

Copper-Catalyzed Xanthine–Chalcogenide Hybrids: Synthesis, DNA Binding & Docking

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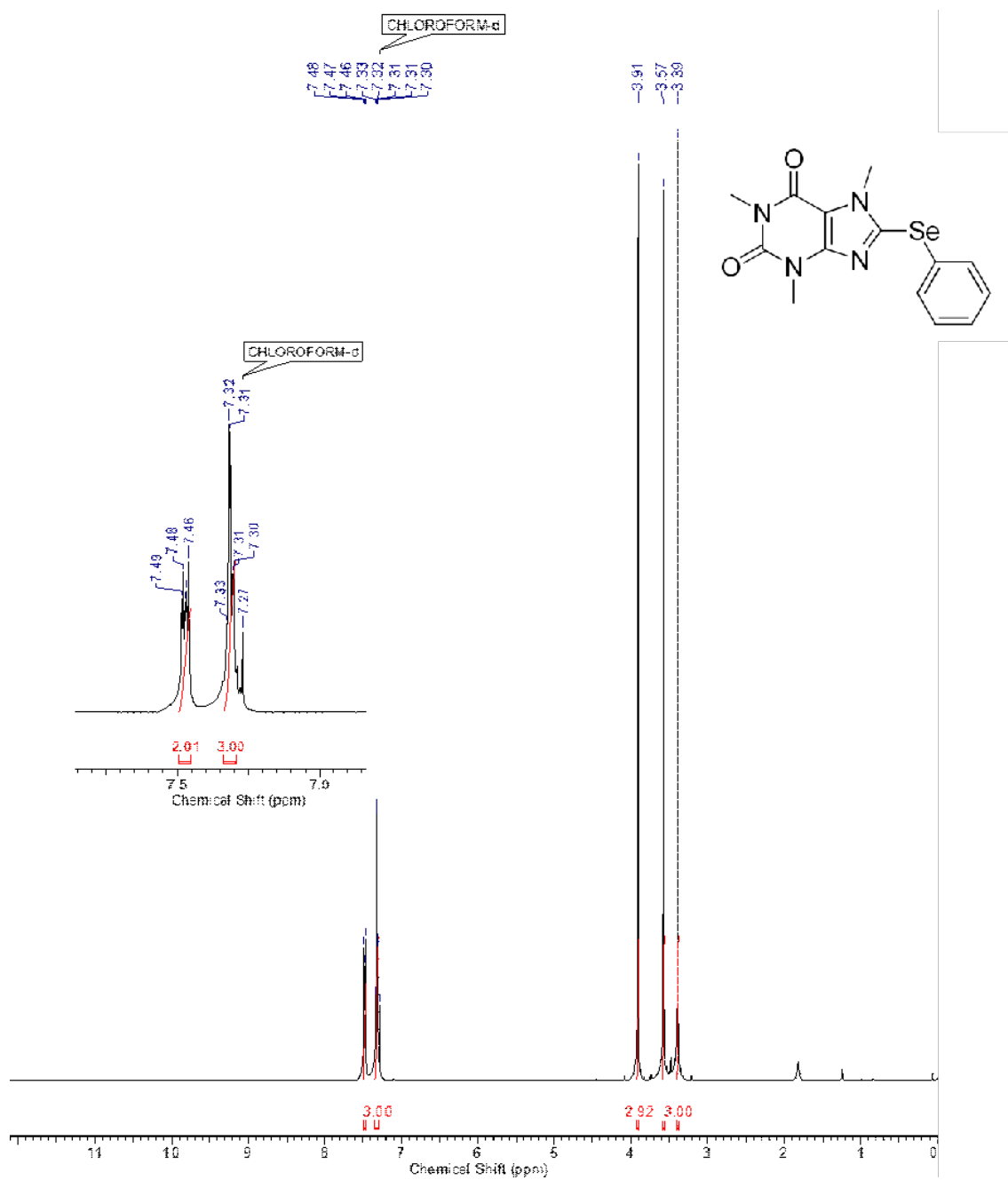
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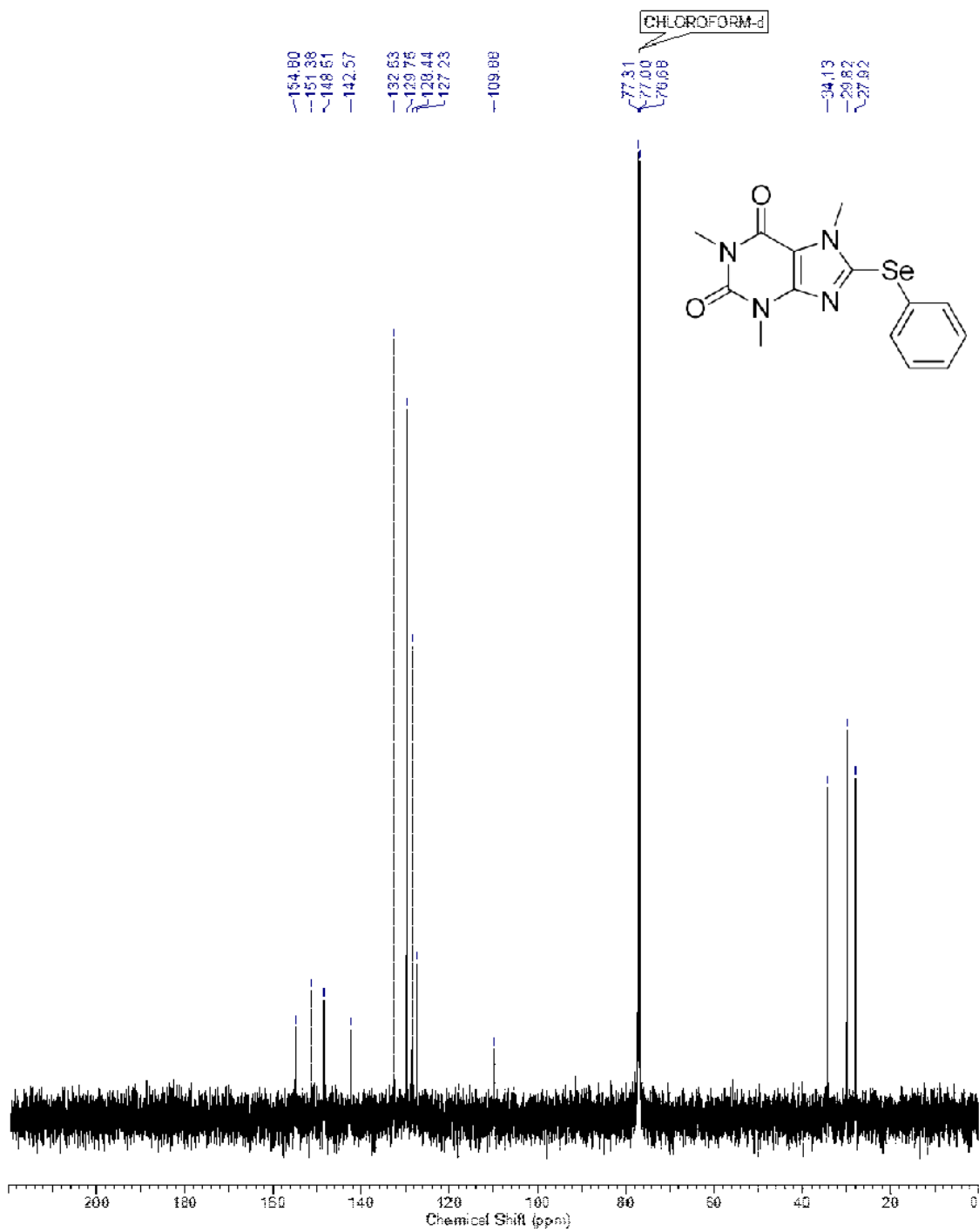
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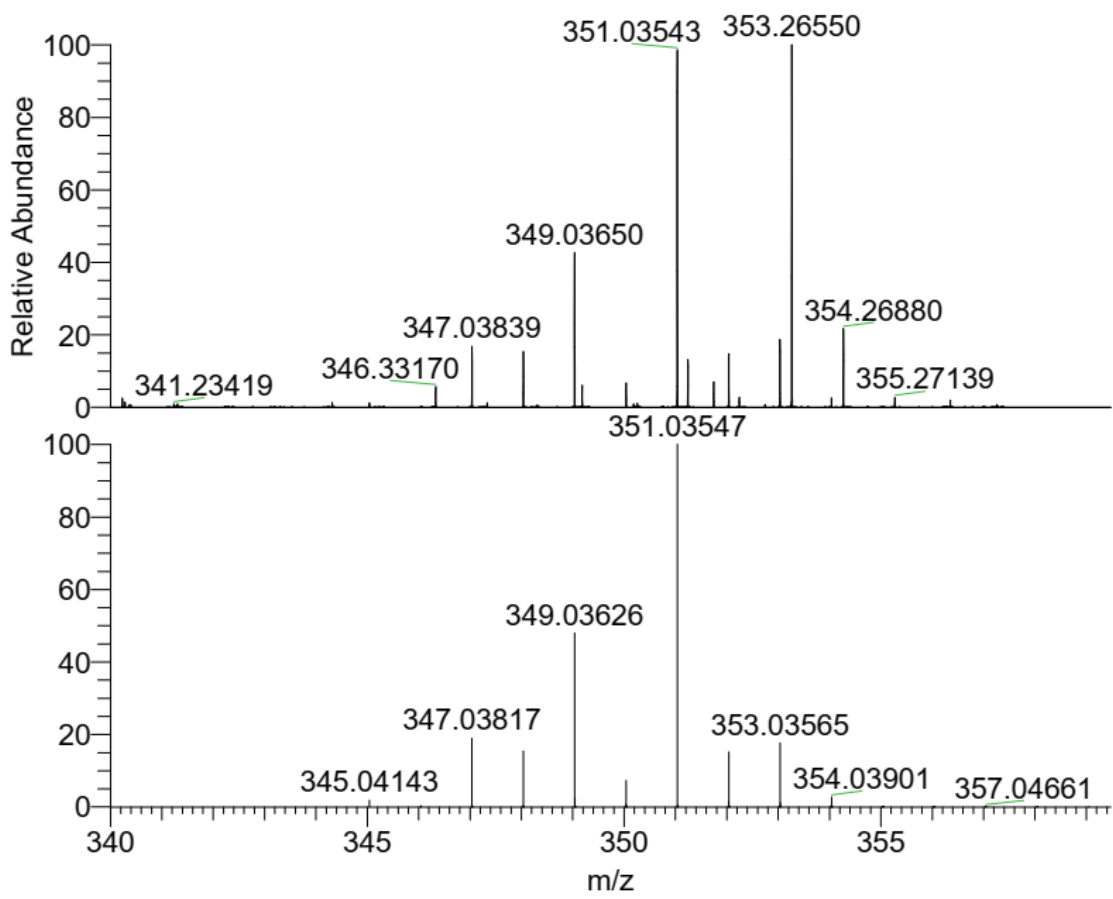
1. NMR spectra



^1H NMR (400 MHz, CDCl_3) spectrum of **3**.

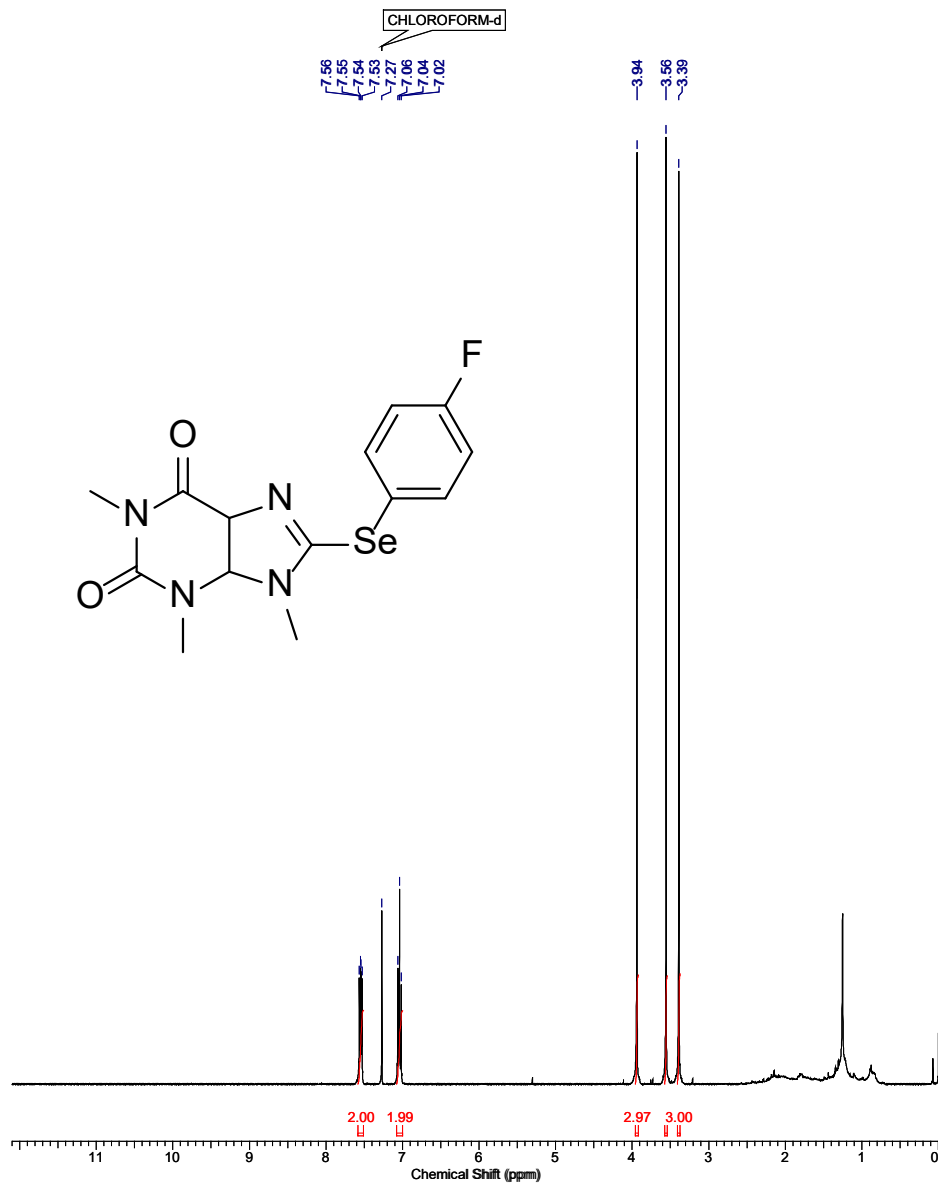


^{13}C NMR (100 MHz, CDCl_3) spectrum of **3**.



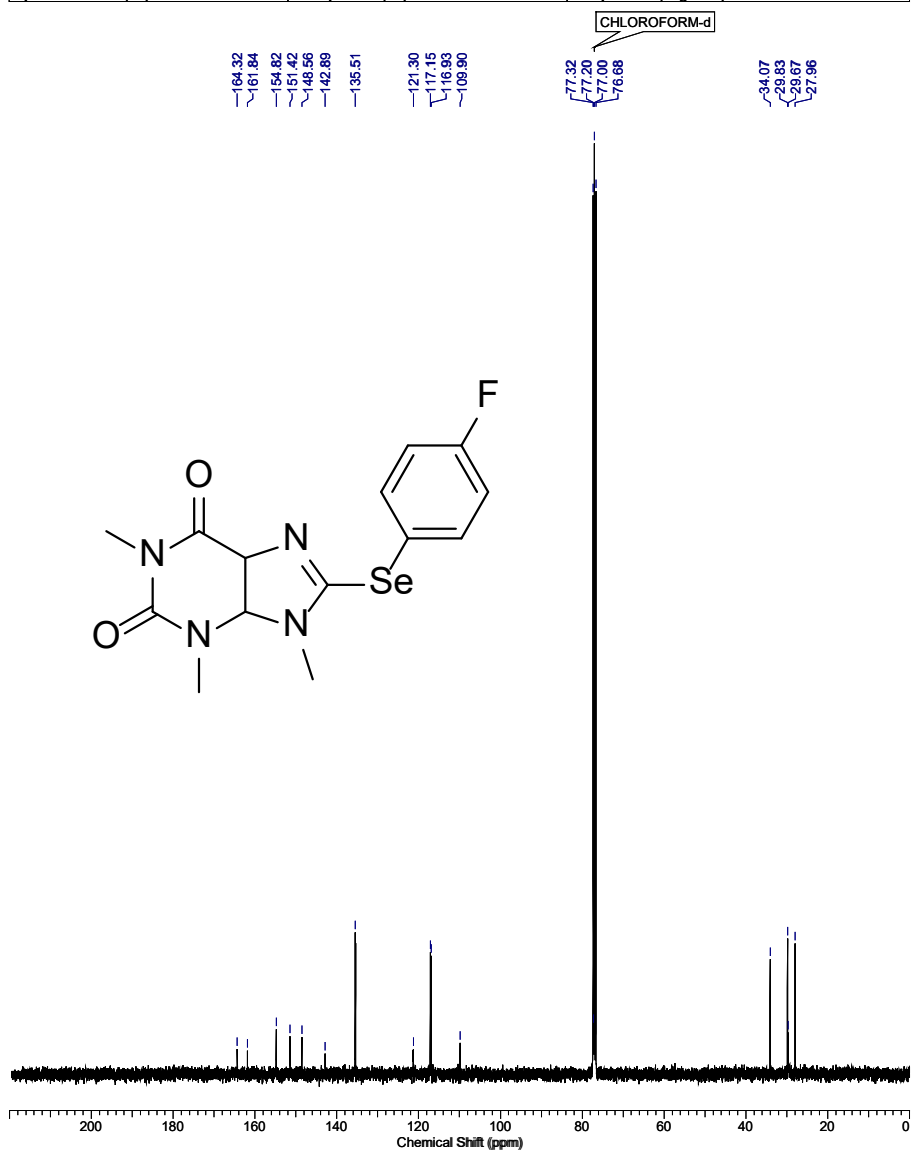
HRMS (ESI) - [M+H]⁺ of 3

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Date Stamp	06 Jun 2024 12:40:48				
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Frequency (MHz)	400.06	Nucleus	1H	Number of Transients	4
Origin	spect	Original Points Count	32768	Owner	root
Points Count	32768	Pulse Sequence	zg30	Receiver Gain	143.70
SW(cyclical) (Hz)	8250.83	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2468.9277	Sweep Width (Hz)	8250.57	Temperature (degree C)	27.000

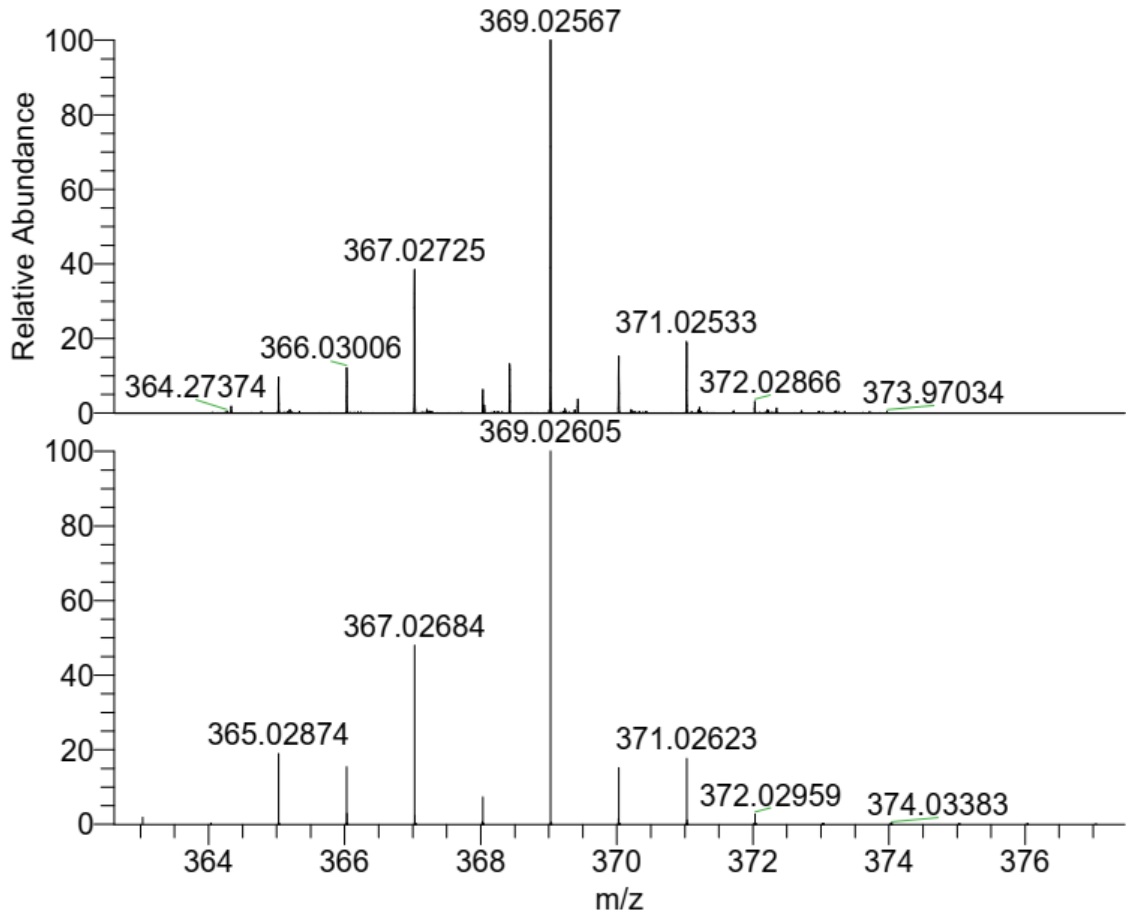


^1H NMR (400 MHz, CDCl_3) spectrum of **4**.

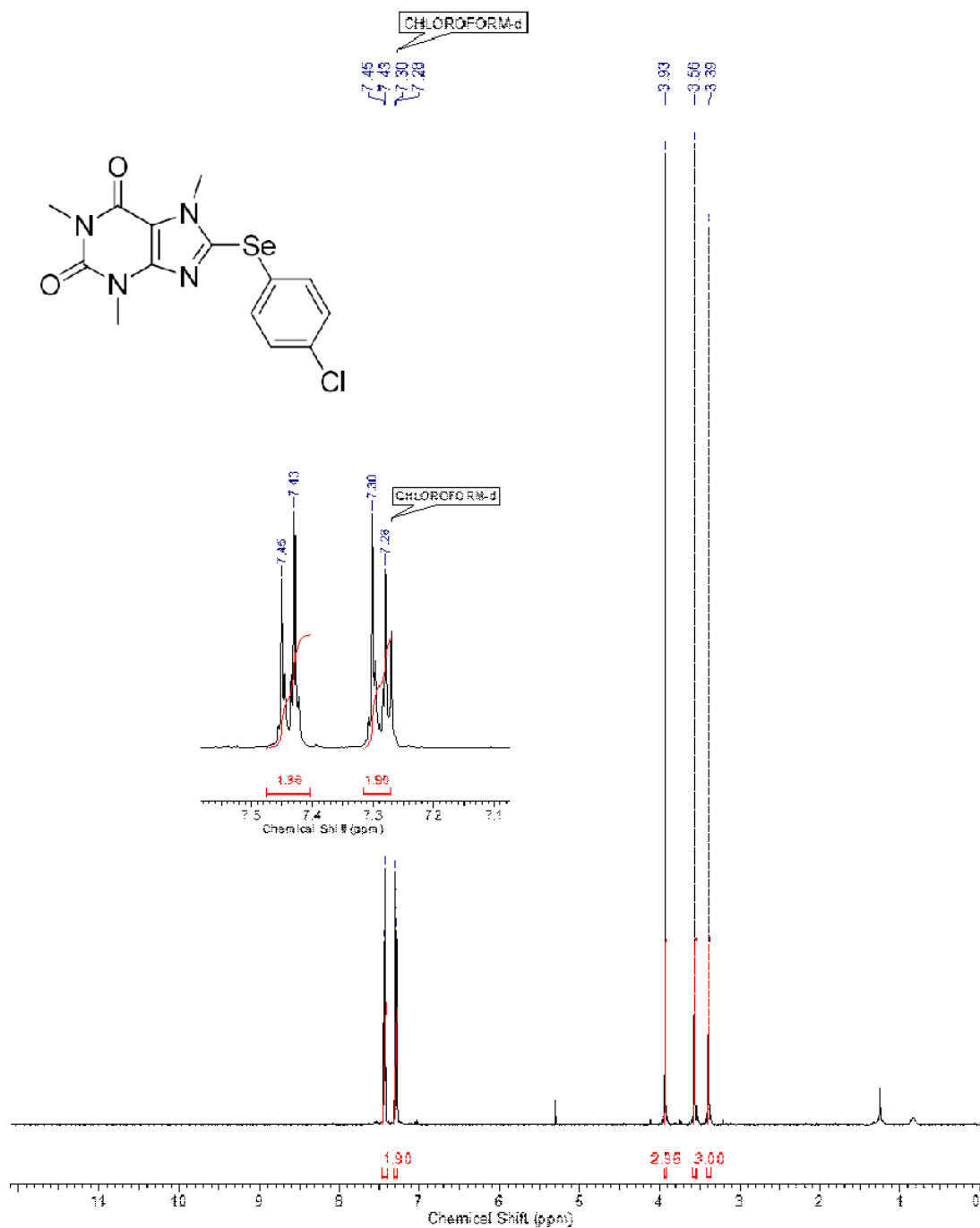
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File Name	C:\Users\suzane\Desktop\RMN_Cafeina\FSe+CAF_CDCl3\024_Junho\NataC_FSe+CAF_CDCl3\2\pdata1\1r				
Frequency (MHz)	100.60	Nucleus	13C	Number of Transients	4352
Origin	spect	Original Points Count	32768	Owner	root
Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	181.00
SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d		
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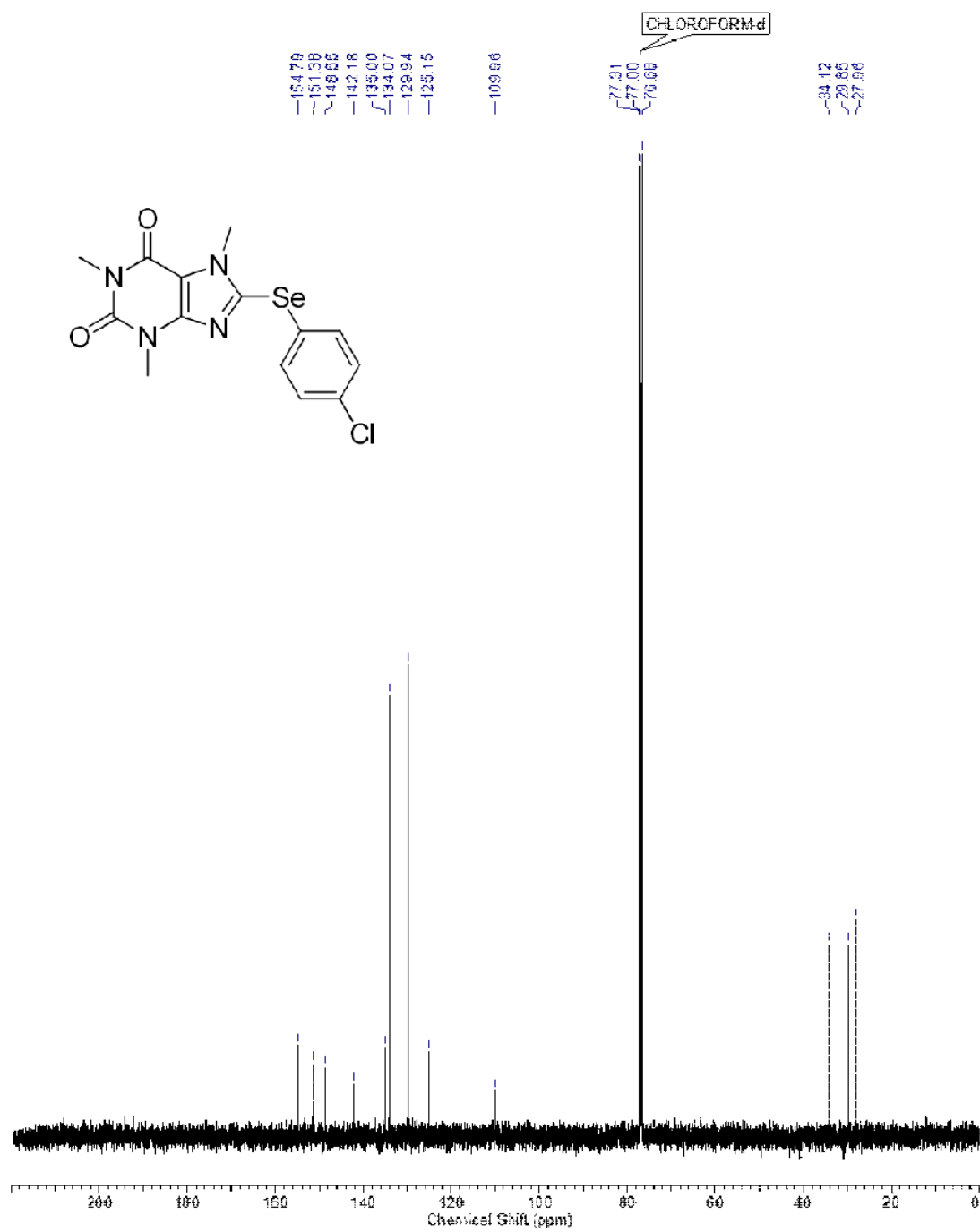
^{13}C NMR (100 MHz, CDCl_3) spectrum of 4.



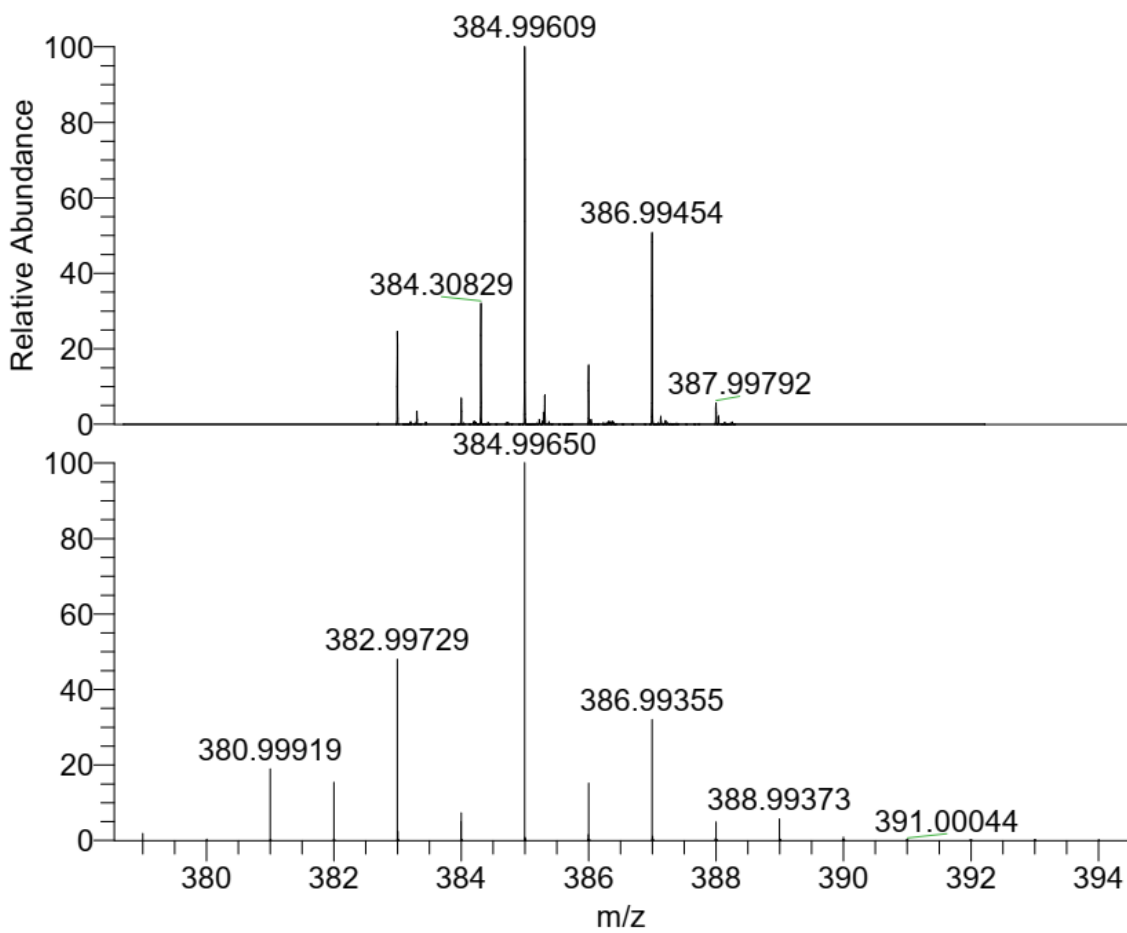
HRMS (ESI) - [M+H]⁺ of 4



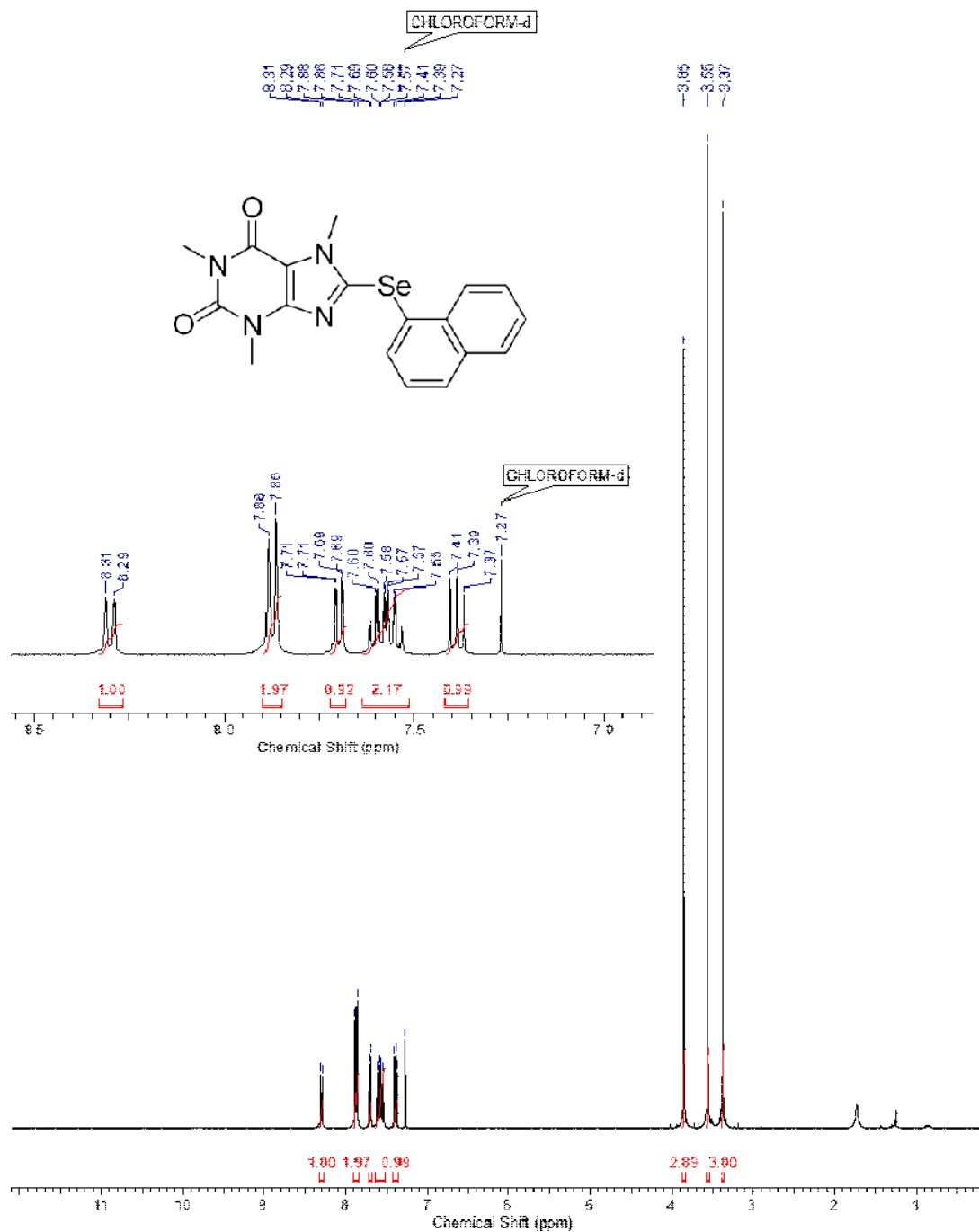
¹H NMR (400 MHz, CDCl₃) spectrum of 5.



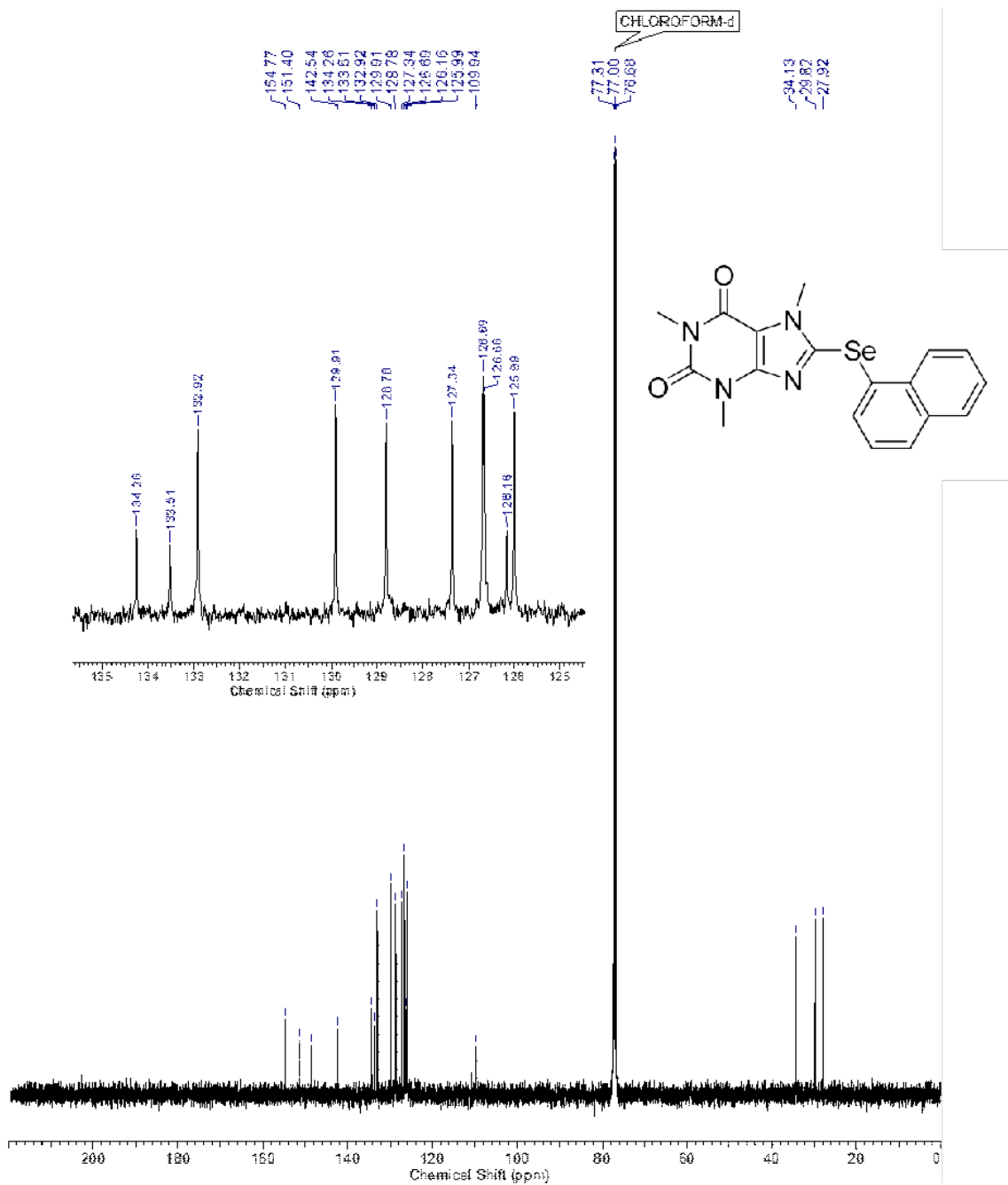
^{13}C NMR (100 MHz, CDCl_3) spectrum of **5**.



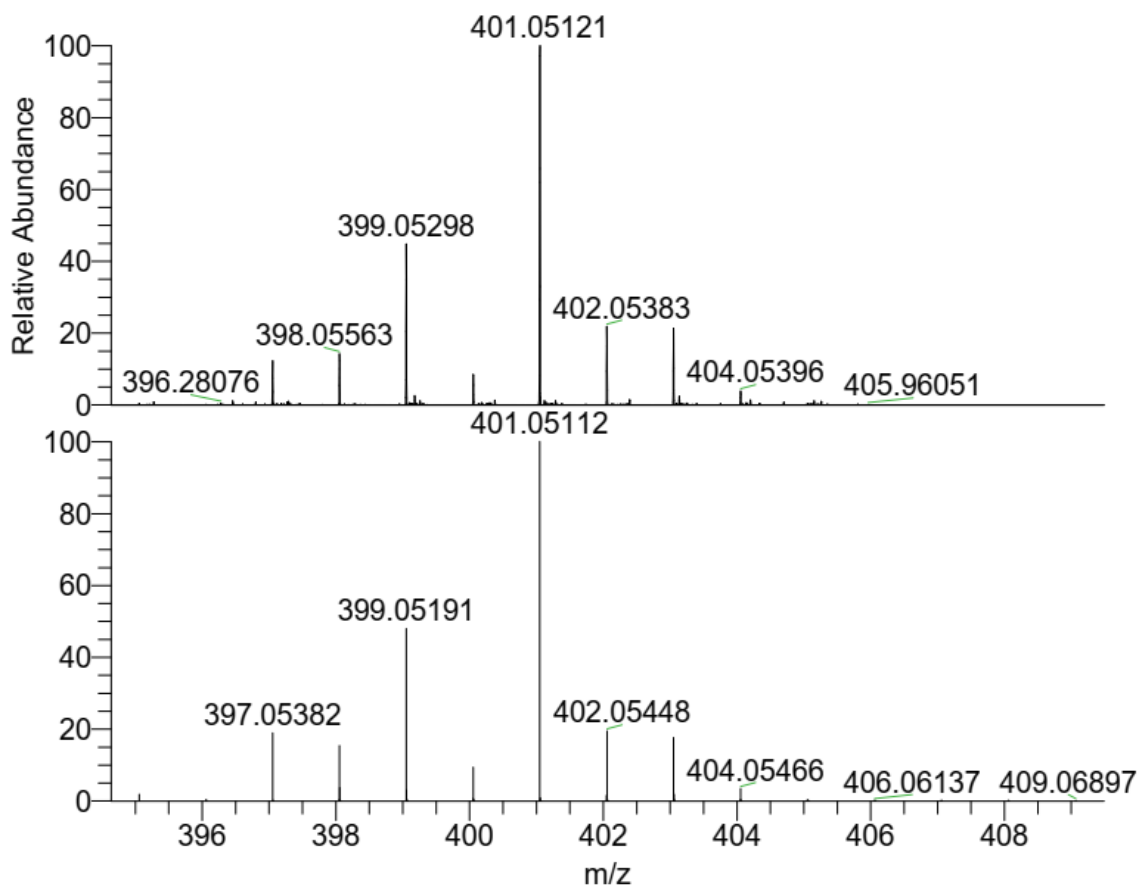
HRMS (ESI) - [M+H]⁺ of 5



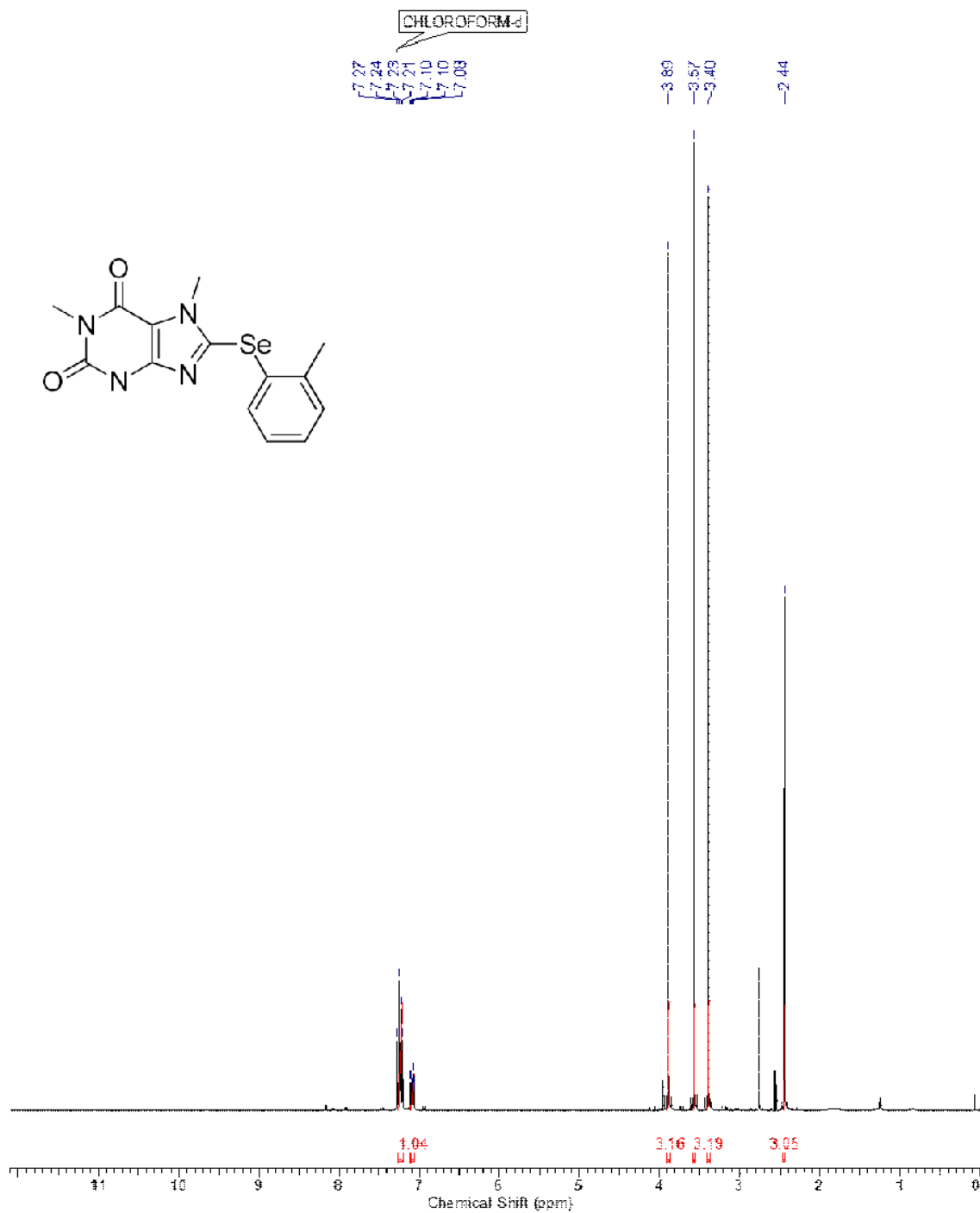
^1H NMR (400 MHz, CDCl_3) spectrum of **6**.



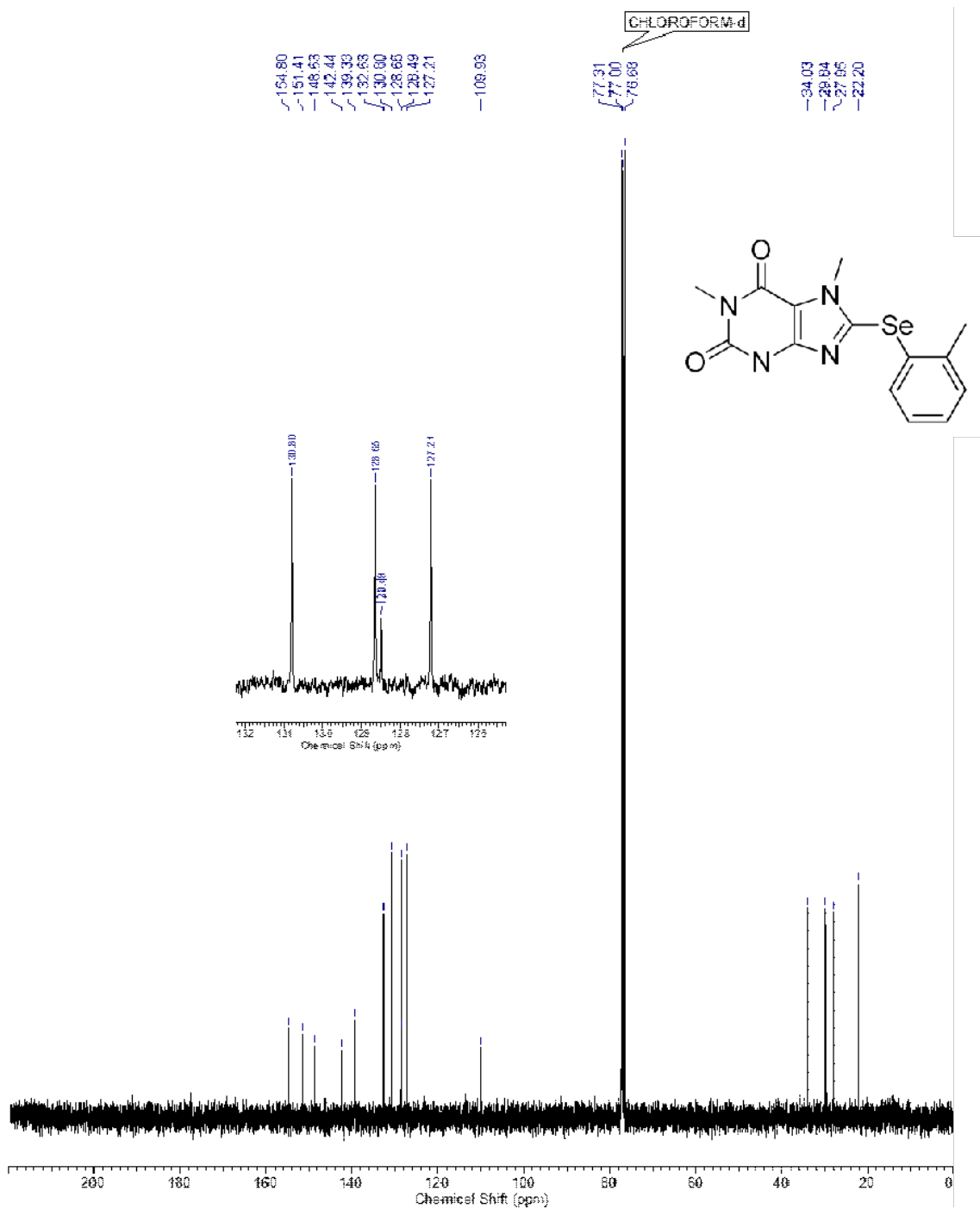
¹³C NMR (100 MHz, CDCl₃) spectrum of 6.



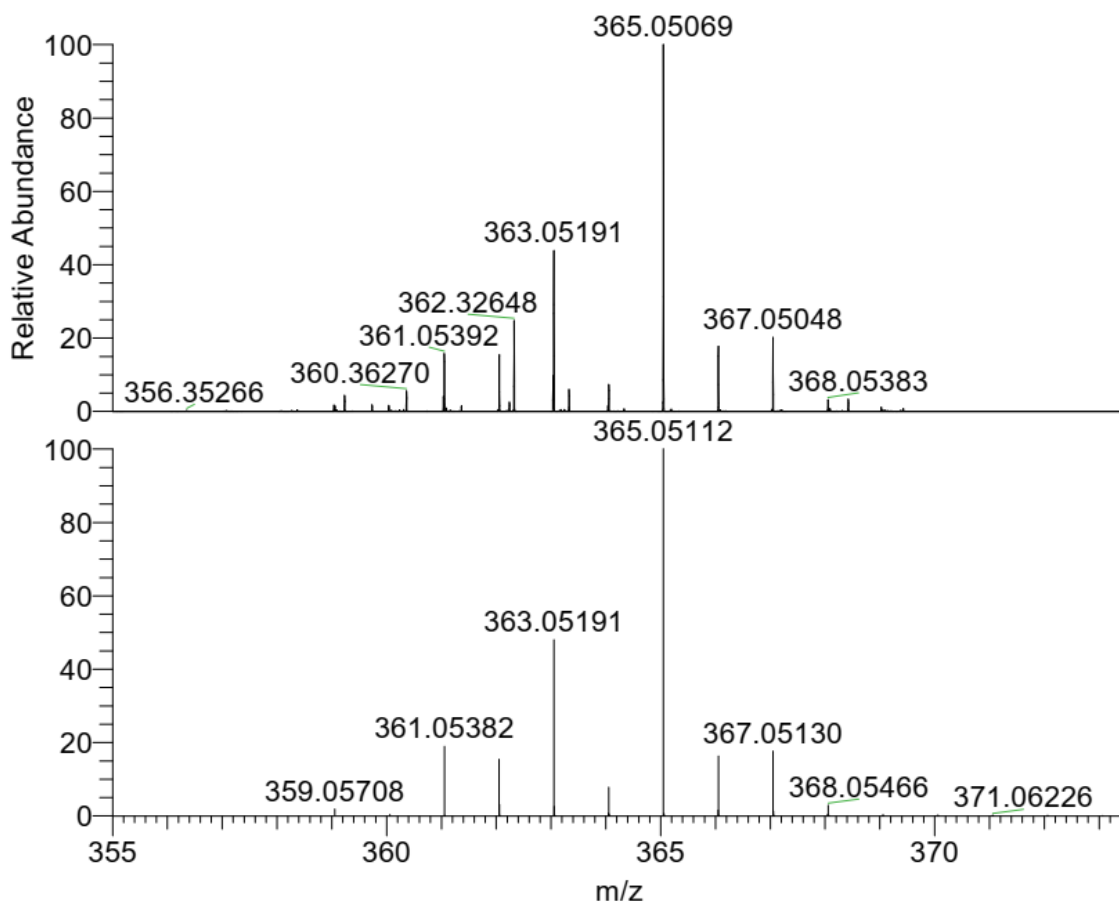
HRMS (ESI) - $[M+H]^+$ of 6



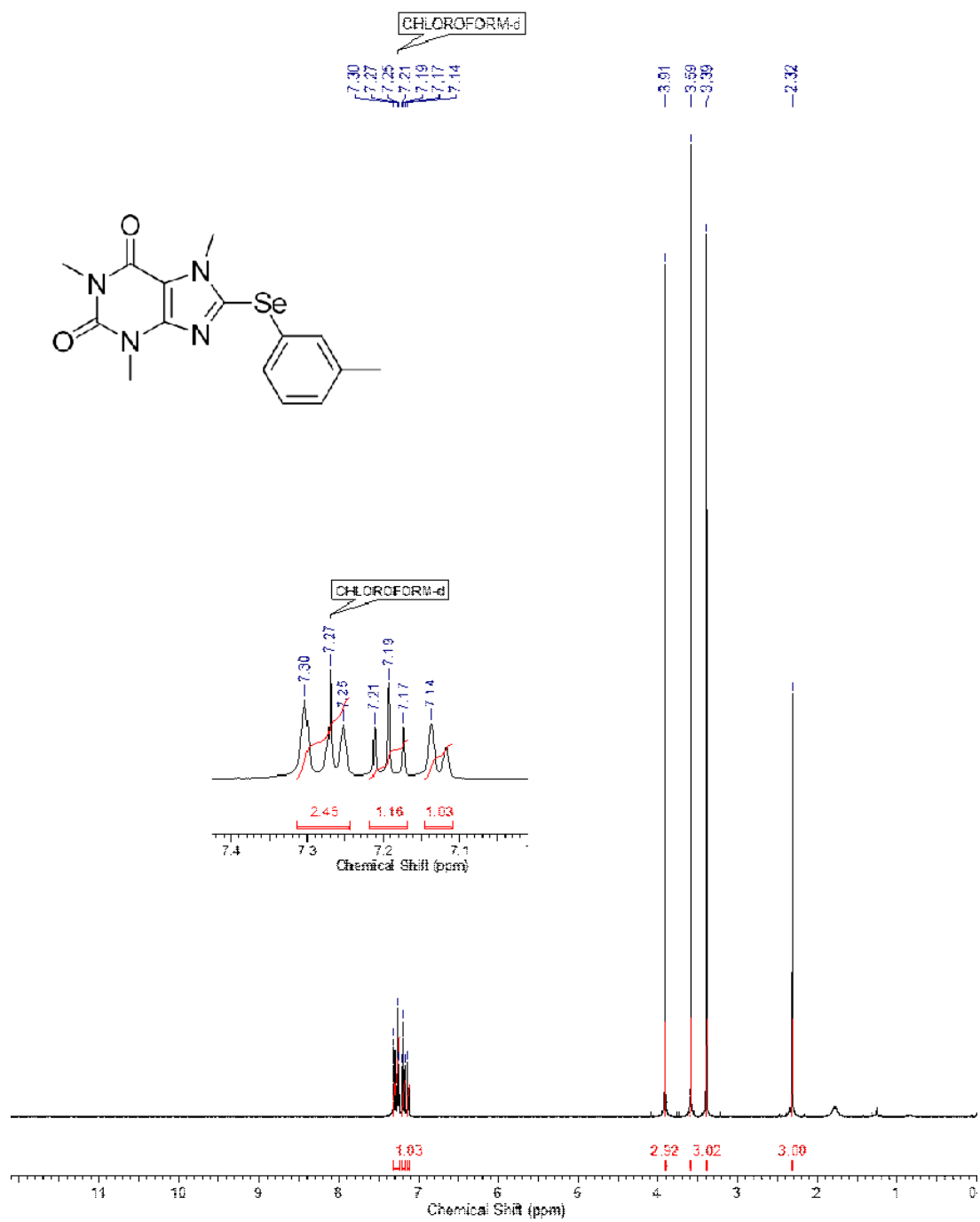
^1H NMR (400 MHz, CDCl_3) spectrum of **7**.



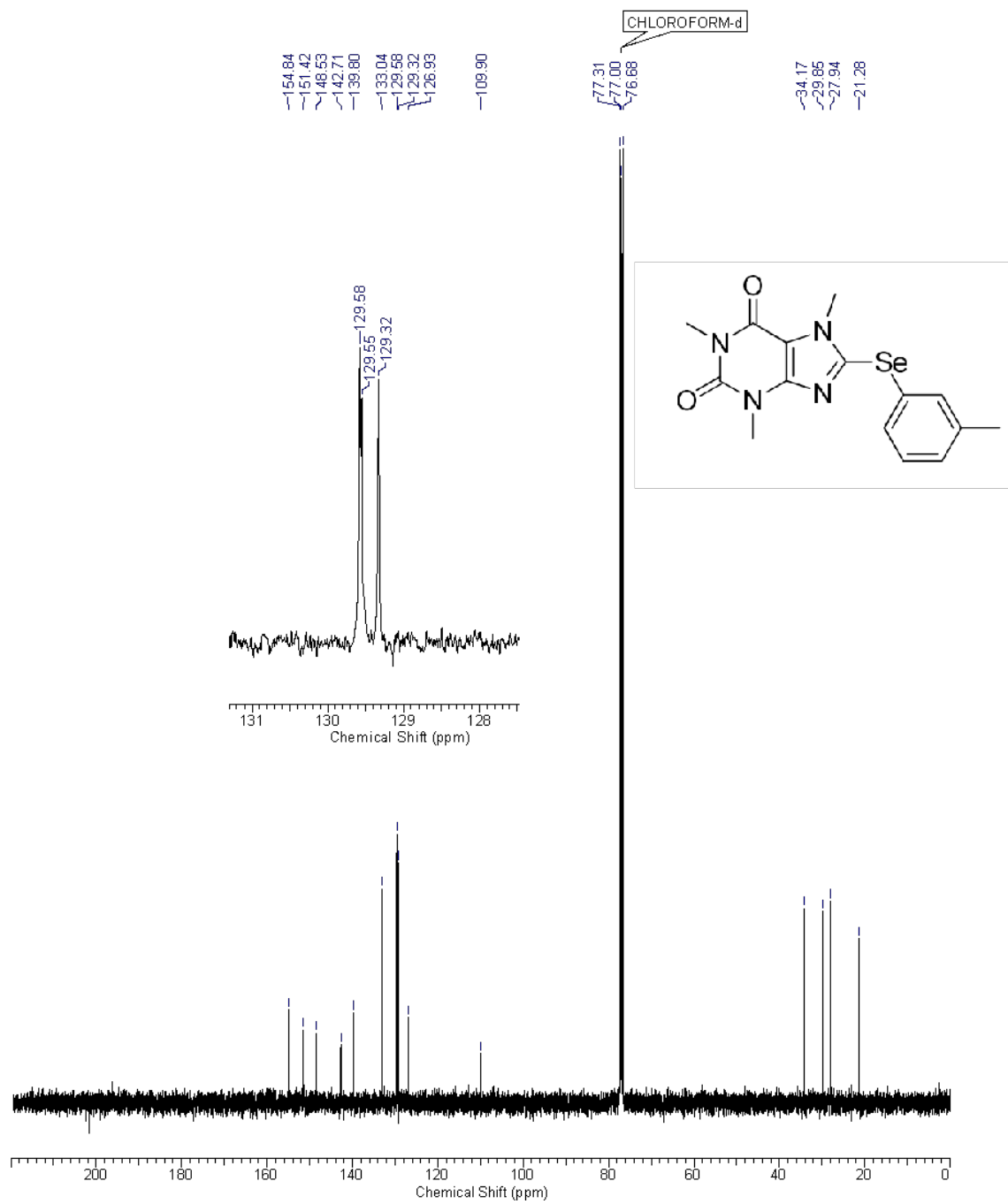
¹³C NMR (100 MHz, CDCl₃) spectrum of 7.



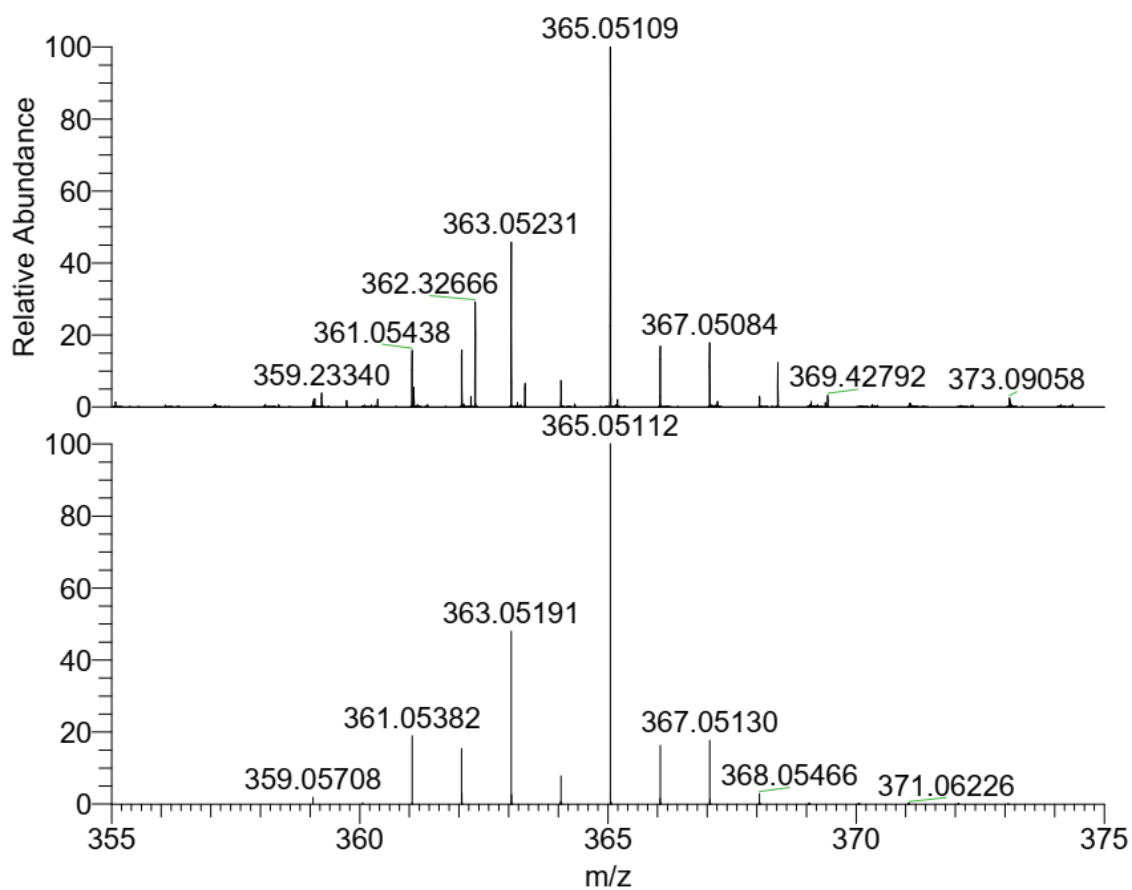
HRMS (ESI) - $[M+H]^+$ of 7



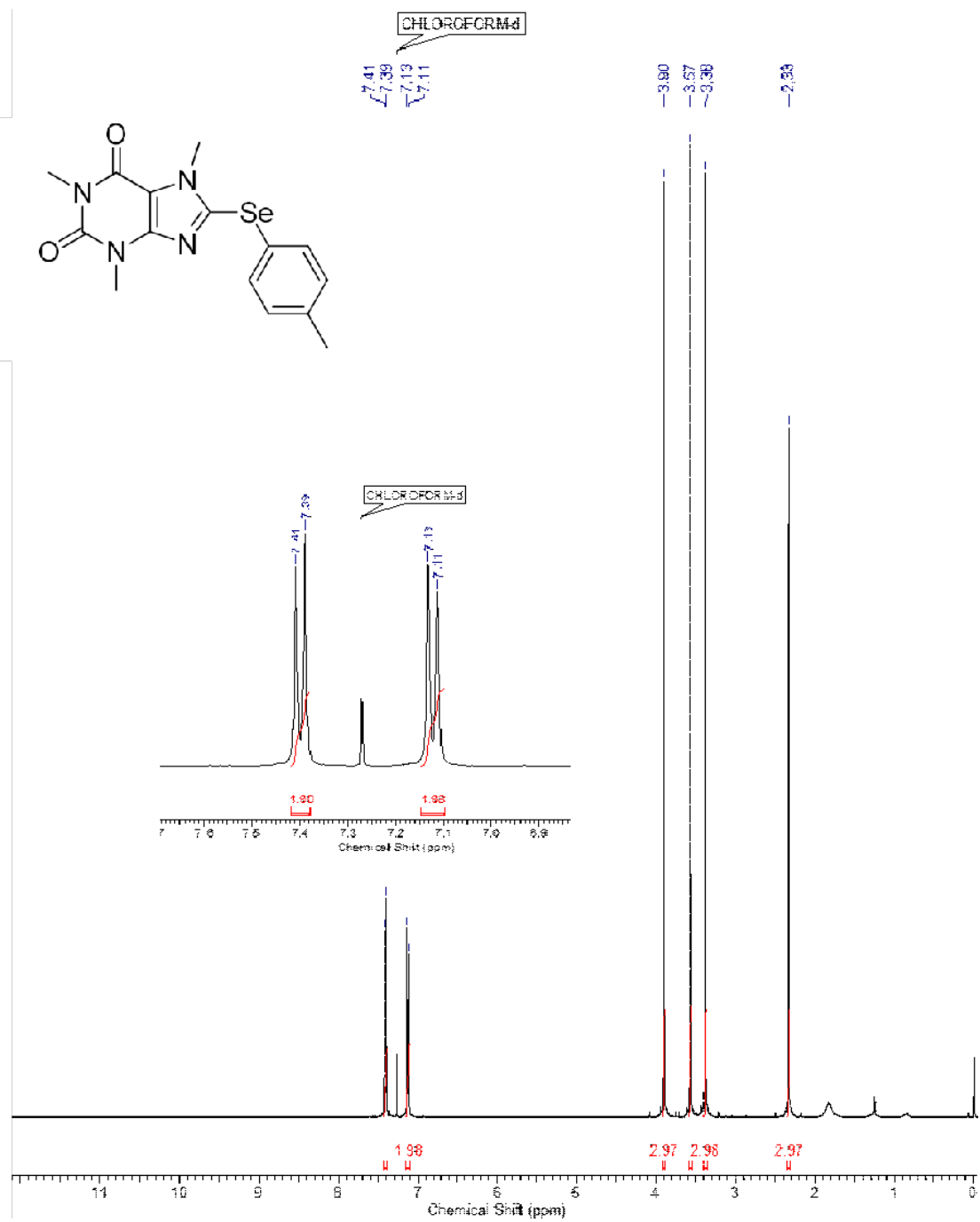
¹H NMR (400 MHz, CDCl₃) spectrum of **8**.



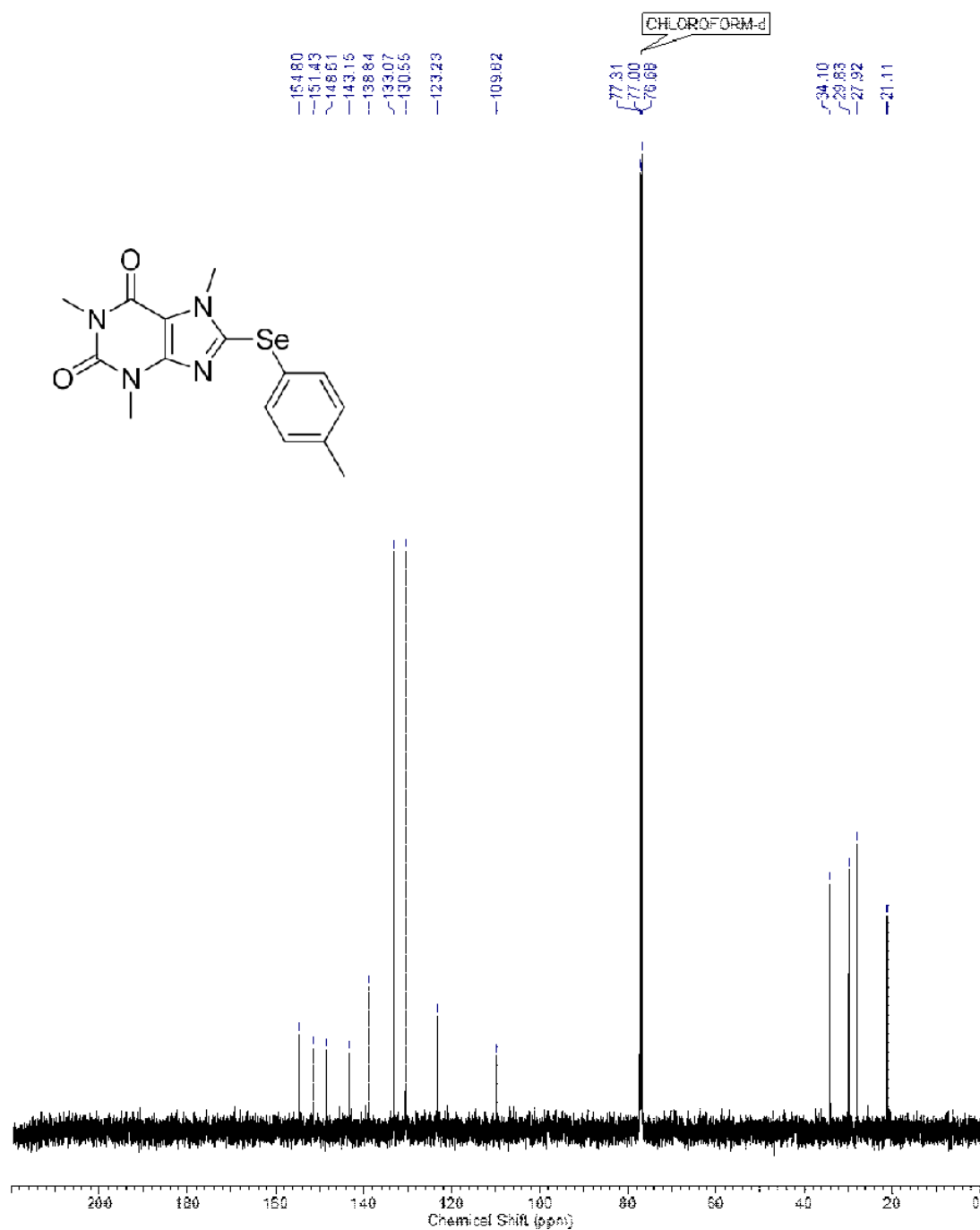
^{13}C NMR (100 MHz, CDCl_3) spectrum of **8**.



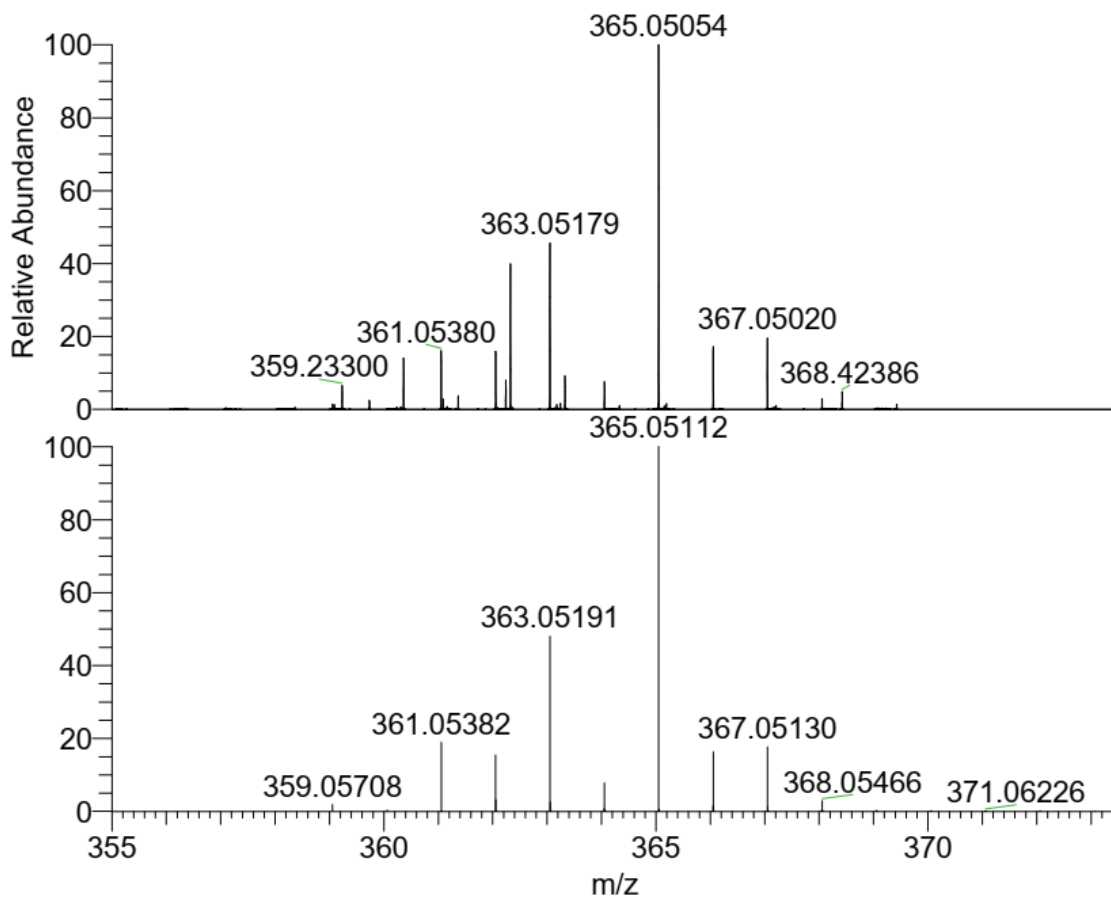
HRMS (ESI) - [M+H]⁺ of 8



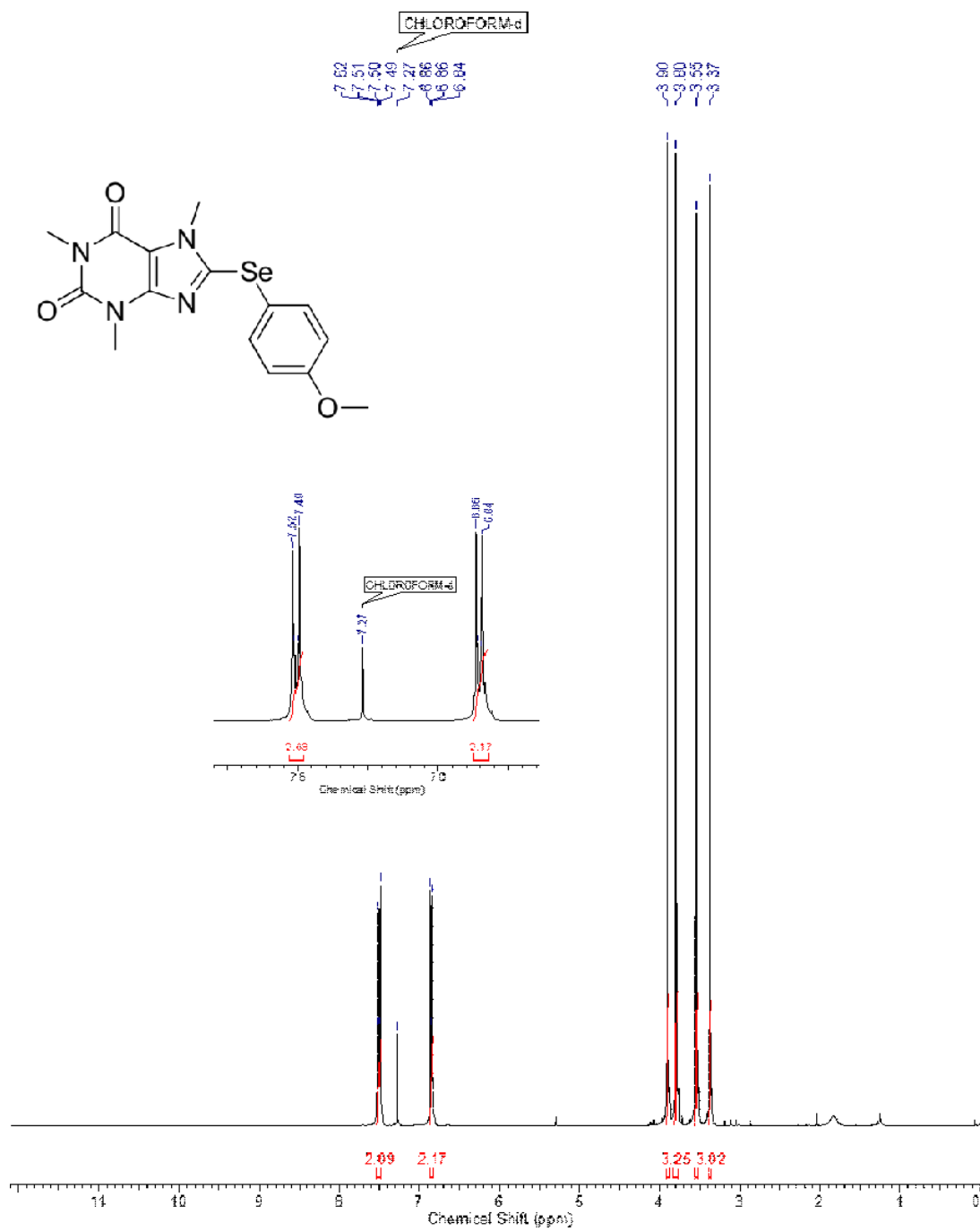
¹H NMR (400 MHz, CDCl₃) spectrum of **9**.



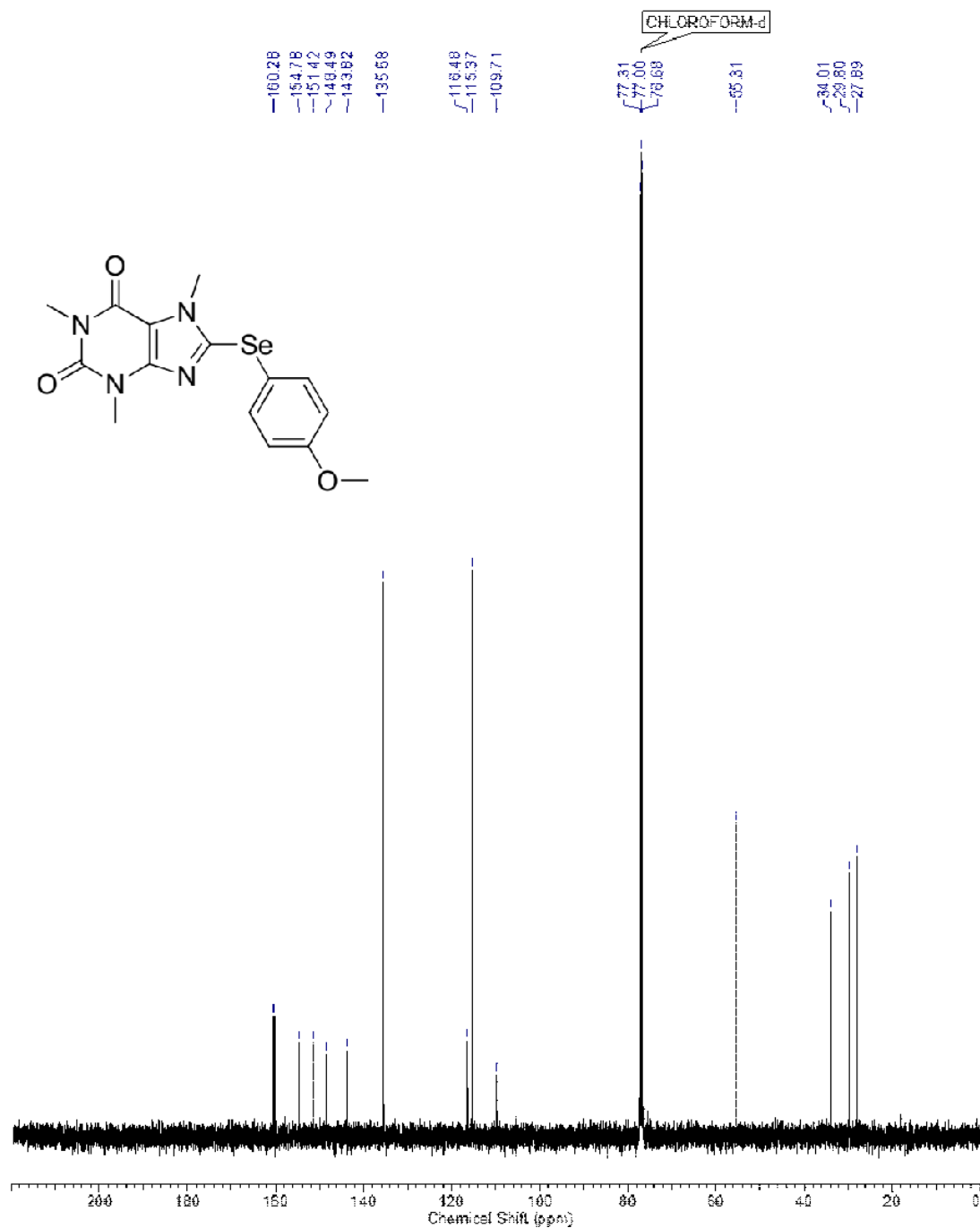
^{13}C NMR (100 MHz, CDCl_3) spectrum of **9**.



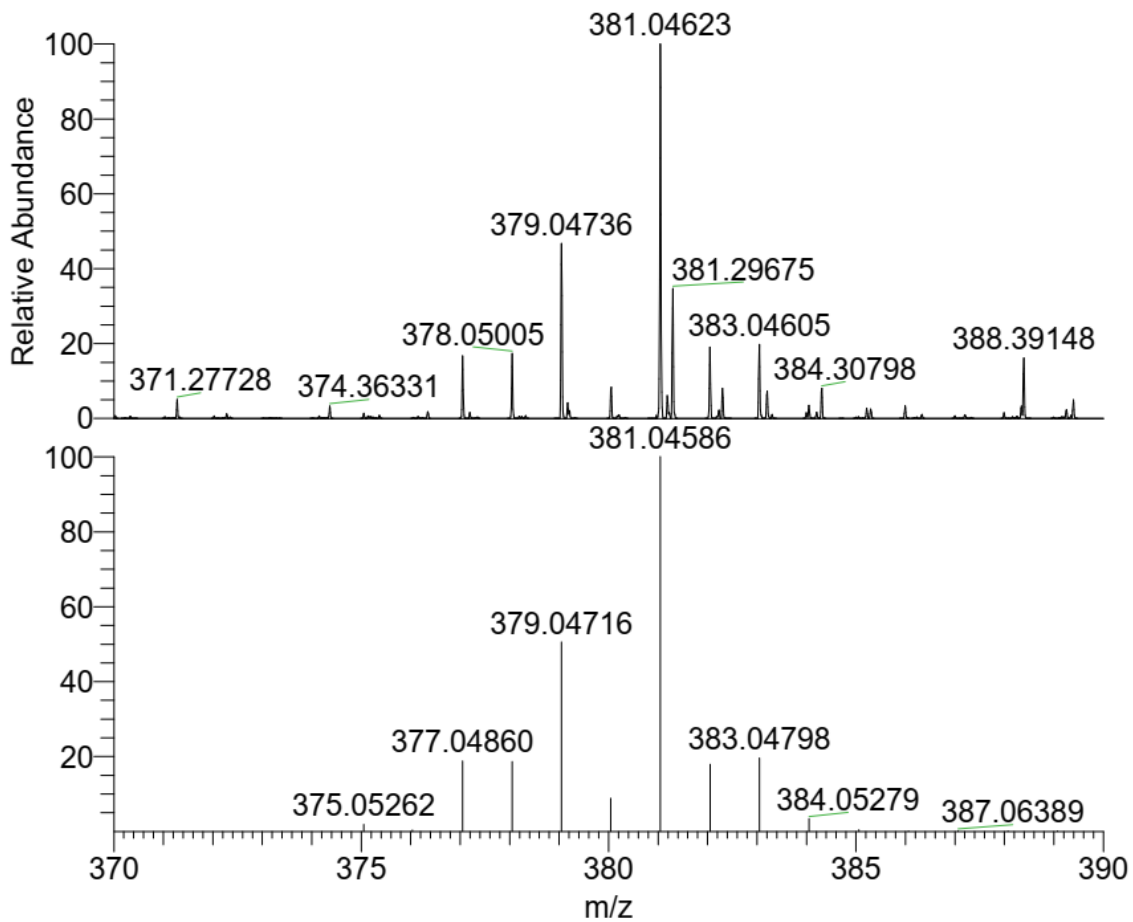
HRMS (ESI) - [M+H]⁺ of 9



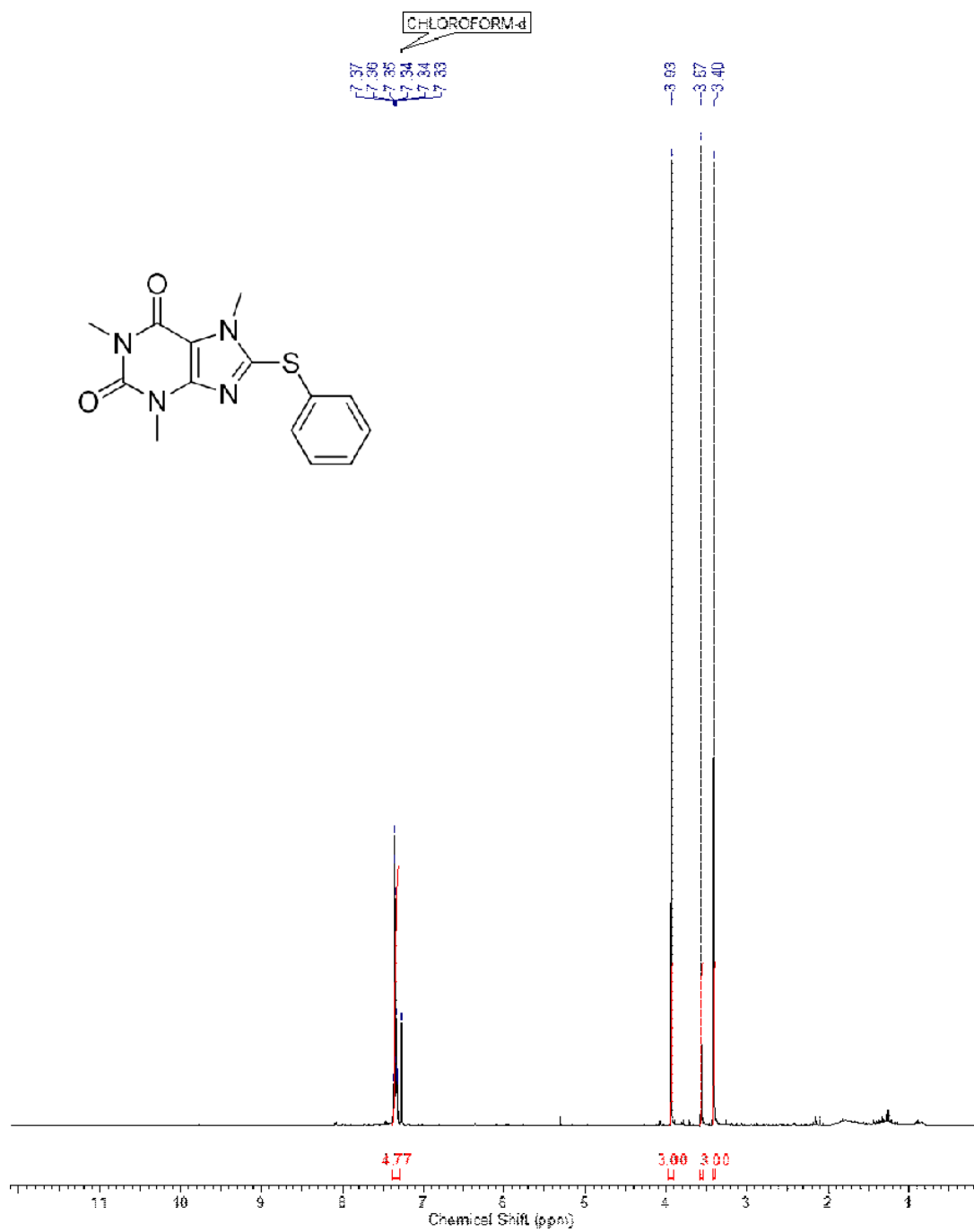
¹H NMR (400 MHz, CDCl₃) spectrum of **10**.



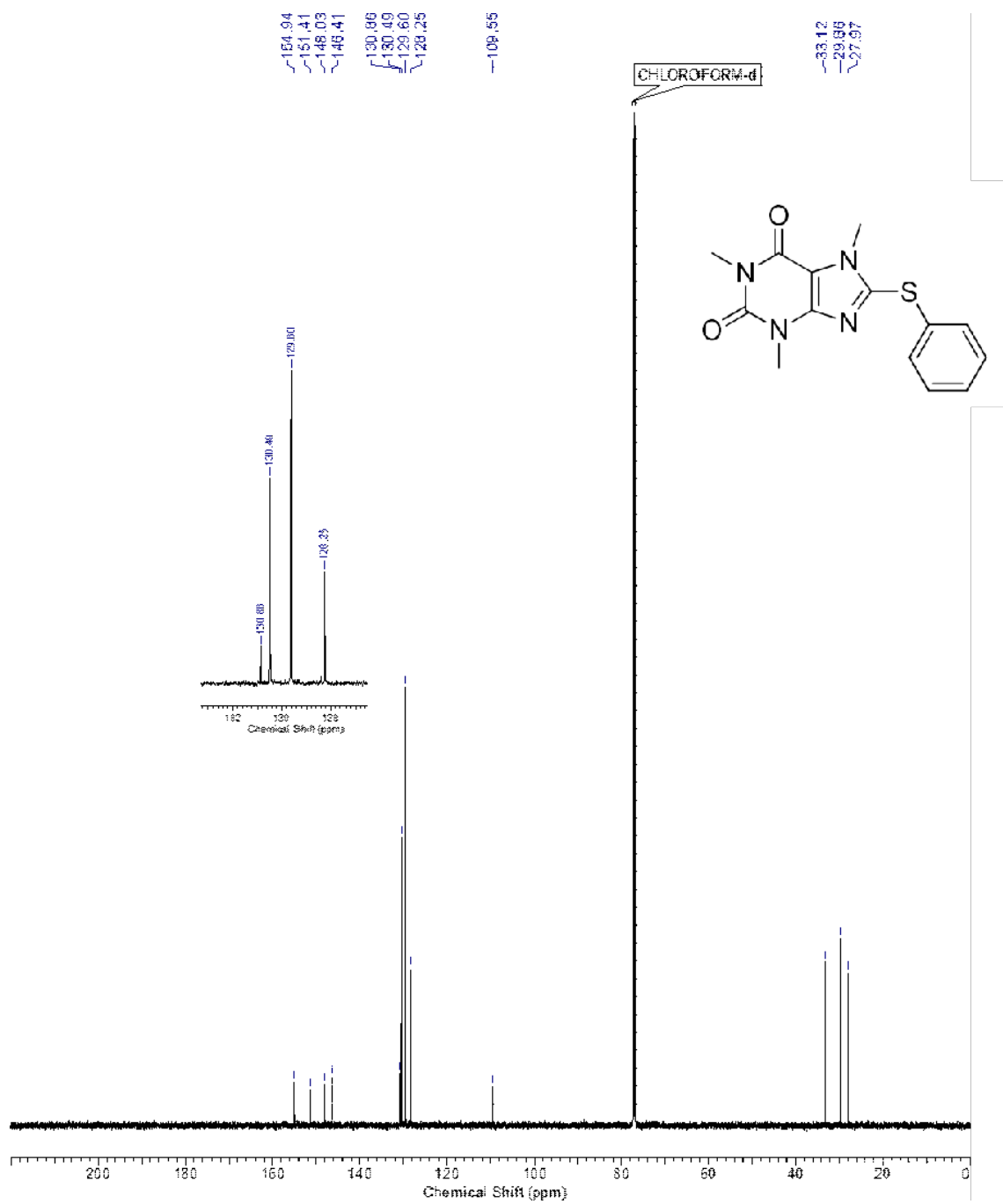
¹³C NMR (100 MHz, CDCl₃) spectrum of **10**.



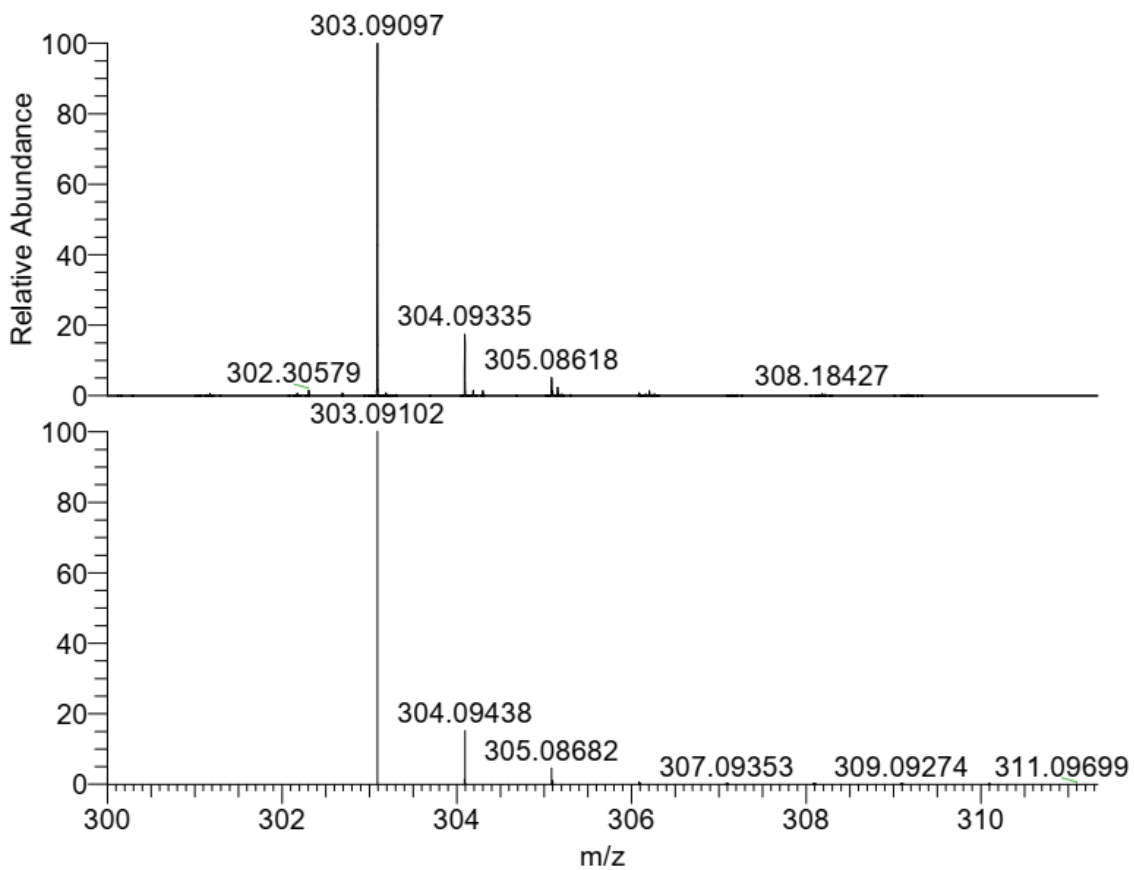
HRMS (ESI) - [M+H]⁺ of 10



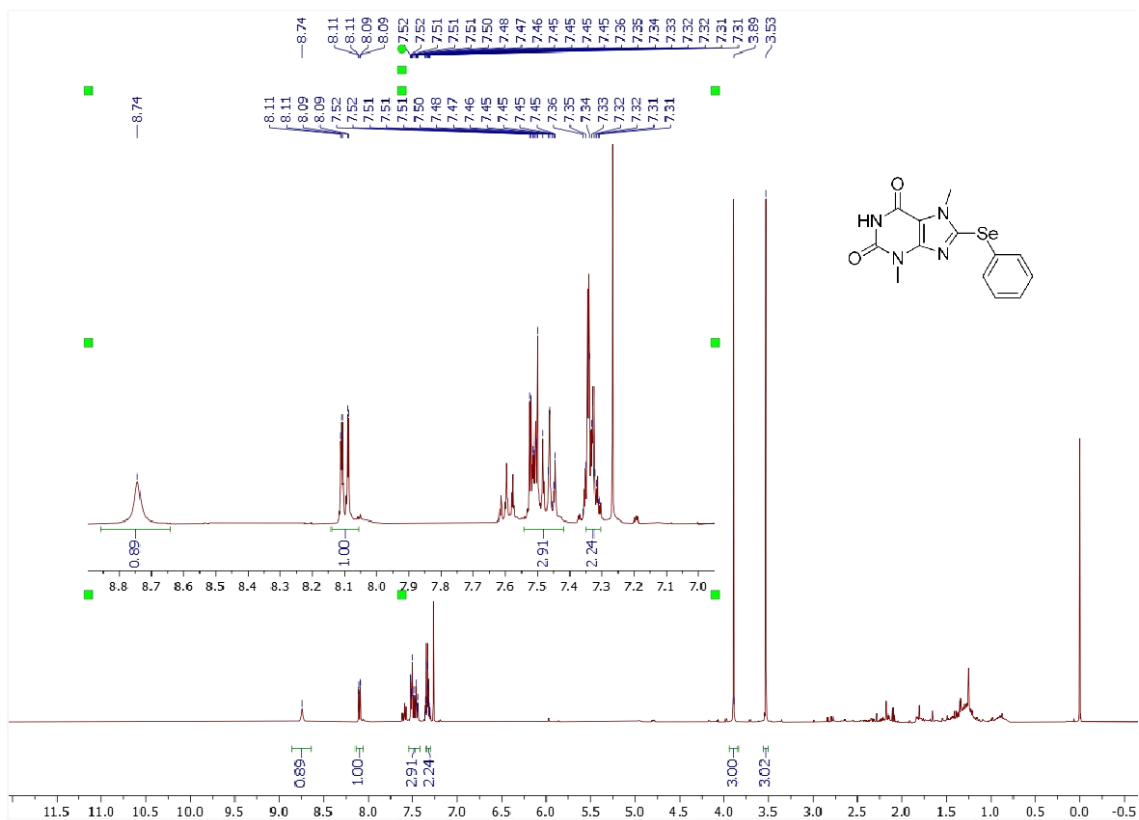
¹H NMR (400 MHz, CDCl₃) spectrum of **11**.



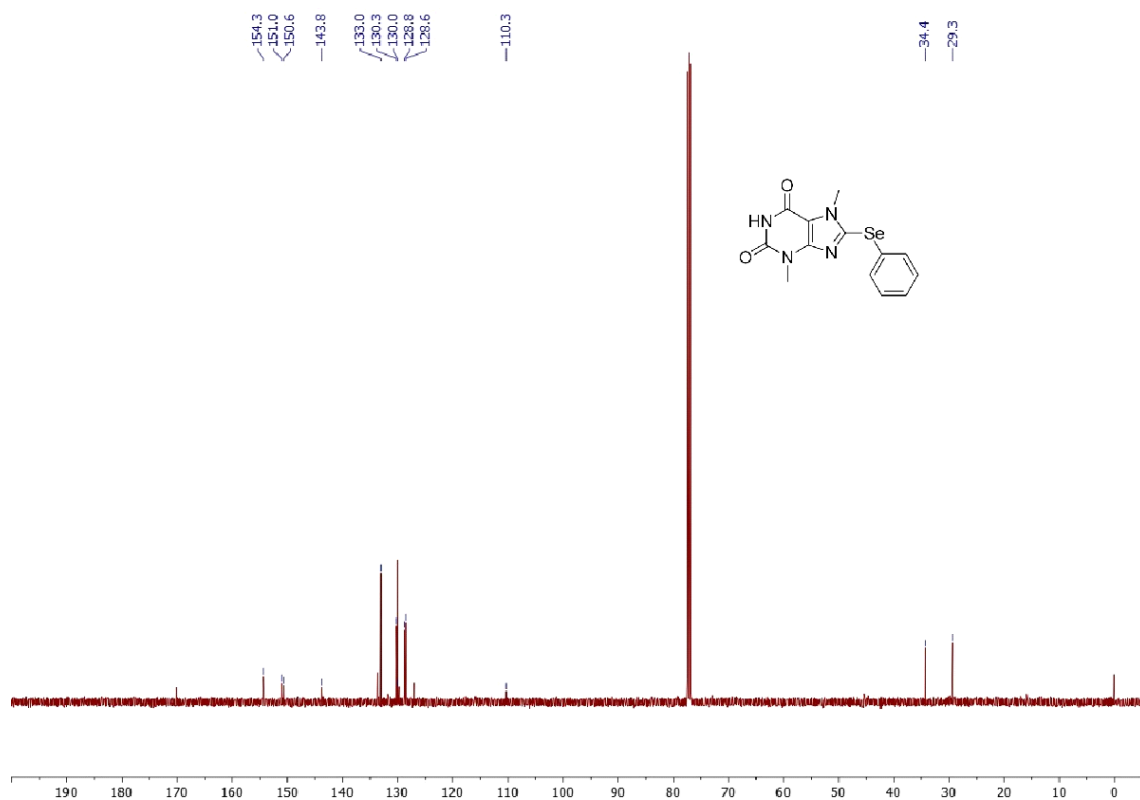
^{13}C NMR (100 MHz, CDCl_3) spectrum of 11.



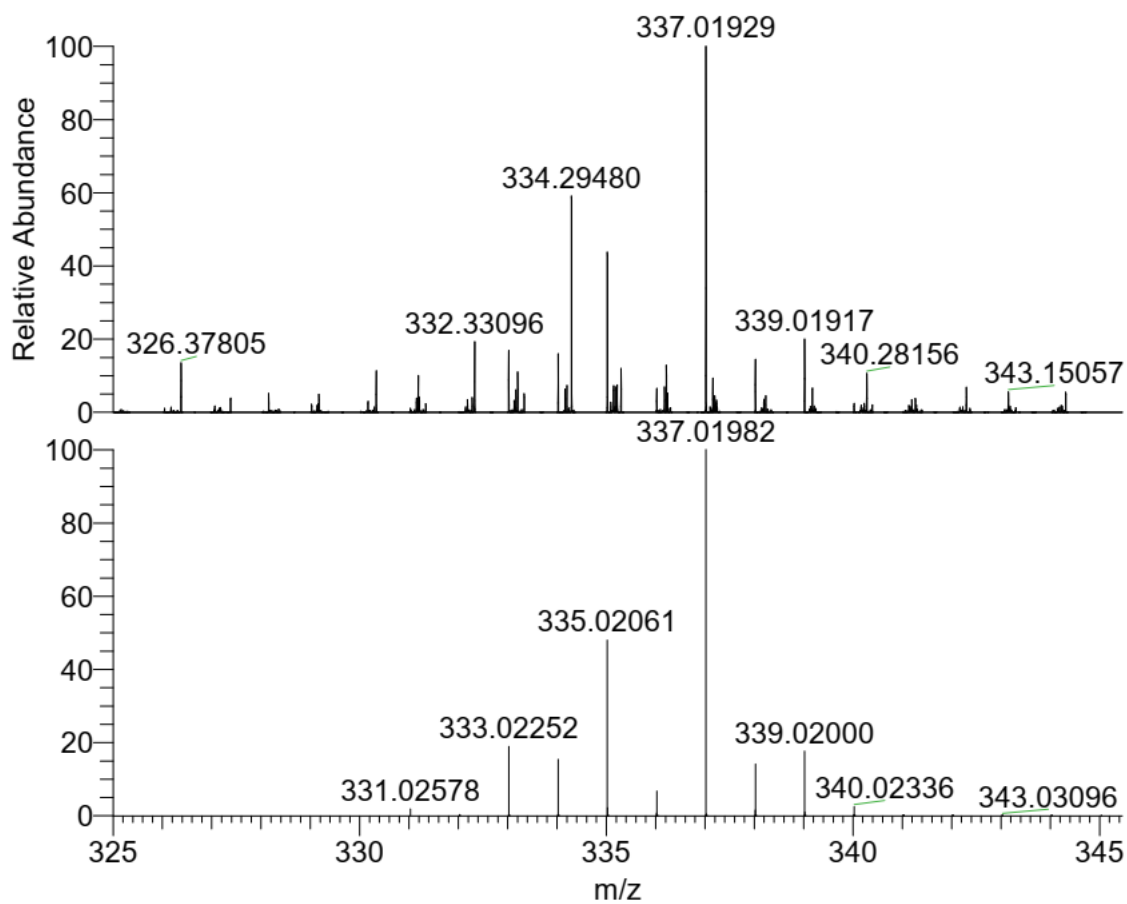
HRMS (ESI) - $[M+H]^+$ of 11



^1H NMR (400 MHz, CDCl_3) spectrum of **12**.

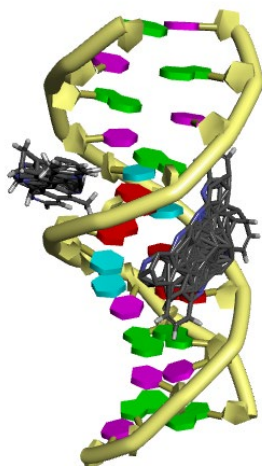


^{13}C NMR (100 MHz, CDCl_3) spectrum of **12**.



HRMS (ESI) - [M+H]⁺ of 12

3. 1BNA Cross-docking



Cross-docking results obtained for crystallographic structure PDB ID: 1BNA with a classic DNA intercalation ligand ellipticine retrieve from crystallographic structure PDB ID: 1Z3F.