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SUPPLEMENTARY MATERIAL TO

Theoretical calculation of newly synthesized tetrazolopyrimidine derivatives as a potential corrosion inhibitor

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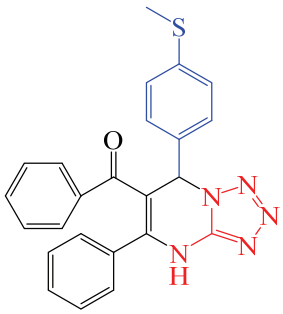
*The spectral data of (7-(4-(methylthio)phenyl)-5-phenyl-4,7-dihydrotetrazolo-[1,5-α]pyrimidin-6-yl)(phenyl) methanone (**6**)*



M.p.: 260-262ºC; IR (KBr, υ, cm^{-1}) 3218, 3084, 2960, 1692, 1623, 1582, 1549; ^{1}H NMR (300 MHz, DMSO-*d*6): δ (ppm) 11.32 (s, 1H, NH), 7.41-6.99 (m, 14H, $H_{arom.}$), 6.88 (s, 1H, CH), 2.40 (s, 3H, SCH_3). ^{13}C-NMR (DMSO-d_6): 194.73 (benzoyl), 149.66, 139.32, 139.27, 136.86, 133.85, 131.69, 130.46, 130.18, 129.06, 128.64, 128.42, 127.95, 126.20, 107.69, 60.54, 14.73.

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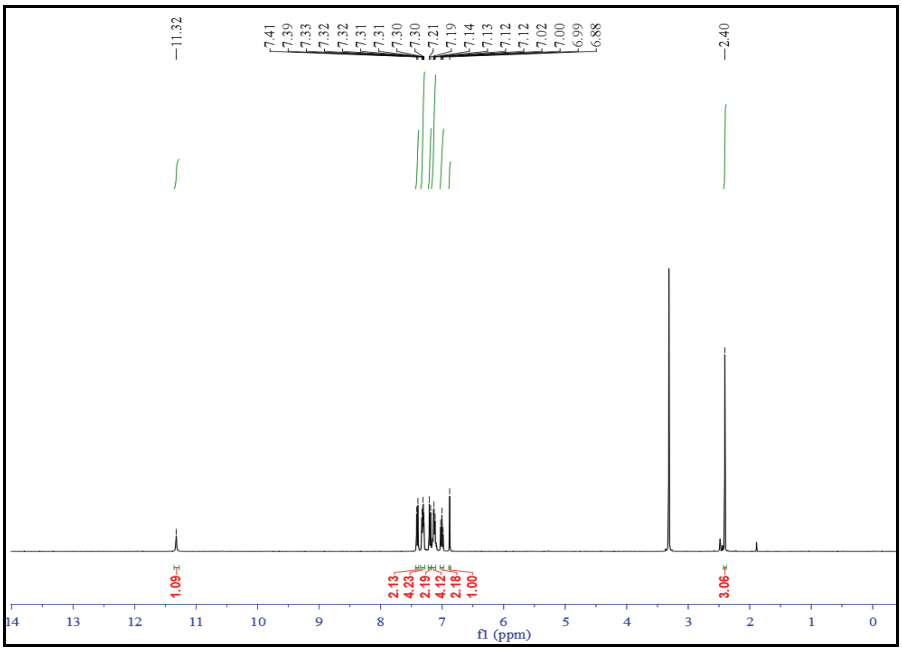


Fig. S-1. ^{1}H-NMR spectra of the compound **6**.

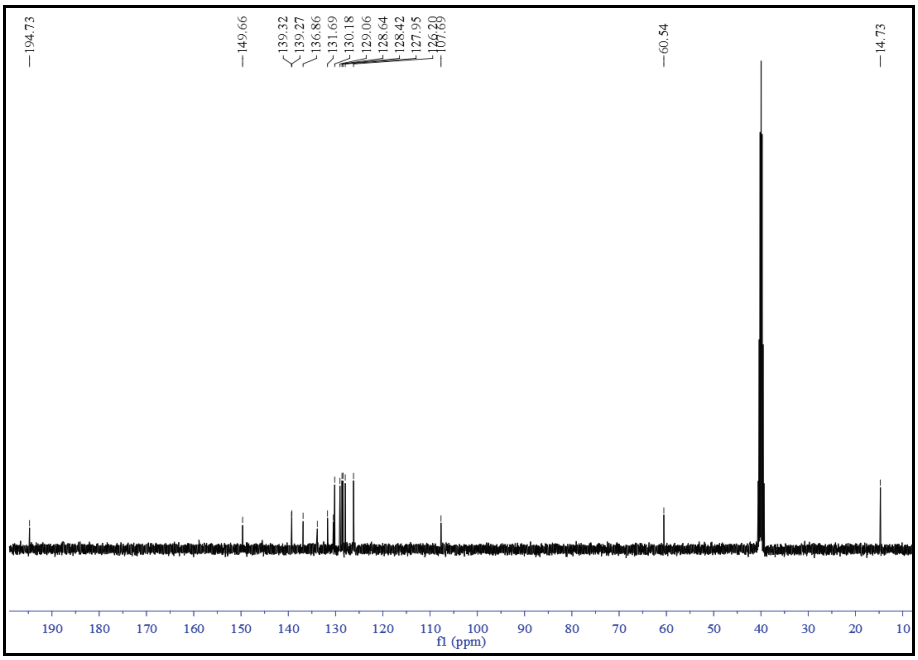
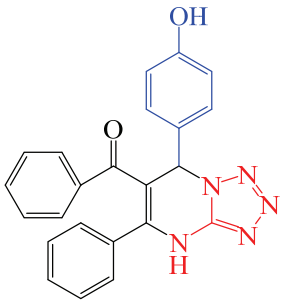


Fig. S-2. ^{13}C-NMR spectra of the compound **6**.

*The spectral data of (7-(4-hydroxyphenyl)-5-phenyl-4,7-dihydrotetrazolo[1,5-α]-pyrimidin-6-yl)(phenyl) methanone (**7**)*



M.p.: 252-253ºC; IR (KBr, υ, cm^{-1}) 3082, 2963, 1690, 1622, 1584, 1541; ^{1}H NMR (300 MHz, DMSO-*d*6): δ (ppm) 11.23 (s, 1H, OH), 9.55 (s, 1H, NH), 7.33-6.99 (m, 12H, $H_{arom.}$) 6.80 (s, 1H, CH), 6.69-6.66 (m, 2H, $H_{arom.}$). ^{13}C-NMR (DMSO-d_6): 194.90 (benzoyl), 157.98, 149.62, 144.47, 139.16, 133.86, 131.75, 130.84, 130.07, 129.34, 129.05, 128.42, 127.96, 123.72, 115.79, 108.29, 60.58.

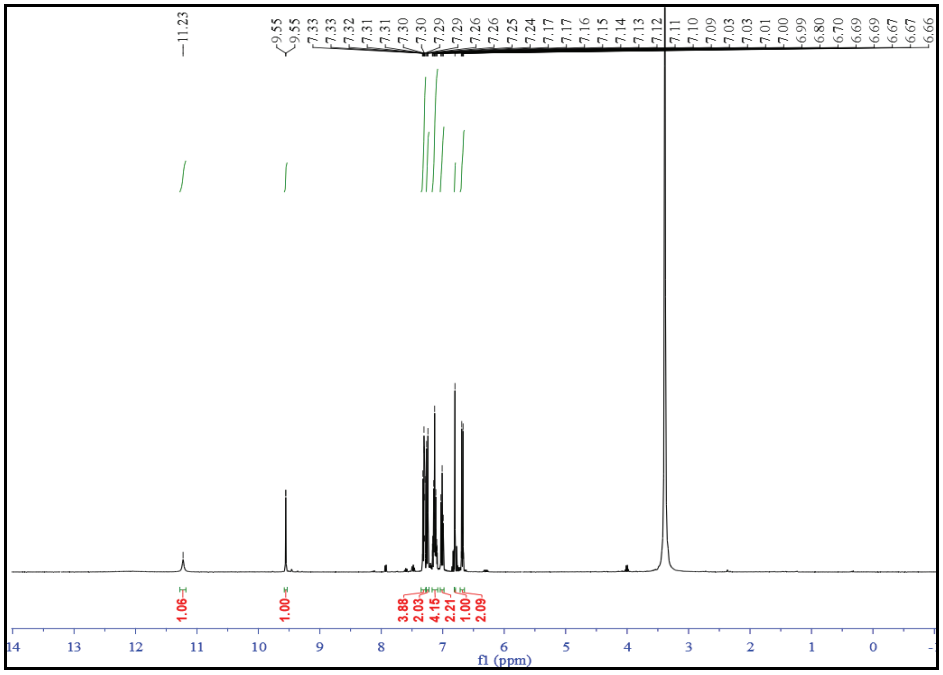


Fig. S-3. ^{1}H-NMR spectra of the compound **7**.

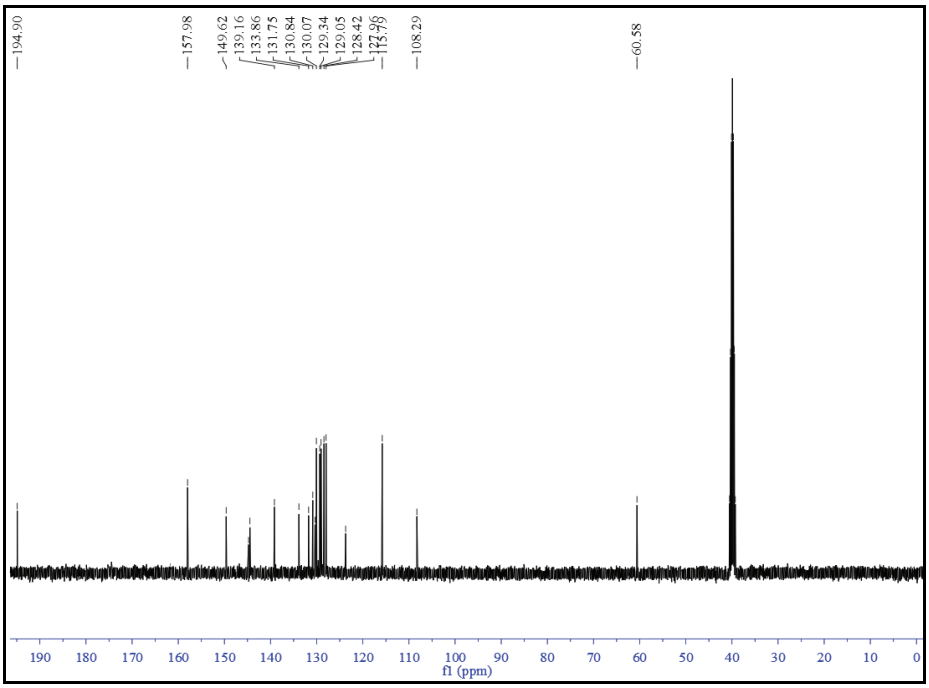
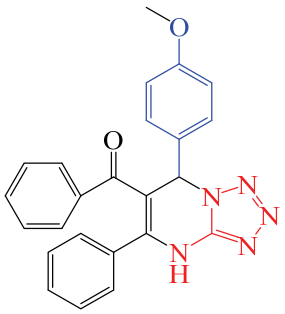


Fig. S-4. ^{13}C-NMR spectra of the compound **7**.

*The spectral data of (7-(4-methoxyphenyl)-5-phenyl-4,7-dihydrotetrazolo[1,5-α]-pyrimidin-6-yl)(phenyl) methanone (**8**)*



M.p.: 267-268ºC; IR (KBr, υ, cm^{-1}) 3216, 2966, 1696, 1628, 1588, 1545; ^{1}H NMR (300 MHz, DMSO-*d*6): δ (ppm) 11.29 (s, 1H, NH), 7.39-6.86 (m, 15H, $H_{arom.}$ and CH), 3.68(s, 3H, O-CH_3). ^{13}C-NMR (DMSO-d_6): 196.27 (benzoyl), 159.22, 145.17, 139.36, 135.39, 132.91, 131.47, 130.38, 130.32, 128.95, 128.26, 128.17, 128.00, 114.40, 110.71, 55.57, 55.31.

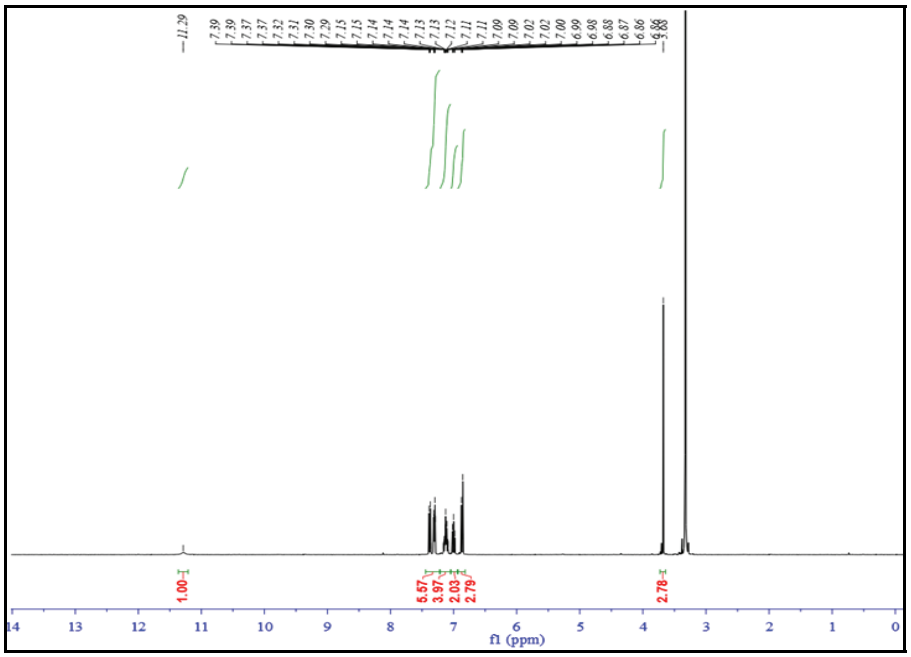


Fig. S-5. ^{1}H-NMR spectra of the compound **8**.

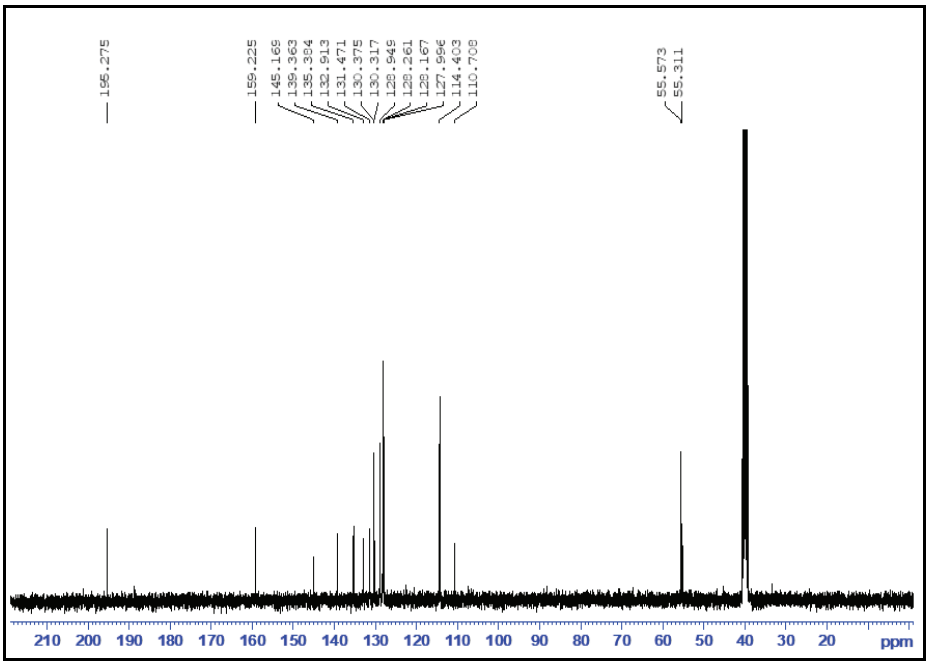
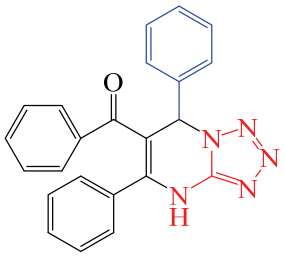


Fig. S-6. ^{13}C-NMR spectra of the compound **8**.

*The spectral data of (5,7-diphenyl-4,7-dihydrotetrazolo[1,5-α]pyrimidin-6-yl)-(phenyl)methanone (**9**)*



M.p.: 260-262ºC; IR (KBr, υ, cm^{-1}) 3218, 2973, 1694, 1628, 1588, 1547; ^{1}H NMR (300 MHz, DMSO-*d*6): δ (ppm) 11.33 (s, 1H, NH), 7.47-6.98 (m, 15H, $H_{arom.}$), 6.91 (s, 1H, CH). ^{13}C-NMR (DMSO-d_6): 194.77 (benzoyl), 149.77, 145.24, 140.37, 139.25, 133.83, 131.68, 130.46, 130.16, 129.19, 129.03, 128.42, 128.03, 127.92, 107.83, 60.96.

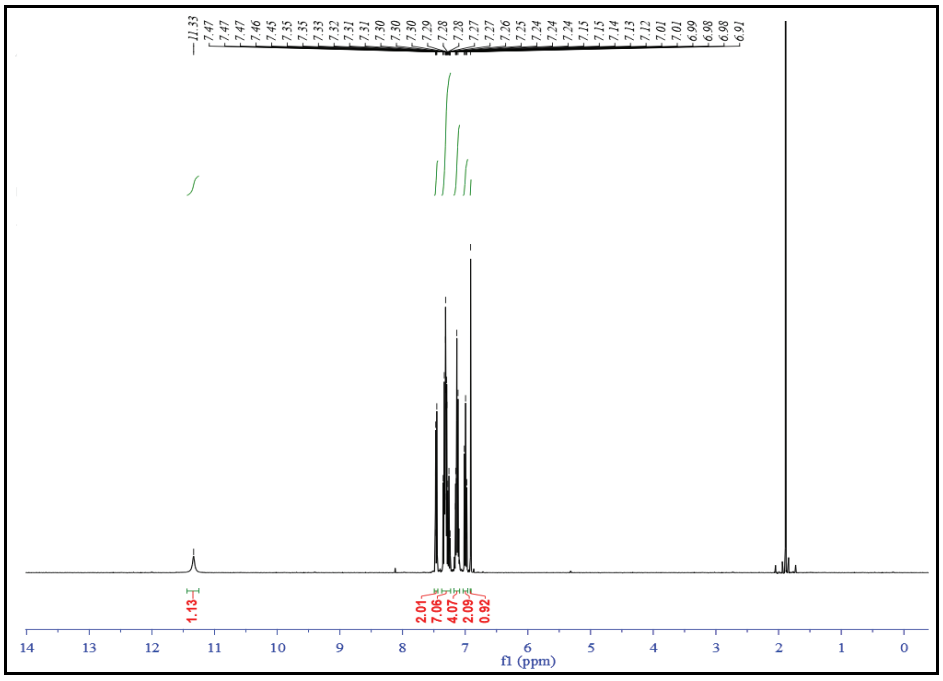


Fig. S-7. ^{1}H-NMR spectra of the compound **9**.

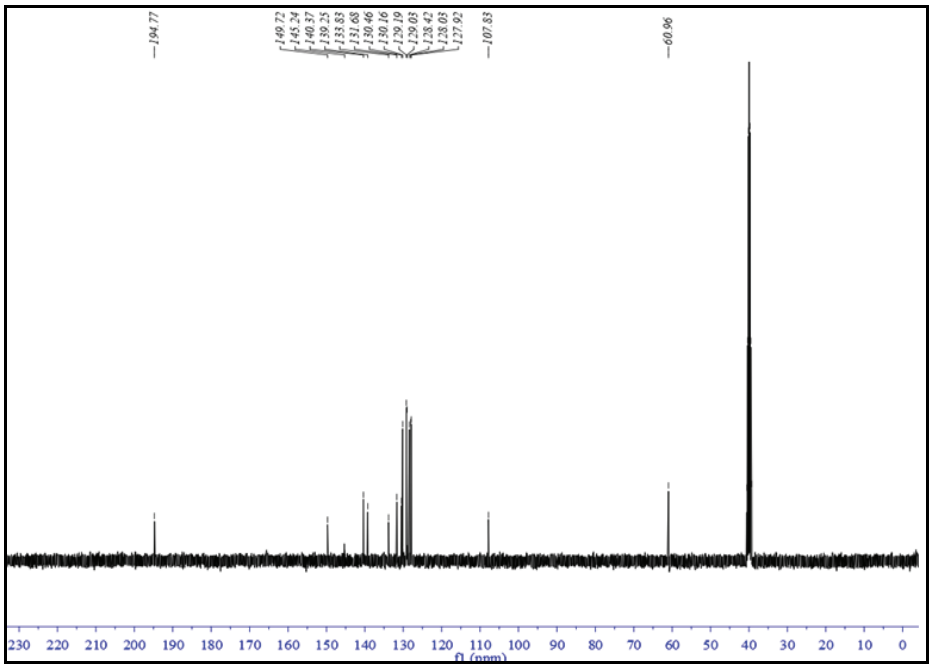


Fig. S-8. ^{13}C-NMR spectra of the compound **9**.