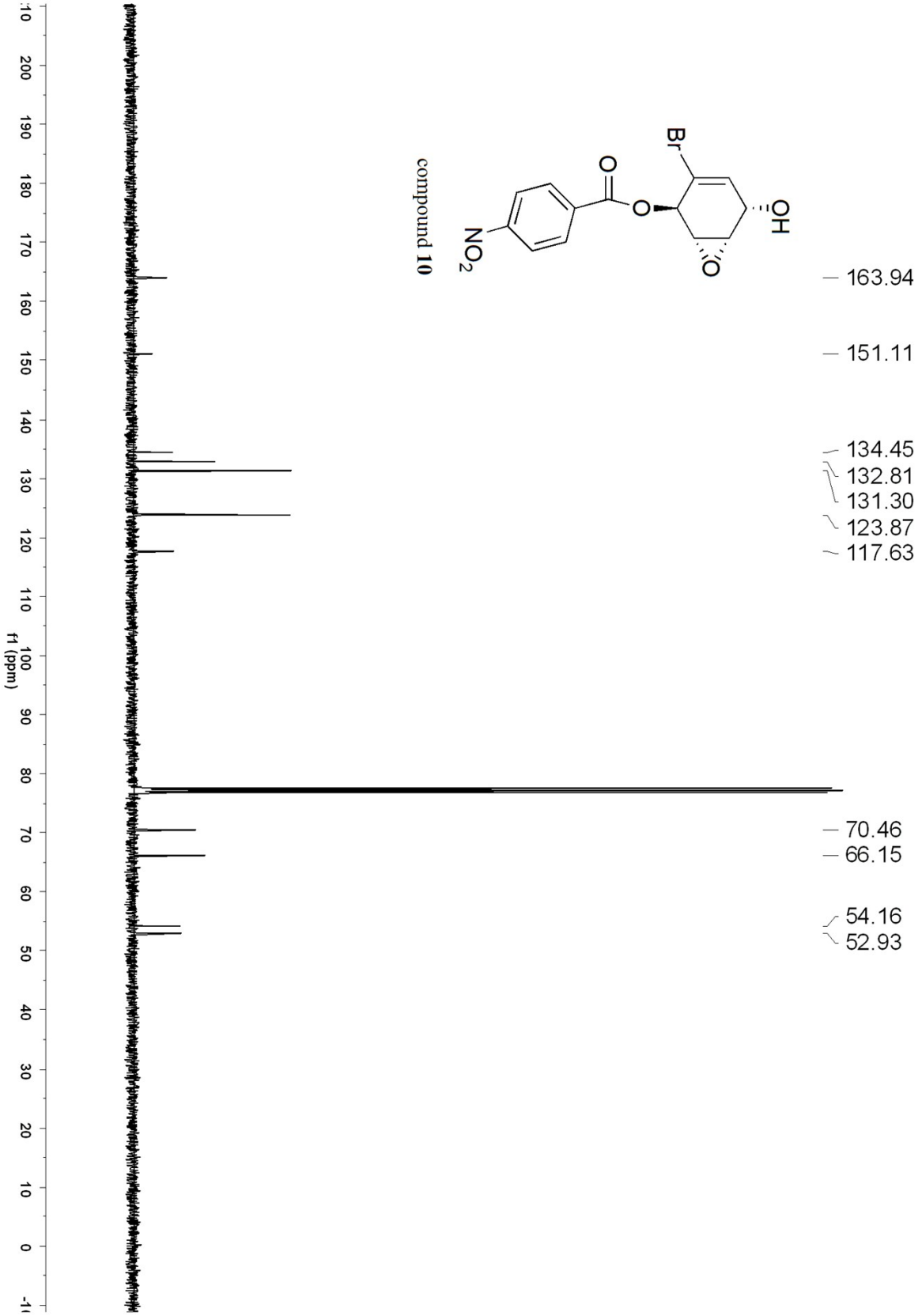



$^{13}$C NMR spectra of compound **9** in $CDCl_3$ (100 MHz)

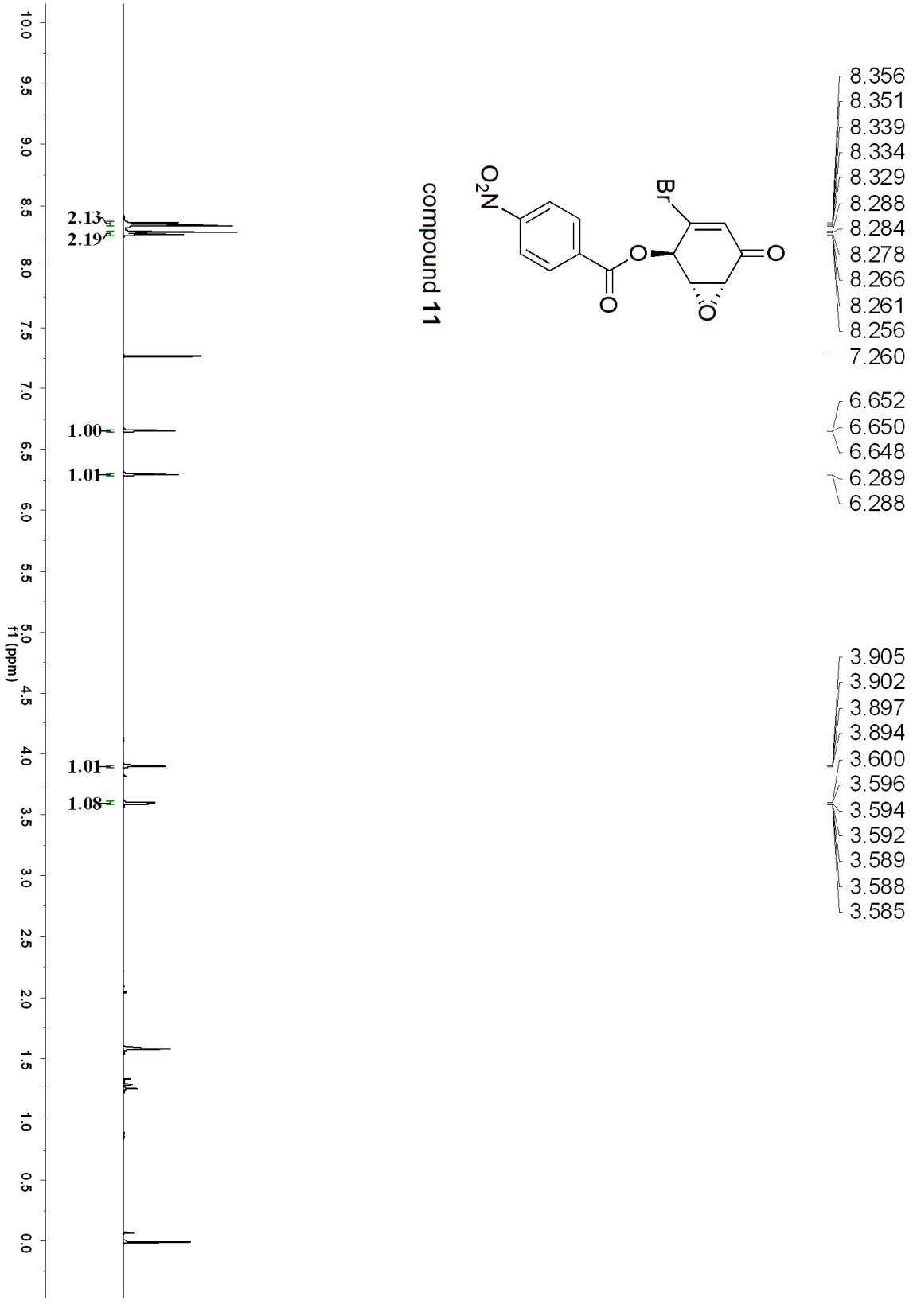
$^{1}$H NMR spectra of compound **10** in $CDCl_3$ (400 MHz)



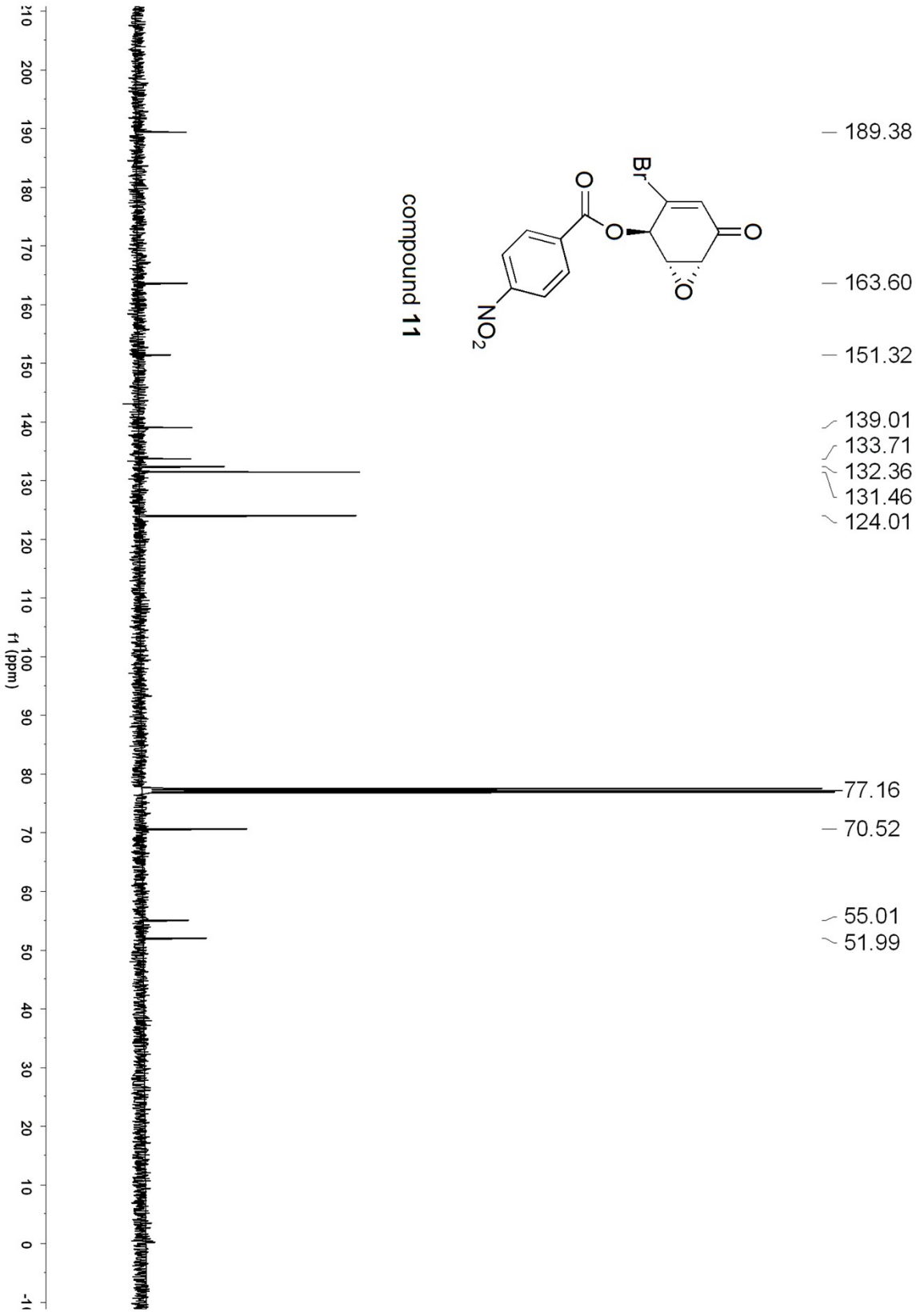
$^{13}C$ NMR spectra of compound **10** in $CDCl_3$ (100 MHz)



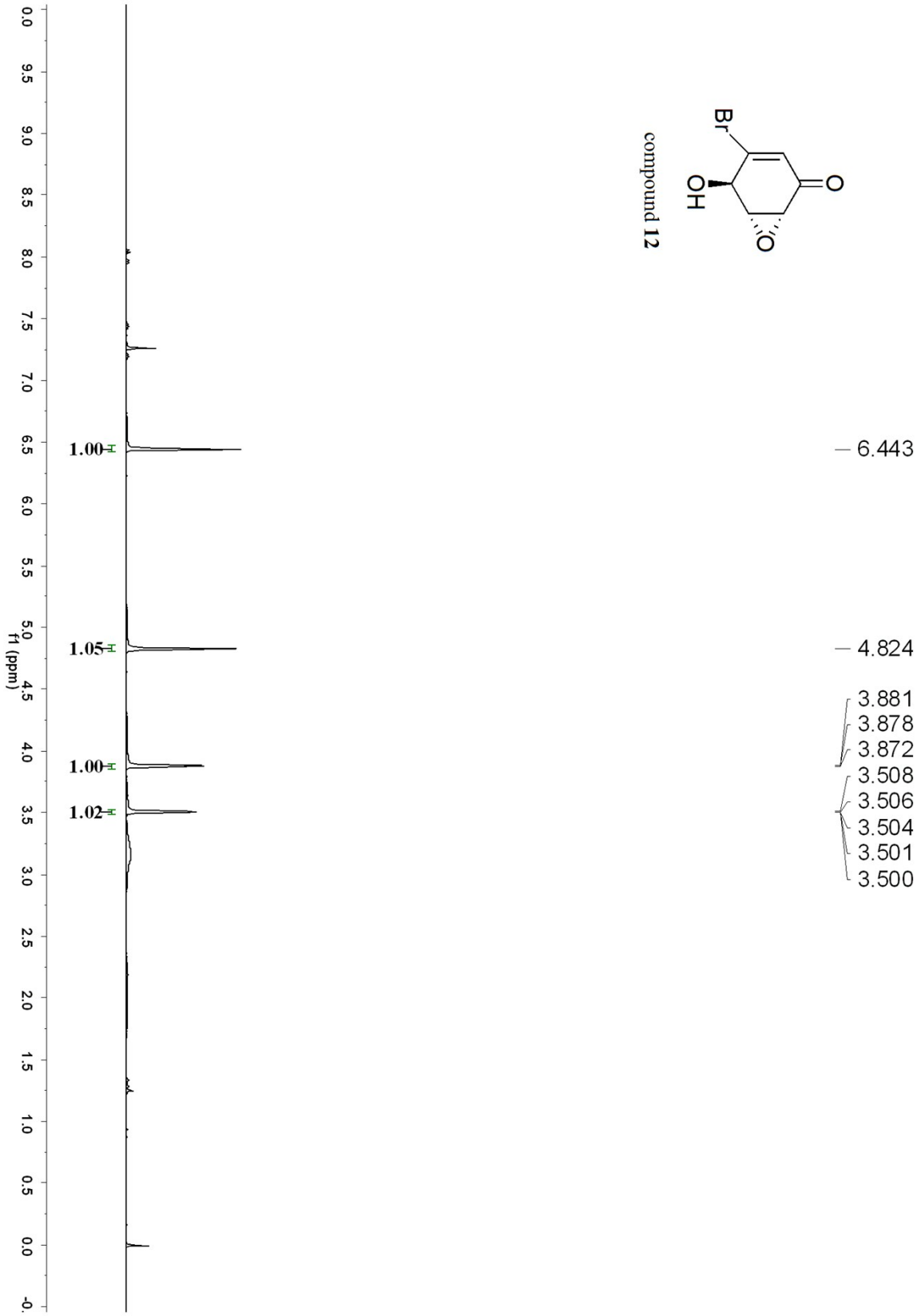
$^{1}$H NMR spectra of compound **11** in $CDCl_3$ (400 MHz)



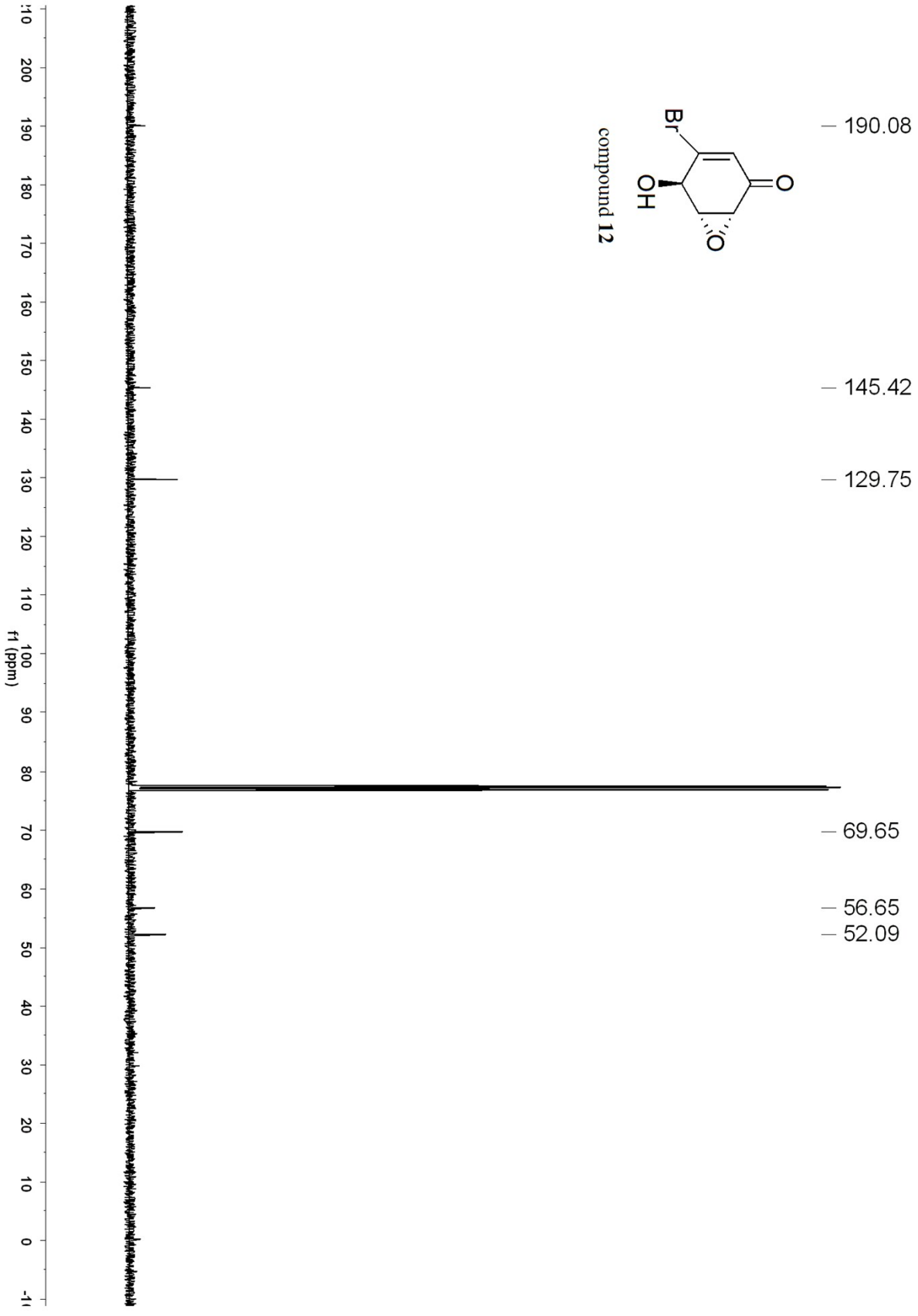
$^{13}C$ NMR spectra of compound **11** in $CDCl_3$ (100 MHz)



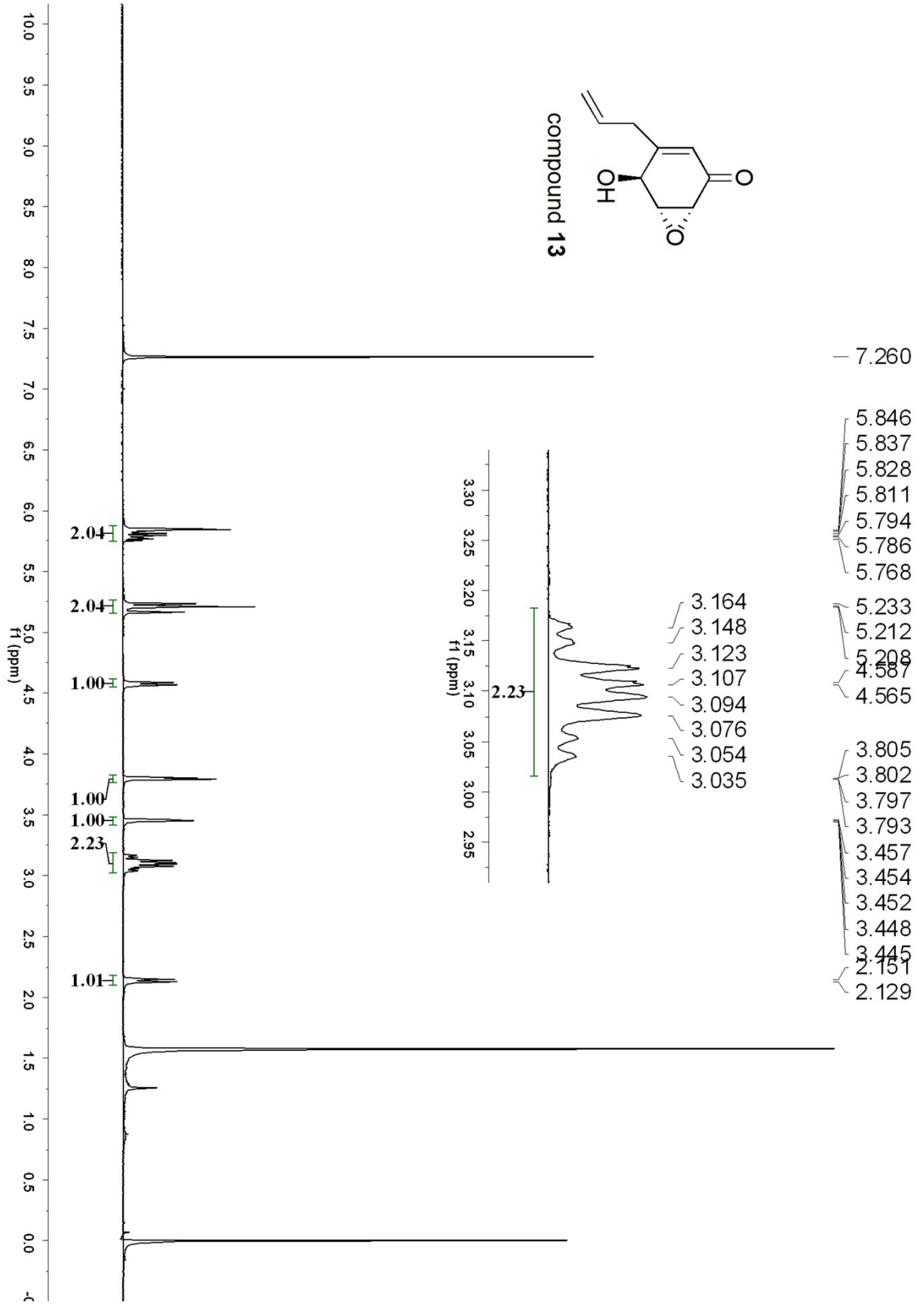
$^{1}$H NMR spectra of compound **12** in $CDCl_3$ (400 MHz)\



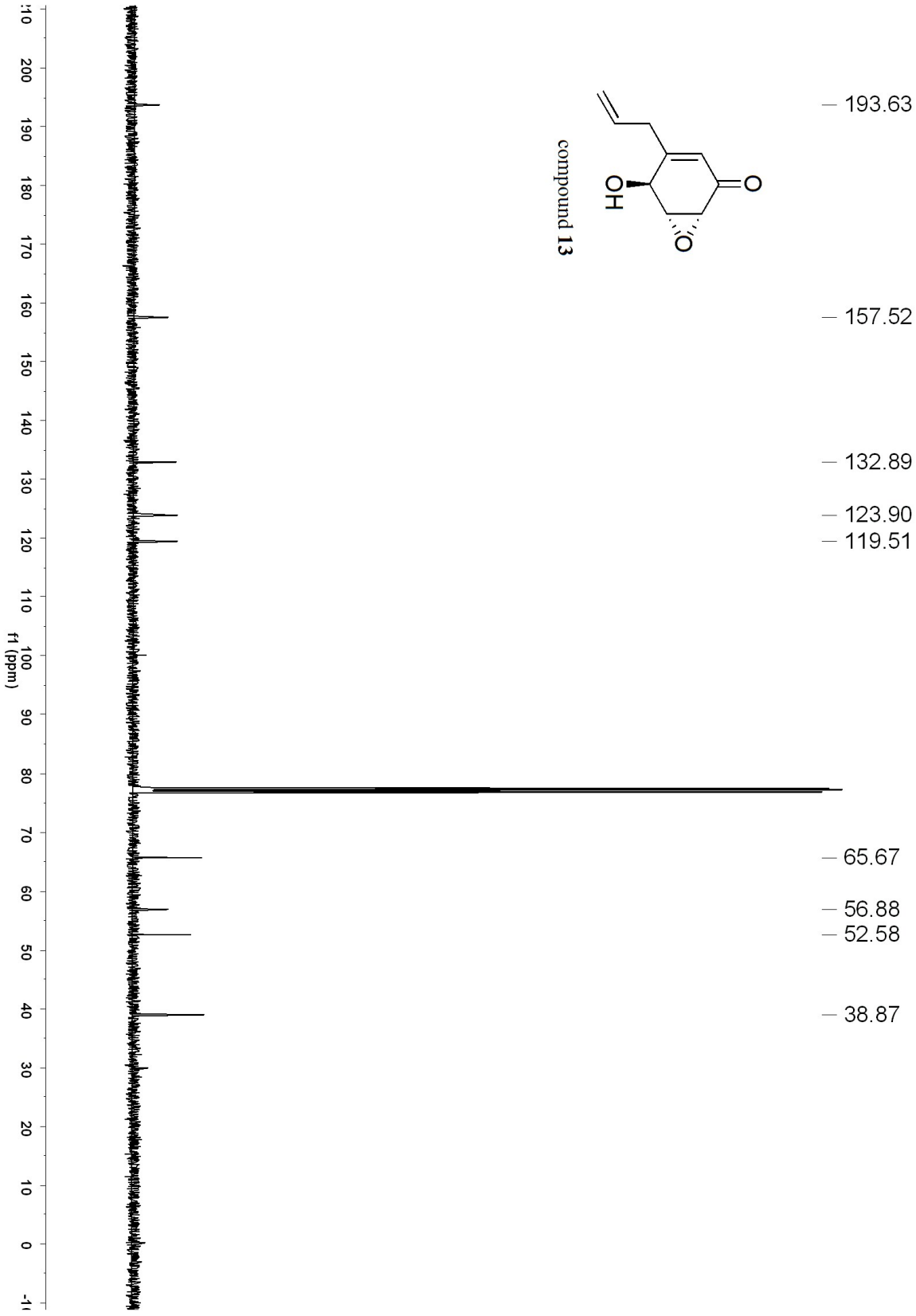
$^{13}C$ NMR spectra of compound **12** in $CDCl_3$ (100 MHz)



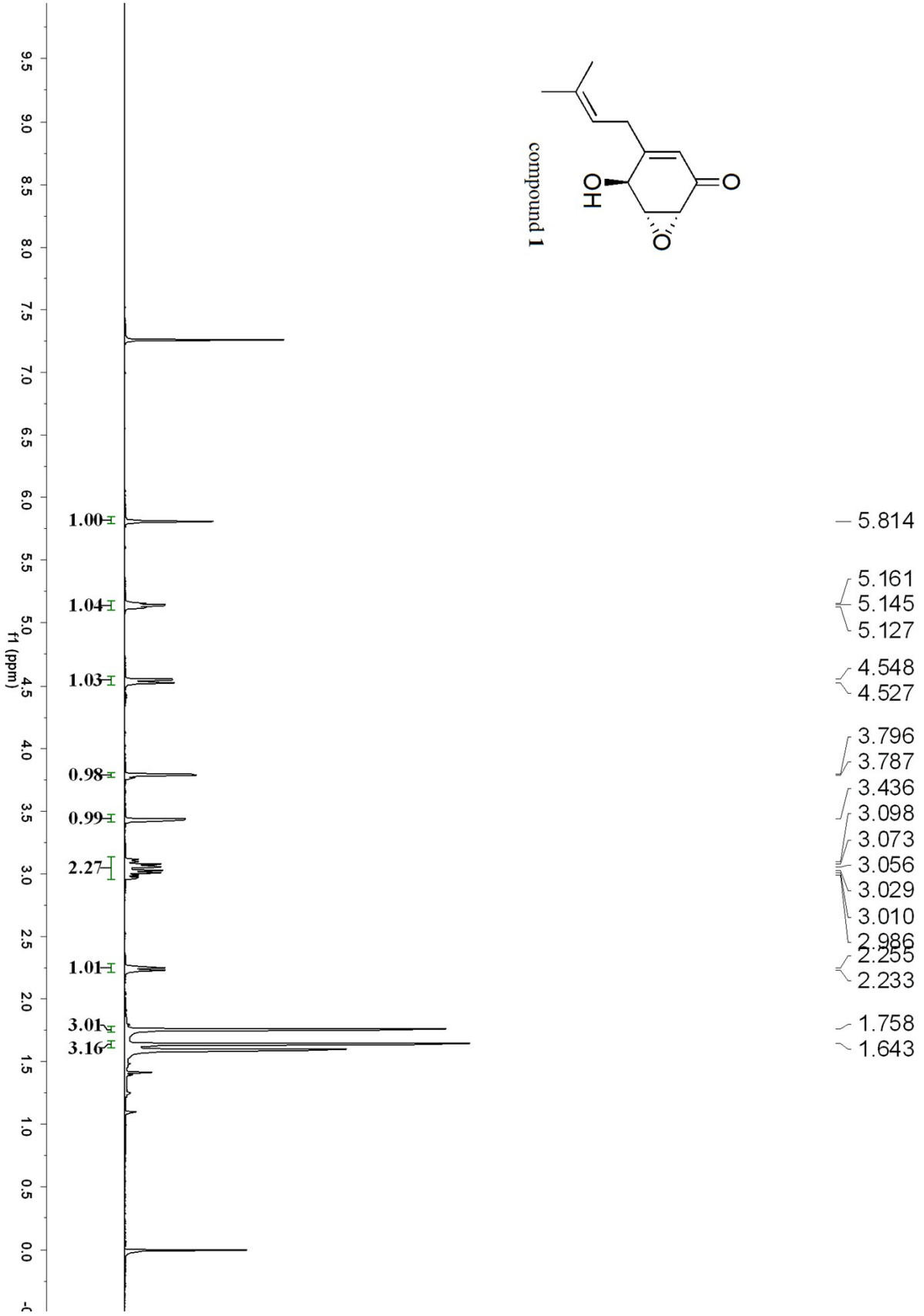
$^{1}$H NMR spectra of compound **13** in $CDCl_3$ (400 MHz)



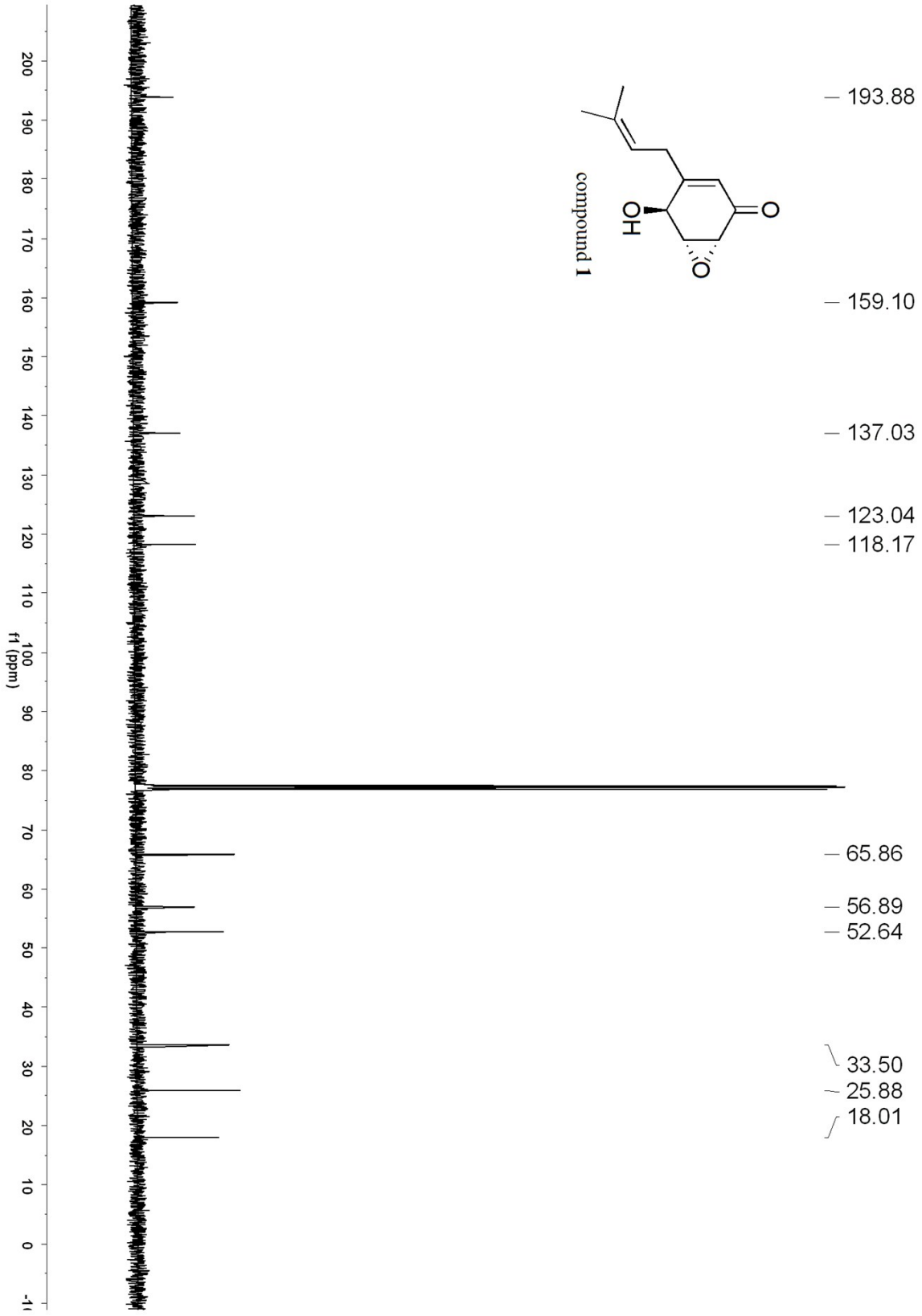
$^{13}C$ NMR spectra of compound **13** in $CDCl_3$ (100 MHz)



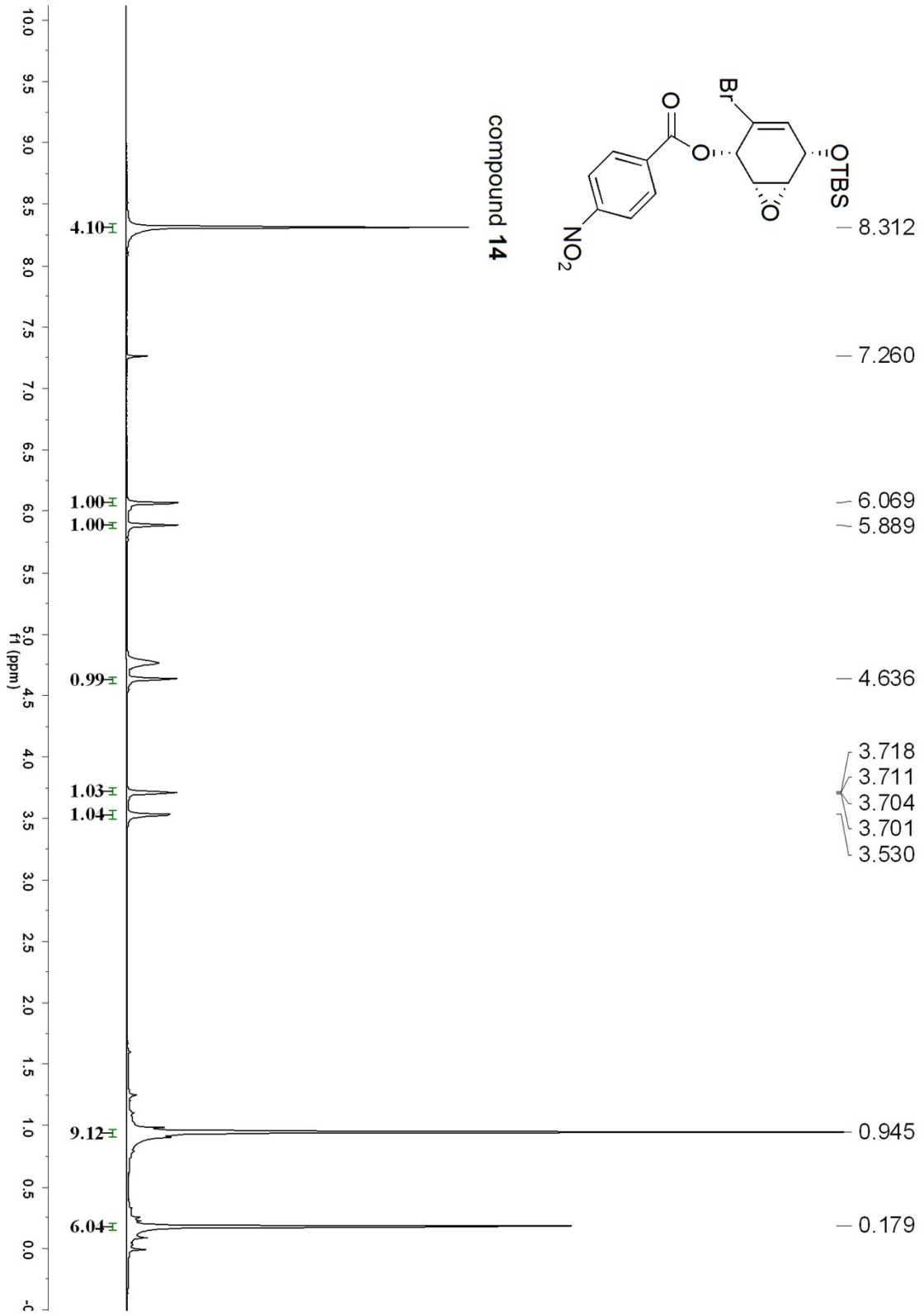
$^{1}H$ NMR spectra of compound **1** in $CDCl_3$ (400 MHz)



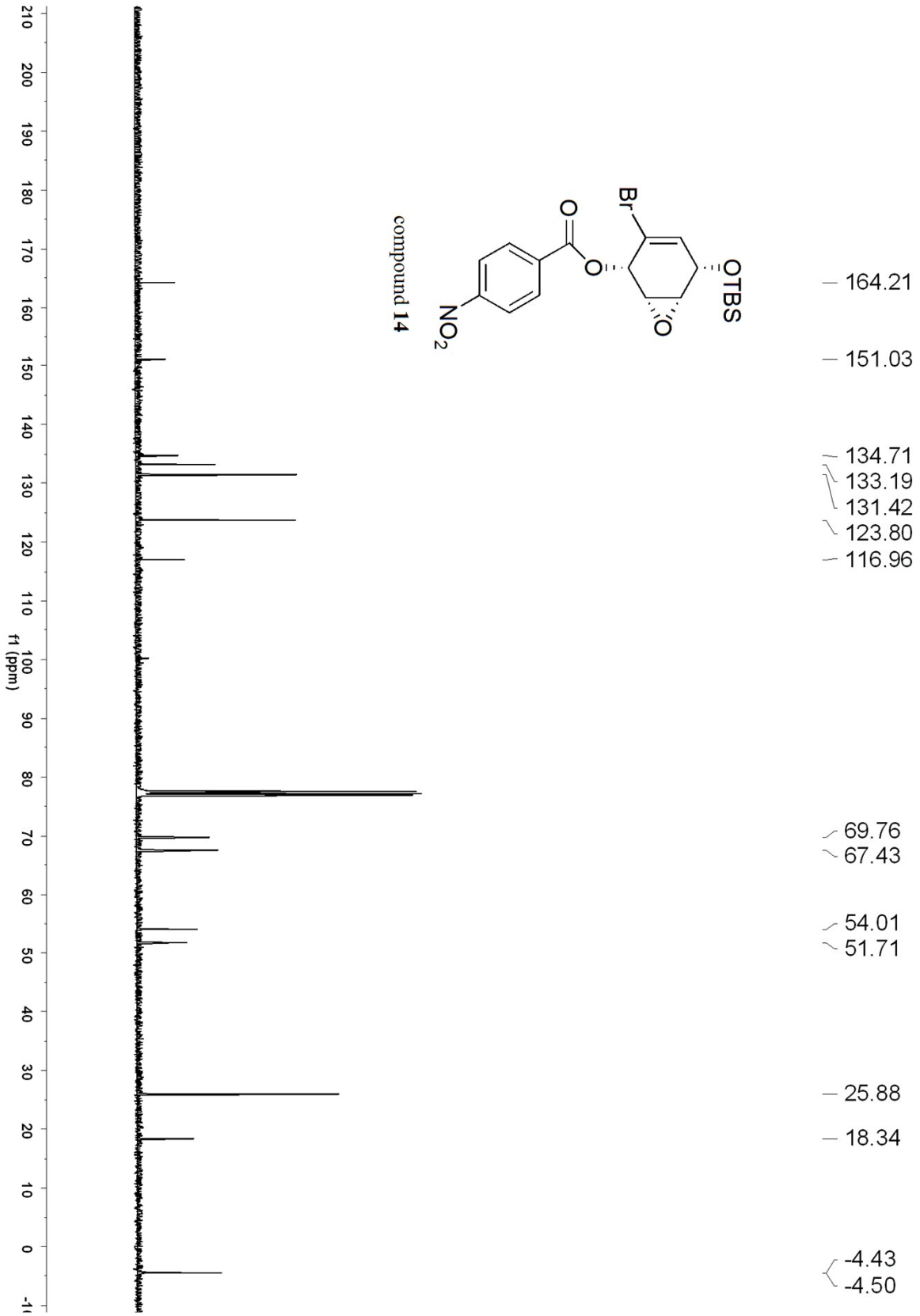
$^{13}C$ NMR spectra of compound **1** in $CDCl_3$ (100 MHz)



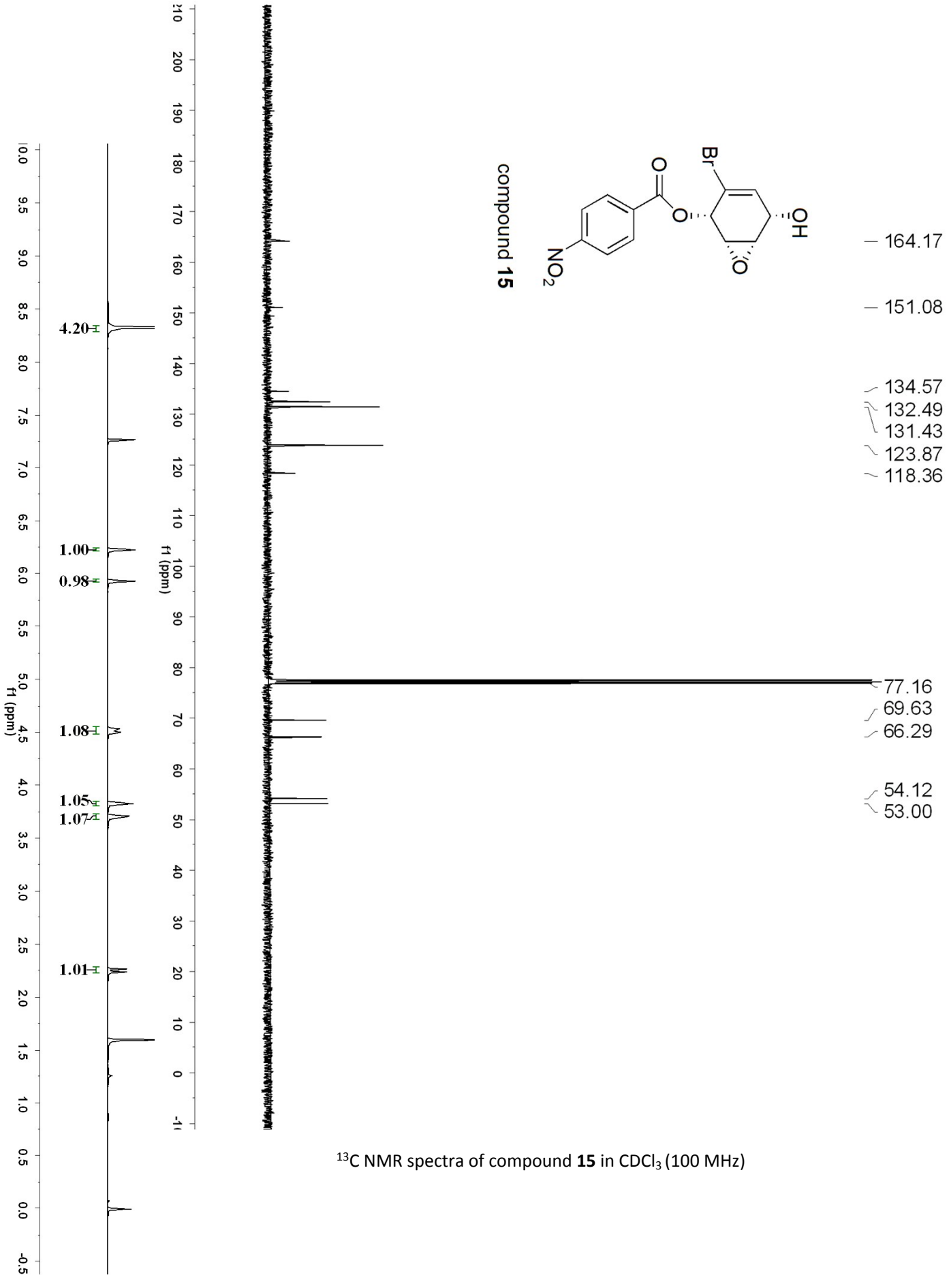
$^{1}$H NMR spectra of compound **14** in $CDCl_3$ and $D_2O$ (400 MHz)



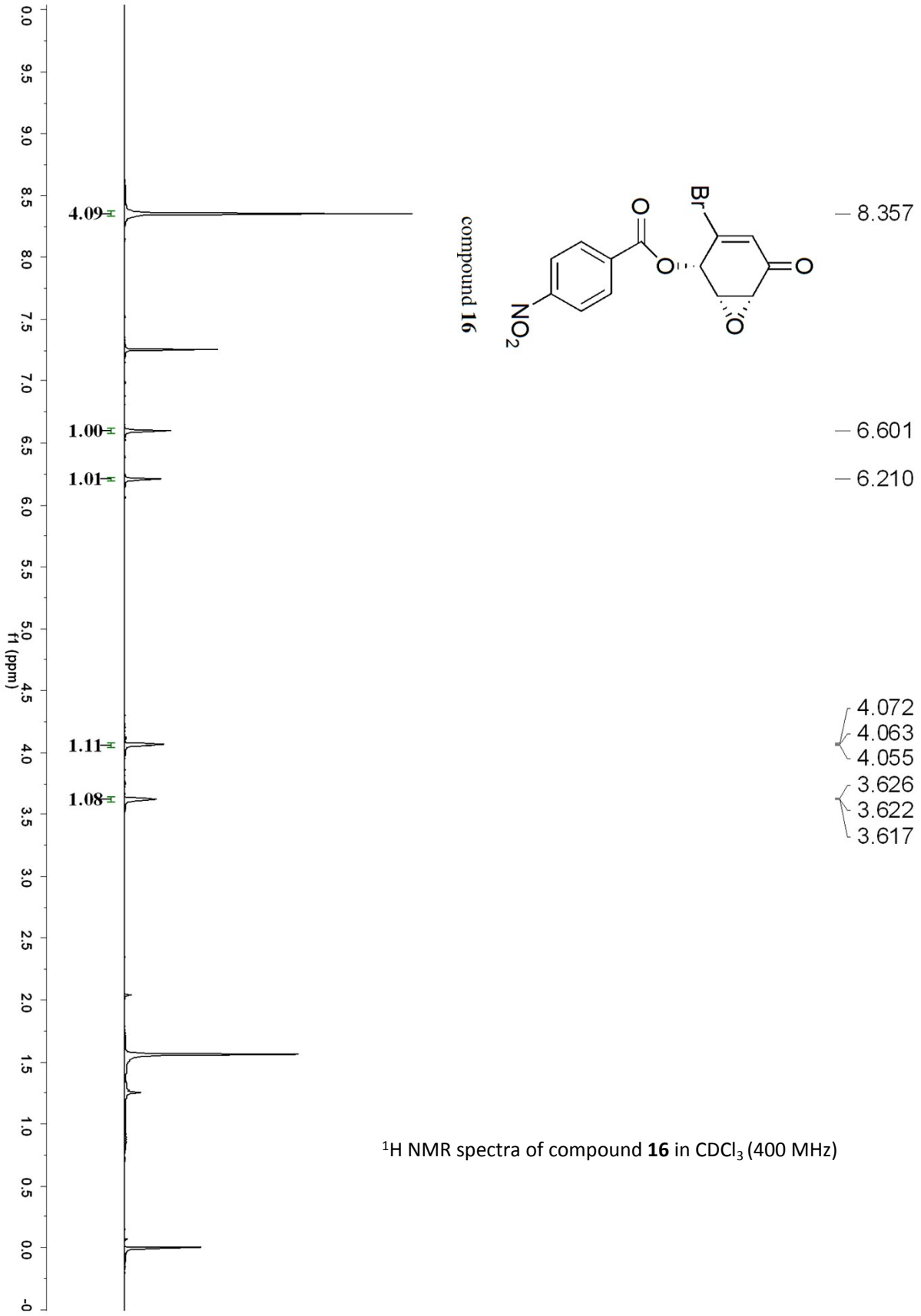
$^{13}C$ NMR spectra of compound **14** in $CDCl_3$ (100 MHz)



$^{1}$H NMR spectra of compound **15** in $CDCl_3$ (400 MHz)

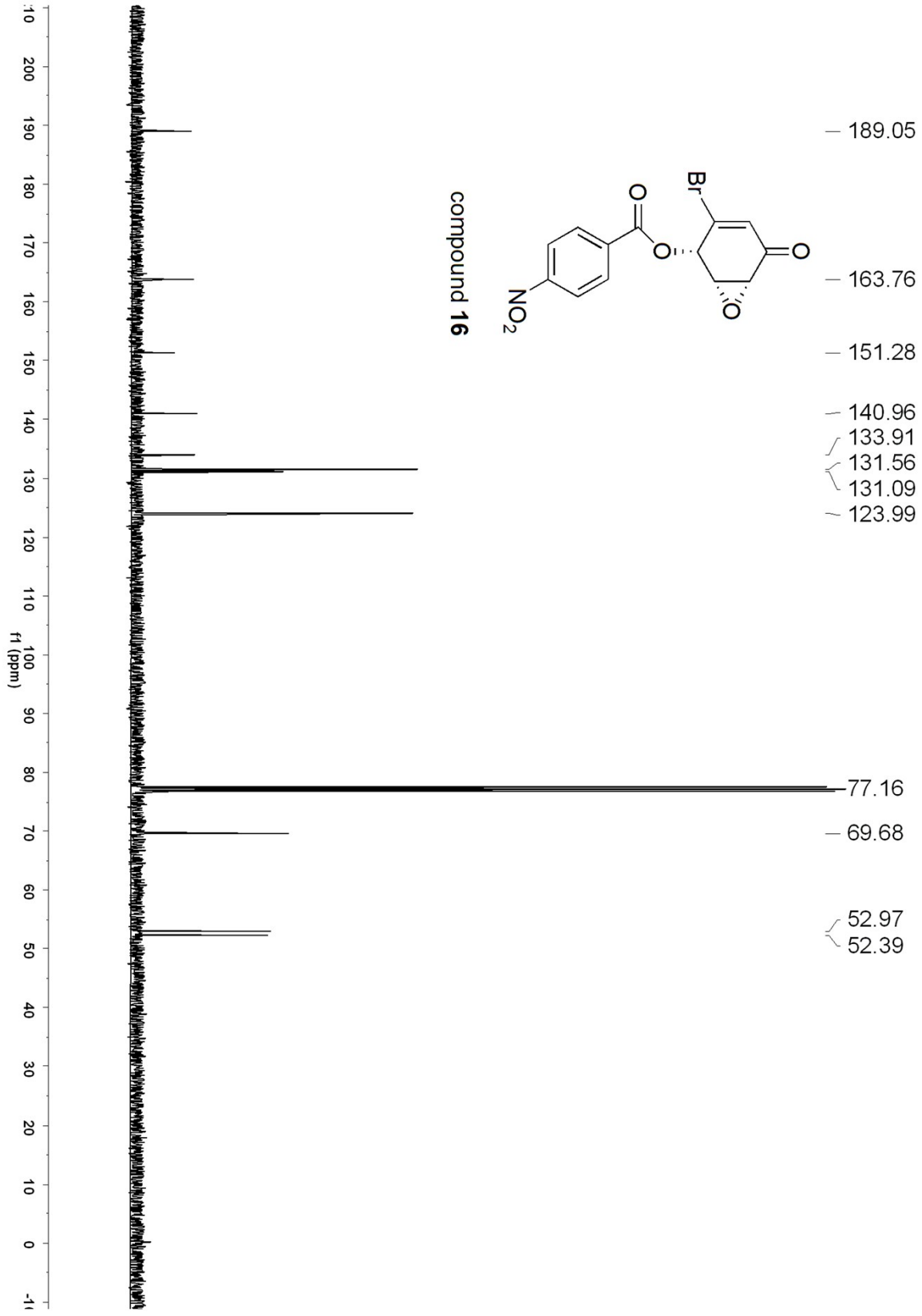



$^{13}$C NMR spectra of compound **15** in $CDCl_3$ (100 MHz)

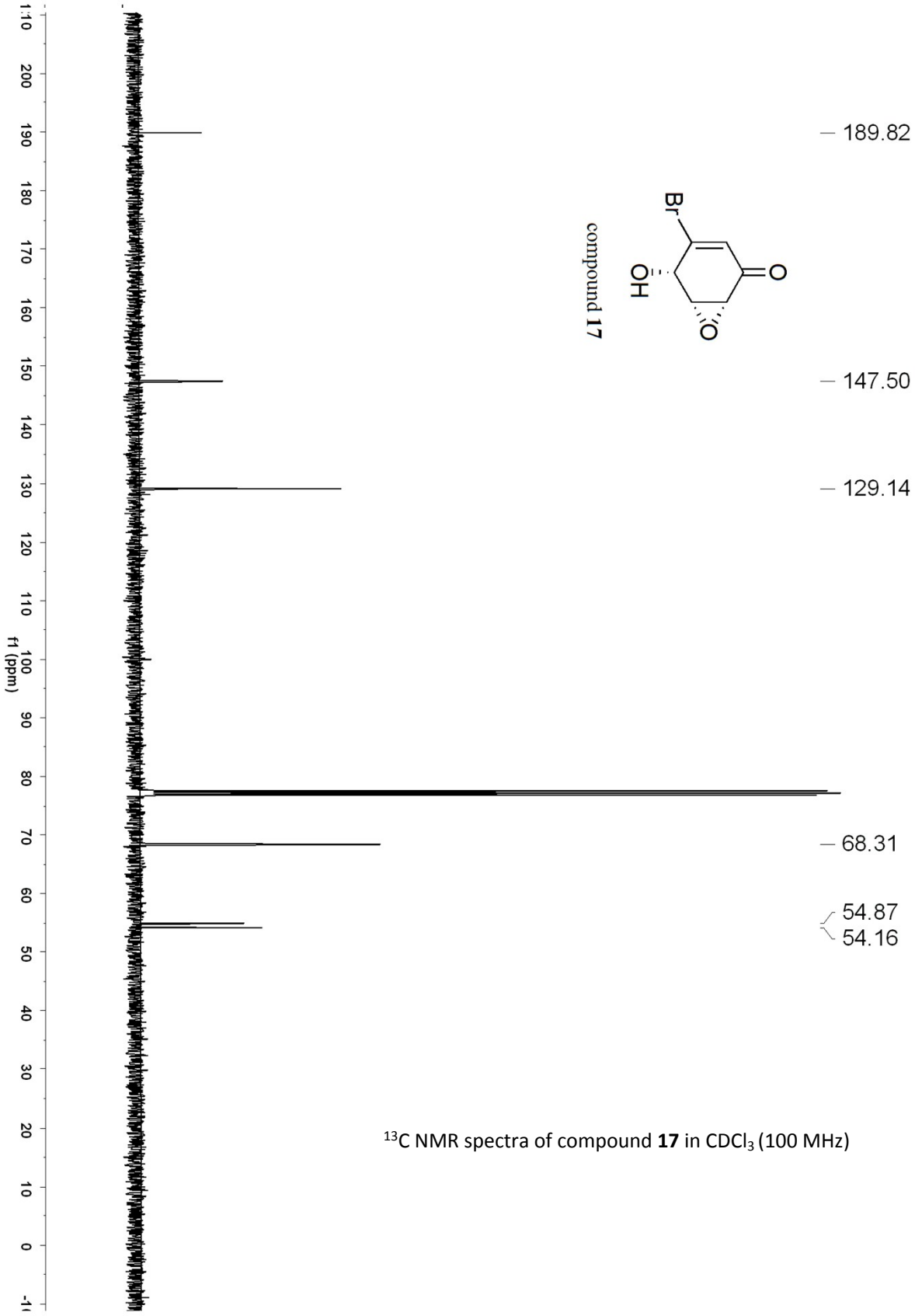



$^1$H NMR spectra of compound **16** in $CDCl_3$ (400 MHz)

$^{13}C$ NMR spectra of compound **16** in $CDCl_3$ (100 MHz)

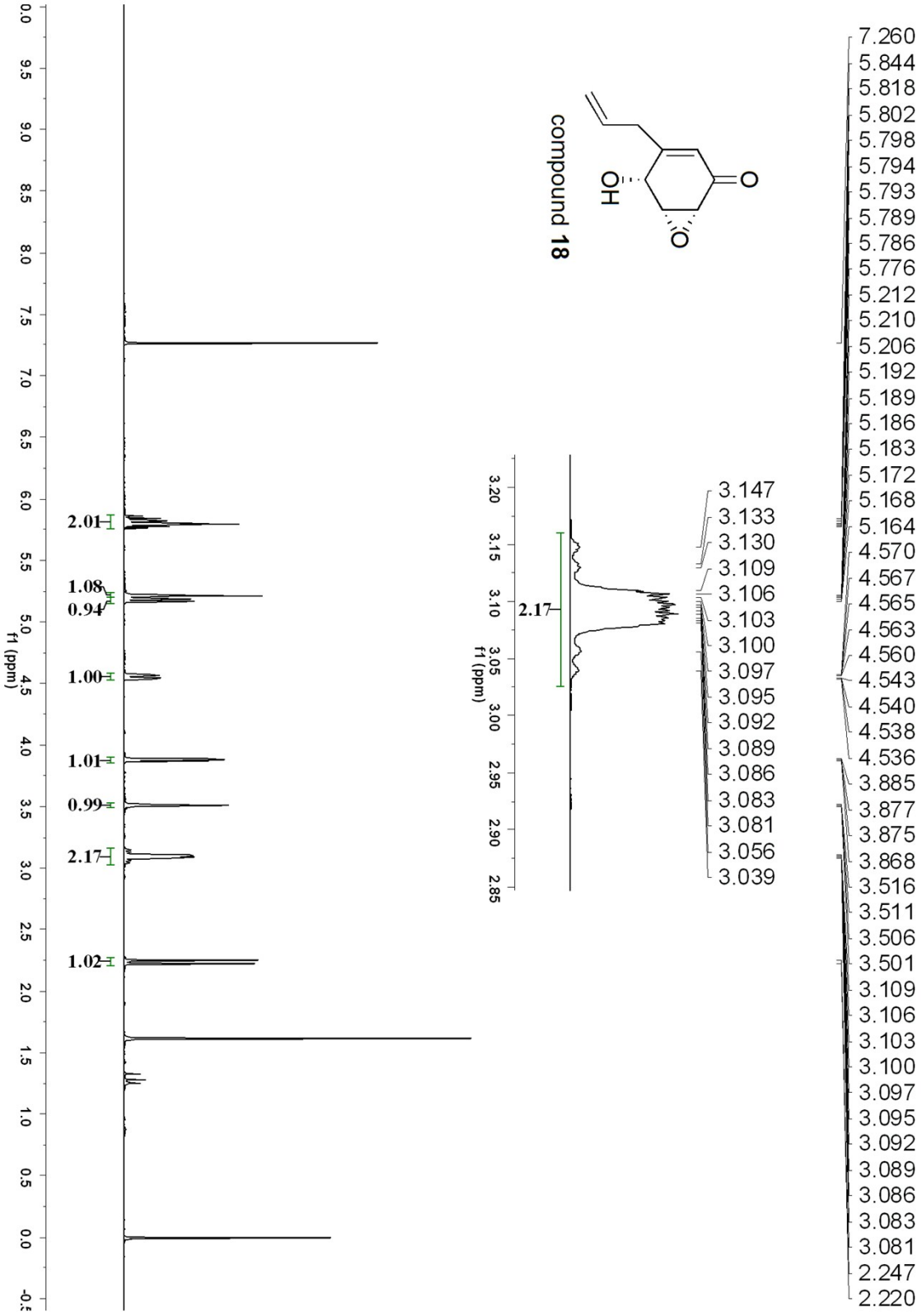


$^{1}$H NMR spectra of compound **17** in $CDCl_3$ (400 MHz)

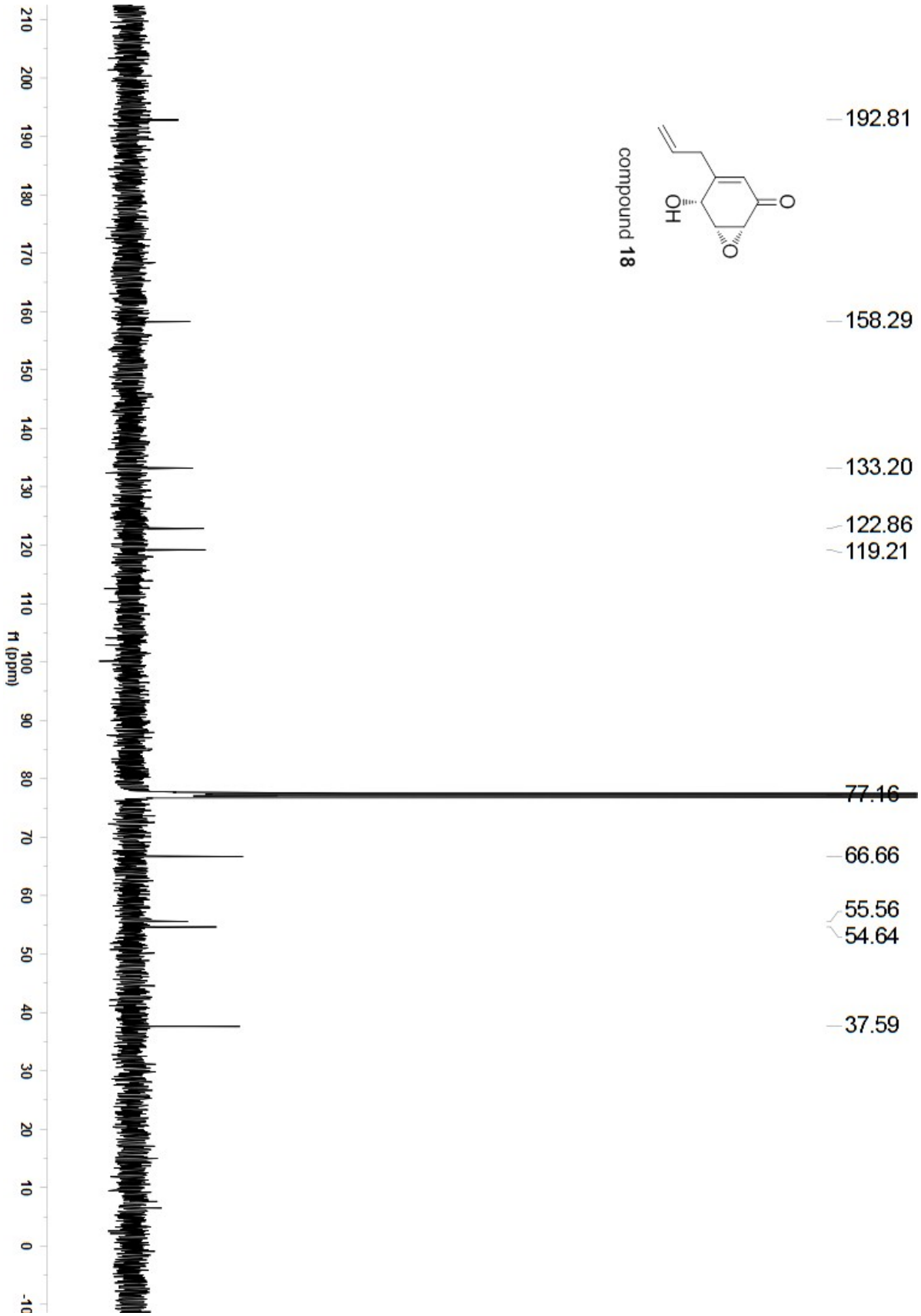



$^{13}$C NMR spectra of compound **17** in $CDCl_3$ (100 MHz)

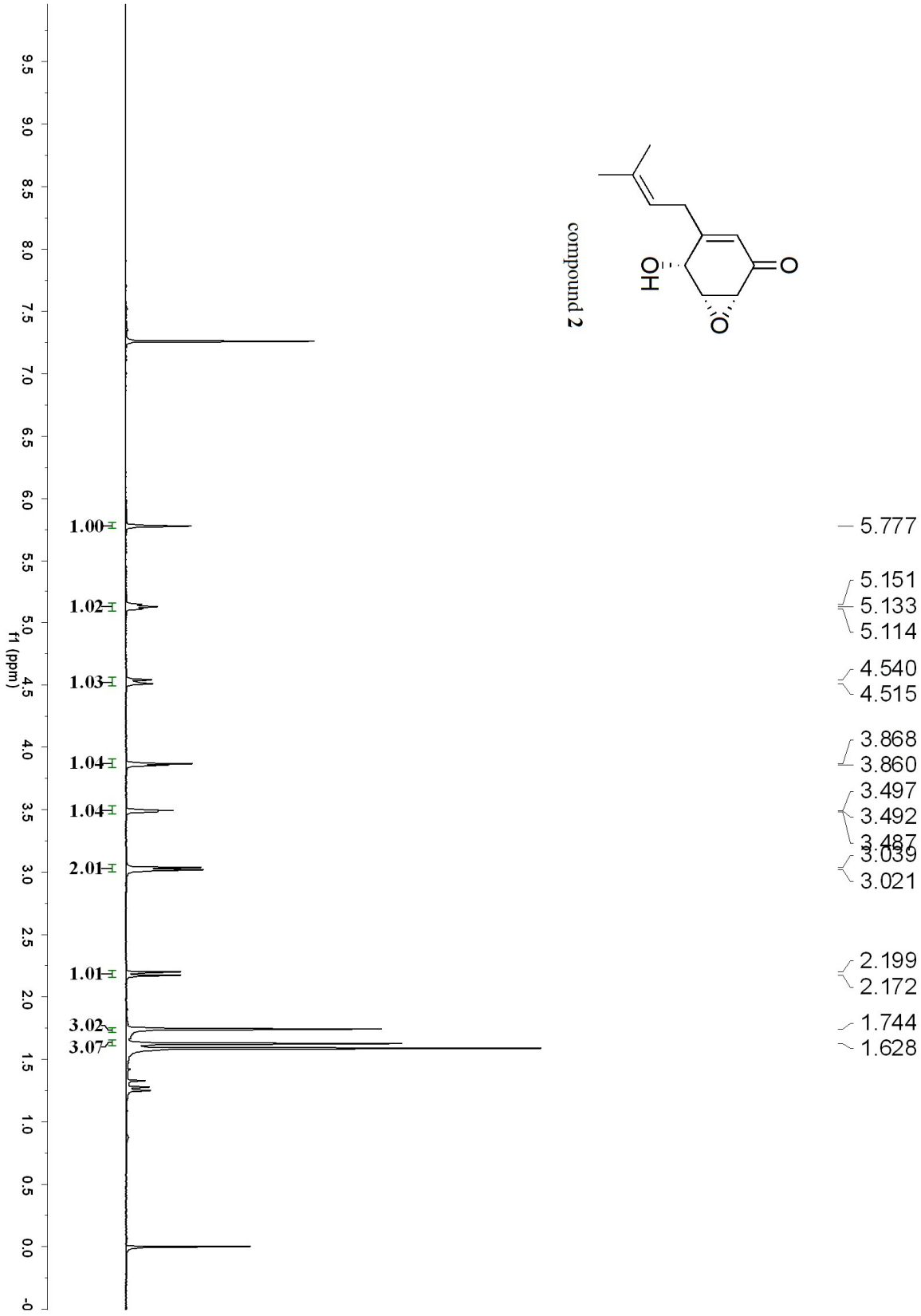
$^{1}$H NMR spectra of compound **18** in $CDCl_3$ (400 MHz)



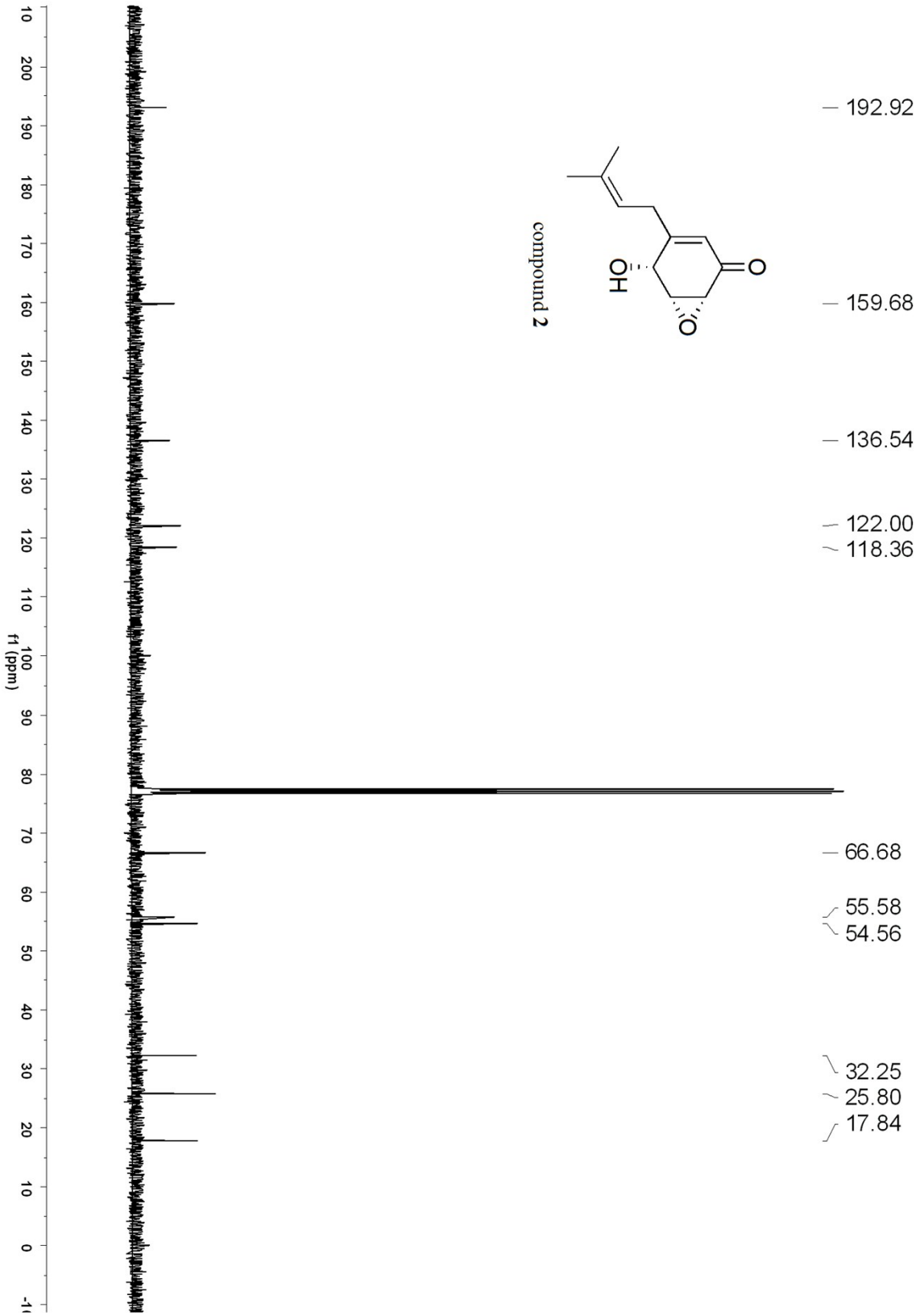
$^{13}C$ NMR spectra of compound **18** in $CDCl_3$ (100 MHz)



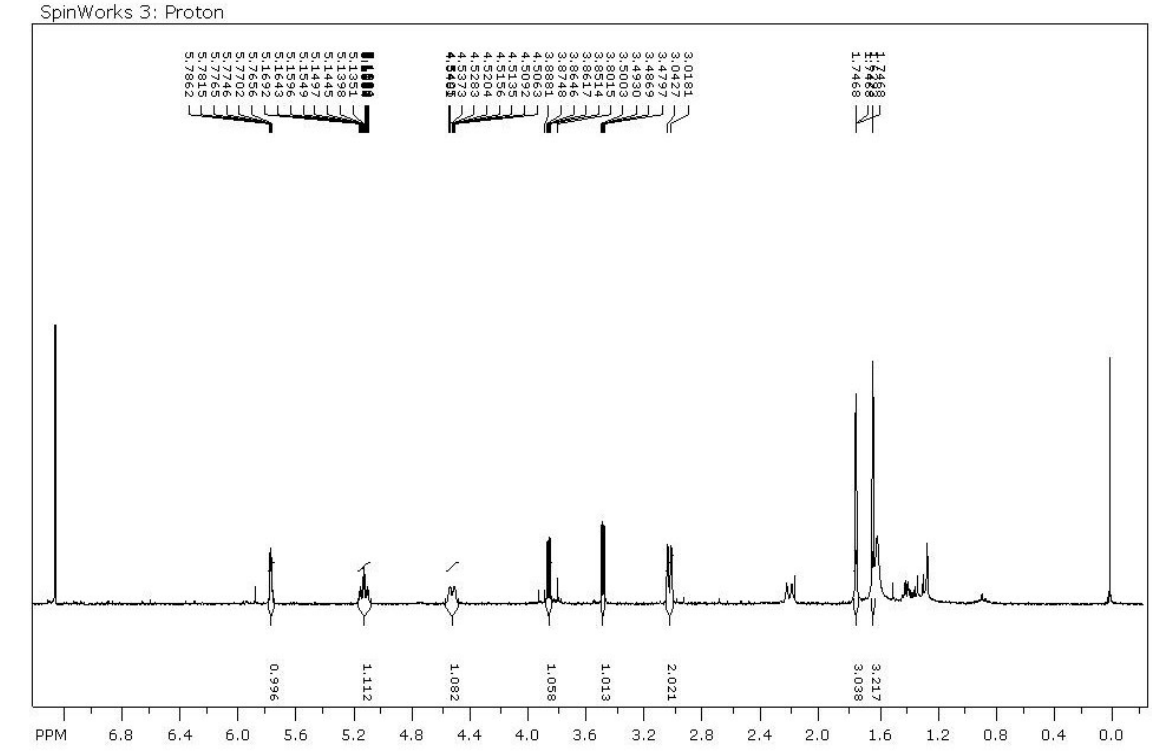
$^{1}$H NMR spectra of compound **2** in $CDCl_3$ (400 MHz)

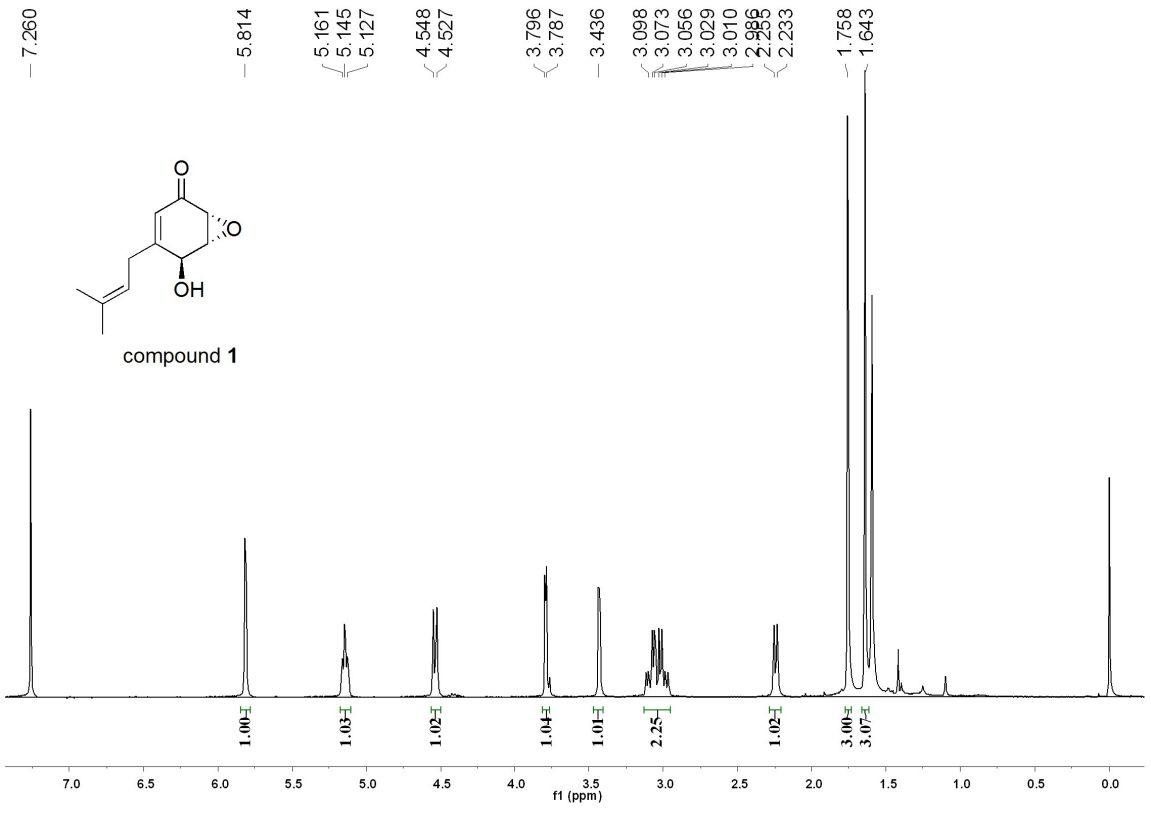


$^{13}C$ NMR spectra of compound **2** in $CDCl_3$ (100 MHz)



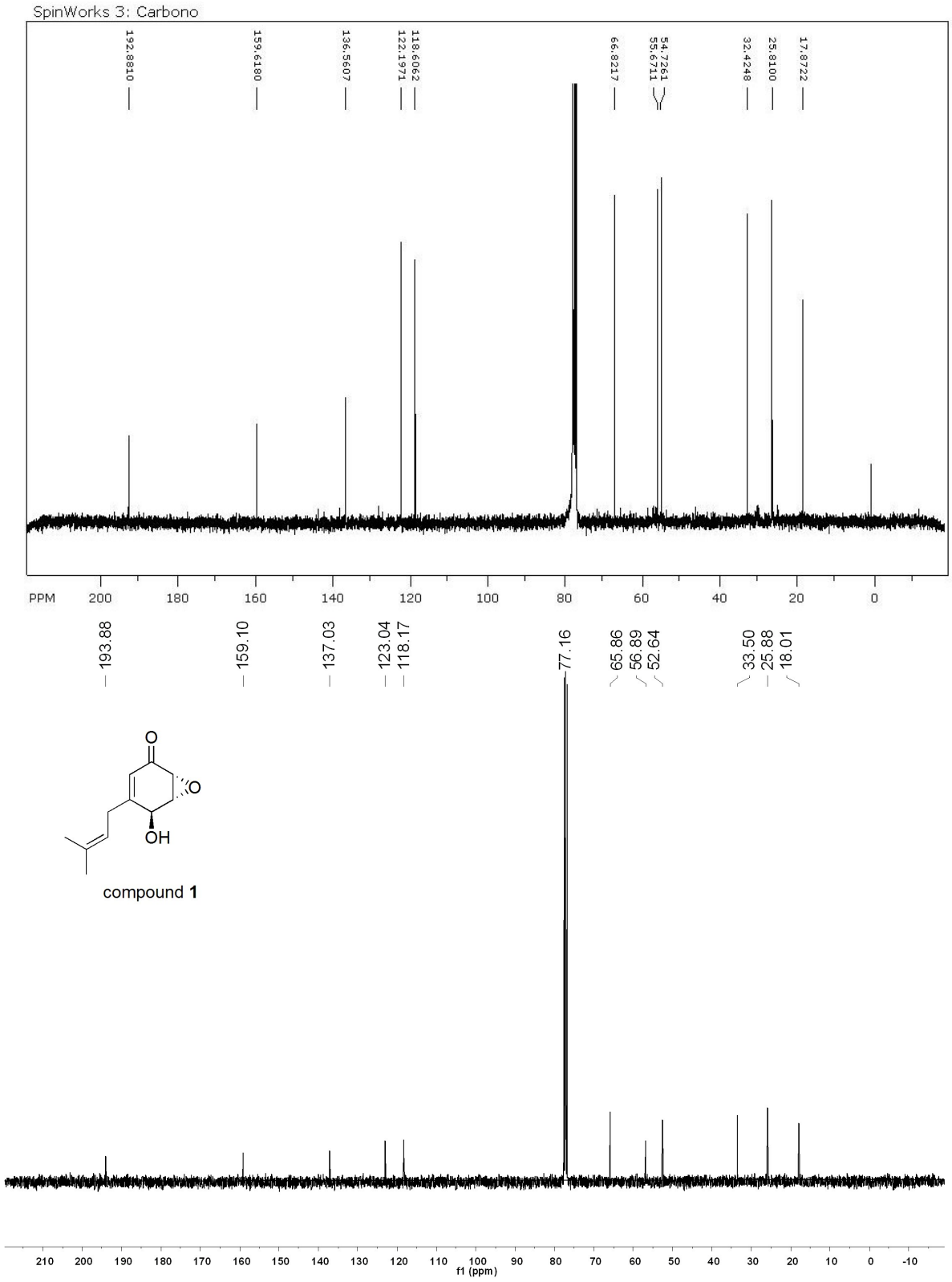
$^{1}$H NMR spectra of compound natural product in $CDCl_3$ (300 MHz) and compound **1** in $CDCl_3$ (400 MHz)



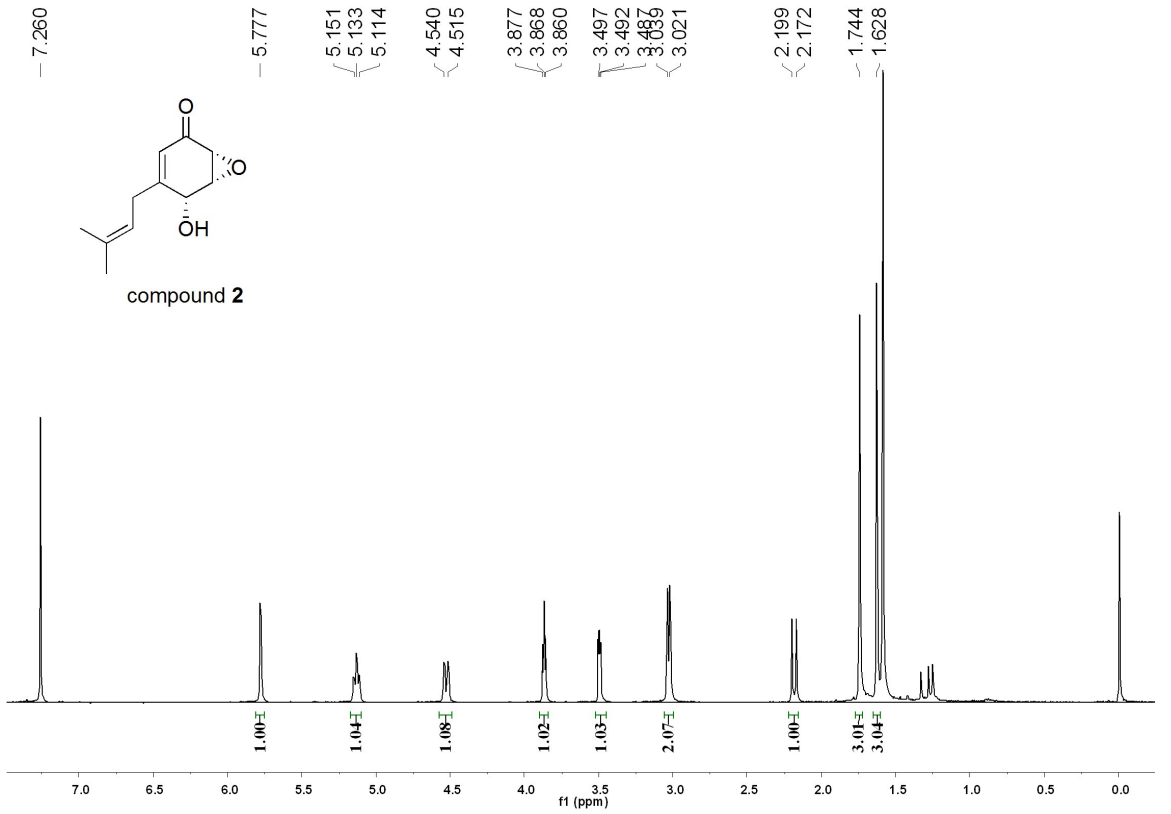




compound **1**

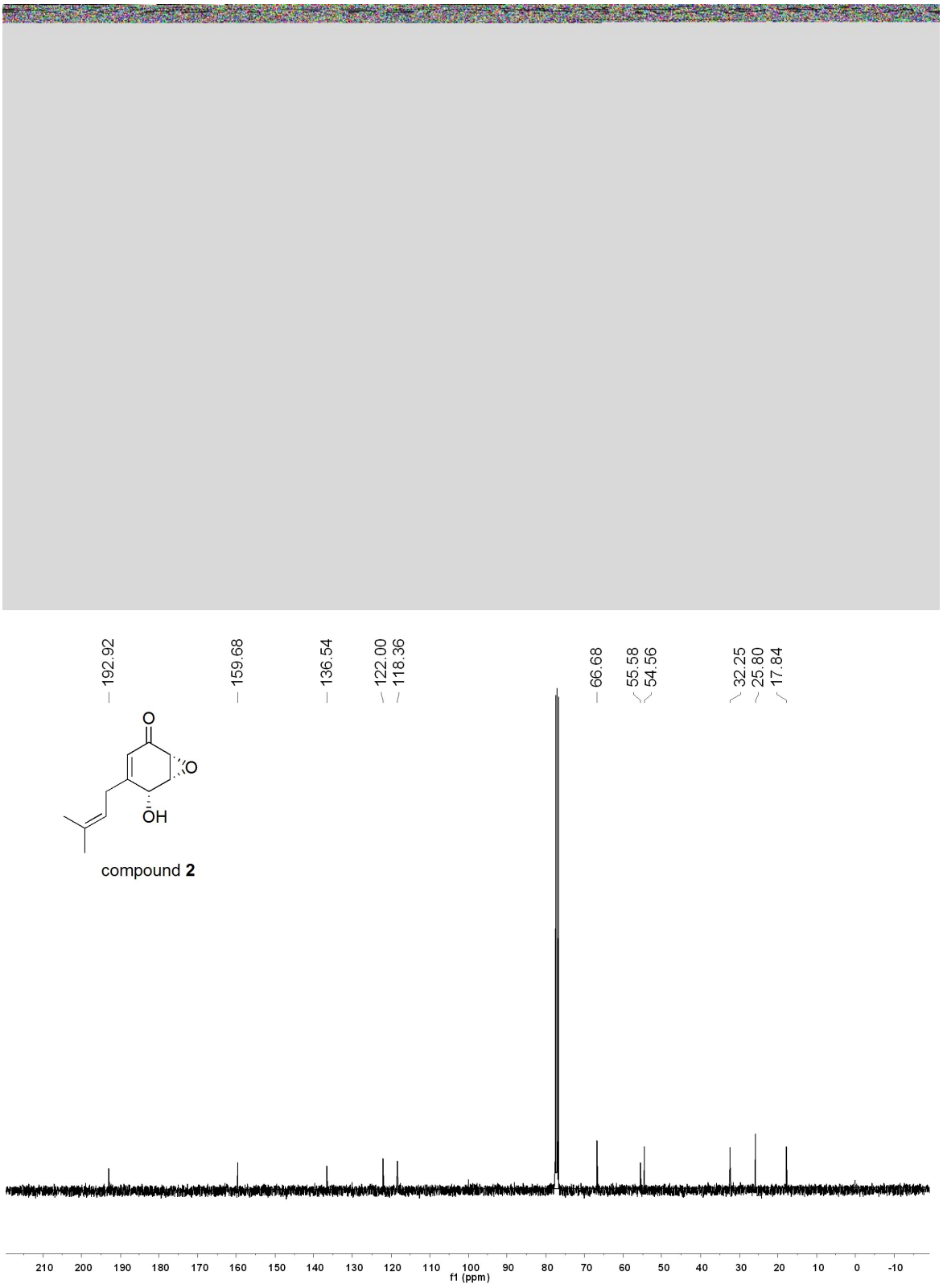
$^{13}C$ NMR spectra of compound natural product in $CDCl_3$ (75 MHz) and **1** in $CDCl_3$ (100 MHz)



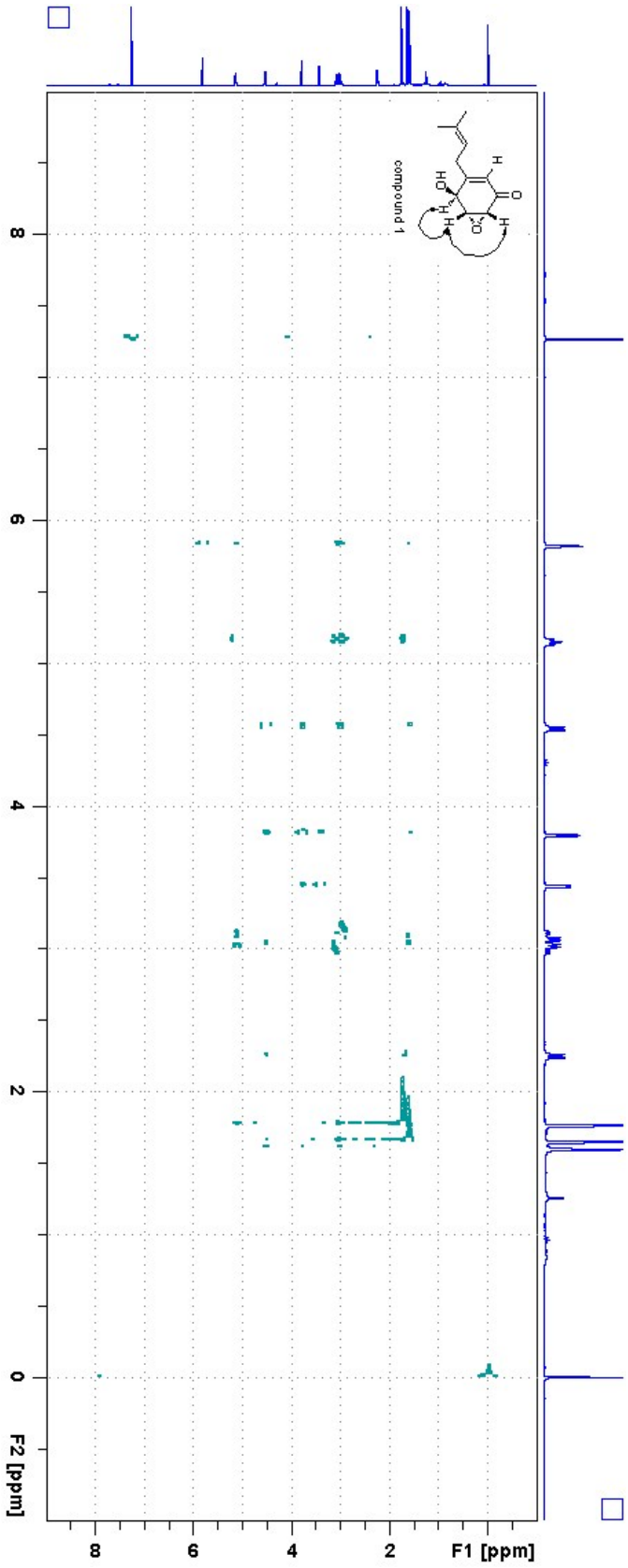
$^{1}$H NMR spectra of compound natural product in $CDCl_3$ (300 MHz) and compound **2** in $CDCl_3$ (400 MHz)

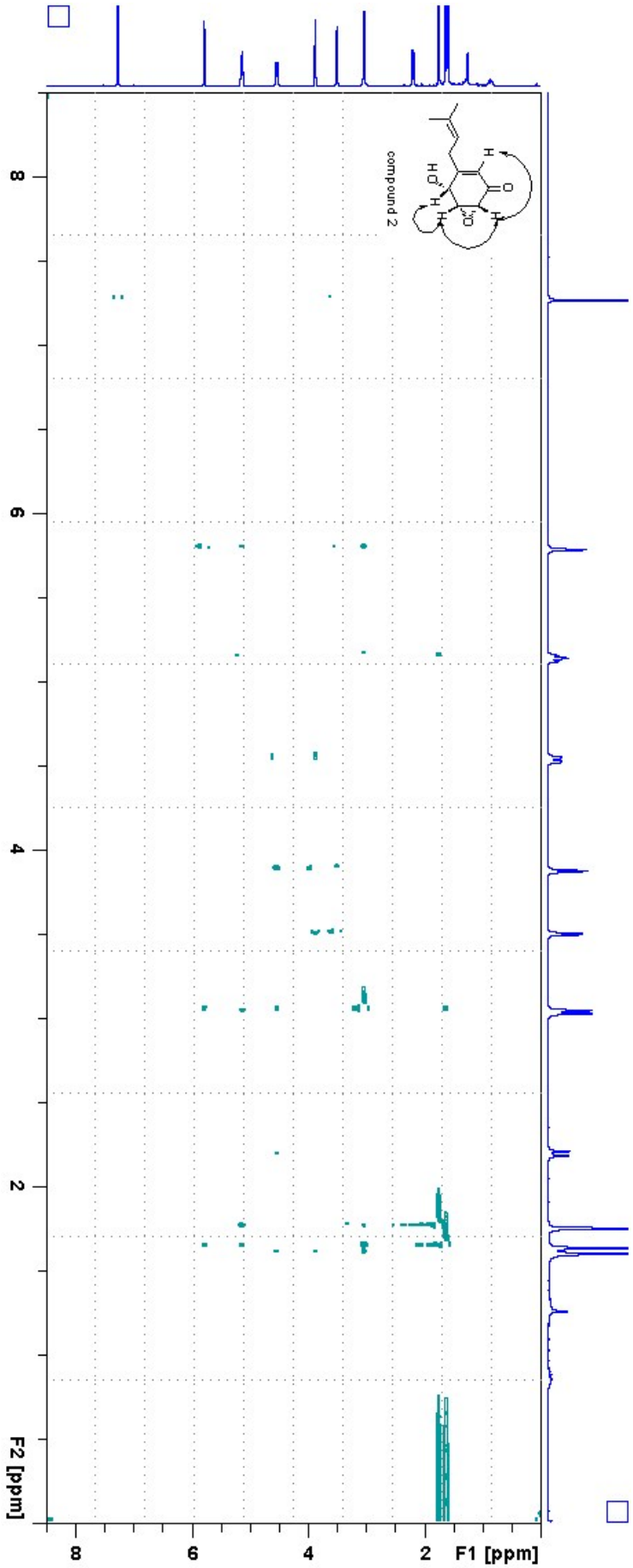


$^{13}C$ NMR spectra of compound natural product in $CDCl_3$ (75 MHz) and **2** in $CDCl_3$ (100 MHz)



$^{1}$H- $^{1}$H NOESY NMR spectra (in $CDCl_3$) of compound **1** and compound **2** (400 MHz)




compound 2
F2 [ppm]
F1 [ppm]
8
6
4
2