

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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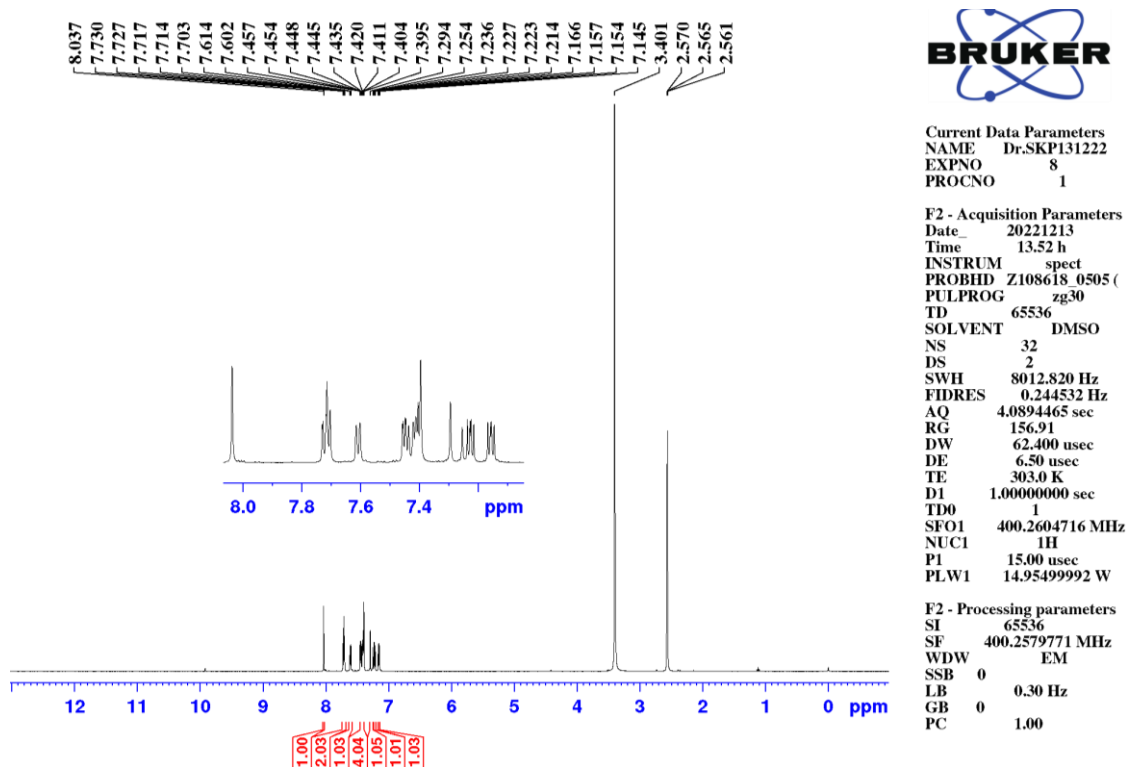


Fig. S1 ^1H NMR spectrum of DTT

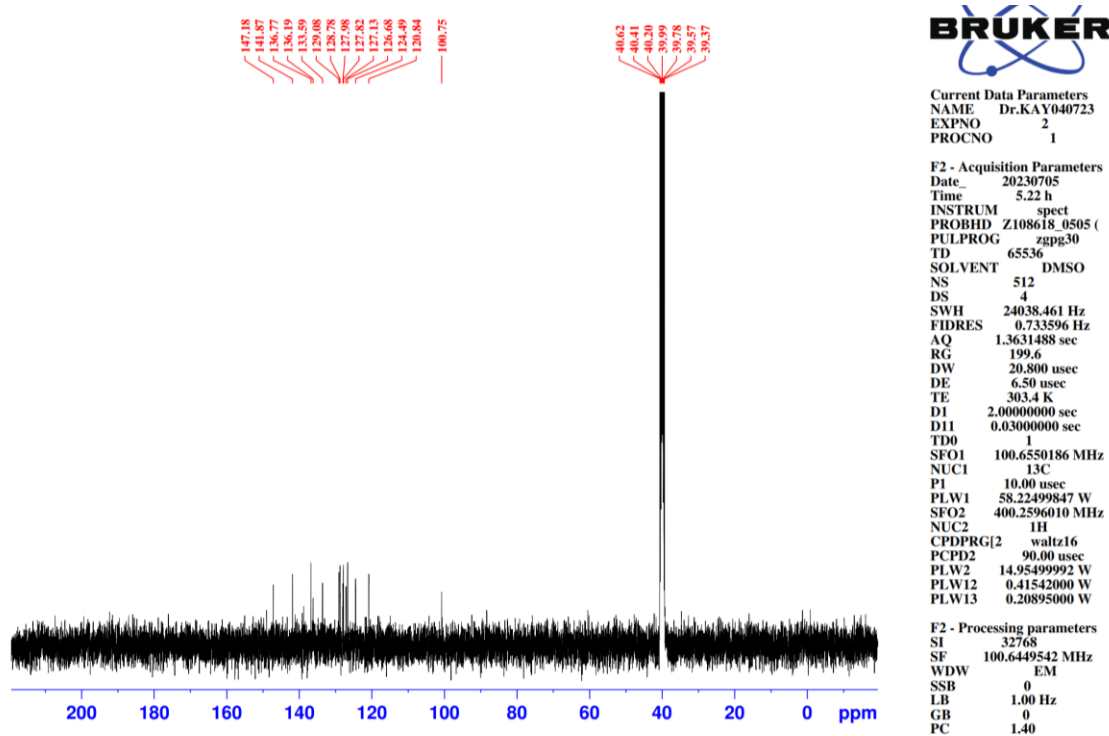


Fig. S2 ^{13}C NMR spectrum of DTT

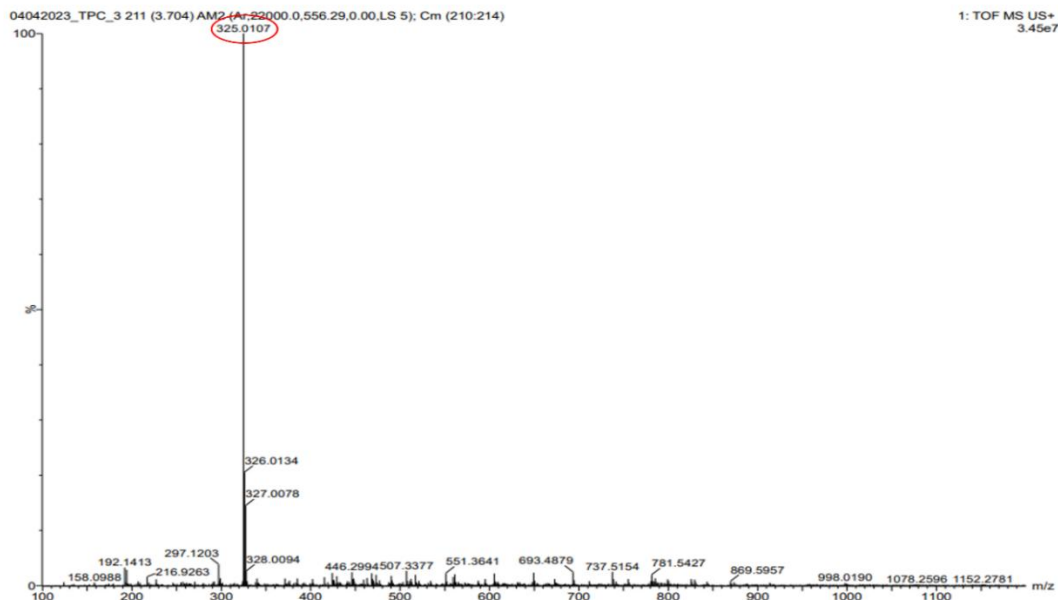
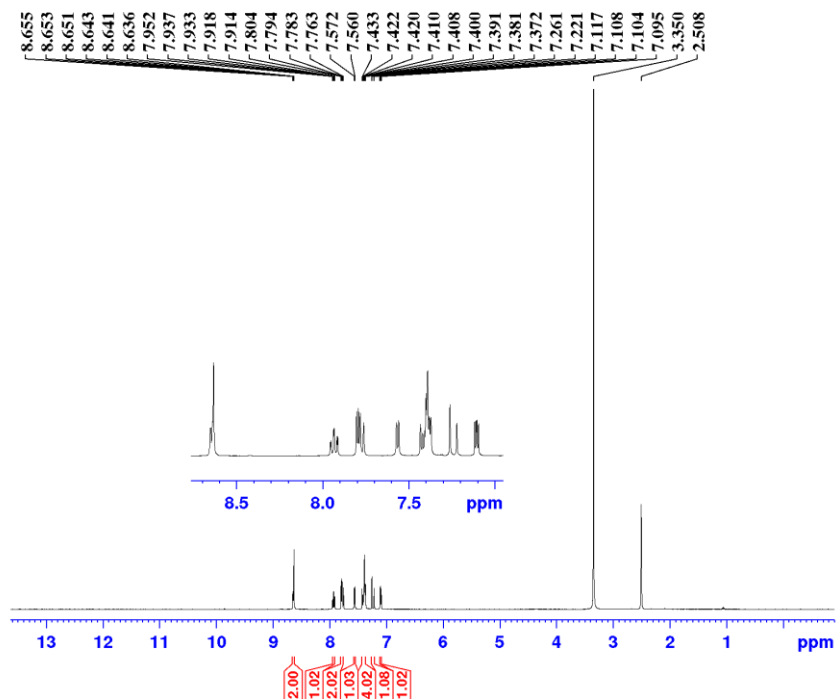


Fig. S3 HRMS data of **DTT**

Signature SIF VIT VELLORE
Thio-2-pyridine



Current Data Parameters
NAME Dr.SKPI31222
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221213
Time 14.02 h
INSTRUM spect
PROBHD Z108618_0505 (Z108618)
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.73
DW 62.400 usec
DE 6.50 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 15.00 usec
PLW1 14.95499992 W

F2 - Processing parameters
SI 65536
SF 400.2580000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Fig. S4 ¹H NMR spectrum of **DTP**

Signature SIF VIT VELLORE
TH-2-PYRIDINE

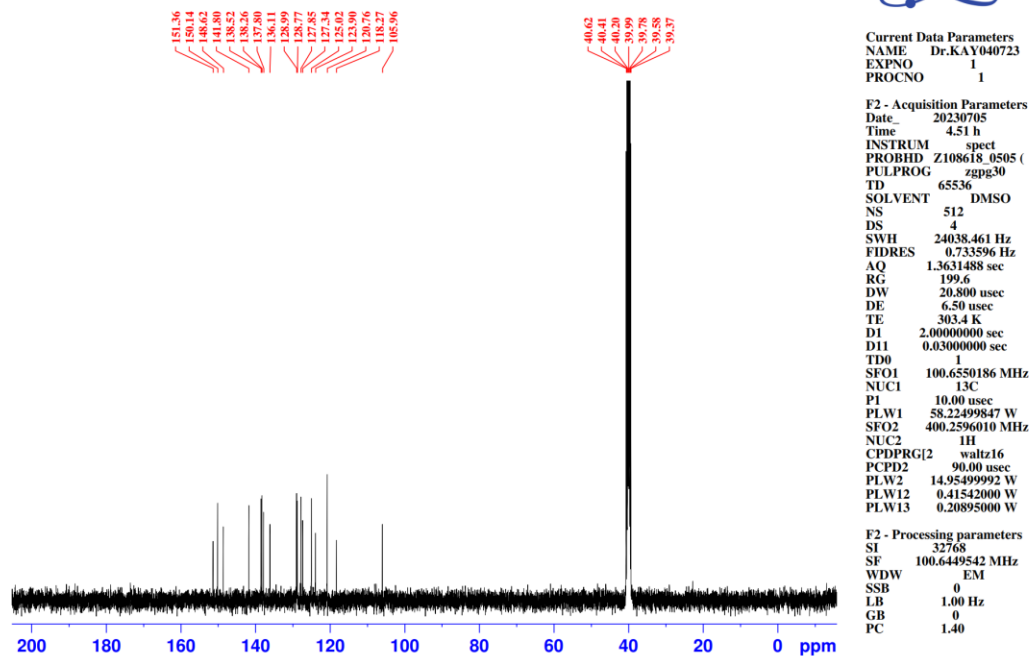


Fig. S5 ^{13}C NMR spectrum of **DTP**

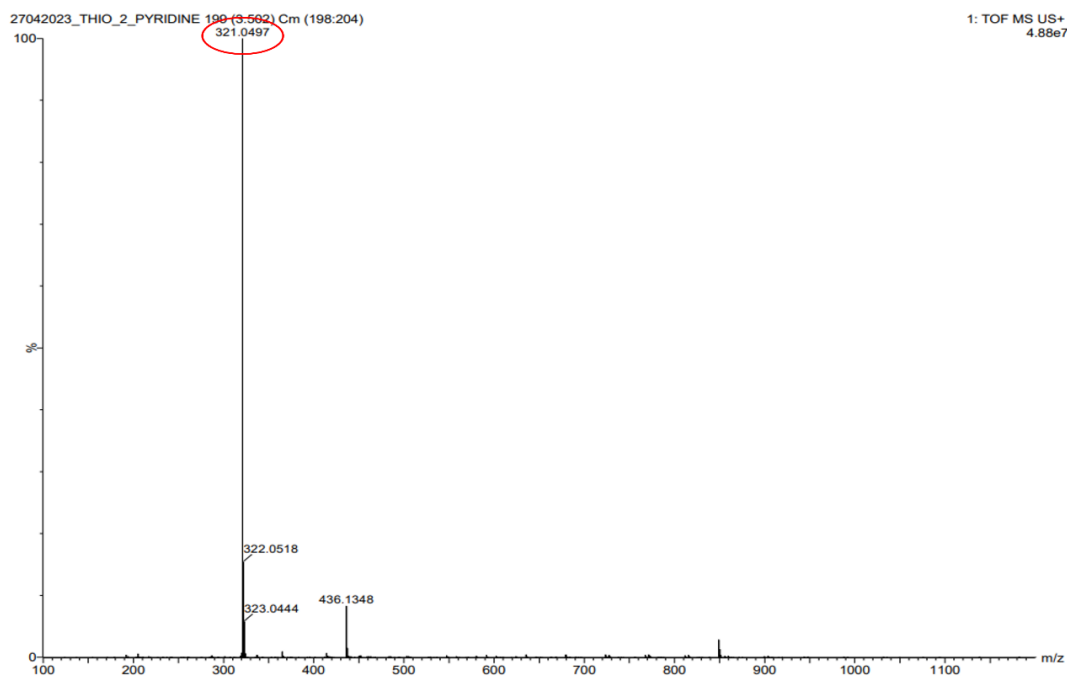


Fig. S6 HRMS data of **DTP**

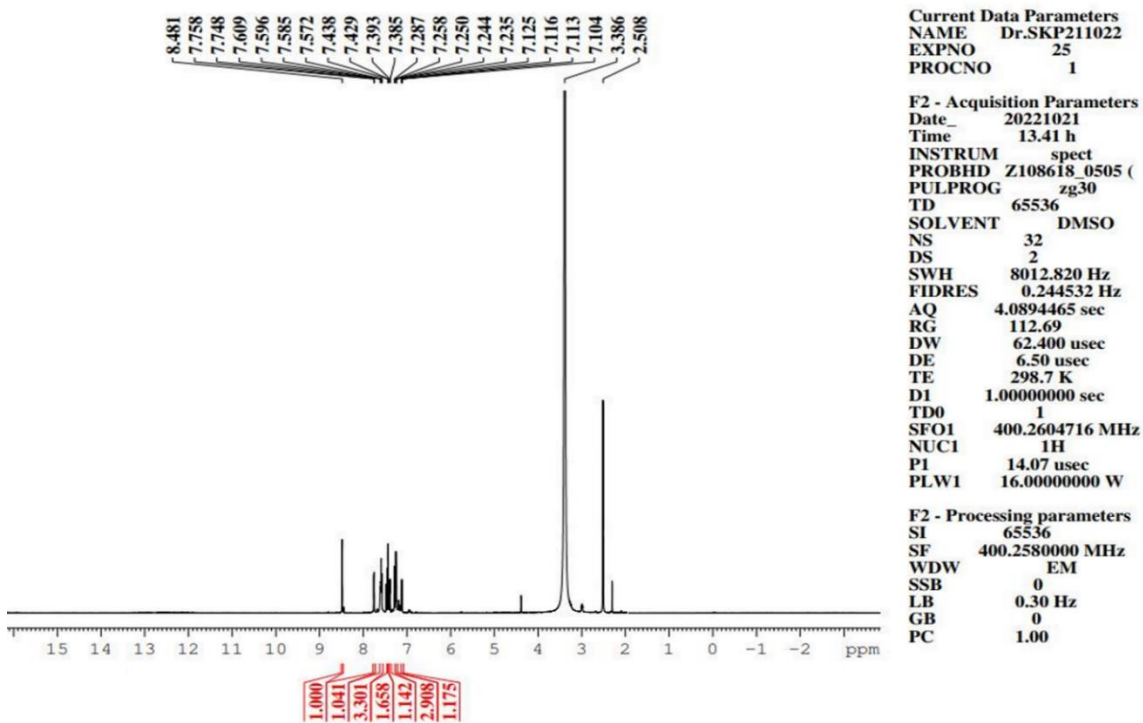


Fig. S7 ^1H NMR spectrum of **DTB**

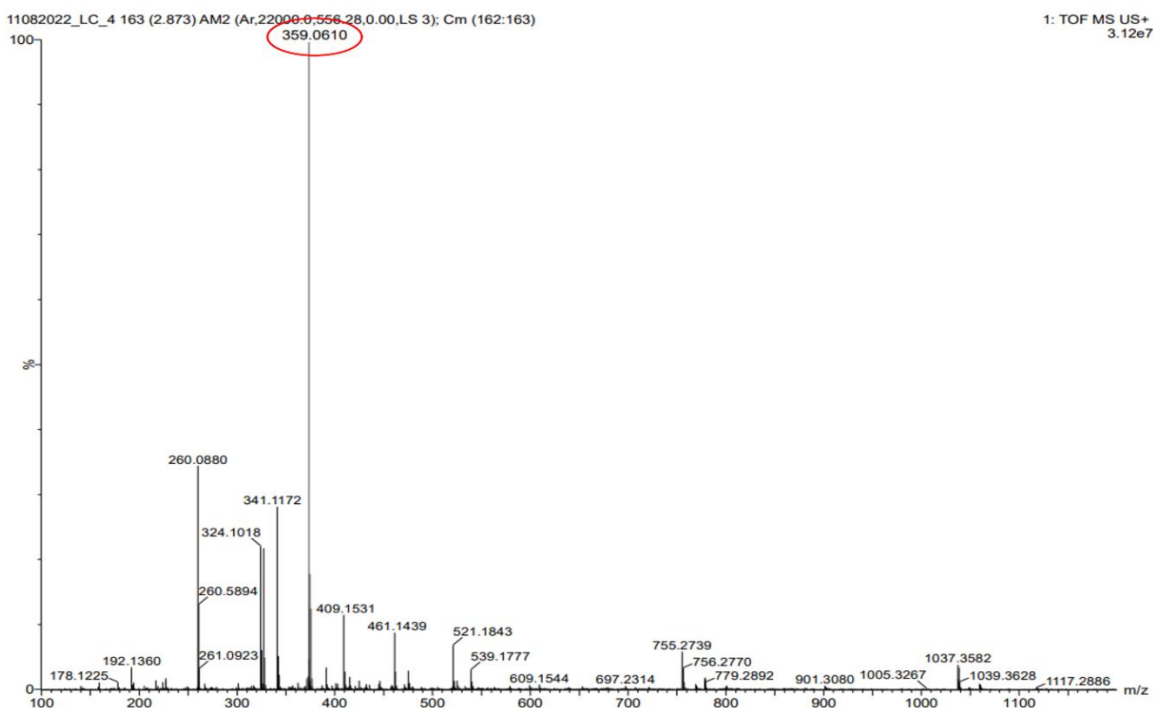


Fig. S8 HRMS data of **DTB**

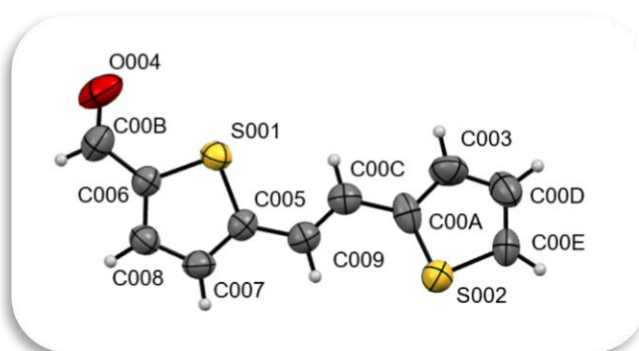


Fig. S9 Single crystal X-ray structure of TH-CHO with atomic labelling (thermal ellipsoid at 50% probability level)

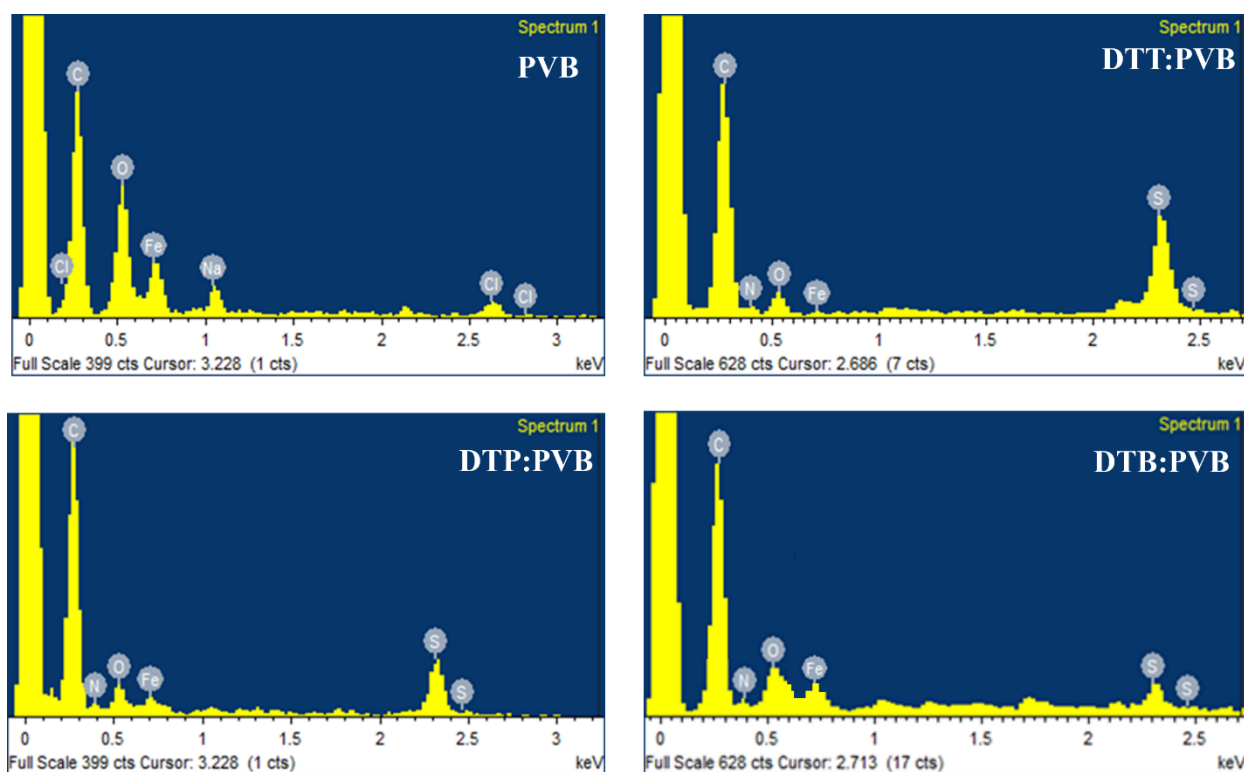


Fig. S10 EDS analysis of MS surface coated with different inhibitor mixture

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<= <i>h</i> <=7, -27<= <i>k</i> <=27, -11<= <i>l</i> <=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>I</i> >2σ(<i>I</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