

Supplementary information

Palladium-catalyzed/copper-mediated carbon-carbon cross-coupling reaction for synthesis of 6-unsubstituted 2-aryldihydropyrimidines

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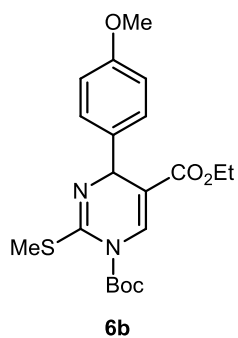
^c*Graduate School of Pharmaceutical Sciences, Tohoku University, 6-3 Aoba, Aramaki, Aoba-ku, Sendai 980-8578, Japan.*

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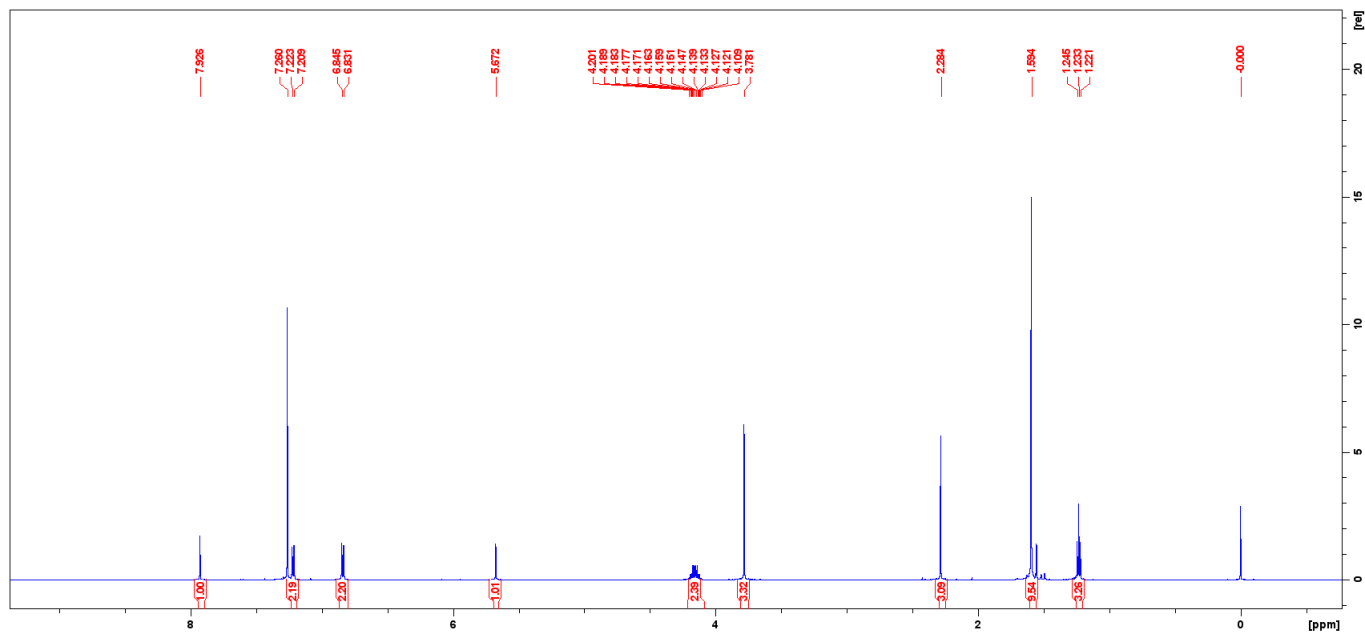
^1H and ^{13}C spectra

Compound 6b	4
Compound 6c	5
Compound 6d	6
Compound 6e	7
Compound 6f	8
Compound 6g	9
Compound 6i	10
Compound 7a	11
Compound 7b	12
Compound 7c	13
Compound 7d	14
Compound 7e	15
Compound 7f	16
Compound 7g	17
Compound 7h	18
Compound 7i	19
Compound 7j	20
Compound 7k	21
Compound 7l	22
Compound 7m	23
Compound 7n	24
Compound 7o	25
Compound 7p	26
Compound 7q	27

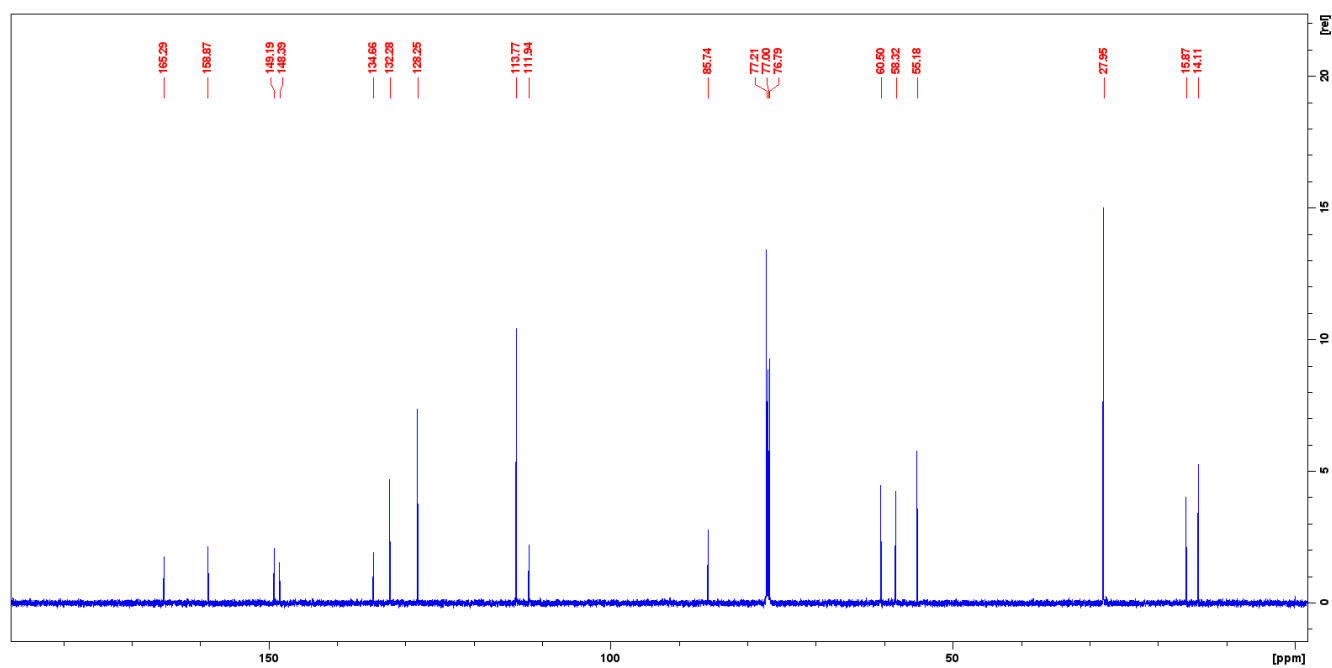
Compound 7r	28
Compound 7s	29
Compound 7t	30
Compound 7u	31
Compound 9	32
Compounds 10a and 11a	34
Compounds 10b and 11b	37
Compounds 10g and 11g	40

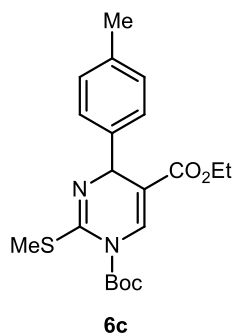


^1H NMR (600 MHz, CDCl_3) spectrum of **6b**.

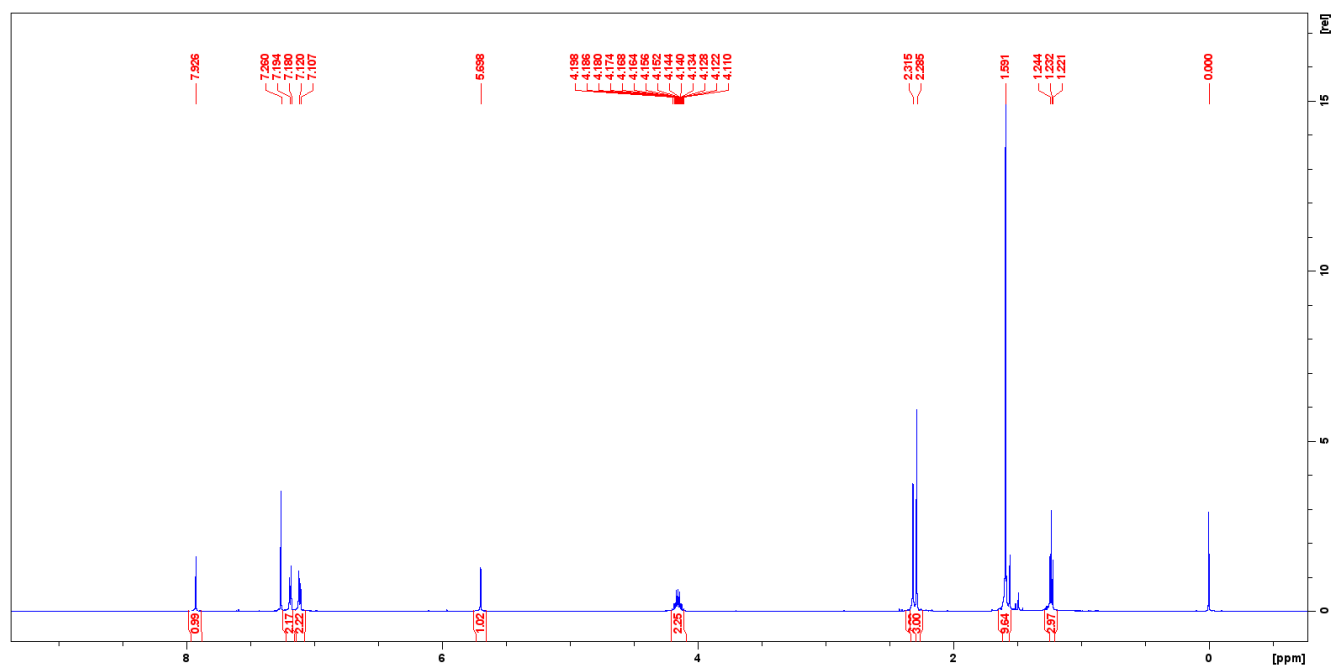


^{13}C NMR (150 MHz, CDCl_3) spectrum of **6b**.

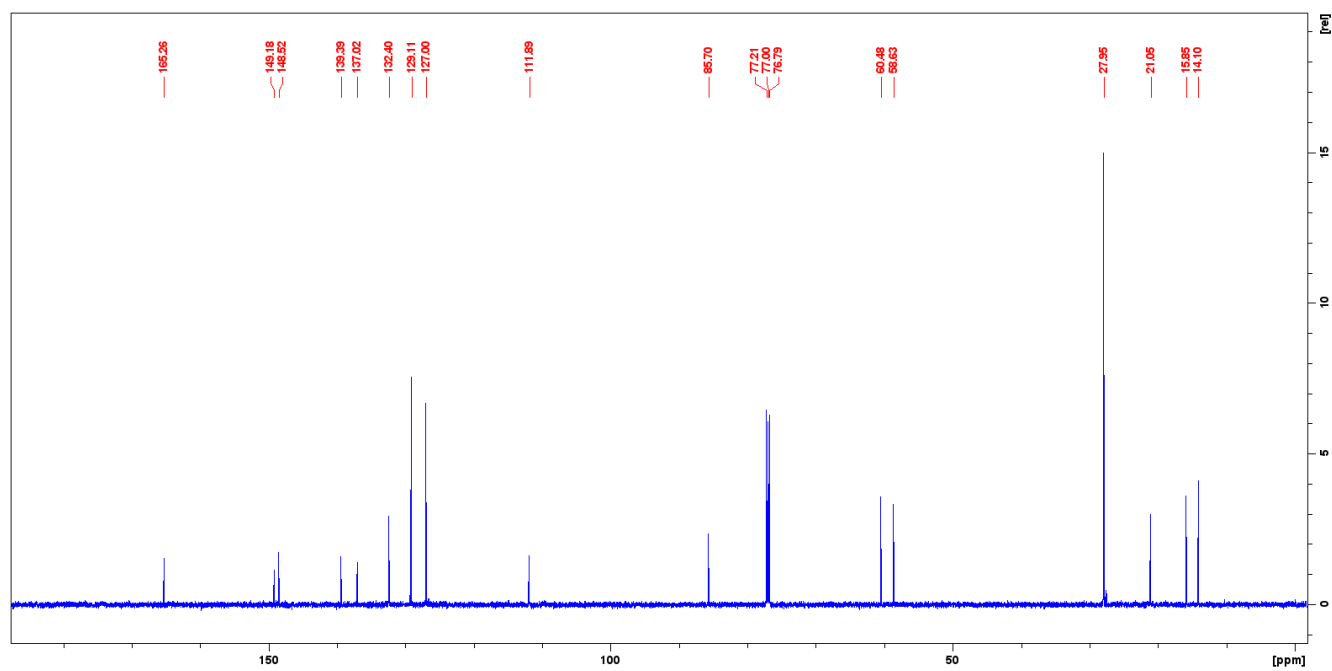


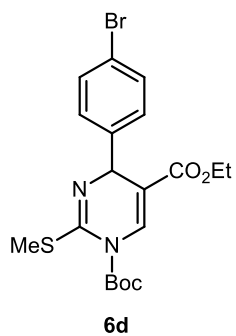


^1H NMR (600 MHz, CDCl_3) spectrum of **6c**.

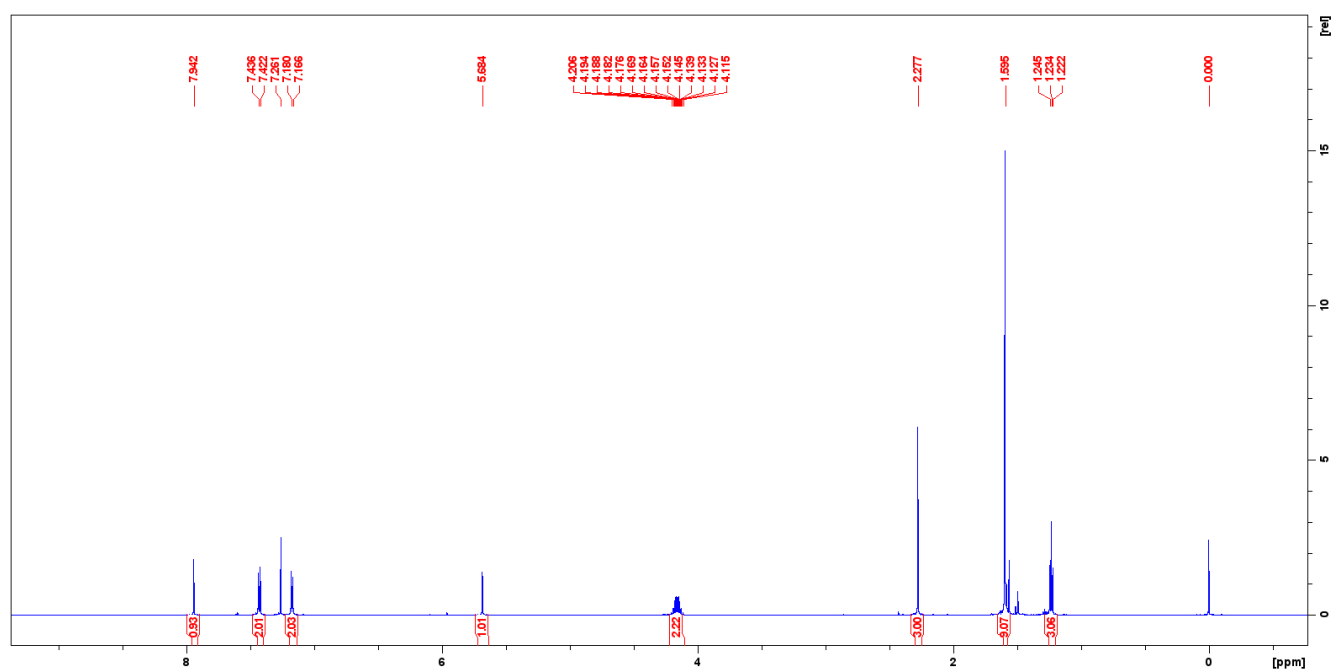


^{13}C NMR (150 MHz, CDCl_3) spectrum of **6c**.

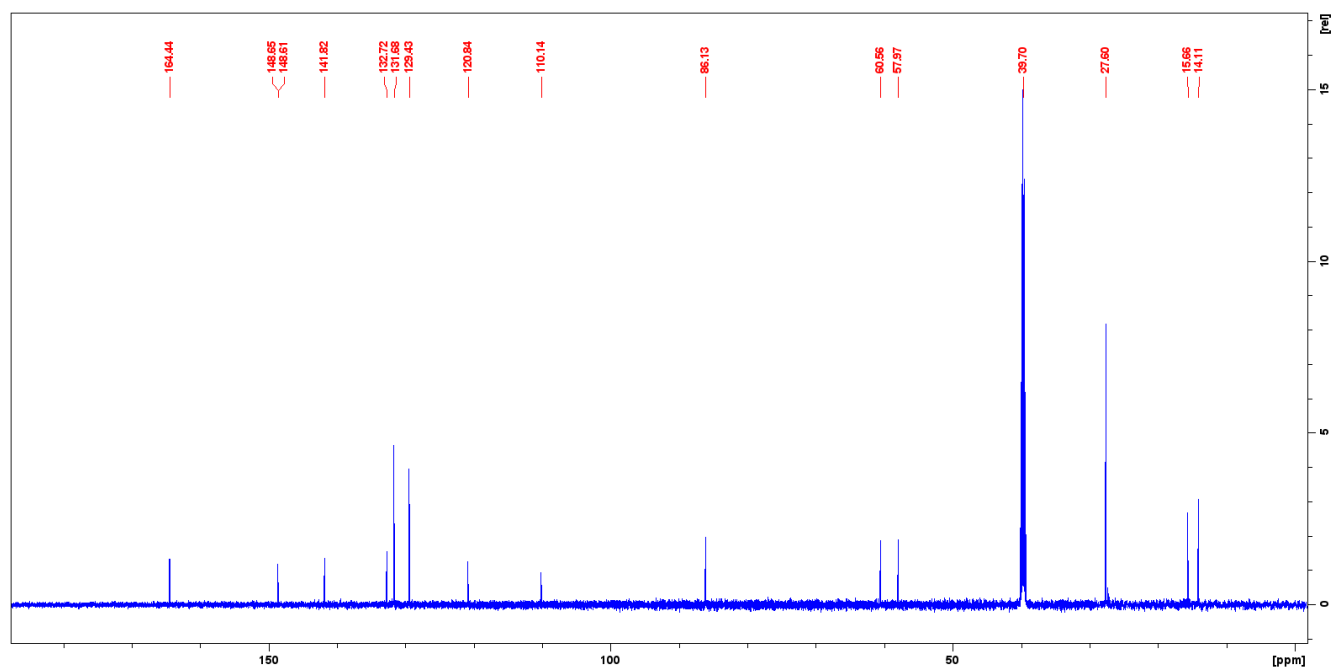


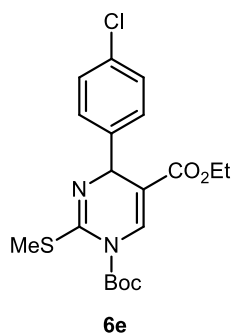


^1H NMR (600 MHz, CDCl_3) spectrum of **6d**.

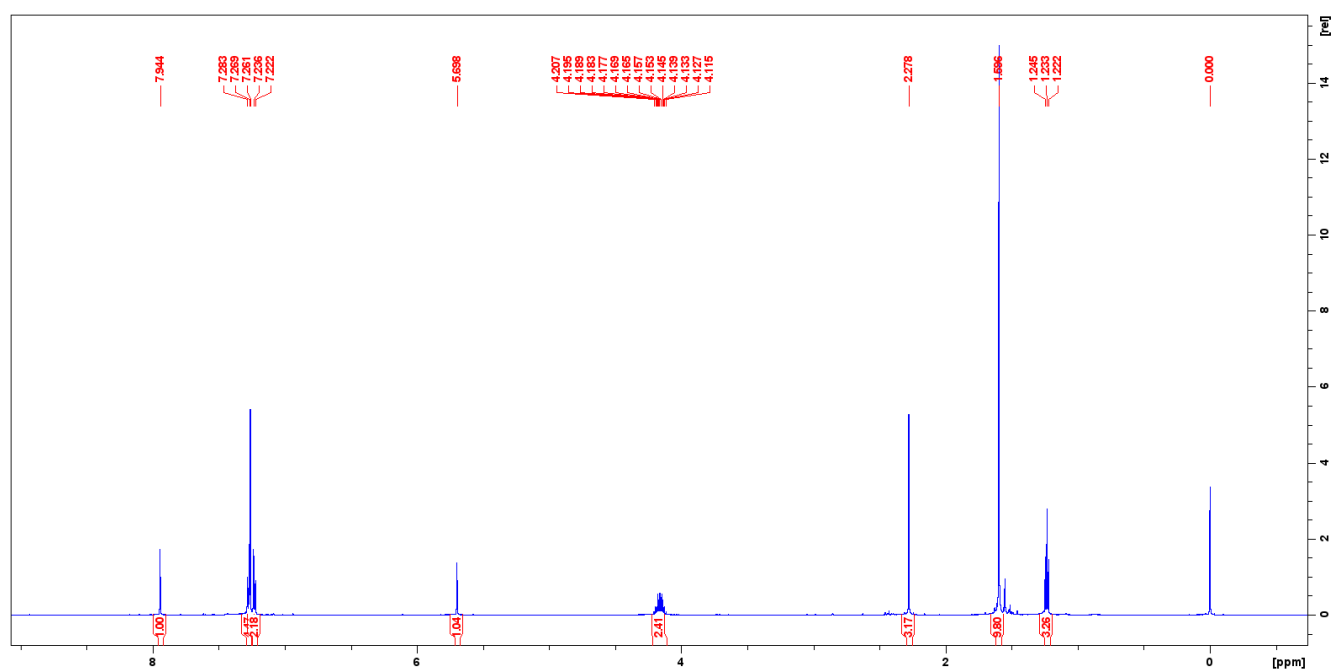


^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) spectrum of **6d**.

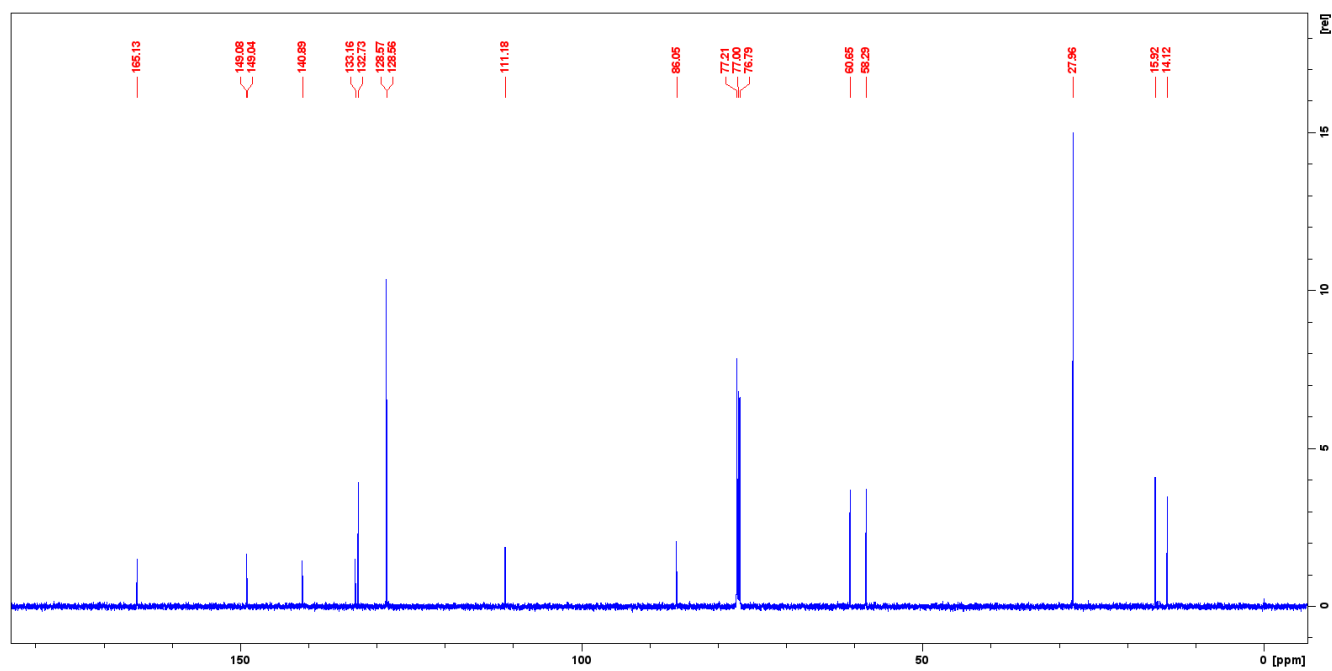


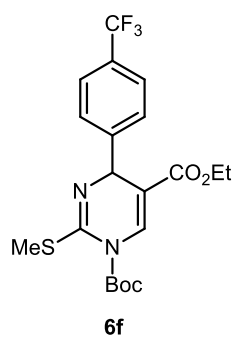


^1H NMR (600 MHz, CDCl_3) spectrum of **6e**.

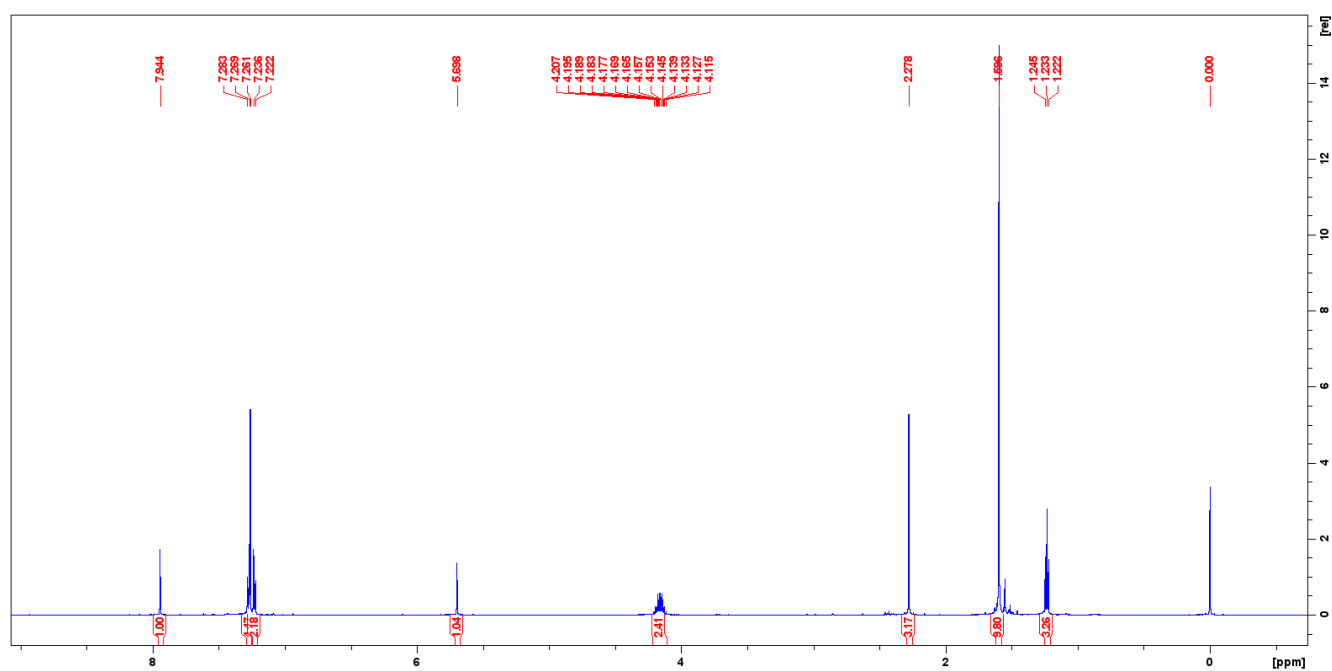


^{13}C NMR (150 MHz, CDCl_3) spectrum of **6e**.

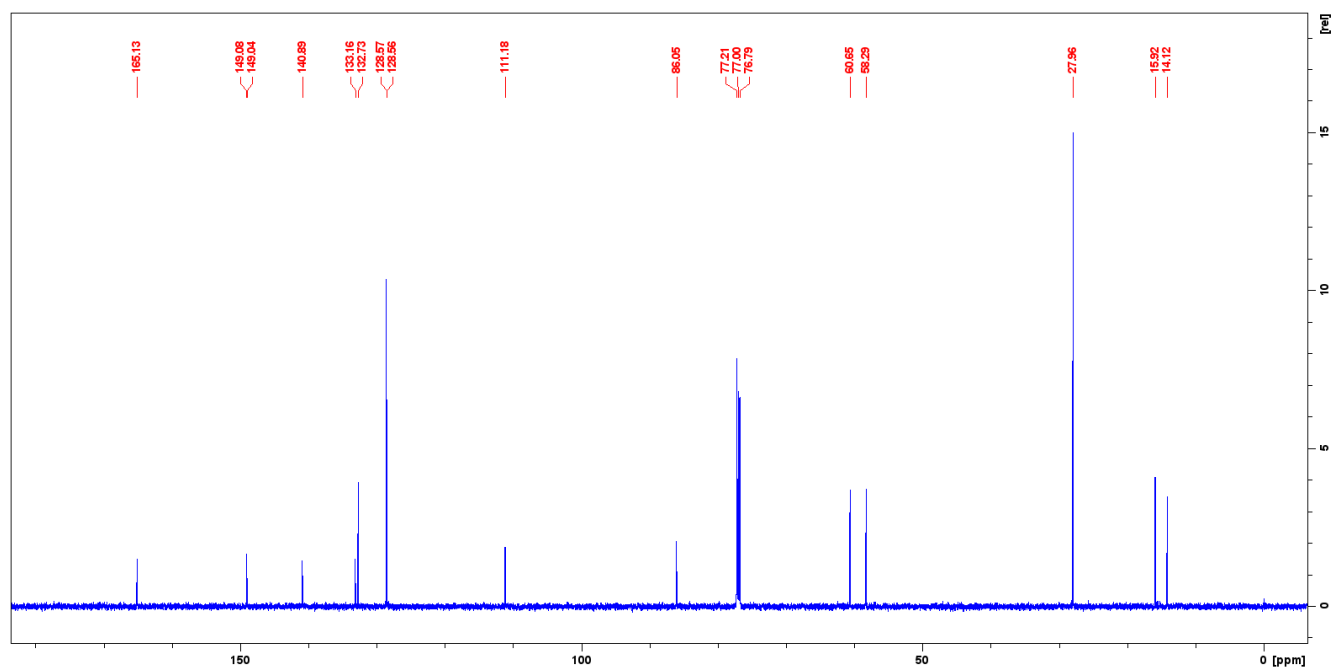


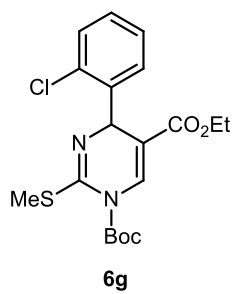


^1H NMR (600 MHz, CDCl_3) spectrum of **6f**.

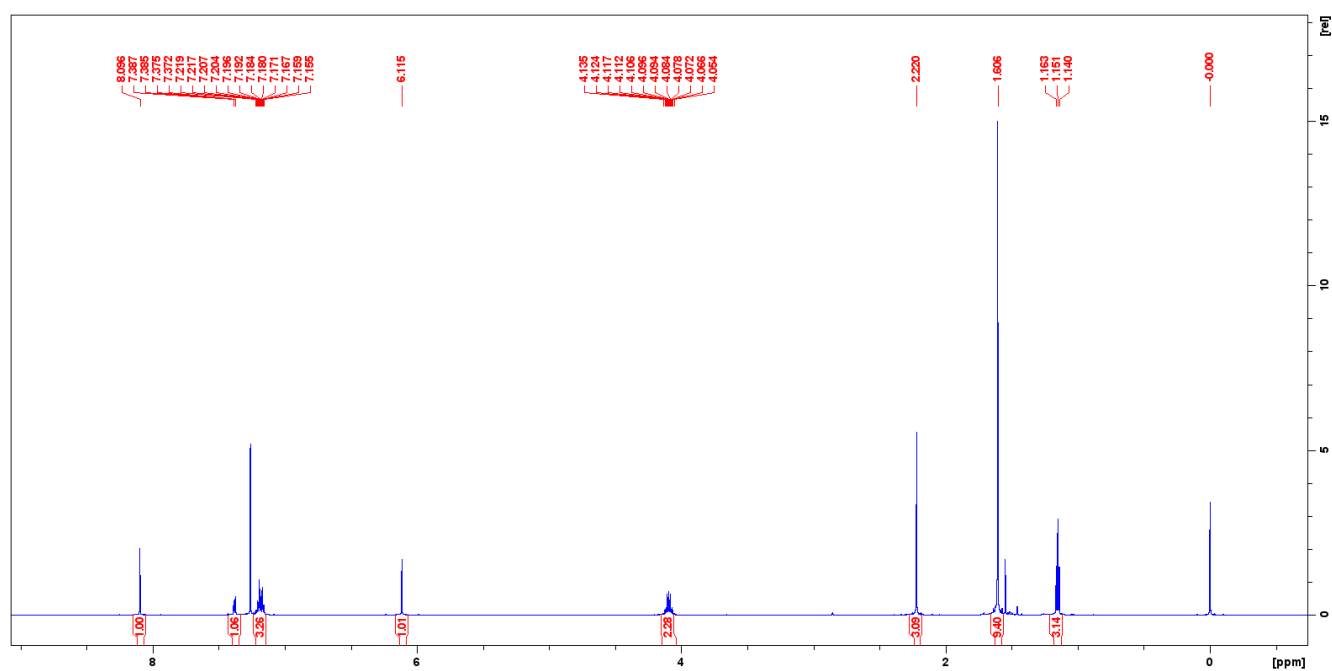


^{13}C NMR (150 MHz, CDCl_3) spectrum of **6f**.

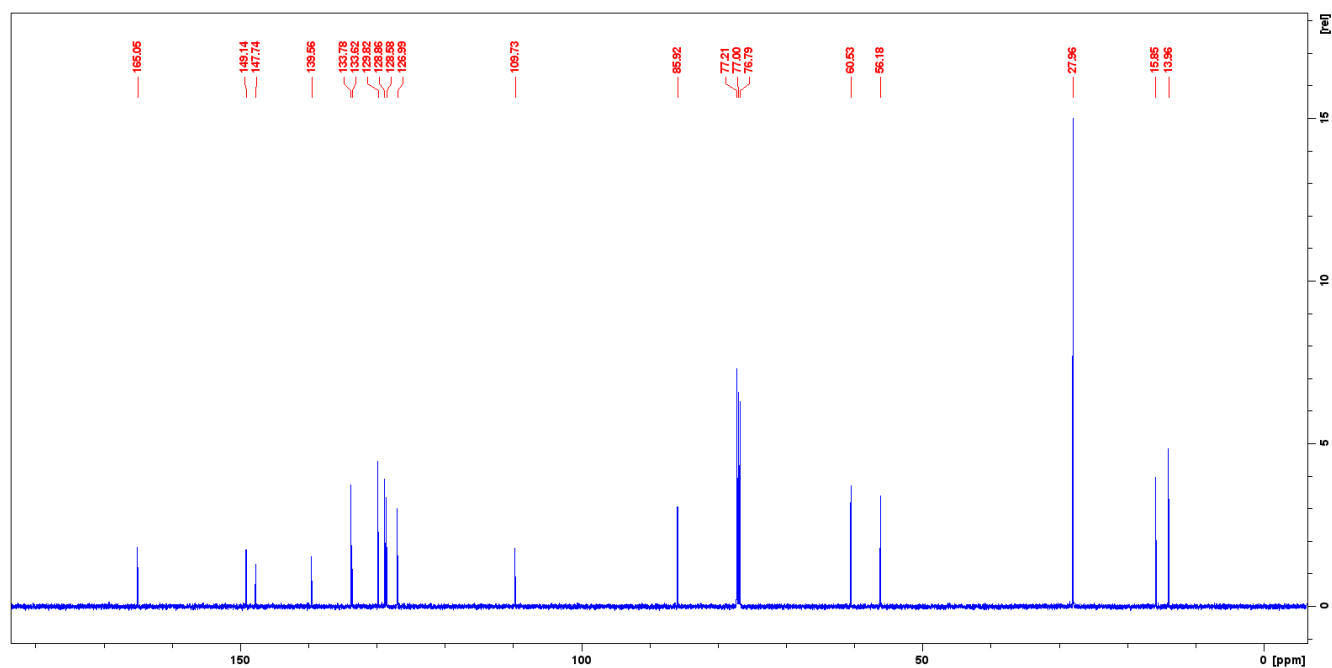


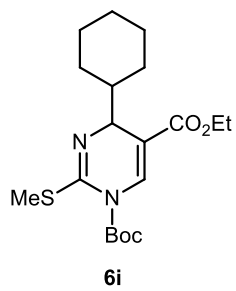


^1H NMR (600 MHz, CDCl_3) spectrum of **6g**.

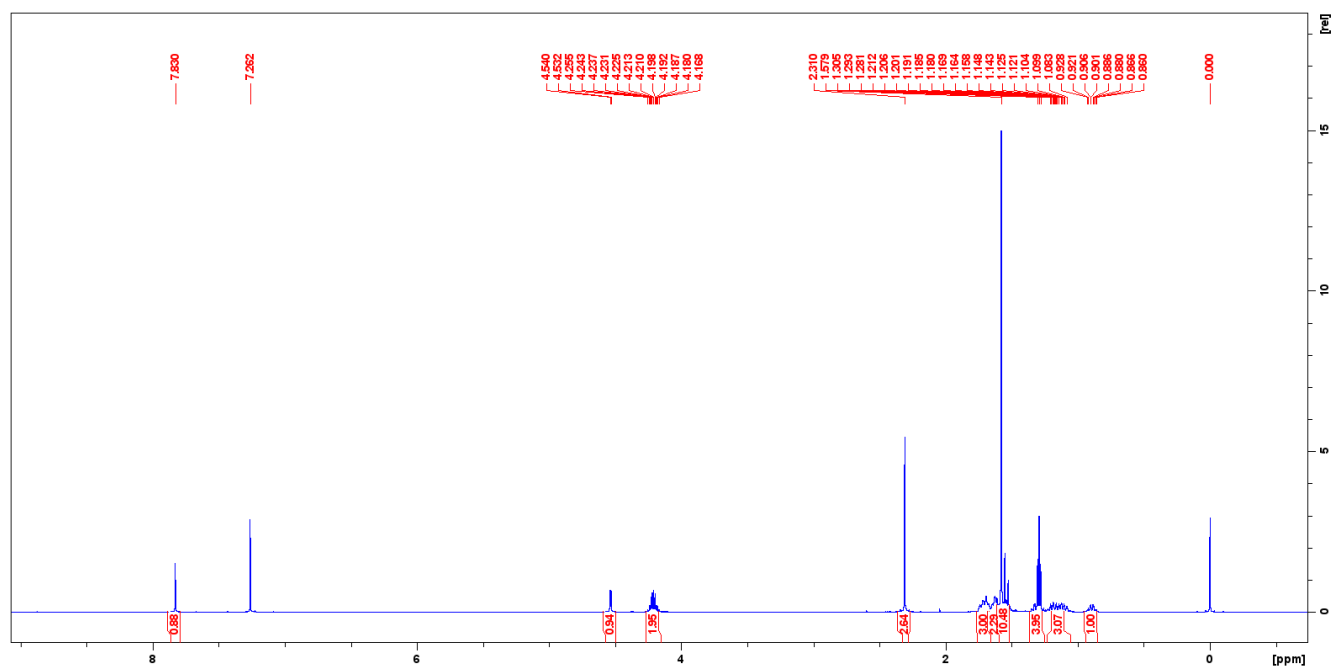


^{13}C NMR (150 MHz, CDCl_3) spectrum of **6g**.

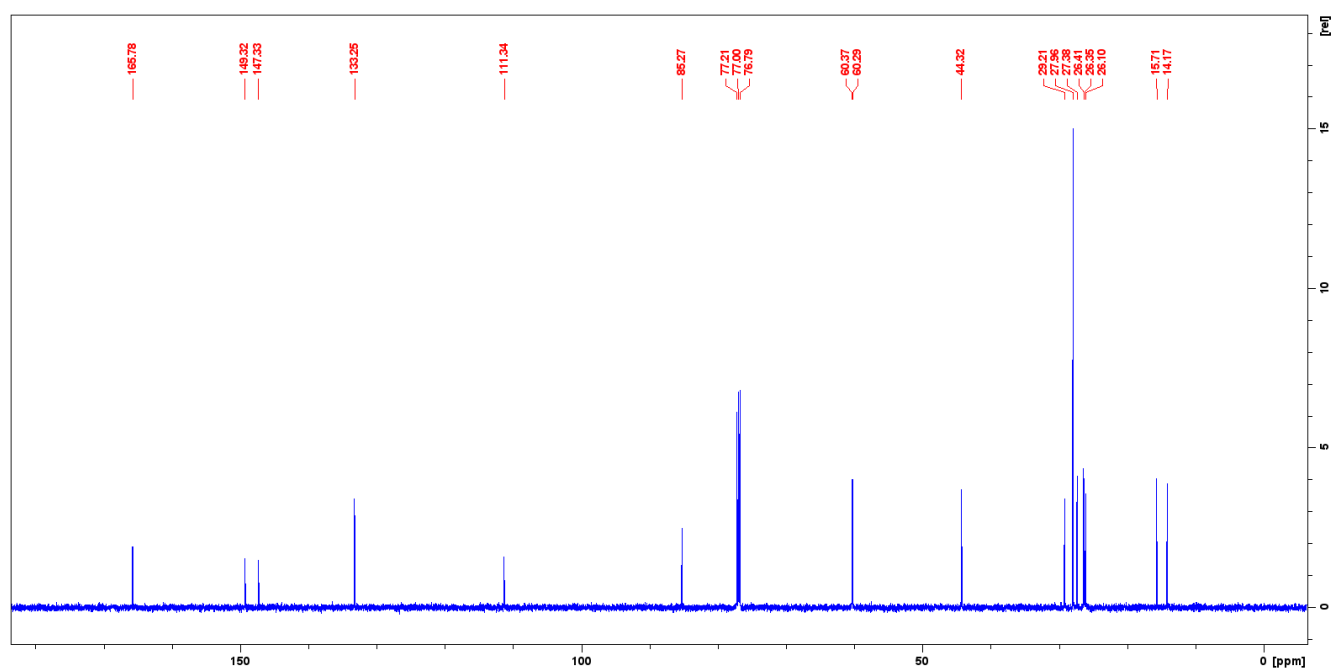


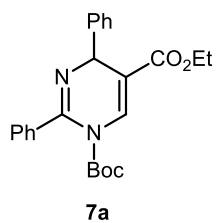


^1H NMR (600 MHz, CDCl_3) spectrum of **6i**.

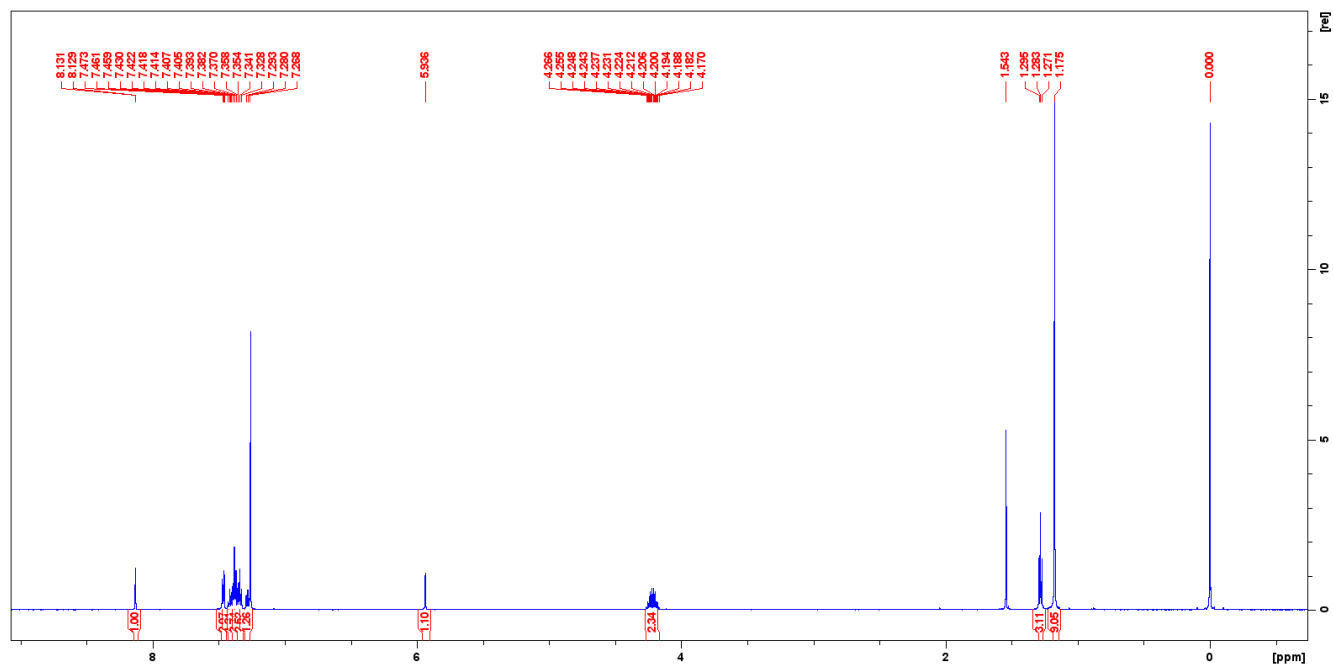


^{13}C NMR (150 MHz, CDCl_3) spectrum of **6i**.

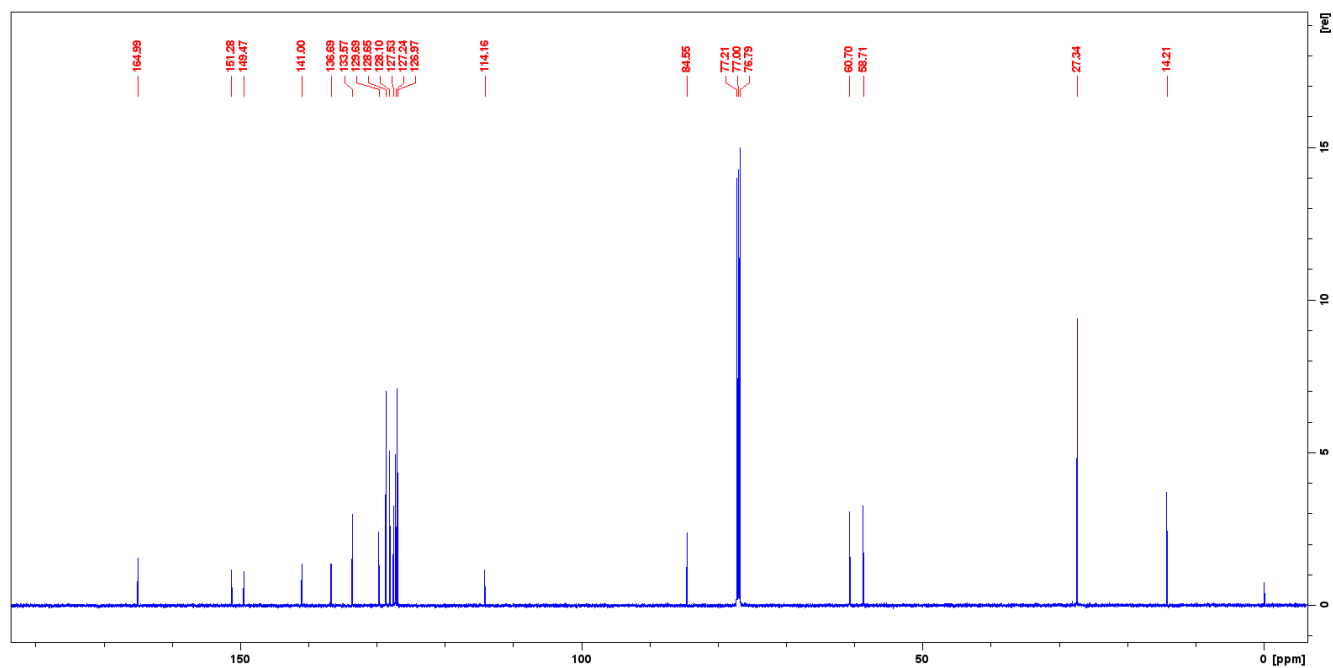


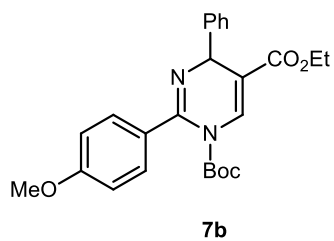


^1H NMR (600 MHz, CDCl_3) spectrum of **7a**.

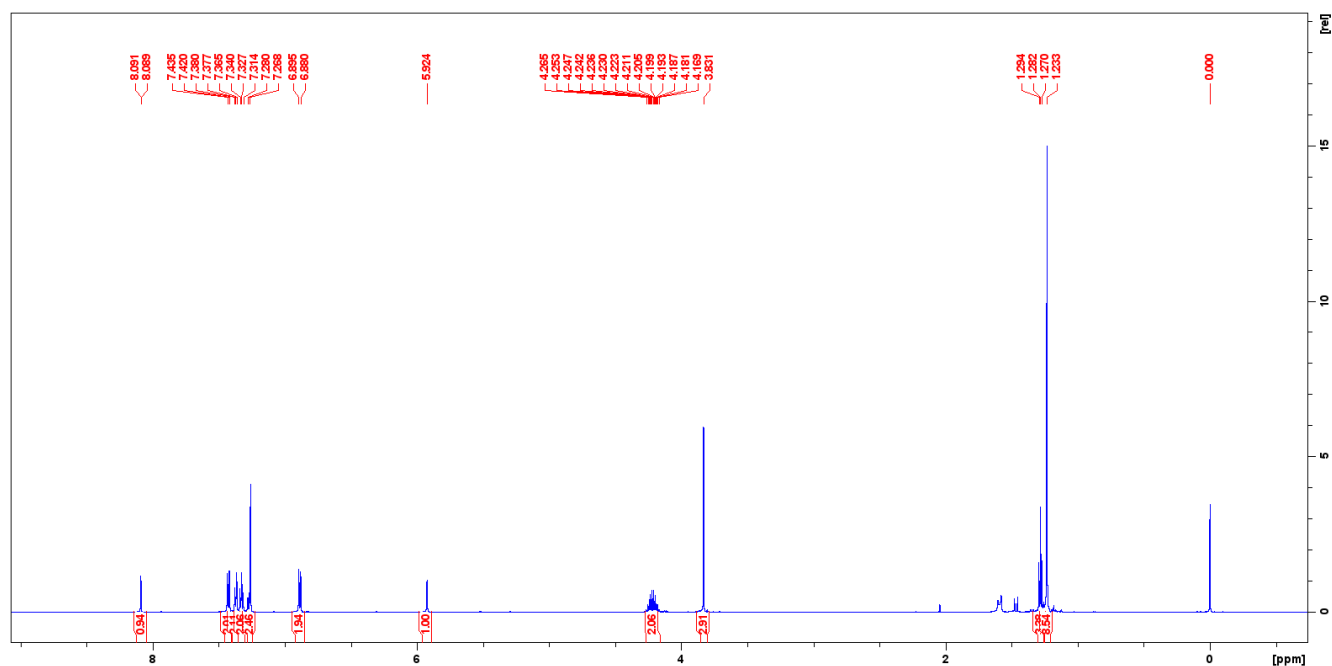


^{13}C NMR (150 MHz, CDCl_3) spectrum of **7a**.

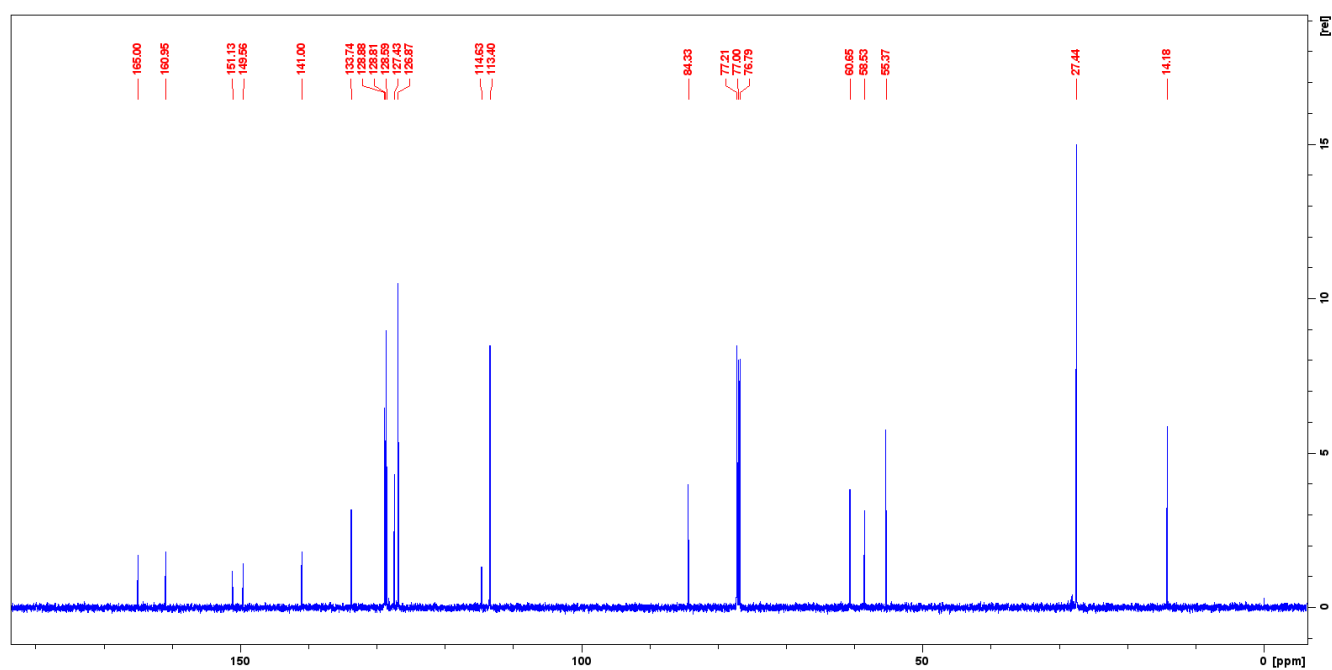


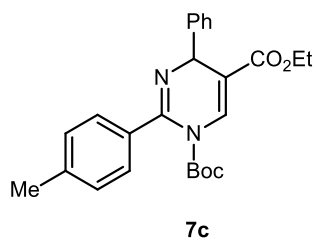


^1H NMR (600 MHz, CDCl_3) spectrum of **7b**.

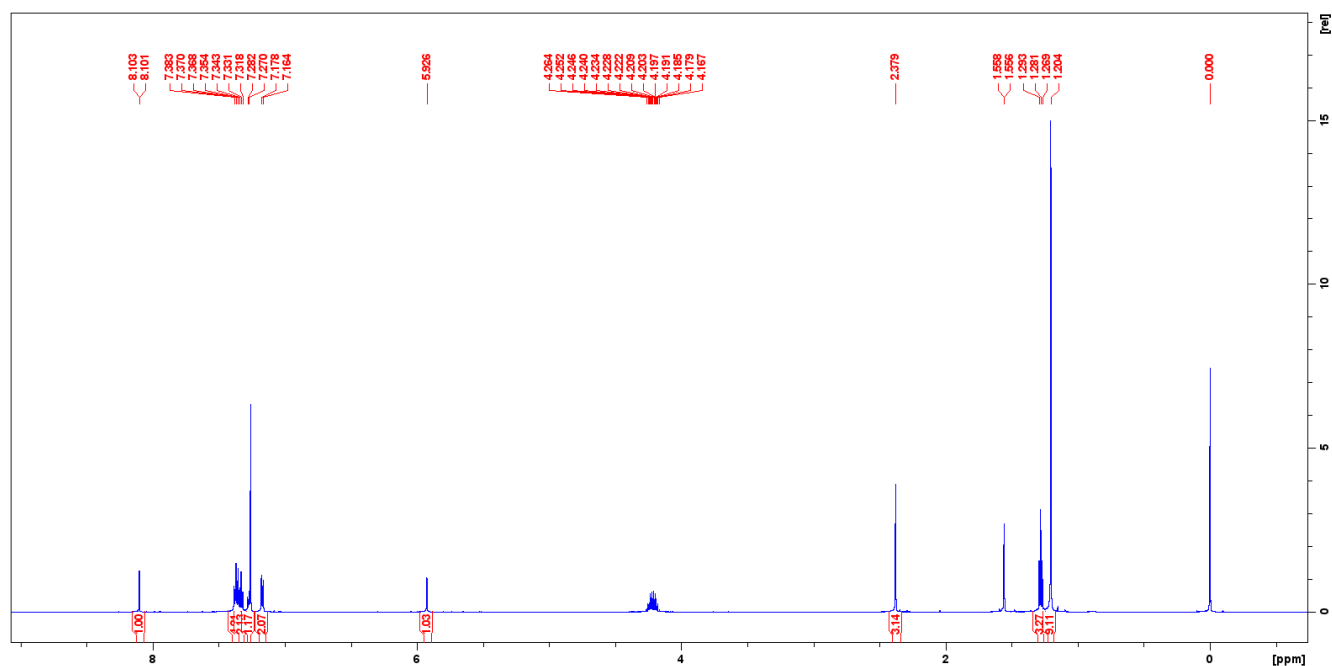


^{13}C NMR (150 MHz, CDCl_3) spectrum of **7b**.

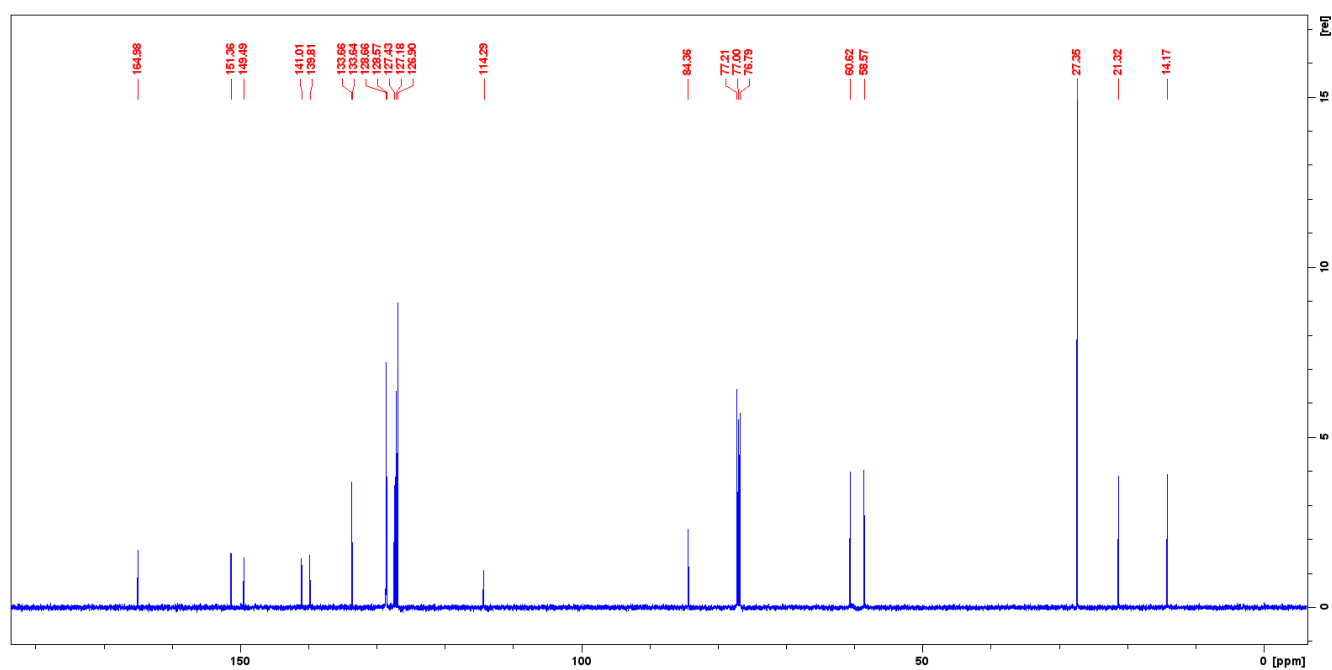


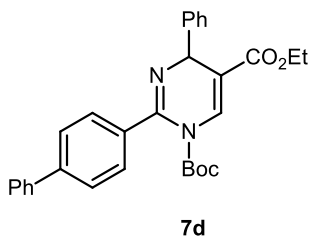
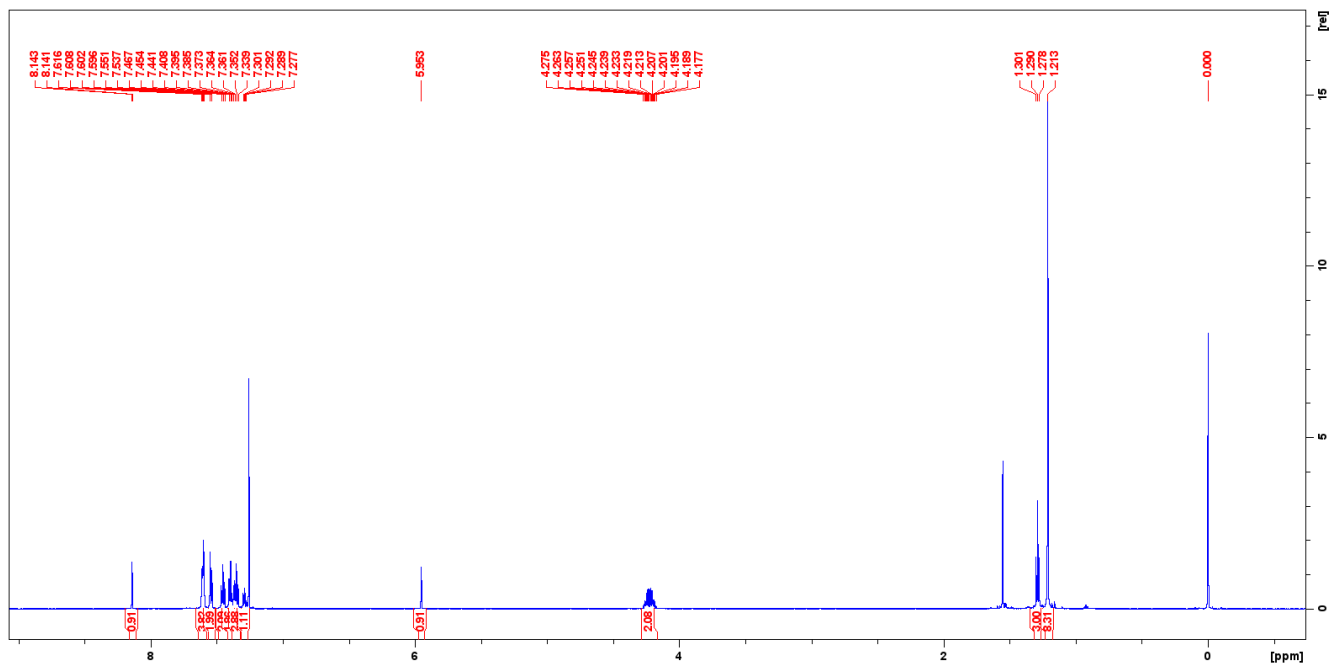


^1H NMR (600 MHz, CDCl_3) spectrum of **7c**.

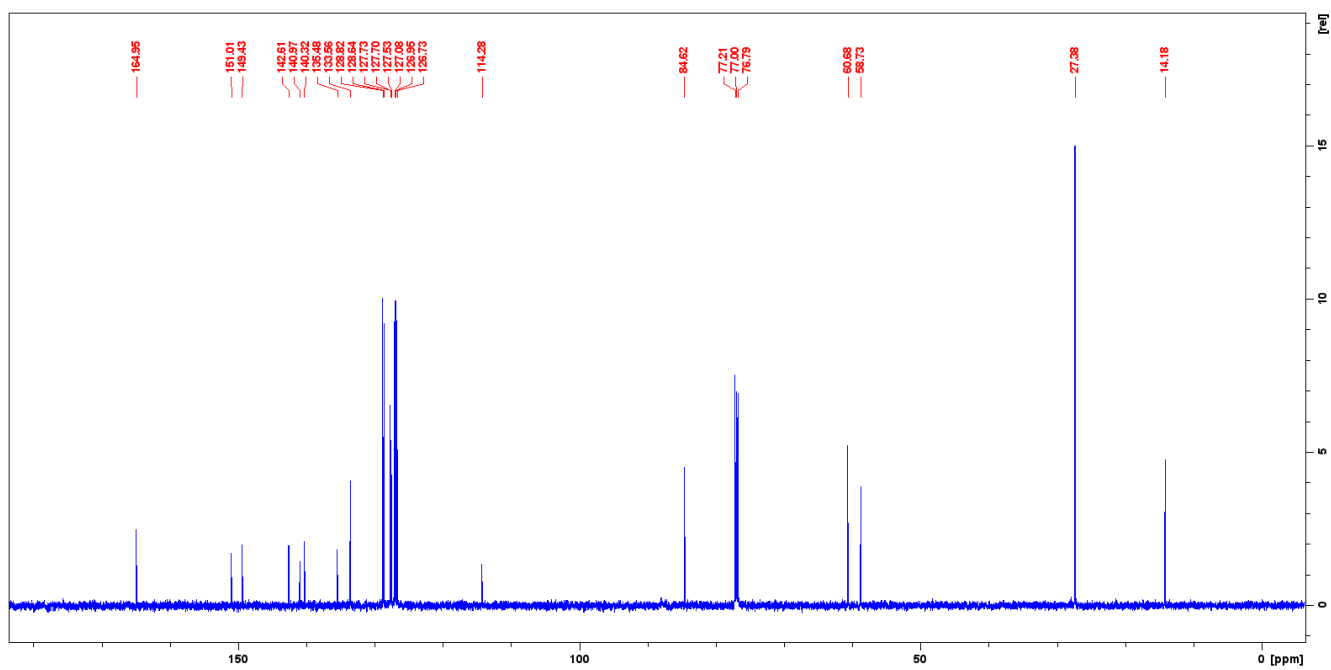


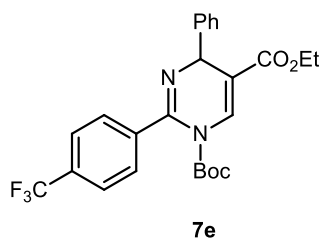
^{13}C NMR (150 MHz, CDCl_3) spectrum of **7c**.



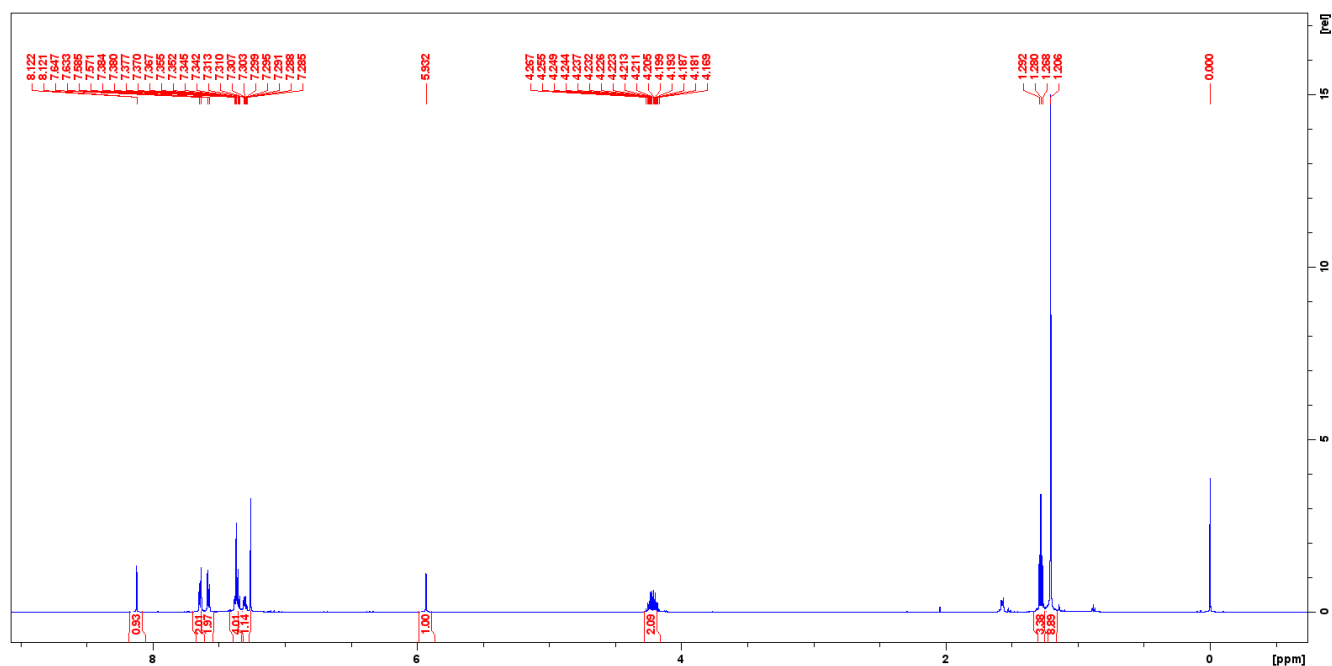
¹H NMR (600 MHz, CDCl₃) spectrum of **7d**.

¹³C NMR (150 MHz, CDCl₃) spectrum of **7d**.

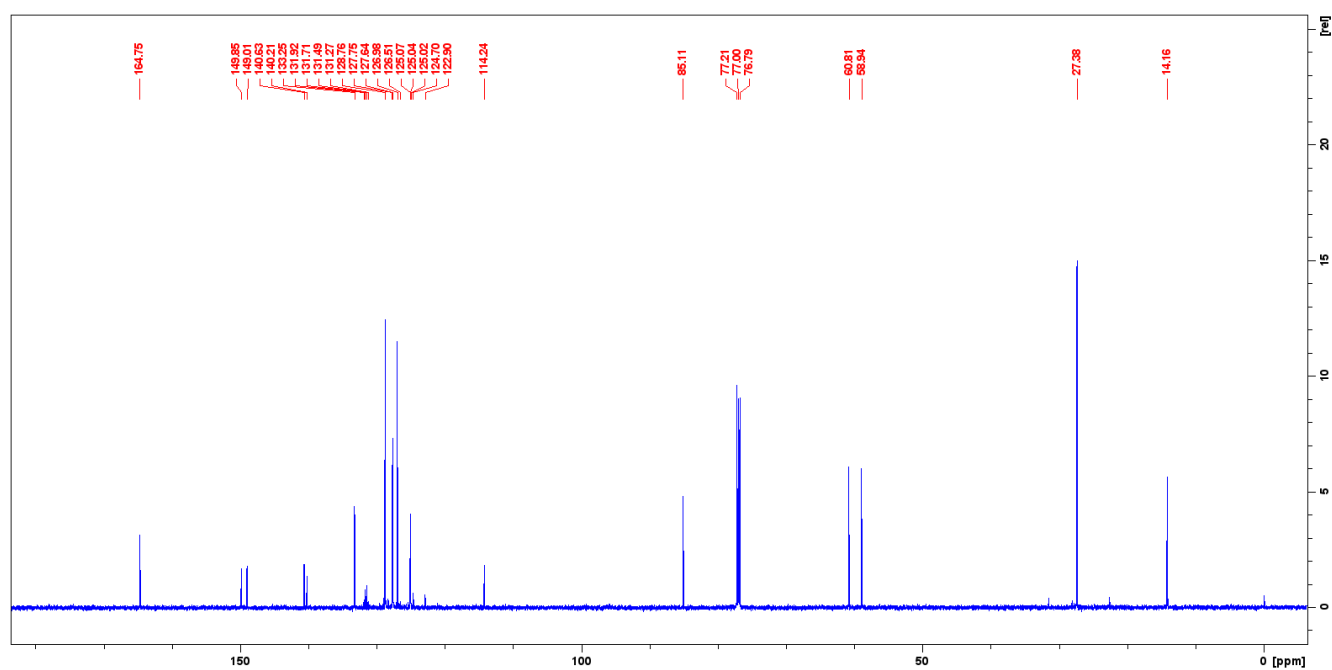


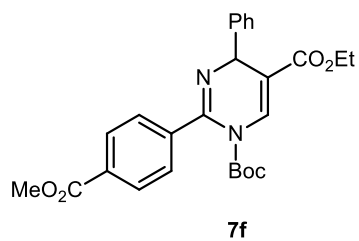


^1H NMR (600 MHz, CDCl_3) spectrum of **7e**.

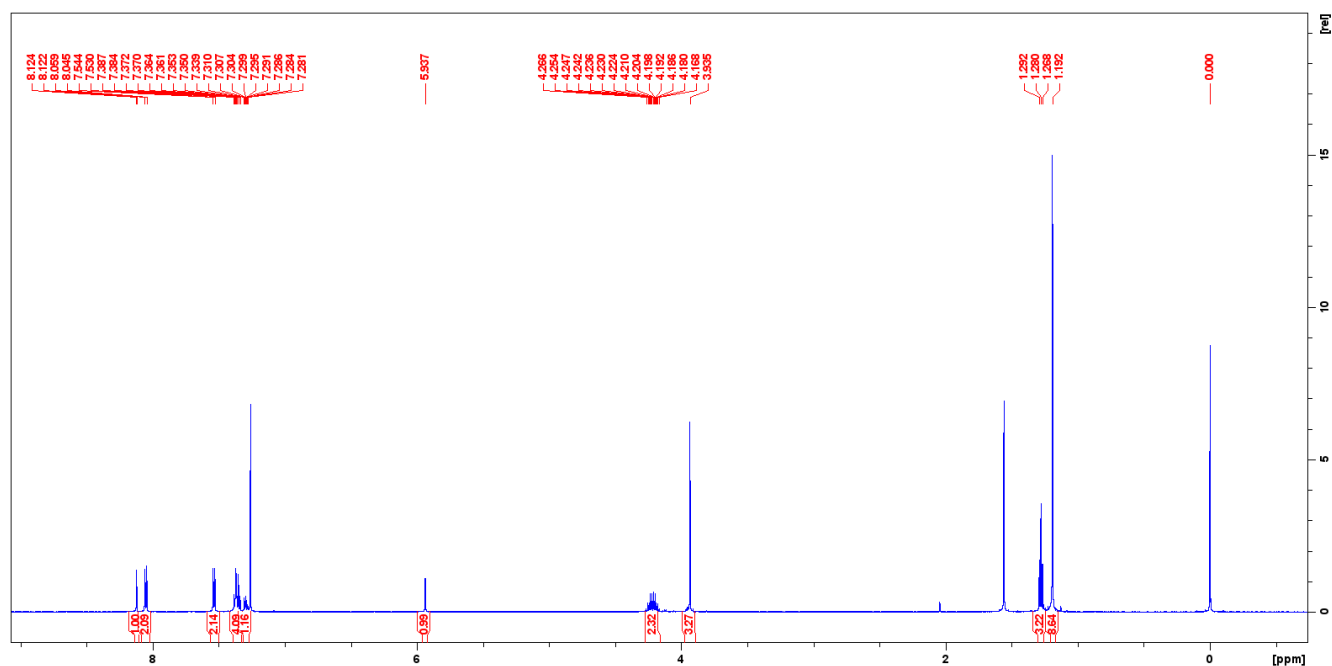


^{13}C NMR (150 MHz, CDCl_3) spectrum of **7e**.

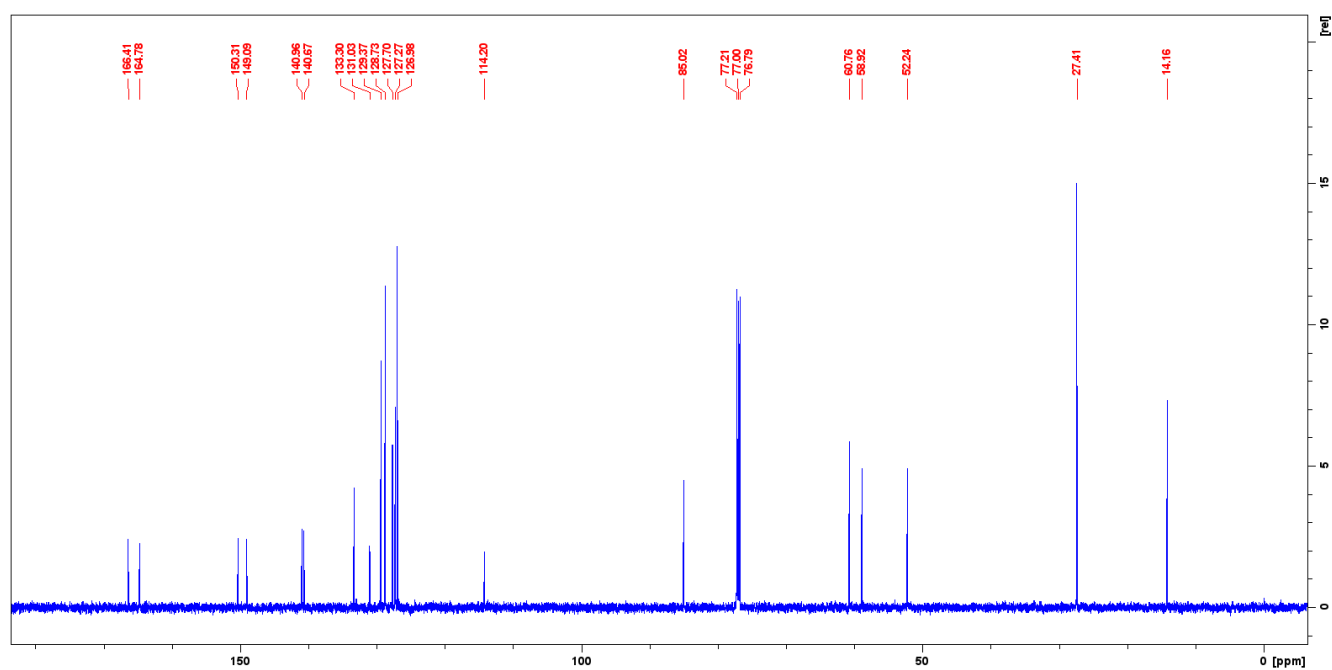


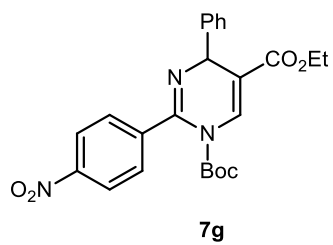


^1H NMR (600 MHz, CDCl_3) spectrum of **7f**.

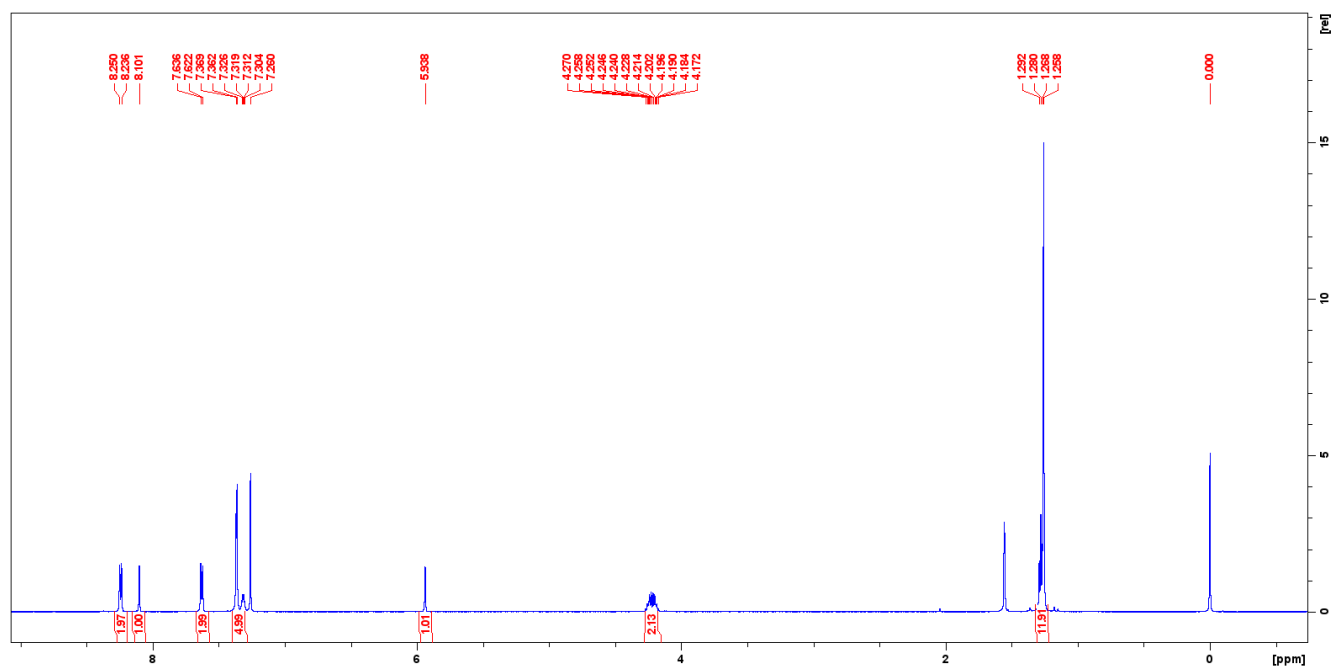


^{13}C NMR (150 MHz, CDCl_3) spectrum of **7f**.

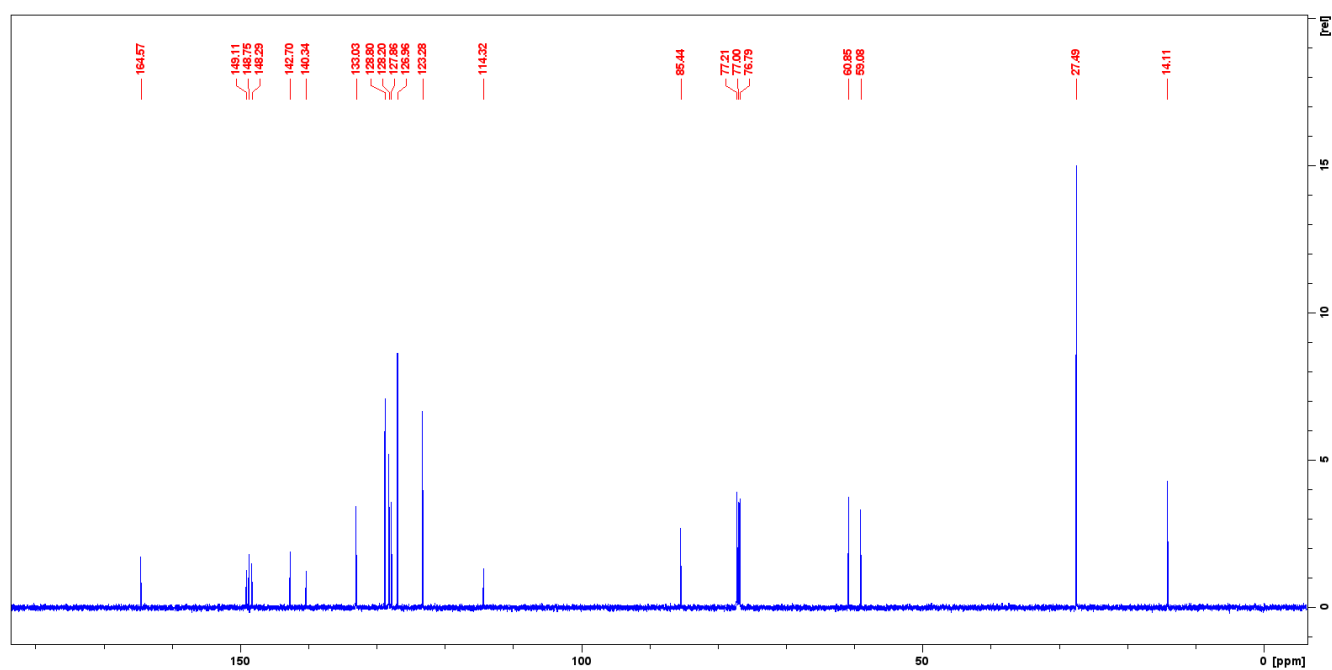


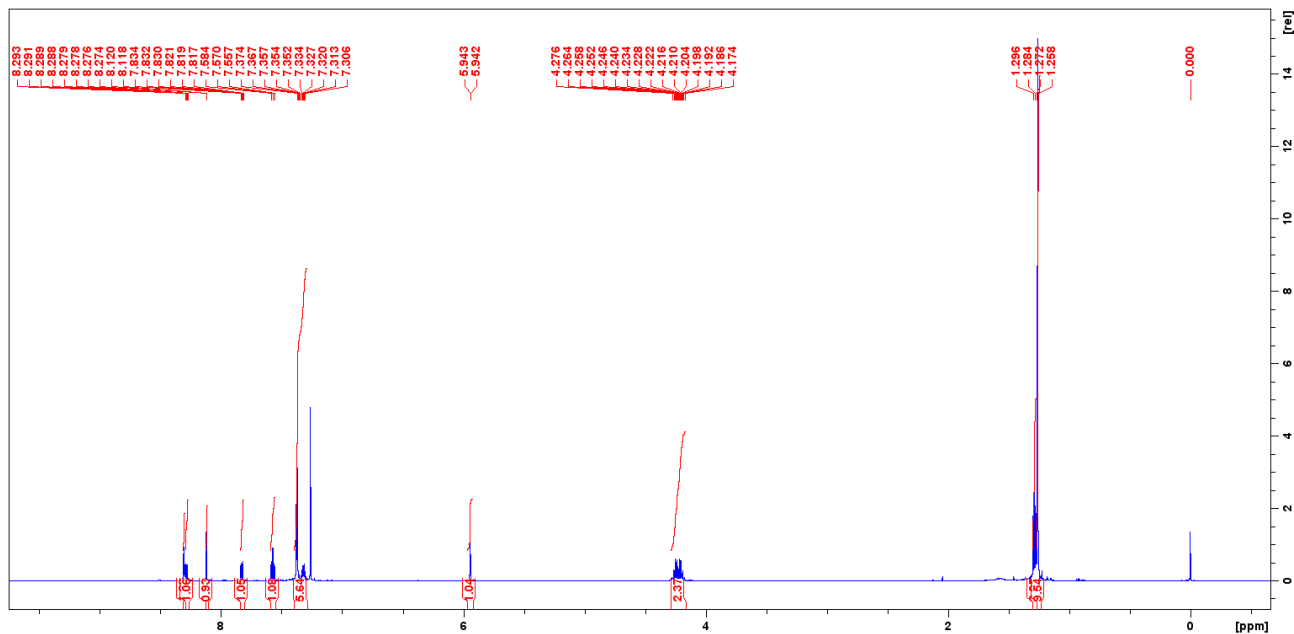


^1H NMR (600 MHz, CDCl_3) spectrum of **7g**.

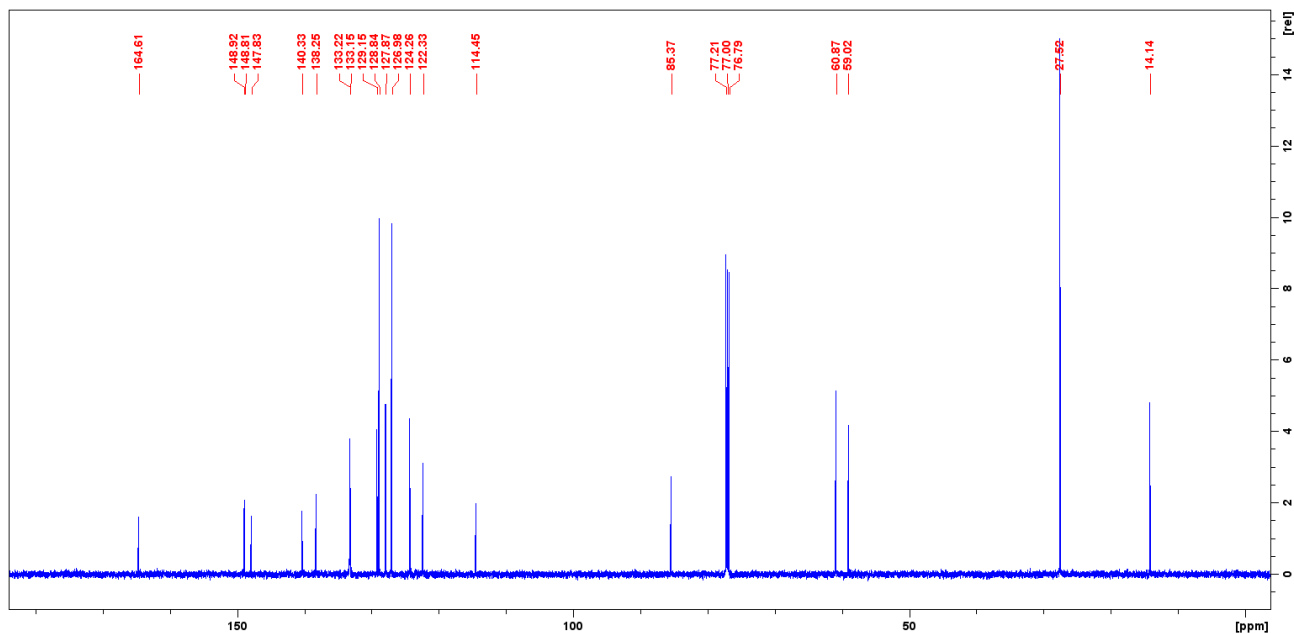


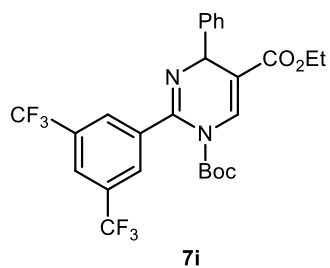
^{13}C NMR (150 MHz, CDCl_3) spectrum of **7g**.



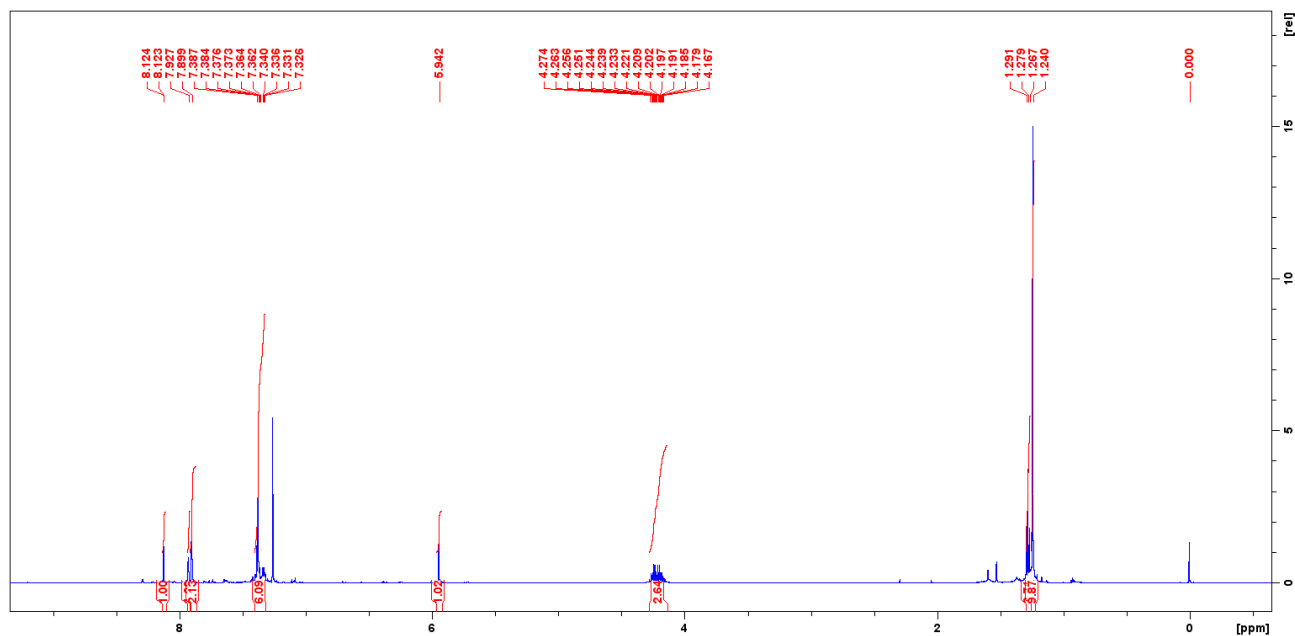
¹H NMR (600 MHz, CDCl₃) spectrum of **7h**.

^{13}C NMR (150 MHz, CDCl_3) spectrum of **7h**.

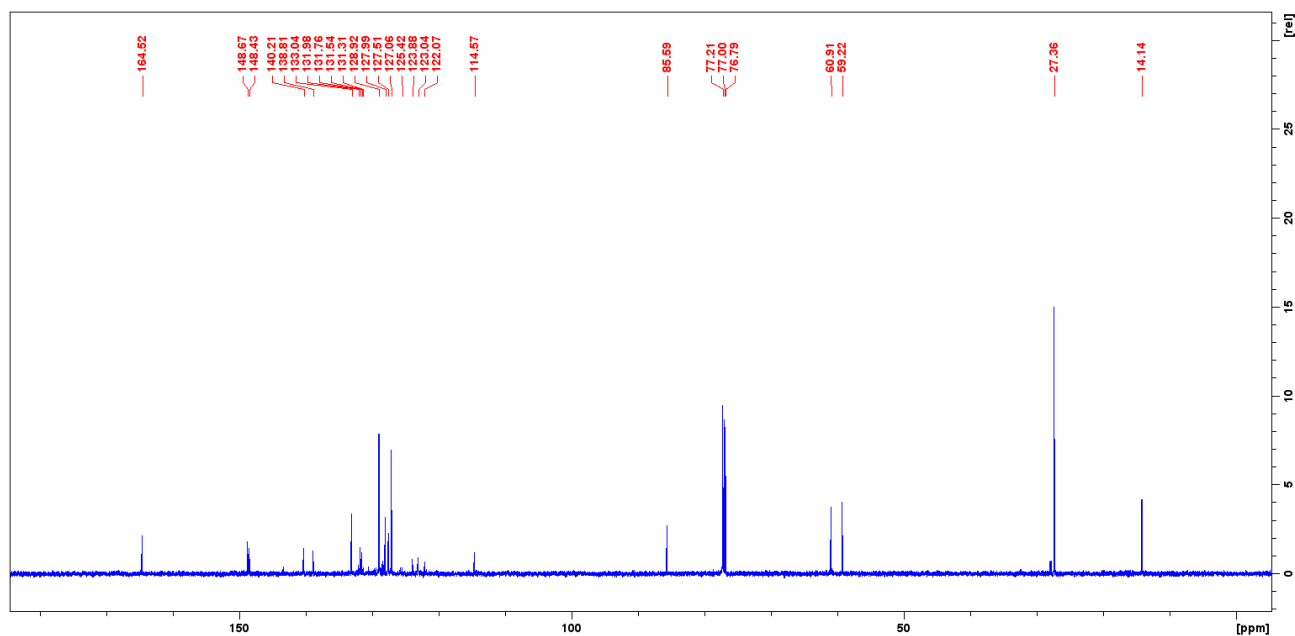


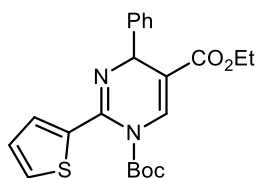


^1H NMR (600 MHz, CDCl_3) spectrum of **7i**.



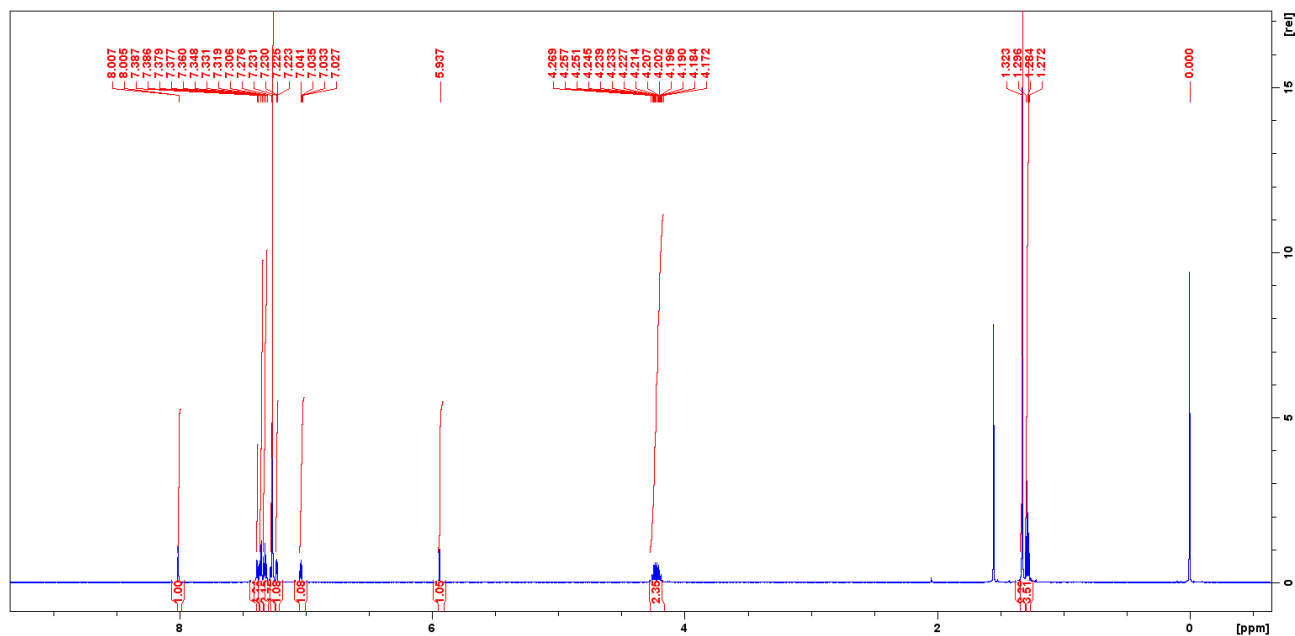
^{13}C NMR (150 MHz, CDCl_3) spectrum of **7i**.



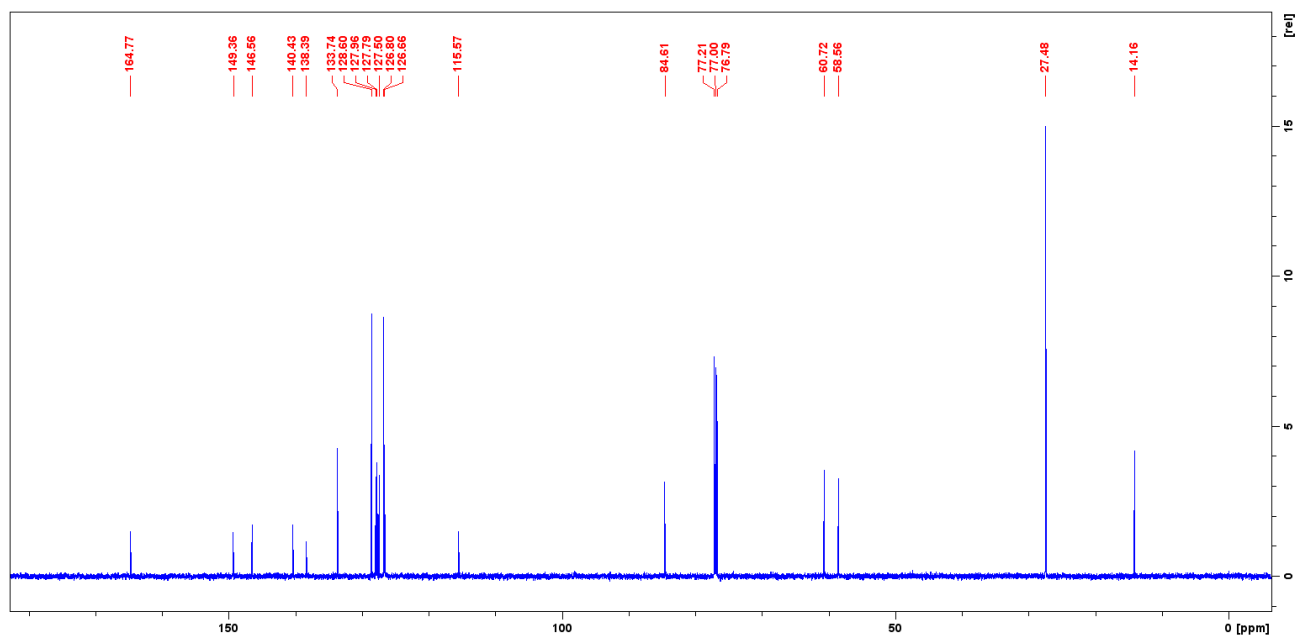


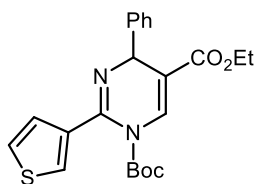
7j

^1H NMR (600 MHz, CDCl_3) spectrum of **7j**.



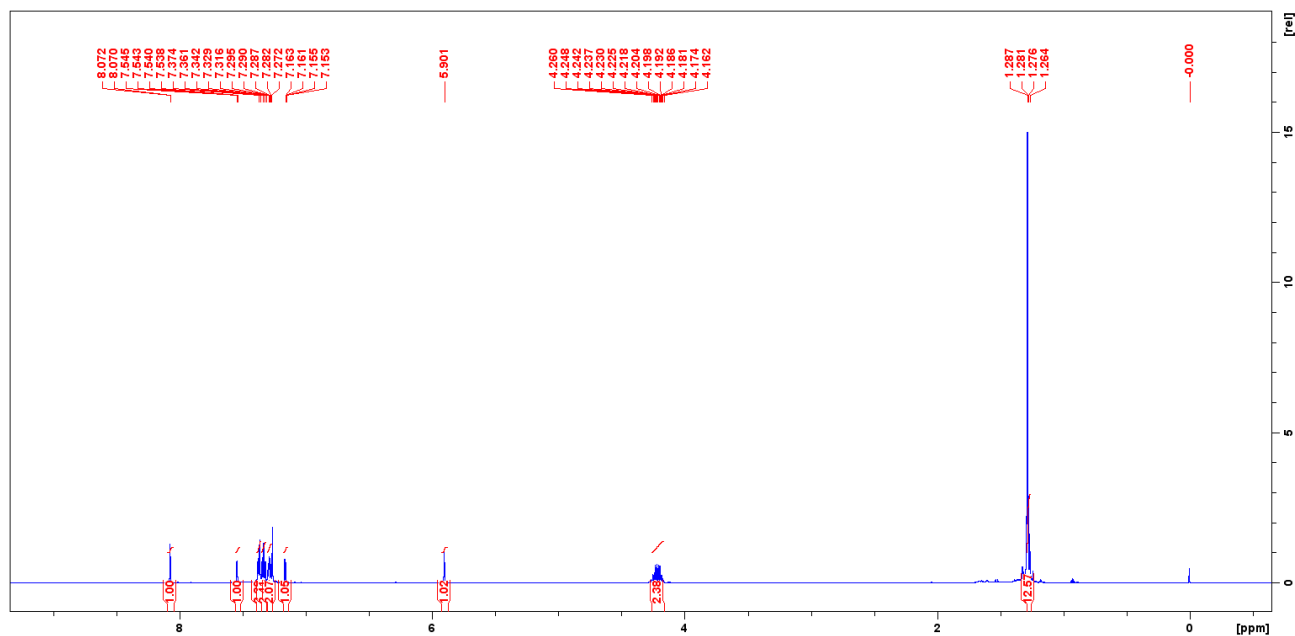
^{13}C NMR (150 MHz, CDCl_3) spectrum of **7j**.



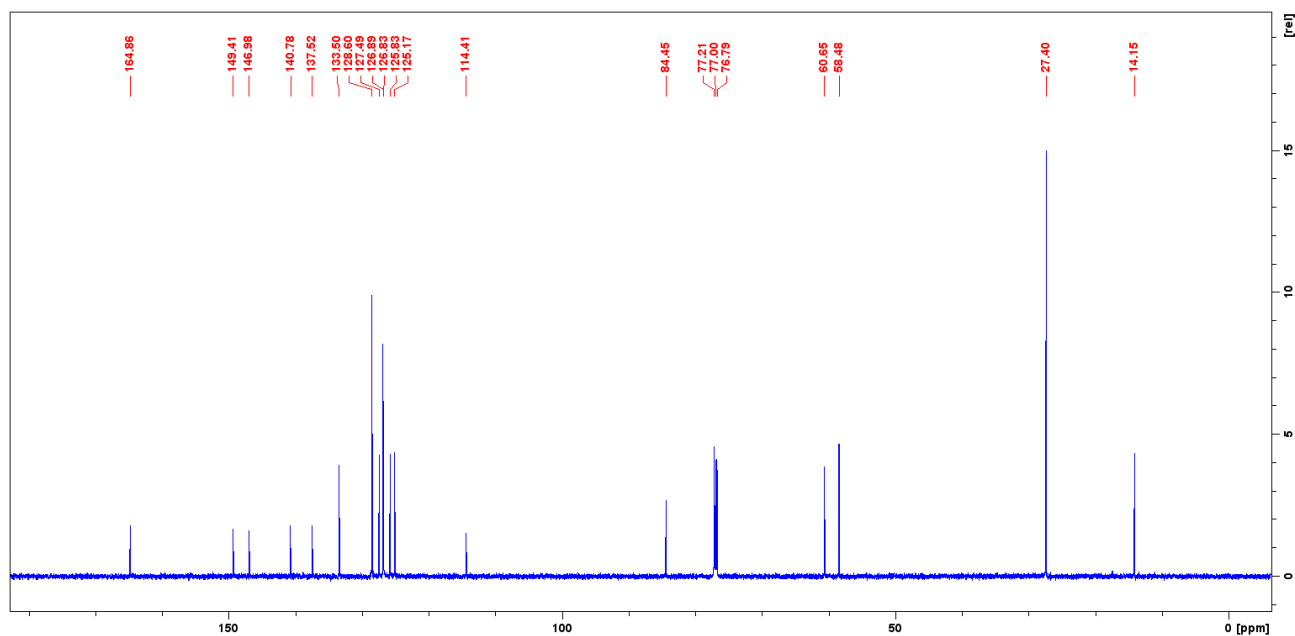


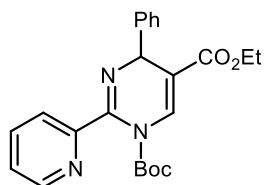
7k

^1H NMR (600 MHz, CDCl_3) spectrum of **7k**.



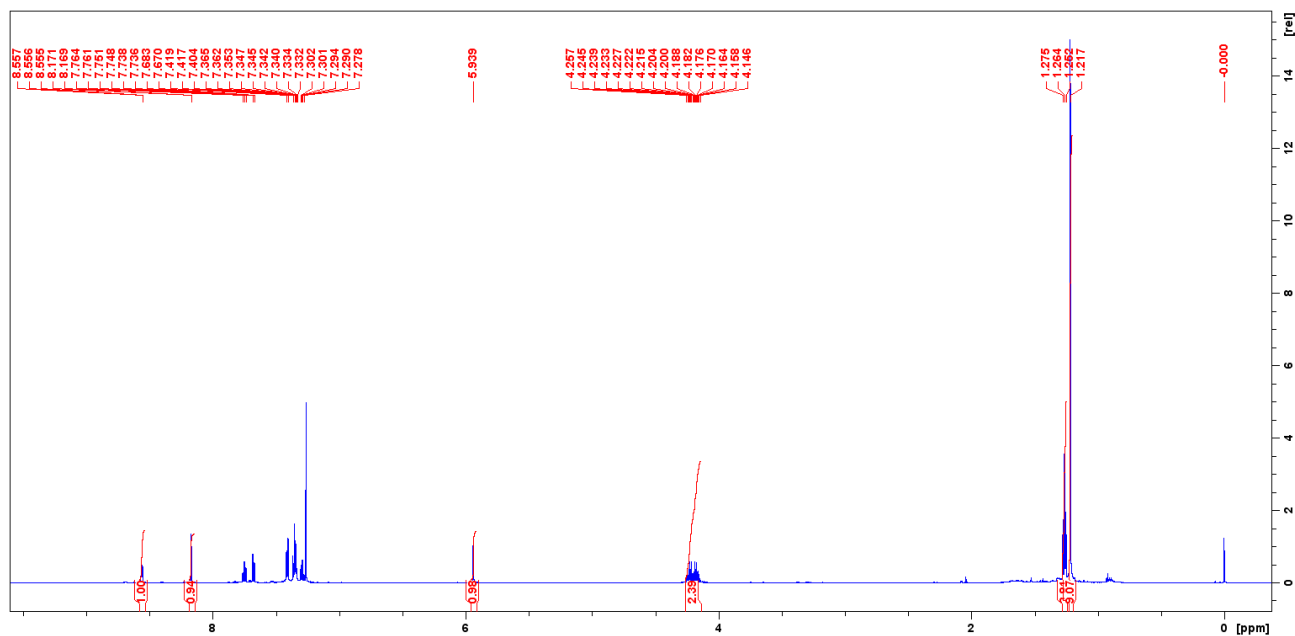
^{13}C NMR (150 MHz, CDCl_3) spectrum of **7k**.



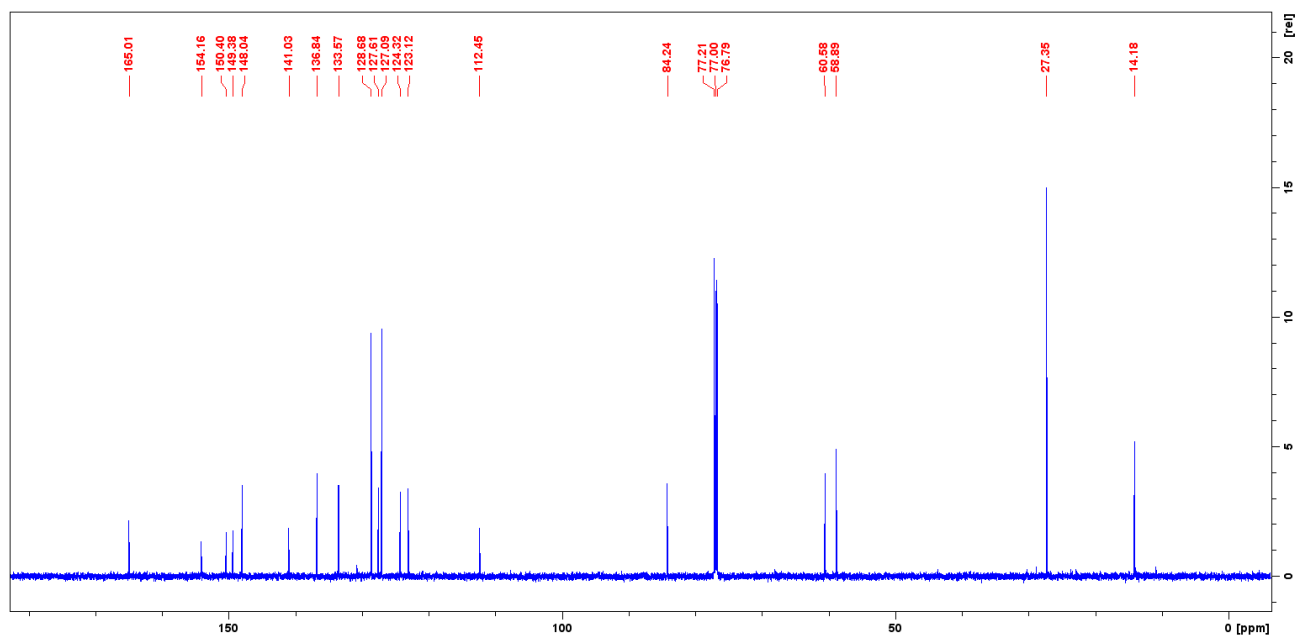


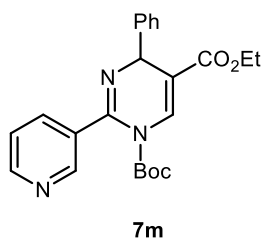
7l

^1H NMR (600 MHz, CDCl_3) spectrum of 7l.

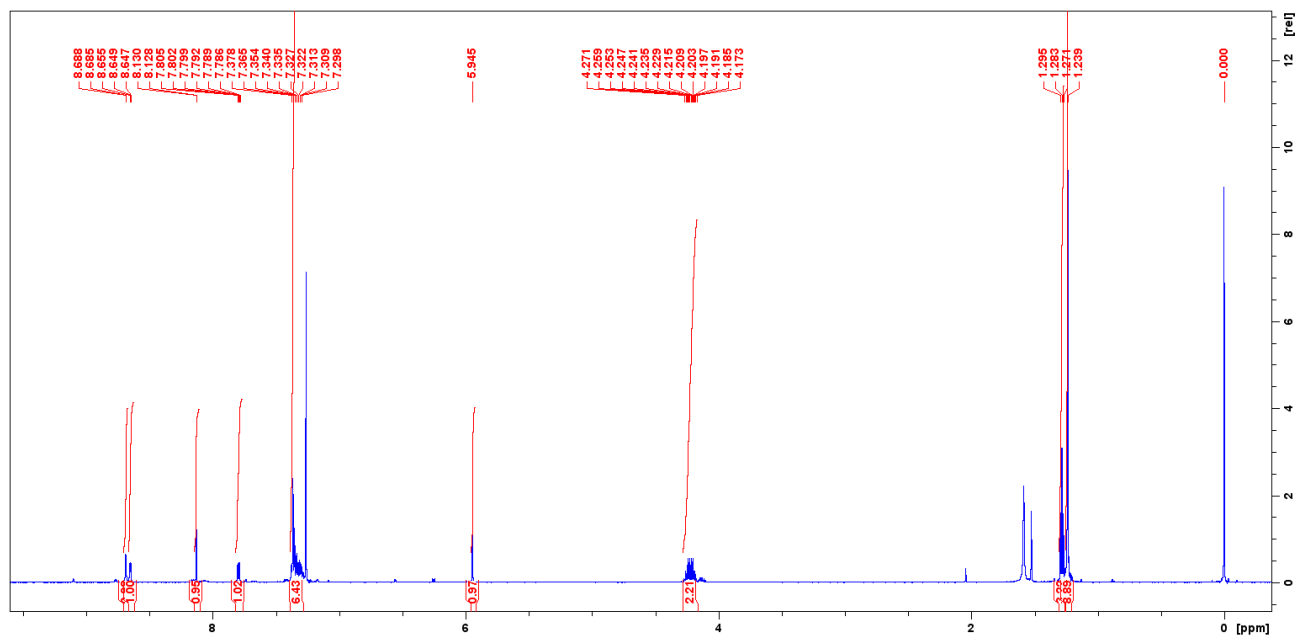


^{13}C NMR (150 MHz, CDCl_3) spectrum of 7l.

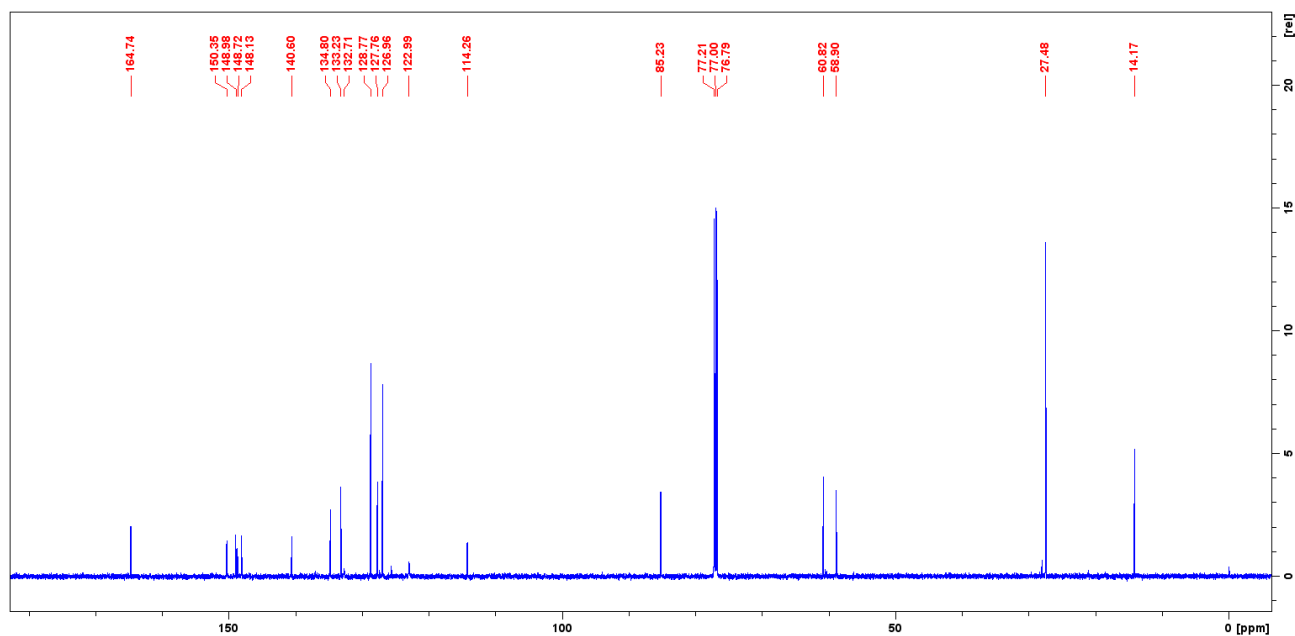


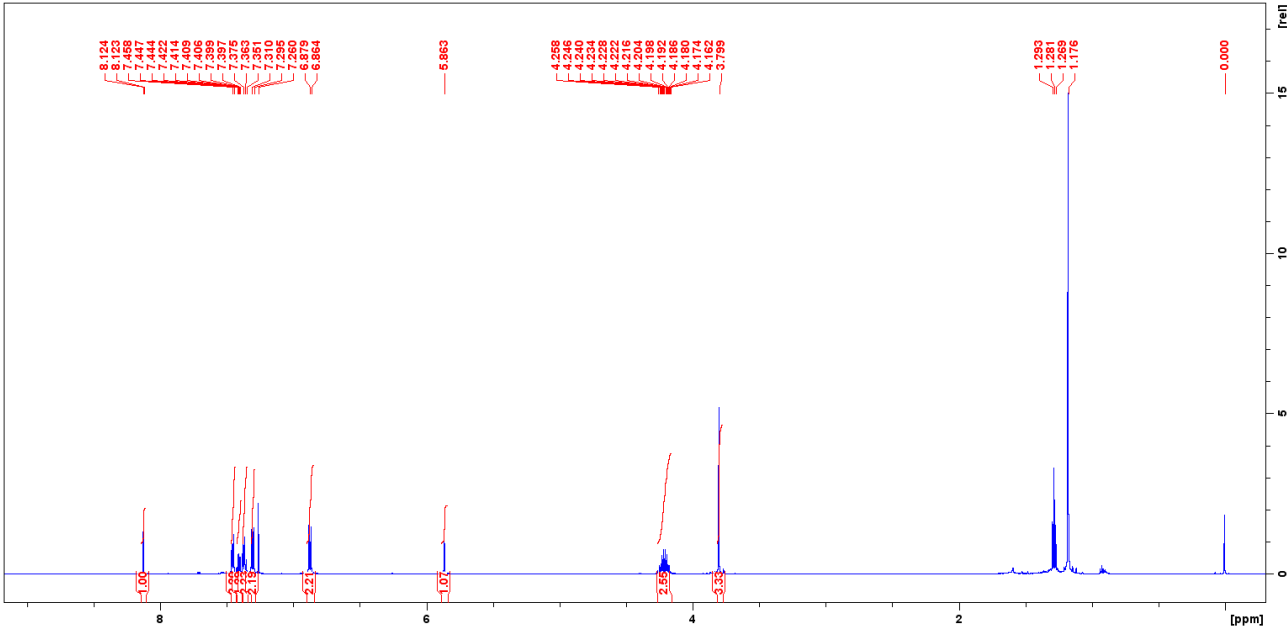
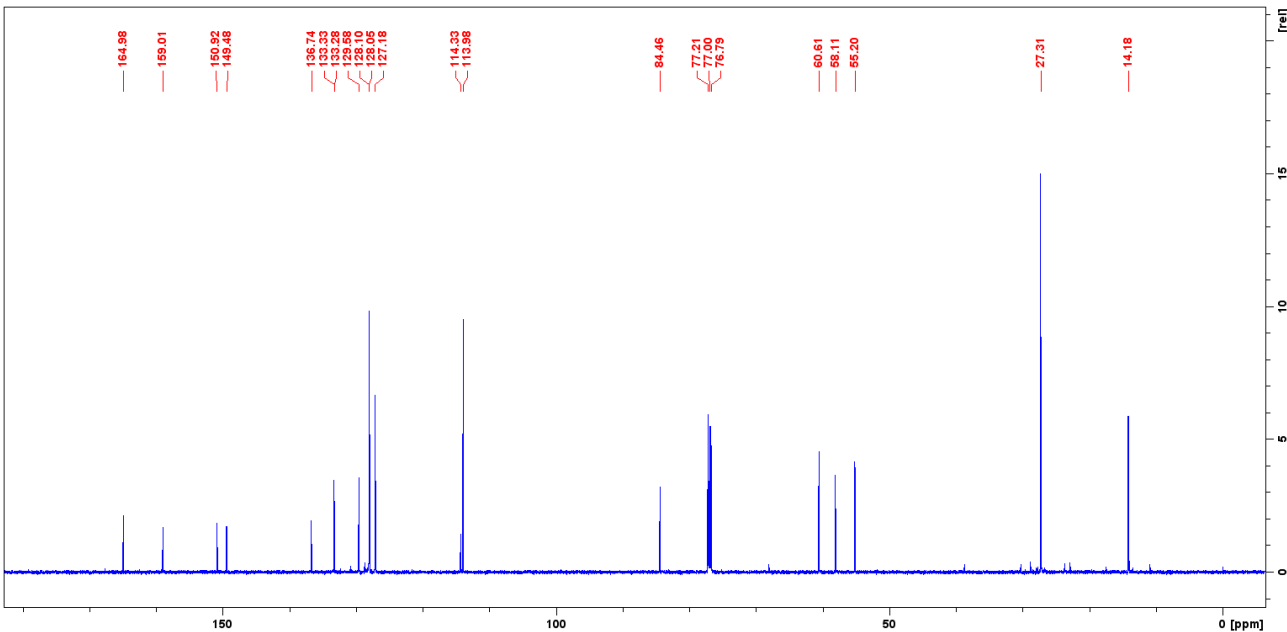


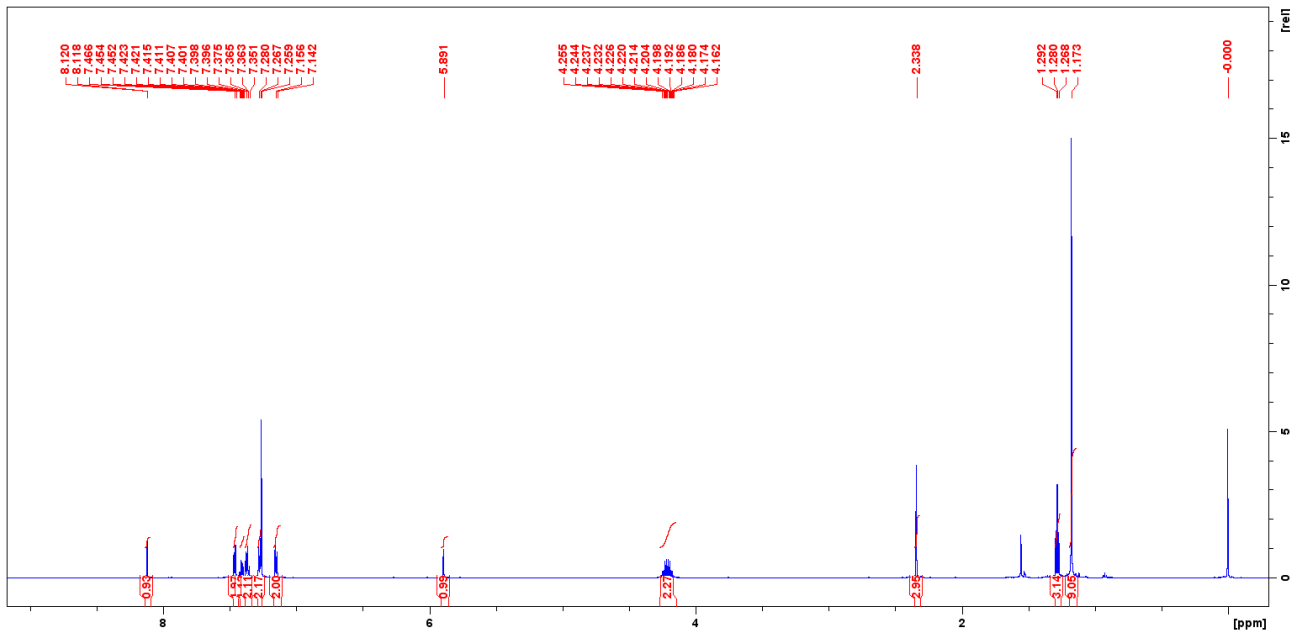
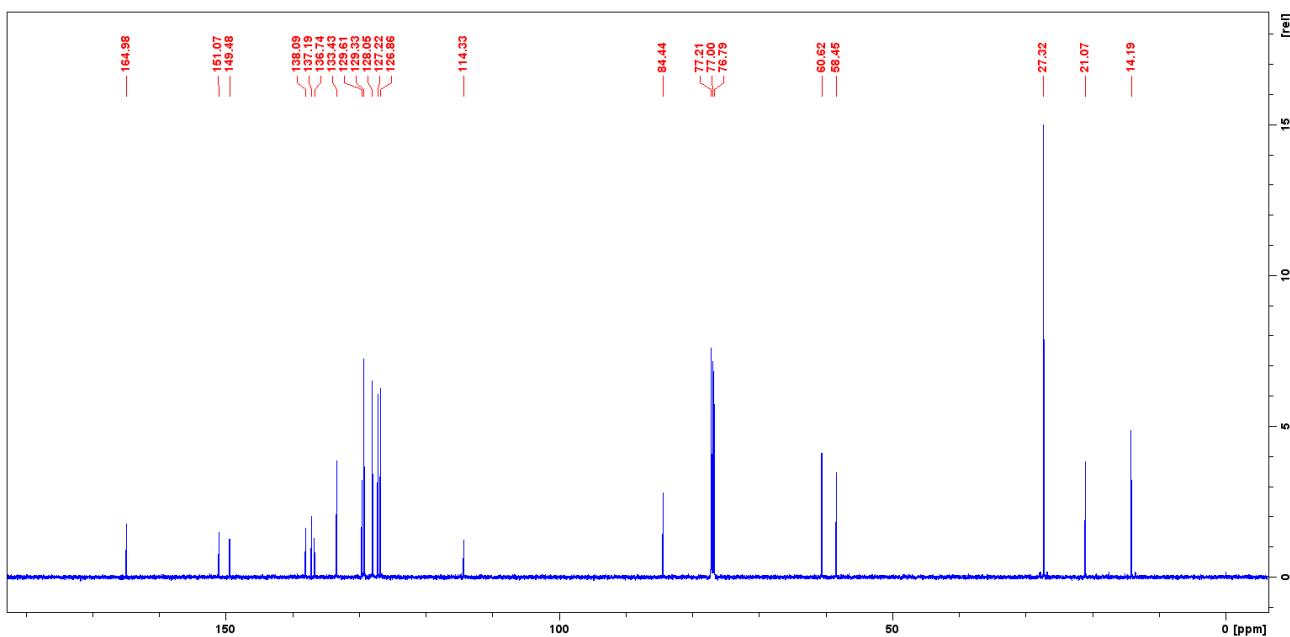
^1H NMR (600 MHz, CDCl_3) spectrum of **7m**.

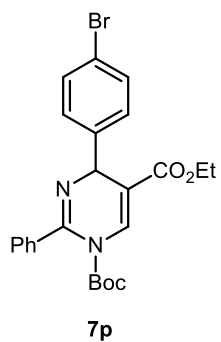


^{13}C NMR (150 MHz, CDCl_3) spectrum of **7m**.

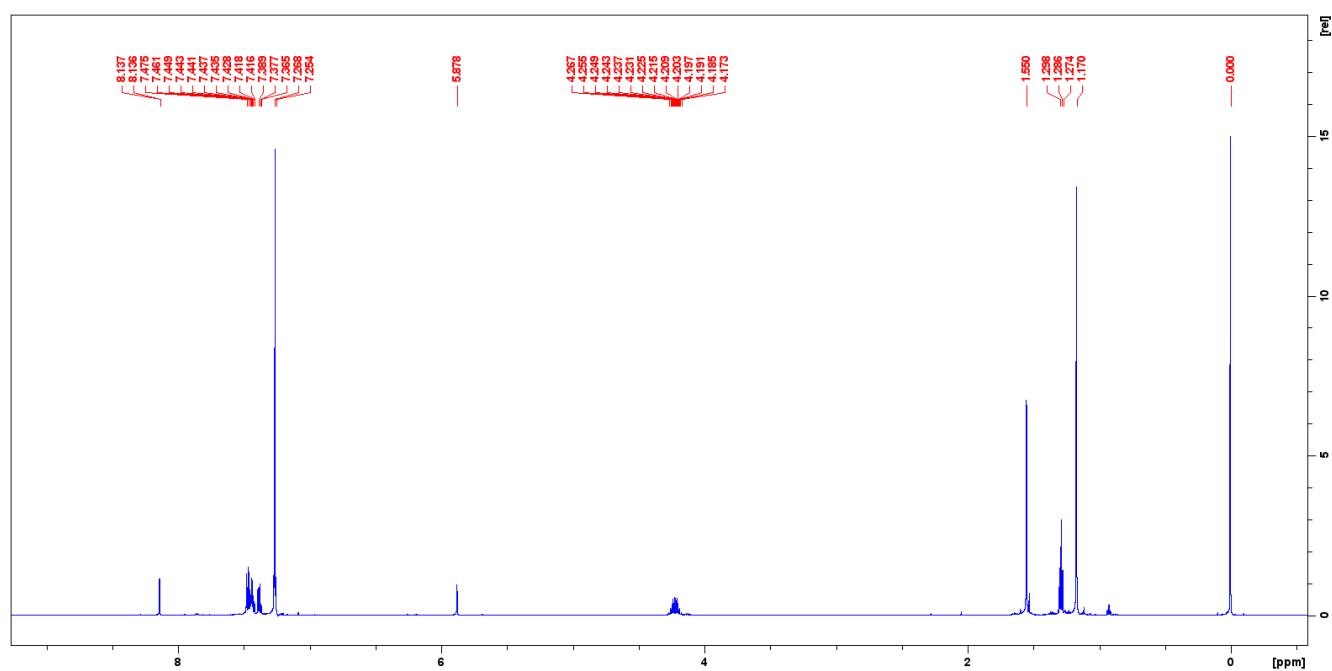


¹H NMR (600 MHz, CDCl₃) spectrum of **7n**. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **7n**.

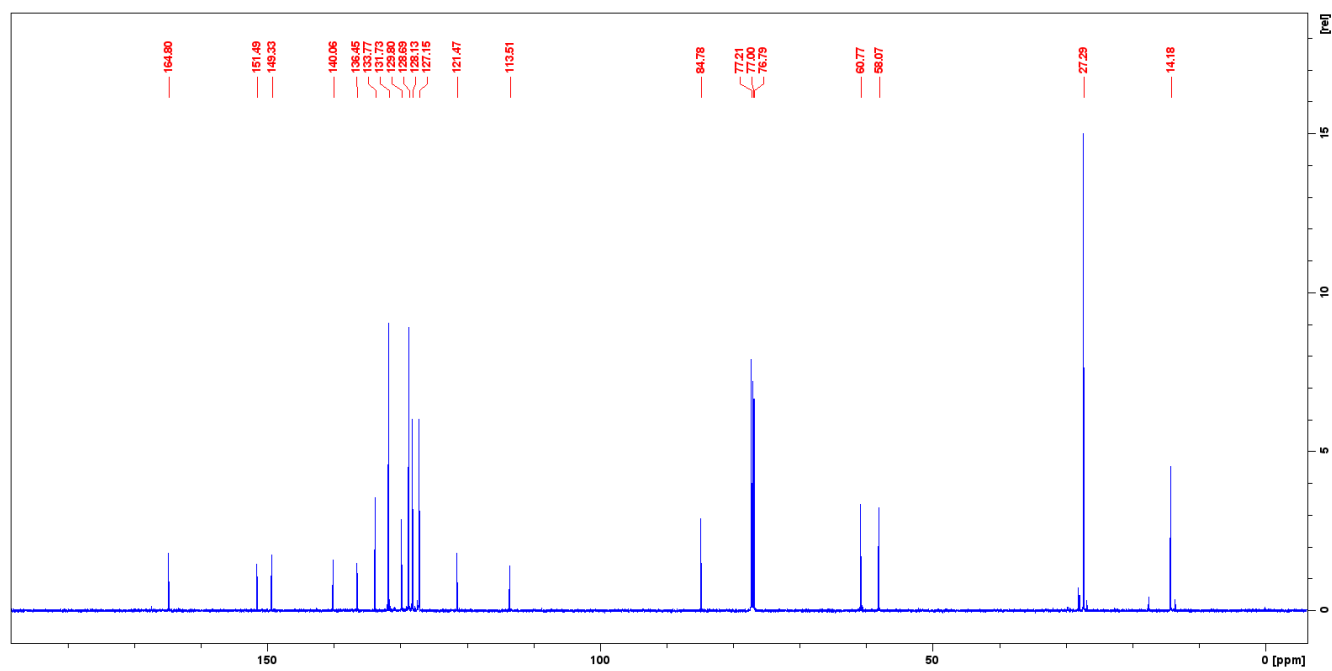
¹H NMR (600 MHz, CDCl₃) spectrum of **7o**. ^{13}C NMR (150 MHz, CDCl_3) spectrum of **7o**.

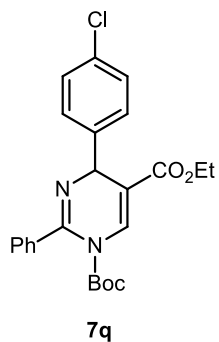


^1H NMR (600 MHz, CDCl_3) spectrum of **7p**.

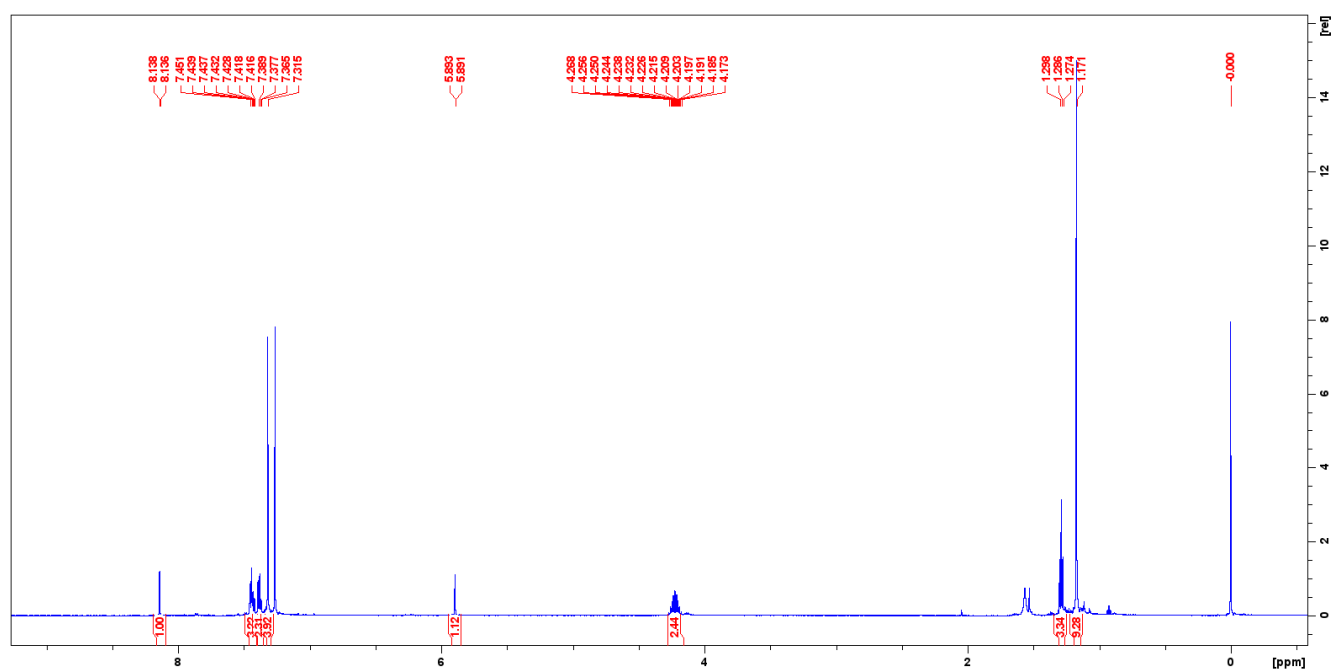


^{13}C NMR (150 MHz, CDCl_3) spectrum of **7p**.

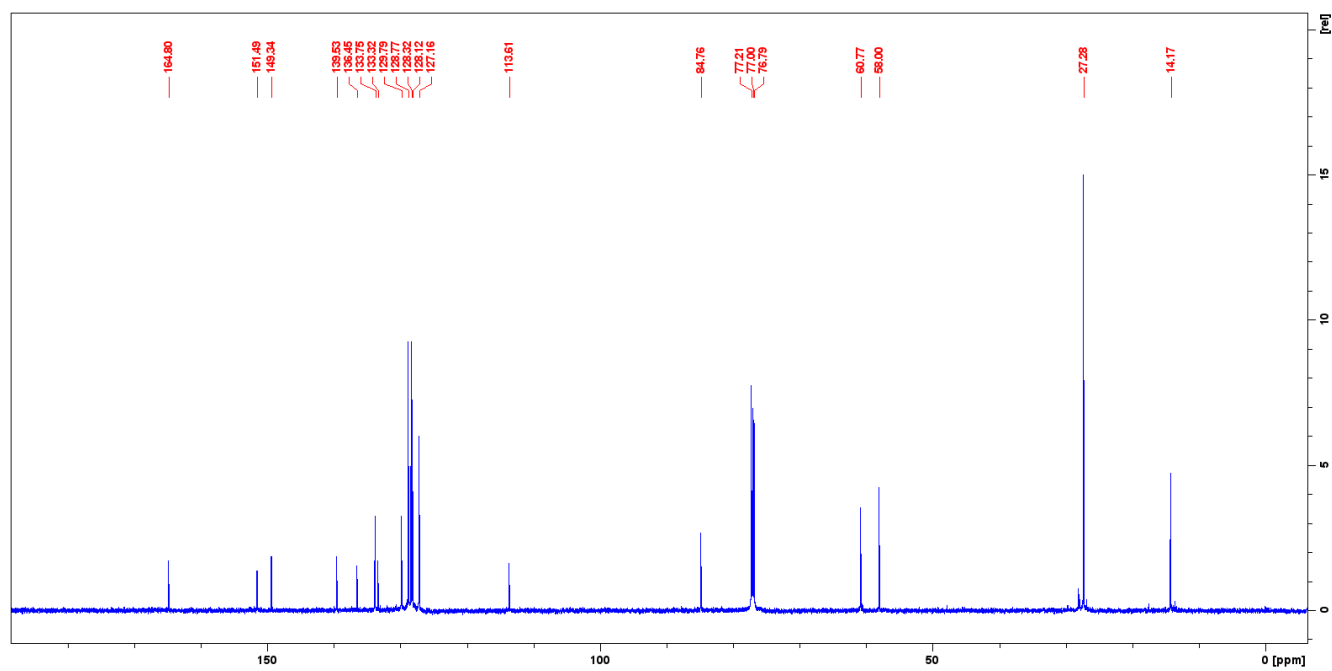


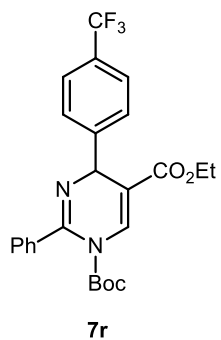


^1H NMR (600 MHz, CDCl_3) spectrum of **7q**.

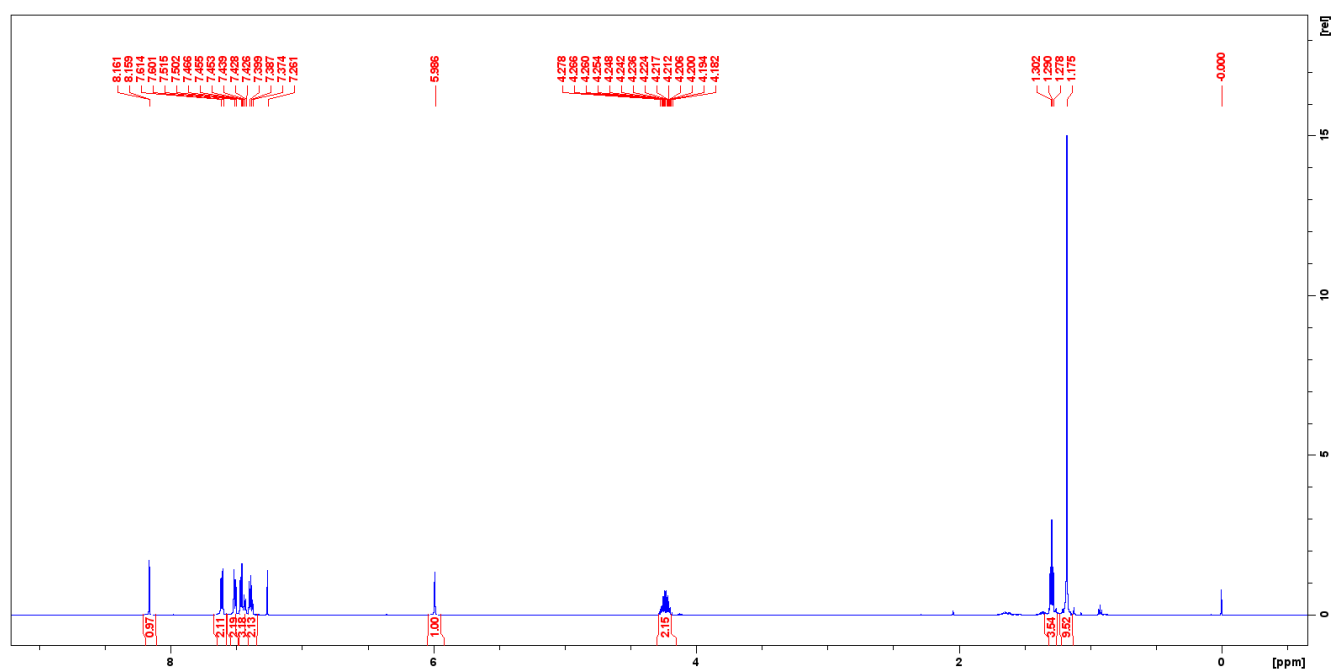


^{13}C NMR (150 MHz, CDCl_3) spectrum of **7q**.

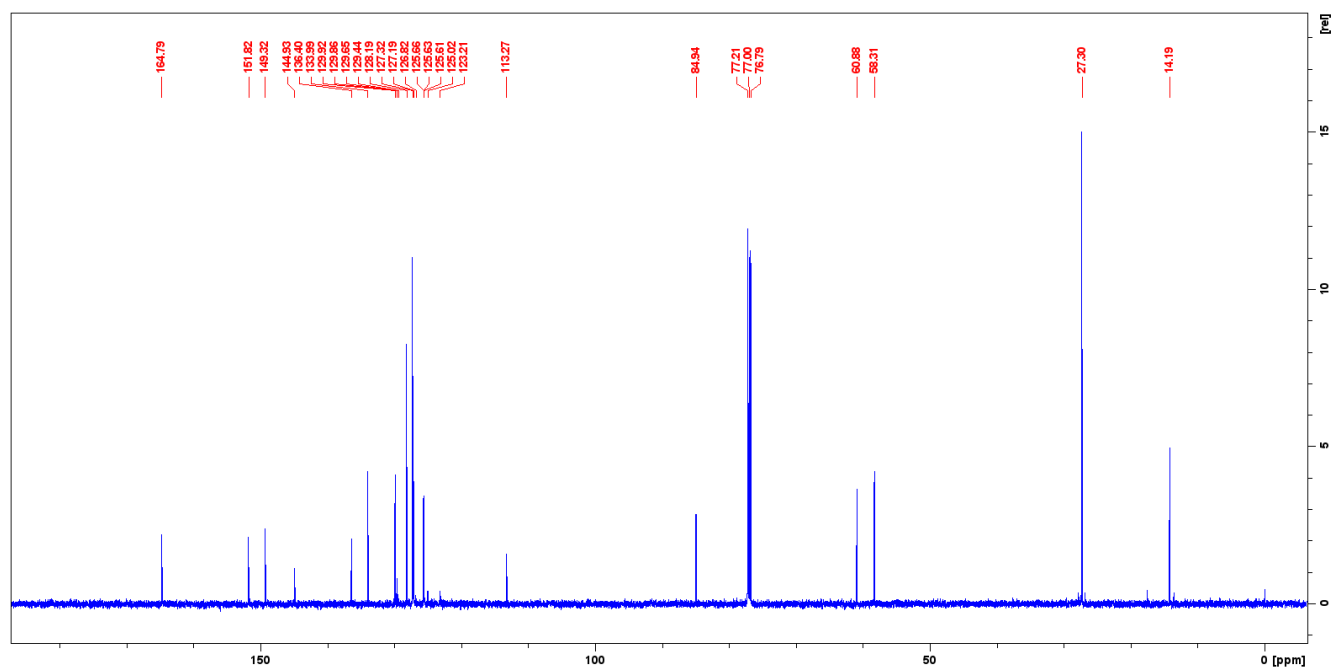




^1H NMR (600 MHz, CDCl_3) spectrum of **7r**.



^{13}C NMR (150 MHz, CDCl_3) spectrum of **7r**.





¹H NMR spectrum of compound 10 in CDCl₃. The x-axis represents chemical shift in ppm, ranging from 0 to 10. The y-axis represents relative intensity. The spectrum shows several peaks: a multiplet between 7.2 and 8.3 ppm (integral 1.00), a multiplet between 4.1 and 4.2 ppm (integral 2.34), a multiplet at 1.6 ppm (integral 3.24), and a sharp singlet at 0.00 ppm (integral 3.24). Integration values are shown in red below the baseline.

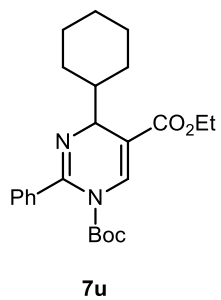
¹³C NMR spectrum (CDCl₃) of compound 10. The x-axis represents chemical shift in ppm, ranging from 0 to 160. The y-axis represents intensity. The spectrum shows several sharp peaks. Key peaks are labeled with their chemical shift values: 164.66, 150.62, 149.53, 138.35, 134.92, 134.14, 130.14, 128.88, 128.66, 127.92, 127.10, 112.30, 84.61, 77.21, 76.79, 60.68, 56.50, 27.29, 14.07, and -0.05. The peaks at 77.21 and 76.79 ppm correspond to the CDCl₃ solvent triplet.



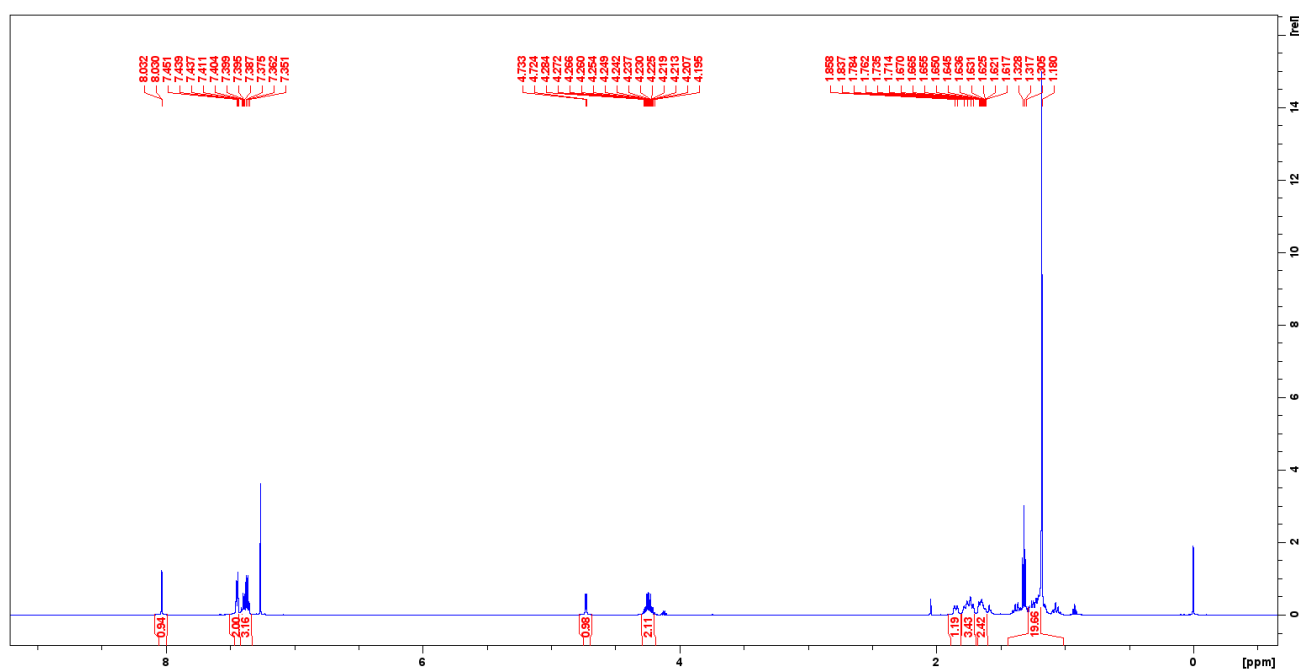
¹H NMR spectrum of compound 10 in CDCl₃. The spectrum shows peaks in the aromatic region (7.3-8.1 ppm), a methine region (4.2-4.9 ppm), and an aliphatic region (1.3-1.7 ppm). Integration values are provided below the peaks, and chemical shifts are listed above them.

Chemical Shift (ppm)	Integration
8.016, 8.014, 8.012, 7.958, 7.933, 7.922, 7.915, 7.912, 7.910, 7.905, 7.900, 7.896, 7.891, 7.885, 7.888, 7.375, 7.375, 7.374, 7.362, 7.361, 7.358	1.00, 5.50
4.815, 4.813, 4.803, 4.794, 4.772, 4.775, 4.269, 4.267, 4.261, 4.254, 4.246, 4.245, 4.240, 4.234, 4.218, 4.212, 4.210	1.15, 2.35
1.655, 1.650, 1.647, 1.646, 1.645, 1.638, 1.632, 1.629, 1.620, 1.615, 1.583, 1.560, 1.553, 1.542, 1.540, 1.536, 1.530, 1.527, 1.502, 1.490, 1.478, 1.475, 1.330, 1.318, 1.306, 0.965, 0.963, 0.971	2.45, 1.05, 1.35, 3.85, 3.32
0.000	

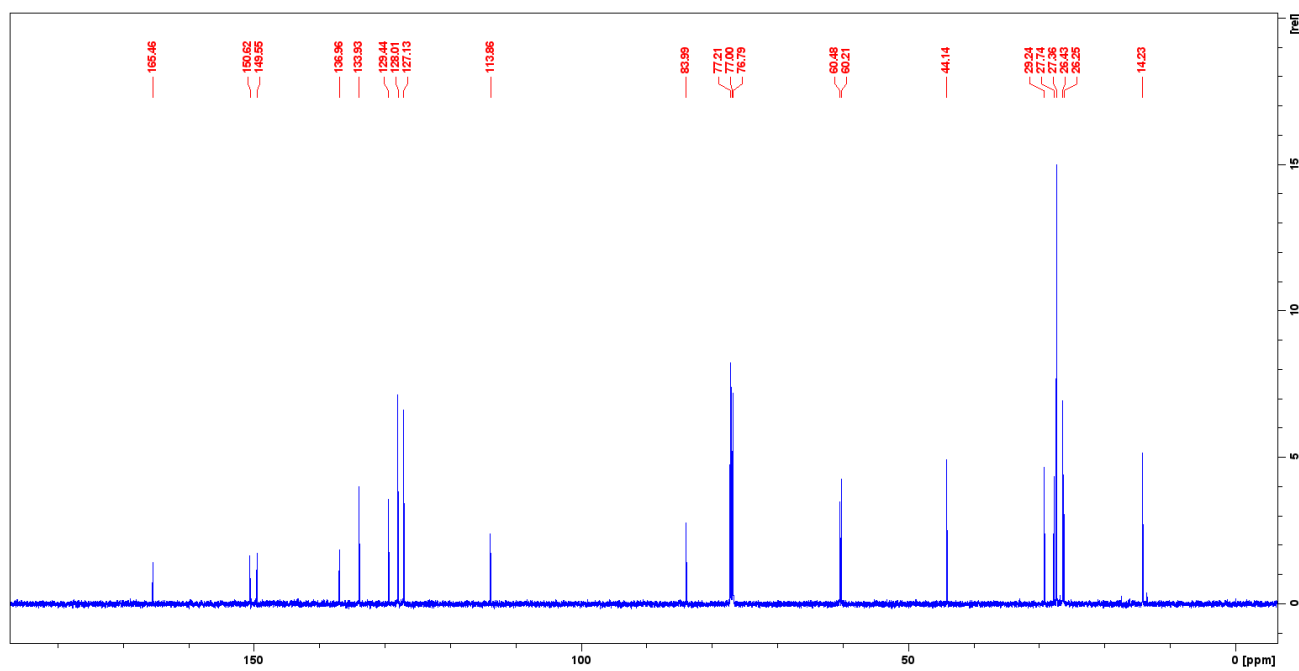
165.17
150.55
149.50
137.02
133.69
129.42
127.11
115.11
84.16
77.21
76.79
60.50
54.98
37.96
27.34
18.37
14.24
14.10

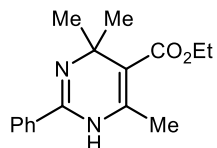


^1H NMR (600 MHz, CDCl_3) spectrum of **7u**.



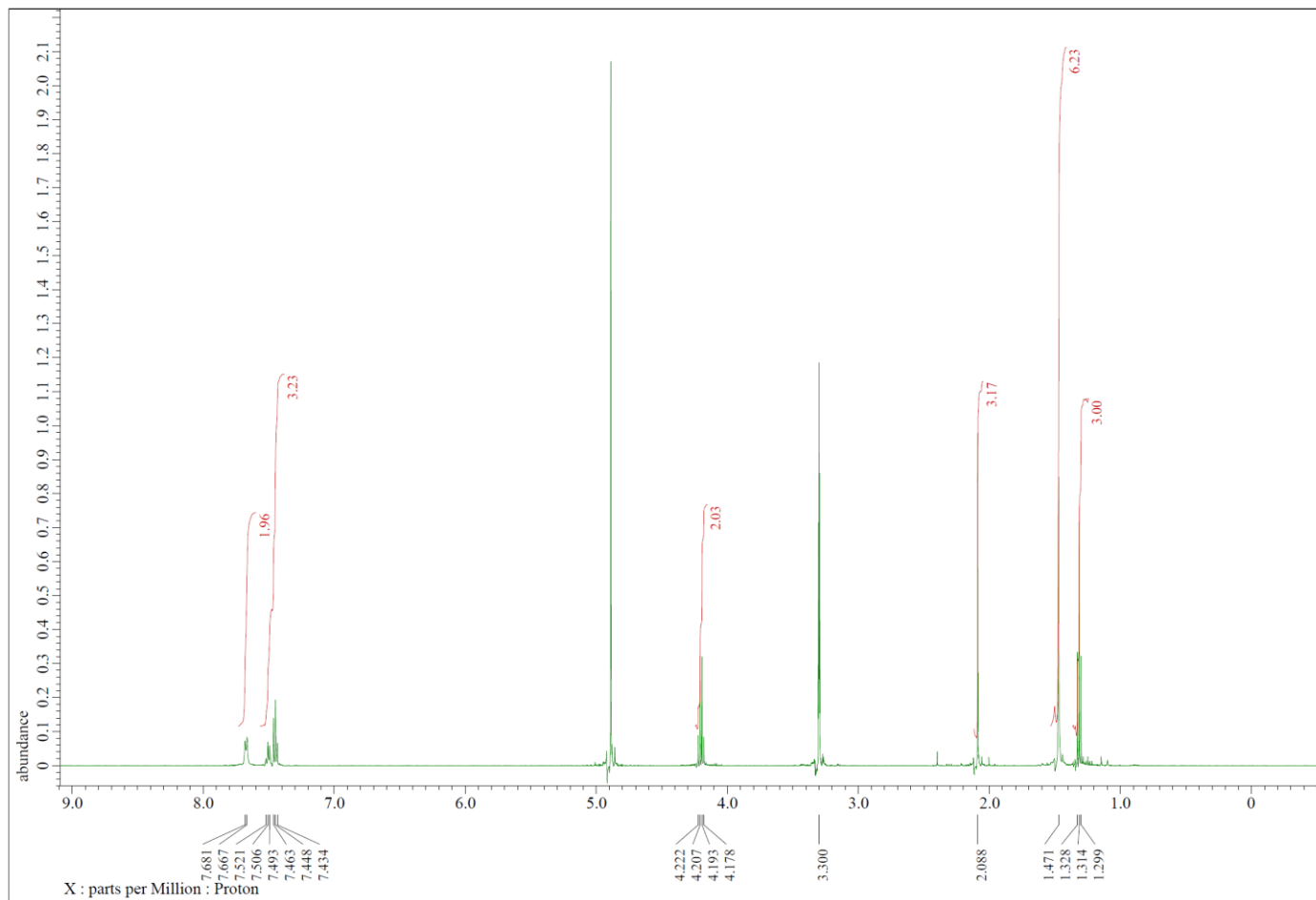
^{13}C NMR (150 MHz, CDCl_3) spectrum of **7u**.



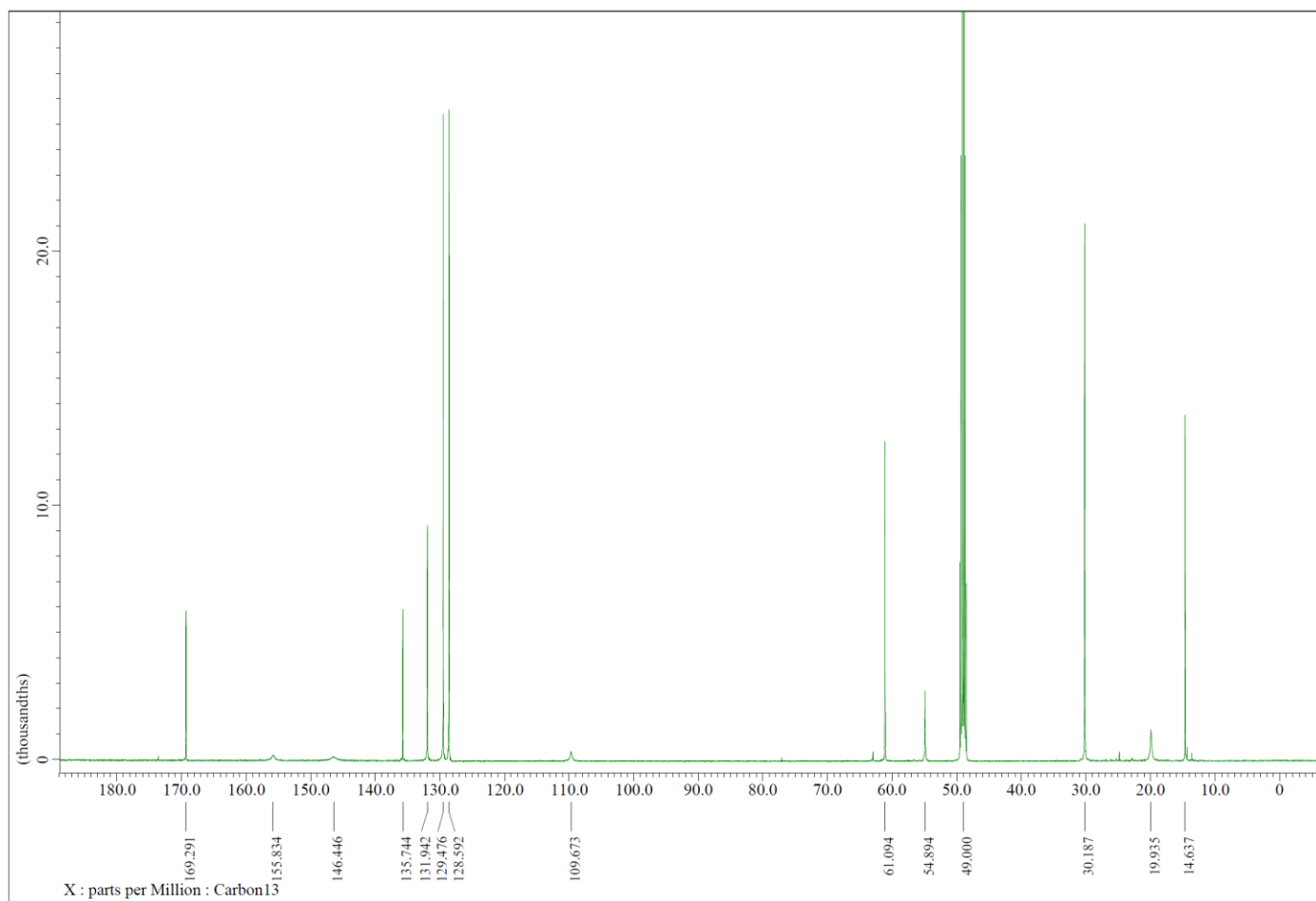


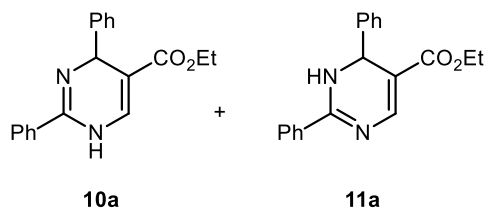
9

^1H NMR (500 MHz, CD_3OD) spectrum of **9**.

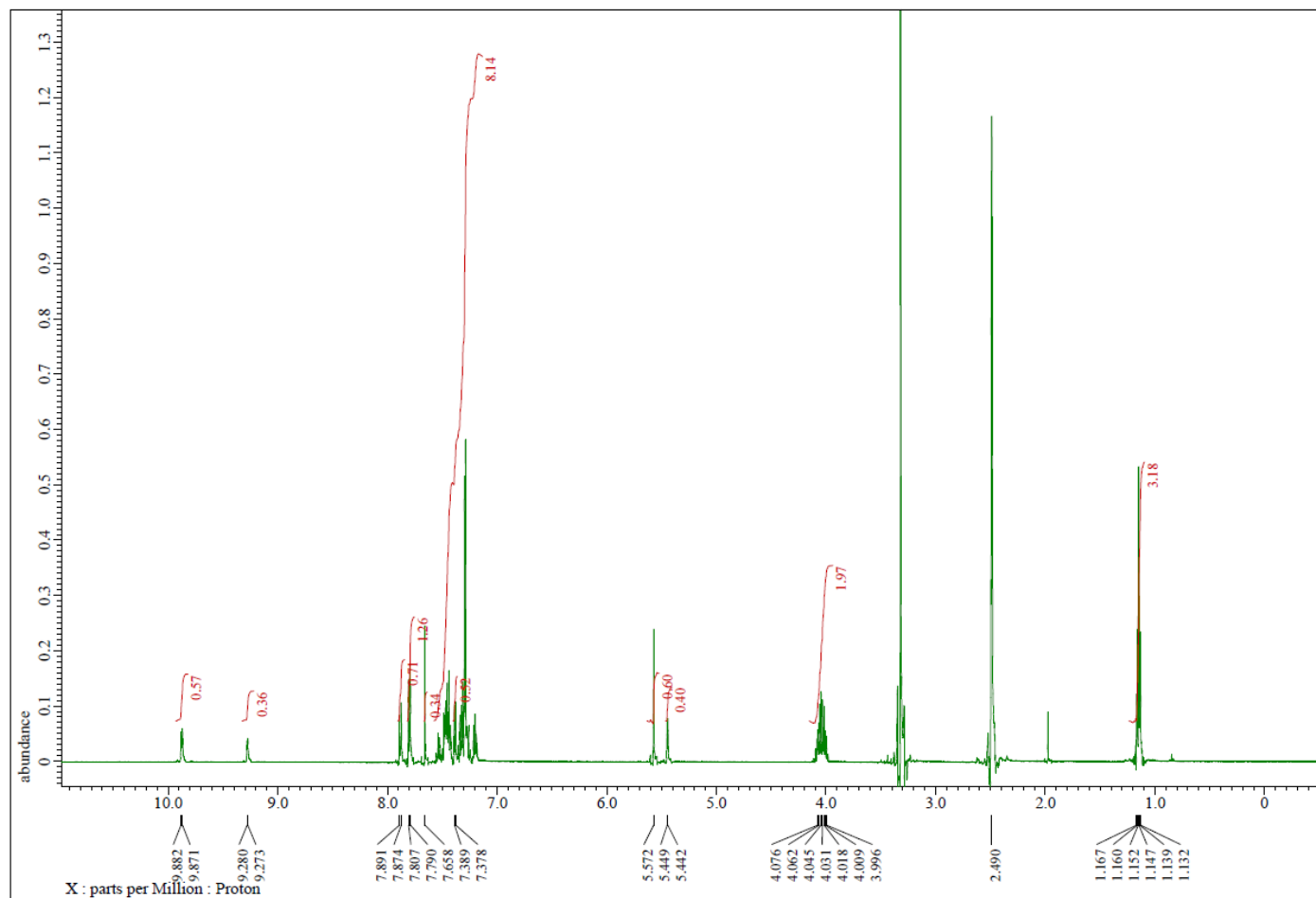


^{13}C NMR (125 MHz, CD_3OD) spectrum of **9**.

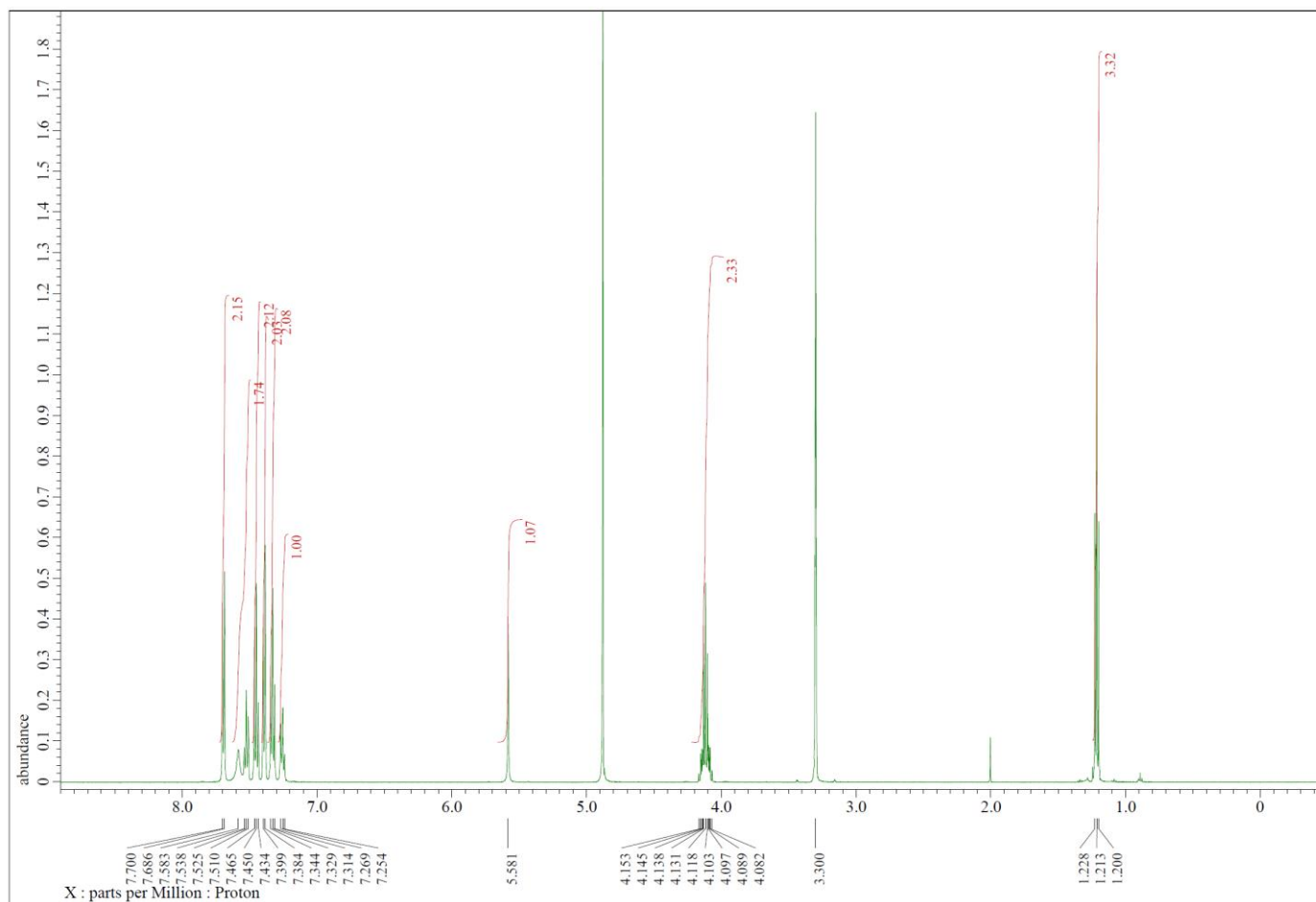




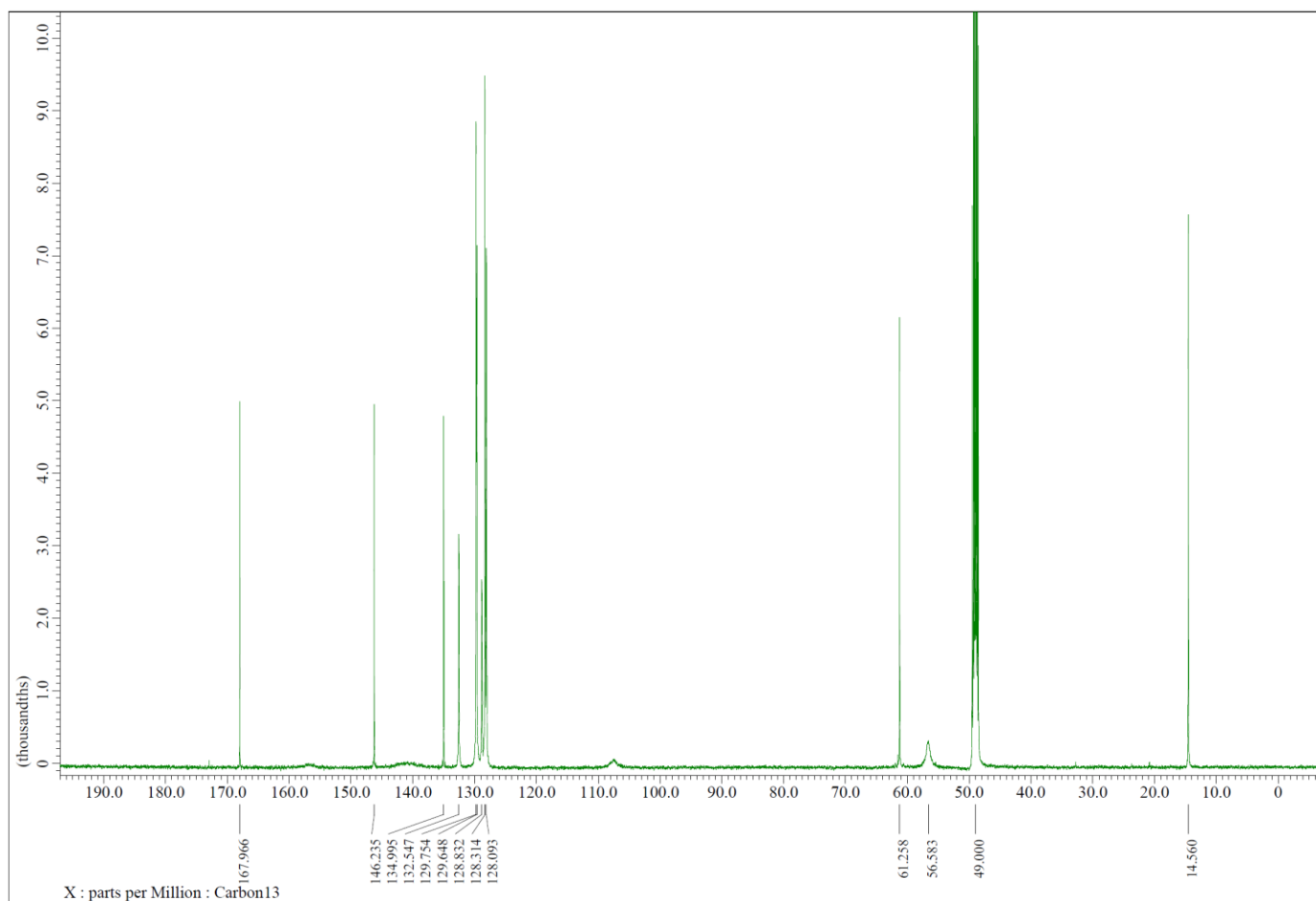
^1H NMR (500 MHz, DMSO- d_6) spectrum of **10a** + **11a**.

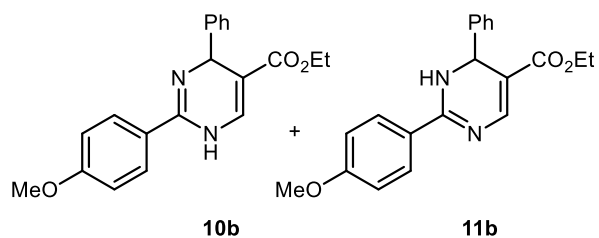


^1H NMR (500 MHz, CD_3OD) spectrum of **10a** + **11a**.

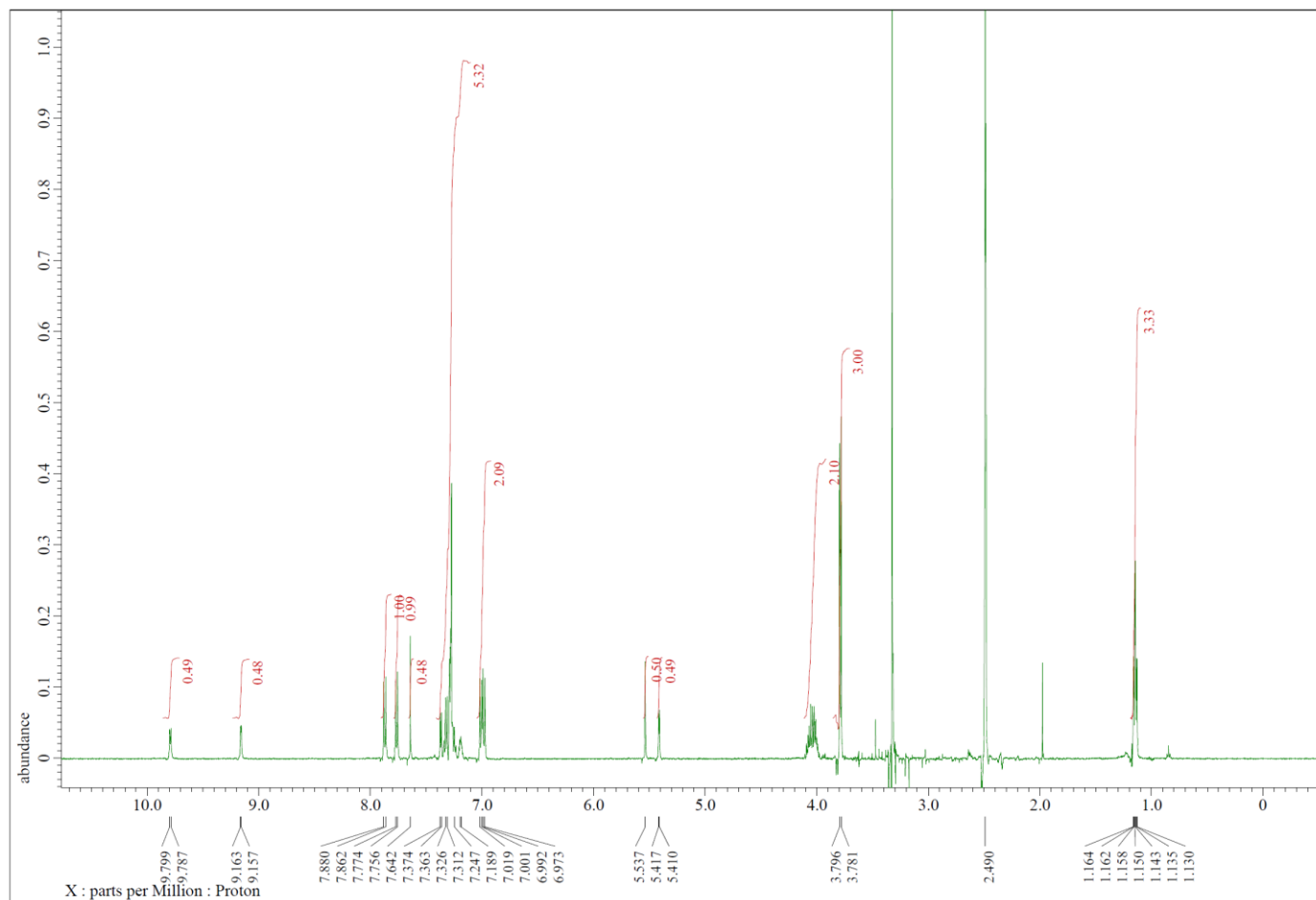


^{13}C NMR (125 MHz, CD_3OD) spectrum of **10a** + **11a**.

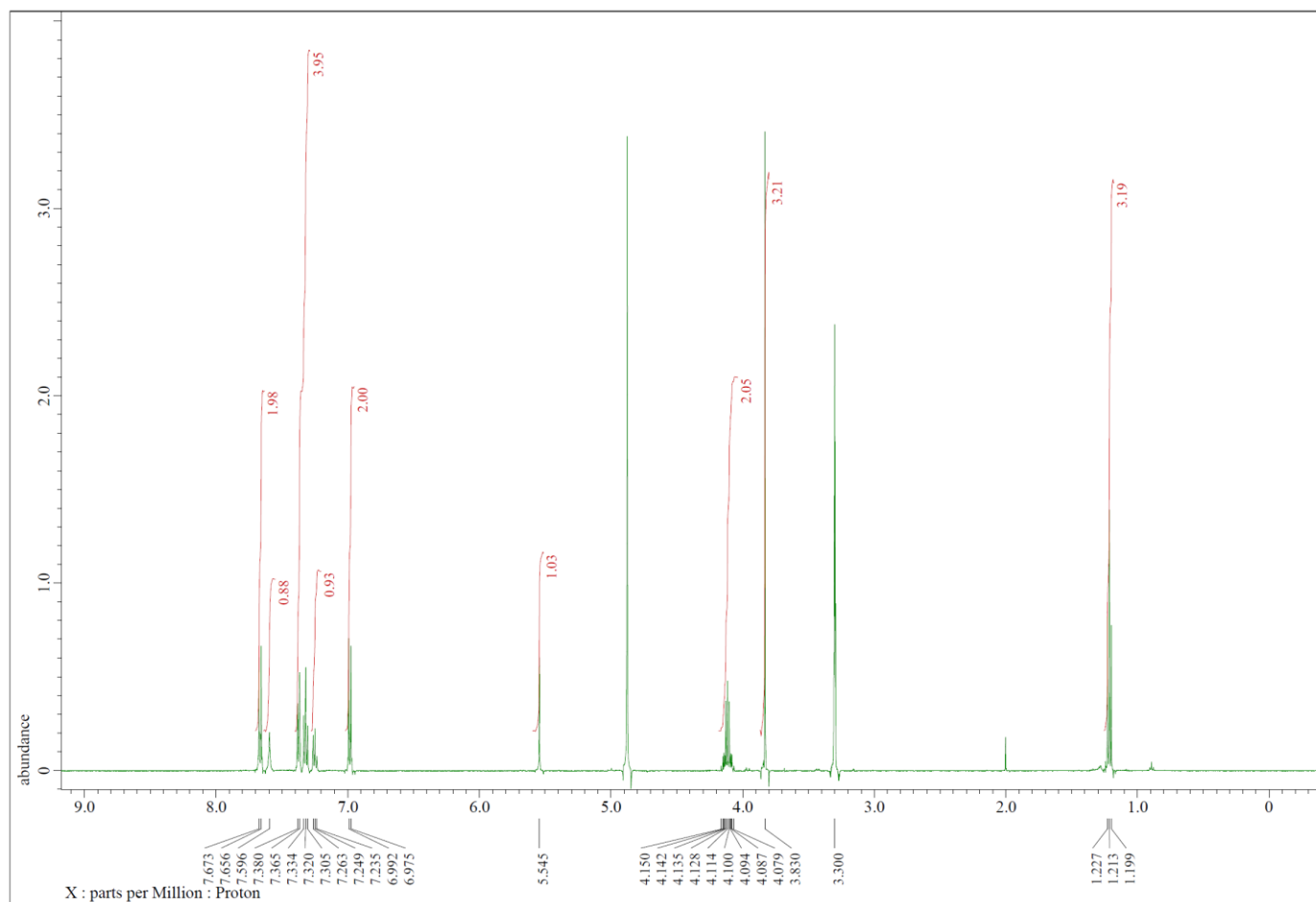




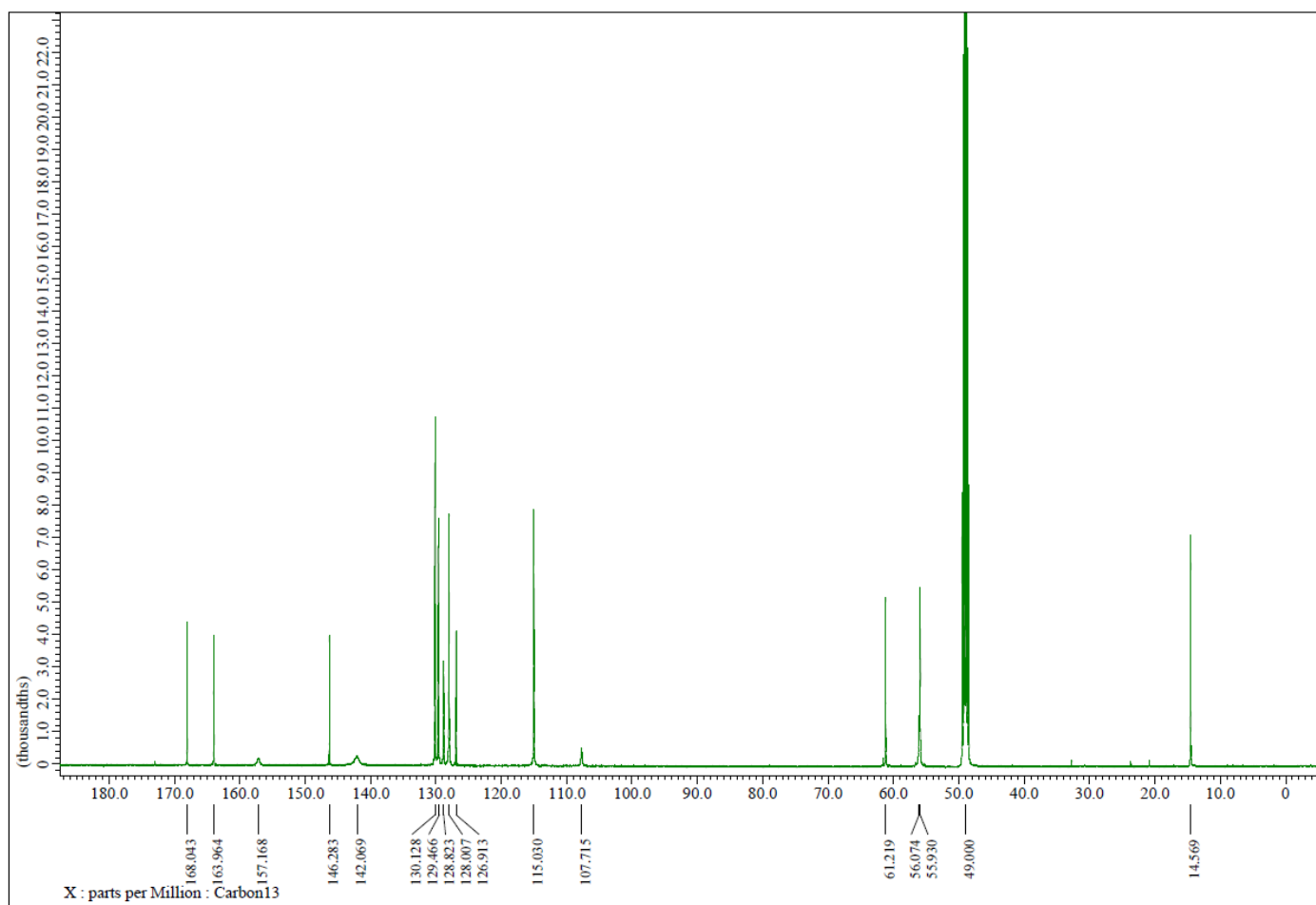
^1H NMR (500 MHz, $\text{DMSO}-d_6$) spectrum of **10b** + **11b**.

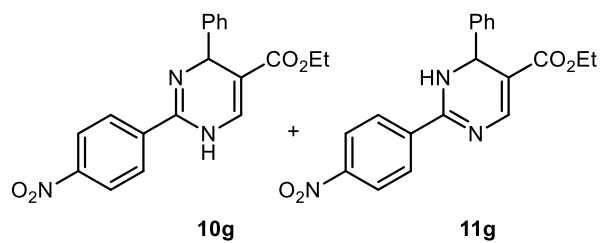


^1H NMR (500 MHz, CD_3OD) spectrum of **10b** + **11b**.

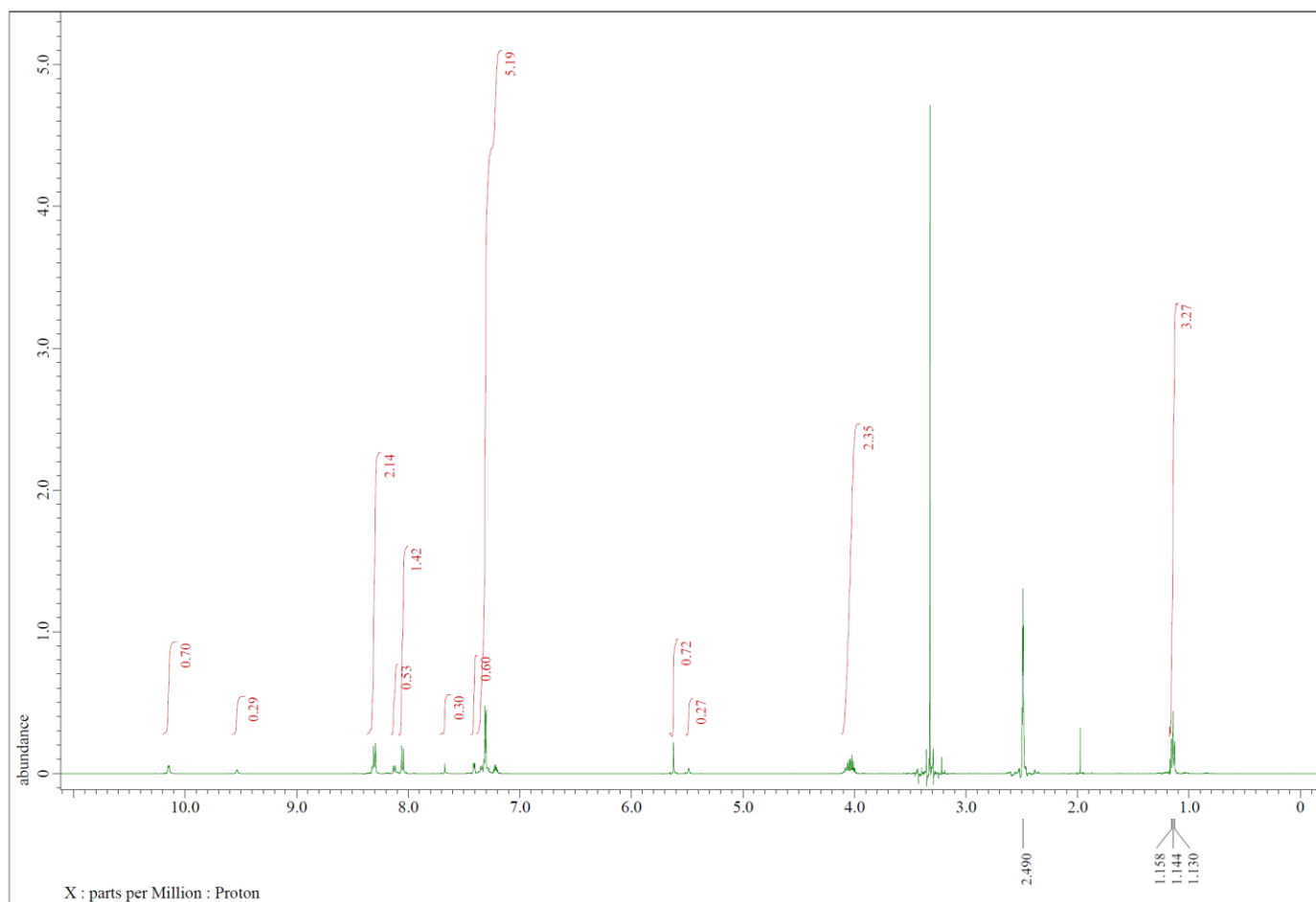


^{13}C NMR (125 MHz, CD_3OD) spectrum of **10b** + **11b**.

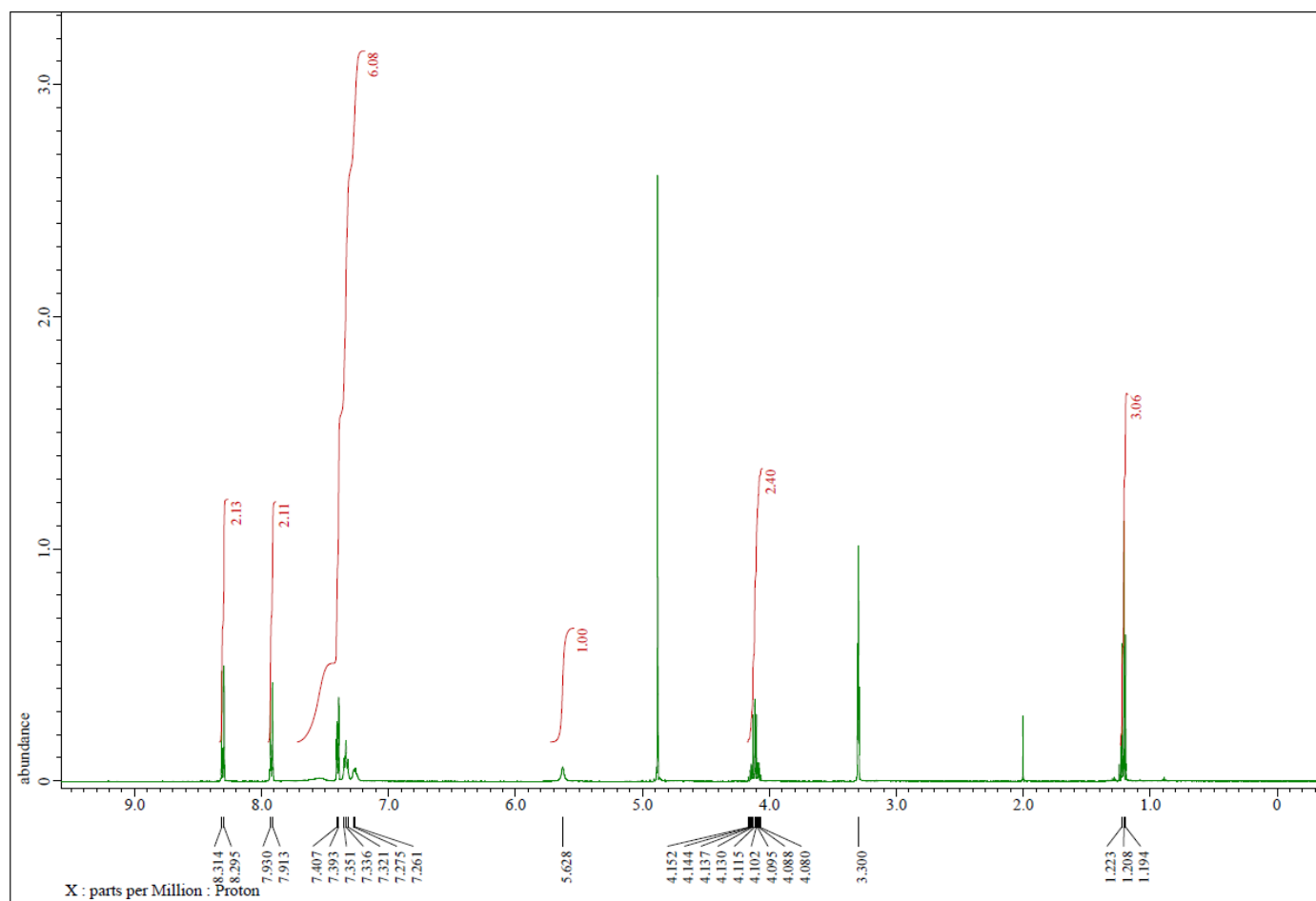




^1H NMR (500 MHz, DMSO- d_6) spectrum of **10g** + **11g**.



^1H NMR (500 MHz, CD_3OD) spectrum of **10g** + **11g**.



^{13}C NMR (125 MHz, CD_3OD) spectrum of **10g** + **11g**.

