Supporting Information

Metal Free TBHP-Promoted Intramolecular Carbonylation of Arenes via Radical Cross-Dehydrogenative Coupling: Synthesis of Indenoquinolinones, 4-Azafluorenones and Fluorenones

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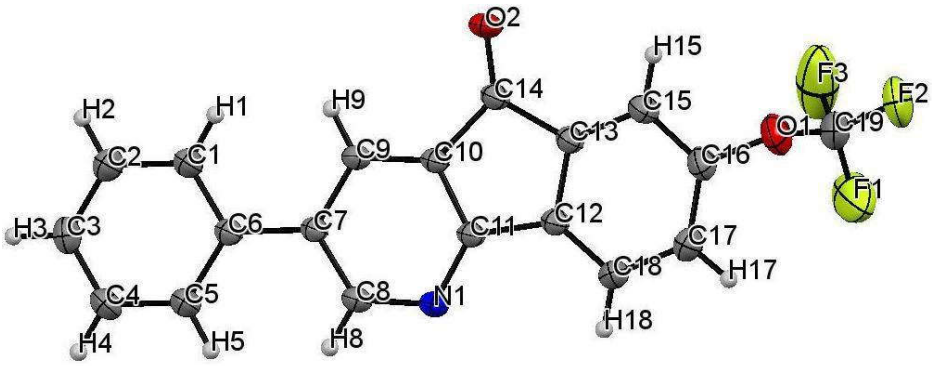
X-Ray Crystallography of compound 7r:

X-ray single crystal structural data of compounds **7r** is collected on Agilent Xcalibur, Eos diffractometer equipped with Enhance (Mo) X-ray source and graphite monochromated Mo-Kα radiation (λ = 0.71073 Å). The program CrysAlis PRO (Agilent, 2012) was used for integration of diffraction profiles and absorption correction was made with SCALE3 ABSPACK scaling algorithm.[1] Structures is solved by SIR 92[2] and refined by full matrix least square method using SHELXL-2014/7[3] and WinGX version 2014.1.[4] All the non-hydrogen atoms were located from the difference Fourier map and refined anisotropically. The crystallographic and structure refinement data of 7r is summarized in Table 1. Selected bond lengths and angles are given in Table 2.

Image of **7r** in mercury
CCDC is **1472053**, Ellipsoid probability = 30%



Oak Ridge Thermal-Ellipsoid Plot (ORTEP) of **7r**
Ellipsoid probability = 30%, Bond line width = 2

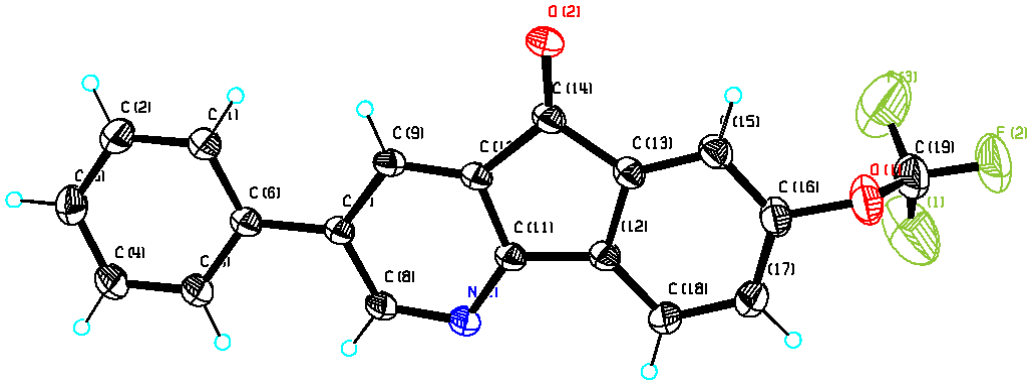


Table 1. Crystal data and structure refinement of **7r**.

Parameters	Molecule 7r
CCDC No.	1472053
Empirical formula	$C_{19}H_{10}F_3NO_2$
Formula Weight	341.28
Crystal system	triclinic
Space group	P-1

a (Å)	5.8910(5)
b (Å)	7.7688(6)
c (Å)	16.6580(14)
α (°)	84.298(6)
β (°)	82.177(7)
γ (°)	84.893(6)
V (A^3)	749.33(11)
Z	2
D_c (g cm^{-3})	1.513
μ (mm^{-1})	0.124
F (000)	348
T (K)	293
λ (Mo K_α)(Å)	0.71073
Crystal size (mm)	0.13 x 0.25 x 0.33
Θ_{min}(°)	3.5
Θ_{max}(°)	32.5
Total data	7945
Unique data	4848
R_{int}	0.021
Data [I>2σ(I)]	2632
R^a	0.0734
$R_w{}^b$	0.2390
S	1.03

Table 2. Selected bond lengths (Å) and angles (º) in **7r.**

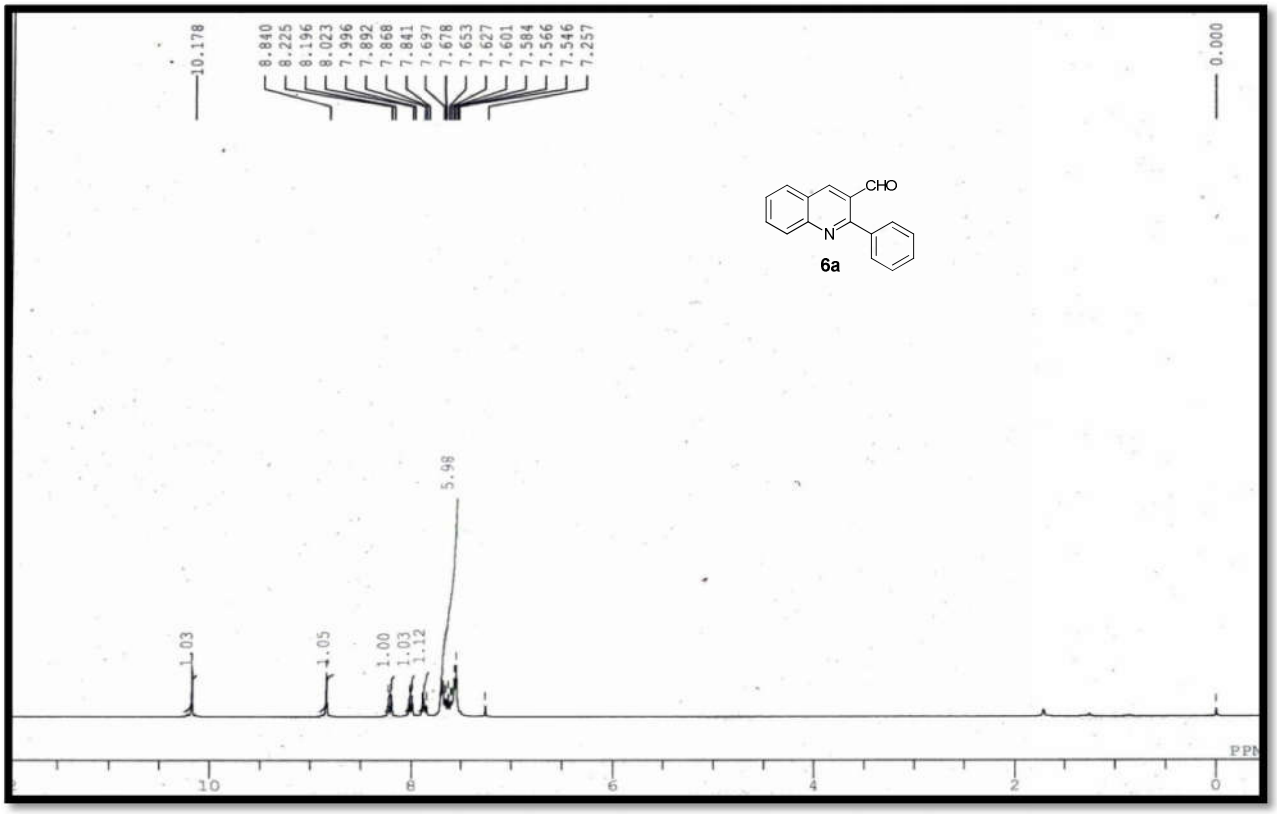
F1-C19	1.275(6)	C10-C14	1.490(3)
F2-C19	1.302(4)	C11 -C12	1.482(3)
F3-C19	1.294(6)	C12-C13	1.403(3)
O1-C16	1.417(3)	C12-C18	1.374(3)
O1-C19	1.308(5)	C13-C14	1.497(3)
O2-C14	1.212(3)	C13-C15	1.381(3)
N1-C8	1.350(3)	C15-C16	1.379(4)
N1-C11	1.332(3)	C16-C17	1.379(4)
C1-C2	1.388(4)	C17-C18	1.391(4)
C1-C6	1.389(3)	C1-H1	0.9300
C2-C3	1.368(4)	C2-H2	0.9300
C3-C4	1.371(4)	C3-H3	0.9300
C4-C5	1.382(4)	C4-H4	0.9300
C5-C6	1.394(4)	C5-H5	0.9300
C6-C7	1.490(3)	C8-H8	0.9300
C7-C8	1.398(3)	C9-H9	0.9300
C7-C9	1.405(3)	C15-H15	0.9300
C9-C10	1.373(3)	C17-H17	0.9300
C10-C11	1.402(3)	C18-H18	0.9300

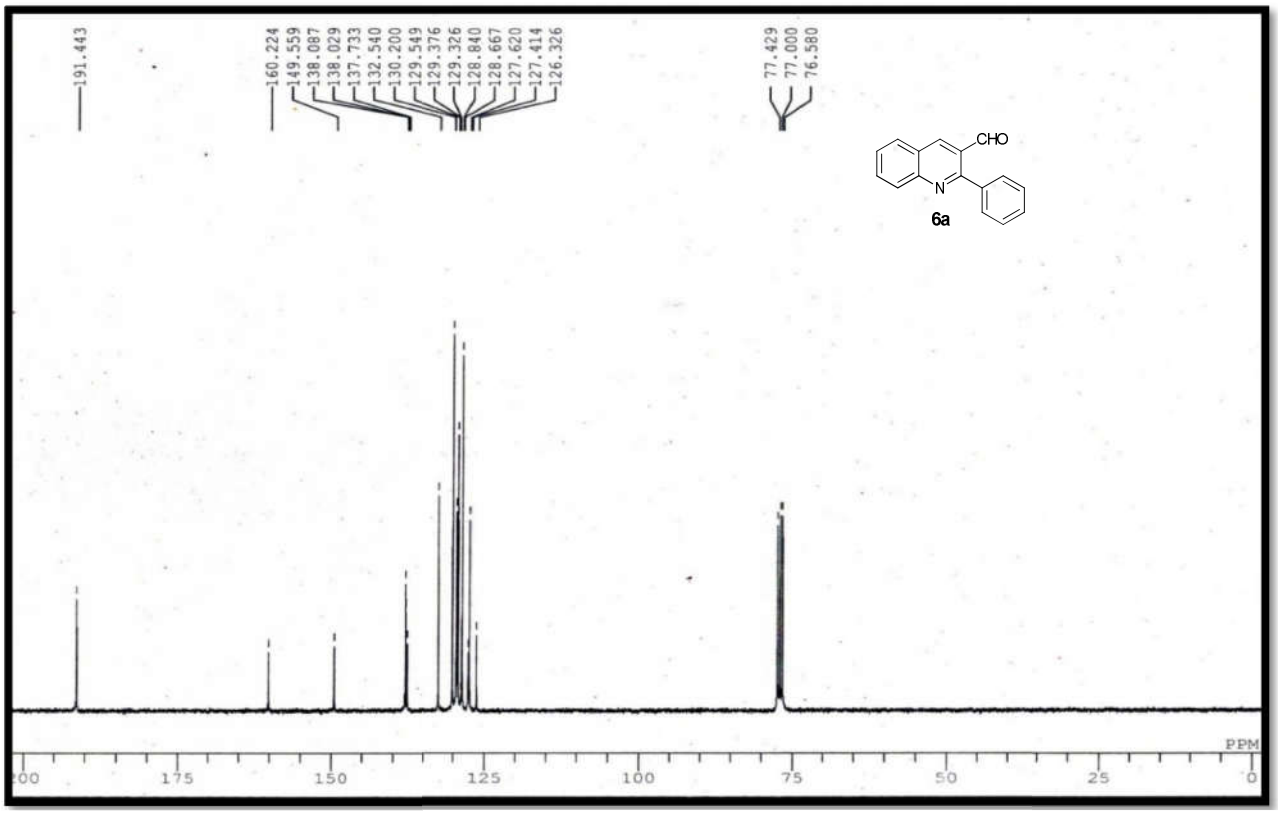
C16-O1-C19	118.5(3)	O2-C14-C13	126.8(2)
C8-N1-C11	115.03(19)	C10-C14-C13	105.43(19)
C2-C1-C6	121.2(2)	C13-C15-C16	117.0(2)
C1-C2-C3	120.7(3)	O1-C16-C15	118.7(2)
C2-C3-C4	119.1(3)	O1-C16-C17	118.3(2)
C3-C4-C5	120.8(3)	C15-C16-C17	122.8(2)
C4-C5-C6	121.2(3)	C16-C17-C18	119.9(2)
C1-C6-C5	117.0(2)	C12-C18-C17	118.6(2)
C1-C6-C7	121.0(2)	F1-C19-F2	107.4(3)
C5-C6-C7	122.0(2)	F1-C19-F3	108.1(4)
C6-C7-C8	120.83(19)	F1-C19-O1	114.3(4)
C6-C7-C9	122.28(19)	F2-C19-F3	106.3(4)
C8-C7-C9	116.9(2)	F2-C19-O1	109.6(4)
N1-C8-C7	126.0(2)	F3-C19-O1	110.8(3)
C7-C9-C10	118.2(2)	C2-C1-H1	119.00
C9-C10-C11	119.9(2)	C6-C1-H1	119.00
C9-C10-C14	131.8(2)	C1-C2-H2	120.00
C11-C10-C14	108.35(19)	C3-C2-H2	120.00
N1-C11-C10	124.0(2)	C2-C3-H3	120.00
N1-C11-C12	126.69(19)	C4-C3-H3	120.00
C10-C11-C12	109.33(18)	C3-C4-H4	120.00
C11-C12-C13	107.88(19)	C5-C4-H4	120.00
C11-C12-C18	131.6(2)	C4-C5-H5	119.00
C13-C12-C18	120.6(2)	C6-C5-H5	119.00
C12-C13-C14	109.0(2)	N1-C8-H8	117.00
C12-C13-C15	121.3(2)	C7-C8-H8	117.00
C14-C13-C15	129.7(2)	C7-C9-H9	121.00
O2-C14-C10	127.8(2)	C10-C9-H9	121.00
C13-C15-H15	122.00	C18-C17-H17	120.00
C16-C15-H15	121.00	C12-C18-H18	121.00
C16-C17-H17	120.00	C17-C18-H18	121.00

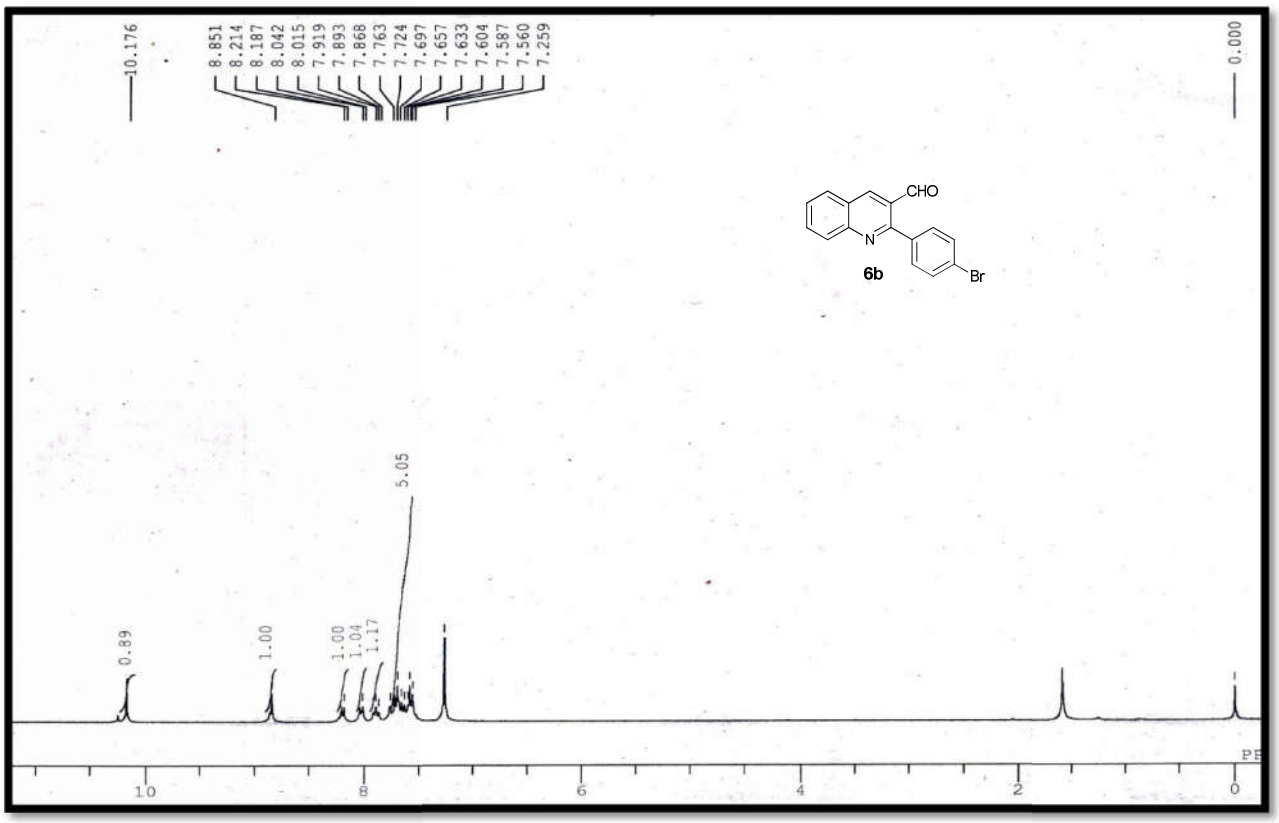
References

1. Agilent, (2012) *CrysAlis PRO* Agilent Technologies, Yarnton, England.
2. a) A. Altomare, G. Cascarano, C. Giacovazzo, and A. Gualaradi, *J. Appl. Cryst*. **1993**, *26*, 343. b) A. Altomare, M. C. Burla, G. Camalli, G. Cascarano, C. Giacovazzo, A. Gualiardi and G. Polidori, J. Appl. Cryst. 1994, **27**, 435.
3. G. M. Sheldrick, *ActaCryst.,* 2008, **A64**, 112-122.
4. L. J. Farrugia, WinGX-A Windows Program for Crystal Structure Analysis, *J. Appl. Cryst.,* 2012, **45**, 849-854.

^{1}H NMR (300 MHz) and ^{13}CNMR (75 MHz) Spectra of starting materials



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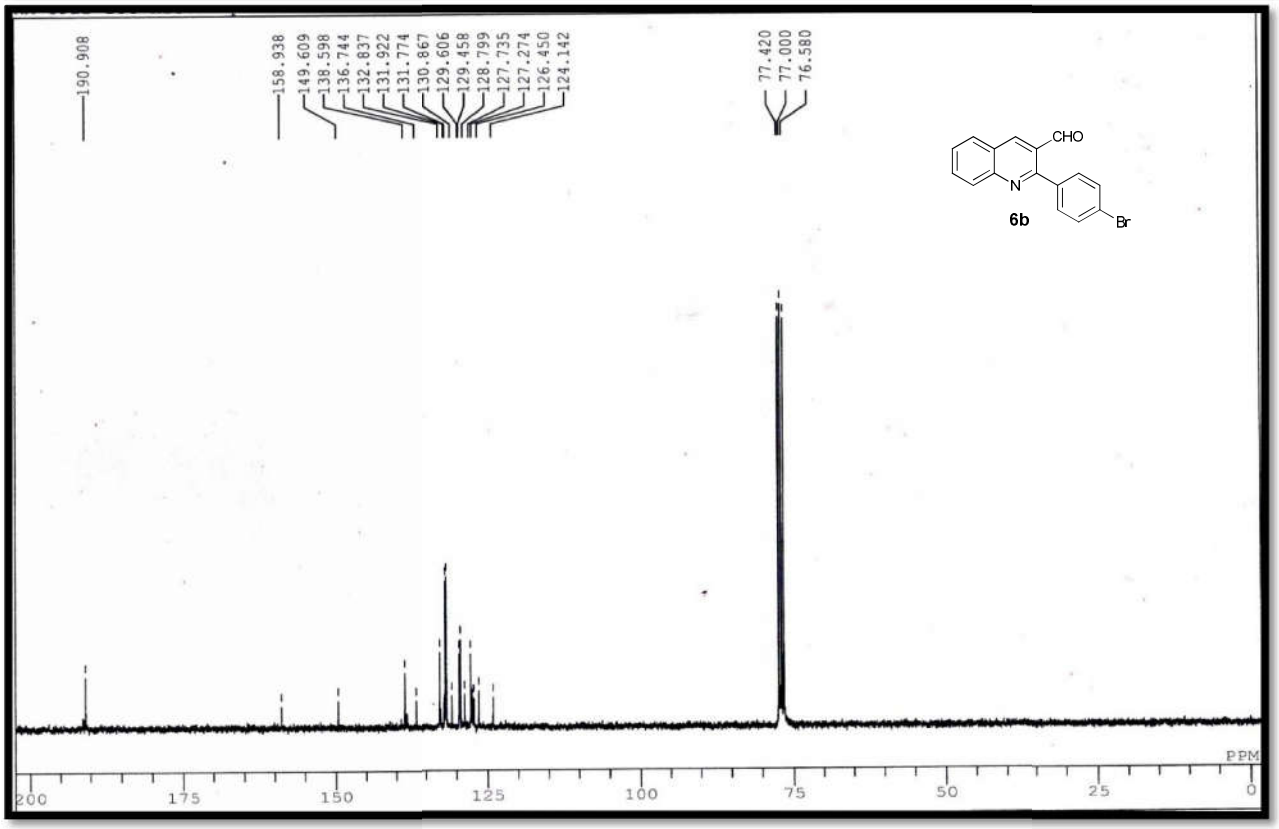
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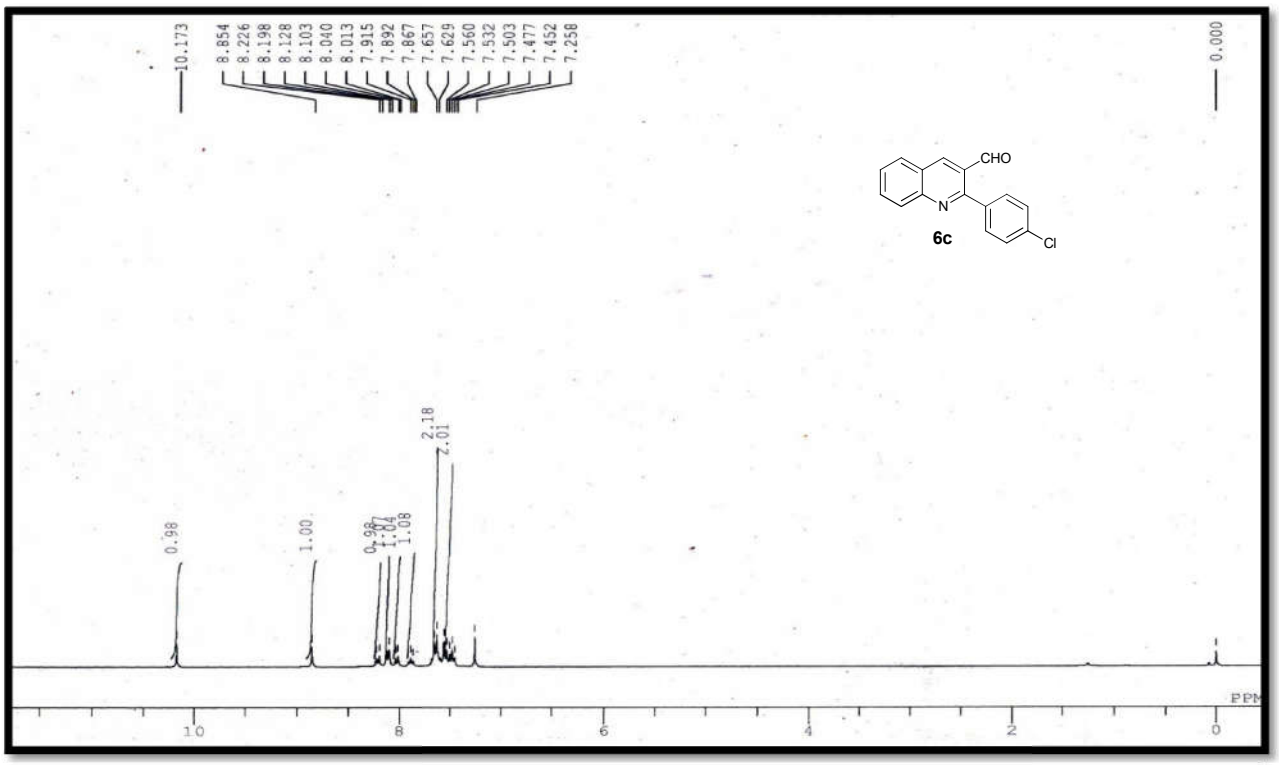
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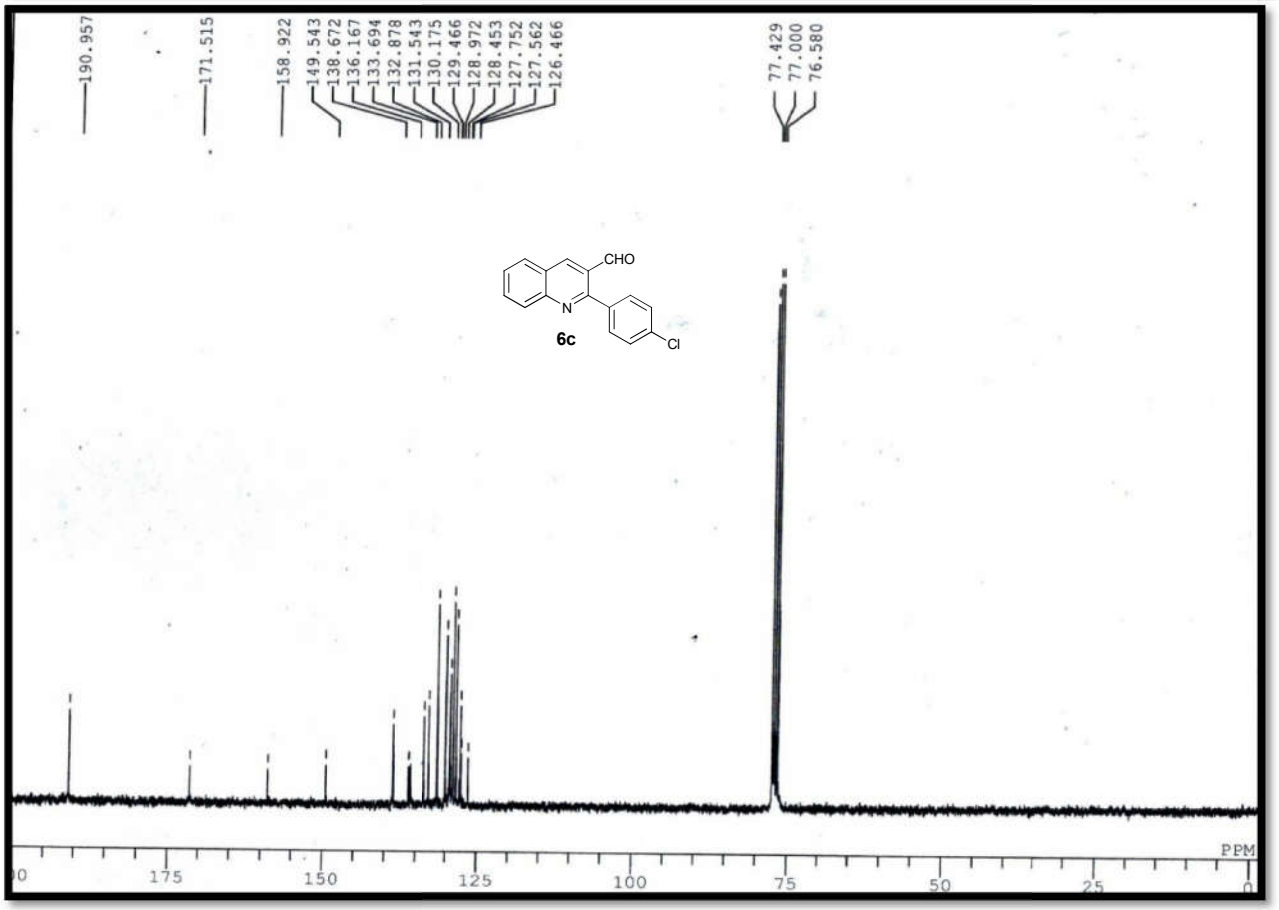
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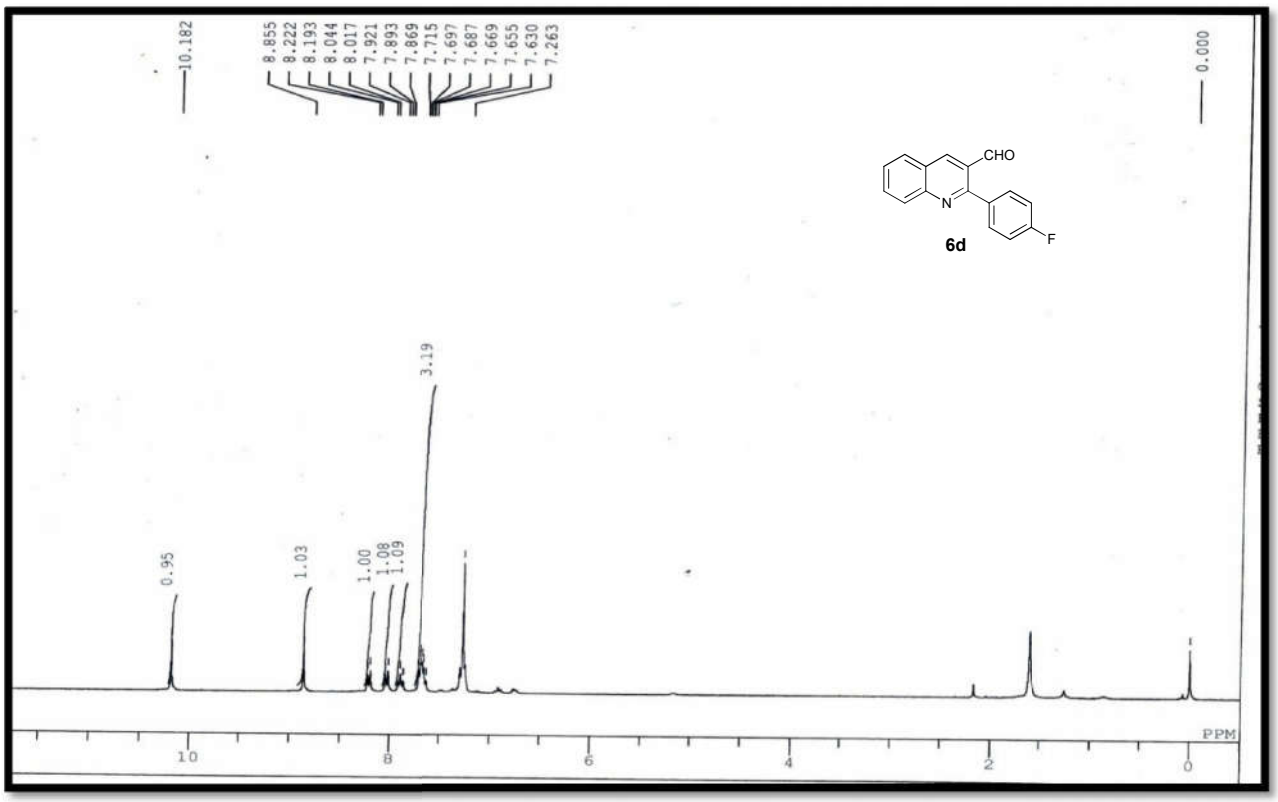
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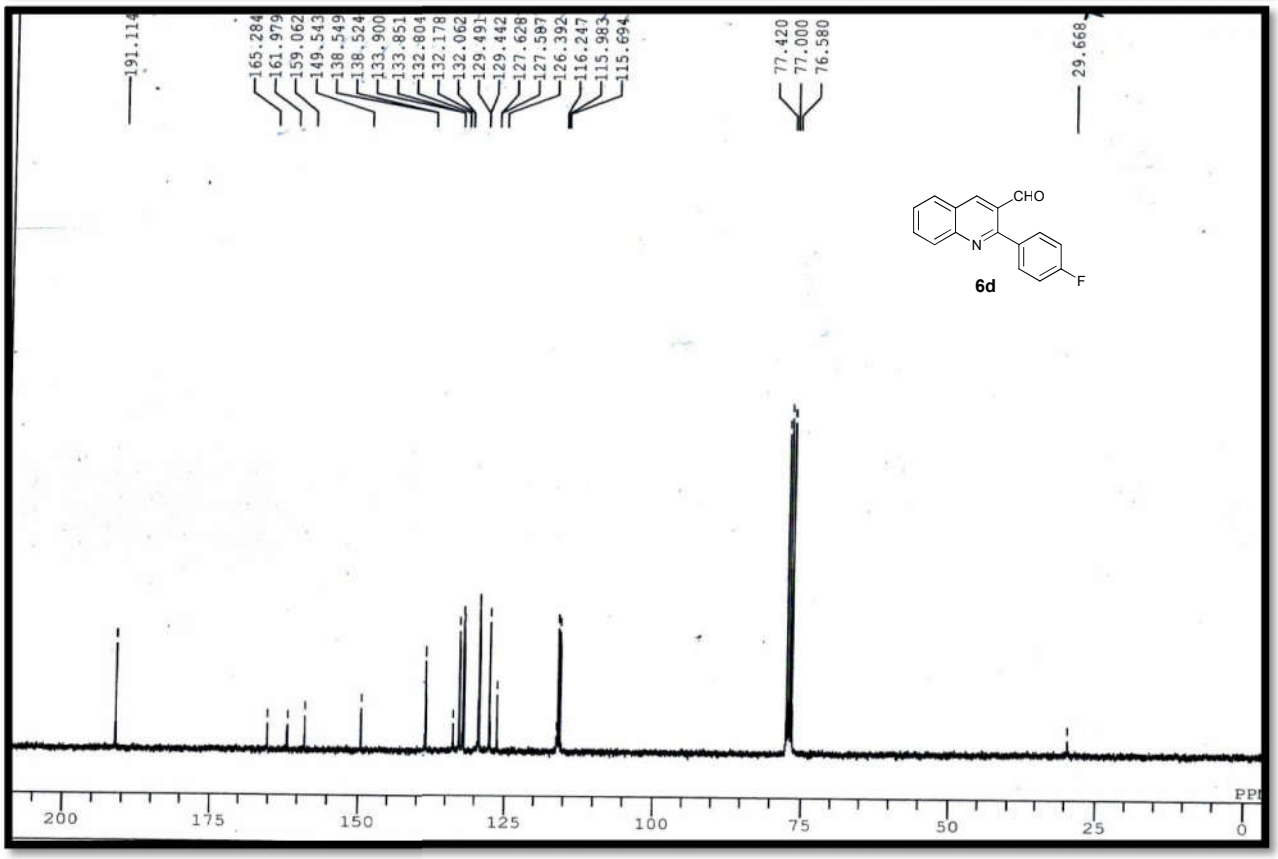
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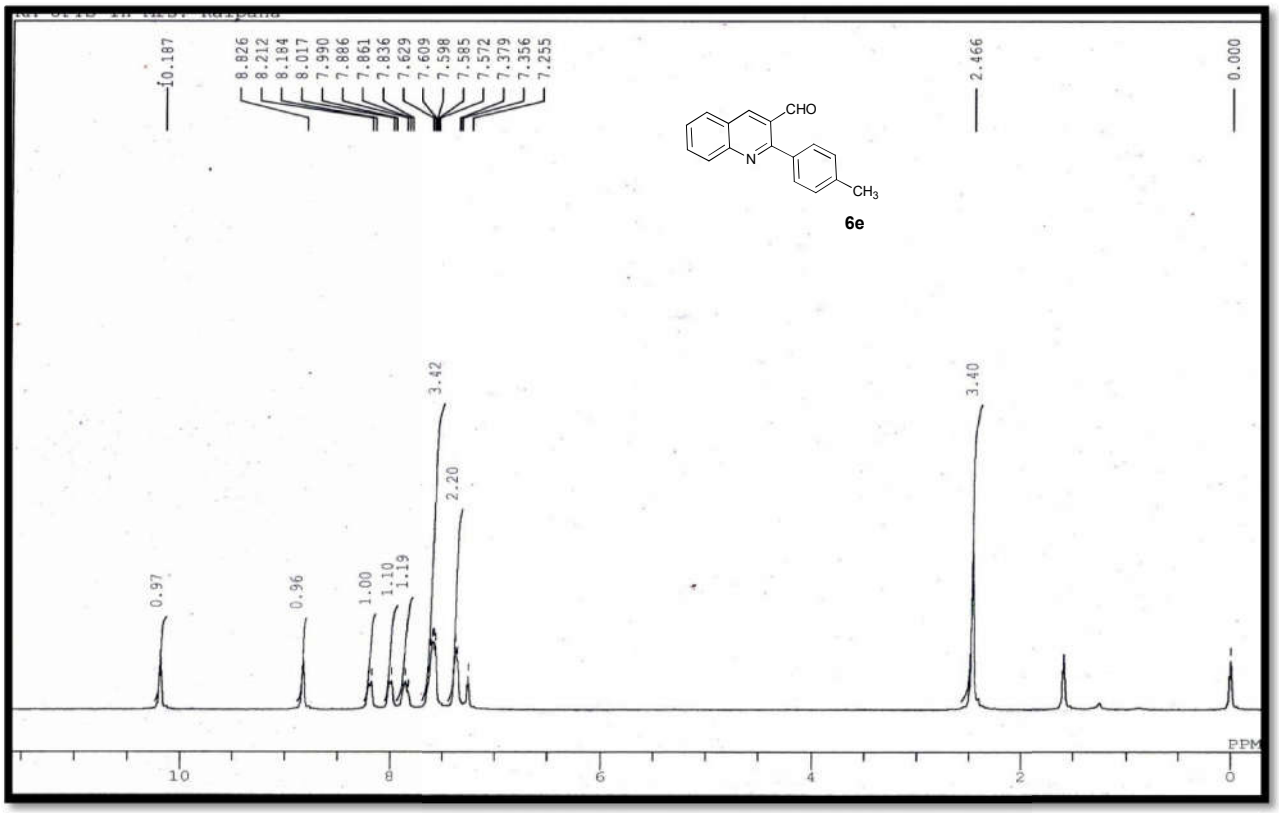
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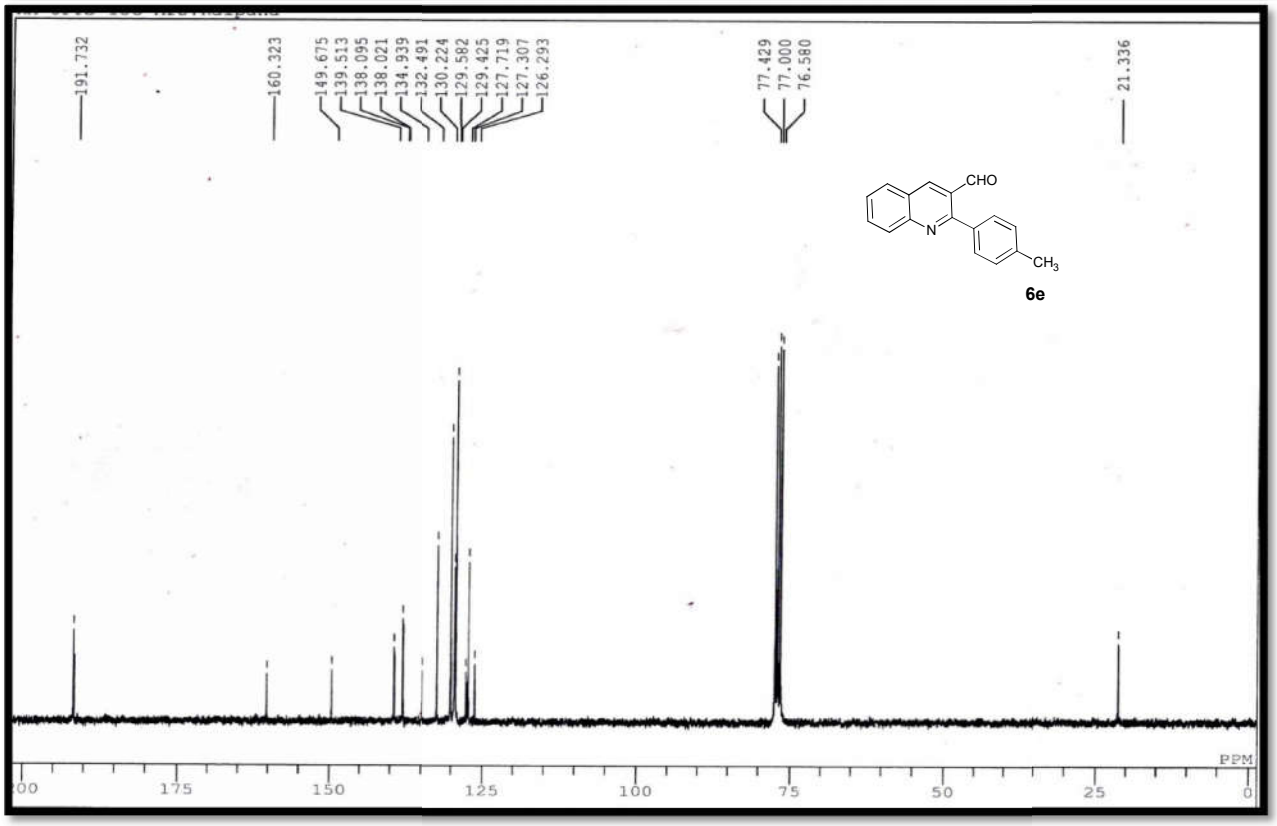
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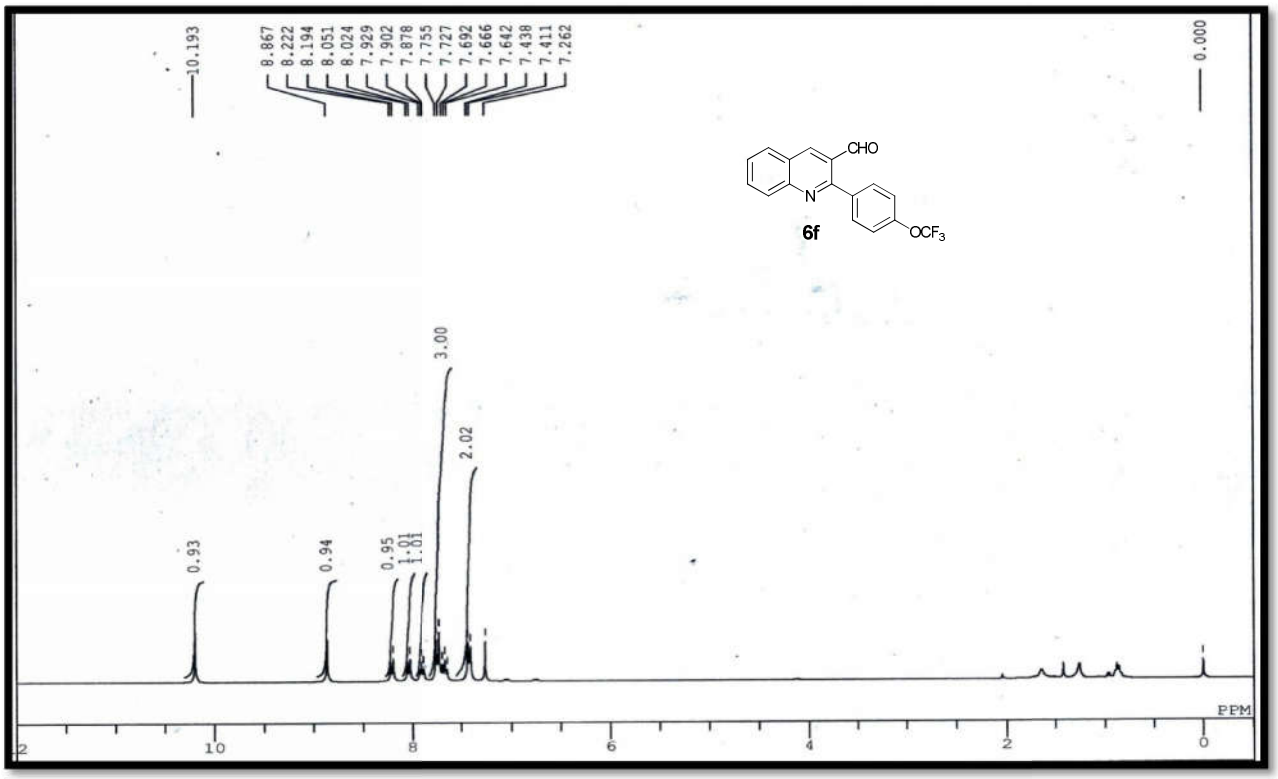
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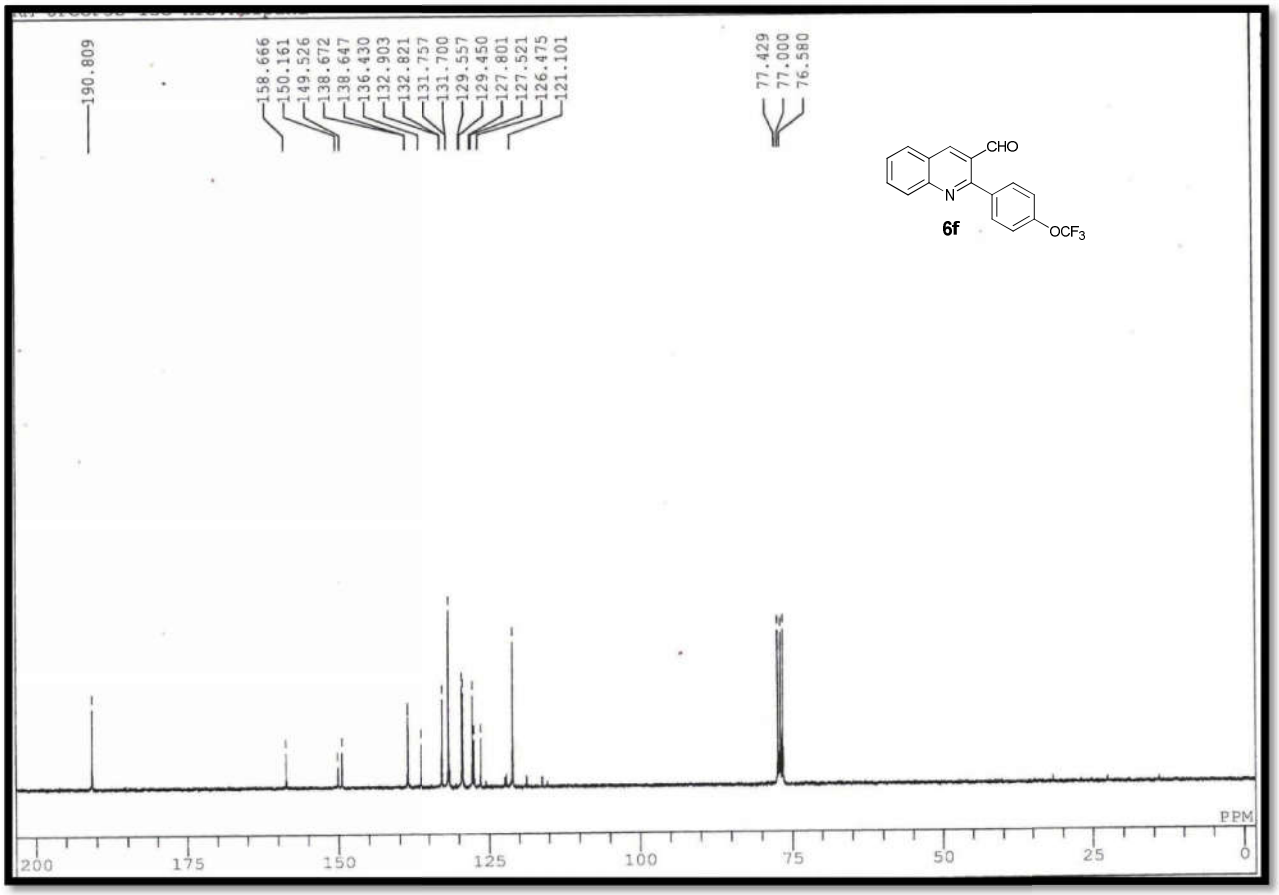
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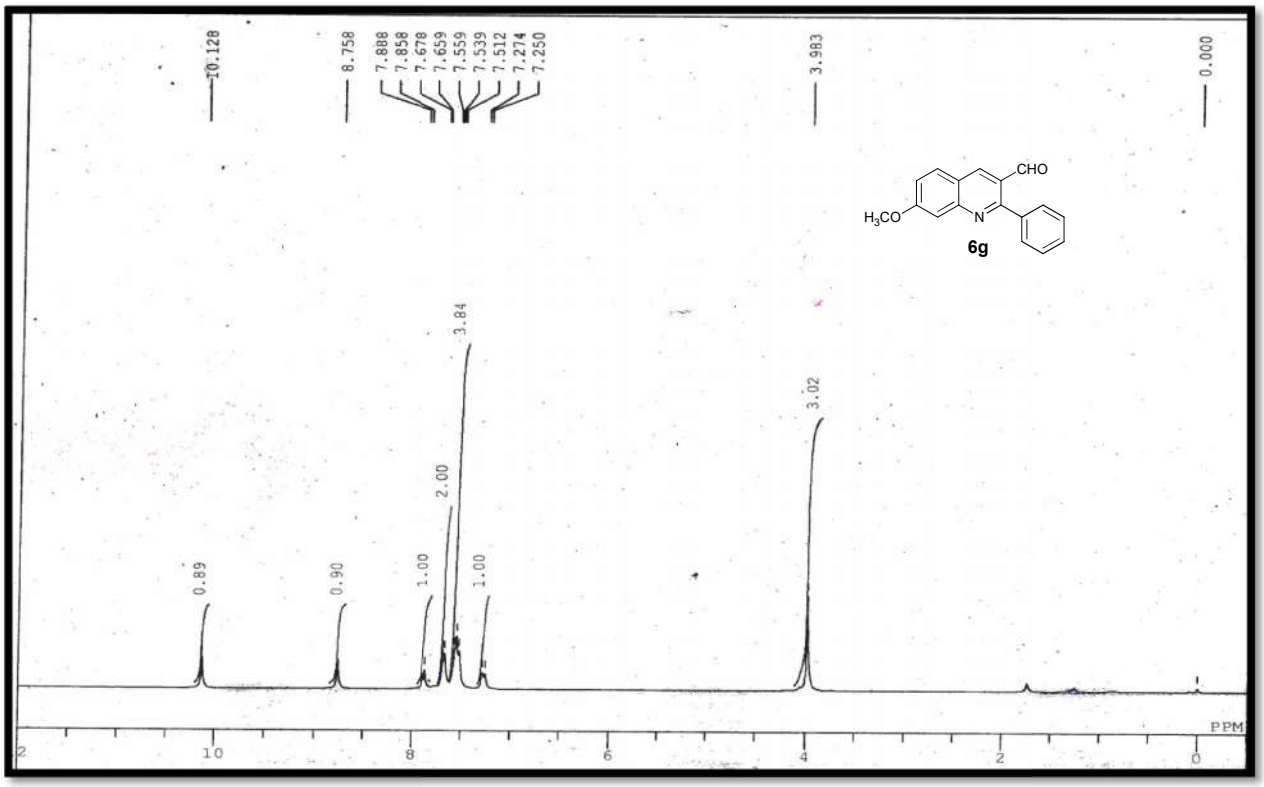
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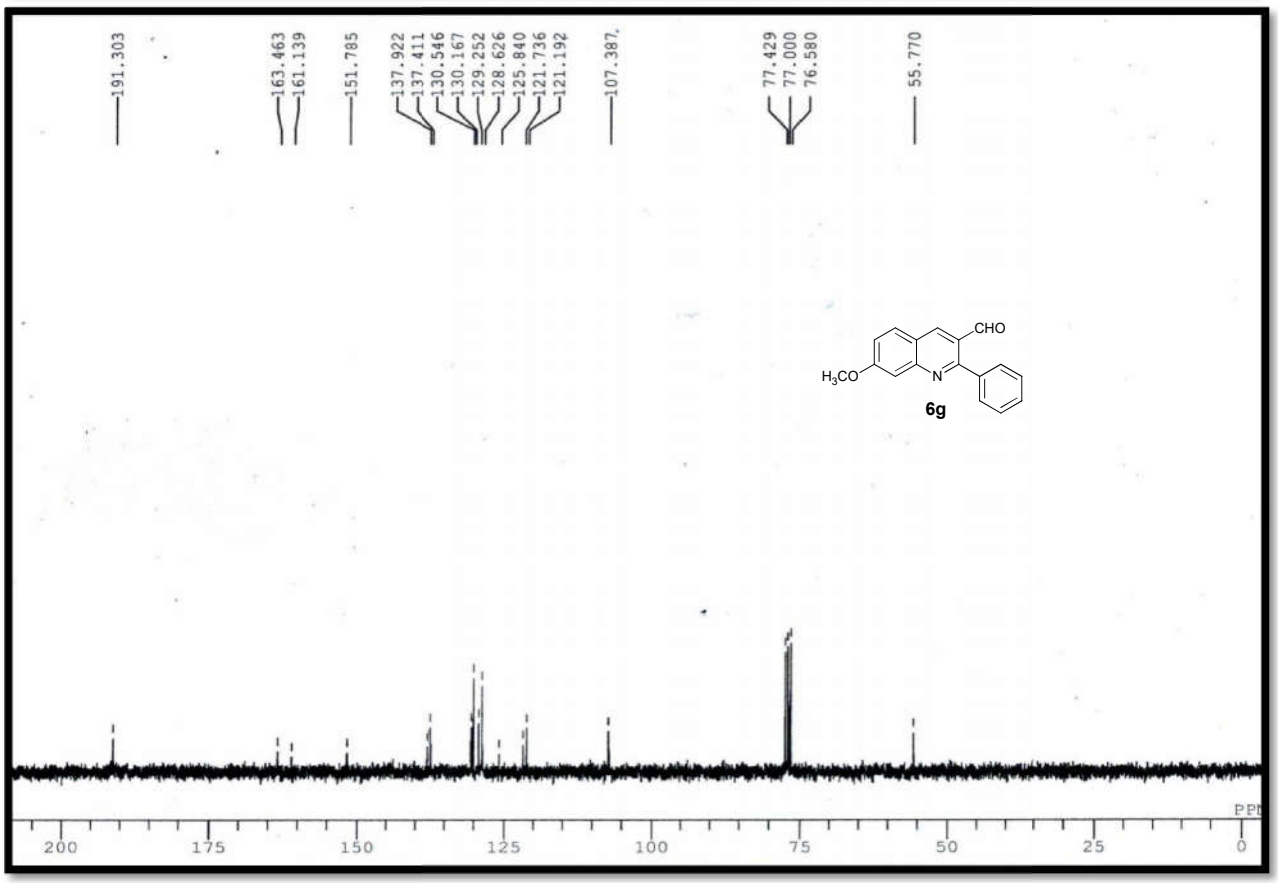
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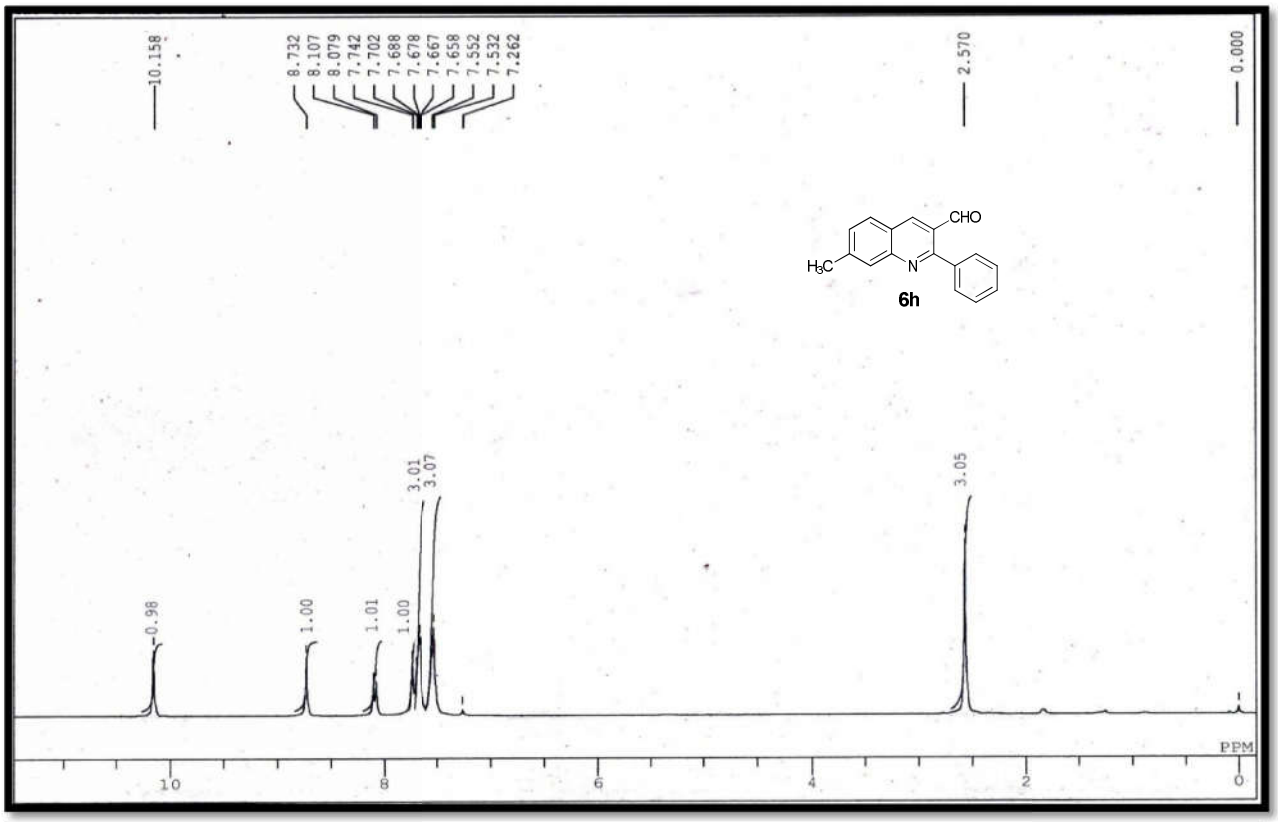
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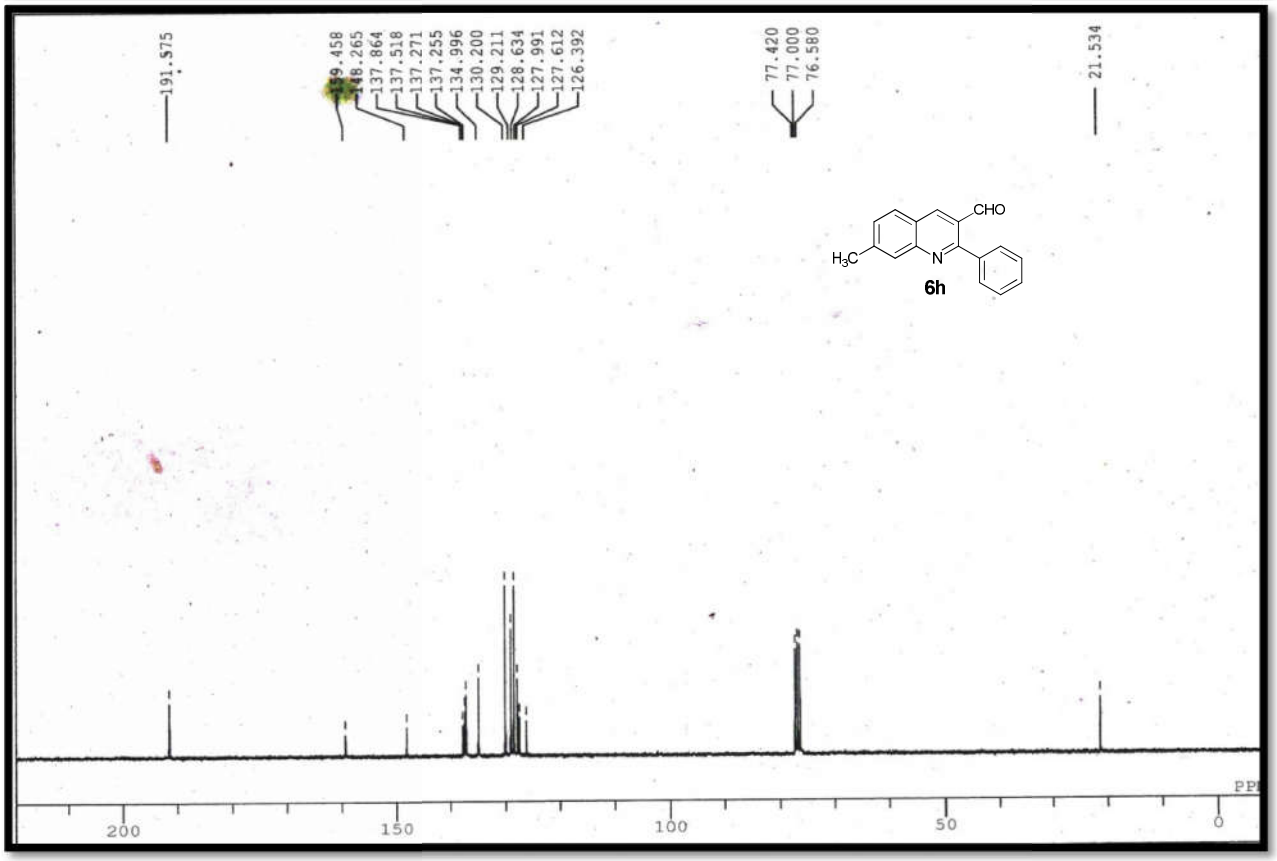
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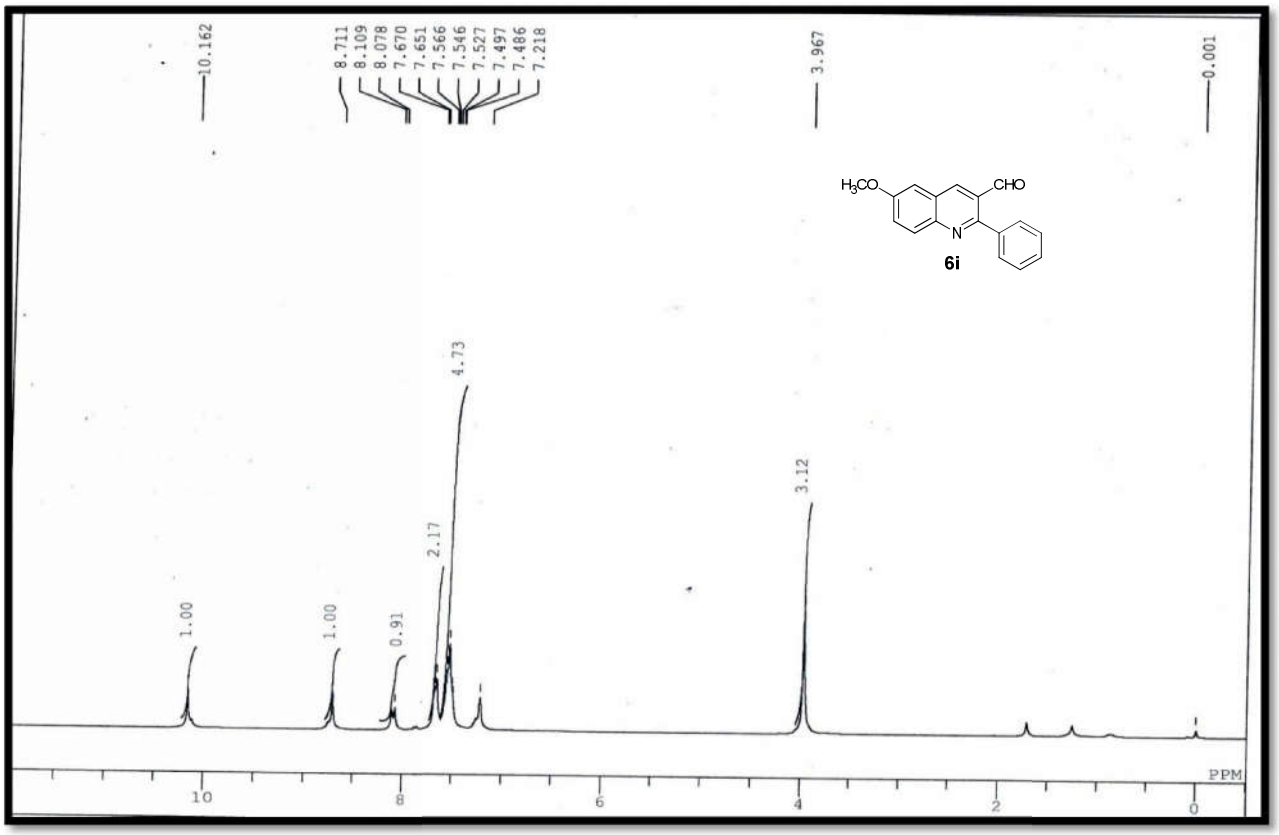
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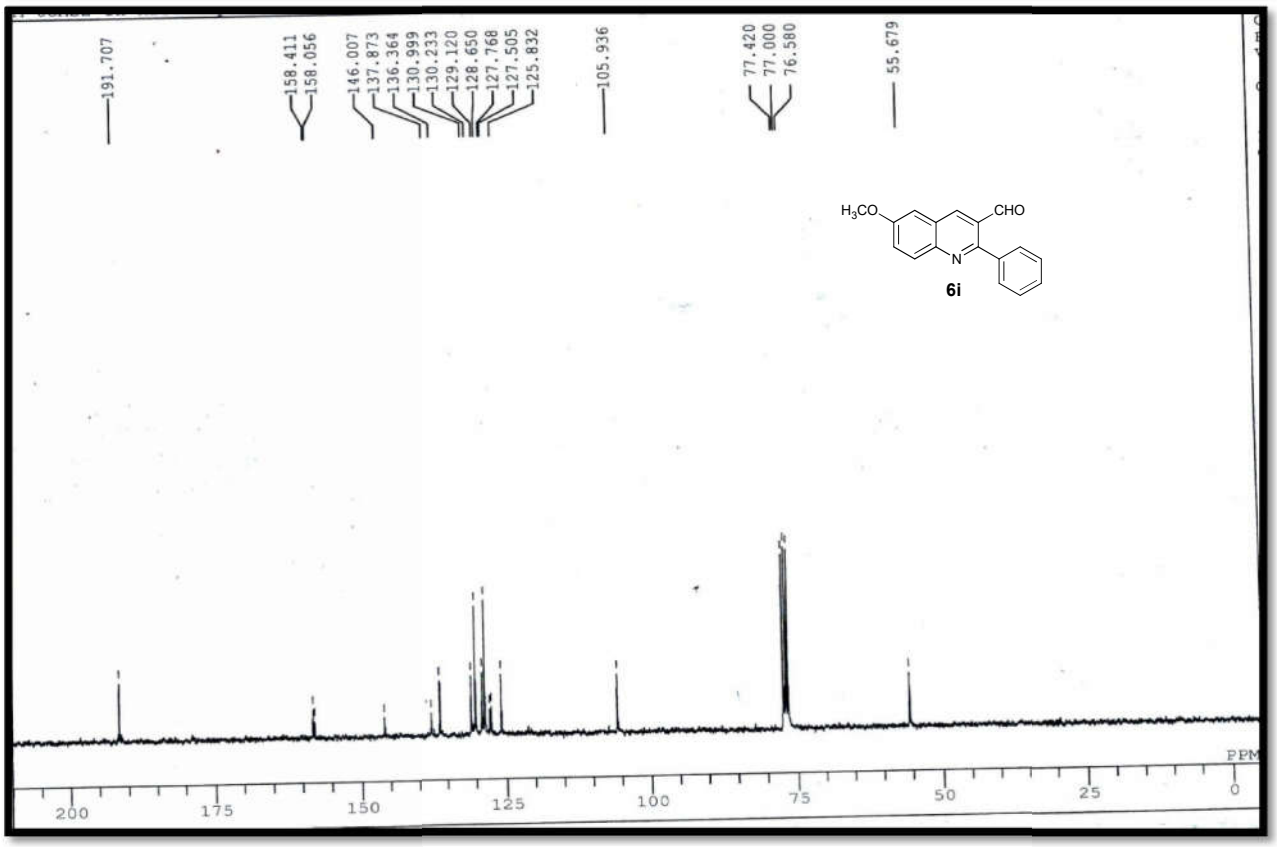
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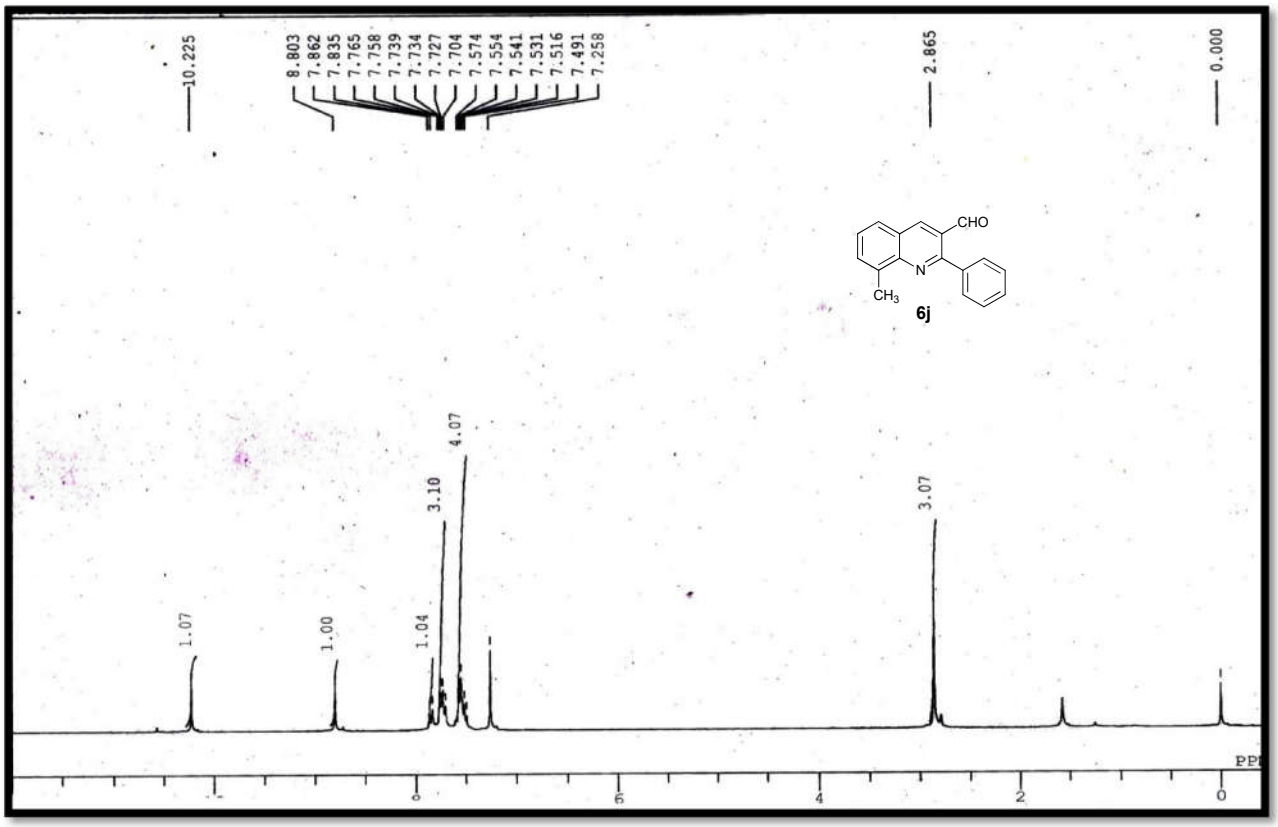
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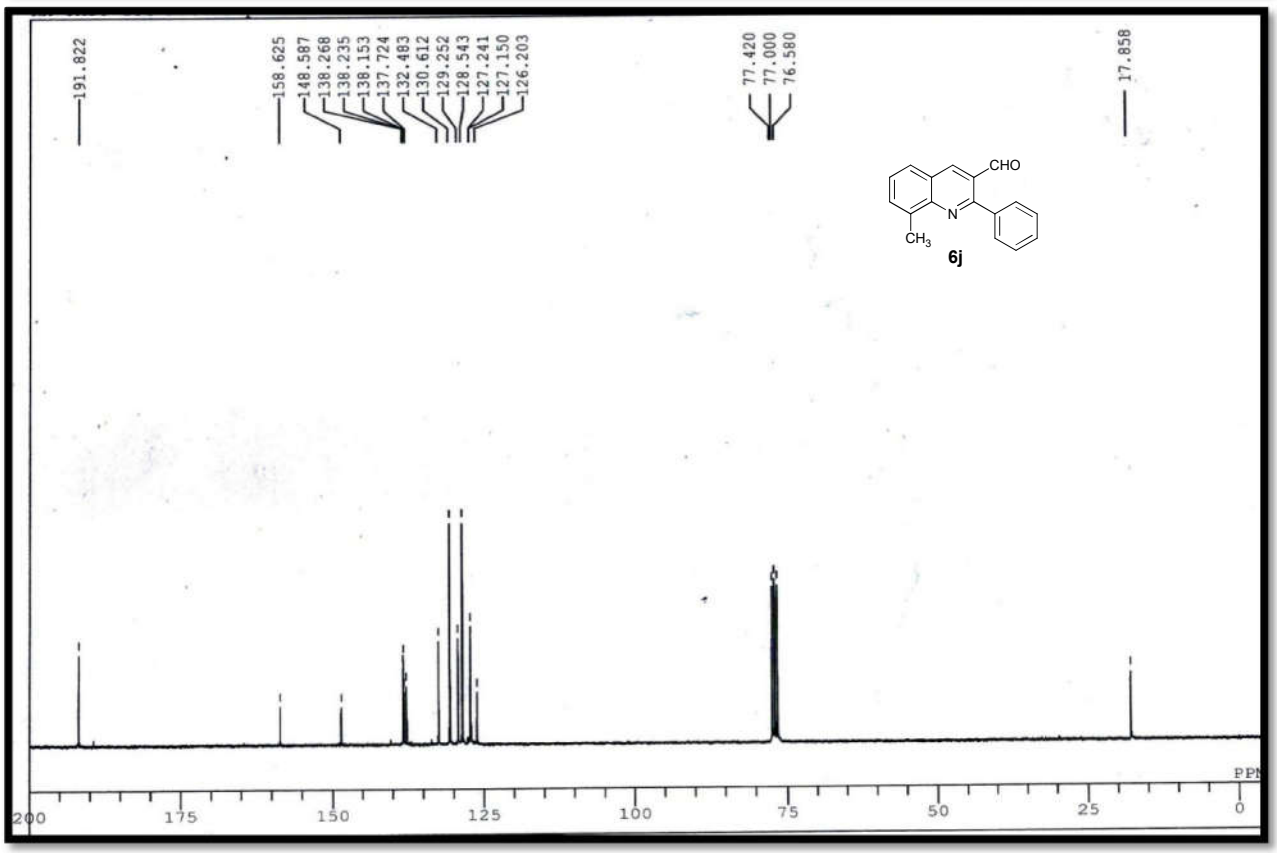
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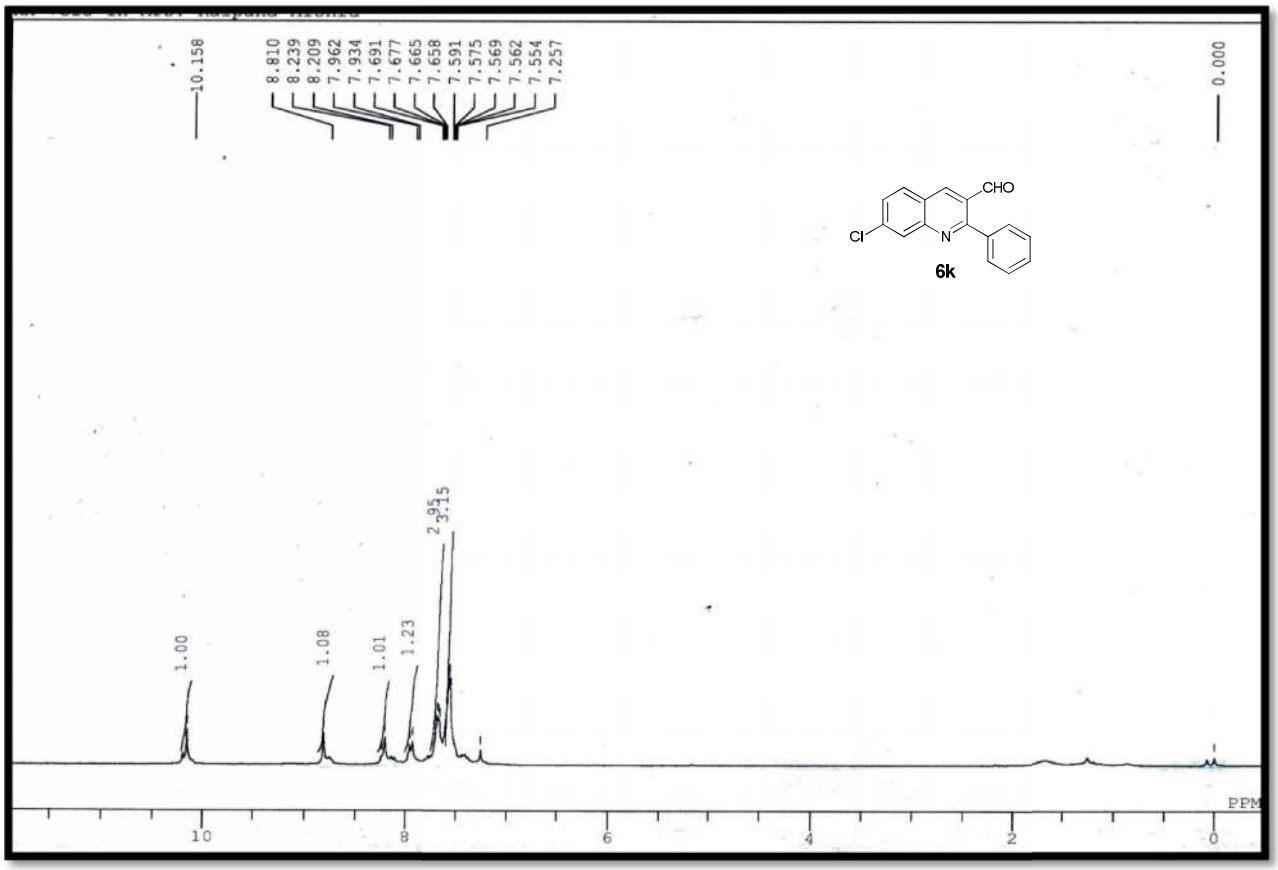
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8.239
8.209
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7.691
7.677
7.665
7.658
7.591
7.575
7.569
7.562
7.554
7.257
0.000
CHO
Cl
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3.15
1.00
1.08
1.01
1.23
PPM
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6
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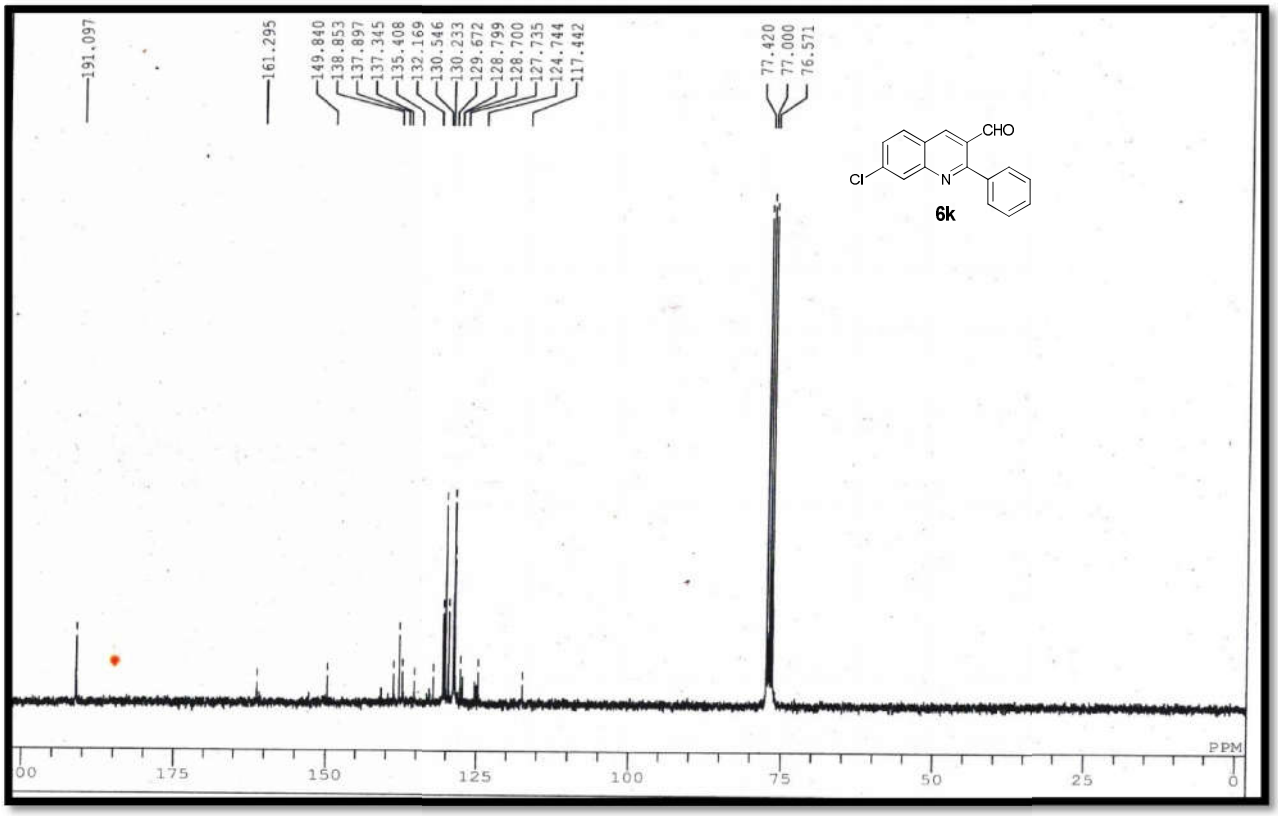
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137.345
135.408
132.169
130.546
130.233
129.672
128.799
128.700
127.735
124.744
117.442
77.420
77.000
76.571
CHO
Cl
N
6k
PPM
00
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100
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50
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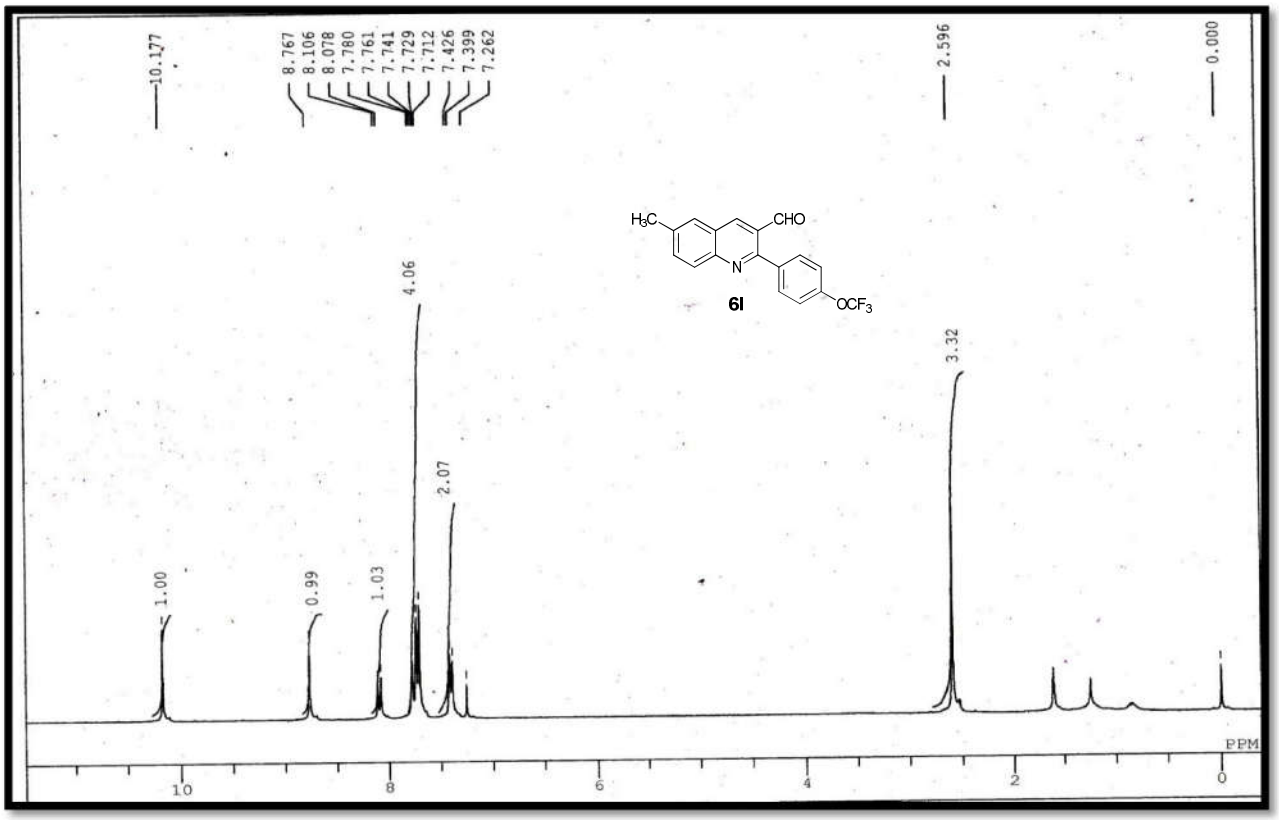
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8.106
8.078
7.780
7.761
7.741
7.729
7.712
7.426
7.399
7.262
2.596
0.000
H3C
CHO
N
OCF3
6l
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3.32
2.07
1.00
0.99
1.03
PPM
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8
6
4
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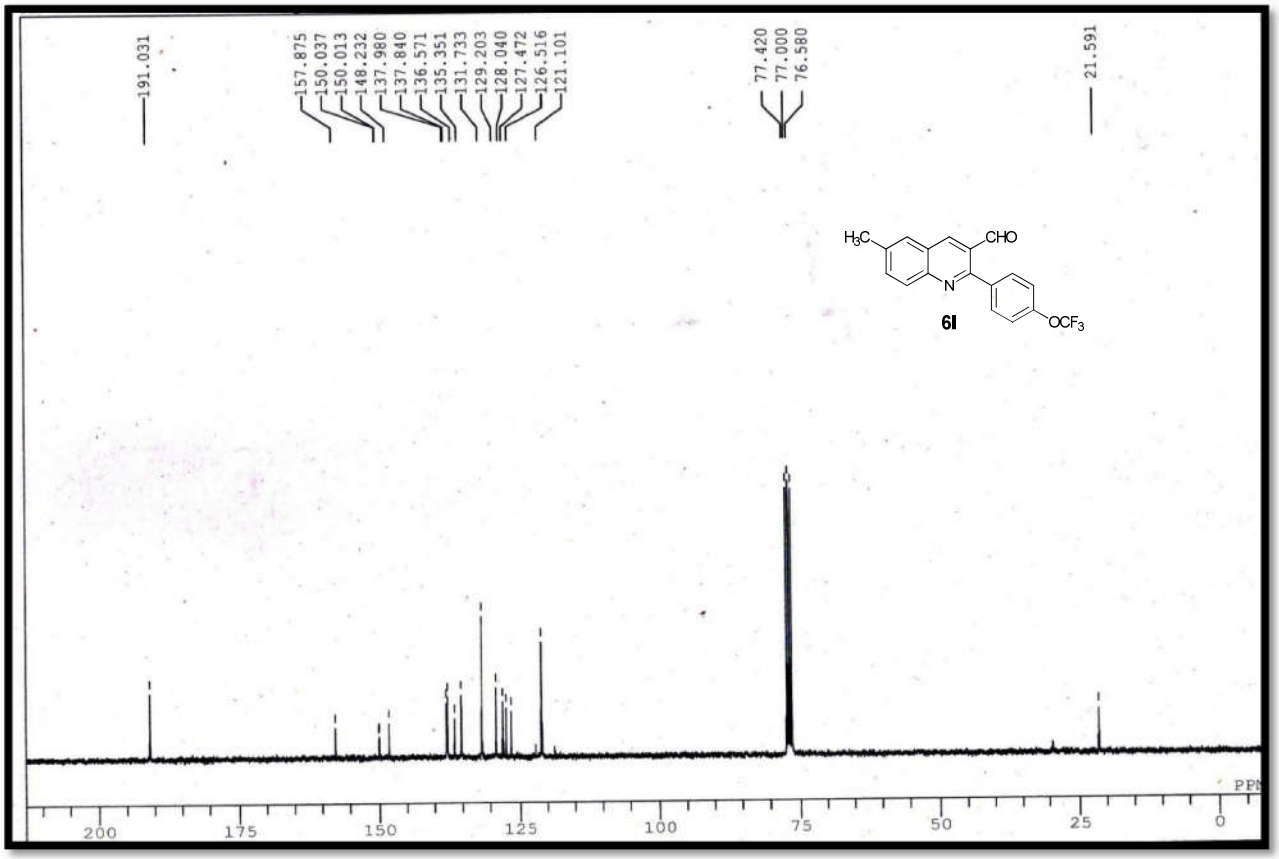
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137.980
137.840
136.571
135.351
131.733
129.203
128.040
127.472
126.516
121.101
77.420
77.000
76.580
21.591
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CHO
N
OCF3
6l
PPM
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175
150
125
100
75
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25
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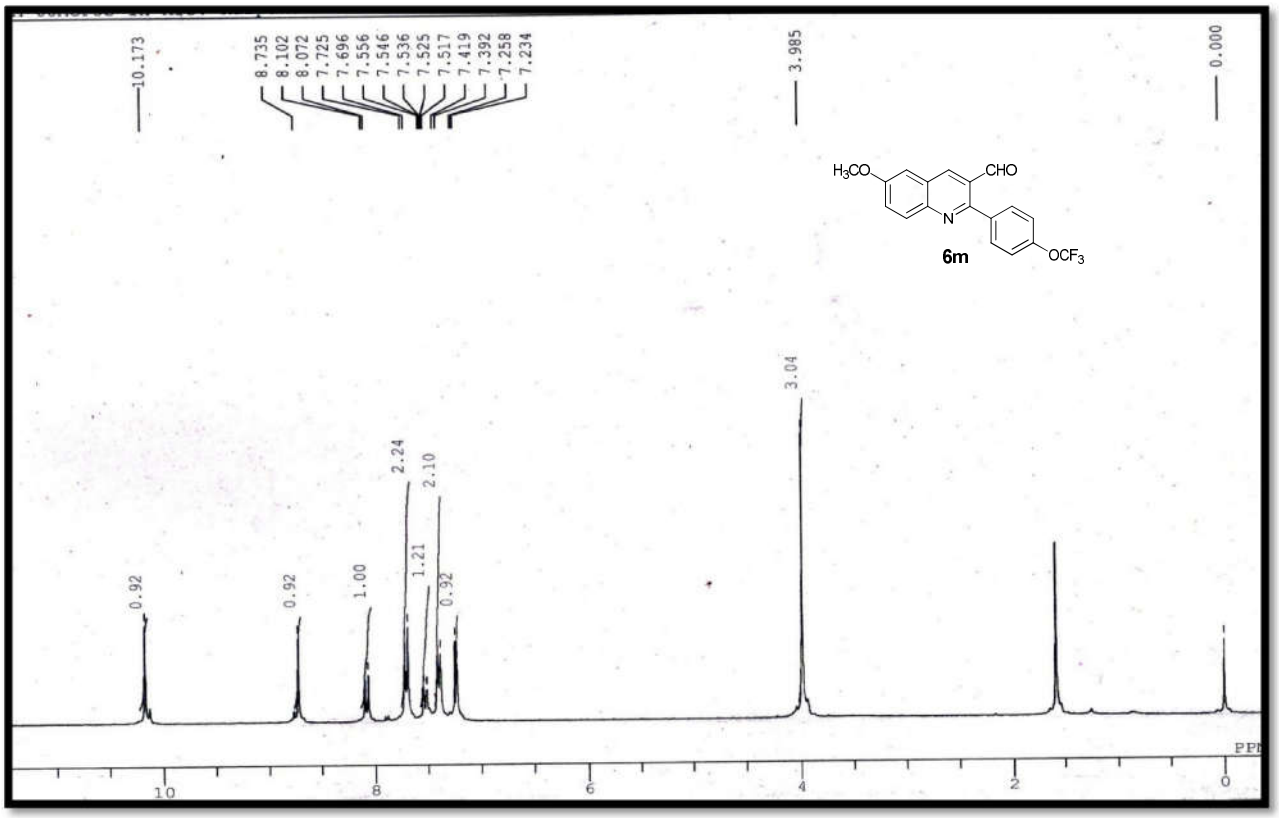
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8.102
8.072
7.725
7.696
7.556
7.546
7.536
7.525
7.517
7.419
7.392
7.258
7.234
3.985
0.000
H3CO
CHO
N
OCF3
6m
3.04
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2.10
1.21
0.92
0.92
1.00
0.92
PPM
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8
6
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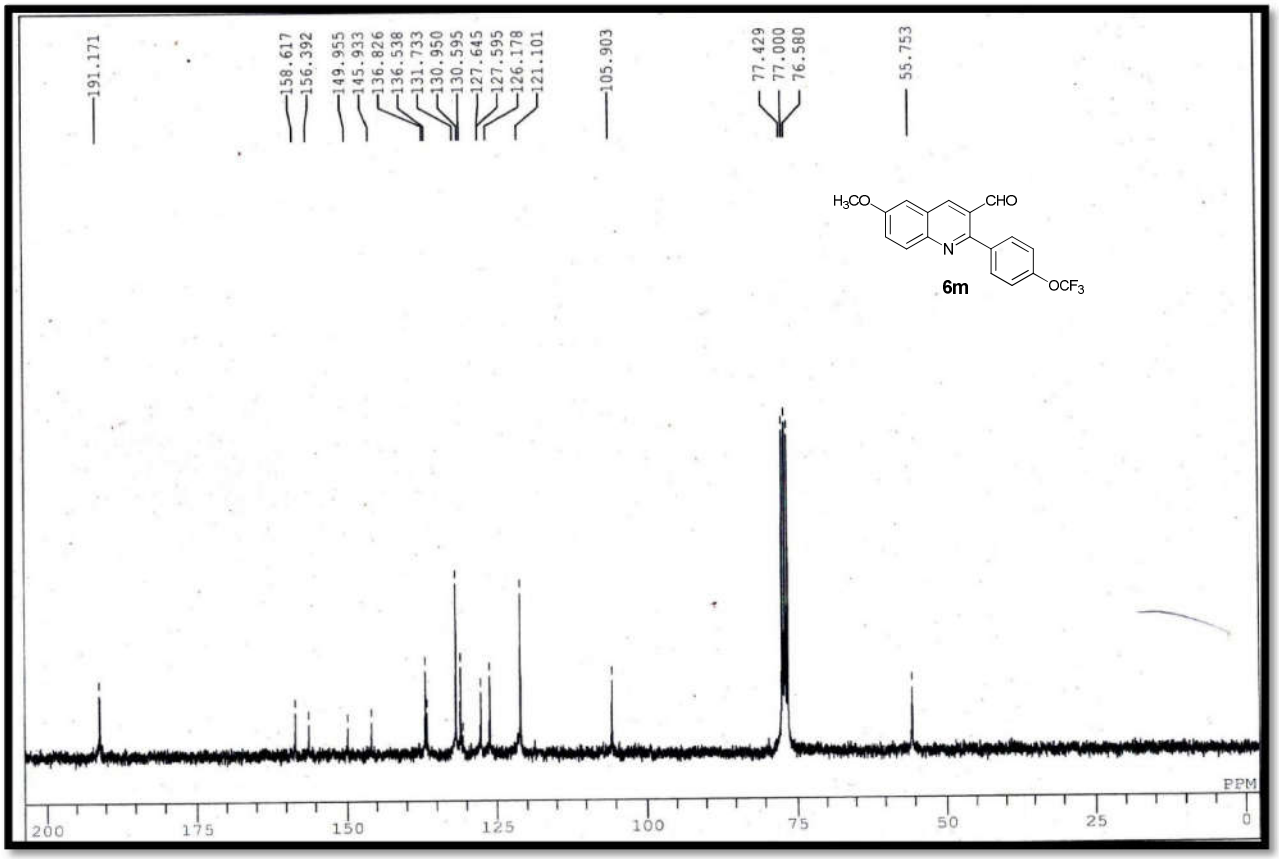
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158.617
156.392
149.955
145.933
136.826
136.538
131.733
130.950
130.595
127.645
127.595
126.178
121.101
105.903
77.429
77.000
76.580
55.753
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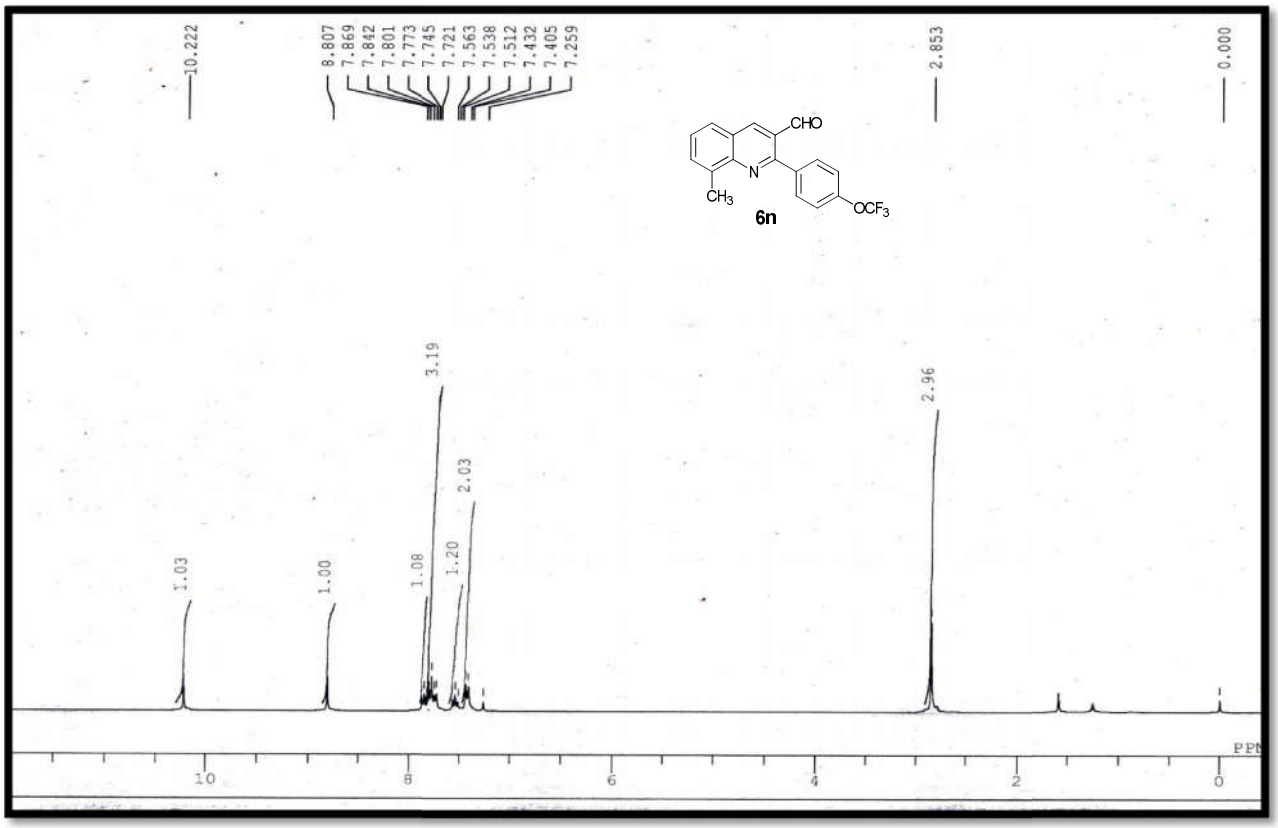
CHO
N
OCF3
6m
PPM
200
175
150
125
100
75
50
25
0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7.869
7.842
7.801
7.773
7.745
7.721
7.563
7.538
7.512
7.432
7.405
7.259
2.853
0.000
CHO
N
CH3
OCF3
6n
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2.96
2.03
1.03
1.00
1.08
1.20
PPM
10
8
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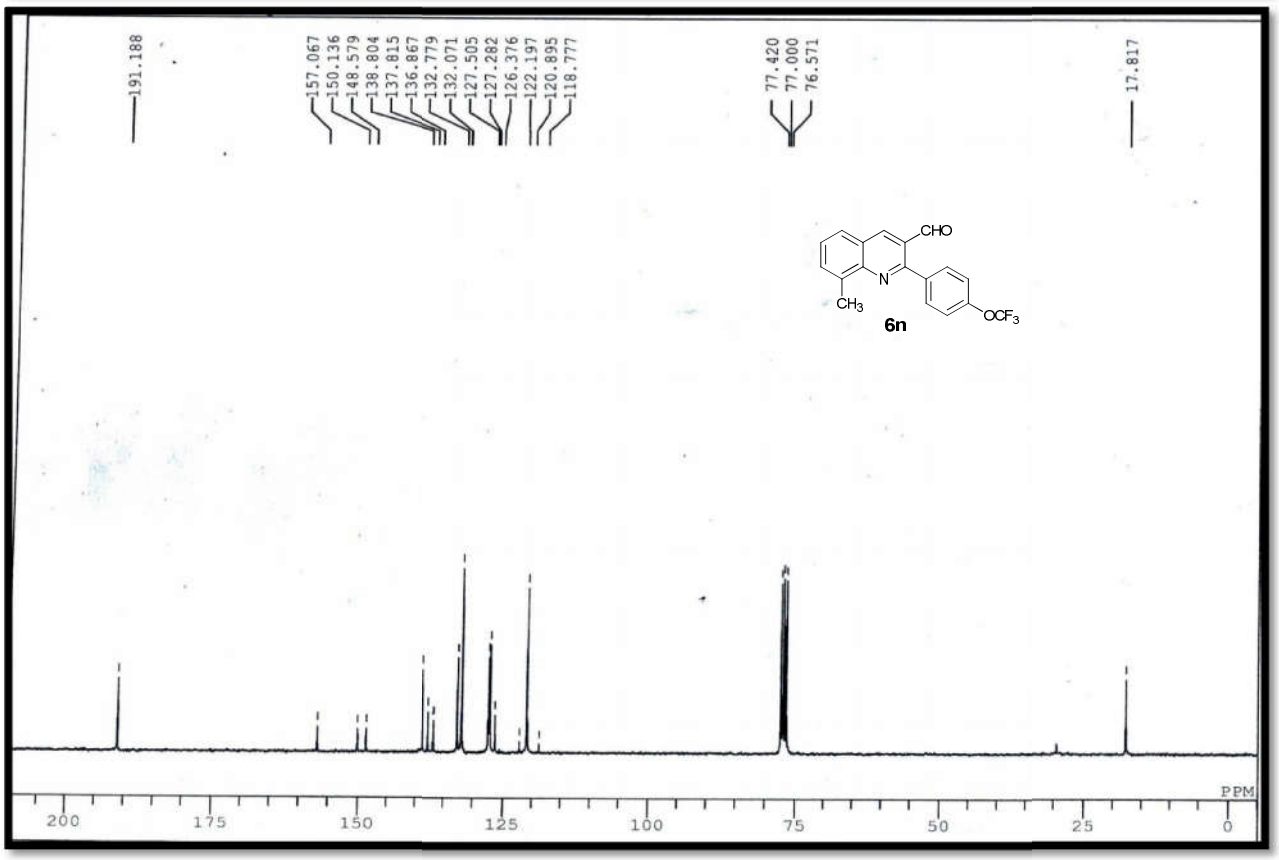
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150.136
148.579
138.804
137.815
136.867
132.779
132.071
127.505
127.282
126.376
122.197
120.895
118.777
77.420
77.000
76.571
17.817
CHO
N
CH3
OCF3
6n
PPM
200
175
150
125
100
75
50
25
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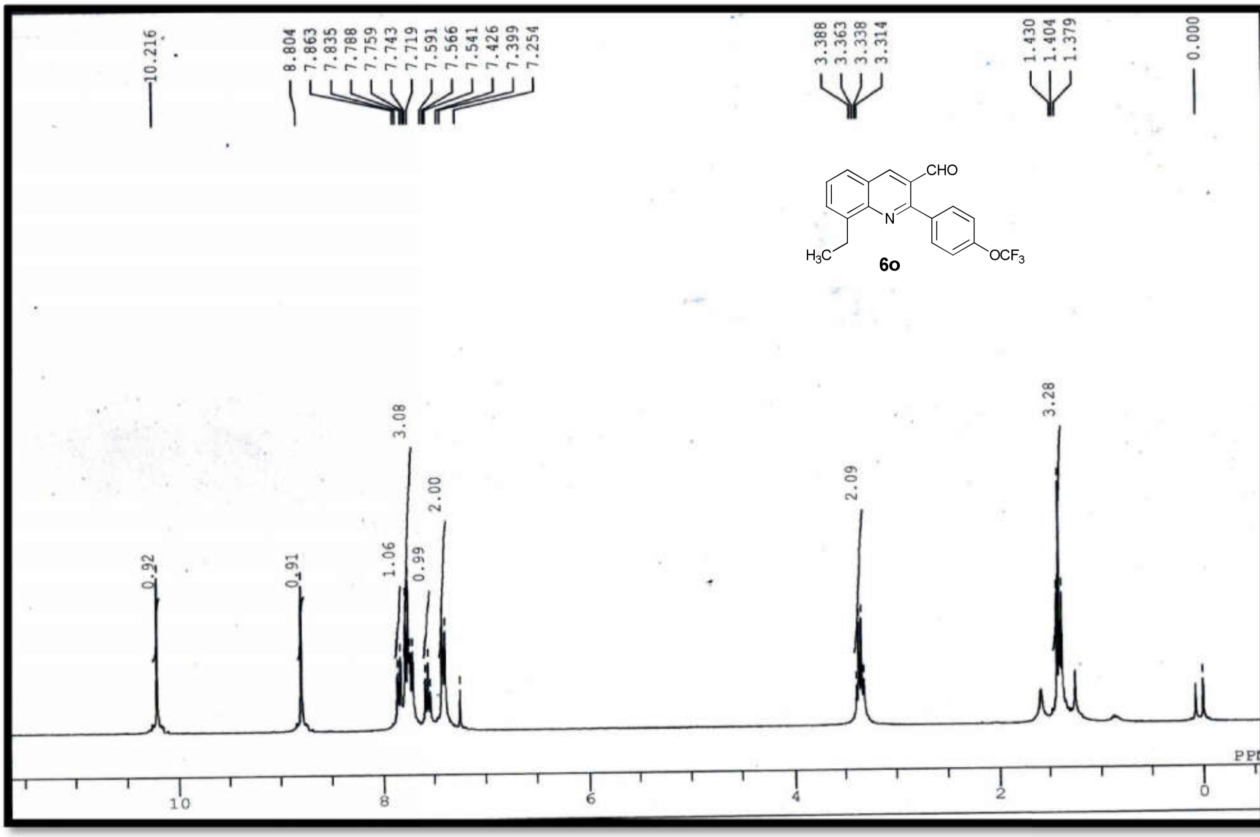
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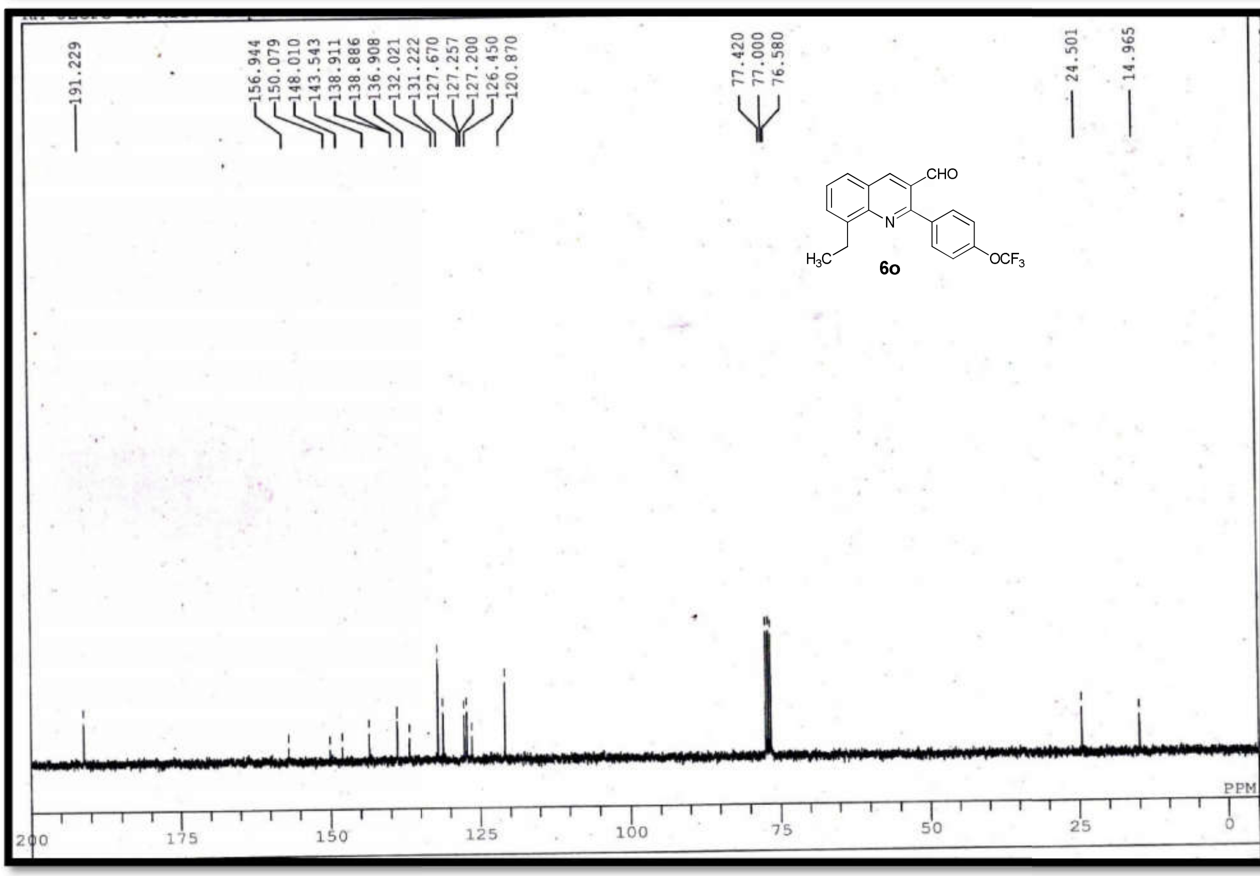
8.804
7.863
7.835
7.788
7.759
7.743
7.719
7.591
7.566
7.541
7.426
7.399
7.254
3.388
3.363
3.338
3.314
1.430
1.404
1.379
0.000
CHO
N
H_3C
OCF_3
6o
0.92
0.91
1.06
3.08
0.99
2.00
2.09
3.28
PPM
10
8
6
4
2
0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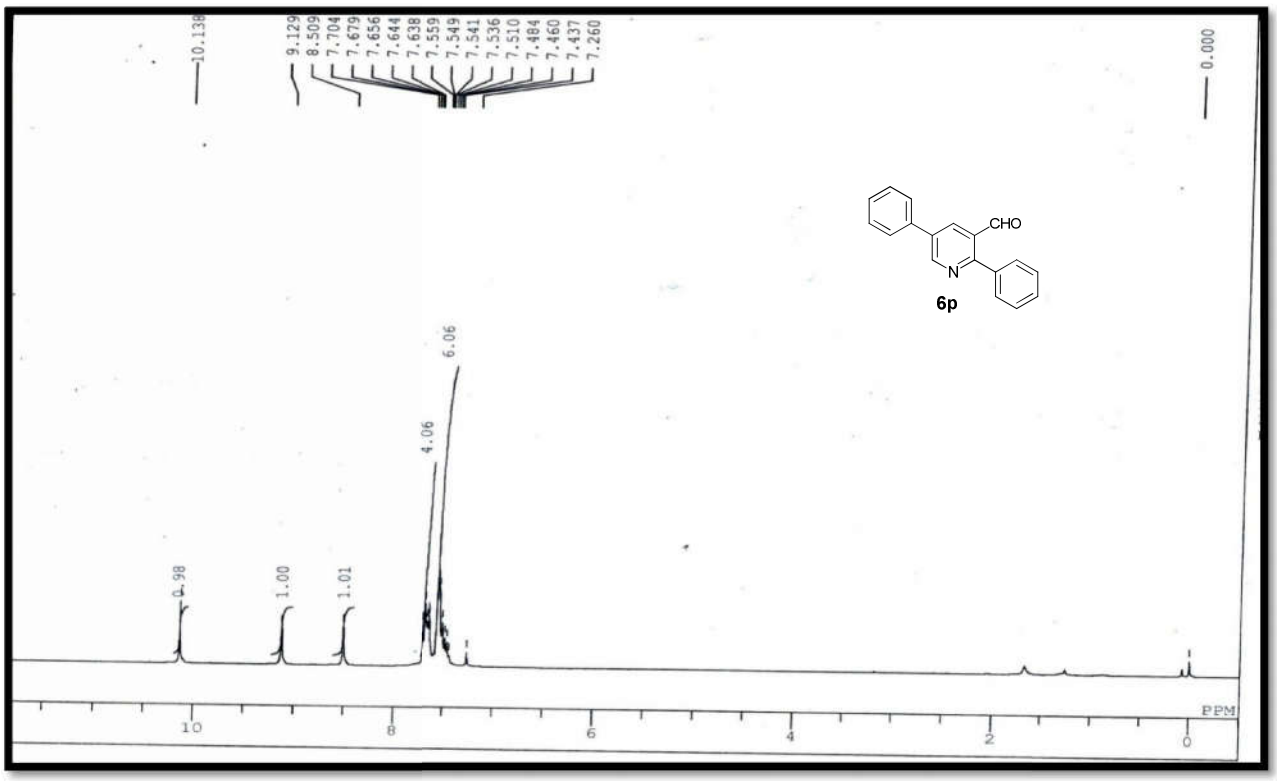
150.079
148.010
143.543
138.911
138.886
136.908
132.021
131.222
127.670
127.257
127.200
126.450
120.870
77.420
77.000
76.580
24.501
14.965
CHO
N
H_3C
OCF_3
6o
PPM
200
175
150
125
100
75
50
25
0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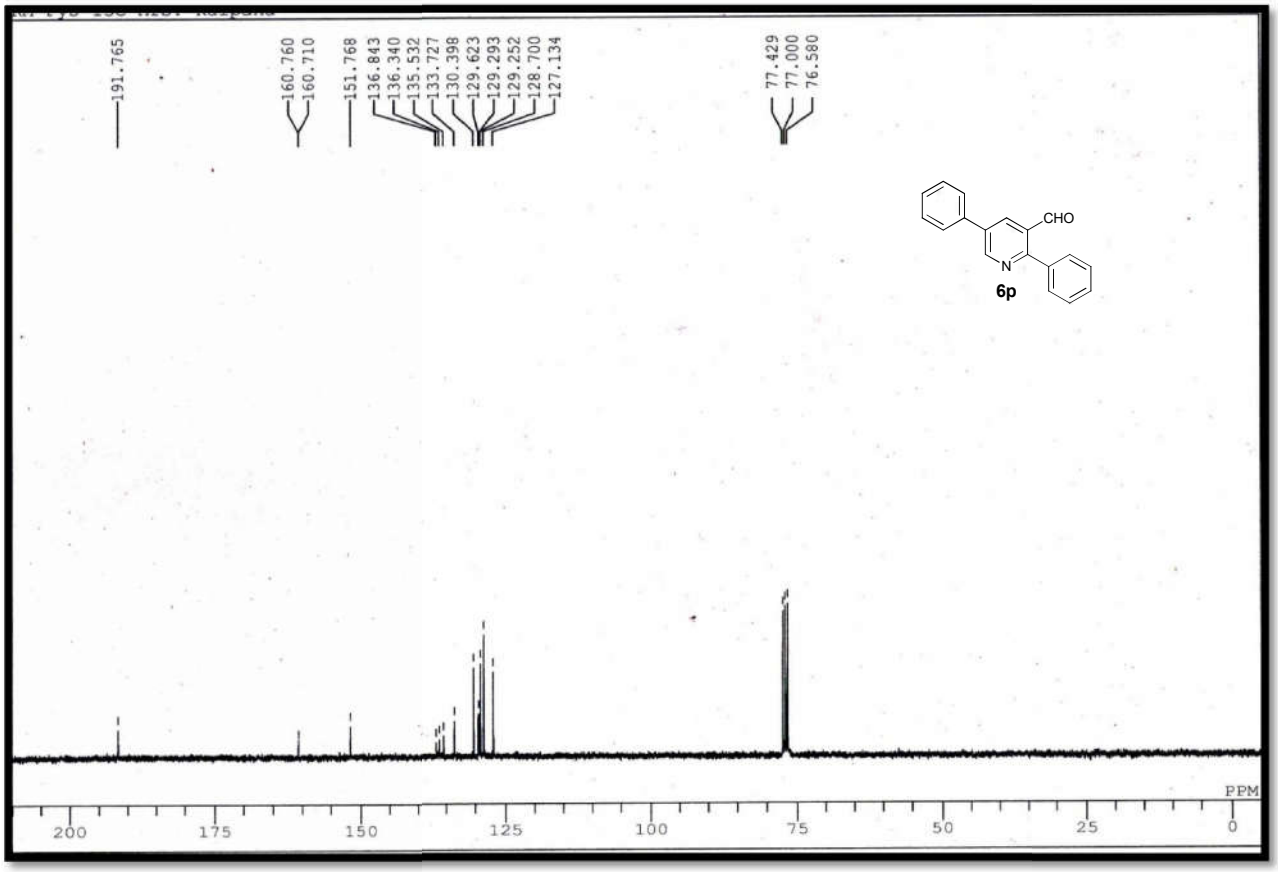
9.129
8.509
7.704
7.679
7.656
7.644
7.638
7.559
7.549
7.541
7.536
7.510
7.484
7.460
7.437
7.260
0.000
CHO
N
6p
6.06
4.06
0.98
1.00
1.01
PPM
10
8
6
4
2
0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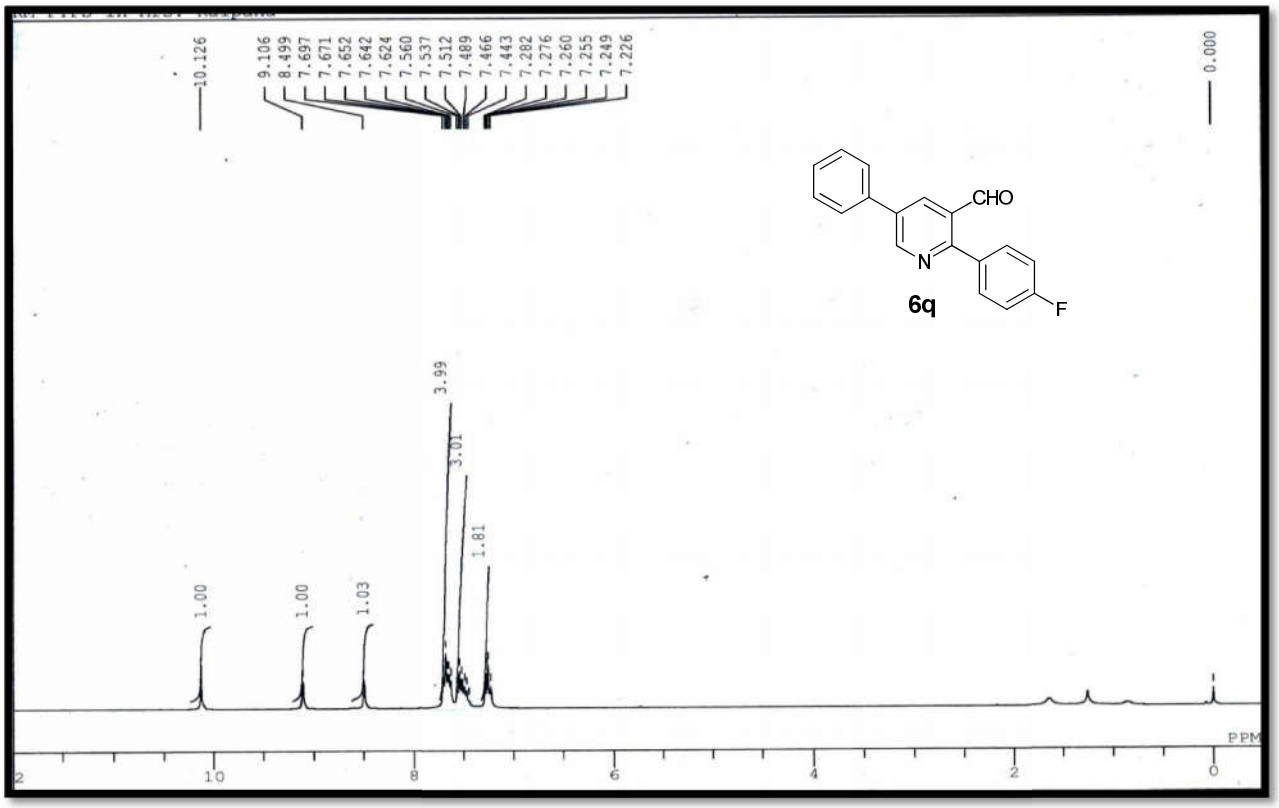
160.760
160.710
151.768
136.843
136.340
135.532
133.727
130.398
129.623
129.293
129.252
128.700
127.134
77.429
77.000
76.580
CHO
N
6p
PPM
200
175
150
125
100
75
50
25
0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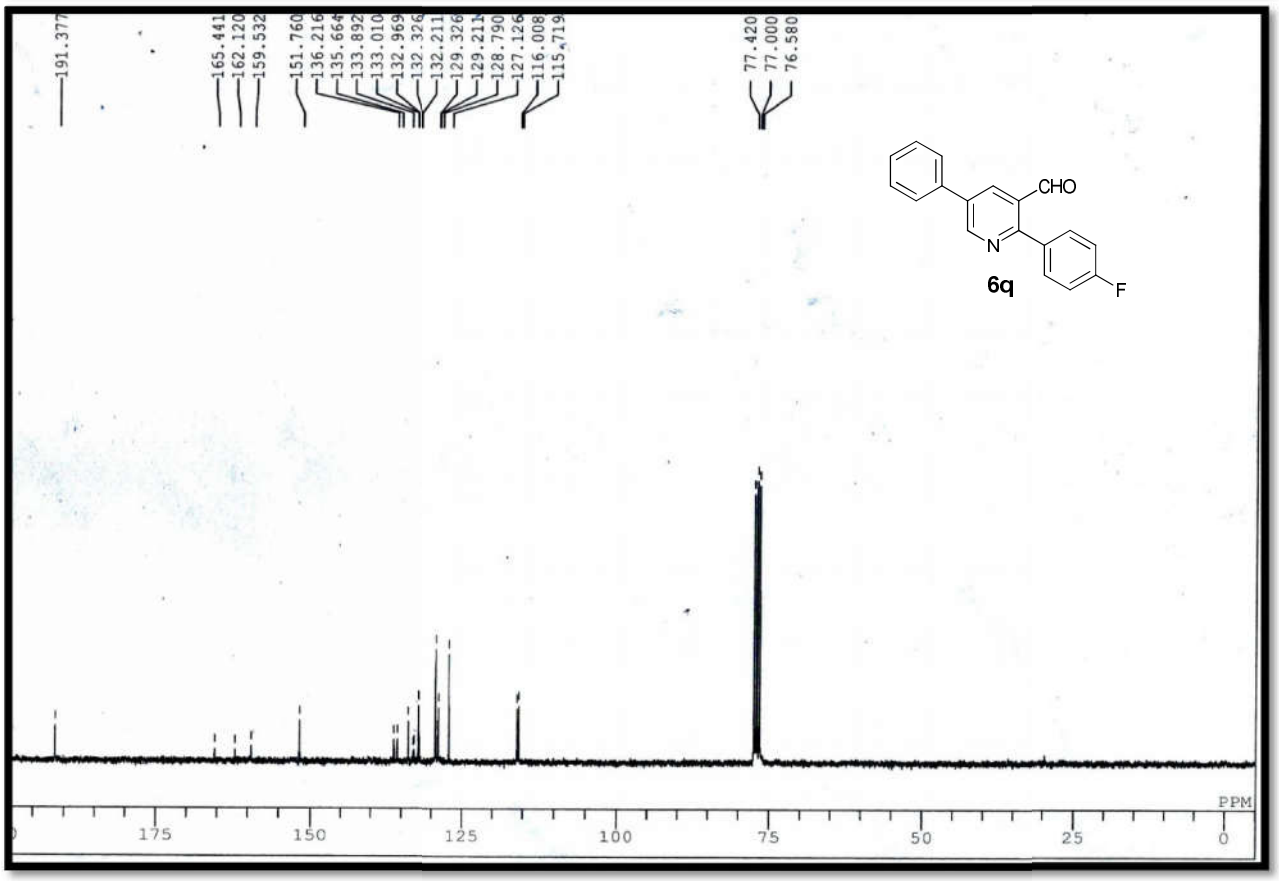
9.106
8.499
7.697
7.671
7.652
7.642
7.624
7.560
7.537
7.512
7.489
7.466
7.443
7.282
7.276
7.260
7.255
7.249
7.226
0.000
CHO
N
F
6q
3.99
3.01
1.81
1.00
1.00
1.03
PPM
10
8
6
4
2
0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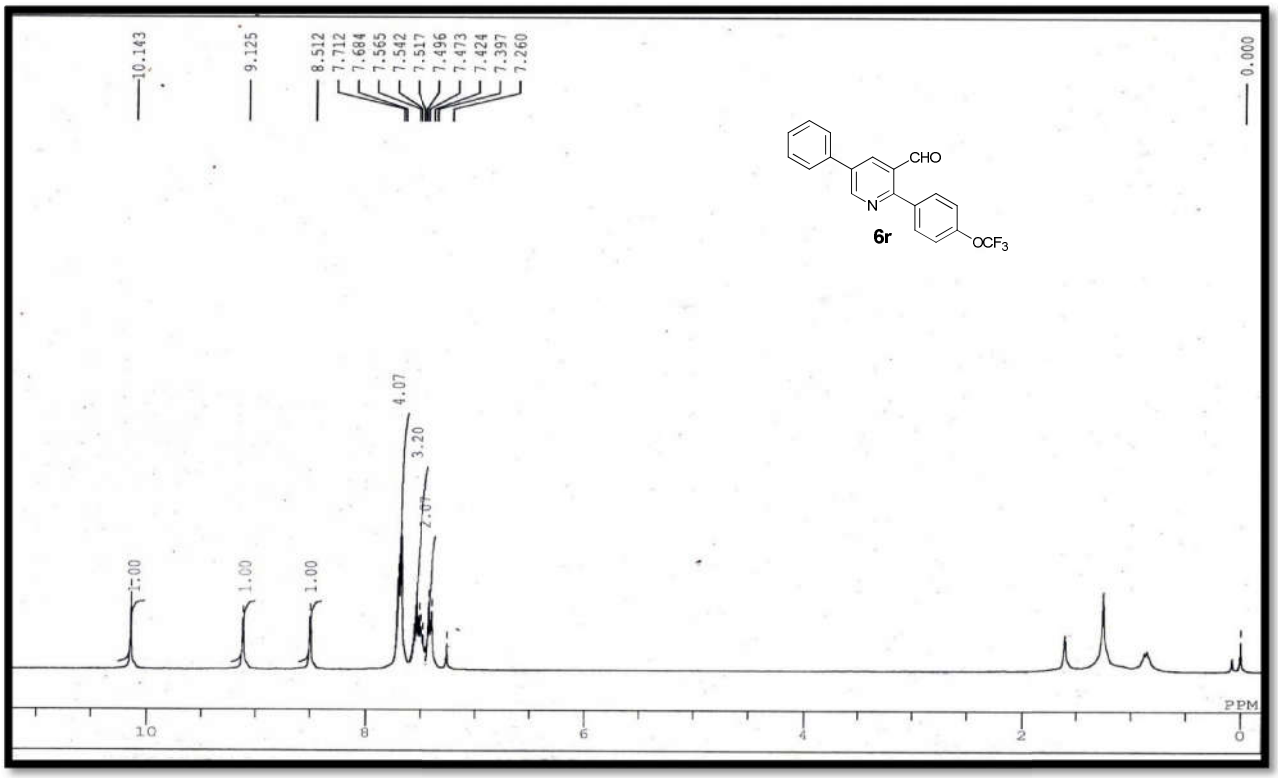
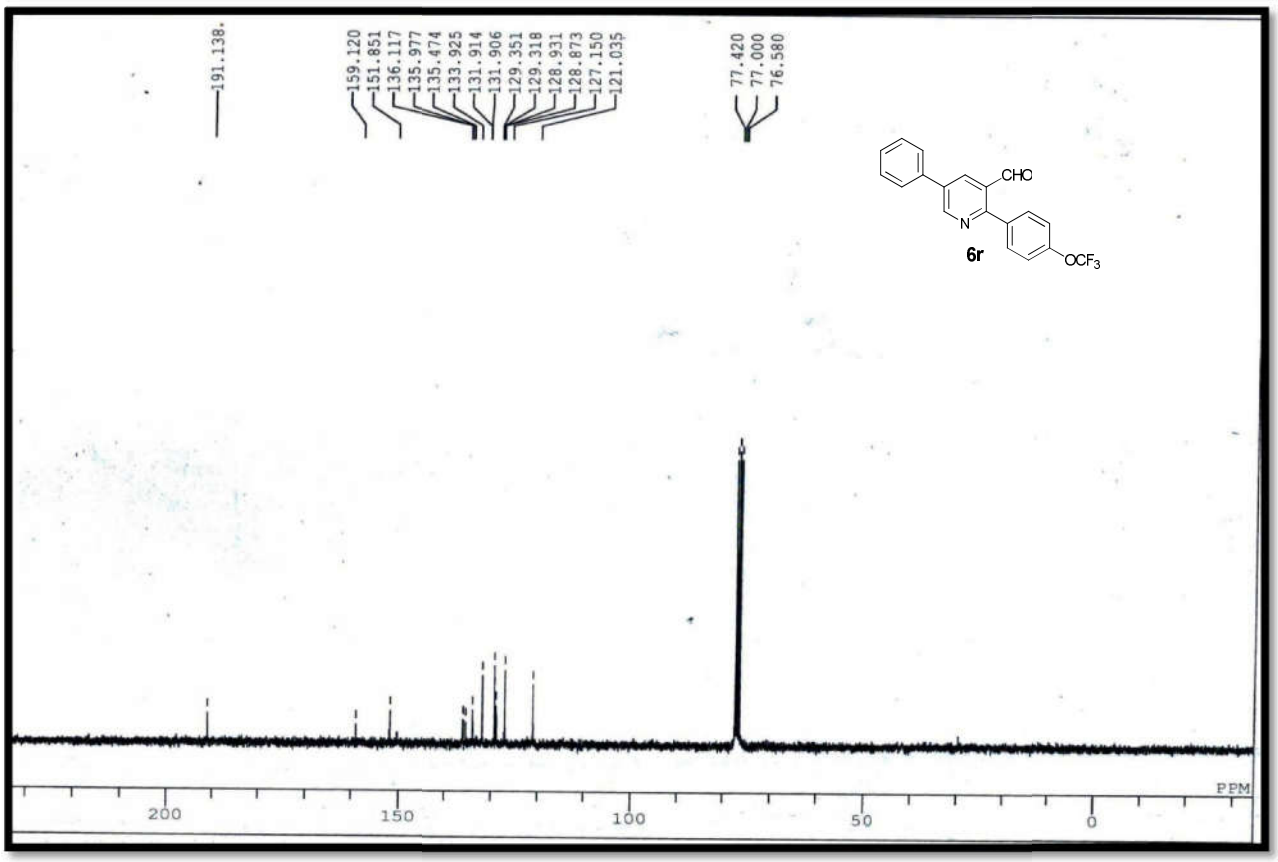
162.120
159.532
151.760
136.216
135.664
133.892
133.010
132.969
132.326
132.211
129.326
129.211
128.790
127.126
116.008
115.719
77.420
77.000
76.580
CHO
N
F
6q
PPM
175
150
125
100
75
50
25
0


10.143
9.125
8.512
7.712
7.684
7.565
7.542
7.517
7.496
7.473
7.424
7.397
7.260
0.000
CHO
N
6r
OCF3
4.07
3.20
2.07
1.00
1.00
1.00
PPM
10
8
6
4
2
0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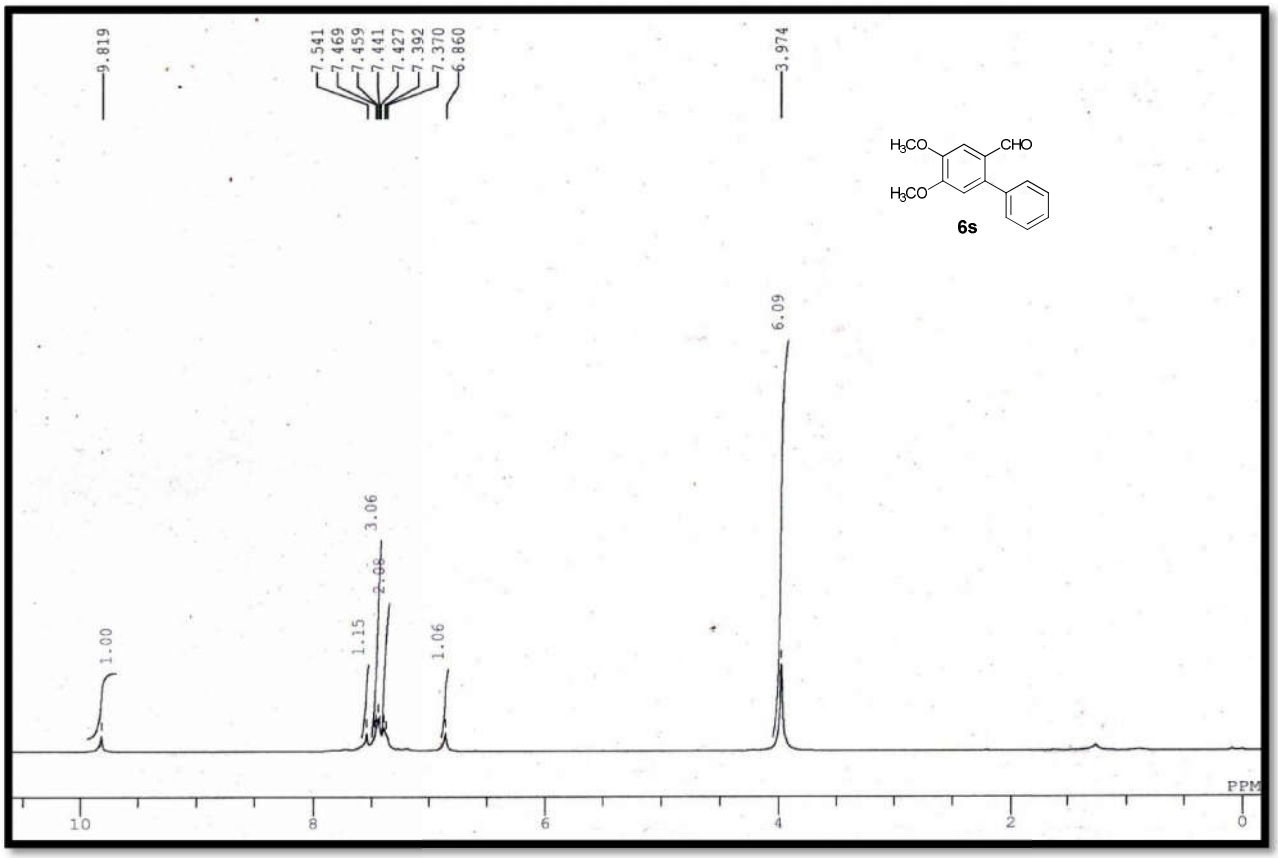
159.120
151.851
136.117
135.977
135.474
133.925
131.914
131.906
129.351
129.318
128.931
128.873
127.150
121.035
77.420
77.000
76.580
CHO
N
6r
OCF3
PPM
200
150
100
50
0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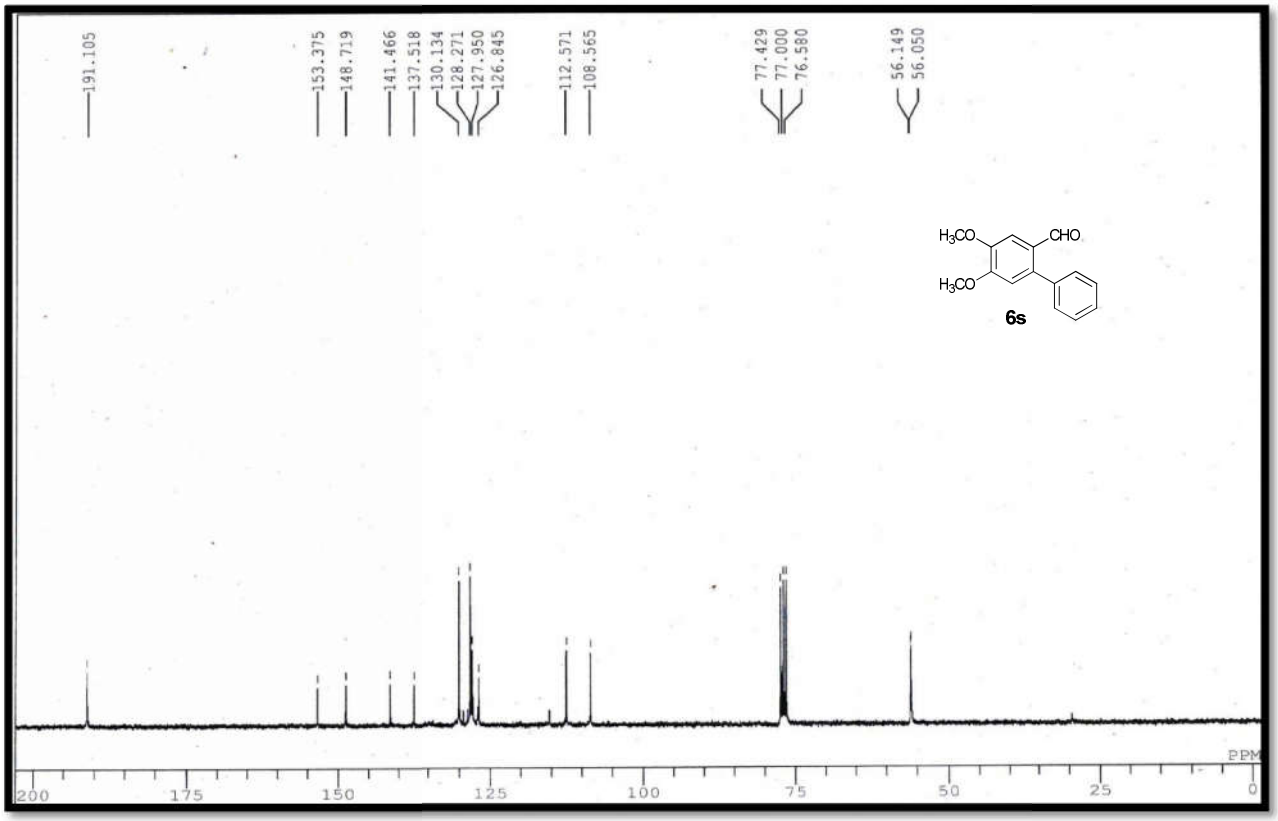
7.469
7.459
7.441
7.427
7.392
7.370
6.860
3.974
6.09
3.06
2.08
1.15
1.06
1.00
PPM
10
8
6
4
2
0

H3CO
CHO
H3CO

6s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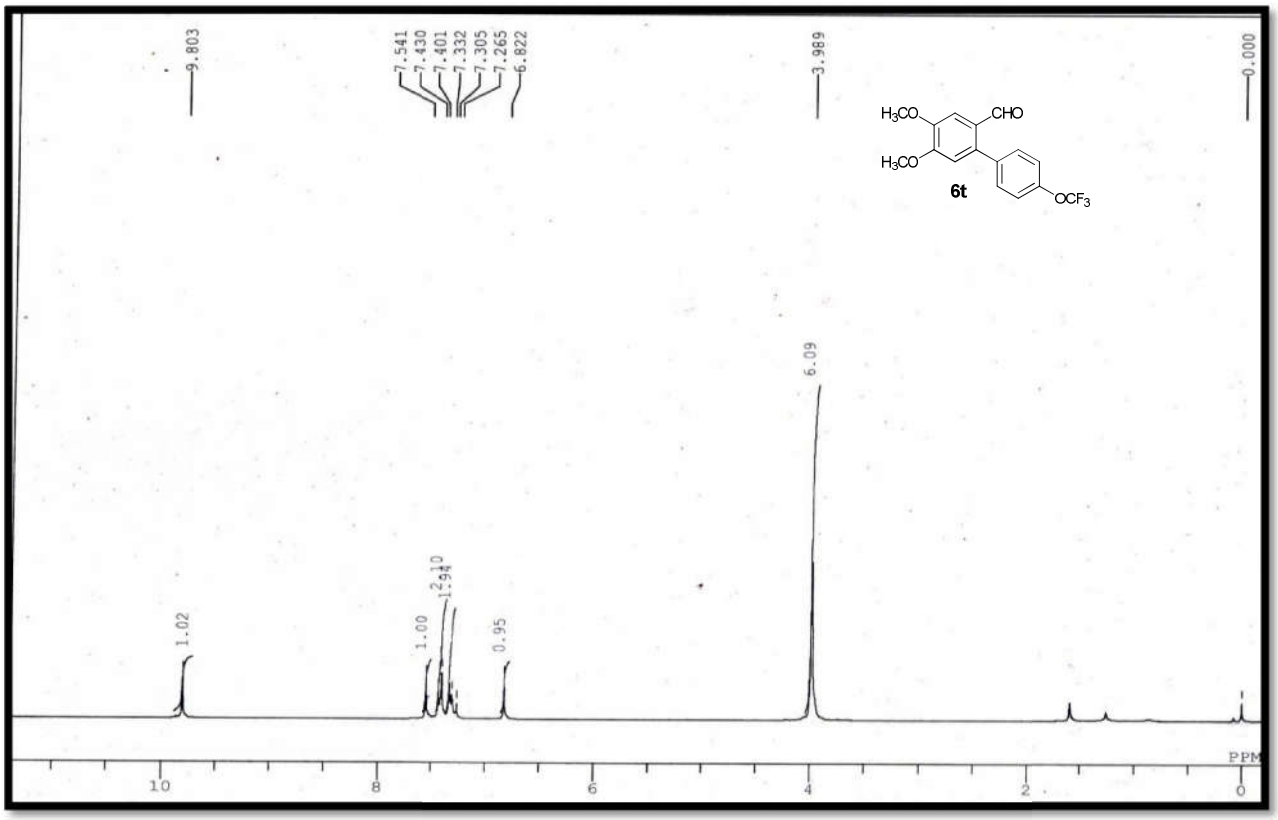
148.719
141.466
137.518
130.134
128.271
127.950
126.845
112.571
108.565
77.429
77.000
76.580
56.149
56.050
PPM
200
175
150
125
100
75
50
25
0

H3CO
CHO
H3CO

6s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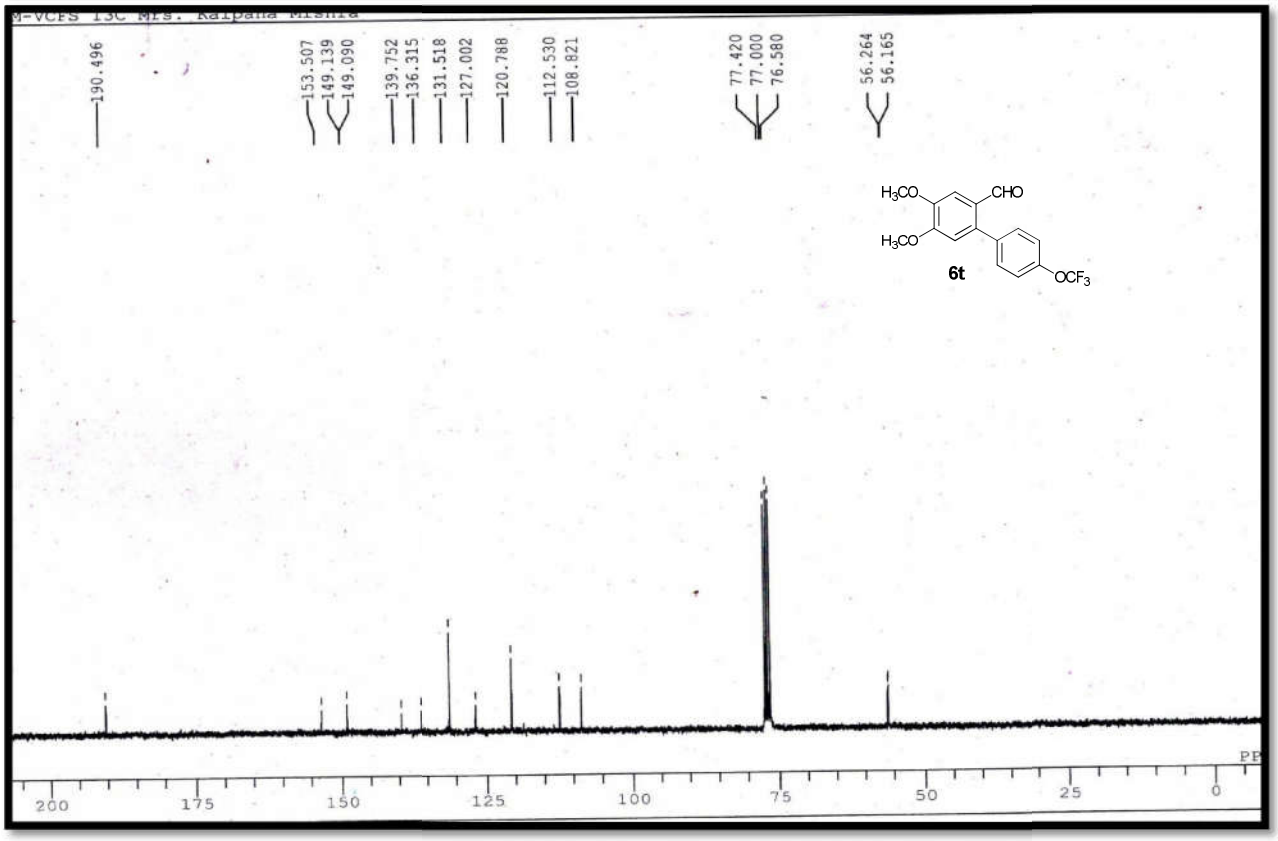
7.430
7.401
7.332
7.305
7.265
6.822
3.989
0.000
6.09
1.02
1.00
2.10
1.94
0.95
PPM
10
8
6
4
2
0
H3CO
CHO
H3CO
OCF3
6t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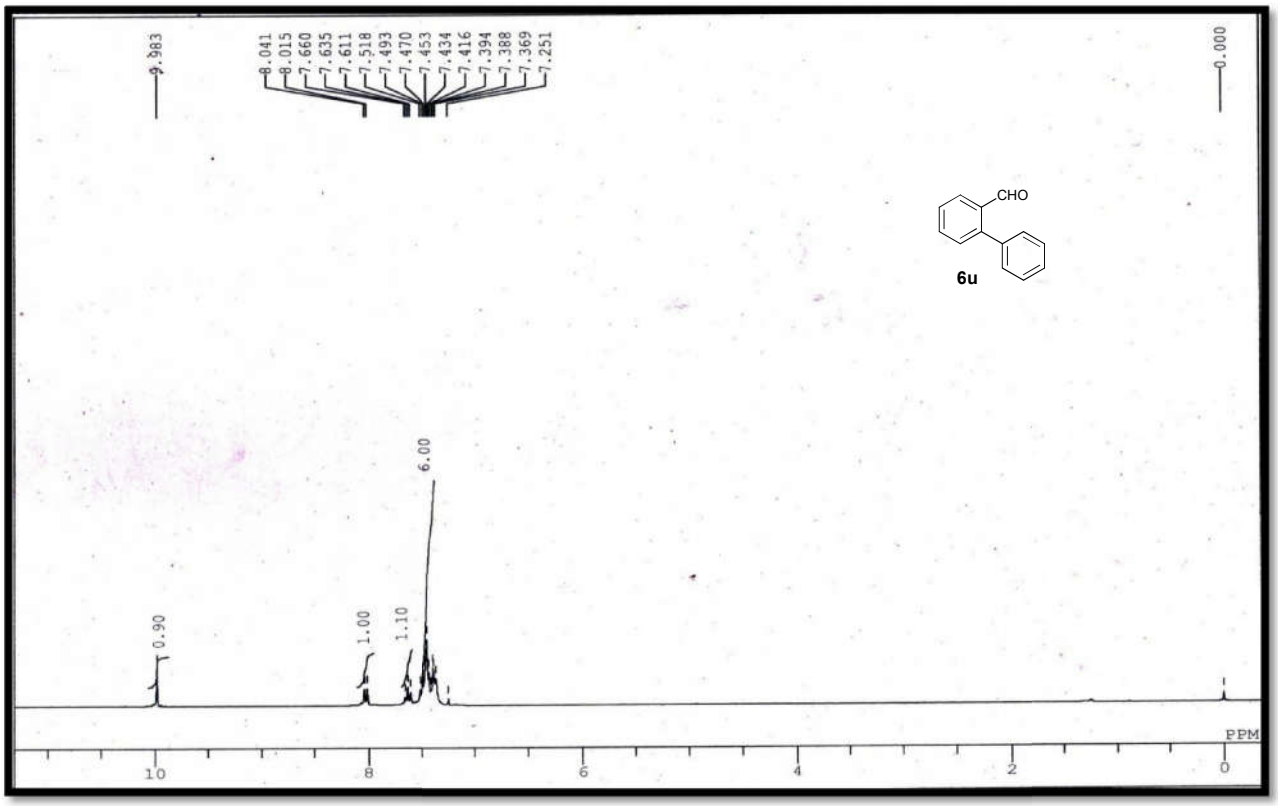
149.139
149.090
139.752
136.315
131.518
127.002
120.788
112.530
108.821
77.420
77.000
76.580
56.264
56.165
200
175
150
125
100
75
50
25
0
H3CO
CHO
H3CO
OCF3
6t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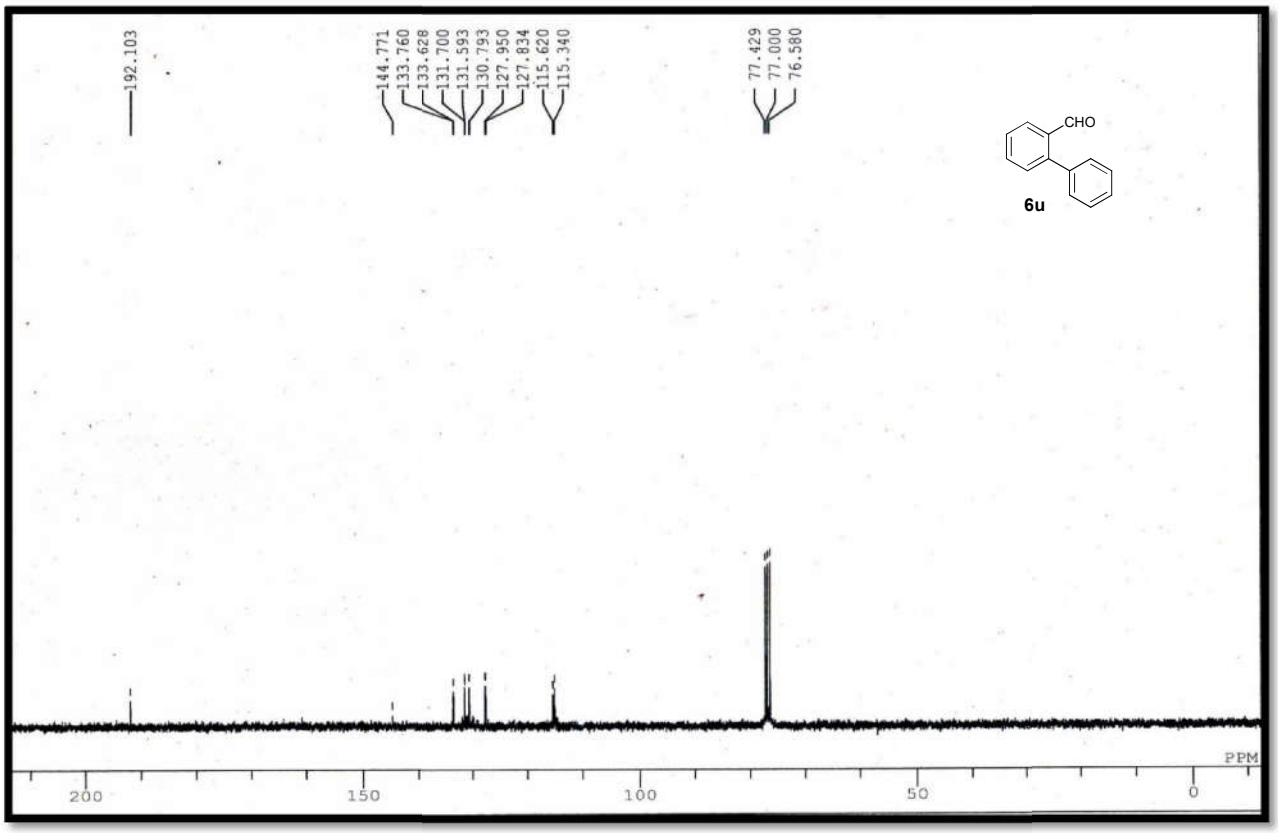
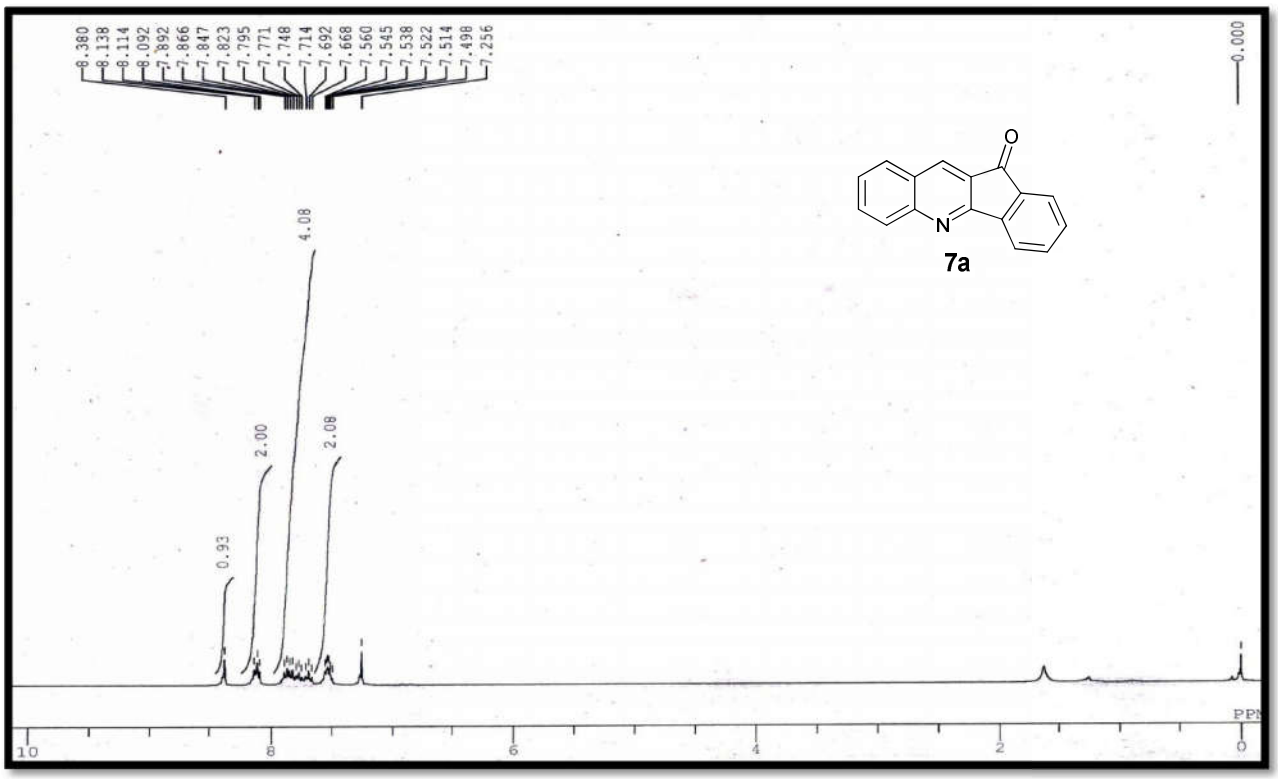
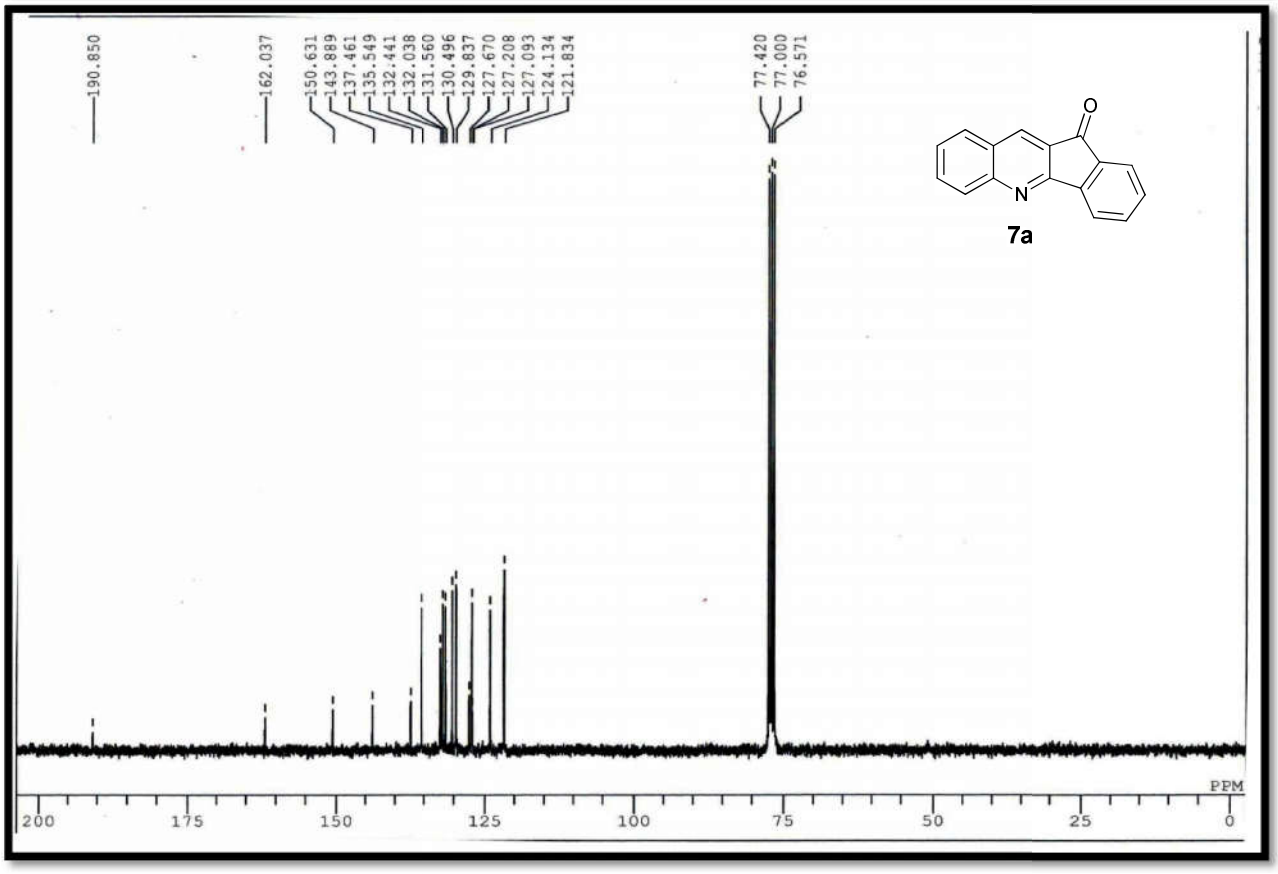
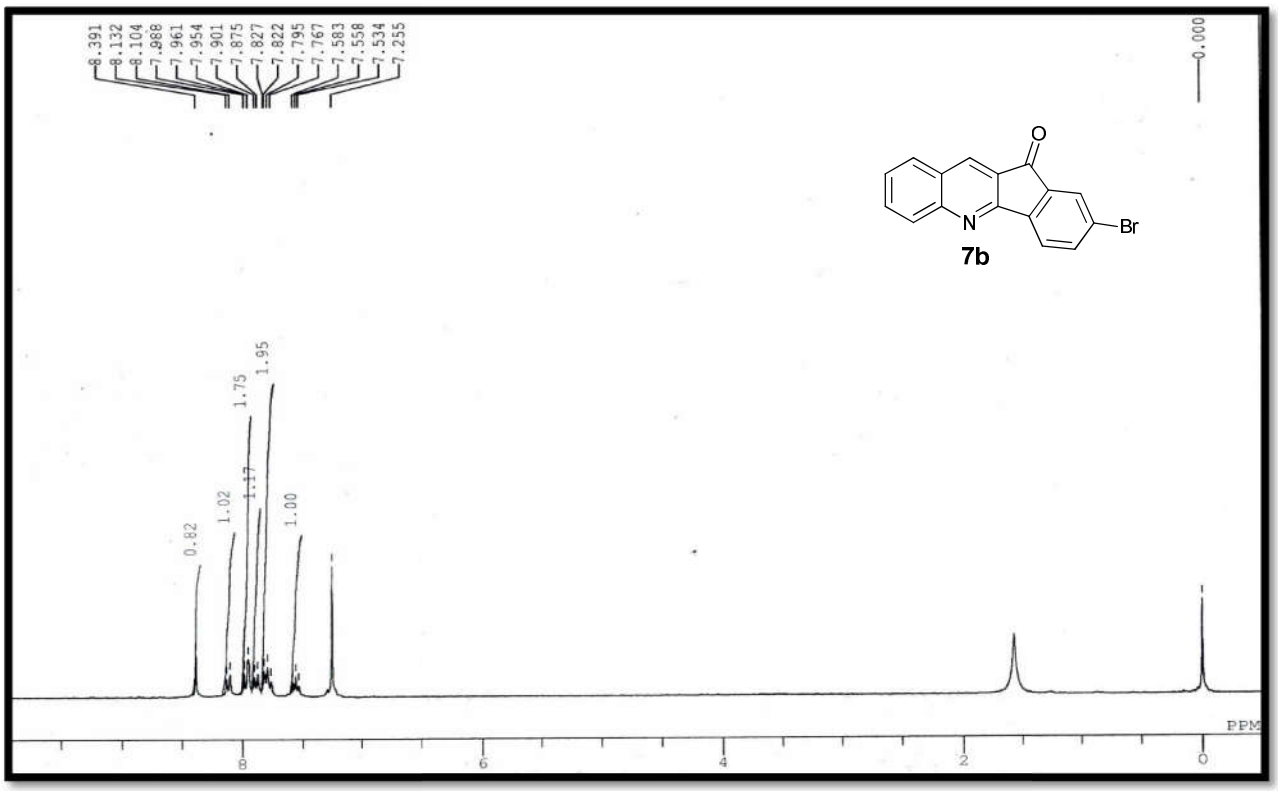
8.015
7.660
7.635
7.611
7.518
7.493
7.470
7.453
7.434
7.416
7.394
7.388
7.369
7.251
0.000
CHO
6u
6.00
1.10
1.00
0.90
PPM
10
8
6
4
2
0


192.103
144.771
133.760
133.628
131.700
131.593
130.793
127.950
127.834
115.620
115.340
77.429
77.000
76.580
CHO
6u
PPM
200
150
100
50
0

^{1}H NMR (300 MHz), ^{13}C NMR (75 MHz) and ^{19}F NMR (500 MHz) spectra of annulated product (7)



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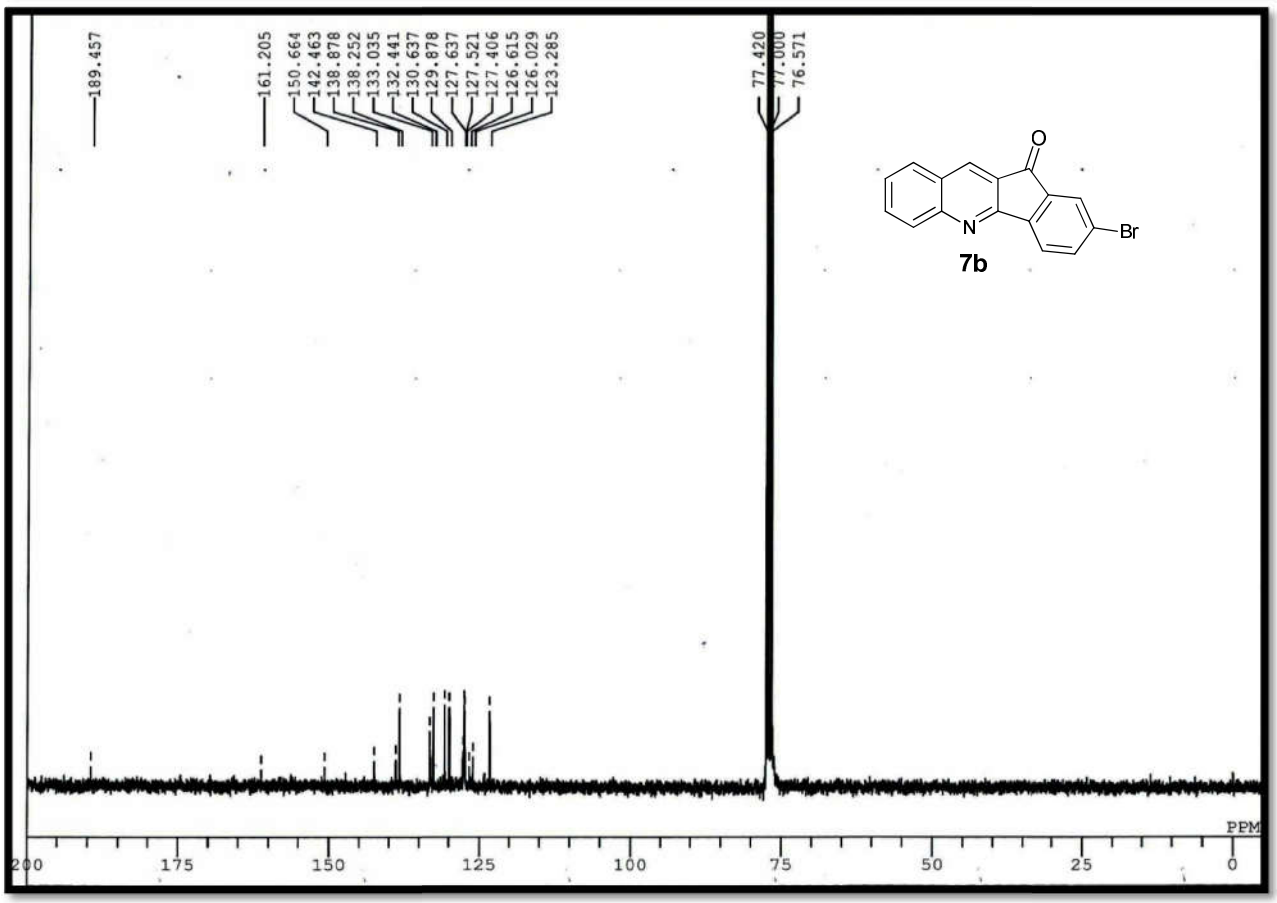
8.104
7.961
7.954
7.901
7.875
7.827
7.822
7.795
7.767
7.583
7.558
7.534
7.255
0.000
O
N
Br
7b
0.82
1.02
1.75
1.17
1.95
1.00
PPM
8
6
4
2
0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161.205
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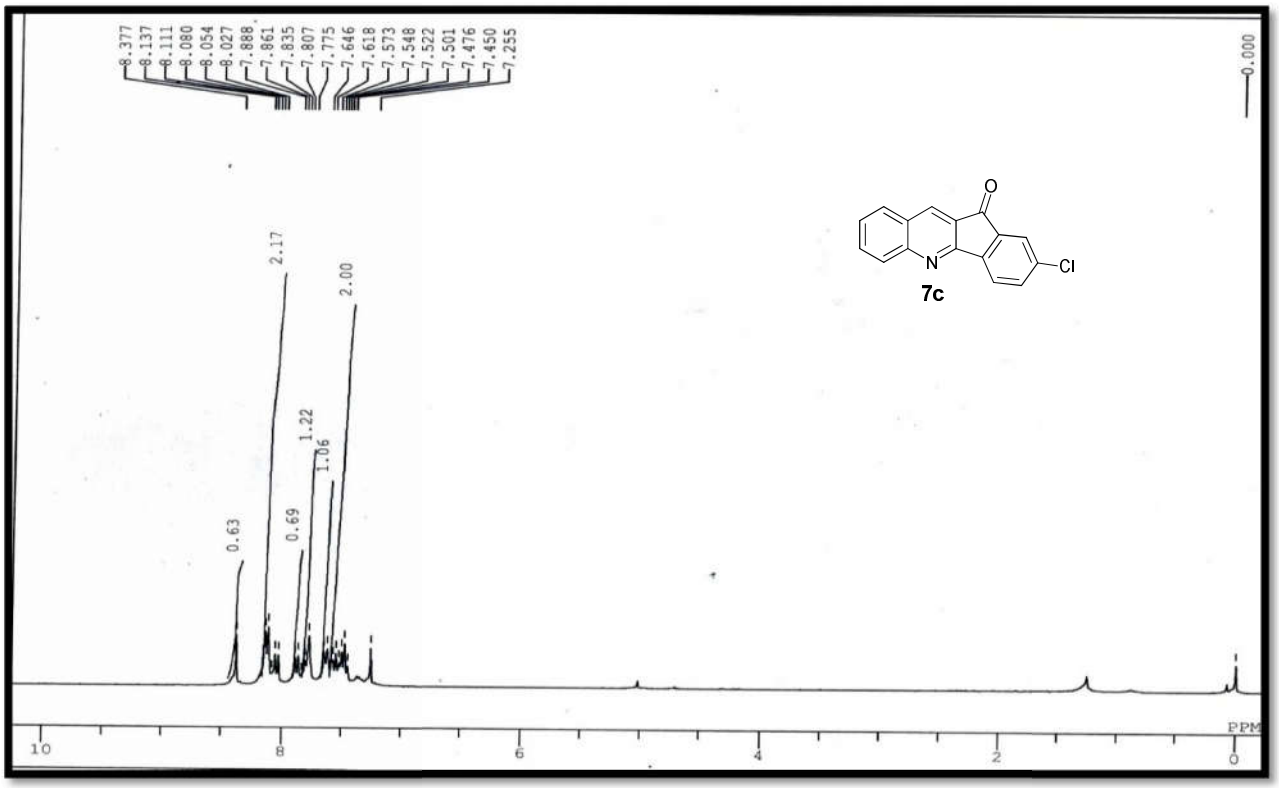
142.463
138.878
138.252
133.035
132.441
130.637
129.878
127.637
127.521
127.406
126.615
126.029
123.285
77.420
77.000
76.571
O
N
Br
7b
PPM
200
175
150
125
100
75
50
25
0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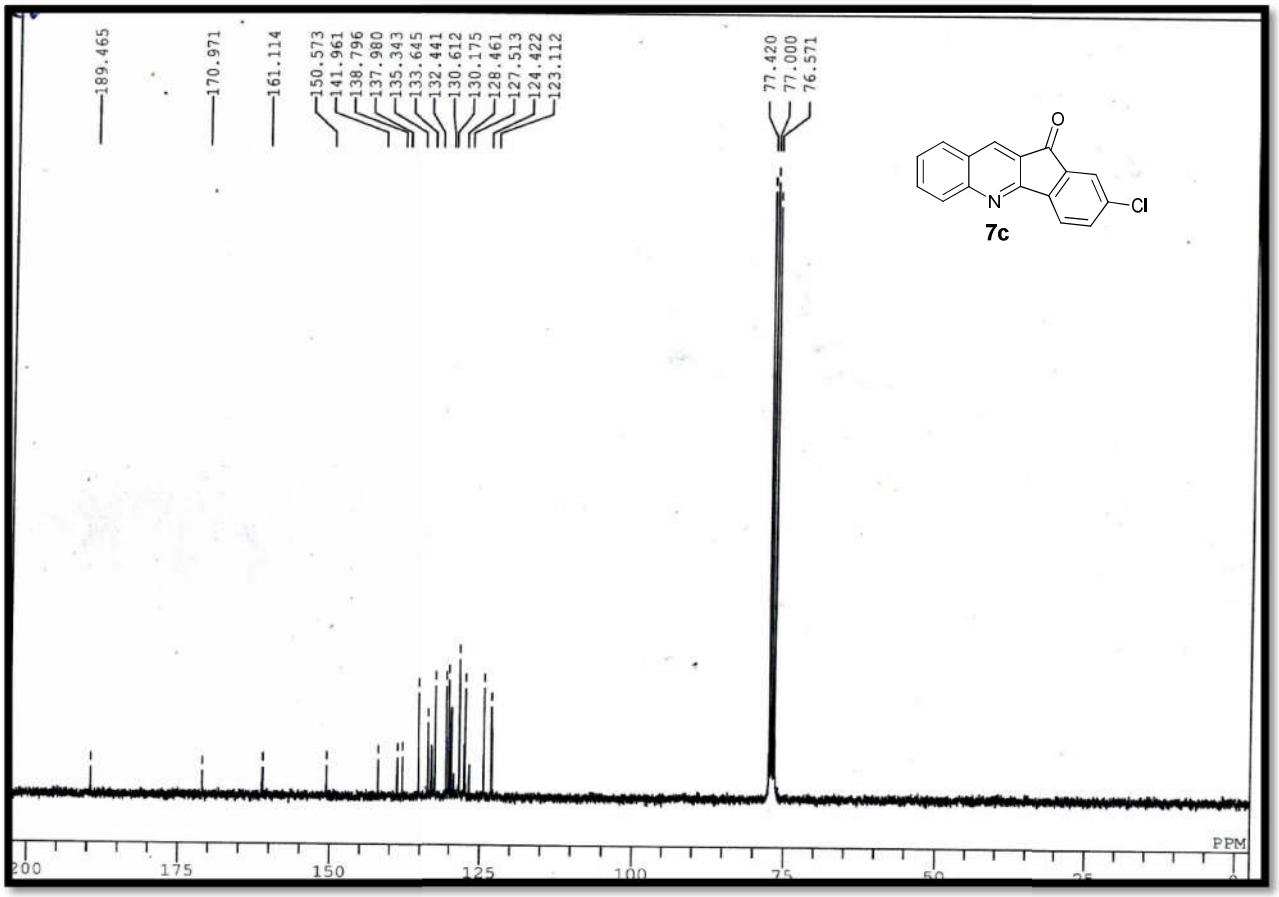
8.137
8.111
8.080
8.054
8.027
7.888
7.861
7.835
7.807
7.775
7.646
7.618
7.573
7.548
7.522
7.501
7.476
7.450
7.255
0.000
2.17
2.00
1.22
1.06
0.69
0.63
O
N
Cl
7c
10
8
6
4
2
0
PPM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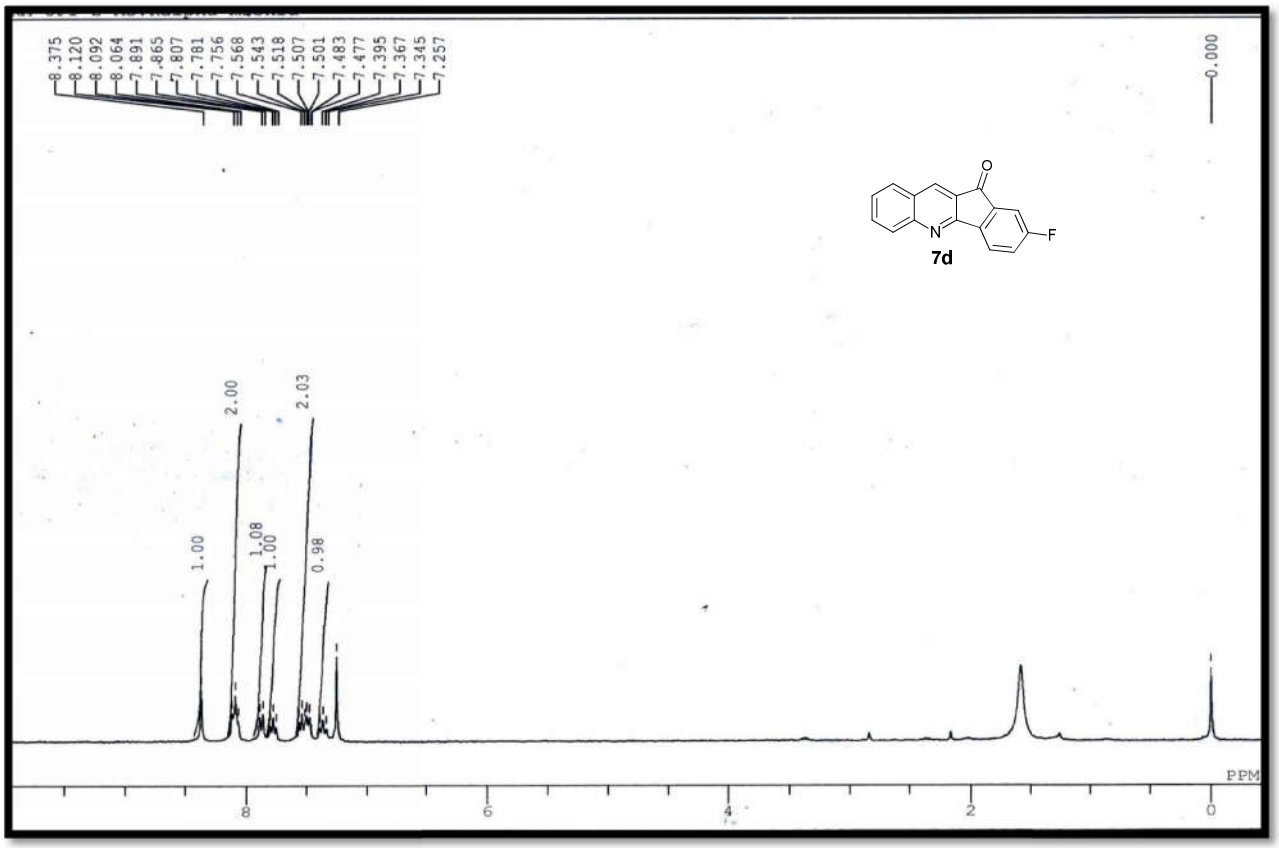
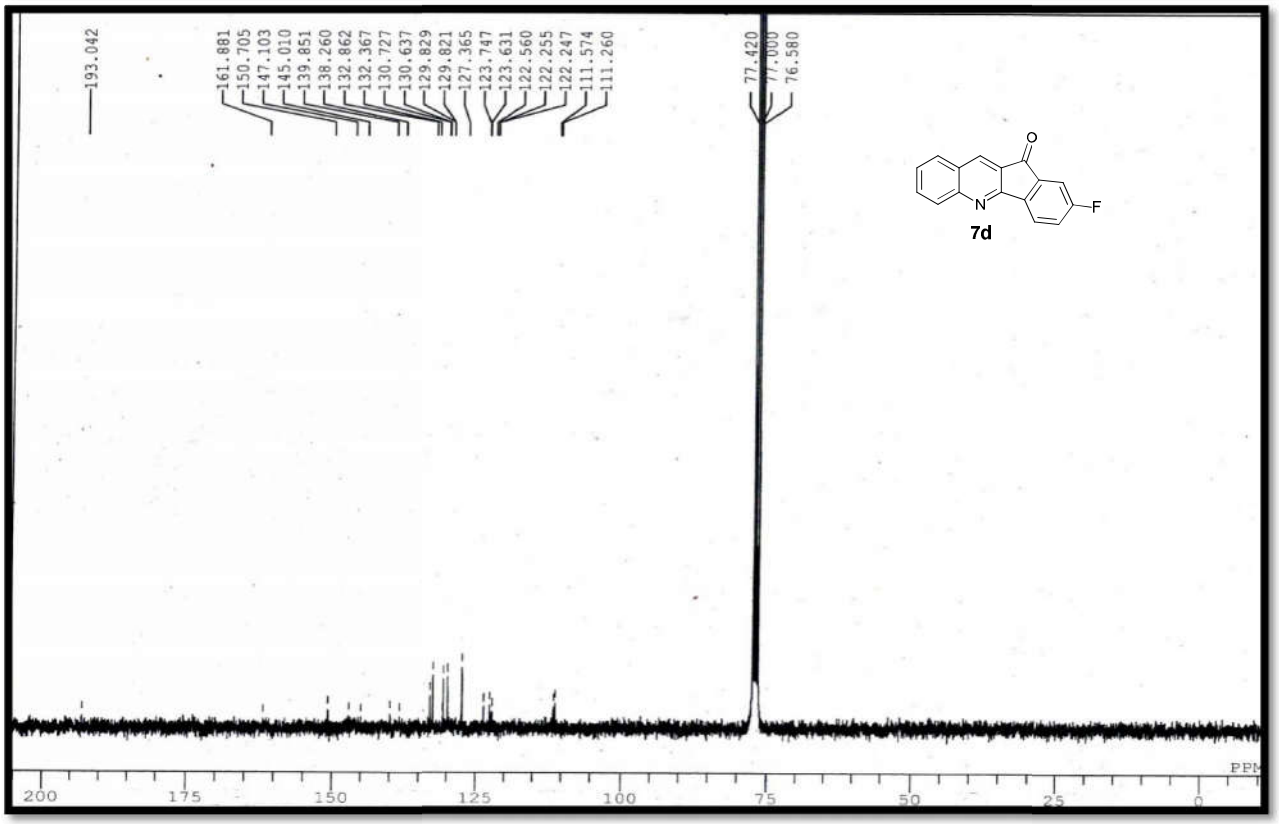
150.573
141.961
138.796
137.980
135.343
133.645
132.441
130.612
130.175
128.461
127.513
124.422
123.112
77.420
77.000
76.571
O
N
Cl
7c
200
175
150
125
100
75
50
25
0
PPM


8.375
8.120
8.092
8.064
7.891
7.865
7.807
7.781
7.756
7.568
7.543
7.518
7.507
7.501
7.483
7.477
7.395
7.367
7.345
7.257
0.000
O
N
F
7d
1.00
2.00
1.08
1.00
2.03
0.98
PPM
8
6
4
2
0


193.042
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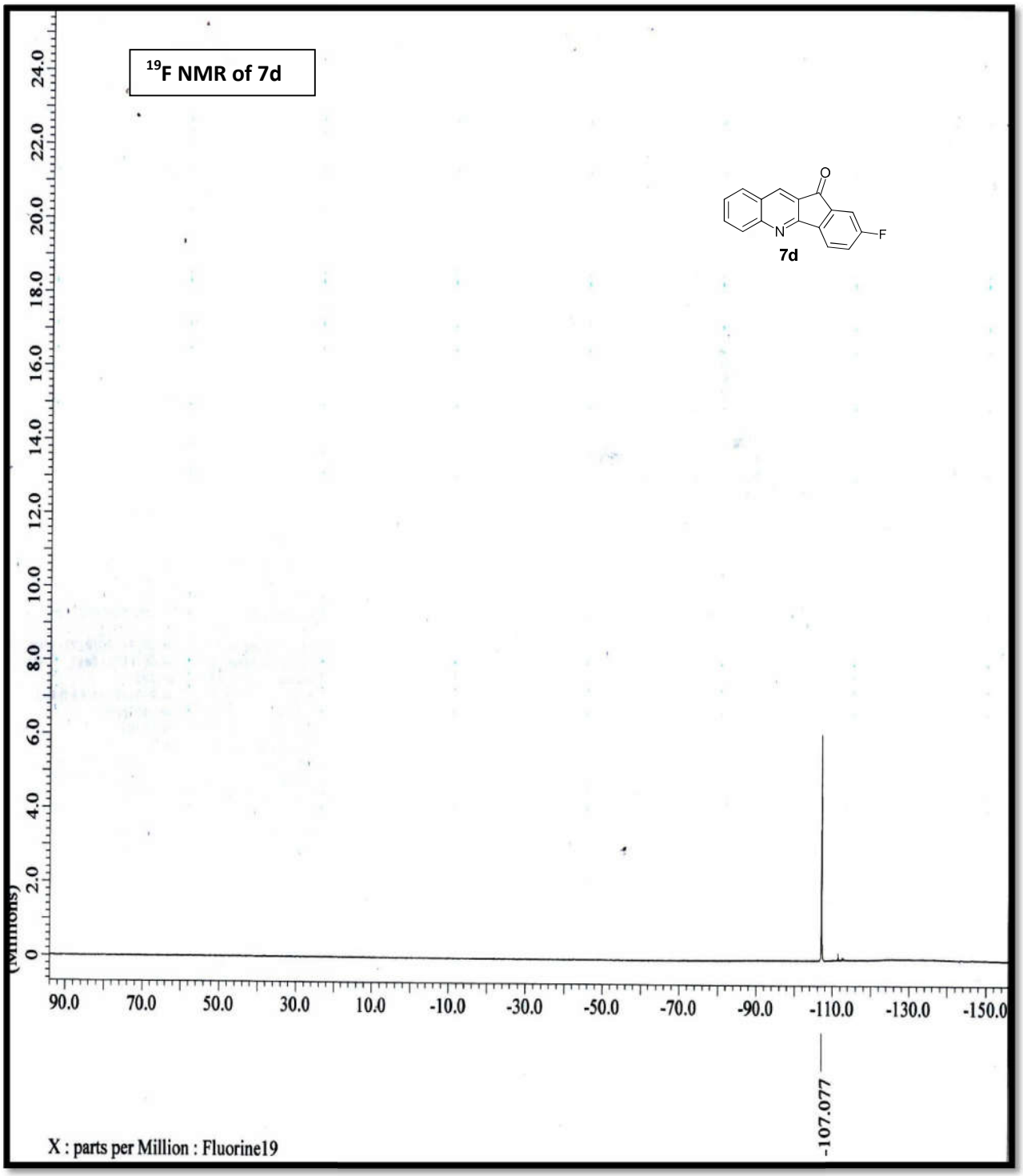
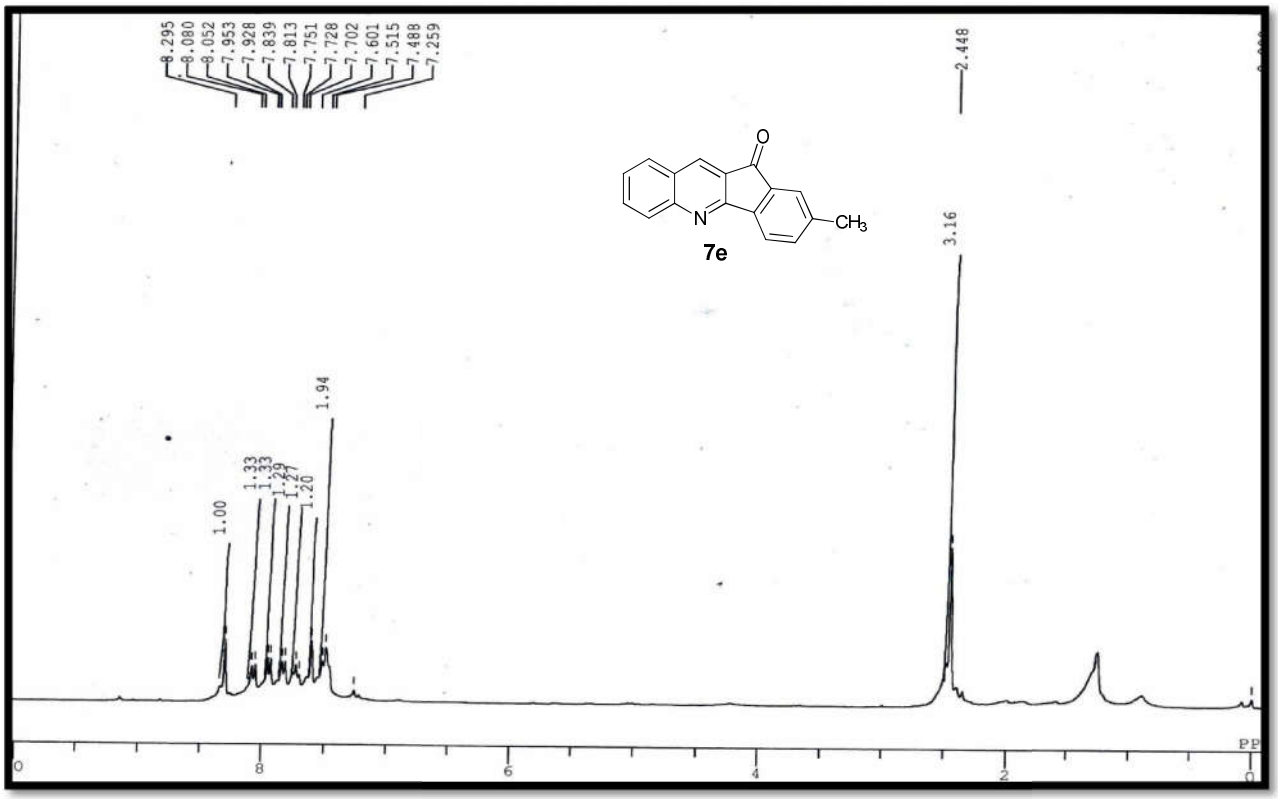
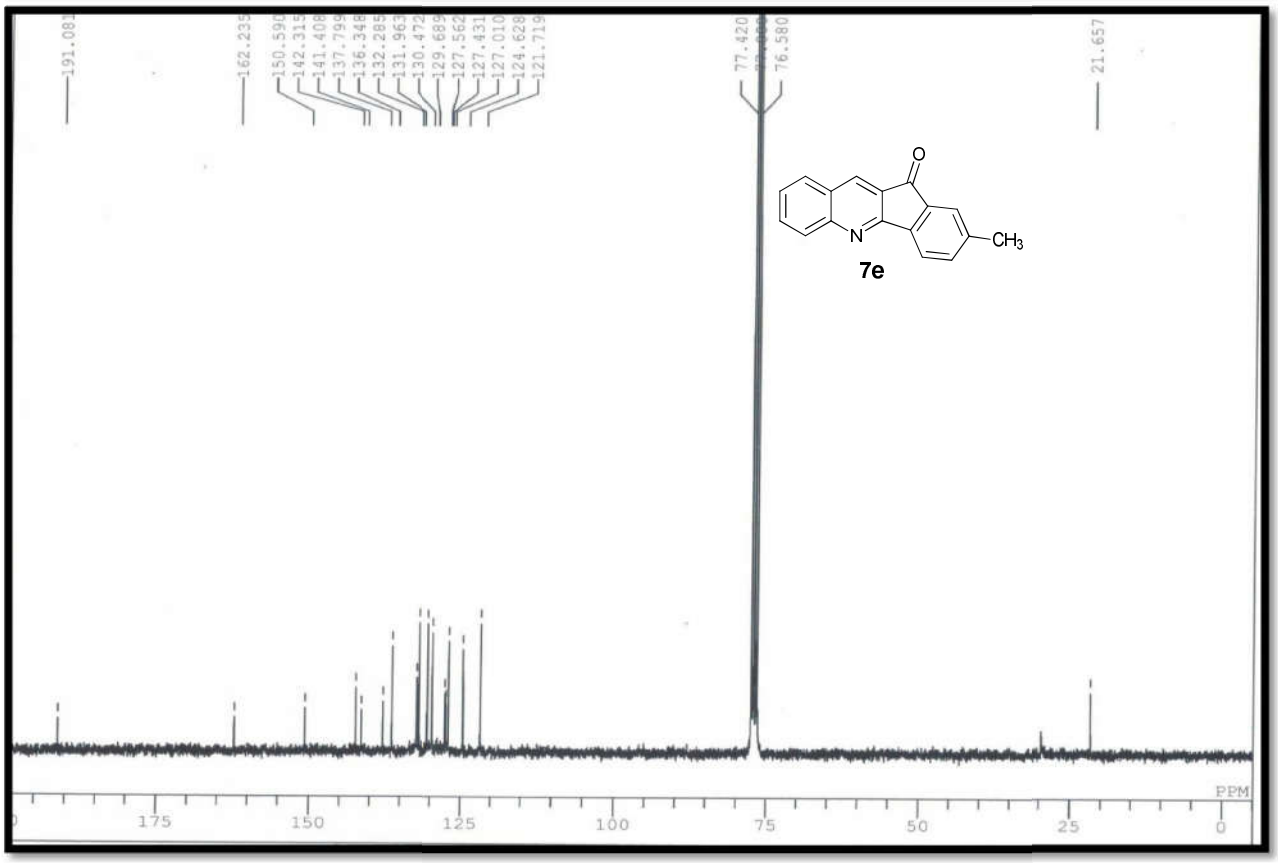
147.103
145.010
139.851
138.260
132.862
132.367
130.727
130.637
129.829
129.821
127.365
123.747
123.631
122.560
122.255
122.247
111.574
111.260
77.420
77.000
76.580
O
N
F
7d
PPM
200
175
150
125
100
75
50
25
0


19F NMR of 7d
O
N
F
7d
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
0
(Millions)
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-107.077
X : parts per Million : Fluorine19


8.295
8.080
8.052
7.953
7.928
7.839
7.813
7.751
7.728
7.702
7.601
7.515
7.488
7.259
2.448
3.16
1.94
1.33
1.33
1.29
1.27
1.20
1.00
O
N
CH3
7e
PP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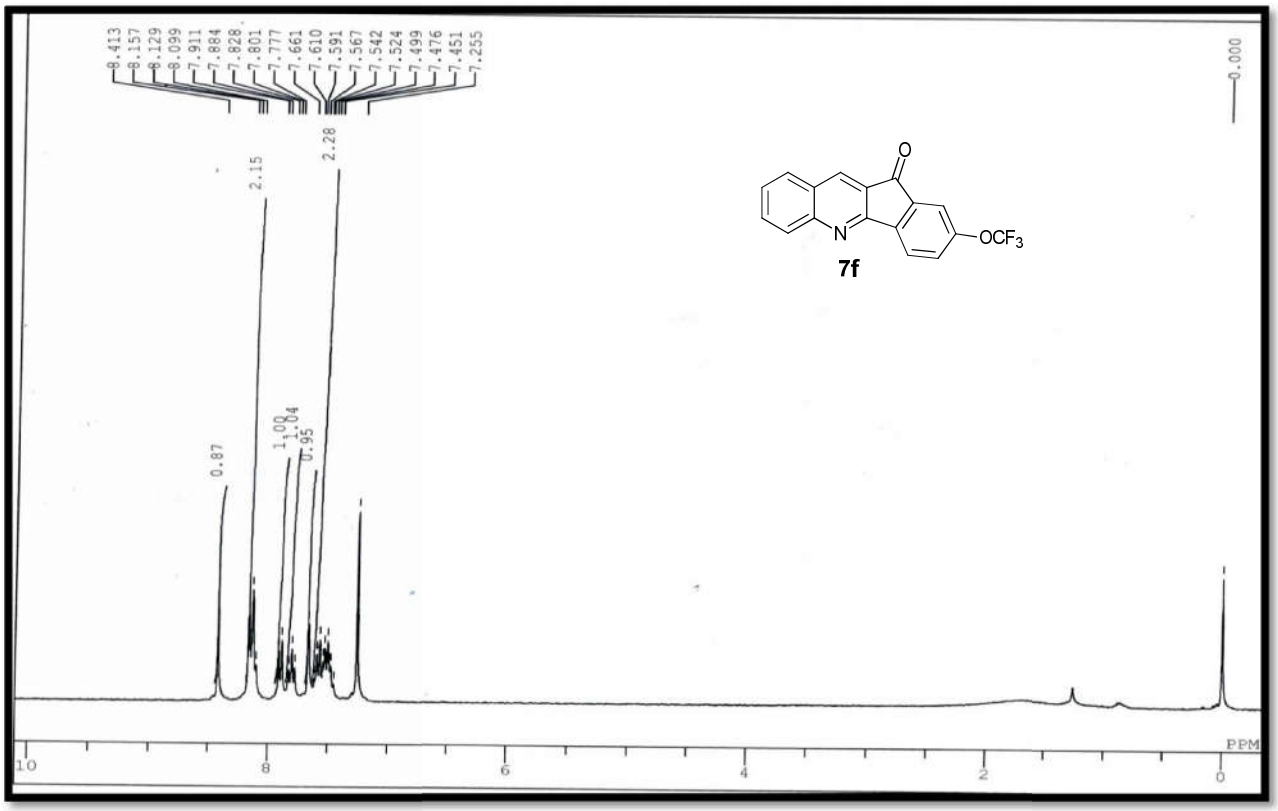
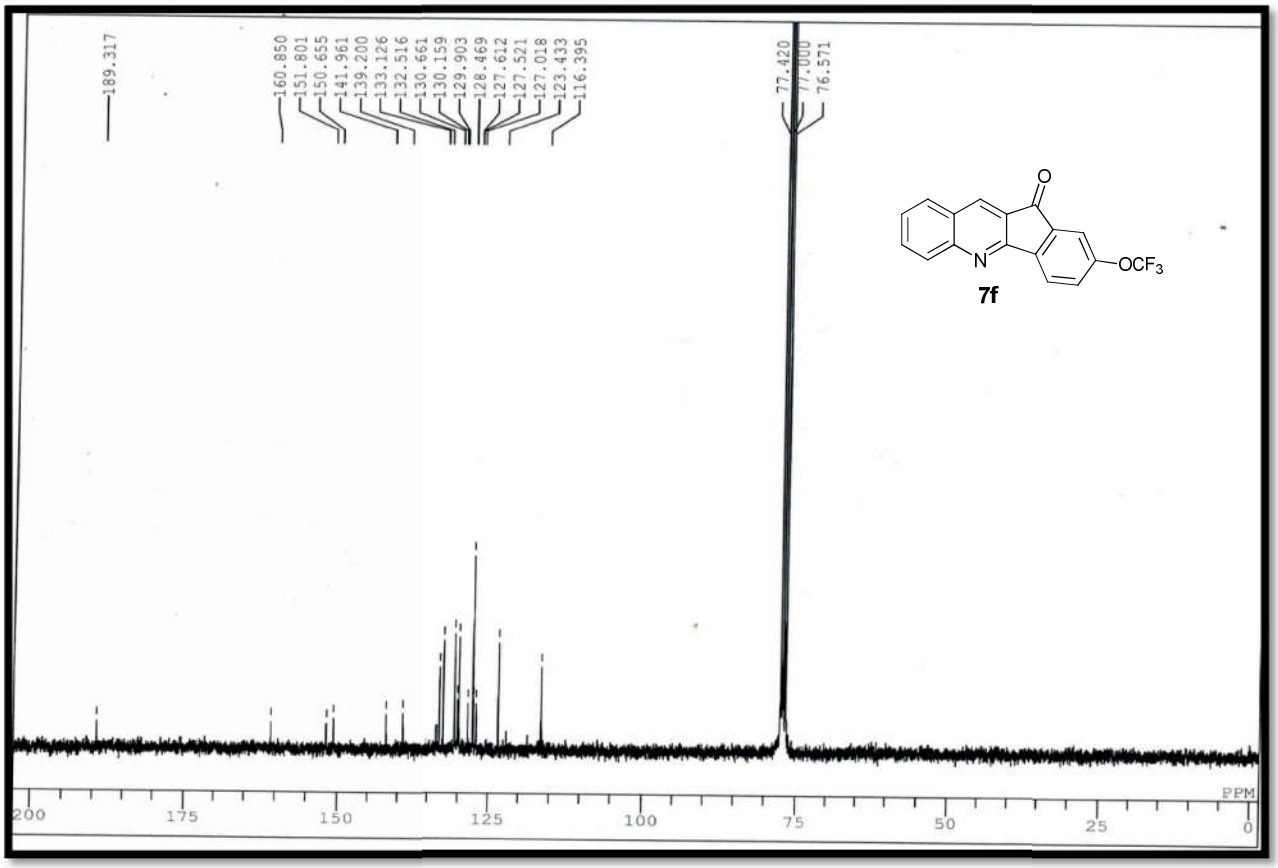
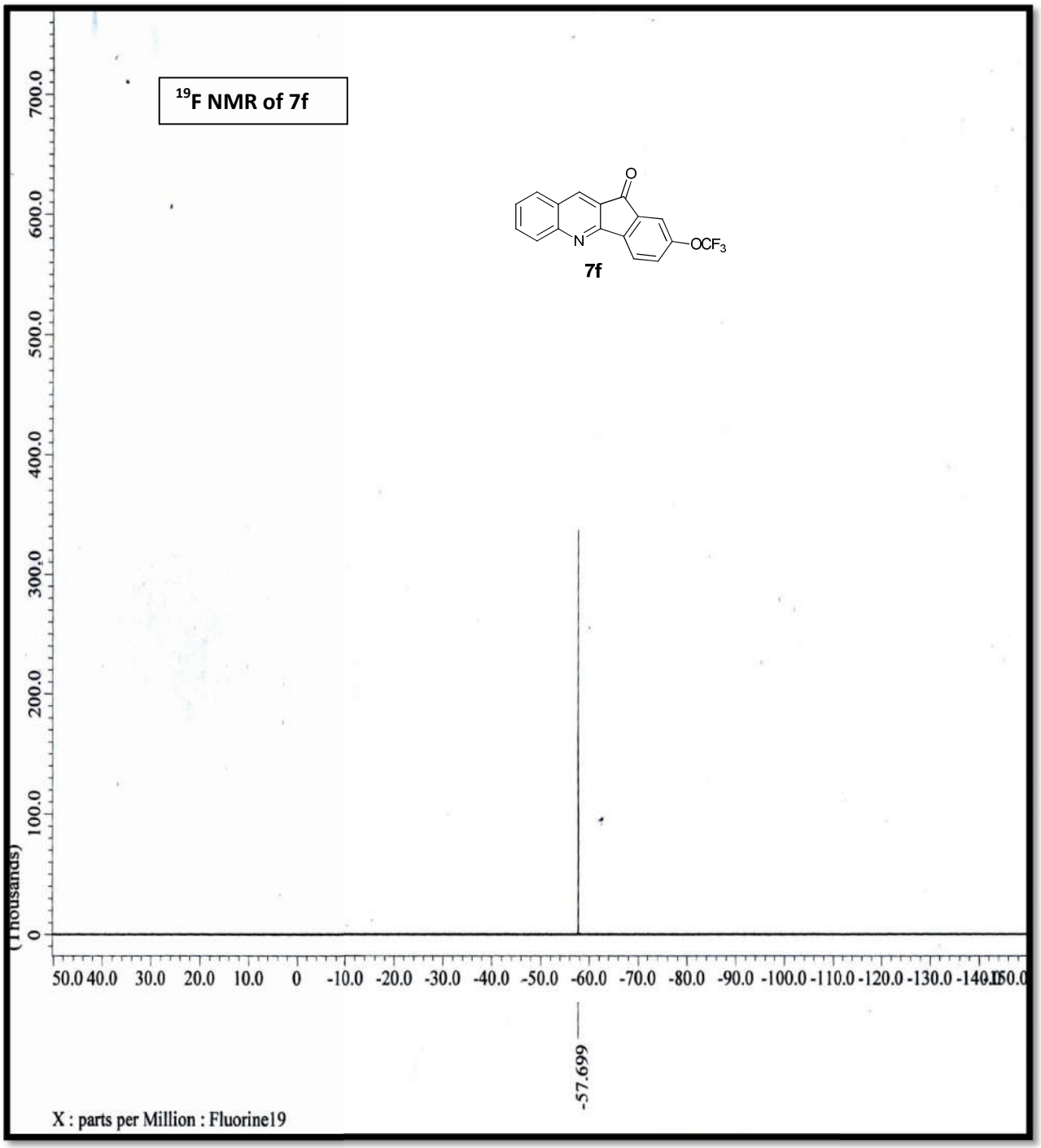
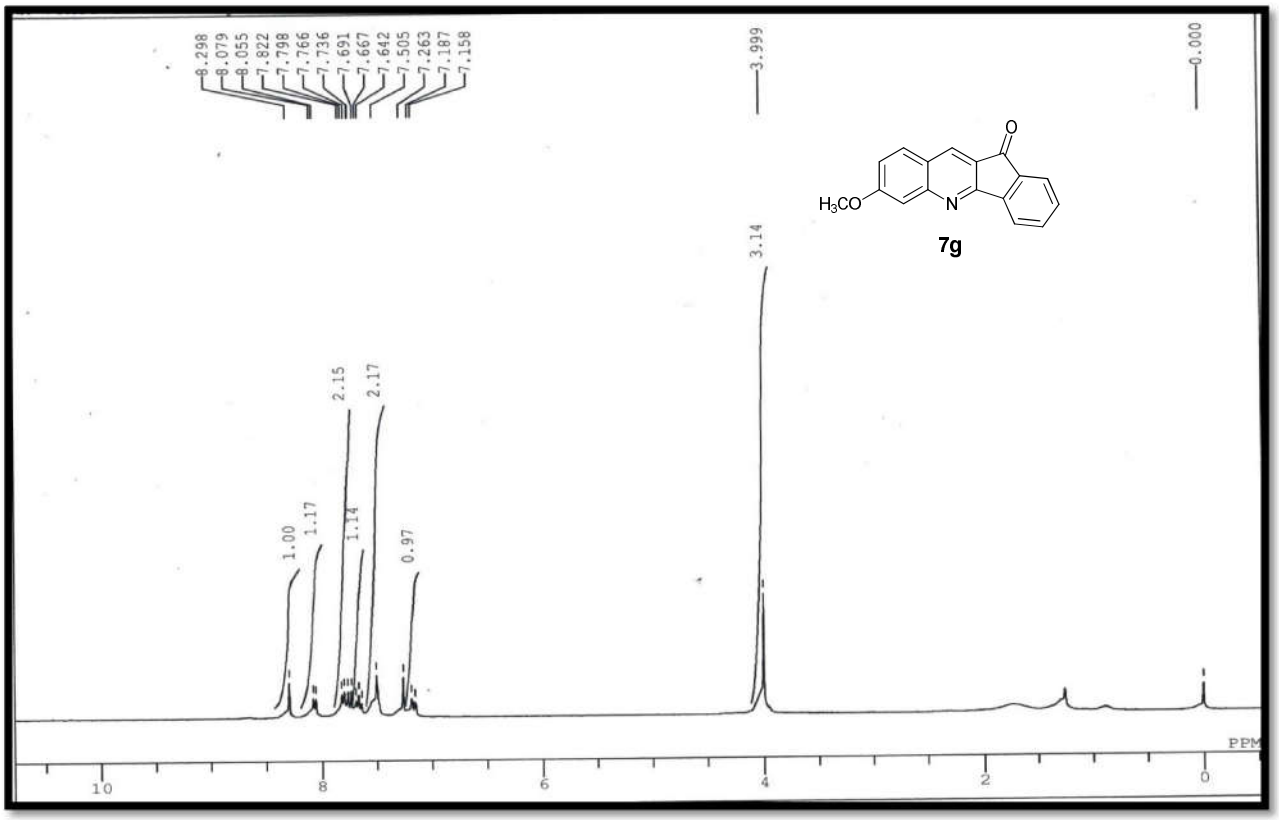
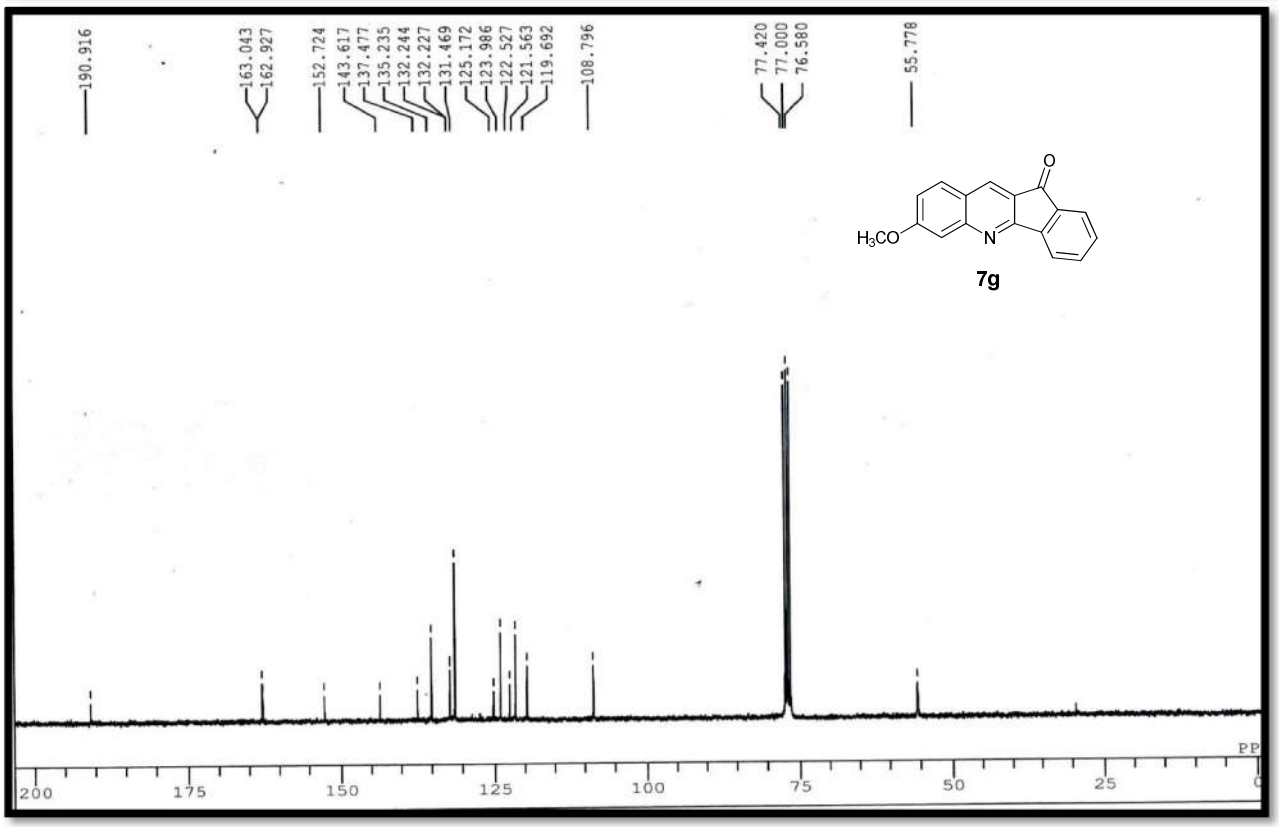
162.235
150.590
142.315
141.408
137.799
136.348
132.285
131.963
130.472
129.689
127.562
127.431
127.010
124.628
121.719
77.420
76.580
21.657
O
N
CH3
7e
PPM
175
150
125
100
75
50
25
0

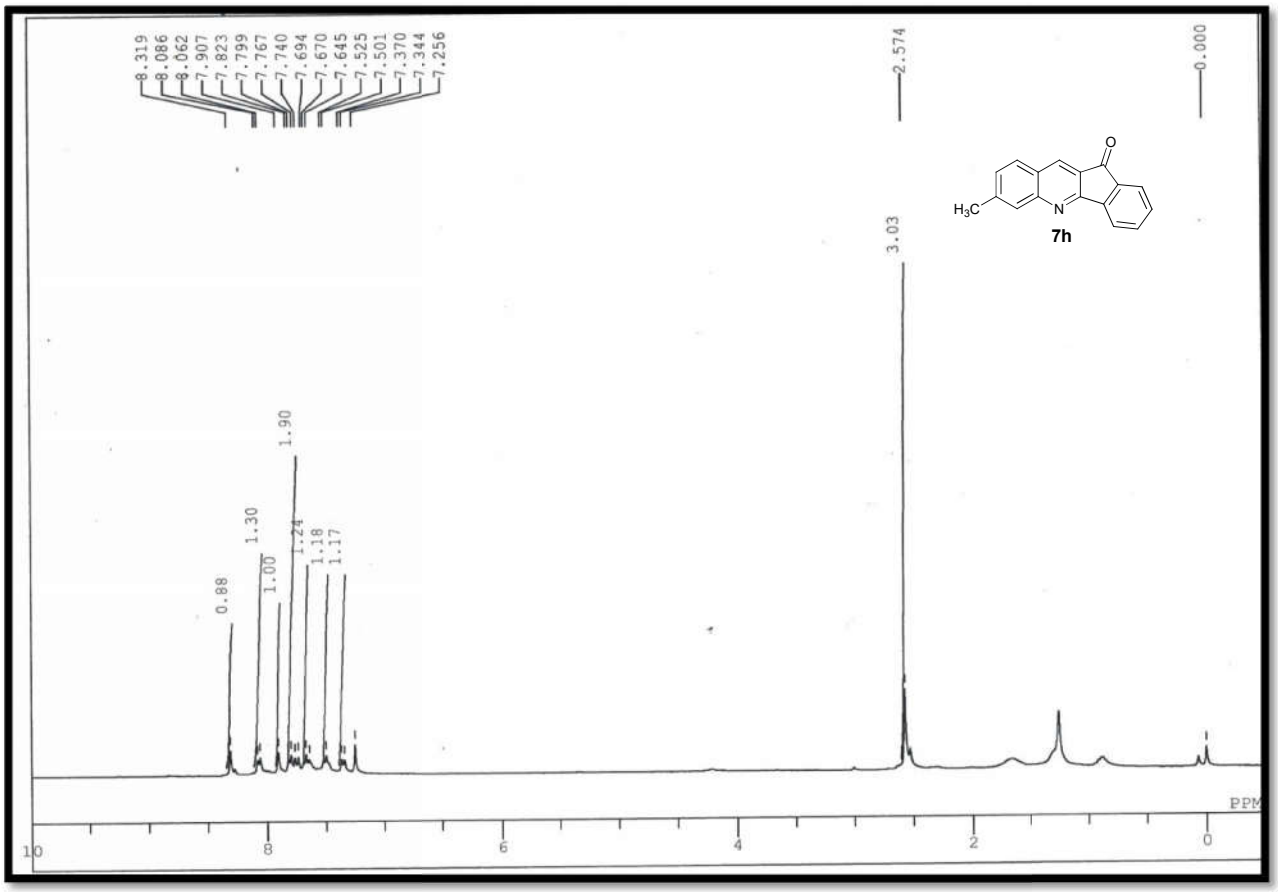

8.413
8.157
8.129
8.099
7.911
7.884
7.828
7.801
7.777
7.661
7.610
7.591
7.567
7.542
7.524
7.499
7.476
7.451
7.255
0.000
2.15
2.28
0.87
1.08
1.04
0.95
O
N
OCF3
7f
PPM
10
8
6
4
2
0

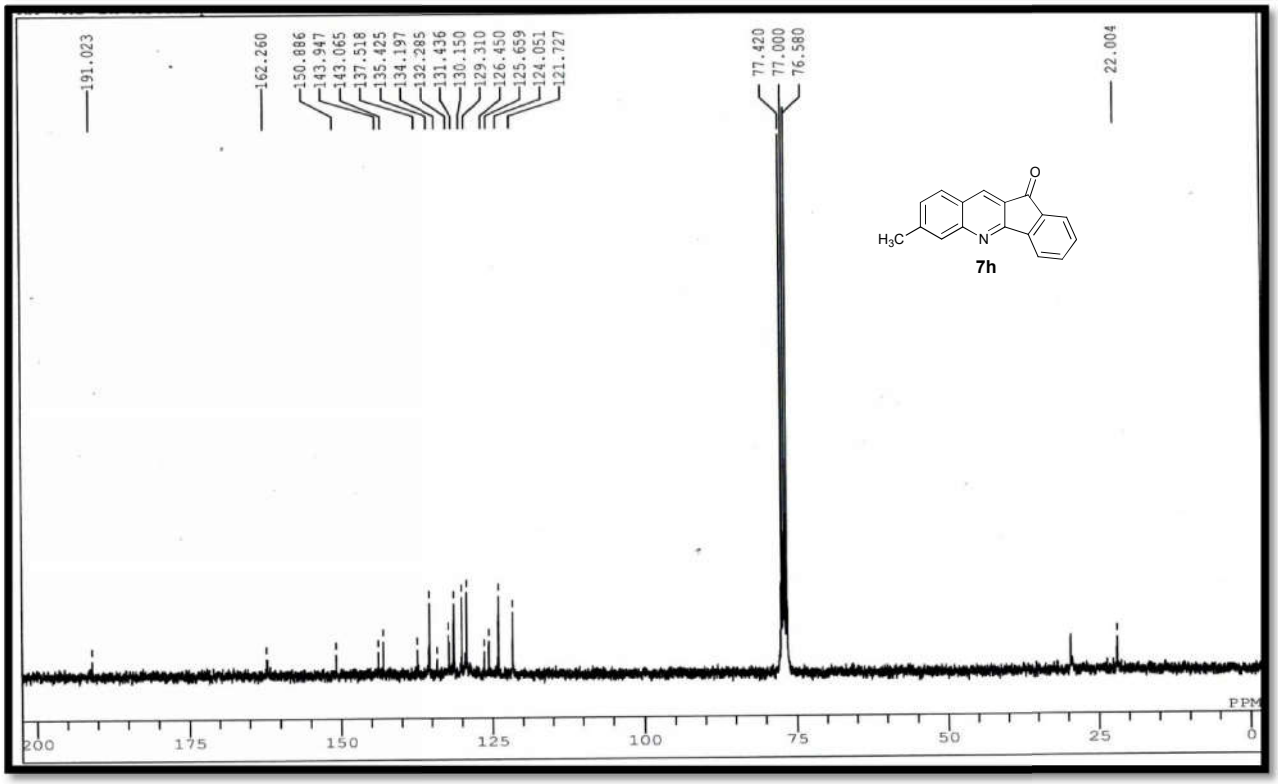

189.317
160.850
151.801
150.655
141.961
139.200
133.126
132.516
130.661
130.159
129.903
128.469
127.612
127.521
127.018
123.433
116.395
77.420
77.000
76.571
O
N
OCF3
7f
PPM
200
175
150
125
100
75
50
25
0

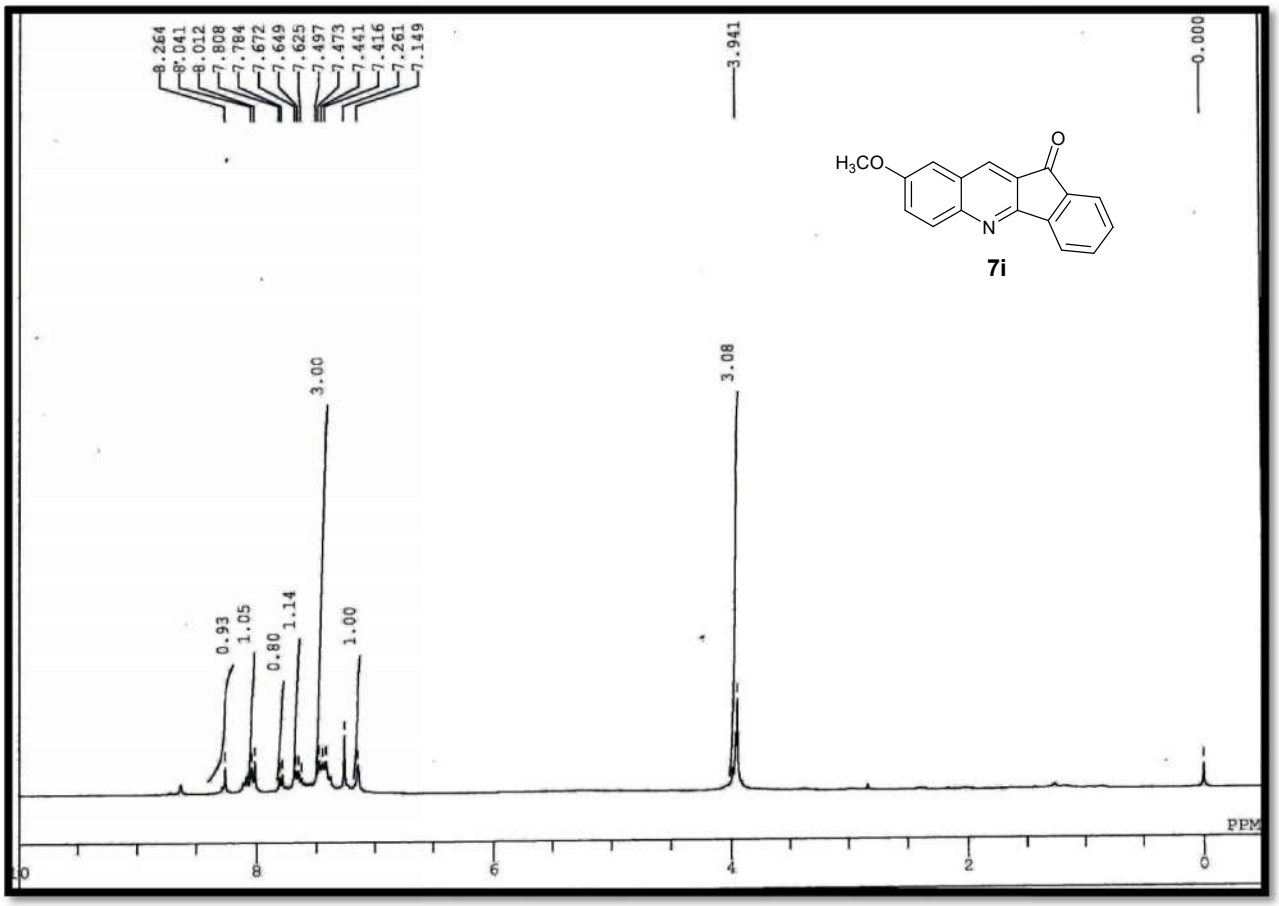

^{19}F NMR of 7f
O
N
OCF3
7f
700.0
600.0
500.0
400.0
300.0
200.0
100.0
0
(Thousands)
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0
-57.699
X : parts per Million : Fluorine19

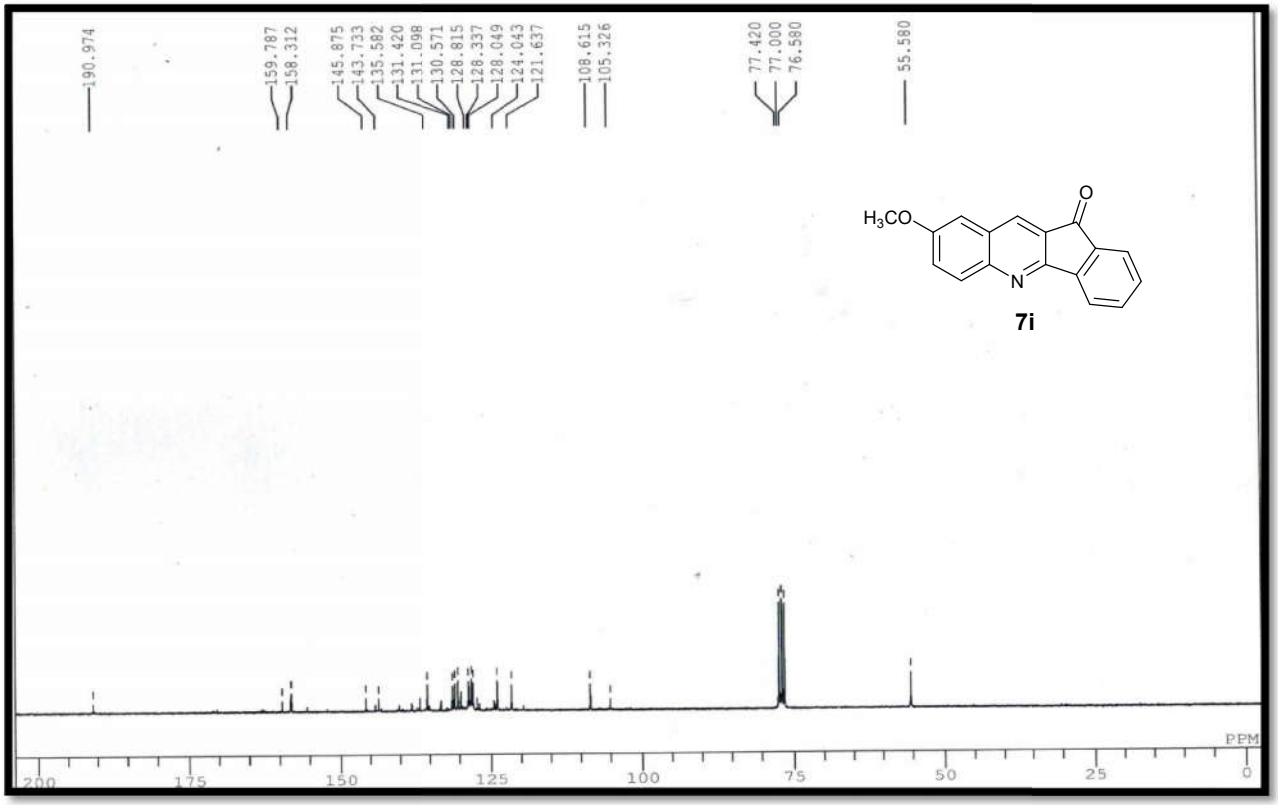

8.298
8.079
8.055
7.822
7.798
7.766
7.736
7.691
7.667
7.642
7.505
7.263
7.187
7.158
3.999
0.000
3.14
2.15
2.17
1.00
1.17
1.14
0.97
PPM
10
8
6
4
2
0
O
H3CO
N
7g


190.916
163.043
162.927
152.724
143.617
137.477
135.235
132.244
132.227
131.469
125.172
123.986
122.527
121.563
119.692
108.796
77.420
77.000
76.580
55.778
200
175
150
125
100
75
50
25
O
H3CO
N
7g


8.319
8.086
8.062
7.907
7.823
7.799
7.767
7.740
7.694
7.670
7.645
7.525
7.501
7.370
7.344
7.256
2.574
0.000
3.03
1.90
1.30
1.24
1.18
1.17
1.00
0.88
O
H3C
N
7h
PPM
10
8
6
4
2
0


191.023
162.260
150.886
143.947
143.065
137.518
135.425
134.197
132.285
131.436
130.150
129.310
126.450
125.659
124.051
121.727
77.420
77.000
76.580
22.004
O
H3C
N
7h
PPM
200
175
150
125
100
75
50
25
0


8.264
8.041
8.012
7.808
7.784
7.672
7.649
7.625
7.497
7.473
7.441
7.416
7.261
7.149
3.941
0.000
H3CO
O
N
7i
3.00
3.08
0.93
1.05
0.80
1.14
1.00
PPM
10
8
6
4
2
0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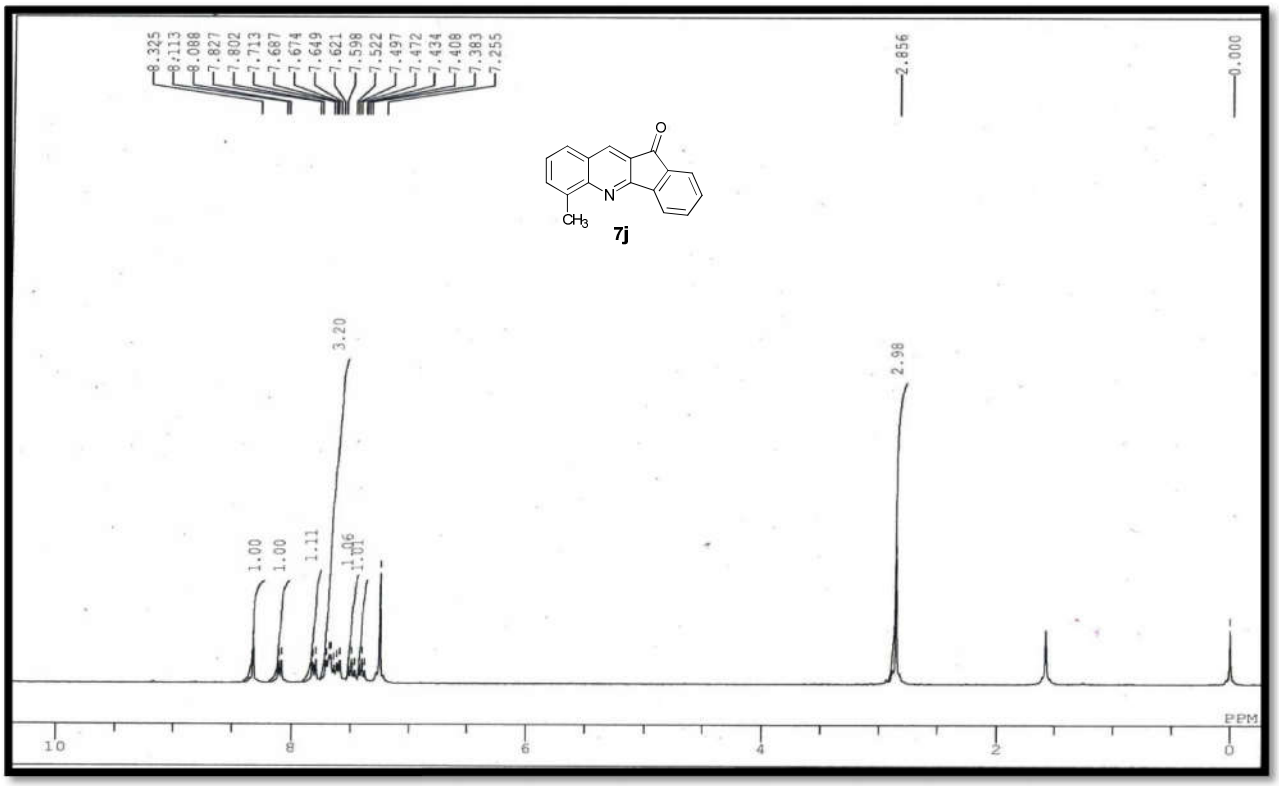
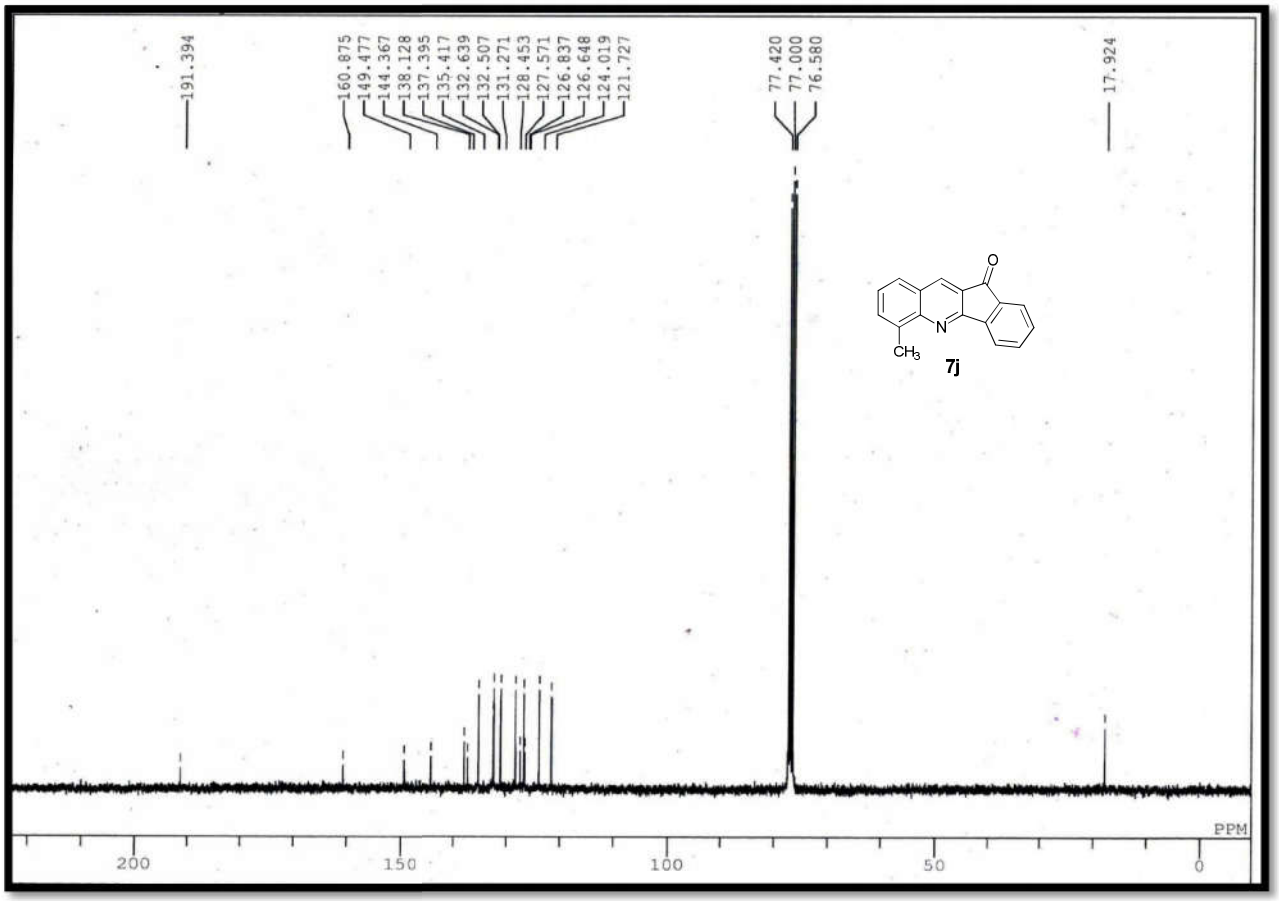
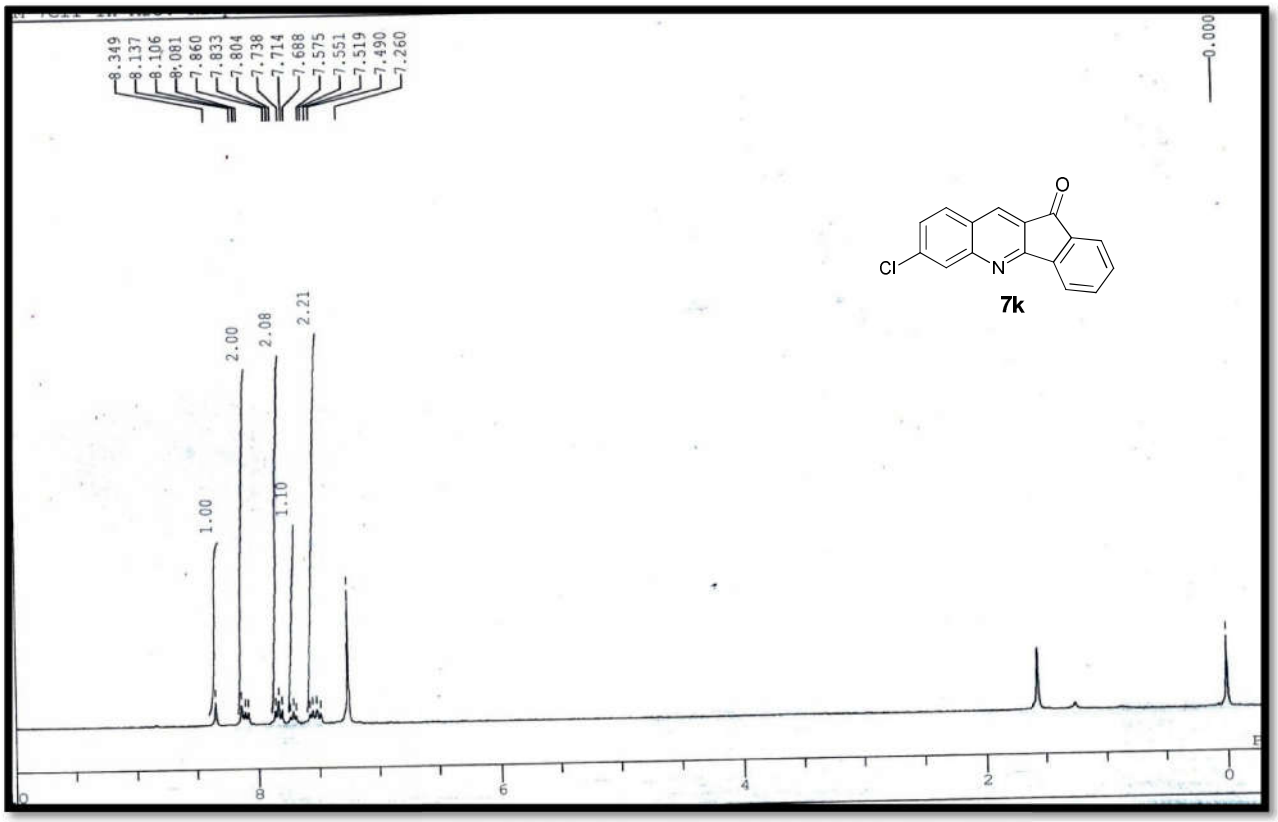
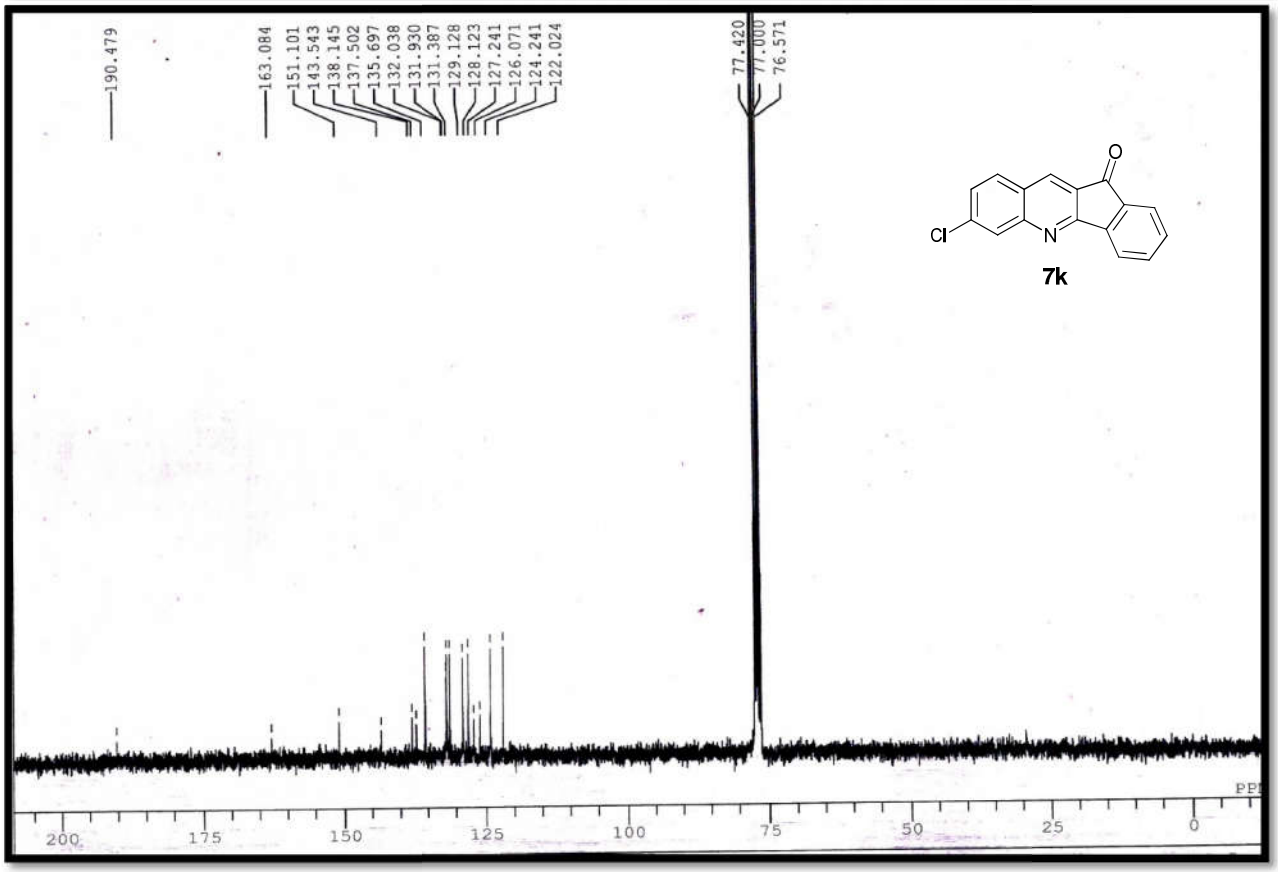
159.787
158.312
145.875
143.733
135.582
131.420
131.098
130.571
128.815
128.337
128.049
124.043
121.637
108.615
105.326
77.420
77.000
76.580
55.580
H3CO
O
N
7i
PPM
200
175
150
125
100
75
50
25
0


8.325
8.113
8.088
7.827
7.802
7.713
7.687
7.674
7.649
7.621
7.598
7.522
7.497
7.472
7.434
7.408
7.383
7.255
2.856
0.000
O
N
CH3
7j
3.20
2.98
1.00
1.00
1.11
1.06
1.01
PPM
10
8
6
4
2
0


191.394
160.875
149.477
144.367
138.128
137.395
135.417
132.639
132.507
131.271
128.453
127.571
126.837
126.648
124.019
121.727
77.420
77.000
76.580
17.924
O
N
CH3
7j
PPM
200
150
100
50
0


8.349
8.137
8.106
8.081
7.860
7.833
7.804
7.738
7.714
7.688
7.575
7.551
7.519
7.490
7.260
0.000
2.00
2.08
2.21
1.00
1.10
Cl
N
O
7k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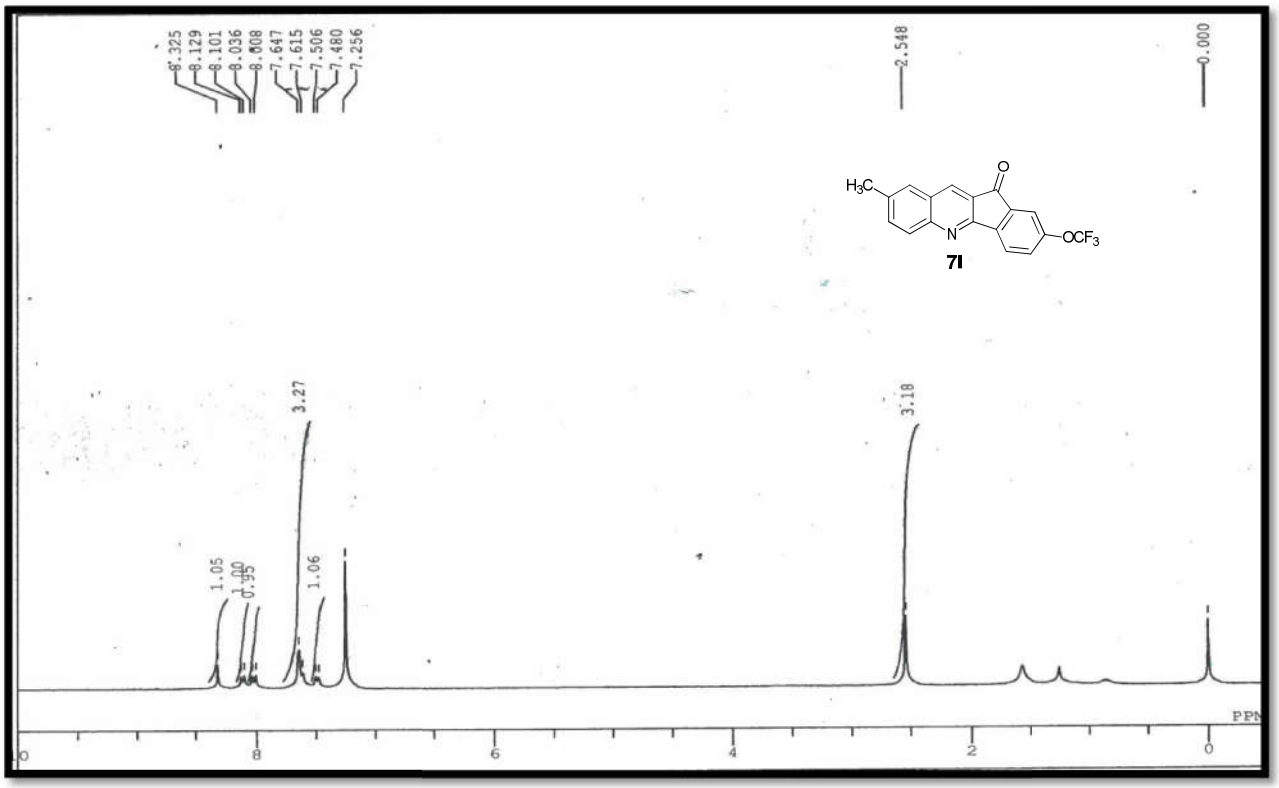
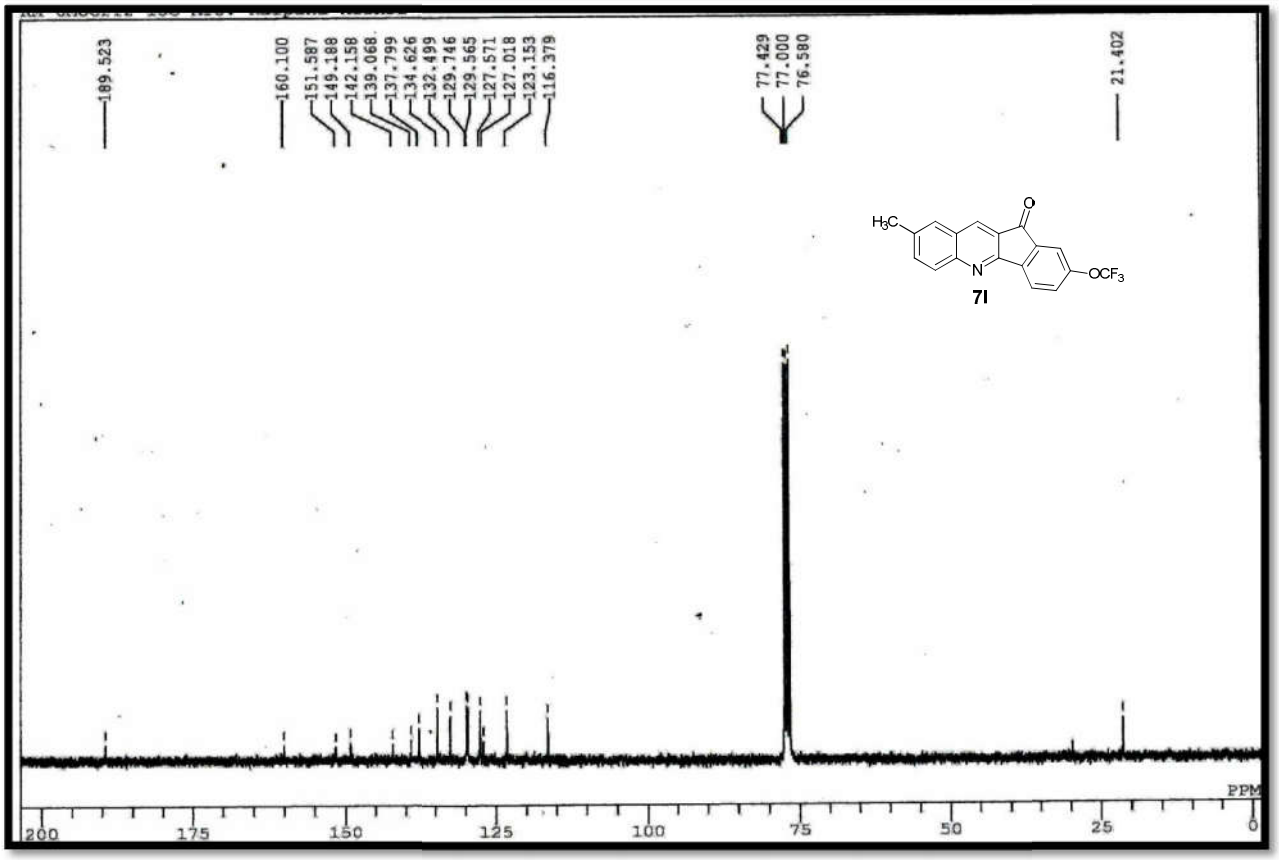
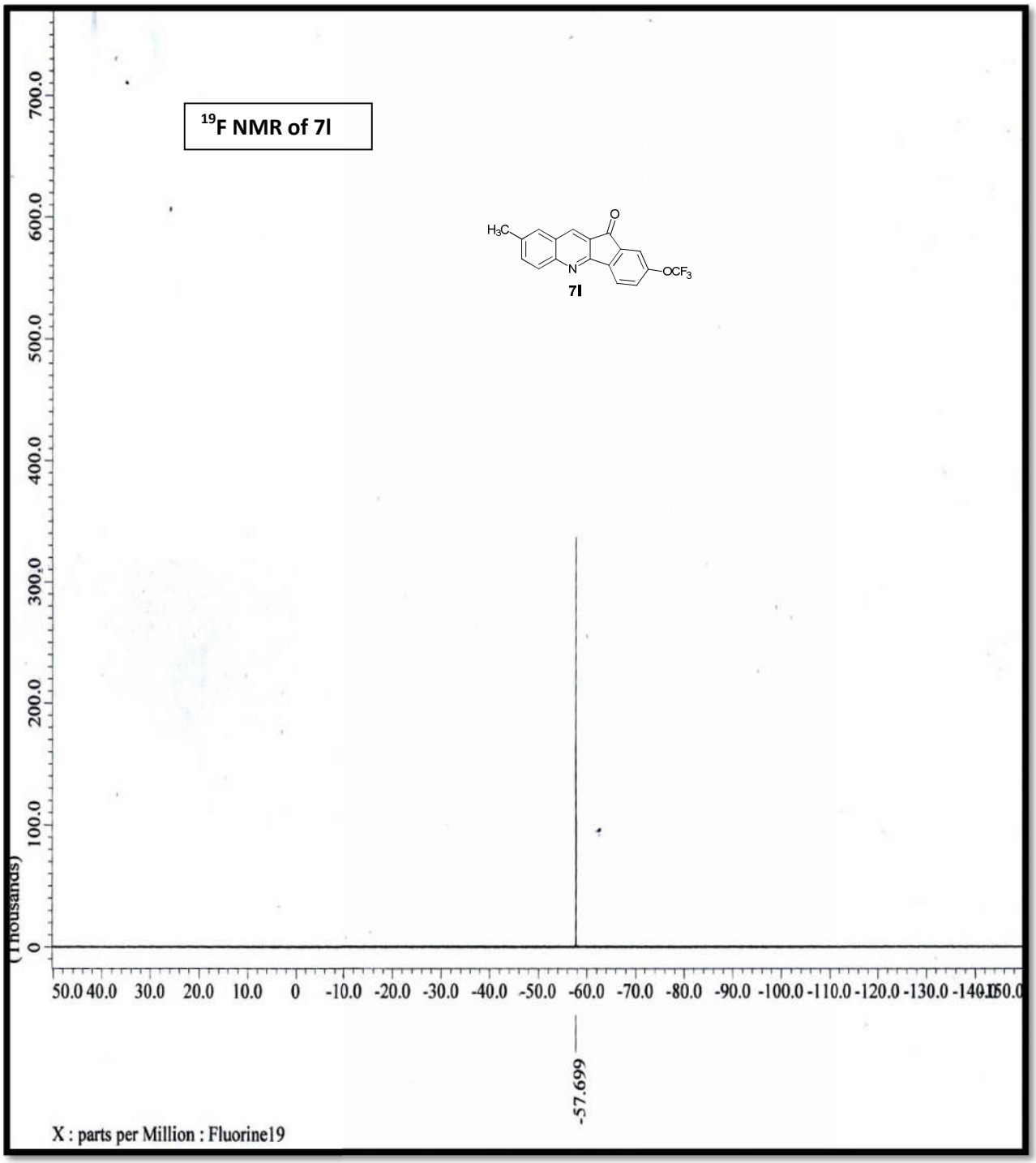
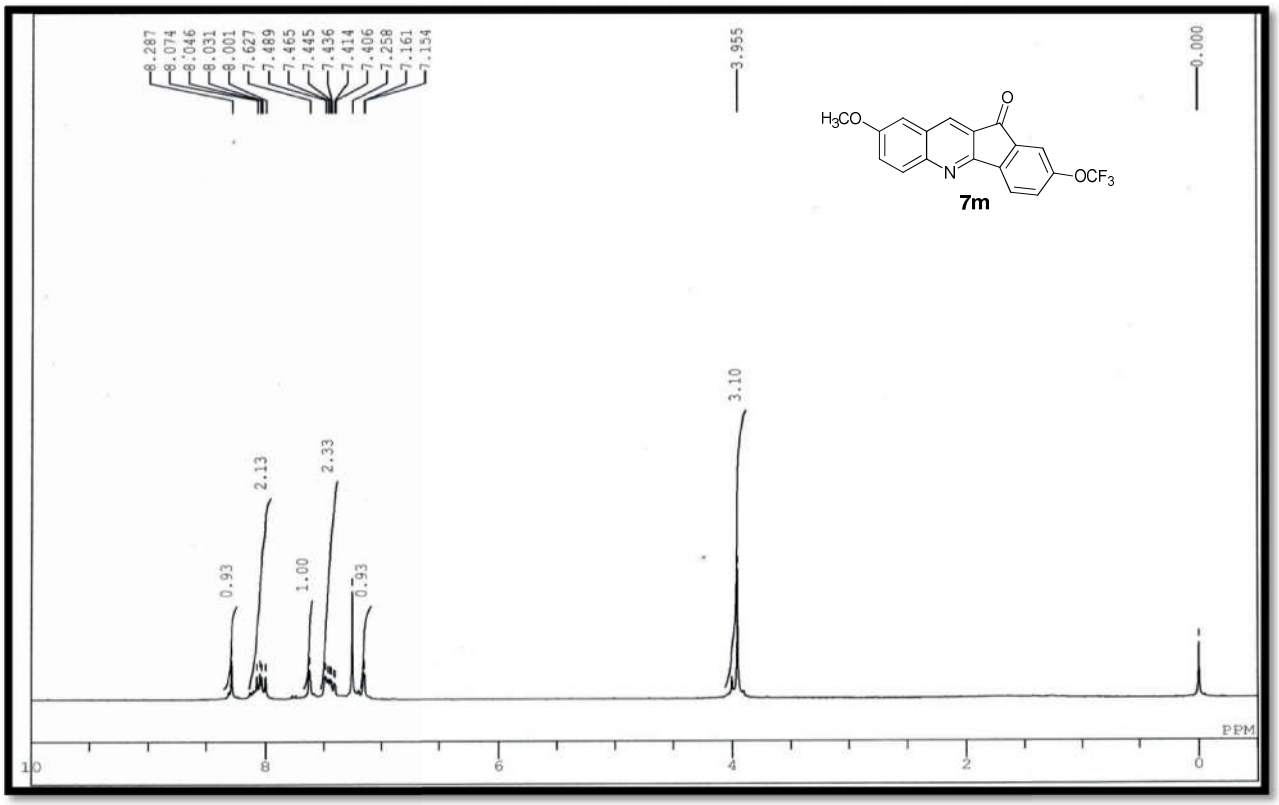
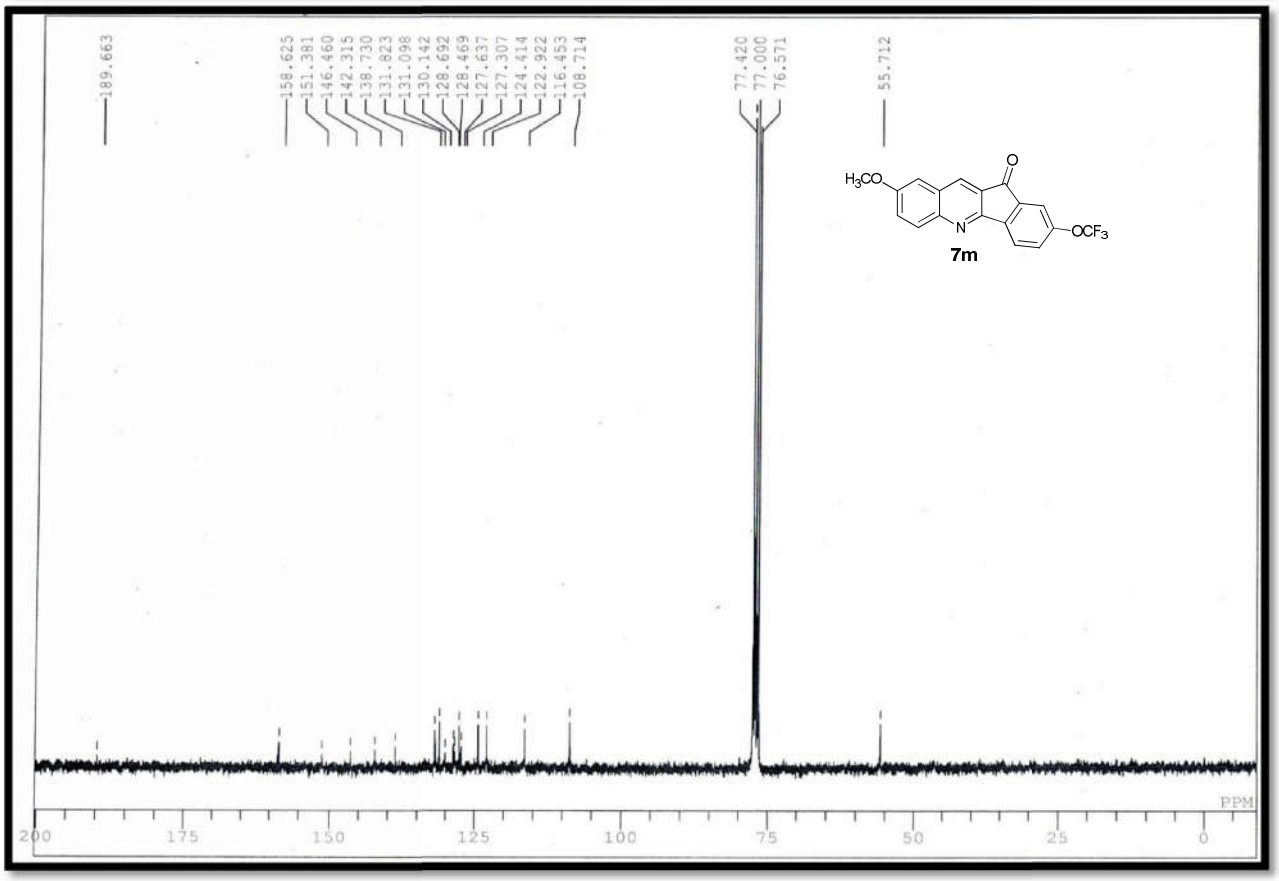
163.084
151.101
143.543
138.145
137.502
135.697
132.038
131.930
131.387
129.128
128.123
127.241
126.071
124.241
122.024
77.420
77.000
76.571
Cl
N
O
7k

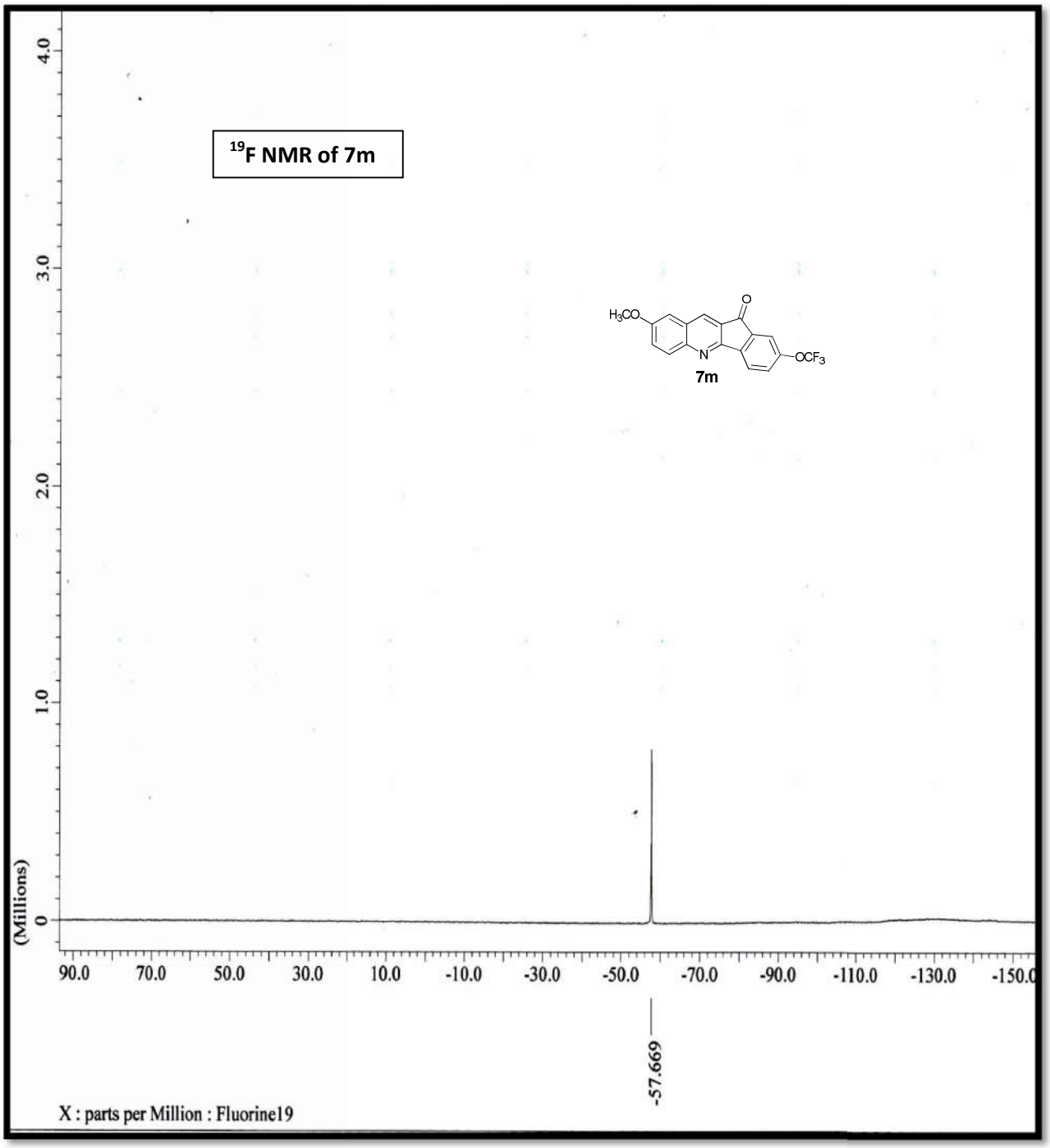

8.325
8.129
8.101
8.036
8.008
7.647
7.615
7.506
7.480
7.256
2.548
0.000
H3C
O
N
OCF3
7l
3.27
3.18
1.05
1.00
0.95
1.06
PPM
0
2
4
6
8

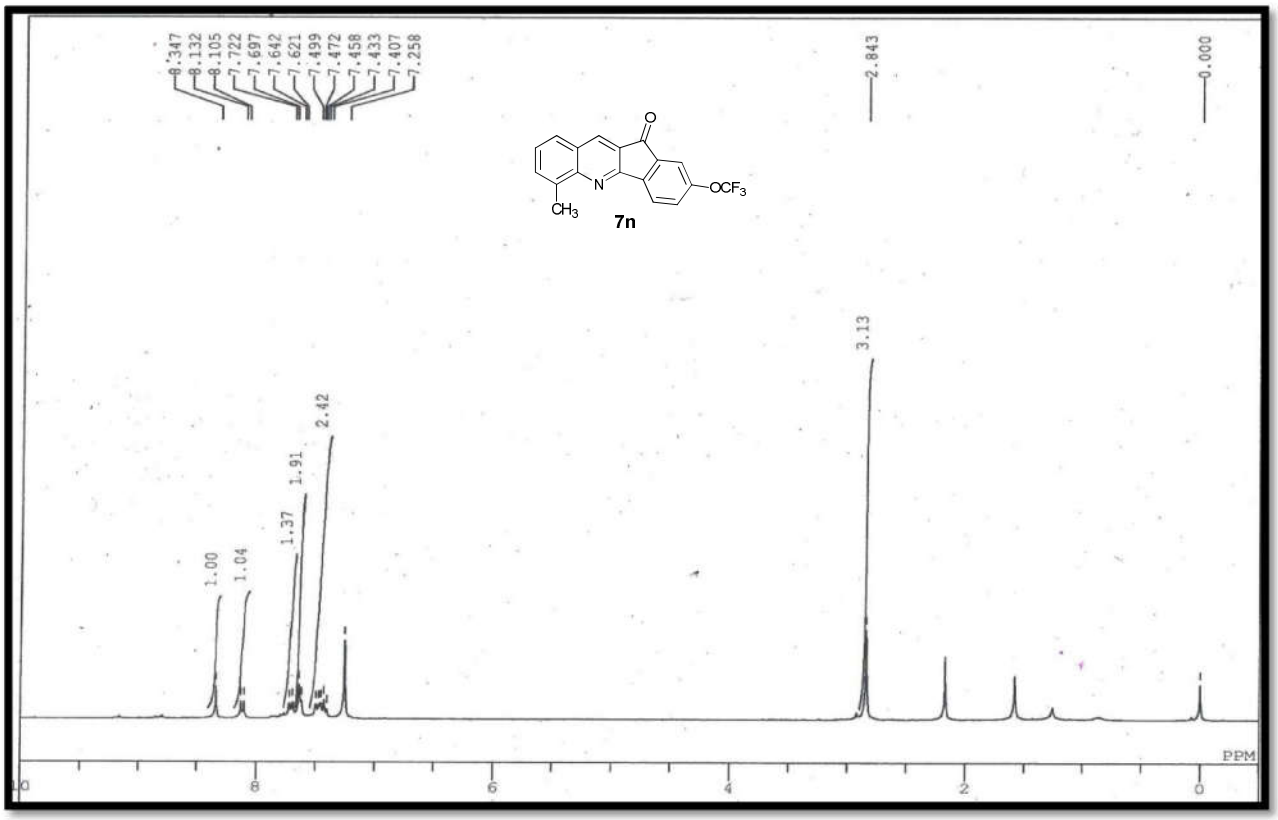

189.523
160.100
151.587
149.188
142.158
139.068
137.799
134.626
132.499
129.746
129.565
127.571
127.018
123.153
116.379
77.429
77.000
76.580
21.402
H3C
O
N
OCF3
7l
PPM
200
175
150
125
100
75
50
25
0

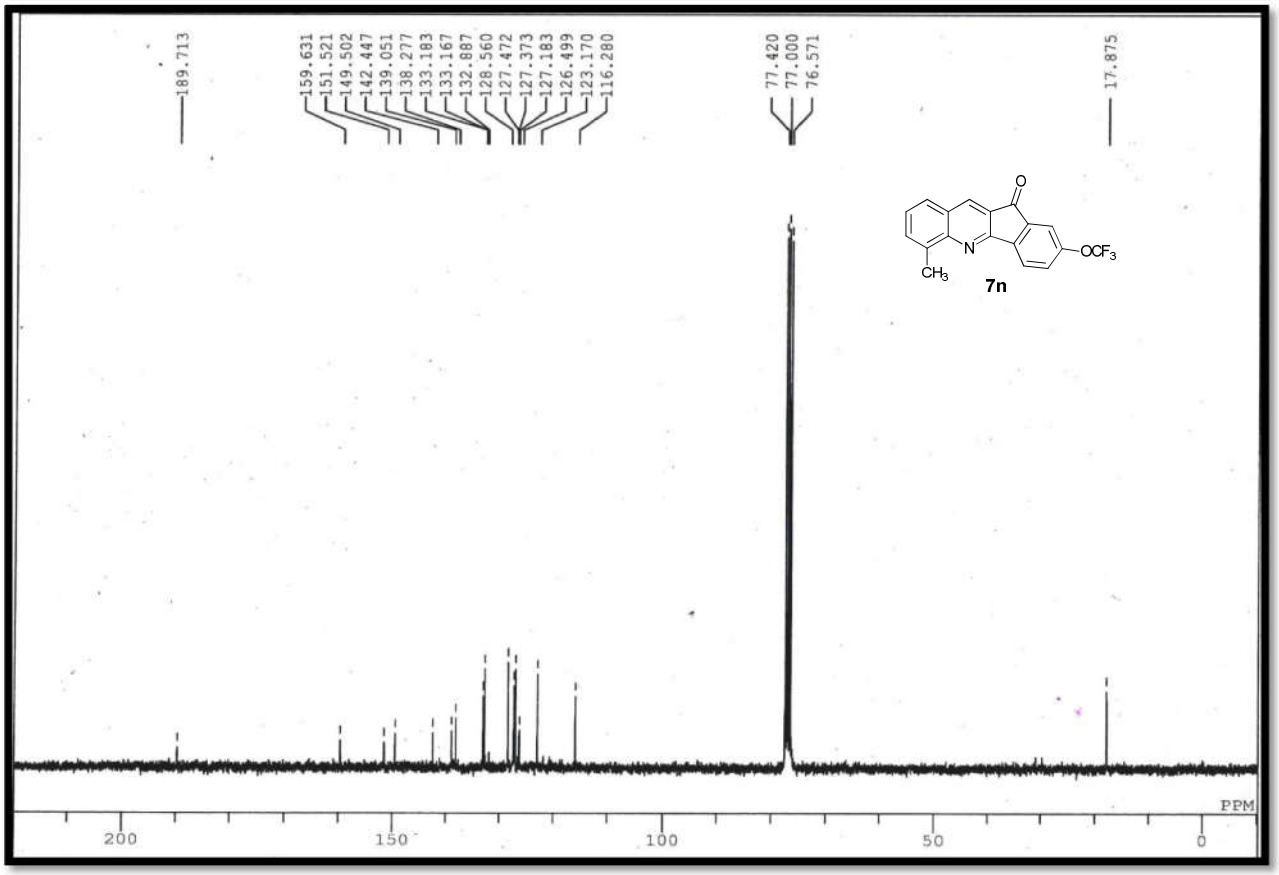

19F NMR of 7l
H3C
O
N
OCF3
7l
700.0
600.0
500.0
400.0
300.0
200.0
100.0
0
(Thousands)
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0
-57.699
X : parts per Million : Fluorine19

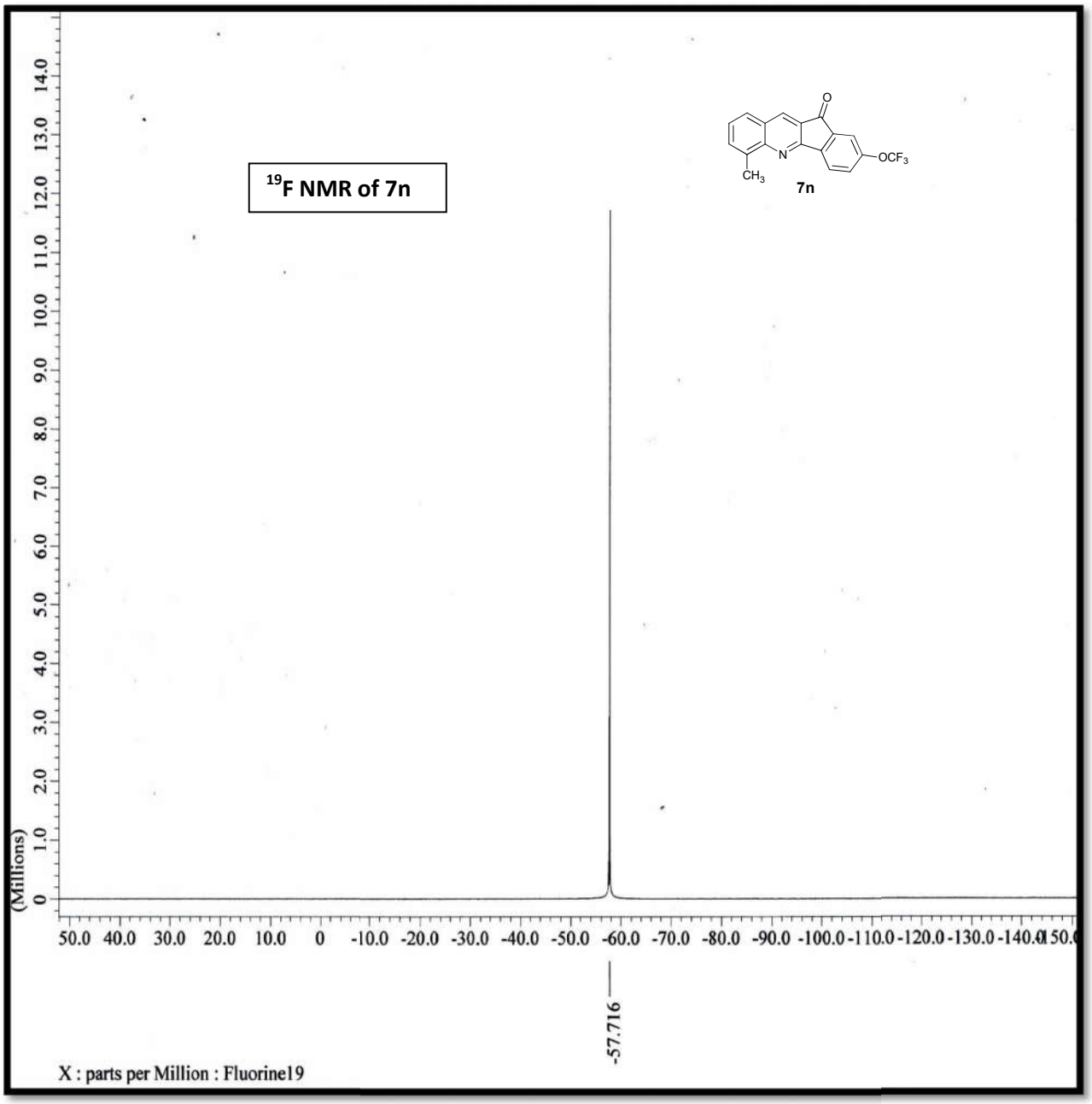

8.287
8.074
8.046
8.031
8.001
7.627
7.489
7.465
7.445
7.436
7.414
7.406
7.258
7.161
7.154
3.955
0.000
3.10
2.13
2.33
0.93
1.00
0.93
PPM
10
8
6
4
2
0
O
H3CO
N
OCF3
7m

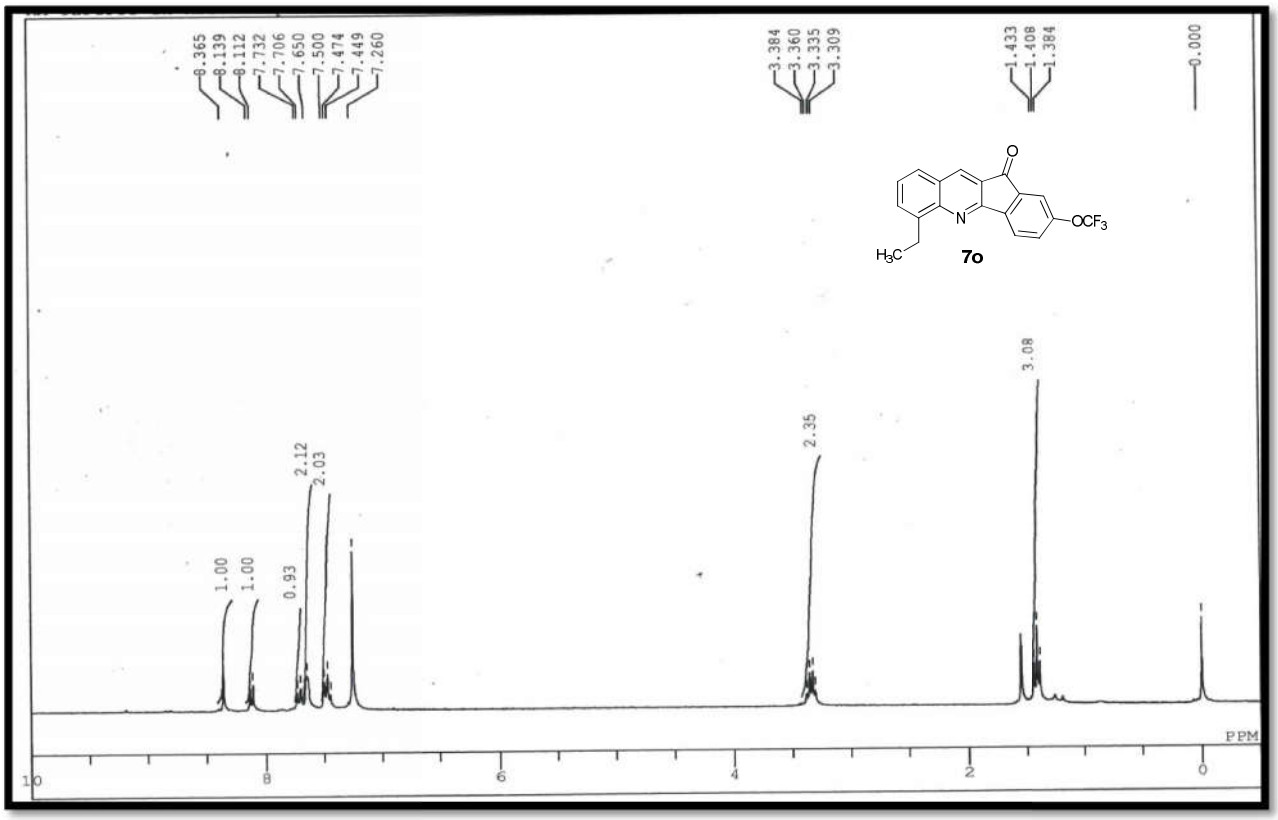

189.663
158.625
151.381
146.460
142.315
138.730
131.823
131.098
130.142
128.692
128.469
127.637
127.307
124.414
122.922
116.453
108.714
77.420
77.000
76.571
55.712
PPM
200
175
150
125
100
75
50
25
0
O
H3CO
N
OCF3
7m

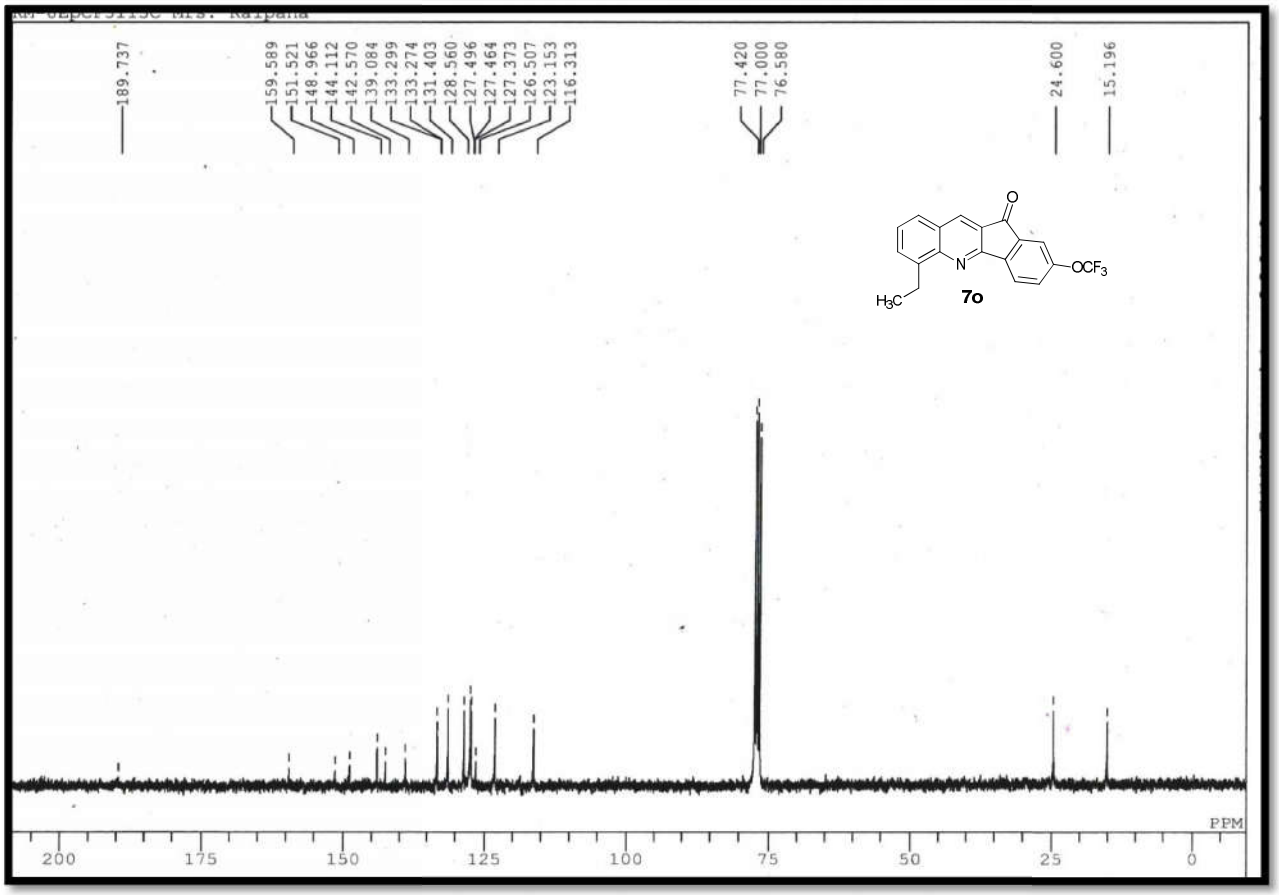

^{19}F NMR of 7m
H3CO
O
N
OCF3
7m
4.0
3.0
2.0
1.0
0
(Millions)
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-57.669
X : parts per Million : Fluorine19

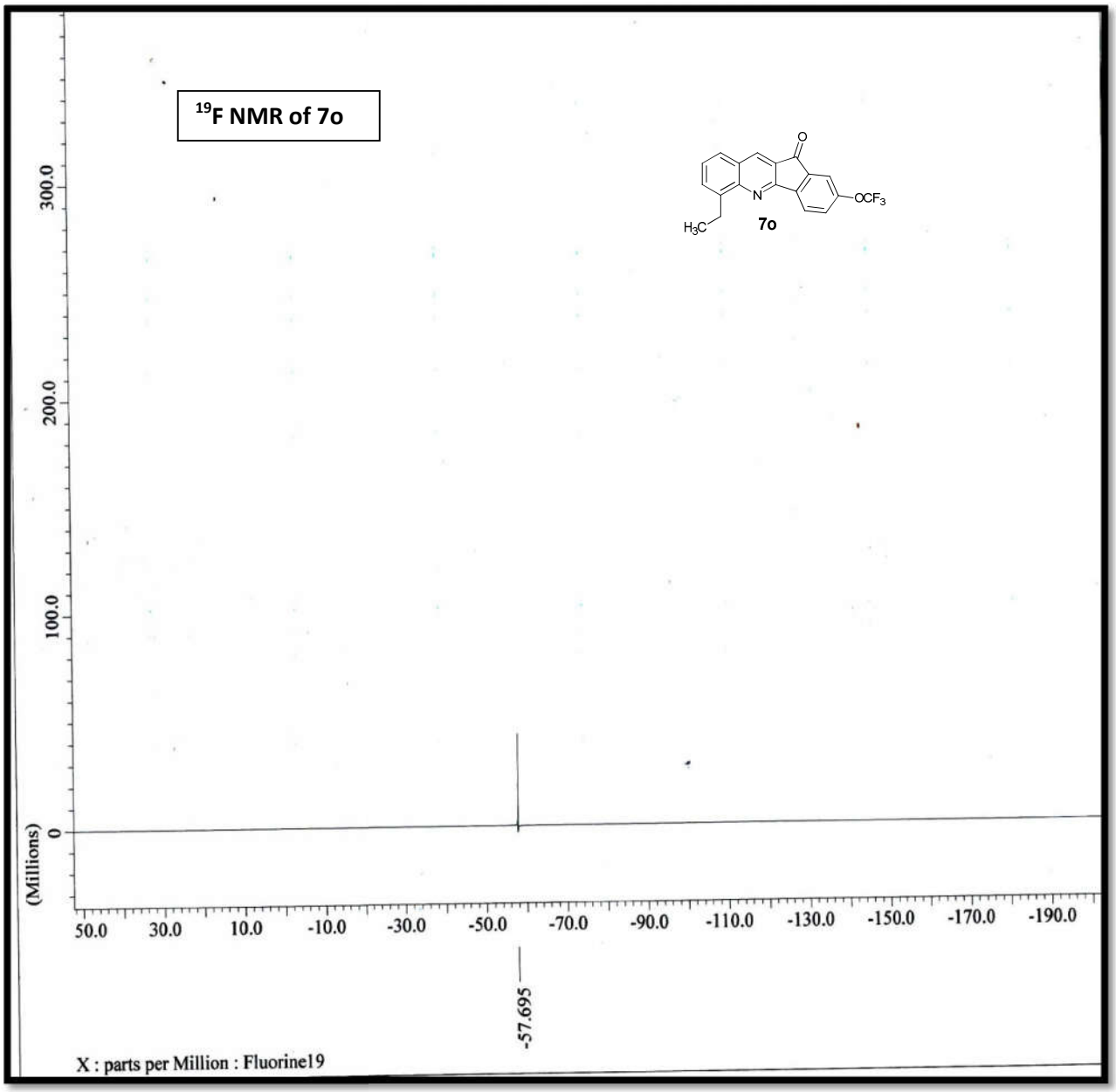

8.347
8.132
8.105
7.722
7.697
7.642
7.621
7.499
7.472
7.458
7.433
7.407
7.258
2.843
0.000
O
N
CH3
OCF3
7n
3.13
2.42
1.91
1.37
1.04
1.00
PPM
10
8
6
4
2
0

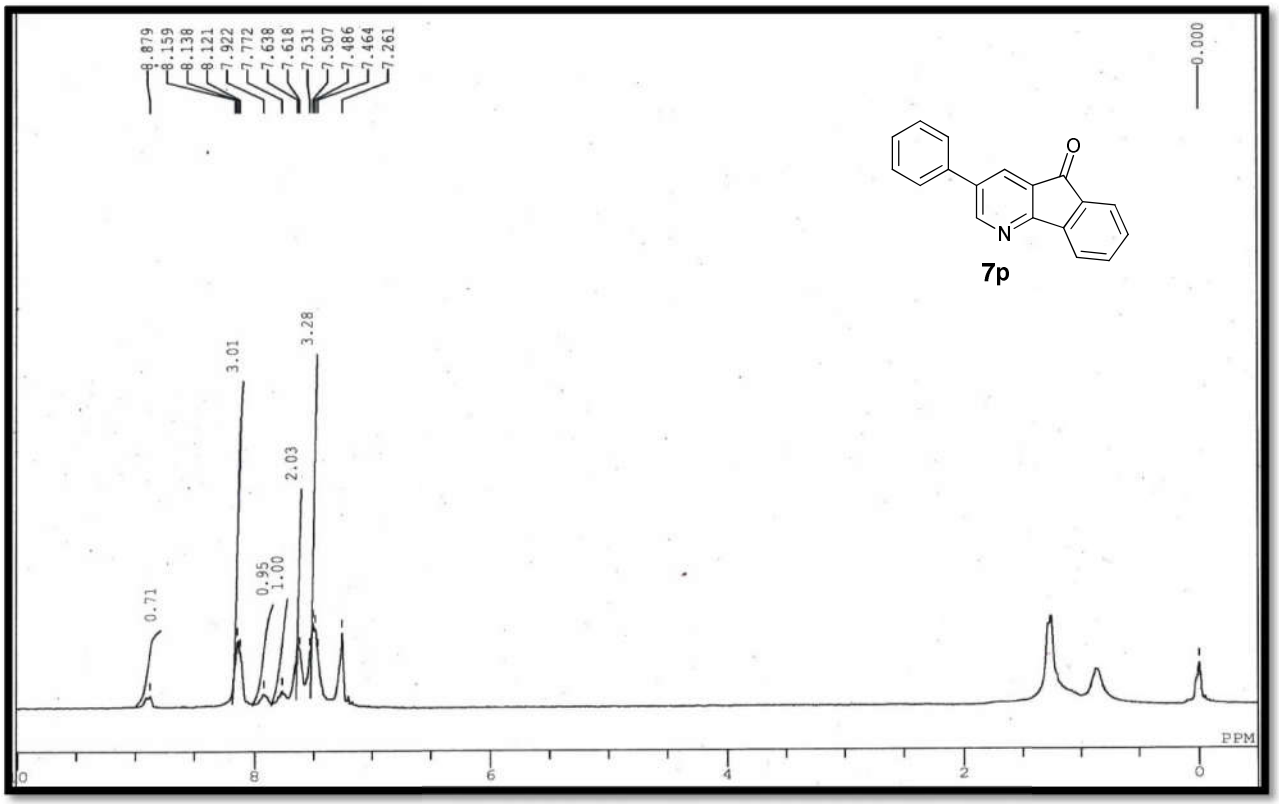

189.713
159.631
151.521
149.502
142.447
139.051
138.277
133.183
133.167
132.887
128.560
127.472
127.373
127.183
126.499
123.170
116.280
77.420
77.000
76.571
17.875
O
N
CH3
OCF3
7n
PPM
200
150
100
50
0

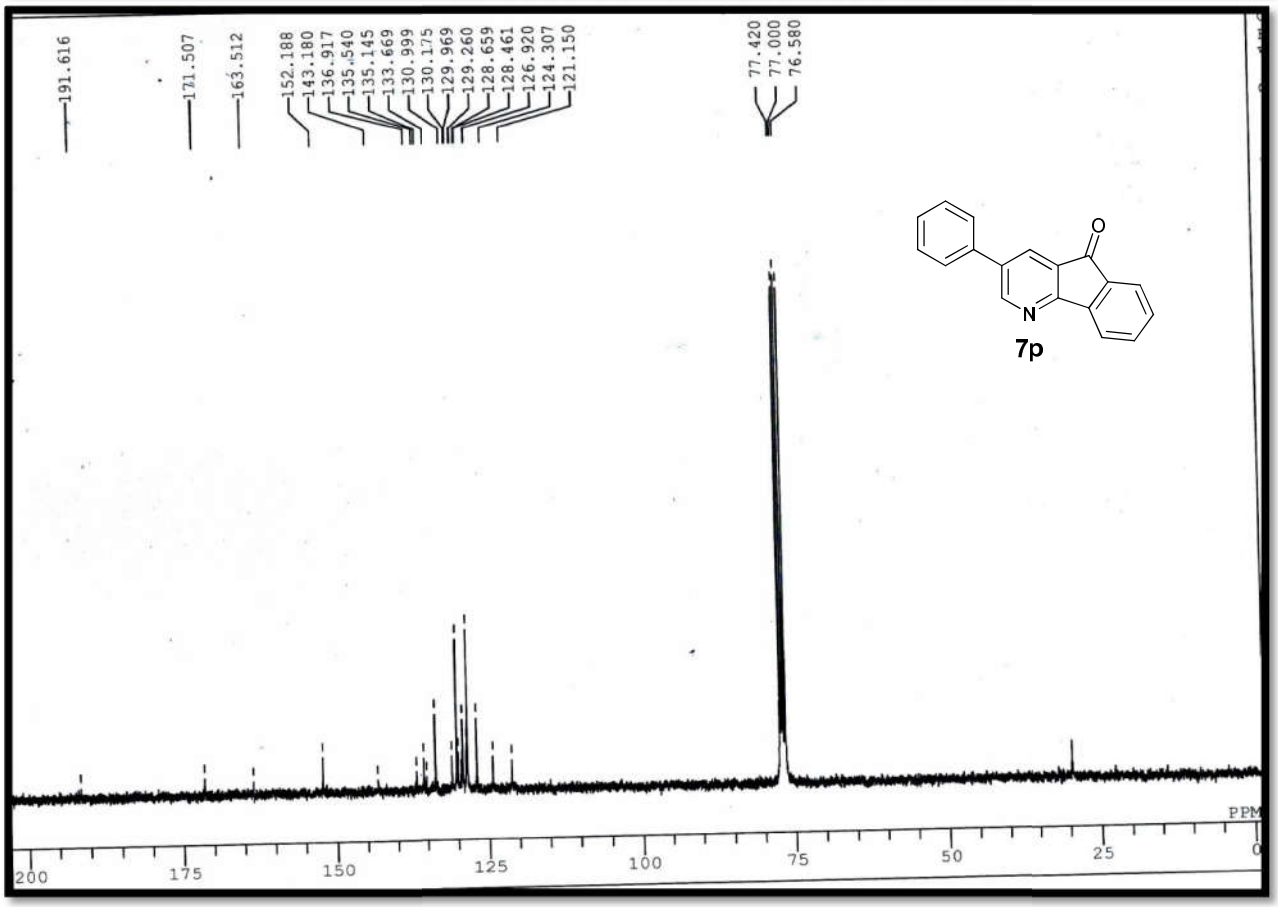

19F NMR of 7n
O
N
CH3
OCF3
7n
(Millions)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0
-57.716
X : parts per Million : Fluorine19

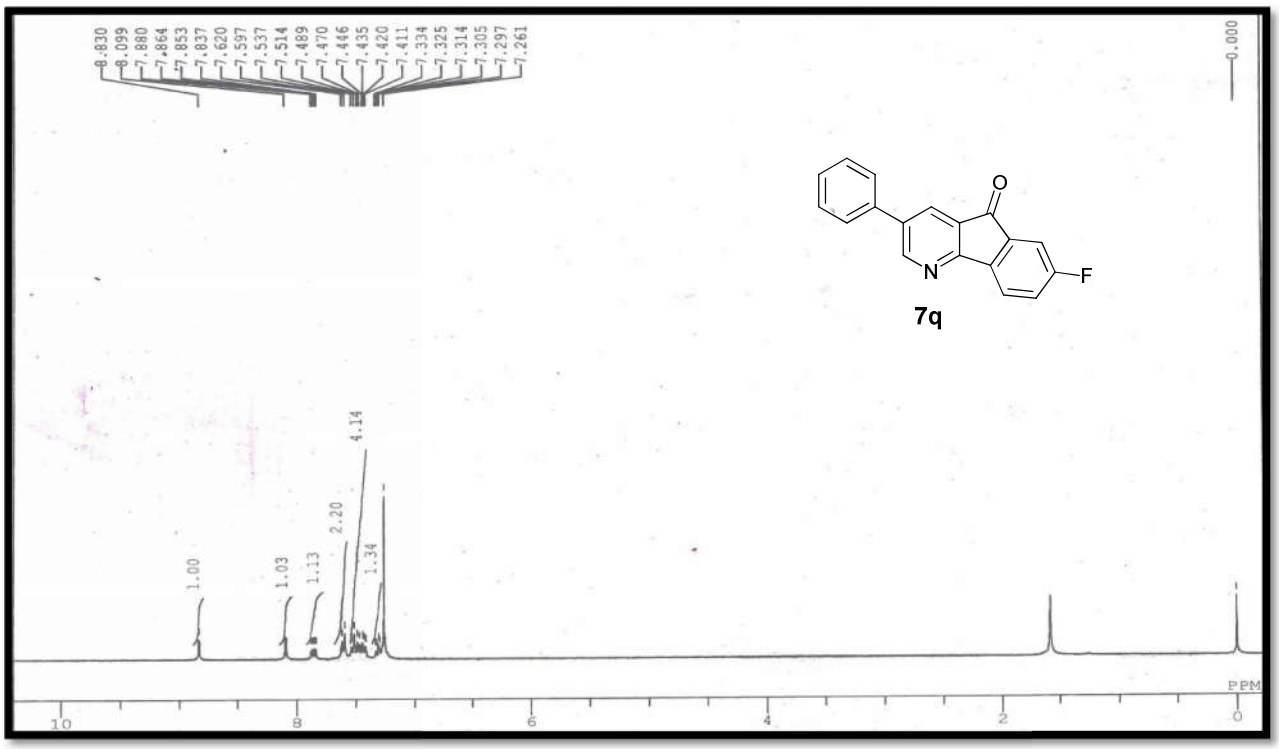

8.365
8.139
8.112
7.732
7.706
7.650
7.500
7.474
7.449
7.260
3.384
3.360
3.335
3.309
1.433
1.408
1.384
0.000
O
N
OCF3
H3C
7o
3.08
2.35
2.12
2.03
1.00
1.00
0.93
PPM
10
8
6
4
2
0

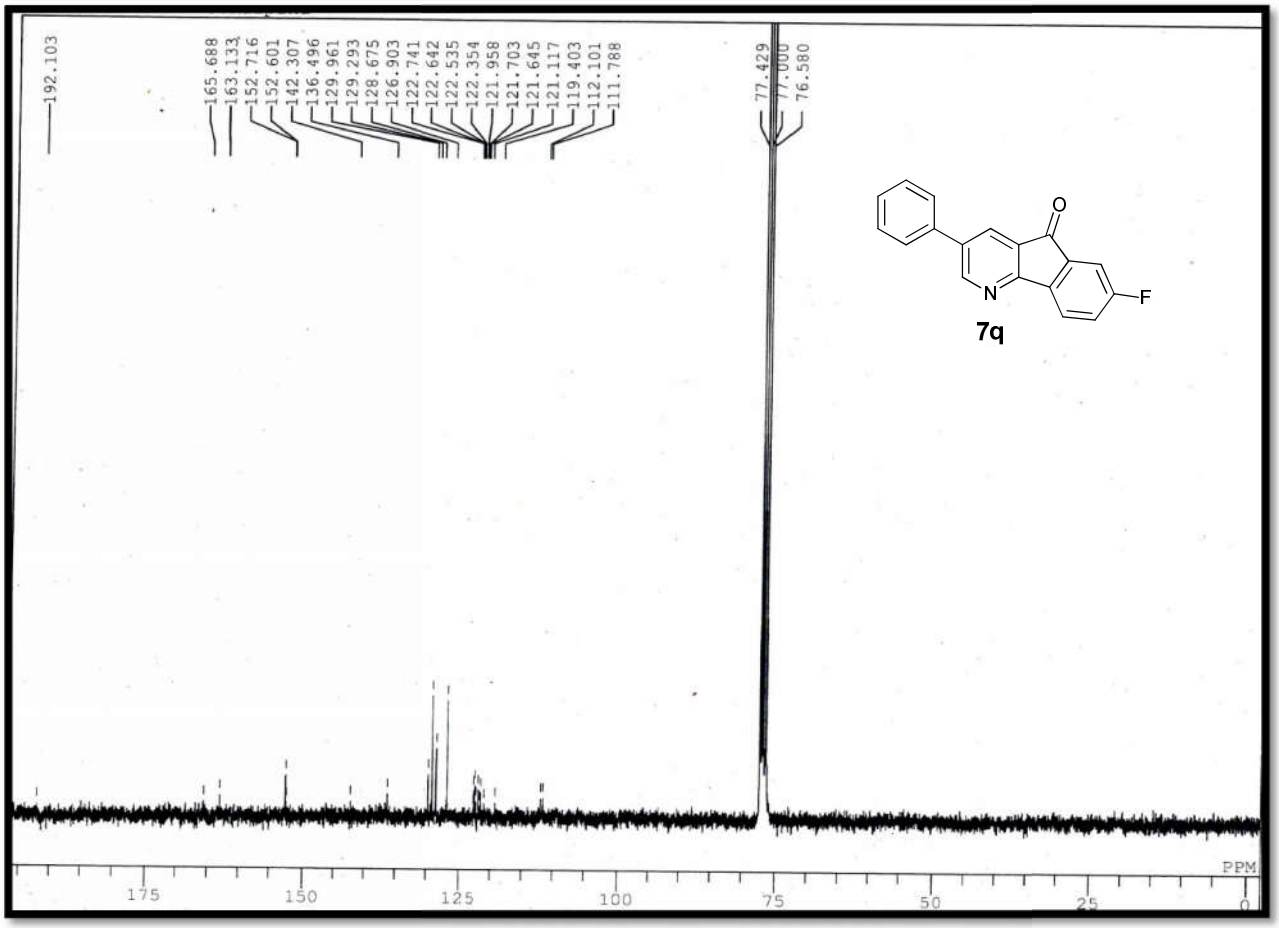

189.737
159.589
151.521
148.966
144.112
142.570
139.084
133.299
133.274
131.403
128.560
127.496
127.464
127.373
126.507
123.153
116.313
77.420
77.000
76.580
24.600
15.196
O
N
OCF3
H3C
7o
PPM
200
175
150
125
100
75
50
25
0

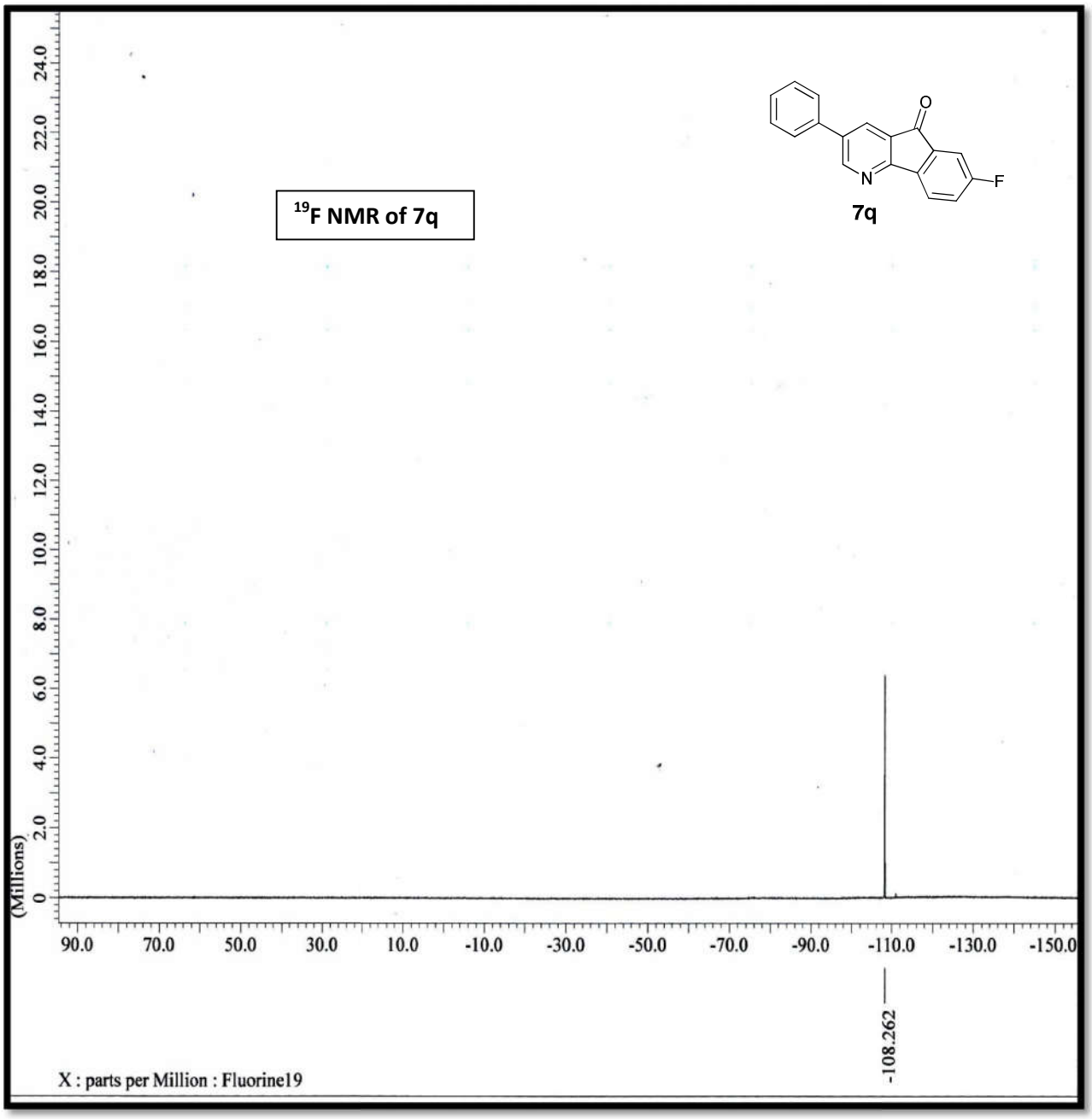

19F NMR of 7o
O
N
OCF3
H3C
7o
300.0
200.0
100.0
0
(Millions)
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-57.695
X : parts per Million : Fluorine19

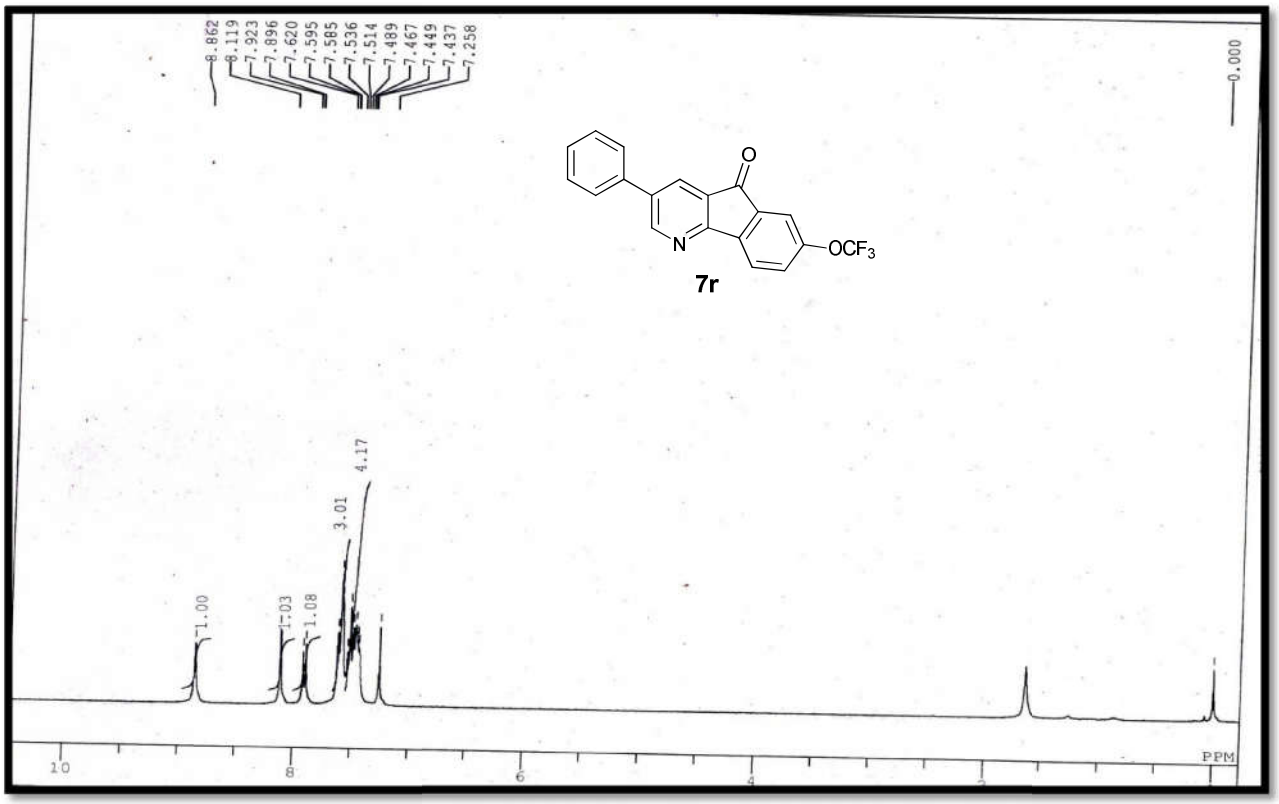

8.879
8.159
8.138
8.121
7.922
7.772
7.638
7.618
7.531
7.507
7.486
7.464
7.261
0.000
O
N
7p
3.01
3.28
2.03
0.95
1.00
0.71
PPM
8
6
4
2
0

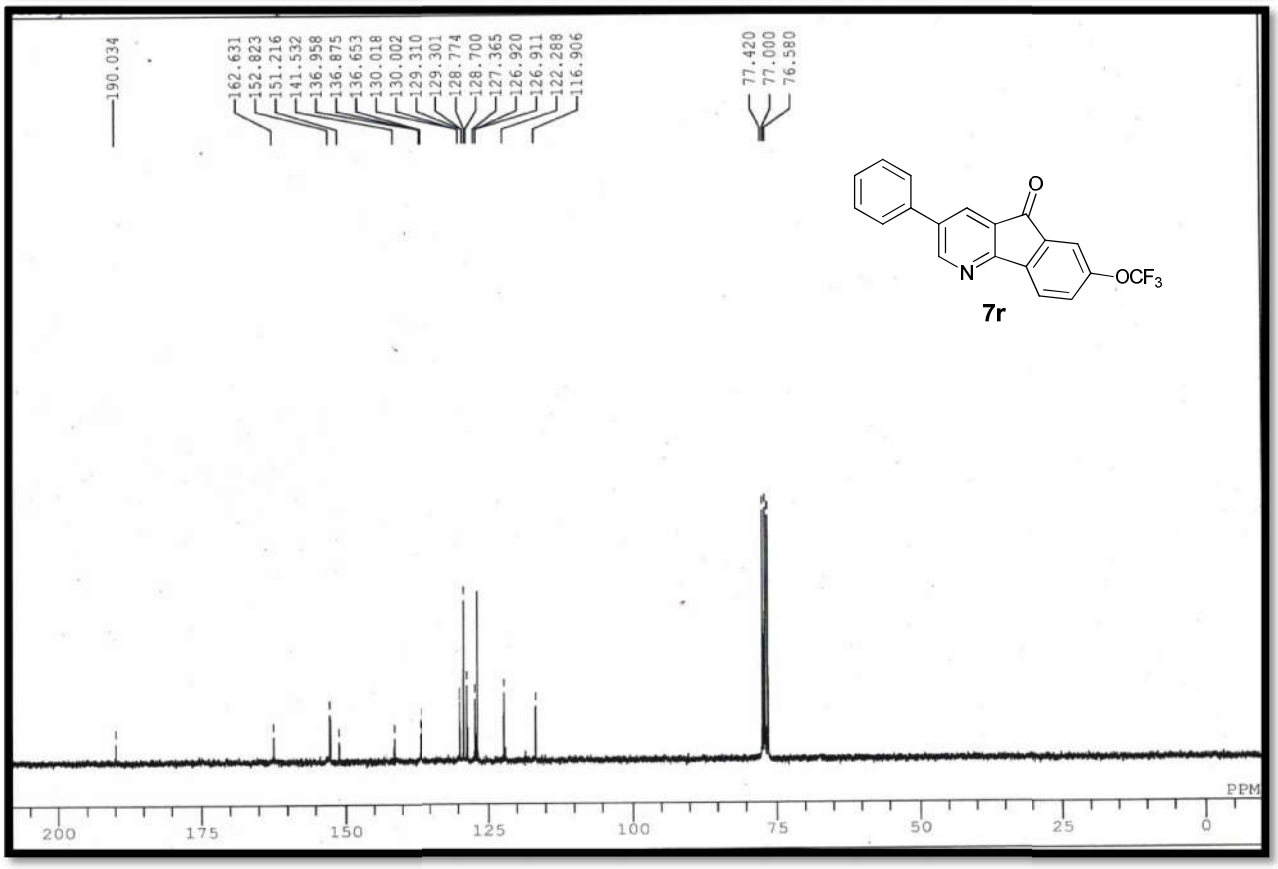

191.616
171.507
163.512
152.188
143.180
136.917
135.540
135.145
133.669
130.999
130.175
129.969
129.260
128.659
128.461
126.920
124.307
121.150
77.420
77.000
76.580
O
N
7p
PPM
200
175
150
125
100
75
50
25
0

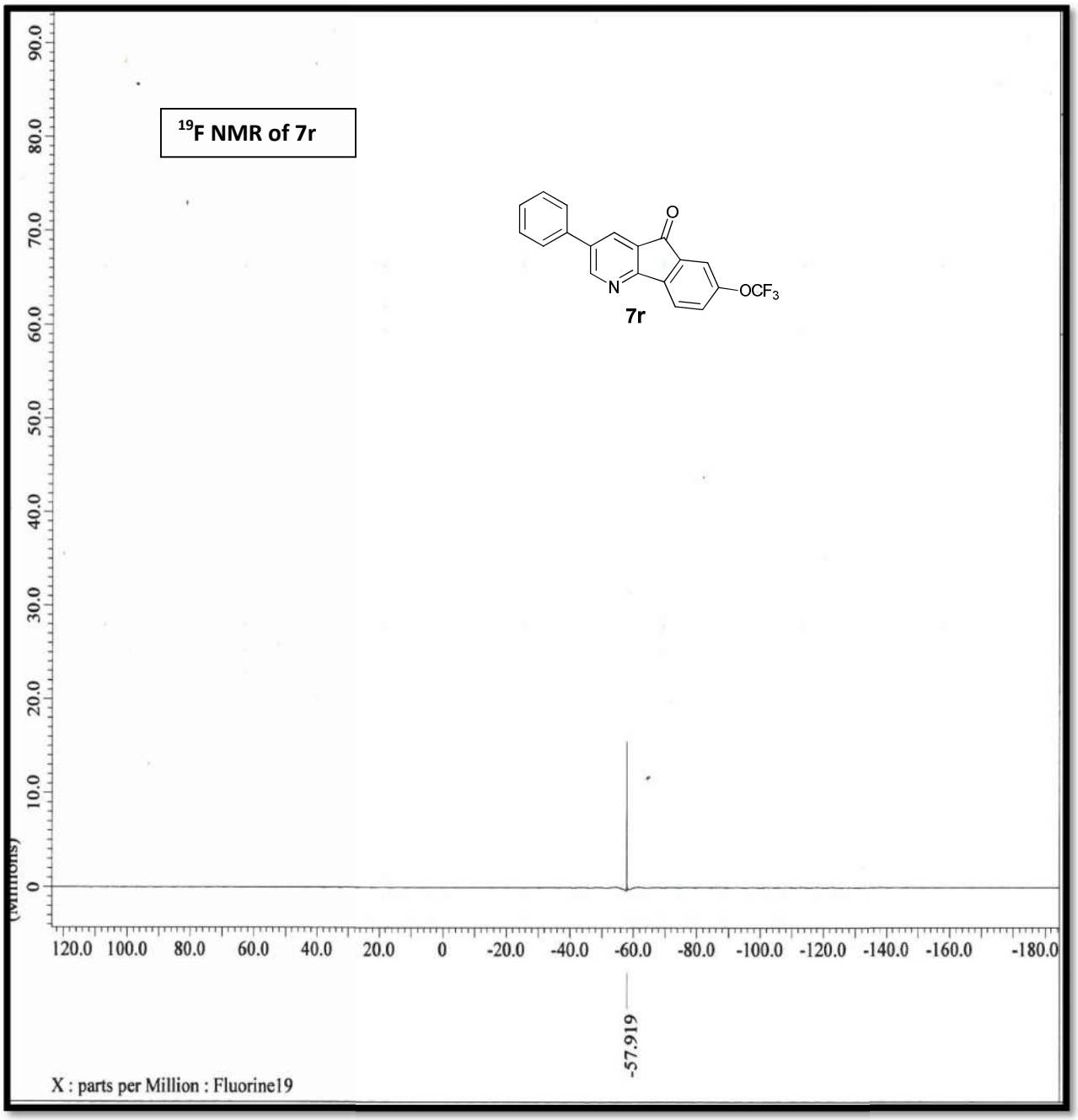

8.830
8.099
7.880
7.864
7.853
7.837
7.620
7.597
7.537
7.514
7.489
7.470
7.446
7.435
7.420
7.411
7.334
7.325
7.314
7.305
7.297
7.261
0.000
O
N
F
7q
1.00
1.03
1.13
2.20
4.14
1.34
PPM
10
8
6
4
2
0

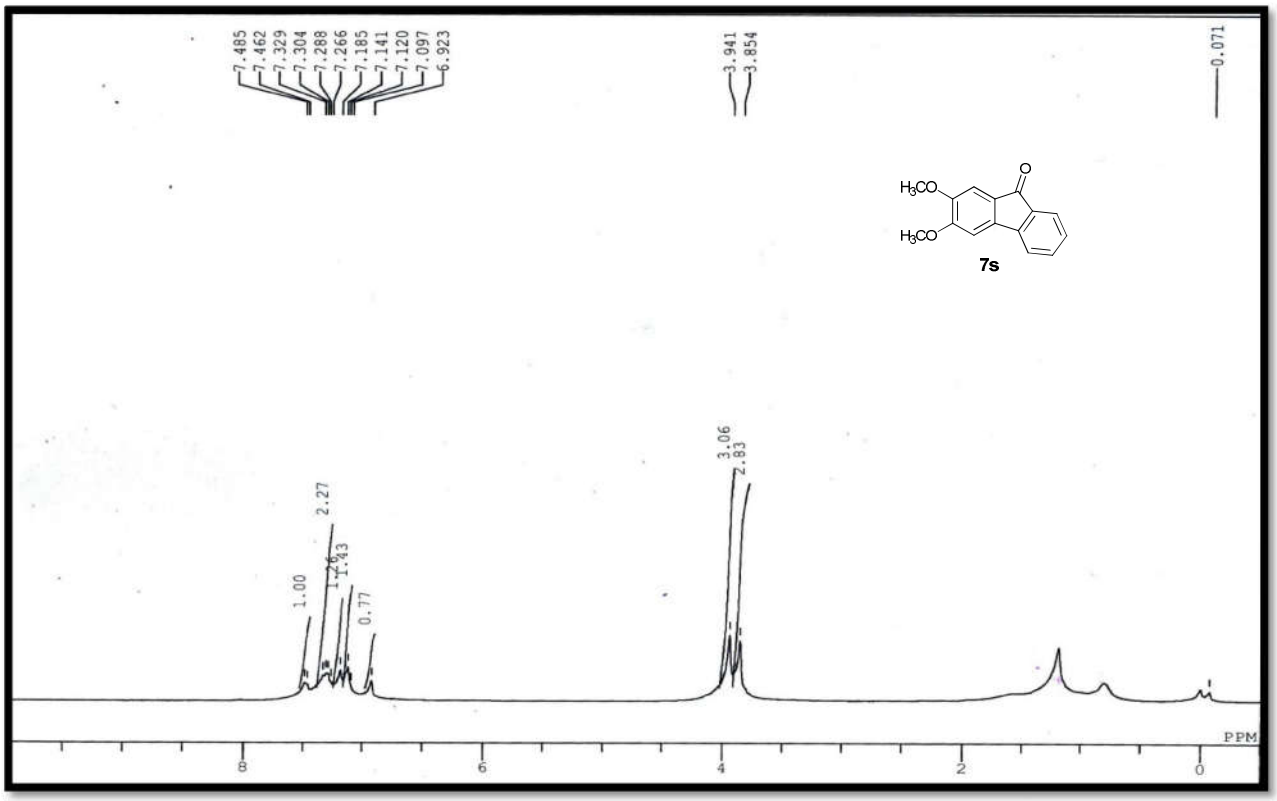

192.103
165.688
163.133
152.716
152.601
142.307
136.496
129.961
129.293
128.675
126.903
122.741
122.642
122.535
122.354
121.958
121.703
121.645
121.117
119.403
112.101
111.788
77.429
77.000
76.580
O
N
F
7q
PPM
175
150
125
100
75
50
25
0

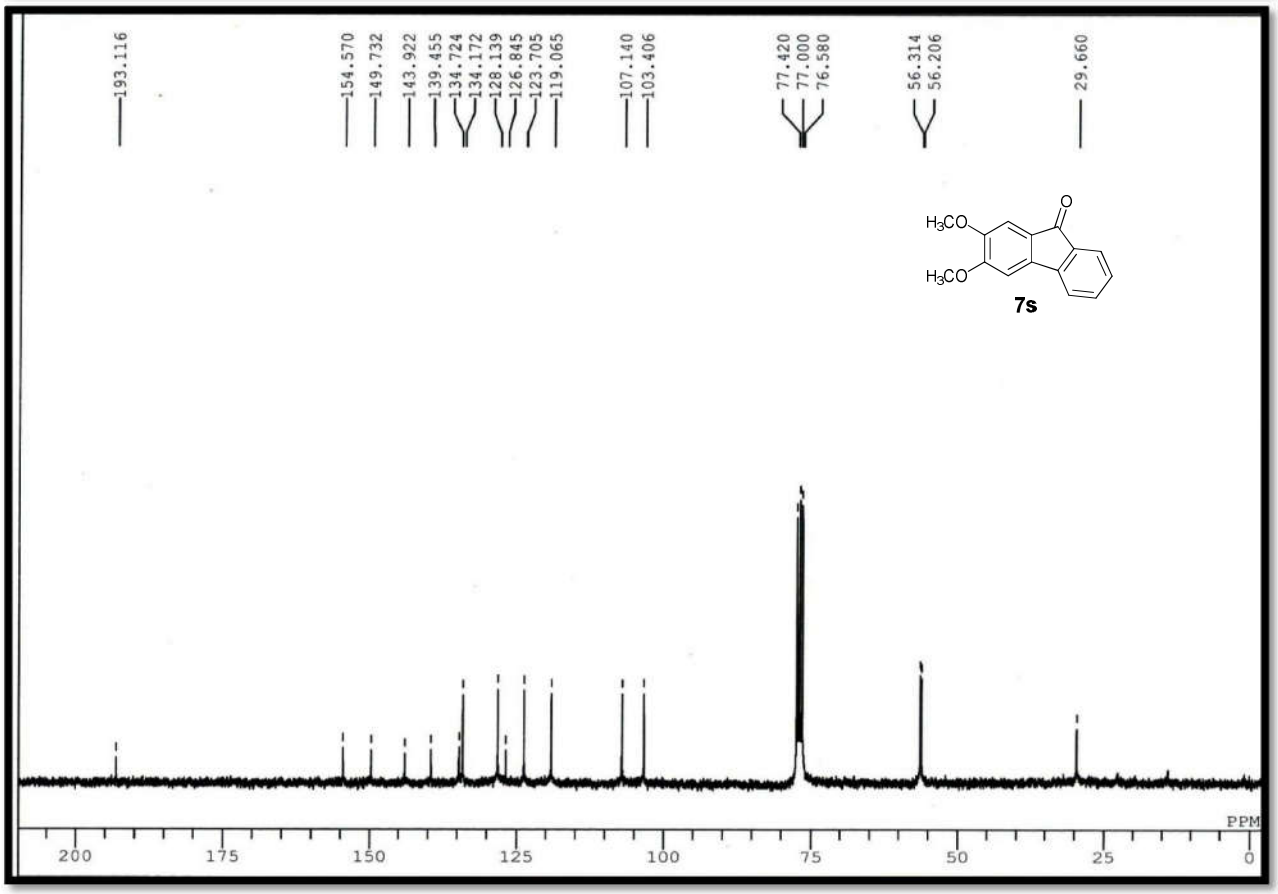

^{19}F NMR of 7q
7q
O
N
F
(Millions)
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
0
90.0
70.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-108.262
X : parts per Million : Fluorine19

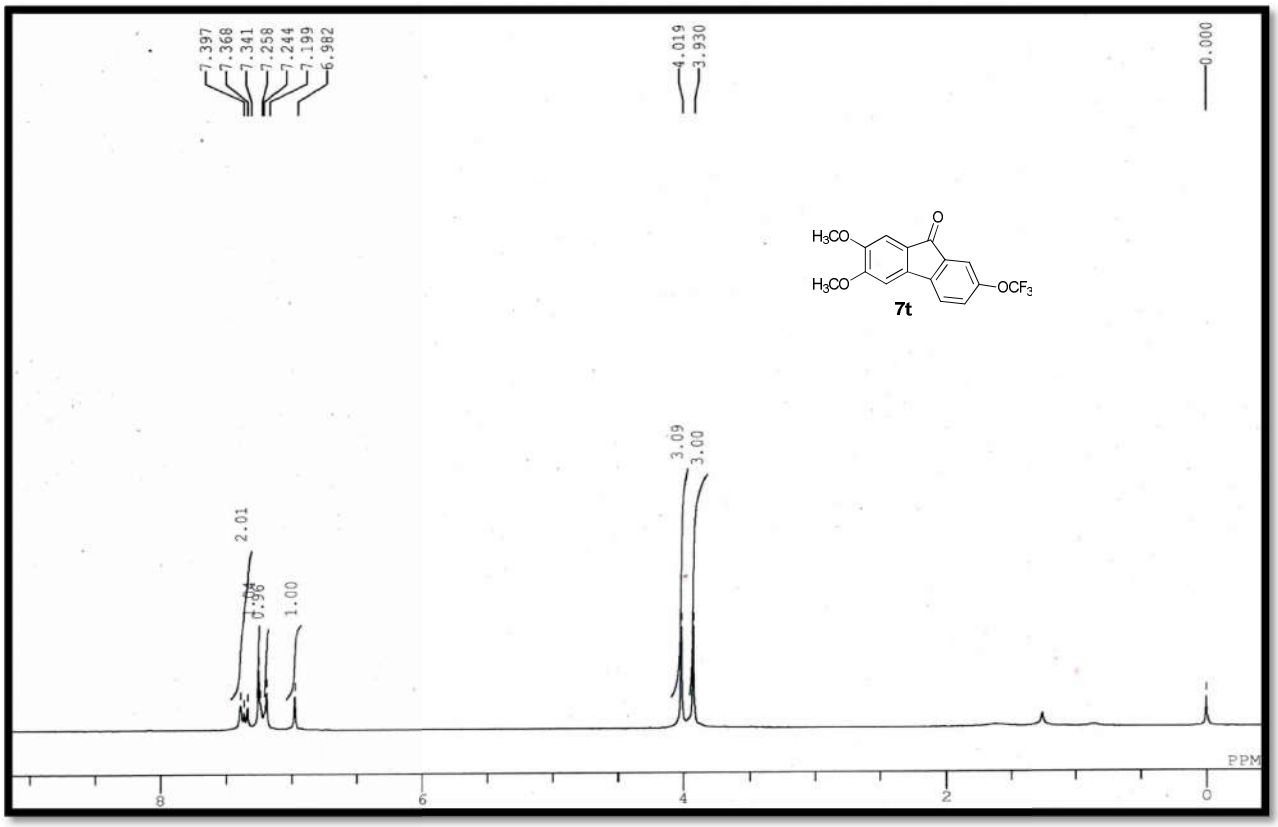

8.862
8.119
7.923
7.896
7.620
7.595
7.585
7.536
7.514
7.489
7.467
7.449
7.437
7.258
0.000
O
N
OCF3
7r
4.17
3.01
1.00
1.03
1.08
10
8
6
PPM

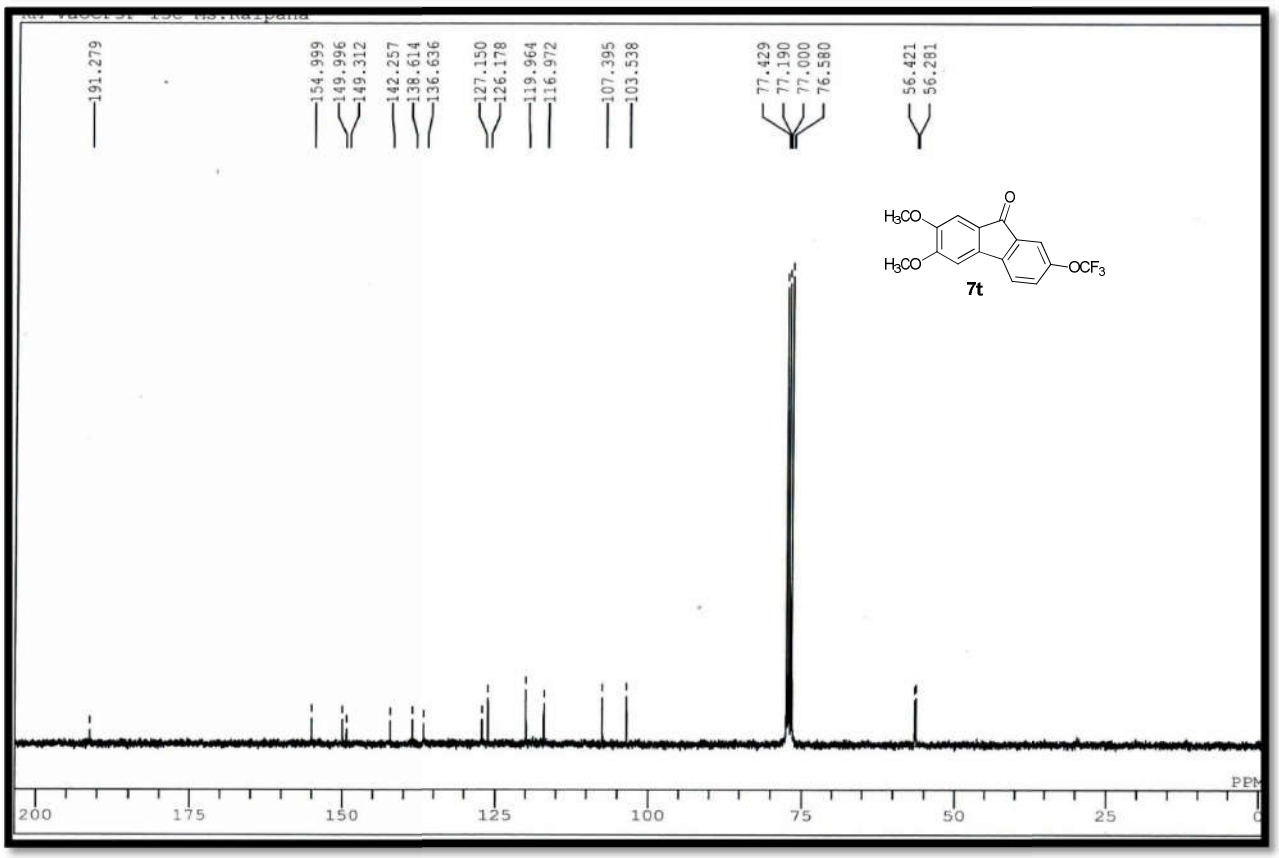

190.034
162.631
152.823
151.216
141.532
136.958
136.875
136.653
130.018
130.002
129.310
129.301
128.774
128.700
127.365
126.920
126.911
122.288
116.906
77.420
77.000
76.580
O
N
OCF3
7r
200
175
150
125
100
75
50
25
0
PPM

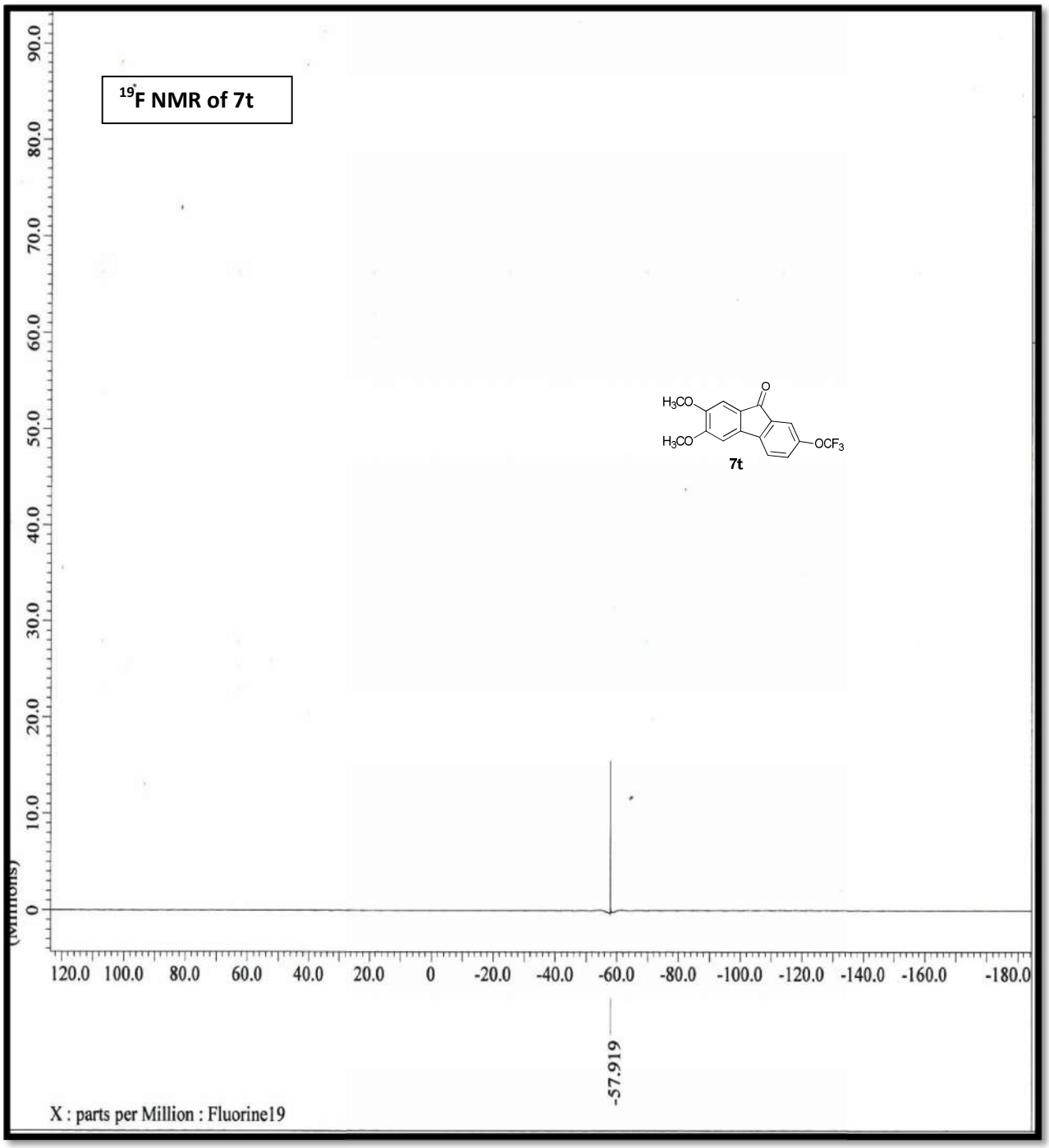

19F NMR of 7r
O
N
OCF3
7r
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
(Millions)
120.0 100.0 80.0 60.0 40.0 20.0 0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0
-57.919
X : parts per Million : Fluorine19

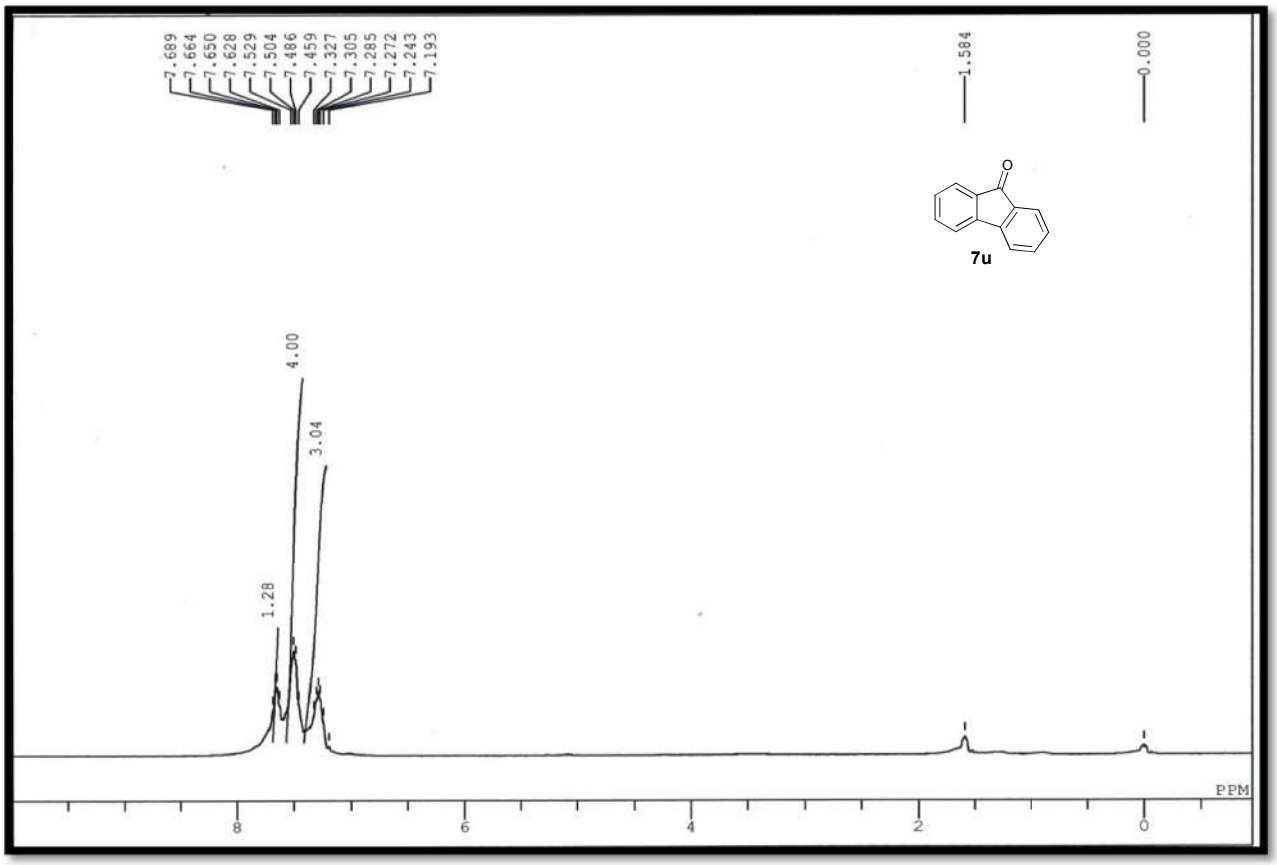

7.485
7.462
7.329
7.304
7.288
7.266
7.185
7.141
7.120
7.097
6.923
3.941
3.854
0.071
H3CO
H3CO
O
7s
3.06
2.83
2.27
1.43
1.00
0.77
PPM
8
6
4
2
0

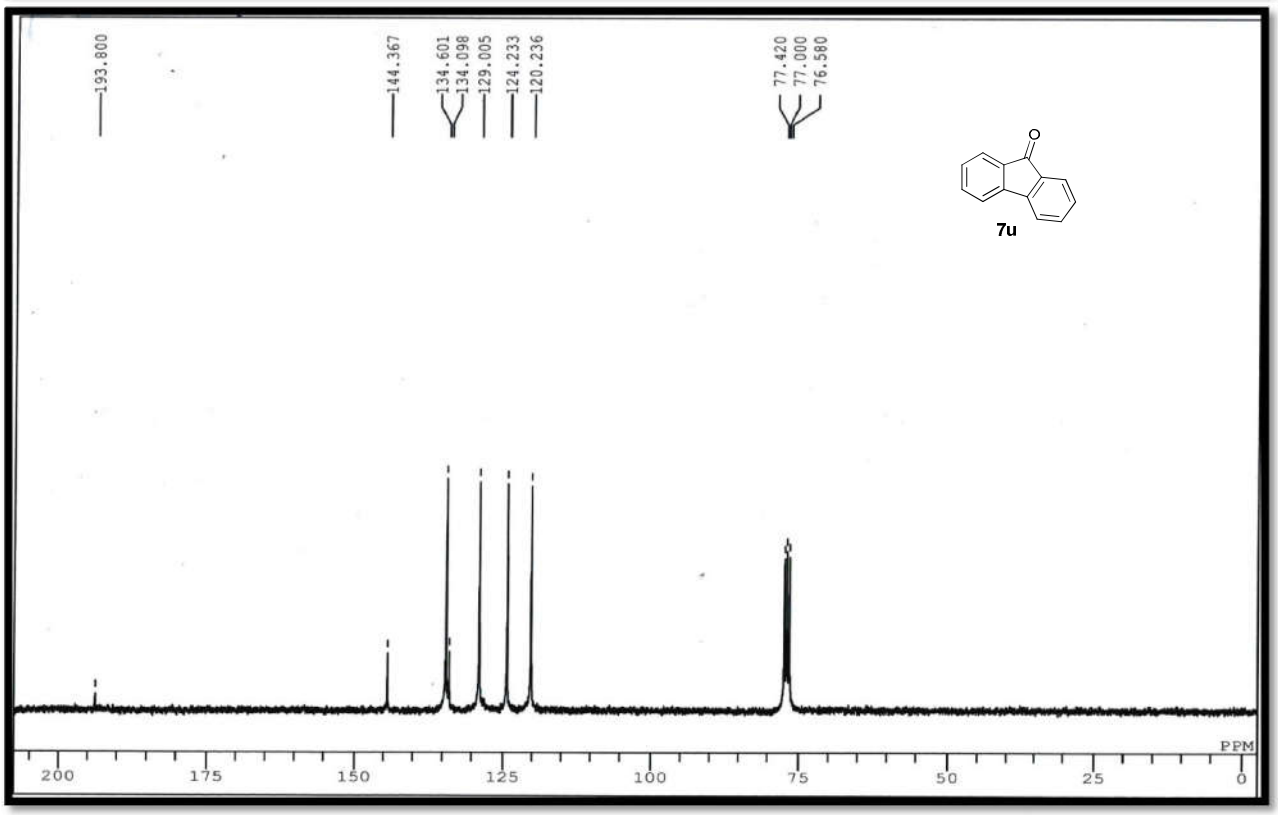

193.116
154.570
149.732
143.922
139.455
134.724
134.172
128.139
126.845
123.705
119.065
107.140
103.406
77.420
77.000
76.580
56.314
56.206
29.660
H3CO
H3CO
O
7s
PPM
200
175
150
125
100
75
50
25
0


7.397
7.368
7.341
7.258
7.244
7.199
6.982
4.019
3.930
0.000
3.09
3.00
2.01
0.98
1.00
PPM
8
6
4
2
0
7t


191.279
154.999
149.996
149.312
142.257
138.614
136.636
127.150
126.178
119.964
116.972
107.395
103.538
77.429
77.190
77.000
76.580
56.421
56.281
PPM
200
175
150
125
100
75
50
25
7t


19F NMR of 7t
H3CO
H3CO
O
OCF3
7t
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
(Millions)
120.0 100.0 80.0 60.0 40.0 20.0 0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0
-57.919
X : parts per Million : Fluorine19


7.689
7.664
7.650
7.628
7.529
7.504
7.486
7.459
7.327
7.305
7.285
7.272
7.243
7.193
1.584
0.000
O
7u
4.00
3.04
1.28
PPM
8
6
4
2
0


193.800
144.367
134.601
134.098
129.005
124.233
120.236
77.420
77.000
76.580
O
7u
PPM
200
175
150
125
100
75
50
25
0