Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Dibenzofuran and Dibenzothiophene based Palladium(II)/NHC Catalysts - Synthesis and Applications in C-C bond formation

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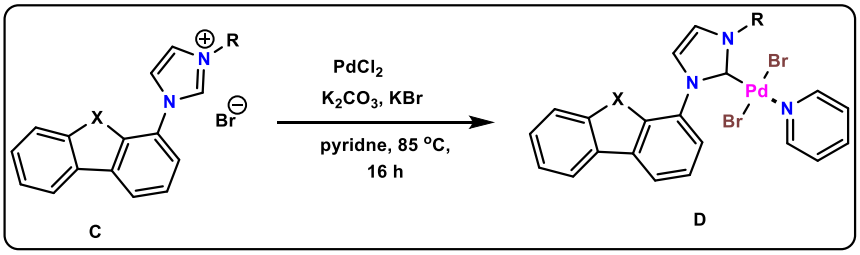
1. General experimental methods and materials

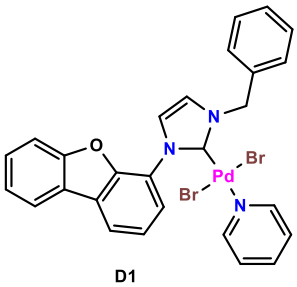
Unless otherwise mentioned all the reactions were carried out in screw capped reaction tubes under an inert atmosphere of nitrogen. Anhydrous acetonitrile, DMSO, Dioxane, Pyridine purchased from commercial sources and used without further purification. Chemicals were purchased from Sigma-Aldrich, Alfa Aesar, AVRA. Thin layer chromatography was carried on 250 mm diameter aluminium supported silica gel TLC plates (MERCK TLC Plates). ^{1}H NMR spectra were recorded on Bruker spectrometer (400 MHz) and reported in units *ppm* (parts per million) relative to the signals for residual chloroform (7.26 *ppm*) and DMSO (2.54 *ppm*) in the deuterated solvent. ^{13}C NMR spectra were recorded on Bruker spectrometer (100 MHz) and are reported in *ppm* relative to deuterated chloroform (77.23 *ppm*) and DMSO (39.52 *ppm*) with tetramethyl silane as an internal standard. Coupling constants (*J*) are reported in Hz; splitting patterns are assigned *s* = singlet, *d* = doublet, *t* = triplet, *q* = quartet, *dd* = doublet of doublets, *br* = broad signal. High-resolution mass spectra (HRMS) were performed on MS-EI analyser.

X-ray crystallography of D4

Single crystal X-ray structural data of the compounds **D4** were collected on a CMOS based Bruker D8 Venture PHOTON 100 diffractometer equipped with a INCOATEC micro-focus source with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) operating at 50 kV and 30 mA. The SAINT[1] program was used for the integration of diffraction profiles and absorption correction was applied with the SADABS[2] Program. Both the structures were initially solved by SIR 92[3] and refined by the full matrix least squares method using SHELXL-2013[4] and WinGX system, Ver 2013.3.[5] The non-hydrogen atoms in both the structures were located using the difference Fourier map and refined anisotropically. The hydrogen atoms were fixed by HFIX and placed in ideal positions and included in the refinement process using a riding model with isotropic thermal parameters. crystallographic and structure refinement data of **D4** are summarized in Table S4. The crystallographic information files are deposited with the **CCDC 1845489.**

2. Synthesised Palladium-NHC Catalysts D1-D6

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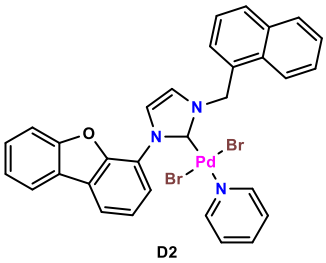
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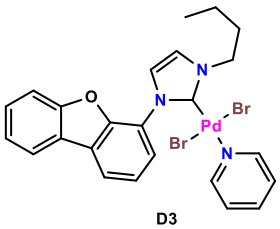
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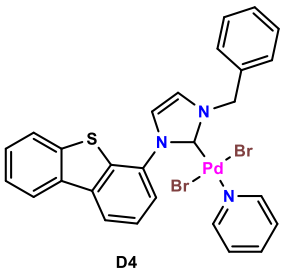
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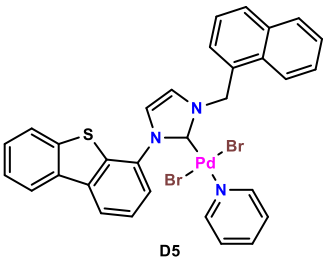
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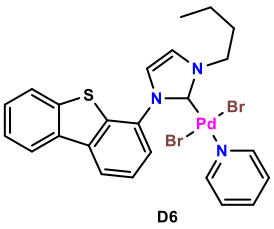
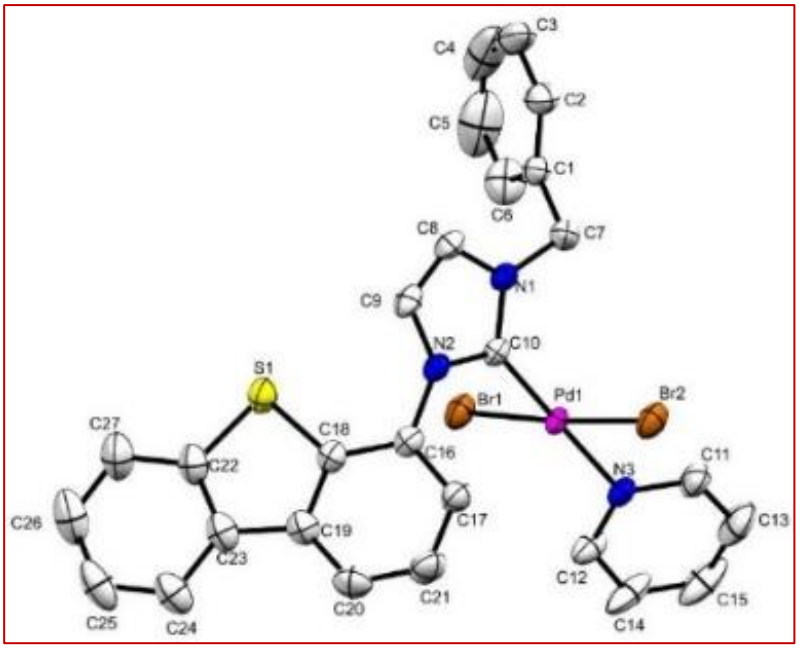

D6

3. Crystallographic data of D4



Bond distance

Atom	Atom	Distance (Å)	Atom	Atom	Distance (Å)
Pd1	Br1	**2.418(9)**	C17	C21	**1.390(5)**
Pd1	Br2	**2.421(9)**	C8	C9	**1.321(5)**
Pd1	N3	**2.105(3)**	C22	C23	**1.390(6)**
Pd1	C10	**1.957(4)**	C22	C27	**1.388(8)**
S1	C18	**1.741(4)**	C21	C20	**1.362(7)**
S1	C22	**1.745(5)**	C23	C24	**1.396(6)**
N2	C16	**1.432(4)**	C24	C25	**1.380(1)**
N2	C10	**1.360(5)**	C25	C26	**1.378(9)**
N2	C9	**1.391(4)**	C26	C27	**1.368(8)**
C15	C13	**1.370(1)**	C2	C3	**1.388(7)**
C15	C14	**1.347(9)**	C6	C5	**1.350(1)**
N1	C10	**1.337(4)**	C3	C4	**1.370(2)**
N1	C8	**1.387(5)**	C4	C5	**1.330(1)**

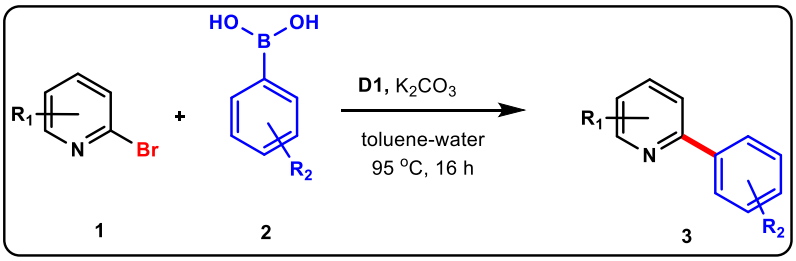
N1	C7	**1.469(5)**	C19	C20	**1.390(6)**
N3	C12	**1.328(5)**	C19	C23	**1.455(7)**
N3	C11	**1.333(5)**	C16	C17	**1.370(5)**
C18	C19	**1.402(5)**	C13	C11	**1.378(7)**
C18	C16	**1.399(5)**	C14	C12	**1.372(7)**
C1	C7	**1.490(5)**	C1	C2	**1.365(5)**

Bond angles

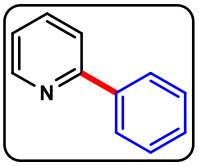
Atom 1	Atom 2	Atom 3	Angle[°]	Atom 1	Atom 2	Atom 3	Angle[°]
Br1	Pd1	Br2	**175.8(2)**	N2	C16	C18	**119.7(3)**
Br1	Pd1	N3	**91.1(8)**	N2	C16	C17	**120.7(3)**
Br1	Pd1	C10	**87.5(1)**	C18	C16	C17	**119.5(3)**
Br2	Pd1	N3	**92.2(8)**	C15	C13	C11	**119.1(6)**
Br2	Pd1	C10	**89.0(1)**	C15	C14	C12	**119.0(5)**
N3	Pd1	C10	**177.7(1)**	C16	C17	C21	**120.1(4)**
C18	S1	C22	**90.8(2)**	Pd1	C10	N2	**128.7(3)**
C16	N2	C10	**125.3(3)**	Pd1	C10	N1	**126.1(3)**
C16	N2	C9	**125.0(3)**	N2	C10	N1	**105.1(3)**
C10	N2	C9	**109.7(3)**	N1	C8	C9	**107.0(3)**
C13	C15	C14	**119.4(6)**	S1	C22	C23	**112.9(3)**
C10	N1	C8	**110.9(3)**	S1	C22	C27	**125.9(4)**
C10	N1	C7	**124.2(3)**	C23	C22	C27	**121.2(5)**
C8	N1	C7	**124.9(3)**	N2	C9	C8	**107.4(3)**
Pd1	N3	C12	**120.6(3)**	N3	C12	C14	**122.7(4)**
Pd1	N3	C11	**121.2(3)**	C17	C21	C20	**120.8(4)**
C12	N3	C11	**118.2(3)**	N1	C7	C1	**112.8(3)**

S1	C18	C19	**113.1(3)**	C19	C20	C21	**120.6(4)**
S1	C18	C16	**126.7(3)**	C19	C23	C22	**112.1(4)**
C19	C18	C16	**120.2(3)**	C19	C23	C24	**128.8(4)**
C7	C1	C2	**120.8(4)**	C22	C23	C24	**119.1(4)**
C7	C1	C6	**120.5(4)**	C23	C24	C25	**119.2(5)**
C2	C1	C6	**118.7(4)**	N3	C11	C13	**121.6(4)**
C18	C19	C20	**118.7(4)**	C24	C25	C26	**120.8(6)**
C18	C19	C23	**111.1(4)**	C25	C26	C27	**121.0(6)**
C20	C19	C23	**130.2(4)**	C22	C27	C26	**118.7(6)**
C1	C2	C3	**120.0(5)**	C1	C6	C5	**121.0(7)**
C2	C3	C4	**118.8(7)**	C3	C4	C5	**120.7(9)**
C6	C5	C4	**120.6(9)**				

4. General procedure for Suzuki-Miyaura coupling using D1



An oven-dried vial equipped with a stir bar was charged with 2-bromo pyridine (0.31 mmol) and the corresponding phenyl boronic acid (0.47 mmol), potassium carbonate (0.63 mmol), **D1** (5 mol%), followed by toluene-water (4:1 mL). Then the reaction mixture was placed in a preheated oil bath at 95 °C and stirred for 16 h. After the indicated time, the reaction mixture was diluted with water (5 mL), extracted with ethyl acetate (5 mL x 2) and concentrated. The crude material was purified by column chromatography on silica gel with n-hexane - ethyl acetate as eluent, to yield the title compound.

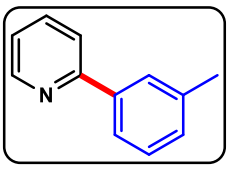


2-phenylpyridine-**3a**, colorless oil, 41 mg, 85% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.8 Hz, 1H), 7.82 (d, *J* = 7.6 Hz, 2H), 7.61-7.55 (m, 2H), 7.33-7.23 (m, 3H), 7.09-7.05 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.76, 144.94, 134.67, 132.01, 124.21, 124.01, 122.18, 117.36, 115.85.

Spectral data match those previously reported.[6]

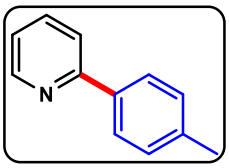


2-(*m*-tolyl)pyridine, **3b**, colorless oil, 43 mg, 81% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.4 Hz, 1H), 7.76 (s, 1H), 7.68-7.63 (m, 3H), 7.29 (t, *J* = 7.6 Hz, 1H), 7.16-7.12 (m, 2H), 2.36 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.67, 149.61, 139.38, 138.42, 136.70, 129.72, 128.64, 127.66, 124.01, 122.01, 120.65, 21.52.

Spectral data match those previously reported.[7]

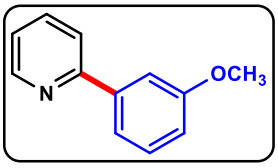


2-(*p*-tolyl)pyridine, **3c**, colorless oil, 45 mg, 86% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.4 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 2H), 7.67-7.61 (m, 2H), 7.21-7.10 (m, 3H), 2.33 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.49, 149.60, 138.95, 136.69, 129.49, 126.78, 121.81, 120.28, 21.28.

Spectral data match those previously reported.[8]

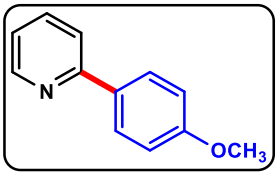


2-(3-methoxyphenyl)pyridine, **3d**, colorless oil, 50 mg, 86% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.8 Hz, 1H), 7.70-7.63 (m, 2H), 7.51-7.45 (m, 2H), 7.31 (t, *J* = 8.0 Hz, 1H), 7.18-7.14 (m, 1H), 6.90 (d, *J* =8.0 Hz, 1H), 3.82 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.05, 156.24, 148.56, 139.85, 135.73, 128.69, 121.22, 119.71, 118.29, 114.08, 110.98, 54.35.

Spectral data match those previously reported.[8]

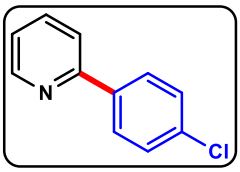


2-(4-methoxyphenyl)pyridine, **3e**, off-white solid, 51 mg, 88% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.8 Hz, 1H), 7.87 (d, *J* = 8.8 Hz, 2H), 7.65-7.57 (m, 2H), 7.11-7.07 (m, 1H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.46, 157.14, 149.55, 136.67, 132.04, 128.17, 121.41, 119.82, 114.13, 55.36.

Spectral data match those previously reported.[8]

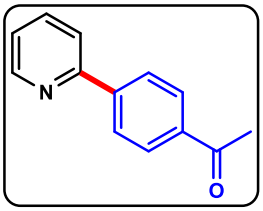


2-(4-chlorophenyl)pyridine, **3f**, off-white solid, 39 mg, 66% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.4 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 2H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.16-7.15 (m, 1H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 156.24, 149.76, 137.82, 136.88, 135.11, 128.94, 128.18, 122.38, 120.35.

Spectral data match those previously reported.[9]

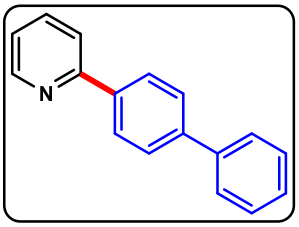


1-(4-(pyridin-2-yl)phenyl)ethan-1-one, **3g**, off-white solid, 37 mg, 60% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 2H), 7.99 (d, *J* = 9.6 Hz, 2H), 7.73-7.71 (m, 2H), 7.24-7.20 (m, 1H), 2.58 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.87, 156.11, 149.94, 143.61, 136.95, 128.83, 127.05, 122.94, 121.05, 26.77.

Spectral data match those previously reported.[10]

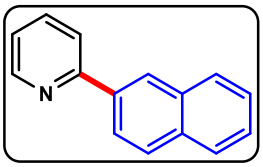


2-([1,1'-biphenyl]-4-yl)pyridine, **3h**, colorless oil, 51 mg, 71% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.4 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 2H), 7.80-7.68 (m, 6H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 6.8 Hz, 1H), 7.27-7.25 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.06, 149.75, 141.72, 140.60, 138.29, 136.77, 128.84, 127.48, 127.30, 127.12, 122.13, 120.46.

Spectral data match those previously reported.[11]

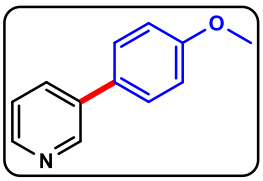


2-(naphthalen-2-yl)pyridine, **3i**, grey solid, 44 mg, 69% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.8 Hz, 1H), 8.51 (s, 1H), 8.18-8.16 (m, 1H), 7.98-7.89 (m, 4H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.55-7.52 (m, 2H), 7.29-7.26 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.35, 149.80, 136.84, 136.69, 133.69, 133.54, 128.75, 128.48, 127.69, 126.55, 126.35, 126.32, 124.58, 122.18, 120.85.

Spectral data match those previously reported.[12]

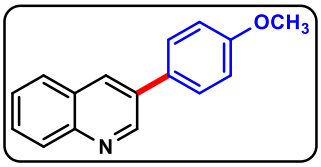


3-(4-methoxyphenyl)pyridine, **3j**, colorless oil, 36 mg, 63% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 2.0 Hz, 1H), 8.46 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.76-7.73 (m, 1H), 7.43 (d, *J* = 8.8 Hz, 2H), 7.26-7.23 (m, 1H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.77 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.78, 147.96, 147.84, 136.27, 133.87, 128.22, 123.50, 114.57, 55.38.

Spectral data match those previously reported.[13]

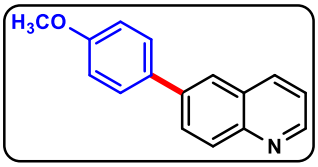


3-(4-methoxyphenyl)quinoline, **3k**, off-white solid, 40 mg, 55% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (d, *J* = 2.4 Hz, 1H), 8.15 (d, *J* = 2.0 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.63-7.56 (m, 3H), 7.47 (t, *J* = 7.2 Hz, 1H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.81, 149.86, 147.02, 133.49, 132.39, 130.29, 129.19, 129.08, 128.52, 128.13, 127.88, 126.95, 114.68, 55.42.

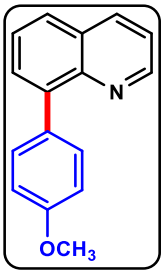
Spectral data match those previously reported.[14]



6-(4-((λ^1-oxidanyl)-λ^5-methyl)phenyl)quinoline **3l**, grey solid, 51 mg, 70% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (dd, *J* = 4.0, 1.6 Hz, 1H), 8.12-8.06 (m, 2H), 7.89-7.87 (m, 2H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.35-7.32 (m, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 159.55, 150.08, 147.41, 138.94, 136.14, 132.78, 129.78, 129.09, 128.51, 124.65, 121.44, 114.44, 55.44.

Spectral data match those previously reported.[8]

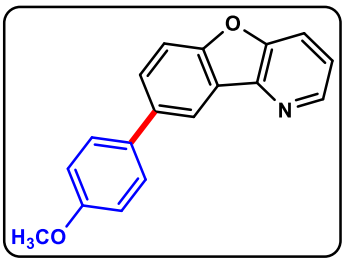


8-(4-methoxyphenyl)quinoline **3m**, colorless oil, 48 mg, 65% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 4.0 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 6.8 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.31-7.28 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 2H), 3.78 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.01, 150.16, 146.16, 140.52, 136.27, 131.76, 130.00, 128.82, 127.13, 126.33, 120.95, 113.61, 55.35.

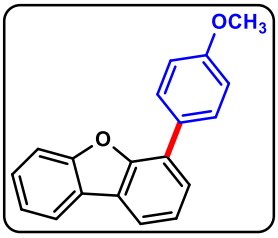
Spectral data match those previously reported.[15]



8-(4-methoxyphenyl)benzofuro[3,2-*b*]pyridine, **3n**, pale yellow solid, 43 mg, 50% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.8 Hz, 1H), 8.32 (s, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.56-7.53 (m, 3H), 7.32-7.29 (m, 1H), 6.94 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.17, 156.63, 150.22, 145.24, 144.34, 136.90, 133.32, 128.39, 123.75, 121.38, 118.92, 118.75, 114.38, 112.26, 55.39.

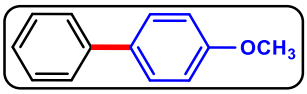


4-(4-methoxyphenyl)dibenzo[*b*,*d*]furan, **3o**, off-white solid, 37 mg, 44% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.6 Hz, 1H), 7.82-7.77 (m, 3H), 7.52-7.47 (m, 2H), 7.39-7.25 (m, 3H), 6.99 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.37, 156.77, 153.31, 129.95, 128.87, 127.16, 126.46, 125.59, 124.85, 124.31, 123.21, 122.73, 120.69, 119.08, 114.16, 111.84, 55.39.

Spectral data match those previously reported.[16]



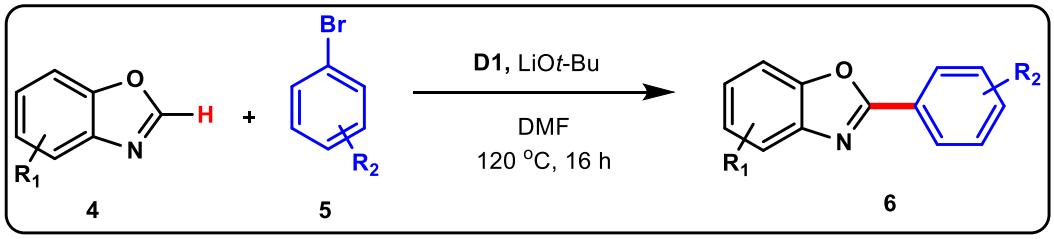
4-methoxy-1,1'-biphenyl, **3p**, off-white solid, 52 mg, 90% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (t, *J* = 8.0 Hz, 4H), 7.33 (t, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 7.2 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 2H), 3.76 (s, 3H).

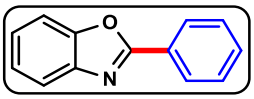
^{13}C NMR (100 MHz, $CDCl_3$) δ 159.16, 140.85, 133.80, 128.75, 128.18, 126.76, 126.68, 114.22, 55.37.

Spectral data match those previously reported.[12]

5. General procedure for direct C-H arylation of benzoxazoles with D1



An oven-dried vial equipped with a stir bar was charged with benzoxazole (0.42 mmol) and the corresponding bromobenzene (0.58 mmol), lithium tertiary butoxide (1.26 mmol), **D1** (5 mol%), followed by DMF (0.5 mL). Then the reaction mixture was placed in a preheated oil bath at 120 °C and stirred for 16 h. After the indicated time, the solvent was removed and purification by flash column chromatography on silica gel with n-hexane - ethyl acetate as eluent, to yield the title compound.

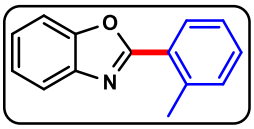


2-phenylbenzo[*d*]oxazole, **6a**, pale yellow solid , 49 mg, 60% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.18 (m, 2H), 7.72-7.69 (m, 1H), 7.53-7.50 (m, 1H), 7.46-7.45 (m, 3H), 7.29-7.27 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.07, 150.79, 142.14, 131.53, 128.92, 127.64, 127.21, 125.12, 124.59, 120.04, 110.60.

Spectral data match those previously reported.[17]

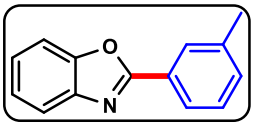


2-(o-tolyl)benzo[*d*]oxazole, **6b**,colorless oil, 35 mg, 41% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.6 Hz, 1H), 7.74-7.72 (m, 1H), 7.53-7.51 (m, 1H), 7.37-7.33 (m, 1H), 7.30-7.28 (m, 4H), 2.74 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.43, 150.31, 142.12, 138.86, 131.80, 130.92, 129.96, 126.07, 125.02, 124.38, 120.15, 110.49, 22.20.

Spectral data match those previously reported.[21]

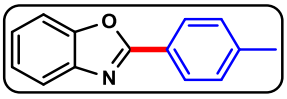


2-(m-tolyl)benzo[*d*]oxazole, **6c**, colorless oil, 48 mg, 55% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.70-7.68 (m, 1H), 7.50-7.48 (m, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.27-7.25 (m, 3H), 2.37 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.28, 150.76, 142.12, 138.76, 132.38, 128.84, 128.21, 127.03, 125.05, 124.79, 124.56, 119.97, 110.57, 21.36.

Spectral data match those previously reported.[18]

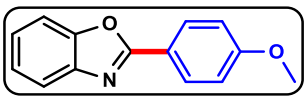


2-(p-tolyl)benzo[*d*]oxazole **6d**, colorless oil, 52 mg, 61% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.0 Hz, 2H), 7.69-7.67 (m, 1H), 7.50-7.47 (m, 1H), 7.27-7.24 (m, 4H), 2.35 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.32, 150.70, 142.18, 142.08, 129.66, 127.61, 124.88, 124.49, 119.85, 110.51.

Spectral data match those previously reported.[17]

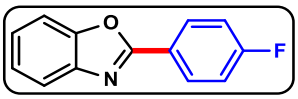


2-(4-methoxyphenyl)benzo[*d*]oxazole, **6e**, off-white solid, 60 mg, 64% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.11 (m, 2H), 7.67-7.65 (m, 1H), 7.49-7.47 (m, 1H), 7.26-7.23 (m, 2H), 6.97-6.94 (m, 2H), 3.82 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.20, 162.35, 150.70, 142.30, 129.41, 124.61, 124.43, 119.73, 119.63, 114.38, 110.39, 55.47.

Spectral data match those previously reported. [18]

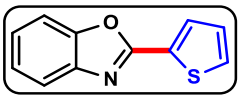


2-(4-fluorophenyl)benzo[*d*]oxazole, **6f**, off-white solid, 48 mg, 55% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19-8.16 (m, 2H), 7.69-7.67 (m, 1H), 7.50-7.48 (m, 1H), 7.28-7.26 (m, 2H), 7.15-7.11 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.09, 163.58, 162.19, 150.78, 142.06, 129.90, 129.81, 125.16, 124.68, 123.53, 123.49, 119.99, 116.32, 116.10, 110.59.

Spectral data match those previously reported.[18]

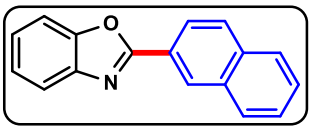


2-(thiophen-2-yl)benzo[*d*]oxazole, **6g**, colorless oil, 40 mg, 48% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.83 (m, 1H), 7.67-7.65 (m, 1H), 7.49-7.46 (m, 2H), 7.28-7.25 (m, 2H), 7.13-7.11 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.07, 150.45, 142.01, 130.27, 129.96, 129.67, 128.27, 125.10, 124.74, 119.82, 110.44.

Spectral data match those previously reported.[19]

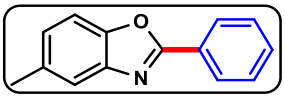


2-(naphthalen-2-yl)benzo[*d*]oxazole, **6h**, off-white solid, 53 mg, 52% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.23 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.91-7.88 (m, 2H), 7.82-7.80 (m, 1H), 7.74-7.72 (m, 1H), 7.55-7.47 (m, 3H), 7.30-7.28 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.23, 150.89, 142.24, 134.77, 133.00, 128.97, 128.80, 128.17, 127.93, 127.82, 126.92, 125.20, 124.66, 124.42, 123.98, 120.04, 110.61.

Spectral data match those previously reported.[20]



5-methyl-2-phenylbenzo[*d*]oxazole, **6i**, colorless oil, 43 mg, 56% of yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18-8.16 (m, 2H), 7.48-7.44 (m, 4H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 2.42 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.14, 149.43, 142.29, 134.42, 131.40, 128.89, 127.56, 126.25, 119.92, 109.96, 21.55.

Spectral data match those previously reported.[21]

6. References

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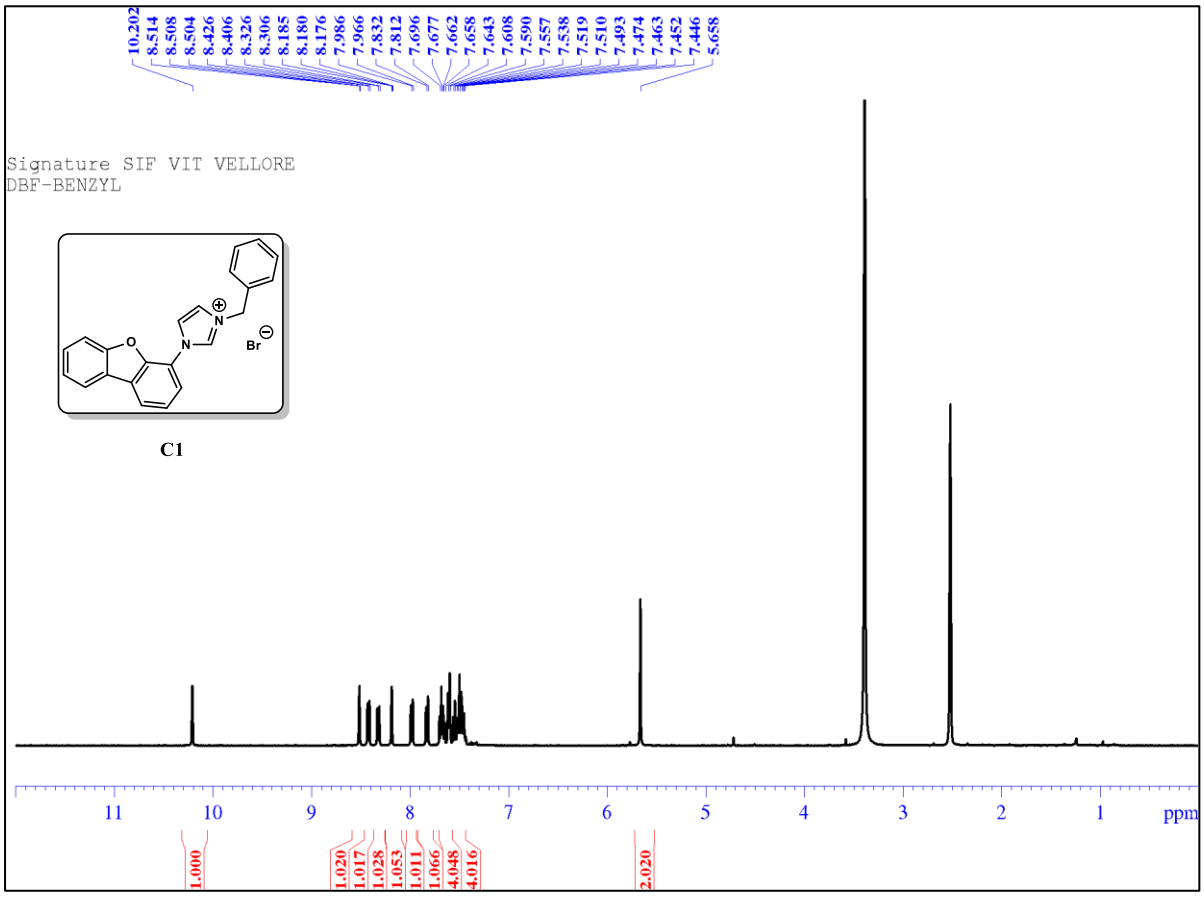
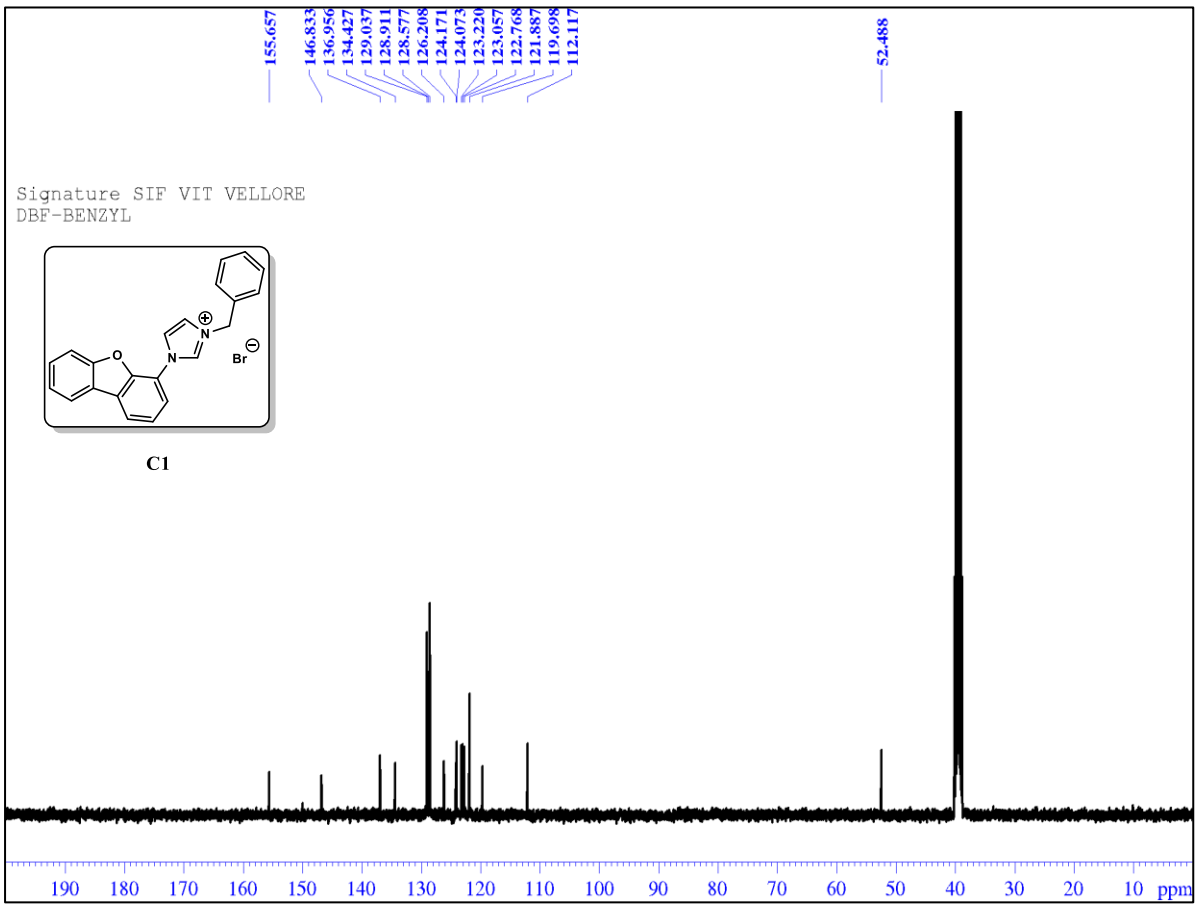
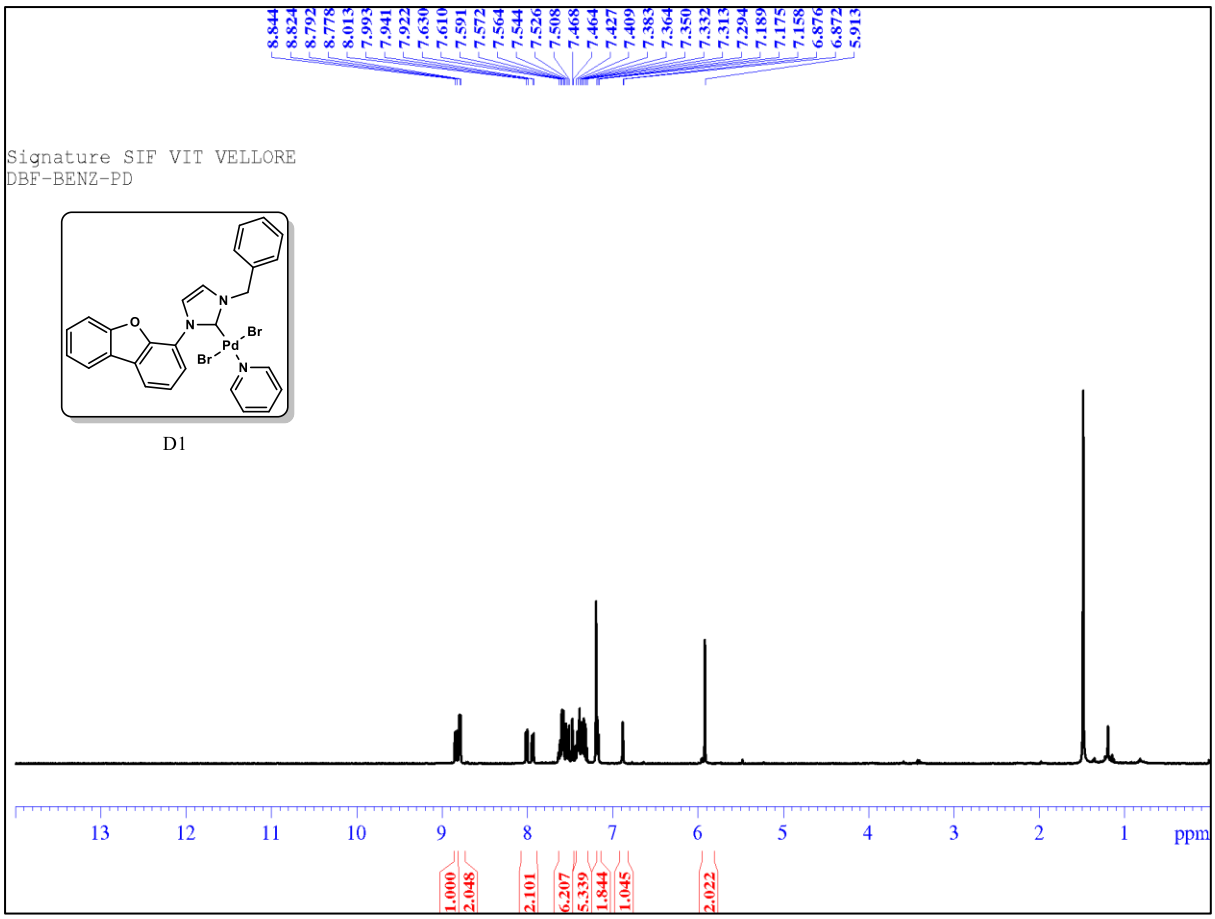
7. Copies of ^{1}H & ^{13}C NMR spectra of synthesized derivatives



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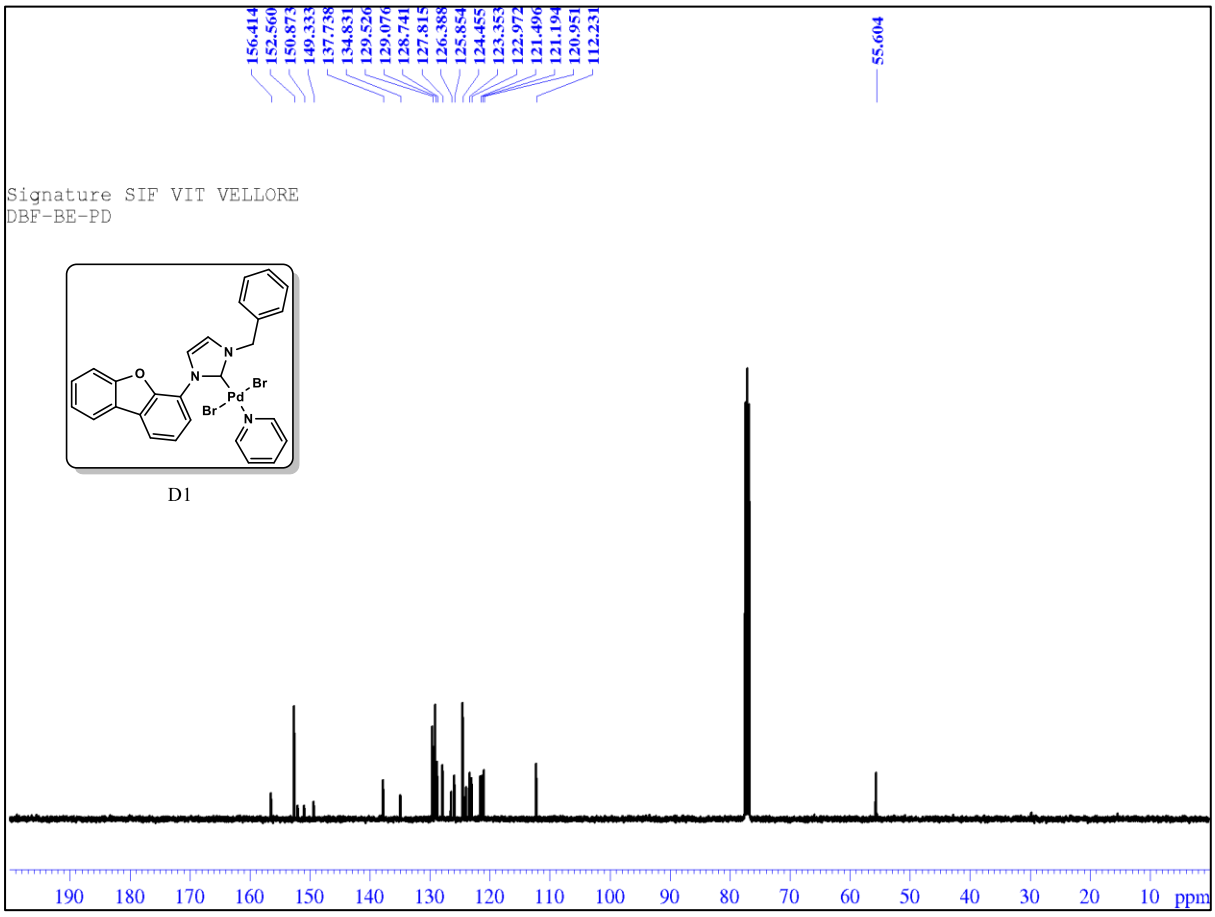
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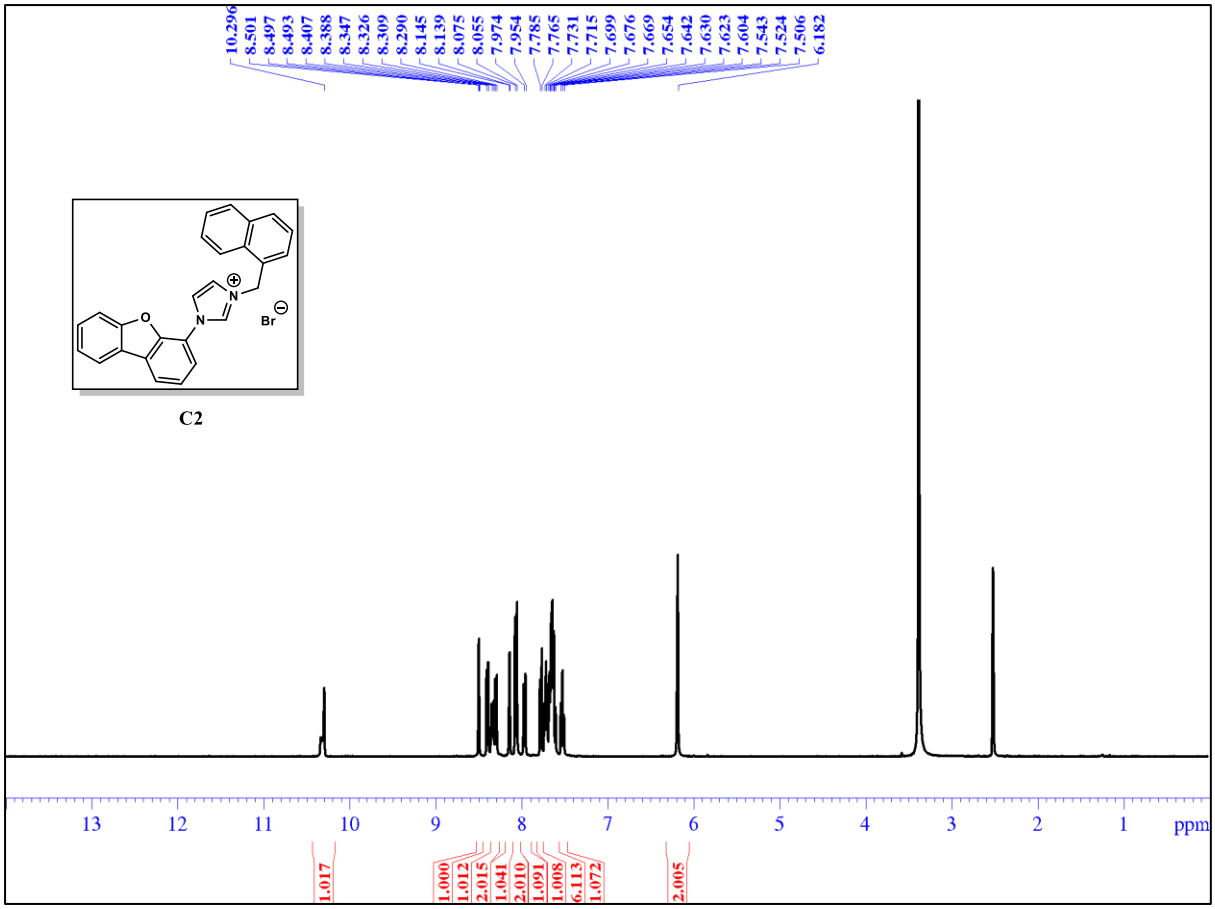
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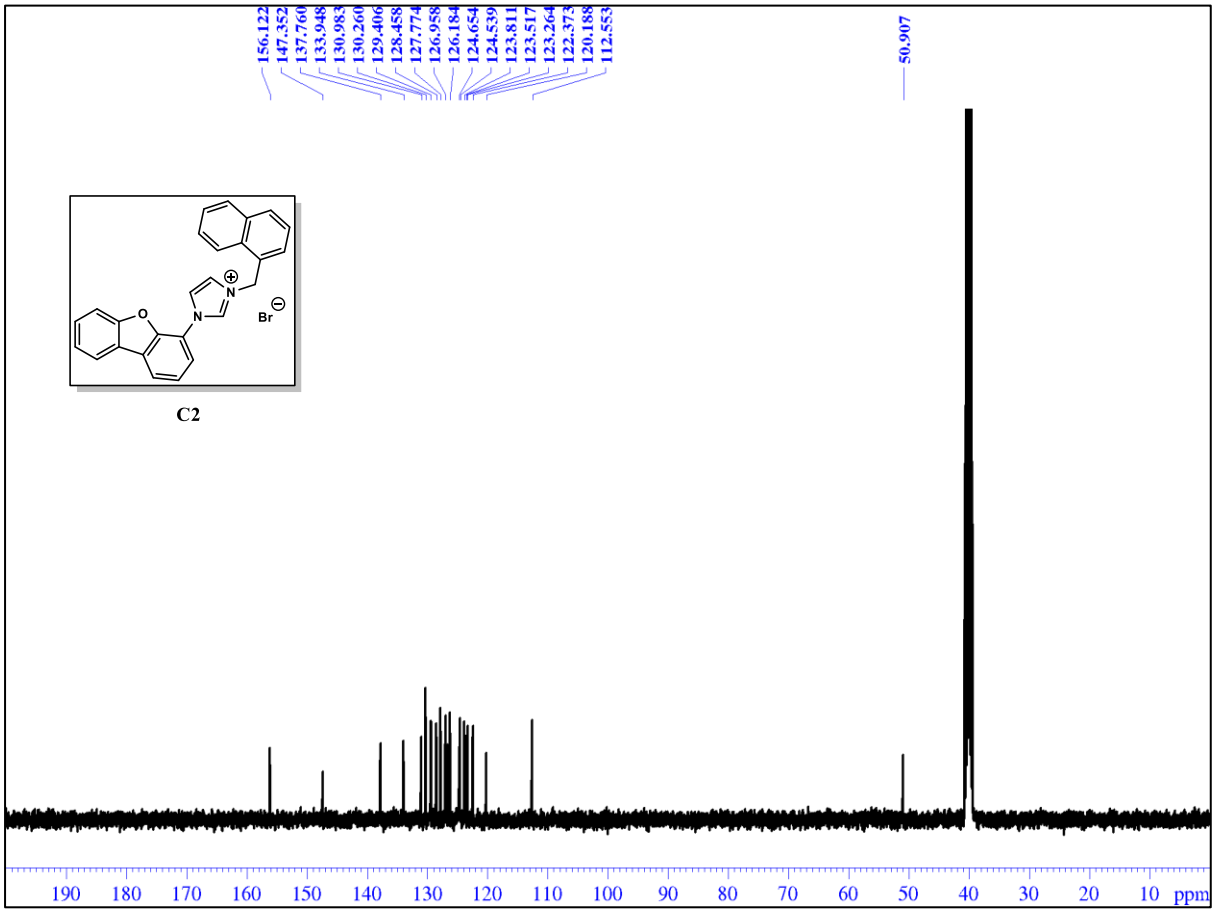
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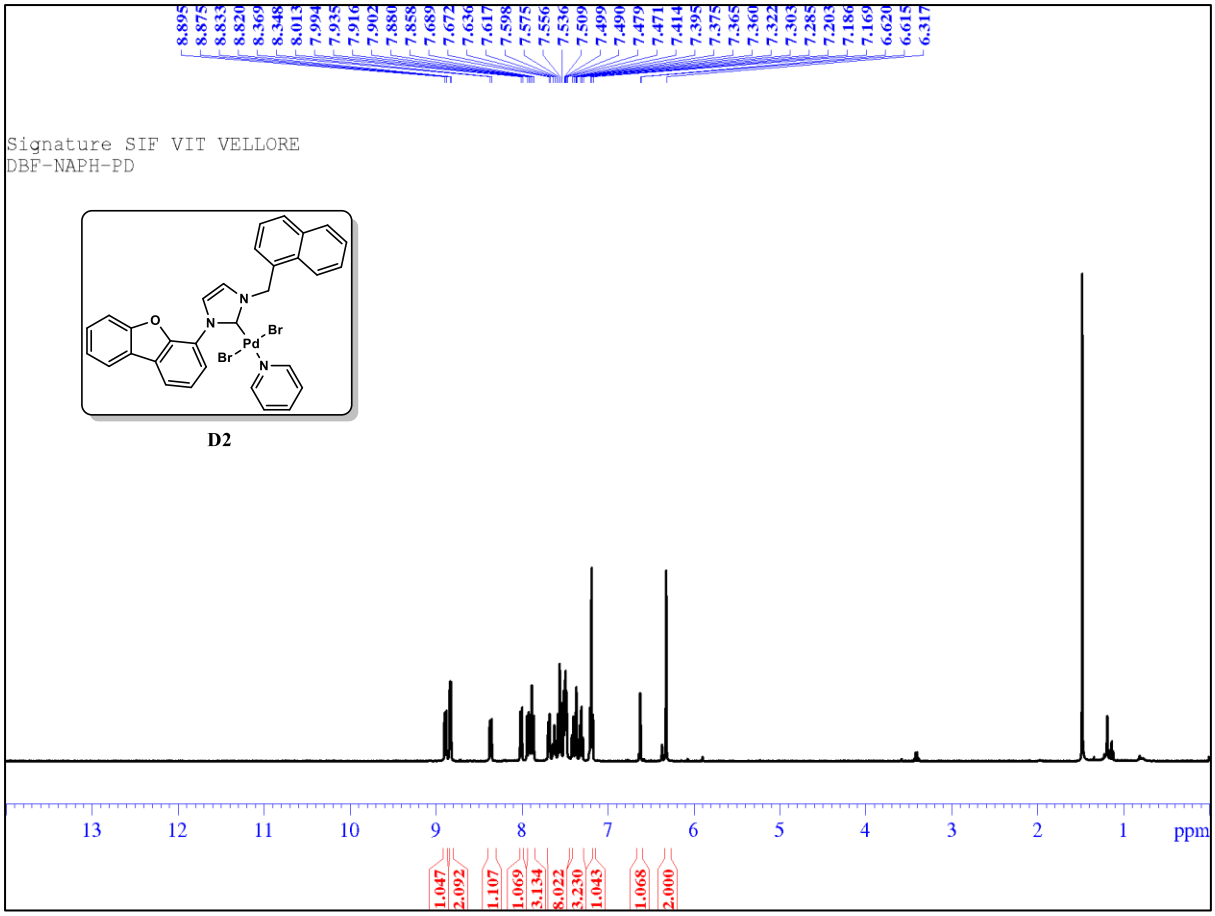
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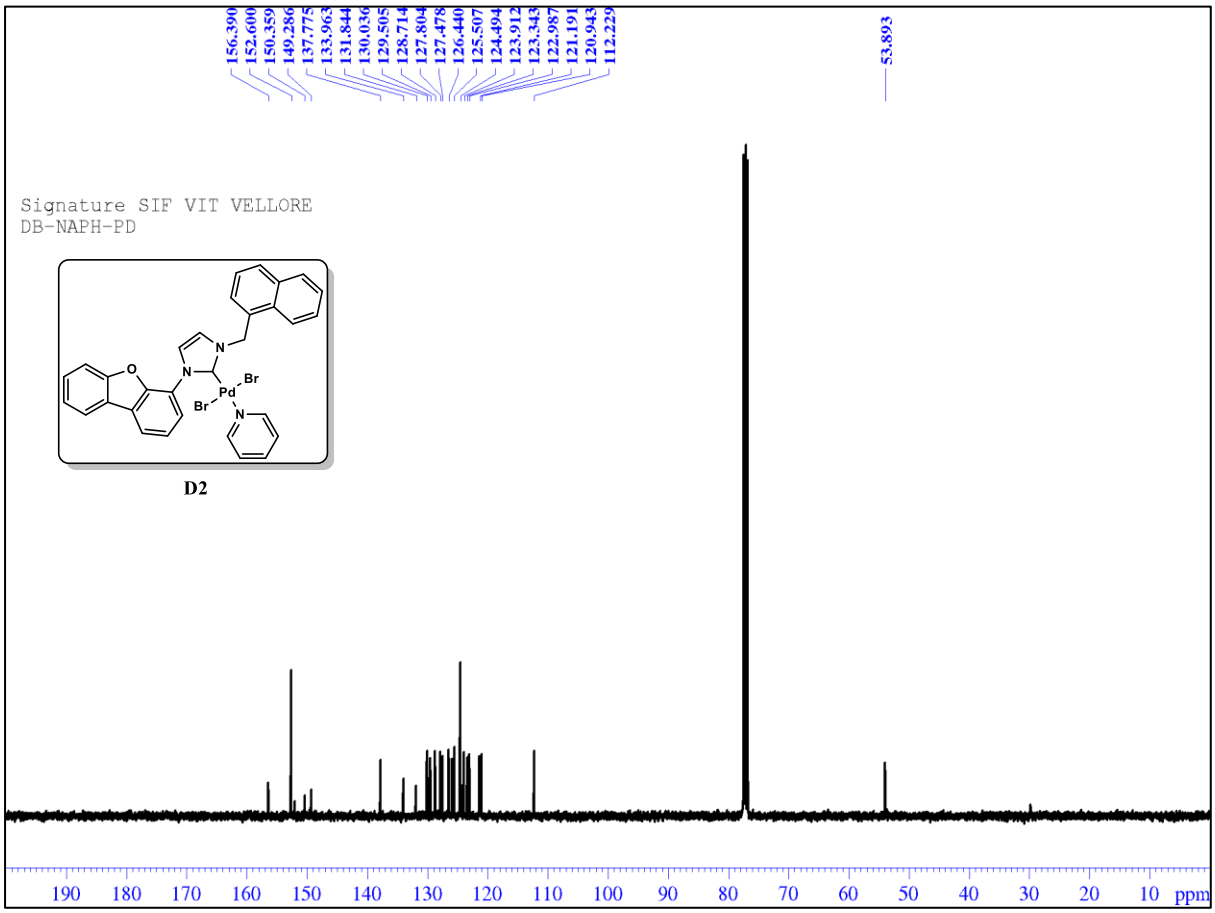
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140
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110
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90
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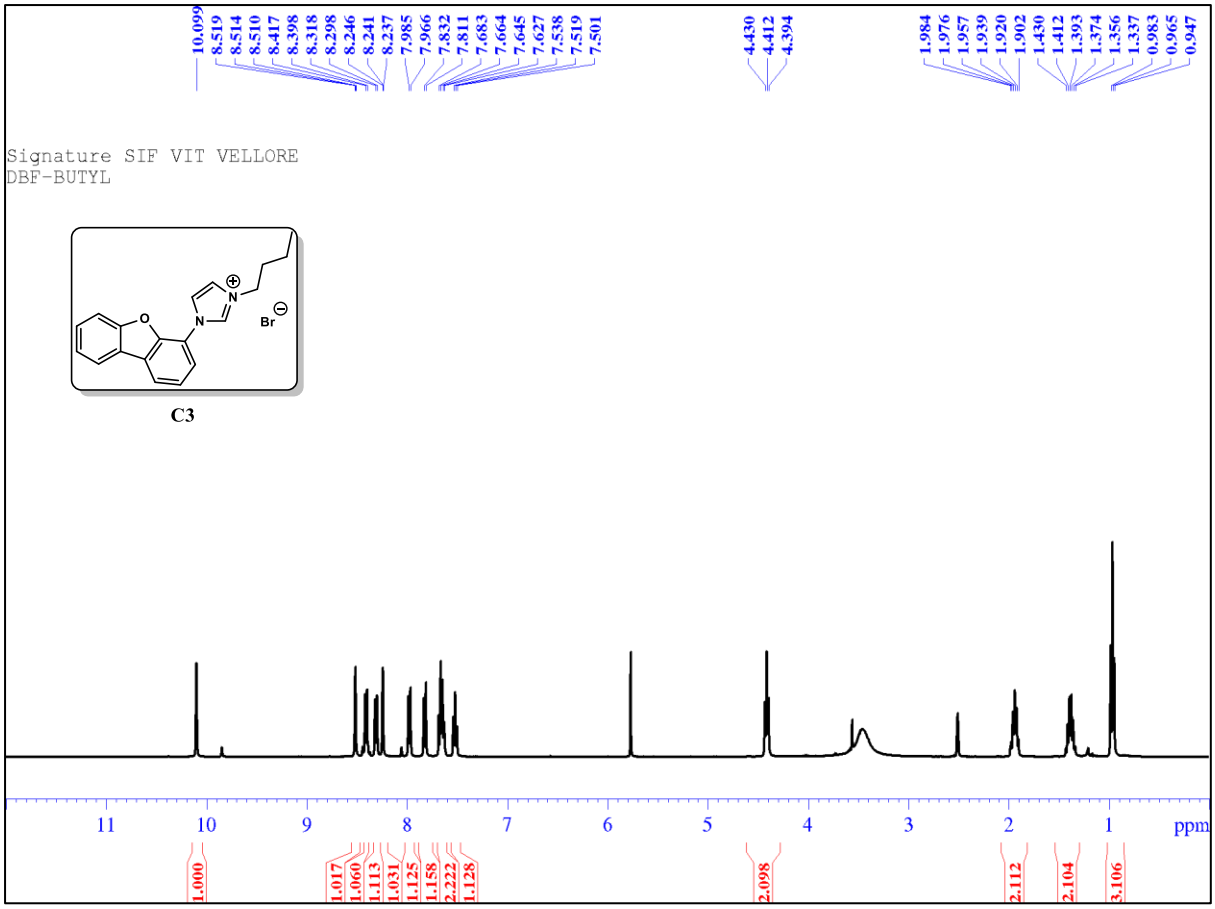
30
20
10
ppm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8.514
8.510
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8.318
8.298
8.246
8.241
8.237
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7.966
7.832
7.811
7.683
7.664
7.645
7.627
7.538
7.519
7.501
4.430
4.412
4.394
1.984
1.976
1.957
1.939
1.920
1.902
1.430
1.412
1.393
1.374
1.356
1.337
0.983
0.965
0.947
Signature SIF VIT VELLORE
DBF-BUTYL
Br
C3
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.017
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1.031
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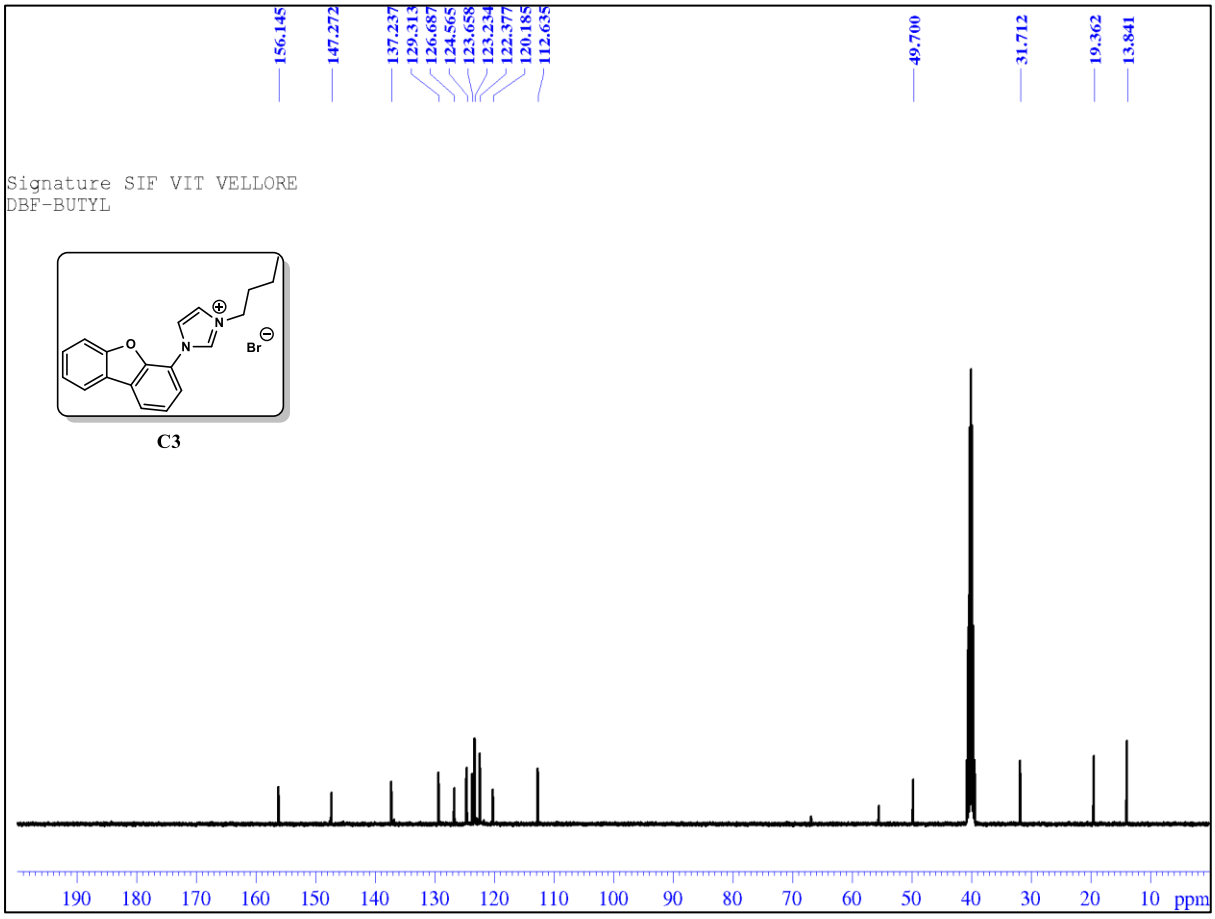
1.158
2.222
1.128
2.098
2.112
2.104
3.106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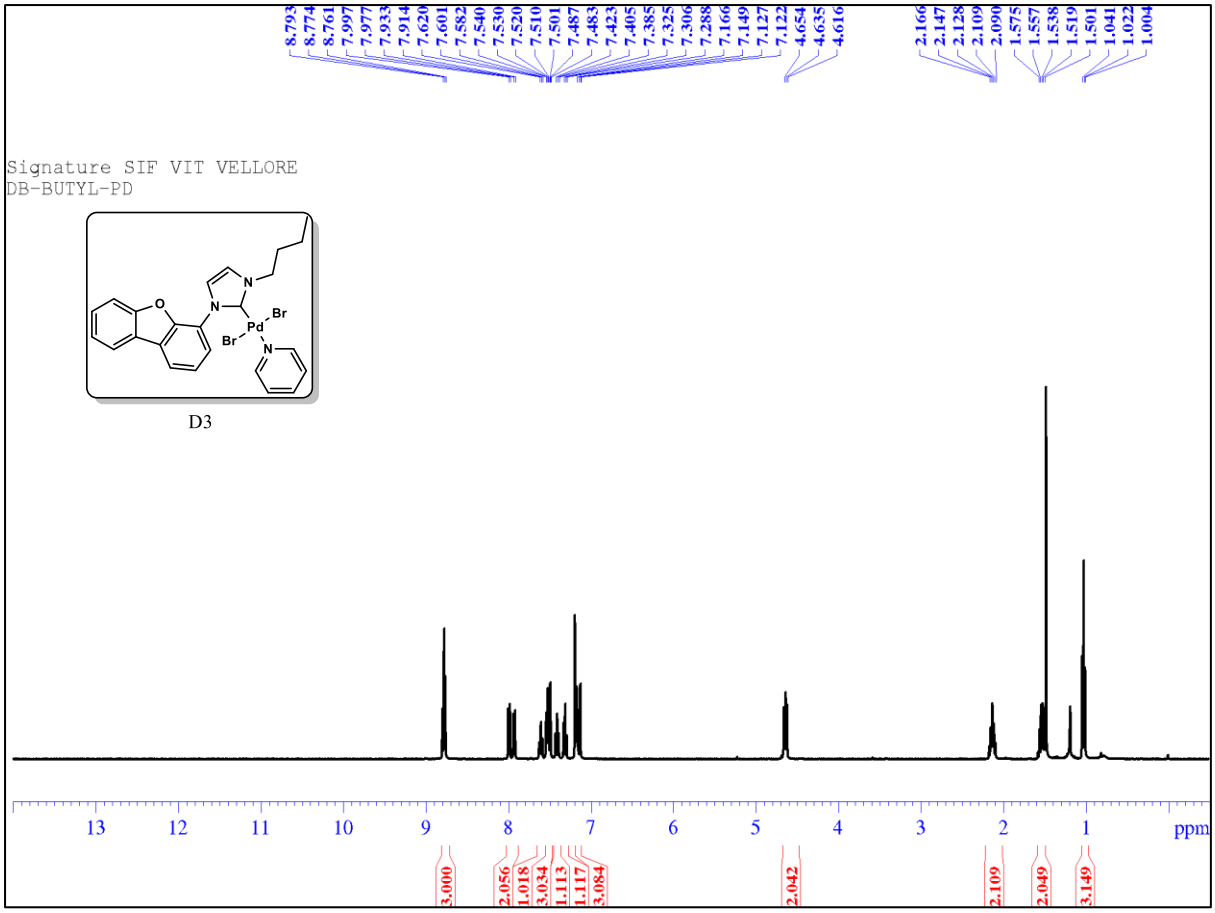
147.272
137.237
129.313
126.687
124.565
123.658
123.234
122.377
120.185
112.635
49.700
31.712
19.362
13.841
Signature SIF VIT VELLORE
DBF-BUTYL
Br
C3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.774
8.761
7.997
7.977
7.933
7.914
7.620
7.601
7.582
7.540
7.530
7.520
7.510
7.501
7.487
7.483
7.423
7.405
7.385
7.325
7.306
7.288
7.166
7.149
7.127
7.122
4.654
4.635
4.616
2.166
2.147
2.128
2.109
2.090
1.575
1.557
1.538
1.519
1.501
1.041
1.022
1.004
Signature SIF VIT VELLORE
DB-BUTYL-PD
D3
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
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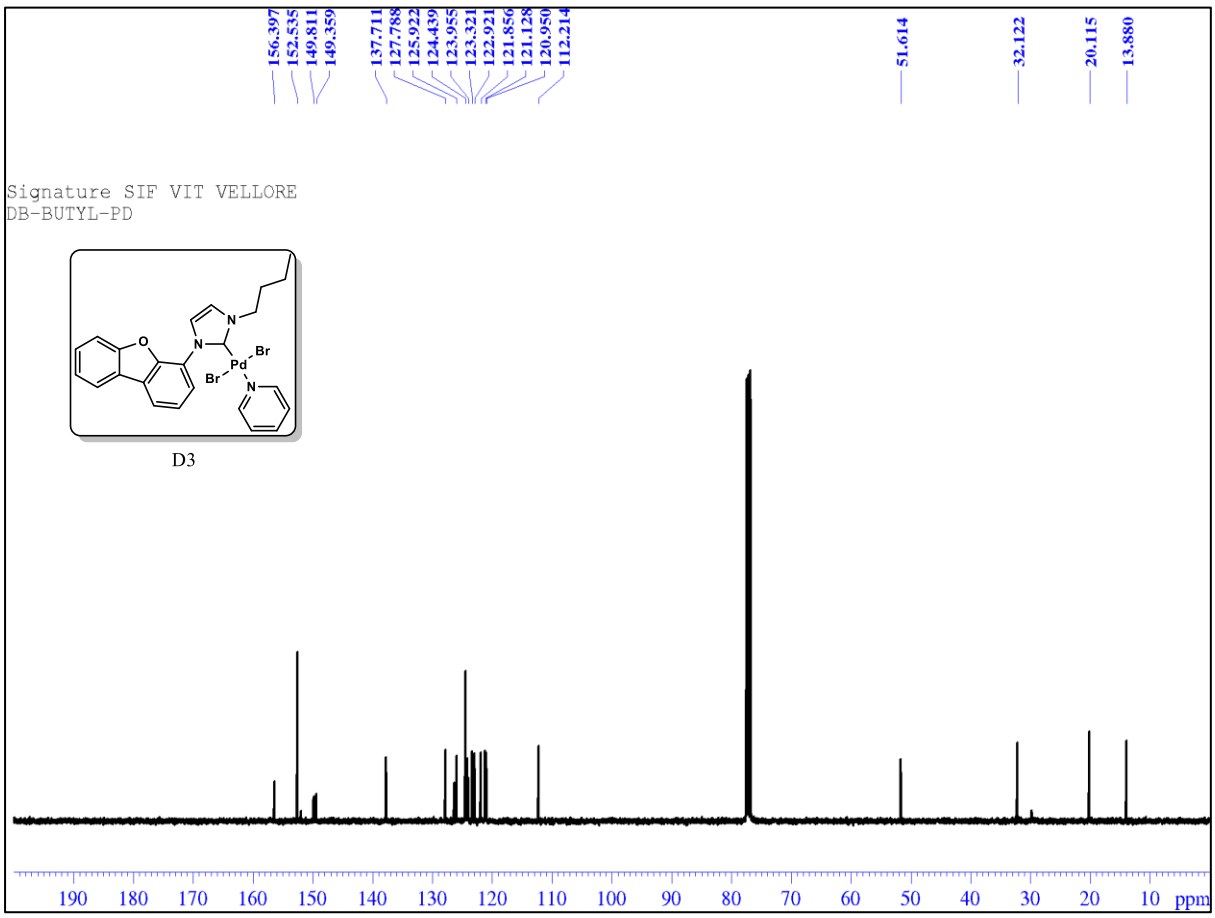
1.018
3.034
1.113
1.117
3.084
2.042
2.109
2.049
3.149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152.535
149.811
149.359
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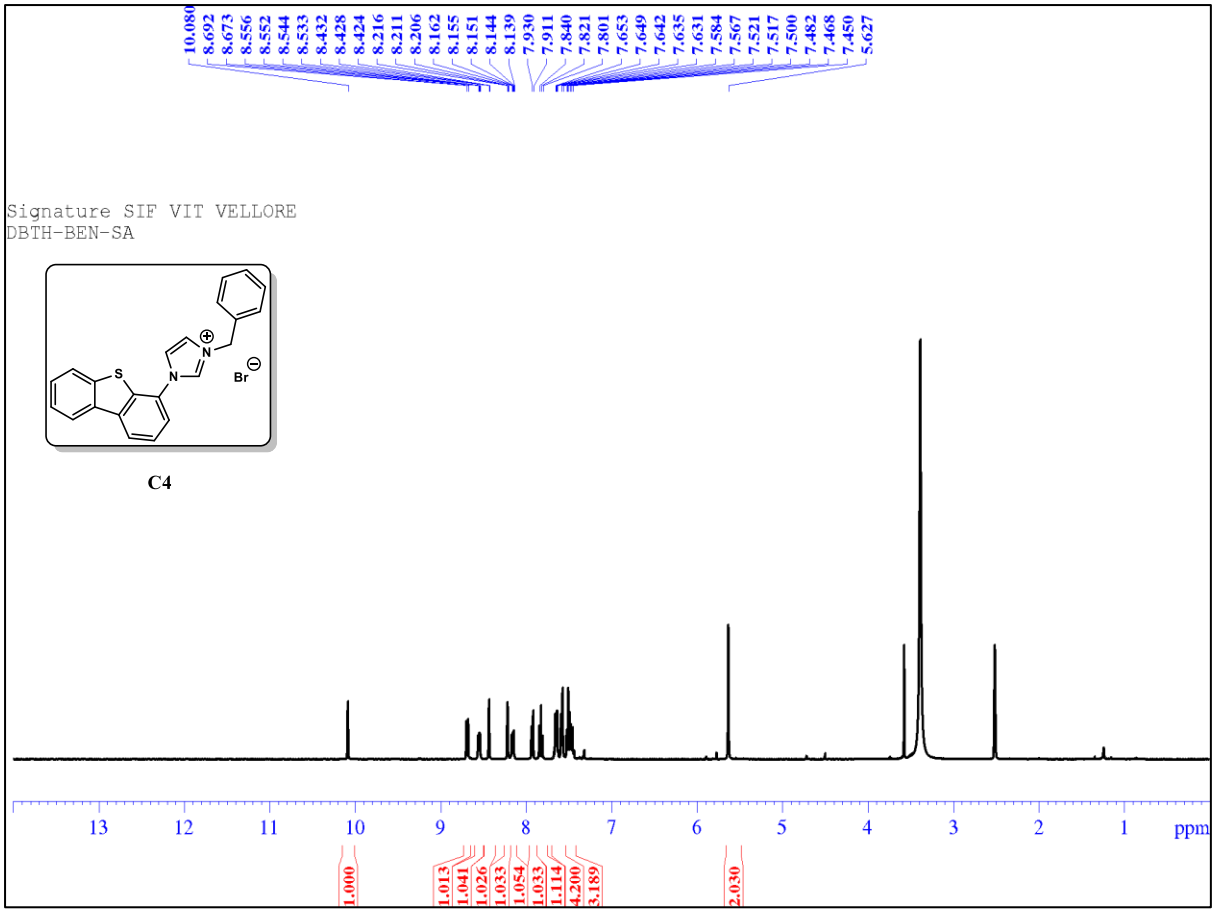
127.788
125.922
124.439
123.955
123.321
122.921
121.856
121.128
120.950
112.214
51.614
32.122
20.115
13.880
Signature SIF VIT VELLORE
DB-BUTYL-PD
D3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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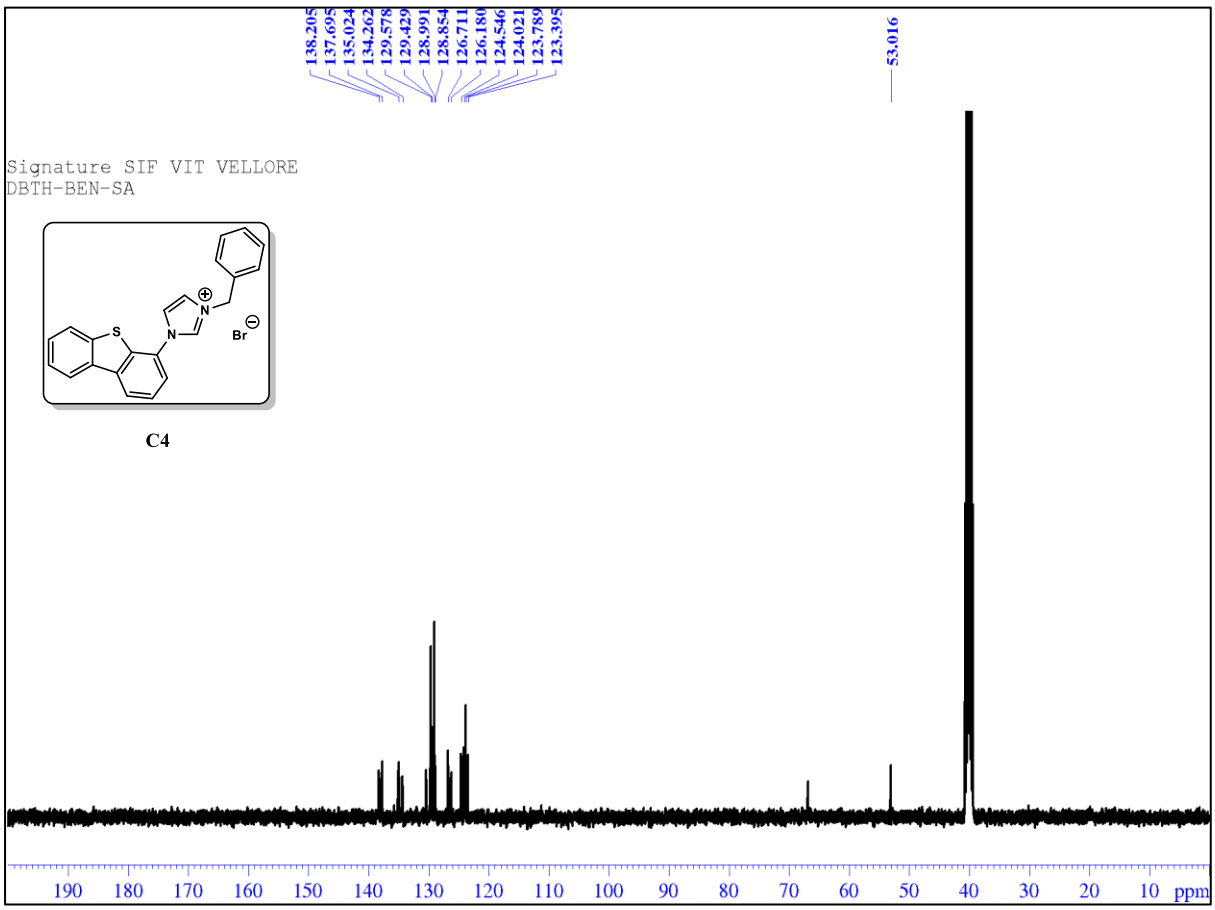
8.432
8.428
8.424
8.216
8.211
8.206
8.162
8.155
8.151
8.144
8.139
7.930
7.911
7.840
7.821
7.801
7.653
7.649
7.642
7.635
7.631
7.584
7.567
7.521
7.517
7.500
7.482
7.468
7.450
5.627
Signature SIF VIT VELLORE
DBTH-BEN-SA
S
N
N
Br
C4
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.013
1.041
1.026
1.033
1.054
1.033
1.114
4.200
3.189
2.030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137.695
135.024
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128.991
128.854
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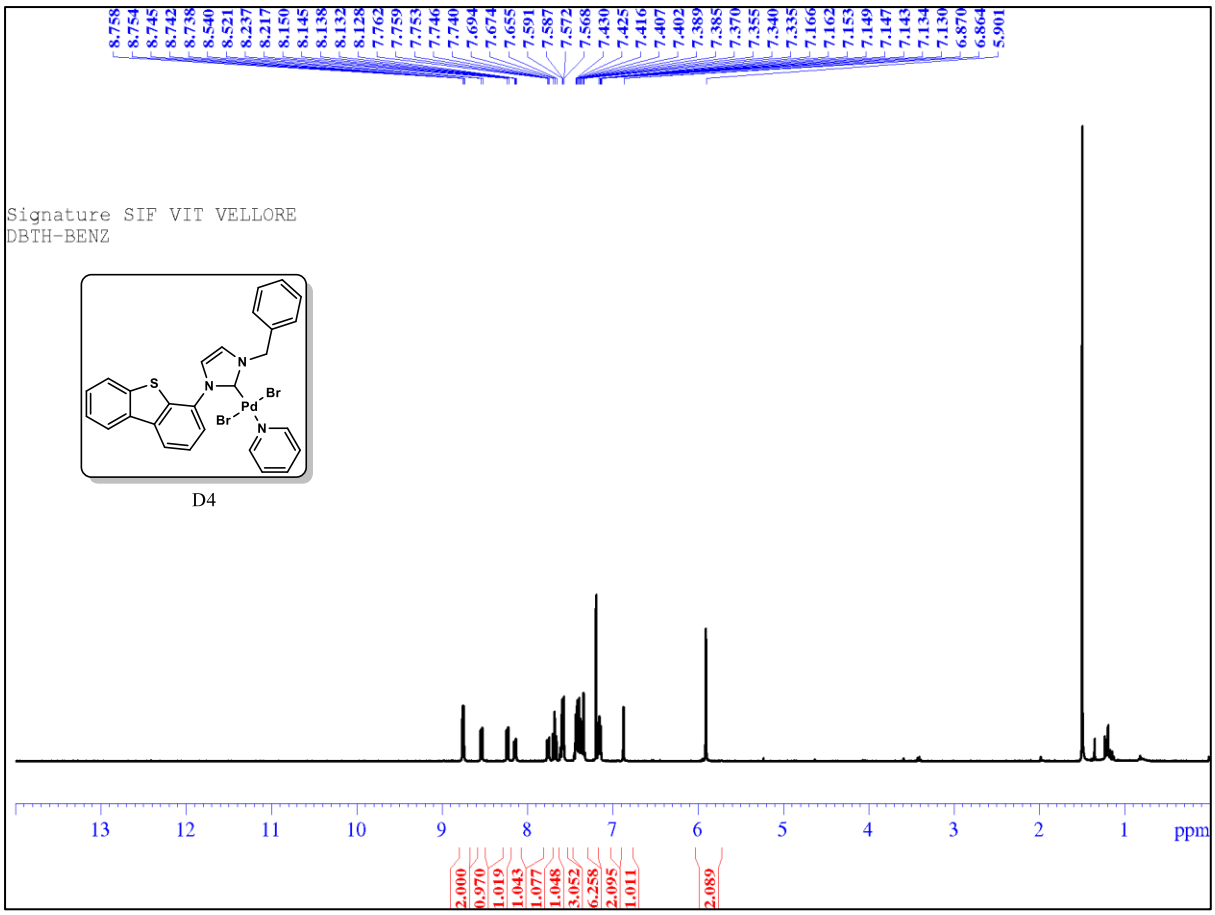
126.180
124.546
124.021
123.789
123.395
53.016
Signature SIF VIT VELLORE
DBTH-BEN-SA
S
N
N
Br
C4
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.754
8.745
8.742
8.738
8.540
8.521
8.237
8.217
8.150
8.145
8.138
8.132
8.128
7.762
7.759
7.753
7.746
7.740
7.694
7.674
7.655
7.591
7.587
7.572
7.568
7.430
7.425
7.416
7.407
7.402
7.389
7.385
7.370
7.355
7.340
7.335
7.166
7.162
7.153
7.149
7.147
7.143
7.134
7.130
6.870
6.864
5.901
Signature SIF VIT VELLORE
DBTH-BENZ
D4
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
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0.970
1.019
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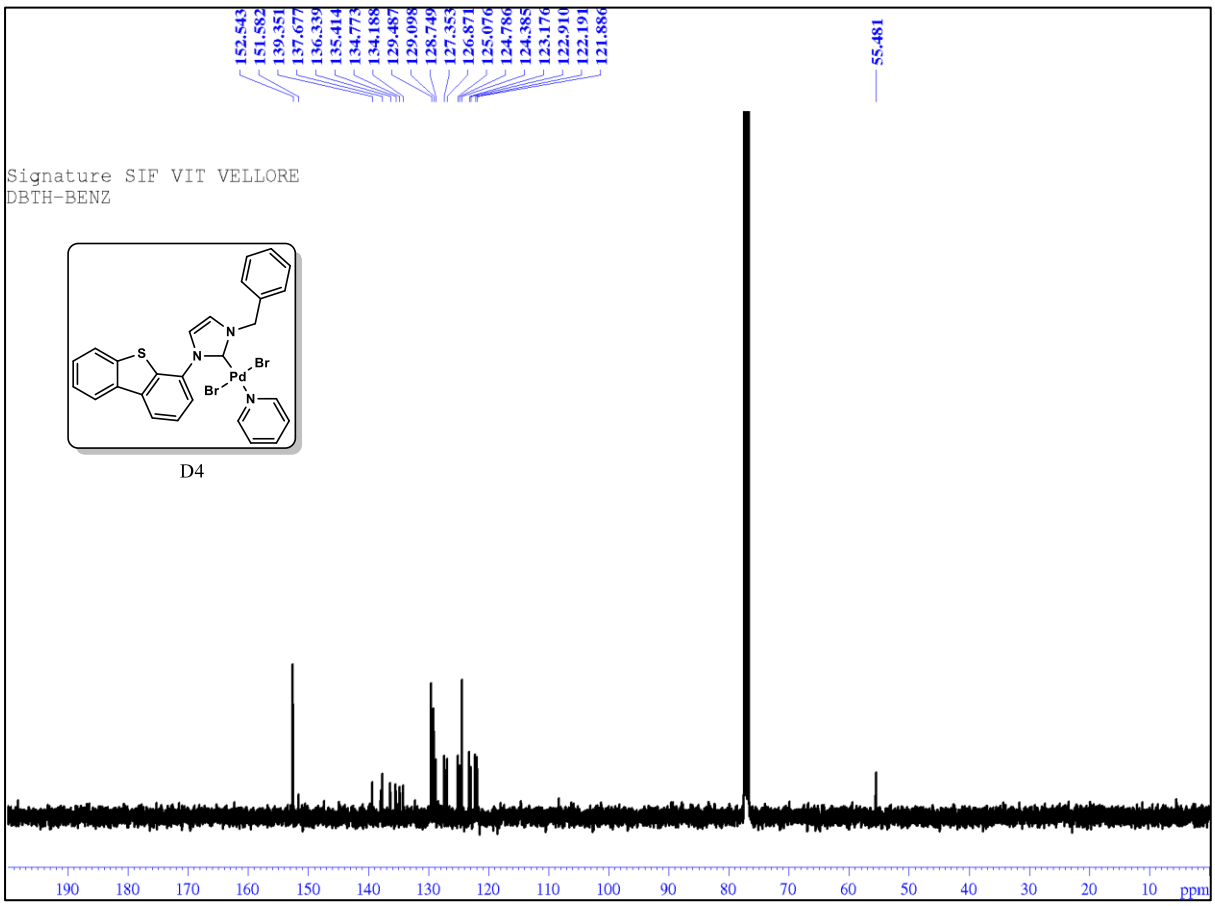
1.077
1.048
3.052
6.258
2.095
1.011
2.089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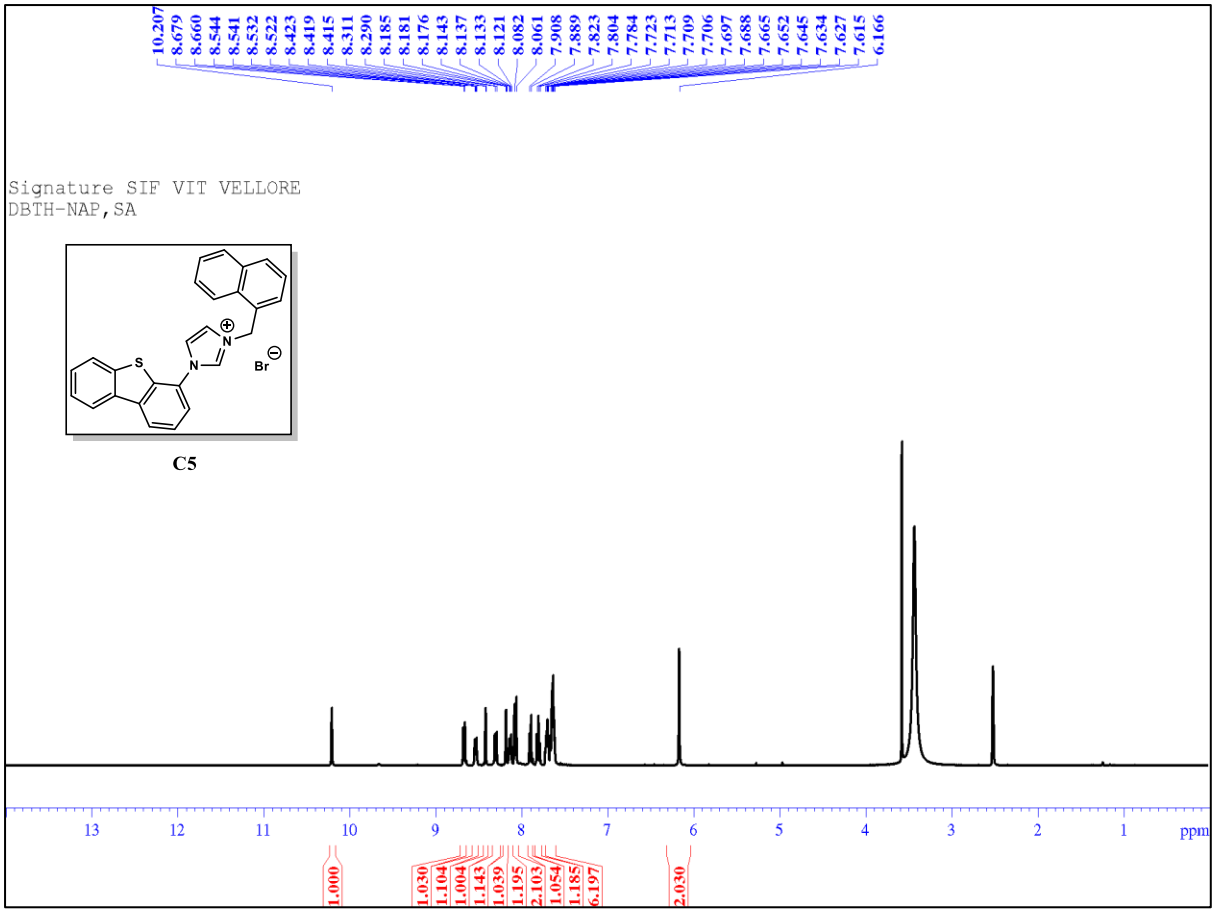
151.582
139.351
137.677
136.339
135.414
134.773
134.188
129.487
129.098
128.749
127.353
126.871
125.076
124.786
124.385
123.176
122.910
122.191
121.886
55.481
Signature SIF VIT VELLORE
DBTH-BENZ
D4
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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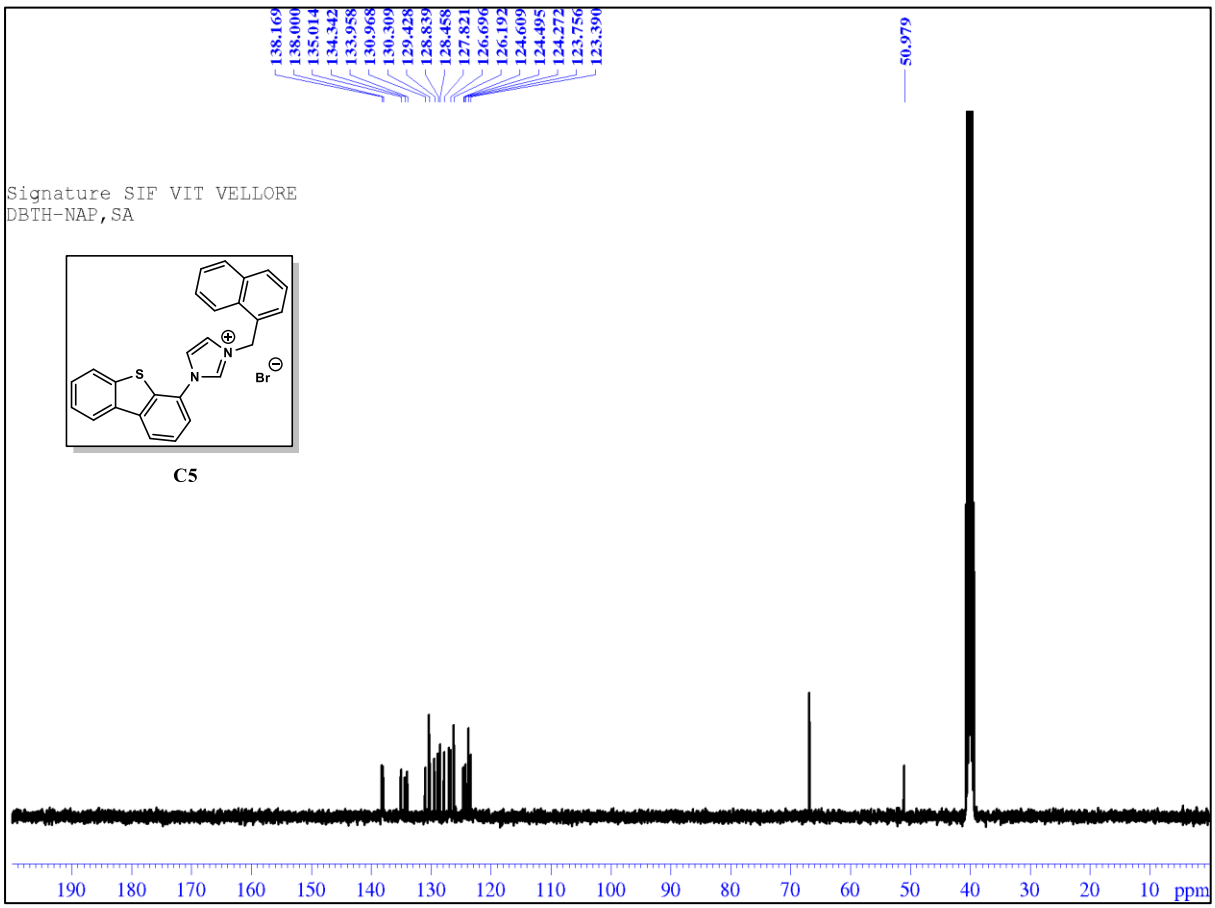
8.660
8.544
8.541
8.532
8.522
8.423
8.419
8.415
8.311
8.290
8.185
8.181
8.176
8.143
8.137
8.133
8.121
8.082
8.061
7.908
7.889
7.823
7.804
7.784
7.723
7.713
7.709
7.706
7.697
7.688
7.665
7.652
7.645
7.634
7.627
7.615
6.166
Signature SIF VIT VELLORE
DBTH-NAP,SA
Br
C5
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.030
1.104
1.004
1.143
1.039
1.195
2.103
1.054
1.185
6.197
2.030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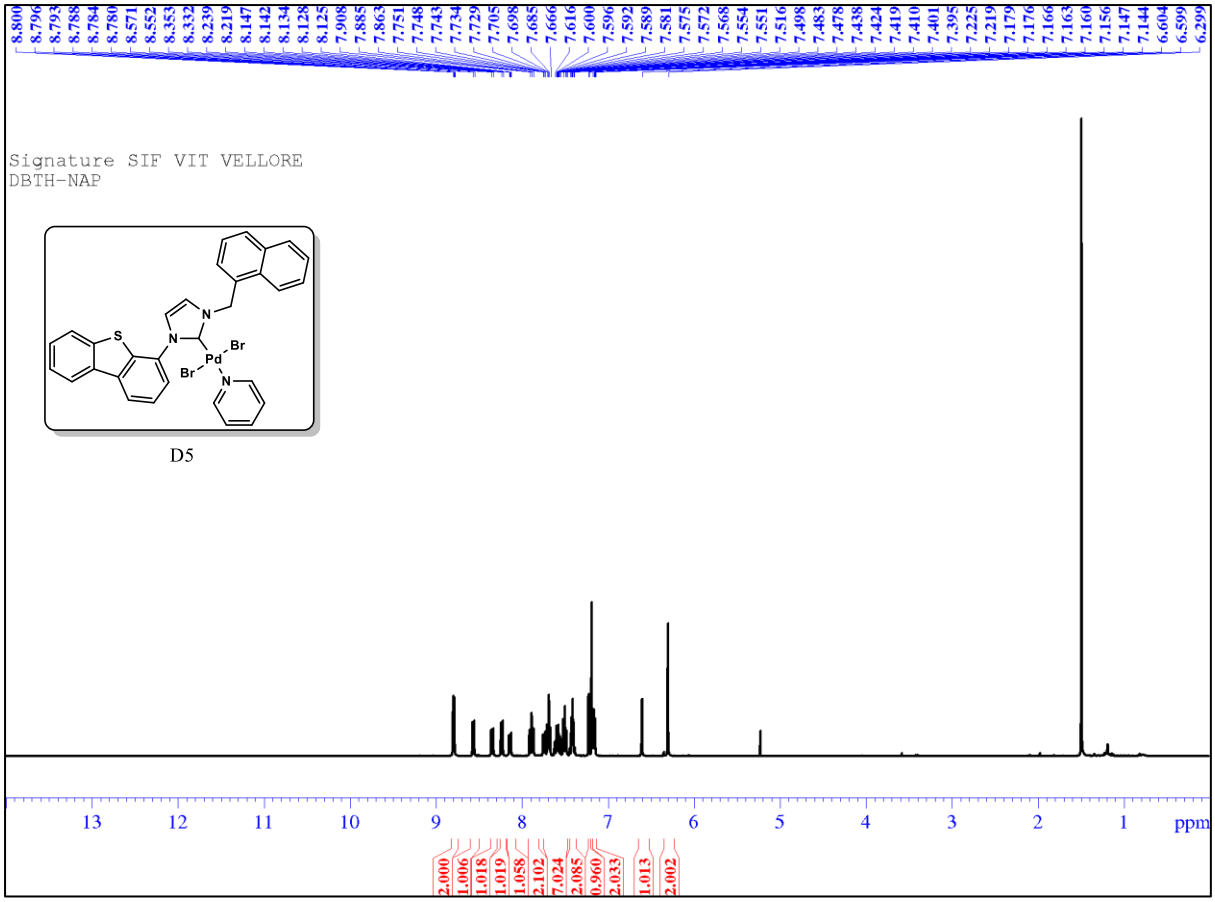
138.000
135.014
134.342
133.958
130.968
130.309
129.428
128.839
128.458
127.821
126.696
126.192
124.609
124.495
124.272
123.756
123.390
50.979
Signature SIF VIT VELLORE
DBTH-NAP,SA
Br
C5
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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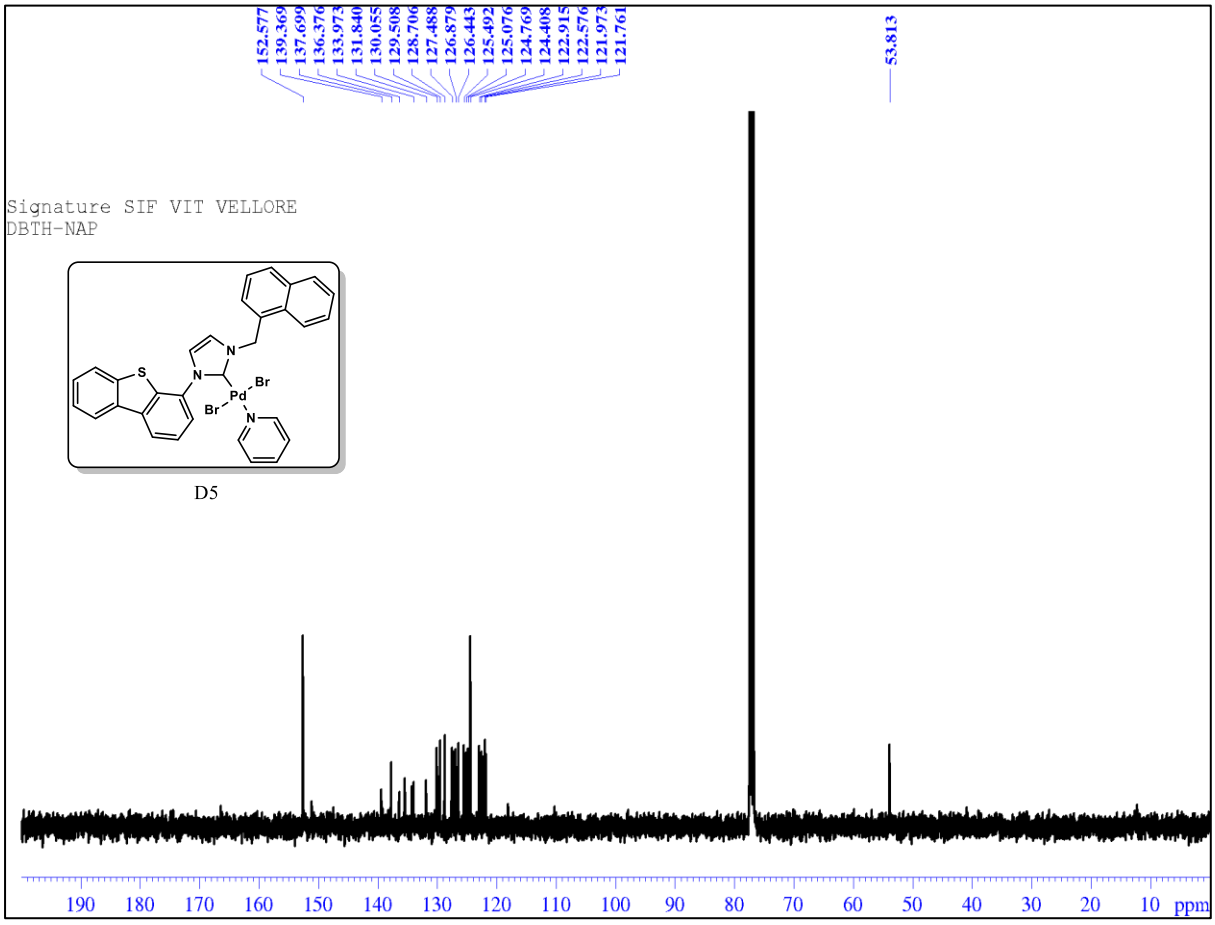
DBTH-NAP
D5
ppm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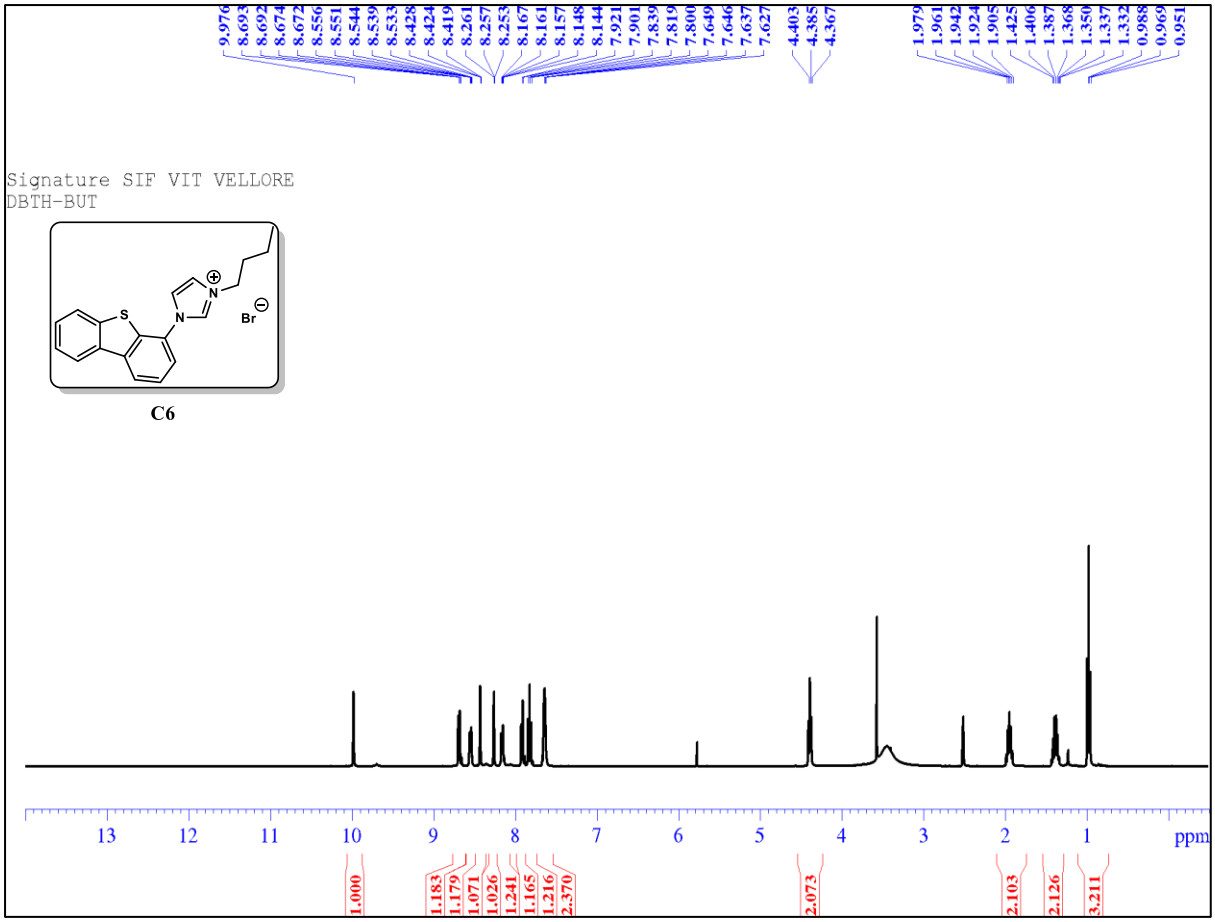
DBTH-NAP
D5
ppm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8.551
8.544
8.539
8.533
8.428
8.424
8.419
8.261
8.257
8.253
8.167
8.161
8.157
8.148
8.144
7.921
7.901
7.839
7.819
7.800
7.649
7.646
7.637
7.627
4.403
4.385
4.367
1.979
1.961
1.942
1.924
1.905
1.425
1.406
1.387
1.368
1.350
1.337
1.332
0.988
0.969
0.951
Signature SIF VIT VELLORE
DBTH-BUT
S
N
N
Br
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.183
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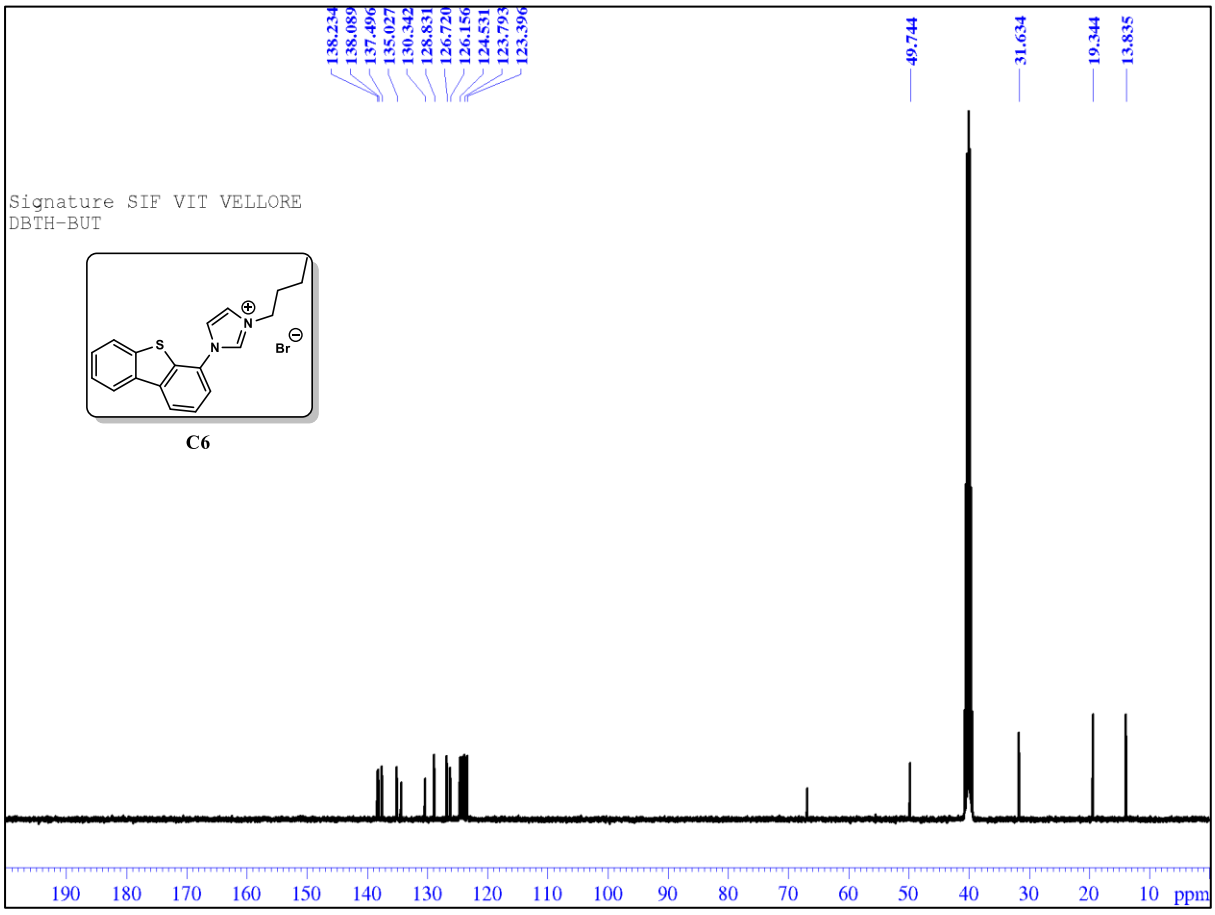
1.026
1.241
1.165
1.216
2.370
2.073
2.103
2.126
3.211

C6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126.156
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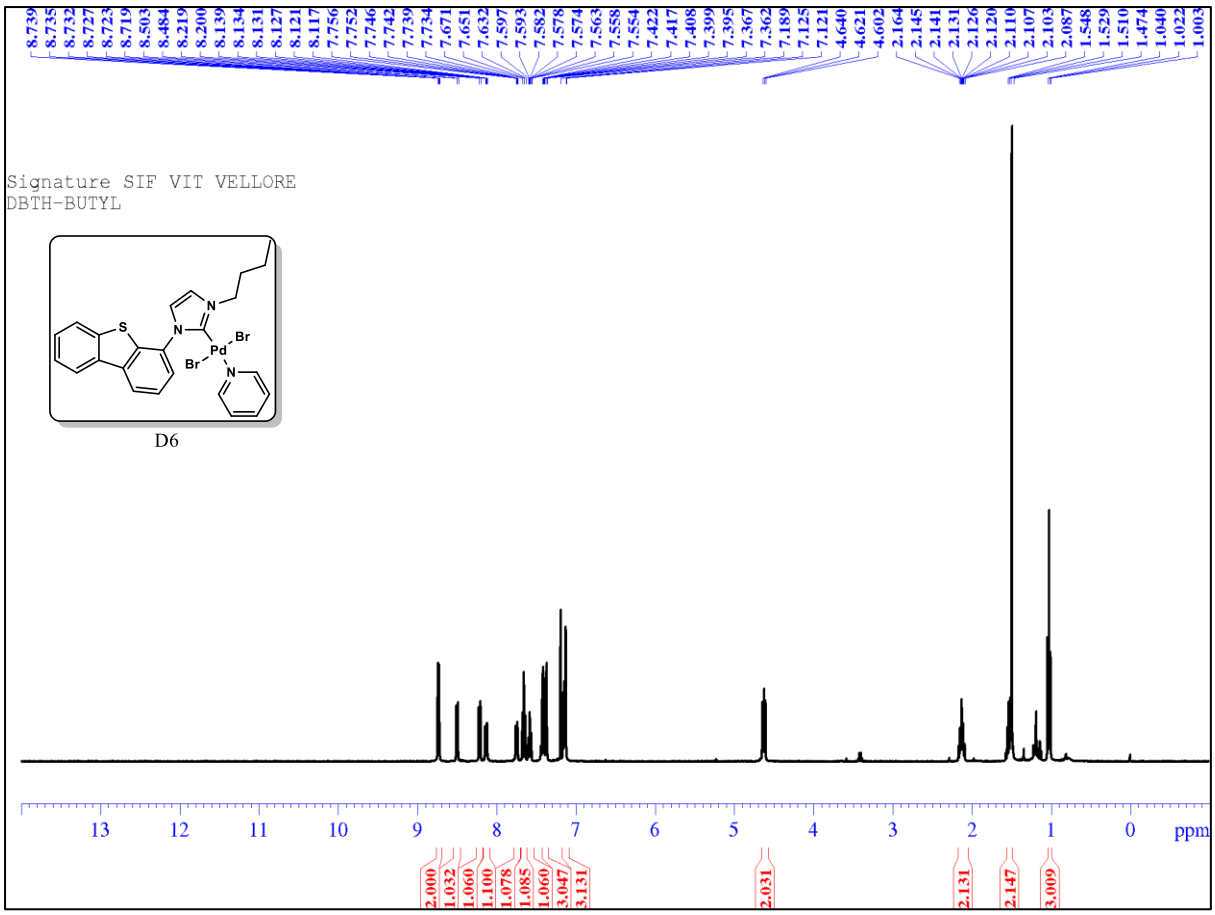
123.793
123.396
49.744
31.634
19.344
13.835
Signature SIF VIT VELLORE
DBTH-BUT
S
N
N
Br
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

C6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8.732
8.727
8.723
8.719
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8.484
8.219
8.200
8.139
8.134
8.131
8.127
8.121
8.117
7.756
7.752
7.746
7.742
7.739
7.734
7.671
7.651
7.632
7.597
7.593
7.582
7.578
7.574
7.563
7.558
7.554
7.422
7.417
7.408
7.399
7.395
7.367
7.362
7.189
7.125
7.121
4.640
4.621
4.602
2.164
2.145
2.141
2.131
2.126
2.120
2.110
2.107
2.103
2.087
1.548
1.529
1.510
1.474
1.040
1.022
1.003
Signature SIF VIT VELLORE
DBTH-BUTYL
D6
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.000
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1.060
1.100
1.078
1.085
1.060
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3.131
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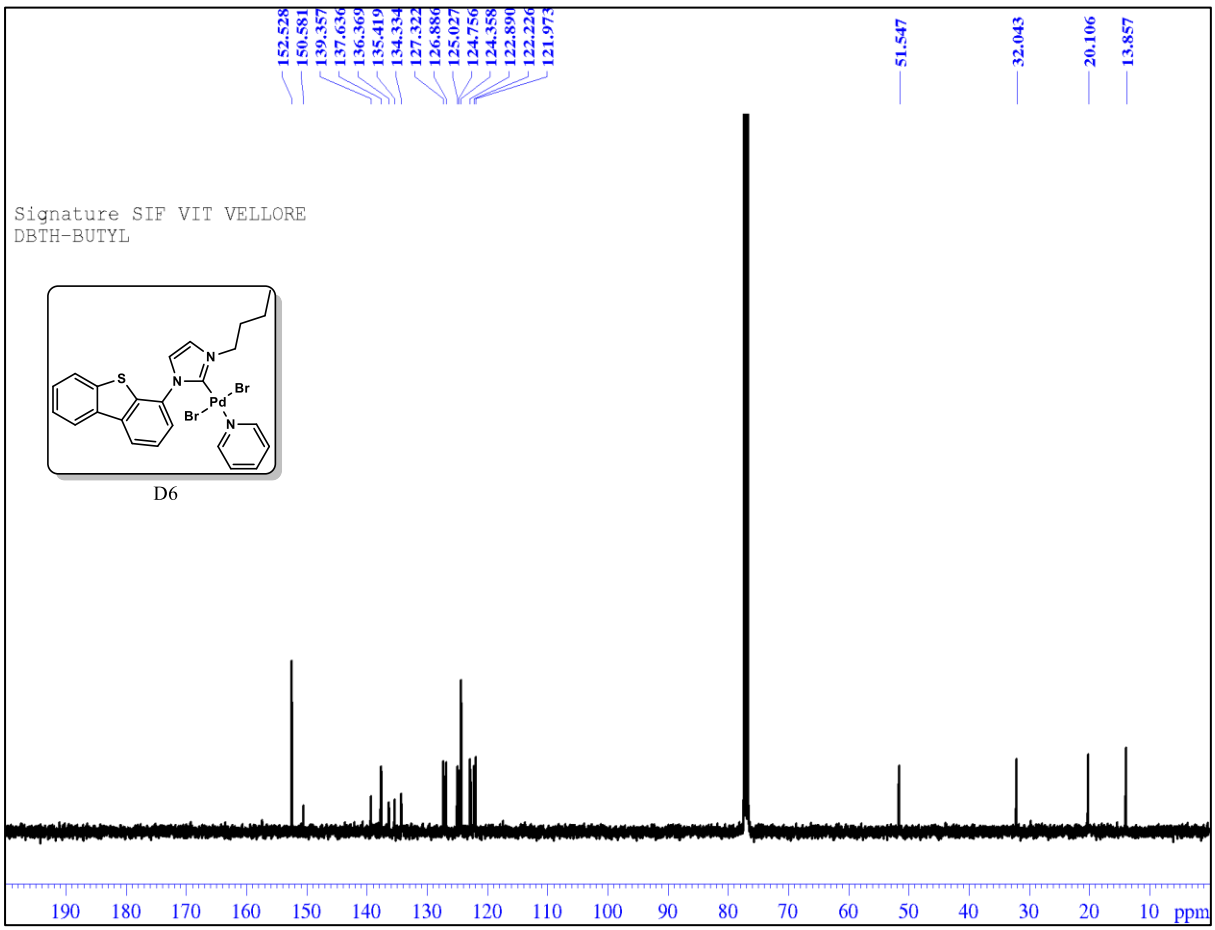
2.131
2.147
3.009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137.636
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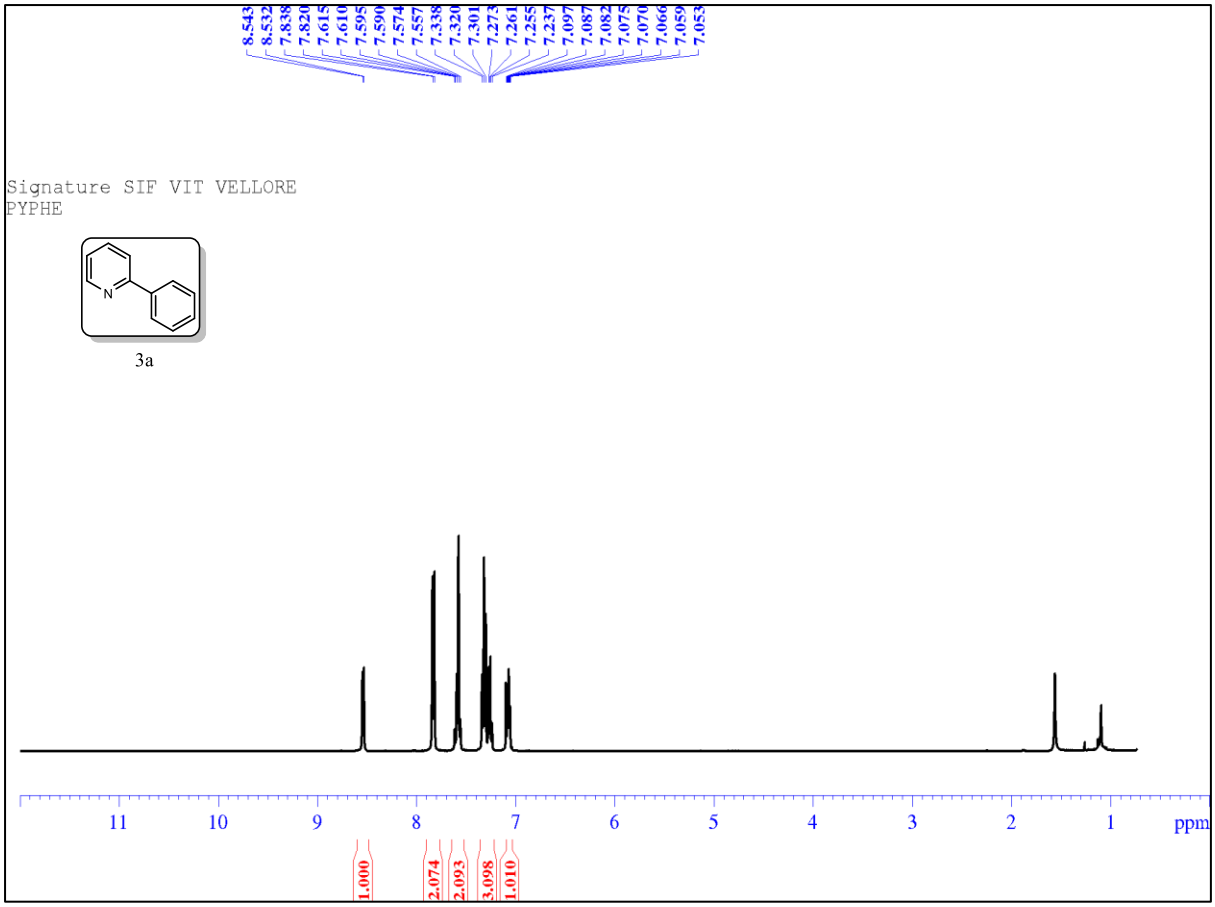
135.419
134.334
127.322
126.886
125.027
124.756
124.358
122.890
122.226
121.973
51.547
32.043
20.106
13.857
Signature SIF VIT VELLORE
DBTH-BUTYL
D6
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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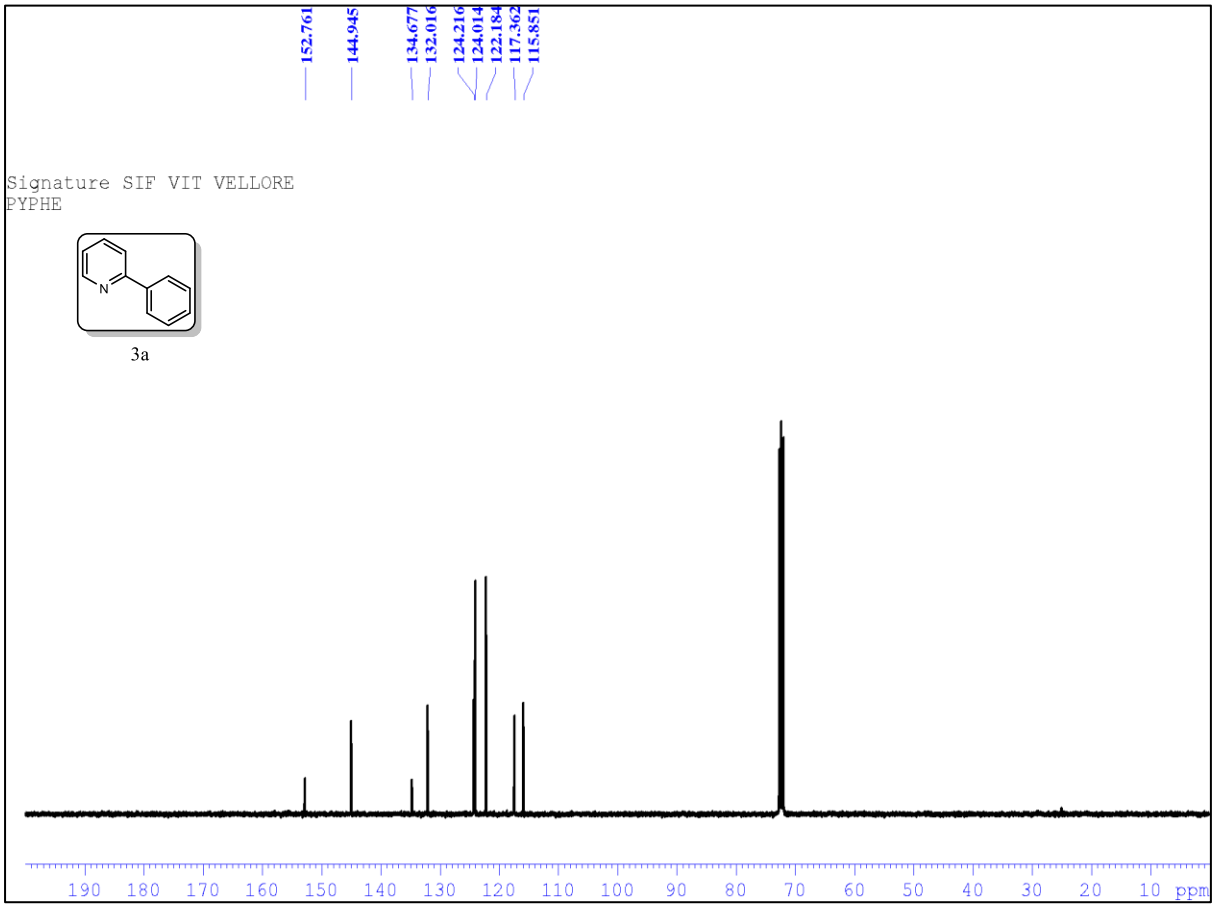
8.532
7.838
7.820
7.615
7.610
7.595
7.590
7.574
7.557
7.338
7.320
7.301
7.273
7.261
7.255
7.237
7.097
7.087
7.082
7.075
7.070
7.066
7.059
7.053
Signature SIF VIT VELLORE
PYPHE
N
3a
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
2.074
2.093
3.098
1.010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132.016
124.216
124.014
122.184
117.362
115.851
Signature SIF VIT VELLORE
PYPHE
N
3a
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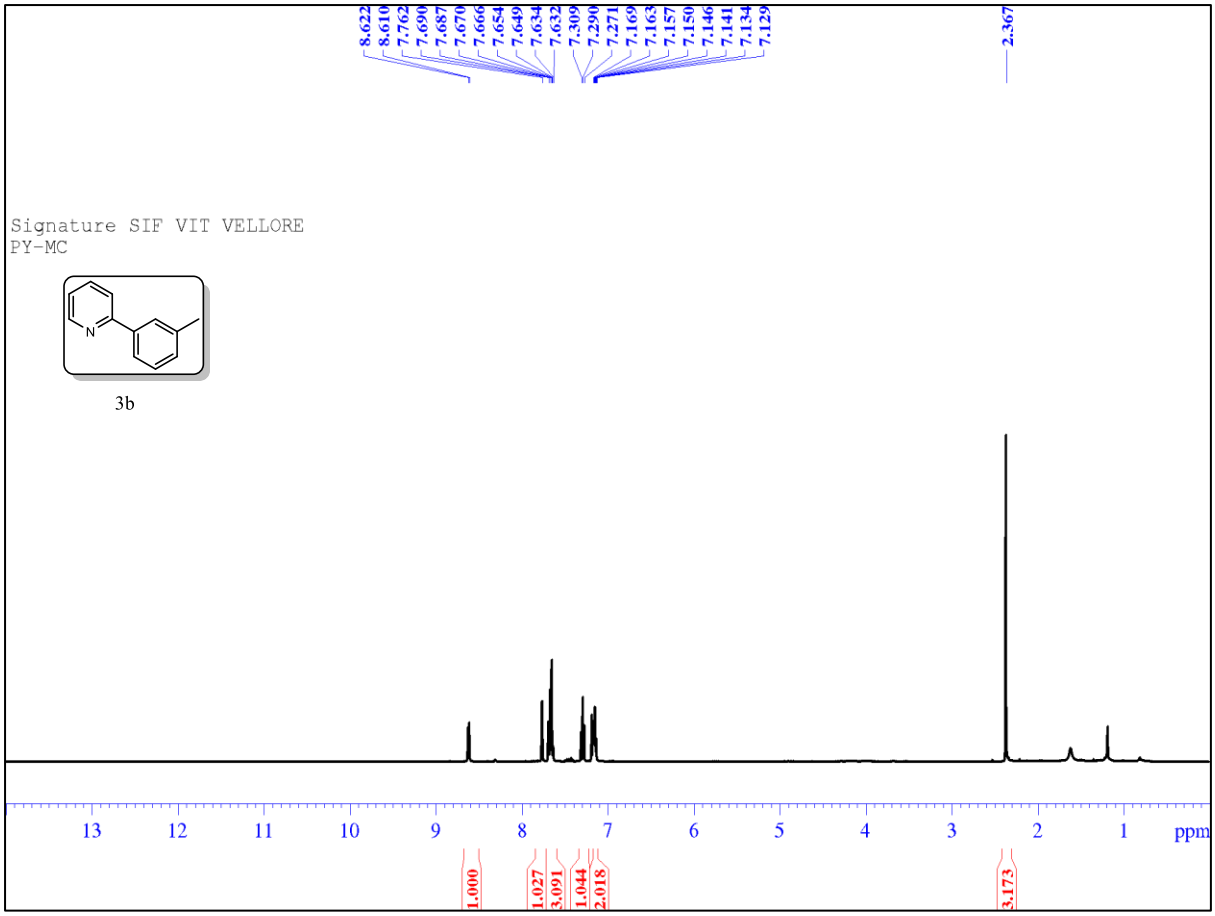
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.610
7.762
7.690
7.687
7.670
7.666
7.654
7.649
7.634
7.632
7.309
7.290
7.271
7.169
7.163
7.157
7.150
7.146
7.141
7.134
7.129
2.367
Signature SIF VIT VELLORE
PY-MC
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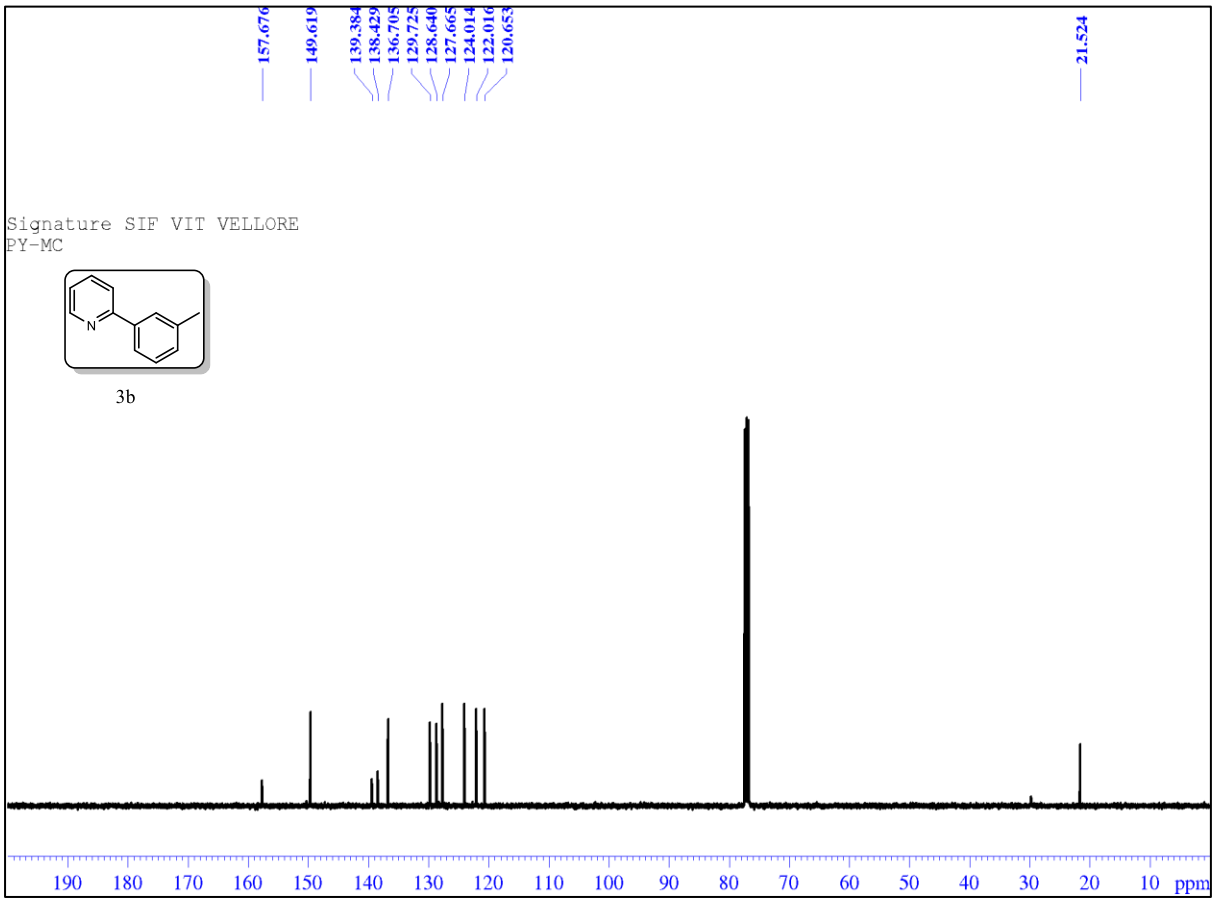
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.027
3.091
1.044
2.018
3.173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136.705
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128.640
127.665
124.014
122.016
120.653
21.524
Signature SIF VIT VELLORE
PY-MC
3b
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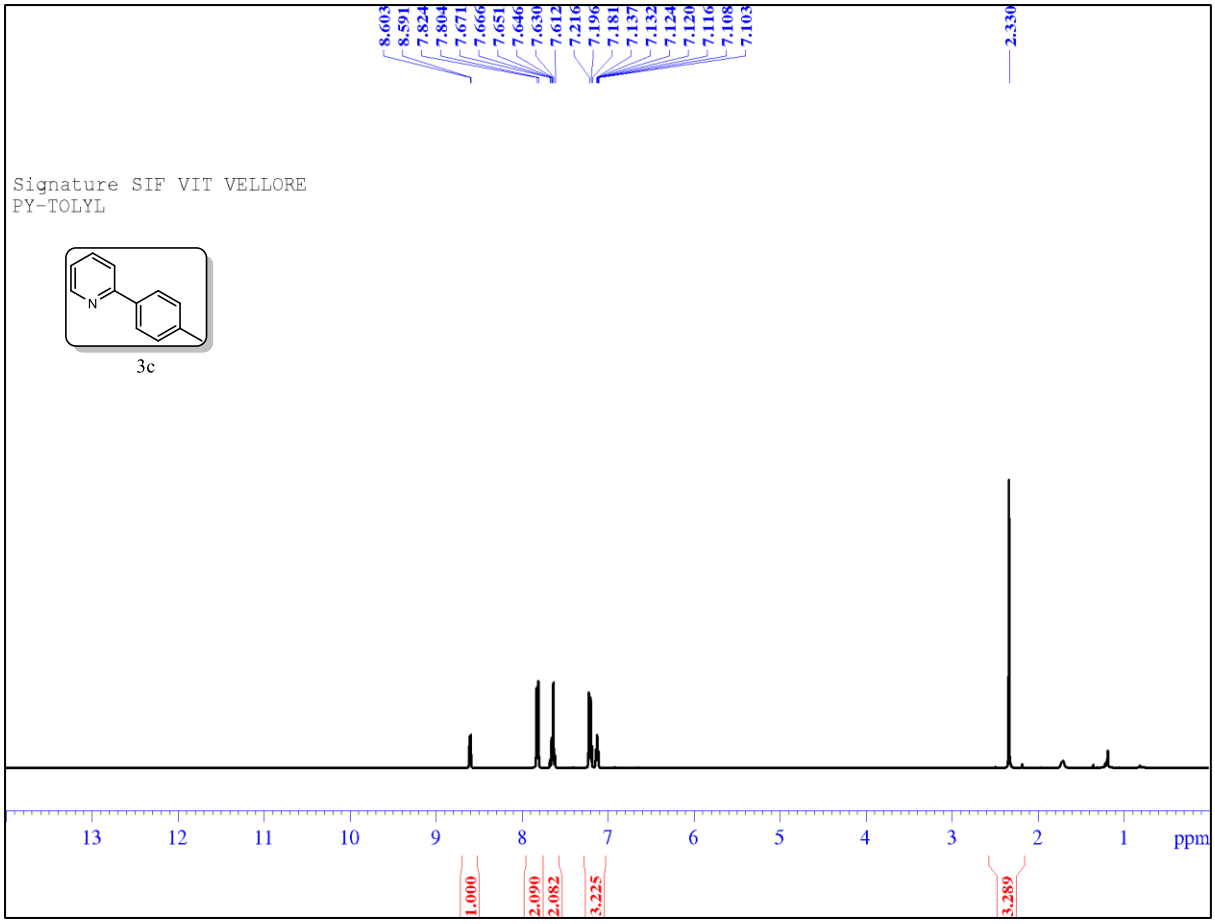
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8.591
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7.804
7.671
7.666
7.651
7.646
7.630
7.612
7.216
7.196
7.181
7.137
7.132
7.124
7.120
7.116
7.108
7.103
2.330
Signature SIF VIT VELLORE
PY-TOLYL
3c
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
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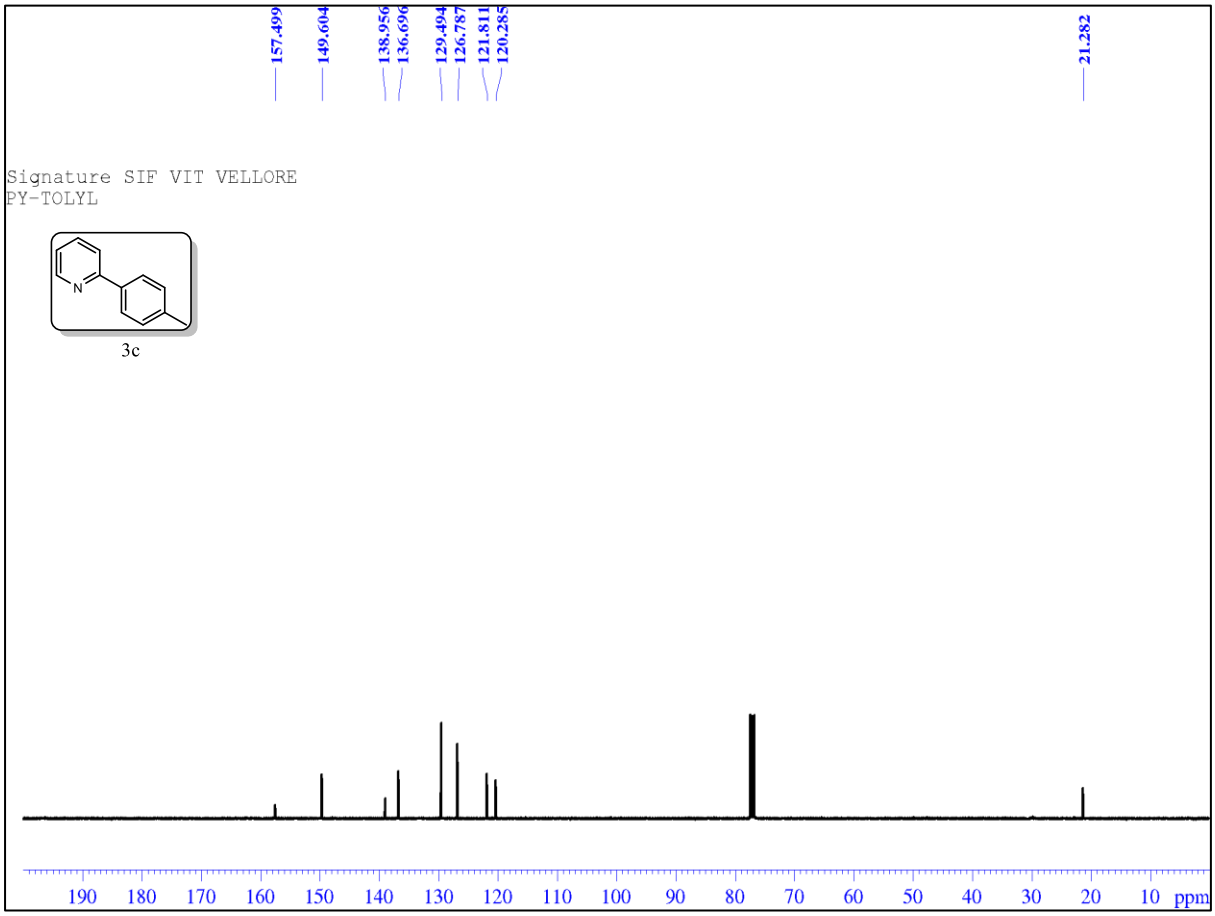
2.090
2.082
3.225
3.289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138.956
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129.494
126.787
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120.285
21.282
Signature SIF VIT VELLORE
PY-TOLYL
3c
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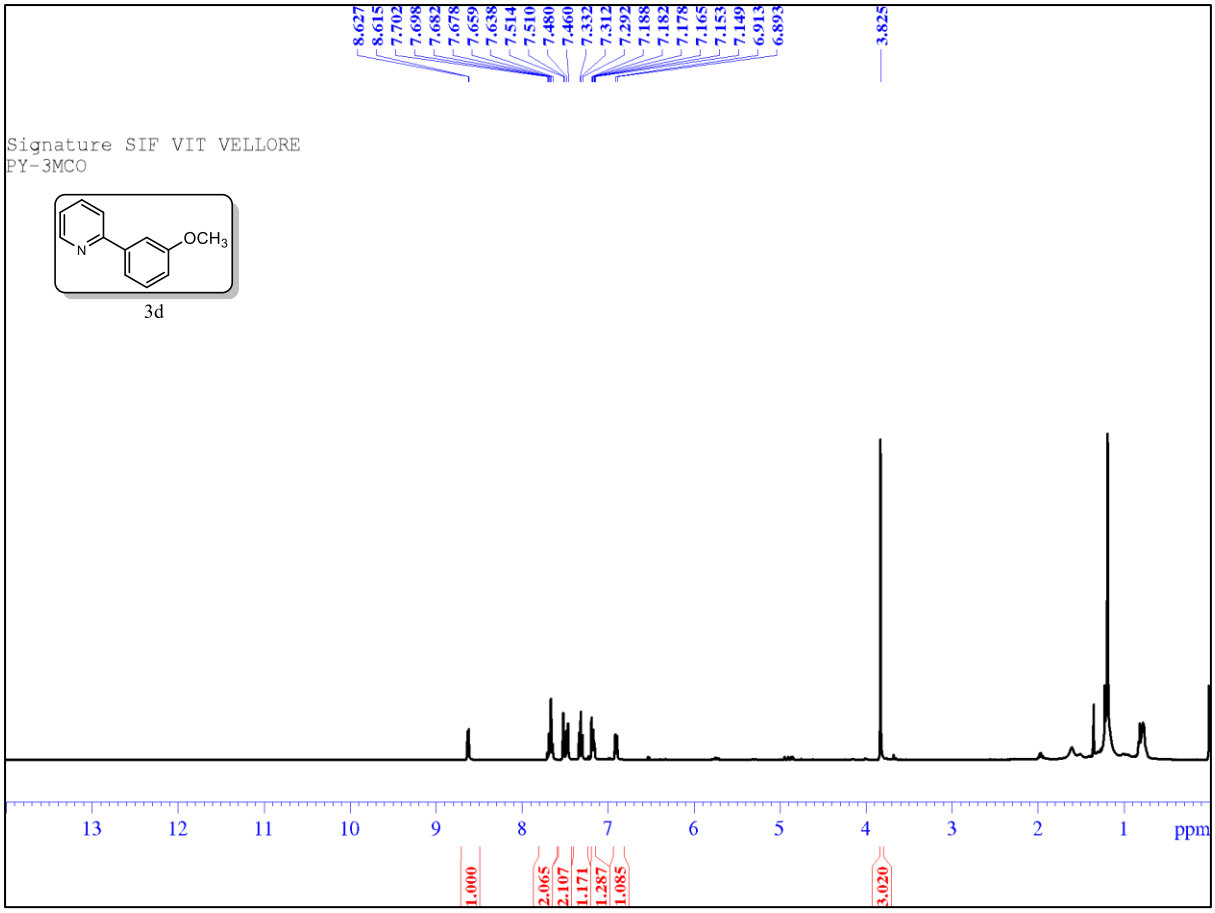
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7.659
7.638
7.514
7.510
7.480
7.460
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7.312
7.292
7.188
7.182
7.178
7.165
7.153
7.149
6.913
6.893
3.825
Signature SIF VIT VELLORE
PY-3MCO
OCH3
3d
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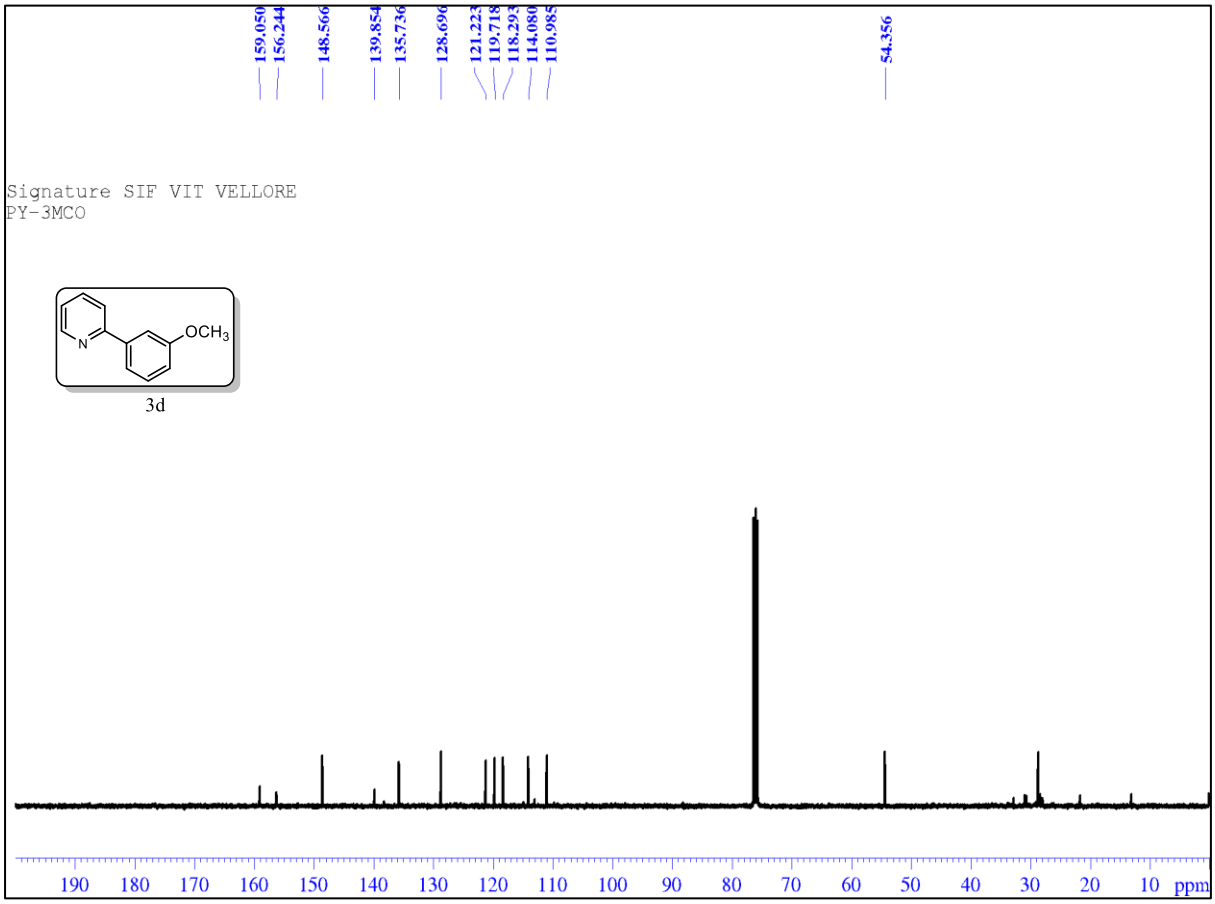
1.000
2.065
2.107
1.171
1.287
1.085
3.020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156.244
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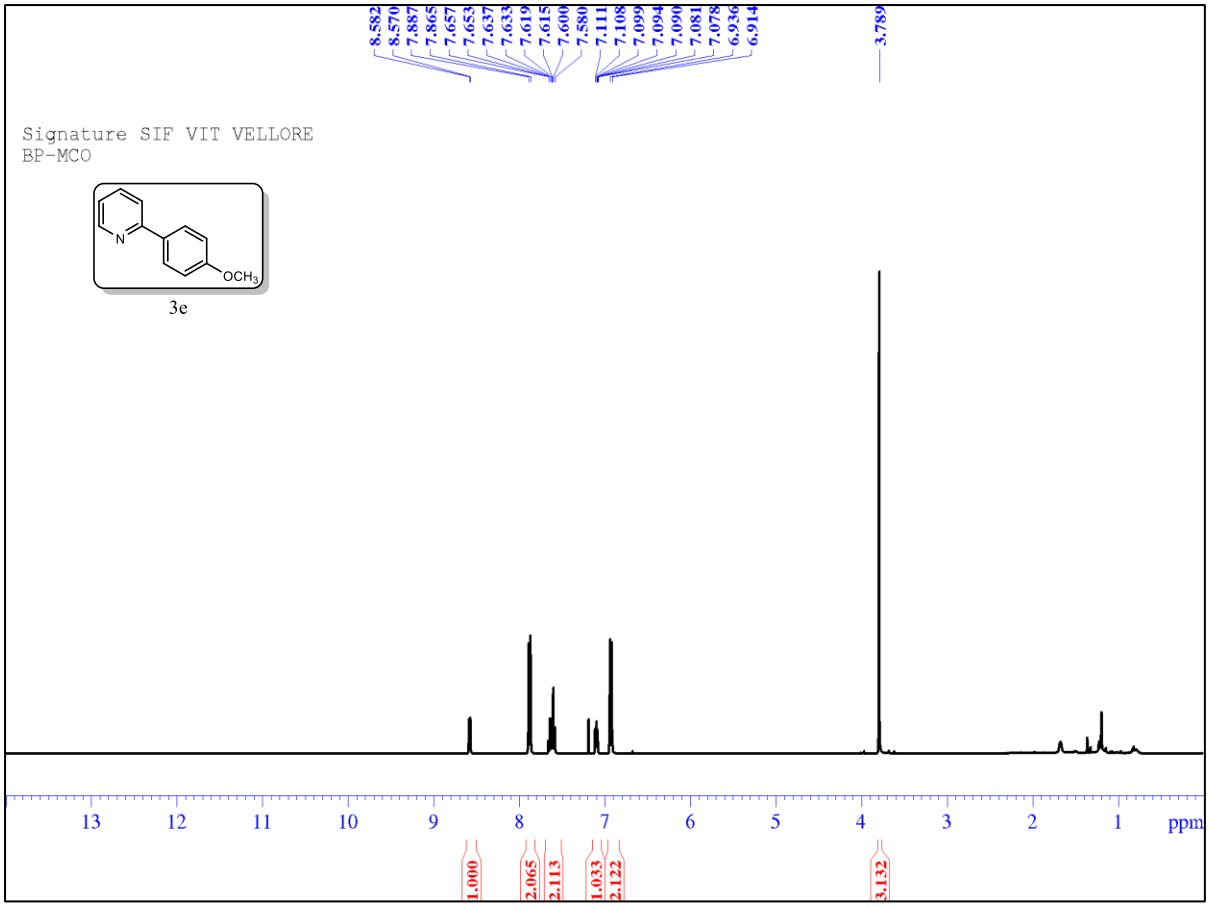
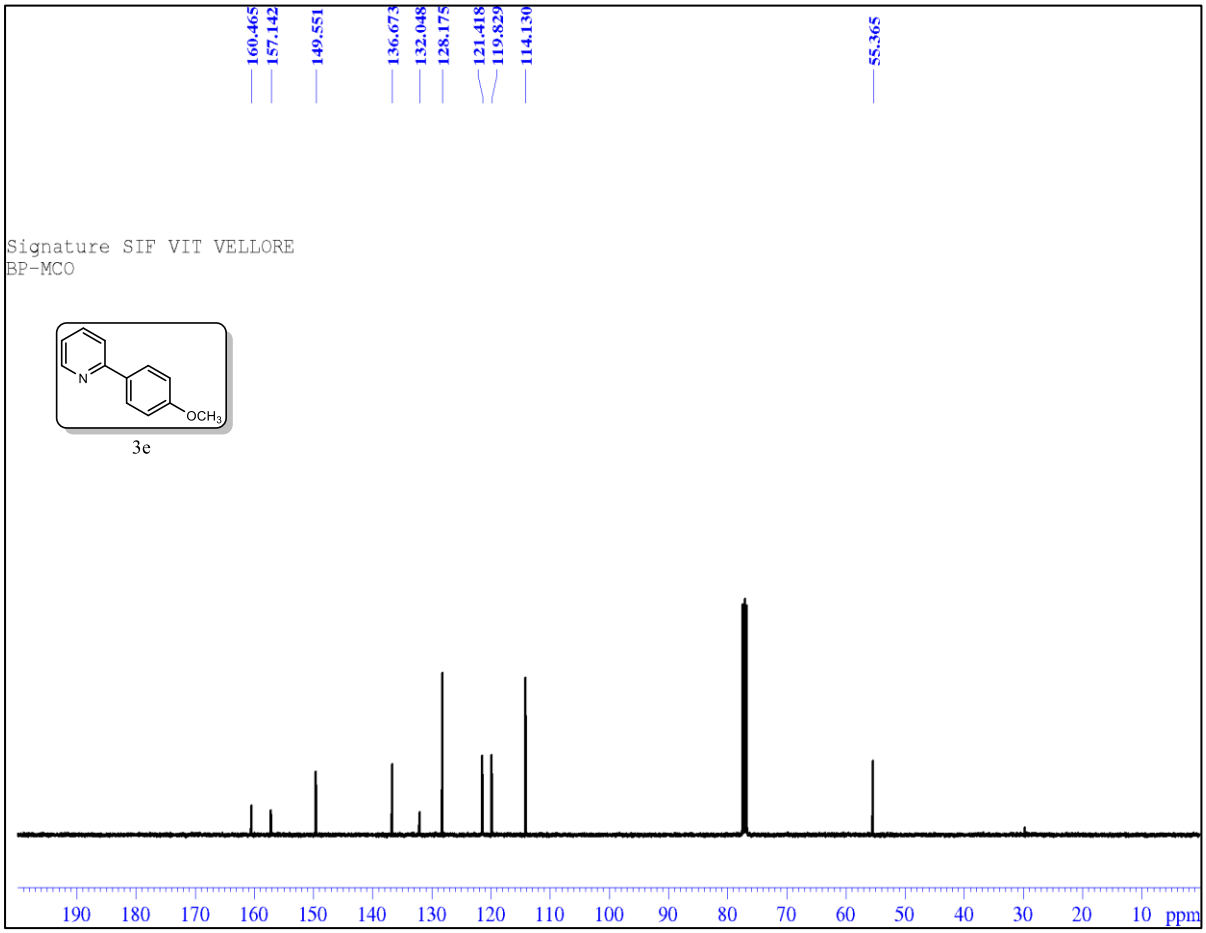
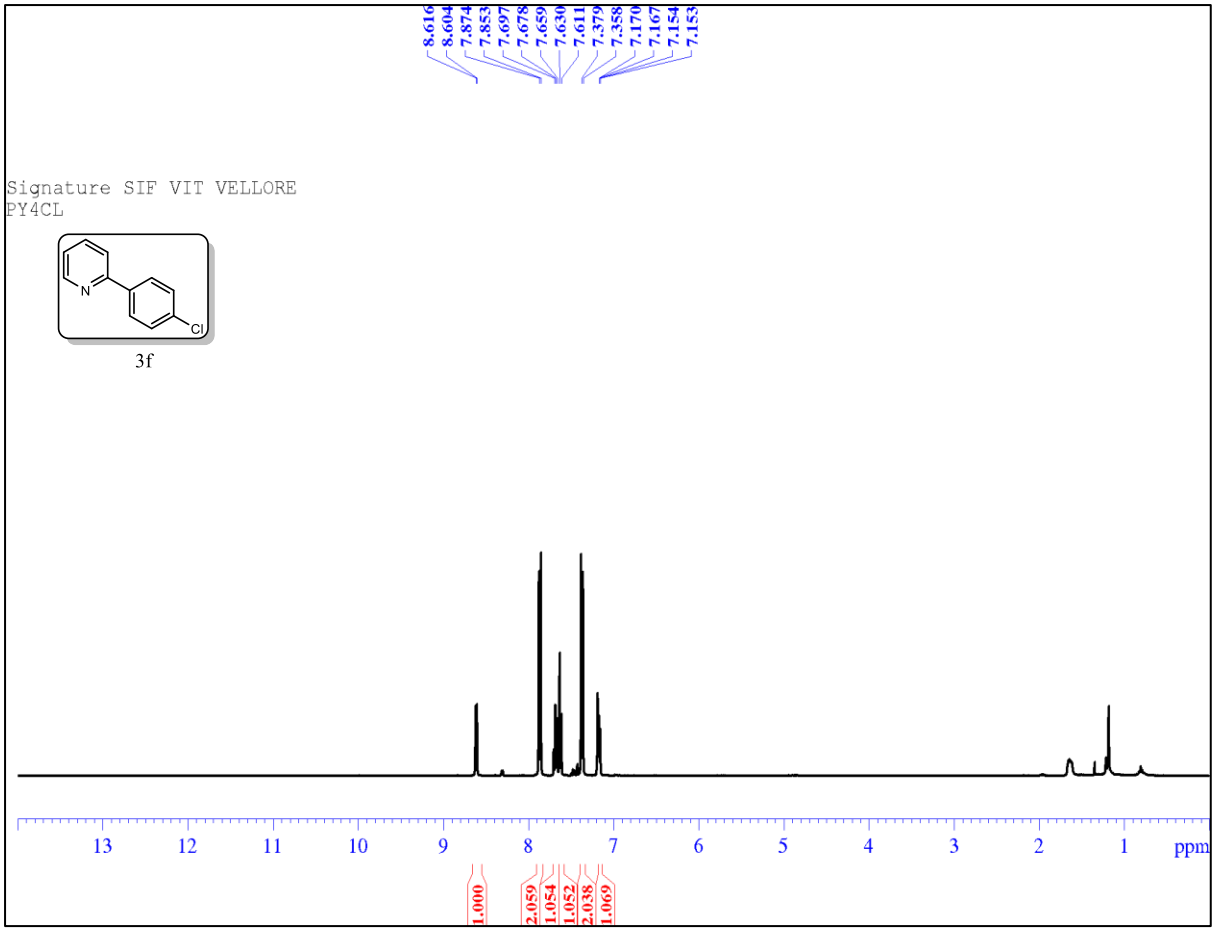
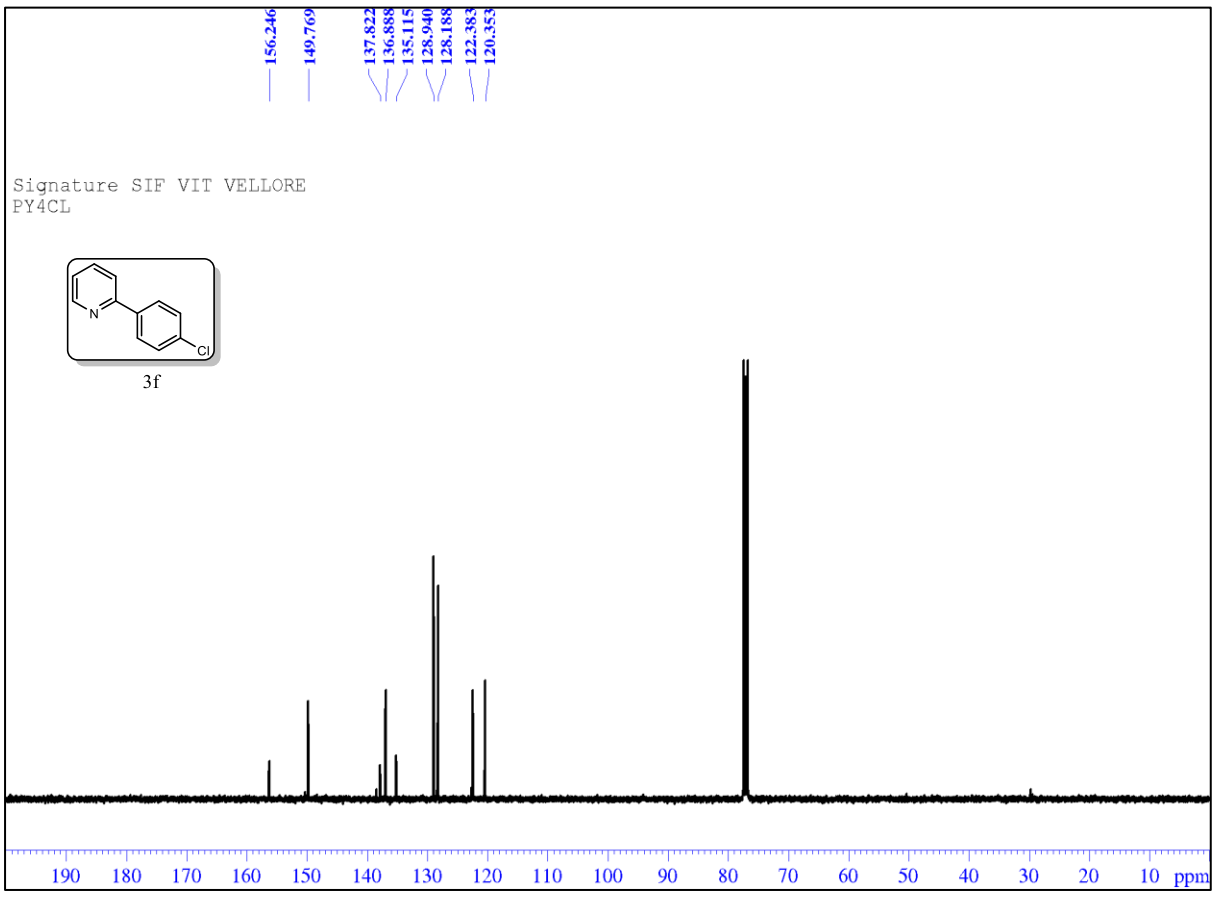
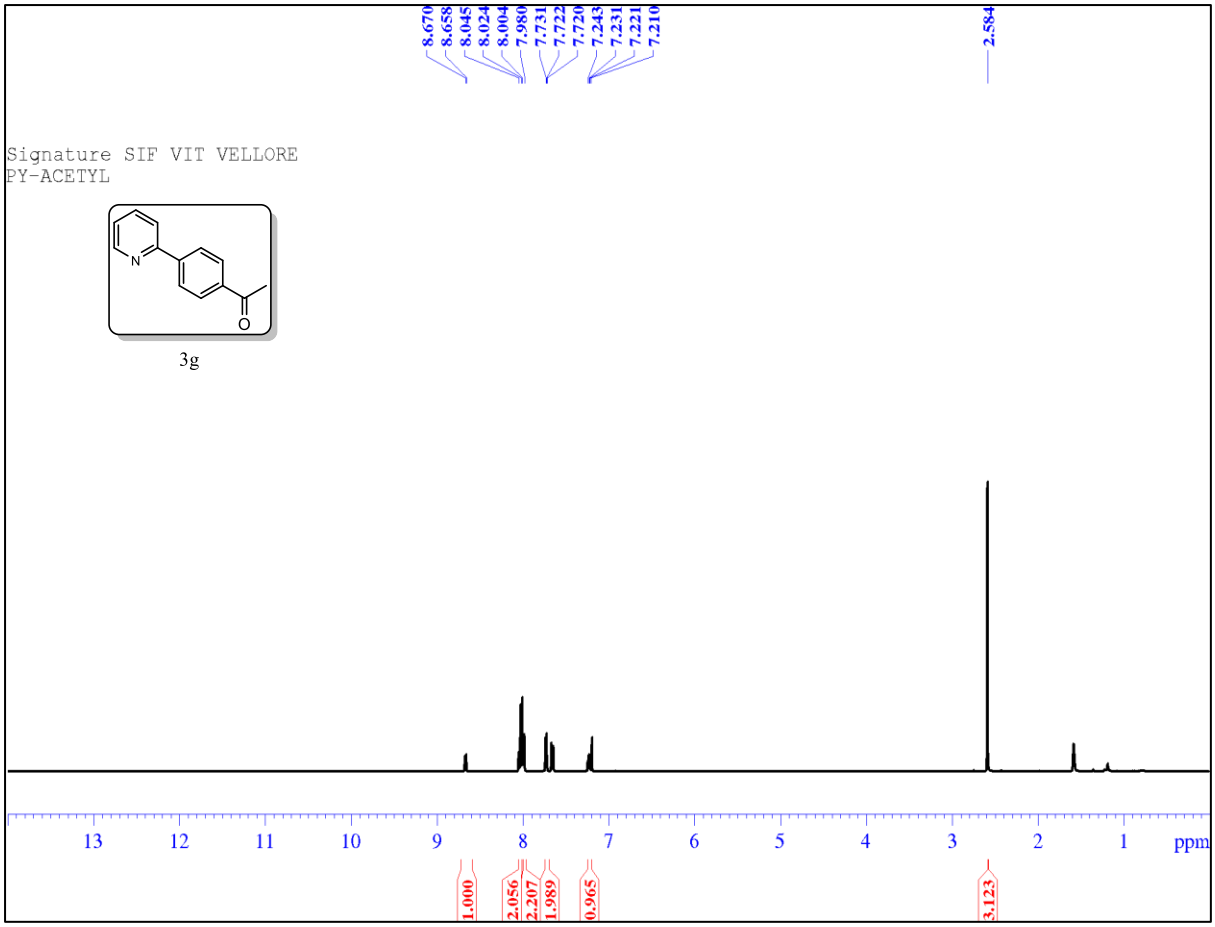
139.854
135.736
128.696
121.223
119.718
118.293
114.080
110.985
54.356
Signature SIF VIT VELLORE
PY-3MCO
OCH3
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

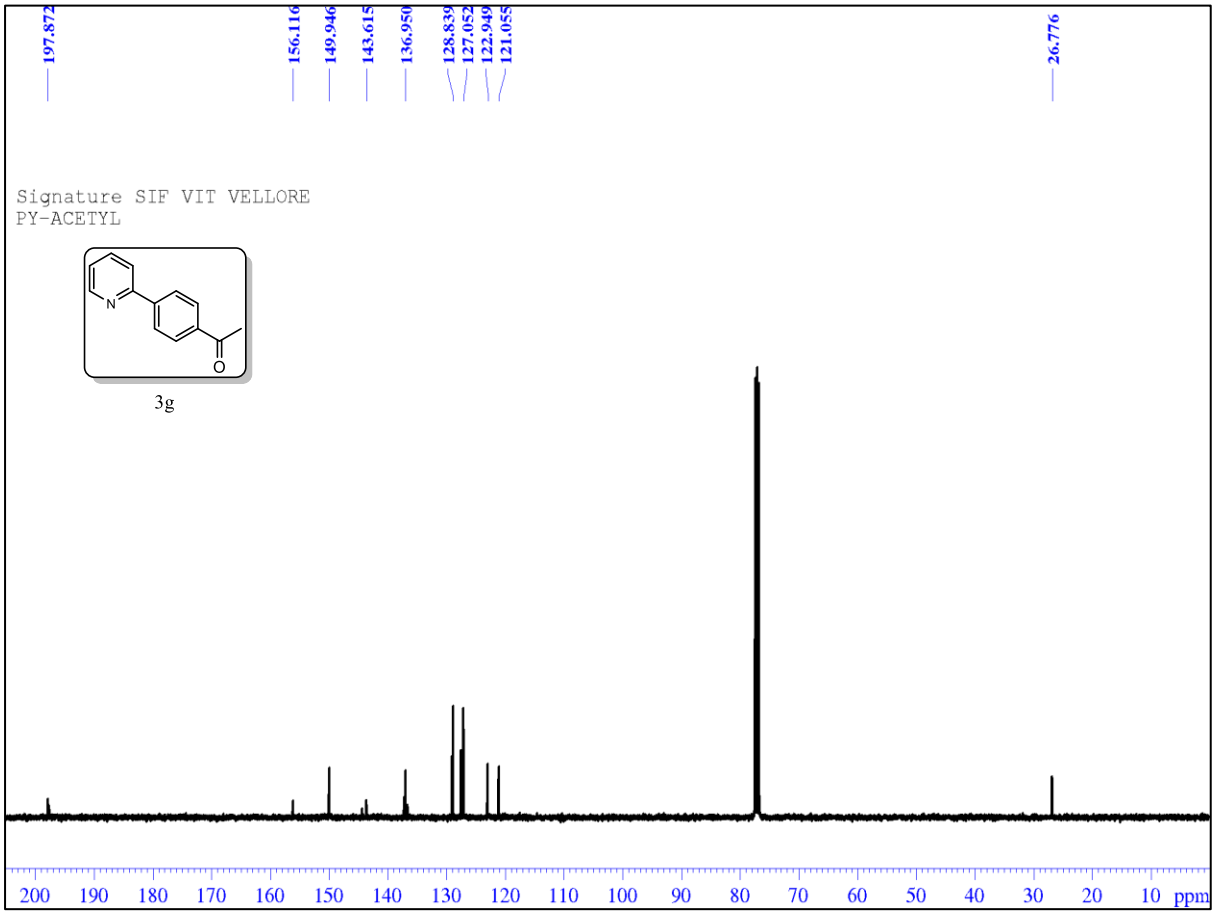

8.582
8.570
7.887
7.865
7.657
7.653
7.637
7.633
7.619
7.615
7.600
7.580
7.111
7.108
7.099
7.094
7.090
7.081
7.078
6.936
6.914
3.789
Signature SIF VIT VELLORE
BP-MCO
N
OCH3
3e
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
2.065
2.113
1.033
2.122
3.132

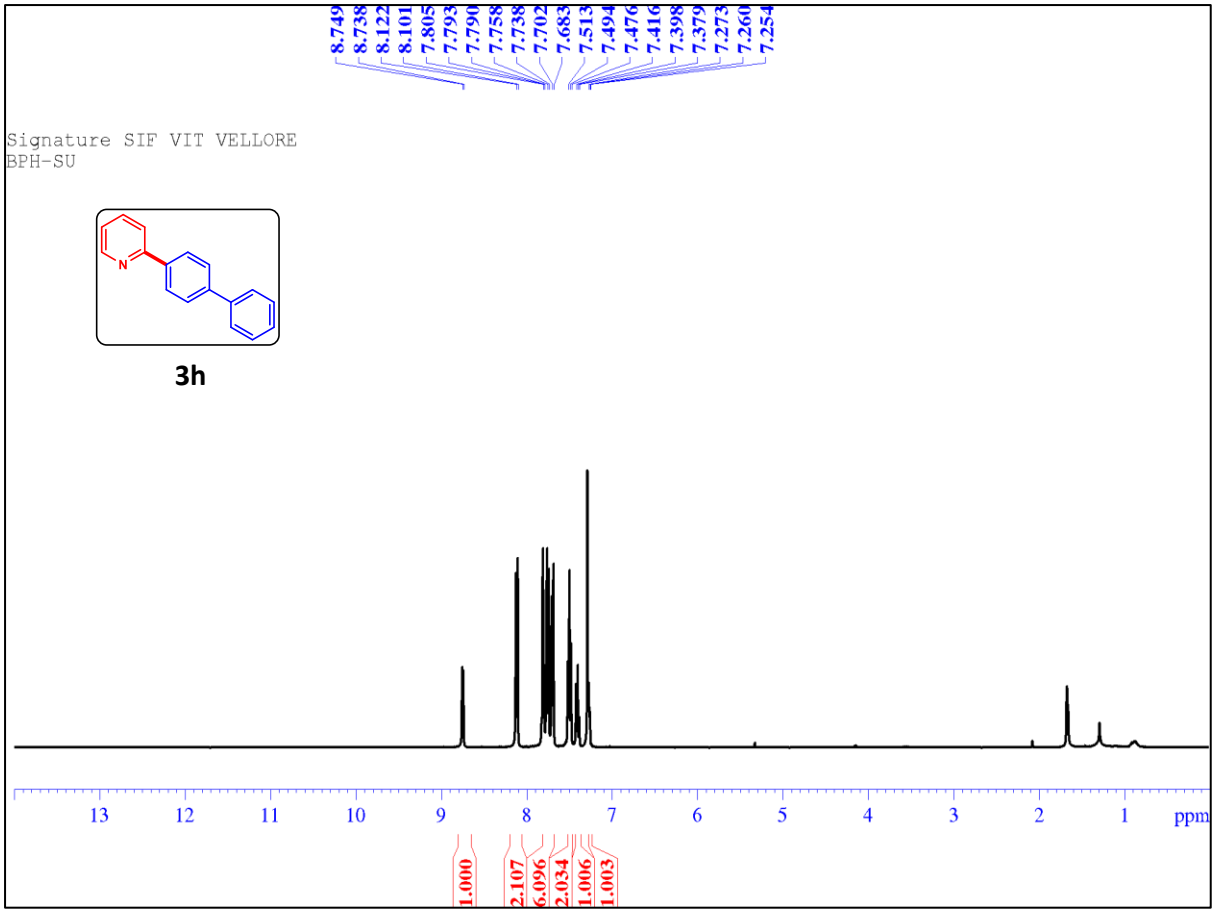

160.465
157.142
149.551
136.673
132.048
128.175
121.418
119.829
114.130
55.365
Signature SIF VIT VELLORE
BP-MCO
N
OCH3
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

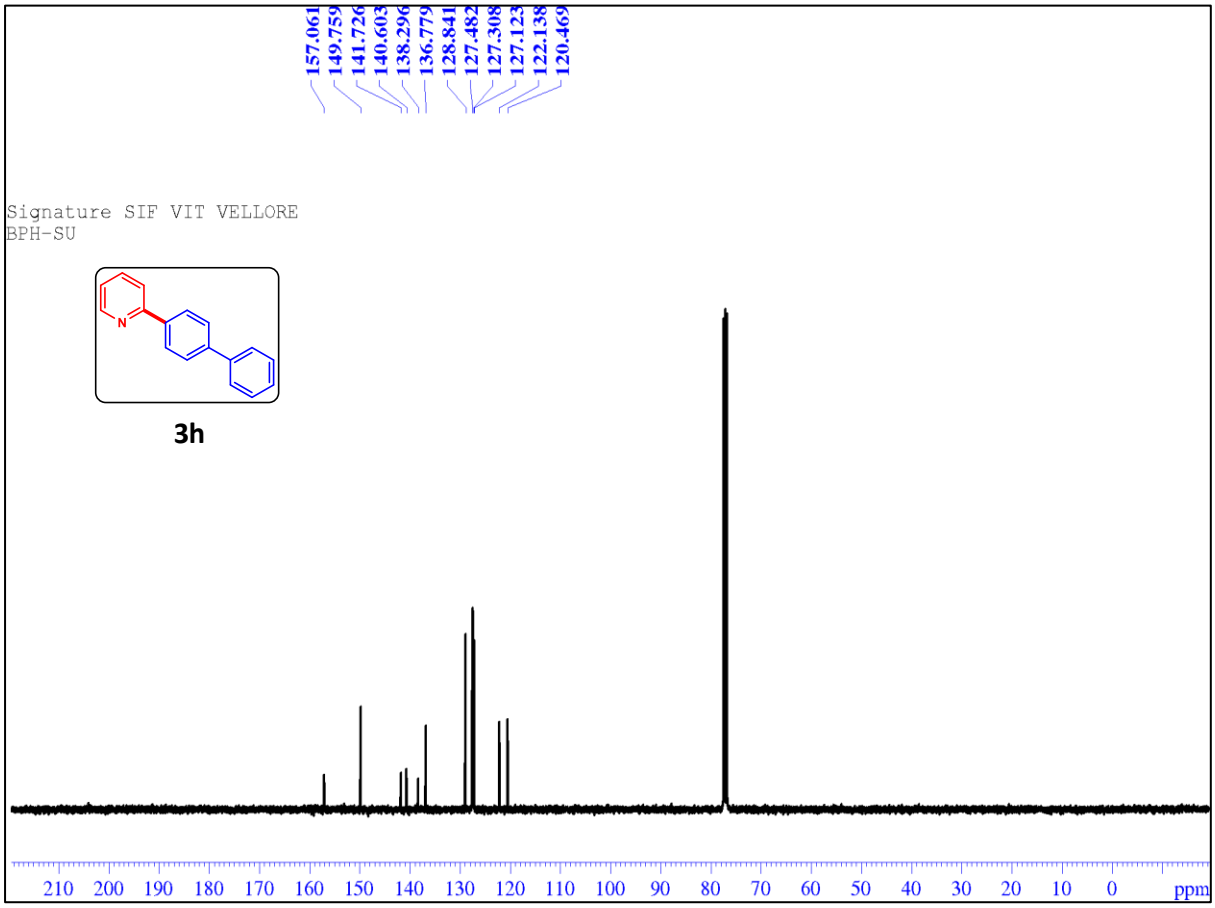

8.616
8.604
7.874
7.853
7.697
7.678
7.659
7.630
7.611
7.379
7.358
7.170
7.167
7.154
7.153
Signature SIF VIT VELLORE
PY4CL
N
Cl
3f
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
2.059
1.054
1.052
2.038
1.069

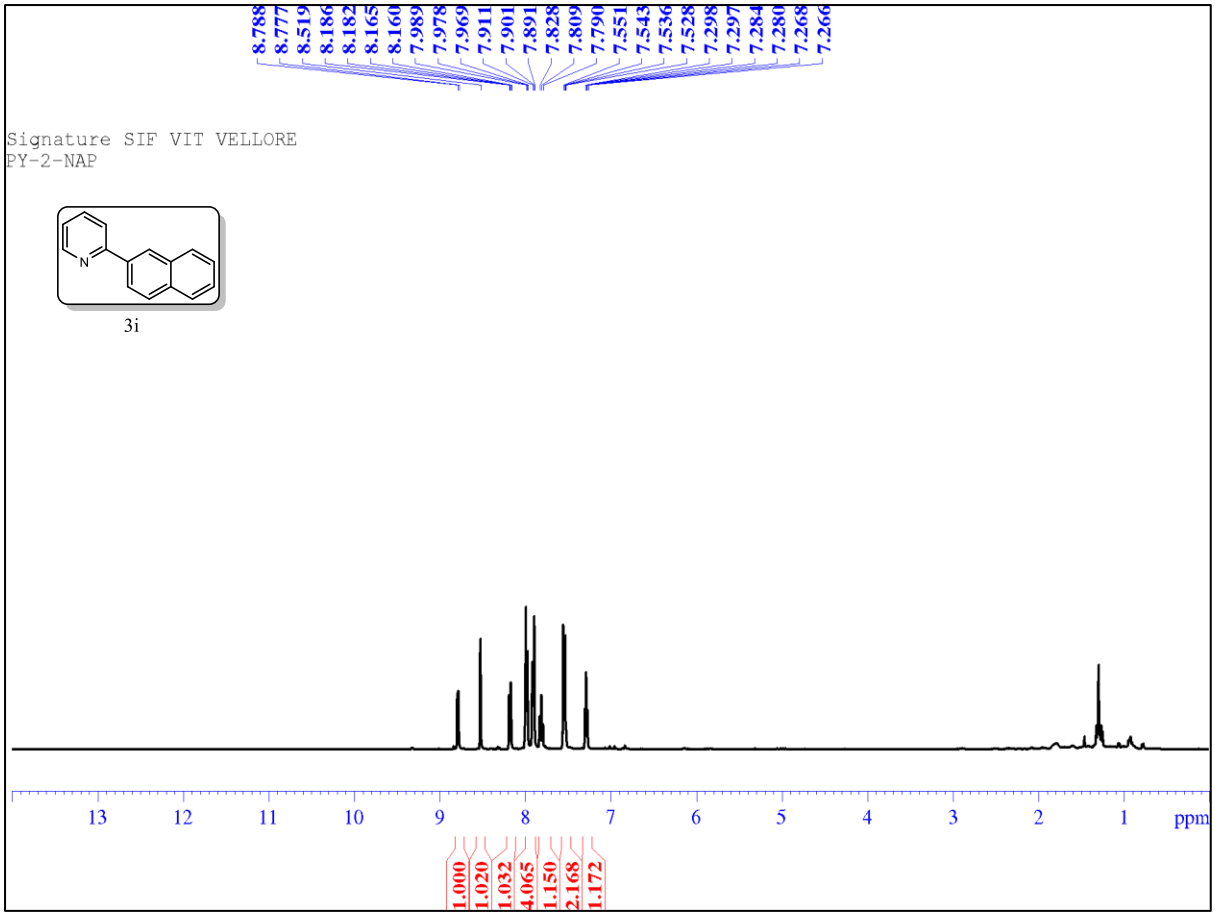

156.246
149.769
137.822
136.888
135.115
128.940
128.188
122.383
120.353
Signature SIF VIT VELLORE
PY4CL
N
Cl
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

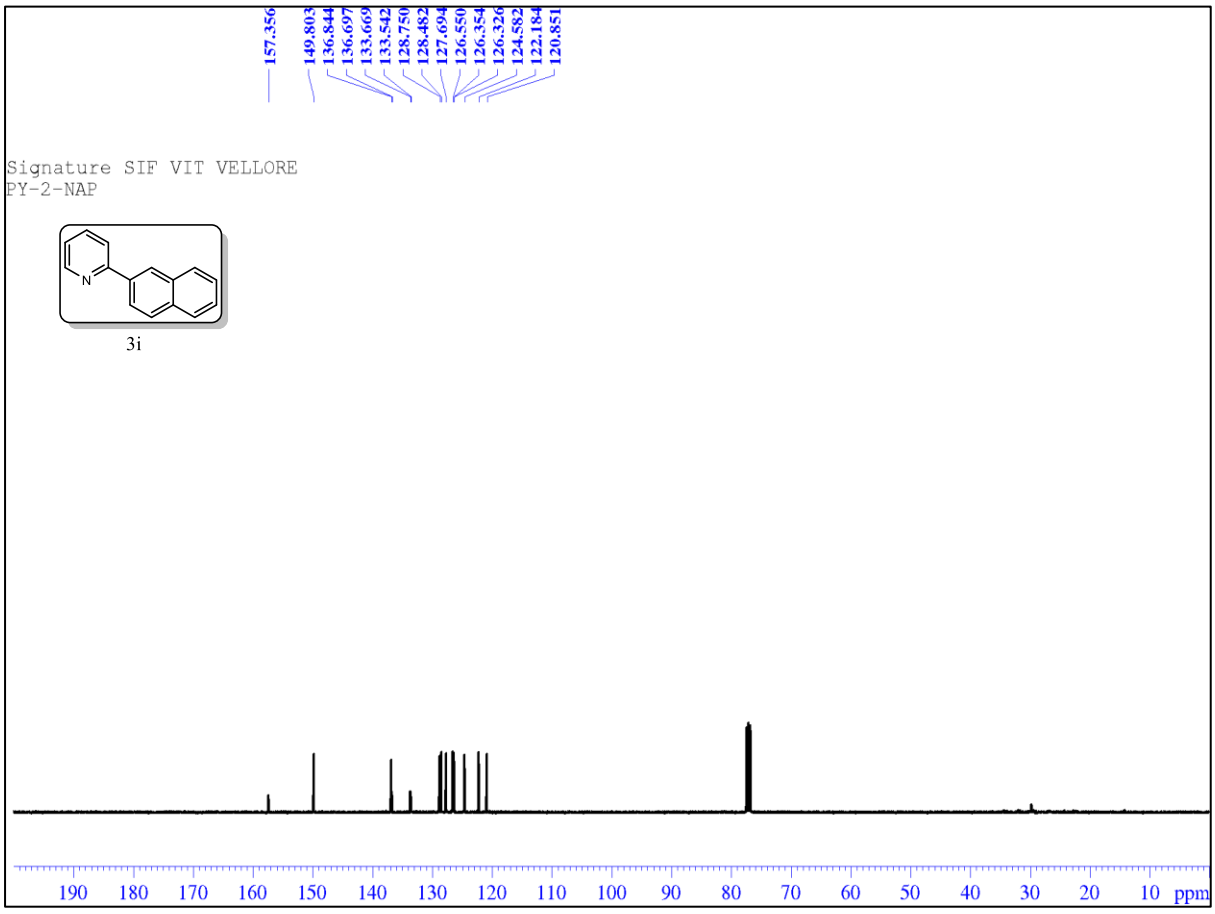

8.670
8.658
8.045
8.024
8.004
7.980
7.731
7.722
7.720
7.243
7.231
7.221
7.210
2.584
Signature SIF VIT VELLORE
PY-ACETYL
N
O
3g
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
2.056
2.207
1.989
0.965
3.123

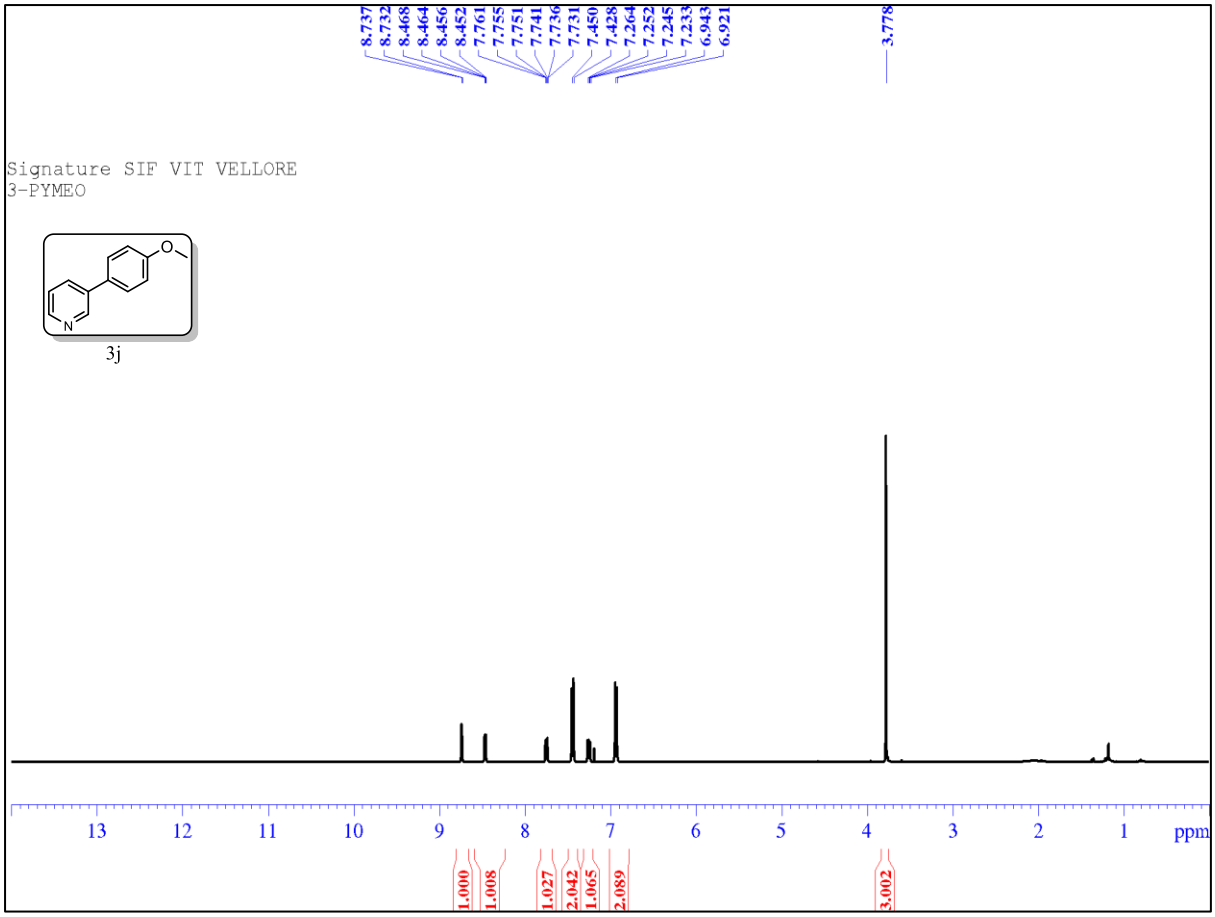

197.872
156.116
149.946
143.615
136.950
128.839
127.052
122.949
121.055
26.776
Signature SIF VIT VELLORE
PY-ACETYL
N
O
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

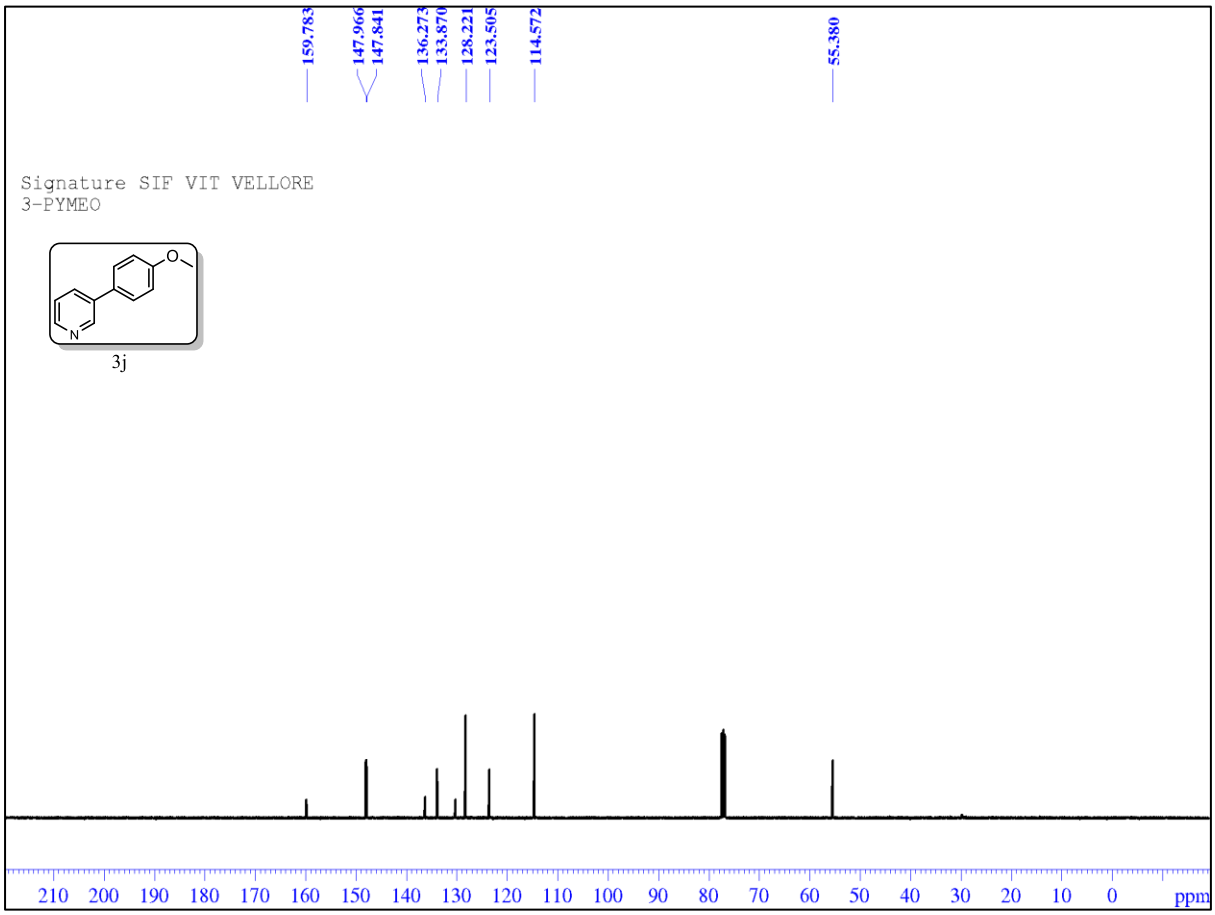

8.749
8.738
8.122
8.101
7.805
7.793
7.790
7.758
7.738
7.702
7.683
7.513
7.494
7.476
7.416
7.398
7.379
7.273
7.260
7.254
Signature SIF VIT VELLORE
BPH-SU
3h
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
2.107
6.096
2.034
1.006
1.003

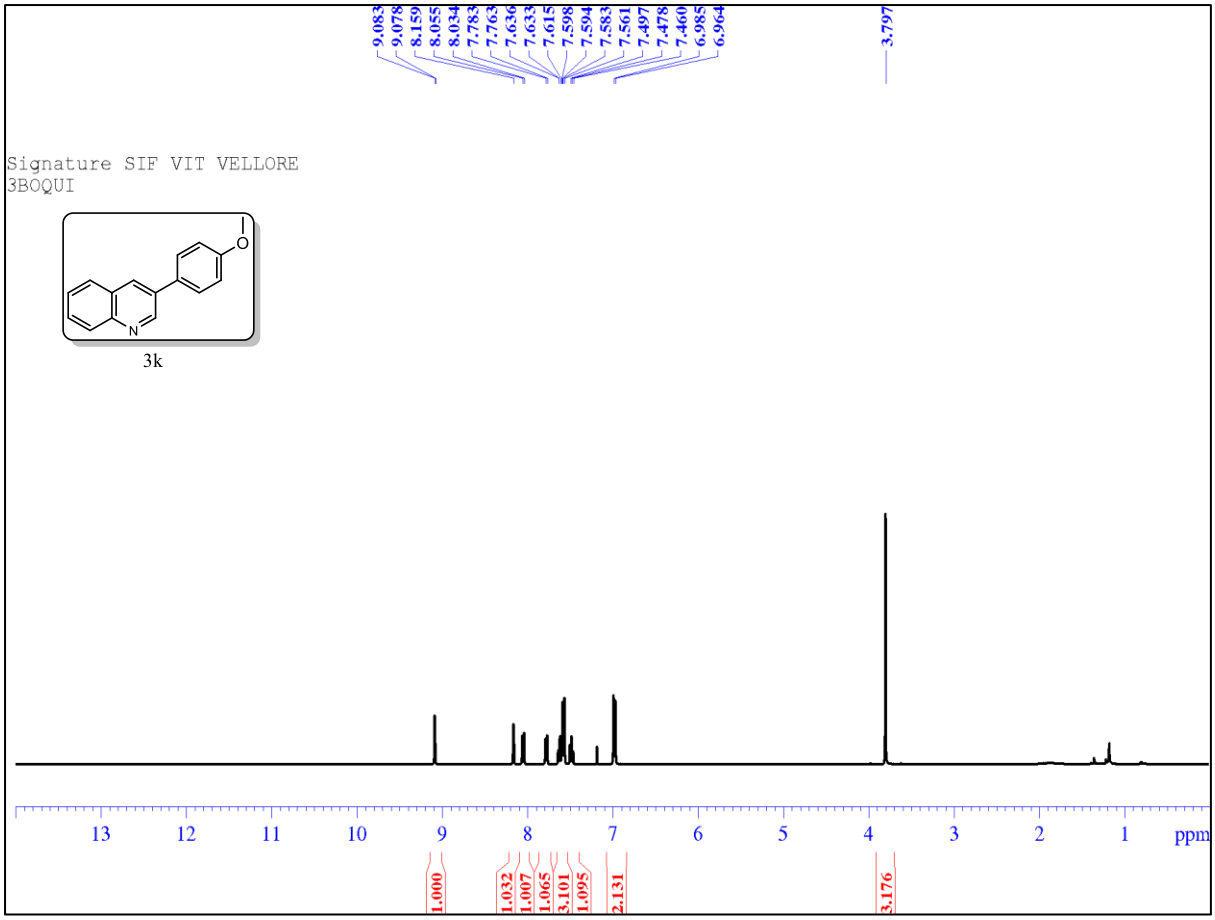

157.061
149.759
141.726
140.603
138.296
136.779
128.841
127.482
127.308
127.123
122.138
120.469
Signature SIF VIT VELLORE
BPH-SU
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

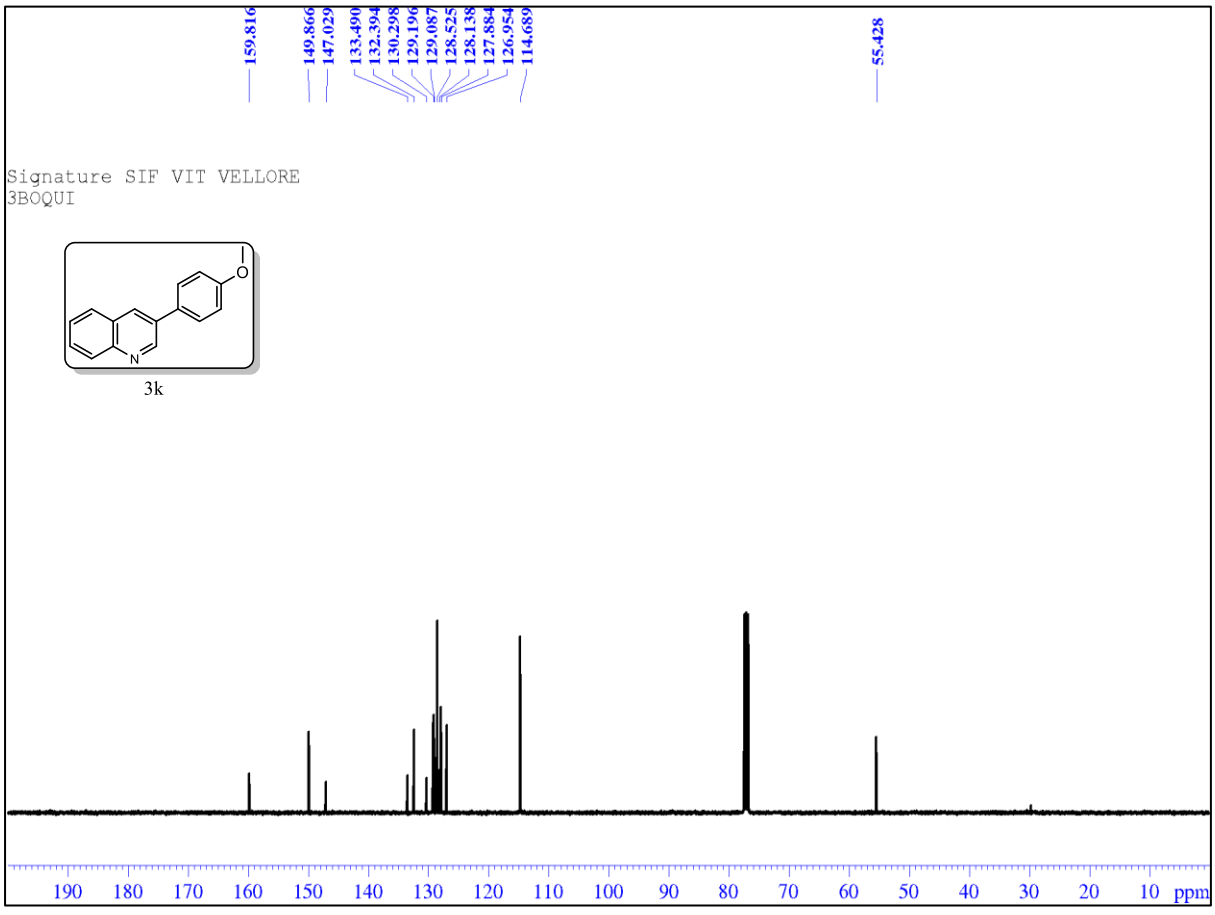

8.788
8.777
8.519
8.186
8.182
8.165
8.160
7.989
7.978
7.969
7.911
7.901
7.891
7.828
7.809
7.790
7.551
7.543
7.536
7.528
7.298
7.297
7.284
7.280
7.268
7.266
Signature SIF VIT VELLORE
PY-2-NAP
3i
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.020
1.032
4.065
1.150
2.168
1.172

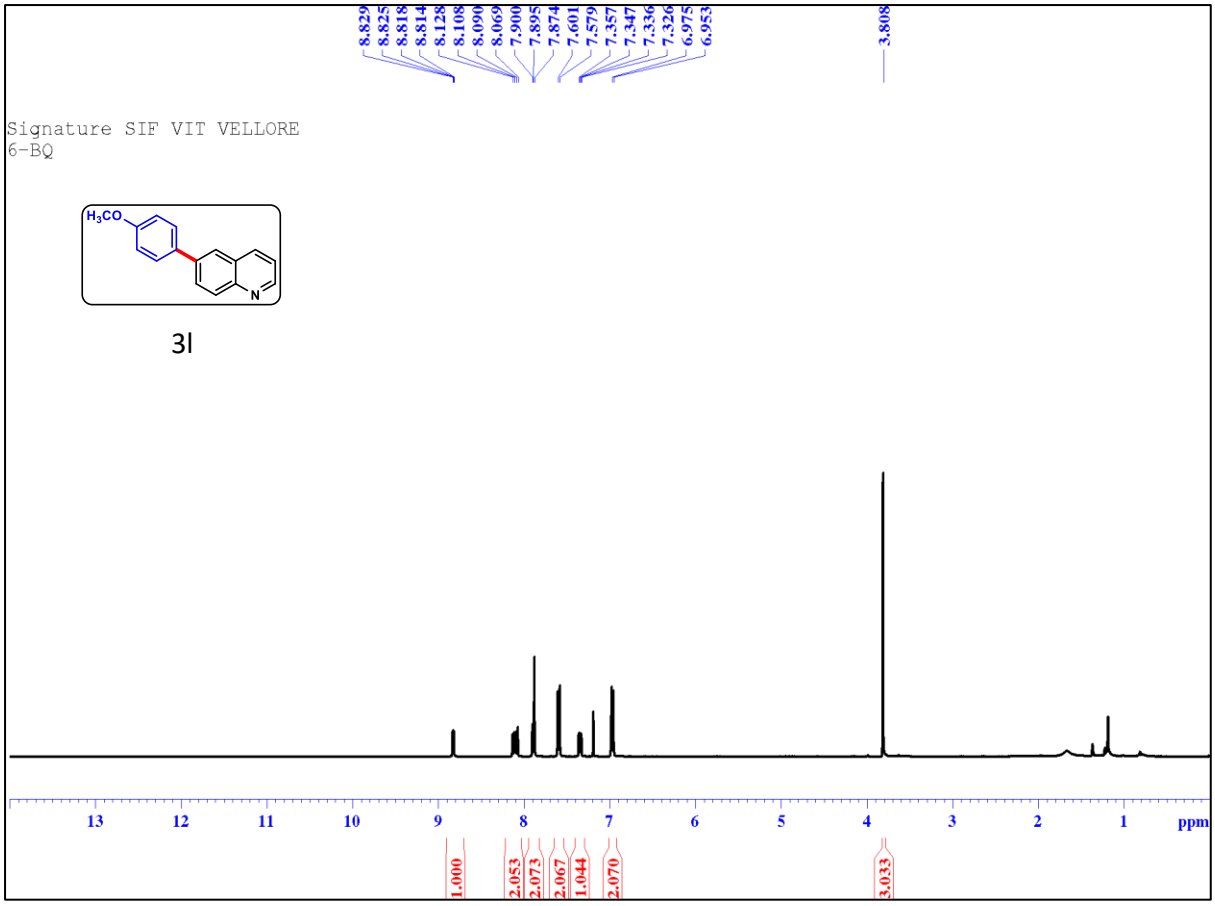

157.356
149.803
136.844
136.697
133.669
133.542
128.750
128.482
127.694
126.550
126.354
126.326
124.582
122.184
120.851
Signature SIF VIT VELLORE
PY-2-NAP
3i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

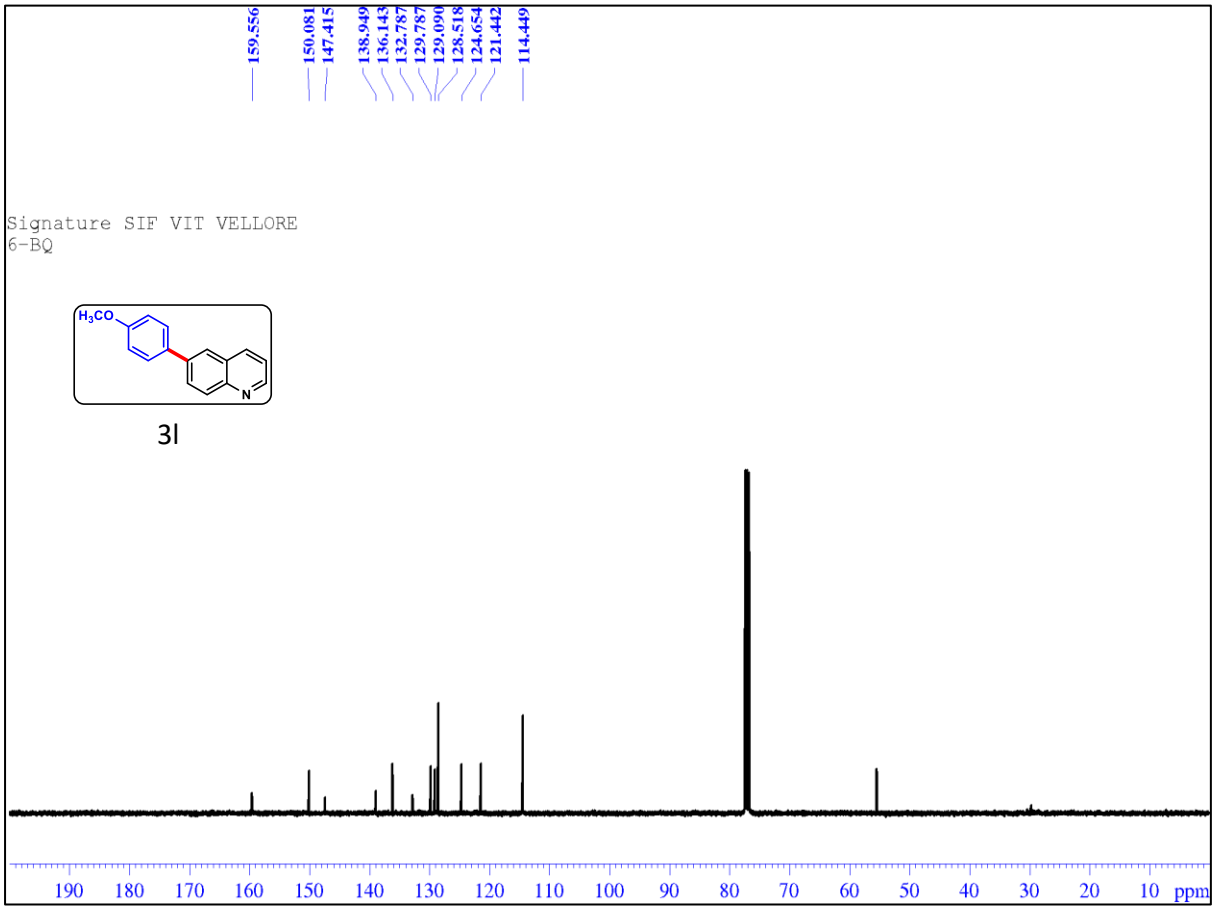

8.737
8.732
8.468
8.464
8.456
8.452
7.761
7.755
7.751
7.741
7.736
7.731
7.450
7.428
7.264
7.252
7.245
7.233
6.943
6.921
3.778
Signature SIF VIT VELLORE
3-PYMEO
3j
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.008
1.027
2.042
1.065
2.089
3.002

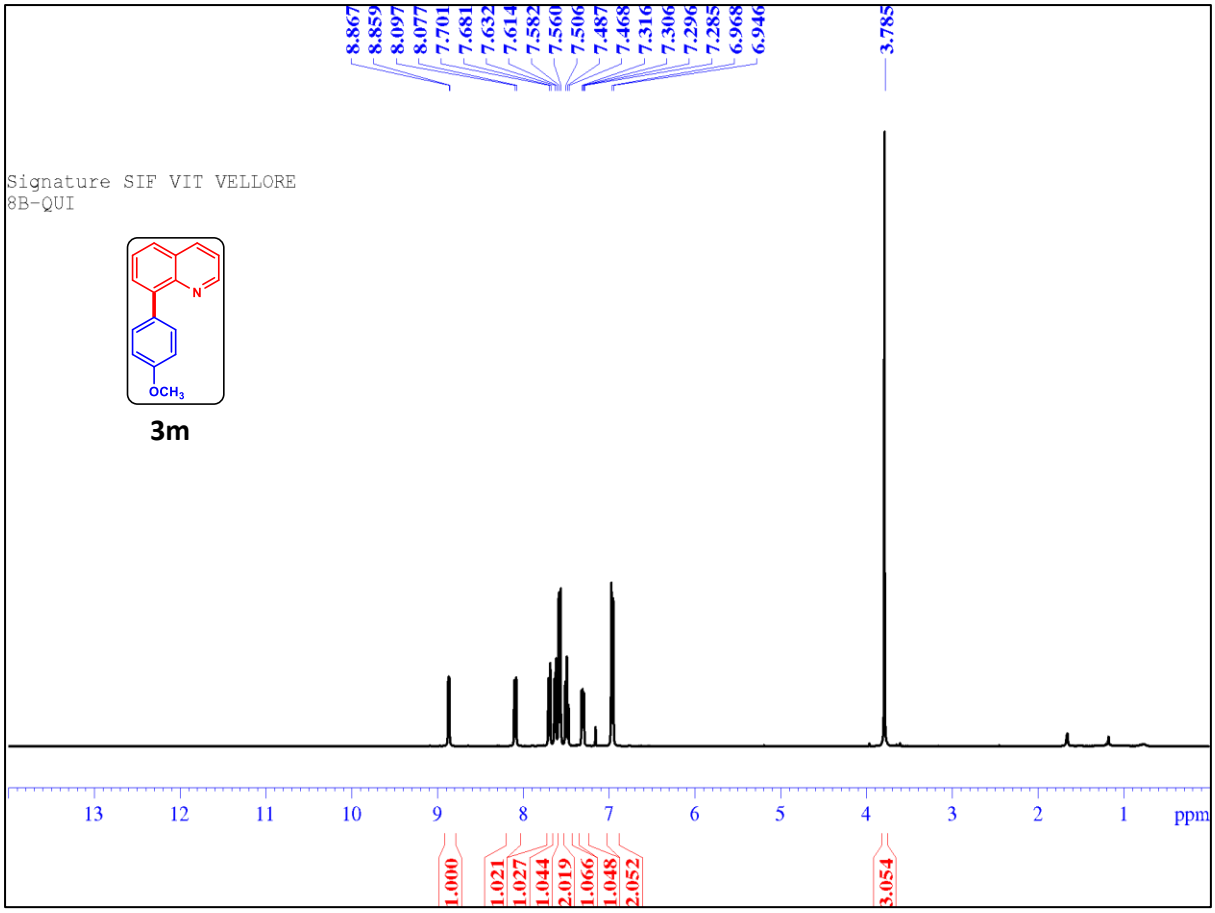

159.783
147.966
147.841
136.273
133.870
128.221
123.505
114.572
55.380
Signature SIF VIT VELLORE
3-PYMEO
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


9.083
9.078
8.159
8.055
8.034
7.783
7.763
7.636
7.633
7.615
7.598
7.594
7.583
7.561
7.497
7.478
7.460
6.985
6.964
3.797
Signature SIF VIT VELLORE
3BOQUI
O
N
3k
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.032
1.007
1.065
3.101
1.095
2.131
3.176

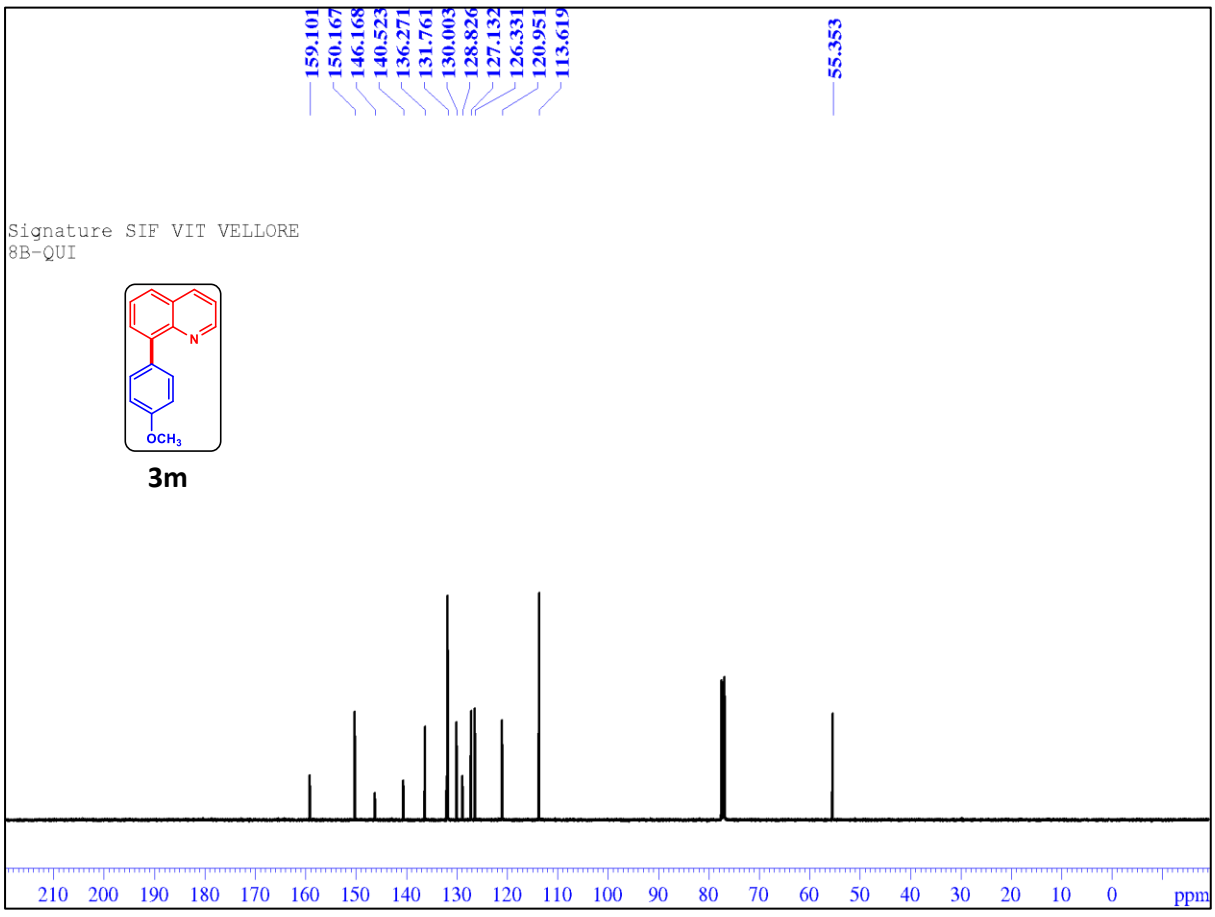

159.816
149.866
147.029
133.490
132.394
130.298
129.196
129.087
128.525
128.138
127.884
126.954
114.689
55.428
Signature SIF VIT VELLORE
3BOQUI
O
N
3k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.829
8.825
8.818
8.814
8.128
8.108
8.090
8.069
7.900
7.895
7.874
7.601
7.579
7.357
7.347
7.336
7.326
6.975
6.953
3.808
Signature SIF VIT VELLORE
6-BQ
H3CO
N
3l
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
2.053
2.073
2.067
1.044
2.070
3.033

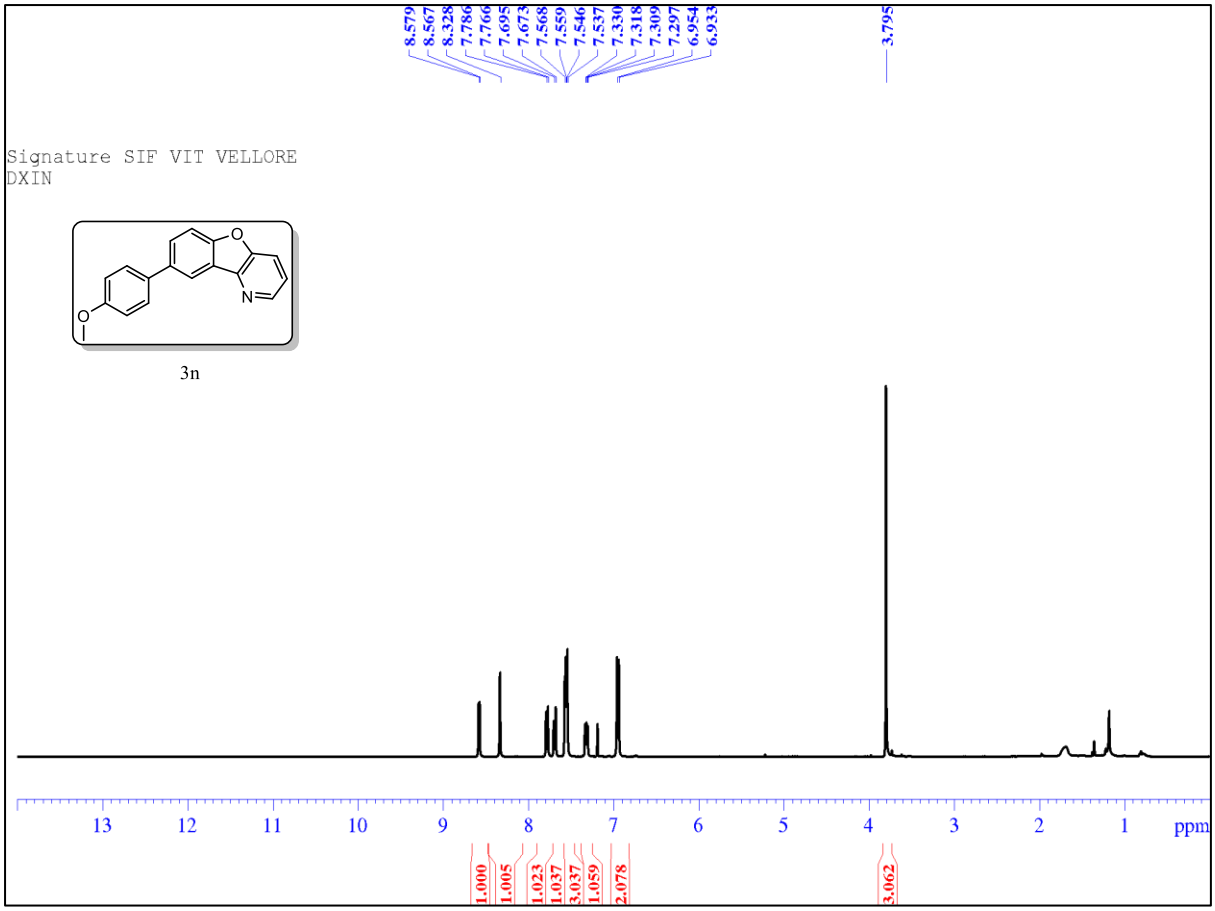

159.556
150.081
147.415
138.949
136.143
132.787
129.787
129.090
128.518
124.654
121.442
114.449
Signature SIF VIT VELLORE
6-BQ
H3CO
N
3l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

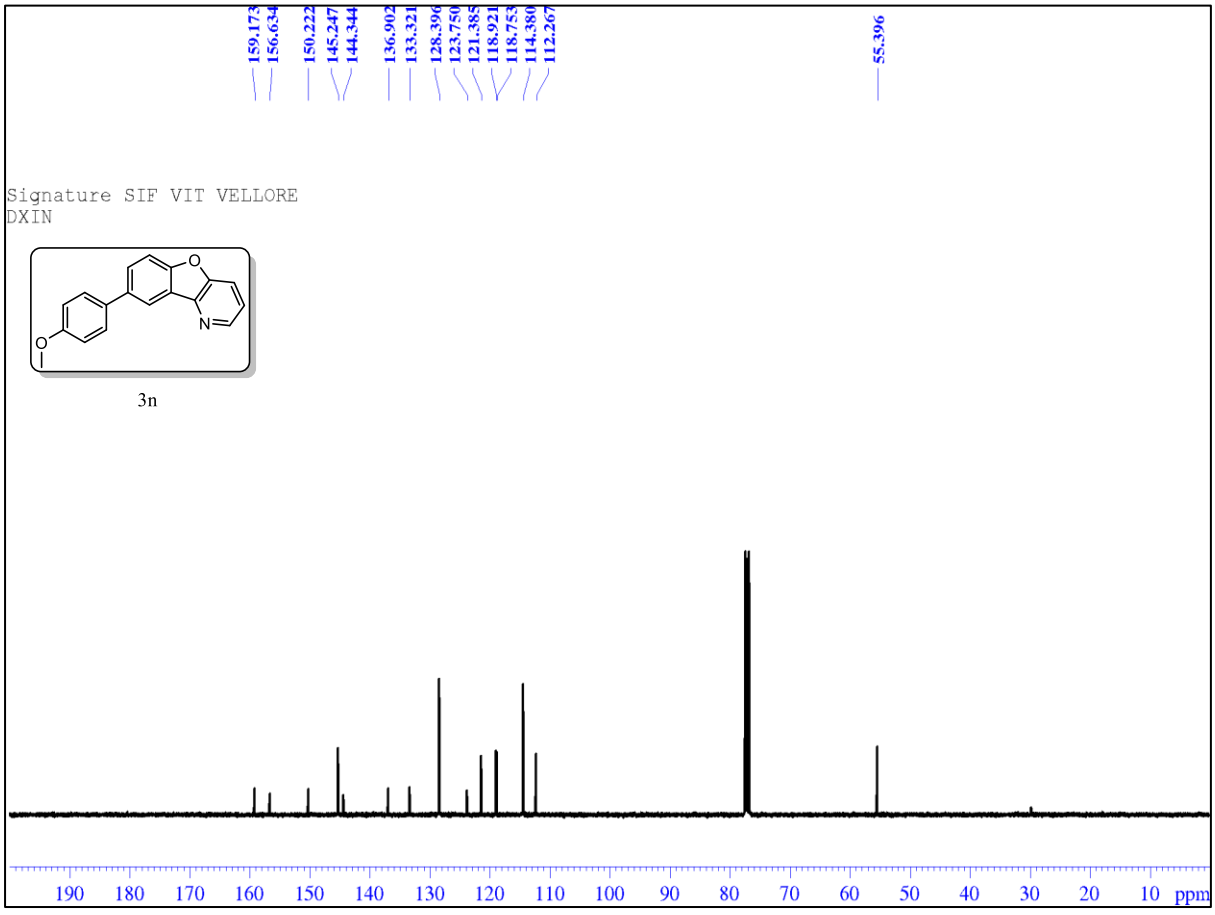

8.867
8.859
8.097
8.077
7.701
7.681
7.632
7.614
7.582
7.560
7.506
7.487
7.468
7.316
7.306
7.296
7.285
6.968
6.946
3.785
Signature SIF VIT VELLORE
8B-QUI
N
OCH3
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
1.021
1.027
1.044
2.019
1.066
1.048
2.052
3.054

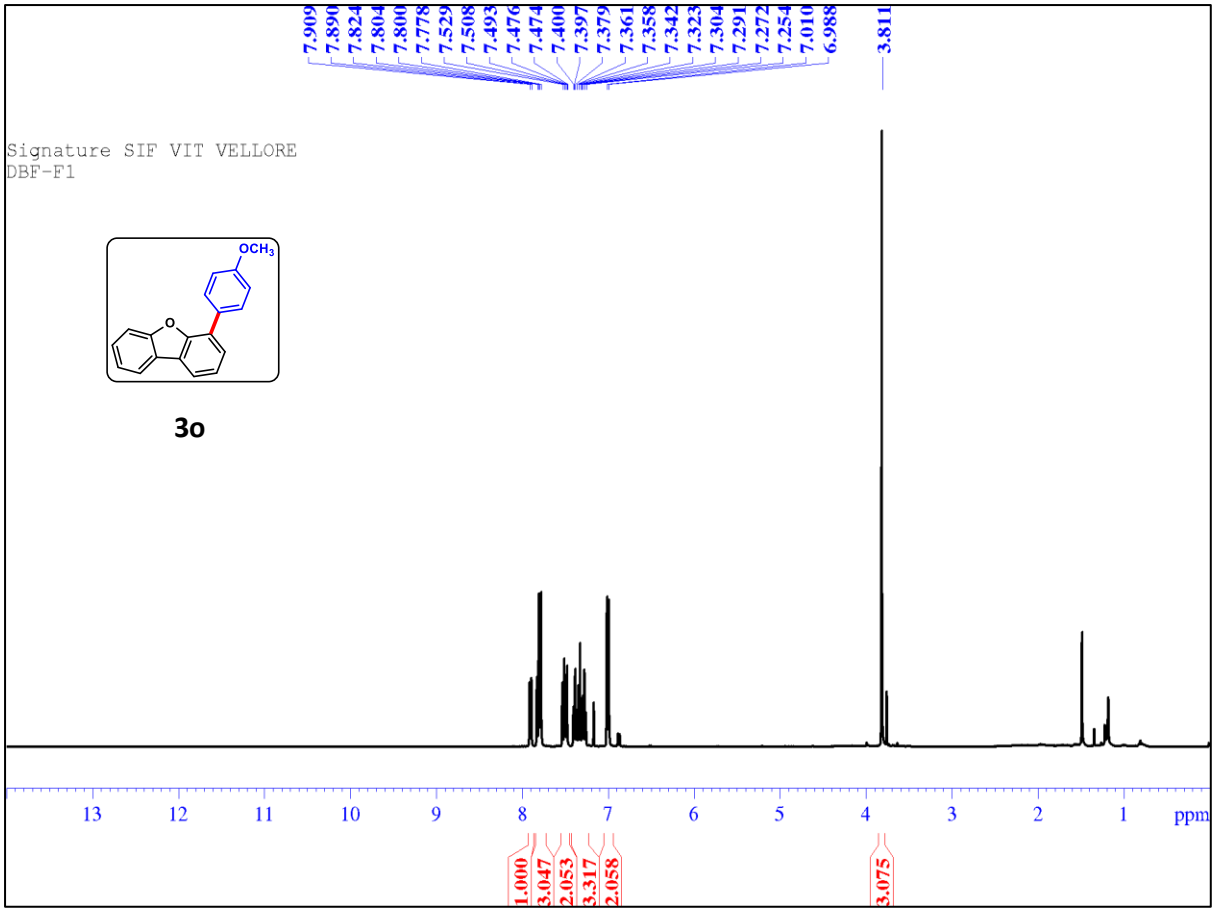
3m


159.101
150.167
146.168
140.523
136.271
131.761
130.003
128.826
127.132
126.331
120.951
113.619
55.353
Signature SIF VIT VELLORE
8B-QUI
N
OCH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

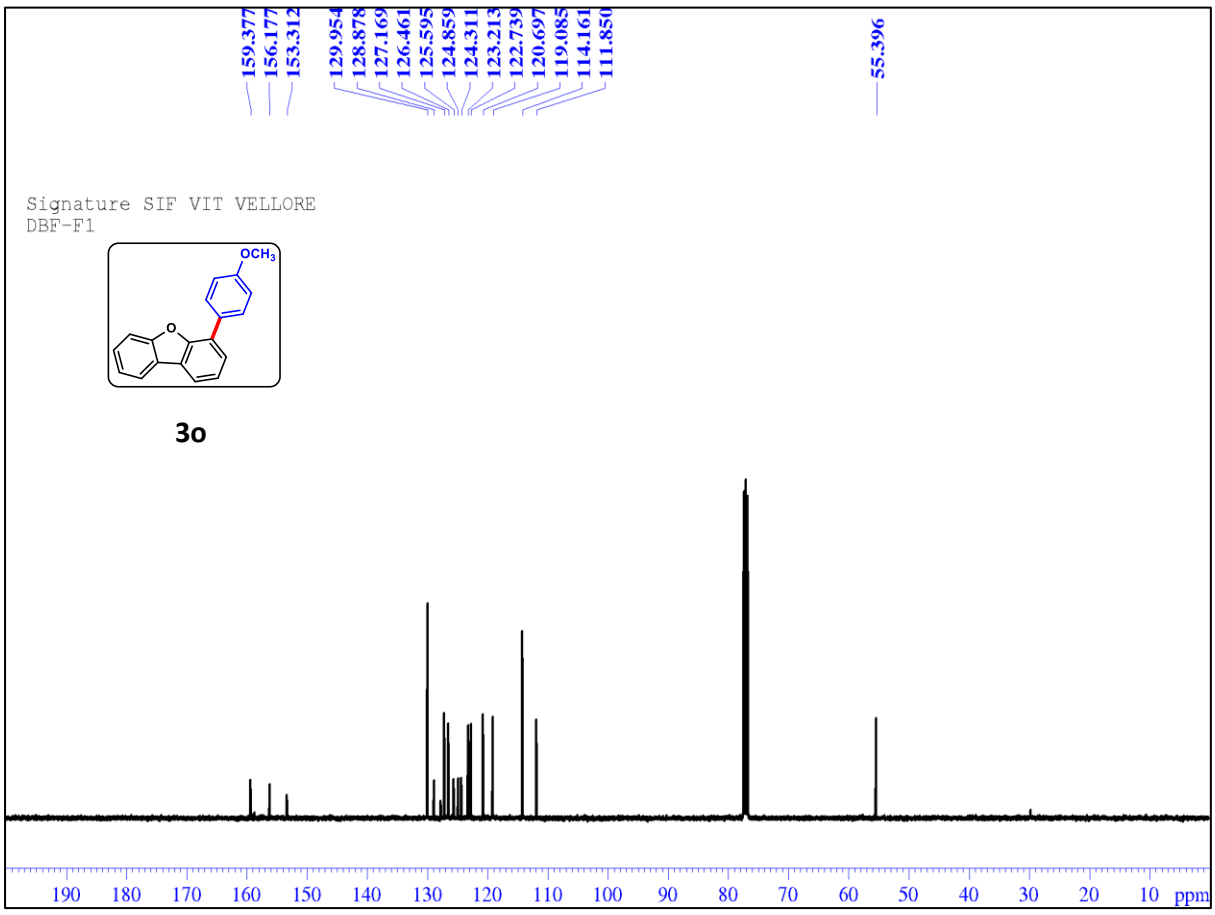
3m


8.579
8.567
8.328
7.786
7.766
7.695
7.673
7.568
7.559
7.546
7.537
7.330
7.318
7.309
7.297
6.954
6.933
3.795
Signature SIF VIT VELLORE
DXIN
O
N
O
3n
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.005
1.023
1.037
3.037
1.059
2.078
3.062


159.173
156.634
150.222
145.247
144.344
136.902
133.321
128.396
123.750
121.385
118.921
118.753
114.380
112.267
55.396
Signature SIF VIT VELLORE
DXIN
O
N
O
3n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.909
7.890
7.824
7.804
7.800
7.778
7.529
7.508
7.493
7.476
7.474
7.400
7.397
7.379
7.361
7.358
7.342
7.323
7.304
7.291
7.272
7.254
7.010
6.988
3.811
Signature SIF VIT VELLORE
DBF-F1
OCH3
O
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.000
3.047
2.053
3.317
2.058
3.075

3o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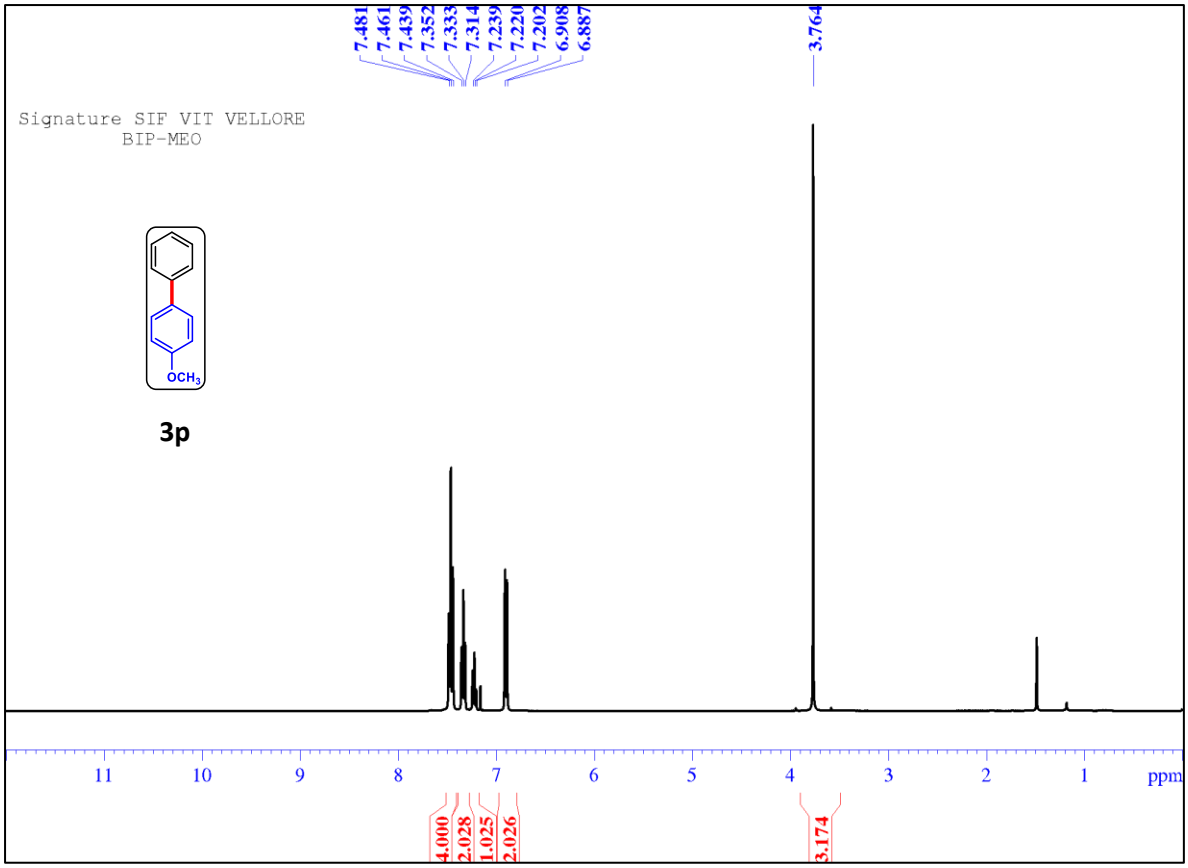
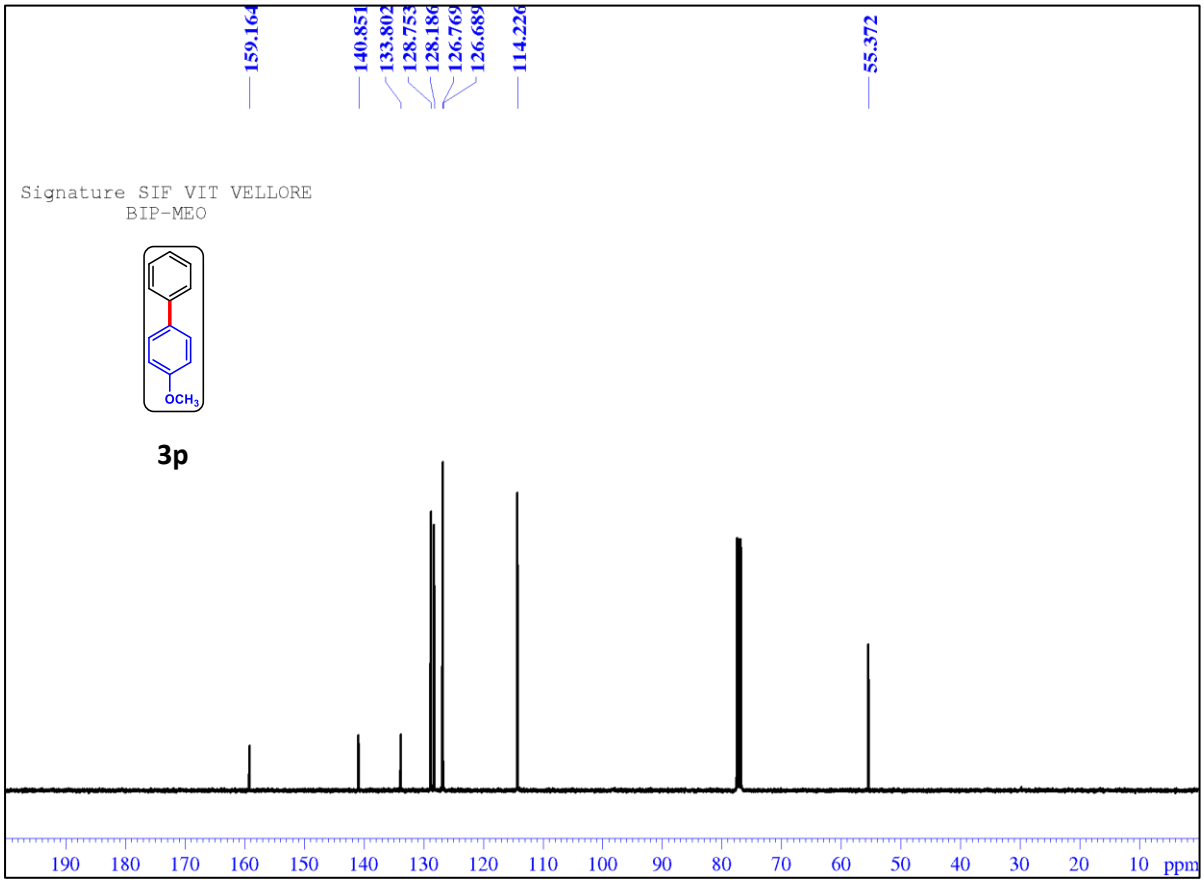
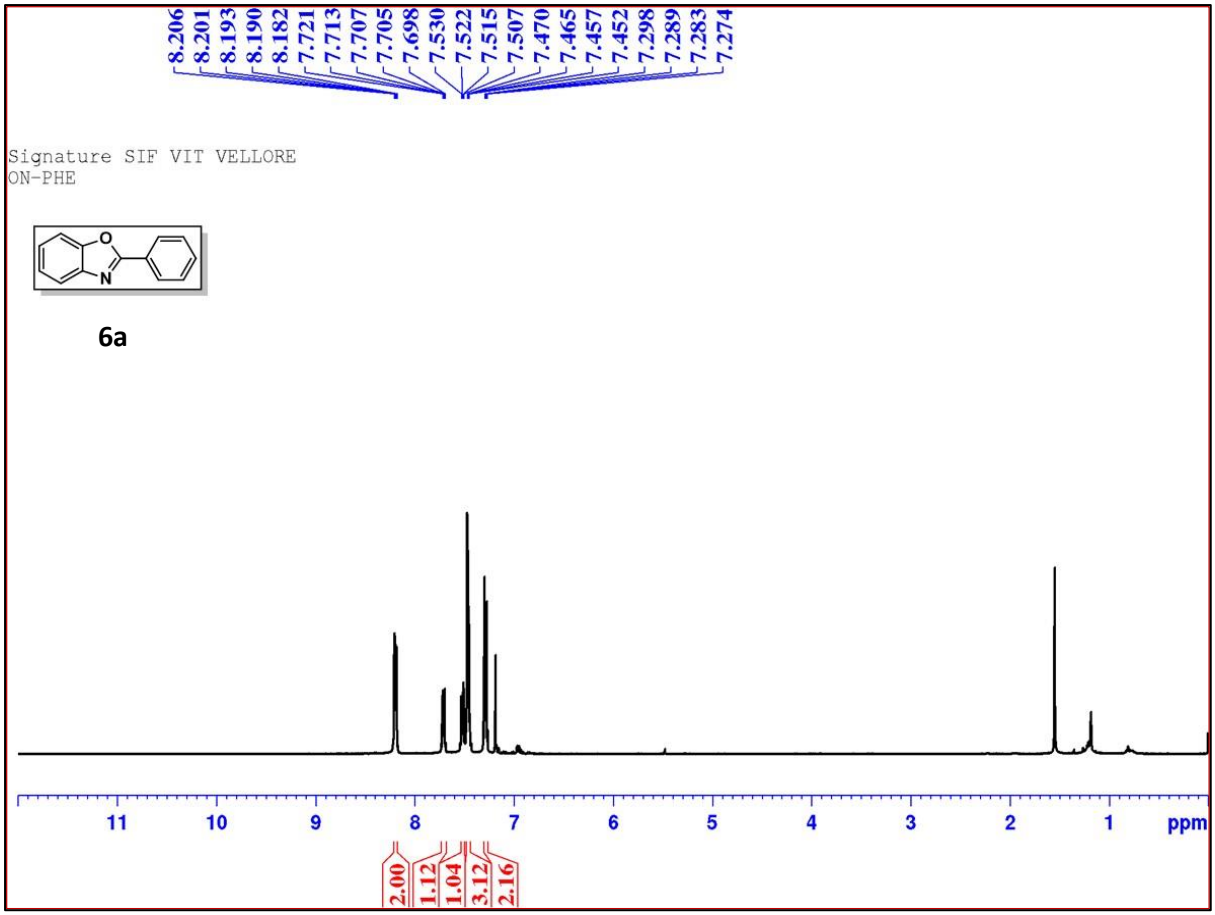
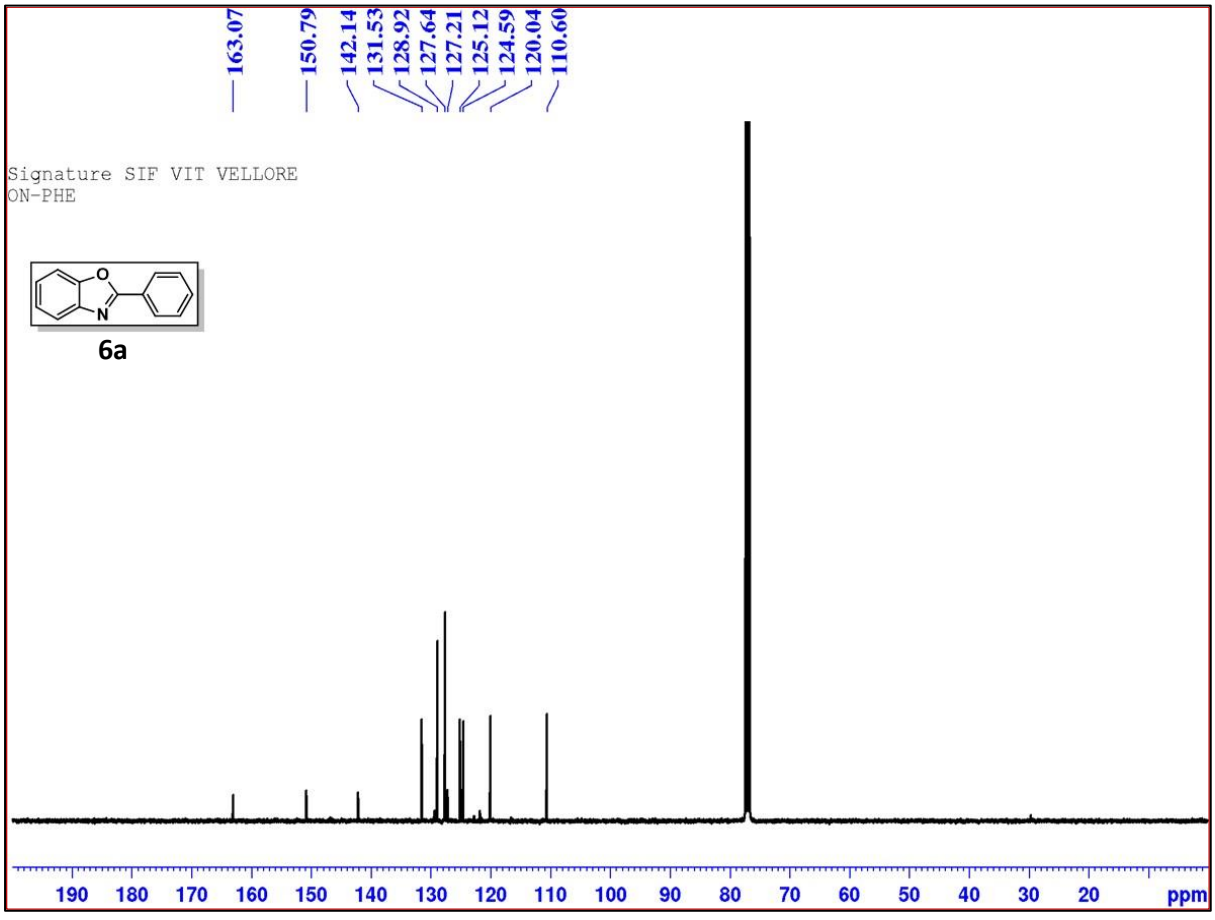
156.177
153.312
129.954
128.878
127.169
126.461
125.595
124.859
124.311
123.213
122.739
120.697
119.085
114.161
111.850
55.396
Signature SIF VIT VELLORE
DBF-F1
OCH3
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

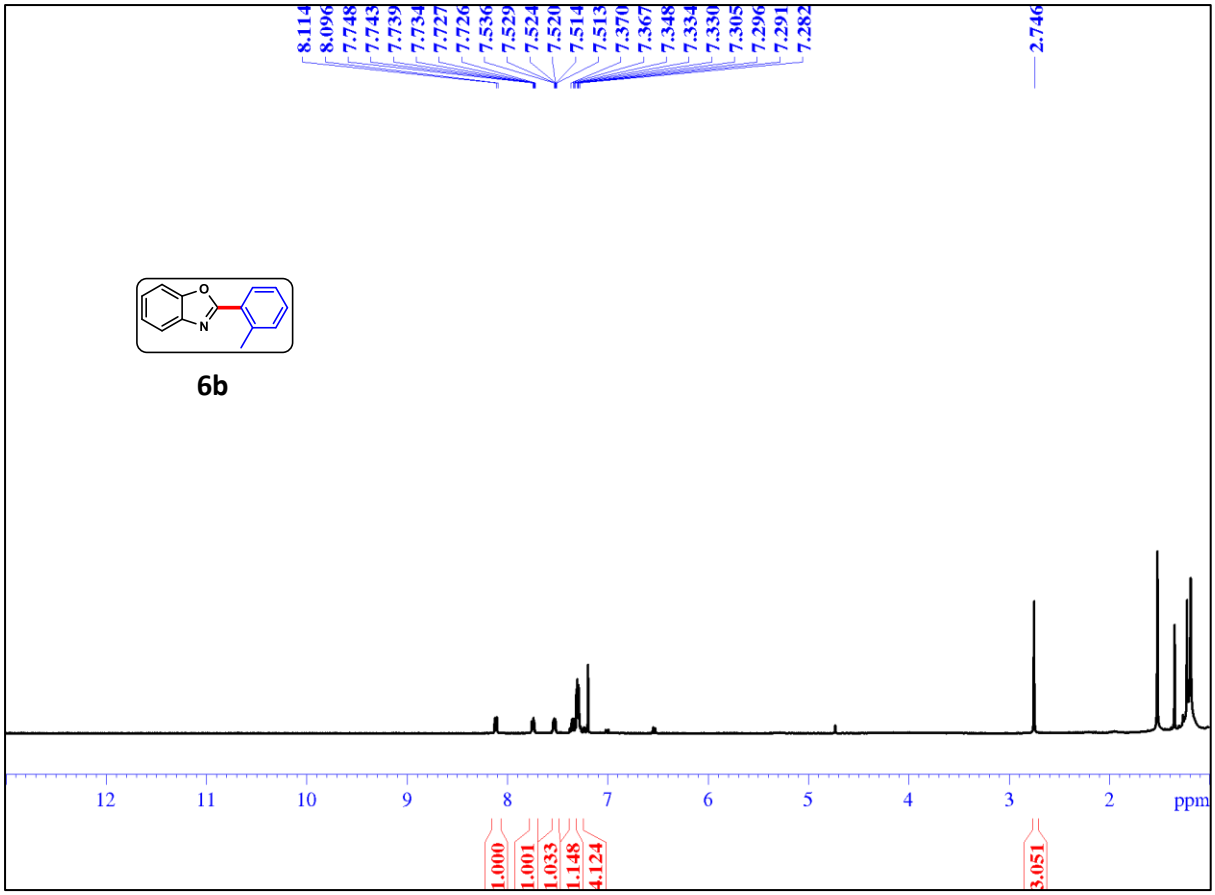
3o


7.481
7.461
7.439
7.352
7.333
7.314
7.239
7.220
7.202
6.908
6.887
3.764
Signature SIF VIT VELLORE
BIP-MEO
OCH3
3p
11
10
9
8
7
6
5
4
3
2
1
ppm
4.000
2.028
1.025
2.026
3.174

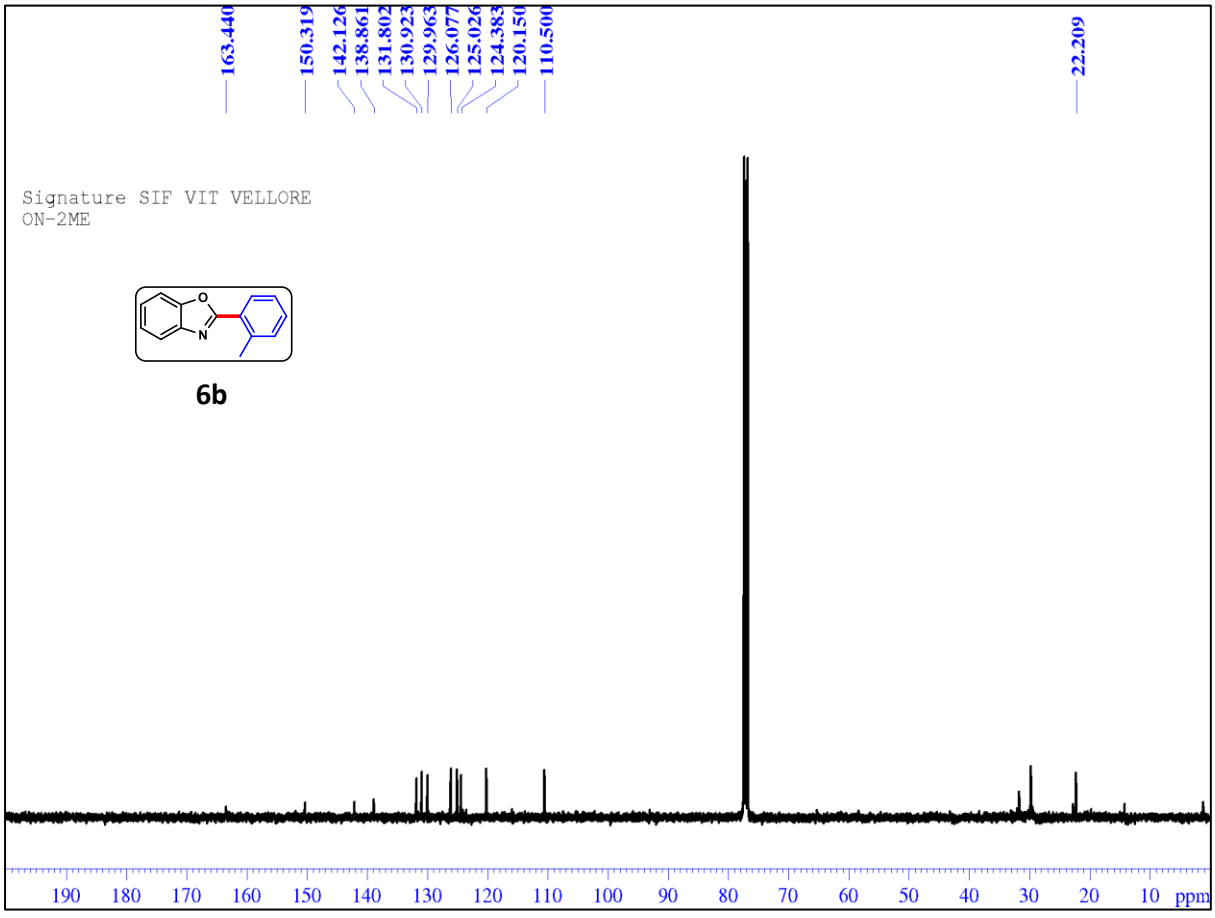

159.164
140.851
133.802
128.753
128.186
126.769
126.689
114.226
55.372
Signature SIF VIT VELLORE
BIP-MEO
OCH3
3p
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.206
8.201
8.193
8.190
8.182
7.721
7.713
7.707
7.705
7.698
7.530
7.522
7.515
7.507
7.470
7.465
7.457
7.452
7.298
7.289
7.283
7.274
Signature SIF VIT VELLORE
ON-PHE
6a
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.12
1.04
3.12
2.16

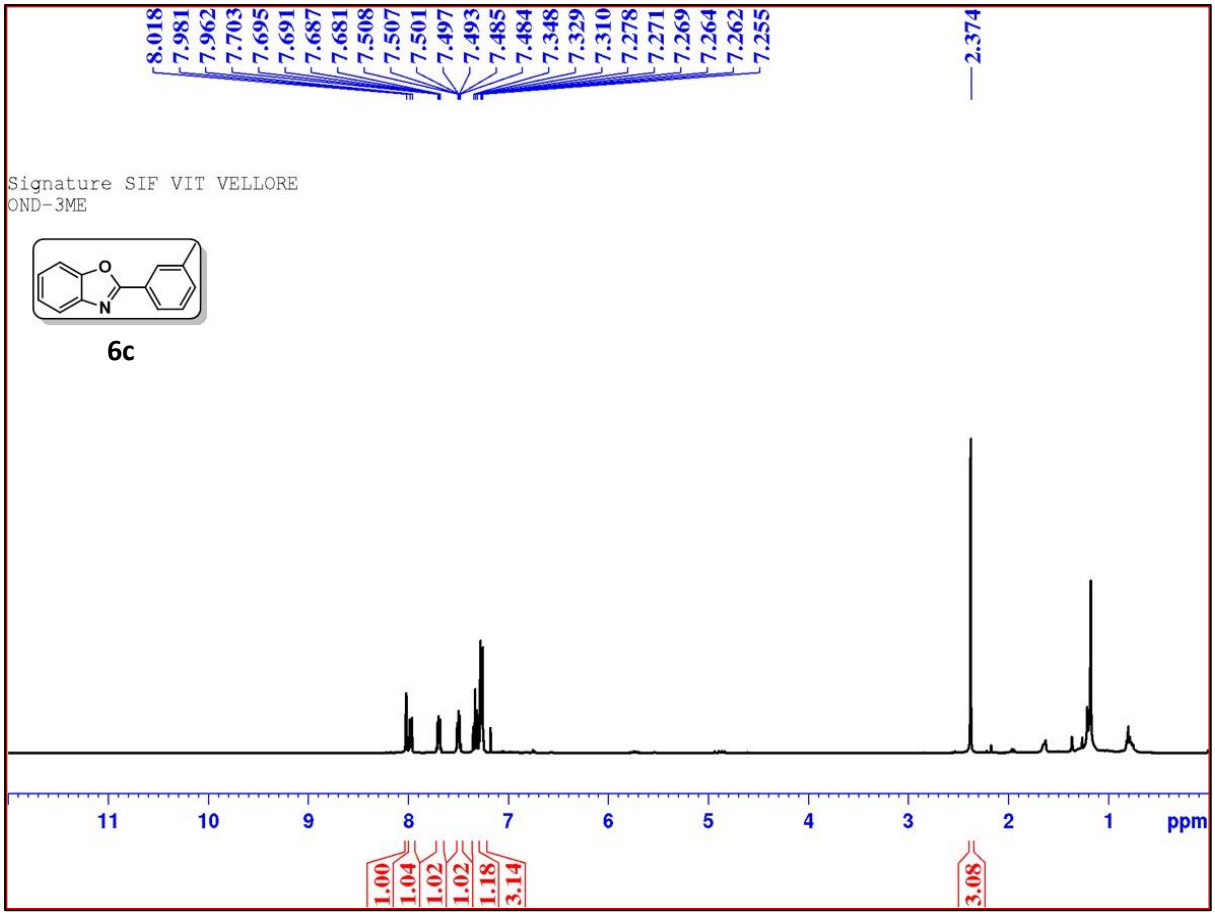

163.07
150.79
142.14
131.53
128.92
127.64
127.21
125.12
124.59
120.04
110.60
Signature SIF VIT VELLORE
ON-PHE
6a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.114
8.096
7.748
7.743
7.739
7.734
7.727
7.726
7.536
7.529
7.524
7.520
7.514
7.513
7.370
7.367
7.348
7.334
7.330
7.305
7.296
7.291
7.282
2.746
12
11
10
9
8
7
6
5
4
3
2
ppm
1.000
1.001
1.033
1.148
4.124
3.051

6b


163.440
150.319
142.126
138.861
131.802
130.923
129.963
126.077
125.026
124.383
120.150
110.500
22.209
Signature SIF VIT VELLORE
ON-2ME
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

6b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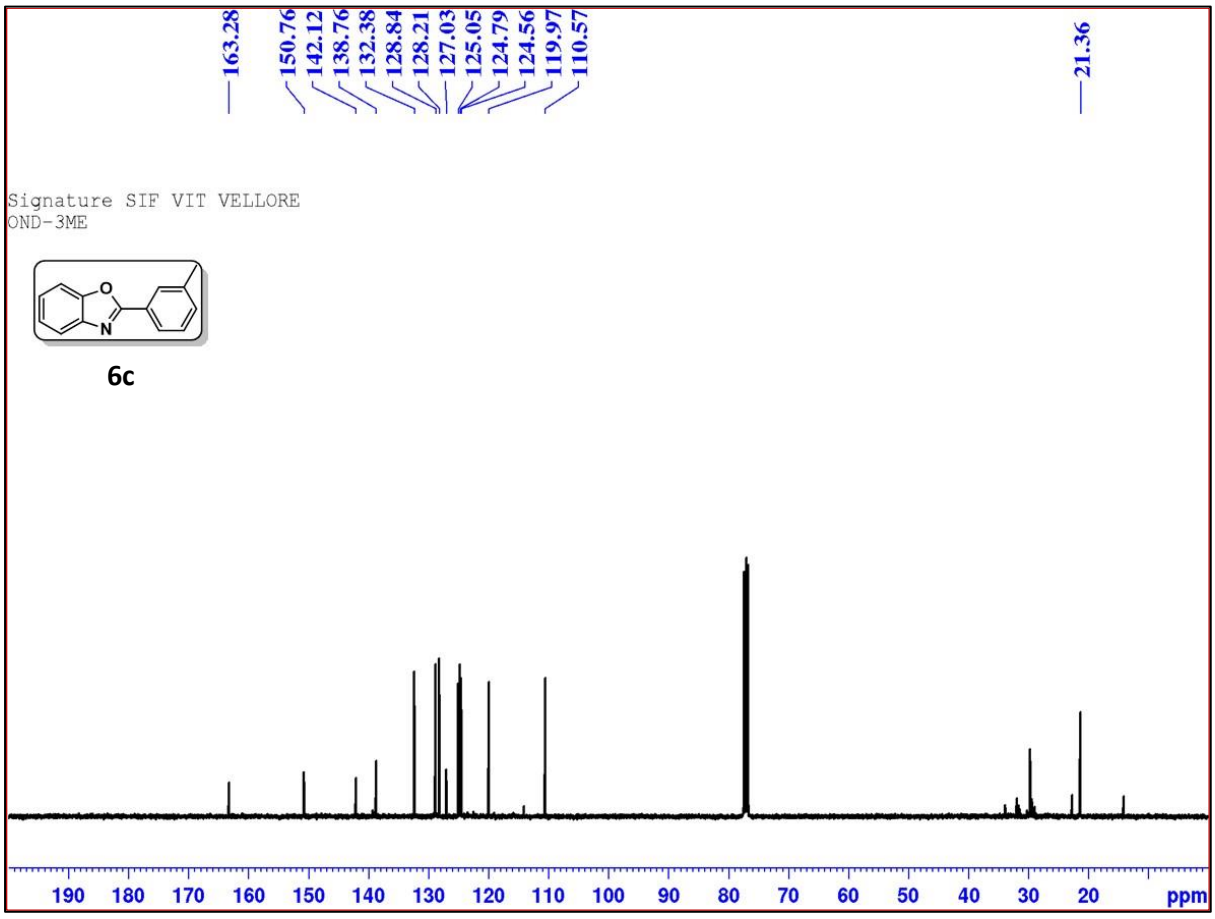
7.981
7.962
7.703
7.695
7.691
7.687
7.681
7.508
7.507
7.501
7.497
7.493
7.485
7.484
7.348
7.329
7.310
7.278
7.271
7.269
7.264
7.262
7.255
2.374
Signature SIF VIT VELLORE
OND-3ME
6c
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.04
1.02
1.02
1.18
3.14
3.08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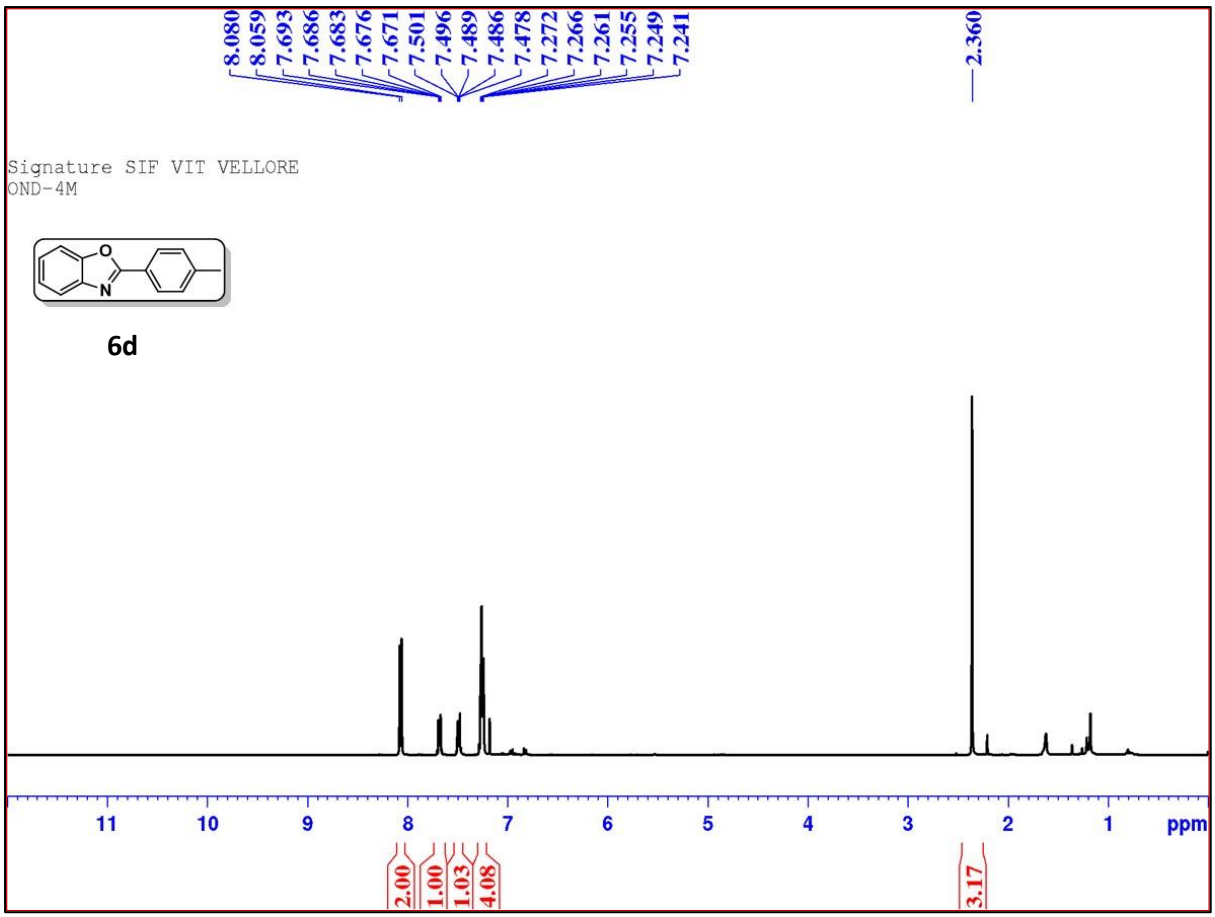
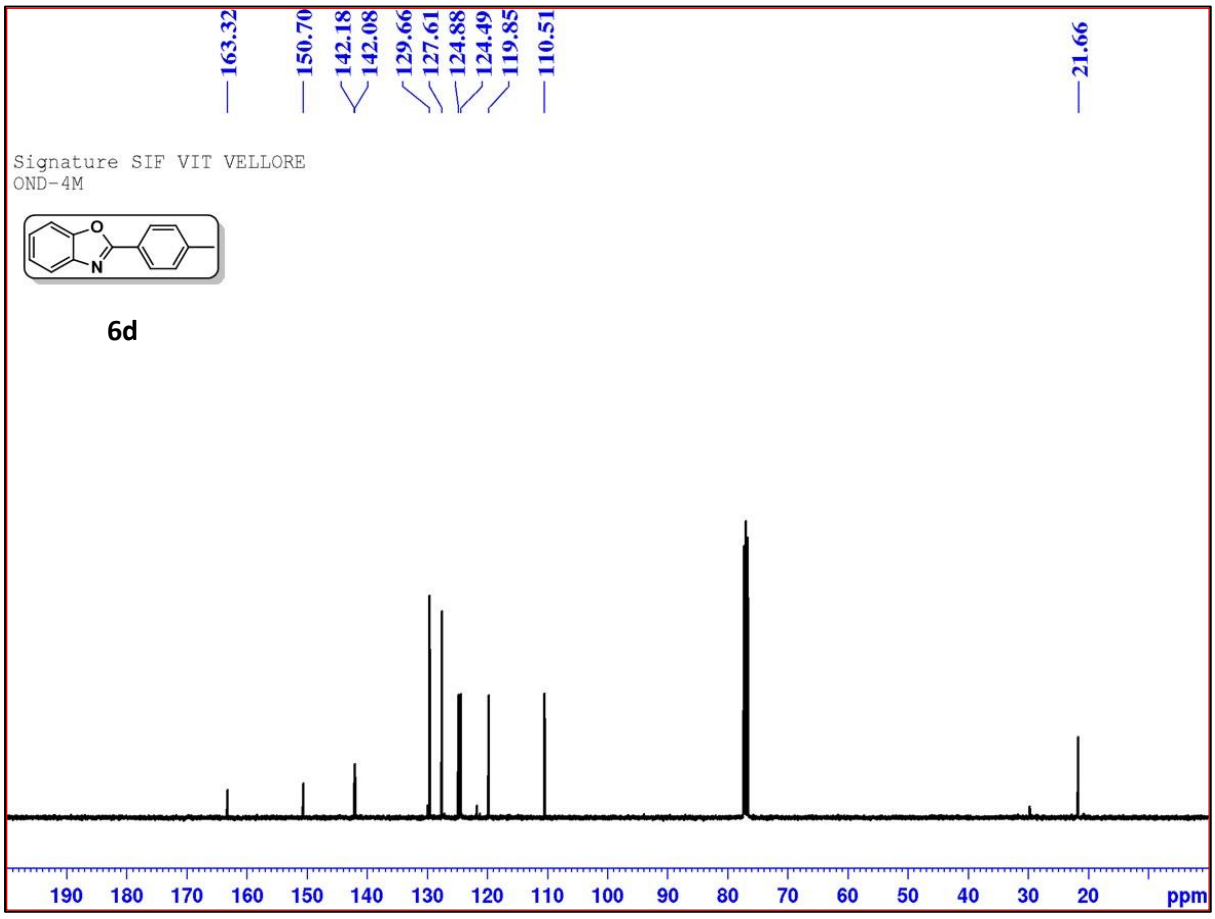
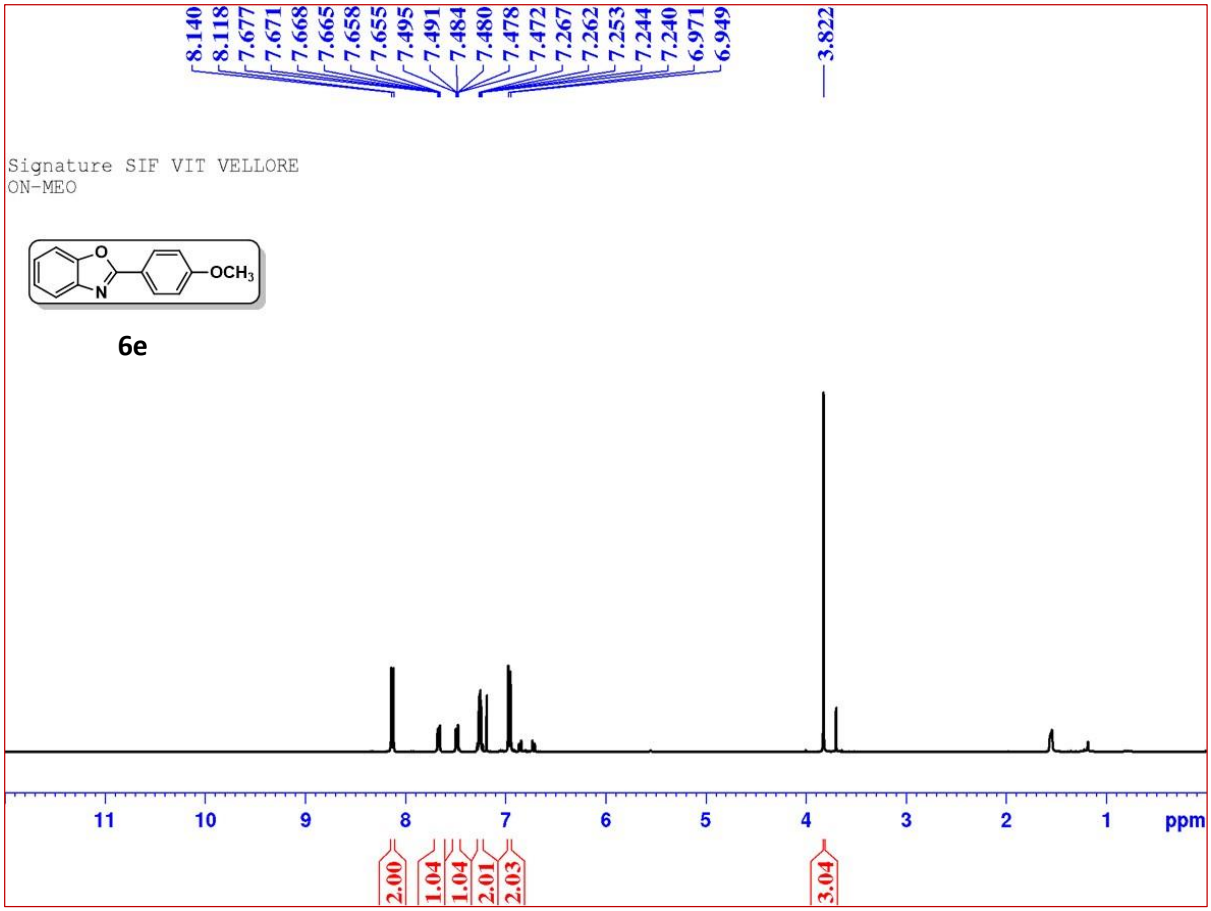
150.76
142.12
138.76
132.38
128.84
128.21
127.03
125.05
124.79
124.56
119.97
110.57
21.36
Signature SIF VIT VELLORE
OND-3ME
6c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.080
8.059
7.693
7.686
7.683
7.676
7.671
7.501
7.496
7.489
7.486
7.478
7.272
7.266
7.261
7.255
7.249
7.241
2.360
Signature SIF VIT VELLORE
OND-4M
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.00
1.03
4.08
3.17

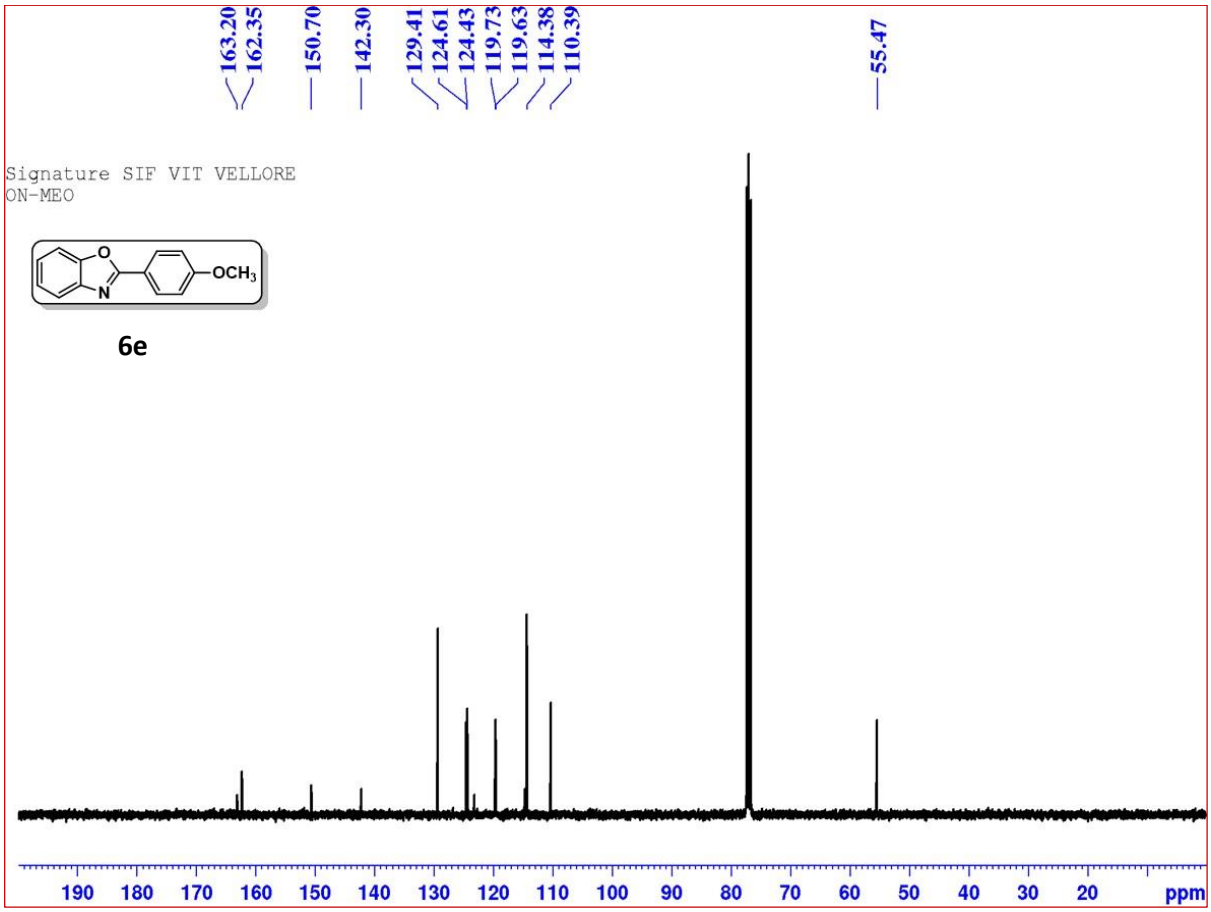
6d


163.32
150.70
142.18
142.08
129.66
127.61
124.88
124.49
119.85
110.51
21.66
Signature SIF VIT VELLORE
OND-4M
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

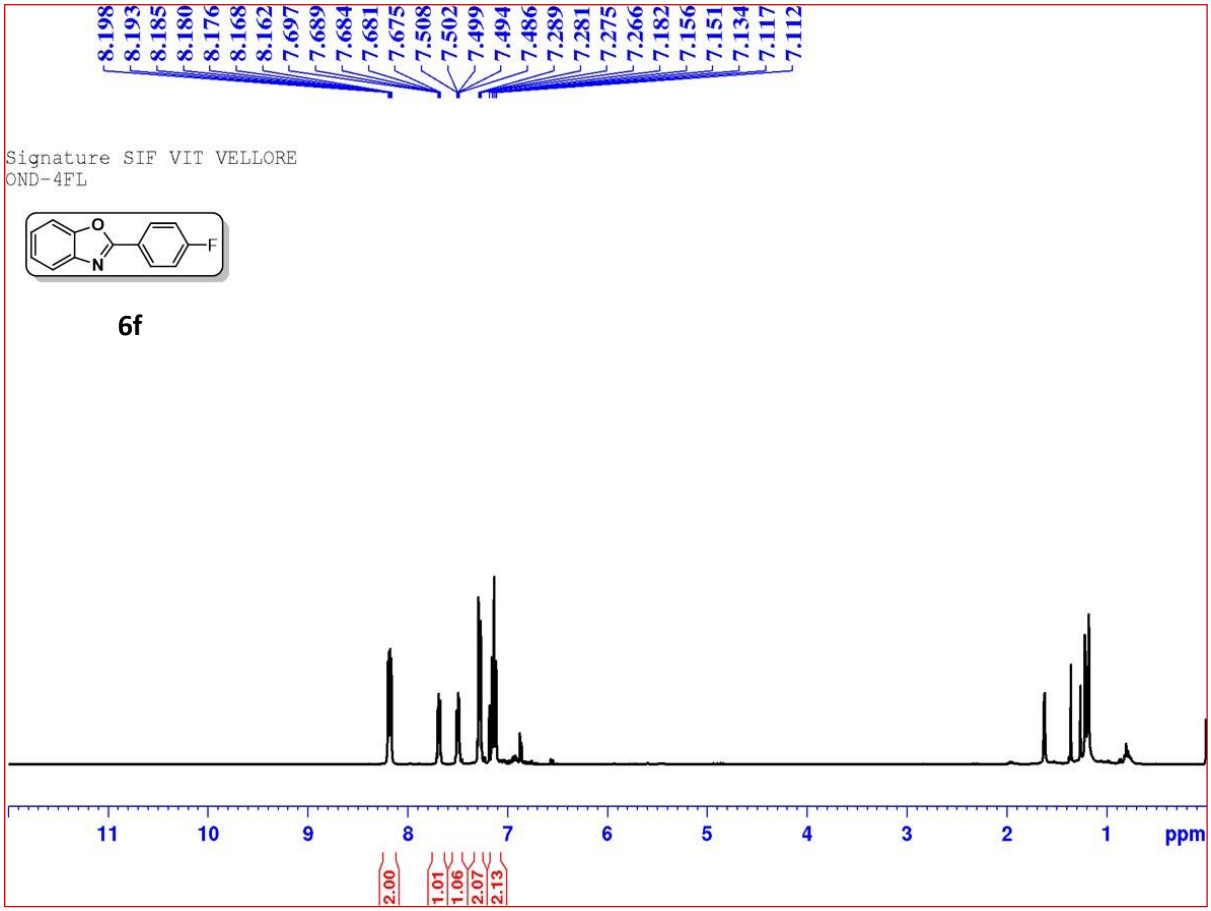
6d

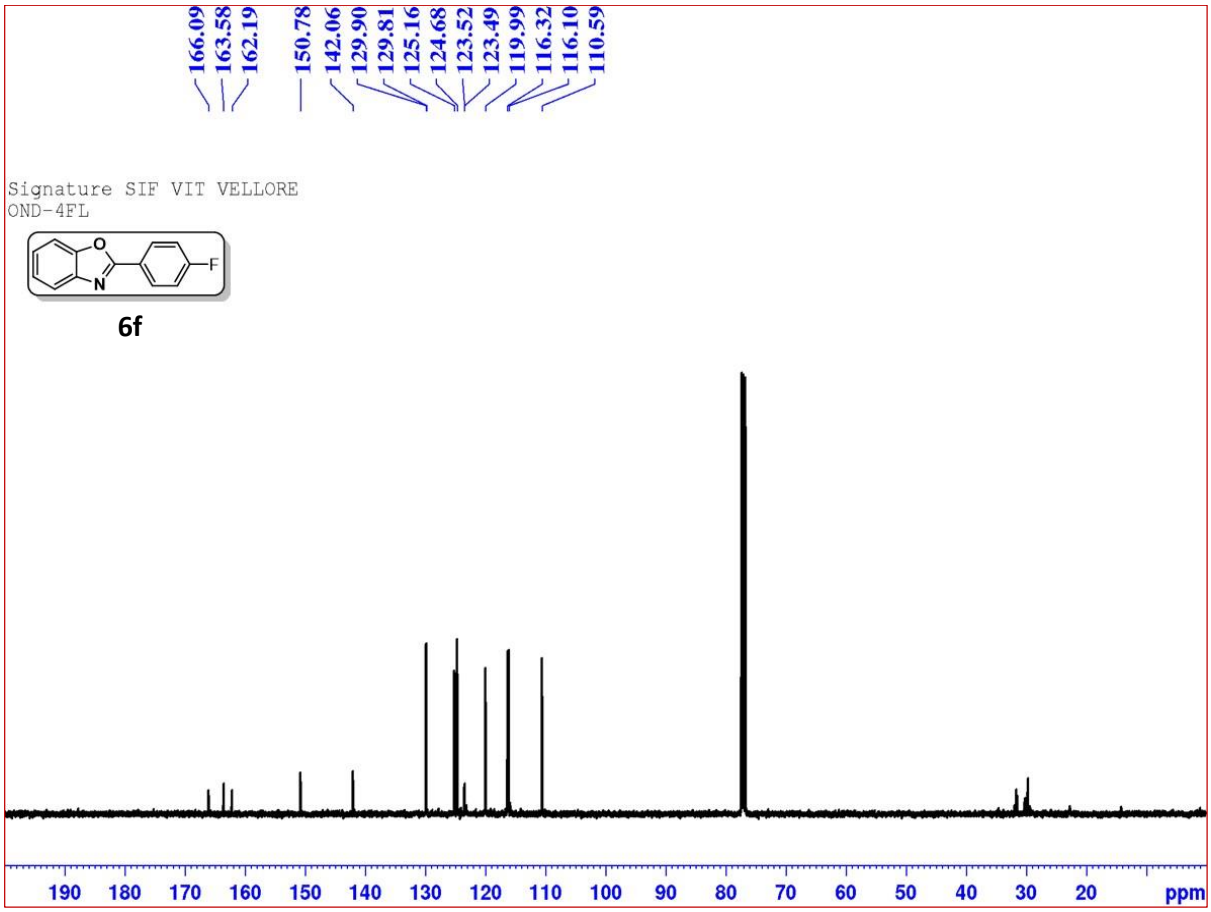

8.140
8.118
7.677
7.671
7.668
7.665
7.658
7.655
7.495
7.491
7.484
7.480
7.478
7.472
7.267
7.262
7.253
7.244
7.240
6.971
6.949
3.822
Signature SIF VIT VELLORE
ON-MEO
OCH3
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.04
1.04
2.01
2.03
3.04

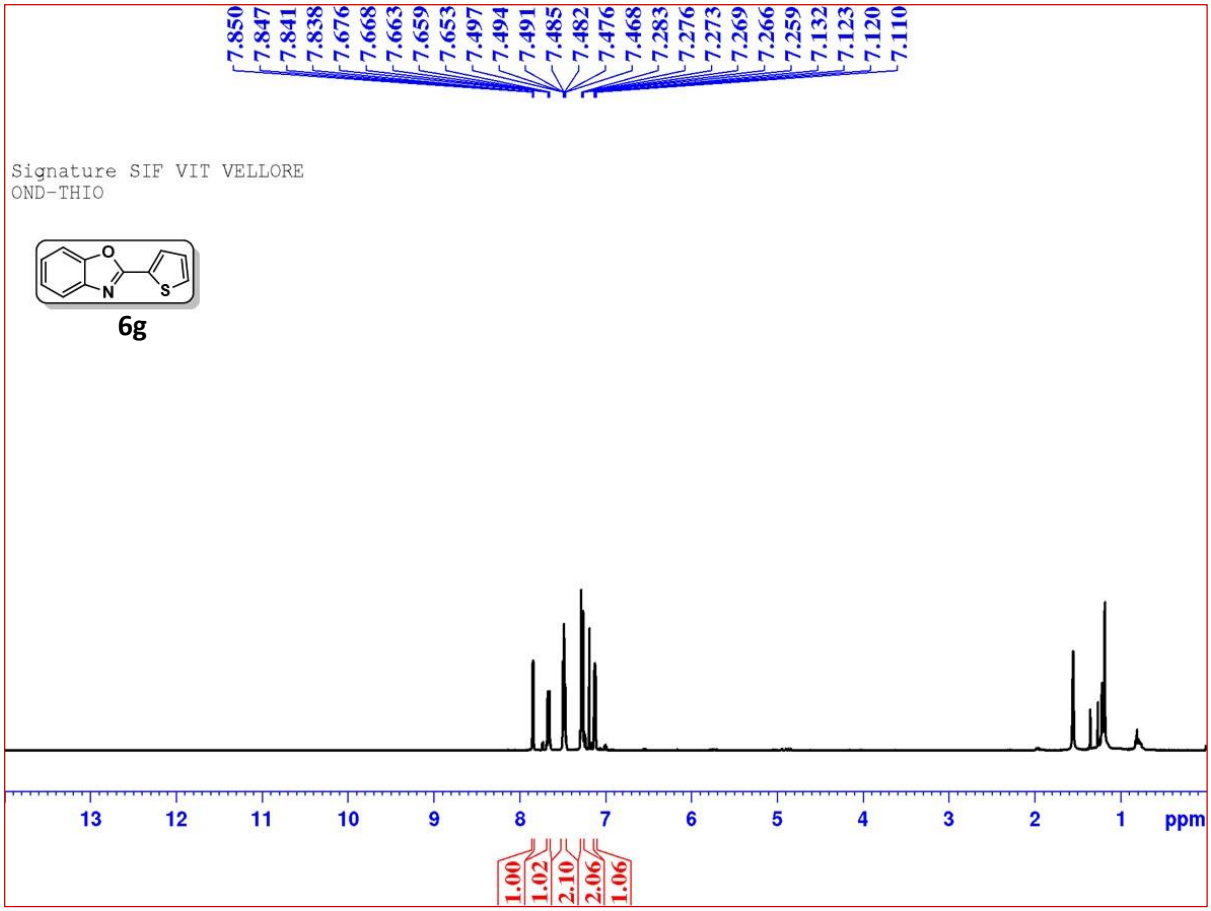
6e

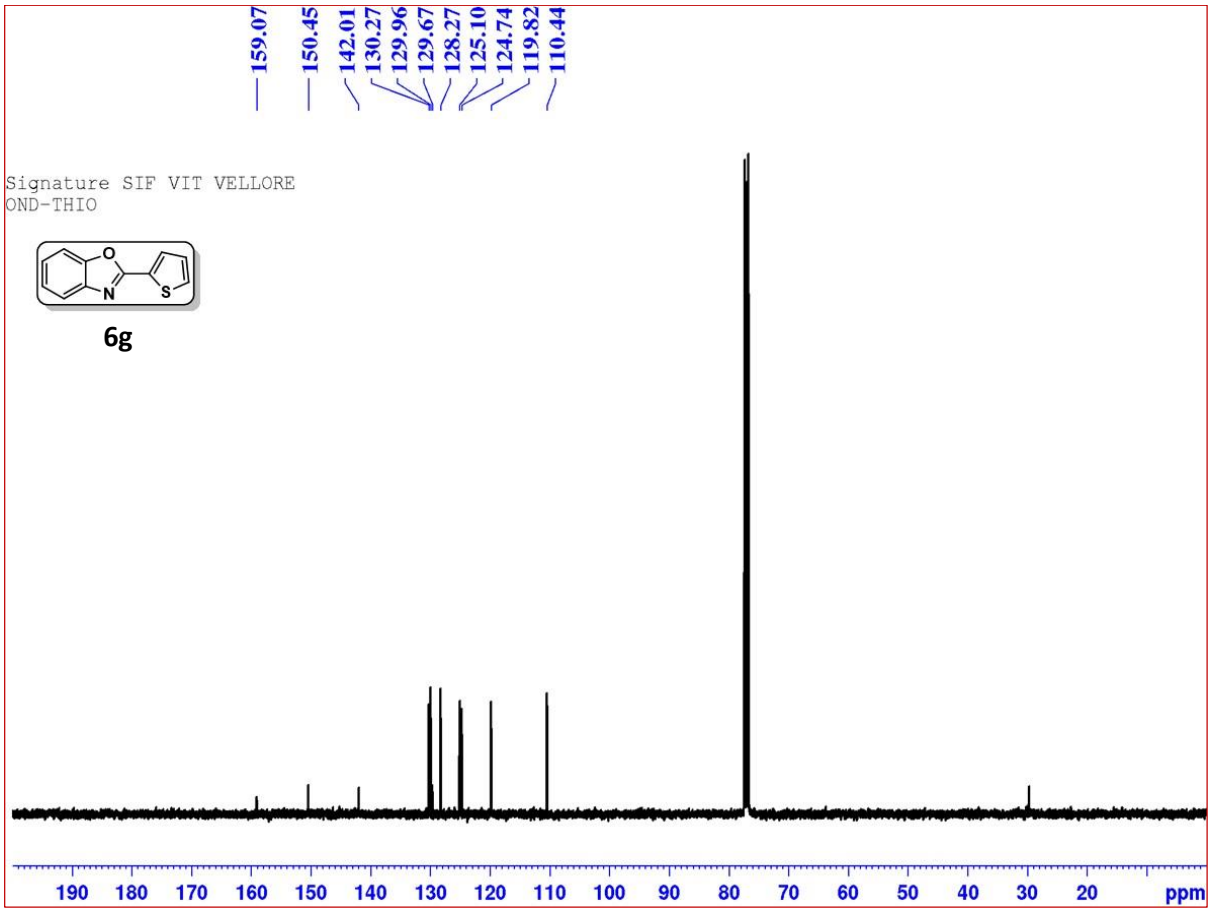

163.20
162.35
150.70
142.30
129.41
124.61
124.43
119.73
119.63
114.38
110.39
55.47
Signature SIF VIT VELLORE
ON-MEO
OCH3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

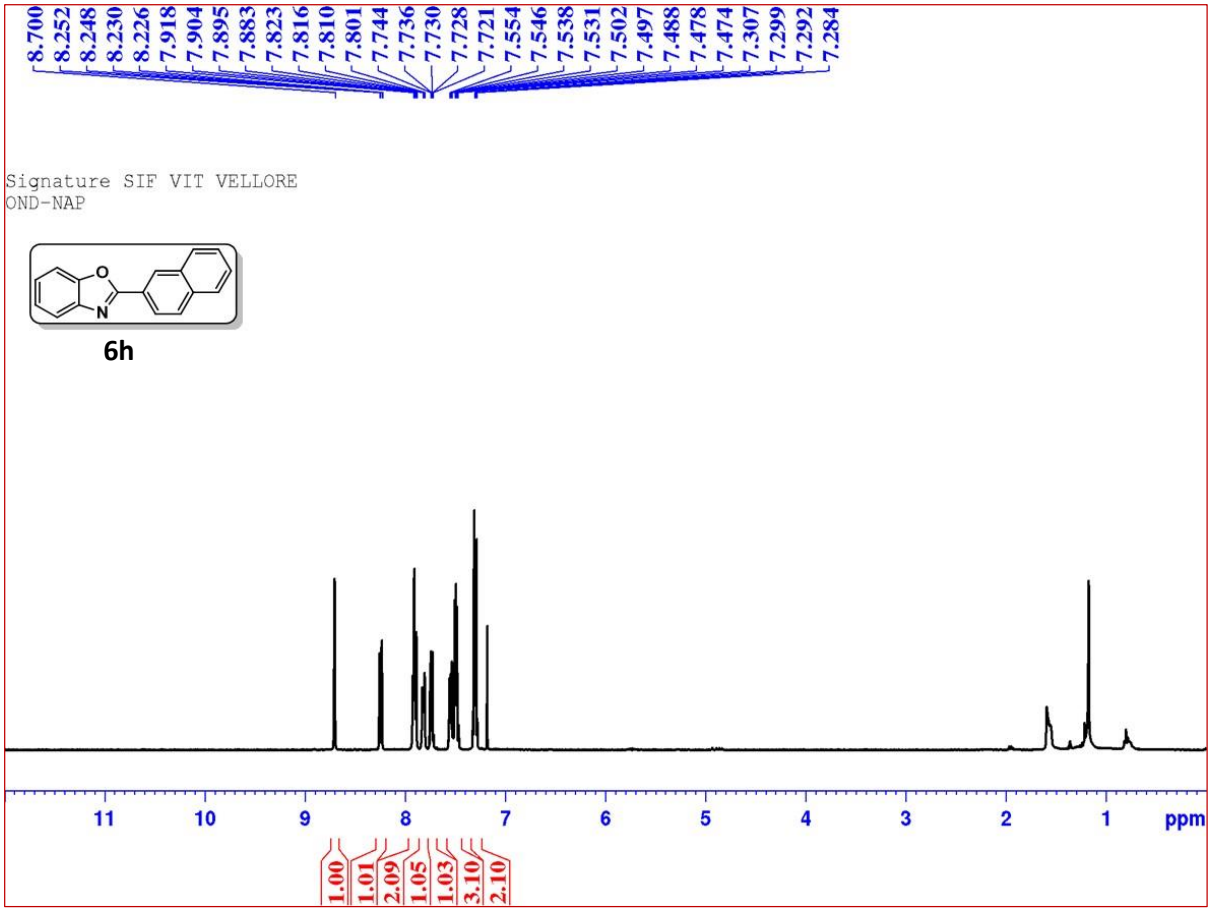
6e

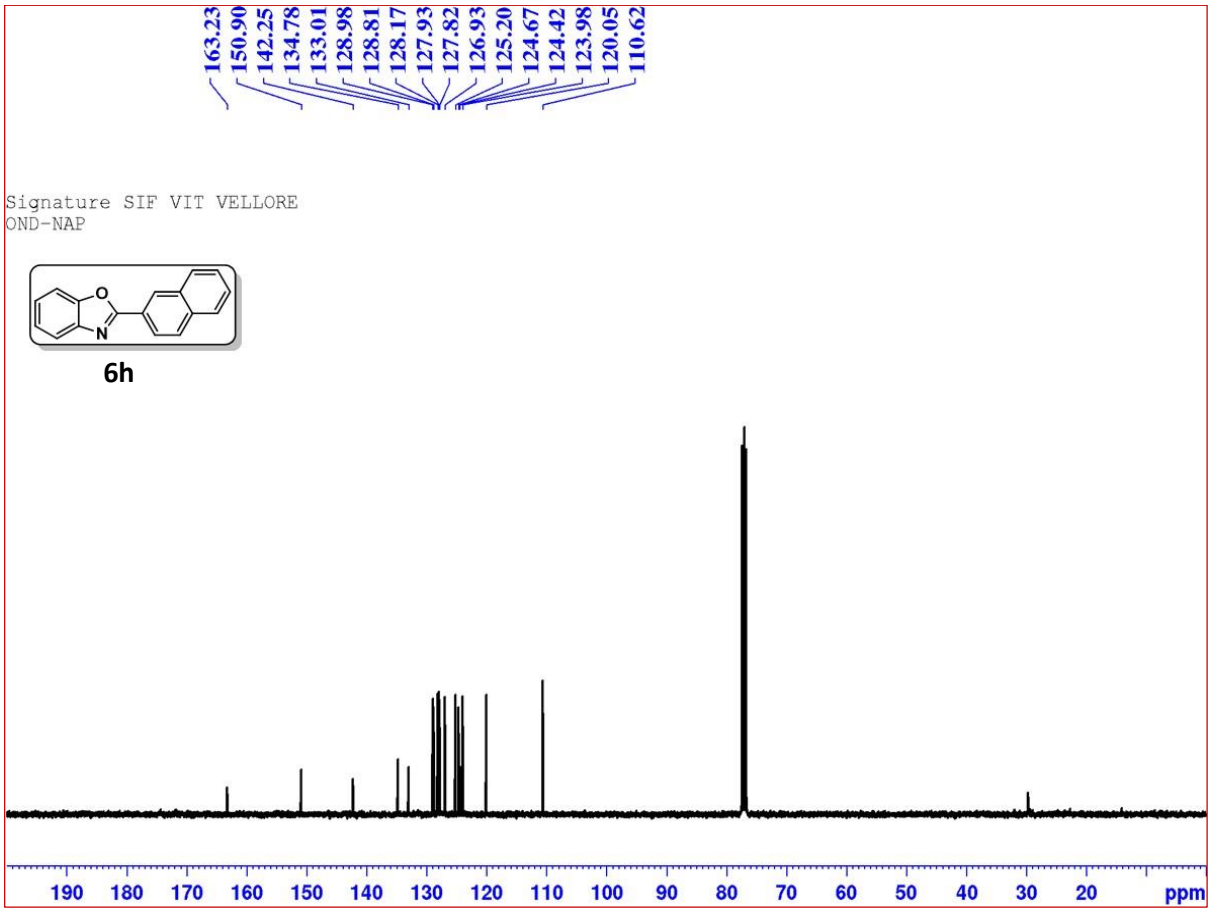

8.198
8.193
8.185
8.180
8.176
8.168
8.162
7.697
7.689
7.684
7.681
7.675
7.508
7.502
7.499
7.494
7.486
7.289
7.281
7.275
7.266
7.182
7.156
7.151
7.134
7.117
7.112
Signature SIF VIT VELLORE
OND-4FL
F
6f
11
10
9
8
7
6
5
4
3
2
1
ppm
2.00
1.01
1.06
2.07
2.13


166.09
163.58
162.19
150.78
142.06
129.90
129.81
125.16
124.68
123.52
123.49
119.99
116.32
116.10
110.59
Signature SIF VIT VELLORE
OND-4FL
F
6f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.850
7.847
7.841
7.838
7.676
7.668
7.663
7.659
7.653
7.497
7.494
7.491
7.485
7.482
7.476
7.468
7.283
7.276
7.273
7.269
7.266
7.259
7.132
7.123
7.120
7.110
Signature SIF VIT VELLORE
OND-THIO
O
N
S
6g
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.02
2.10
2.06
1.06


159.07
150.45
142.01
130.27
129.96
129.67
128.27
125.10
124.74
119.82
110.44
Signature SIF VIT VELLORE
OND-THIO
O
N
S
6g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.700
8.252
8.248
8.230
8.226
7.918
7.904
7.895
7.883
7.823
7.816
7.810
7.801
7.744
7.736
7.730
7.728
7.721
7.554
7.546
7.538
7.531
7.502
7.497
7.488
7.478
7.474
7.307
7.299
7.292
7.284
Signature SIF VIT VELLORE
OND-NAP
6h
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
2.09
1.05
1.03
3.10
2.10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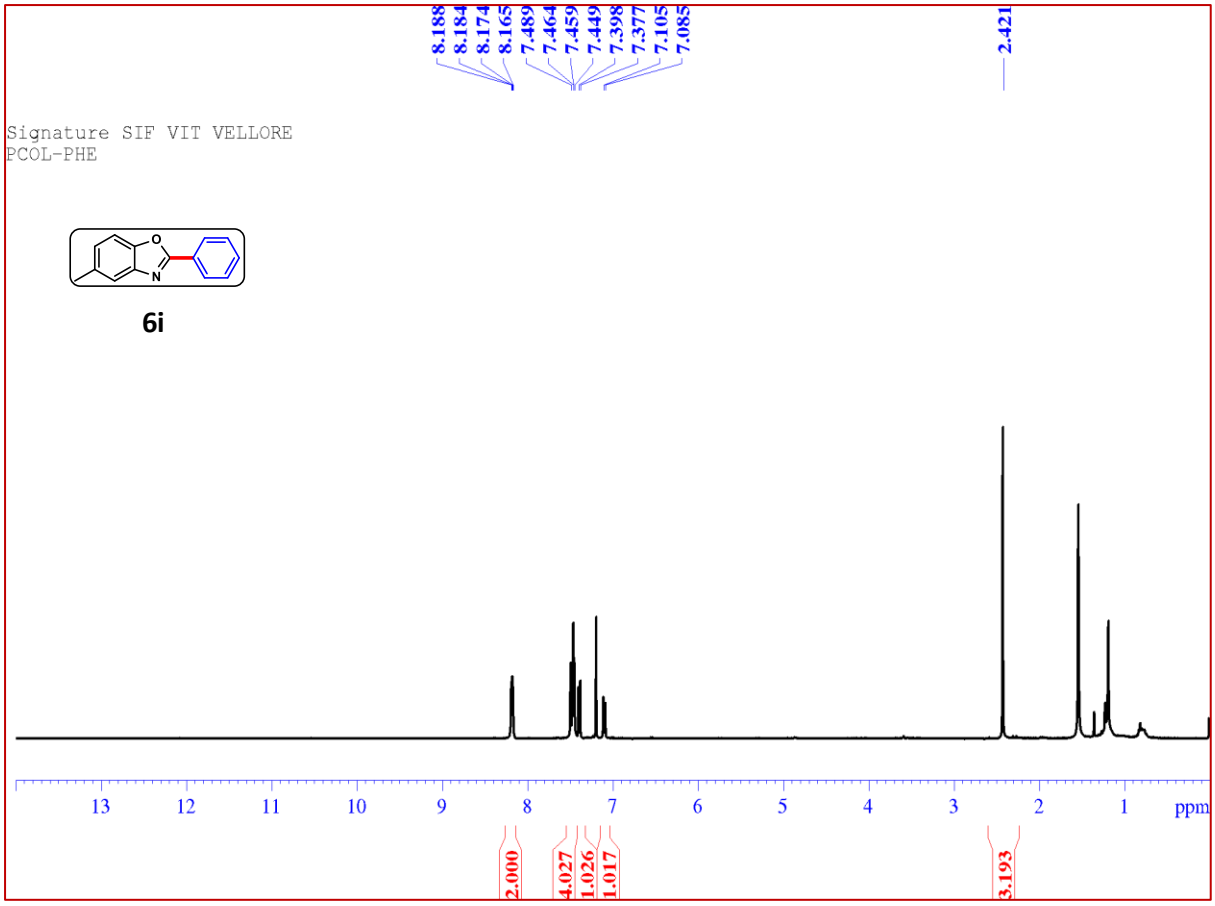
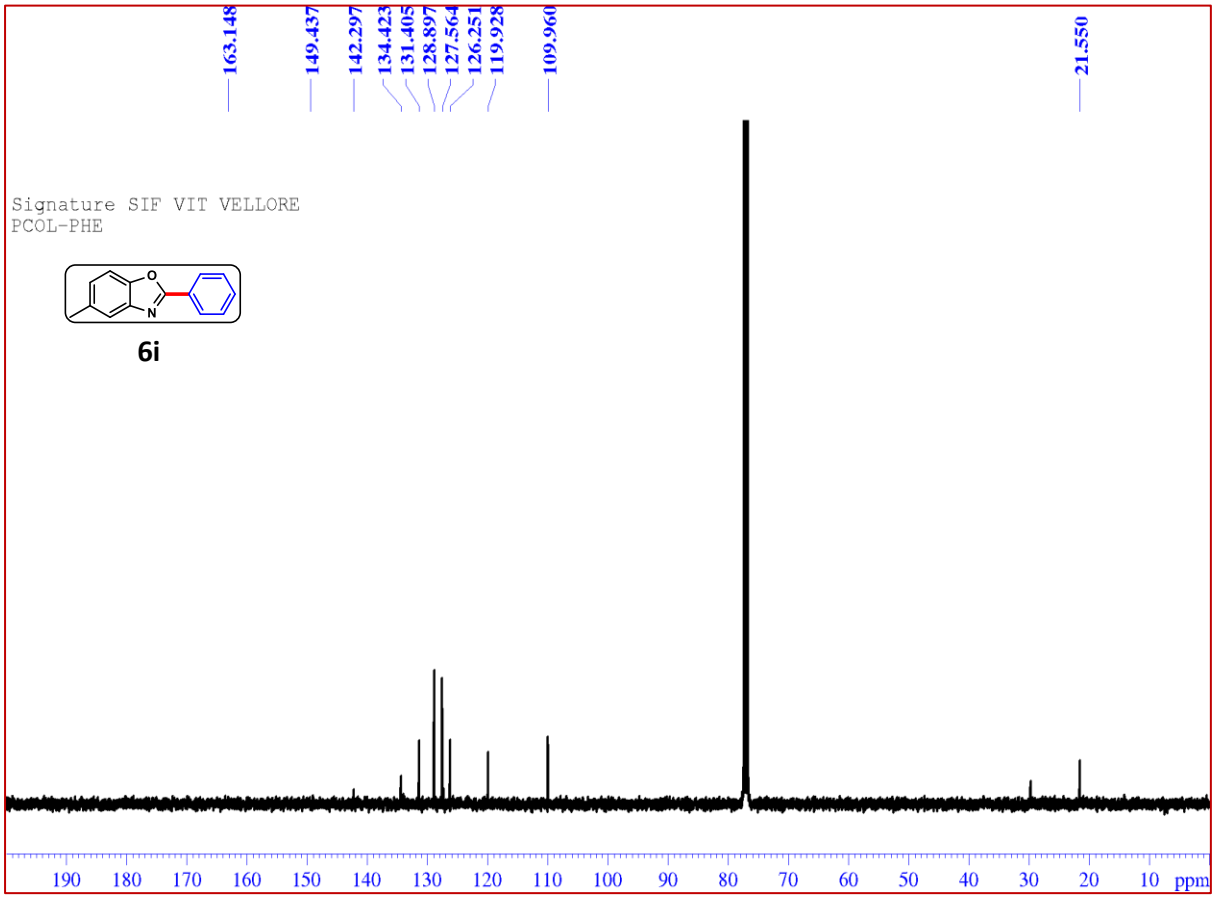
142.25
134.78
133.01
128.98
128.81
128.17
127.93
127.82
126.93
125.20
124.67
124.42
123.98
120.05
110.62
Signature SIF VIT VELLORE
OND-NAP
6h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


8.188
8.184
8.174
8.165
7.489
7.464
7.459
7.449
7.398
7.377
7.105
7.085
2.421
Signature SIF VIT VELLORE
PCOL-PHE
6i
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
2.000
4.027
1.026
1.017
3.193


163.148
149.437
142.297
134.423
131.405
128.897
127.564
126.251
119.928
109.960
21.550
Signature SIF VIT VELLORE
PCOL-PHE
6i
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm