Structurally Isomeric Ditopic 2-Mercaptobenzoxazole and 2-Hydroxybenzothiazole as Ligands for Design of 2D Sodium-Based Luminescent Coordination Polymers

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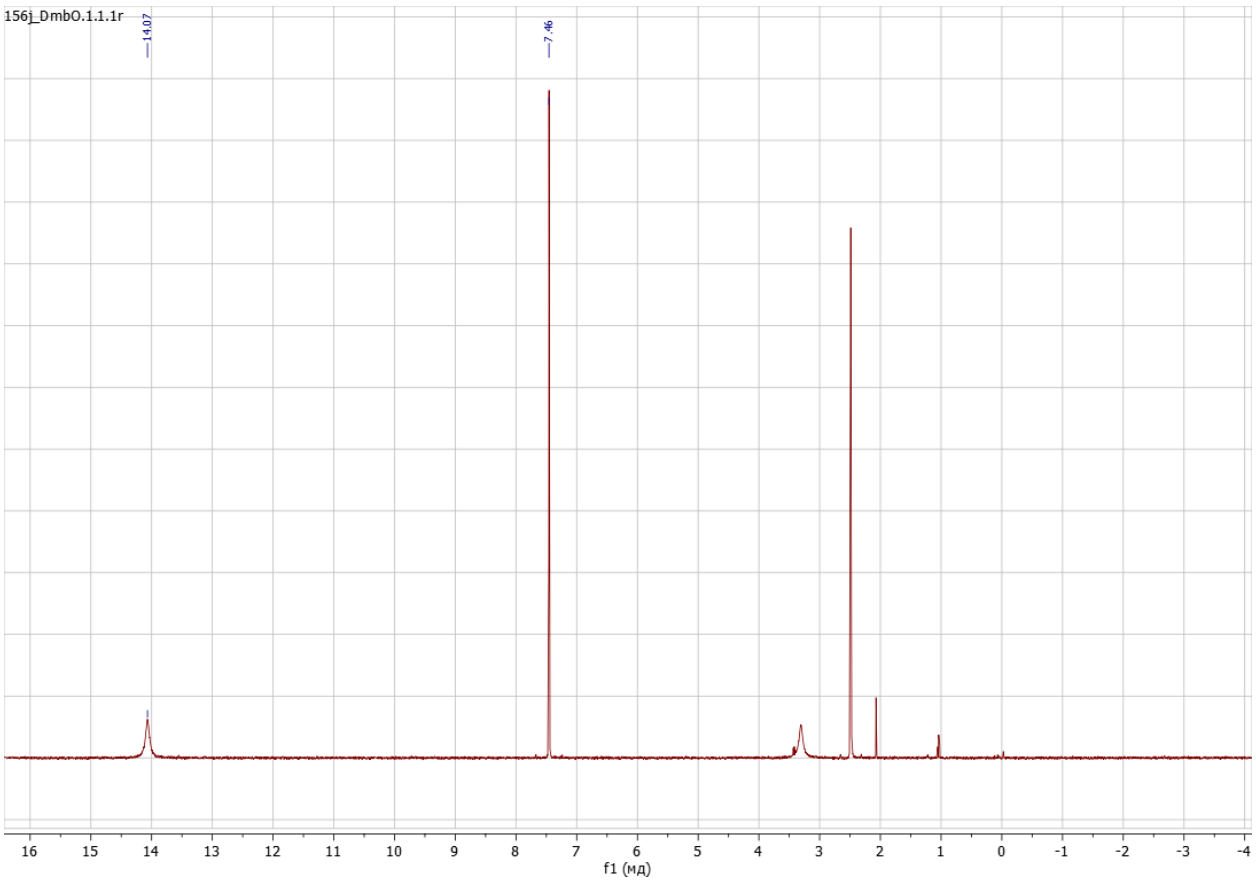

Figure S1. ^{1}H NMR spectrum of $H_2\mathbf{L^1}$ in DMSO-d6.

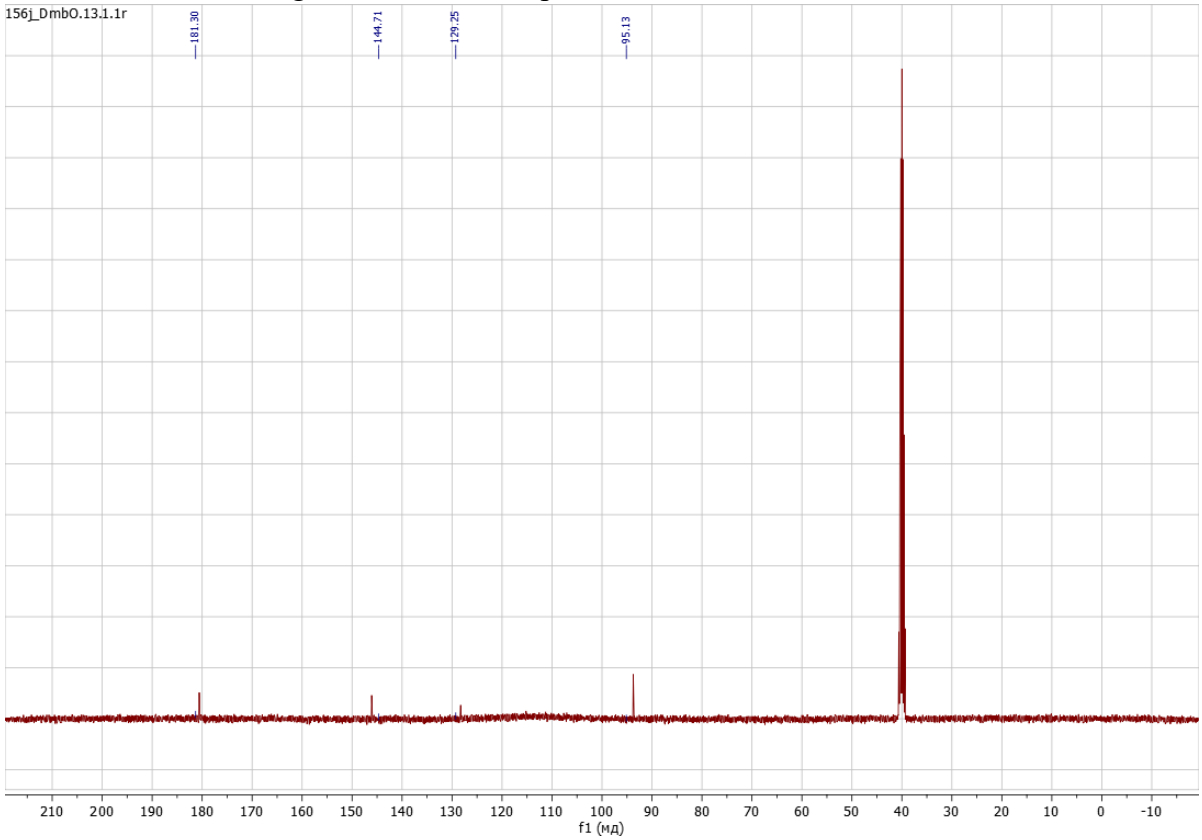

Figure S2. ^{13}C NMR spectrum of $H_2\mathbf{L^1}$ in DMSO-d6.

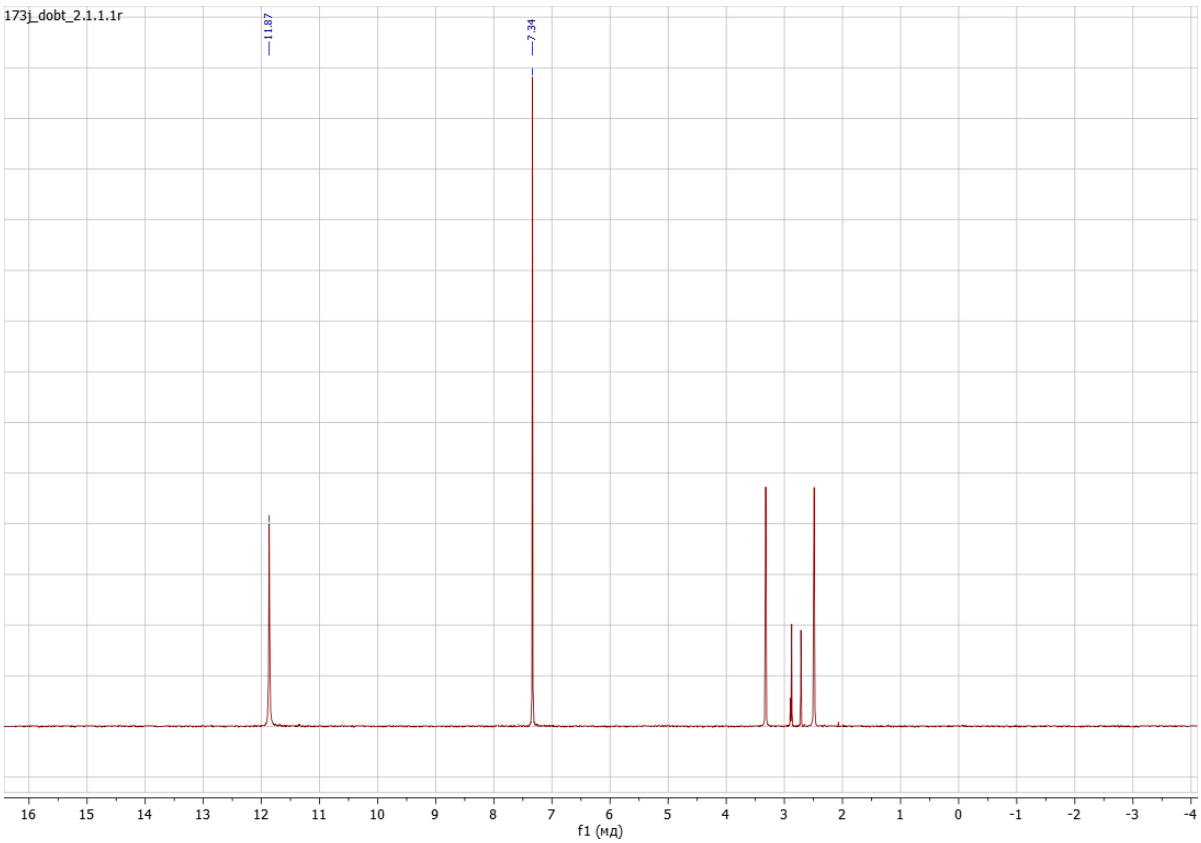

Figure S3. ^{1}H NMR spectrum of $H_2\mathbf{L^2}$ in DMSO-d6.

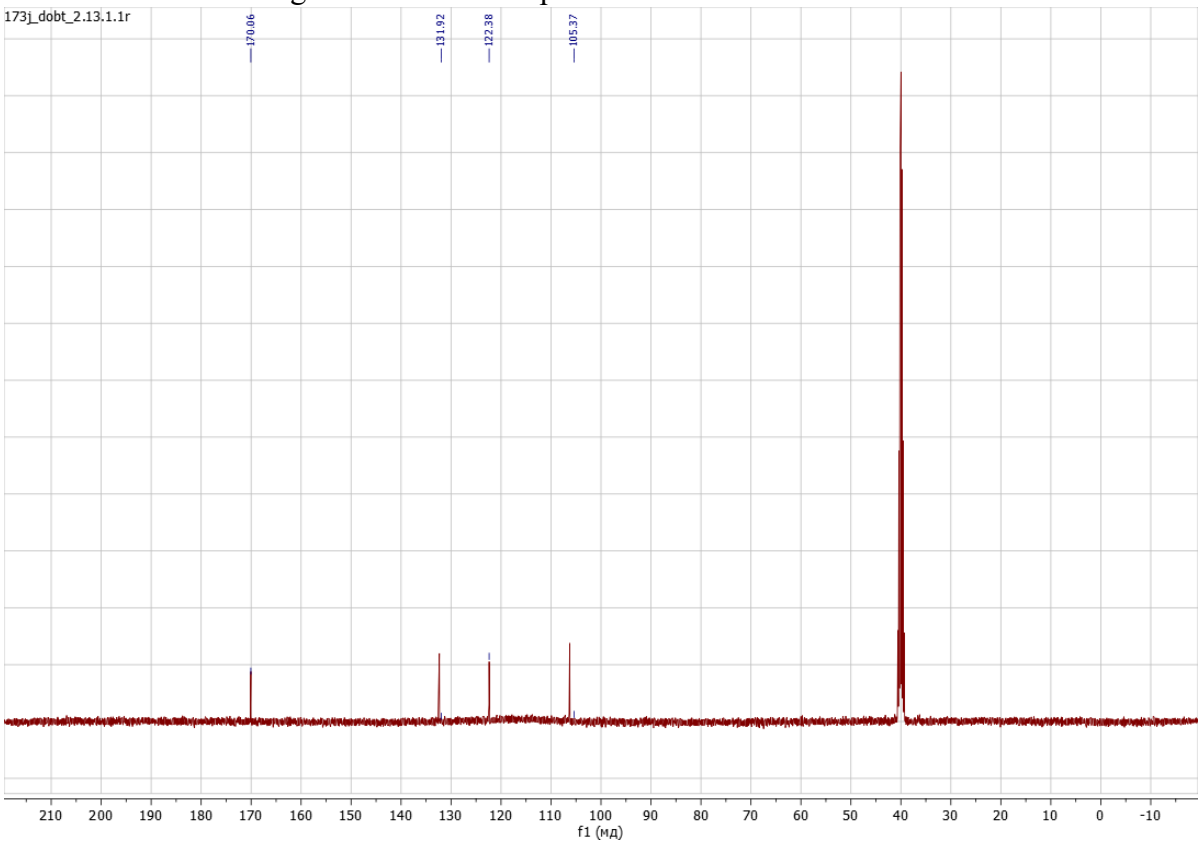

Figure S4. ^{13}C NMR spectrum of $H_2\mathbf{L^2}$ in DMSO-d6.

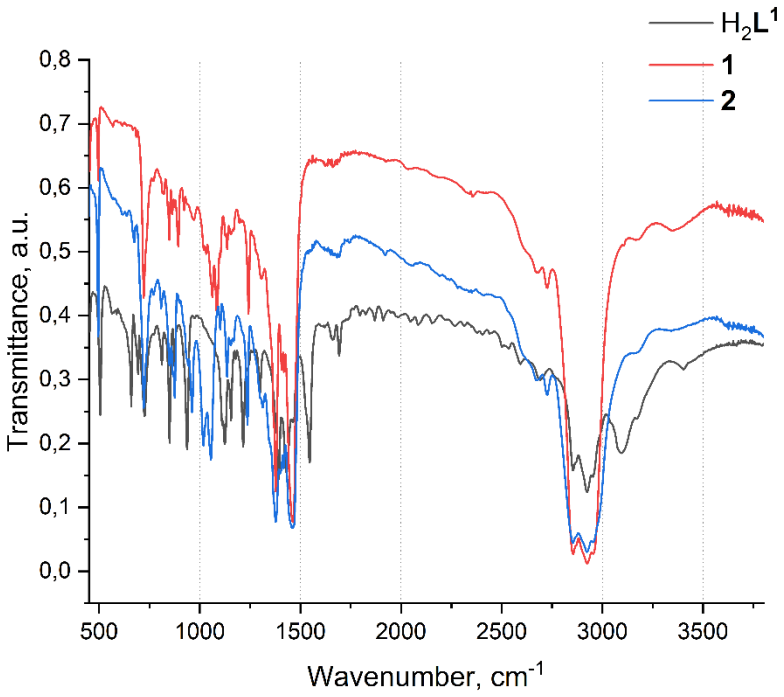

Figure S5. FTIR spectra of H_2**L**^{1} and CPs **1** and **2**.

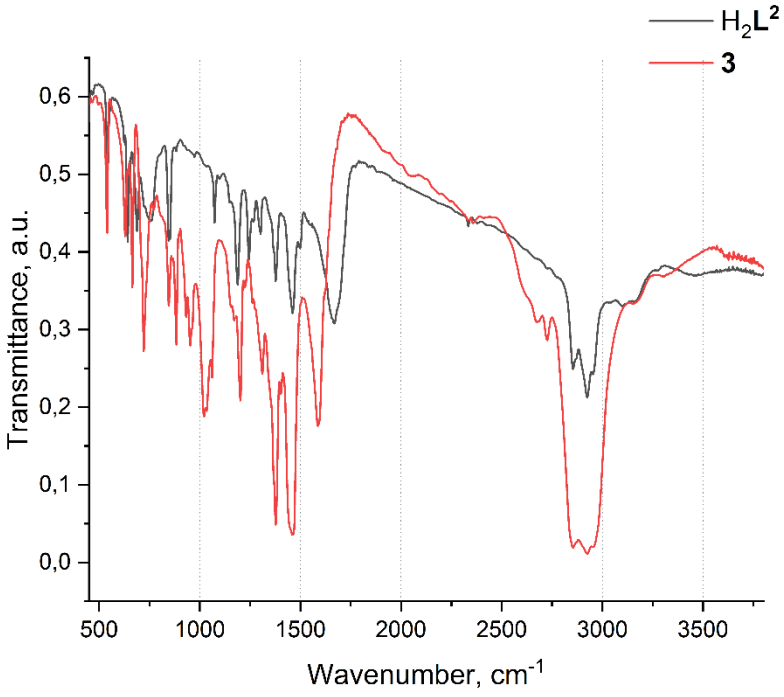

Figure S6. FTIR spectra of H_2**L**^{2} and CP **3**.

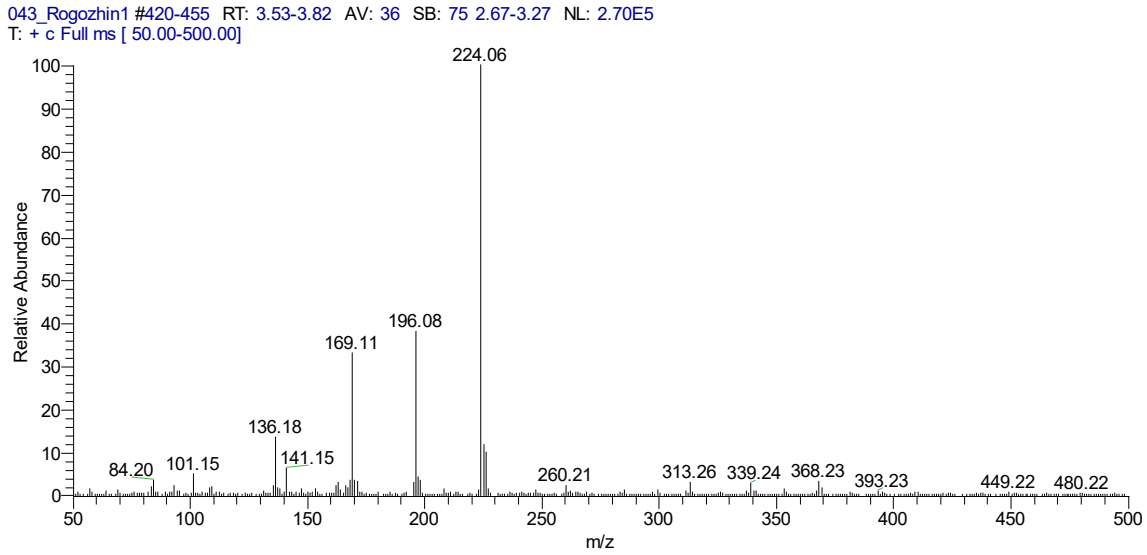

Figure S7. Mass-spectrum of $H_2\mathbf{L}^1$.

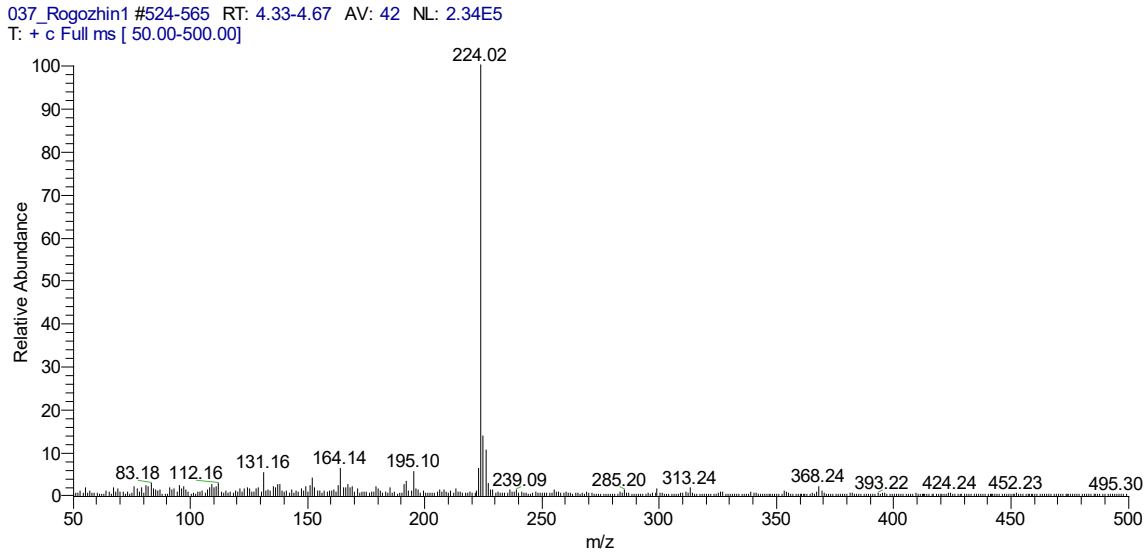

Figure S8. Mass-spectrum of $H_2\mathbf{L}^2$.

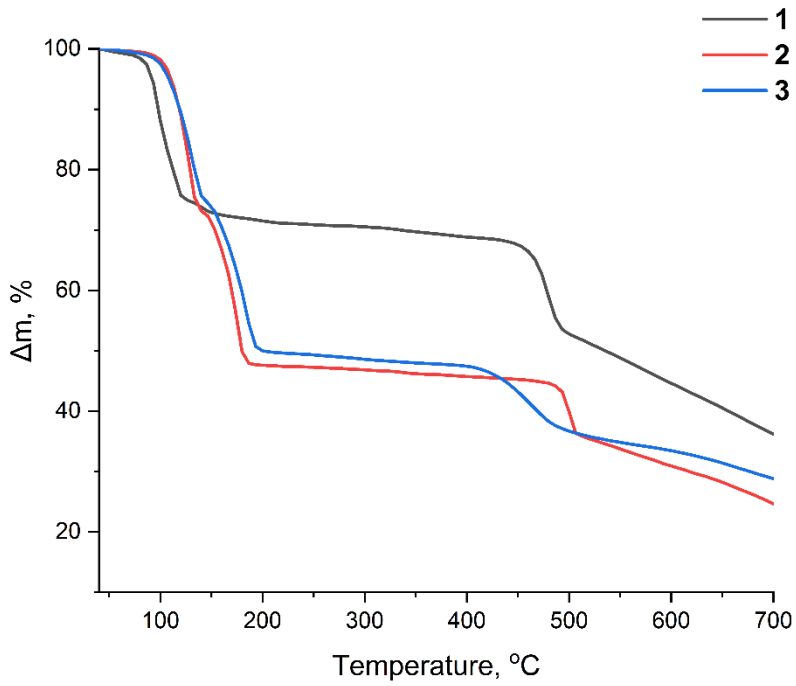

Figure S9. TG curves of **1**-**3**.

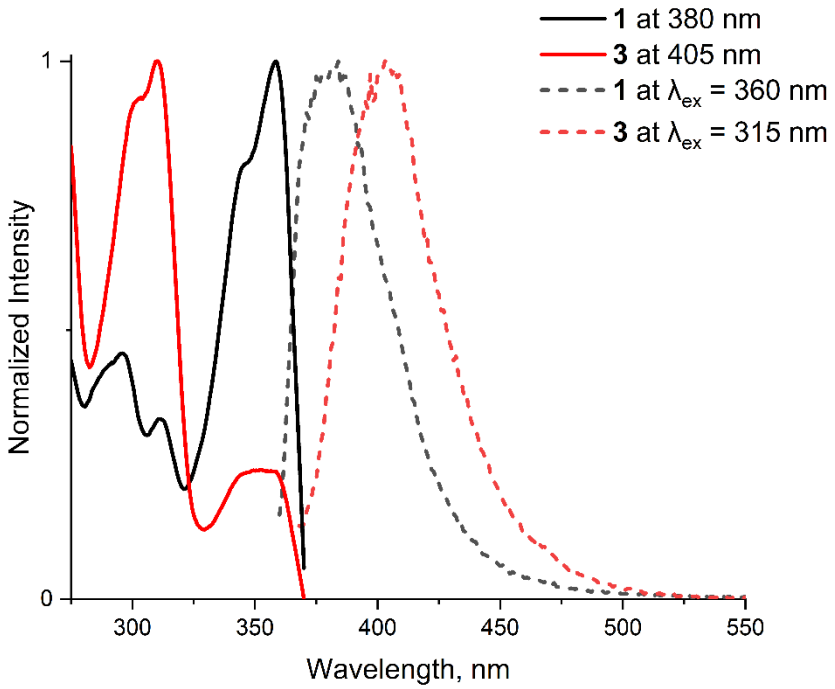

Figure S10. PL and PL excitation spectra of **1** and **3** in DME solution.

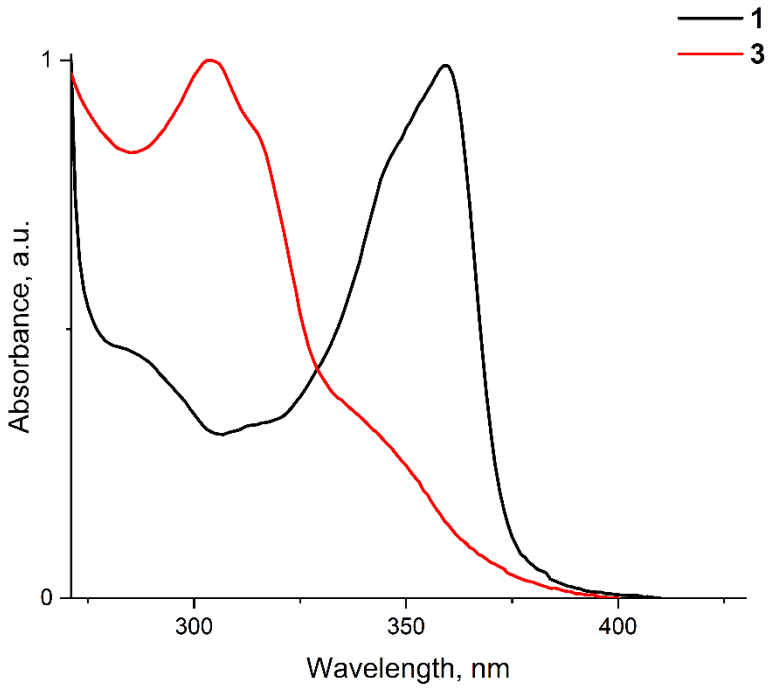

Figure S11. Absorption spectra of **1** and **3** in DME.

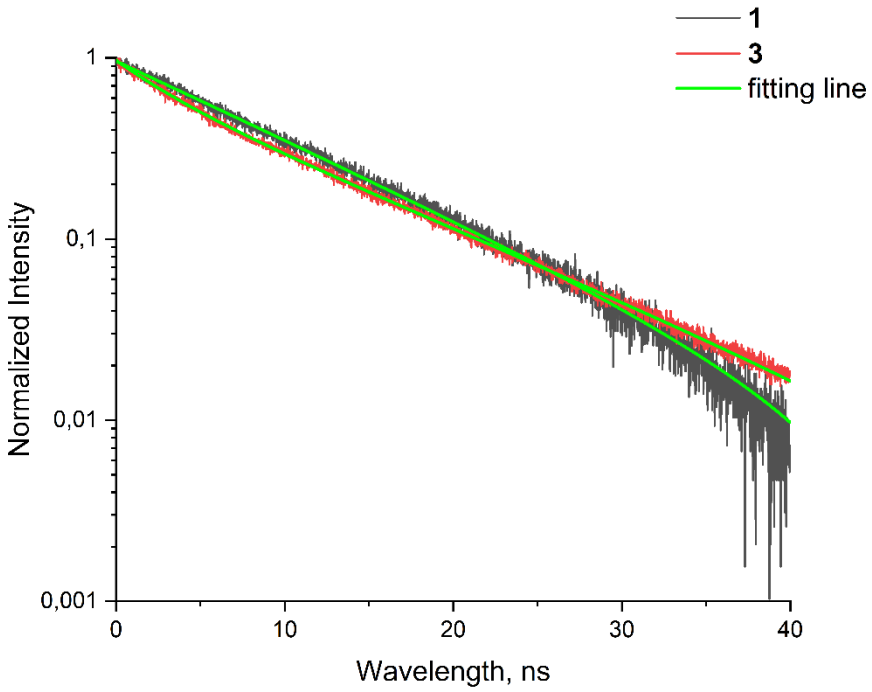

Figure S12. PL decay curves of **1** at 380 nm and **3** at 405 nm in DME solution at 298 K.

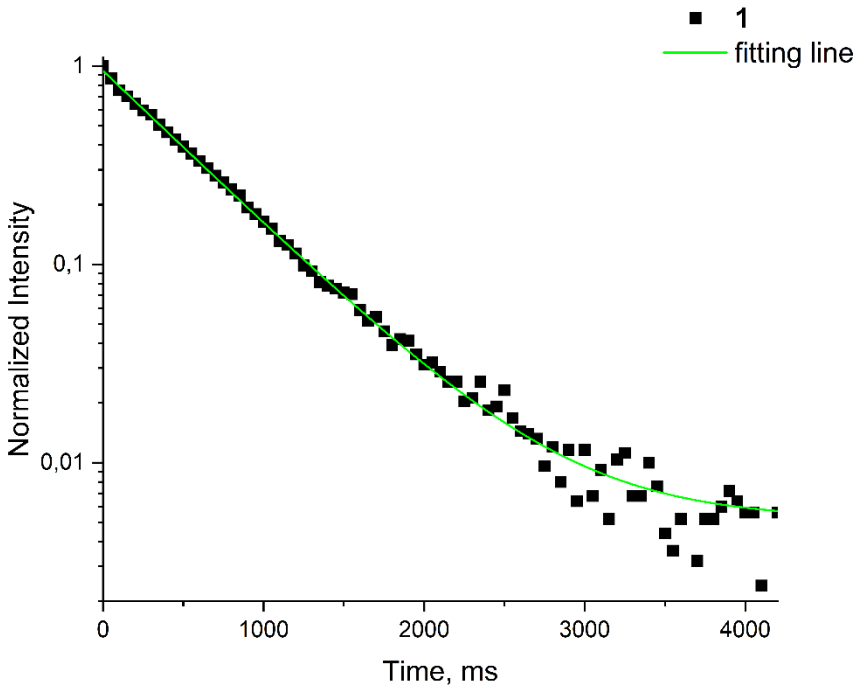

Figure S13. PL decay curve of **1** at 530 nm in DME solution at 77 K.

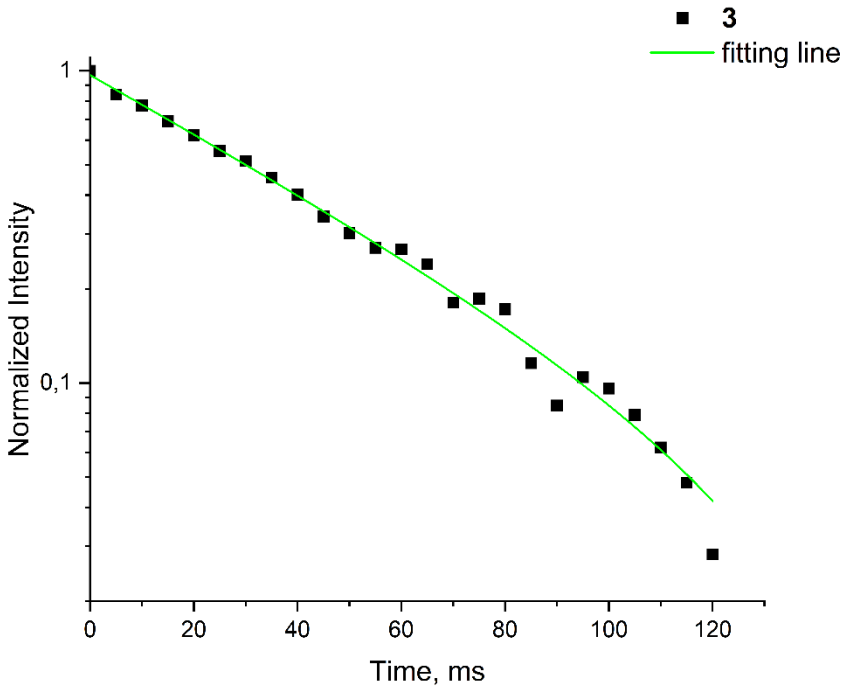

Figure S14. PL decay curve of **2** at 530 nm in DME solution at 77 K.

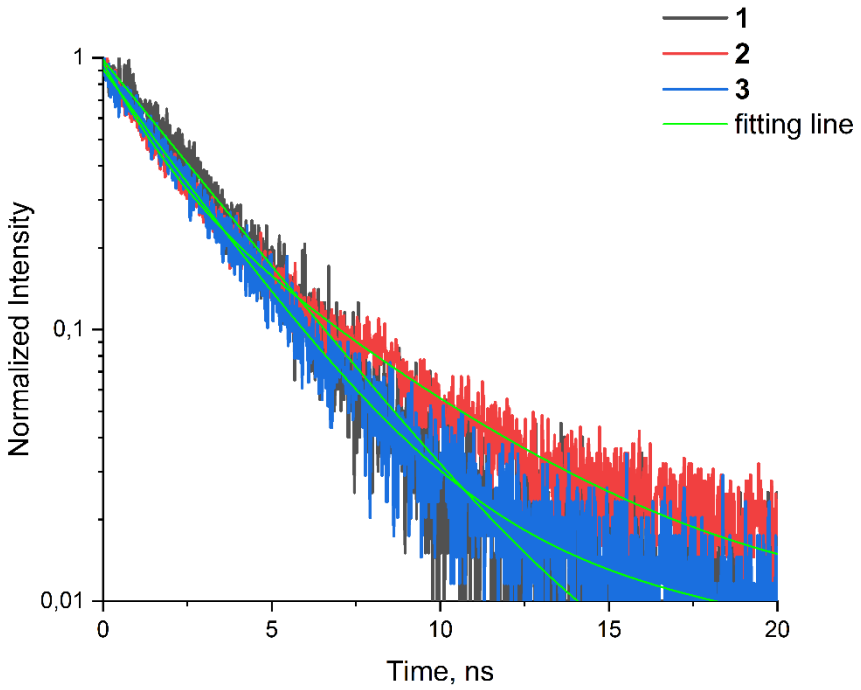

Figure S15. PL decay curves of **1**-**3** at 405 nm in solid state at 298 K.

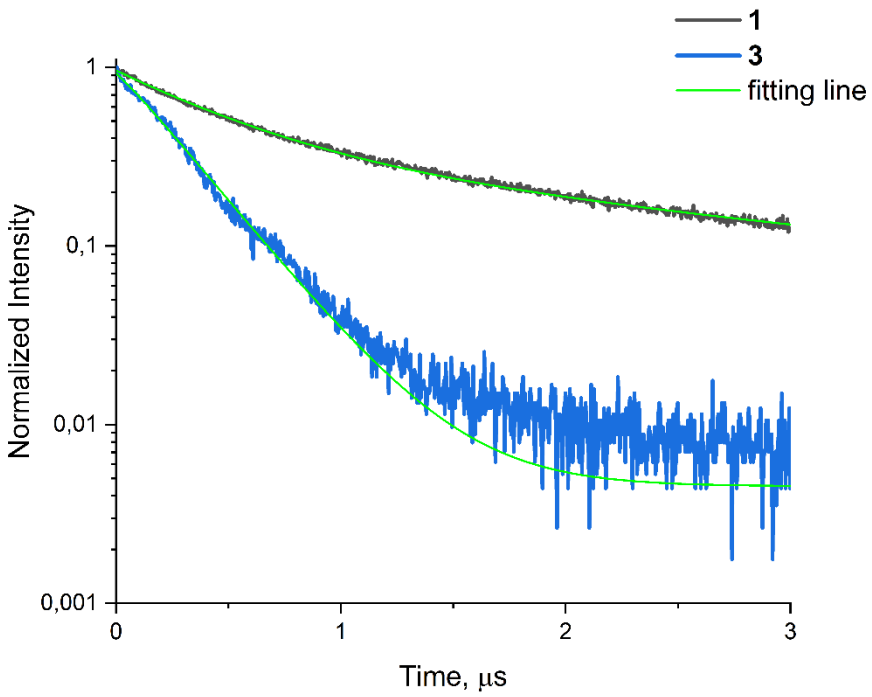

Figure S16. PL decay curves of **1**-**3** at 530 nm in solid state at 298 K.

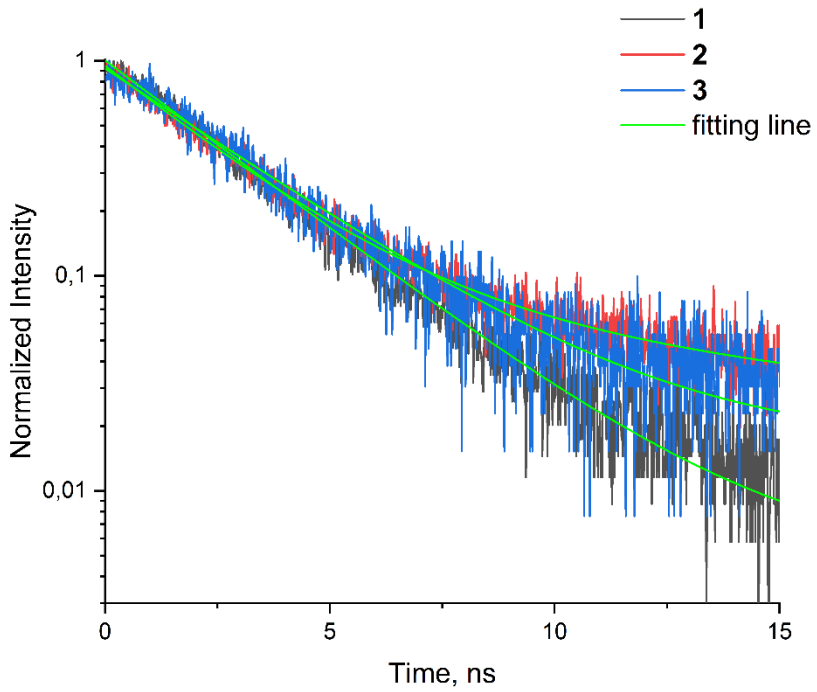

Figure S17. PL decay curves of **1-3** at 405 nm in solid state at 77 K.

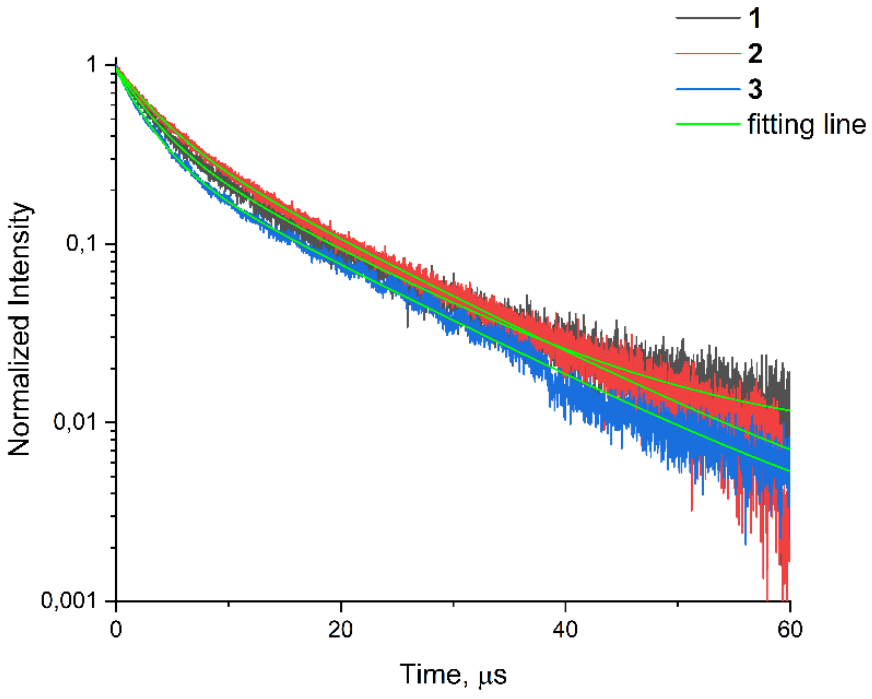

Figure S18. PL decay curves of **1-3** at 530 nm in solid state at 77 K.

Table S1. Crystal data for **1**-**3**.

Compound	**1**	**2**	**3**
Chemical formula	$C_8H_{11}NO_3SNa$	$C_{16}H_{26}N_2O_6S_6Na_2$	$C_{24}H_{39}N_3Na_3O_9S_9$
M_r	224.23	580.73	871.09
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/c$
Temperature (K)	220	150	150
a, b, c (Å)	6.2801 (5), 11.4240 (8), 14.7832 (9)	14.4519 (7), 13.6441 (7), 14.8205 (8)	9.6370 (3), 21.2068 (7), 19.2452 (7)
β (°)	95.063 (2)	112.633 (2)	95.360 (1)
V (Å^3)	1056.47 (13)	2697.3 (2)	3915.9 (2)
Z	4	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.33	0.57	0.59
Crystal size (mm)	0.20 × 0.08 × 0.06	0.20 × 0.12 × 0.12	0.12 × 0.03 × 0.03
T_{min}, T_{max}	0.689, 0.745	0.693, 0.741	0.671, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10153, 2158, 1864	15929, 15929, 10678	36188, 7462, 4482
R_{int}	0.031	-	0.121
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.716	0.611
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.082, 1.08	0.063, 0.165, 1.05	0.055, 0.120, 1.01
No. of reflections	2158	15929	7462
No. of parameters	129	346	484
No. of restraints	-	48	36
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.20	1.20, −1.22	0.70, −0.51