Supplementary Materials

Methoxyquinolone–Benzothiazole Hybrids as New Aggregation-Induced Emission Luminogens and Efficient Fluorescent Chemosensors for Cyanide Ions

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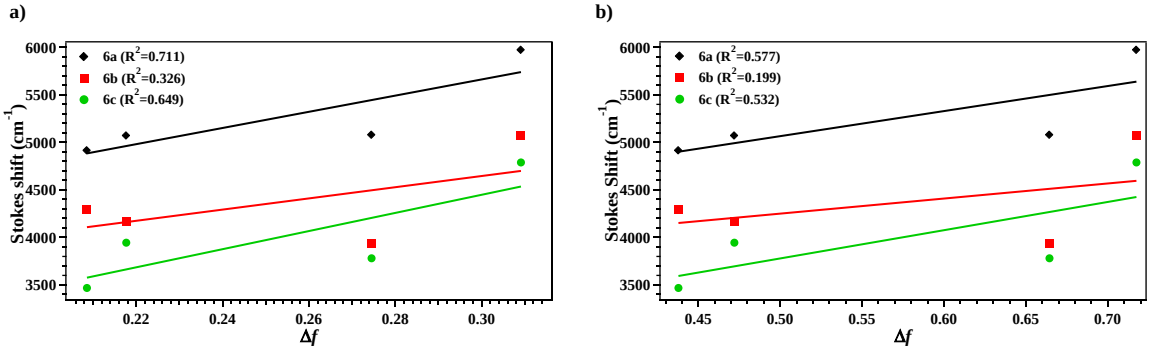


Figure S1. (**a**) Lippert-Mataga and (**b**) McRae plots of chromophores **6a–c**.

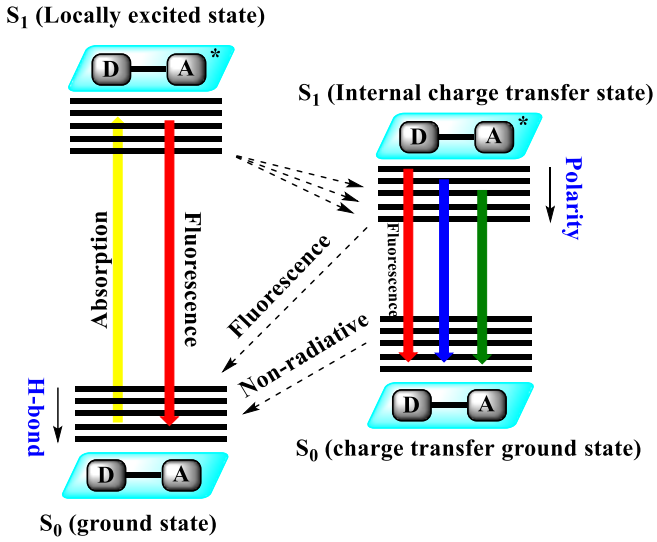


Figure S2. Jablonski diagrams of intermolecular charge transfer.

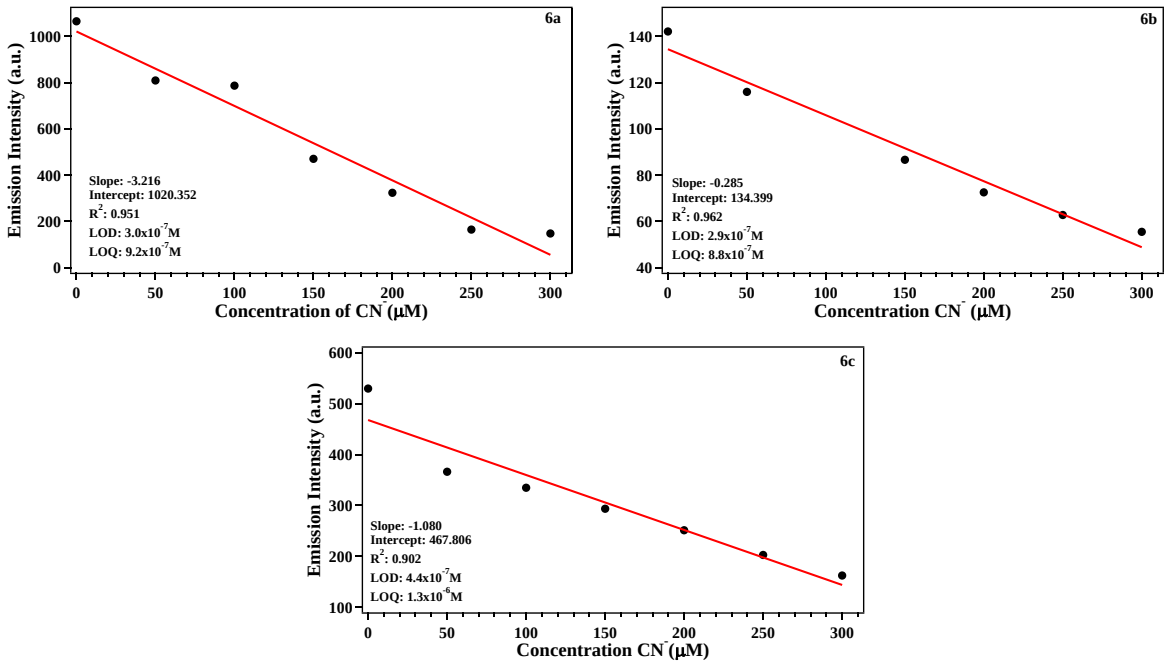
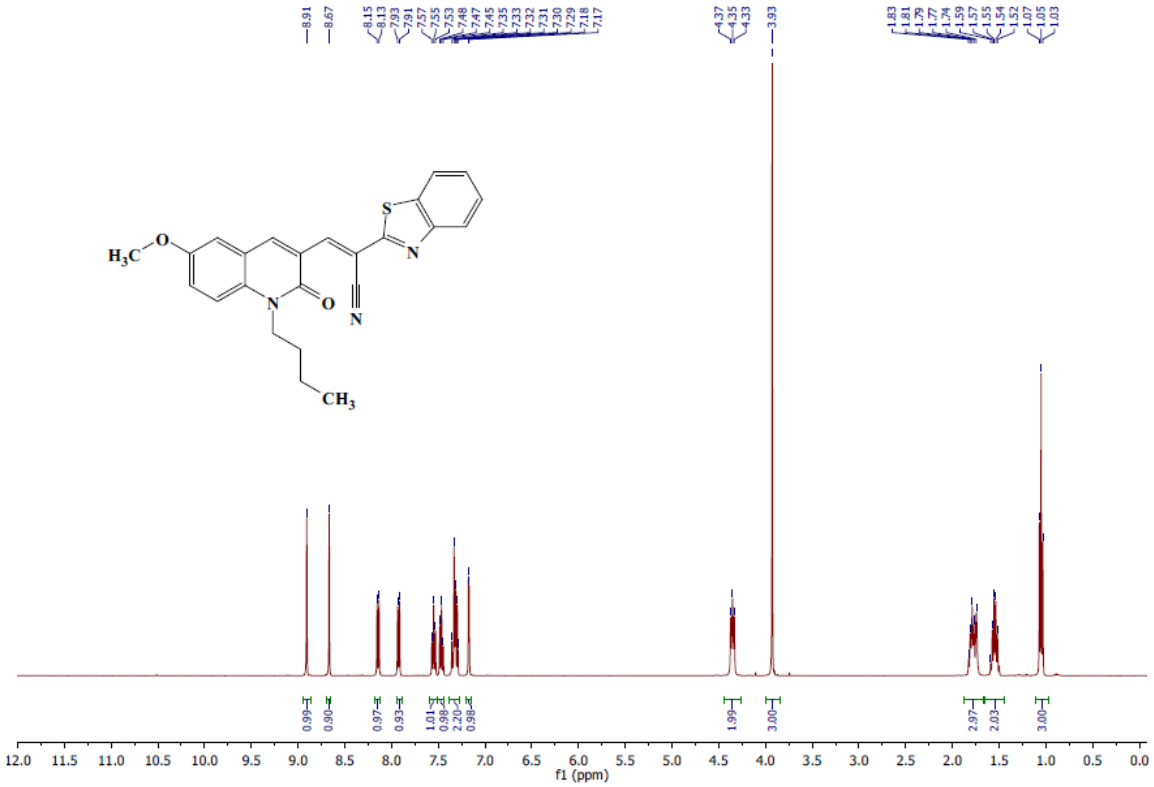


Figure S3. The calibration plot for determination of LOD and LOQ of **6a**, **6b,** and **6c**.



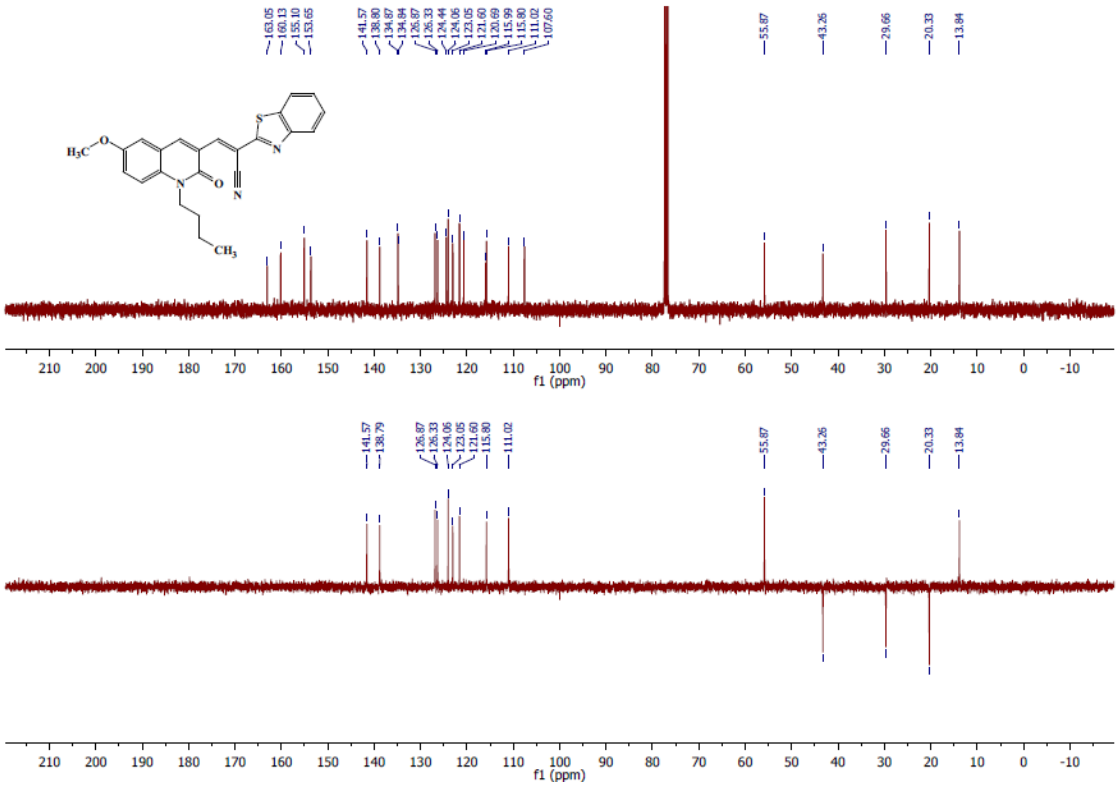
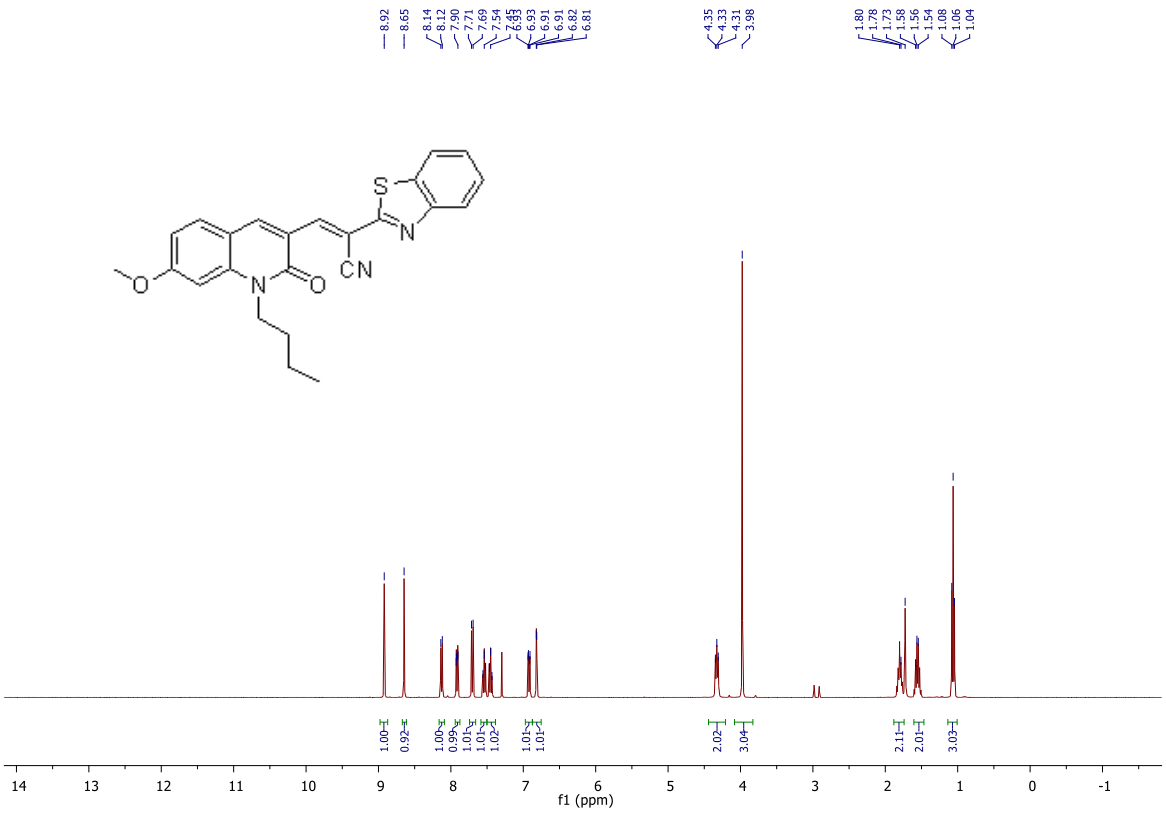


Figure S4. [1]H-NMR and [13]C-NMR Spectra of compound **6a.**



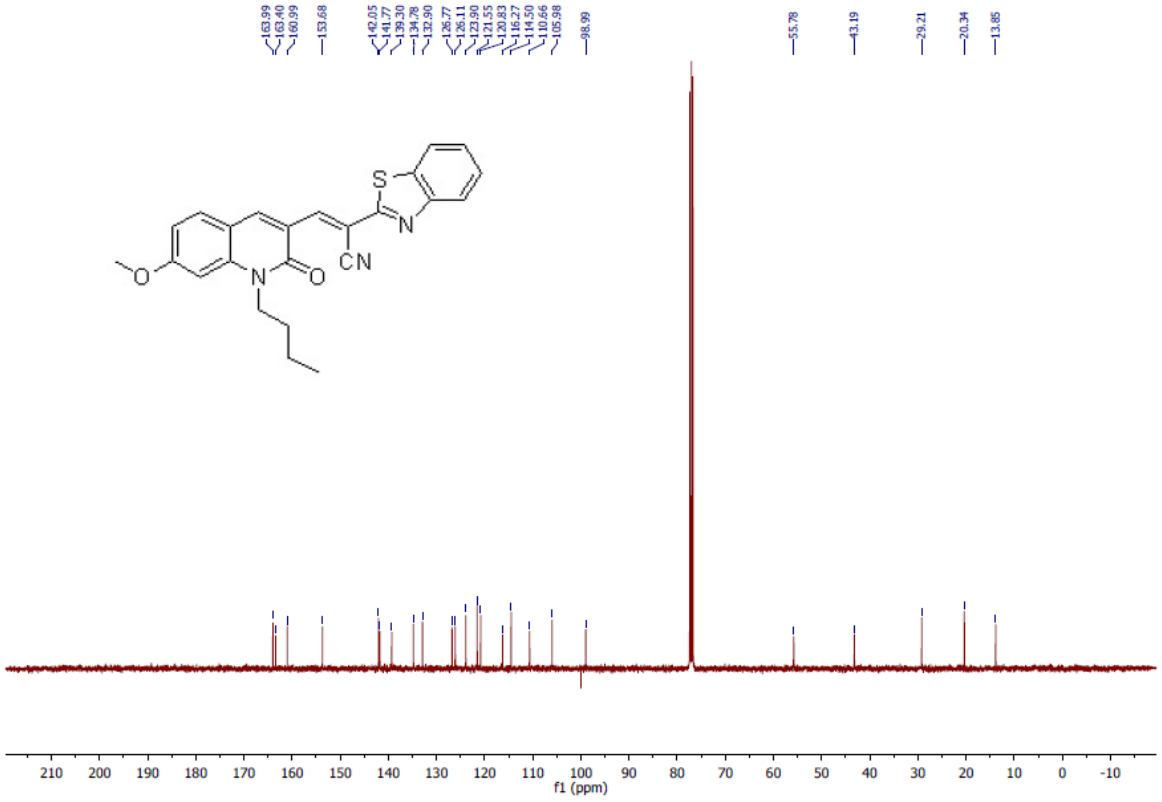
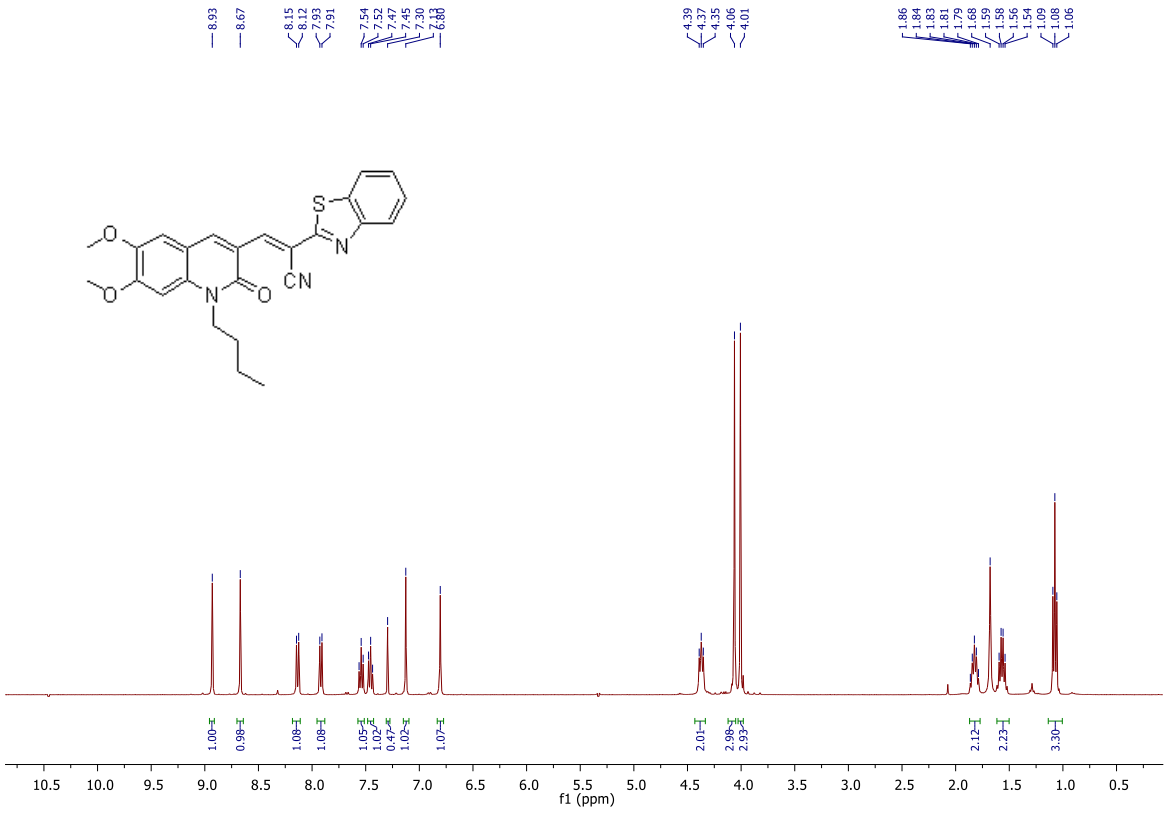


Figure S5. ^{1}H-NMR and ^{13}C-NMR Spectra of compound **6b.**



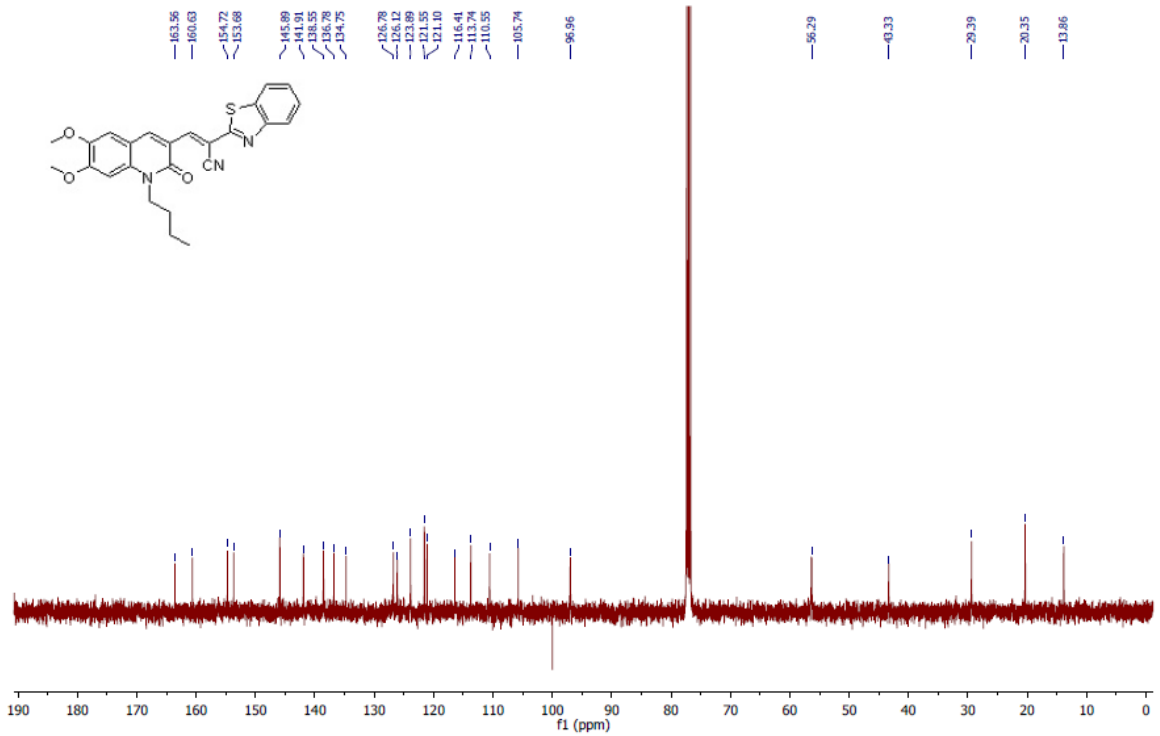
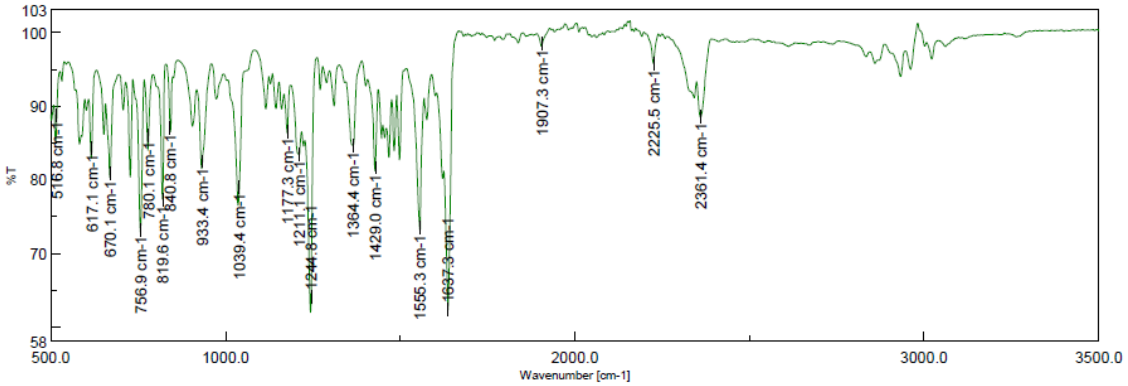


Figure S6. ^{1}H-NMR and ^{13}C-NMR Spectra of compound **6c.**



[Comments]
Sample name
Comment
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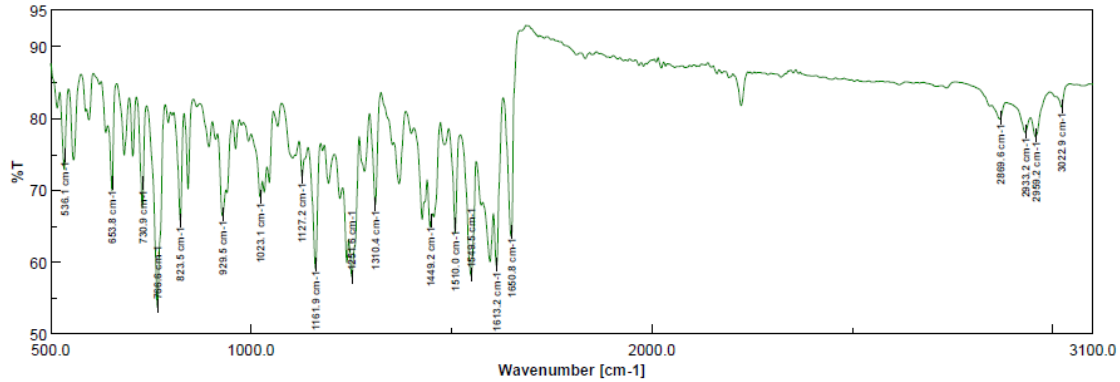
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Data points	3736

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Accessory S/N	C179361809
Incident angle	45 deg
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Detector	TGS
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Apodization	Cosine
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Scanning Speed	Auto (2 mm/sec)
Filter	Auto (30000 Hz)

Figure S7. FT-IR Spectra of compound **6a.**



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Sample name
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User
Division
Company Universidad Del Atlantico

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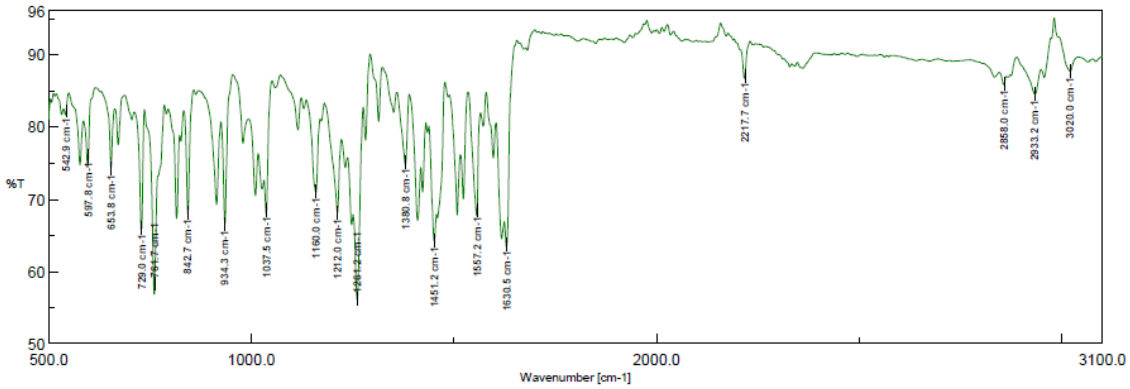
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Incident angle 45 deg

Measurement Date 23/04/2024 1:05 p. m.

Light Source Standard
Detector TGS
Accumulation 16
Resolution 4 cm-1
Zero Filling On
Apodization Cosine
Gain Auto (8)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (30000 Hz)

Figure S8. FT-IR Spectra of compound **6b.**



[Comments]
Sample name
Comment
User
Division
Company Universidad Del Atlantico

[Detailed Information]
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Data points 3736

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Serial Number F058861788

Accessory ATR PRO ONE
Accessory S/N C179361809
Incident angle 45 deg

Measurement Date 23/04/2024 11:57 a. m.

Light Source Standard
Detector TGS
Accumulation 16
Resolution 4 cm-1
Zero Filling On
Apodization Cosine
Gain Auto (8)
Aperture Auto (7.1 mm)
Scanning Speed Auto (2 mm/sec)
Filter Auto (30000 Hz)

Figure S9. FT-IR Spectra of compound **6c.**

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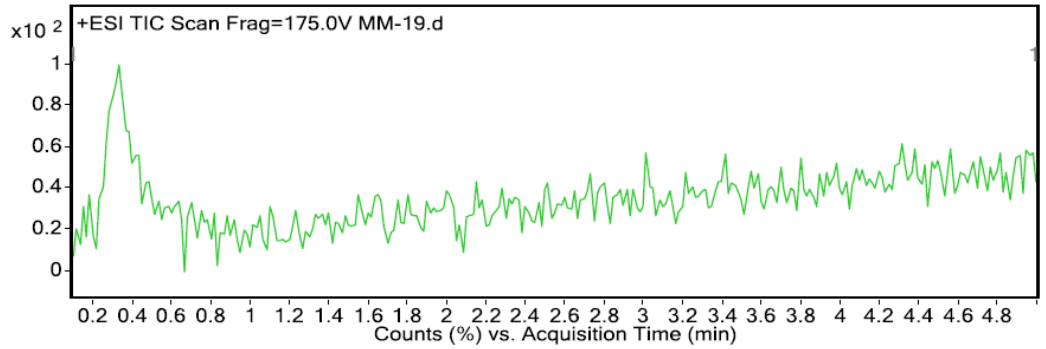
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Sample Group **Info.**

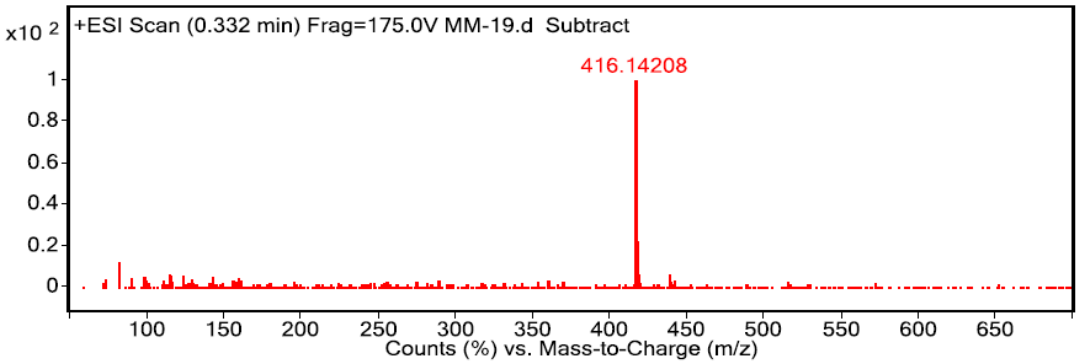
User Chromatograms

Fragmentor Voltage 175 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage 175 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund	Abund %
81.93788		3728.8	12.27
97.96818		1722.5	5.67
113.96391		1952.8	6.43
114.98515		1737.8	5.72
122.96392		1848.4	6.08
141.95778		1684.5	5.54
416.14208	1	30380.9	100
416.25461		1847.6	6.08

Figure S10. HRMS of compound 6a.

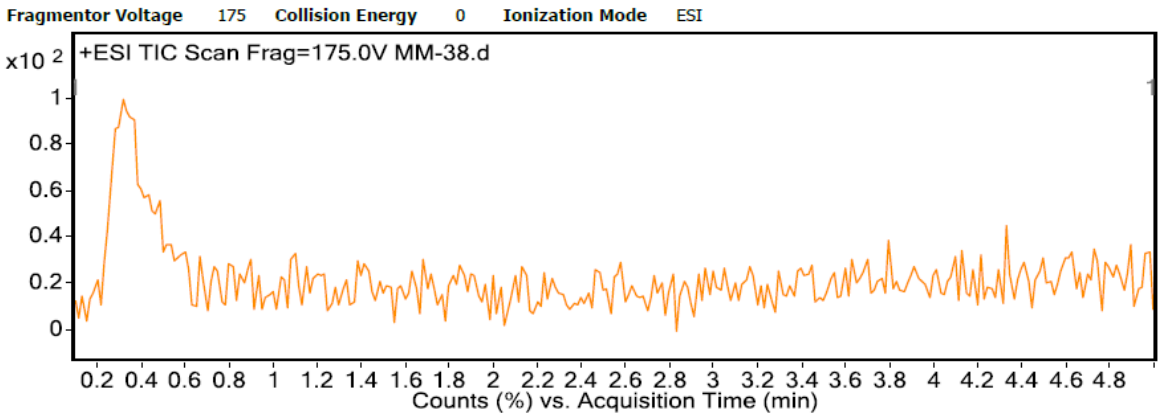
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Reporte de Análisis Cualita

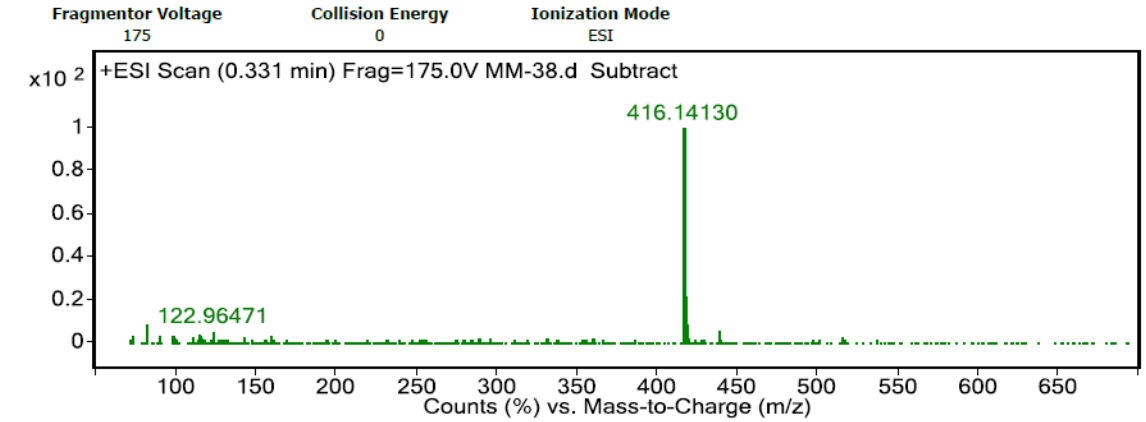
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Comentario			

Sample Group **Info.**

User Chromatograms



User Spectra



Peak List

m/z	z	Abund	Abund %
81.9379		3702.9	8.46
122.96471		2464.6	5.63
416.1413	1	43755.8	100
416.27933		2281.1	5.21
417.14569	1	9409.3	21.5
418.14222	1	3714.7	8.49
438.12681		2578.4	5.89

Figure S11. HRMS of compound **6b.**

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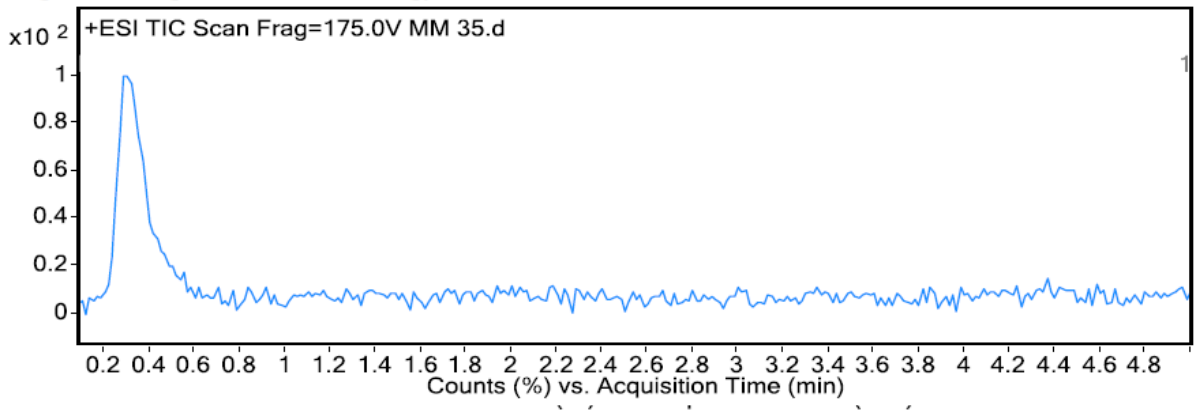
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Comentario			

Sample Group **Info.**

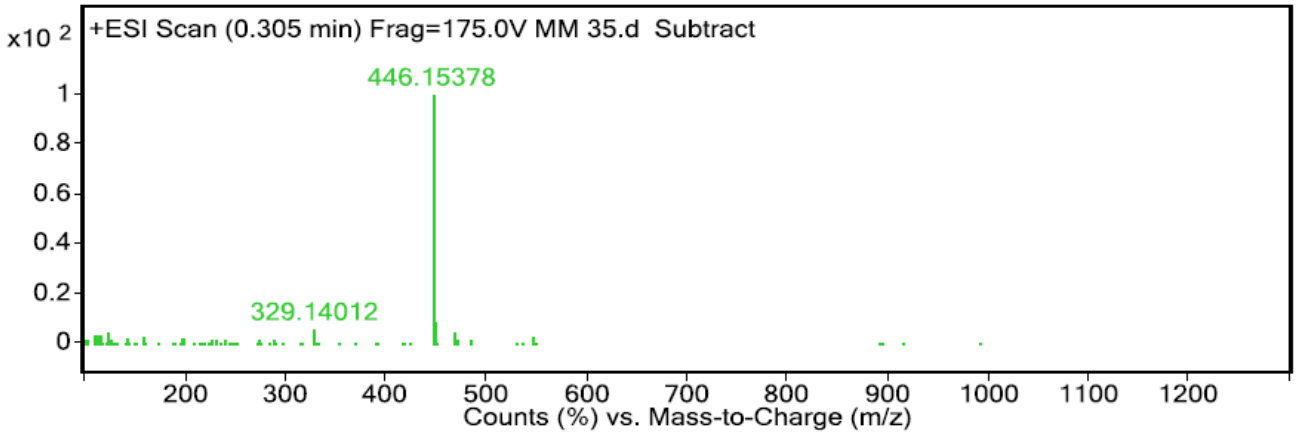
User Chromatograms

Fragmentor Voltage 175 **Collision Energy** 0 **Ionization Mode** ESI



User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
175	0	ESI



Peak List

m/z	z	Abund	Abund %
81.93819		6827.2	10.33
329.14012		3829.2	5.79
446.15378	1	66085.7	100
447.156	1	18502.9	28
448.15603	1	5832.3	8.83

Figure S12. HRMS of compound **6c.**

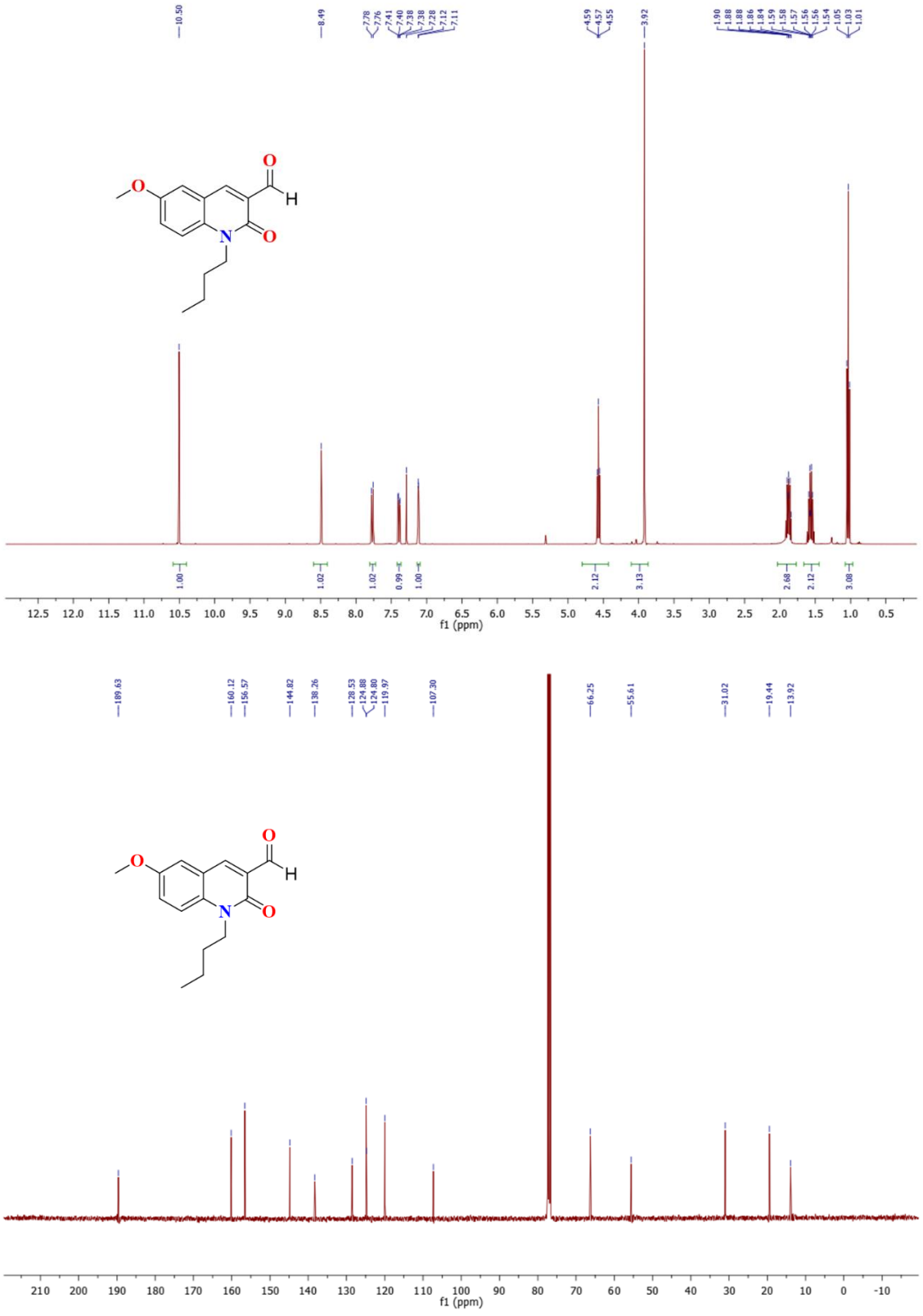


Figure S13. ^{1}H-NMR and ^{13}C-NMR Spectra of compound **4a.**

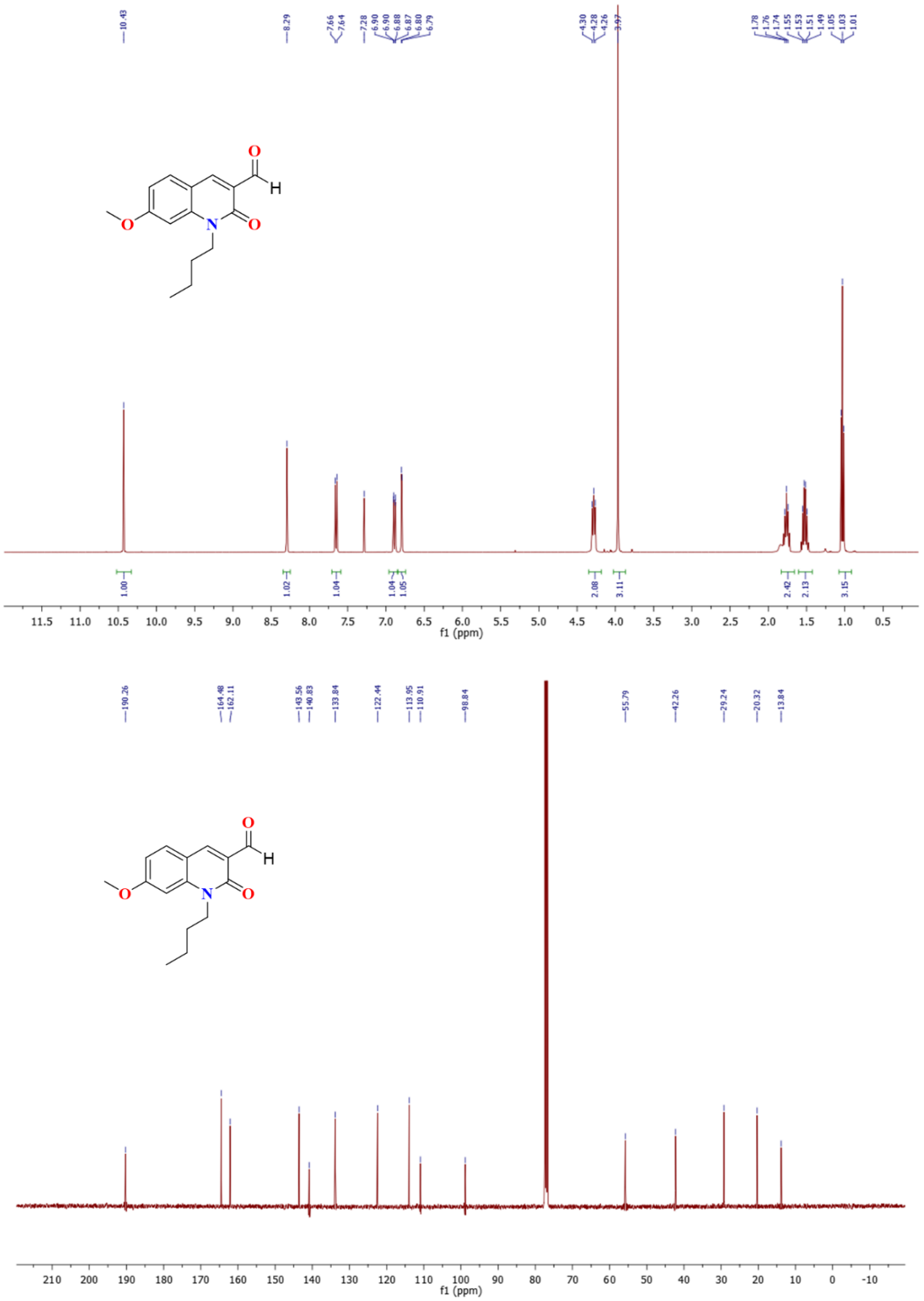


Figure S14. ^{1}H-NMR and ^{13}C-NMR Spectra of compound **4b.**

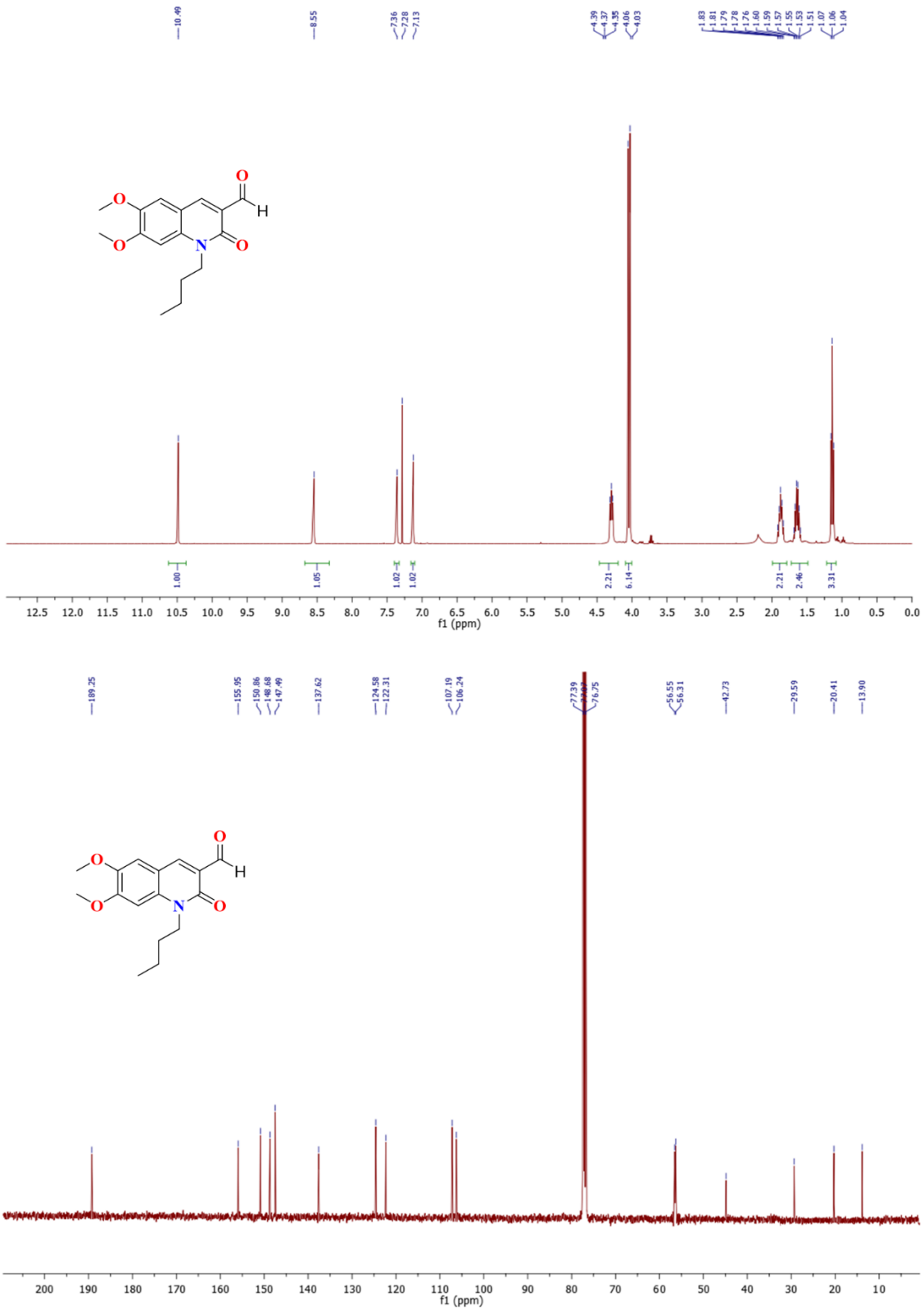


Figure S15. ^{1}H-NMR and ^{13}C-NMR Spectra of compound **4c.**

Table S1. Crystal data and structure refinement for **6c** compound.

Identification Code	
Empirical formula	$C_{25}H_{23}N_3O_3S$
Formula weight	445.52
Temperature/K	298
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	9.8965(4)
b/Å	17.8620(9)
c/Å	12.6989(5)
α (°)	90
β (°)	96.575(4)
γ (°)	90
Volume/ Å^3	2230.04(17)
Z	4
ϱ_{calc} mg/mm3	1.327
μ/mm^{-1}	1.554
F(000)	936
2θ range for data collection/°	4.3 to 76.2
Reflections collected	11605
Independent reflections	4620
Data / restraints / parameters	4620/0/292
Goodness-of-fit on F^2	1.05
Completeness (%)	99
Final R indices [I>2sigma(I)]	R1 = 0.0531, wR2 = 0.1652
Largest diff. Peak/hole/ e.Å^{-3}	-0.32 and 0.33