

Supporting Information

Synthesis of *N,N*-disubstituted 2-aminothiophenes by the cyclization of *gem*-difluoroalkenes with β -keto thioamides

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*Corresponding author. Tel: +86-21-64253452; fax: +86-21-64252603

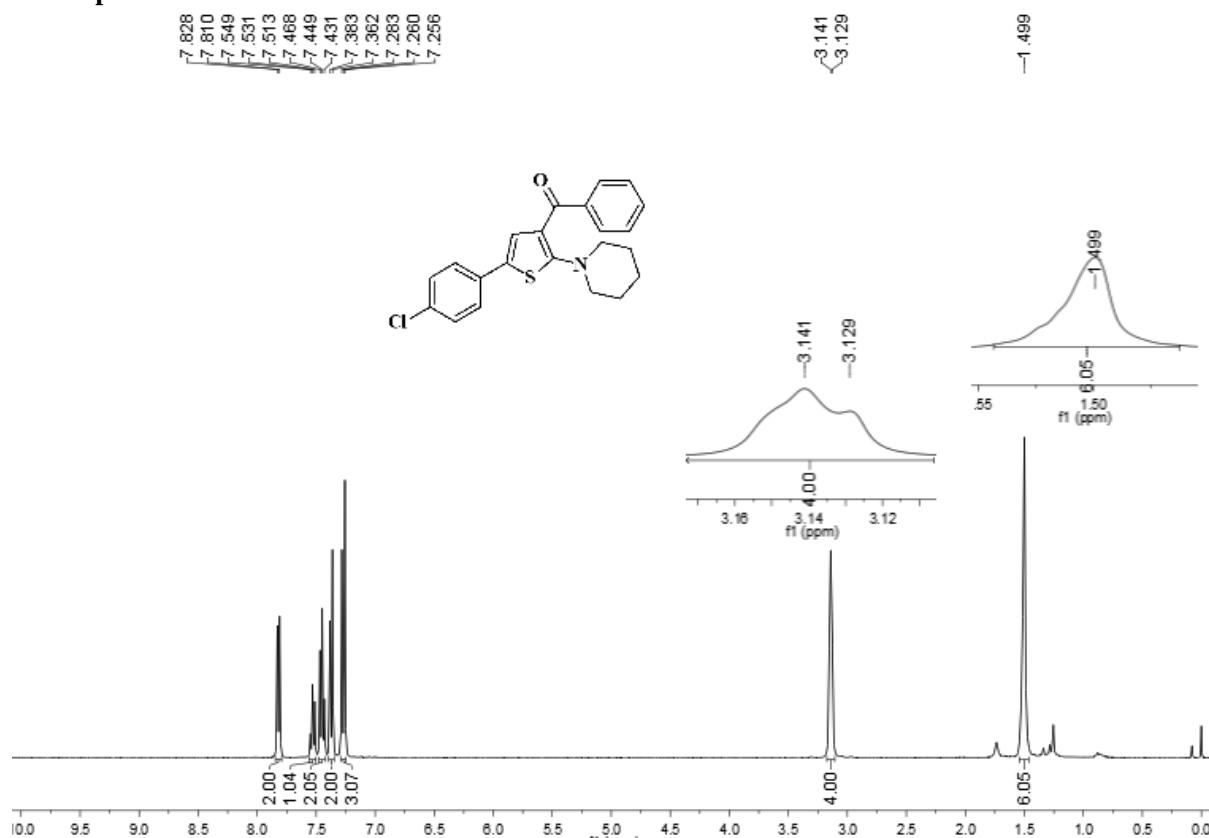
E-mail address: scao@ecust.edu.cn

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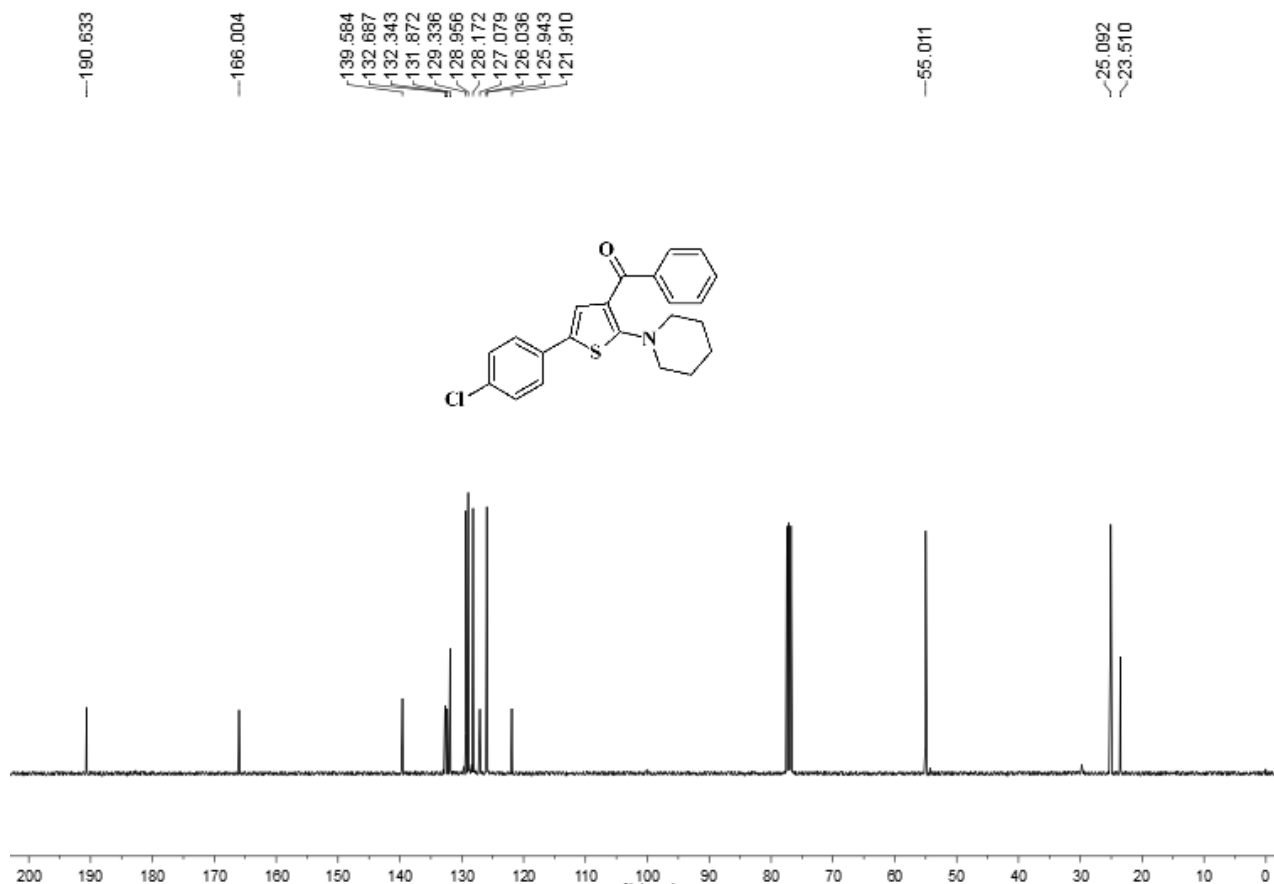
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1. ^1H , ^{13}C , ^{19}F NMR and HRMS (EI) spectra of compounds 3

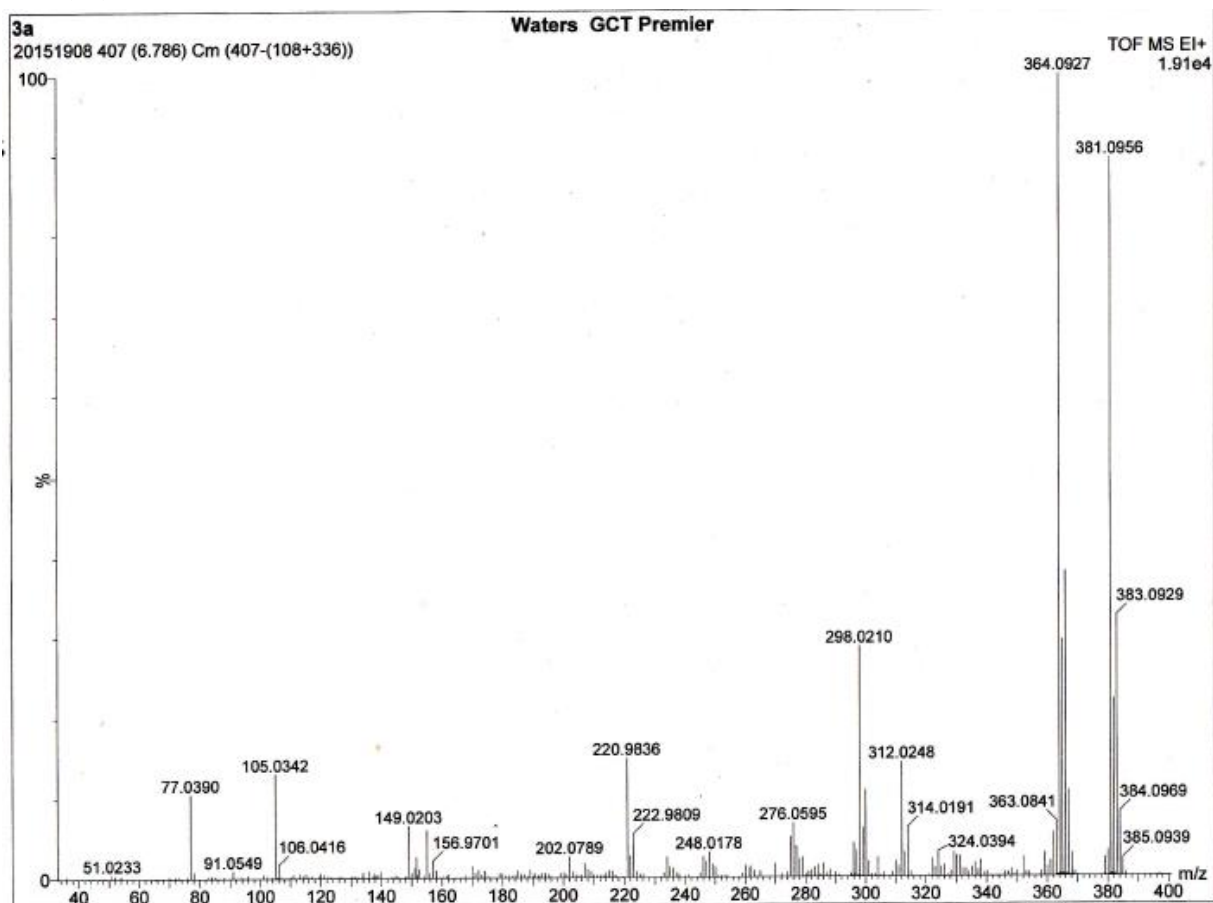
^1H NMR spectrum of 3aa



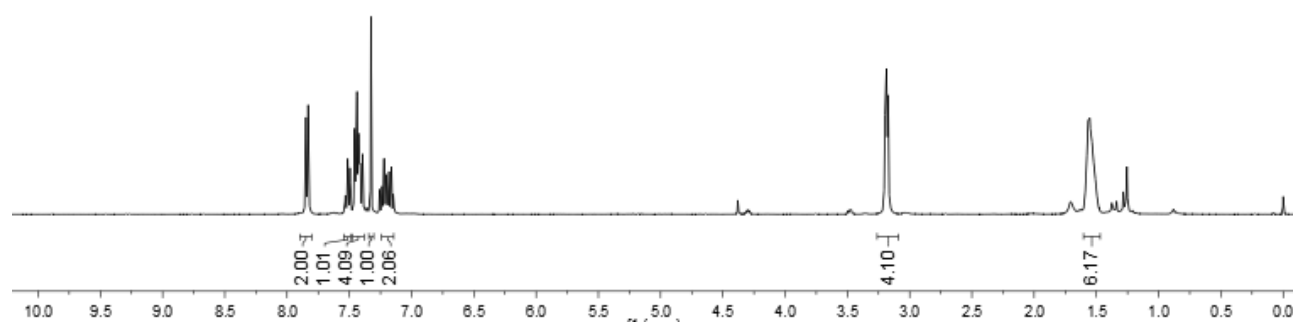
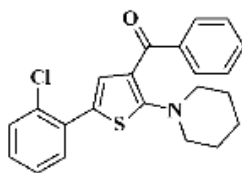
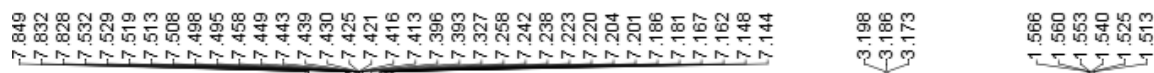
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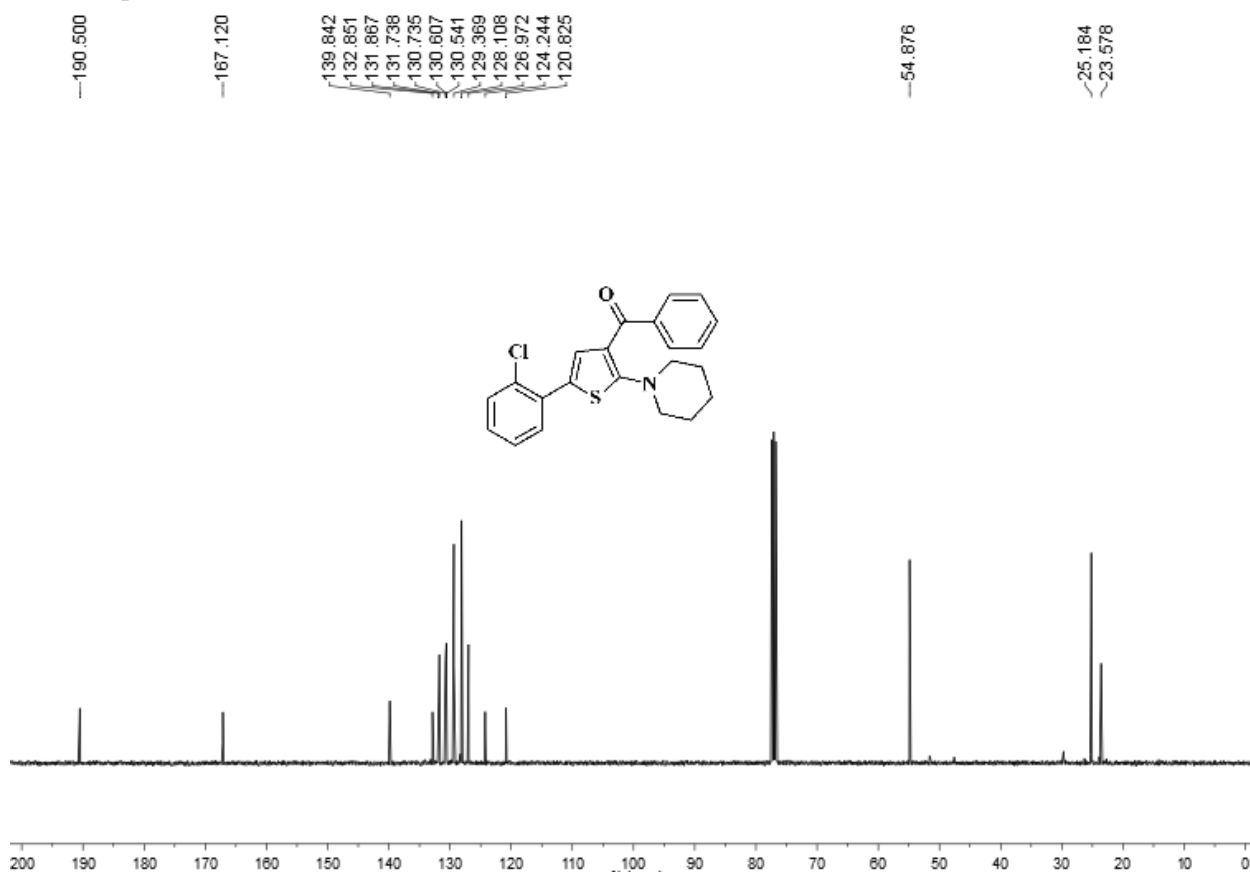
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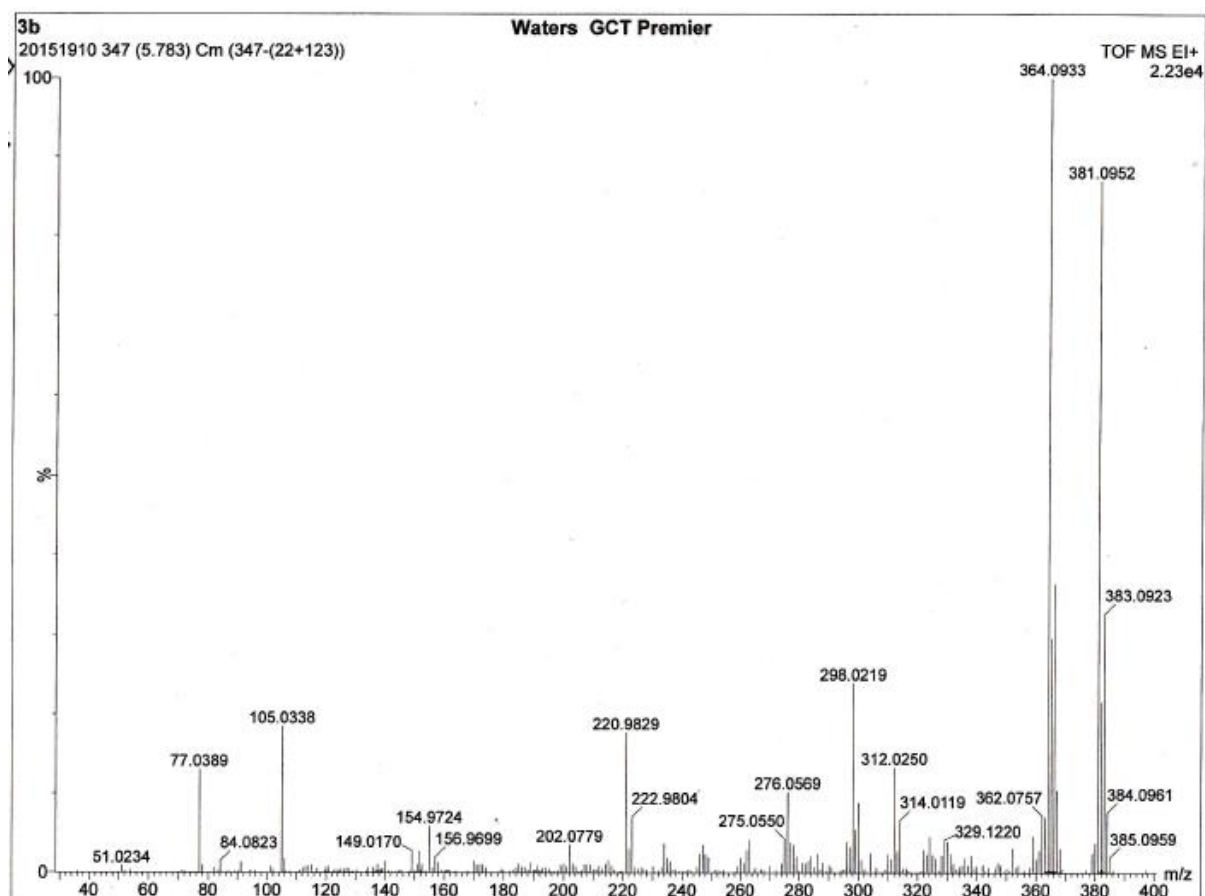
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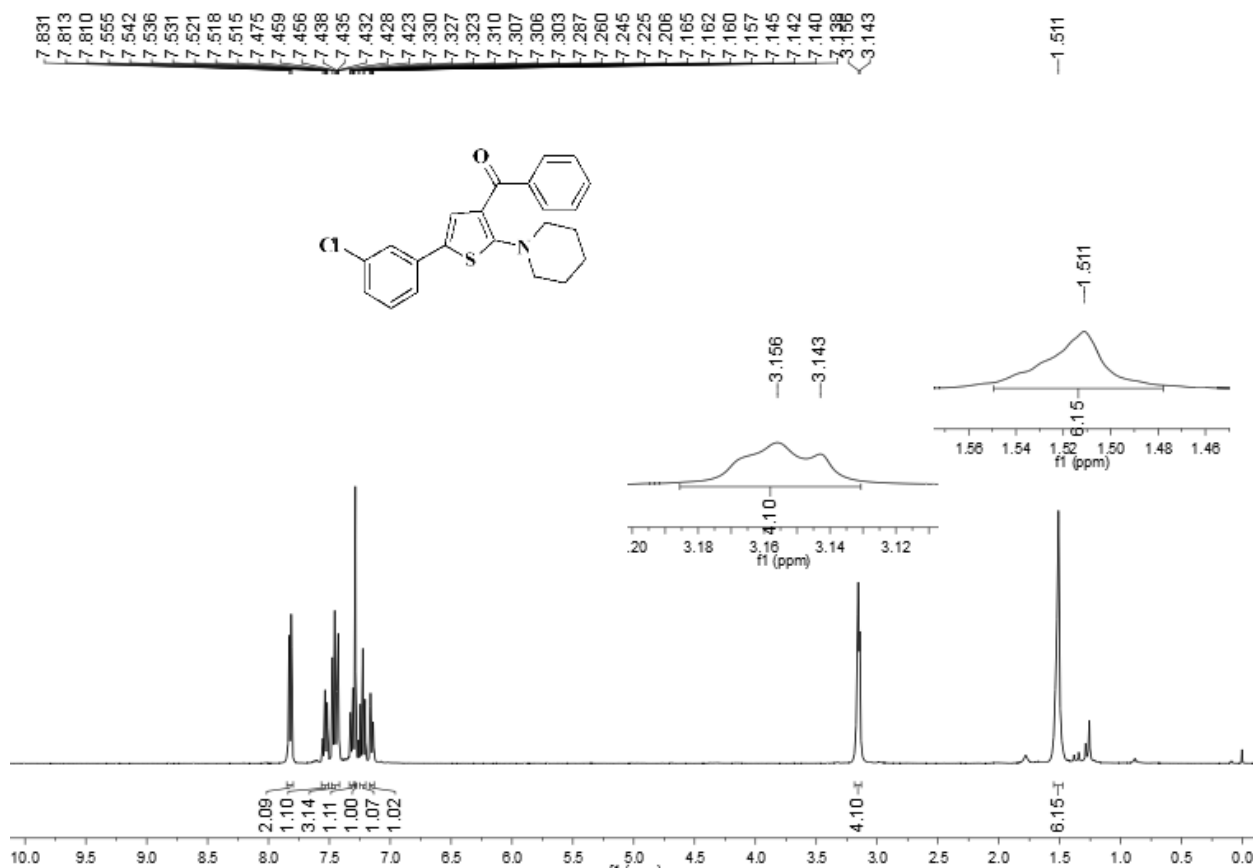
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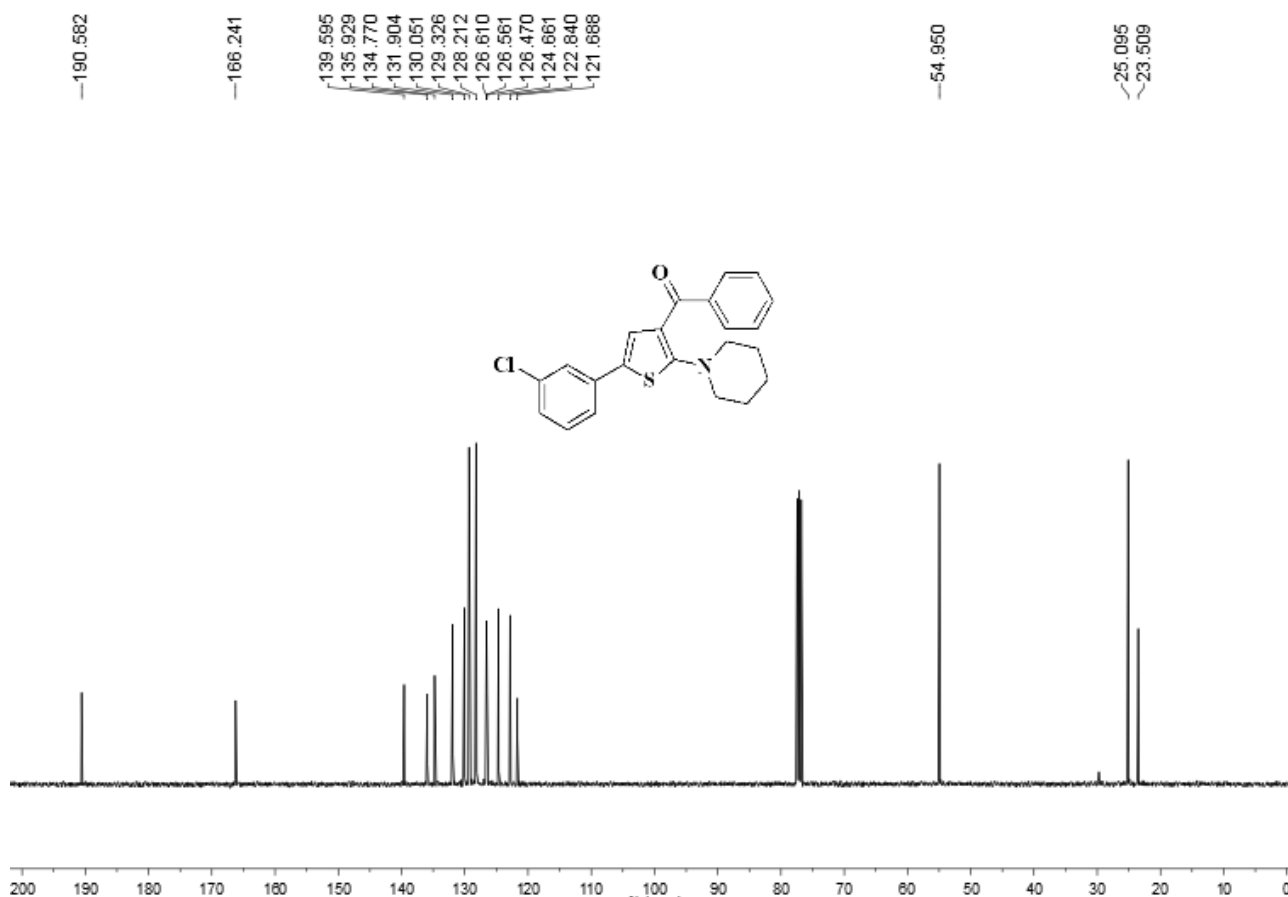
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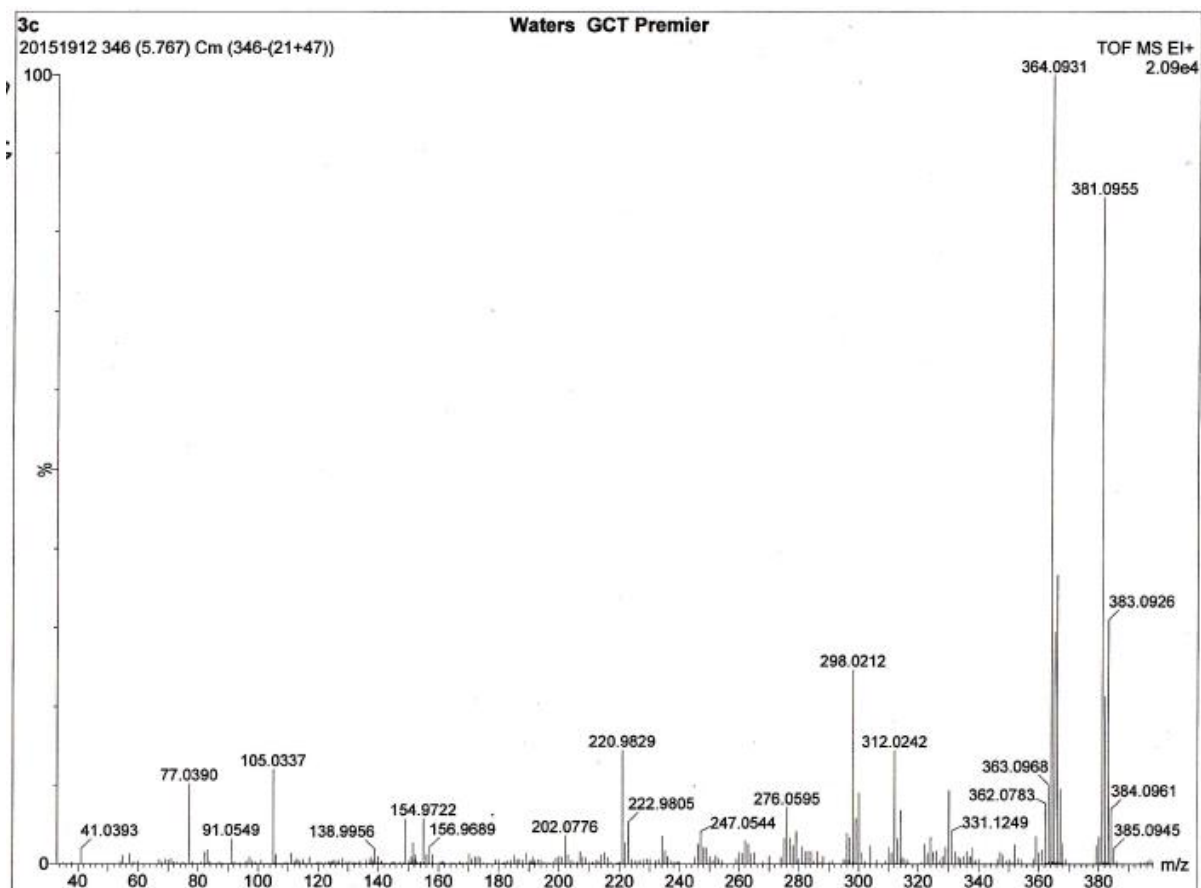
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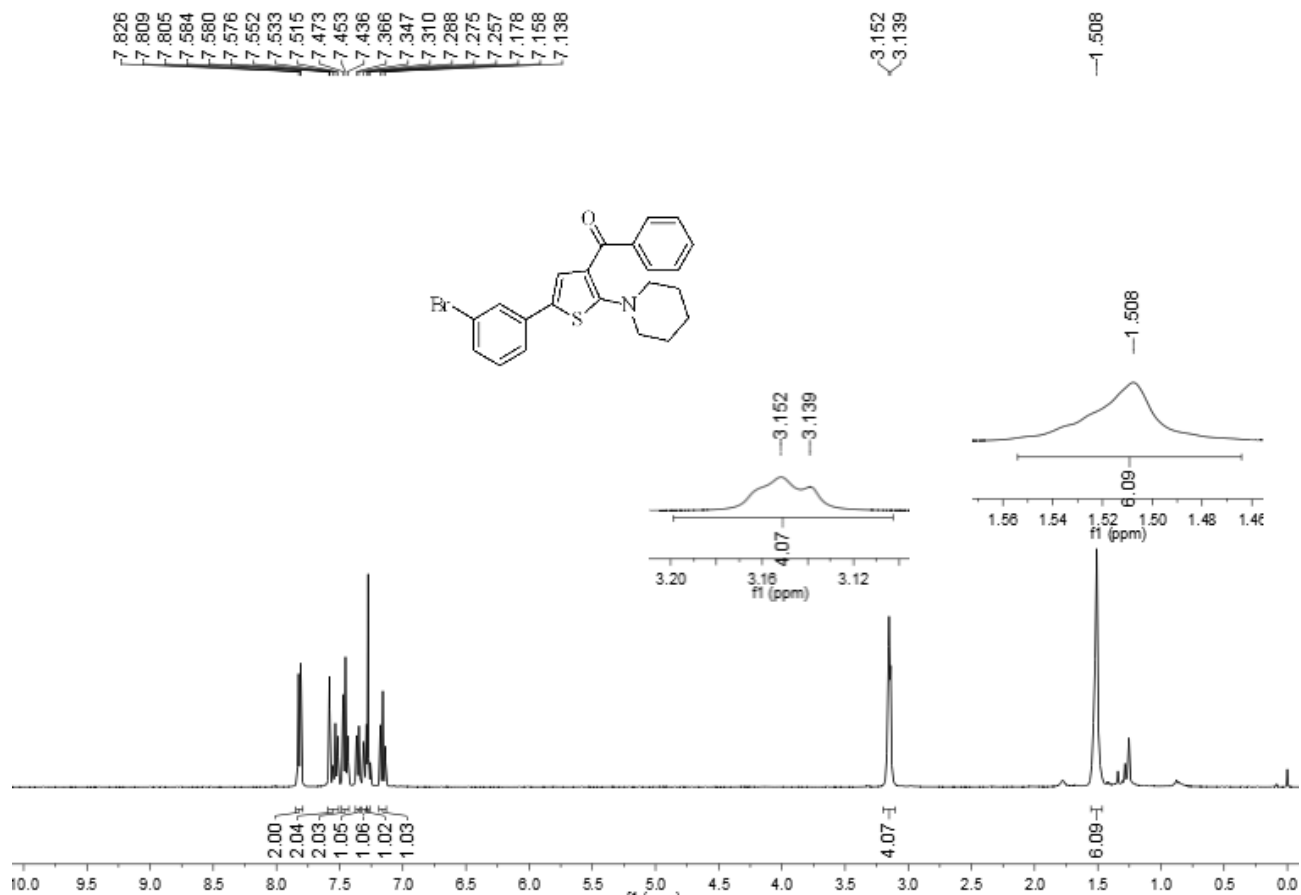
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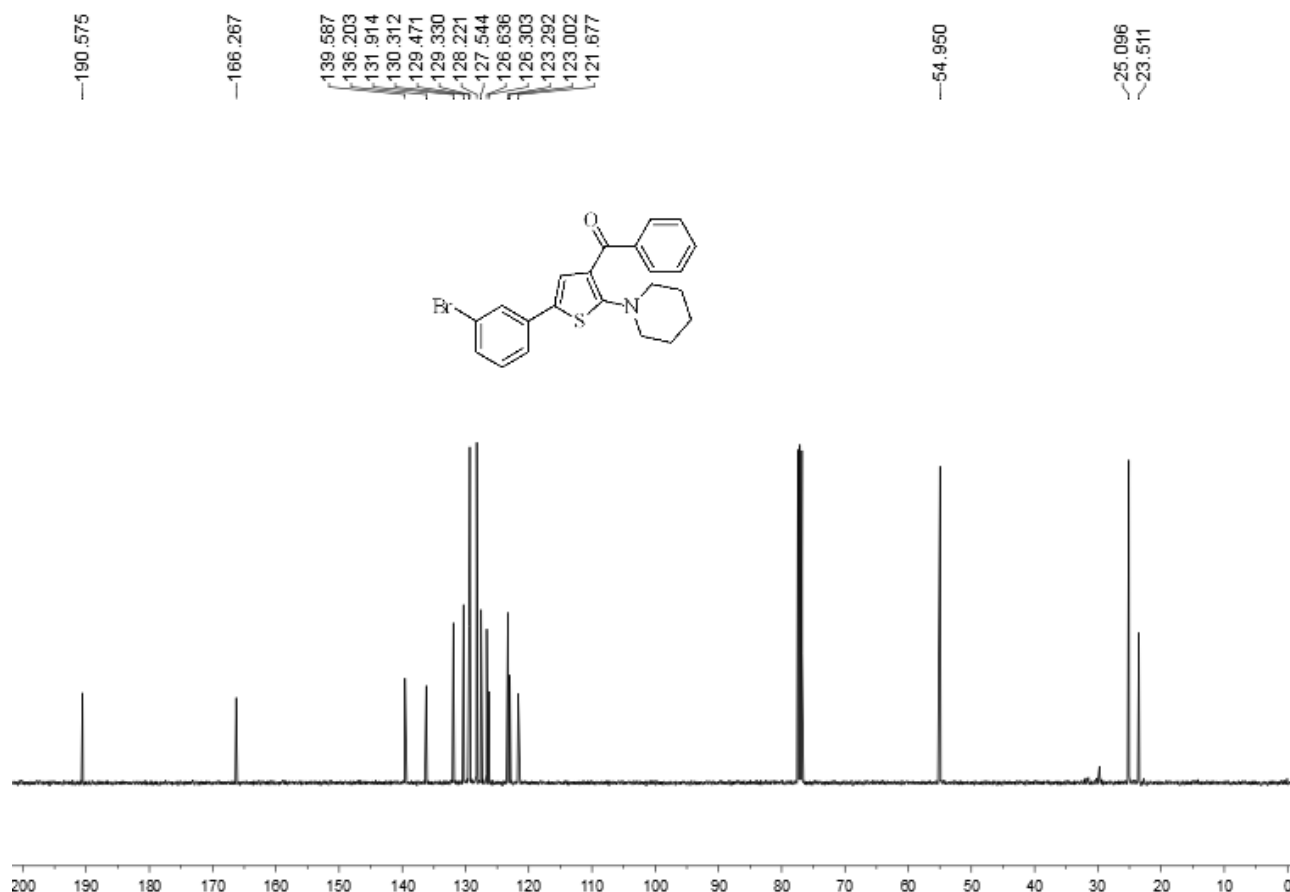
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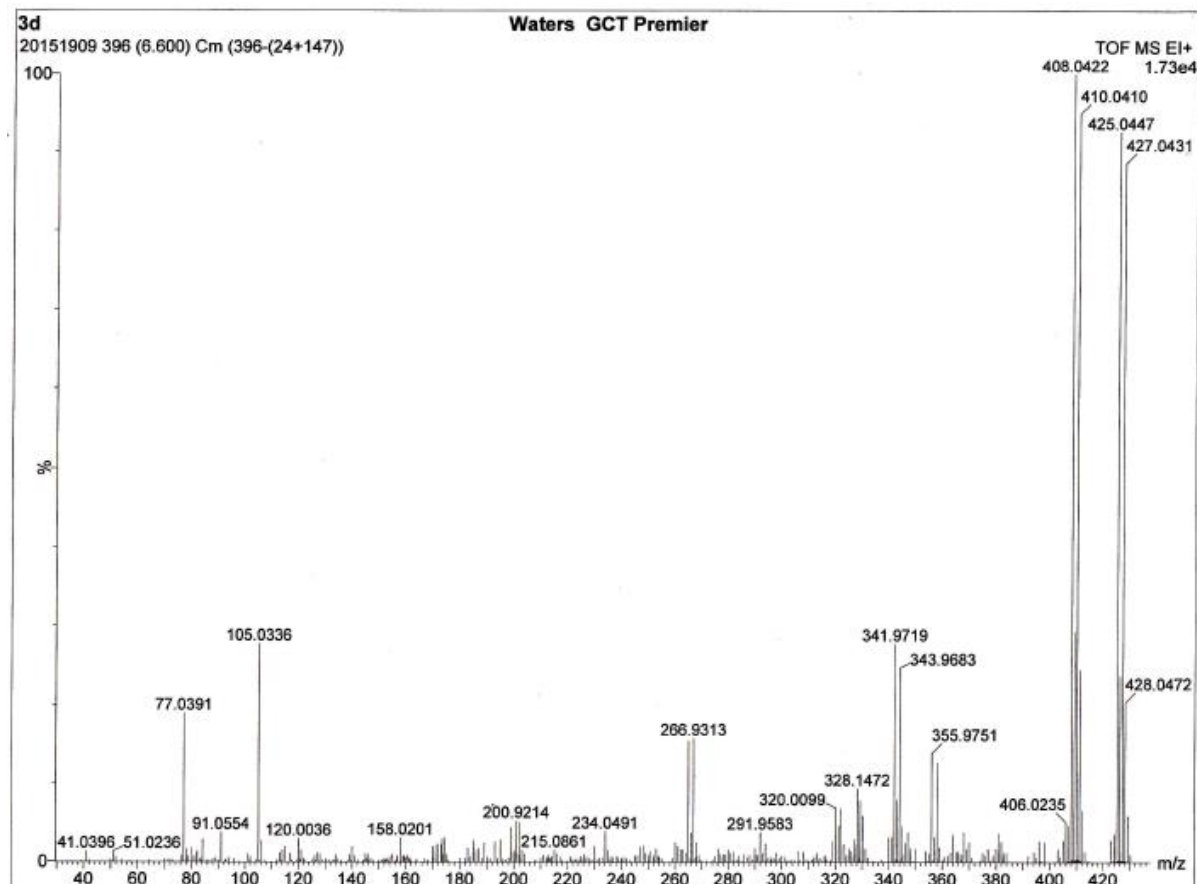
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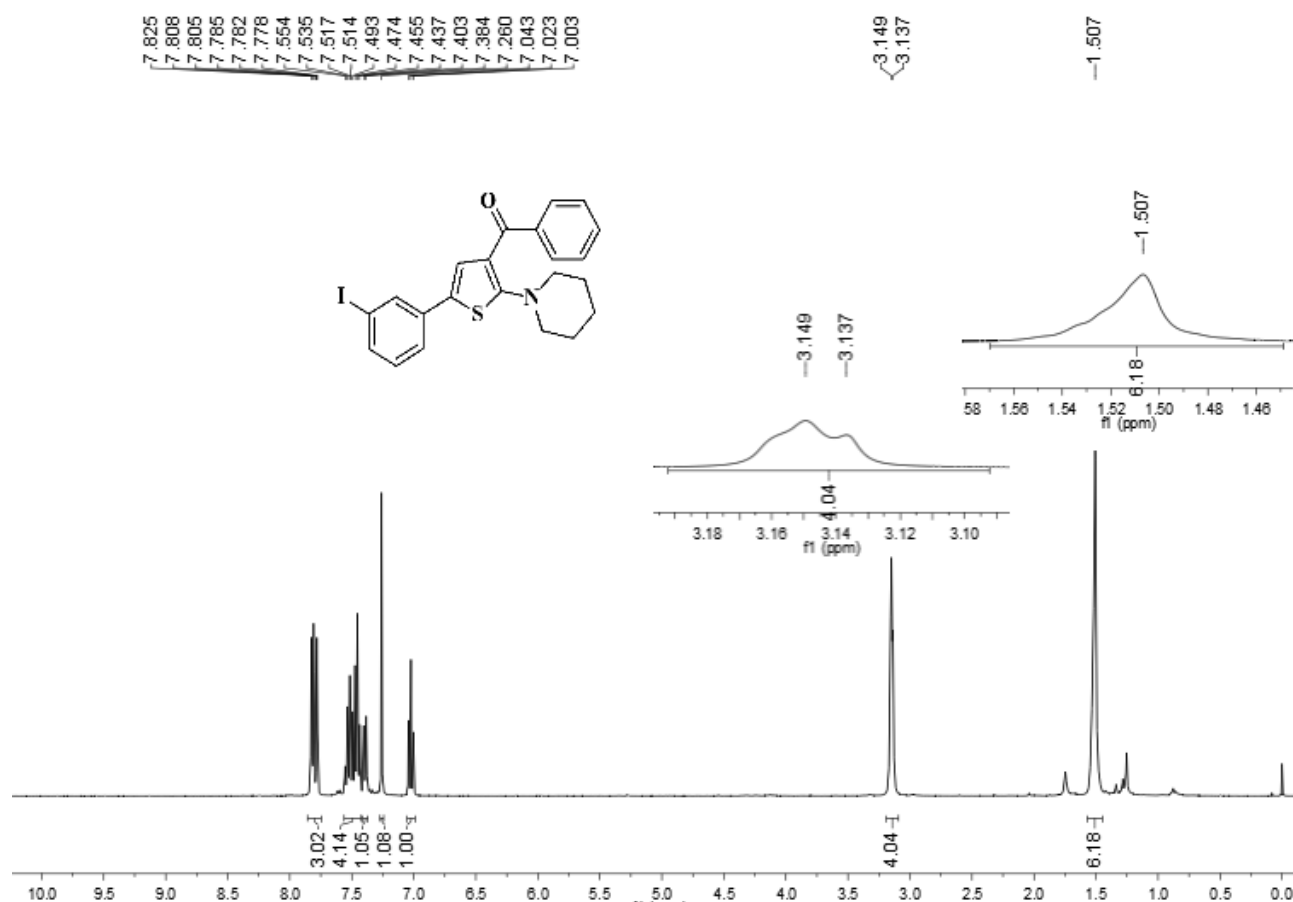
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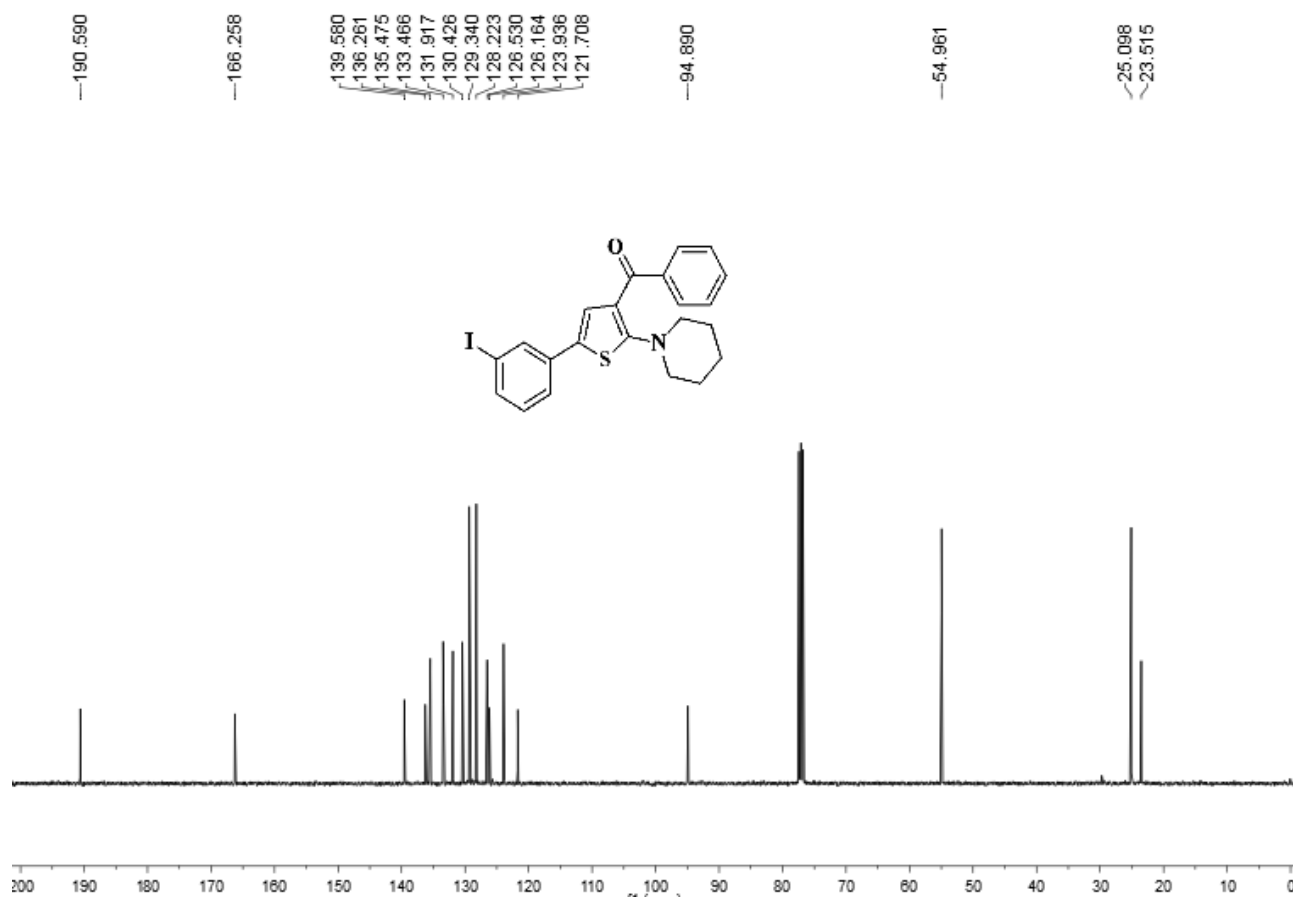
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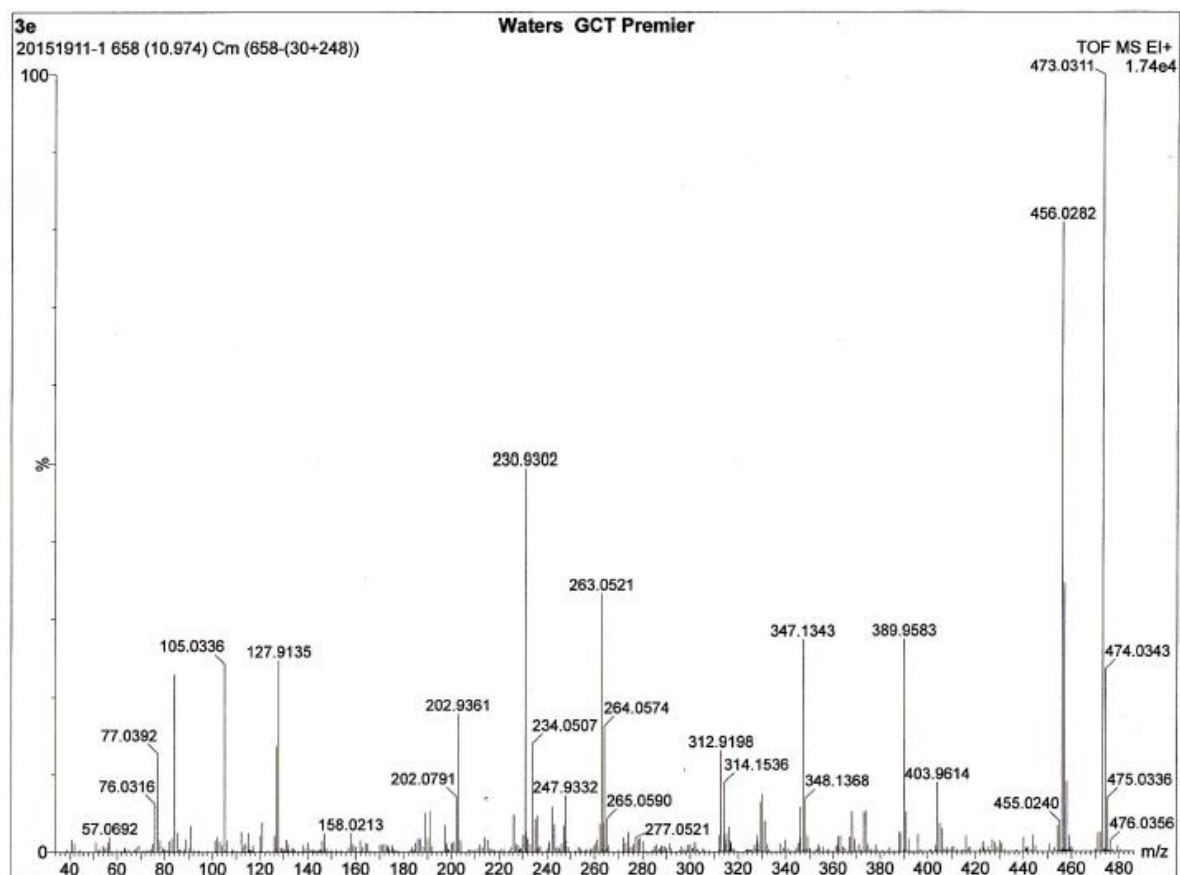
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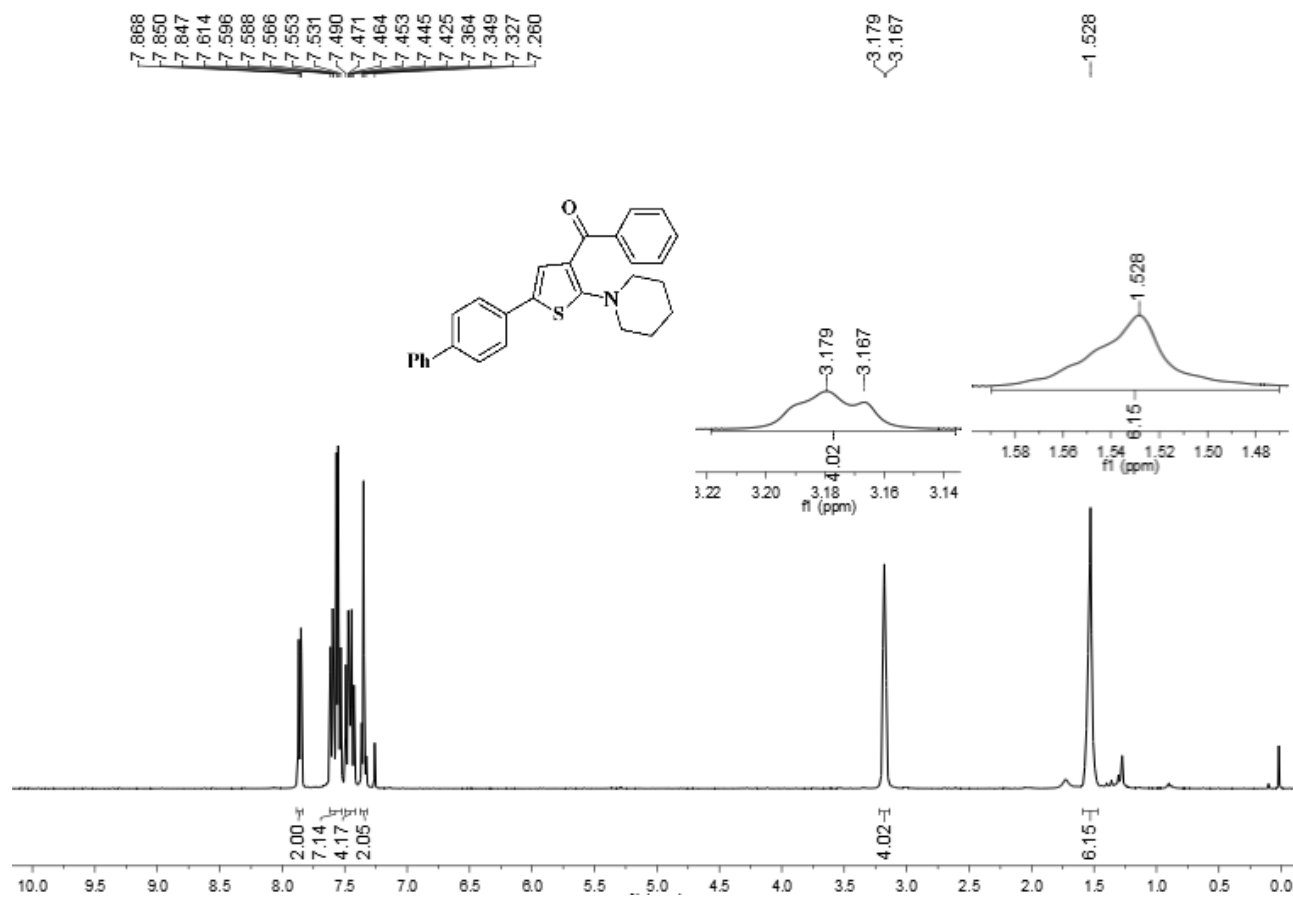
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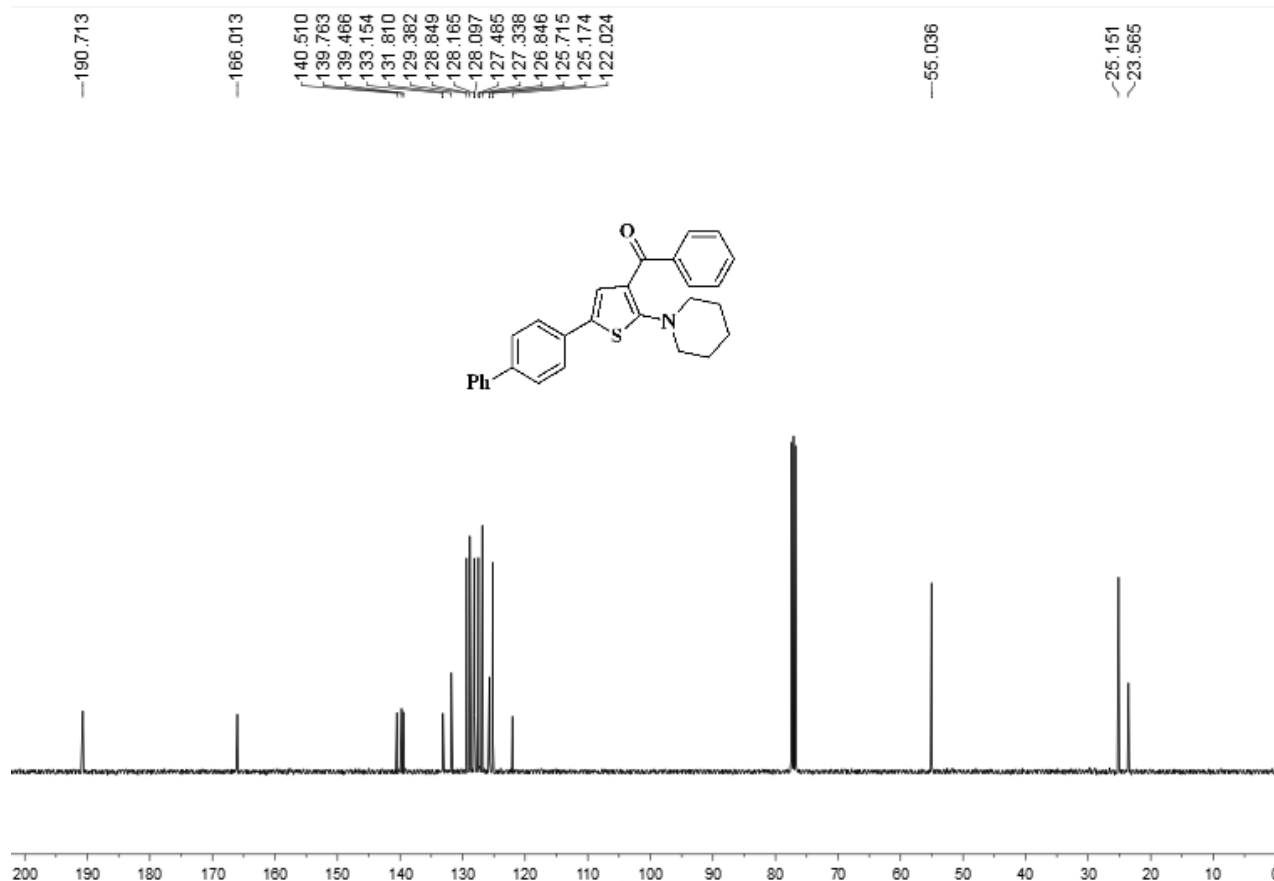
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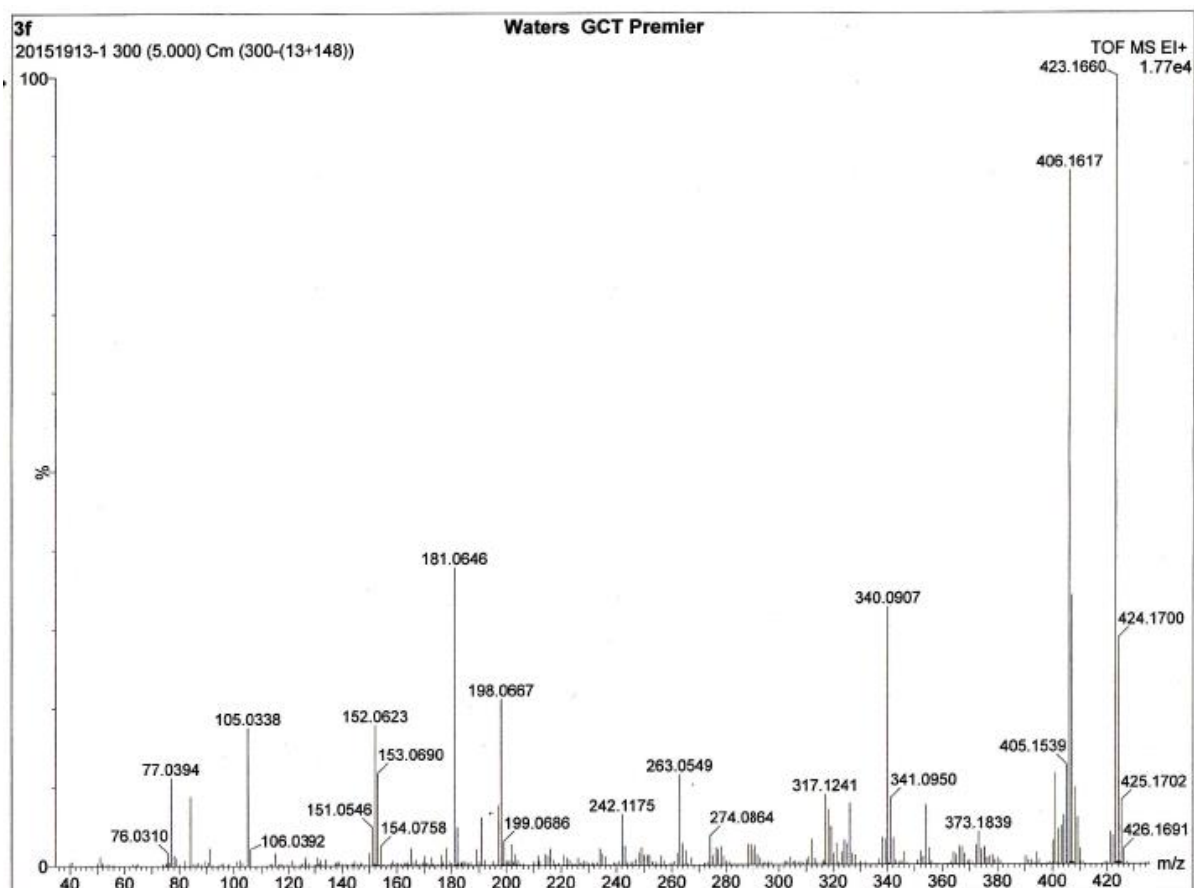
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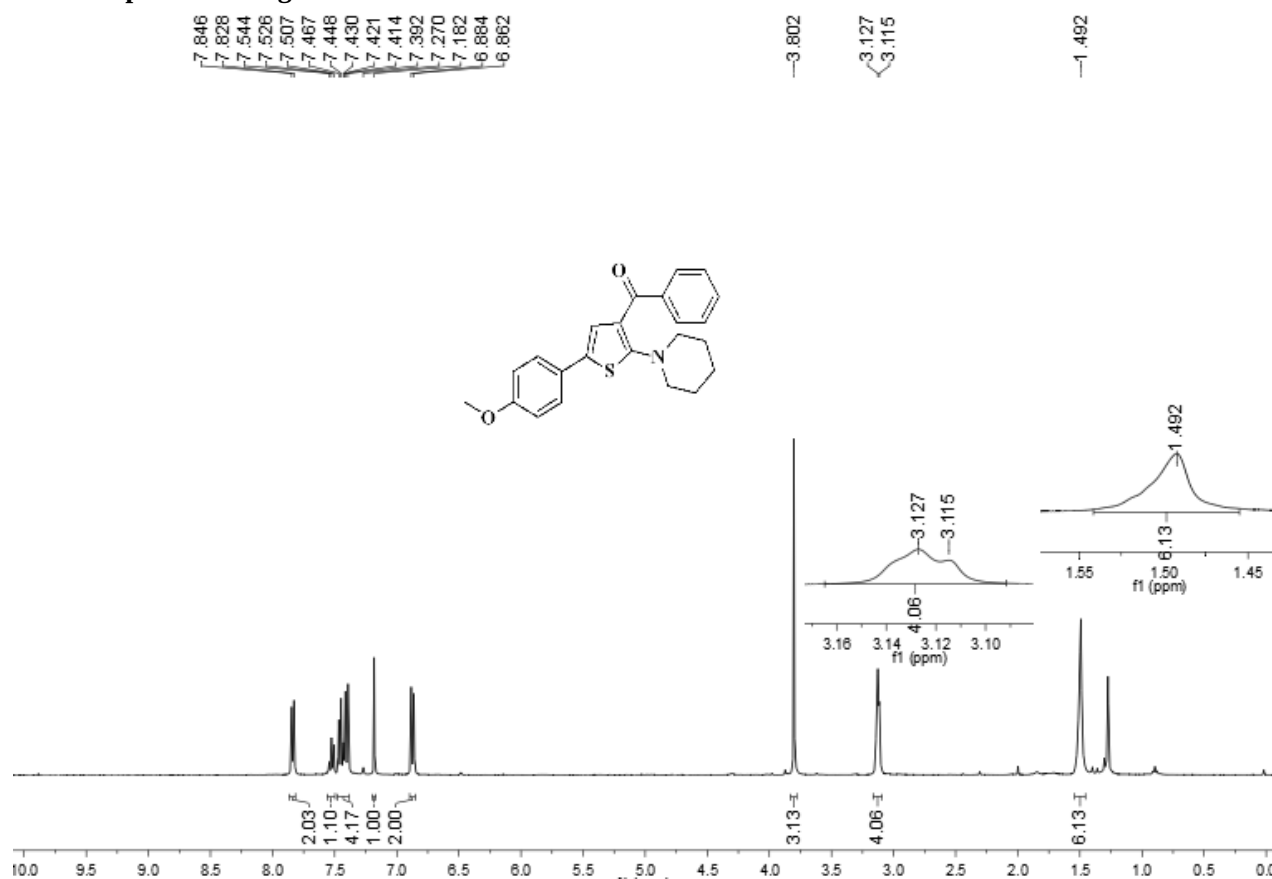
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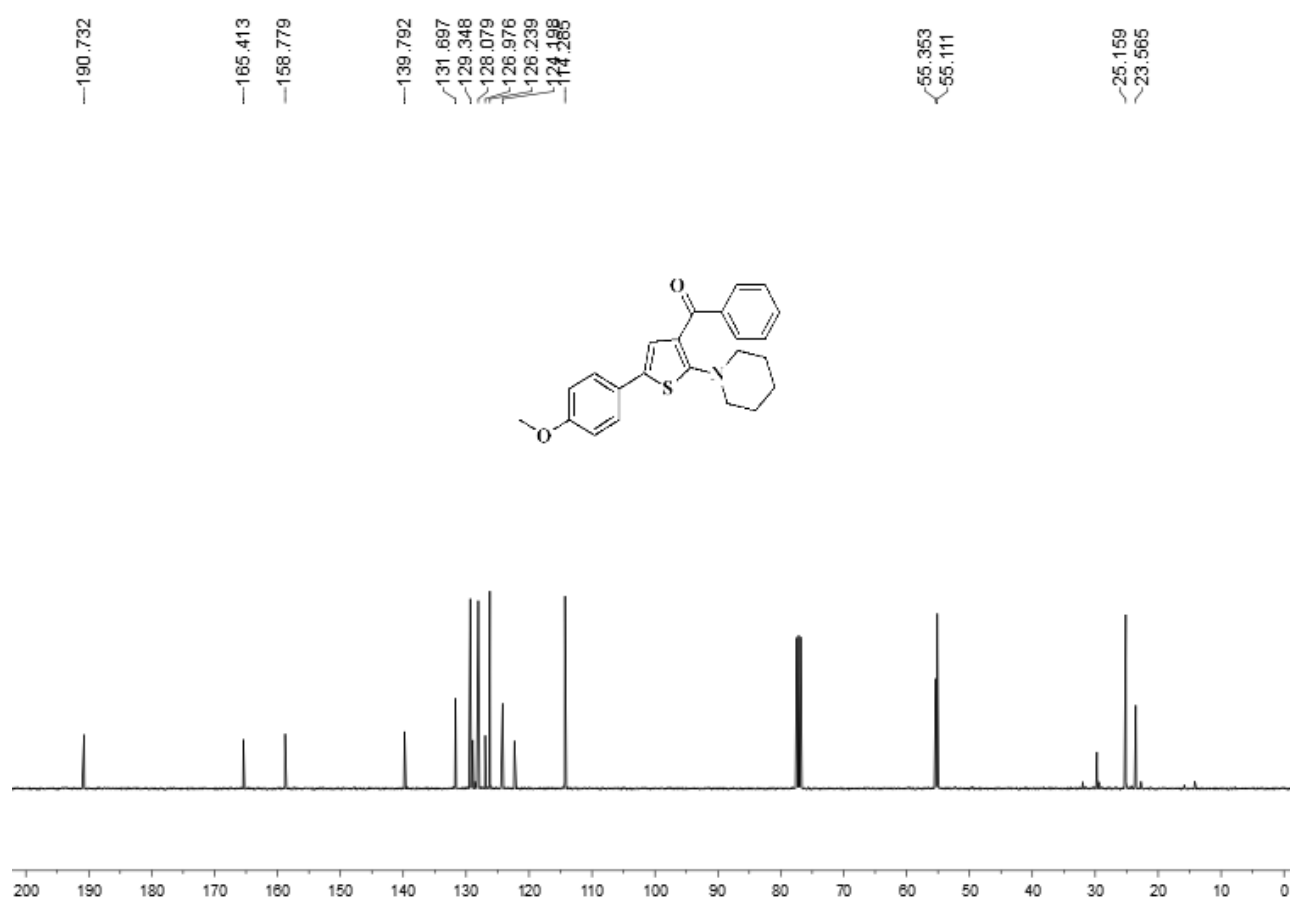
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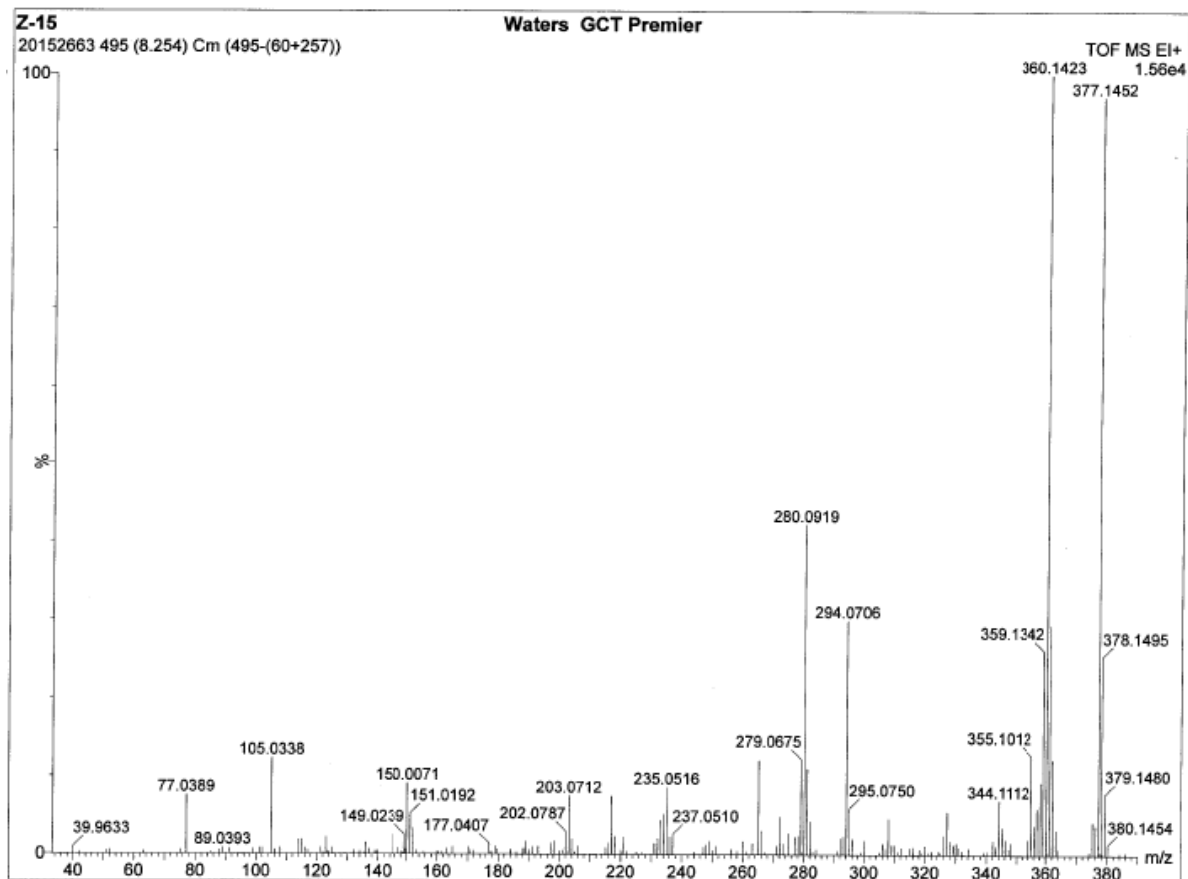
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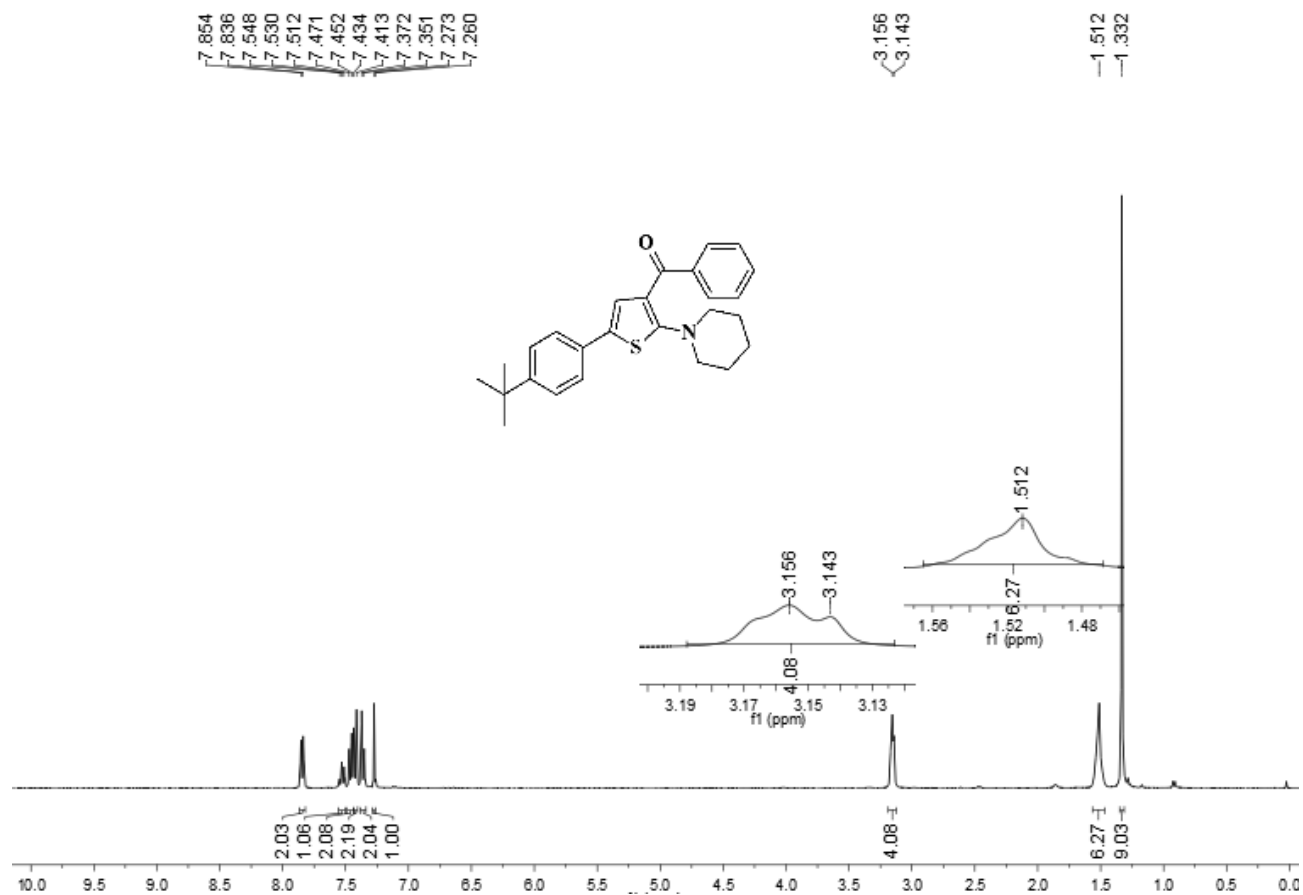
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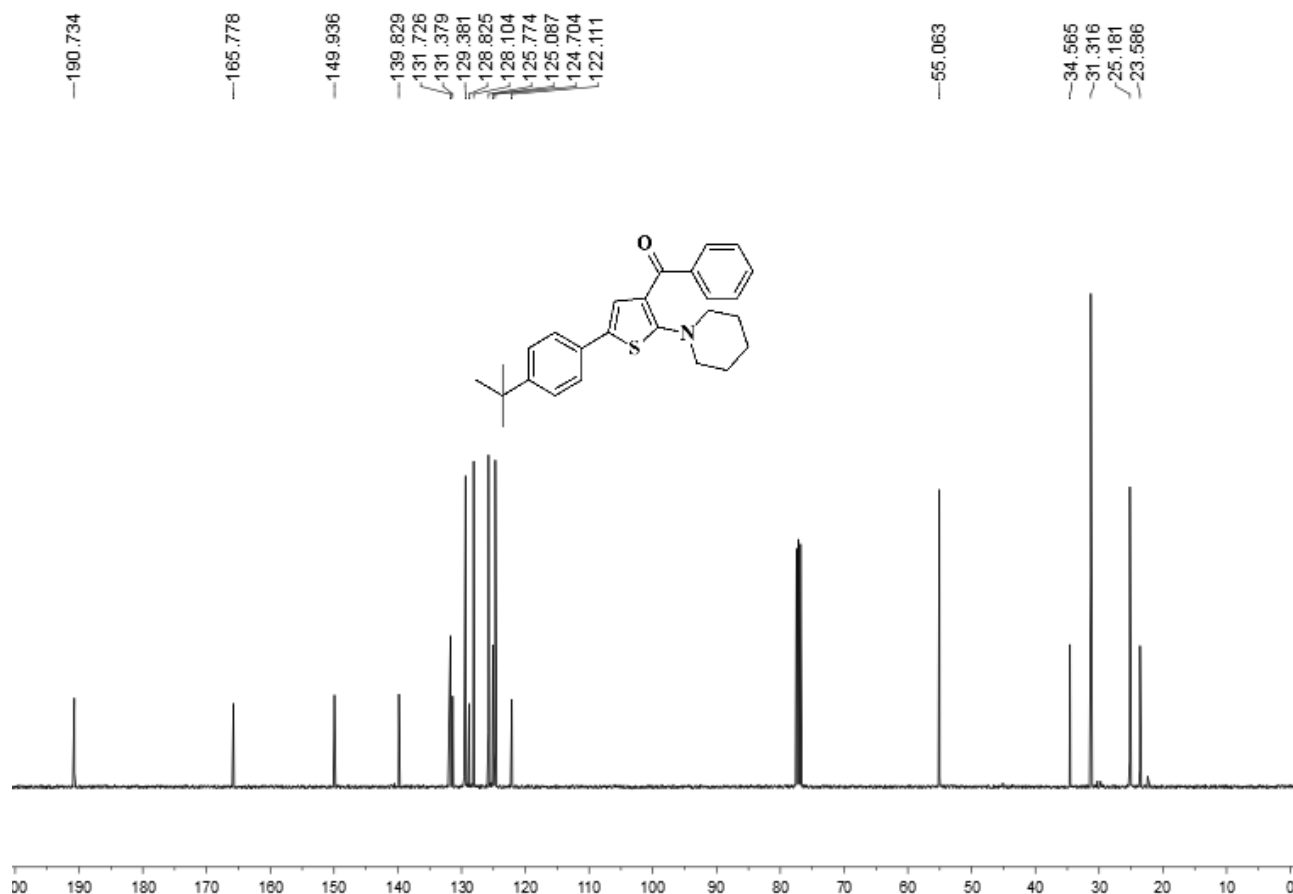
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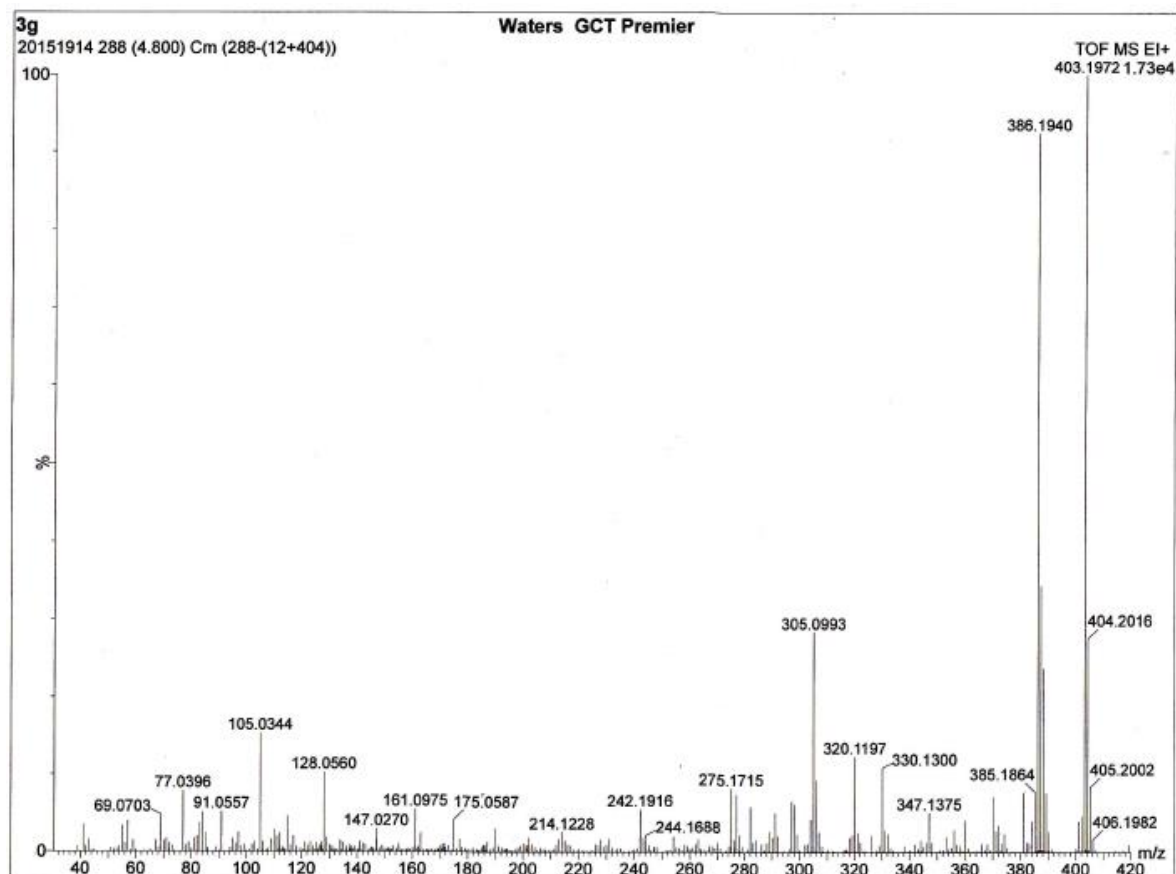
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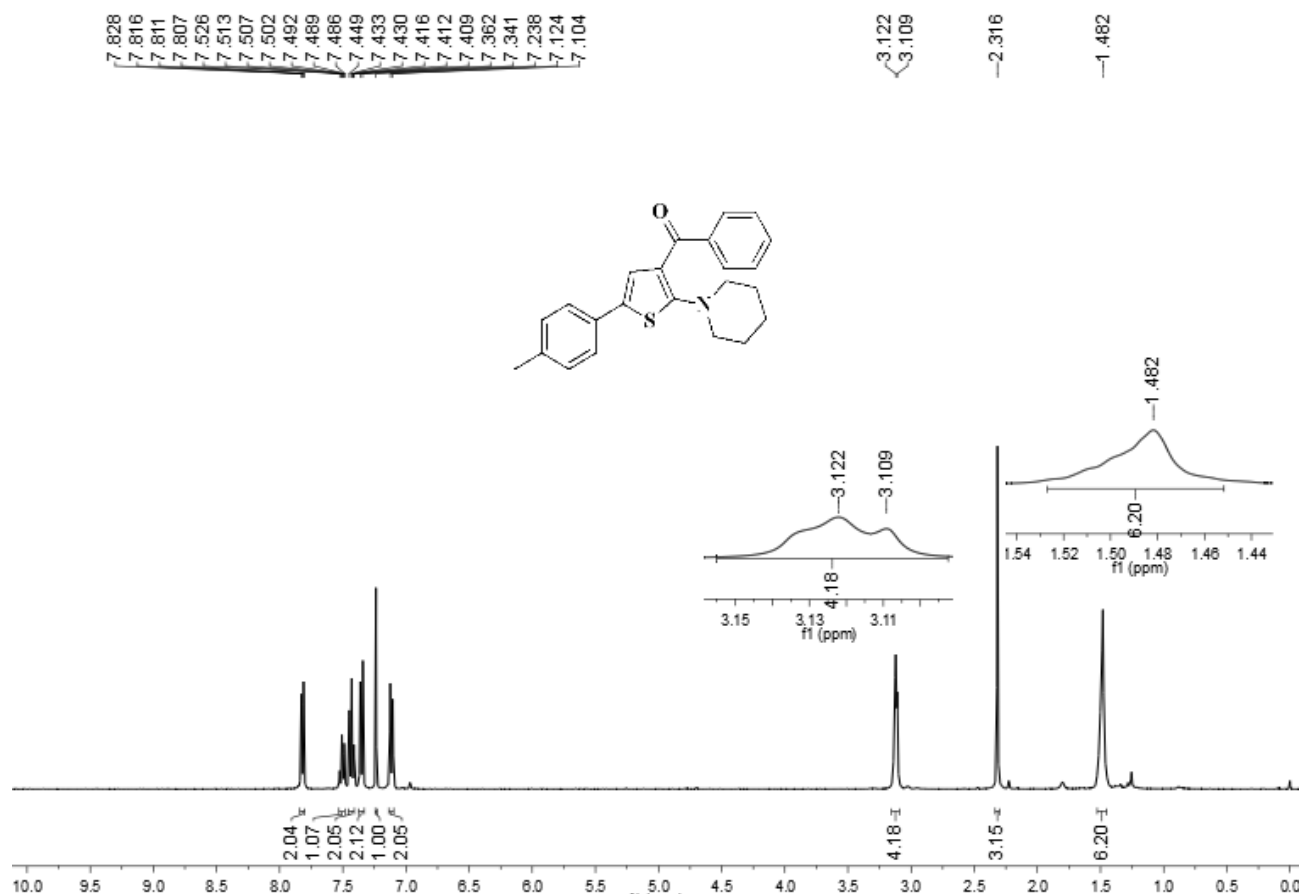
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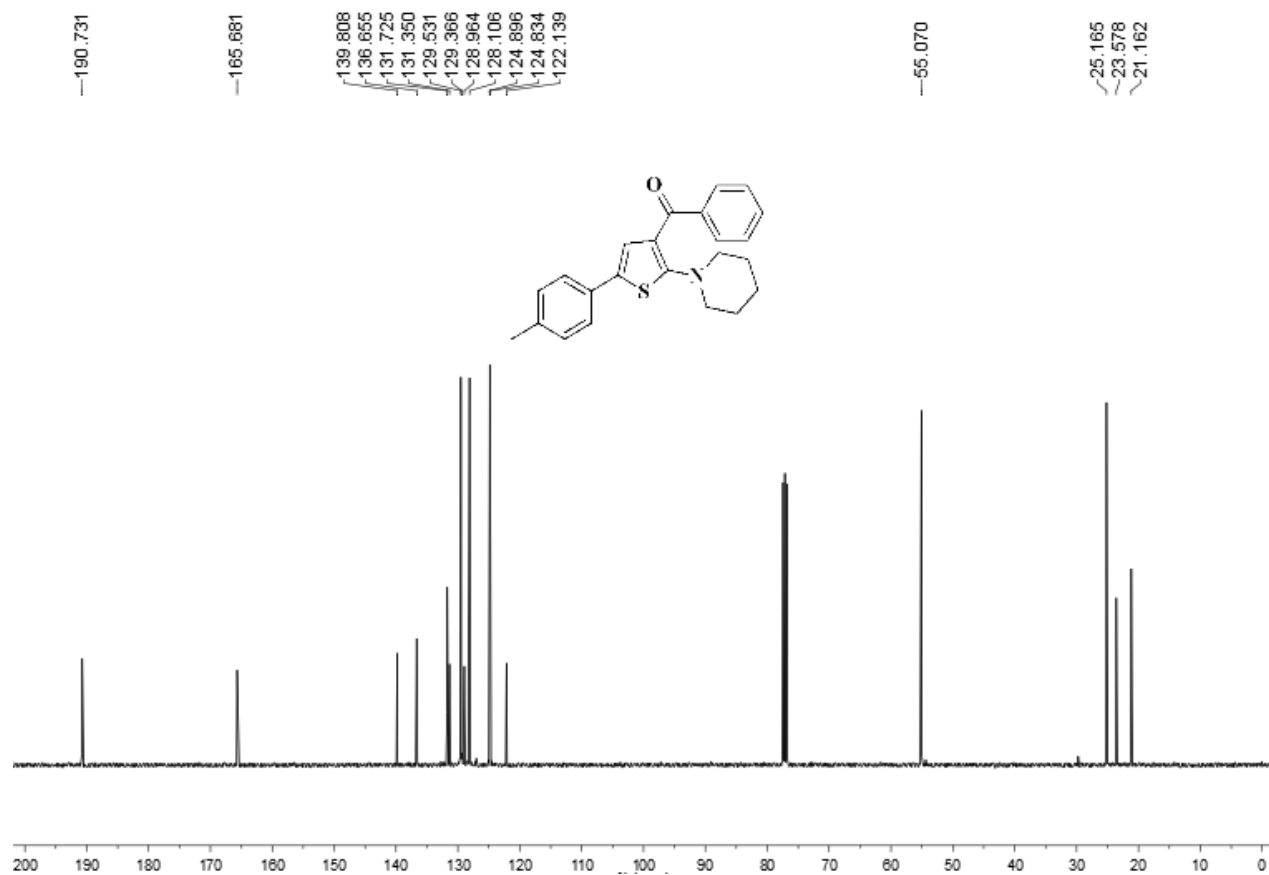
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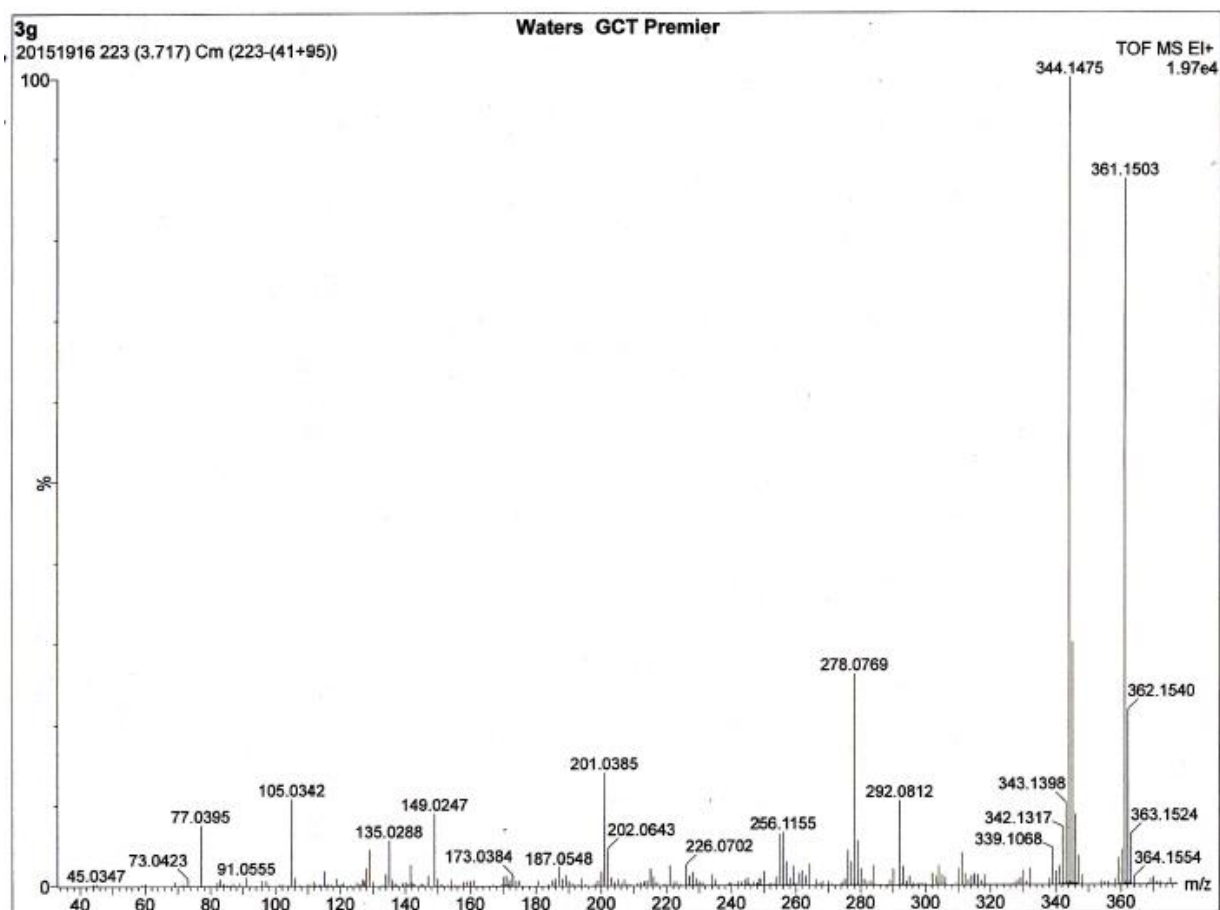
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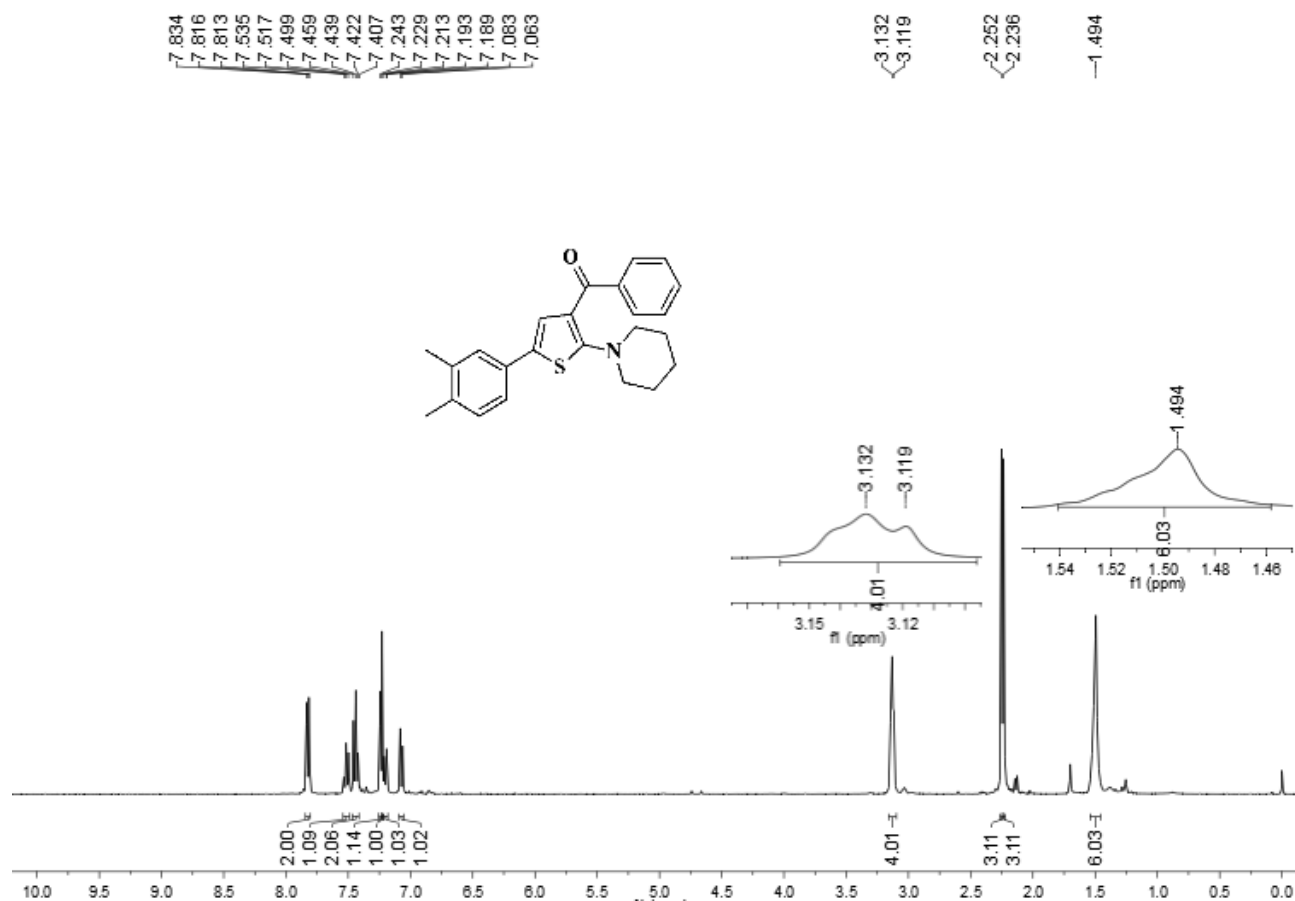
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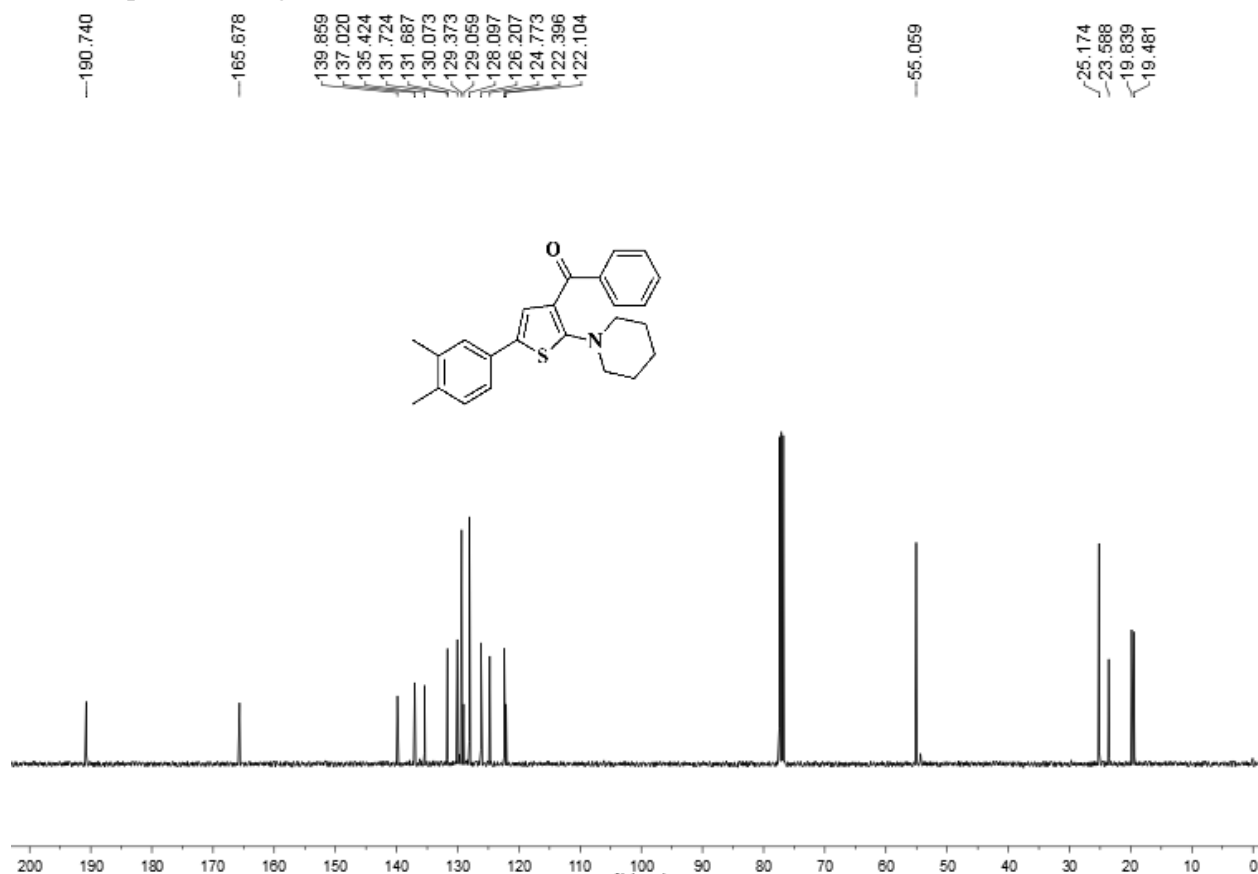
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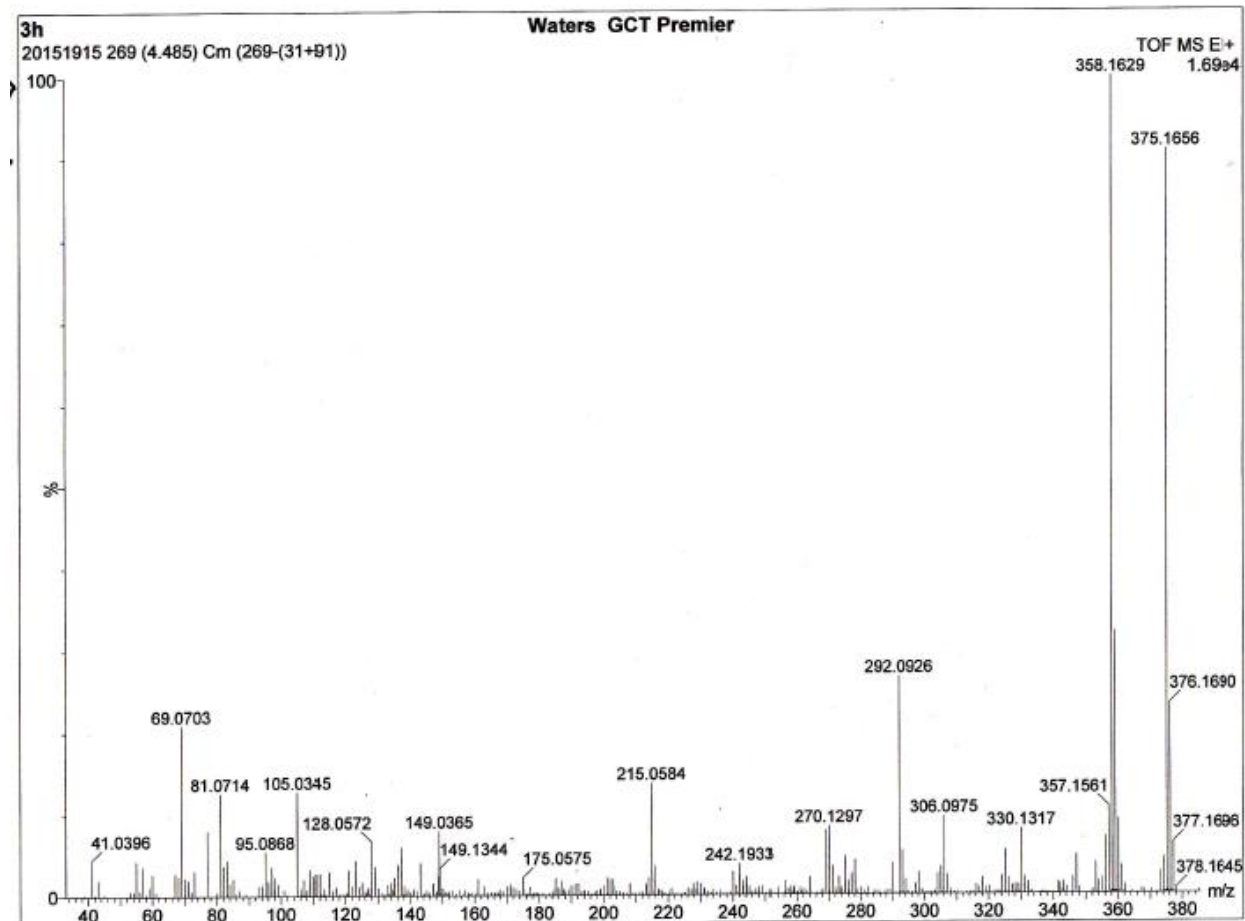
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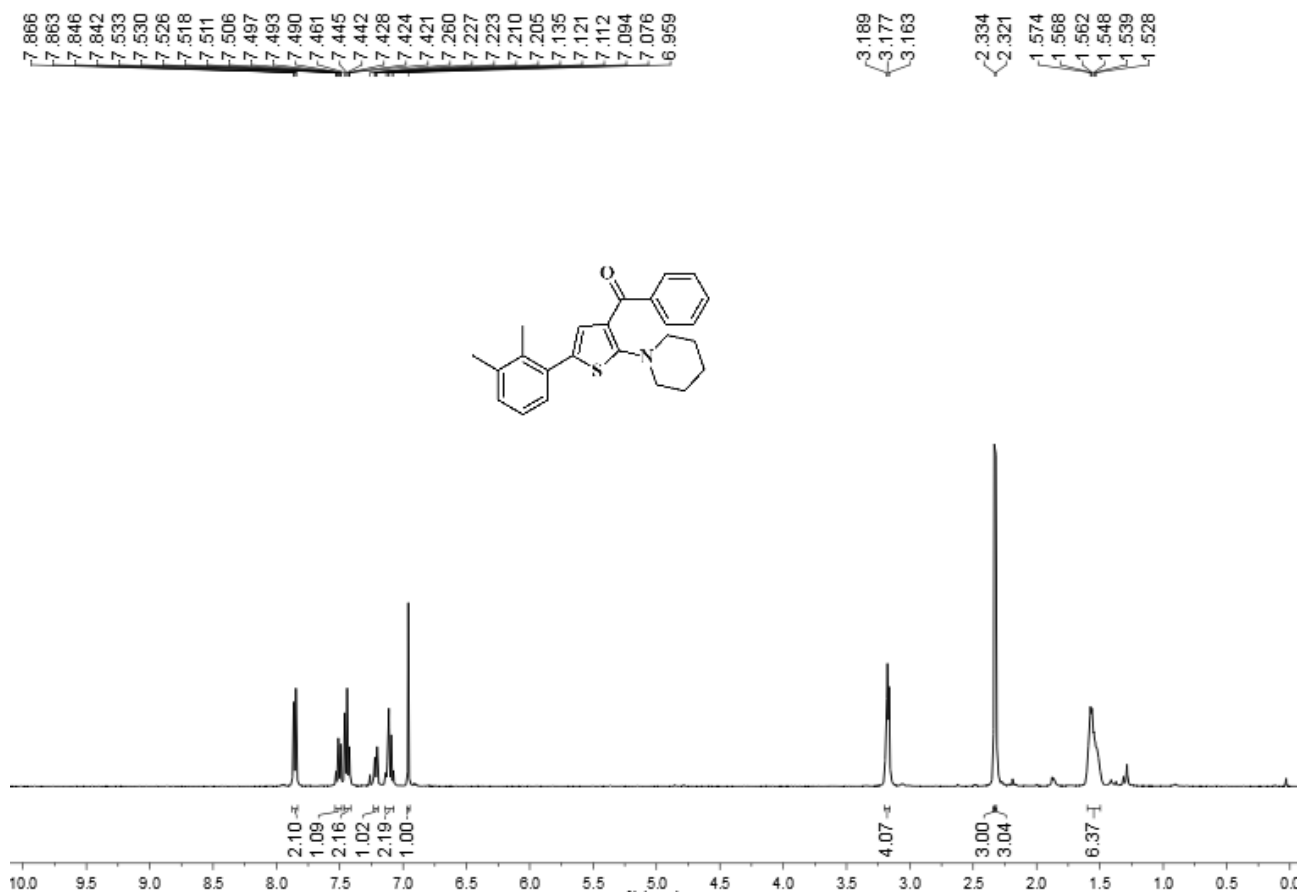
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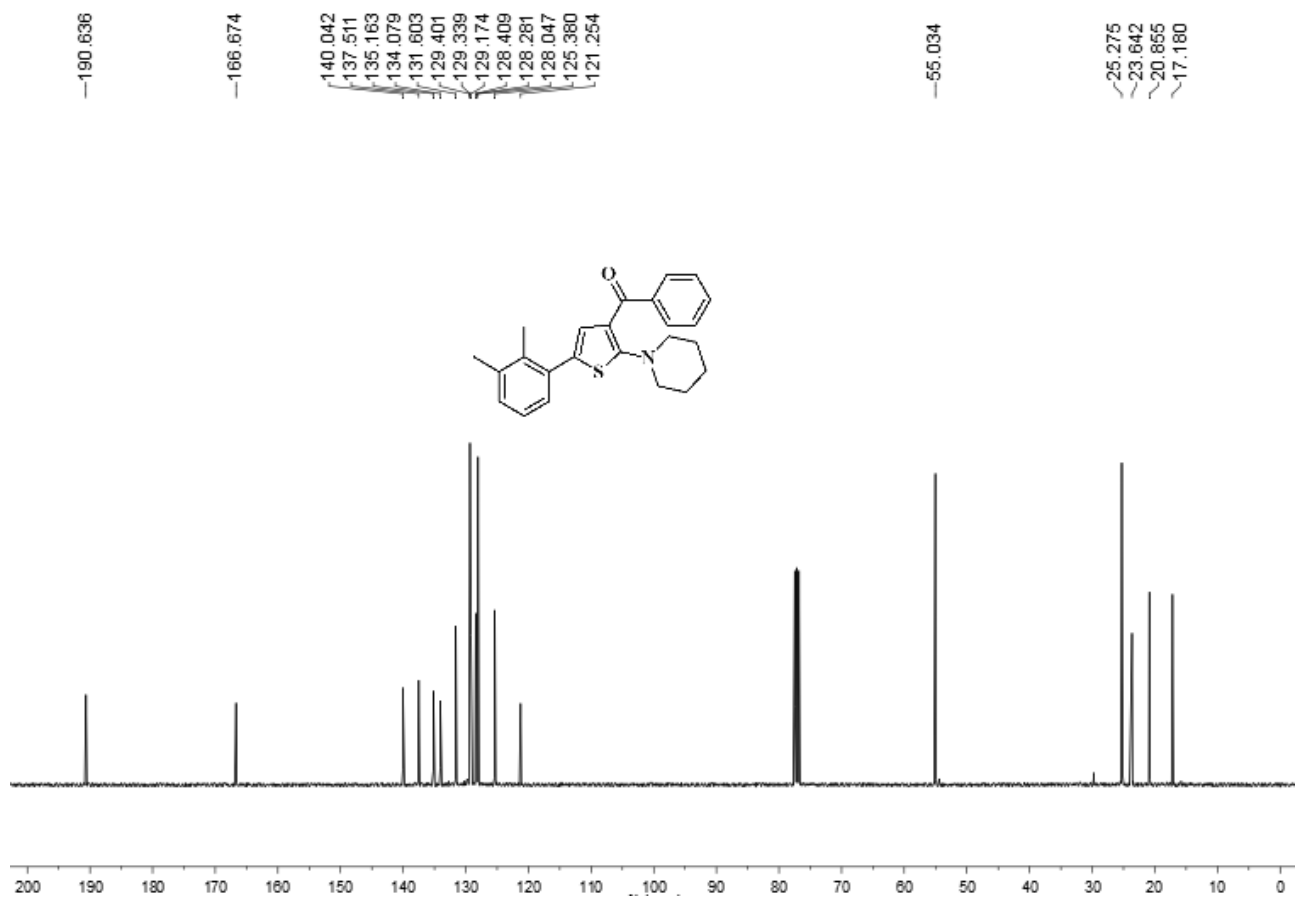
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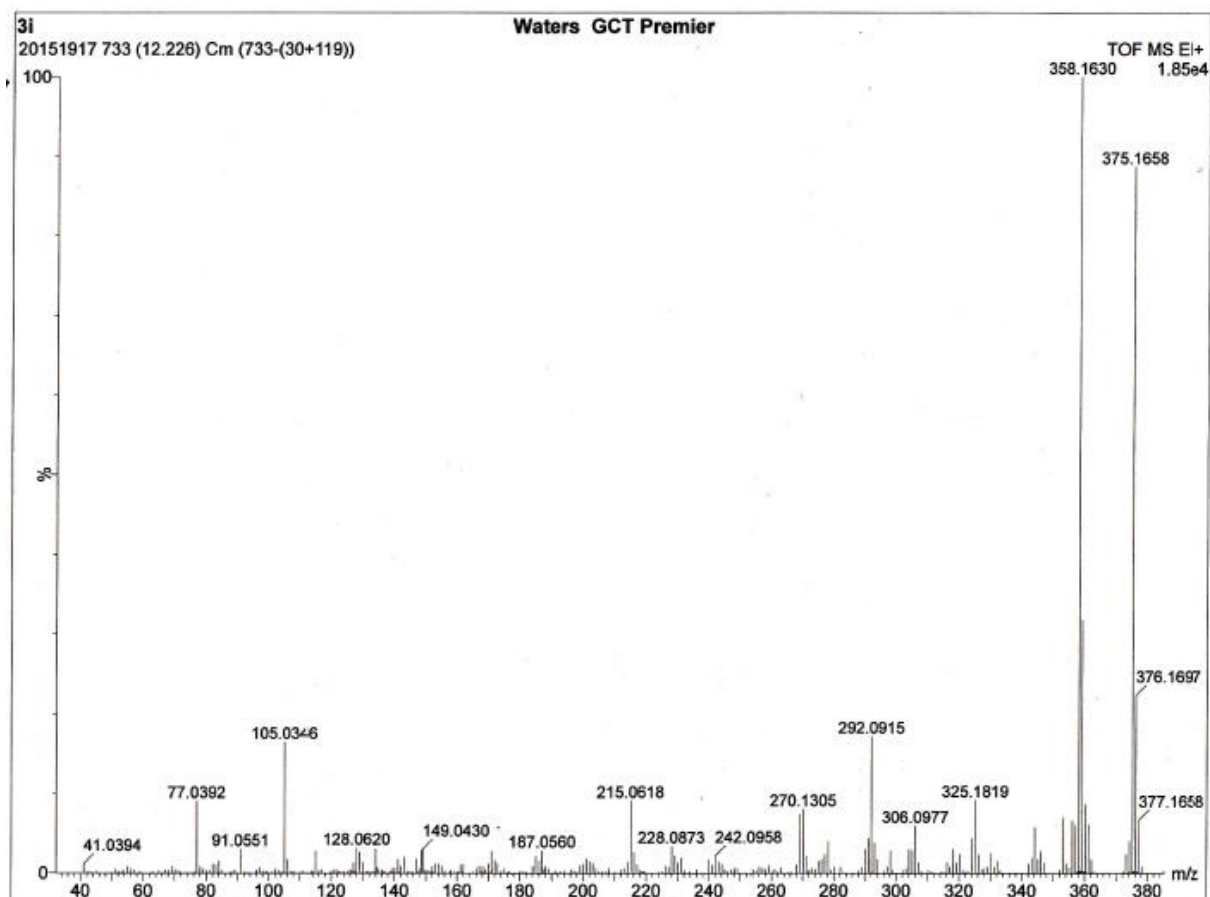
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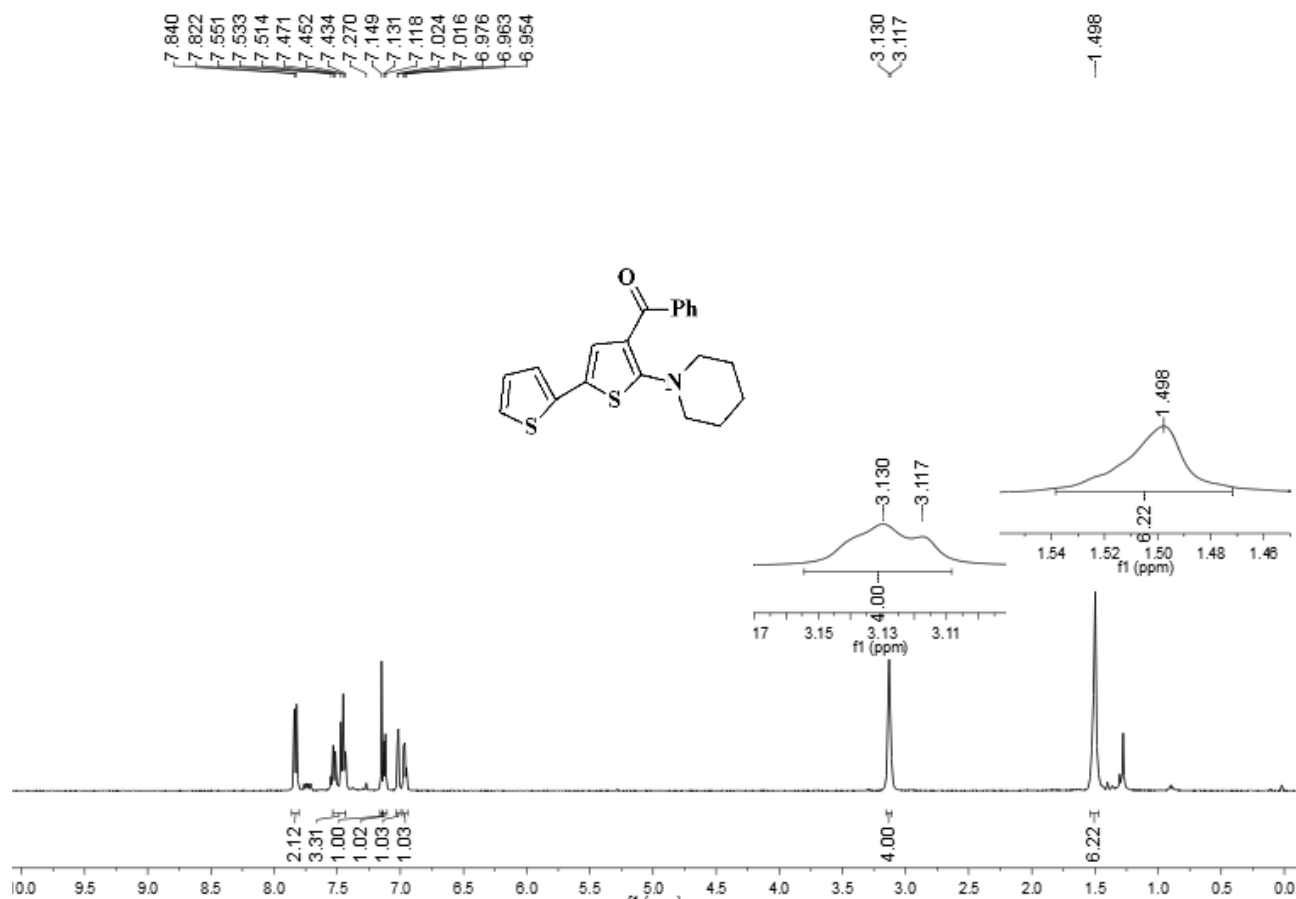
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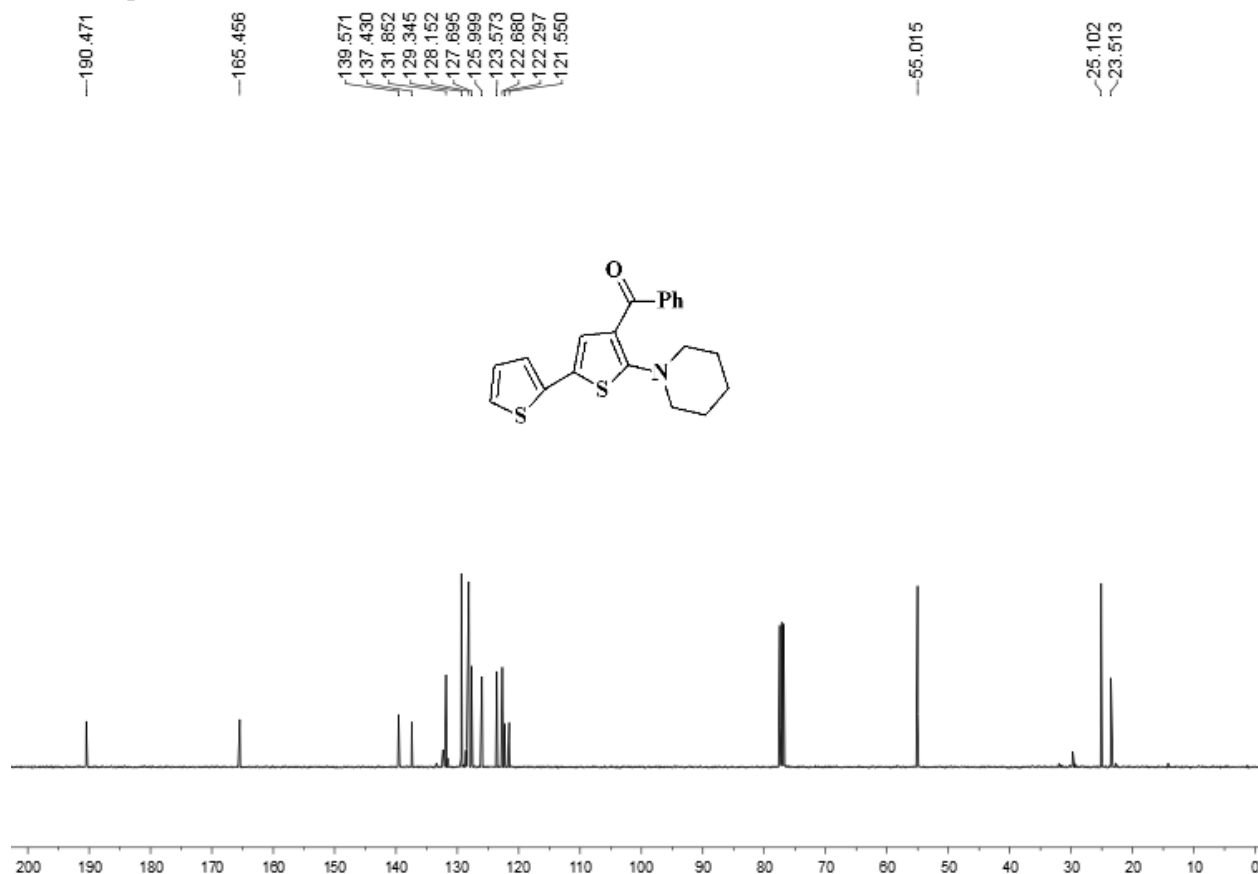
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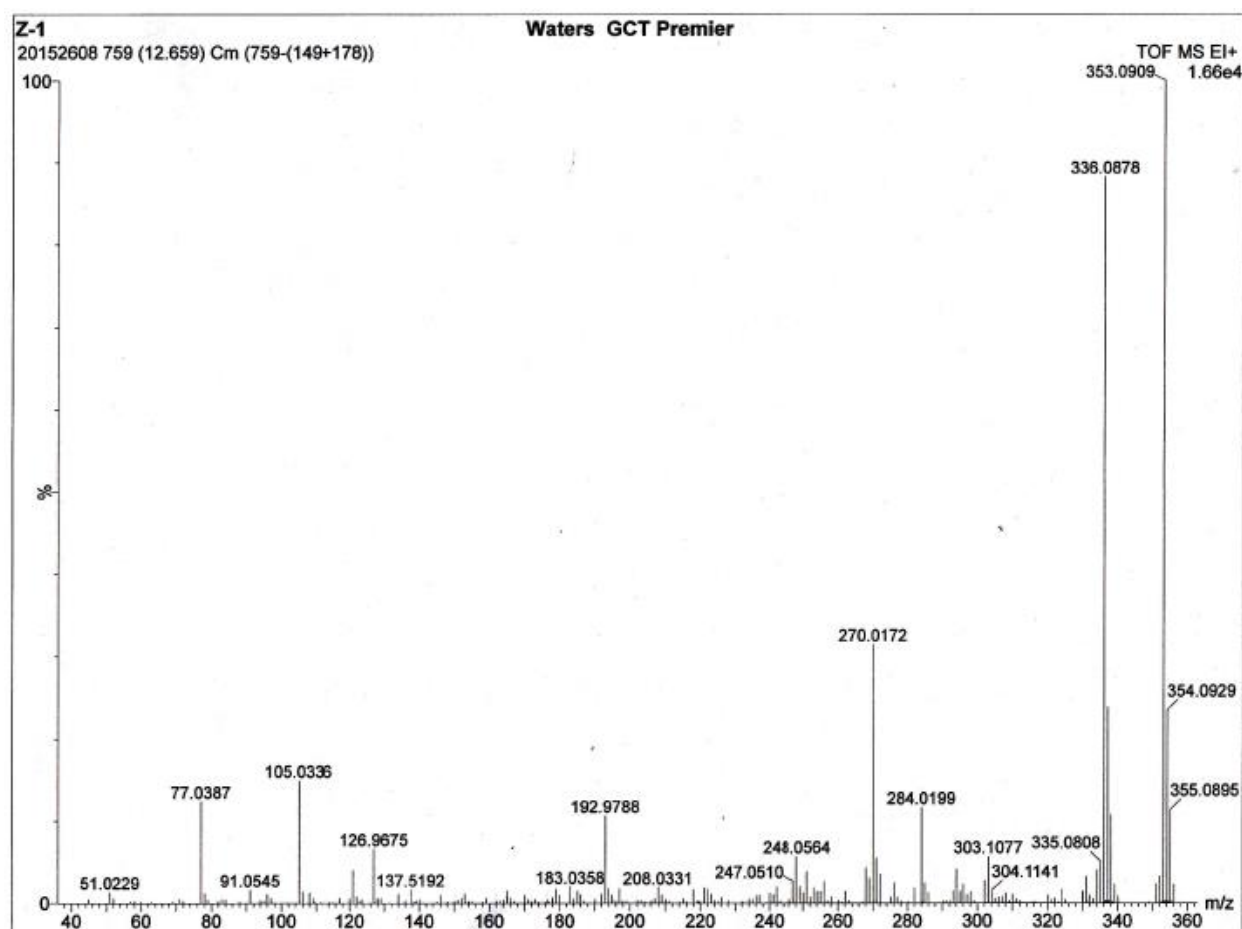
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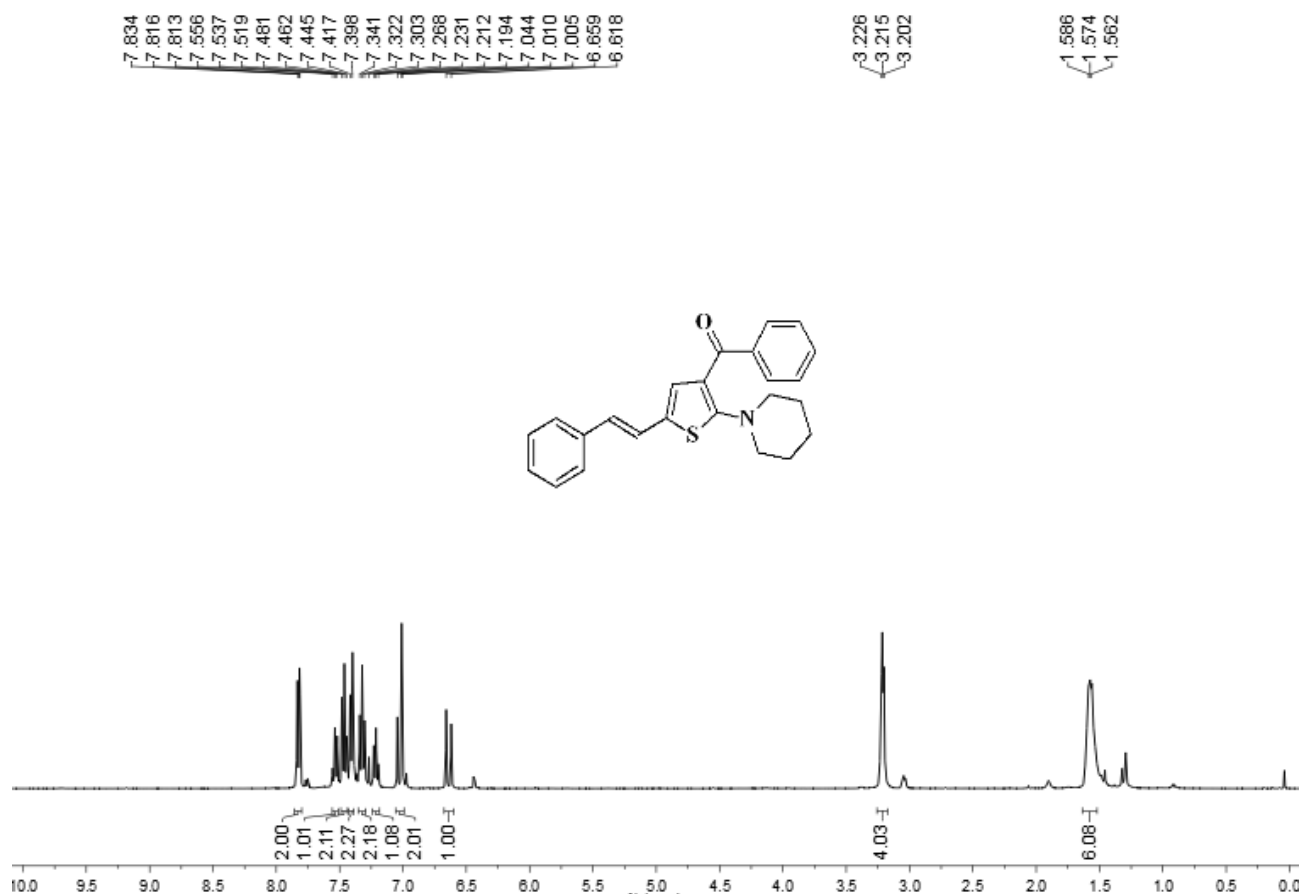
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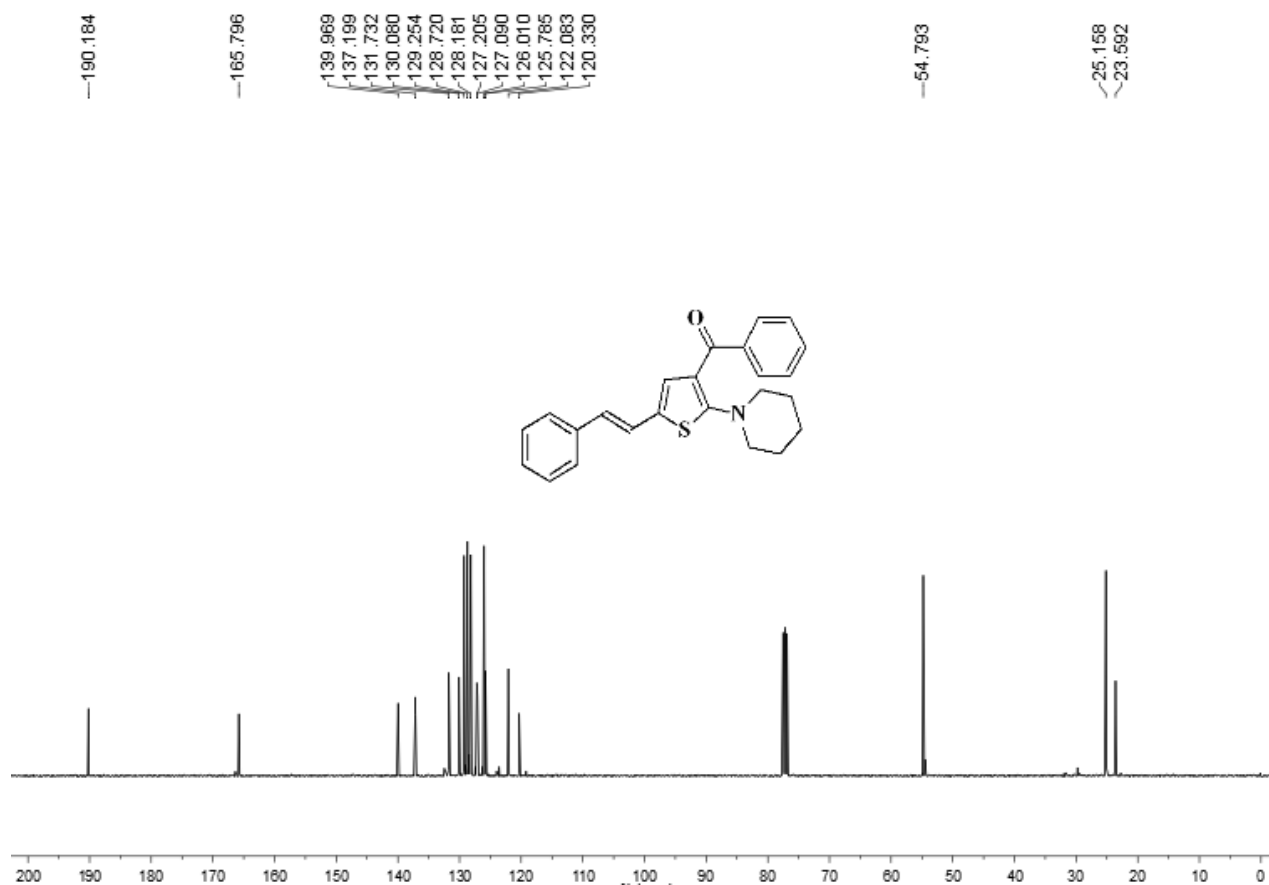
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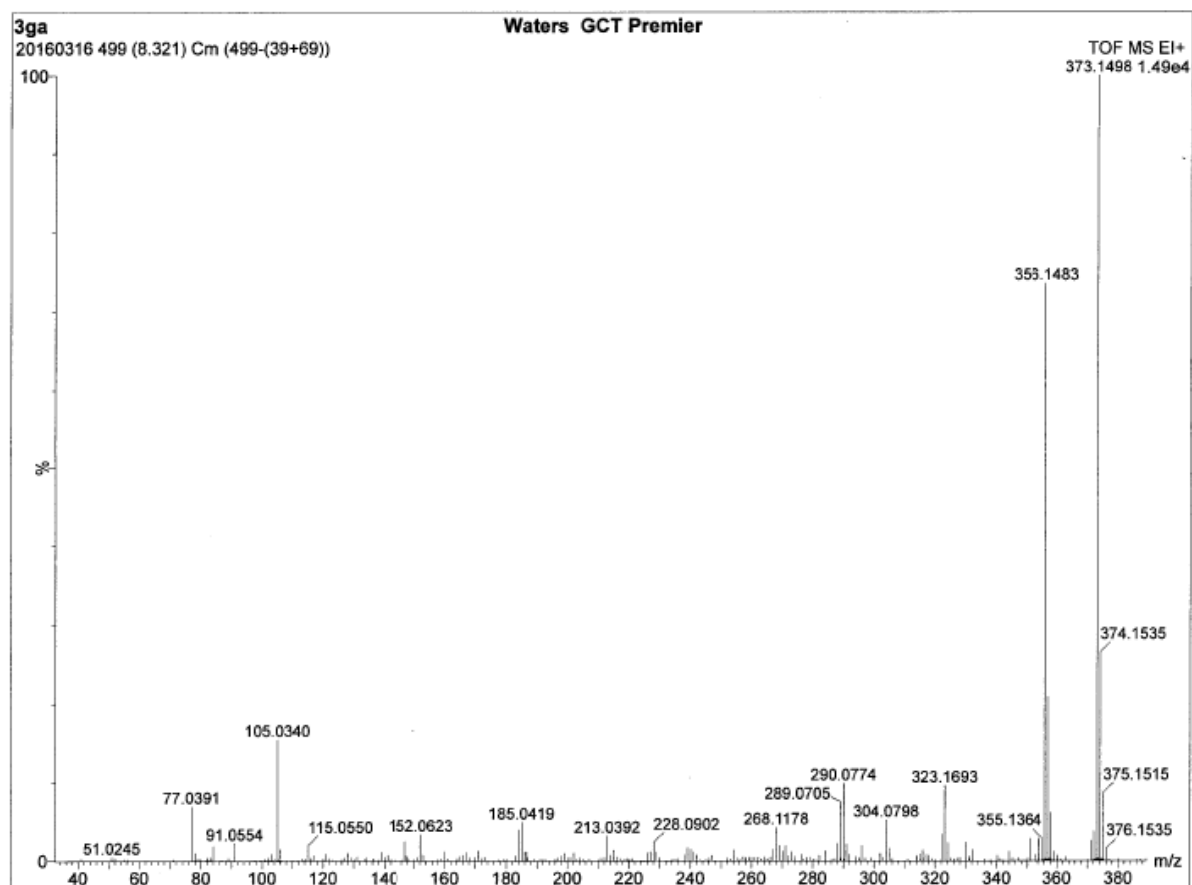
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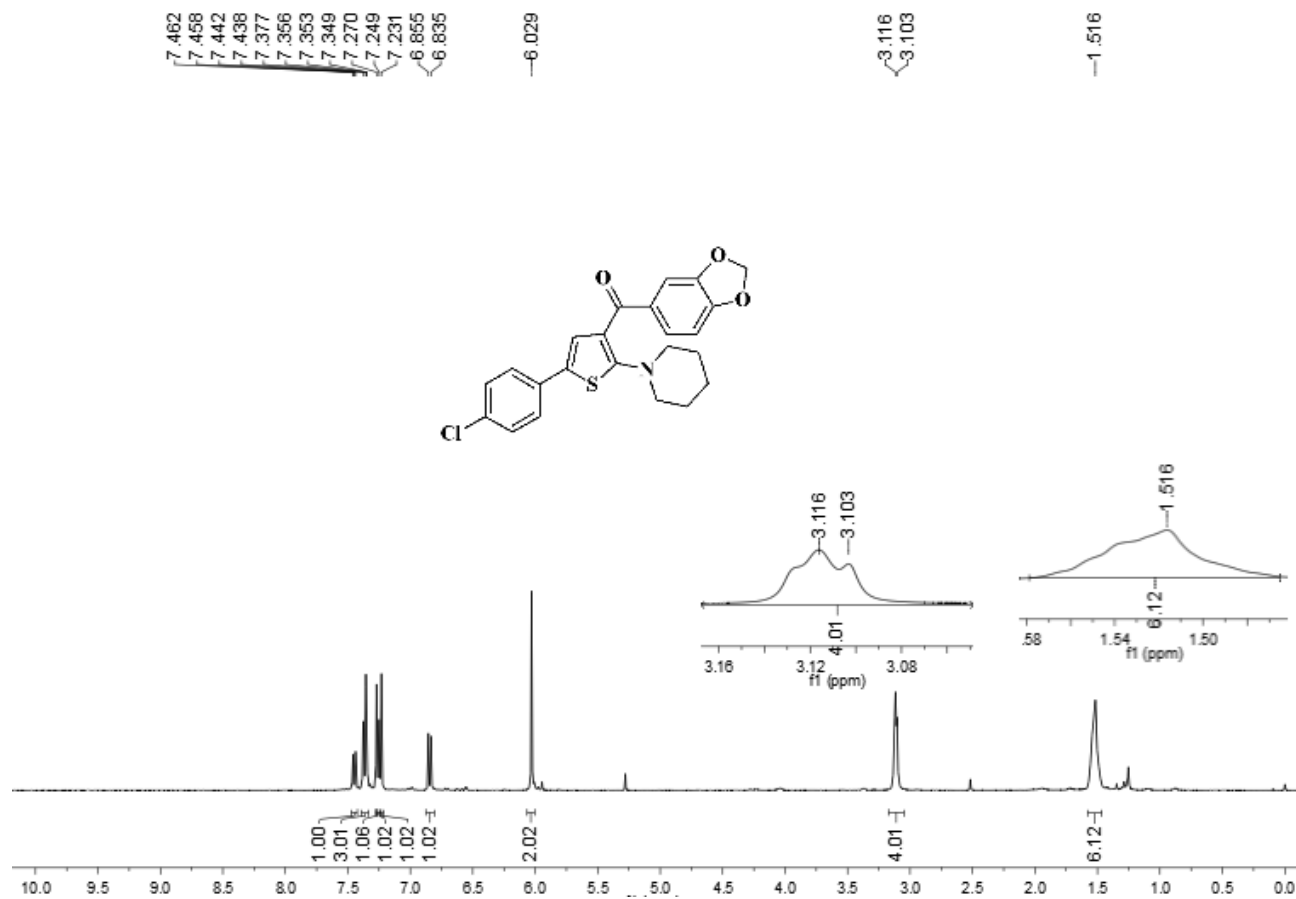
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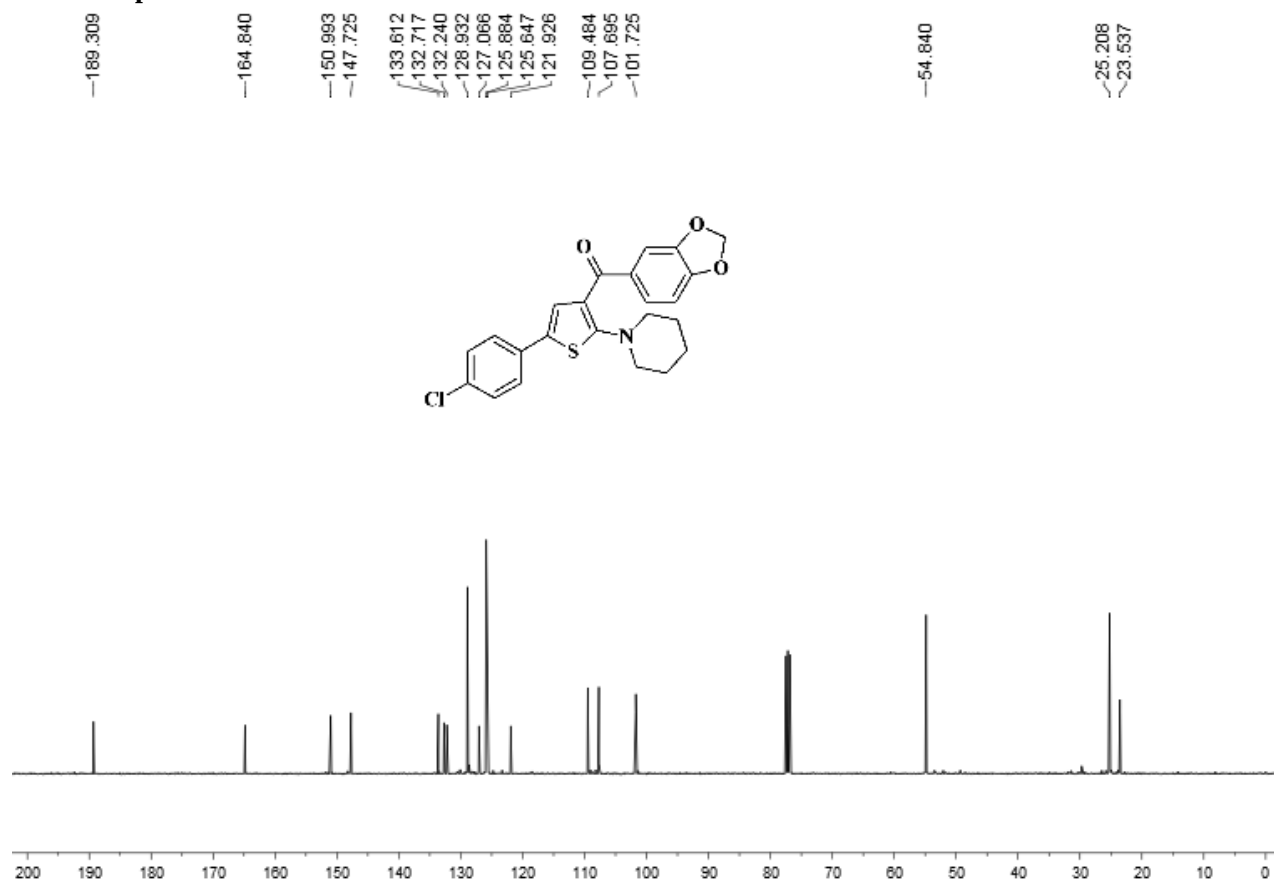
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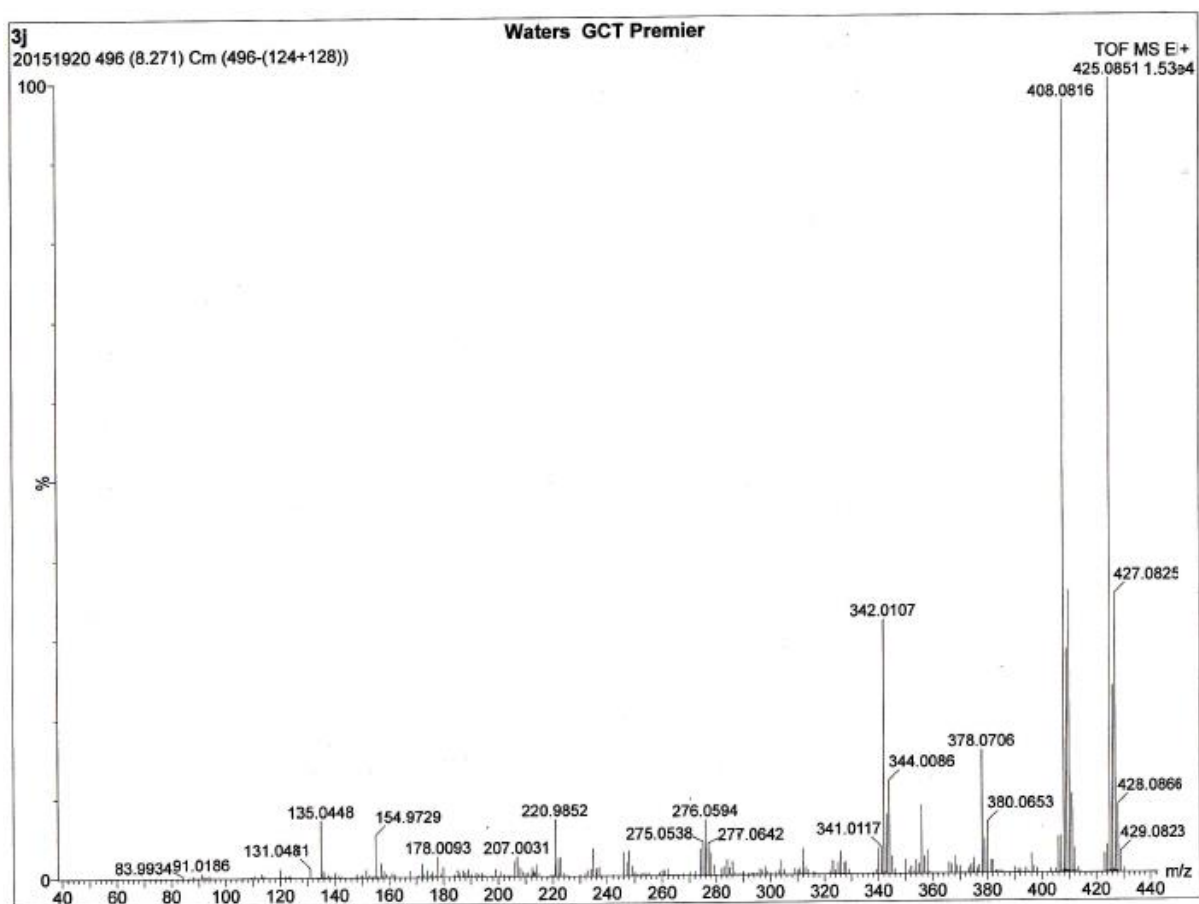
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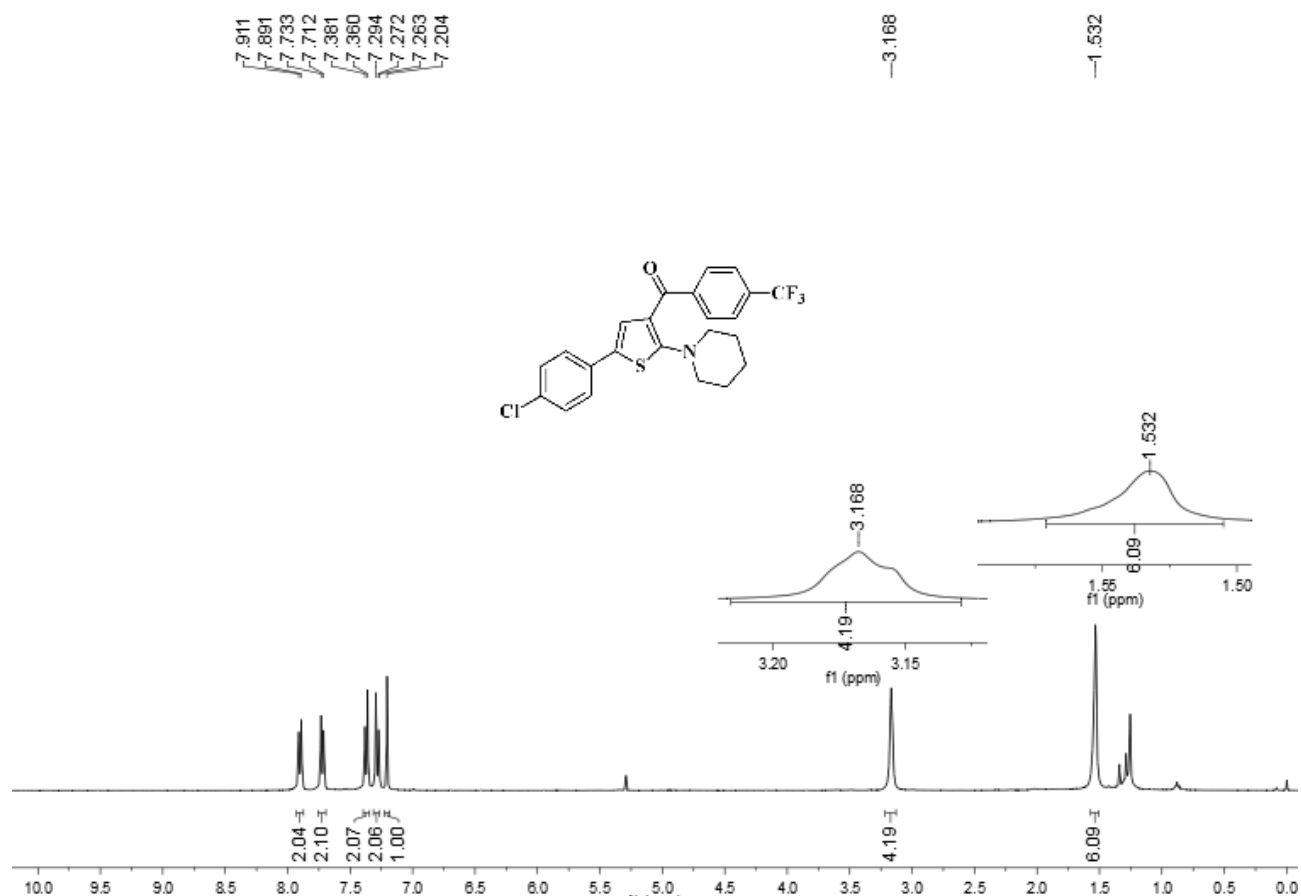
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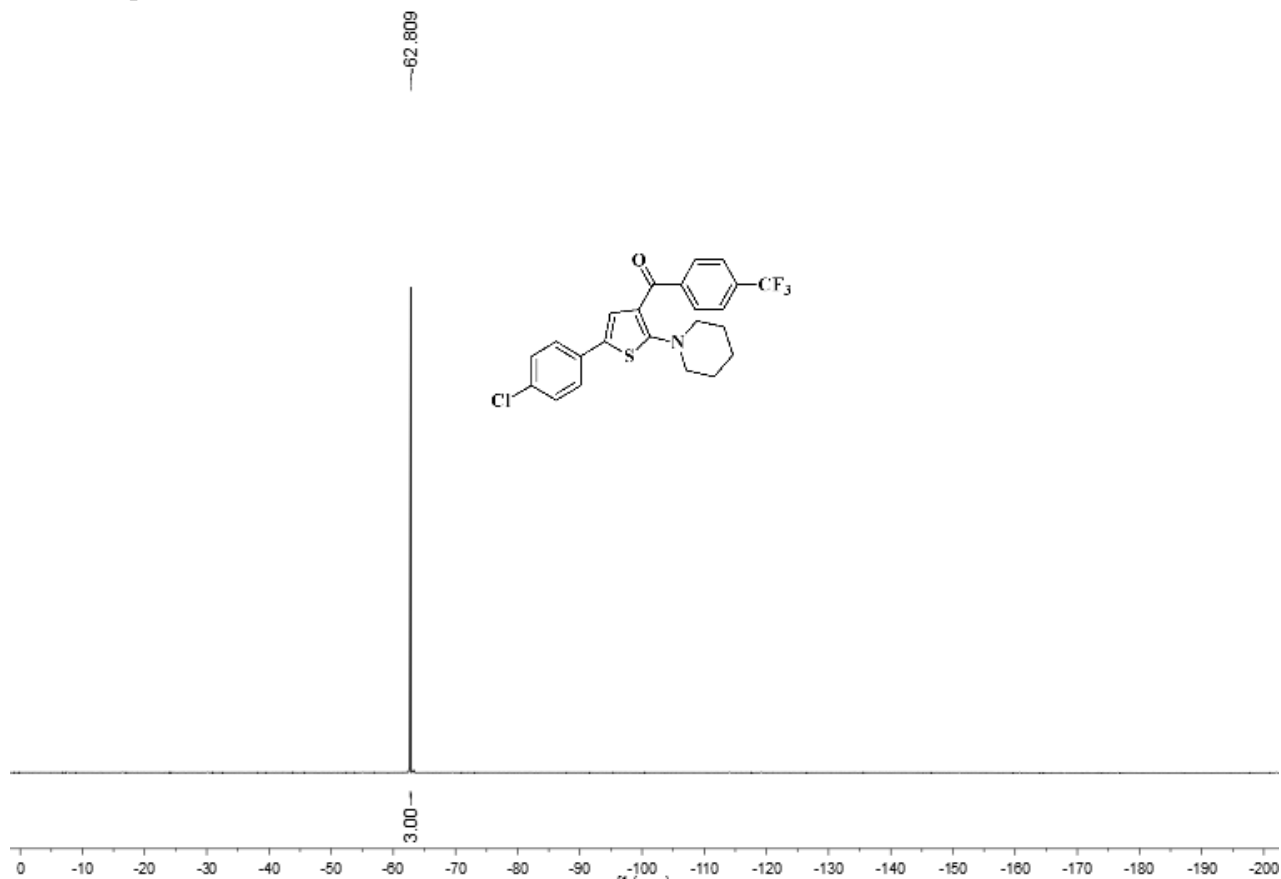
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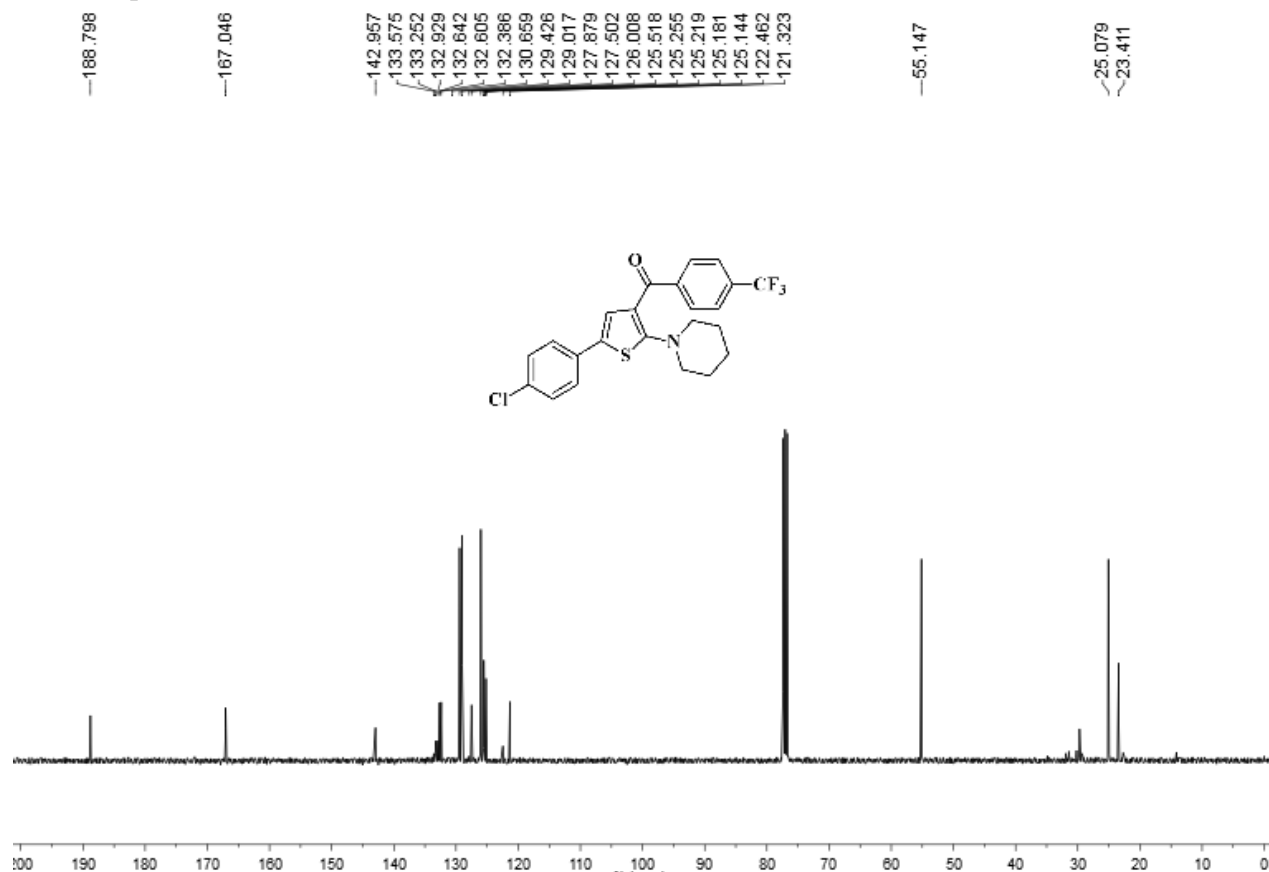
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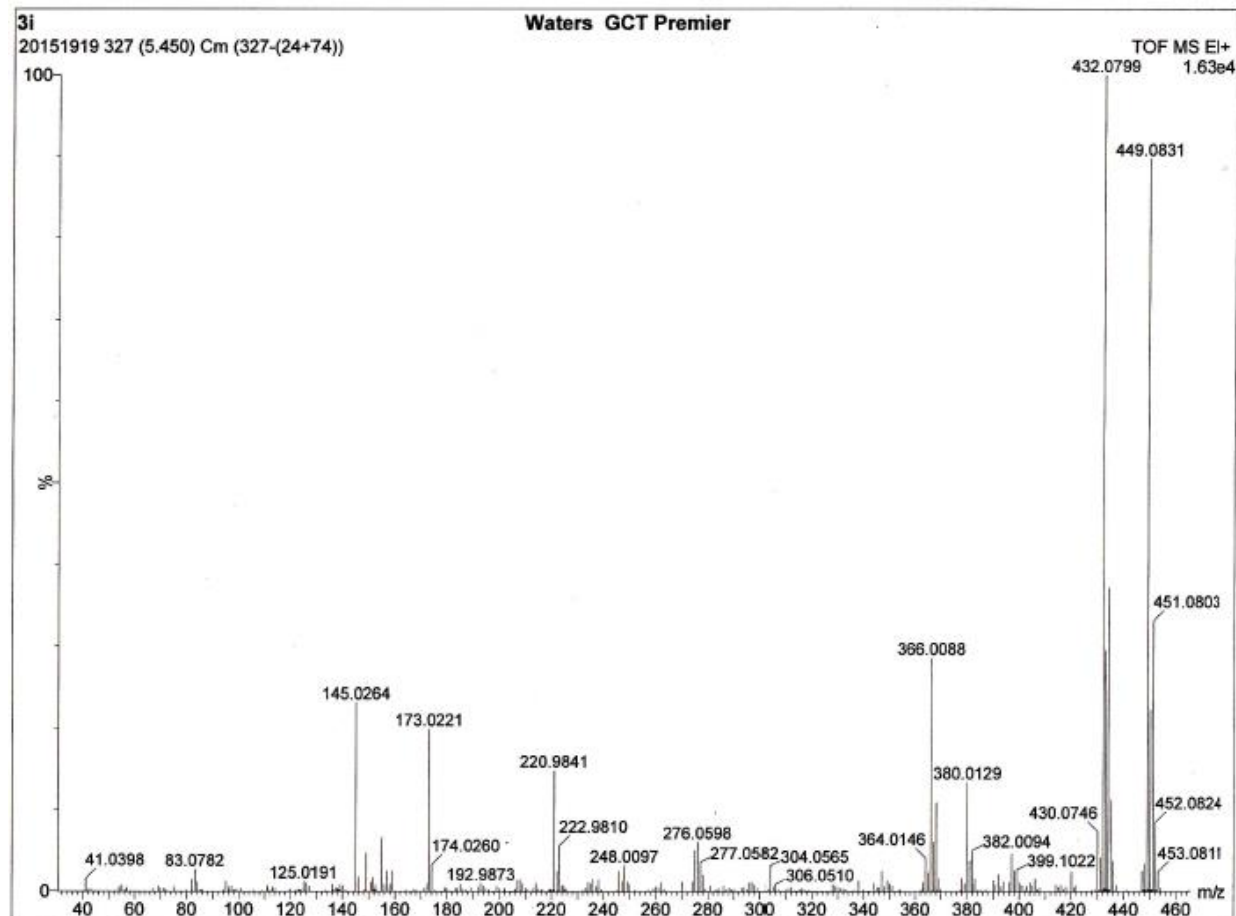
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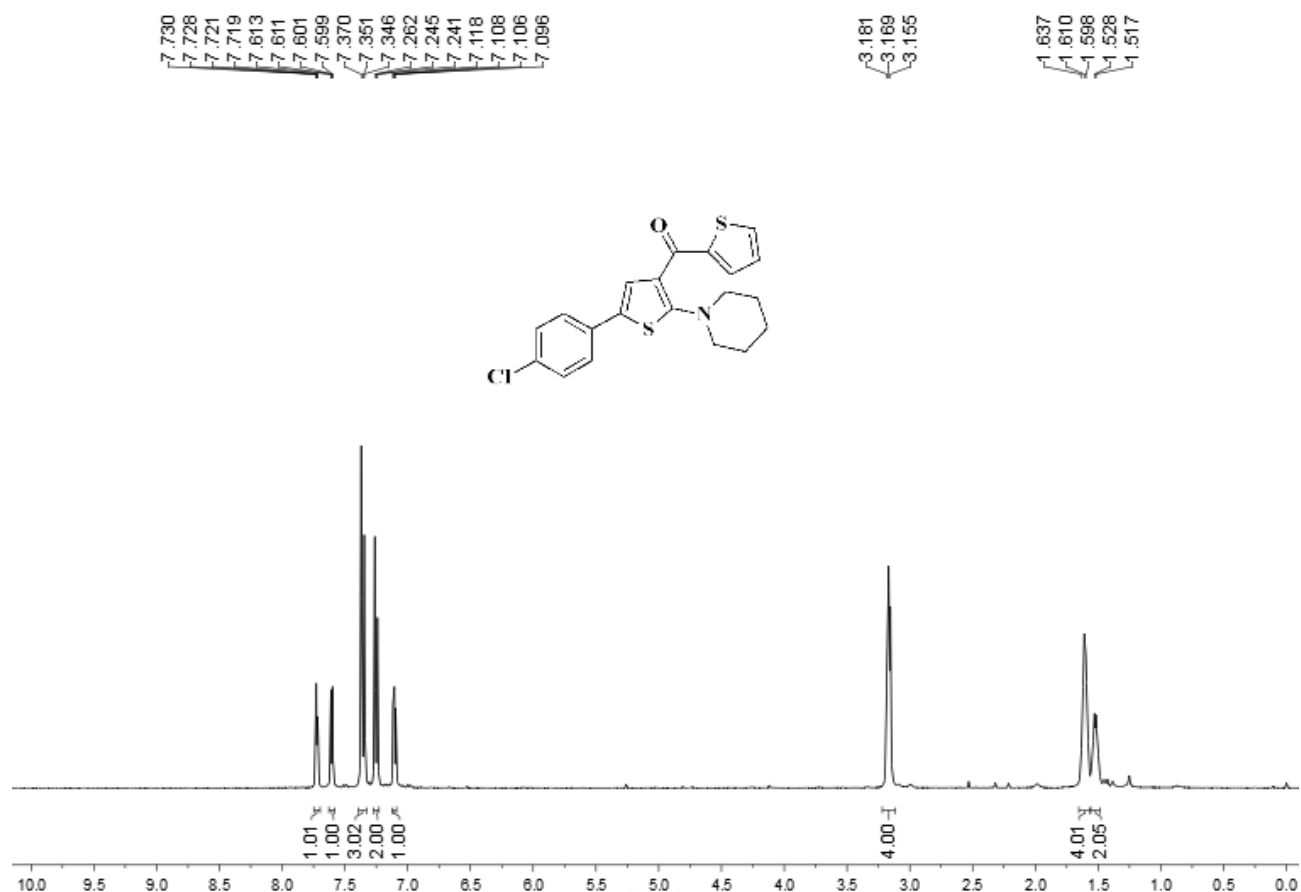
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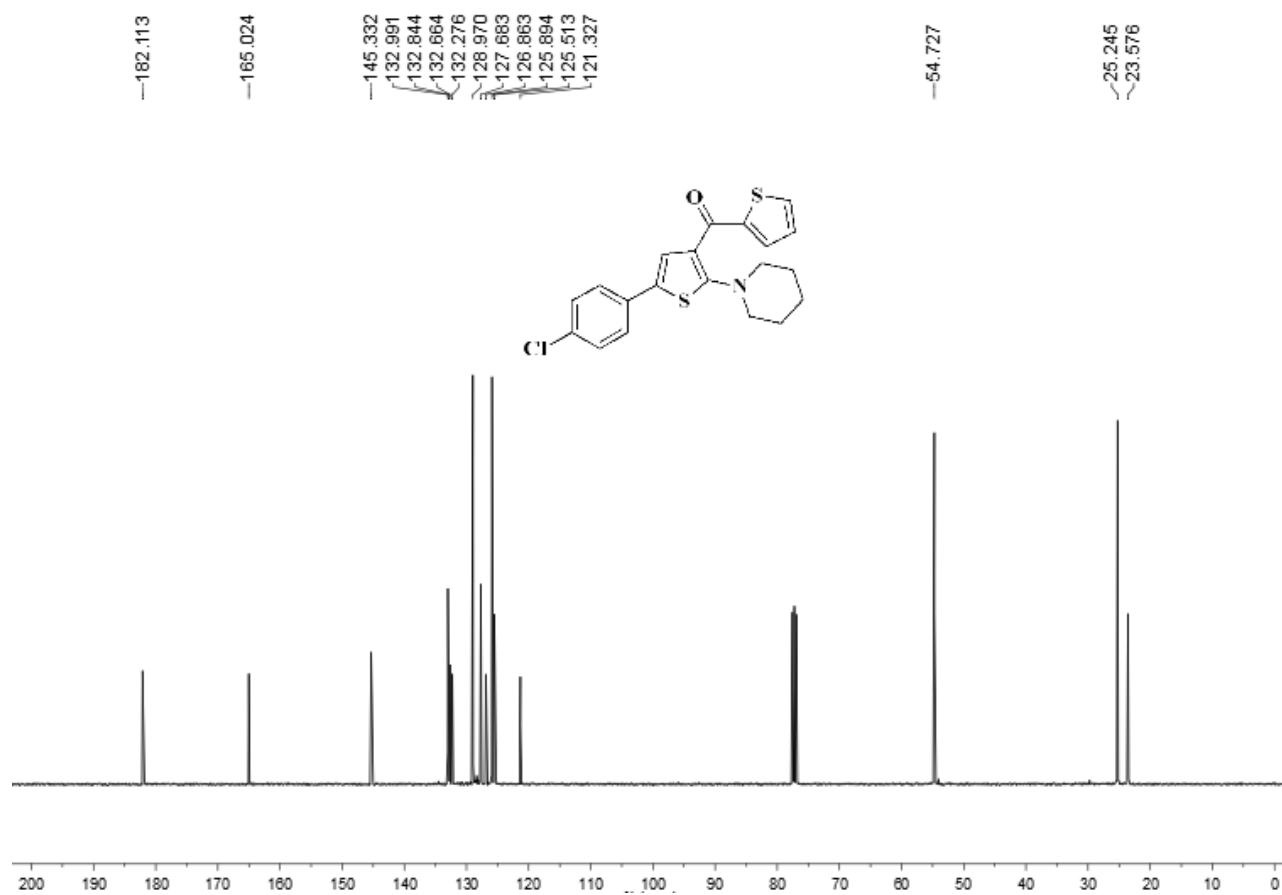
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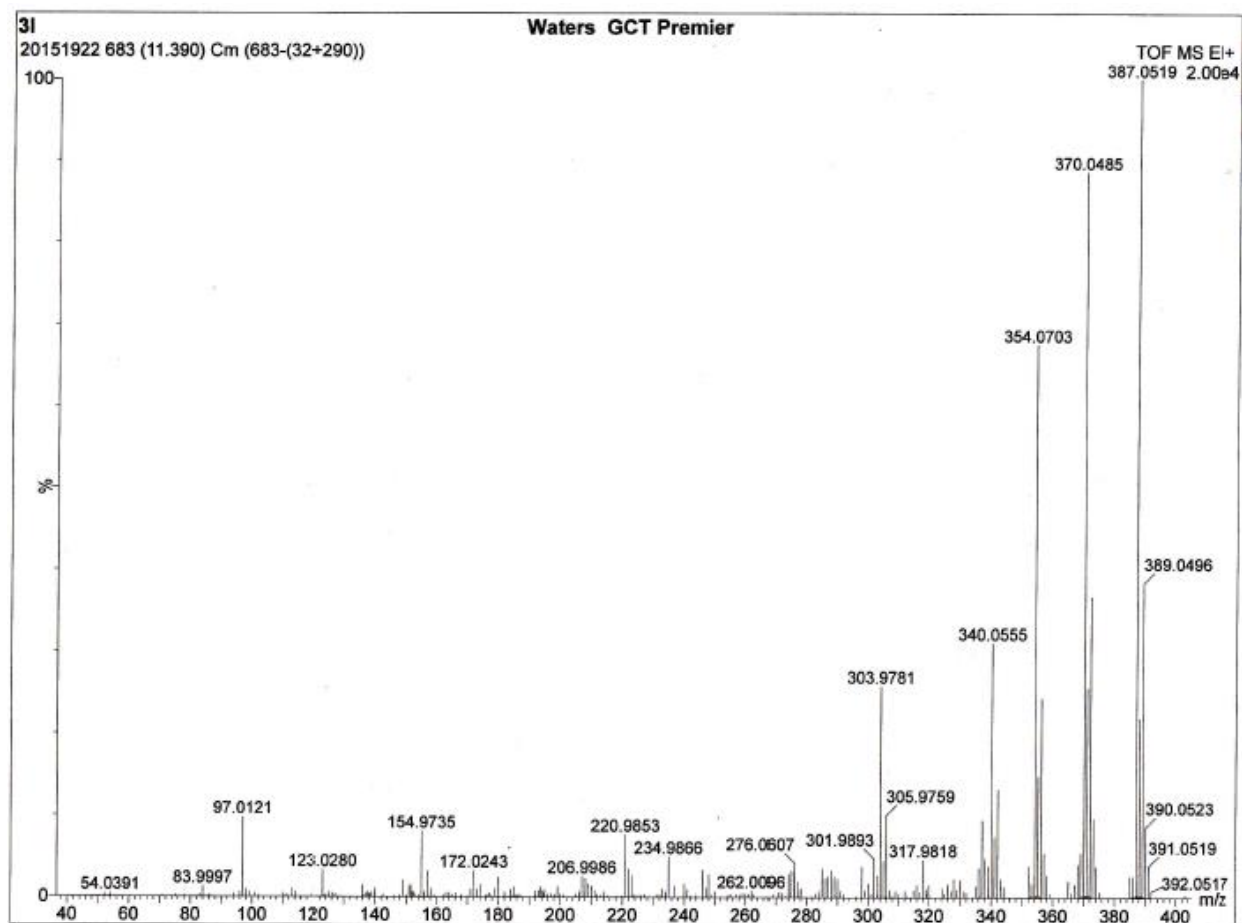
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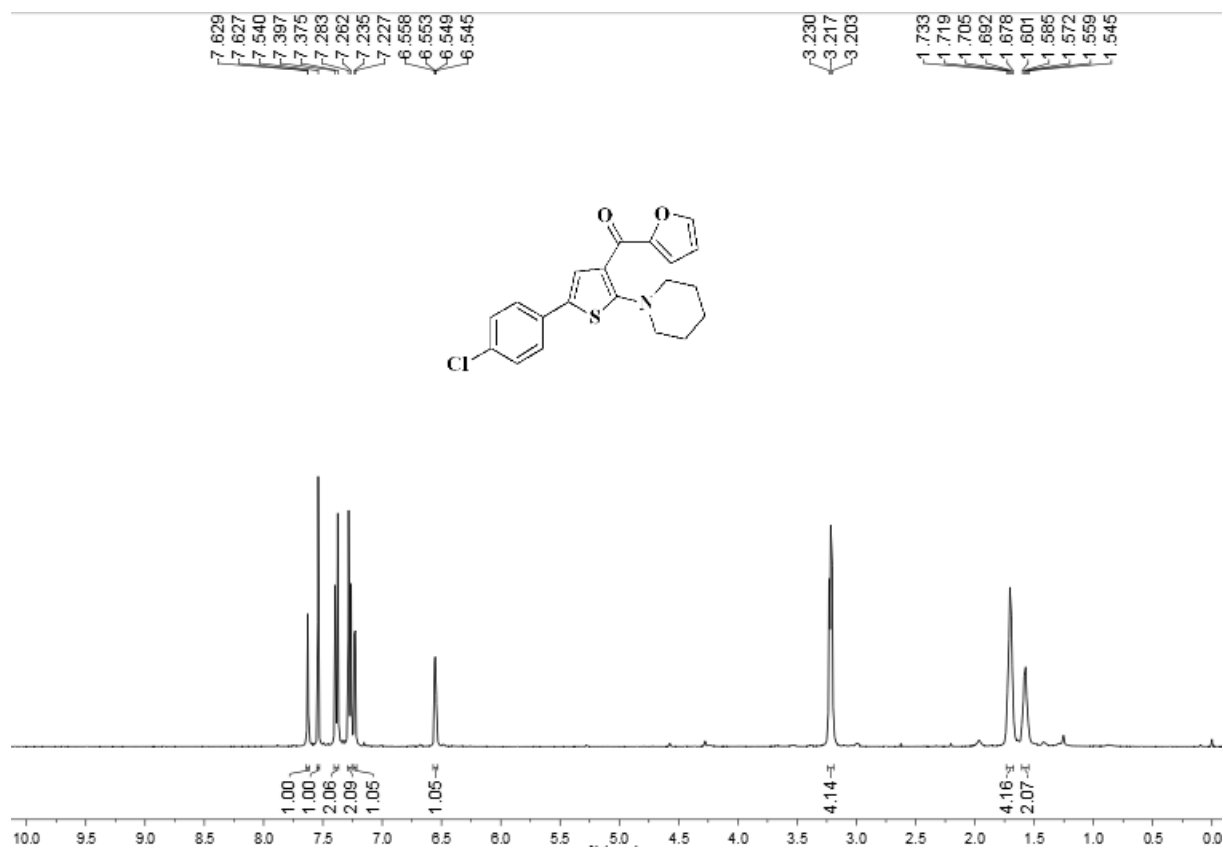
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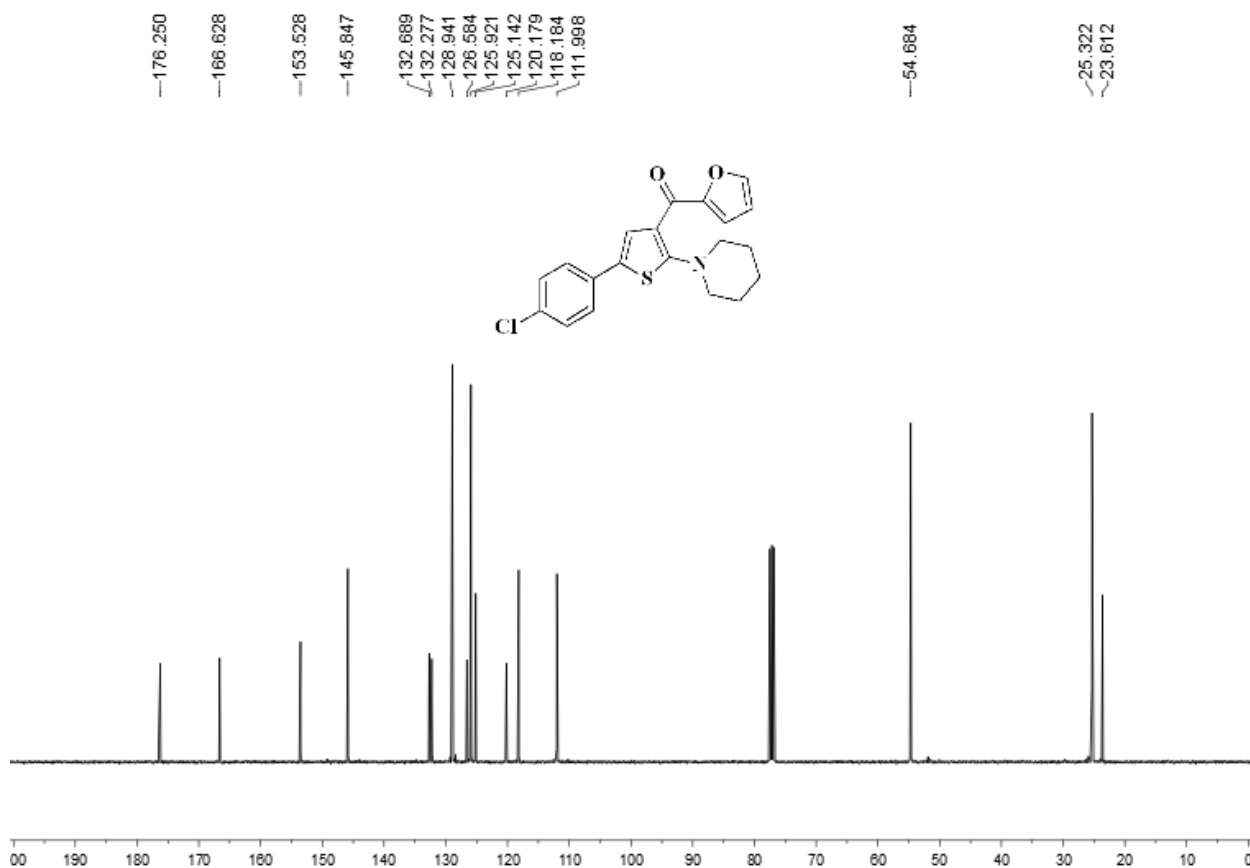
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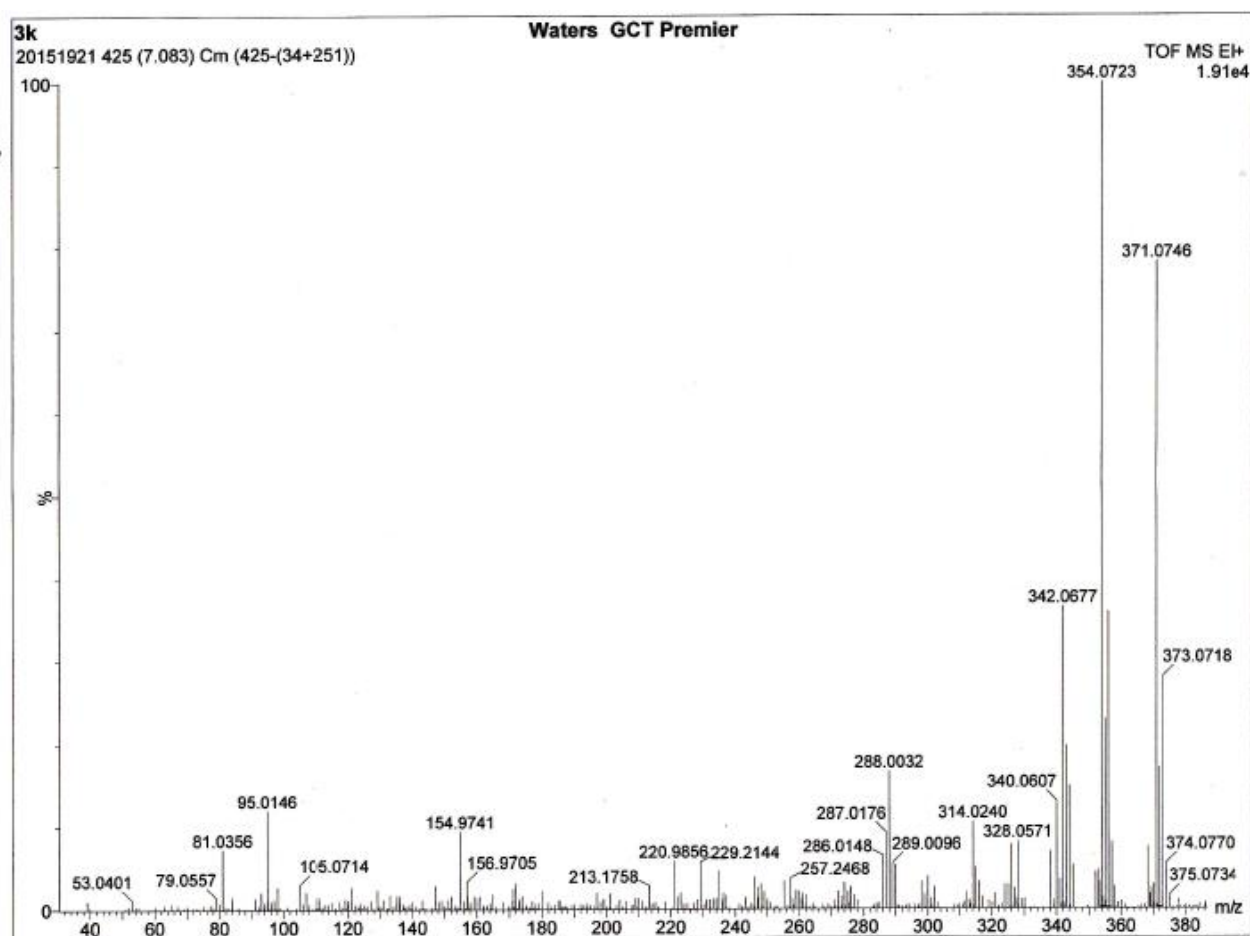
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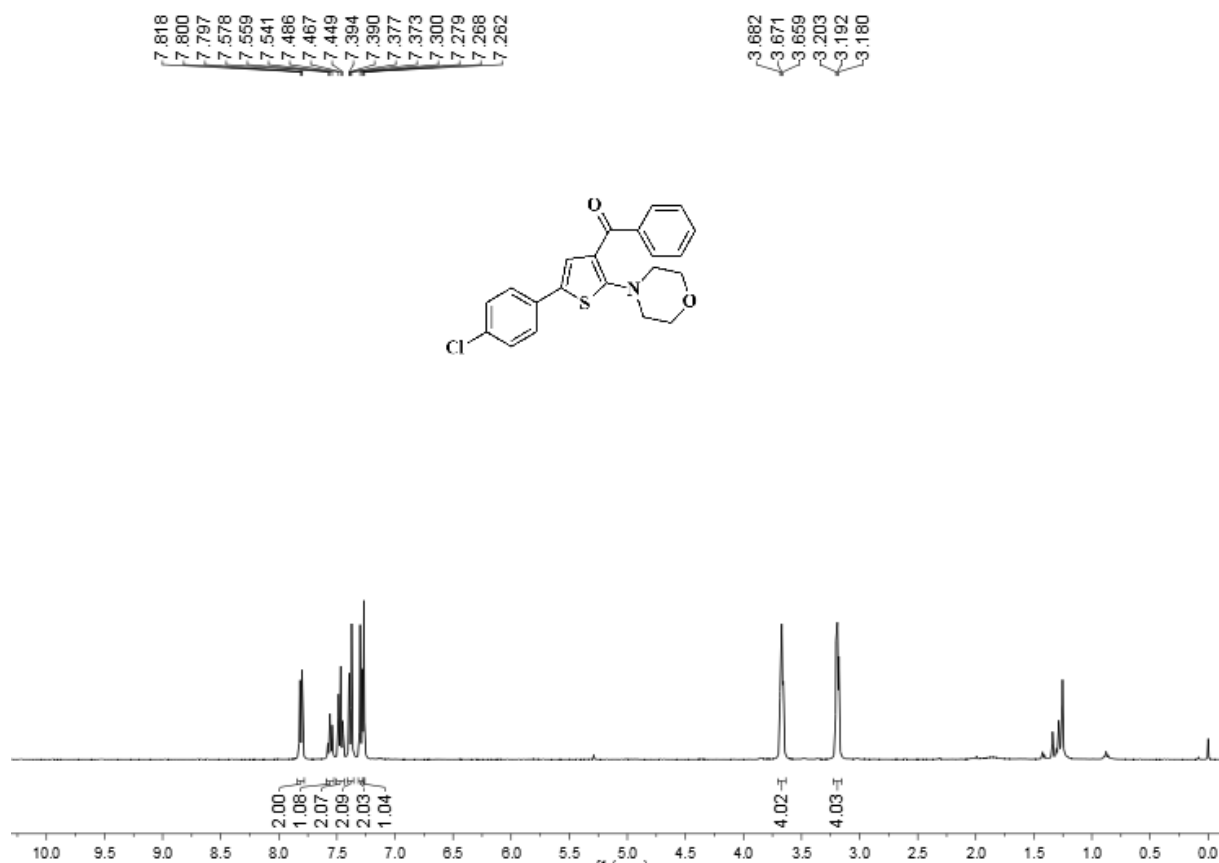
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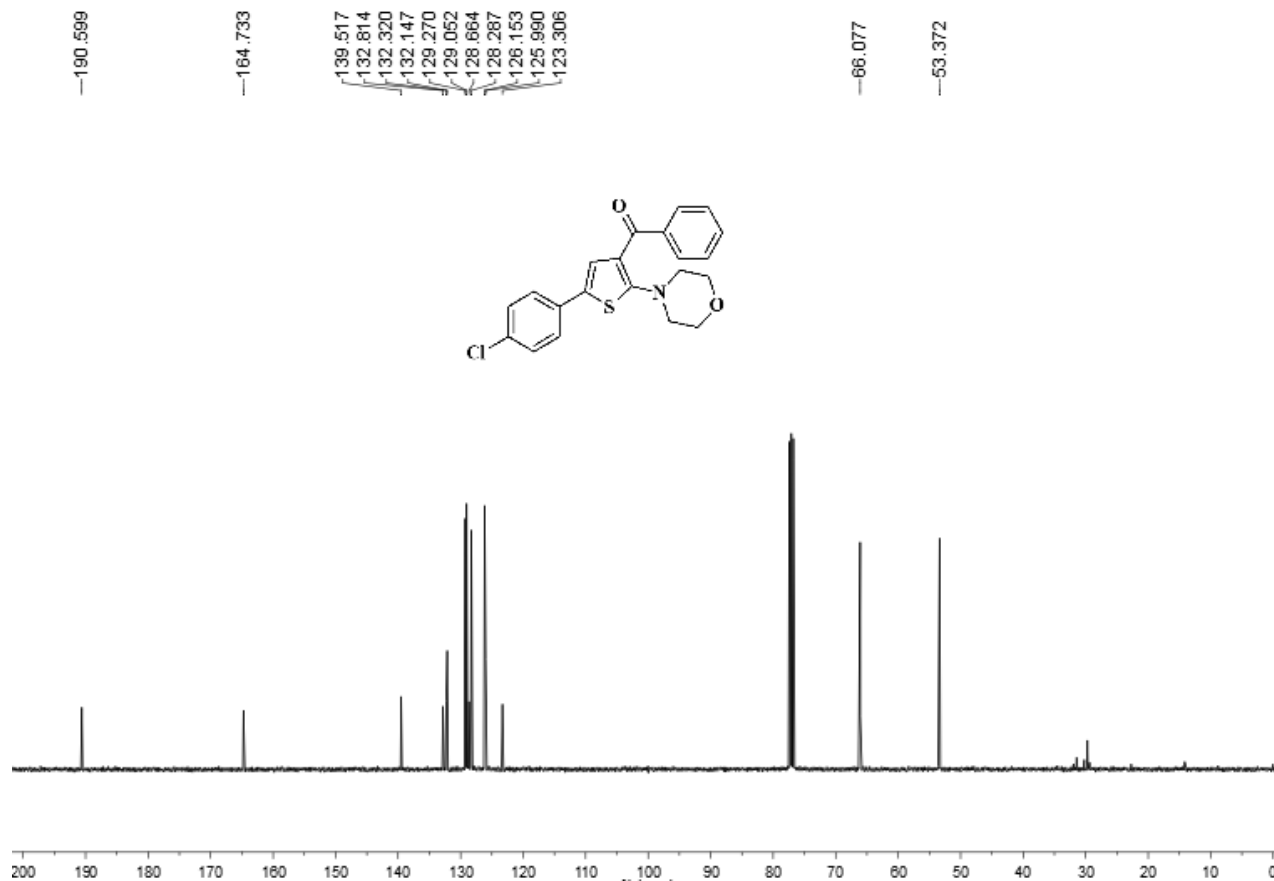
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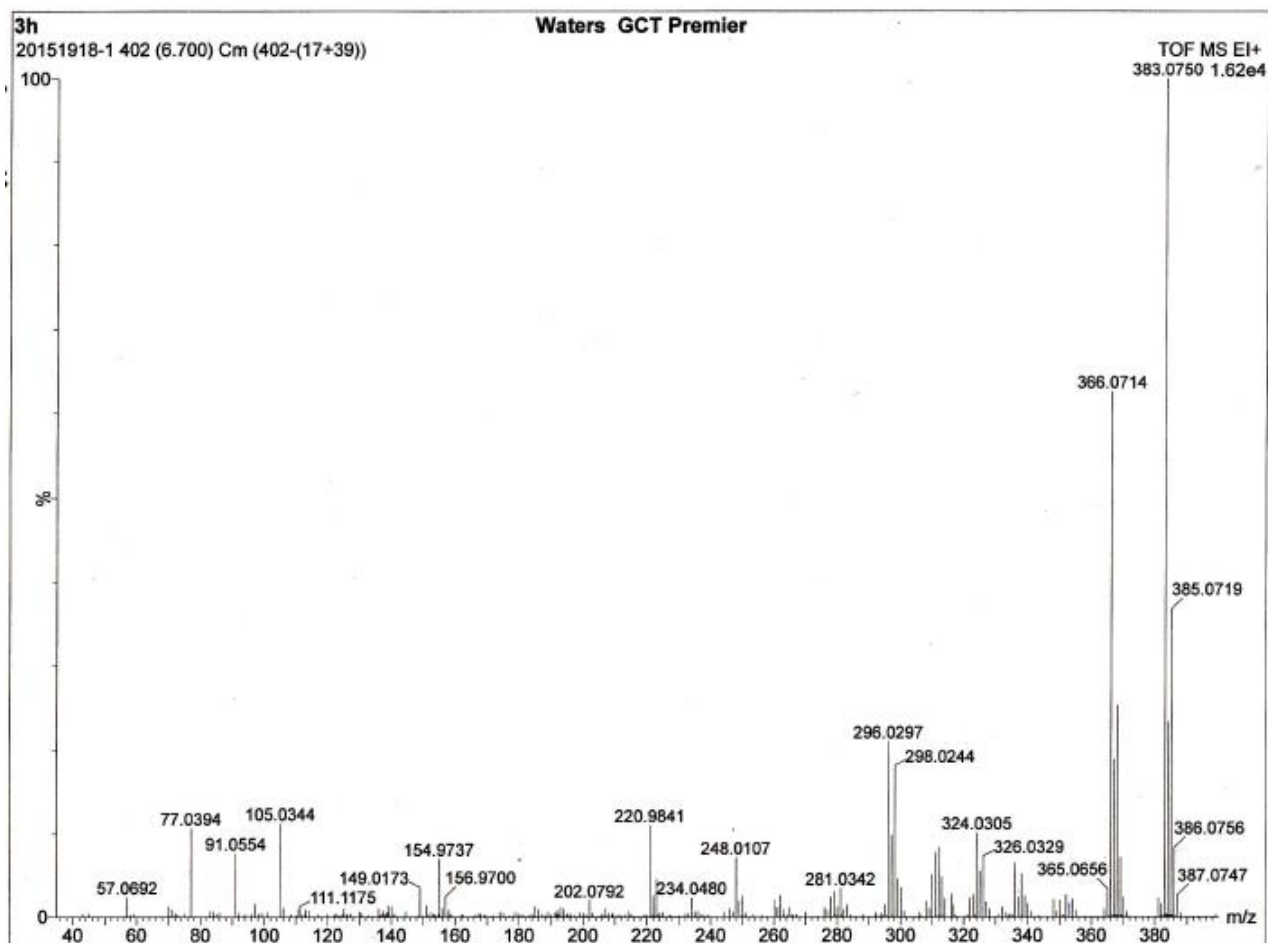
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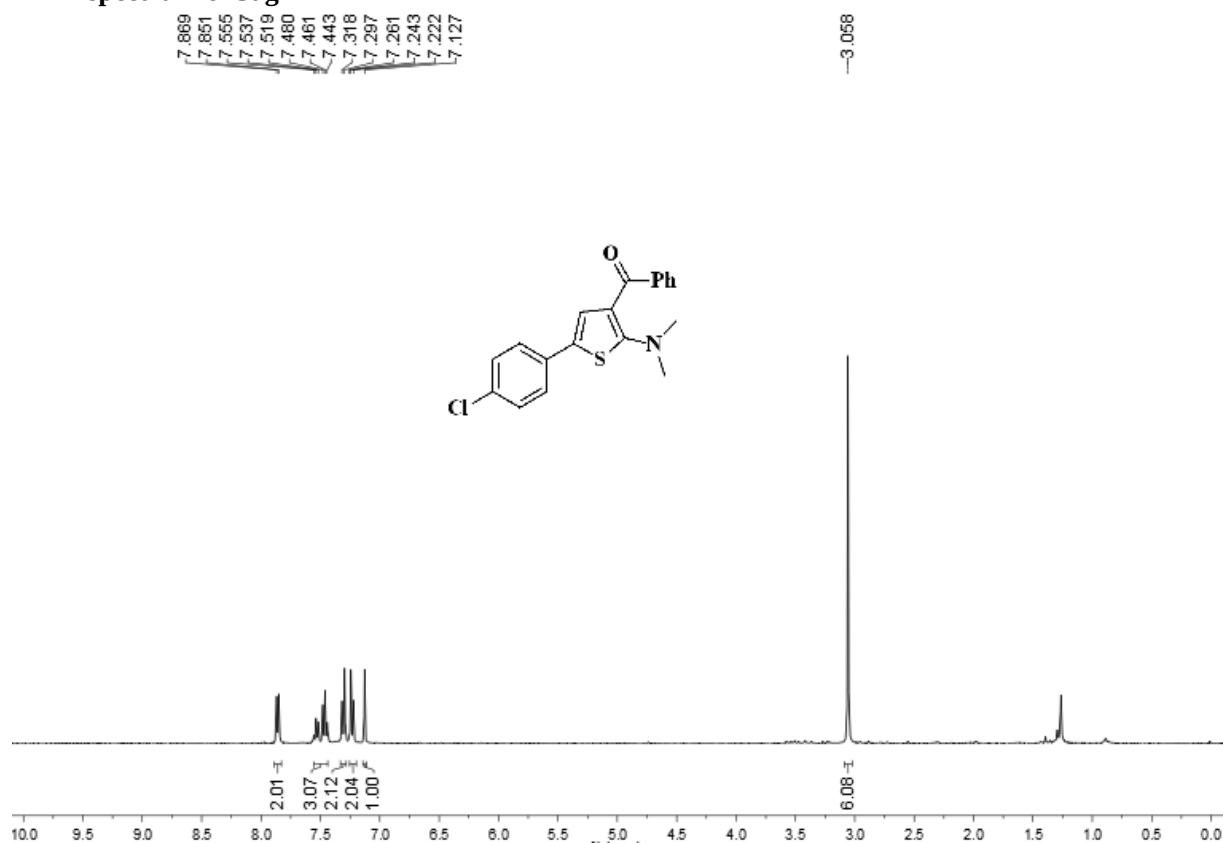
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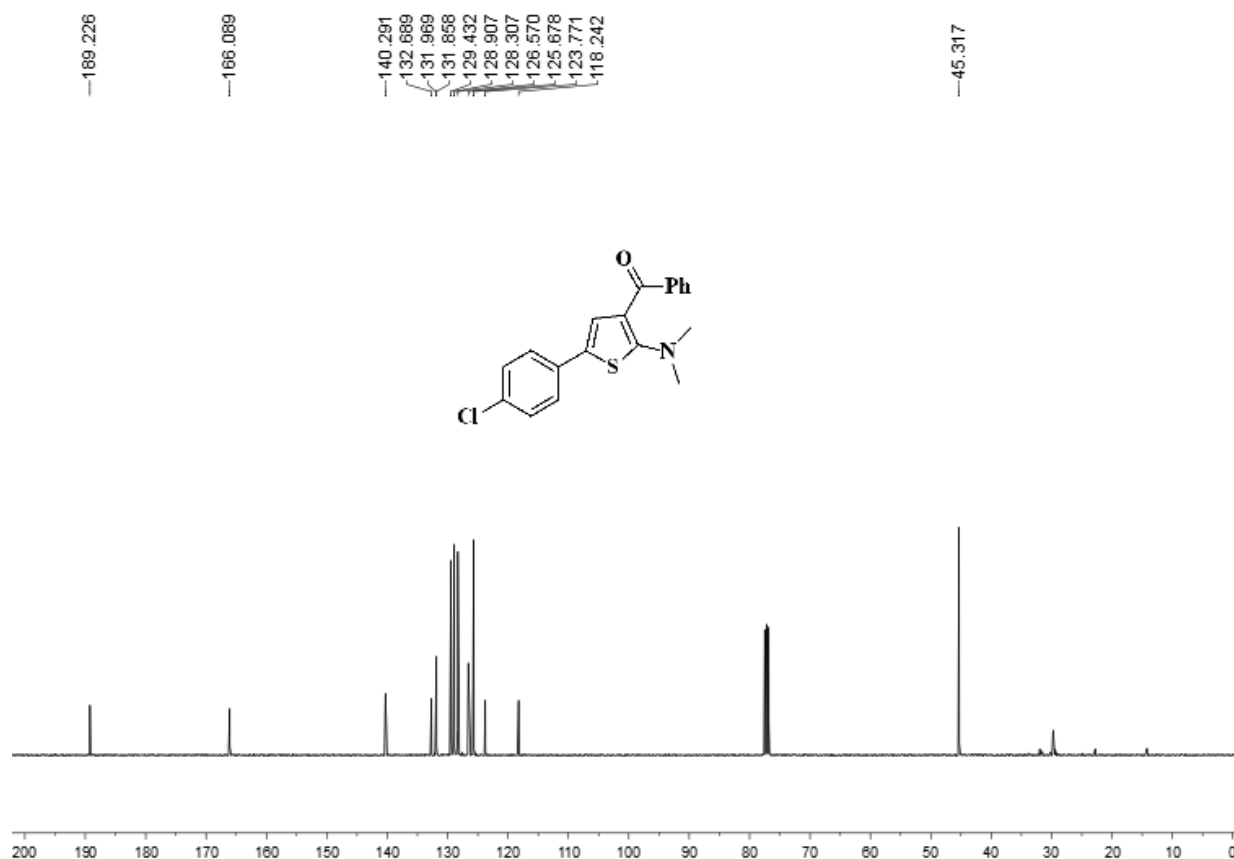
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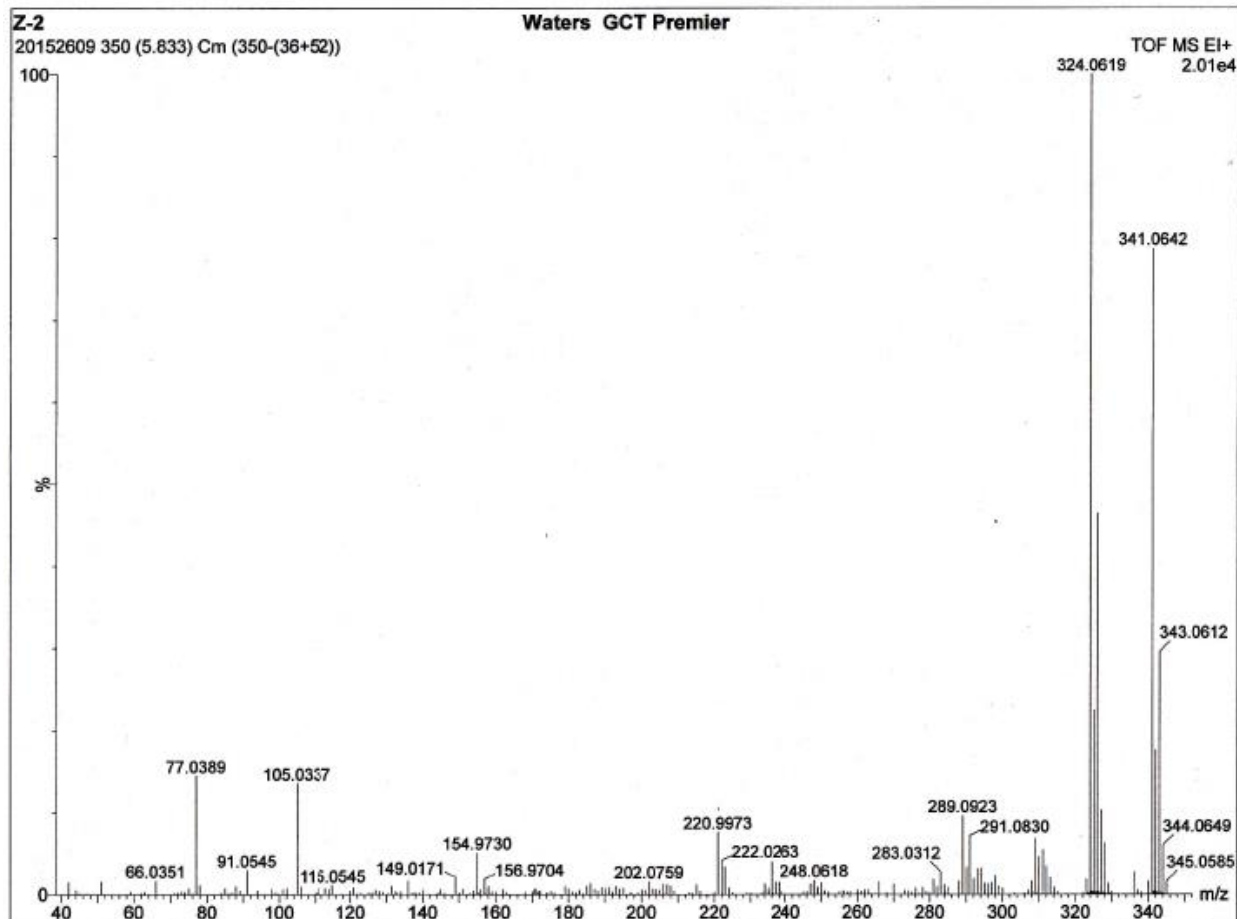
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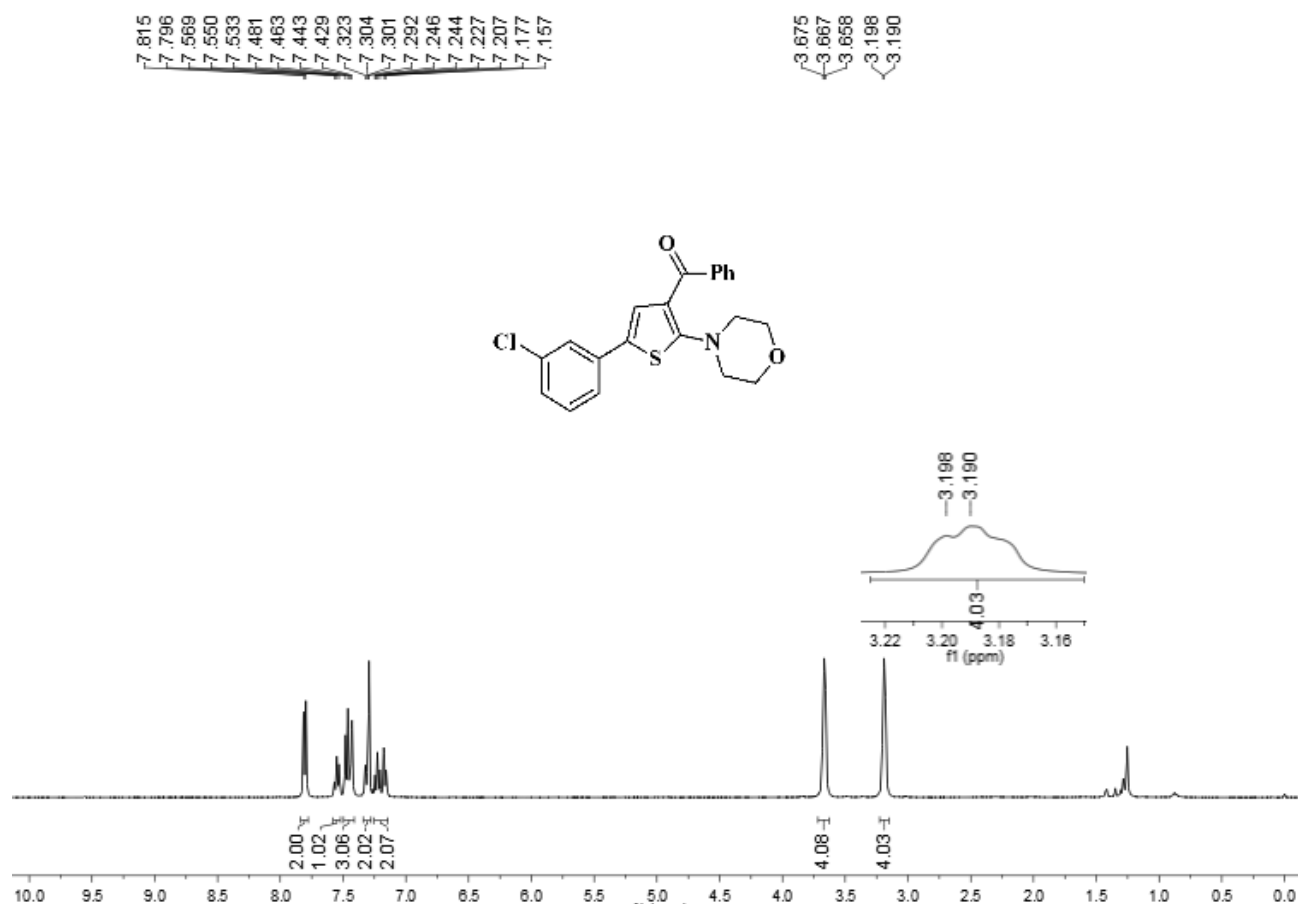
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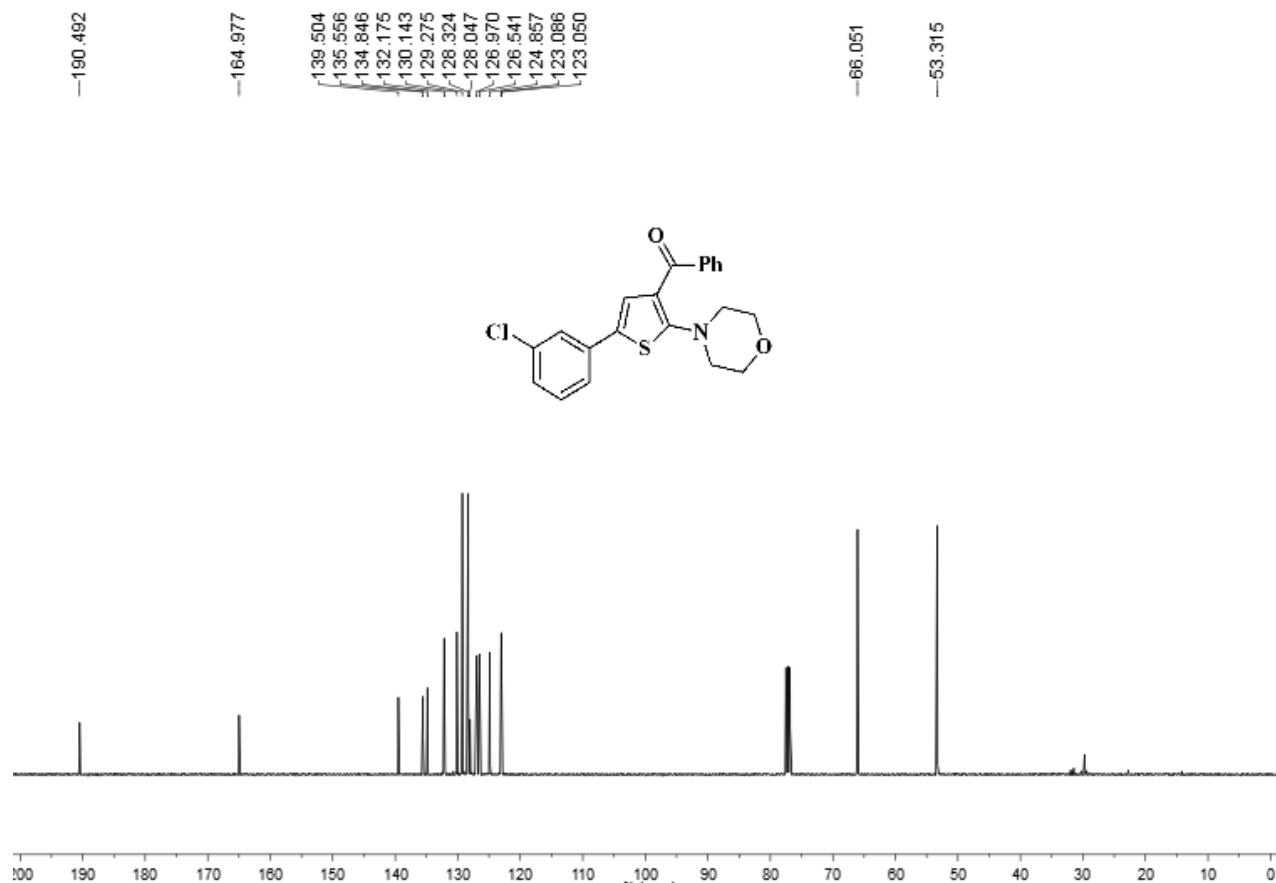
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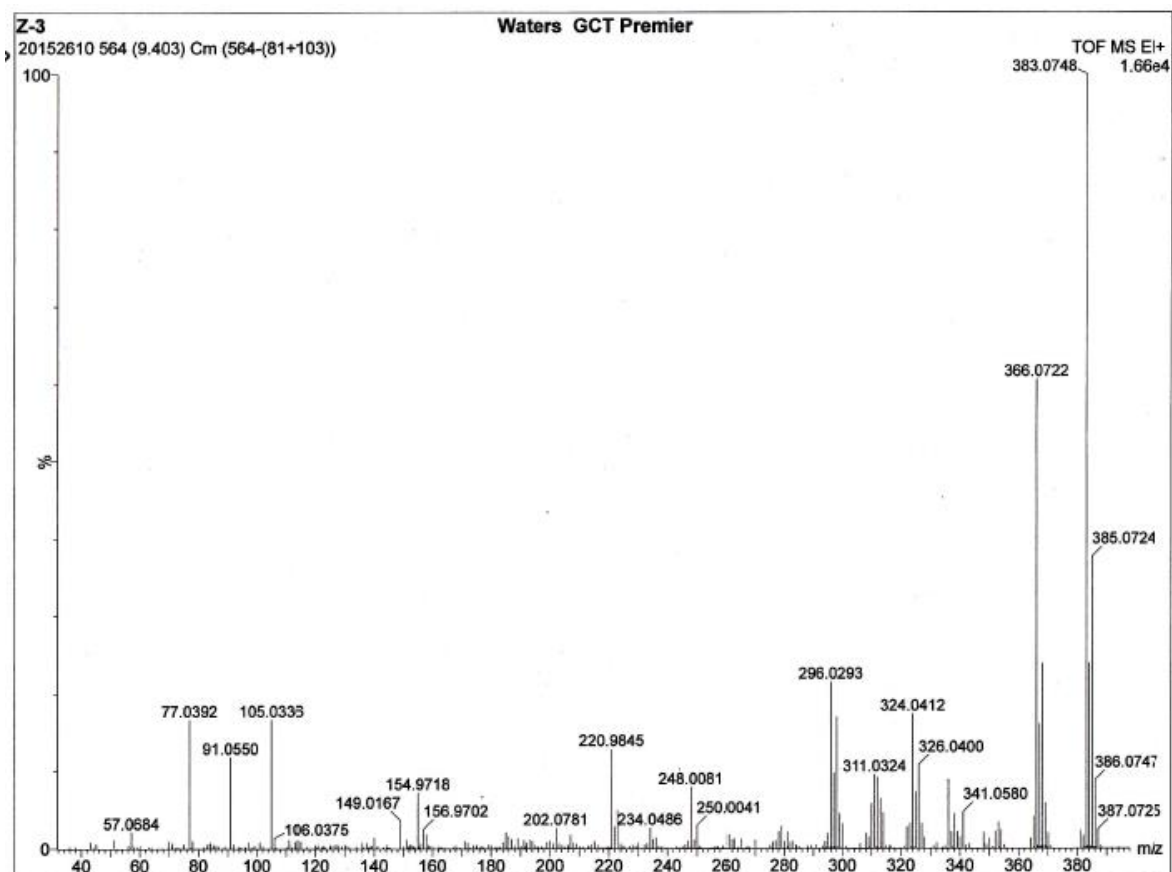
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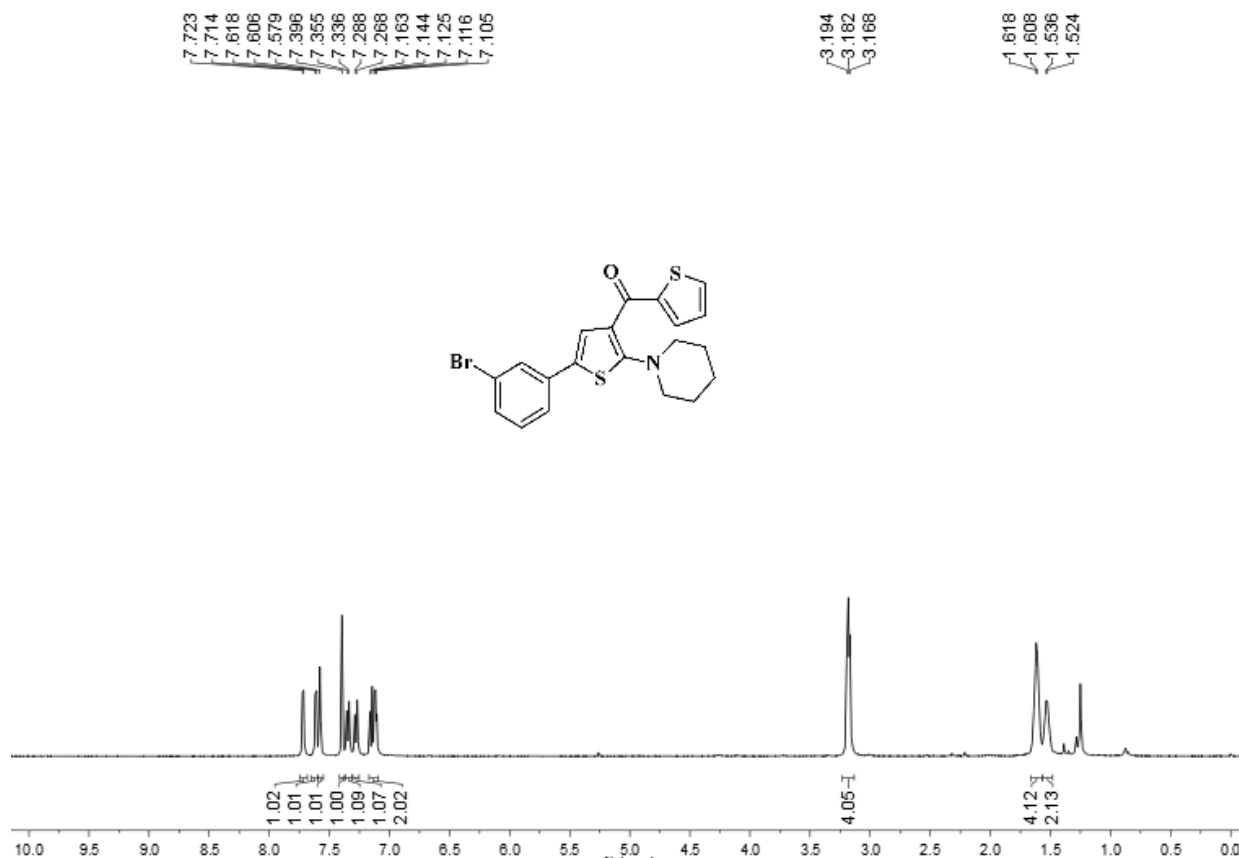
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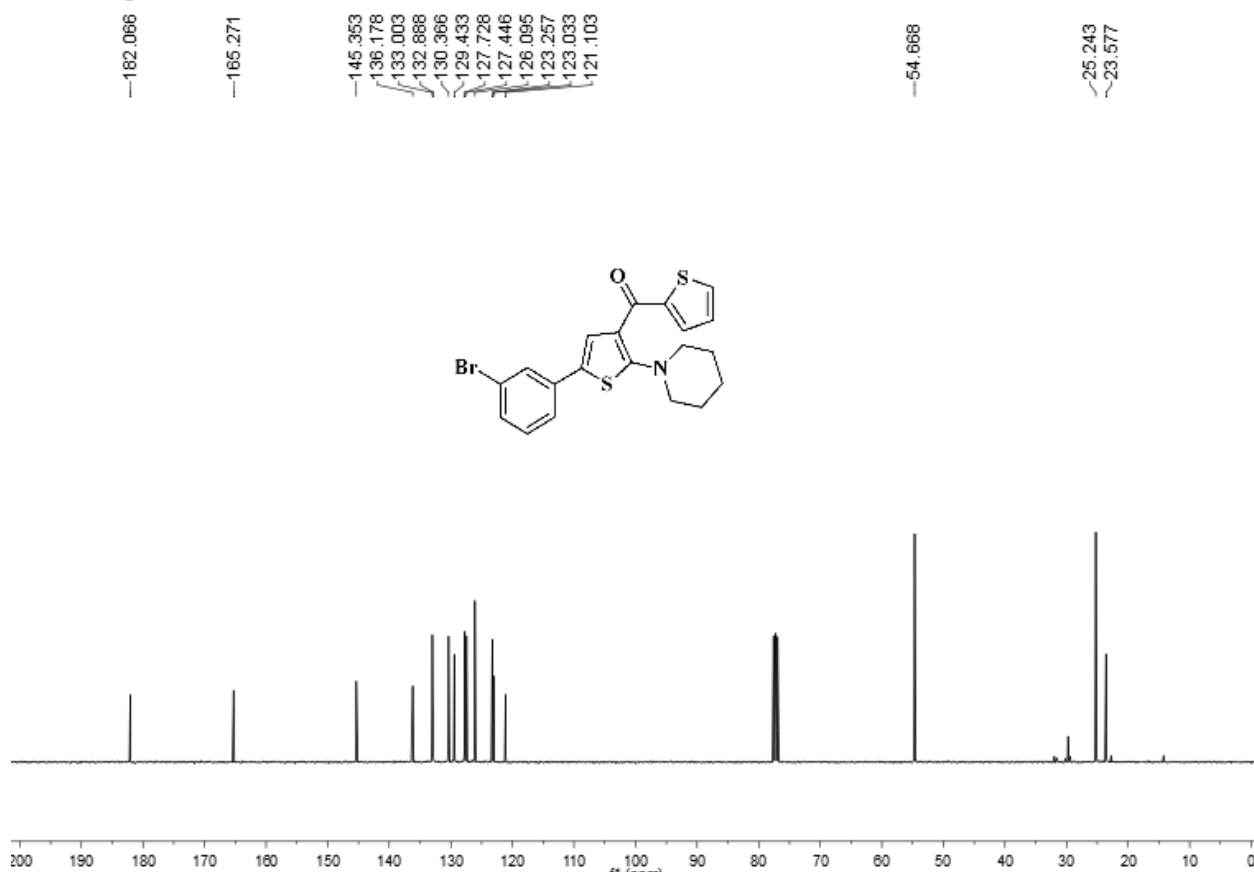
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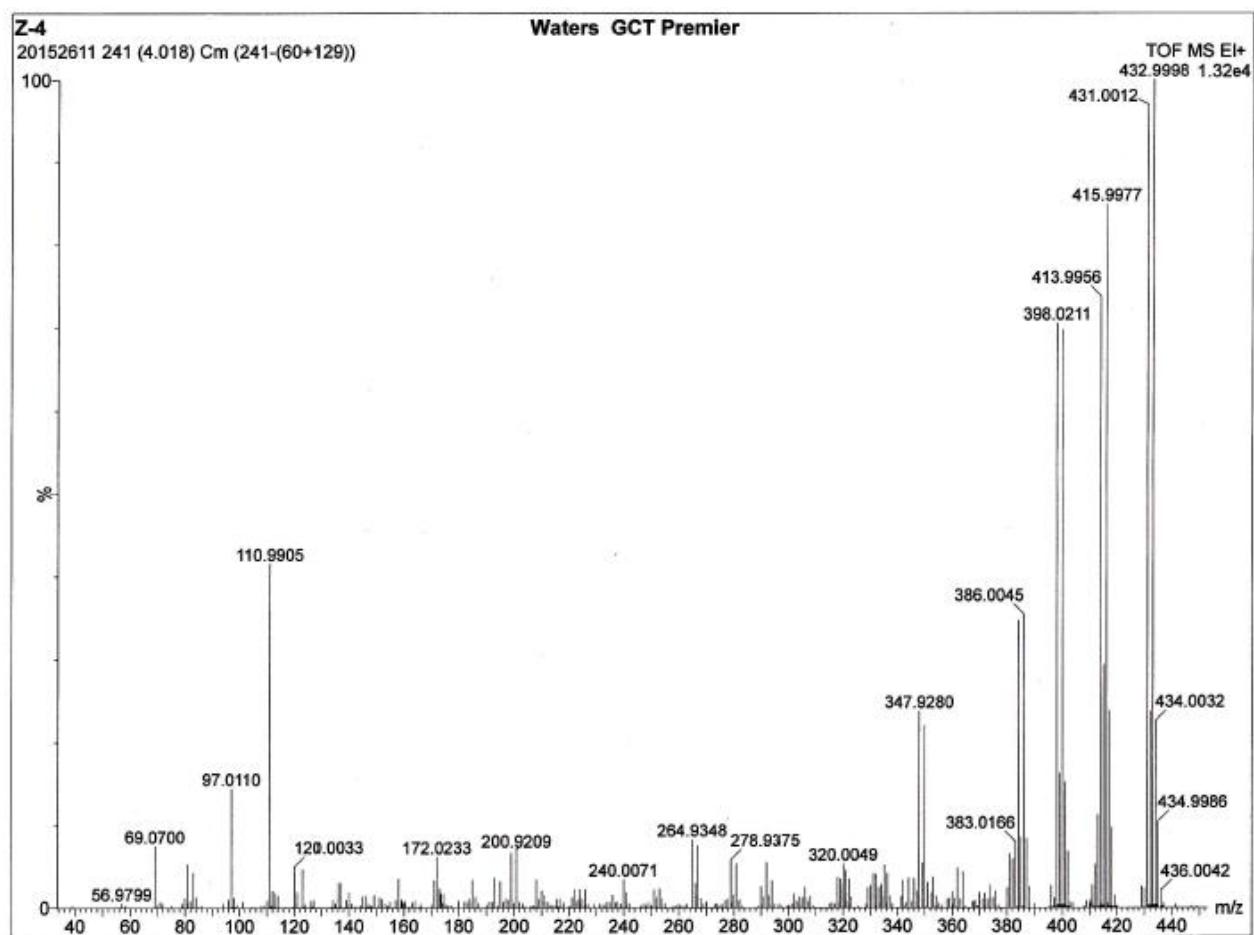
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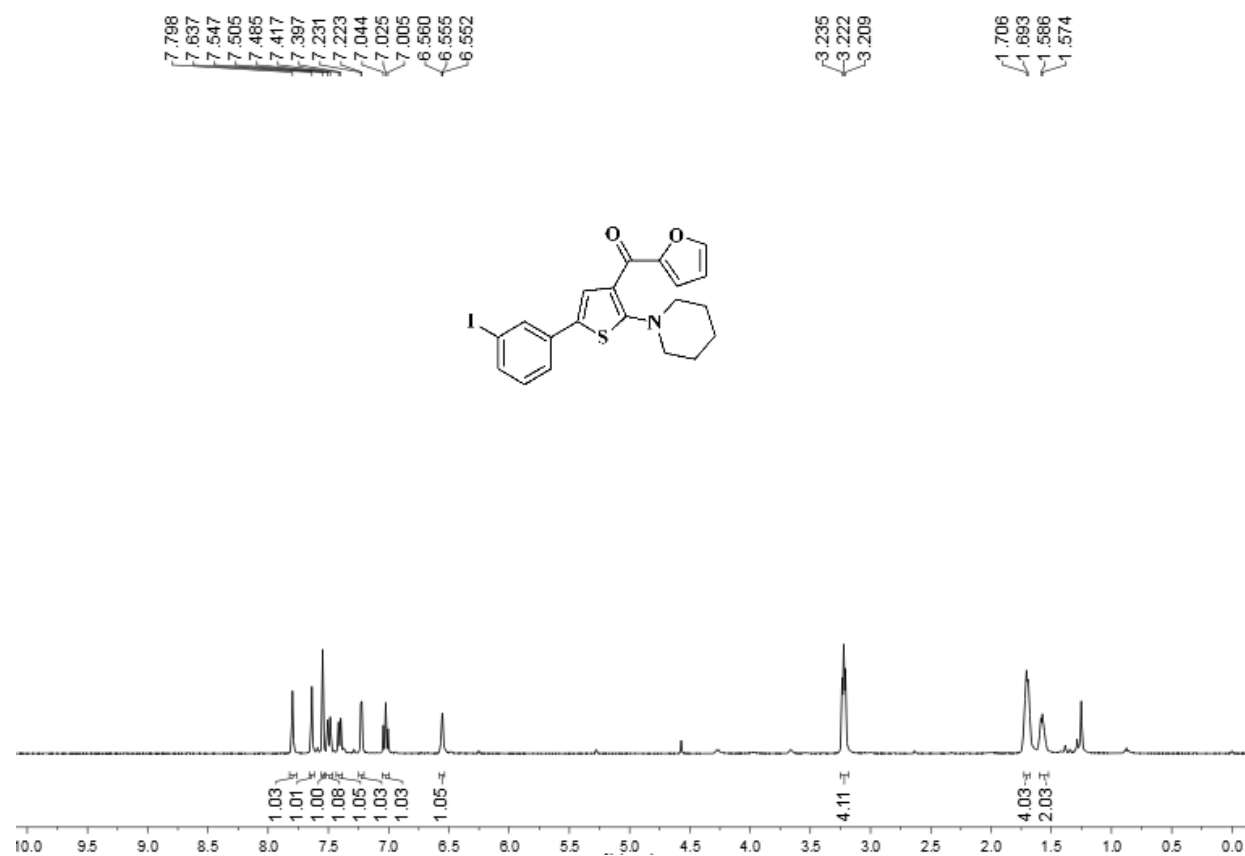
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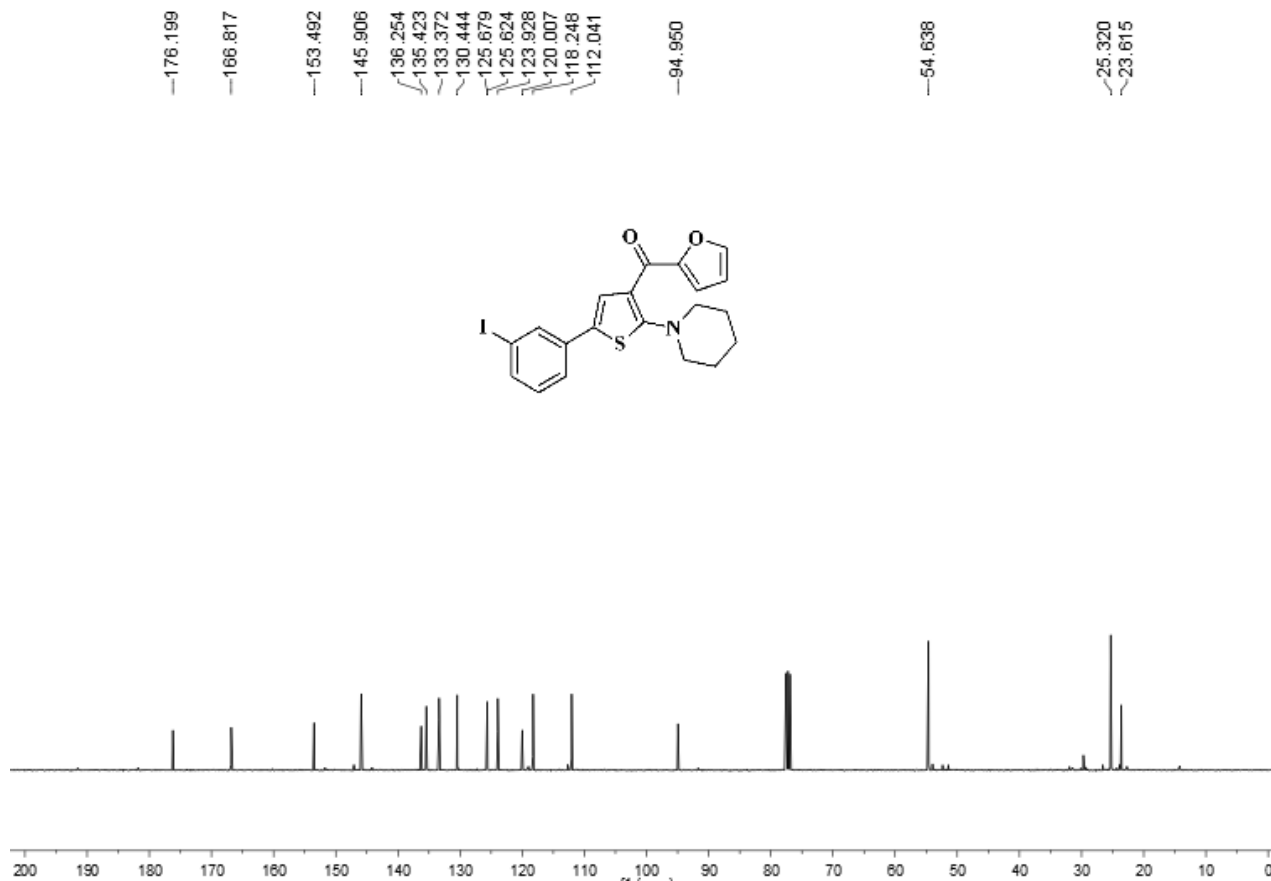
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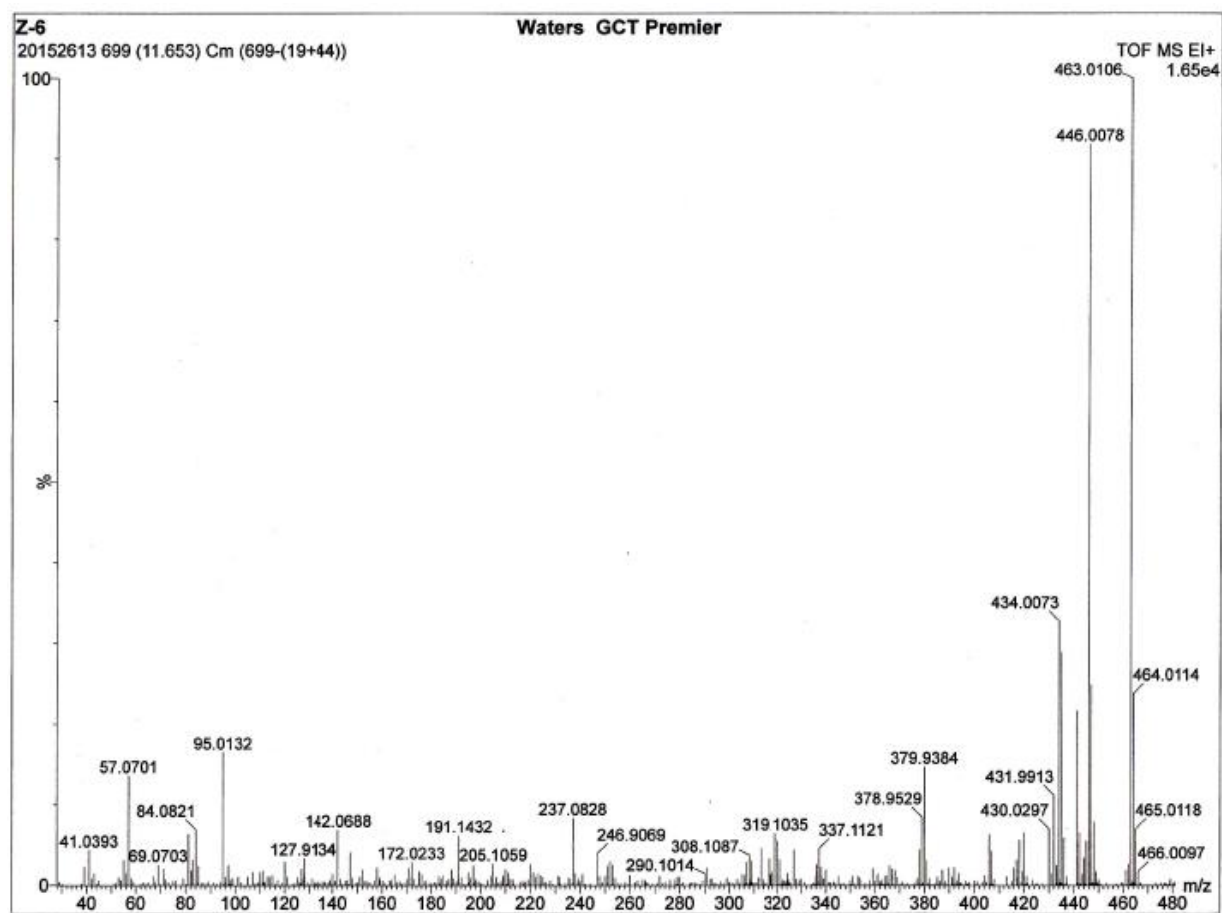
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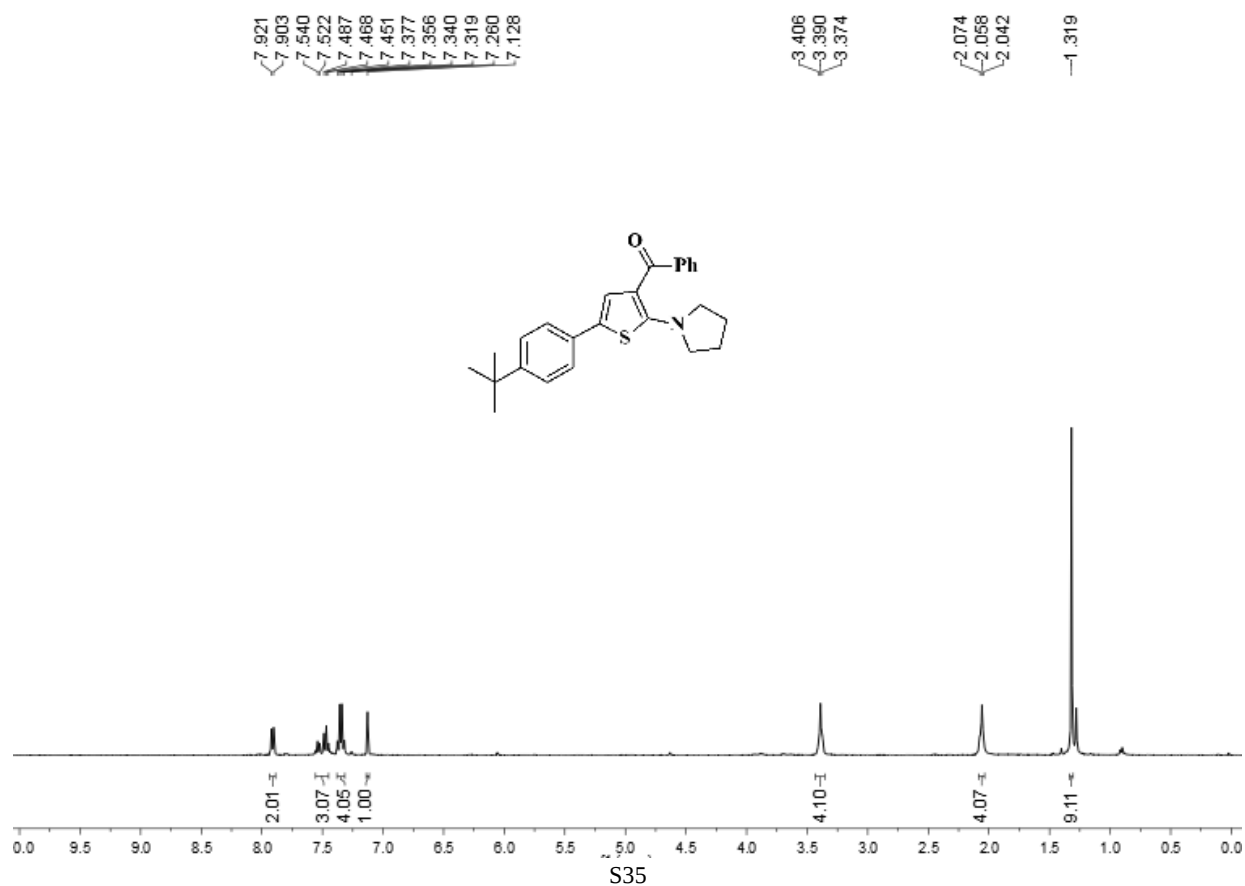
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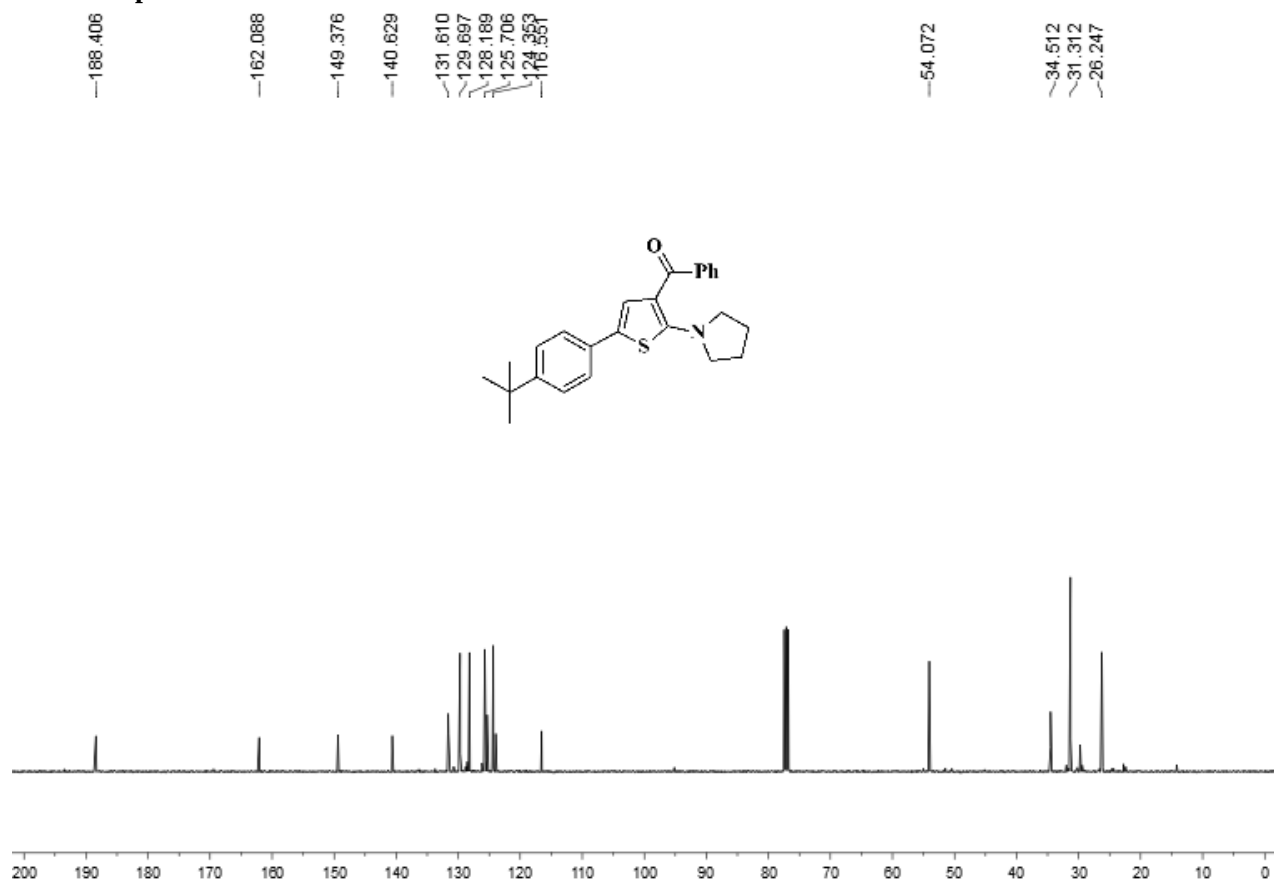
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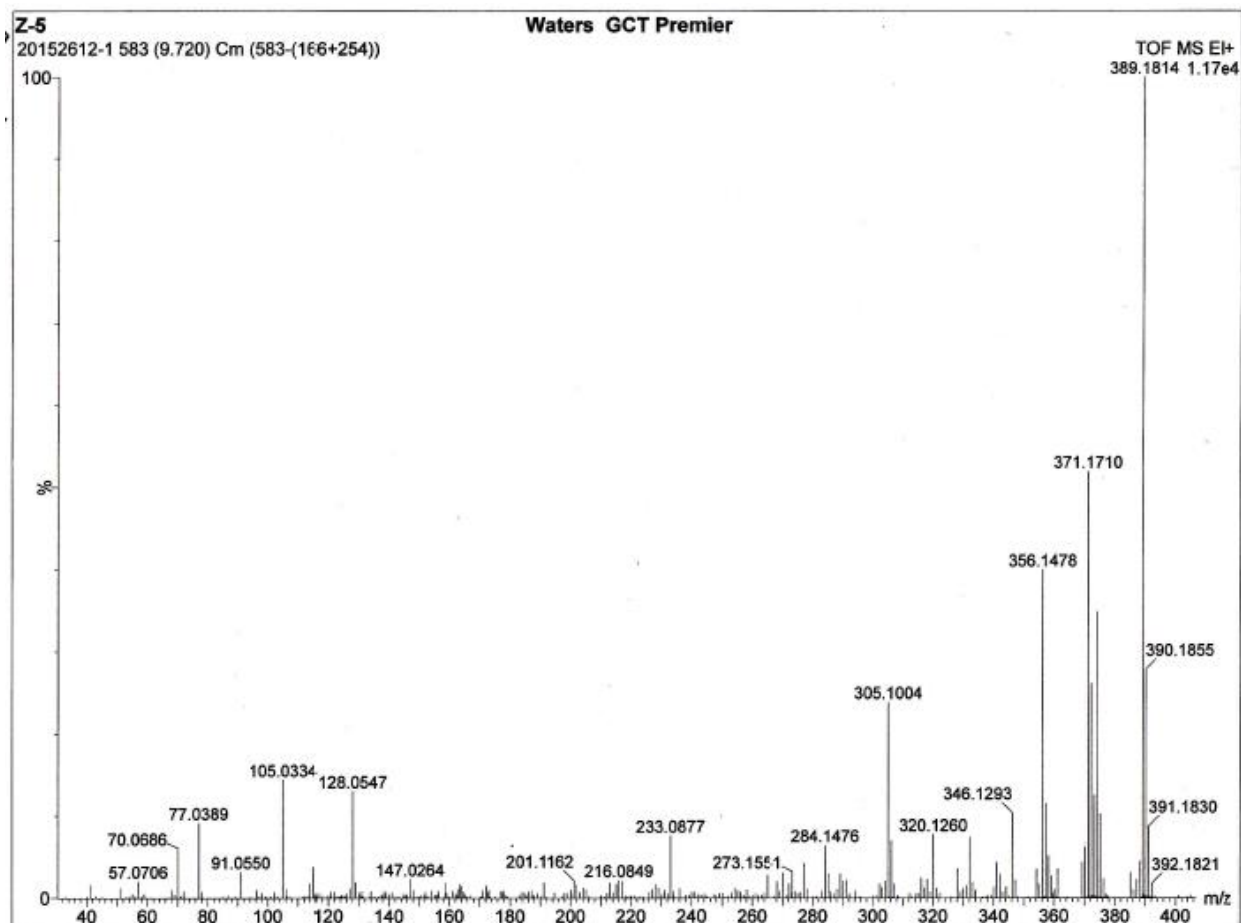
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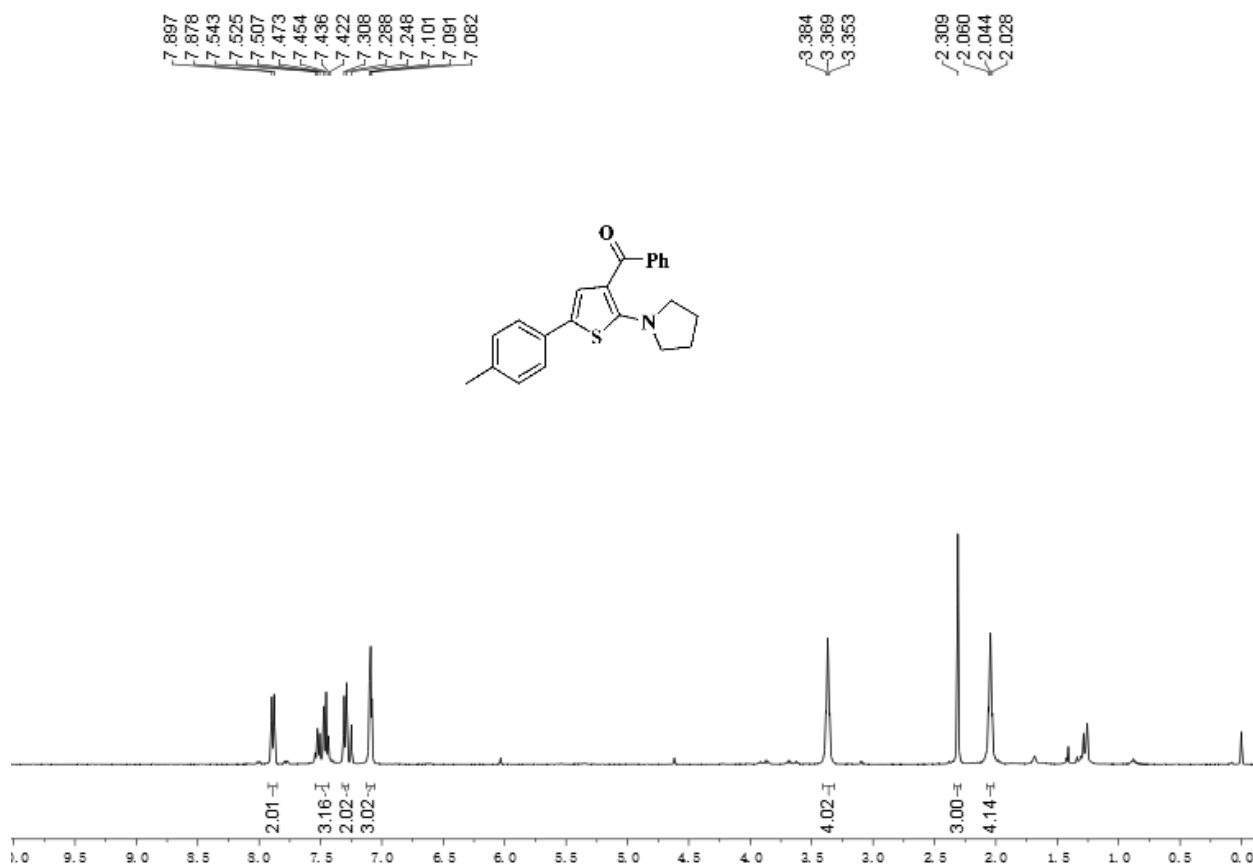
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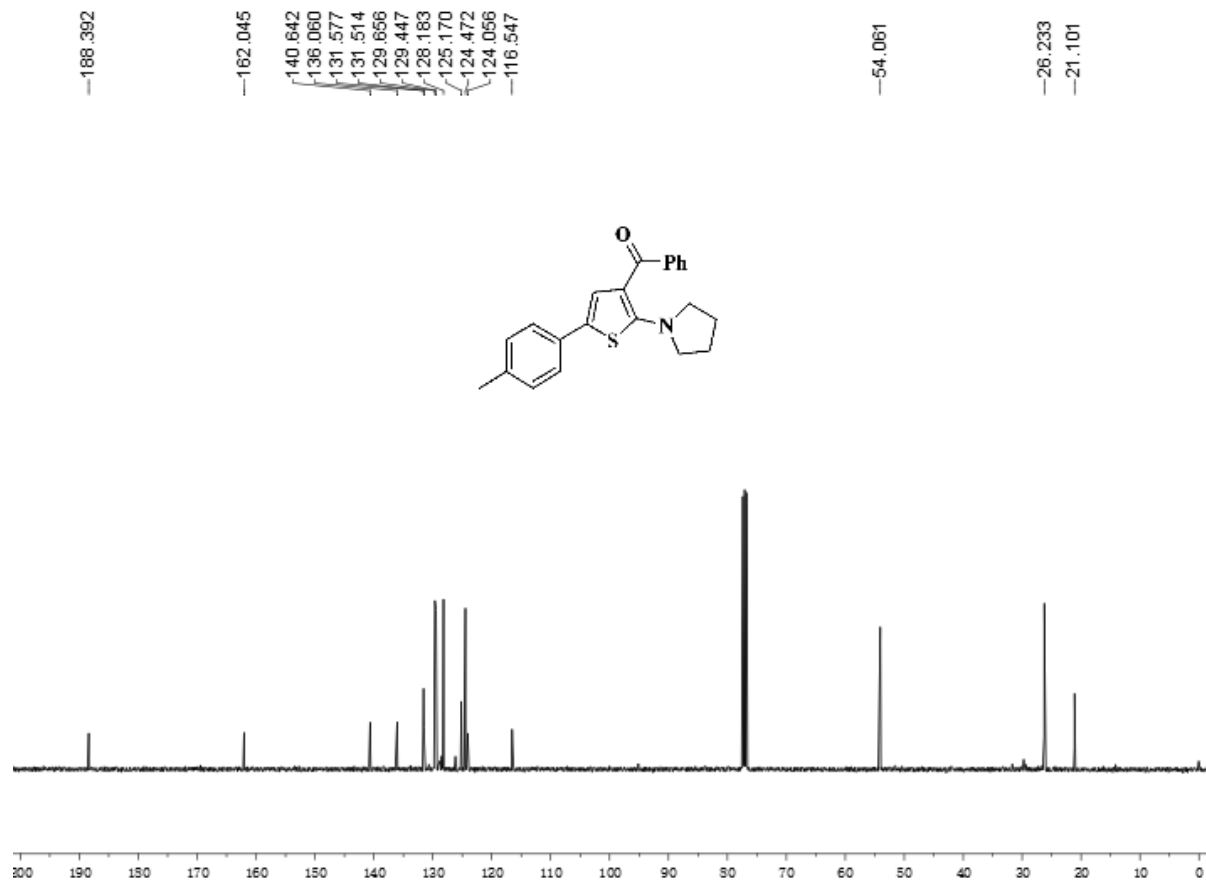
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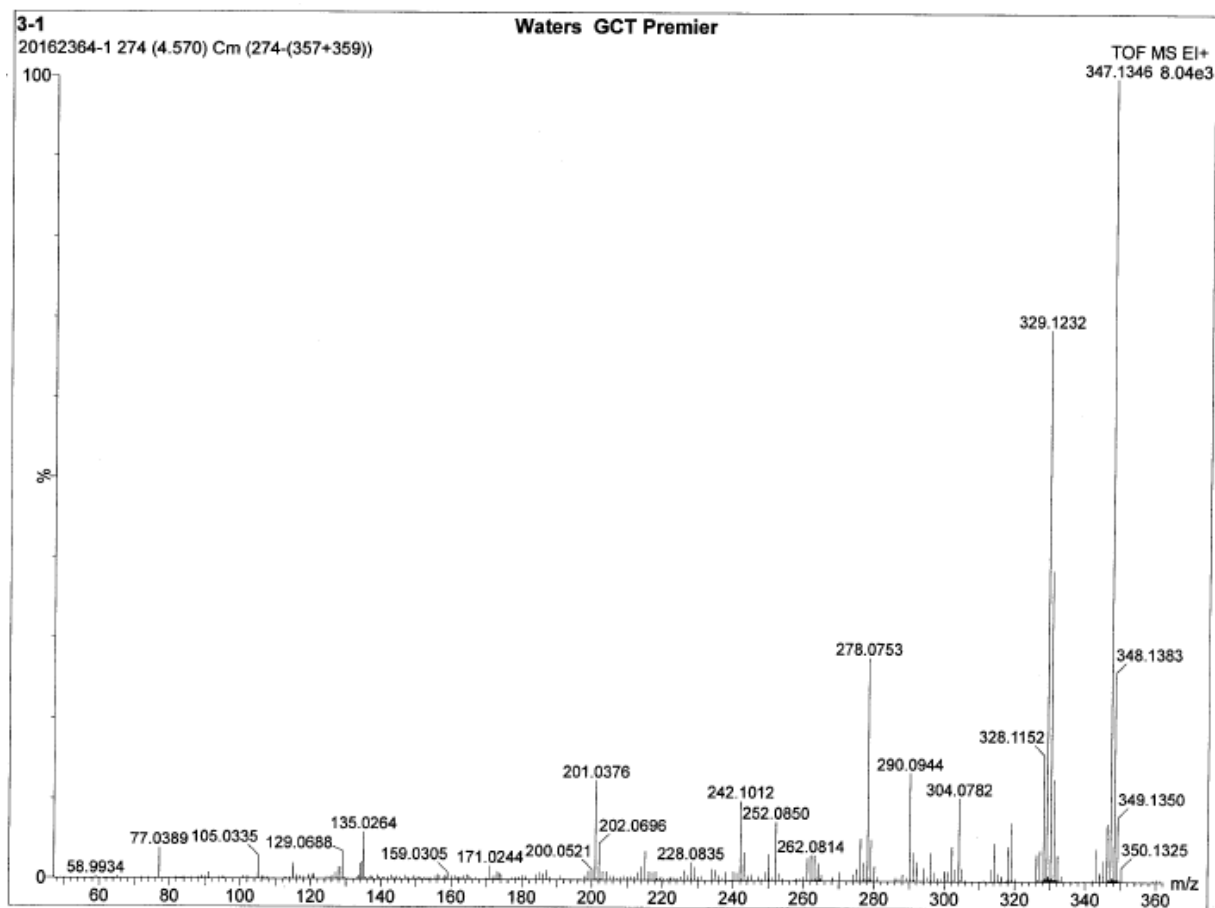
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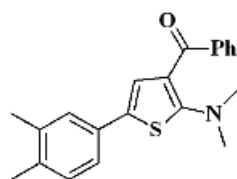
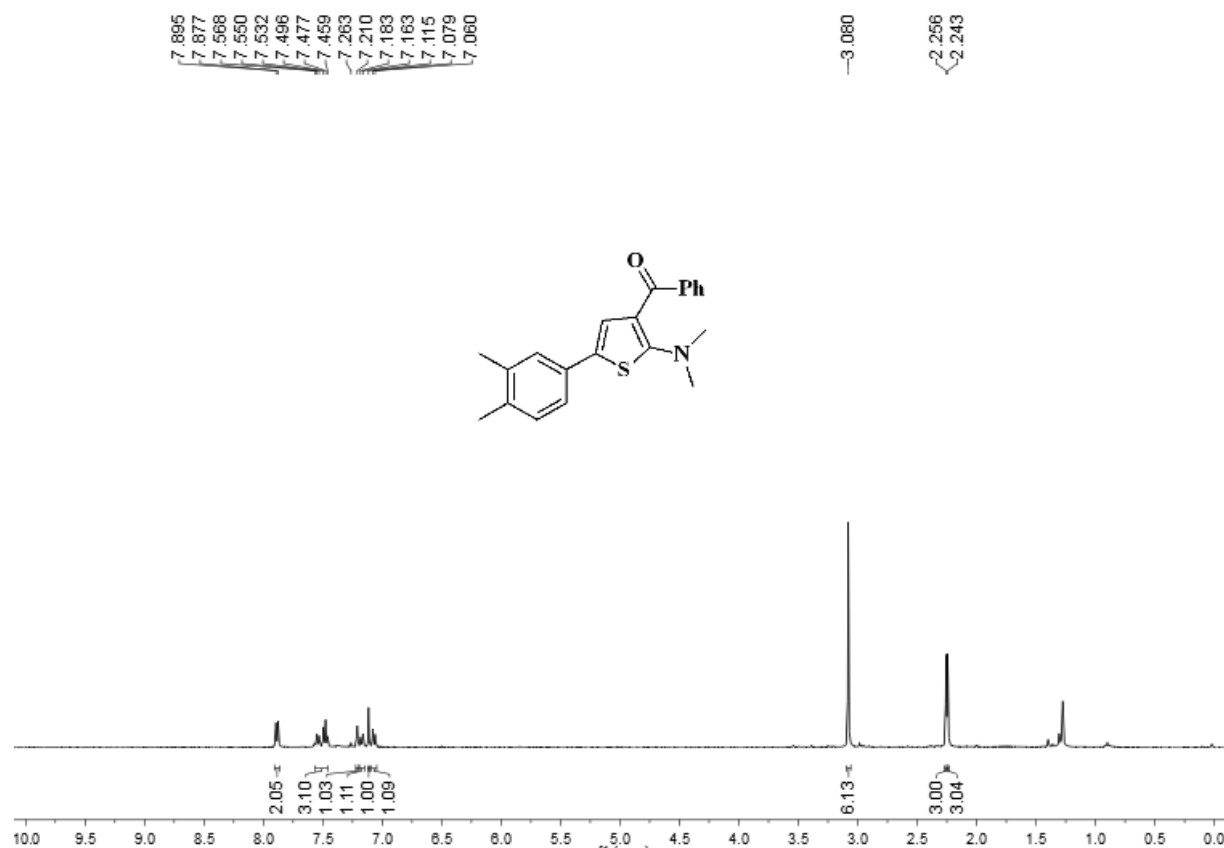
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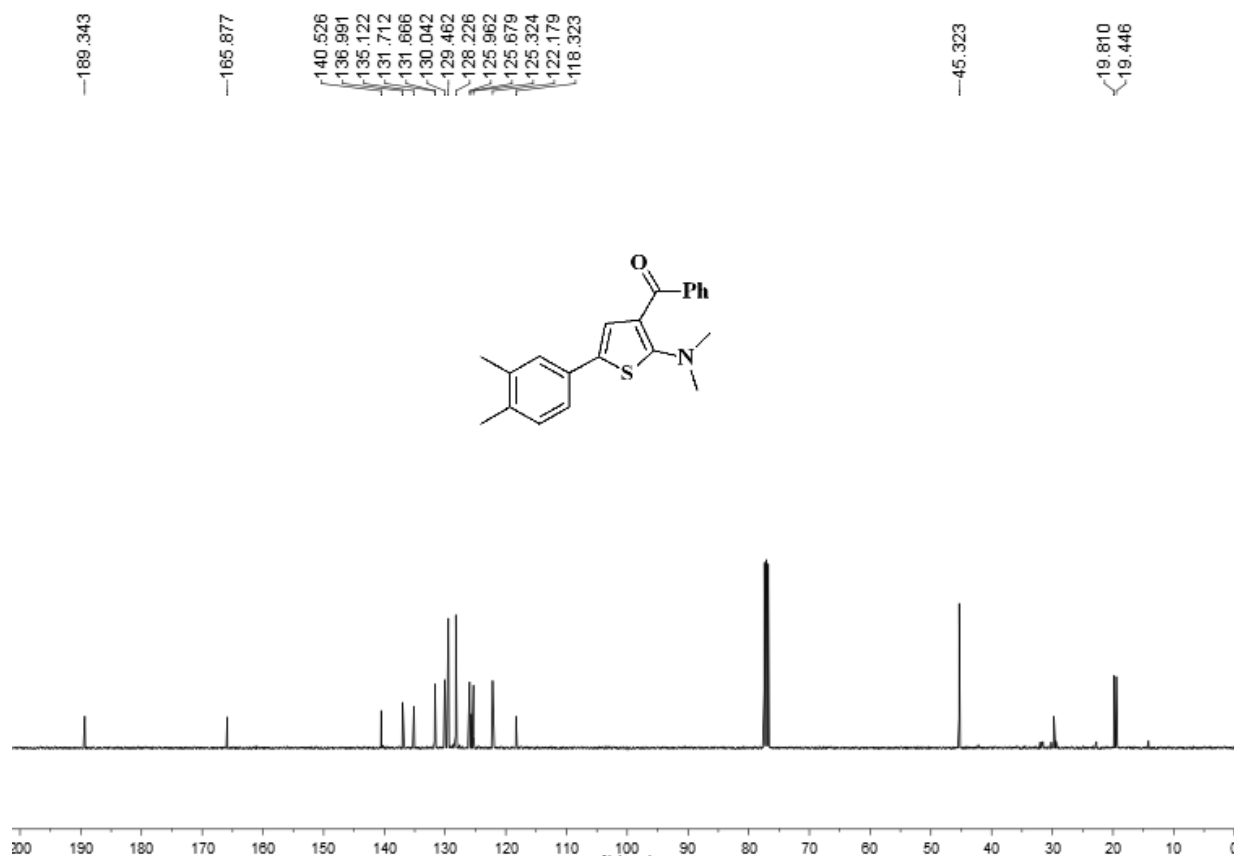
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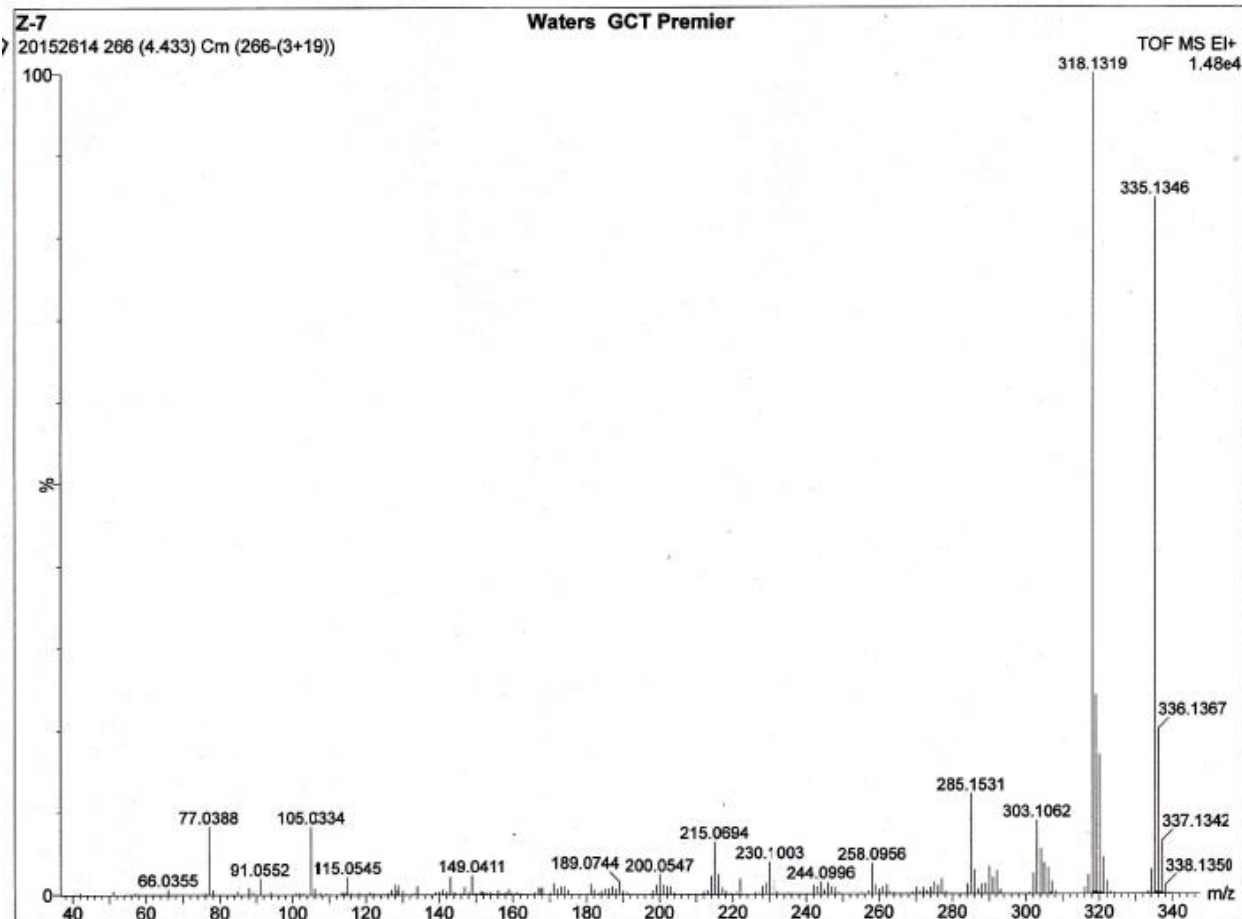
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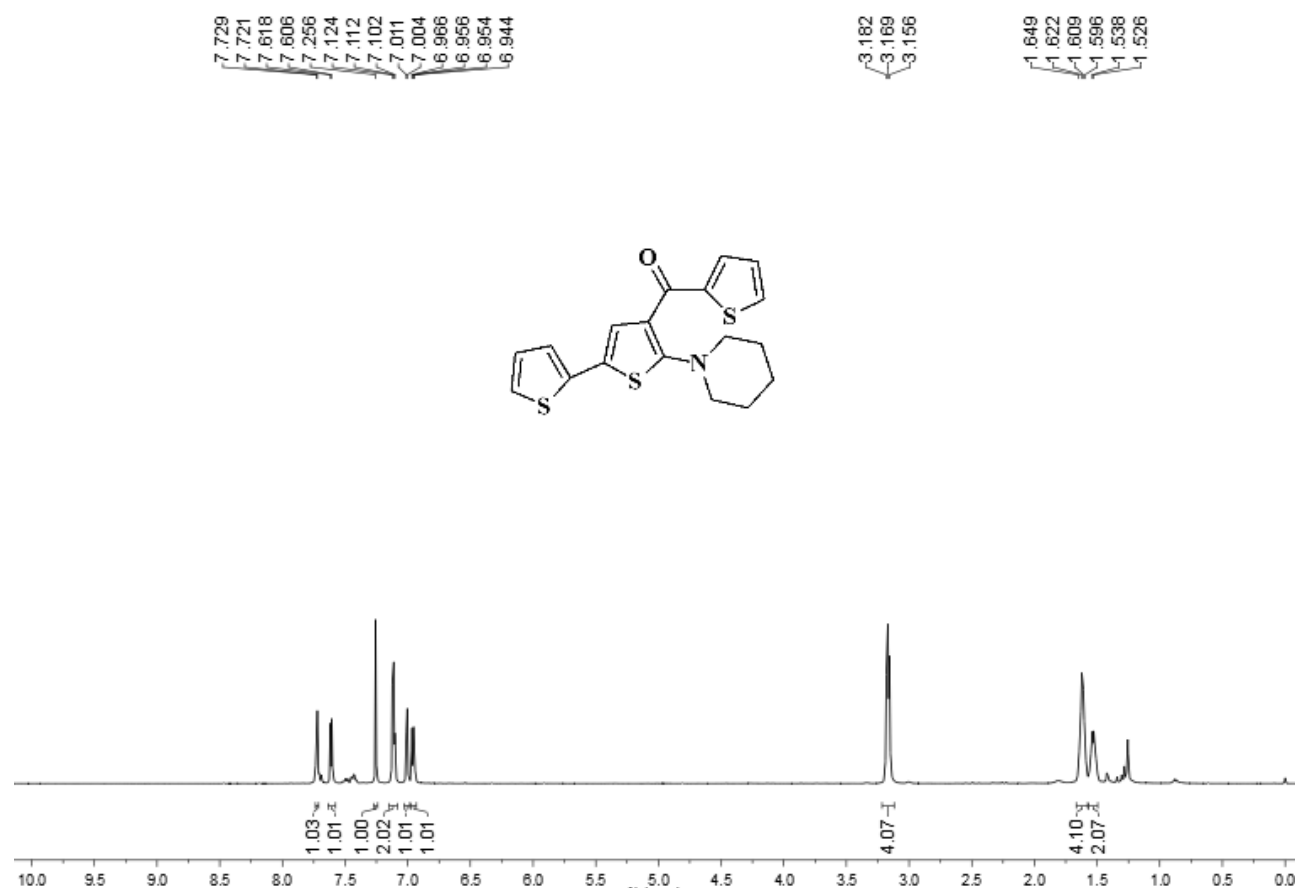
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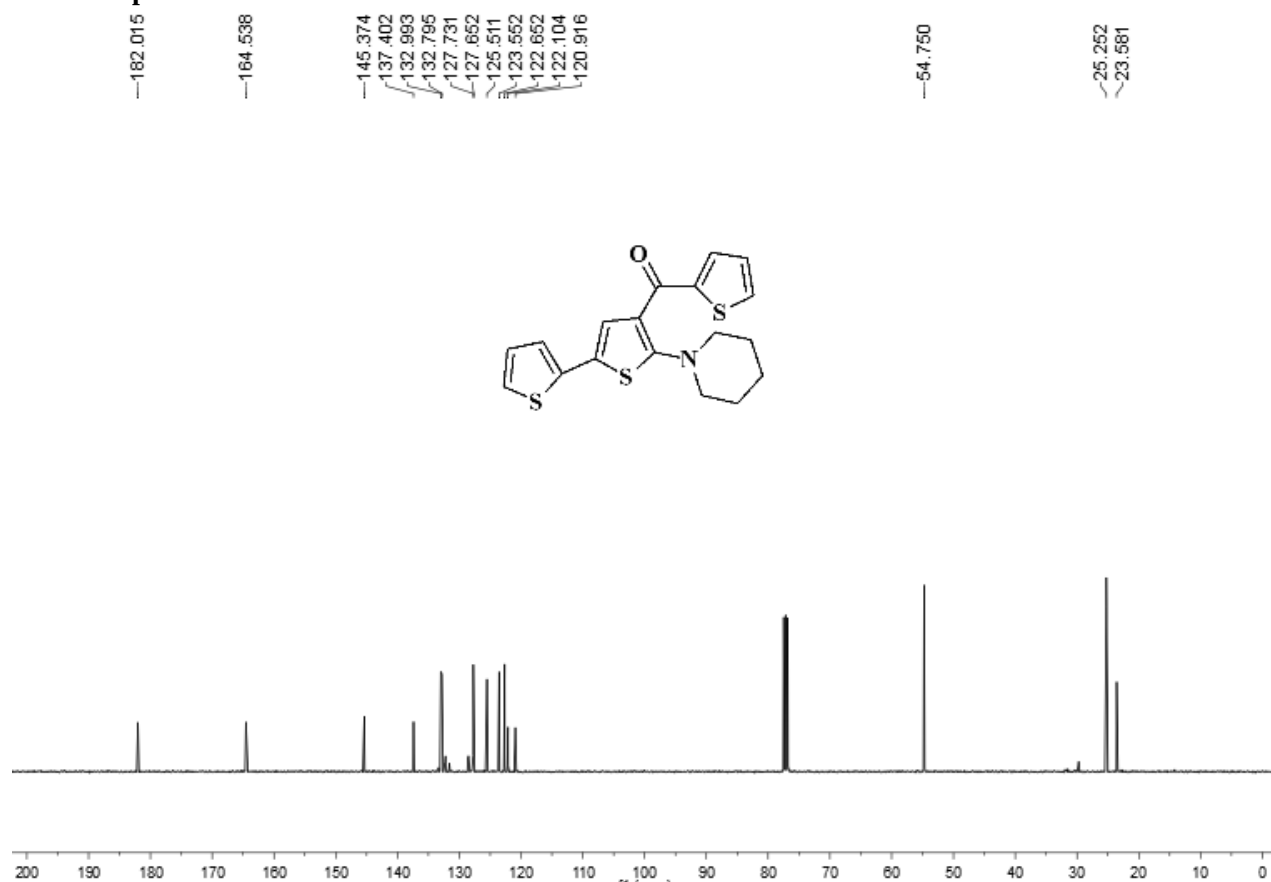
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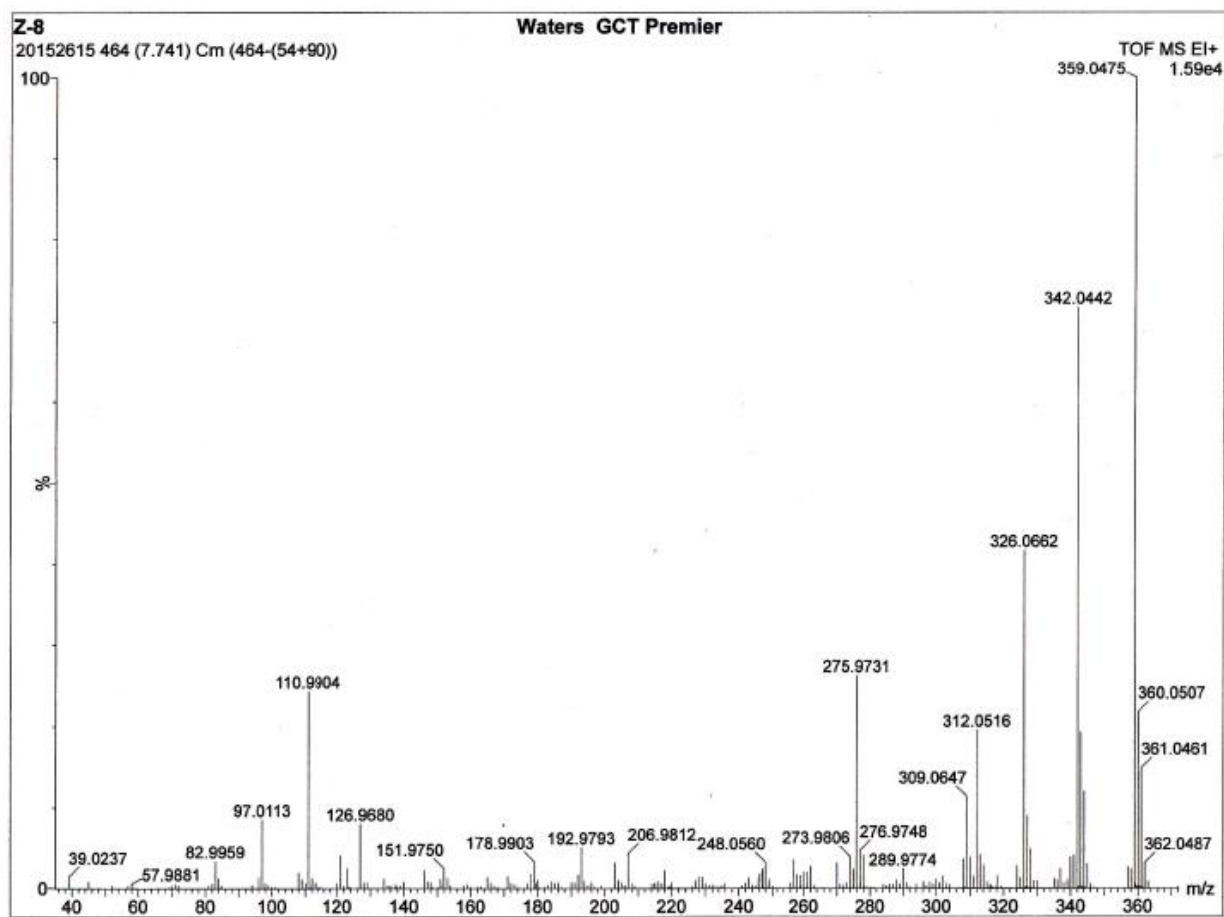
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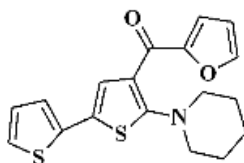
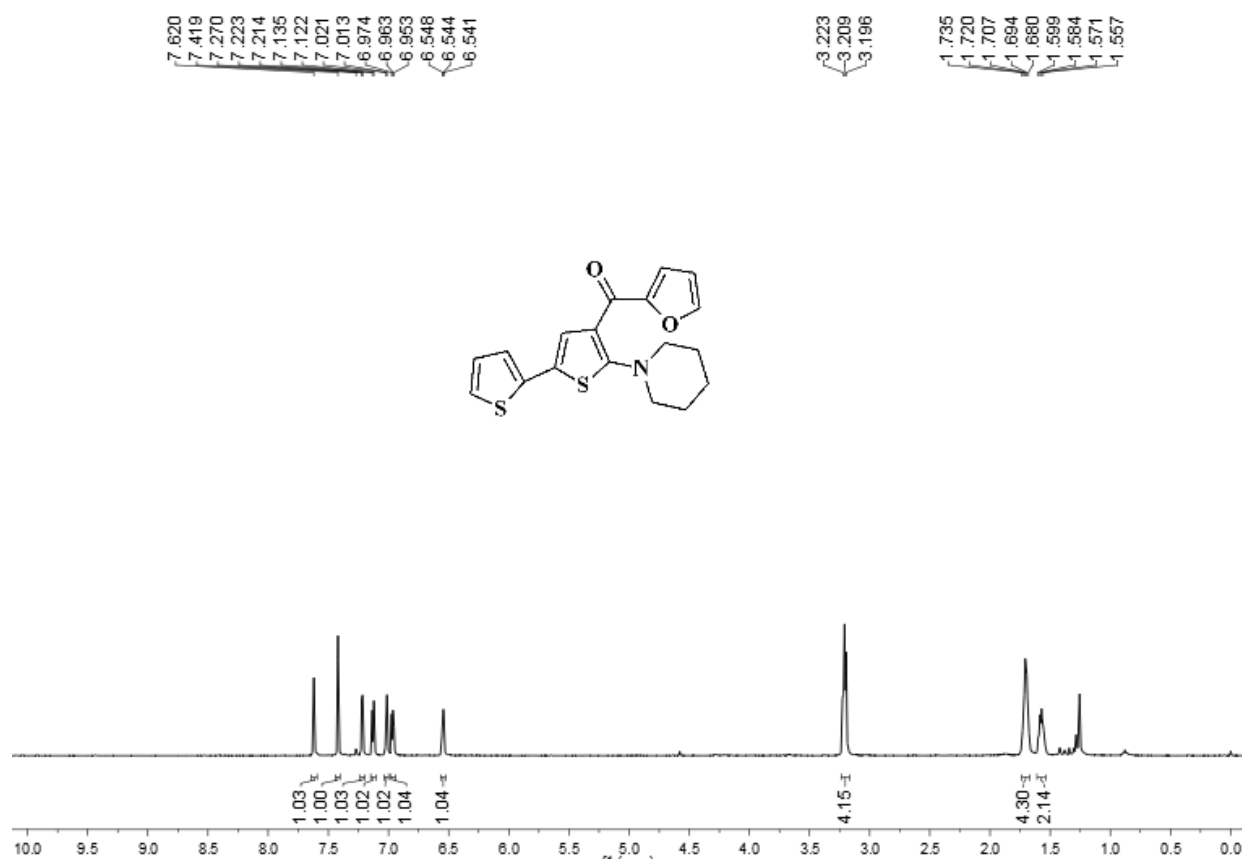
¹³C NMR spectrum of 3ld



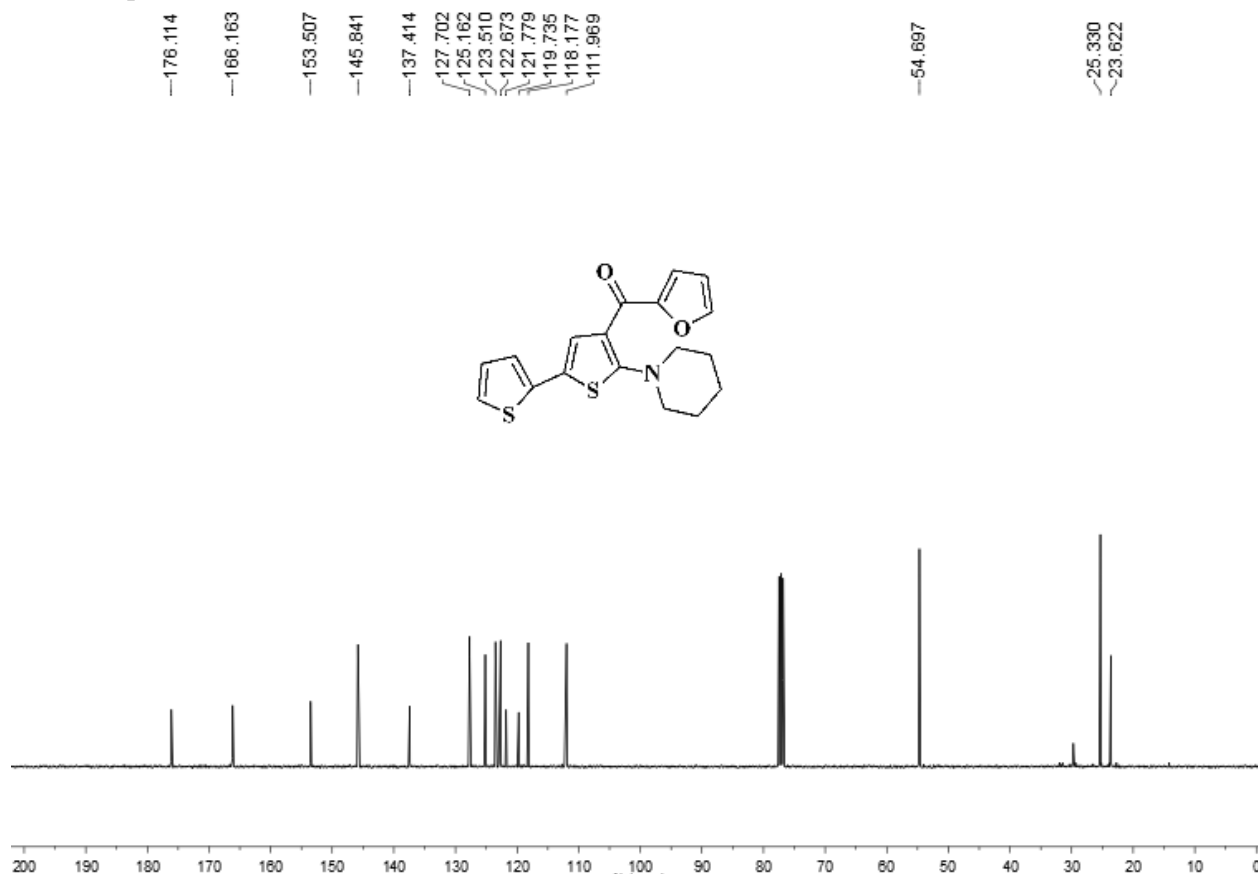
HRMS (EI) of 3ld



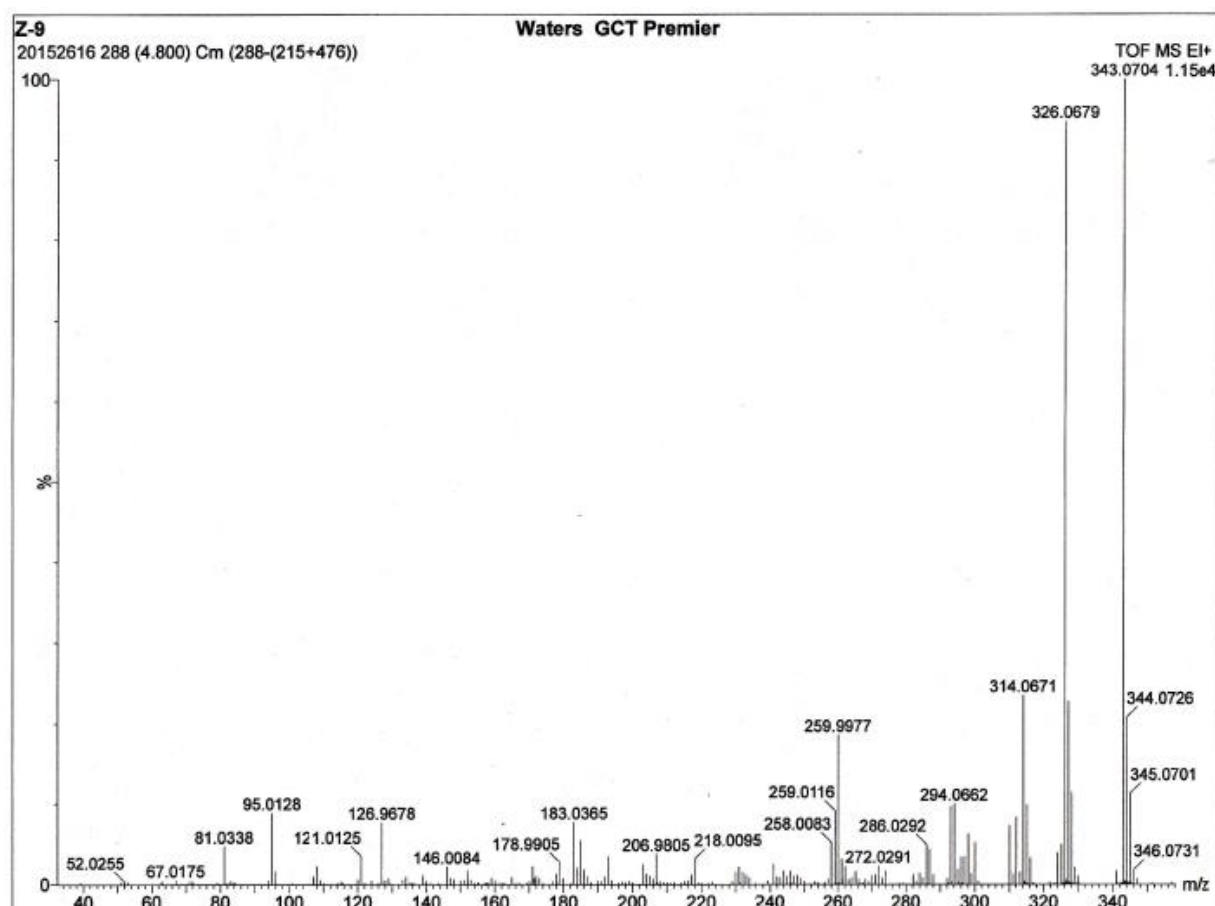
¹H NMR spectrum of 3le



¹³C NMR spectrum of 3le



HRMS (EI) of 3le



2. X-ray crystal structure of compound 3fa

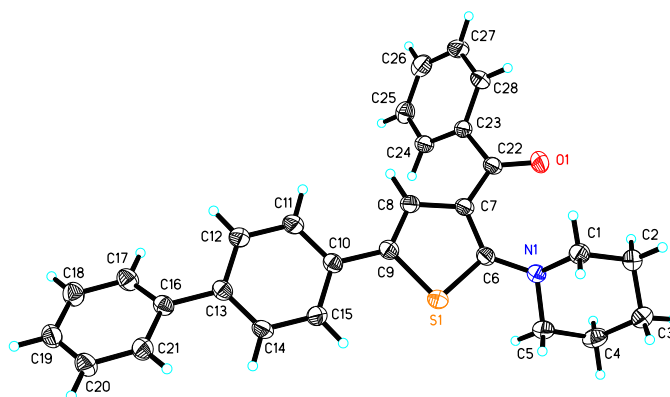


Figure S1. X-ray crystal structure of **3fa**.

Single crystals of **3fa** (yellowish prisms) suitable for diffraction study were obtained by slow diffusion of hexane into a dichloromethane solution of compound **3fa**. X-ray crystallographic data for compound **3fa** (CCDC 1434922) has been deposited in the Cambridge Crystallographic Data Center. The data can be obtained free of charge via http://www.ccdc.ac.uk/data_request/cif. The X-ray crystallography data of **3fa** are listed below.

Empirical formula	C ₂₈ H ₂₅ NOS	
Formula weight	423.55	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 6.9949(9) Å	α = 90 °
	b = 10.2229(14) Å	β = 95.443(3) °
	c = 15.438(2) Å	γ = 90 °
Volume	1099.0(3) Å ³	
Z	2	
Density (calculated)	1.280 Mg/m ³	
Absorption coefficient	0.168 mm ⁻¹	
F(000)	448	
Crystal size	0.25 x 0.22 x 0.1 mm ³	
Theta range for data collection	1.325 to 28.080 °	
Index ranges	-8 ≤ h ≤ 9, -13 ≤ k ≤ 12, -20 ≤ l ≤ 20	
Reflections collected	9424	
Independent reflections	4639 [R(int) = 0.0234]	
Completeness to theta = 25.242 °	100.0 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6383
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4639 / 1 / 280
Goodness-of-fit on F^2	1.023
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0367$, $wR_2 = 0.0801$
R indices (all data)	$R_1 = 0.0499$, $wR_2 = 0.0862$
Absolute structure parameter	-0.02(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.135 and -0.152 e.Å ⁻³