frontiers

Supplementary Material

Synthesis of 2,1,3-Benzoxadiazole Derivatives as New Fluorophores—Combined Experimental, Optical, Electro, and Theoretical Study

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1. TABLE:

Table 1S: Excited state lifetimes and their relative amplitudes at emission maxima of **9a-d** in chloroform solution

Compounds	τ_1 / ns	A_1 / %	τ_2 /ns	A_2 / %	χ^2	λ^{max}_{FL}/nm
9a	3.28±0.04	47.85	2.23±0.04	52.15	0.970	494
9b	3.61±0.05	29.90	2.28±0.03	70.10	0.983	498
9c	3.85±0.06	23.65	2.31±0.03	76.35	0.981	495
9d	3.95±0.07	21.91	2.32±0.03	78.09	1.005	498

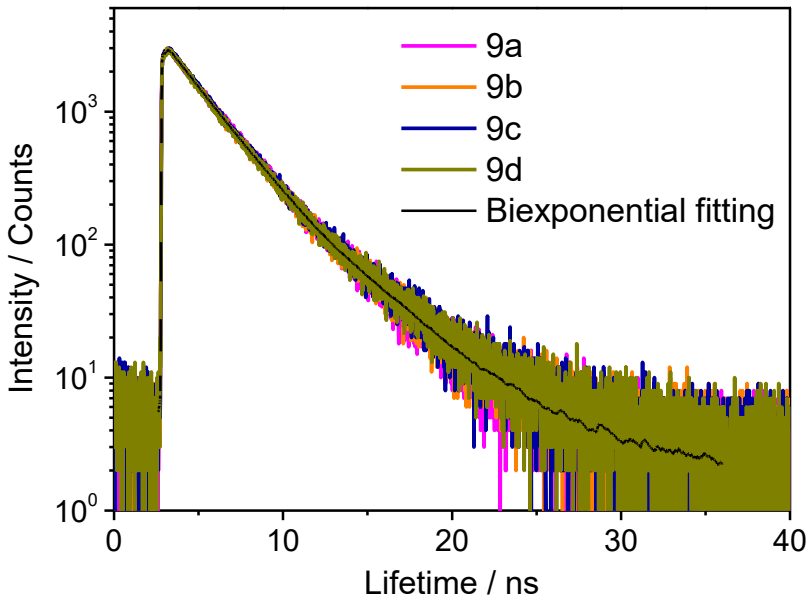
Table 2S: Fluorescence properties of compound **9a** at 10^{-5}M in heptane, toluene, tetrahydrofuran (THF) and acetone solutions

Solvents	τ_1 /ns	A_1 /%	τ_2 / ns	A_2 / %	χ^2	$<\tau_f>^a$ /ns	$\lambda^{b,c}_{em}$ / nm	$\Phi_{FL}{}^d$
Heptane	2.11±0.03	47.76	1.44±0.03	52.24	0.968	1.80	457	0.27
Toluene	3.27±0.08	11.68	1.85±0.02	88.32	1.084	2.12	474	0.44
THF	3.37±0.06	18.80	1.97±0.02	81.20	1.006	2.42	478	0.53
Acetone	3.88±0.07	25.71	2.20±0.04	74.29	1.030	2.84	486	0.71

[a]Average lifetimes were calculated using $<\tau_f> = \Sigma\tau_i^2 A_i/\Sigma\tau_i A_i$; [b]Excited at maximum absorption; [c]Maxima emission wavelength; [d]Relative quantum yields in solution determined using quinine sulfate as standard (Φ_{Fl} = 0.546 in 1N H_2SO_4);

2. FLUORESCENCE DECAY CURVES:

Figure 1S: Fluorescence decay curves for compounds **9a-d** in chloroform solution (10^{-5} mol L^{-1}) using a 401 nm excitation wavelength recorded at emission maxima fitted by a bi-exponential function



3. ABSORPTION (ABS) AND FLUORESCENCE EXCITATION (EX)

Figure 2S: Absorption (Abs) and fluorescence excitation (Ex) spectra of compounds **9a-d** in chloroform solution

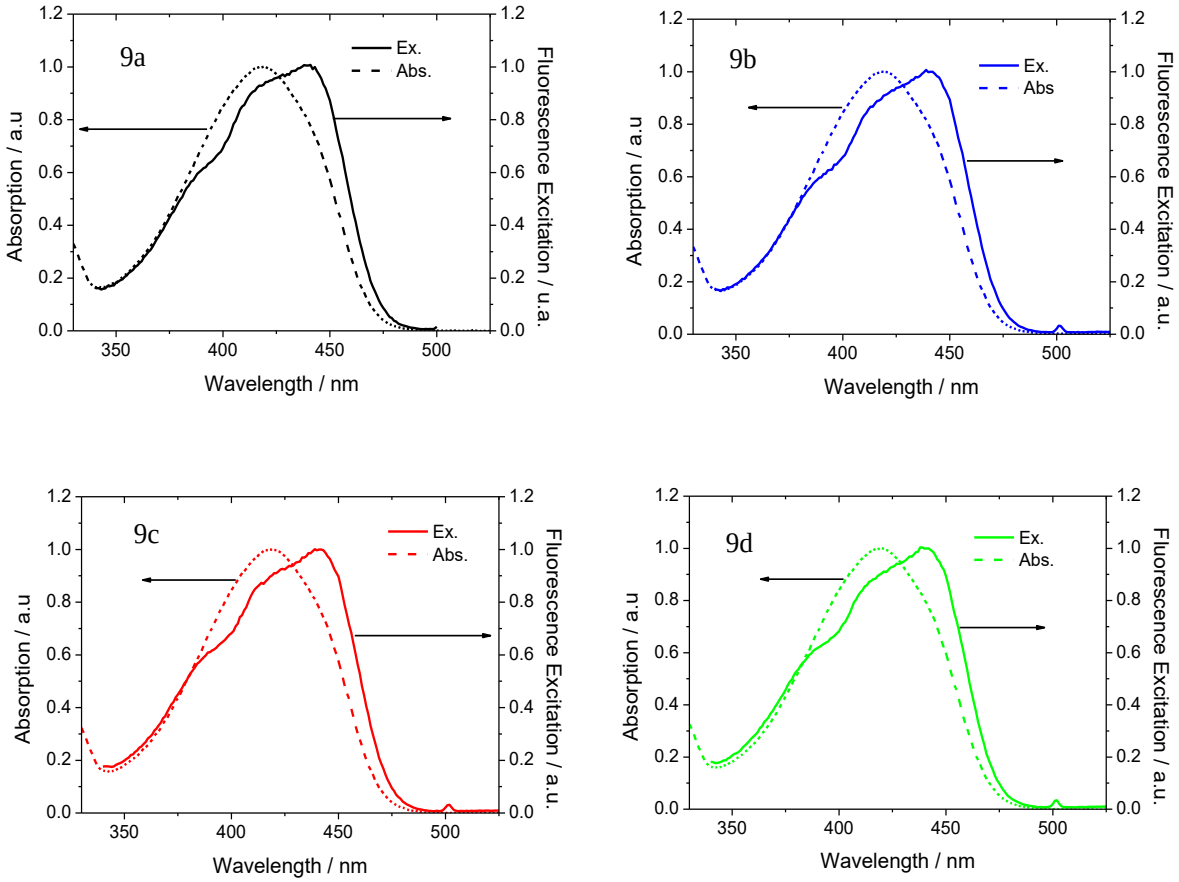
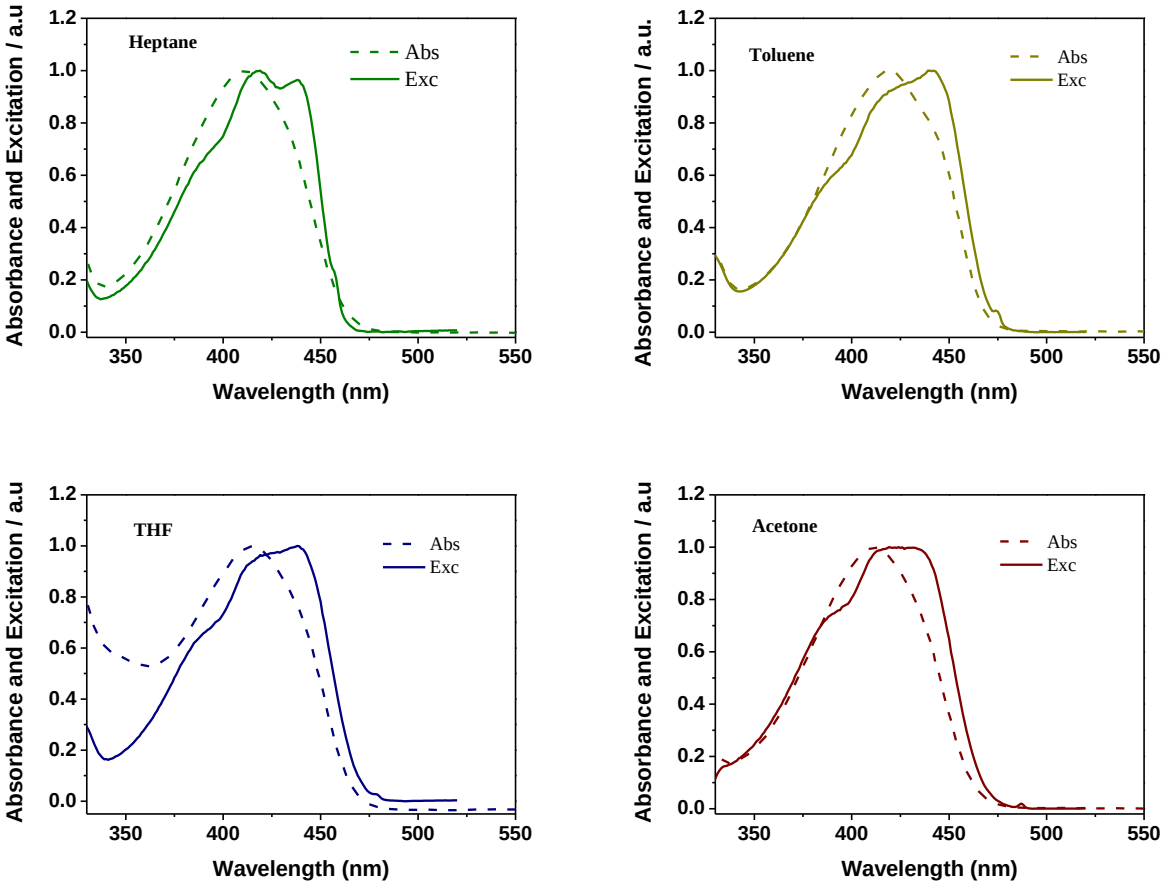


Figure 3S: Absorption (Abs) and fluorescence excitation (Ex) spectra of compounds **9a** in heptane, toluene, tetrahydrofuran (THF) and acetone solutions



4. NMR SPECTRA:

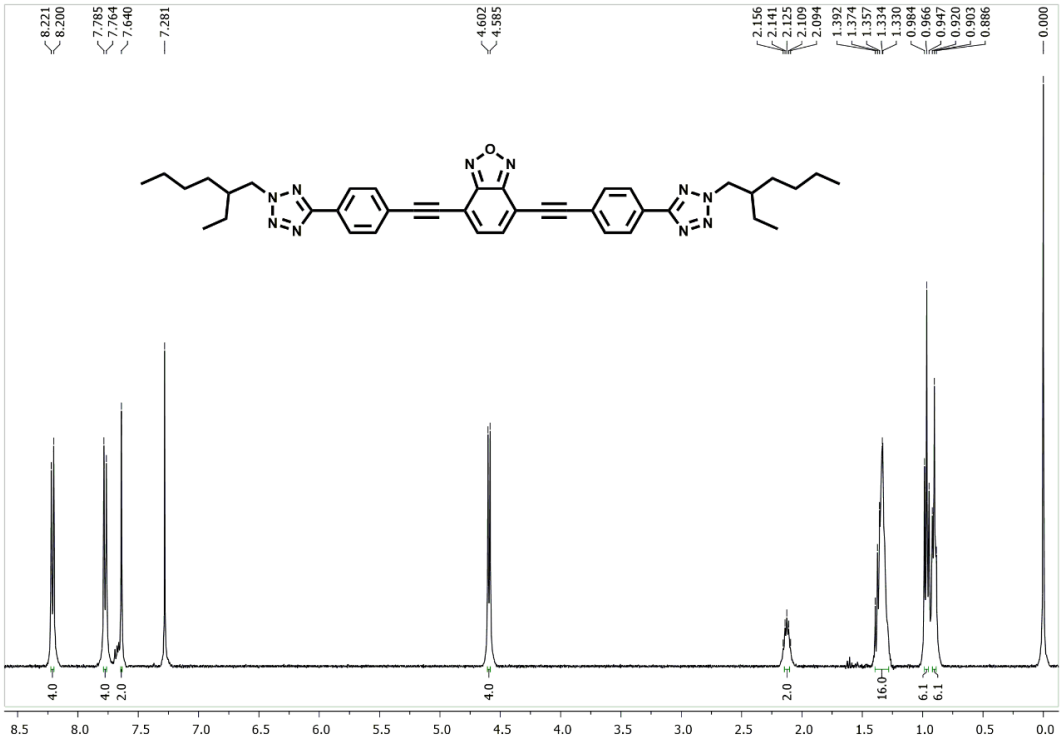


Figure 4S. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **9a**.

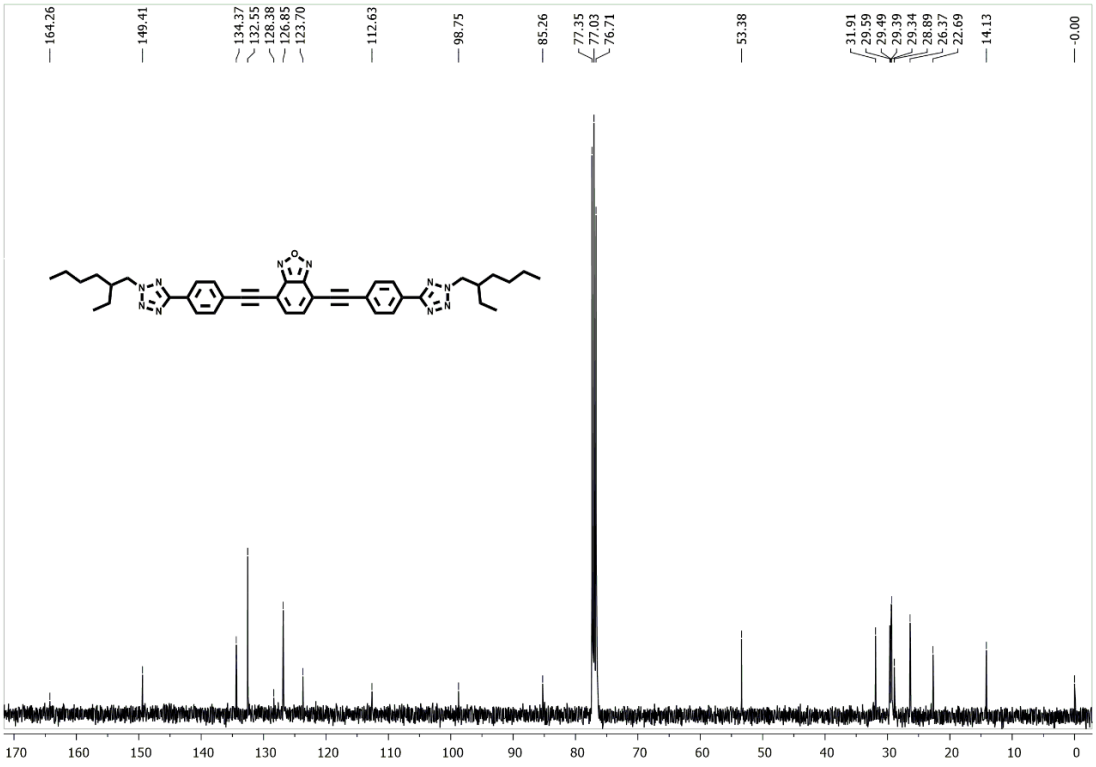


Figure 5S. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **9a**.

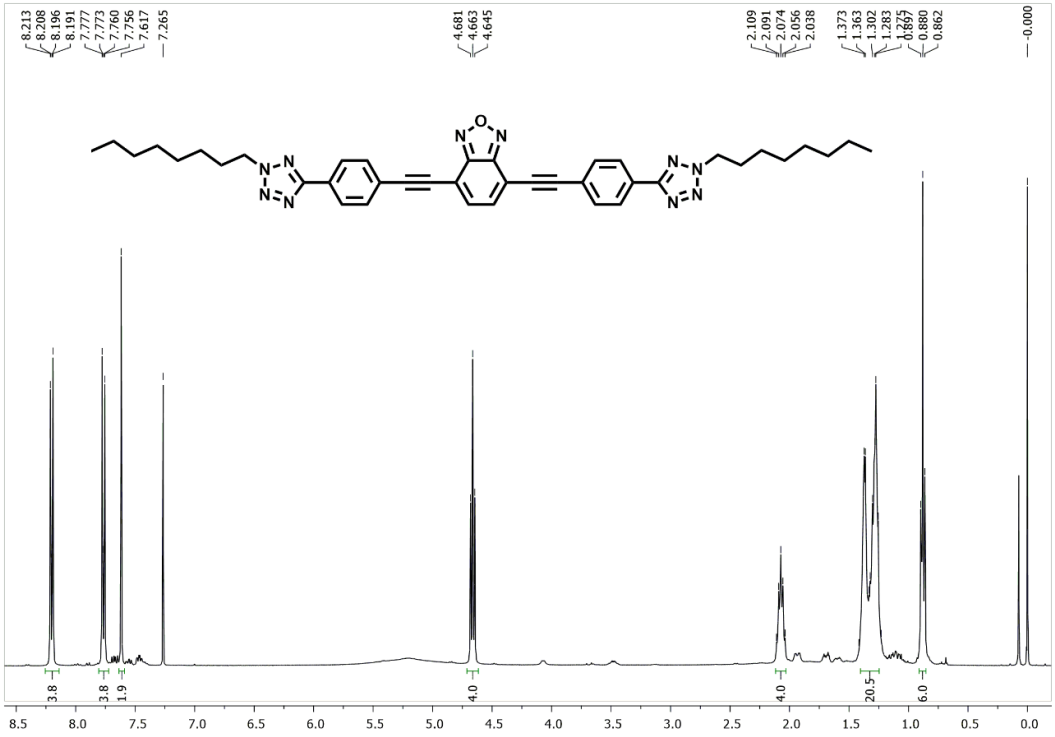


Figure 6S. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **9b**.

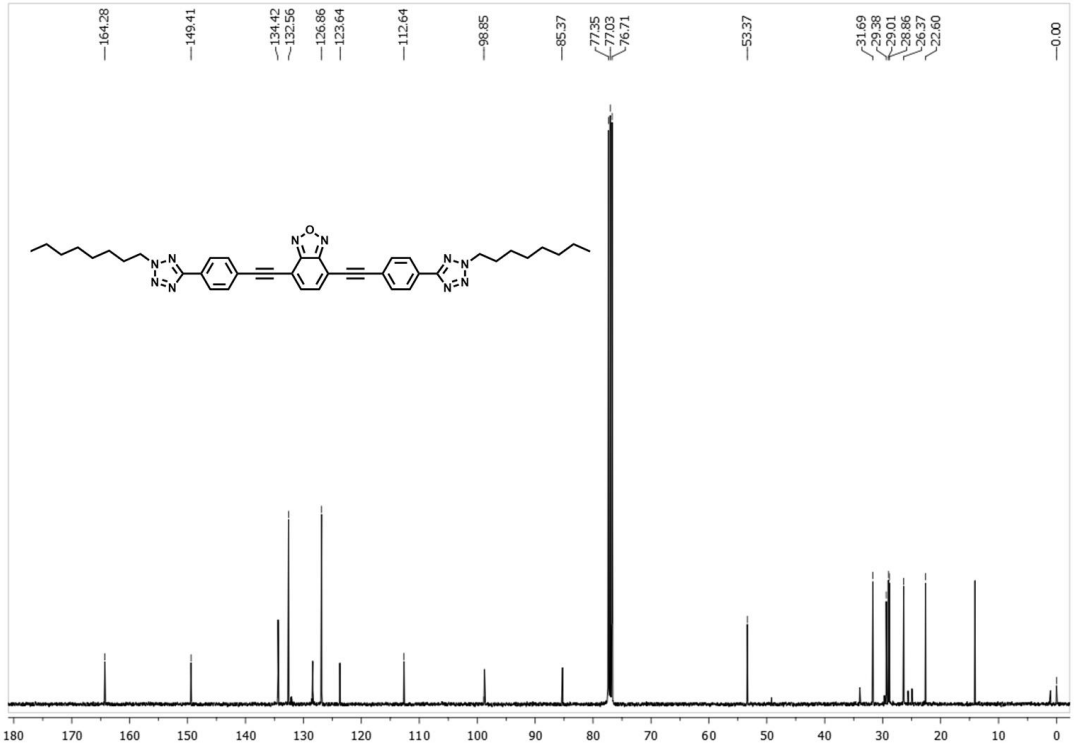


Figure 7S. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **9b**.

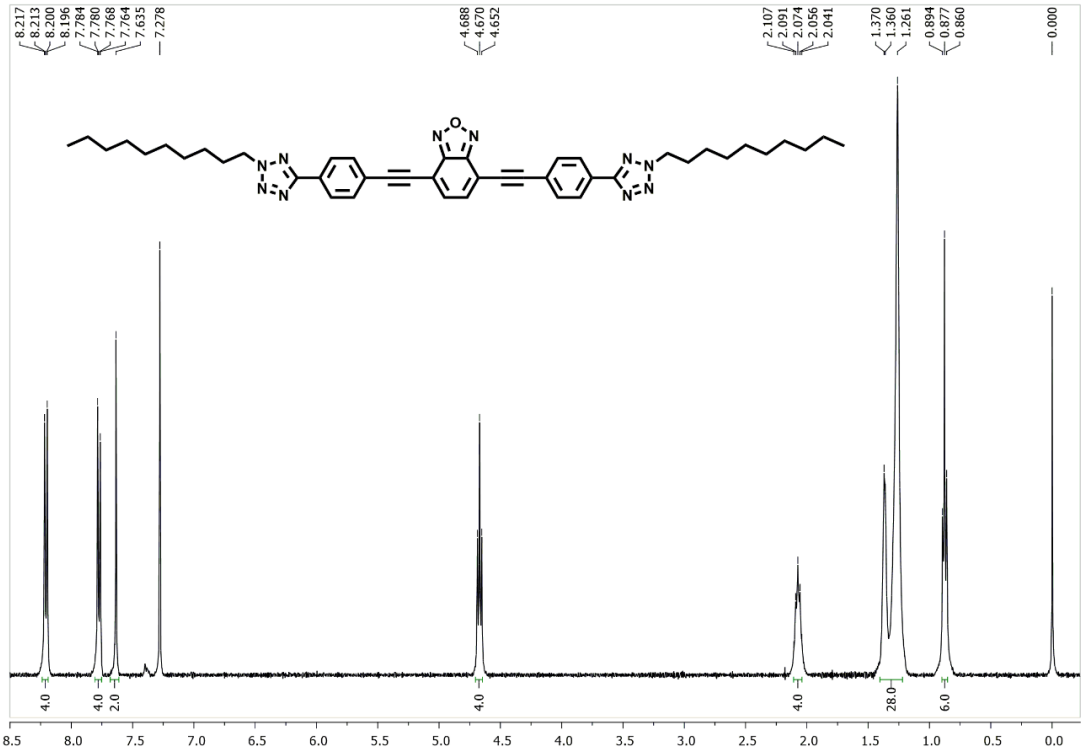


Figure 8S. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **9c**.

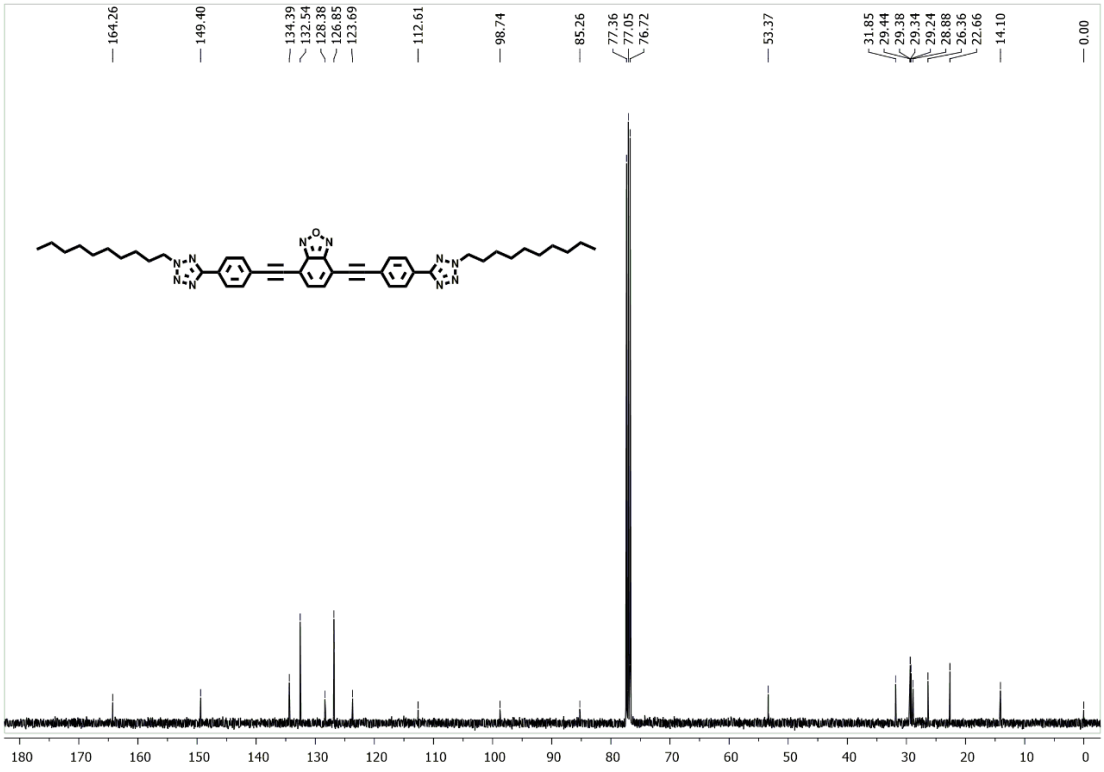


Figure 9S. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **9c**.

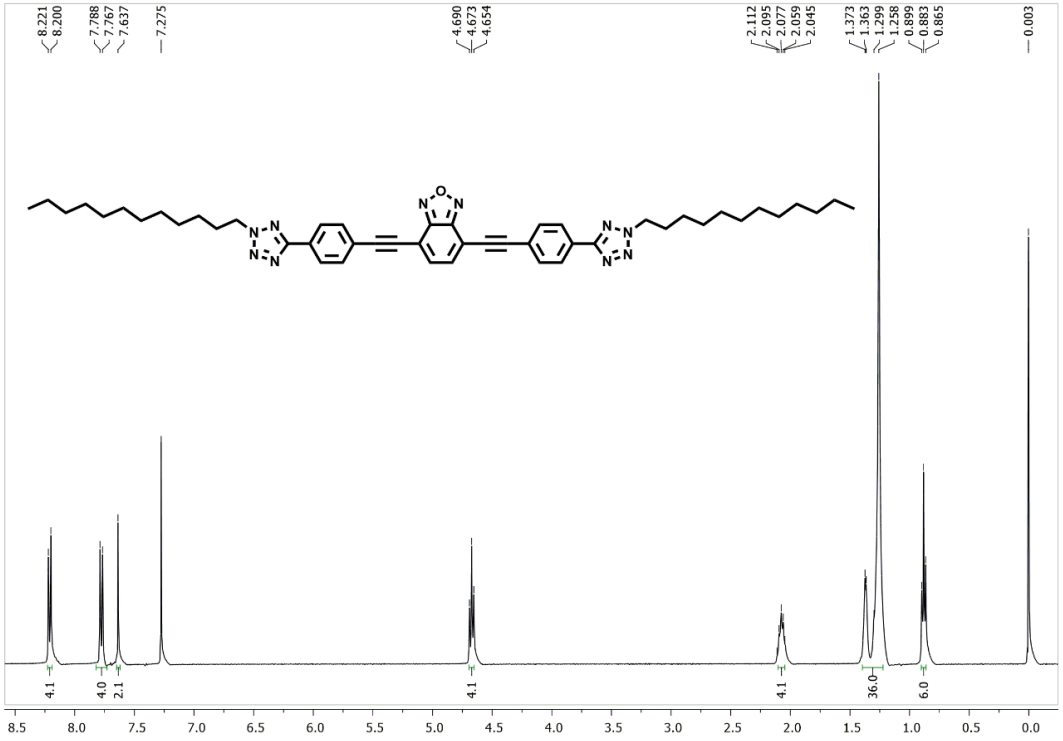


Figure 10S. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **9d**.

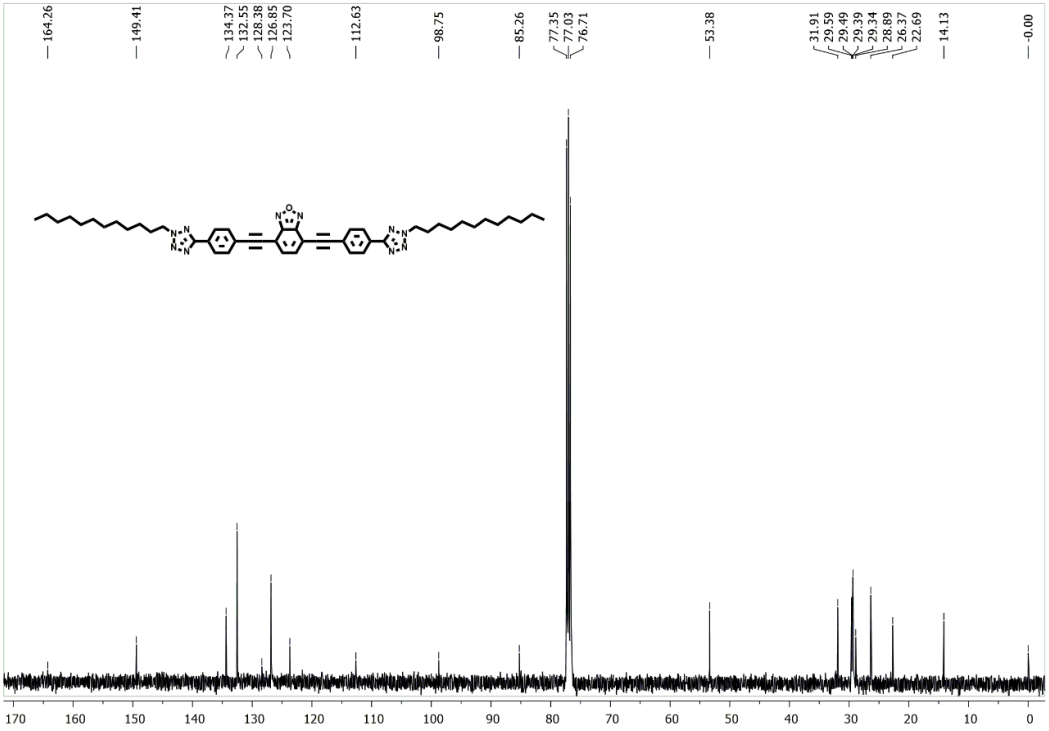


Figure 11S. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **9d**.

5. Fourier transform infrared spectroscopy (*FTIR*)

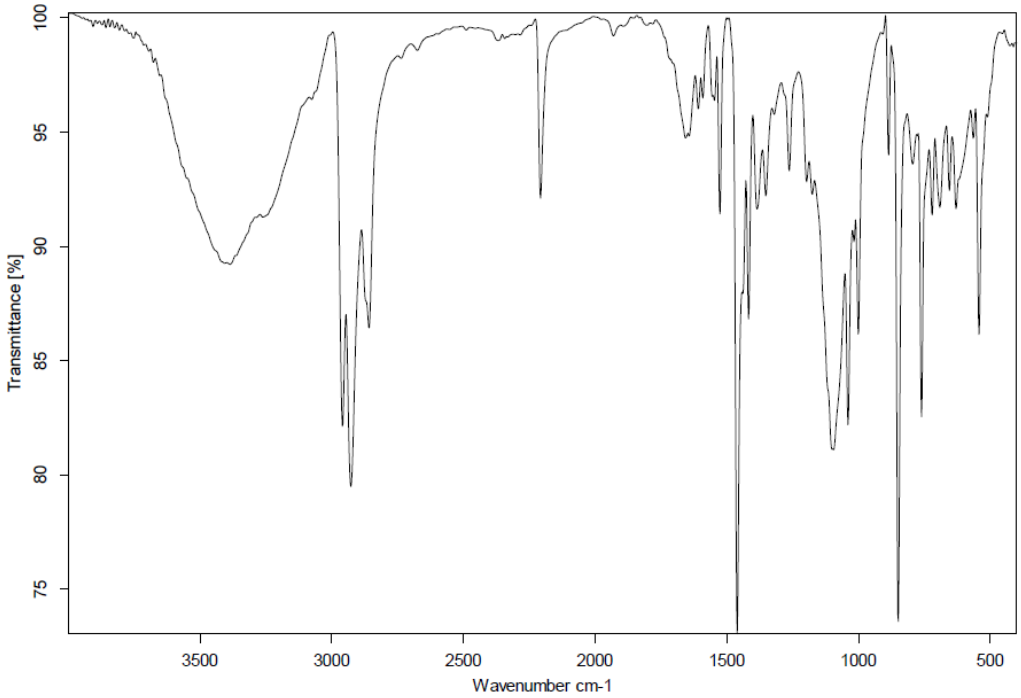


Figure 12S. The FTIR absorption spectrum (KBr disk) of **9a.**

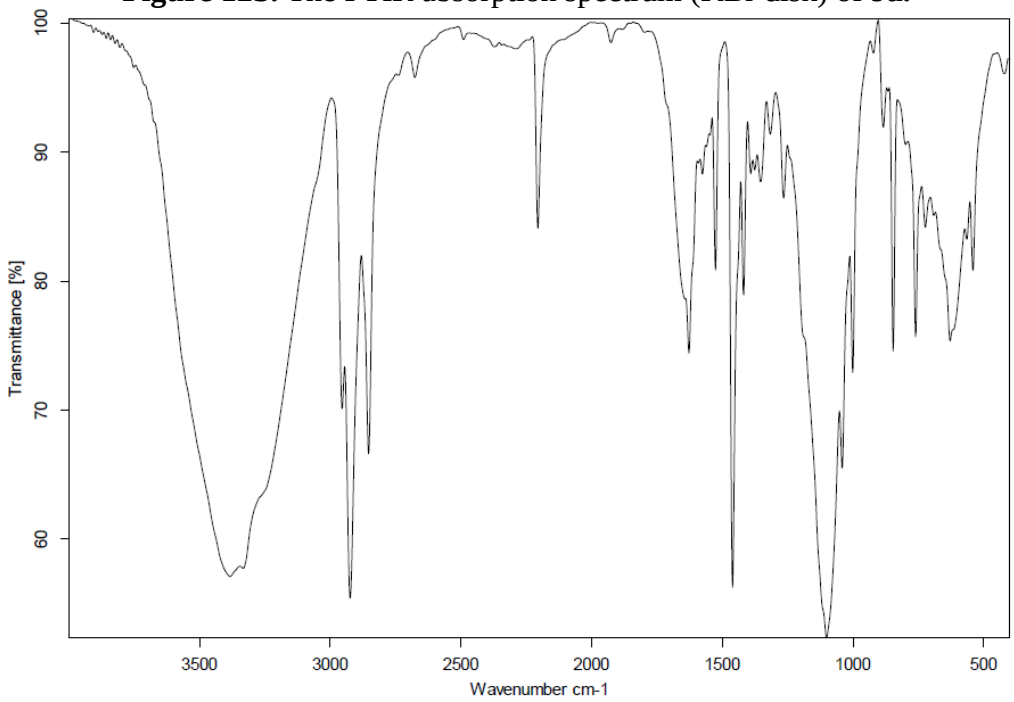


Figure 13S. The FTIR absorption spectrum (KBr disk) of **9b.**

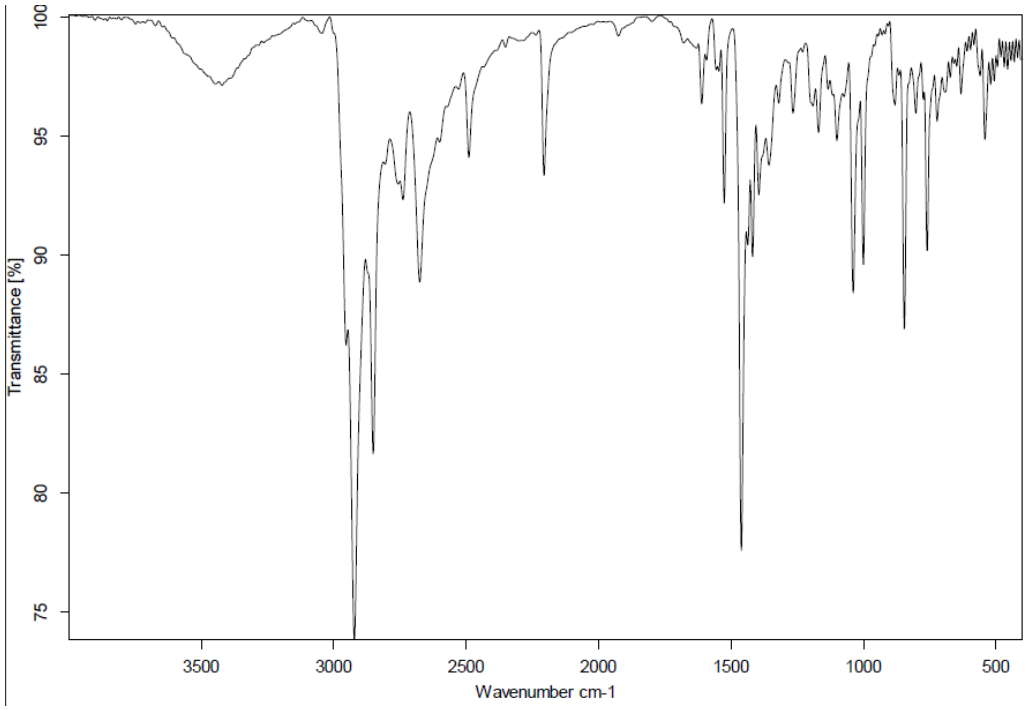


Figure 14S. The FTIR absorption spectrum (KBr disk) of **9c**.

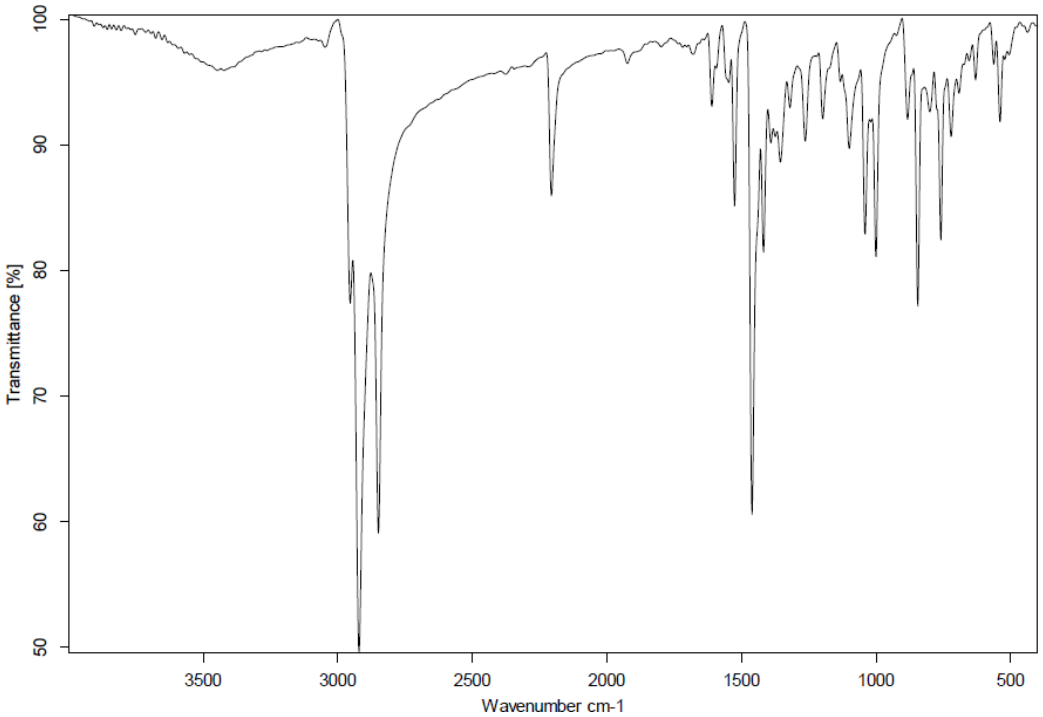


Figure 15S. The FTIR absorption spectrum (KBr disk) of **9d**.

6. HRMS:

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Source

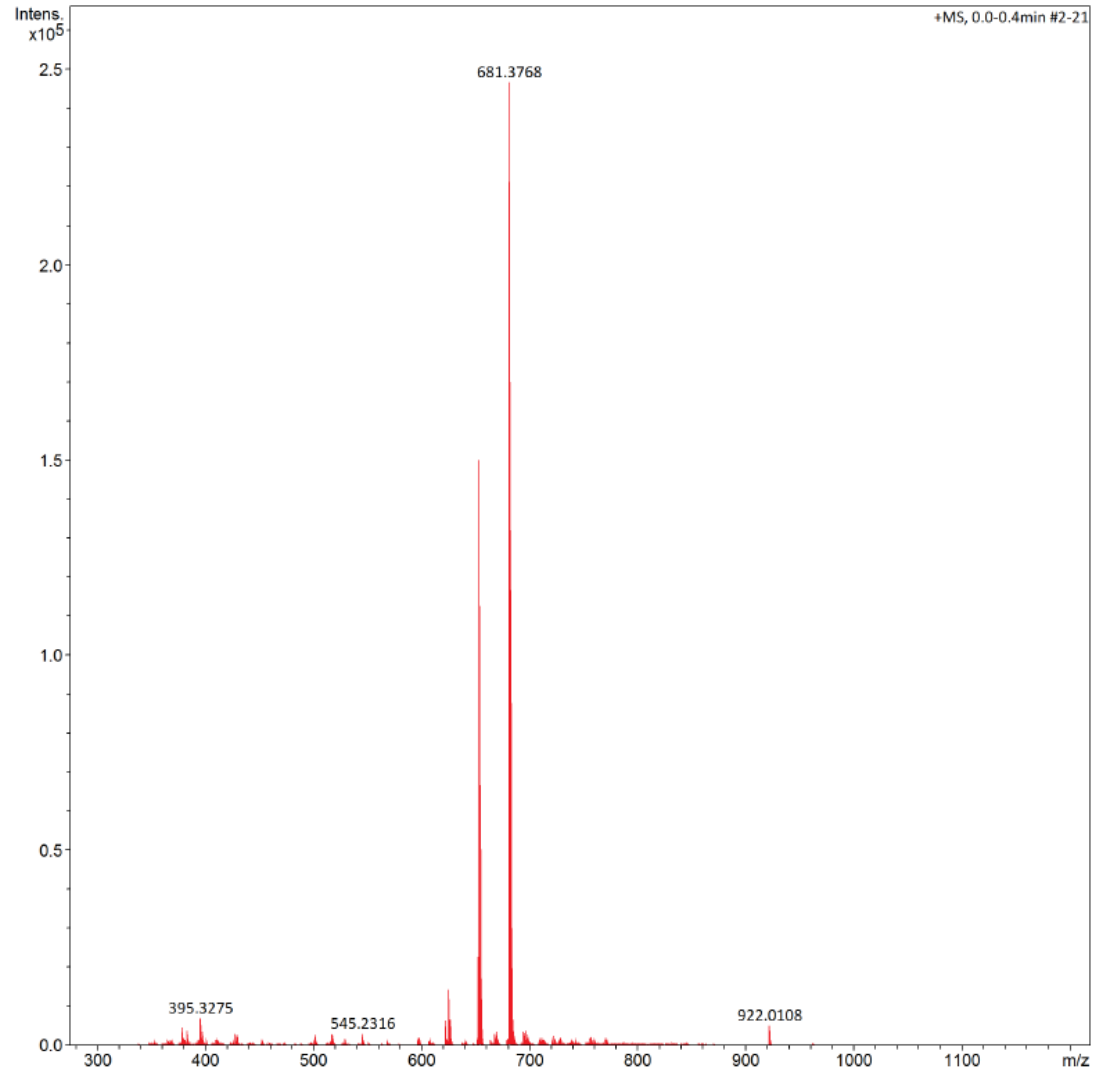


Figure 16S. High-Resolution Mass Spectrum of **9a**.

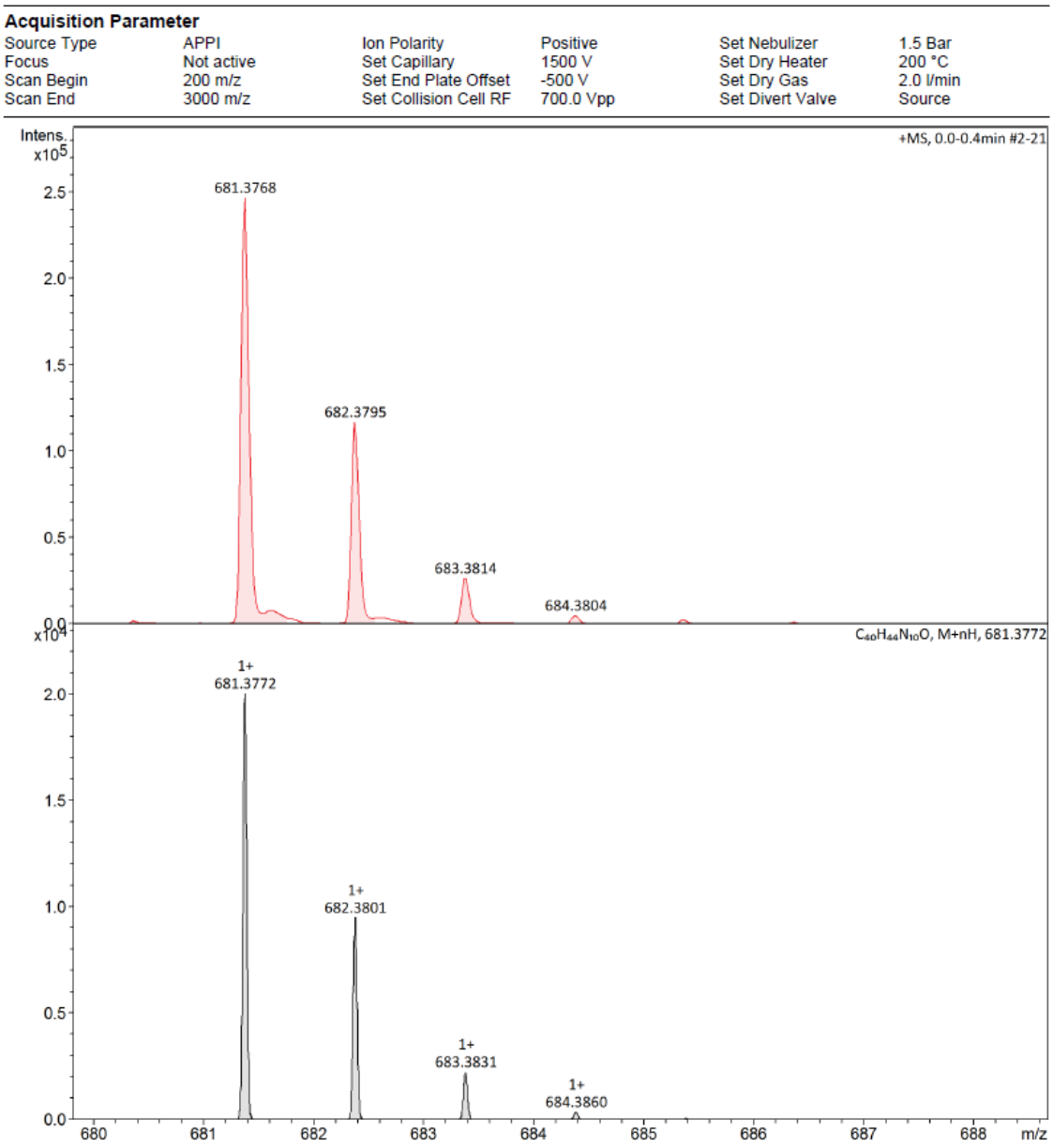


Figure 17S. Isotope Distribution Mass Spectrum of **9a**.

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active	Set Capillary	1500 V	Set Dry Heater	200 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	700.0 Vpp	Set Divert Valve	Source

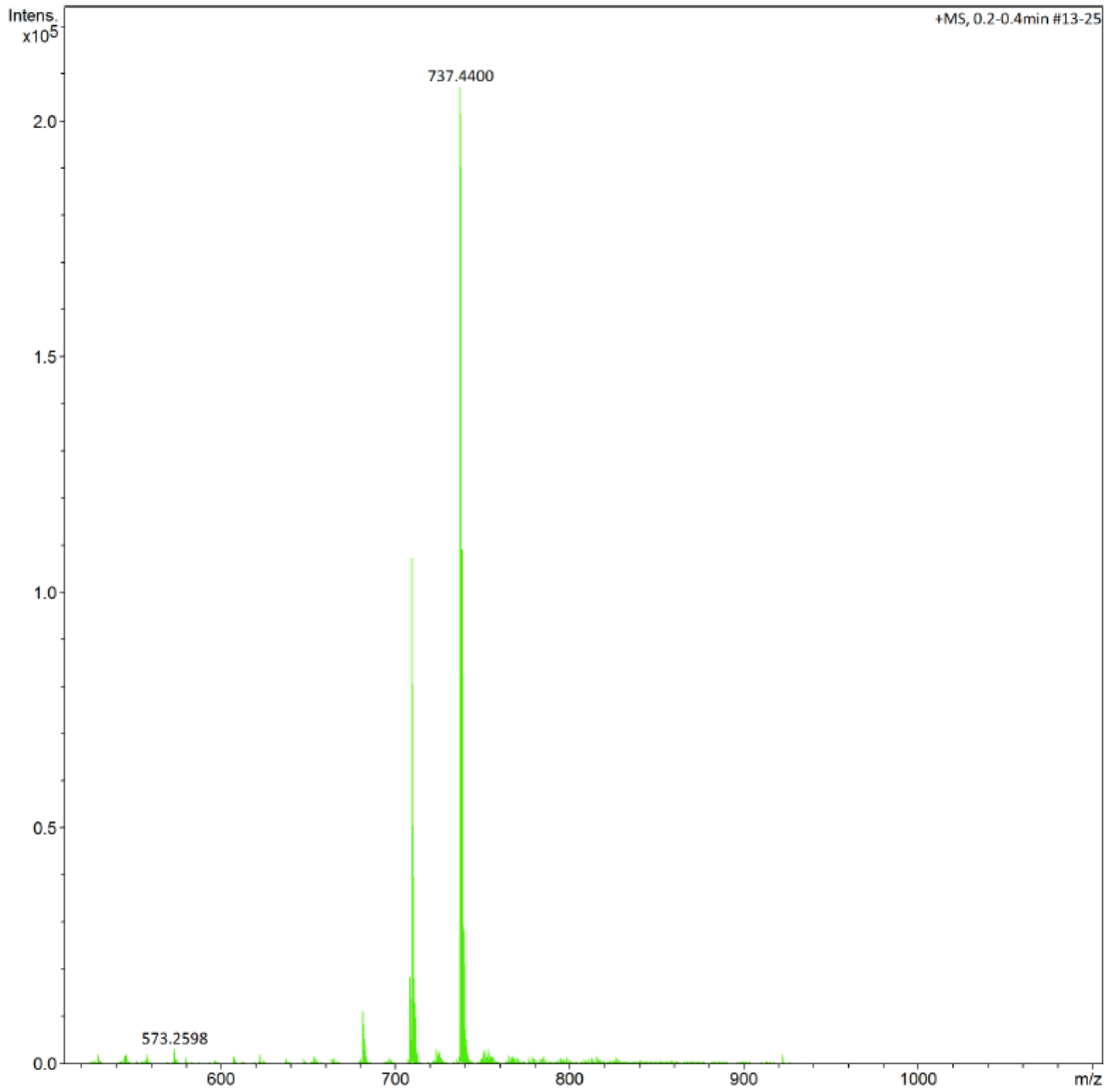


Figure 18S. High-Resolution Mass Spectrum of **9b**.

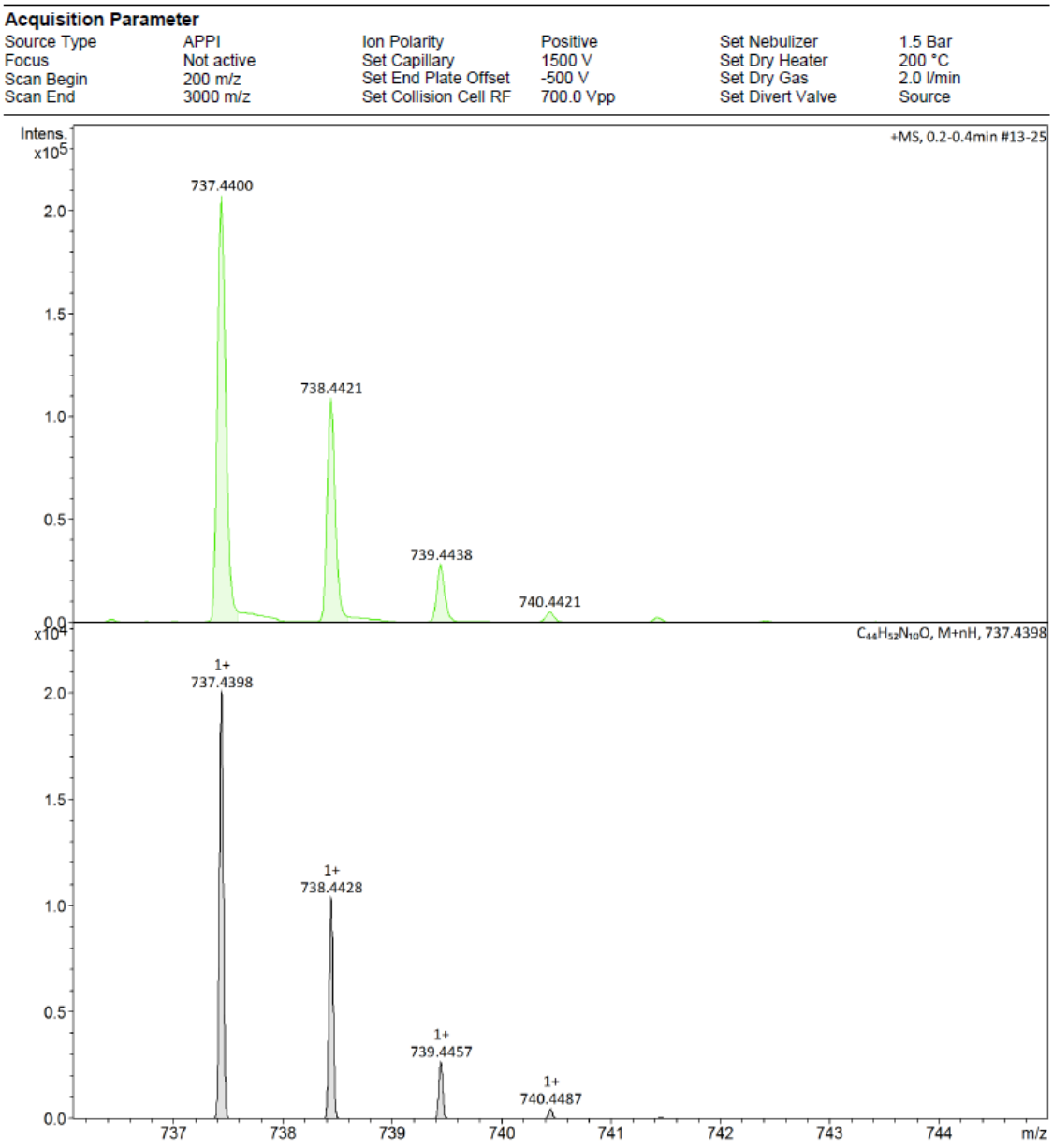


Figure 19S. Isotope Distribution Mass Spectrum of **9b**.

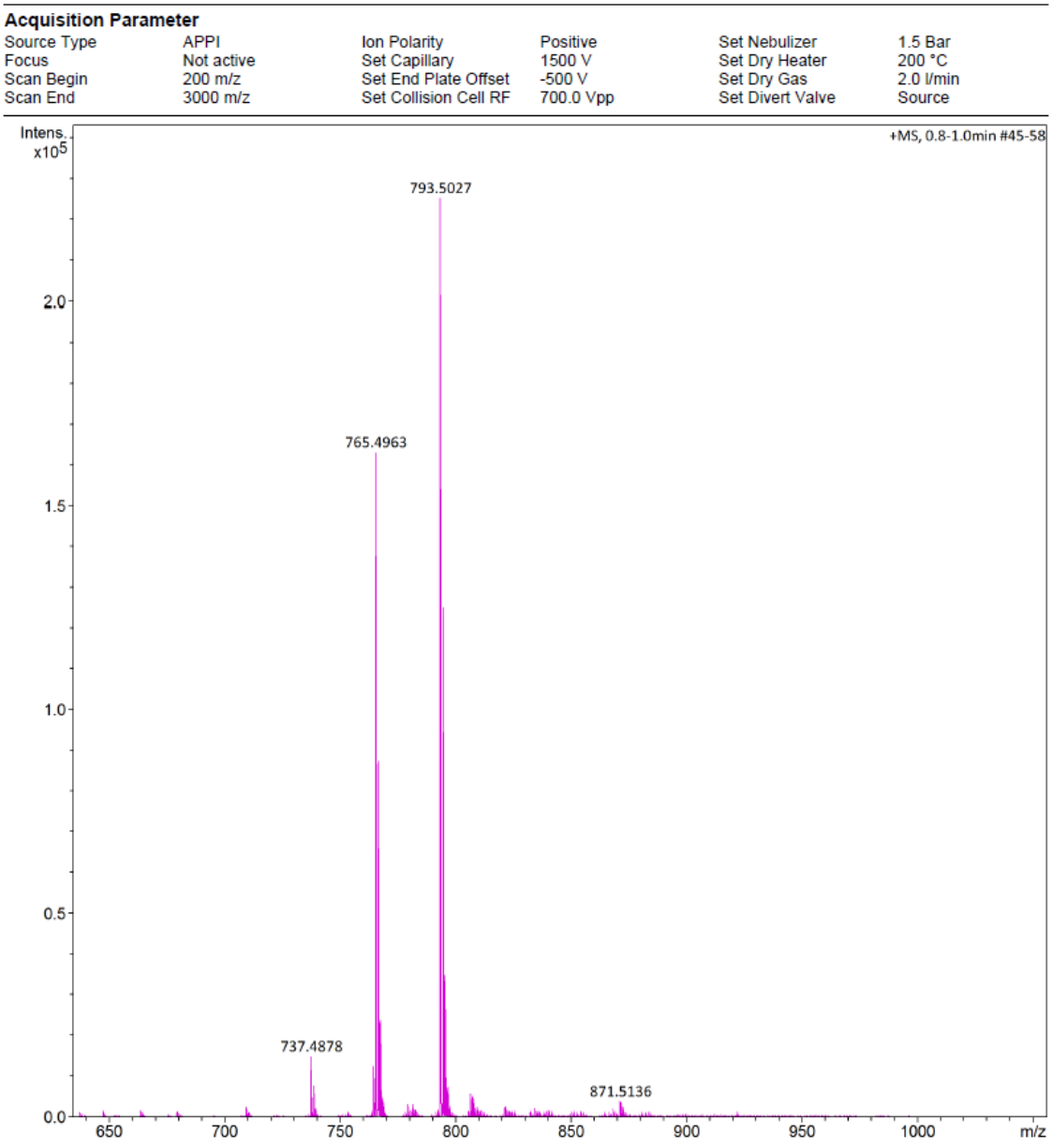


Figure 20S. High-Resolution Mass Spectrum of **9c**.

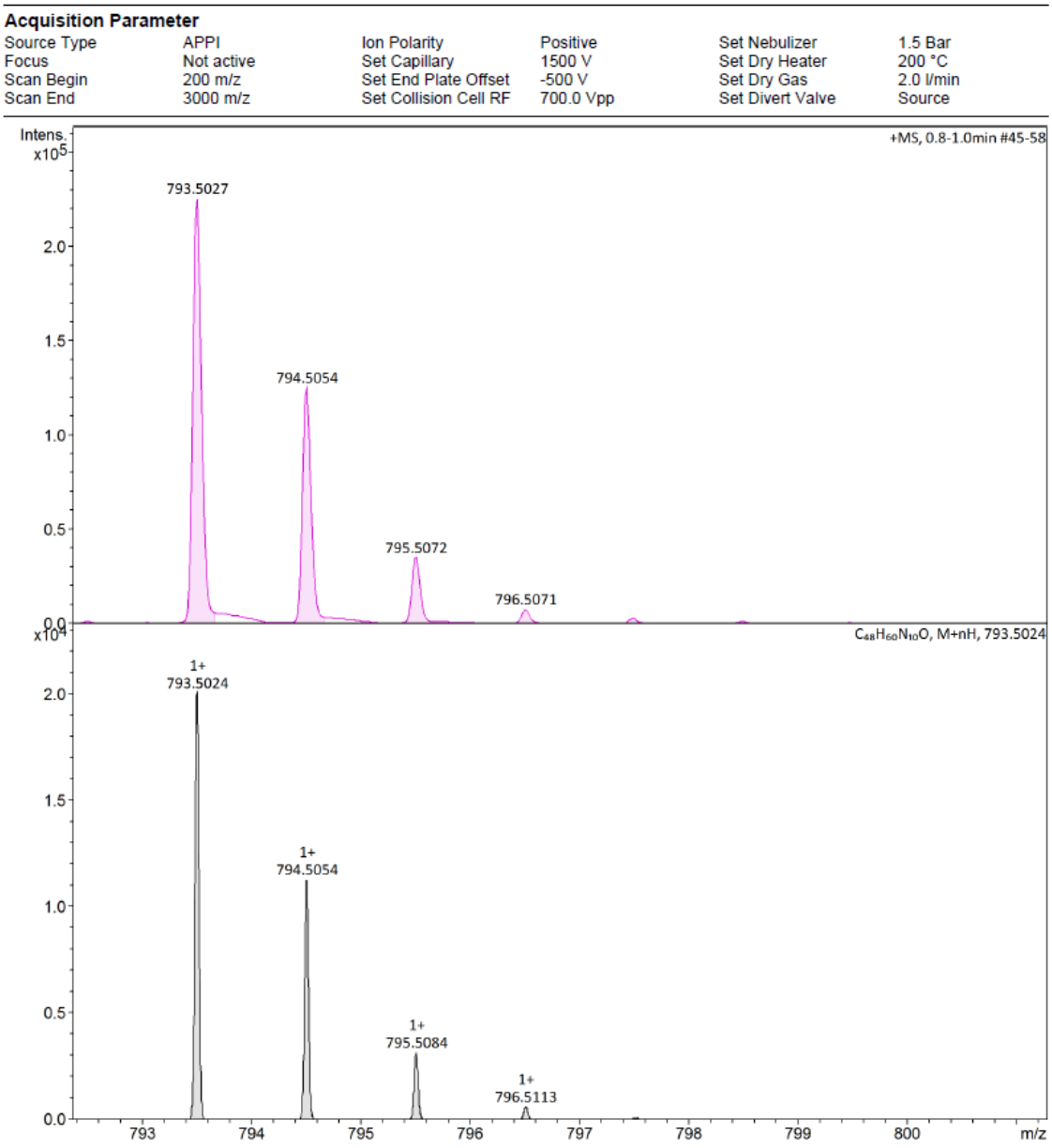


Figure 21S. Isotope Distribution Mass Spectrum of **9c**.

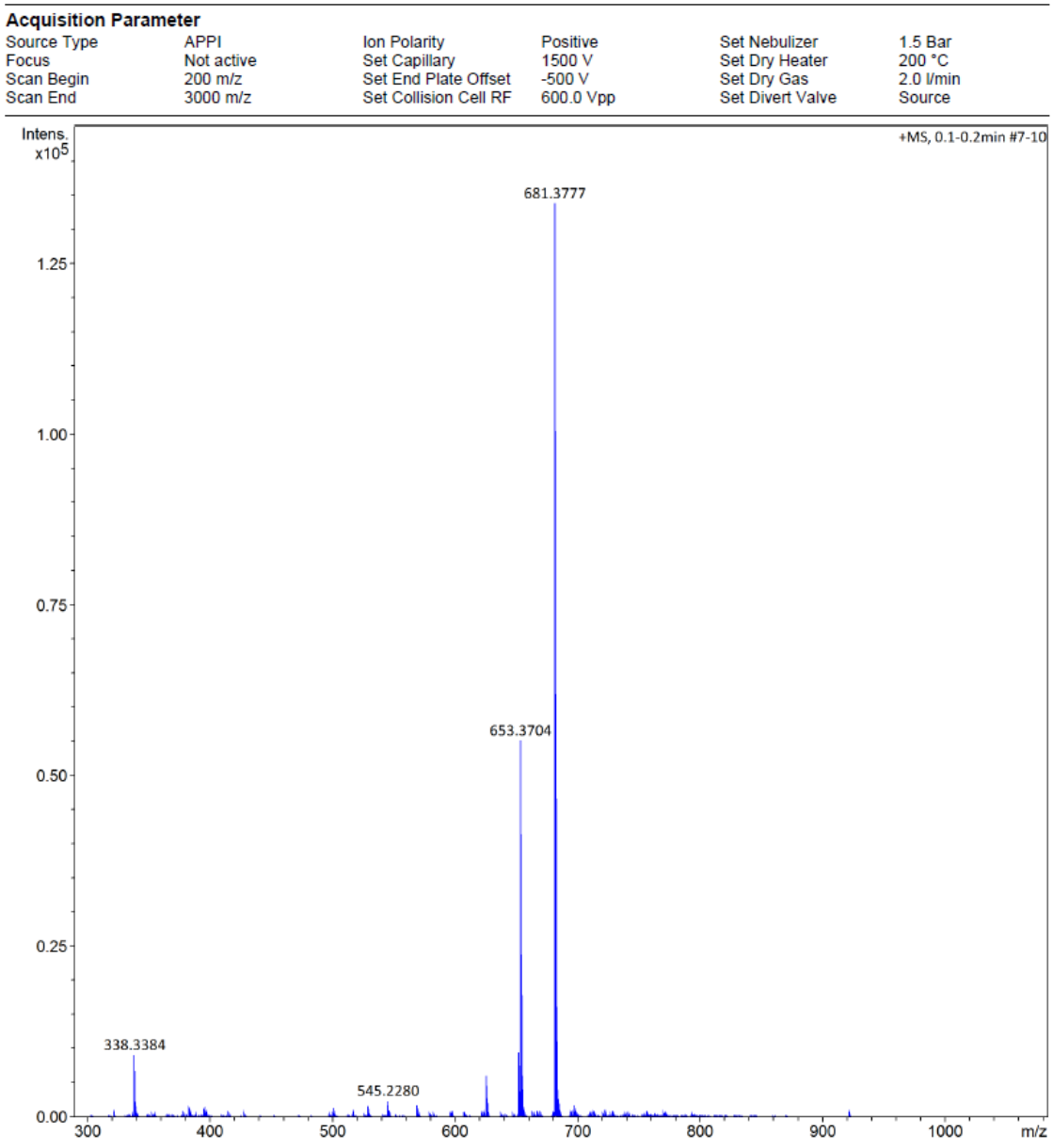


Figure 22S. High-Resolution Mass Spectrum of **9d**.

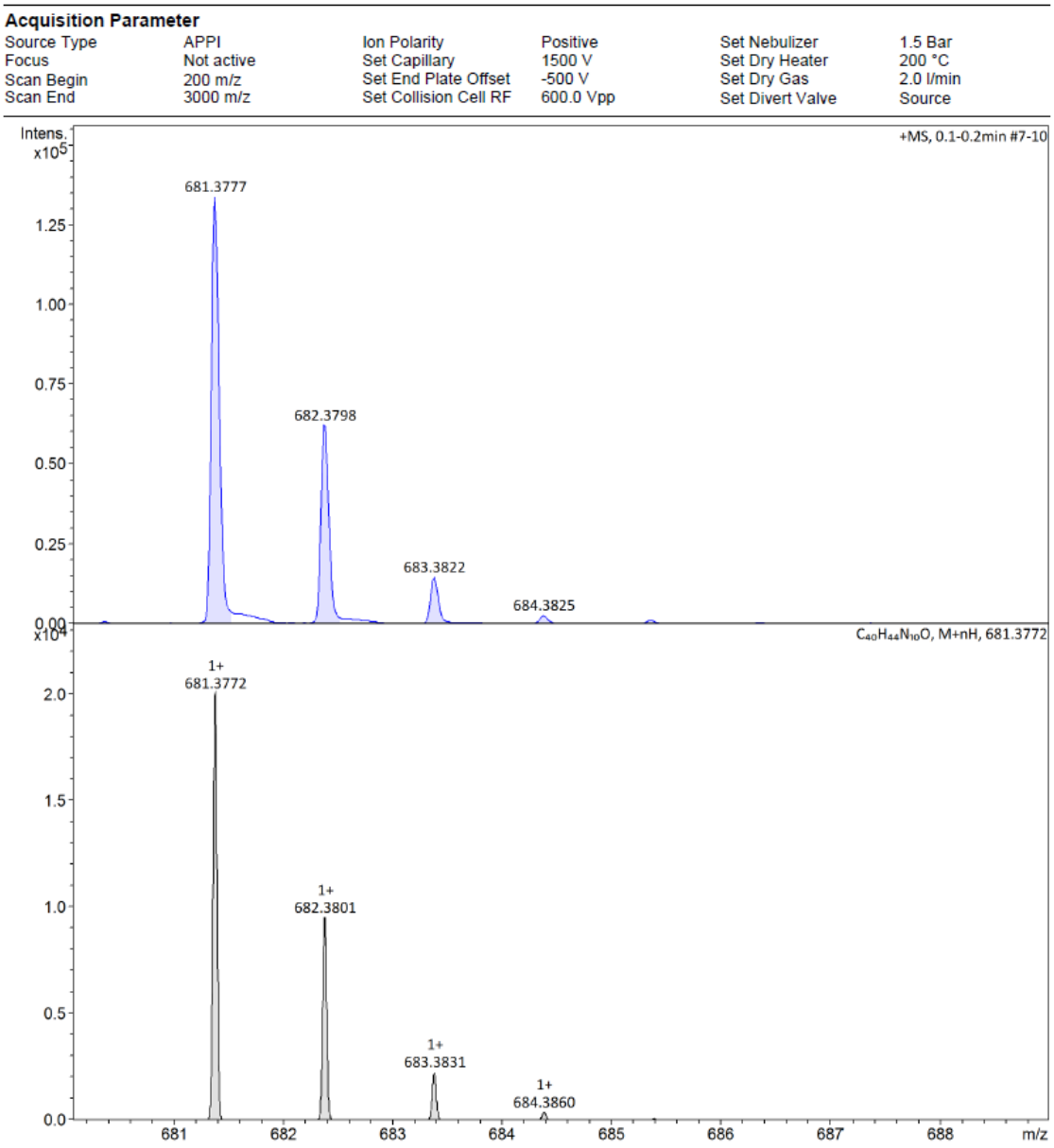


Figure 23S. Isotope Distribution Mass Spectrum of **9d**.