Supporting Information

Heteroaryl chalcone allied triazole conjugated organosilatranes: Synthesis, Spectral Analysis, Antimicrobial Screening, Photophysical and Theoretical Investigations

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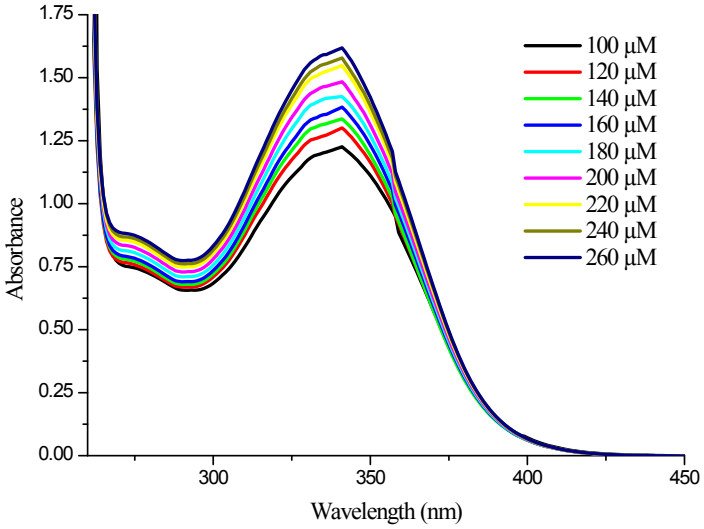
Synthesis of 3-Azidopropyltriethoxysilane (AzPTES)

To the stirred solution of sodium azide (5.4 g, 83.1 mmol) in dry DMF (150 ml), (5.0 g, 20.7 mmol) of 3-chloropropyltriethoxysilane was added dropwise within 10 min. The reaction mixture was stirred at 90 ˚C for 4 h. The removal of DMF was carried out under reduced pressure. The crude mixture was then diluted with diethylether and filtered under inert atmosphere. The diethyl ether was removed in vacuo and the crude oil obtained was distilled at 130 ˚C under reduced pressure of 5 mm of Hg resulting into AzPTES as colourless oil. Yield: 91 %; NMR (300 MHz, $CDCl_3$, 25 °C): δ_H = 0.57 (t, 2H, -Si*CH*$_2$-, *J* = 8.1 Hz), 1.15 (d, 9H, -OCH$_2$*CH*$_3$, *J* = 7.1 Hz), 1.63 (m, 2 H, -C*CH*$_2$C-), 3.18 (t, 2H, N$_3$*CH*$_2$CH$_2$, *J* = 6.9 Hz), 3.73 (q, 6H, -O*CH*$_2$CH$_3$, *J* = 7.0 Hz) ppm.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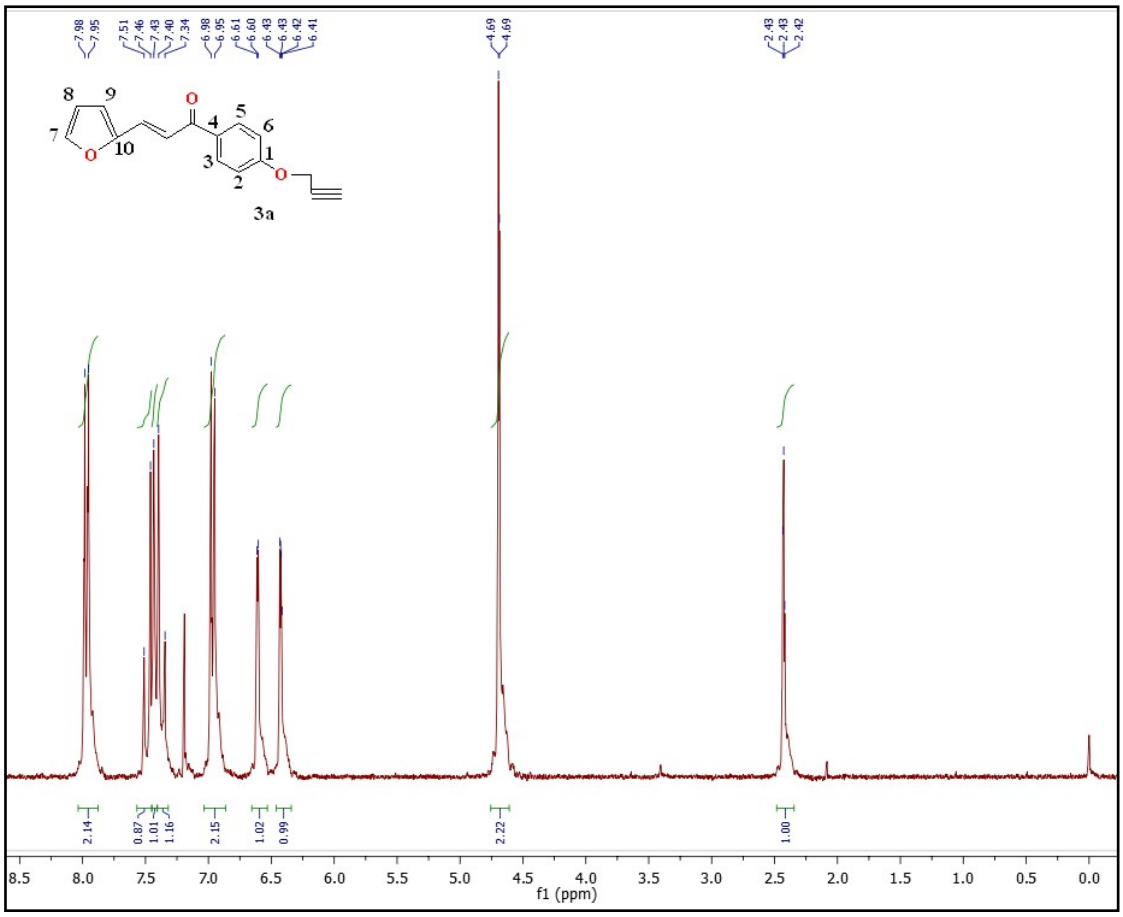
260 μM

Figure S1.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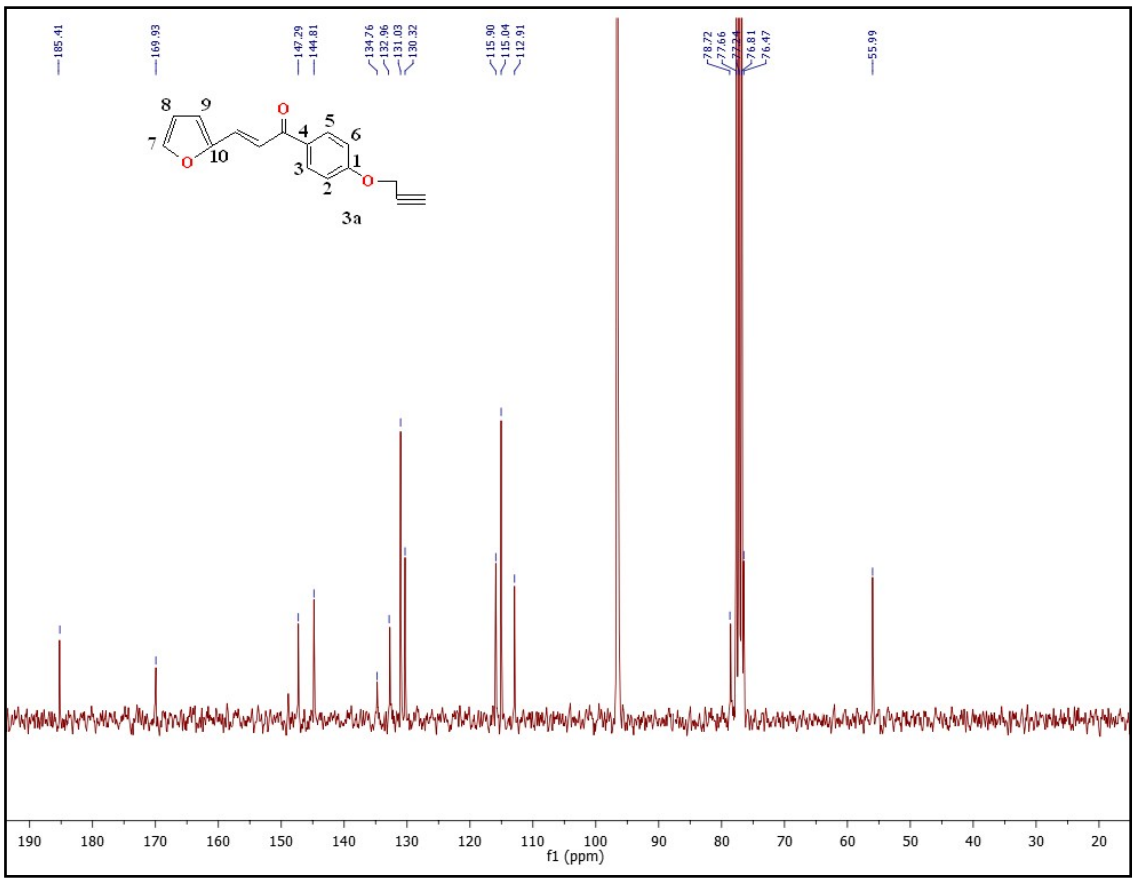
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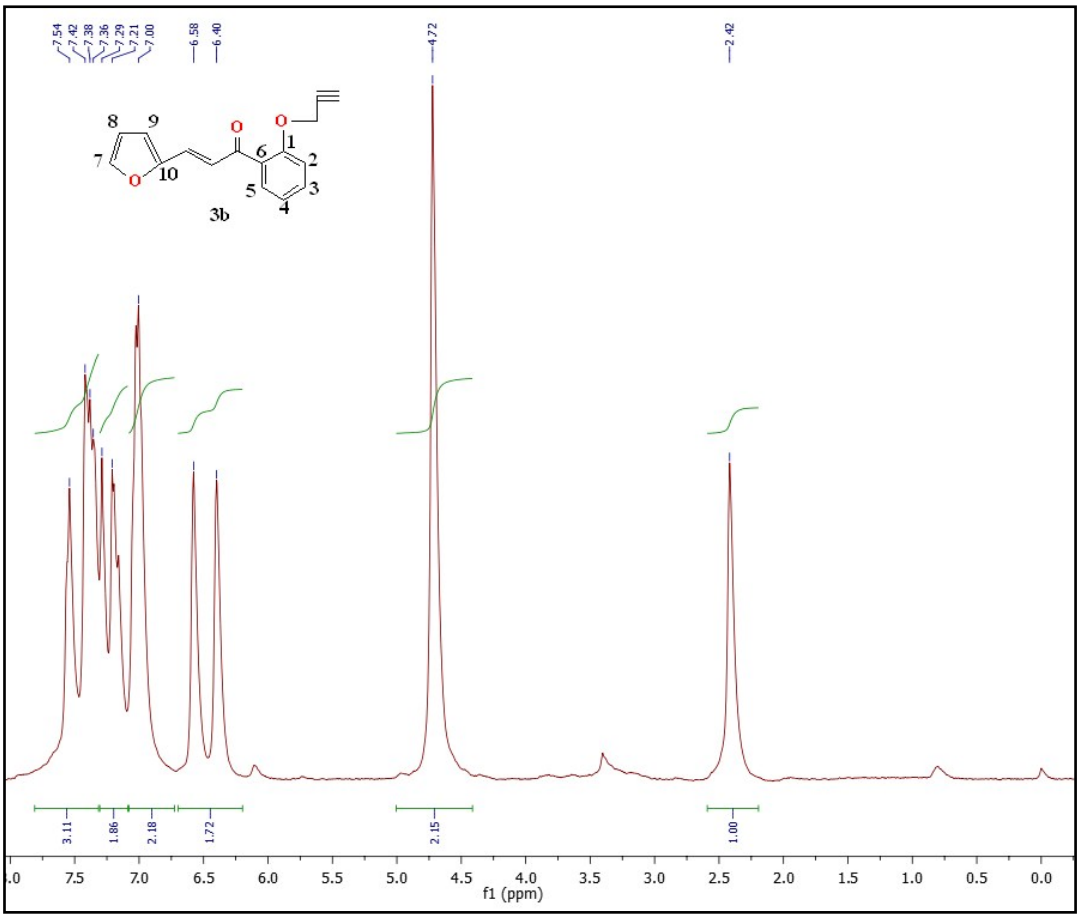
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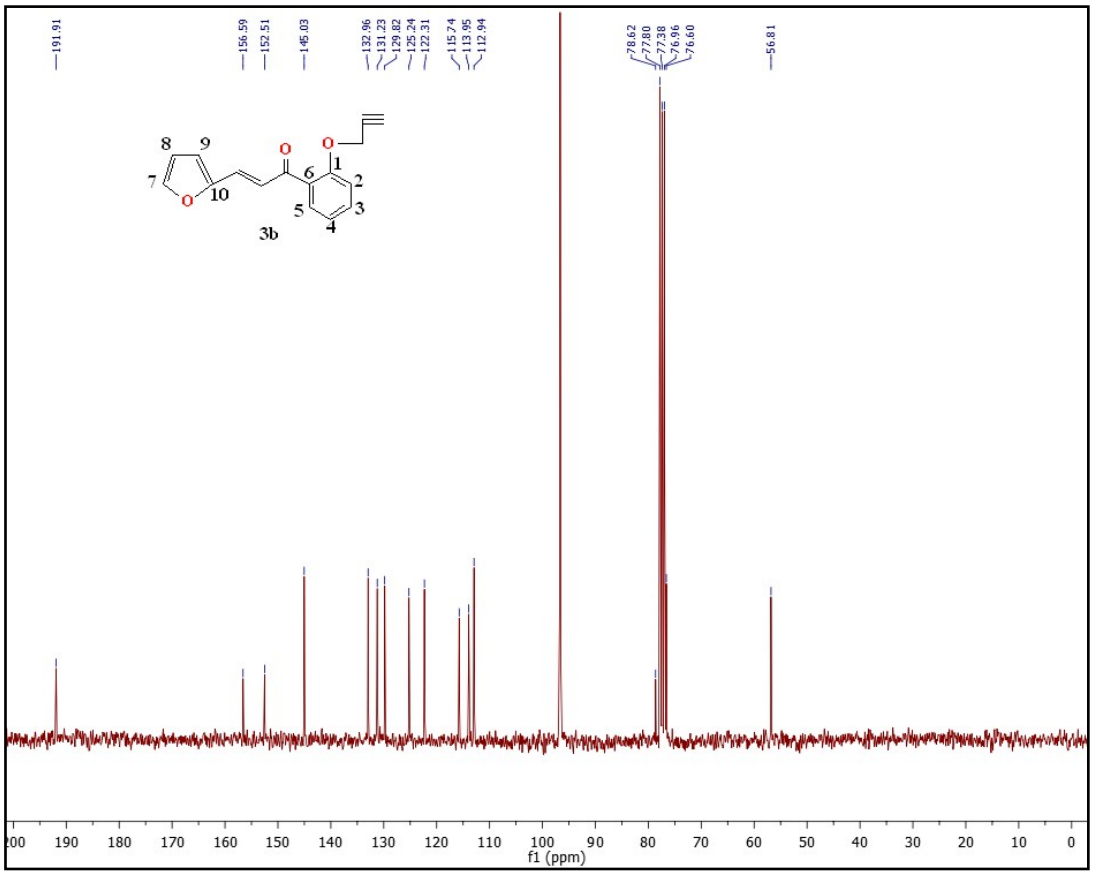
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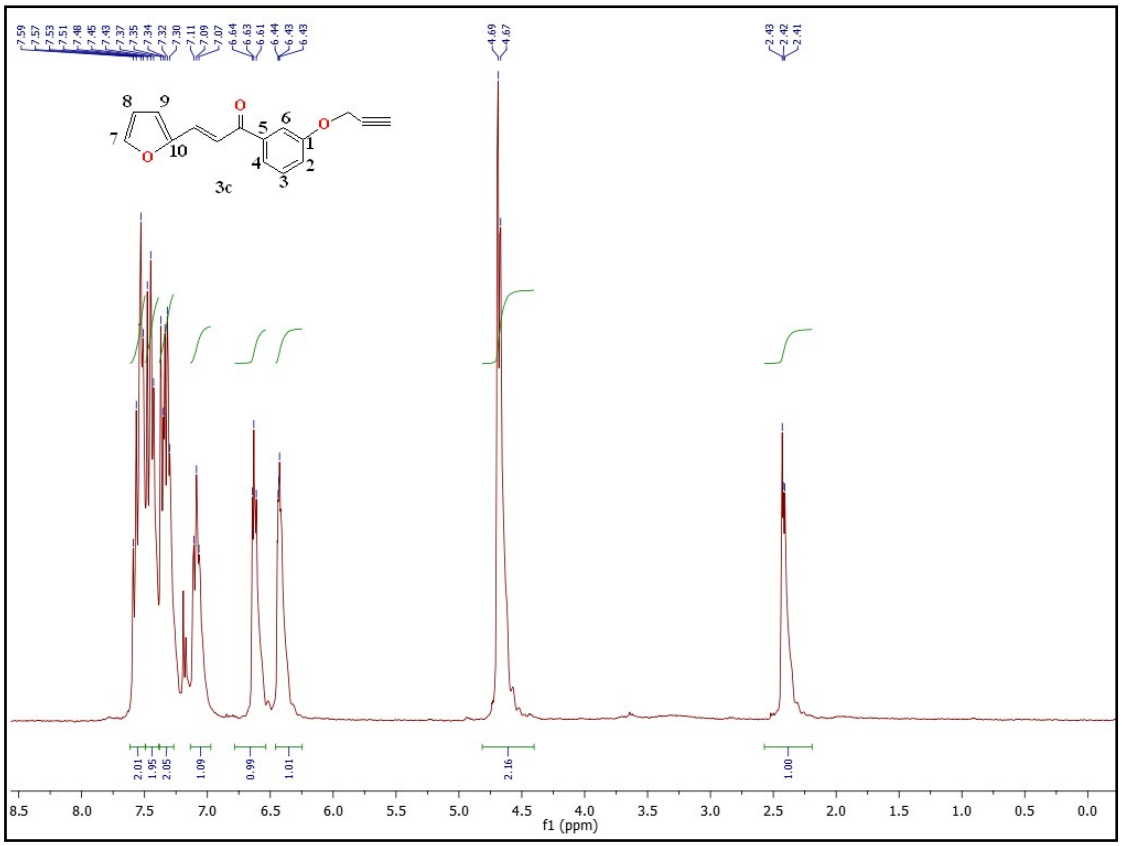
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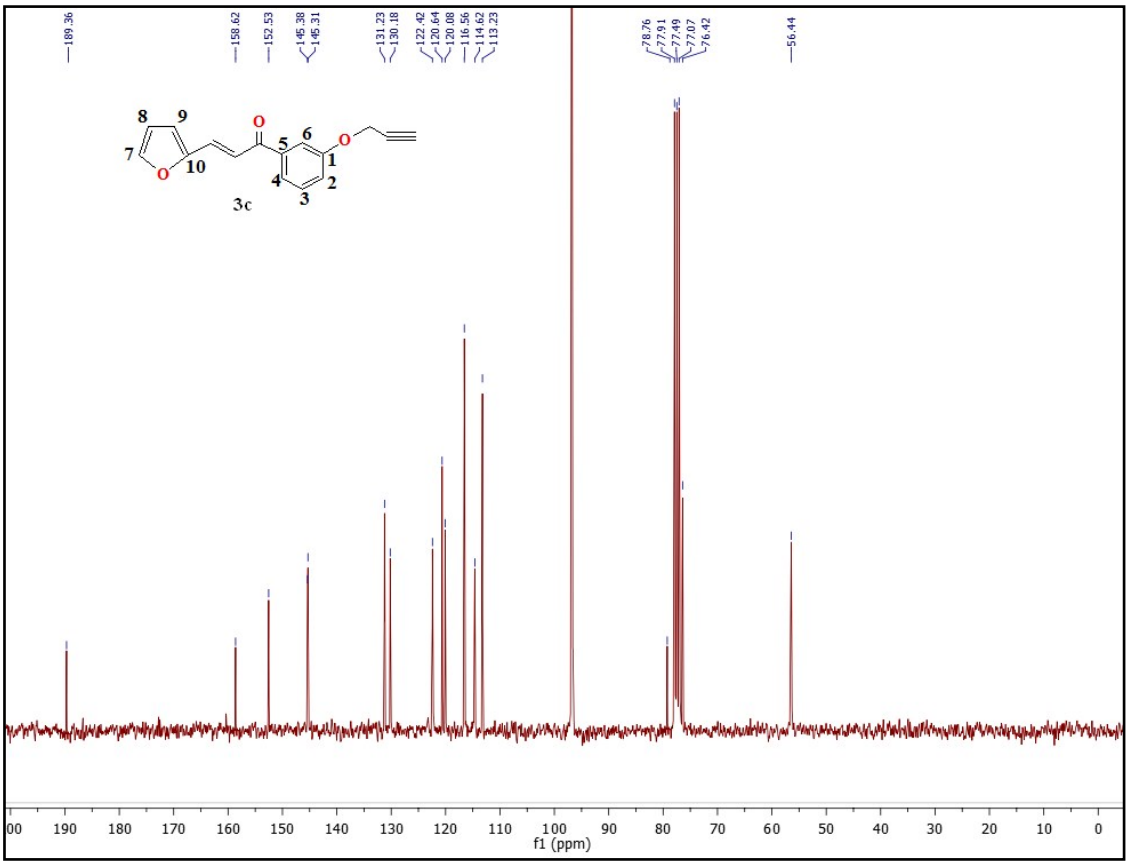
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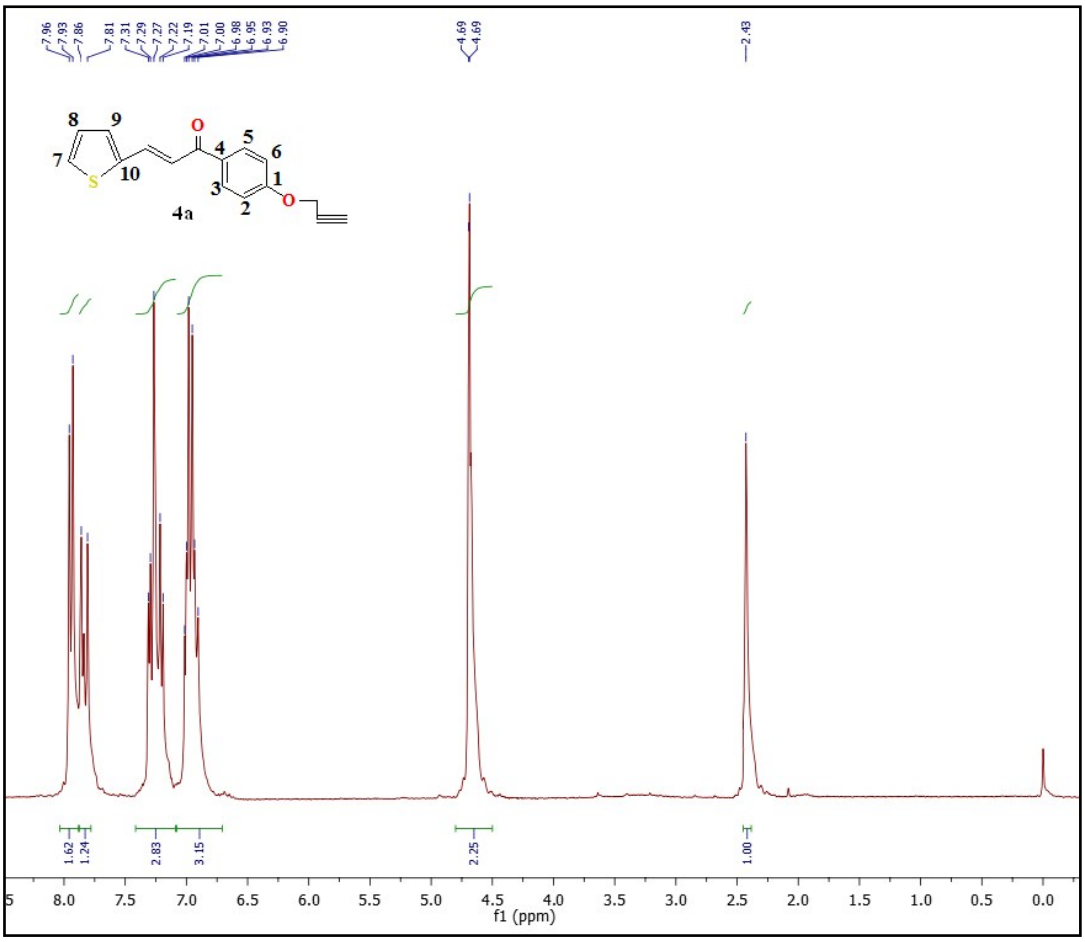
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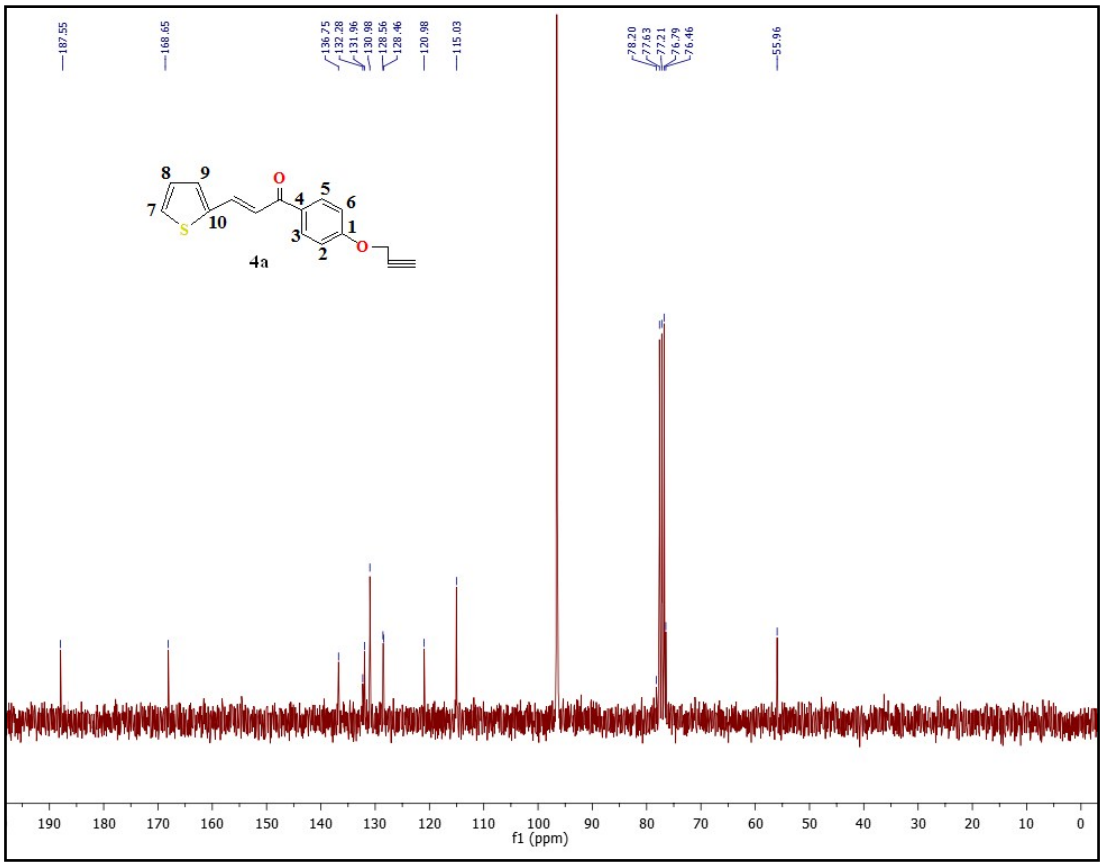
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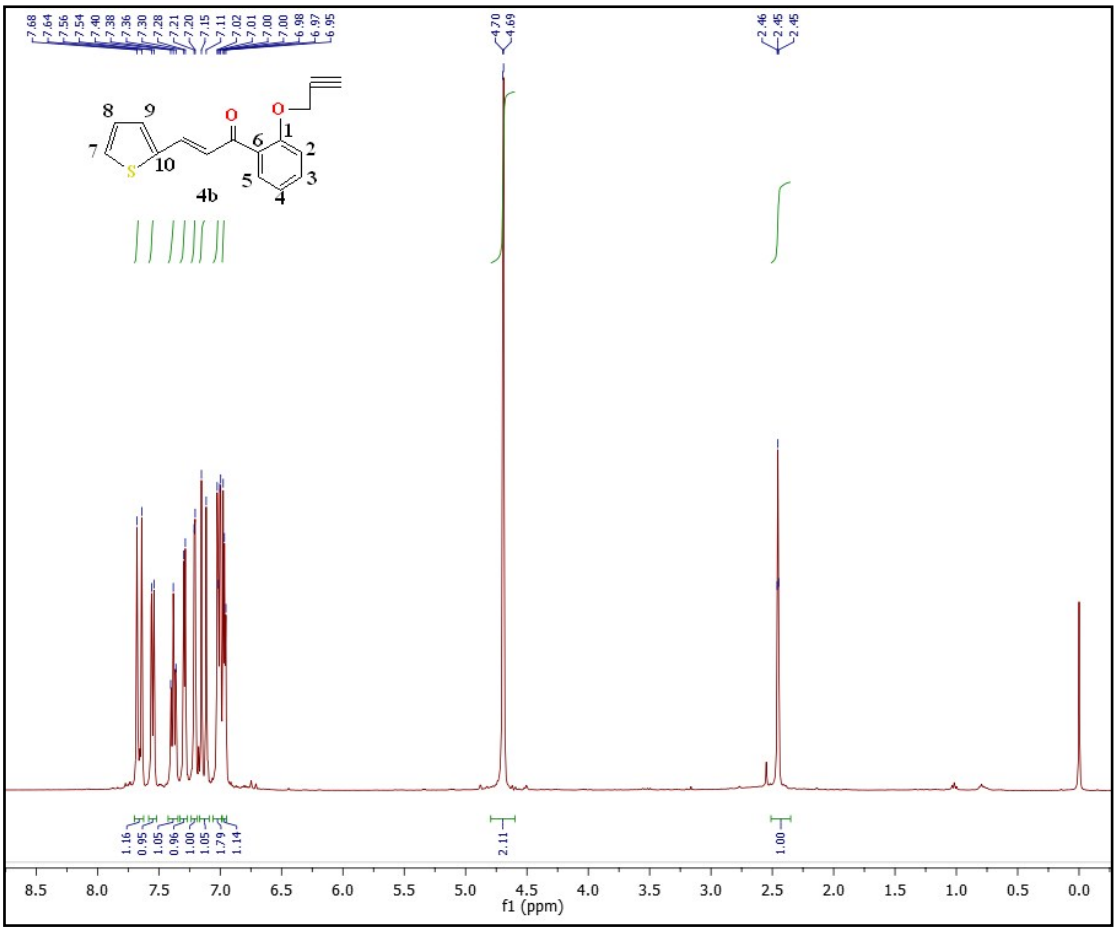
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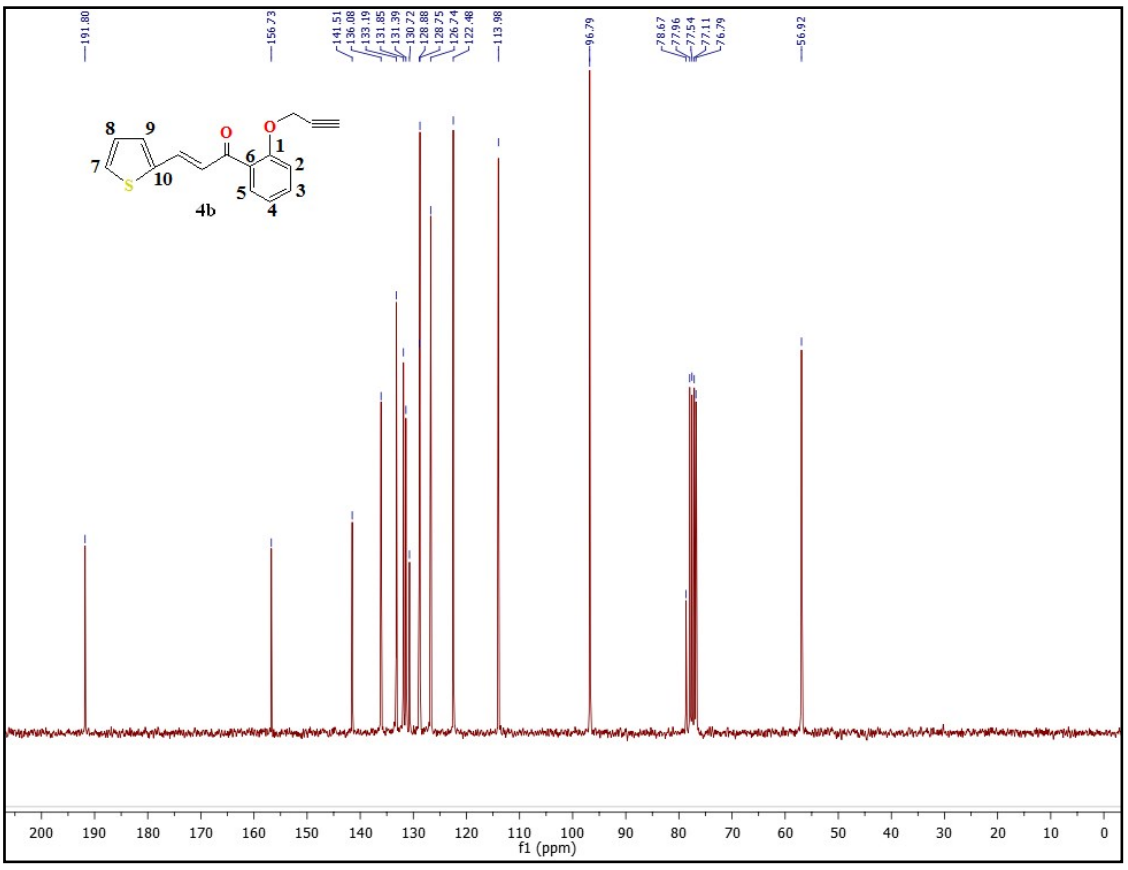
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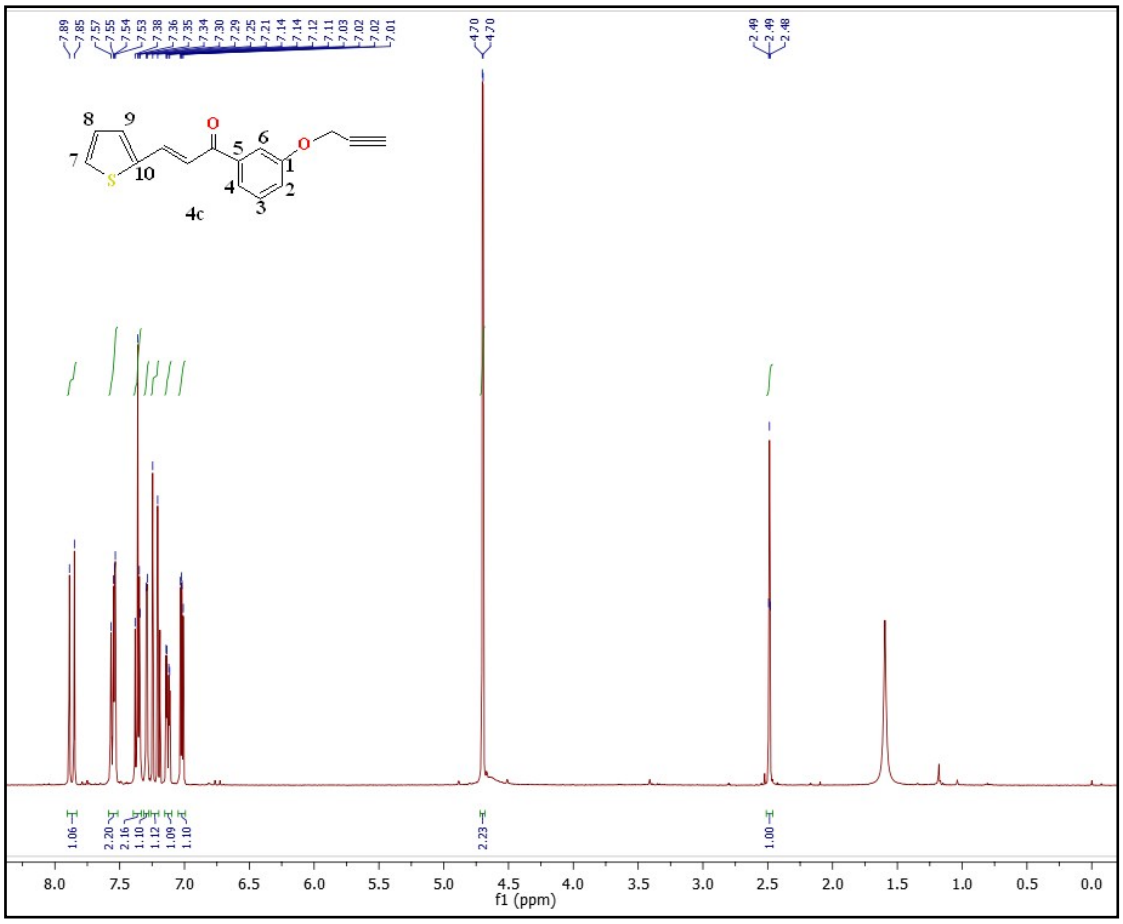
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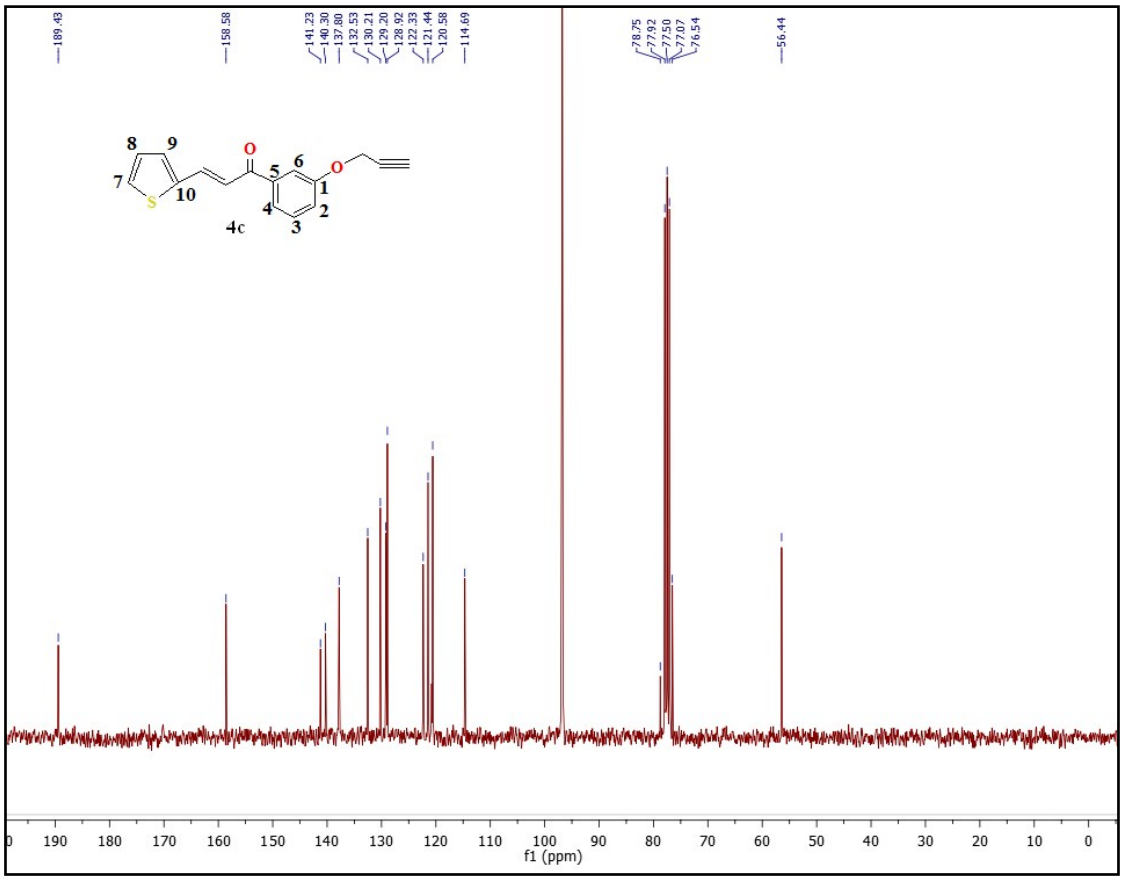
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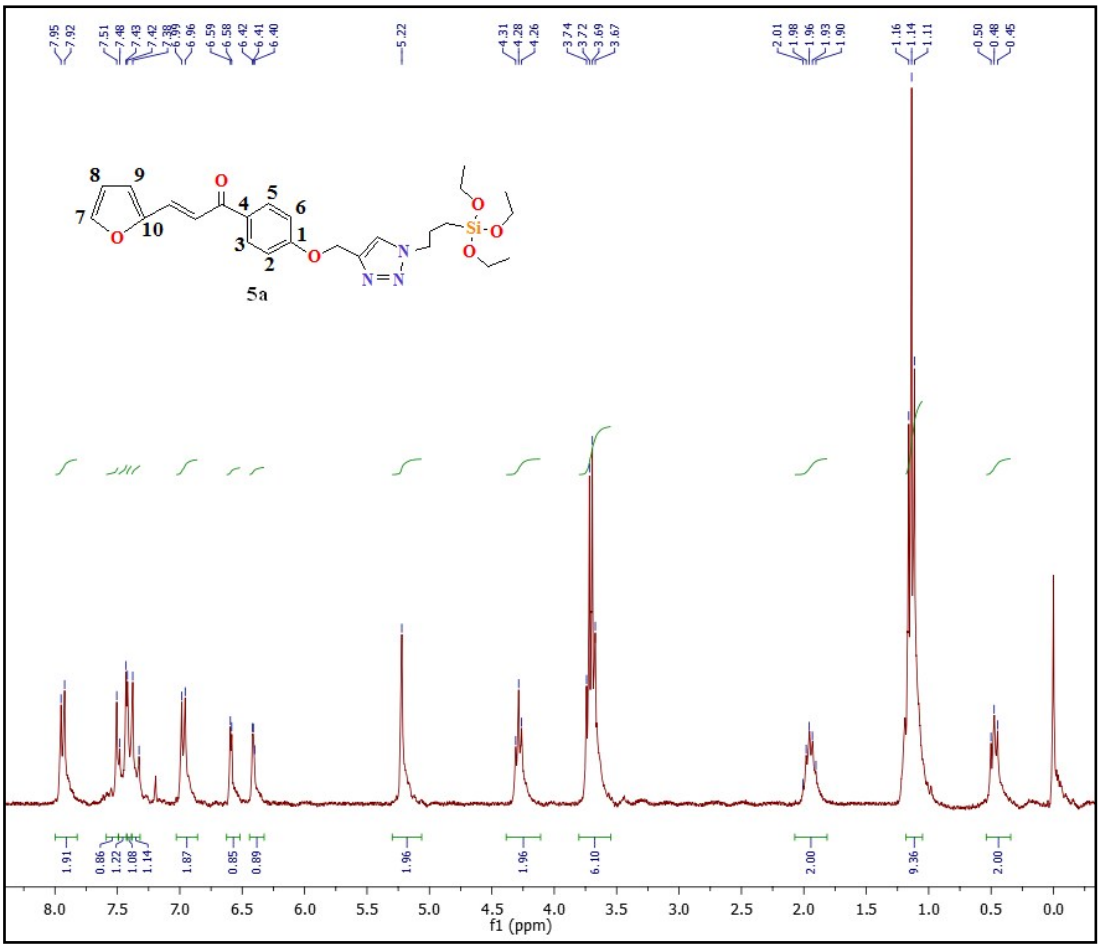
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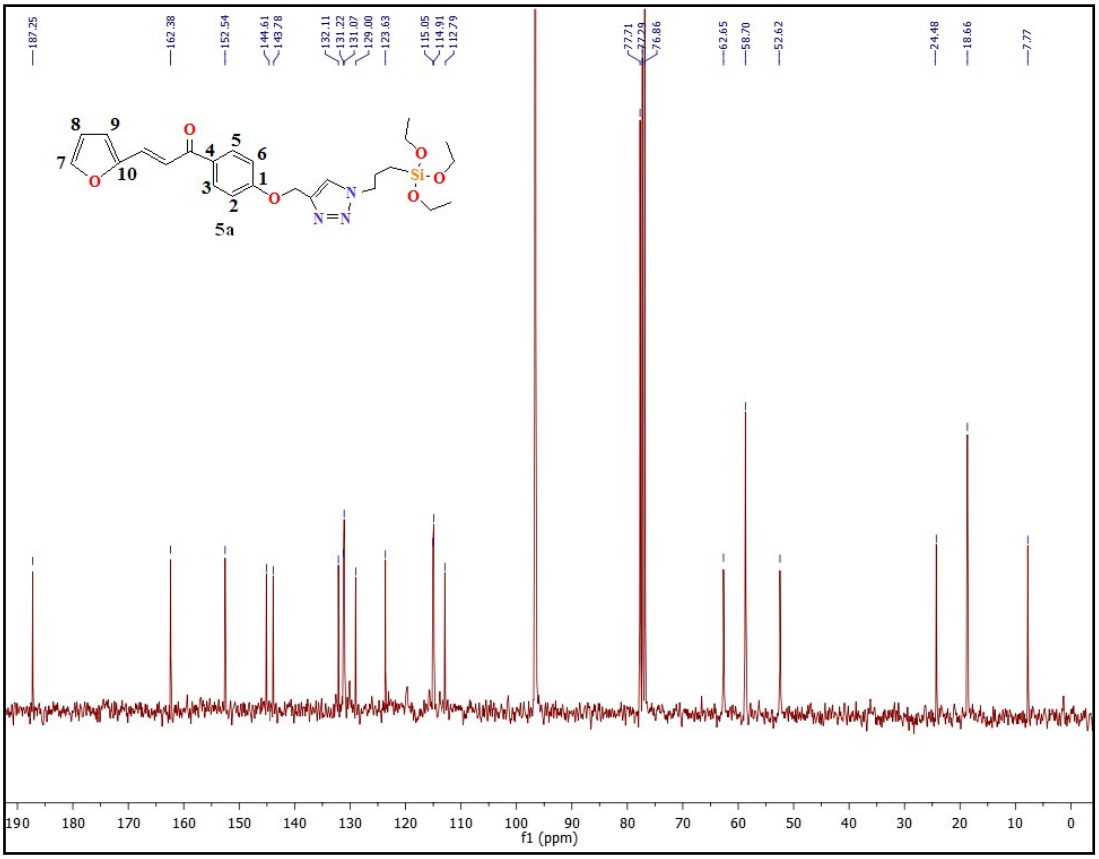
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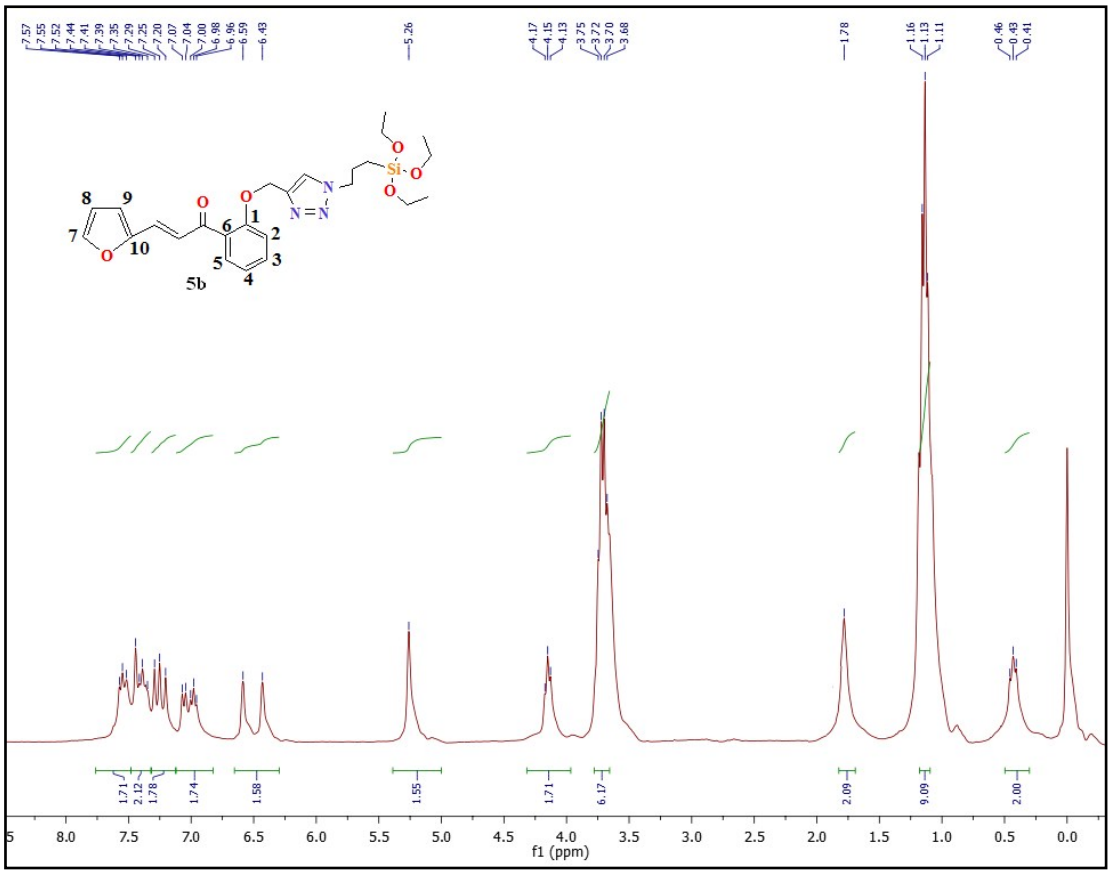
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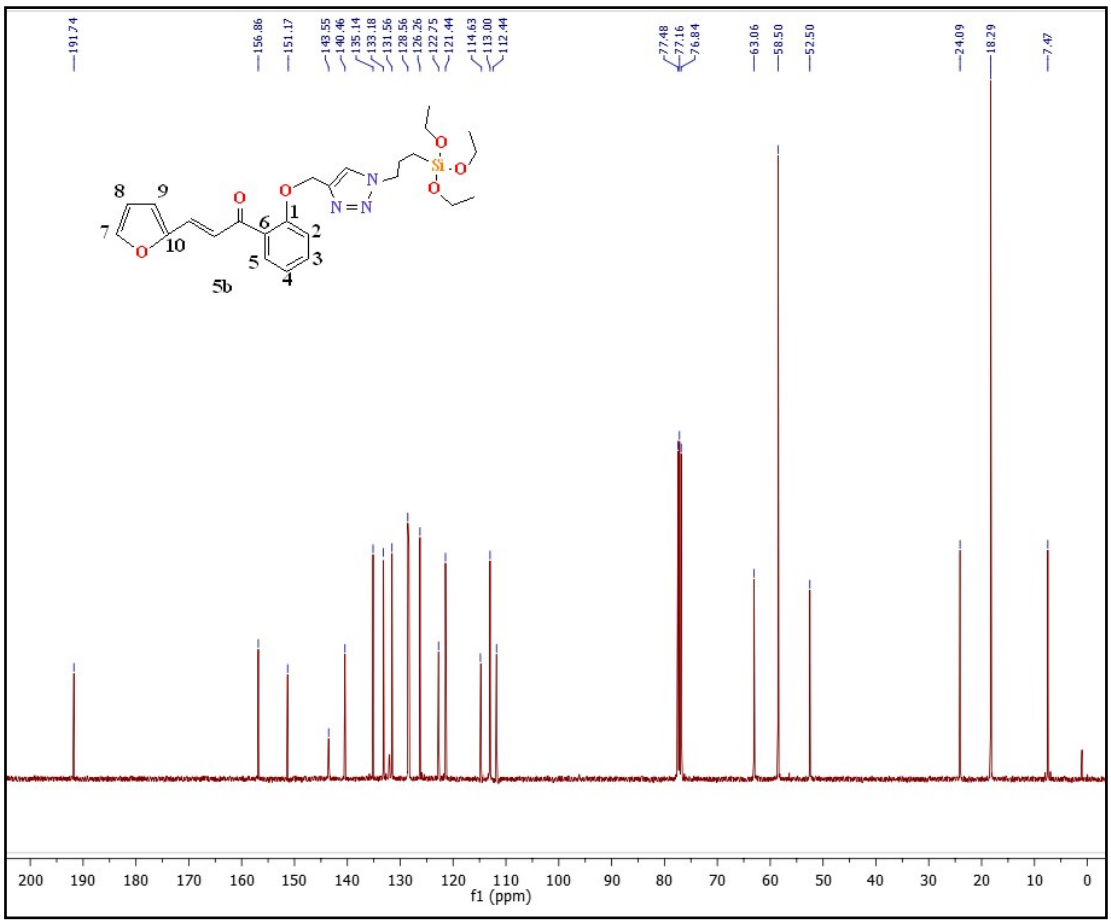
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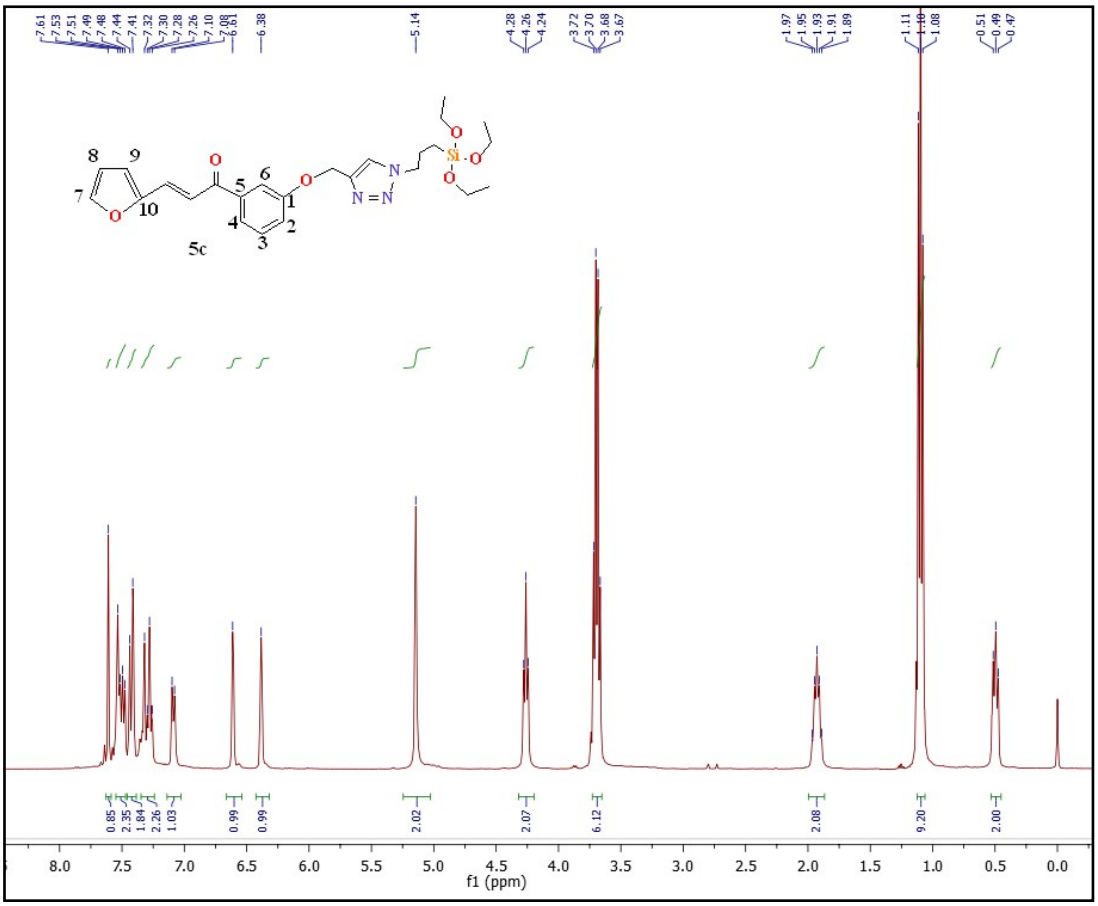
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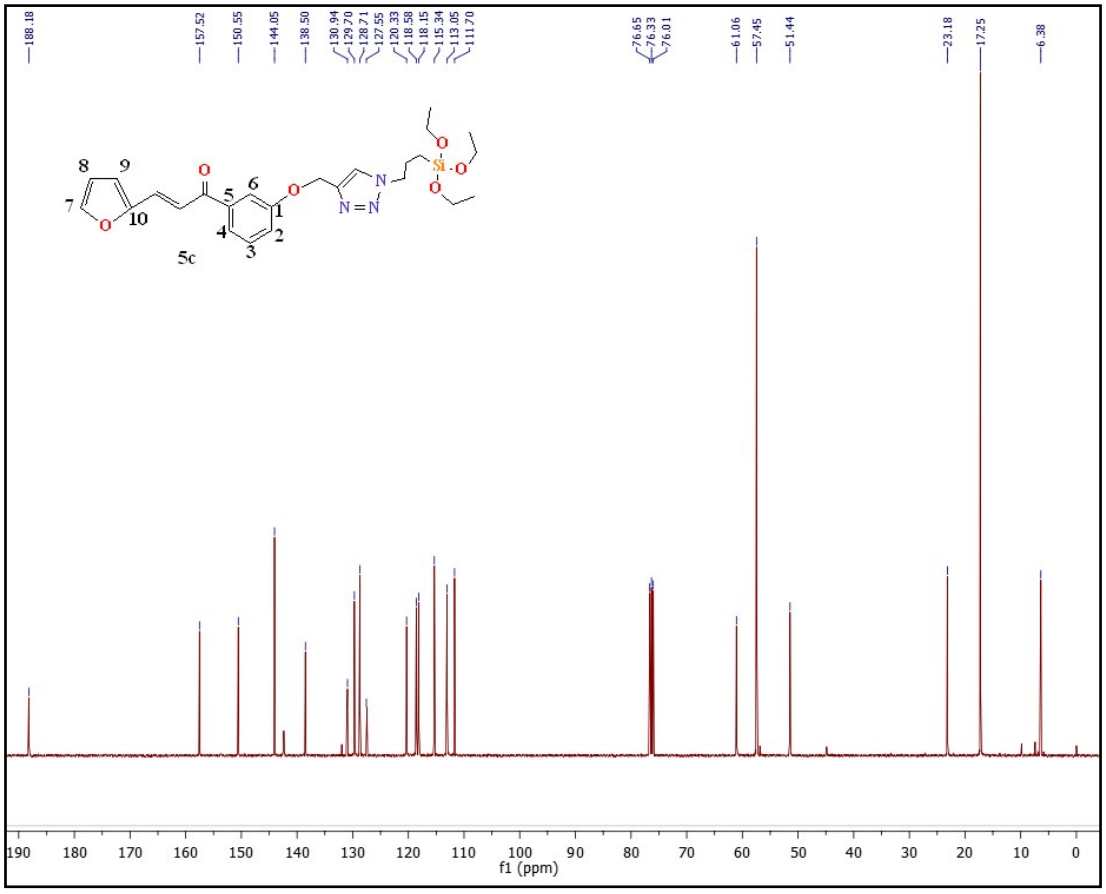
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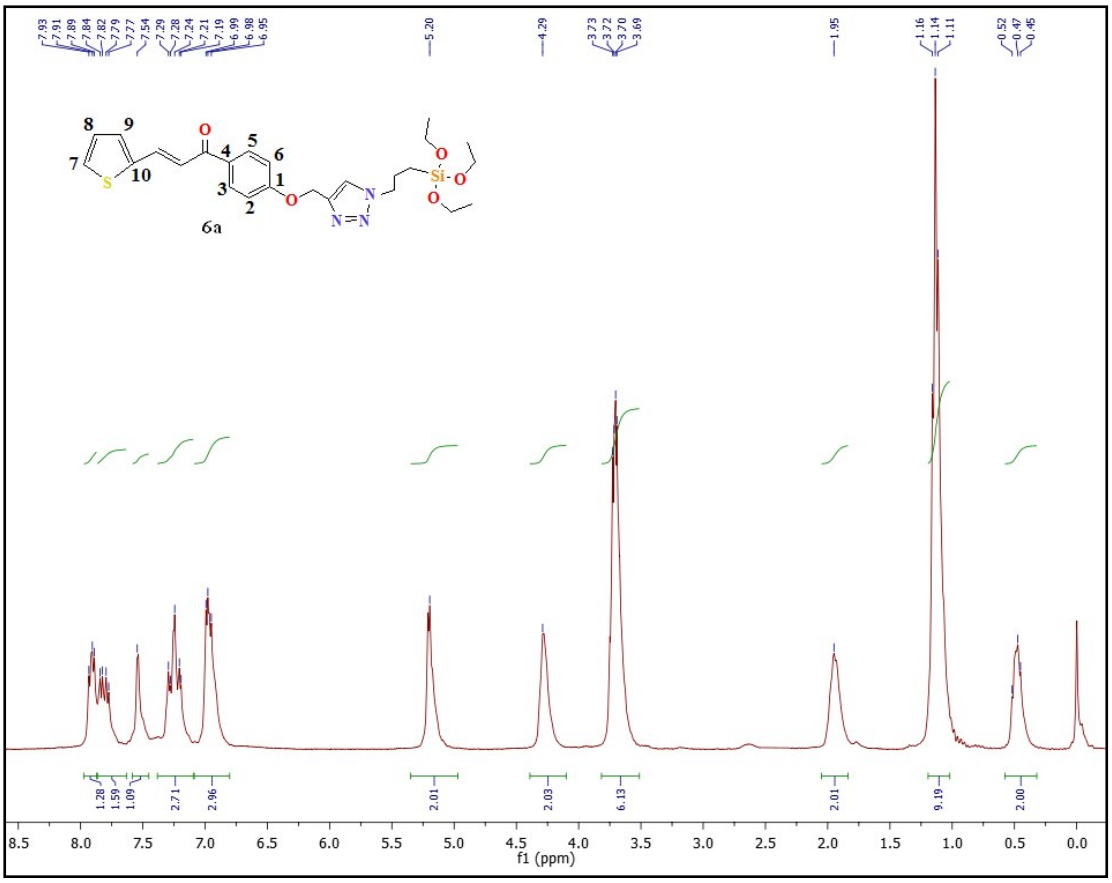
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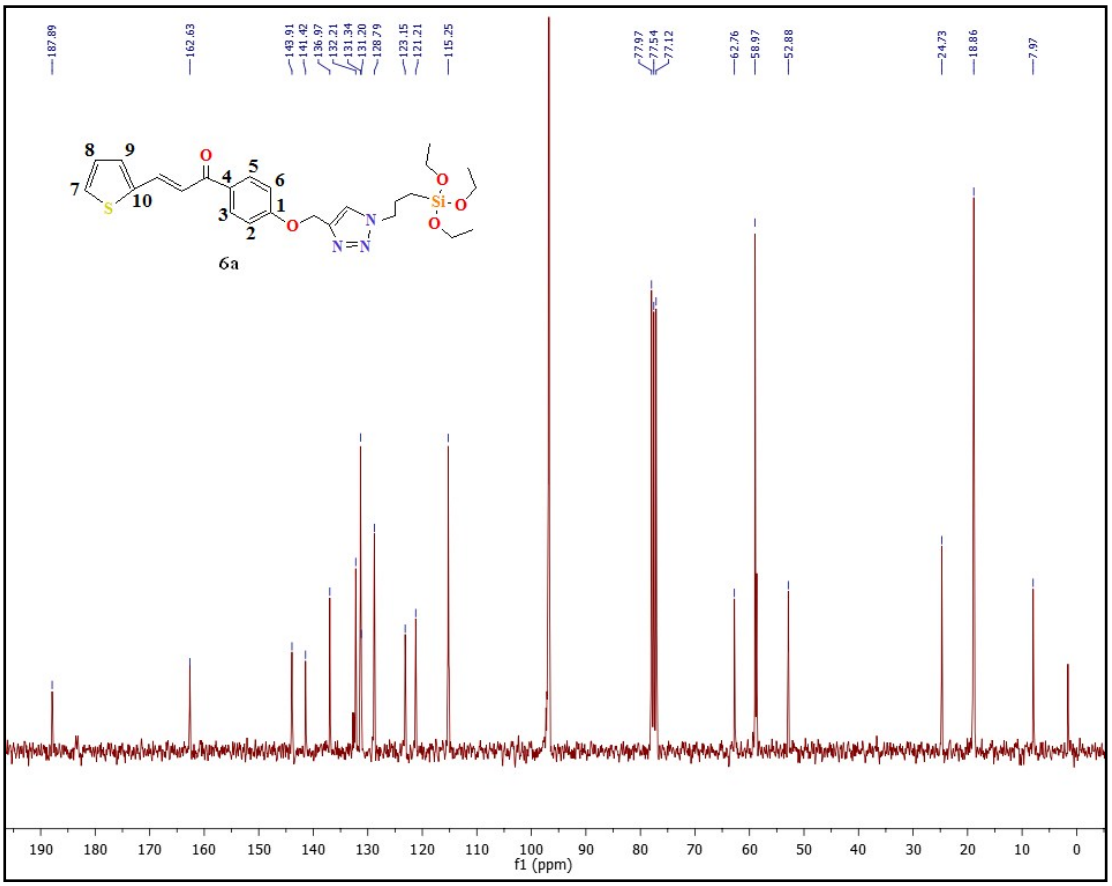
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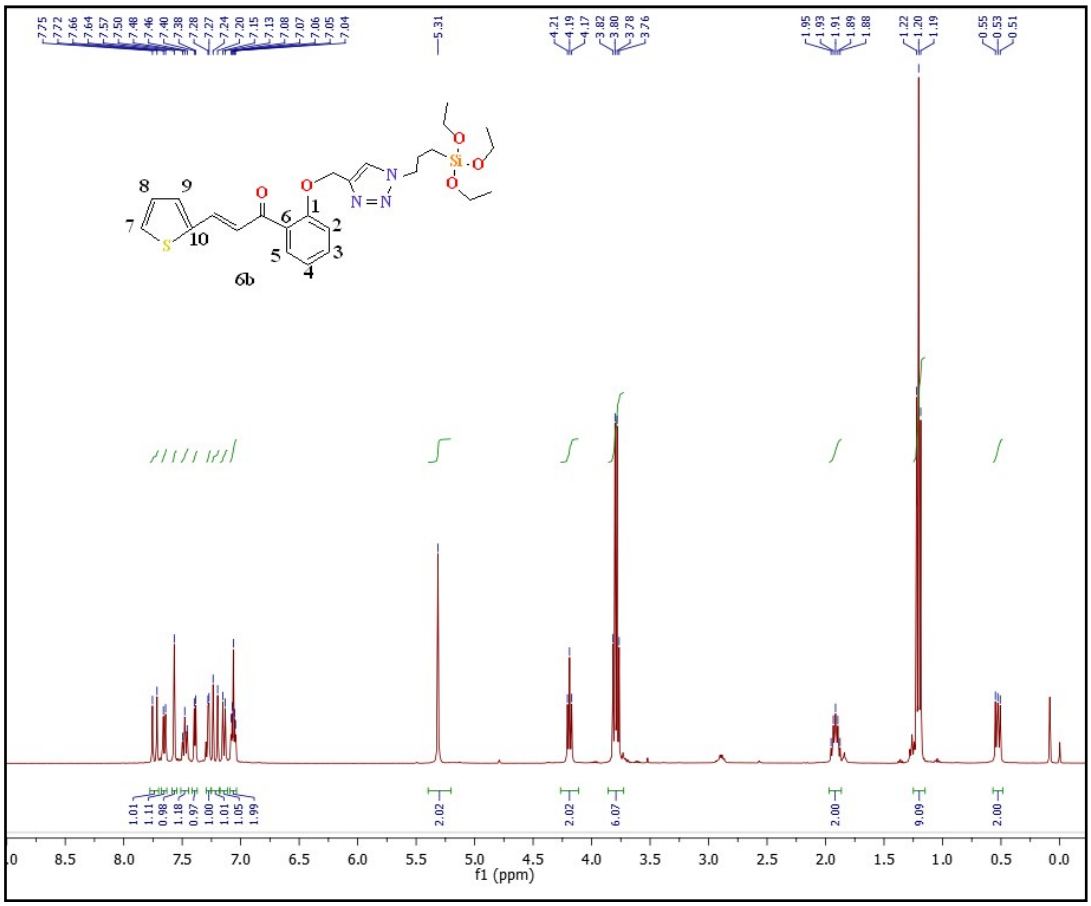
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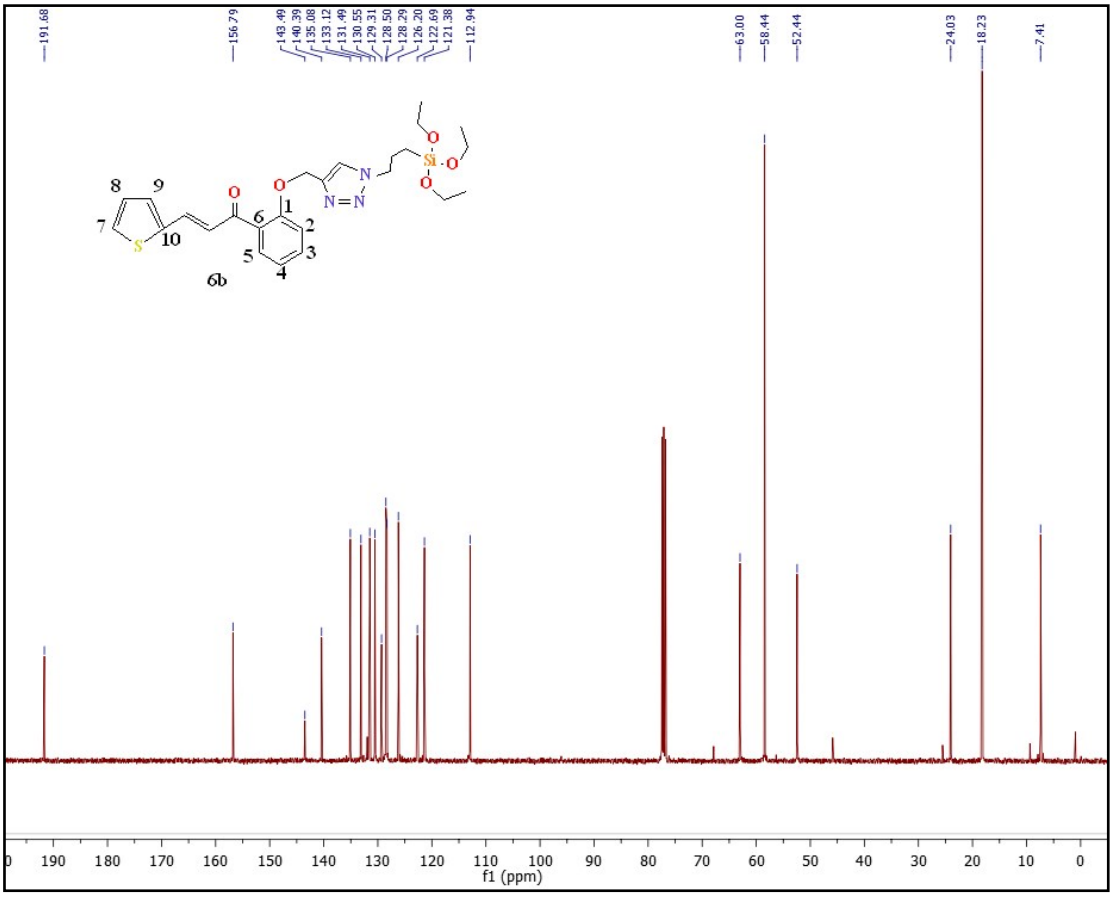
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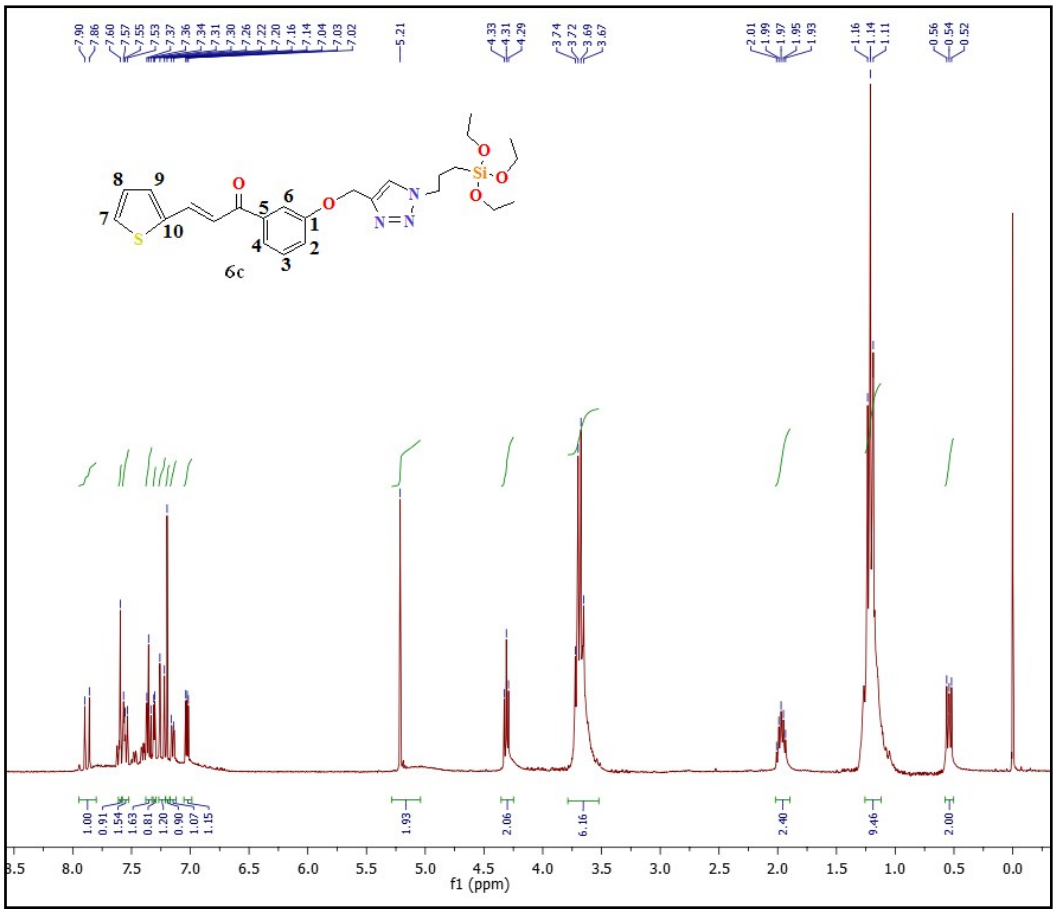
156.79
143.49
140.39
135.08
133.12
131.49
130.55
129.31
128.50
128.29
126.20
122.69
121.38
112.94
63.00
58.44
52.44
24.03
18.23
7.41
6b
f1 (ppm)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7.86
7.60
7.57
7.55
7.53
7.37
7.36
7.34
7.31
7.30
7.26
7.22
7.20
7.16
7.14
7.04
7.03
7.02
5.21
4.33
4.31
4.29
3.74
3.72
3.69
3.67
2.01
1.99
1.97
1.95
1.93
1.16
1.14
1.11
0.56
0.54
0.52
6c
1.00
0.91
1.54
1.63
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1.93
2.06
6.16
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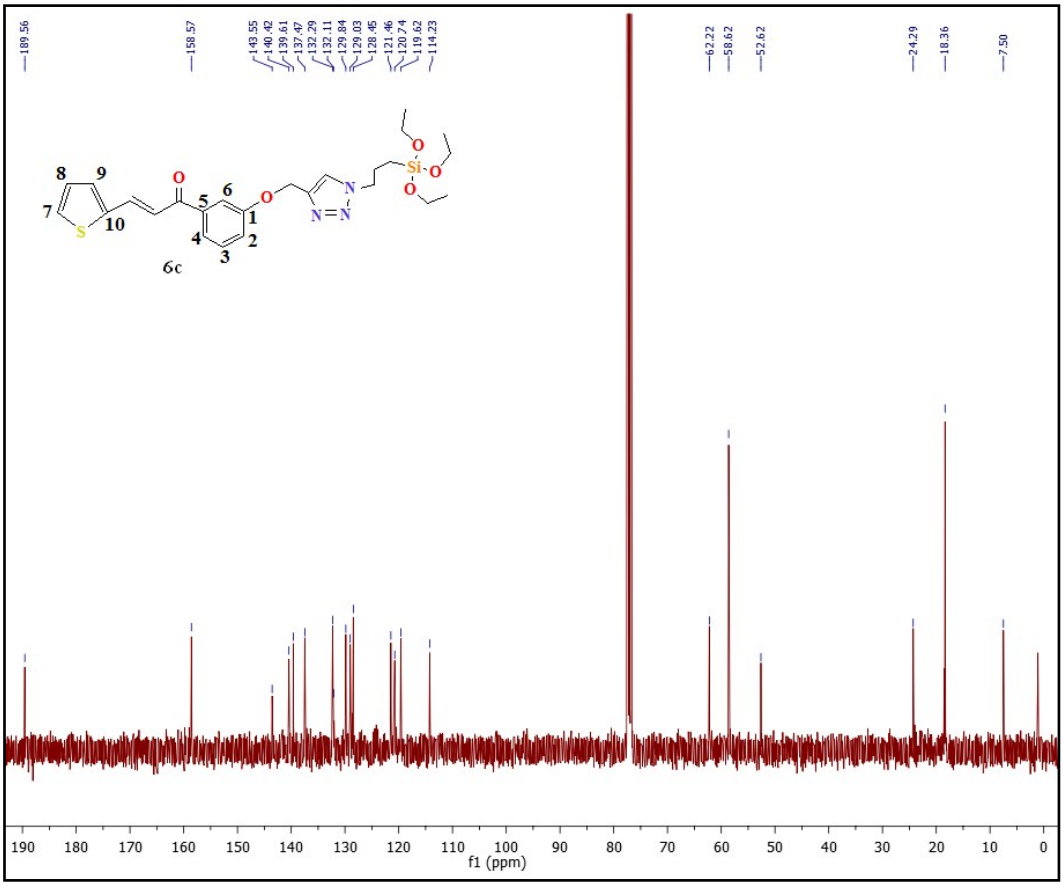
2.00
f1 (ppm)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132.11
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120.74
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114.23
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58.62
52.62
24.29
18.36
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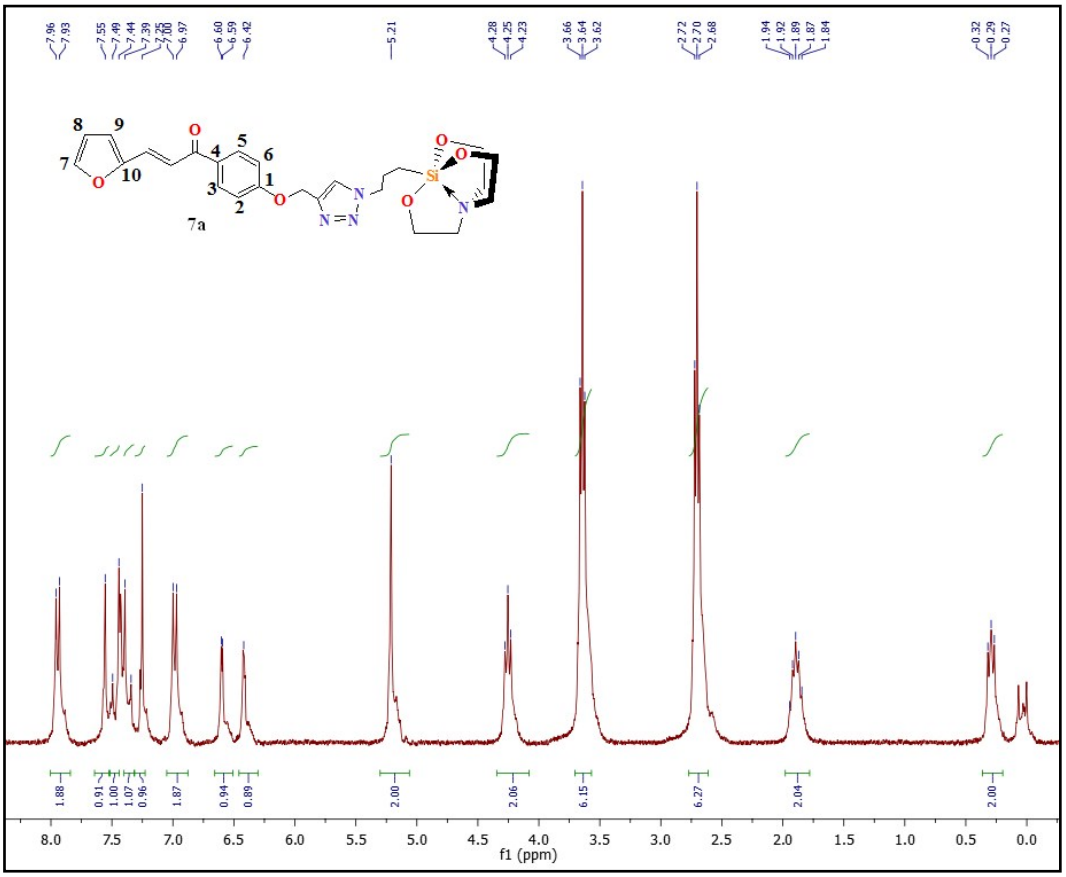
6c
f1 (ppm)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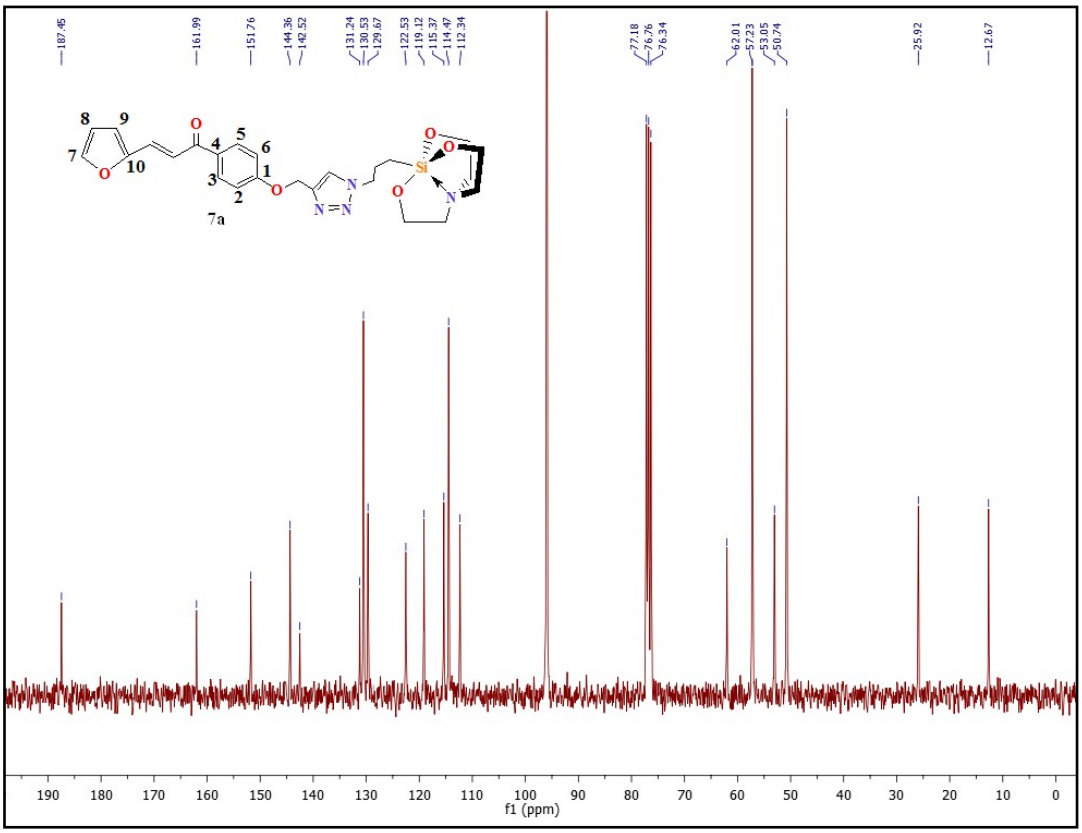
7.39
7.08
6.97
6.60
6.59
6.42
5.21
4.28
4.25
4.23
3.66
3.64
3.62
2.72
2.70
2.68
1.94
1.92
1.89
1.87
1.84
0.32
0.29
0.27
7a
1.88
0.91
1.00
1.07
0.96
1.87
0.94
0.89
2.00
2.06
6.15
6.27
2.04
2.00
f1 (ppm)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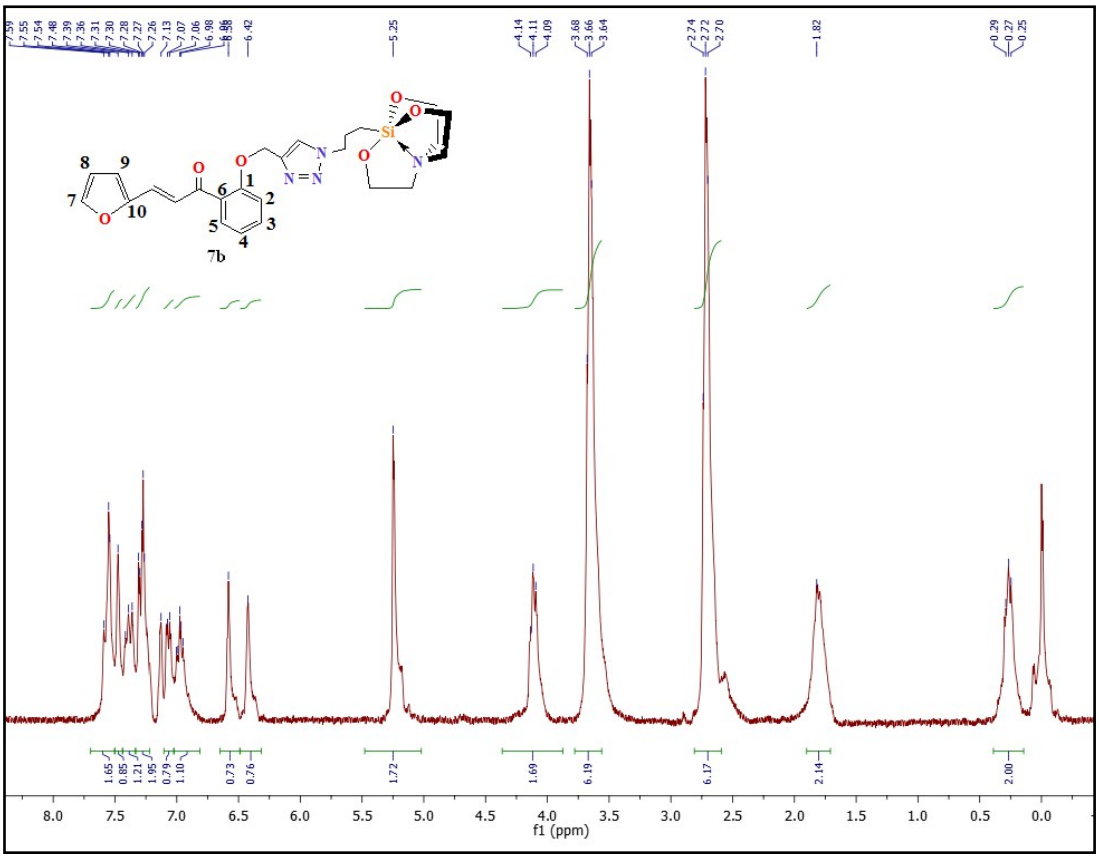
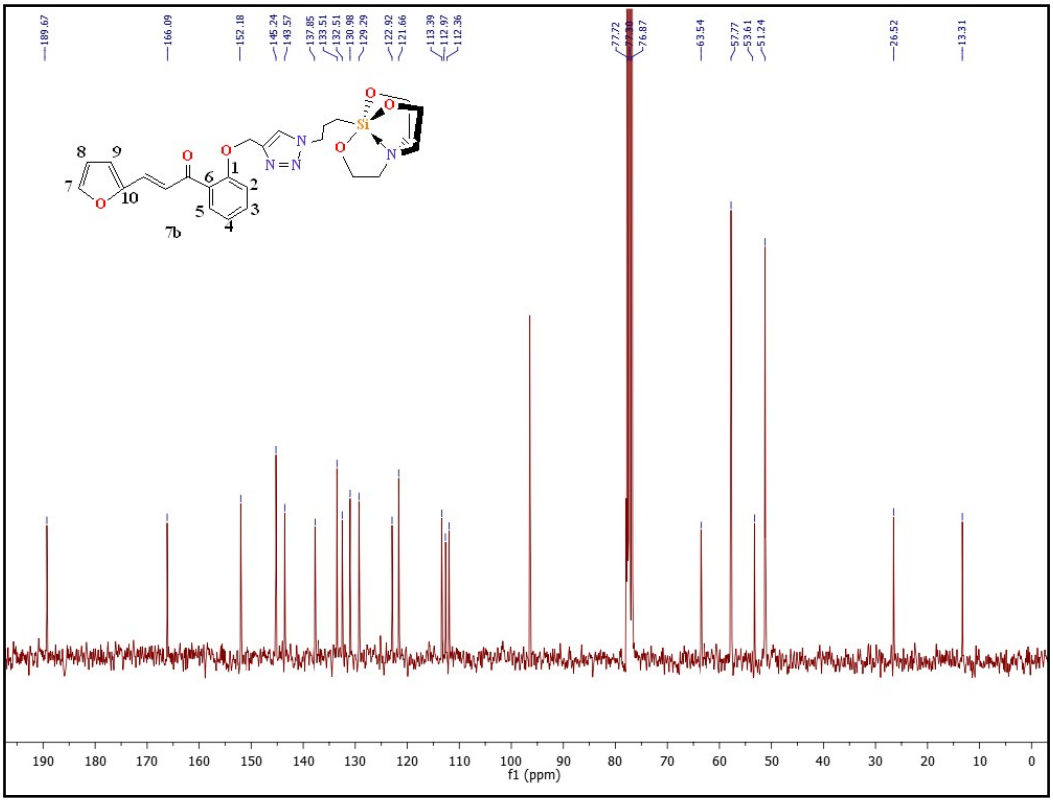
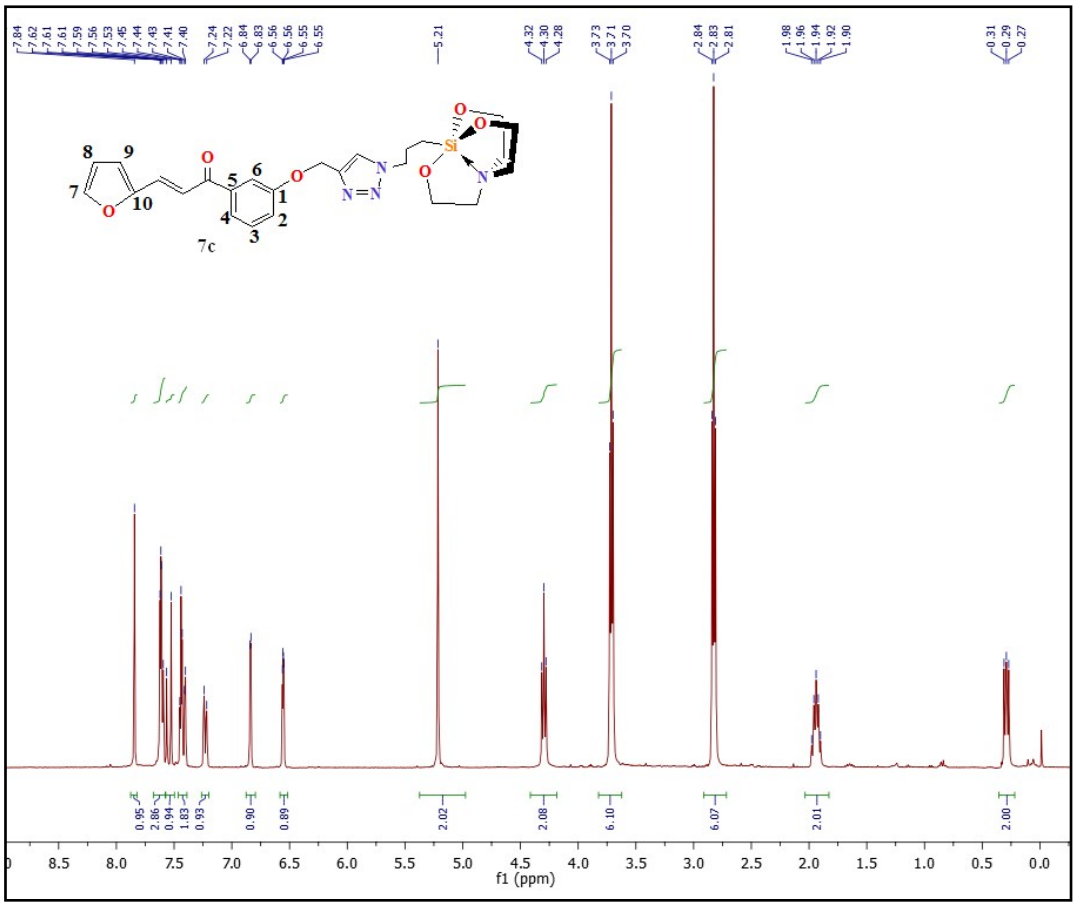
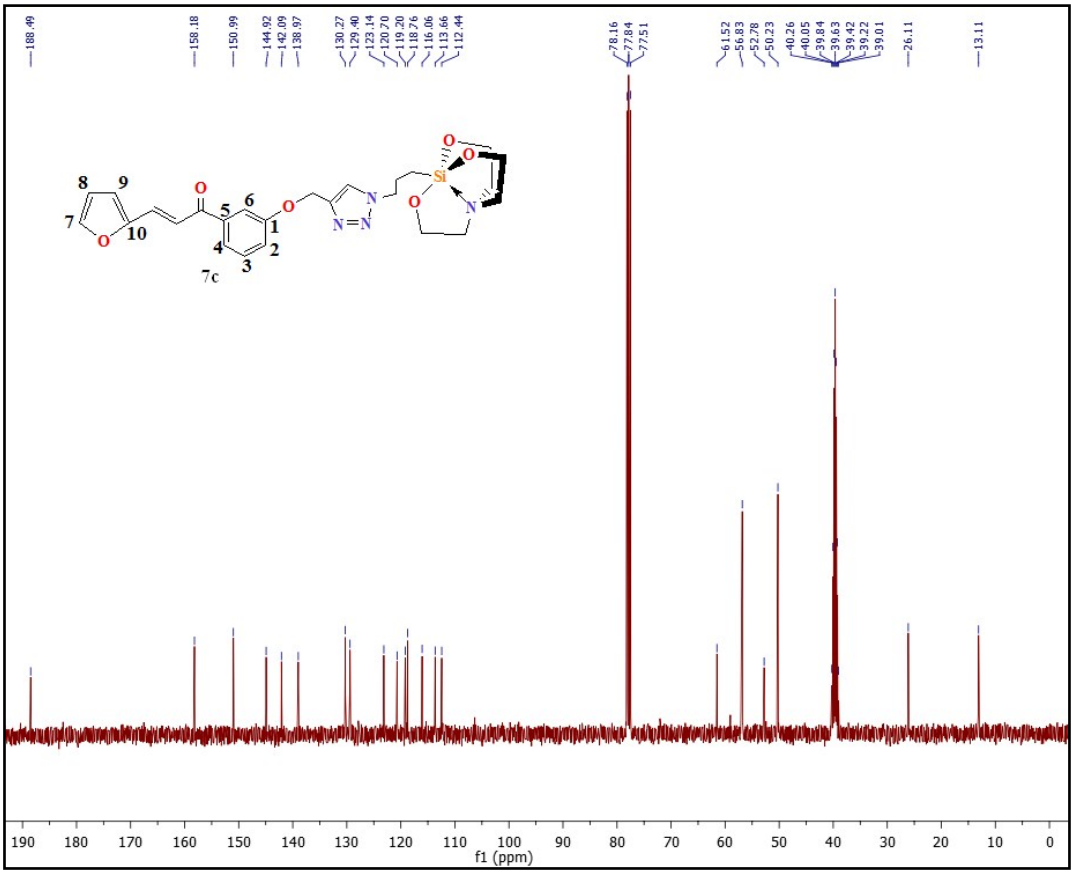
161.99
151.76
144.36
142.52
131.24
130.53
129.67
122.53
119.12
115.37
114.47
112.34
77.18
76.76
76.34
62.01
57.23
53.05
50.74
25.92
12.67
7a
f1 (ppm)


7b
f1 (ppm)


7b
f1 (ppm)


7.84
7.62
7.61
7.61
7.59
7.56
7.53
7.45
7.44
7.43
7.41
7.40
7.24
7.22
6.84
6.83
6.56
6.56
6.55
6.55
5.21
4.32
4.30
4.28
3.73
3.71
3.70
2.84
2.83
2.81
1.98
1.96
1.94
1.92
1.90
0.31
0.29
0.27
7c
0.95
2.86
0.94
1.83
0.93
0.90
0.89
2.02
2.08
6.10
6.07
2.01
2.00
f1 (ppm)


188.49
158.18
150.99
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142.09
138.97
130.27
129.40
123.14
120.70
119.20
118.76
116.66
113.66
112.44
78.16
77.84
77.51
61.52
56.83
52.78
50.23
40.26
40.05
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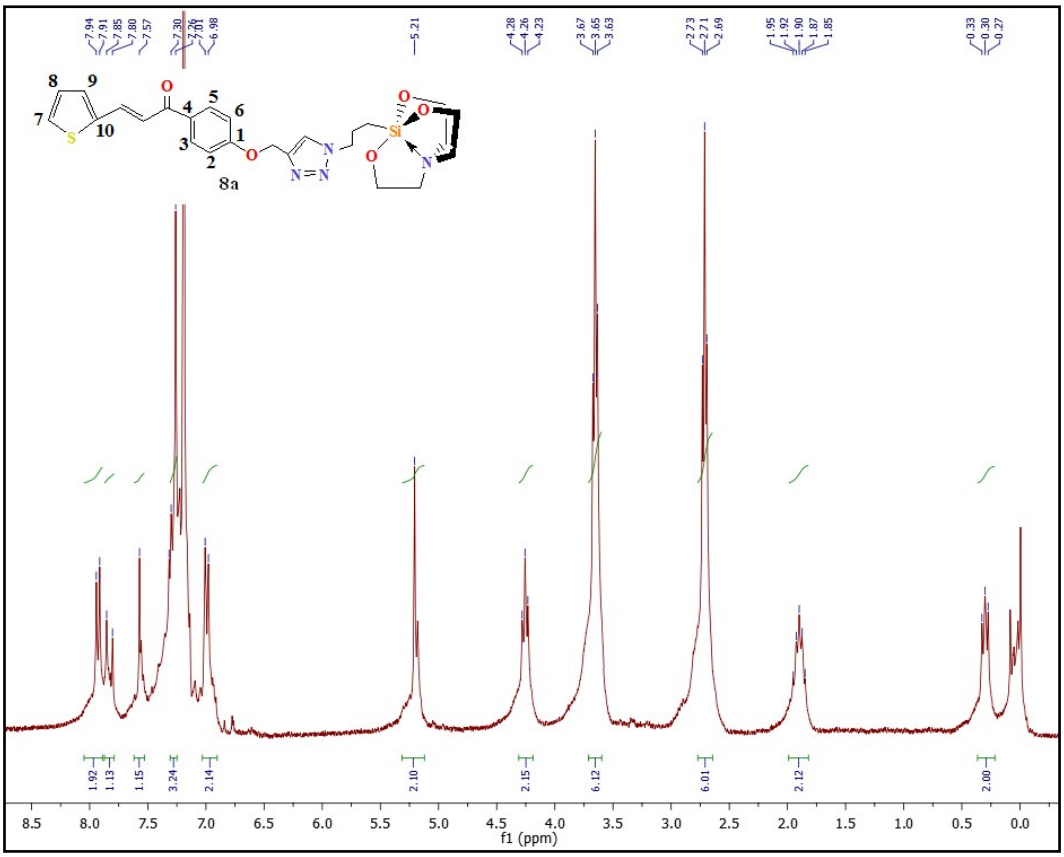
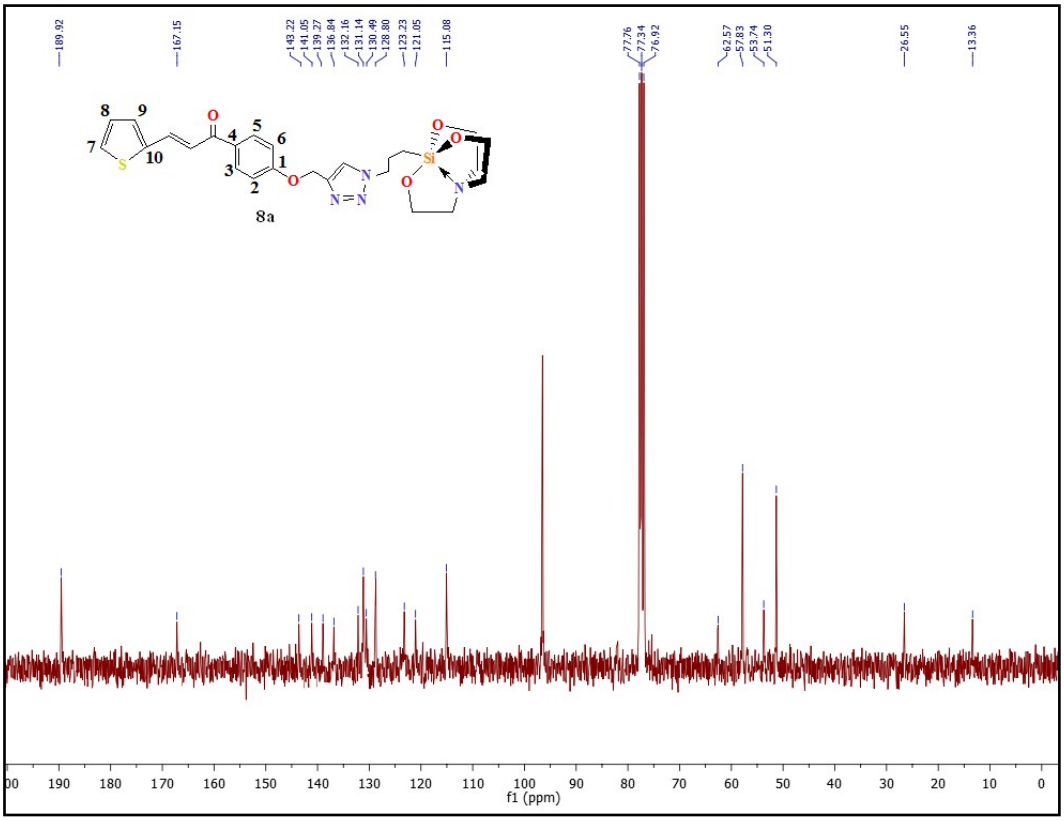
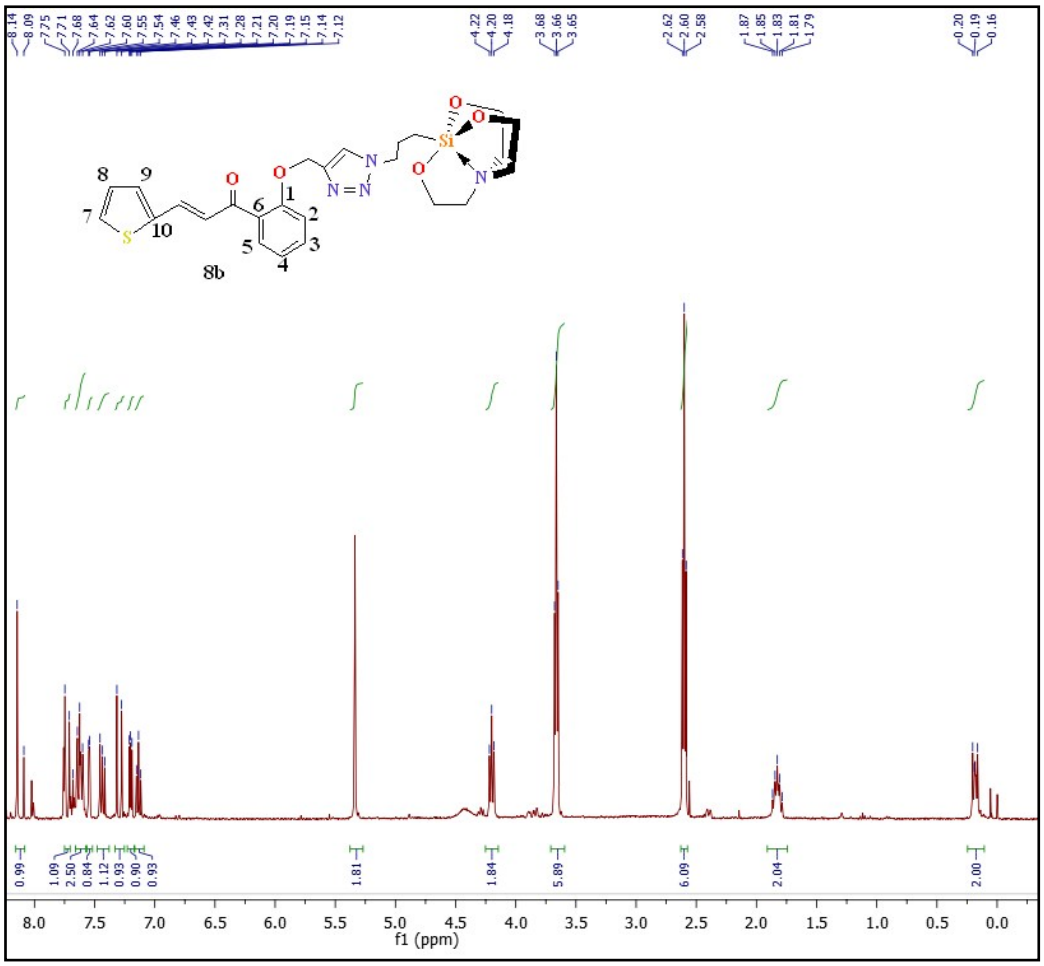
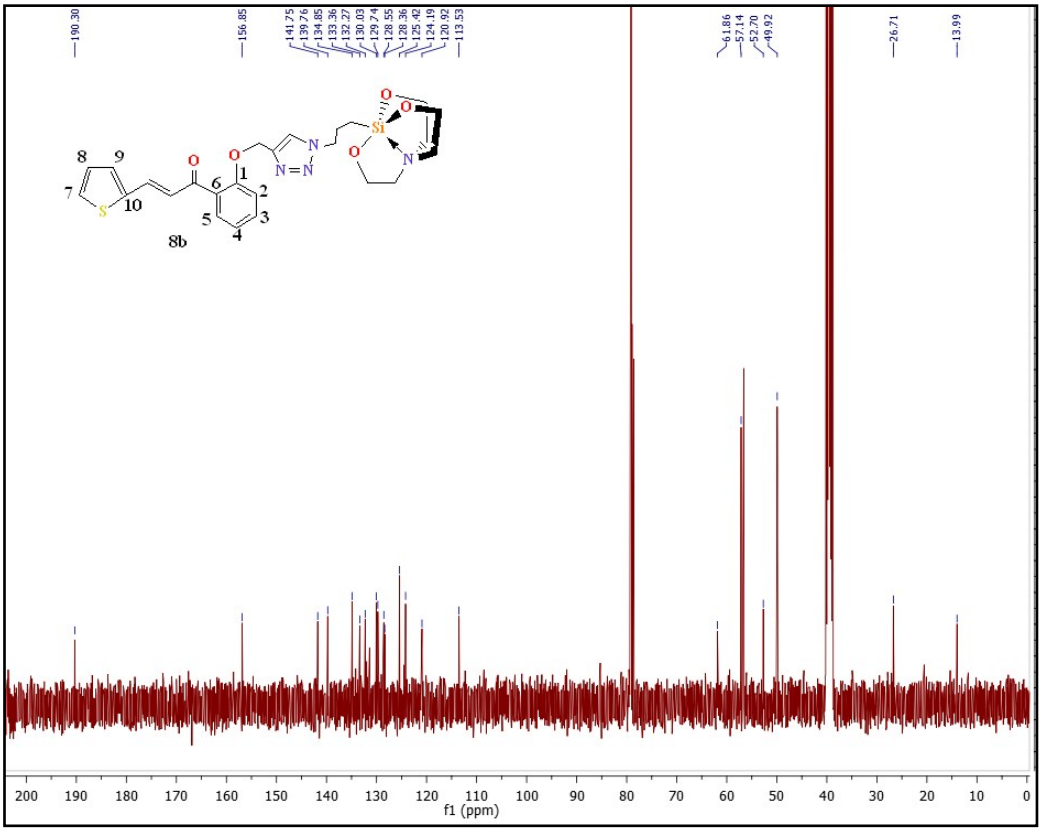
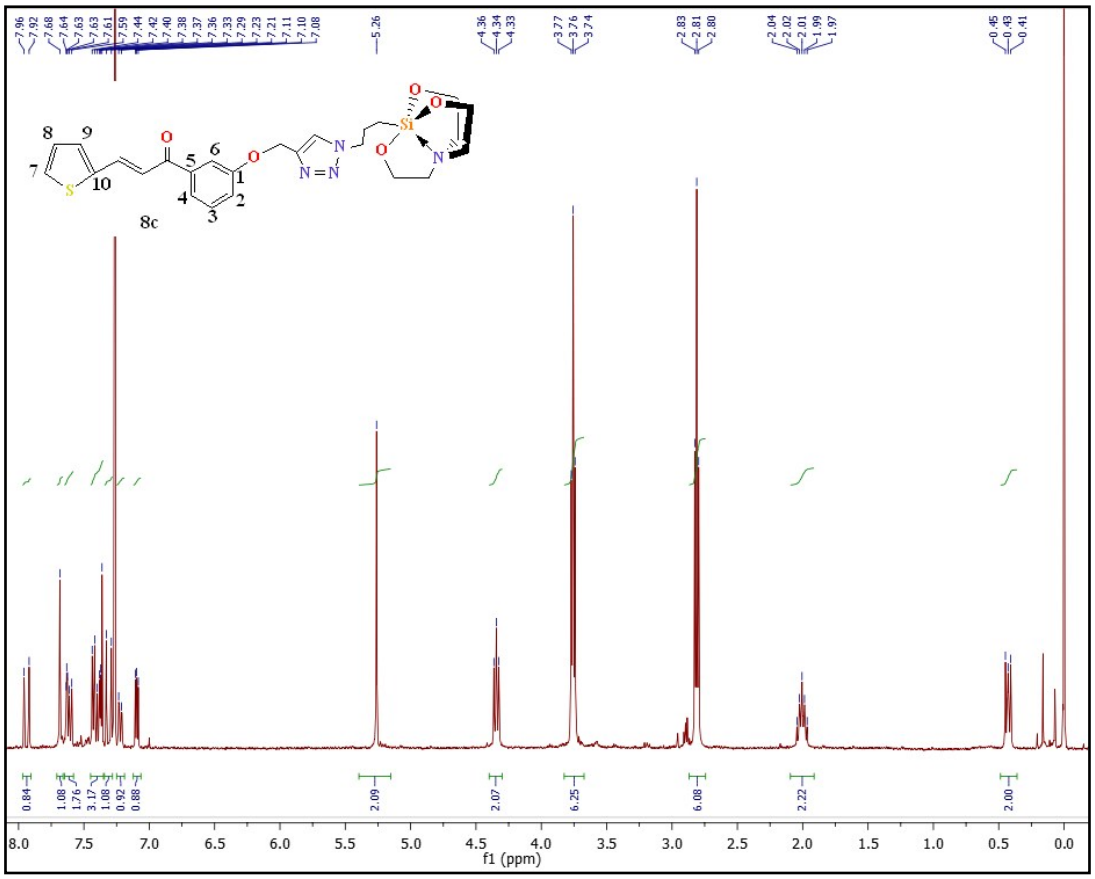
39.63
39.42
39.22
39.01
26.11
13.11
7c
f1 (ppm)

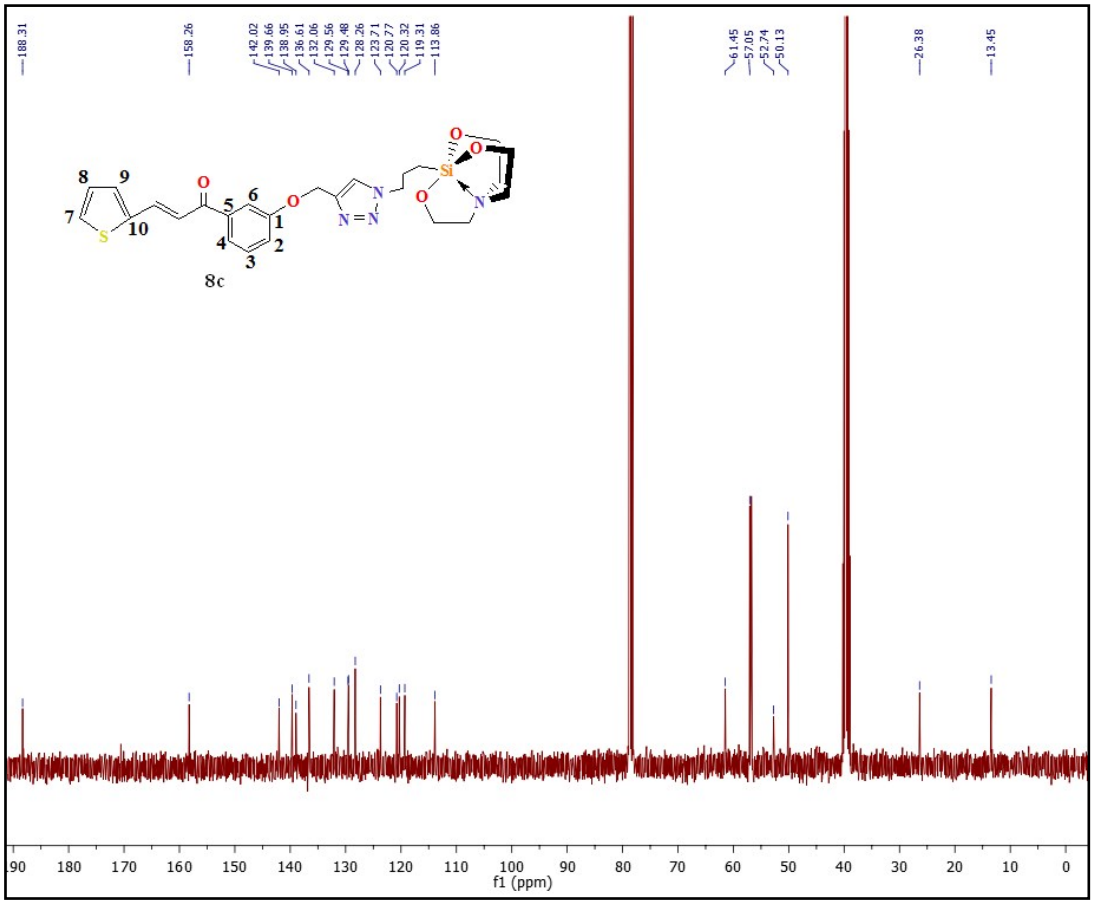

8a
f1 (ppm)


8a
f1 (ppm)


8b
f1 (ppm)


8b
f1 (ppm)


8c
f1 (ppm)


8c
f1 (ppm)

Comments on A alert: Various attempts to rectify the A alert (observed/unique reflections (too) low 19% for **7a** and 26% for **8a**) were made, however due to the weakly diffracting crystals, the data quality could not be improved in these cases. To obtain better signal to noise ratio, the data was cut at 1.1 Å, which eliminated the alert, however, this gave rise to many resolution alerts. As the purpose of this crystal structure determination is to determine the general connectivity of atoms and their conformations, we believe that the obtained results will present reasonable structure models. In addition, attempts were made to grow bigger/better crystals as well but similar data sets were obtained.

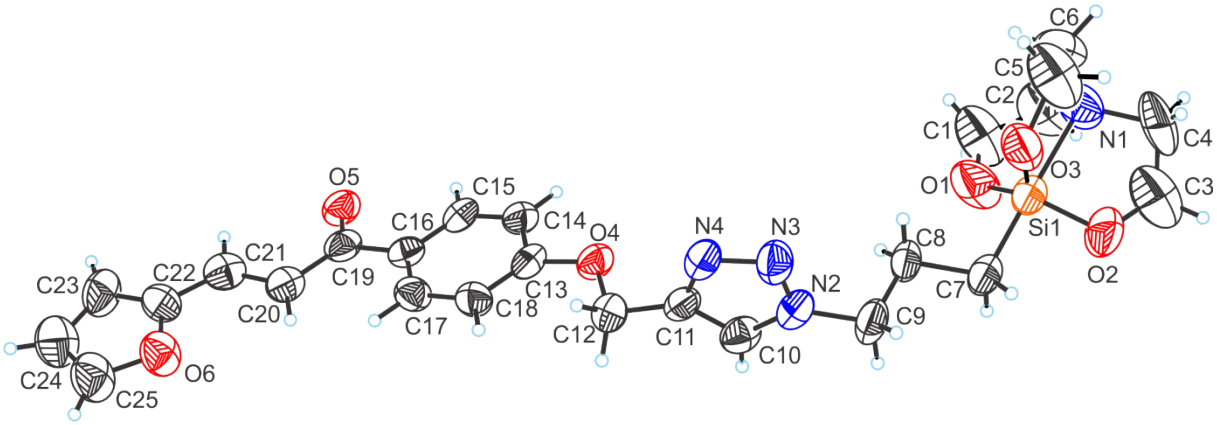


Figure S2.

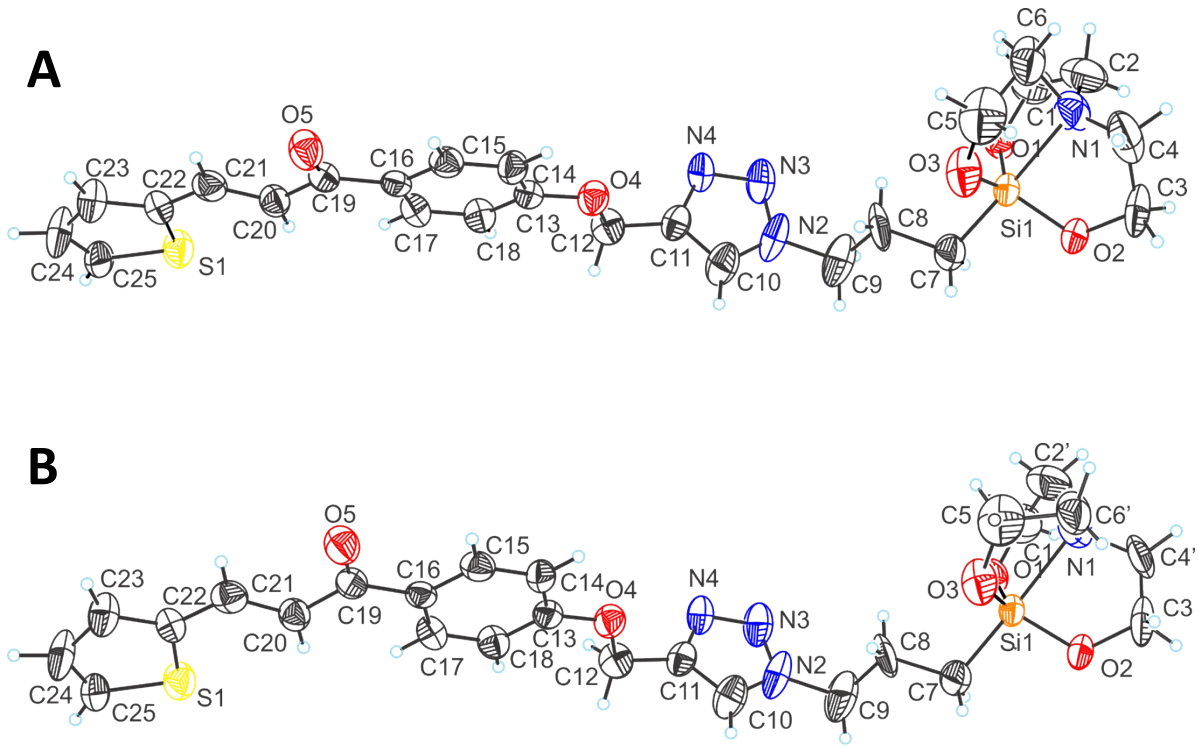
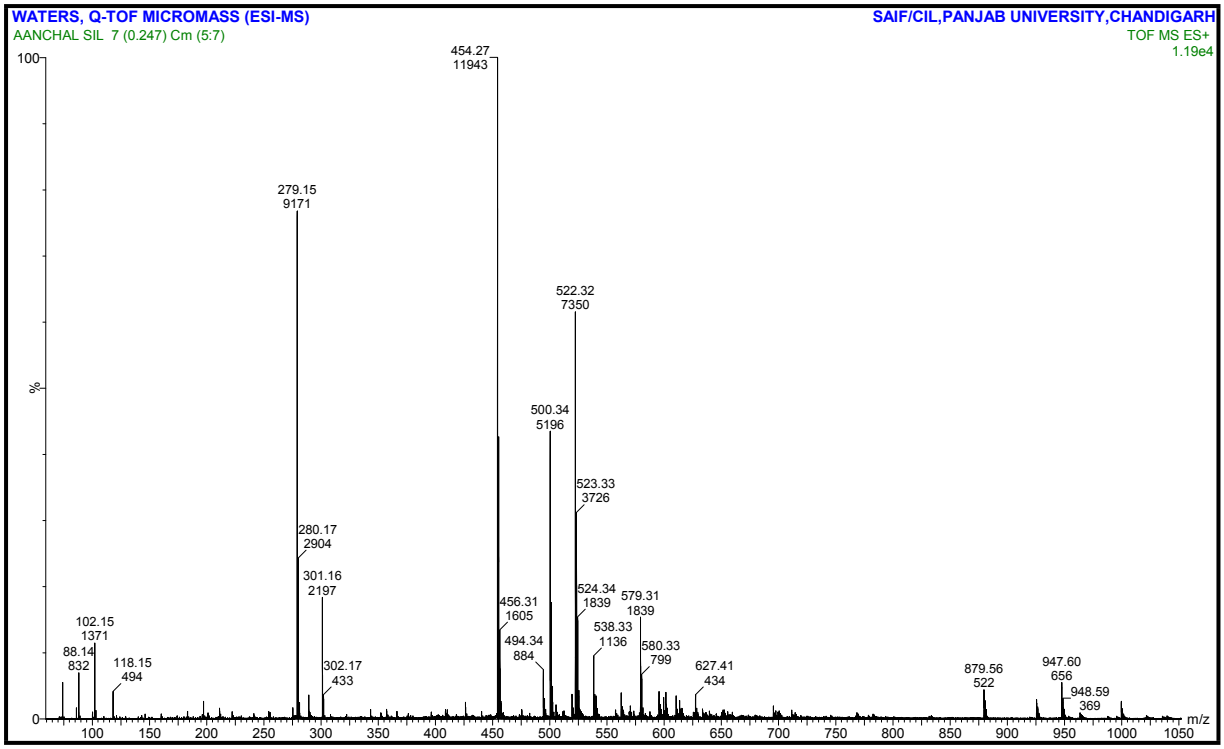

A
C6
C2
C5
C1
N1
C4
O3
O1
C3
Si1
O2
O5
C16
C15
C14
O4
N4
N3
C23
C22
C21
C19
C20
C13
N2
C8
C12
C11
C10
C9
C7
C17
C18
C24
C25
S1
B
C2'
C5
C6'
C1
N1
C4'
O3
O1
C3
Si1
O2
O5
C16
C15
C14
O4
N4
N3
C23
C22
C21
C19
C20
C13
N2
C8
C12
C11
C10
C9
C7
C17
C18
C24
C25
S1

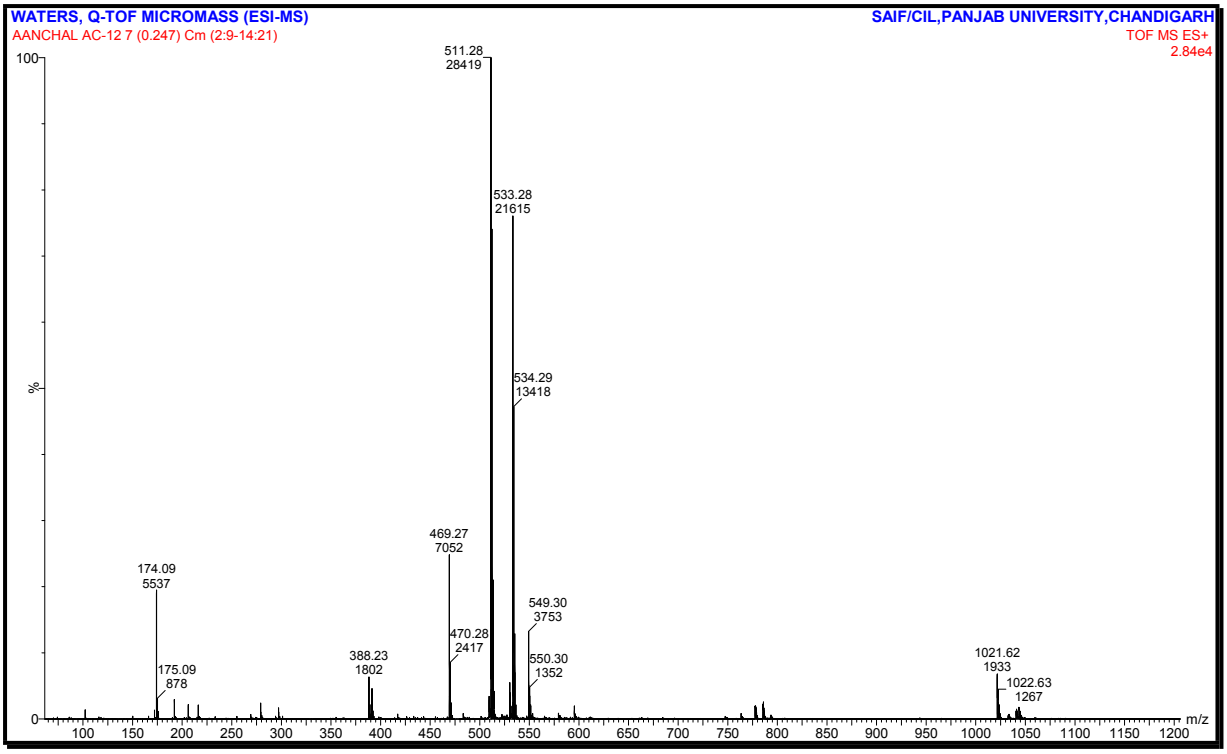
Figure S3.

Table S1.

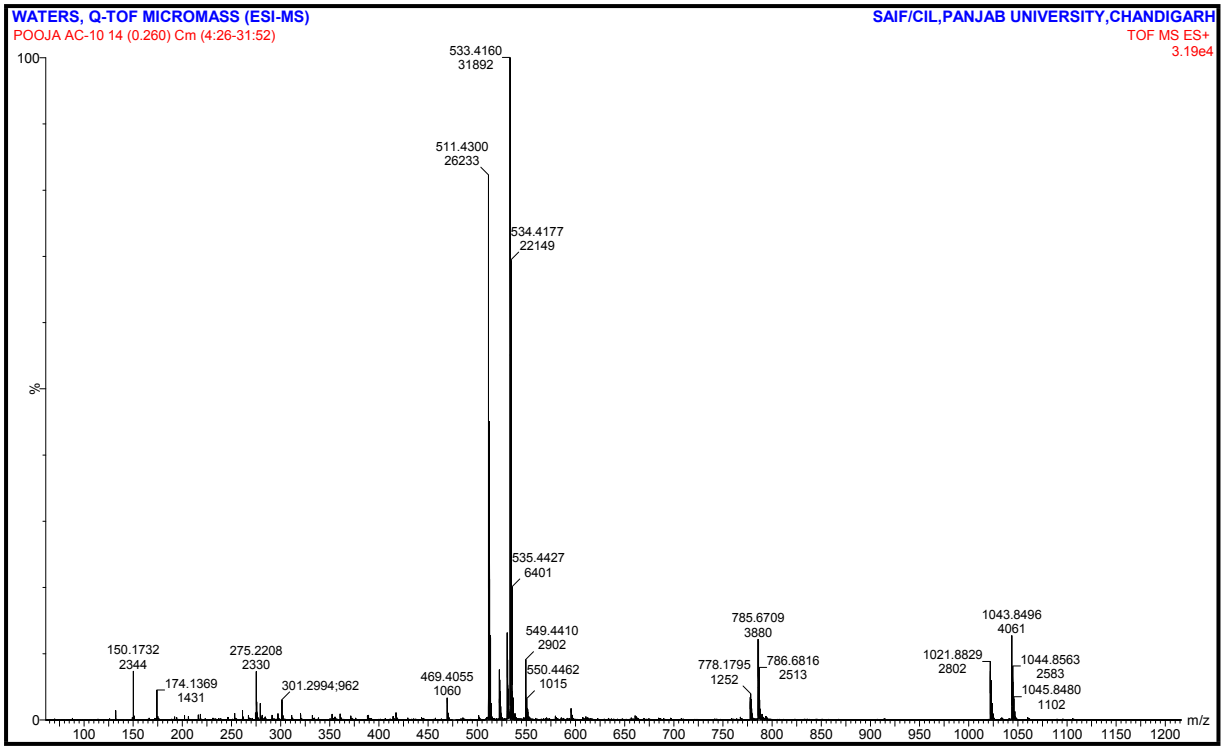
	7a	**8a**
Si(1)-O(1)	1.658(4)	1.656(3)
Si(1)-O(2)	1.668(4)	1.661(3)
Si(1)-O(3)	1.673(4)	1.664(3)
Si(1)-C(7)	1.879(5)	1.857(5)
Si(1)-N(1)	2.138(5)	2.151(5)
X(1)-C(22)	1.375(6)	1.724(5)
X(1)-C(25)	1.357(7)	1.711(6)
O(1)-Si(1)-O(2)	117.8(2)	118.27(17)
O(2)-Si(1)-O(3)	119.0(2)	118.81(18)
O(3)-Si(1)-O(2)	119.4(2)	118.44(18)
O(1)-Si(1)-N(1)	83.8(2)	83.03(19)
O(2)-Si(1)-N(1)	83.67(19)	83.55(18)
O(3)-Si(1)-N(1)	83.08(18)	82.21(17)
O(1)-Si(1)-C(7)	96.5(2)	97.5(2)
O(2)-Si(1)-C(7)	96.4(2)	98.44(19)
O(3)-Si(1)-C(7)	96.7(2)	95.3(2)
C(7)-Si(1)-N(1)	179.7(2)	177.3(2)



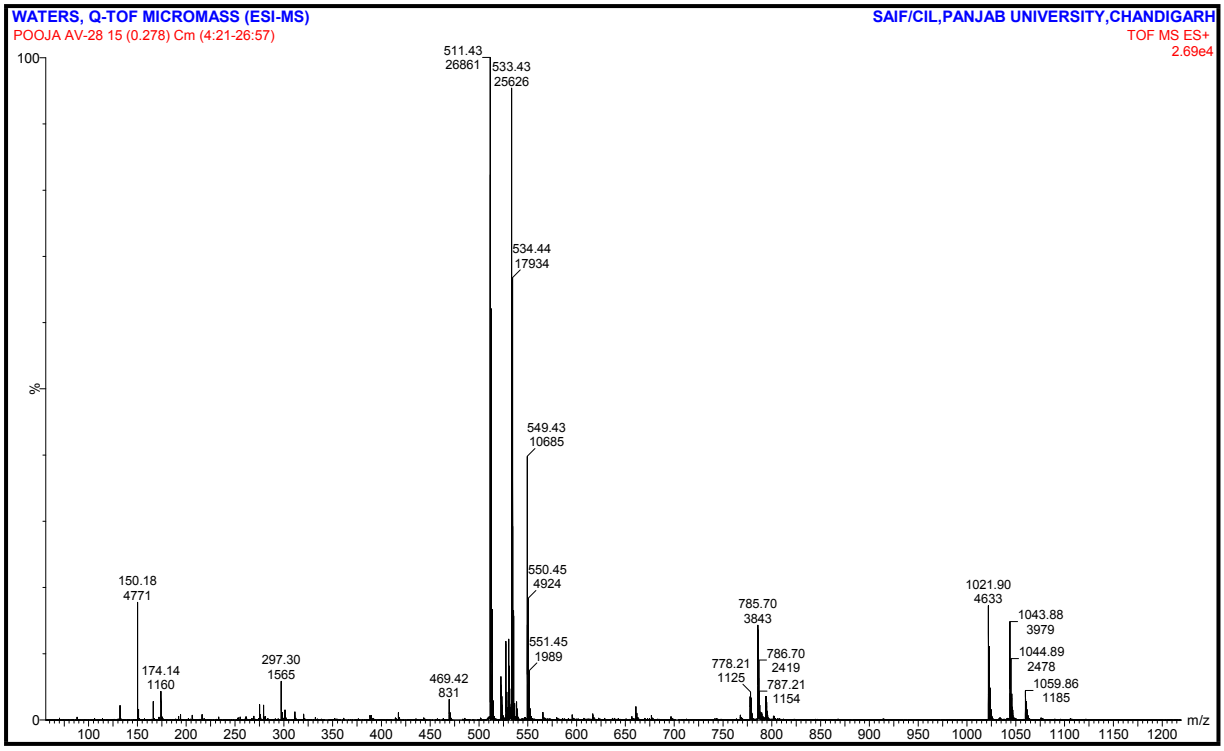
Mass spectrum of **5a**.



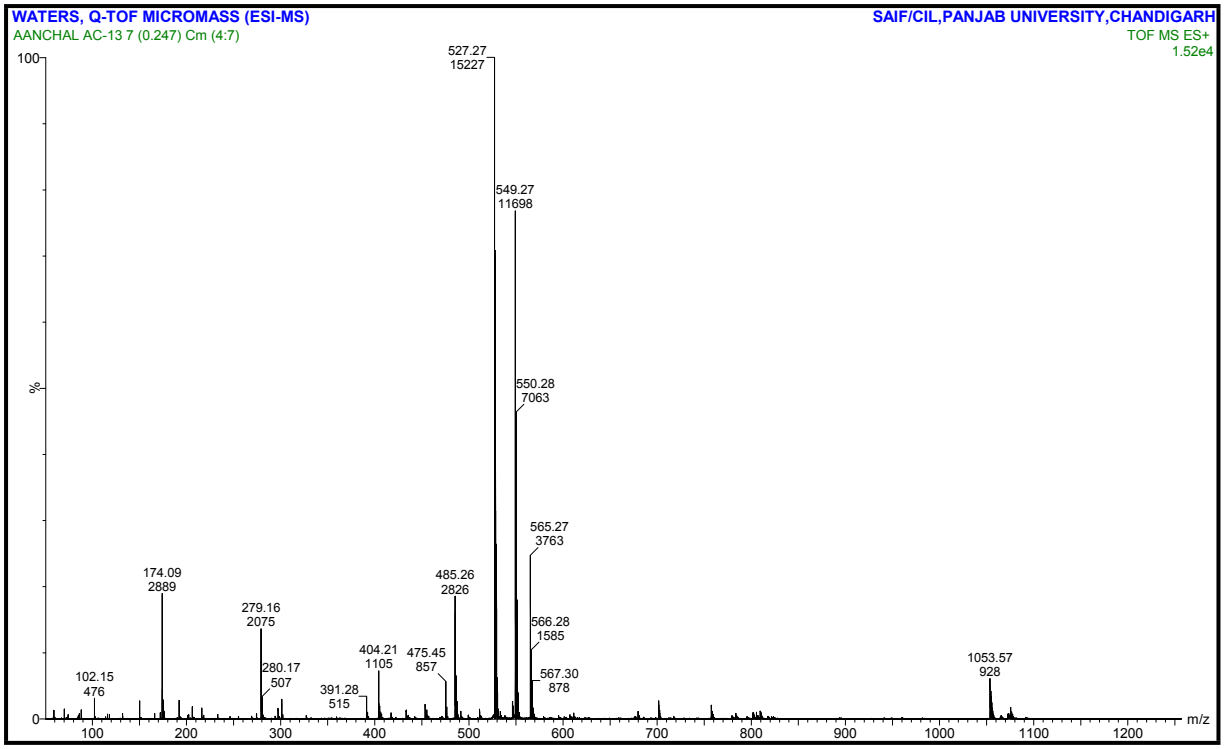
Mass spectrum of **7a**.



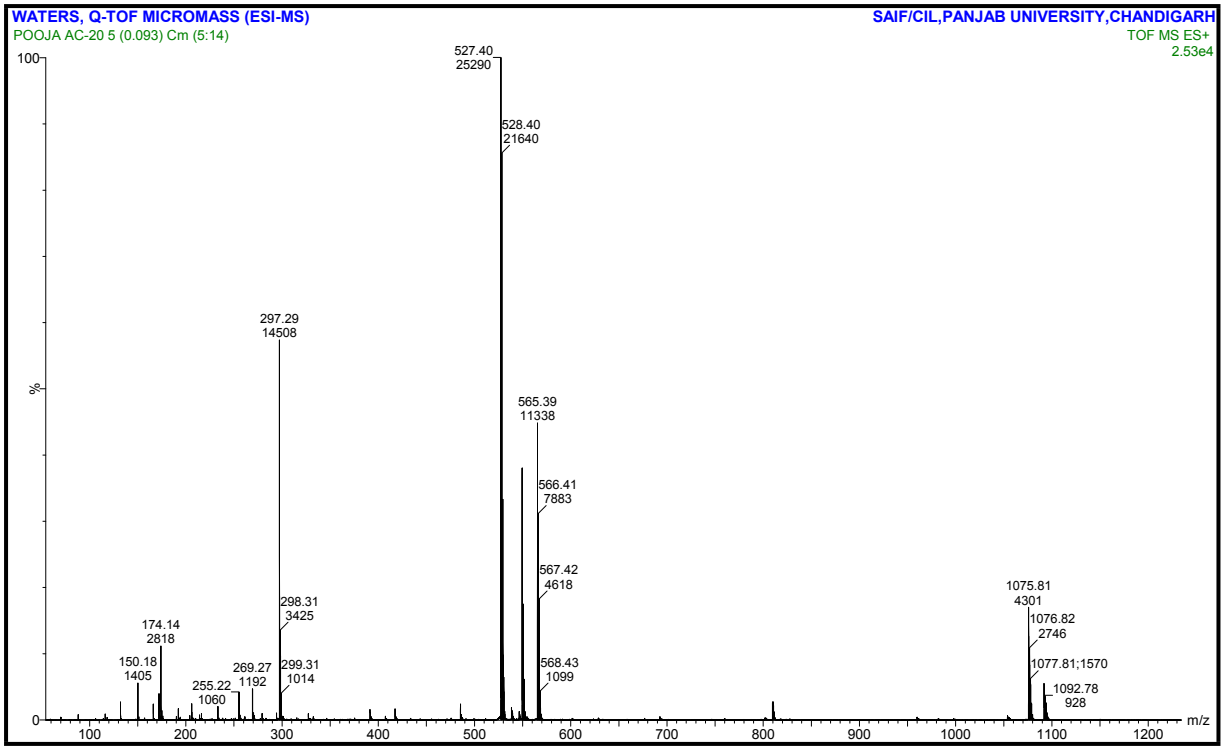
Mass spectrum of **7b**.



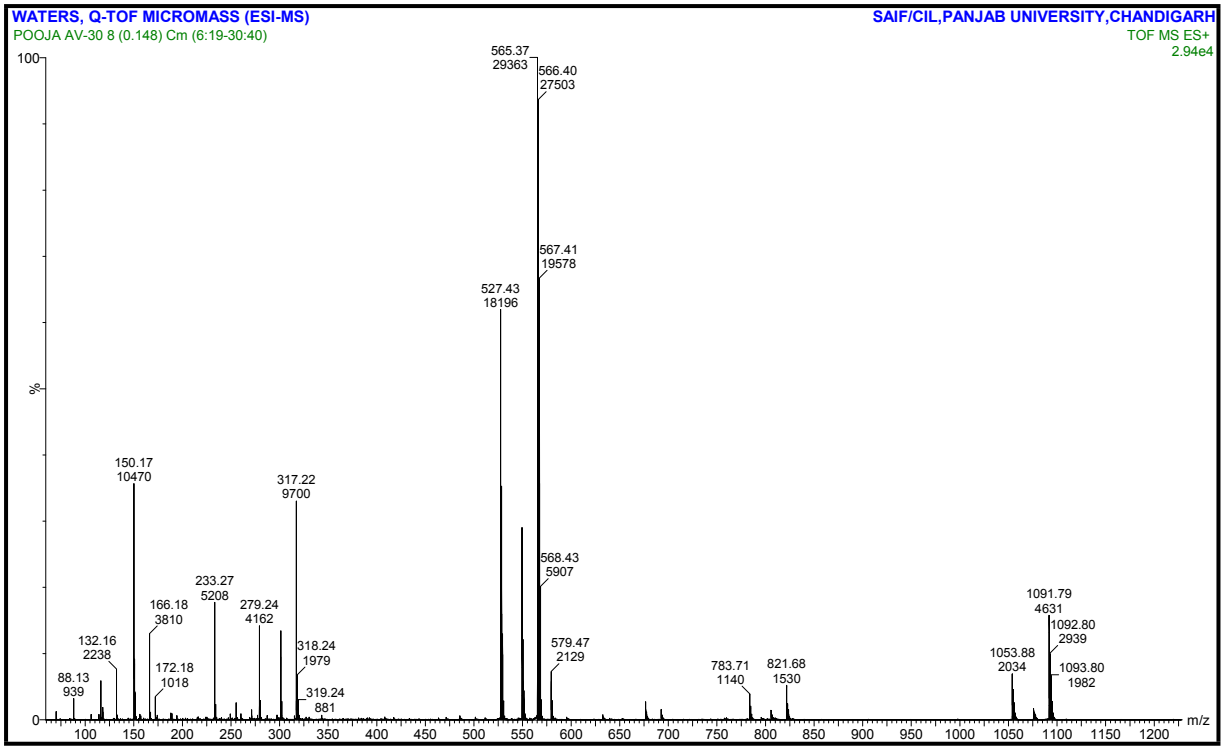
Mass spectrum of **7c**.



Mass spectrum of **8a**.



Mass spectrum of **8b**.



Mass spectrum of **8c**.