

**Ring formation and ring opening reactions of a dihydrothiadiazine cycle fused to 1,2,4-triazole**

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*Spectral characteristics for compounds 3–5.*

**3:**  $^1\text{H NMR}$  ( $[\text{D}_6]\text{DMSO}$ )  $\delta$ : 3.74, 3.79 (2s, 3H, OMe), 4.35, 4.86 (2d, 1H,  $\text{CH}_2$ ,  $J$  16.1 Hz), 6.77, 7.14 (2s, 1H,  $\text{H}_{\text{Ar}}$ ), 7.4 (m, 3H, Ph), 7.52 (d, 2H, Ph,  $J$  6.9 Hz), 7.66, 8.12 (2d, 2H,  $\text{H}_{\text{Ar}}$ ,  $J$  8.6 Hz), 14.13 (s, 1H,  $\text{NH}_{\text{triazole}}$ ). MS,  $m/z$  (%): 492 (1), 477 (5), 445 (5), 317 (67), 301 (40), 273 (28), 192 (43), 177 (100), 164 (40), 139 (90). Found (%): C, 55.81; H, 3.74; N, 14.27. Calc. for  $\text{C}_{24}\text{H}_{20}\text{ClN}_5\text{O}_4\text{S}$  (%): C, 56.52; H, 3.95; N, 13.73.

**4:**  $^1\text{H NMR}$  ( $\text{CDCl}_3$ )  $\delta$ : 3.96, 3.97 (2s, 3H, OMe), 4.40 (s, 4H,  $\text{CH}_2$ ,  $\text{SCH}_2$ ), 6.79, 7.28 (2s, 1H,  $\text{H}_{\text{Ar}}$ ), 7.31–7.45 (m, 5H, Ph), 7.78 (m, 4H,  $\text{H}_{\text{Ar}}$ ), 8.10 (m, 4H,  $\text{H}_{\text{Ar}}$ ). MS,  $m/z$  (%): 586 (0.5), 444 (1), 313 (2), 274 (2), 196 (7), 177 (5), 164 (13), 151 (10), 136 (44), 103 (100). Found (%): C, 57.64; H, 4.13; N, 13.21. Calc. for  $\text{C}_{31}\text{H}_{25}\text{ClN}_6\text{O}_6\text{S}$  (%): C, 57.72; H, 3.91; N, 13.03.

**5:**  $^1\text{H NMR}$  ( $\text{CDCl}_3$ )  $\delta$ : 3.95 (s, 6H, OMe), 4.63 (s, 1H,  $\text{CH}_2$ ), 6.70 (s, 1H,  $\text{H}_{\text{Ar}}$ ), 7.47 (d, 2H, 4- $\text{ClC}_6\text{H}_4$ ,  $J$  8.5 Hz), 7.77 (s, 1H,  $\text{H}_{\text{Ar}}$ ), 7.97 (d, 2H, 4- $\text{ClC}_6\text{H}_4$ ,  $J$  8.5 Hz). MS,  $m/z$  (%): 335  $[\text{M}]^+$  (5), 289 (14), 248 (1), 180 (15), 164 (3), 139 (100), 111 (28), 92 (5), 75 (12). Found (%): C, 57.37; H, 4.42; N, 4.23. Calc. for  $\text{C}_{16}\text{H}_{14}\text{ClNO}_5$  (%): C, 57.24; H, 4.20; N, 4.17.