Electronic Supplementary Information

Mesoporous Fe-SBA-15 catalyzed synthesis of 2-alkoxyimidazo[1, 2-a]pyridines and evaluation of in-silico selectivity and binding affinity to biological targets

Soumen Payra[a], Arijit Saha[a], Chia-Ming Wu[b], Balaranjan Selvaratnam[b], Thorn Dramstad[b], Luther Mahoney[b], Sant K. Verma[c], Suresh Thareja[c], Ranjit Koodali[b], Subhash Banerjee[a,*]

[a]Department of Chemistry, Guru Ghasidas Vishwavidyalaya, Bilaspur-495009,Chhattisgarh, India.

[b]Department of Chemistry, University of South Dakota, Vermillion, SD 57069 USA

[C]Department of Pharmacy, Guru Ghasidas Vishwavidyalaya, Bilaspur-495009, Chhattisgarh, India.

*Corresponding author; E-mail: ocsb2009@yahoo.com; Fax: +91 7752 260148; Tel: 91-7587401979

ESI 1. General Information:

All the chemicals were purchased from Sigma Aldrich, Sd-Fine, Merk and HIMEDIA (India) and no further purification. The solvents were distilled before use. All the reactions were performed with hot air oven-dried glassware under atmospheric condition. Distilled petroleum ether and ethyl acetate were used for performing column chromatography after. Analytical TLC was performed on Merck 60F254 silica gel plates (0.25 mm thickness).

Column chromatography was performed on silica gel (60-120 mesh size, HIMEDIA, India).

^{1}H NMR spectra were recorded on Bruker AV 300, AV 400 and AV 500. The ^{1}H NMR chemical shifts are reported relative to the center of solvent resonance ($CDCl_3$: 7.26 (1H). Chemical shifts are expressed in parts per million (δ) and the signals were reported as s (singlet), d (doublet), t (triplet), q(quartet), m (multiplet) and coupling constants *J* were given in Hz. ^{13}C NMR spectra were recorded at 125, 100 and 75 MHz in $CDCl_3$ solution. Chemical shifts are expressed in parts per million (δ) and are referenced to $CDCl_3$ (δ = 77.16) as internal standard. The powder XRD patterns of the Fe-SBA-15 catalysts were performed on a Rigaku Ultima IV X-ray diffractometer using Cu Kα radiation of λ= 1.540806 Å. The diffractometer was operated at 40 kV and 40 mA with a step width of 0.02° and the scan rate was used 0.24°/min. The Surface area was determined using the Brunauer-Emmett-Teller (BET) method in the relative pressure range of (P/P_0) = 0.05 to 0.30. The pore size was calculated by applying the Non-Local Density Functional Theory (NLDFT) equation to the desorption isotherm. The pore volume was calculated from the amount of nitrogen adsorbed at the highest relative pressure (P/P_0) ~ 0.98. The TEM images were recorded using a Tecnai G^2 instrument operating at 120 kV.

ESI 2. Method for the preparation of Mesoporous Fe-SBA-15:

The synthesis of Fe-SBA-15 was carried out as follows.[1] First, 19.2 g of P123 polymer was dissolved in 300 ml of water. Then, 0.22 g of NH_4F was added to the resulting solution. After NH_4F was dissolved in the solution, 2.37 g of $Fe(NO_3)_3 \bullet 9H_2O$ and 420 ml of water were added. Finally, the silica precursor, 43.7 ml of TEOS was added to the resulting solution under constant stirring. 1 M HCl and 1M aqueous ammonia solution were used to adjust the pH value to 3 for the resulting solution. The solution was stirred at 40 ^oC for 24 hours and then allowed to further react at 100^oC for 48 hours. After this, the white solid powder obtained was filtered, washed thoroughly by deionized water, and the wet powder was dried at 80 ^oC for overnight in an oven. The as-synthesized Fe-SBA-15 material (Fe is perhaps present in the form of finely dispersed iron oxide nanoclusters) was then calcined in air at 550 ^oC (3 ^oC/min heating rate) for 12 hours to remove the P123 polymer. Standard solutions of Fe^{3+} were first prepared and their absorbance values determined using Atomic Absorption Spectrometry (AAS) and a calibration plot was made. A known amount of Fe-SBA-15 was stirred with Con. HCl overnight. The solid was separated and the supernatant solution that contains (Fe^{3+}) was then carefully diluted to known volume. The absorbance value of the supernatant solution was determined using three trials and the average value was noted. The concentration of Fe^{3+} was then determined from the calibration graph and the amount of Fe^{3+} (mol%) was then calculated using the weight of Fe-SBA-15.The AAS studies indicate the loading of Fe to be 1.59 mole % on the silica SBA-15 support.

ESI 3. (a) Nitrogen adsorption-desorption isotherm and pore size distribution of Fe-SBA-15.

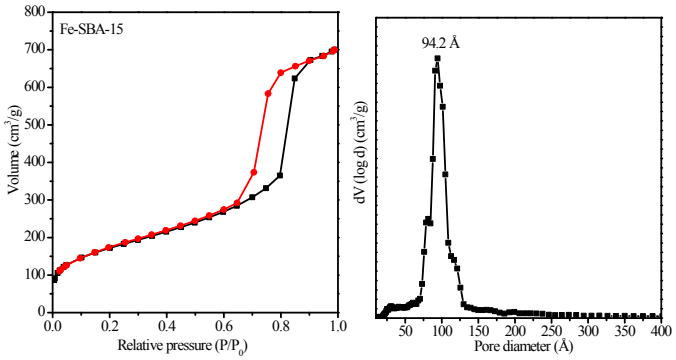


Figure 1S: Nitrogen adsorption-desorption isotherm (left) and (b) pore size distribution of Fe-SBA-15 (right).

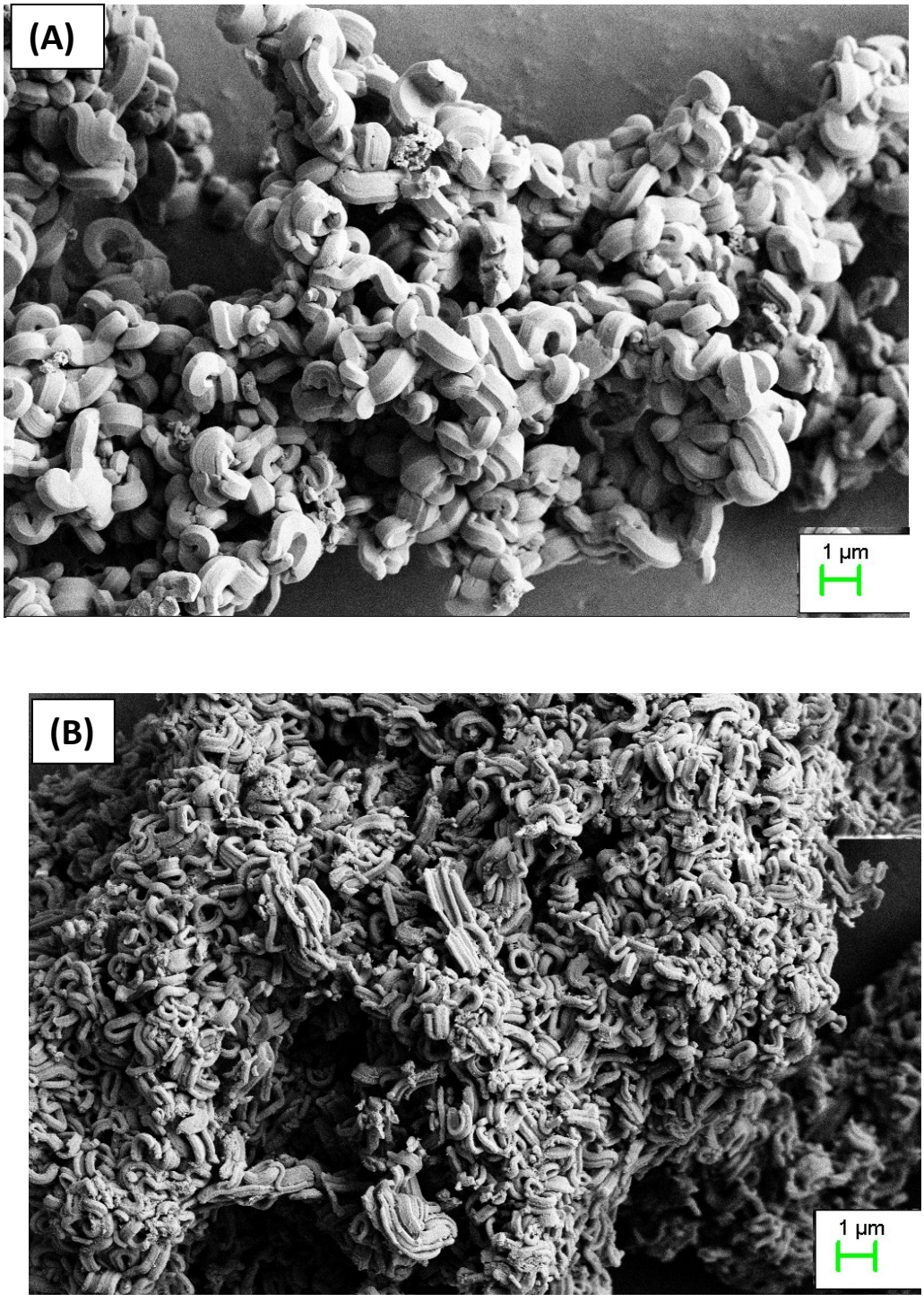


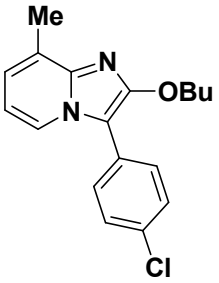
Figure 2S: Scanning electron microscopic (SEM) images of SBA-15 (A) and Fe-SBA-15 (B).

ESI 4. General procedure for the synthesis of 2-alkoxy-3-arylimidazo[1,2-a]pyridines: Representative experimental procedure for the 2-ethoxy-3-phenylimidazo[1,2-*a*]pyridine (4p, Table 2):

A mixture of *β*-nitrostyrene (149 mg, 1 mmol), 2-aminopyridine (113 mg, 1.2 mmol) and ethanol (2 ml) was taken in an oven dried round bottomed flask (25 ml, Borosil glass) in the presence of Fe-SBA-15 (15 mg) and was stirred at reflux condition in air for 1.5 hours under open atmosphere. After completion of the reaction monitored by TLC the reaction mixture was cooled to room temperature. After that the catalyst was separated by simple filtration and the reaction mixture was extracted from ethyl acetate. The organic layer was dried over anhydrous Na_2SO_4. The crude product was obtained after evaporating the solvent under vacuum. The crude product was purified by column chromatography on silica gel (60–120 mesh) using a mixture of distilled petroleum ether and ethyl acetate (85:15) as an eluting solvent to afford the pure 2-ethoxy-3-phenylimidazo[1,2-*a*]pyridine (4p) in 85% yield (203 mg). The product was confirmed by ^{1}H NMR and ^{13}C NMR spectroscopy and elemental analysis. The spectroscopic data and elemental analysis of all the compounds has been given in S5.

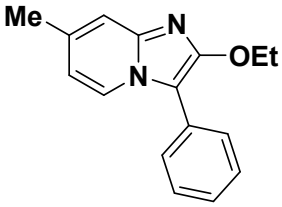
ESI 5. Detailed spectral data of the 2-alkoxy-imidazopyridine derivatives listed in Scheme 2.

The ^{1}H and ^{13}C NMR spectra were recorded on 300 MHz, 400 MHz or 500 MHz Bruker NMR spectrometer and $CDCl_3$ was used as solvent.



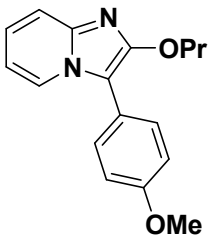
2-butoxy-3-(4-chlorophenyl)-8-methyl*H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4a, Isolated yield 86%); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.33 (d, *J* = 9.0 Hz, 1H), 7.99 (d, *J* = 8.7 Hz, 2H), 7.91 (d, *J* = 7.5 Hz, 2H), 7.36 (d, *J* = 6.3 Hz, 1H), 7.14 (t, *J* = 8.4 Hz, 1H) 4.15-4.08 (q, *J* = 6.9 Hz, 2H), 2.42 (s, 3H), 1.81 (m, *J* = 4.2 Hz, 2H), 1.53 (m, *J* = 5.4 Hz, 2H), 1.00 (t, *J* = 4.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.03, 149.14, 148.59, 136.40, 130.36, 130.17, 128.44, 119.77, 116.78, 63.16, 30.14, 21.09, 19.94, 14.37. Anal calc for $C_{18}H_{19Cl}N_2O$: C, 68.67; H, 6.08; N, 8.90 %; Found: C, 68.69; H, 6.12; N, 8.89 %.



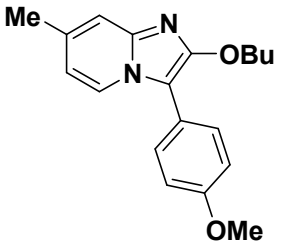
2-ethoxy-7-methyl-3-phenyl *H*-imidazo [1,2-*a*]pyridine

Gummy mass (Scheme , entry 4b, Isolated yield 81%); ^{1}H NMR (500MHz, $CDCl_3$): δ 8.15 (d, *J* = 5.0 Hz, 1H), 7.32-7.27 (m, 3 H), 7.23-7.19 (m, 2H), 6.70 (d, *J* = 5.0 Hz, 1H), 6.41 (s, 1H), 4.46 (q, 2H), 2.19 (s, 3H), 1.45 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125MHz, $CDCl_3$): δ 161.25, 160.70, 149.04, 148.30, 131.78, 130.25, 129.22, 128.94, 127.36, 119.53, 116.92, 63.03, 21.04, 14.39. Anal calc for $C_{16}H_{16}N_2O$: C, 76.16; H, 6.39; N, 11.10 %; Found: C, 76.14; H, 6.43; N, 11.05 %.



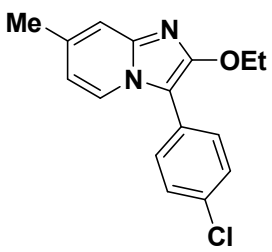
3-(4-methoxyphenyl)-2-propoxy *H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme , entry 4d, Isolated yield 80%); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.17 (d, *J* = 4.8 Hz, 1H), 7.32 (d, *J*= 4.8 Hz, 2H), 7.27 (d, *J* = 4.8 Hz, 2H), 6.67 (d, *J* = 5.2 Hz, 1H), 6.44 (s, 1H), 4.41 (t, *J* = 8.0 Hz, 2H), 3.76 (s, 3H), 1.70 (m, 2H), 0.91 (t, *J* = 6.5 Hz. 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 160.98, 148.86, 147.92, 131.64, 130.23, 129.19, 128.92, 128.08, 120.01, 116.43, 60.54, 30.85, 19.11, 14.34; Anal calc for $C_{17}H_{18}N_2O_2$: C, 72.32; H, 6.43; N, 9.92 %; Found: C, 72.35; H, 6.47; N, 9.90.



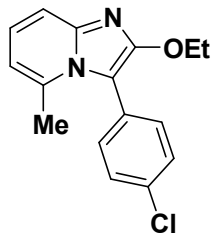
2-butoxy-3-(4-methoxyphenyl)-7-methyl*H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4g, Isolated yield 79%); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.37 (d, *J* = 5.1 Hz, 1H), 7.67 (d, *J*= 6.3 Hz, 2H), 7.59 (d, *J* = 6.3 Hz, 2H), 6.68 (d, *J* = 5.1 Hz, 1H), 6.46 (s, 1H), 4.46 (q, *J* = 8.0 Hz, 2H), 3.85 (s, 3H), 2.31 (s, 3H), 1.76 (m, 2H), 1.5 (m, 1H), 0.91 (t, *J* = 8.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.15, 148.07, 147.17, 131.14, 129.13, 125.14, 119.43, 118.13, 113.50, 62.95, 55.39, 55.38, 29.84, 21.17, 14.43; Anal calc for $C_{19}H_{22}N_2O_2$: C, 73.52; H, 7.14; N, 9.03 %; Found: C, 73.57; H, 7.18; N, 9.07 %.



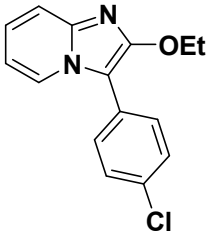
3-(4-chlorophenyl)-2-ethoxy-7-methyl*H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4i, Isolated yield 86%); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.16 (d, *J* = 5.1 Hz, 1H), 7.26 (d, *J*= 6.3 Hz, 2H), 7.19 (d, *J* = 6.3 Hz, 2H), 6.72 (d, *J* = 5.1 Hz, 1H), 6.44 (s, 1H), 4.44 (q, *J* = 6.8 Hz, 2H), 2.22 (s, 3H), 1.42 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.02, 149.16, 148.59, 139.65, 138.01, 136.40, 130.66, 130.17, 128.41, 119.77, 116.78, 63.16, 21.09, 14.37; Anal calc for $C_{16}H_{15}ClN_2O$: C, 67.02; H, 5.27; N, 9.75 %; Found: C, 67.08; H, 5.22; N, 9.76 %.



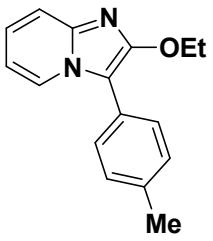
3-(4-chlorophenyl)-2-ethoxy-5-methyl*H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4j, Isolated yield 78%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, *J* = 6.5 Hz, 1H), 7.91 (d, *J* = 8,5 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 6.96 (d, *J* = 6.5 Hz, 1H), 6.70 (t, *J* = 6.5 Hz, 1H), 4.43 (q, 2H), 2.45 (s, 3H), 1.41 (t, *J* = 9.0 Hz, 3H); ^{13}C NMR (125MHz, $CDCl_3$): δ 161.17, 149.29, 148.55, 139.21, 137.82, 135.90, 130.68, 130.07, 128.63, 119.17, 116.66, 63.93, 21.01, 14.67; Anal calc. for $C_{16}H_{15}ClN_2O$: C, 67.02; H, 5.27; N, 9.77 %; Found: C, 66.95; H, 5.32; N, 9.82 %.



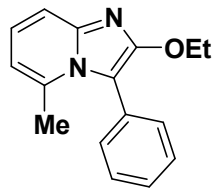
3-(4-chlorophenyl)-2-ethoxy *H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4k, Isolated yield 87%); ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.32 (d, *J* = 3.0 Hz, 1H), 7.46-7.26-7.32 (m, 4H), 7.20 (t, *J* = 4.5 Hz, 1H), 6.86 (t, *J* = 4.5 Hz, 1H), 6.53 (d, *J* = 3.0 Hz), 4.49-4.42 (m, 2H), 1.44 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.38, 161.02, 148.87, 137.69, 131.69, 131.64, 130.27, 129.21, 128.10, 118.22, 116.48, 63.08, 14.37; Anal calc for $C_{17}H_{17}ClN_2O$: C, 66.06; H, 4.80; N, 10.27 %; Found: C, 66.03; H, 4.84; N, 10.22 %.



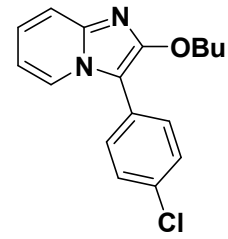
2-ethoxy-3-*p*-tolyl
H-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4l, Isolated yield 83%); ^{1}H NMR (500MHz, $CDCl_3$): δ 8.16 (d, *J* = 5.0 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 1H), 7.02 (d, *J* = 8.0 Hz,. 1H), 6.89 (d, *J* = 5.0 Hz, 1H), 6.70 (d, *J* = 5.0 Hz 1H), 4.42 (q, 2H), 2.24 (s, 3H), 1.40 (t, *J* = 7.0 Hz,3H); ^{13}C NMR (125MHz, $CDCl_3$): δ 161.28, 149.16, 148.57, 138.46, 138.01, 135.19, 131.61, 130.28, 128.56, 119.33, 116.68, 63.66, 21.13, 14.21. Anal calc. for $C_{16}H_{16}N_2O$: C, 76.16; H, 6.39; N, 11.10 %; Found: C, 76.11; H, 6.44; N, 11.09 %.



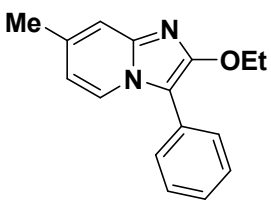
2-ethoxy-5-methyl-3-phenyl
H-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4m, Isolated yield 77%); ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.31-7.25 (m, 4H), 7.19 (t, *J* = 6.9 Hz, 2H), 6.71 (d, *J* = 6.0 Hz, 1H), 6.23 (d, *J* = 8.1 Hz, 1H), 4.44 (q, 2H), 2.45 (s, 3H), 1.40 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 160.86, 160.81, 157.72, 137.90, 131.66, 130.21, 129.23, 128.01, 117.50, 113.09, 62.98, 24.48, 14.36. Anal calc for $C_{16}H_{16}N_2O$: C, 76.16; H, 6.39; N, 11.10 %; Found: C, 76.10; H, 6.43; N, 11.12 %.



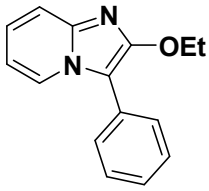
2-butoxy-3-(4-chlorophenyl)
H-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4n, Isolated yield 87%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (d, *J* = 4.8Hz, 1H), 7.52 (t, *J* = 8.8Hz, 1H), 7.25-7.17 (m, 4H), 6.91 (t, *J* = 8.8 Hz, 1H), 6.59 (d, *J* = 7.6 Hz, 1H), 4.39 (t, *J* = 8.8 Hz, 2H), 1.81-1.77 (m, 2H), 1.53-1.48 (m, 2H), 0.99 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ 161.31, 157. 75, 148.82, 138.60, 137.67, 134.40, 132.31, 129.17, 128.10, 118.20, 116.47, 67.44, 30.85, 21.17, 14.45. Anal calc for $C_{17}H_{17}ClN_2O$: C, 67.88; H, 5.70; N, 9.31 %; Found: C, 67.86; H, 5.76; N, 9.36 %.



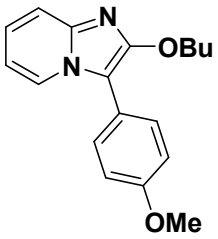
2-ethoxy-7-methyl-3-phenyl
H-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4o, Isolated yield 81%); ^{1}H NMR (500MHz, $CDCl_3$): δ 8.15 (d, *J* = 5.0 Hz, 1H), 7.33-7.29 (m, 3 H), 7.26-7.21 (m, 2H), 6.70 (d, *J* = 5.0 Hz 1H), 6.41 (s, 1H), 4.44 (q, 2H), 2.19 (s, 1H), 1.44 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125MHz, $CDCl_3$): δ 161.25, 160.70, 149.04, 148.30, 131.78, 130.25, 129.22, 128.94, 127.36, 119.53, 116.92, 63.03, 21.04, 14.39. Anal calc for $C_{16}H_{16}N_2O$: C, 76.16; H, 6.39; N, 11.10 %; Found: C, 76.11; H, 6.34; N, 11.15 %.



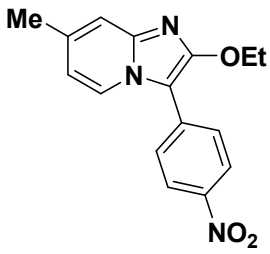
2-ethoxy-3-phenyl
H-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4p, Isolated yield 85%); ^{1}H NMR (500MHz, $CDCl_3$): δ 8.33 (d, *J* = 4.2 Hz, 1H), 7.46 (t, *J* = 6.0 Hz, 1 H), 7.32-7.27 (m, 5H), 6.90 (d, *J* = 4.8 Hz, 1H), 6.56 (d, *J* = 8.0 Hz, 1H), 4.48 (q, 2H), 1.26 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75MHz, $CDCl_3$): δ 161.37, 160.98, 148.86, 147.92, 131.67, 130.26, 129.19, 128.90, 127.37, 120.00, 116.46, 63.06, 14.35. Anal calc for $C_{15}H_{14}N_2O$: C, 75.65; H, 6.92; N, 11.76 %; Found: C, 75.59; H, 6.96; N, 11.80 %.



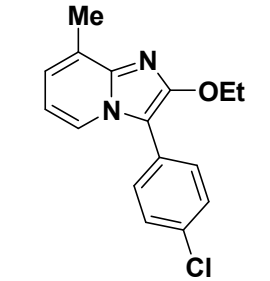
2-butoxy-3-(4-methoxyphenyl)
H-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4q, Isolated yield 76%); ^{1}H NMR (500MHz, $CDCl_3$): δ 8.35 (d, *J* = 4.3 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.27 (t, *J* = 4.5 Hz, 1H), 6.90 (d, *J* = 5.5 Hz 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 6.58 (d, *J* = 8.0 Hz 1H), 4.39 (t, *J* = 6.5 Hz, 2H), 1.83-1.77 (m, 2H), 1.56-1.49 (m, 2H), 0.99 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 165.95, 161.31, 148.56, 144.79, 137.73, 133.67, 130.61, 128.55, 128.49, 118.48, 118.43, 116.57, 67.48, 30.80, 21.16, 19.61. Anal calc for $C_{18}H_{20}N_2O_2$: C, 72.95; H, 6.80; N, 9.45 %; Found: C, 72.98; H, 6.74; N, 9.49 %.



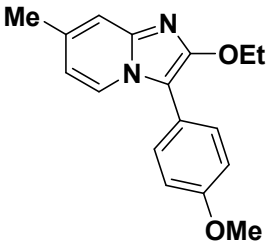
2-ethoxy-7-methyl-3-(4-nitrophenyl) *H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4r, Isolated yield 87%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.15 (d, *J* = 4.0 Hz, 1H), 7.92 (d, *J*= 8.0 Hz, 2H), 7.79 (d, *J* = 1.0 Hz, 2H), 6.92 (d, *J* = 8.5 Hz, 1H), 6.37 (s, 1H), 4.40 (q, *J* = 11.5 Hz, 2H), 2.41 (s, 3H), 1.29 (t, *J* = 5.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.11, 151.43, 131.80, 130.32, 129.14, 128.94, 128.87, 128.12, 127.33, 119.47, 116.96, 63.07, 21.06, 14.43; Anal calc for $C_{16}H_{15}N_3O_3$: C, 64.64; H, 5.09; N, 14.13 %; Found: C, 64.67; H, 5.13; N, 14.11 %.



3-(4-chlorophenyl)-2-ethoxy-8-methyl*H*-imidazo[1,2-*a*]pyridine

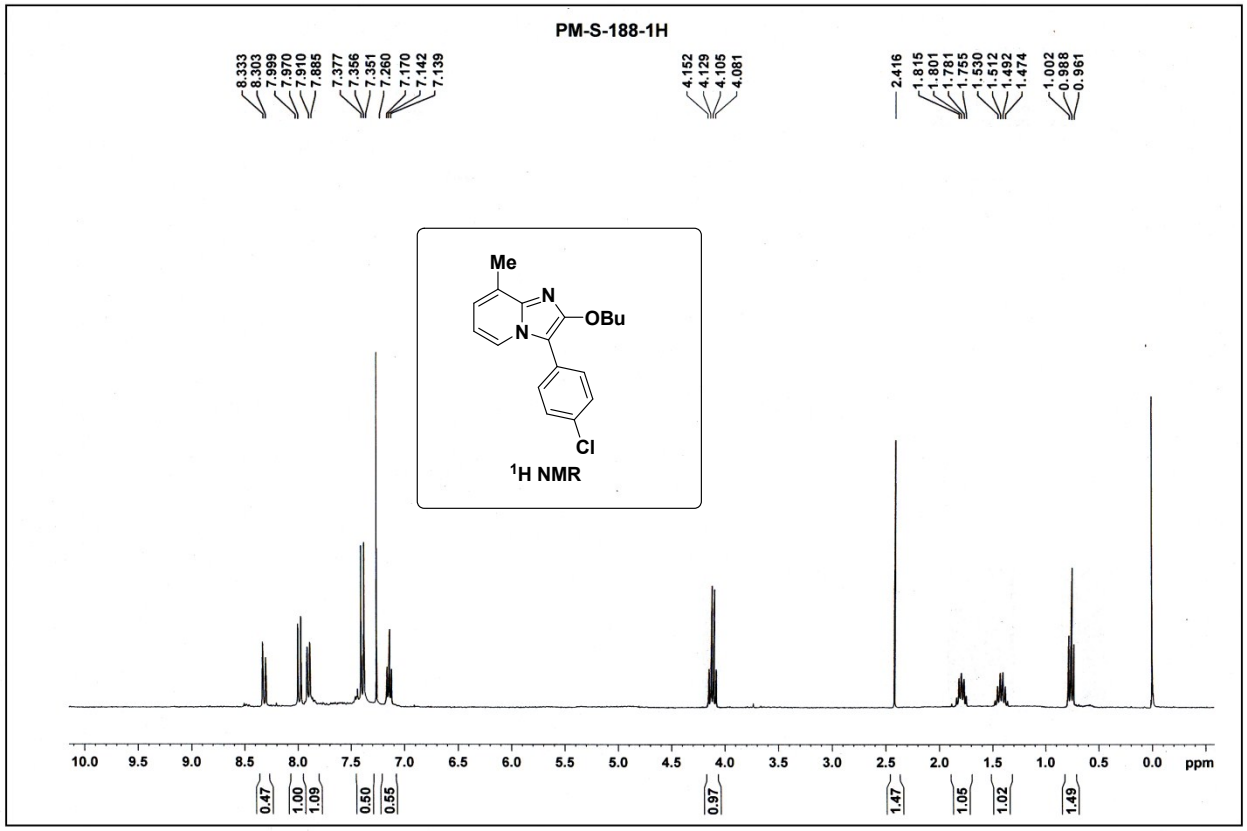
Gummy mass (Scheme 2, entry 4s, Isolated yield 83%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.98 (d, *J* = 6.5 Hz, 1H), 7.90 (d, *J* = 8,5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 6.97 (d, *J* = 6.5 Hz, 1H), 6.70 (t, *J* = 6.5 Hz, 1H), 4.13 (q, 2H), 2.65 (s, 3H), 1.28 (t, *J* = 9.0 Hz, 3H); ^{13}C NMR (125MHz, $CDCl_3$): δ 161.17, 149.29, 148.55, 139.21, 137.82, 135.90, 130.68, 130.07, 128.63, 119.17, 116.66, 63.93, 21.01, 14.67; Anal calc. for $C_{16}H_{15}ClN_2O$: C, 66.84; H, 5.27; N, 9.77 %; Found: C, 66.93; H, 5.23; N, 9.80 %.

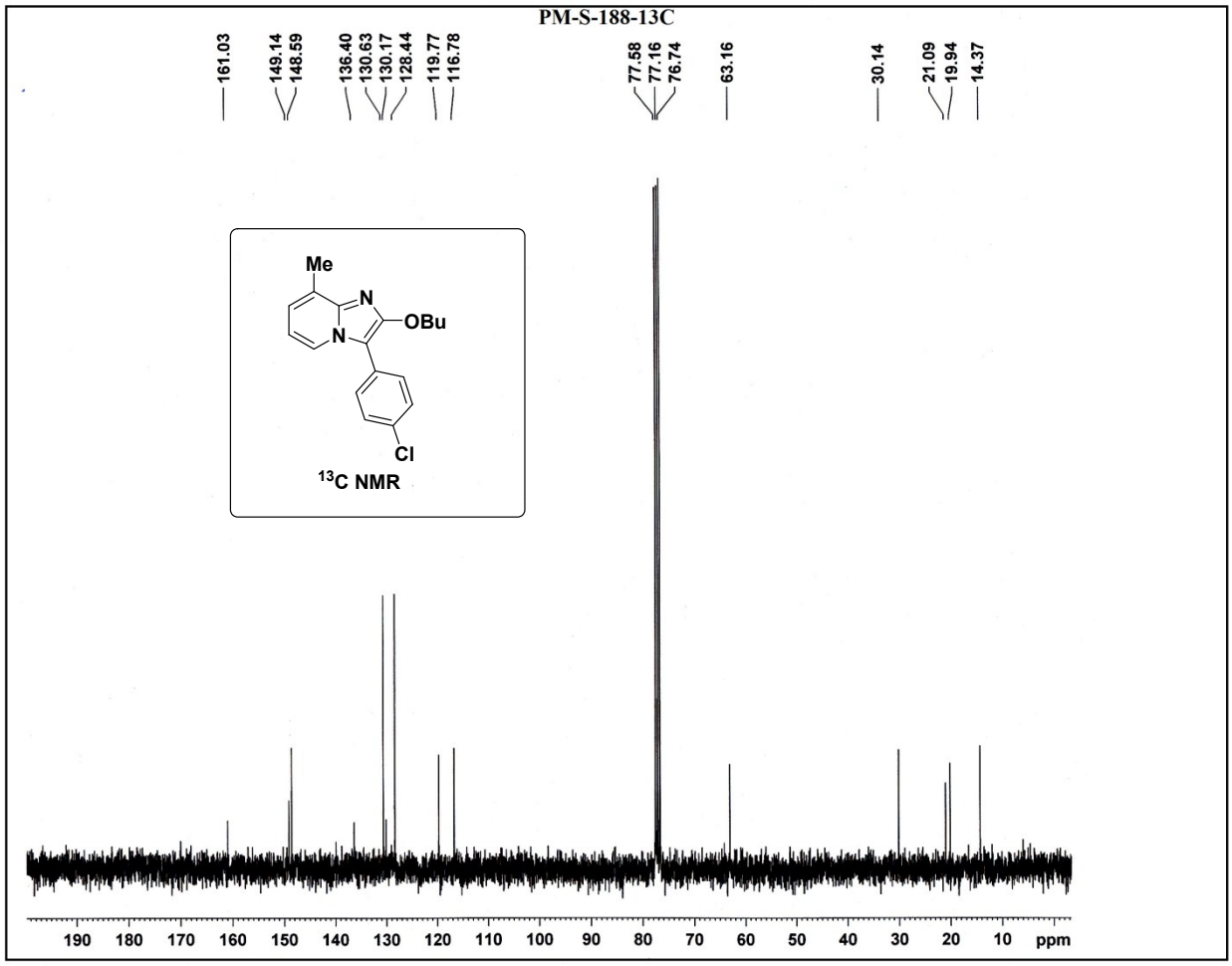


2-ethoxy-3-(4-methoxyphenyl) -7-methyl*H*-imidazo[1,2-*a*]pyridine

Gummy mass (Scheme 2, entry 4t, Isolated yield 86%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.23 (d, *J* = 3.5 Hz, 1H), 7.87 (d, *J* = 14.5 Hz, 2H), 7.47 (d, *J* = 14.5 Hz, 2H), 6.46 (d, *J* = 8.5 Hz, 1H), 6.33 (s, 1H), 4.45-4.33 (q, *J* = 11.5 Hz, 2H), 3.23 (s, 3H), 2.40 (s, 3H), 1.30 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.04, 149.16, 148.57, 136.41, 131.02, 130.66, 130.16, 129.40, 128.41, 119.88, 116.78, 63.14, 59.19, 21.07, 14.34; Anal calc for $C_{17}H_{18}N_2O_2$: C, 72.32; H, 6.43; N, 9.92 %; Found: C, 72.36; H, 6.45; N, 9.89 %.

ESI 6. Copy of ^{1}H NMR and ^{13}C NMR spectra of the 2-alkoxy-imidazopyridine derivatives:

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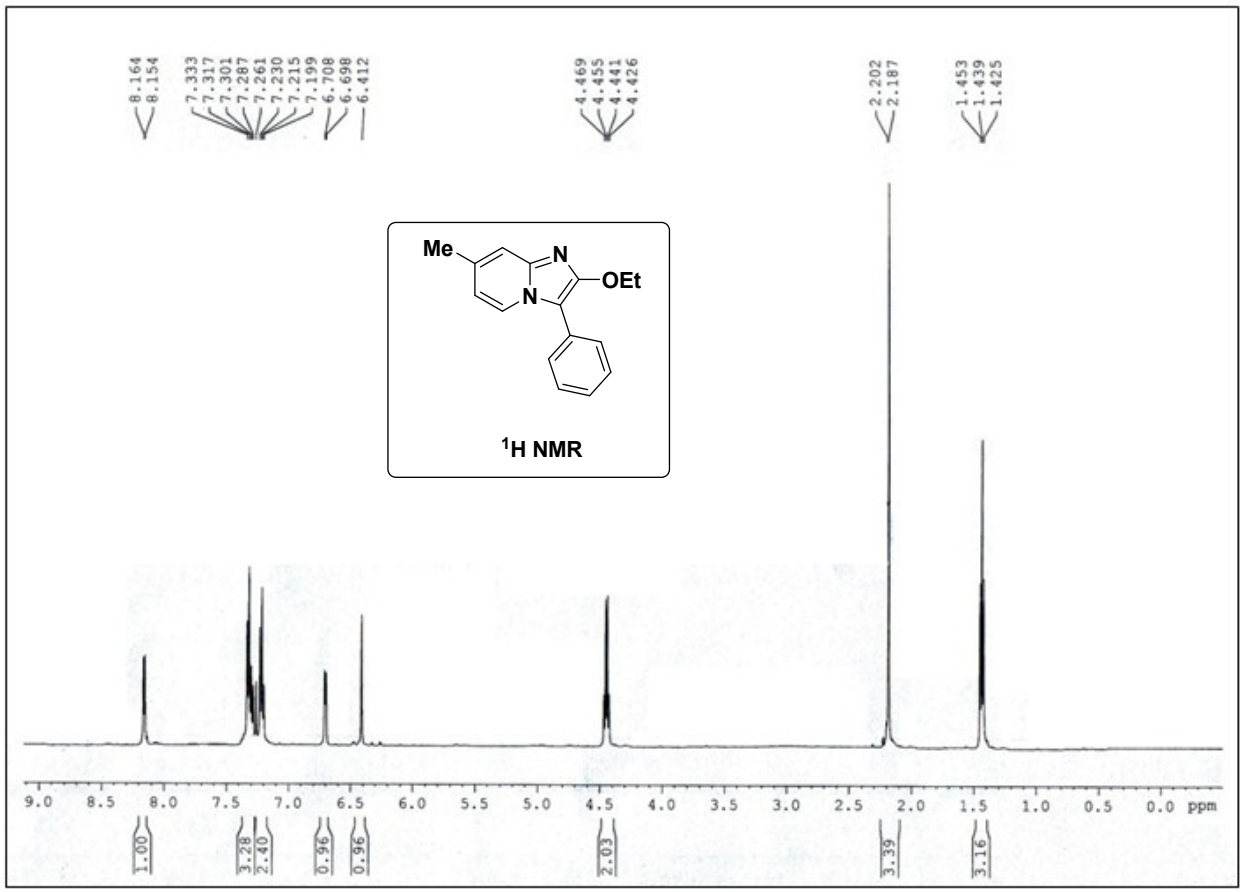
149.14
148.59
136.40
130.63
130.17
128.44
119.77
116.78
77.58
77.16
76.74
63.16
30.14
21.09
19.94
14.37
Me
N
N
OBu
Cl
13C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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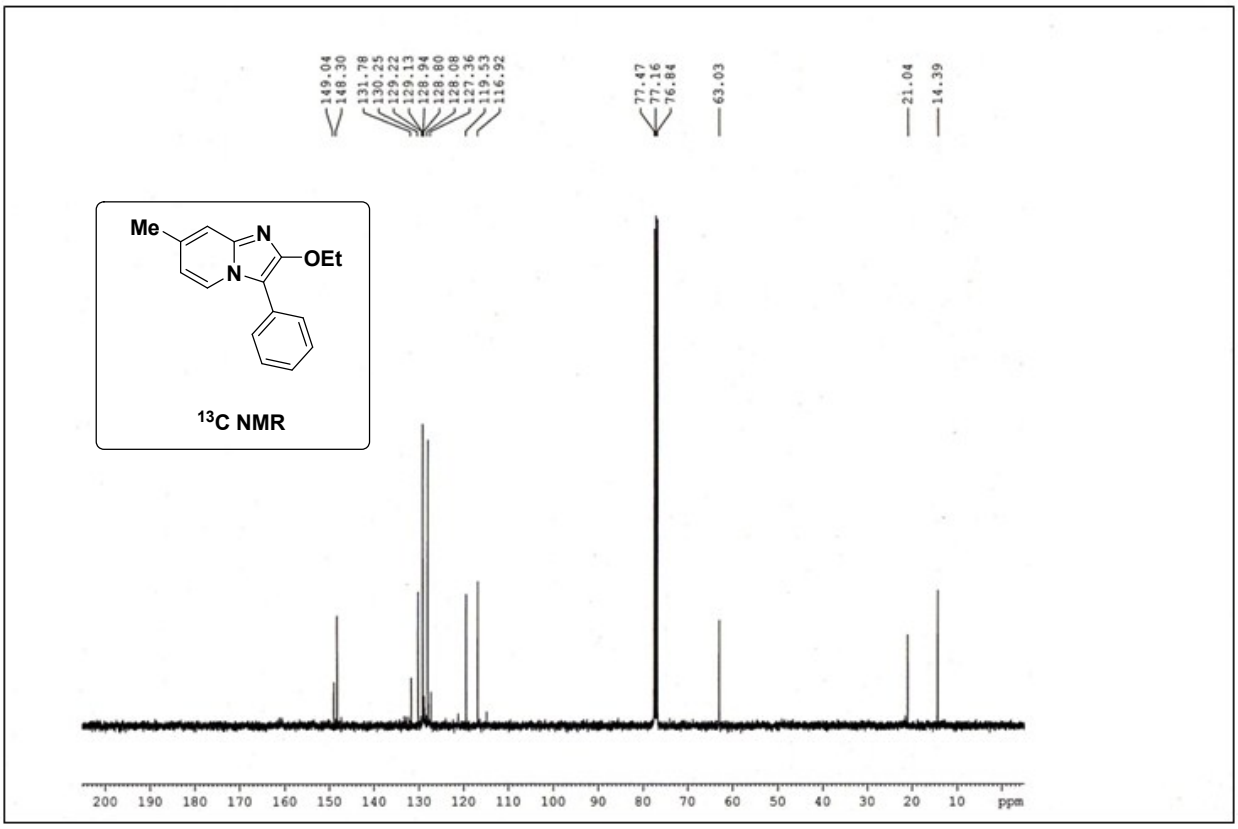
8.154
7.333
7.317
7.301
7.287
7.261
7.230
7.215
7.199
6.708
6.698
6.412
4.469
4.455
4.441
4.426
2.202
2.187
1.453
1.439
1.425
Me
N
N
OEt
1H NMR
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
1.00
3.28
2.40
0.96
0.96
2.03
3.39
3.16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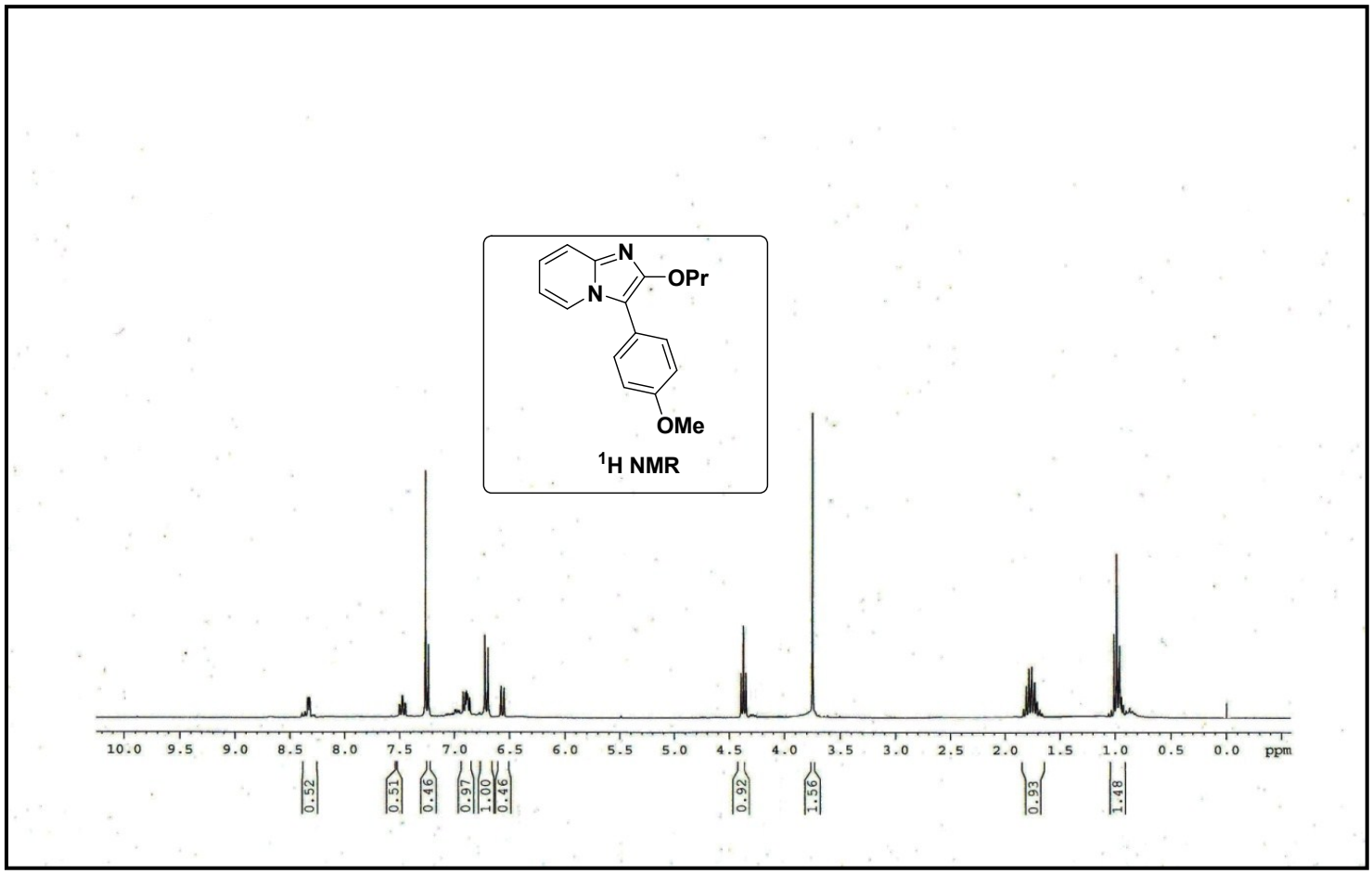
148.30
131.78
130.25
129.22
129.13
128.94
128.80
128.08
127.36
119.53
116.92
77.47
77.16
76.84
63.03
21.04
14.39
Me
N
N
OEt
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


N
N
OPr
OMe
1H NMR
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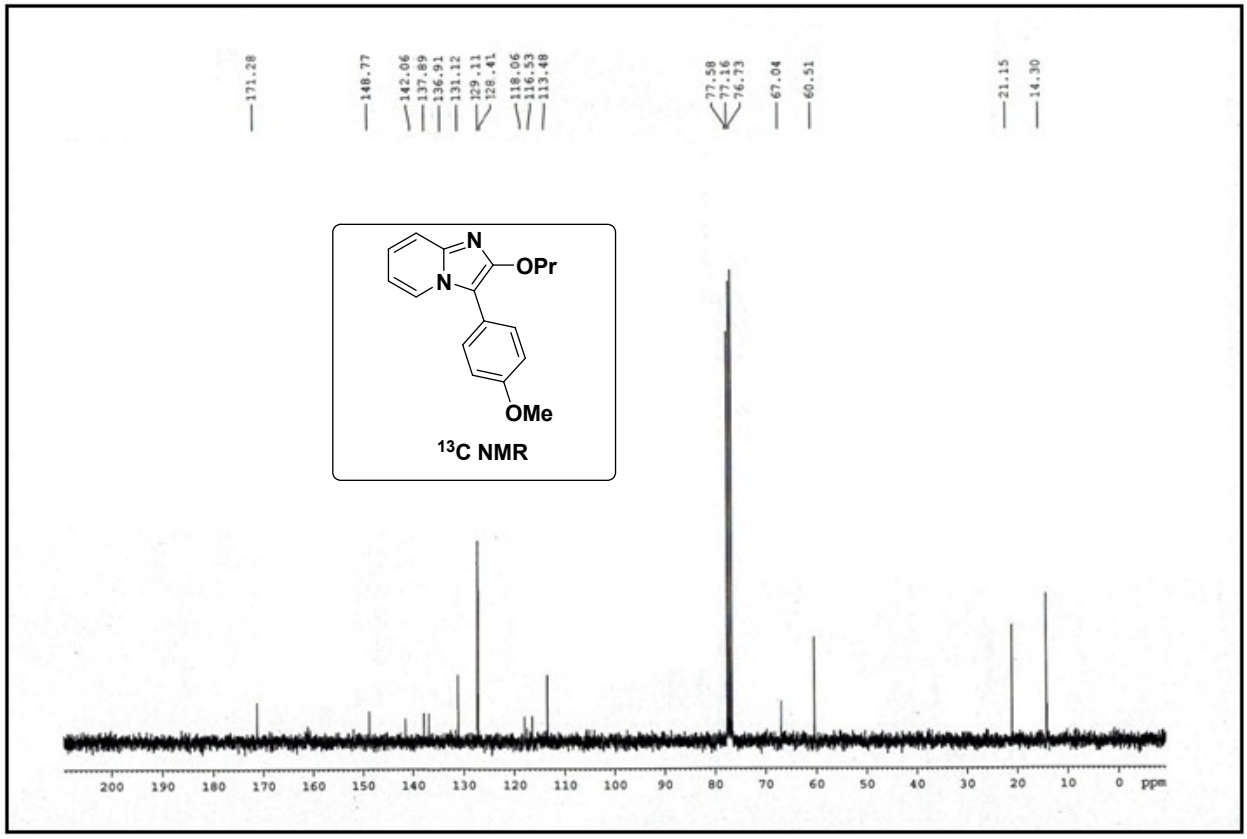
0.51
0.46
0.97
1.00
0.46
0.92
1.56
0.93
1.48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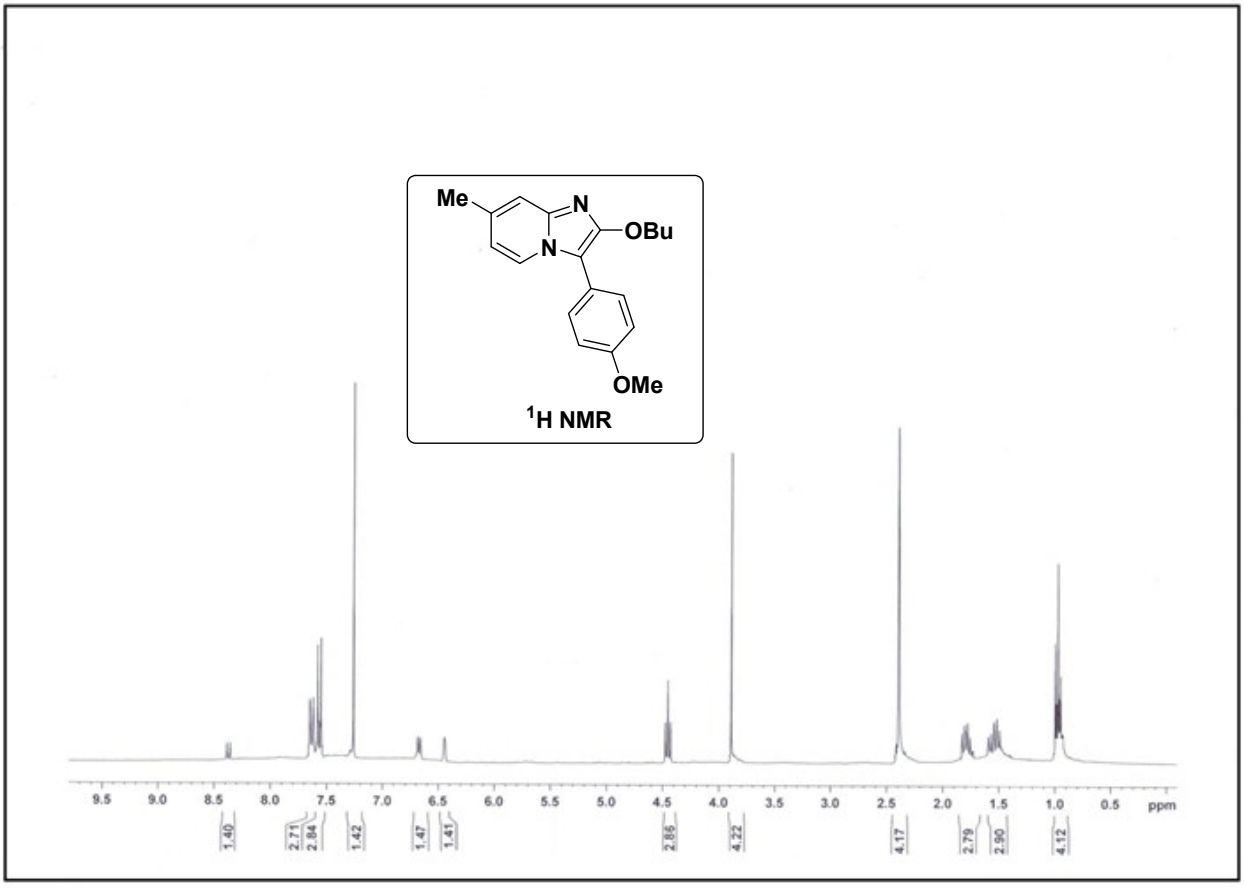
148.77
142.06
137.89
136.91
131.12
129.11
128.41
118.06
116.53
113.48
77.58
77.16
76.73
67.04
60.51
21.15
14.30
N
N
OPr
OMe
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Me
N
N
OBu
OMe
1H NMR
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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1.42
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1.41
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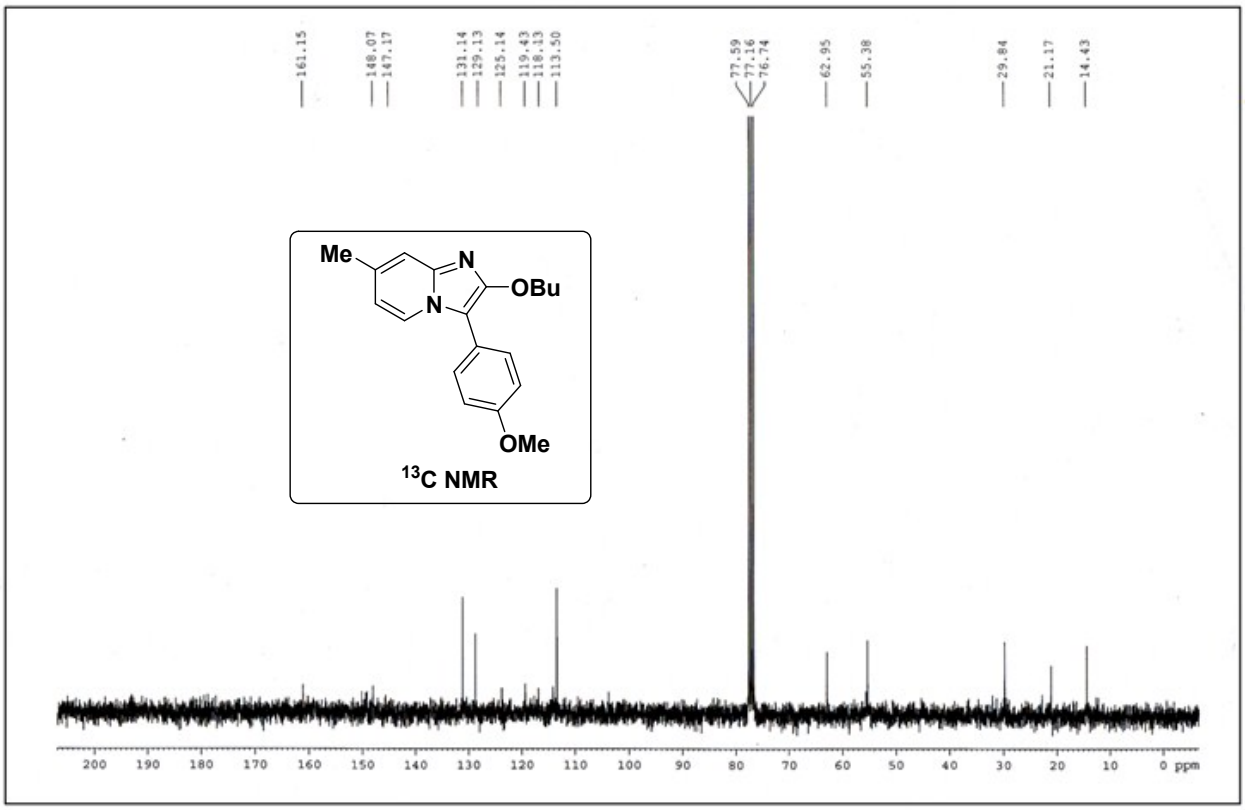
4.22
4.17
2.79
2.90
4.12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131.14
129.13
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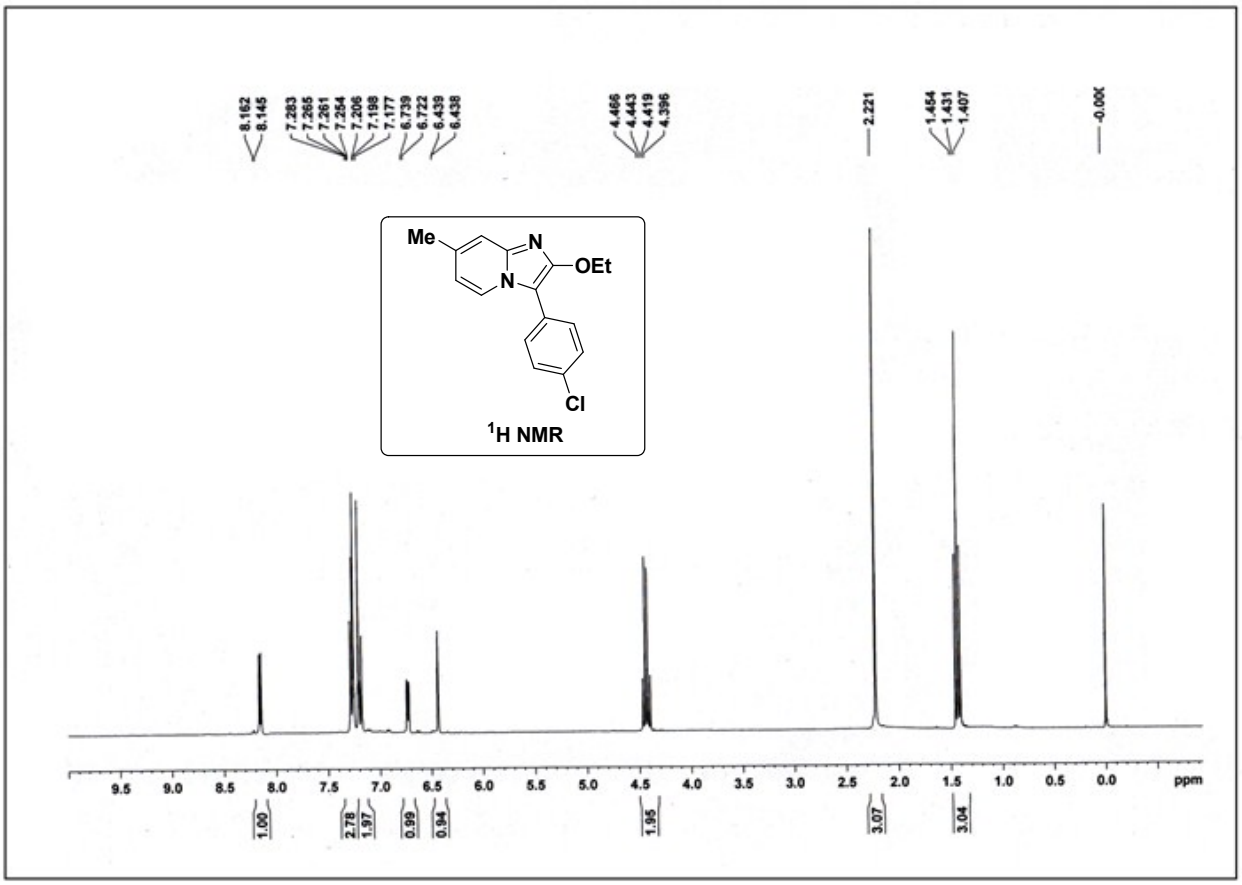
118.13
113.50
77.59
77.16
76.74
62.95
55.38
29.84
21.17
14.43
Me
N
N
OBu
OMe
13C NMR
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.206
7.198
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6.722
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6.438
4.466
4.443
4.419
4.396
2.221
1.454
1.431
1.407
-0.00
Me
N
N
OEt
Cl
1H NMR
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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0.0
ppm
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0.99
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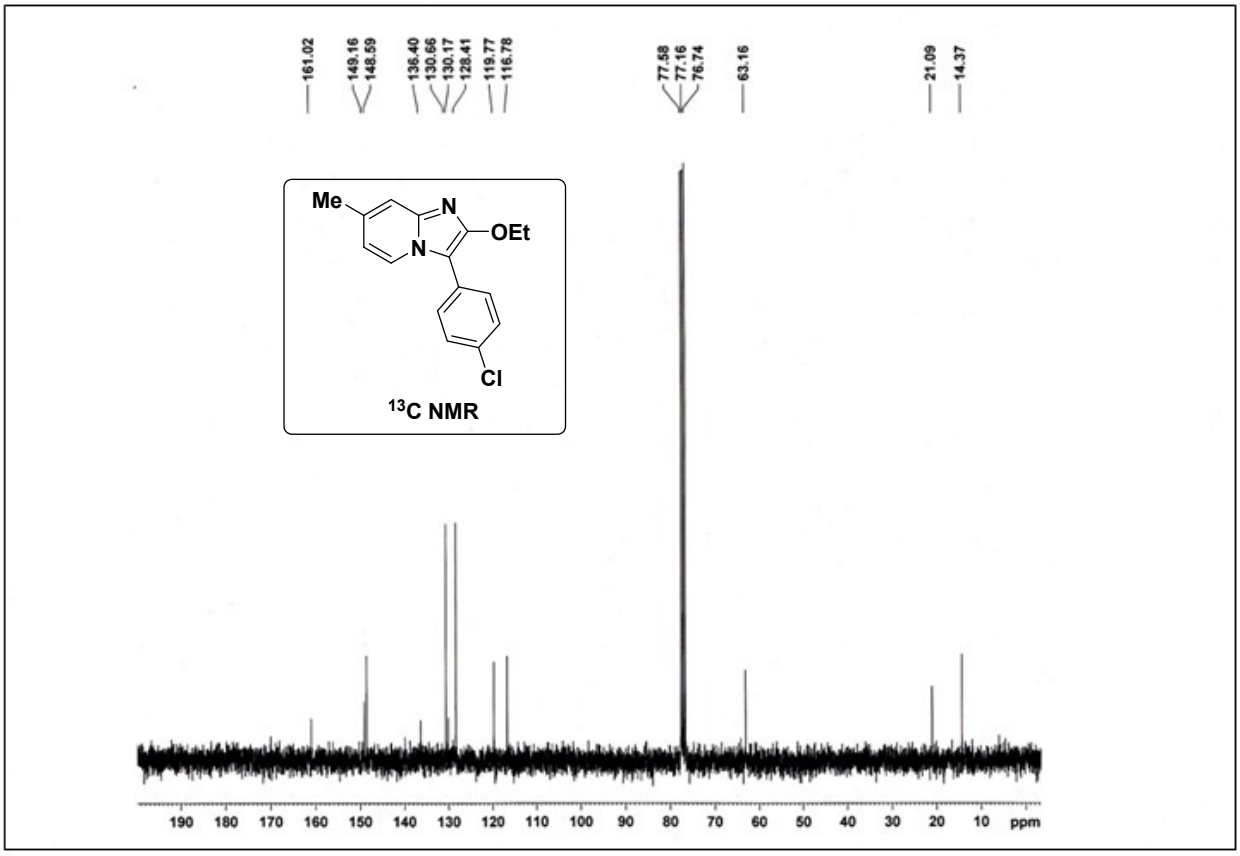
1.95
3.07
3.04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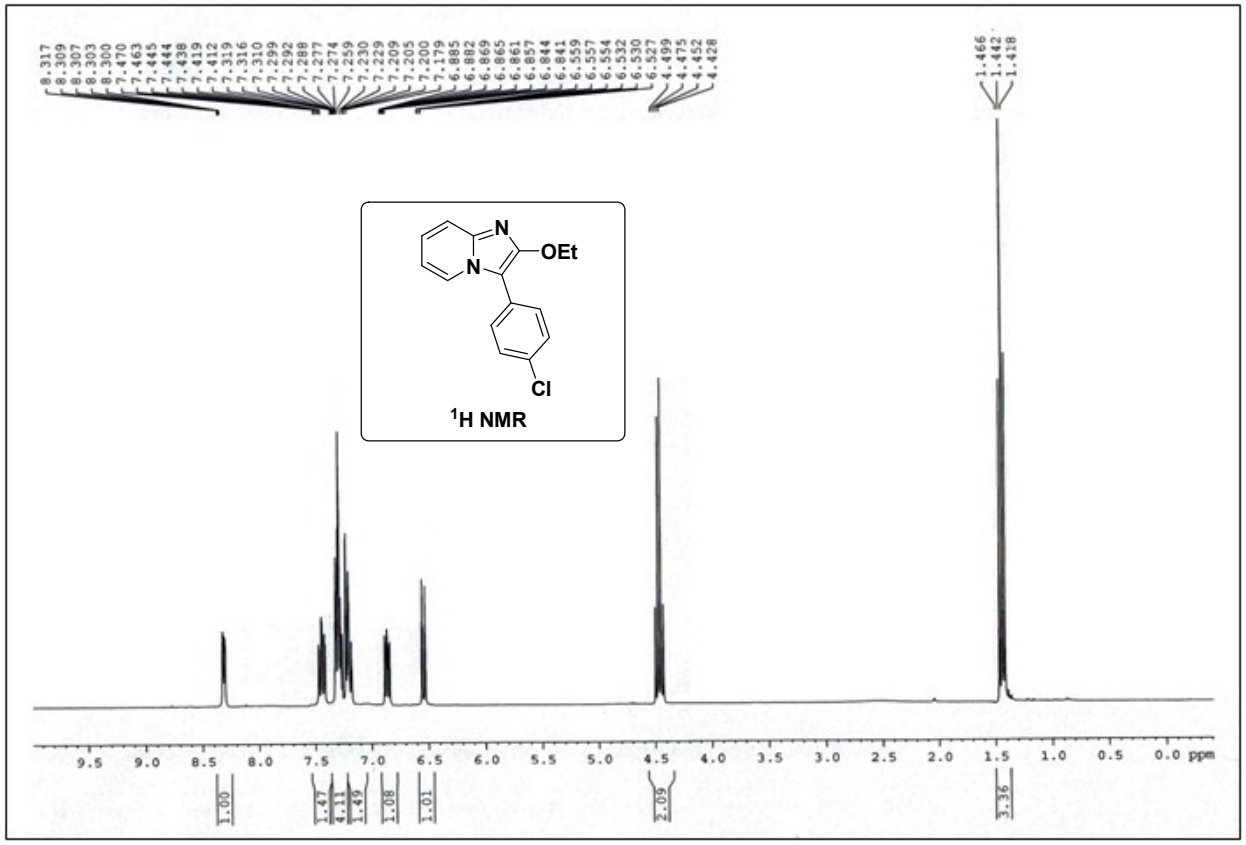
148.59
136.40
130.66
130.17
128.41
119.77
116.78
77.58
77.16
76.74
63.16
21.09
14.37
Me
N
N
OEt
Cl
13C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.445
7.444
7.438
7.419
7.412
7.319
7.316
7.310
7.299
7.292
7.288
7.277
7.274
7.259
7.230
7.229
7.209
7.205
7.200
7.179
6.885
6.882
6.869
6.865
6.861
6.857
6.844
6.841
6.559
6.557
6.554
6.532
6.530
6.527
4.499
4.475
4.452
4.428
1.466
1.442
1.418
N
N
OEt
Cl
1H NMR
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
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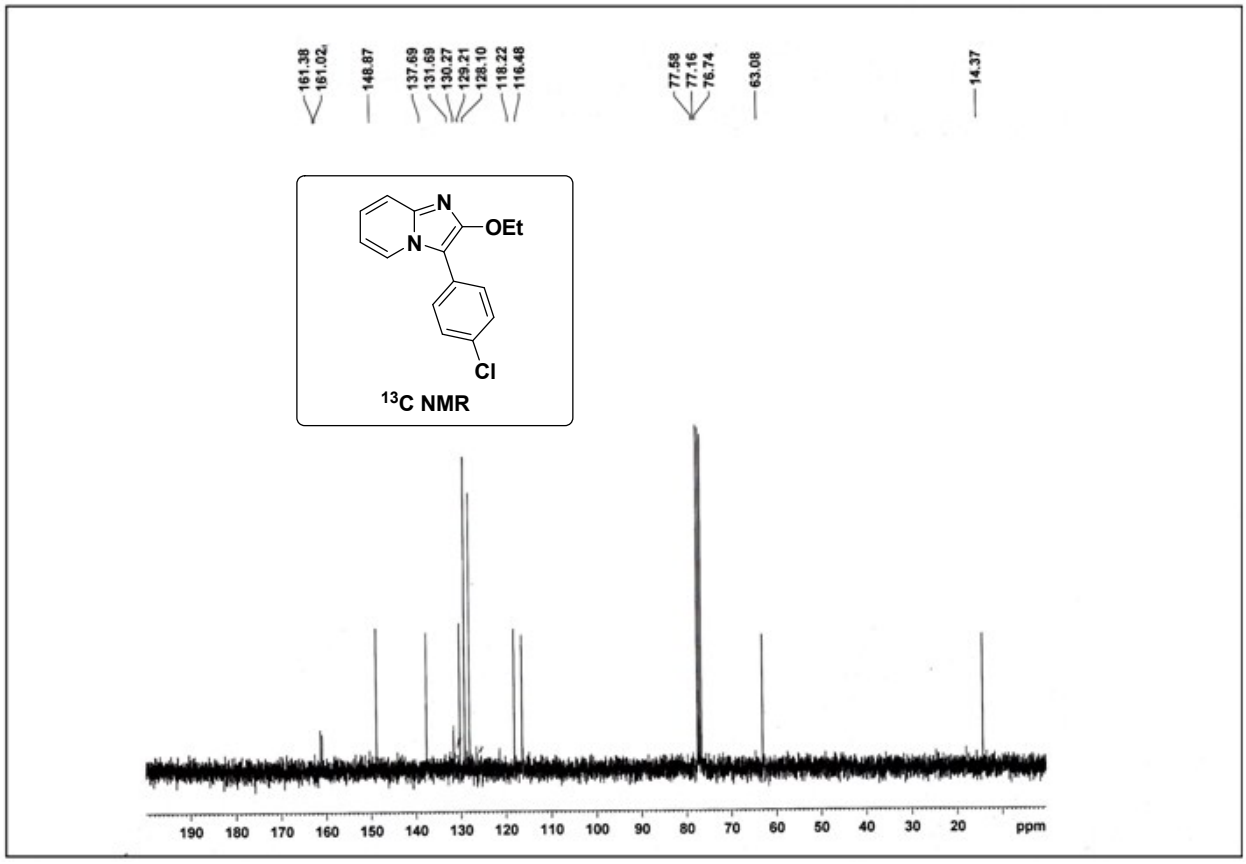
4.11
1.49
1.08
1.01
2.09
3.36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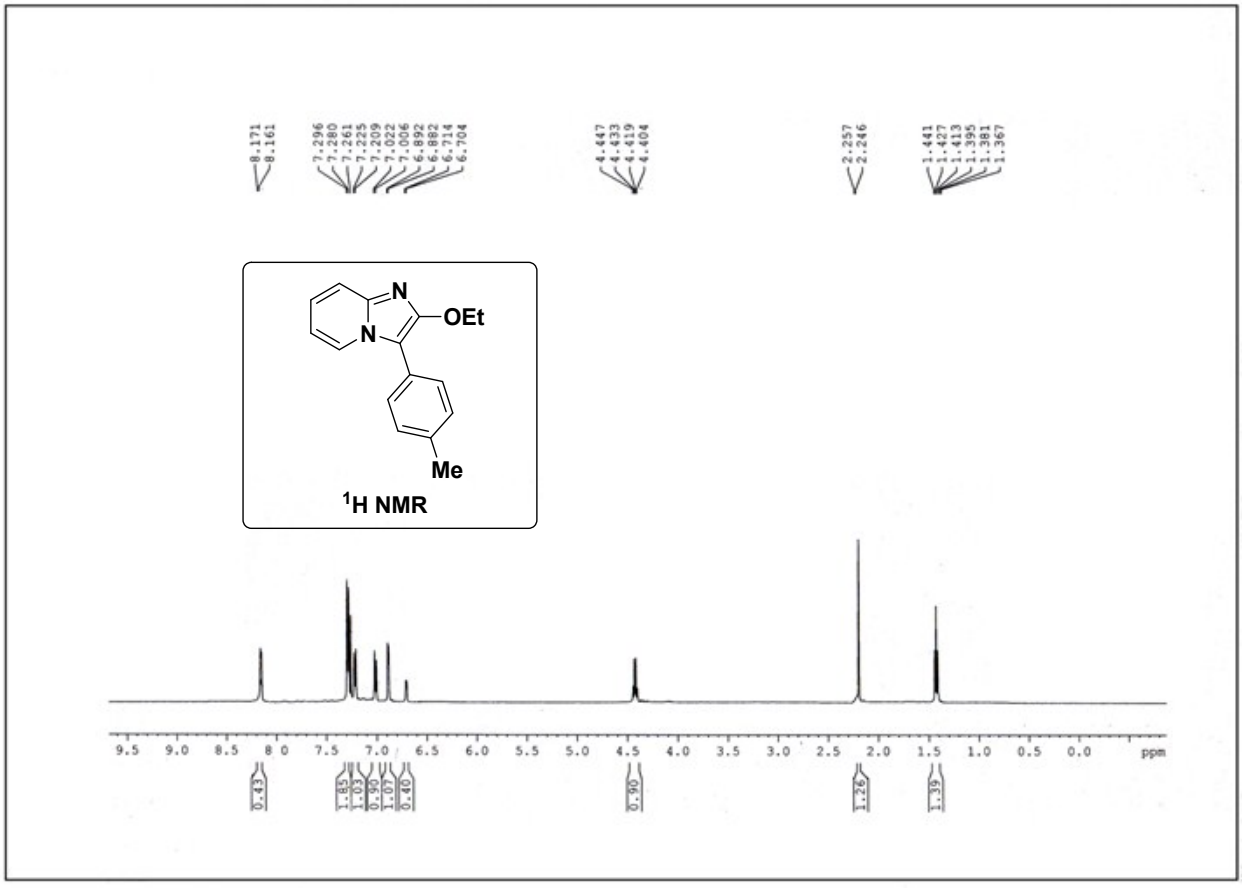
131.69
130.27
129.21
128.10
118.22
116.48
77.58
77.16
76.74
63.08
14.37
N
N
OEt
Cl
13C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.022
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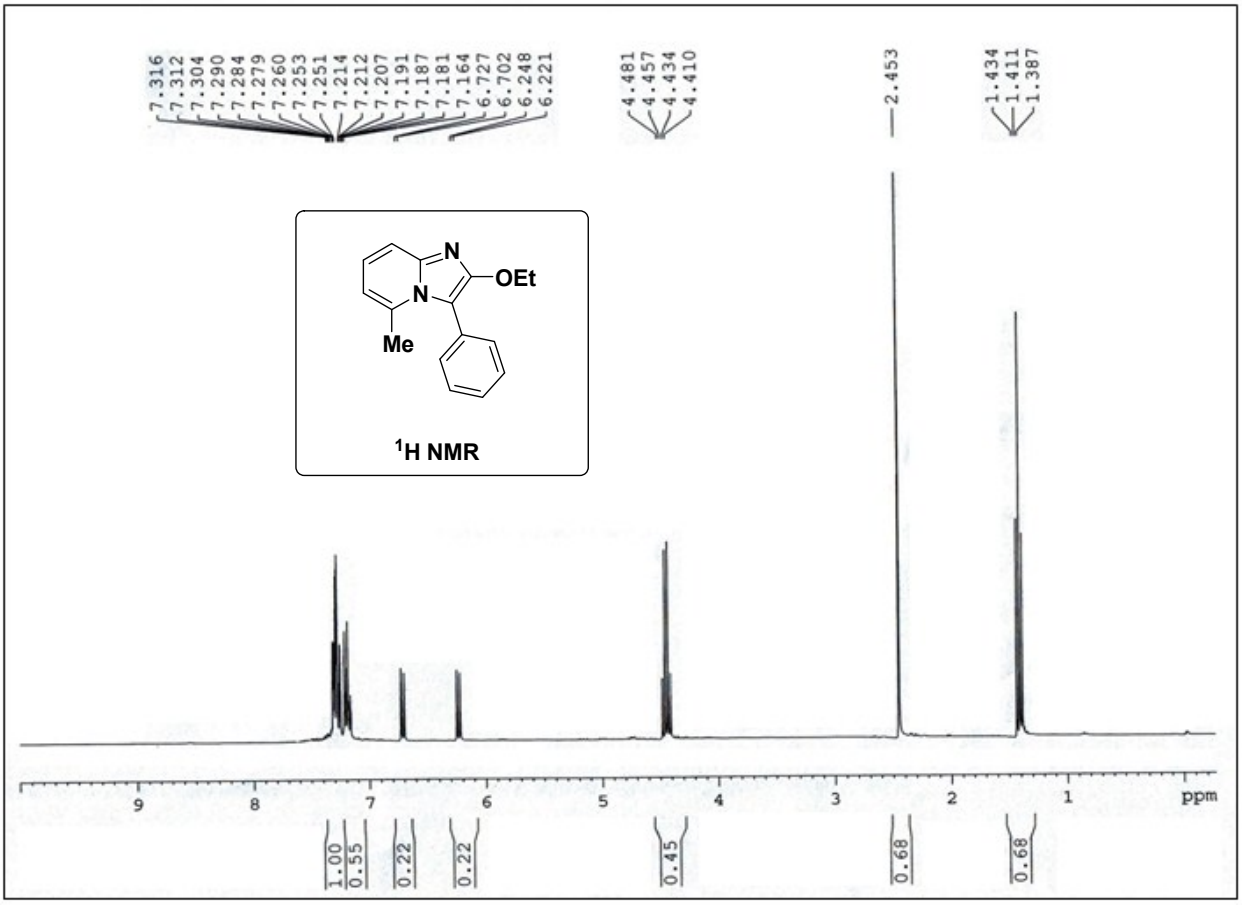
6.882
6.714
6.704
4.447
4.433
4.419
4.404
2.257
2.246
1.441
1.427
1.413
1.395
1.381
1.367
N
N
OEt
Me
1H NMR
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.43
1.85
1.03
0.90
1.07
0.40
0.90
1.26
1.39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7.279
7.260
7.253
7.251
7.214
7.212
7.207
7.191
7.187
7.181
7.164
6.727
6.702
6.248
6.221
4.481
4.457
4.434
4.410
2.453
1.434
1.411
1.387
N
N
OEt
Me
1H NMR
9
8
7
6
5
4
3
2
1
ppm
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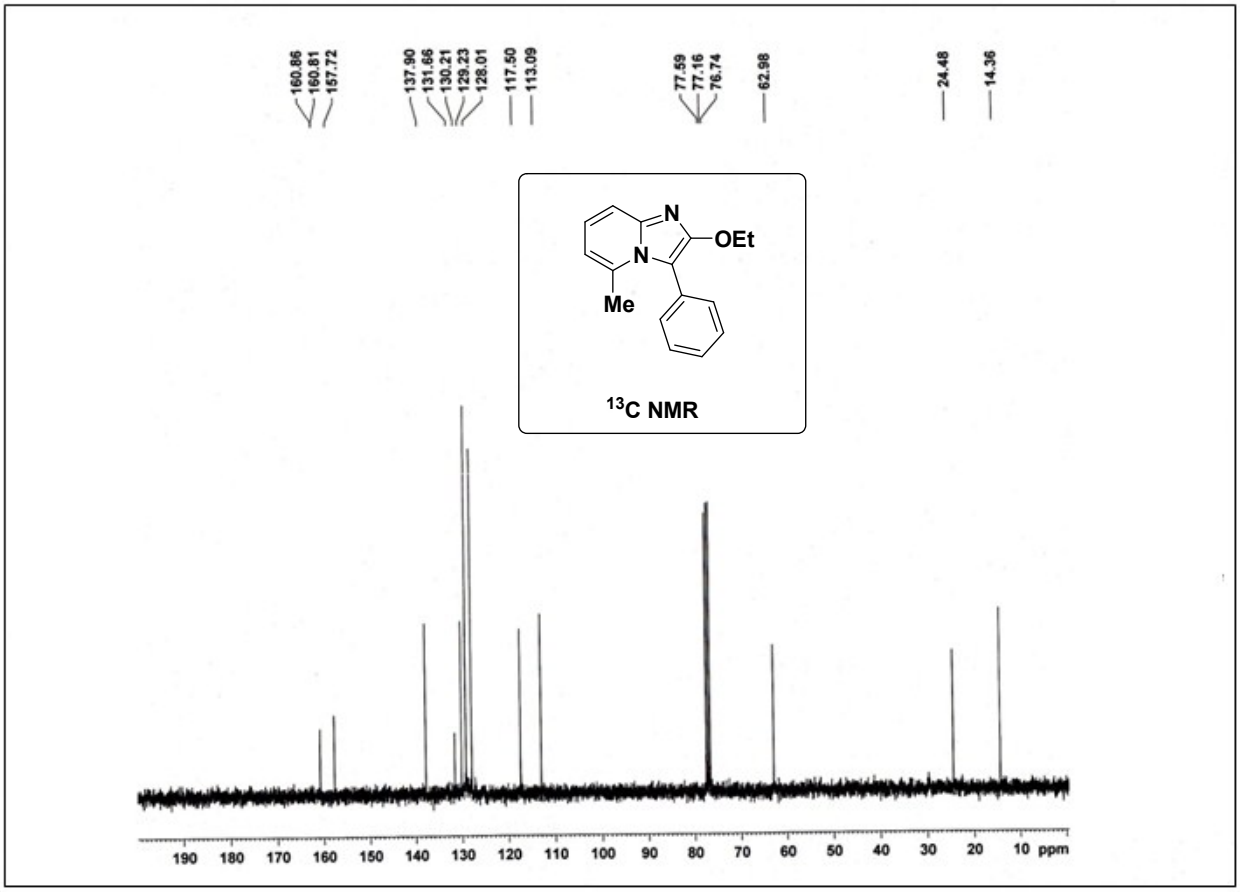
0.55
0.22
0.22
0.45
0.68
0.68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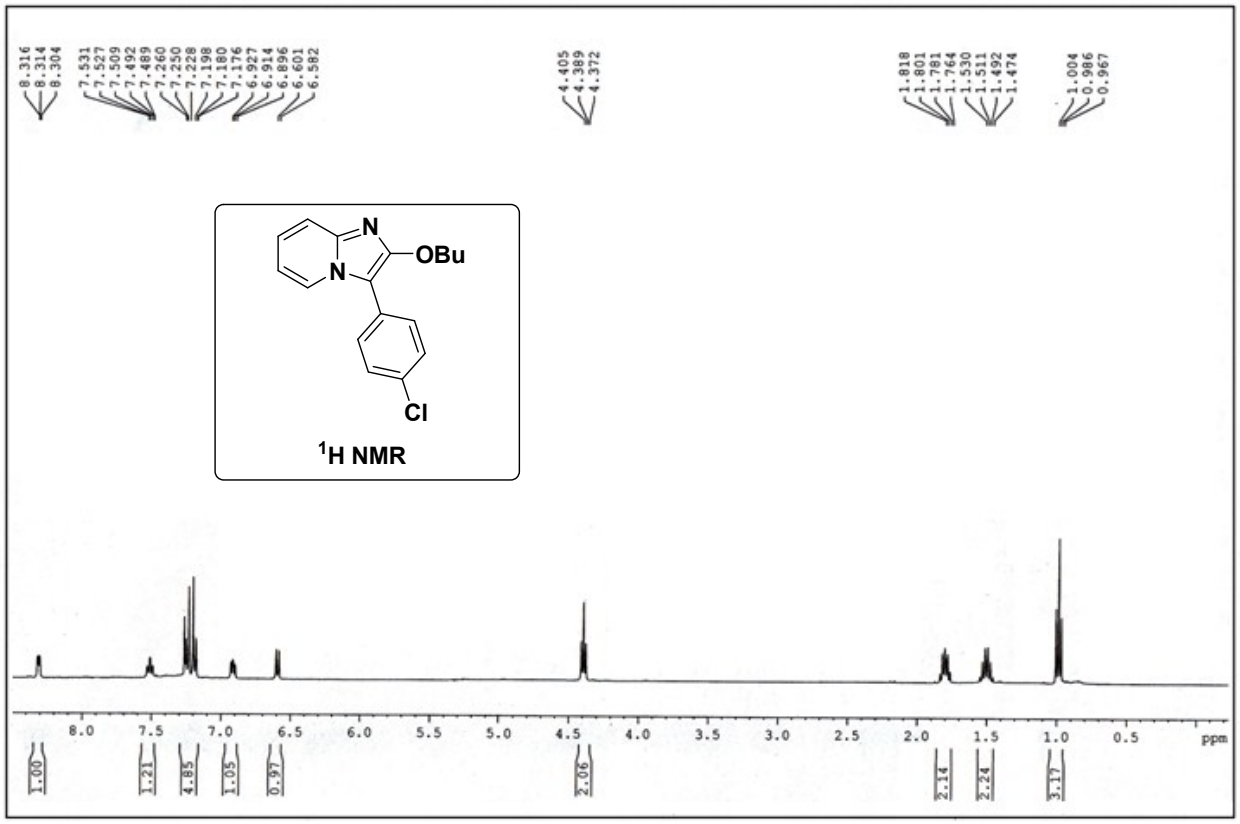
137.90
131.66
130.21
129.23
128.01
117.50
113.09
77.59
77.16
76.74
62.98
24.48
14.36
N
OEt
N
Me
13C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.489
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7.250
7.228
7.198
7.180
7.176
6.927
6.914
6.896
6.601
6.582
4.405
4.389
4.372
1.818
1.801
1.781
1.764
1.530
1.511
1.492
1.474
1.004
0.986
0.967
N
N
OBu
Cl
1H NMR
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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ppm
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0.97
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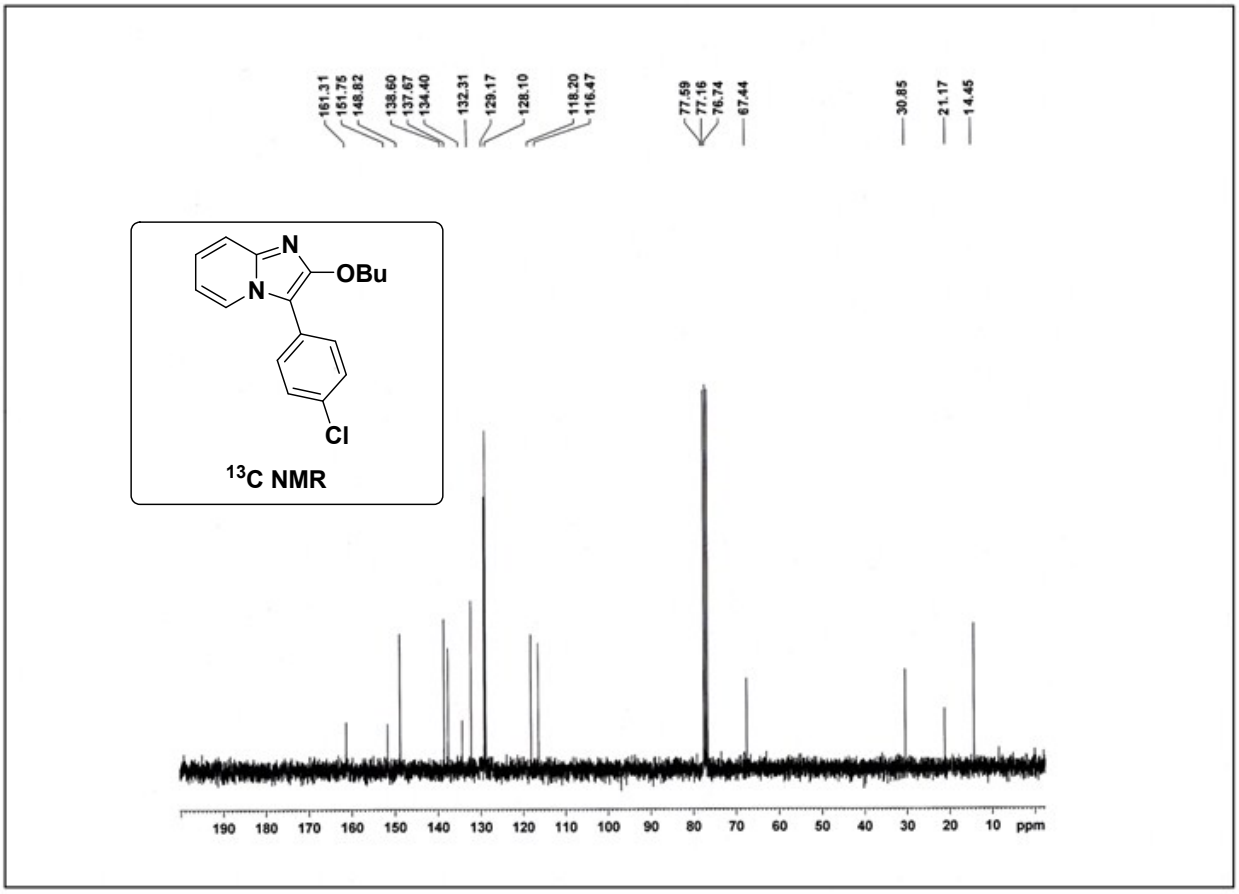
2.24
3.17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129.17
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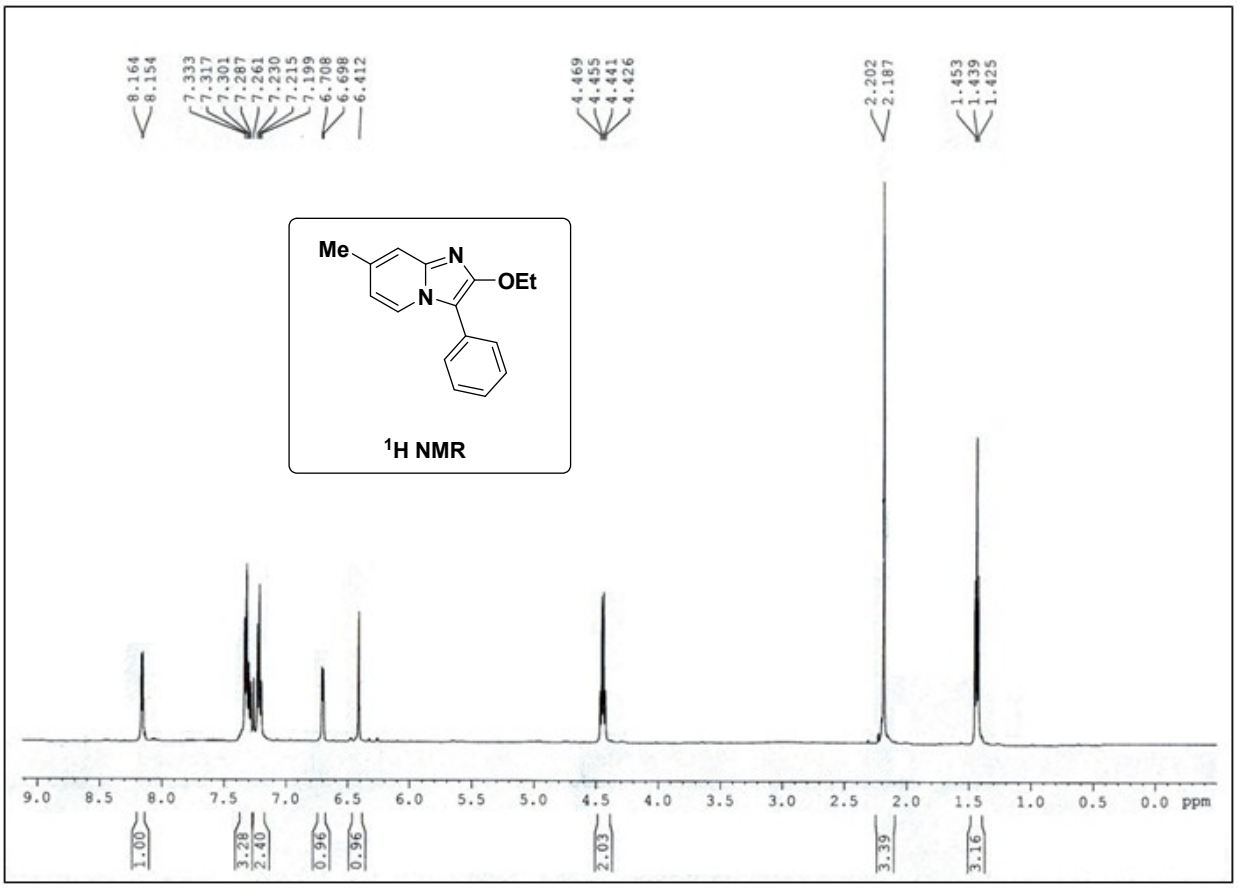
118.20
116.47
77.59
77.16
76.74
67.44
30.85
21.17
14.45
N
N
OBu
Cl
13C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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6.698
6.412
4.469
4.455
4.441
4.426
2.202
2.187
1.453
1.439
1.425
Me
N
OEt
N
1H NMR
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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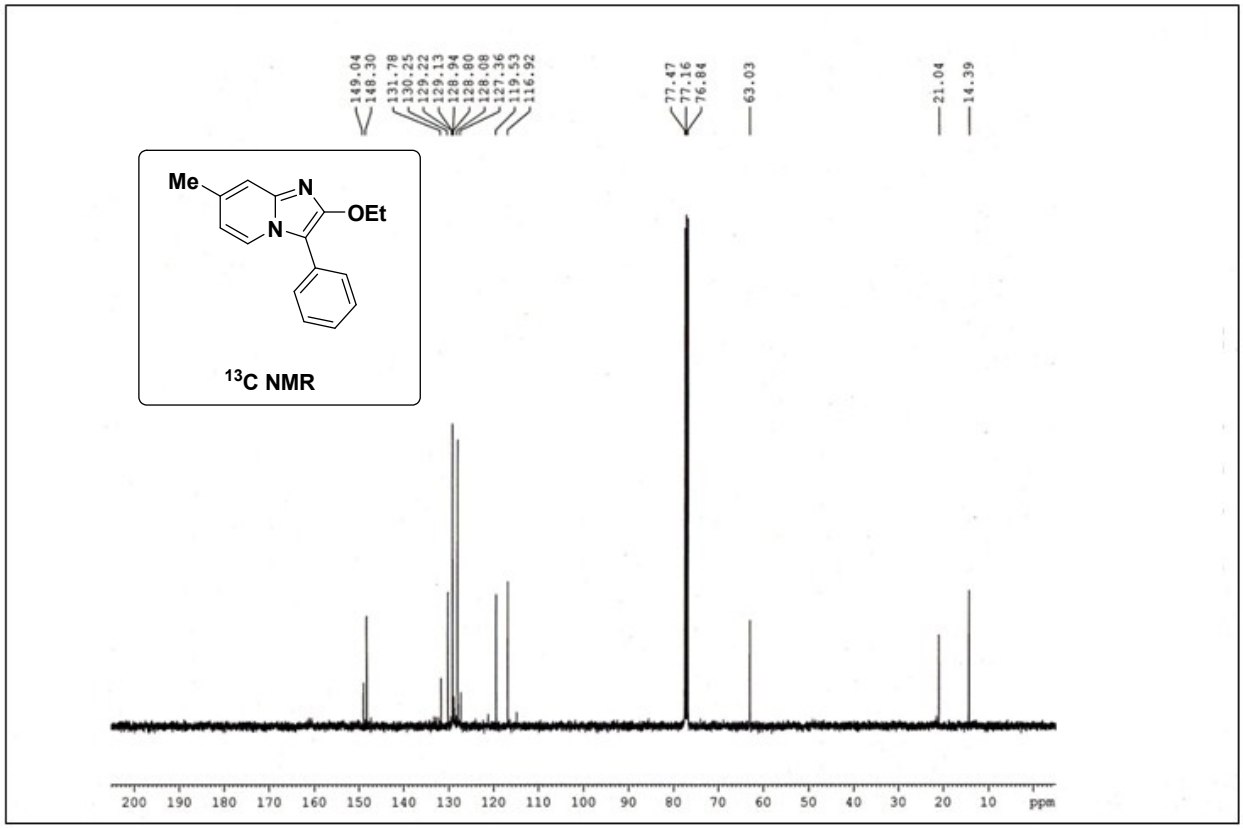
0.96
0.96
2.03
3.39
3.16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129.13
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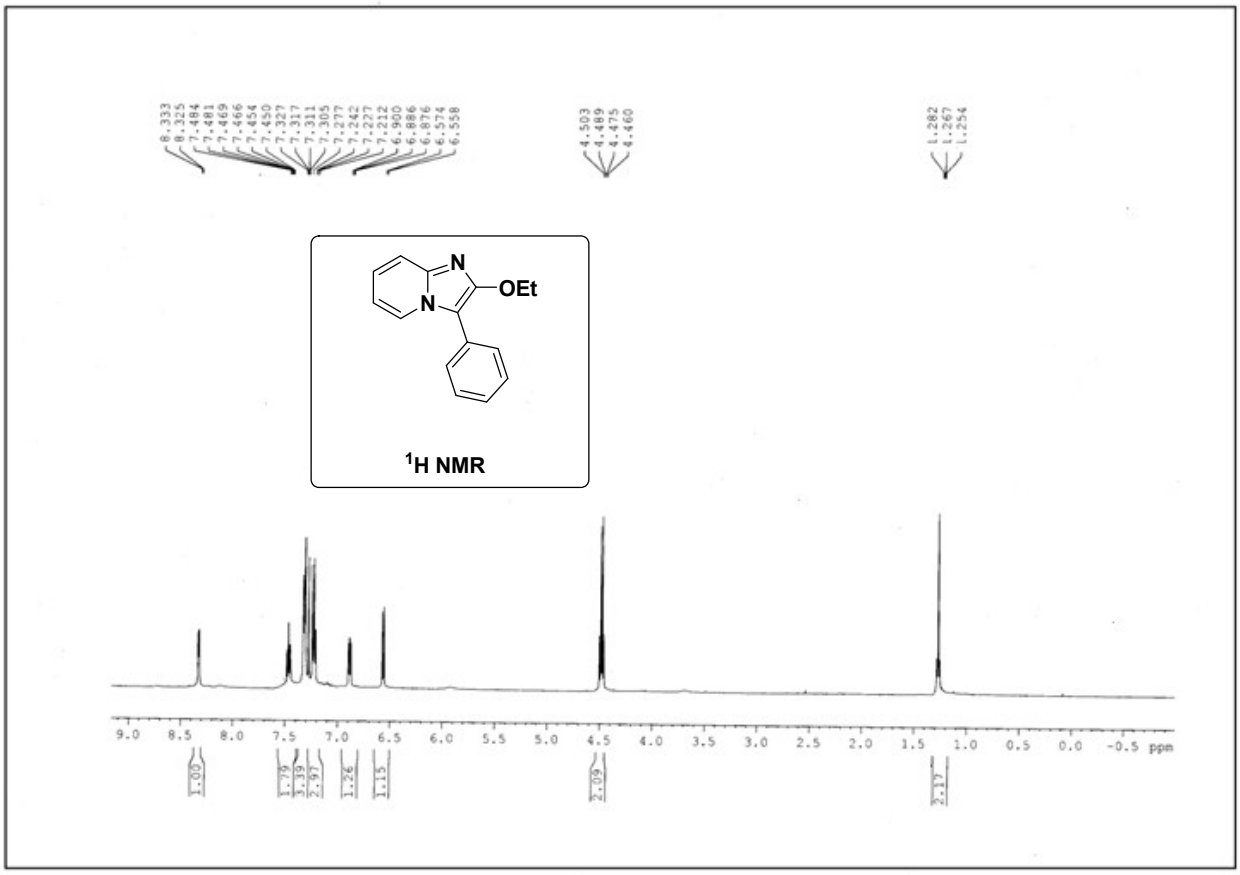
128.80
128.08
127.36
119.53
116.92
77.47
77.16
76.84
63.03
21.04
14.39
Me
N
N
OEt
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.327
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7.311
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7.242
7.227
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6.574
6.558
4.503
4.489
4.475
4.460
1.282
1.267
1.254
N
N
OEt
1H NMR
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
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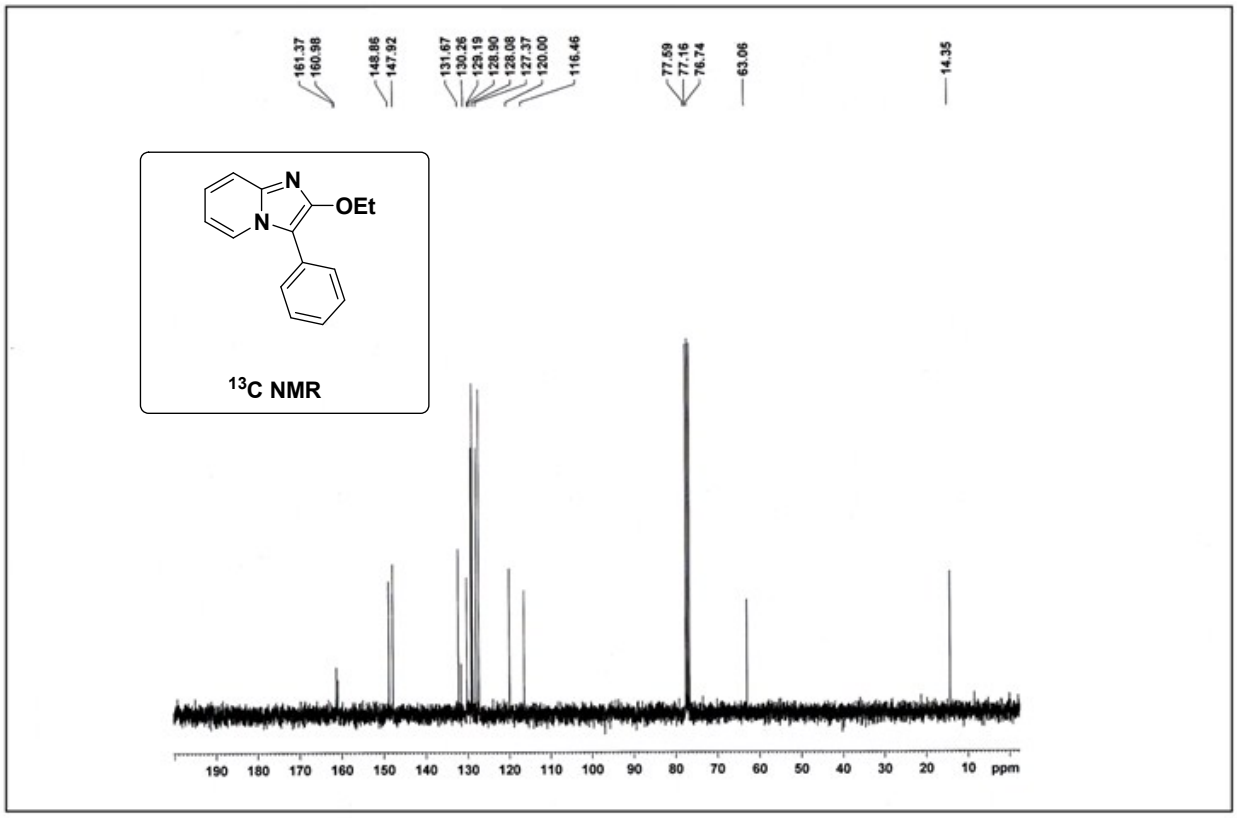
2.97
1.26
1.15
2.09
3.17


161.37
160.98
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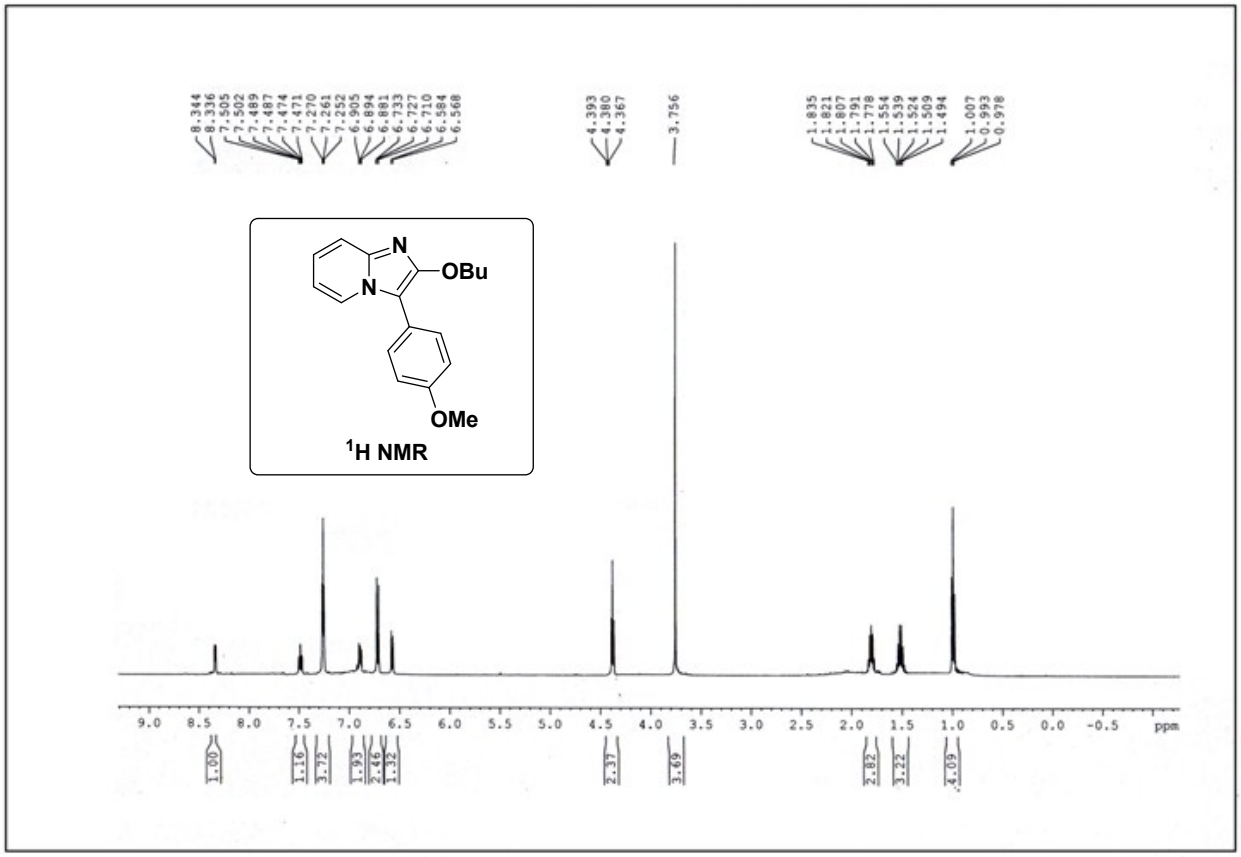
147.92
131.67
130.26
129.19
128.90
128.08
127.37
120.00
116.46
77.59
77.16
76.74
63.06
14.35
N
N
OEt
13C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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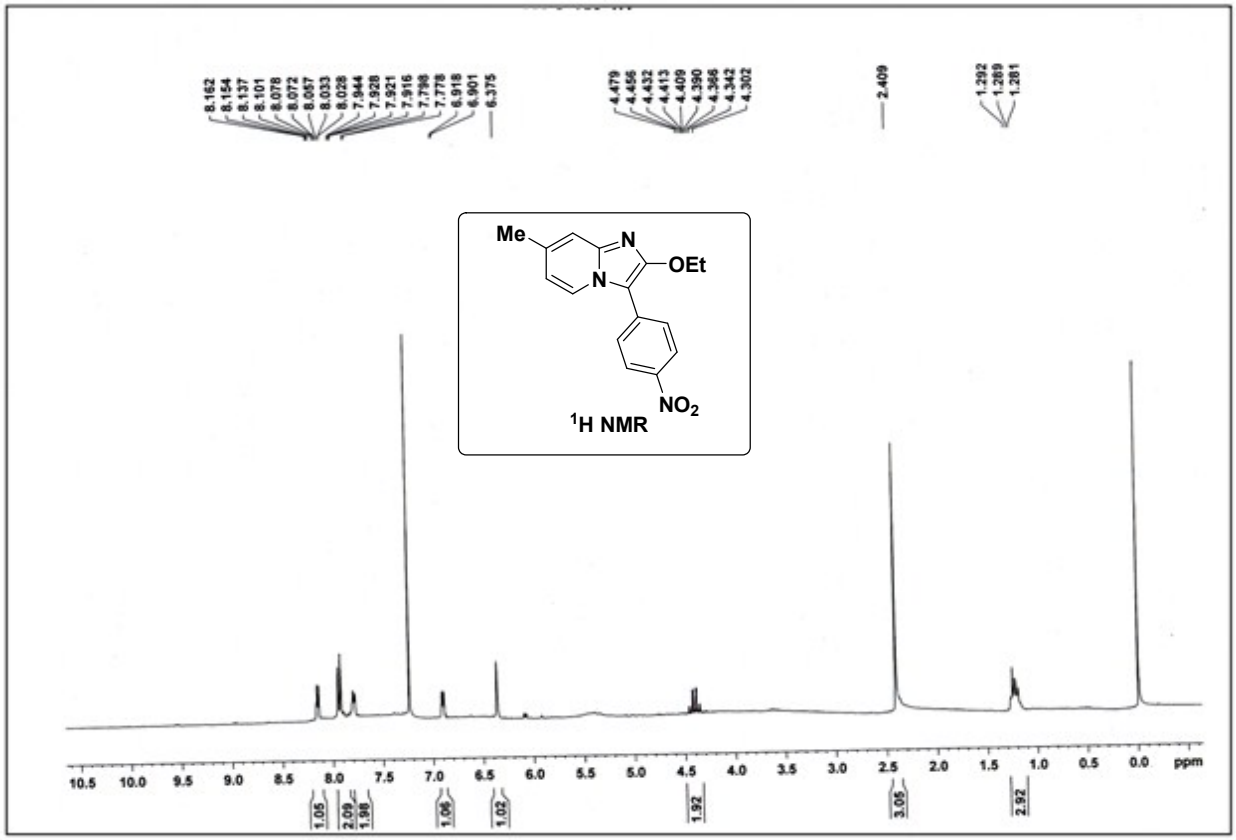
8.336
7.505
7.502
7.489
7.487
7.474
7.471
7.270
7.261
7.252
6.905
6.894
6.881
6.733
6.727
6.710
6.584
6.568
4.393
4.380
4.367
3.756
1.835
1.821
1.807
1.791
1.778
1.554
1.539
1.524
1.509
1.494
1.007
0.993
0.978
N
N
OBu
OMe
1H NMR
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
1.00
1.16
3.72
1.93
2.46
1.32
2.37
3.69
2.82
3.22
4.09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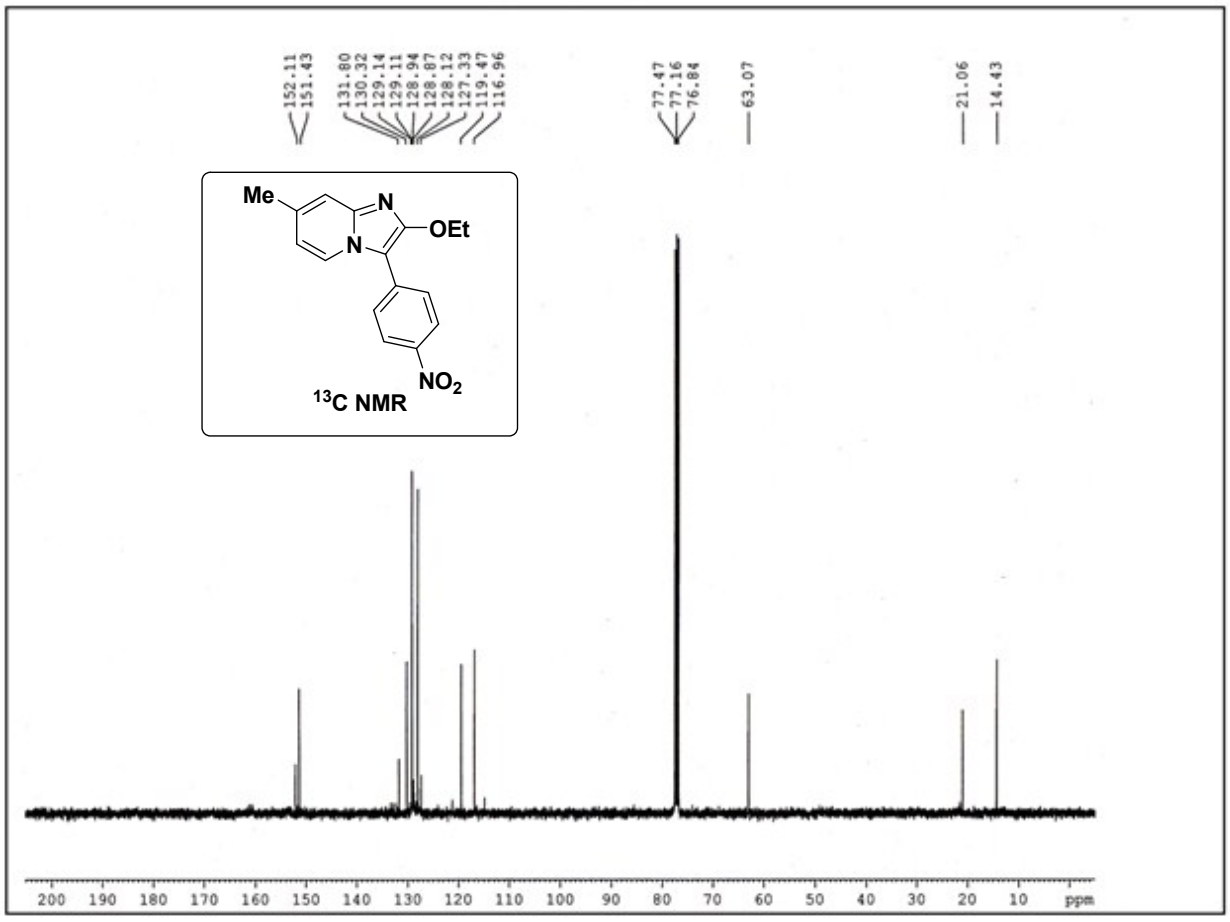
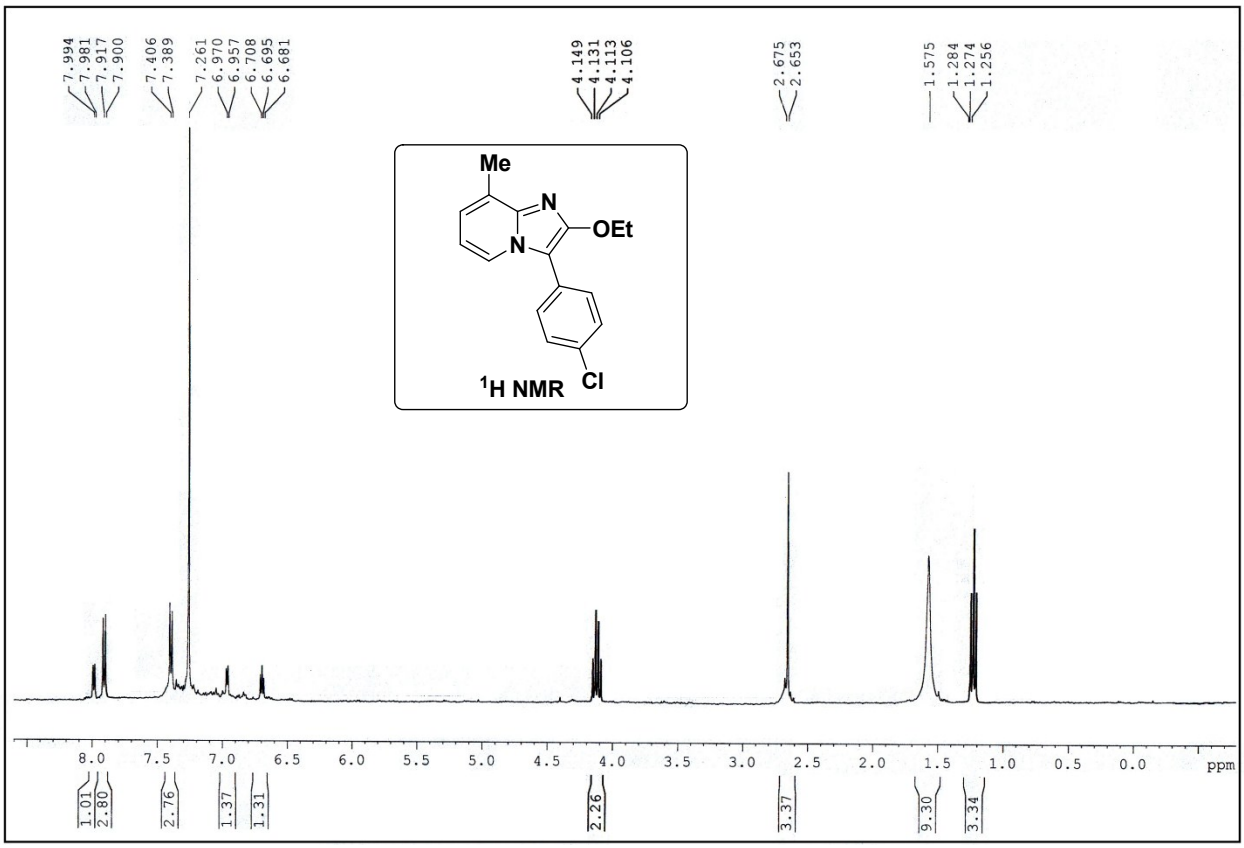
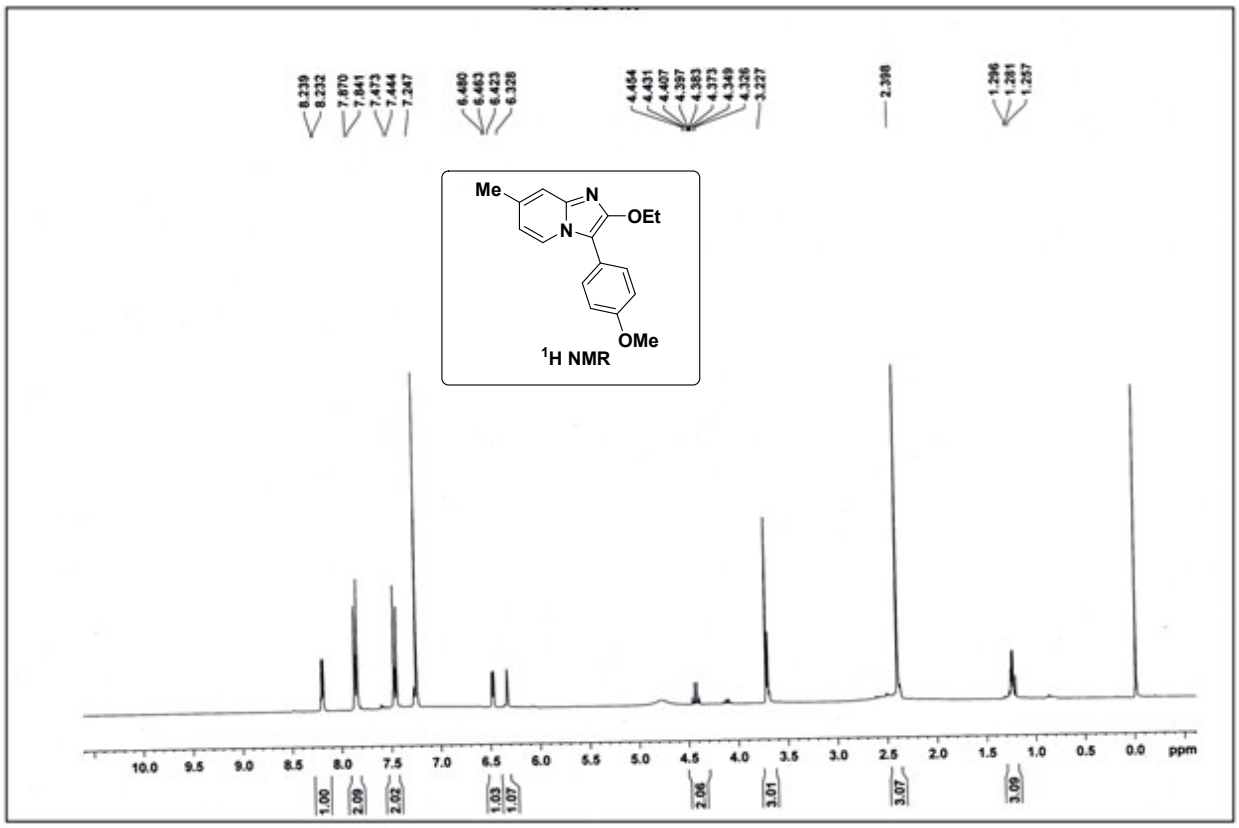
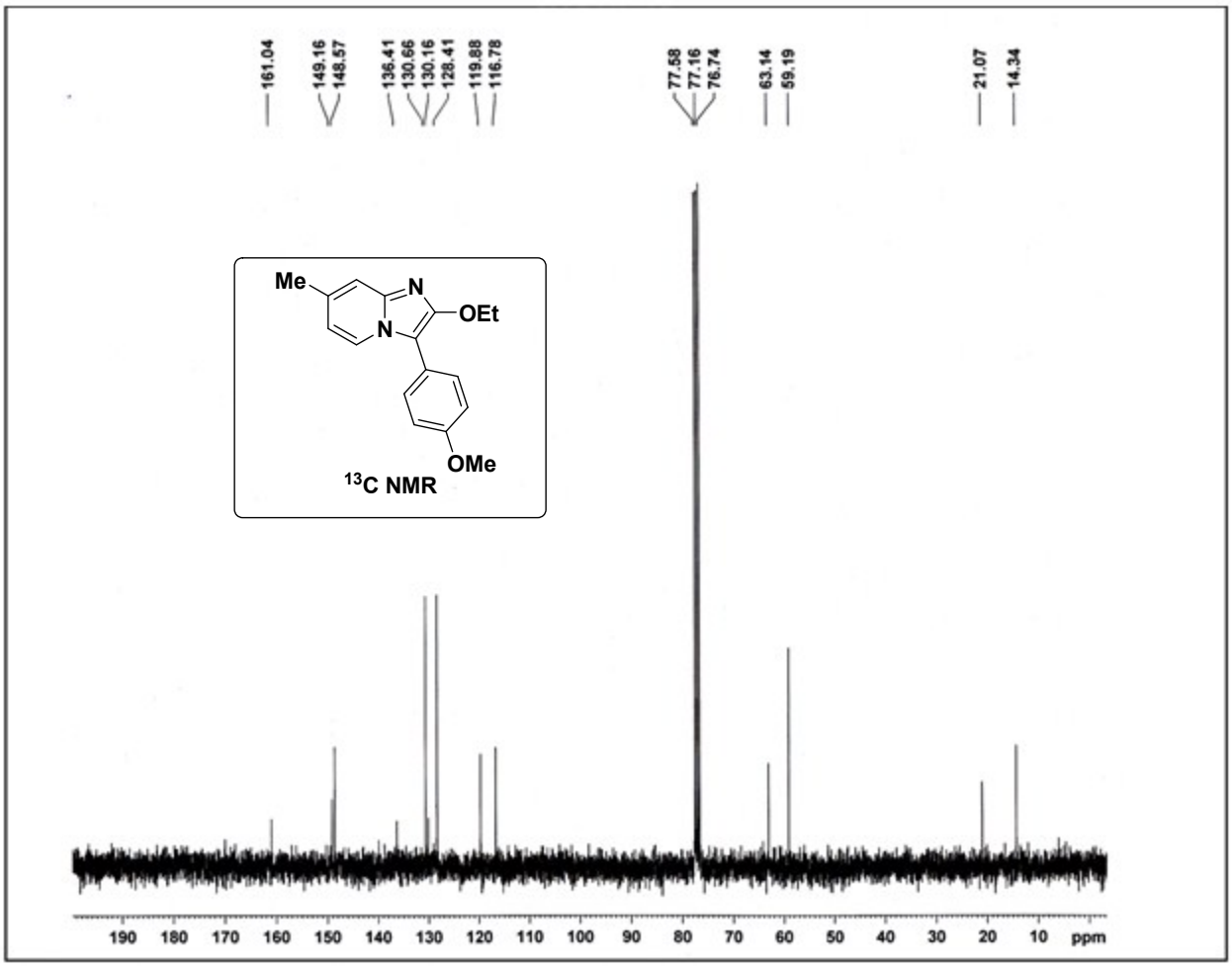
8.154
8.137
8.101
8.078
8.072
8.057
8.033
8.028
7.944
7.928
7.921
7.916
7.798
7.778
6.918
6.901
6.375
4.479
4.456
4.432
4.413
4.409
4.390
4.366
4.342
4.302
2.409
1.292
1.289
1.281
Me
N
N
OEt
NO2
1H NMR
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.05
2.09
1.98
1.06
1.02
1.92
3.05
2.92


152.11
151.43
131.80
130.32
129.14
129.11
128.94
128.87
128.12
127.33
119.47
116.96
77.47
77.16
76.84
63.07
21.06
14.43
Me
N
N
OEt
NO2
13C NMR
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.994
7.981
7.917
7.900
7.406
7.389
7.261
6.970
6.957
6.708
6.695
6.681
4.149
4.131
4.113
4.106
2.675
2.653
1.575
1.284
1.274
1.256
Me
N
N
OEt
Cl
1H NMR
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.01
2.80
2.76
1.37
1.31
2.26
3.37
9.30
3.34


8.239
8.232
7.870
7.841
7.473
7.444
7.247
6.480
6.463
6.423
6.328
4.454
4.431
4.407
4.397
4.383
4.373
4.349
4.326
3.227
2.398
1.296
1.281
1.257
Me
N
N
OEt
OMe
1H NMR
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.09
2.02
1.03
1.07
2.06
3.01
3.07
3.09


161.04
149.16
148.57
136.41
130.66
130.16
128.41
119.88
116.78
77.58
77.16
76.74
63.14
59.19
21.07
14.34
Me
N
OEt
N
OMe
13C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

ESI 7. Docking scores (MolDock, re-rank, H-bond and steric) of imidazopyridine derivatives (**4a-4t**) docked with different targets selected for screening

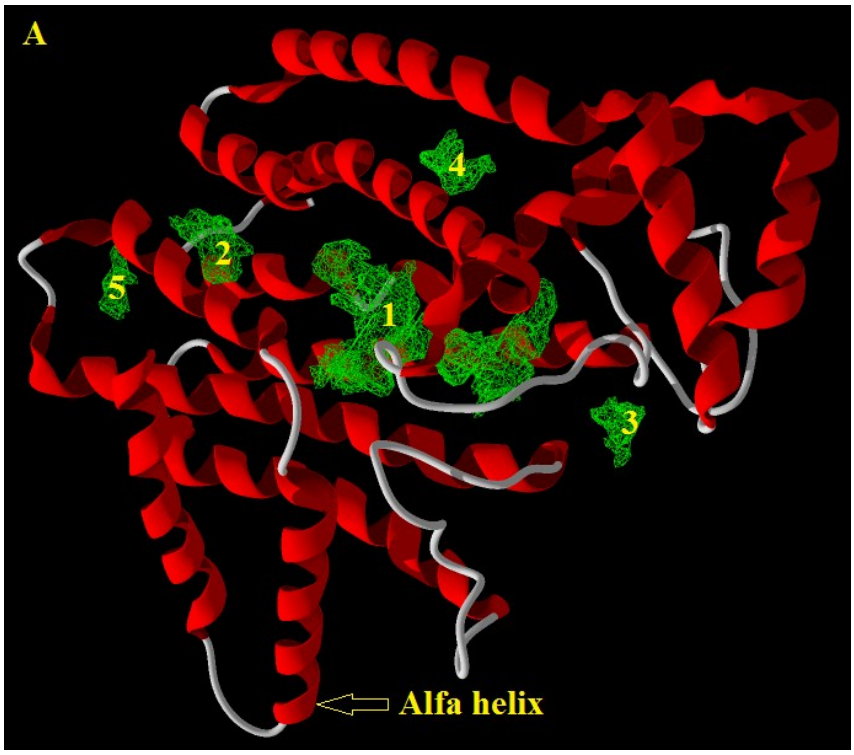
Table 1S. Docking scores (MolDock, re-rank, H-bond and steric)

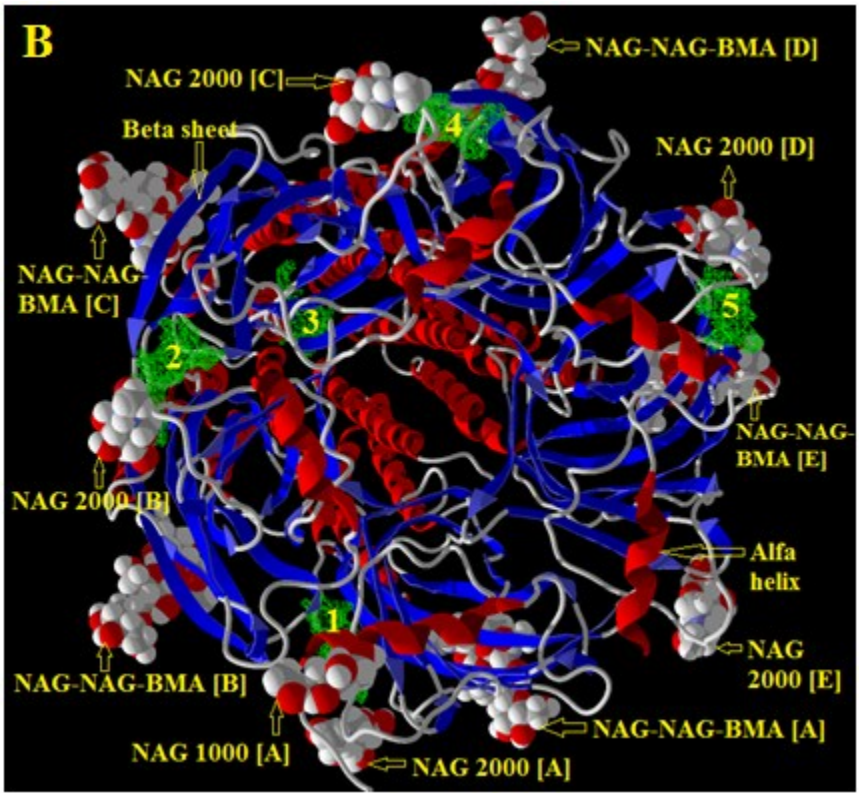
Target	Compound No.	Docking scores			
		MolDock	**Re-rank**	**H-Bond**	**Steric**
Farnesyl diphosphate synthase	4aa	-118.894	-94.567	-3.645	-116.408
	4ab	-110.717	-85.991	0.000	-110.651
	4ac	-124.122	-93.709	-4.448	-119.069
	4ad	-118.992	-98.642	0.000	-120.560
	4ae	-130.001	-104.945	-5.231	-122.627
	4af	-128.924	-76.445	-10.143	-115.993
	4ag	**-135.390**	**-113.326**	0.000	**-136.430**
	4ah	-124.094	-98.269	-2.500	-118.541
	4ai	-121.150	-87.403	-2.473	-119.836
	4aj	-118.092	-86.754	-4.970	-114.438
	4ak	-106.866	-80.000	0.000	-108.121
	4al	-113.230	-84.912	0.000	-110.985
	4am	-110.045	-86.578	-3.776	-107.927
	4an	-116.845	-96.248	-0.130	-118.693
	4ao	-113.937	-88.107	-5.062	-110.490
	4ap	-106.892	-84.494	-4.799	-105.440
	4aq	-126.657	-94.306	-6.079	-121.496
	4ar	-126.991	-103.873	-3.465	-121.834
	4as	-110.925	-87.357	-3.956	-105.878
	4at	-122.666	-84.444	-7.918	-115.452
	Minodronic acid	-97.925	-81.223	-14.548	-89.640

GABAa	4aa	-128.654	-95.298	-0.069	-129.686
	4ab	-115.668	-91.955	-0.458	-115.723
	4ac	-129.366	**-103.099**	-0.094	-133.227
	4ad	-131.563	-100.674	-0.733	-129.072
	4ae	-134.520	-93.780	-0.609	-133.819
	4af	-129.593	-91.870	-2.159	-127.590
	4ag	**-140.075**	-101.404	-0.384	**-136.975**
	4ah	-128.334	-99.842	-0.080	-130.049
	4ai	-125.602	-96.181	-0.631	-122.138
	4aj	-116.297	-56.835	-0.220	-117.141
	4ak	-120.374	-93.189	-0.741	-117.986
	4al	-125.970	-95.253	-0.585	-122.589
	4am	-116.507	-87.308	0.000	-119.762
	4an	-129.328	-78.135	-0.104	-127.982
	4ao	-119.177	-89.205	-0.334	-119.222
	4ap	-112.834	-89.727	0.000	-114.031
	4aq	-134.705	**-106.674**	0.000	-134.040
	4ar	-129.043	-98.990	-0.239	-127.421
	4as	-119.349	-93.524	-0.519	-118.838
	4at	-128.841	-98.450	-0.537	-126.314
	Alpidem	**-149.261**	-96.039	-0.592	**-153.605**
	Necopidem	**-142.306**	-83.686	-0.683	**-144.012**
	Saripidem	-135.442	-62.150	-0.319	-134.996
	Zolpidem	-127.959	-94.655	-0.634	-131.210
CXCR4	4aa	-100.797	-65.423	-1.991	-102.374
	4ab	-98.076	-75.417	0.000	-98.311
	4ac	-111.556	-85.081	0.000	-110.111
	4ad	-101.679	-80.483	-2.500	-99.772

	4ae	-108.843	-80.604	-5.628	-106.948
	4af	-101.554	-78.059	-1.218	-100.011
	4ag	-105.800	-81.494	-1.148	-105.449
	4ah	-106.885	-76.043	-2.049	-109.366
	4ai	-99.383	-79.323	-2.500	-97.368
	4aj	-95.632	-73.120	0.000	-97.400
	4ak	-98.677	-72.307	-1.832	-94.912
	4al	-100.196	-76.897	-1.165	-99.773
	4am	-97.663	-72.271	0.000	-97.763
	4an	-100.278	-70.344	-0.675	-99.526
	4ao	-91.862	-70.230	-2.500	-90.839
	4ap	-90.859	-72.290	0.000	-94.821
	4aq	-101.582	-58.212	-2.228	-99.658
	4ar	-104.217	-80.891	-6.626	-97.201
	4as	-100.757	-72.275	-2.706	-97.533
	4at	-105.511	-73.737	-1.749	-103.089
	GSK812397	**-119.863**	**-93.391**	-1.880	**-129.993**

ESI 8. The secondary structure of all the selected targets with detected active sites


A
4
2
5
1
3
Alfa helix


B
NAG-NAG-BMA [D]
NAG 2000 [C]
Beta sheet
4
NAG 2000 [D]
NAG-NAG-
BMA [C]
3
5
2
NAG-NAG-
BMA [E]
NAG 2000 [B]
Alfa
helix
1
NAG
2000 [E]
NAG-NAG-BMA [B]
NAG-NAG-BMA [A]
NAG 1000 [A]
NAG 2000 [A]

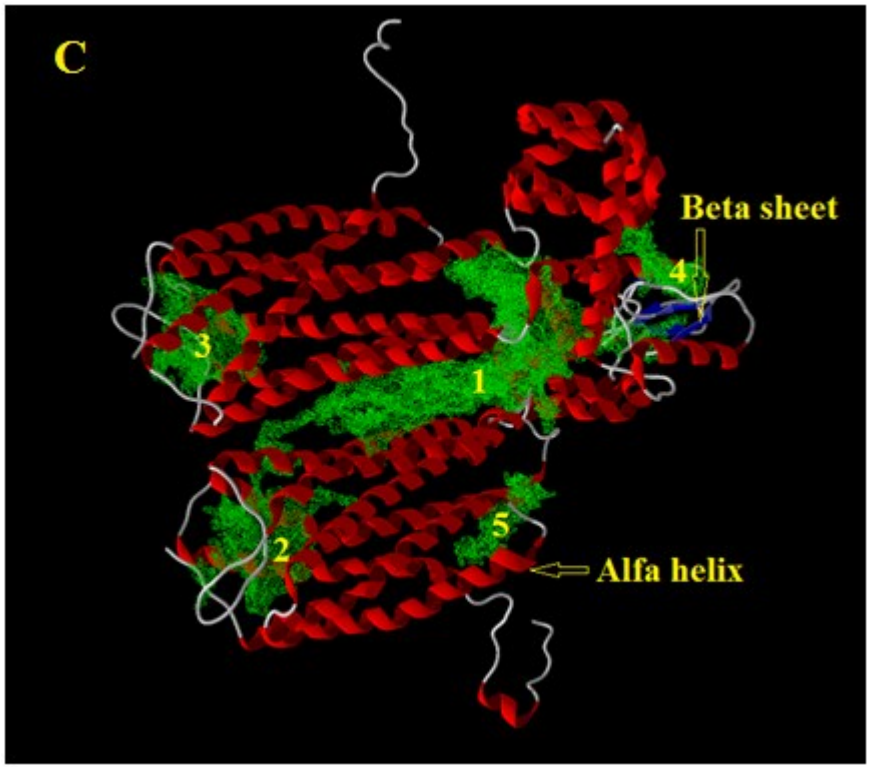


Figure 3S Secondary structure of farnesyl diphosphate synthase (A), GABAa (B), and CXCR4 (C) along with active sites (1-5) (green in colour)

ESI 9.

Table 2S: The active sites (cavities) (1-5) detected in different selected targets along with their volume and surface area

Target	Cavity No.	Volume (Å^3)	Surface area (Å^2)
Phosphodiesterase 3B	1	1920.510	4992.000
	2	379.904	1149.440
	3	374.784	1050.880
	4	349.184	1016.32
	5	339.456	988.160
Farnesyl diphosphate synthase	1	278.016	695.040
	2	33.280	117.760
	3	23.552	84.480
	4	22.016	97.280
	5	15.872	70.400
GABAa	1	124.416	335.360
	2	103.424	360.960
	3	96.256	418.560
	4	81.408	277.760
	5	81.408	266.240
CXCR4	1	3771.900	7645.440
	2	924.672	2040.320
	3	873.472	1719.040
	4	248.320	879.360
	5	197.120	664.320

ESI 10.

Table 3S. The key amino acid residues present in largest cavity (cavity 1) of each target

Target	Key amino acid residues present in cavity 1
Phosphodiesterase 3B	Cys 792, Ilu 671, Lys 790, Ser 788, Ser 789, Ser 791, Ser 793, Cys 1059, Gln 1012, Gln 1060, Glu 1067, His 1063, His 1064, Phe 1058, Val 944
Farnesyl diphosphate synthase	Arg 126, Asp 117, Asp 118, Asp 121, Asp 188, Asp 257, Asp 258, Asp 261, Asp 275, Cys 281, Gln 185, Gln 254, Gly 273, Ile 272, Leu 114, Lys 214, Lys 271, Lys 280, Phe 113, Ser 123, Ser 282, Thr 125, Thr 181, Thr 215, Thr 274, Tyr 207, Tyr 218
GABAa	Arg 169, Arg 180, Asn 41, Asp 43, Gln 64, Gly 127, Leu 128, Met 115, Tyr 62, Ala 201, Arg 207, Glu 155, Leu 99, Phe 200, Ser 156, Thr 202, Tyr 97, Tyr 157, Tyr 205
CXCR4	Arg 1014, Asp 1020, Gln 1100, Glu 1022, Leu 1033, Lys 1019, Thr 1026, Tys 1018, Tyr 1024

ESI 11. Recyclability of the catalyst

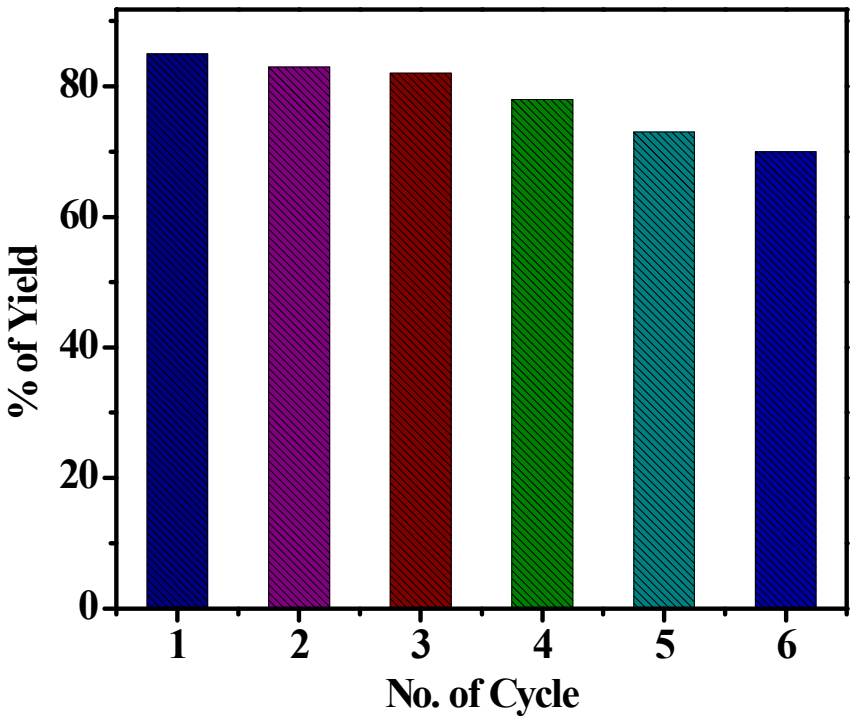


Figure 4S: Recyclability of Fe-SBA-15 catalyst

ESI 12. Reference:

1 A. Murali, Z. Chang, K. T. Ranjit, R. M. Krishna, V. Kurshev and L. Kevan, *J. Phys. Chem.* B., 2002, **106**, 6913.