Electronic Supplementary Material (ESI) for RSC Advances


# Supporting Information

## Palladium catalyzed novel monoarylation and symmetrical/unsymmetrical diarylation of imidazo[1,2-*a*]pyrazines and their *in vitro* anticancer activities

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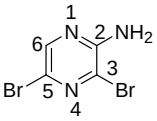
**Instrumentations and chemicals:**

All commercially available compounds (Spectrochem, Aldrich, Merck etc.) were used without purification. Unless otherwise noted, all reactions were performed in oven-dried glassware. All reactions were run under argon or nitrogen atmosphere. All solvents used in the reactions were purified before use. The reactions were carried out in an oil bath using Microwave Vials (10-15 ml). Melting points were determined in open capillaries and were uncorrected. $^{1}H$ and $^{13}C$ NMR spectra were performed on Jeol 400 NMR spectrometer, which was operated at 400 MHz for $^{1}H$ nuclei and 100 MHz for $^{13}C$ nuclei, using $CDCl_3$ as solvent. Chemical shifts are reported in parts per million (ppm) with TMS as internal reference and *J* values are given in hertz. Mass Spectra of the synthesized compounds were recorded at MAT 120 in SAIF, Punjab University. Gas chromatography–mass spectrometry analyses were carried out on an Agilent Technologies with Scion Mass spectrometer. The Bruker AXS KAPPA APEX II system is used for single crystal X-ray diffraction. Reactions were monitored by thin layer chromatography (TLC) with silica plate coated with silica gel HF-254 and column chromatography was performed with silica gel 60-120/100-200 mesh. Hexane/ethyl acetate and chloroform/methanol were adopted solvent systems.

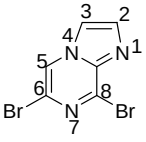
**Typical procedure for synthesis of 2-amino-3,5-dibromopyrazine (2)**

N-Bromosuccinamide (14.95 g, 83.99 mmol) was added over 50 min to a mixture of 2-aminopyrazine (3.80 g, 40 mmol) in 80 ml DMSO and 2 ml $H_2O$ below 15 $^0$C. Mixture was then stirred for 6 h at room temperature. After completion of reaction, mixture was then extracted with water and ethyl acetate. Ethyl acetate layer was dried over sodium sulphate and concentrated in vacuum. Crude product was purified by column chromatography using hexane: ethyl acetate (9:1) as eluents.



**Spectral data 2-amino-3,5-dibromopyrazine (2)**: White solid; Yield: 90%; mp 115-116 $^0$C (lit. M.p. 117-118 $^0$C) [1]; $^1$H NMR ($CDCl_3$, 400 MHz): δ 5.12 (bs, 1H, $NH_2$), 8.04 (s, 1H, $C_6H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 123.57, 123.90, 143.09, 151.84; MS (EI): m/z 254 ($M^+$+1).

**Typical procedure for synthesis of 6,8-dibromo-imidazo[1,2-*a*]pyrazine (3)**: To 2-amino-3,5-dibromopyrazine (5.0 g, 19.8 mmol) in 100 ml of isopropyl alcohol (IPA), 50% aqueous solution of chloroacetaldehyde (99 mmol) was added dropwise. The reaction mixture was refluxed at 110 $^0$C for 24 h. After the completion of the reaction, cooled to room temperature and then extracted with water and chloroform. Chloroform layer was dried over sodium sulphate and concentrated in vacuum to get the crude product. The product was purified by column chromatography using hexane:ethyl acetate (6:4) as eluent.



**Spectral data 6,8-dibromoimidazo[1,2-*a*]pyrazine (3):** White solid; Yield: 80%; mp 163-165 $^0$C (lit. M.p. 165-166 $^0$C)[2]; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.80 (d, $J$ = 0.92 Hz, 1H, $C_2H$), 7.86 (d, $J$ = 1.36 Hz, 1H, $C_3H$), 8.29 (s, 1H, $C_5H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 115.92, 119.32, 119.97, 137.03, 137.39, 142.54; MS (EI): m/z 278 ($M^+$+1).

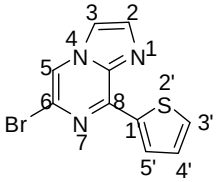
**Typical procedure for synthesis of compounds 4-15:** A vial equipped with stirring bar was charged with 6,8-dibromo-imidazo[1,2-*a*]pyrazine (0.5 g, 1.8 mmol), $Cs_2CO_3$ (0.6 g, 1.8 mmol)

(1) B. Jiang, C.-G. Yang, W.-N.. Xiong and J. Wang, *Bioorg. Med. Chem.*, 2001**, 9,** 1149-1154.

(2) J. Bradac, Z. Furek, D. Janezic, S. Molan, I. Smerkolj, B. Stanovnik, M. Tisler and B. Vercek, *J. Org. Chem.*, 1977, **42**, 4197-4201.

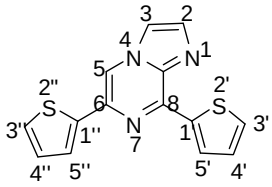
and boronic acid (1.8 mmol), dissolved in MeCN:$H_2O$ (9:1) at 100 $^0$C under inert atmosphere. Then, 5 mol% of $Pd(PPh_3)_4$ was added and vial was capped. The reaction mixture was refluxed for 7-12 h. After the completion of the reaction (monitored by TLC), cooled the reaction mixture, and then extract with water and chloroform. Organic layer was dried over sodium sulphate, filtered and concentrated under *vacuo* to get crude product. The residue was purified by silica gel (60-120 mesh) column chromatography using hexane: ethyl acetate as eluents to give pure solid.

**Spectral data 6-bromo-8-(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine (4a) :** Green solid; Yield:



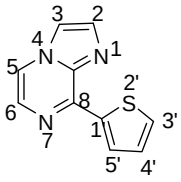

70%; mp 149-151 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.23 (t, *J* = 4.12 Hz, 1H, $C_4$'H), 7.62 (d, *J* = 5.04 Hz, 1H, $C_5$'H), 7.67 (s, 1H, $C_2$H), 7.83 (s, 1H, $C_3$H), 8.14 (s, 1H, $C_5$H), 8.77 (d, *J* = 3.68 Hz, 1H, $C_3$'H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.19, 117.25, 122.37, 128.57, 131.67, 132.99, 135.97, 137,10 138.96, 144.62 (ArC); GC-MS: m/z 279 ($M^+$).

**Spectral data 6,8-di(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine (4b)**: Green solid; Yield: 10%;



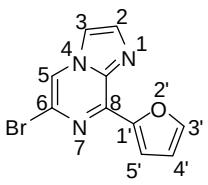

mp 140-142 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.12 (t, *J* = 4.36 Hz, 1H, $C_4$"H), 7.24 (t, *J* = 4.36 Hz, 1H, $C_4$'H), 7.38 (d, *J* = 5.04 Hz, 1H, $C_5$"H), 7.56 (d, *J* = 3.68 Hz, 1H, $C_3$"H), 7.59 (d, *J* = 5.04 Hz, 1H, $C_5$'H), 7.69 (d, *J* = 0.92 Hz, 1H, $C_2$H), 7.81 (d, *J* = 0.92 Hz, 1H, $C_3$H), 8.29 (s, 1H, $C_5$H), 8.79 (d, *J* = 3.64 Hz, 1H, $C_3$'H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 111.52, 114.52, 123.53, 126.67, 128.11, 128.46, 130.74, 132.19, 134.90, 135.33, 137.22, 140.34, 141.38, 144.29 (ArC); GC-MS: m/z 283 ($M^+$).

**Spectral data 8-(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine (4c)**: Light green solid; Yield: 60%;



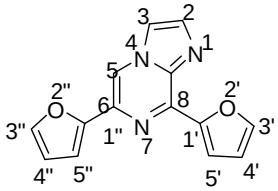

mp 135-137 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.26-7.23 (m, 1H, $C_4$'H), 7.58 -7.57 (dd, $^2J$ = 5.04 Hz, $^3J$ = 0.92 Hz, 1H, $C_5$'H), 7.77 (d, *J* = 0.92 Hz, 1H, $C_2$H), 7.85 (d, *J* = 0.95 Hz, 1H, $C_3$H), 7.87 (d, *J* = 4.56 Hz, 1H, $C_5$H), 7.99 (d, *J* = 4.56 Hz, 1H, $C_6$H), 8.82-8.80 (dd, $^2J$ = 4.16 Hz, $^3J$ = 1.1 Hz, 1H, $C_3$'H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.06, 117.33, 128.58, 129.05, 130.23, 132.12, 134.93 (ArC); MS (EI): m/z 202 ($M^+$+1).

**Spectral data 6-bromo-8-(furan-2'-yl)imidazo[1,2-*a*]pyrazine (5a):** Light brown solid;



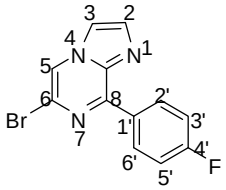
Yield: 56%; mp 124-126 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 6.68-6.67 (dd, $^{2}J$ = 3.20 Hz, $^{3}J$ = 1.60 Hz, 1H, $C_{5'}H$), 7.69 (d, $J$ = 0.92 Hz, 1H, $C_2H$), 7.77 (t, $J$ = 0.92 Hz, 1H, $C_{4'}H$), 7.83 (d, $J$ = 0.92 Hz, 1H, $C_3H$), 8.10 (d, $J$ = 3.2 Hz, 1H, $C_{3'}H$), 8.17 (s, 1H, $C_5H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 112.82, 114.30, 117.42, 118.88, 122.57, 136.05, 136.46, 140.30, 146.42, 148.30 (ArC); GC-MS: m/z 263 ($M^+$).

**Spectral data 6,8-di(furan-2'-yl)imidazo[1,2-*a*]pyrazine (5b)**: Light brown solid; Yield:



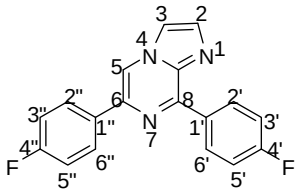
12%; mp 140-142 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 6.56-6.55 (dd, $^{2}J$ = 3.20 Hz, $^{3}J$ = 1.82 Hz, 1H, $C_{4''}H$), 6.68-6.67 (dd, $^{2}J$ = 3.64 Hz, $^{3}J$ = 1.62 Hz, 1H, $C_{4'}H$), 7.13 (d, $J$ = 2.76 Hz, 1H, $C_{5''}H$), 7.50 (d, $J$ = 1.8 Hz, 1H, $C_{5'}H$), 7.73 (d, $J$ = 1.4 Hz, 1H, $C_2H$), 7.77 (d, $J$ = 1.36 Hz, 1H, $C_{3''}H$), 7.81 (d, $J$ = 1.36 Hz, 1H, $C_3H$), 8.07 (d, $J$ = 4.12 Hz, 1H, $C_{3'}H$), 8.36 (s, 1H, $C_5H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 108.66, 111.79, 111.98, 112.37, 114.69, 117.44, 132.01, 135.18, 136.50, 140.62, 142.61, 145.58, 149.18, 151.16 (ArC); GC-MS: m/z 251 ($M^+$).

**Spectral data 6-bromo-8-(4'-fluorophenyl)imidazo[1,2-*a*]pyrazine (6a)**: Light yellow solid;



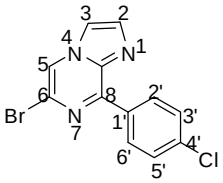
Yield: 52%; mp 157-159 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): 7.23-7.18 (m, 2H, $C_{2'}H$ and $C_{6'}H$), 7.70 (s, 1H, $C_2H$), 7.84 (s, 1H, $C_3H$), 8.21 (s, 1H, $C_5H$), 8.81-8.79 (dd, $^{2}J$ = 8.68 Hz, $^{3}J$ = 5.48 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.12, 115.49, 115.71, 118.08, 122.62, 130.99, 132.19, 132.28, 136.17, 138.45, 148.10 (ArC); GC-MS: m/z 291($M^+$).

**Spectral data 6,8-bis(4'-fluorophenyl)imidazo[1,2-*a*]pyrazine (6b)**: Light yellow solid;



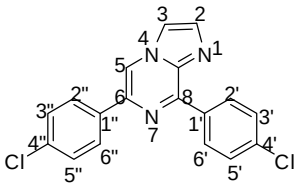
Yield: 25%; mp 162-164 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 7.27-7.17 (m, 4H, $C_{2'}H$, $C_{6'}H$, $C_{2''}H$ and $C_{6''}H$), 7.78 (d, $J$ = 1.36 Hz, 1H, $C_2H$), 7.86 (d, $J$ = 1.36 Hz, 1H, $C_3H$), 8.04-8.00 (m, 2H, $C_{3''}H$ and $C_{5''}H$), 8.40 (s, 1H, $C_5H$), 8.89 - 8.92 (m, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 113.65, 114.48, 115.38, 115.59, 115.87, 116.09, 128.04, 128.12, 131.91, 131.99, 132.21, 132.78, 135.46, 138.07, 138.61, 147.72, 162.10, 163.21, 164.57, 165.71 (ArC); GC-MS: m/z 307 ($M^+$).

**Spectral data 6-bromo-8-(4'-chlorophenyl)imidazo[1,2-*a*]pyrazine (7a)**: White solid; Yield:



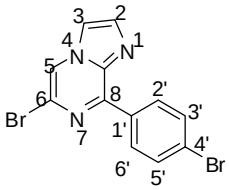
70%; mp 157-159 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.50 (d, *J* = 8.72 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.72 (d, *J* = 0.88 Hz, 1H, $C_2H$), 7.86 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.24 (s, 1H, $C_5H$), 8.74 (d, *J* = 8.72 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.14, 118.35, 122.63, 128.78, 131.31, 133.22, 136.25, 137.44, 138.49, 148.02 (ArC); GC-MS: m/z 309 ($M^+$).

**Spectral data 6,8-bis(4'-chlorophenyl)imidazo[1,2-*a*]pyrazine (7b)**: Off white solid; Yield:



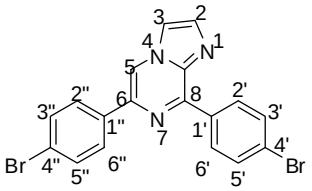
16%; mp 139-141 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.47 (d, *J* = 8.72 Hz, 2H, $C_{2''}H$ and $C_{6''}H$), 7.53 (d, *J* = 8.72 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.78 (s, 1H, $C_2H$), 7.86 (s, 1H, $C_3H$), 7.98 (d, *J* = 8.72 Hz, 2H, $C_{3''}H$ and $C_{5''}H$), 8.43 (s, 1H, $C_5H$), 8.84 (d, *J* = 8.72 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.13, 114.58, 127.52, 128.71, 129.20, 131.12, 134.41, 134.87, 135.01, 135.57, 136.86, 137.80, 138.63, 147.60 (ArC); GC-MS: m/z 340 ($M^+$).

**Spectral data 6-bromo-8-(4'-bromophenyl)imidazo[1,2-*a*]pyrazine (8a)**: White solid; Yield:



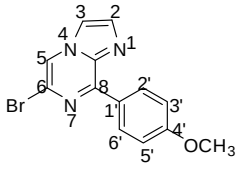
68%; mp 138-140 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.65 (d, *J* = 8.72 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.71 (d, *J* = 0.92 Hz, 1H, $C_2H$), 7.85 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.24 (s, 1H, $C_5H$), 8.66 (d, *J* = 8.72 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.13, 118.38, 122.63, 126.08, 131.50, 131.73, 133.65, 136.26, 138.45, 148.05 (ArC); Mass (EI): m/z 351 ($M^+$+1).

**Spectral data 6,8-bis(4'-bromophenyl)imidazo[1,2-*a*]pyrazine (8b)**: White solid; Yield: 20%;



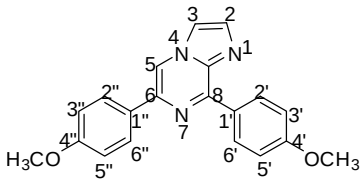
mp 145-147 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.63 (d, *J* = 8.72 Hz, 2H, $C_{2''}H$ and $C_{6''}H$), 7.69 (d, *J* = 8.24 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.79 (s, 1H, $C_2H$), 7.87 (d, *J* = 0.80 Hz, 1H, $C_3H$), 7.92 (d, *J* = 8.68 Hz, 2H, $C_{3''}H$ and $C_{5''}H$), 8.45 (s, 1H, $C_5H$), 8.76 (d, *J* = 8.72 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.17, 114.59, 123.15, 125.47, 127.82, 131.14, 131.68, 132.16, 134.85, 135.47, 135.60, 137.88, 138.62, 147.73 (ArC); Mass (EI): m/z 428 ($M^+$+1).

**Spectral data 6-bromo-8-(4'-methoxyphenyl)imidazo[1,2-*a*]pyrazine (9a):** White solid; Yield



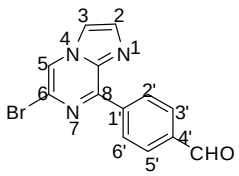
: 69%; mp 138-140 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 3.89 (s, 3H, $OCH_3$), 7.05 (d, *J* = 9.16 Hz, 2H, $C_2$'H and $C_6$'H), 7.67 (d, *J* = 1.36 Hz, 1H, $C_2$H), 7.83 (d, *J* = 0.92 Hz, 1H, $C_3$H), 8.16 (s, 1H, $C_5$H), 8.77 (d, *J* = 9.16 Hz, 2H, $C_3$'H and $C_5$'H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 55.53 ($OCH_3$), 113.93 117.28, 122.37, 122.80, 127.48, 131.76, 135.83, 138.52, 148.95, 162.10 (ArC); GC-MS: m/z 303 ($M^+$).

**Spectral data 6,8-bis(4'-methoxyphenyl)imidazo[1,2-*a*]pyrazine (9b)**: White solid; Yield: 14%;



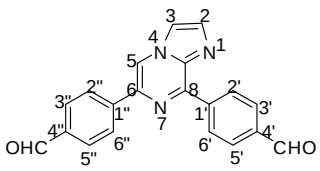
mp 162-164 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 3.86 (s, 3H, $OCH_3$), 3.90 (s, 3H, $OCH_3$), 7.01 (d, *J* = 9.16 Hz, 2H, $C_2$"H and $C_6$"H), 7.07 (d, *J* = 9.16 Hz, 2H, $C_2$'H and $C_6$'H), 7.67 (d, *J* = 1.36 Hz, 1H, $C_2$H), 7.80 (d, *J* = 0.92 Hz, 1H, $C_3$H), 7.97 (d, *J* = 9.16 Hz, 2H, $C_3$"H and $C_5$"H), 8.27 (s, 1H, $C_5$H), 8.87 (d, *J* = 8.72 Hz, 2H, $C_3$'H and $C_5$'H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 55.49 (2×$OCH_3$), 112.38, 113.79, 114.15, 114.28, 127.52, 129.03, 129.44, 131.40, 134.90, 138.61, 148.17, 160.13, 161.52, 161.91 (ArC); GC-MS: m/z 331 ($M^+$).

**Spectral data 4'-(6-bromoimidazo[1,2-*a*]pyrazin-8-yl)benzaldehyde (10a):** Yellow solid;



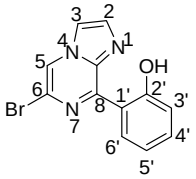
Yield: 70%; mp 176-178 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.76 (d, *J* = 1.36 Hz, 1H, $C_2$H), 7.90 (d, *J* = 0.88 Hz, 1H, $C_3$H), 8.03 (d, *J* = 8.68 Hz, 2H, $C_2$'H and $C_6$'H), 8.30 (s, 1H, $C_5$H), 8.93 (d, *J* = 8.24 Hz, 2H, $C_3$'H and $C_5$'H), 10.11 (s, 1H, CHO); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 111.42, 119.04 122.69, 129.70, 130.57, 136.66, 137.59, 138.71, 140.16, 147.76 (ArC), 192.20 (CHO); GC-MS: m/z 301 ($M^+$).

**Spectral data 4',4"-imidazo[1,2-*a*]pyrazine-6,8-diyl)dibenzaldehyde (10b)**: Light yellow



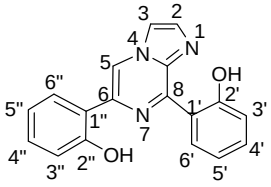
solid; Yield: 15%; mp 229-231 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.86 (s, 1H, $C_2$H), 7.93 (d, *J* = 0.92 Hz, 1H, $C_3$H), 8.03 (d, *J* = 8.24 Hz, 2H, $C_2$"H and $C_6$"H), 8.08 (d, *J* = 8.24 Hz, 2H, $C_2$'H and $C_6$'H), 8.25 (d, *J* = 8.28 Hz, 2H, $C_3$"H and $C_5$"H), 8.63 (s, 1H, $C_5$H), 9.06 (d, *J* = 8.28 Hz, 2H, $C_3$'H and $C_5$'H), 10.09 (s, 1H, CHO), 10.14 (s, 1H, CHO); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.93, 115.97, 126.76, 129.73, 130.43, 130.49, 136.19, 136.44, 137.44, 137.61, 138.92, 141.29, 142.07, 147.67 (ArC), 191.83, 192.25 (CHO); GC-MS: m/z 327 ($M^+$).

**Spectral data 2'-(6-bromoimidazo[1,2-*a*]pyrazin-8-yl) phenol (11a):** Yellow solid; Yield:



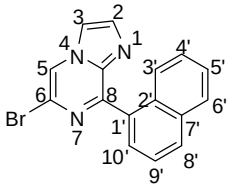
57%; mp 190-192 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): 7.32-7.26 (m, 2H, $C_{5'}$H and $C_{6'}$H), 7.45-7.40 (m, 2H, $C_{3'}$H and $C_{4'}$H), 7.65 (d, *J* = 0.88 Hz, 1H, $C_2$H), 7.75 (d, *J* = 0.92 Hz, 1H, $C_3$H), 7.97 (s, 1H, $C_5$H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 115.34, 115.51, 119.30, 121.76, 125.89, 129.58, 132.63, 135.24 152.11, 152.16 (ArC); Mass (EI): m/z 290 ($M^+$+1).

**Spectral data 2',2"-(imidazo[1,2-*a*]pyrazin-6,8-diyl)diphenol (11b)**: Yellow solid; Yield:



30%; mp 228-230 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 6.97–6.92 (m, 1H, $C_{5"}$H), 7.03 (d, *J* = 8.24 Hz, 1H, $C_{6"}$H), 7.11-7.07 (m, 1H, $C_{5'}$H), 7.15-7.13 (dd, $^2J$ = 8.28 Hz, $^3J$ = 1.38 Hz, 1H, $C_{6'}$H), 7.33-7.29 (m, 1H, $C_{4"}$H), 7.49-7.45 (m, 1H, $C_{4'}$H), 7.63-7.60 (dd, $^2J$ = 7.76 Hz, $^3J$ = 1.38 Hz, 1H, $C_{3"}$H), 7.84 (d, *J* = 1.40 Hz, 1H, $C_2$H), 7.85 (d, *J* = 0.92 Hz, 1H, $C_3$H), 8.29-8.26 (dd, $^2J$ = 8.28Hz, $^3J$ = 1.82 Hz 1H, $C_{3'}$H), 8.55 (s, 1H, $C_5$H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 113.28, 115.25, 117.78, 118.59, 119.92, 120.73, 121.38, 125.67, 130.87, 131.23, 133.56, 133.70, 137.60, 139.84, 147.88, 157.56, 158.02 (ArC); Mass (EI): m/z 303 ($M^+$+1).

**Spectral data 6-bromo-8-(napthalen-1'-yl)imidazo[1,2-*a*]pyrazine (12a):** White solid;



Yield: 64%; mp 192-194 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.53-7.46 (m, 2H, $C_{8'}$H and $C_{10'}$H), 7.62 (t, *J* = 7.79 Hz, 1H, $C_{9'}$H), 7.78 (d, *J* = 0.92 Hz, 1H, $C_2$H), 7.83 (d, *J* = 0.92 Hz, 1H, $C_3$H), 7.91 - 7.93 (m, 1H, $C_{6'}$H), 8.08-8.00 (m, 3H, $C_{3'}$H, $C_{4'}$H and $C_{5'}$H), 8.36 (s, 1H, $C_5$H); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.28, 118.50, 122.53, 125.02, 125.29, 126.22, 126.94, 128.61, 129.27, 130.94, 131.26, 131.86, 134.12, 136.85, 139.93, 152.17 (ArC); GC-MS: m/z 323 ($M^+$).

**Typical procedure for synthesis of compounds 16-30:** A vial equipped with stirring bar was charged with 6-bromo-8-substituted-imidazo[1,2-*a*]pyrazine (0.1 g, 0.323 mmol), $Cs_2CO_3$ (0.105 g, 0.323 mmol) and boronic acid (0.323 mmol), dissolved in MeCN:$H_2O$ (9:1) at 100 $^0$C under inert atmosphere. Then, 5 mol% of $Pd(PPh_3)_4$ was added, vial was capped and refluxed for 6-12 h. After the completion of the reaction (monitored by TLC), cooled the reaction mixture, and then extracted the reaction mixture with water and chloroform. Organic layer was dried over sodium

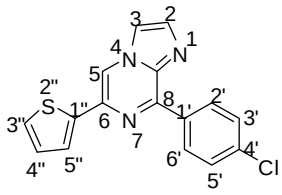
sulphate, filtered and concentrated under *vacuo* to get crude product. The residue was purified by silica gel (100-200 mesh) column chromatography using hexane:ethyl acetate as eluent to give pure solid.

**Spectral data 4”-(8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (16)**: Off white solid; Yield: 82%; mp 208-210 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 7.29-7.25 (m, 2H, $C_{2'}H$ and $C_{6'}H$), 7.83 (d, *J* = 0.92 Hz, 1H, $C_2H$), 7.90 (d, *J* = 1.36 Hz, 1H, $C_3H$), 8.03 (d, *J* = 8.68 Hz, 2H, $C_{2''}H$ and $C_{6''}H$), 8.26 (d, *J* = 8.72 Hz, 2H, $C_{3''}H$ and $C_{5''}H$), 8.58 (s, 1H, $C_5H$), 8.95-8.92 (dd, $^{2}J$ = 9.16 Hz, $^{3}J$ = 5.70 Hz, 2H, $C_{3'}H$ and $C_{5'}H$), 10.10 (s, 1H, CHO); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.71, 115.11, 115.37, 115.58, 126.61, 130.34, 131.88, 131.97, 135.68, 136.19, 137.27, 138.64, 142.27, 147.95, 163.22, 165.73 (ArC), 191.83 (CHO); Mass (EI): m/z 318 ($M^{+}$+1).

**Spectral data 2”-(8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol (17)**: Yellow solid; Yield: 80%; mp 158-160 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 6.96 (t, *J* = 7.56 Hz, 1H, $C_{5''}H$), 7.06 (d, *J* = 8.24 Hz, 1H, $C_{6''}H$), 7.35 -7.26 (m, $C_{2'}H$, 3H, $C_{6'}H$ and $C_{4''}H$), 7.65-7.63 (dd, $^{2}J$ = 8.24 Hz, $^{3}J$ = 1.40 Hz, 1H, $C_{3''}H$), 7.87 (s, 1H, $C_2H$), 7.95 (s, 1H, $C_3H$), 8.58 (s, 1H, $C_5H$), 8.69-8.66 (dd, $^{2}J$ = 8.68 Hz, $^{3}J$ = 5.50 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 113.41, 115.00, 115.79, 116.00, 117.32, 118.59, 119.55, 124.88, 130.73, 130.76, 130.95, 131.69, 131.77, 136.50, 137.61, 139.06, 146.35, 157.97, 163.32, 165.83 (ArC); Mass (EI): m/z 306 ($M^{+}$+1).

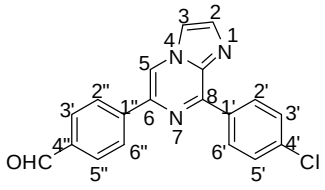
**Spectral data 6-(4”-chlorophenyl)-8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazine (18)**: Light green solid; Yield: 62%; mp 136-138 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 7.27-7.23 (m, 2H, $C_{2'}H$ and $C_{6'}H$), 7.47 (d, *J* = 8.72 Hz, 2H, $C_{2''}H$ and $C_{6''}H$), 7.78 (d, *J* = 1.40 Hz, 1H, $C_2H$), 7.86 (d, *J* = 0.92 Hz, 1H, $C_3H$), 7.98 (d, *J* = 8.72 Hz, 2H, $C_{3''}H$ and $C_{5''}H$), 8.42 (s, 1H, $C_5H$), 8.92-8.88 (dd, $^{2}J$ = 9.16 Hz, $^{3}J$ = 5.74 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 113.73, 114.40, 115.20, 115.42, 127.29, 128.98, 131.75, 131.83, 131.98, 132.01, 134.63, 134.88, 135.32, 137.49, 138.44, 147.46, 163.06, 165.56 (ArC); Mass (EI): m/z 324 ($M^{+}$+1).

**Spectral data 8-(4'-chlorophenyl)-6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazine (19)**: Green



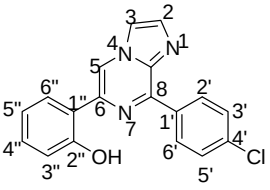
solid; Yield: 70%; mp 135-137 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 7.14 (t, *J* = 4.36 Hz, 1H, $C_{4"}H$), 7.40 (d, *J* = 5.04 Hz, 1H, $C_{5"}H$), 7.51 (d, *J* = 8.72 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.56 (d, *J* = 3.20 Hz, 1H, $C_{3'}H$), 7.74 (s, 1H, $C_2H$), 7.84 (s, 1H, $C_3H$), 8.39 (s, 1H, $C_5H$), 8.85 (d, *J* = 9.16 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 112.31, 114.44, 123.31, 126.76, 128.17, 128.66, 131.16, 134.16, 134.87, 135.46, 136.86, 138.52, 141.57, 147.37 (ArC); Mass (EI): m/z 312 ($M^+$+1).

**Spectral data 4"-(8-(4'-chlorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (20)**: Light



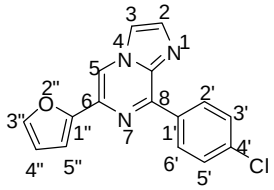
yellow solid; Yield: 65%; mp 204-207 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 7.56 (d, *J* = 8.68 Hz, 2H, $C_{2"}H$ and $C_{6"}H$), 7.84 (d, *J* = 0.92 Hz, 1H, $C_2H$), 7.91 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.04 (d, *J* = 8.28 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 8.25 (d, *J* = 8.28 Hz, 2H, $C_{3'}H$ and $C_{5'}H$), 8.60 (s, 1H, $C_5H$), 8.88 (d, *J* = 8.68 Hz, 2H, $C_{3"}H$ and $C_{5"}H$), 10.10 (s, 1H, CHO); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 114.82, 115.41, 126.71, 128.77, 130.46, 131.16, 134.28, 135.84, 136.31, 137.05, 137.39, 138.72, 142.29, 147.91 (ArC), 191.94 (CHO); Mass (EI): m/z 334 ($M^+$+1).

**Spectral data 2"-(8-(4'-chlorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol (21)**: Yellow solid;



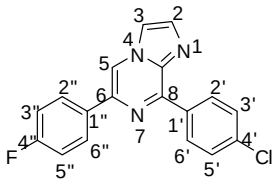
Yield: 68%; mp 172-174 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 6.97- 6.93 (m, 1H, $C_{5"}H$), 7.06-7.04 (dd, $^{2}J$ = 8.24 Hz, $^{3}J$ = 0.92 Hz, 1H, $C_{6"}H$), 7.34-7.30 (m, 1H, $C_{4"}H$), 7.56 (d, *J* = 8.72 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.64-7.62 (dd, $^{2}J$ = 8.24 Hz, $^{3}J$ = 1.62 Hz, 1H, $C_{3'}H$), 7.87 (d, *J* = 0.92 Hz, 1H, $C_2H$), 7.95 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.59 (s, 1H, $C_5H$), 8.61 (d, *J* = 8.68 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 113.77, 115.14, 117.45, 118.77, 119.73, 125.05, 129.17, 130.95, 131.15, 133.12, 136.72, 137.59, 137.76, 139.30, 146.44, 158.07 (ArC); Mass (EI): m/z 322 ($M^+$+1).

**Spectral data 8-(4'-chlorophenyl)-6-(furan-2"-yl)imidazo[1,2-*a*]pyrazine (22)**: White solid;



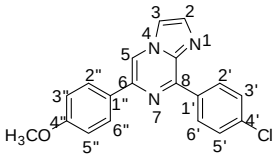
Yield: 72%; mp 159-161 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 6.58-6.56 (dd, $^2J$ = 3.2 Hz, $^3J$ = 1.84 Hz, 1H, $C_{4"}H$), 7.12 (d, $J$ = 2.72 Hz, 1H, $C_{5"}H$), 7.54-7.51 (m, 3H, $C_{3"}H$, $C_{2'}H$ and $C_{6'}H$), 7.76 (d, $J$ = 1.4 Hz, 1H, $C_2H$), 7.84 (d, $J$ = 1.36 Hz, 1H, $C_3H$), 8.43 (s, 1H, $C_5H$), 8.80 (d, ($J$ = 6.88 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): 108.72, 112.14, 112.49, 114.73, 128.68, 131.14, 132.08, 134.28, 135.38, 136.83, 138.50, 142.78, 148.06, 151.58 (ArC); Mass (EI): m/z 296 ($M^+$+1).

**Spectral data 8-(4'-chlorophenyl)-6-(4"-fluorophenyl)imidazo[1,2-*a*]pyrazine (23)**: White



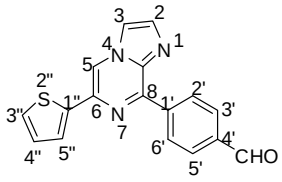
solid; Yield: 70%; mp 134-135 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.19 (t, $J$ = 8.72 Hz, 2H, $C_{2"}H$ and $C_{6"}H$), 7.52 (d, $J$ = 8.72 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.77 (d, $J$ = 1.36 Hz, 1H, $C_2H$), 7.85 (d, $J$ = 0.92 Hz, 1H, $C_3H$), 8.03-7.99 (dd, $^2J$ = 9.16 Hz, $^3J$ = 5.26 Hz, 2H, $C_{3"}H$ and $C_{5"}H$), 8.39 (s, 1H, $C_5H$), 8.84 (d, $J$ = 8.68 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): 113.68, 114.33, 115.67, 115.89, 127.81, 127.89, 128.47, 130.92, 132.45, 134.28, 135.27, 136.59, 137.78, 138.34, 147.17, 161.92, 164.39 (ArC); Mass (EI): m/z 324 ($M^+$+1).

**Spectral data 8-(4'-chlorophenyl)-6-(4"-methoxyphenyl)imidazo[1,2-*a*]pyrazine (24)**: White



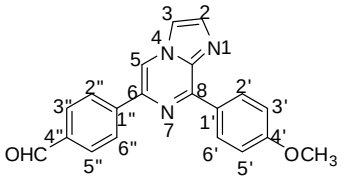
solid; Yield: 74%; mp 115-117 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 3.88 (s, 3H, $OCH_3$), 7.03 (d, $J$ = 8.68 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.52 (d, $J$ = 8.72 Hz, 2H, $C_{2"}H$ and $C_{6"}H$), 7.75 (d, $J$ = 1.4 Hz, 1H, $C_2H$), 7.83 (d, $J$ = 1.36 Hz, 1H, $C_3H$), 7.97 (2H, d, $J$ = 8.68 Hz, $C_{3'}H$ and $C_{5'}H$), 8.36 (s, (1H, $C_5H$), 8.85 (d, $J$ = 8.28 Hz, 2H, $C_{3"}H$ and $C_{5"}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): 108.72, 112.14, 112.49, 114.73, 128.68, 131.14, 132.08, 134.28, 135.38, 136.83, 138.50, 142.78, 148.06, 151.58 (ArC); Mass (EI): m/z 336 ($M^+$+1).

**Spectral data 4'-(6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazin-8-yl)benzaldehyde (25)**: Green



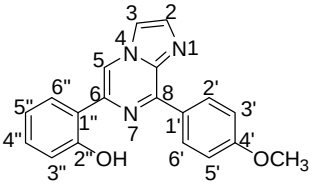
solid; Yield: 52%; mp 165-167 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 7.14 (t, *J* = 4.36 Hz, 1H, $C_{4"}H$), 7.42-7.40 (dd, $^2J$ = 5.04 Hz, $^3J$ = 1.36 Hz, 1H, $C_{5"}H$), 7.59-7.57 (dd, $^2J$ = 3.64 Hz, $^3J$ = 0.92 Hz, 1H, $C_{3"}H$), 7.77 (d, *J* = 0.92 Hz, 1H, $C_2H$), 7.86 (d, *J* = 0.8 Hz, 1H, $C_3H$), 8.05 (d, *J* = 8.24 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 8.43 (s, 1H, $C_5H$), 9.03 (d, *J* = 8.24 Hz, 2H, $C_{3'}H$ and $C_{5'}H$), 10.12 (s, 1H, CHO); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 112.92, 114.56, 123.56, 126.96, 128.26, 129.70, 130.41, 135.14, 135.86, 137.30, 138.76, 141.19, 141.31, 147.20 (ArC), 192.36 (CHO); Mass (EI): m/z 306 ($M^+$+1).

**Spectral data 4”-(8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (26)**: Off



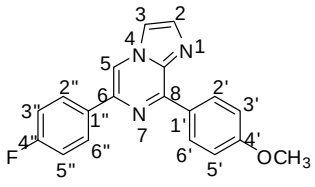
white solid; Yield: 85%; mp 190-192 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 3.92 (s, 3H, $OCH_3$), 7.11 (d, *J* = 9.16 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.80 (d, *J* = 0.92 Hz, 1H, $C_2H$), 7.88 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.03 (d, *J* = 8.72 Hz, 2H, $C_{2"}H$ and $C_{6"}H$), 8.27 (d, *J* = 8.28 Hz, 2H, $C_{3"}H$ and $C_{5"}H$), 8.54 ( s, 1H, $C_5H$), 8.90 (d, *J* = 9.16 Hz, 2H, $C_{3'}H$ and $C_{5'}H$), 10.10 (s, 1H, CHO); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 55.37 ($OCH_3$), 113.75, 114.47, 114.51, 126.48, 128.44, 130.21, 131.37, 135.27, 136.00, 137.64, 138.59, 142.48, 148.46, 161.68 (ArC), 191.84 (CHO); Mass (EI): m/z 330 ($M^+$+1).

**Spectral data 2”-(8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol (27)**: Yellow



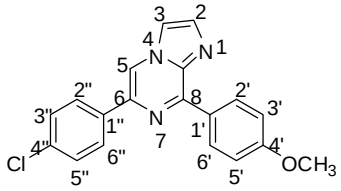
solid; Yield: 75%; mp 125-127 $^0$C; $^1$H NMR ($CDCl_3$, 400 MHz): δ 3.92 (s, 3H, $OCH_3$), 6.97-6.93 (m, 1H, $C_{5"}H$), 7.07-7.05 (dd, $^2J$ = 8.28 Hz, $^3J$ = 0.92 Hz, 1H, $C_{6"}H$), 7.11 (d, *J* = 9.16 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.34-7.30 (m, 1H, $C_{4"}H$), 7.66-7.63 (dd, $^2J$ = 7.80 Hz, $^3J$ = 1.60 Hz, 1H, $C_{3"}H$), 7.84 (d, *J* = 0.92 Hz, 1H, $C_2H$), 7.93 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.54 (s, 1H, $C_5H$), 8.66 (d, *J* = 9.16 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 55.40 ($OCH_3$), 112.66, 114.12, 114.82, 117.43, 118.48, 119.34, 124.77, 127.09, 130.71, 131.21, 136.05, 137.60, 138.89, 146.85, 158.09, 161.97 (ArC); Mass (EI): m/z 318 ($M^+$+1).

**Spectral data 6-(4”-fluorophenyl)-8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazine (28)**: White



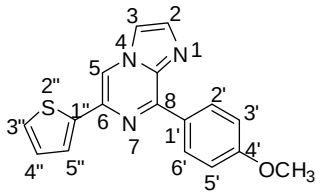
solid; Yield: 68%; mp 108-110 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 3.91 (s, 3H, $OCH_3$), 7.09 (d, *J* = 9.16 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.19 (t, *J* = 8.46 Hz, 2H, $C_{2''}H$ and $C_{6''}H$), 7.75 (s, 1H, $C_2H$), 7.84 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.05-8.02 (dd, $^{2}J$ = 8.72 Hz, $^{3}J$ = 5.50 Hz, 2H, $C_{3''}H$ and $C_{5''}H$), 8.36 (s, 1H, $C_5H$), 8.87 (d, *J* = 9.16 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 55.37 ($OCH_3$), 112.92, 113.71, 114.20, 115.62, 115.83, 127.87, 127.94, 128.67, 131.30, 132.86, 132.89, 134.97, 137.81, 138.50, 148.22, 161.52, 161.88, 164.34 (ArC); Mass (EI): m/z 320 ($M^{+}$+1).

**Spectral data 6-(4”-chlorophenyl)-8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazine (29)**: White



solid; Yield: 76%; mp 119-121 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 3.91 (s, 3H, $OCH_3$), 7.09 (d, *J* = 9.16 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.46 (d, *J* = 8.68 Hz, 2H, $C_{2''}H$ and $C_{6''}H$), 7.74 (d, *J* = 1.36 Hz, 1H, $C_2H$), 7.84 (d, *J* = 0.92 Hz, 1H, $C_3H$), 7.99 (d, *J* = 8.68 Hz, 2H, $C_{3''}H$ and $C_{5''}H$), 8.37 (s, 1H, $C_5H$), 8.86 (d, 2H, *J* = 9.16 Hz, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 55.35 ($OCH_3$), 113.15, 113.69, 114.26, 127.32, 128.59, 128.91, 137.29, 134.44, 135.00, 135.17, 137.46, 138.50, 148.20, 161.53 (ArC), Mass (EI): m/z 336 ($M^{+}$+1).

**Spectral data 8-(4’-methoxyphenyl)-6-(thiophen-2”-yl)imidazo[1,2-*a*]pyrazine (30)**: White



solid; Yield: 70%; mp 120-122 $^{0}$C; $^{1}$H NMR ($CDCl_3$, 400 MHz): δ 3.91 (s, 3H, $OCH_3$), 7.09 (d, *J* = 9.20 Hz, 2H, $C_{2'}H$ and $C_{6'}H$), 7.15 -7.13 (dd, $^{2}J$ = 5.04 Hz, $^{3}J$ = 3.68 Hz, 1H, $C_{4''}H$), 7.40-7.39 (dd, $^{2}J$ = 5.04 Hz, $^{3}J$ = 0.92 Hz, 1H, $C_{5''}H$), 7.58-7.57 (dd, $^{2}J$ = 3.68 Hz, $^{3}J$ = 0.92 Hz, 1H, $C_{3''}H$), 7.72 (d, *J* = 1.36 Hz, 1H, $C_2H$), 7.85 (d, *J* = 0.92 Hz, 1H, $C_3H$), 8.35 (s, 1H, $C_5H$), 8.87 (d, *J* = 9.16 Hz, 2H, $C_{3'}H$ and $C_{5'}H$); $^{13}$C NMR ($CDCl_3$, 100 MHz): δ 55.38 ($OCH_3$), 113.74, 114.42, 114.16, 123.01, 126.45, 127.99, 128.40, 131.43, 134.76, 135.04, 138.54, 141.94, 148.32, 161.23 (ArC); Mass (EI): m/z 308 ($M^{+}$+1).

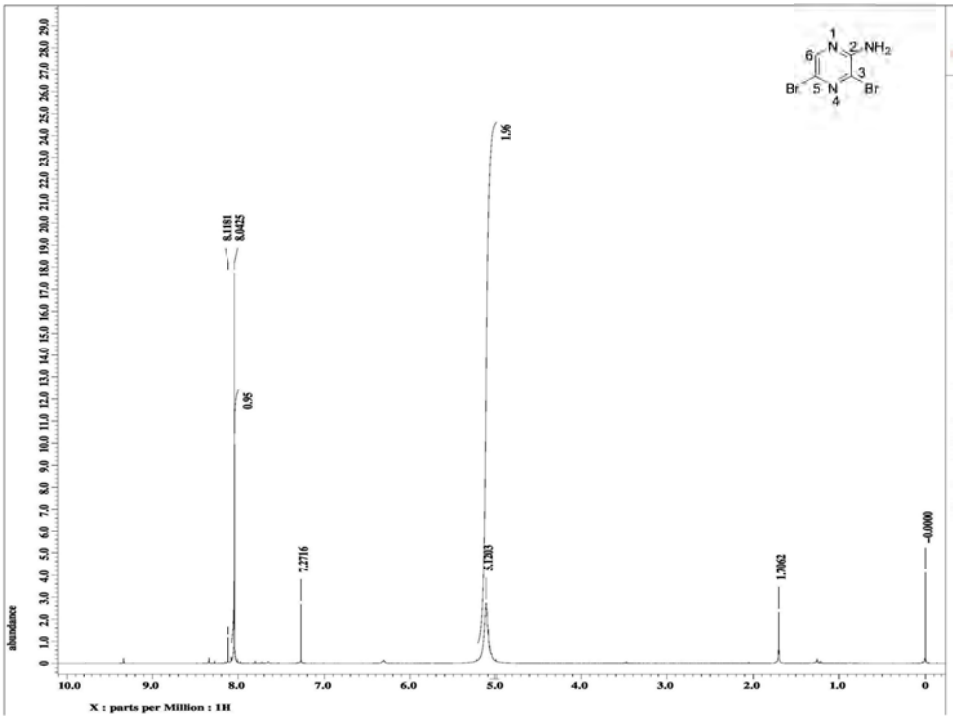



Fig. S1: $^{1}$H NMR Spectrum of 2-amino-3,5-dibromopyrazine **(2)**

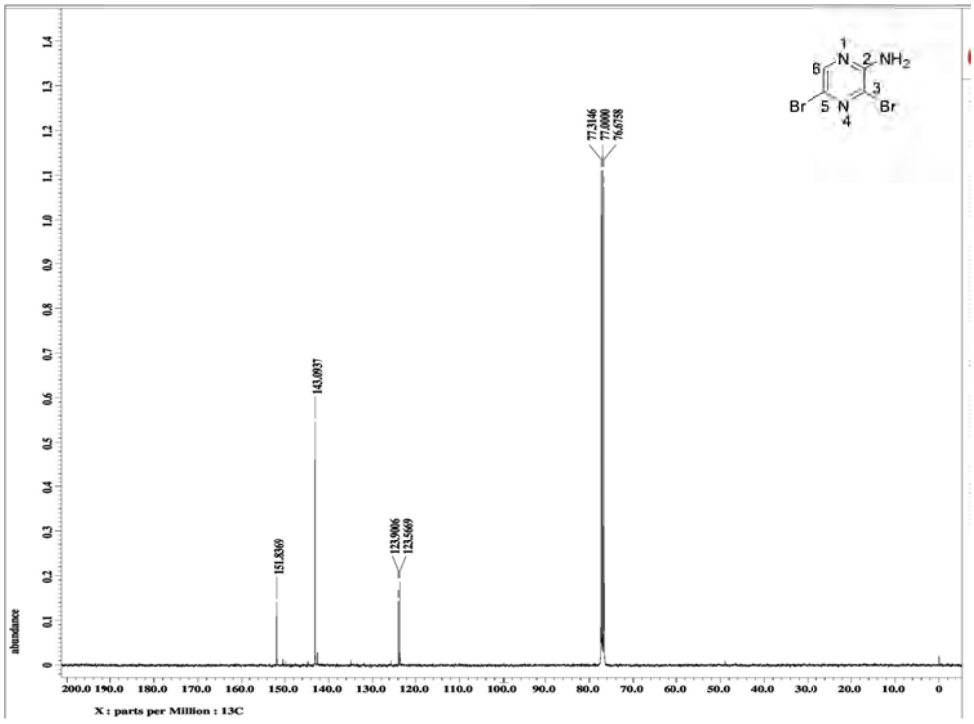



Fig. S2: $^{13}$C NMR Spectrum of 2-amino-3,5-dibromopyrazine **(2)**

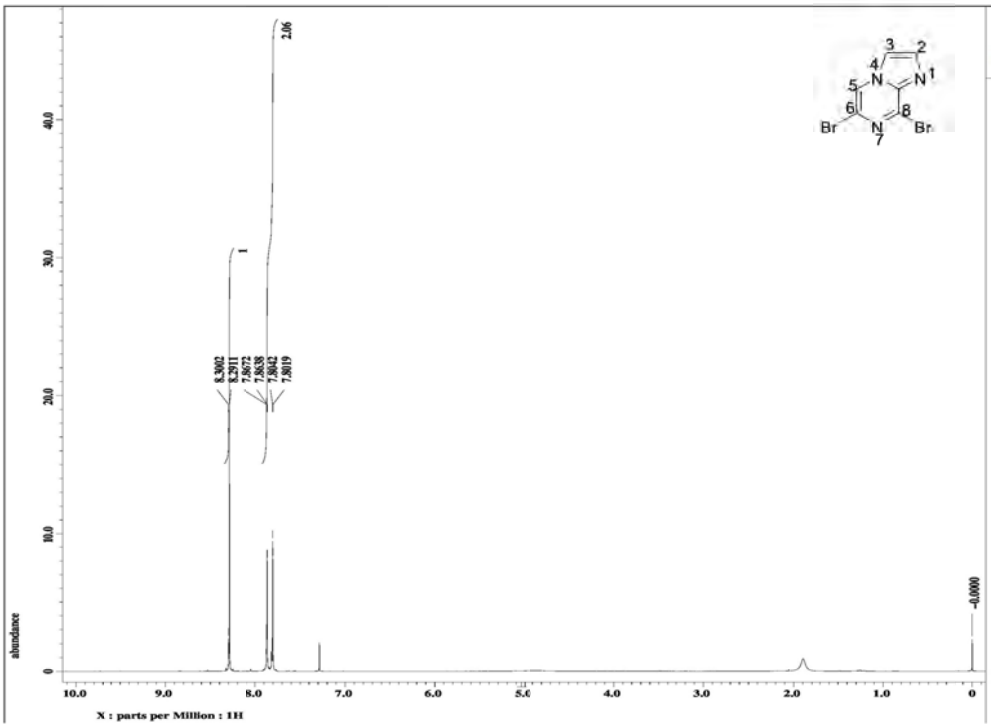



Fig. S3: $^{1}$H NMR Spectrum of 6,8-dibromoimidazo[1,2-*a*]pyrazine **(3)**

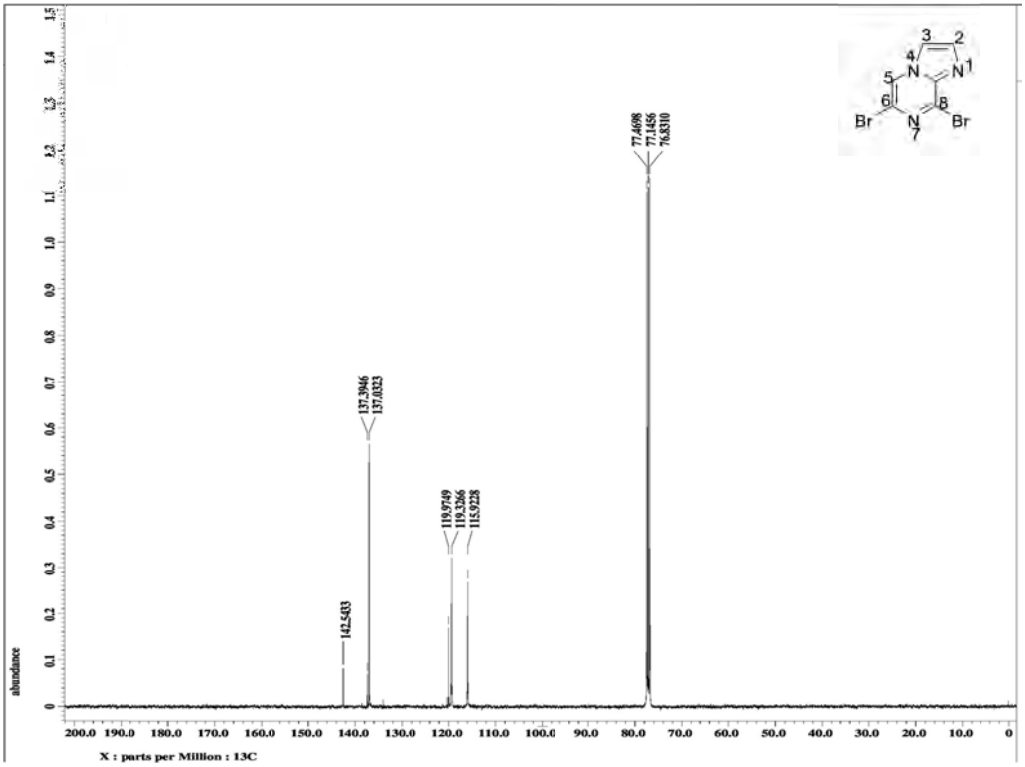



Fig. S4: $^{13}$C NMR Spectrum of 6,8-dibromoimidazo[1,2-*a*]pyrazine **(3)**

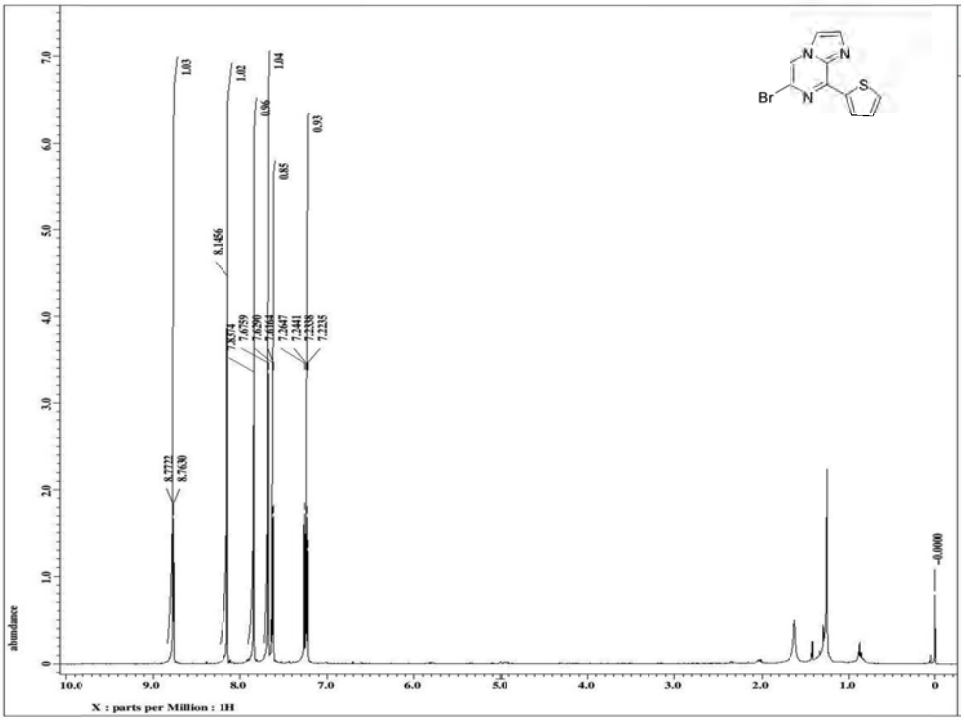



Fig. S5: $^{1}$H NMR Spectrum of 6-bromo-8-(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine **(4a)**

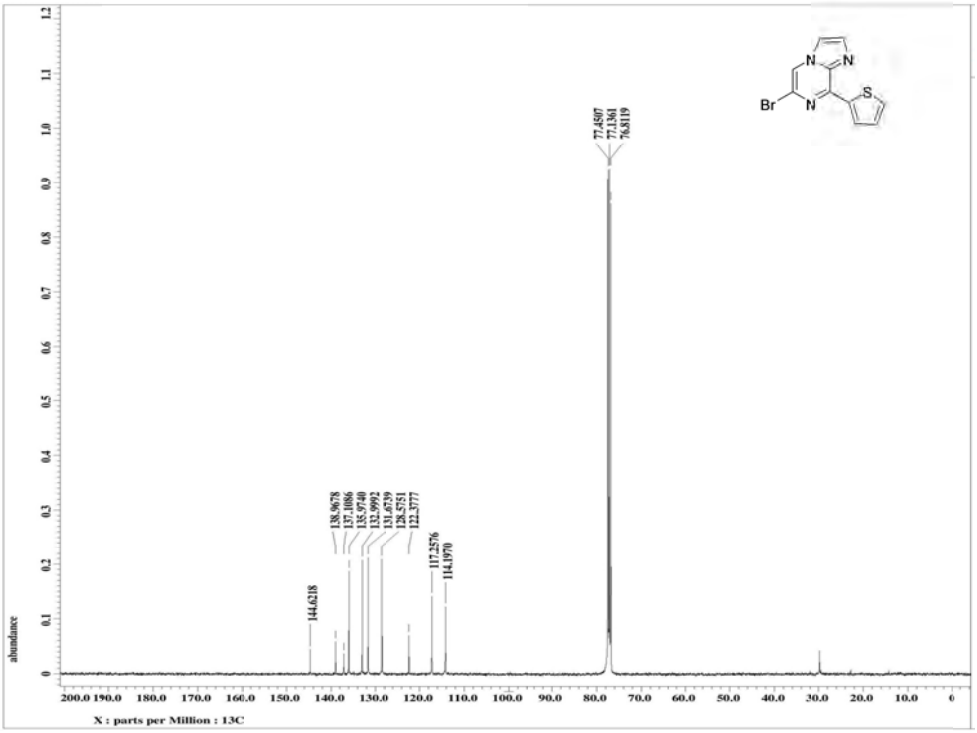



Fig. S6: $^{13}$C NMR Spectrum of 6-bromo-8-(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine **(4a)**

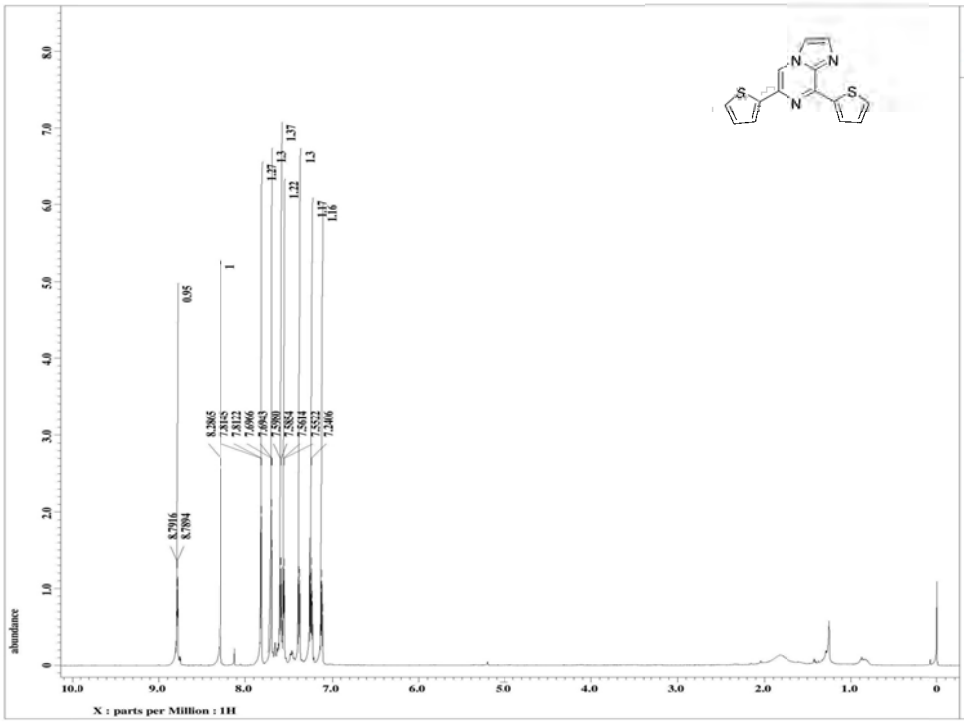



Fig. S7: $^{1}$H NMR Spectrum of 6,8-di(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine **(4b)**

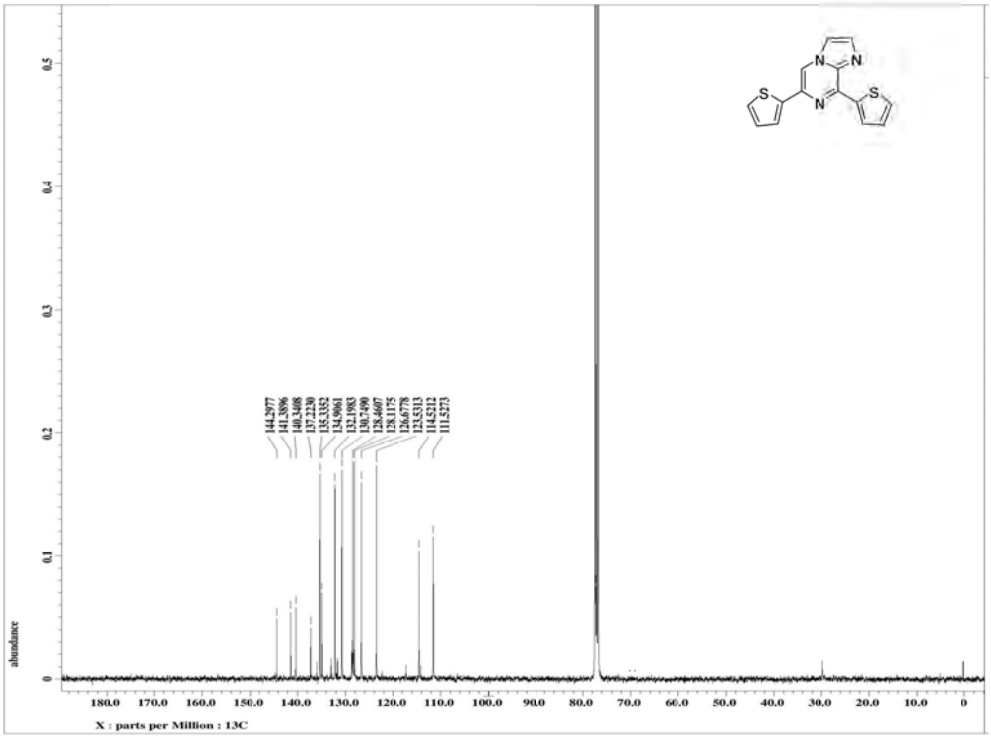



Fig. S8: $^{13}$C NMR Spectrum of 6,8-di(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine **(4b)**

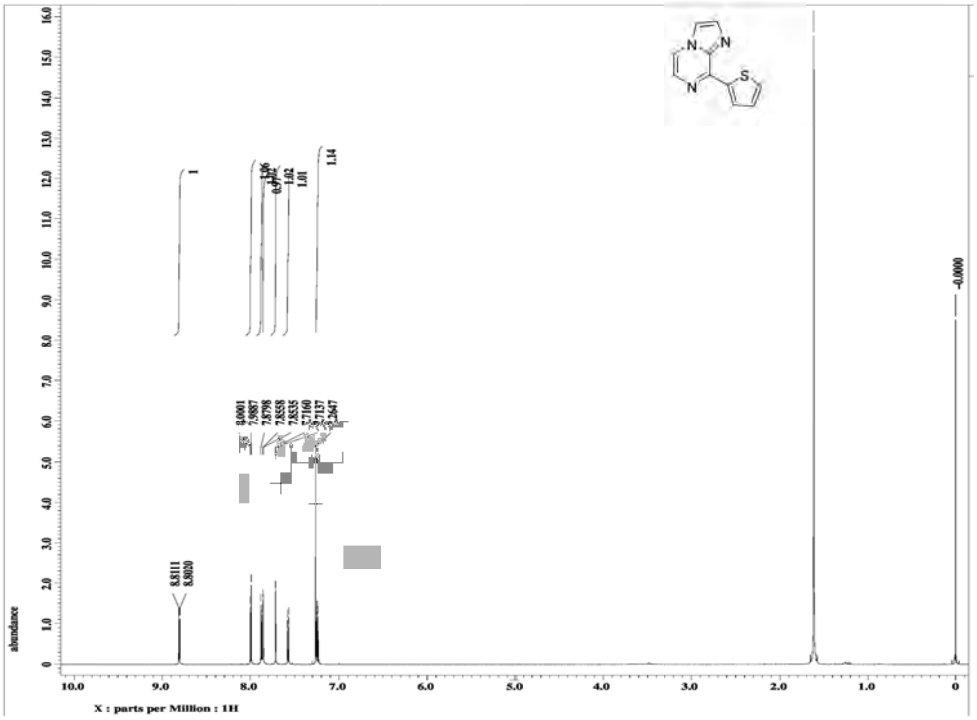



Fig. S9: $^{1}$H NMR Spectrum of 8-(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine **(4c)**

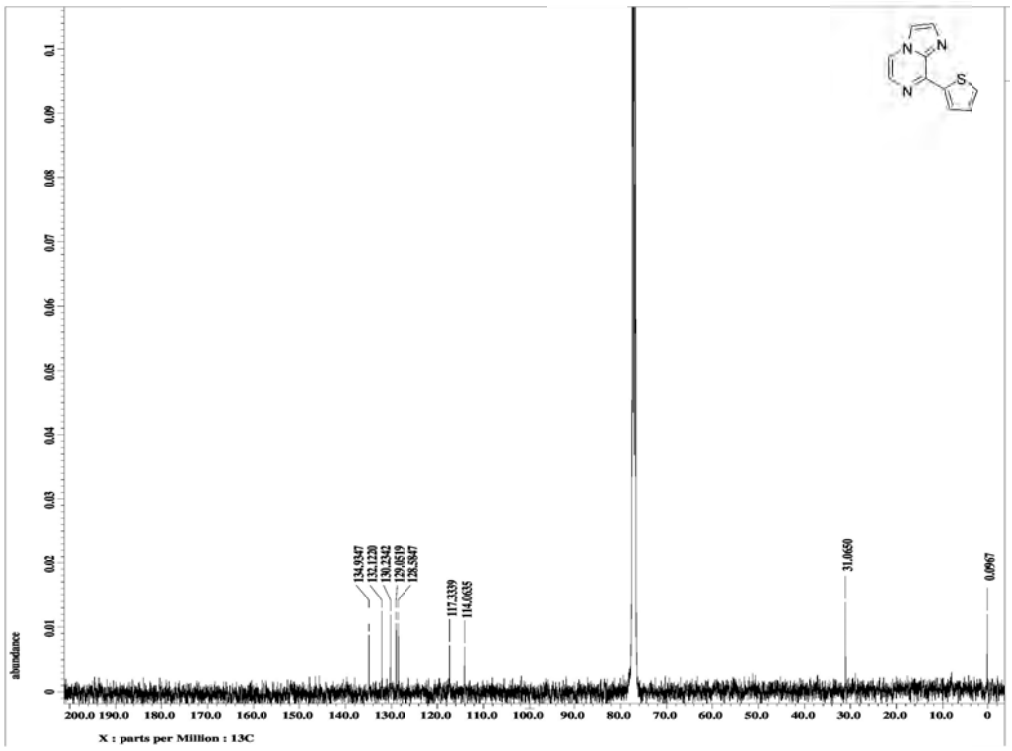



Fig. S10: $^{13}$C NMR Spectrum of 8-(thiophen-2'-yl)imidazo[1,2-*a*]pyrazine **(4c)**

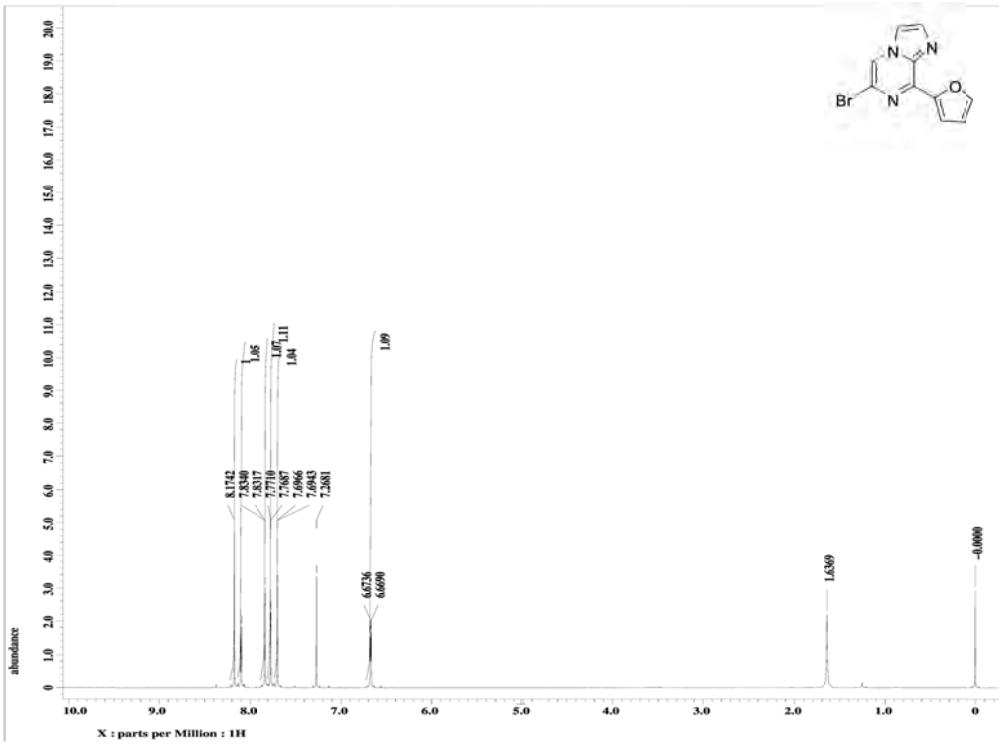



Fig. S11: $^{1}$H NMR Spectrum of 6-bromo-8-(furan-2'-yl)imidazo[1,2-*a*]pyrazine **(5a)**

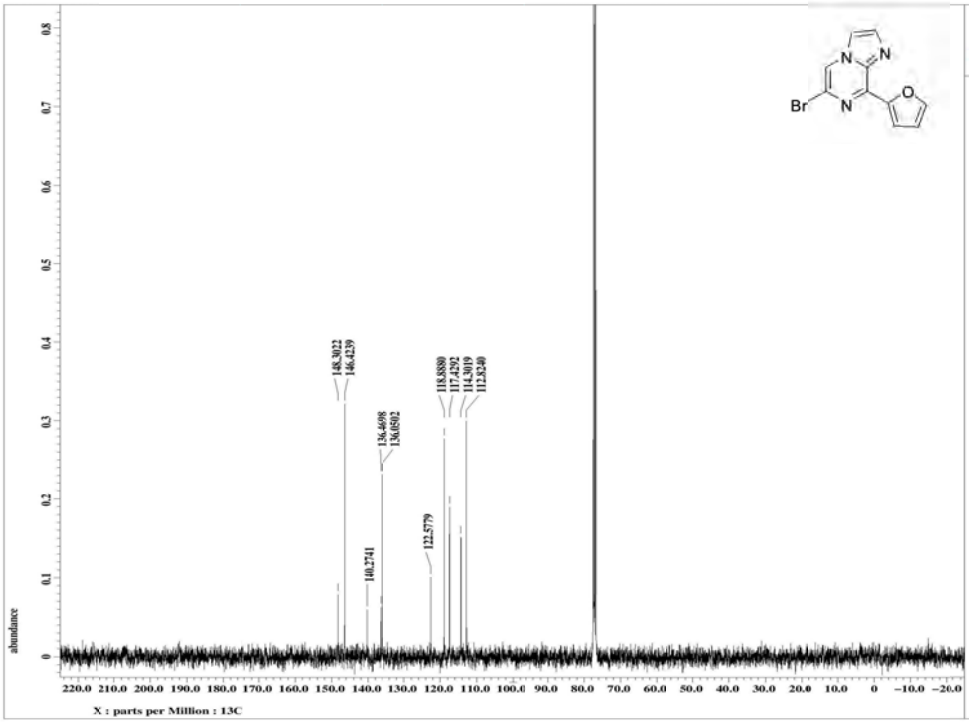



Fig. S12: $^{13}$C NMR Spectrum of 6-bromo-8-(furan-2'-yl)imidazo[1,2-*a*]pyrazine **(5a)**

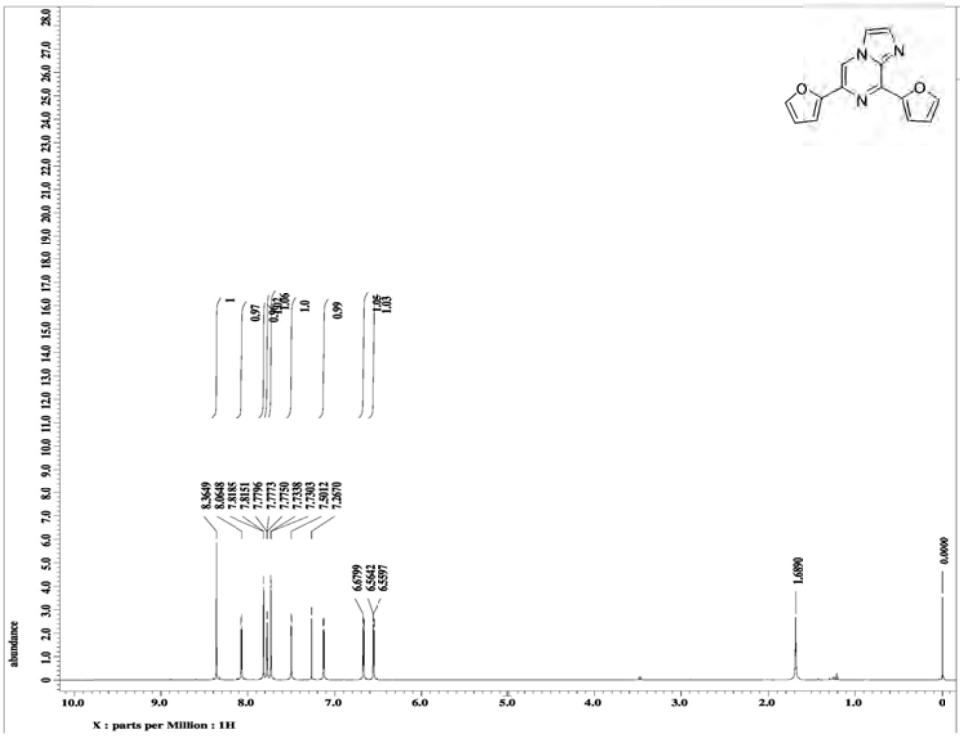



Fig. S13: $^{1}$H NMR Spectrum of 6,8-di(furan-2'-yl)imidazo[1,2-*a*]pyrazine **(5b)**

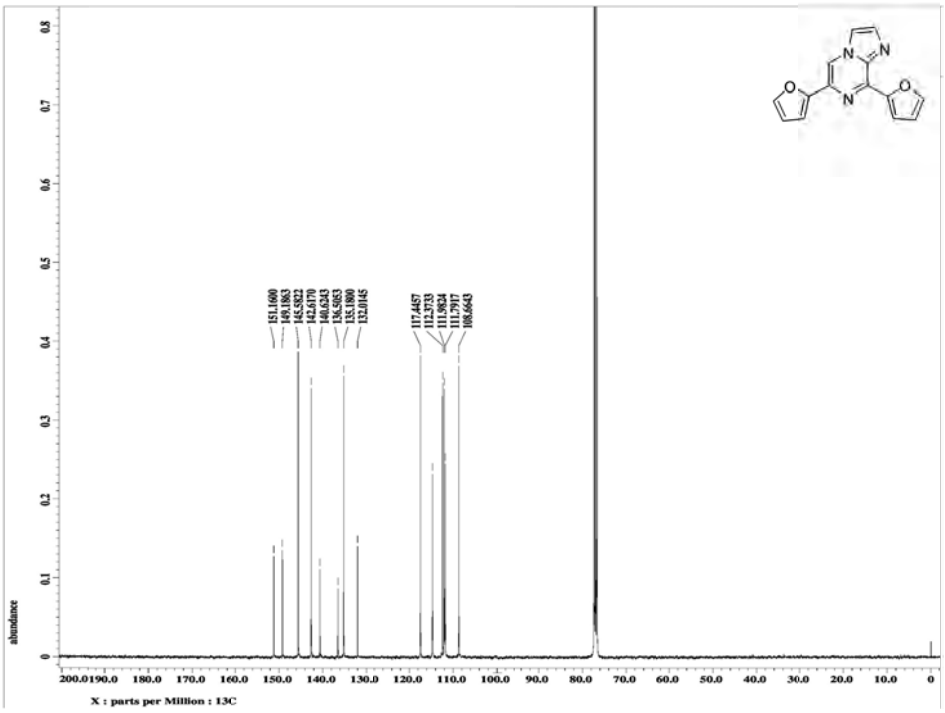



Fig. S14: $^{13}$C NMR Spectrum of 6,8-di(furan-2'-yl)imidazo[1,2-*a*]pyrazine **(5b)**

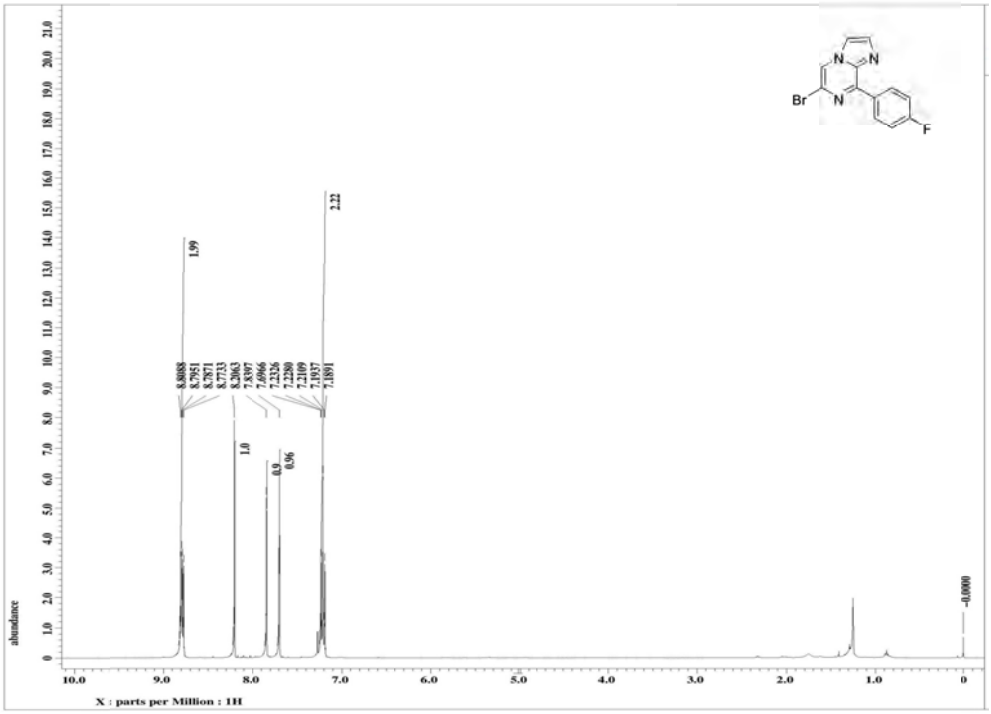



Fig. S15: $^{1}$H NMR Spectrum of 6-bromo-8-(4'-fluorophenyl)imidazo[1,2-*a*]pyrazine **(6a)**

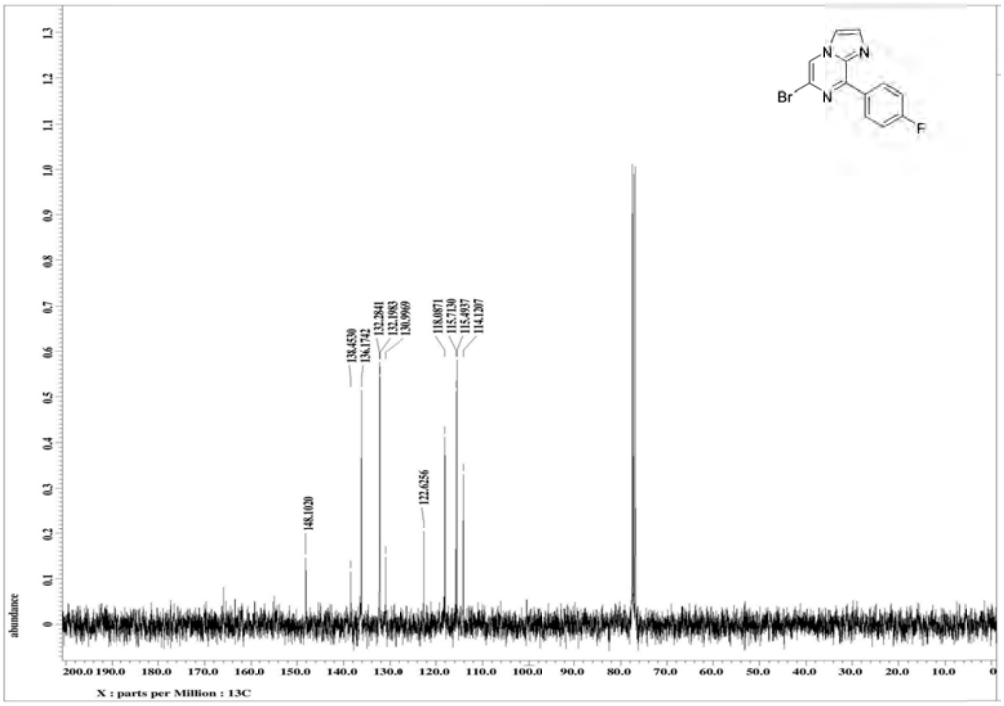



Fig. S16: $^{13}$C NMR Spectrum of 6-bromo-8-(4'-fluorophenyl)imidazo[1,2-*a*]pyrazine **(6a)**

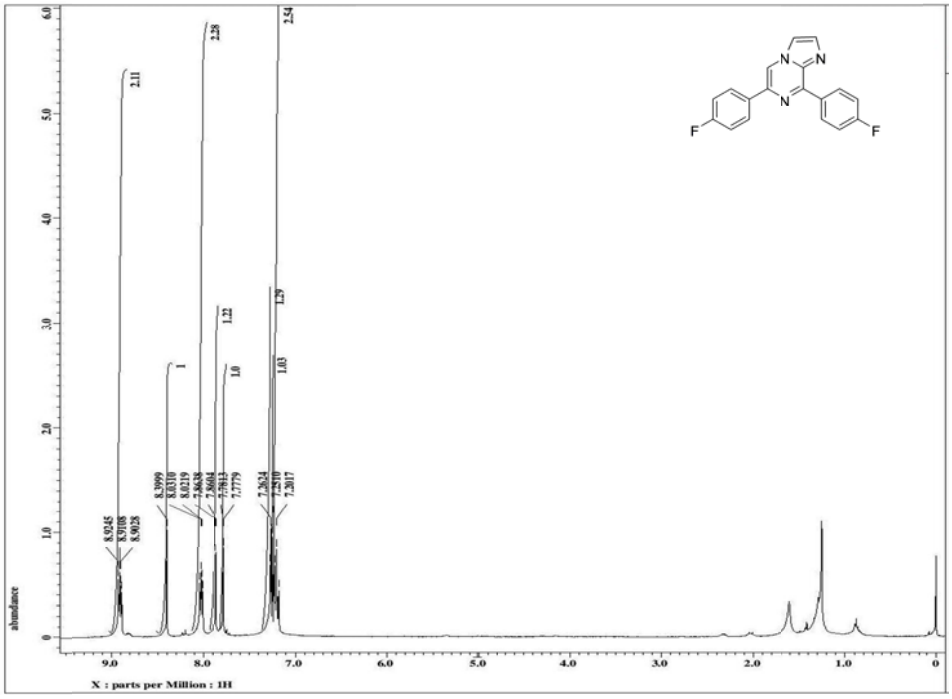



Fig. S17: $^{1}$H NMR Spectrum of 6,8-bis(4'-fluorophenyl)imidazo[1,2-*a*]pyrazine **(6b)**

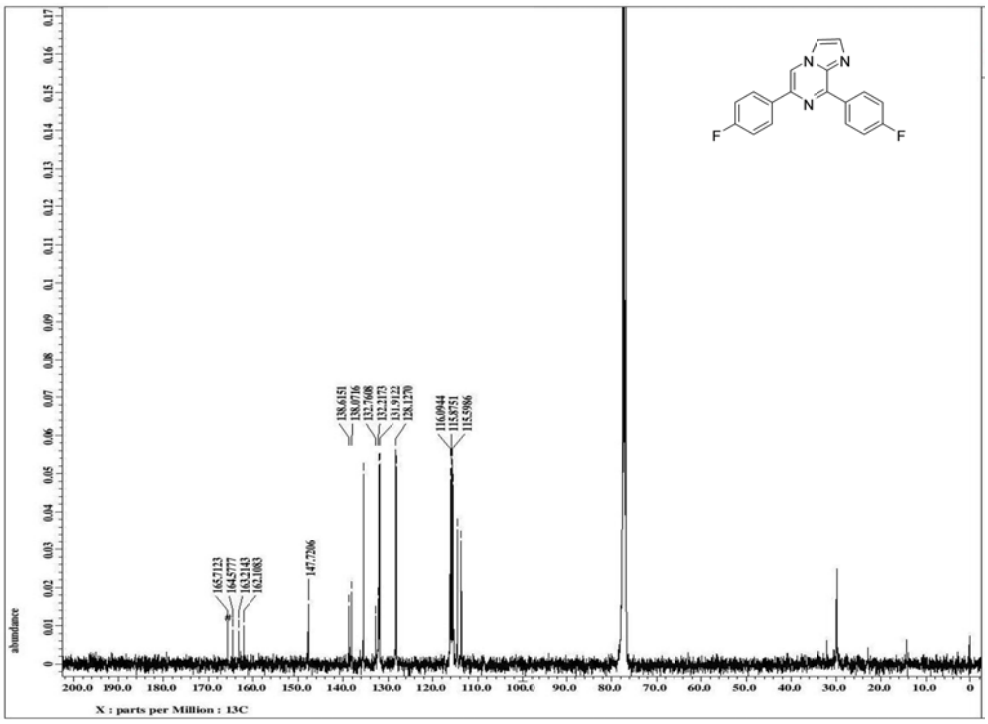



Fig. S18: $^{13}$C NMR Spectrum of 6,8-bis(4'-fluorophenyl)imidazo[1,2-*a*]pyrazine **(6b)**

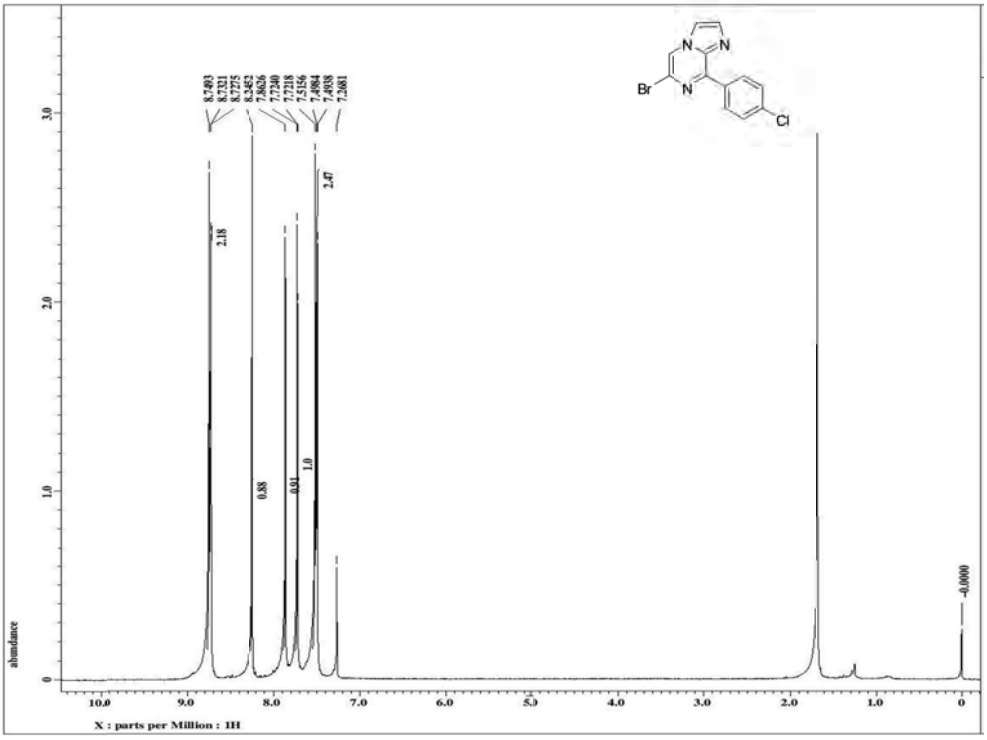



Fig. S19: $^{1}$H NMR Spectrum of 6-bromo-8-(4'-chlorophenyl)imidazo[1,2-*a*]pyrazine **(7a)**

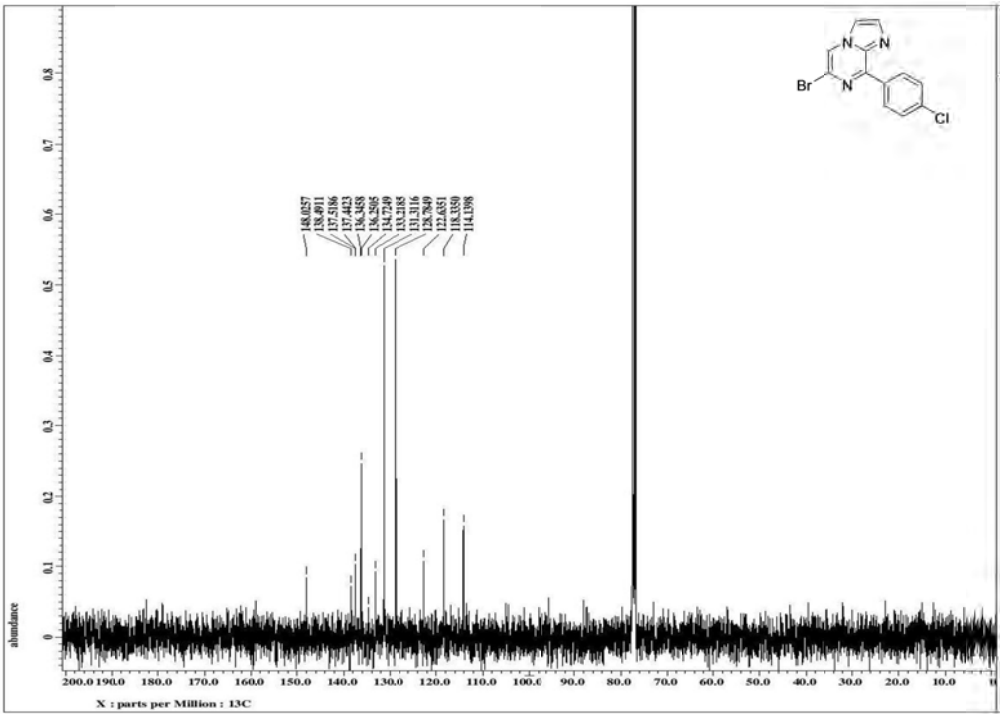



Fig. S20: $^{13}$C NMR Spectrum of 6-bromo-8-(4'-chlorophenyl)imidazo[1,2-*a*]pyrazine **(7a)**

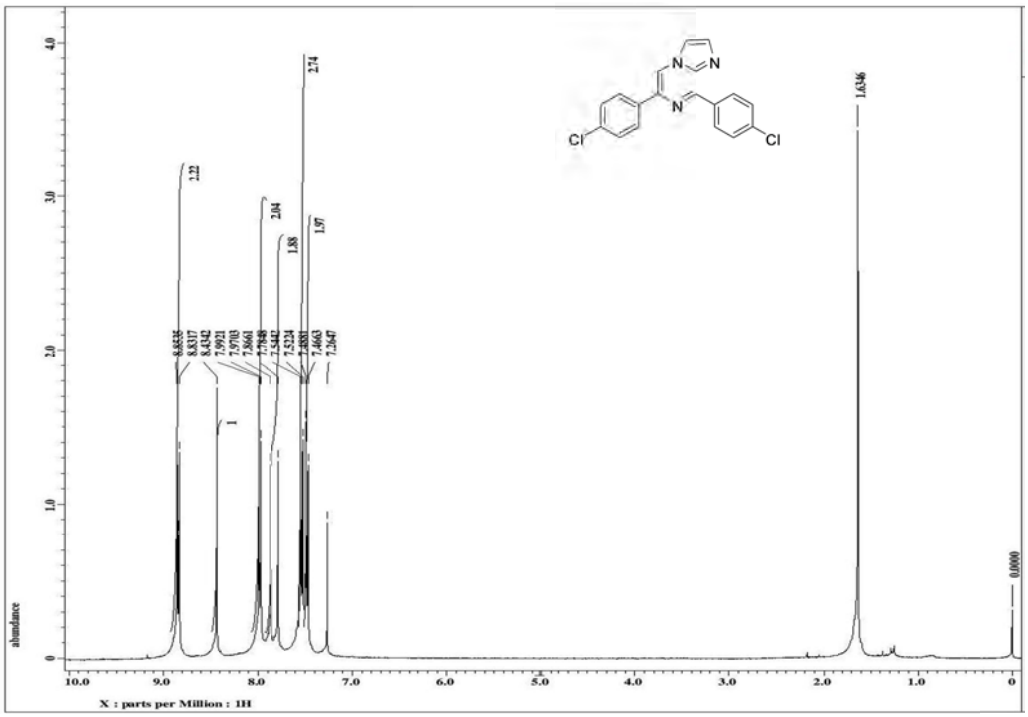



Fig. S21: $^{1}$H NMR Spectrum of 6,8-bis(4'-chlorophenyl)imidazo[1,2-*a*]pyrazine **(7b)**

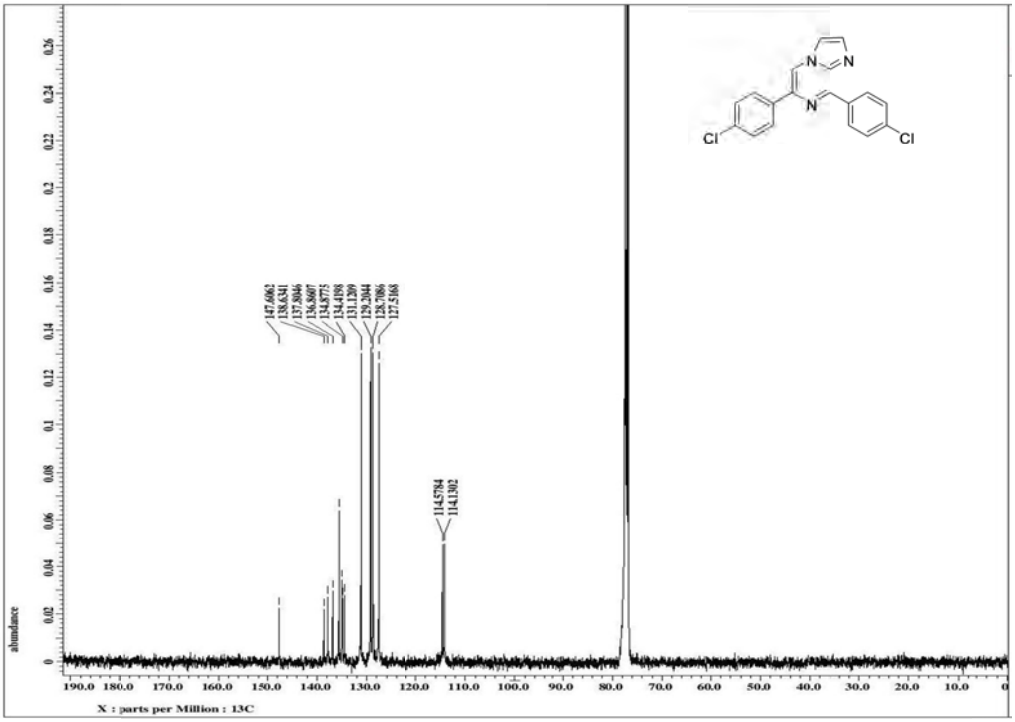



Fig. S22: $^{13}$C NMR Spectrum of 6,8-bis(4'-chlorophenyl)imidazo[1,2-*a*]pyrazine **(7b)**

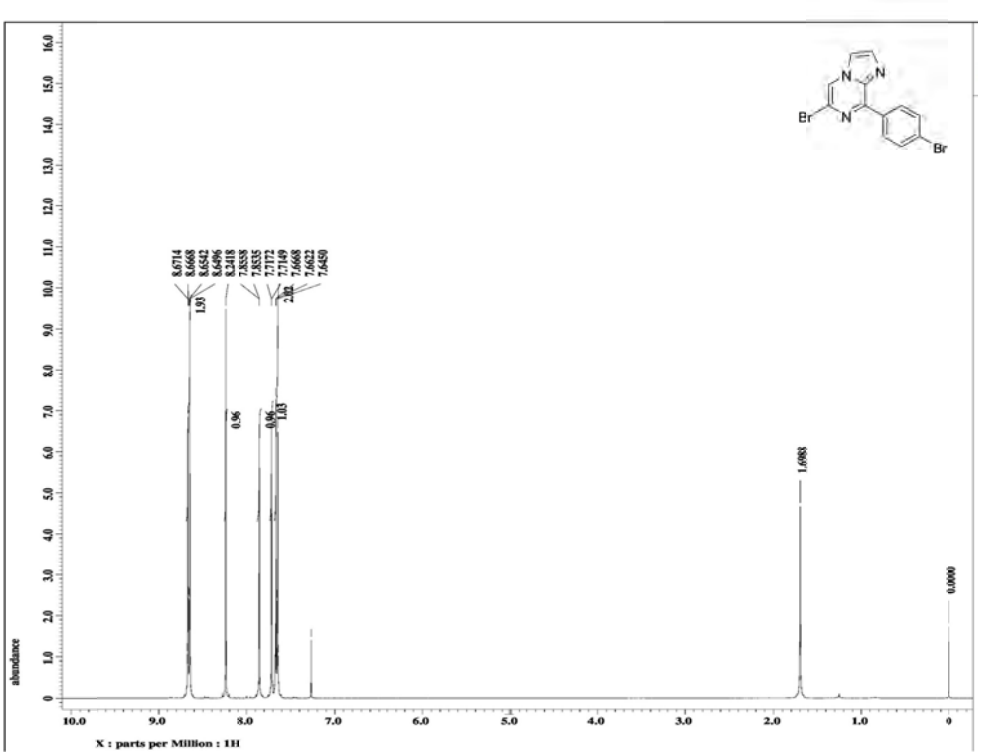



Fig. S23: $^{1}$H NMR spectrum of 6-bromo-8-(4'-bromophenyl)imidazo[1,2-*a*]pyrazine **(8a)**

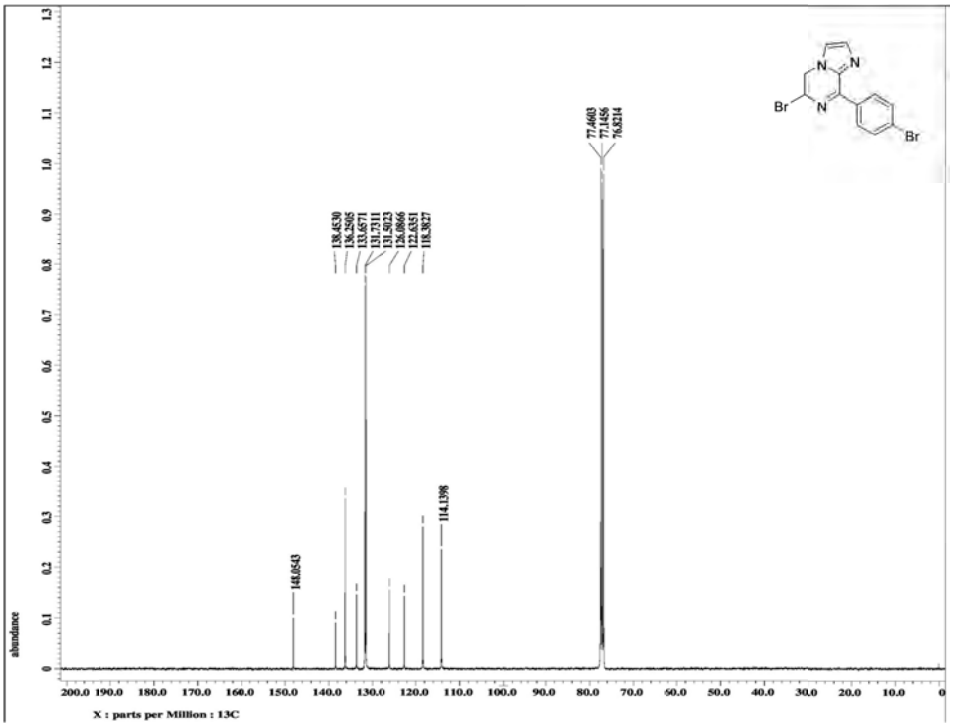



Fig. S24: $^{13}$C NMR spectrum of 6-bromo-8-(4'-bromophenyl)imidazo[1,2-*a*]pyrazine **(8a)**

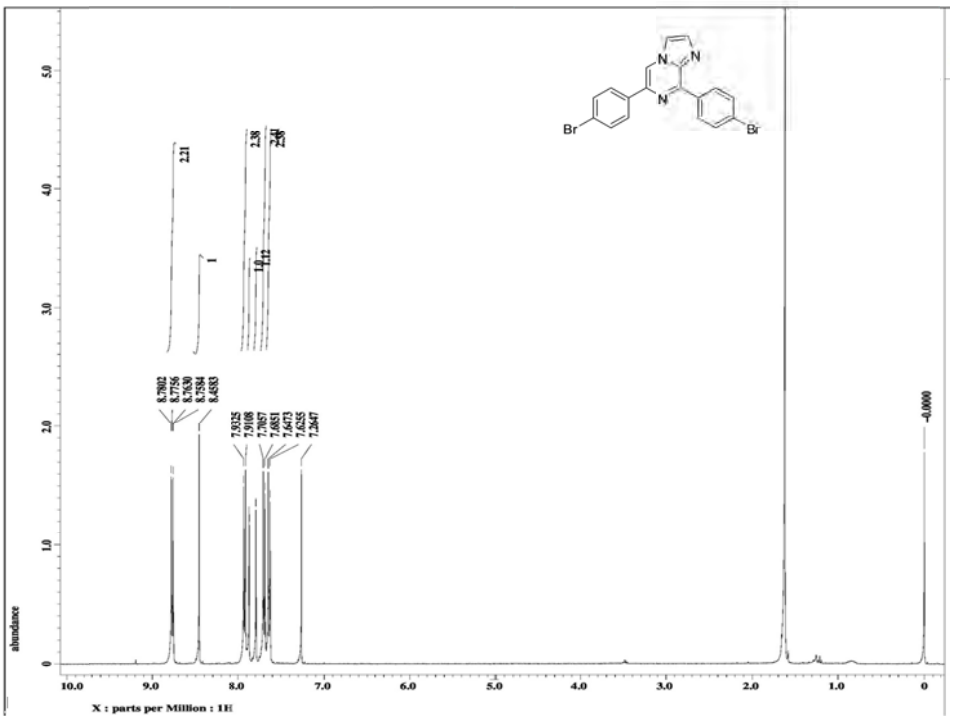



Fig. S25: $^{1}$H NMR spectrum of 6,8-bis(4'-bromophenyl)imidazo[1,2-*a*]pyrazine **(8b)**

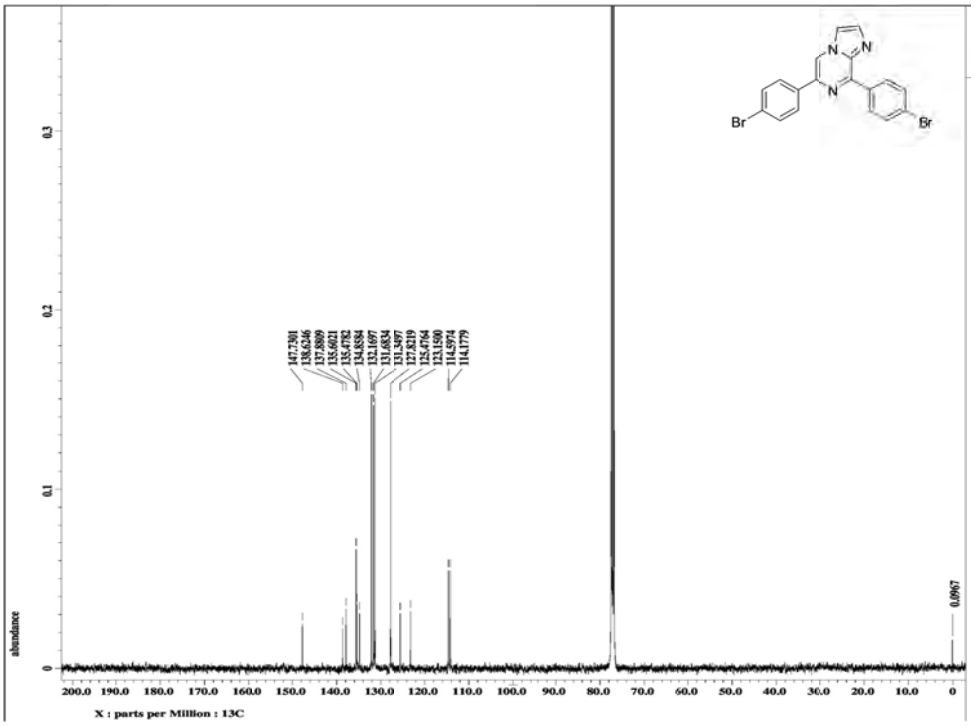



Fig. S26: $^{13}$C NMR spectrum of 6,8-bis(4'-bromophenyl)imidazo[1,2-*a*]pyrazine **(8b)**

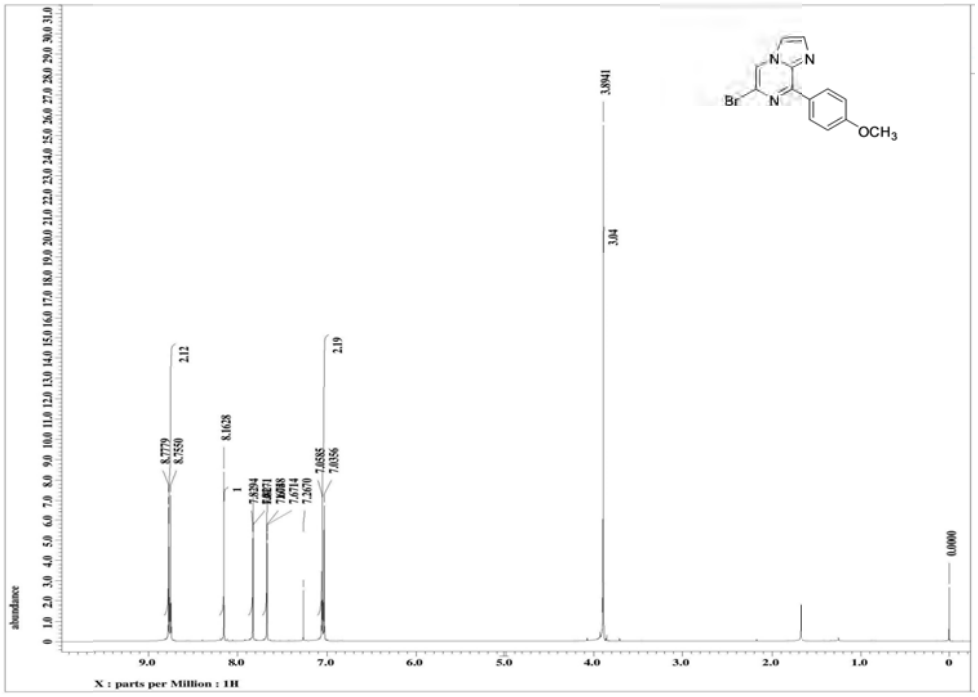



Fig. S27: $^{1}$H NMR Spectrum of 6-bromo-8-(4'-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(9a)**

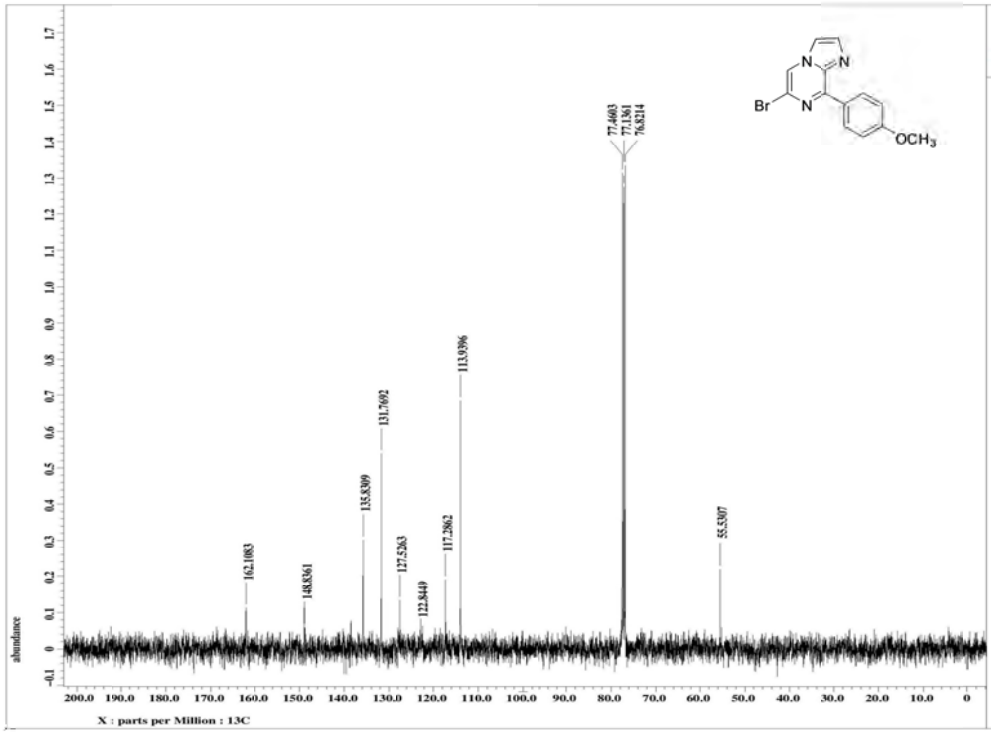



Fig. S28: $^{13}$C NMR Spectrum of 6-bromo-8-(4'-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(9a)**

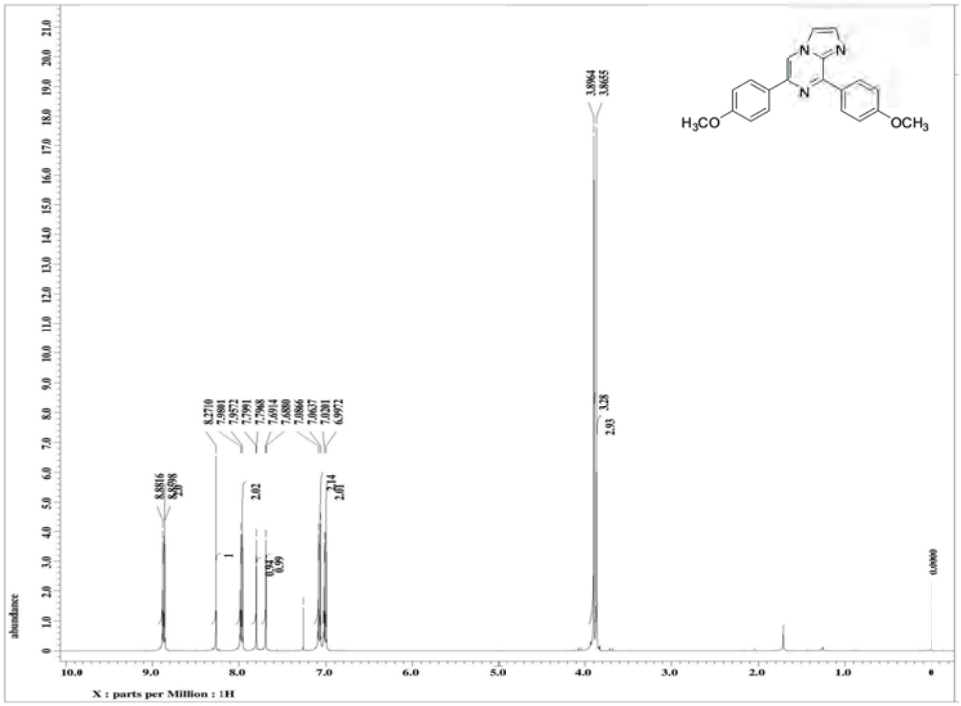



Fig. S29: $^{1}$H NMR Spectrum of 6,8-bis(4'-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(9b)**

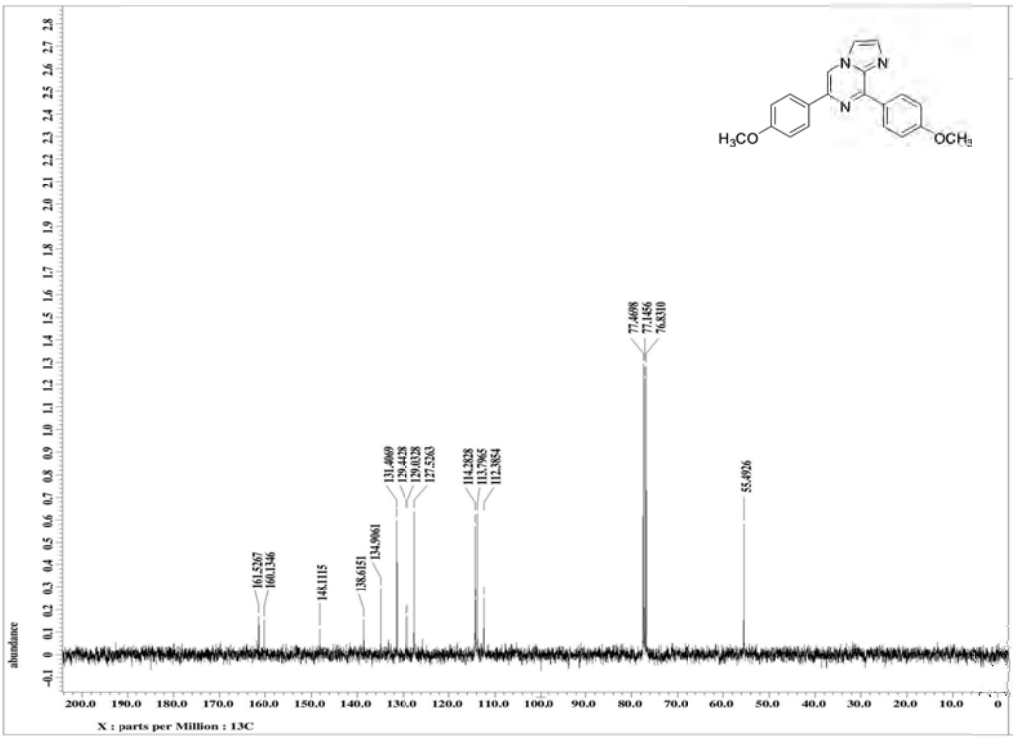



Fig. S30: $^{13}$C NMR Spectrum of 6,8-bis(4'-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(9b)**

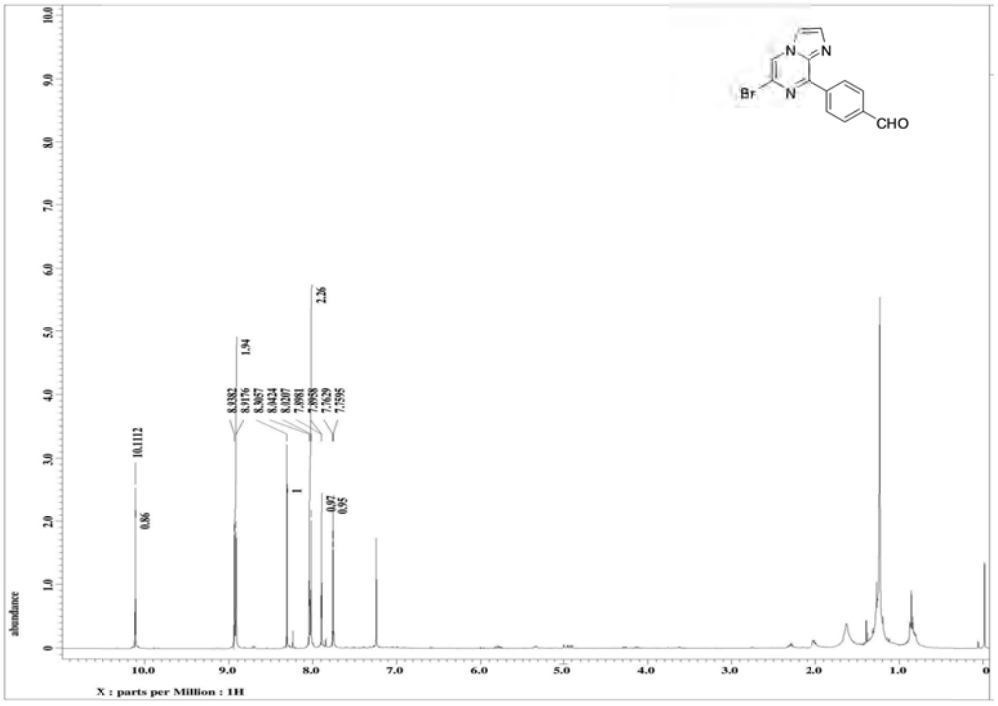



Fig. S31: $^{1}$H NMR Spectrum of 4’-(6-bromo-imidazo[1,2-*a*]pyrazin-8-yl)benzaldehyde **(10a)**

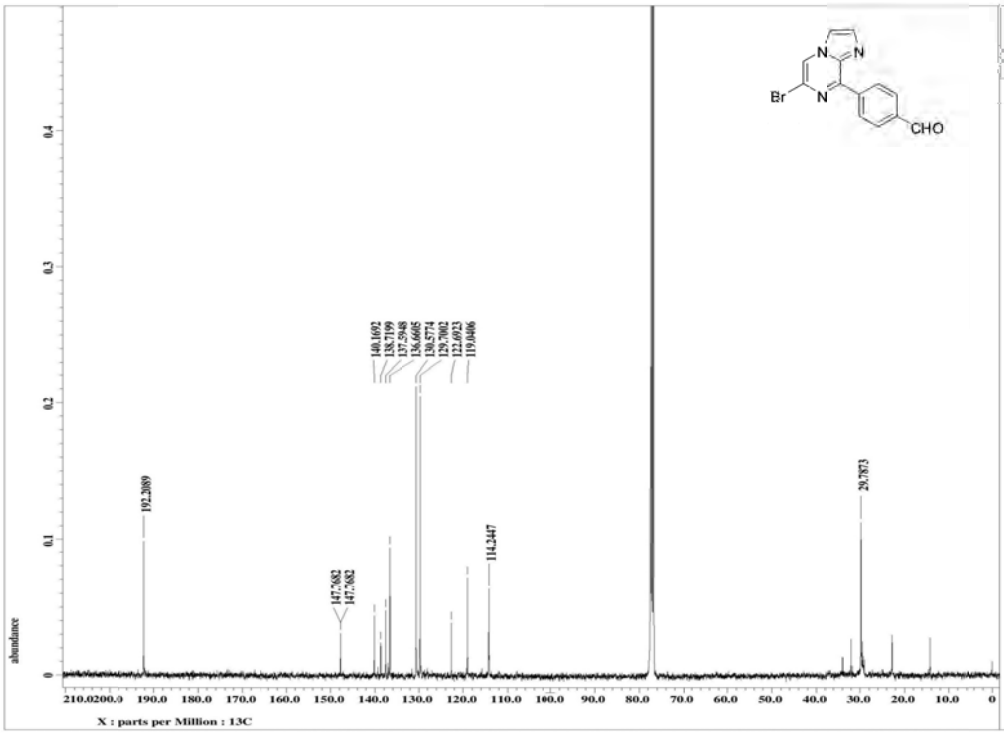



Fig. S32: $^{13}$C NMR Spectrum of 4’-(6-bromo-imidazo[1,2-*a*]pyrazin-8-yl)benzaldehyde **(10a)**

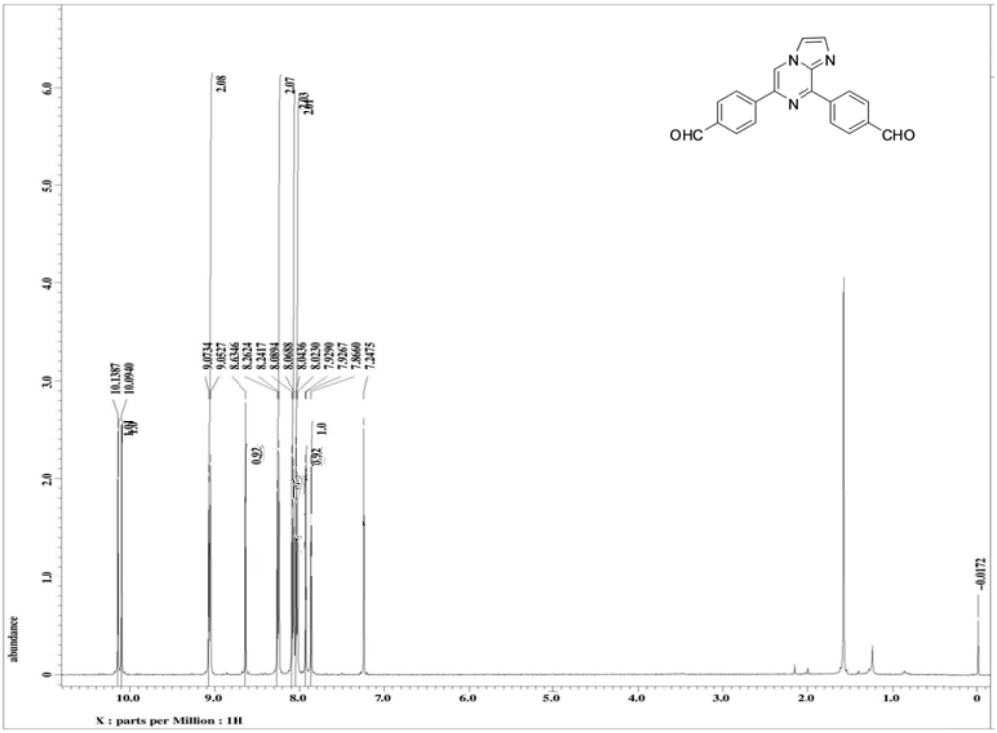



Fig. S33: $^{1}$H NMR Spectrum of 4',4"-imidazo[1,2-*a*]pyrazine-6,8-diyl)dibenzaldehyde **(10b)**

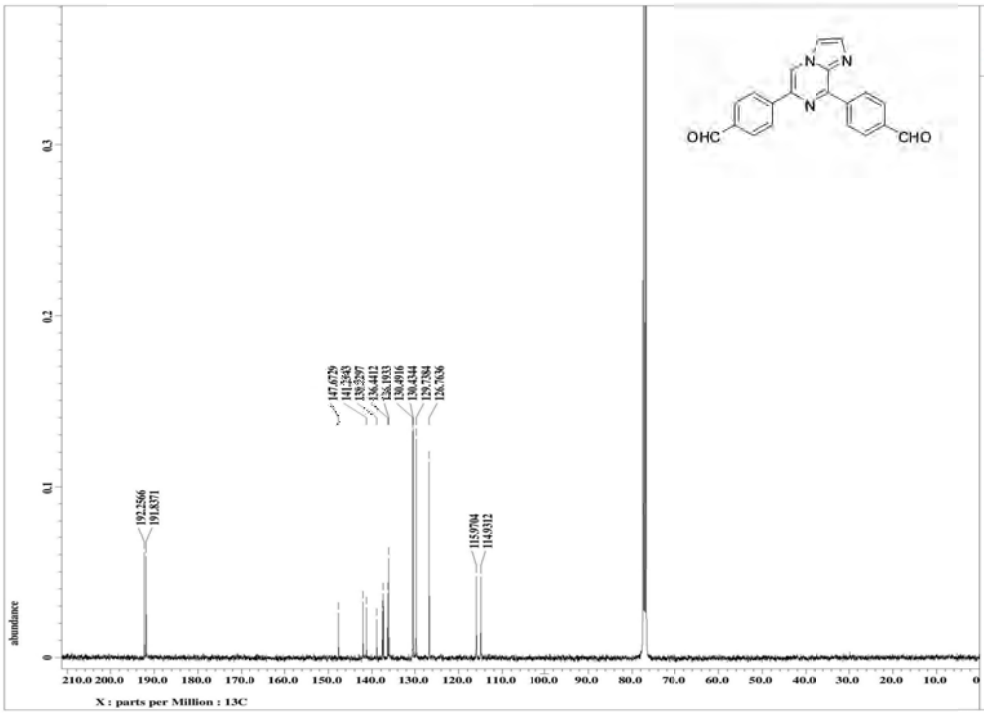



Fig. S34: $^{13}$C NMR Spectrum of 4',4"-imidazo[1,2-*a*]pyrazine-6,8-diyl)dibenzaldehyde **(10b)**

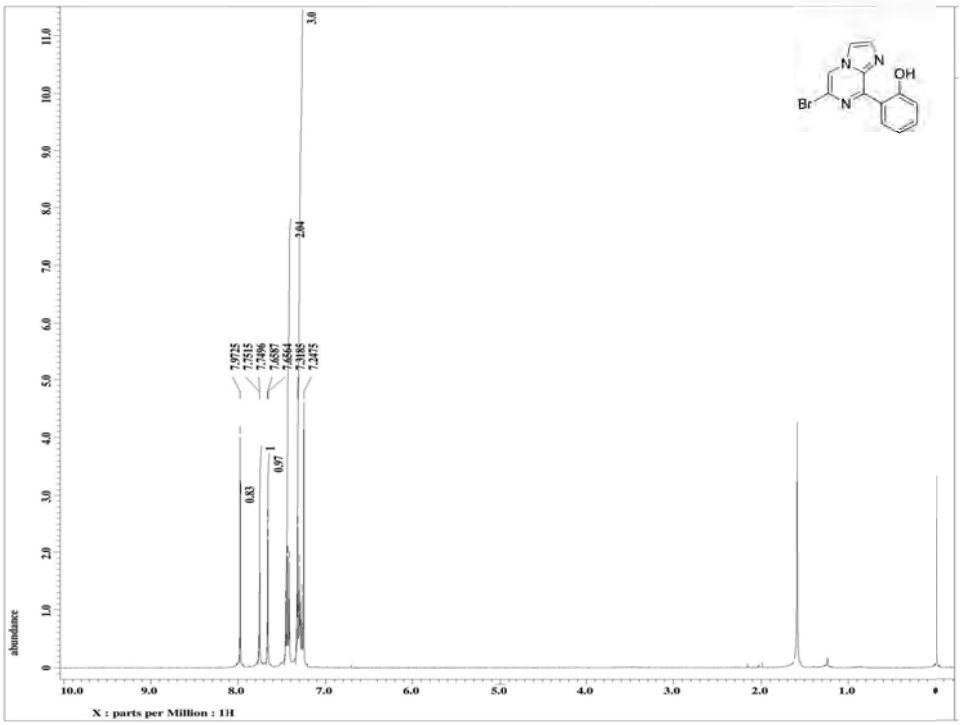



Fig. S35: $^{1}$H NMR Spectrum of 2'-(6-bromoimidazo[1,2-*a*]pyrazin-8-yl)phenol **(11a)**

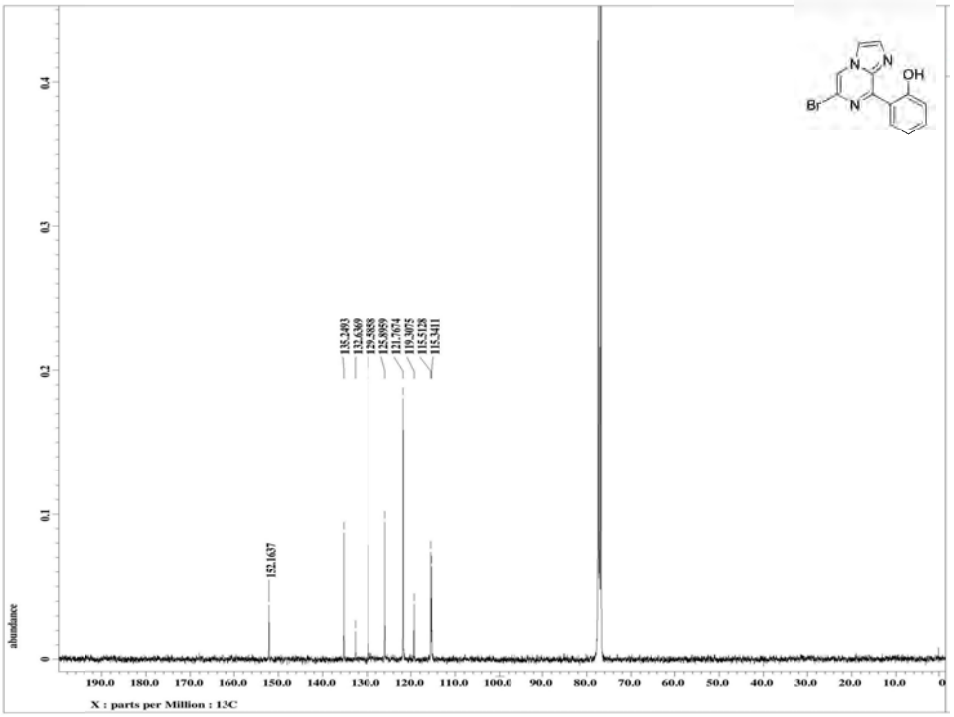



Fig. S36: $^{13}$C NMR Spectrum of 2'-(6-bromoimidazo[1,2-*a*]pyrazin-8-yl) phenol **(11a)**

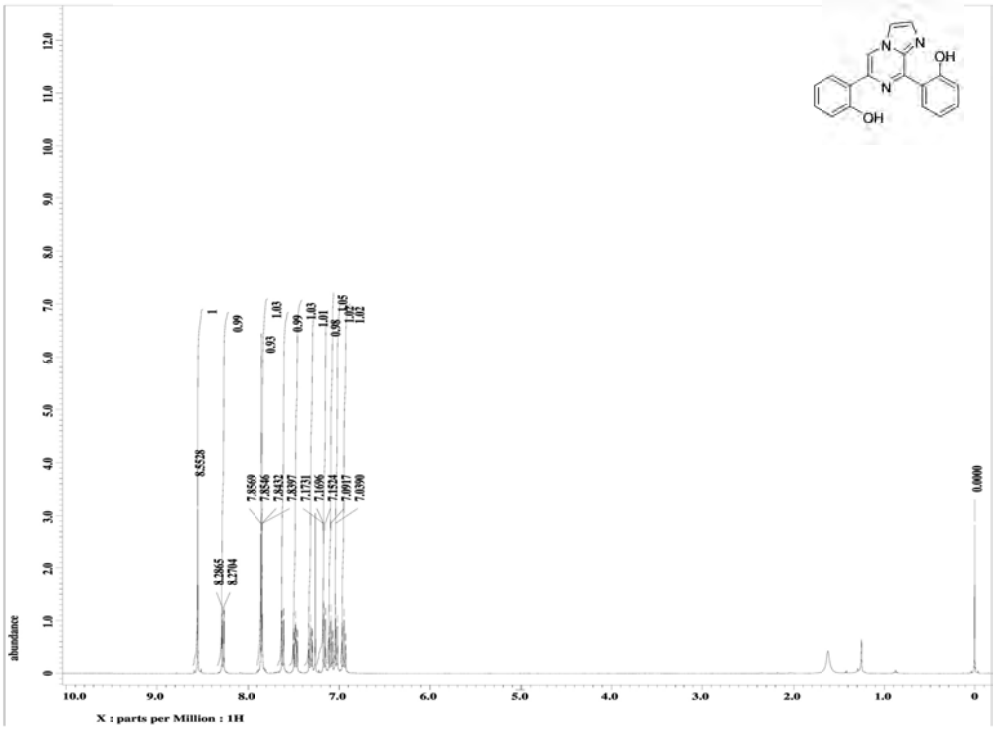



Fig. S37:[1]H NMR Spectrum of 2',2"-(imidazo[1,2-*a*]pyrazin-6,8-diyl)diphenol **(11b)**

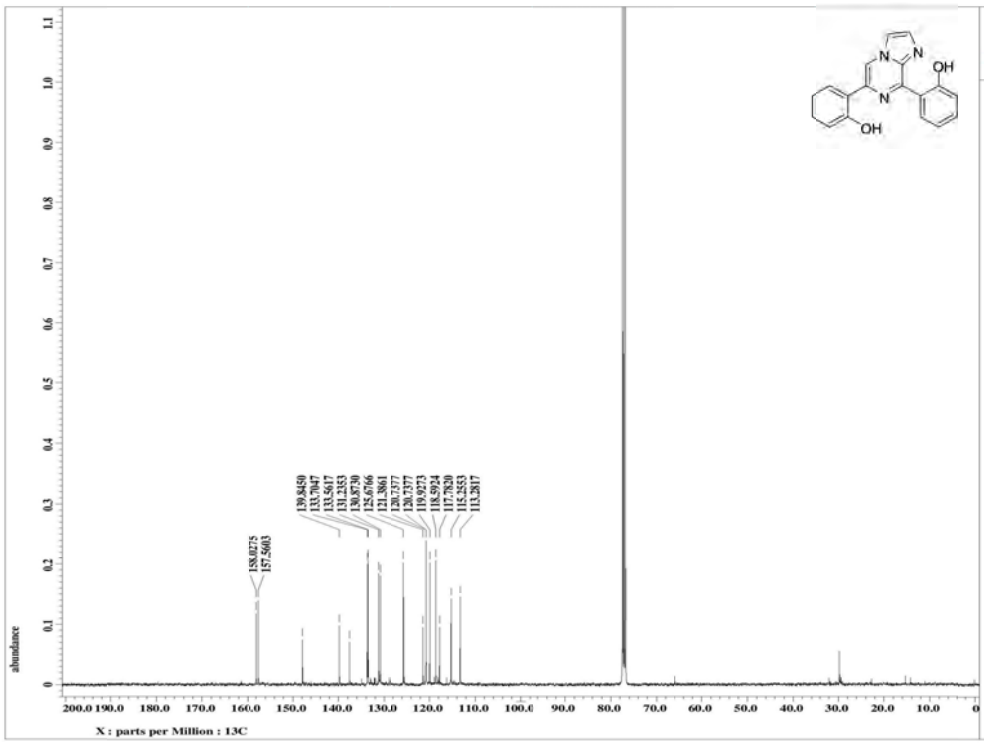



Fig. S38: [13]C NMR Spectrum of 2',2"-(imidazo[1,2-*a*]pyrazin-6,8-diyl)diphenol **(11b)**

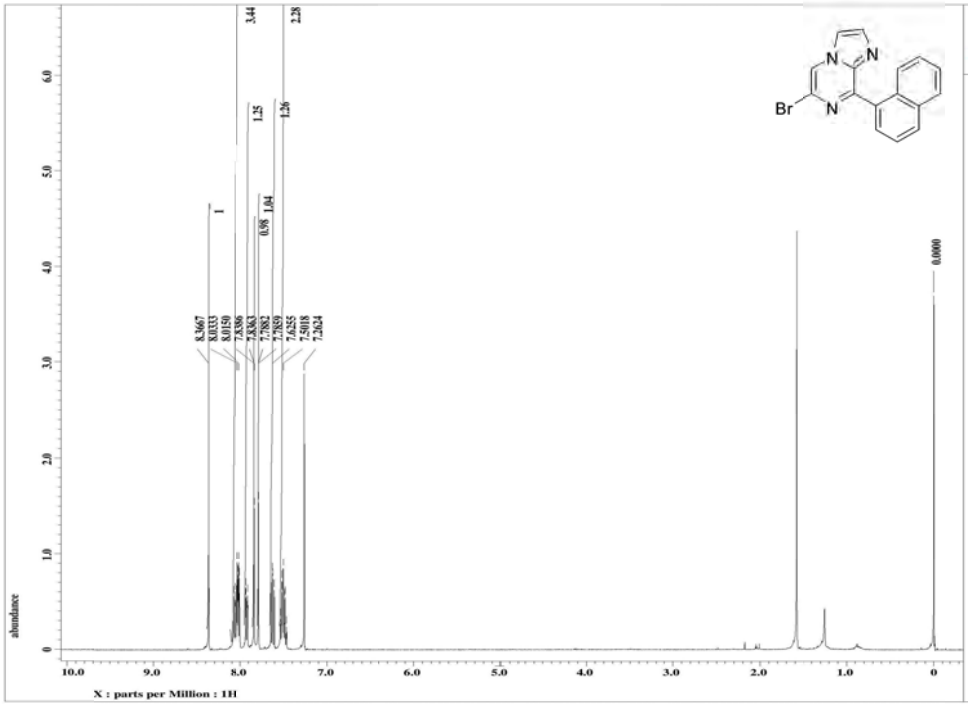



Fig. S39: $^{1}$H NMR Spectrum of 6-bromo-8-(napthalen-1'-yl)imidazo[1,2-*a*]pyrazine **(12a)**

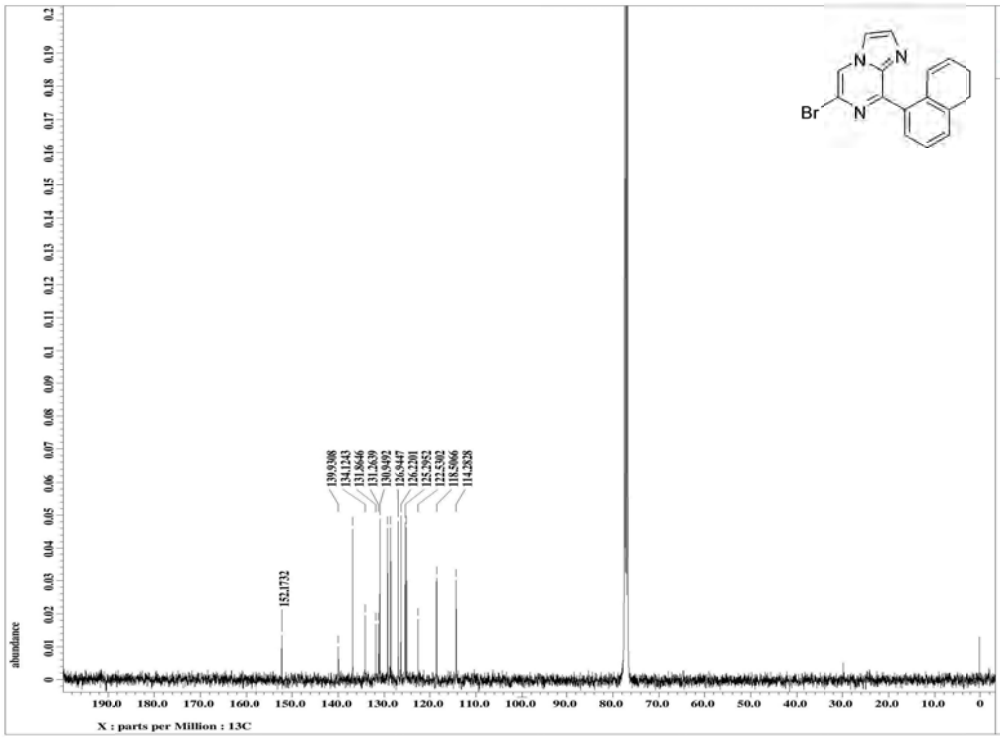



Fig. S40: $^{13}$C NMR Spectrum of 6-bromo-8-(napthalen-1'-yl)imidazo[1,2-*a*]pyrazine **(12a)**

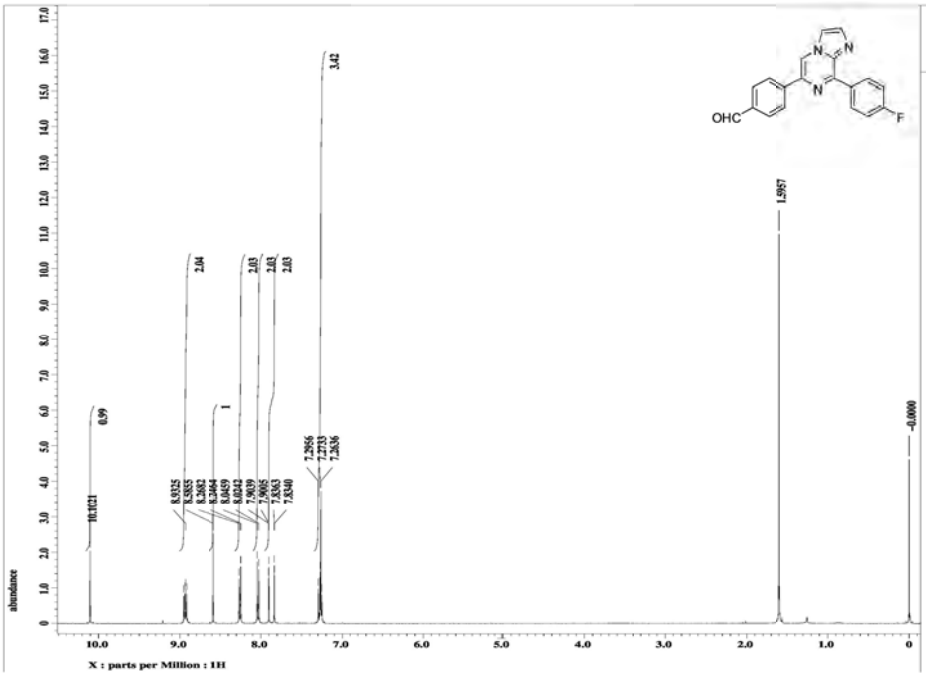



Fig. S41: $^{1}$H NMR spectrum of 4”-(8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde **(16)**

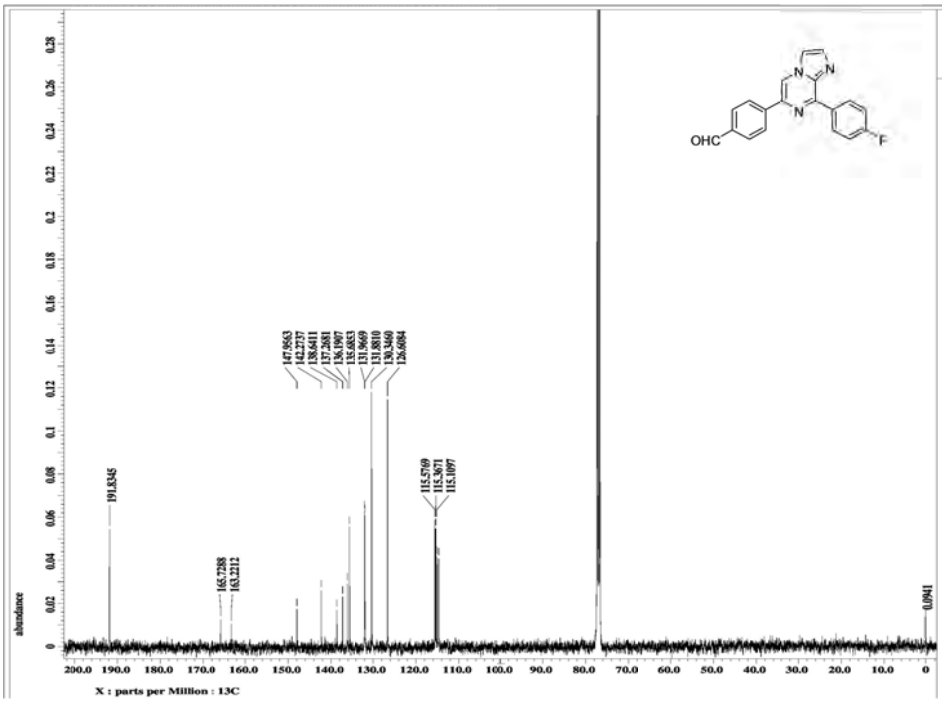



Fig. S42: $^{13}$C NMR spectrum of 4”-(8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde **(16)**

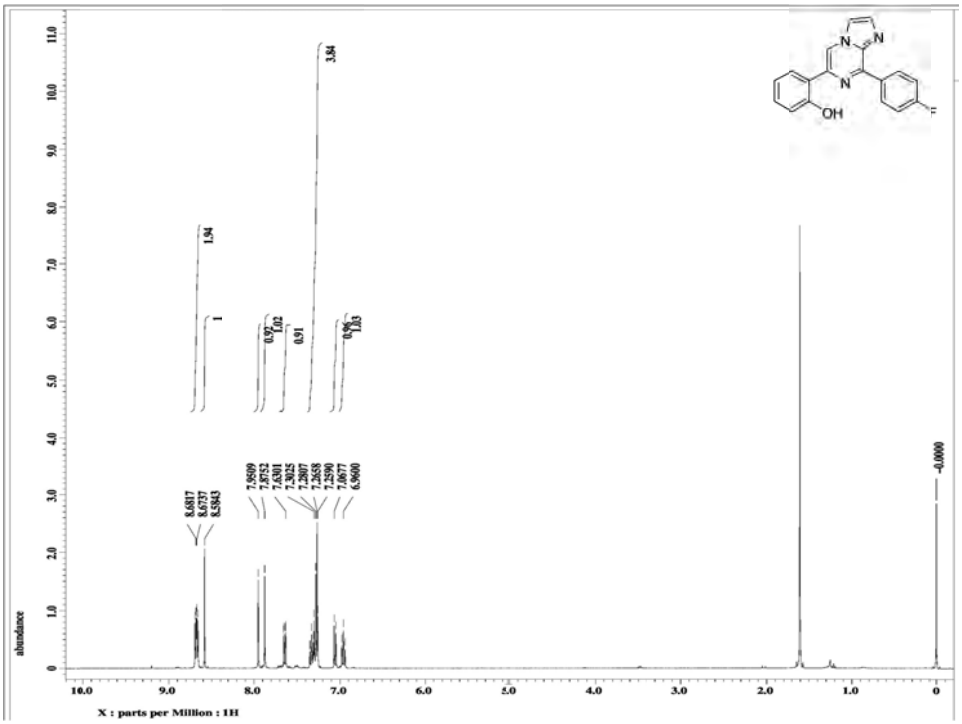



Fig. S43: [1] H NMR spectrum of 2”-(8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol **(17)**

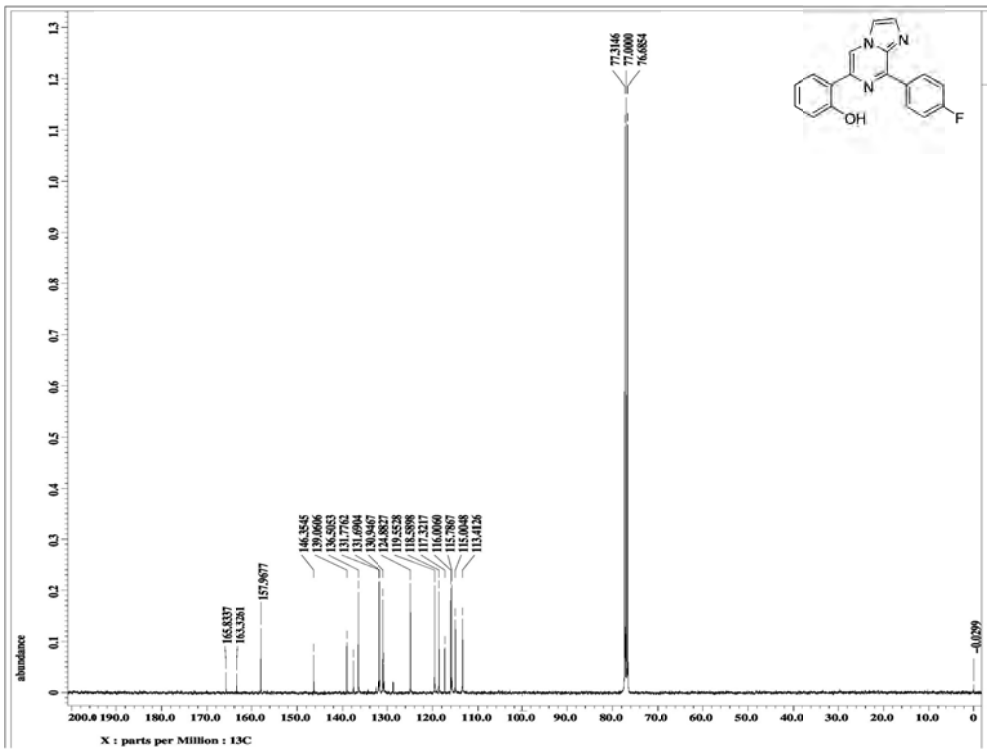



Fig. S44: [13]C NMR spectrum of 2”-(8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol **(17)**

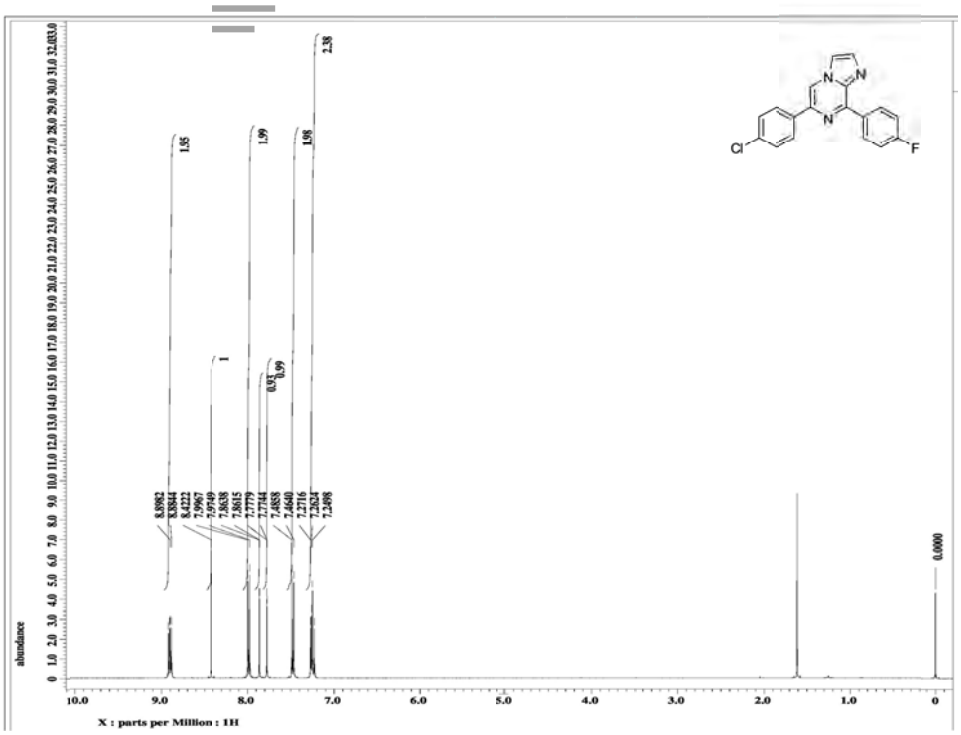



Fig. S45: $^{1}$H NMR spectrum of 6-(4”-chlorophenyl)-8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazine **(18)**

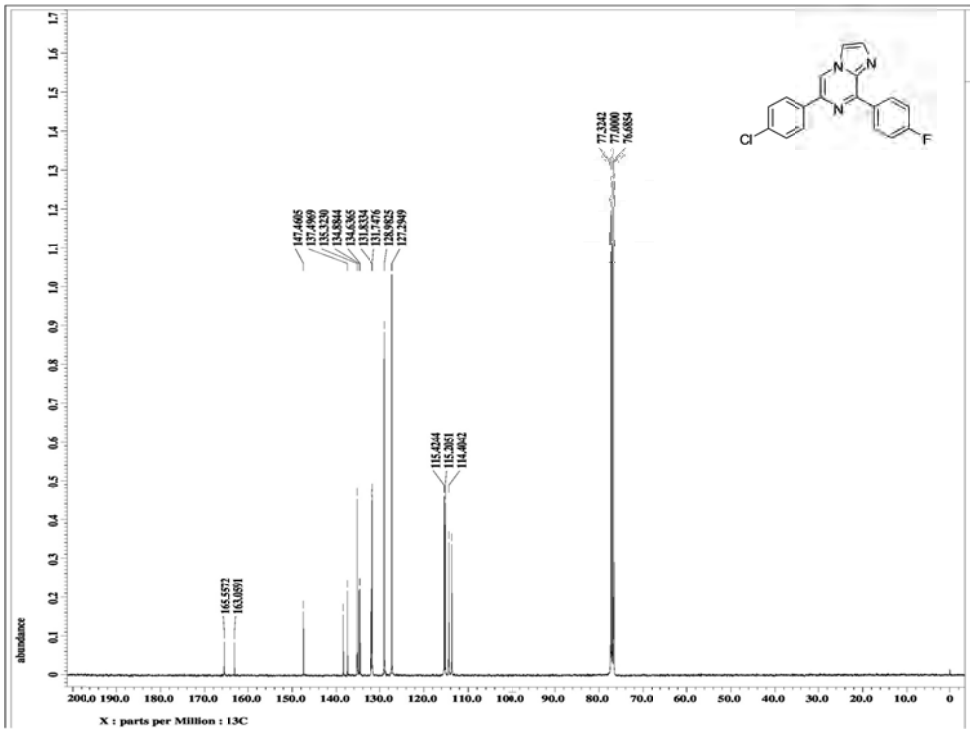



Fig. S46: $^{13}$C NMR spectrum of 6-(4”-chlorophenyl)-8-(4’-fluorophenyl)imidazo[1,2-*a*]pyrazine **(18)**

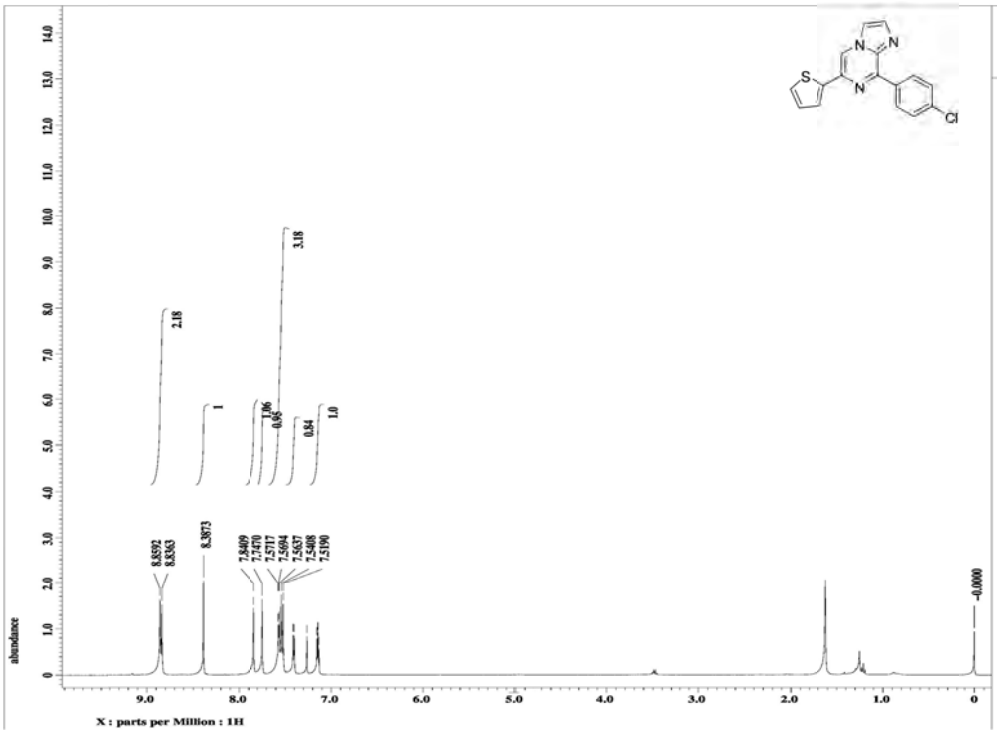



Fig. S47: [1]H NMR Spectrum of 8-(4'-chlorophenyl)-6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazine **(19)**

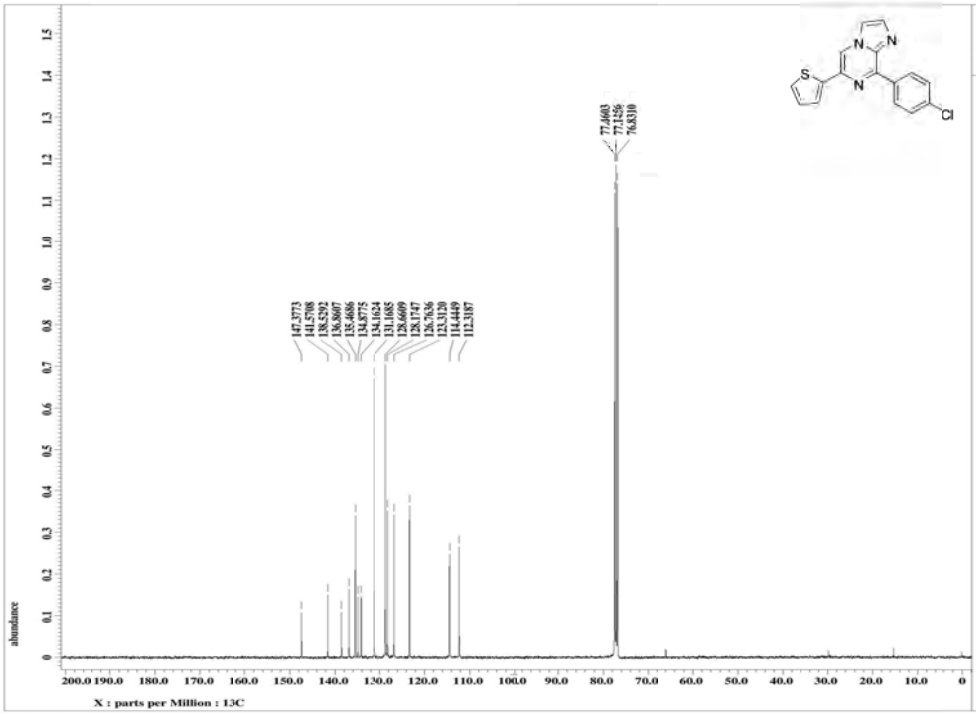



Fig. S48: [13]C NMR Spectrum of 8-(4'-chlorophenyl)-6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazine **(19)**

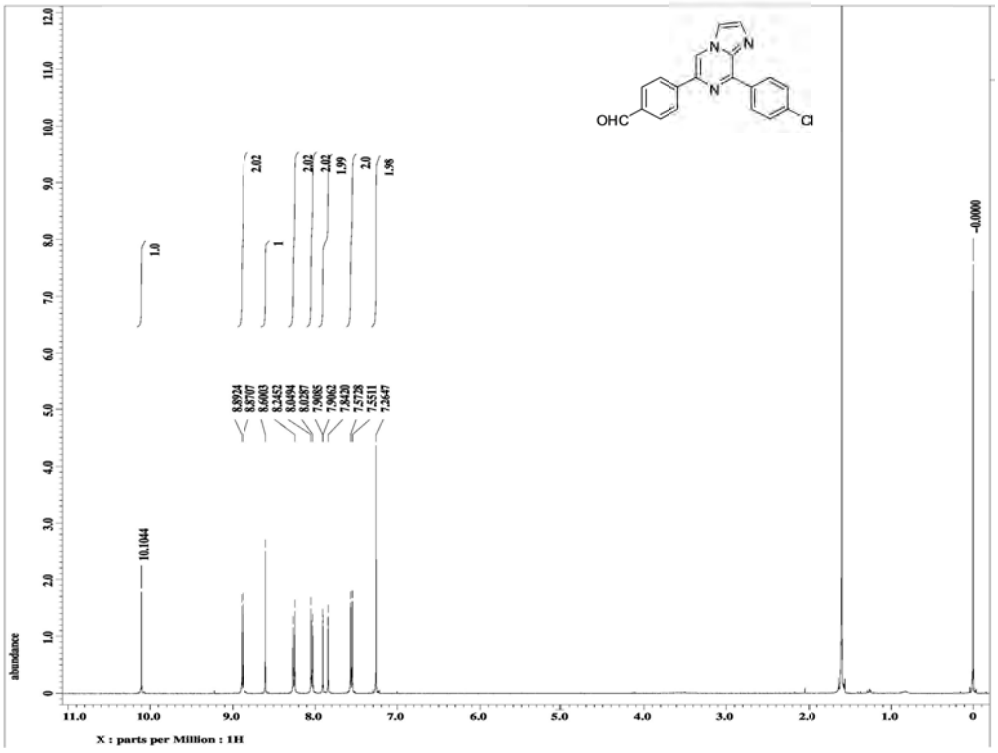



Fig. S49: $^{1}$H NMR Spectrum of 4”-(8-(4’-chlorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde **(20)**

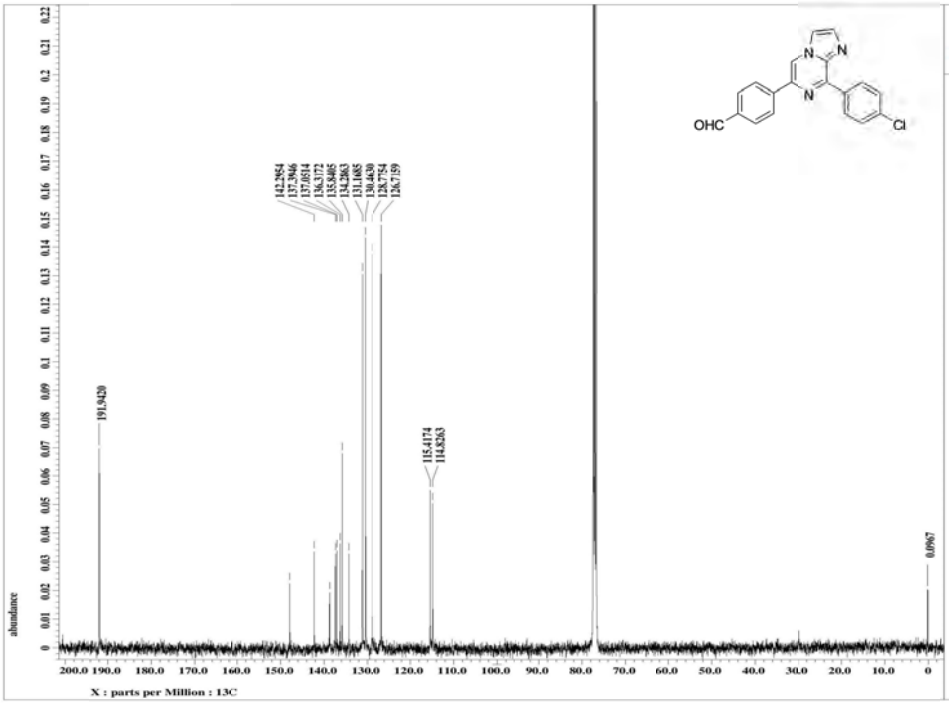



Fig. S50: $^{13}$C NMR Spectrum of 4”-(8-(4’-chlorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde **(20)**

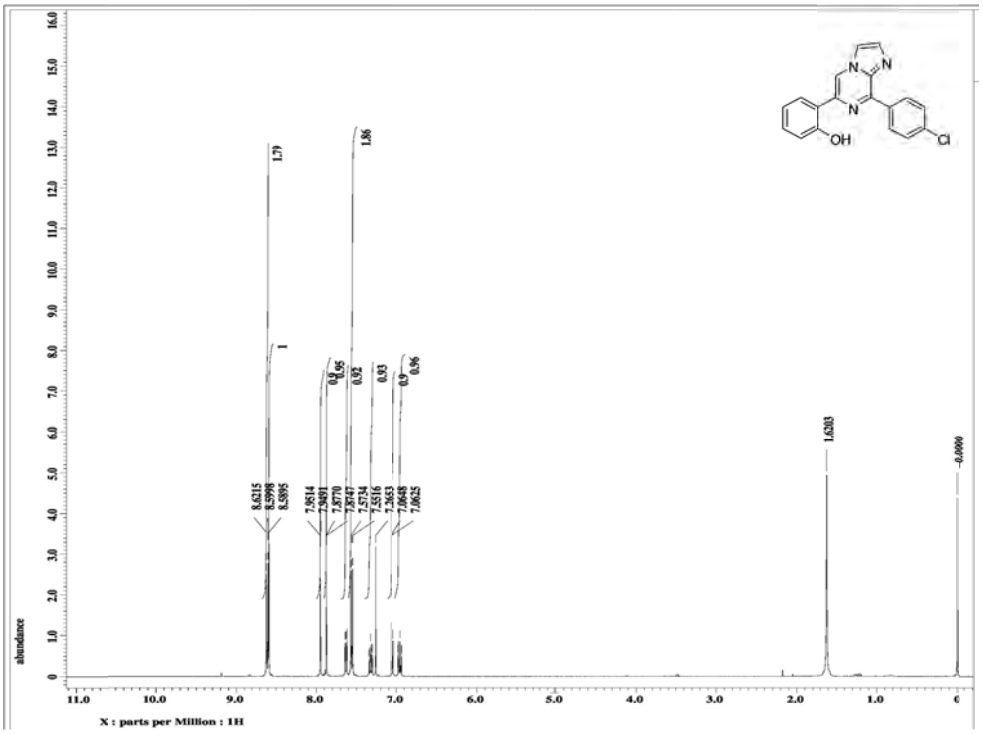



Fig. S51: $^{1}$H NMR spectrum of 2”-(8-(4’-chlorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol **(21)**

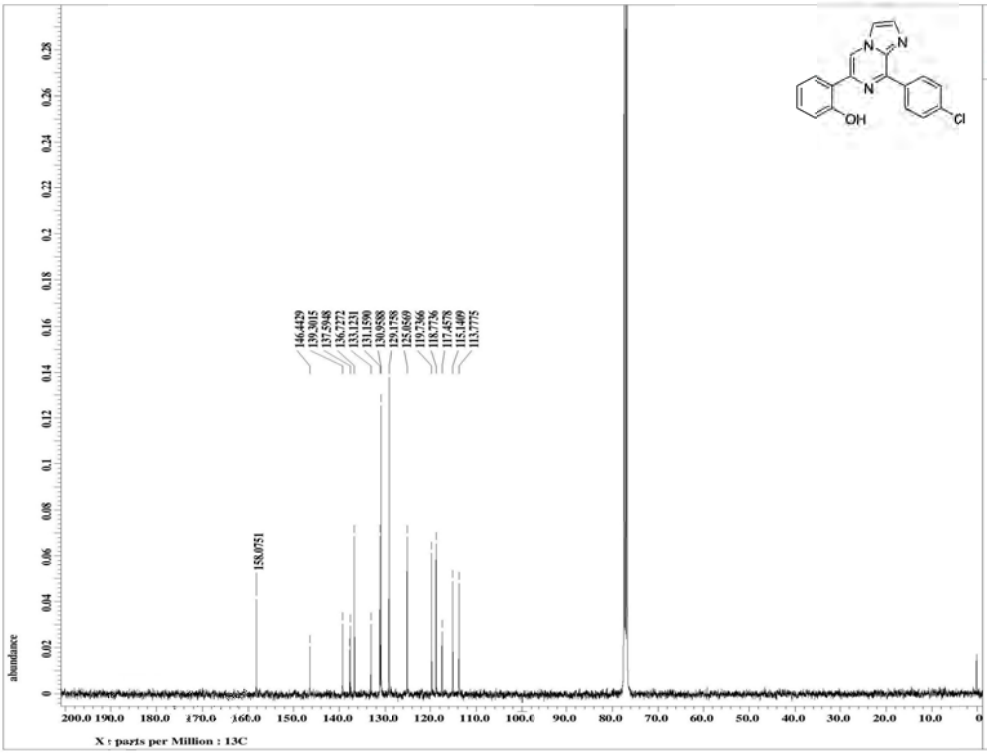



Fig. S52: $^{13}$C NMR spectrum of 2”-(8-(4’-chlorophenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol **(21)**

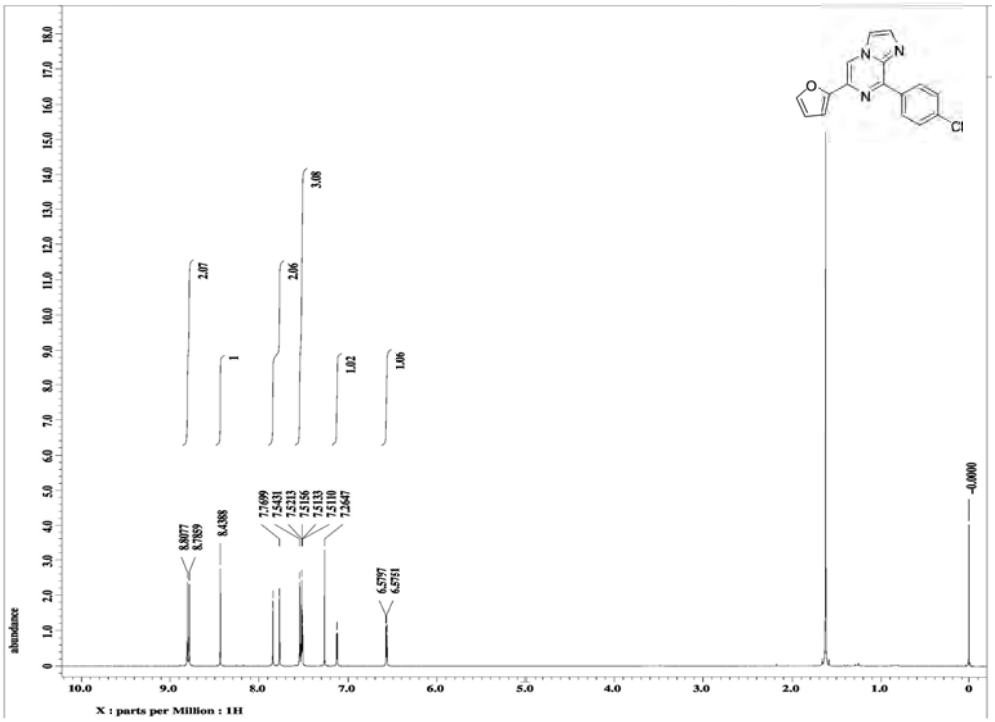



Fig. S53: $^{1}$H NMR spectrum of 8-(4'-chlorophenyl)-6-(furan-2"-yl)imidazo[1,2-*a*]pyrazine **(22)**

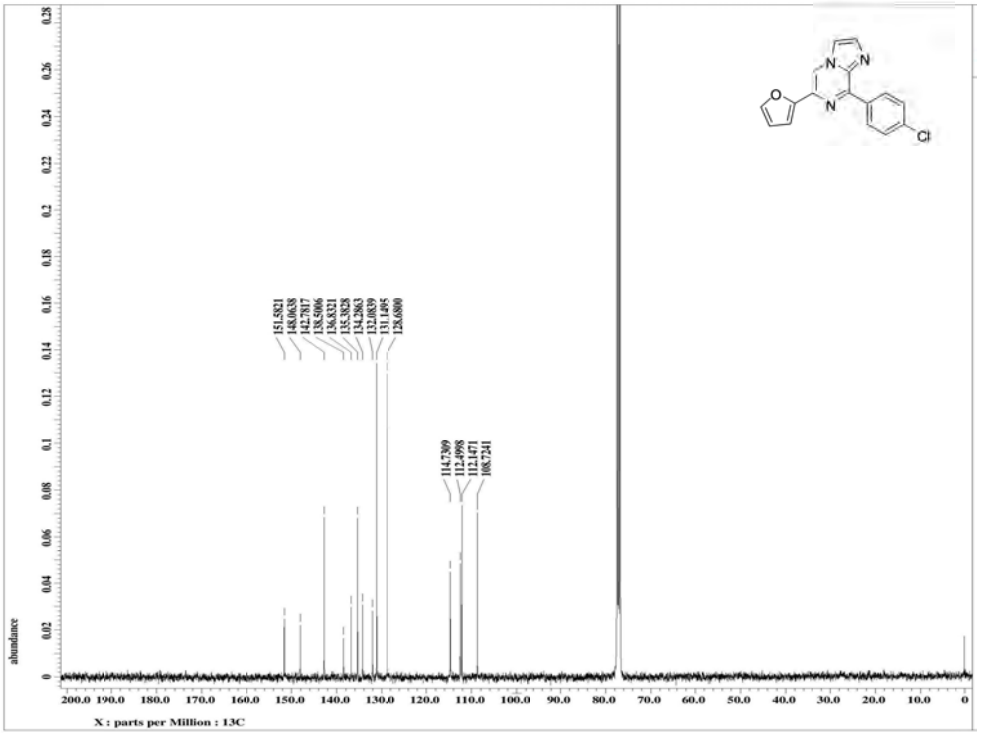



Fig. S54: $^{13}$C NMR spectrum of 8-(4'-chlorophenyl)-6-(furan-2"-yl)imidazo[1,2-*a*]pyrazine **(22)**

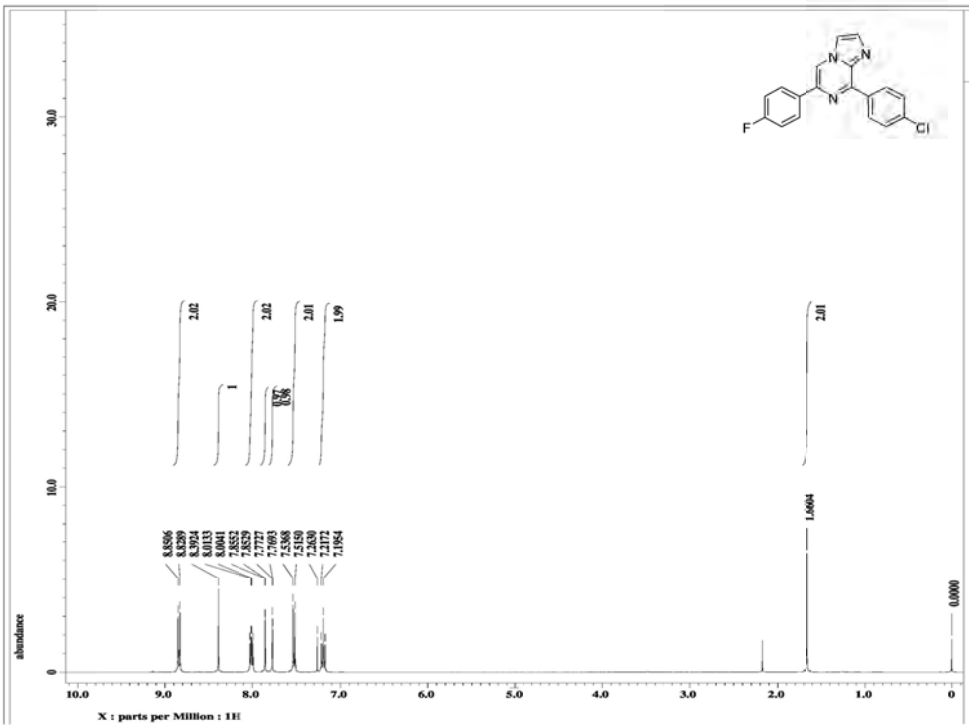



Fig. S55: $^{1}$H NMR spectrum 8-(4'-chlorophenyl)-6-(4"-fluorophenyl)imidazo[1,2-*a*]pyrazine **(23)**

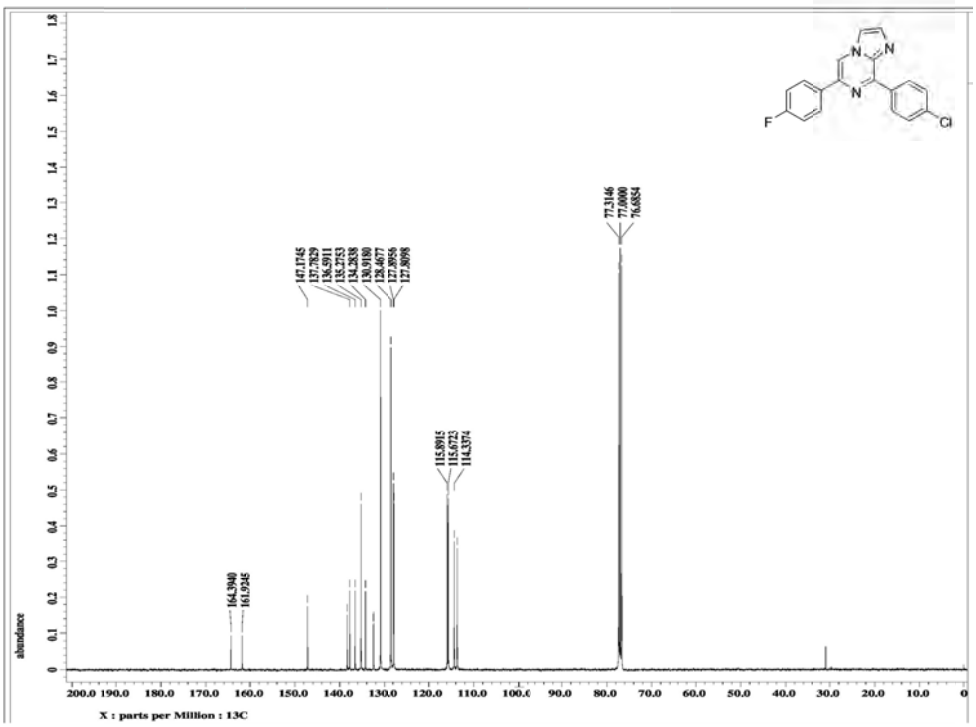



Fig. S56: $^{13}$C NMR spectrum of 8-(4'-chlorophenyl)-6-(4"-fluorophenyl)imidazo[1,2-*a*]pyrazine **(23)**

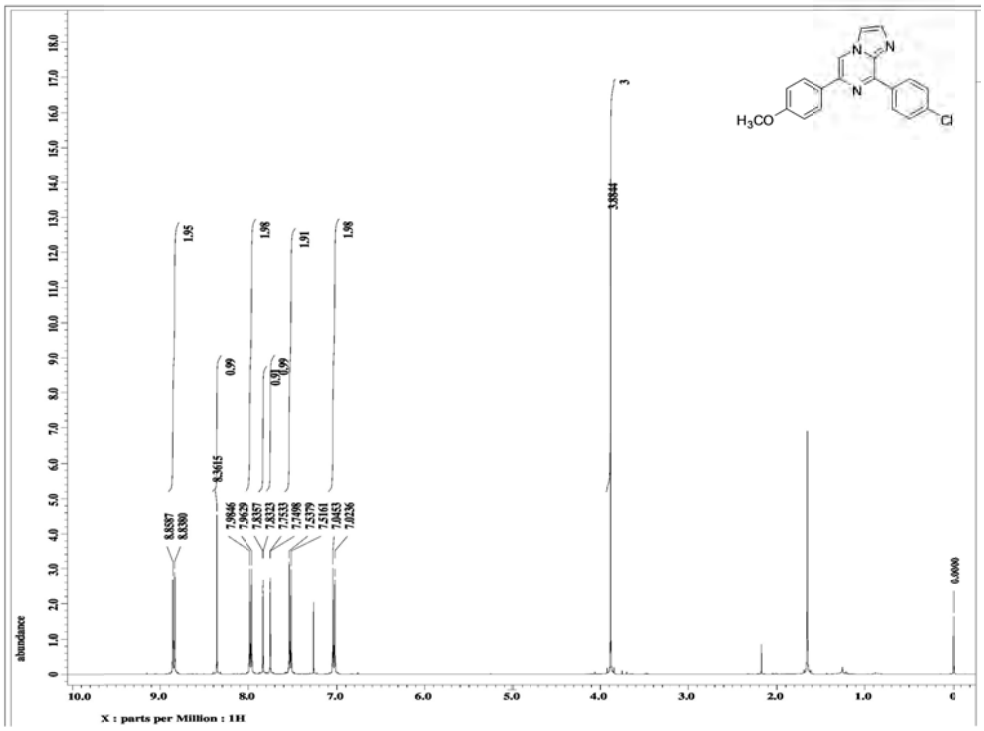



Fig. S57: $^{1}$H NMR spectrum of 8-(4'-chlorophenyl)-6-(4"-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(24)**

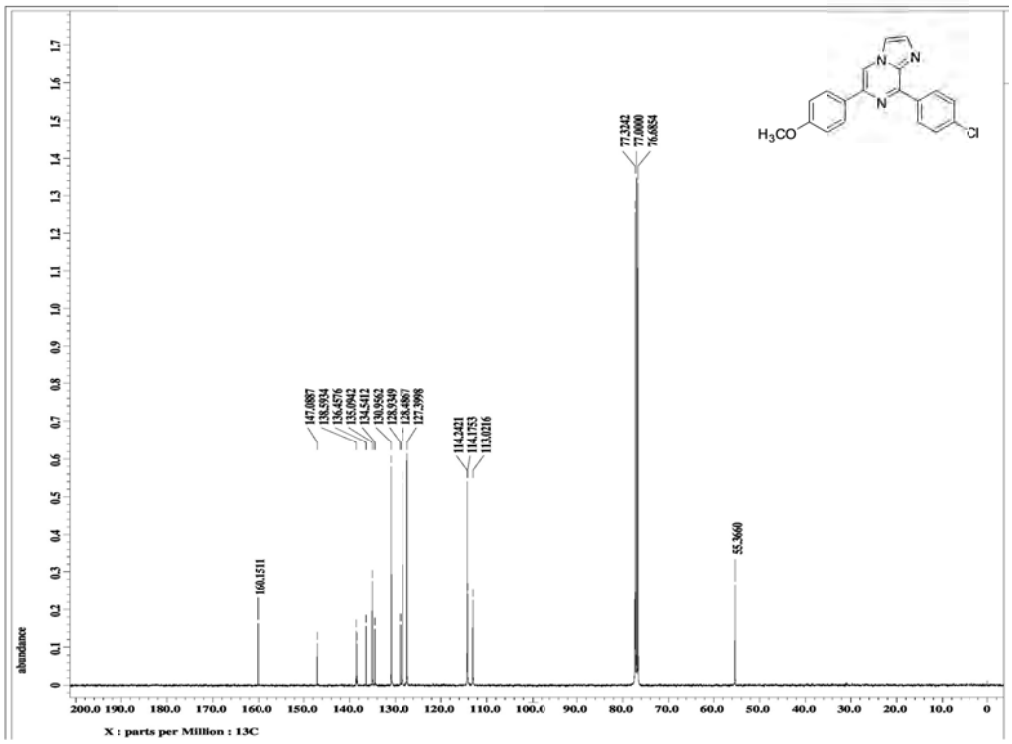



Fig. S58: $^{13}$C NMR spectrum of 8-(4'-chlorophenyl)-6-(4"-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(24)**

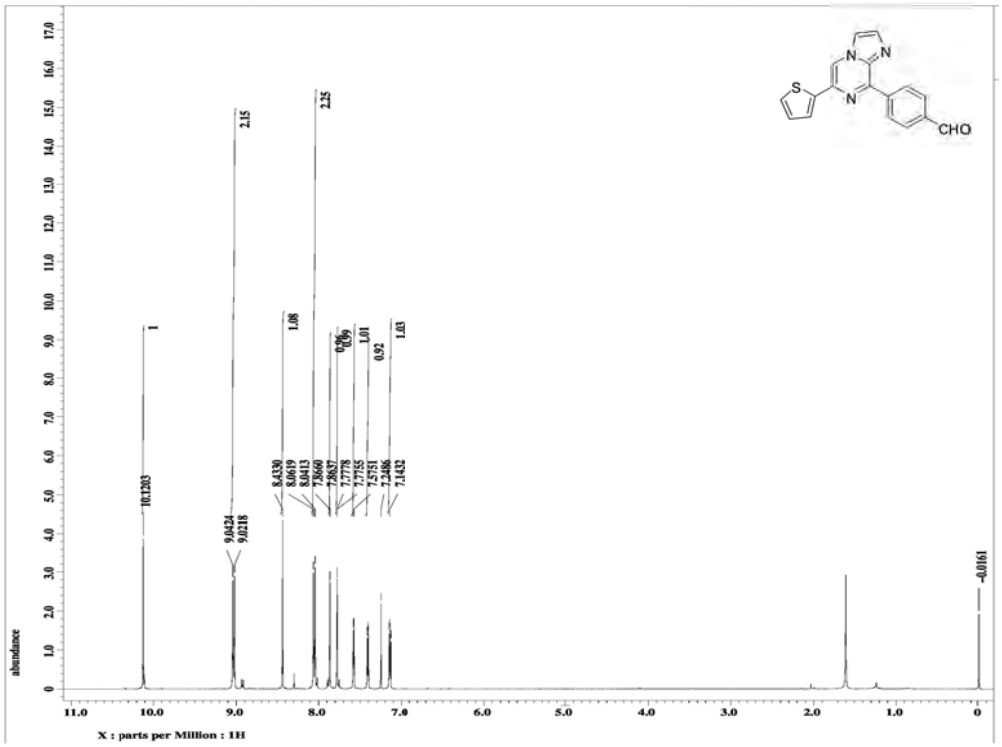



Fig. S59: $^{1}$H NMR Spectrum of 4'-(6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazin-8-yl)benzalehyde **(25)**

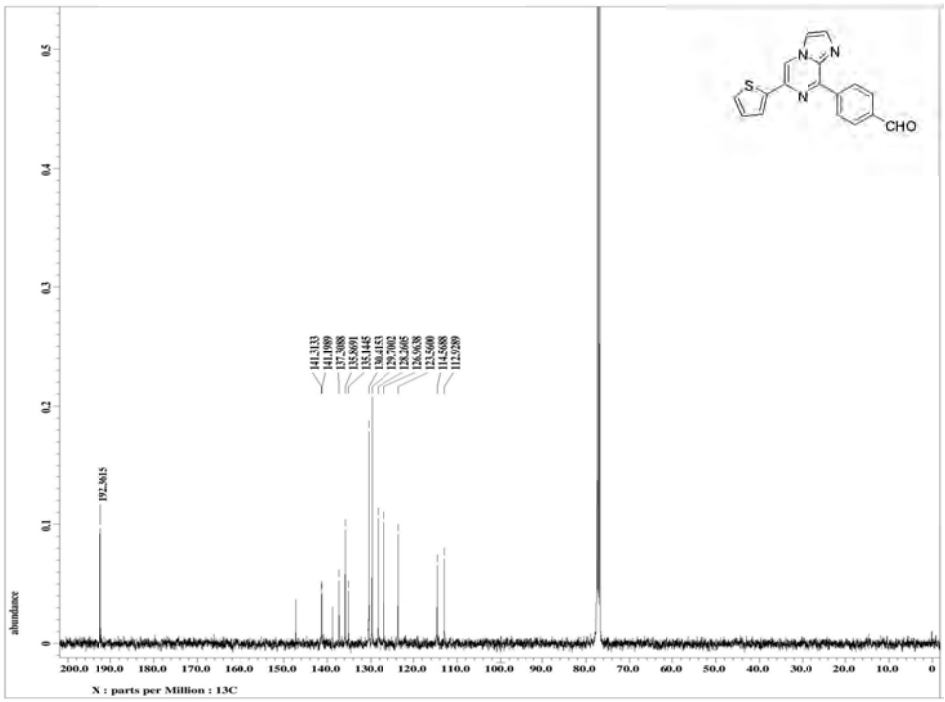



Fig. S60: $^{13}$C NMR Spectrum of 4'-(6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazin-8-yl)benzalehyde **(25)**

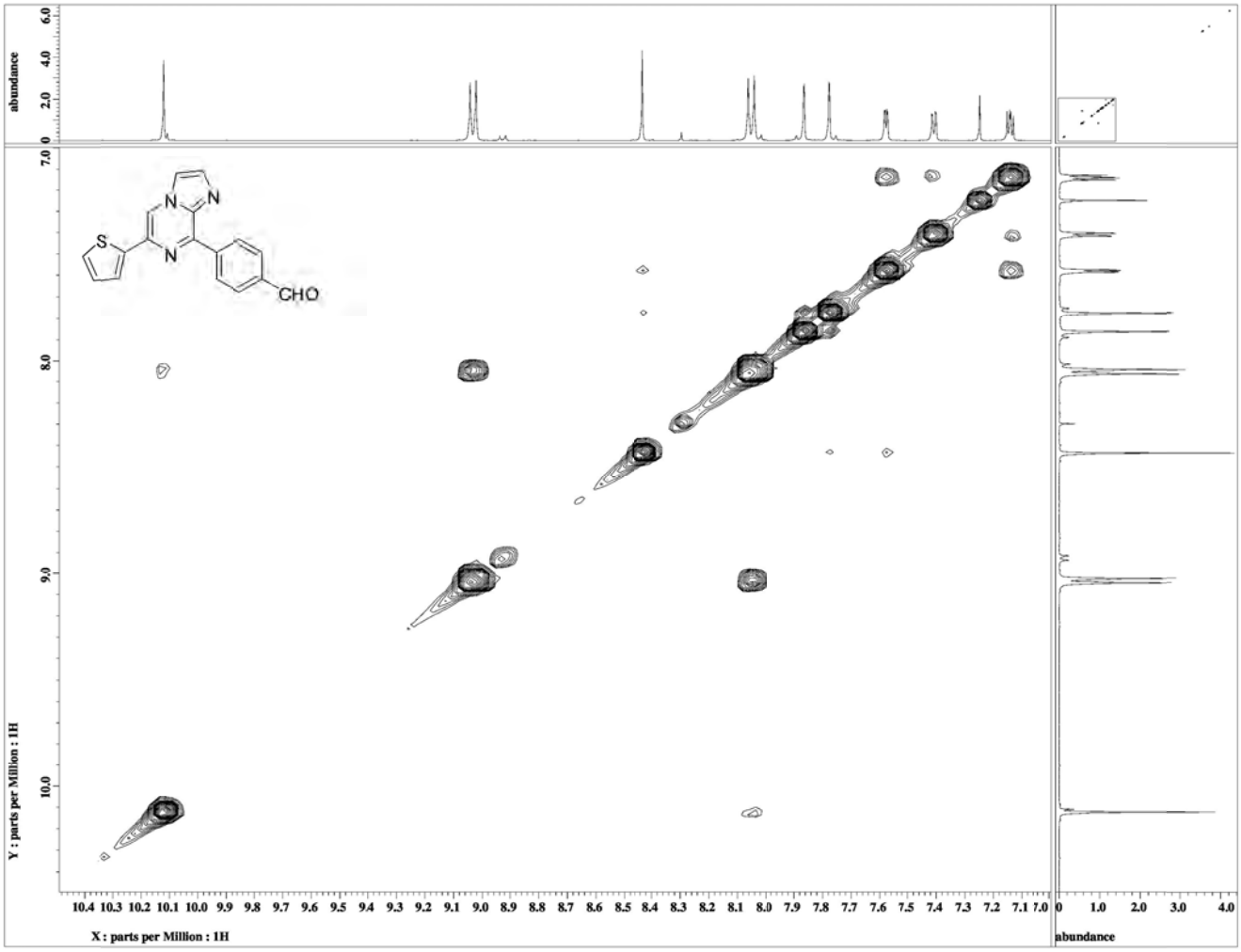



Fig. S61: NOESY Spectrum of 4'-(6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazin-8-yl)benzalehyde **(25)**

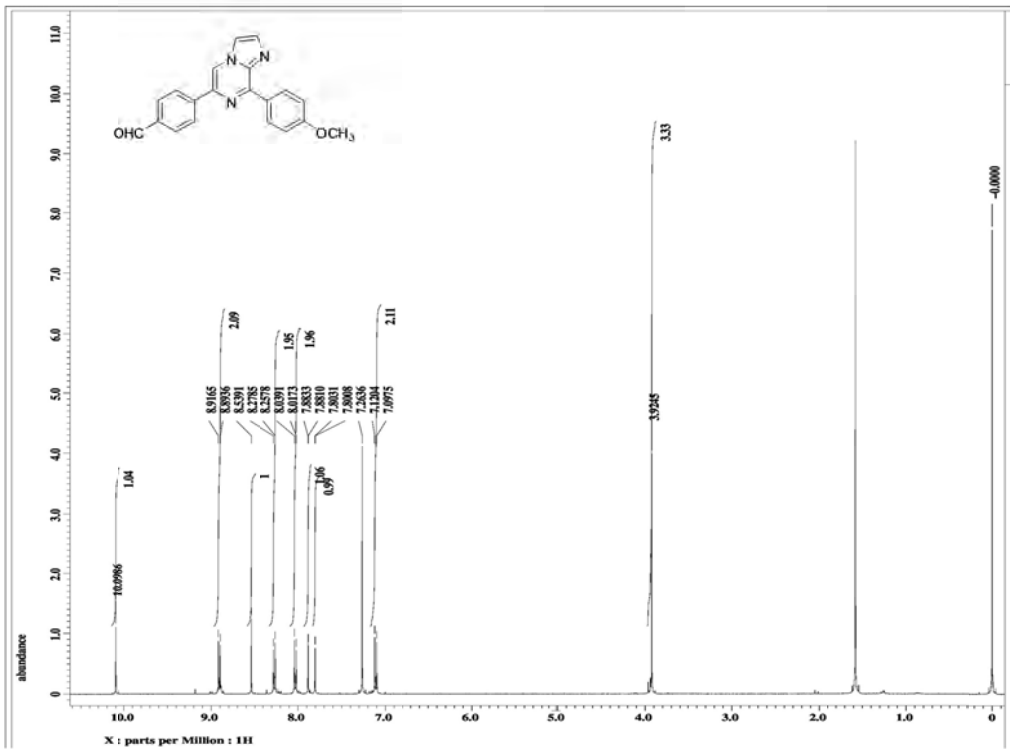



Fig. S62: $^{1}$H NMR spectrum of 4”-(8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde **(26)**

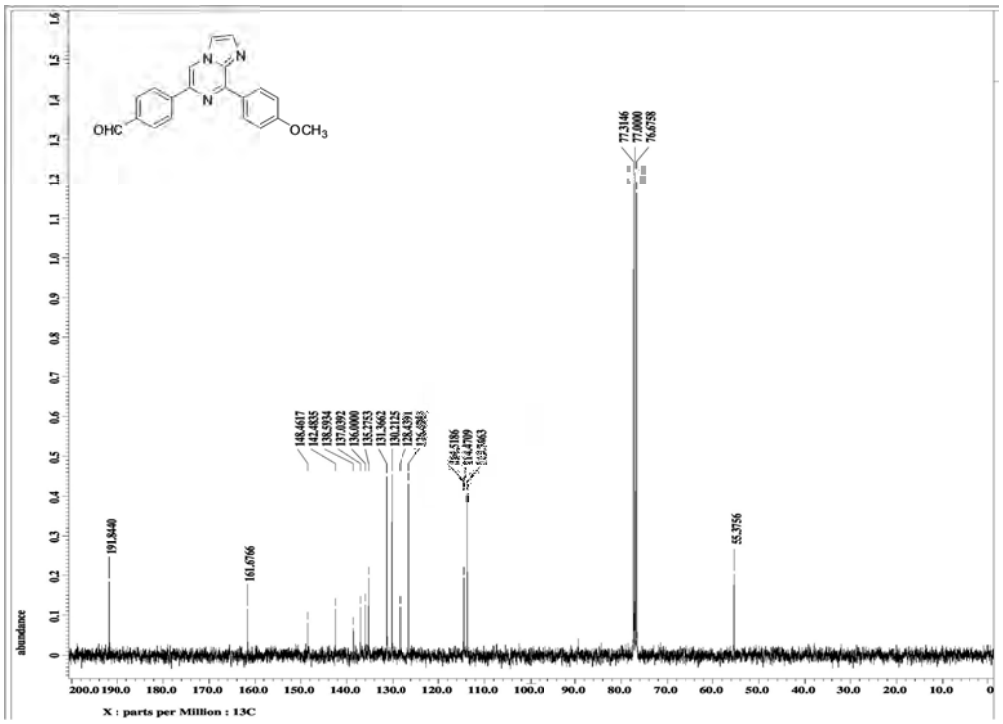



Fig. S63: $^{13}$C NMR spectrum of 4”-(8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde **(26)**

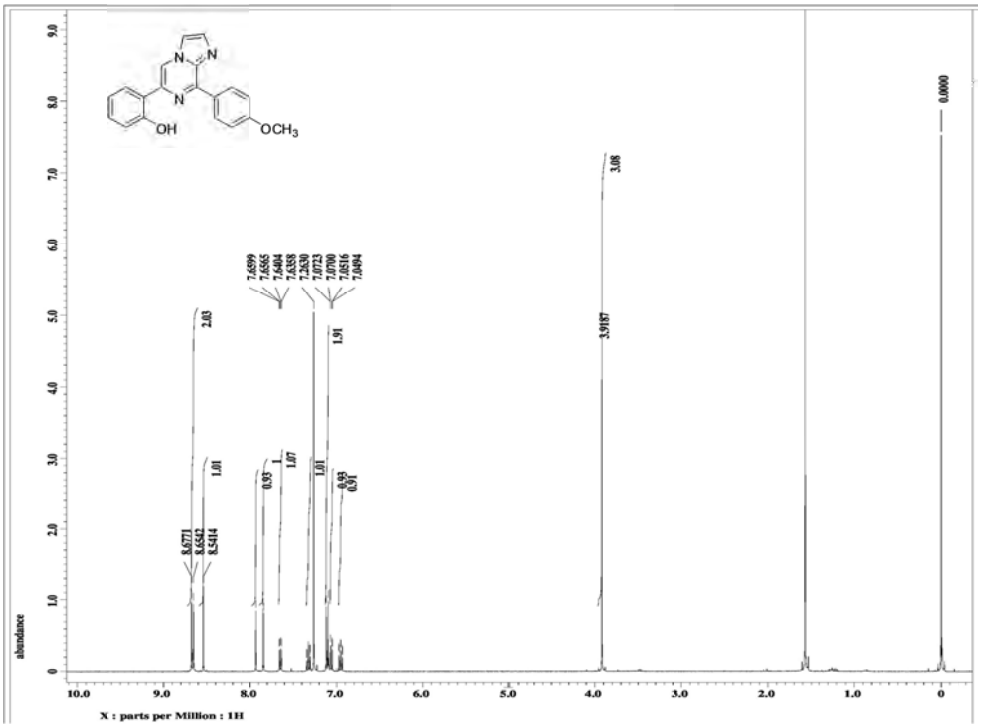



Fig. S64: $^{1}$H NMR spectrum of 2”-(8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol **(27)**

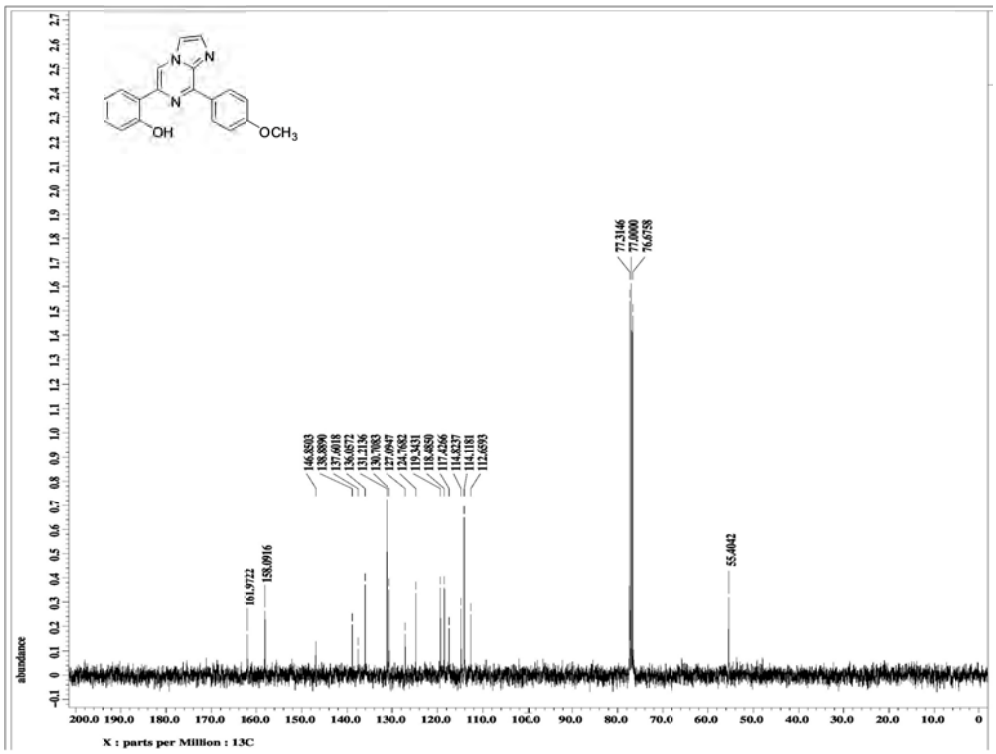



Fig. S65: $^{13}$C NMR spectrum of 2”-(8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazin-6-yl)phenol **(27)**

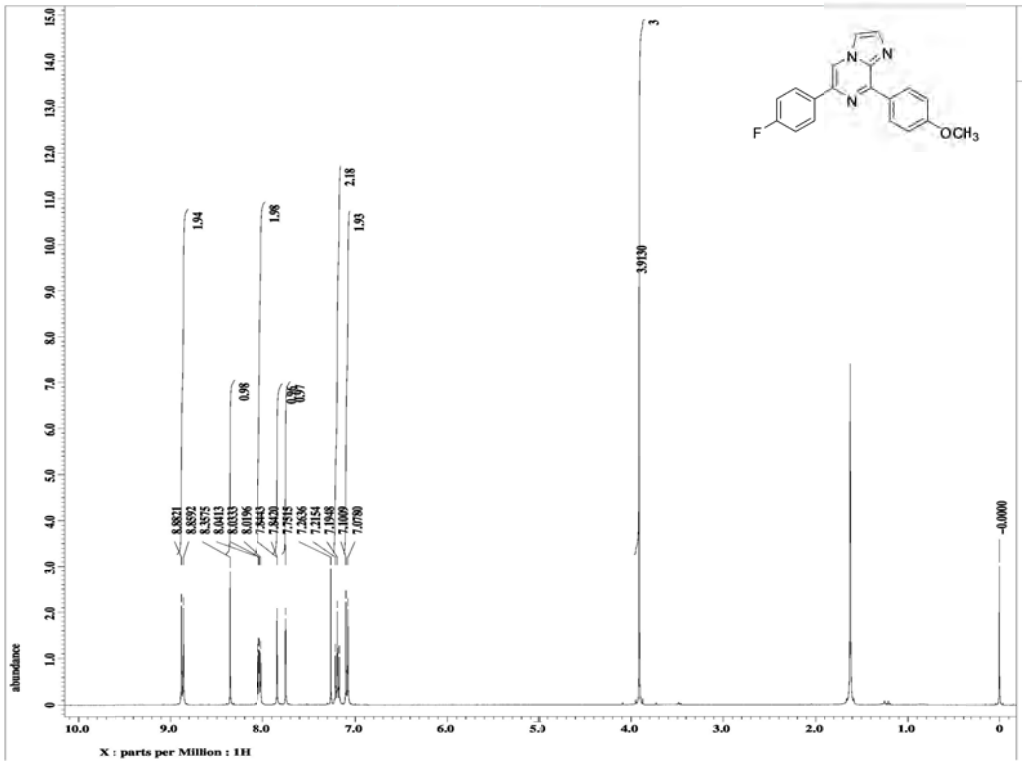



Fig. S66: $^{1}$H NMR spectrum of 6-(4”-fluorophenyl)-8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(28)**

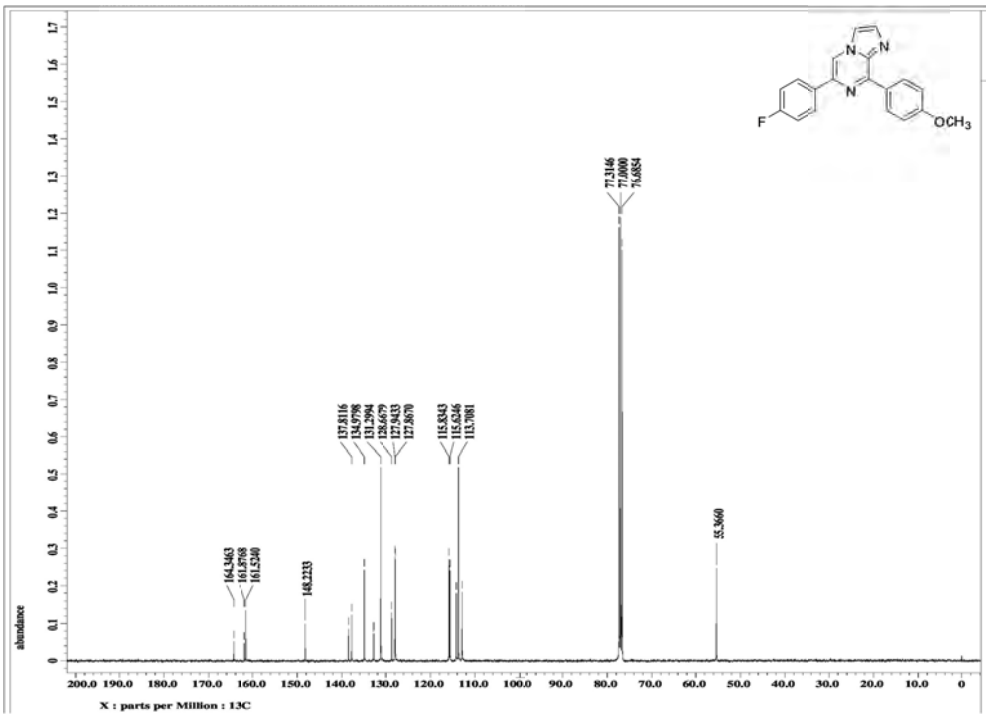



Fig. S67: $^{13}$C NMR spectrum of 6-(4”-fluorophenyl)-8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(28)**

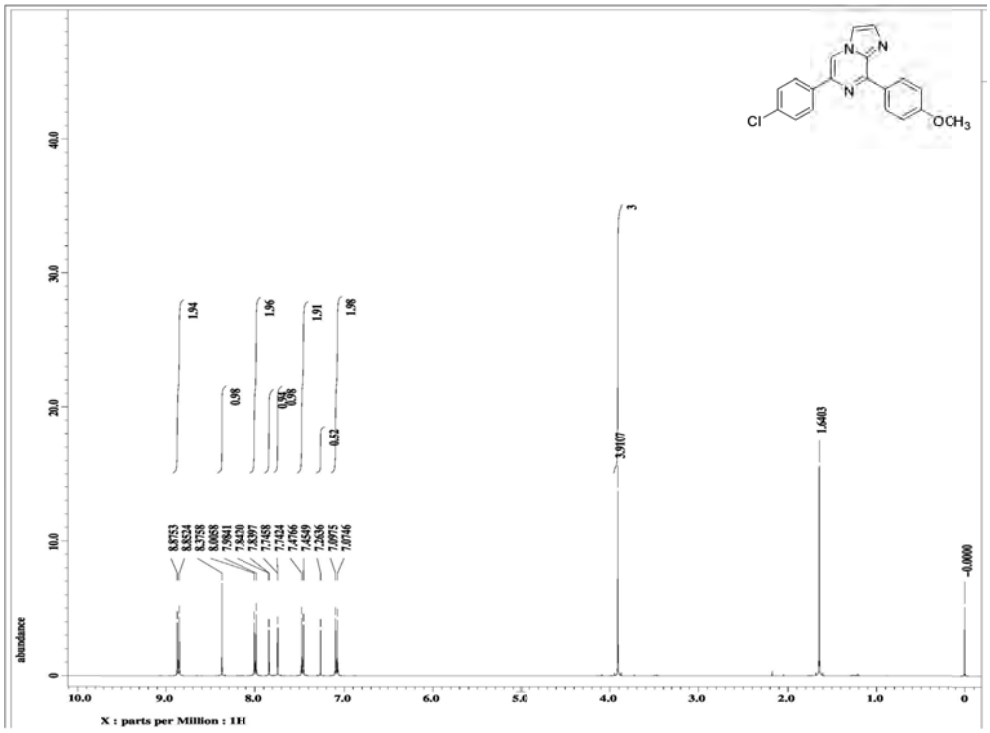



Fig. S68: $^{1}$H NMR spectrum of 6-(4”-chlorophenyl)-8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(29)**

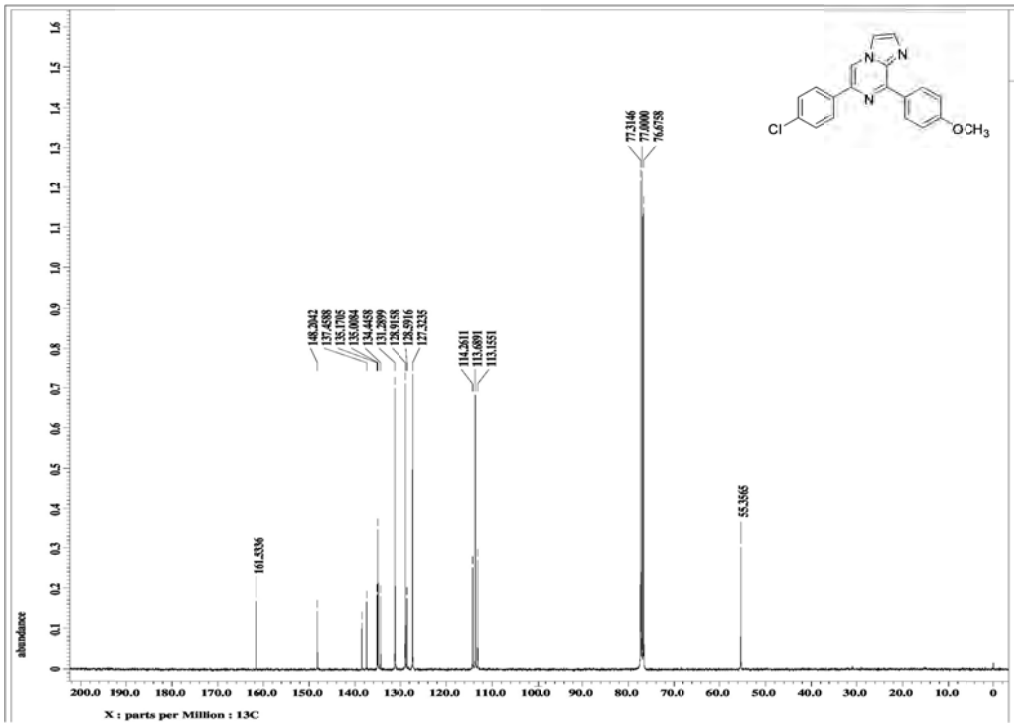



Fig. S69: $^{13}$C NMR spectrum of 6-(4”-chlorophenyl)-8-(4’-methoxyphenyl)imidazo[1,2-*a*]pyrazine **(29)**

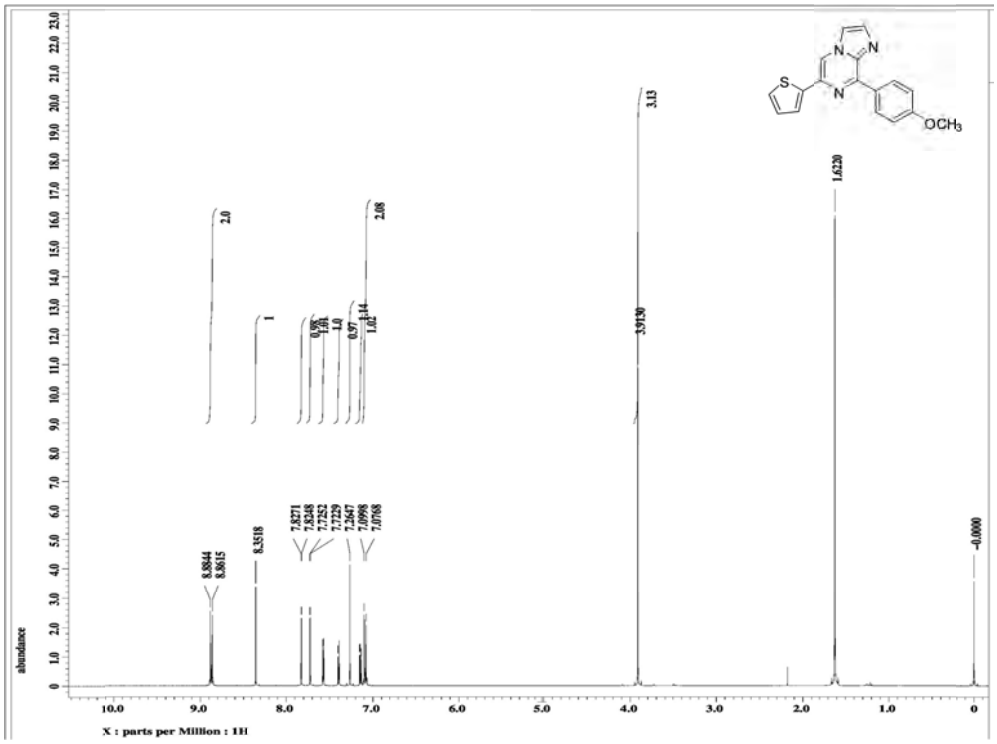



Fig. S70: $^{1}$H NMR spectrum of 8-(4'-methoxyphenyl)-6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazine **(30)**

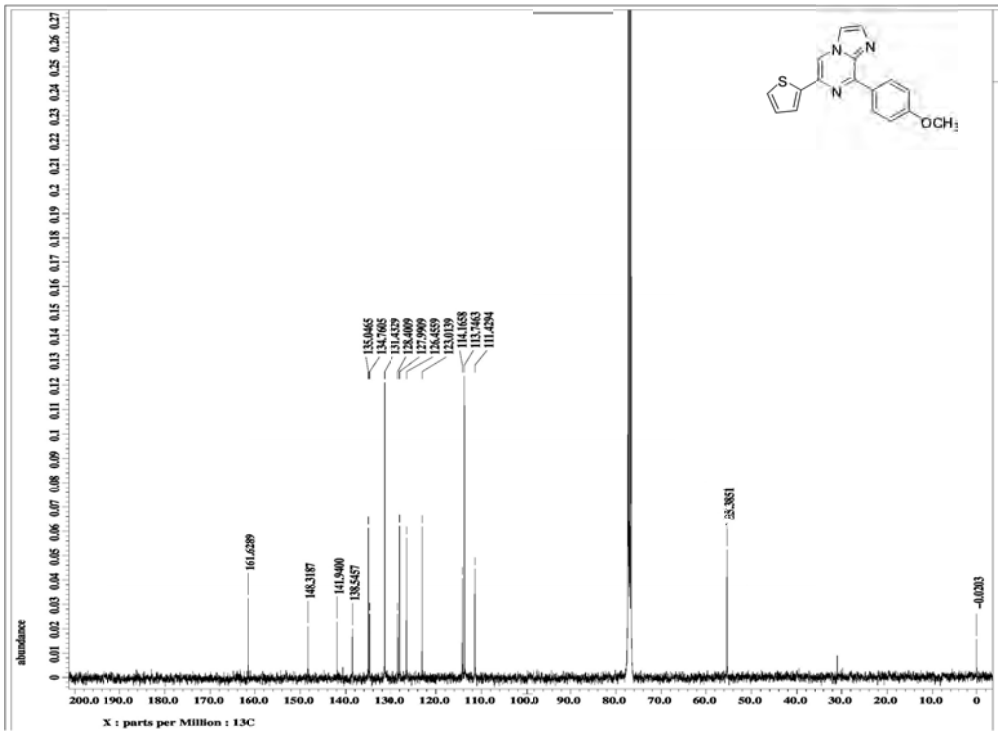



Fig.S71: $^{13}$C NMR spectrum of 8-(4'-methoxyphenyl)-6-(thiophen-2"-yl)imidazo[1,2-*a*]pyrazine **(30)**

**Antitumor methodology:** The human tumor cell lines of the cancer screening panel were grown in RPMI 1640 medium containing 5% fetal bovine serum and 2.0 mM L-glutamine. For a typical screening experiment, cells were inoculated into 96 well microtiter plates in 100 µl at plating densities ranging from 5000 to 40,000 cells/well depending on the doubling time of individual cell lines. After cell inoculation, the microtiter plates were incubated at 37 $^0$C, 5% $CO_2$, 95% air and 100% relative humidity for 24 h prior to addition of experimental drugs. After 24 h, two plates of each cell line were fixed in situ with TCA, to represent a measurement of the cell population for each cell line at the time of drug addition (Tz). Experimental drugs were solubilized in dimethyl sulfoxide at 400-fold the desired final maximum test concentration and stored frozen prior to use. At the time of drug addition, an aliquot of frozen concentrate was thawed and diluted to twice the desired final maximum test concentration with complete medium containing 50 µg/ml gentamicin. Aliquot of 100 µl of this drug dilution was added to the appropriate microtiter wells already containing 100 µl of medium, resulting in the required final drug concentrations. Following drug addition, the plates were incubated for an additional 48 h at 37 $^0$C, 5% $CO_2$, 95% air, and 100% relative humidity. For adherent cells, the assay was terminated by the addition of cold TCA. Cells were fixed in situ by the gentle addition of 50 µl of cold 50% (w/v) TCA (final concentration, 10% TCA) and incubated for 60 min at 4 $^0$C. The supernatant was discarded, and the plates were washed five times with tap water and air dried. Sulforhodamine B (SRB) solution (100 µl) at 0.4% (w/v) in 1% acetic acid was added to each well, and plates were incubated for 10 min at room temperature. After staining, unbound dye was removed by washing 5 times with 1% acetic acid and the plates were air dried. Bound stain was subsequently solubilized with 10 mM trizma base, and the absorbance is read on an automated plate reader at a wavelength of 515 nm. For suspension cells, the methodology is the same except that the assay is terminated by fixing settled cells at the bottom of the wells by gently adding 50 µl of 80% TCA (final concentration, 16% TCA).

**Table-1** Percentage (%) growth inhibition (GI) of compounds **4a-b**, **5a-b**, **7a, 8a-b**, **9a-b**, **11a-b** and **13b** over the full panel of 60 tumor cell lines at concentration of 10 µM.

| Cell line type | Cell line name | 4a | 4b | 5a | 5b | 7a | 8a | 8b | 9a | 9b | 11a | 11b | 13b |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Leukemia** | CCRF-CEM | - | - | - | - | - | - | 55.21 | - | - | - | 45.26 | - |
| | HL-60(TB) | NT | NT | - | - | NT | - | 69.76 | NT | NT | NT | NT | NT |
| | K-562 | - | - | - | - | - | - | **83.21** | - | - | - | 42.90 | - |
| | MOLT-4 | - | NT | - | - | 21.13 | - | 69.64 | - | - | 29.90 | 36.39 | NT |
| | RPMI-8226 | - | - | - | - | - | - | 41.74 | - | - | - | 45.84 | - |
| | SR | - | - | - | - | - | - | **86.61** | - | - | - | 46.69 | - |
| **Non-Small Cell Lung Cancer** | A549/ATCC | - | - | - | - | - | - | 68.14 | - | - | - | 29.47 | - |
| | HOP-62 | - | - | - | - | - | 32.79 | 66.79 | - | - | - | - | - |
| | HOP-92 | - | - | - | - | 46.37 | 33.11 | 44.22 | 29.33 | 48.62 | - | 44.57 | - |
| | NCI-H226 | - | - | - | - | 25.39 | 21.94 | 29.38 | - | 20.68 | - | 26.51 | - |
| | NCI-H23 | - | - | - | - | - | 27.75 | 40.18 | - | - | - | - | - |
| | NCI-H322M | - | - | - | - | - | - | - | - | - | - | - | - |
| | NCI-H460 | - | - | - | - | - | - | **83.24** | - | - | - | 35.82 | - |
| | NCI-H522 | - | - | - | - | - | - | **L** | - | - | - | 49.20 | - |
| **Colon Cancer** | COLO 205 | - | - | - | - | - | - | **92.17** | - | - | - | - | - |
| | HCC-2998 | - | - | - | - | - | - | 39.76 | - | - | - | 25.73 | - |
| | HCT-116 | - | - | - | - | 22.16 | - | 69.96 | - | - | - | 32.49 | - |
| | HCT-15 | - | 45.55 | - | - | - | - | **78.38** | - | - | - | 59.04 | - |
| | HT29 | - | - | - | - | - | - | **90.12** | - | - | - | - | - |
| | KM12 | - | 25.06 | - | - | - | - | 65.37 | - | - | - | 58.16 | - |
| | SW-620 | - | - | - | - | - | - | **74.59** | - | - | - | - | - |
| **CNS Cancer** | SF-268 | - | - | - | - | - | - | 43.09 | - | - | - | 40.05 | - |
| | SF-295 | - | - | - | - | - | - | 69.38 | - | - | - | - | - |
| | SF-539 | - | - | - | - | - | 21.39 | 47.52 | - | - | - | 33.12 | - |
| | SNB-19 | - | - | - | - | - | - | 24.23 | - | - | - | 26.43 | - |
| | SNB-75 | - | - | - | - | - | 37.71 | 64.36 | 21.70 | - | - | 44.13 | 29.36 |
| | U251 | - | - | - | - | 21.82 | - | 60.82 | - | - | - | 36.88 | - |
| **Melanoma** | LOX IMVI | - | - | - | - | 22.16 | - | 56.82 | - | - | - | 36.88 | - |
| | MALME-3M | - | - | - | - | - | - | 60.53 | - | - | - | - | - |
| | M14 | - | - | - | - | - | - | 47.52 | - | - | - | 35.81 | - |
| | MDA-MB-435 | - | - | - | - | - | - | **96.92** | - | - | - | 29.94 | - |
| | SK-MEL-2 | NT | NT | - | - | NT | - | 69.23 | NT | NT | NT | NT | NT |
| | SK-MEL-28 | - | - | - | - | - | - | 37.85 | - | 25.31 | - | 46.19 | - |
| | SK-MEL-5 | - | 31.97 | - | - | - | - | 53.74 | - | - | - | - | - |
| | UACC-257 | - | - | - | - | - | - | 32.55 | - | - | - | - | - |
| | UACC-62 | - | - | - | - | 22.63 | - | 56.36 | - | - | - | 29.21 | - |
| **Ovarian Cancer** | IGROV1 | - | - | - | - | 25.74 | 23.89 | 44.23 | - | - | - | 25.30 | - |
| | OVCAR-3 | - | - | - | - | - | - | 68.10 | - | - | - | 39.82 | - |
| | OVCAR-4 | - | 47.97 | - | - | - | - | 37.80 | - | - | - | 29.44 | - |
| | OVCAR-5 | - | - | - | - | - | - | - | - | - | - | - | - |
| | OVCAR-8 | - | - | - | - | - | - | 48.40 | - | - | - | 23.89 | - |
| | NCI/ADR-RES | NT | NT | - | - | NT | - | **80.29** | NT | NT | NT | NT | NT |
| | SK-OV-3 | - | - | - | - | - | 25.17 | 44.78 | - | - | - | 27.05 | - |
| **Renal Cancer** | 786-0 | - | - | - | - | - | - | 42.16 | - | - | - | - | - |
| | A498 | - | - | - | - | 23.41 | - | 64.07 | - | 29.32 | - | 68.01 | 22.64 |
| | ACHN | - | - | - | - | - | 22.54 | 45.39 | - | - | - | 27.88 | - |
| | CAKI-1 | - | - | - | 45.67 | 27.04 | 28.35 | 60.43 | - | - | - | 48.21 | - |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | RXF 393 | - | - | - | - | - | - | 53.04 | - | - | - | 50.82 | - |
| | SN12C | - | - | - | - | - | 20.44 | 46.25 | - | - | - | 39.90 | - |
| | TK-10 | - | - | - | - | - | - | - | - | - | - | 30.23 | - |
| | UO-31 | - | - | - | - | 59.68 | 49.62 | 58.36 | 23.14 | 27.69 | - | 53.71 | 23.29 |
| **Prostate Cancer** | PC-3 | - | - | - | - | - | 21.59 | 33.77 | - | - | - | 29.85 | - |
| | DU-145 | - | - | - | - | - | - | 27.33 | - | - | - | - | - |
| **Breast Cancer** | MCF7 | 36.45 | **75.44** | 38.14 | **75.20** | 35.87 | 29.97 | **77.96** | 33.19 | - | 32.29 | 59.64 | 42.69 |
| | MDA-MB-231/ATCC | - | - | - | - | 30.38 | 28.08 | 53.45 | - | - | - | 69.32 | - |
| | HS 578T | - | - | - | - | - | - | 38.90 | - | 20.77 | - | 37.38 | - |
| | BT-549 | - | - | 38.09 | - | - | 33.42 | **82.44** | - | - | - | 37.67 | - |
| | T-47D | - | **78.80** | - | 49.11 | 45.59 | 47.04 | 62.84 | 22.95 | - | 32.42 | 47.07 | 42.48 |
| | MDA-MB-468 | - | **88.28** | - | 64.74 | 21.12 | - | 66.82 | - | - | - | 48.29 | 30.62 |

NT-not tested, L- lethal

**Table-2** Percentages (%) growth inhibition (GI) of compounds **18**-**19**, **21**- **23**, **27**- **28** and **30** over the full panel of 60 tumor cell lines at concentration of 10 µM.

| Cell line type | Cell line name | 18 | 19 | 21 | 22 | 23 | 27 | 28 | 30 |
|---|---|---|---|---|---|---|---|---|---|
| **Leukemia** | CCRF-CEM | - | 34.75 | 25.29 | 21.65 | 33.43 | - | - | 22.66 |
| | HL-60(TB) | - | - | - | - | - | - | - | - |
| | K-562 | - | **73.90** | **78.51** | 31.05 | **70.71** | - | - | 37.83 |
| | MOLT-4 | 23.61 | 37.56 | 53.12 | 20.05 | 28.64 | - | 20.53 | 24.60 |
| | RPMI-8226 | - | 35.34 | - | 47.08 | - | 30.11 | - | 28.61 |
| | SR | 20.98 | 40.51 | 58.89 | 36.61 | 41.09 | 30.77 | - | 29.92 |
| **Non-Small Cell Lung Cancer** | A549/ATCC | 25.93 | 42.59 | 48.62 | **L** | 32.55 | - | 22.65 | - |
| | HOP-62 | 22.21 | 42.27 | 49.45 | 68.64 | 41.11 | 21.79 | 30.09 | 38.49 |
| | HOP-92 | 30.33 | - | 28.35 | 65.30 | 30.62 | - | 22.34 | 32.10 |
| | NCI-H226 | 22.22 | 28.04 | 21.60 | 53.72 | 30.49 | 21.69 | - | 30.91 |
| | NCI-H23 | - | 28.90 | 27.89 | 38.99 | - | - | - | - |
| | NCI-H322M | - | - | - | **88.56** | - | - | - | - |
| | NCI-H460 | - | - | 22.26 | **85.47** | - | - | - | - |
| | NCI-H522 | 24.24 | 72.01 | **82.59** | 38.45 | 47.09 | 27.13 | - | 50.23 |
| **Colon Cancer** | COLO 205 | - | 28.91 | - | 24.95 | 26.84 | - | - | - |
| | HCC-2998 | - | 52.20 | 23.30 | 41.81 | - | - | - | 28.38 |
| | HCT-116 | 20.00 | 31.98 | 48.02 | 49.85 | 37.95 | - | - | 21.97 |
| | HCT-15 | 21.20 | 68.84 | 60.41 | NT | 63.12 | 35.05 | - | 51.50 |
| | HT29 | - | 58.37 | 41.70 | 59.69 | 43.15 | - | - | 20.93 |
| | KM12 | - | 49.45 | 38.53 | 51.30 | 39.34 | - | - | 32.70 |
| | SW-620 | - | 42.67 | 56.77 | 27.26 | 44.25 | - | - | - |
| **CNS Cancer** | SF-268 | - | - | 24.20 | 35.73 | - | - | - | - |
| | SF-295 | - | - | 22.27 | **84.86** | 27.87 | - | - | 26.78 |
| | SF-539 | - | 23.30 | 29.70 | 37.84 | - | - | - | 26.14 |
| | SNB-19 | - | - | 21.09 | 69.43 | 20 | - | - | - |
| | SNB-75 | 26.73 | 31.87 | 32.81 | 67.97 | 52.25 | 36.35 | 33.53 | 39.07 |
| | U251 | - | - | 31.37 | **L** | 23.29 | - | - | 24.92 |
| **Melanoma** | LOX IMVI | - | 38.60 | 46.47 | 44.76 | 29.61 | 25.46 | - | 31.06 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | MALME-3M | - | - | 22.40 | 22.96 | - | - | - | - |
| | M14 | - | 38.48 | 46.18 | - | 46.88 | 25.49 | - | 41.72 |
| | MDA-MB-435 | - | **76.92** | **81.62** | 21.44 | - | 23.60 | - | 51.97 |
| | SK-MEL-2 | - | 29.41 | 34.10 | - | - | - | - | 32.65 |
| | SK-MEL-28 | - | - | - | - | - | - | - | - |
| | SK-MEL-5 | - | 46.78 | 27.13 | 42.03 | 27.87 | 26.32 | - | 43.51 |
| | UACC-257 | - | 29.76 | 23.60 | 24.77 | - | - | - | - |
| | UACC-62 | - | 39.83 | 43.90 | - | 38.69 | - | - | 28.30 |
| **Ovarian Cancer** | IGROV1 | 20.33 | 39.06 | 42.46 | 59.29 | 33.81 | - | - | - |
| | OVCAR-3 | - | 27.40 | 24.26 | 49.26 | - | - | - | 21.05 |
| | OVCAR-4 | - | 35.44 | - | 58.70 | 21.48 | - | - | 25.52 |
| | OVCAR-5 | - | - | - | - | - | - | - | - |
| | OVCAR-8 | - | - | 25.34 | 50.21 | - | - | - | - |
| | NCI/ADR-RES | - | 44.46 | 54.11 | 29.85 | 34.08 | 31.88 | - | 34.70 |
| | SK-OV-3 | 22.64 | 49.84 | 43.58 | **L** | 35.01 | - | 27.57 | 41.97 |
| **Renal Cancer** | 786-0 | - | - | - | **L** | - | - | - | - |
| | A498 | 21.83 | - | 26.82 | 63.21 | 23.22 | - | - | - |
| | ACHN | - | - | - | **91.41** | - | - | - | - |
| | CAKI-1 | 30.38 | 41.01 | 34.72 | 49.82 | 43.45 | 31.71 | 25.42 | 36.11 |
| | RXF 393 | - | - | 20.90 | 58.40 | 38.85 | - | - | 33.85 |
| | SN12C | - | - | 20.55 | 34.30 | 22.85 | - | - | - |
| | TK-10 | - | 39.27 | - | **88.07** | - | - | - | - |
| | UO-31 | 40.53 | 54.06 | 51.83 | **92.94** | 52.29 | 46.56 | 40.95 | 45.06 |
| **Prostate Cancer** | PC-3 | 22.49 | 37.62 | 27.31 | 39.85 | 27.36 | 21.00 | 20.87 | 21.61 |
| | DU-145 | - | - | - | 32.73 | - | - | - | - |
| **Breast Cancer** | MCF7 | 39.00 | **80.94** | 56.98 | **72.83** | 57.41 | 25.48 | 24.89 | 42.68 |
| | MDA-MB-231/ATCC | 23.35 | 33.47 | 47.39 | 26.00 | 37.60 | 36.97 | 21.64 | 39.19 |
| | HS 578T | - | - | 23.39 | - | 20.47 | 20.07 | - | 22.18 |
| | BT-549 | - | NT | NT | NT | NT | 39.50 | NT | 33.41 |
| | T-47D | 36.98 | **83.67** | 29.74 | 59.78 | 35.2 | 36.65 | 40.92 | **76.26** |
| | MDA-MB-468 | - | **L** | - | **L** | 23.47 | - | - | 69.70 |

NT-not tested, L- lethal