Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION (SI)

Experimental and theoretical investigation on anti-corrosion characteristics of Pyridine substituted benzothiazole derivatives for mild steel in aqueous HCl

Fig. S1 A

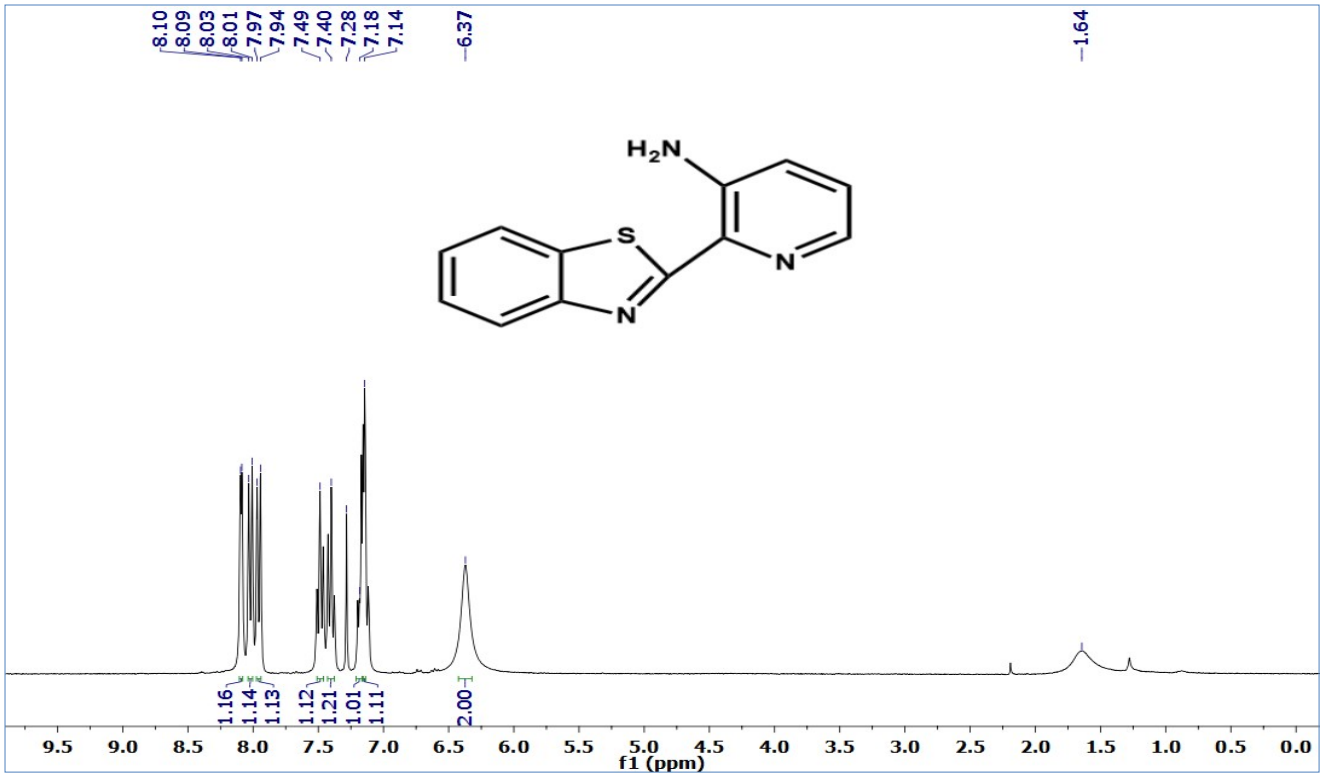


Fig. S1 B

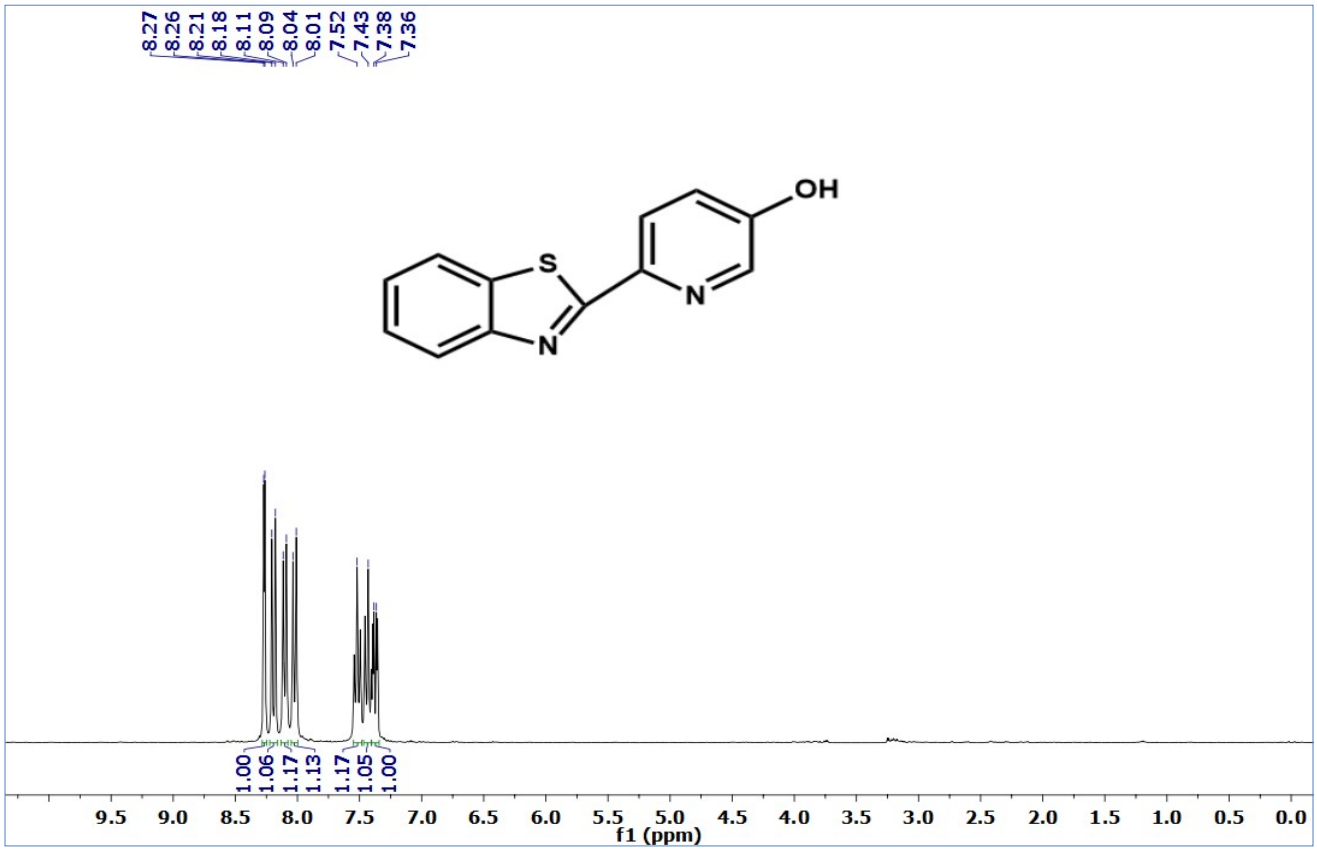


Fig. S1 C

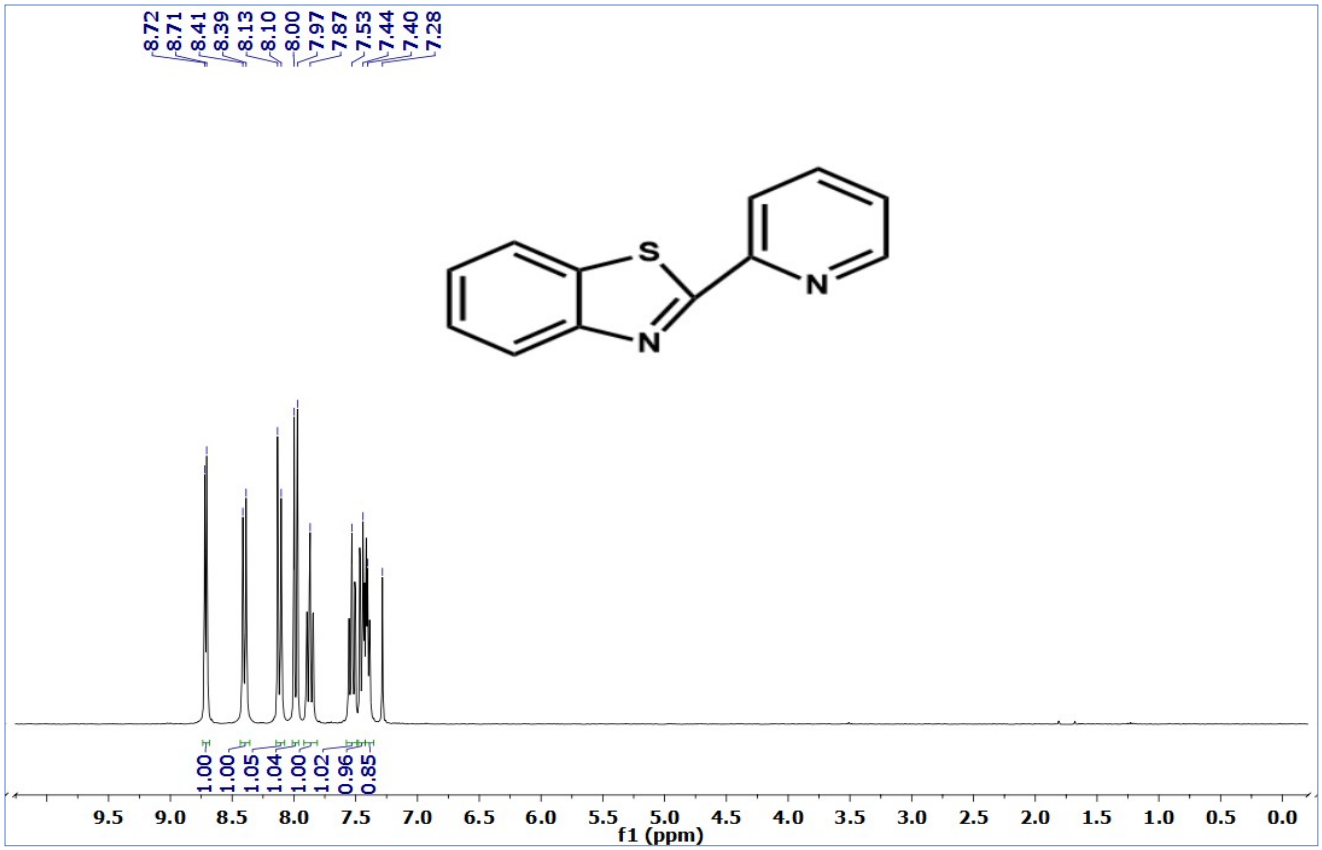


Fig. S1 (A-C) ^{1}H-NMR spectrum of (A) APYBT, (B) HPYBT and (C) PYBT inhibitors in CDCl3 at 400 MHz

Fig. S2 A

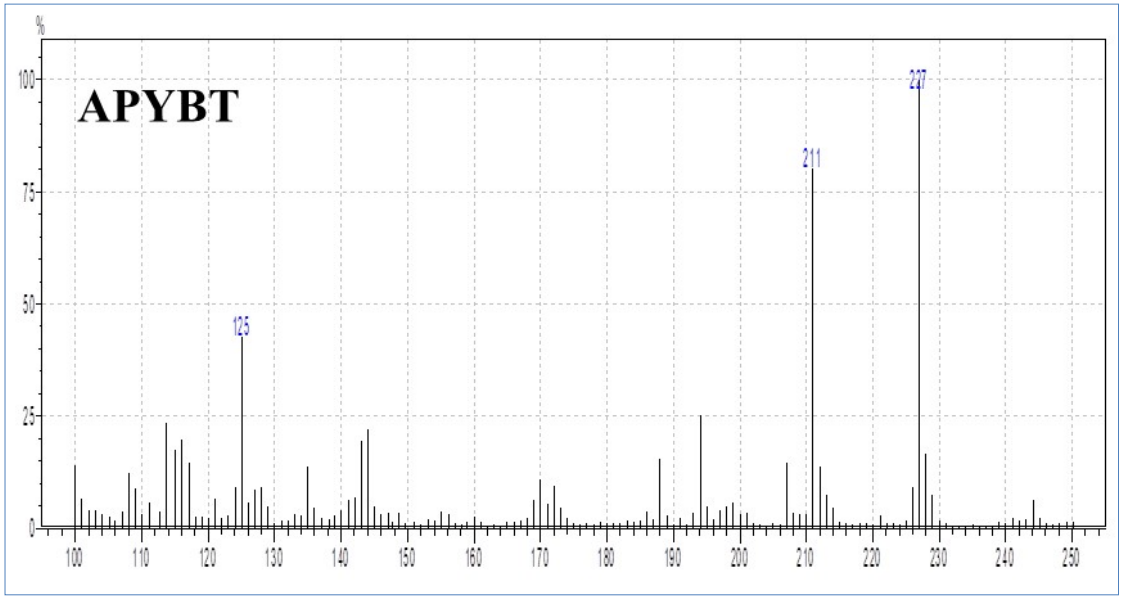


Fig. S2 B

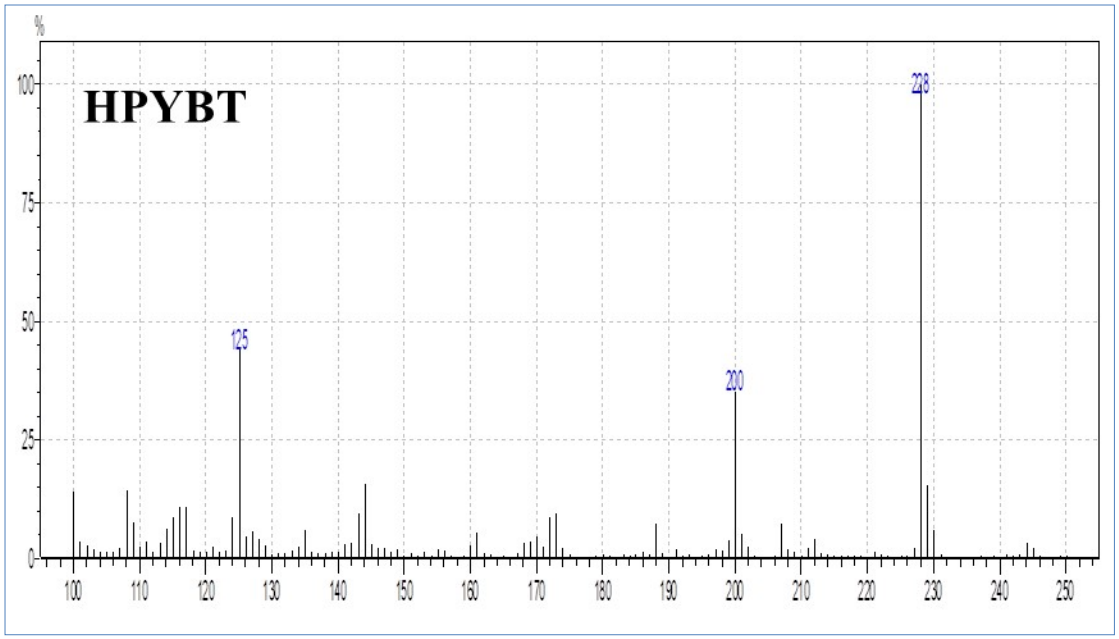


Fig. S2 C

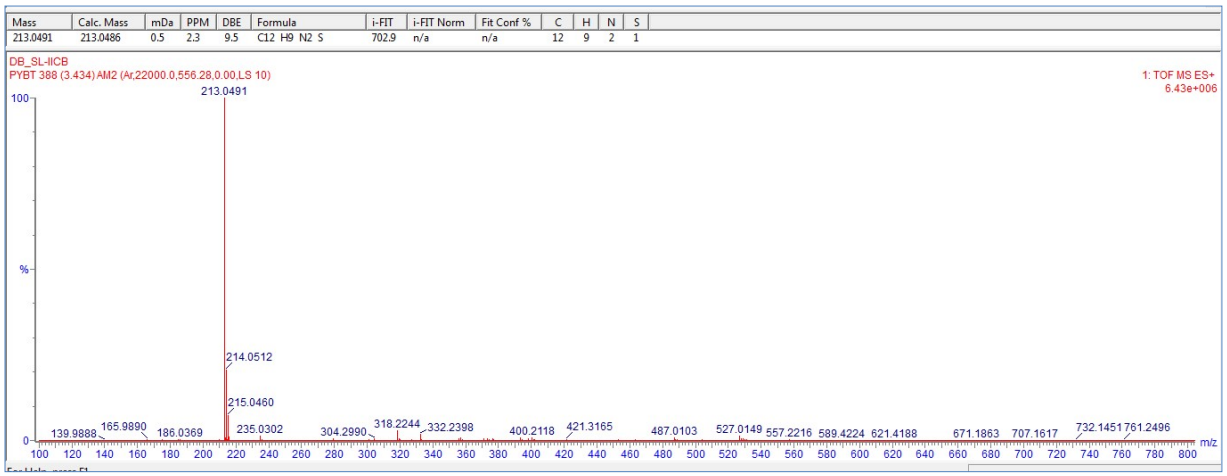


Fig. S2 (A-C) EI-MS spectrum of (A) APYBT (B) HPYBT and ESI-MS spectrum of (C) PYBT inhibitors in methanol.

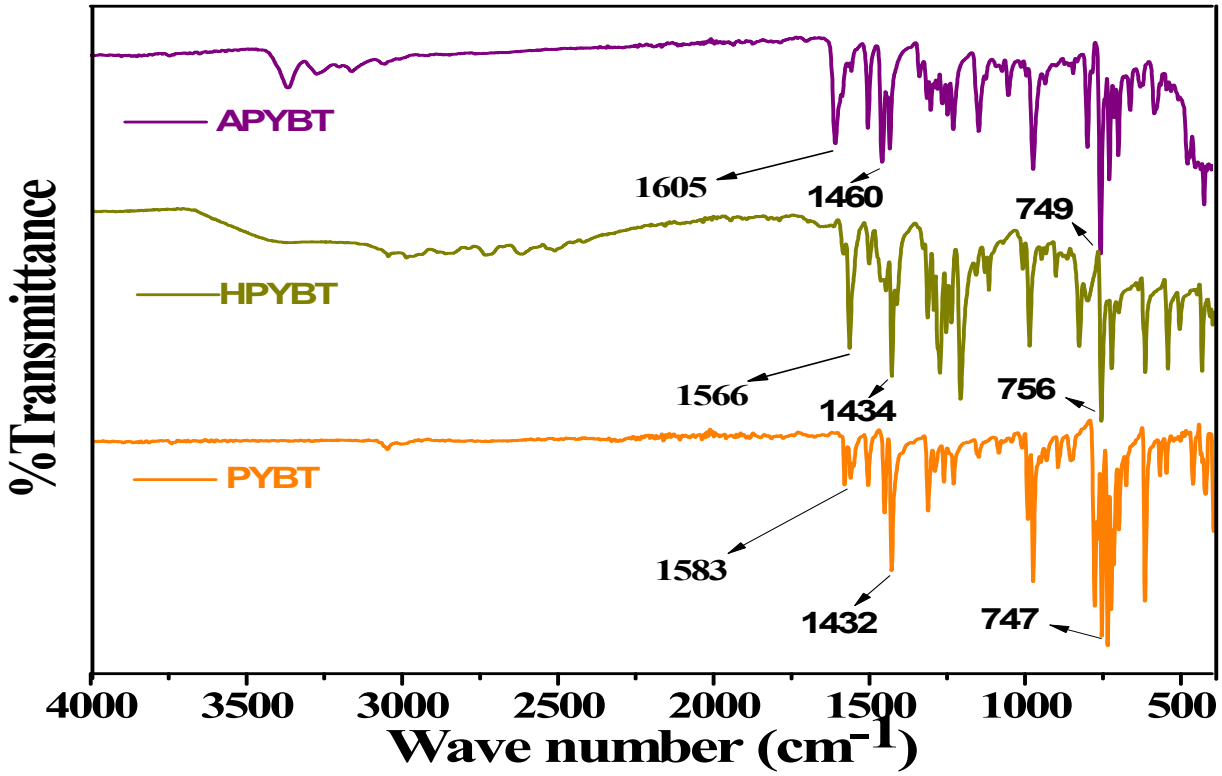


Fig. S3 FTIR spectrum of APYBT, HPYBT and PYBT inhibitors

Fig. S4 A

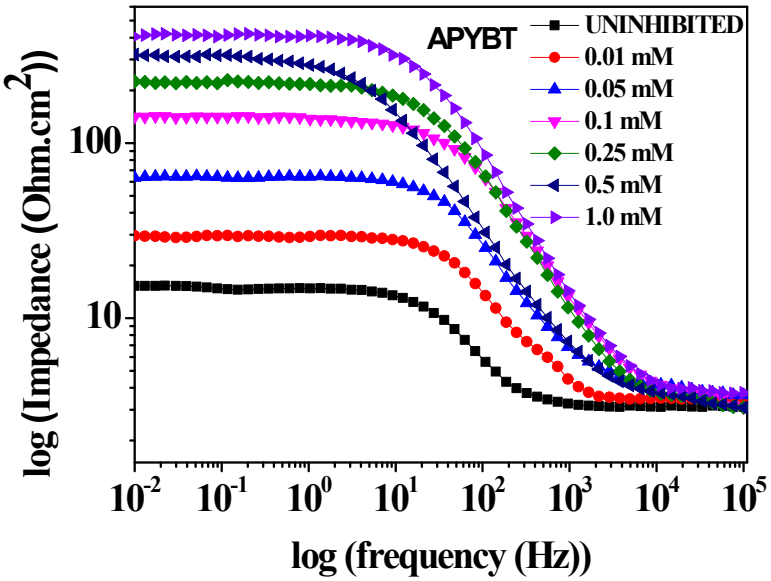


Fig. S4 B

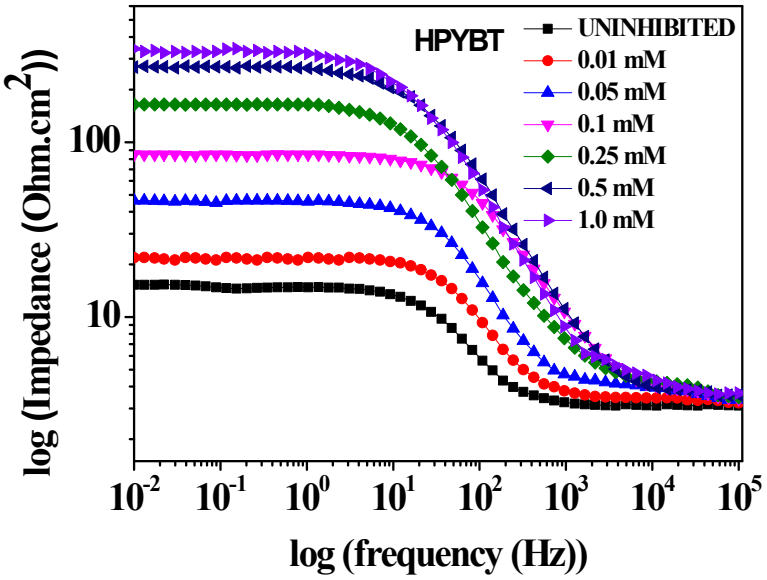


Fig. S4 C

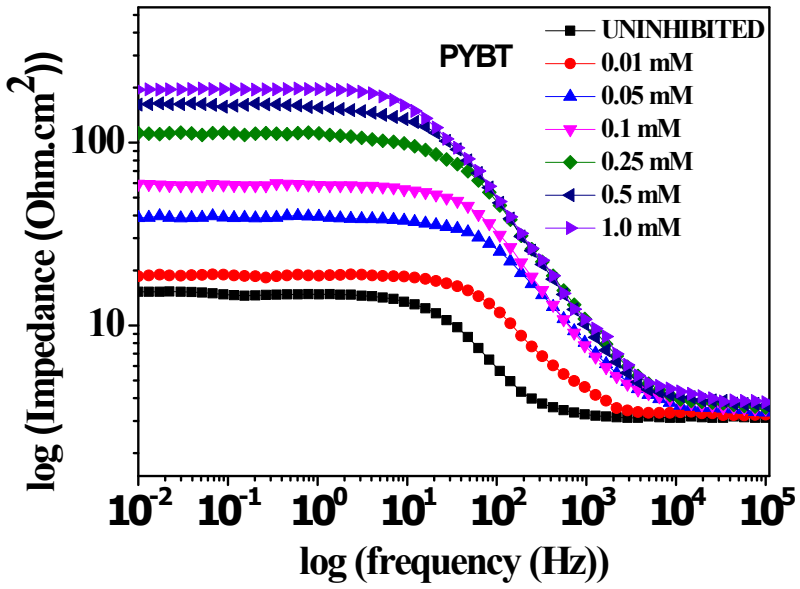


Fig. S4 (A-C) Bode impedance plots of mild steel in 1M HCl containing (A) APYBT (B) HPYBT and (C) PYBT inhibitors.

Fig S5 A

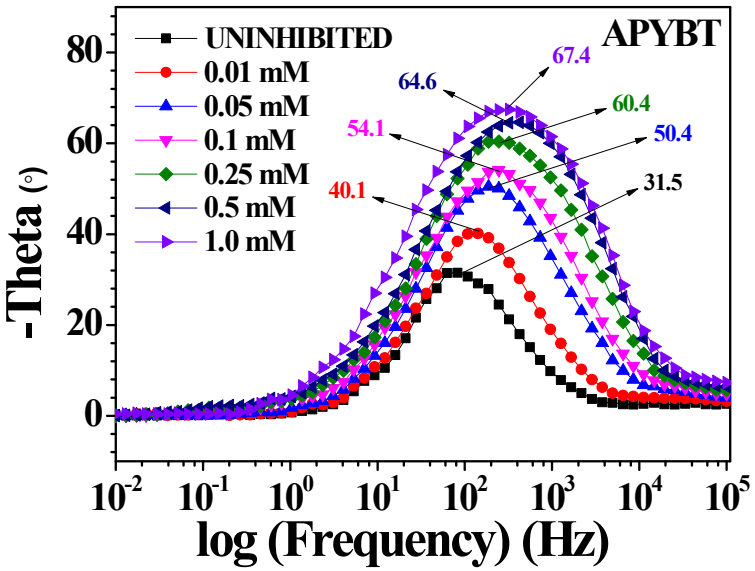


Fig. S5 B

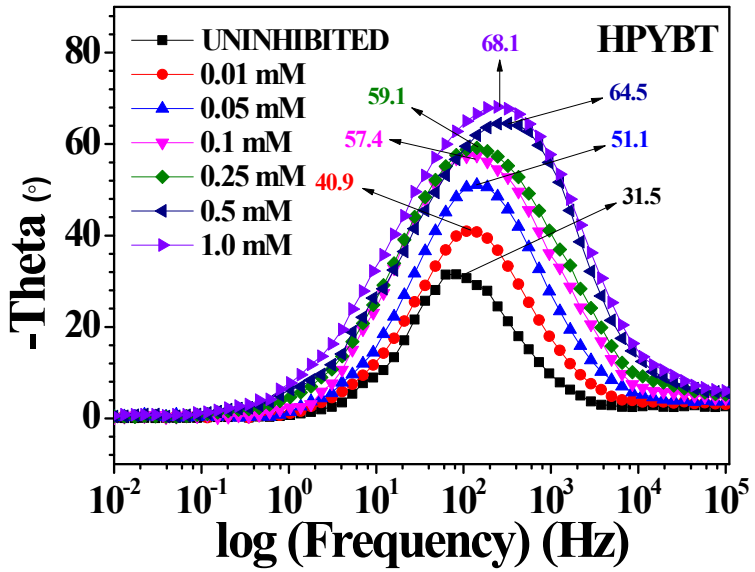


Fig. S5 C

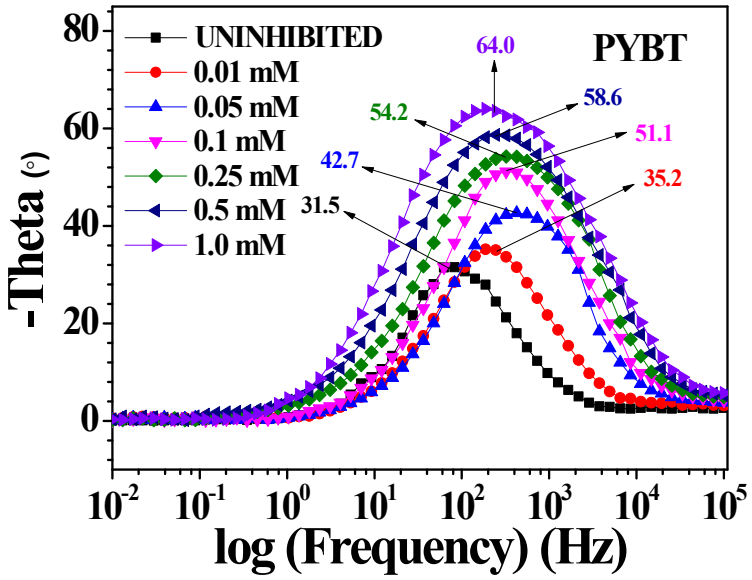


Fig. S5 (A-C) Bode phase angle plots of mild steel in 1M HCl containing (A) APYBT (B) HPYBT and (C) PYBT inhibitors.

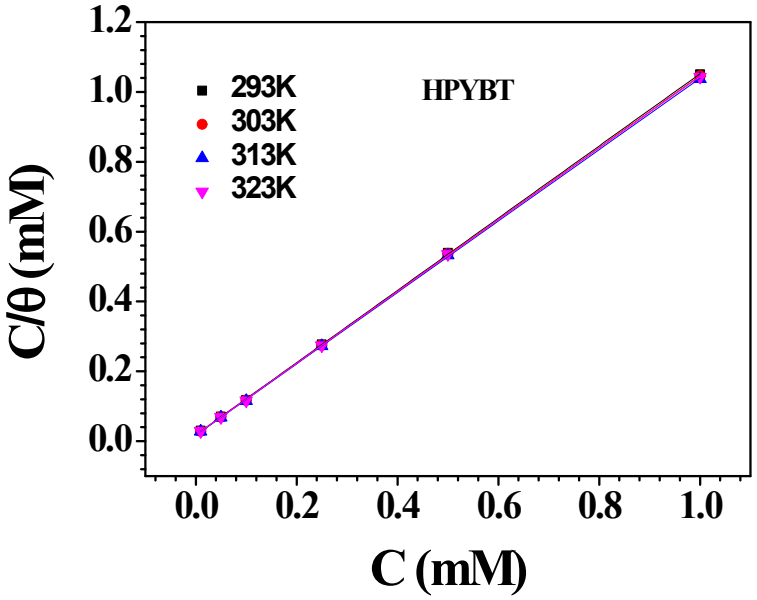


Fig. S6 Langmuir adsorption isotherm for mild steel in 1M HCl with HPYBT inhibitor

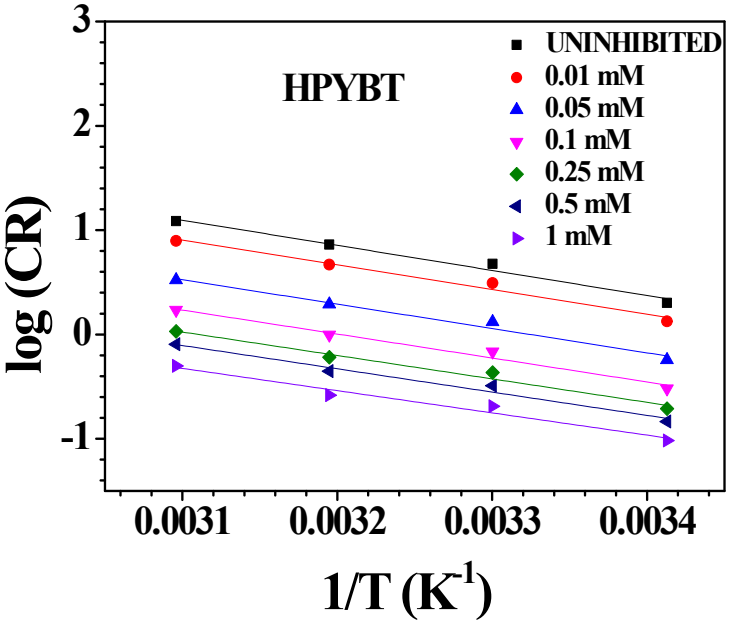


Fig. S7 Arrhenius plots for mild steel in 1M HCl solution with HPYBT inhibitor

Fig. S8 A

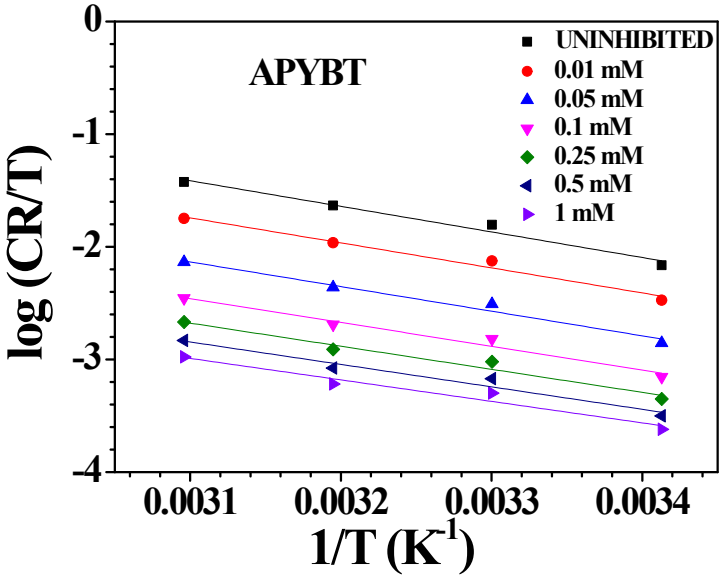


Fig. S8 B

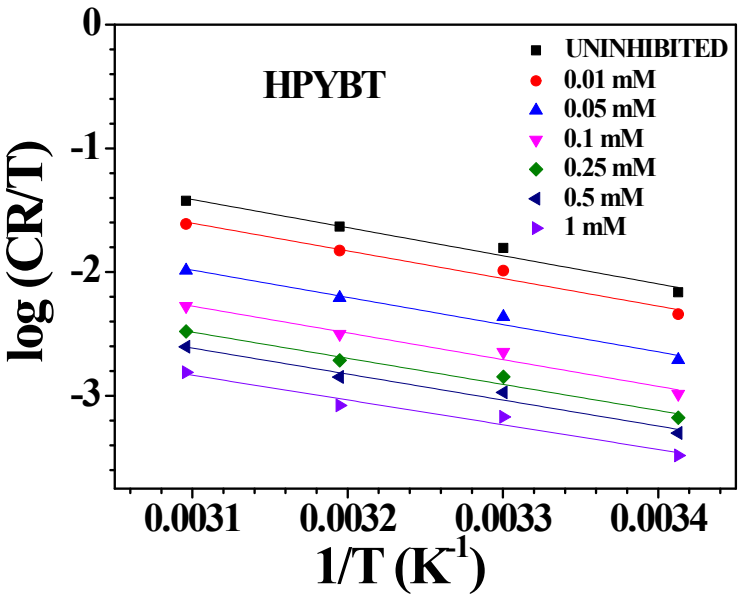


Fig. S8 C

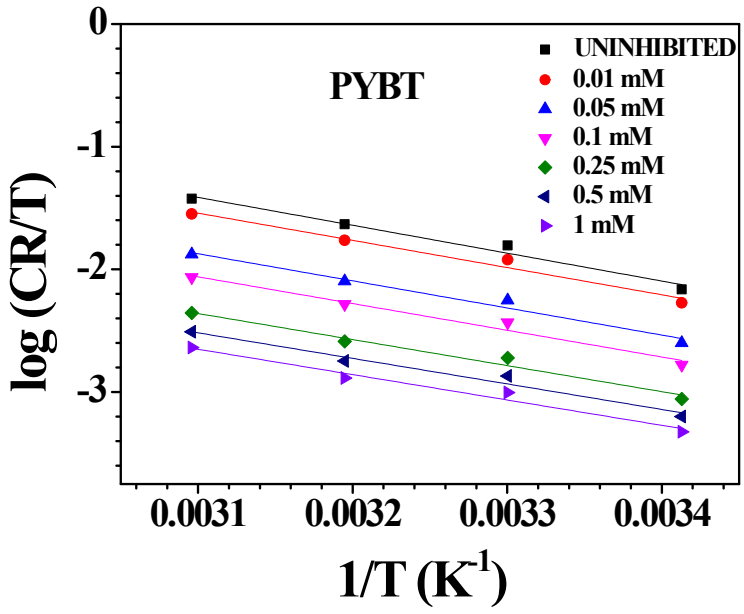


Fig. S8 (A-C) Arrhenius plots for mild steel in 1M HCl containing (A) APYBT, (B) HPYBT and (C) PYBT

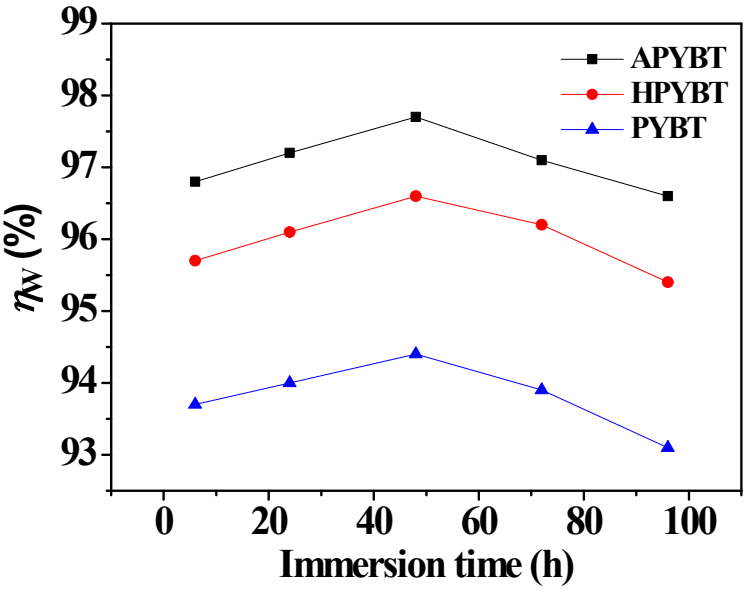


Fig. S9 Variation of the inhibition efficiency at 1 mM inhibitor concentration against immersion time at 30 ºC

Fig. S10 A

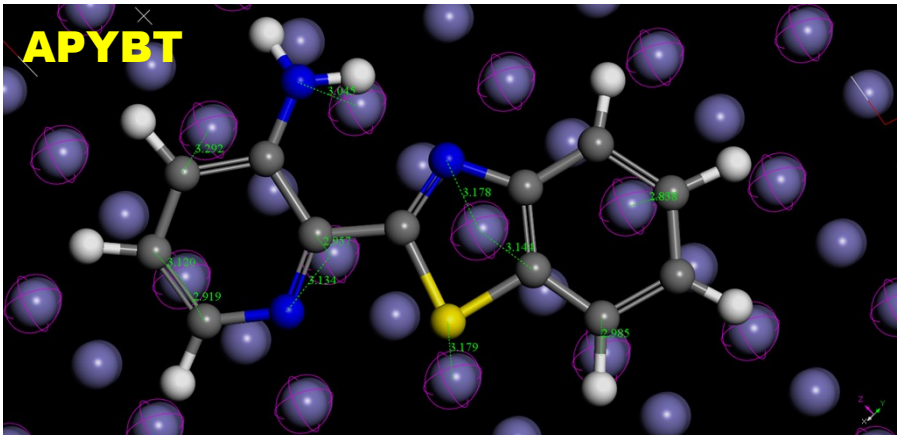


Fig. S10 B

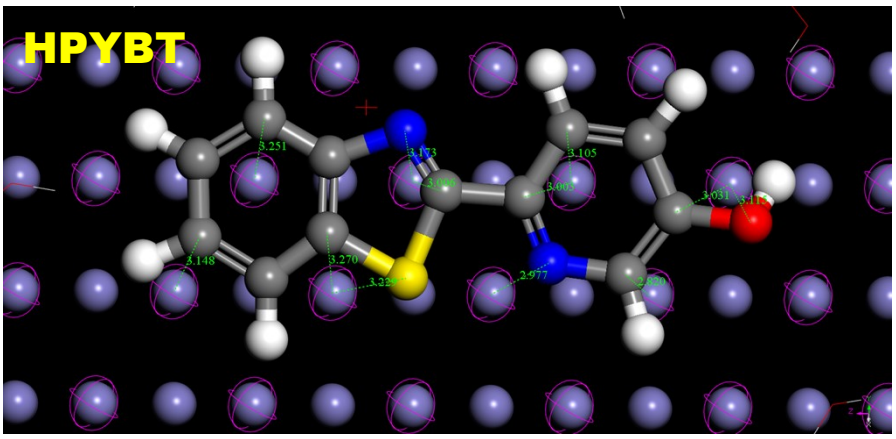


Fig. S10 C

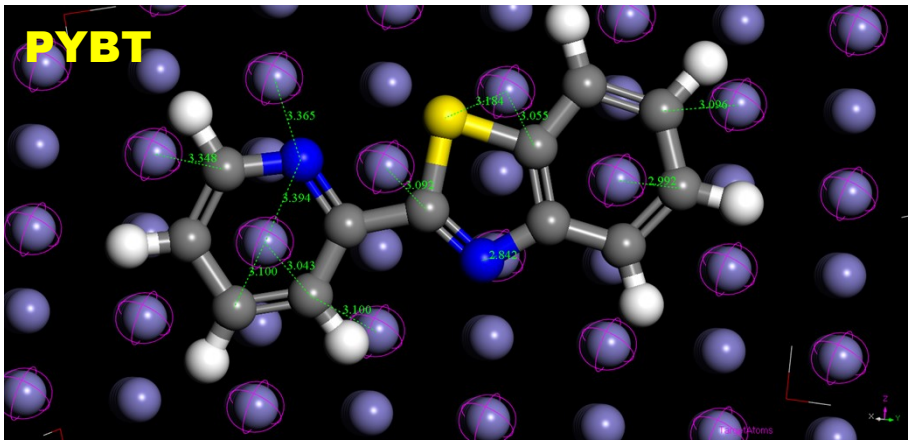


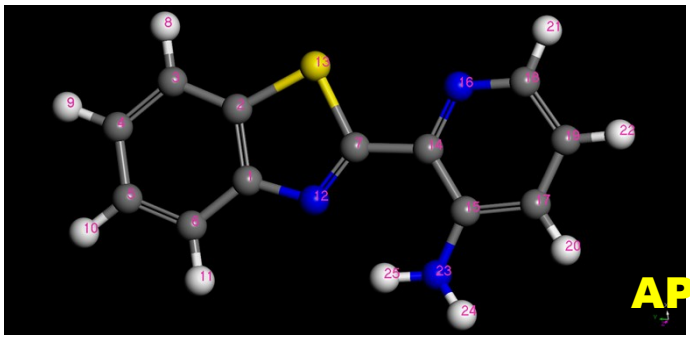
Fig. S10 (A-C) Closest distance of mild steel surface and atoms of APYBT, HPYBT & PYBT as obtained from MD simulation study

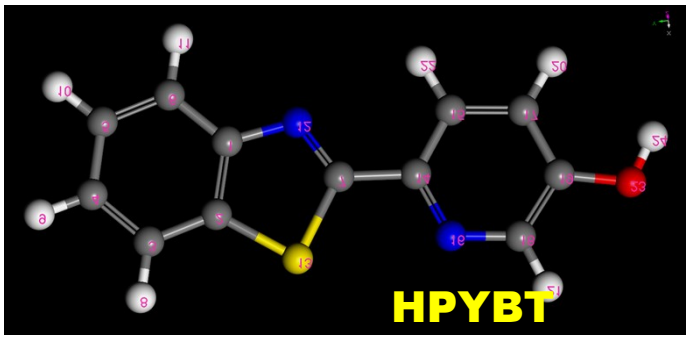
Table S1 Corrosion rate of mild steel in 1 M HCl in absence and presence of inhibitors (1 mM concentration) at different exposure times at 30 °C

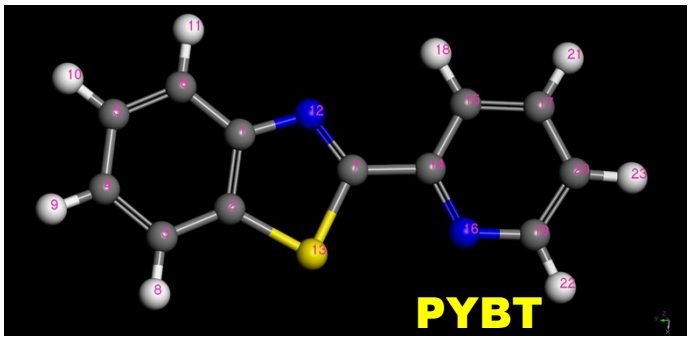
Exposure Time (h)	Inhibitor	Weight loss (mg)	Corrosion Rate (mg cm^{-2} h^{-1})	η_w (%)
6	UNINHIBITED	384.9	4.752	
	APYBT	12.3	0.152	96.8
	HPYBT	16.6	0.204	95.7
	PYBT	24.2	0.299	93.7
24	UNINHIBITED	1630.4	5.032	
	APYBT	45.7	0.141	97.2
	HPYBT	63.6	0.196	96.1
	PYBT	97.8	0.302	94.0
48	UNINHIBITED	2547.6	3.931	
	APYBT	58.6	0.090	97.7
	HPYBT	86.6	0.134	96.6
	PYBT	142.7	0.220	94.4
72	UNINHIBITED	2970.3	3.056	
	APYBT	86.1	0.089	97.1
	HPYBT	112.9	0.116	96.2
	PYBT	181.2	0.186	93.9
96	UNINHIBITED	3279.8	2.532	
	APYBT	111.5	0.086	96.6
	HPYBT	150.9	0.116	95.4
	PYBT	226.3	0.175	93.1

Table S2 Calculated Fukui functions of the atoms present in APYBT, HPYBT & PYBT respectively

	APYBT		HPYBT		PYBT	
Atoms	f_k^+	f_k^-	f_k^+	f_k^-	f_k^+	f_k^-
C (1)	0.022	0.031	0.024	0.053	0.022	0.073
C (2)	0.025	0.031	0.026	0.047	0.026	0.059
C (3)	0.028	0.019	0.031	0.029	0.029	0.039
C (4)	0.046	0.041	0.049	0.070	0.047	0.095
C (5)	0.025	0.029	0.027	0.045	0.026	0.059
C (6)	0.039	0.024	0.043	0.037	0.040	0.046
C (7)	0.074	0.017	0.083	0.039	0.078	0.057
H (8)	0.015	0.012	0.017	0.018	0.016	0.024
H (9)	0.020	0.017	0.022	0.027	0.021	0.036
H (10)	0.014	0.014	0.015	0.022	0.014	0.028
H (11)	0.019	0.013	0.021	0.020	0.020	0.026
N (12)	0.071	0.038	0.084	0.052	0.085	0.053
S (13)	0.105	0.070	0.115	0.079	0.113	0.089
C (14)	0.048	0.073	0.054	0.052	0.063	0.031
C (15)	0.037	0.058	0.048	0.049	0.052	0.049
N (16)	0.071	0.035	0.069	0.037	0.066	0.030
C (17)	0.063	0.051	0.043	0.037	0.052	0.026
C (18)	0.045	0.087	0.040	0.062	-	-
H (18)	-	-	-	-	0.027	0.021
C (19)	0.080	0.047	0.063	0.061	0.040	0.040
H (20)	0.029	0.026	0.022	0.020	-	-
C (20)	-	-	-	-	0.080	0.060
H (21)	0.024	0.035	0.022	0.027	0.026	0.015
H (22)	0.035	0.025	0.026	0.023	0.023	0.019
N (23)	0.032	0.127	-	-	-	-
O (23)	-	-	0.040	0.070	-	-
H (23)	-	-	-	-	0.034	0.023
H (24)	0.017	0.044	0.017	0.024	-	-
H (25)	0.017	0.039	-	-	-	-




HPYBT


PYBT