Supporting Information

Blue LED-driven C-N Bond formation for Synthesis of Imidazopyridines

Amardeep Ramprasad Jadhao,[a] Shankesh Chandrakant Zyate,[b] Sanjay Subhash Gaikwad[c]*

[a] Department of Chemistry, Late Pushpadevi Patil Arts and Science College, Risod, Dist Washim, Maharashtra, India-444506.

[b] Department of Chemistry, Shri R. L. T. College, Akola, Maharashtra, India-444001.

[c] Department of Chemistry, MES, Abasaheb Garware College, Pune, Maharashtra, India-411004

Corresponding author: E-mail: sanjchem99@gmail.com

Tel: +919765939988

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1. General information:

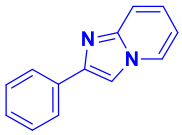
All reagents and solvents used were obtained commercially from sigma Aldrich, Alfa aesar and Spectrochem. Reactions were magnetically stirred, sunlight exposer 1h, microwave at 300 W and monitored by analytical thin-layer chromatography (TLC). Merck 0.25 mm silica gel 60 F254. TLC plates were pictured by exposing to ultraviolet light (UV, 254 nm) and/or exposure to an aqueous solution of potassium permanganate ($KMnO_4$) followed by heating with a heat gun. Isolation of compounds was performed using silica gel (100-200 mesh) column chromatography with solvents distilled prior to use. ^1H NMR spectra were recorded on a 400 MHz spectrometer and ^{13}C NMR spectra were obtained at a 101 MHz spectrometer using $CDCl_3$ as a solvent. TMS (0.00 ppm) and $CDCl_3$ (77.0 ppm) served as internal standards in ^1H NMR and ^{13}C NMR respectively. Chemical shifts were recorded in δ ppm, and coupling constants (*J*) in Hz. s: singlet, d: doublet, t: triplet, m: multiplet, bs: broad singlet dd: doublet of doublet for proton spectra are the abbreviations used to denote multiplicities in NMR spectra.

General procedure for preparation of 2-substituted imidazo [1,2-a]pyridine (2):

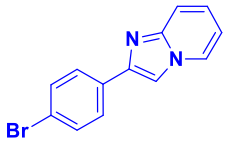
N-Bromosuccinimide (2.0 mmole) was added to the flask containing styrene (1.0 mmol) and H_2O at room temperature under an N_2 atmosphere. The Reaction flask was immersed in Blue LED for 10 min. then 2 aminopyridines (1.0 mmol) were added to the reaction flask in the same reaction condition for 40 min. The reaction mixture was then cooled to room temperature. After completion of the reaction, as indicated by TLC, the crude product was extracted with ethyl acetate (3 x 30 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated in vaccuo. The crude product was purified by silica gel column chromatography with hexane: ethyl acetate to give 2-substituted imidazo [1,2-a]pyridine derivative (2a- 2h & 2a'- 2i') with good yield.

The spectroscopic data of all the products are presented below. All the known compounds gave satisfactory spectroscopic values and are analogue to spectroscopic data reported in the literature.

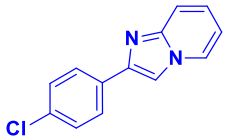
Spectral data:



2-phenylimidazo[1,2-a]pyridine (2a): Isolated yield: 88%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96-7.92 (m, 3H), 7.73 (s, 1H), 7.58 (d, *J* = 9.0 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 2H), 7.31 (d, *J* = 7Hz, 1H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.65 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ146.0, 145.8, 134.0, 128.9, 128.2, 126.2, 125.8, 124.8, 117.7, 112.6, 108.4

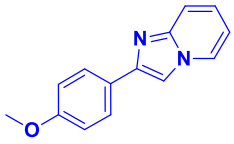


2-(4-bromophenyl)imidaz[1,2-a]pyridine (2b): Isolated yield: 39%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.08 (d, *J* = 6.6 Hz, 1H),7.82-7.80 (m, 3H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.19 (t, *J* = 7.8 Hz, 1H), 6.79 (t, *J* = 6.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.0, 144.9, 133.0, 132.0, 127.8, 125.8, 125.2, 122.1, 117.8, 112.8, 108.4.

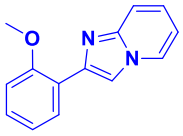


2-(4-chlorophenyl)imidazo[1,2-a]pyridine (2c): Isolated yield: 53%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.09 (d, *J* = 6.5 Hz, 1H), 7.88 (d, *J* = 8.5 Hz, 2H), 7.82 (s, 1H), 7.61 (d, *J* = 8.8 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 2H), 7.17 (t, *J* = 7.2 Hz, 1H), 6.77 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.0, 144., 133.9, 132.6, 129.1, 127.5, 125.8, 125.1, 117.8, 112.8, 108.4.

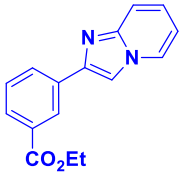
2-(p-tolyl)imidazo[1,2-a]pyridine(2d): Isolated yield: 82%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.98 (d, *J* = 6.4 Hz, 1H), 7.82 (d, *J* = 7.8 Hz, 2H), 7.73 (s, 1H), 7.58 (d, *J* = 8.8 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.5 Hz, 1H), 6.66 (t, *J* = 6.2 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 145.9, 145.6, 137.9, 131.0, 129.5, 126.0, 125.6, 124.6, 117.4, 112.4, 107.9, 21.4.



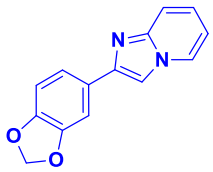
2-(4-methoxyphenyl)imidazo[1,2-a]pyridine (2e): Isolated yield: 60%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.05 (d, *J* = 6.4 Hz, 1H), 7.87 (d, *J* = 8.2 Hz, 2H), 7.74 (s, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.13 (t, *J* = 7.8 Hz, 1H), 6.96 (d, *J* = 8.2 Hz, 2H), 6.72 (t, *J* = 6.4 Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 159.7, 145.8, 127.5, 126.6, 125.6, 124.6, 117.4, 114.3, 112.5, 107.4, 55.5.



2-(2-methoxyphenyl)imidazo[1,2-a]pyridine(2f): Isolated yield: 62%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.41 (d, *J* = 7.5 Hz, 1H), 8.156 (s,1H), 8.05 (d, *J* = 6.4 Hz, 1H), 7.59 (d, *J* = 9.0 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.11 (t, *J* = 7.3 Hz, 2H), 6.96 (d, *J* = 7.9 Hz, 1H), 6.67 (t, *J* = 6.4 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 156.8, 144.5, 141.2, 128.9, 128.7, 125.7, 124.5, 122.4, 121.1, 117.3, 112.6, 112.0, 111.9, 55.5.

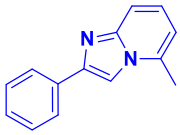


Ethyl 3-(imidazo[1,2-a]pyridin-2-yl)benzoate(2g): Isolated yield: 76%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.55 (s, 1H), 8.16 (d, *J* = 7.8 Hz,1H), 8.06 (d, *J* = 6.7 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.88 (s, 1H), 7.61 (d, *J* = 9.0 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.73 (t, *J* = 6.4 Hz, 1H), 4.40 (q, *J* = 7.0 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.7, 145.8, 144.8, 134.2, 131.0, 130.4, 129.1, 129.0, 127.1, 125.0, 125.0, 117.5, 112.7, 108.7, 61.2, 14.5.



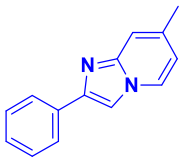
2-(benzo[1,3]dioxol-5-yl)imidazo[1,2-a]pyridine(2h): Isolated yield: 38%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 6.3 Hz, 1H), 7.73 (s,1H), 7.59 (d, *J* = 8.9 Hz, 1H), 7.45 (d, *J* = 7.8 Hz,

1H), 7.43 (s, 1H), 7.14 (t, *J* = 7.8 Hz, 1H), 6.87 (d, *J* = 7.8 Hz, 1H), 6.75 (t, *J* = 6.6 Hz, 1H), 5.99 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 148.3, 147.7, 145.9, 145.7, 128.3, 125.7, 124.8, 120.0, 117.5, 112.5, 108.8, 107.6, 106.8, 101.3.

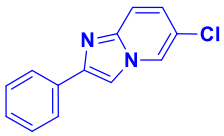


5-methyl-2-phenylimidazo[1,2-a]pyridine (2a'): Isolated yield: 73%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.96 (d, *J* = 7.0 Hz, 2H), 7.64 (s, 1H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.28 (t, *J* = 7.3 Hz, 1H), 7.06 (t, *J* = 7.8 Hz, 1H), 6.51 (d, *J* = 6.7 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.2, 145.7, 134.4, 134.1, 128.7, 128.0, 126.1, 124.9, 114.8, 111.6, 105.4, 18.8.

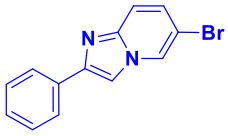
6-methyl-2-phenylimidazo[1,2-a]pyridine(2b'): Isolated yield: 78%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J* = 7.8 Hz, 2H), 7.84 (s, 1H), 7.74 (s, 1H), 7.51 (d, *J* = 9.1 Hz, 1H), 7.41 (t, *J* = 7.1 Hz, 2H), 7.30 (t, *J* = 7.2 Hz,1H), 6.99 (d, *J* = 9.1 Hz, 1H), 2.53 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 145.7, 144.9, 134.1, 128.9, 128.1, 128.0, 126.1, 123.5, 122.2, 117.0, 108.0, 18.3.



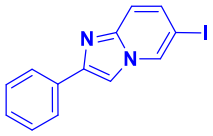
7-methyl-2-phenylimidazo[1,2-a]pyridine(2c'): Isolated yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.4 Hz, 3H), 7.73 (s, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.37 (s, 1H), 7.30 (t, *J* = 7.2 Hz, 1H), 6.55 (d, *J* = 6.2 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.3, 145.6, 135.7, 134.1, 128.8, 128.0, 126.1, 125.0, 116.0, 115.2, 107.7, 21.6.



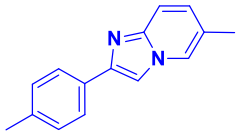
6-chloro-2-phenylimidazo[1,2-a]pyridine(2e'): Isolated yield: 72%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.13 (s, 1H), 7.92 (d, *J* = 7.3 Hz, 2H), 7.81(s, 1H), 7.56 (d, *J* = 9.4 Hz, 1H), 7.41 (t, *J* = 7.3 Hz, 2H), 7.34 (t, *J* = 7.0 Hz,1H), 7.12 (d, *J* = 9.4 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 147.1, 144.3, 133.5, 129.0, 128.5, 126.3, 123.5, 120.8, 118.1, 108.7.



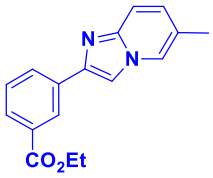
6-bromo-2-phenylimidazo[1,2-a]pyridine(2d'): Isolated yield: 73%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.21 (s, 1H), 7.91 (d, *J* = 7.6 Hz, 2H), 7.78 (s, 1H), 7.50 (d, *J* = 9.4 Hz, 1H), 7.43 (t, *J* = 7.2 Hz, 2H), 7.33 (t, *J* = 7.1 Hz, 1H), 7.20 (d, *J* = 9.3 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.9, 144.4, 133.5, 129.0, 128.5, 128.3, 126.3, 125.8, 118.3, 108.5, 107.2.



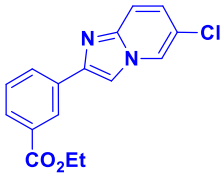
6-iodo-2-phenylimidazo[1,2-a]pyridine(2f'): Isolated yield: 75%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.36 (s, 1H), 7.93-7.91 (m, 2H),7.78 (s, 1H), 7.43-7.41 (m, 3H), 7.34-7.31 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 146.4, 144.4, 133.3, 132.8, 130.6, 129.0, 128.5, 126.3, 118.7, 108.0.



6-methyl-2-(p-tolyl)imidazo[1,2a]pyridine(2g'): Isolated yield: 55%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.82-7.78 (m, 3H), 7.64 (s, 1H),7.47 (d, *J* = 9.1 Hz, 1H), 7.21 (d, *J* = 7.6 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 1H), 2.36 (s,3H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ145.7, 144.8, 137.7, 131.3, 129.5,127.8, 126.0, 123.4, 122.0, 116.8, 107.7, 21.5, 18.2.

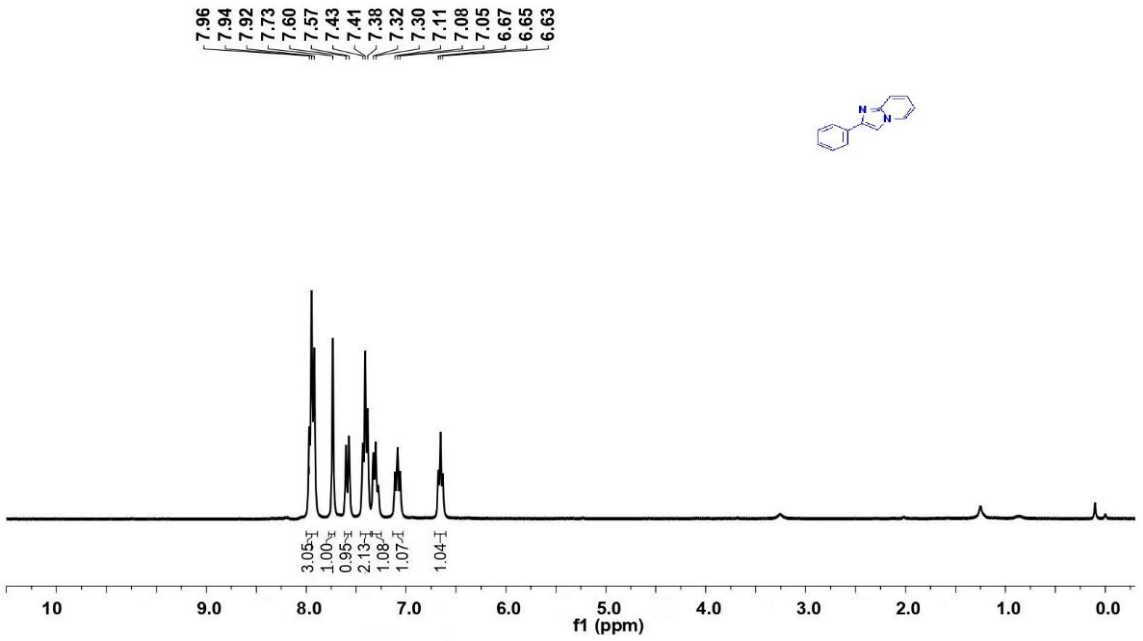


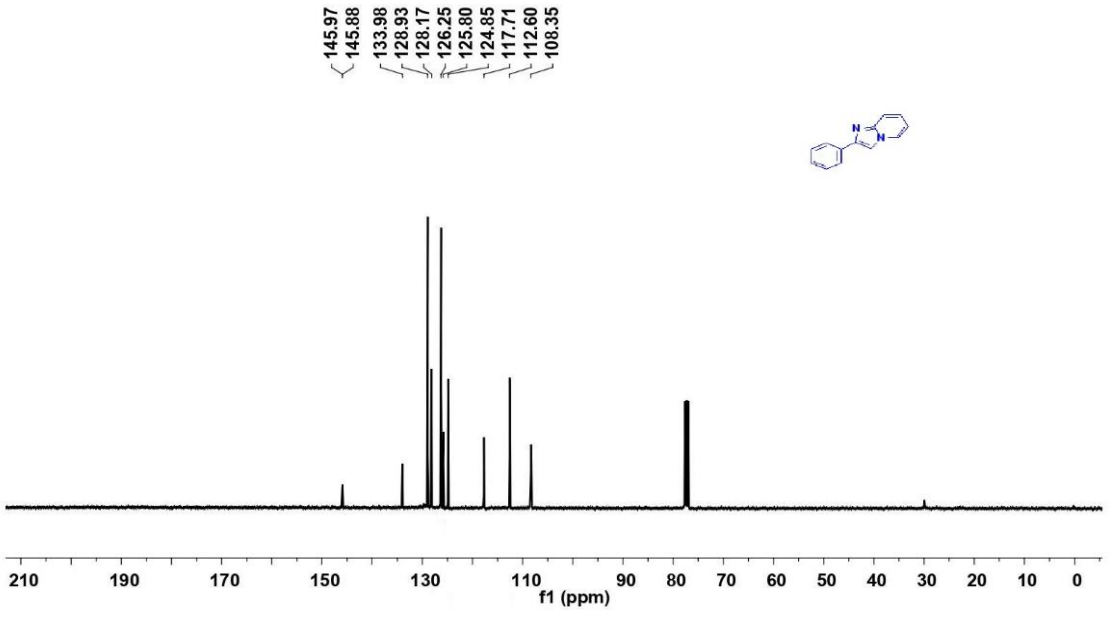
ethyl 3-(6-methylimidazo[1,2a]pyridin-2-yl)benzoate(2h'): Isolated yield: 60%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.52 (s, 1H), 8.10 (d, *J* = 7.2 Hz,1H), 7.98 (d, *J* = 7.0 Hz, 1H), 7.74-7.71 (m, 2H), 7.48-7.43 (m, 2H), 6.93 (d, *J* = 8.8 Hz, 1H), 4.9 (q, 6.5 Hz, 2H), 2.19 (s, 3H), 1.40 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.6, 144.8, 144.4, 134.4, 130.9, 130.2, 128.8, 128.1, 126.8, 123.4, 122.2, 116.7, 108.4, 61.1, 18.0, 14.4.

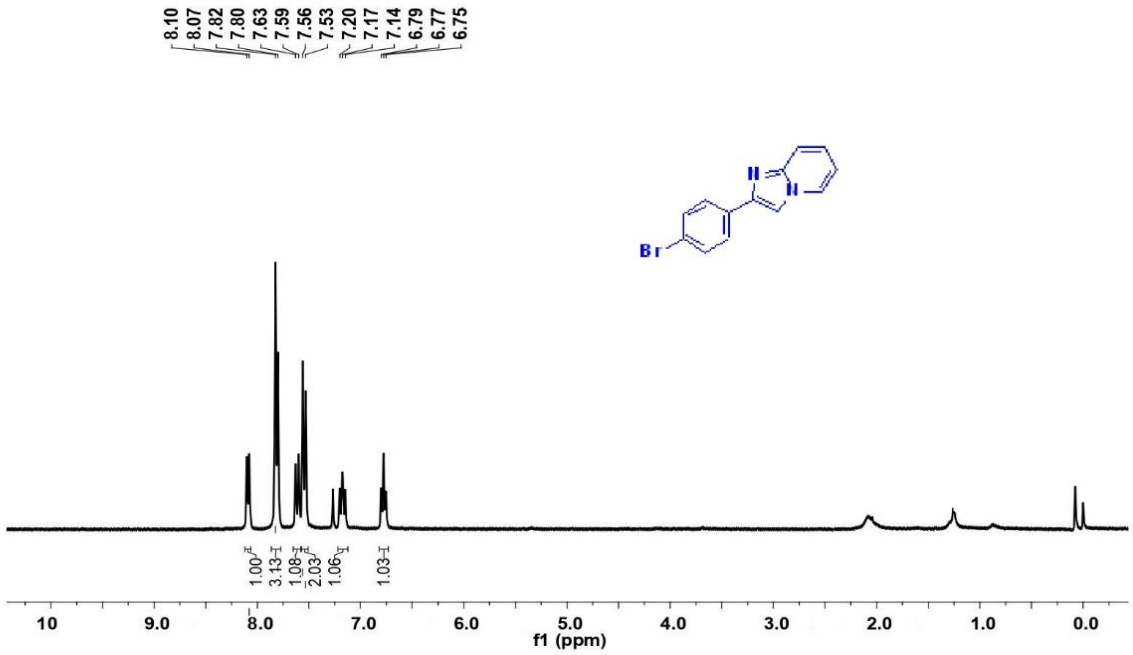


Ethyl 3-(6-chloroimidazo[1,2-a]pyridin-2-yl)benzoate(2i'): Isolated yield: 51%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.50 (s, 1H), 8.12-8.08 (m, 2H), 8.00 (d, *J* = 7.5 Hz, 1H), 7.81 (s, 1H), 7.54-7.45 (m, 2H), 7.08 (d, *J* = 9.1 Hz, 1H), 4.40 (q, *J* = 6.7 Hz, 2H), 1.41 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$): δ166.5, 145.7, 144.1, 130.3,129.3, 129.0, 127.0, 126.4, 123.6, 117.8, 109.1, 61.2, 14.5.

^{1}H & ^{13}C NMR spectra:



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7.59
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6.75
Br
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1.06
1.03
10
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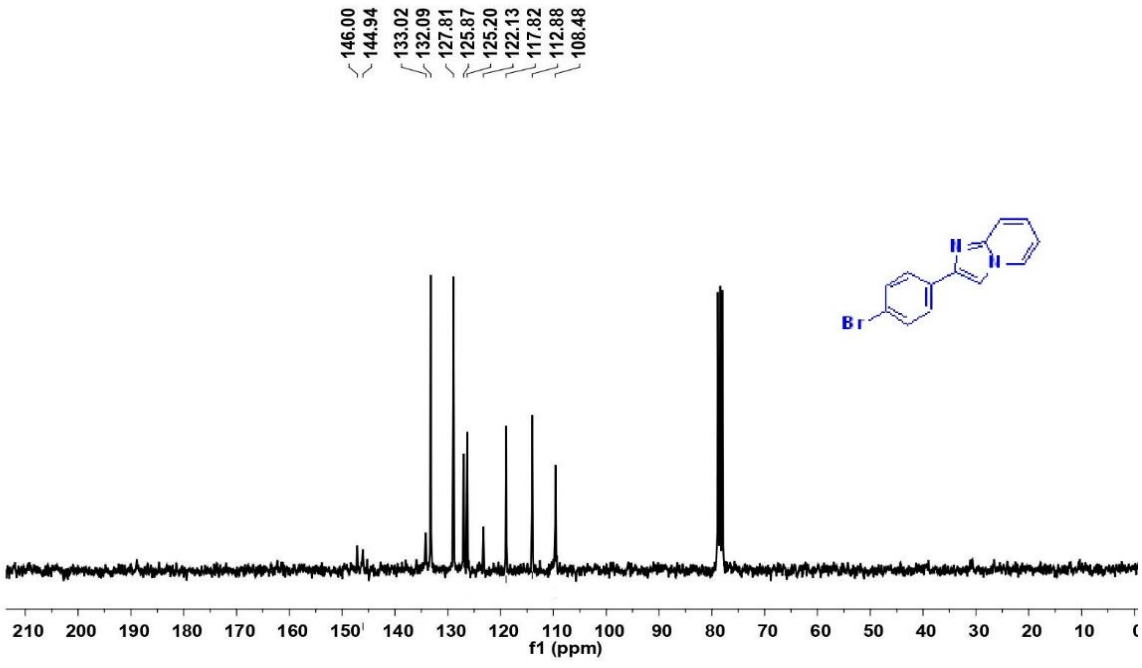
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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112.88
108.48
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60
50
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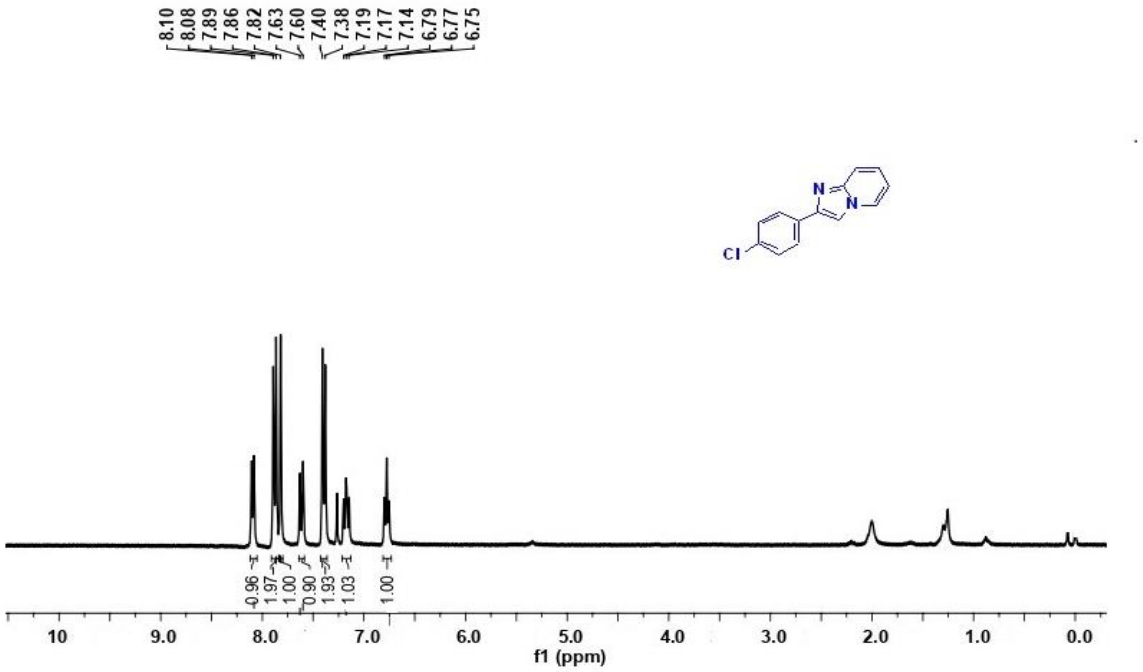
30
20
10
f1 (ppm)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6.77
6.75
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N
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1.97
1.00
0.90
1.93
1.03
1.00
10
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5.0
4.0
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2.0
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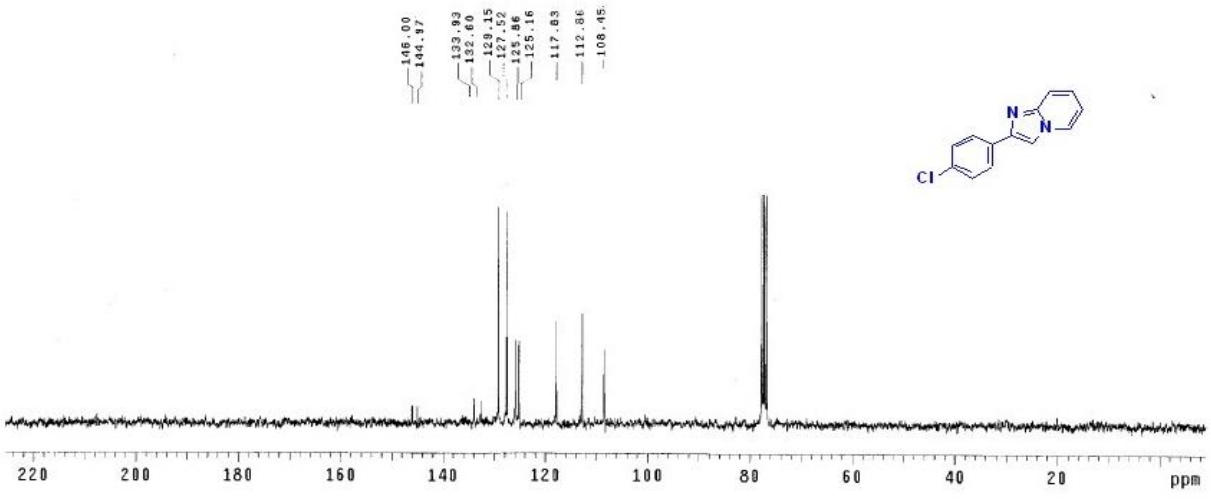
0.0
f1 (ppm)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Cl
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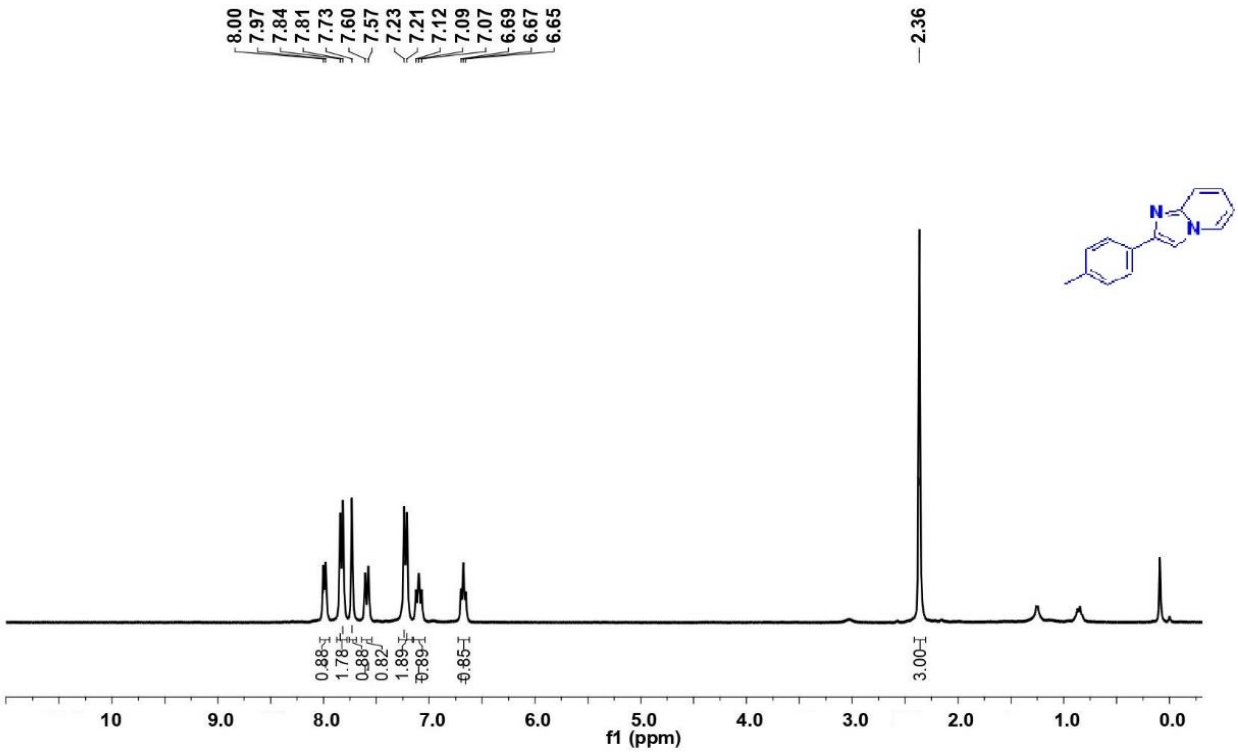
20
ppm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7.09
7.07
6.69
6.67
6.65
2.36
0.88
1.78
0.88
0.82
1.89
0.89
0.85
3.00
10
9.0
8.0
7.0
6.0
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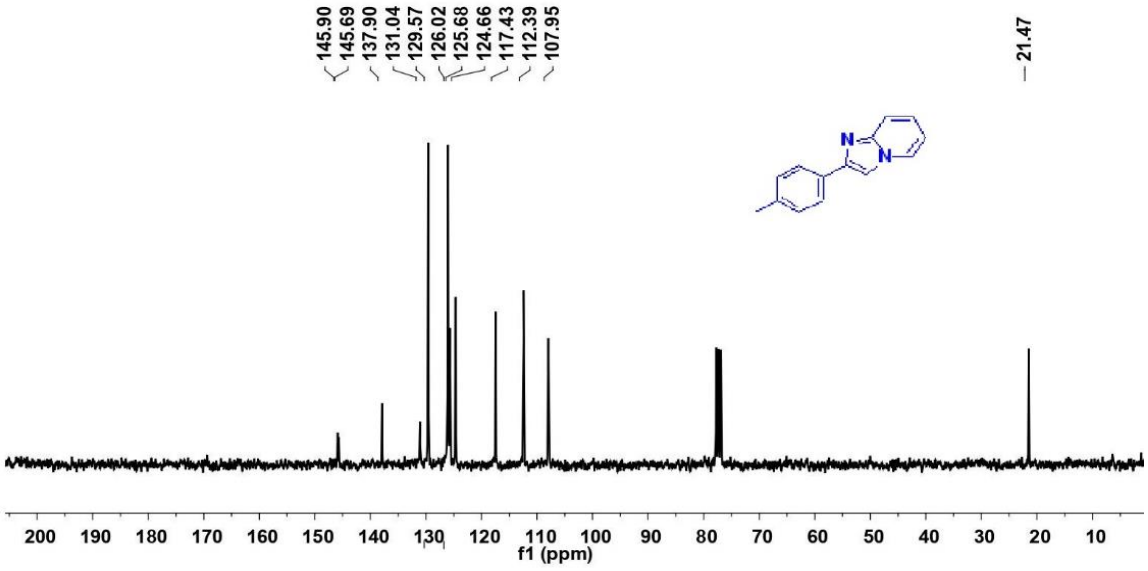
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126.02
125.68
124.66
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112.39
107.95
21.47
200
190
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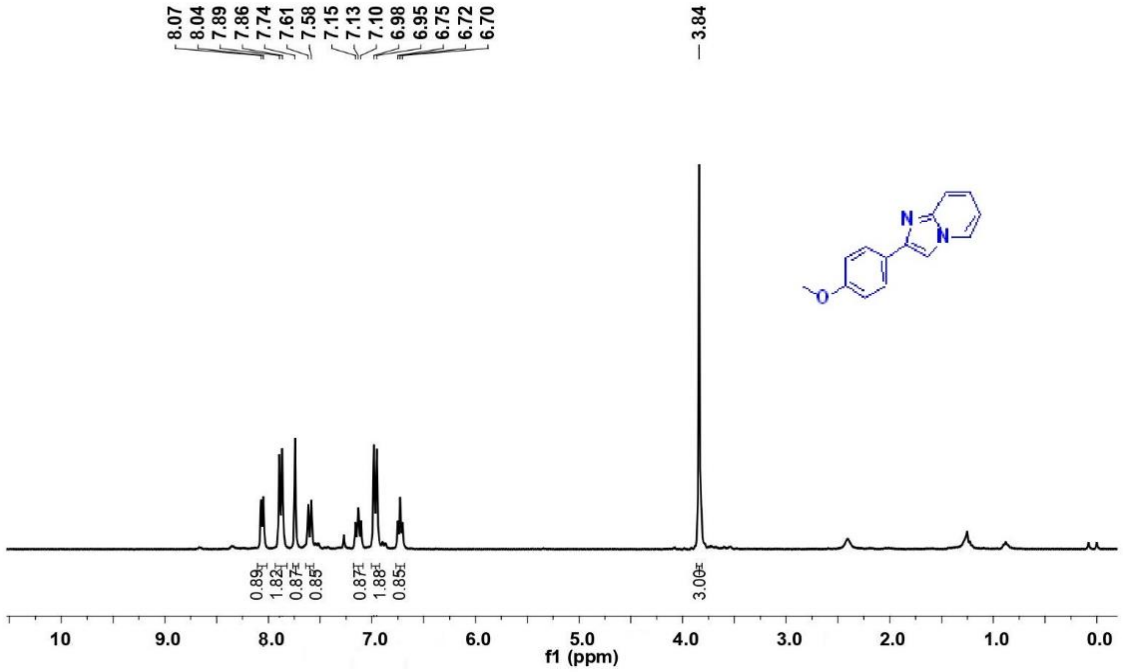
f1 (ppm)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7.15
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7.10
6.98
6.95
6.75
6.72
6.70
3.84
0.89
1.82
0.87
0.85
0.87
1.88
0.85
3.00
10
9.0
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3.0
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1.0
0.0
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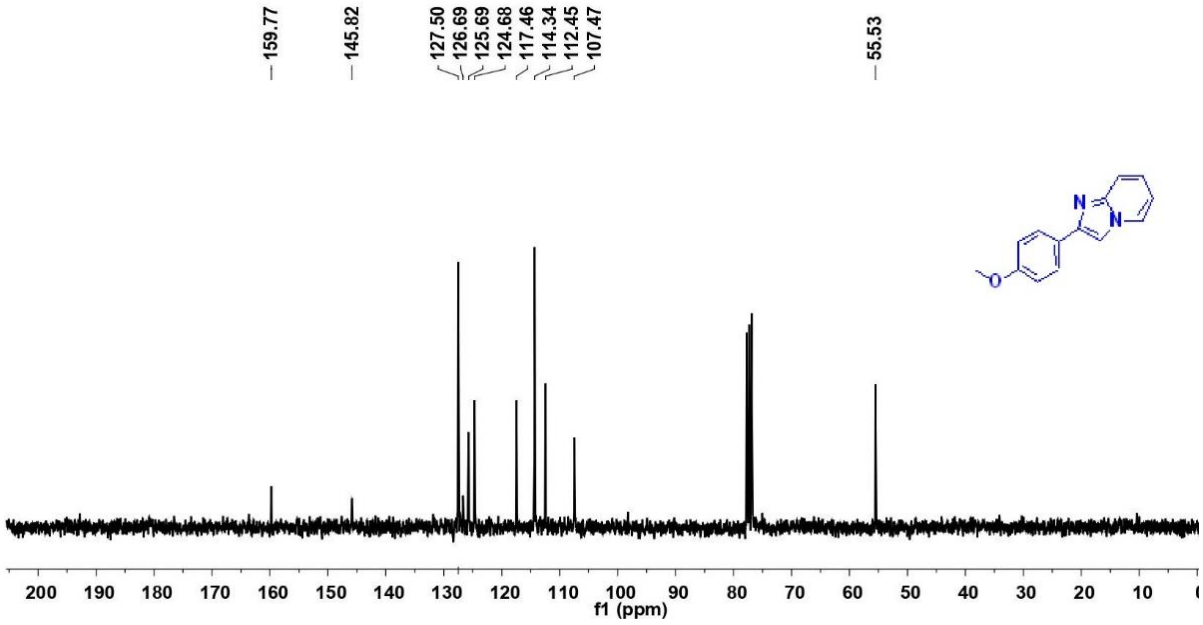
N
O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170
160
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20
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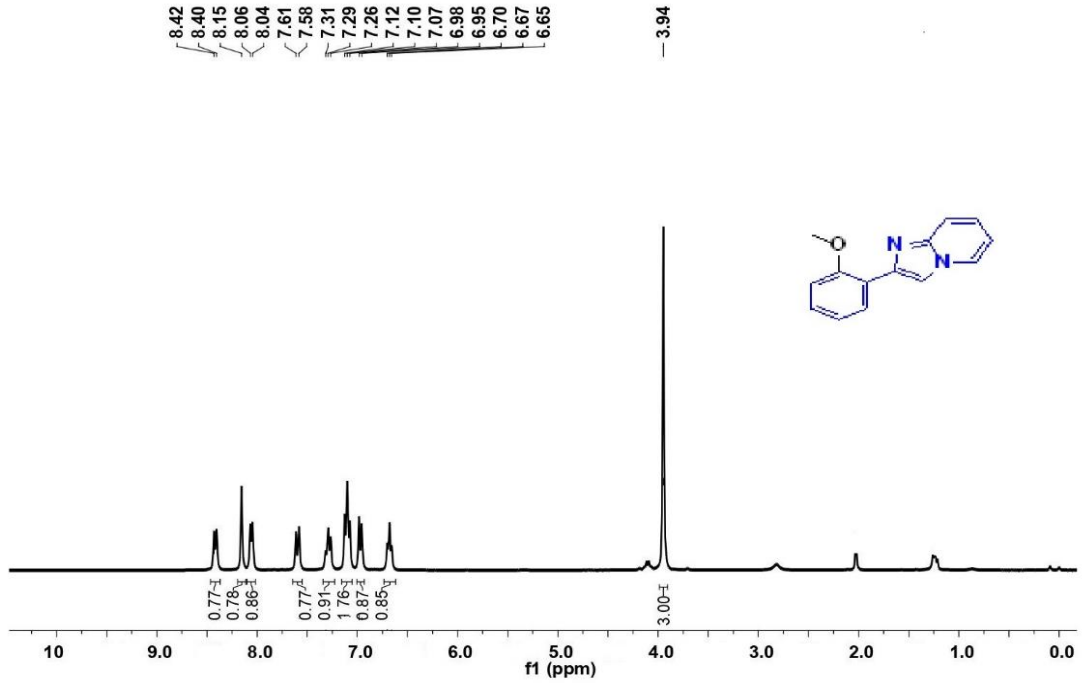
f1 (ppm)
N
N
O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7.07
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6.95
6.70
6.67
6.65
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0.77
0.91
1.76
0.87
0.85
3.00
10
9.0
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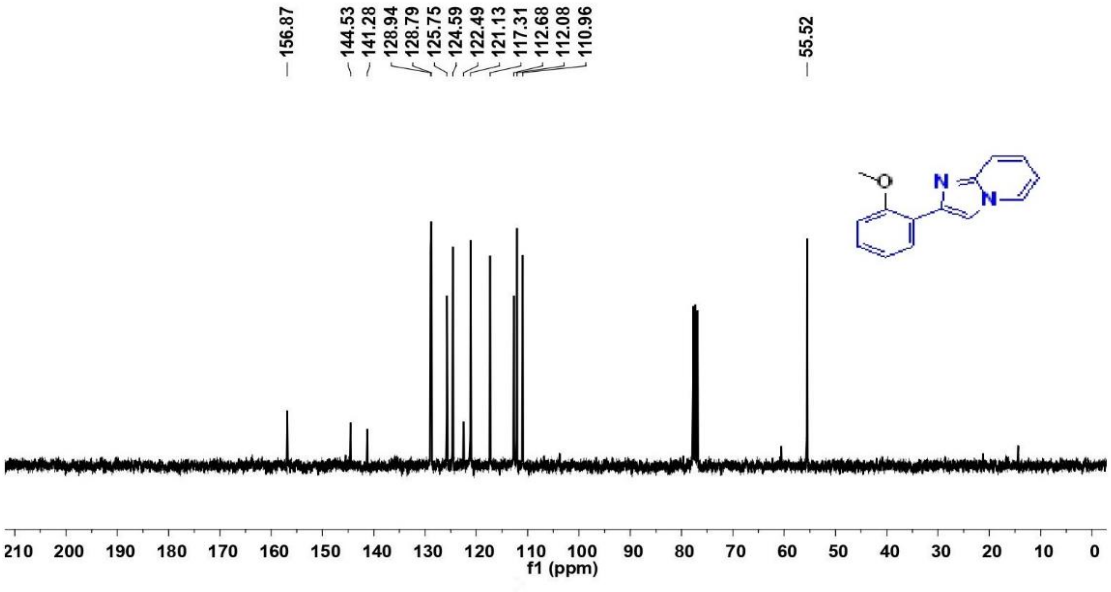
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180
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160
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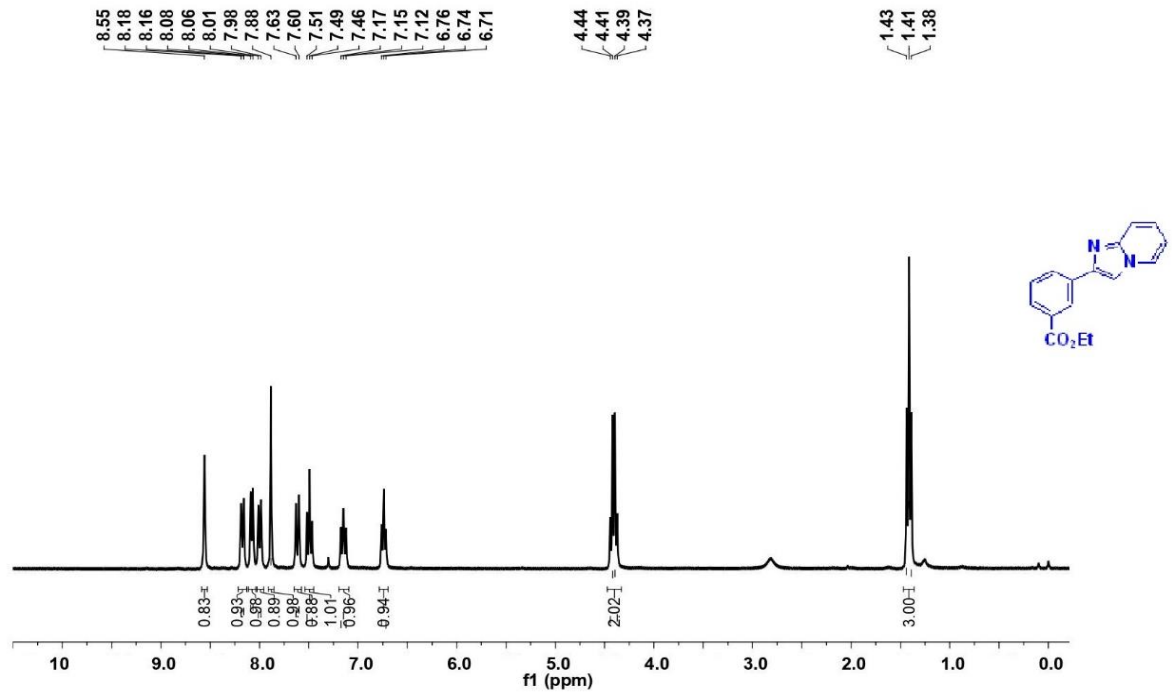
O
N
N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7.51
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7.17
7.15
7.12
6.76
6.74
6.71
4.44
4.41
4.39
4.37
1.43
1.41
1.38
0.83
0.93
0.98
0.89
0.98
0.88
1.01
0.96
0.94
2.02
3.00
N
N
CO2Et
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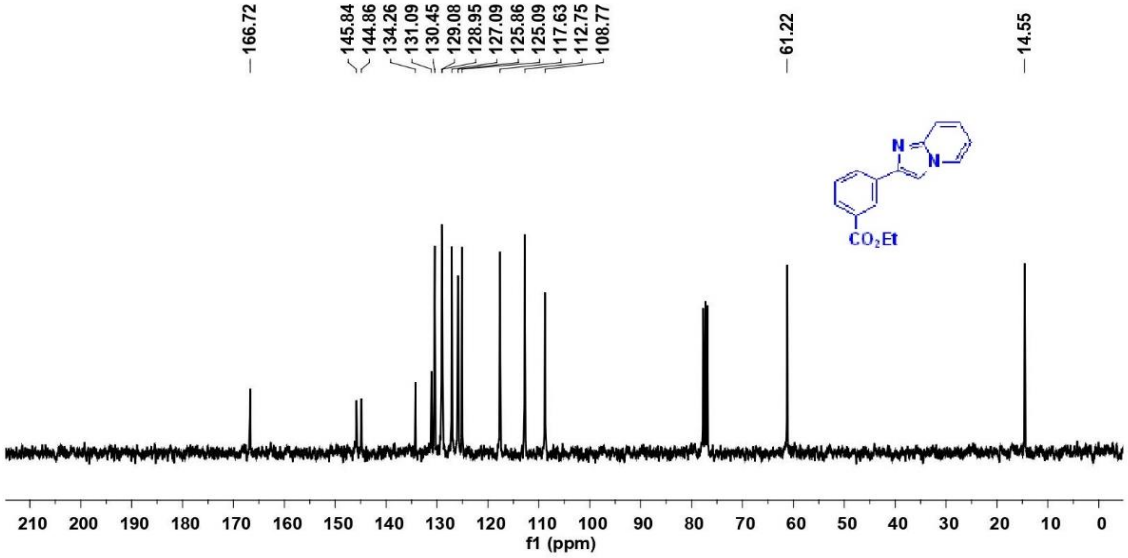
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117.63
112.75
108.77
61.22
14.55
N
N
CO2Et
210
200
190
180
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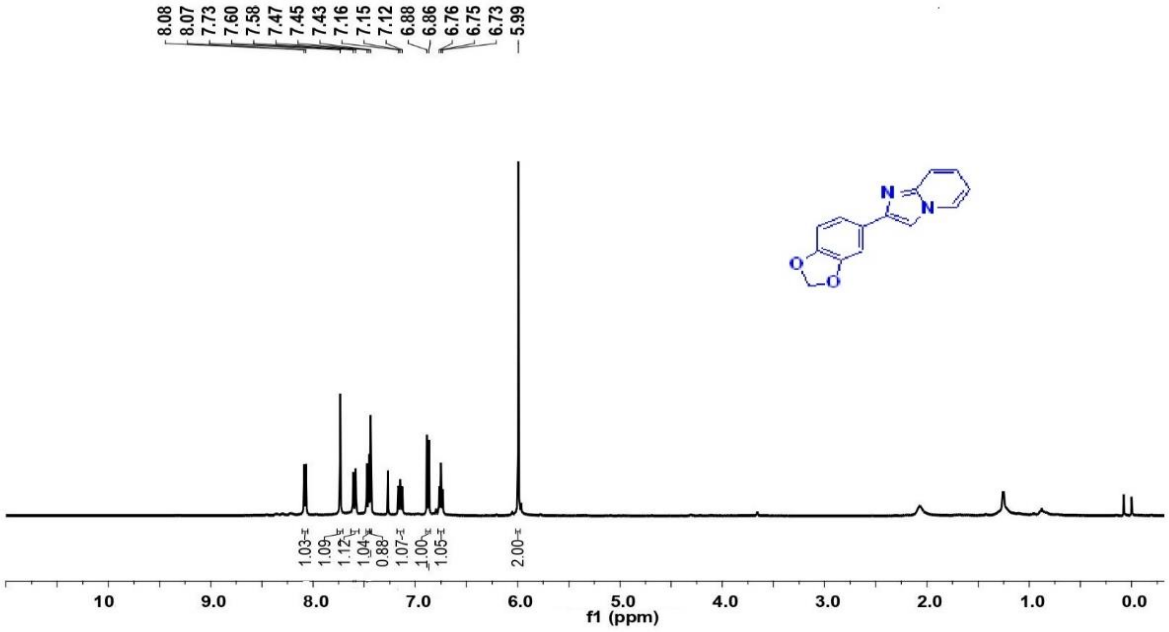
f1 (ppm)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7.43
7.16
7.15
7.12
6.88
6.86
6.76
6.75
6.73
5.99
1.03
1.09
1.12
1.04
0.88
1.07
1.00
1.05
2.00
10
9.0
8.0
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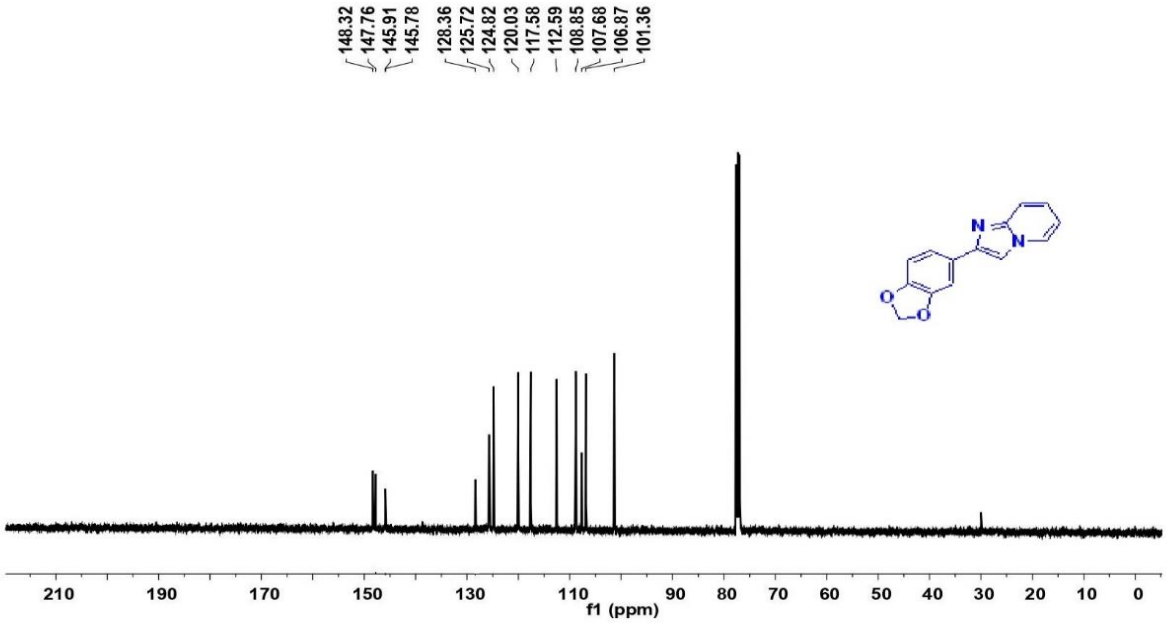
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
N
N
O
O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112.59
108.85
107.68
106.87
101.36
210
190
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90
80
70
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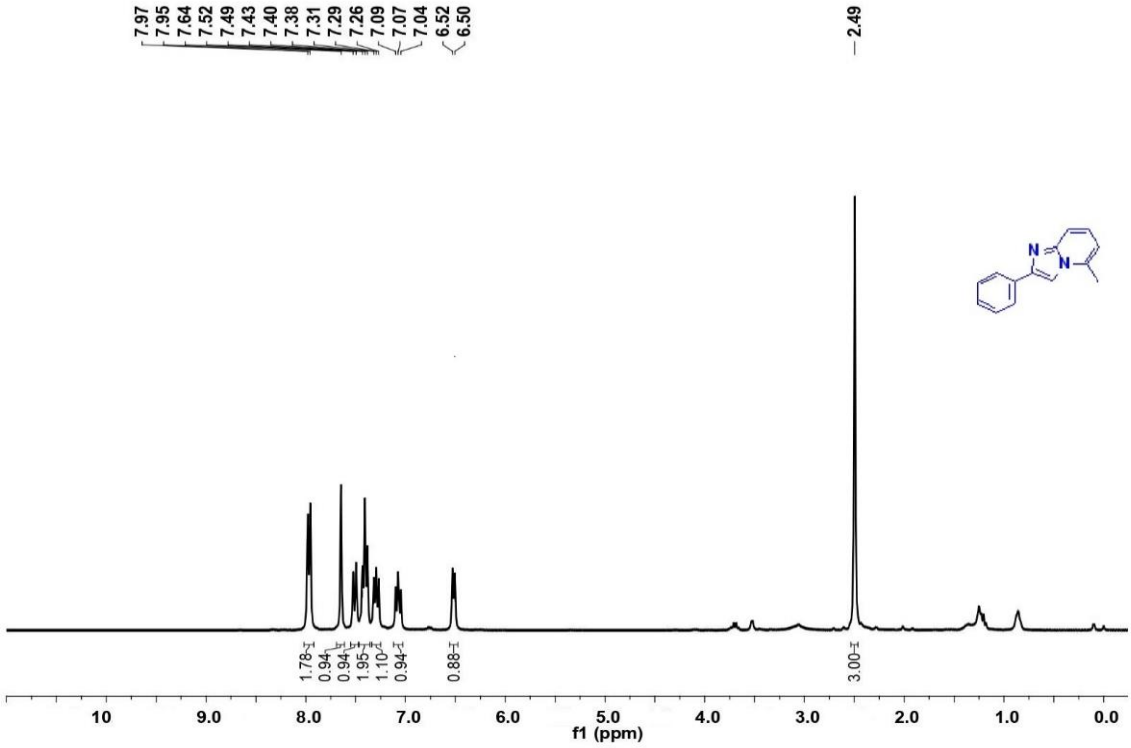
50
40
30
20
10
0
f1 (ppm)
N
N
O
O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7.09
7.07
7.04
6.52
6.50
2.49
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N
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0.94
0.94
1.95
1.10
0.94
0.88
3.00
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5.0
4.0
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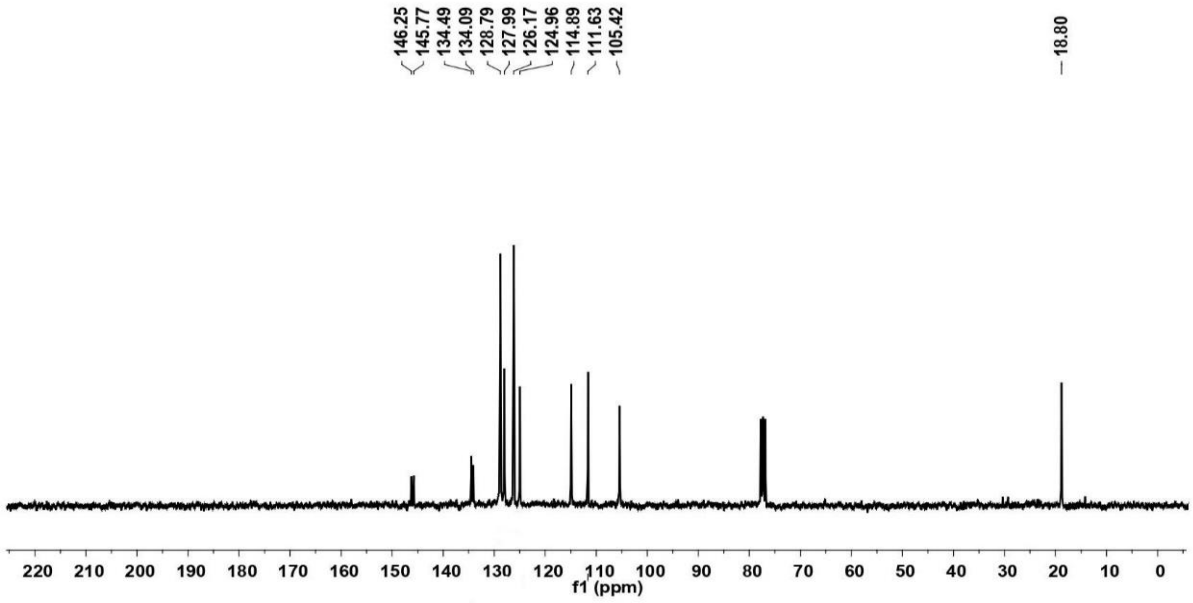
2.0
1.0
0.0
f1 (ppm)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114.89
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105.42
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200
190
180
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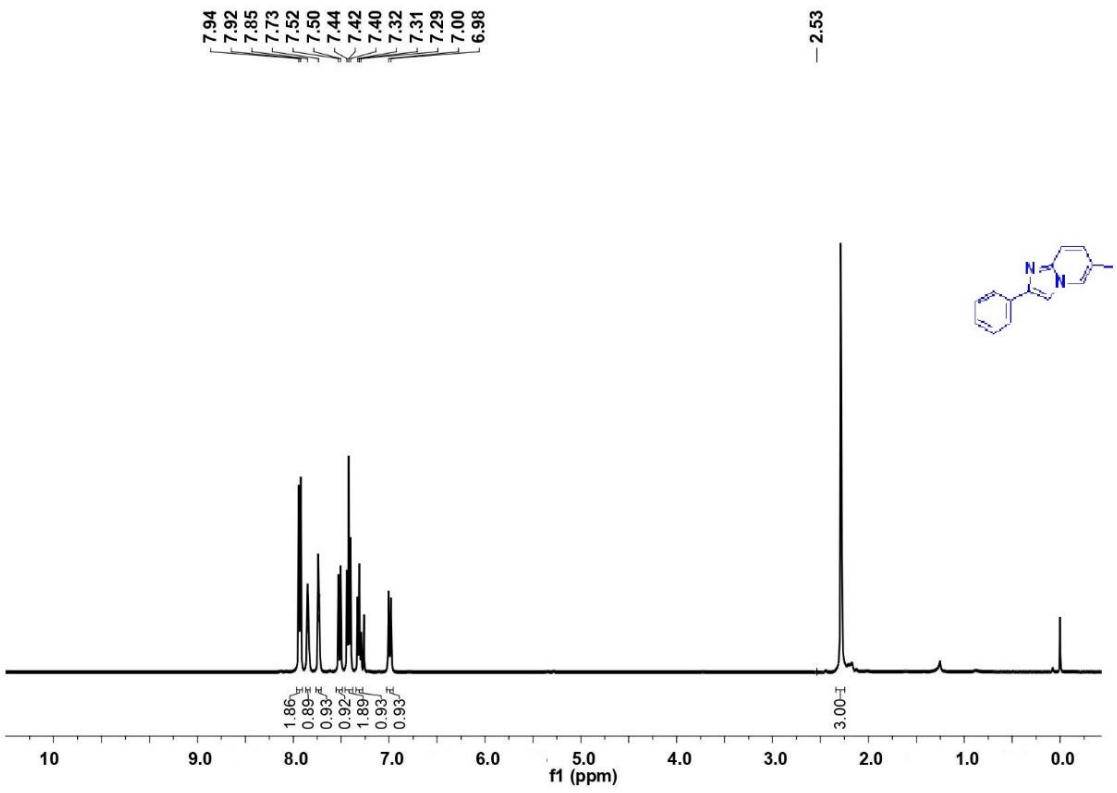
10
0
f1 (ppm)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7.92
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7.29
7.00
6.98
2.53
1.86
0.89
0.93
0.92
1.89
0.93
0.93
3.00
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7.0
6.0
5.0
4.0
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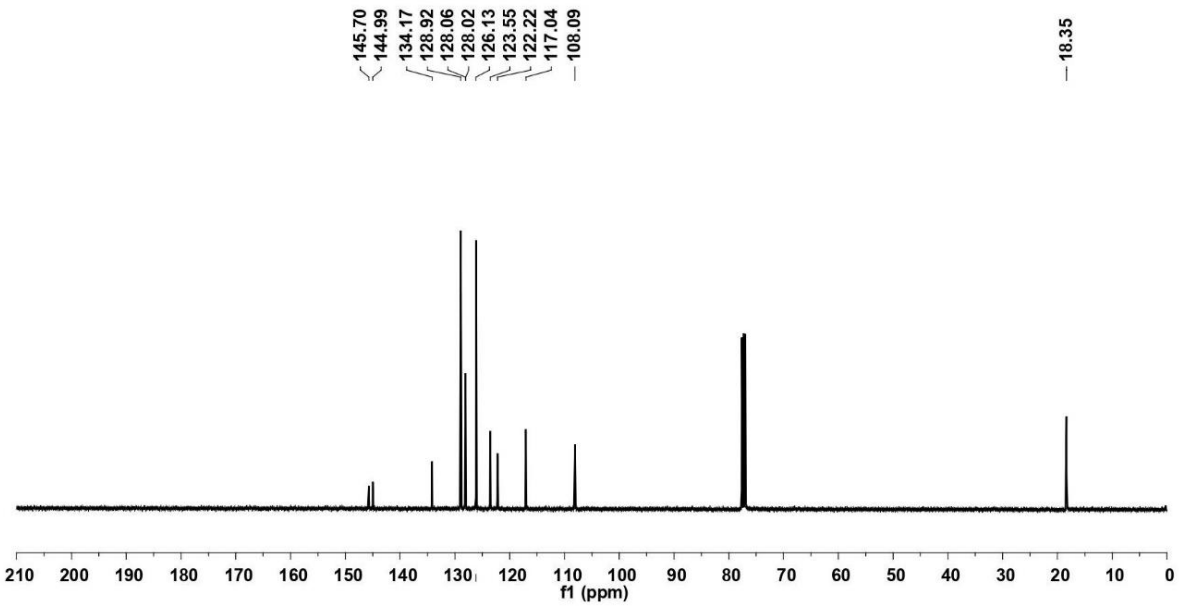
2.0
1.0
0.0
f1 (ppm)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123.55
122.22
117.04
108.09
18.35
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200
190
180
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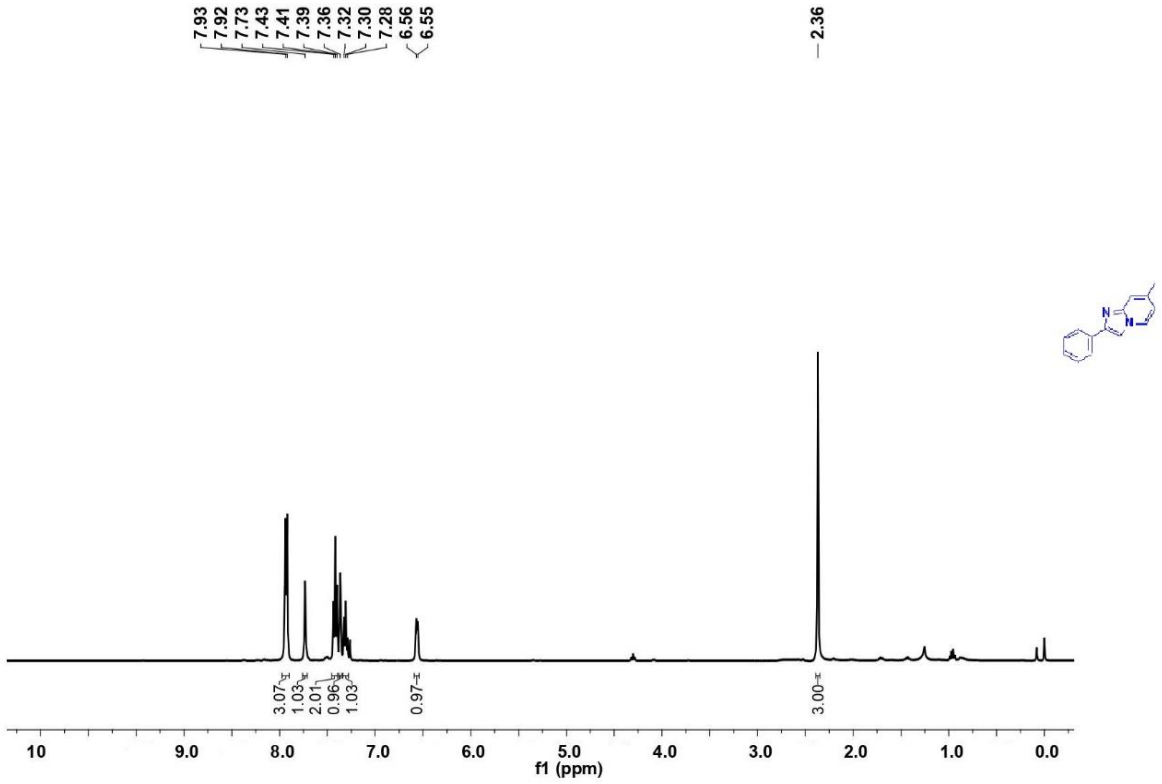
f1 (ppm)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6.55
2.36
3.07
1.03
2.01
0.96
1.03
0.97
3.00
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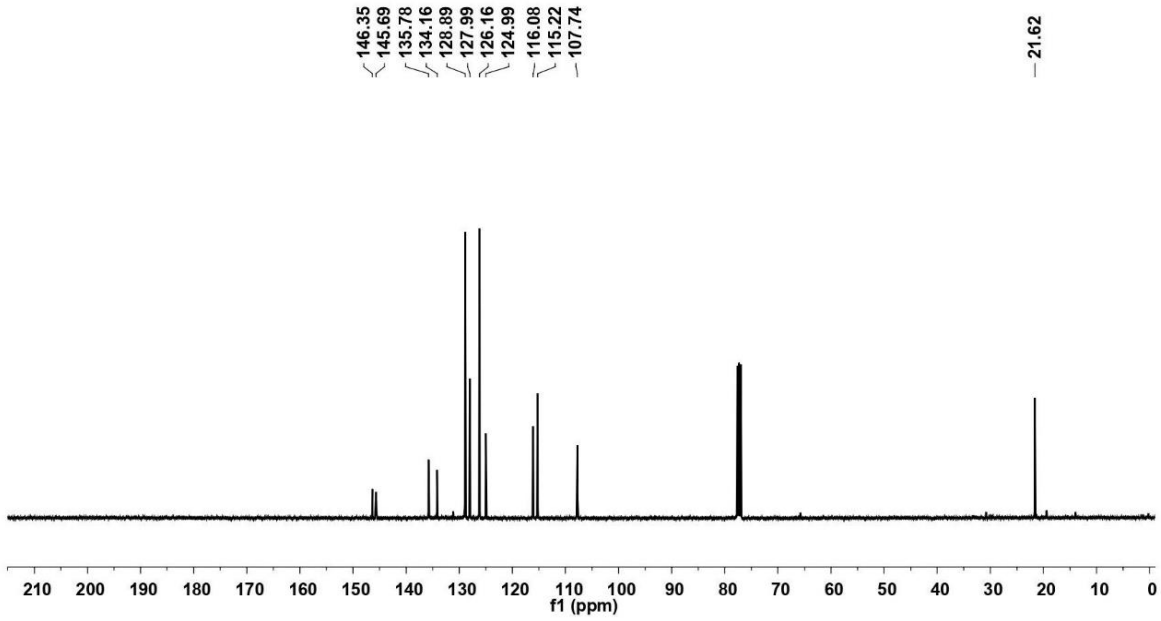
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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115.22
107.74
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200
190
180
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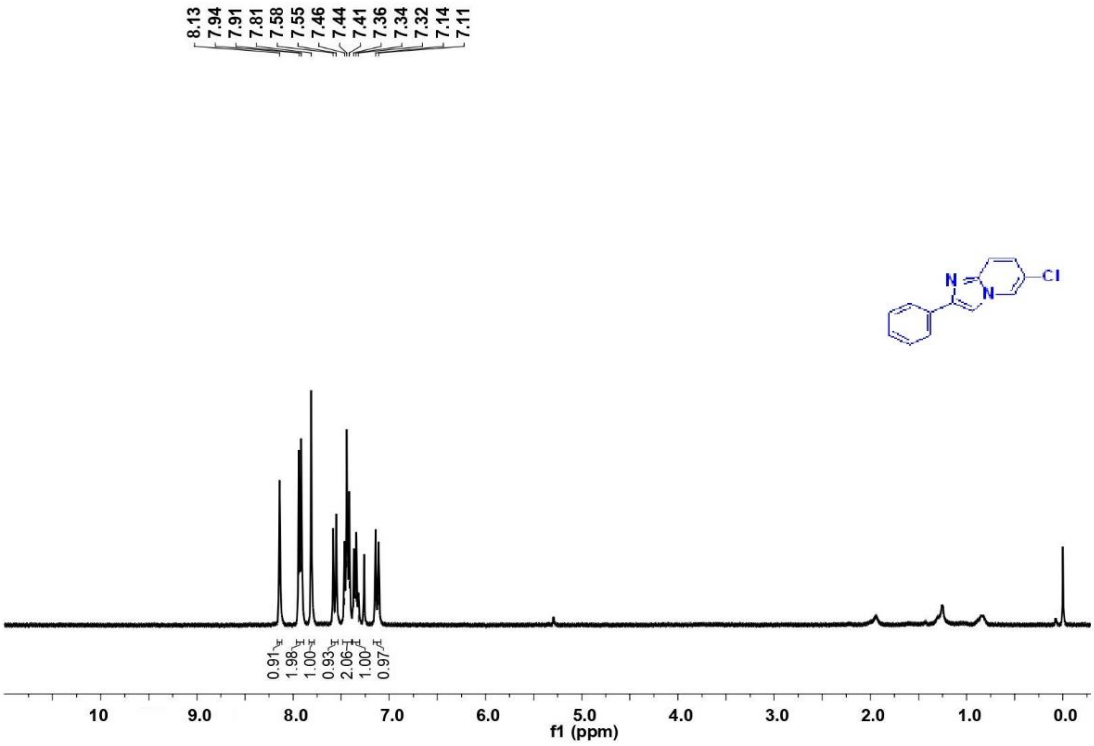
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7.32
7.14
7.11
Cl
0.91
1.98
1.00
0.93
2.06
1.00
0.97
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7.0
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5.0
4.0
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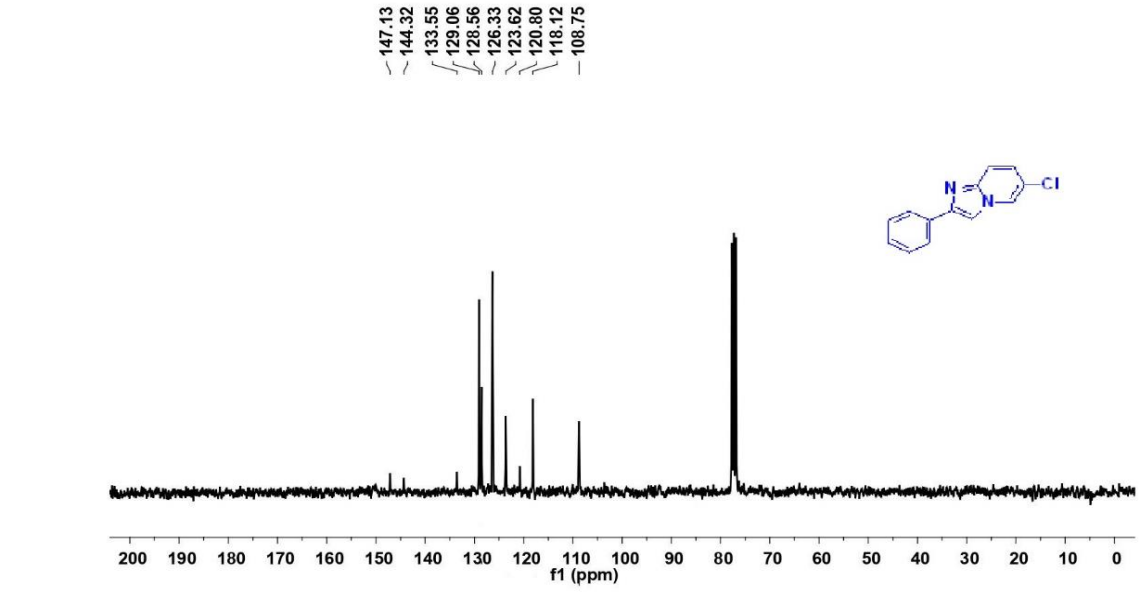
2.0
1.0
0.0
f1 (ppm)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108.75
Cl
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180
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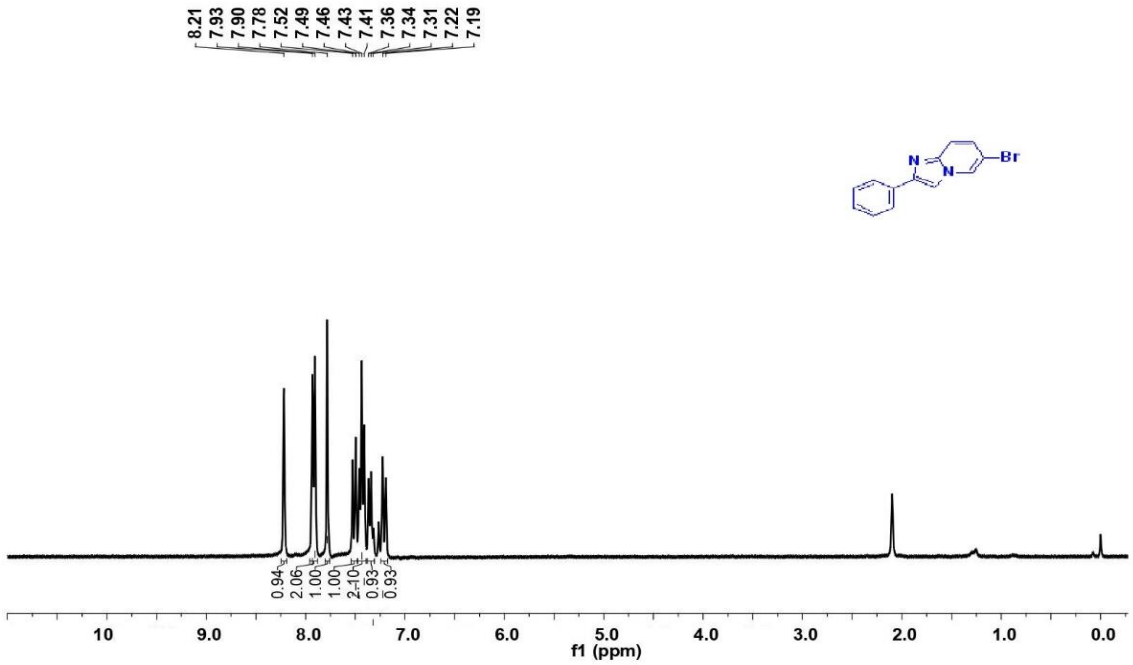
f1 (ppm)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7.36
7.34
7.31
7.22
7.19
Br
0.94
2.06
1.00
1.00
2.10
0.93
0.93
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6.0
5.0
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3.0
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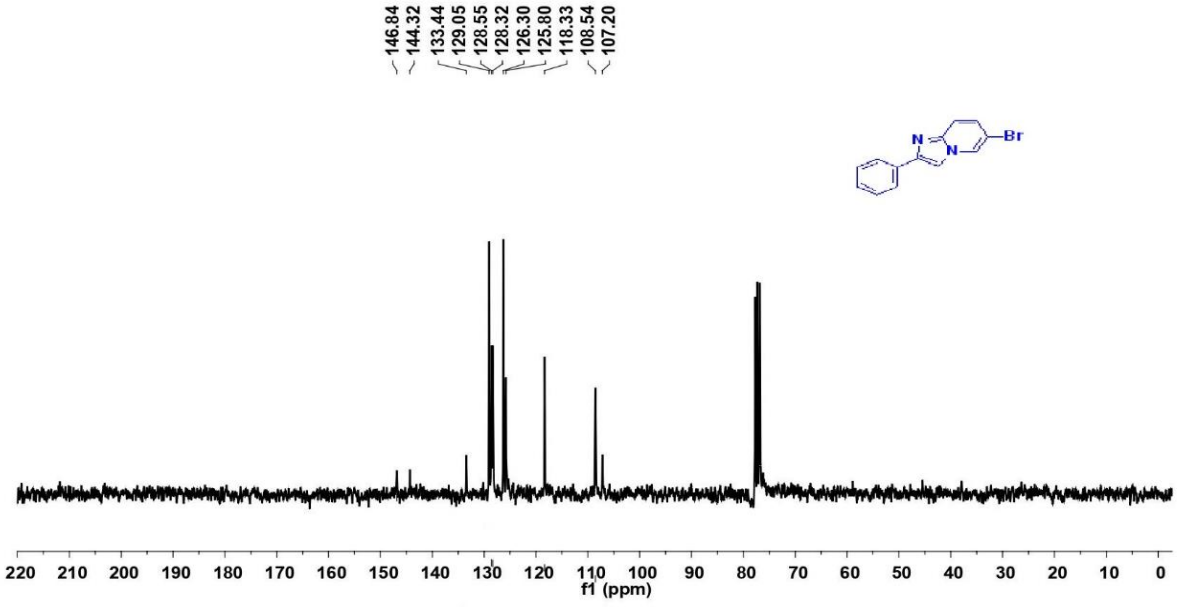
1.0
0.0
f1 (ppm)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128.32
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125.80
118.33
108.54
107.20
Br
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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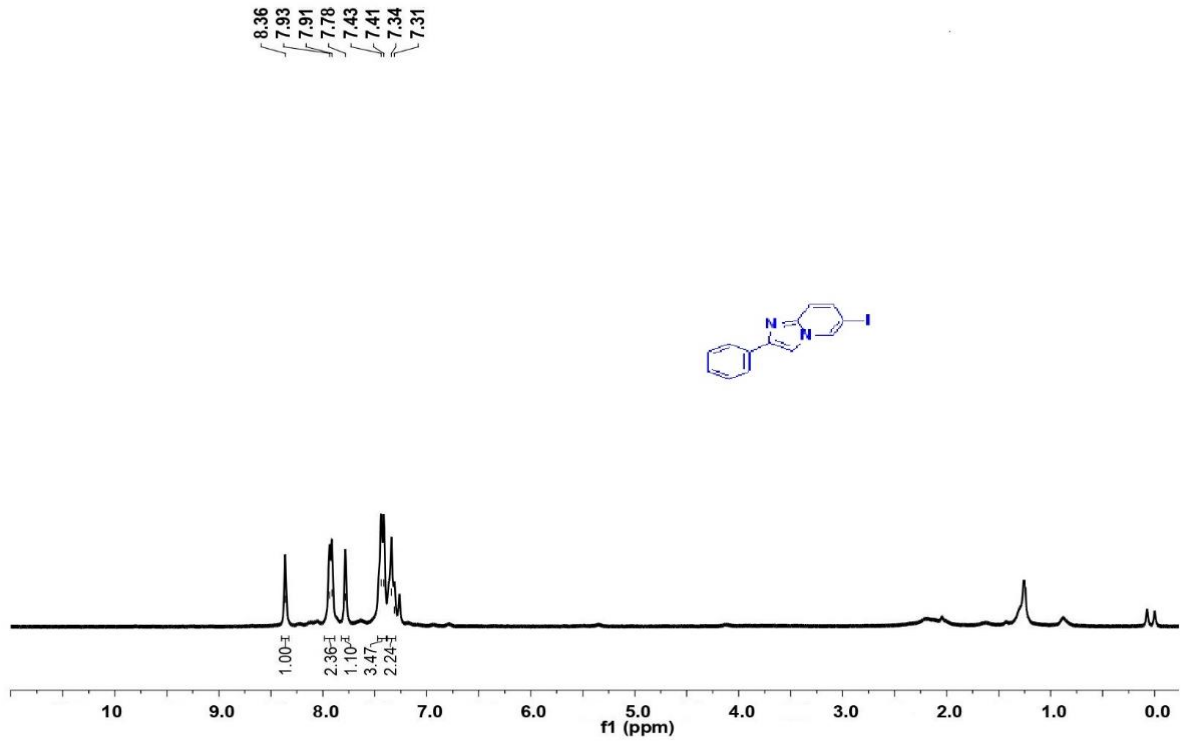
f1 (ppm)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7.34
7.31
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2.36
1.10
3.47
2.24
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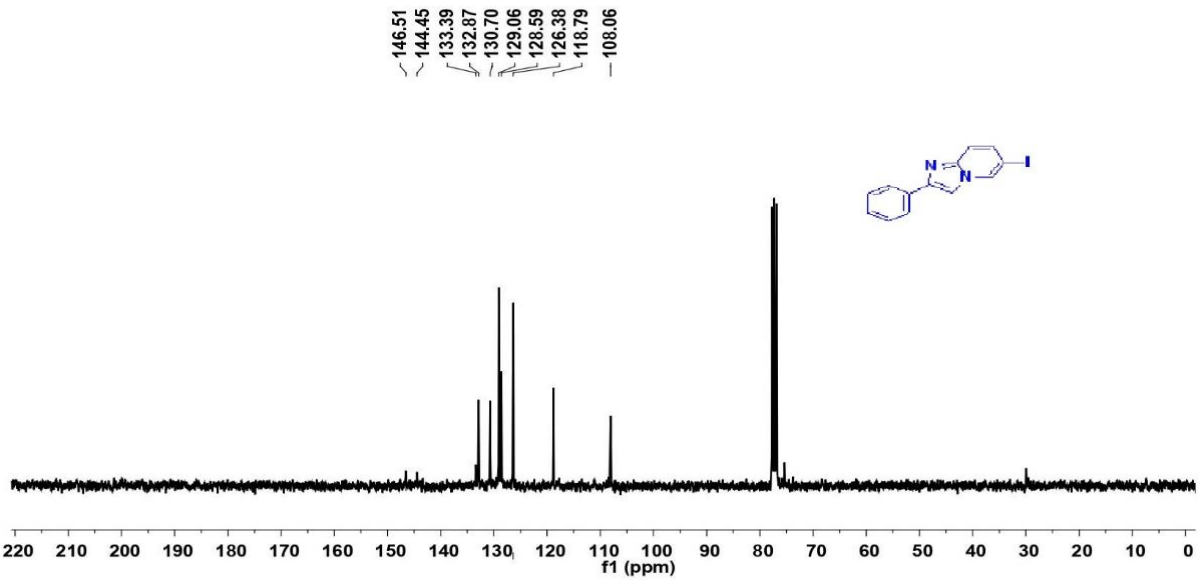
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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128.59
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108.06
220
210
200
190
180
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130
120
110
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90
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70
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50
40
30
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10
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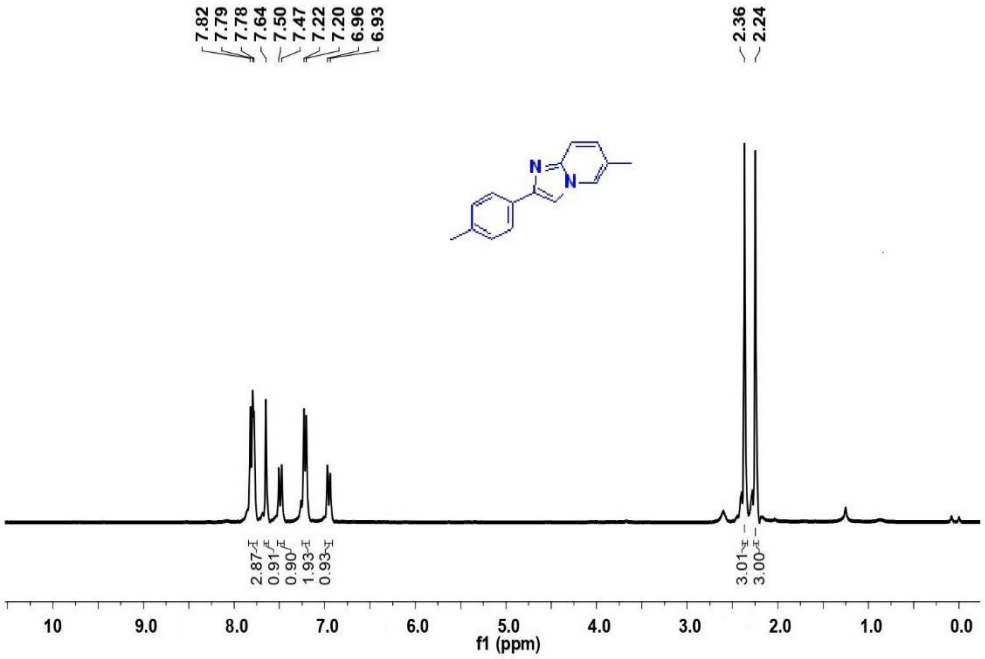
f1 (ppm)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7.47
7.22
7.20
6.96
6.93
2.36
2.24
2.87
0.91
0.90
1.93
0.93
3.01
3.00
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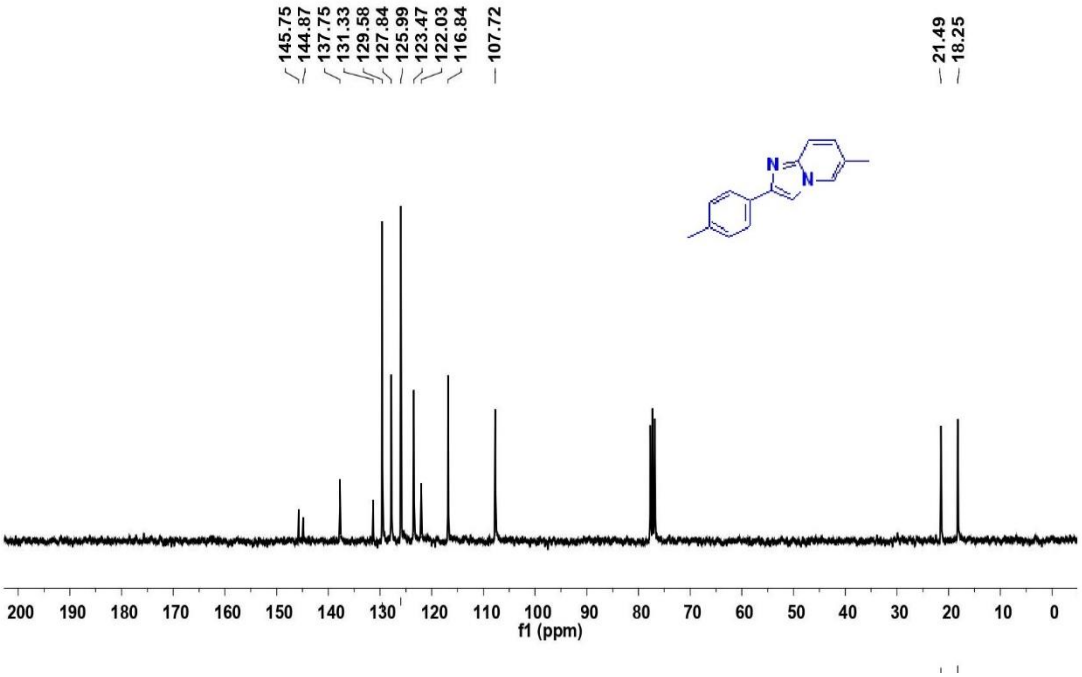
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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122.03
116.84
107.72
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18.25
200
190
180
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130
120
110
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10
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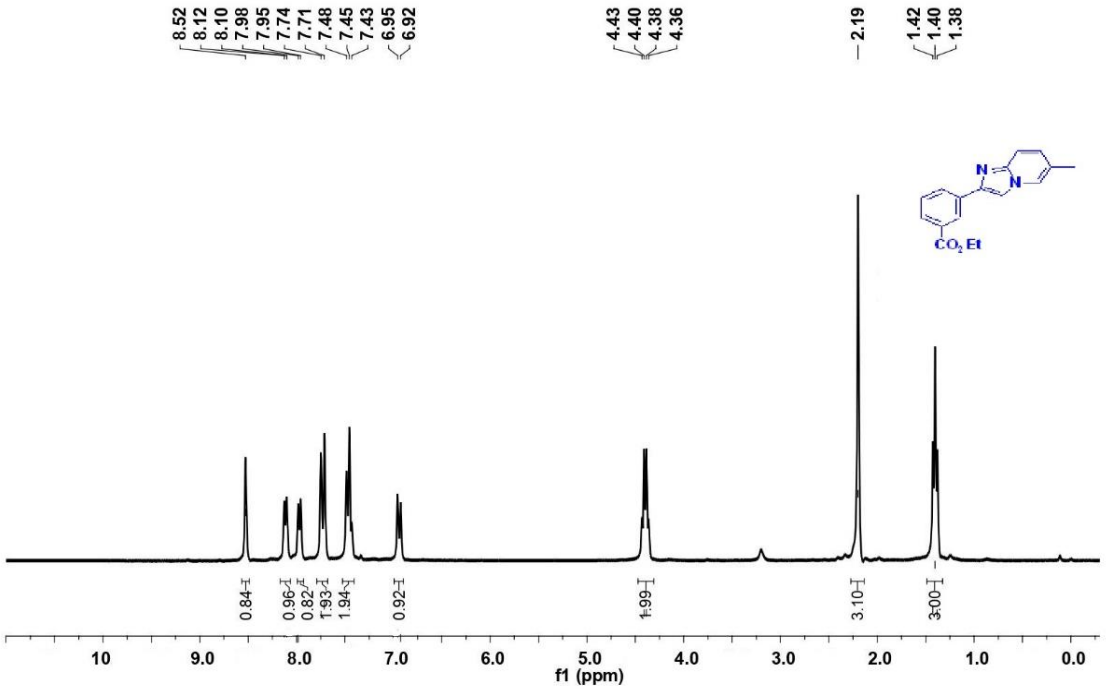
f1 (ppm)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7.74
7.71
7.48
7.45
7.43
6.95
6.92
4.43
4.40
4.38
4.36
2.19
1.42
1.40
1.38
N
N
CO2 Et
0.84
0.96
0.82
1.93
1.94
0.92
1.99
3.10
3.00
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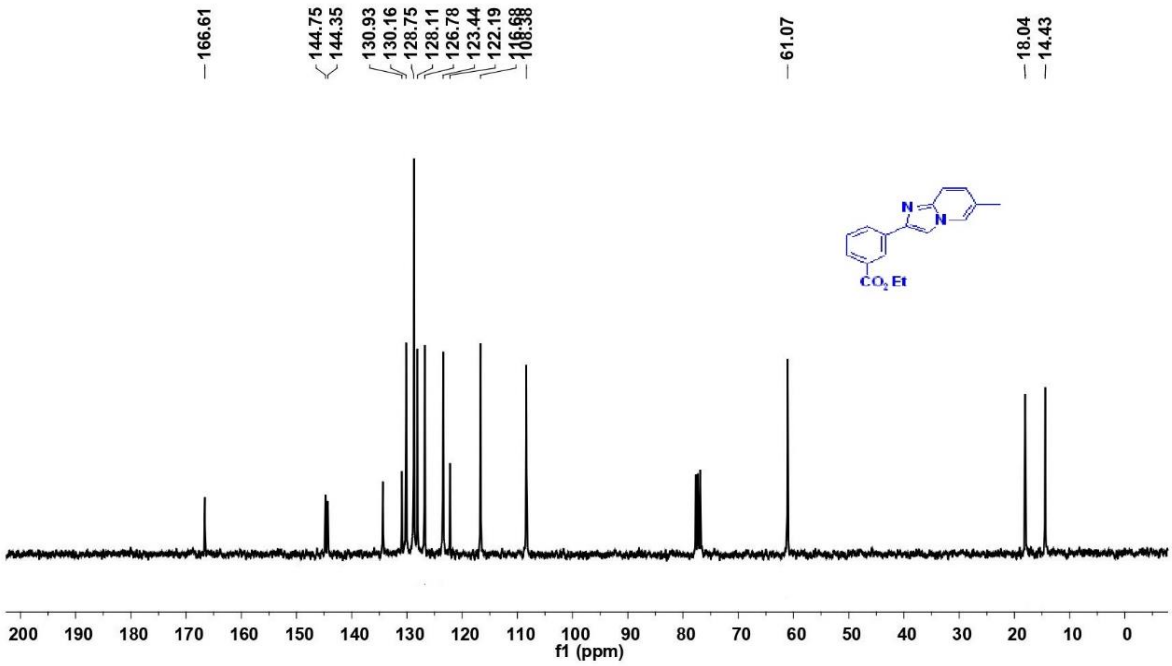
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128.11
126.78
123.44
122.19
116.68
108.38
61.07
18.04
14.43
N
N
CO2 Et
200
190
180
170
160
150
140
130
120
110
100
90
80
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50
40
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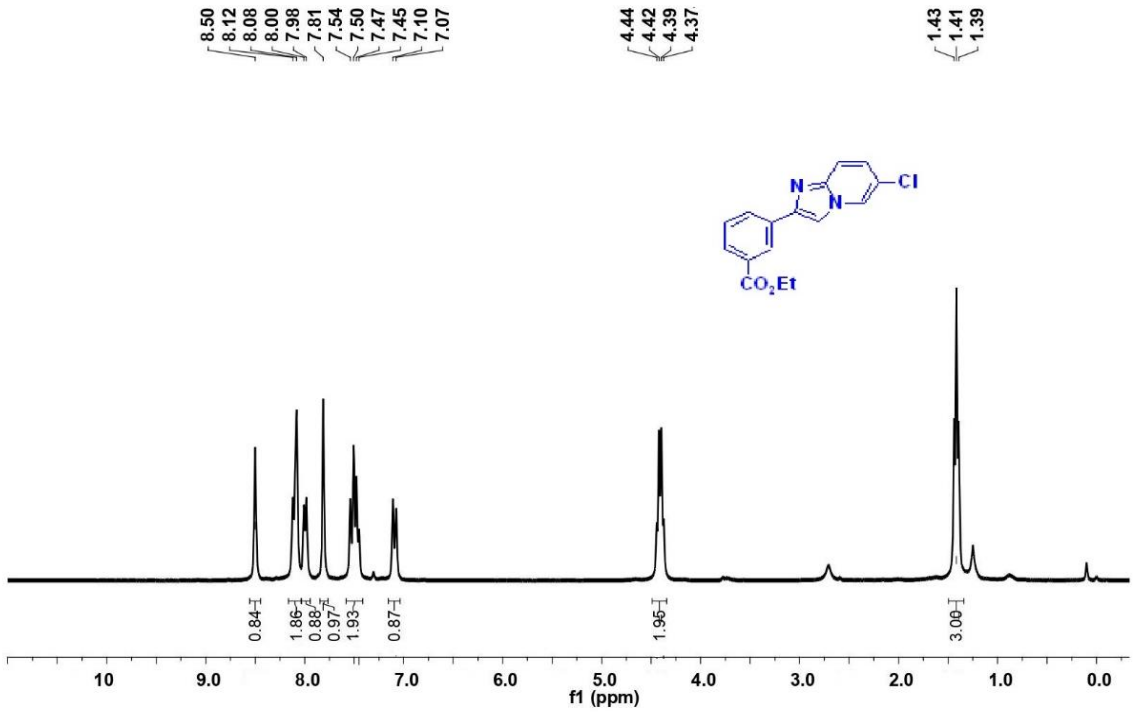
10
0
f1 (ppm)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7.47
7.45
7.10
7.07
4.44
4.42
4.39
4.37
1.43
1.41
1.39
Cl
N
N
CO2Et
0.84
1.86
0.88
0.97
1.93
0.87
1.96
3.00
10
9.0
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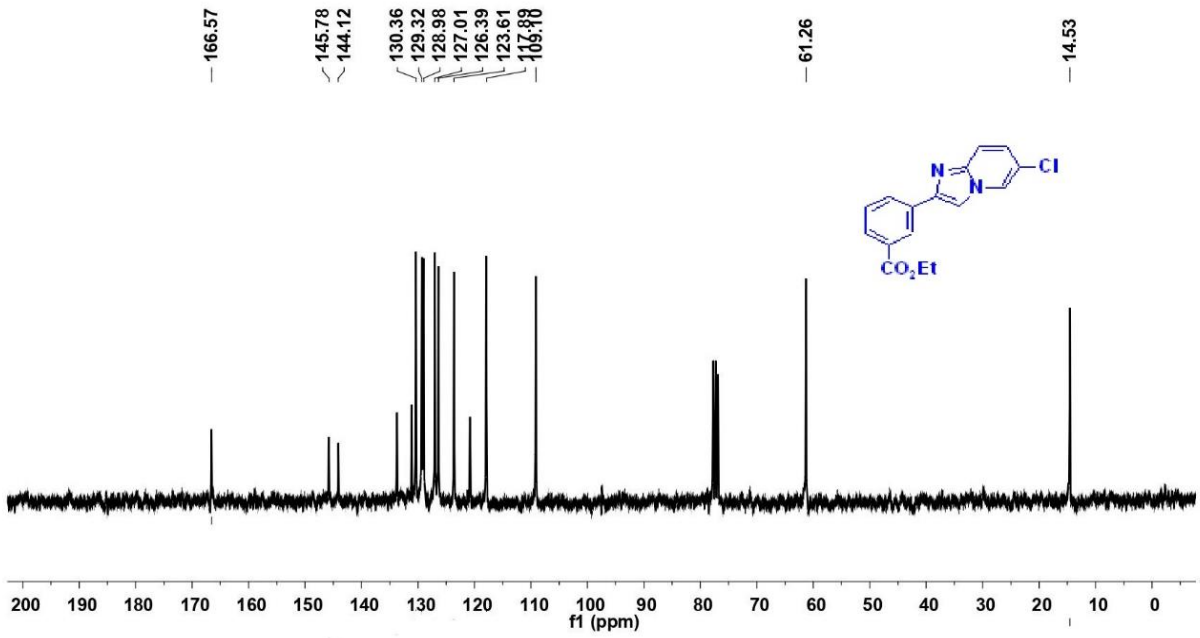
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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127.01
126.39
123.61
61.26
14.53
Cl
N
N
CO2Et
200
190
180
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120
110
100
90
80
70
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50
40
30
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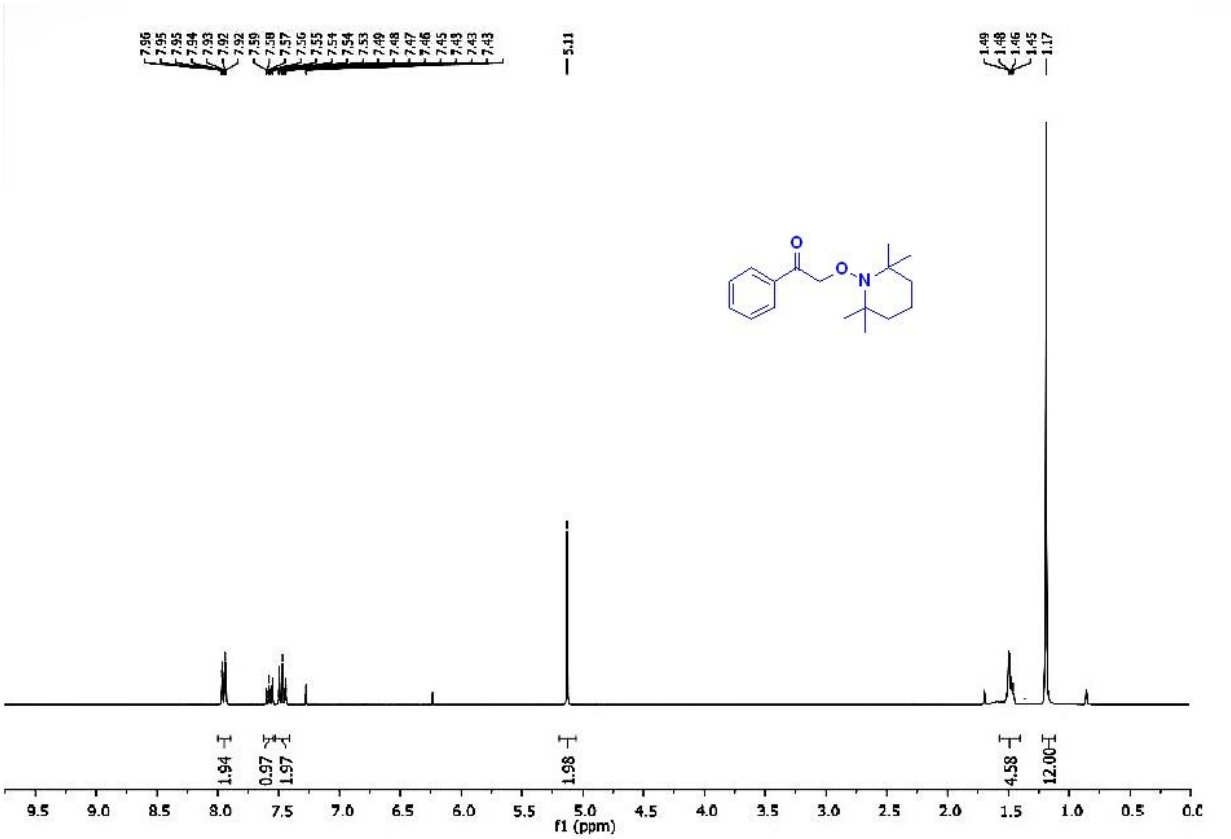
10
0
f1 (ppm)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7.47
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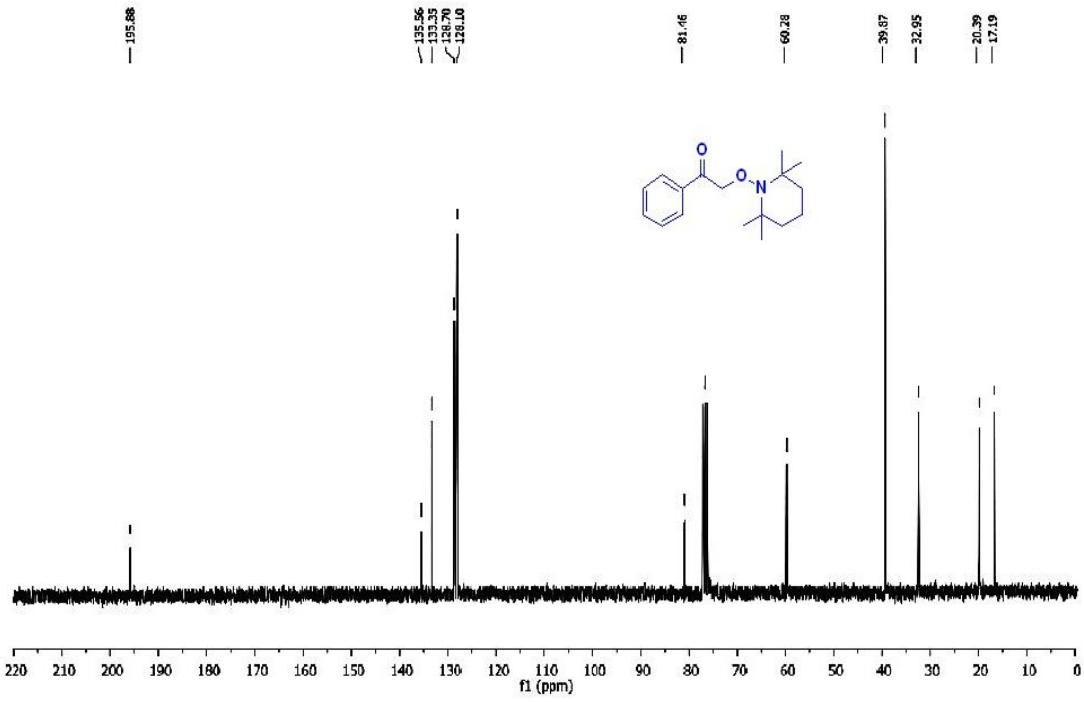
7.45
7.43
7.43
5.11
1.49
1.48
1.46
1.45
1.17
O
O
N
1.94
0.97
1.97
1.98
4.58
12.00
f1 (ppm)


195.88
135.56
133.35
128.70
128.10
81.46
60.28
39.87
32.95
20.39
17.19
O
O
N
f1 (ppm)