Supporting Information

An Approach to 6-Trifluoromethyl-Phenanthridines through Visible-Light-Mediated Intramolecular Radical Cyclization of Trifluoroacetimidoyl Chlorides

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General……..……. …..…..…….S2

General Procedures for Experiments and Analytical Data……..…….… ...S2-S9

NMR Spectra……...……..…..……..…..….. S10-S35

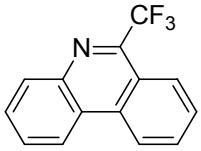
General: Solvents were purified or dried in a standard manner. Reactions were monitored by TLC on silica gel plates (GF254), and the analytical thin-layer chromatography (TLC) was performed on precoated, glass-backed silica gel plates. ^{1}H NMR , ^{13}C NMR spectra and ^{19}F NMR spectra were recorded on a 400 or 500 MHz NMR spectrometers at room temperature. Chemical shifts (δ) are reported in ppm downfield from tetramethylsilane. Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; m, multiplet. Trifluoroacetimidoyl chlorides were prepared according to the literature. [1]

General experimental details

To a mixture of **1a-t** (0.3 mmol) and $Ru(bpy)_3Cl_2•6H_2O$ (3 mol%) in 3.0 mL of CH_3CN was added $(n\text{Bu})_3N$ (0.6 mmol) under N_2 atmosphere. The solution was stirred at room temperature under 5 W blue LED irradiation for 6 h. When the reaction finished, the solvent was evaporated under vacuum. Then, the crude products were directly purified using flash column chromatography on silica gel (petroleum ether/ethyl acetate 10:1 as the eluant) to afford the desired 6-trifluoromethyl-phenanthridines **2a-t**.

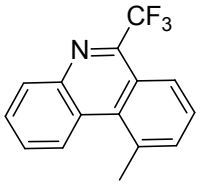
Characterization data of compounds

6-(trifluoromethyl)phenanthridine (2a)[2]



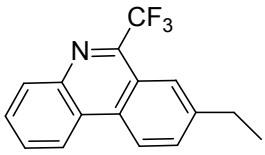
Yield 86%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.59 (d, *J* = 8.5 Hz, 1H), 8.49-8.50 (m, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 8.19-8.20 (m, 1H), 7.81-7.84 (m, 1H), 7.66-7.73 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 146.5(q, *J* = 33.0 Hz), 141.8, 134.0, 131.4, 131.1, 129.3, 129.2, 128.1, 125.9 (q, *J* = 4.1 Hz), 125.1, 122.5, 122.1, 121.9 (q, *J* =275.6 Hz), 121.8.

6-(trifluoromethyl)-10-methylphenanthridine (2b)[3]



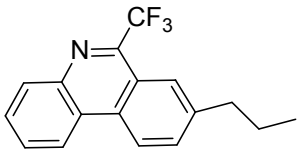
Yield 88%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.85-8.87 (m, 1H), 8.30-8.34 (m, 2H), 7.75-7.83 (m, 3H), 7.66-7.69 (m, 1H), 3.15(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 147.1(q, *J* = 32.2 Hz), 142.8, 135.8, 135.6, 133.5, 131.5, 128.5, 128.4, 127.4, 126.6, 126.5, 124.3 (q, *J* = 3.6 Hz), 123.2, 122.1 (q, *J* =275.6 Hz), 27.1.

8-ethyl-6-(trifluoromethyl)phenanthridine(2c)



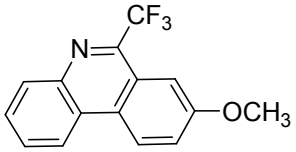
Yield 85%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.49-8.54 (m, 2H), 8.22-8.25 (m, 1H), 8.12 (s, 1H), 7.70-7.76 (m, 3H), 2.90 (q, *J* = 8.0 Hz, 2H), 1.36 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.3 (q, *J* = 32.3 Hz), 144.4, 141.4, 132.1, 131.0, 129.1, 128.9, 125.2, 124.0 (q, *J* =3.5 Hz), 122.5, 122.1 (q, *J* =275.2 Hz), 122.0, 121.9, 29.2, 15.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.4 (s, 3 F); EI-MS (m/z): 276 $[M+1]^+$

6-(trifluoromethyl)-8-propylphenanthridine(2d)



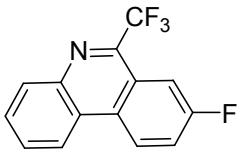
Yield 87%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.48-8.54 (m, 2H), 8.22-8.25 (m, 1H), 8.10 (s, 1H), 7.69-7.74 (m, 3H), 2.82 (t, *J* = 7.2 Hz, 2H), 1.73-1.78 (m, 2H), 1.00 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.3 (q, *J* = 32.4 Hz), 142.9, 141.4, 132.5,132.1, 131.0, 129.1, 128.8, 125.2, 124.7 (q, *J* =2.8 Hz), 124.4, 122.0 (q, *J* =275.3 Hz), 121.93, 121.89, 38.2, 24.5, 13.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.43; EI-MS (m/z): 290 $[M+1]^+$

6-(trifluoromethyl)-8-methoxyphenanthridine(2e) [3]



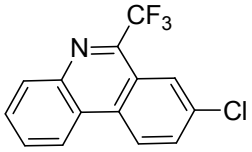
Yield 83%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.44 (d, *J* = 9.2 Hz, 1H), 8.37-8.39 (m, 1H), 8.19-8.21 (m, 1H), 7.66-7.70 (m, 2H), 7.59 (s, 1H), 7.42-7.45 (m, 1H), 3.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 158.9, 145.4(q, *J* = 33.1 Hz), 140.9, 131.0, 129.2, 128.3, 128.26, 125.2, 124.0, 123.0, 122.4, 122.1 (q, *J* =275.1 Hz), 121.5, 105.4(q, *J* = 3.6 Hz), 55.5.

8-fluoro-6-(trifluoromethyl)phenanthridine(2f)



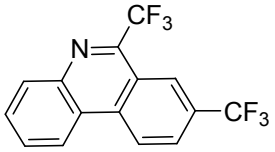
Yield 76%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56-8.60 (m, 1H), 8.42-8.44 (m, 1H), 8.21-8.23 (m, 1H), 7.93-7.95 (m, 1H), 7.72-7.77 (m, 2H), 7.58-7.63 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.4 (d, *J* = 248.9 Hz), 145.6(q, *J* = 29.4 Hz), 141.3, 131.2, 130.6(d, *J* = 1.9 Hz), 129.6, 129.2, 125.1(d, *J* = 9.0 Hz), 124.6, 122.7(d, *J* = 8.8 Hz), 121.8, 121.7(q, *J* = 275.1 Hz), 120.8 (d, *J* = 23.8 Hz), 110.7 (dq, *J* = 23.2 Hz, *J* = 3.4 Hz).^{19}F NMR (376 MHz, $CDCl_3$) δ -63.99 (s, 3 F), -109.92 (s, 1 F); EI-MS (m/z): 266 $[M+1]^+$

8-chloro-6-(trifluoromethyl)phenanthridine(2g) [3]



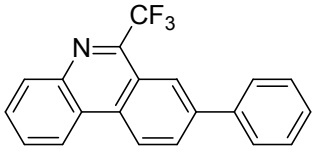
Yield 81%.^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.48 (d, *J* = 8.8 Hz, 1H), 8.41-8.43 (m, 1H), 8.25-8.27 (m, 1H), 8.19-8.22 (m, 1H), 7.71-7.79 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.6(q, *J* = 33.1 Hz), 141.6, 134.2, 132.2, 132.0, 131.2, 129.67, 129.66, 125.1 (q, *J* =3.0 Hz), 124.4, 124.1, 122.4, 121.9, 121.6 (q, *J* = 274.6 Hz).

6,8-bis(trifluoromethyl)phenanthridine(2h) [3]



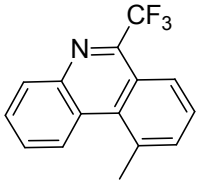
Yield 70%.^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.80 (t, *J* = 8.5 Hz, 1H), 8.60-8.63 (m, 2H), 8.31-8.32 (m, 1H), 8.10-8.11 (m, 1H), 7.83-7.90 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 146.3 (q, *J* = 33.5 Hz), 142.4, 136.0, 131.4, 130.6, 130.1, 129.9, 129.8 (q, *J* = 4.1 Hz), 127.3, 124.2, 123.8, 123.6 (q, *J* = 270.9 Hz), 122.4, 121.6 (q, *J* = 275.3 Hz), 121.0.

6-(trifluoromethyl)-8-phenylphenanthridine(2i) [3]



Yield 62%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.70 (d, *J* = 8.8 Hz, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 8.55-8.58 (m, 1H), 8.53 (s, 1H), 8.26-8.28 (m, 1H), 8.10-8.13 (m, 1H), 7.71-7.79 (m, 4H), 7.51-7.55 (m, 2H), 7.44-7.46 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.6 (q, *J* = 32.7 Hz), 141.7, 140.9, 139.8, 132.9, 131.2, 130.7, 129.4, 129.3, 129.2, 128.3, 127.5, 125.0, 123.8 (q, *J* = 3.3 Hz), 123.1, 122.2, 122.1, 122.0 (q, *J* = 275.4 Hz).

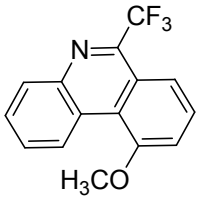
6-(trifluoromethyl)-10-methylphenanthridine(2j) [3]



Yield 56%.^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.85-8.87 (m, 1H), 8.30-8.34 (m, 2H), 7.75-7.83 (m, 3H), 7.66-7.69 (m, 1H), 3.15(s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 147.1(q,

J = 32.2 Hz), 142.8, 135.8, 135.6, 133.5, 131.5, 128.5, 128.4, 127.4, 126.6, 126.5, 124.3 (q, *J* = 3.6 Hz), 123.2, 122.1 (q, *J* =275.6 Hz), 27.1.

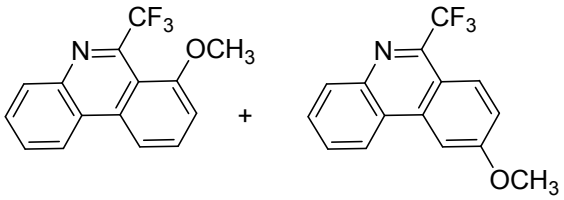
6-(trifluoromethyl)-10-methoxyphenanthridine(2k) [3]



Yield 53%.^{1}H NMR (500 MHz, $CDCl_3$): δ = 9.56-9.59 (m, 1H), 8.29-8.32 (m, 1H), 8.03-8.05 (m, 1H), 7.72-7.82 (m, 3H), 7.41 (d, *J* = 8.5 Hz, 1H), 4.19 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 158.3, 146.2 (q, *J* = 33.5 Hz), 142.3, 130.9, 129.1, 128.6, 128.2, 128.0, 125.0, 124.6, 123.8, 122.1 (q, *J* = 275.4 Hz), 118.0, 112.2, 55.9.

6-(trifluoromethyl)-7-methoxyphenanthridine(2l)

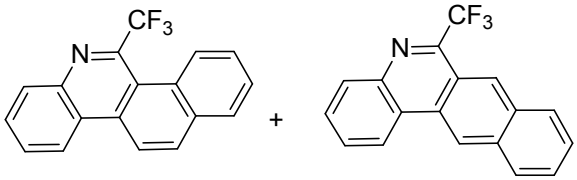
and 6-(trifluoromethyl)-9-methoxyphenanthridine(2l′) [4] **(2l : 2l′ = 3:2)**



Yield 72%.^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.39 (d, *J* = 8.0 Hz, 1H), 8.34 (d, *J* = 8.4 Hz, 0.69H), 8.16-7.20 (m, 2.2H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.74-7.80 (m, 0.67H), 7.64-7.73 (m, 4.32H), 7.21-7.24 (m, 0.63H), 7.03 (d, *J* = 8.0 Hz, 1H), 3.98 (s, 3H), 3.97 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ = 161.6, 156.6, 146.0 (q, *J* = 32.5 Hz), 144.5 (q, *J* = 35.0Hz), 142.0, 141.4, 136.2, 136.1, 131.9, 130.9, 130.8, 129.3, 129.28, 129.0, 128.5, , 127.6 (q, *J* = 3.0 Hz), 124.7, 124.5, 122.4, 122.0, 122.0 (q, *J* = 273.2Hz), 122.0 (q, *J* = 275.2Hz), 118.4, 116.5, 114.4, 114.1, 109.1, 102.9, 56.0, 55.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.23 (s, 2 F), -63.55 (s, 3 F).

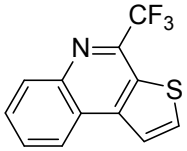
5-(trifluoromethyl)benzo[i]phenanthridine and 6-

(trifluoromethyl)benzo[j]phenanthridine (2m: 2m′ = 10:1)



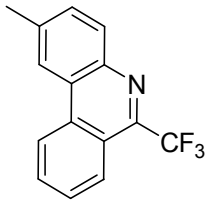
Yield 67%.^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.78 (d, *J* = 8.4 Hz, 1H), 8.53 (d, *J* = 8.0 Hz, 1H), 8.47(d, *J* = 8.8 Hz, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 9.2 Hz, 1H), 7.92-7.94 (m, 1H), 7.63-7.82 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 144.3 (q, *J* = 33.1 Hz), 142.4,135.1, 133.0, 132.8, 130.4, 129.6, 129.1, 128.4, 128.2, 127.7 (q, *J* = 8.2 Hz), 127.4, 127.2, 124.8, 122.6 (q, *J* = 274.6Hz), 122.5, 119.9, 119.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.68 (s, 0.34 F), -60.03 (s, 3 F).

4-(trifluoromethyl)thieno[2,3-c]quinoline (2n) [3]



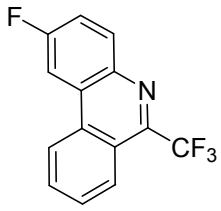
Yield 42%.^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.33 (d, *J* = 8.0 Hz, 1H), 8.17-7.20 (m, 1H), 7.69-7.82 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 147.9, 142.9(q, *J* = 34.6 Hz), 141.9, 131.0, 129.4, 129.1, 128.9, 127.5, 125.1, 123.3, 123.1 (q, *J* = 3.0 Hz), 121.8 (q, *J* = 274.9Hz).

6-(trifluoromethyl)-2-methylphenanthridine (2o) [3]



Yield 81%.^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.53 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 8.4 Hz, 1H), 8.23 (s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.78-7.82 (m, 1H), 7.65-7.69 (m, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 2.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 145.0(q, *J* = 32.5 Hz), 140.0, 139.5, 133.5, 131.05, 131.04, 130.7, 127.8, 125.7 (q, *J* = 3.0 Hz), 124.9, 122.4, 122.1 (q, *J* = 276.2Hz), 121.8, 12`1.6, 22.1.

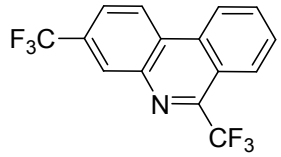
2-fluoro-6-(trifluoromethyl)phenanthridine(2p) [2]



Yield 77%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.44 (d, *J* = 8.4 Hz, 1H), 8.33 (d, *J* = 8.4 Hz, 1H), 8.20-8.24 (m, 1H), 8.06-8.09 (m, 1H), 7.84-7.88 (m, 1H), 7.73-7.77 (m, 1H), 7.46-

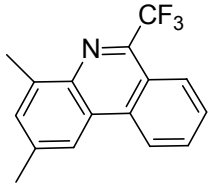
7.51 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.6 (d, *J* = 249.0 Hz), 145.8 (dq, *J* = 33.0, 2.8 Hz), 138.5, 133.5 (d, *J* = 9.5 Hz), 133.2 (d, *J* = 4.4 Hz), 131.4, 128.7, 126.7 (d, *J* = 9.6 Hz), 125.9 (q, *J* = 3.5 Hz), 122.6, 121.9 (q, *J* = 276.1 Hz), 121.7, 118.4 (d, *J* = 25.4 Hz), 107.1 (d, *J* = 23.7 Hz).

3,6-bis(trifluoromethyl)phenanthridine(2q) [3]



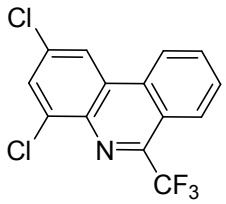
Yield 80%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.63 (t, *J* = 8.5 Hz, 2H), 8.61 (s, 1H), 8.39 (d, *J* = 8.5 Hz, 1H), 7.92-7.98 (m, 2H), 7.82-7.85 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 147.9 (q, *J* = 33.4 Hz), 140.9, 133.1, 132.0, 131.2 (q, *J* = 33.2 Hz), 129.2, 128.6 (q, *J* = 3.4 Hz), 127.2, 126.1 (q, *J* = 3.4 Hz), 124.9 (q, *J* = 3.3 Hz), 123.7 (q, *J* = 270.9 Hz), 123.1, 122.8, 122.2, 121.6 (q, *J* = 275.1 Hz).

6-(trifluoromethyl)-2,4-dimethylphenanthridine(2r) [2]



Yield 75%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59 (d, *J* = 8.4 Hz, 1H), 8.31-8.33 (m, 1H), 8.13 (s, 1H), 7.79-7.84 (m, 1H), 7.67-7.71 (m, 1H), 7.43 (s, 1H), 2.81 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 143.8 (q, *J* = 33.0 Hz), 138.96, 138.91, 138.86, 133.9, 131.7, 130.7, 127.6, 125.6 (q, *J* = 3.4 Hz), 124.9, 122.7, 122.2 (q, *J* = 275.1Hz), 121.6, 119.4, 22.2, 17.9.

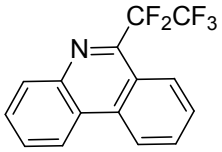
2,4-dichloro-6-(trifluoromethyl)phenanthridine(2s) [3]



Yield 72%.^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.36 (d, *J* = 8.5 Hz, 1H), 8.29-8.31 (m, 1H), 8.22 (d, *J* = 2.0 Hz, 1H), 7.84-7.87 (m, 1H), 7.74-7.77 (m, 1H), 7.73 (d, *J* = 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ = 146.7 (q, *J* = 33.6 Hz), 136.6, 136.5, 134.7, 132.5,

131.9, 129.9, 129.3, 127.0, 125.9 (q, J = 4.0 Hz), 122.6, 121.8, 121.6 (q, J = 270.3 Hz), 120.4.

6-(perfluoroethyl)phenanthridine(2t)



Yield 79%. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.55 (d, J = 8.0 Hz, 1H), 8.39-8.45 (m, 2H), 8.16-8.18 (m, 1H), 7.78-7.82 (m, 1H), 7.65-7.73 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 146.5(t, J = 26.3 Hz), 141.5, 133.8, 131.2, 131.1, 129.3, 129.2, 127.9, 125.9 (t, J = 6.8 Hz), 124.7, 122.5, 122.4, 121.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -80.16 (s, 2 F), -106.80 (s, 3 F).

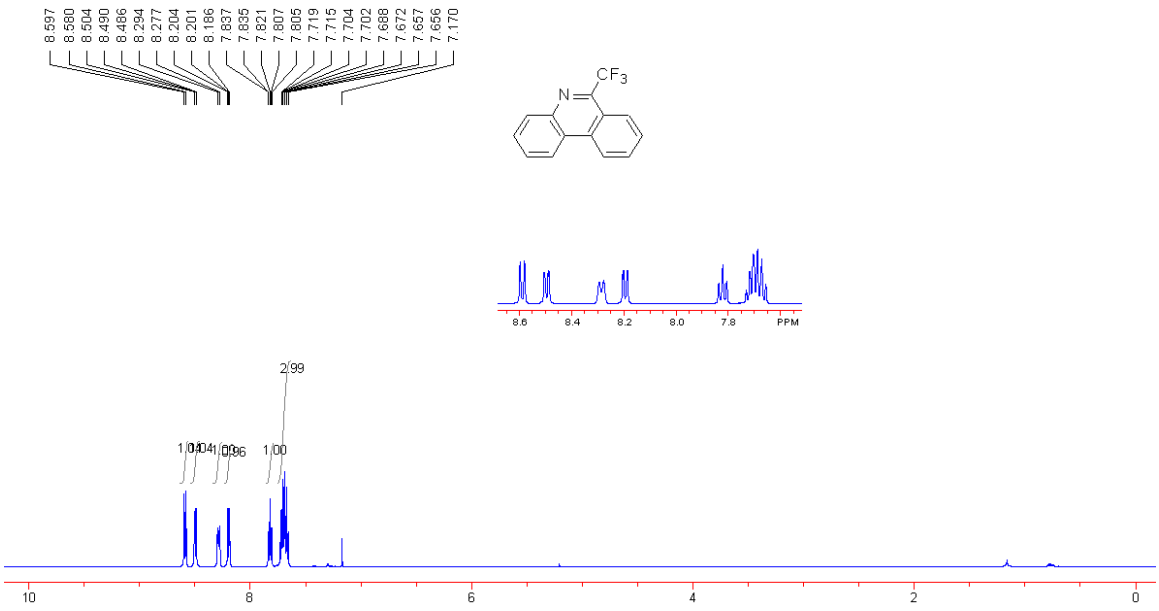
Reference：

(1) K. J. Tamura, H. Mizukami, K. Maeda, H. Watanabe and K. J. Uneyama, *J. Org. Chem.* 1993, **58**, 32.

(2) B. Zhang, C. Mück-Lichtenfeld, C. G. Daniliuc and A. Studer, *Angew. Chem., Int. Ed.,* 2013, **52**, 10792

(3) (a) Q. Wang, X. Dong, T. Xiao and L. Zhou, *Org. Lett.,* 2013, **15**, 4846 (b) Y. Chen, H. Jiang, Y. Zhang and S. Yu, *Org. Lett.,* 2013, **15**, 5520.

(4) W.-Y. Wang, X. Feng, B.-L. Hu, C.-L. Deng and X.-G. Zhang, *J. Org. Chem.,* 2013, **78**, 6025.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7.807
7.805
7.719
7.715
7.704
7.702
7.688
7.672
7.657
7.656
7.170
CF3
N
8.6
8.4
8.2
8.0
7.8
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1.04
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1.00
10
8
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2
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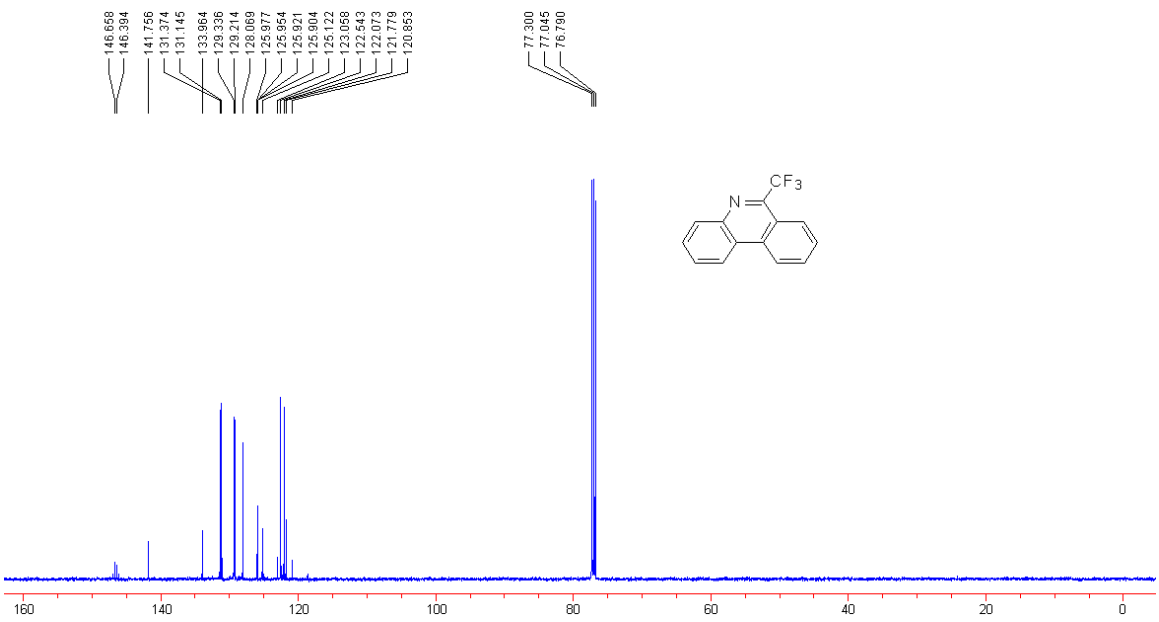
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125.122
123.058
122.543
122.073
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140
120
100
80
60
40
20
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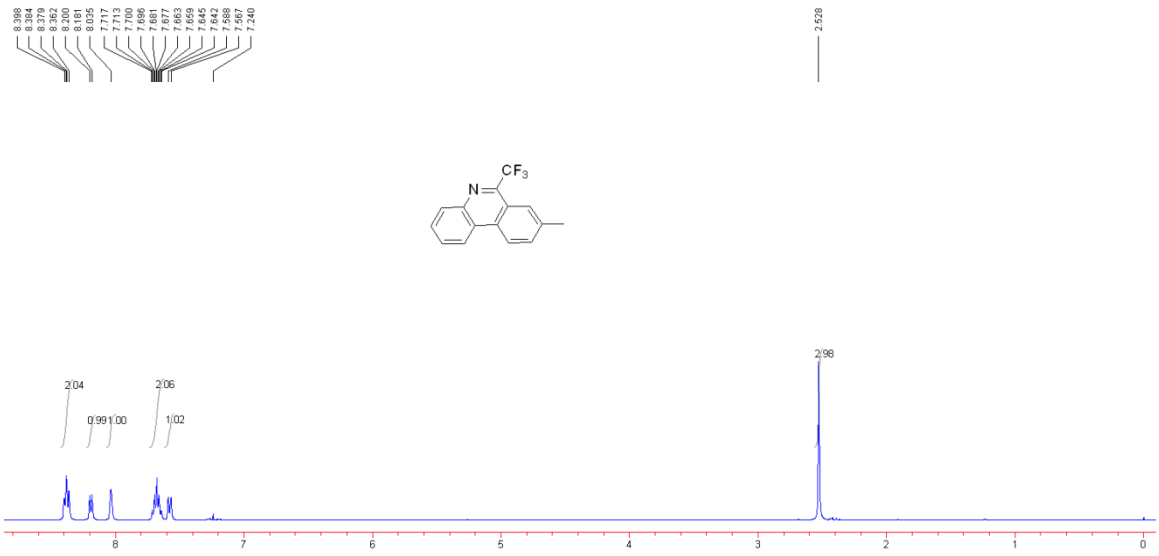
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7.677
7.663
7.659
7.645
7.642
7.568
7.564
7.240
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CF3
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1.02
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7
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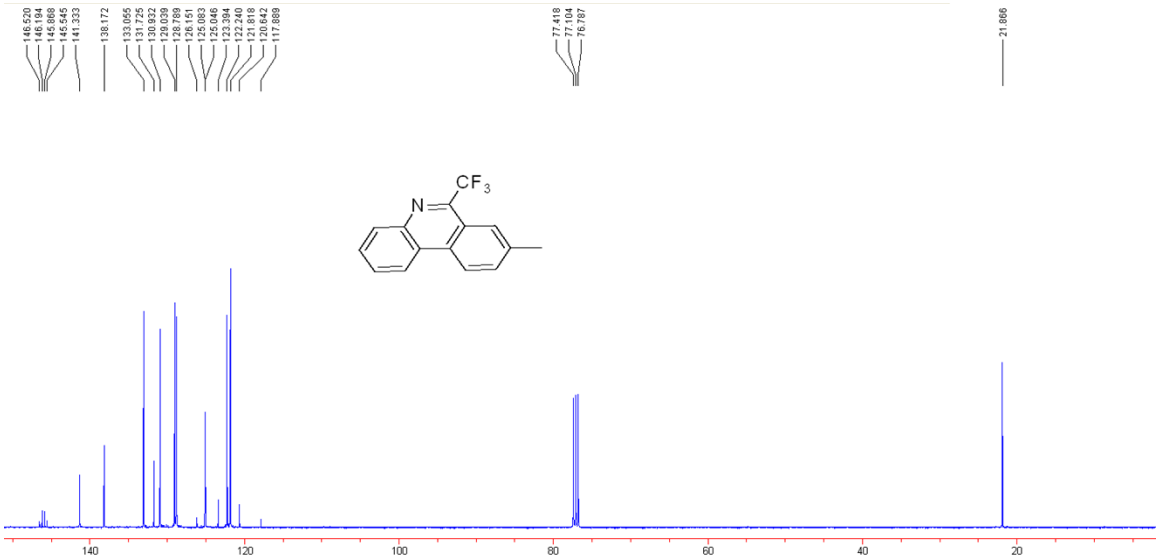
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126.151
125.083
125.046
123.294
122.240
121.818
120.642
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77.418
77.104
76.787
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80
60
40
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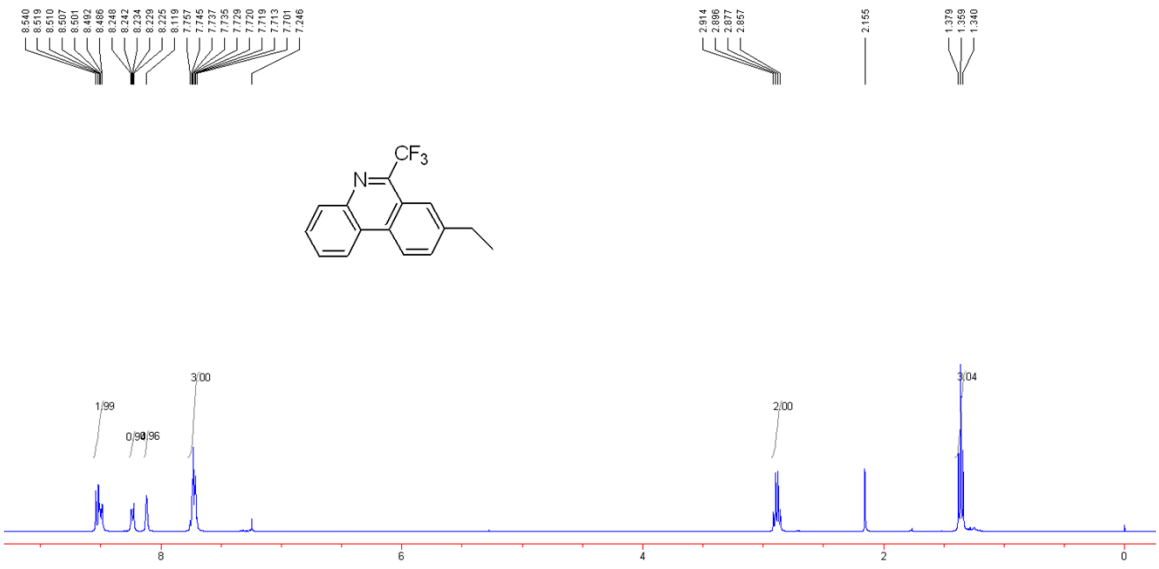
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8.234
8.229
8.225
8.119
7.757
7.745
7.737
7.735
7.729
7.720
7.719
7.713
7.701
7.246
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2.896
2.877
2.857
2.155
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2.00
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8
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2
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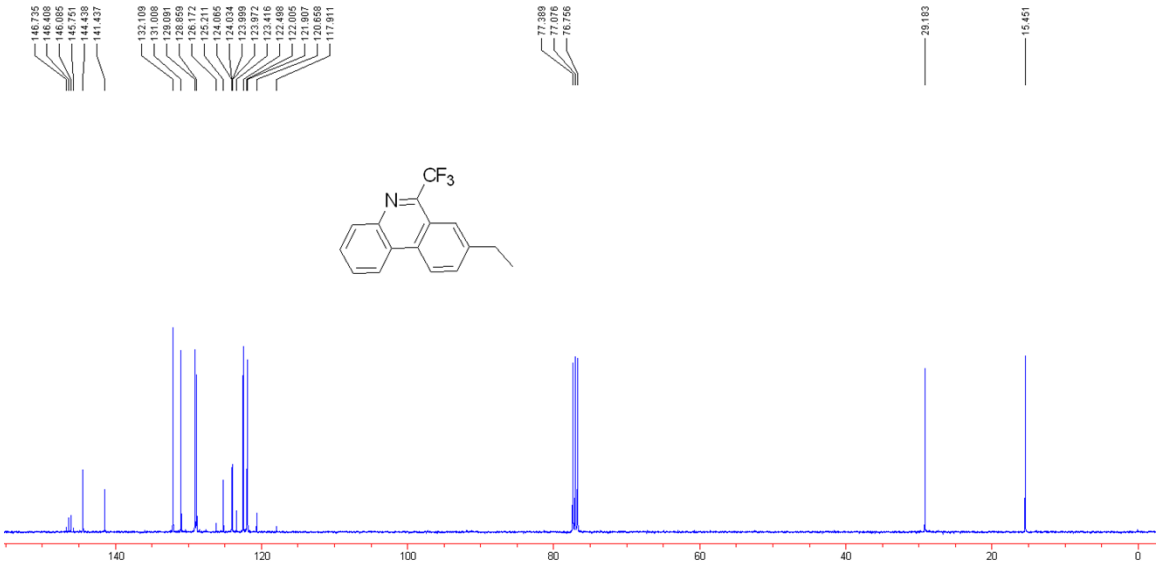
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122.498
122.005
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29.183
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CF3
N
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120
100
80
60
40
20
0


-63.434
CF3
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-100
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-140
-160


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8.241
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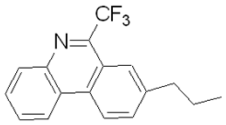
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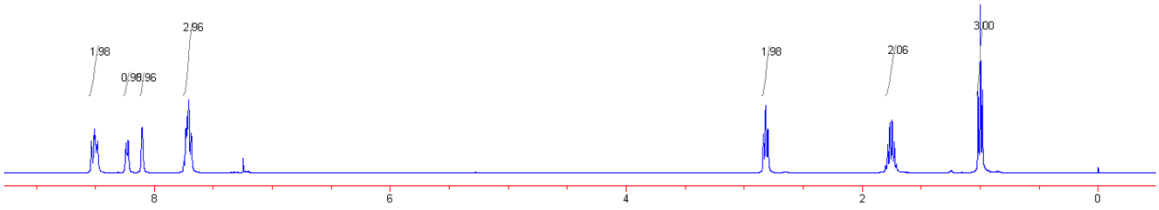
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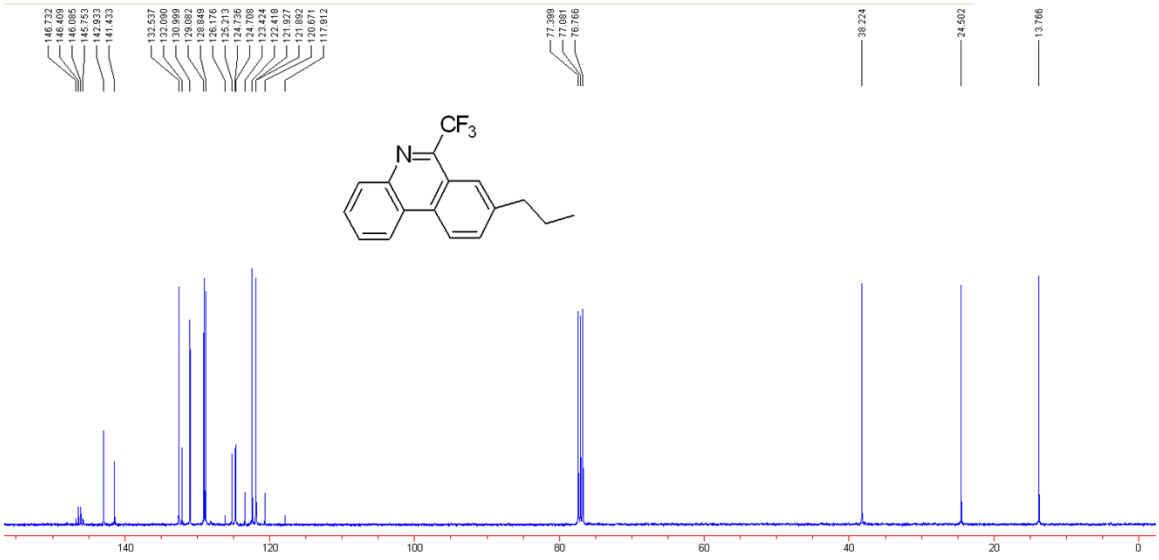
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20
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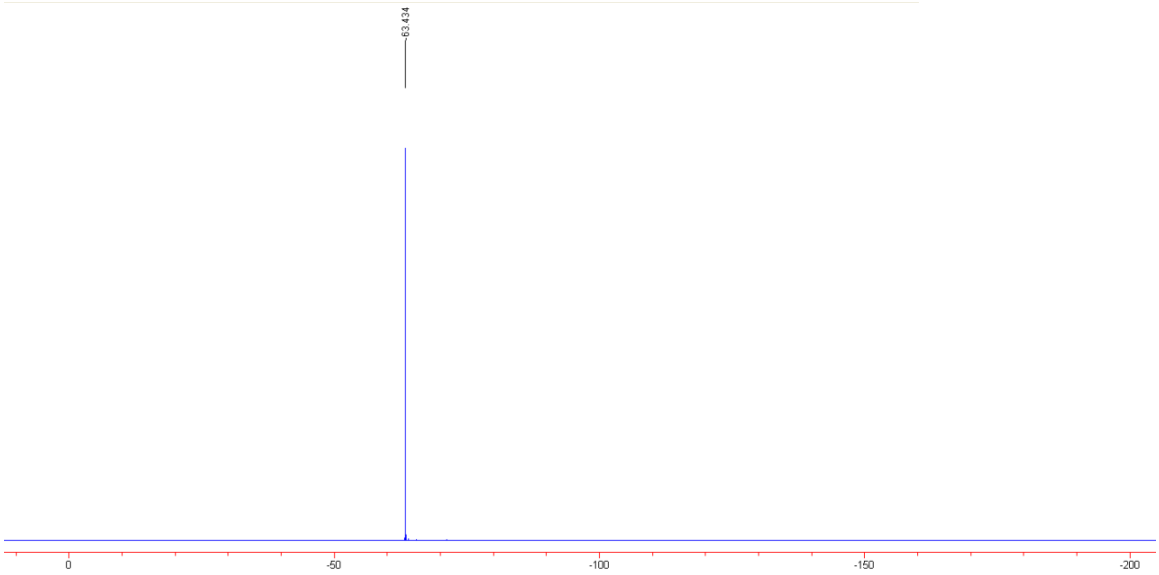
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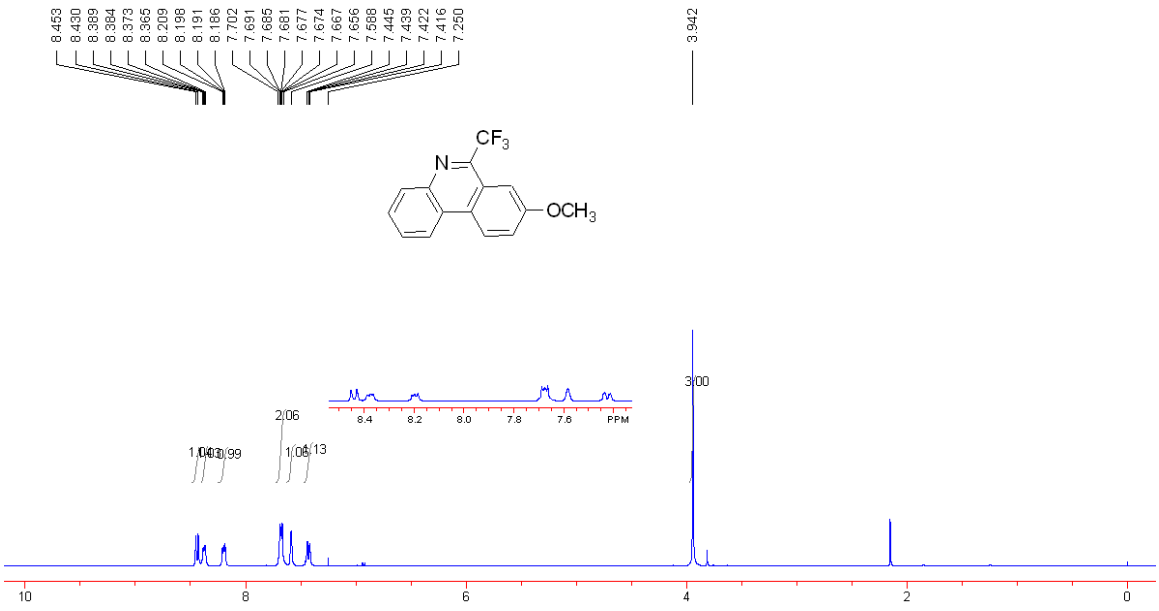
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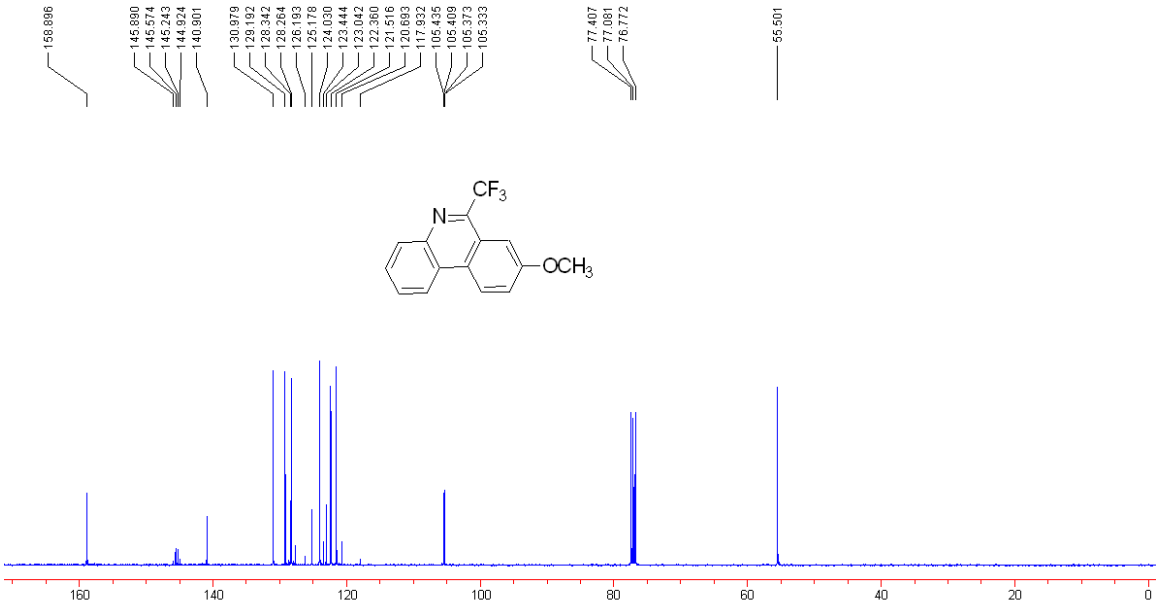
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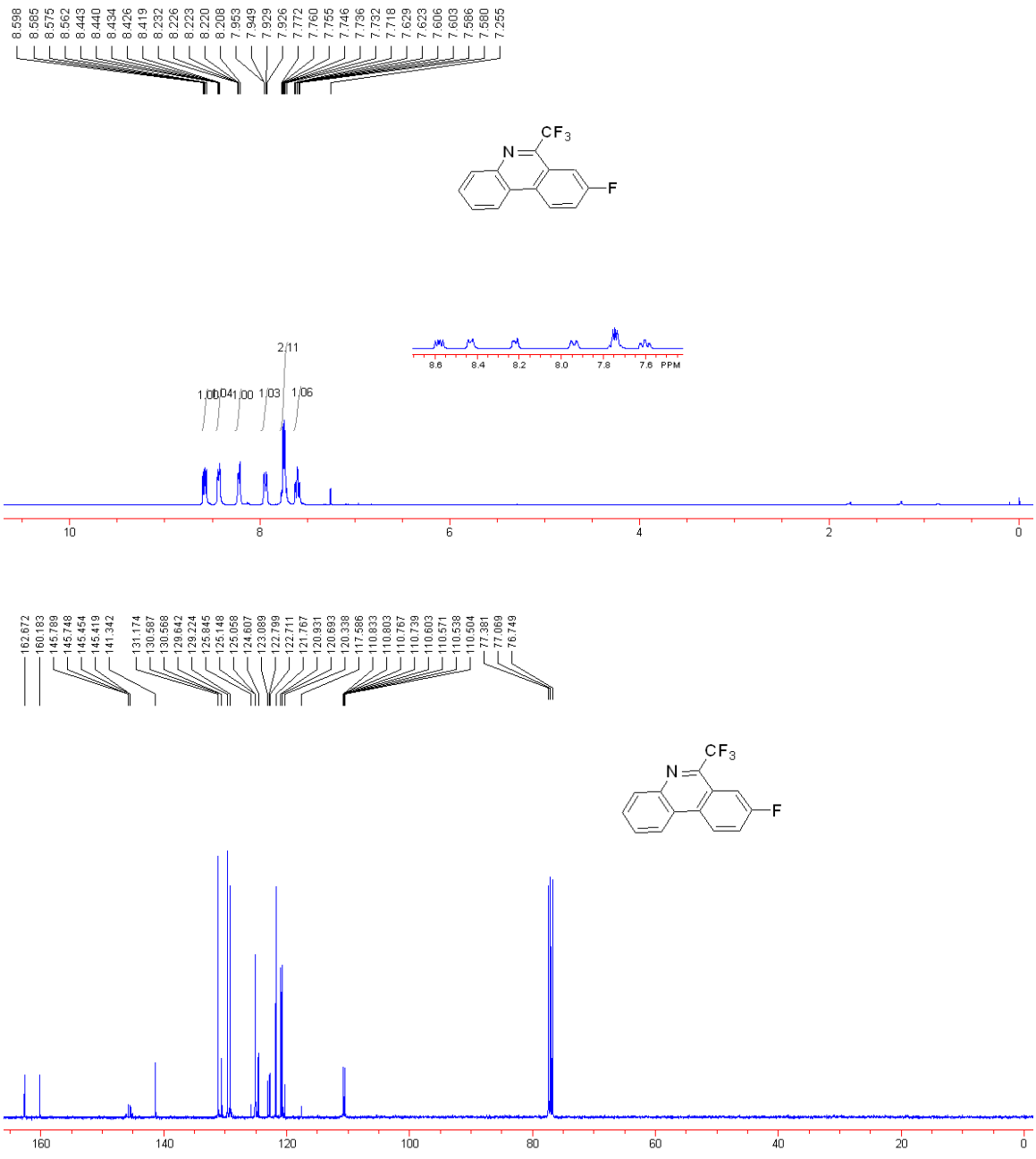
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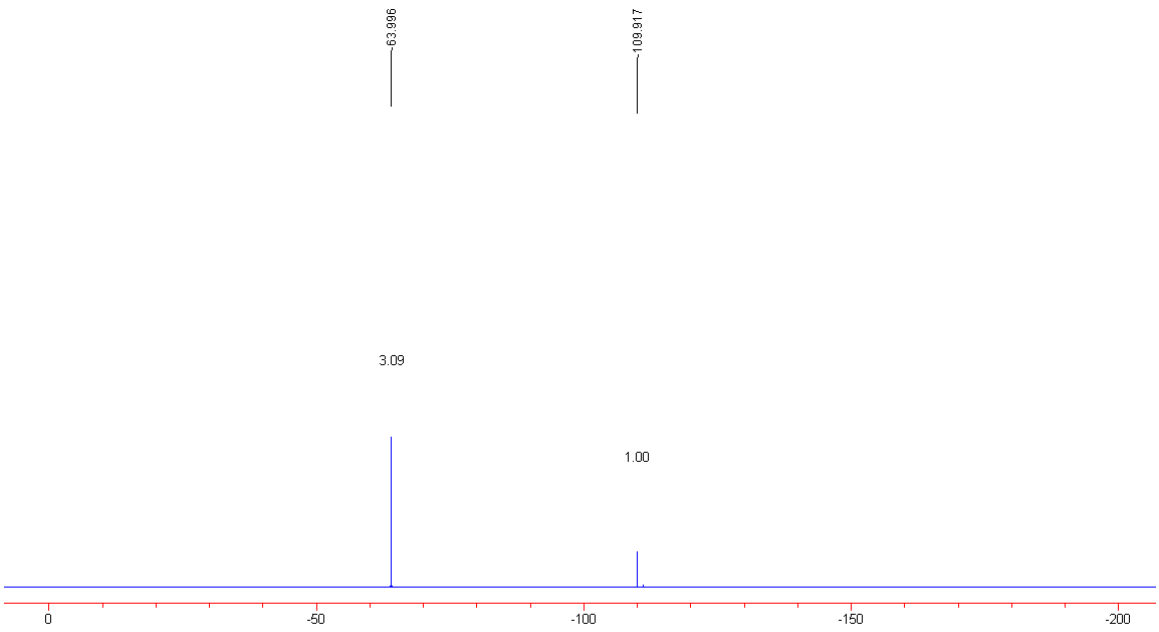
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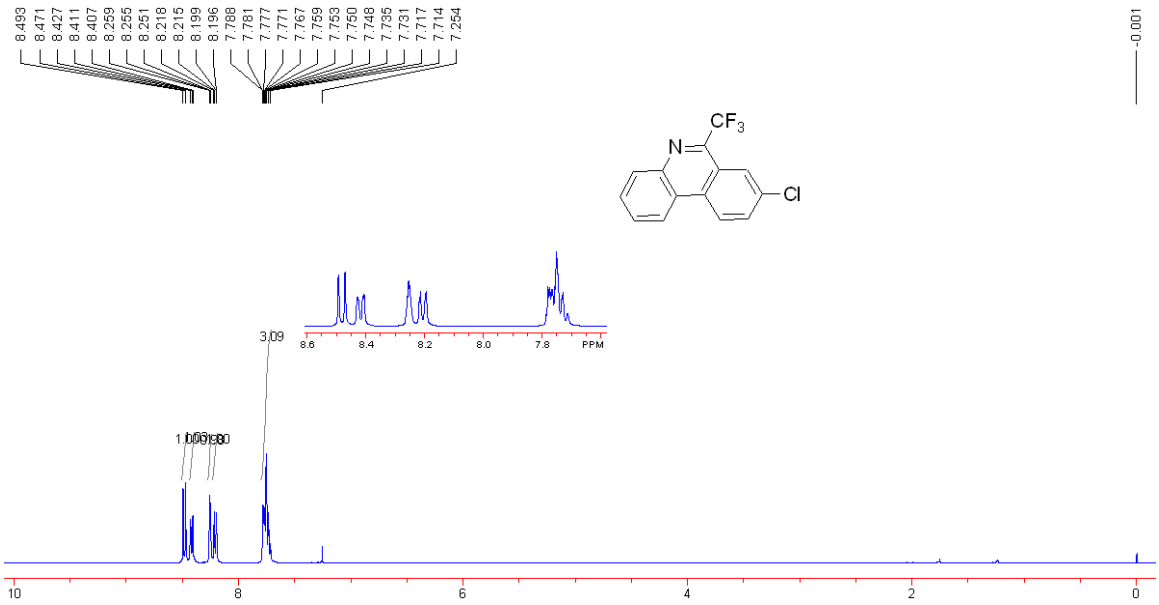
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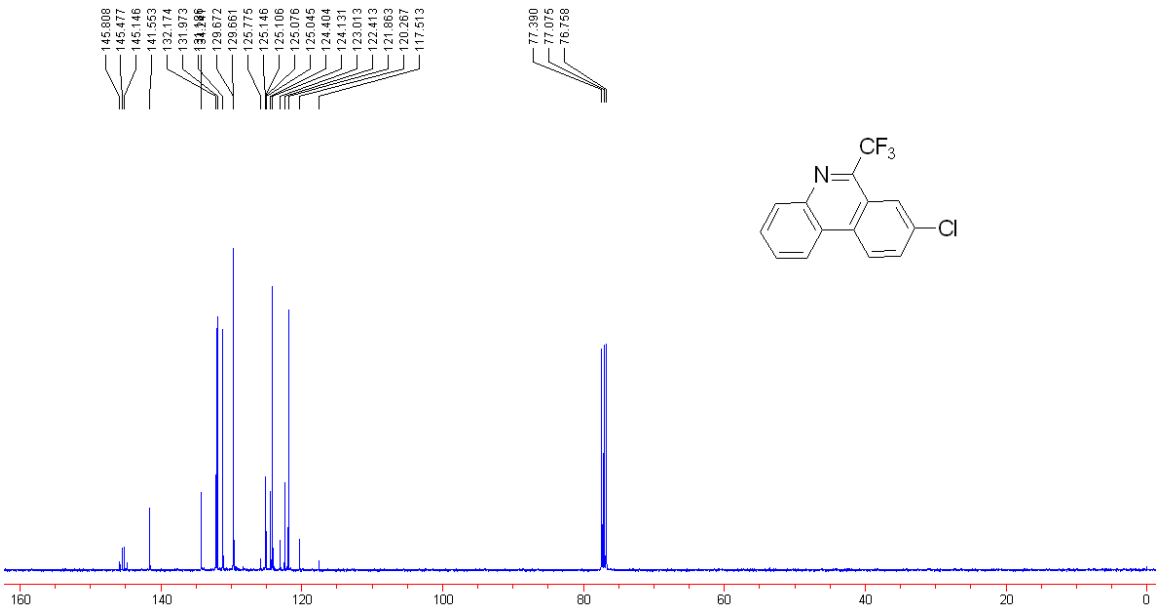
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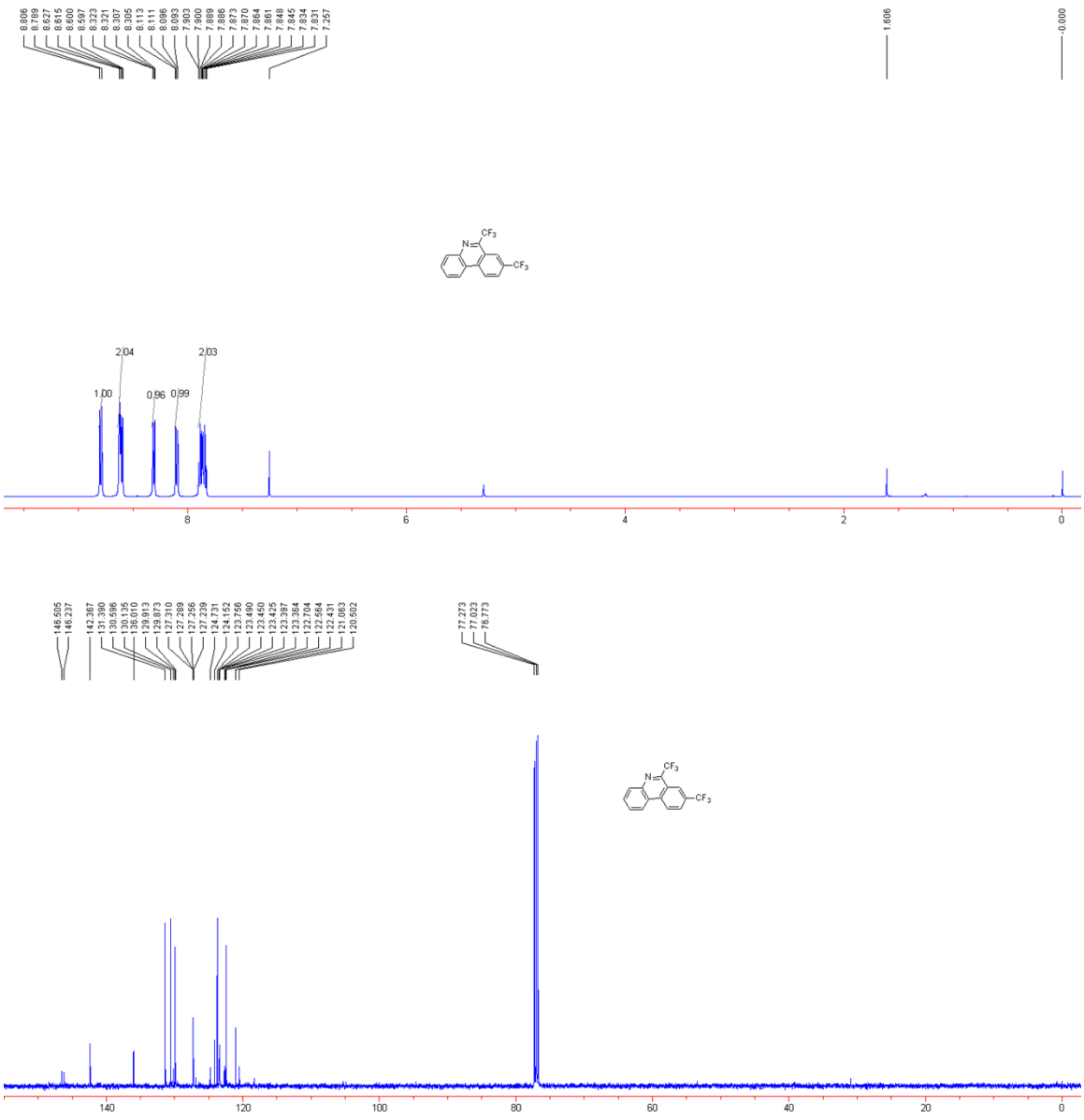
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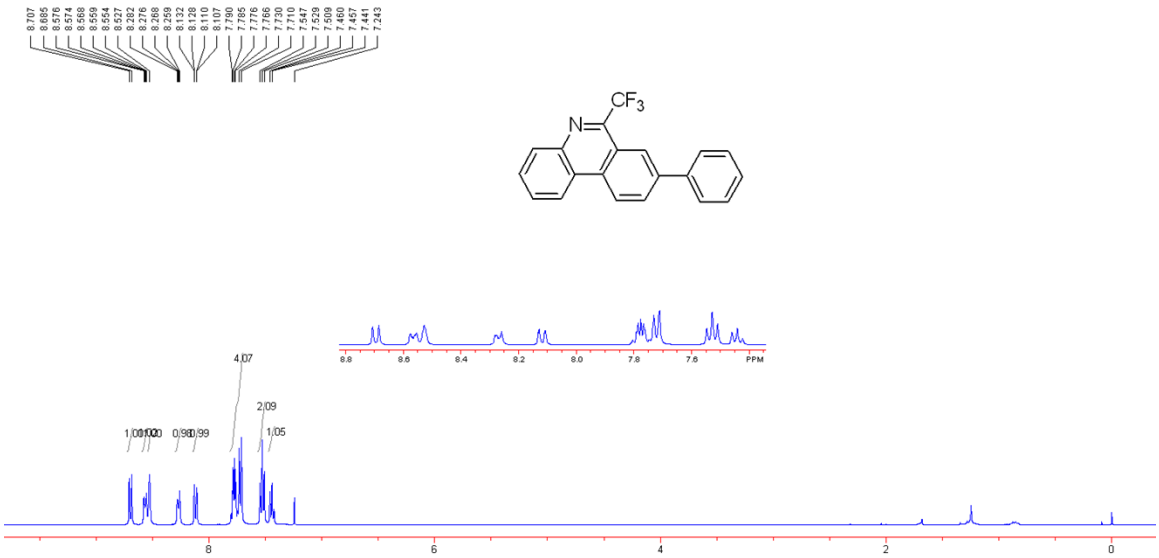
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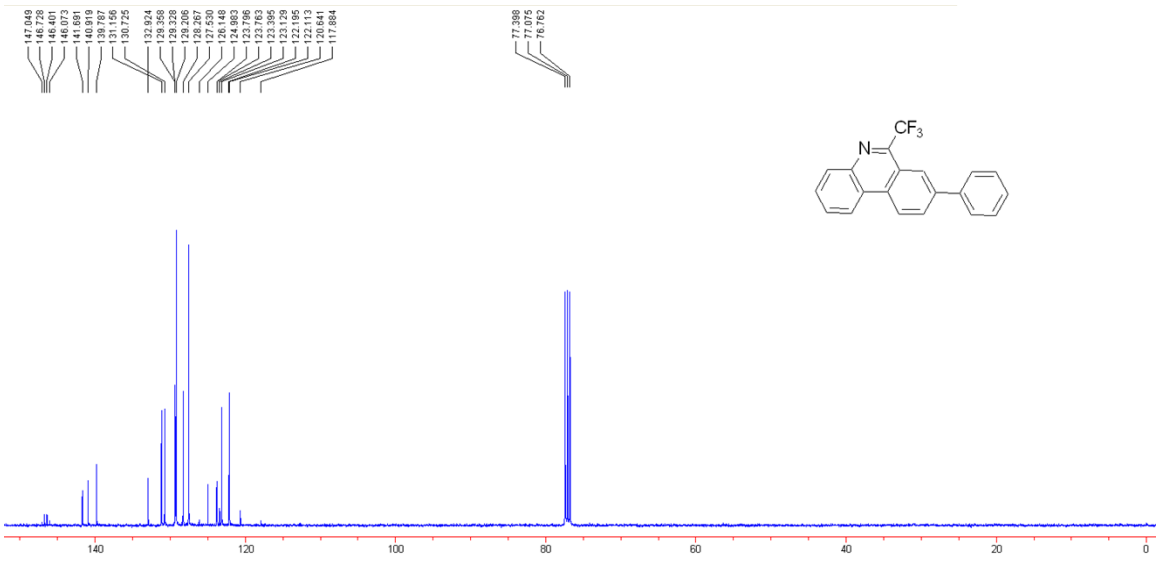
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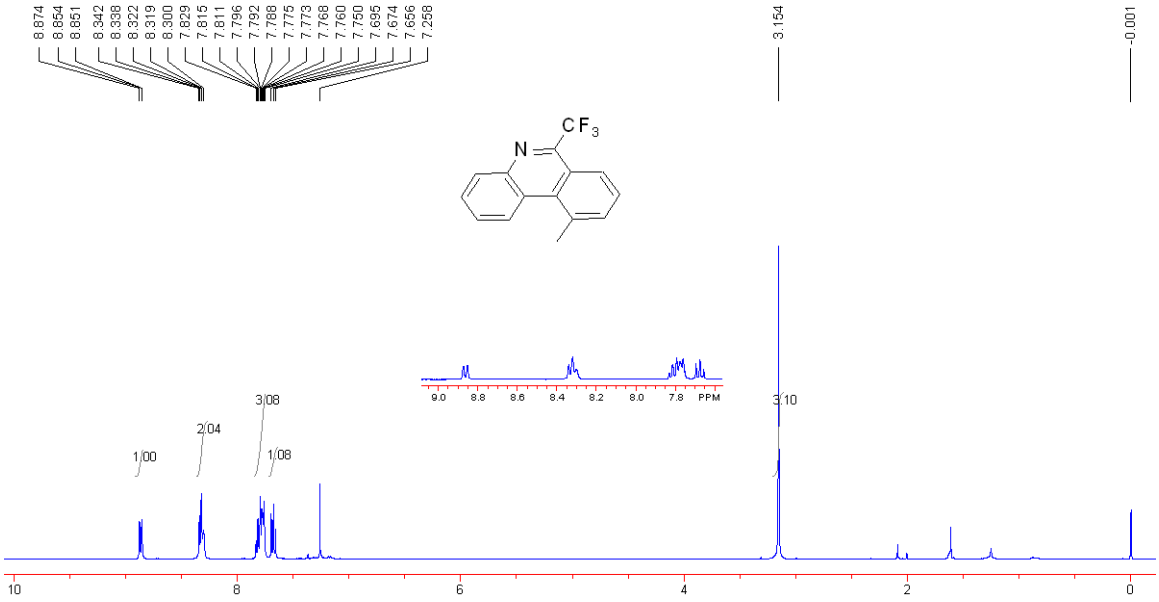
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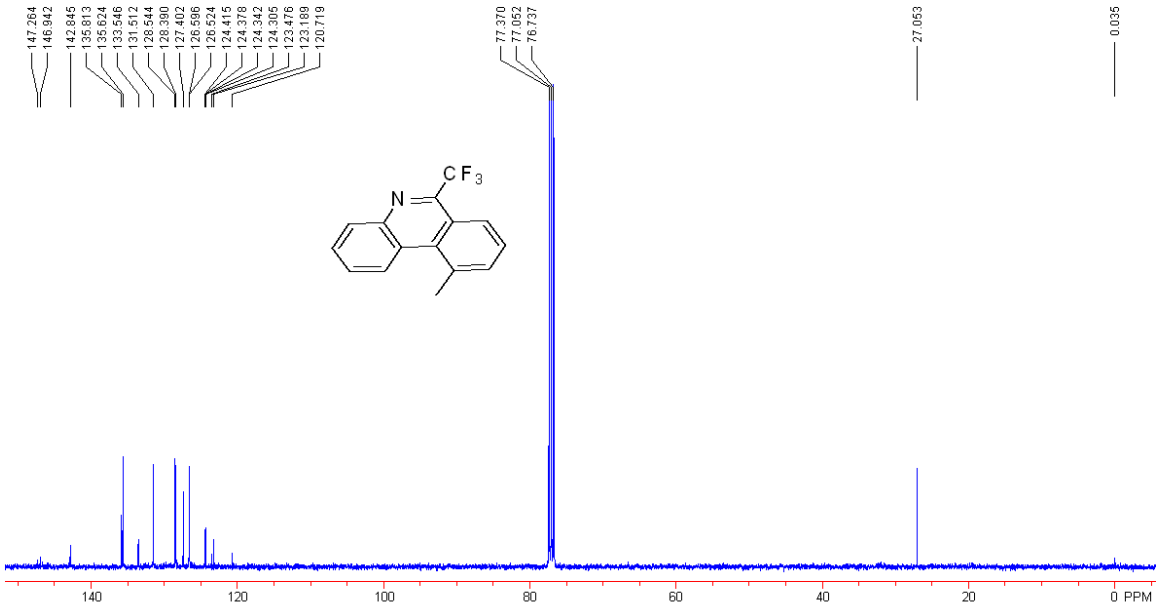
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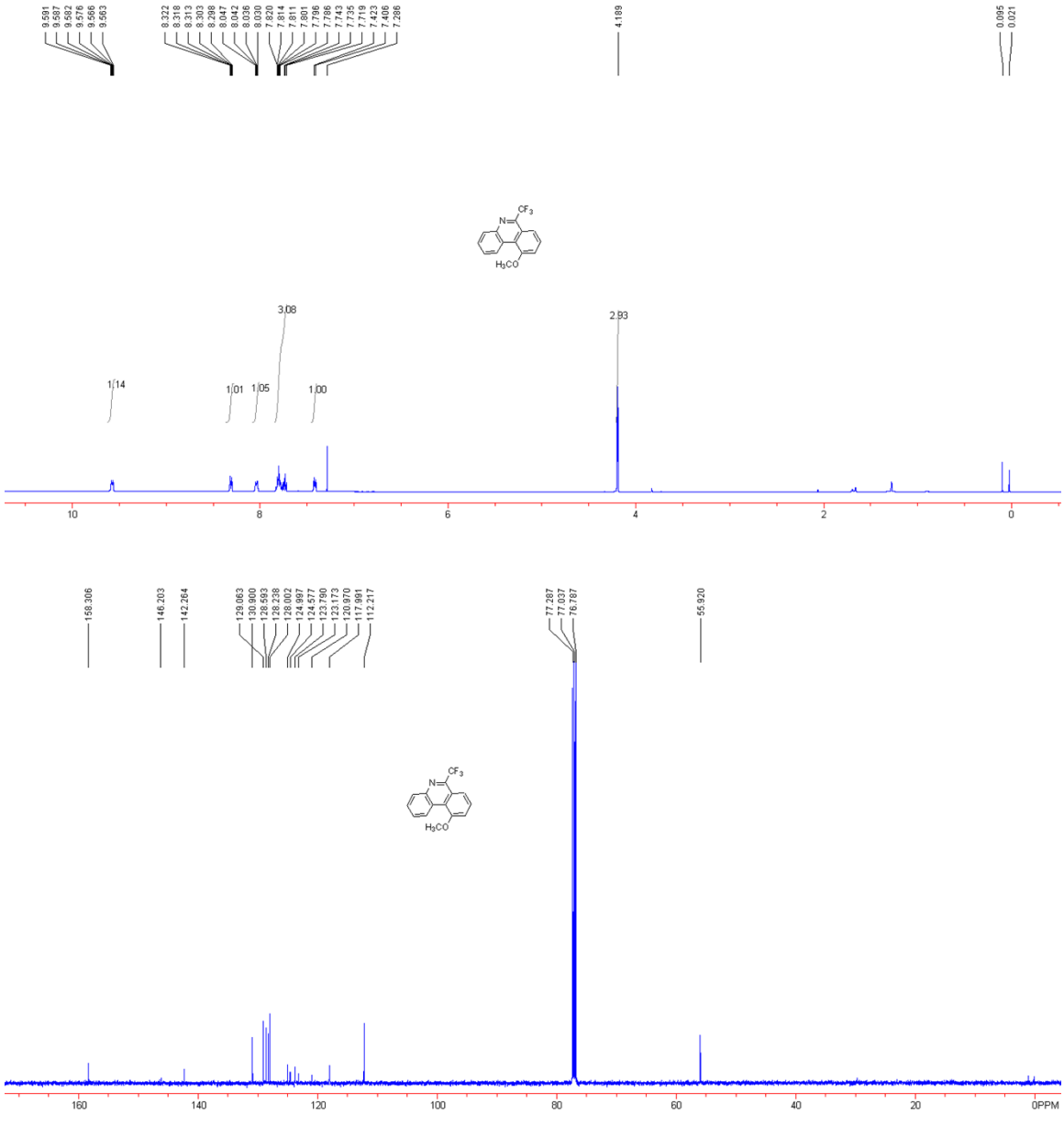
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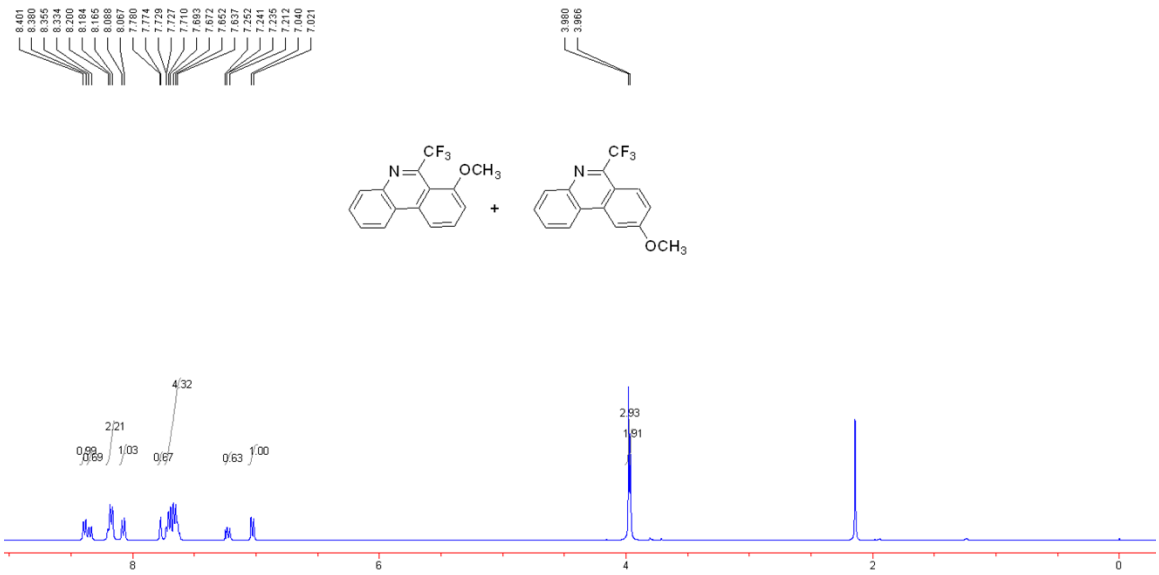
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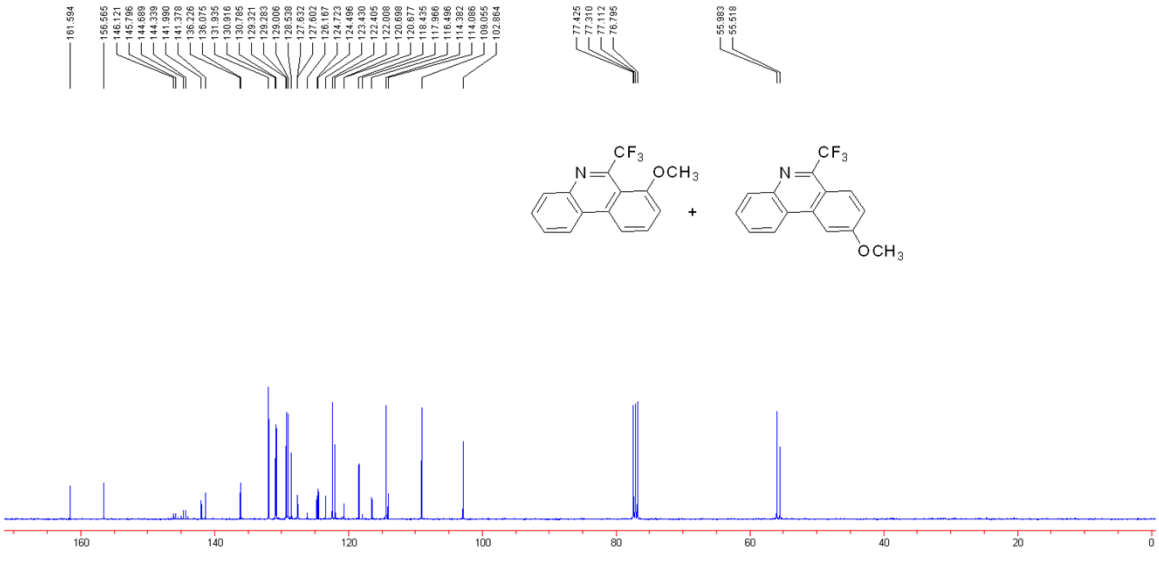
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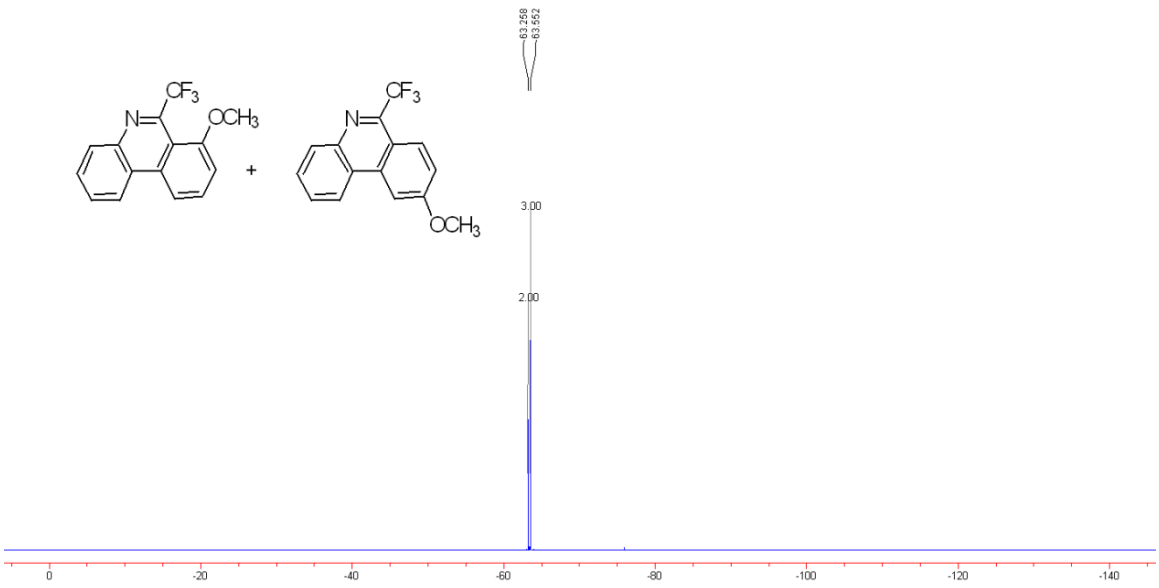
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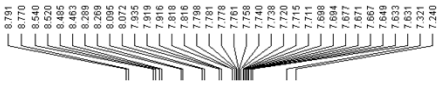
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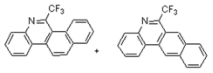
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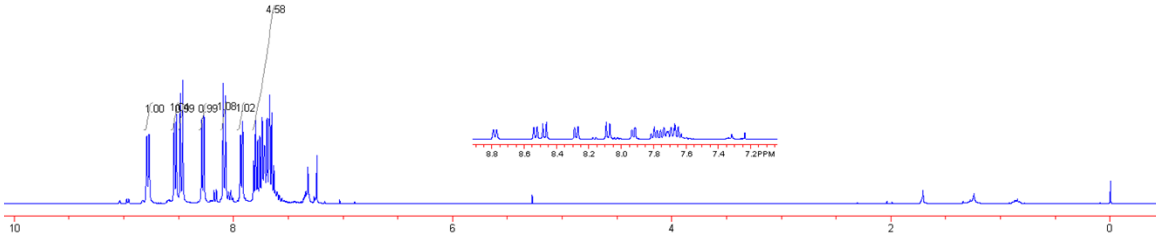
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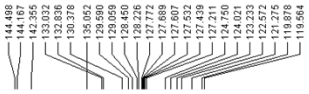
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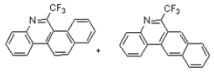
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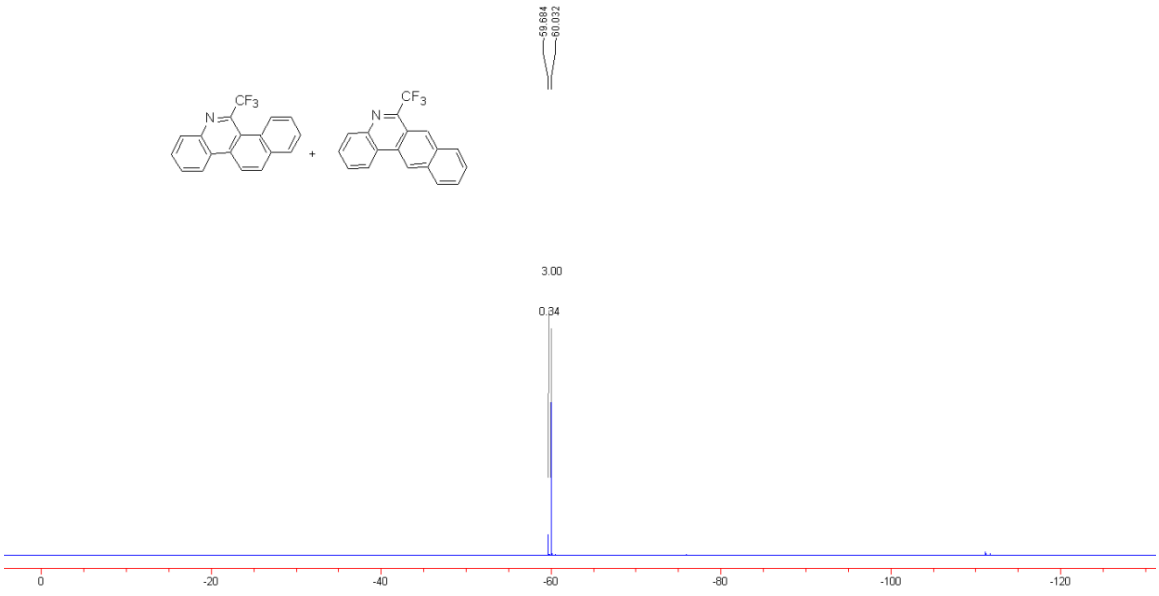
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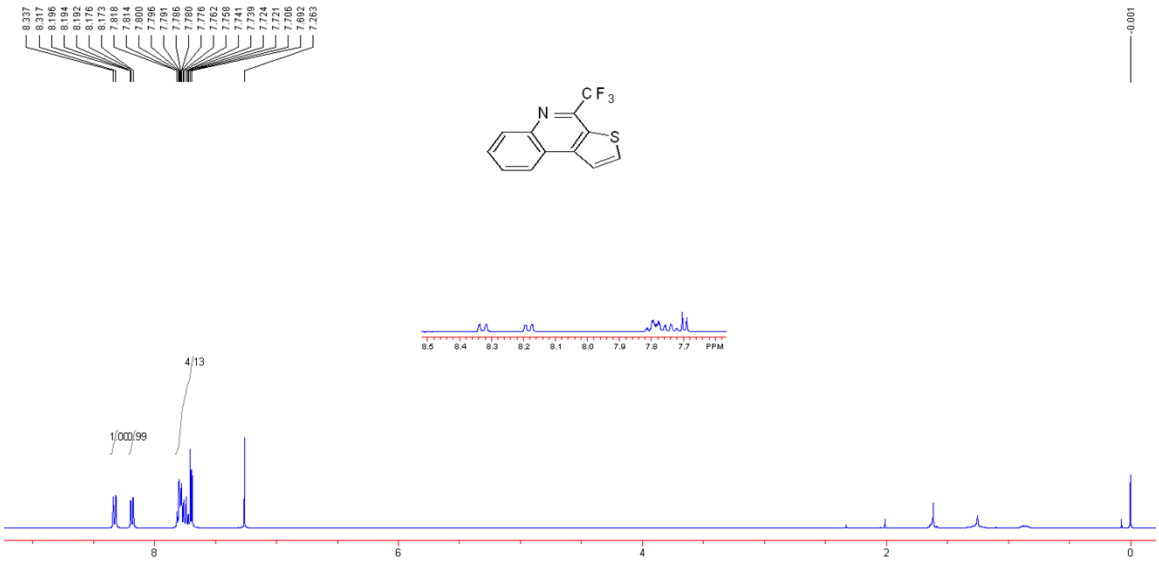
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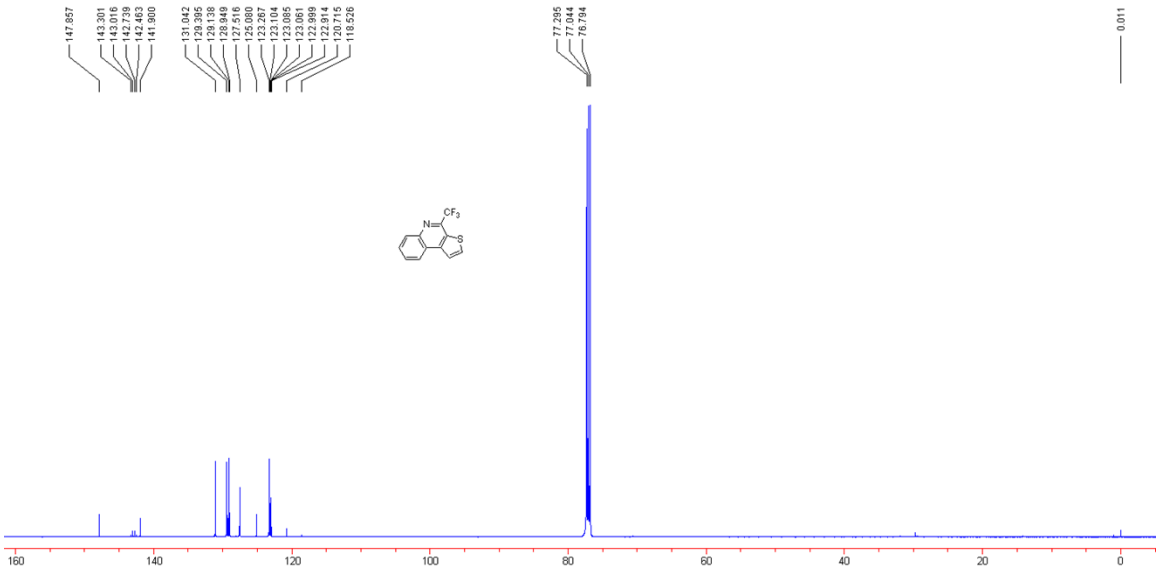
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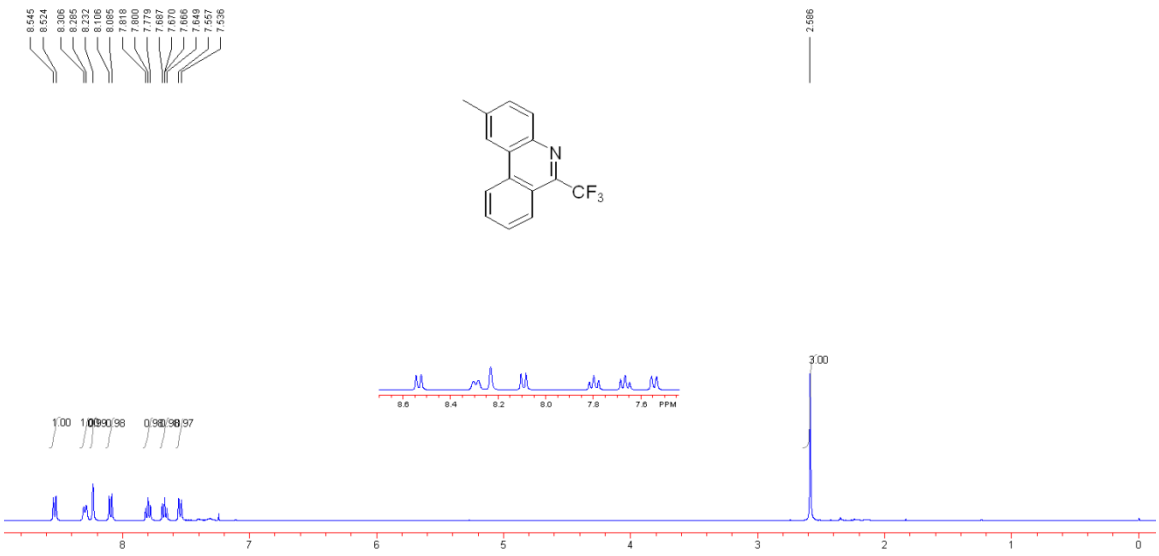
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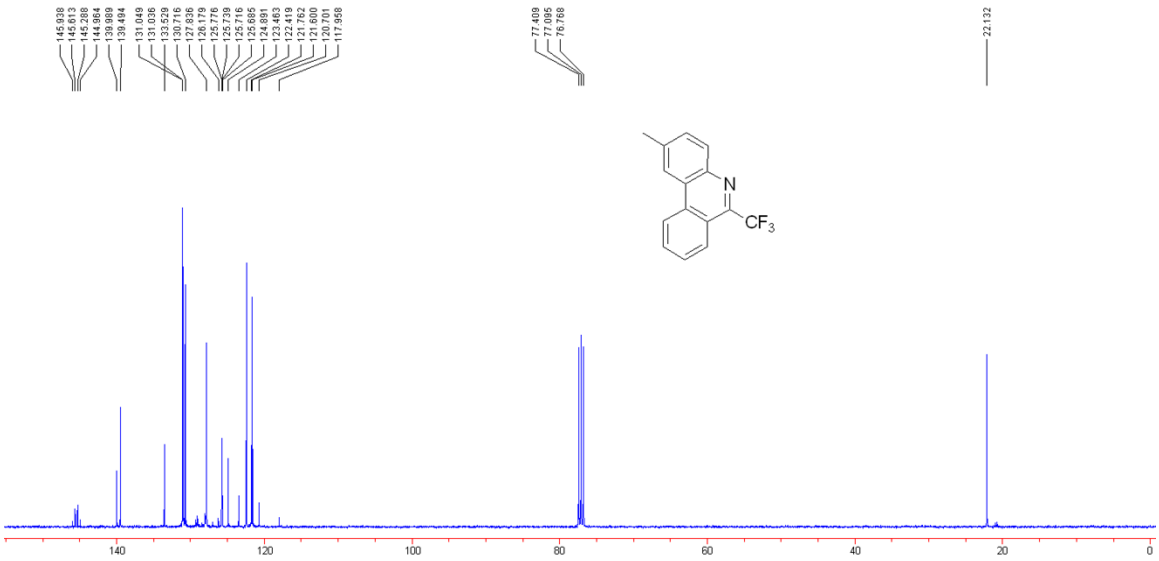
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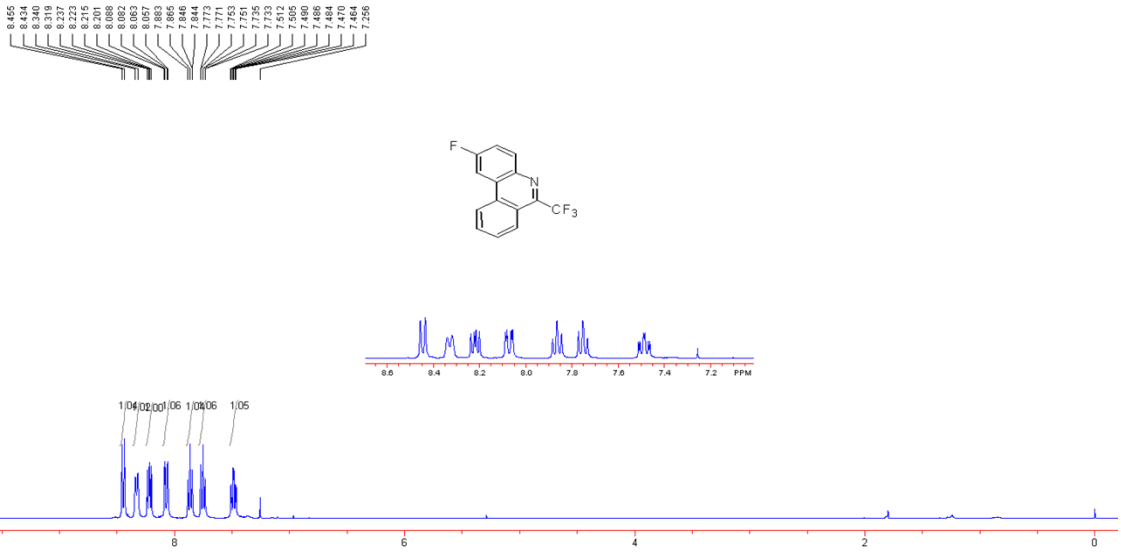
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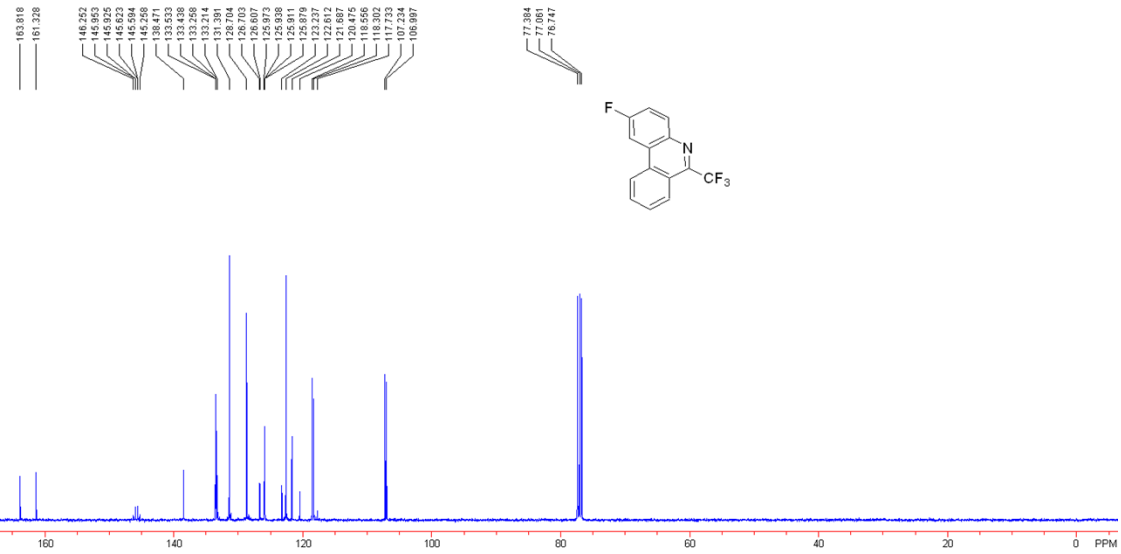
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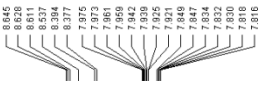
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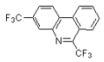
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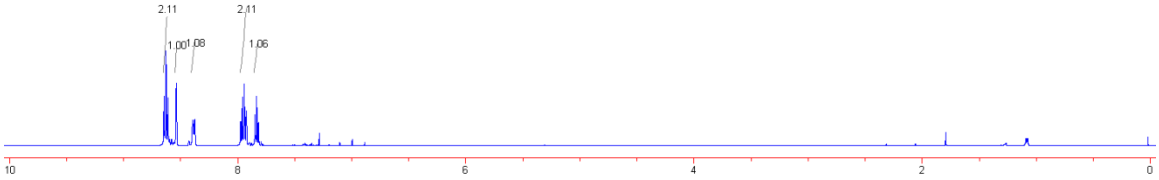
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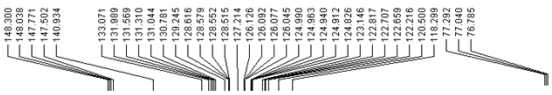
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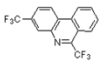
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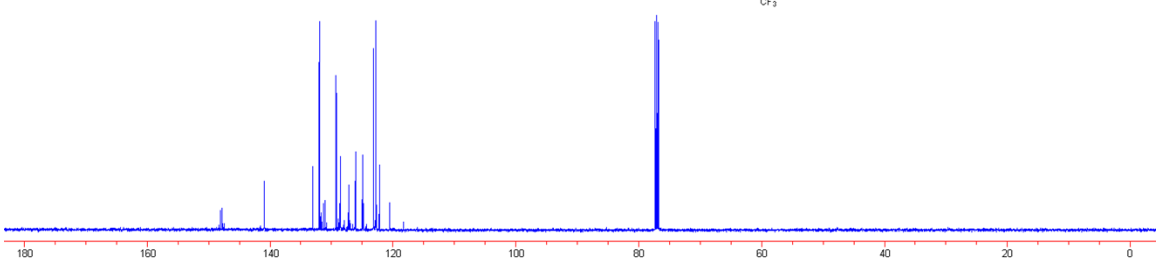
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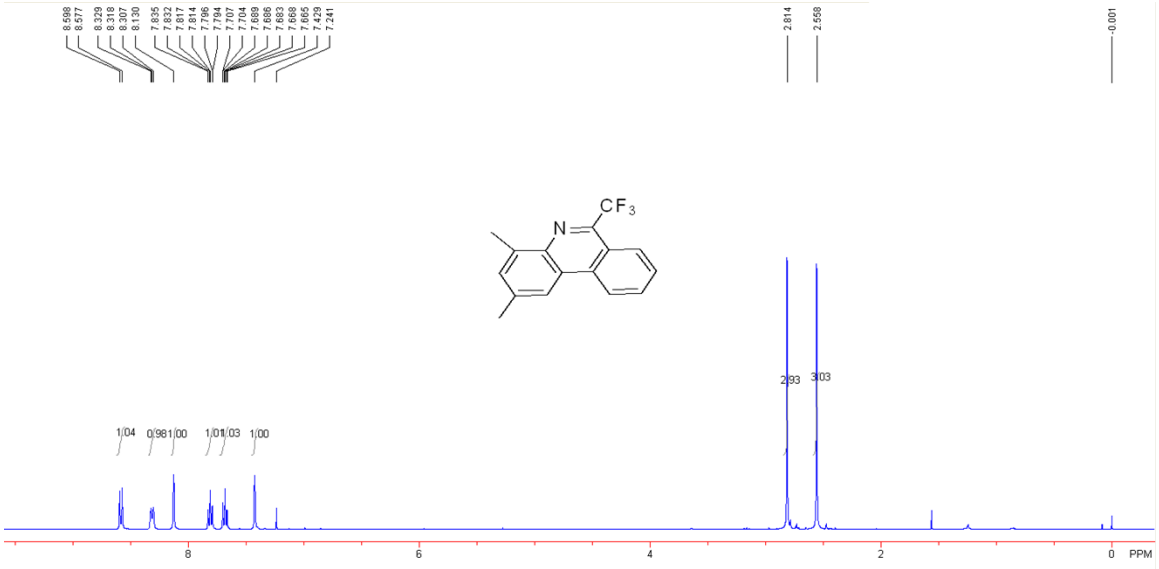
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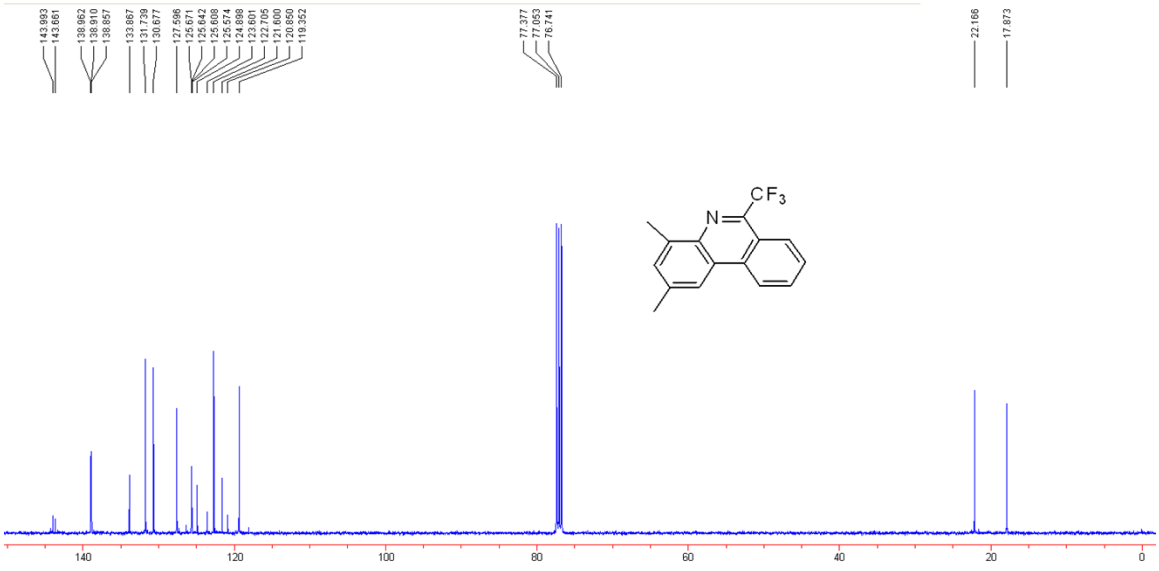
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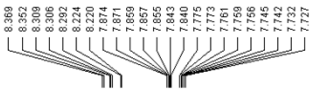
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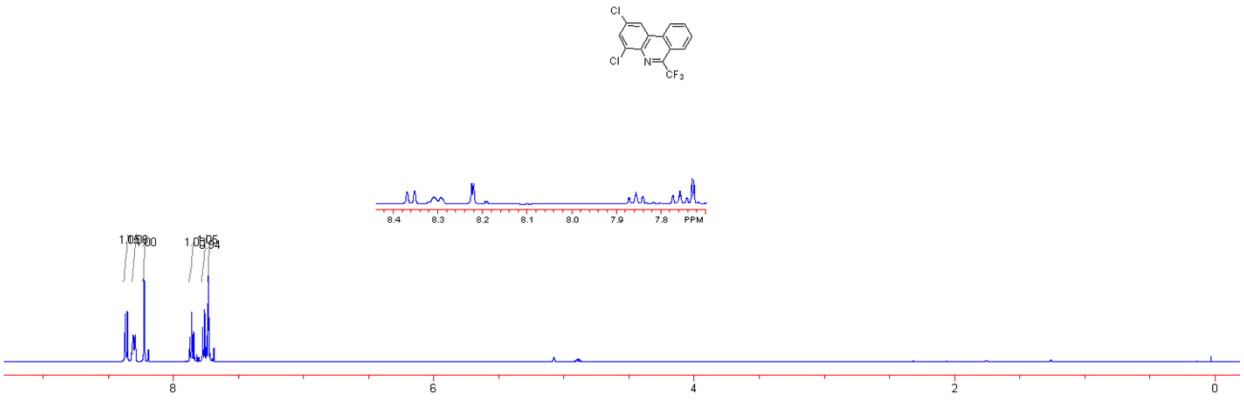
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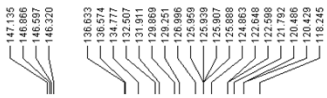
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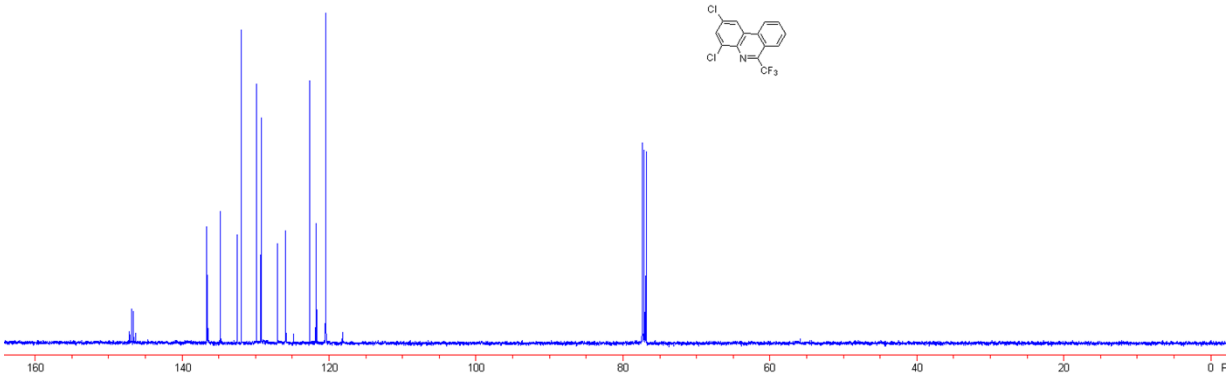
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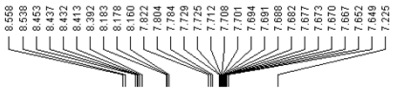
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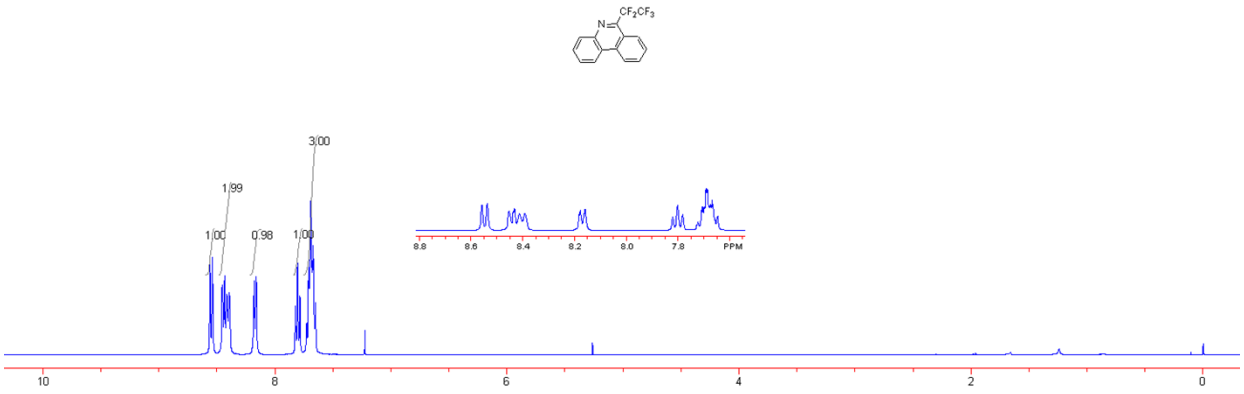
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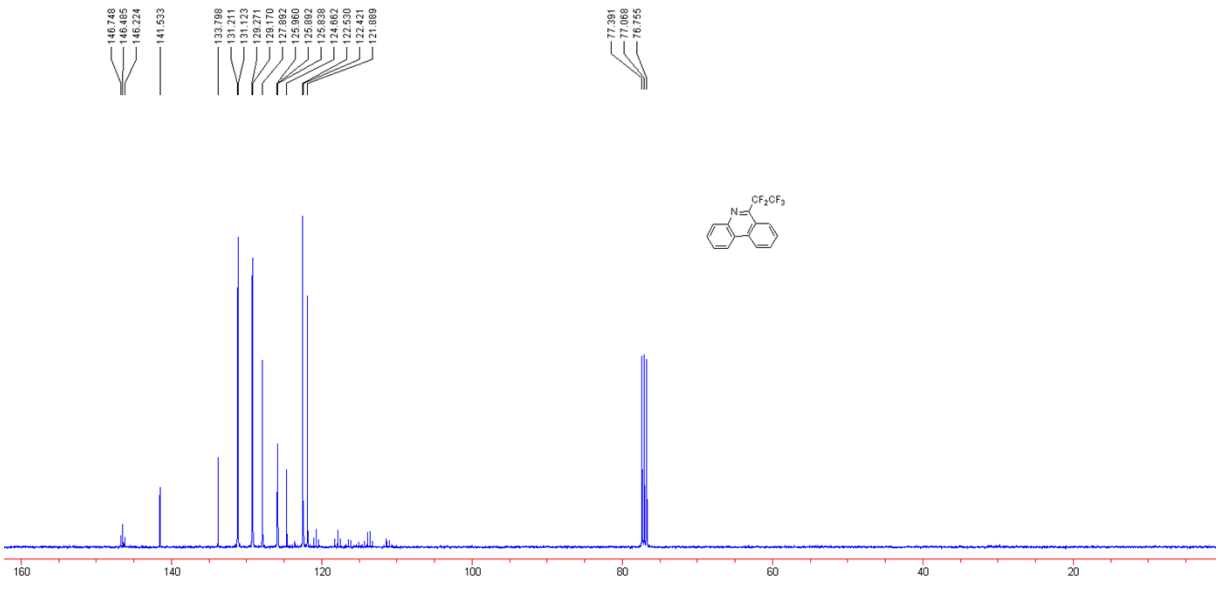
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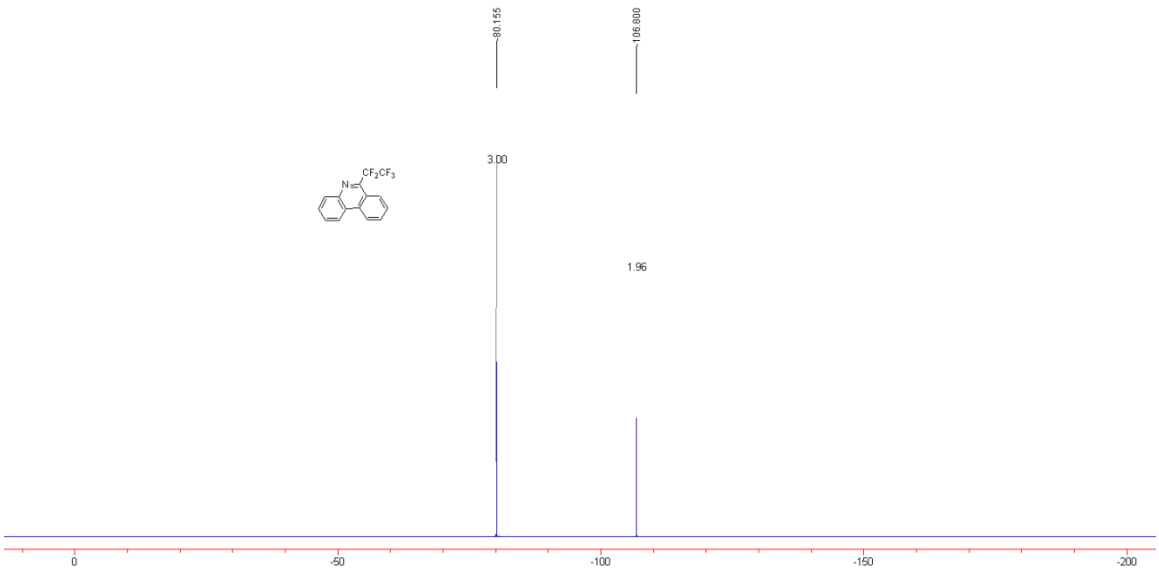
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