4-Methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarine

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Supporting Information

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1. NMR spectra of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole 2

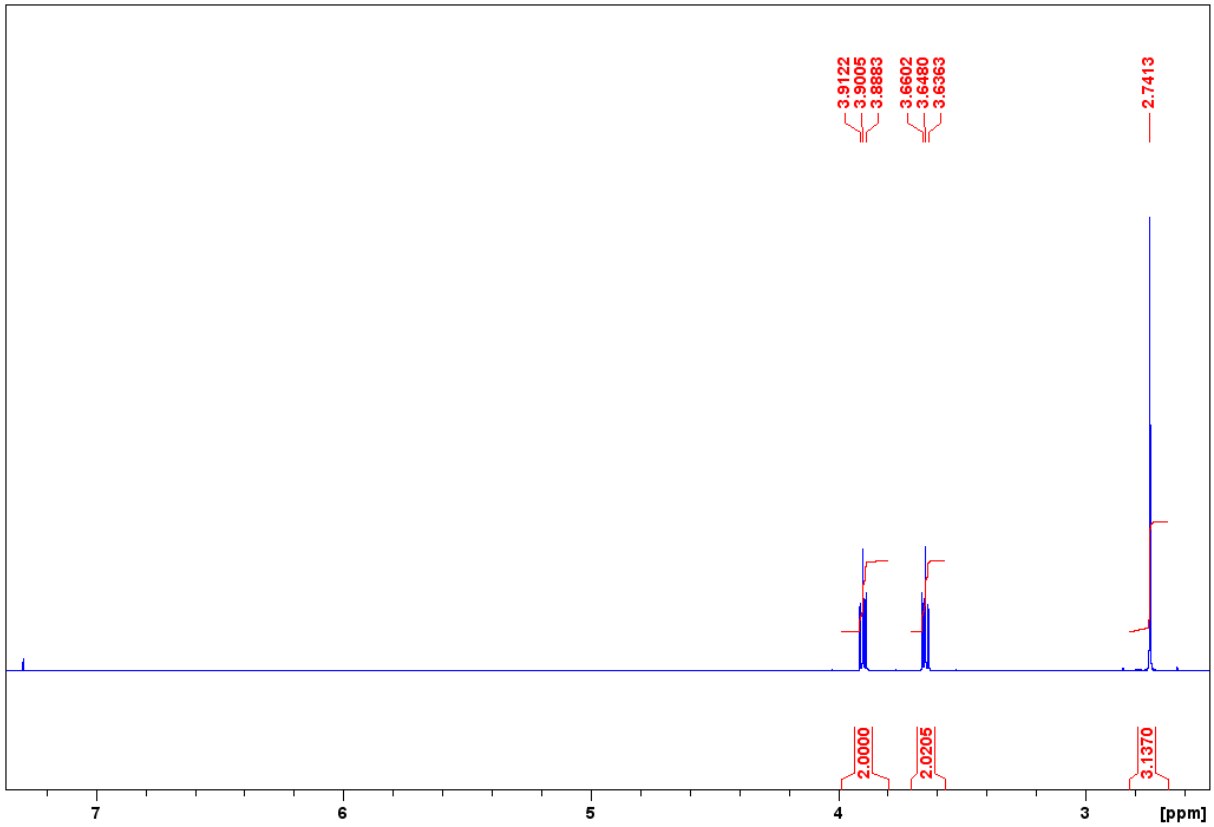

Figure S1. ^{1}H NMR spectrum of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole in $CDCl_3$.

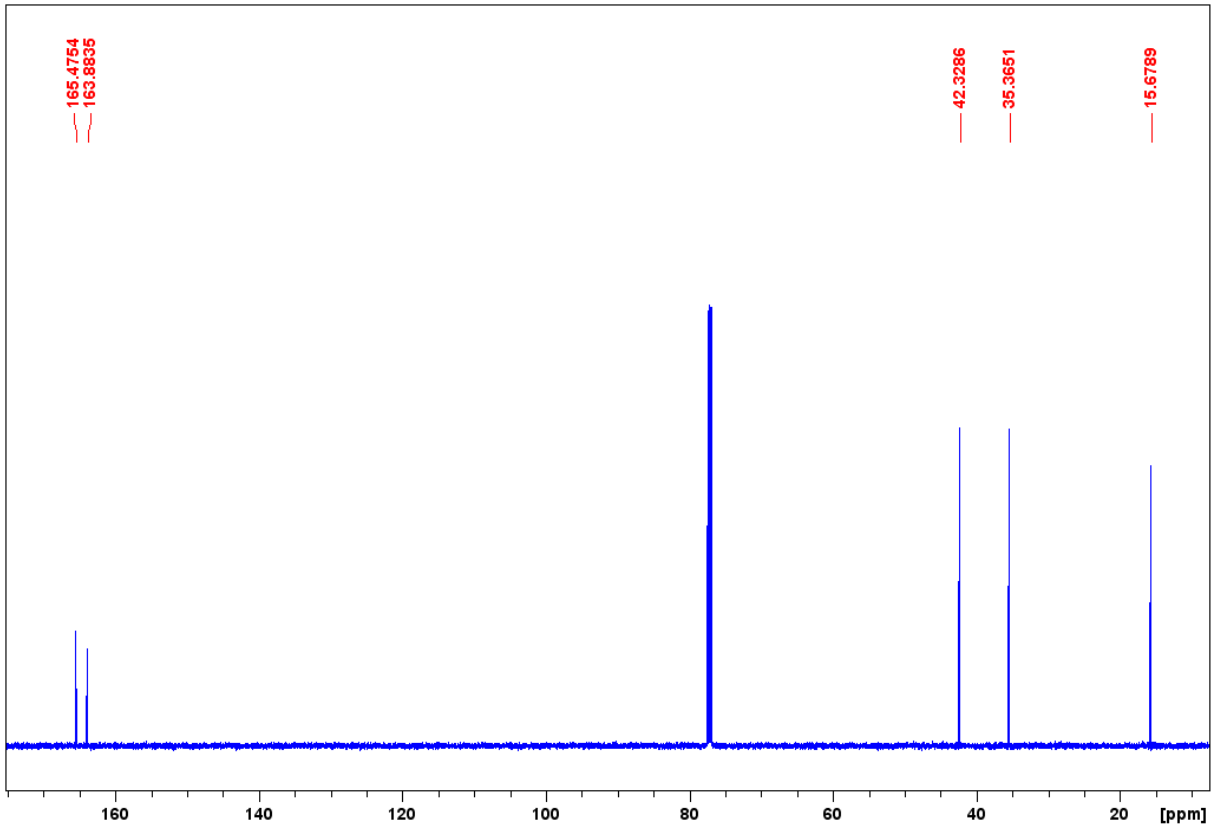

Figure S2. ^{13}C NMR spectrum of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole in $CDCl_3$.

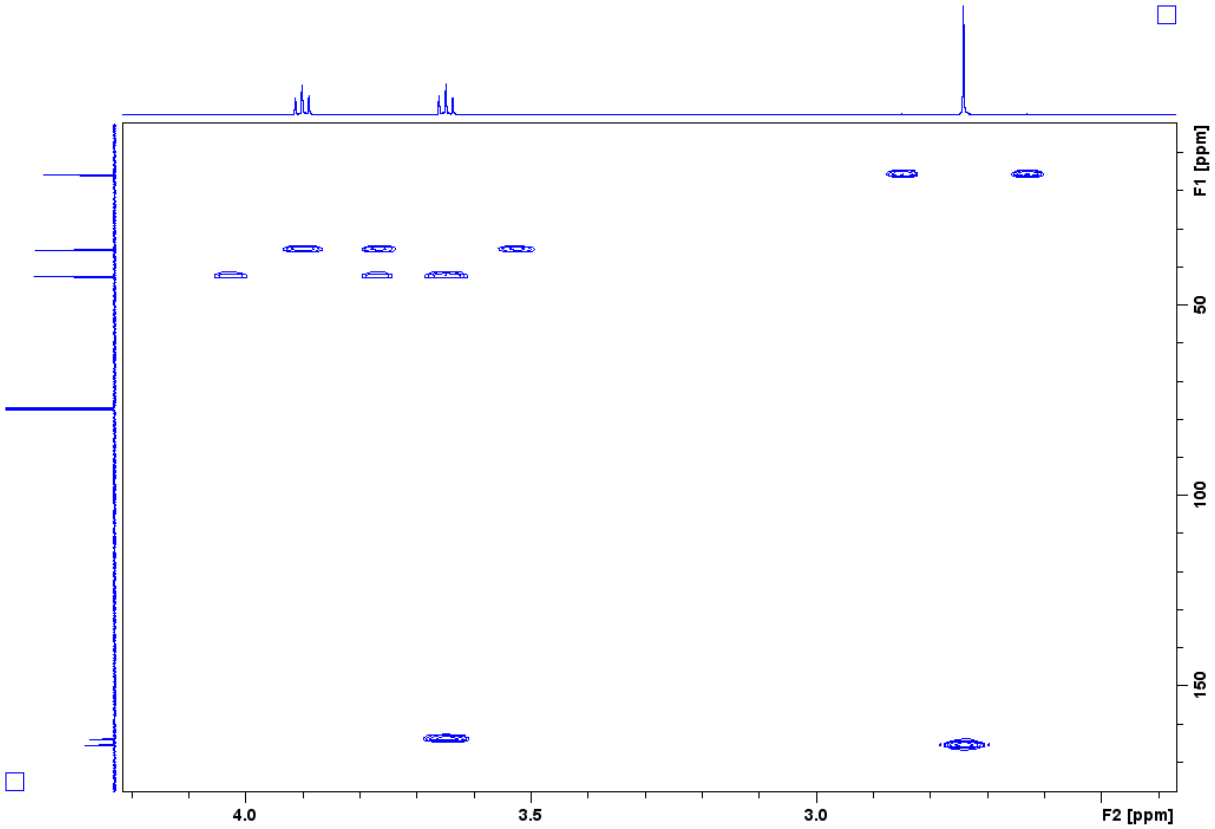

Figure S3. HMBC spectrum of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole in $CDCl_3$.

2. NMR spectra of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin 3

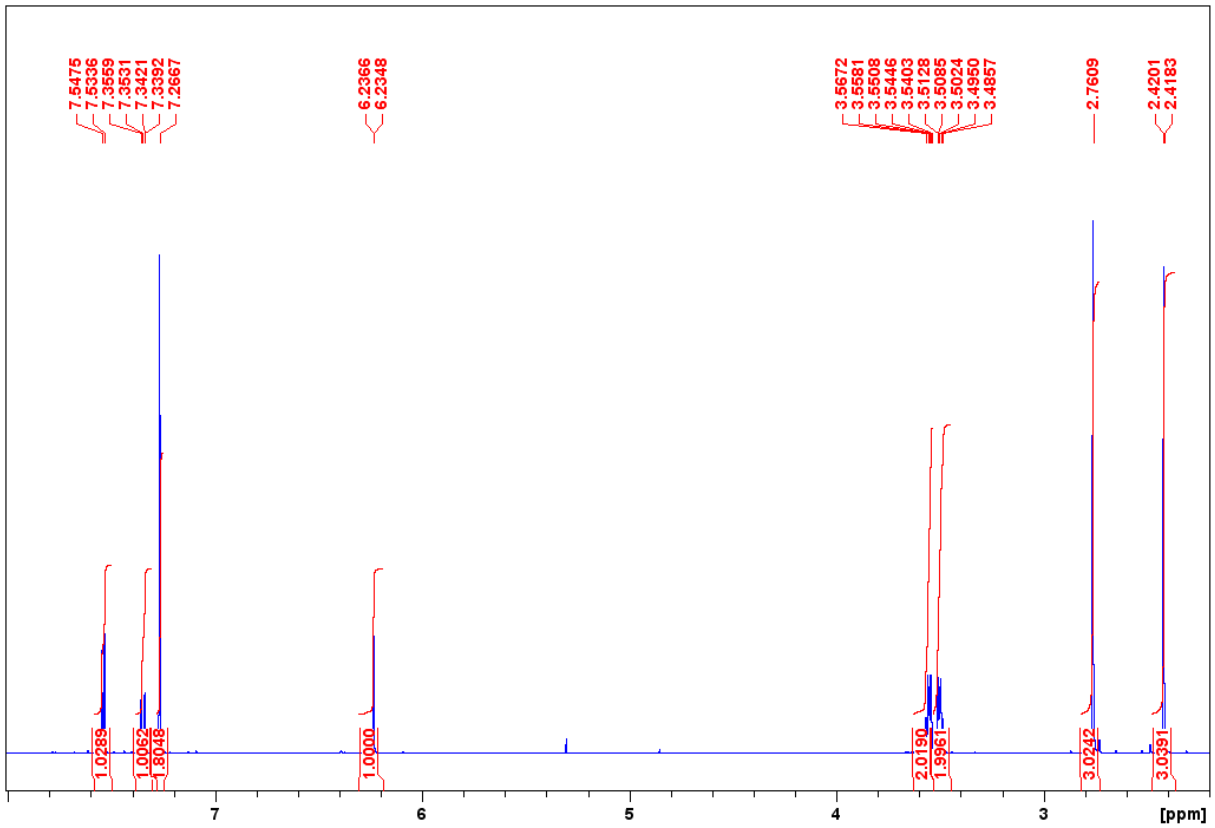

Figure S4. ^1H NMR spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin in $CDCl_3$.

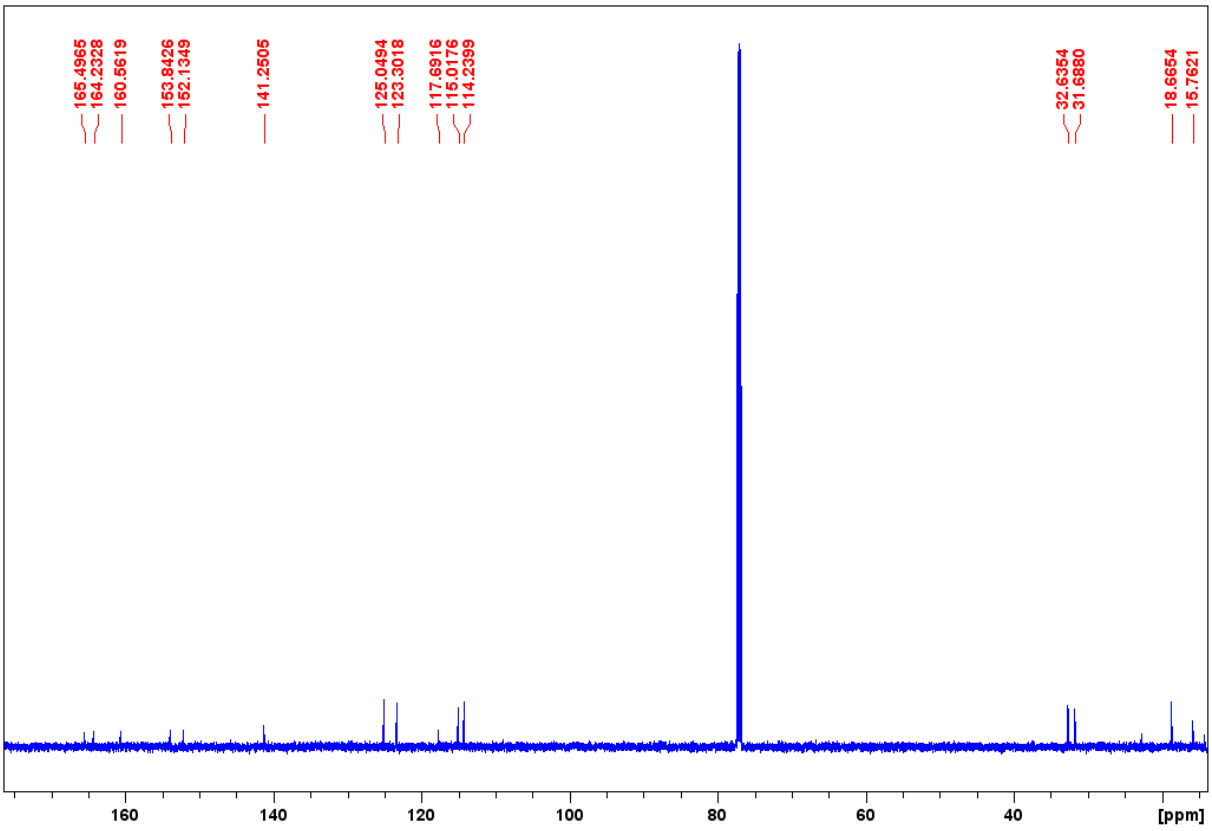

Figure S5. ^{13}C NMR spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin in $CDCl_3$.

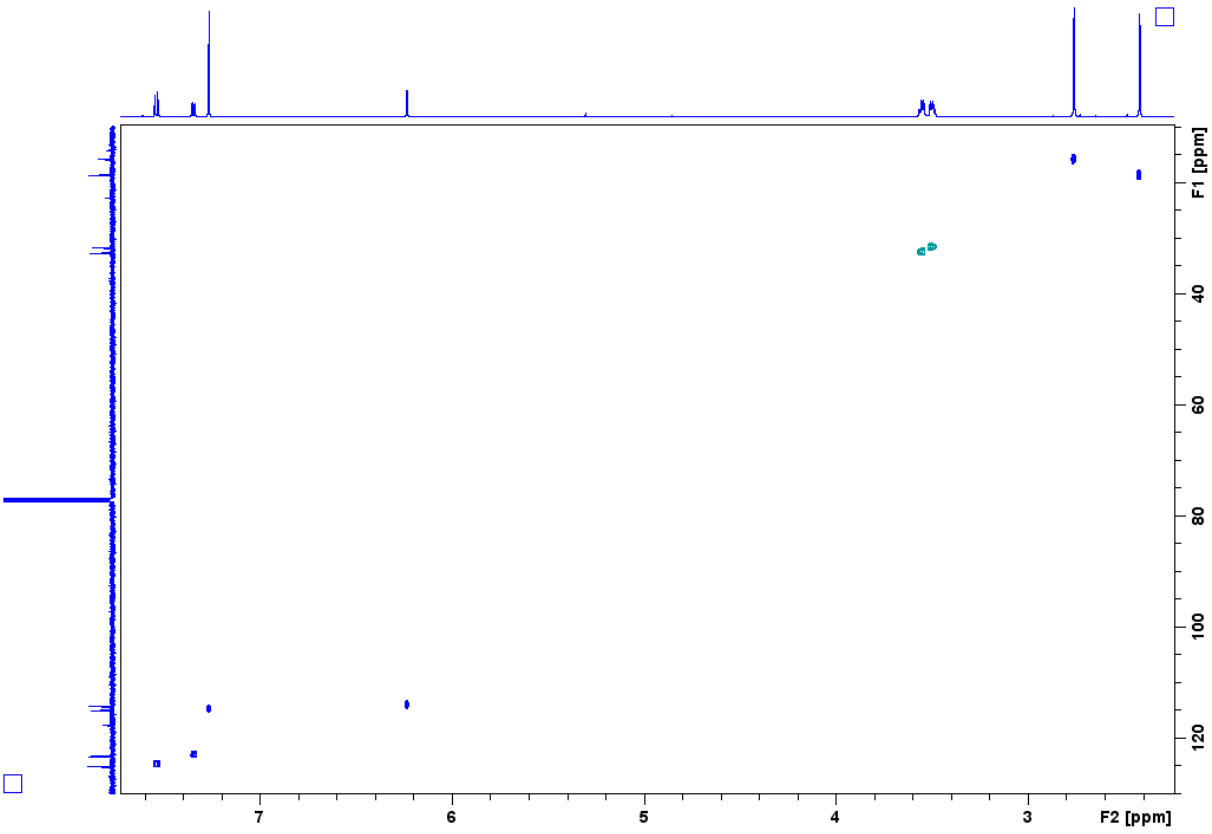

Figure S6. HSQC spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin in $CDCl_3$.

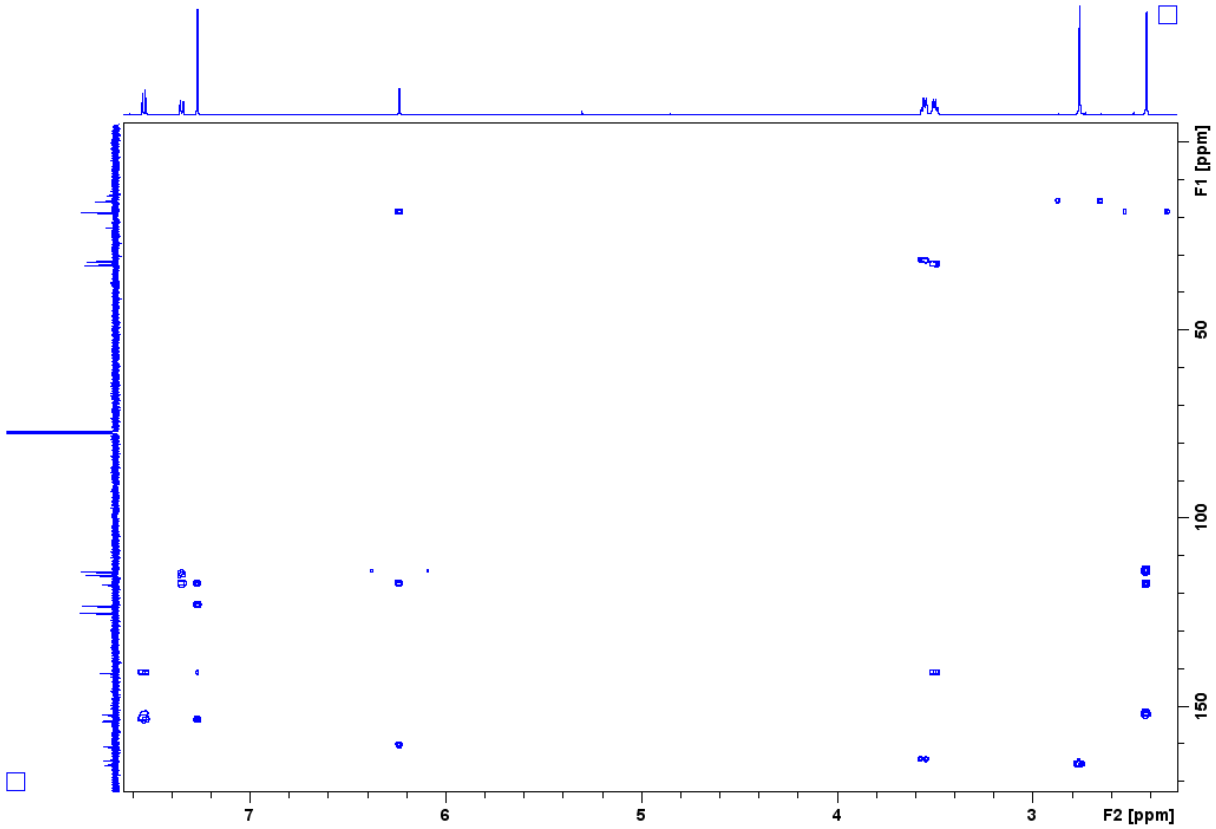

Figure S7. HMBC spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin in $CDCl_3$.

3. HRMS spectrum of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole 2

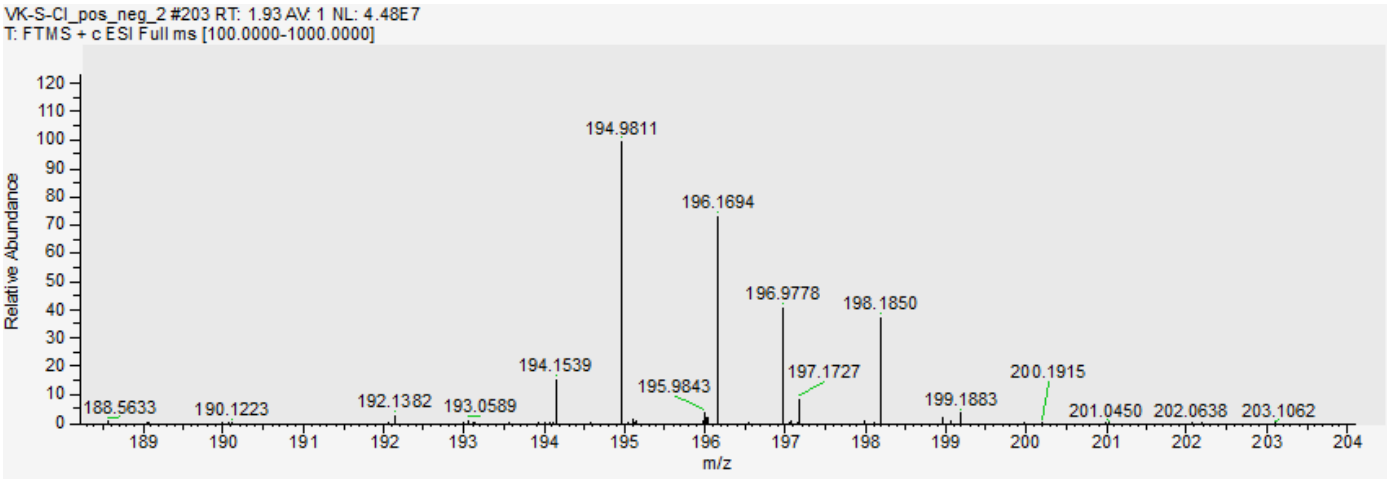

Figure S8. HRMS spectrum of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole 2**.**

4. HRMS spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin 3

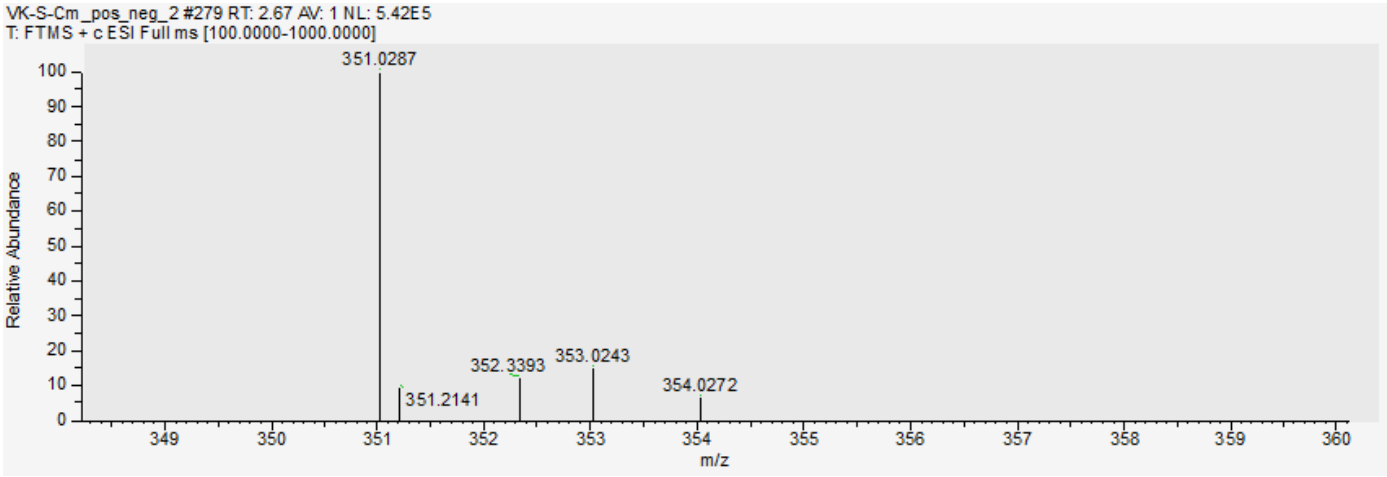

Figure S9. HRMS spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin 3**.**

5. IR spectrum of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole 2

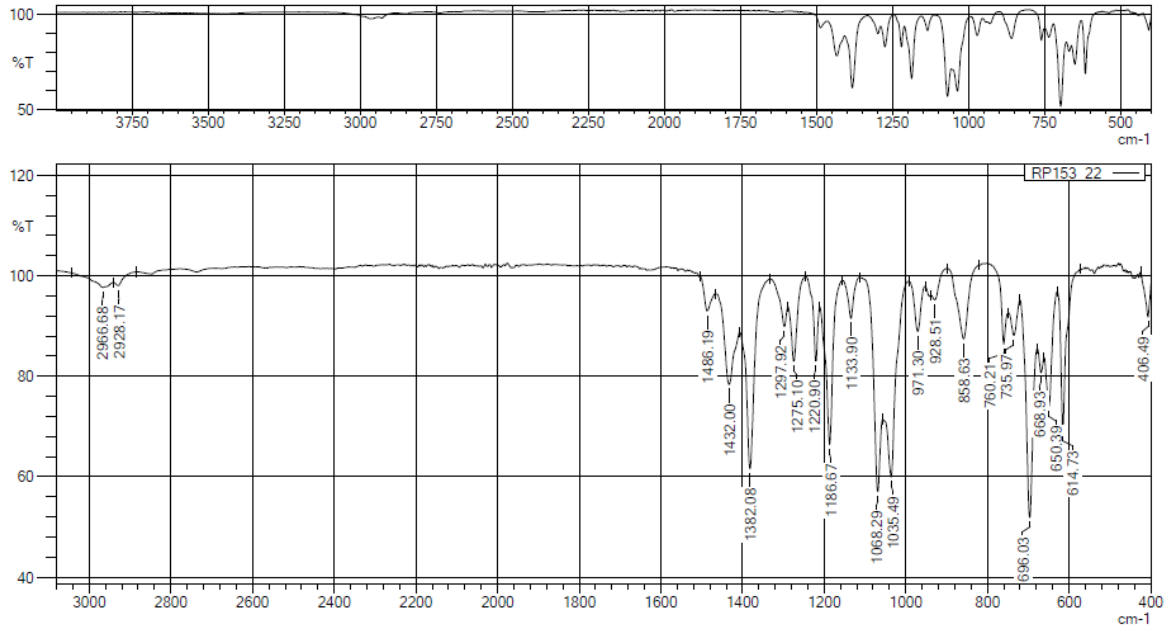

Figure S10. IR spectrum of 2-((2-chloroethyl)thio)-5-methyl-1,3,4-thiadiazole **2**.

6. IR spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin 3

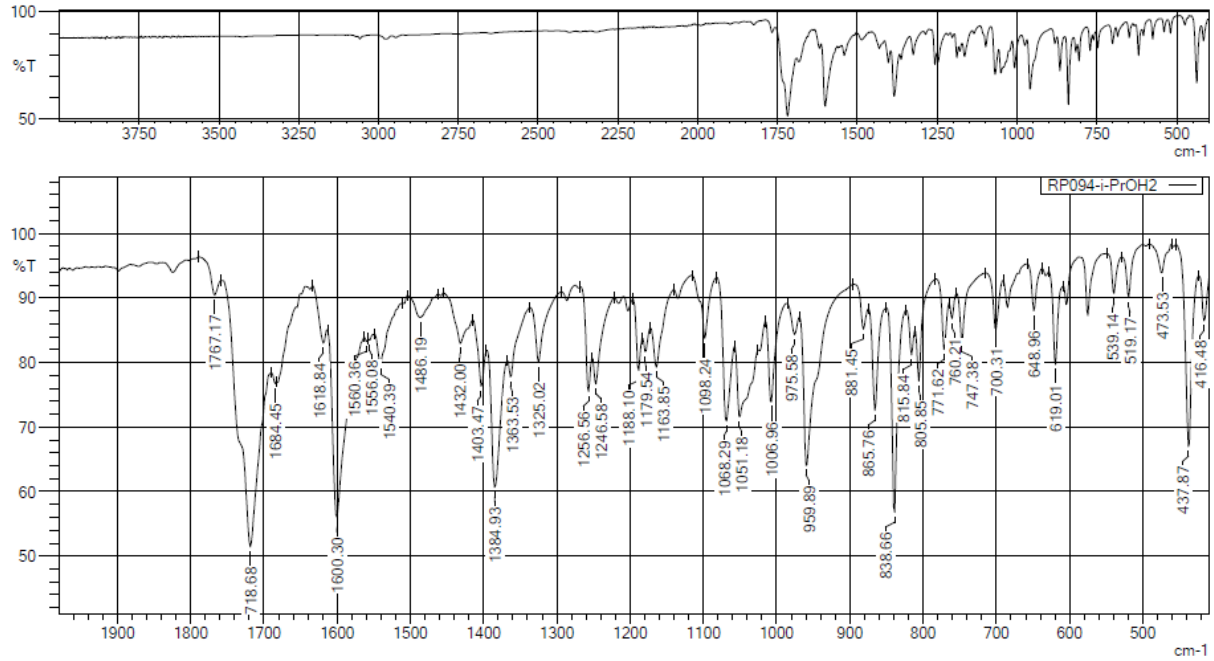

Figure S11. IR spectrum of 4-methyl-7-((2-((5-methyl-1,3,4-thiadiazol-2-yl)thio)ethyl)thio)-coumarin 3.

7. Table S1. The most important data collection and crystallographic refinement parameters for 3.

$C_{15}H_{14}N_2O_2S_3$
M_r = 350.46
Monoclinic, $P2_1/n$
a = 13.515 (3) Å
b = 4.1892 (12) Å
c = 27.577 (7) Å
β = 94.12 (2)°
V = 1557.2 (7) Å^3
Z = 4
F(000) = 728
D_x = 1.495 Mg m^{-3}
Melting point : 157.2–157.7 °C;
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2099 reflections
θ = 2.6–31.7°
μ = 0.48 mm^{-1}
T = 290 K
Block, orange
0.25 × 0.2 × 0.1 mm^3
ω and φ scans
Absorption correction: multi-scan
T_{min} = 0.588, T_{max} = 1.000
16797 measured reflections
3168 independent reflections
2330 reflections with $I > 2\sigma(I)$
R_{int} = 0.154
θ_{max} = 26.4°, θ_{min} = 1.6°
h = −16 15
k = −5 5
l = −34 34
Refinement on F^2 Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.094
$wR(F^2)$ = 0.285
S = 1.06
3168 reflections
202 parameters; 0 restraints
Primary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1874P)^2 + 0.0072P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}
Extinction correction: SHELXL-2019/1[2],
$Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.020(8)
CCDC deposition number 2215392