Anticorrosive performance of thiophene based inhibitor-reinforced PVB coating on mild steel; An Inclusive approach on the structural advantage of corrosion inhibitor

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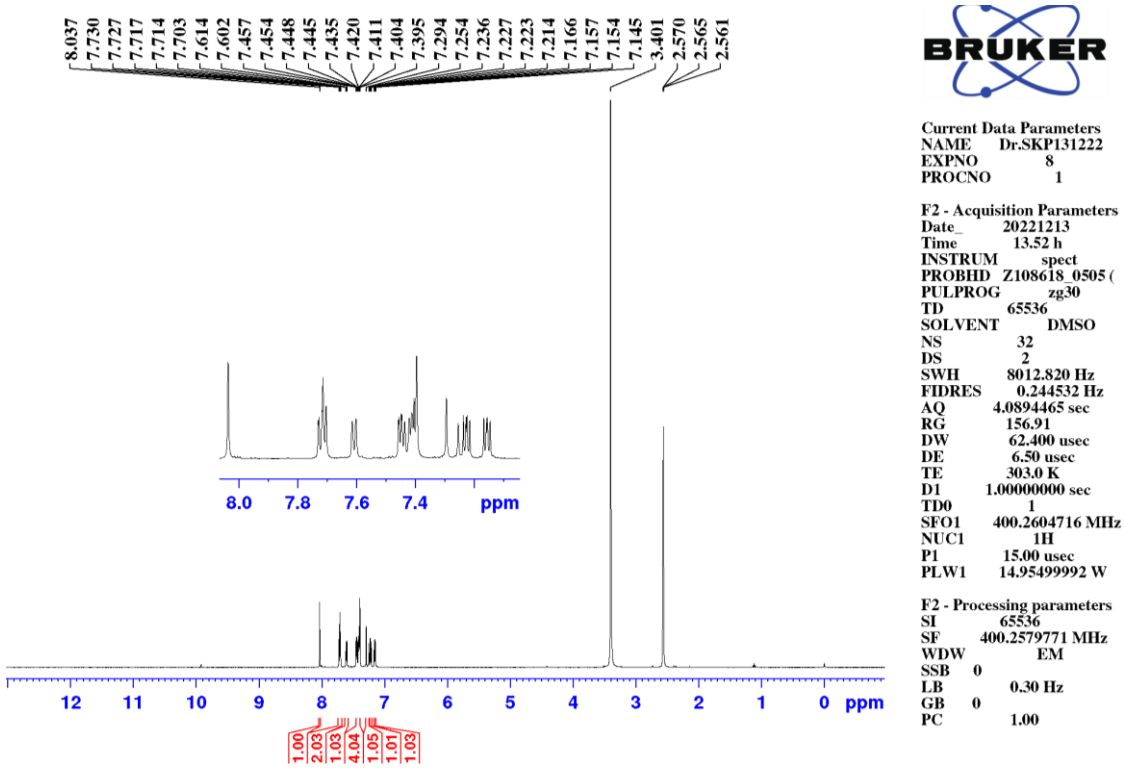

Fig. S1 ^{1}H NMR spectrum of **DTT**

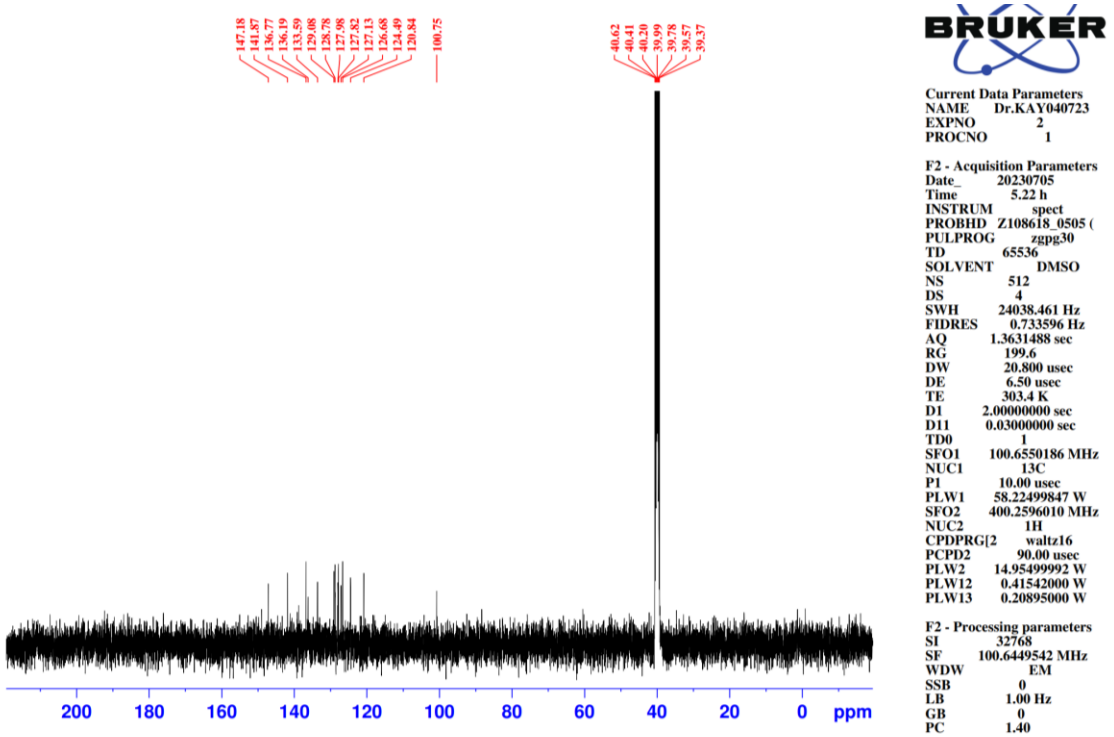

Fig. S2 ^{13}C NMR spectrum of **DTT**

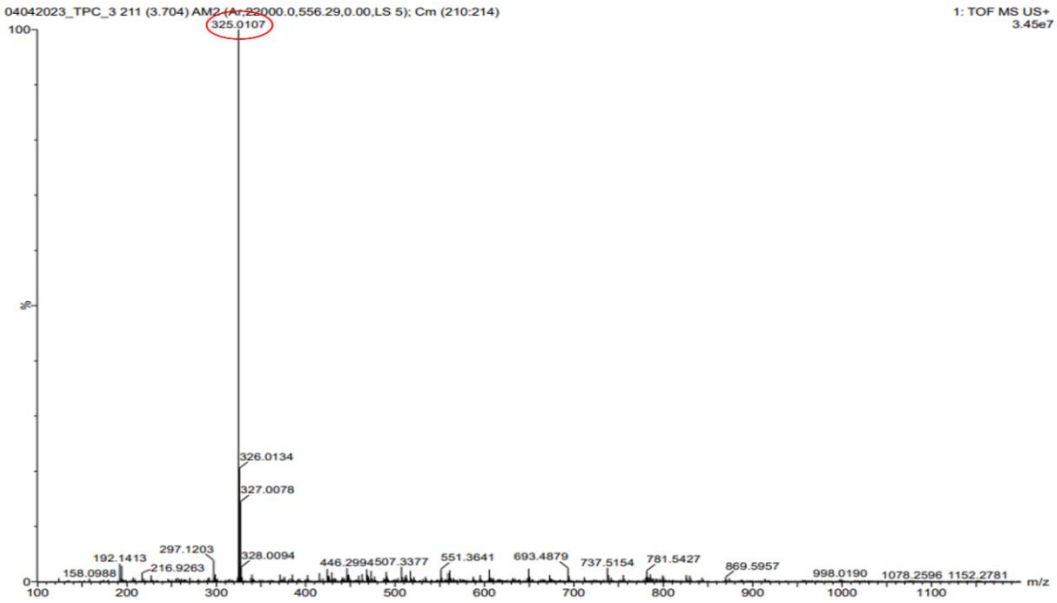

Fig. S3 HRMS data of **DTT**

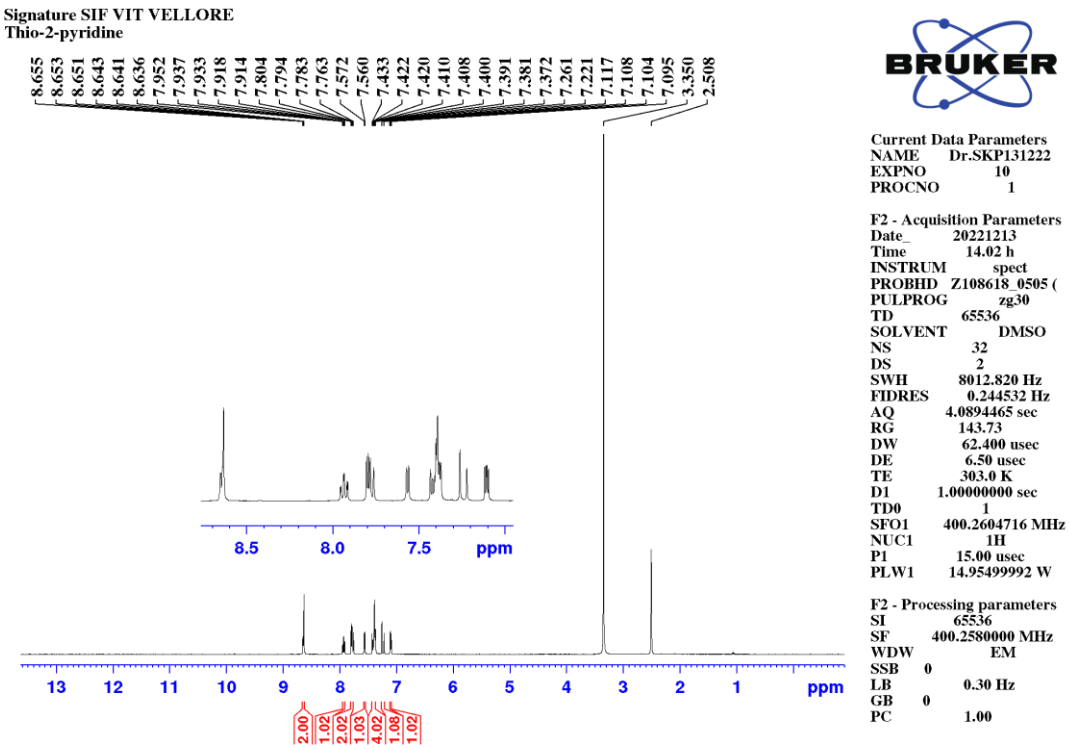

Fig. S4 ^{1}H NMR spectrum of **DTP**

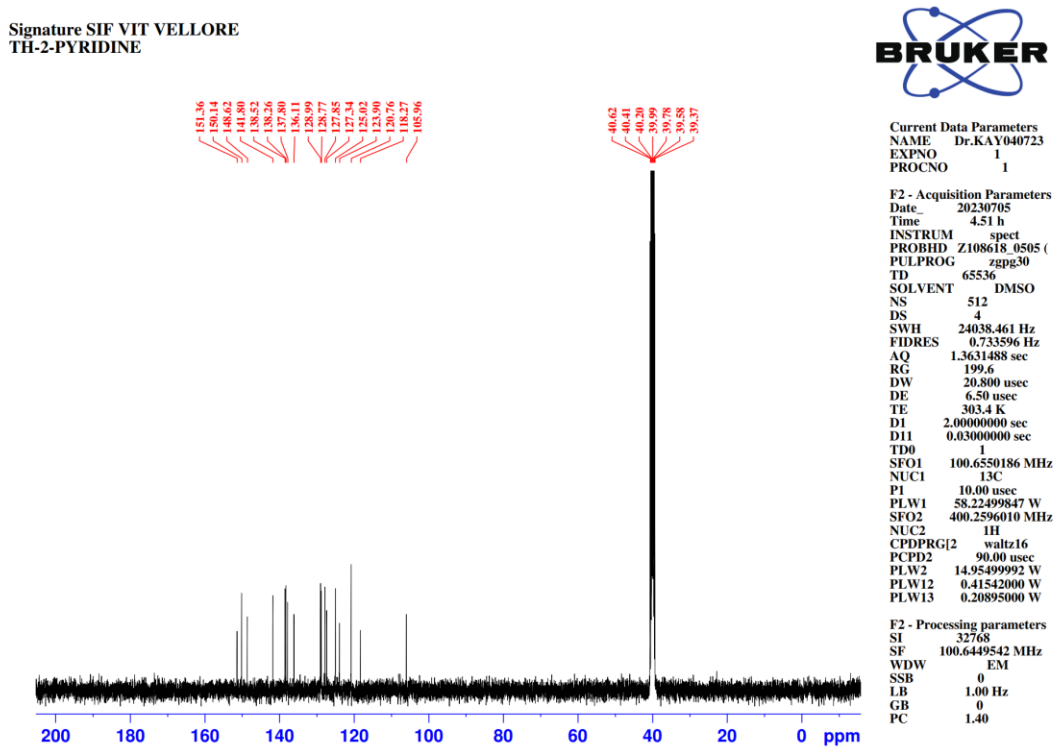

Fig. S5 ^{13}C NMR spectrum of **DTP**

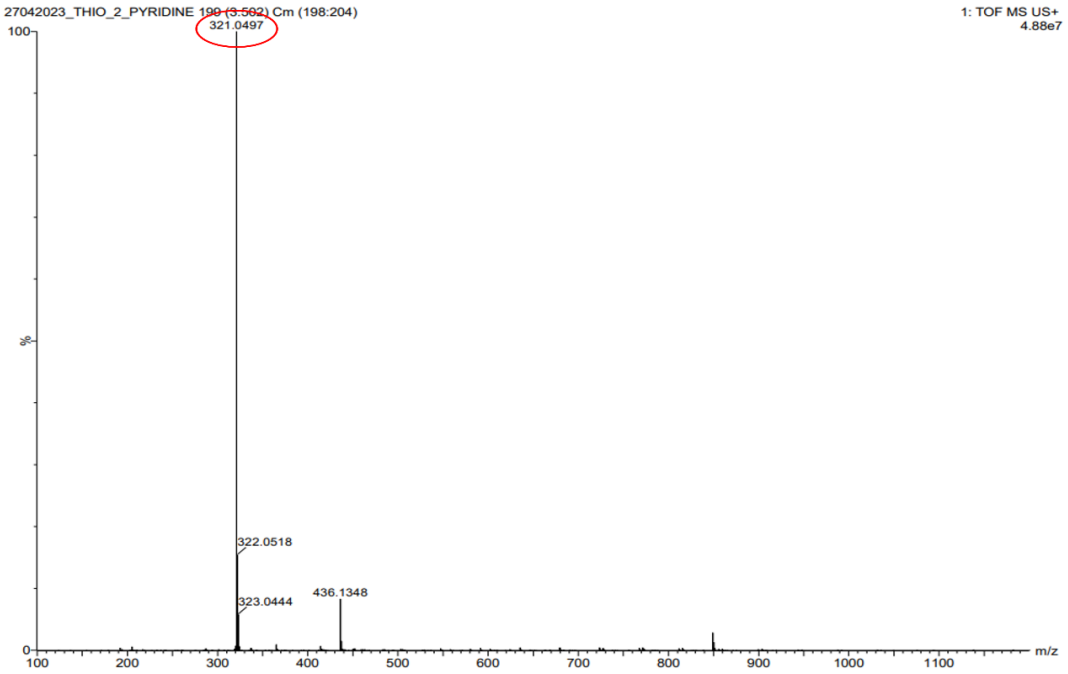

Fig. S6 HRMS data of **DTP**

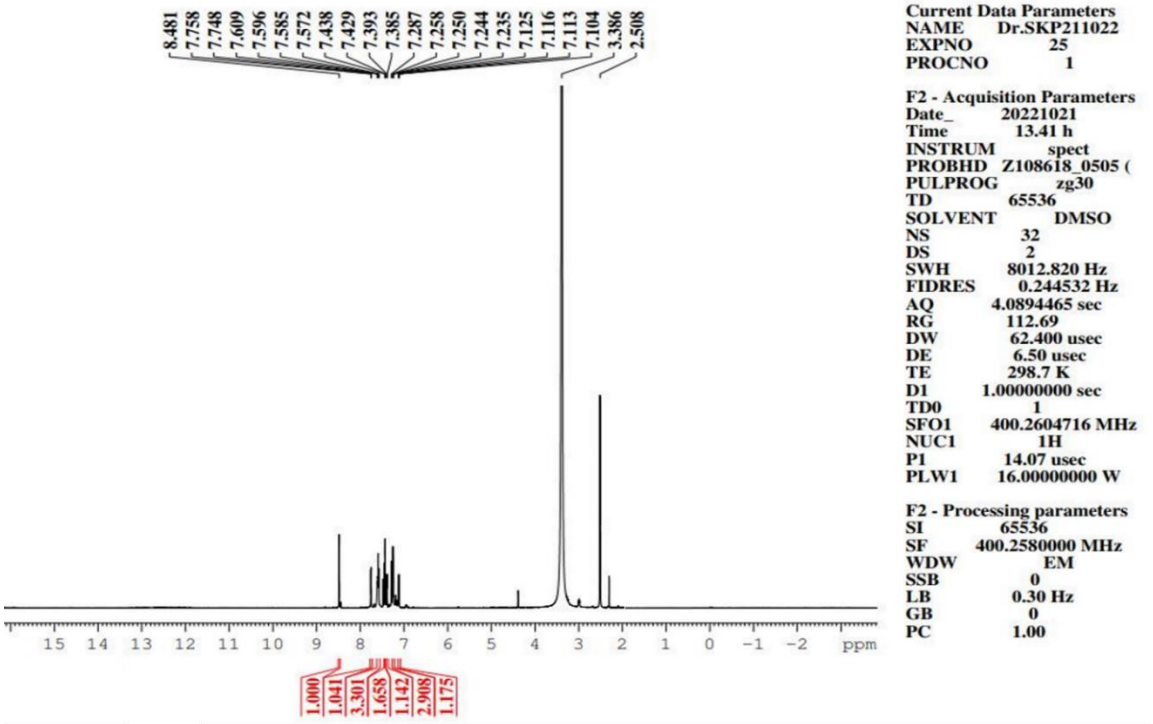

Fig. S7 ^{1}H NMR spectrum of **DTB**

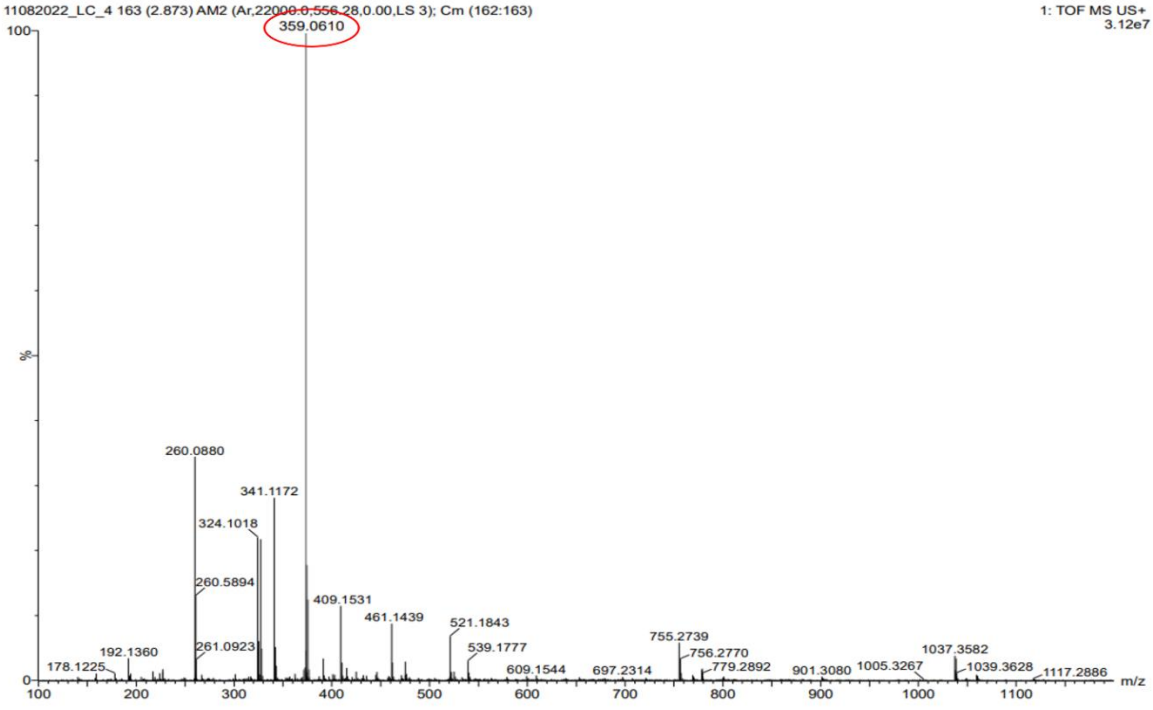

Fig. S8 HRMS data of **DTB**

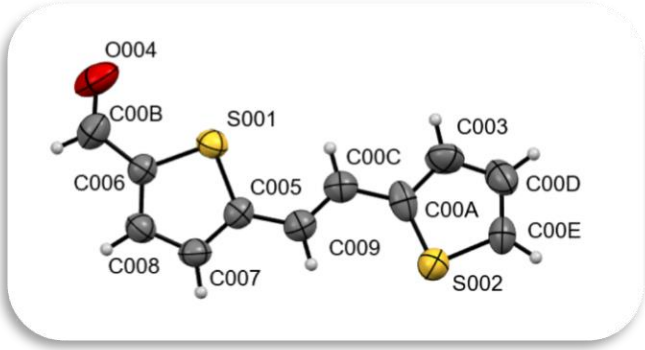

Fig. S9 Single crystal X-ray structure of TH-CHO with atomic labelling (thermal ellipsoid at 50% probability level)

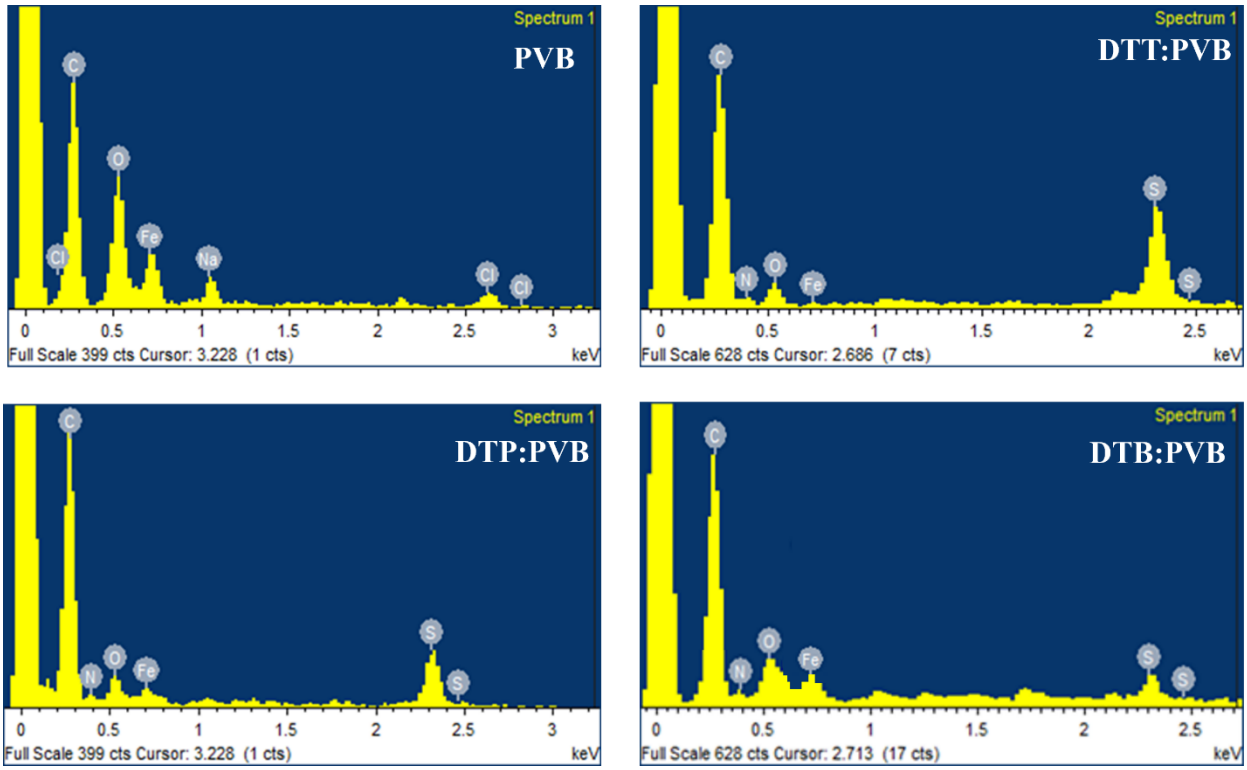

Fig. S10 EDS analysis of MS surface coated with different inhibitor mixture

Table S1. Crystal data and structural refinement of receptor **L2**.

CCDC number	2270806
Empirical formula	C_{11} H_8 O S_2
Formula weight	220.318
Temperature	300 K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P1-21/n 1
Unit cell dimensions	a = 6.0042(9) Å α = 90° b = 20.645(3) Å β = 103.459(5)° c = 8.6691(13) Å γ = 90°
Volume	1045.1(3) $Å^3$
Z, Calculated density	4, 1.400 Mg/m^3
Absorption coefficient	0.6406 (min), 0.7457 (max) mm^{-1}
F(000)	457.196
Crystal size	0.1 x 0.14 x 0.25 mm
Theta range for data collection	2.61 to 28.21 deg.
Limiting indices	-7<=h<=7, -27<=k<=27, -11<=l<=11
Reflections collected / unique	2564/197 [R(int) = 0.0611]
Completeness to theta = 28.28	99.5 %
Max transmission	0.8591
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2574 / 26 / 149
Goodness-of-fit on F^2	1.1054
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1070
R indices (all data)	R1 = 0.0661, wR2 = 0.1259
Largest diff. peak and hole	0.5757 and -0.2703 e. $Å^{-3}$

Table S2. Coating proportion of PVB:Inhibitors on MS surface.

Percentage ratio (PVB:Inhibitors)	DTT Code	DTP Code	DTB Code
100:0	DTT-0	DTP-0	DTB-0
80:20	DTT-20	DTP-20	DTB-20
50:50	DTT-50	DTP-50	DTB-50
20:80	DTT-80	DTP-80	DTB-80

Table S3. Elemental composition obtained from EDS analysis (Atomic weight percentage)

Element	**PVB**	**DTT: PVB**	**DTP: PVB**	**DTB: PVB**
C	58.02	71.9	72.58	76.50
O	24.17	6.32	5.71	6.75
N	-	8.3	10	9.29
S	-	12.5	10.05	6.88
Fe	11.42	0.98	1.68	0.59