Journal of the Serbian Chemical Society
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J. Serb. Chem. Soc. *87* (12) S480–S487 (2022) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Anticorrosion activity of 2-thiohydantoin–Shiff base derivatives for mild steel in 0.5 M HCl

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J. Serb. Chem. Soc. *87* (12) (2022) 1409–1423

*3-[(phenylmethylene)amino]-2-thioxo-4-imidazolidinone (**1**)*

Yield 1.158 g (72 %). IR (KBr): 3419m, 3055m, 3032w, 2967m, 2768m, 1711s, 1645s, 1591s, 1490w, 1445w, 1409w, 1345m, 1327m, 1310m, 1249s, 1225m, 1213m, 1074w, 1039w, 969m, 877m, 854m, 835m, 788m, 756m, 734m, 713m 695m, 629w cm^{-1}. ^1H NMR (200 MHz, DMSO-d_6, δ): 8.40 (*s*, 1H), 7.75 (*m*, 2H), 7.45 (*m*, 3H), 3.89 (*s*, 2H). ^{13}C NMR (50 MHz, DMSO-d_6, δ): 174.33, 165.51, 156.31, 134.31, 130.76, 128.96, 127.76, 33.26.

*3-[(2-hydroxybenzylidene)amino]-2-thioxoimidazolidin-4-one (**2**)*

Yield 2.102 g (89 %). IR (KBr): 3441m, 3318m, 3031w, 2958m, 2776m, 1718s, 1640s, 1623s, 1568w, 1492w, 1469w, 1334m, 1317m, 1266m, 1254m, 1204m, 1149w, 890w, 838w, 757m, 735m, 710m, 637w cm^{-1}. ^1H NMR (200 MHz, DMSO-d_6, δ): 12.09 (*bs*, NH, exchangeable with D_2O), 10.88 (*s*, OH, exchangeable with D_2O), 8.64 (*s*, 1H), 7.58 (*dd*, 1H, J_1 = 8.0, J_2 = 1.9 Hz), 7.32 (*dt*, 1H, J_1 = 7.8, J_2 = 1.8 Hz), 6.95 (*m*, 2H), 3.97 (*s*, 2H). ^{13}C NMR (50 MHz, DMSO-d_6, δ): 173.77, 164.44, 158.01, 157.76, 132.17, 130.62, 119.54, 118.50, 116.38, 33.46.

*3-[(2-furanylmethylene)amino]-2-thioxo-4-imidazolidinone (**3**)*

Yield 1.186 g (57 %). IR (KBr): 3434m, 3153w, 3114m, 3023m, 2949m, 2752m, 1713s, 1642s, 1594s, 1476m, 1436m, 1390w, 1360m, 1320s, 1249s, 1206m, 1154m, 1074w, 1044w, 1018m, 964w, 939m, 895m, 884m, 852m, 824m, 787m, 771m, 732m, 677w, 599w, 514m cm^{-1}. ^1H NMR (200 MHz,

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DMSO-d_6, δ): 8.21 (*s*, 1H), 7.85 (*d*, 1H, J = 1.8 Hz), 6.95 (*d*, 1H, J = 3.4 Hz), 6.64 (*dd*, 1H, J_1 = 3.6, J_2 = 1.8 Hz), 3.87 (*s*, 2H). ^{13}C NMR (50 MHz, DMSO-d_6, δ): 174.32, 165.00, 149.48, 146.00, 145.77, 115.88, 112.59, 33.40.

*3-[[(4-hydroxy-3-methoxyphenyl)methylene]amino]-2-thioxo-4-imidazolidinone (**4**)*

Yield 2.540 g (96 %). IR (KBr): 3393m, 2938m, 2774m, 1696s, 1640s, 1613s, 1513m, 1472m, 1435m, 1398w, 1326m, 1271m, 1248s, 1210m, 1167m, 1123w, 1042w, 803w, 768w, 737w, 155w, 519w cm^{-1}. ^{1}H NMR (200 MHz, DMSO-d_6, δ): 11.83 (*bs*, NH, exchangeable with D_2O), 9.63 (*s*, OH, exchangeable with D_2O), 8.26 (*s*, 1H), 7.32 (*d*, 1H, J = 1.6 Hz), 7.19 (*dd*, 1H, J_1 = 8.2, J_2 = 1.6 Hz), 3.87 (*s*, 2H), 3.80 (*s*, 3H). ^{13}C NMR (50 MHz, DMSO-d_6, δ): 174.13, 163.50, 156.22, 149.50, 147.91, 125.75, 122.18, 115.69, 110.66, 55.70, 33.08.

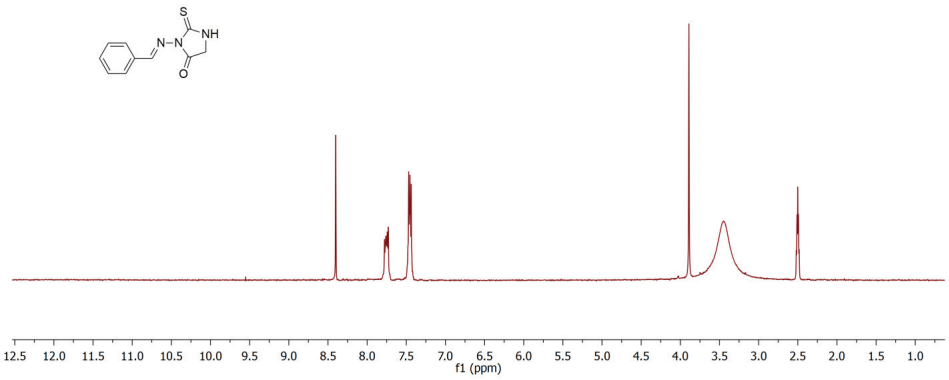

Fig. S-1. ^{1}H NMR spectra of 3-[(phenylmethylene)amino]-2-thioxo-4-imidazolidinone (**1**)

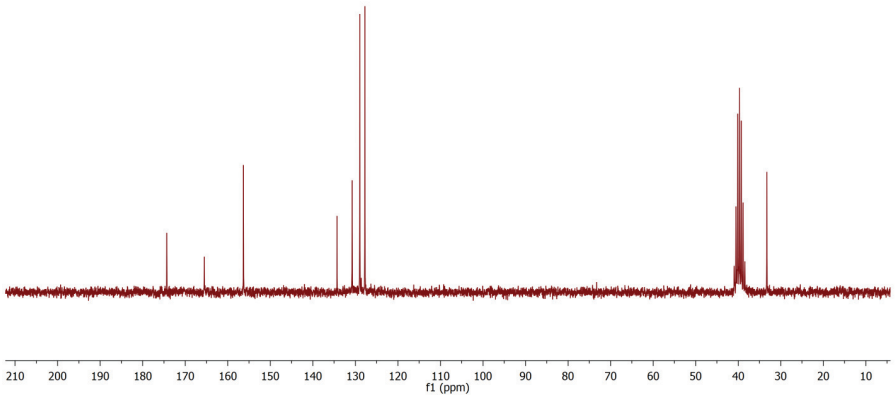

Fig. S-2. ^{13}C NMR spectra of 3-[(phenylmethylene)amino]-2-thioxo-4-imidazolidinone (**1**)

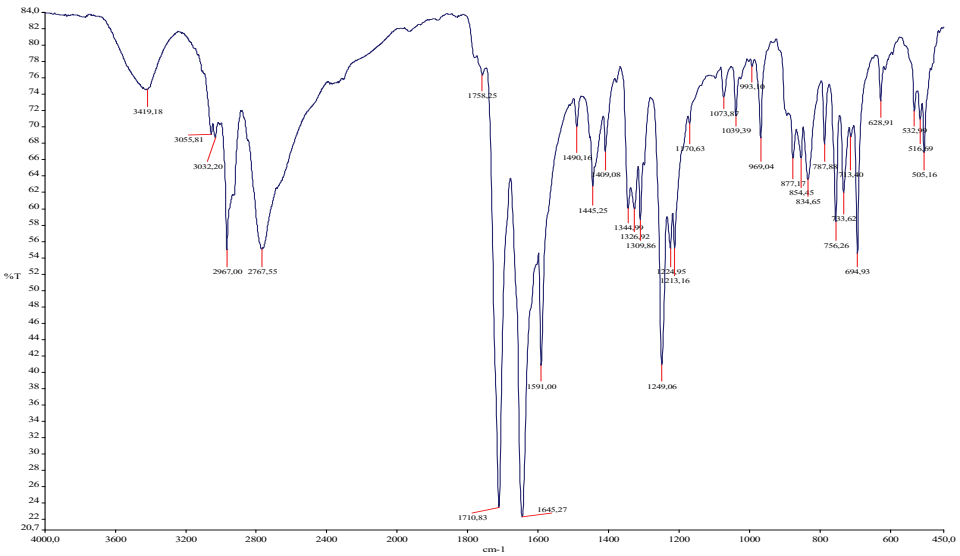

Fig. S-3. IR spectra of 3-[(phenylmethylene)amino]-2-thioxo-4-imidazolidinone (**1**)

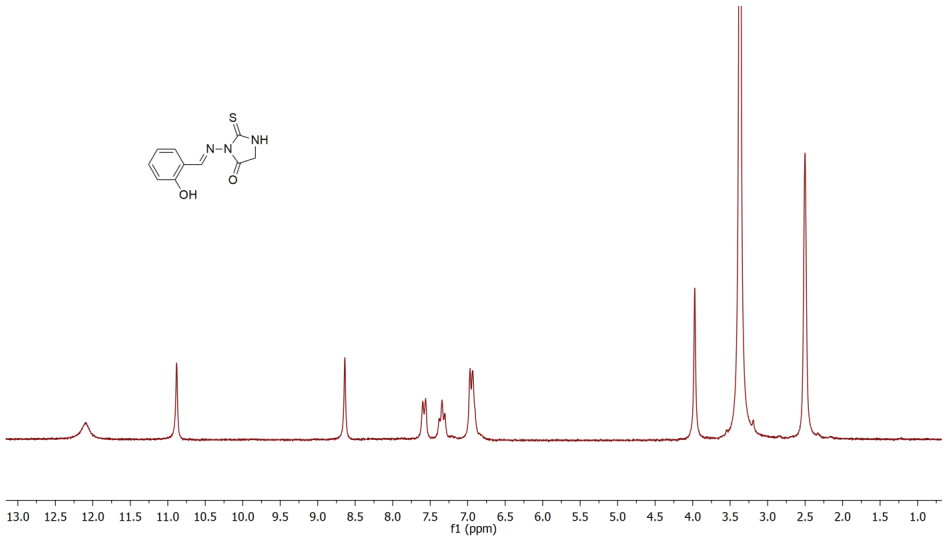

Fig. S-4. ^{1}H NMR spectra of 3-[(2-hydroxybenzylidene)amino]-2-thioxoimidazolidin-4-one (**2**)

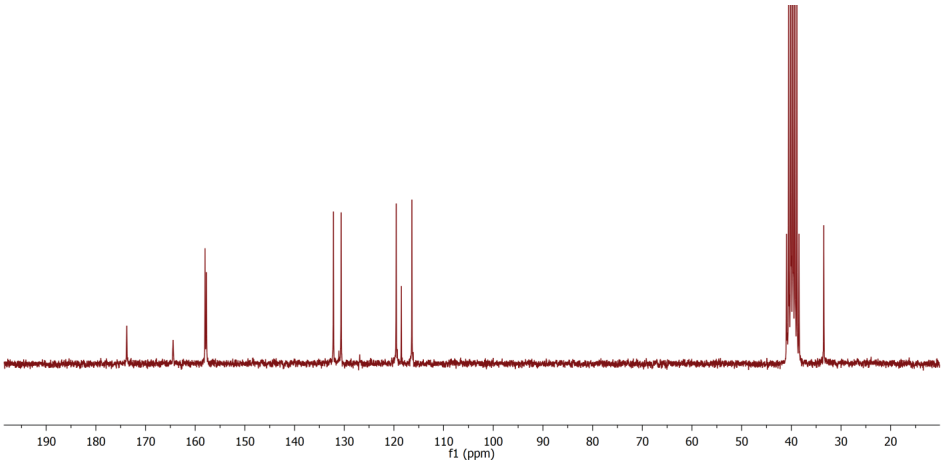

Fig. S-5. ^{13}C NMR spectra of 3-[(2-hydroxybenzylidene)amino]-2-thioxoimidazolidin-4-one (**2**)

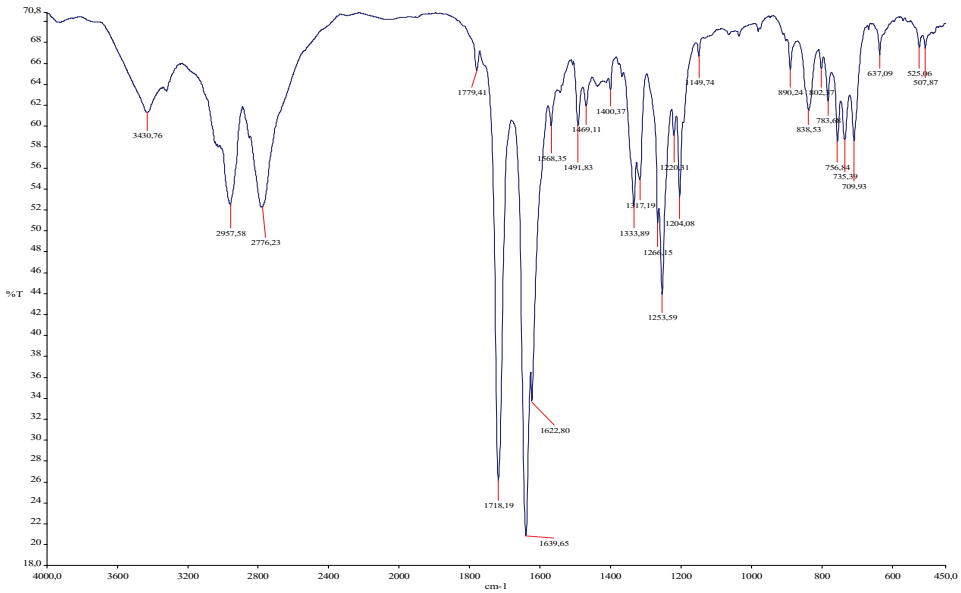

Fig. S-6. IR spectra of 3-[(2-hydroxybenzylidene)amino]-2-thioxoimidazolidin-4-one (**2**)

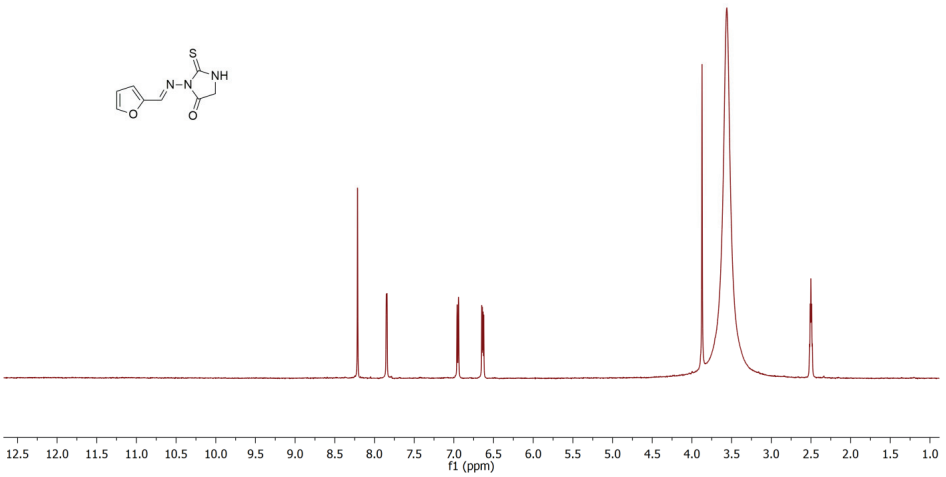

Fig. S-7. ^{1}H NMR spectra of 3-[(2-furanylmethylene)amino]-2-thioxo-4-imidazolidinone (**3**)

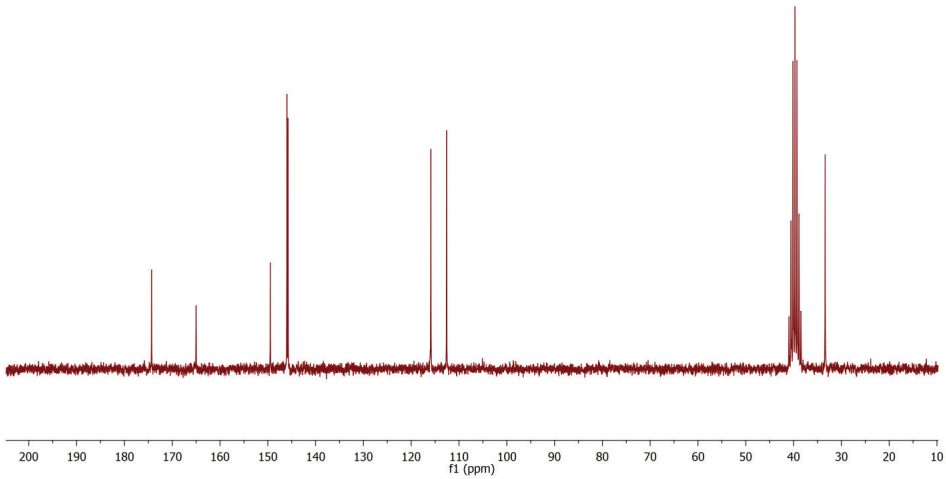

Fig. S-8. ^{13}C NMR spectra of 3-[(2-furanylmethylene)amino]-2-thioxo-4-imidazolidinone (**3**)

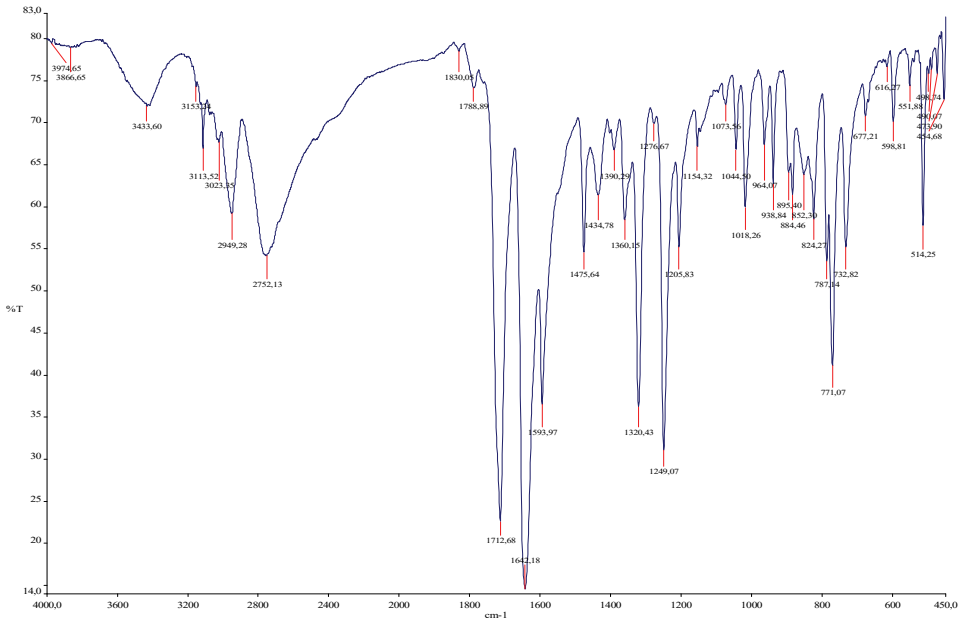

Fig. S-9. IR spectra of 3-[(2-furanylmethylene)amino]-2-thioxo-4-imidazolidinone (**3**)

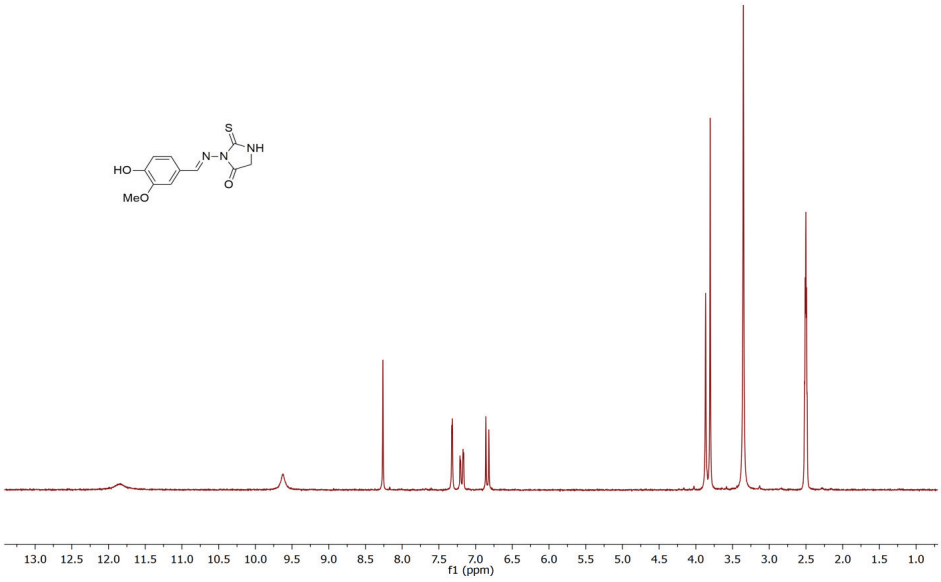

Fig. S-10. ^{1}H NMR spectra of 3-[[(4-hydroxy-3-methoxyphenyl)methylene]amino]-2-thioxo-4-imidazolidinone (**4**)

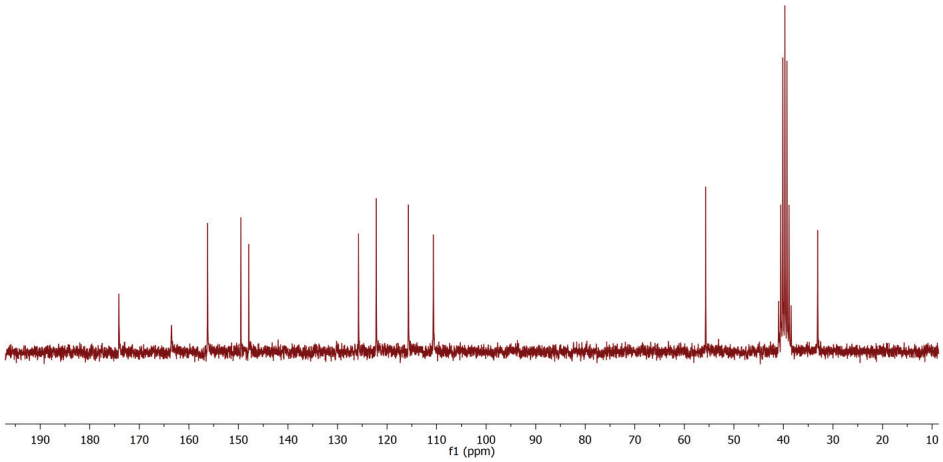

Fig. S-11. ^{13}C NMR spectra of 3-[[(4-hydroxy-3-methoxyphenyl)methylene]amino]-2-thioxo-4-imidazolidinone (**4**)

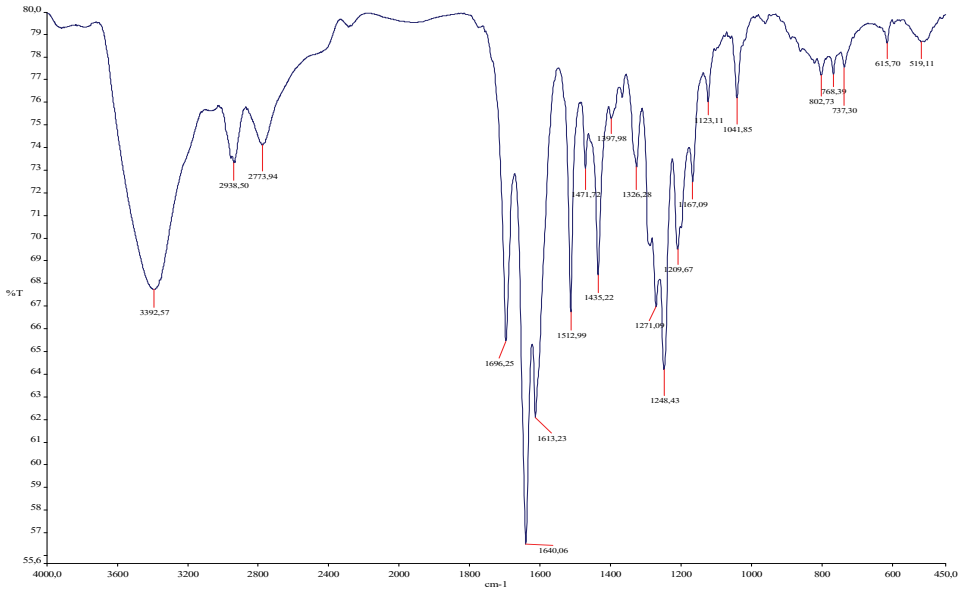

Fig. S-12. IR spectra of 3-[[(4-hydroxy-3-methoxyphenyl)methylene]amino]-2-thioxo-4-imidazolidinone (**4**)

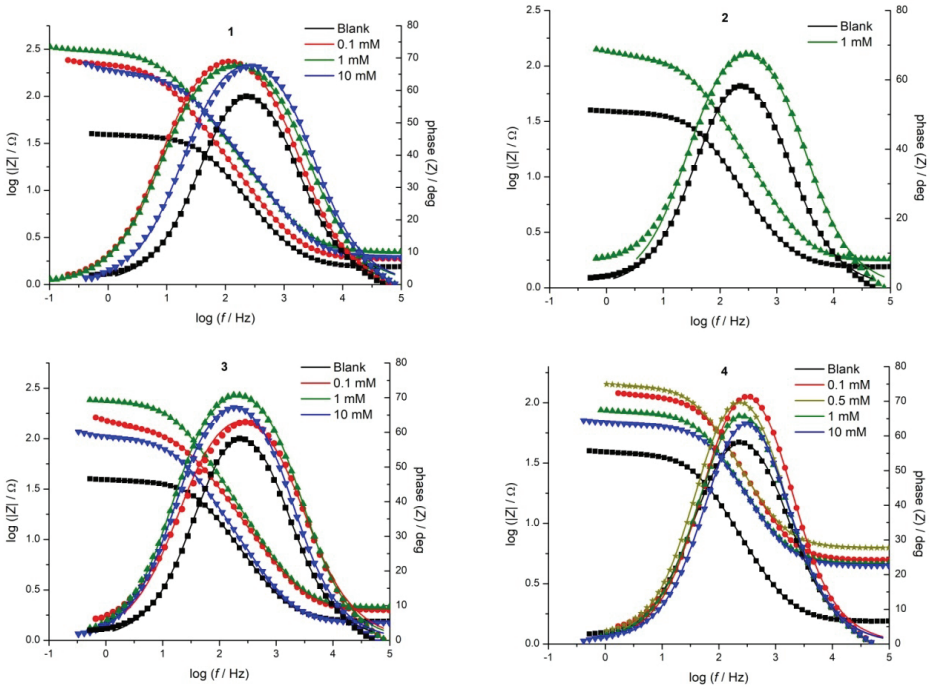

Fig. S-13. Bode plots for MS electrode and different inhibitors compounds **1**-**4** at various concentrations with respect to blank 0.5 M HCl. Scattered dots represent experimental data, while solid lines represent calculated and fitted results.