Supplementary file

Corrosion Inhibition and In Silico Toxicity Assessment of Imidazo[1,2-a]pyrimidine-Schiff Base Derivatives as Effective and Environmentally Friendly Corrosion Inhibitors for Mild Steel

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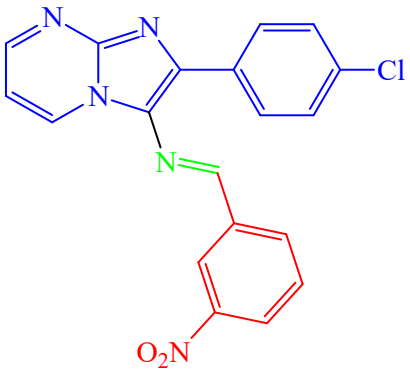
The chemicals and solvents used in the synthesis were of analytical grade, sourced from Sigma-Aldrich, and employed without further purification. NMR spectra (^{1}H and ^{13}C) were recorded using a JNM-ECZ500R/S1 FT NMR system from JEOL, with $CDCl_3$ as the solvent. Mass spectrometry data were obtained using the Thermo Scientific TSQ 8000 Evo Triple Quadrupole GC-MS/MS spectrometer. FT-IR spectra were collected with a JASCO FT/IR-4700 spectrophotometer. Melting points were determined using a Stuart SMP20 melting point apparatus. The Bio-Logic Science Instruments SAS Model SP-150 Potentiostat, controlled by EC-lab software V11.33 were used to conduct the electrochemical measurements.

^{1}H-NMR , ^{13}C-NMR , FT-IR and **LC-MS**(ESI^{+}) **of**

(E)-2-(4-chlorophenyl)-N-(3-nitrobenzylidene)imidazo[1,2-a]pyrimidin-3-amine **(IPY 1).**



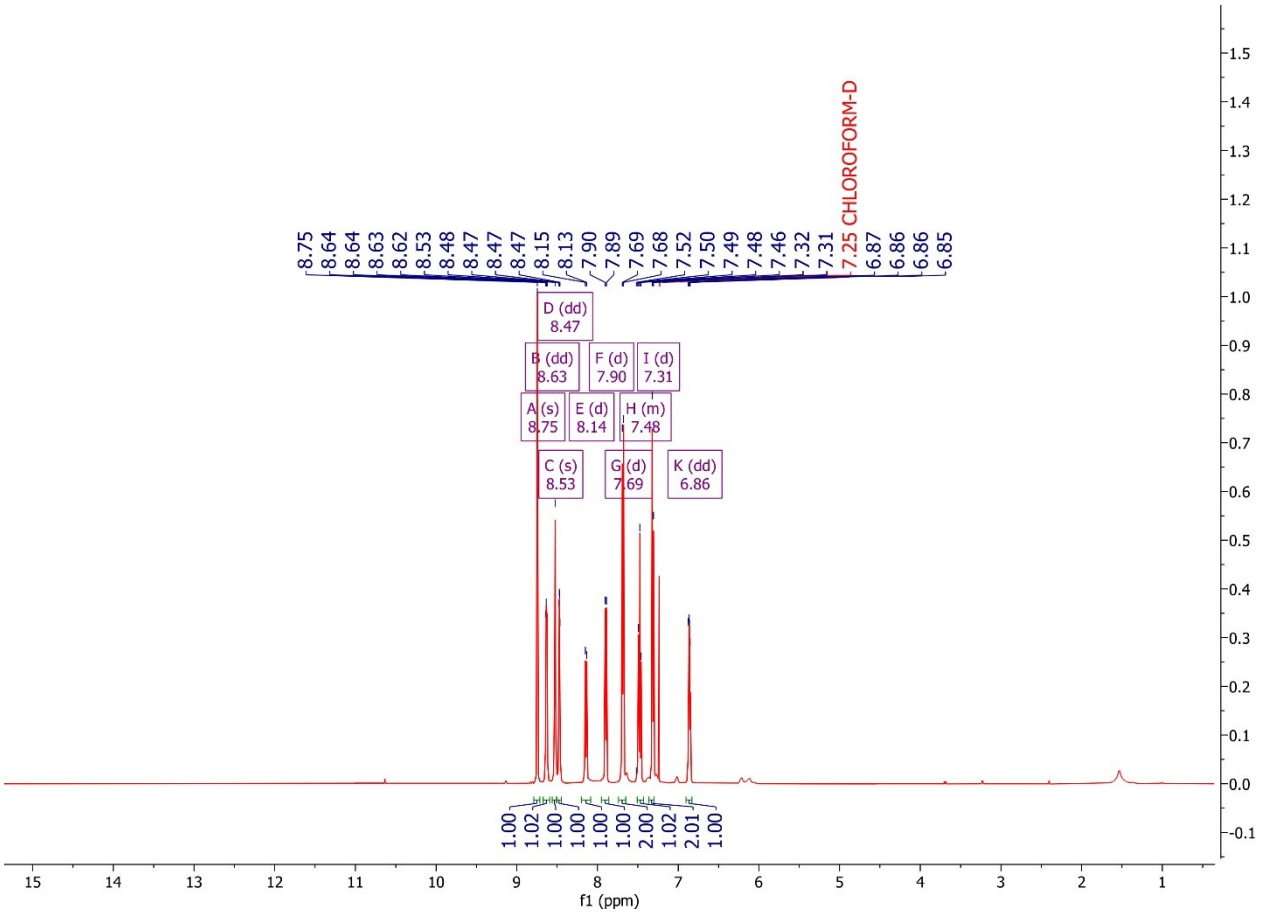


Figure S1. ^{1}H NMR spectra of **(IPY 1)**

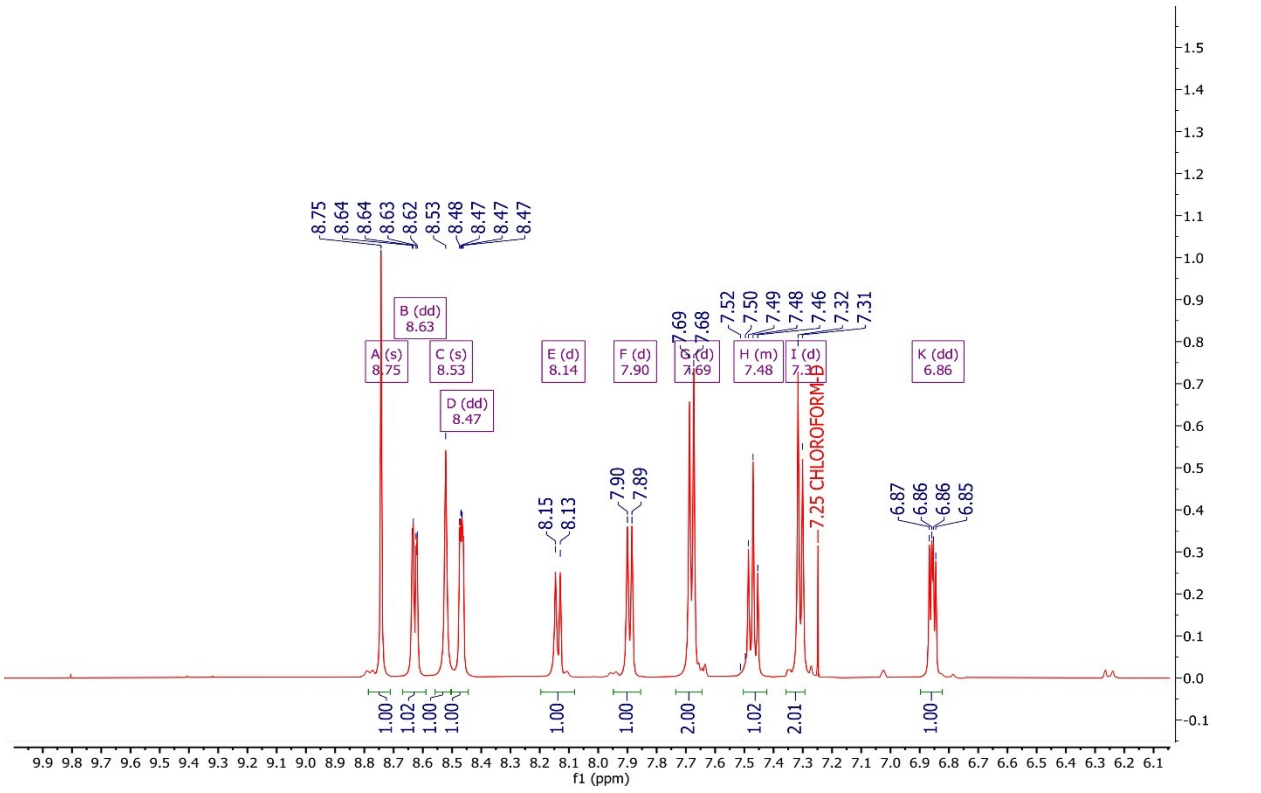


Figure S2. ^{1}H NMR spectra (10-6 ppm) of **(IPY 1)**

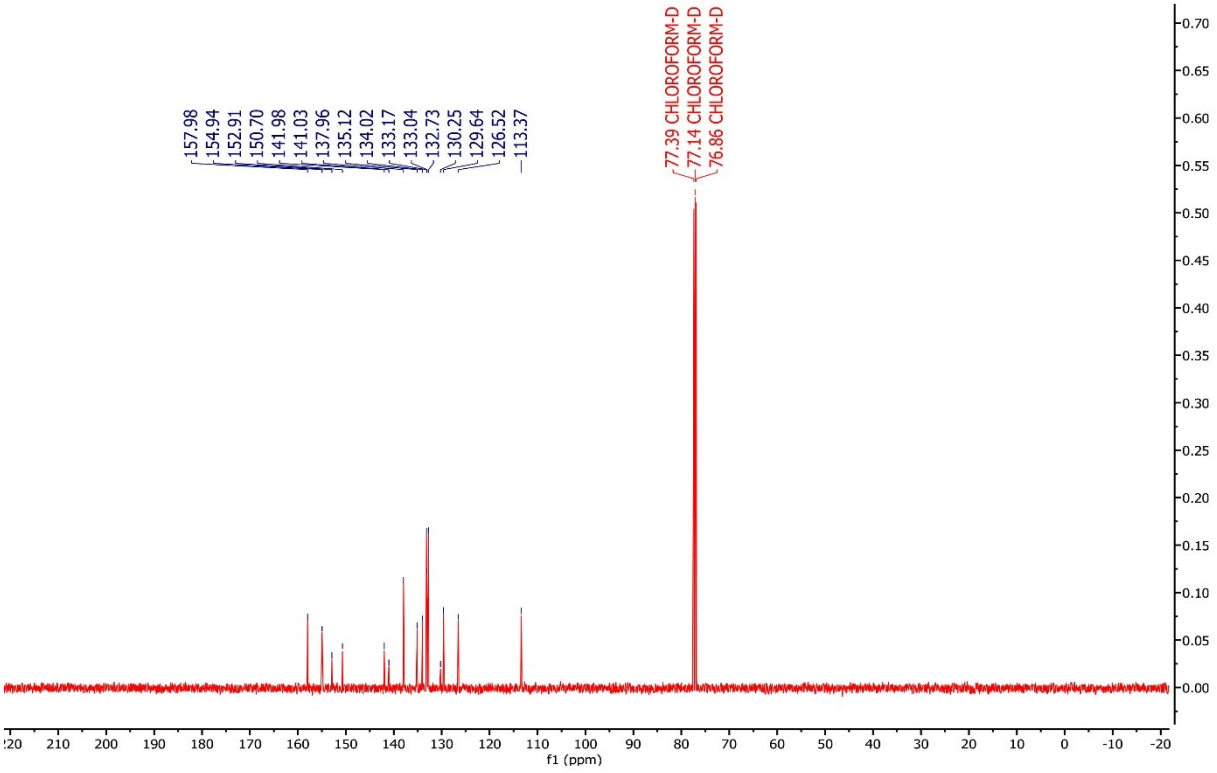


Figure S3. ^{13}C NMR spectra of **(IPY 1)**

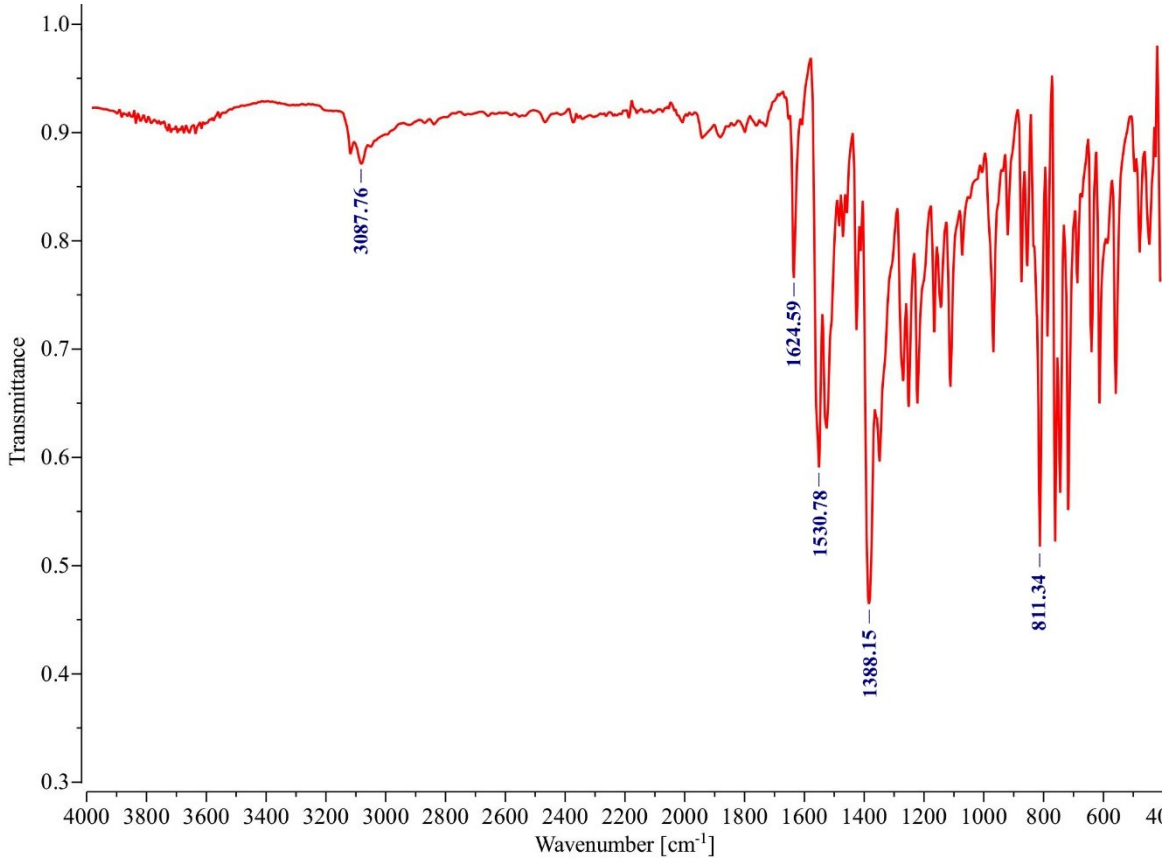


Figure S4. FT-IR spectra of **(IPY 1)**

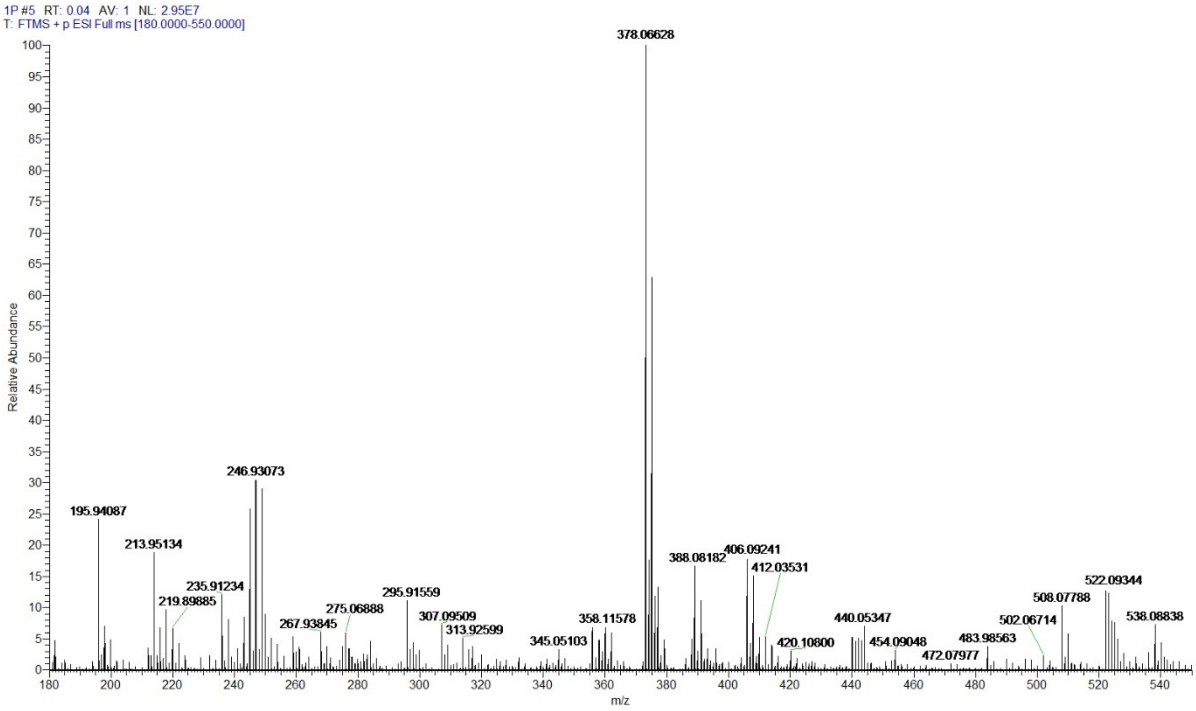
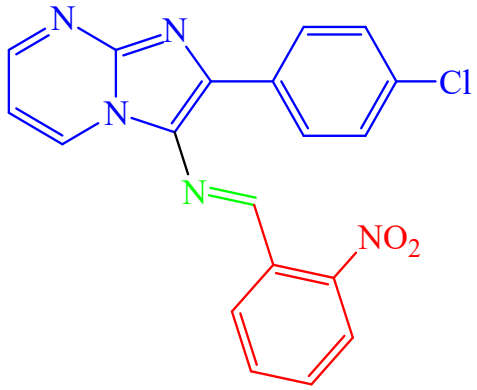


Figure S5. ESI$^+$-MS spectra of **(IPY 1)**

^{1}**H-NMR ,** ^{13}**C-NMR , FT-IR** and **LC-MS**(ESI$^+$) **of**

(E)-2-(4-chlorophenyl)-N-(2-nitrobenzylidene)imidazo[1,2-a]pyrimidin-3-amine (**IPY 2**).



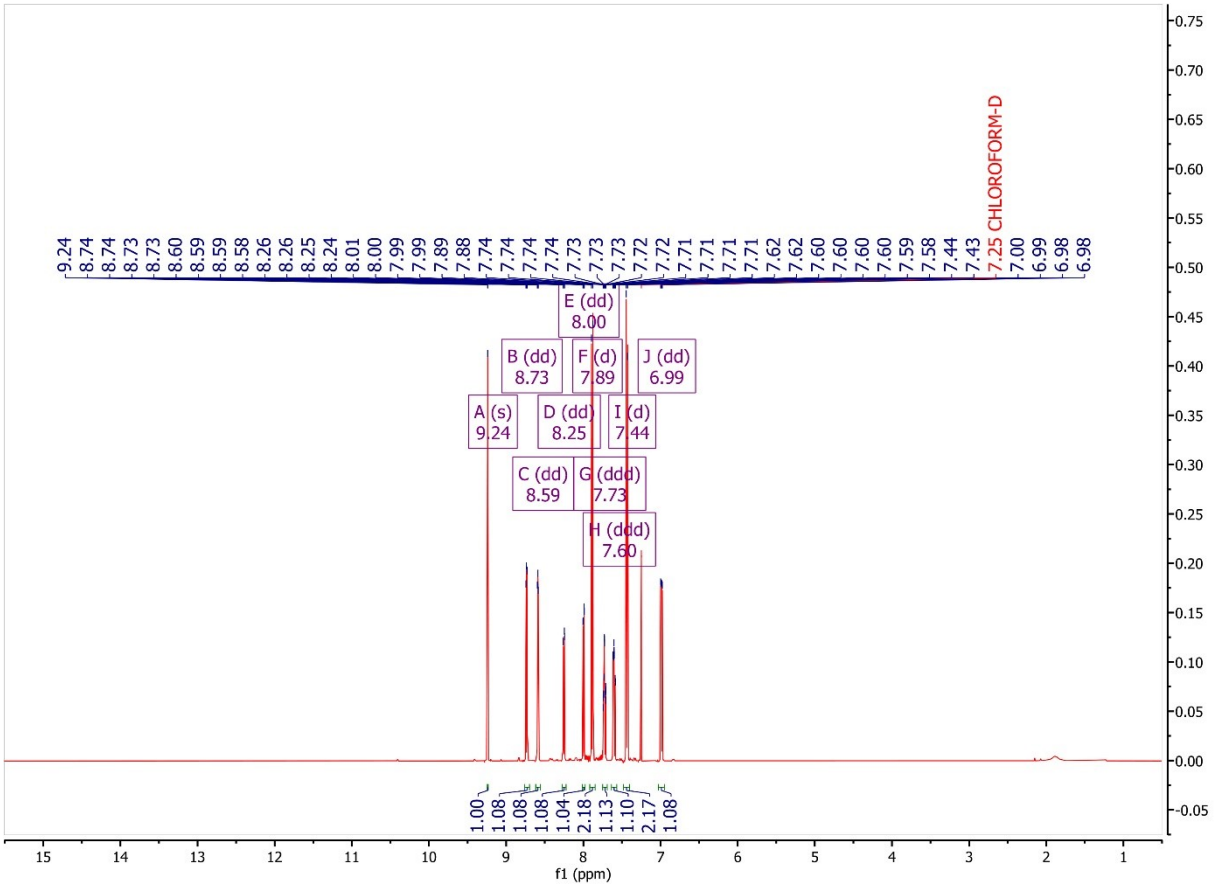


Figure S6. ^{1}H NMR spectra of **(IPY 2)**

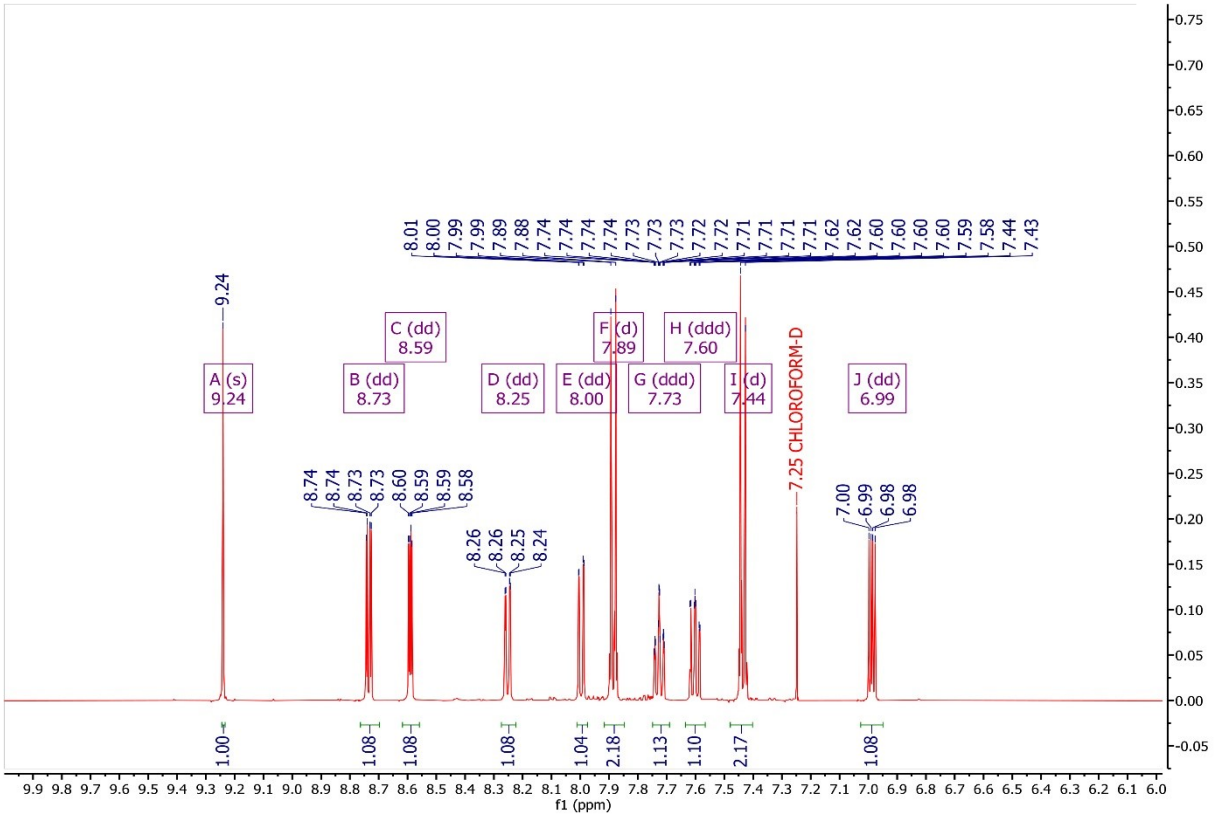


Figure S7. ^{1}H NMR spectra (10-6 ppm) of **(IPY 2)**

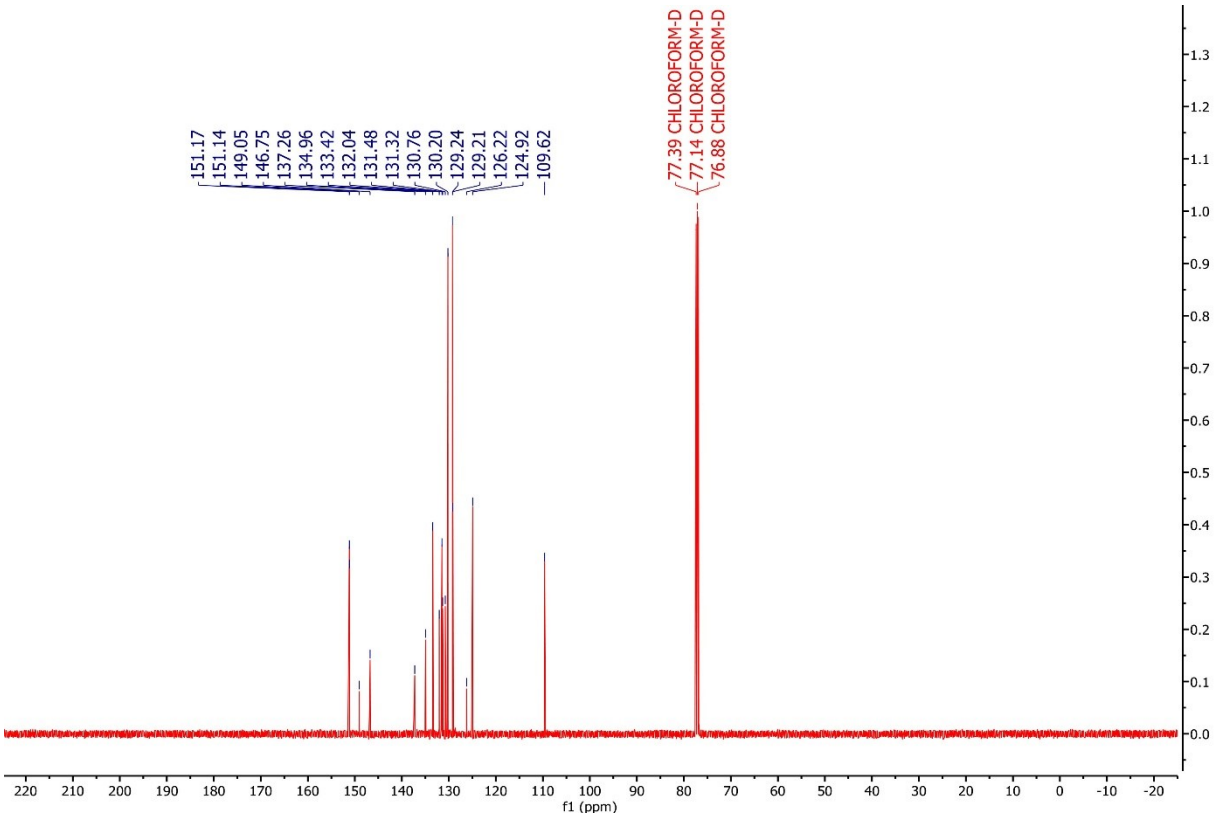


Figure S8. ^{13}C NMR spectra of **(IPY 2)**

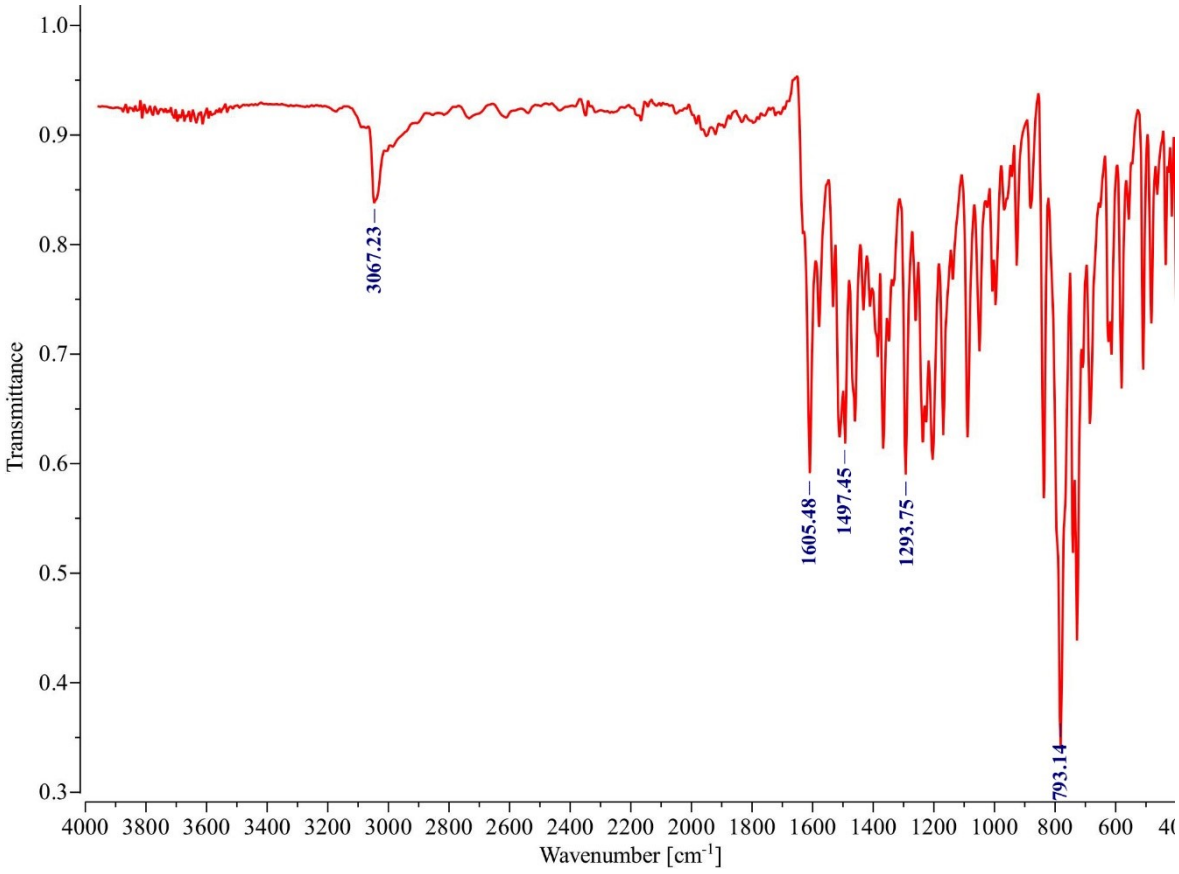


Figure S9. FT-IR spectra of **(IPY 2)**

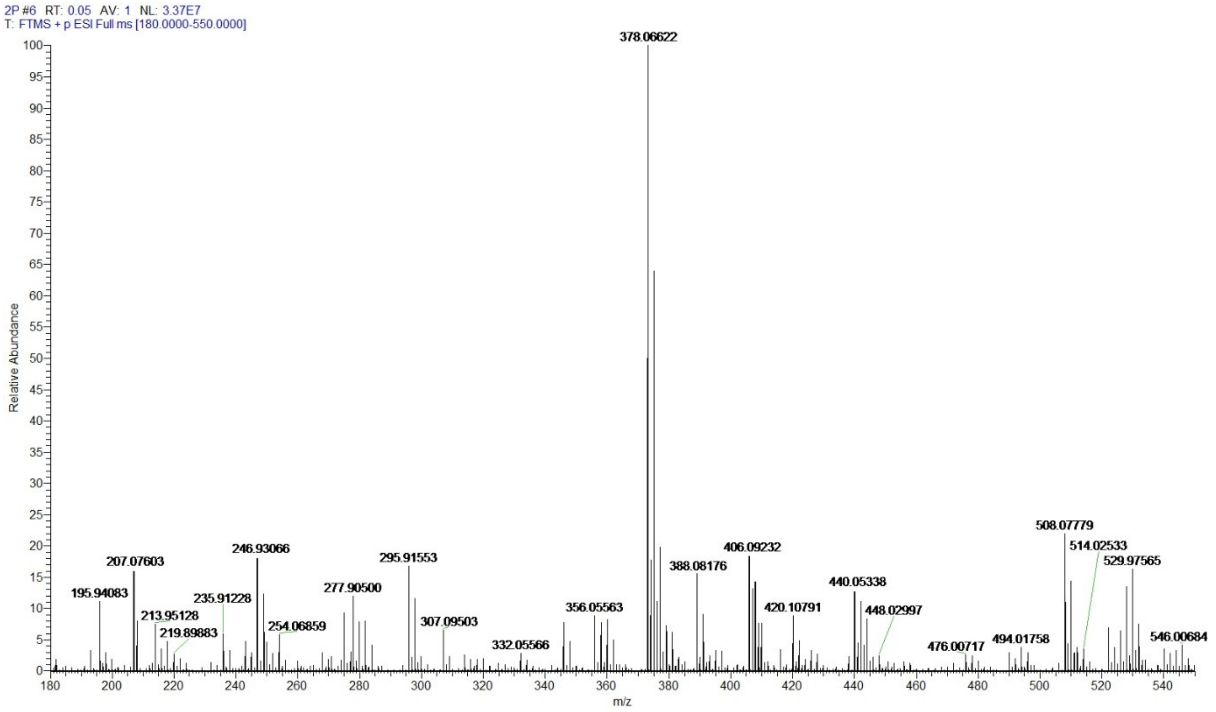


Figure S10. ESI^{+}-MS spectra of **(IPY 2)**

Tables

Table SI1: Characteristics of the new inhibitors (IPY 1) and (IPY 2).

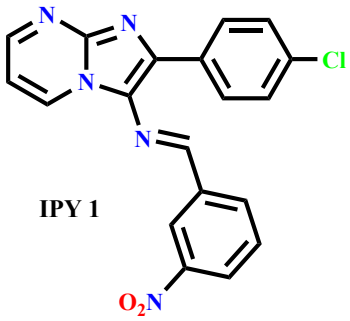
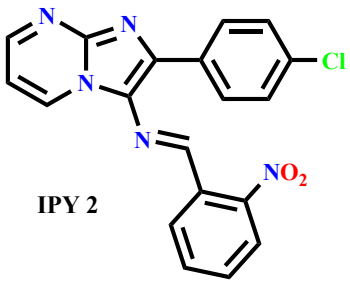
Compound	Aspect	Structural characterization of IPY 1 and IPY 2
 IPY 1	Obtained as yellow powder; yield 85%, mp; 272-274 °C.	**FT-IR (υ_{max}/cm^{-1})**
		υ(C-H) = 3087 ; υ(C=N) = 1624; υ(C=C) = 1530; υ(N=O) = 1388 ;υ(C-Cl) = 811.
		^{1}H NMR (500 MHz, CHLOROFORM-D)
		δ 8.75 (s, 1H), 8.63 (dd, *J* = 6.7, 1.9 Hz, 1H), 8.53 (s, 1H), 8.47 (dd, *J* = 4.2, 1.9 Hz, 1H), 8.14 (d, *J* = 7.7 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 2H), 7.55 – 7.43 (m, 1H), 7.31 (d, *J* = 7.8 Hz, 2H), 6.86 (dd, *J* = 6.7, 4.2 Hz, 1H).
		^{13}C NMR (126 MHz, CHLOROFORM-*D*)
		δ 157.98, 154.94, 152.91, 150.70, 141.98, 141.03, 137.96, 135.12, 134.02, 133.17, 133.04, 132.73, 130.25, 129.64, 126.52, 113.37.
		LC-MS
		m/z= 378.066 (M+1)
 IPY 2	Obtained as yellow powder; yield 92%, mp; 205-207 °C.	**FT-IR (υ_{max}/cm^{-1})**
		υ(C-H) = 3067 ; υ(C=N) = 1605; υ(C=C) = 1497; υ(N=O) = 1293; υ(C-Cl) = 793.
		^{1}H NMR (500 MHz, CHLOROFORM-D)
		δ 9.24 (s, 1H), 8.73 (dd, *J* = 6.8, 2.0 Hz, 1H), 8.59 (dd, *J* = 4.1, 2.0 Hz, 1H), 8.25 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.00 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.89 (d, *J* = 8.7 Hz, 2H), 7.73 (ddd, *J* = 7.9, 7.4, 1.3 Hz, 1H), 7.60 (ddd, *J* = 8.2, 7.4, 1.4 Hz, 1H), 7.44 (d, *J* = 8.7 Hz, 2H), 6.99 (dd, *J* = 6.8, 4.1 Hz, 1H).
		^{13}C NMR (126 MHz, CHLOROFORM-*D*)
		δ 151.17, 151.14, 149.05, 146.75, 137.26, 134.96, 133.42, 132.04, 131.48, 131.32, 130.76, 130.20, 129.24, 129.21, 126.22, 124.92, 109.62.
		LC-MS
		378.066 (M+1)

Table SI2. Adsorption Isotherms parameters of IPY 1 and IPY 2 obtained from PDP at 298 K.

Sample	Langmuir			Temkin			Frumkin			Freundlish		
	R^2	K_{ads} (M^{-1})	ΔG°_{ads} (Kj/mol)	R^2	K_{ads} (M^{-1})	ΔG°_{ads} (Kj/mol)	R^2	K_{ads} (M^{-1})	ΔG°_{ads} (Kj/mol)	R^2	K_{ads} (M^{-1})	ΔG°_{ads} (Kj/mol)
IPY 1	0,999	1.39×10^{5}	-39.29	0.931	6.65×10^{21}	-134.45	0.805	4.62×10^{16}	-105.02	0.941	1.12	-10.23
IPY 2	0,999	1.48×10^{5}	-39.44	0.917	3.06×10^{18}	-115.41	0.844	4.48×10^{14}	-93.54	0.917	1.15	-10.29

Table SI3. Activation parameters for MS dissolution in 1.0 M HCl, both in the presence of 10^{-3} M IPY 1 and IPY 2 and in their absence.

Sample	E_a (kJ/mol)	ΔH_a (kJ/mol)	ΔS_a (j mol^{-1} K^{-1})
Blank	26.34	23.74	-193.40
IPY 1	54.87	52.28	-185.11
IPY 2	51.79	49.23	-186.01