molecules

MDPI

Supporting Information for

Practical Synthesis of Quinoline-Caged Morpholino Oligomers for the Light-Triggered Regulation of Gene Function

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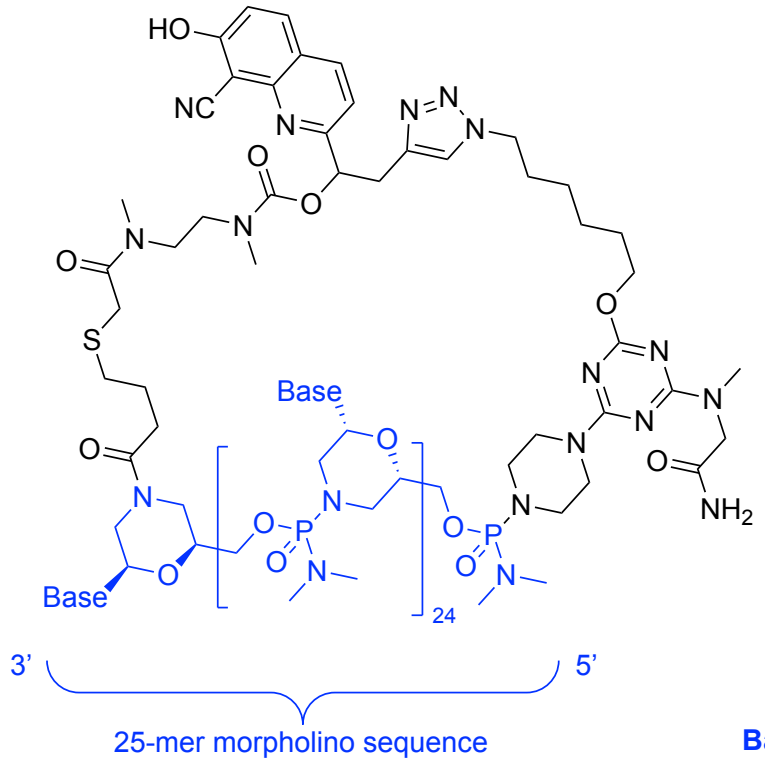
Table of Contents



Base:

A = Adenine
G = Guanine
T = Thymine
C = Cytosine

7a: 5′-AAGGTGCAGAAGACGCCATCAGTCC-3′

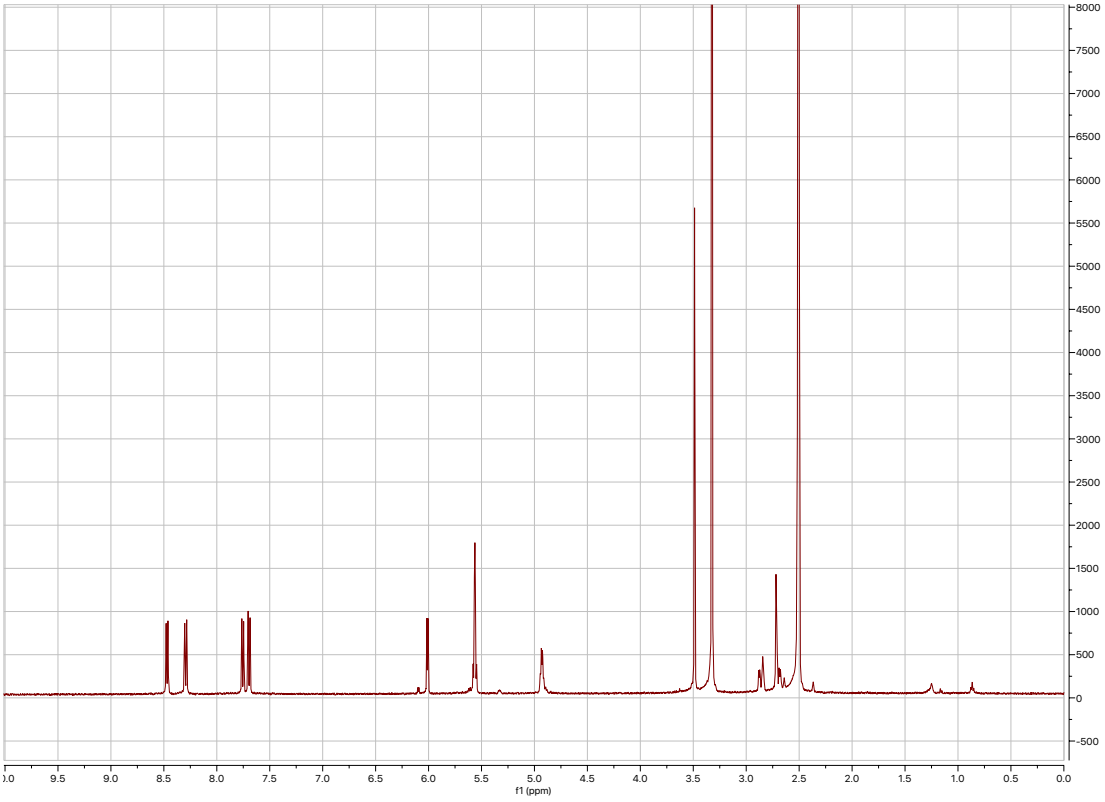
7b: 5′-GAAACCAAAACCCGTGTGATGCCAT-3′

Figure S1. Full structures of compounds **7a** and **7b**.

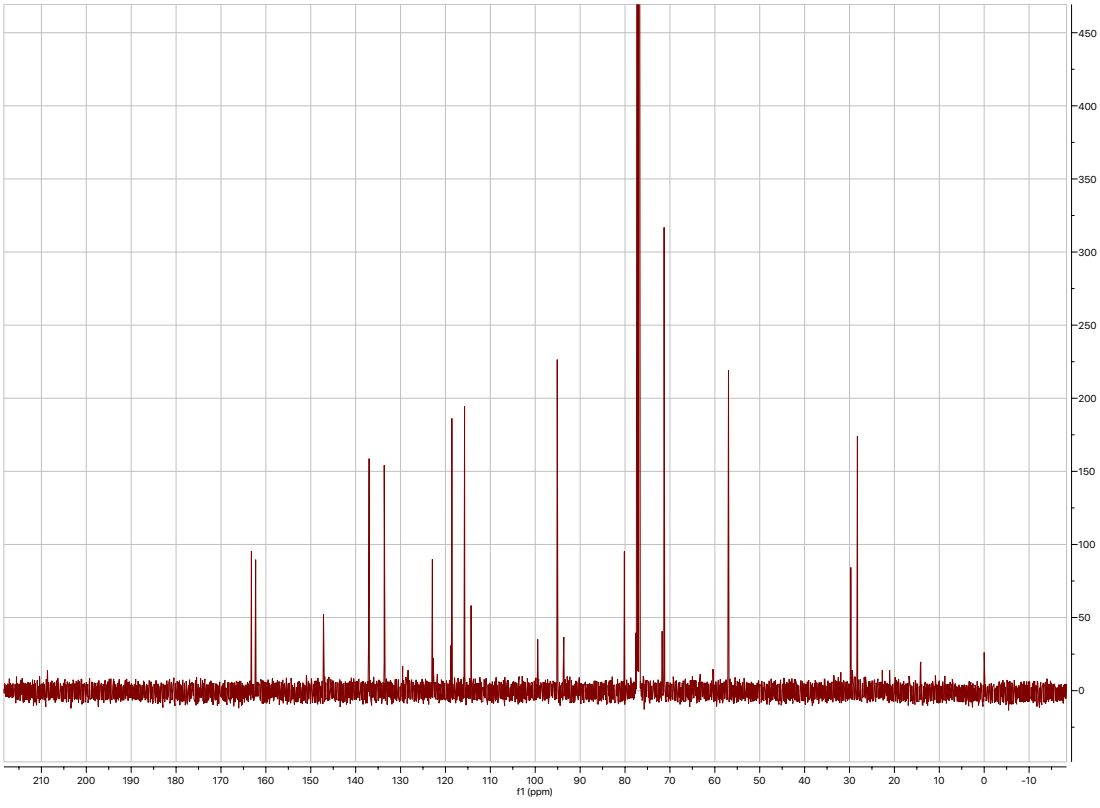
^{1}H and ^{13}C NMR Spectra

*2-(1-hydroxybut-3-yn-1-yl)-7-(methoxymethoxy)quinoline-8-carbonitrile (**1**).*

^{1}H NMR (500 MHz, DMSO-d_6)

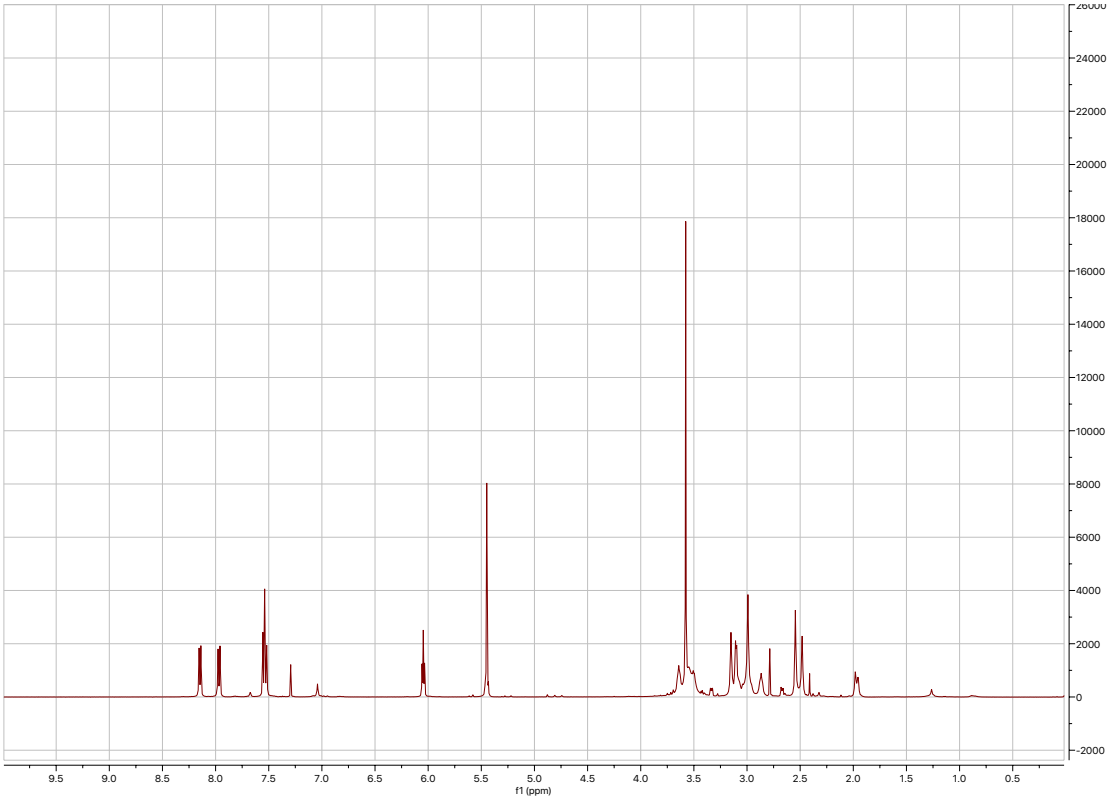


^{13}C NMR (126 MHz, chloroform-*d*)

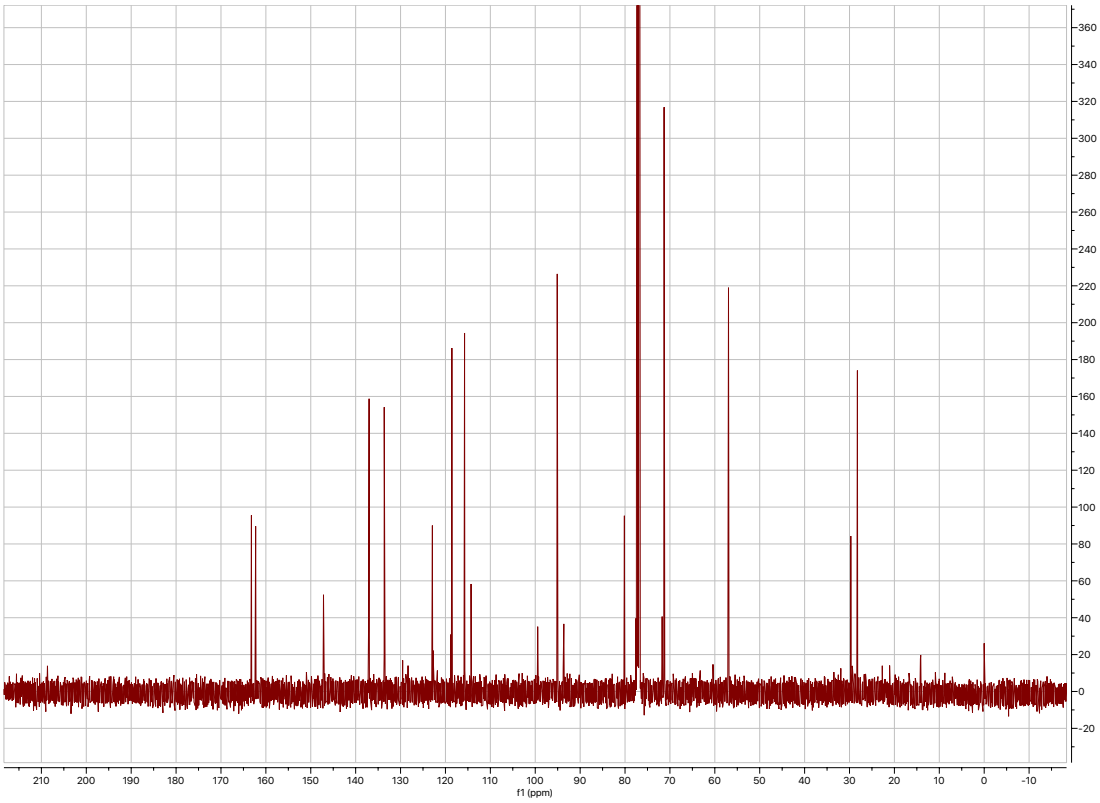


1-(8-cyano-7-(methoxymethoxy)quinolin-2-yl)but-3-yn-1-yl-methyl(2-(methylamino)ethyl)carbamate (**2**).

^{1}H NMR (500 MHz, chloroform-*d*)

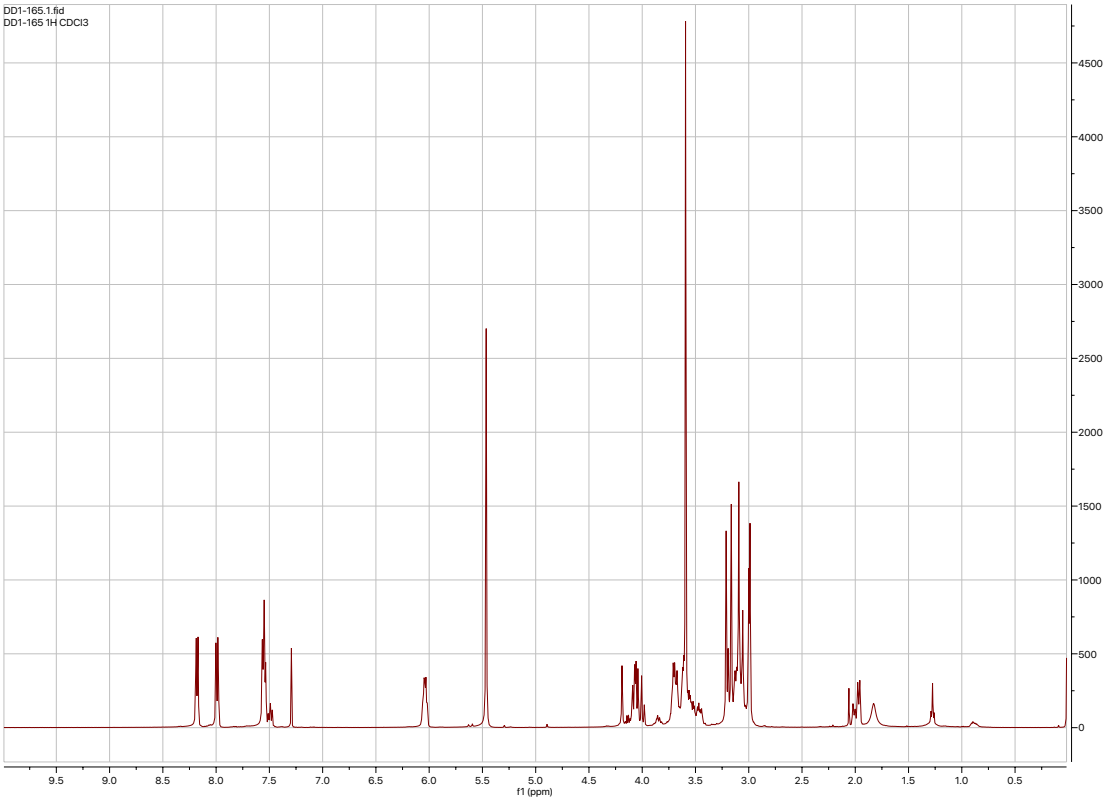


^{13}C NMR (126 MHz, chloroform-*d*)

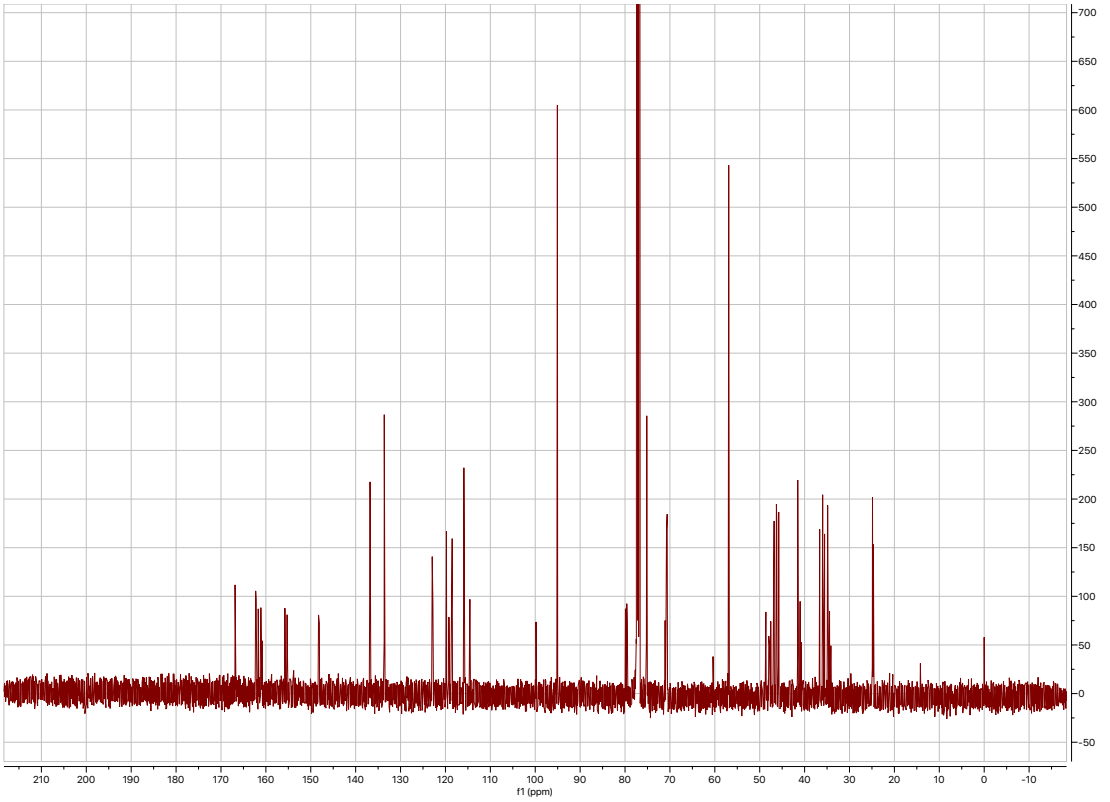


*1-(8-cyano-7-(methoxymethoxy)quinolin-2-yl)but-3-yn-1-yl-(2-(2-chloro-N-methylacetamido)ethyl)(methyl)carbamate (**3**).*

^{1}H NMR (500 MHz, chloroform-*d*)

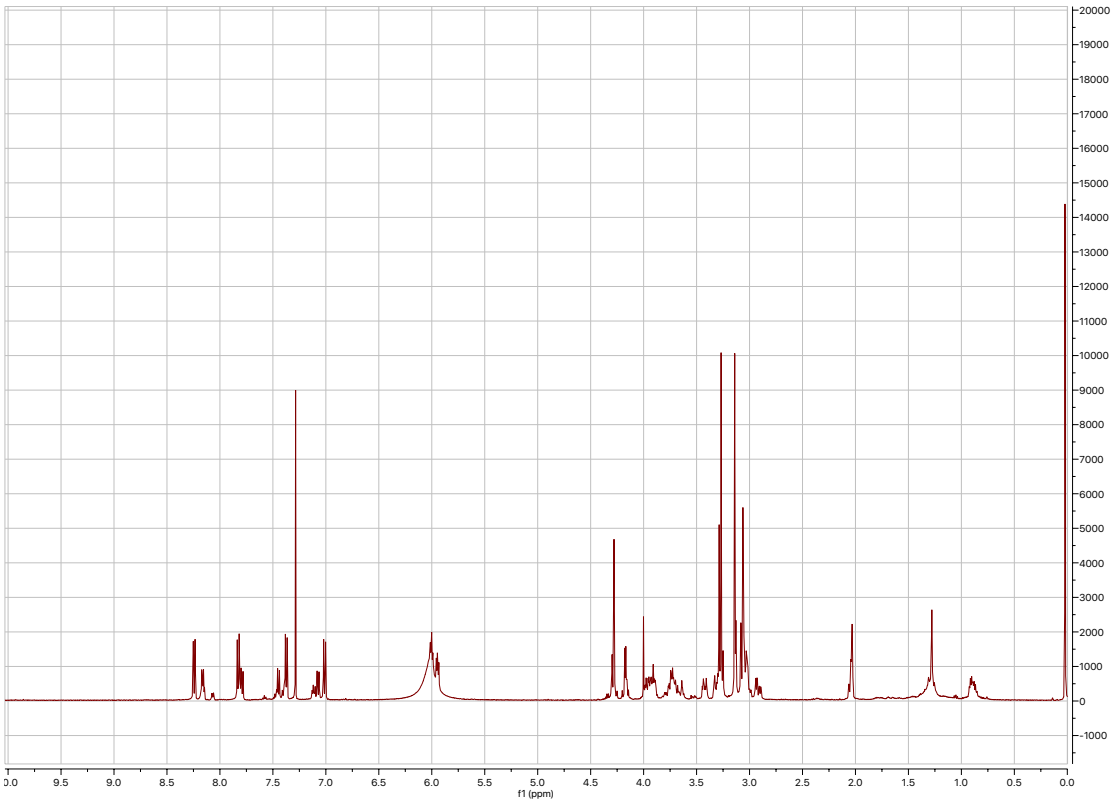


^{13}C NMR (126 MHz, chloroform-*d*)

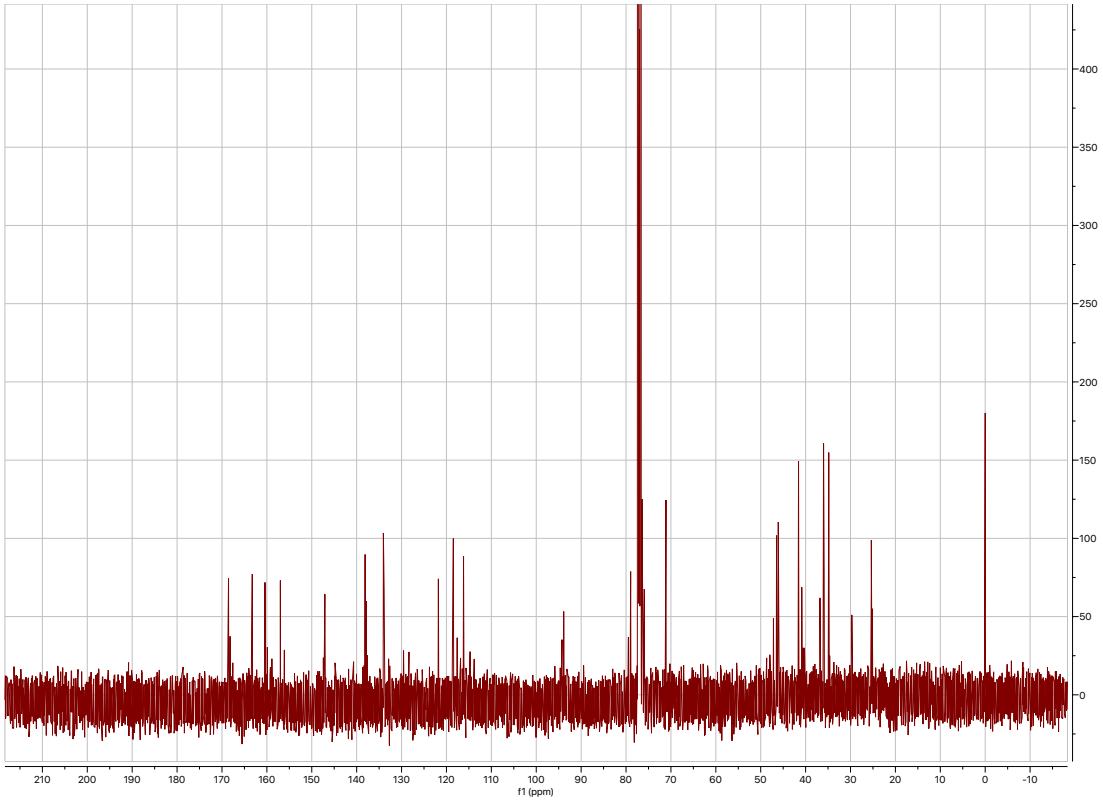


*1-(8-cyano-7-hydroxyquinolin-2-yl)but-3-yn-1-yl-(2-(2-chloro-N-methylacetamido)ethyl)(methyl)carbamate (**4**).*

^{1}H NMR (500 MHz, chloroform-*d*)



^{13}C NMR (126 MHz, chloroform-*d*)

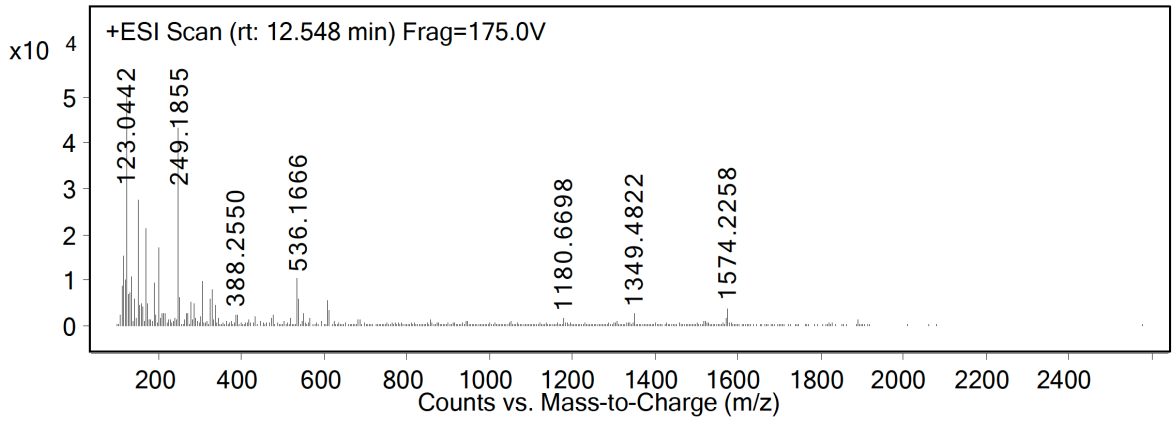


HRMS Spectra

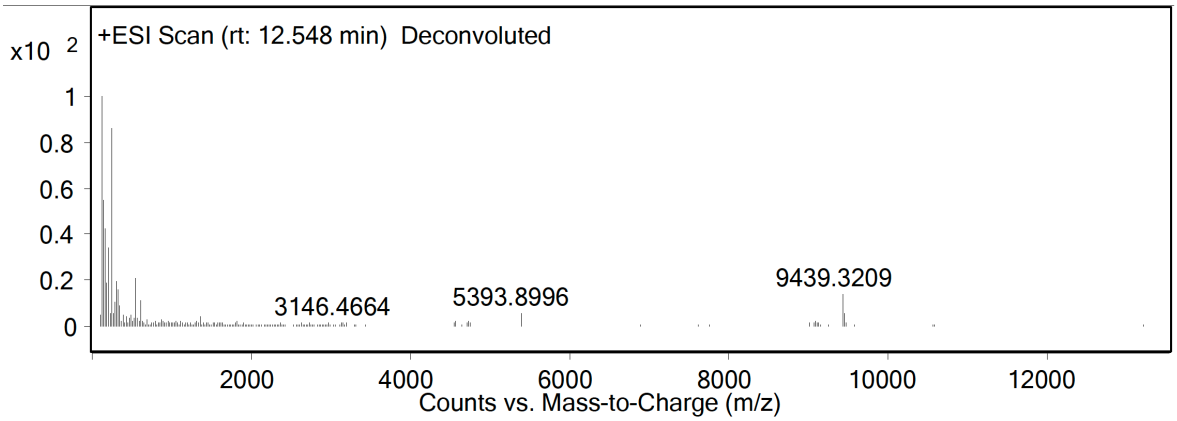
*CyHQ-MO-gad1 (**6a**)*

[M] calculated for $C_{338}H_{515}N_{167}O_{103}S_2P_{25}Cl$ = 9439.7029

HRMS trace



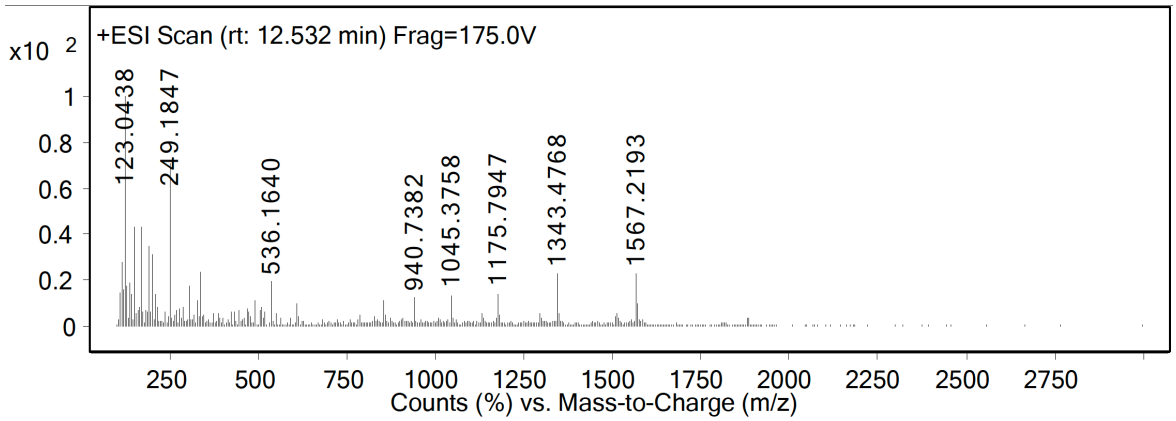
Deconvolution



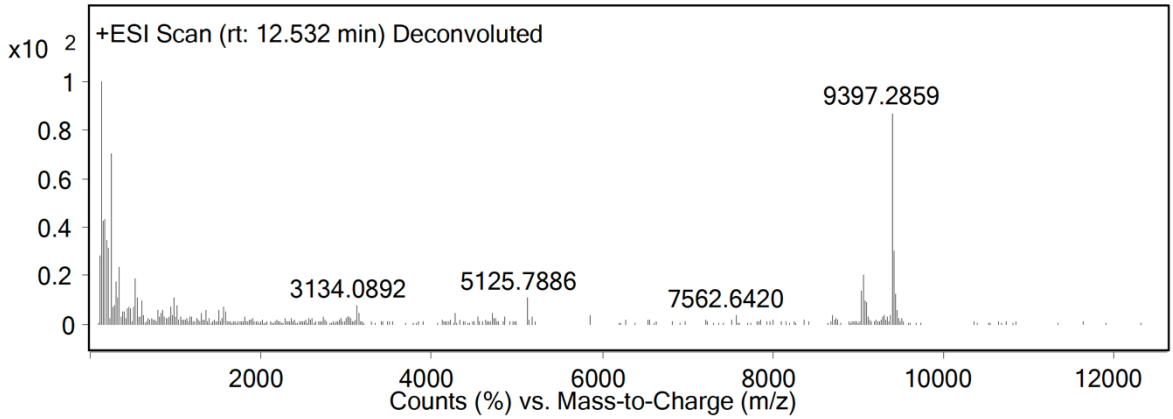
*CyHQ-MO-gad2 (**6b**)*

[M] calculated for $C_{338}H_{515}N_{164}O_{103}S_2P_{25}Cl$ = 9397.6828

HRMS trace



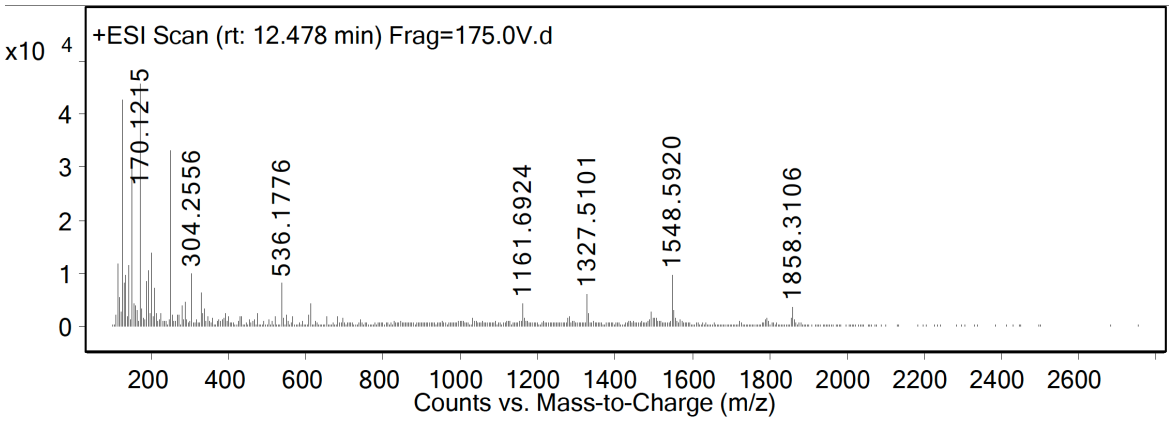
Deconvolution



*CyHQ-ccMO-gad1 (**7a**)*

[M] calculated for $C_{334}H_{507}N_{166}O_{102}SP_{25}$ = 9285.0646

HRMS trace



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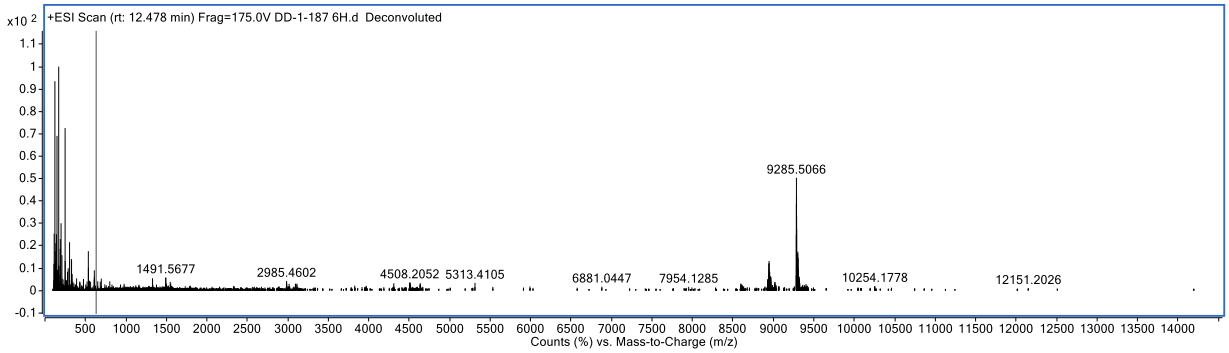
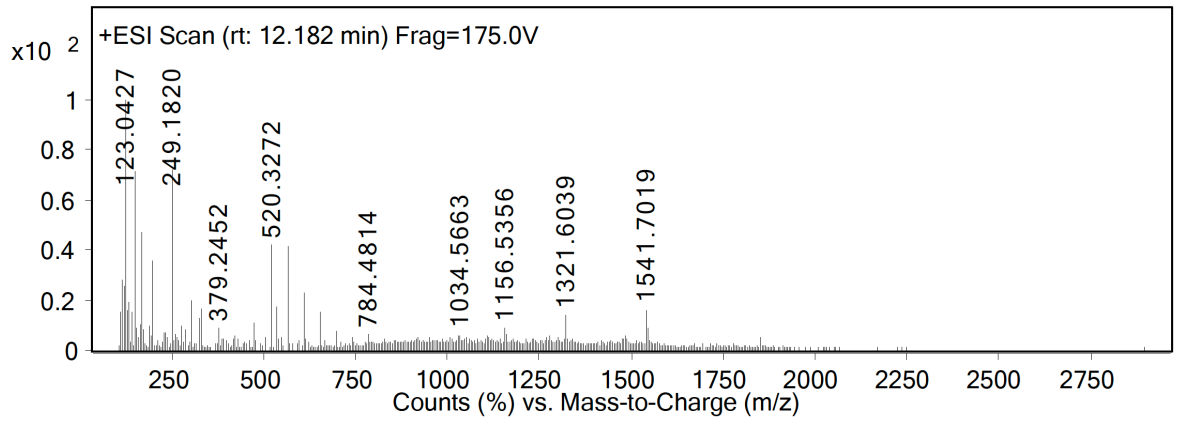


*CyHQ-ccMO-gad2 (**7b**)*

[M] calculated for $C_{334}H_{507}N_{163}O_{102}SP_{25}$ = 9244.0525

HRMS trace



Deconvolution