Supporting Materials for article:

An alternative way to analogues of avenanthramides and their antiradical activity

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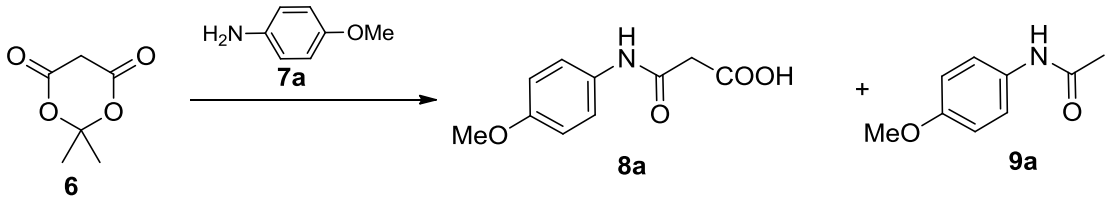
CONTENTS

OPTIMIZATION OF THE CLEAVAGE OF MELDRUM`S ACID (7) WITH P-ANISIDINE (8A)

Table S1



Entry	Solvent	Temp., °C	$E_T(30)$, kcal/mol[41]	Time	Composition of product mixture, %		Yield, %[a]
					Comp. **8a**	Comp. **9a**	
1	Water	100	63.1	1 h 20 min	91	5	67
2	Water	90	63.1	6 h 30 min	91	4	93
3	Water	82	63.1	3 h 10 min	90	0	55
4	Water	77	63.1	4 h 15 min	93	0	61
5	Methanol	65	55.4	7 h 40 min	85	9	79
6	Ethanol	78	51.9	2 h 50 min	85	10	47
7	*n*-Butanol	118	49.7	45 min	40	53	-
8	Acetonitrile	82	45.6	1 h 55 min	59	40	-
9	Chloroform	61	39.1	8 h	88	10	58
10	Ethyl propanoate	99	38.1[b]	1 h	25	66	-
11	Ethyl acetate	77	38.1	1 h 40 min	96	2	75
12	1,4-Dioxane	101	36.0	3 h 15 min	0	100	92
13	Isooctane	99	31.1[c]	4 h 10 min	0	100	88
14	Toluene	75	33.9	8 h 40 min	96	1	87
15	Toluene	65	33.9	9 h 30 min	97	0	75

[a]The isolated yield of the main compound **6a** or **9a** (the content of the main compound was more than 80% of the product mixture).
[b]$E_T(30)$ value of ethyl acetate.
[c]$E_T(30)$ value of *n*-octane.

CORRELATIONS BETWEEN INHIBITION OF FREE RADICAL DPPH OR GO AND HAMMETT SUBSTITUENT CONSTANTS FOR ANILIDES OF FERULIC AND SINAPIC ACID

The position of substituents in the aniline moiety was detected with respect to the cinnamoylamino group - *ortho*-, *meta*- or *para*-, respectively. Hammett substituent constants for *meta*- and *para*- substituents were obtained from data summarized by Hansch *et al.*;[1] equation $\sigma_o=0.66\cdot\sigma_p$ was used to calculate predictable Hammett substituent constants for *ortho*-substituents.[2] Antiradical activity data for the compounds containing COOH group in the aniline moiety were obtained by our group previously.[3] The correlations were established for anilides **1** of ferulic and sinapic acids (Fig. S1-S4).

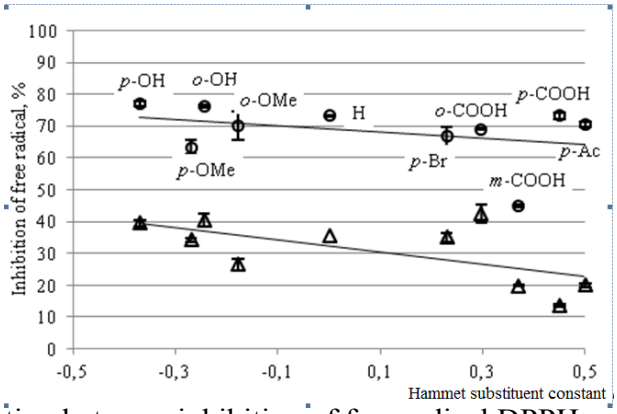


Fig. S1. Correlation between inhibition of free radical DPPH or GO and Hammett substituent constants for anilides of ferulic acid. Abbreviations in this and following figures 3-5: ○ – inhibition of DPPH; Δ - inhibition of GO. Data are presented as mean ± standard deviation.

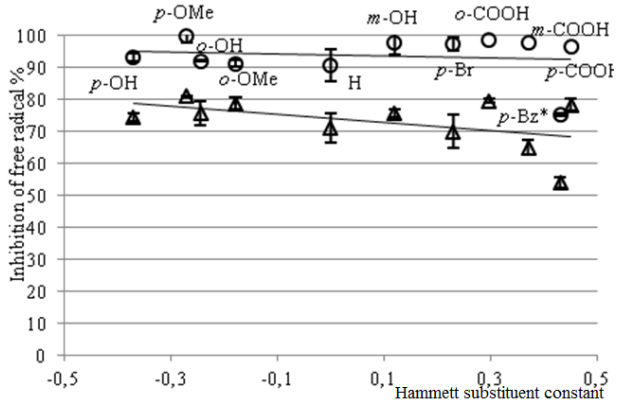
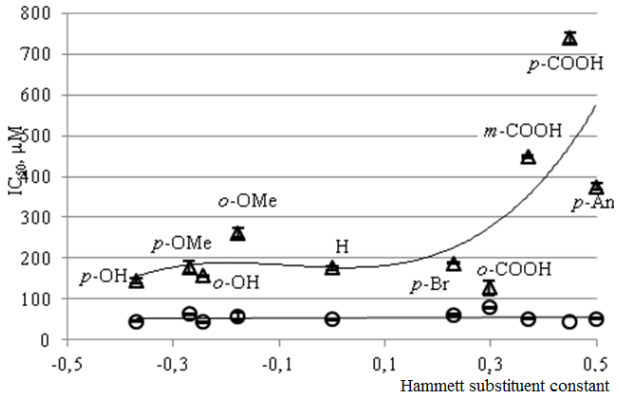
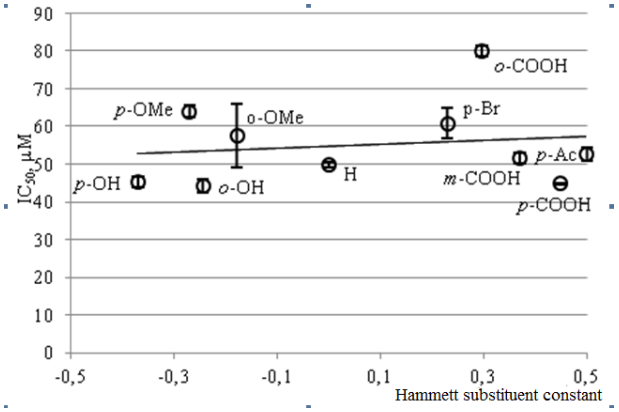


Fig. S2. Correlation between inhibition of free radical DPPH or GO and Hammett substituent constants for anilides of sinapic acid. * Hammett substituent constants for 3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2(*E*)-enoyl was not available, data for benzoyl substituent was used to predict the electronic factor of the group.

[1] Hansch, C.; Leo, A.; Taft, R. W. *Chem. Rev*. **1991**, *91*, 165.
[2] Ali, H. M.; Abo-Shady, A.; Sharaf Eldeen, H. A.; Soror, H. A.; Shousha, W. G.; Abdel-Barry, O. A.; Saleh, A. M. *Chem. Cent. J.* **2013**, *7*, doi:10.1186/1752-153X-7-53.
[3] Mierina, I.; Zaharova, M.; Jure, M.; Neibolte, I. *J. Chem. Pharm. Res.* **2015**, *7*(6), 416.



a)



b)

Fig. S3. Correlation between IC_{50} values and Hammett substituent constants for ferulic acid derivatives. Fig. 8a) demonstrates inhibition concentration both for GO and DPPH. Fig. 8b) is expanded view for DPPH data.

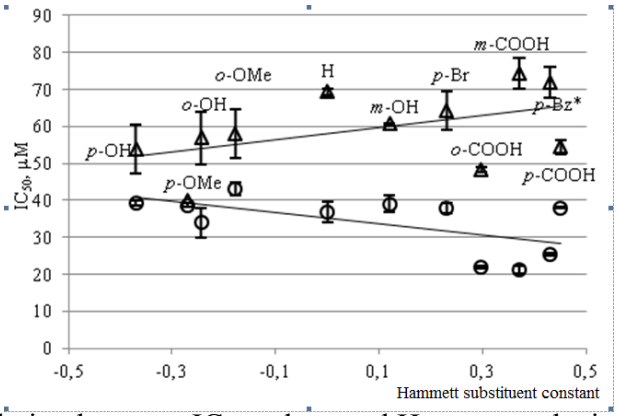
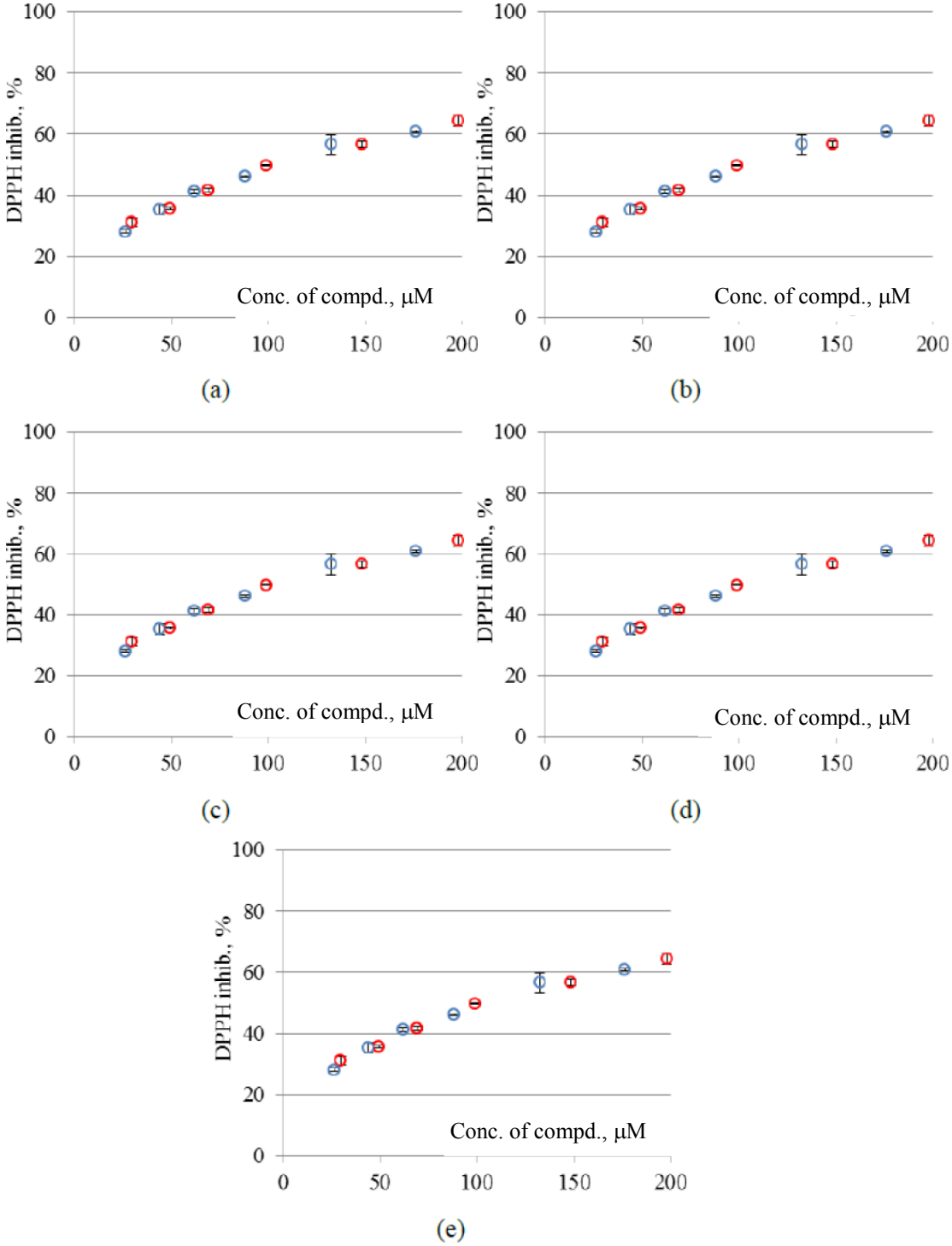


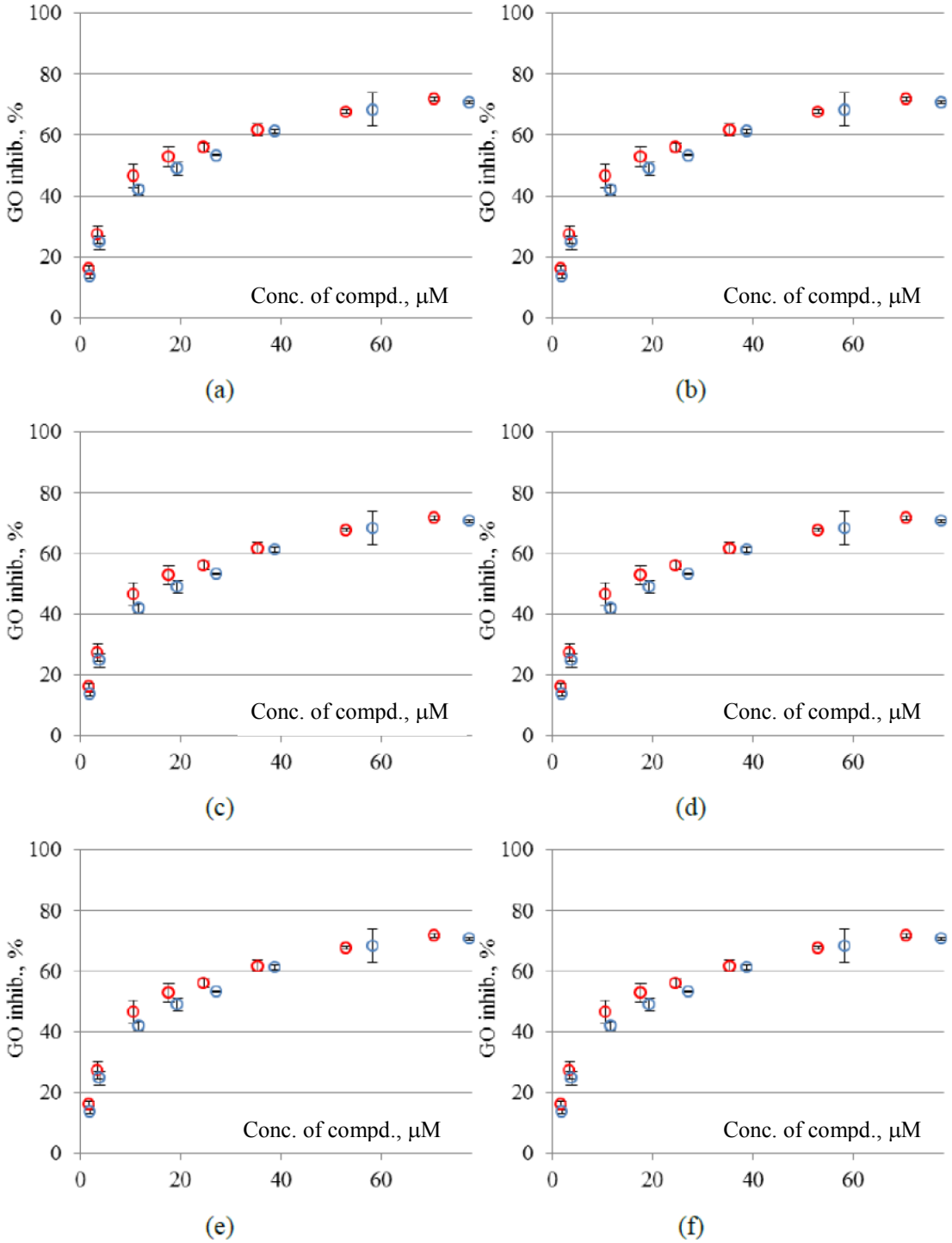
Fig. S4. Correlation between IC_{50} values and Hammett substituent constants for sinapic acid derivatives.

INHIBITION OF DPPH DEPENDING ON THE CONCENTRATION OF ARYLIDENE MALONIC ACID MONOANILIDES



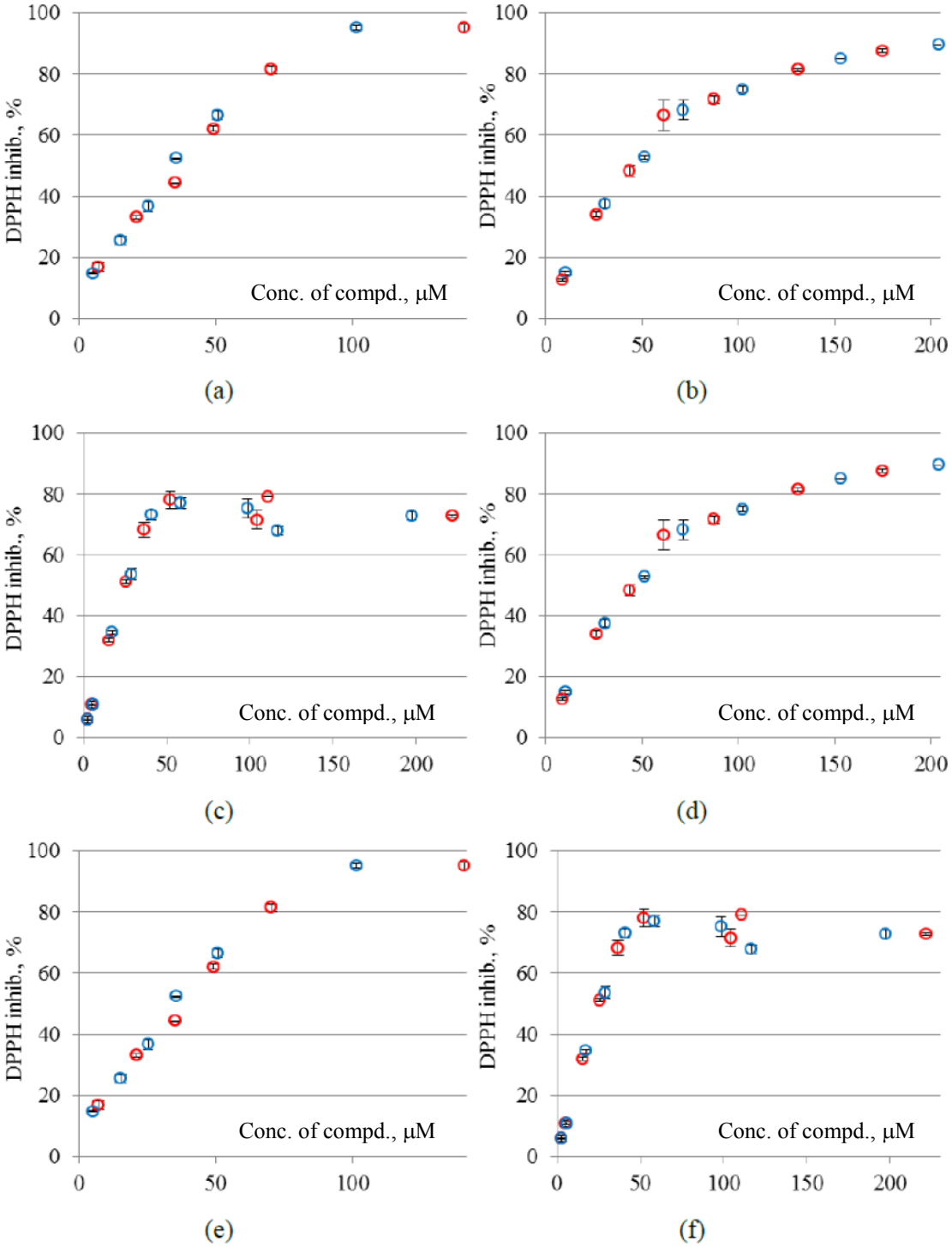
Inhibition of DPPH depending on the concentration of arylidene malonic acid monoanilide **11bA** (a), **11cA** (b), **11cH** (c), **11eH** (d), **11dA** (e).

INHIBITION OF GO DEPENDING ON THE CONCENTRATION OF ARYLIDENE MALONIC ACID MONOANILIDES

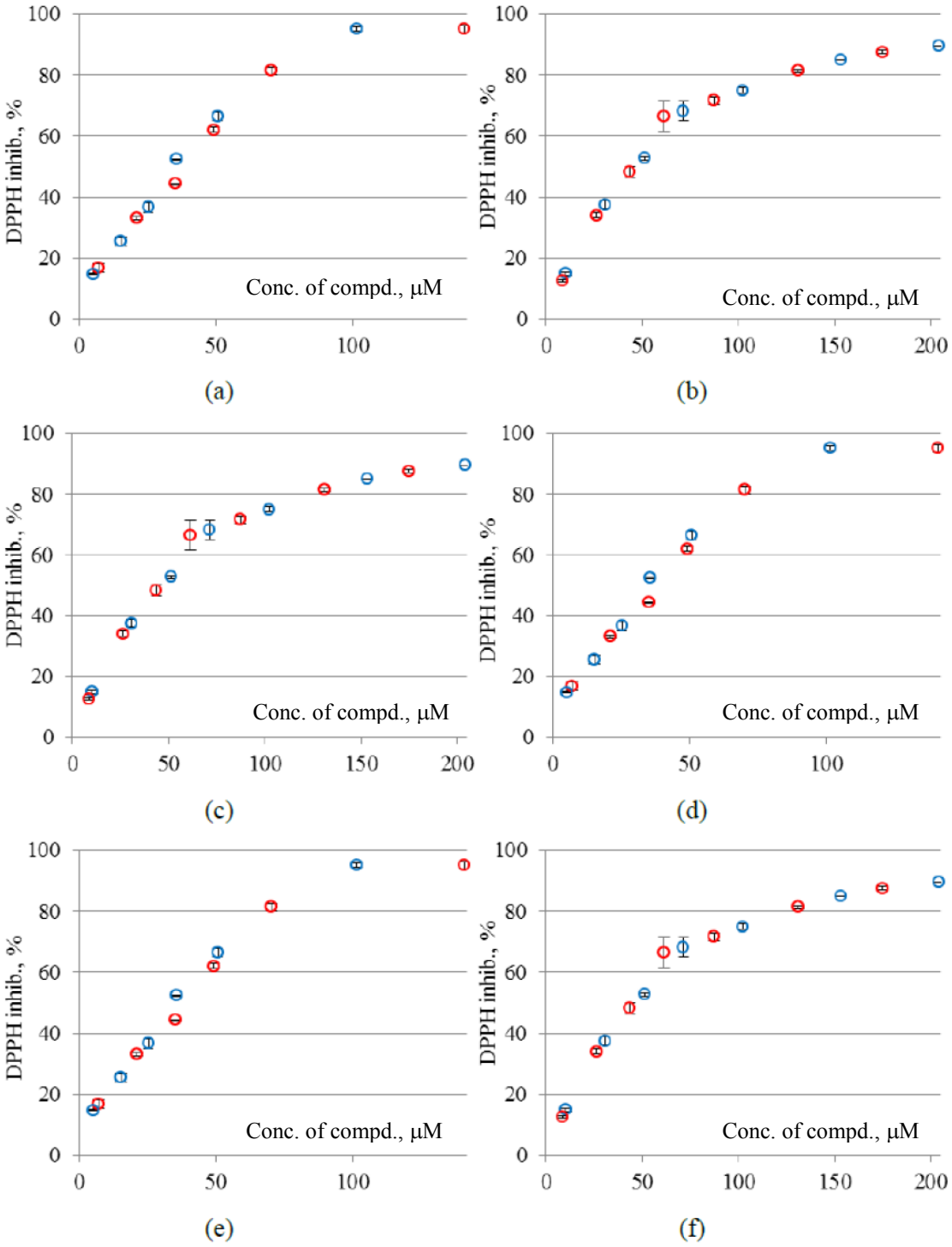


Inhibition of GO depending on the concentration of arylidene malonic acid monoanilide **11bA** (a), **11aA** (b), **11cA** (c), **11cH** (d), **11eH** (e), **11dA** (f).

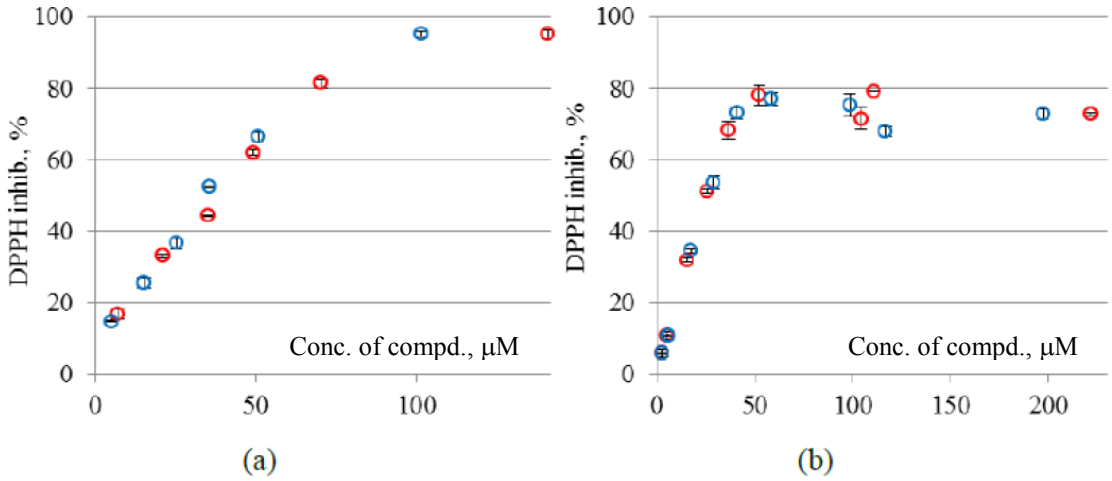
INHIBITION OF DPPH DEPENDING ON THE CONCENTRATION OF CINNAMOYL ANILINES



Inhibition of DPPH depending on the concentration of cinnamoyl aniline **12hA** (a), **12gA** (b), **12gH** (c), **12fA** (d), **12fH** (e), **12bA** (f).

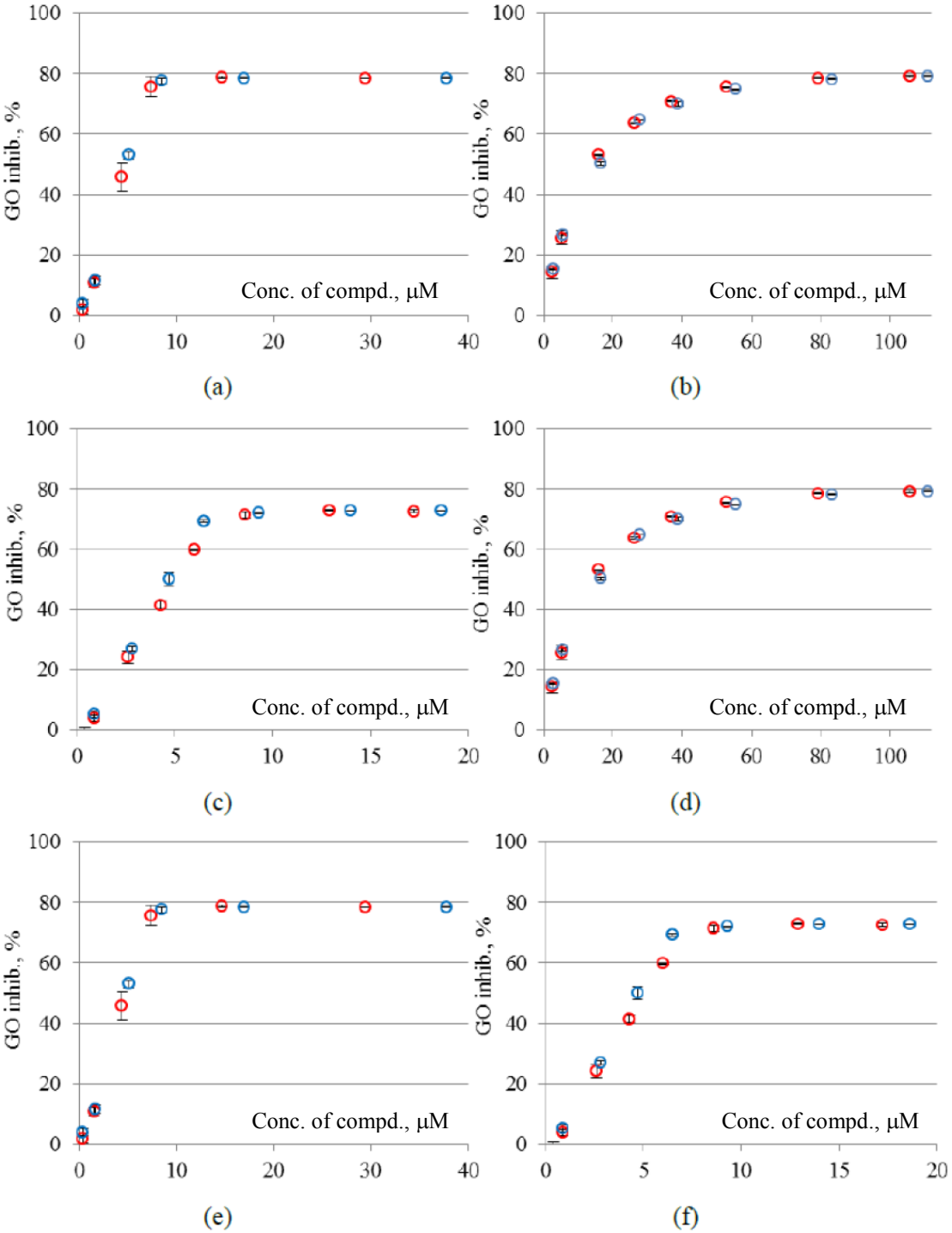


Inhibition of DPPH depending on the concentration of cinnamoyl aniline **12bH** (a), **12aH** (b), **12cA** (c), **12cH** (d), **12eH** (e), **12dA** (f).

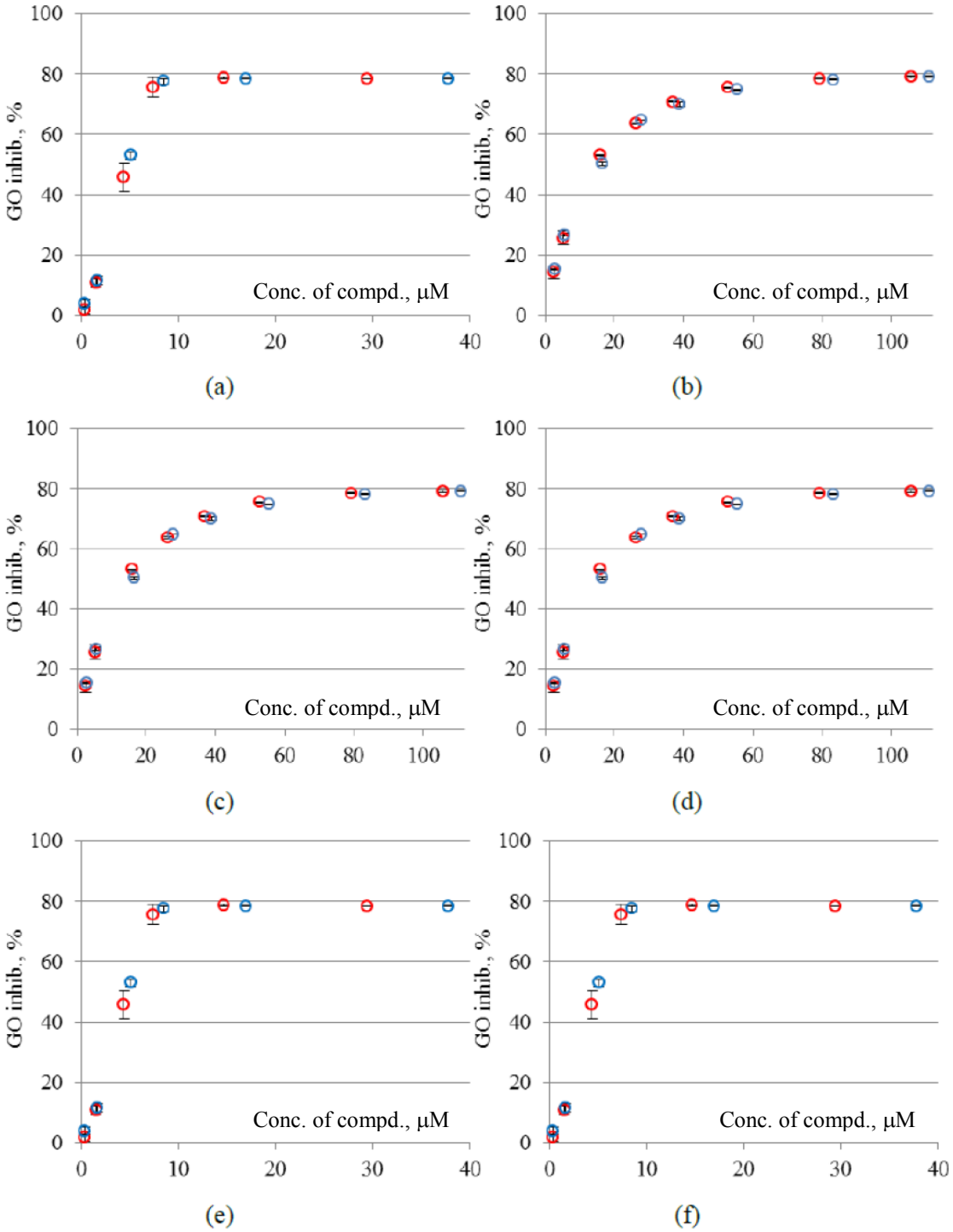


Inhibition of DPPH depending on the concentration of cinnamoyl aniline **12dH** (a) un **12hH`** (b).

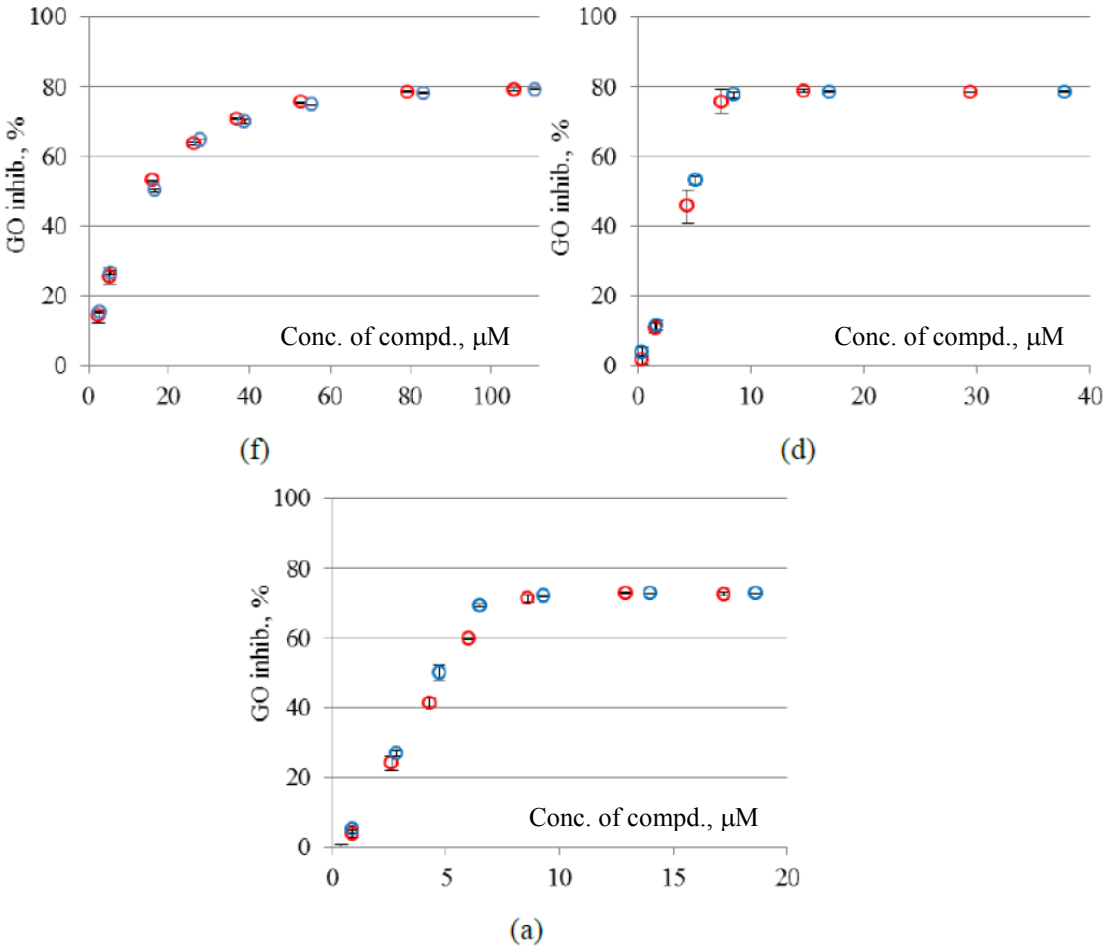
INHIBITION OF GO DEPENDING ON THE CONCENTRATION OF CINNAMOYL ANILINES



Inhibition of GO depending on the concentration of cinnamoyl aniline **12hA** (a), **12gA** (b), **12gH** (c), **12fA** (d), **12fH** (e), **12bA** (f).



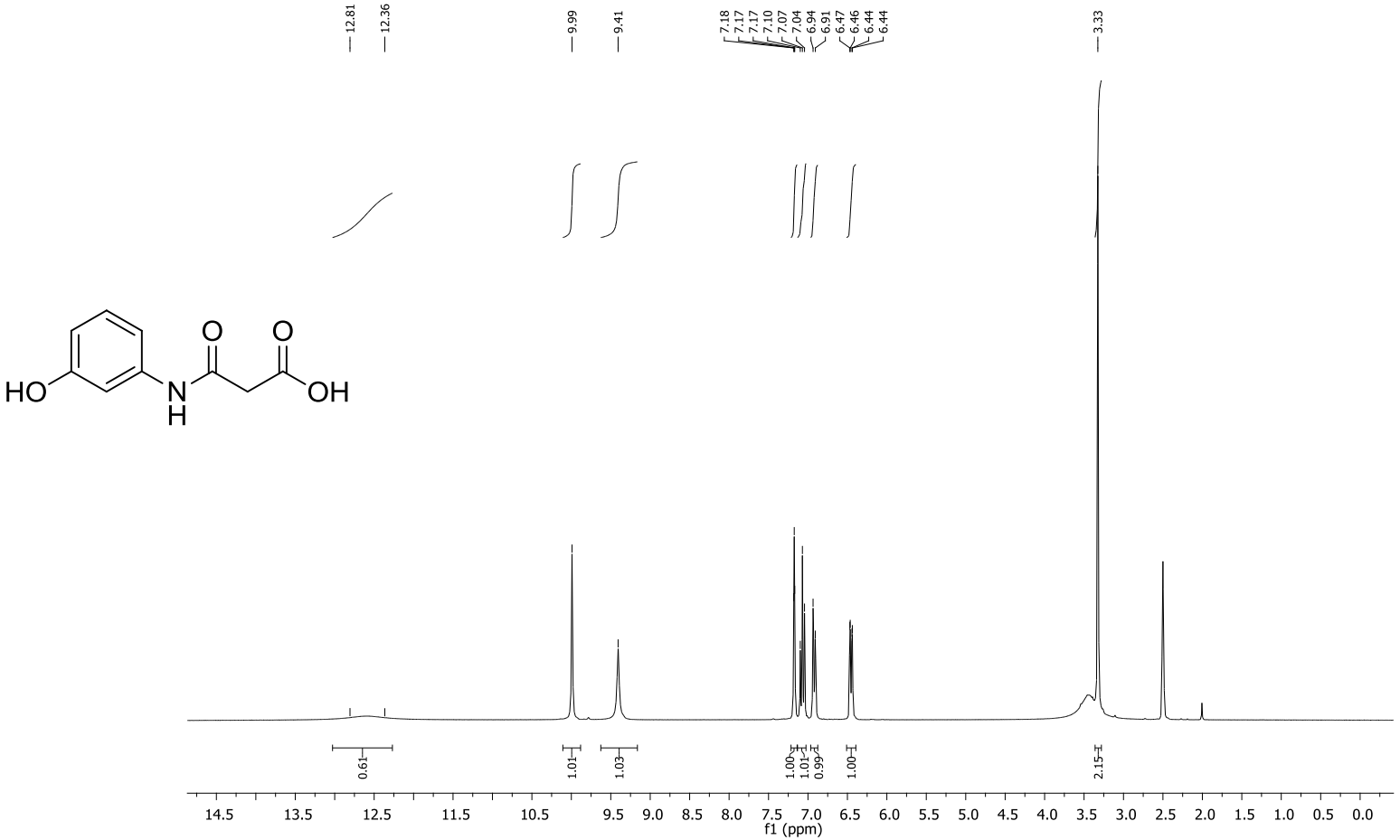
Inhibition of GO depending on the concentration of cinnamoyl aniline **12bH** (a), **12aA** (b), **12bH12cA** (c), **12cA** (d), **12cH** (e), **12eH** (f).



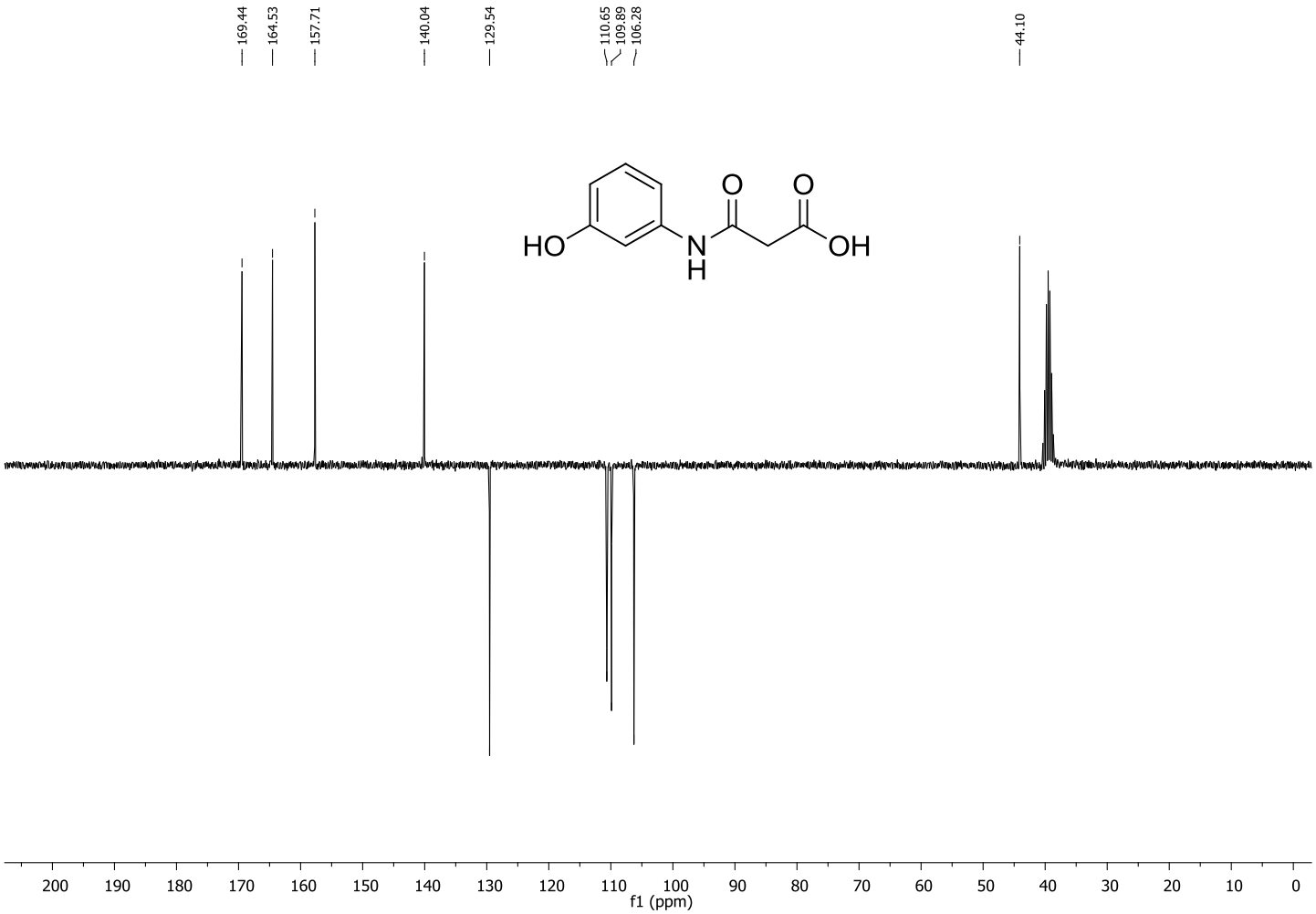
Inhibition of GO depending on the concentration of cinnamoyl aniline **12dA** (a), **12dH** (b), **12hH`** (c).

NMR SPECTRA OF MALONIC ACID MONOANILIDES 8

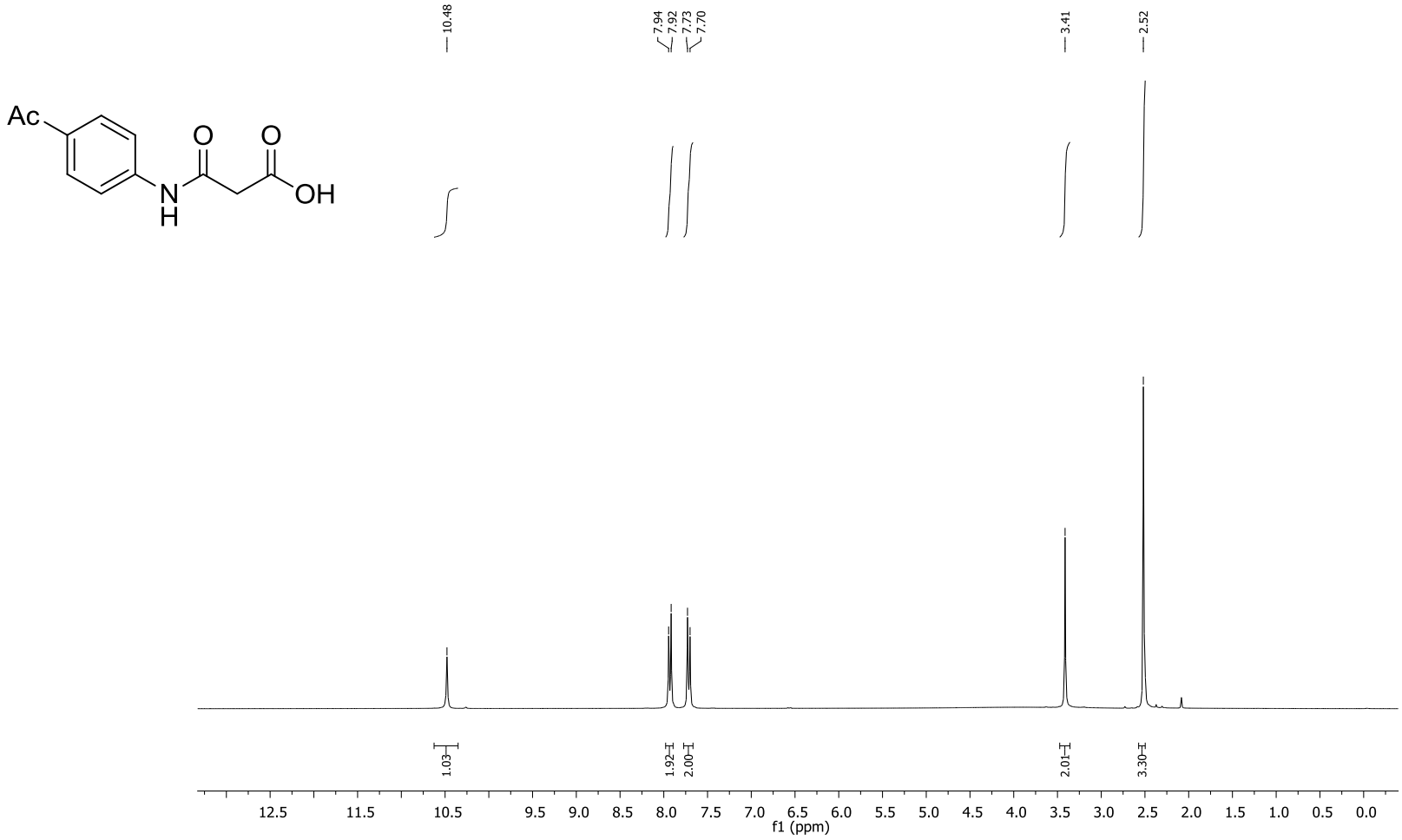
^{1}H NMR spectra of compound 8e:



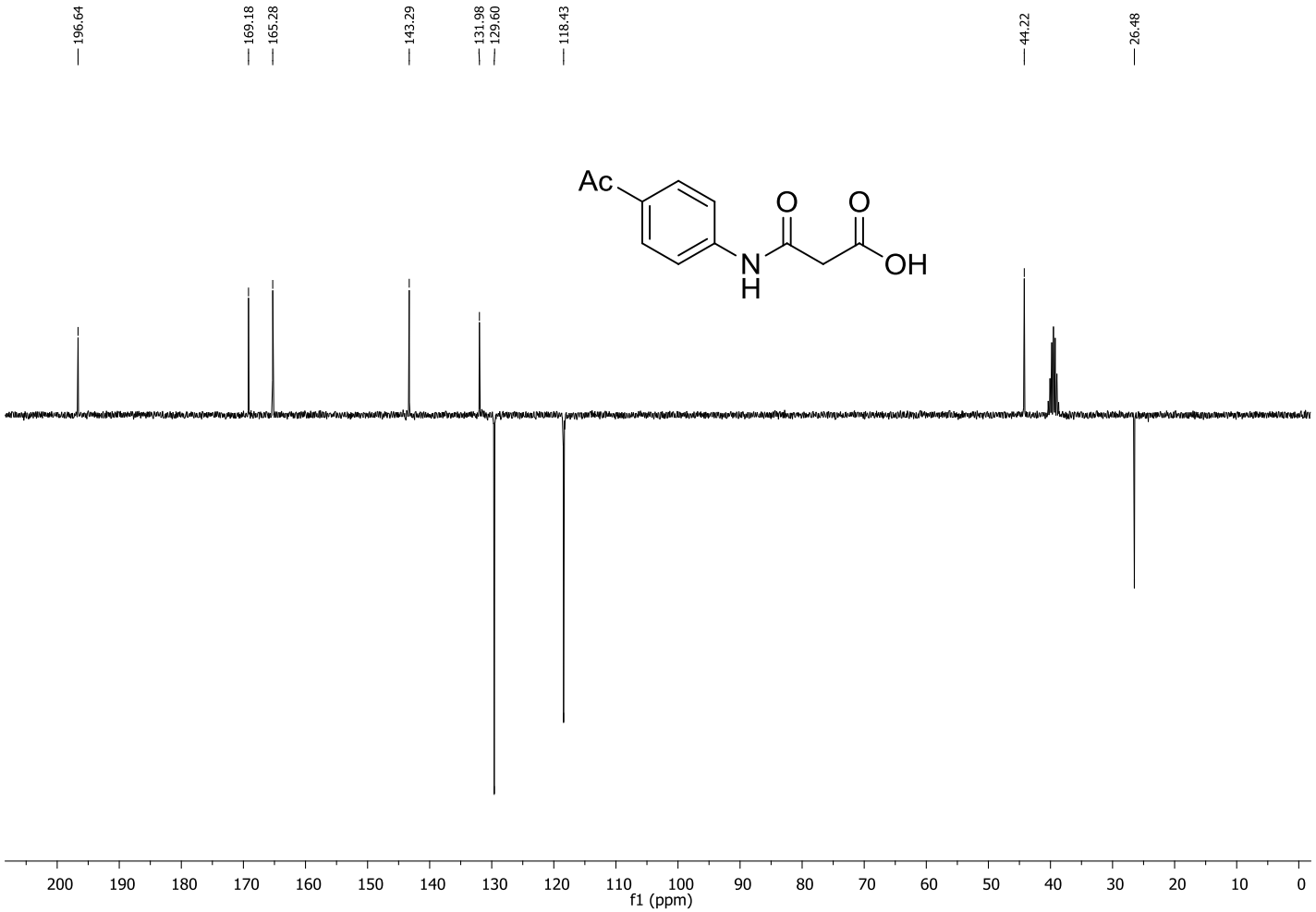
^{13}C NMR spectra of compound 8e:



^{1}H NMR spectra of compound 8h:

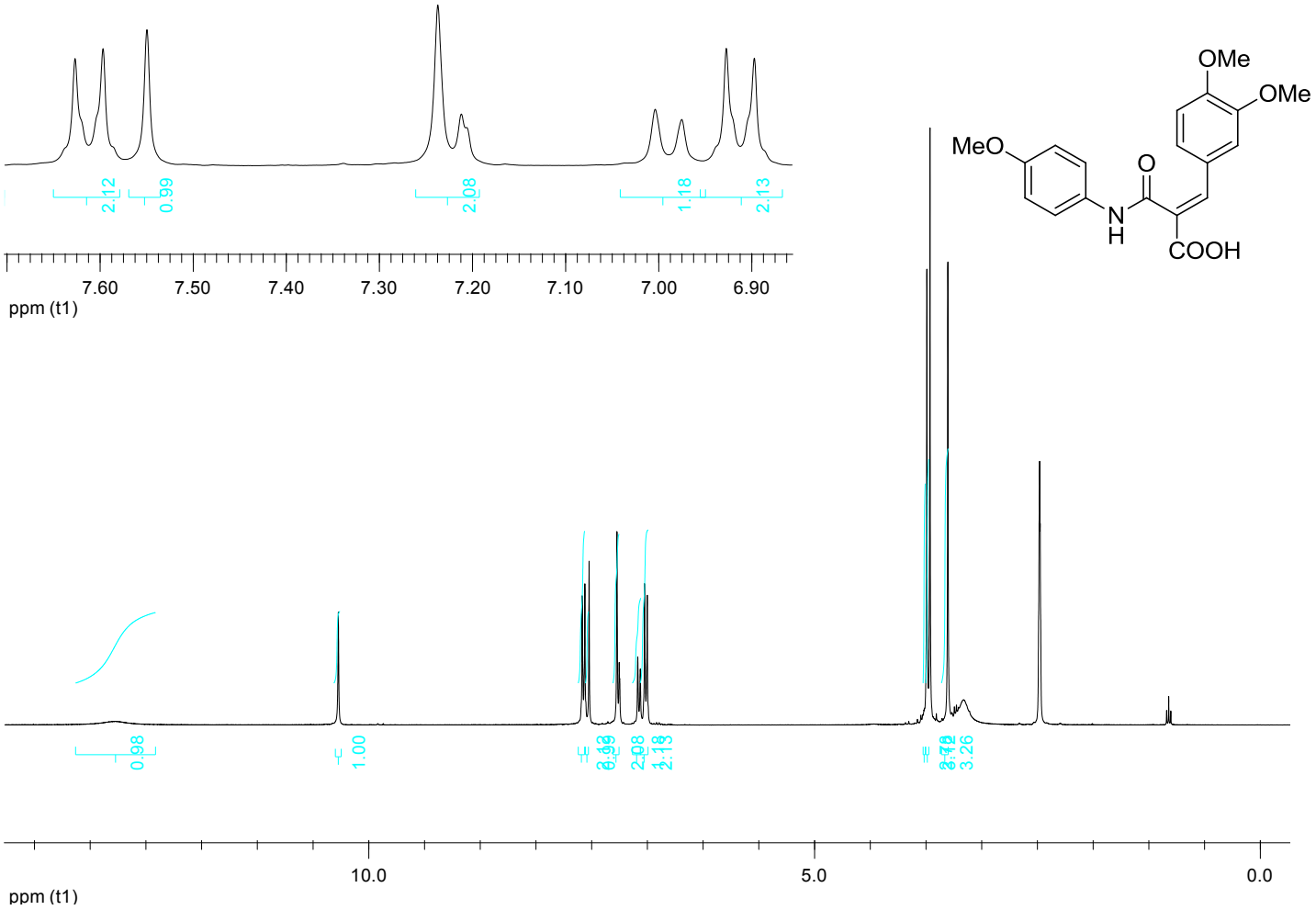


^{13}C NMR spectra of compound 8h:

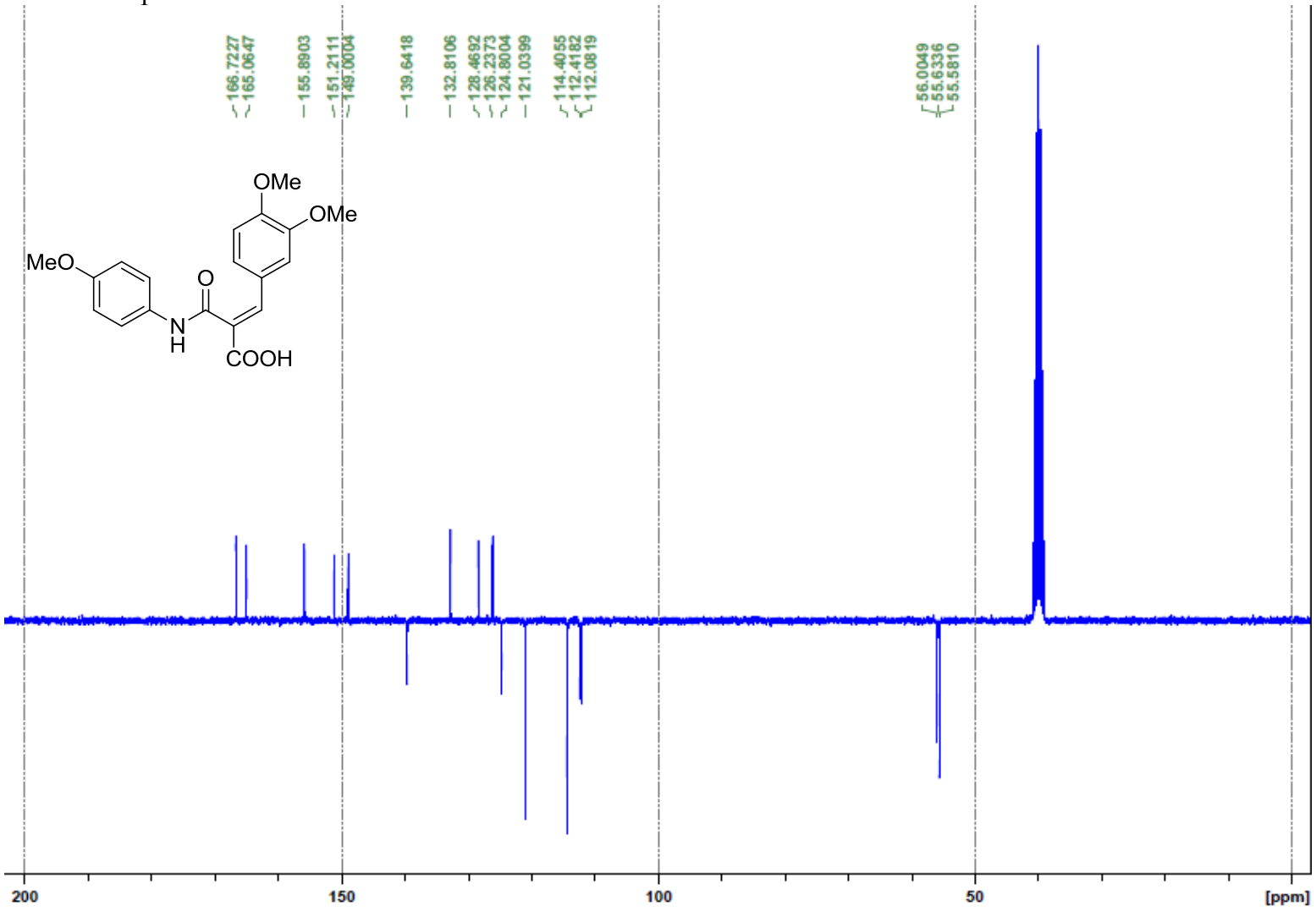


NMR SPECTRA OF ARYLIDENE MALONIC ACID MONOANILIDES 11

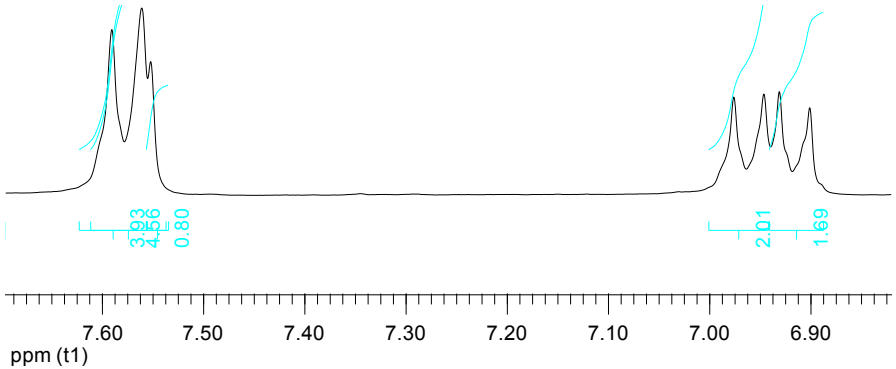
^{1}H NMR spectra of compound 11aB:

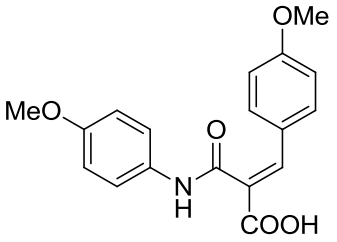


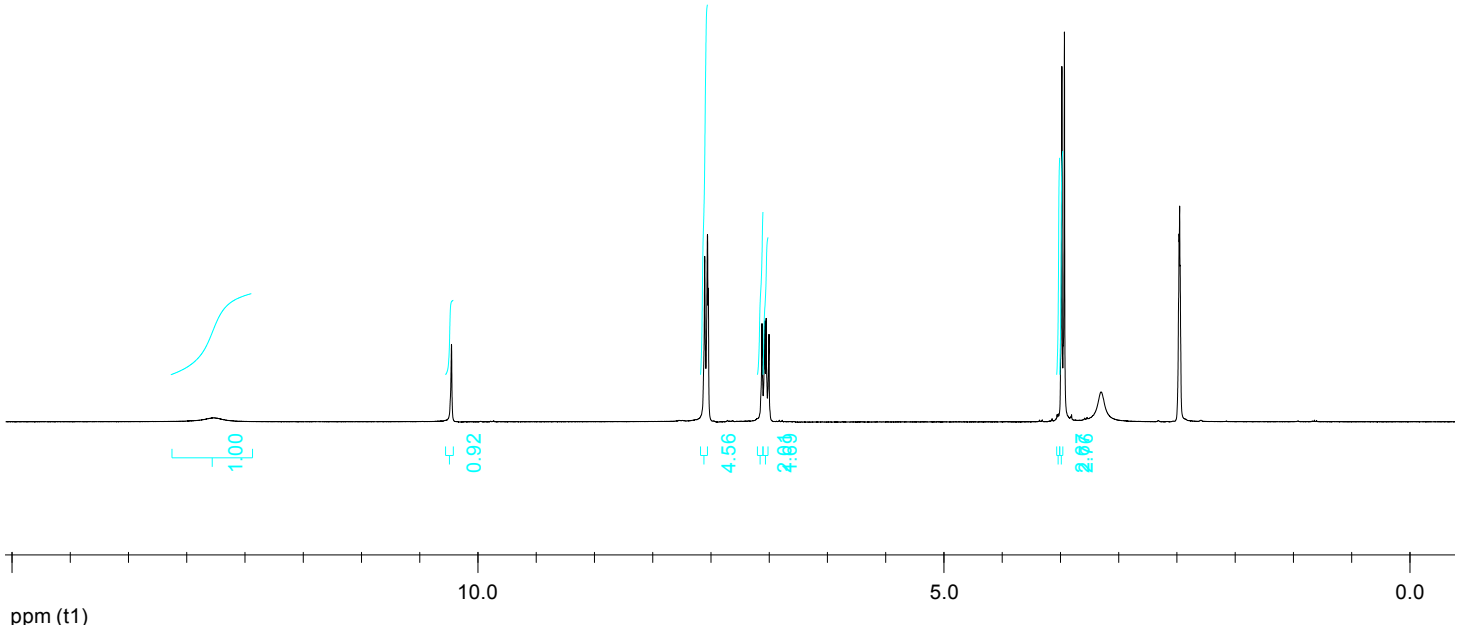
^{13}C NMR spectra of compound **11aB**:



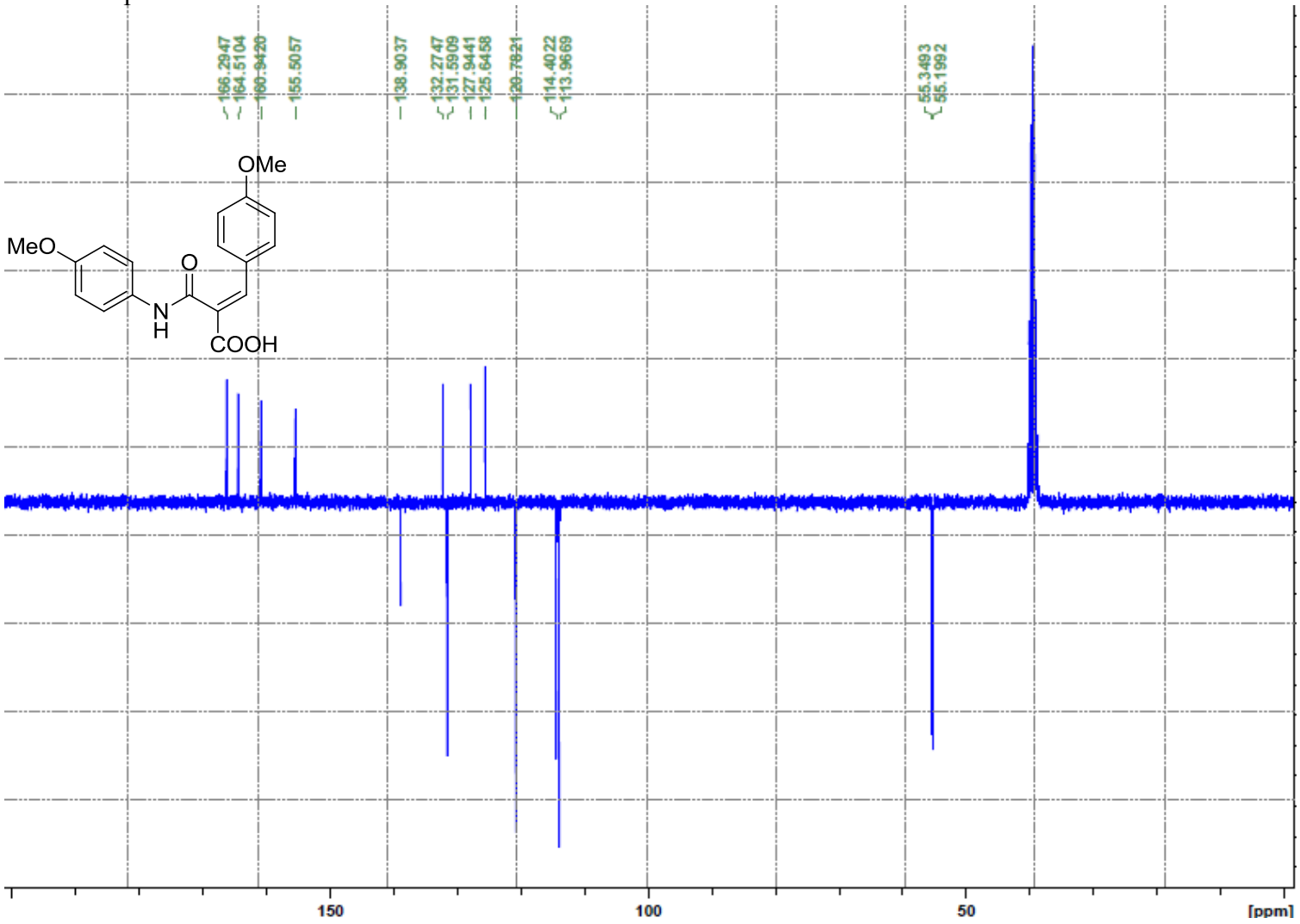
^{1}H NMR spectra of compound 11aC:



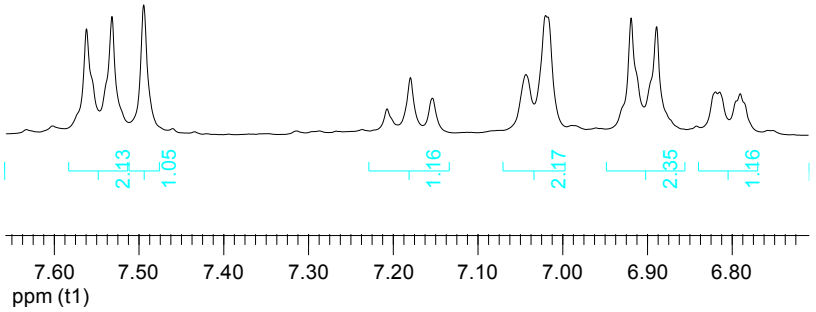


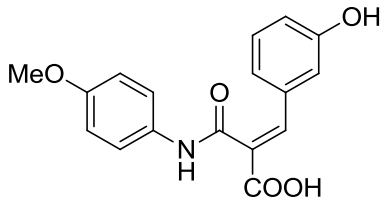


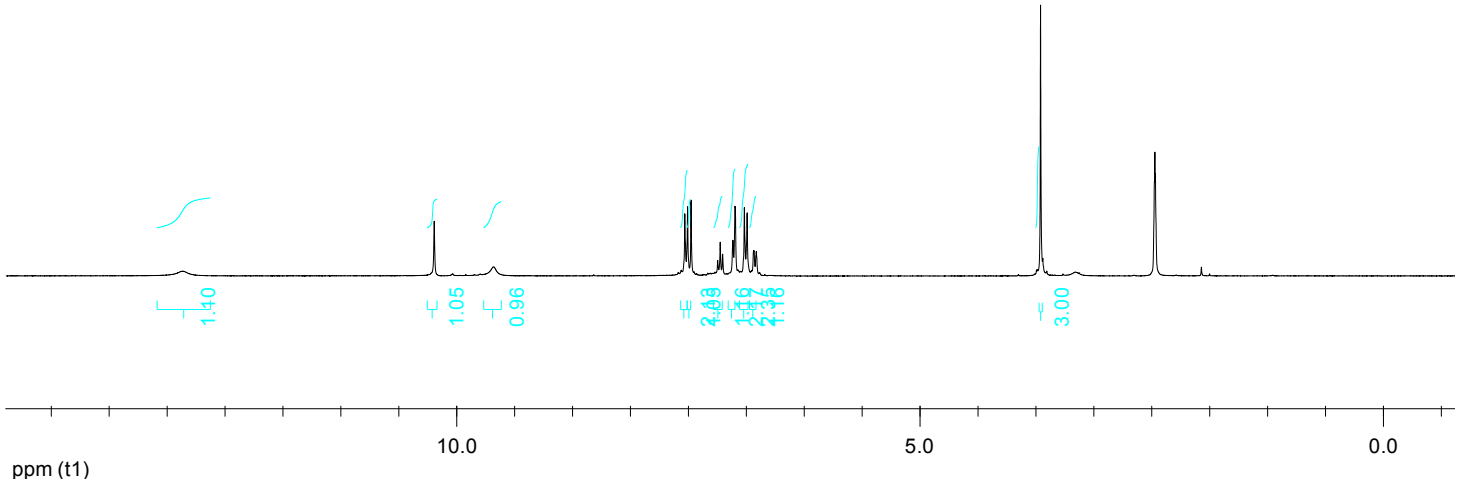
^{13}C NMR spectra of compound **11aC**:



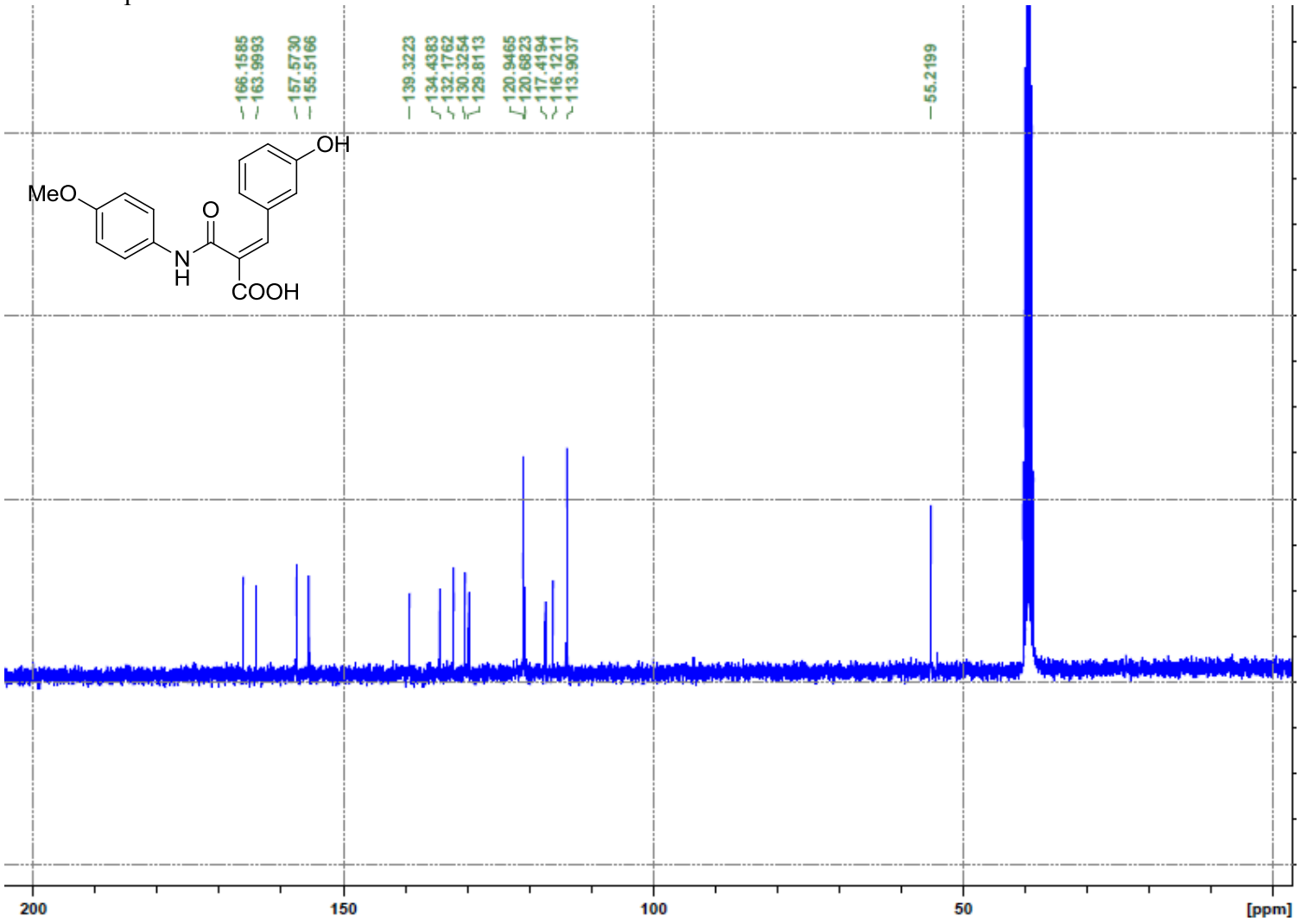
^{1}H NMR spectra of compound 11aE:



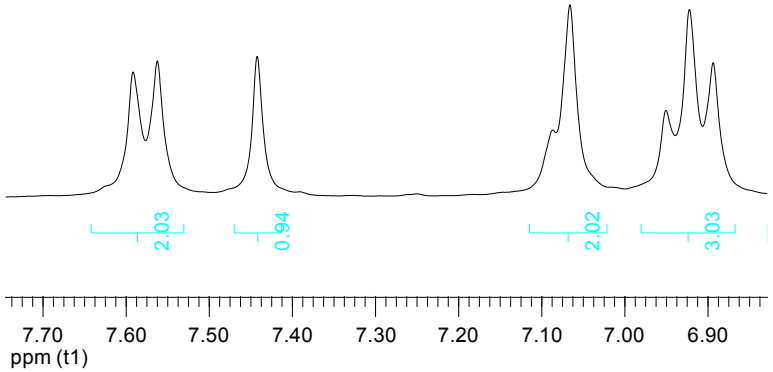


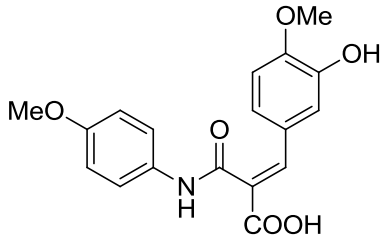


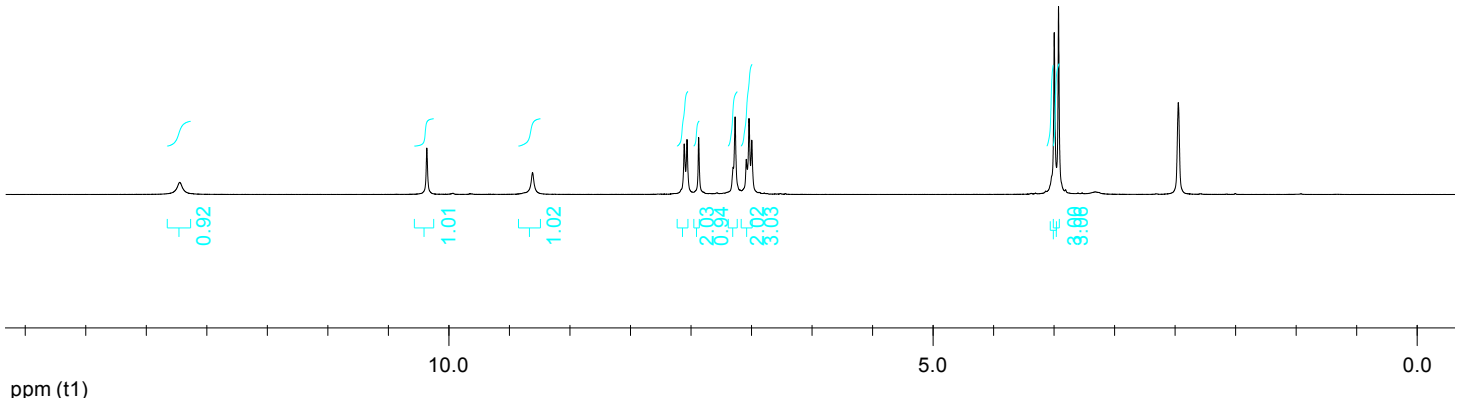
^{13}C NMR spectra of compound **11aE**:



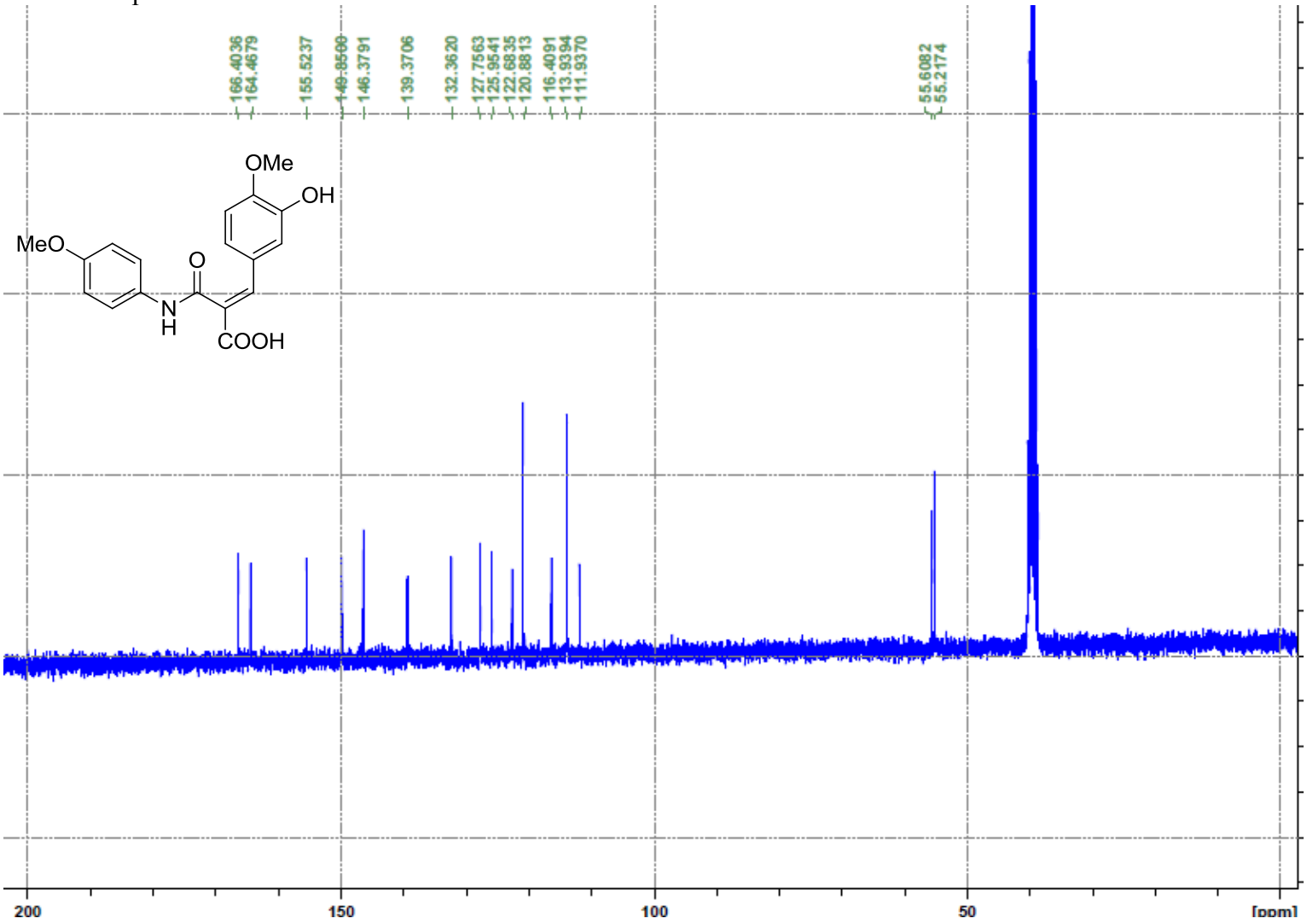
^{1}H NMR spectra of compound 11aF:



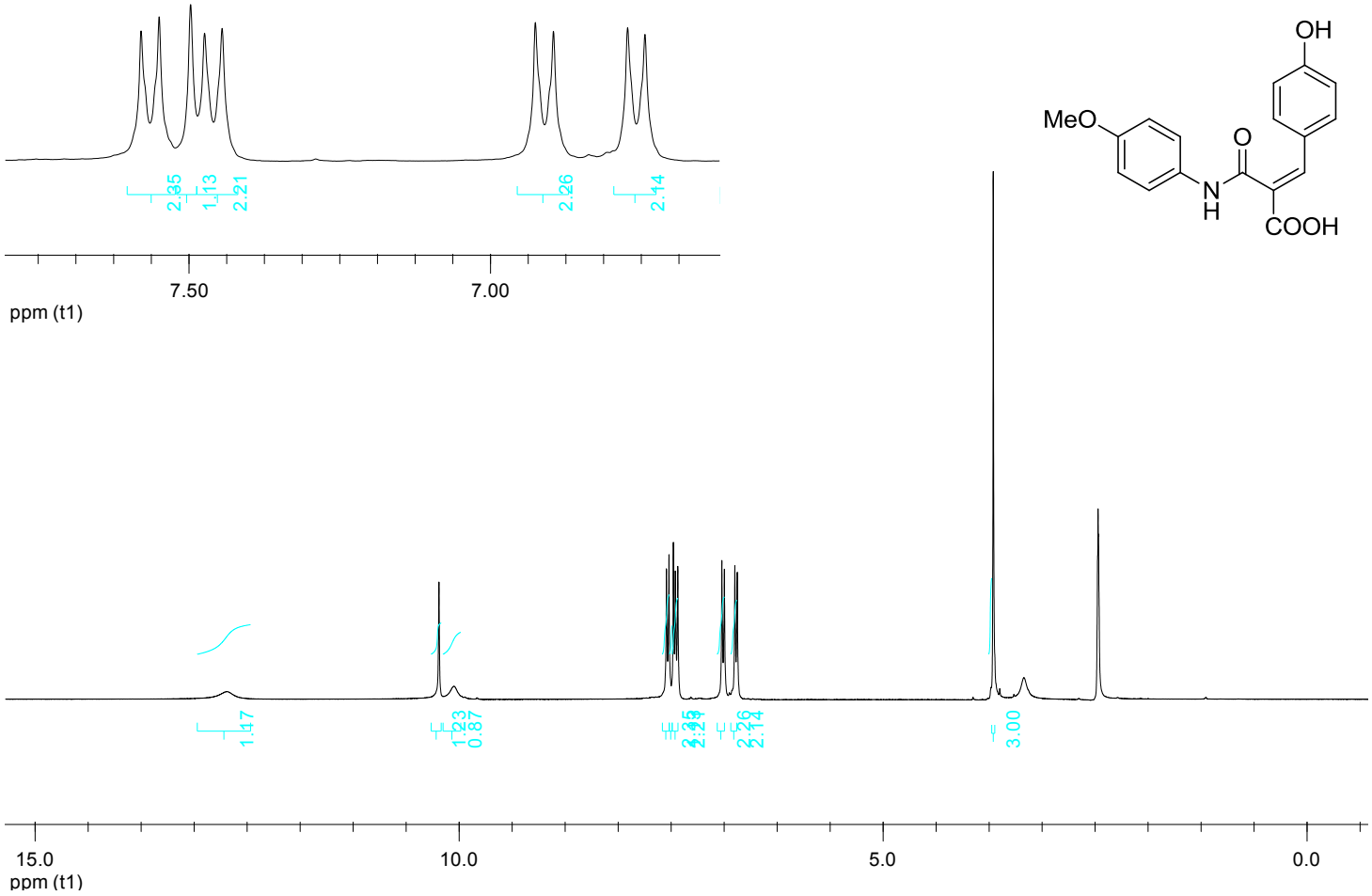




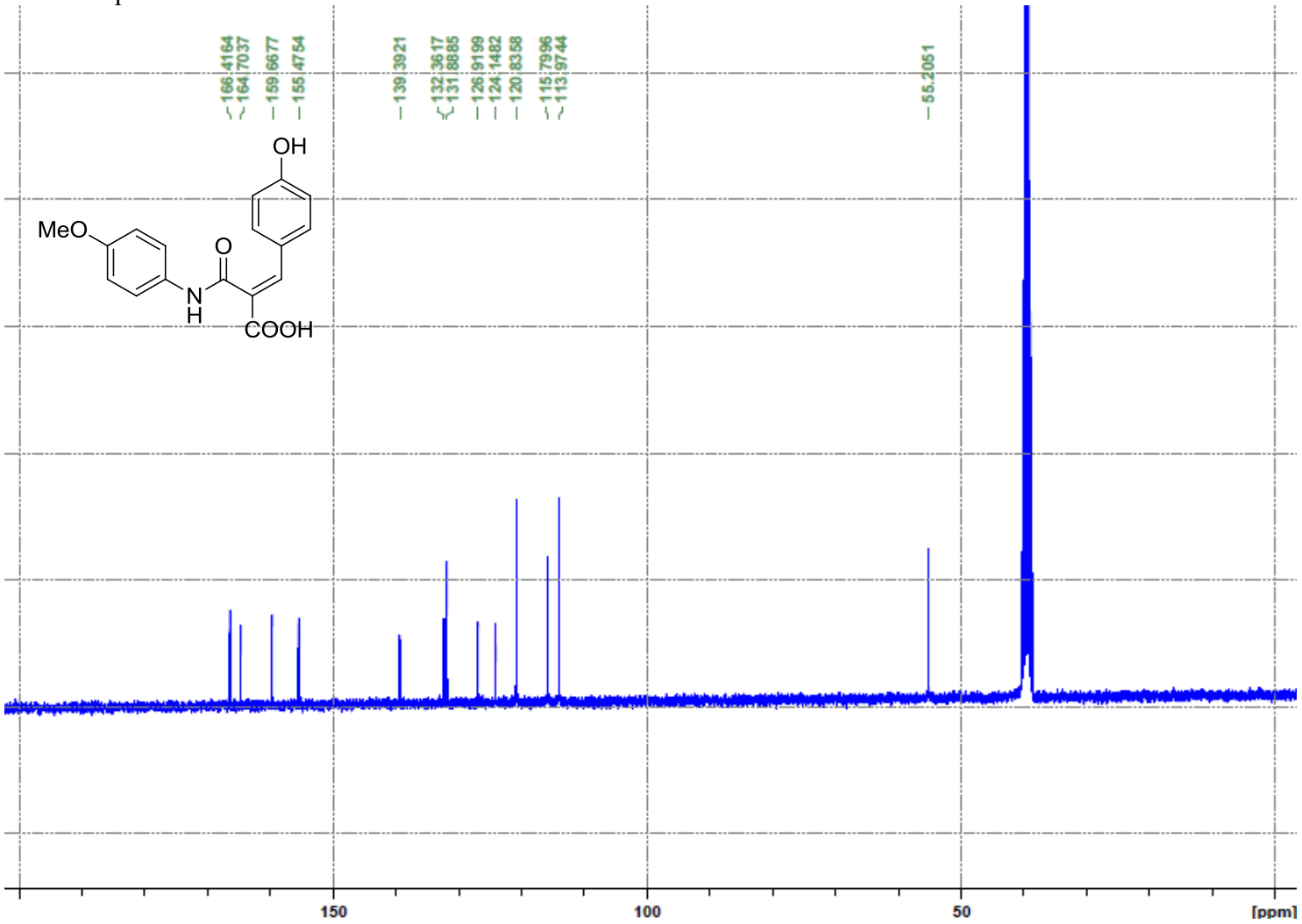
^{13}C NMR spectra of compound **11aF**:



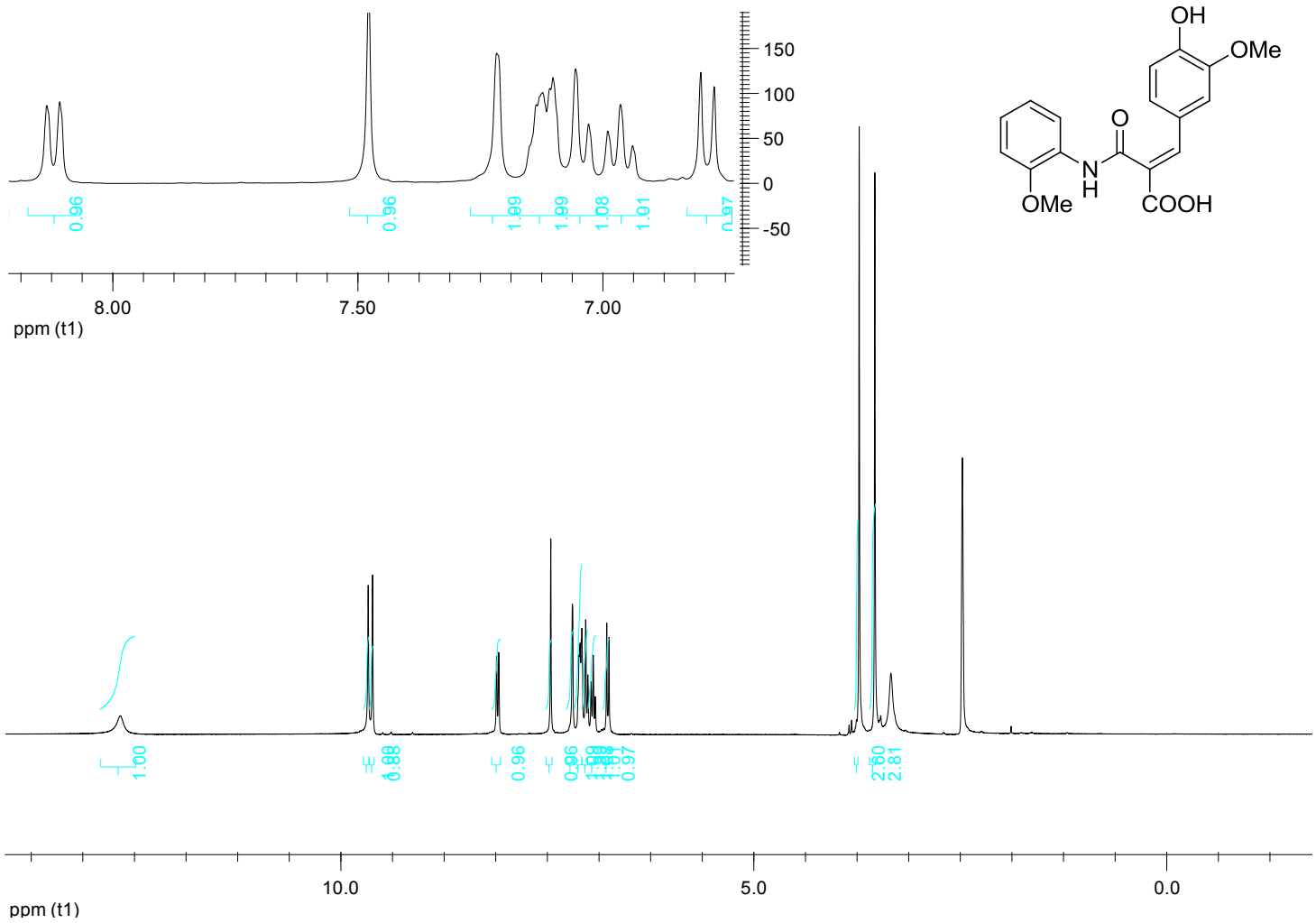
^{1}H NMR spectra of compound 11aG:



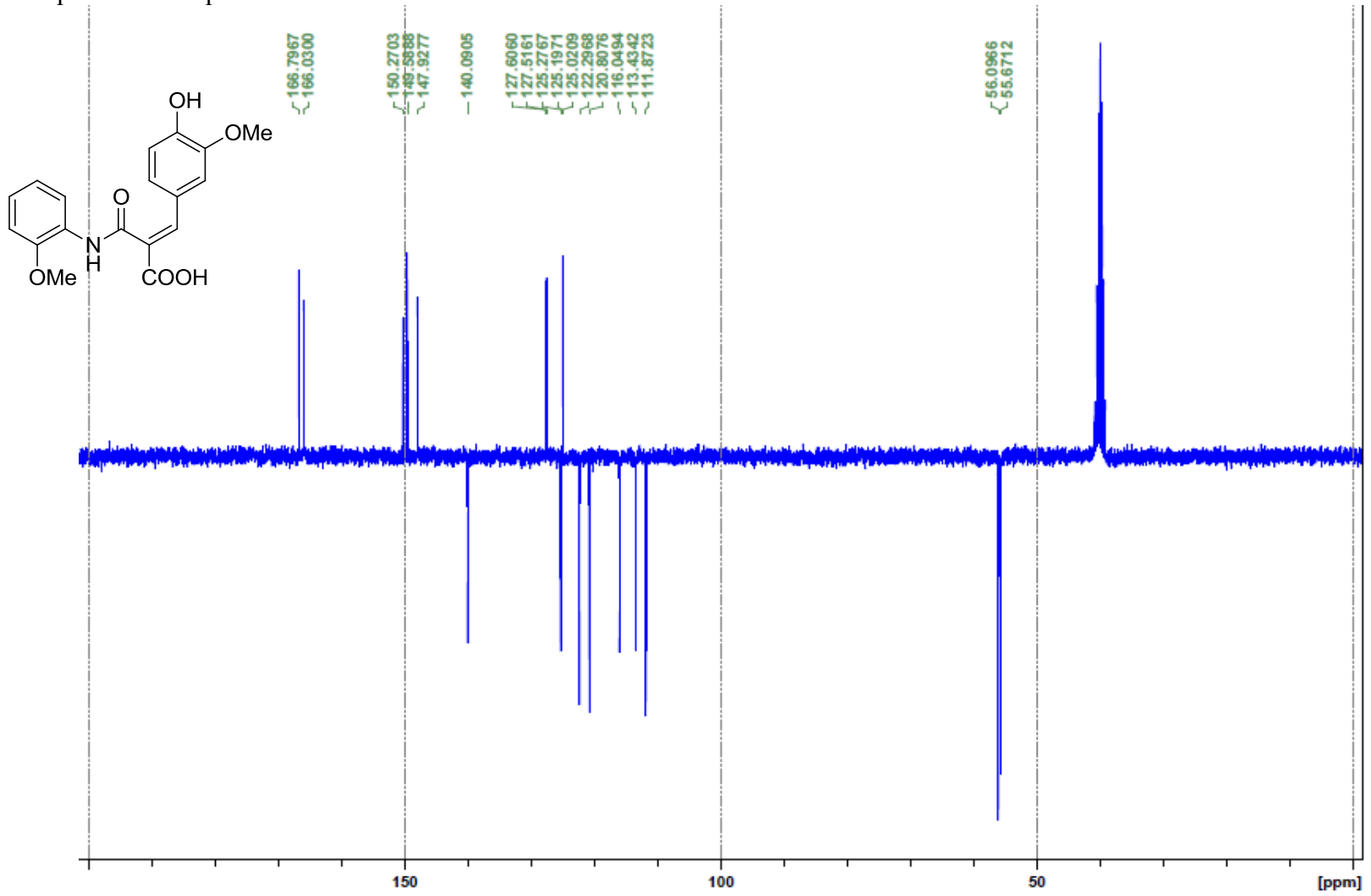
^{13}C NMR spectra of compound **11aG**:



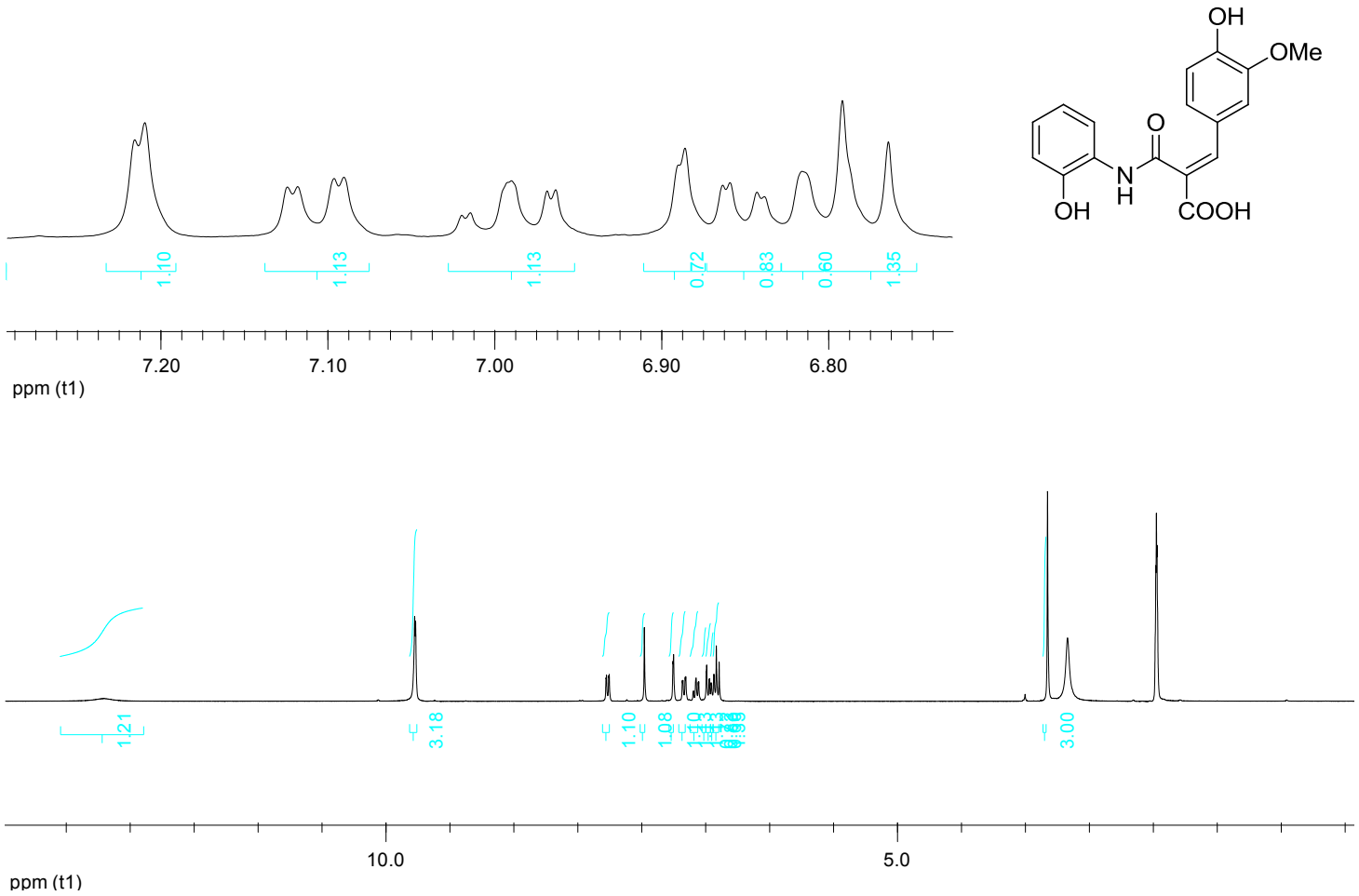
^{1}H NMR spectra of compound 11bA:



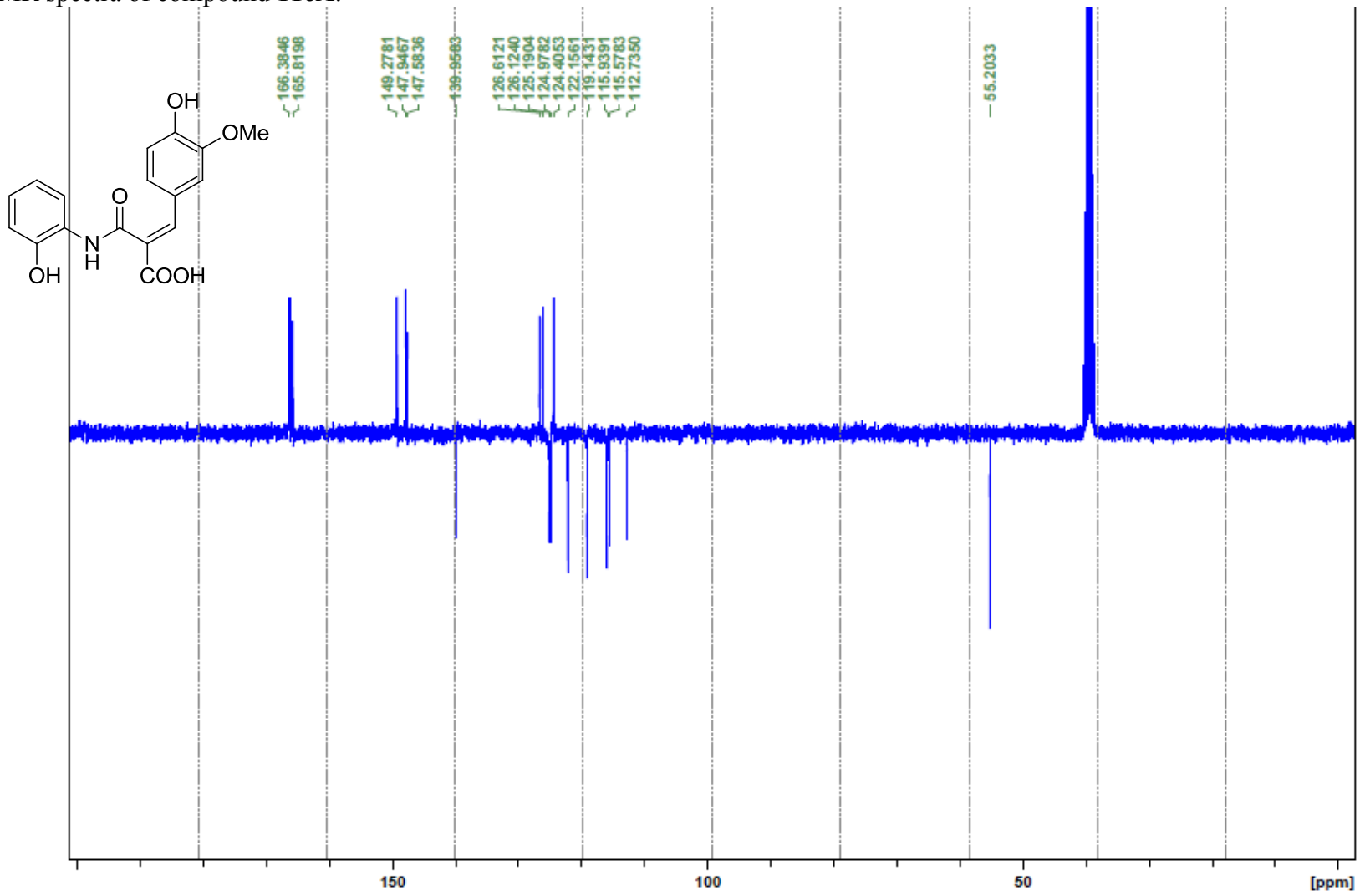
^{13}C NMR spectra of compound **11bA**:



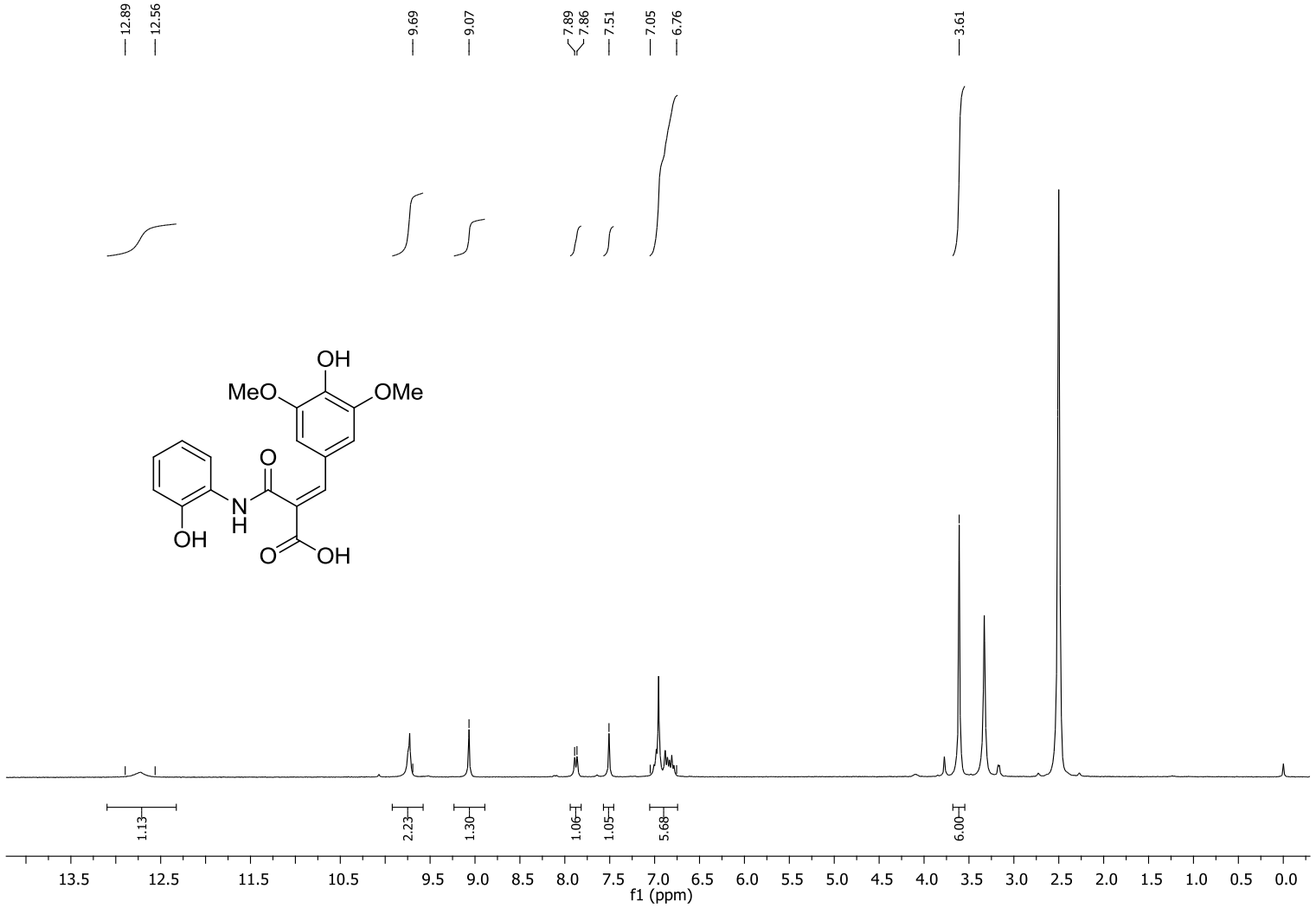
^{1}H NMR spectra of compound 11cA:



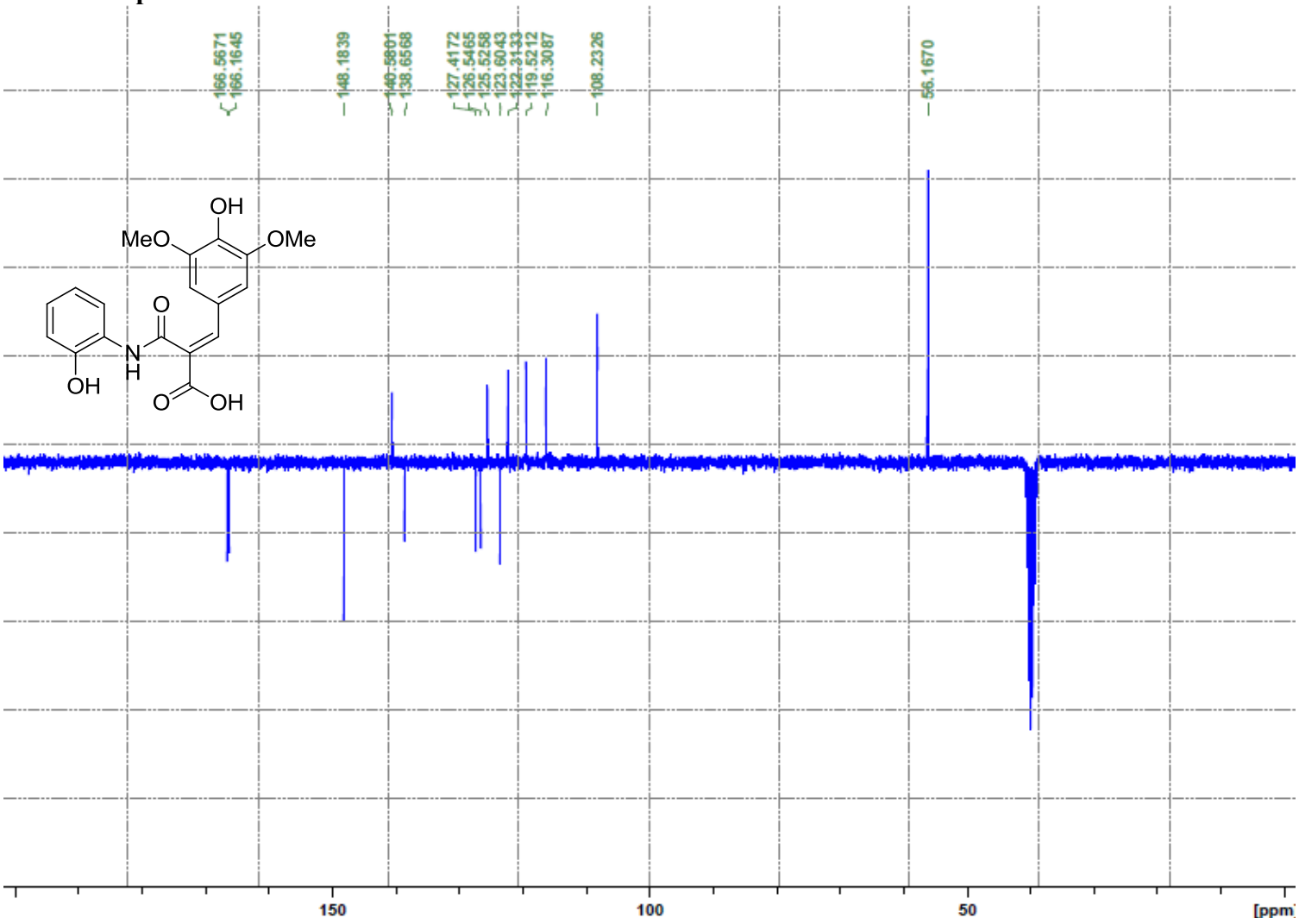
^{13}C NMR spectra of compound **11cA**:



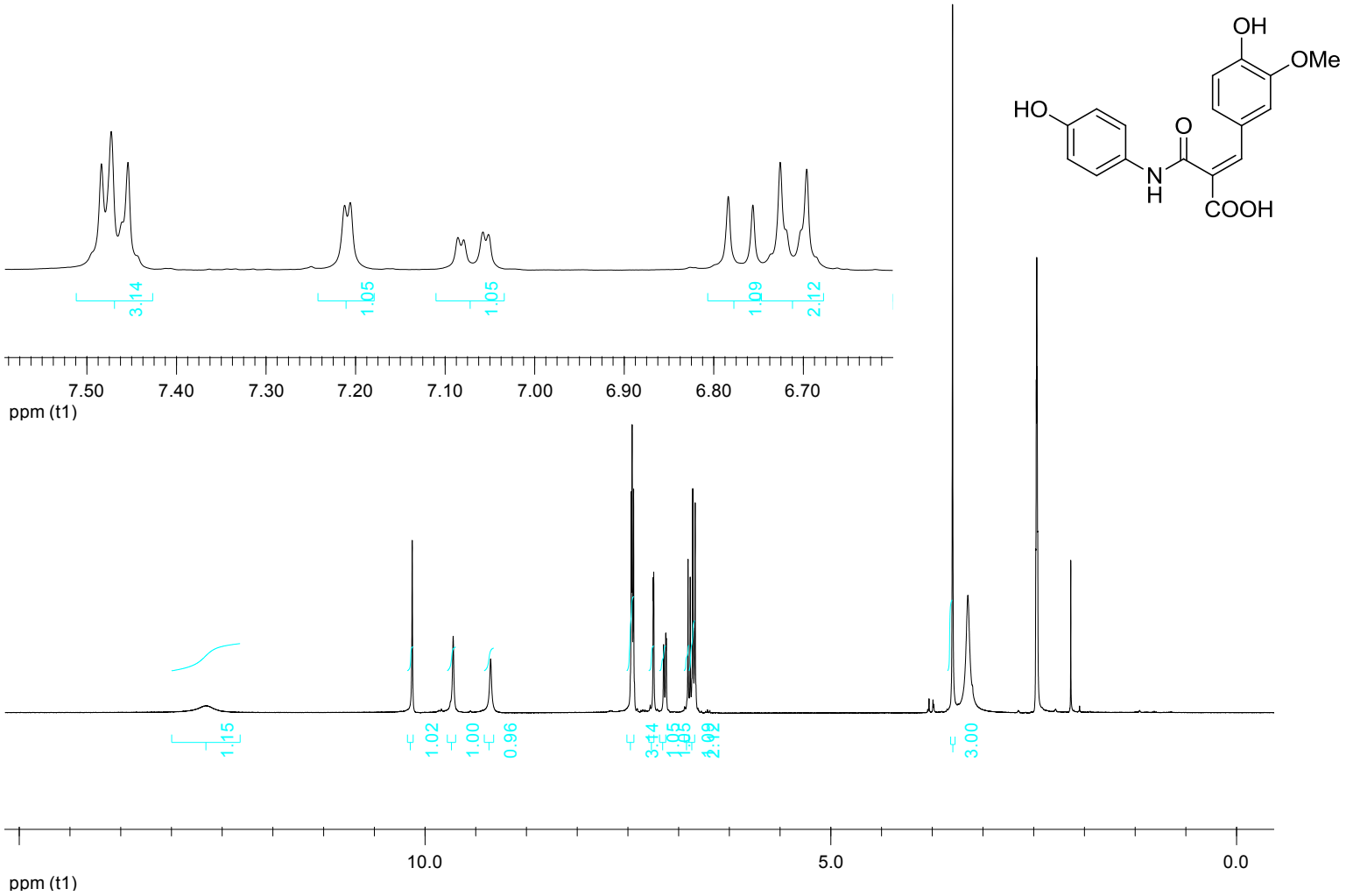
^{1}H NMR spectra of compound 11cH:


12.89
12.56
9.69
9.07
7.89
7.86
7.51
7.05
6.76
3.61
OH
MeO
OMe
O
N
H
OH
O
OH
1.13
2.23
1.30
1.06
1.05
5.68
6.00
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

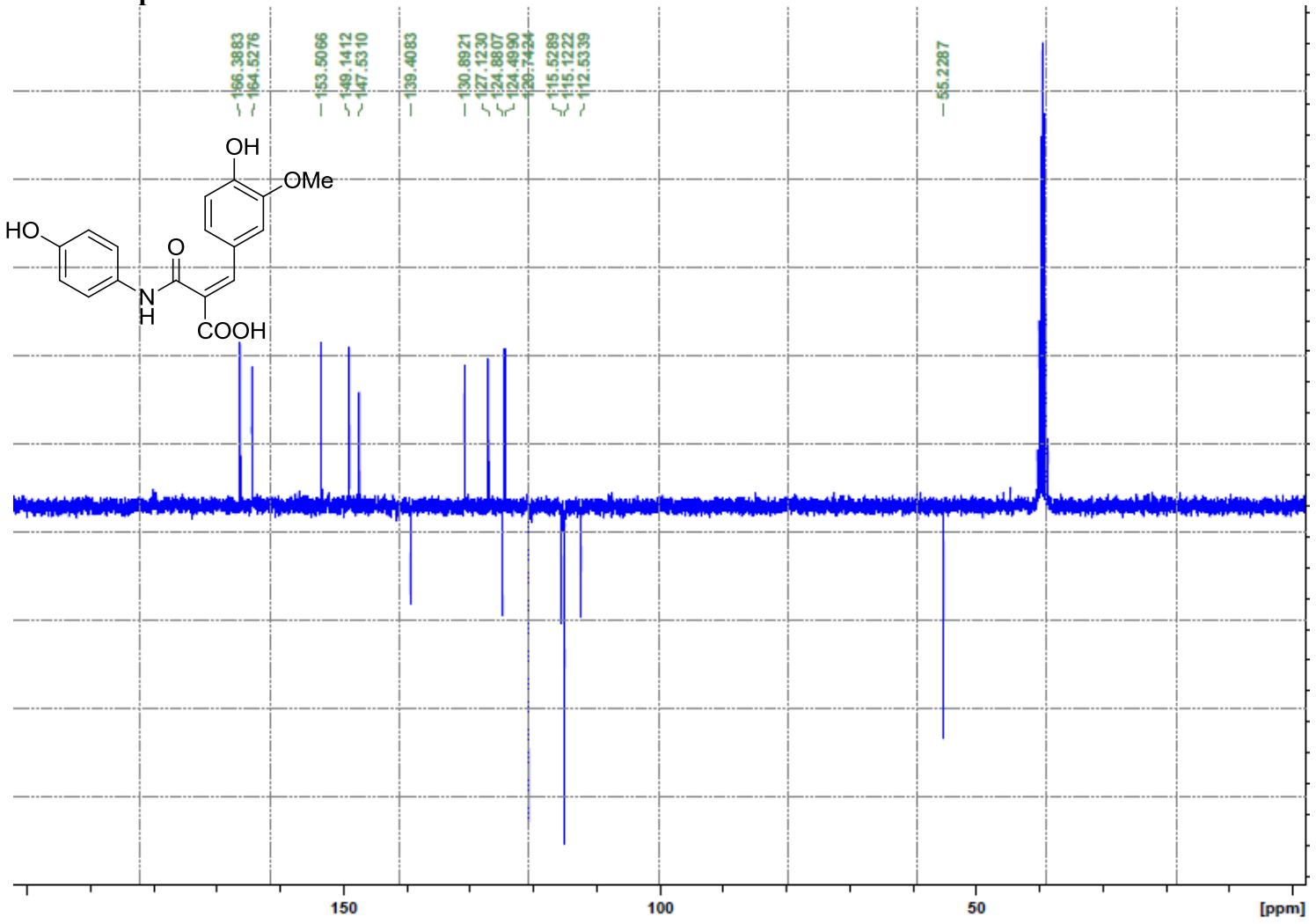
^{13}C NMR spectra of compound 11cH:



^{1}H NMR spectra of compound 11dA:



^{13}C NMR spectra of compound 11dA:



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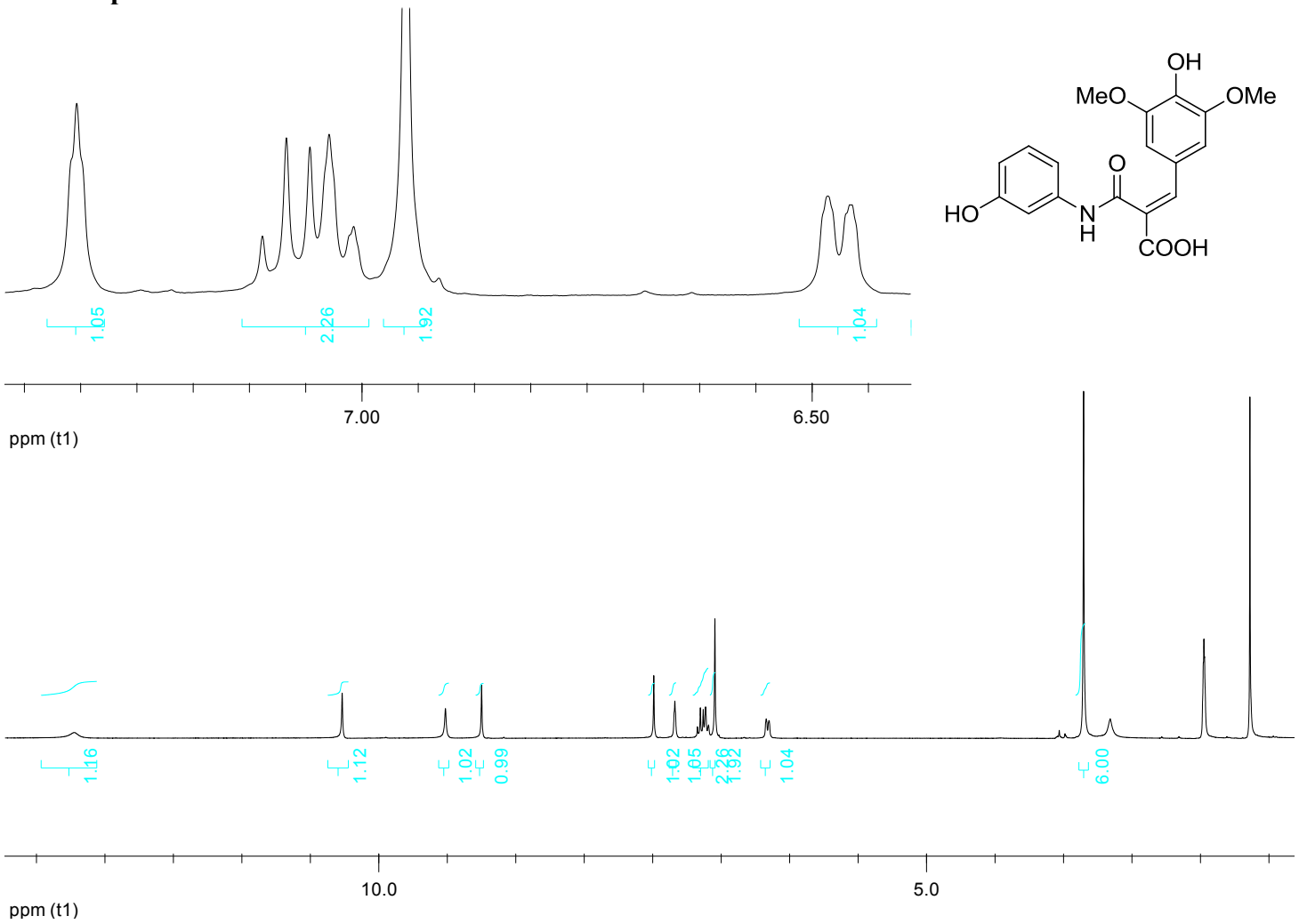
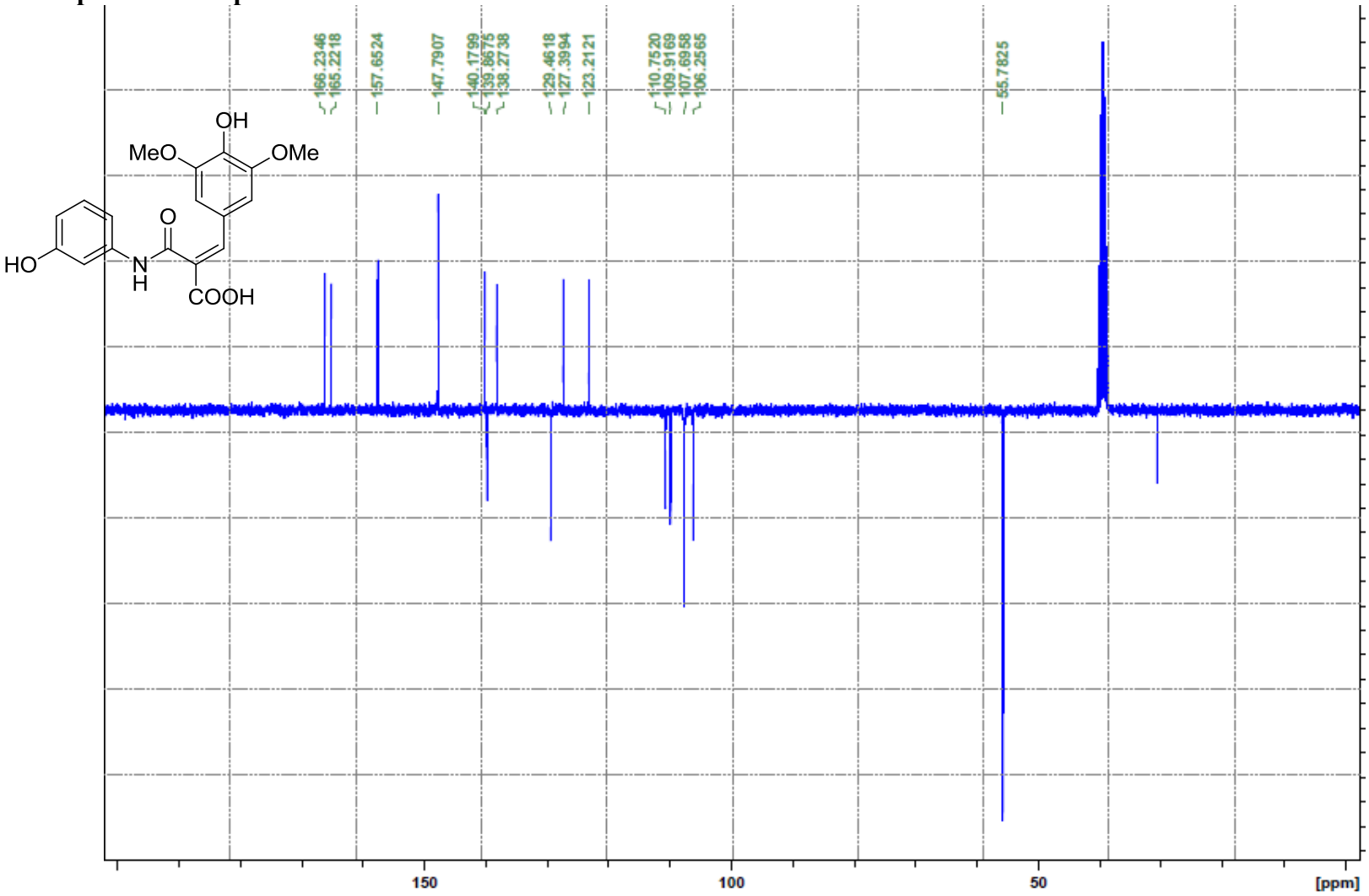
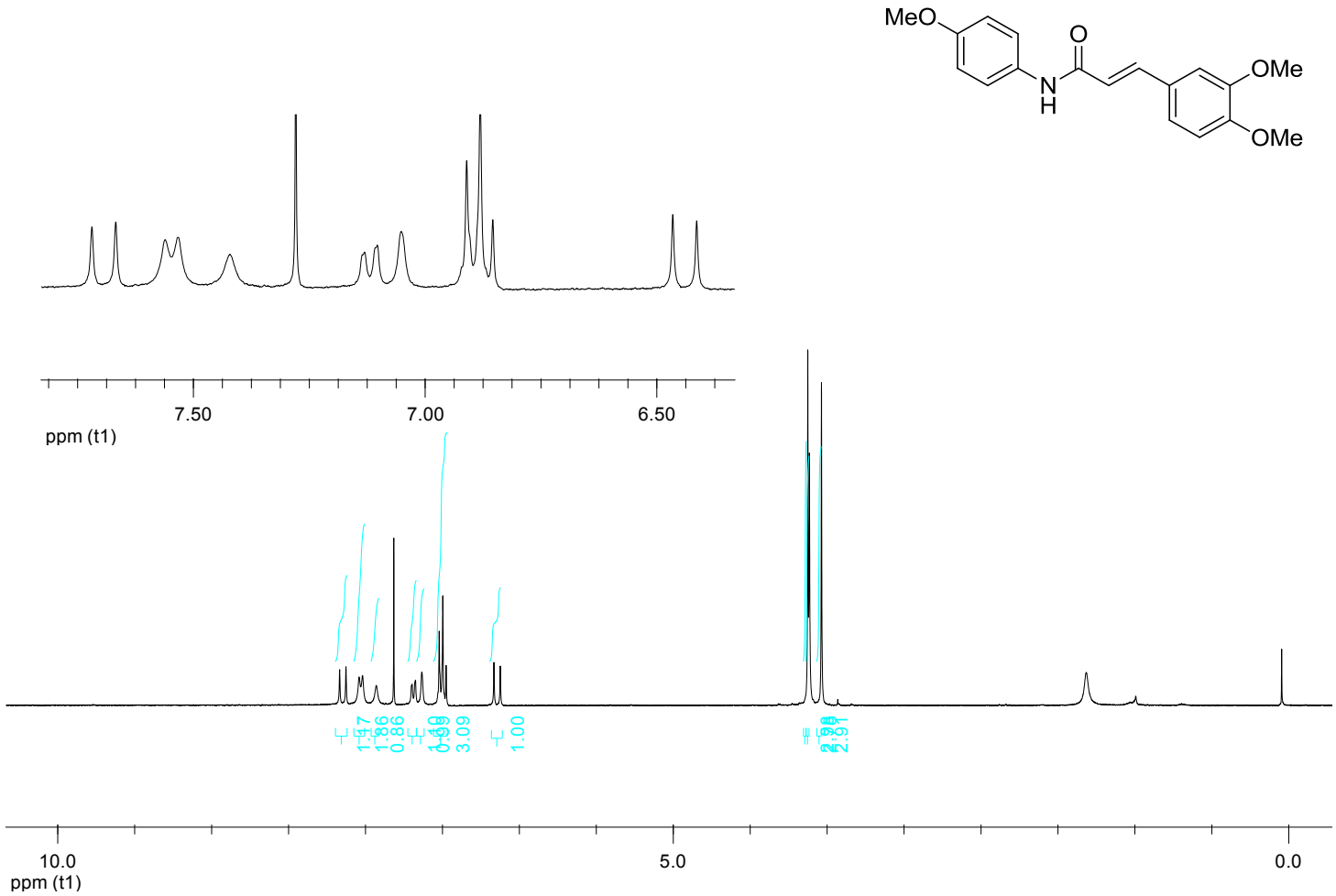


^{13}C NMR spectra of compound 11eH:

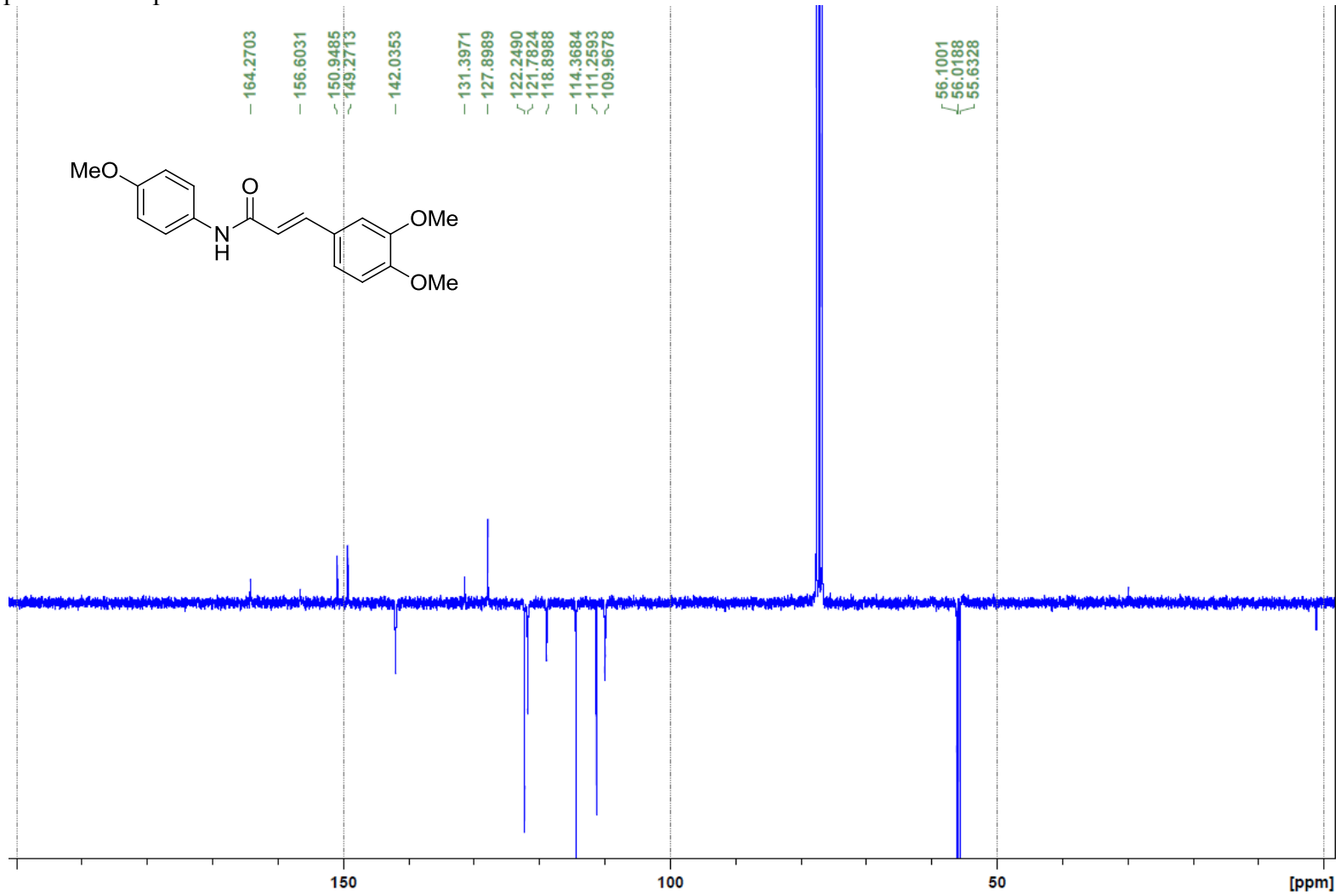


NMR SPECTRA OF CINNAMOYL ANILINES 12

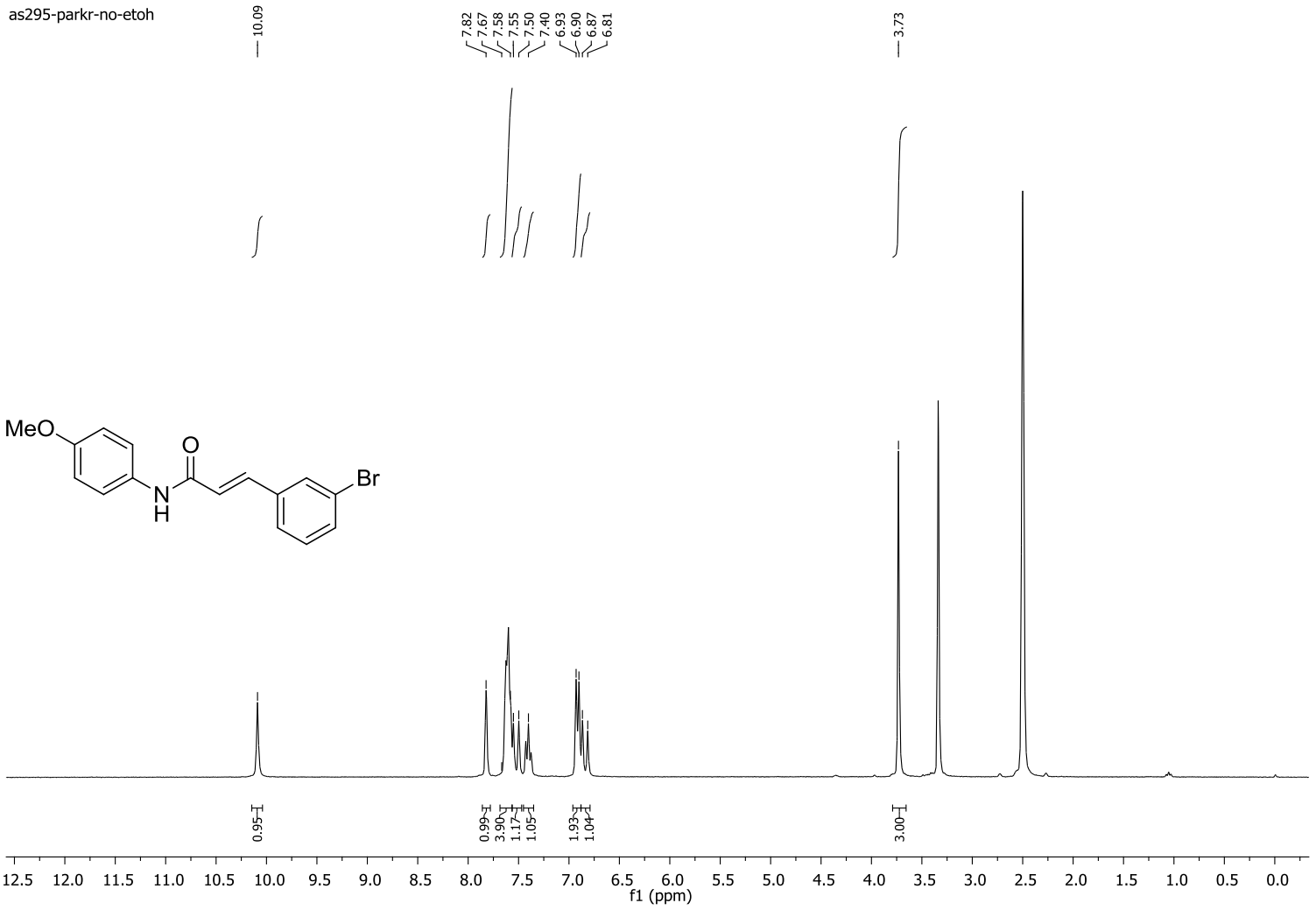
^{1}H NMR spectra of compound 12aB:



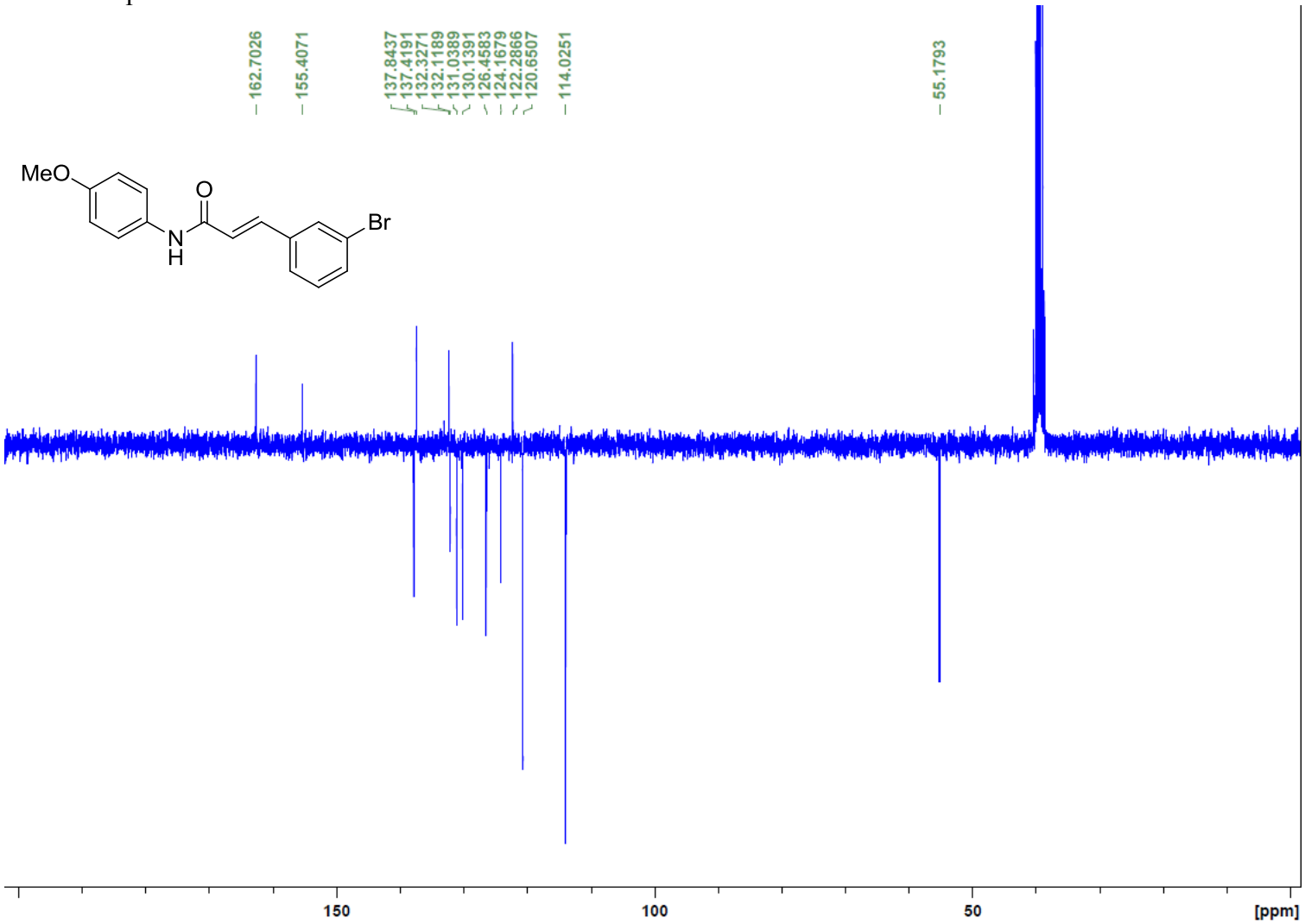
^{13}C NMR spectra of compound **12aB**:



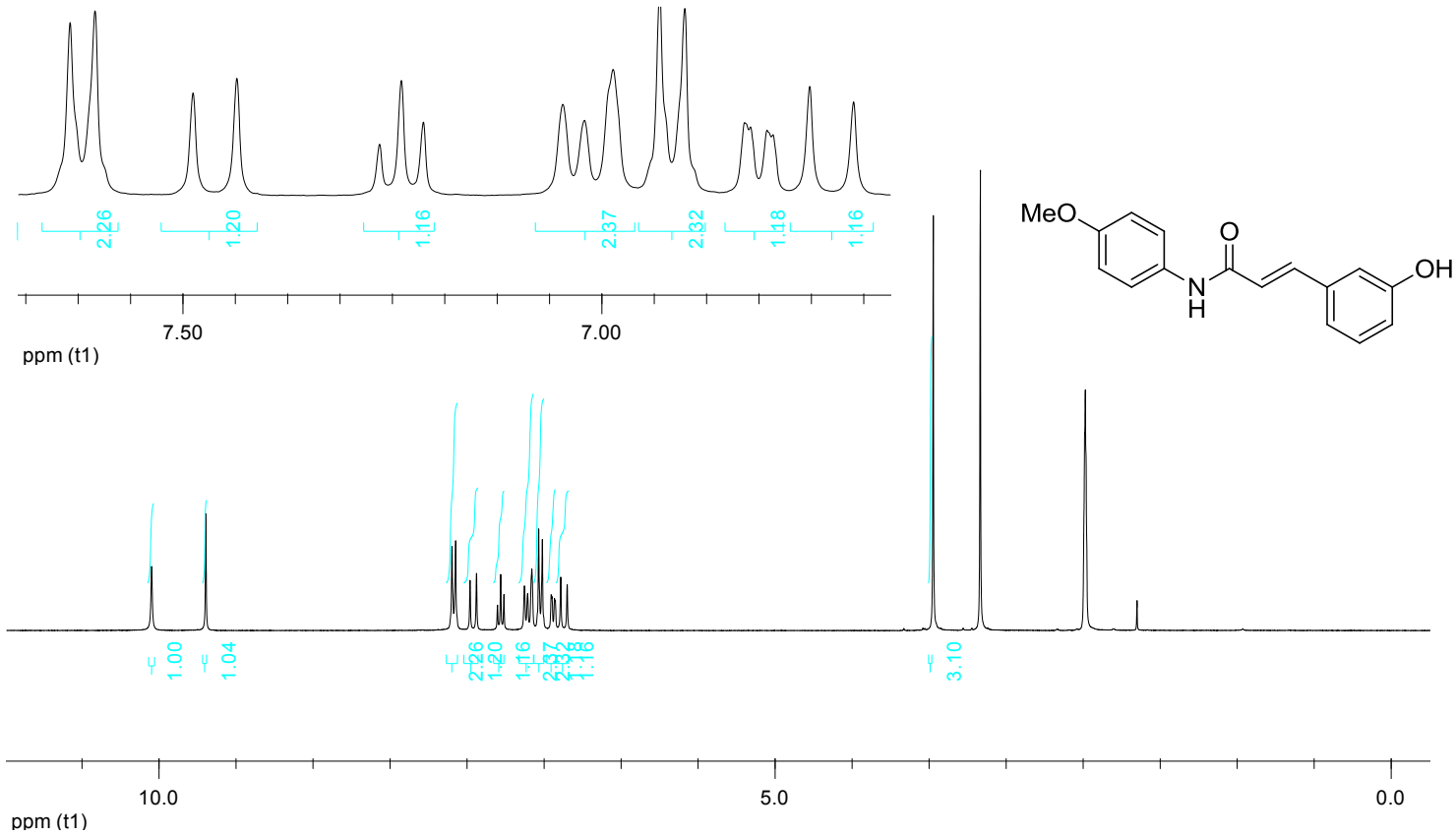
^{1}H NMR spectra of compound 12aD:



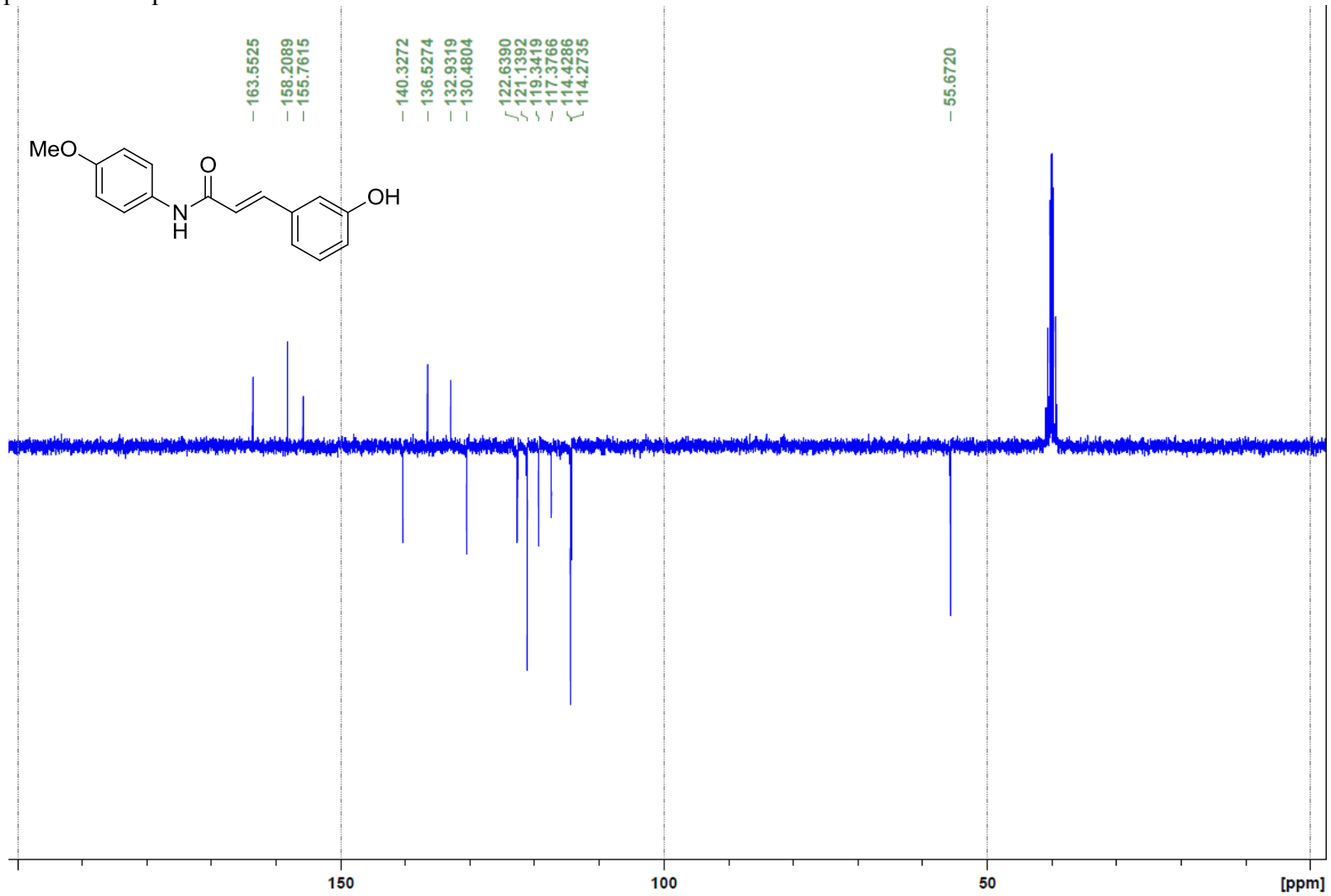
^{13}C NMR spectra of compound **12aD**:



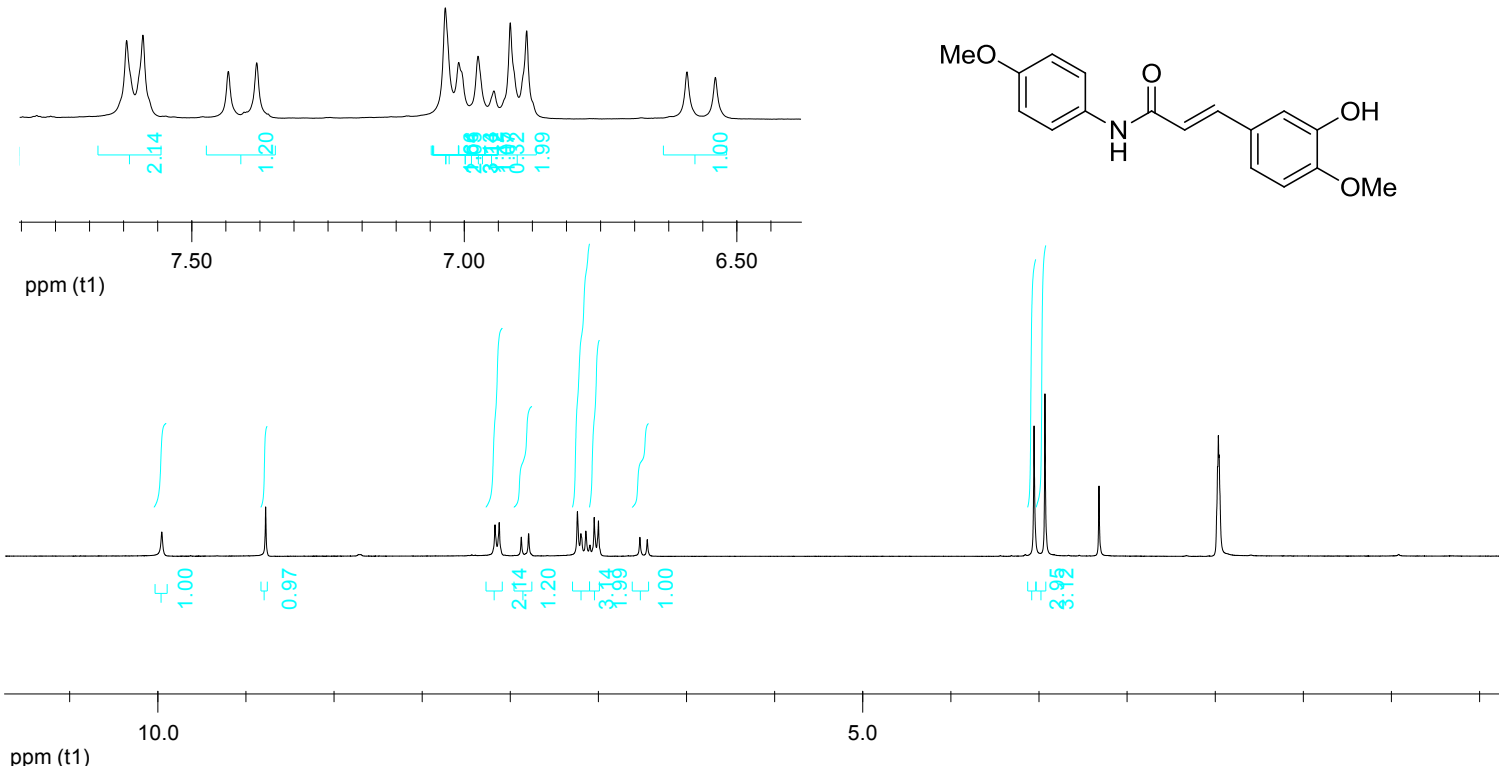
^{1}H NMR spectra of compound 12aE:



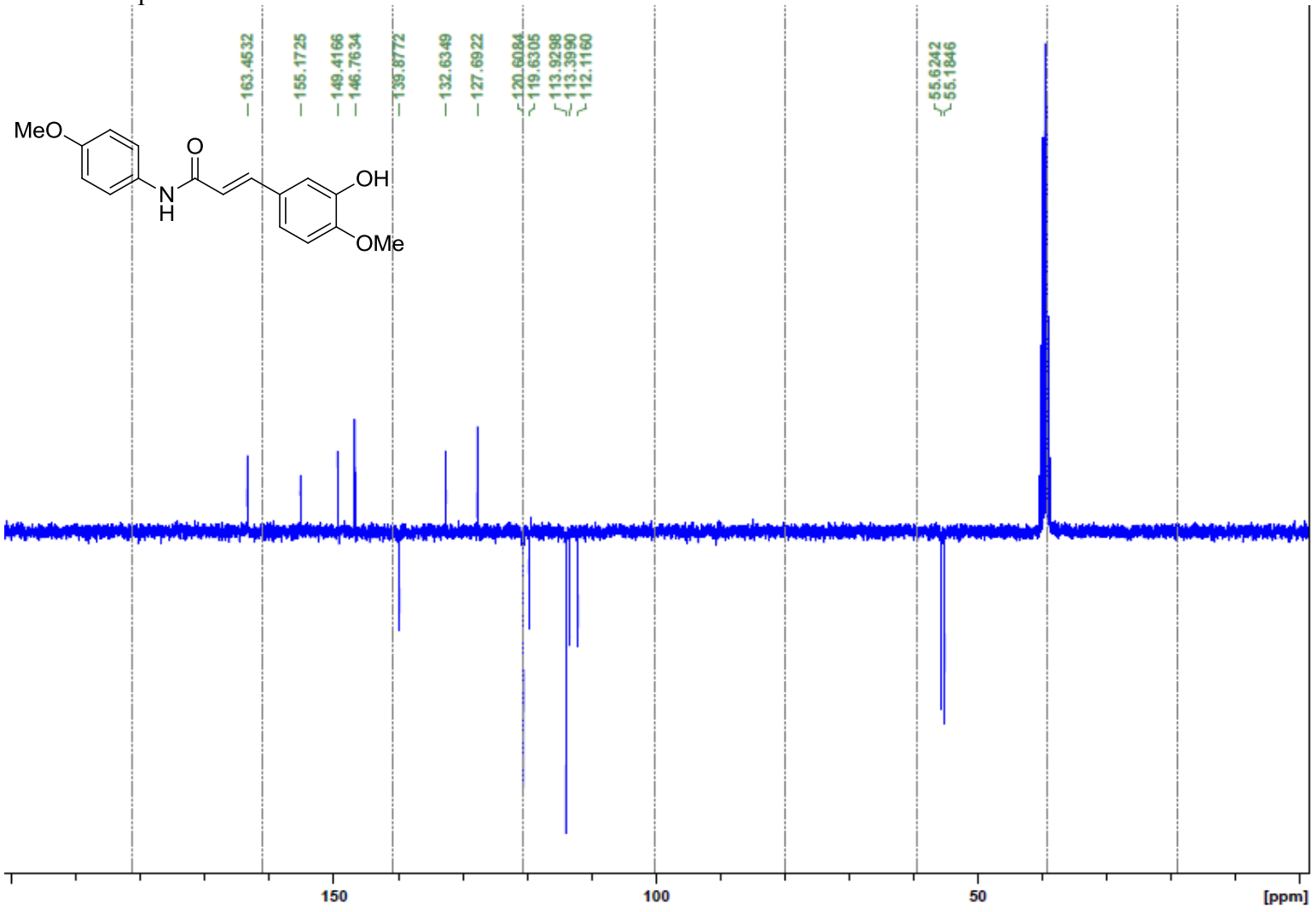
^{13}C NMR spectra of compound **12aE**:



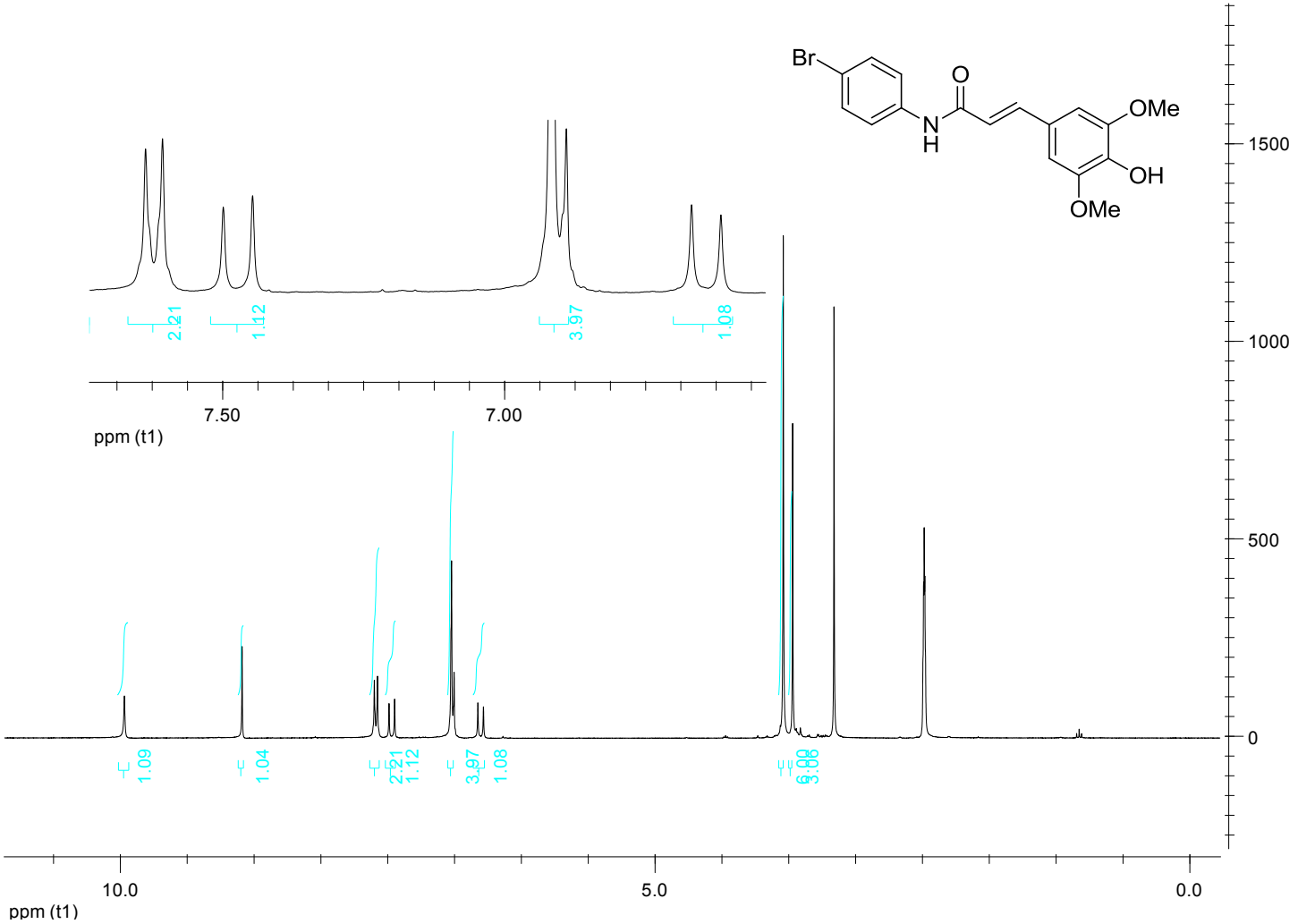
[1]H NMR spectra of compound 12aF:



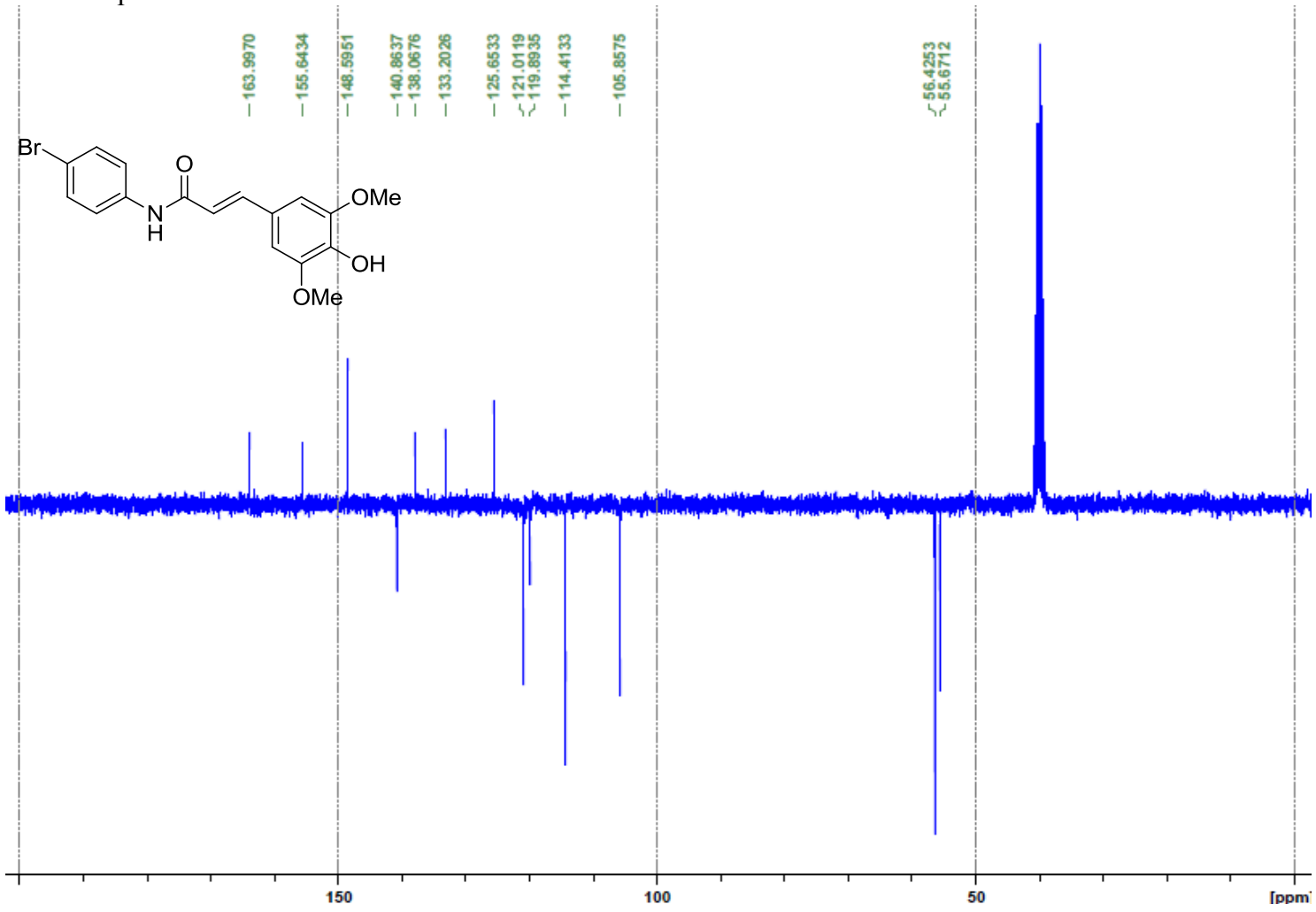
^{13}C NMR spectra of compound **12aF**:



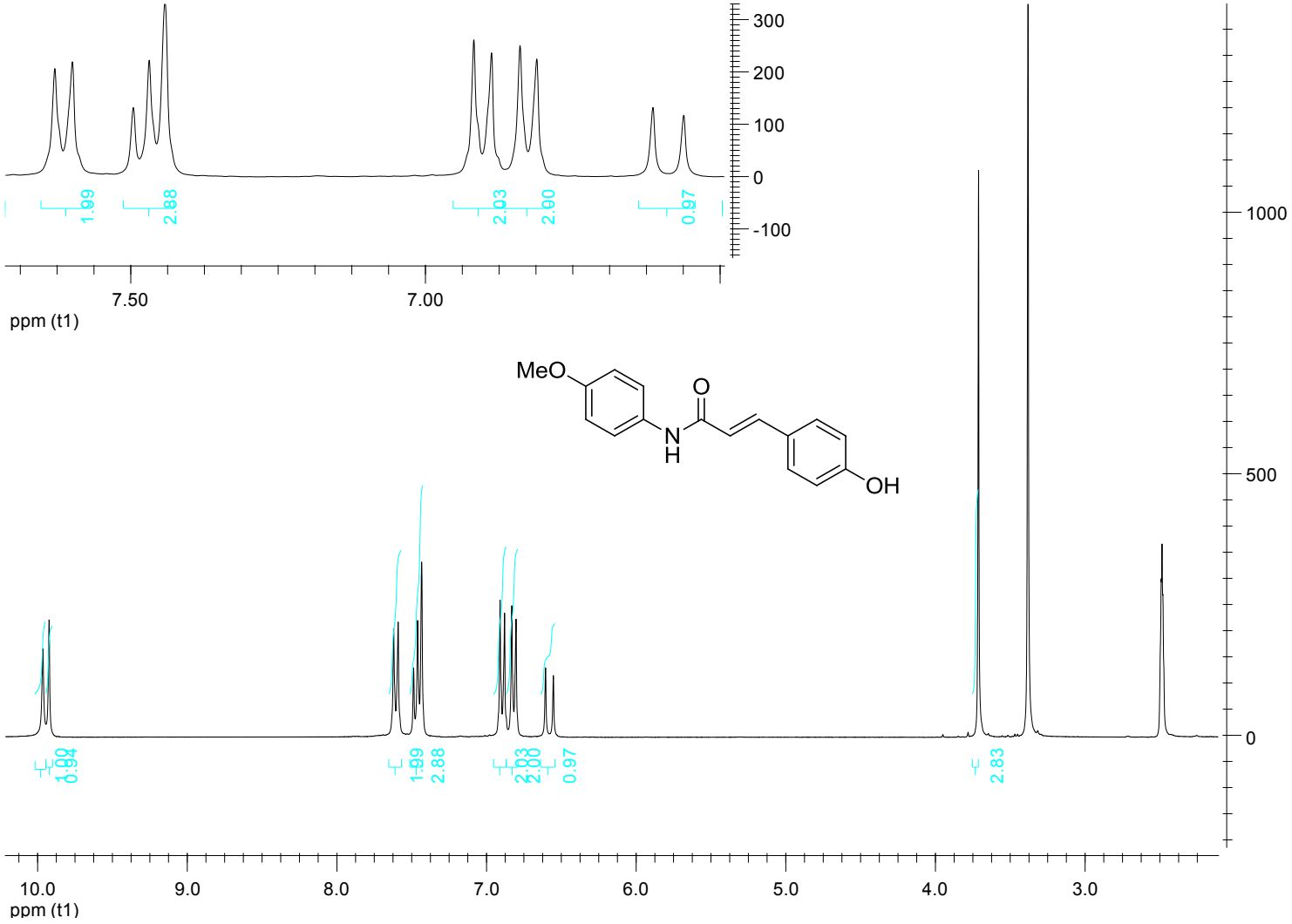
^{1}H NMR spectra of compound 12aH:



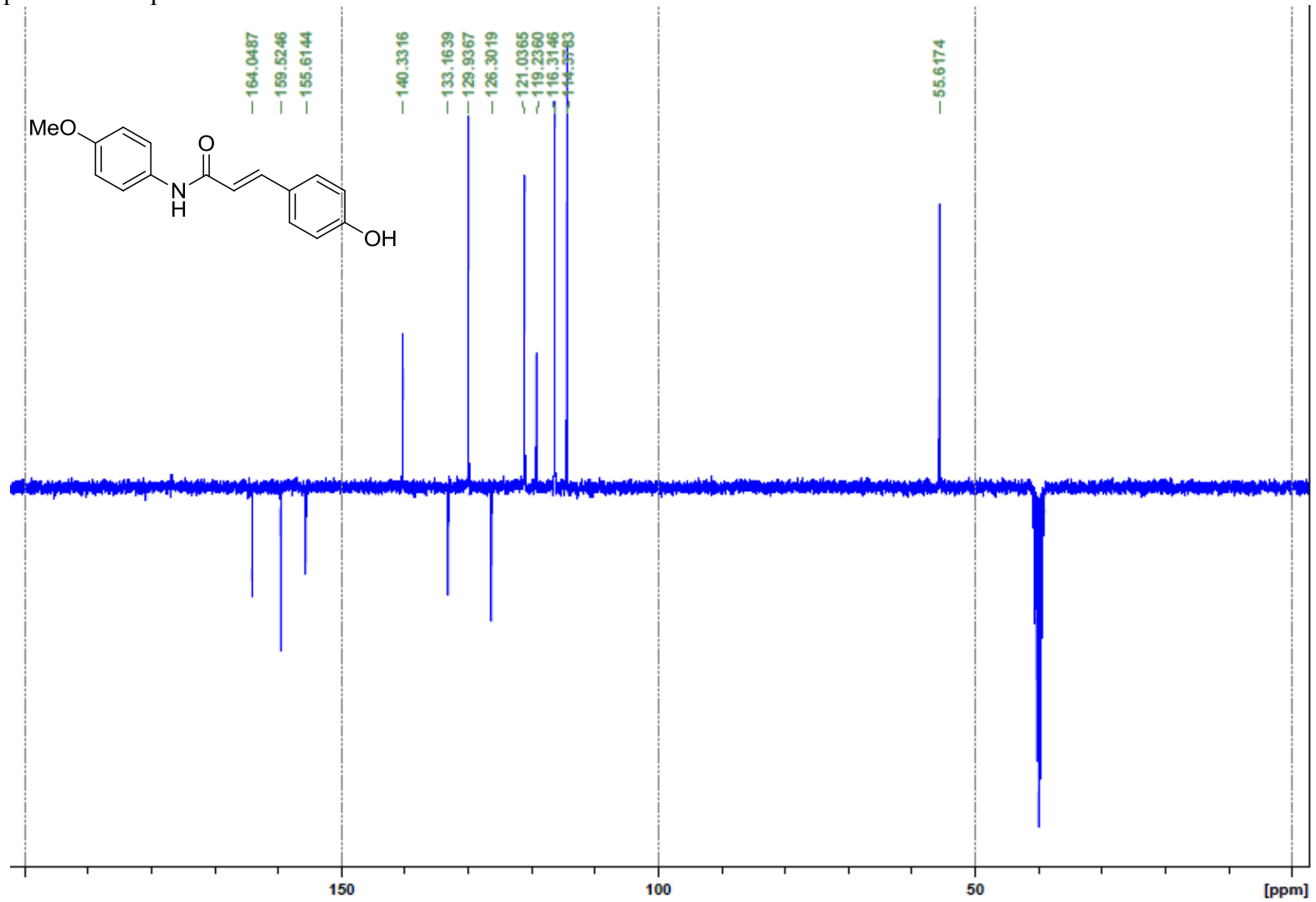
^{13}C NMR spectra of compound **12aH**:



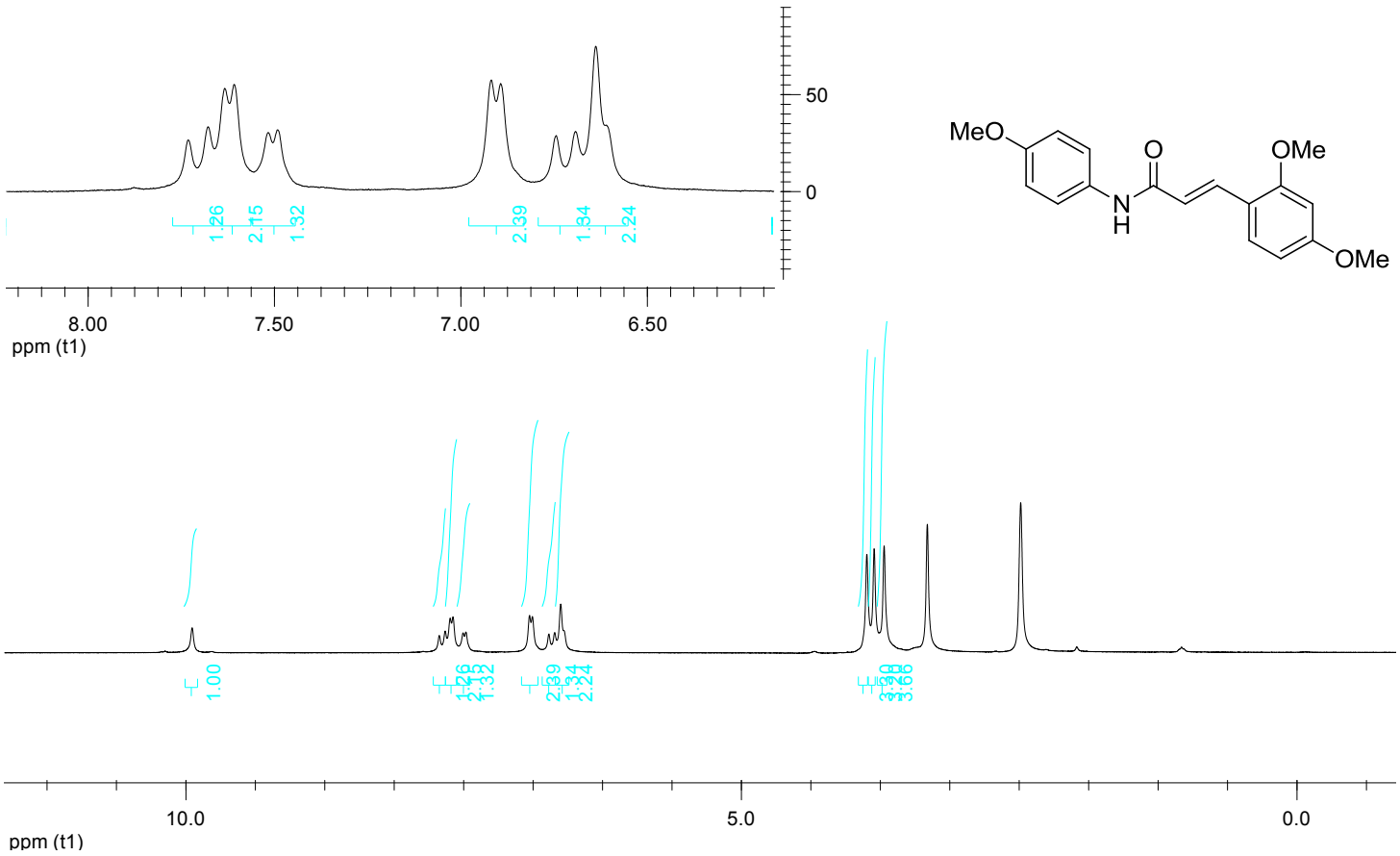
^{1}H NMR spectra of compound 12aG:



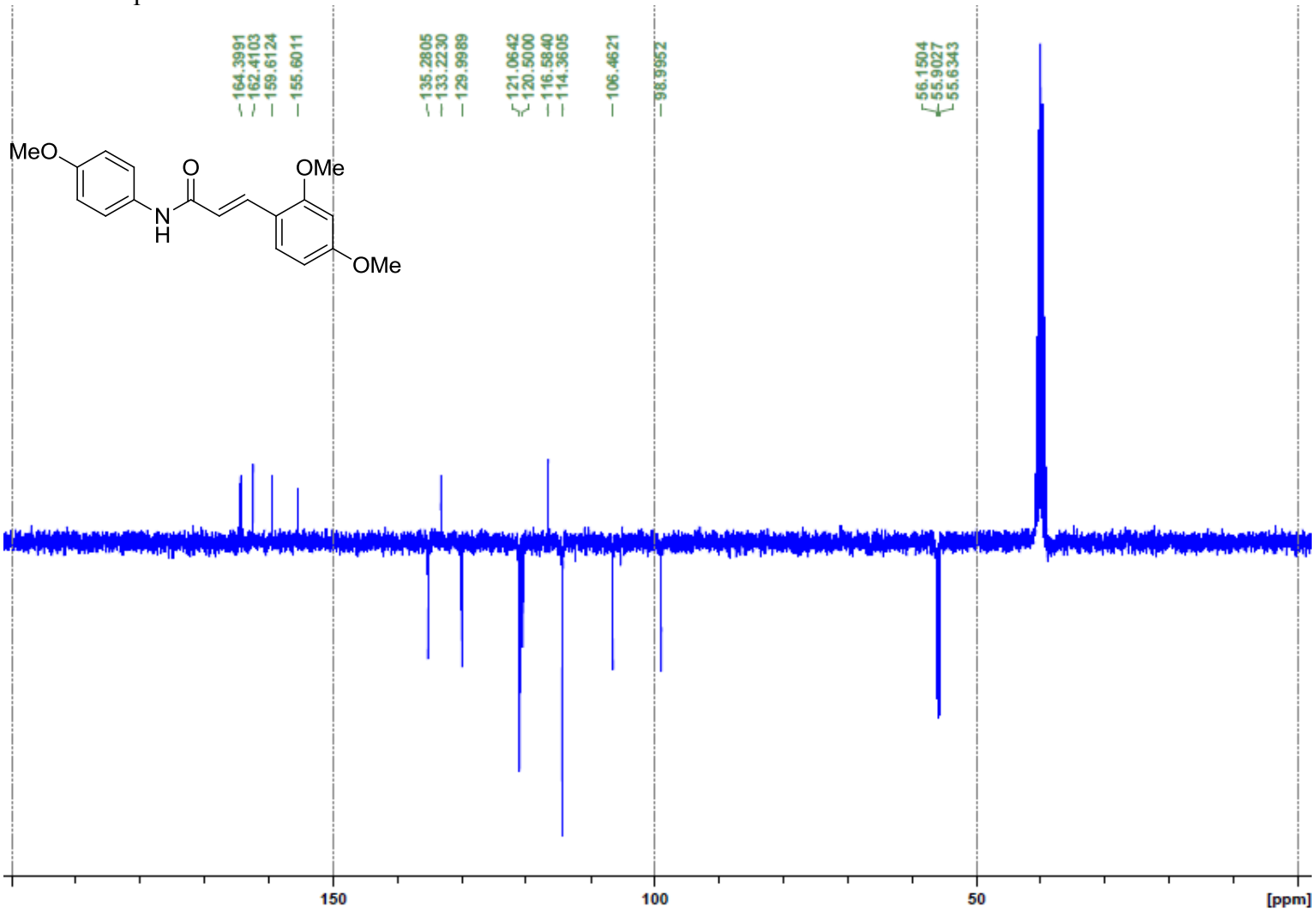
^{13}C NMR spectra of compound **12aG**:



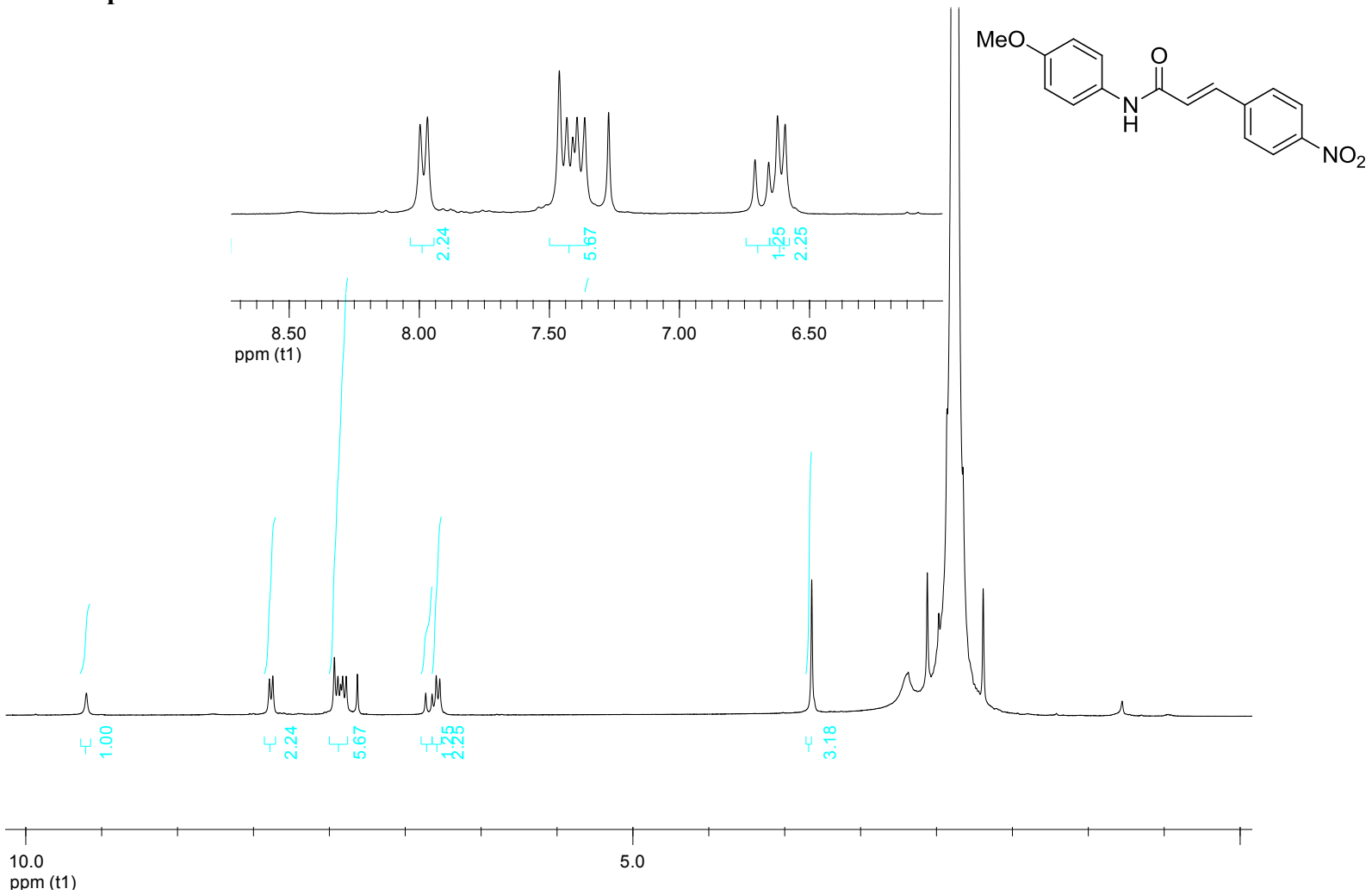
^{1}H NMR spectra of compound 12aI:



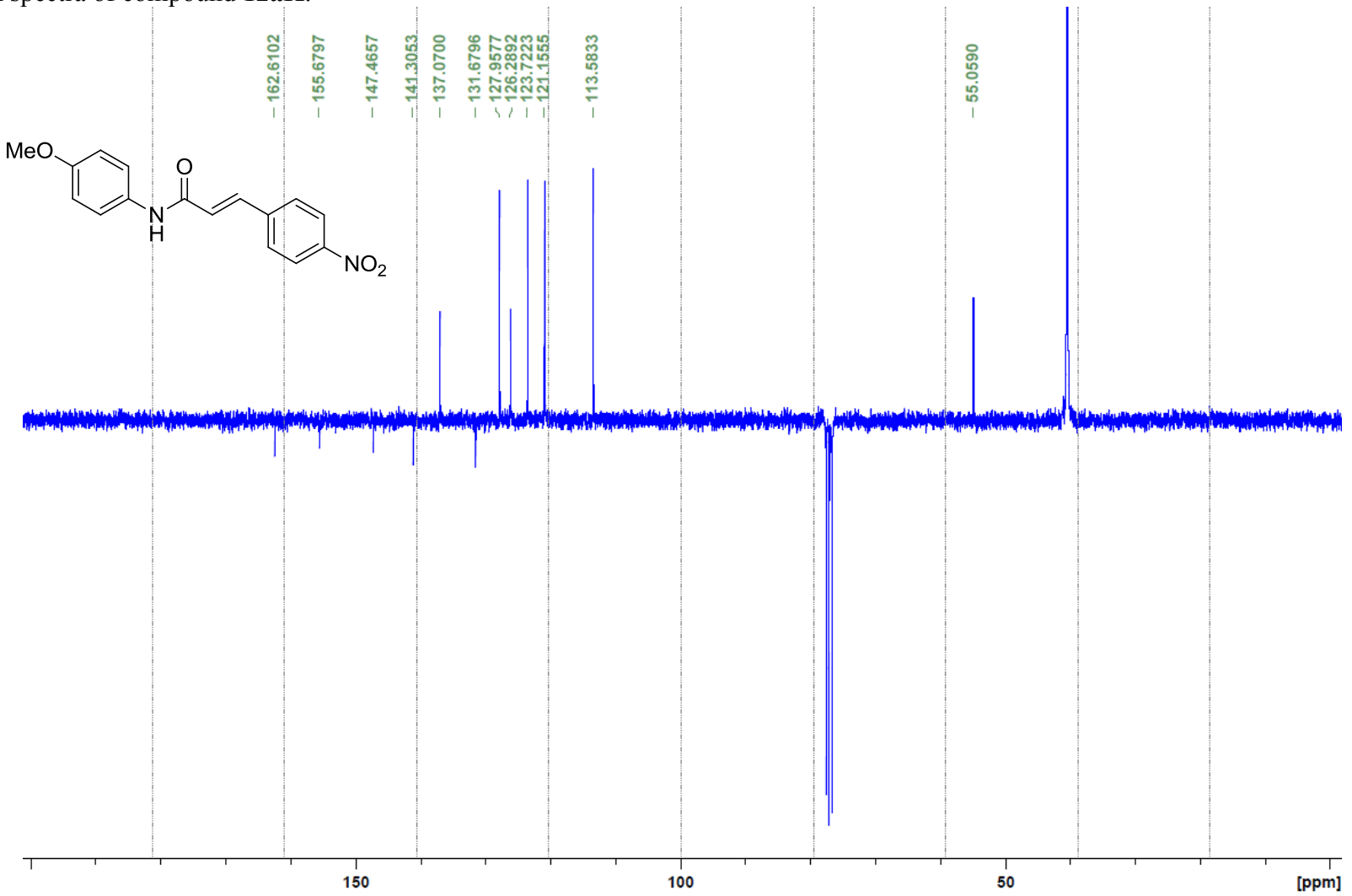
^{13}C NMR spectra of compound **12aI**:



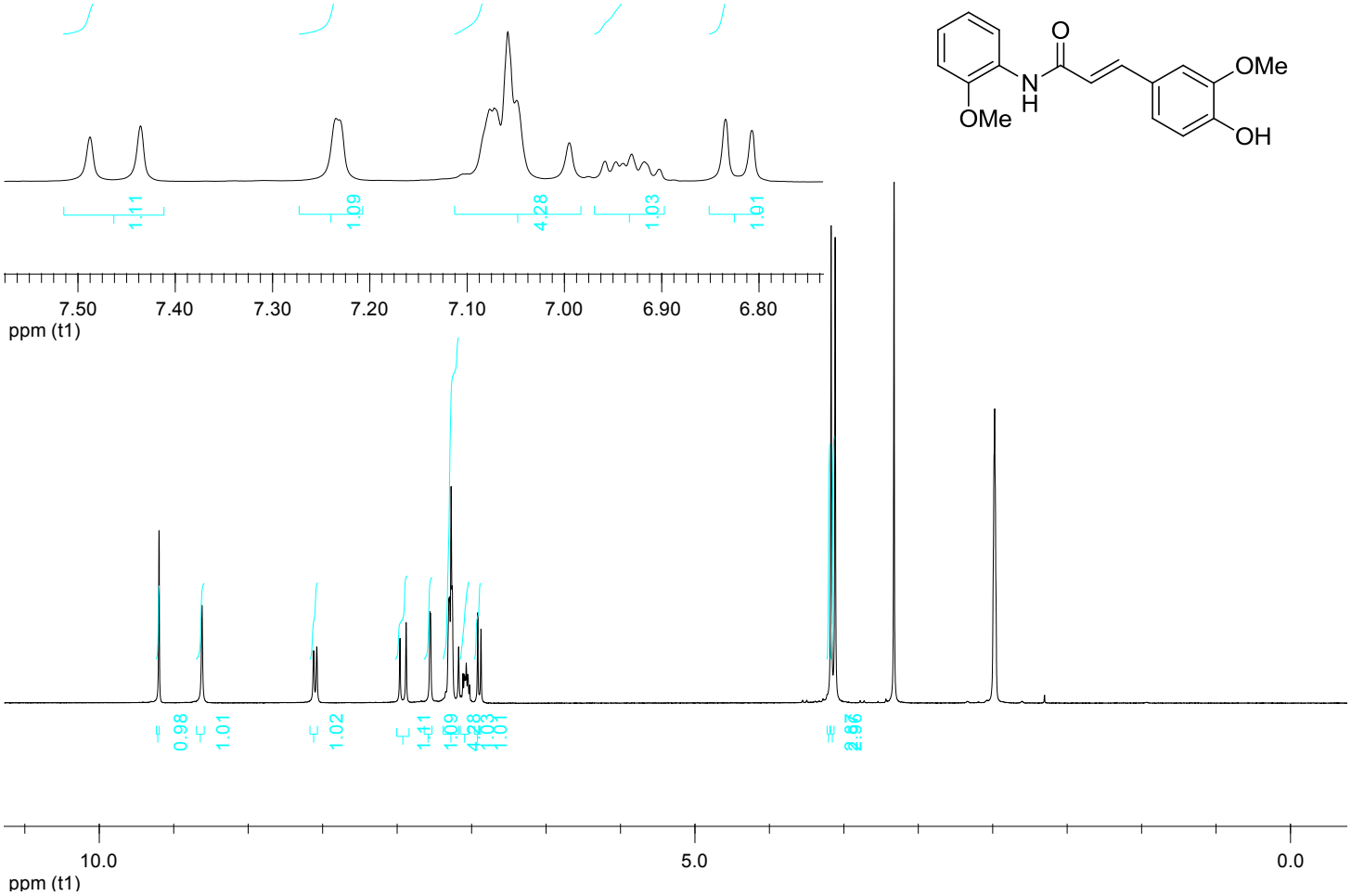
^{1}H NMR spectra of compound 12aK:



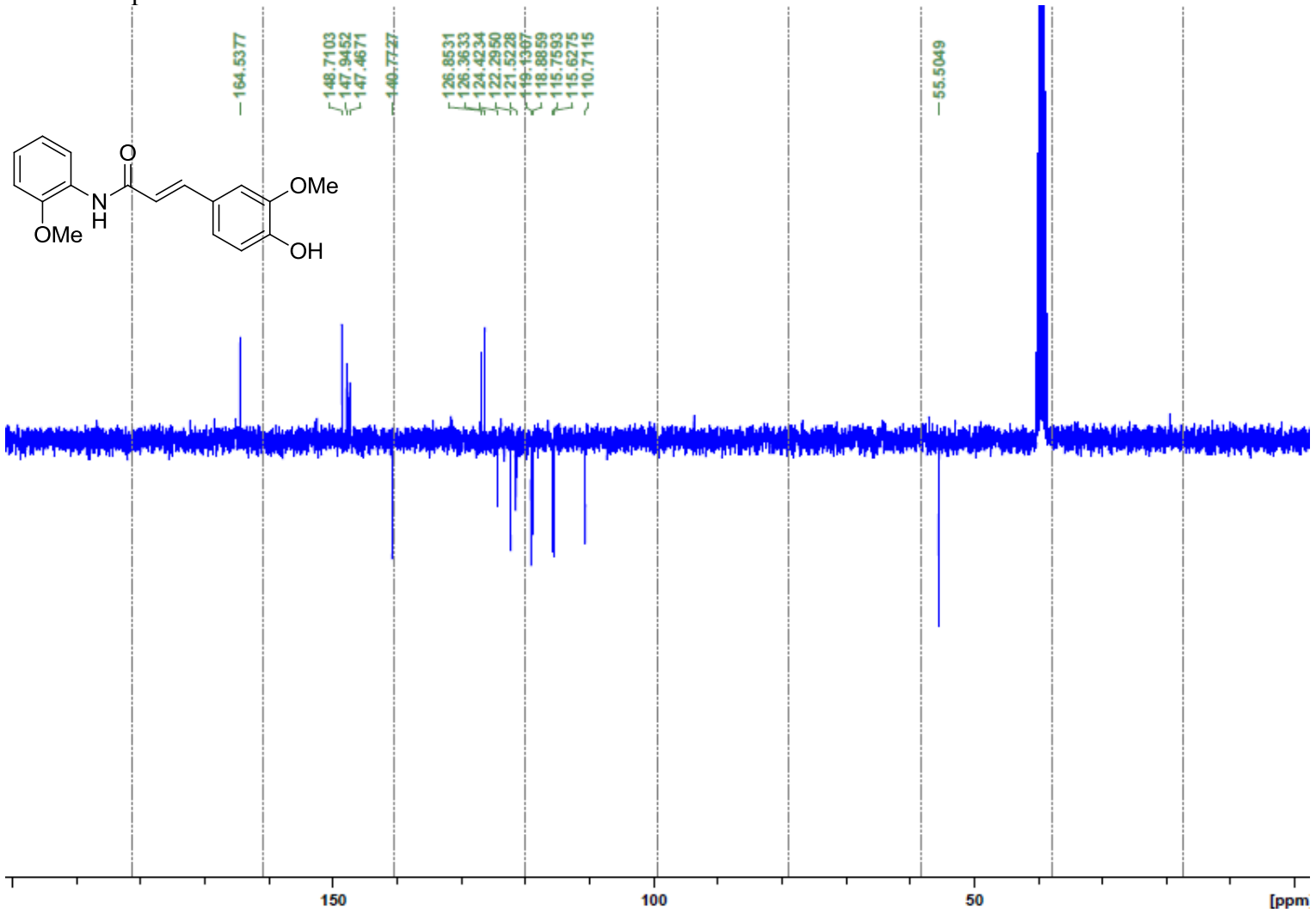
^{13}C NMR spectra of compound **12aK**:



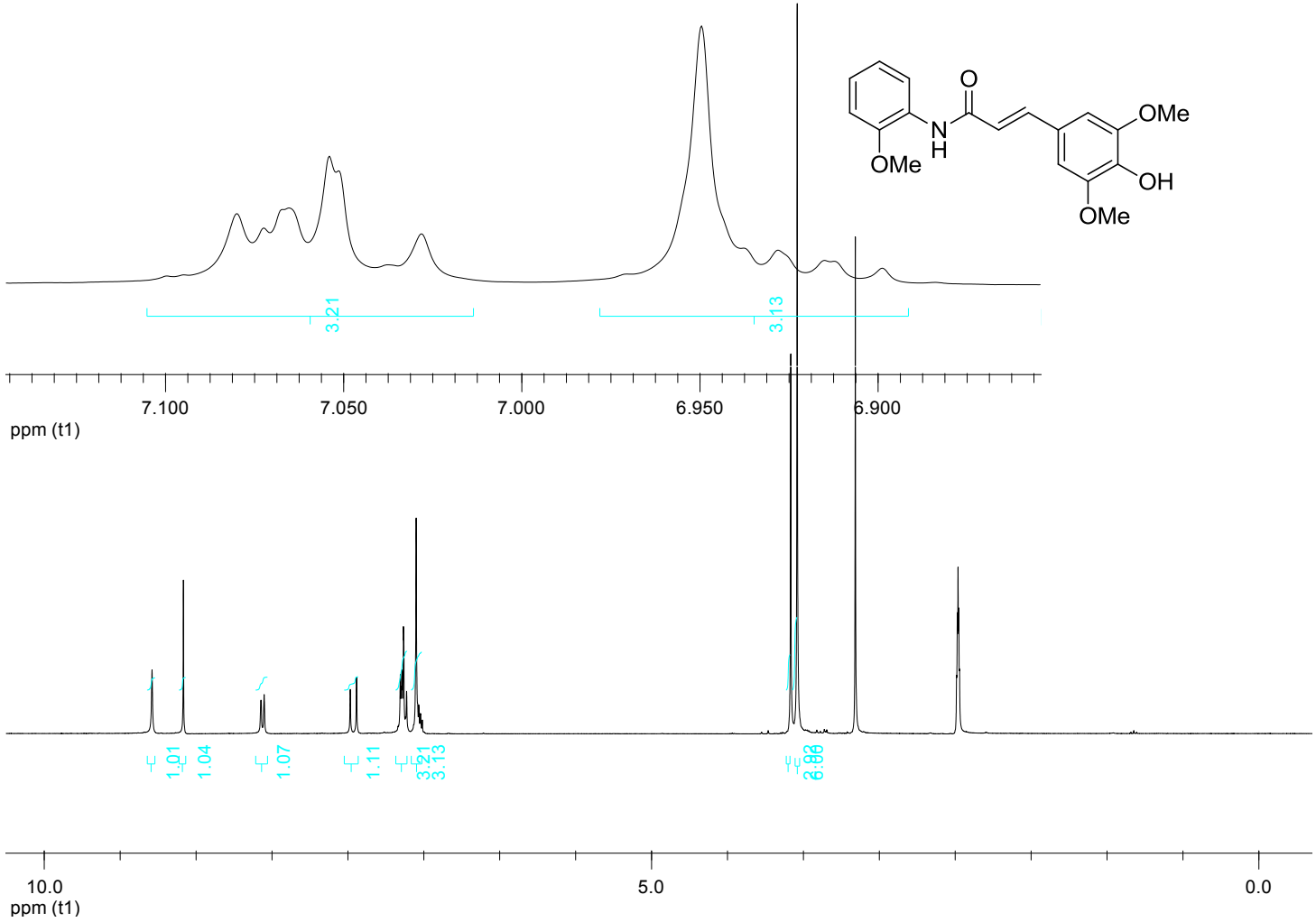
^{1}H NMR spectra of compound 12bA:



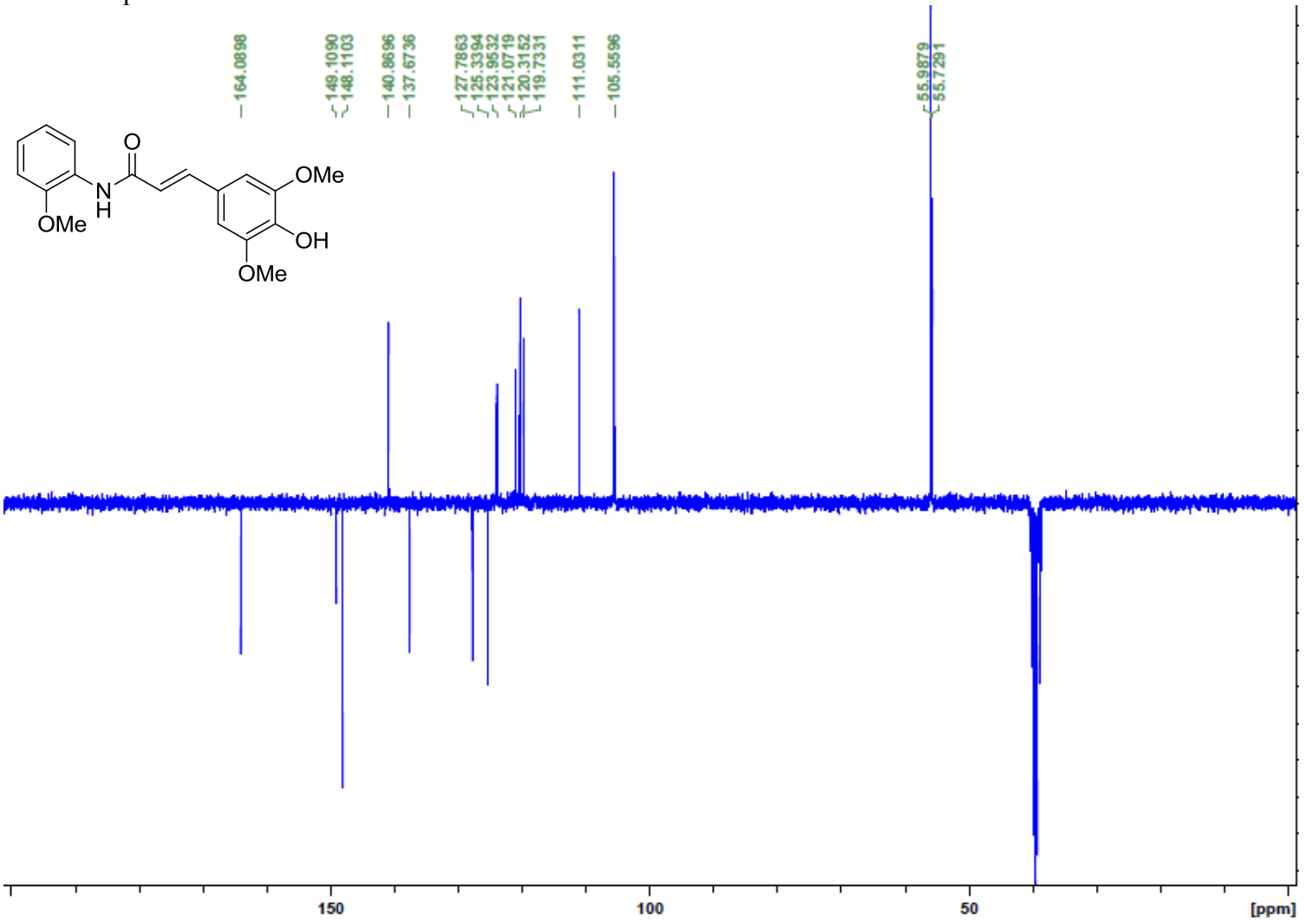
^{13}C NMR spectra of compound **12bA**:



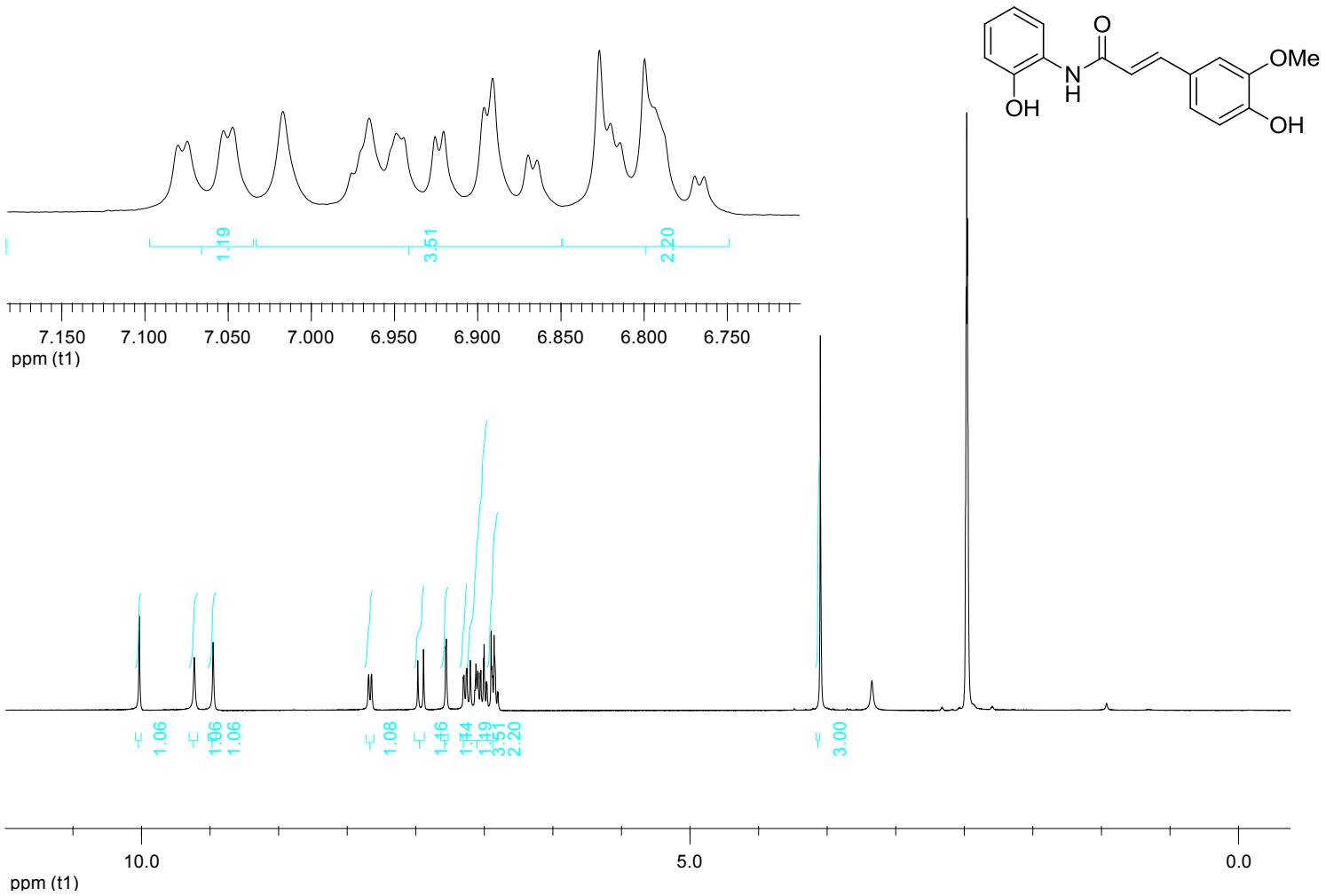
[1]H NMR spectra of compound 12bH:



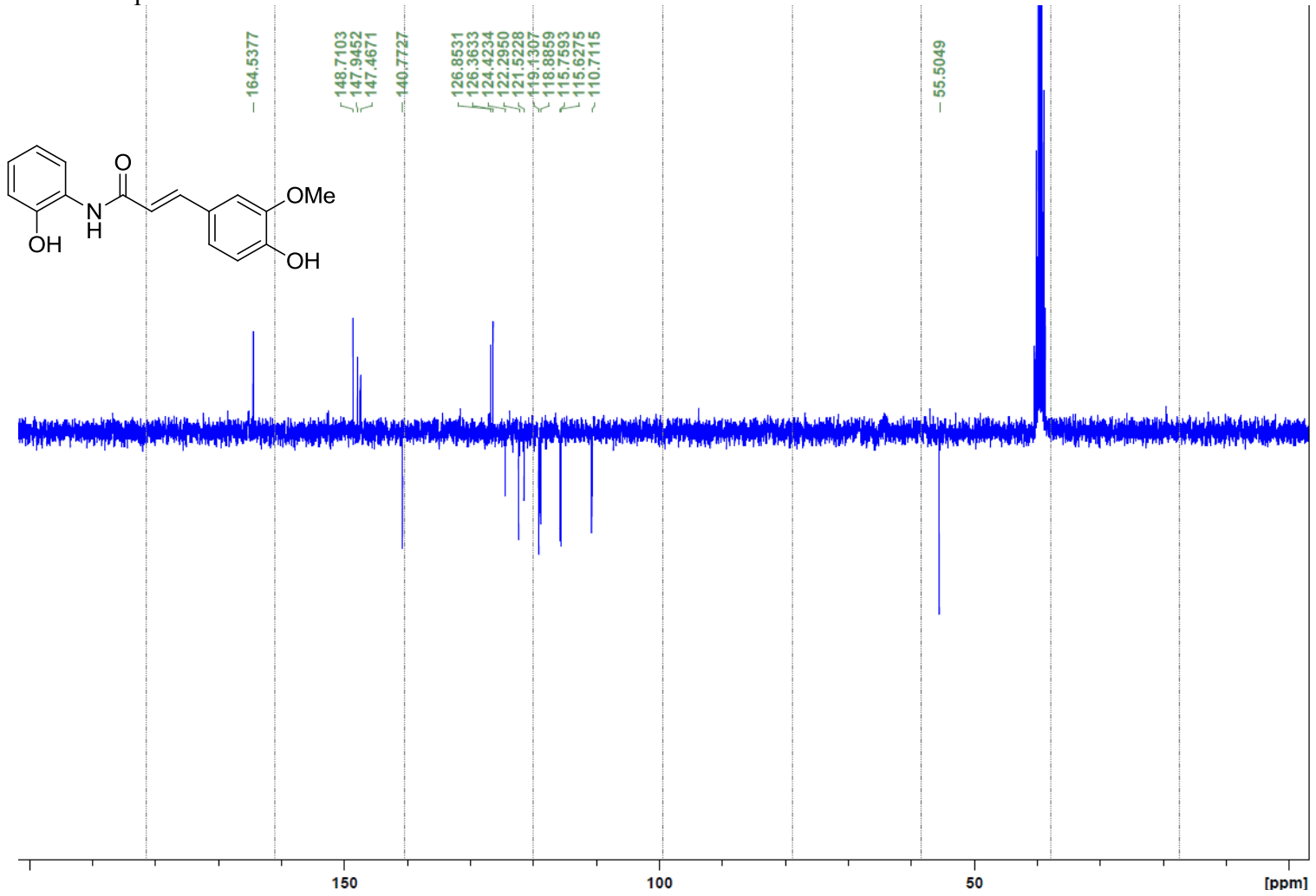
^{13}C NMR spectra of compound **12bH**:



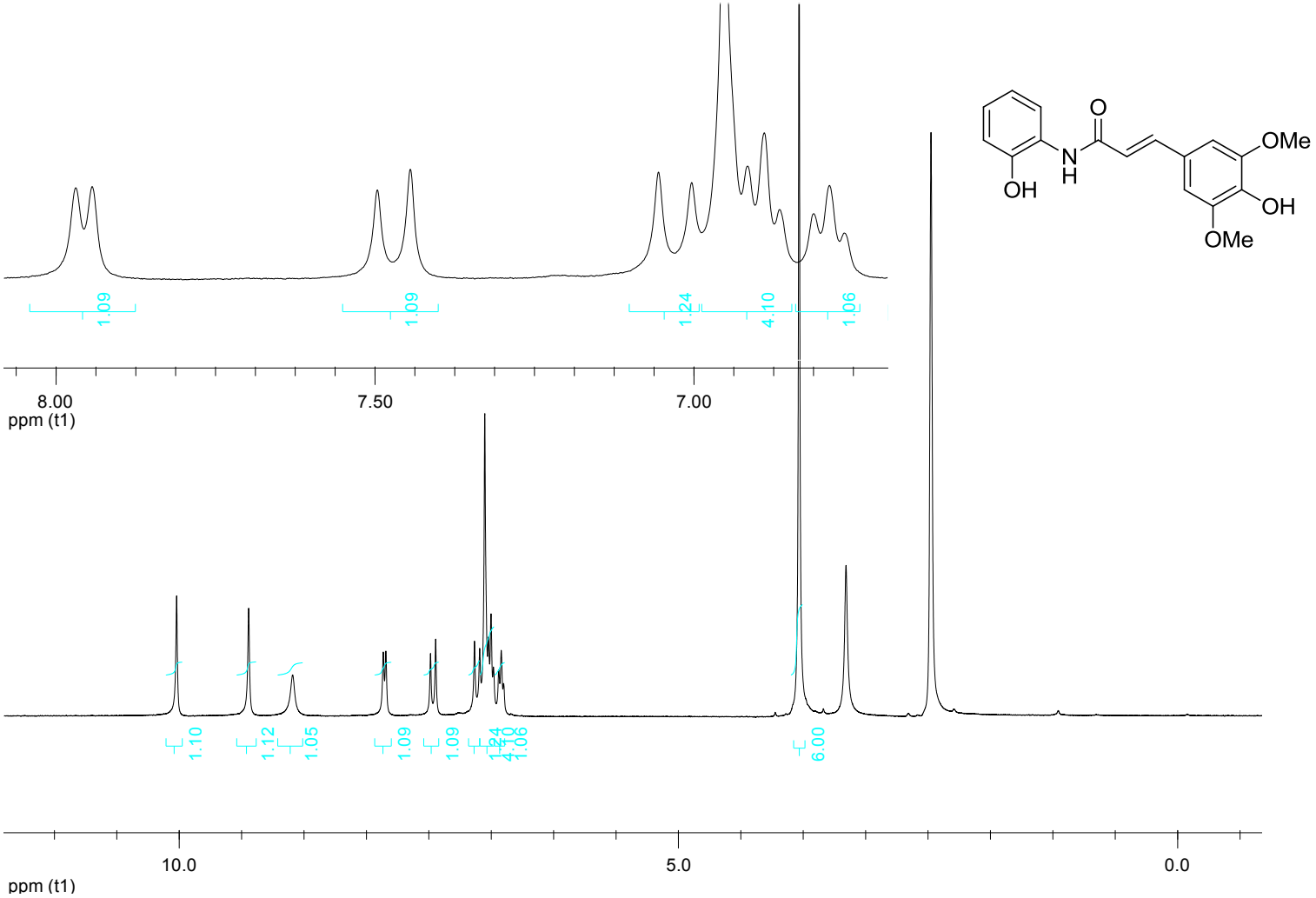
[1]H NMR spectra of compound 12cA:



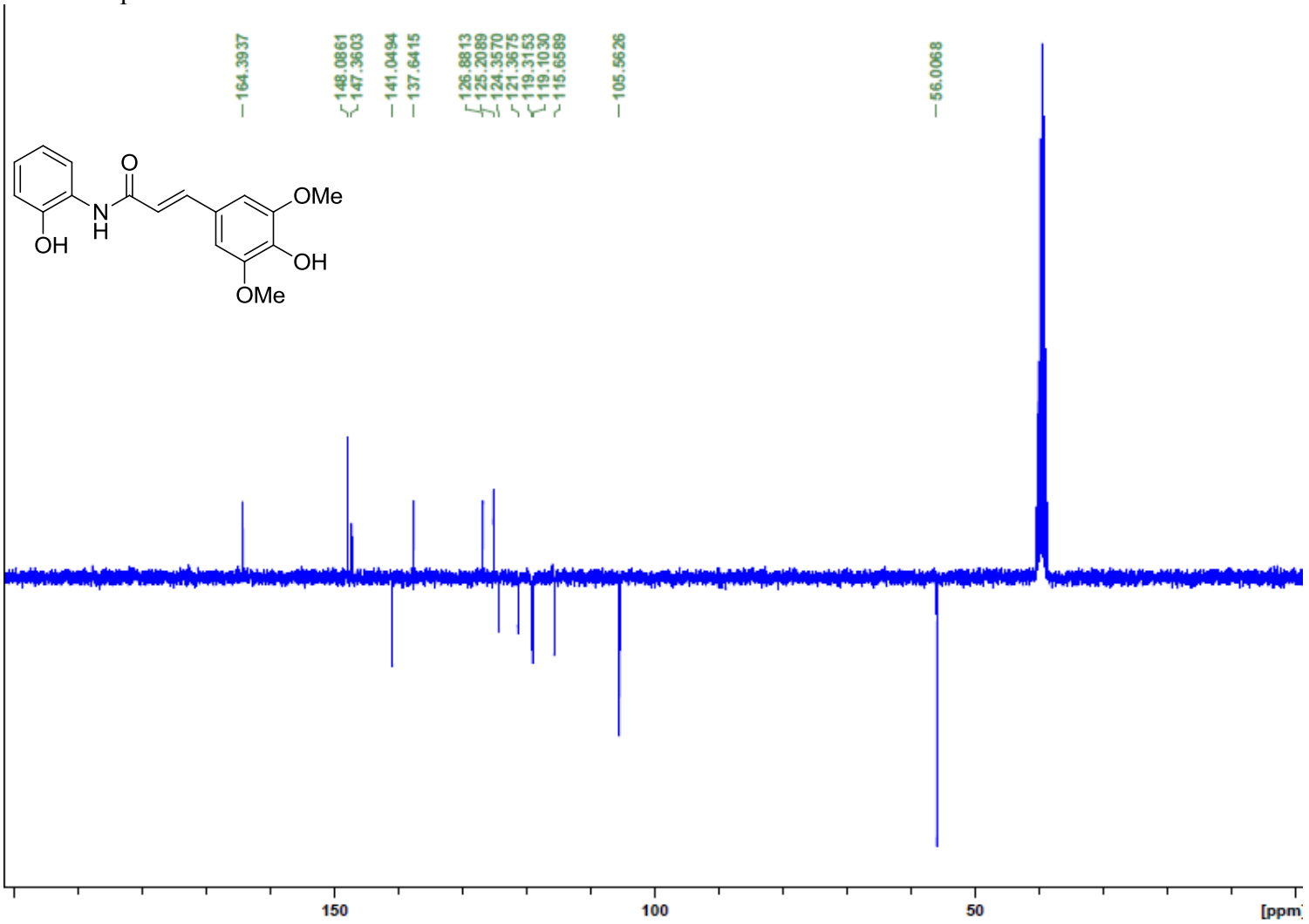
^{13}C NMR spectra of compound **12cA**:



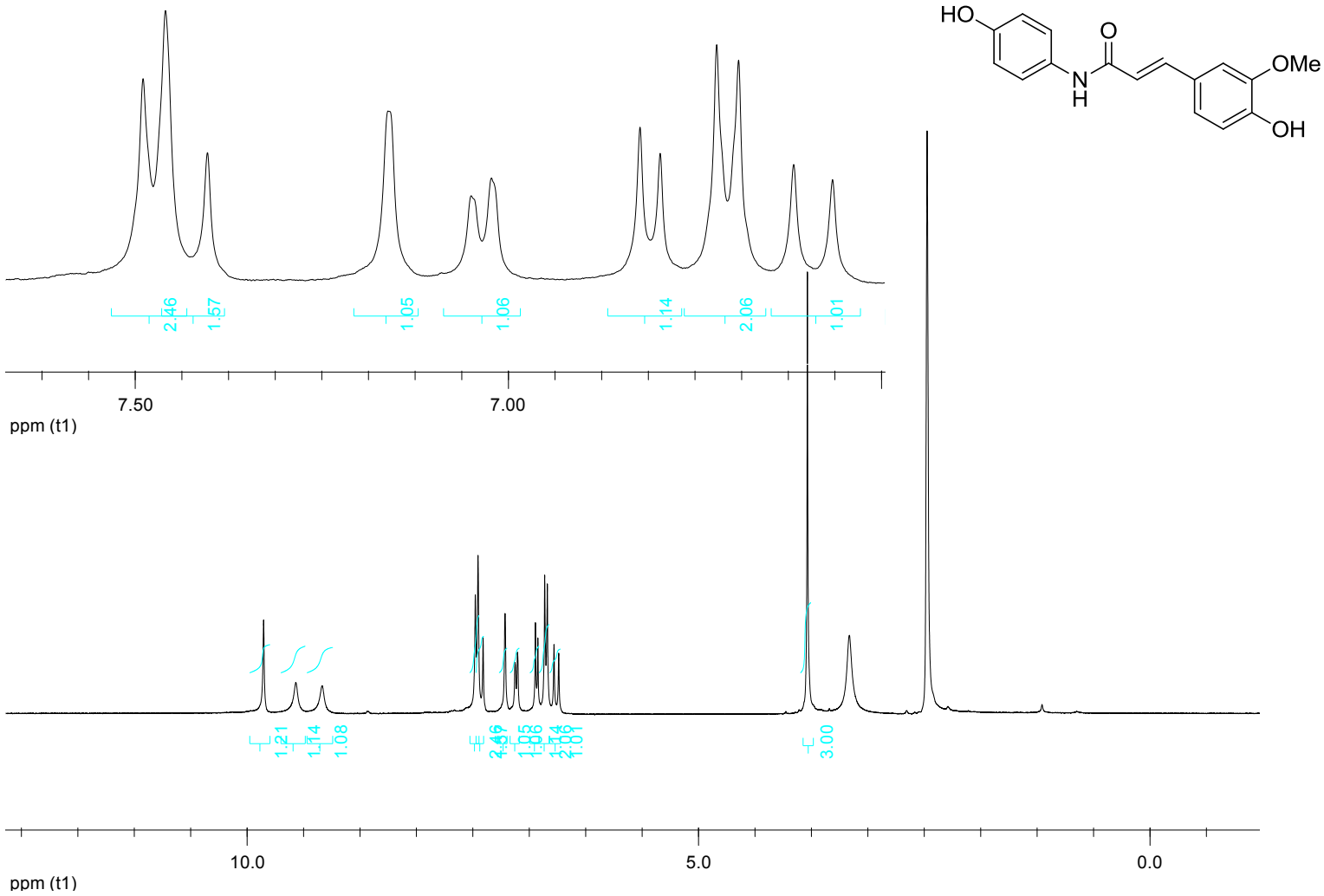
[1]H NMR spectra of compound 12cH:



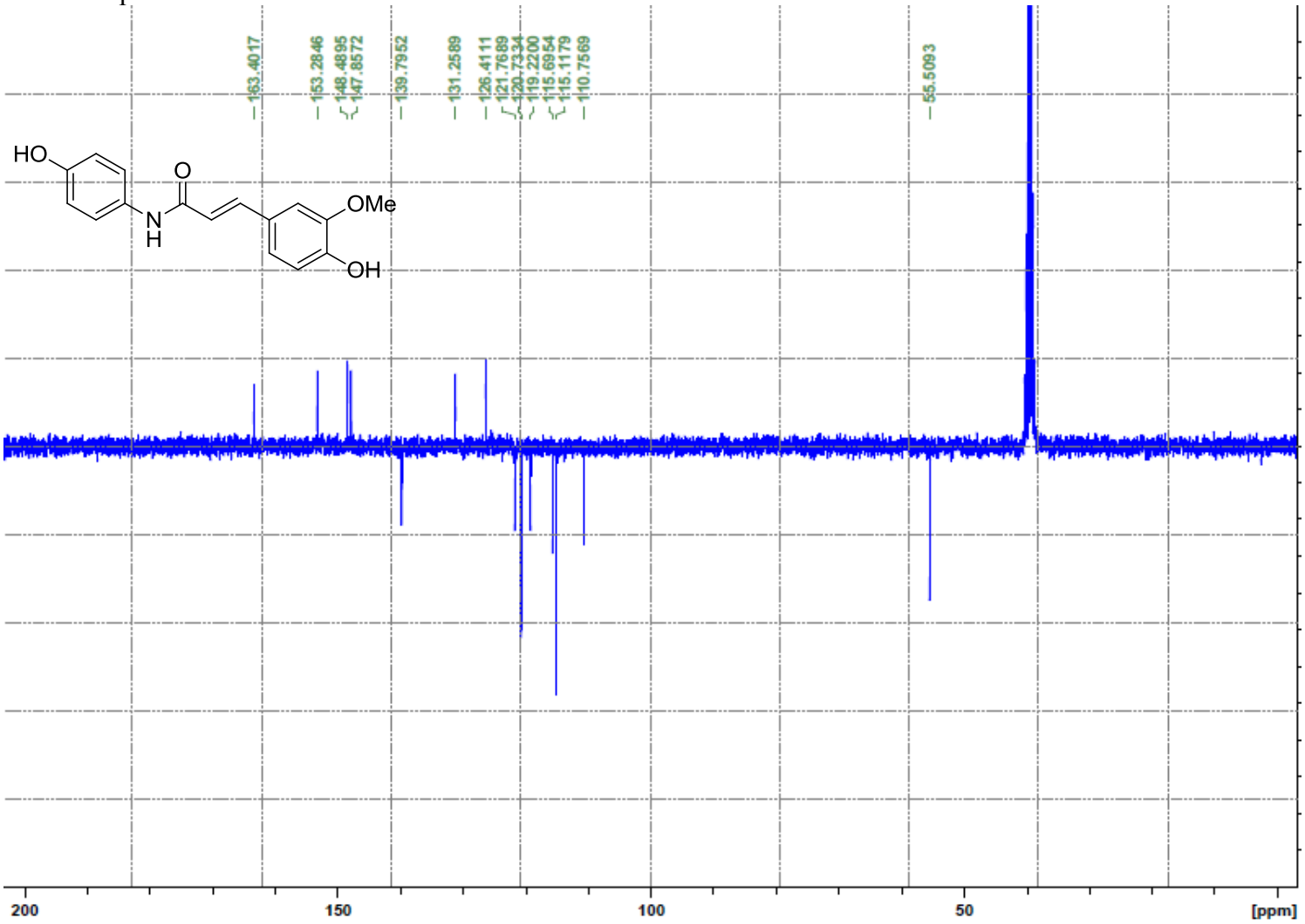
^{13}C NMR spectra of compound **12cH**:



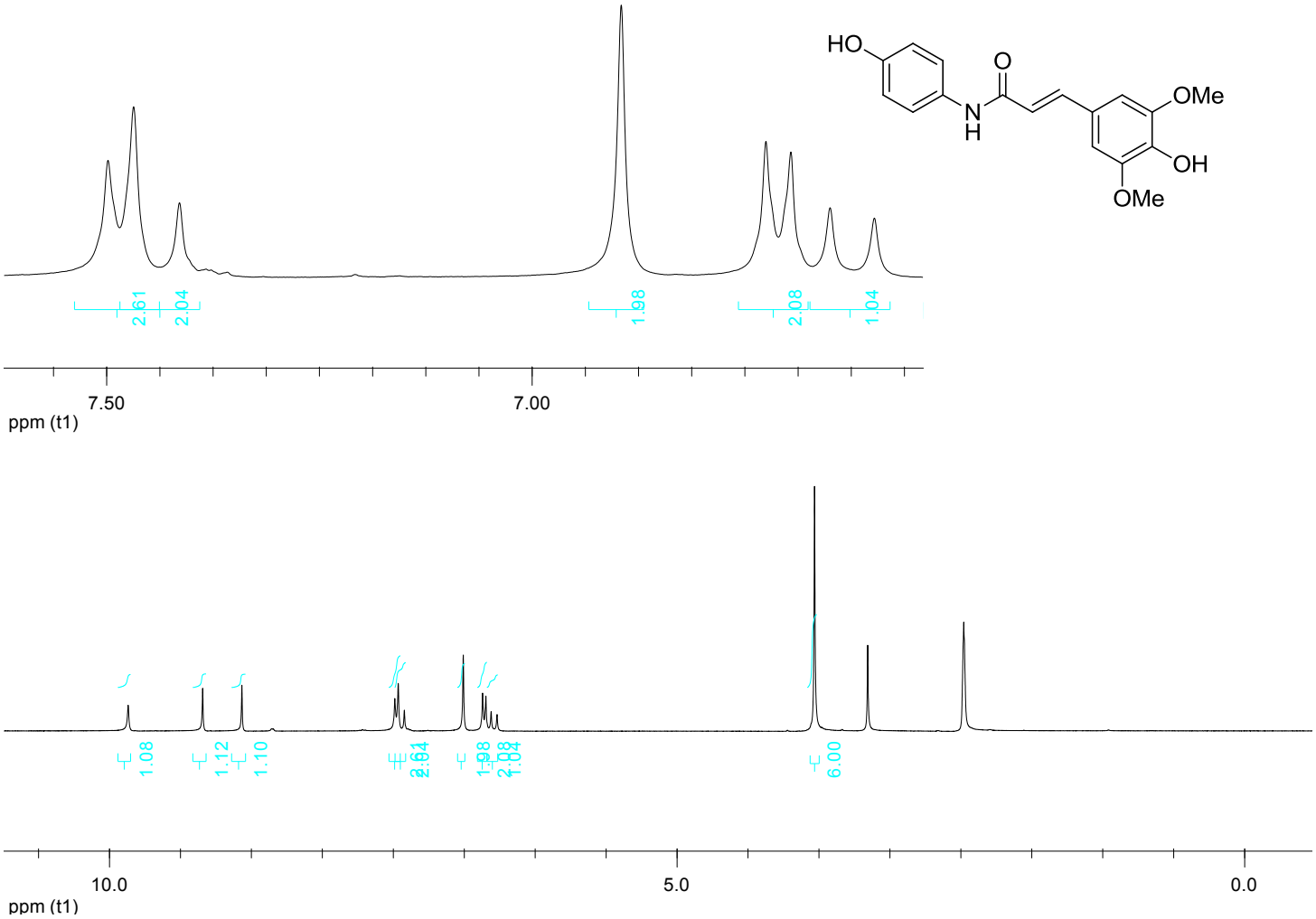
^{1}H NMR spectra of compound 12dA:



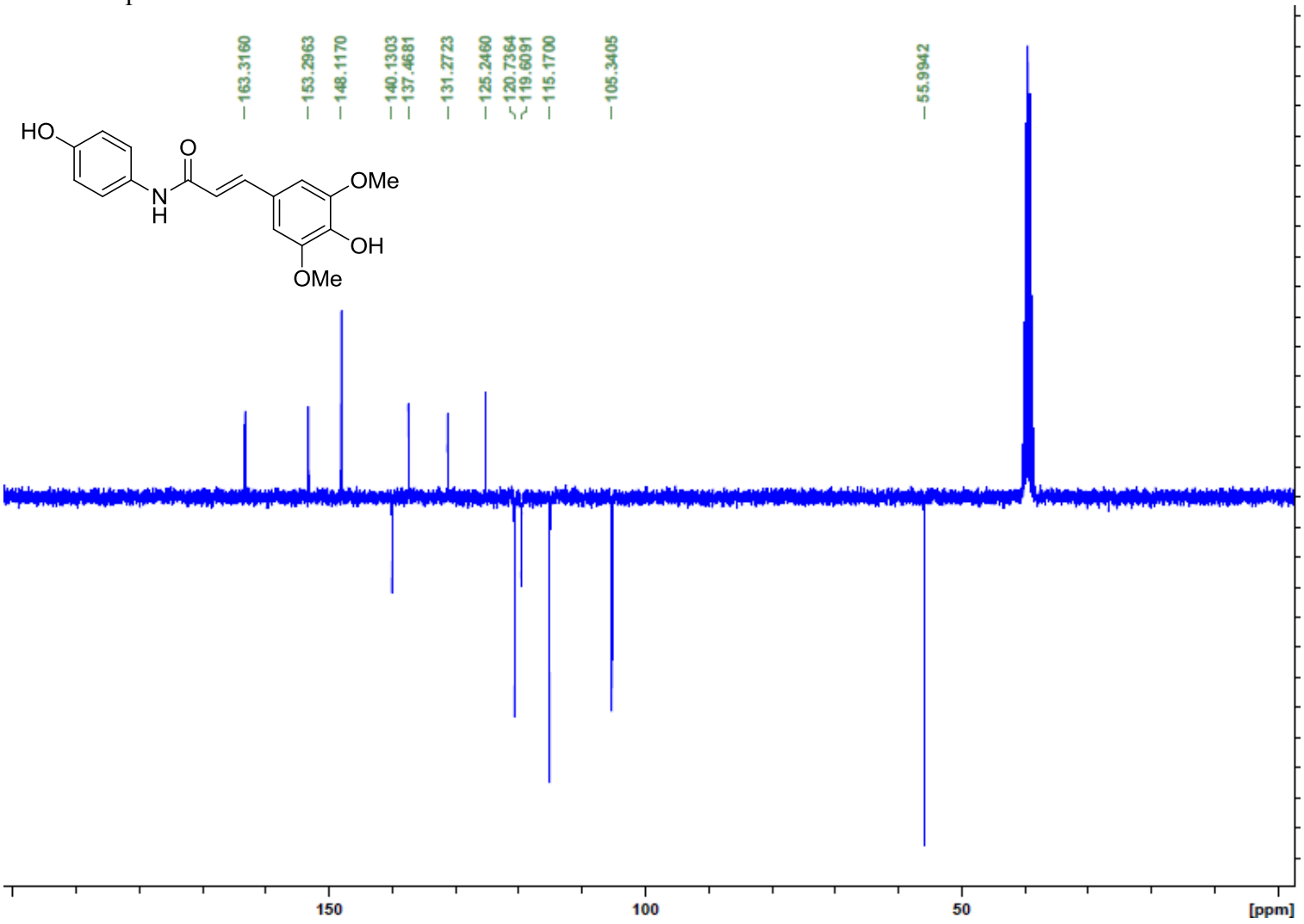
^{13}C NMR spectra of compound **12dA**:



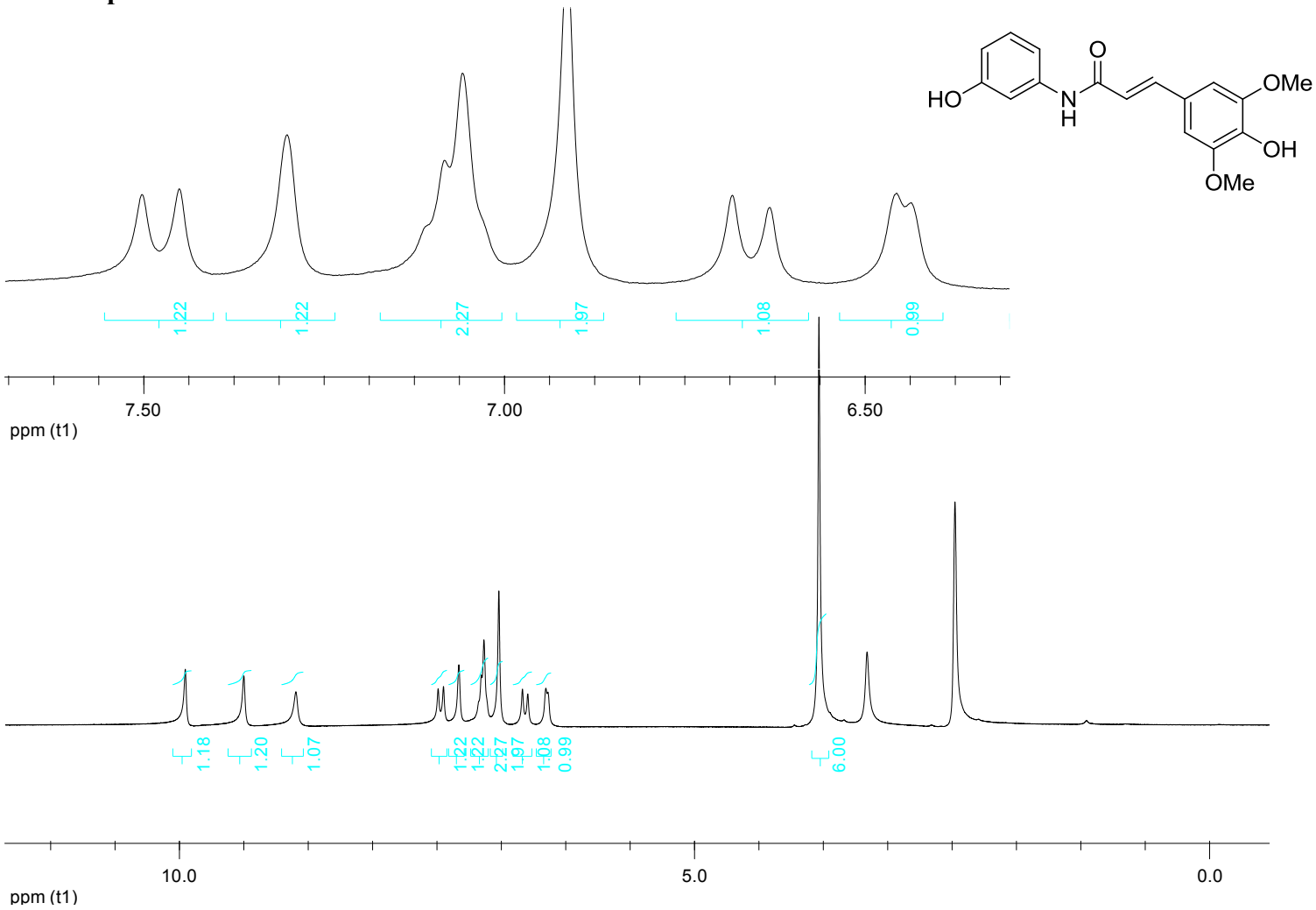
^{1}H NMR spectra of compound 12dH:



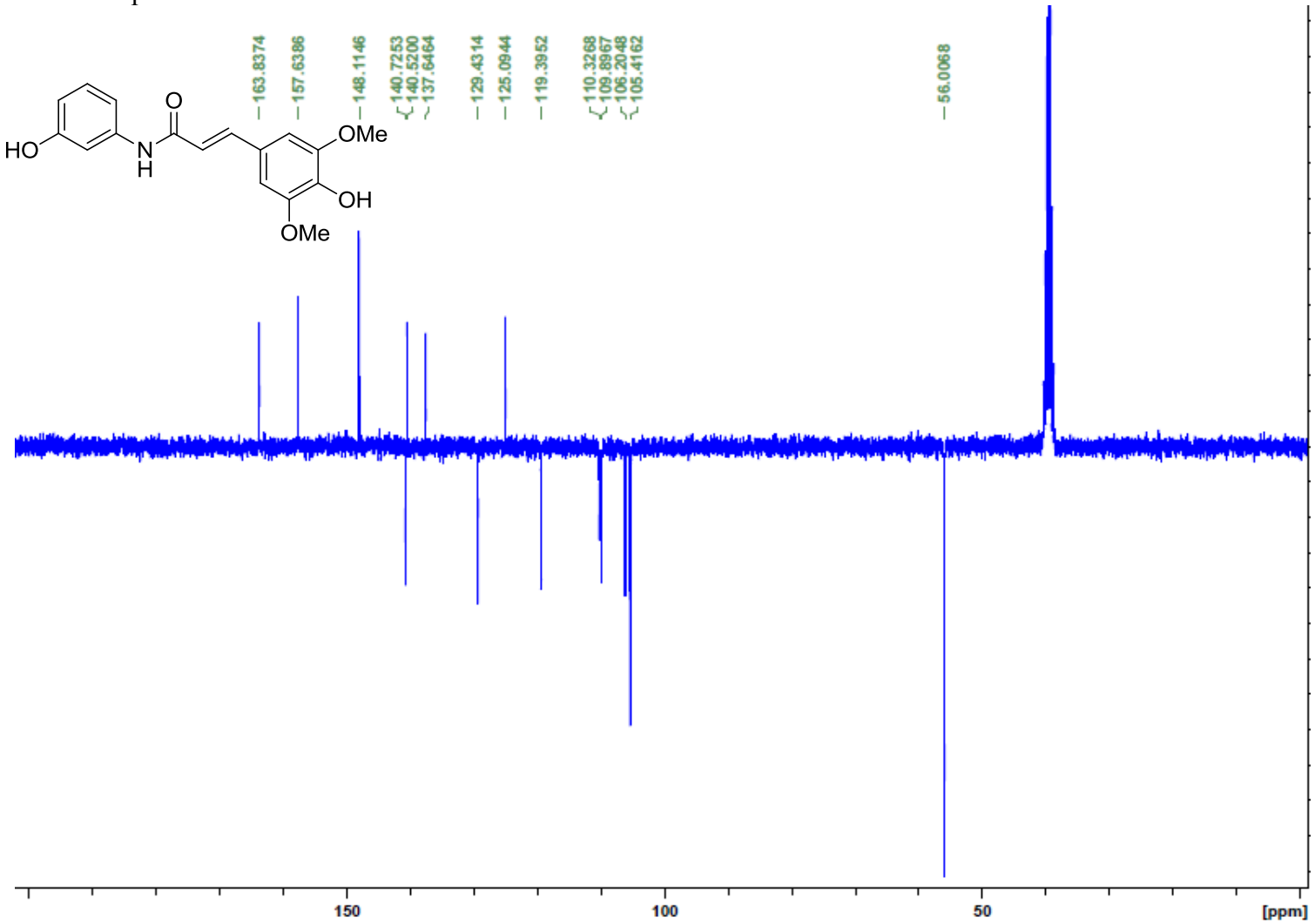
^{13}C NMR spectra of compound **12dH**:



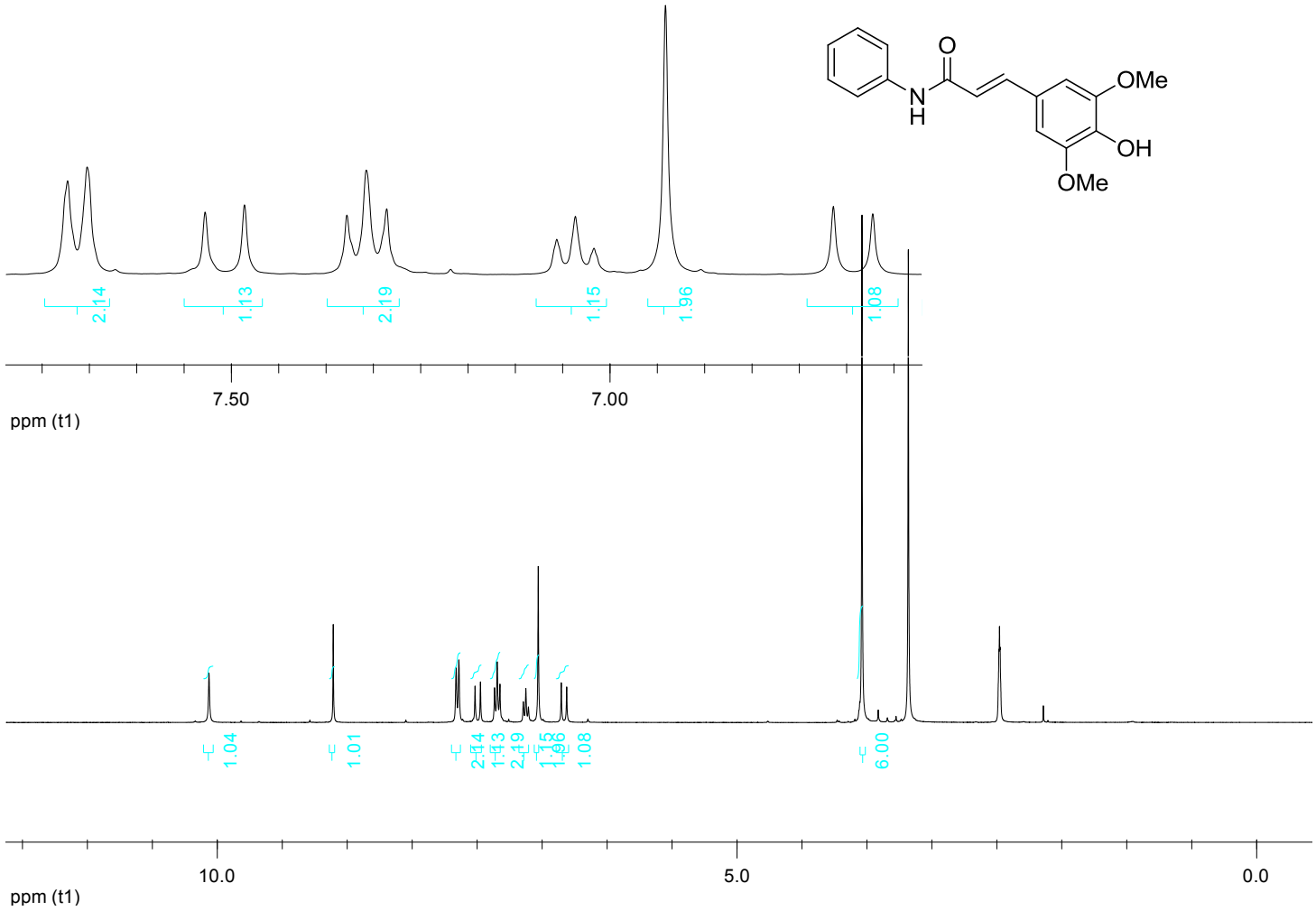
^{1}H NMR spectra of compound 12eH:



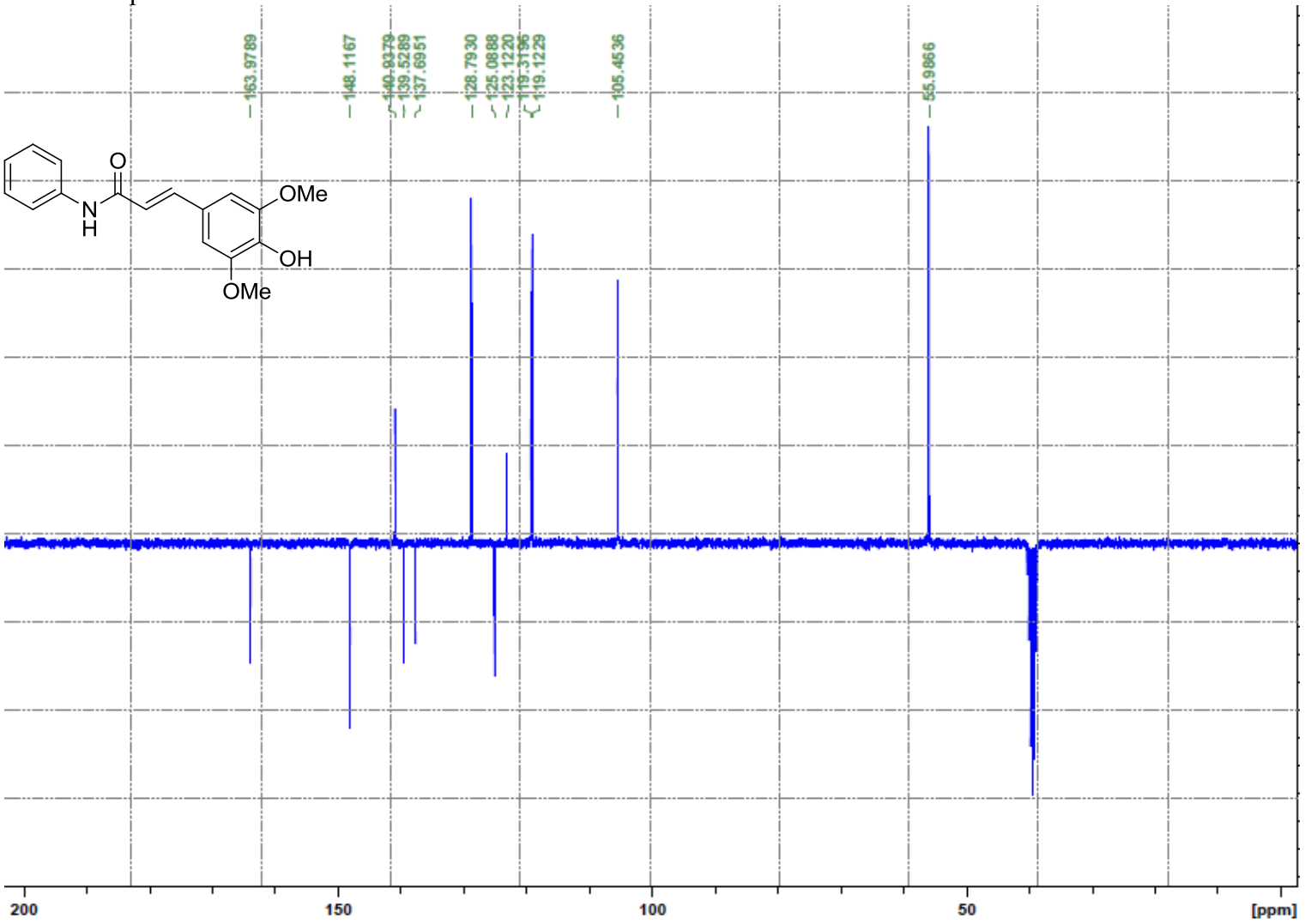
^{13}C NMR spectra of compound **12eH**:



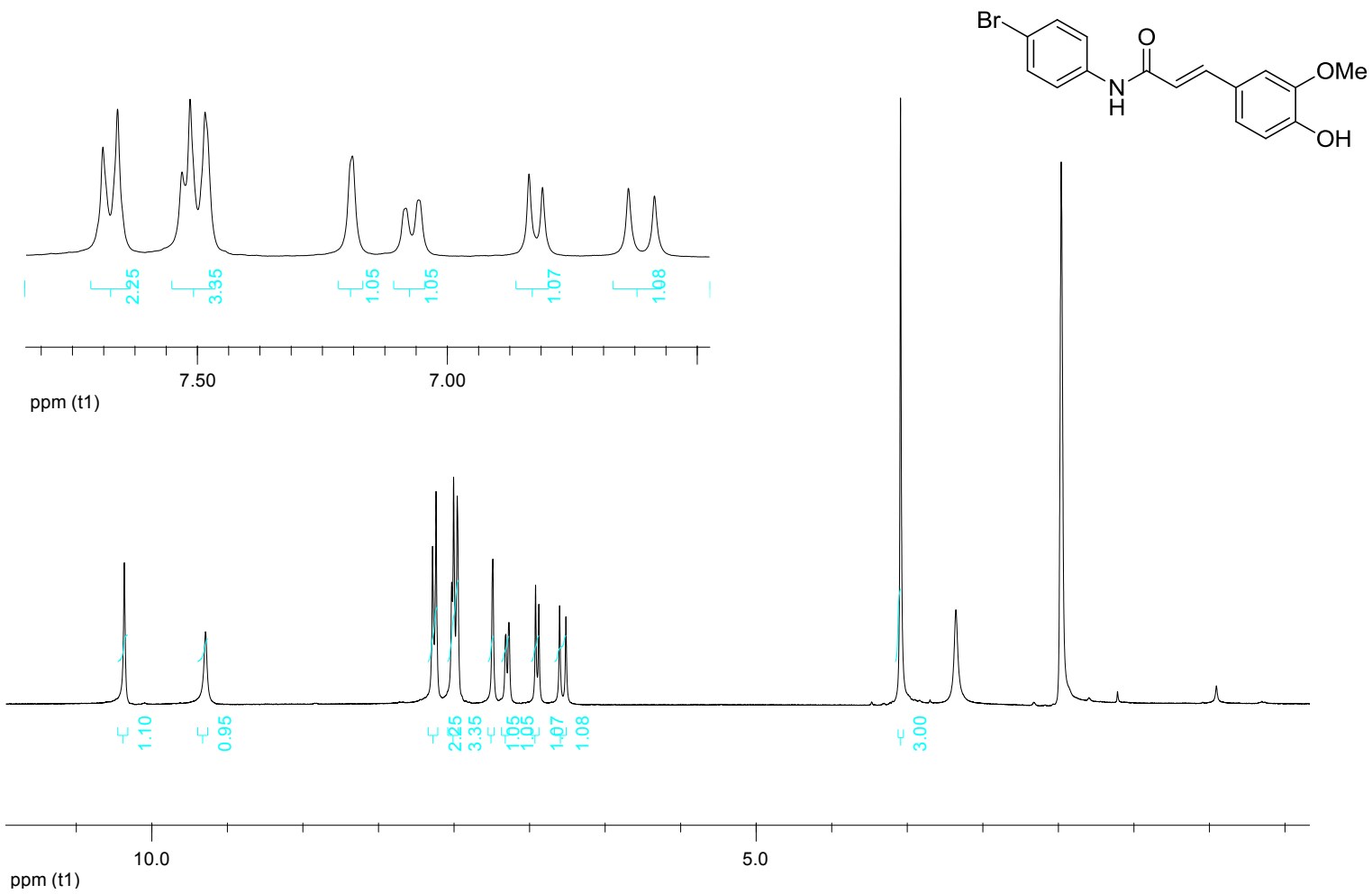
^{1}H NMR spectra of compound 12fH:



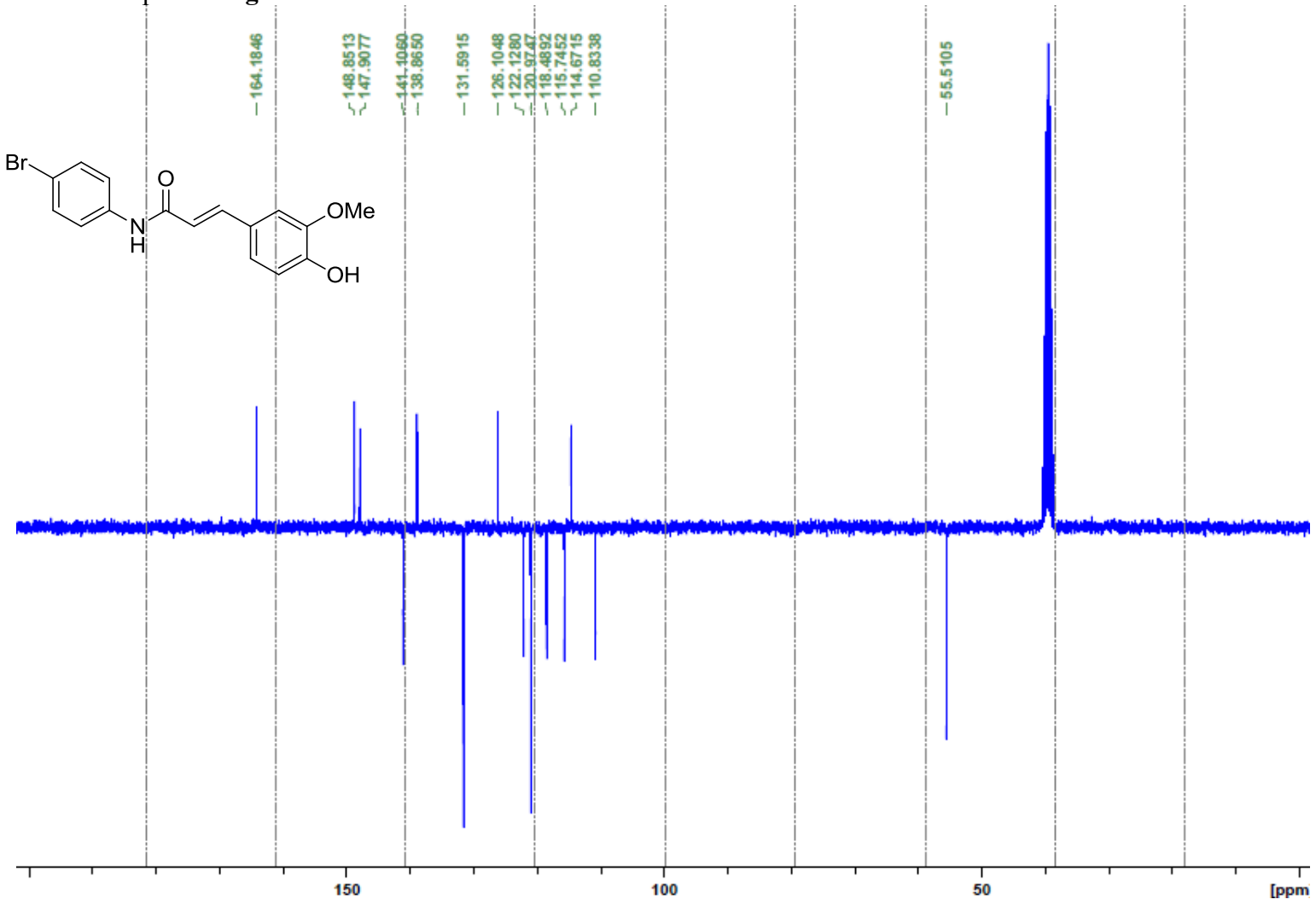
^{13}C NMR spectra of compound **12fH**:



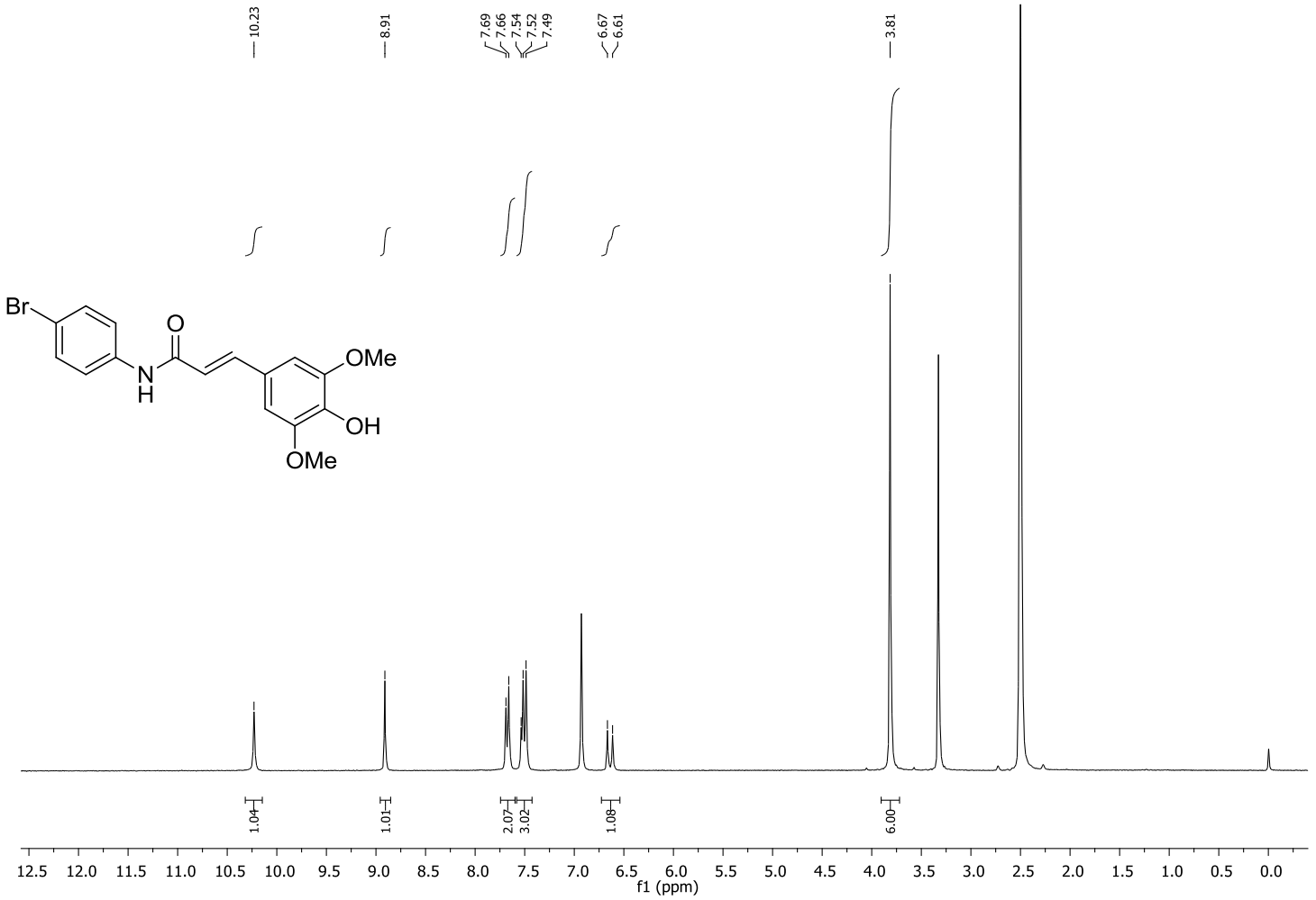
^{1}H NMR spectra of compound 12gA:



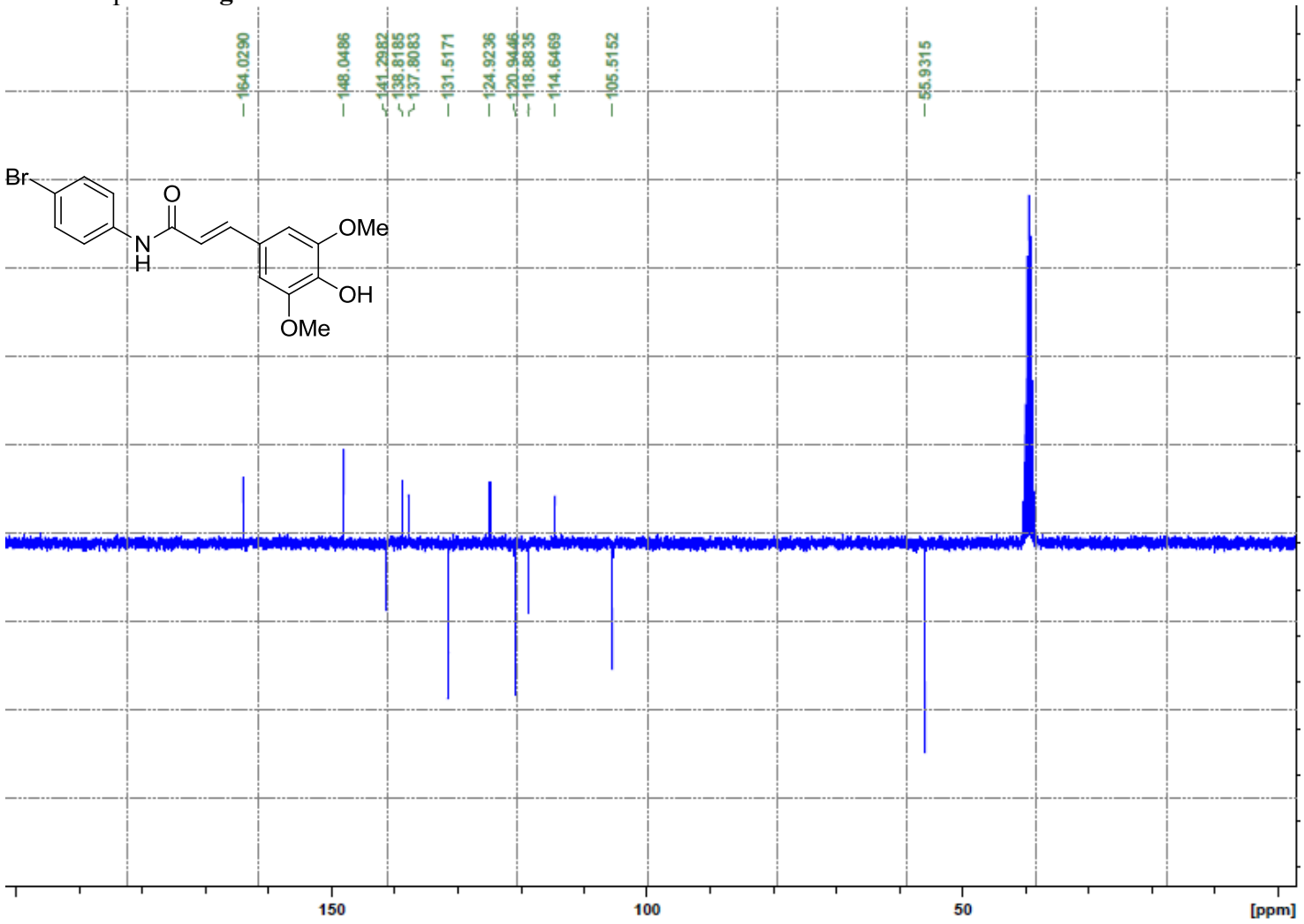
^{13}C NMR spectra of compound **12gA**:



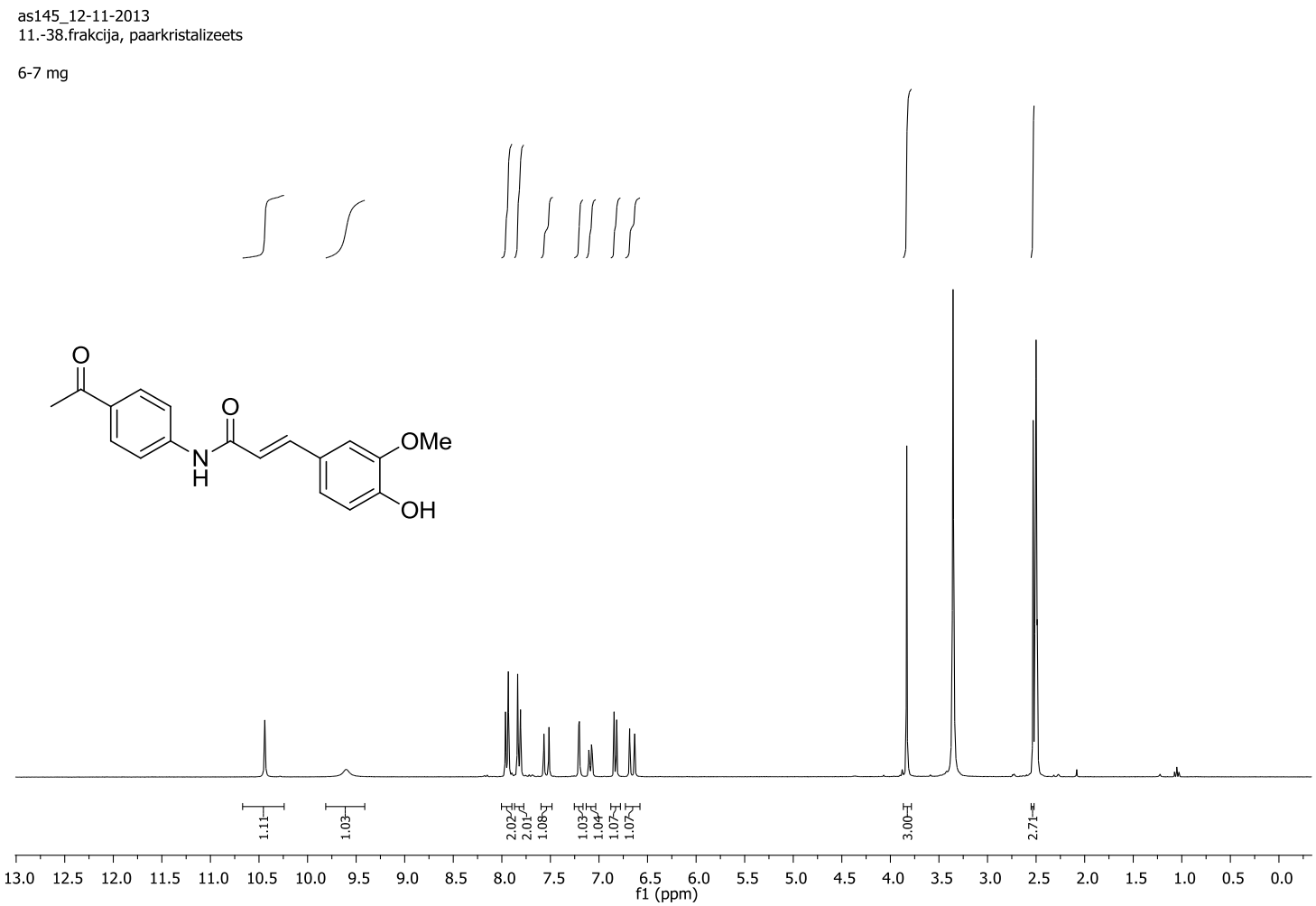
^{1}H NMR spectra of compound 12gH:



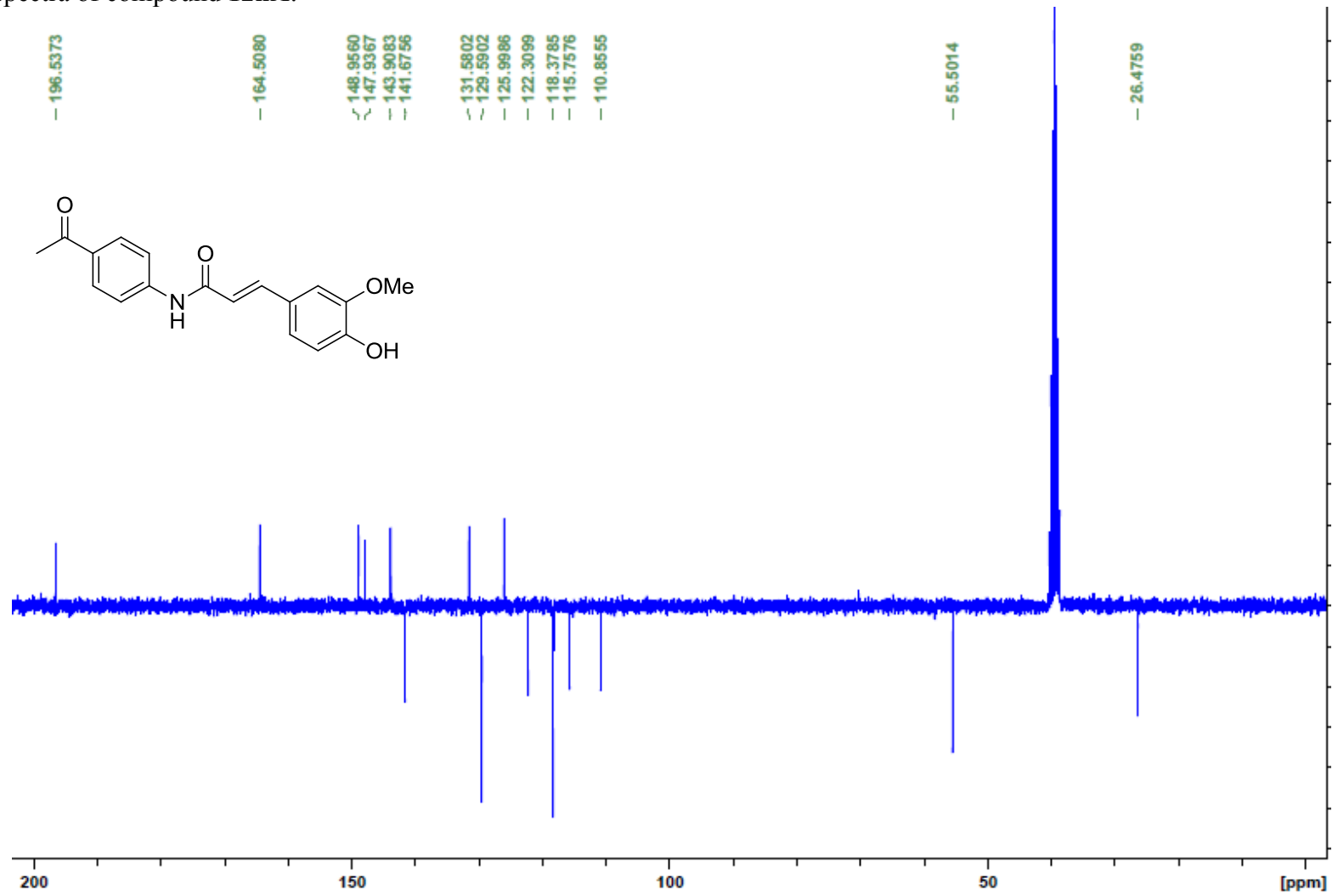
^{13}C NMR spectra of compound **12gH**:



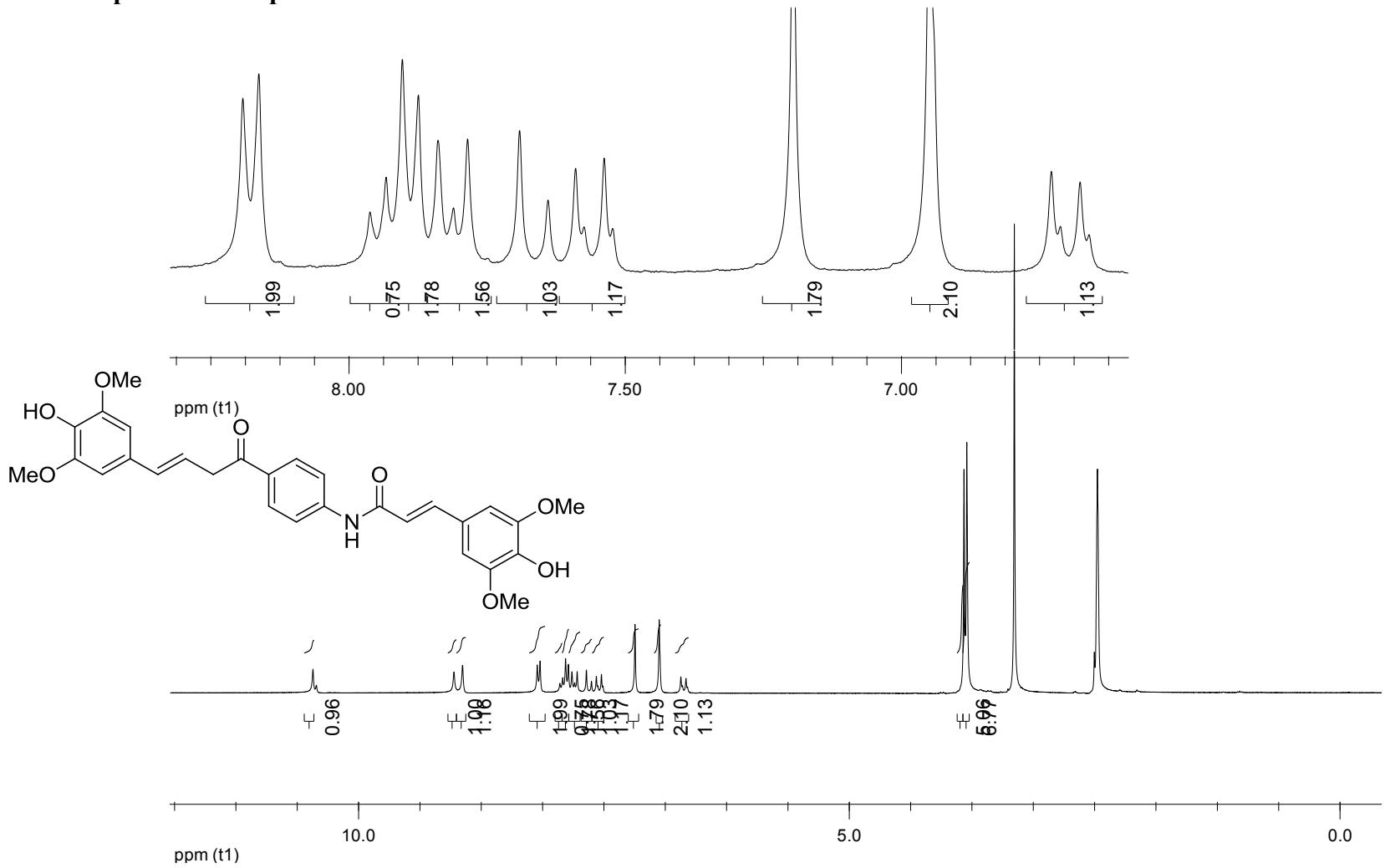
^{1}H NMR spectra of compound 12hA:



^{13}C NMR spectra of compound **12hA**:



[1]H NMR spectra of compound 12hH`:



^{13}C NMR spectra of compound **12hH`**: