

Supplementary material

Design, spectroscopy, and assessment of cholinesterase inhibition and antimicrobial activities of novel coumarin-thiadiazole hybrids

Dariusz Karcz^{1*}, Karolina Starzak¹, Ewa Ciszkowicz², Katarzyna Lecka-Szlachta², Daniel Kamiński³, Bernadette Creaven⁴, Anna Miłoś⁵, Hollie Jenkins⁶, Lidia Ślusarczyk⁷, and Arkadiusz Matwiczuk⁷

¹*Department of Chemical Technology and Environmental Analytics (C1), Faculty of Chemical Engineering and Technology, Cracow University of Technology, Cracow, Poland;*

²*Department of Biotechnology and Bioinformatics, Faculty of Chemistry, Rzeszow University of Technology, Rzeszow, Poland;*

³*Department of General and Coordination Chemistry and Crystallography, Institute of Chemical Sciences, Maria Curie-Skłodowska University in*

Lublin, Lublin, Poland;

⁴*School of Chemical and Pharmaceutical Sciences, Technological University Dublin, Dublin, Ireland;*

⁵*Department of Biotechnology and Bioinformatics, Faculty of Chemistry, Doctoral School of Engineering and Technical Sciences at the Rzeszow*

University of Technology, Rzeszow, Poland,

⁶*Department of Applied Science, Technological University Dublin, Tallaght, Ireland;*

⁷*Department of Biophysics, University of Life Sciences in Lublin, Lublin, Poland;*

*Correspondence: dariusz.karcz@pk.edu.pl ; Tel.: +48(12)6282177

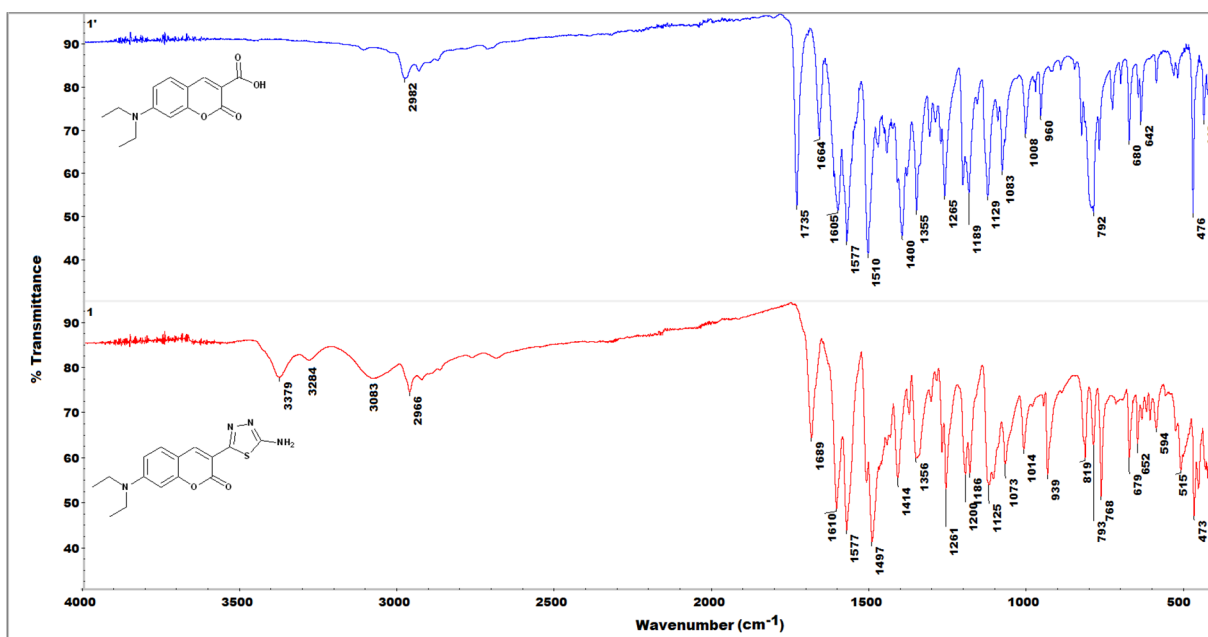


Figure S1. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **1'** (top) and the corresponding coumarin-thiadiazole hybrid **1** (bottom).

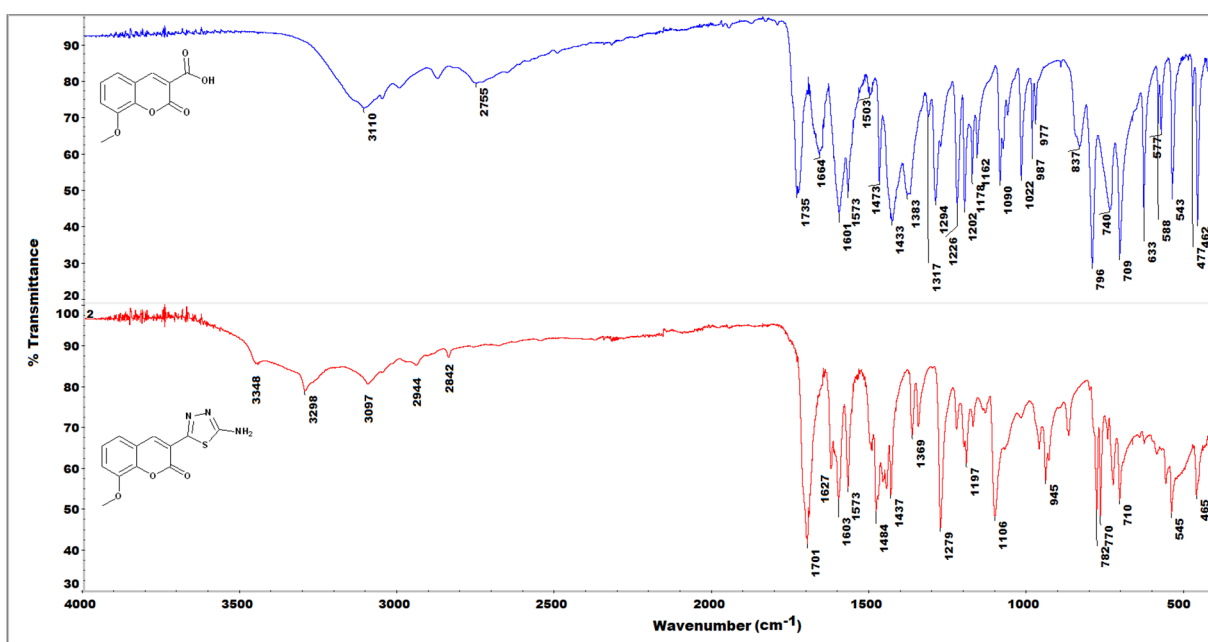


Figure S2. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **2'** (top) and the corresponding coumarin-thiadiazole hybrid **2** (bottom).

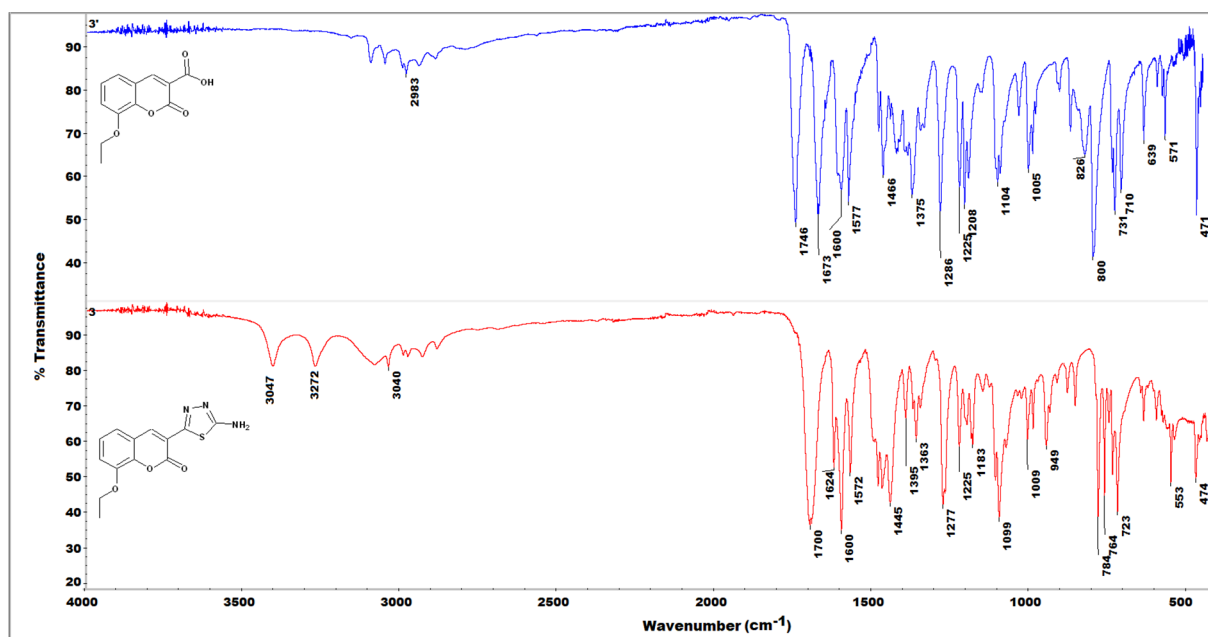


Figure S3. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **3'** (top) and the corresponding coumarin-thiadiazole hybrid **3** (bottom).

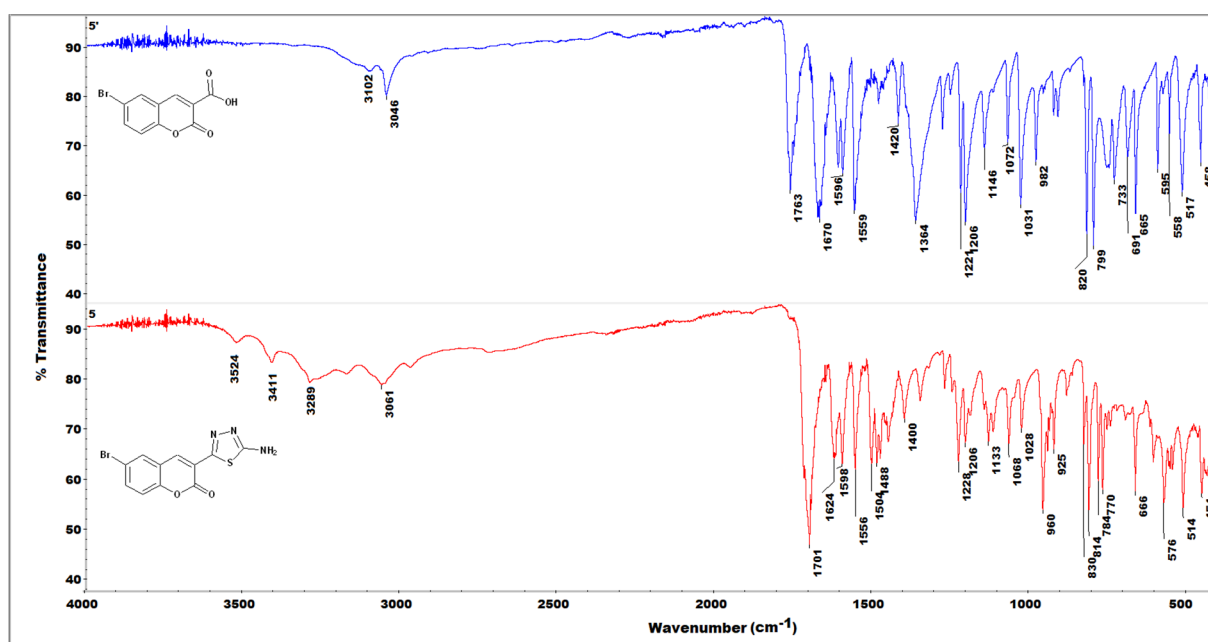


Figure S4. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **5'** (top) and the corresponding coumarin-thiadiazole hybrid **5** (bottom).

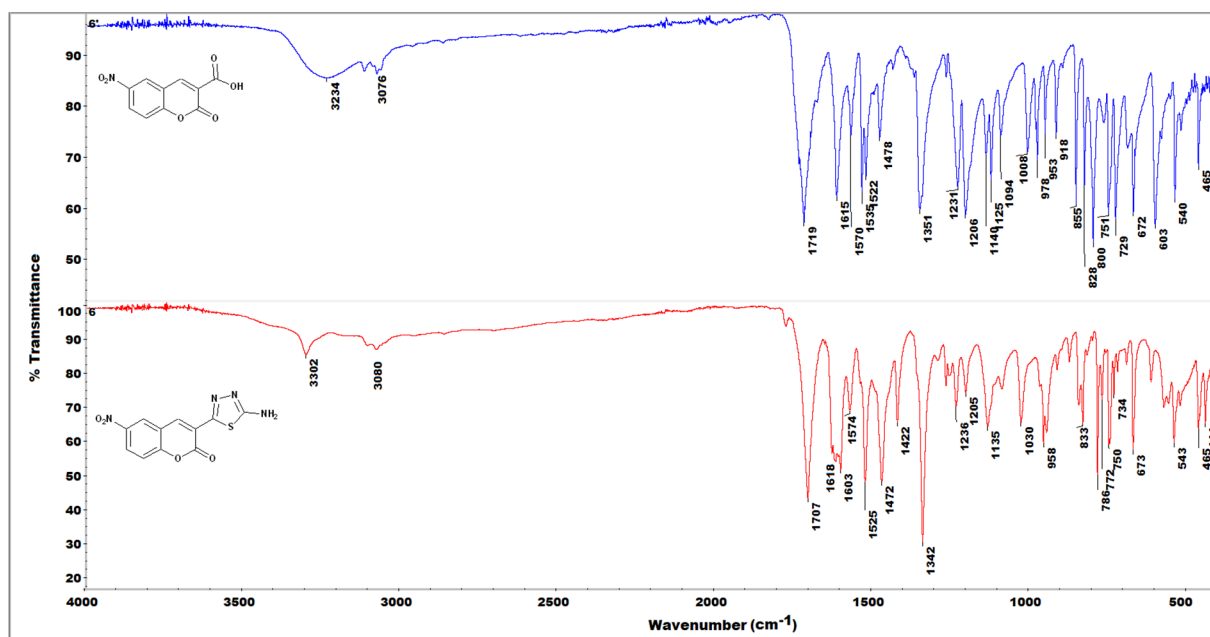


Figure S5. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **6'** (top) and the corresponding coumarin-thiadiazole hybrid **6** (bottom).

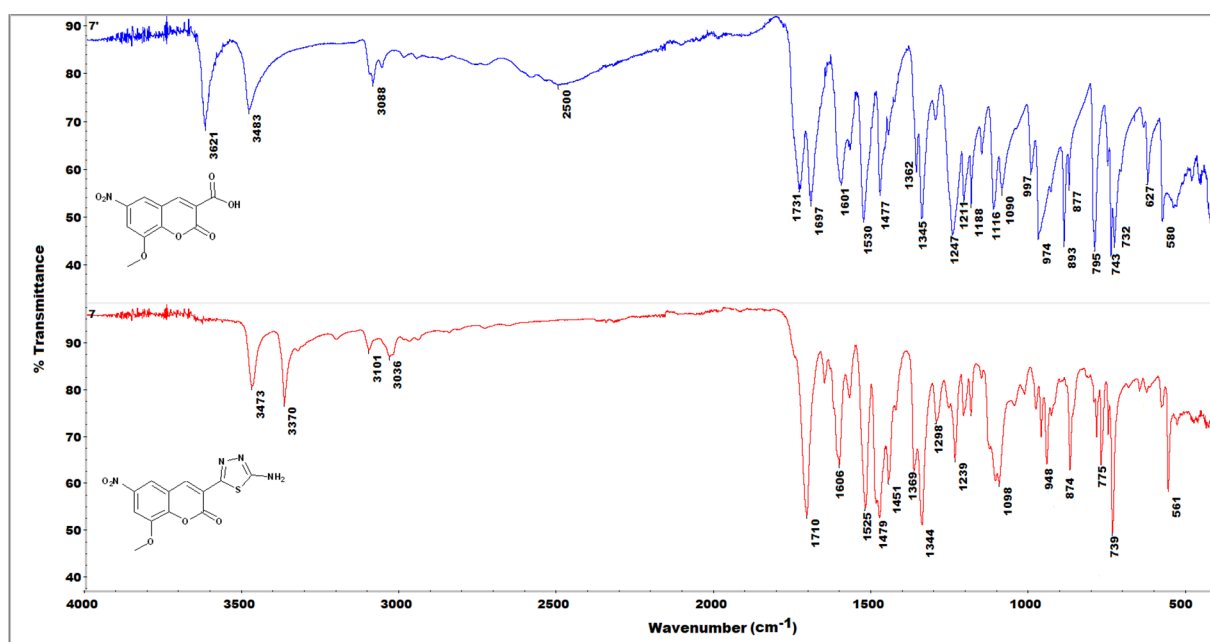


Figure S6. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **7'** (top) and the corresponding coumarin-thiadiazole hybrid **7** (bottom).

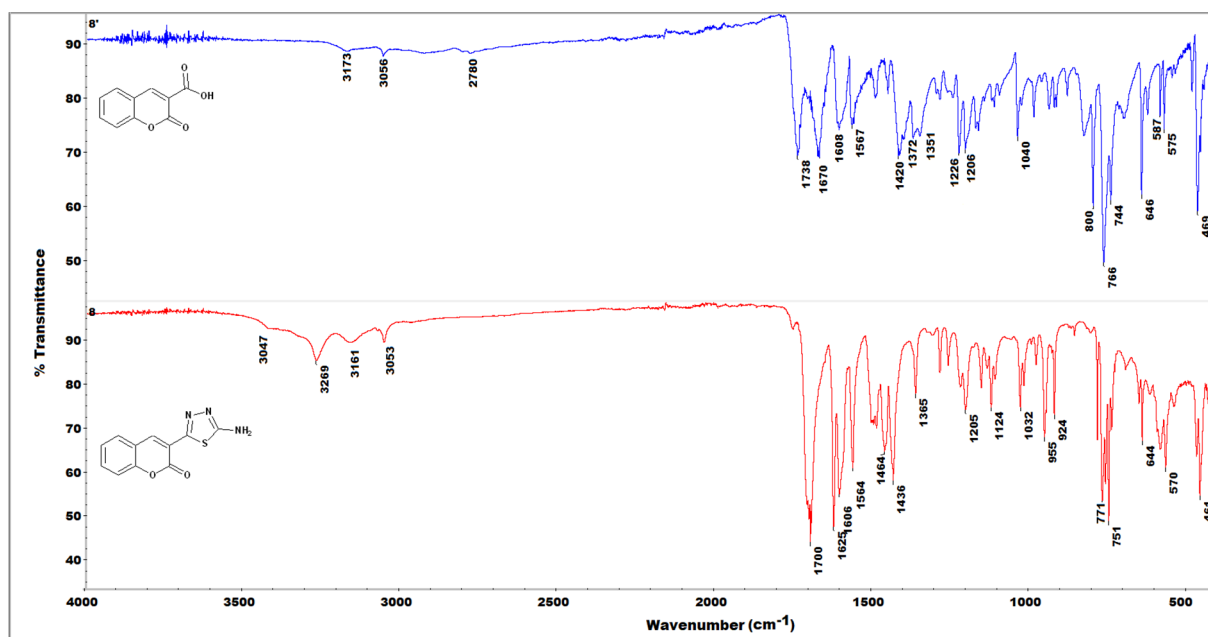


Figure S7. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **8'** (top) and the corresponding coumarin-thiadiazole hybrid **8** (bottom).

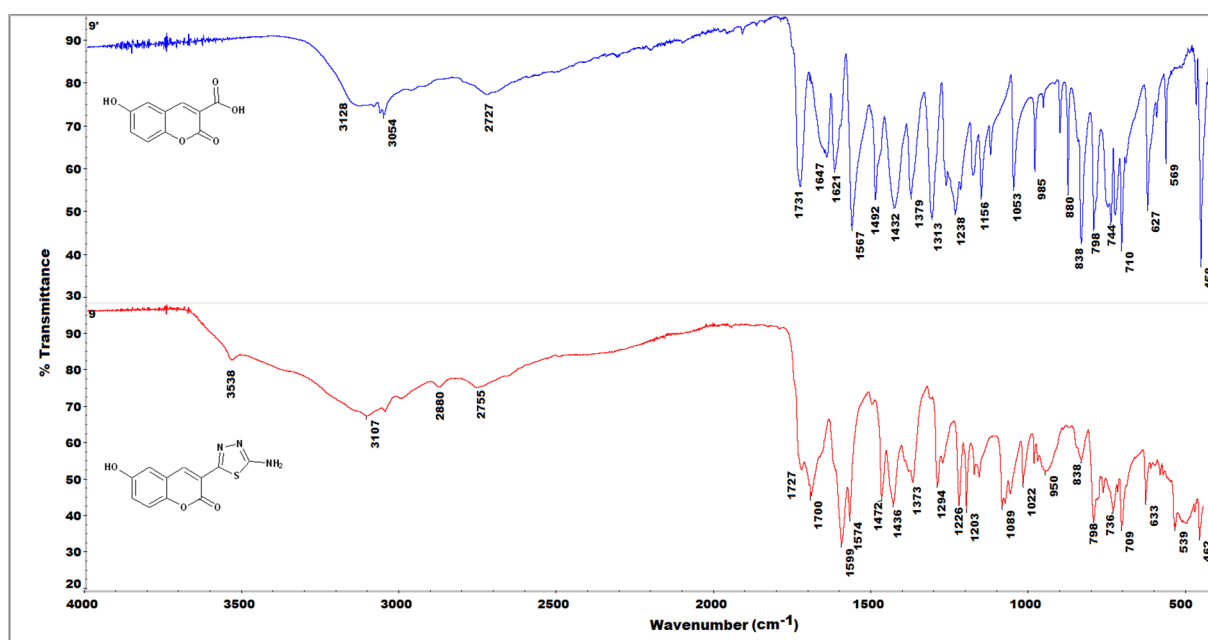


Figure S8. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **9'** (top) and the corresponding coumarin-thiadiazole hybrid **9** (bottom).

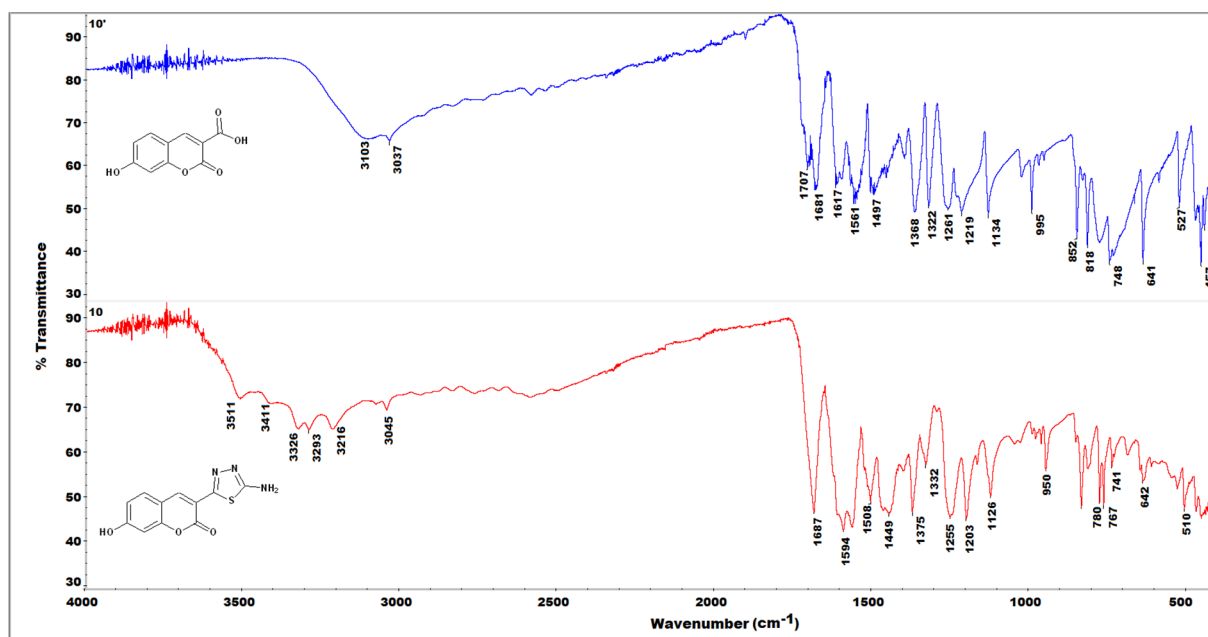


Figure S9. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **10'** (top) and the corresponding coumarin-thiadiazole hybrid **10** (bottom).

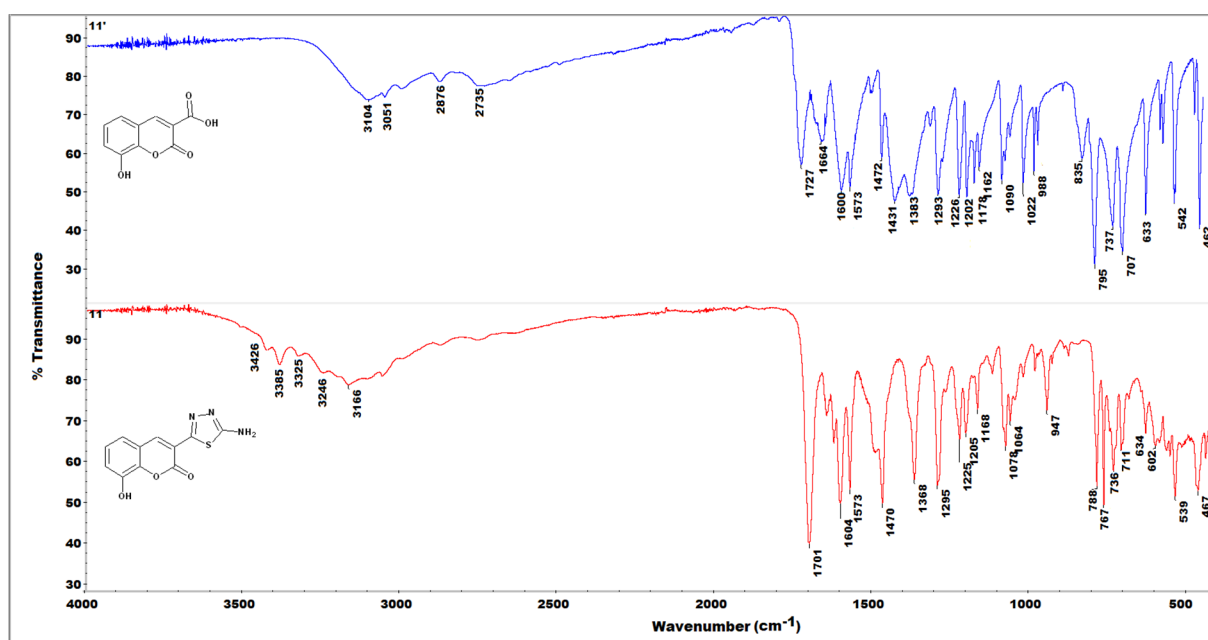


Figure S10. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **11'** (top) and the corresponding coumarin-thiadiazole hybrid **11** (bottom).

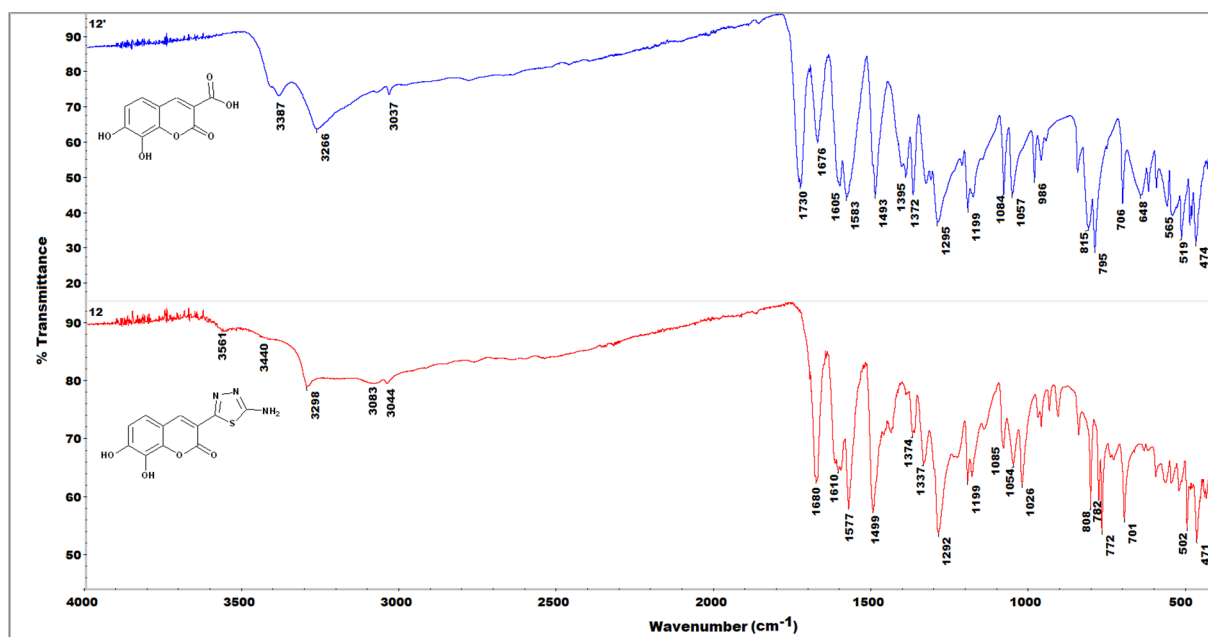


Figure S11. Comparison of the IR(ATR) spectra of coumarin-3-carboxylic acid **12'** (top) and the corresponding coumarin-thiadiazole hybrid **12** (bottom).

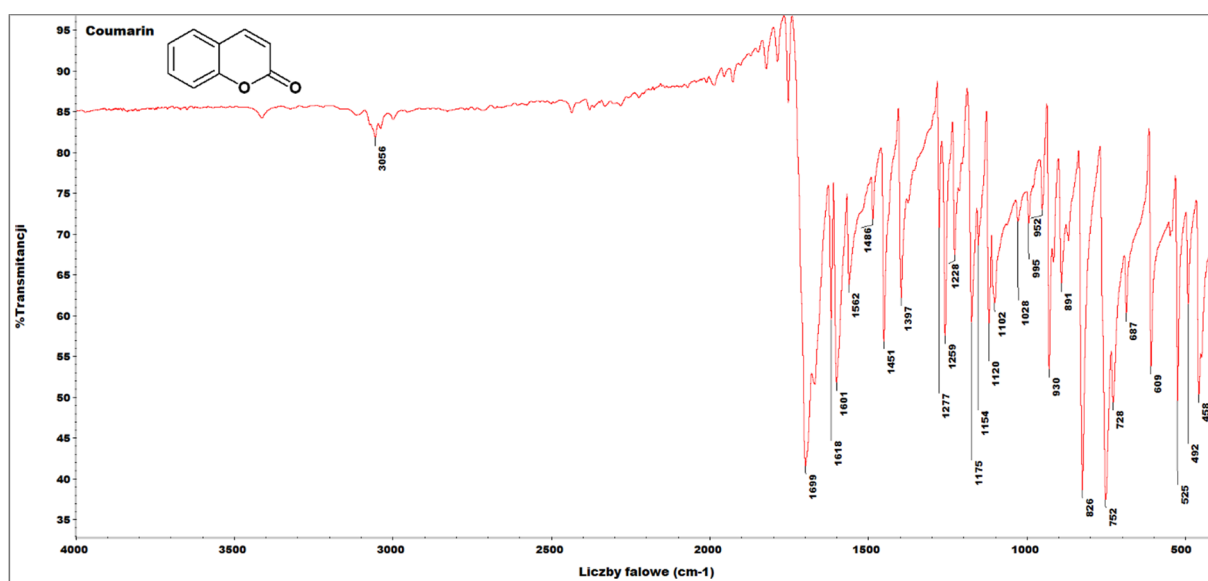


Figure S12. IR(ATR) spectrum of coumarin.

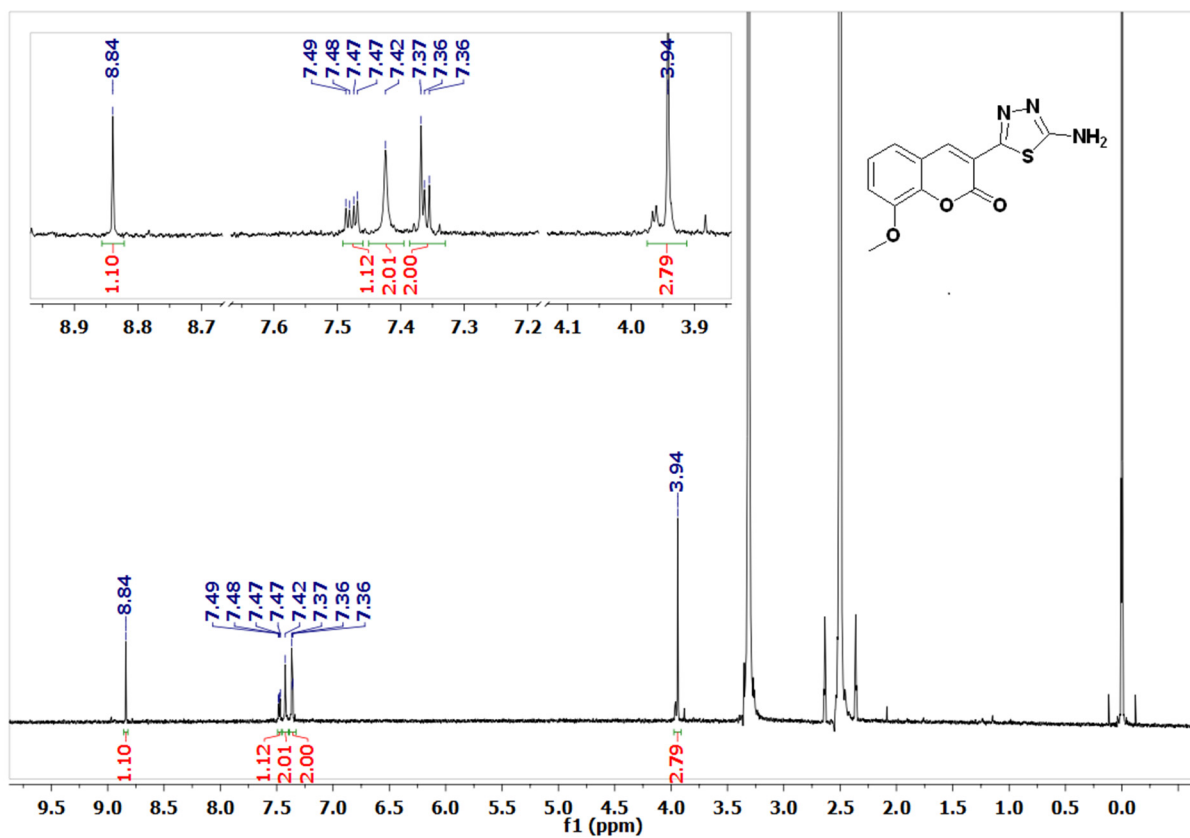


Figure S13. ¹H-NMR (DMSO-d₆) spectrum of coumarin-thiadiazole hybrid **2**.

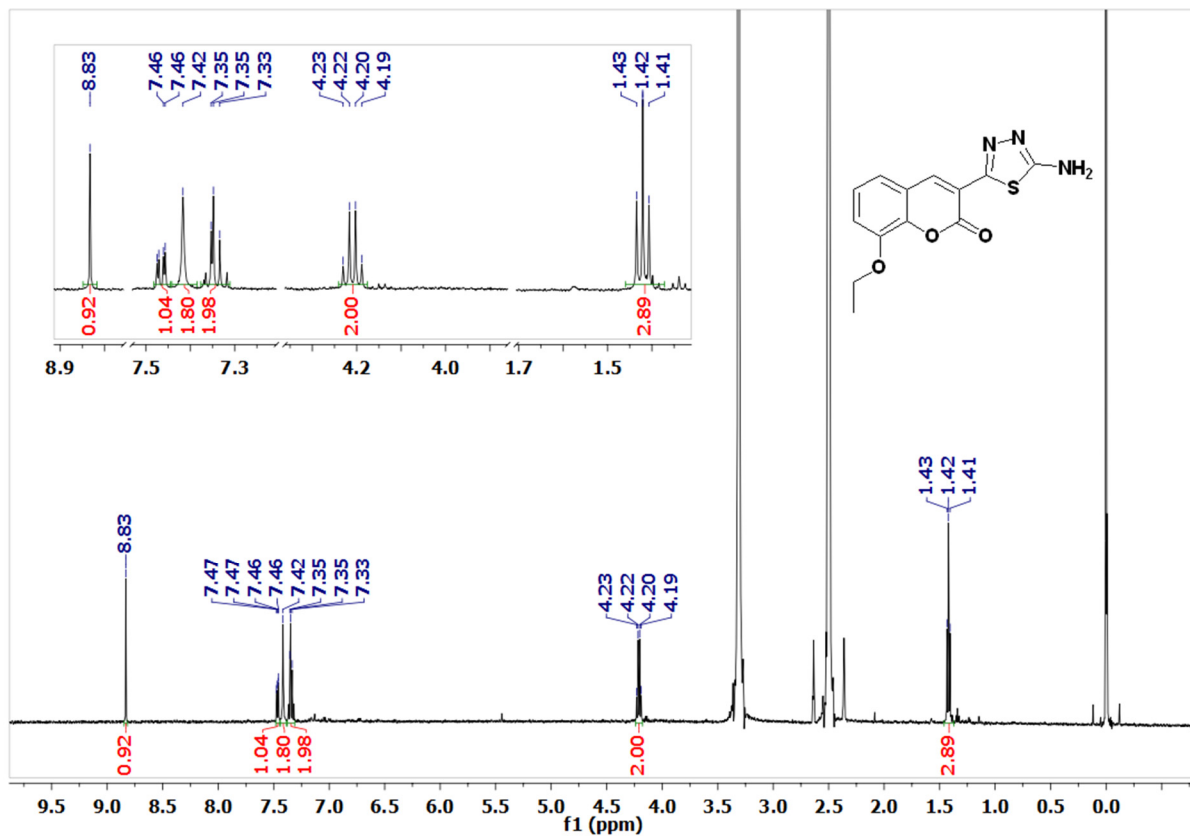


Figure S14. ¹H-NMR (DMSO-d₆) spectrum of coumarin-thiadiazole hybrid **3**.

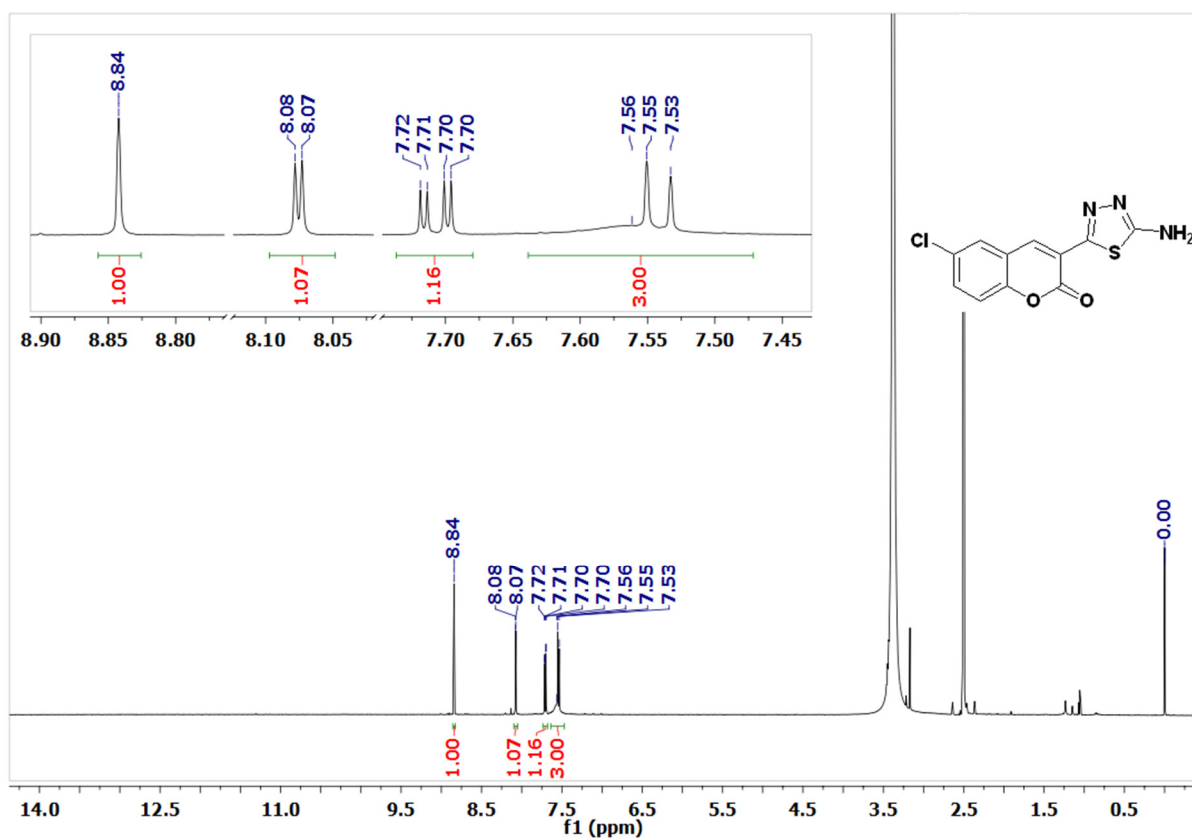


Figure S15. ^1H -NMR (DMSO-d_6) spectrum of coumarin-thiadiazole hybrid **4**.

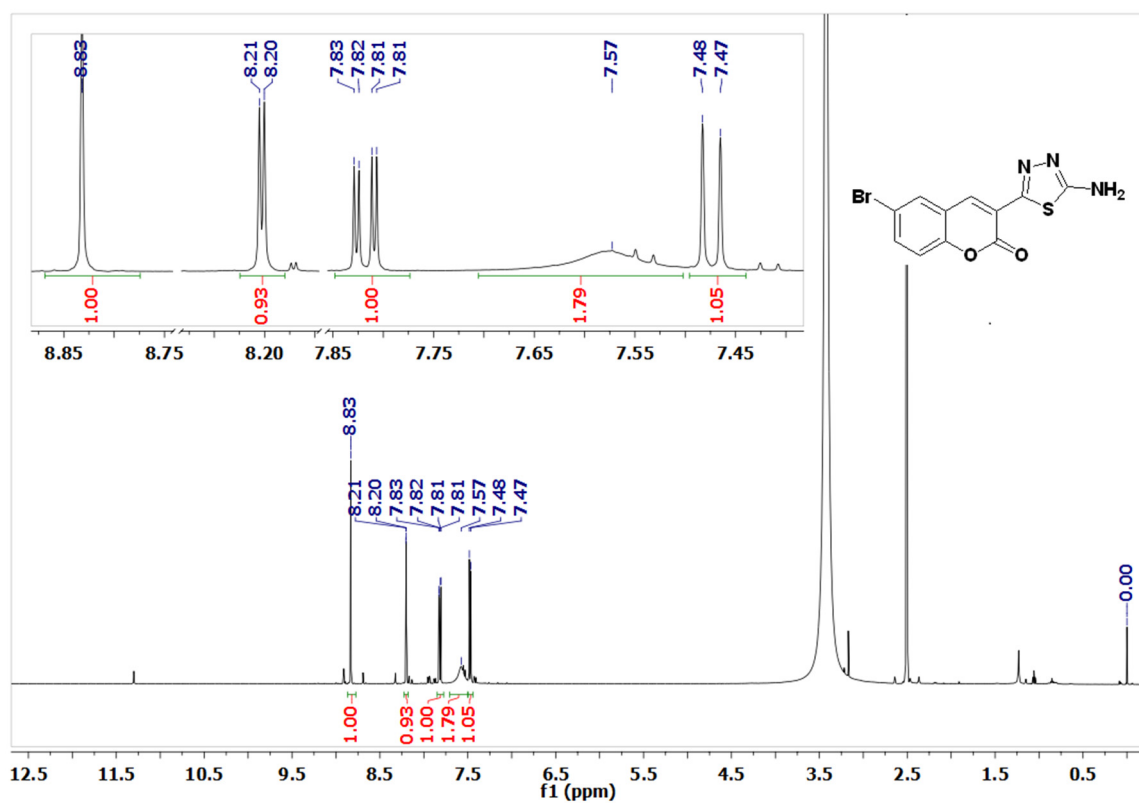


Figure S16. ^1H -NMR (DMSO-d_6) spectrum of coumarin-thiadiazole hybrid **5**.

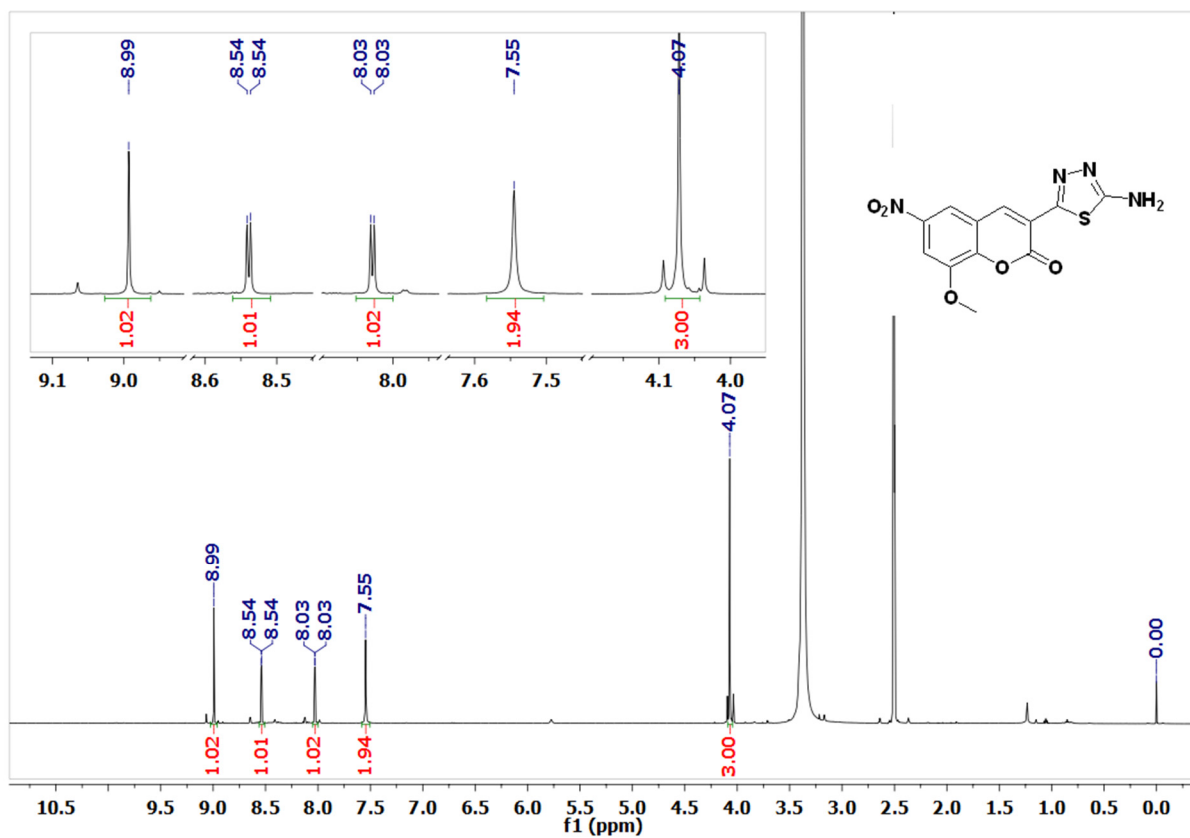


Figure S17. ^1H -NMR (DMSO-d_6) spectrum of coumarin-thiadiazole hybrid **7**.

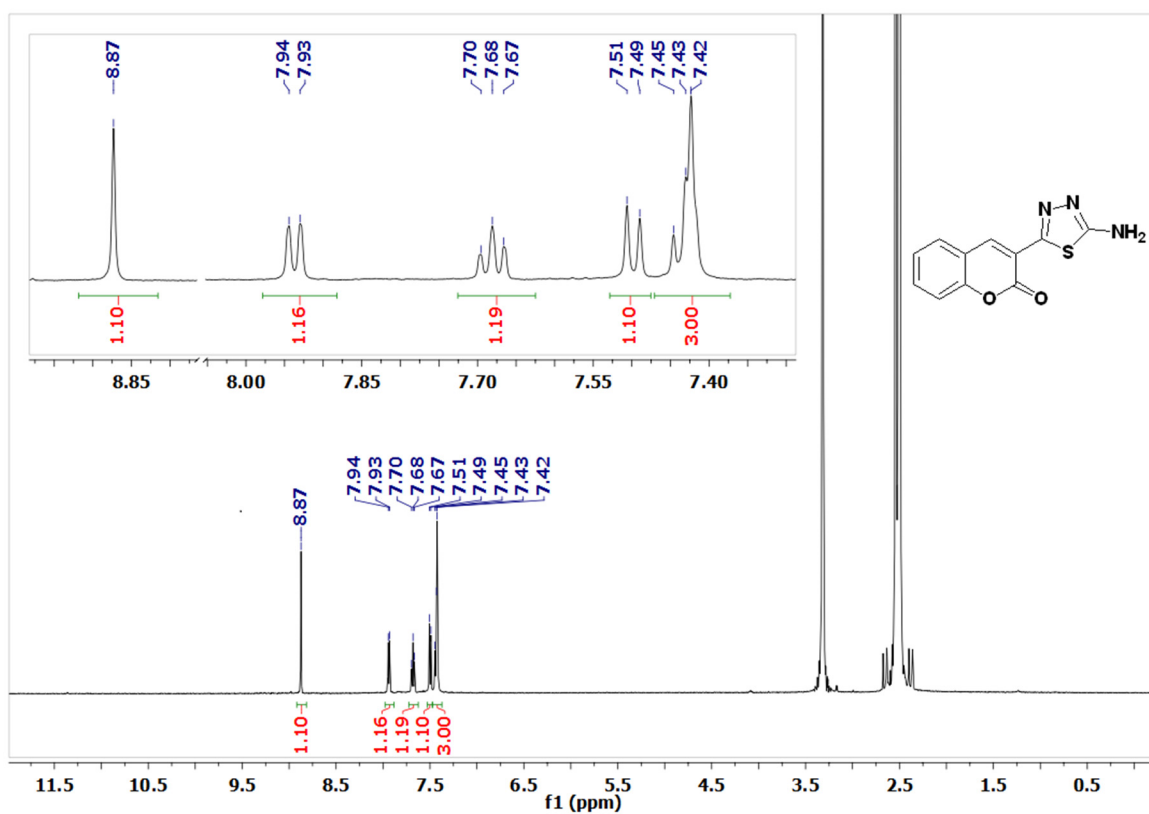


Figure S18. ^1H -NMR (DMSO-d_6) spectrum of coumarin-thiadiazole hybrid **8**.

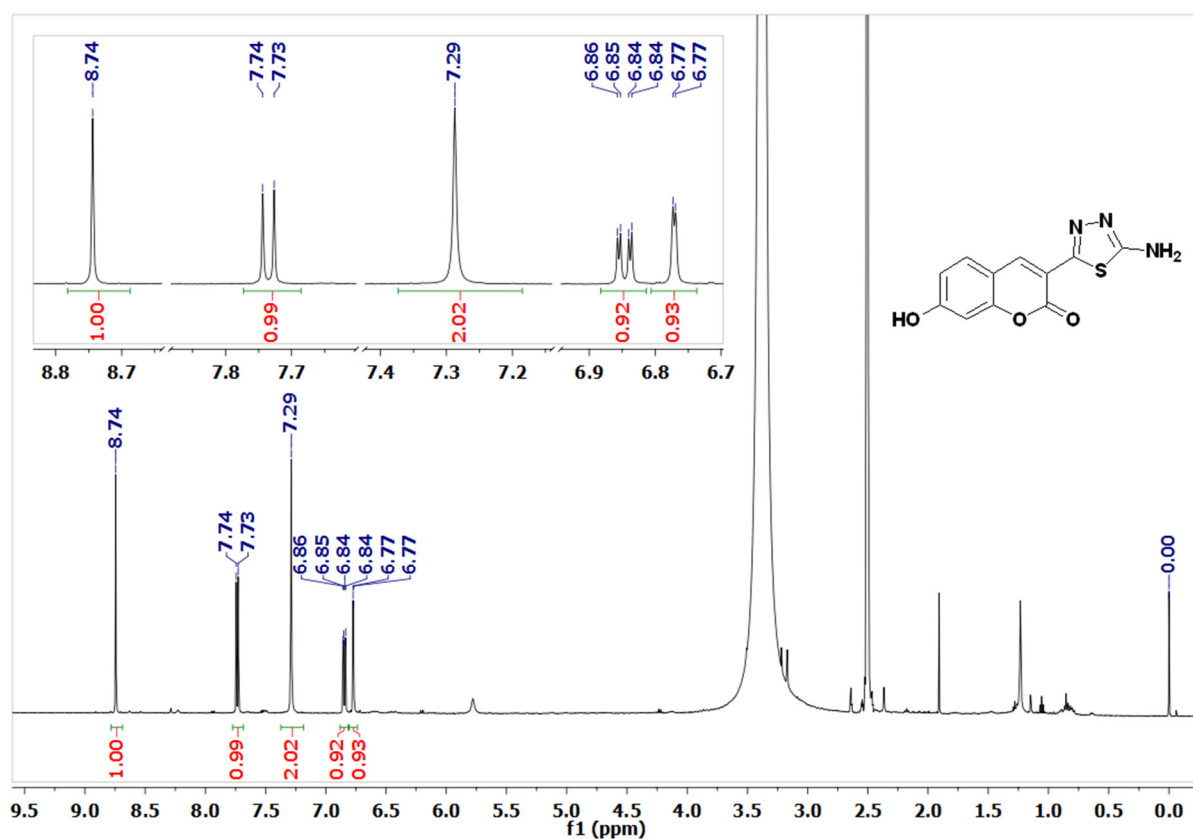


Figure S19. ^1H -NMR (DMSO-d_6) spectrum of coumarin-thiadiazole hybrid **10**.

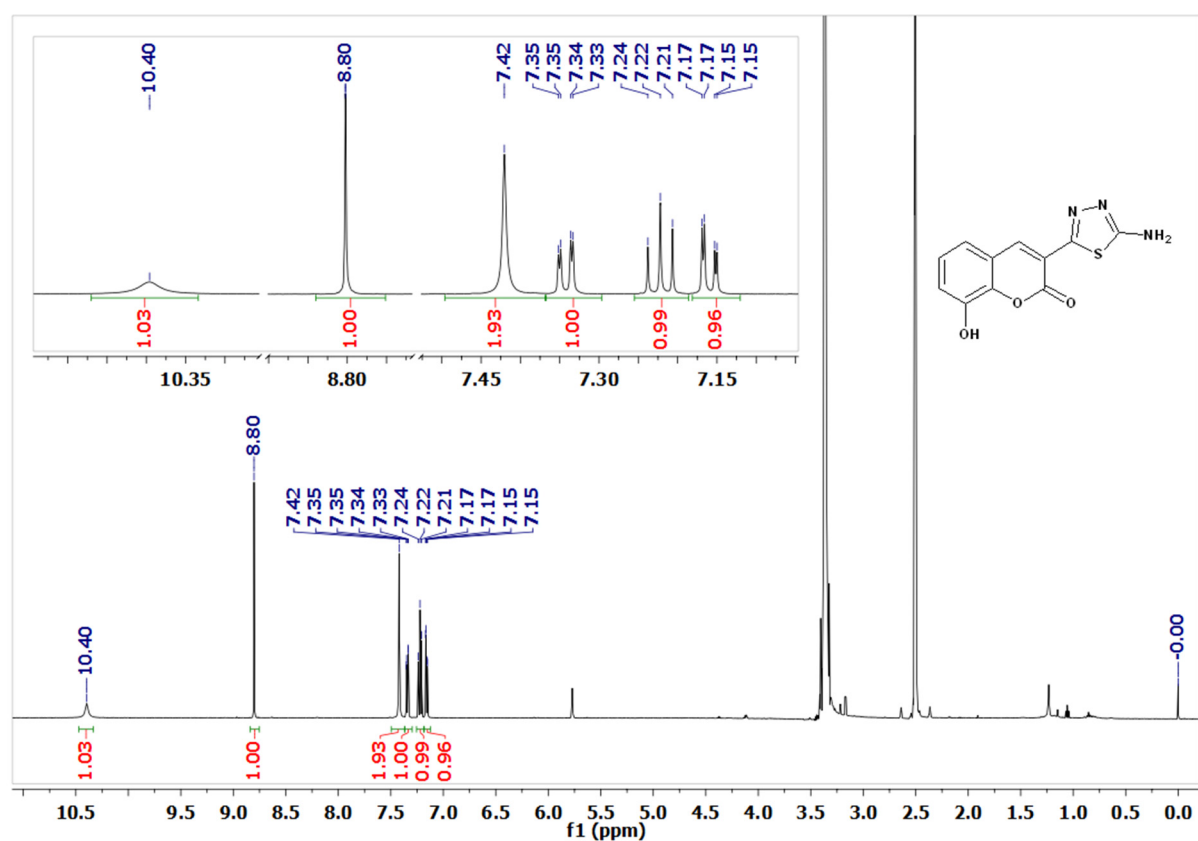


Figure S20. ^1H -NMR (DMSO-d_6) spectrum of coumarin-thiadiazole hybrid **11**.

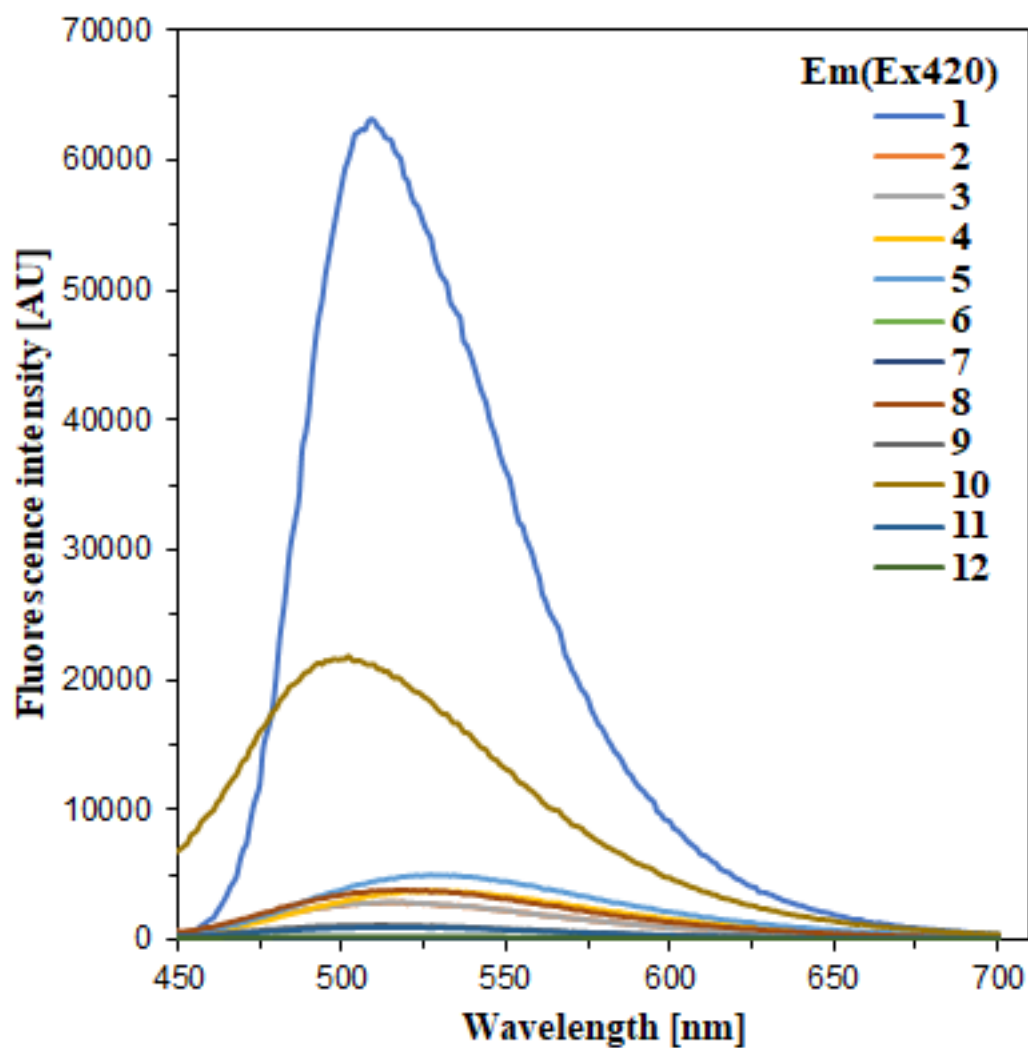


Figure S21. Fluorescence emission spectra of coumarin-thiadiazole hybrids **1-12** in methanol. The spectra were recorded at the $\lambda_{\text{ex}} = 420$ nm and concentration of 0.01 mM, except **1** which was recorded at the concentration of 0.002 mM.