**Supplementary data**

## 1. Synthesis of compound ZM-093

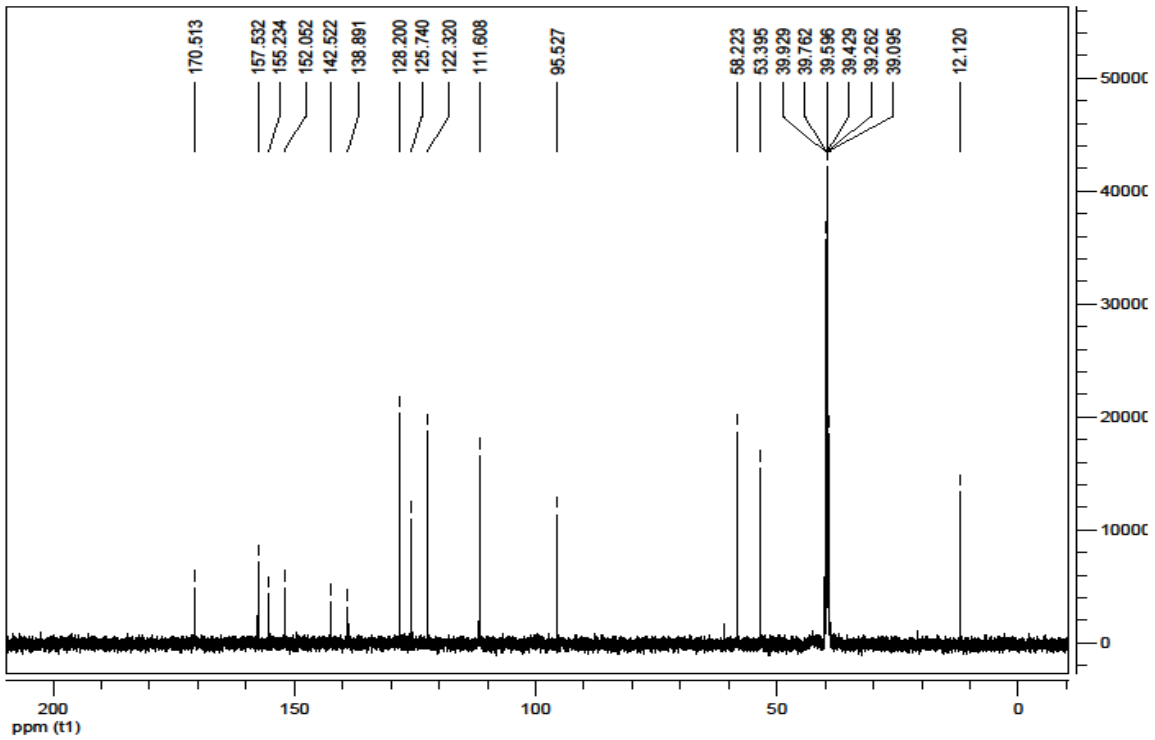
Sulfamethoxazole-based azo dye (ZM-093) was obtained in high yield via common diazotization-coupling reactions. The diazonium salt was prepared from an equimolar mixture of sulfonamide derivative (2 mmol of sulfonamide derivative, 4 mL of acetonitrile, and some drops of acetic acid) and in situ-prepared $HNO_2$ ($NaNO_2$ & HCl). Then, the diazonium salt in the previous step was added dropwise to a solution containing the coupling reagent (N-phenyl-2,2`-imino diethanol in ethanol). The solution was vigorously stirred at 0–4 °C for 2 h. After that, the pH of the solution was maintained at 6.5–7.5 by adding NaOH (0.5 M). TLC evaluated the reaction progress. The raw product was filtered and washed with water (three times). ZM-093 was isolated by recrystallization from EtOH/$H_2O$. FT-IR, $^1$H NMR, and $^{13}$C NMR spectroscopy confirmed the structure of the obtained azo dye. Compound ZM-093: orange solid; yield 92%; M.p. 185°C (Section 4-1).

### *1.1. Spectroscopic characterization of the ZM-093*

In the $^1$H NMR spectrum of ZM-093, the dominant NH hydrogen of the sulfonamide group (-$NHSO_2$) appeared as a broad signal at low frequency (10.66 ppm). Additionally, a distinct signal at 1.42 ppm is attributed to the methyl group of the sulfamethoxazole component. Other characteristic peaks are observed at corresponding chemical shifts (S. Fig. 1). In the FT-IR spectrum of ZM-093, a broad peak at 3420 $cm^{-1}$ is assigned to the overlapping of the hydroxyl and amine functional groups. Furthermore, a characteristic peak at 1512 $cm^{-1}$ is assigned to the azo (N=N) group (S. Fig. 2).

**S. Figure 1. NMR spectrum of ZM-093. a)** C-NMR spectrum of ZM-093. **b)** H-NMR spectrum of ZM-093. Due to the characteristics of the methyl group of the sulfamethoxazole component and the hydrogen atom of the sulfonamide group (-$NHSO_2$), two broad signals at frequencies of 1.42 ppm and 10.66 ppm appeared.

**1. a)**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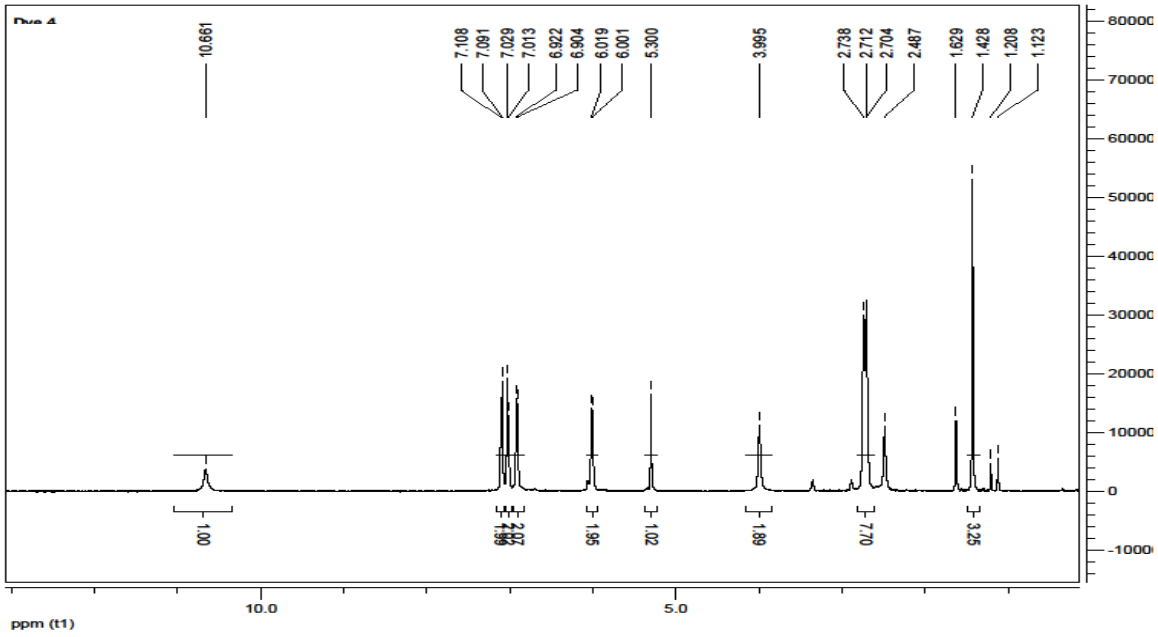
157.532
155.234
152.052
142.522
138.891
128.200
125.740
122.320
111.608
95.527
58.223
53.395
39.929
39.762
39.596
39.429
39.262
39.095
12.120
50000
40000
30000
20000
10000
0
200
150
100
50
0
ppm (t1)

**1. b)**


10.661
7.108
7.091
7.029
7.013
6.922
6.904
6.019
6.001
5.300
3.995
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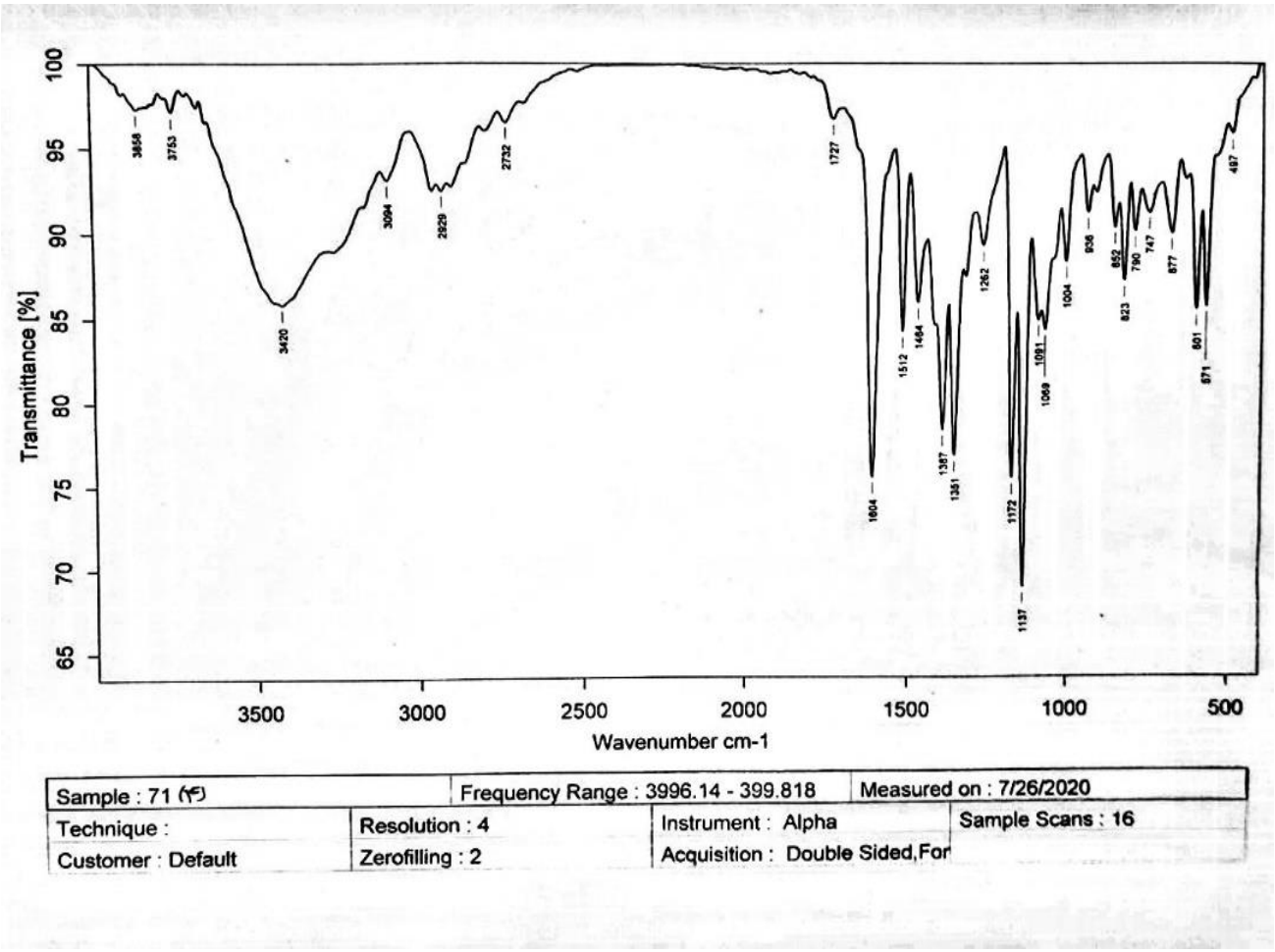
2.712
2.704
2.487
1.629
1.428
1.208
1.123
1.00
1.96
2.02
1.88
7.70
3.25
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.0
5.0
ppm (t1)

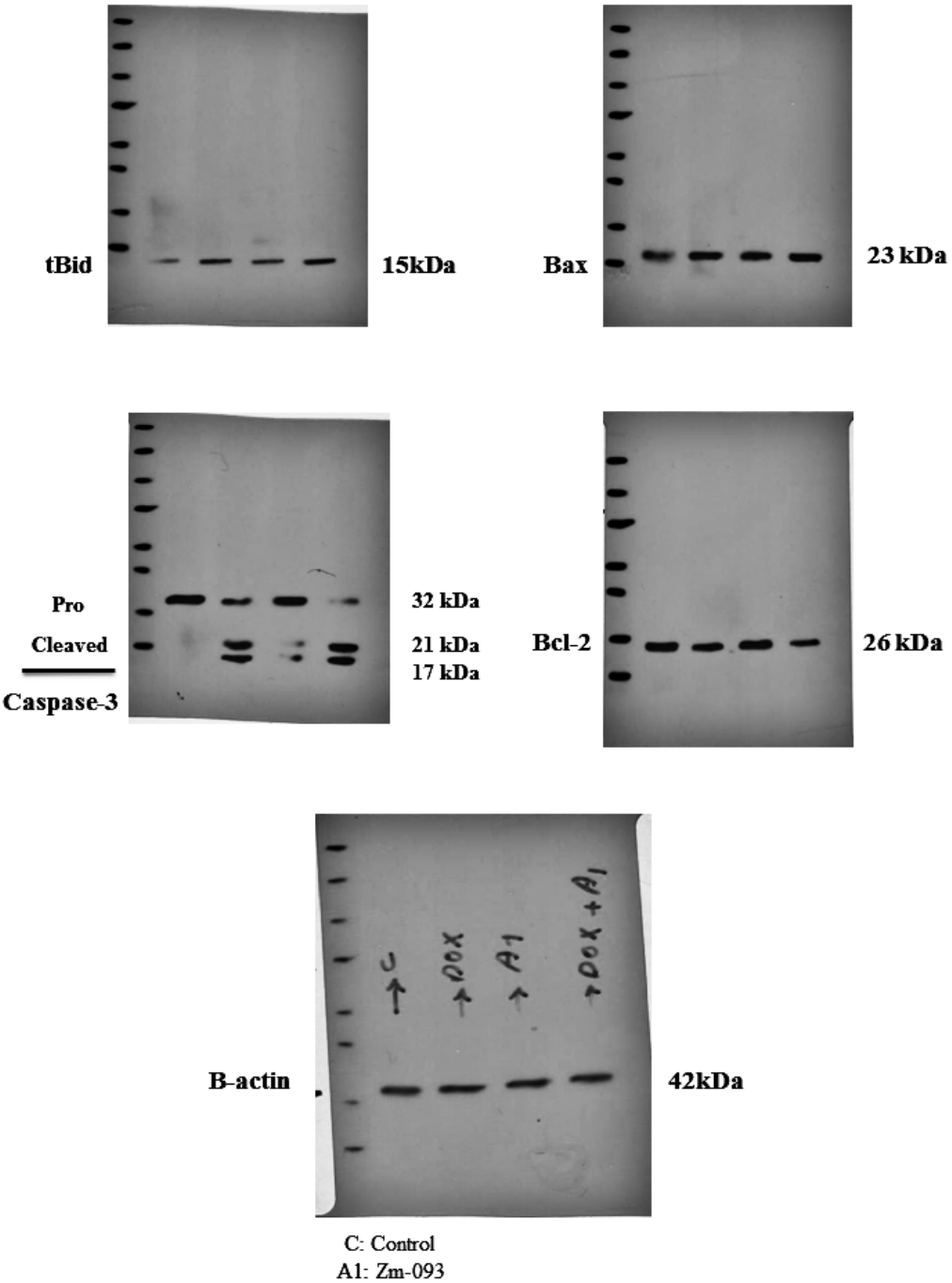
**S. Figure 2. FT-IR spectrum of ZM-093.** FT-IR (KBr, $cm^{-1}$): 3420 (OH, NH, overlapped), 3094 (C-H, aromatic), 2929 (C-H, aliphatic), 1604 (C=C), 1512 (N=N), 1464, 1387, 1351, 1172, 1137, 1089, 823, 601, 571. $^{1}$H NMR (400 MHz, DMSO-$d_6$, 298 K), δ (ppm): 1.42 (s, 3H ($H_j$), $CH_3$), 2.71 (t, 8H ($H_b$ & $H_c$), -$CH_2$-), 3.99 (s, 2H ($H_a$), OH), 5.30 (s, 1H ($H_i$), Ar-H), 6.01 (d, 2H ($H_d$), *J* = 7.2 Hz, Ar-H), 6.91 (d, 2H ($H_g$), *J* = 7.2 Hz, Ar-H), 7.02 (d, 2H ($H_f$), *J* = 7.2 Hz, Ar-H), 7.10 (d, 2H ($H_e$), *J* = 7.2 Hz, Ar-H), 10.66 (s, 1H ($H_i$), NH). $^{13}$C NMR (100 MHz, DMSO-$d_6$, 298 K): δ (ppm) 12.1, 53.3, 58.2, 95.5, 111.6, 122.3, 125.7, 128.2, 138.8, 142.5, 152.0, 155.2, 157.5, 170.5.



**2. Original photos of the western blot gel**

Pictures are related to the expression of tBid, Bax, Caspase-3, and Bcl-2 proteins in MCF-7 cells (Section 2-3; S. Fig. 3).

S. Figure 3. Relative expression of proteins in MCF-7 cells.




C: Control
A1: Zm-093