Review of: "Design, Synthesis, and In-Silico Analysis of Thiazole-Embedded Schiff Base Derivatives for Breast Cancer Therapeutic Potential"

Nasser A. Hassan[1]

1 Organic Chemistry, National Research Centre, Cairo, Egypt

Potential competing interests: No potential competing interests to declare.

Review of the Manuscript Titled: "Thiazole Schiff Bases as Potential Breast Cancer Drugs through Design, Synthesis, and In Silico Analysis"

I would like to sincerely thank the authors for their work on the manuscript. The writing is clear, precise, and well-structured, making it easy to follow and understand. The language used is good, reflecting a high level of expertise and attention to detail. Overall, the manuscript is a well-written and comprehensive piece, and I commend the authors for their effort in presenting their research so effectively. However, I have identified some areas where corrections are needed, which I have outlined below.

In the experimental section

Corrections:

1. Nuclear Magnetic Resonance (NMR) Spectrum:

Original: "Nuclear Magnetic Resonance (NMR) spectra, including 1H and 13C, were recorded using a BRUKER AVANCE III HD (400 MHz)"

Corrected: "Nuclear Magnetic Resonance (NMR) spectra, including ^{1}H NMR at 400 MHz and ^{13}C NMR at 100 MHz, were recorded on a Bruker Avance III HD spectrometer."

Or

The 400 MHz must be corrected in all experimental parts: ^{13}C NMR (DMSO-d6, 400 MHz) to ^{13}C NMR (DMSO-d6, 100 MHz).

2. Synthesis of Thiazole-Embedded Schiff Base Derivatives (TZ1-TZ3):

The procedure in the experimental section should be updated as follows:

Original:

2.2.2. Synthesis of Thiazole-Embedded Schiff Base Derivatives (TZ1-TZ3)

A mixture of 0.013 mol of 3-chloroacetic acetone (3) and 0.015 mol of thiosemicarbazone derivatives (4-6) was dissolved in acetone and refluxed for 6 h. After completing the reaction, the crude mixture was cooled in an ice bath. The cooled mixture was then added to ice-cold water to induce precipitation. The precipitate was filtered and recrystallized from ethanol, with compounds TZ1-TZ3 subsequently purified via column chromatography. Reaction shown in Scheme 1. All the reactions proceeded smoothly with diverse substituted thiosemicarbazone, and products were obtained in moderate

yields. The structures of the synthesized compounds were elucidated by 1H NMR, 13C NMR, DEPT, HMBC spectroscopic method.

Corrected:

2.2.2. Synthesis of Thiazole-Embedded Schiff Base Derivatives (TZ1-TZ3)

General Procedure: A solution of 0.013 mol of 3-chloroacetic acetone and 0.015 mol of thiosemicarbazone derivatives (4-6) was prepared in acetone. The mixture was refluxed for 6 hours. Upon completion of the reaction, the crude mixture was cooled in an ice bath. Ice-cold water was then added to the cooled mixture to induce precipitation. The precipitate was filtered, crystallized from ethanol, and further purified by column chromatography to afford the products TZ1-TZ3.

Note: Remove the scheme and the following parts: "Reaction shown in Scheme 1. All the reactions proceeded smoothly with diverse substituted thiosemicarbazone, and products were obtained in moderate yields. The structures of the synthesized compounds were elucidated by 1H NMR, 13C NMR, DEPT, HMBC spectroscopic method."

3. 13C NMR for Compound 4:

Original: "40.2N (CH3)2."

Corrected: "40.2 $N(CH_3)_2$."

4. Physical Properties of 2-(4-(dimethylamino) benzylidene) hydrazine-1-carbothioamide (Compound 4):

Original: "Physical properties of 2-(4-(dimethylamino) benzylidene) hydrazine-1-carbothioamide, 4: Orange colored powder, Yield 90%, m. p. 210~212 °C, IR (KBr, cm-1, 5): 3406,3251(w, NH2), 3051(C-H, Ar), 1593.99(C=N), 1184.29 (C=S), 815.85 (C-S-C). 1HNMR (400 MHz, DMSO-d6, δ ppm, 5): 7.59 (1H, d, J= 8.8 Hz, H-2′); 6.71 (1H, d, J= 8.4 Hz, H-3′);6.71 (1H, d, J= 8.4 Hz, H-5′) and 7.59 (1 H, d, J= 8.8 Hz, H-6′); 7.98 (1H, s, CH=N);3.36 (1H, s);11.04 (2H, s); 2.95 (2H, s). ^{13}C NMR (400 MHz, DMSO-d6, δ ppm, 5): 121.8(C1'), 129.0(C2'), 112.1(C3'), 151.8(C4'), 112.1(C5'), 129.0(C6'), 143.8 (CH=N), 177.4(C=S),40.2N (CH3)2."

Corrected:

Physical properties of 2-(4-(dimethylamino) benzylidene) hydrazine-1-carbothioamide (Compound 4): Orange-colored powder, Yield 90%, m.p. 210–212 °C, IR (KBr, cm^{-1}): 3406, 3251 (w, NH_2), 3051 (C-H, Ar), 1593.99 (C=N), 1184.29 (C=S), 815.85 (C-S-C). ^{1}H NMR (400 MHz, DMSO-d_6, δ ppm): 7.59 (1H, d, J = 8.8 Hz, H-2′); 6.71 (1H, d, J = 8.4 Hz, H-3′); 6.71 (1H, d, J = 8.4 Hz, H-5′); 7.59 (1H, d, J = 8.8 Hz, H-6′); 7.98 (1H, s, CH=N); 3.36 (1H, s); 11.04 (2H, s); 2.95 (2H, s). ^{13}C NMR (100 MHz, DMSO-d_6, δ ppm): 121.8 (C1′), 129.0 (C2′), 112.1 (C3′), 151.8 (C4′), 112.1 (C5′), 129.0 (C6′), 143.8 (CH=N), 177.4 (C=S), 40.2 $N(CH_3)_2$.

5. Physical Properties of Other Compounds:

The same corrections should be applied to the physical properties and spectral data for compound 5 and compound 6 as done for compound 4. Ensure the correct formatting and NMR data.

By incorporating these corrections, the manuscript will be clearer and more accurate.